CHEMICAL INVESTIGATIONS AND ANTIPROLIFERATIVE ACTIVITIES OF THE ALKALOIDS FROM *Tabernaemontana polyneura*

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FACULTY OF SCIENCE
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KUALA LUMPUR

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THESIS SUBMITTED IN FULFILMENT OF THE REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCE
UNIVERSITI MALAYA
KUALA LUMPUR

2024

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Field of Study:

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CHEMICAL INVESTIGATIONS AND ANTIPROLIFERATIVE ACTIVITIES OF THE ALKALOIDS FROM *Tabernaemontana polyneura*

ABSTRACT

The alkaloidal content of a Malaysian plant, *Tabernaemontana polyneura* (family: Apocynaceae), was investigated. A total of 72 alkaloids (**1**–**72**) were isolated and characterized from the bark and leaf extracts of *T. polyneura*, collected from Fraser's Hill, in the state of Pahang, Peninsular Malaysia. The bark extract yielded 16 new alkaloids, including ten iboga (**1**–**10**), one chippiine (**30**), three vobasine (**33**–**35**), one cleavamine (**54**), and one vobasinyl-iboga bisindole alkaloids (**66**), while the leaf extract only yielded known alkaloids. Among the new alkaloids, polyneurine A (**1**) is characterized by a γ-lactone unit embedded within the iboga skeleton, while polyneurines I (**30**) and J (**9**) are the first examples of chippiine and *seco*-coronaridine alkaloids that incorporate an additional pyrrolidine ring. The biosynthetic pathways toward alkaloids **1**, **3**–**5**, **9**, and **30** were also proposed. Polyneurine P and four known bisindole alkaloids (**66**–**70**) displayed pronounced growth inhibitory activity (IC_{50} 0.34–9.02 μM) against HT-29, HCT 116, MDA-MB-231, A549, and MCF7 cancer cells.

Keywords: *Tabernaemontana polyneura*, alkaloids, bisindole, cytotoxic

KAJIAN KIMIA DAN AKTIVITI ANTIPROLIFERATIF ALKALOIDA DARIPADA *Tabernaemontana polyneura*

ABSTRAK

Kandungan alkaloida untuk suatu tumbuhan Malaysia, *Tabernaemontana polyneura* (famili: Apocynaceae), telah dikaji. Sebanyak 72 alkaloida (**1**–**72**) telah diasing dan dikenalpasti daripada ekstrak kulit pokok dan daun *T. polyneura*, yang diambil dari Bukit Fraser, Pahang, Malaysia. Ekstrak kulit pokok *T. polyneura* telah memberikan 16 alkaloida baharu, termasuk sepuluh iboga (**1**–**10**), satu chippiine (**30**), tiga vobasine (**33**–**35**), satu cleavamine (**54**) dan satu vobasinyl-iboga bisindola (**66**), manakala ekstrak daun hanya memberikan alkaloida yang diketahui. Antara alkaloida yang baharu, alkaloida **1** mempunyai unit γ-lakton dalam rangka iboga, manakala alkaloid **30** dan **9** mempunyai satu unit pyrrolidina tambahan yang digabungkan bersama rangka chippiine atau *seco*-coronaridine. Laluan biosintitek alkaloida **1**, **3**–**5**, **9** dan **30** juga telah dicadangkan. Satu alkaloida bisindola baharu dan empat alkaloida bisindola yang telah diketahui menunjukkan aktiviti sitotoksik (**66**–**70**, IC_{50} 0.34–9.02 μM) terhadap sel kanser HT-29, HCT 116, MDA-MB-231, A549 dan MCF7.

Kata kunci: *Tabernaemontana polyneura*, alkaloida, bisindola, sitotoksik

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α	:	Alpha
Å	:	Angstrom
β	:	Beta
J	:	Coupling constant
°C	:	Degree Celsius
δ	:	Delta
ε	:	Epsilon / molar absorptivity
γ	:	Gamma
g	:	Gram
K	:	Kelvin
kg	:	Kilogram
λ	:	Lambda
m/z	:	Mass-to-charge ratio
MHz	:	Megahertz
μg	:	Microgram
μL	:	Microliter
mg	:	Milligram
mL	:	Milliliter
mm	:	Millimeter
nm	:	Nanometer
$[\alpha]_D$	:	Specific rotation
cm^{-1}	:	Wavenumber
Ac	:	Acetyl

br	:	Broad
CCDC	:	Cambridge Crystallographic Data Centre
$CDCl_3$	:	Deuterated chloroform
CD_3OD	:	Deuterated methanol
CH_2Cl_2	:	Dichloromethane
$CHCl_3$	:	Chloroform
^{13}C NMR	:	Carbon-13 Nuclear Magnetic Resonance
COSY	:	Correlation Spectroscopy
DBE	:	Degree of unsaturation
d	:	Doublet
dd	:	Doublet of doublets
ddd	:	Doublet of doublet of doublets
dddd	:	Doublet of doublet of doublet of doublets
ddt	:	Doublet of doublet of triplets
DMSO	:	Dimethyl sulfoxide
2D NMR	:	Two-Dimensional Nuclear Magnetic Resonance
D_2O	:	Deuterium oxide
DP4+	:	Dispersion Corrected Probability for the Fourth Order
dq	:	Doublet of quartets
dt	:	Doublet of triplets
ECD	:	Electronic Circular Dichroism
EtOH	:	Ethanol
GIAO	:	Gauge-Including Atomic Orbital
HMBC	:	Heteronuclear Multiple Bond Correlation
^1H NMR	:	Proton Nuclear Magnetic Resonance
HRDARTMS	:	High Resolution Direct Analysis in Real Time Mass Spectrometry

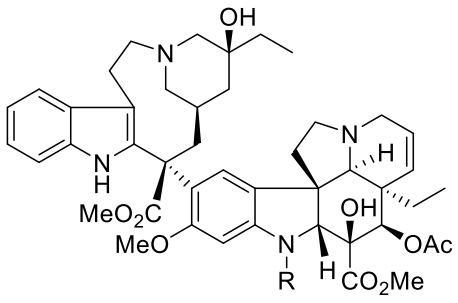
HRESIMS	:	High Resolution Electrospray Ionization Mass Spectrometry
HSQC	:	Heteronuclear Single Quantum Coherence
IC_{50}	:	Half maximal inhibitory concentration
IR	:	Infrared
m	:	Multiplet
Me	:	Methyl
MeOH	:	Methanol
mp	:	Melting point
MS	:	Mass Spectrometry
Na_2CO_3	:	Sodium carbonate
Na_2SO_4	:	Sodium sulfate
NMR	:	Nuclear Magnetic Resonance
NOE	:	Nuclear Overhauser Effect
NOESY	:	Nuclear Overhauser Effect Spectroscopy
OMe	:	Methoxy
PCM	:	Polarizable Continuum Model
ppm	:	Parts per million
q	:	Quartet
qd	:	Quartet of doublet
s	:	Singlet
SiO_2	:	Silica
t	:	Triplet
td	:	Triplet of doublets
TDDFT	:	Time-Dependent Density Functional Theory
TMS	:	Tetramethylsilane
UV	:	Ultraviolet

CHAPTER 1: INTRODUCTION AND LITERATURE REVIEW

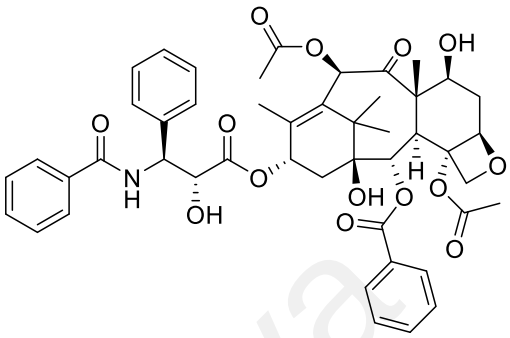
1.1 Natural Products

Natural products are organic compounds isolated from various natural sources (plants, marine, microbes, and terrestrial organisms). Many of these compounds and their derivatives (*via* semisynthetic modification of a natural product) have been used as drugs for the treatment of human diseases (Atanasov *et al.*, 2015; Beutler, 2009; Chin *et al.*, 2006; Jabeen *et al.*, 2014; Kinghorn *et al.*, 2009; Krause & Tobi, 2013; Newman & Cragg, 2020). The bisindole alkaloids from *Catharanthus roseus* and their derivatives such as vincristine, vinblastine (Cragg & Newman, 2013; Ishikawa *et al.*, 2009; Kuboyama *et al.*, 2004; Maccormack, 1990), vindesine (Barnett *et al.*, 1978; Ishikawa *et al.*, 2009), vinorelbine (Gueritte *et al.*, 1983; Ishikawa *et al.*, 2009), as well as the camptothecins (*e.g.*, topotecan, irinotecan) (Kauh & Bjornsti, 1995; Wall *et al.*, 1966), the epipodophyllotoxins (Kamal *et al.*, 2011; Thakur, 2011), and the taxanes (*e.g.*, Taxol or paclitaxel, docetaxel) (Rose, 1995; Wani *et al.*, 1971) are plant-derived natural products or derivatives which have been clinically used for chemotherapeutic purposes (Figure 1.1). Antitumor antibiotics from microbes that are used clinically include doxorubicin (Takemura & Fujiwara, 2007; Wouters *et al.*, 2005), bleomycin (Galm *et al.*, 2005; Kawai & Akaza, 2003; Ohno, 1989; Takita *et al.*, 1978; Umezawa *et al.*, 1966), dactinomycin (*e.g.*, actinomycin D) (Bullock & Johnson, 1957; Fernbach & Martyn, 1966; Ginell *et al.*, 1988; Kirk, 1960), and mitomycin C (Galm *et al.*, 2005; Schiltz & Kohn, 1993) (Figure 1.1). In addition, it has been established that natural products can be used to combat malaria. The discovery of artemisinin, which has contributed to the treatment of malaria, is one of the famous examples (Tu *et al.*, 1981; Tu, 2011). Potential antipsychotic activity has also been reported for galantamine,

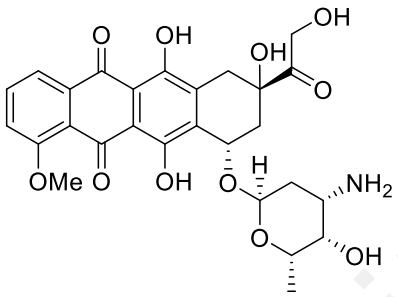
reserpine, emodin, and lobeline, as well as in botanical drugs such as the *Ginkgo biloba* extract (Skalicka-Woźniak & Gertsch, 2020). However, further studies are still needed to substantiate their findings as antipsychotic agents.



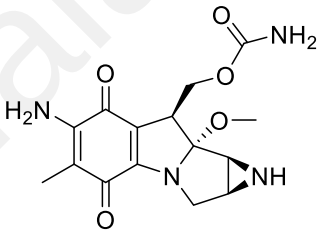
R = CHO Vincristine
R = Me Vinblastine



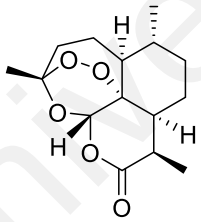
Paclitaxel



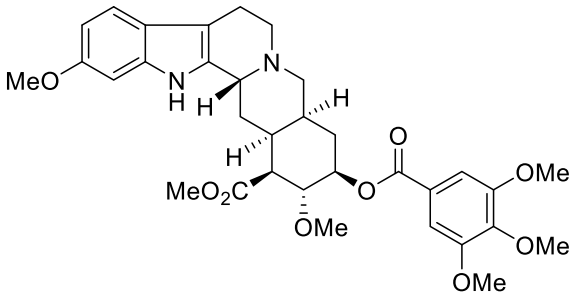
Doxorubicin



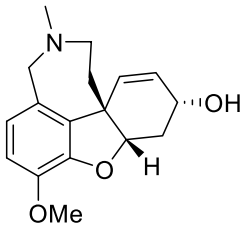
Mitomycin C



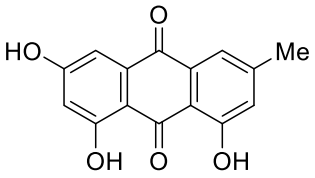
Artemisinin



Reserpine



Galanthamine



Emodin

Figure 1.1: Examples of bioactive natural products

As one of the world's biodiversity rich countries, Malaysia has tropical rainforests that prevails in natural resources. The natural products research and pharmaceutical sectors are therefore in a great position to benefit from this. As part of our efforts in searching bioactive alkaloids from medicinal plants, the Malayan *Tabernaemontana polyneura* (family: Apocynaceae) was selected as the plant material in this research as it was previously used by natives in Malaysia to treat ulcerations (Clivio, Richard, Hadi *et al.*, 1990).

1.2 Alkaloids

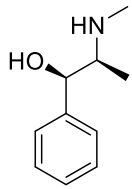
Alkaloids are one of the major classes of natural products (Jabeen *et al.*, 2014). Plant alkaloids or alkaloid-containing extracts were used as remedies, potions, teas, poultices, poisons, and psychoactive or recreational drugs in ancient times. The beginning of alkaloid chemistry was marked by the isolation of morphine by Friedrich Sertürner (a German pharmacist) in 1806 (Jabeen *et al.*, 2014). The term 'alkaloid' was first mentioned by the pharmacist W. Meissner, and it simply meant to describe substances of plant origin with an alkali-like or basic character (Aniszewski, 2007; Funayama & Cordell, 2015; Hesse, 2002). After years of studies, this definition was no longer comprehensive enough to describe all alkaloids. Pelletier had once modified the definition of alkaloids as cyclic compounds containing nitrogen in a negative oxidation state which is of limited distribution in living organisms. Hesse subsequently presented a more general definition of alkaloids, *i.e.*, nitrogen-containing organic substances of natural origin with a greater or lesser degree of basic character (Hesse, 2002). A more recent and pragmatic definition of alkaloids encompasses naturally occurring nitrogen-containing compounds, excluding peptides, non-protein amino acids, amines,

cyanogenic glycosides, glucosinolates, cofactors, phytohormones, and primary metabolites (Funayama & Cordell, 2015; Wink, 2016).

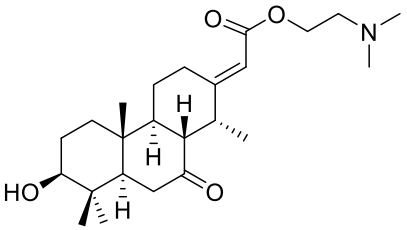
Alkaloids can be classified into five classes based on the position of the *N*-atom in the main structural element (Cordell, 1981; Hesse, 2002; Pelletier, 1983) (Figure 1.2).

i. Heterocyclic alkaloids
ii. Alkaloids with exocyclic *N*-atoms and aliphatic amines (*e.g.*, ephedrine, (–)-cassaine, mescaline)
iii. Putrescine, spermidine, and spermine alkaloids (*e.g.*, agleptine, inandenin-12-one, paucine)
iv. Peptide alkaloids (*e.g.*, celenamide E, mucronine A)
v. Terpene and steroid alkaloids (*e.g.*, solanidine, conessine)

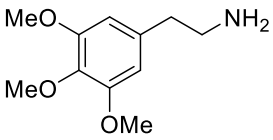
Alkaloids with exocyclic *N*-atoms and aliphatic amines



(–)-Ephedrine

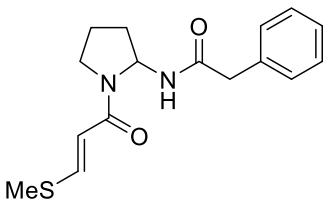


(–)-Cassaine

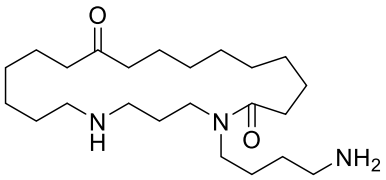


Mescaline

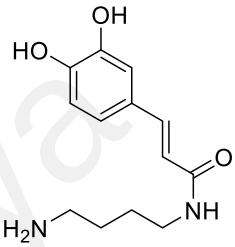
Putrescine, spermidine, and spermine alkaloids



Agleptine

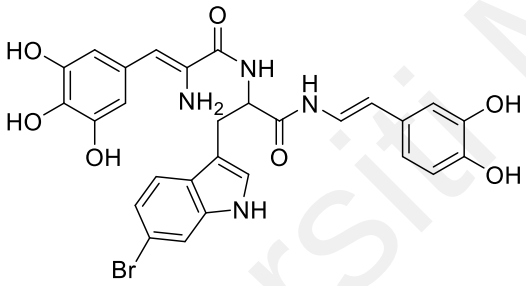


Inandenin-12-one

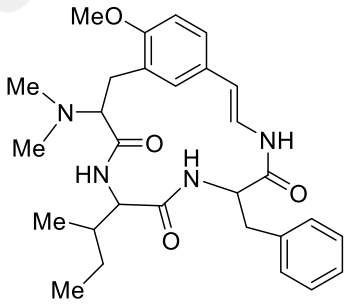


Paucine

Peptide alkaloids

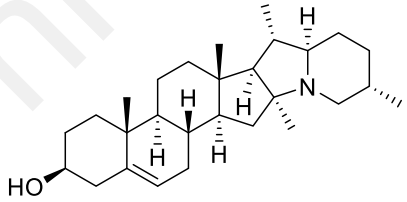


Celenamide E

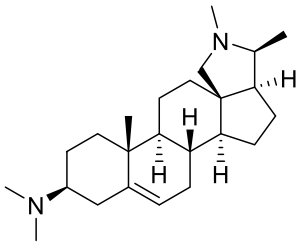


Mucronine A

Terpene and steroid alkaloids



Solanidine



Conessine

Figure 1.2: Examples of alkaloids from the five alkaloid classes

Among the five classes, heterocyclic alkaloids constitute the largest group, and the term alkaloids usually refers to heterocyclic alkaloids. Based on the carbon-nitrogen skeleton, heterocyclic alkaloids can be further classified into 15 subclasses as shown in Figure 1.3 (Cordell, 1981; Gutiérrez-Grijalva *et al.*, 2020; Hesse, 2002; Pelletier, 1983).

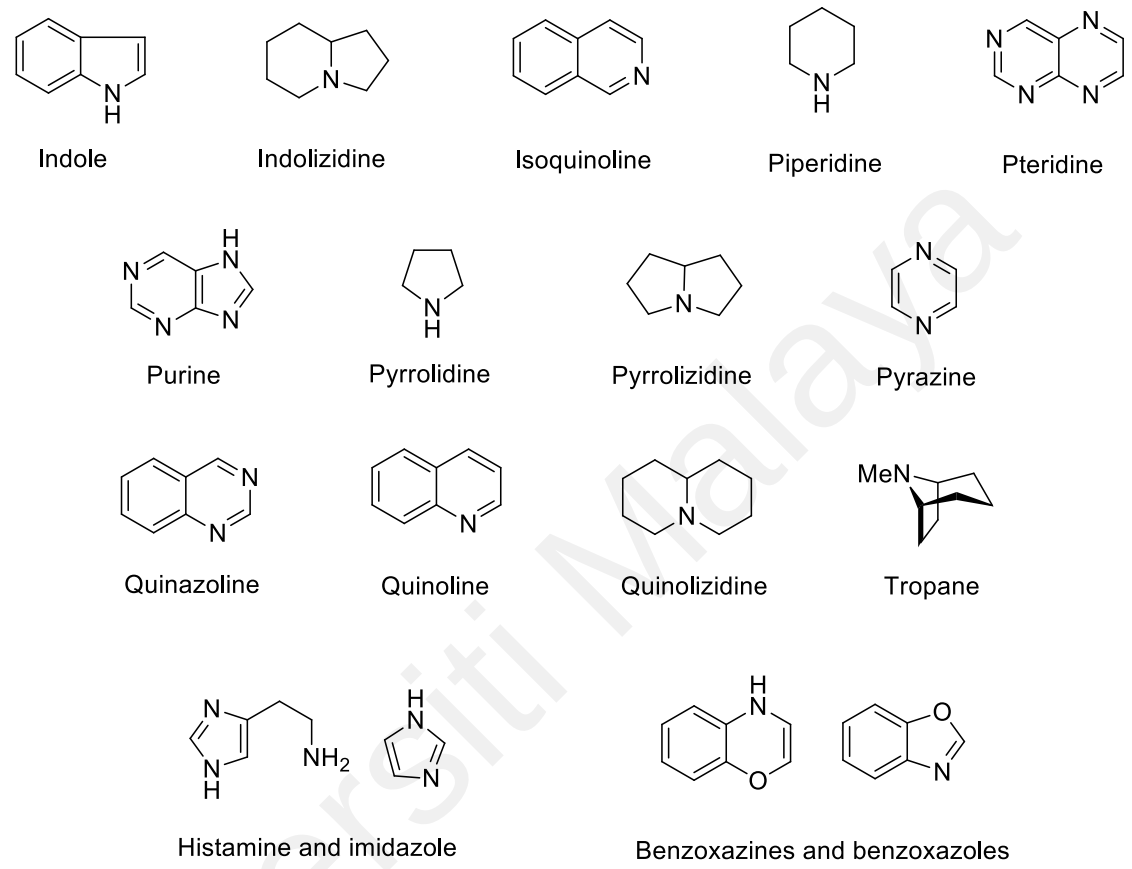


Figure 1.3: 15 Subclasses of the heterocyclic alkaloids

1.3 Indole Alkaloids of the Apocynaceae

1.3.1 General

Indole alkaloids constitute the largest class of alkaloids (Dey *et al.*, 2020). The indole alkaloids consist of (i) compounds that incorporate the actual indole chromophore, (ii) those containing its derivatives, namely indoline (or dihydroindole), indolenine, hydroxyindolenine, α-methylideneindoline, pseudoindoxyl, and oxindole, (iii) alkaloids in which the nucleus incorporates an additional benzene or pyridine ring, *e.g.*, carbazole, or β- and γ-carbolines, and their derivatives (Cordell, 1981; Hesse, 2002; Pelletier, 1983) (Figure 1.4).

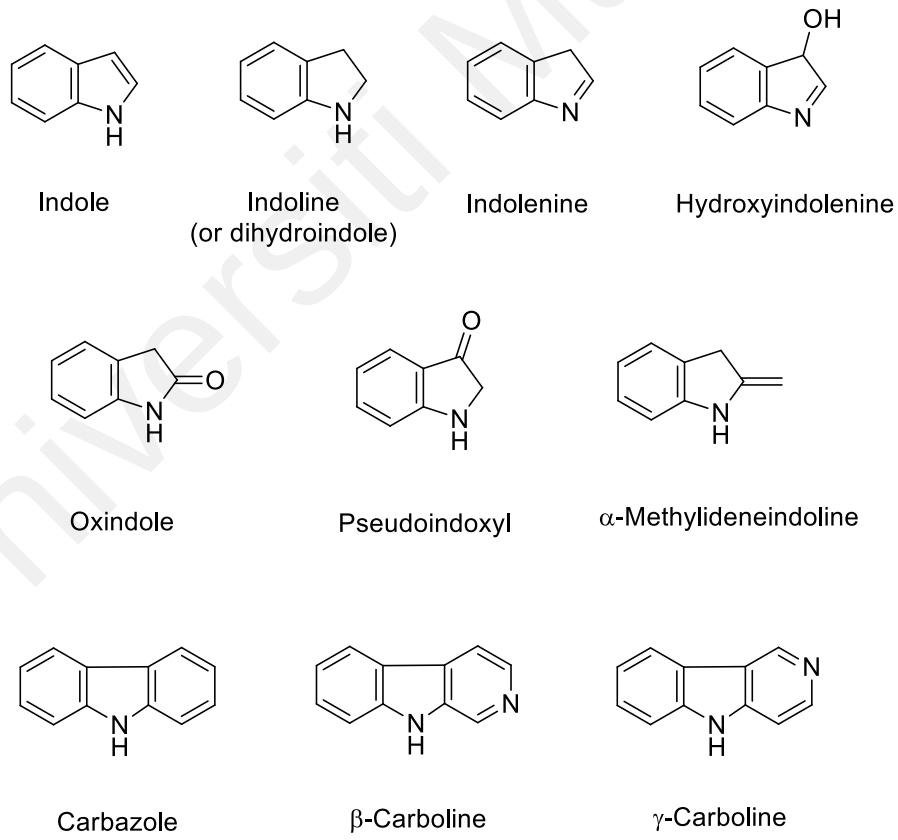


Figure 1.4: Indole and its derivatives

1.3.2 Classification of the Indole Alkaloids

Indole alkaloids can be further classified into two main classes. Simple indole alkaloids that do not possess a structural uniformity but have only the indole nucleus or a direct derivative as a common feature (*e.g.*, harmane), constitute the first class. The second class, known as monoterpene indole alkaloids (MIAs), contains two structural units, *viz.*, tryptamine (or tryptophan) with the indole nucleus and a C_9- or C_{10}-monoterpene moiety derived from secologanin (Figure 1.5) (Cordell, 1981; Hesse, 2002; Pelletier, 1983). Most of the plant-derived indole alkaloids belong to the second class (Pan *et al.*, 2016).

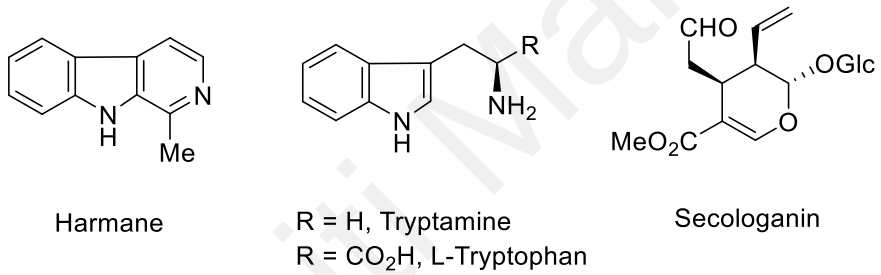
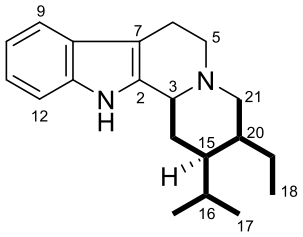


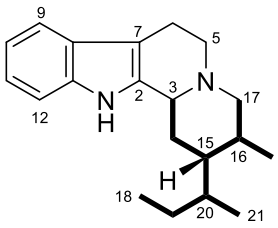
Figure 1.5: Harmane, tryptamine/L-tryptophan, and secologanin

The MIAs share a common biogenetic origin or precursor, namely strictosidine, which is a condensation product of tryptamine and secologanin (Cordell, 1974; O'Connor & Maresh, 2006; Stöckigt & Panjikar, 2007). On the basis of their biogenesis, MIAs have been structurally grouped into ten main skeletal types, comprising of corynanthean (C), vallesiachotaman (V), vincosan (D), strychnan (S), aspidospermatan (A), heynean (H), capuronan (K), tacaman (T), plumeran (P), and eburnan (E) (Figure 1.6) (Atta-ur-Rahman & Basha, 1983; Hibino & Choshi, 2001 & 2002; Higuchi & Kawasaki, 2007; Hill & Sutherland, 2009 & 2010; Ihara & Fukumoto, 1995, 1996 & 1997; Ishikura & Yamada, 2009; Ishikura *et al.*, 2010, 2013 & 2015; Kawasaki & Higuchi, 2005; Kisakurek & Hesse, 1980; Kisakurek *et al.*, 1983; Leonard, 1999;

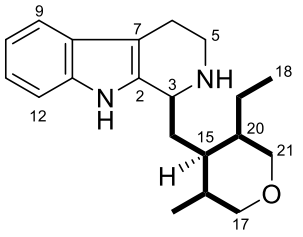
Lounasmaa & Tolvanen, 2000; O'Connor & Maresh, 2006; Saxton, 1984, 1985, 1986, 1987, 1989, 1990, 1991, 1993, 1994, 1995, 1996 & 1997; Somei & Yamada, 2003, 2004 & 2005; Stöckigt & Panjikar, 2007; Toyota & Ihara, 1998; Van Beek & Van Gessel, 1988; Van Beek, Verpoorte, Baerheim Svendsen *et al.*, 1984). Indole alkaloids of the C-, V-, D-, S-, and A-types possess skeletons with a non-rearranged secologanin moiety, whereas alkaloids of H-, K-, T-, P-, and E-types contain skeletons with a rearranged secologanin moiety. These alkaloids are biogenetically related and the plausible biogenetic relationships between them are shown in Scheme 1.1 (Cordell, 1981; Hesse, 2002; Kisakurek & Hesse, 1980; Kisakurek *et al.*, 1983; Pelletier, 1983; Van Beek & Van Gessel, 1988; Van Beek, Verpoorte, Baerheim Svendsen *et al.*, 1984). The ten main skeletal types can be subdivided according to the increasing complexity of their basic carbon skeleton.



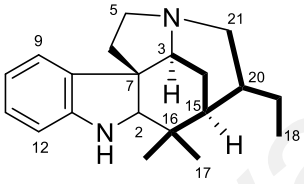
(C)



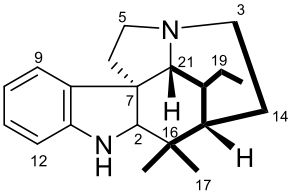
(V)



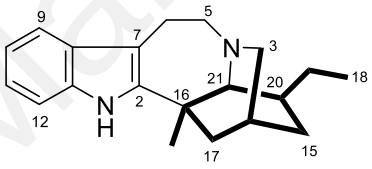
(D)



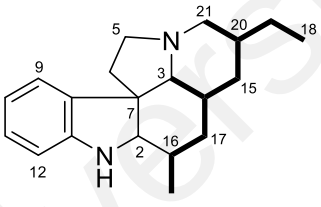
(S)



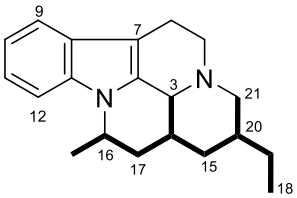
(A)



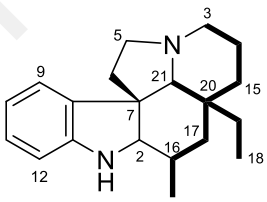
(H)



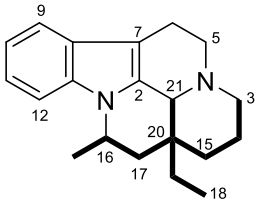
(K)



(T)

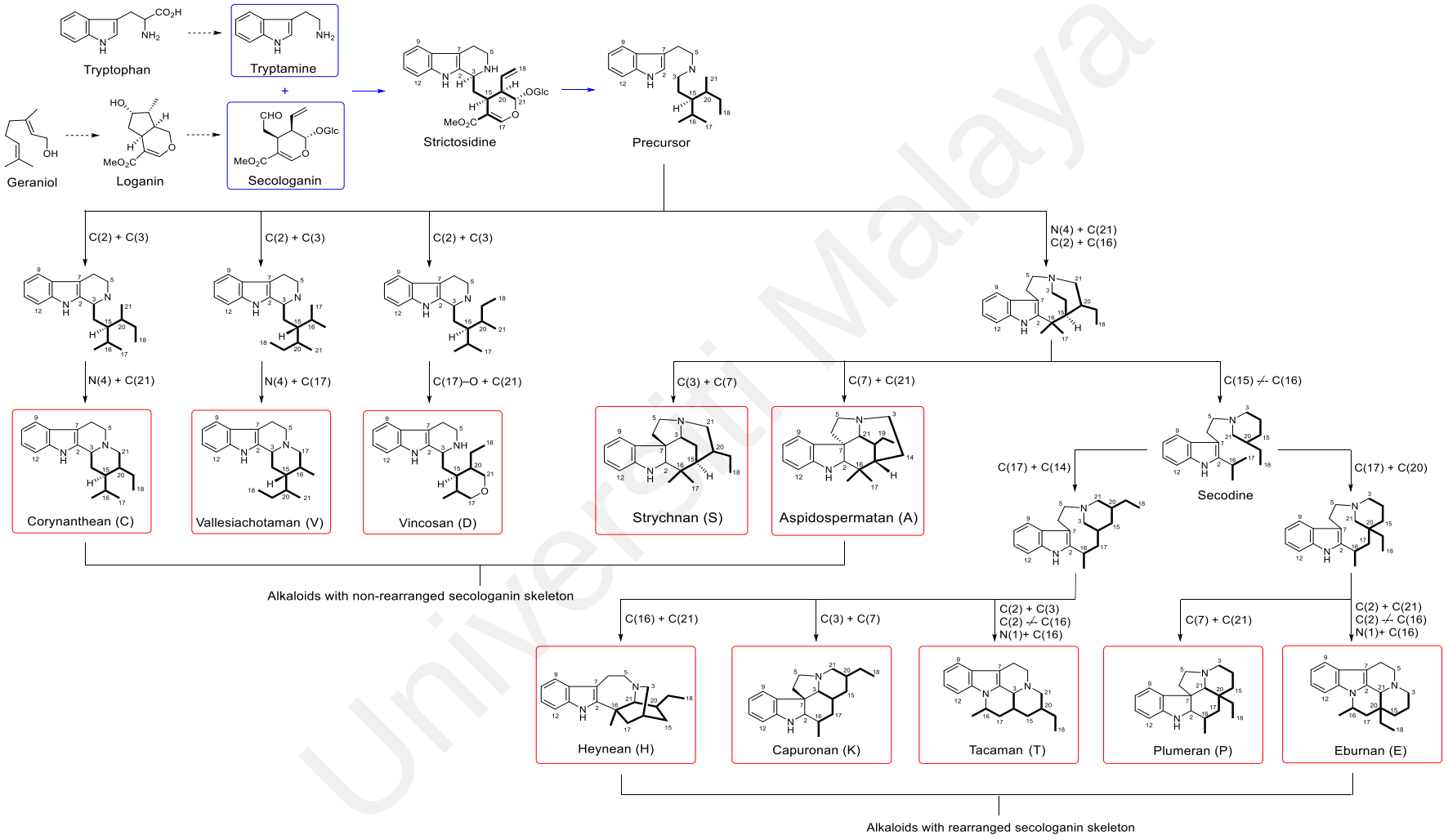


(P)



(E)

Figure 1.6: Classification of the monoterpenoid indole alkaloids



Scheme 1.1: Biogenetic inter-relationships of the ten main skeletal types of indole alkaloids with C_9- or C_{10}-monoterpene components

1.4 The Genus *Tabernaemontana*

1.4.1 General

The genus *Tabernaemontana* (tribe Tabernaemontaneae, subfamily Rauvolfioideae or Plumerioideae, family Apocynaceae) (Endress & Bruyns, 2000; Leeuwenberg, 1991) was named by Linnaeus after the birthplace of the German herbalist, Jacobus Theodorus von, who was usually known by the latinized form of the name of his birthplace, Tabernaemontanus (which means 'mountain tavern' in German) (Pratchayasakul *et al.*, 2008). It comprises of about 110 species (19 genera) distributed throughout the tropical and some subtropical regions of the world, *viz.*, 55 in America, 21 in Asia, Oceania and Australia, 18 in Africa, 15 in Madagascar, and one in Mascarene Island (Leeuwenberg, 1991). A list of the synonyms of the genus *Tabernaemontana* is listed in Table 1.1 (Leeuwenberg, 1991; Van Beek & Van Gessel, 1988; Van Beek, Verpoorte, Baerheim Svendsen *et al.*, 1984).

Table 1.1: Synonyms of the Genus *Tabernaemontana*

Anacampta	*Hazunta*	*Phrissocarpus*
Anartia	*Leptopharyngia*	*Protogabunia*
Bonafousia	*Merizadenia*	*Pterotaberna*
Camerunia	*Muntafara*	*Quadricasaea*
Capuronetta	*Ochronerium*	*Rejoua*
Codonemma	*Oisthanthera*	*Sarcopharyngia*
Conopharyngia	*Pagiantha*	*Stenosolen*
Domkeocarpa	*Pandaca*	*Taberna*
Ervatamia	*Pandacastrum*	*Testupides*
Gabunia	*Peschiera*	

The *Tabernaemontana* species found in Malaysia (Peninsular Malaysia and Malaysian Borneo) are listed below (Leeuwenberg, 1991; Middleton, 2011).

i. *T. antheonycta* Leeuwenberg
ii. *T. corymbosa* Roxb. ex Wall.
iii. *T. crispa* Roxb. ex Wall.
iv. *T. dichotoma* Roxb. ex Wall.
v. *T. divaricata* (L) R. Br. ex Roem. & Schult.
vi. *T. hirta* Hook. f.
vii. *T. macrocarpa* Jack
viii. *T. malaccensis* Hook. f.
ix. *T. pandacaqui* Lam.
x. *T. pauciflora* Bl.
xi. *T. peduncularis* Wall.
xii. *T. polyneura* (King & Gamble) D.J.Middleton
xiii. *T. polysperma* Merr.

The *Tabernaemontana* genus plants have long been a prodigious producer of alkaloids. The heynean- (or iboga)-type alkaloids have been identified as a characteristic and useful chemical marker of these plants. These plants have also been reported to contain many bisindole alkaloids with prominent bioactivities (Danieli & Palmisano, 1986; Kam & Choo, 2006; Kitajima & Takayama, 2016; Van Beek & Van Gessel, 1988; Van Beek, Verpoorte, Baerheim Svendsen *et al.*, 1984).

The *Tabernaemontana* species have been employed in folk medicine, *e.g.*, as stimulants or analgesics, as decoctions for cleansing wounds, or used in steam-baths for curing syphilis. Some examples are shown in Table 1.2 (Amelia *et al.*, 2019; Ebede *et*

al., 2021; Li *et al.*, 2019; Lien & Sung, 2000; Yuwen *et al.*, 2019). It is also one of the genera used in Chinese, Ayurvedic, and Thai traditional medicine to treat dysentery, fever, and pain (Pratchayasakul *et al.*, 2008). In addition to their medicinal uses, the root extracts are used as ingredients in arrow poisons, latex as birdlime, and wood as a fuel source (Van Beek & Van Gessel, 1988; Van Beek, Verpoorte, Baerheim Svendsen *et al.*, 1984).

Table 1.2: Medicinal Uses of *Tabernaemontana* Plants

Species	Part(s) of plant	Uses
T. bovina	Roots	Used as a traditional medicine in Vietnam for the treatment of fever and jaundice.
T. bufalina	Roots	Traditionally used for anti-hypertension, anti-rheumatalgia, and anti-snake poisoning in China.
T. contorta	Leaves	To prevent keloids formation. As an antiseptic.
	Milky juice	To treat eye infections and intestinal worms.
T. divaricata	Roots	Traditionally used for treating hypertension, headache, and scabies in Guangdong and Guangxi provinces of China.
	Roots, leaves, and flowers	To treat snake and scorpion poisoning.
T. macrocarpa	Exudate from the bark	Used traditionally to cure dental disorders, herpes, and eczema in Borneo, Indonesia.

1.4.2 *Tabernaemontana polyneura*

T. polyneura (King & Gamble) D.J.Middleton (basionym: *Ervatamia polyneura*) is endemic in Peninsular Malaysia (Middleton, 2011). It can be found in the states of Kelantan, Perak, Selangor, Melaka, Pahang, and Johor (Middleton, 2011). This plant usually grows in lower montane forest at 800–1500 m altitude (Middleton, 2011). It was used by natives in Malaysia as a traditional medicine to treat ulcerations (Clivio, Richard, Hadi *et al.*, 1990). A prior investigation of the same plant from a different

location (Genting Sempah, Selangor, Peninsular Malaysia) by Clivio *et al.* in 1990 yielded a total of 23 monomeric indole alkaloids, of which only four of them were reported as new compounds, *viz.*, two vobasine and two iboga alkaloids (Clivio, Richard, Hadi *et al.*, 1990). Another two new Aspidosperma-aspidosperma bisindole alkaloids were subsequently reported from the leaves of *E. polyneura* (Clivio, Guillaume *et al.*, 1995). Since no further studies of this plant have been reported, and in view of our interest in probing the variation of alkaloid content as a function of geographical location in this genus, an extensive study on the chemical and biological aspects of a sample collected from Fraser's Hill, Pahang, Peninsular Malaysia (Figure 1.7) was carried out.

Figure 1.7: *T. polyneura* (collected from Fraser's Hill, Pahang)

1.4.3 Occurrence and Distribution of Alkaloids in the Genus *Tabernaemontana*

The occurrence of alkaloids in *Tabernaemontana* as reported in the literature (up to June 2023) is summarized in Table 1.3. The structures of the alkaloids are shown in Figure 1.8.

Table 1.3: Occurrence of Alkaloids in *Tabernaemontana*

Plant	Plant part	Alkaloids	References
T. accedens Müll. Arg. (*Peschiera accedens*)	Root-bark	Accedine (**199**)	Achenbach & Schaller, 1975; Achenbach, 1983
		Accedinine (**651**)	Achenbach & Schaller, 1976a
		Accedinisine (**647**)	Achenbach & Schaller, 1976a
		Affinisine (**161**)	Achenbach & Schaller, 1976a
		N(1)-Demethyl-16-*epi*-accedine (**200**)	Achenbach & Schaller, 1976b
		N(4)-Demethylvoacamine (**724**)	Achenbach & Schaller, 1976a
		N(1)-Methyl-16-*epi*-affinine (**204**)	Achenbach & Schaller, 1975
		Voacamidine (**660**)	Achenbach & Schaller, 1976a
		Voacamine (**720**)	Achenbach & Schaller, 1976a
		Voacamine *N*-oxide (**721**)	Achenbach & Schaller, 1976a
T. affinis Müll. Arg. (*P. affinis*)	Root-bark	Affinine (**202**)	Weisbach *et al.*, 1963; Cava *et al.*, 1964
		Affinisine (**161**)	Weisbach *et al.*, 1963; Cava *et al.*, 1964; Matos *et al.*, 1976
		Coronaridine (**14**)	Matos *et al.*, 1976
		Coronaridine pseudoindoxyl (**27**)	Matos *et al.*, 1976
		19-*Epi*-heyneanine (**17**)	Matos *et al.*, 1976
		Heyneanine (**16**)	Matos *et al.*, 1976
		19(*R*)-Hydroxyibogamine (**13**)	Wolter Filho *et al.*, 1985
		Iboxygaine (**547**)	Wolter Filho *et al.*, 1985;
		Olivacine (**77**)	Fonteles *et al.*, 1974; Matos *et al.*, 1976
		Voacangine (**23**)	Wolter Filho *et al.*, 1985
		Voacristine (= Voacangarine) (**24**)	Wolter Filho *et al.*, 1985
		Vobasine (**37**)	Weisbach *et al.*, 1963
	Roots,	Affinisine (**161**)	Santos *et al.*, 2009

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	stems	Coronaridine (**14**)	Santos *et al.*, 2009
		Iboxygaine (**547**)	Santos *et al.*, 2009
		Voacangine (**23**)	Santos *et al.*, 2009
		Voacristine (= Voacangarine) (**24**)	Santos *et al.*, 2009
		Voacristine hydroxyindolenine (**508**)	Santos *et al.*, 2009
	Roots	6*N*-Hydroxy-olivacine (**81**)	Santos *et al.*, 2012
		Olivacine (**77**)	Santos *et al.*, 2012
		2*N*-oxide-olivacine (**82**)	Santos *et al.*, 2012
T. alba Mill.	Seeds	Coronaridine (**14**)	Collera *et al.*, 1962
		Tabersonine (**281**)	Collera *et al.*, 1962
T. albiflora (Miq.) Pulle	Stem-bark	(–)-Albifloranine (**15**)	Kan *et al.*, 1981a
		Coronaridine (**14**)	Kan *et al.*, 1980a
		Desethylibophyllidine (**632**)	Kan *et al.*, 1980a
		(+)-20(*R*)-18,19-Dihydroxy-pseudovincadifformine (**614**)	Kan *et al.*, 1981b
		20-*Epi*-ibophyllidine (**628**)	Kan *et al.*, 1980a
		18-Hydroxy-20-*epi*-ibophyllidine (**629**)	Kan *et al.*, 1980b
		19(*R*)-Hydroxy-20-*epi*-ibophyllidine (**630**)	Kan *et al.*, 1980b
		19(*S*)-Hydroxy-20-*epi*-ibophyllidine (**631**)	Kan *et al.*, 1980b
		(+)-19-Hydroxy-20-*epi*-pandoline (**618**)	Kan *et al.*, 1980b
		19-Hydroxyibophyllidine (**635**)	Kan *et al.*, 1981b
		Ibophyllidine (**633**)	Kan *et al.*, 1980a
T. amblyocarpa Urb.	Stems	(+)-Tubotaiwine (**60**)	Perez & Sierra, 1980
		Vallesamine (**270**)	Perez & Sierra, 1980
		Voacristine (= Voacangarine) (**24**)	Perez & Sierra, 1980
	Leaves, stems, flowers	Heyneanine (**16**)	Perez & Sierra, 1983; Perez & Sierra, 1985; Perez *et al.*, 1995
		Ibogamine (**11**)	Perez & Sierra, 1980; Perez & Sierra, 1983; Perez & Sierra, 1985; Perez *et al.*, 1995
		19-Oxovoacangine (**469**)	Perez & Sierra, 1983; Perez, 1984; Perez & Sierra, 1985; Perez *et al.*, 1995
	Stems, flowers	Iboxygaine (**547**)	Perez, 1984; Perez & Sierra, 1985
		Voacangine (**23**)	Perez & Sierra, 1980; Perez, & Sierra, 1983; Fajardo *et al.*, 1984
	Leaves, flowers	Coronaridine (**14**)	Perez & Sierra, 1980; Perez & Sierra, 1983; Fajardo *et al.*, 1984
		Isovoacristine (**471**)	Perez & Sierra, 1980; Fajardo *et al.*, 1984

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Leaves, stems	Isovoacangine (**430**)	Perez & Sierra, 1980; Perez, 1984
	Leaves	Akuammidine (**172**)	Perez & Sierra, 1980
	Flowers	Tabersonine (**281**)	Perez & Sierra, 1985
T. amygdalifolia Jacq.	Roots	Coronaridine (**14**)	Achenbach, 1967b
		Cylindrocarpidine (**319**)	Achenbach, 1967b
		12-Demethoxycylindrocarpidine (**320**)	Achenbach, 1967a
		12-Demethylaspidospermine (**318**)	Achenbach, 1967b
		O-Demethylpalosine (**323**)	Achenbach, 1966a
		Homocylindrocarpidine (**321**)	Achenbach, 1967a
		5-Oxocylindrocarpidine (**322**)	Achenbach, 1967b
		Voacangine (**23**)	Achenbach, 1967b
T. angulata Mart. (*Anacampta angulata*)	Bark	Voacristine-7-hydroxyindolenine (**508**)	Garnier, Mahuteau *et al.*, 1984
	Stem	Coronaridine (**14**)	De Assis *et al.*, 2009
		Voacangine (**23**)	De Assis *et al.*, 2009
T. apoda Wr. ex Sauv. (*T. armeniaca*, *P. apoda*)	Leaves, flowers	Apodine (**328**)	Iglesias & Diatta, 1975a, 1975b
		Voacristine (= Voacangarine) (**24**)	Perez & Iglesias, 1976; Laguna & Iglesias, 1977
		Voacristine-7-hydroxyindolenine (**508**)	Perez & Iglesias, 1976; Laguna & Iglesias, 1977
	Leaves, roots, flowers	Coronaridine (**14**)	Sierra & Iglesias, 1975; Iglesias & Diatta, 1975b; Lagunas & Iglesias, 1977
		Ibogamine (**11**)	Sierra & Iglesias, 1975; Lagunas & Iglesias, 1977; Perez *et al.*, 1979
		Voacangine (**23**)	Sierra & Iglesias, 1975; Iglesias, 1976; Lagunas & Iglesias, 1977; Perez *et al.*, 1979
	Root-bark, flowers	Voacangine-7-hydroxyindolenine (**507**)	Laguna & Iglesias, 1977; Iglesias Lores, 1979
		Voacangine pseudoindoxyl (= Voaluteine) (**520**)	Iglesias, 1976; Sierra *et al.*, 1977
	Fruits	Ibogaine-7-hydroxyindolenine (**513**)	Iglesias, 1976
		Iboluteine (= Ibogaine pseudoindoxyl) (**556**)	Iglesias, 1976
		Voacristine pseudoindoxyl (**521**)	Laguna & Iglesias, 1977
	Leaves	Apodinine (**330**)	Iglesias Lores, 1979
		Deoxoapodine (**329**)	Iglesias & Diatta, 1975b
	Root-bark	Heyneanine (**16**)	Sierra *et al.*, 1977

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Leaves, roots	Isovoacangine (**430**)	Sierra & Iglesias, 1975; Perez *et al.*, 1979
	Leaves, roots	Isovoacangine (**430**)	Sierra & Iglesias, 1975; Perez *et al.*, 1979
T. arborea Rose	Seeds	Isovoacangine (**430**)	Chaverri & Ciccio, 1980
		Tabersonine (**281**)	Chaverri & Ciccio, 1980
	Latex, trunk	19-*Epi*-voacristine (= 19-*Epi*-voacangarine) (**470**)	Ciccio *et al.*, 1985; Cabezas & Ciccio, 1986
		19(*R*)-Hydroxyconopharyngine (**472**)	Ciccio *et al.*, 1985; Cabezas & Ciccio, 1986
		Vobasine (**37**)	Ciccio *et al.*, 1985; Cabezas & Ciccio, 1986
	Twigs	Conopharyngine (**25**)	Ciccio *et al.*, 1985
	Latex, trunk	19-*Epi*-voacorine (**726**)	Ciccio *et al.*, 1985; Kingston, 1978
	Latex, leaves	Voacamine (**720**)	Kingston, 1978; Cabezas & Ciccio, 1986
	Seeds, latex, twigs	Voacangine (**23**)	Kingston, 1978; Chaverri & Ciccio, 1980; Ciccio *et al.*, 1985
T. attenuata (Miers) Urb. (*A. meyeri*)	Leaves	16-*Epi*-pleiocarpamine (**153**)	Ladhar *et al.*, 1981
		11-Hydroxycoronaridine (**428**)	Ladhar *et al.*, 1981
		10-Hydroxyheyneanine (**459**)	Ladhar *et al.*, 1981
		11-Hydroxyheyneanine (**460**)	Ladhar *et al.*, 1981
	Stem-bark, root-bark	Angustine (**158**)	Ladhar *et al.*, 1981
		Conopharyngine (**25**)	Ladhar *et al.*, 1981
		Coronaridine (**14**)	Ladhar *et al.*, 1981
		Coronaridine-7-hydroxyindolenine (**29**)	Ladhar *et al.*, 1981
		Eglandine (**432**)	Ladhar *et al.*, 1981
		19-*Epi*-Heyneanine (**17**)	Ladhar *et al.*, 1981
		Heyneanine (**16**)	Ladhar *et al.*, 1981
		Ibophyllidine (**633**)	Ladhar *et al.*, 1981
		Isovoacangine (**430**)	Ladhar *et al.*, 1981
		Jollyanine (= Conopharyngine-7-hydroxyindolenine) (**509**)	Ladhar *et al.*, 1981
		6(*R*)-3,6-Oxidocoronaridine (**486**)	Ladhar *et al.*, 1981
		(+)-Tubotaiwine (**60**)	Ladhar *et al.*, 1981
		Voacangine (**23**)	Ladhar *et al.*, 1981
T. aurantiaca Gaud. (*Rejouna aurantiaca*, *E. aurantiaca*)	Bark, leaves, flowers	Iboluteine (= Ibogaine pseudoindoxyl) (**556**)	Guise, Rasmussen *et al.*, 1965; Guise, Ritchie *et al.*, 1965
		Voaluteine (= Voacangine pseudoindoxyl) (**520**)	Guise, Rasmussen *et al.*, 1965; Guise, Ritchie *et al.*, 1965
		Vobtusine (**823**)	Guise, Rasmussen *et al.*, 1965; Ganzinger & Hesse, 1976

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Bark	Voacangine (**23**)	Guise, Rasmussen *et al.*, 1965
T. australis Müll. Arg. (*P. australis*)	Stems	Voacamine (**720**)	Gorman *et al.*, 1960
		Voacangine (**23**)	Gorman *et al.*, 1960
	Seeds	Coronaridine-7-hydroxyindolenine (**29**)	Rates *et al.*, 1993
		Tabersonine (**281**)	Rates *et al.*, 1993
	Roots	16'-Decarbomethoxyvoacamine (**718**)	Rates *et al.*, 1993
		Tabernamine (**67**)	Rates *et al.*, 1993
	Leaves	Catharinensine (**146**)	Rates *et al.*, 1993
	Leaves, root-bark	Olivacine (**77**)	Rates *et al.*, 1993
	Seeds, root-bark	Coronaridine (**14**)	Rates *et al.*, 1993
T. bovina Lour.	Leaves, stems	14α,15β-Dihydroxy-*N*(1)-methylaspidospermine (**317**)	Lien, Ripperger *et al.*, 1998
		19(*R*)-*Epi*-voacristine (**470**)	Lien, Ripperger *et al.*, 1998
		Hecubine (= *N*(1)-Methylvoaphylline) (**345**)	Lien, Ripperger *et al.*, 1998
		20-Hydroxyconopharyngine (**431**)	Lien, Ripperger *et al.*, 1998
		Ibogaine (**536**)	Lien, Ripperger *et al.*, 1998
		Ibogaline (**539**)	Lien, Ripperger *et al.*, 1998
		Isovoacristine (**471**)	Lien, Kamperdick *et al.*, 1998
		(−)-Mehranine (**314**)	Lien, Ripperger *et al.*, 1998
		Methylene-bis-mehranine (**836**)	Lien, Kamperdick *et al.*, 1998
		3-Oxomehranine (**315**)	Lien, Ripperger *et al.*, 1998
		Pedunculine (= Conofoline) (**848**)	Lien, Ripperger *et al.*, 1998
		Tabernaebovine (**837**)	Lien, Kamperdick *et al.*, 1998
	Seeds	Tabernaemontabovine (**838**)	Ripperger *et al.*, 1999
		Tabernaemontavine (**839**)	Ripperger *et al.*, 1999
	Stems, leaves	Apovincamine (**381**)	Yu, Bao, Huang *et al.*, 2021
		Cononitarine B (**765**)	Liu, Liu *et al.*, 2018
		10,11-Dimethoxy-criocerine (**388**)	Yu, Bao, Huang *et al.*, 2021

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		10,11-Dimethoxy-14,15-didehydrovincamine (**373**)	Yu, Bao, Huang *et al.*, 2021
		10,11-Dimethoxy-16-*epi*-14,15-didehydrovincamine (**370**)	Yu *et al.*, 2021
		10,11-Dimethoxy-16-*epi*-14,15-didehydrovincamine *N*(4)-oxide (**372**)	Yu *et al.*, 2021
		10,11-Dimethoxy-14,15-didehydrovincamine *N*(4)-oxide (**377**)	Yu *et al.*, 2021
		10,11-Dimethoxy-14,15-didehydrovincamenine (**382**)	Yu *et al.*, 2021
		10,11-Dimethoxy-14,15-didehydroapovincamine (**383**)	Yu *et al.*, 2021
		10,11-Dimethoxy-isoeburnamenine (**397**)	Yu *et al.*, 2021
		10,11-Dimethoxy-16-*O*-methyl-isoeburnamenine (**396**)	Yu *et al.*, 2021
		16-*Epi*-14,15-didehydrovincamine (**59**)	Yu *et al.*, 2021
		19-*Epi*-heyneanine (**17**)	Liu, Liu *et al.*, 2018
		Ervachinine C (**676**)	Liu, Liu *et al.*, 2018
		14-Formylcriocerine (**389**)	Yu *et al.*, 2021
		Heyneanine (**16**)	Liu, Liu *et al.*, 2018
		10-Hydroxy-14,15-didehydrovincamine (**375**)	Yu *et al.*, 2021
		10-Hydroxy-11-methoxy-14,15-didehydrovincamine (**369**)	Yu *et al.*, 2021
		10-Hydroxy-11-methoxy-16-*epi*-14,15-didehydrovincamine (**371**)	Yu *et al.*, 2021
		10-Hydroxy-11-methoxyvincapusine (**387**)	Yu *et al.*, 2021
		10-Methoxy-14,15-didehydroapovincamine (**384**)	Yu *et al.*, 2021
		10-Methoxy-14α-hydroxymeloyunine (**386**)	Yu *et al.*, 2021
		N(1)-Methylvoaphylline (= Hecubine) (**345**)	Liu, Liu *et al.*, 2018
		3-(2-Oxopropyl)-10,11-dimethoxy-16-*epi*-14,15-didehydrovincamine (**379**)	Yu *et al.*, 2021
		3-(2-Oxopropyl)-16-*epi*-14,15-didehydrovincamine (**378**)	Yu *et al.*, 2021
		Taberbovcamine A (**391**)	Yu *et al.*, 2021
		Taberbovcamine B (**376**)	Yu *et al.*, 2021
		Taberbovcamine C (**380**)	Yu *et al.*, 2021
		Taberbovcamine D (**392**)	Yu *et al.*, 2021
		Taberbovcamine E (**393**)	Yu *et al.*, 2021
		Tabernaecorymbosine A (**767**)	Liu, Liu *et al.*, 2018
		Tabernaecorymbosine B (**769**)	Liu, Liu *et al.*, 2018
		Tabernaricatine E (**677**)	Liu, Liu *et al.*, 2018
		10,11,12-Trimethoxy-14,15-didehydrovincamine (**374**)	Yu *et al.*, 2021
		Vobasonidine (**652**)	Liu, Liu *et al.*, 2018
	Stems	Taberbovine A (**89**)	Wu *et al.*, 2019
		Taberbovine B (**90**)	Wu *et al.*, 2019
		Taberbovine C (**91**)	Wu *et al.*, 2019
		Taberbovine D (**92**)	Wu *et al.*, 2019
		(±)-Tabovine A (**107**)	Yu, Bao, & Cai., 2021
		(−)-(3*R*,7*S*,14*R*,20*S*)-Tabovine B (**361**)	Yu, Bao, & Cai., 2021
		(±)-Tabovine C (**108**)	Yu, Bao, & Cai., 2021
		(+)-(3*R*,14*R*,20*R*)-Tabovine D (**109**)	Yu, Bao, & Cai., 2021

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Coronaridine (**14**)	Zhang, Du *et al.*, 2021
		Coronaridine hydroxyindolenine (**29**)	Zhang, Du *et al.*, 2021
		3-Oxocoronaridine (**19**)	Zhang, Du *et al.*, 2021
		Taberibogine A (**443**)	Zhang, Du *et al.*, 2021
		Taberibogine B (**465**)	Zhang, Du *et al.*, 2021
		Voacangine (**23**)	Zhang, Du *et al.*, 2021
	Leaves	17(*R*)-Acetyljerantinine A (**343**)	Yu *et al.*, 2023
		Apotacamine (= 16,17-Anhydrotacamine) (**398**)	Yu, Bao, Wang *et al.*, 2019
		16(*R*)-Descarbomethoxy-tacamine (**427**)	Yu, Bao, Wang *et al.*, 2019
		16(*S*)-Descarbomethoxy-tacamine (**428**)	Yu, Bao, Wang *et al.*, 2019
		10-*O*-Methyljerantinine D (**299**)	Yu *et al.*, 2023
		15-*O*-Methyljerantinine E (**301**)	Yu *et al.*, 2023
		10-*O*-Methylmelodinine M (**309**)	Yu *et al.*, 2023
		3(*S*)-Methyljerantinine A (**306**)	Yu *et al.*, 2023
		3(*S*)-Methyl-10-*O*-methyljerantinine A (**286**)	Yu *et al.*, 2023
		Mehranine (**314**)	Zhao *et al.*, 2022
		N(4)-Oxidejerantinine A (**288**)	Yu *et al.*, 2023
		N(4)-Oxidejerantinine E (**308**)	Yu *et al.*, 2023
		Taberbovermine A (**289**)	Yu *et al.*, 2023
		Taberbovermine B (**312**)	Yu *et al.*, 2023
		Taberbovermine C (**290**)	Yu *et al.*, 2023
		Taberbovermine D (**311**)	Yu *et al.*, 2023
		Taberbovermine E (**307**)	Yu *et al.*, 2023
		Taberbovermine F (**287**)	Yu *et al.*, 2023
		Taberbovermine G (**298**)	Yu *et al.*, 2023
		Taberbovermine H (**302**)	Yu *et al.*, 2023
		Taberbovermine I (**360**)	Yu *et al.*, 2023
		Tabercamine A (**420**)	Yu, Bao, Wang *et al.*, 2019
		Tabercamine B (**423**)	Yu, Bao, Wang *et al.*, 2019
		Tabercamine C (**421**)	Yu, Bao, Wang *et al.*, 2019
		Tabercamine D (**418**)	Yu, Bao, Wang *et al.*, 2019
		Tabercamine E (**424**)	Yu, Bao, Wang *et al.*, 2019
		Tabercamine F (**401**)	Yu, Bao, Wang *et al.*, 2019
		Tabercamine G (**422**)	Yu, Bao, Wang *et al.*, 2019
		Tabercamine H (**419**)	Yu, Bao, Wang *et al.*, 2019
		Tabercamine I (**402**)	Yu, Bao, Wang *et al.*, 2019
		Tabercamine J (**413**)	Yu, Bao, Wang *et al.*, 2019
		Tabercamine K (**425**)	Yu, Bao, Wang *et al.*, 2019
		Taberibogine C (**351**)	Zhao *et al.*, 2022
		Taberibogine D (**358**)	Zhao *et al.*, 2022
		Tabernabovine A (**641**)	Yu, Bao, Wu *et al.*, 2019
		Tabernabovine B (**99**)	Yu, Bao, Wu *et al.*, 2019
		Tabernabovine C (**110**)	Yu, Bao, Wu *et al.*, 2019

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Tabernaemontine A (**862**)	Yu *et al.*, 2020
		Tabernaemontine B (**865**)	Yu *et al.*, 2020
		Tabernaemontine C (**867**)	Yu *et al.*, 2020
		Tabernaemontine D (**869**)	Yu *et al.*, 2020
		Tabernaemontine E (**863**)	Yu *et al.*, 2020
		Tabernaemontine F (**864**)	Yu *et al.*, 2020
		Tabernaemontine G (**871**)	Yu *et al.*, 2020
		Tabernaemontine H (**868**)	Yu *et al.*, 2020
		Tabernaemontine I (**866**)	Yu *et al.*, 2020
		Tabernaemontine J (**872**)	Yu *et al.*, 2020
		Tabernaemontine K (**870**)	Yu *et al.*, 2020
		Tabernaemontine L (**873**)	Yu *et al.*, 2020
		Tabersonine (**281**)	Zhao *et al.*, 2022
		Tacamodinine (**417**)	Yu, Bao, Wang *et al.*, 2019
		Tacamonine (**415**)	Yu *et al.*, 2019
	Leaves, twigs	14α,15β-Dihydroxy-N(1)-methylaspidospermine (**317**)	Ngoc *et al.*, 2022
		Hecubine (= N(1)-Methylvoaphylline) (**345**)	Ngoc *et al.*, 2022
		Mehranine (**314**)	Ngoc *et al.*, 2022
		Taberbovinine A (**316**)	Ngoc *et al.*, 2022
		Taberbovinine B (**147**)	Ngoc *et al.*, 2022
		Voacangarine (= Voacristine) (**24**)	Ngoc *et al.*, 2022
		Voafinidine (**357**)	Ngoc *et al.*, 2022
T. brachyantha Stapf. (*Conopharyngia brachyantha*)	Stem-bark	Anhydrovobasindiol (= Taberpsychine) (**212**)	Patel *et al.*, 1973
		Normacusine B (**168**)	Patel *et al.*, 1973
		Voacorine (**725**)	Patel *et al.*, 1973
T. bufalina Lour. (Ervatamia hainanensis)	Roots	Coronaridine (**14**)	Feng *et al.*, 1982
		Coronaridine-7-hydroxyindolenine (**29**)	Feng *et al.*, 1982
		Ervahaimidine A (**704**)	Feng *et al.*, 1989
		Ervahaimidine B (**689**)	Feng *et al.*, 1989
		Ervahaimine A (**69**)	Feng *et al.*, 1989
		Ervahaimine B (**70**)	Feng *et al.*, 1989
		Ervahanine A (**701**)	Feng *et al.*, 1981
		Ervahanine B (**678**)	Feng *et al.*, 1981
		Ervahanine C (**746**)	Feng *et al.*, 1981
		Geissoschizol (**136**)	Feng *et al.*, 1982
		Heyneanine (**16**)	Feng *et al.*, 1982
		3(*S*)-3-(β-Hydroxyethyl)-coronaridine (**442**)	Feng *et al.*, 1982
		10-Hydroxygeissoscchizol (**137**)	Feng *et al.*, 1982
		10-Hydroxyheyneanine (**459**)	Feng *et al.*, 1982
		Ibogamine (**11**)	Feng *et al.*, 1982
		3-Oxocoronaridine (= Eglandulosine) (**19**)	Feng *et al.*, 1982
		Perivine (**40**)	Feng *et al.*, 1982
		Vobasine (**37**)	Feng *et al.*, 1982
	Stems	Coronaridine (**14**)	Zhan *et al.*, 2010
		Coronaridine-7-hydroxyindolenine (**29**)	Zhan *et al.*, 2010
		Ervahainanmine (**176**)	Zhan *et al.*, 2009
		19(*R*)-Heyneanine (**17**)	Zhan *et al.*, 2010
		19(*S*)-Heyneanine (**16**)	Zhan *et al.*, 2010
		Heyneanine-7-hydroxyindolenine (**512**)	Zhan *et al.*, 2010

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		10-Hydroxycoronaridine (**427**)	Zhan *et al.*, 2010
		Voacangine (**23**)	Zhan *et al.*, 2010
		Vobasine (**37**)	Zhan *et al.*, 2010
	Twigs, Leaves	Coronaridine (**14**)	Yang *et al.*, 2013; Liu *et al.*, 2016
		Coronaridine hydroxyindolenine (**29**)	Yang *et al.*, 2013
		7(*S*)-Coronaridine hydroxyindolenine (**499**)	Liu *et al.*, 2016
		Coronaridine pseudoindoxyl (**27**)	Liu *et al.*, 2016
		3(*S*)-Cyano-7(*S*)-coronaridine hydroxyindolenine (**497**)	Liu *et al.*, 2016
		19-*Epi*-heyneanine (**17**)	Yang *et al.*, 2013
		Ervahainine A (**479**)	Liu *et al.*, 2013
		Heyneanine (**16**)	Yang *et al.*, 2013
		3(*R*)-Hydroxy-7(*S*)-coronaridine hydroxyindolenine (**498**)	Liu *et al.*, 2016
		3(*S*)-[24(*R*)-Hydroxyethyl]-coronaridine (**519**)	Liu *et al.*, 2016
		3(*S*)-[24(*S*)-Hydroxyethyl]-coronaridine (**518**)	Liu *et al.*, 2016
		3-Oxocoronaridine (**19**)	Liu *et al.*, 2016
		5-Oxocoronaridine (**526**)	Liu *et al.*, 2016
		3-Oxo-7(*R*)-coronaridine hydroxyindolenine (**516**)	Liu *et al.*, 2016
		3-Oxo-7(*S*)-coronaridine hydroxyindolenine (**502**)	Liu *et al.*, 2016
		5-Oxo-6(*S*)-hydroxycoronaridine (**527**)	Liu *et al.*, 2016
		5-Oxo-6(*S*)-methoxycoronaridine (**528**)	Liu *et al.*, 2016
		Vobasine (**37**)	Yang *et al.*, 2013
	Aerial parts	Antirhine (**58**)	Shi *et al.*, 2019
		Apparicine (**272**)	Shi *et al.*, 2019
		Conolobine (**275**/**276**)	Shi *et al.*, 2019
		Conolidine (**273**)	Shi *et al.*, 2019
		Conophyllidine (**853**)	Shi *et al.*, 2019
		Conophylline (**71**)	Shi *et al.*, 2019
		Coronaridine (**14**)	Shi *et al.*, 2019; Zhang, Yu *et al.*, 2015; Zhou *et al.*, 2018
		Coronaridine hydroxyindolenine (**29**)	Shi *et al.*, 2019
		14,15-Didehydro-10,11-dimethoxyvincamine (**373**)	Shi *et al.*, 2019
		14,15-Didehydro-10,11-dimethoxy-16-*epi*-vincamine (**370**)	Shi *et al.*, 2019
		Ervatamine A (**569**)	Zhang, Yu *et al.*, 2015
		Ervatamine B (**114**)	Zhang, Yu *et al.*, 2015
		Ervatamine C (**115**)	Zhang, Yu *et al.*, 2015
		Ervatamine D (**116**)	Zhang, Yu *et al.*, 2015
		Ervatamine E (**117**)	Zhang. Yu *et al.*, 2015
		Ervatamine F (**524**)	Shi *et al.*, 2019; Zhang, Yu *et al.*, 2015
		Ervatamine G (= Taberdivarine G) (**21**)	Shi *et al.*, 2019; Zhang, Yu *et al.*, 2015
		Ervatamine H (**483**)	Shi *et al.*, 2019; Zhang, Yu *et al.*, 2015
		Ervatamine I (**476**)	Shi *et al.*, 2019; Zhang, Yu *et al.*, 2015

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Heyneanine (**16**)	Shi *et al.*, 2019; Zhang, Yu *et al.*, 2015
		3-(2'-Oxopropyl)-19-*epi*-heyneanine (**457**)	Shi *et al.*, 2019; Zhang, Yu *et al.*, 2015
		Pandine (**636**)	Shi *et al.*, 2019; Zhang, Yu *et al.*, 2015
		Conodurine (**748**)	Shi *et al.*, 2019; Zhou *et al.*, 2018
		19,20-Dihydroisotabernamine (**757**)	Zhou *et al.*, 2018
		19,20-Dihydrotabernamine (**706**)	Chen *et al.*, 2022; Zhou *et al.*, 2018
		Ervadivaricatine B (**695**)	Chen *et al.*, 2022; Zhou *et al.*, 2018
		Ibogamine (**11**)	Zhou *et al.*, 2018
		3-(2-Oxopropyl)-conodurine (**577**)	Zhou *et al.*, 2018
		3-(2-Oxopropyl)-coronaridine (**456**)	Zhou *et al.*, 2018
		3'-(2-Oxopropyl)-19,20-dihydrotabernamine (**712**)	Zhou *et al.*, 2018
		3'-(2-Oxopropyl)-ervahanine B (**703**)	Zhou *et al.*, 2018
		Taberdivarine C (**662**)	Zhou *et al.*, 2018
		Taberdivarine D (**663**)	Zhou *et al.*, 2018
		Taberdivarine E (**710**)	Zhou *et al.*, 2018
		Taberdivarine F (**711**)	Zhou *et al.*, 2018
		Tabernaecorymbosine A (**767**)	Chen *et al.*, 2022; Zhou *et al.*, 2018
		Tabernaelegantine A (**733**)	Zhou *et al.*, 2018
		Tabernaelegantine B (**664**)	Zhou *et al.*, 2018
		Tabernaelegantine C (**734**)	Zhou *et al.*, 2018
		Tabernaelegantinine B (**668**)	Zhou *et al.*, 2018
		Voacangine (**23**)	Shi *et al.*, 2019; Zhou *et al.*, 2018
		14,15-Didehydro-10-hydroxy-11-methoxy-16-*epi*-vincamine (**302**)	Shi *et al.*, 2019
		16-*Epi*-vobasine (**39**)	Shi *et al.*, 2019
		Epi-dehydrovincamine (**298**)	Shi *et al.*, 2019
		Ervahanine A (**701**)	Chen *et al.*, 2022; Shi *et al.*, 2019
		Ervahanine B (**678**)	Chen *et al.*, 2022
		Ervahanine C (**746**)	Shi *et al.*, 2019
		Fluorocarpamine (**53**)	Shi *et al.*, 2019
		Geissoschizol (**136**)	Shi *et al.*, 2019
		Heyneanine hydroxyindolenine (**512**)	Shi *et al.*, 2019
		10-Hydroxycoronaridine (**427**)	Shi *et al.*, 2019
		10-Hydroxygeissoschizol (**137**)	Shi *et al.*, 2019
		10-Hydroxyheyneanine (**459**)	Shi *et al.*, 2019
		16-Hydroxyibogaine (**154**)	Chen *et al.*, 2022
		19(*S*)-Hydroxyibogamine (**12**)	Chen *et al.*, 2022; Shi *et al.*, 2019
		3(*S*)-(24*R*-hydroxyethyl)-coronaridine (**519**)	Chen *et al.*, 2022
		3(*S*)-(24*S*-hydroxyethyl)-coronaridine (**518**)	Chen *et al.*, 2022
		Iboluteine (= Ibogaine pseudoindoxyl) (**556**)	Chen *et al.*, 2022
		Isositsirikine (**51**)	Shi *et al.*, 2019
		Isovallesiachotamine (**156**)	Shi *et al.*, 2019
		Normacusine B (**168**)	Shi *et al.*, 2019
		O-Acetyl-vallesamine (**271**)	Shi *et al.*, 2019
		3-Oxocoronaridine (**19**)	Chen *et al.*, 2022; Shi *et al.*, 2019
		3-(2-Oxopropyl)-coronaridine (**456**)	Shi *et al.*, 2019
		Pachysiphine (**291**)	Shi *et al.*, 2019

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Pandoline (**609**)	Shi *et al.*, 2019
		Pseudoindoxyl coronaridine (**27**)	Shi *et al.*, 2019
		Pseudovincadifformine (**608**)	Shi *et al.*, 2019
		Rhazimal (= rhazinaline) (**231**)	Shi *et al.*, 2019
		Strictamine (**232**)	Shi *et al.*, 2019
		Taberbufamine A (**638**)	Chen *et al.*, 2022
		Taberbufamine B (**639**)	Chen *et al.*, 2022
		Taberbufamine C (**556**)	Chen *et al.*, 2022
		Taberbufamine D (**544**)	Chen *et al.*, 2022
		Taberhaine B (= 3-*O*-methyl-10,11-demethoxychippiine) (**32**)	Shi *et al.*, 2019
		Taberhaine C (**277**)	Shi *et al.*, 2019
		Taberhaine D (**278**)	Shi *et al.*, 2019
		Tabernamine (**67**)	Chen *et al.*, 2022
		Tetrahydroalstonine (**130**)	Shi *et al.*, 2019
		Tubotaiwine (**60**)	Shi *et al.*, 2019
		Vallesamine (**270**)	Shi *et al.*, 2019
		Vallesiachotamine (**155**)	Shi *et al.*, 2019
		Velbanamine (**604**)	Shi *et al.*, 2019
		Voacristine (= Voacangarine) (**24**)	Shi *et al.*, 2019
		Vobasine (**37**)	Shi *et al.*, 2019
		Voaphylline (= Conoflorine) (**55**)	Shi *et al.*, 2019
		Vobatensine C (**727**)	Chen *et al.*, 2022
	Branches, leaves	Conophylline (**71**)	Xu *et al.*, 2019
		(3*R*,7*S*,14*R*,19*S*,20*R*)-19-hydroxypseudovincadifforamine (**616**)	Xu *et al.*, 2019
		12-Methoxyvoaphylline (**346**)	Xu *et al.*, 2019
		Voachalotine (**162**)	Xu *et al.*, 2019
T. calcarea Pichon (*Pandaca calcarea*, *P. caducifolia*)	Leaves	Apparicine (**272**)	Hoizey *et al.*, 1974
		Dregamine (**41**)	Hoizey *et al.*, 1974
		20-*Epi*-pandoline (**610**)	Zeches *et al.*, 1975
		16-*Epi*-silicine (**252**)	Clivio, Richard *et al.*, 1995
		Pandine (**636**)	Hoizey *et al.*, 1974; Zeches *et al.*, 1975
		Pandoline (**470**)	Hoizey *et al.*, 1974; Zeches *et al.*, 1975
		Pseudotabersonine (**607**)	Zeches *et al.*, 1975
		(+)-20(*R*)-Pseudovincadifformine (**608**)	Zeches *et al.*, 1975
		Silicine (**250**)	Zeches *et al.*, 1975; Clivio, Richard *et al.*, 1995
	Leaves, flowers	Coronaridine (**14**)	Chaturvedula *et al.*, 2003
		19-*Epi*-heyneanine (**17**)	Chaturvedula *et al.*, 2003
		19-*Epi*-3-oxo-voacristine (**462**)	Chaturvedula *et al.*, 2003
		19-*Epi*-voacristine (= 19-*Epi*-voacangarine) (**470**)	Chaturvedula *et al.*, 2003
		19-*Epi*-voacristine-7-hydroxyindolenine (**511**)	Chaturvedula *et al.*, 2003
		Heyneanine (**16**)	Chaturvedula *et al.*, 2003
		11-Hydroxycoronaridine (**428**)	Chaturvedula *et al.*, 2003
		3(*R*/*S*)-Hydroxytabernanthine (**540**)	Chaturvedula *et al.*, 2003

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Ibogamine (**11**)	Chaturvedula *et al.*, 2003
		Isovoacangine (**430**)	Chaturvedula *et al.*, 2003
		Isovoacristine (**471**)	Chaturvedula *et al.*, 2003
		10-Methoxyibogamine (**536**)	Chaturvedula *et al.*, 2003
		11-Methoxyibogamine (**538**)	Chaturvedula *et al.*, 2003
		Voacangine (**23**)	Chaturvedula *et al.*, 2003
		Voacristine (= Voacangarine) (**24**)	Chaturvedula *et al.*, 2003
T. capuronii Leeuwenberg (*Capuronetta elegans*)	Leaves, stem-bark	14,15-Anhydrocapuronidine (**621**)	Chardon-Loriaux *et al.*, 1978
		14,15-Anhydro-1,2-dihydrocapuronidine (**620**)	Chardon-Loriaux *et al.*, 1978
		Capuronidine (**624**)	Chardon-Loriaux & Husson, 1975
		Capuronine (**606**)	Chardon-Loriaux & Husson, 1975
		20'(*R*)-Capuvosidine (**797**)	Chardon-Loriaux *et al.*, 1978; Husson *et al.*, 1978
		Capuvosine (**796**)	Chardon-Loriaux & Husson, 1975; Husson *et al.*, 1978
		20'(*R*)-Dehydroxycapuvosine (**794**)	Chardon-Loriaux *et al.*, 1978; Husson *et al.*, 1978
		N(4)-Demethylcapuvosine (**795**)	Chardon-Loriaux *et al.*, 1978
		20'(*R*)-1,2-Dihydrocapuvosidine (**798**)	Husson *et al.*, 1978
T. catharinensis A.DC. (*P. catharinensis*)	Root-bark	Catharinensine (**146**)	Araujo *et al.*, 1984
		Conodurine (**748**)	Araujo *et al.*, 1984
		Coronaridine (**14**)	Araujo *et al.*, 1984; Pereira *et al.*, 1999; Rizo *et al.*, 2013
		Coronaridine-7-hydroxyindolenine (**29**)	Pereira *et al.*, 1999
		16'-Decarbomethoxyvoacamine (**718**)	Araujo *et al.*, 1984
		16-*Epi*-affinine (**203**)	Araujo *et al.*, 1984
		Heyneanine (**16**)	Araujo *et al.*, 1984; Pereira *et al.*, 1999; Rizo *et al.*, 2013
		3(*S*)-Hydroxycoronaridine hydroxyindolenine (**496**)	Pereira *et al.*, 2008
		Ibogamine (**11**)	Pereira *et al.*, 2008
		Isovoacangine (**430**)	Araujo *et al.*, 1984
		12-Methoxy-*N*(4)-methylvoachalotine (**180**)	Pereira *et al.*, 1999; De Fatima *et al.*, 2000
		3-Oxocoronaridine (**19**)	Pereira *et al.*, 2008
		Voacangine (**23**)	Pereira *et al.*, 2008; Rizo *et al.*, 2013
		Voacangine-7-hydroxyindolenine (**507**)	Pereira *et al.*, 1999
		Voachalotine (**162**)	Pereira *et al.*, 2008
		Voacristine (**24**)	Pereira *et al.*, 2008
		Voacristine-7-hydroxyindolenine (**508**)	Pereira *et al.*, 2008
		Vobasine (**37**)	Pereira *et al.*, 1999

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Roots	12-Methoxy-*N*(4)-methylvoachalotine (**180**)	Gonçalves *et al.*, 2011
		Voachalotine (**162**)	Gonçalves *et al.*, 2011
	Latex	Affinisine (**161**)	da Silva Menecucci *et al.*, 2019
		Coronaridine (**14**)	da Silva Menecucci *et al.*, 2019
		16-*Epi*-affinisine (**165**)	da Silva Menecucci *et al.*, 2019
		10-Hydroxy-*N*(1)-methyl-vellosimine (**160**)	da Silva Menecucci *et al.*, 2019
		Ibogamine (**11**)	da Silva Menecucci *et al.*, 2019
		12-Methoxy-voachalotine (**185**)	da Silva Menecucci *et al.*, 2019
		Voachalotine (**162**)	da Silva Menecucci *et al.*, 2019
		Vincamine (**720**)	da Silva Menecucci *et al.*, 2019
T. cerifera Pancher & Sebert (*Pagiantha cerifera*)	Leaves	Apparicine (**272**)	Ros *et al.*, 1978
		Ibogaine (**536**)	Harmouche *et al.*, 1976
		Olivacine (**77**)	Ros *et al.*, 1978
		Voacangine (**23**)	Harmouche *et al.*, 1976
		Voacangine-7-hydroxyindolenine (**507**)	Harmouche *et al.*, 1976
		Vobasine (**37**)	Ros *et al.*, 1978
	Stem-bark	Pagicerine (**211**)	Bert *et al.*, 1985 & 1989
		Pagisulfine (**218**)	Bert *et al.*, 1986 & 1989
	Bark	Ceridimine (**645**)	Wolter Filho *et al.*, 1985; Bert *et al.*, 1989
T. chippii (Stapf) Pichon	Root-bark	Akuammiline (**229**)	Van Beek, Verpoorte, Baerheim *et al.*, 1985
		Anhydrovobasindiol (= Taberpsychine) (**212**)	Van Beek *et al.*, 1985
		Apparicine (**272**)	Van Beek *et al.*, 1985
		Chippiine (**596**)	Van Beek *et al.*, 1985
		Conoduramine (**682**)	Van Beek *et al.*, 1985
		Conodurine (**748**)	Van Beek *et al.*, 1985
		Conopharyngine (**25**)	Van Beek *et al.*, 1985
		Conopharyngine-7-hydroxyindolenine (**509**)	Van Beek *et al.*, 1985
		Coronaridine (**14**)	Van Beek *et al.*, 1985
		Deacetylakuammiline (**228**)	Van Beek *et al.*, 1985
		16-*Epi*-affinisine (**165**)	Van Beek *et al.*, 1985
		16-*Epi*-isositsirikine (**138**)	Van Beek *et al.*, 1985
		12-Hydroxyakuammicine (**257**)	Van Beek *et al.*, 1985
		3'(*R*/*S*)-Hydroxyconoduramine (**686**)	Van Beek *et al.*, 1985
		3'(*R*/*S*)-Hydroxyconodurine (**752**)	Van Beek *et al.*, 1985
		3(*R*/*S*)-Hydroxyconopharyngine (**441**)	Van Beek *et al.*, 1985
		3'(*R*/*S*)-Hydroxy-16'-decarbomethoxyconodurine (**754**)	Van Beek *et al.*, 1985
		3'(*R*/*S*)-Hydroxyvoacamine (**723**)	Van Beek *et al.*, 1985

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Ibogaline (**539**)	Van Beek *et al.*, 1985
		Isositsirikine (**51**)	Van Beek *et al.*, 1985
		Isovoacangine (**430**)	Van Beek *et al.*, 1985
		Monogagaine (**656**)	Van Beek *et al.*, 1985
		Normacusine B (**168**)	Van Beek *et al.*, 1985
		3-Oxoconopharyngine (**440**)	Van Beek *et al.*, 1985
		Pericyclivine (**47**)	Van Beek *et al.*, 1985
		Picraline (**236**)	Van Beek *et al.*, 1985
		Pleiocarpamine (**152**)	Van Beek *et al.*, 1985
		(+)-Tubotaiwine (**60**)	Van Beek *et al.*, 1985
		Voaphylline (= Conoflorine) (**55**)	Van Beek *et al.*, 1985
		Vobasine (**37**)	Van Beek *et al.*, 1985
		Vobasinol (**209**)	Van Beek *et al.*, 1985
		Vobparicine (**653**)	Van Beek *et al.*, 1985
		Vobparicine *N*-oxide (**654**)	Van Beek *et al.*, 1985
T. ciliata Pichon	Leaves	Pandicine (**874**)	Kan-Fan *et al.*, 1981
T. citrifolia L. (*T. oppositifolia*)	Leaves	Akuammidine (**172**)	Kutney & Perez, 1982
		Apparicine (**272**)	Iglesias & Rodriguez, 1979; Kutney & Perez, 1982; Abaul *et al.*, 1989
		12,12'-Bis(11-hydroxycoronaridinyl) (**821**)	Abaul *et al.*, 1989
		Conoflorine (= Voaphylline) (**55**)	Abaul *et al.*, 1989
		14,15-Dehydrotetrastachyne (**809**)	Abaul *et al.*, 1984 & 1989
		14,15-Dehydrotetrastachynine (**811**)	Abaul *et al.*, 1989
		16-*Epi*-isositsirikine (**138**)	Abaul *et al.*, 1989
		20-*Epi*-pandoline (**610**)	Abaul *et al.*, 1989
		Fluorocarpamine (**53**)	Abaul *et al.*, 1989
		10-Hydroxycoronaridine (**427**)	Abaul *et al.*, 1989
		11-Hydroxycoronaridine (**428**)	Abaul *et al.*, 1989
		Ibogaine (**536**)	Abaul *et al.*, 1989
		Iboxygaine (**547**)	Kutney & Perez, 1982
		Lochnericine (**292**)	Kutney & Perez, 1982
		3-Oxovoacangine (**437**)	Kutney & Perez, 1982
		3-Oxovoacristine (**461**)	Kutney & Perez, 1982
		Pandine (**636**)	Abaul *et al.*, 1989
		Pleiocarpamine (**152**)	Abaul *et al.*, 1989
		Sitsirikine (**50**)	Abaul *et al.*, 1989
		Tabersonine (**281**)	Collera *et al.*, 1962; Kutney & Perez, 1982; Abaul *et al.*, 1989
		(+)-Tubotaiwine (**60**)	Abaul *et al.*, 1989
		Vallesamine (**270**)	Kutney & Perez, 1982; Abaul *et al.*, 1989
		Voacamine (**720**)	Gorman *et al.*, 1960
		Voacangine-7-hydroxyindolenine (**507**)	Kutney & Perez, 1982
		Voacristine (= Voacangarine) (**24**)	Kutney & Perez, 1982
	Leaves, roots	Coronaridine (**14**)	Gorman *et al.*, 1960; Collera *et al.*, 1962; Iglesias & Rodriguez, 1979; Kutney & Perez, 1982
		Ibogamine (**11**)	Gorman *et al.*, 1960; Kutney & Perez, 1982; Abaul *et al.*, 1989

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Voacangine (**23**)	Gorman *et al.*, 1960; Iglesias & Rodriguez, 1979; Kutney & Perez, 1982; Abaul *et al.*, 1989
T. coffeoides Boj. ex A.DC. (*T. modesta*, *T. membranacea*, *Hazunta angustifolia*, *H. coffeoides*, *H. membranacea* , *H. modesta*, *H. modesta methuenii*, *H. silicola*, *H. velutina*)	Leaves	Akuammidine (**172**)	Bui *et al.*, 1979
		Deoxoapodine (**329**)	Bui *et al.*, 1980
		14,15-Dihydroxyvincadifformine (**300**)	Bui *et al.*, 1980
		Heyneanine (**16**)	Bui *et al.*, 1979
		10-Hydroxy-11-methoxytabersonine (= Jerantinine A) (**284**)	Bui *et al.*, 1979
		Lochnericine (**292**)	Bui *et al.*, 1980
		Methuenine (**241**)	Bui *et al.*, 1980
		3-Oxotabersonine (**283**)	Bui *et al.*, 1980
		Pericyclivine (**47**)	Bui *et al.*, 1980
		Polyneuridine (**171**)	Bui *et al.*, 1979
		Stemmadenine (**266**)	Bui *et al.*, 1977
		Tabersonine (**281**)	Bui *et al.*, 1980
		Vallesamine (**270**)	Bui *et al.*, 1980
		Vincanidine (**258**)	Bui *et al.*, 1977
		Voaphylline (= Conoflorine) (**55**)	Bui *et al.*, 1979
	Stem-bark	19'(*R*)-Hydroxytabernaelegantine A (**735**)	Bui *et al.*, 1977; Urrea *et al.*, 1981
		Isoreserpiline (**132**)	Bui *et al.*, 1977
		6-Oxomethuenine (**245**)	Bui *et al.*, 1977
		Reserpiline (**131**)	Bui *et al.*, 1977
		Tetraphyllicine (**223**)	Bui *et al.*, 1977
		Tetraphyllicine dimethoxybenzoate (**224**)	Bui *et al.*, 1977
		Tetraphyllicine monomethoxybenzoate (**225**)	Bui *et al.*, 1977
		Tetraphyllicine trimethoxybenzoate (**226**)	Bui *et al.*, 1977
	Roots	Coronaridine (**14**)	Vecchietti *et al.*, 1978
		Ibogamine (**11**)	Bui *et al.*, 1977, 1979 & 1980; Ferrari *et al.*, 1971
		Voacangine (**23**)	Vecchietti *et al.*, 1978
	Root-bark	20'(*S*)-19',20'-Dihydrotabernamine (**706**)	Urrea *et al.*, 1981
		20-*Epi*-silicine (**251**)	Bui *et al.*, 1977
		Tabernaelegantine A (**733**)	Bui *et al.*, 1977; Urrea *et al.*, 1981
	Stem-bark, root-bark	3,14-Dihydroellipticine (**76**)	Bui *et al.*, 1977, 1979 & 1980
		Isomethuenine (**244**)	Bui *et al.*, 1977 & 1979
		6-Oxo-16-*epi*-silicine (**254**)	Bui *et al.*, 1980
	Leaves, twigs	Hazuntine (**293**)	Potier *et al.*, 1968
		Hazuntinine (**294**)	Potier *et al.*, 1968
		Tabernaemontanine (**42**)	Potier *et al.*, 1968
	Leaves, stem-bark, root-bark	Apparicine (**272**)	Bui *et al.*, 1980
		Isovoacangine (**430**)	Bui *et al.*, 1977
		Silicine (**250**)	Bui *et al.*, 1977 & 1980

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Root-bark, roots	6-Oxosilicine (**253**)	Bui *et al.*, 1977, 1979 & 1980; Vecchietti *et al.*, 1978
	Leaves, roots	19-*Epi*-heyneanine (**17**)	Bui *et al.*, 1979
	Leaves, stem-bark	Normacusine B (**168**)	Bui *et al.*, 1977
	Leaves, twigs, stem-bark	Voacarpine (**201**)	Potier *et al.*, 1968
	Leaves, twigs, stem-bark, roots	Dregamine (**41**)	Potier *et al.*, 1968
	Leaves, twigs, stem-bark, root-bark	Vobasine (**37**)	Bui *et al.*, 1977, 1979 & 1980; Potier *et al.*, 1968
T. contorta Stapf.	Stem-bark	Conopharyngine (**25**)	Patel *et al.*, 1967
		Coronaridine (**14**)	Patel *et al.*, 1967
		Ibogaine (**536**)	Patel *et al.*, 1967
		Voacangine (**23**)	Foudjo Melacheu *et al.*, 2019; Patel *et al.*, 1967
		Voacristine (= Voacangarine) (**24**)	Patel *et al.*, 1967
	Roots	Contortarine A (**875**)	Ndongo *et al.*, 2017
		16-E*pi*-pleiomutinine (**876**)	Ndongo *et al.*, 2017
		N(4)-Chloromethyl-pleiomutinine (**877**)	Ndongo *et al.*, 2017
		Pleiocarpamine (**152**)	Ndongo *et al.*, 2017
	Fruits	(−)-Apparicin-21-one (**274**)	Foudjo Melacheu *et al.*, 2019
		5,6-Dioxo-11-methoxy-voacangine (**534**)	Foudjo Melacheu *et al.*, 2019
T. corymbosa Roxb. ex Wall. (*E. corymbosa*, *E. officinalis, E. chinensis* (Merr.) Tsiang, *E. yunnanensis* Tsiang)	Leaves	Apparicine (**272**)	Sim, 2001
		Bistabercarpamine A (**802**)	Ma *et al.*, 2014b
		Bistabercarpamine B (**803**)	Ma *et al.*, 2014b
		Conodiparine A (**673**)	Kam, Sim *et al.*, 2003
		Conodiparine B (**759**)	Kam, Sim *et al.*, 2003
		Conodiparine C (**674**)	Kam, Sim *et al.*, 2003
		Conodiparine D (**760**)	Kam, Sim *et al.*, 2003
		Conodiparine E (**675**)	Kam, Sim *et al.*, 2003
		Conodiparine F (**761**)	Kam, Sim *et al.*, 2003
		Conodirinine A (**773**)	Kam & Sim, 2003a
		Conodirinine B (**774**)	Kam & Sim, 2003a
		Conodurine (**748**)	Ma *et al.*, 2014a

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Conodutarine A (**762**)	Kam, Sim *et al.*, 2003
		Conodutarine B (**763**)	Kam, Sim *et al.*, 2003
		Conofolidine (**858**)	Kam, Sim *et al.*, 2003
		Conolodinine A (**844**)	Sim *et al.*, 2019
		Conolodinine B (= Taberyunine C) (**842**)	Sim *et al.*, 2019
		Conolodinine C (**860**)	Sim *et al.*, 2019
		Conolodinine D (**861**)	Sim *et al.*, 2019
		Cononitarine A (**764**)	Kam, Sim *et al.*, 2003
		Cononitarine B (**765**)	Kam, Sim *et al.*, 2003
		Conophylline (**71**)	Sim *et al.*, 2019
		Conophyllinine (**857**)	Sim *et al.*, 2019
		Coronaridine (**14**)	Ma *et al.*, 2014a
		Corymbosic acid A (**123**)	Nugroho *et al.*, 2018
		Corymbosic acid B (**124**)	Nugroho *et al.*, 2018
		19,20-Dehydroervatamine (**49**)	Kam & Loh, 1993
		14,15-Didehydro-10-hydroxy-11-methoxyvincamine (**369**)	Lim, Thomas *et al.*, 2009
		Dippinine A (**594**)	Kam & Sim, 1999a & 2001
		Dippinine D (**602**)	Kam & Sim, 2001
		Dregamine *N*(4)-oxide (**191**)	Sim *et al.*, 2022
		16-*Epi*-accedine (**159**)	Sim *et al.*, 2022
		16-*Epi*-affinisine *N*(4)-oxide (**166**)	Sim *et al.*, 2022
		19-*Epi*-isovoacristine (**474**)	Ma *et al.*, 2014a
		Ervachinine C (**676**)	Ma *et al.*, 2014a
		Heyneanine (**16**)	Ma *et al.*, 2014a
		Ibogaine (**536**)	Trinh *et al.*, 2001a
		Ibogamine (**11**)	Ma *et al.*, 2014a
		7(*S*)-16(*R*)-19,20-*E*-Isositsirikine oxindole (**143**)	Lim, Thomas *et al.*, 2009
		7(*S*)-Geissoschizol oxindole *N*(4)-oxide (**142**)	Sim *et al.*, 2022
		3(*S*)-Hydroxyibogaine (**541**)	Sim *et al.*, 2022
		Isovoacangine (**430**)	Ma *et al.*, 2014a
		Isovoacristine (**471**)	Kam & Sim, 2002a
		Jerantinine A (**284**)	Lim *et al.*, 2008
		Jerantinine B (**296**)	Lim *et al.*, 2008
		Jerantinine C (**285**)	Lim *et al.*, 2008
		Jerantinine D (**297**)	Lim *et al.*, 2008
		Jerantinine E (**305**)	Lim *et al.*, 2008
		Jerantinine F (**333**)	Lim *et al.*, 2008
		Jerantinine G (**310**)	Lim *et al.*, 2008
		Jerantinine H (**313**)	Lim, Thomas *et al.*, 2009
		Jerantiphylline A (**340**)	Lim, Thomas *et al.*, 2009
		Jerantiphylline B (**342**)	Lim, Thomas *et al.*, 2009
		N(1)-Methoxy-19,20-dehydroervatamine (**243**)	Kam & Loh, 1993
		11-Methoxytronocarpine (**102**)	Sim, 2001
		Methuenine (**241**)	Kam & Loh, 1993
		Modestanine (= Deoxoapodine) (**329**)	Zeches *et al.*, 1995
		Norfluorocurarine (**259**)	Sim, 2001
		Normacusine B (**168**)	Zeches *et al.*, 1995
		5-Oxo-19,20-dehydroervatamine (**242**)	Kam & Loh, 1993
		3-(2'-Oxopropyl)-coronaridine (**456**)	Trinh *et al.*, 2001b
		3-(2'-Oxopropyl)-19-*epi*-heyneanine (**457**)	Trinh *et al.*, 2001b

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Tabercarpamine A (**800**)	Ma *et al.*, 2014a
		Tabercarpamine B (**801**)	Ma *et al.*, 2014a
		Tabercarpamine C (**336**)	Ma *et al.*, 2014a
		Tabercarpamine D (**337**)	Ma *et al.*, 2014a
		Tabercarpamine E (**338**)	Ma *et al.*, 2014a
		Tabercarpamine F (**339**)	Ma *et al.*, 2014a
		Tabercarpamine G (**597**)	Ma *et al.*, 2014a
		Tabercarpamine H (**598**)	Ma *et al.*, 2014a
		Tabercarpamine I (**599**)	Ma *et al.*, 2014a
		Tabercarpamine J (**600**)	Ma *et al.*, 2014a
		Taberisidine (**93**)	Nge, Sim *et al.*, 2016
		Tabernaecorymbosine A (**767**)	Ma *et al.*, 2014a
		Tacamenine (**399**)	Sim *et al.*, 2022
		Tacamenine *N*(4)-oxide (**400**)	Sim *et al.*, 2022
		Vandrikine (**331**)	Zeches *et al.*, 1995
		Vincarudine (= tabernaecorymine C) (**385**)	Sim *et al.*, 2022
		Voacangine (**23**)	Ma *et al.*, 2014a
		Voafinisine A (**354**)	Sim *et al.*, 2022
		Voafinisine B (**355**)	Sim *et al.*, 2022
		Vobasidine E (**45**)	Sim *et al.*, 2022
		Vobasidine F (**46**)	Sim *et al.*, 2022
		Vobasidine G (**214**)	Sim *et al.*, 2022
		Yohimbine (**119**)	Nugroho *et al.*, 2018; Zeches *et al.*, 1995
		β-Yohimbine (**118**)	Nugroho *et al.*, 2018; Zeches *et al.*, 1995
		β-Yohimbine oxindole (**127**)	Nugroho *et al.*, 2018; Zeches *et al.*, 1995
		β-Yohimbine pseudoindoxyl (**128**)	Zeches *et al.*, 1995
		(2*S*)-*β*-Yohimbine-pseudoindoxyl-*β*-*N*-oxide (**129**)	Nugroho *et al.*, 2018
		(7*S*)-3-Oxo-7-hydroxy-3,7-seco-*β*-yohimbine-oxindole (**125**)	Nugroho *et al.*, 2018
		(7*R*)-3-Oxo-7-hydroxy-3,7-seco-*β*-yohimbine-oxindole (**126**)	Nugroho *et al.*, 2018
	Leaves, twigs	19-Acetonylvoacangine (**448**)	Zhang, Ding *et al.*, 2020; Zhang, Teng *et al.*, 2015
		17-Acetyl-tabernaecorymbosine A (**766**)	Zhang, Guo *et al.*, 2015
		Akuammicine (**255**)	Zhang, Lu *et al.*, 2018
		Akuammicine *N*(4)-oxide (**256**)	Zhang, Lu *et al.*, 2018
		Apparicine (**272**)	Zhang, Teng *et al.*, 2015; Zhang, Yuan *et al.*, 2018
		Conodurine (**748**)	Zhang, Ding *et al.*, 2020; Zhang, Guo *et al.*, 2015
		Conofoline (**848**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		Conopharyngine (**25**)	Tang *et al.*, 2014
		Conophyllidine (**853**)	Zhang, Lu *et al.*, 2018
		Conophylline (**71**)	Zhang, Lu *et al.*, 2018
		Coronaridine (**14**)	Zhang, Ding *et al.*, 2020; Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015; Liu *et al.*, 2017
		Coronaridine hydroxyindolenine (**29**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		16'-Decarbomethoxydihydrovoacamine (**707**)	Zhang, Yuan *et al.*, 2018
		16'-Decarbomethoxyvoacamine (**718**)	Zhang, Guo *et al.*, 2015
		19,20-Dehydroervatamine (**49**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		2α,7α-Dihydrodihydroxyvoaphylline (**350**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		19,20-Dihydroervahanine A (**705**)	Zhang, Teng *et al.*, 2015
		Dregamine (**41**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		Eglandine (**432**)	Zhang, Teng *et al.*, 2015
		20-*Epi*-ervatarnine (**80**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		19-*Epi*-heyneanine (**17**)	Zhang, Ding *et al.*, 2020
		19-*Epi*-5-oxovoacristine (**535**)	Tang *et al.*, 2014
		Ervachinine C (**676**)	Zhang, Yuan *et al.*, 2018
		Ervadivaricatine A (**694**)	Zhang, Teng *et al.*, 2015
		Ervadivaricatine B (**695**)	Zhang, Teng *et al.*, 2015
		Ervaoffine A (**559**)	Tang *et al.*, 2014
		Ervaoffine B (= Ervaluteine) (**560**)	Tang *et al.*, 2014
		Ervaoffine C (**561**)	Tang *et al.*, 2014
		Ervaoffine D (**568**)	Tang *et al.*, 2014
		Ervaoffine E (**579**)	Liu *et al.*, 2017
		Ervaoffine F (**581**)	Liu *et al.*, 2017
		Ervaoffine G (**582**)	Liu *et al.*, 2017
		Ervatamine (**247**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		Heyneanine (**16**)	Tang *et al.*, 2014; Zhang, Ding *et al.*, 2020; Zhang, Teng *et al.*, 2015
		Heyneanine hydroxyindolenine (**512**)	Zhang, Ding *et al.*, 2020
		19(*S*)-Hydroxyibogamine (**12**)	Tang *et al.*, 2014
		Ibogaine (**536**)	Tang *et al.*, 2014
		Ibogaine-5,6-dione (**563**)	Tang *et al.*, 2014
		7(*S*)-Ibogaine hydroxyindolenine (**513**)	Tang *et al.*, 2014
		Ibogaine *N*(4)-oxide (**537**)	Tang *et al.*, 2014
		Ibogaline (**539**)	Tang *et al.*, 2014
		Ibogamine (**11**)	Zhang, Teng *et al.*, 2015
		Iboluteine (= Ibogaine pseudoindoxyl) (**556**)	Tang *et al.*, 2014
		Isovallesiachotamine (**156**)	Zhang, Lu *et al.*, 2018
		Isovoacangine (**430**)	Zhang, Ding *et al.*, 2020; Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		Isovoacristine (**471**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		Lirofoline A (**573**)	Liu *et al.*, 2017
		Lirofoline B (**574**)	Liu *et al.*, 2017
		3-Oxocoronaridine (**19**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		5-Oxocoronaridine (**526**)	Liu *et al.*, 2017
		6-Oxoibogaine (**564**)	Liu *et al.*, 2017
		7(*S*)-3-Oxoibogaine hydroxyindolenine (**551**)	Tang *et al.*, 2014
		8-Oxoibogaine lactam (**565**)	Liu *et al.*, 2017
		3-(2'-Oxopropyl)-coronaridine (**456**)	Zhang, Ding *et al.*, 2020; Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		3-(2'-Oxopropyl)-coronaridine hydroxyindolenine (**506**)	Zhang, Teng *et al.*, 2015

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		3'-Oxotabernaelegantine B (**671**)	Zhang, Lu *et al.*, 2018
		3-Oxotabersonine (**283**)	Zhang, Lu *et al.*, 2018
		Tabercorine A (**778**)	Zhang, Guo *et al.*, 2015
		Tabercorine B (**780**)	Zhang, Ding *et al.*, 2020; Zhang, Guo *et al.*, 2015; Zhang, Yuan *et al.*, 2018
		Tabercorine C (**787**)	Zhang, Guo *et al.*, 2015
		Tabernaecorymbosine A (**767**)	Zhang, Ding *et al.*, 2020; Zhang, Yuan *et al.*, 2018
		Tabernaecorymbosine B (**769**)	Zhang, Yuan *et al.*, 2018
		Tabercorymine A (**790**)	Yuan *et al.*, 2017
		Tabercorymine B (**784**)	Yuan *et al.*, 2017
		Taberdivarine A (**791**)	Zhang, Teng *et al.*, 2015
		Taberdivarine B (**792**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		Taberdivarine C (**662**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		Taberdivarine D (**663**)	Zhang, Teng *et al.*, 2015
		Taberdivarine E (**710**)	Zhang, Teng *et al.*, 2015; Zhang, Yuan *et al.*, 2018
		Taberdivarine F (**711**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		Taberdivarine G (= Ervatamine G) (**21**)	Zhang, Teng *et al.*, 2015
		Taberdivarine H (**426**)	Zhang, Teng *et al.*, 2015
		Taberine A (**771**)	Zhang, Ding *et al.*, 2020
		Taberine B (**758**)	Zhang, Ding *et al.*, 2020
		Taberine C (**779**)	Zhang, Ding *et al.*, 2020
		Taberine D (**785**)	Zhang, Ding *et al.*, 2020
		Taberine E (**467**)	Zhang, Ding *et al.*, 2020
		Taberine F (**468**)	Zhang, Ding *et al.*, 2020
		Taberine G (**501**)	Zhang, Ding *et al.*, 2020
		Taberine H (**210**)	Zhang, Ding *et al.*, 2020
		Taberine I (**576**)	Zhang, Ding *et al.*, 2020
		Tabernaelegantine B (**664**)	Zhang, Ding *et al.*, 2020; Zhang, Lu *et al.*, 2018
		Tabernaelegantine D (**666**)	Zhang, Teng *et al.*, 2015; Zhang, Yuan *et al.*, 2018
		Tabernaemontanine (**42**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
		Tabernaricatine A (**775**)	Zhang, Guo *et al.*, 2015
		Tabernaricatine B (**776**)	Zhang, Guo *et al.*, 2015
		Tabernaricatine C (**781**)	Zhang, Ding *et al.*, 2020; Zhang, Yuan *et al.*, 2018
		Tabernaricatine D (**789**)	Zhang, Ding *et al.*, 2020; Zhang, Guo *et al.*, 2015
		Tabersonine (**281**)	Zhang, Lu *et al.*, 2018
		Taberyunine A (**843**)	Zhang, Lu *et al.*, 2018
		Taberyunine B (**856**)	Zhang, Lu *et al.*, 2018
		Taberyunine C (= Conolodinine B) (**842**)	Zhang, Lu *et al.*, 2018
		Taberyunine D (**847**)	Zhang, Lu *et al.*, 2018
		Taberyunine E (**849**)	Zhang, Lu *et al.*, 2018
		Taberyunine F (**850**)	Zhang, Lu *et al.*, 2018
		Taberyunine G (**852**)	Zhang, Lu *et al.*, 2018
		Taberyunine H (**731**)	Zhang, Lu *et al.*, 2018
		Taberyunine I (**732**)	Zhang, Lu *et al.*, 2018

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Taburnaemine A (**782**)	Zhang, Yuan *et al.*, 2018
		Taburnaemine B (**788**)	Zhang, Yuan *et al.*, 2018
		Taburnaemine C (**783**)	Zhang, Yuan *et al.*, 2018
		Taburnaemine D (**786**)	Zhang, Ding *et al.*, 2020; Zhang, Yuan *et al.*, 2018
		Taburnaemine E (**777**)	Zhang, Yuan *et al.*, 2018
		Taburnaemine F (**770**)	Zhang, Yuan *et al.*, 2018
		Taburnaemine G (**768**)	Zhang, Yuan *et al.*, 2018
		Taburnaemine H (**691**)	Zhang, Yuan *et al.*, 2018
		Taburnaemine I (**772**)	Zhang, Ding *et al.*, 2020; Zhang, Yuan *et al.*, 2018
		Vallesiachotamine (**155**)	Zhang, Lu *et al.*, 2018
		Vincadifformine (**325**)	Zhang, Lu *et al.*, 2018
		Voacangine (**23**)	Tang *et al.*, 2014; Zhang, Ding *et al.*, 2020
		Voacangine hydroxyindolenine (**507**)	Zhang, Lu *et al.*, 2018
		Voacristine (**24**)	Tang *et al.*, 2014; Zhang, Ding *et al.*, 2020; Zhang, Lu *et al.*, 2018
		Voaphylline (= conoflorine) (**55**)	Zhang, Lu *et al.*, 2018
		Voaphylline-7-hydroxyindolenine (**56**)	Zhang, Teng *et al.*, 2015
		Vobasine (**37**)	Zhang, Lu *et al.*, 2018; Zhang, Teng *et al.*, 2015
	Leaves, stem-bark	Conodurinine (**755**)	Kam & Sim, 2003b
		Coronaridine (**14**)	Trinh *et al.*, 2001a; Kam & Sim, 2002a
		19-*Epi*-heyneanine (**17**)	Trinh *et al.*, 2001a; Kam & Sim, 2002a
		Heyneanine (**16**)	Trinh *et al.*, 2001a; Kam & Sim, 2002a
		19'(*S*)-Hydroxyconoduramine (**687**)	Kam & Sim, 2003b
		Ibogamine (**11**)	Trinh *et al.*, 2001a; Kam & Sim, 2002a
		Isovoacryptine (**473**)	Kam & Sim, 2002a
		Vobasonidine (**652**)	Kam & Sim, 2002c
	Stems	Coronaridine (**14**)	Jin *et al.*, 2010
		Coronaridine-7-hydroxyindolenine (**29**)	Jin *et al.*, 2010
		Dregamine (**41**)	Takayama *et al.*, 1998
		20-*Epi*-ervatamine (**248**)	Takayama *et al.*, 1998
		Ervataine (**567**)	Jin *et al.*, 2010
		Ervatamine (**247**)	Takayama *et al.*, 1998
		Heyneanine (**16**)	Jin *et al.*, 2010
		Ibogaine (**536**)	Jin *et al.*, 2010
		Tabercarpamine K (**395**)	Yang *et al.*, 2016
		Tabernaemontanine (**42**)	Takayama *et al.*, 1998
		Voacangine (**23**)	Kam & Sim, 2002a; Takayama *et al.*, 1998
		Voacristine (= Voacangarine) (**24**)	Takayama *et al.*, 1998
	Stem-bark	Affinisine (**161**)	Sim, 2001; Lim *et al.*, 2015
		Akuammidine (**172**)	Fan, Zhang *et al.*, 2023;
		Antirhine (**58**)	Lim *et al.*, 2015
		Apocidine A (**334**)	Nge, Chong *et al.*, 2016
		Apocidine B (**332**)	Nge, Chong *et al.*, 2016
		N(4)-Chloromethylnorfluorocurarine chloride (**262**)	Lim *et al.*, 2015; Nge, Chong *et al.*, 2016

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Conodurine (**748**)	Kam & Sim, 2003b
		Conodusine A (**553**)	Nge, Chong *et al.*, 2016
		Conodusine B (**554**)	Nge, Chong *et al.*, 2016
		Conodusine C (**555**)	Nge, Chong *et al.*, 2016
		Conodusine D (**515**)	Nge, Chong *et al.*, 2016
		Conodusine E (**475**)	Nge, Chong *et al.*, 2016
		Conoduzidine A (**394**)	Nge, Chong *et al.*, 2016
		Conoliferine (**590**)	Lim & Kam, 2009a; Lim *et al.*, 2015
		Conolutinine (**98**)	Lim, Etoh *et al.*, 2009; Lim *et al.*, 2015
		Conomicidine A (**588**)	Lim & Kam, 2009b; Lim *et al.*, 2015
		Conomicidine B (**589**)	Lim & Kam, 2009b; Lim *et al.*, 2015
		Cononuridine (**566**)	Nge, Sim *et al.*, 2016
		Cononusine (**587**)	Lim *et al.*, 2015
		Coronaridine (**14**)	Lim *et al.*, 2015
		Coronaridine-7-hydroxyindolenine (**29**)	Kam & Sim, 2002a
		Criofolinine (**135**)	Nge *et al.*, 2014
		16'-Decarbomethoxy-19,20-dihydro-20-*epi*-voacamine (**708**)	Sim *et al.*, 2016
		16'-Decarbomethoxyvoacamine (**718**)	Lim *et al.*, 2015; Nge, Chong *et al.*, 2016; Sim *et al.*, 2016
		16'-Decarbomethoxyvoacamine pseudoindoxyl (**728**)	Lim *et al.*, 2015; Sim *et al.*, 2016
		Decarbomethoxyvoacristine *N*(4)-oxide (**548**)	Fan, Ding *et al.*, 2022
		19,20-Dehydroyohimbine (**122**)	Nge, Chong *et al.*, 2016
		19,20-Dehydro-α-yohimbine (**121**)	Nge, Chong *et al.*, 2016
		N(4)-Demethyltaberpsychine (**213**)	Lim, Sim *et al.*, 2009
		Deoxoapodine (**329**)	Nge, Chong *et al.*, 2016
		19,20-Dihydroisositsirikine (**140**)	Fan, Zhang *et al.*, 2023; Nge, Chong *et al.*, 2016
		Dippinine B (**595**)	Kam & Sim, 2001
		Dippinine C (**601**)	Kam & Sim, 1999b & 2001
		19-*Epi*-heyneanine (**17**)	Lim *et al.*, 2015
		19-*Epi*-isovoacristine (**474**)	Kam & Sim, 2002a
		19-*Epi*-voacristine (**470**)	Fan, Zhang *et al.*, 2023
		16-*Epi*-normacusine B (**169**)	Sim, 2001
		16-*Epi*-vobasenal (**198**)	Sim *et al.*, 2014
		16-*Epi*-vobasine (**39**)	Sim *et al.*, 2014
		Ervahanine A (**701**)	Kam & Sim, 2003b
		Ervaluteine (= Ervaoffine B) (**560**)	Lim *et al.*, 2015
		Ervatensine A (= Ervachinine B) (**714**)	Lim *et al.*, 2015
		Ervatensine B (**715**)	Lim *et al.*, 2015
		3(*R*/*S*)-Ethoxycoronaridine (**433**)	Kam & Sim, 2002a
		3(*R*/*S*)-Ethoxy-19-*epi*-heyneanine (**455**)	Kam & Sim, 2002a
		3(*R*/*S*)-Ethoxyheyneanine (**454**)	Kam & Sim, 2002a
		16-Ethoxytronocarpine (**103**)	Sim, 2001
		Fluorocarpamine (**53**)	Fan, Zhang *et al.*, 2023
		7(*R*)-Geissoschizol oxindole (**144**)	Lim, Sim, *et al.*, 2009; Lim *et al.*, 2015
		7(*S*)-Geissoschizol oxindole (**141**)	Lim, Sim *et al.*, 2009; Lim *et al.*, 2015
		Hedrantherine (**335**)	Nge, Chong *et al.*, 2016
		Heyneanine (**16**)	Lim *et al.*, 2015

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		19'(*S*)-Hydroxyconodurine (**753**)	Kam & Sim, 2003b
		20(*S*)-Hydroxy-1,2-dehydropseudoaspidospermidine (**625**)	Lim *et al.*, 2015
		19'(*S*)-Hydroxyervahanine A (**702**)	Kam & Sim, 2003b
		19(*R*)-Hydroxyibogamine (**13**)	Nge, Chong *et al.*, 2016
		19(*S*)-Hydroxyibogamine (**12**)	Kam & Sim, 2002a; Nge, Chong *et al.*, 2016
		12-Hydroxynorfluorocurarine (**261**)	Sim, 2001
		20(*R*)-18-Hydroxypseudovincadifformine (**612**)	Fan, Ding *et al.*, 2022
		20(*R*)-18-Hydroxypseudovincadifformine *N*(4)-oxide (**613**)	Fan, Ding *et al.*, 2022
		(3*R*, 7*S*, 14*R*, 19*S*, 20*R*)-19-Hydroxypseudovincadifformine (**616**)	Fan, Ding *et al.*, 2022
		(3*R*, 7*S*, 14*R*, 19*S*, 20*R*)-19-Hydroxypseudovincadifformine *N*(4)-oxide (**617**)	Fan, Ding *et al.*, 2022
		3-Hydroxy-3,4-*seco*-coronaridine (**22**)	Kam & Sim, 2002a
		19'(*R*)-Hydroxytabernamine (**68**)	Kam & Sim, 2002b
		19'(*S*)-Hydroxytabernamine (**699**)	Kam & Sim, 2002b
		19(*S*)-Hydroxytacamine *N*(4)-oxide (**408**)	Fan, Ding *et al.*, 2022
		19(*S*)-Hydroxy-16-*epi*-tacamine *N*(4)-oxide (**406**)	Fan, Ding *et al.*, 2022
		Ibogaine (**536**)	Fan, Zhang *et al.*, 2023; Lim *et al.*, 2015
		Ibogaine-7-hydroxyindolenine (**513**)	Fan, Zhang *et al.*, 2023; Lim *et al.*, 2015
		Ibogamine (**11**)	Lim *et al.*, 2015
		Iboluteine (= Ibogaine pseudoindoxyl) (**556**)	Lim *et al.*, 2015
		Iboxygaine (**547**)	Lim *et al.*, 2015
		Isoconoliferine (**591**)	Lim & Kam, 2009a
		Isoconomicidine A (**592**)	Lim & Kam, 2009b
		Isoconomicidine B (**593**)	Lim & Kam, 2009b
		7(*R*)-16(*R*)-19,20-*E*-Isositsirikine oxindole (**145**)	Lim, Sim *et al.*, 2009; Lim *et al.*, 2015
		Isovoacangine (**430**)	Kam & Sim, 2002a
		Lirofoline A (**573**)	Low *et al.*, 2010; Lim *et al.*, 2015
		Modestanine (= Deoxoapodine) (**329**)	Trinh *et al.*, 2001b
		12-Methoxyvoaphylline (**346**)	Fan, Zhang *et al.*, 2023
		Norfluorocurarine (**259**)	Lim *et al.*, 2015; Nge, Chong *et al.*, 2016
		Norfluorocurarine *N*(4)-oxide (**260**)	Sim, 2001
		Normacusine B (**168**)	Trinh *et al.*, 2001b
		3-Oxocoronaridine (**19**)	Kam & Sim, 2002a
		3-Oxo-19-*epi*-heyneanine (**18**)	Kam & Sim, 2002a
		6-Oxoibogaine (**564**)	Lim *et al.*, 2015
		19'-Oxotabernamine (**541**)	Kam & Sim, 2002b
		Pagicerine (**211**)	Fan, Zhang *et al.*, 2023
		Pandine (**636**)	Fan, Zhang *et al.*, 2023
		Pericyclivine (**47**)	Sim, 2001
		Strictamine (**232**)	Sim, 2001
		Tabernaecorymine A (**619**)	Fan, Zhang et al., 2022
		Tabernaecorymine B (**615**)	Fan, Zhang et al., 2023
		Tabernaecorymine C (= Vincarudine) (**385**)	Fan, Zhang et al., 2023
		Tabernaecorymine D (**410**)	Fan, Zhang et al., 2023
		Tabernaecorymine E (**412**)	Fan, Zhang et al., 2023
		Tabernaemontanine (**42**)	Fan, Zhang *et al.*, 2023; Sim *et al.*, 2014

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Tabernamidine A (**692**)	Nge, Chong *et al.*, 2016
		Tabernamidine B (**693**)	Nge, Chong *et al.*, 2016
		Tabernamine (**67**)	Sim, 2001; Nge, Chong *et al.*, 2016
		Taberpsychine (= Anhydrovobasindiol) (**212**)	Sim, 2001
		Tabertinggine (**578**)	Nge *et al.*, 2013
		Tacamine *N*-oxide (**403**)	Fan, Zhang *et al.*, 2023; Sim *et al.*, 2014
		Tacamodinine (**417**)	Lim *et al.*, 2015
		Tacamonine (**415**)	Fan, Zhang *et al.*, 2023
		Tacamonine *N*-oxide (**414**)	Sim *et al.*, 2014
		Taipinisine (**642**)	Sim *et al.*, 2014
		Tronocarpine (**101**)	Kam *et al.*, 2000
		Tronoharine (**97**)	Kam *et al.*, 1999
		Tronoharine (**97a**, revised structure)	Sim *et al.*, 2014
		Vandrikine (**331**)	Nge, Chong *et al.*, 2016
		Velbanamine (**604**)	Lim *et al.*, 2015
		Vernavosine (**133**)	Nge *et al.*, 2014
		Vernavosine ethyl ether (**134**)	Nge *et al.*, 2014
		Vincamajicine (**221**)	Lim *et al.*, 2015
		Voacangine (**23**)	Nge, Chong *et al.*, 2016
		Voachalotine (**162**)	Fan, Ding *et al.*, 2022; Lim *et al.*, 2015
		19(*R*)-Voacristine hydroxyindolenine (**511**)	Fan, Zhang *et al.*, 2023
		Voaphylline (**55**)	Fan, Zhang *et al.*, 2023
		Voastrictine (**104**)	Kam *et al.*, 2001
		Voatinggine (**577**)	Nge *et al.*, 2013
		Vobasenal (**43**)	Sim *et al.*, 2014
		Vobasidine A (**196**)	Sim *et al.*, 2014
		Vobasidine B (**197**)	Sim *et al.*, 2014
		Vobasidine C (**195**)	Sim *et al.*, 2014
		Vobasidine D (**44**)	Sim *et al.*, 2014
		Vobasine (**37**)	Sim *et al.*, 2014
		Vobatensine A (**716**)	Sim *et al.*, 2016
		Vobatensine B (**709**)	Sim *et al.*, 2016
		Vobatensine C (**727**)	Sim *et al.*, 2016
		Vobatensine D (**729**)	Sim *et al.*, 2016
		Vobatensine E (**661**)	Sim *et al.*, 2016
		Vobatensine F (**717**)	Sim *et al.*, 2016
		Vobatricine (**659**)	Kam & Sim, 2002c; Sim *et al.*, 2016
		Yohimbine (**119**)	Nge, Chong *et al.*, 2016
		β-Yohimbine (**118**)	Trinh *et al.*, 2001b
		β-Yohimbine oxindole (**127**)	Trinh *et al.*, 2001b
		7(*R*)-*β*-yohimbine oxindole (**127**)	Nge, Chong *et al.*, 2016
		7(*S*)-*β*-yohimbine oxindole (**127**)	Nge, Chong *et al.*, 2016
		β-Yohimbine pseudoindoxyl (**128**)	Trinh *et al.*, 2001b
		β-Yohimbine pseudoindoxyl *N*(4)-oxide (**129**)	Nge, Chong *et al.*, 2016
	Aerial parts	Eglandine (**432**)	Tang, Li *et al.*, 2022
		Ervaoffine H (**571**)	Tang, Li *et al.*, 2022
		Ervaoffine I (**572**)	Tang, Li *et al.*, 2022
		Ervaoffine J (**583**)	Tang, Li *et al.*, 2022
		Ervaoffine K (**586**)	Tang, Li *et al.*, 2022
		Ervatamine G (= Taberdivarine G) (**21**)	Tang, Li *et al.*, 2022
		Isovoacangine (**430**)	Tang, Li *et al.*, 2022

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Roots	Erchinine A (= Ervaoffine E) (**579**)	Yu, Qin *et al.*, 2018
		Erchinine B (**580**)	Yu, Qin *et al.*, 2018
	Whole plant	19-Acetonylisovoacangine (**449**)	Guo, He *et al.*, 2012
		Conophyllidine (**853**)	Zhang, Wang *et al.*, 2007
		Coronaridine (**14**)	Guo, He *et al.*, 2012
		16'-Decarbomethoxy-19,20-dihydro-20-*epi*-voacamine (**708**)	Zhang, Wang *et al.*, 2007
		16'-Decarbomethoxyvoacamine (**718**)	Zhang, Wang *et al.*, 2007; Guo, He *et al.*, 2012
		10-Demethoxynorvincorine (**227**)	Zhang, Wang *et al.*, 2007
		14,15-Didehydro-10,11-dimethoxy-16-*epi*-vincamine (**370**)	Zhang, Wang *et al.*, 2007
		14,15-Didehydro-10,11-dimethoxyvincamine (**373**)	Zhang, Wang *et al.*, 2007
		14,15-Didehydro-10-hydroxy-11-methoxy-16-*epi*-vincamine (**371**)	Zhang, Wang *et al.*, 2007
		14,15-Didehydro-10-hydroxy-11-methoxyvincamine (**369**)	Zhang, Wang *et al.*, 2007
		Difforlemenine (**217**)	Guo, He *et al.*, 2012
		Dihydroevocarpine (**84**)	Guo, Zhang *et al.*, 2012
		Ervachinine A (**713**)	Guo, He *et al.*, 2012
		Ervachinine B (= Ervatensine A) (**714**)	Guo, He *et al.*, 2012
		Ervachinine C (**676**)	Guo, He *et al.*, 2012
		Ervachinine D (**690**)	Guo, He *et al.*, 2012
		Ervachinine E (**575**)	Guo, Zhang *et al.*, 2012
		Evocarpine (**83**)	Guo, Zhang *et al.*, 2012
		(+)-Hecubine (= *N*(1)-Methylvoaphylline) (**345**)	Guo, He *et al.*, 2012
		Heyneanine (**16**)	Guo, He *et al.*, 2012
		19(*S*)-Hydroxyconopharyngine (**26**)	Zhang, Wang *et al.*, 2007
		20(*S*)-Hydroxy-1,2-dehydropseudoaspidospermidine (**625**)	Zhang, Wang *et al.*, 2007
		Ibogaine (**536**)	Zhang, Wang *et al.*, 2007
		Ibogaine-7-hydroxyindolenine (**513**)	Zhang, Wang *et al.*, 2007
		Isovoacangine (**430**)	Guo, He *et al.*, 2012
		1-Methyl-2-nonyl-4(1*H*)-quinolone (**85**)	Guo, Zhang *et al.*, 2012
		1-Methyl-2-[(*Z*)-6-undecenyl]-4(1*H*)-quinolone (**86**)	Guo, Zhang *et al.*, 2012
		12-Methoxyvoaphylline (**346**)	Zhang, Wang *et al.*, 2007
		3-(2'-Oxopropyl)-voacangine (**448**)	Guo, He *et al.*, 2012
		Picrinine (**237**)	Zhang, Wang *et al.*, 2007
		Rhazinaline (= Rhazimal) (**231**)	Zhang, Wang *et al.*, 2007
		Rutaecarpine (**157**)	Guo, Zhang *et al.*, 2012
		Strictamine (**232**)	Zhang, Wang *et al.*, 2007
		Tabernaecorymbosine A (**767**)	Guo, He *et al.*, 2012
		(−)-Velbanamine (**604**)	Zhang, Wang *et al.*, 2007
		Vincadiffine (**206**)	Guo, He *et al.*, 2012
		Voacangine (**23**)	Zhang, Wang *et al.*, 2007
		Voachalotine (**162**)	Zhang, Wang *et al.*, 2007
		Voacristine (**24**)	Zhang, Wang *et al.*, 2007
		Voaphylline (= Conoflorine) (**55**)	Zhang, Wang *et al.*, 2007; Guo, He *et al.*, 2012;
		Vobasine (**37**)	Guo, He *et al.*, 2012

Table 1.3, continued

Plant	Plant part	Alkaloids	References
T. crassa Benth. (*T. durissima Conopharyngia crassa, C. durissima, C. jollyana, Gabunia odoratissima, Sarcopharyngia crassa*)	Seeds	Coronaridine (**14**)	Batchily *et al.*, 1986
		Ibogaine (**536**)	Batchily *et al.*, 1986
		3-Oxotabersonine (**283**)	Batchily *et al.*, 1986
		Pachysiphine (**291**)	Batchily *et al.*, 1986
		Sarcopharyngine (**450**)	Batchily *et al.*, 1986
		Tabersonine (**281**)	Batchily *et al.*, 1986
		Voacangine (**23**)	Batchily *et al.*, 1986
		Voacangine-7-hydroxyindolenine (**507**)	Batchily *et al.*, 1986
		Voacangine pseudoindoxyl (**520**)	Batchily *et al.*, 1986
	Stem-bark	*O*-Acetylpolyneuridine (**173**)	Hootele, Levy *et al.*, 1967
		Akuammiline (**229**)	Dugan *et al.*, 1969
		Anhydrovobasindiol (= Taberpsychine) (**212**)	Dugan *et al.*, 1969
		Conoduramine (**682**)	Renner *et al.*, 1959; Cava, Talapatra *et al.*, 1965
		Conodurine (**748**)	Renner *et al.*, 1959; Cava, Talapatra *et al.*, 1965
		Conopharyngine (**25**)	Renner *et al.*, 1959; Van Beek, De Smidt *et al.*, 1985
		Conopharyngine-7-hydroxyindolenine (**509**)	Hootele, Levy *et al.*, 1967
		Coronaridine (**14**)	Hootele, Pecher *et al.*, 1964; Cava, Talapatra *et al.*, 1965
		Coronaridine hydroxyindolenine (**29**)	Li *et al.*, 2023
		Crassanine (**477**)	Cava, Watanabe *et al.*, 1968
		Ervatamine (**247**)	Li *et al.*, 2023
		Gabunine (**747**)	Cava, Talapatra *et al.*, 1965
		Heyneanine (**16**)	Hootele, Levy *et al.*, 1967
		19(*S*)-Hydroxyconopharyngine (**26**)	Hootele, Levy *et al.*, 1967; Hootele, Pecher *et al.*, 1964; Cava, Watanabe *et al.*, 1968
		10-Hydroxycoronaridine (**427**)	Li *et al.*, 2023
		Ibogaine (**536**)	Van Beek, De Smidt *et al.*, 1985
		Ibogamine (**11**)	Cava, Talapatra *et al.*, 1965
		Isovoacangine (**430**)	Cava, Talapatra *et al.*, 1965; Li *et al.*, 2023; Renner *et al.*, 1959
		3-Oxoconopharyngine (**440**)	Hootele & Pecher, 1968
		3-Oxocoronaridine (**19**)	Hootele & Pecher, 1968
		5-Oxocoronaridine (**526**)	Hootele, Pecher *et al.*, 1964
		3-Oxoheyneanine (**452**)	Hootele & Pecher, 1968
		3-(2'-Oxopropyl)-coronaridine (**456**)	Li *et al.*, 2023
		Pericyclivine (**47**)	Cava, Talapatra *et al.*, 1965
		Perivine (**40**)	Hootele, Levy *et al.*, 1967
		Tabercrassine A (**806**)	Li *et al.*, 2023
		Tabercrassine B (**451**)	Li *et al.*, 2023
		Tabercrassine C (**341**)	Li *et al.*, 2023
		Voacangine (**23**)	Li *et al.*, 2023
		Voacristine (= Voacangarine) (**24**)	Hootele, Levy *et al.*, 1967; Li *et al.*, 2023

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Vobasine (**37**)	Cava, Talapatra *et al.*, 1965
T. crassifolia Pichon	Stem-bark	Ibogamine (**11**)	Hoizey *et al.*, 1970
		Tabernanthine (= 11-Methoxyibogamine) (**538**)	Hoizey *et al.*, 1970
T. cymosa Jacq. (*P. buchtieni*)	Leaves	Angustine (**158**)	Ghorbel *et al.*, 1981
		Apodine (**328**)	Azoug *et al.*, 1995
		14,15-Dehydrotetrastachyne (**809**)	Ghorbel *et al.*, 1981
		16-*Epi*-isositsirikine (**138**)	Ghorbel *et al.*, 1981
		19-*Epi*-voacristine (= 19-*Epi*-voacangarine) (**470**)	Ghorbel *et al.*, 1981
		10-Hydroxyheyneanine (**459**)	Ghorbel *et al.*, 1981
		(+)-Tubotaiwine (**60**)	Ghorbel *et al.*, 1981
		Voacristine (= Voacangarine) (**24**)	Azoug *et al.*, 1995
		Voacristine-7-hydroxyindolenine (**508**)	Azoug *et al.*, 1995
	Stem-bark	Affinisine (**161**)	Azoug *et al.*, 1995
		Affinisine *N*(4)-oxide (= *N*(4)-Oxyaffinisine) (**164**)	Azoug *et al.*, 1995
		Buchtienine (**643**)	Azoug *et al.*, 1995
		Ceridimine (**645**)	Azoug *et al.*, 1995
		Chloromethylene-affinisinium (**177**)	Azoug *et al.*, 1995
		Coronaridine (**14**)	Azoug *et al.*, 1995
		Coronaridine-7-hydroxyindolenine (**29**)	Azoug *et al.*, 1995
		N(4)-Demethylaccedinisine (**648**)	Azoug *et al.*, 1995
		N(4)-Demethylceridimine (**646**)	Azoug *et al.*, 1995
		N(4)-Demethyltabernamine (**696**)	Azoug *et al.*, 1995
		3,14-Dihydroolivacine (**80**)	Azoug *et al.*, 1995
		4',17(*β*)-Dihydrotchibangensine (**644**)	Azoug *et al.*, 1995
		18,19(*R*)-Dihydroxycoronaridine (**458**)	Azoug *et al.*, 1995
		Eglandine (**432**)	Azoug *et al.*, 1995
		Eglandulosine (= 3-Oxocoronaridine) (**19**)	Azoug *et al.*, 1995
		19-*Epi*-heyneanine (**17**)	Azoug *et al.*, 1995
		19-*Epi*-voacorine (**726**)	Azoug *et al.*, 1995
		Heyneanine (**16**)	Azoug *et al.*, 1995
		18-Hydroxyaffinisine (**178**)	Azoug *et al.*, 1995
		3'(*R*/*S*)-Hydroxy-*N*(4)-demethyltabernamine (**698**)	Azoug *et al.*, 1995
		3-Hydroxytetrahydroolivacine (**79**)	Azoug *et al.*, 1995
		Ibogaine-7-hydroxyindolenine (**513**)	Ghorbel *et al.*, 1981
		Ibogamine (**11**)	Azoug *et al.*, 1995
		Isositsirikine (**51**)	Azoug *et al.*, 1995
		Janetine (**63**)	Azoug *et al.*, 1995
		10-Methoxyeglandine (**444**)	Ghorbel *et al.*, 1981
		N(1)-Methylpericyclivine (**170**)	Azoug *et al.*, 1995
		Normacusine B (**168**)	Azoug *et al.*, 1995
		Ochropamine (**207**)	Azoug *et al.*, 1995
		Vallesamine (**270**)	Azoug *et al.*, 1995
		Voacangine pseudoindoxyl (= Voaluteine) (**520**)	Ghorbel *et al.*, 1981
		Voachalotine (**162**)	Azoug *et al.*, 1995
		Voaphylline (= Conoflorine) (**55**)	Azoug *et al.*, 1995
		Voaphylline-7-hydroxyindolenine (**56**)	Azoug *et al.*, 1995

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Seeds	(+)-Condylocarpine (**264**)	Achenbach *et al.*, 1997
		(+)-14,15-Dehydro-16-*epi*-vincamine (**59**)	Achenbach *et al.*, 1997
		Heyneanine (**16**)	Achenbach *et al.*, 1997
		Isositsirikine (**51**)	Achenbach *et al.*, 1997
		3-Oxotabersonine (**283**)	Achenbach *et al.*, 1997
		3-Oxovoacangine (**437**)	Monsalve-Escudero *et al.*, 2021
		Rupicoline (= Voacangine pseudoindoxyl) (**520**)	Monsalve-Escudero *et al.*, 2021
		Stemmadenine (**266**)	Achenbach *et al.*, 1997
		Stemmadenine *N*-oxide (**267**)	Achenbach *et al.*, 1997
		Tabersonine (**281**)	Achenbach *et al.*, 1997
		Tabersonine *N*-oxide (**282**)	Achenbach *et al.*, 1997
		Tetrahydroalstonine (**130**)	Achenbach *et al.*, 1997
		Voacangine-7-hydroxyindolenine (**507**)	Monsalve-Escudero *et al.*, 2021
	Stem-bark, root-bark	16'-Decarbomethoxyvoacamine (**718**)	Ghorbel *et al.*, 1981
		N(4)-Demethylvoacamine (**724**)	Ghorbel *et al.*, 1981
		Ibogaine (**536**)	Ghorbel *et al.*, 1981
		Olivacine (**77**)	Ghorbel *et al.*, 1981
		Voacamidine (**660**)	Ghorbel *et al.*, 1981
		Voacamine (**720**)	Ghorbel *et al.*, 1981
	Leaves, seeds	10-Hydroxycoronaridine (**427**)	Ghorbel *et al.*, 1981; Achenbach *et al.*, 1997
		Voacristine (= Voacangarine) (**24**)	Ghorbel *et al.*, 1981; Achenbach *et al.*, 1997
	Stem-bark, seeds	Coronaridine (**14**)	Ghorbel *et al.*, 1981; Achenbach *et al.*, 1997
		3-Oxovoacangine (**437**)	Ghorbel *et al.*, 1981; Achenbach *et al.*, 1997
	Leaves, root-bark	Vobasine (**37**)	Ghorbel *et al.*, 1981
	Leaves, stem-bark	Olivacine (**77**)	Azoug *et al.*, 1995
		Pleiocarpamine (**152**)	Ghorbel *et al.*, 1981
	Leaves, stem-bark, root-bark	Voacangine-7-hydroxyindolenine (**507**)	Ghorbel *et al.*, 1981
	Seeds, leaves, stem-bark, root-bark	Voacangine (**23**)	Ghorbel *et al.*, 1981; Achenbach *et al.*, 1997
T. debrayi (Markgr.) Leeuwenberg (*Pandaca debrayi*)	Leaves	Pandine (**636**)	Hoizey *et al.*, 1974
		Pandoline (**609**)	Hoizey *et al.*, 1974
	Leaves, stem-bark, root-bark	Dregamine (**41**)	Hoizey *et al.*, 1974

Table 1.3, continued

Plant	Plant part	Alkaloids	References
T. dichotoma Roxb. Ex Wall (*Ervatamia dichotoma, Pagiantha dichotoma*, *Rejuoa dichotoma*)	Leaves	19-*Epi*-iboxygaine (**546**)	Vittrup *et al.*, 1981
		19-*Epi*-voacristine (= 19-*Epi*-voacangarine) (**470**)	Vittrup *et al.*, 1981
		16-Hydroxy-16,22-dihydroappariceine (**269**)	Perera, Van Beek *et al.*, 1984
		Perivine (**40**)	Vittrup *et al.*, 1981
		Voaphylline-7-hydroxyindolenine (**56**)	Perera, Van Beek *et al.*, 1984
	Flowers	*O*-Acetylvallesamine (**271**)	Perera, Sandberg *et al.*, 1984
		Dichomine (**637**)	Perera, Sandberg, *et al.*, 1984
		19-*Epi*-heyneanine (**17**)	Perera, Sandberg, *et al.*, 1984
		Voaphylline (= Conoflorine) (**55**)	Perera, Sandberg, *et al.*, 1984
		Vobasine (**37**)	Perera, Sandberg, *et al.*, 1984
	Stem-bark	Monogagaine (**656**)	Van Beek, Lankhorst *et al.*, 1985
	Stem-bark, roots	*N*(4)-Demethyltabernamine (**696**)	Perera, Sandberg *et al.*, 1985
		Heyneanine (**16**)	Perera, Sandberg *et al.*, 1985
		3'(*R*/*S*)-Hydroxy-*N*(4)-demethylervahanine A (**719**)	Perera, Sandberg *et al.*, 1985
		3'(*R*/*S*)-Hydroxy-*N*(4)-demethylervahanine B (**684**)	Perera, Sandberg *et al.*, 1985
		3'(*R*/*S*)-Hydroxy-*N*(4)-demethyltabernamine (**698**)	Perera, Sandberg *et al.*, 1985
		3'(*R*/*S*)-Hydroxytabernamine (**697**)	Perera, Sandberg *et al.*, 1985
		3'(*R*/*S*)-Hydroxyvoacamine (**723**)	Perera, Sandberg *et al.*, 1985
		Ibogamine (**11**)	Perera, Sandberg *et al.*, 1985
		Isomethuenine (**244**)	Perera, Sandberg *et al.*, 1985
		3-Ketopropyl-19(*R*)-heyneanine (**453**)	Perera, Sandberg *et al.*, 1985
		3,19(*R*)-Oxidocoronaridine (**492**)	Perera, Sandberg *et al.*, 1985
		3-Oxocoronaridine (**19**)	Perera, Sandberg *et al.*, 1985
		Perivine (**40**)	Perera, Sandberg *et al.*, 1985
		Tabernamine (**67**)	Perera, Sandberg *et al.*, 1985
		Voacamine (**720**)	Perera, Sandberg *et al.*, 1985

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Leaves, flowers	12-Methoxyvoaphylline (**346**)	Vittrup *et al.*, 1981; Perera, Sandberg, *et al.*, 1984
		Vallesamine (**270**)	Perera, Sandberg, *et al.*, 1984; Perera, Van Beek, *et al.*, 1984
	Stem-bark, flowers	3-Ketopropylcoronaridine (**434**)	Perera, Sandberg, *et al.*, 1984; Perera, Sandberg *et al.*, 1985
	Leaves, stem-bark	Vobasine (**37**)	Vittrup *et al.*, 1981; Perera, Sandberg *et al.*, 1985
	Leaves, stems, roots, flowers	Apparicine (**272**)	Vittrup *et al.*, 1981; Perera, Sandberg, *et al.*, 1984; Perera, Sandberg *et al.*, 1985
	Stem-bark, flowers, roots	Coronaridine (**14**)	Perera, Sandberg, *et al.*, 1984; Perera, Sandberg *et al.*, 1985
T. divaricata (L.) R. Br. ex Roem. & Schult. *(T. coronaria, Ervatamia coronaria, E. divaricata)*	Leaves	Apparicine (**272**)	Gomez Gonzalez, Navajas *et al.*, 1981; Kam & Anuradha, 1995; Kam, Pang *et al.*, 2003
		Conofoline (= Pedunculine) (**848**)	Chen *et al.*, 2021; Kam & Anuradha, 1995
		Conolodinine A (**844**)	Chen *et al.*, 2021
		Conolodinine B (**842**)	Chen *et al.*, 2021
		Conophyllidine (**853**)	Chen *et al.*, 2021; Kam, Loh *et al.*, 1993
		Conophylline (**71**)	Chen *et al.*, 2021; Kam, Loh *et al.*, 1992 & 1993
		Conophyllinine (**857**)	Kam, Pang, *et al.*, 2003
		19-*Epi*-heyneanine (**17**)	Arambewela & Ranatunge, 1991
		16-Hydroxy-16,22-dihydroapparicine (**269**)	Kam, Pang *et al.*, 2003
		Ibogaine (**536**)	Kam, Pang *et al.*, 2003
		Ibogamine (**11**)	Kam, Pang *et al.*, 2003
		16(*R*)-19,20-*E*-Isositsirikine (**138**)	Kam, Pang *et al.*, 2003
		16(*R*)-19,20-*E*-Isositsirikine oxindole (**143**)	Kam, Pang *et al.*, 2003
		Isovoacristine (**471**)	Karawya & Aboutabl, 1982; Arambewela & Ranatunge, 1991
		Lochnericine (**292**)	Raj *et al.*, 1974; Talapatra, Patra *et al.*, 1975
		(−)-Mehranine (**314**)	Kam & Anuradha, 1995; Kam, Pang, *et al.*, 2003
		N(1)-Methylvoafinine (**348**)	Kam, Pang, *et al.*, 2003
		N(1)-Methylvoaphylline (= Hecubine) (**345**)	Kam & Anuradha, 1995; Kam, Pang, *et al.*, 2003
		Pachysiphine (**291**)	Kam & Anuradha, 1995; Kam, Pang, *et al.*, 2003

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Peduncularidine (**851**)	Kam, Pang, *et al.*, 2003
		Taberdivarine A (**881**)	Chen *et al.*, 2021
		Taberdivarine B (**882**)	Chen *et al.*, 2021
		Taberdivarine C (**845**)	Chen *et al.*, 2021
		Taberdivarine D (**840**)	Chen *et al.*, 2021
		Taberdivarine E (**841**)	Chen *et al.*, 2021
		Taberdivarine F (**854**)	Chen *et al.*, 2021
		Taberdivarine G (**855**)	Chen *et al.*, 2021
		Taberdivarine H (**846**)	Chen *et al.*, 2021
		Taberhanine (**295**)	Kam, Pang, *et al.*, 2003
		Taberyunine A (**843**)	Chen *et al.*, 2021
		Taberyunine B (**856**)	Chen *et al.*, 2021
		Taberyunine D (**847**)	Chen *et al.*, 2021
		Taberyunine E (**849**)	Chen *et al.*, 2021
		Voacangine (**23**)	Kam, Pang, *et al.*, 2003
		Voacristine (**24**)	Kam, Pang, *et al.*, 2003
		Voafinidine (**357**)	Kam, Pang, *et al.*, 2003
		Voafinine (**347**)	Kam, Pang, *et al.*, 2003
		Voaharine (**106**)	Kam, Loh *et al.*, 1992; Kam & Anuradha, 1995
		Voalenine (**349**)	Kam, Pang, *et al.*, 2003
		Voaphylline (**55**)	Kam & Anuradha, 1995; Kam, Pang, *et al.*, 2003
		Voastrictine (**104**)	Kam, Pang, *et al.*, 2003
	Root-bark	Coronaridine-7-hydroxyindolenine (**29**)	Rastogi *et al.*, 1980
		5-Hydroxy-6-oxocoronaridine (**530**)	Rastogi *et al.*, 1980
		3-Oxocoronaridine (**19**)	Delle Monache *et al.*, 1972; Rastogi *et al.*, 1980
		5-Oxocoronaridine (**526**)	Rastogi *et al.*, 1980
		6-Oxocoronaridine (**529**)	Rastogi *et al.*, 1980
		Pseudovobparicine (**655**)	Van Beek, Verpoorte, & Kinh, 1985
	Roots	19,20-Dihydroervahanine A (**705**)	Liu *et al.*, 2018
		Divaricamine A (**878**)	Hirasawa *et al.*, 2021
		Ervadivamine A (**879**)	Liu *et al.*, 2018
		Ervadivamine B (**880**)	Liu *et al.*, 2018
		Ibogaine (**536**)	Liu *et al.*, 2018
		Ibogamine (**11**)	Liu *et al.*, 2018
	Stems	(−)-Apparicine (**272**)	Cai *et al.*, 2018
		16'-Decarbomethoxyvoacamine (**718**)	Henriques *et al.*, 1996
		19,20-Dihydroervahanine A (**705**)	Henriques *et al.*, 1996
		19,20-Dihydrotabernamine (**706**)	Cai *et al.*, 2018
		19,20-Dihydrovobparicine (**657**)	Cai *et al.*, 2018
		Ervahanine A (**701**)	Cai *et al.*, 2018
		Flabellipparicine (**658**)	Cai *et al.*, 2018
		3-(2-Oxopropyl)-coronaridine hydroxyindolenine (**506**)	Cai *et al.*, 2018
		3'(*R*/*S*)-Hydroxyvoacamine (**723**)	Chaiyana *et al.*, 2013
		3'-(2-Oxopropyl)-ervahanine A (**703**)	Cai *et al.*, 2018
		3-(2'-Oxopropyl)-coronaridine (**456**)	Delle Monache *et al.*, 1972
		Tabercetimine A (**148**)	Zhu *et al.*, 2021
		Tabercetimine B (**149**)	Zhu *et al.*, 2021
		Tabercetimine C (**150**)	Zhu *et al.*, 2021
		Tabercetimine D (**151**)	Zhu *et al.*, 2021

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Taberdivarine E (**710**)	Cai *et al.*, 2018
		Tabernamine (**67**)	Cai *et al.*, 2018
		Taberniacin A (**95**)	Hirasawa *et al.*, 2019
		Taberniacin B (**96**)	Hirasawa *et al.*, 2019
		Tubotaiwine (**60**)	Cai *et al.*, 2018
		Vobparicine (**653**)	Cai *et al.*, 2018
	Flowers	Tabersonine (**281**)	Gomez Gonzalez *et al.*, 1981
		3,14;4,19-Tetrahydroolivacine (= Janetine) (**78**)	Gomez Gonzalez & Corzo Rodriguez, 1978
	Leaves, stems	Akuammicine (**255**)	Zhang, Wang *et al.*, 2007
		Apparicine (**272**)	Zhang, Wang *et al.*, 2007
		Coronaridine (**14**)	Gorman *et al.*, 1960; Raj *et al.*, 1974; Talapatra *et al.*, 1975; Gomez Gonzalez & Lorincz, 1976; Arambewela & Ranatunge, 1991; Henriques *et al.*, 1996; Zhang, Wang *et al.*, 2007
		Coronaridine-7-hydroxyindolenine (**29**)	Zhang, Wang *et al.*, 2007
		Dehydroxyervataminol (**240**)	Zhang, Wang *et al.*, 2007
		19,20-Didehydro-6α-hydroxyervatamine (**239**)	Zhang, Wang *et al.*, 2007
		19,20-Dihydrotabernamine (**706**)	Zhang, Wang *et al.*, 2007
		Dregamine (**41**)	Gorman *et al.*, 1960; Raj *et al.*, 1974; Talapatra *et al.*, 1975; Arambewela & Ranatunge, 1991; Zhang, Wang *et al.*, 2007
		20-*Epi*-ervatamine (**248**)	Zhang, Wang *et al.*, 2007
		14,15-β-Epoxytabersonine (= Pachysiphine) (**291**)	Zhang, Wang *et al.*, 2007
		Ervadivaricatine A (**694**)	Zhang, Wang *et al.*, 2007
		Ervadivaricatine B (**695**)	Zhang, Wang *et al.*, 2007
		Ervatamine (**247**)	Zhang, Wang *et al.*, 2007
		Ibogamine (**11**)	Zhang, Wang *et al.*, 2007
		(−)-Mehranine (**314**)	Zhang, Wang *et al.*, 2007
		11-Methoxy-*N*(1)-methyldihydropericyclivine (**179**)	Arambewela & Ranatunge, 1991
		Tabernaemontanine (**42**)	Zhang, Wang *et al.*, 2007
		Tabersonine (**281**)	Zhang, Wang *et al.*, 2007
		Tubotaiwine (**60**)	Zhang, Wang *et al.*, 2007
		Voacangine (**23**)	Zhang, Wang *et al.*, 2007
		Voacangine-7-hydroxyindolenine (**507**)	Zhang, Wang *et al.*, 2007
		Voaphylline (**55**)	Zhang, Wang *et al.*, 2007
	Root-bark, stems	Heyneanine (**16**)	Rastogi *et al.*, 1980; Henriques *et al.*, 1996
		Voacamine (**720**)	Rastogi *et al.*, 1980; Karawya & Aboutabl, 1982; Henriques *et al.*, 1996

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Voacristine (= Voacangarine) (**24**)	Raj *et al.*, 1974; Talapatra *et al.*, 1975; Arambewela & Ranatunge, 1991; Henriques *et al.*, 1996
	Leaves, flowers	*N*(1)-Methylvoaphylline (= Hecubine) (**345**)	Gomez Gonzalez & Martinez, 1976; Gomez Gonzalez & Corzo Rodriguez, 1978; Gomez Gonzalez *et al.*, 1981
		Voaphylline (= Conoflorine) (**55**)	Raj *et al.*, 1974; Talapatra *et al.*, 1975; Gomez Gonzalez & Martinez, 1976; Gomez Gonzalez *et al.*, 1981
	Leaves, stem-bark	Voacangine (**23**)	Raj *et al.*, 1974; Talapatra *et al.*, 1975; Gomez Gonzalez & Lorincz, 1976; Karawya & Aboutabl, 1982; Arambewela & Ranatunge, 1991
	Root-bark, stem-bark	Ibogamine (**11**)	Gomez Gonzalez & Lorincz, 1976; Rastogi *et al.*, 1980
	Stem-bark	*O*-Acetylvallesamine (**271**)	Kam *et al.*, 2004
		Apparicine (**272**)	Kam *et al.*, 2004
		Conodusarine (**722**)	Kam & Pang, 2004
		Conofoline (**848**)	Kam *et al.*, 2004
		Conolobine A (**275**)	Kam *et al.*, 2004
		Conolobine B (**276**)	Kam *et al.*, 2004
		Conolodine (**273**)	Kam *et al.*, 2004
		Coronaridine (**14**)	Kam *et al.*, 2004
		3(*S*)-Cyanocoronaridine (**20**)	Kam *et al.*, 2004
		3(*S*)-Cyanoisovoacangine (**495**)	Kam *et al.*, 2004
		3(*S*)-Cyanovoacangine (**494**)	Kam *et al.*, 2004
		19,20-Dehydroervatamine (**49**)	Kam *et al.*, 2004
		10,11-Demethoxychippiine (**31**)	Kam *et al.*, 2004
		3(*R*/*S*)-Ethoxycoronaridine (**433**)	Kam *et al.*, 2004
		3(*R*/*S*)-Ethoxyvoacangine (**464**)	Kam *et al.*, 2004
		Heyneanine (**16**)	Kam *et al.*, 2004
		10-Hydroxycoronaridine (**427**)	Kam *et al.*, 2004
		16(*S*)-Hydroxy-16,22-dihydroapparicine (**269**)	Kam *et al.*, 2004
		19(*S*)-Hydroxyibogamine (**12**)	Kam *et al.*, 2004
		Ibogaine (**536**)	Kam *et al.*, 2004
		Ibogamine (**11**)	Kam *et al.*, 2004
		Iboxygaine (**547**)	Kam *et al.*, 2004
		(16*R*,19*E*)-Isositsirikine (**51**)	Kam *et al.*, 2004
		Isovoacangine (**430**)	Gomez Gonzalez & Lorincz, 1976; Arambewela & Ranatunge, 1991; Kam *et al.*, 2004
		Lirofoline B (**574**)	Low *et al.*, 2010

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		(–)-Mehranine (**314**)	Kam *et al.*, 2004
		Methuenine (**241**)	Kam *et al.*, 2004
		3-Oxocoronaridine (**19**)	Kam *et al.*, 2004
		3-Oxovoacangine (**437**)	Kam *et al.*, 2004
		Pachysiphine (**291**)	Kam *et al.*, 2004
		Pericyclivine (**47**)	Kam *et al.*, 2004
		Tubotaiwine (**60**)	Kam *et al.*, 2004
		Vallesamine (**270**)	Kam *et al.*, 2004
		Voacamine (**720**)	Kam *et al.*, 2004
		Voacangine (**23**)	Kam *et al.*, 2004
		Voacangine-7-hydroxyindolenine (**507**)	Kam *et al.*, 2004
		Voacristine (**24**)	Kam *et al.*, 2004
		Voafinidine (**357**)	Kam *et al.*, 2004
		Voafinine (**347**)	Kam *et al.*, 2004
		Voalenine (**349**)	Kam *et al.*, 2004
		Voaphylline (**55**)	Kam *et al.*, 2004
		Voastrictine (**104**)	Kam *et al.*, 2004
		Vobasine (**37**)	Kam *et al.*, 2004
	Leaves, branches	3*α*-Acetatemethoxyl-ibogamine (**545**)	Deng *et al.*, 2018
		Coronaridine (**14**)	Deng *et al.*, 2018
		Coronaridine hydroxyindolenine (**29**)	Deng *et al.*, 2018
		Heyneanine (**16**)	Deng *et al.*, 2018
		3*α*-Hydroxymethyl-ibogamine (**542**)	Deng *et al.*, 2018
		16*α*-Hydroxyl-ibogamine (**517**)	Deng *et al.*, 2018
		Isovoacangine (**430**)	Deng *et al.*, 2018
		Taberdicatine A (**111**)	Deng *et al.*, 2021
		Taberdicatine B (**100**)	Deng *et al.*, 2021
		Taberdicatine C (**324**)	Deng *et al.*, 2021
		Taberdicatine D (**585**)	Deng *et al.*, 2021
		Taberdicatine E (**570**)	Deng *et al.*, 2021
		Taberdicatine F (**112**)	Deng *et al.*, 2021
		Taberdicatine G (**113**)	Deng *et al.*, 2021
		Taberdivarine G (= Ervatamine G) (**21**)	Deng *et al.*, 2018
		Voacangine (**23**)	Deng *et al.*, 2018
	Leaves, twigs	Conodurine (**748**)	Li *et al.*, 2019
		Conophylline (**71**)	Li *et al.*, 2019
		Coronaridine (14)	Zhang, Bai *et al.*, 2021
		(3*R*)-7,19-Di-*epi*-3-methoxytabernoxidine (**482**)	Li *et al.*, 2019
		Ervadivaricatine B (**695**)	Yuwen *et al.*, 2019
		Hecubine (**345**)	Li *et al.*, 2019
		(3*R*,19*R*)-19-Hydroxy-3-(2-oxopropyl)-voacangine (**466**)	Li *et al.*, 2019
		Ibogaine (**536**)	Li *et al.*, 2019
		Ibogamine (**11**)	Zhang, Bai *et al.*, 2021
		Isovoacangine (**430**)	Yuwen *et al.*, 2019; Zhang, Bai *et al.*, 2021
		N-methylvoaphylline (= Hecubine) (**345**)	Zhang, Bai *et al.*, 2021
		Pedunculine (= Conofoline) (**848**)	Yuwen *et al.*, 2019
		Taberdine A (**344**)	Zhang, Bai *et al.*, 2021
		Taberdine B (**356**)	Zhang, Bai *et al.*, 2021
		Taberdine C (**359**)	Zhang, Bai *et al.*, 2021
		Taberdine D (**490**)	Zhang, Bai *et al.*, 2021
		Taberdine E (**446**)	Zhang, Bai *et al.*, 2021
		Taberdine F (**447**)	Zhang, Bai *et al.*, 2021
		Taberdine G (**445**)	Zhang, Bai *et al.*, 2021
		Taberdine H (**480**)	Zhang, Bai *et al.*, 2021

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Taberdine I (**481**)	Zhang, Bai *et al.*, 2021
		Taberdine J (**279**)	Zhang, Bai *et al.*, 2021
		Taberdine K (**280**)	Zhang, Bai *et al.*, 2021
		Taberdine L (**484**)	Han *et al.*, 2022
		Taberdine M (**105**)	Han *et al.*, 2022
		Taberdivamine A (**640**)	Zhu *et al.*, 2020
		Taberdivamine B (**65**)	Zhu *et al.*, 2020
		Taberdivarine H (**846**)	Li *et al.*, 2019
		Taberine E (**467**)	Zhang, Bai *et al.*, 2021
		Taberine F (**468**)	Zhang, Bai *et al.*, 2021
		Taberine H (**210**)	Zhang, Bai *et al.*, 2021
		Tabernaemontanine (**42**)	Yuwen *et al.*, 2019
		Tabernanthine (= 11-Methoxyibogamine) (**538**)	Li *et al.*, 2019
		Tabervarine A (**503**)	Yuwen *et al.*, 2019
		Tabervarine B (**504**)	Yuwen *et al.*, 2019
		19,20-(*E*)-vallesamine (**270**)	Li *et al.*, 2019
		Voacangine (**23**)	Yuwen *et al.*, 2019; Zhang, Bai *et al.*, 2021
		Voafinidine (**357**)	Li *et al.*, 2019
		Vobasidine C (**195**)	Yuwen *et al.*, 2019
	Leaves, stems, roots	Vobasine (**37**)	Karawya & Aboutabl, 1982; Arambewela & Ranatunge, 1991
	Leaves, stems, roots, flowers	Tabernaemontanine (**42**)	Gorman *et al.*, 1960; Raj *et al.*, 1974; Talapatra *et al.*, 1975; Karawya & Aboutabl, 1982; Arambewela & Ranatunge, 1991
	Whole plant	Conofoline (**848**)	Bao *et al.*, 2013
		Cononitarine B (**765**)	Bao *et al.*, 2013
		Conophylline (**71**)	Bao *et al.*, 2013
		19-*Epi*-isovoacristine (**474**)	Bao *et al.*, 2013
		Ervachinine A (**713**)	Bao *et al.*, 2013
		Ervachinine B (= Ervatensine A) (**714**)	Bao *et al.*, 2013
		Ervachinine C (**676**)	Bao *et al.*, 2013
		Heyneanine (**16**)	Bao *et al.*, 2013
		Ibogaine (**536**)	Bao *et al.*, 2013
		Isovoacangine (**430**)	Bao *et al.*, 2013
		N(1)-Methylvoaphylline (**345**)	Bao *et al.*, 2013
		3-(2'-Oxopropyl)-voacangine (**448**)	Bao *et al.*, 2013
		Picrinine (**237**)	Bao *et al.*, 2013
		Tabernaecorymbosine A (**767**)	Bao *et al.*, 2013
		Tabernaecorymbosine B (**769**)	Bao *et al.*, 2013
		Tabernanthine (**538**)	Bao *et al.*, 2013
		Tabernaricatine A (**775**)	Bao *et al.*, 2013
		Tabernaricatine B (**776**)	Bao *et al.*, 2013
		Tabernaricatine C (**781**)	Bao *et al.*, 2013
		Tabernaricatine D (**789**)	Bao *et al.*, 2013
		Tabernaricatine E (**677**)	Bao *et al.*, 2013
		Tabernaricatine F (**552**)	Bao *et al.*, 2013
		Tabernaricatine G (**543**)	Bao *et al.*, 2013
		19,20-*E*-Vallesamine (**270**)	Bao *et al.*, 2013
		Voacangine-7-hydroxyindolenine (**507**)	Bao *et al.*, 2013

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Voacristine (**24**)	Bao *et al.*, 2013
		Voacristine-7-hydroxyindolenine (**508**)	Bao *et al.*, 2013
		Voaphyllinediol (**57**)	Bao *et al.*, 2013
T. eglandulosa Stapf (*T. chartacea, Gabunia eglandulosa, G. longifera*)	Leaves, twigs	16,17-Anhydrotacamine (**398**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		(+)-20(*R*)-1,2-Dehydropseudoaspidospermidine (**622**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		16(*R*)-Descarbomethoxytacamine (**409**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		16(*S*)-Descarbomethoxytacamine (**411**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		(+)-20(*R*)-15,20-Dihydrocleavamine (**603**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		(−)-20(*S*)-15,20-Dihydrocleavamine (**605**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		16-*Epi*-tacamine (**405**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		11-Hydroxycoronaridine (**428**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		(+)-20(*S*)-Hydroxy-1,2-dehydropseudo-aspidospermidine (**625**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		19(*S*)-Hydroxytacaine (**407**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		17-Hydroxytacamonine (**416**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		Ibogamine (**11**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		Norfluorocurarine (**259**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		20(*R*)-Pseudovincadifformine (**608**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		Tacamine (**404**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		Tacamonine (**415**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		(+)-Tubotaiwine (**60**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
		Voaphylline (= Conoflorine) (**55**)	Van Beek, Verpoorte, & Baerheim Svendsen, 1984a

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Root-bark	Isovoacangine (**430**)	Agwada *et al.*, 1975
		Perivine (**40**)	Agwada *et al.*, 1975
		Voacamine (**720**)	Agwada *et al.*, 1975
	Root-bark	3(*R*/*S*)-Hydroxycoronaridine (**432**)	Agwada *et al.*, 1975
		3(*R*/S)-Hydroxyisovoacangine (**436**)	Agwada *et al.*, 1975
	Stem-bark	Conopharyngine (**25**)	Patel *et al.*, 1967
	Roots, stems	Eglandine (**432**)	Le Men-Olivier *et al.*, 1985
		Eglandulosine (= 3-Oxocoronaridine) (**19**)	Le Men-Olivier *et al.*, 1985
	Leaves, twigs, stem-bark	Coronaridine (**14**)	Le Men *et al.*, 1974; Van Beek, Verpoorte, & Baerheim Svendsen, 1984a
T. elegans Stapf (*Conopharyngia elegans*)	Leaves	Alasmontamine A (**883**)	Hirasawa *et al.*, 2009;
		Dregamine (**41**)	Mansoor, Ramalho *et al.*, 2009
		Eleganine A (**220**)	Mansoor, Ramalho *et al.*, 2009
		Tabernaemontanine (**42**)	Mansoor, Ramalho *et al.*, 2009
		Tabernine A (**73**)	Mansoor, Ramalhete *et al.*, 2009
		Tabernine B (**74**)	Mansoor, Ramalhete *et al.*, 2009
		Tabernine C (**75**)	Mansoor, Ramalhete *et al.*, 2009
		Vobasine (**37**)	Mansoor, Ramalhete *et al.*, 2009
		Vobtusine (**823**)	Mansoor, Ramalhete *et al.*, 2009
		Vobtusine lactone (**824**)	Mansoor, Ramalhete *et al.*, 2009
	Whole plant	Apparicine (**272**)	Van der Heijden *et al.*, 1986
		Dregaminol (**188**)	Van der Heijden *et al.*, 1986
		Dregaminol methyl ether (**190**)	Van der Heijden *et al.*, 1986
		3'(*R*/S)-Hydroxyconodurine (**752**)	Van der Heijden *et al.*, 1986
		16(*S*)-Hydroxy-16,22-dihydroapparicine (**269**)	Van der Heijden *et al.*, 1986
		3'(*R*/*S*)-Hydroxytabernaelegantine B (**665**)	Van der Heijden *et al.*, 1986
		Isovoacangine (**430**)	Van der Heijden *et al.*, 1986
		3'-Methoxytabernaeelegantine C (**736**)	Van der Heijden *et al.*, 1986
		Tabernaemontaninol (**187**)	Van der Heijden *et al.*, 1986

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		(+)-Tubotaiwine (**60**)	Van der Heijden *et al.*, 1986
		Vobasine (**37**)	Van der Heijden *et al.*, 1986
		Vobasinol (**209**)	Van der Heijden *et al.*, 1986
	Roots	Dregamine (**41**)	Mansoor *et al.*, 2013
		16-*Epi*-dregamine (**194**)	Mansoor *et al.*, 2013
		19'(*S*)-Hydroxytabernaelegantine A (**739**)	Paterna *et al.*, 2016b
		3'(*R*)-Hydroxytabernaelegantine C (**742**)	Paterna *et al.*, 2016a
		3'-Oxotabernaelegantine C (**741**)	Paterna *et al.*, 2016b
		3'-Oxotabernaelegantine D (**672**)	Paterna *et al.*, 2016b
		Tabernaelegantine A (**733**)	Paterna *et al.*, 2016b
		Tabernaelegantine B (**664**)	Mansoor *et al.*, 2013
		Tabernaelegantine C (**734**)	Mansoor *et al.*, 2013
		Tabernaelegantine D (**666**)	Paterna *et al.*, 2016b
		Tabernaemontanine (**42**)	Mansoor *et al.*, 2013
		Voacangine (**23**)	Mansoor *et al.*, 2013
	Root-bark	Conoduramine (**682**)	Gabetta *et al.*, 1975
		Tabernaelegantinine A (**738**)	Bombardelli *et al.*, 1976
		Tabernaelegantinine B (**668**)	Bombardelli *et al.*, 1976
		Tabernaelegantinine C (**737**)	Bombardelli *et al.*, 1976
		Tabernaelegantinine D (**667**)	Bombardelli *et al.*, 1976
	Whole plant, root-bark	Dregamine (**41**)	Gabetta *et al.*, 1975; Van der Heijden *et al.*, 1986
		Tabernaelegantine A (**733**)	Gabetta *et al.*, 1975; Bombardelli *et al.*, 1976; Van der Heijden *et al.*, 1986
		Tabernaelegantine B (**664**)	Gabetta *et al.*, 1975; Bombardelli *et al.*, 1976; Van der Heijden *et al.*, 1986
		Tabernaelegantine C (**734**)	Gabetta *et al.*, 1975; Bombardelli *et al.*, 1976; Van der Heijden *et al.*, 1986
		Tabernaelegantine D (**666**)	Gabetta *et al.*, 1975; Bombardelli *et al.*, 1976; Van der Heijden *et al.*, 1986
		Tabernaemontanine (**42**)	Gabetta *et al.*, 1975; Van der Heijden *et al.*, 1986
T. eusepala Aug.DC. (*Pandaca eusepala*)	Stem-bark	Apparicine (**272**)	Quirin *et al.*, 1975
		(+)-20(*S*)-1,2-Dehydropseudoaspidospermidine (**623**)	Quirin *et al.*, 1975
		(+)-20(*R*)-15,20-Dihydrocleavamine (**603**)	Quirin *et al.*, 1975
		(−)-20(*S*)-15,20-Dihydrocleavamine (**605**)	Quirin *et al.*, 1975
		19-*Epi*-voacristine (= 19-*Epi*-voacangarine) (**470**)	Quirin *et al.*, 1975
		Ibogaine (**536**)	Quirin *et al.*, 1975
		Ibogaine-7-hydroxyindolenine (**513**)	Quirin *et al.*, 1975
		Vobasine (**37**)	Quirin *et al.*, 1975

Table 1.3, continued

Plant	Plant part	Alkaloids	References
T. flavicans Willd. (*Anartia flavicans*)	Stems	Ibophyllidine (**633**)	Achenbach & Raffelsberger, 1980c; Achenbach, 1983
		Ibophyllidine *N*(4)-oxide (**634**)	Achenbach & Raffelsberger, 1980c; Achenbach, 1983
T. fuchsiaeifolia A.DC. (*Peschiera fuchsiaeifolia*)	Stem-bark	Affinisine (**161**)	Achenbach, 1966b
		16'-Decarbomethoxyvoacamine (**718**)	Braga *et al.*, 1980; Federici *et al.*, 2000
		N(4)-Demethylvoacamine (**724**)	Braga *et al.*, 1980; Federici *et al.*, 2000
		Ervahanine A (**701**)	Federici *et al.*, 2000
		Euchsiaefoline (**183**)	Braga & Reis, 1987; Federici *et al.*, 2000
		Heyneanine (**16**)	Federici *et al.*, 2000
		3(*R*/*S*)-Hydroxycoronaridine (**432**)	Federici *et al.*, 2000
		Ibogamine (**11**)	Federici *et al.*, 2000
		12-Methoxy-*N*(4)-methylvoachalotine (**180**)	Braga & Reis, 1987
		12-Methoxy-*N*(4)-methylvoachalotine ethyl ester (**181**)	Braga & Reis, 1987
		Perivine (**40**)	Braga *et al.*, 1980; Federici *et al.*, 2000
		Tabernamine (**67**)	Federici *et al.*, 2000
		Voacamidine (**660**)	Braga *et al.*, 1980; Federici *et al.*, 2000
		Voacamine (**720**)	Fernandez *et al.*, 1967
		Voacangine (**23**)	Fernandez *et al.*, 1967
		Voachalotine (**162**)	Achenbach, 1966b; Fernandez *et al.*, 1967
		Voacristine (= Voacangarine) (**24**)	Federici *et al.*, 2000
		Vobasinol (**209**)	Federici *et al.*, 2000
T. glandulosa (Stapf) Pichon	Leaves, stems	Conophylline (**71**)	Achenbach *et al.*, 1994
		Coronaridine (**14**)	Achenbach *et al.*, 1994
		12-Demethoxytabernulosine (**235**)	Achenbach *et al.*, 1982
		Difforlemenine (**217**)	Achenbach *et al.*, 1994
		Difforlemenitine (**215**)	Achenbach *et al.*, 1994
		10,12-Dimethoxynareline (**233**)	Achenbach *et al.*, 1994
		19-*Epi*-difforlemenitine (**216**)	Achenbach *et al.*, 1994
		3(*R*/*S*)-Ethoxycoronaridine (**433**)	Achenbach & Raffelsberger, 1980d
		3(*R*/*S*)-Hydroxycoronaridine (**432**)	Achenbach, Raffelsberger, & Brillinger, 1980
		Tabernulosine (**234**)	Achenbach *et al.*, 1994
		Vincadiffine (**206**)	Achenbach *et al.*, 1994
		Voacangine (**23**)	Achenbach *et al.*, 1994
		Vobasine (**37**)	Achenbach *et al.*, 1994

Table 1.3, continued

Plant	Plant part	Alkaloids	References
T. grandiflora L.	Stem-bark	Coronaridine-7-hydroxyindolenine (**29**)	Tessier *et al.*, 1984
		Heyneanine (**16**)	Tessier *et al.*, 1984
		3-Hydroxyvoacangarine (**463**)	Tessier *et al.*, 1984
		3(*R*/*S*)-Hydroxyvoacangine (**438**)	Tessier *et al.*, 1984
		Voacangarine (= Voacristine) (**24**)	Tessier *et al.*, 1984
		Voacangine (**23**)	Tessier *et al.*, 1984
		Voacangine-7-hydroxyindolenine (**507**)	Tessier *et al.*, 1984
	Seeds	Conoflorine (= Voaphylline) (**55**)	Torrenegra *et al.*, 1988
		14,15-Dehydrotetrastachynine (**811**)	Torrenegra *et al.*, 1988
		11-Hydroxycoronaridine (**428**)	Torrenegra *et al.*, 1988
		14β-Hydroxyquebrachamine (**353**)	Torrenegra *et al.*, 1988
		3-Oxotabersonine (**283**)	Torrenegra *et al.*, 1988
		3-Oxovincadifformine (**303**)	Torrenegra *et al.*, 1988
		Pachysiphine (**291**)	Torrenegra *et al.*, 1988
		Quebrachamine (**352**)	Torrenegra *et al.*, 1988
		Tabersonine (**281**)	Torrenegra *et al.*, 1988
	Seeds, stem-bark	Coronaridine (**14**)	Tessier *et al.*, 1984; Torrenegra *et al.*, 1988
T. heterophylla Vahl (*T. tenuiflora, Peschiera heterophylla, P. diversifolia, P. tenuifolia, Stenosolen heterophyllus*)	Leaves	Affinisine (**161**)	Kan *et al.*, 1984
		Apparicine (**272**)	Kan *et al.*, 1984
		Coronaridine (**14**)	Kan *et al.*, 1984
		16'-Decarbomethoxyvoacamine (**718**)	Kan *et al.*, 1984
		3-*Epi*-ervafolidine (**814**)	Henriques *et al.*, 1982
		Ervafolene (**819**)	Henriques *et al.*, 1980; Henriques *et al.*, 1982
		Ervafolidine (**813**)	Henriques *et al.*, 1982
		Ervafoline (**817**)	Henriques *et al.*, 1980 & 1982
		19'(*S*)-Hydroxy-3-*epi*-ervafolidine (**816**)	Henriques *et al.*, 1982
		19'-Hydroxyervafolene (**820**)	Henriques *et al.*, 1980 & 1982
		19'(*R*)-Hydroxyervafolidine (**815**)	Henriques *et al.*, 1982
		19'-Hydroxyervafoline (**818**)	Henriques *et al.*, 1980 & 1982
		Ibogaine (**536**)	Kan *et al.*, 1984
		Ibogamine (**11**)	Kan *et al.*, 1984
		Olivacine (**77**)	Kan *et al.*, 1984
		Pandine (**636**)	Henriques *et al.*, 1980; Kan *et al.*, 1984
		Pandoline (**609**)	Henriques *et al.*, 1980; Kan *et al.*, 1984
		Tabernamine (**67**)	Kan *et al.*, 1984
		3,14;4,19-Tetrahydroolivacine (**78**)	Kan *et al.*, 1984
		Vallesamine (**270**)	Kan *et al.*, 1984
		Voacamine (**720**)	Kan *et al.*, 1984
		Voacangine (**23**)	Henriques *et al.*, 1980
		Voacangine-7-hydroxyindolenine (**507**)	Henriques *et al.*, 1980
		Voaphylline (= Conoflorine) (**55**)	Henriques *et al.*, 1980; Kan *et al.*, 1984
		Vobasine (**37**)	Kan *et al.*, 1984

Table 1.3, continued

Plant	Plant part	Alkaloids	References
T. heyneana Wall. (*Ervatamia heyneana, Pagiantha heyneana*)	Flowers	Coronaridine-7-hydroxyindolenine (**29**)	Srivastava *et al.*, 2001
		Ervatine (**523**)	Srivastava *et al.*, 2001
		15β-Stemmadenine (**268**)	Grover *et al.*, 2002
		Tabersonine (**281**)	Srivastava *et al.*, 2001
		Voacristine-7-hydroxyindolenine (**508**)	Srivastava *et al.*, 2001
	Stem-bark	*O*-Acetylvallesamine (**271**)	Gunasekera *et al.*, 1980
		Apparicine (**272**)	Gunasekera *et al.*, 1980
		Camptothecine (**87**)	Gunasekera *et al.*, 1979
		10-Hydroxycoronaridine (**427**)	Gunasekera *et al.*, 1980
		9-Methoxycamptothecine (**88**)	Gunasekera *et al.*, 1979
		19(*S*)-3,19-Oxidovoacangine (**491**)	Gunasekera *et al.*, 1980
		6(*R*)-3,6-Oxidovoacangine *N*(4)-oxide (**489**)	Gunasekera *et al.*, 1980
		19-Oxovoacangine (= Voacryptine) (**469**)	Gunasekera *et al.*, 1980
		(+)-Tubotaiwine (**60**)	Gunasekera *et al.*, 1980
		Voacangine-7-hydroxyindolenine (**507**)	Gunasekera *et al.*, 1980
	Roots	Ibogamine (**11**)	Meyer *et al.*, 1973
		3-Oxocoronaridine (**19**)	Meyer *et al.*, 1973
		Voacangine pseudoindoxyl (= Voaluteine) (**520**)	Meyer *et al.*, 1973
	Leaves	Isovoacristine (**471**)	Rao & Singri, 1979
	Stem-bark, flowers	Heyneanine (**16**)	Govindachari *et al.*, 1965; Saradamma *et al.*, 1971; Gunasekera *et al.*, 1980; Srivastava *et al.*, 2001
		Voacristine (= Voacangarine) (**24**)	Gunasekera *et al.*, 1980; Srivastava *et al.*, 2001
	Stem-bark, leaves	Tabernoxidine (**478**)	Joshi *et al.*, 1984
	Stem-bark, roots	Voacangine (**23**)	Meyer *et al.*, 1973; Gunasekera *et al.*, 1980
	Stem-bark, flowers, seeds, roots	Coronaridine (**14**)	Ramiah & Mohandas, 1966; Saradamma *et al.*, 1971; Meyer *et al.*, 1973; Gunasekera *et al.*, 1980; Joshi *et al.*, 1984; Srivastava *et al.*, 2001
T. hilariana Müll. Arg.	Root-bark	Catharanthine (**584**)	Cardoso *et al.*, 1998
		Coronaridine (**14**)	Cardoso *et al.*, 1998
		Coronaridine pseudoindoxyl (**27**)	Cardoso *et al.*, 1998
		3(*R*/*S*)-Hydroxycoronaridine (**432**)	Cardoso *et al.*, 1998
		3(*R*/*S*)-Hydroxyvoacangine (**438**)	Cardoso *et al.*, 1998
		Ibogamine (**11**)	Cardoso *et al.*, 1998
		Isovoacangine (**430**)	Cardoso *et al.*, 1998
		3-Oxocoronaridine (**19**)	Cardoso *et al.*, 1998
		3-(2'-Oxopropyl)-coronaridine (**456**)	Cardoso *et al.*, 1998

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Tabernanthine (**538**)	Cardoso *et al.*, 1998
		Tetraphyllicine (**223**)	Cardoso *et al.*, 1998
		Voacangine (**23**)	Cardoso *et al.*, 1998
		Voacangine-7-hydroxyindolenine (**507**)	Cardoso *et al.*, 1998
		Voacangine pseudoindoxyl (= Voaluteine) (**520**)	Cardoso *et al.*, 1998
T. hirta Hook. f. (*E. hirta*)	Leaves, root-bark	*O*-Acetyl-16-*epi*-affinisine (**167**)	Clivio *et al.*, 1991
		Affinisine (**161**)	Clivio *et al.*, 1991
		Affinisine *N*(4)-oxide (**164**)	Clivio *et al.*, 1991
		Apparicine (**272**)	Clivio *et al.*, 1991
		16'-Decarbomethoxy-19,20-dihydrovoacamine (**707**)	Clivio *et al.*, 1991
		16'-Decarbomethoxyvoacamine (**718**)	Clivio *et al.*, 1991
		16'-Decarbomethoxyvoacamine pseudoindoxyl (**728**)	Clivio *et al.*, 1991
		Dehydro-16-*epi*-affinisine (**186**)	Clivio *et al.*, 1991
		19,20-Dehydro-*β*-yohimbine (**120**)	Clivio *et al.*, 1991
		4',17(*β*)-Dihydrotchibangensine (**644**)	Clivio *et al.*, 1991
		Dregamine (**41**)	Clivio *et al.*, 1991
		16-*Epi*-affinisine (**165**)	Clivio *et al.*, 1991
		16-*Epi*-normacusine B (**169**)	Clivio *et al.*, 1991
		12-Hydroxynorfluorocurarine (**261**)	Clivio *et al.*, 1991
		Ibogaine (**536**)	Clivio *et al.*, 1991
		Iboxygaine (**547**)	Clivio *et al.*, 1991
		Iboxygaine-7-hydroxyindolenine (**514**)	Clivio *et al.*, 1991
		Isositsirikine (**51**)	Clivio *et al.*, 1991
		Norfluorocurarine (**259**)	Clivio *et al.*, 1991
		Norfluorocurarine *N*(4)-oxide (**260**)	Clivio *et al.*, 1991
		Normacusine B (**168**)	Clivio *et al.*, 1991
		Tabernaemontanine (**42**)	Clivio *et al.*, 1991
		Voacristine (= Voacangarine) (**24**)	Clivio *et al.*, 1991
		Vobasine (**37**)	Clivio *et al.*, 1991
		Yohimbine (**119**)	Clivio *et al.*, 1991
		β-Yohimbine (**118**)	Clivio *et al.*, 1991
		β-Yohimbine oxindole (**127**)	Clivio *et al.*, 1991
		β-Yohimbine pseudoindoxyl (**128**)	Clivio *et al.*, 1991
T. humblotii (Baill.) Pichon (*T. ochrascens*, *Pandaca ochrascens*, *P. speciosa*)	Leaves	Akuammicine (**255**)	Panas *et al.*, 1974
		Akuammidine (**172**)	Panas *et al.*, 1974
		Apparicine (**272**)	Panas *et al.*, 1974
		(+)-14,15-Dehydro-16-*epi*-vincamine (**59**)	Panas *et al.*, 1974
		19-*Epi*-iboxygaine (**546**)	Panas *et al.*, 1974
		19-*Epi*-iboxygaline (**549**)	Panas *et al.*, 1974
		Ibogaine (**536**)	Panas *et al.*, 1974
		Iboxygaline (**550**)	Panas *et al.*, 1974
	Leaves, stem-bark	Voacangine (**23**)	Levy *et al.*, 1975
		Voacristine (= Voacangarine) (**24**)	Levy *et al.*, 1975

Table 1.3, continued

Plant	Plant part	Alkaloids	References
T. hystrix Steud. (*T. echinata* Vell., *Peschiera echinata*)	Root-bark	Affinine (**202**)	Monnerat *et al.*, 2005
		Affinisine (**161**)	Monnerat *et al.*, 2005
		Coronaridine (**14**)	De Souza *et al.*, 2010
		Coronaridine hydroxyindolenine (**29**)	De Souza *et al.*, 2010
		Hystrixnine (**208**)	Monnerat *et al.*, 2005
		Ibogamine (**11**)	Monnerat *et al.*, 2005
		Ibogamine-7,8-dione (**562**)	De Souza *et al.*, 2010
		12-Methoxyvoachalotine (**185**)	De Souza *et al.*, 2010
		N(4)-Methylaffinisine (**175**)	Monnerat *et al.*, 2005
		Olivacine (**77**)	Monnerat *et al.*, 2005; De Souza *et al.*, 2010
		3-Oxocoronaridine (**19**)	De Souza *et al.*, 2010
		5-Oxocoronaridine (**526**)	De Souza *et al.*, 2010
		3-Oxocoronaridine hydroxyindolenine (**510**)	De Souza *et al.*, 2010
		Vobasine (**37**)	De Souza *et al.*, 2010
	Leaves, stem, root-bark	Angustine (**158**)	Ghorbel *et al.*, 1981
		Coronaridine (**14**)	Ghorbel *et al.*, 1981
		16'-Decarbomethoxyvoacamine (**718**)	Ghorbel *et al.*, 1981
		N(4)-Demethylvoacamine (**724**)	Ghorbel *et al.*, 1981
		16-*Epi*-isositsirikine (**138**)	Ghorbel *et al.*, 1981
		10-Hydroxycoronaridine (**427**)	Ghorbel *et al.*, 1981
		10-Hydroxyheyneanine (**459**)	Ghorbel *et al.*, 1981
		Ibogaine (**536**)	Ghorbel *et al.*, 1981
		Ibogaine-7-hydroxyindolenine (**513**)	Ghorbel *et al.*, 1981
		Olivacine (**77**)	Ghorbel *et al.*, 1981
		6(*R*)-3,6-Oxidovoacangine (**488**)	Ghorbel *et al.*, 1981
		3-Oxovoacangine (**437**)	Ghorbel *et al.*, 1981
		Pleiocarpamine (**152**)	Ghorbel *et al.*, 1981
		Tubotaiwine (**60**)	Ghorbel *et al.*, 1981
		Voacamine (**720**)	Ghorbel *et al.*, 1981
		Voacangine (**23**)	Ghorbel *et al.*, 1981
		Voacangine-7-hydroxyindolenine (**507**)	Ghorbel *et al.*, 1981
		Voacangine pseudoindoxyl (**520**)	Ghorbel *et al.*, 1981
		Voacristine (**24**)	Ghorbel *et al.*, 1981
		Vobasine (**37**)	Ghorbel *et al.*, 1981
T. inconspicua	Stems	5,6-Dioxo-11-hydroxyvoacangine (**533**)	Foudjo Melacheu Laura *et al.*, 2021
		Vocangine (**23**)	
T. laeta Mart.	Root-bark	Coronaridine (**14**)	Medeiros *et al.*, 2001
		Heyneanine (**16**)	Medeiros *et al.*, 2001
		N(4)-Methylvoachalotine (**174**)	Medeiros *et al.*, 2001
		Tabernamine (**67**)	Medeiros *et al.*, 2001
		Voacangine (**23**)	Medeiros *et al.*, 2001
	Leaves, stems	Affinine (**202**)	Jahodář *et al.*, 1974; Votický *et al.*, 1977
		Akuammidine (**172**)	Votický *et al.*, 1977
		Conodurine (**748**)	Jahodář *et al.*, 1974
		Geissoschizol (**136**)	Jahodář *et al.*, 1974; Votický *et al.*, 1977
		Normacusine B (**168**)	Votický *et al.*, 1977
		Voacamine (**720**)	Jahodář *et al.*, 1974
		Vobasine (**37**)	Jahodář *et al.*, 1974; Votický *et al.*, 1977

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Leaves, stems, root-bark	Conodurine (**748**)	Votický *et al.*, 1977; Medeiros *et al.*, 2001
		Voacamine (**720**)	Votický *et al.*, 1977; Medeiros *et al.*, 2001
T. litoralis (Kunth)	Fruits	Coronaridine (**14**)	Qu *et al.*, 2016
		Heyneanine (**16**)	Qu *et al.*, 2016
		18-Hydroxypseudovincadifformine (**611**)	Qu *et al.*, 2016
		Isoakuammiline (**230**)	Qu *et al.*, 2016
		3,19-Oxidocoronaridine (**493**)	Qu *et al.*, 2016
		Strictosidine (**94**)	Qu *et al.*, 2016
		Tabersonine (**281**)	Qu *et al.*, 2016
T. longipes Donn. Sm.	Seeds	Tabersonine (**281**)	Ciccio, 1979
		Voacangine (**23**)	Ciccio, 1979
	Seeds, leaves	Coronaridine (**14**)	Ciccio, 1979; Ciccio & Hoet, 1981
T. lundii A.DC. (*Peschiera lundii*)	Leaves, stem-bark	Coronaridine (**14**)	Hwang *et al.*, 1969
		19-*Epi*-voacristine (= 19-*Epi*-voacangarine) (**470**)	Hwang *et al.*, 1969
		Ibogaine (**536**)	Hwang *et al.*, 1969
		Iboxygaine (**547**)	Hwang *et al.*, 1969
		Iboxygaine-7-hydroxyindolenine (**514**)	Hwang *et al.*, 1969
		Voacangine (**23**)	Hwang *et al.*, 1969
		Voacristine (= Voacangarine) (**24**)	Hwang *et al.*, 1969
		Voacristine pseudoindoxyl (**521**)	Hwang *et al.*, 1969
		Vobasine (**37**)	Hwang *et al.*, 1969
T. macrocalyx Müll. Arg. (*Anacampta macrocalix*)	Stem-bark	Coronaridine-7-hydroxyindolenine (**29**)	Garnier *et al.*, 1984
		19-*Epi*-voacangarine (= 19-*Epi*-voacristine) (**470**)	Garnier *et al.*, 1984
		Heyneanine (**16**)	Garnier *et al.*, 1984
		3-Oxocoronaridine-7-hydroxyindolenine (**510**)	Garnier *et al.*, 1984
		Voacangarine-7-hydroxyindolenine (**508**)	Garnier *et al.*, 1984
		Voacangine-7-hydroxyindolenine (**507**)	Garnier *et al.*, 1984
	Leaves	10-Hydroxycoronaridine (**427**)	Garnier *et al.*, 1984
	Seeds	Tabersonine (**281**)	Bruneton *et al.*, 1979
	Stem-bark, leaves	Voacangarine (= Voacristine) (**24**)	Garnier *et al.*, 1984
		Voacangine (**23**)	Garnier *et al.*, 1984
	Seeds, stem-bark	Coronaridine (**14**)	Bruneton *et al.*, 1979; Garnier *et al.*, 1984

Table 1.3, continued

Plant	Plant part	Alkaloids	References
T. macrocarpa Jack (*Ervatamia macrocarpa, Pagiantha macrocarpa*)	Roots	Coronaridine pseudoindoxyl (**27**)	Husain *et al.*, 1997
		19-*Epi*-heyneanine (**17**)	Husain *et al.*, 1997
		3-Oxocoronaridine (**19**)	Husain *et al.*, 1997
		Voacangine pseudoindoxyl (= Voaluteine) (**520**)	Husain *et al.*, 1997
	Seeds	Voacangine (**23**)	Miet & Poisson, 1977
		Voaphylline (= Conoflorine) (**55**)	Miet & Poisson, 1977
	Seeds, roots	Coronaridine (**14**)	Miet & Poisson, 1977; Husain *et al.*, 1997
		Voacangine-7-hydroxyindolenine (**507**)	Miet & Poisson, 1977; Husain *et al.*, 1997
	Bark	Affinine (**202**)	Amelia *et al.*, 2019
		Affinisine (**161**)	Amelia *et al.*, 2019
		Bisnaecarpamine A (**649**)	Amelia *et al.*, 2021
		Bisnaecarpamine B (**650**)	Amelia *et al.*, 2021
		22-Deetyl fuchsiaefoline (**184**)	Amelia *et al.*, 2019
		22-Demethyl-12-methoxy-4-methyl-voachalotine (**182**)	Amelia *et al.*, 2019
		Isositsirikine (**51**)	Amelia *et al.*, 2019
		12-Methoxy-4-methylvoachalotine (**180**)	Amelia *et al.*, 2019
T. malaccensis Hook. f.	Leaves, root-bark	19,20-Dehydroervatamine (**49**)	Clivio, Richard, Zeches *et al.*, 1990
		Dregamine (**41**)	Clivio *et al.*, 1990
		16-*Epi*-ervatamine (**249**)	Clivio *et al.*, 1990
		16-*Epi*-methuenine (= Isomethuenine) (**244**)	Clivio *et al.*, 1990
		N(1)-Methoxy-19,20-dehydroervatamine (**243**)	Clivio *et al.*, 1990
		N(1)-Methoxymethuenine (**246**)	Clivio *et al.*, 1990
		Methuenine (**241**)	Clivio *et al.*, 1990
		6-Oxomethuenine (**245**)	Clivio *et al.*, 1990
T. markgrafiana J. F. Macbr.	Bark	*O*-Acetylvallesamine (**271**)	Nielsen *et al.*, 1994
		Akuammidine (**172**)	Nielsen *et al.*, 1994
		Coronaridine (**14**)	Nielsen *et al.*, 1994
		Coronaridine-7-hydroxyindolenine (**29**)	Nielsen *et al.*, 1994
		5,6-Dehydrocoronaridine (**525**)	Nielsen *et al.*, 1994
		10,11-Demethoxychippiine (**31**)	Nielsen *et al.*, 1994
		16(*R*)-19,20-(*E*)-*Epi*-isositsirikine (**138**)	Nielsen *et al.*, 1994
		Heyneanine (**16**)	Nielsen *et al.*, 1994
		Heyneanine-7-hydroxyindolenine (**512**)	Nielsen *et al.*, 1994
		3(*R*/*S*)-Hydroxycoronaridine (**432**)	Nielsen *et al.*, 1994
		Ibogaine (**536**)	Nielsen *et al.*, 1994
		Ibogamine (**11**)	Nielsen *et al.*, 1994
		3(*R*)-Methoxycoronaridine (**435**)	Nielsen *et al.*, 1994
		3(*R*)-Methoxyvoacangine (**439**)	Nielsen *et al.*, 1994
		3-Oxocoronaridine (**19**)	Nielsen *et al.*, 1994
		3-Oxovoacangine (**437**)	Nielsen *et al.*, 1994
		Vallesamine (**270**)	Nielsen *et al.*, 1994
		Voacangine (**23**)	Nielsen *et al.*, 1994
		Voacristine (= Voacangarine) (**24**)	Nielsen *et al.*, 1994

Table 1.3, continued

Plant	Plant part	Alkaloids	References
T. mauritiana Poir. (*Pandaca mauritiana*)	Roots, stem-bark	Dregamine (**41**)	Miet & Poisson, 1977
		Vobasine (**37**)	Miet & Poisson, 1977
	Roots, stem-bark, leaves	(+)-Tubotaiwine (**60**)	Miet & Poisson, 1977
T. minutiflora Pichon (*Pandaca minutiflora*)	Leaves	(+)-Condylocarpine (**264**)	Petitfrere *et al.*, 1975
		Coronaridine (**14**)	Petitfrere *et al.*, 1975
		Stemmadenine (**266**)	Petitfrere *et al.*, 1975
		Stereoisomer of 15,20; 15',20'-tetrahydro-presecamine (**808**)	Petitfrere *et al.*, 1975
		(+)-Tubotaiwine (**60**)	Petitfrere *et al.*, 1975
		(+)-Vincadifformine (**325**)	Petitfrere *et al.*, 1975
		Vobasine (**37**)	Petitfrere *et al.*, 1975
T. mocquerysii Aug.DC. (*T. boiteaui, Pandaca boiteaui, P. callosa, P. mocquerysii*)	Stem-bark	20'(*R*)-Capuvosidine (**797**)	Husson *et al.*, 1978; Andriantsiferana *et al.*, 1979
		16'-Decarbomethoxyvoacamine (**718**)	Andriantsiferana *et al.*, 1979
		19,20-Dehydroervatamine (**49**)	Andriantsiferana *et al.*, 1979
		20(*S*)-1,2-Dehydropseudoaspidospermidine (**623**)	Andriantsiferana *et al.*, 1979
		20'(*R*)-Dehydroxycapuvosine (**794**)	Andriantsiferana *et al.*, 1979
		20'(*R*)-Dehydroxyisocapuvosine (**793**)	Andriantsiferana *et al.*, 1979
		20'(*R*)-1,2-Dihydrocapuvosidine (**798**)	Andriantsiferana *et al.*, 1979
		20'(*S*)-1,2-Dihydrocapuvosidine (**799**)	Andriantsiferana *et al.*, 1979
		(+)-20(*R*)-15,20-Dihydrocleavamine (**603**)	Andriantsiferana *et al.*, 1979
		(−)-20(*S*)-15,20-Dihydrocleavamine (**605**)	Andriantsiferana *et al.*, 1979
		20(*R*)-Pseudoaspidospermidine (**626**)	Andriantsiferana *et al.*, 1979
		20(*S*)-Pseudoaspidospermidine (**627**)	Andriantsiferana *et al.*, 1979
		(+)-Tubotaiwine (**60**)	Andriantsiferana *et al.*, 1979
		Voacamine (**720**)	Andriantsiferana *et al.*, 1979
	Root-bark	Coronaridine (**14**)	De Bellefon *et al.*, 1975
		19-*Epi*-heyneanine (**17**)	De Bellefon *et al.*, 1975
		19-*Epi*-voacristine (= 19-*Epi*-voacangarine) (**470**)	De Bellefon *et al.*, 1975
		Heyneanine (**16**)	De Bellefon *et al.*, 1975
		Voacangine (**23**)	De Bellefon *et al.*, 1975
		Voacristine (= Voacangarine) (**24**)	De Bellefon *et al.*, 1975

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Root-bark, stem-bark	Ervitsine (**238**)	Andriantsiferana *et al.*, 1977 & 1979
		Methuenine (**241**)	Andriantsiferana *et al.*, 1977 & 1979
T. mucronata Merr. (*Ervatamia mucronata*)	Bark	Coronaridine (**14**)	Santos *et al.*, 1965
		Tabernaemontanine (**42**)	Santos *et al.*, 1965
T. olivacea Müll. Arg.	Stems	Akuammidine (**172**)	Achenbach & Raffelsberger, 1980b
		Condylocarpine *N*(4)-oxide (**265**)	Achenbach & Raffelsberger, 1980b
		Coronaridine (**14**)	Achenbach & Raffelsberger, 1980b
		Coronaridine-7-hydroxyindolenine (**29**)	Achenbach & Raffelsberger, 1980b
		Coronaridine pseudoindoxyl (**27**)	Achenbach & Raffelsberger, 1980b
		Heyneanine (**16**)	Achenbach & Raffelsberger, 1980b
		Ibogaine (**536**)	Achenbach & Raffelsberger, 1980b
		Ibogamine (**11**)	Achenbach & Raffelsberger, 1980b
		Voacangine (**23**)	Achenbach & Raffelsberger, 1980b
		Voacangine-7-hydroxyindolenine (**507**)	Achenbach & Raffelsberger, 1980b
		Voacangine pseudoindoxyl (= Voaluteine) (**520**)	Achenbach & Raffelsberger, 1980b
		Voacristine (= Voacangarine) (**24**)	Achenbach & Raffelsberger, 1980b
T. orientalis R. Br. (*Ervatamia lifuana*, *E. daemeliana*)	Bark	16'-Decarbomethoxy-19,20-dihydro-20-*epi*-voacamine (**708**)	Knox & Slobbe, 1975
		16'-Decarbomethoxy-19,20-dihydrovoacamine (**707**)	Knox & Slobbe, 1975
		16'-Decarbomethoxyvoacamine (**718**)	Knox & Slobbe, 1975
		Dregamine (**41**)	Knox & Slobbe, 1975
		Voacamine (**720**)	Knox & Slobbe, 1975
		Voacristine (= Voacangarine) (**24**)	Knox & Slobbe, 1975
	Leaves	Apparicine (**272**)	Knox & Slobbe, 1975
		Ibogaine (**536**)	Knox & Slobbe, 1975
		Iboxygaine (**547**)	Knox & Slobbe, 1975
	Leaves, twigs	Conopharyngine (**25**)	Bruneton *et al.*, 1980
		Coronaridine (**14**)	Bruneton *et al.*, 1980
		20-*Epi*-pandoline (**610**)	Bruneton *et al.*, 1980
		Ervatamine (**247**)	Bruneton *et al.*, 1980
		Pandine (**636**)	Bruneton *et al.*, 1980
		Pandoline (**609**)	Knox & Slobbe, 1975

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Leaves, stem-bark	19,20-Dehydroervatamine (**49**)	Knox & Slobbe, 1975
	Bark, leaves, twigs	Tabernaemontanine (**42**)	Knox & Slobbe, 1975; Bruneton *et al.*, 1980;
	Leaves, twigs, bark	Dregamine (**41**)	Knox & Slobbe, 1975
	Leaves, twigs, stem-bark	20-*Epi*-ervatamine (**248**)	Knox & Slobbe, 1975
T. pachysiphon Stapf. (*T. cumminsii, T. holstii*)	Leaves	Conopharyngine-7-hydroxyindolenine (**509**)	Crooks & Robinson, 1970
		Conopharyngine pseudoindoxyl (**522**)	Crooks & Robinson, 1973
		19(*S*)-Hydroxyconopharyngine (**26**)	Crooks & Robinson, 1973
		Tabernaesine A (**830**)	Yi *et al.*, 2020
		Tabernaesine B (**831**)	Yi *et al.*, 2020
		Tabernaesine C (**825**)	Yi *et al.*, 2020
		Tabernaesine D (**828**)	Yi *et al.*, 2020
		Tabernaesine E (**829**)	Yi *et al.*, 2020
		Tabernaesine F (**832**)	Yi *et al.*, 2020
		Tabernaesine G (**833**)	Yi *et al.*, 2020
		Tabernaesine H (**834**)	Yi *et al.*, 2020
		Tabernaesine I (**835**)	Yi *et al.*, 2020
		Tabernaesine J (**390**)	Yi *et al.*, 2022
		Vobtusine (**823**)	Yi *et al.*, 2020
		Vobtusine lactone (**824**)	Yi *et al.*, 2020
	Seeds	Pachysiphine (**291**)	Patel & Poisson, 1966
		Voacangine (**23**)	Patel & Poisson, 1966
	Root-bark, stem-bark	Affinine (**202**)	Van Beek, Kuijlaars *et al.*, 1984
		Anhydrovobasindiol (= Taberpsychine) (**212**)	Van Beek, Kuijlaars *et al.*, 1984
		Conoduramine (**682**)	Van Beek, Kuijlaars *et al.*, 1984
		Conodurine (**748**)	Van Beek, Kuijlaars *et al.*, 1984
		Coronaridine (**14**)	Van Beek, Kuijlaars *et al.*, 1984
		11'-Demethylconoduramine (**681**)	Van Beek, Kuijlaars *et al.*, 1984
		16-*Epi*-affinisine (**165**)	Van Beek, Kuijlaars *et al.*, 1984
		16-*Epi*-isositsirikine (**138**)	Van Beek, Kuijlaars *et al.*, 1984
		Gabunine (**747**)	Van Beek, Kuijlaars *et al.*, 1984
		3(*R*/*S*)-Hydroxyconopharyngine (**441**)	Van Beek, Kuijlaars *et al.*, 1984
		Ibogaline (**539**)	Van Beek, Kuijlaars *et al.*, 1984
		Isositsirikine (**51**)	Van Beek, Kuijlaars *et al.*, 1984

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Lochnericine (**292**)	Van Beek, Kuijlaars *et al.*, 1984
		Normacusine B (**168**)	Van Beek, Kuijlaars *et al.*, 1984
		3'-Oxoconodurine (**749**)	Van Beek, Kuijlaars *et al.*, 1984
		3-Oxocoronaridine (**19**)	Van Beek, Kuijlaars *et al.*, 1984
		3'-(2-Oxopropyl)-conodurine (**750**)	Van Beek, Kuijlaars *et al.*, 1984
		Pericyclivine (**47**)	Van Beek, Kuijlaars *et al.*, 1984
		Perivine (**40**)	Van Beek, Kuijlaars *et al.*, 1984
	Leaves, stem-bark, root-bark	Apparicine (**272**)	Renner & Kernweisz, 1963; Van Beek, Kuijlaars *et al.*, 1984
		Conopharyngine (**25**)	Thomas & Starmer, 1963; Van Beek, Kuijlaars *et al.*, 1984
		Isovoacangine (**430**)	Van Beek, Kuijlaars *et al.*, 1984; Hoft *et al.*, 1998
		(+)-Tubotaiwine (**60**)	Patel & Poisson, 1966; Hoft *et al.*, 1998; Ingkaninan *et al.*, 1999
		(+)-Tubotaiwine *N*(4)-oxide (**61**)	Van Beek, Kuijlaars *et al.*, 1984; Hoft *et al.*, 1998
T. pandacaqui Poir. (*T. laurifolia, Ervatamia pandacaqui*)	Leaves	*O*-Acetylvallesamine (**271**)	Abe *et al.*, 1993
		Akuammicine (**255**)	Abe *et al.*, 1993
		3-*Epi*-ervafolidine (**814**)	Lathuilliere *et al.*, 1970
		(+)-20-*Epi*-lochneridine (**263**)	Lathuilliere *et al.*, 1966
		Ervafolidine (**813**)	Lathuilliere *et al.*, 1970
		Ervafoline (**817**)	Lathuilliere *et al.*, 1970
		Pericyclivine (**47**)	Lathuilliere *et al.*, 1970
		Vallesamine (**270**)	Abe *et al.*, 1993
	Bark	Coronaridine (**14**)	Aguilar-Santos *et al.*, 1963; Cava, Mowdood *et al.*, 1965
		Ibogamine (**11**)	Cava, Mowdood *et al.*, 1965
		Iboxygaine (**547**)	Cava, Mowdood *et al.*, 1965
		Isovoacangine (**430**)	Cava, Mowdood *et al.*, 1965
		Isovoacristine (**471**)	Cava, Mowdood *et al.*, 1965
		Tabernanthine (**538**)	Cava, Mowdood *et al.*, 1965
	Stems	Ervatamine (**247**)	Abe *et al.*, 1993
		Voaluteine (= Voacangine pseudoindoxyl) (**520**)	Abe *et al.*, 1993

Table 1.3, continued

Plant	Plant part	Alkaloids	References
	Leaves, stems	Pandine (**636**)	Abe *et al.*, 1993
		Tabernaemontanine (**42**)	Lathuilliere *et al.*, 1970; Abe *et al.*, 1993
		Voacangine (**23**)	Okuyama *et al.*, 1992; Abe *et al.*, 1993
		Voacristine (= Voacangarine) (**24**)	Abe *et al.*, 1993
	Roots	*N*(4)-Demethylervahanine A (**700**)	Kitajima *et al.*, 2019
		N(4)-Demethylervahanine B (**680**)	Kitajima *et al.*, 2019
		3-*O*-Methyl-10,11-demethoxychippiine (= Taberhaine B) (**32**)	Kitajima *et al.*, 2019
		Voacangine (**23**)	Okuyama *et al.*, 1992
T. peduncularis Wall. (*E. peduncularis*)	Leaves, stem-bark	Coronaridine (**14**)	Zèches-Hanrot *et al.*, 1995
		Heyneanine (**16**)	Zèches-Hanrot *et al.*, 1995
		Heyneanine-7-hydroxyindolenine (**512**)	Zèches-Hanrot *et al.*, 1995
		Peduncularidine (**851**)	Zèches-Hanrot *et al.*, 1995
		Pedunculine (= Conofoline) (**848**)	Zèches-Hanrot *et al.*, 1995
T. penduliflora K. Schum. (*Conopharyngia penduliflora*)	Stem-bark	Conopharyngine (**25**)	Patel *et al.*, 1967
		Coronaridine (**14**)	Patel *et al.*, 1967; Ambujam & Parimoo, 1985
		10-Hydroxycoronaridine (**427**)	Masuda *et al.*, 2000
		Voacangine (**23**)	Patel *et al.*, 1967; Masuda *et al.*, 2000
	Trunk-bark	Tabernaemontine (**429**)	Bitombo *et al.*, 2021
	Leaves	7,10-Dihydroindolenine (**500**)	Nama *et al.*, 2023
		10-Hydroxycoronaridine (**427**)	Nama *et al.*, 2023
		10-Hydroxyheyneanine (**459**)	Nama *et al.*, 2023
		Pendulifloramine (**805**)	Nama *et al.*, 2023
		Voacristine (**24**)	Nama *et al.*, 2023
		Vobasine (**37**)	Nama *et al.*, 2023
T. polyneura (King & Gamble) D.J.Middleton (*Ervatamia coriacea* Ridl., *E. polyneura*)	Stem-bark	Anhydrovobasindiol (= Taberpsychine) (**212**)	Clivio, Richard, Hadi *et al.*, 1990
		Apparicine (**272**)	Clivio, Richard, Hadi *et al.*, 1990
		Coronaridine (**14**)	Clivio, Richard, Hadi *et al.*, 1990
		Coronaridine hydroxyindolenine (**29**)	Clivio, Richard, Hadi *et al.*, 1990
		3,14-Dihydroellipticine (**76**)	Clivio, Richard, Hadi *et al.*, 1990
		Dregamine (**41**)	Clivio, Richard, Hadi *et al.*, 1990

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Eglandine (**432**)	Clivio, Richard, Hadi *et al.*, 1990
		Egalndulosine (**19**)	Clivio, Richard, Hadi *et al.*, 1990
		19-*Epi*-heyneanine (**17**)	Clivio, Richard, Hadi *et al.*, 1990
		16-*Epi*-vobasenal (**198**)	Clivio, Richard, Hadi *et al.*, 1990
		16-*Epi*-vobasine (**39**)	Clivio, Richard, Hadi *et al.*, 1990
		Heyneanine (**16**)	Clivio, Richard, Hadi *et al.*, 1990
		3-Hydroxy-3,4-*seco*-coronaridine (**22**)	Clivio, Richard, Hadi *et al.*, 1990
		3-Oxo-19-*epi*-heyneanine (**18**)	Clivio, Richard, Hadi *et al.*, 1990
		Pericyclivine (**47**)	Clivio, Richard, Hadi *et al.*, 1990
		Perivine (**40**)	Clivio, Richard, Hadi *et al.*, 1990
		(+)-Tubotaiwine (**60**)	Clivio, Richard, Hadi *et al.*, 1990
		Voacangine (**23**)	Clivio, Richard, Hadi *et al.*, 1990
		Voaphylline (= Conoflorine) (**55**)	Clivio, Richard, Hadi *et al.*, 1990
		Vobasenal (**43**)	Clivio, Richard, Hadi *et al.*, 1990
		Vobasine (**37**)	Clivio, Richard, Hadi *et al.*, 1990
		Vobasinol (**209**)	Clivio, Richard, Hadi *et al.*, 1990
	Leaves	Dregamine (**41**)	Clivio, Richard, Hadi *et al.*, 1990
		Polyervine (**71**)	Clivio, Guillaume *et al.*, 1995
		Polyervinine (**859**)	Clivio, Guillaume *et al.*, 1995
		Vobasenal (**43**)	Clivio, Richard, Hadi *et al.*, 1990
		Vobasine (**37**)	Clivio, Richard, Hadi *et al.*, 1990
		Vobasine *N*(4)-oxide (**38**)	Clivio, Richard, Hadi *et al.*, 1990
	Bark	Polyneurine A (**1**)	Tang *et al.*, 2023
		Polyneurine B (**2**)	Tang *et al.*, 2023
		Polyneurine C (**3**)	Tang *et al.*, 2023
		Polyneurine D (**4**)	Tang *et al.*, 2023
		Polyneurine E (**5**)	Tang *et al.*, 2023
		Polyneurine F (**6**)	Tang *et al.*, 2023
		Polyneurine G (**7**)	Tang *et al.*, 2023
		Polyneurine H (**8**)	Tang *et al.*, 2023

Table 1.3, continued

Plant	Plant part	Alkaloids	References
T. psorocarpa (Pierre ex Stapf) Pichon	Stem-bark	Coronaridine (**14**)	Van Beek *et al.*, 1983
		16-*Epi*-isositsirikine (**138**)	Van Beek *et al.*, 1983
		Isovallesiachotamine (**156**)	Van Beek *et al.*, 1983
		12-Methoxy-14,15-dehydrovincamine (**368**)	Van Beek *et al.*, 1983
		Tetrahydroalstonine (**130**)	Van Beek *et al.*, 1983
		Vallesiachotamine (**155**)	Van Beek *et al.*, 1983
		Voacangine (**23**)	Van Beek *et al.*, 1983
T. psychotriifolia H. B. K.	Leaves	16-*Epi*-isositsirikine (**138**)	Ghorbel *et al.*, 1981
		19-*Epi*-voacristine (= 19-*Epi*-voacangarine) (**470**)	Ghorbel *et al.*, 1981
		10-Hydroxycoronaridine (**427**)	Ghorbel *et al.*, 1981
		10-Hydroxyheyneanine (**459**)	Ghorbel *et al.*, 1981
		(+)-Tubotaiwine (**60**)	Ghorbel *et al.*, 1981
		Voacristine (= Voacangarine) (**24**)	Ghorbel *et al.*, 1981
	Stem-bark	Anhydrovobasindiol (= Taberpsychine) (**212**)	Burnell & Medina, 1971
		16-*Epi*-vobasinic acid (**205**)	Burnell & Medina, 1971
		Ibogaine-7-hydroxyindolenine (**513**)	Ghorbel *et al.*, 1981
		6(*R*)-3,6-Oxidovoacangine (**488**)	Ghorbel *et al.*, 1981
		3-Oxovoacangine (**437**)	Ghorbel *et al.*, 1981
	Roots	Voacamine (**720**)	Ghorbel *et al.*, 1981
	Root-bark	Voacamidine (**660**)	Ghorbel *et al.*, 1981
	Leaves, root-bark	Vobasine (**37**)	Ghorbel *et al.*, 1981
		Pleiocarpamine (**152**)	Ghorbel *et al.*, 1981
	Stem-bark, root-bark	16'-Decarbomethoxyvoacamine (**718**)	Ghorbel *et al.*, 1981
		N(4)-Demethylvoacamine (**724**)	Ghorbel *et al.*, 1981
		Ibogaine (**536**)	Ghorbel *et al.*, 1981
	Roots, stem-bark	Coronaridine (**14**)	Ghorbel *et al.*, 1981
	Root-bark, stem-bark	Affinine (**202**)	Burnell & Medina, 1971
	Leaves, stem-bark, root-bark	Voacangine (**23**)	Ghorbel *et al.*, 1981
T. quadrangularis[b]	Roots	Coronaridine (**14**)	Achenbach & Raffelsberger, 1980a
		19-*Epi*-heyneanine (**17**)	Achenbach & Raffelsberger, 1980a
		Heyneanine (**16**)	Achenbach & Raffelsberger, 1980a
		19(*R*)-Hydroxyibogamine (**13**)	Achenbach & Raffelsberger, 1980a
		19(*R*)-Hydroxyibogamine pseudoindoxyl (**558**)	Achenbach & Raffelsberger, 1980a

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Ibogaine (**536**)	Achenbach & Raffelsberger, 1980a
		Ibogamine (**11**)	Achenbach & Raffelsberger, 1980a
		Ibogamine pseudoindoxyl (**557**)	Achenbach & Raffelsberger, 1980a
		3-Oxocoronaridine (**19**)	Achenbach & Raffelsberger, 1980a
		3-Oxovoacangine (**437**)	Achenbach & Raffelsberger, 1980a
		Voacangine (**23**)	Achenbach & Raffelsberger, 1980a
		Voacangine-7-hydroxyindolenine (**507**)	Achenbach & Raffelsberger, 1980a
T. retusa (Lam.) Pichon (*T. noronhiana*, *Conopharyngia retusa*, *Pandaca retusa*, *Plumeria retusa)*	Leaves	Coronaridine (**14**)	Picot *et al.*, 1973
		Heyneanine (**16**)	Picot *et al.*, 1973
		3-Oxovoacangine (**437**)	Picot *et al.*, 1973
		Voacangine (**23**)	Picot *et al.*, 1973
		Voacristine (= Voacangarine) (**24**)	Picot *et al.*, 1973
	Seeds	Pachysiphine (**291**)	Le Men-Olivier *et al.*, 1974
		Tabersonine (**281**)	Le Men-Olivier *et al.*, 1974
		Voaphylline (= Conoflorine) (**55**)	Le Men-Olivier *et al.*, 1974
T. riedelii Müll. Arg.	Leaves, seeds	(+)-Minovincine (**326**)	Cava, Tjoa *et al.*, 1968
		(+)-3-Oxominovincine (**327**)	Cava, Tjoa *et al.*, 1968
		(+)-Vincadifformine (**325**)	Cava, Tjoa *et al.*, 1968
		rac-Vincadifformine (*rac*-**325**)[a]	Cava, Tjoa *et al.*, 1968
T. rigida (Miers) Leeuwenberg (*T. Macrophylla, Anacampta rigida, Phrissocarpus rigidus*)	Stem-bark	(+)-Apovincamine (**381**)	Cava, Tjoa *et al.*, 1968
		rac-16-*Epi*-vincamine (*rac*-**364**)[a]	Cava, Tjoa *et al.*, 1968
		(−)-16-*Epi*-vincamine (**365**)	Cava, Tjoa *et al.*, 1968
		(+)-21-*Epi*-vincamine (**366**)	Cava, Tjoa *et al.*, 1968
		(−)-21-*Epi*-vincamine (**367**)	Cava, Tjoa *et al.*, 1968
		rac-Vincamine (*rac*-**363**)[a]	Cava, Tjoa *et al.*, 1968
		(+)-Vincamine (**362**)	Cava, Tjoa *et al.*, 1968
T. rupicola Benth. (*Anacampta rupicola*)	Leaves, twigs	Voacangine pseudoindoxyl (= Voaluteine) (**520**)	Niemann & Kessel, 1966
		Voacristine pseudoindoxyl (**521**)	Niemann & Kessel, 1966

Table 1.3, continued

Plant	Plant part	Alkaloids	References
T. salzmannii (A.DC.) (*P. salzmannii*)	Leaves	3(*S*)-Hydroxyisovoacangine (**436**)	Figueiredo *et al.*, 2010
		Isovoacangine (**430**)	Figueiredo *et al.*, 2010
		Isovoacristine (**471**)	Figueiredo *et al.*, 2010
	Root-bark	Coronaridine (**14**)	Figueiredo *et al.*, 2010
		Heyneanine (**16**)	Figueiredo *et al.*, 2010
		Olivacine (**77**)	Figueiredo *et al.*, 2010
		3-Oxocoronaridine (**19**)	Figueiredo *et al.*, 2010
		Voacangine (**23**)	Figueiredo *et al.*, 2010
		Voachalotine (**162**)	Figueiredo *et al.*, 2010
T. sananho Ruíz & Pav.	Bark	Coronaridine (**14**)	Delle Monache *et al.*, 1977
		Heyneanine (**16**)	Delle Monache *et al.*, 1977
		3(*R*/*S*)-Hydroxycoronaridine (**432**)	Delle Monache *et al.*, 1977
		Ibogamine (**11**)	Delle Monache *et al.*, 1977
		Voacangine (**23**)	Delle Monache *et al.*, 1977
T. sessilifolia Baker (*Muntafara sessilifolia*)	Leaves, stem-bark	Apparicine (**272**)	Panas *et al.*, 1975
		Coronaridine (**14**)	Panas *et al.*, 1975
		Dregamine (**41**)	Panas *et al.*, 1975
		6-Hydroxy-3-oxocoronaridine (**531**)	Panas *et al.*, 1975
		6-Hydroxy-3-oxoisovaocangine (**532**)	Panas *et al.*, 1975
		Isovoacangine (**430**)	Panas *et al.*, 1975
		6(*R*)-3,6-Oxidocoronaridine (**486**)	Panas *et al.*, 1975
		6(*R*)-3,6-Oxidoisovoacangine (**487**)	Panas *et al.*, 1975
		Tabernaemontanine (**42**)	Panas *et al.*, 1975
	Stem-bark	Coronaridine (**14**)	Girardot *et al.*, 2012a
		19,20α-Dihydroeleganine A (**219**)	Girardot *et al.*, 2012a
		Dregamine (**41**)	Girardot *et al.*, 2012b
		Dregamine acetate (**192**)	Girardot *et al.*, 2012b
		19(*S*)-Heyneanine (**16**)	Girardot *et al.*, 2012b
		3'(*R*)-Hydroxyconodurine (**752**)	Girardot *et al.*, 2012b
		3(*R*/*S*)-Hydroxycoronaridine (= Eglandine) (**432**)	Girardot *et al.*, 2012a
		3'(*R*)-Hydroxytabernaelegantine A (**744**)	Girardot *et al.*, 2012b
		3'(*R*/*S*)-Hydroxytabernaelegantine A (**744**)	Girardot *et al.*, 2012a
		3'(*R*)-Hydroxytabernaelegantine B (**665**)	Girardot *et al.*, 2012b
		3'(*R*)-Hydroxytabernaelegantine C (**742**)	Girardot *et al.*, 2012b
		3'(*S*)-Hydroxytabernaelegantine C (**743**)	Girardot *et al.*, 2012a
		3'(*R*)-Hydroxytabernaelegantine D (**670**)	Girardot *et al.*, 2012b
		3-Oxocoronaridine (= Eglandulosine) (**19**)	Girardot *et al.*, 2012a
		3-Oxocoronaridine hydroxyindolenine (**510**)	Girardot *et al.*, 2012a
		3'-Oxotabernaelegantine A (**740**)	Girardot *et al.*, 2012a
		3'-Oxotabernaelegantine B (**671**)	Girardot *et al.*, 2012a
		3'(*R*)-Tabernaelegantinal A (**745**)	Girardot *et al.*, 2012b
		3'(*R*)-Tabernaelegantinal B (**669**)	Girardot *et al.*, 2012b
		3'(*R*)-Tabernaelegantinal E (**756**)	Girardot *et al.*, 2012b
		Tabernaelegantine A (**733**)	Girardot *et al.*, 2012a
		Tabernaelegantine B (**664**)	Girardot *et al.*, 2012b
		Tabernaelegantine D (**666**)	Girardot *et al.*, 2012a

Table 1.3, continued

Plant	Plant part	Alkaloids	References
		Tabernaemontanine (**42**)	Girardot *et al.*, 2012a
		Tabernaemontanine acetate (**193**)	Girardot *et al.*, 2012b
		Tabernaemontanol (**189**)	Girardot *et al.*, 2012b
T. siphilitica (L.f.) Leeuwenberg (*T. tetratachia, Bonafousia tetrastachia, Echites siphilitica*)	Leaves	Apparicine (**272**)	Damak *et al.*, 1981
		12,12'-Bis(11-hydroxycoronaridinyl) (**821**)	Damak, Poupat *et al.*, 1976
		Bonafousine (**804**)	Damak, Ahond *et al.*, 1976; Damak *et al.*, 1980
		Coronaridine (**14**)	Damak, Poupat *et al.*, 1976
		Geissoschizine (**139**)	Damak, Ahond *et al.*, 1976
		12-Hydroxyvincadifformine (**304**)	Damak *et al.*, 1981
		Isobonafousine (**807**)	Damak *et al.*, 1980
		Isovoacangine (**430**)	Damak *et al.*, 1981; Damak, Poupat *et al.*, 1976
		Pleiocarpamine (**152**)	Damak *et al.*, 1981
		Tetrahydroalstonine (**130**)	Damak *et al.*, 1981
		Tetrastachyne (**859**)	Damak *et al.*, 1981
		Tetrastachynine (**810**)	Damak *et al.*, 1981
		(+)-Tubotaiwine (**60**)	Damak *et al.*, 1981
		(+)-Vincadifformine (**325**)	Damak *et al.*, 1981
		Voacangine (**23**)	Damak, Poupat, *et al.*, 1976; Damak *et al.*, 1981
T. solanifolia A.DC. (*P. campestris* (Rizz.) Rizz.)	Leaves, bark, roots	Coronaridine (**14**)	Gower *et al.*, 1986
		Heyneanine (**16**)	Gower *et al.*, 1986
		Isovoacangine (**430**)	Gower *et al.*, 1986
		Isovoacristine (**471**)	Gower *et al.*, 1986
		12-Methoxy-*N*(4)-methylvoachalotine (**180**)	Gower *et al.*, 1986
		Voacamine (**720**)	Gower *et al.*, 1986
		Voacangine (**23**)	Gower *et al.*, 1986
		Voacangine-7-hydroxyindolenine (**507**)	Gower *et al.*, 1986
		Voachalotine (**162**)	Gower *et al.*, 1986
		Vobasine (**37**)	Gower *et al.*, 1986
T. sphaerocarpa Blume (*Pagiantha sphaerocarpa*)	Leaves, seeds	Dregamine (**41**)	Chatterjee *et al.*, 1968
		Tabernaemontanine (**42**)	Chatterjee *et al.*, 1968
	Stem	Biscarpamontamine A (**812**)	Zaima *et al.*, 2009
		Biscarpamontamine B (**827**)	Zaima *et al.*, 2009
		3-Hydroxyvoacangine (**438**)	Zaima *et al.*, 2009
		3-Hydroxyvobtusine (**826**)	Zaima *et al.*, 2009
		Ibogamine (**11**)	Zaima *et al.*, 2009
		Voacangine (**23**)	Zaima *et al.*, 2009
		Vobasine (**37**)	Zaima *et al.*, 2009

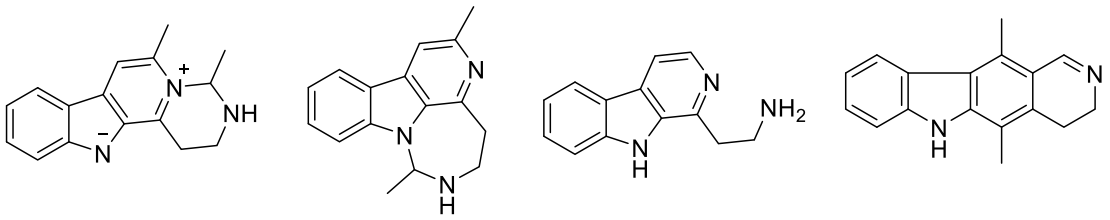
Table 1.3, continued

Plant	Plant part	Alkaloids	References
T. stapfiana Britten (*T. johnstonii* (Stapf) Pichon, *Conopharyngia johnstonii*)	Stem-bark	Conoduramine (**682**)	Kingston *et al.*, 1978
		Conodurine (**748**)	Kingston *et al.*, 1978
		19',20'-Epoxyconoduramine (**683**)	Kingston *et al.*, 1978
		Gabunamine (**679**)	Kingston *et al.*, 1978
		Gabunine (**747**)	Kingston *et al.*, 1978
		Ibogamine (**11**)	Kingston *et al.*, 1978
		Pericyclivine (**47**)	Kingston *et al.*, 1978
		Perivine (**40**)	Kingston *et al.*, 1978
		Tabernamine (**67**)	Kingston *et al.*, 1978
	Root-bark	Ibogamine (**11**)	Kingston *et al.*, 1976
		Tabernamine (**67**)	Kingston *et al.*, 1976
		Tubotaiwine (**60**)	Pinar *et al.*, 1972
		Tubotaiwine *N*-oxide (**61**)	Pinar *et al.*, 1972
T. stellata Pichon (*P. stellata*)	Root-bark	Coronaridine (**14**)	Picot *et al.*, 1973
T. subglobosa Merr.	Twigs	Ervatamine (**247**)	Huang *et al.*, 1991
		Vobasine (**37**)	Huang *et al.*, 1991
	Leaves, roots	Conoduramine (**682**)	Takayama *et al.*, 1994
		Conodurine (**748**)	Takayama *et al.*, 1994
		Coronaridine (**14**)	Takayama *et al.*, 1994
		Heyneanine (**16**)	Takayama *et al.*, 1994
		19'(*R*)-Hydroxyconoduramine (**685**)	Takayama *et al.*, 1994
		19'(*R*)-Hydroxyconodurine (**751**)	Takayama *et al.*, 1994
		Isovoacangine (**430**)	Takayama *et al.*, 1994
		Tabernaelegantine A (**733**)	Takayama *et al.*, 1994
		Tabernaelegantine B (**664**)	Takayama *et al.*, 1994
		Tabernamine (**67**)	Takayama *et al.*, 1994
	Leaves, roots, twigs	Dregamine (**41**)	Huang *et al.*, 1991; Takayama *et al.*, 1994
		Tabernaemontanine (**42**)	Huang *et al.*, 1991; Takayama *et al.*, 1994
T. undulata Vahl (*Bonafusia undulata*)	Seeds, stem-bark	Coronaridine (**14**)	Picot *et al.*, 1973; Van Beek & Verpoorte, 1985
		Voaphylline (= Conoflorine) (**55**)	Bruneton *et al.*, 1979
	Stem-bark	19-*Epi*-heyneanine (**17**)	Bruneton *et al.*, 1979; Van Beek & Verpoorte, 1985
		19-*Epi*-voacristine (= 19-*Epi*-voacangarine) (**470**)	Van Beek & Verpoorte, 1985
		18-Hydroxycoronaridine (**15**)	Van Beek & Verpoorte, 1985
		18-Hydroxyvoacangine (**485**)	Van Beek & Verpoorte, 1985
		Quebrachidine (**222**)	Bruneton *et al.*, 1979
		Voacangine (**23**)	Garnier *et al.*, 1984; Van Beek & Verpoorte, 1985

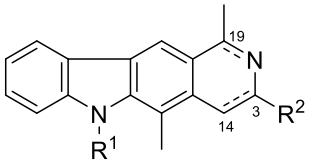
Table 1.3, continued

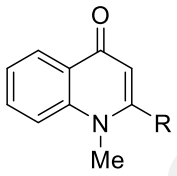
Plant	Plant part	Alkaloids	References
T. ventricosa Hochst. ex A. DC.	Whole plant	Akuammicine (**255**)	Schripsema *et al.*, 1986
		Akuammicine *N*-oxide (**256**)	Schripsema *et al.*, 1986
		Apparicine (**272**)	Schripsema *et al.*, 1986
		16-*Epi*-isositsirikine (**138**)	Schripsema *et al.*, 1986
		10-Hydroxycoronaridine (**427**)	Schripsema *et al.*, 1986
		10-Hydroxyheyneanine (**459**)	Schripsema *et al.*, 1986
		Norfluorocurarine (**259**)	Schripsema *et al.*, 1986
		(+)-Tubotaiwine (**60**)	Schripsema *et al.*, 1986
T. wallichiana Steud.	Leaves	Isovoacangine (**430**)	Talapatra *et al.*, 1976
	Leaves, stem-bark	Coronaridine (**14**)	Talapatra *et al.*, 1976
		Voacangine (**23**)	Talapatra *et al.*, 1976
		Voacristine (= Voacangarine) (**24**)	Talapatra *et al.*, 1976

[a]*rac* = racemic; [b]Not listed in the botanical literature.



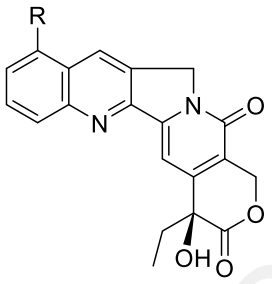
73 **74** **75** **76**

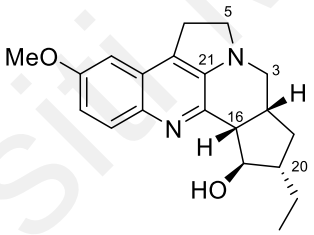


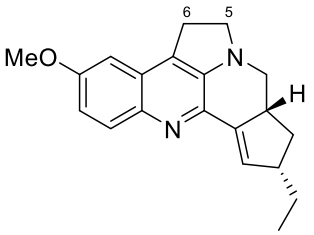


77 $R^1 = R^2 = H$, $\Delta^{3,14;4,19}$
78 $R^1 = R^2 = H$
79 $R^1 = H$, $R^2 = OH$
80 $R^1 = R^2 = H$, $\Delta^{4,19}$
81 $R^1 = OH$, $R^2 = H$, $\Delta^{3,14;4,19}$
82 $R^1 = R^2 = H$, $\Delta^{3,14;4,19}$, N(4)→O

83 R =
84 R =
85 R =
86 R =



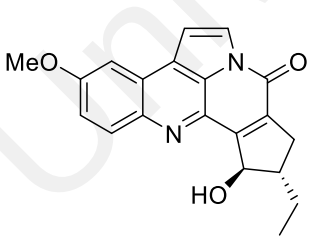


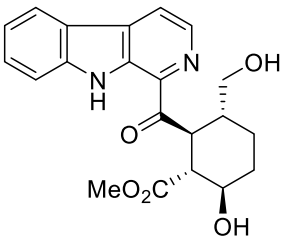


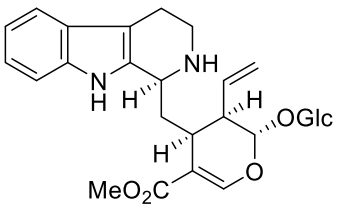
87 R = H
88 R = OMe

89

90
91 $\Delta^{5,6}$

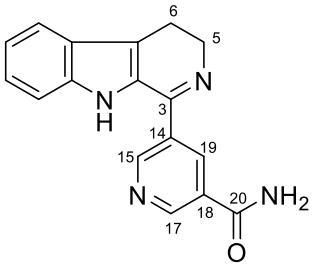






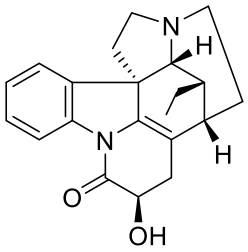
92 **93** **94**

Figure 1.8: Structures of alkaloids in *Tabernaemontana*



95

96 $\Delta^{5,6}$



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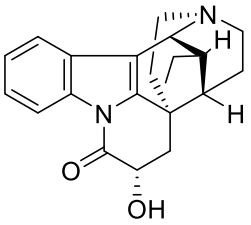

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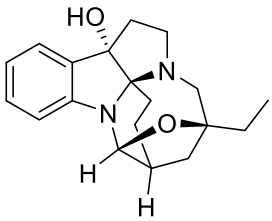

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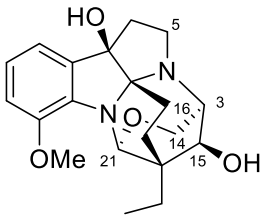

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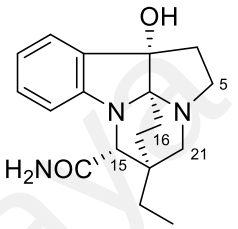

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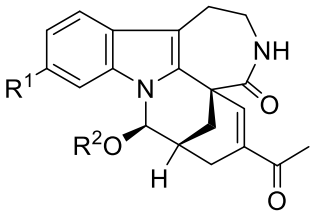
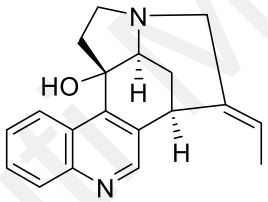


101 $R^1 = R^2 = H$

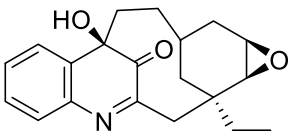
102 $R^1 = OMe$, $R^2 = H$

103 $R^1 = H$, $R^2 = Et$



104

105 N(4)→O



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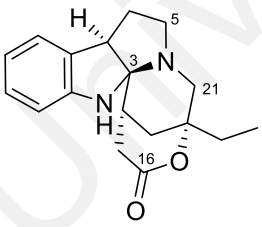

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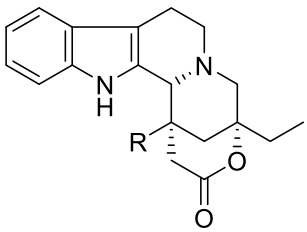

108 R = OH

109 R = H

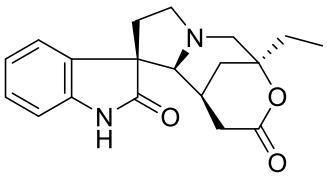

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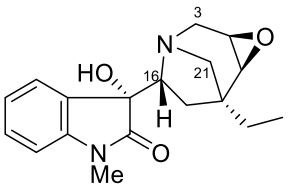
Figure 1.8, continued



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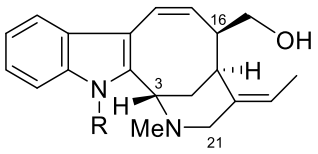
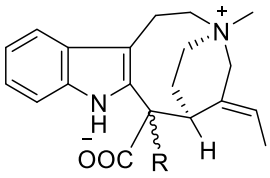
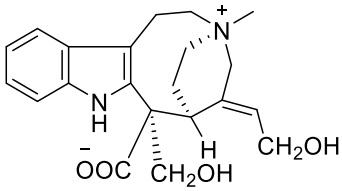
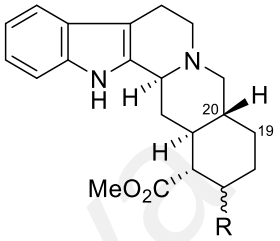


112 R = H
113 R = Me



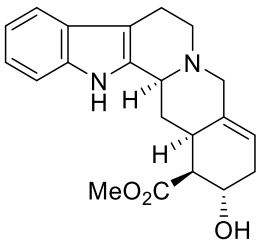


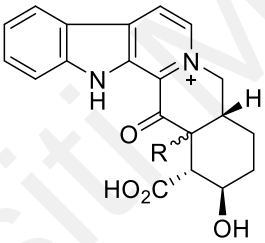


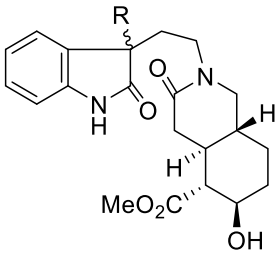
114 R = β-H
115 R = α-H
116 R = α-CH_2OH

117

118 R = β-OH
119 R = α-OH
120 R = β-OH, $\Delta^{19,20}$
121 R = α-OH, $\Delta^{19,20}$



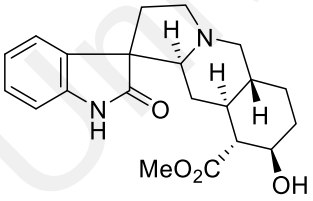


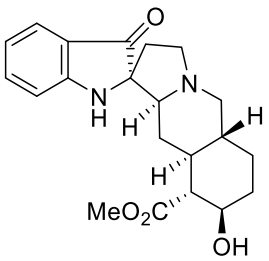


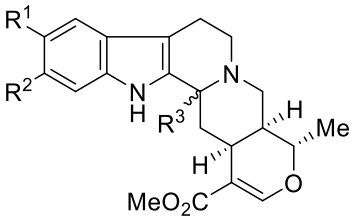
122

123 R = α-OH
124 R = β-OH

125 R = α-OH
126 R = β-OH





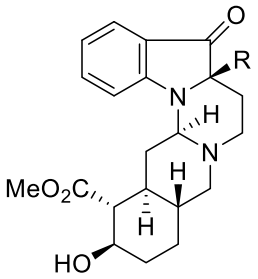


127

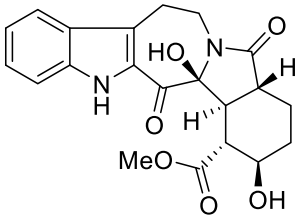
128
129 N(4)→O

130 R^1 = R^2 = H, R^3 = α-H
131 R^1 = R^2 = OMe, R^3 = β-H
132 R^1 = R^2 = OMe, R^3 = α-H

Figure 1.8, continued



133 R = OH
134 R = OEt



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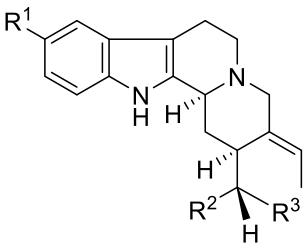
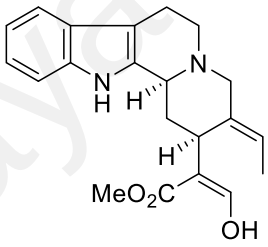


136 $R^1 = R^3 = H$, $R^2 = CH_2OH$
137 $R^1 = OH$, $R^2 = CH_2OH$, $R^3 = H$
138 $R^1 = H$, $R^2 = CH_2OH$, $R^3 = CO_2Me$
51 $R^1 = H$, $R^2 = CO_2Me$, $R^3 = CH_2OH$



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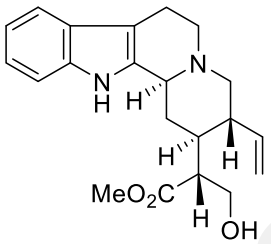

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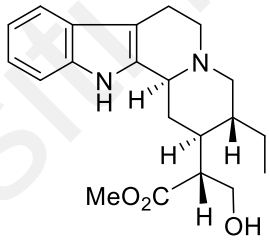

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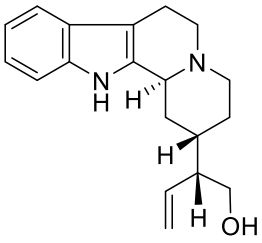

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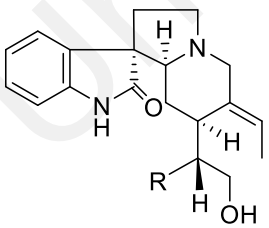
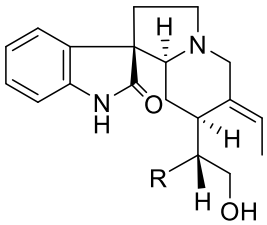
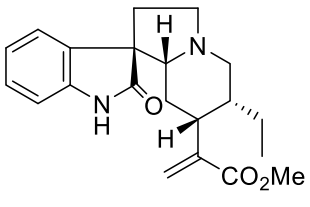


141 R = H
142 R = H, N(4)→O
143 R = CO_2Me

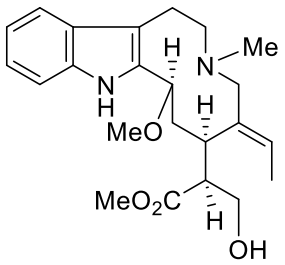


144 R = H
145 R = CO_2Me



146

Figure 1.8, continued



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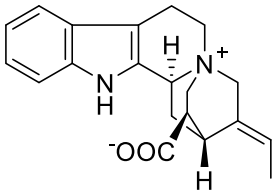

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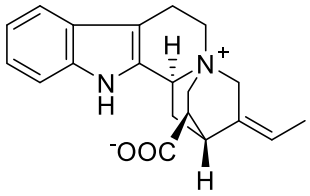

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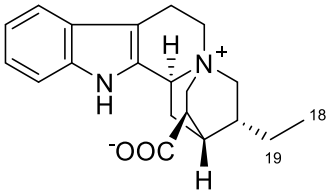
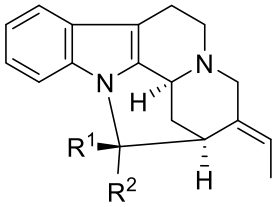


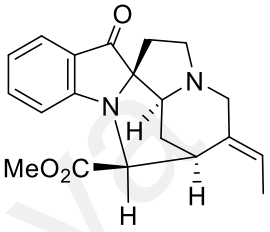
150

151 $\Delta^{18,19}$



152 $R^1 = CO_2Me$, $R^2 = H$

153 $R^1 = H$, $R^2 = CO_2Me$



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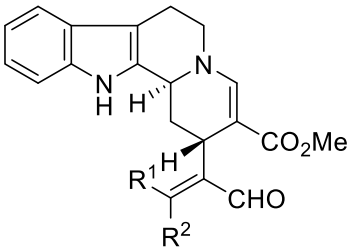
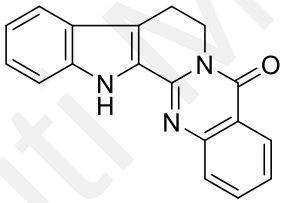


155 $R^1 = H$, $R^2 = Me$

156 $R^1 = Me$, $R^2 = H$



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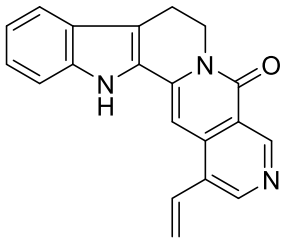

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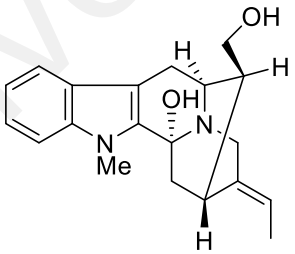

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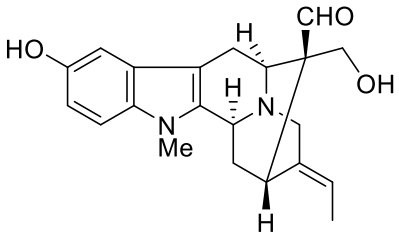

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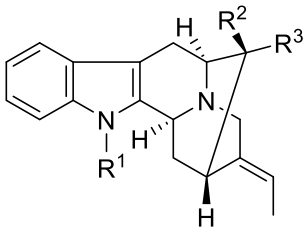
Figure 1.8, continued



161 R^1 = Me, R^2 = H, R^3 = CH_2OH

162 R^1 = Me, R^2 = CH_2OH, R^3 = CO_2Me

163 R^1 = Me, R^2 = CH_2OH, R^3 = CO_2Me, N(4)→O

47 R^1 = R^3 = H, R^2 = CO_2Me

164 R^1 = Me, R^2 = H, R^3 = CH_2OH, N(4)→O

165 R^1 = Me, R^2 = CH_2OH, R^3 = H

166 R^1 = Me, R^2 = CH_2OH, R^3 = H, N(4)→O

167 R^1 = Me, R^2 = CH_2OAc, R^3 = H

168 R^1 = R^2 = H , R^3 = CH_2OH

169 R^1 = R^3 = H , R^2 = CH_2OH

170 R^1 = Me, R^2 = CO_2Me, R^3 = H

171 R^1 = H , R^2 = CH_2OH, R^3 = CO_2Me

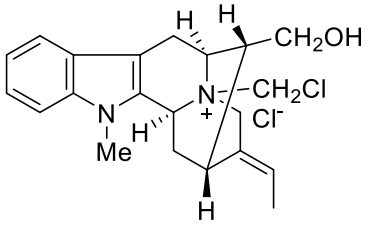
172 R^1 = H , R^2 = CO_2Me, R^3 = CH_2OH

173 R^1 = H , R^2 = CH_2OAc, R^3 = CO_2Me

174 R^1 = Me, R^2 = CH_2OH, R^3 = CO_2Me, $MeN(4)^+$

175 R^1 = Me, R^2 = CH_2OH, R^3 = H, $MeN(4)^+$

176 R^1 = R^3 = H, R^2 = CH_2OH, N(4)→O



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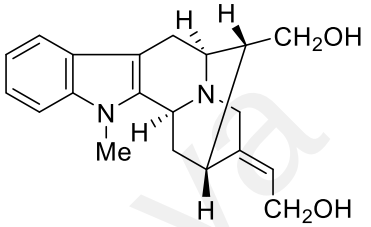

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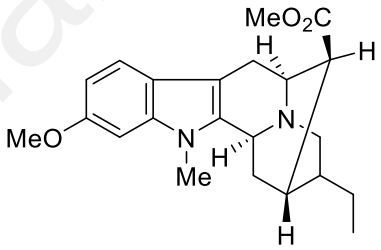

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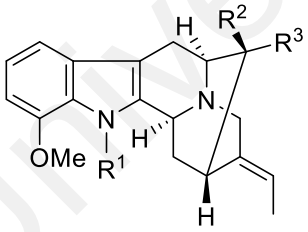


180 R^1 = Me, R^2 = CH_2OH, R^3 = CO_2Me, $MeN(4)^+$

181 R^1 = Me, R^2 = CH_2OH, R^3 = CO_2Et, $MeN(4)^+$

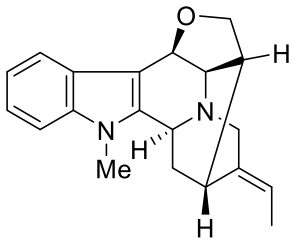
182 R^1 = Me, R^2 = CH_2OH, R^3 = CO_2H, $MeN(4)^+$

183 R^1 = Me, R^2 = H, R^3 = CO_2Et, $MeN(4)^+$

184 R^1 = Me, R^2 = H, R^3 = CO_2H, $MeN(4)^+$

185 R^1 = Me, R^2 = CH_2OH, R^3 = CO_2Me

Figure 1.8, continued



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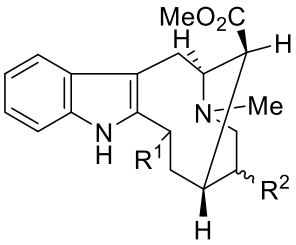
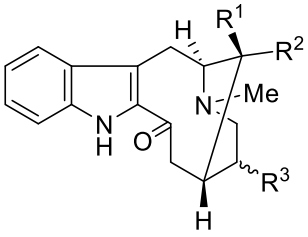
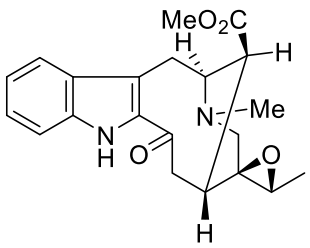


187 R^1 = α-OH, R^2 = β-Et
188 R^1 = α-OH, R^2 = α-Et
189 R^1 = β-OH, R^2 = β-Et
190 R^1 = OMe, R^2 = α-Et



41 R^1 = CO_2Me, R^2 = H, R^3 = α-Et
191 R^1 = CO_2Me, R^2 = H, R^3 = α-Et, N(4)→O
192 R^1 = CO_2Me, R^2 = H, R^3 = α-Et (acetate salt)
42 R^1 = CO_2Me, R^2 = H, R^3 = β-Et
193 R^1 = CO_2Me, R^2 = H, R^3 = β-Et (acetate salt)
194 R^1 = H, R^2 = CO_2Me, R^3 = α-Et
195 R^1 = H, R^2 = CO_2Me, R^3 = β-Et



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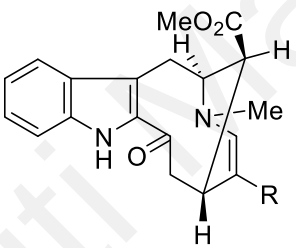
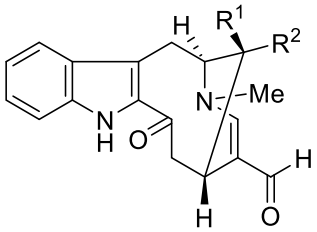
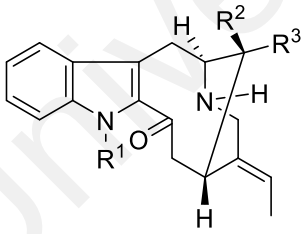


197 R = Et
44 R = Ac

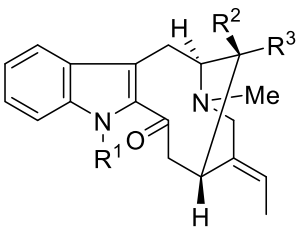


43 R^1 = CO_2Me, R^2 = H
198 R^1 = H, R^2 = CO_2Me

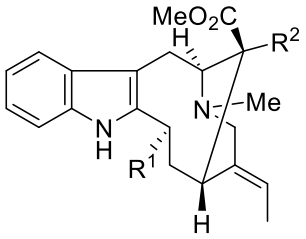


40 R^1 = R^3 = H, R^2 = CO_2Me
199 R^1 = Me, R^2 = H, R^3 = CH_2OH
200 R^1 = R^3 = H, R^2 = CH_2OH
201 R^1 = H, R^2 = CO_2Me, R^3 = CH_2OH

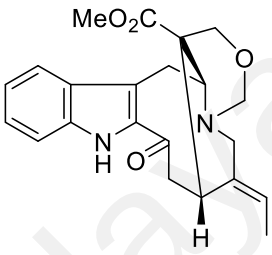
Figure 1.8, continued



37 $R^1 = R^3 = H$, $R^2 = CO_2Me$
202 $R^1 = R^3 = H$, $R^2 = CH_2OH$
39 $R^1 = R^2 = H$, $R^3 = CO_2Me$
203 $R^1 = R^2 = H$, $R^3 = CH_2OH$
204 $R^1 = Me$, $R^2 = H$, $R^3 = CH_2OH$
205 $R^1 = R^2 = H$, $R^3 = COOH$
206 $R^1 = H$, $R^2 = CO_2Me$, $R^3 = CH_2OH$
207 $R^1 = Me$, $R^2 = CO_2Me$, $R^3 = H$
208 $R^1 = R^2 = H$, $R^3 = CH_2OMe$



209 $R^1 = OH$, $R^2 = H$
210 $R^1 = OMe$, $R^2 = CH_2OH$



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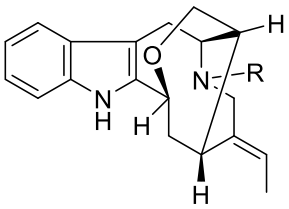
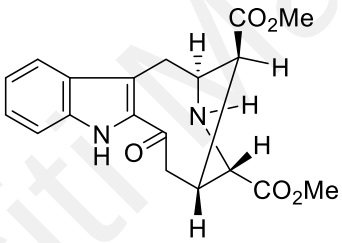


212 R = Me
213 R = H



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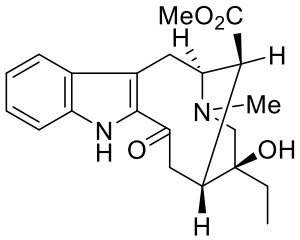
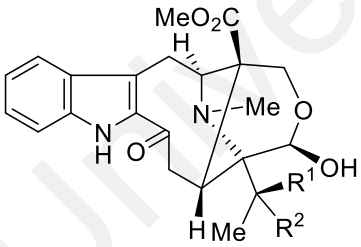
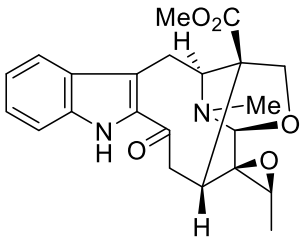


46
214 N(4)→O



215 $R^1 = OH$, $R^2 = H$
216 $R^1 = H$, $R^2 = OH$



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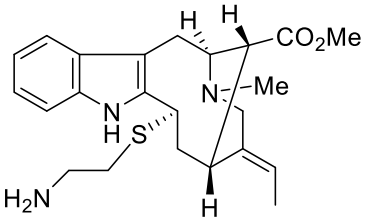

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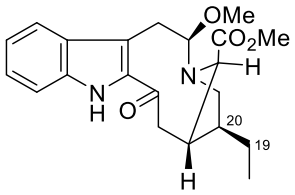
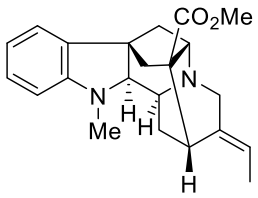
Figure 1.8, continued



219

220 $\Delta^{19,20}$



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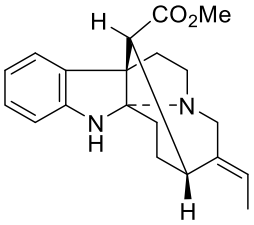

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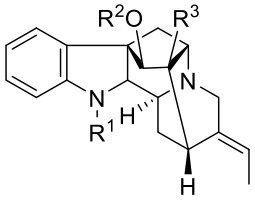


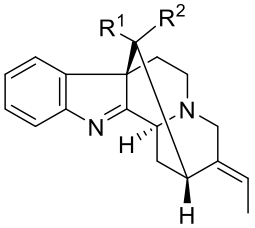
222 $R^1 = R^2 = H$, $R^3 = CO_2Me$

223 $R^1 = Me$, $R^2 = R^3 = H$

224 $R^1 = Me$, $R^2 = COC_6H_4(OMe)$, $R^3 = H$

225 $R^1 = Me$, $R^2 = COC_6H_3(OMe)_2$, $R^3 = H$

226 $R^1 = Me$, $R^2 = COC_6H_2(OMe)_3$, $R^3 = H$



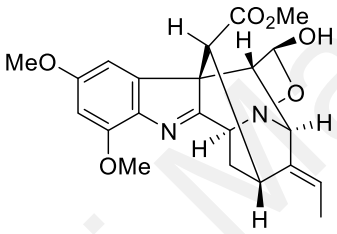
228 $R^1 = CH_2OH$, $R^2 = CO_2Me$

229 $R^1 = CH_2OAc$, $R^2 = CO_2Me$

230 $R^1 = CO_2Me$, $R^2 = CH_2OAc$

231 $R^1 = CO_2Me$, $R^2 = CHO$

232 $R^1 = H$, $R^2 = CO_2Me$



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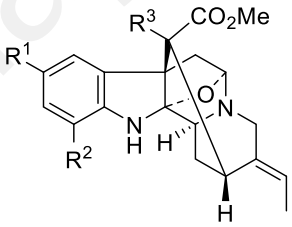
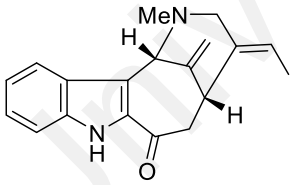


234 $R^1 = R^2 = OMe$, $R^3 = H$

235 $R^1 = OMe$, $R^2 = R^3 = H$

236 $R^1 = R^2 = H$, $R^3 = CH_2OAc$

237 $R^1 = R^2 = R^3 = H$



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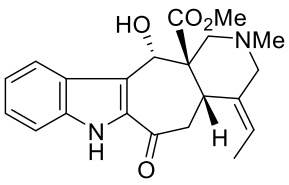

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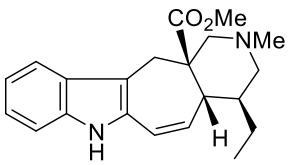

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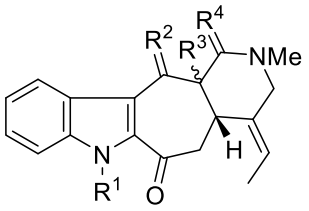
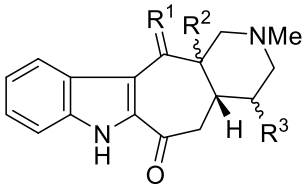
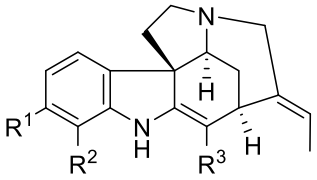
Figure 1.8, continued



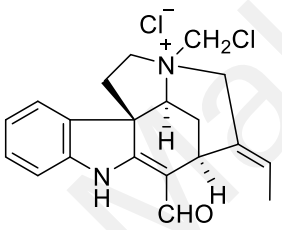


49 R^1 = H, R^2 = R^4 = H,H, R^3 = β-CO_2Me
241 R^1 = H, R^2 = R^4 = H,H, R^3 = β-H
242 R^1 = H, R^2 = H,H, R^3 = β-CO_2Me, R^4 = O
243 R^1 = OMe, R^2 = R^4 = H,H, R^3 = β-CO_2Me
244 R^1 = H, R^2 = R^4 = H,H, R^3 = α-H
245 R^1 = H, R^2 = O, R^3 = β-H, R^4 = H,H
246 R^1 = OMe, R^2 = R^4 = H,H, R^3 = β-H

247 R^1 = H,H, R^2 = β-CO_2Me, R^3 = β-Et
248 R^1 = H,H, R^2 = β-CO_2Me, R^3 = α-Et
249 R^1 = H,H, R^2 = α-CO_2Me, R^3 = β-Et
250 R^1 = H,H, R^2 = β-H, R^3 = α-Et
251 R^1 = H,H, R^2 = β-H, R^3 = β-Et
252 R^1 = H,H, R^2 = α-H, R^3 = α-Et
253 R^1 = O, R^2 = β-H, R^3 = α-Et
254 R^1 = O, R^2 = α-H, R^3 = α-Et



255 R^1 = R^2 = H, R^3 = CO_2Me
256 R^1 = R^2 = H, R^3 = CO_2Me, N(4)→O
257 R^1 = H, R^2 = OH, R^3 = CO_2Me
258 R^1 = OH, R^2 = H, R^3 = CHO
259 R^1 = R^2 = H, R^3 = CHO
260 R^1 = R^2 = H, R^3 = CHO, N(4)→O
261 R^1 = H, R^2 = OH, R^3 = CHO



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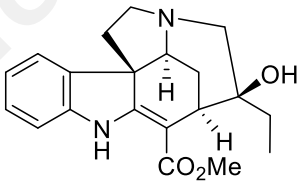

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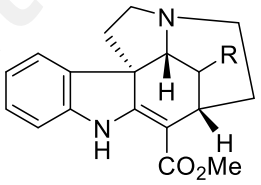
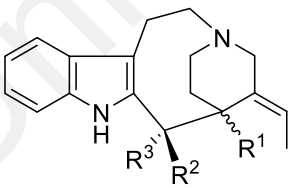
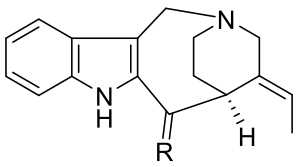


264 R = =CHMe
60 R = α-Et
265 R = =CHMe, N(4)→O
61 R = α-Et, N(4)→O

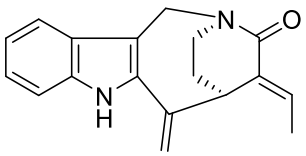


266 R^1 = α-H, R^2 = CH_2OH, R^3 = CO_2Me
267 R^1 = α-H, R^2 = CH_2OH, R^3 = CO_2Me, N(4)→O
268 R^1 = β-H, R^2 = CH_2OH, R^3 = CO_2Me
269 R^1 = α-H, R^2 = Me, R^3 = OH
270 R^1 = α-H, R^2 = CH_2OH, R^3 = CO_2Me
271 R^1 = α-H, R^2 = CH_2OAc, R^3 = CO_2Me

Figure 1.8, continued



272 R = CH_2
273 R = O



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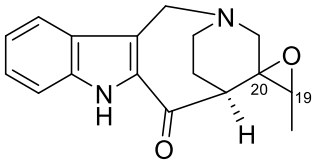
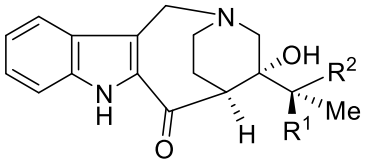
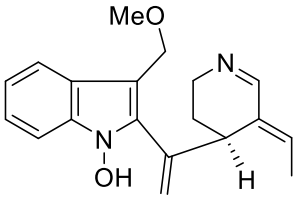


275 R = 19(*R*),20(*R*)
276 R = 19(*S*),20(*R*)



277 R^1 = H, R^2 = OH
278 R^1 = OH, R^2 = H



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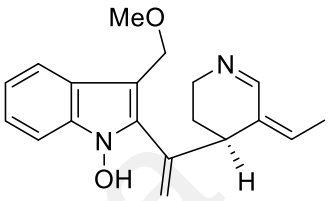

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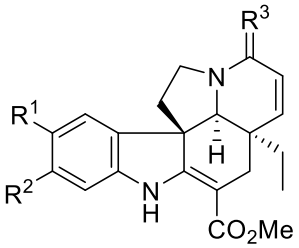
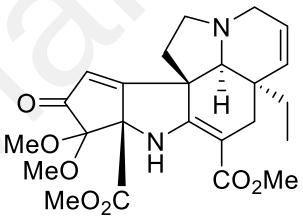


281 R^1 = R^2 = R^3 = H,H
282 R^1 = R^2 = H, R^3 = H,H, N(4)→O
283 R^1 = R^2 = H, R^3 = O
284 R^1 = OH, R^2 = OMe, R^3 = H,H
285 R^1 = OH, R^2 = OMe, R^3 = O
286 R^1 = R^2 = OMe, R^3 = α-CH_2OH
287 R^1 = R^2 = OMe, R^3 = $CHCOCH_3$
288 R^1 = OH, R^2 = OMe, R^3 = H,H, N(4)→O



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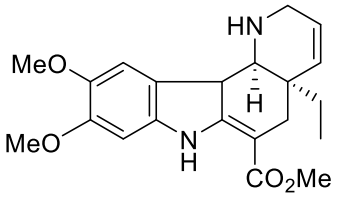

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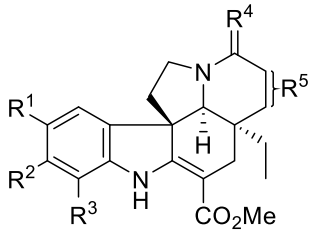
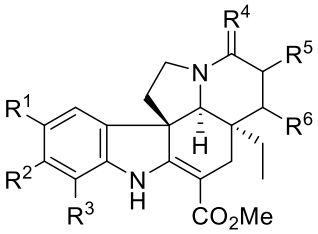
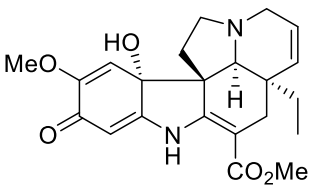


291 $R^1 = R^2 = R^3 = H$, $R^4 = H,H$, $R^5 = 14,15\text{-}\beta\text{-O}$
292 $R^1 = R^2 = R^3 = H$, $R^4 = H,H$, $R^5 = 14,15\text{-}\alpha\text{-O}$
293 $R^1 = R^3 = H$, $R^2 = OMe$, $R^4 = H,H$, $R^5 = 14,15\text{-O}$
294 $R^1 = R^2 = OMe$, $R^3 = H$, $R^4 = H,H$, $R^5 = 14,15\text{-}\beta\text{-O}$
295 $R^1 = OH$, $R^2 = R^3 = OMe$, $R^4 = H,H$, $R^5 = 14,15\text{-}\beta\text{-O}$
296 $R^1 = OH$, $R^2 = OMe$, $R^3 = H$, $R^4 = H,H$, $R^5 = 14,15\text{-}\alpha\text{-O}$
297 $R^1 = OH$, $R^3 = H$, $R^2 = OMe$, $R^4 = O$, $R^5 = 14,15\text{-}\alpha\text{-O}$
298 $R^1 = OH$, $R^2 = OMe$, $R^3 = H$, $R^4 = \alpha\text{-}CH_2COCH_3$, $R^5 = 14,15\text{-}\alpha\text{-O}$
299 $R^1 = R^2 = OMe$, $R^3 = H$, $R^4 = O$, $R^5 = 14,15\text{-}\alpha\text{-O}$



300 $R^1 = R^2 = R^3 = H$, $R^4 = H,H$, $R^5 = R^6 = OH$
301 $R^1 = OH$, $R^2 = OMe$, $R^3 = R^5 = H$, $R^4 = H,H$, $R^6 = \beta\text{-OMe}$
302 $R^1 = OH$, $R^2 = OMe$, $R^3 = R^5 = H$, $R^4 = O$, $R^6 = \beta\text{-OH}$
303 $R^1 = R^2 = R^3 = H$, $R^4 = O$, $R^5 = R^6 = H$
304 $R^1 = R^2 = H$, $R^3 = OH$, $R^4 = H,H$, $R^5 = R^6 = H$
305 $R^1 = OH$, $R^2 = OMe$, $R^3 = H$, $R^4 = H,H$, $R^5 = R^6 = H$
306 $R^1 = OH$, $R^2 = OMe$, $R^3 = H$, $R^4 = \alpha\text{-}CH_2OH$, $R^5 = R^6 = H$
307 $R^1 = OH$, $R^2 = OMe$, $R^3 = H$, $R^4 = CHCOCH_3$, $R^5 = R^6 = H$
308 $R^1 = OH$, $R^2 = OMe$, $R^3 = H$, $R^4 = H,H$, $R^5 = R^6 = H$, $N(4)\rightarrow O$



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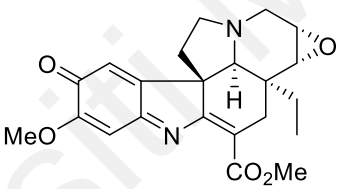

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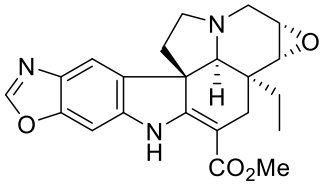

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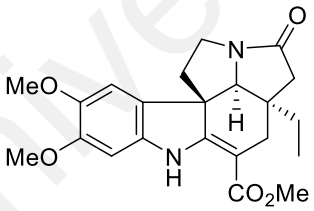

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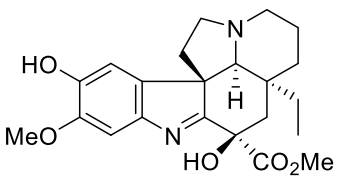

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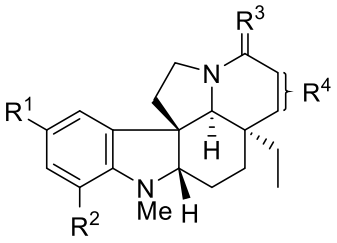
Figure 1.8, continued

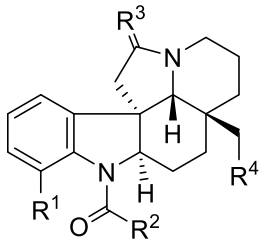


314 $R^1 = R^2 = H$, $R^3 = H,H$, $R^4 = 14,15\text{-}\beta\text{-}O$

315 $R^1 = R^2 = H$, $R^3 = O$, $R^4 = 14,15\text{-}\beta\text{-}O$

316 $R^1 = CHO$, $R^2 = H$, $R^3 = H,H$, $R^4 = 14,15\text{-}\beta\text{-}O$

317 $R^1 = H$, $R^2 = OH$, $R^3 = H,H$, $R^4 = 14\text{-}\alpha OH,15\text{-}\beta OH$



318 $R^1 = OH$, $R^2 = R^4 = Me$, $R^3 = H,H$

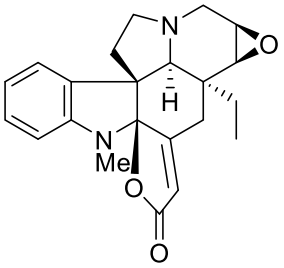
319 $R^1 = OMe$, $R^2 = Me$, $R^3 = H,H$, $R^4 = CO_2Me$

320 $R^1 = H$, $R^2 = Me$, $R^3 = H,H$, $R^4 = CO_2Me$

321 $R^1 = OMe$, $R^2 = Et$, $R^3 = H,H$, $R^4 = CO_2Me$

322 $R^1 = OMe$, $R^2 = Me$, $R^3 = O$, $R^4 = CO_2Me$

323 $R^1 = OH$, $R^2 = Et$, $R^3 = H,H$ $R^4 = Me$



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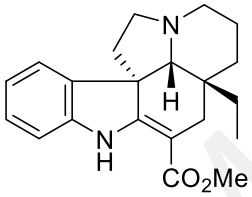

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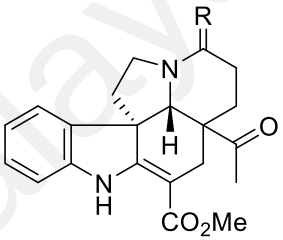
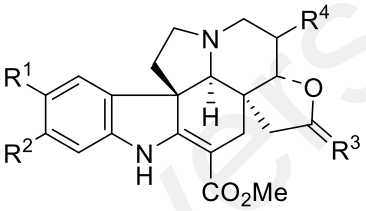


326 R = H,H

327 R = O



328 $R^1 = R^2 = R^4 = H$, $R^3 = O$

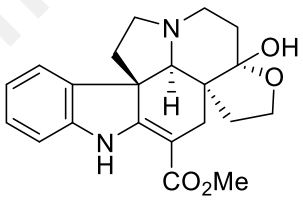
329 $R^1 = R^2 = R^4 = H$, $R^3 = H,H$

330 $R^1 = R^2 = H$, $R^3 = O$, $R^4 = OH$

331 $R^1 = R^4 = H$, $R^2 = OMe$, $R^3 = H,H$

332 $R^1 = R^2 = H$, $R^3 = H,H$, $R^4 = \beta\text{-}OH$

333 $R^1 = OH$, $R^2 = OMe$, $R^3 = H,H$, $R^4 = H$



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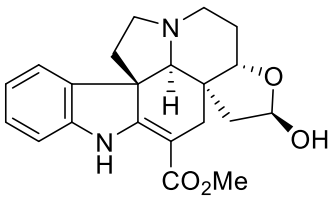

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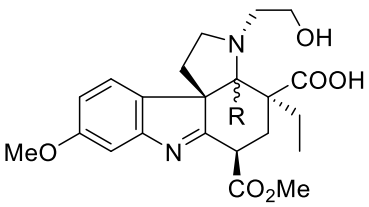
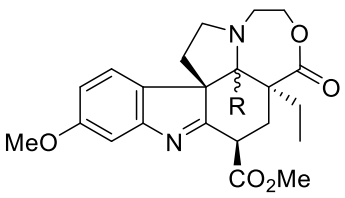
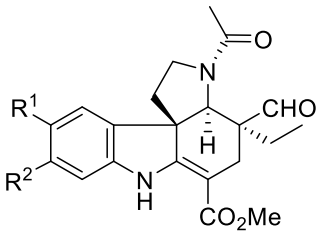
Figure 1.8, continued



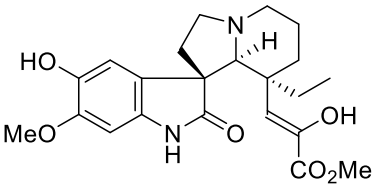
336 R = α-H
337 R = β-H



338 R = α-H
339 R = β-H



340 R^1 = OH, R^2 = OMe
341 R^1 = R^2 = H



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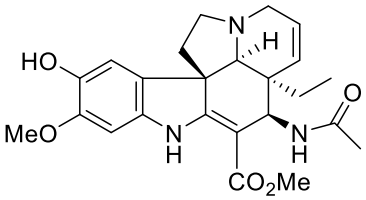

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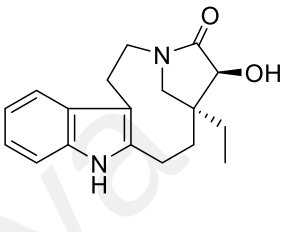

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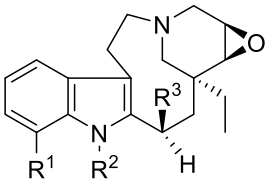
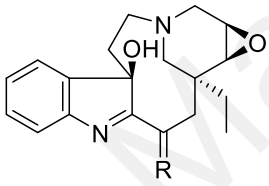
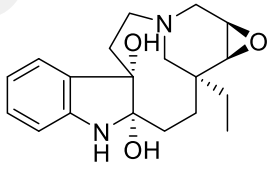


55 R^1 = R^2 = R^3 = H
345 R^1 = R^3 = H, R^2 = Me
346 R^1 = OMe, R^2 = R^3 = H
347 R^1 = R^2 = H, R^3 = OH
348 R^1 = H, R^2 = Me, R^3 = OH



56 R = H,H
349 R = O



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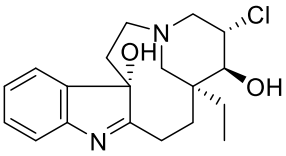

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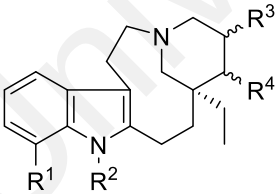
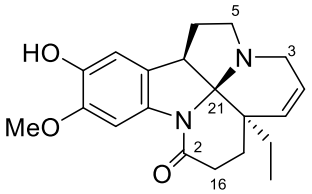


352 R^1 = R^2 = R^3 = R^4 = H
353 R^1 = R^2 = R^4 = H, R^3 = β-OH
354 R^1 = OMe, R^2 = H, R^3 = β-OH, R^4 = α-OH
355 R^1 = OMe, R^2 = H, R^3 = β-OH, R^4 = α-Cl
356 R^1 = H, R^2 = Me, R^3 = β-OH, R^4 = α-Cl
357 R^1 = H, R^2 = Me, R^3 = α-OH, R^4 = β-OH
358 R^1 = H, R^2 = Me, R^3 = α-OMe, R^4 = β-OH
57 R^1 = R^2 = H, R^3 = R^4 = OH
359 R^1 = H, R^2 = Me, R^3 = R^4 = β-OH

Figure 1.8, continued



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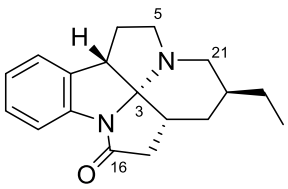

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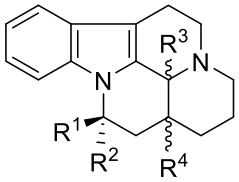
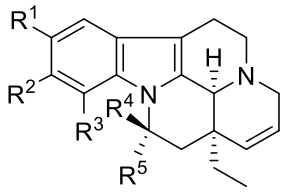
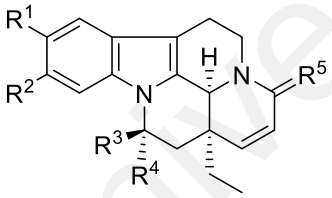


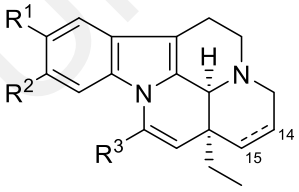
362 R^1 = OH, R^2 = CO_2Me, R^3 = α-H, R^4 = β-Et
363 R^1 = CO_2Me, R^2 = OH, R^3 = β-H, R^4 = α-Et
364 R^1 = OH, R^2 = CO_2Me, R^3 = β-H, R^4 = β-Et
365 R^1 = CO_2Me, R^2 = OH, R^3 = α-H, R^4 = α-Et
366 R^1 = OH, R^2 = CO_2Me, R^3 = β-H, R^4 = α-Et
367 R^1 = CO_2Me, R^2 = OH, R^3 = α-H, R^4 = β-Et



59 R^1 = R^2 = R^3 = H, R^4 = CO_2Me, R^5 = OH
368 R^1 = R^2 = H, R^3 = OMe, R^4 = OH, R^5 = CO_2Me
369 R^1 = OH, R^2 = OMe, R^3 = H, R^4 = OH, R^5 = CO_2Me
370 R^1 = R^2 = OMe, R^3 = H, R^4 = CO_2Me, R^5 = OH
371 R^1 = OH, R^2 = OMe, R^3 = H, R^4 = CO_2Me, R^5 = OH
372 R^1 = R^2 = OMe, R^3 = H, R^4 = CO_2Me, R^5 = OH, N(4)→O
373 R^1 = R^2 = OMe, R^3 = H, R^4 = OH, R^5 = CO_2Me
374 R^1 = R^2 = R^3 = OMe, R^4 = OH, R^5 = CO_2Me
375 R^1 = OH, R^2 = R^3 = H, R^4 = OH, R^5 = CO_2Me
376 R^1 = OH, R^2 = OMe, R^3 = H, R^4 = OH, R^5 = CO_2H
377 R^1 = R^2 = OMe, R^3 = H, R^4 = OH, R^5 = CO_2Me, N(4)→O

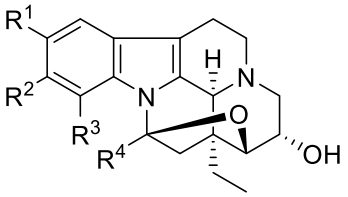


378 R^1 = R^2 = H, R^3 = CO_2Me, R^4 = OH, R^5 = α-H,β-CH_2COMe
379 R^1 = R^2 = OMe, R^3 = CO_2Me, R^4 = OH, R^5 = α-H,β-CH_2COMe
380 R^1 = R^2 = OMe, R^3 = OH, R^4 = CO_2Me, R^5 = O



381 R^1 = R^2 = H, R^3 = CO_2Me
382 R^1 = R^2 = OMe, R^3 = H, $\Delta^{14,15}$
383 R^1 = R^2 = OMe, R^3 = CO_2Me, $\Delta^{14,15}$
384 R^1 = OMe, R^2 = H, R^3 = CO_2Me, $\Delta^{14,15}$

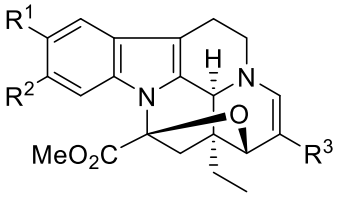
Figure 1.8, continued



385 $R^1 = R^2 = H$, $R^3 = OMe$, $R^4 = H$

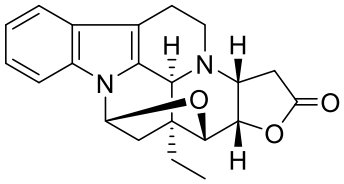
386 $R^1 = OMe$, $R^2 = R^3 = H$

387 $R^1 = OH$, $R^2 = OMe$, $R^3 = CO_2Me$



388 $R^1 = R^2 = OMe$, $R^3 = H$

389 $R^1 = R^2 = H$, $R^3 = CHO$



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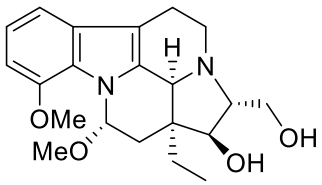

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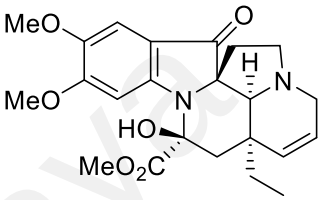

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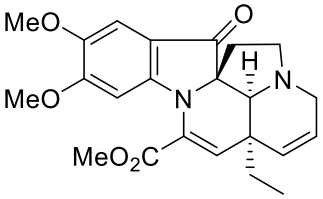

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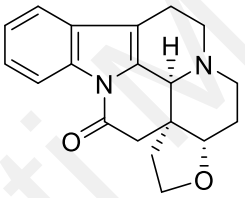

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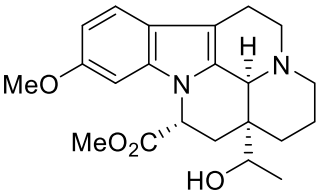

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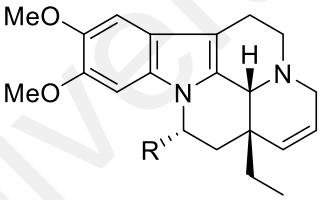
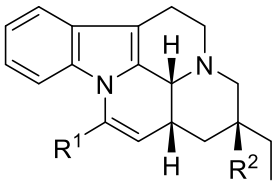


396 R = OMe

397 R = OH



398 $R^1 = CO_2Me$, $R^2 = H$

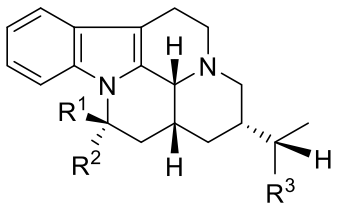
399 $R^1 = R^2 = H$

400 $R^1 = R^2 = H$, N(4)→O

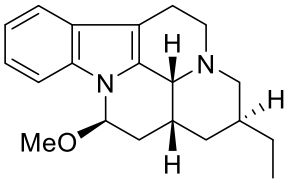
401 $R^1 = H$, $R^2 = OH$

402 $R^1 = H$, $R^2 = OH$, N(4)→O

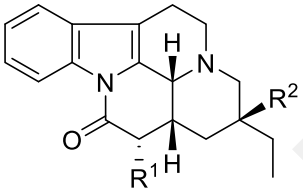
Figure 1.8, continued



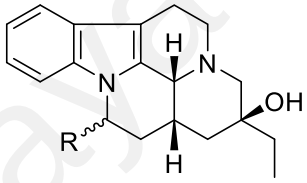
403 R^1 = OH, R^2 = CO_2Me, R^3 = H, N(4)→O
404 R^1 = CO_2Me, R^2 = OH, R^3 = H
405 R^1 = OH, R^2 = CO_2Me, R^3 = H
406 R^1 = R^3 = OH, R^2 = CO_2Me, N(4)→O
407 R^1 = CO_2Me, R^2 = R^3 = OH
408 R^1 = CO_2Me, R^2 = R^3 = OH, N(4)→O
409 R^1 = OH, R^2 = R^3 = H
410 R^1 = OMe, R^2 = R^3 = H
411 R^1 = R^3 = H, R^2 = OH
412 R^1 = R^3 = H, R^2 = OMe



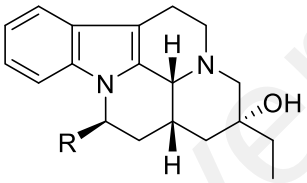
413



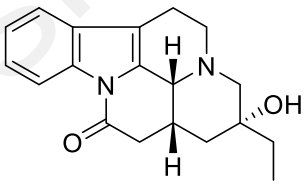
414 R^1 = R^2 = H, N(4)→O
415 R^1 = R^2 = H
416 R^1 = OH, R^2 = H
417 R^1 = H, R^2 = OH



418 R = α-OH
419 R = α-OH, N(4)→O
420 R = β-OMe
421 R = β-OH
422 R = β-OH, N(4)→O



423 R = OMe
424 R = OH



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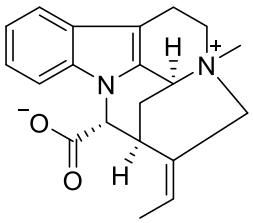

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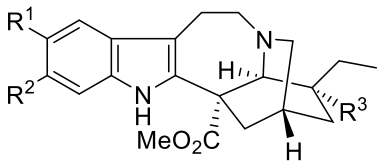
Figure 1.8, continued



14 $R^1 = R^2 = R^3 = H$

427 $R^1 = OH$, $R^2 = R^3 = H$

428 $R^1 = R^3 = H$, $R^2 = OH$

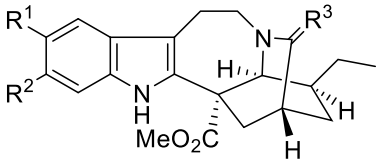
23 $R^1 = OMe$, $R^2 = R^3 = H$

429 $R^1 = OMe$, $R^2 = R^3 = H$, N(4)→O

430 $R^1 = R^3 = H$, $R^2 = OMe$

25 $R^1 = R^2 = OMe$, $R^3 = H$

431 $R^1 = R^2 = OMe$, $R^3 = OH$



432 $R^1 = R^2 = H$, $R^3 = H,OH,(R/S)$

433 $R^1 = R^2 = H$, $R^3 = H,OEt,(R/S)$

19 $R^1 = R^2 = H$, $R^3 = O$

434 $R^1 = R^2 = H$, $R^3 = H,CH_2COMe,(R/S)$

435 $R^1 = R^2 = H$, $R^3 = H,OMe,(R)$

436 $R^1 = H$, $R^2 = OMe$, $R^3 = H,OH,(R/S)$

437 $R^1 = OMe$, $R^2 = H$, $R^3 = O$

438 $R^1 = OMe$, $R^2 = H$, $R^3 = H,OH,(R/S)$

439 $R^1 = OMe$, $R^2 = H$, $R^3 = H,OMe,(R)$

440 $R^1 = R^2 = OMe$, $R^3 = O$

441 $R^1 = R^2 = OMe$, $R^3 = H,OH,(R/S)$

442 $R^1 = R^2 = H$, $R^3 = H,CH(OH)Me,(S)$

443 $R^1 = H$, $R^2 = OMe$, $R^3 = H,CH(OH)Me,(S)$

444 $R^1 = OMe$, $R^2 = H$, $R^3 = H,OH,(R)$

21 $R^1 = R^2 = H$, $R^3 = H,CH_2OH,(S)$

445 $R^1 = OMe$, $R^2 = H$, $R^3 = H,CH_2OAc,(S)$

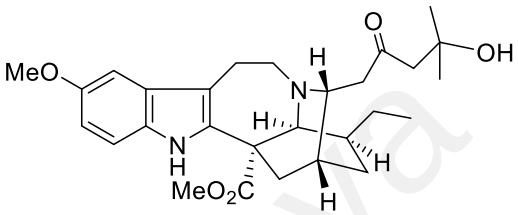
446 $R^1 = R^2 = H$, $R^3 = H,CO_2Me,(S)$

447 $R^1 = OMe$, $R^2 = H$, $R^3 = H,CO_2Me,(S)$

448 $R^1 = OMe$, $R^2 = H$, $R^3 = H,CH_2COMe,(S)$

449 $R^1 = H$, $R^2 = OMe$, $R^3 = H,CH_2COMe,(S)$

450 $R^1 = OMe$, $R^2 = H$, $R^3 = H,CH_2OH,(R)$



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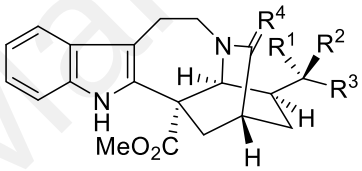


16 $R^1 = H$, $R^2 = OH$, $R^3 = Me$, $R^4 = H,H$

17 $R^1 = OH$, $R^2 = H$, $R^3 = Me$, $R^4 = H,H$

452 $R^1 = H$, $R^2 = OH$, $R^3 = Me$, $R^4 = O$

453 $R^1 = OH$, $R^2 = H$, $R^3 = Me$, $R^4 = H,CH_2COMe$, (R/S)

18 $R^1 = OH$, $R^2 = H$, $R^3 = Me$, $R^4 = O$

454 $R^1 = H$, $R^2 = OH$, $R^3 = Me$, $R^4 = H,OEt,(R/S)$

455 $R^1 = OH$, $R^2 = H$, $R^3 = Me$, $R^4 = H,OEt,(R/S)$

456 $R^1 = R^2 = H$, $R^3 = Me$, $R^4 = H,CH_2Ac,(R/S)$

457 $R^1 = OH$, $R^2 = H$, $R^3 = Me$, $R^4 = H,CH_2Ac,(R/S)$

458 $R^1 = H$, $R^2 = OH$, $R^3 = CH_2OH$, $R^4 = H,H$

7 $R^1 = OH$, $R^2 = H$, $R^3 = CH_2OH$, $R^4 = H,H$

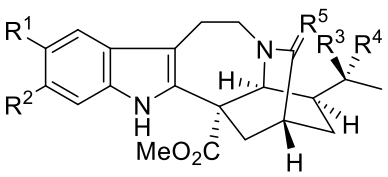
3 $R^1 = OH$, $R^2 = H$, $R^3 = Me$, $R^4 = H,CH_2OH,(S)$

4 $R^1 = OH$, $R^2 = H$, $R^3 = Me$, $R^4 = H,CH_2CHO,(S)$

5 $R^1 = R^2 = H$, $R^3 = Me$, $R^4 = H,CH_2CHO,(S)$

6 $R^1 = R^2 = H$, $R^3 = CH_2OH$, $R^4 = O$

Figure 1.8, continued



459 $R^1 = R^3 = OH$, $R^2 = R^4 = H$, $R^5 = H,H$

460 $R^1 = R^4 = H$, $R^2 = R^3 = OH$, $R^5 = H,H$

461 $R^1 = OMe$, $R^2 = R^4 = H$, $R^3 = OH$, $R^5 = O$

462 $R^1 = OMe$, $R^2 = R^3 = H$, $R^4 = OH$, $R^5 = O$

463 $R^1 = OMe$, $R^2 = R^4 = H$, $R^3 = OH$, $R^5 = H,OH,(R/S)$

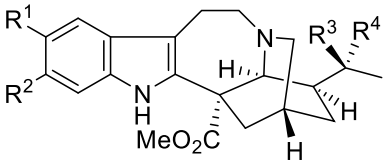
464 $R^1 = OMe$, $R^2 = R^3 = R^4 = H$, $R^5 = H,OEt,(R/S)$

465 $R^1 = R^3 = H$, $R^2 = OMe$, $R^4 = OH$, $R^5 = H,CH_2COMe,(R)$

466 $R^1 = OMe$, $R^2 = R^3 = H$, $R^4 = OH$, $R^5 = H,CH_2COMe,(R)$

467 $R^1 = OMe$, $R^2 = R^4 = H$, $R^3 = OH$, $R^5 = H,CH_2COMe,(R)$

468 $R^1 = R^4 = H$, $R^2 = OMe$, $R^3 = OH$, $R^5 = H,CH_2COMe,(R)$



469 $R^1 = OMe$, $R^2 = H$, $R^3,R^4 = O$

24 $R^1 = OMe$, $R^2 = R^4 = H$, $R^3 = OH$

470 $R^1 = OMe$, $R^2 = R^3 = H$, $R^4 = OH$

471 $R^1 = R^3 = H$, $R^2 = OMe$, $R^4 = OH$

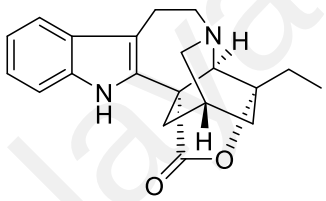
472 $R^1 = R^2 = OMe$, $R^3 = OH$, $R^4 = H$

26 $R^1 = R^2 = OMe$, $R^3 = H$, $R^4 = OH$

473 $R^1 = H$, $R^2 = OMe$, $R^3,R^4 = O$

474 $R^1 = R^4 = H$, $R^2 = OMe$, $R^3 = OH$

475 $R^1 = R^2 = H$, $R^3,R^4 = O$



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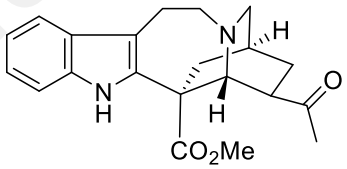

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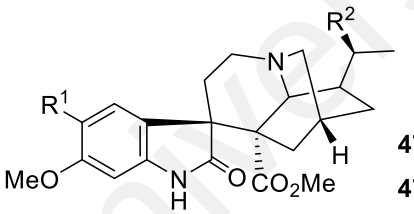
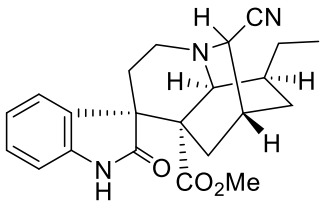


477 $R^1 = OMe$, $R^2 = H$

478 $R^1 = H$. $R^2 = OH$



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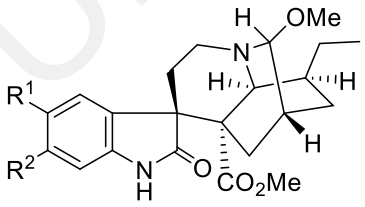
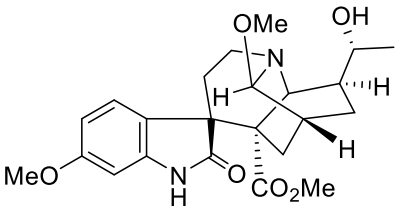


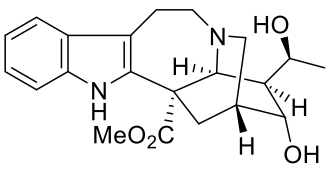
480 $R^1 = H$, $R^2 = OMe$

481 $R^1 = OMe$, $R^2 = H$



482

Figure 1.8, continued



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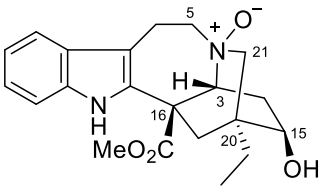

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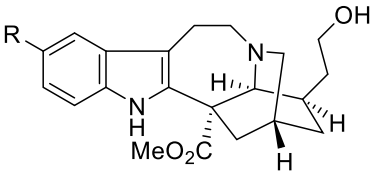
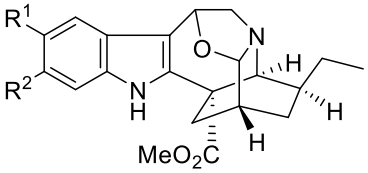
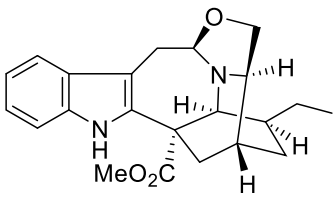


15 R = H
485 R = OMe



486 $R^1 = R^2 = H$
487 $R^1 = H$, $R^2 = OMe$
488 $R^1 = OMe$, $R^2 = H$
489 $R^1 = OMe$, $R^2 = H$, N(4)→O



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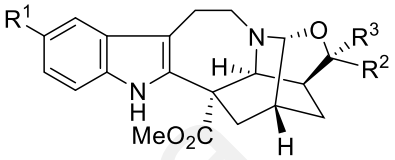
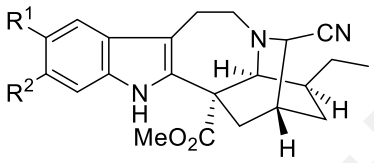
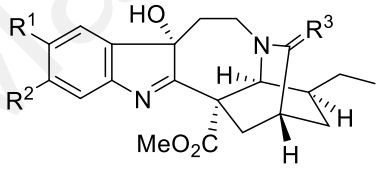


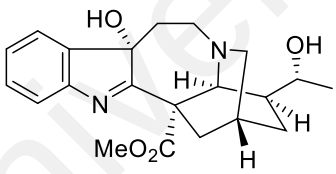
491 $R^1 = OMe$, $R^2 = Me$, $R^3 = H$
492 $R^1 = R^2 = H$, $R^3 = Me$
493 $R^1 = R^3 = H$, $R^2 = Me$



20 $R^1 = R^2 = H$
494 $R^1 = H$, $R^2 = OMe$
495 $R^1 = OMe$, $R^2 = H$

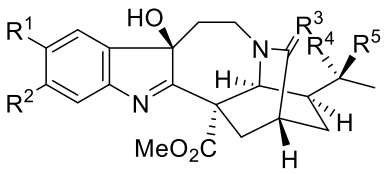


496 $R^1 = R^2 = H$, $R^3 = H,OH$ (*S*)
497 $R^1 = R^2 = H$, $R^3 = H,CN$ (*S*)
498 $R^1 = R^2 = H$, $R^3 = H,OH$ (*R*)
499 $R^1 = R^2 = H$, $R^3 = H,H$
500 $R^1 = OH$, $R^2 = H$, $R^3 = H,H$
501 $R^1 = H$, $R^2 = OMe$, $R^3 = H,H$
502 $R^1 = R^2 = H$, $R^3 = O$
503 $R^1 = OMe$, $R^2 = H$, $R^3 = H,CH_2COMe,(R)$
504 $R^1 = H$, $R^2 = OMe$, $R^3 = H,CH_2COMe,(R)$



505

Figure 1.8, continued



29 $R^1 = R^2 = R^4 = R^5 = H$, $R^3 = H,H$

506 $R^1 = R^2 = R^4 = R^5 = H$, $R^3 = H,CH_2Ac$

507 $R^1 = OMe$, $R^2 = R^4 = R^5 = H$, $R^3 = H,H$

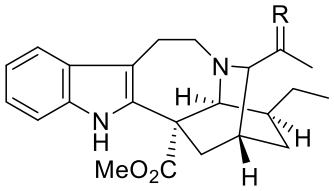
508 $R^1 = OMe$, $R^2 = R^4 = H$, $R^3 = H,H$, $R^5 = OH$

509 $R^1 = OMe$, $R^2 = R^4 = R^5 = H$, $R^3 = H,H$

510 $R^1 = R^2 = R^4 = R^5 = H$, $R^3 = O$

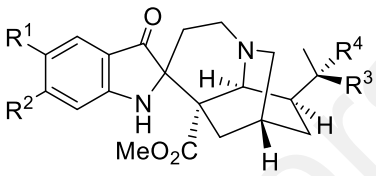
511 $R^1 = R^2 = OMe$, $R^3 = H,H$, $R^5 = H$, $R^4 = OH$

512 $R^1 = R^2 = R^4 = H$, $R^3 = H,H$, $R^5 = OH$



518 R = H,OH,(*S*)

519 R = H,OH,(*R*)



27 $R^1 = R^2 = R^3 = R^4 = H$

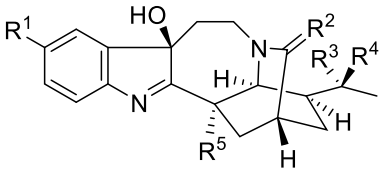
520 $R^1 = OMe$, $R^2 = R^3 = R^4 = H$

521 $R^1 = OMe$, $R^2 = R^4 = H$, $R^3 = OH$

522 $R^1 = R^2 = OMe$, $R^3 = R^4 = H$

523 $R^1 = R^3 = H$, $R^2 = OMe$, $R^4 = OH$

524 $R^1 = R^2 = R^4 = H$, $R^3 = OH$

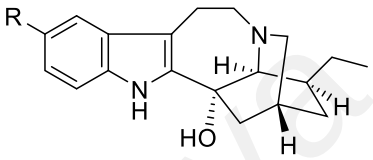


513 $R^1 = OMe$, $R^2 = H,H$, $R^3 = R^4 = R^5 = H$

514 $R^1 = OMe$, $R^2 = H,H$, $R^3 = R^5 = H$, $R^4 = OH$

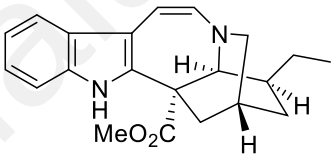
515 $R^1 = R^5 = H$, $R^2 = O$, $R^3,R^4 = O$

516 $R^1 = R^3 = R^4 = H$, $R^2 = O$, $R^5 = CO_2Me$



154 R = OMe

517 R = H



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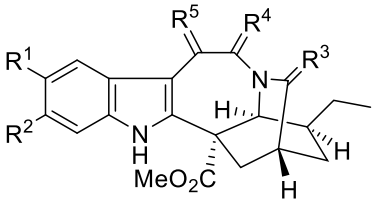


526 $R^1 = R^2 = H$, $R^3 = R^5 = H,H$, $R^4 = O$

527 $R^1 = R^2 = H$, $R^3 = H,H$, $R^4 = O$, $R^5 = H,OH,(S)$

528 $R^1 = R^2 = H$, $R^3 = H,H$, $R^4 = O$, $R^5 = H,OMe,(S)$

529 $R^1 = R^2 = H$, $R^3 = R^4 = H,H$, $R^5 = O$

530 $R^1 = R^2 = H$, $R^3 = H,H$, $R^4 = H,OH$, $R^5 = O$

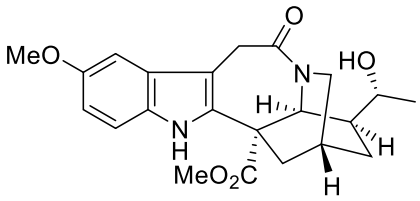
531 $R^1 = R^2 = H$, $R^3 = O$, $R^4 = H,H$, $R^5 = H,OH$

532 $R^1 = H$, $R^2 = OMe$, $R^3 = O$, $R^4 = H,H$, $R^5 = H,OH$

533 $R^1 = OMe$, $R^2 = OH$, $R^3 = H,H$, $R^4 = R^5 = O$

534 $R^1 = R^2 = OMe$, $R^3 = H,H$, $R^4 = R^5 = O$

Figure 1.8, continued



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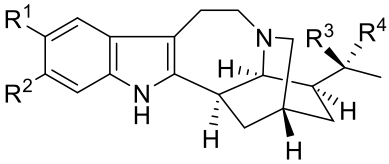


546 R^1 = OMe, R^2 = R^3 = H, R^4 = OH

12 R^1 = R^2 = R^4 = H, R^3 = OH

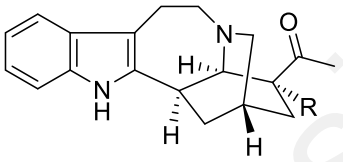
547 R^1 = OMe, R^2 = R^4 = H, R^3 = OH

548 R^1 = OMe, R^2 = R^4 = H, R^3 = OH, N(4)→O

549 R^1 = R^2 = OMe, R^3 = OH, R^4 = H

13 R^1 = R^2 = R^3 = H, R^4 = OH

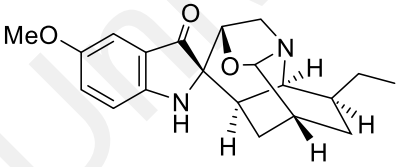
550 R^1 = R^2 = OMe, R^3 = H, R^4 = OH



553 R = α-H

554 R = β-H

555 R = β-H, N(4)→O



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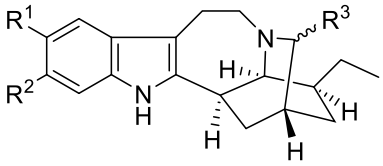


536 R^1 = OMe, R^2 = R^3 = H

11 R^1 = R^2 = R^3 = H

537 R^1 = OMe, R^2 = R^3 = H, N(4)→O

538 R^1 = R^3 = H, R^2 = OMe

539 R^1 = R^2 = OMe, R^3 = H

540 R^1 = H, R^2 = OMe, R^3 = OH,(*R*/*S*)

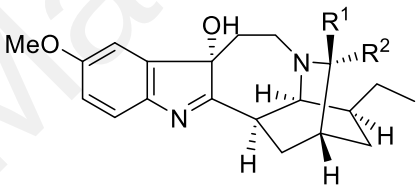
541 R^1 = OMe, R^2 = H, R^3 = OH,(*R*)

542 R^1 = R^2 = H, R^3 = CH_2OH,(*S*)

543 R^1 = OMe, R^2 = H, R^3 = α-CH_2COMe

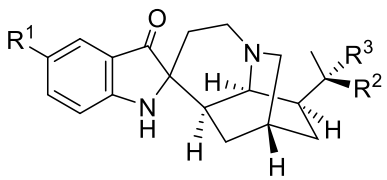
544 R^1 = R^2 = H, R^3 = CH(OH)Me,(*S*)

545 R^1 = R^2 = H, R^3 = CH_2CO_2Me,(*R*)



551 R^1,R^2 = O

552 R^1 = H, R^2 = CH_2Ac

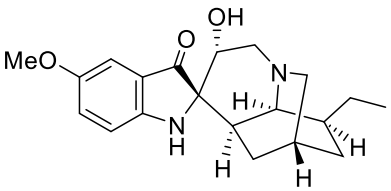


556 R^1 = OMe, R^2 = R^3 = H

557 R^1 = R^2 = R^3 = H

558 R^1 = R^2 = H, R^3 = OH

Figure 1.8, continued



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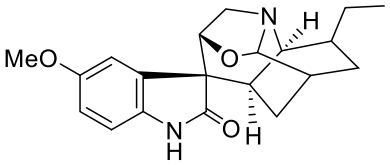

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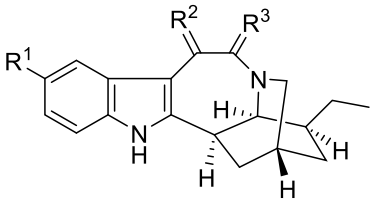
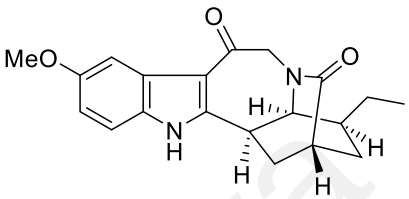


562 R^1 = H, R^2 = R^3 = O

563 R^1 = OMe, R^2 = R^3 = O

564 R^1 = OMe, R^2 = O, R^3 = H,H



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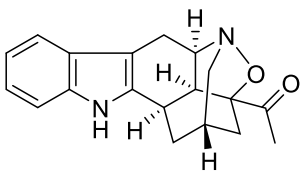

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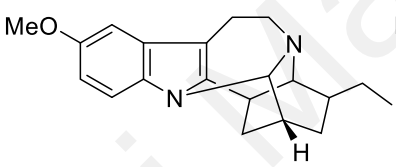

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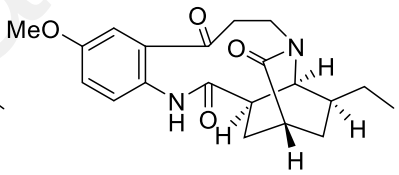

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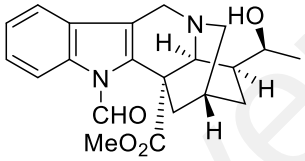

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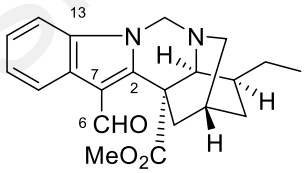

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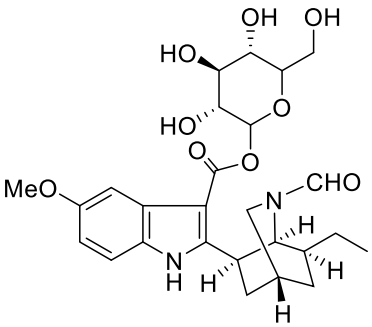

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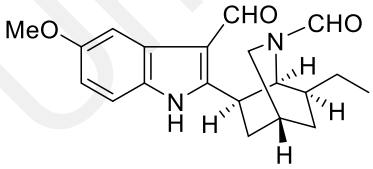

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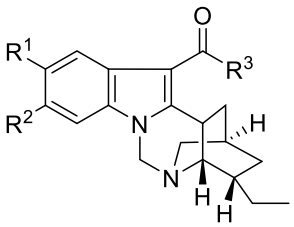
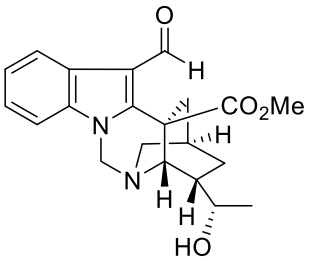


573 R^1 = OMe, R^2 = R^3 = H

574 R^1 = OMe, R^2 = H, R^3 = CH_2OH

575 R^1 = R^3 = H, R^2 = OMe

Figure 1.8, continued



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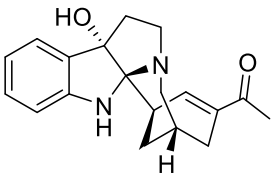

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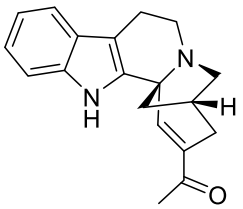

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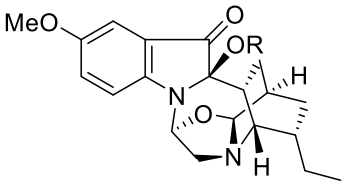
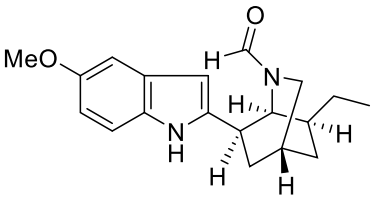


579 R = H

580 R = Me



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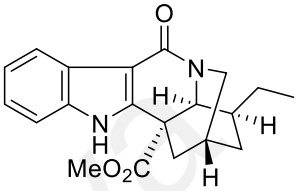

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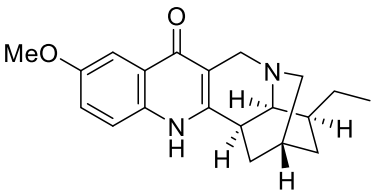

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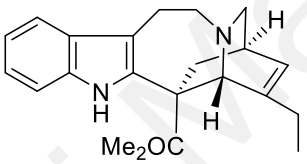

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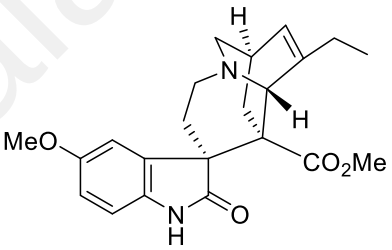

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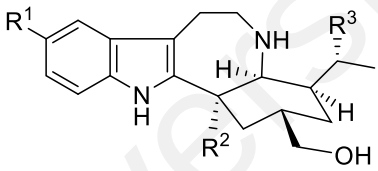
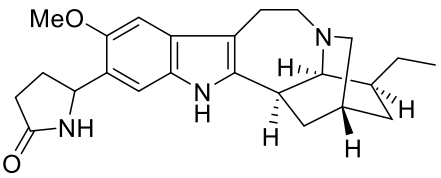


22 $R^1 = R^3 = H$, $R^2 = CO_2Me$

2 $R^1 = H$, $R^2 = CO_2Me$, $R^3 = OH$

586 $R^1 = OMe$, $R^2 = R^3 = H$



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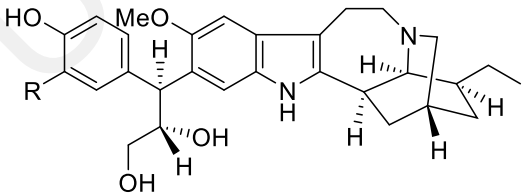
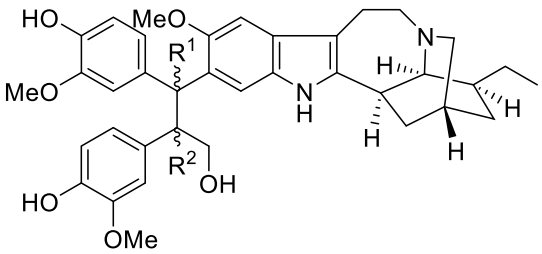


588 R = OMe

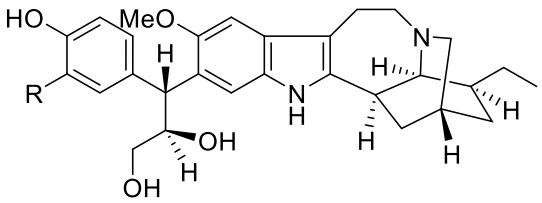
589 R = H



590 R^1 = α-H, R^2 = β-H

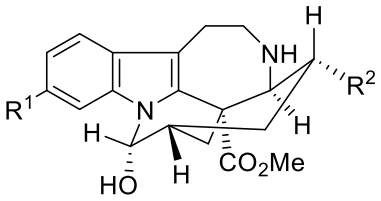
591 R^1 = β-H, R^2 = α-H

Figure 1.8, continued



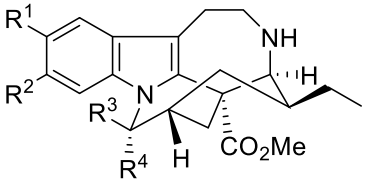
592 R = OMe

593 R = H



594 R^1 = OMe, R^2 = $CH_3CH(OH)$

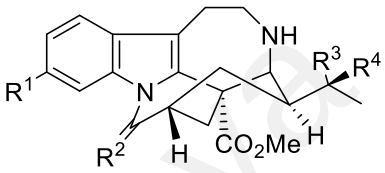
595 R^1 = H, R^2 = CH_3CO



596 R^1 = R^2 = OMe, R^3 = OH, R^4 = H

31 R^1 = R^2 = R^4 = H, R^3 = OH

32 R^1 = R^2 = R^3 = H, R^4 = OH

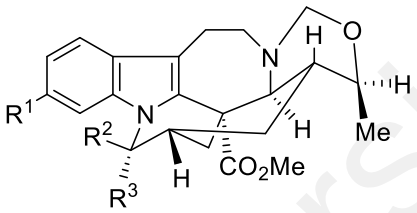


597 R^1 = OMe, R^2 = H,H, R^3 = R^4 = H

598 R^1 = OMe, R^2 = H,H, R^3 = H, R^4 = OH

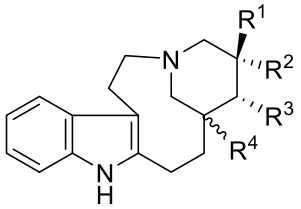
599 R^1 = OMe, R^2 = O, R^3 = R^4 = H

600 R^1 = R^3 = H, R^2 = H,H, R^4 = OH



601 R^1 = R^2 = H, R^3 = OH

602 R^1 = OMe, R^2,R^3 = O

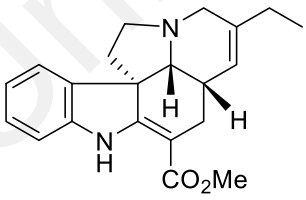


603 R^1 = R^3 = H, R^2 = Et, R^4 = β-H

604 R^1 = OH, R^2 = Et, R^3 = H, R^4 = α-H

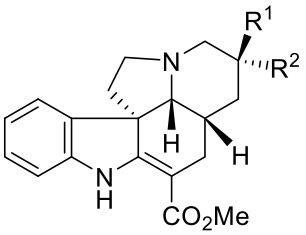
605 R^1 = Et, R^2 = R^3 = H, R^4 = β-H

606 R^1 = H, R^2 = Et, R^3 = OH, R^4 = β-H

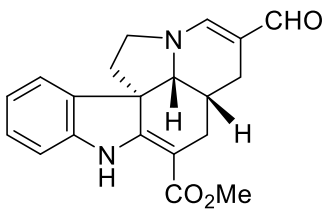


607

Figure 1.8, continued



608 R^1 = H, R^2 = Et
609 R^1 = Et, R^2 = OH
610 R^1 = OH, R^2 = Et
611 R^1 = H, R^2 = CH_2CH_2OH
612 R^1 = CH_2CH_2OH, R^2 = H
613 R^1 = CH_2CH_2OH, R^2 = H, N(4)→O
614 R^1 = H, R^2 = $CH(OH)CH_2OH$
615 R^1 = $CH(OH)CH_2OH$, R^2 = H
616 R^1 = H, R^2 = CH(OH)Me
617 R^1 = H, R^2 = CH(OH)Me, N(4)→O
618 R^1 = OH, R^2 = CH(OH)Me



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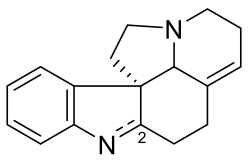
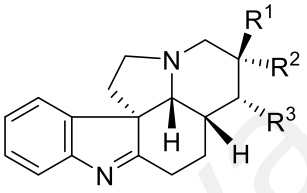
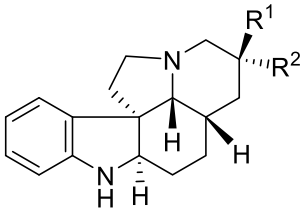


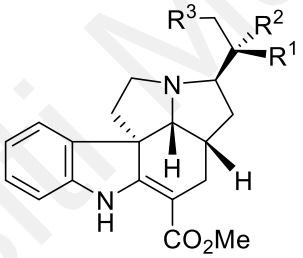
620
621 $\Delta^{1,2}$



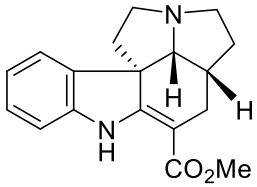
622 R^1 = R^3 = H, R^2 = Et
623 R^1 = Et, R^2 = R^3 = H
624 R^1 = H, R^2 = Et, R^3 = OH
625 R^1 = OH, R^2 = Et, R^2 = H



626 R^1 = H, R^2 = Et
627 R^1 = Et, R^2 = H



628 R^1 = R^2 = R^3 = H
629 R^1 = R^2 = H, R^3 = OH
630 R^1 = OH, R^2 = R^3 = H
631 R^1 = R^3 = H, R^2 = OH



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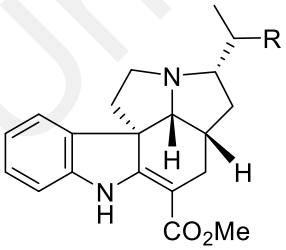
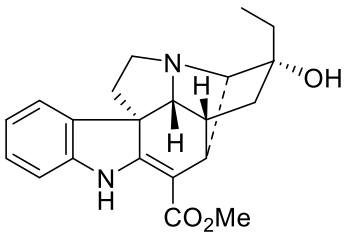


633 R = H
634 R = H, N(4)→O
635 R = OH



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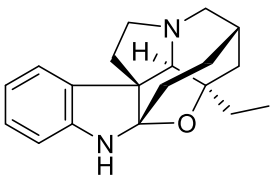

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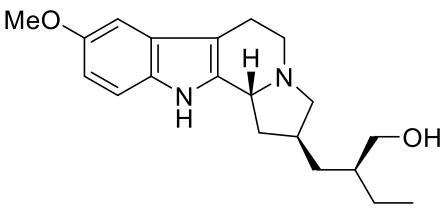
Figure 1.8, continued



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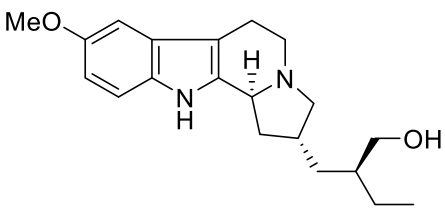

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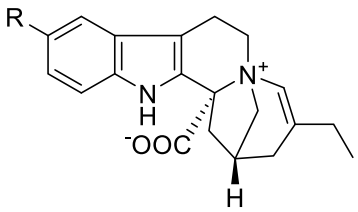
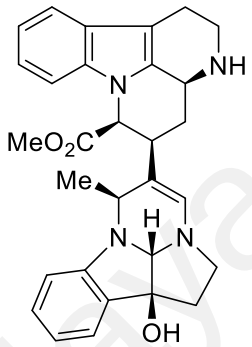


640 R = OMe

65 R = H



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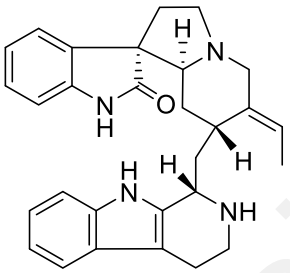

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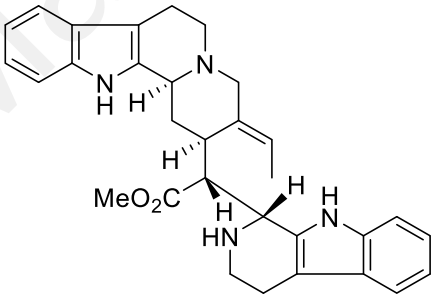

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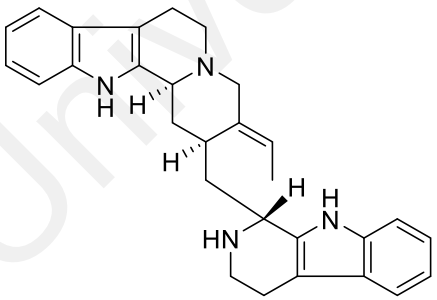

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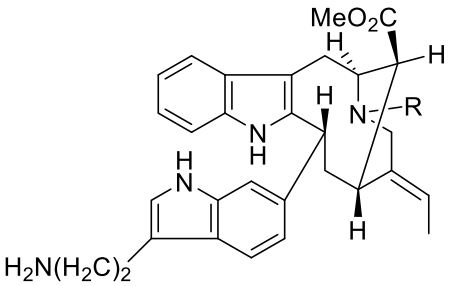
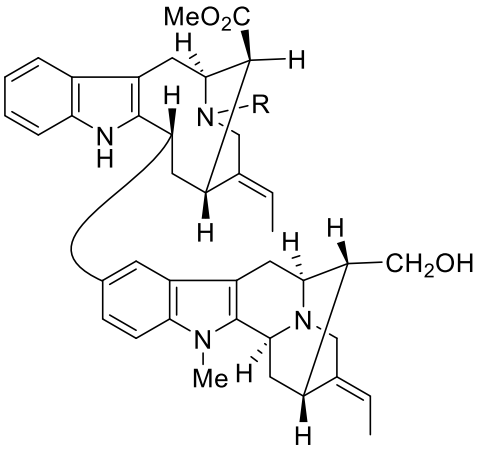


645 R = Me

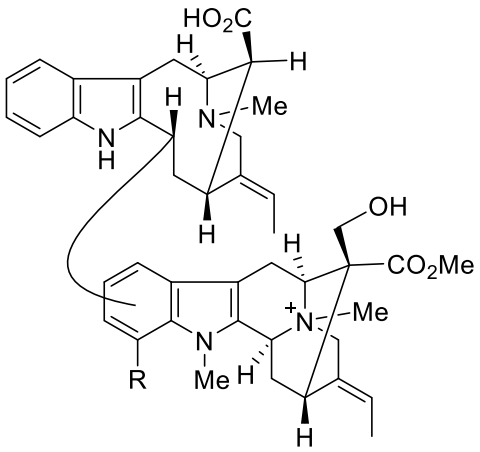
646 R = H

Figure 1.8, continued



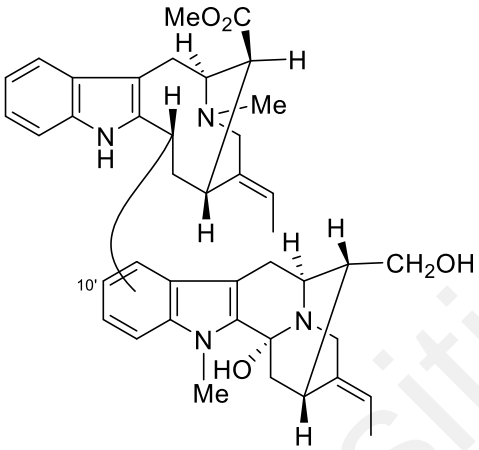
647 R = Me

648 R = H



649 R = OMe, C(3)-C(9')

650 R = OH, C(3)-C(11')



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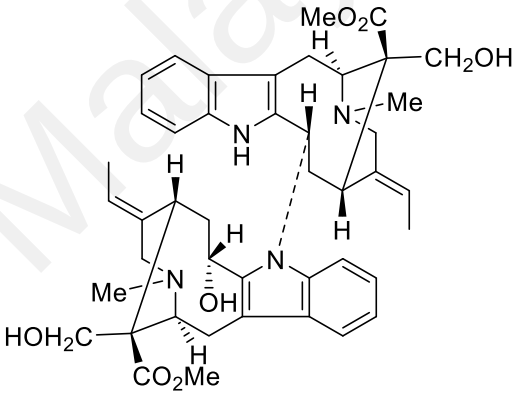

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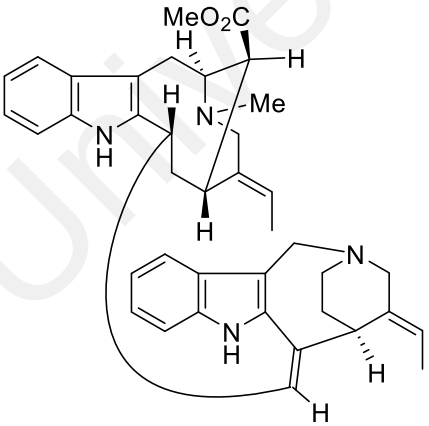

653

654 N(4')→O

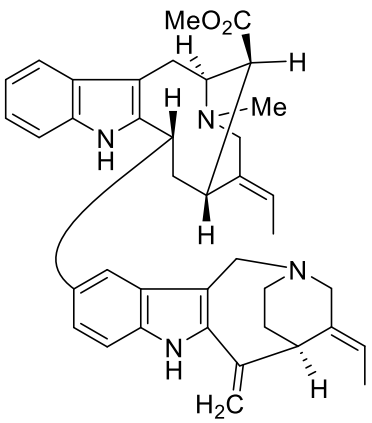

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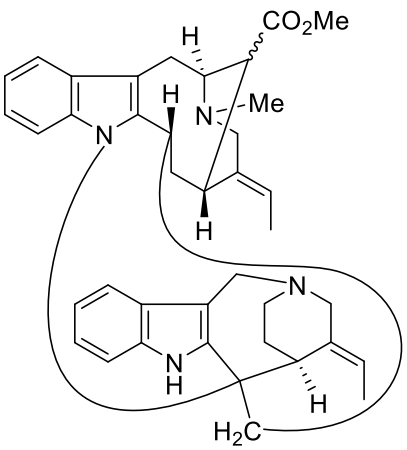
Figure 1.8, continued



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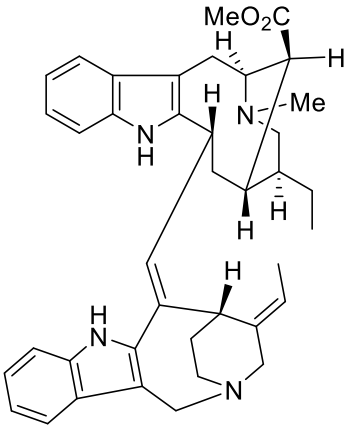

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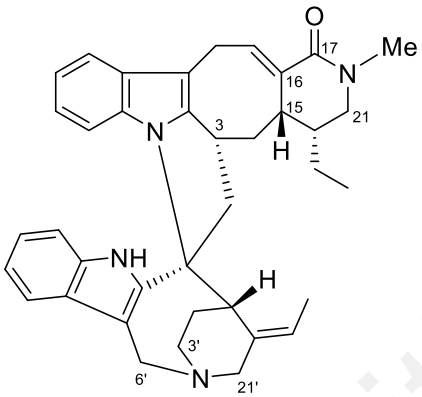

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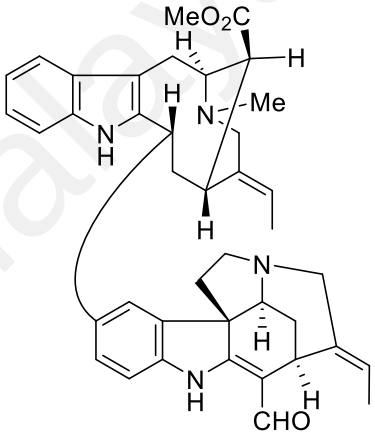

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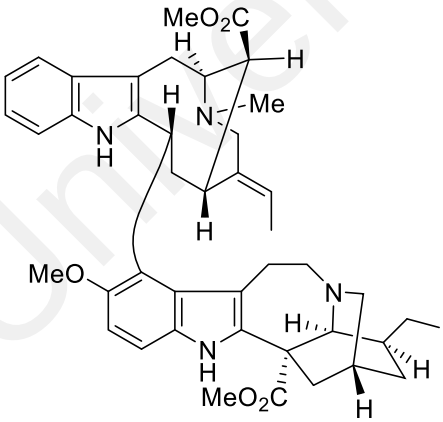

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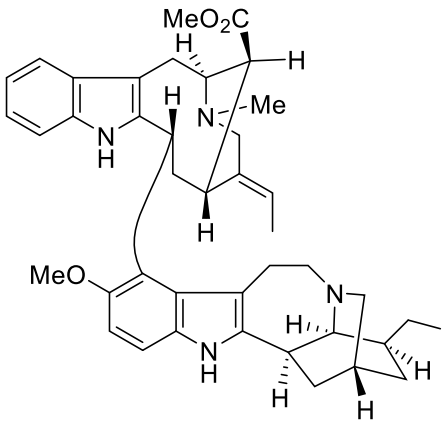

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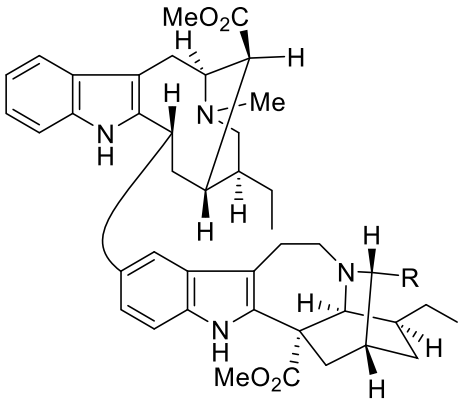
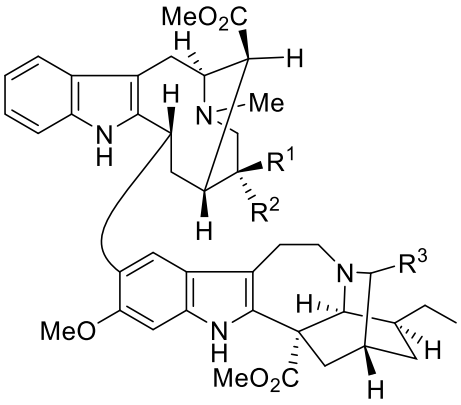
Figure 1.8, continued



662 R = H

663 R = $COCH_3$



664 R^1 = Et, R^2 = R^3= H

665 R^1 = Et, R^2 = H, R^3 = OH,(*R*/*S*)

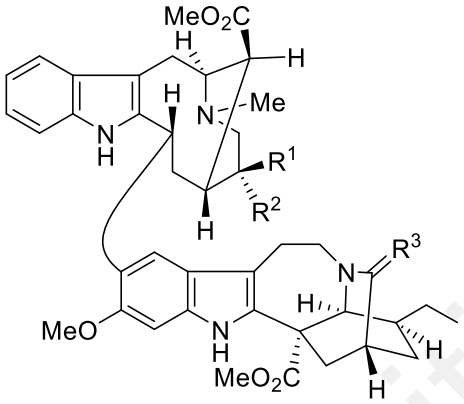
666 R^1 = R^3 = H, R^2 = Et,

667 R^1 = H, R^2 = Et, R^3 = CN

668 R^1 = Et, R^2 = H, R^3 = CH_2Ac

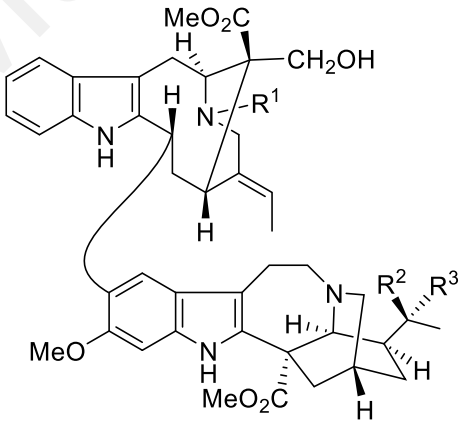
669 R^1 = Et, R^2 = H, R^3 = CHO,(*R*)

670 R^1 = H, R^2 = Et, R^3 = OH,(*R*)



671 R^1 = Et, R^2 = H, R^3 = O

672 R^1 = H, R^2 = Et, R^3 = O



673 R^1 = Me, R^2 = OH, R^3 = H

674 R^1 = Me, R^2,R^3 = O

675 R^1 = R^3 = H, R^2 = OH

676 R^1 = Me, R^2 = R^3 = H

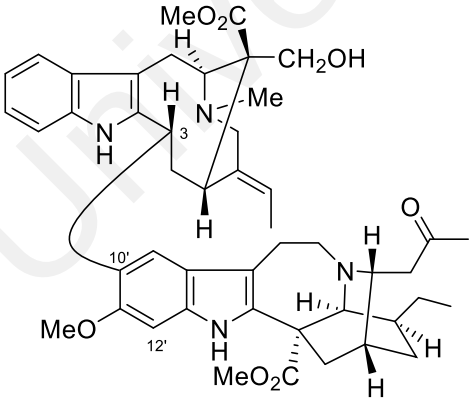


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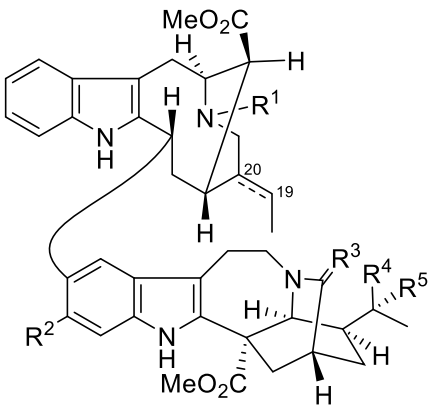
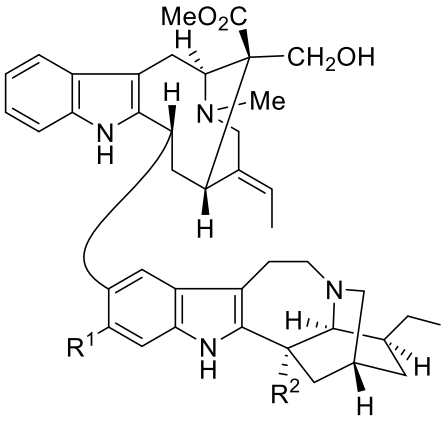
Figure 1.8, continued





678 R^1 = Me, R^2 = R^4 = R^5 = H, R^3 = H,H

679 R^1 = R^4 = R^5 = H, R^2 = OMe, R^3 = H,H

680 R^1 = R^2 = R^4 = R^5 = H, R^3 = H,H

681 R^1 = Me, R^2 = OH, R^3 = H,H, R^4 = R^5 = H

682 R^1 = Me, R^2 = OMe, R^3 = H,H, R^4 = R^5 = H

683 R^1 = Me, R^2 = OMe, R^3 = H,H, R^4 = R^5 = H, 19,20-epoxy

684 R^1 = R^2 = R^4 = R^5 = H, R^3 = H,OH,(*R*/*S*)

685 R^1 = Me, R^2 = OMe, R^3 = H,H, R^4 = H, R^5 = OH

686 R^1 = Me, R^2 = OMe, R^3 = H,OH,(*R*/*S*), R^4 = R^5 = H

687 R^1 = Me, R^2 = OMe, R^3 = H,H, R^4 = OH, R^5 = H

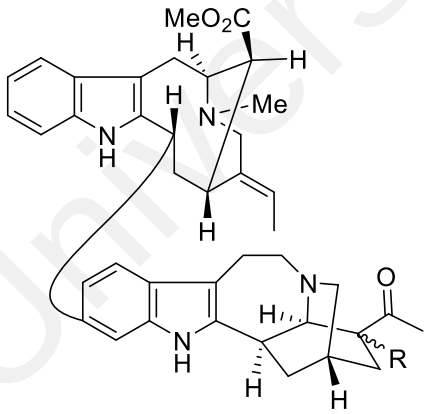
70 R^1 = Me, R^2 = R^4 = R^5 = H, R^3 = O

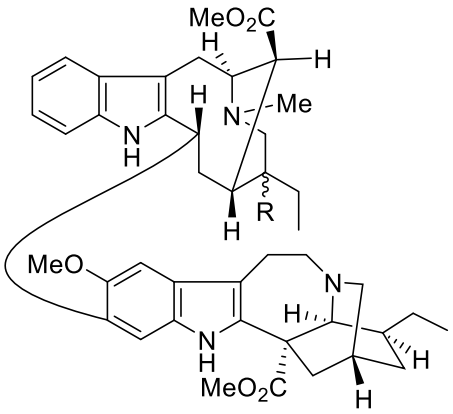
688 R^1 = Me, R^2 = R^4 = R^5 = H, R^3 = CH_2COMe

689 R^1 = Me, R^2 = R^4 = R^5 = H, R^3 = H,CH(OH)Me

690 R^1 = OMe, R^2 = H

691 R^1 = H, R^2 = CO_2Me





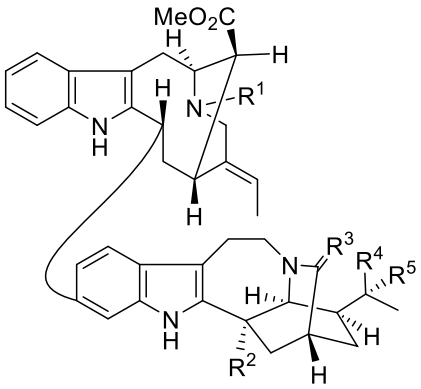
692 R = α-H

693 R = β-H

694 R = β-H

695 R = α-H

Figure 1.8, continued



67 R^1 = Me, R^2 = R^4 = R^5 = H, R^3 = H,H

696 R^1 = R^2 = R^4 = R^5 = H, R^3 = H,H

697 R^1 = Me, R^2 = R^4 = R^5 = H, R^3 = H,OH,(*R*/*S*)

698 R^1 = R^2 = R^4 = R^5 = H, R^3 = H,OH,(*R*/*S*)

68 R^1 = Me, R^2 = R^4 = H, R^3 = H,H, R^5 = OH

699 R^1 = Me, R^2 = R^5 = H, R^3 = H,H, R^4 = OH

700 R^1 = R^4 = R^5 = H, R^2 = CO_2Me, R^3 = H,H

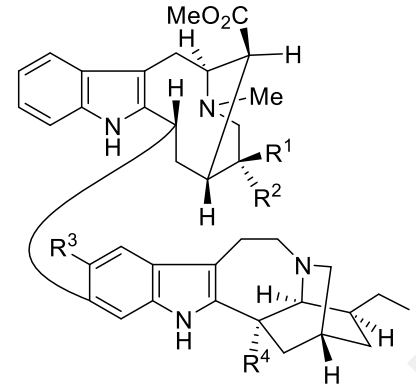
701 R^1 = Me, R^2 = CO_2Me, R^3 = H,H, R^4 = R^5 = H

702 R^1 = Me, R^2 = CO_2Me, R^3 = H,H, R^4 = OH, R^5 = H

703 R^1 = Me, R^2 = CO_2Me, R^3 = CH_2COMe, R^4 = R^5 = H

69 R^1 = Me, R^2 = CO_2Me, R^3 = O, R^4 = R^5 = H

704 R^1 = Me, R^2 = CO_2Me, R^3 = H,CH(OH)Me, R^4 = R^5 = H

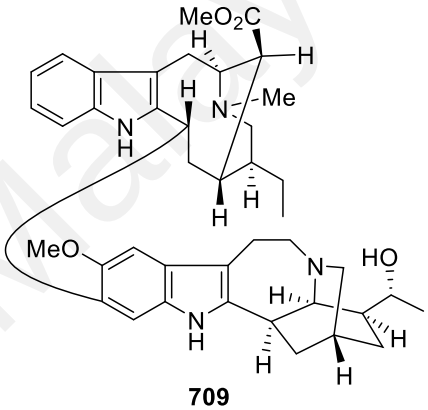


705 R^1 = Et, R^2 = R^3 = H, R^4 = CO_2Me

706 R^1 = Et, R^2 = R^3 = R^4 = H

707 R^1 = R^4 = H, R^2 = Et, R^3 = OMe

708 R^1 = Et, R^2 = R^4 = H, R^3 = OMe



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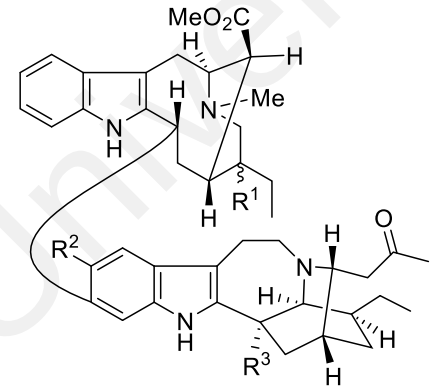
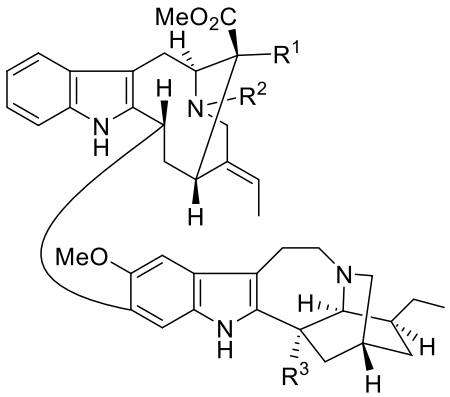


710 R^1 = α-H, R^2 = H, R^3 = CO_2Me

711 R^1 = α-H, R^2 = OMe, R^3 = CO_2Me

712 R^1 = β-H, R^2 = R^3 = H

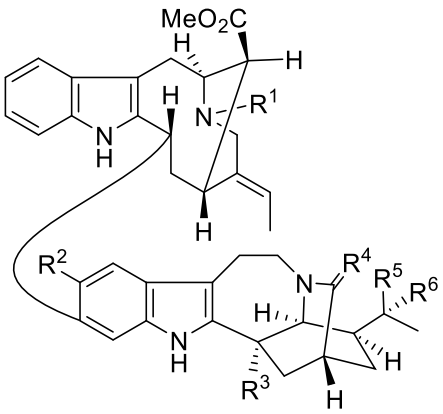


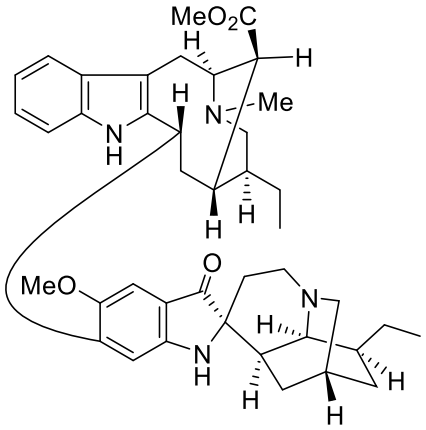
713 R^1 = CH_2OH, R^2 = Me, R^3 = CO_2Me

714 R^1 = CH_2OH, R^2 = Me, R^3 = H

715 R^1 = R^2 = R^3 = H

Figure 1.8, continued





716 R^1 = Me, R^2 = OMe, R^3 = R^5 = H, R^4 = H,H, R^6 = OH

717 R^1 = Me, R^2 = OMe, R^3 = R^5 = R^6 = H, R^4 = H,H, N(4)→O

718 R^1 = Me, R^2 = OMe, R^3 = R^5 = R^6 = H, R^4 = H,H

719 R^1 = R^2 = R^5 = R^6 = H, R^3 = CO_2Me, R^4 = H,OH,(*R*/*S*)

720 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = H,H, R^5 = R^6 = H

721 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = H,H, R^5 = R^6 = H, N(4)→O

722 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = O, R^5 = R^6 = H

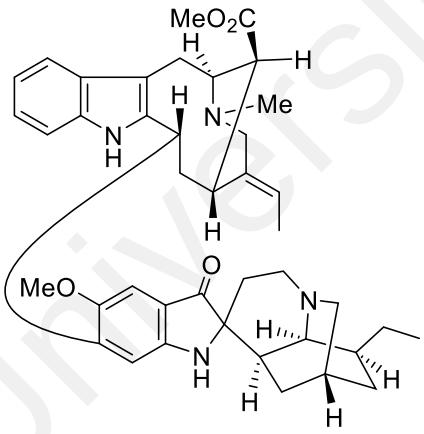
723 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = H,OH,(*R*/*S*), R^5 = R^6 = H

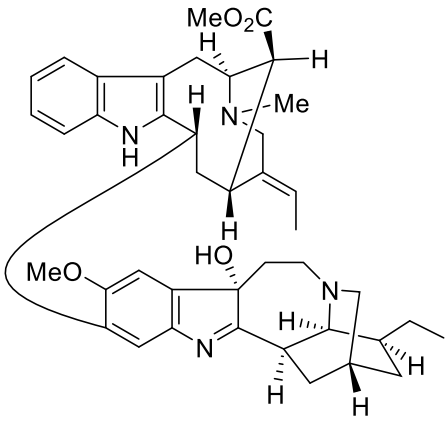
724 R^1 = R^5 = R^6 = H, R^2 = OMe, R^3 = CO_2Me, R^4 = H,H

725 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = H,H, R^5 = OH, R^6 = H

726 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = H,H, R^5 = H, R^6 = OH

727

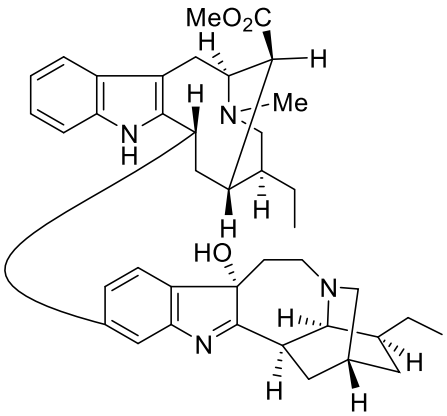




728

729

Figure 1.8, continued



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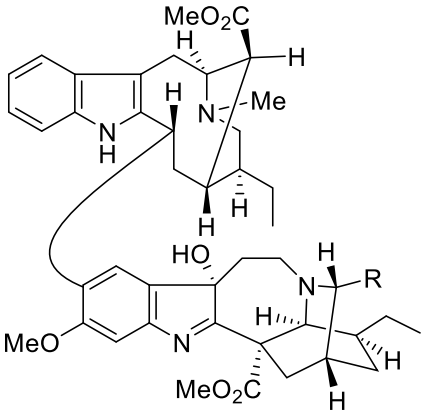
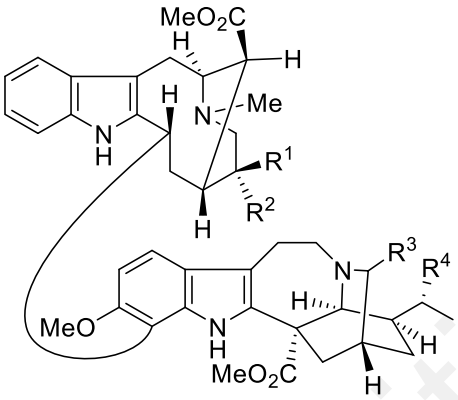


731 R = H

732 R = CH_2COMe



733 R^1 = Et, R^2 = R^3 = R^4 = H

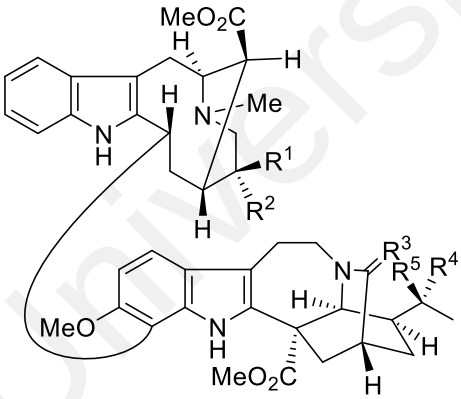
734 R^1 = R^3 = R^4 = H, R^2 = Et

735 R^1 = Et, R^2 = R^3 = H, R^4 = OH

736 R^1 = R^4 = H, R^2 = Et, R^3 = OMe

737 R^1 = R^4 = H, R^2 = Et, R^3 = CN

738 R^1 = Et, R^2 = R^4 = H, R^3 = CH_2COMe



739 R^1 = R^4 = H, R^2 = Et, R^3 = H,H, R^5 = OH

740 R^1 = Et, R^2 = R^4 = R^5 = H, R^3 = O

741 R^1 = R^4 = R^5 = H, R^2 = Et, R^3 = O

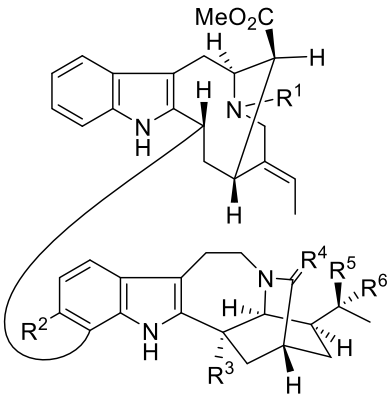
742 R^1 = R^4 = R^5 = H, R^2 = Et, R^3 = H,OH,(*R*)

743 R^1 = R^4 = R^5 = H, R^2 = Et, R^3 = H,OH,(*S*)

744 R^1 = Et, R^2 = R^4 = R^5 = H, R^3 = H,OH,(*R*/*S*)

745 R^1 = Et, R^2 = R^4 = R^5 = H, R^3 = H,CHO,(*R*)

Figure 1.8, continued



746 R^1 = Me, R^2 = R^5 = R^6 = H, R^3 = CO_2Me, R^4 = H,H

747 R^1 = R^5 = R^6 = H, R^2 = OMe, R^3 = CO_2Me, R^4 = H,H

748 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = H,H, R^5 = R^6 = H

749 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = O, R^5 = R^6 = H

750 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = H,CH_2COMe, R^5 = R^6 = H

751 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = H,H, R^5 = H, R^6 = OH

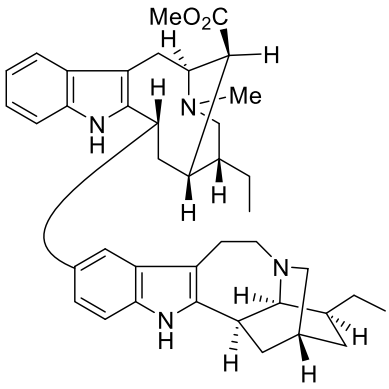
752 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = H,OH,(*R*/*S*), R^5 = R^6 = H

753 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = H,H, R^5 = OH, R^6 = H

754 R^1 = Me, R^2 = OMe, R^3 = R^5 = R^6 = H, R^4 = H,OH,(*R*/*S*)

755 R^1 = R^6 = H, R^2 = OMe, R^3 = CO_2Me, R^4 = H,H, R^5 = OH

756 R^1 = Me, R^2 = OMe, R^3 = CO_2Me, R^4 = H,CHO,(*R*), R^5 = R^6 = H



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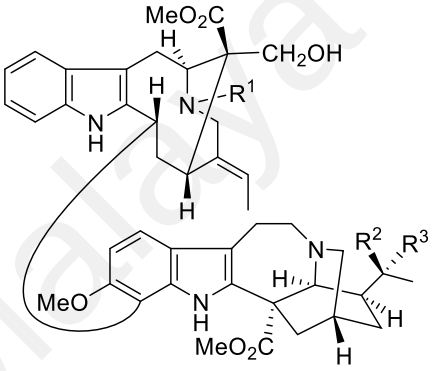
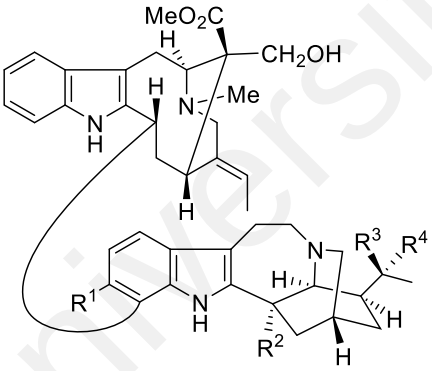


758 R^1 = Me, R^2 = R^3 = H

759 R^1 = Me, R^2 = OH, R^3 = H

760 R^1 = Me, R^2,R^3 = O

761 R^1 = R^3 = H, R^2 = OH

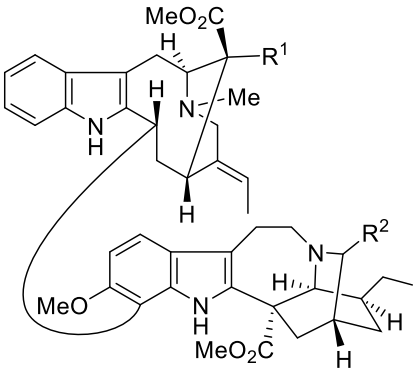


762 R^1 = OMe, R^2 = R^4 = H, R^3 = OH

763 R^1 = OMe, R^2 = H, R^3,R^4 = O

764 R^1 = OH, R^2 = CO_2Me, R^3 = OH, R^4 = H

765 R^1 = OH, R^2 = CO_2Me, R^3 = R^4 = H



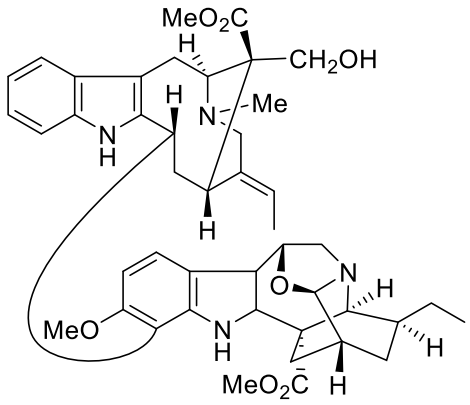
766 R^1 = CH_2OAc, R^2 = H

767 R^1 = CH_2OH, R^2 = H

768 R^1 = R^2 = CH_2OH

769 R^1 = CH_2OH, R^2 = CH_2COCH_3

Figure 1.8, continued



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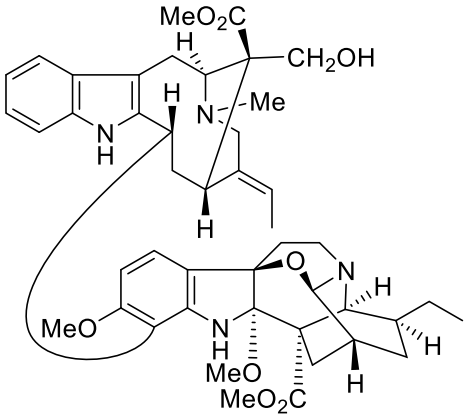

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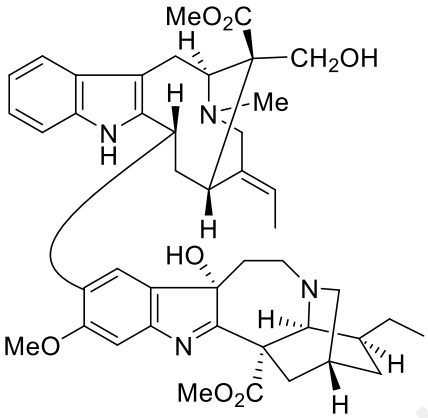

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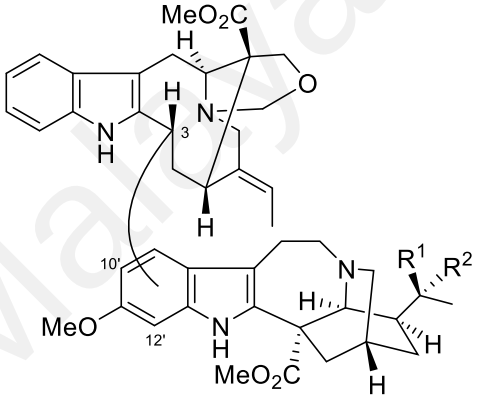
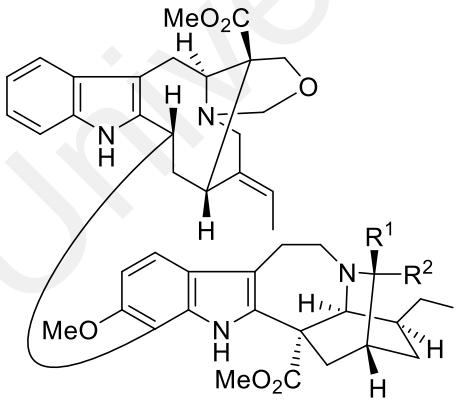


773 C(3)-C(10'), R^1 = OH, R^2 = H

774 C(3)-C(12'), R^1 = OH, R^2 = H

775 C(3)-C(10'), R^1 = R^2 = H

776 C(3)-C(12'), R^1 = R^2 = H



777 R^1 = H, R^2 = CH_2OH

778 R^1 = H, R^2 = CH_2COMe

779 R^1,R^2 = O

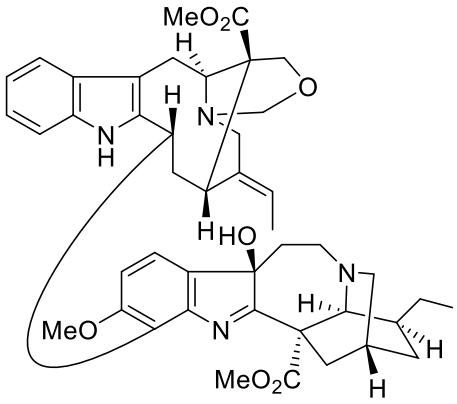


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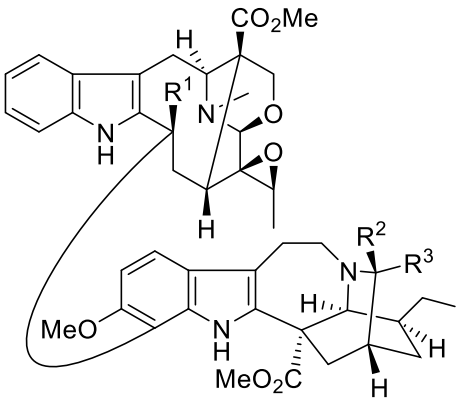
Figure 1.8, continued

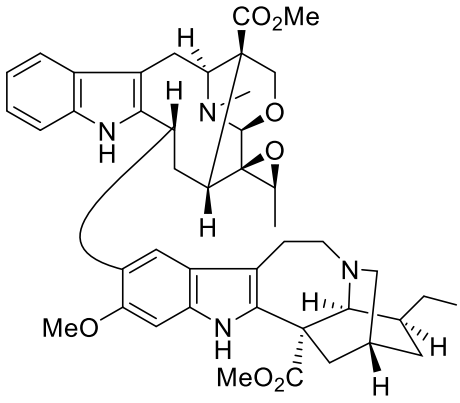


781 $R^1 = R^2 = R^3 = H$

782 $R^1 = R^2 = H$, $R^3 = CH_2COMe$

783 $R^1 = H$, R^2,$R^3 = O$

784 $R^1 = OH$, $R^2 = R^3 = H$



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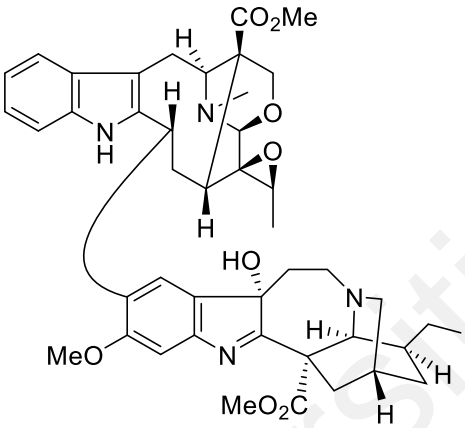

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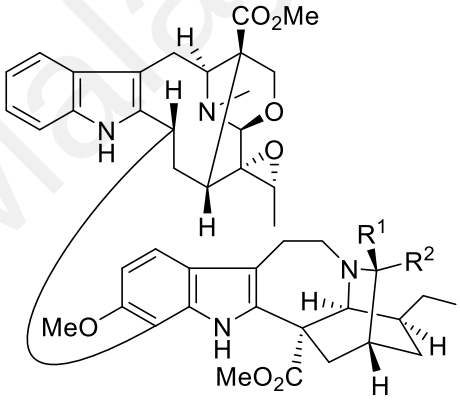
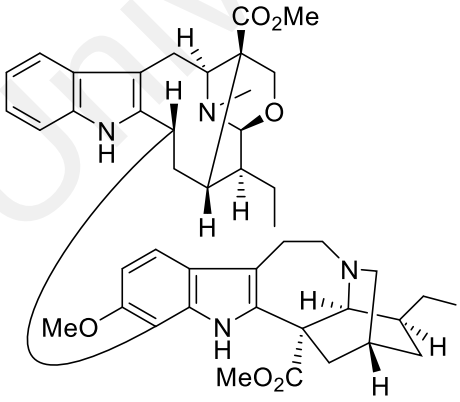


787 $R^1 = R^2 = H$

788 $R^1 = H$, $R^2 = CH_2COMe$



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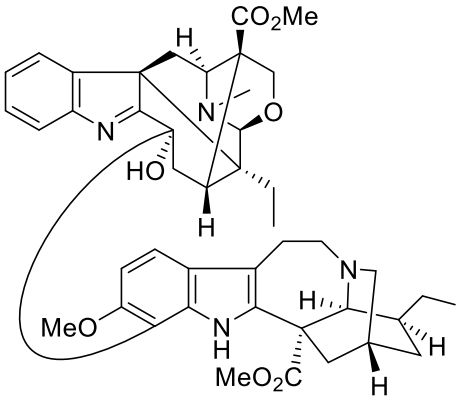

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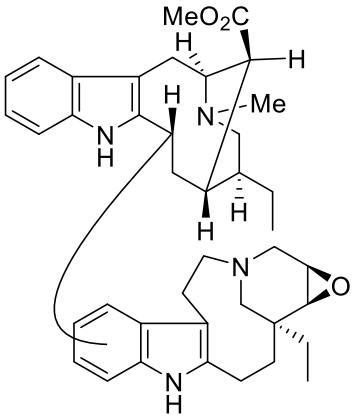
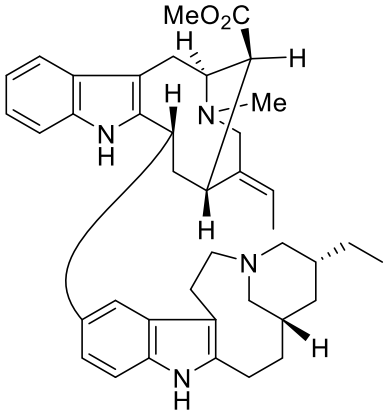


791 C(3)-C(11')

792 C(3)-C(10')



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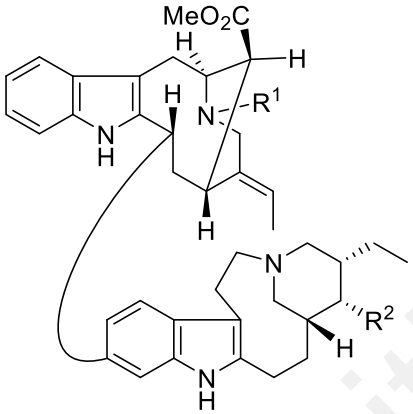
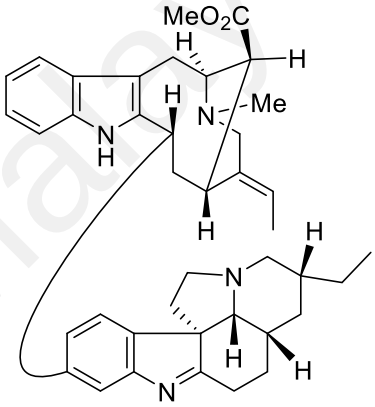


794 R^1 = H, R^2 = Me

795 R^1 = OH, R^2 = H

796 R^1 = OH, R^2 = Me



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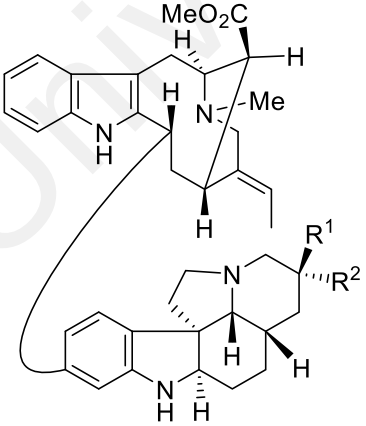
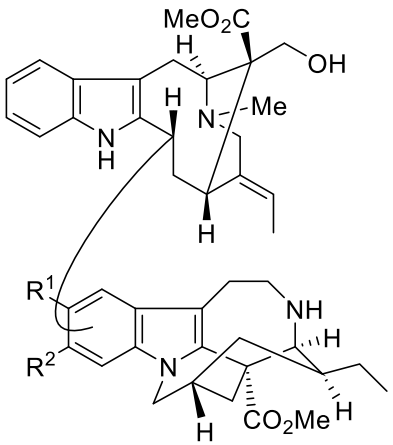


798 R^1 = H, R^2 = Et

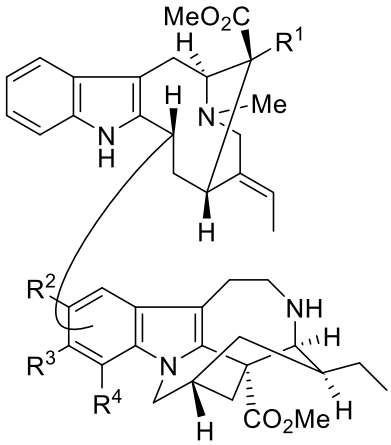
799 R^1 = Et, R^2 = H



800 C(3)-C(10'), R^1 = H, R^2 = OMe

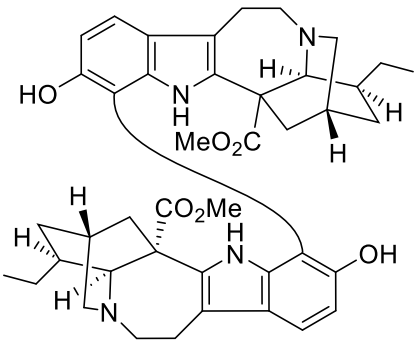
801 C(3)-C(11'), R^1 = OMe, R^2 = H

Figure 1.8, continued



802 C(3)-C(12'), R^1 = CH_2OH, R^2 = H, R^3 = OMe

803 C(3)-C(10'), R^1 = R^4 = H, R^3 = OMe



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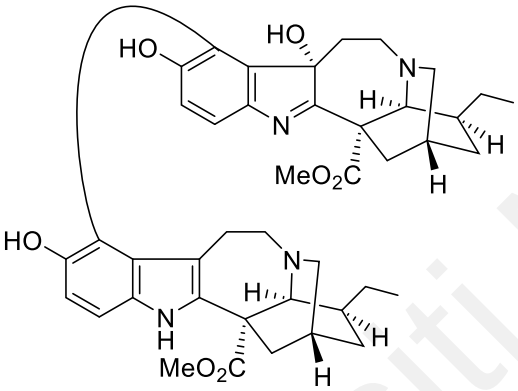

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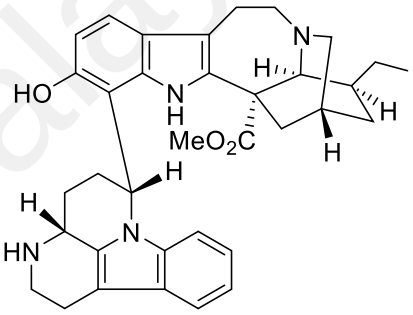

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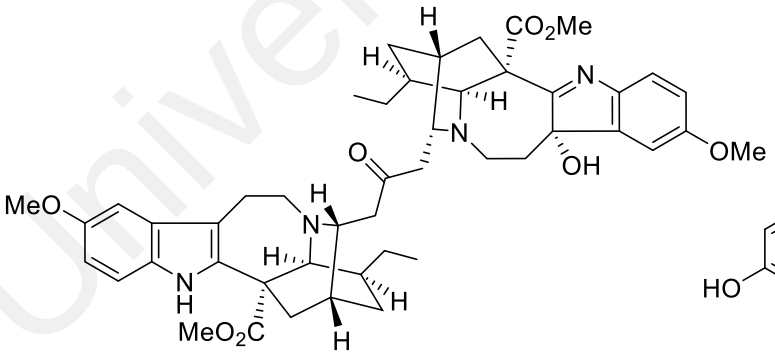

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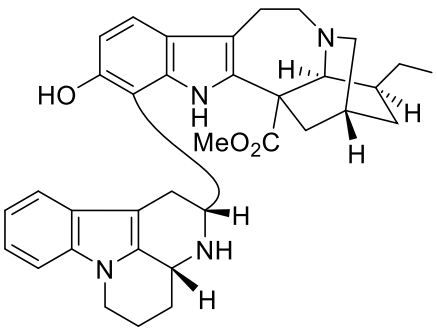

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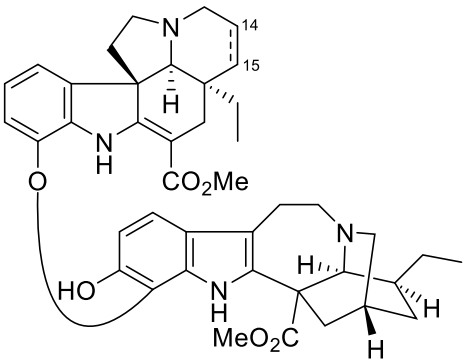
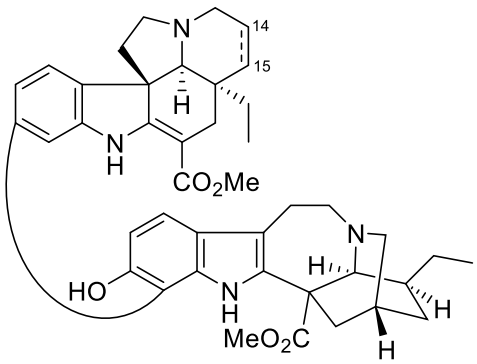
Figure 1.8, continued



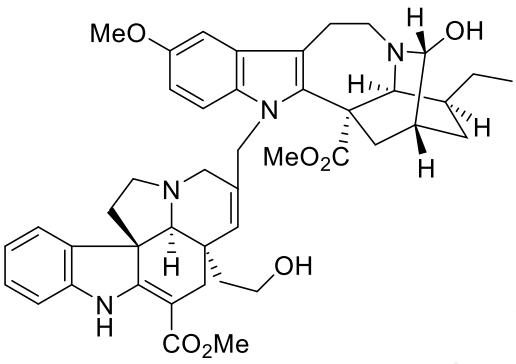
809

810 $\Delta^{14,15}$



811

812 $\Delta^{14,15}$



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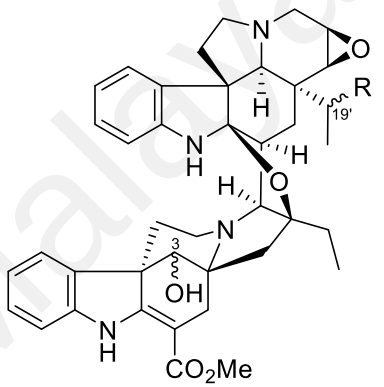
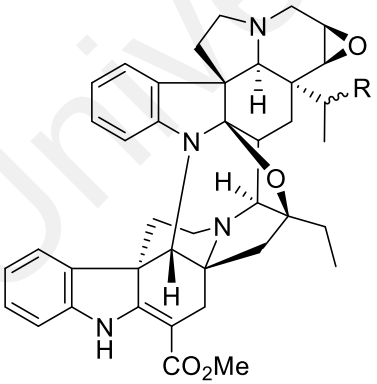


814 R = H, 3(*R*)

815 R = H, 3(*S*)

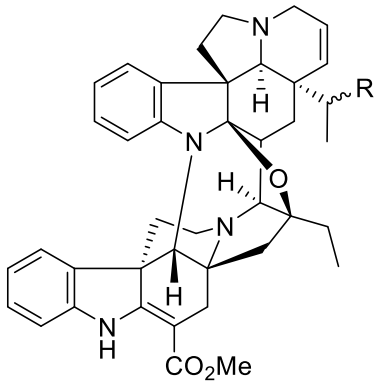
816 R = OH, 3(*S*), 19'(*R*)

817 R = OH, 3(*S*), 19'(*S*)



818 R = H

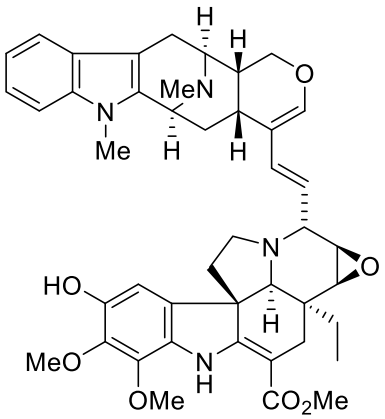
819 R = OH



820 R = H

821 R = OH

Figure 1.8, continued



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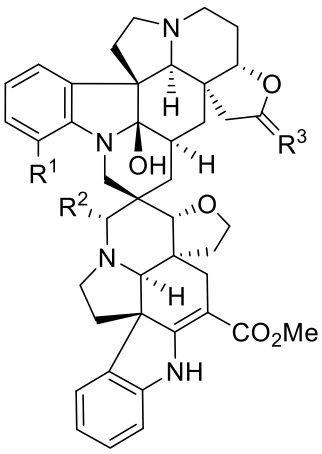
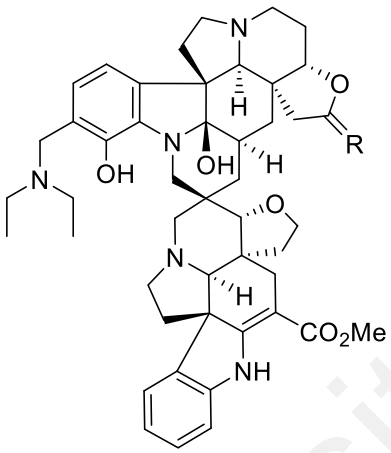
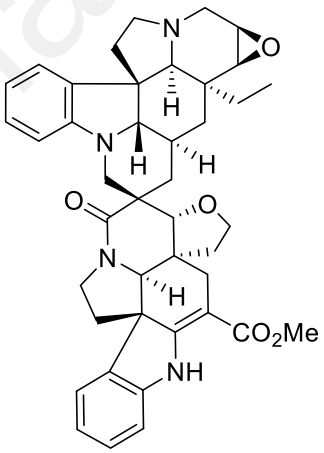


823 R^1 = OMe, R^2 = H, R^3 = H,H
824 R^1 = OMe, R^2 = H, R^3 = O
825 R^1 = OH, R^2 = H, R^3 = O
826 R^1 = OMe, R^2 = OH, R^3 = H,H
827 R^1 = OMe, R^2 = OH, R^3 = O



828 R = O
829 R = H,H



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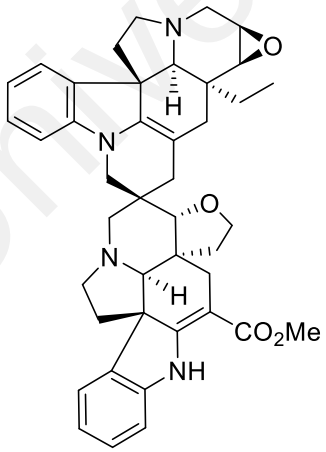
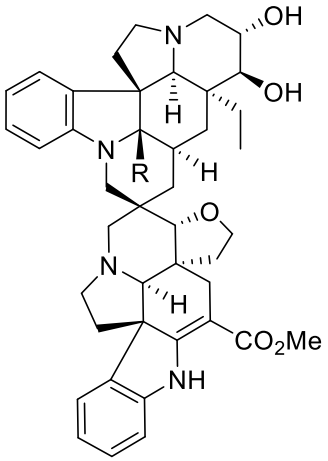
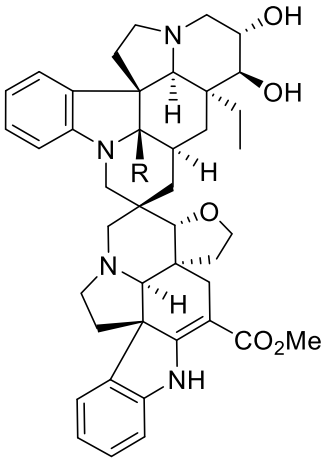


831

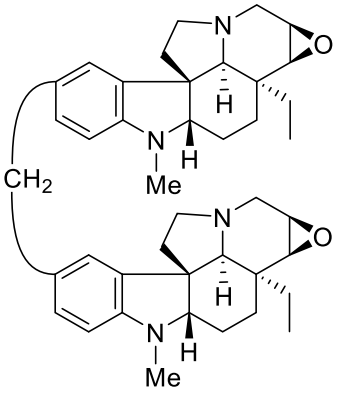
Figure 1.8, continued



832 R = H
833 R = OH



834 R = H
835 R = OH



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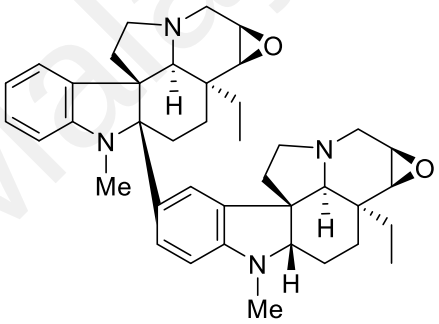

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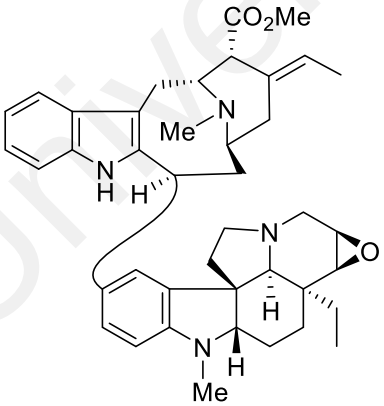

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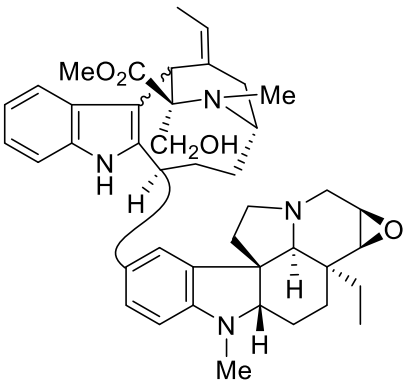

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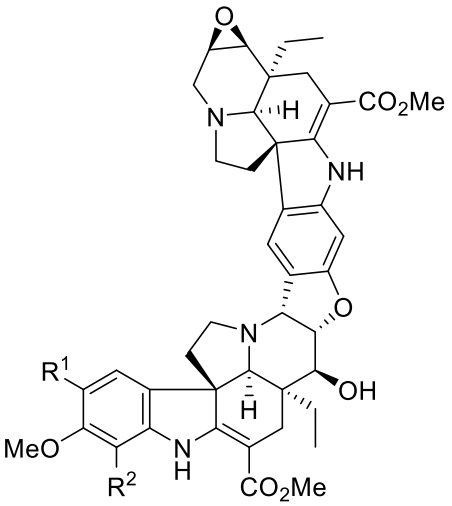
Figure 1.8, continued



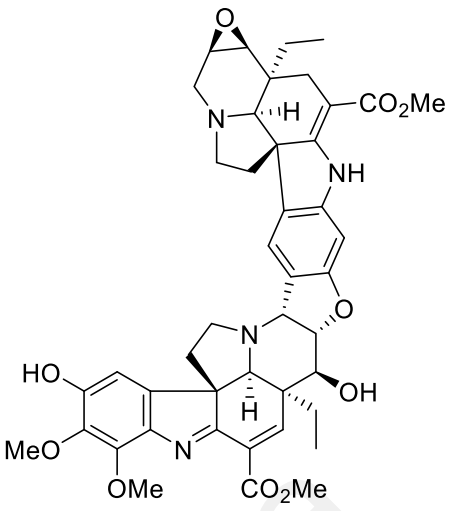
71 R^1 OH, R^2 = OMe

840 R^1 = OH, R^2 = OMe, N(4)→O

841 R^1 = OH, R^2 = H

842 R^1 = H, R^2 = OH

843 R^1 = R^2 = H



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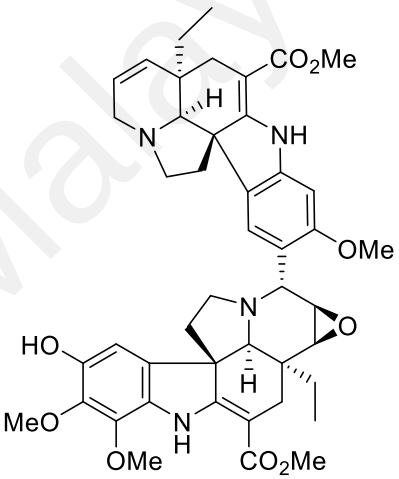

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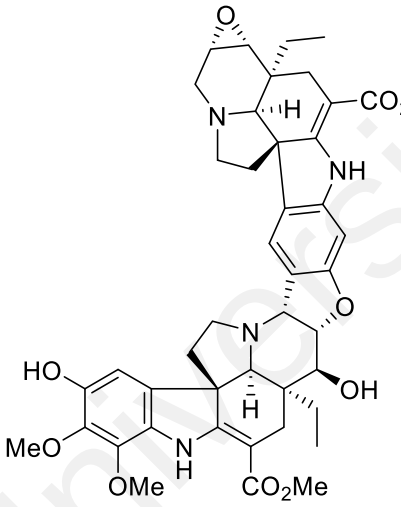

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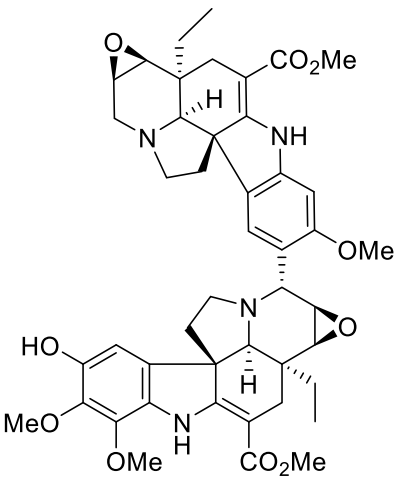

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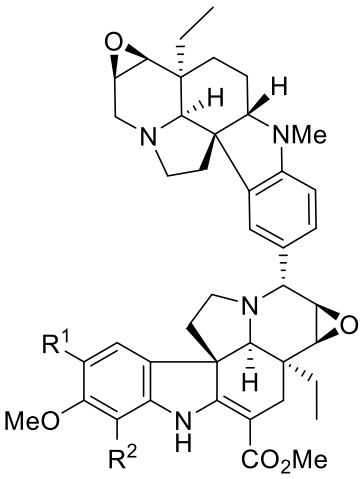
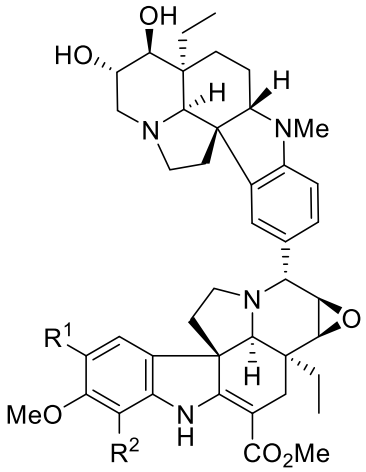
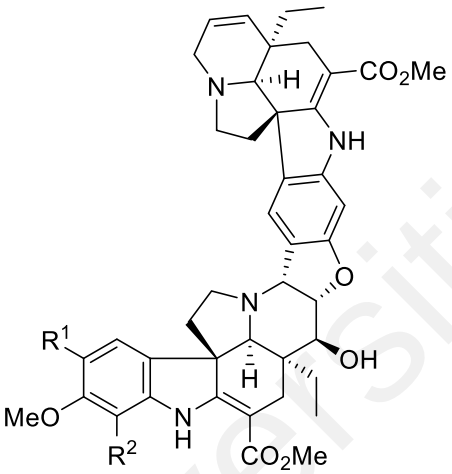
Figure 1.8, continued



848 R^1 = OH, R^2 = OMe
849 R^1 = R^2 = H
850 R^1 = H, R^2 = OMe



851 R^1 = OH, R^2 = OMe
852 R^1 = R^2 = H, N(4)'→O



853 R^1 = OH, R^2 = OMe
854 R^1 = H, R^2 = OMe
855 R^1 = H, R^2 = OH
856 R^1 = R^2 = H

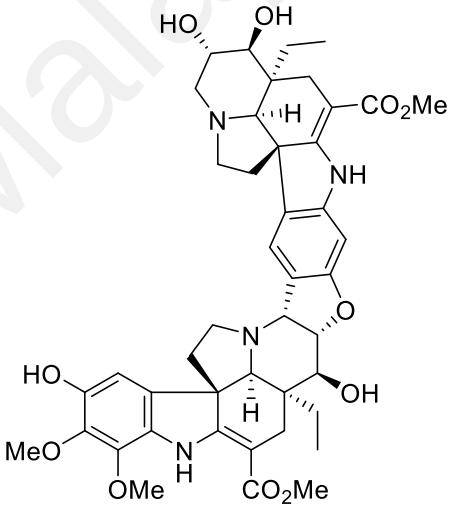


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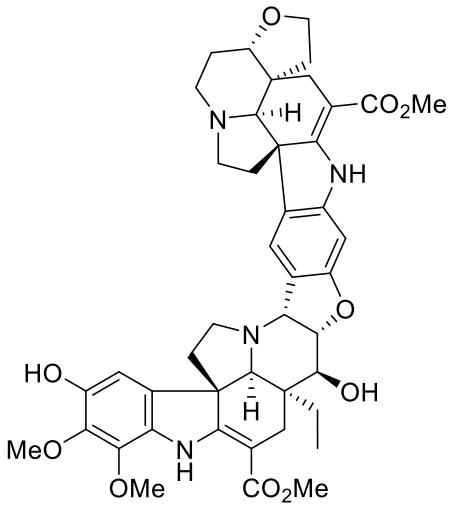
Figure 1.8, continued



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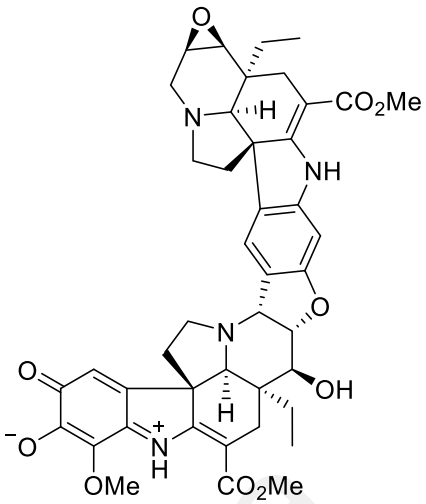

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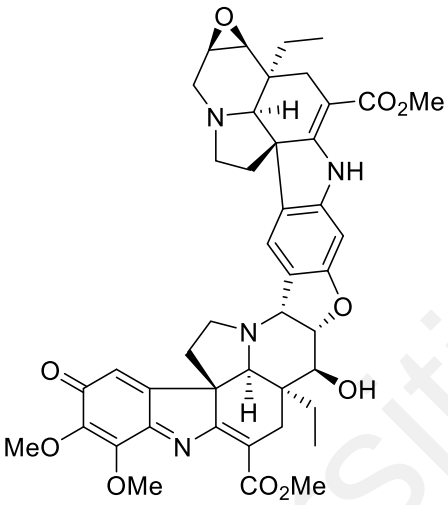

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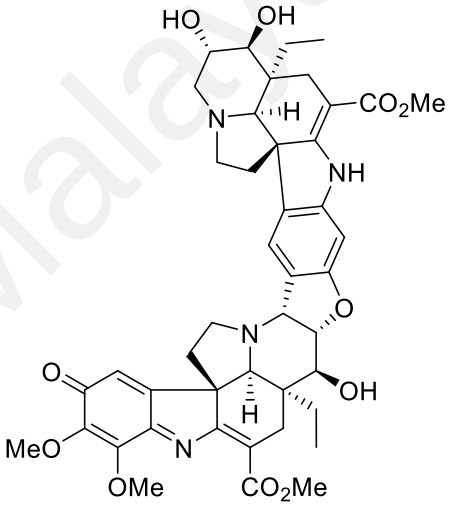

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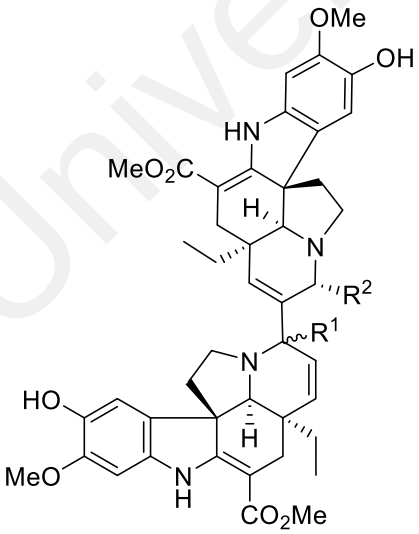
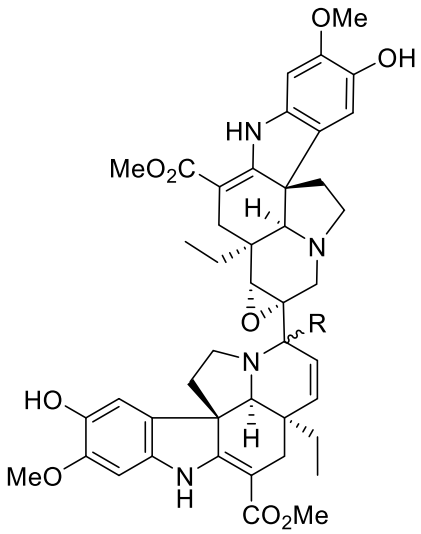


862 R^1 = α-H, R^2 = H

863 R^1 = β-H, R^2 = H

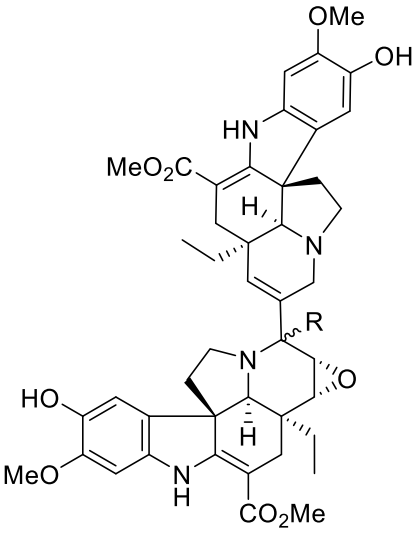
864 R^1 = β-H, R^2 = CH_2COMe



865 R = α-H

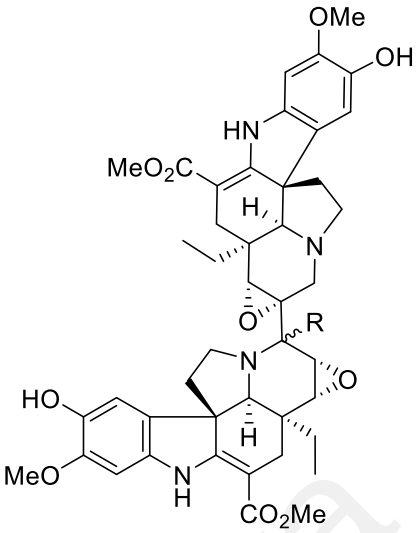
866 R = β-H

Figure 1.8, continued



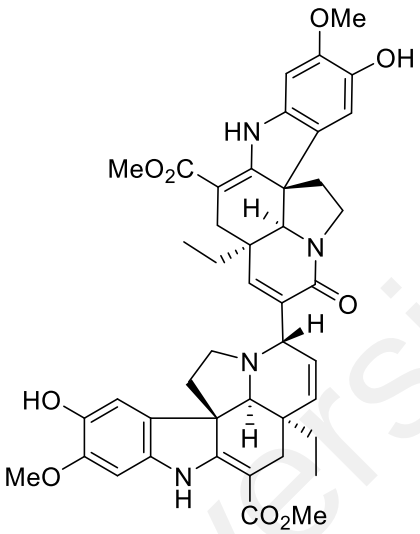
867 R = α-H

868 R = β-H



869 R = α-NHNH$_2$

870 R = β-H



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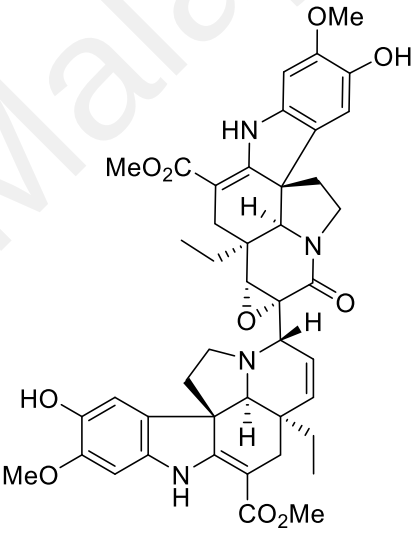

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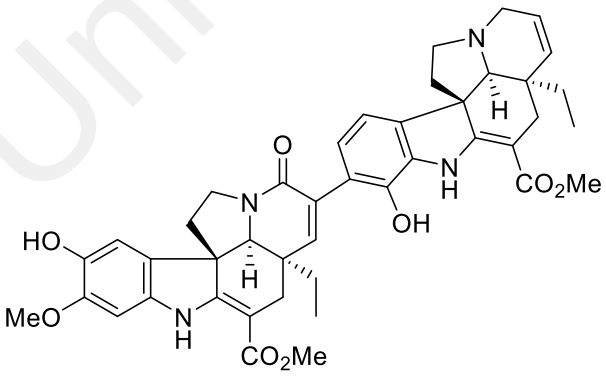

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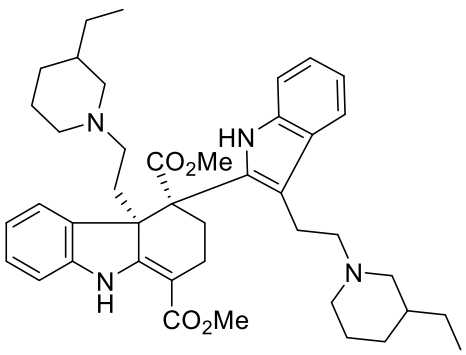

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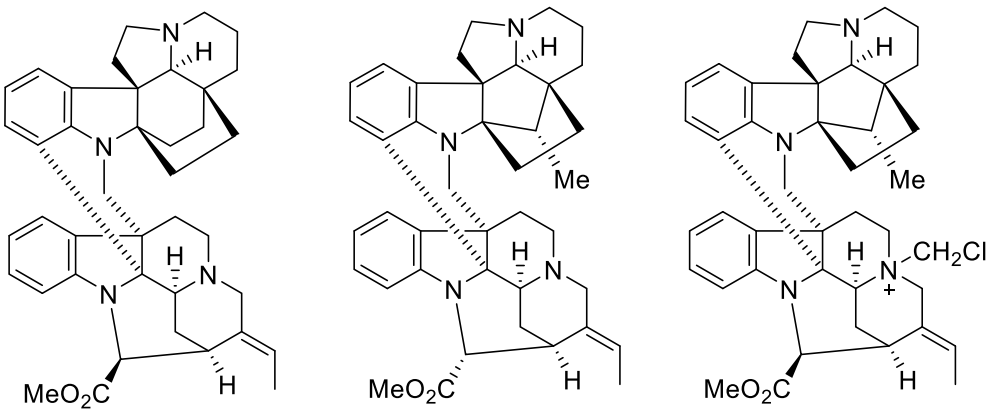
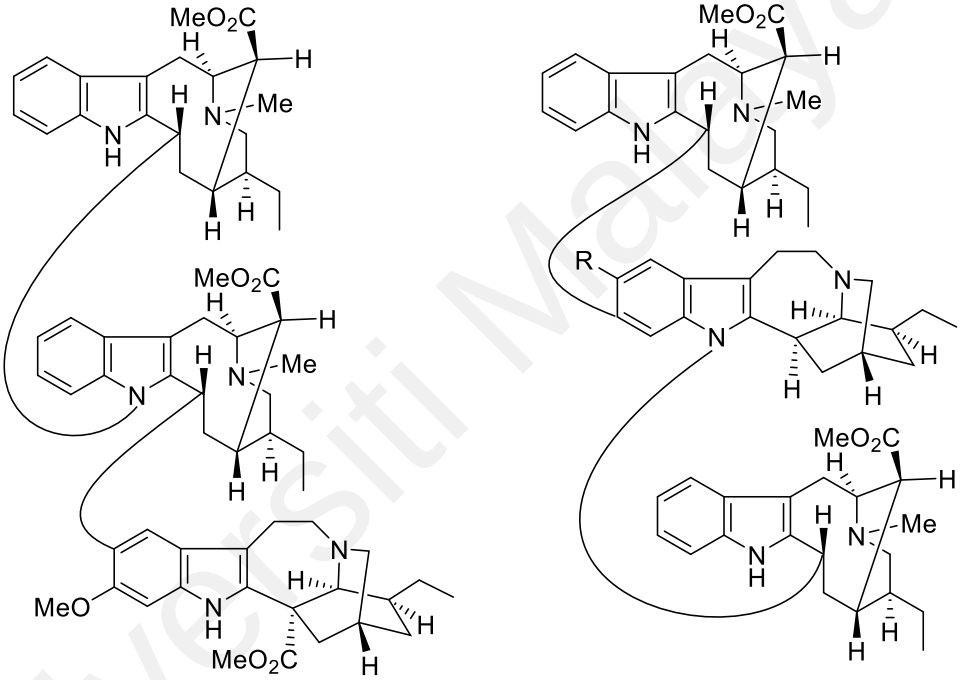
Figure 1.8, continued



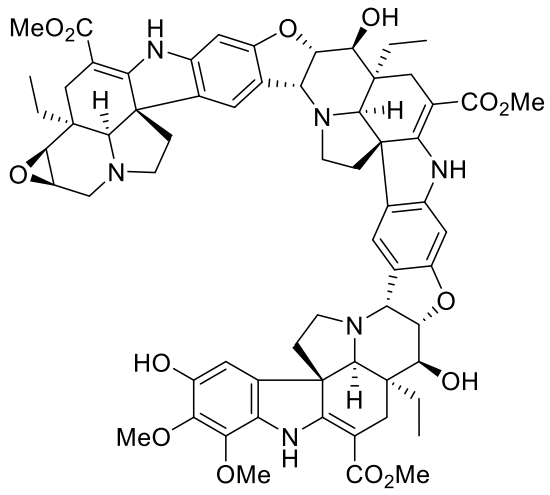
875 **876** **877**



878 **879** R = H

880 R = OMe

Figure 1.8, continued



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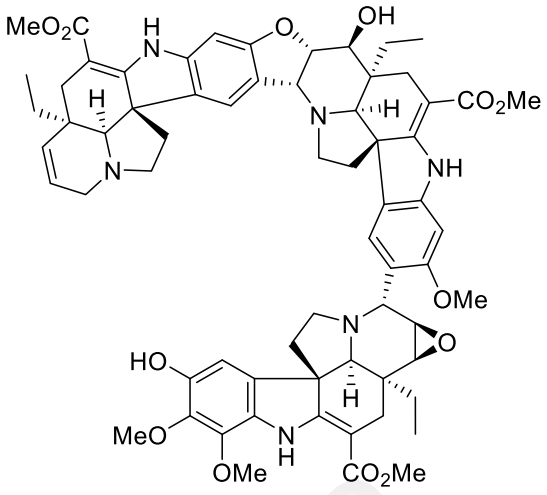

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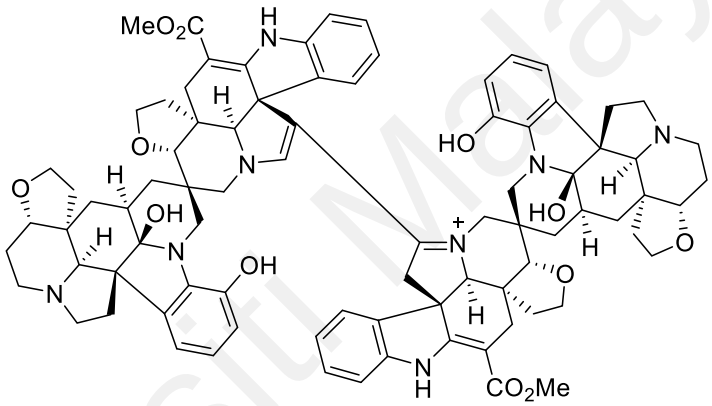


883

Figure 1.8, continued

1.5 Objective of the Present Research

The present study aims to examine the alkaloid composition of *Tabernaemontana polyneura* (collected from Fraser's Hill, Pahang, Peninsular Malaysia). The investigation encompasses several key aspects as follows:

(i) the isolation and structure elucidation of new alkaloids,

(ii) an exploration of the biogenesis of new alkaloids,

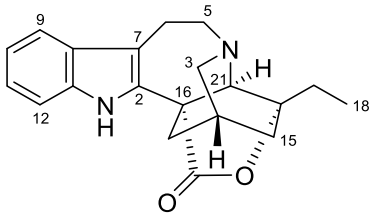
(iii) an examination of variations in alkaloid content, and

(iv) an evaluation of the cytotoxicity of the isolated alkaloids.

CHAPTER 2: RESULTS AND DISCUSSION

2.1 Alkaloids from *Tabernaemontana polyneura*

A total of 72 alkaloids were isolated and characterized from the bark and leaf extracts of *Tabernaemontana polyneura* (collected from Fraser's Hill, Pahang) (Figure 2.1). The results are summarized in Table 2.1. The bark extract of *T. polyneura* yielded 16 new alkaloids, which include ten iboga (polyneurines A–H, J, and K, **1**–**10**), one chippiine (polyneurine I, **30**), three vobasine (polyneurines M–O, **33**–**35**), one cleavamine (polyneurine L, **54**) and one vobasinyl-iboga bisindole alkaloids (polyneurine P, **66**).



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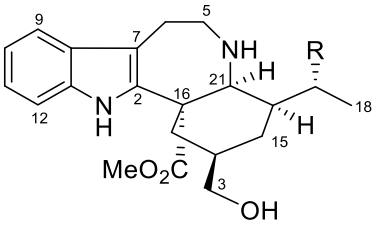
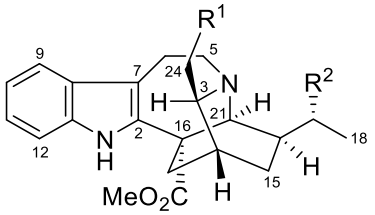
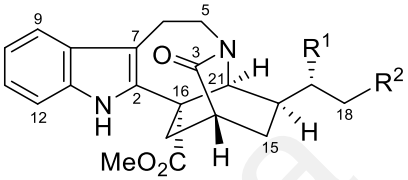


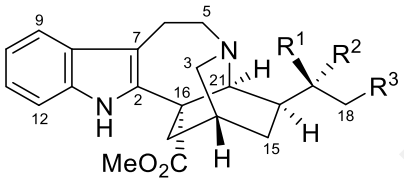
2 R = OH [new]
22 R = H



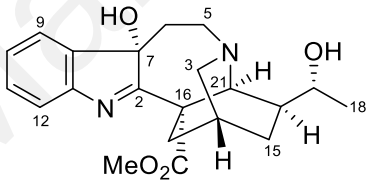
3 R^1 = OH, R^2 = OH [new]
4 R^1 = CHO, R^2 = OH [new]
5 R^1 = CHO, R^2 = H [new]
21 R^1 = OH, R^2 = H



6 R^1 = H, R^2 = OH [new]
18 R^1 = OH, R^2 = H
19 R^1 = R^2 = H



7 R^1 = H, R^2 = R^3 = OH [new]
14 R^1 = R^2 = R^3 = H
15 R^1 = R^2 = H, R^3 = OH
16 R^1 = OH, R^2 = R^3 = H
17 R^1 = H, R^2 = OH, R^3 = H



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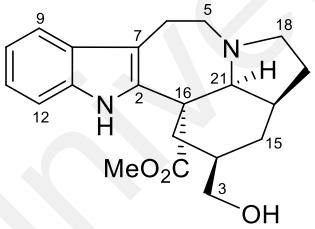

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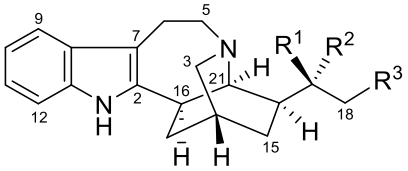
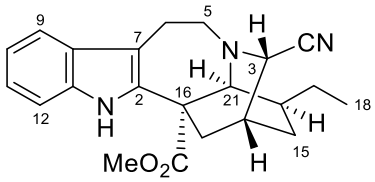


10 R^1 = R^2 = H, R^3 = OH [new]
11 R^1 = R^2 = R^3 = H
12 R^1 = OH, R^2 = R^3 = H
13 R^1 = H, R^2 = OH, R^3 = H



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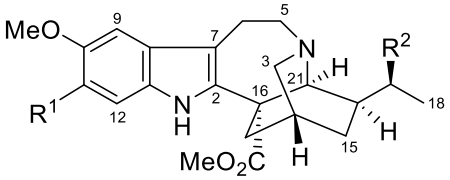
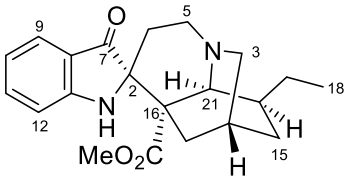


23 R^1 = R^2 = H
24 R^1 = H, R^2 = OH
25 R^1 = OMe, R^2 = H
26 R^1 = OMe, R^2 = OH

Figure 2.1: Structures of compounds **1**–**72**



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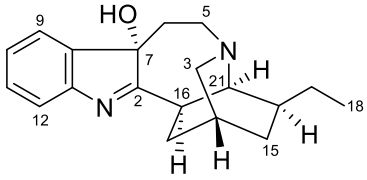

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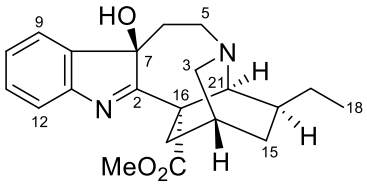

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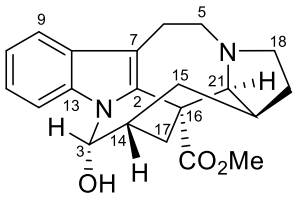

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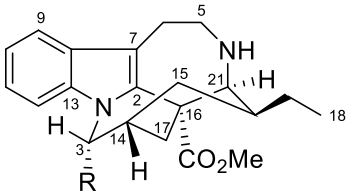
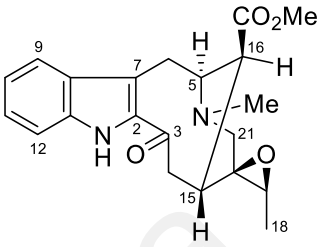


31 R = OH
32 R = OMe



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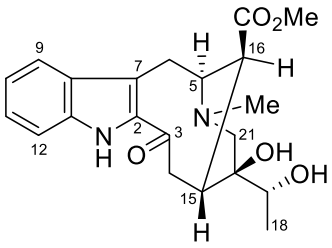
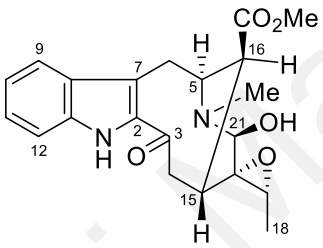


34 [new]



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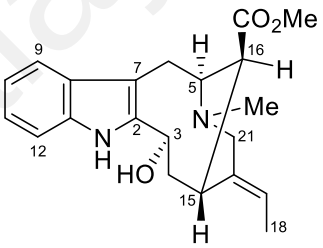

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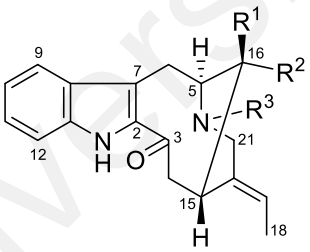
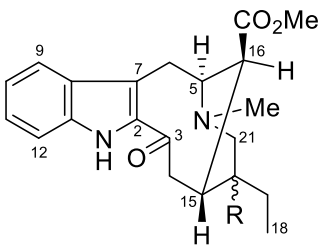
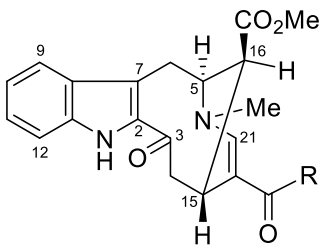


37 R^1 = CO_2Me, R^2 = H, R^3 = Me
38 R^1 = CO_2Me, R^2 = H, R^3 = Me, N(4)→O
39 R^1 = H, R^2 = CO_2Me, R^3 = Me
40 R^1 = CO_2Me, R^2 = R^3 = H

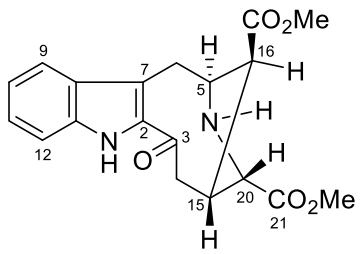




41 R = β-H
42 R = α-H
46 R = β-OH

43 R = H
44 R = Me

Figure 2.1, continued



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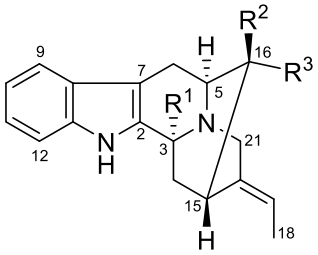
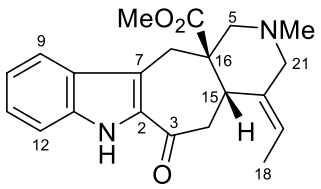


47 R^1 = H, R^2 = CO_2Me, R^3 = H
48 R^1 = OH, R^2 = CH_2OH, R^3 = CO_2Me



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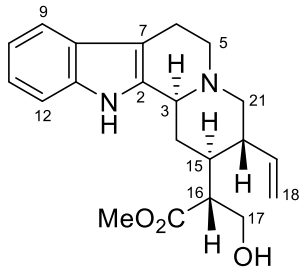

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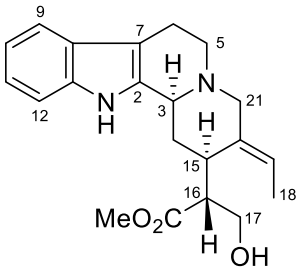

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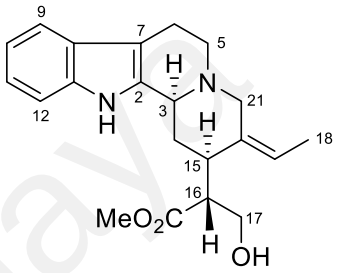

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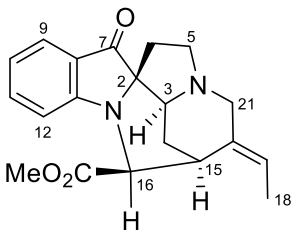

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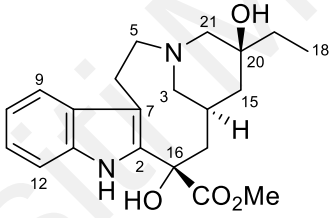

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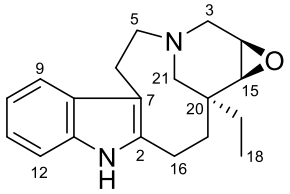

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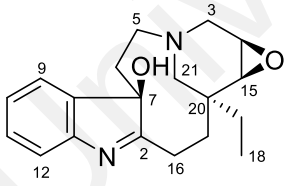

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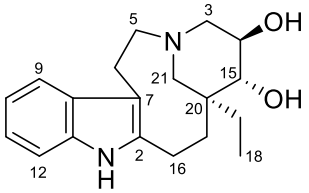

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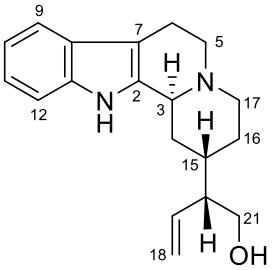

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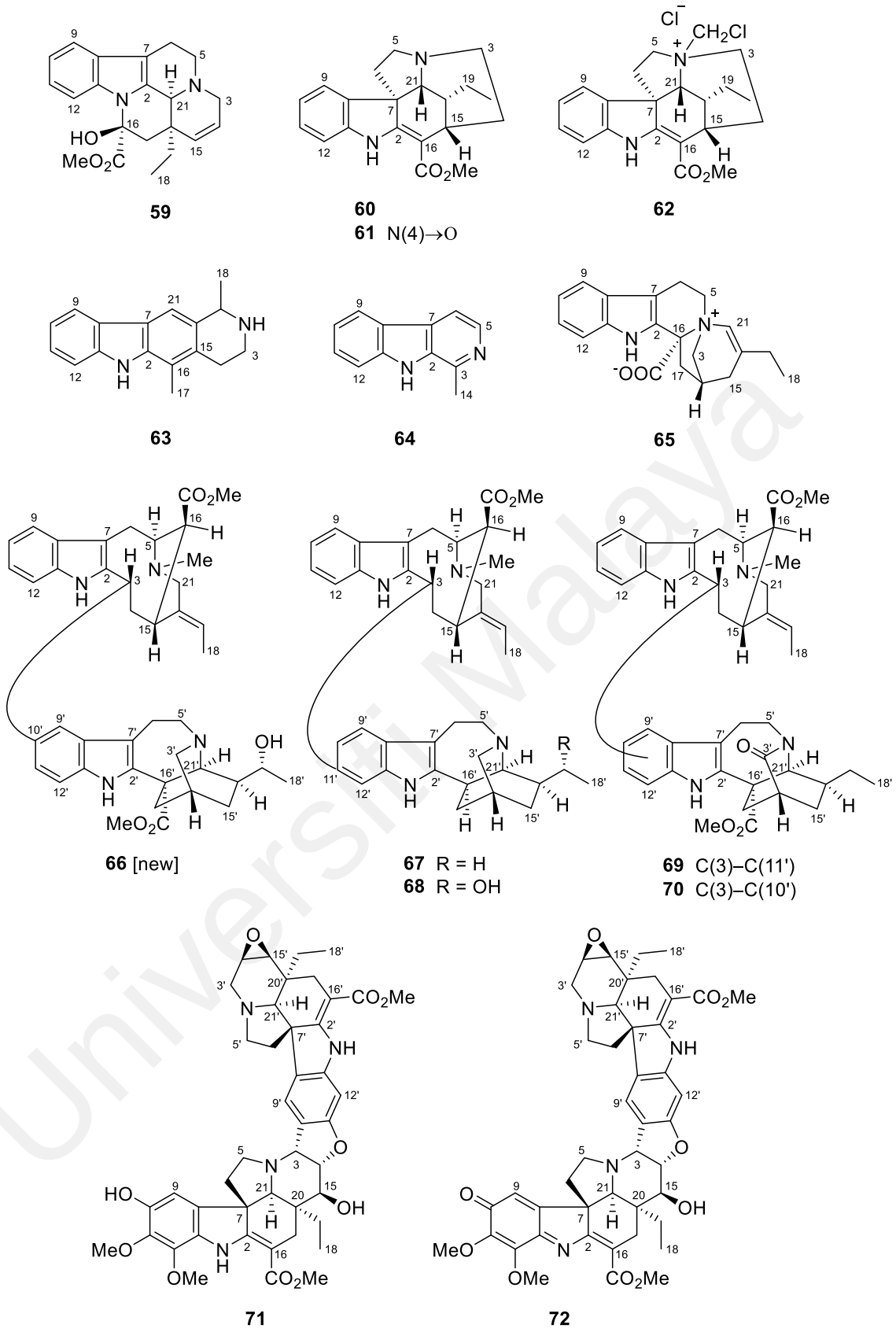


Figure 2.1, continued

Table 2.1: Alkaloid Composition of *T. polyneura*

Plant part	Alkaloid	Yield (mg kg^{-1})
Bark (11.9 kg)	Polyneurine A (**1**) [new]	0.37
	Polyneurine B (**2**) [new]	36.51
	Polyneurine C (**3**) [new]	0.31
	Polyneurine D (**4**) [new]	0.14
	Polyneurine E (**5**) [new]	0.13
	Polyneurine F (**6**) [new]	2.55
	Polyneurine G (**7**) [new]	0.86
	Polyneurine H (**8**) [new]	0.34
	Polyneurine J (**9**) [new]	5.91
	Polyneurine K (**10**) [new]	0.28
	Ibogamine (**11**)	17.96
	19(*S*)-Hydroxyibogamine (**12**)	0.34
	19(*R*)-Hydroxyibogamine (**13**)	2.27
	Coronaridine (**14**)	188.28
	(–)-Albifloranine (**15**)	3.54
	(–)-Heyneanine (**16**)	53.02
	19-*Epi*-heyneanine (**17**)	65.17
	3-Oxo-19-*epi*-heyneanine (**18**)	37.98
	3-Oxo-coronaridine (**19**)	9.86
	3(*S*)-Cyanocoronaridine (**20**)	0.76
	Ervatamine G (**21**)	1.47
	3-Hydroxy-3,4-*seco*coronaridine (**22**)	15.16
	Voacangine (**23**)	1.85
	Coronaridine pseudoindoxyl (**27**)	1.21
	Ibogamine 7(*S*)-hydroxyindolenine (**28**)	0.29
	Coronaridine-7-hydroxyindolenine (**29**)	2.70
	Polyneurine I (**30**) [new]	0.47
	10,11-Demethoxychippiine (**31**)	0.07
	3-Methoxy-10,11-demethoxychippiine (**32**)	0.36
	Polyneurine M (**33**) [new]	1.13
	Polyneurine N (**34**) [new]	0.15
	Polyneurine O (**35**) [new]	0.26
	3-*Epi*-vobasinol (**36**)	1.56
	Vobasine (**37**)	1567.34
	Vobasine *N*(4)-oxide (**38**)	3.10
	16-*Epi*-vobasine (**39**)	13.84
	Perivine (**40**)	14.40
	Dregamine (**41**)	0.17
	Tabernaemontanine (**42**)	0.24
	Vobasenal (**43**)	60.80
	Vobasidine D (**44**)	2.45

Table 2.1, continued

Plant part	Alkaloid	Yield (mg kg^{-1})
	Vobasidine F (**46**)	0.52
	Pericyclivine (**47**)	1.06
	16-*Epi*-voacarpine (**48**)	1.16
	19,20-Dehydroervatamine (**49**)	0.17
	16(*R*)-Sitsirikine (**50**)	0.54
	16(*R*)-19,20-*E*-isositsirikine (**51**)	1.82
	16(*R*)-19,20-*Z*-isositsirikine (**52**)	0.80
	Fluorocarpamine (**53**)	0.13
	Polyneurine L (**54**) [new]	0.53
	Voaphylline (**55**)	3.12
	Voaphylline-7-hydroxyindolenine (**56**)	0.47
	Voaphyllinediol (**57**)	0.39
	Antirhine (**58**)	13.84
	14,15-Dehydro-16-*epi*-vincamine (**59**)	0.08
	Tubotaiwine (**60**)	1.03
	N(4)-Chloromethyl-tubotaiwine chloride (**62**)	6.75
	Taberdivamine B (**65**)	1.22
	Polyneurine P (**66**) [new]	2.45
	Tabernamine (**67**)	51.71
	19'(*R*)-Hydroxytabernamine (**68**)	4.34
	Ervahaimine A (**69**)	5.66
	Ervahaimine B (**70**)	1.48
Leaf (11.1 kg)	Coronaridine (**14**)	0.35
	Voacristine (**24**)	1.52
	Conopharyngine (**25**)	1.41
	19(*S*)-Hydroxy-conopharyngine (**26**)	0.25
	Vobasine (**37**)	4.55
	Vobasidine E (**45**)	0.88
	Tubotaiwine *N*(4)-oxide (**61**)	0.68
	Janetine (**63**)	5.81
	Harmane (**64**)	82.2
	Conophylline (**71**)	2.96
	Conophylline quinone (**72**)	1.21

2.1.1 Iboga Alkaloids

2.1.1.1 Polyneurine A (1)

Polyneurine A (**1**) was obtained as a light orange oil, $[\alpha]^{25}_{D}$ –44 (*c* 0.22, $CHCl_3$). The UV spectrum showed absorption maxima at 226, 284, and 291 nm, indicating the presence of an indole chromophore, while the IR spectrum showed absorption bands at 3427 and 1756 cm^{-1}, suggesting the presence of NH and γ-lactone functions, respectively. The HRMS data showed an $[M + H]^+$ peak at *m/z* 323.1761, corresponding to the molecular formula $C_{20}H_{22}N_2O_2 + H$.

The ^1H NMR spectrum (Figure 2.5) showed the presence of an indolic NH (δ_H 9.59), four aromatic resonances (δ_H 7.10–7.49) due to an unsubstituted indole moiety, as well as an ethyl side chain (δ_H 1.03, t, *J* = 7.5 Hz, Me-18; δ_H 1.80, dq, *J* = 14.5, 7.5 Hz, H-19a; δ_H 1.98, dq, *J* = 14.5, 7.5 Hz, H-19b). The ^{13}C NMR data (Table 2.2) showed a total of 20 carbon resonances comprising one methyl, six methylenes, six methines, one ester carbonyl, one tertiary carbon linked to an ester oxygen, two tertiary carbons bonded to indolic nitrogen, and three quaternary carbon atoms. The COSY data revealed the presence of NCH_2CH_2, CH_2CHCH_2, and CH_2CH_3 partial structures, corresponding to N–C-5–C-6, C-15–C-14–C-17 and C-19–C-18, respectively (Figure 2.2). These structural features are reminiscent of the iboga skeleton, *e.g.*, coronaridine (**14**) (Santos *et al*., 2009), except for the absence of signals due to H-20 and the ester methyl in **1**. This is in agreement with the molecular formula of **1**, which differs from that of **14** by 16 mass units (CH_3 + H). In addition, the ^{13}C NMR data of **1** displayed an upfield shift of the C-16 resonance from *ca.* δ_C 55 in **14** to δ_C 45.7 in **1**, whereas the signal of C-20 (usually observed at *ca.* δ_C 40 as in **14**) was significantly shifted downfield to δ_C 88.1, likely due to being linked to an oxygen atom. These observations suggested the

presence of a lactone bridge that connects C-16 and C-20, which was confirmed by the three-bond correlations observed from H-17 to *C*OO, as well as from H-14 to C-16 and C-20 in the HMBC spectrum (Figure 2.2). Examination of the NOE data (Figure 2.3) indicated that the relative configuration of **1** was similar to that of **14**.

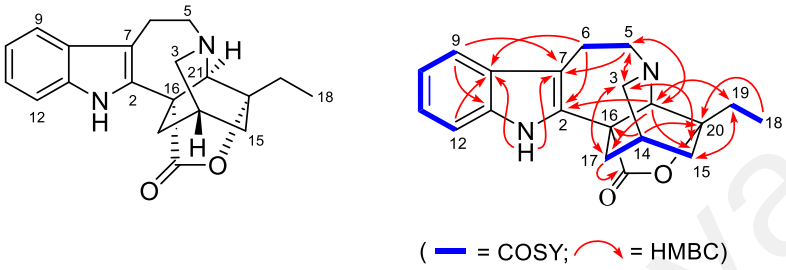


Figure 2.2: COSY and selected HMBCs of **1**

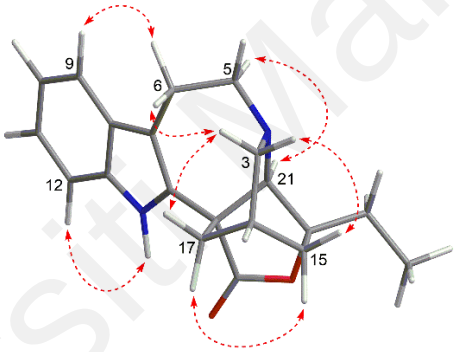


Figure 2.3: Selected NOEs of **1**

A search of the literature revealed that a compound similar to **1** was obtained as a by-product during a total synthesis of vinblastine (Ishikawa *et al.*, 2009). Compound **1** has similar ^{1}H and ^{13}C NMR, MS, and IR spectroscopic data compared to those of the synthetic compound (catharanthine lactone) but showed opposite sign for the specific rotation ($[\alpha]^{25}_{D}$ –44 for **1** *vs* $[\alpha]^{22}_{D}$ +33 for catharanthine lactone), suggesting an enantiomeric relationship between **1** and the synthetic compound. In any case, the absolute configuration of **1** (14*S*, 16*S*, 20*R*, 21*R*) was further confirmed by TDDFT-ECD (Figure 2.4). The experimental ECD data also matches with the experimental ECD data of voacangalactone, a 10-methoxy derivative of **1** (Harada *et al.*, 2012), and this provided further confirmation of the structure and absolute configuration of **1**.

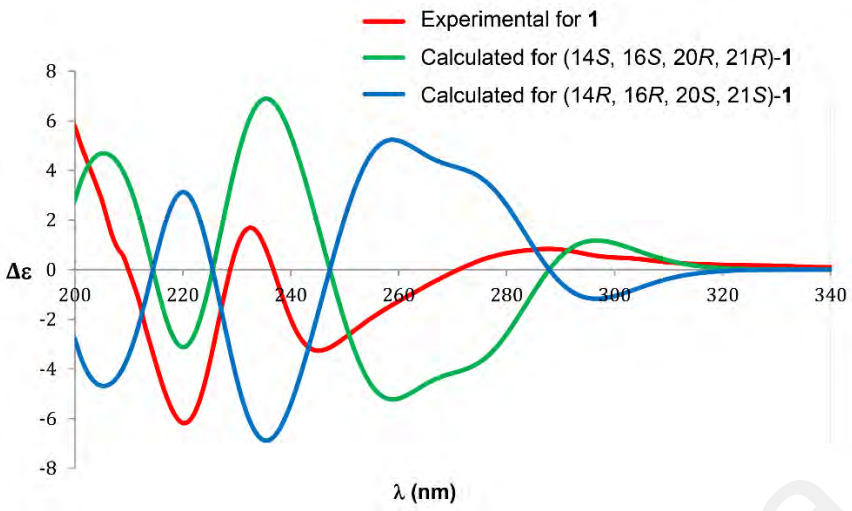
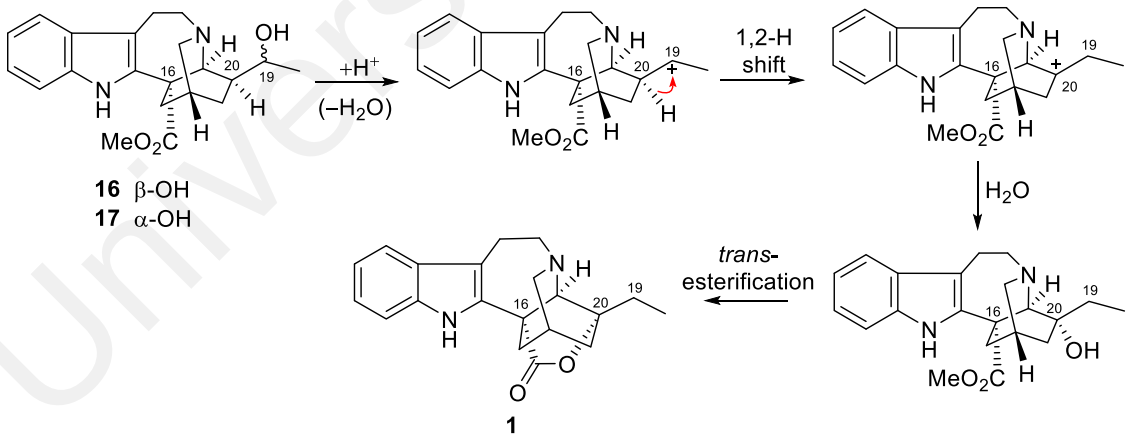


Figure 2.4: Experimental ECD spectrum of (–)-**1** and calculated ECD spectra of (14*S*, 16*S*, 20*R*, 21*R*)-**1** and (14*R*, 16*R*, 20*S*, 21*S*)-**1**

A plausible biosynthetic pathway to **1** from an iboga precursor, heyneanine (**16**, **17**), is shown in Scheme 2.1. Generation of a secondary carbocation at C-19 followed by a 1,2-H shift provides a tertiary carbocation at C-20, which on nucleophilic attack by a water molecule and a subsequent intramolecular transesterification furnish **1**.



Scheme 2.1: Possible biosynthetic pathway to **1**

Table 2.2: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of Polyneurine A (**1**)[a]

H/C	δ_H (J/Hz)	δ_C
2	-	136.2
3a	3.09 dt (10.0, 2.9)	50.2
3b	3.21 dt (10.0, 2.5)	
5α	3.23 ddd (14.5, 13.0, 3.0)	54.0
5β	3.34 dt (14.5, 3.0)	
6α	2.79 dt (16.5, 3.0)	20.0
6β	3.44 ddd (16.5, 13.0, 3.0)	
7	-	109.9
8	-	128.3
9	7.49 d (8.0)	117.7
10	7.10 td (8.0, 1.0)	119.4
11	7.16 td (8.0, 1.0)	121.6
12	7.35 d (8.0)	111.2
13	-	134.1
14	2.24 m	26.1
15β	1.80 dt (14.7, 2.2)	35.8
15α	2.05 m	
16	-	45.7
17β	2.05 m	37.5
17α	2.32 dt (14.3, 3.3)	
18	1.03 t (7.5)	7.2
19a	1.80 dq (14.5, 7.5)	29.3
19b	1.98 dq (14.5, 7.5)	
20	-	88.1
21	3.51 s	65.6
*C*OO	-	178.1
N(1)-H	9.59 br s	-

[a]$CDCl_3$, 600 (^{1}H) and 150 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and 1D/2D NOESY.

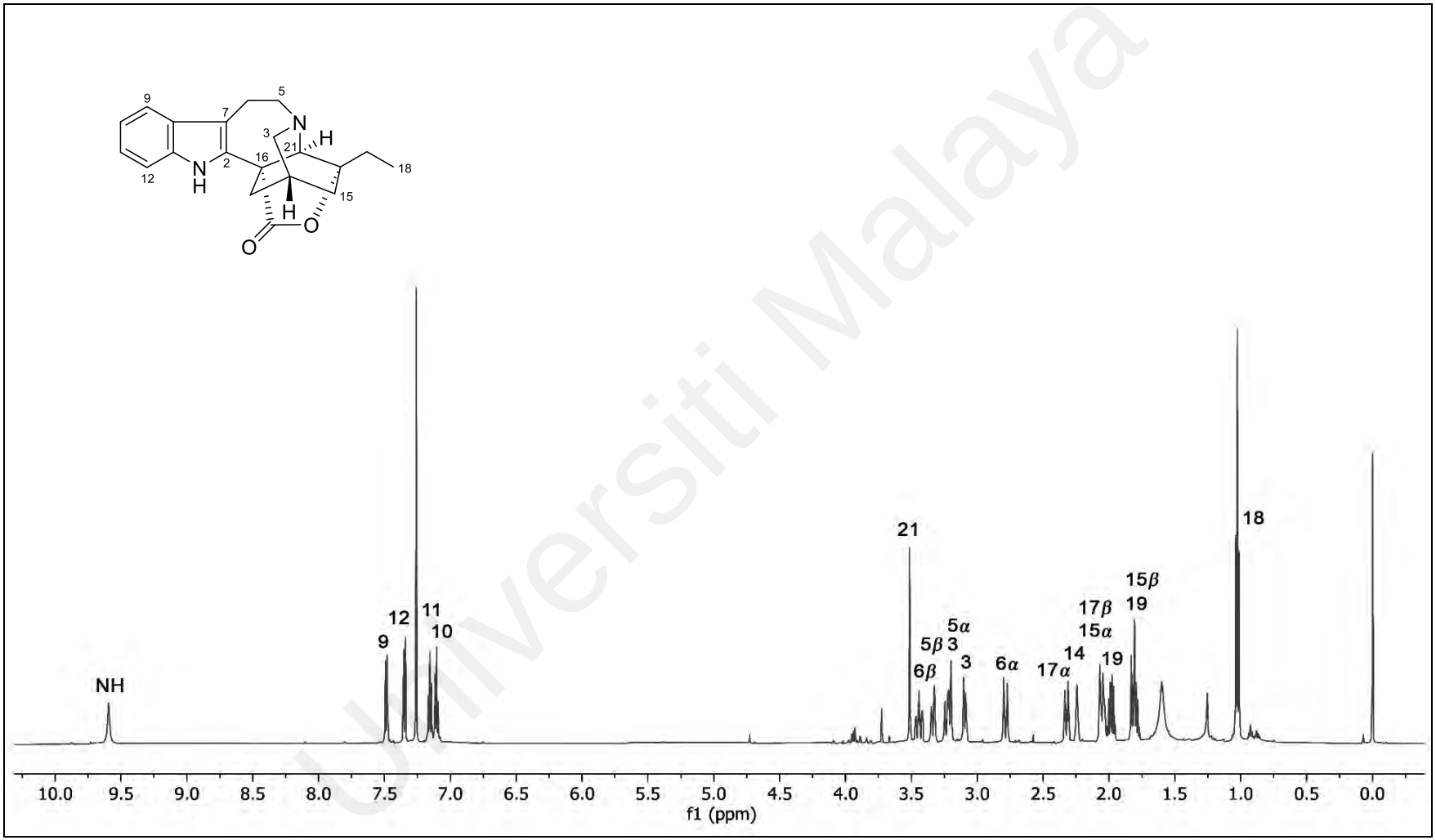


Figure 2.5: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Polyneurine A (**1**)

2.1.1.2 Polyneurine B (2)

Polyneurine B (**2**) was initially isolated as a colorless oil, $[\alpha]^{25}_{D}$ –44 (*c* 0.46, $CHCl_3$), and subsequently as colorless plates from CCl_4/MeOH (mp 175–177 °C). The UV spectrum showed absorption maxima at 217, 220, 285, and 292 nm, indicating the presence of an indole chromophore, while the IR spectrum showed absorption bands at 3259 and 1716 cm^{-1}, suggesting the presence of NH/OH and ester carbonyl functions, respectively. The HRMS data showed an $[M + H]^+$ peak at *m/z* 373.2139, which corresponds to the molecular formula, $C_{21}H_{28}N_2O_4 + H$.

The ^1H and ^{13}C NMR data (Table 2.3) of **2** were generally similar to those of 3-hydroxy-3,4-*seco*coronaridine (**22**) (Clivio, Richard, Hadi *et al.*, 1990), suggesting that they share a similar basic skeleton. The ^1H NMR data of **2** showed the presence of an indolic NH (δ_H 8.55), four aromatic hydrogens (δ_H 7.07–7.46) and a methyl ester (δ_H 3.65), while the ^{13}C NMR data showed a total of 21 resonances, including the notable downfield shift of the C-3 methylene resonance to δ_C 67.3 (which was commonly observed at *ca.* δ_C 52 in **14**), indicating a cleavage of the C-3–N-4 bond and substitution of an OH at C-3.

The most pronounced difference in the NMR data between **2** and **22** was the presence of a hydroxyethyl group at C-20 in **2**, in place of the ethyl side chain in **22**. This is consistent with the observed oxymethine resonance at δ_C 72.0 in the ^{13}C NMR spectrum, as well as the signals due to a hydroxyethyl side chain (δ_H 1.39, d, J = 6.5 Hz, Me-18; δ_H 3.86, qd, J = 6.5, 3.0 Hz, H-19) in the ^1H NMR spectrum. Analysis of the COSY data also revealed the presence of a $CHCHCH_3$ fragment in **2** (Figure 2.6), in place of the $CHCH_2CH_3$ fragment in **22**, due to C-20–C-19–C-18. Attachment of the hydroxyethyl side chain at C-20 was further supported by the following three-bond correlations in the HMBC spectrum, *viz.*, from H-19 (δ_H 3.86) to C-15 (δ_C 27.7) and C-

21 (δ_C 53.1), as well as from H-18 (δ_H 1.39) to C-20 (δ_C 42.3) (Figure 2.6). The relative configurations at all the stereogenic centers in **2**, except for C-19, were readily determined *via* analysis of the NOE data (Figure 2.7). Since suitable crystals of **2** were obtained, an X-ray diffraction analysis was carried out, which confirms the structure and the absolute configuration of **2** as (14*R*, 16*S*, 19*R*, 20*S*, 21*S*) (Figure 2.8). The crystal data and structure refinement parameters of **2** are summarized in Table 2.4.

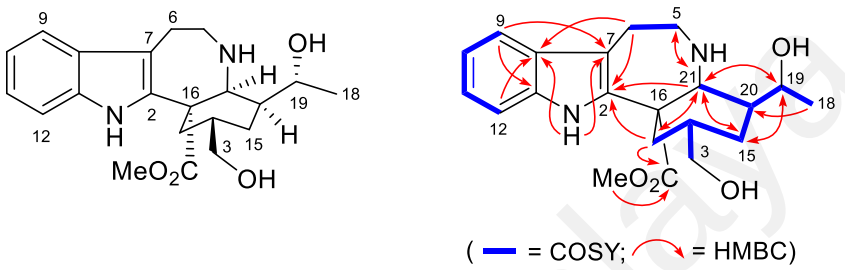


Figure 2.6: COSY and selected HMBCs of **2**

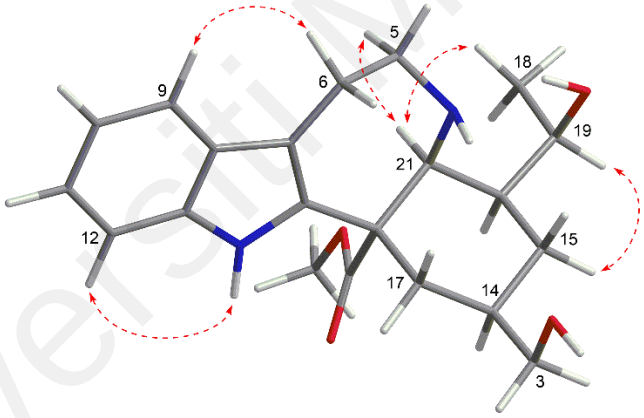


Figure 2.7: Selected NOEs of **2**

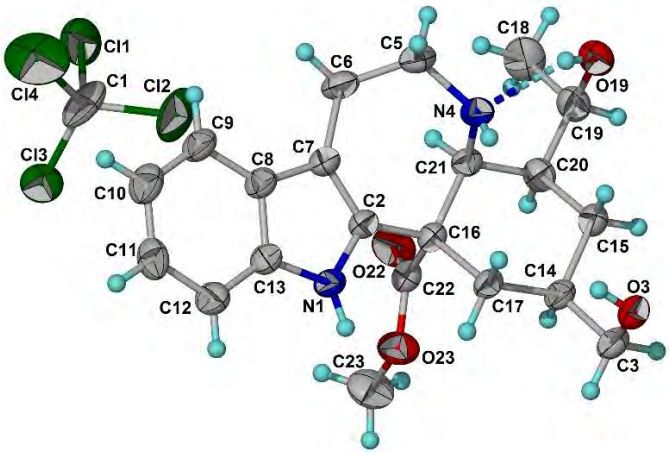


Figure 2.8: X-ray crystal structure of **2**

Table 2.3: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of Polyneurine B (**2**)[a]

H/C	δ_H (J/Hz)	δ_C
2	-	133.2
3	3.48 dd (10.8, 5.5)	67.3
3	3.56 dd (10.8, 5.5)	
5	3.14 m	47.2
5	3.25 m	
6	2.90 m	23.4
6	3.18 m	
7	-	110.0
8	-	128.0
9	7.46 d (8.0)	118.2
10	7.07 td (8.0, 1.0)	119.4
11	7.14 td (8.0, 1.0)	122.2
12	7.27 d (8.0)	110.7
13	-	135.5
14	1.76 m	36.9
15α	1.51 m	27.7
15β	1.62 q (13.0)	
16	-	55.7
17β	1.44 t (13.0)	33.8
17α	2.68 d (13.0)	
18	1.39 d (6.5)	22.7
19	3.86 qd (6.5, 3.0)	72.0
20	1.37 m	42.3
21	4.43 d (3.0)	53.1
*C*O$_2$Me	-	173.3
CO$_2$*Me*	3.65 s	52.8
N(1)-H	8.55 br s	-

[a]$CDCl_3$, 400 (^{1}H) and 100 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and NOESY.

Table 2.4: Crystal Data and Structure Refinement Parameters of Polyneurine B (**2**)

Molecular formula	$C_{21}H_{28}N_2O_4.CCl_4$
Molecular weight, M_r	526.26
Melting point	175–177 °C
Temperature during diffraction experiment, T	293(2) K
X-ray source	Mo $K\alpha$ (λ = 0.71073 Å)
Crystal system	monoclinic
Space group	$P2_1$
a	9.7036(3) Å
b	9.7698(3) Å
c	13.5325(5) Å
α	90°
β	100.585(3)°
γ	90°
Volume, V	1261.08(7) $Å^3$
No. of molecule per unit cell, Z	2
Density (calcd)	1.386 g/cm^3
μ	0.500 mm^{-1}
$F(000)$	548
Crystal size	0.5 × 0.4 × 0.01 mm^3
2θ range for data collection	6.794 to 59.63°
Index ranges	$-13 \le h \le 13$, $-13 \le k \le 13$, $-17 \le l \le 17$
Reflections collected	22886
Independent reflections	6472 [R_{int} = 0.0340, R_{sigma} = 0.0331]
Data/restraints/parameters	6472/1/297
Goodness-of-fit on F^2	1.207
Final R indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0930, wR_2 = 0.2790
Final R indexes [all data]	R_1 = 0.1205, wR_2 = 0.3117
Largest diff. peak/hole / e $Å^{-3}$	0.77/–0.68
Flack parameter, x	0.02(3)
Hooft parameter, y	0.05(2)
Parson parameter, z	0.01(3)
CCDC Number	2169029

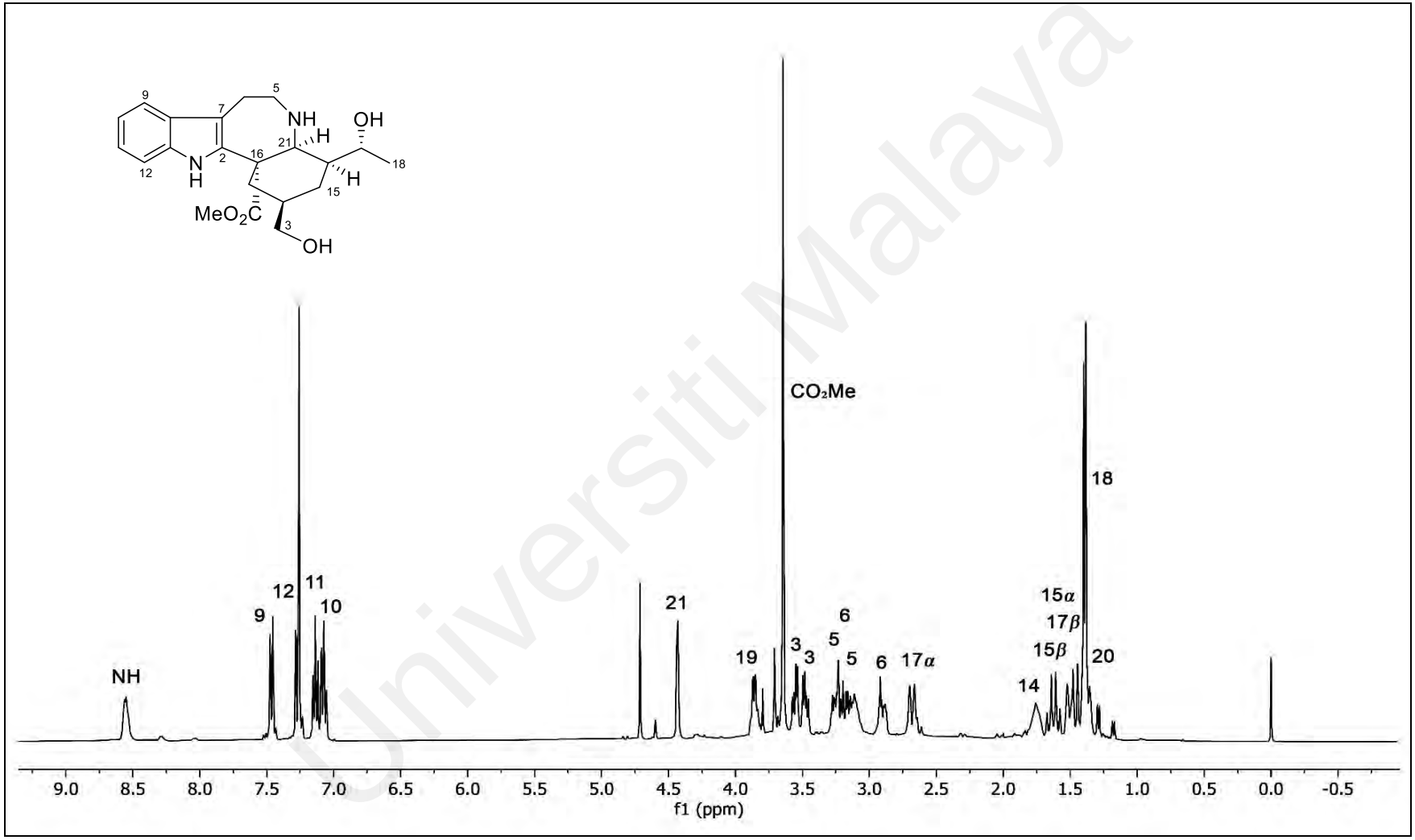


Figure 2.9: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Polyneurine B (**2**)

2.1.1.3 Polyneurines C–E (3–5)

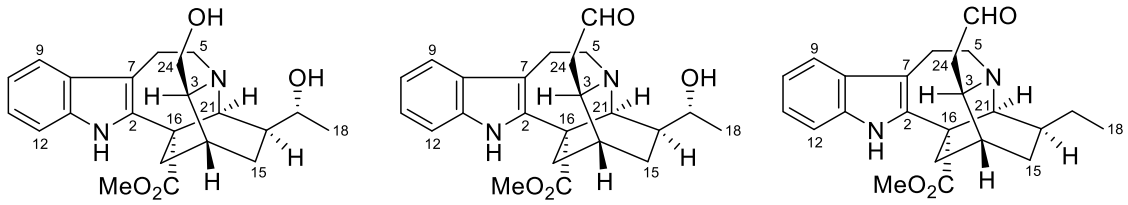


Figure 2.10: Structures of Polyneurines C–E

Polyneurine C (**3**) was isolated as a light yellowish oil, $[\alpha]^{25}_{D}$ –28 (*c* 0.19, $CHCl_3$). The UV spectrum showed absorption maxima at 223 and 286 nm, indicating the presence of an indole chromophore, while the IR spectrum showed absorption bands at 3374 and 1726 cm^{-1}, suggesting the presence of OH/NH and ester carbonyl functions, respectively. The HRMS data showed an $[M + H]^+$ peak at *m/z* 385.2130, corresponding to the molecular formula, $C_{22}H_{28}N_2O_4 + H$.

The ^{1}H NMR spectrum (Figure 2.20) showed the presence of an indolic NH (δ_H 7.89), four aromatic resonances of an unsubstituted indole moiety (δ_H 7.10–7.47), a methyl ester (δ_H 3.72), and a hydroxyethyl side chain (δ_H 1.27, d, *J* = 6.4 Hz, Me-18; δ_H 3.88, qd, *J* = 6.4, 3.2 Hz, H-19). The ^{13}C NMR data (Table 2.6) showed the presence of one methyl, five methylenes, nine methines, one methyl ester, one ester carbonyl, two tertiary carbons bonded to indolic NH, and three quaternary carbons, for a total of 22 carbon resonances.

The ^{1}H and ^{13}C NMR data of **3** showed features typical of iboga alkaloids with some differences, *viz.*, the presence of a hydroxymethyl linked to C-3 and a hydroxyethyl side chain attached to C-20. These observations were supported by the presence of the corresponding oxymethylene (C-3) and oxymethine resonances (C-19), at δ_C 60.5 and 70.8, respectively. These assignments were also supported by the HMBC data which

showed three-bond correlations from H-24 to C-14, H-15 and H-21 to C-19, and H-18 to C-20 (Figure 2.11).

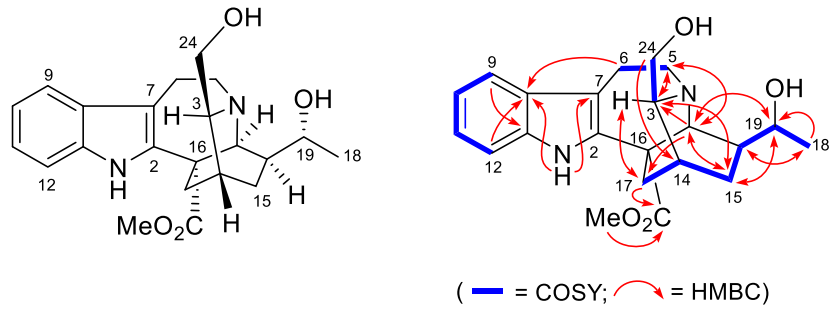


Figure 2.11: COSY and selected HMBCs of **3**

The relative configuration was determined *via* analysis of the NOE data (Figure 2.12) as well as from analysis of the vicinal coupling constants (Table 2.5). The configuration at C-3 was determined to be *S* based on the NOEs observed between H-3 and H-5β, H-6β, H-17β as well as between H-24 and H-15β (Figure 2.12). The β-orientation of the hydroxyethyl side chain at C-20 was determined based on the H-15α/H-20 NOE (Figure 2.12) as well as the observed $J_{15\alpha-20}$ coupling value of 11.0 Hz, which requires the H-20α/H-15α dihedral angle to be ~0° (Nge, Chong *et al.*, 2016).

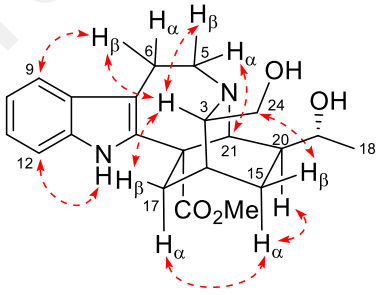


Figure 2.12: Selected NOEs of **3**

The 19*R* configuration was assigned based on the chemical shifts of H-18 (δ_H 1.27), H-19 (δ_H 3.88), H-21 (δ_H 4.18), and C-21 resonance (δ_C 54.7), which correspond to those of the 19*R* series of iboga alkaloids with a β-substituted hydroxyethyl side chain at C-20 (Sim *et al.*, 2016; Takayama *et al.*, 1994; Wenkert, Cochran *et al.*, 1976). The 19*R* configuration was further confirmed by the Gauge-Including Atomic Orbital (GIAO) NMR calculations and DP4+ probability analysis (Grimblat *et al.*, 2015). The

experimental NMR data were compared with the calculated ^{1}H and ^{13}C NMR shifts of **3** and its C-19 epimer, using DP4+ probability analysis. Compound **3** with 19*R* configuration showed DP4+ probability score of 100% (based on all NMR data). Finally, the absolute configuration of **3** was established as (3*S*, 14*R*, 16*S*, 19*R*, 20*S*, 21*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.13).

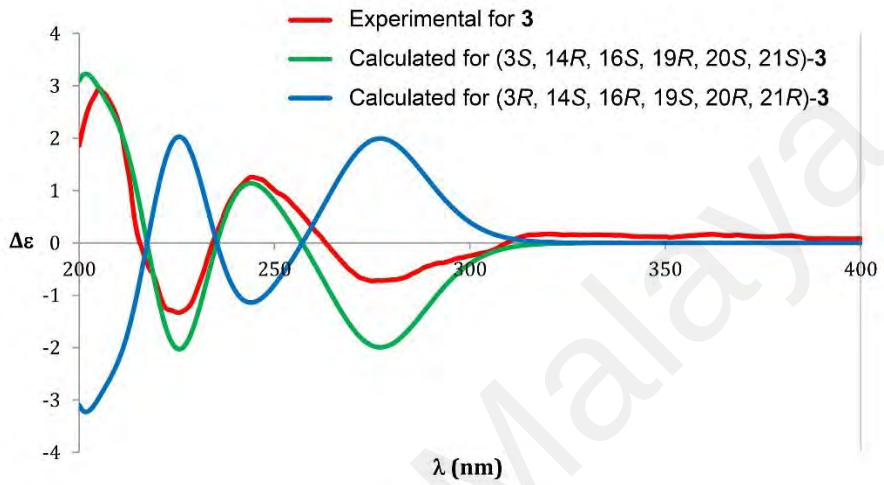


Figure 2.13: Experimental ECD spectrum of **3** and calculated ECD spectra of (3*S*, 14*R*, 16*S*, 19*R*, 20*S*, 21*S*)-**3** and (3*R*, 14*S*, 16*R*, 19*S*, 20*R*, 21*R*)-**3**

Polyneurine D (**4**) was isolated in minute amount as a light yellowish oil, $[\alpha]^{25}_{D}$ −36 (*c* 0.09, $CHCl_3$). The UV spectrum showed absorption maxima at 225, 285, and 293 nm, indicating the presence of an indole chromophore, while the IR spectrum showed absorption bands at 3376, 1725 and 1718 cm^{-1}, suggesting the presence of OH/NH, ester, and aldehyde carbonyl functionalities, respectively. The HRMS data showed an $[M + H]^+$ peak at *m/z* 397.2126, corresponding to the molecular formula, $C_{23}H_{28}N_2O_4$, which is 12 mass units higher than that of **4**.

The ^{13}C NMR data (Table 2.6) accounted for all 23 carbon resonances, including one methyl, five methylenes, nine methines, one methyl ester, one ester carbonyl, one formyl, two tertiary carbons bonded to indolic NH, and three quaternary carbons. The ^{1}H NMR data (Table 2.5) showed some common features with that of **3**, *viz.*, an indolic NH (δ_H 7.85), an unsubstituted indole ring (δ_H 7.11–7.47), a methyl ester (δ_H 3.73), and

a hydroxyethyl side chain (δ_H 1.28, d, J = 7.0 Hz, Me-18; δ_H 3.89, qd, J = 7.0, 2.8 Hz, H-19).

However, unlike **3**, a formylmethyl is attached at C-3 in **4** in place of the hydroxymethyl in **3**. This is evident from the presence of the aldehyde signal (δ_H 9.76; δ_C 201.4) in **4**, as well as the upfield shifts observed for C-3 (δ_C 53.6 in **4** *vs* δ_C 60.5 in **3**) and C-24 (δ_C 46.3 in **4** *vs* δ_C 62.0 in **3**). Furthermore, the COSY data (Figure 2.14) revealed an extended spin system $NCHCH_2CHO$, corresponding to the N-4–C-3–C-24–CHO partial structure. These observations were also consistent with the HMBC data which showed three-bond correlations from the formyl hydrogen to C-3 and from H-3 to the formyl carbon (Figure 2.14).

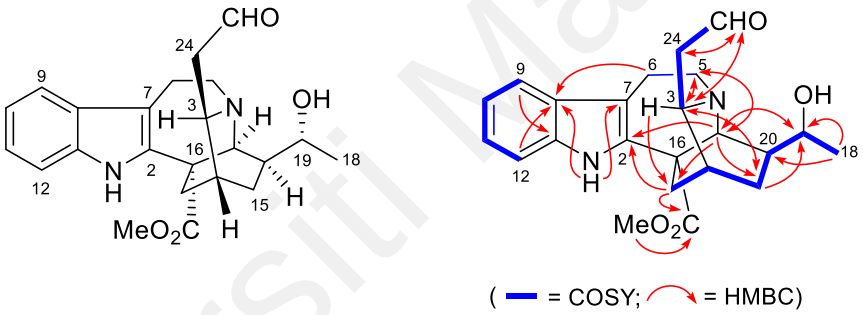


Figure 2.14: COSY and selected HMBCs of **4**

The relative configuration at C-3 was deduced to be *R* based on the observed NOE interactions for H-24/H-15β and H-3/H-5β, H-17β (Figure 2.15). The relative configurations of the remaining stereogenic centers were similar to those in **3**, based on comparison of the NOE as well as chemical shift data. Similar to **3**, the 19*R* configuration was assigned based on the chemical shifts of H-18 (δ_H 1.28), H-19 (δ_H 3.89), H-21 (δ_H 4.14), and C-21 resonance (δ_C 55.0) (*vide supra*). In addition, the GIAO NMR calculations and DP4+ analysis supported **4** with 19*R* configuration as the correct relative configuration, with 100% DP4+ probability (all data). Finally, the absolute configuration of **4** was established as (3*R*, 14*R*, 16*S*, 19*R*, 20*S*, 21*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.16).

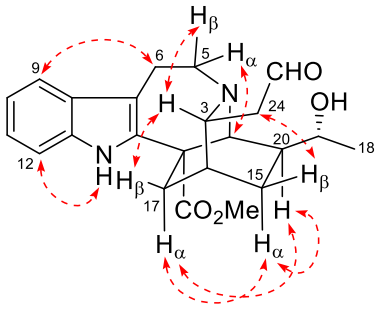


Figure 2.15: Selected NOEs of **4**

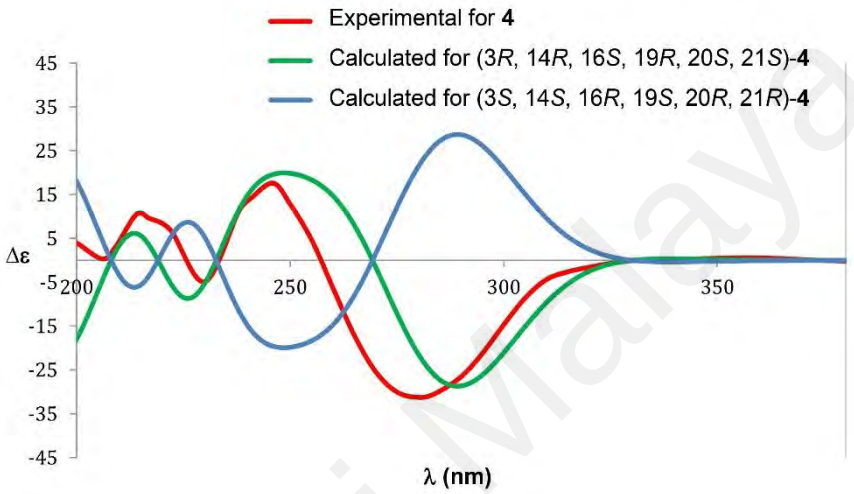


Figure 2.16: Experimental ECD spectrum of **4** and calculated ECD spectra of (3*R*, 14*R*, 16*S*, 19*R*, 20*S*, 21*S*)-**4** and (3*S*, 14*S*, 16*R*, 19*S*, 20*R*, 21*R*)-**4**

Polyneurine E (**5**) was obtained in minute amount as a light orange oil, $[\alpha]^{25}_{D}$ –29 (*c* 0.09, $CHCl_3$). The UV spectrum showed typical indole absorption maxima at 227, 286, and 293 nm, while the IR spectrum showed absorption bands due to NH (3378 cm^{-1}), ester (1726 cm^{-1}), and aldehyde carbonyl (1717 cm^{-1}) functions. The HRMS ($[M + H]^+$ *m/z* 381.2174) data established the molecular formula of **5** as $C_{23}H_{28}N_2O_3$, which is 16 mass units less than **4**, suggesting a deoxy derivative of **4**.

The ^1H and ^{13}C NMR data (Tables 2.5 and 2.6) of **5** showed similarities with those of **4**, such as the presence of a formyl group (δ_H 9.77; δ_C 202.5), an indolic NH (δ_H 7.80), four aromatic hydrogens (δ_H 7.09–7.47) and a methyl ester group (δ_H 3.71; δ_C 52.7, 175.4). The only notable difference in the ^1H and ^{13}C NMR data between **5** and **4** was

the replacement of signals due to the hydroxyethyl side chain present in **4** with signals due to an ethyl side chain in **5**. This observation was also consistent with the presence of a fragment, $CH_2CHCH_2CHCH_2CH_3$, which corresponds to the C-17–C-14–C-15–C-20–C-19–C-18 partial structure (Figure 2.17). The ethyl side chain substitution at C-20 was also indicated from the HMBC data (Figure 2.17) which showed the following three-bond correlations, H-18/C-20, H-15/C-19, and H-19/C-21.

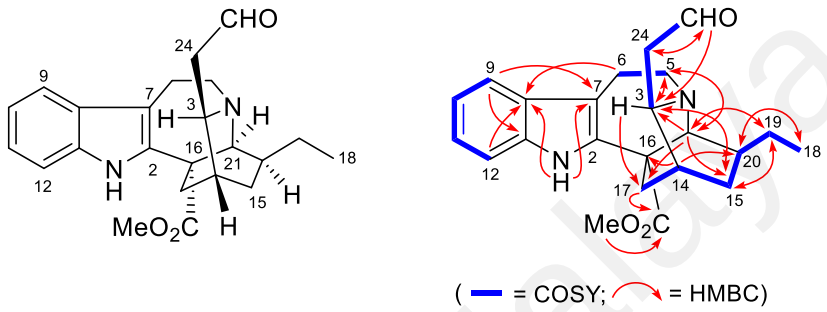


Figure 2.17: COSY and selected HMBCs of **5**

Examination of the NOE data (Figure 2.18) of **5** showed that its relative configuration was similar to those of **3** and **4**. The absolute configuration of **5** was established as (3*R*, 14*R*, 16*S*, 20*S*, 21*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.19).

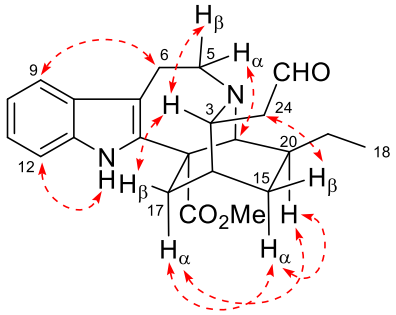


Figure 2.18: Selected NOEs of **5**

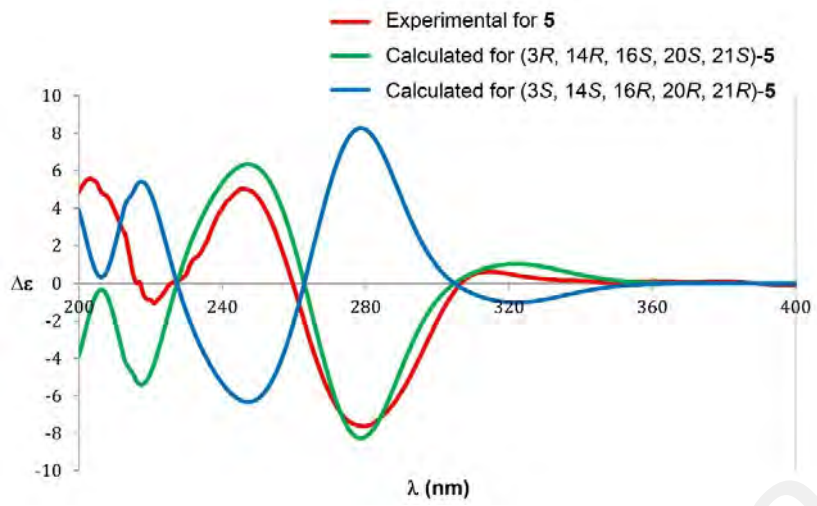
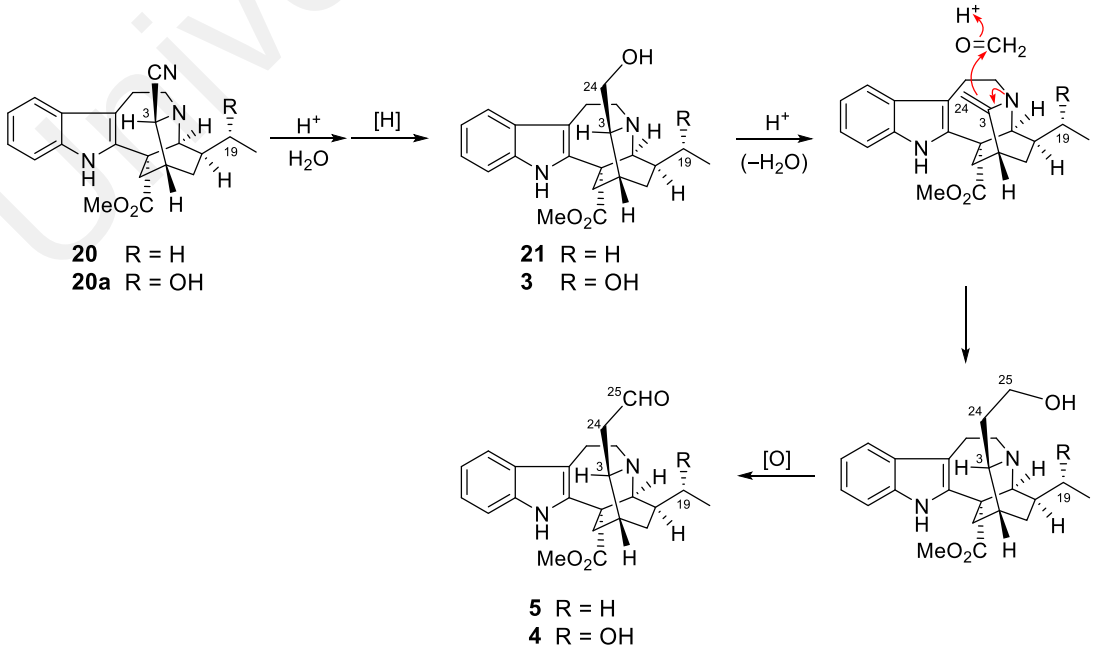


Figure 2.19: Experimental ECD spectrum of **5** and calculated ECD spectra of (3*R*, 14*R*, 16*S*, 20*S*, 21*S*)-**5** and (3*S*, 14*S*, 16*R*, 20*R*, 21*R*)-**5**

A plausible biosynthetic pathway to **3**, **4**, and **5** from an iboga precursor, 3(*S*)-cyanocoronaridine (**20**) (Kam, Pang *et al.*, 2004) is shown in Scheme 2.2. Hydrolysis of **20** followed by reduction leads to ervatamine G (**21**) (Zhang, Yu *et al.*, 2015). Subsequent formation of the enamine, followed by an intermolecular enamine-formaldehyde reaction leads to the C-25 hydroxy intermediate, which upon oxidation leads to **5**. Compounds **3** and **4** may have formed from a similar biosynthetic pathway with the hypothetical 19*R*-hydroxy derivative of 3(*S*)-cyanocoronaridine **20a**.



Scheme 2.2: Possible biosynthetic pathway to **3**, **4**, and **5**

Table 2.5: ^{1}H NMR Spectroscopic Data (δ) of Polyneurines C (**3**), D (**4**), and E (**5**)

H	**3**^{a} (J/Hz)	**4**^{b} (J/Hz)	**5**^{a} (J/Hz)
3	2.94 t (6.0)	3.45 t (5.7)	3.42 dd (8.0, 4.4)
5β	3.26 m	3.15 m	3.19 m
5α	3.39 m	3.39 m	3.32 m
6	3.14 m	3.15 m	3.04 dt (16.0, 6.0)
6	3.14 m	3.15 m	3.19 m
9	7.47 d (8.0)	7.47 d (8.0)	7.47 d (8.0)
10	7.10 td (8.0, 1.0)	7.11 td (8.0, 1.0)	7.09 td (8.0, 1.0)
11	7.17 td (8.0, 1.0)	7.18 td (8.0, 1.0)	7.15 td (8.0, 1.0)
12	7.26 d (8.0)	7.27 d (8.0)	7.25 d (8.0)
14	2.09 m	1.88 m	1.73 m
15	1.61 ddd (13.0, 11.0, 3.1) (α)	1.64 ddd (12.4, 10.5, 4.8) (α)	1.24 m (β)
15	1.93 ddt (13.0, 7.5, 2.1) (β)	1.88 m (β)	1.60 m (α)
17β	2.08 m	2.12 dt (14.0, 3.4)	2.00 ddd (13.7, 4.3, 2.6)
17α	2.66 dd (15.0, 3.5)	2.65 dd (14.0, 1.4)	2.66 m
18	1.27 d (6.4)	1.28 d (7.0)	0.89 t (7.5)
19	3.88 qd (6.4, 3.2)	3.89 qd (7.0, 2.8)	1.44 m
19	-	-	1.60 m
20	1.36 ddd (11.0, 7.5, 2.6)	1.38 ddd (10.5, 7.0, 2.5)	1.30 m
21	4.18 s	4.14 s	3.61 br s
24	3.68 m	2.75 m	2.53 ddd (16.0, 8.0, 2.5)
24	3.68 m	2.75 m	2.67 ddd (16.0, 8.0, 2.5)
CO_2Me	3.72 s	3.73 s	3.71 s
C*H*O	-	9.76 t (2.0)	9.77 t (2.5)
N(1)-H	7.89 br s	7.85 br s	7.80 br s

^{a}$CDCl_3$, 600 MHz; ^{b}$CDCl_3$, 400 MHz; assignments based on COSY, HSQC, and NOESY.

Table 2.6: ^{13}C NMR Spectroscopic Data (δ) of Polyneurines C (**3**), D (**4**), and E (**5**)

C	**3**[a]	**4**[b]	**5**[a]
2	135.5[c]	135.8[d]	136.4
3	60.5	53.6	54.3
5	51.1	50.5	51.4
6	21.6	21.8	22.0
7	109.9	109.9	110.1
8	128.3	128.6	128.7
9	118.4	118.7	118.4
10	119.5	119.8	119.4
11	122.3	122.7	122.1
12	110.5	110.7	110.4
13	135.6[c]	135.6[d]	135.5
14	28.6	31.1	31.5
15	24.3	24.1	26.7
16	53.9	53.9	54.8
17	38.0	37.7	37.7
18	22.2	22.3	11.7
19	70.8	71.0	27.0
20	40.3	40.2	38.5
21	54.7	55.0	58.0
24	62.0	46.3	47.6
*C*O$_2$Me	174.8	174.9	175.4
CO$_2$*Me*	52.9	53.1	52.7
*C*HO	-	201.4	202.5

[a]$CDCl_3$, 150 MHz; [b]$CDCl_3$, 100 MHz; [c–d]Interchangeable; assignments based on HSQC and HMBC.

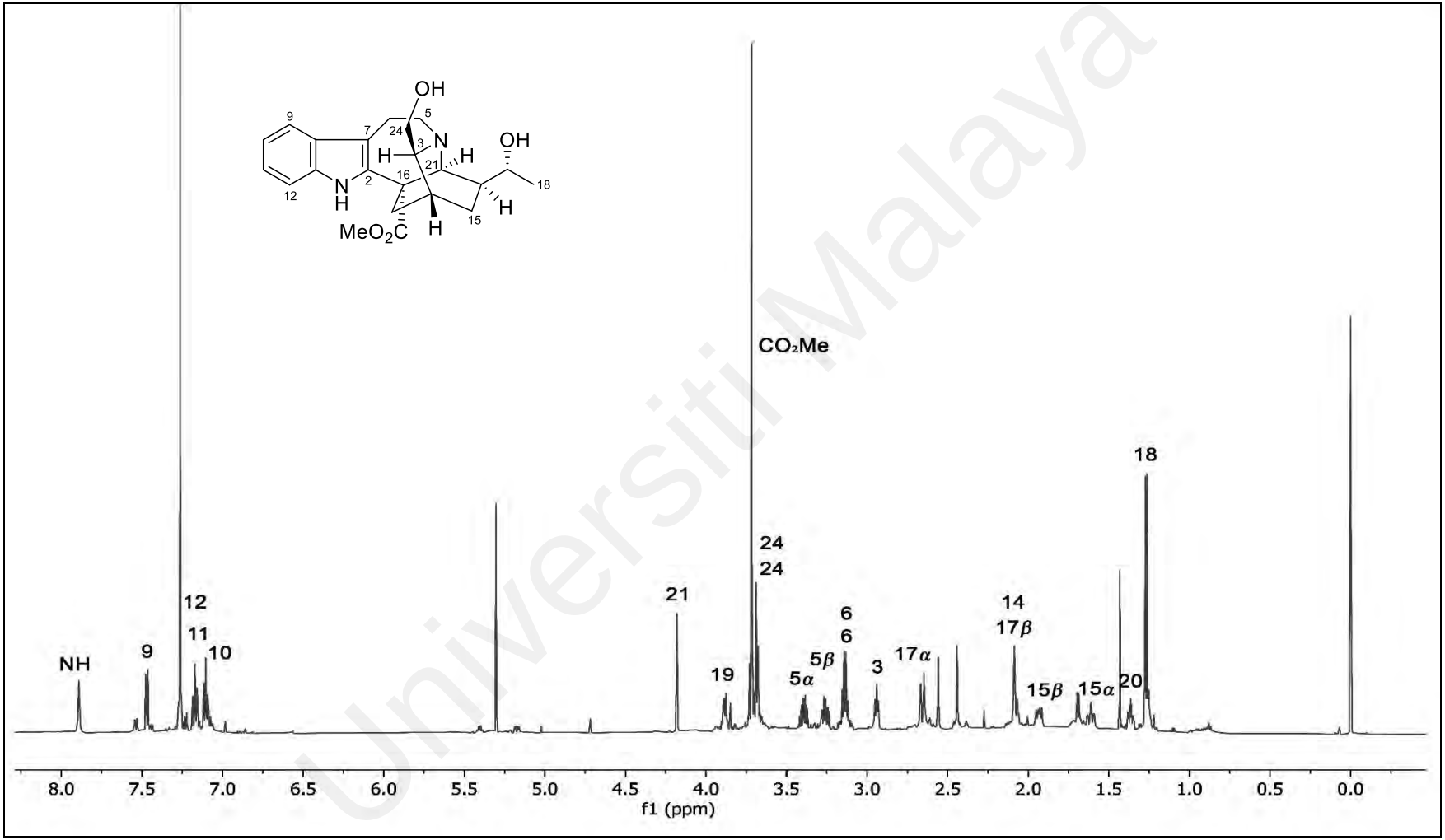


Figure 2.20: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Polyneurine C (**3**)

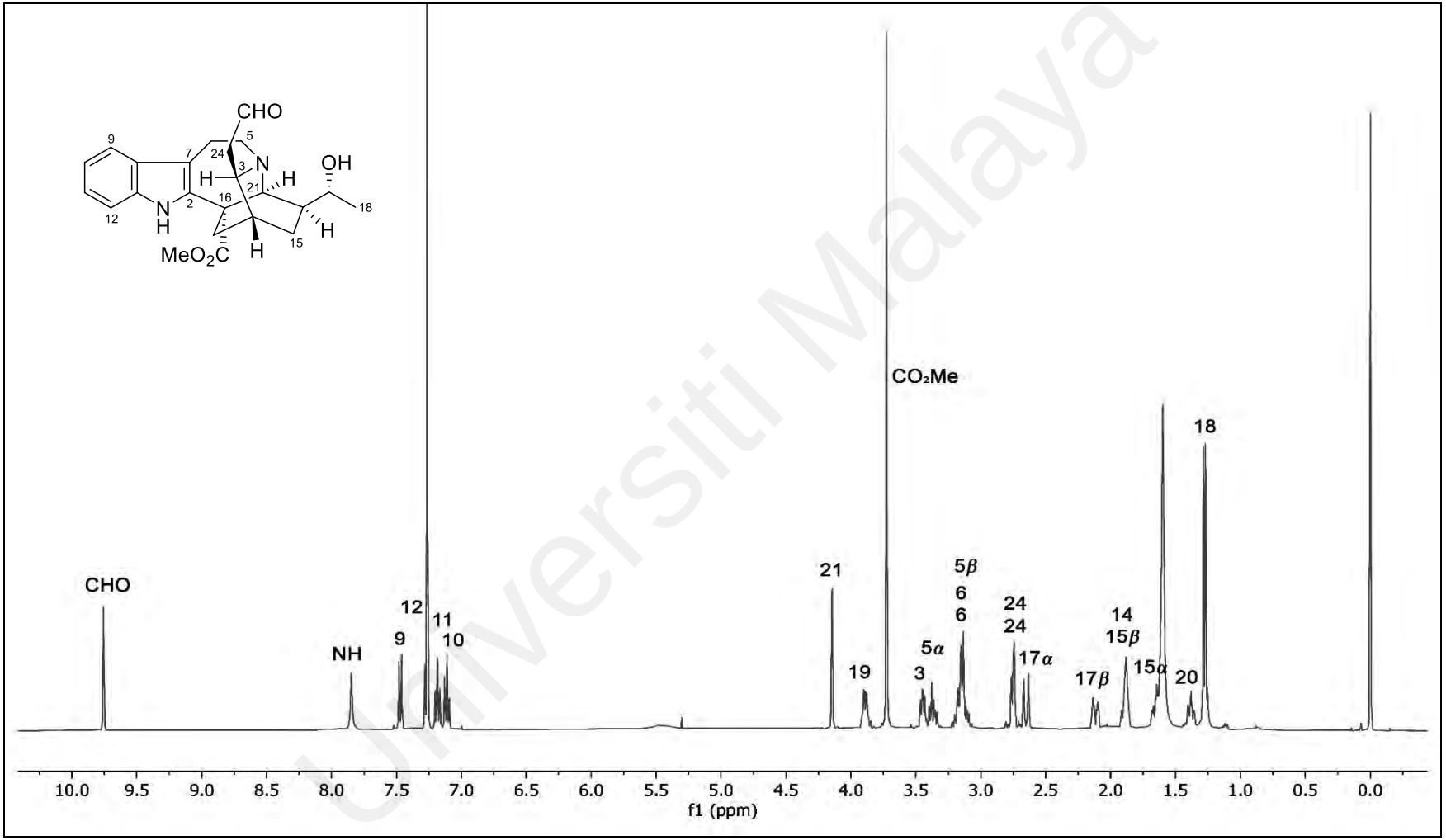


Figure 2.21: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Polyneurine D (**4**)

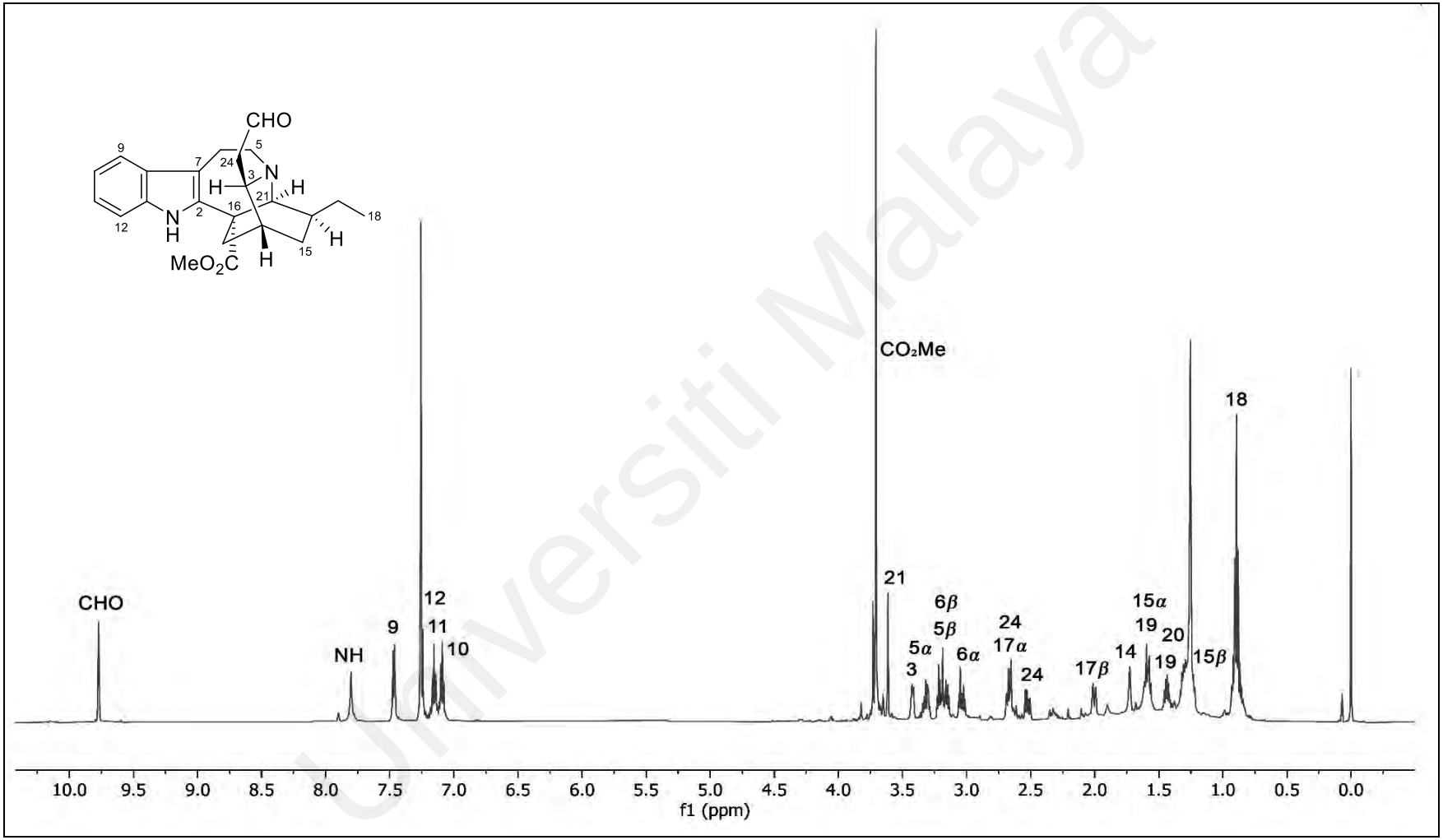


Figure 2.22: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Polyneurine E (**5**)

2.1.1.4 Polyneurine F (6)

Polyneurine F (**6**) was initially obtained as a light yellowish oil, $[\alpha]^{25}_{D}$ –43 (*c* 0.35, $CHCl_3$), and subsequently as light yellowish block crystals from EtOH (mp 153−154 °C). The UV spectrum showed absorption maxima at 223, 285, and 293 nm, which were characteristic of an indole chromophore, while the IR spectrum showed the presence of NH/OH (3331 cm^{-1}), ester (1732 cm^{-1}), and lactam (1657 cm^{-1}) functions. The HRMS data ($[M + H]^+$ *m/z* 369.1817) established the molecular formula of **6** as $C_{21}H_{24}N_2O_4$ + H.

The ^{13}C NMR data (Table 2.7) displayed a total of 21 carbon resonances, comprising six methylenes, seven methines, one methyl ester, one ester carbonyl, one amide carbonyl, two tertiary carbons linked to indolic NH, and three quaternary carbons, in agreement with the molecular formula. The ^{1}H NMR spectrum (Figure 2.26) showed the presence of an indolic NH (δ_H 8.12), an unsubstituted indole moiety (δ_H 7.09–7.48), a methyl ester (δ_H 3.72), and a 1-hydroxyethyl side chain (δ_H 3.74, 3.81, H-18; δ_H 1.64, 1.77, H-19).

The ^{13}C NMR data showed the presence of an oxymethylene at δ_C 60.2 and a methylene at δ_C 37.5, which were attributed to C-18 and C-19, respectively from the HSQC and COSY data (Figure 2.23). The COSY data indicated the presence of a $CH_2CHCH_2CHCH_2CH_2$ partial structure, which corresponds to C-17–C-14–C-15–C-20–C-19–C-18 in **6**. This was further confirmed by the three-bond correlations from H-18 (δ_H 3.74 and 3.81) to C-20 (δ_C 30.6), and from H-20 (δ_H 2.05) to C-18 (δ_C 60.2) (Figure 2.23). In addition, the presence of an amide carbonyl at C-3 was in agreement with the three-bond correlations observed from H-5, H-15, H-17, and H-21 to C-3 (δ_C 176.3) (Figure 2.23). Additionally, the presence of the C-3 carbonyl has resulted in a noticeable anisotropic deshielding of H-5β (δ_H 4.48) (Nge, Chong *et al.*, 2016),

compared to δ_H 3.1–3.4 for H-5β in **1**, **3**–**5**. The NOE data (Figure 2.24) also showed that the relative configuration of **6** was similar to that of compounds **1**–**5**.

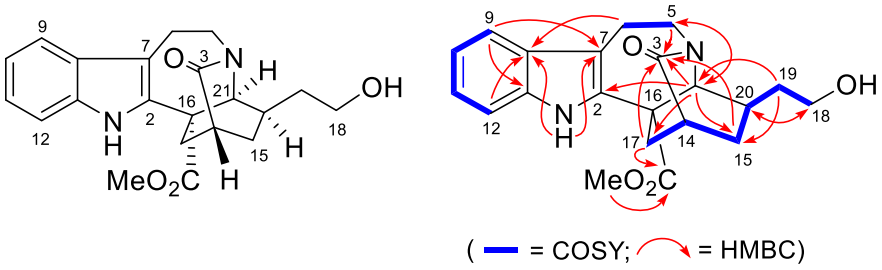


Figure 2.23: COSY and selected HMBCs of **6**

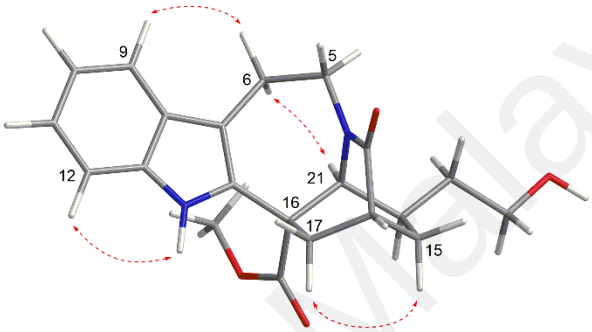


Figure 2.24: Selected NOEs of **6**

Since suitable crystals were obtained, an X-ray diffraction analysis was also carried out which confirmed the structure and provided the absolute configuration of **6** (14*R*, 16*S*, 20*R*, 21*S*) (Figure 2.25). The crystal data and structure refinement parameters of **6** are summarized in Table 2.8.

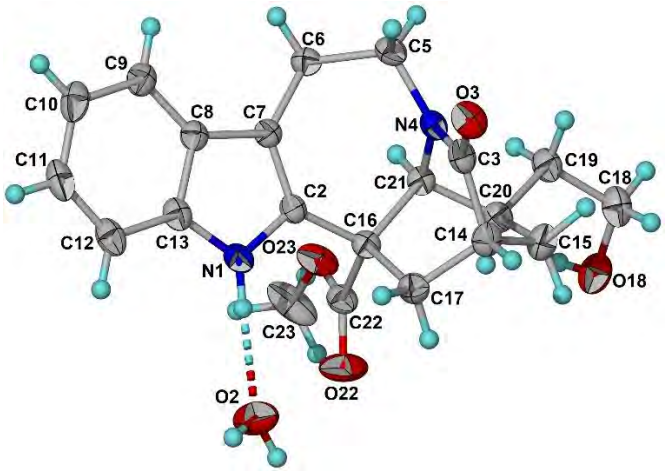


Figure 2.25: X-ray crystal structure of **6**

Table 2.7: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of Polyneurines F (**6**) and G (**7**)[a]

H/C	**6**		**7**	
	δ_H (J/Hz)	δ_C	δ_H (J/Hz)	δ_C
2	-	133.9	-	135.7[b]
3	-	176.3	2.81 d (9.6)	50.9
3	-		3.05 m	
5	3.23 m (α)	42.9	3.10 m (β)	52.1
5	4.48 m (β)		3.42 m (α)	
6	3.23 m	21.1	3.13 m	21.6
6	3.23 m		3.13 m	
7	-	109.5	-	109.8
8	-	127.9	-	128.6
9	7.48 d (8.0)	118.5	7.47 d (8.0)	118.6
10	7.09 t (8.0)	119.7	7.08 td (8.0, 1.0)	119.6
11	7.15 t (8.0)	122.5	7.16 td (8.0, 1.0)	122.5
12	7.25 d (8.0)	110.9	7.26 d (8.0)	110.7
13	-	135.9	-	135.6[b]
14	2.61 m	38.2	2.00 m	26.9
15	1.41 m	31.1	1.83 m	28.3
15	2.02 m		1.83 m	
16	-	55.6	-	53.8
17β	2.33 ddd (13.7, 4.2, 2.6)	35.9	2.00 m	36.8
17α	2.63 m		2.59 dd (12.0, 2.8)	
18	3.74 m	60.2	3.61 m	65.8
18	3.81 m		3.76 m	
19	1.64 m	37.5	3.78 m	75.5
19	1.77 m			
20	2.05 m	30.6	1.64 t (8.8)	35.8
21	4.61 br s	56.4	4.08 s	54.9
*C*O$_2$Me	-	173.2	-	175.0
CO$_2$*Me*	3.72 s	53.3	3.73 s	53.1
N(1)-H	8.12 br s	-	8.13 br s	-

[a]$CDCl_3$, 400 (^{1}H) and 100 MHz (^{13}C); [b]Interchangeable; assignments based on COSY, HSQC, HMBC, and 1D/2D NOESY.

Table 2.8: Crystal Data and Structure Refinement Parameters of Polyneurine F (**6**)

Molecular formula	$C_{21}H_{24}N_2O_4.H_2O$
Molecular weight, M_r	386.44
Melting point	153–154 °C
Temperature during diffraction experiment, T	293(2) K
X-ray source	Cu $K\alpha$ (λ = 1.54184 Å)
Crystal system	triclinic
Space group	$P1$
a	7.8152(6) Å
b	9.4777(9) Å
c	13.9307(12) Å
α	77.234(8)°
β	79.526(7)°
γ	89.595(7)°
Volume, V	988.98(15) $Å^3$
No. of molecule per unit cell, Z	2
Density (calcd)	1.298 g/cm^3
μ	0.763 mm^{-1}
$F(000)$	412
Crystal size	0.2 × 0.1 × 0.03 mm^3
2θ range for data collection	9.578 to 149.212°
Index ranges	$-9 \le h \le 9$, $-11 \le k \le 11$, $-17 \le l \le 17$
Reflections collected	15960
Independent reflections	7405 [R_{int} = 0.0594, R_{sigma} = 0.0665]
Data/restraints/parameters	7405/3/519
Goodness-of-fit on F^2	1.029
Final R indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0507, wR_2 = 0.1071
Final R indexes [all data]	R_1 = 0.0889, wR_2 = 0.1546
Largest diff. peak/hole / e $Å^{-3}$	0.17/–0.18
Flack parameter, x	–0.09(19)
Hooft parameter, y	–0.10(18)
Parson parameter, z	–0.1(2)
CCDC Number	2169030

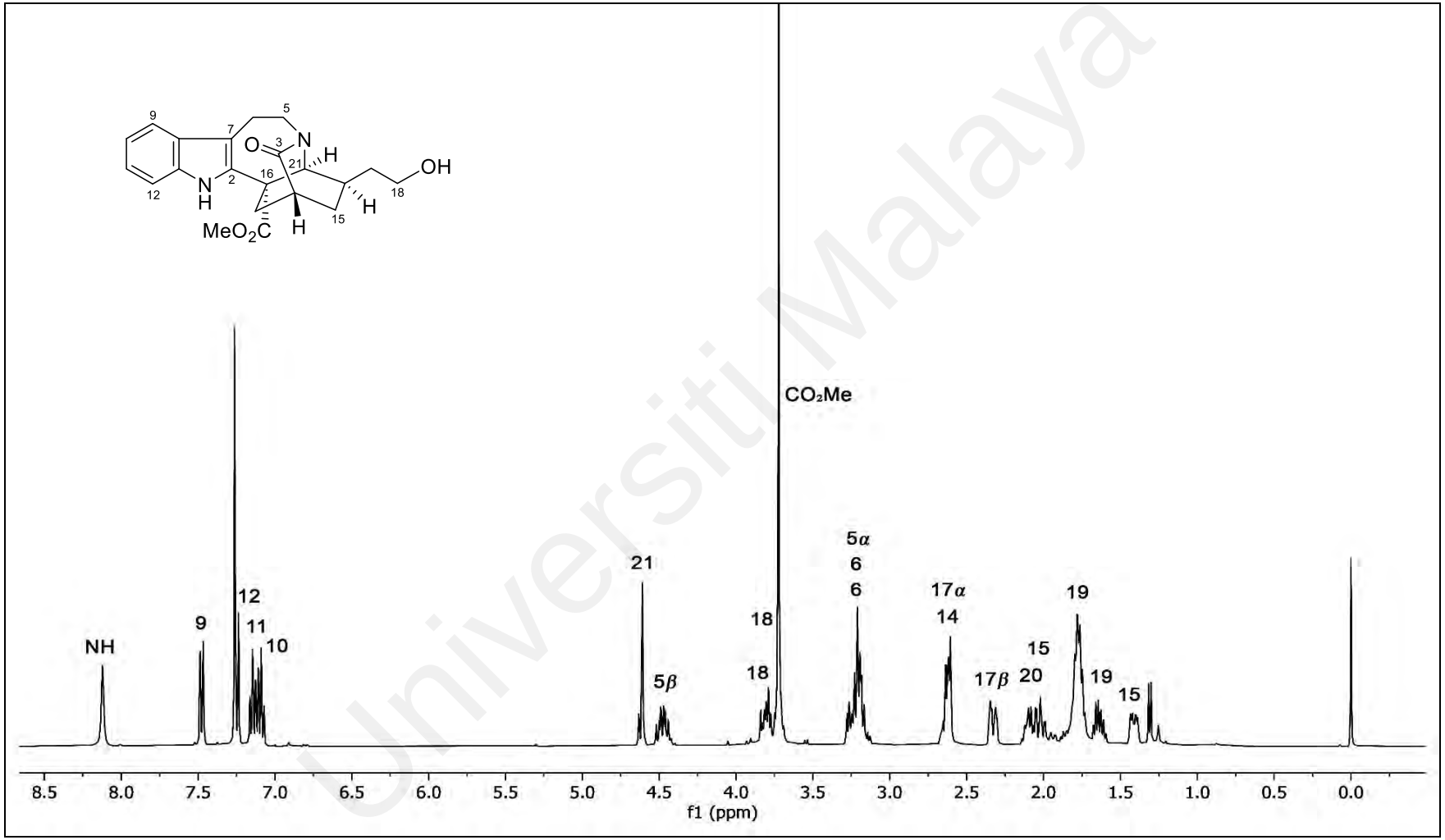


Figure 2.26: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Polyneurine F (**6**)

2.1.1.5 Polyneurine G (7)

Polyneurine G (**7**) was isolated as an orange oil, $[\alpha]^{25}_{D}$ –25 (*c* 0.46, $CHCl_3$). The UV spectrum showed absorption maxima indicative of an indole chromophore at 225, 285, and 293 nm, while the IR spectrum showed the presence of NH/OH and ester groups at 3376 and 1728 cm^{-1}, respectively. The HRMS data ($[M + H]^+$ *m/z* 371.1984) established the molecular formula of **7** as $C_{21}H_{26}N_2O_4 + H$.

The ^1H NMR spectrum (Figure 2.31) showed the presence of an indolic NH (δ_H 8.13), four aromatic hydrogens (δ_H 7.08–7.47), a methyl ester (δ_H 3.73) and a 1,2-disubstituted ethyl side chain (δ_H 3.61, 3.76, H-18; δ_H 3.78, H-19). The ^{13}C NMR data (Table 2.7) indicated 21 carbon resonances, comprising six methylenes, eight methines, one methyl ester, one ester carbonyl, two tertiary carbons linked to indolic NH, and three quaternary carbons.

The COSY and HMBC data (Figure 2.27) led to the elucidation of the structure for the compound as the vicinally-dihydroxysubstituted coronaridine derivative (18,19-dihydroxycoronaridine). The oxymethylene and oxymethine resonances corresponding to the vicinally-dihydroxysubstituted C-18–C-19 were seen at δ_C 65.8 and 75.5, respectively.

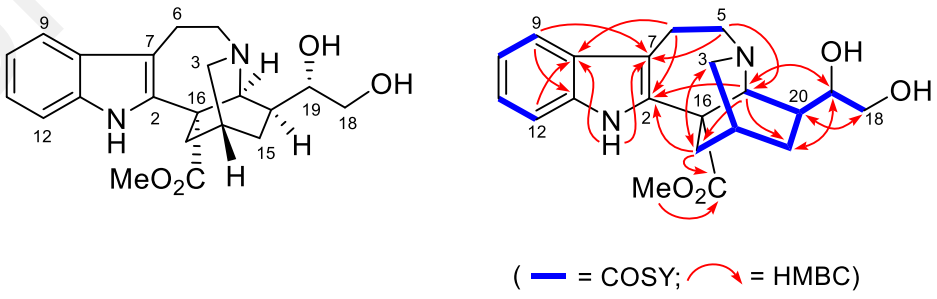


Figure 2.27: COSY and selected HMBCs of **7**

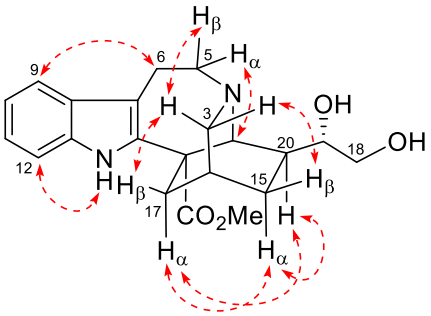
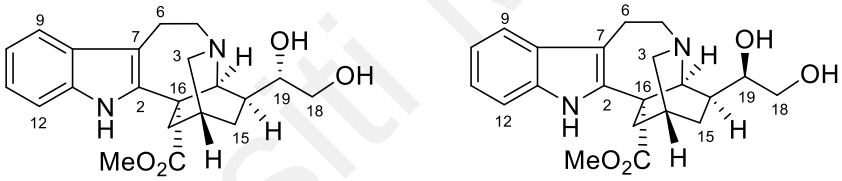


Figure 2.28: Selected NOEs of **7**

A search of the literature revealed that this 2D structure was previously assigned to 18,19-dihydroxycoronaridine (**458**) (Azoug *et al.*, 1995), which does not possess identical ^{1}H and ^{13}C NMR data to those of **7**, suggesting **7** to be an epimer of **458** (Figure 2.29). Since the relative configurations at C-14, C-16, C-20, and C-21 were found to be identical to those of compounds **1**–**6**, the only stereochemical difference between compounds **7** and **458** must be at C-19.



7 **458**

Figure 2.29: Structures of **7** and **458**

The stereochemistry at C-19 was assigned by comparing the ^{13}C NMR data of **7** and **458** with those of 19*R*- and 19*S*-heyneanine (Takayama *et al.*, 1994; Wenkert, Cochran *et al.*, 1976). In **7**, C-15 and C-21 were observed at δ_C 28.3 and δ_C 54.9, respectively, which correspond to the corresponding carbon shifts in the 19*R*-hydroxyiboga alkaloid series such as 19-*epi*-heyneanine (i.e., C-15 at *ca.* δ_C 29; C-21 at *ca.* δ_C 55). On the contrary, C-15 and C-21 of **458** were found at δ_C 23.7 and δ_C 59.2, respectively (Azoug *et al.*, 1995), which are consistent with those found in the 19*S*-hydroxyiboga alkaloid series such as heyneanine. We can therefore deduce that compound **7** possesses an opposite relative configuration at C-19 (*i.e.*, *S*), compared to **458** with a 19*R*

configuration (Azoug *et al.*, 1995). The deduction was further confirmed by GIAO NMR calculations and DP4+ analysis. The experimental NMR data were compared with the calculated ^{1}H and ^{13}C NMR shifts of **7** and its C-19 epimer using DP4+ analysis. The DP4+ results supported **7** with 19*S* configuration as the correct relative configuration, with 100% DP4+ probability (all data). Finally, the absolute configuration of **7** was established as (14*R*, 16*S*, 19*S*, 20*S*, 21*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.30). Compound **7** is thus identified as 18,19(*S*)-dihydroxycoronaridine.

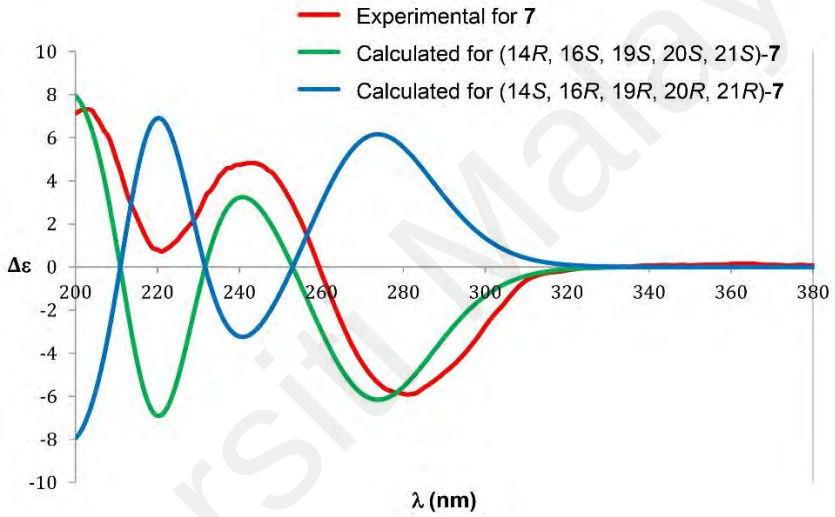


Figure 2.30: Experimental ECD spectrum of **7** and calculated ECD spectra of (14*R*, 16*S*, 19*S*, 20*S*, 21*S*)-**7** and (14*S*, 16*R*, 19*R*, 20*R*, 21*R*)-**7**

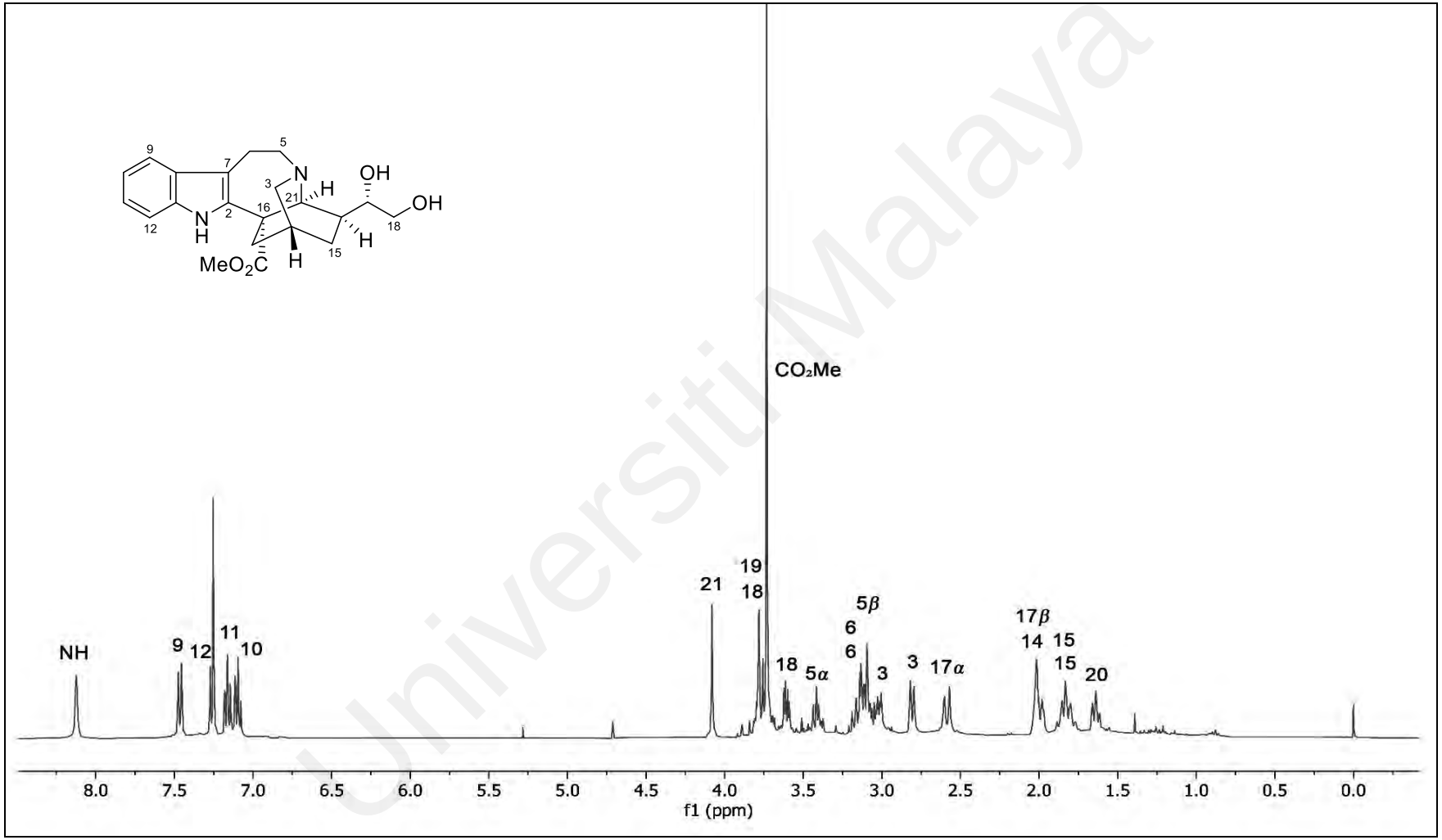


Figure 2.31: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Polyneurine G (**7**)

2.1.1.6 Polyneurine H (8)

Polyneurine H (**8**) was obtained as a yellowish oil, $[\alpha]^{25}_{D}$ –30 (*c* 0.12, $CHCl_3$). The UV spectrum exhibited absorption maxima indicative of a hydroxyindolenine chromophore at 223, 232 sh, 266, and 292 nm, while the IR spectrum showed the presence of OH and ester carbonyl groups at 3301 and 1732 cm^{-1}, respectively. The HRMS data ($[M + H]^+$ *m/z* 371.1952) established the molecular formula of **8** as $C_{21}H_{26}N_2O_4 + H$.

The ^1H and ^{13}C NMR data (Table 2.9) revealed the presence of four aromatic resonances of an unsubstituted indole moiety (δ_H 7.25–7.48), a methyl ester group (δ_H 3.71; δ_C 53.4, 172.9), a hydroxyethyl side chain (δ_H 1.24, 3.85; δ_C 22.2, 70.3), and a broad singlet at δ_H 3.26 due to an OH group (confirmed by D_2O exchange experiment). The imine function in **8** was readily identified from the characteristic C-2 resonance observed at δ_C 188.6, in addition to the absence of an indolic NH signal in the ^1H NMR spectrum (Figure 2.36). The oxygenated tertiary carbon (C-7) associated with the hydroxyindolenine was clearly observed at δ_C 88.0. Examination of the COSY and HMBC data (Figure 2.32) led to the structure as shown in **8**.

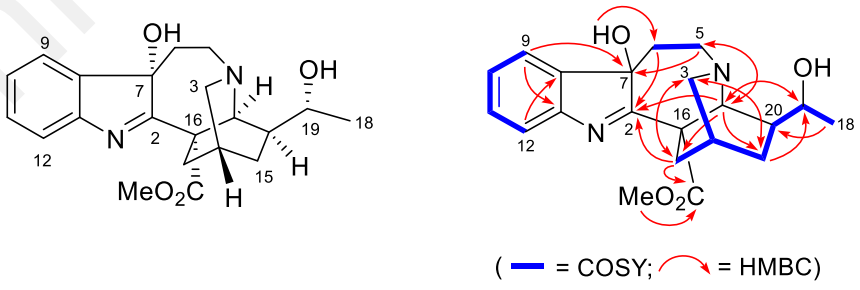


Figure 2.32: COSY and selected HMBCs of **8**

A search of the literature revealed that this 2D structure was previously assigned to heyneanine hydroxyindolenine (**512**) (Sharma *et al.*, 1988; Zèches-Hanrot *et al.*, 1995), which does not have identical NMR data to those of **8**, suggesting **8** to be a diastereomer

of **512** (Figure 2.33). Since the relative configurations at C-14, C-16, C-20, and C-21 were established to be the same as those of compounds **1**–**7**, the stereochemical differences between compounds **8** and **512** must be at C-7 and/or C-19.

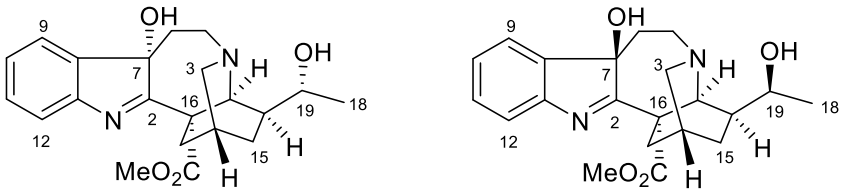


Figure 2.33: Structures of **8** and **512**

As with compounds **3**, **4**, and **7**, the C-19 configuration of **8** was readily determined as *R* from the observed carbon shifts of C-15 (δ_C 28.5) and C-21 (δ_C 54.2), which correspond to those of the 19*R*-hydroxyiboga alkaloid series (*vide supra*) such as 19-*epi*-heyneanine (C-15 at *ca.* δ_C 29 and C-21 at *ca.* δ_C 55) (Takayama *et al.*, 1994; Wenkert, Cochran *et al.*, 1976). The 19*R* configuration was also supported by the GIAO NMR calculations and DP4+ analysis of **8**, which showed 100% probability (all data). The 7*S*-configuration was assigned based on the NOE interaction observed between H-21 and 7-OH (Figure 2.34). Finally, the absolute configuration of **8** was established as (7*S*, 14*R*, 16*S*, 19*R*, 20*S*, 21*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.35). Compound **8** is therefore the 7*S*, 19*R* diastereomer of 7*R*, 19*S*-heyneanine hydroxyindolenine (**512**).

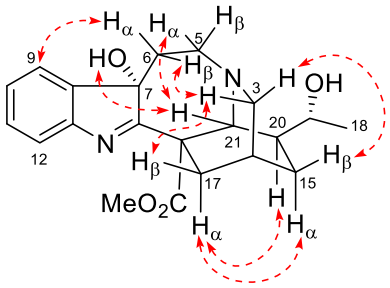


Figure 2.34: Selected NOEs of **8**

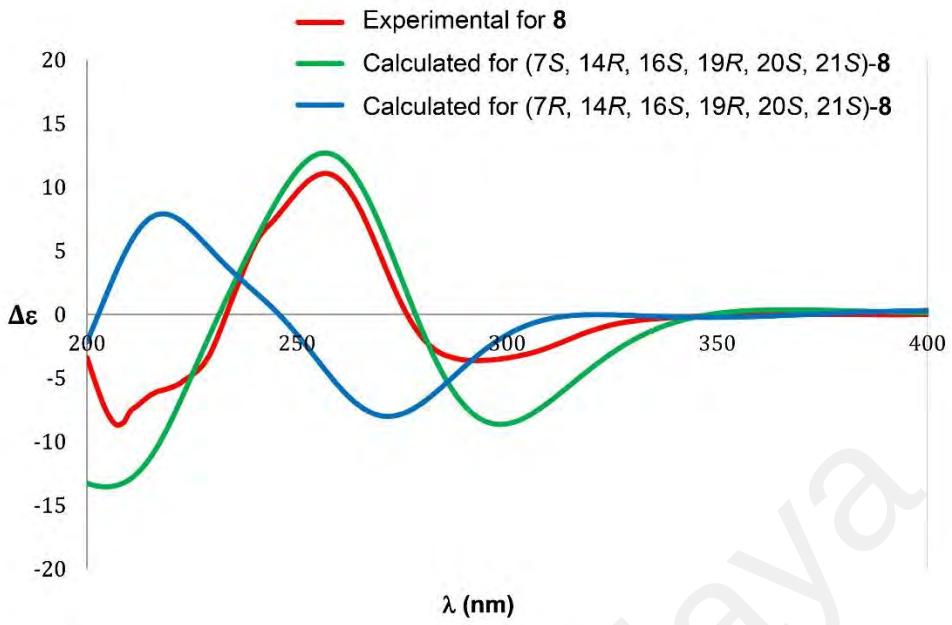


Figure 2.35: Experimental ECD spectrum of **8** and calculated ECD spectra of (7*S*, 14*R*, 16*S*, 19*R*, 20*S*, 21*S*)-**8** and (7*R*, 14*R*, 16*S*, 19*R*, 20*S*, 21*S*)-**8**

Table 2.9: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of Polyneurine H (**8**)[a]

H/C	δ_H (*J*/Hz)	δ_C	H/C	δ_H (*J*/Hz)	δ_C
2	-	188.6	14	2.06 m	26.8
3	2.72 d (9.2)	48.1	15	1.78 m	28.5
3	2.85 dt (9.2, 3.9)		15	1.78 m	
5β	2.89 ddd (14.5, 4.6, 1.8)	47.8	16	-	57.6
5α	3.61 td (14.5, 3.1)		17β	2.51 ddd (14.0, 4.6, 2.6)	35.2
6β	1.83 m	33.0	17α	2.80 dt (14.0, 2.1)	
6α	2.07 m		18	1.24 d (6.5)	22.2
7	-	88.0	19	3.85 qd (6.5, 3.1)	70.3
8	-	142.1	20	1.46 ddd (10.9, 7.7, 3.3)	39.3
9	7.36 d (8.0)	121.5	21	4.39 br s	54.2
10	7.25 td (8.0, 1.0)	127.0	*C*O$_2$Me	-	172.9
11	7.34 td (8.0, 1.0)	129.5	CO$_2$*Me*	3.71 s	53.4
12	7.48 d (8.0)	121.0	7-OH	3.26 s	-
13	-	151.3			

[a]$CDCl_3$, 600 (^{1}H) and 150 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and NOESY.

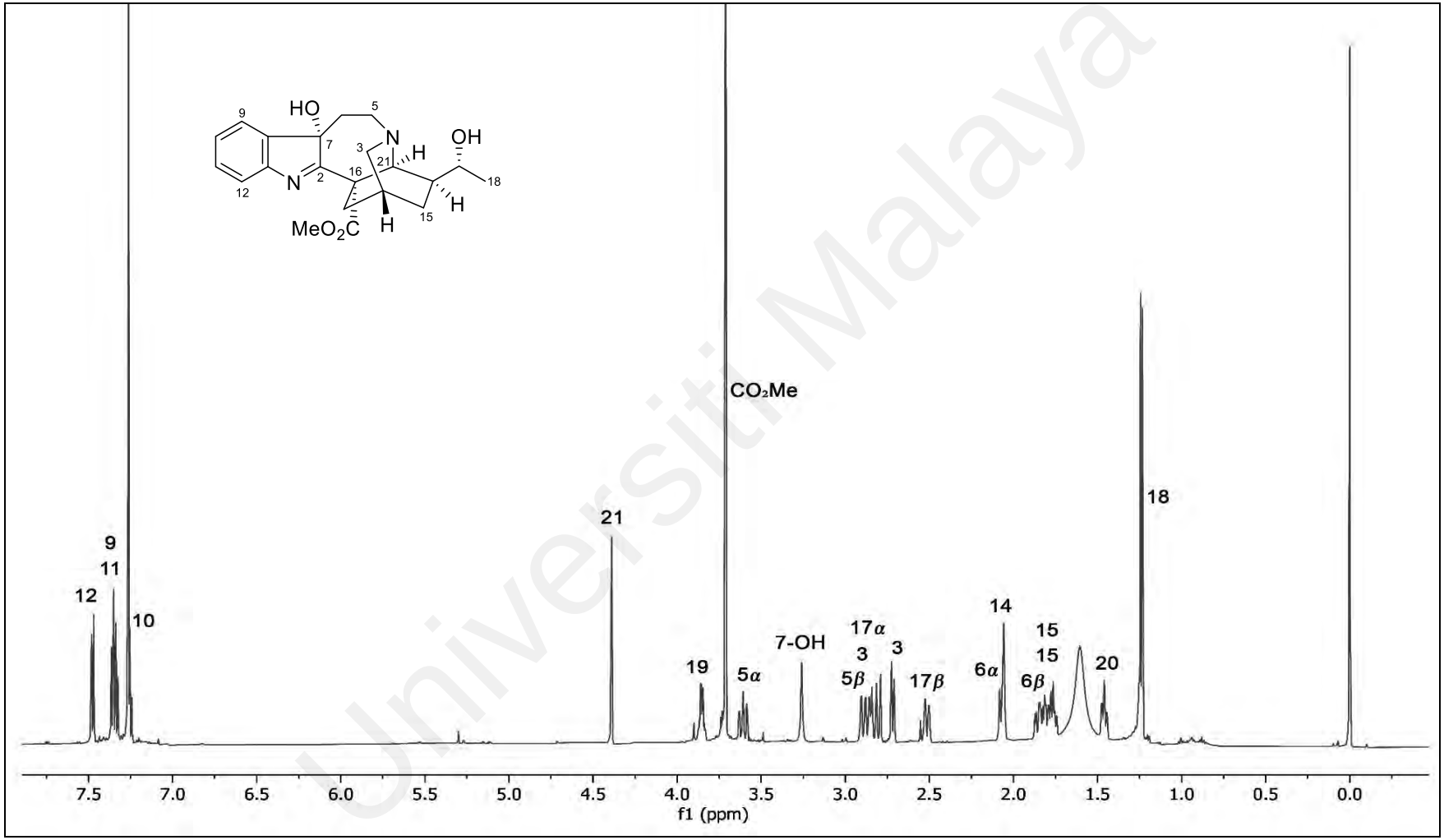


Figure 2.36: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Polyneurine H (**8**)

2.1.1.7 Polyneurine J (9)

Polyneurine J (**9**) was obtained as a light yellowish oil, $[\alpha]^{25}_{D}$ −14 (*c* 0.2, $CHCl_3$). The UV spectrum showed absorption maxima at 221 and 284 nm, indicating the presence of an indole chromophore, while the IR spectrum showed absorption bands at 3384 and 1719 cm^{-1}, suggesting the presence of OH/NH and ester carbonyl functions, respectively. The HRMS data showed an $[M + H]^+$ peak at *m/z* 355.2024, corresponding to the molecular formula $C_{21}H_{26}N_2O_3$ + H (DBE = 10).

The ^{1}H NMR spectrum (Figure 2.40) showed the presence of an indolic NH (δ_H 8.13), four aromatic resonances (δ_H 7.06–7.46) due to an unsubstituted indole moiety, and a methyl ester group (δ_H 3.83; δ_C 52.9, 175.0). The ^{13}C NMR data (Table 2.10) showed a total of 21 carbon resonances, including the characteristic downfield C-3 methylene resonance at δ_C 67.9, indicative of a *seco*-iboga skeleton. The ^{13}C NMR data of **9** closely resembled those of 3-hydroxy-3,4-*seco*coronaridine (**22**) (Clivio, Richard, Hadi *et al.*, 1990), except for the absence of the C-18 methyl triplet at δ_H 0.97 (δ_C 11.7), being replaced instead by a pair of methylene signals at δ_H 2.62 and 3.52 (δ_C 56.6).

The COSY data revealed the presence of NCH_2CH_2 and $CH_2CH(CH_2)CH_2CH(CH)CH_2CH_2$ partial structures, corresponding to N–C-5–C-6 and C-17–C-14(C-3)–C-15–C-20(C-21)–C-19–C-18, respectively (Figure 2.37). The methylene carbon at C-18 was deduced to be linked to N-4, forming an additional pyrrolidine ring, based on the observed three-bond correlations from H-5 to C-18 and C-21, as well as from H-18 to C-5 and C-21 in the HMBC spectrum (Figure 2.37). The presence of an additional pyrrolidine ring is in agreement with the DBE number of **9** (DBE = 10), *cf.*, DBE number of **22** is 9.

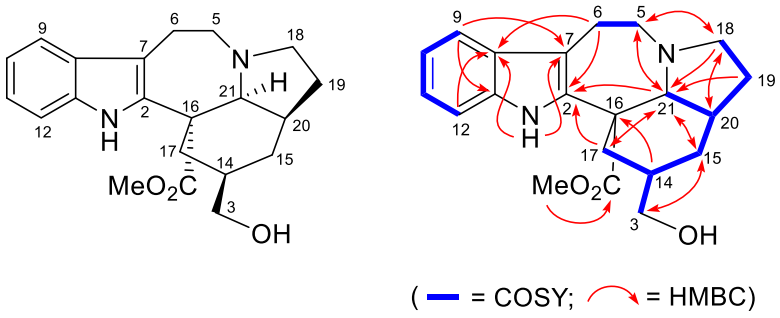


Figure 2.37: COSY and selected HMBCs of **9**

The relative configuration of **9** was determined based on the NOE data (Figure 2.38). The configurations at C-14 and C-20 were determined to be *R*, based on the observed H-20/H-14, H-15α NOEs, while the configuration at C-21 were found to be *S*, based on the H-21/H-5α, H-18α, and H-19α NOEs. The remaining configuration at C-16 was deduced to be *S*, based on the biogenetic grounds (iboga precursor). Finally, the absolute configuration of **9** was established as (14*R*, 16*S*, 20*R*, 21*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.39).

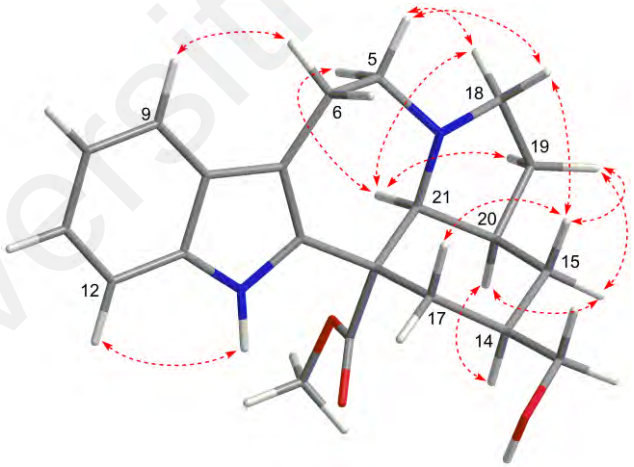


Figure 2.38: Selected NOEs of **9**

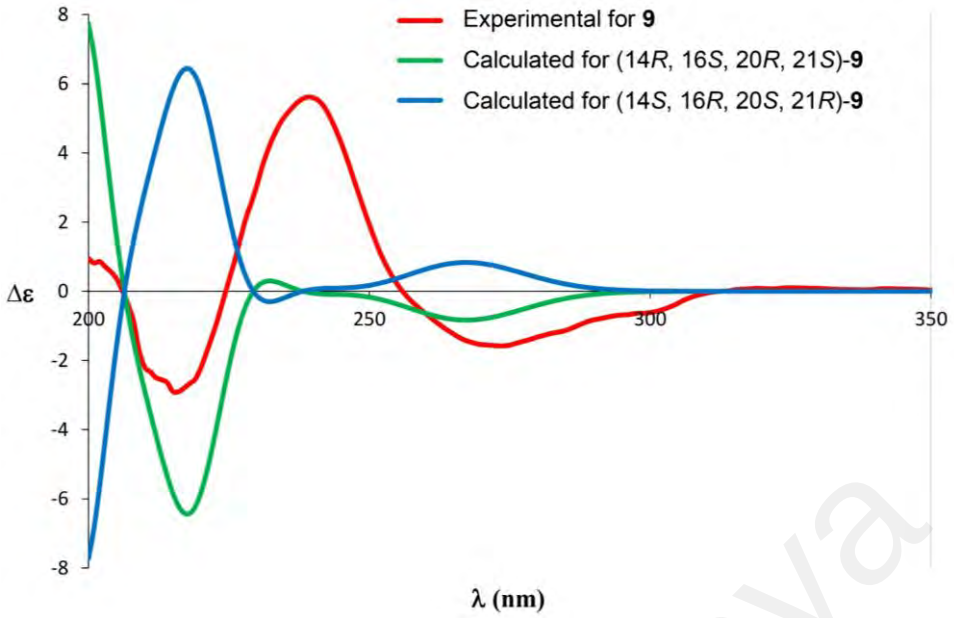
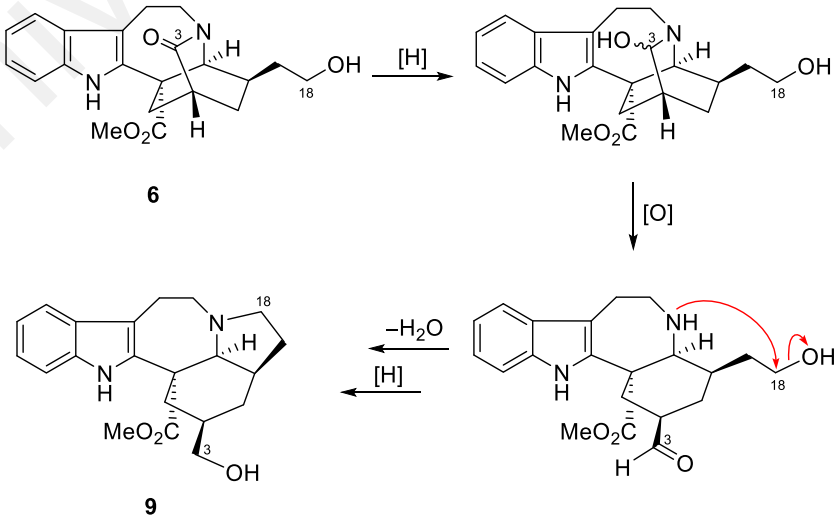


Figure 2.39: Experimental ECD spectrum of **9** and calculated ECD spectra of (14*R*, 16*S*, 20*R*, 21*S*)-**9** and (14*S*, 16*R*, 20*S*, 21*R*)-**9**

The precursor compound for **9** is postulated to be polyneurine E (**6**), an iboga alkaloid which was also found in the same system (Scheme 2.3). The reduction of **6**, followed by a hemiaminal cleavage of C-3–N-4 bond leads to a *seco*-coronaridine intermediate, which then undergoes a cyclization between N-4 and C-18 followed by a reduction to give **9**. Compound **9** represents the first example of a *seco*-iboga alkaloid that incorporates an additional pyrrolidine ring.



Scheme 2.3: Proposed biosynthetic pathway to **9**.

Table 2.10: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) for Polyneurine J (**9**)[a]

H/C	δ_H (J/Hz)	δ_C
2	-	134.3
3	3.44 d (5.5)	67.9
3	3.44 d (5.5)	
5α	2.65 ddd (14.7, 11.5, 2.5)	57.3
5β	3.29 dt (12.2, 4.0)	
6β	2.84 ddd (15.7, 11.5, 4.0)	25.1
6α	3.03 ddd (15.7, 4.0, 2.5)	
7	-	112.2
8	-	128.8
9	7.46 d (7.8)	118.4
10	7.06 td (7.8, 1.1)	119.4
11	7.13 td (7.8, 1.2)	122.1
12	7.24 d (7.8)	110.7
13	-	134.7
14	1.71 m	37.1
15β	1.25 q (12.5)	31.2
15α	1.55 m	
16	-	53.8
17β	1.68 m	34.2
17α	2.20 m	
18α	2.62 td (10.6, 3.8)	56.6
18β	3.52 q (9.1)	
19β	1.41 ddd (12.3, 9.0, 3.8)	28.9
19α	2.00 m	
20	2.24 m	39.8
21	3.36 d (3.8)	67.7
CO_2*Me*	3.83 s	52.9
CO_2Me	-	175.0
N(1)-H	8.13 br s	-

[a]$CDCl_3$, 400 (^{1}H) and 100 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and 1D/2D NOESY.

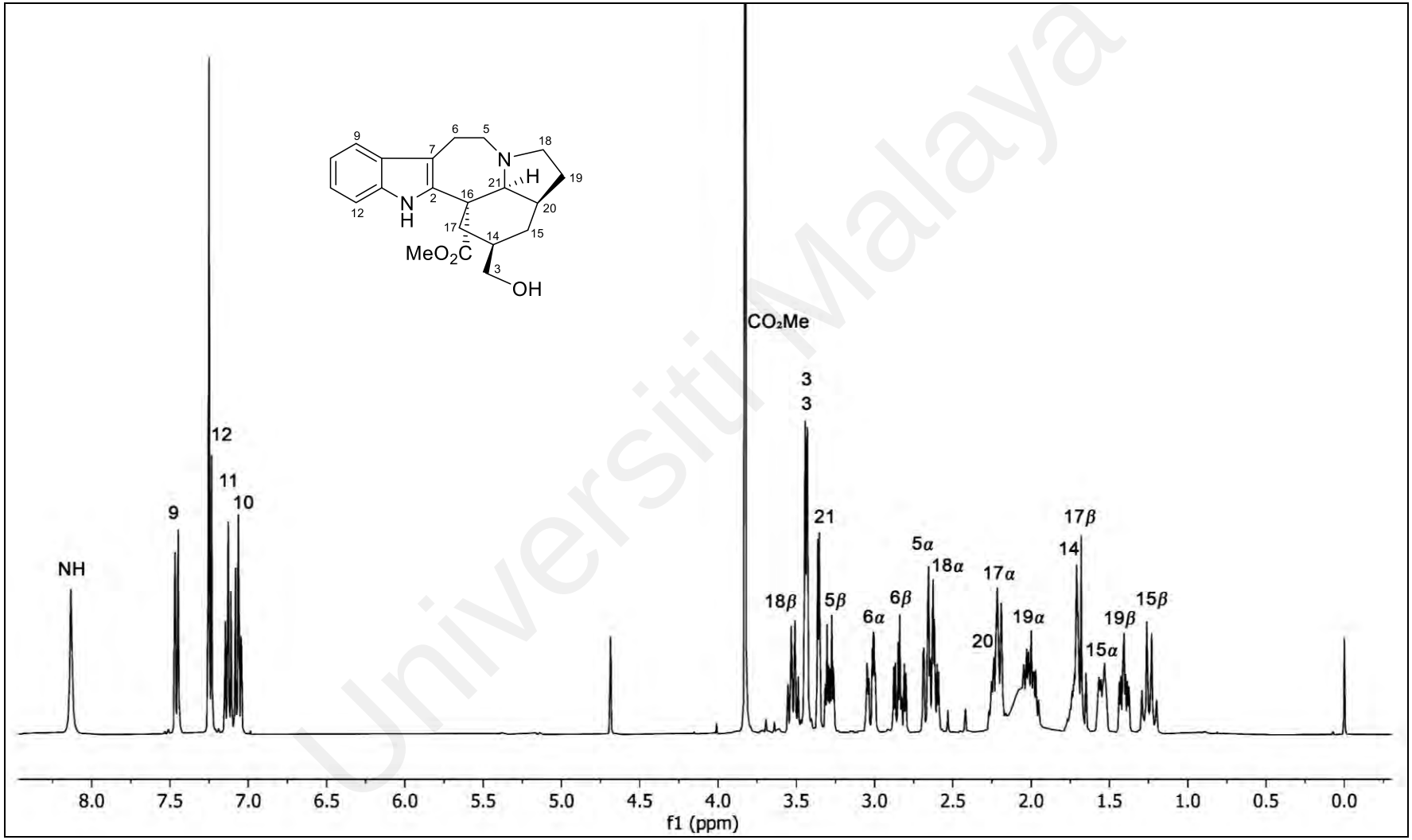


Figure 2.40: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Polyneurine J (**9**)

2.1.1.8 Polyneurine K (10)

Polyneurine K (**10**) was isolated as a yellowish oil, $[\alpha]^{25}_{D}$ −39 (*c* 0.2, $CHCl_3$). The UV spectrum showed absorption maxima at 220 and 286 nm, indicating the presence of an indole chromophore, while the IR spectrum showed the presence of OH/NH function (3267 cm^{-1}). The HRMS data showed an $[M + H]^+$ peak at *m/z* 297.1974, corresponding to the molecular formula $C_{19}H_{24}N_2O$ + H.

The ^{13}C NMR data (Table 2.11) showed resonances for all 19 carbons, including seven methylenes, eight methines, two tertiary carbons bonded to indolic NH, and two quaternary carbons, in agreement with the molecular formula. The ^{1}H NMR spectrum (Figure 2.44) showed the presence of an indolic NH (δ_H 7.72), four aromatic resonances of an unsubstituted indole moiety (δ_H 7.09–7.46), and a 1-hydroxyethyl side chain (δ_H 3.61, 3.85, CH_2-18; δ_H 1.80, 1.90, CH_2-19).

The COSY spectrum showed the presence of NCH_2CH_2 and $CHCH_2CH(CH_2)CH_2CH(CH)CH_2CH_2$ partial structures (Figure 2.41). The former corresponds to C-5–C-6 while the latter corresponds to C-16–C-17–C-14(C-3)–C-15–C-20(C-21)–C-19–C-18, suggesting an iboga-type carbon skeleton. The presence of the 1-hydroxyethyl side chain was confirmed by the carbon resonances of an oxymethylene and methylene at δ_C 58.3 and 37.0, attributed to C-18 and C-19, respectively. This was further confirmed by the three-bond correlations from H-18 to C-20, from H-20 to C-18, and from H-19 to C-15 and C-21 in the HMBC spectrum (Figure 2.41). The relative configuration was determined by analysis of the NOE data (Figure 2.42). The 14*R*, 16*R*, 20*R* and 21*S* configurations were consistent with the NOEs observed for N-H/H-16, H-16/H-20 and H-21/H-5α.

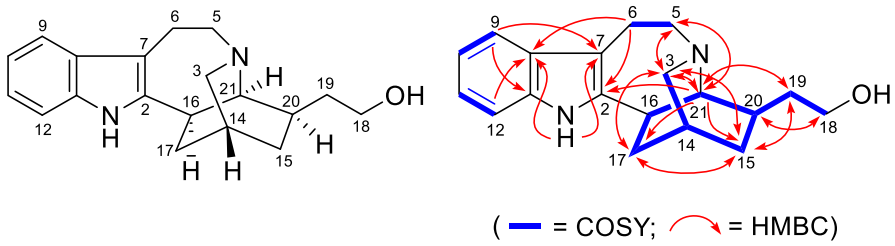


Figure 2.41: COSY and selected HMBCs of **10**

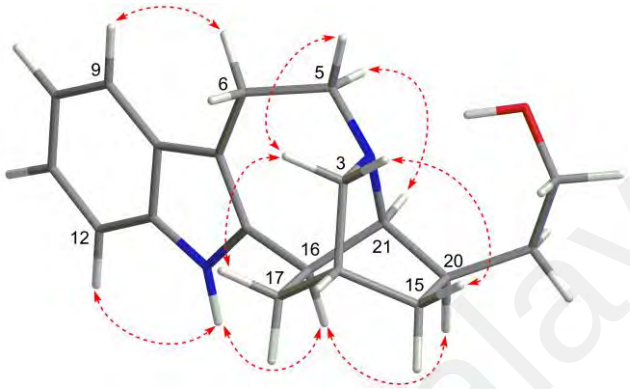


Figure 2.42: Selected NOEs of **10**

Compound **10** was first encountered as a synthetic product obtained during the total syntheses of racemic albifloranine and its congeners by Kuehne and co-workers (Bandarage *et al.*, 1999). Synthetic **10** was obtained from the decarbomethoxylation of racemic albifloranine and it has similar ^{1}H and ^{13}C NMR, MS, and IR spectroscopic data with those of natural **10**.

Finally, the absolute configuration of **10** was established as (14*R*, 16*R*, 20*R*, 21*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.43).

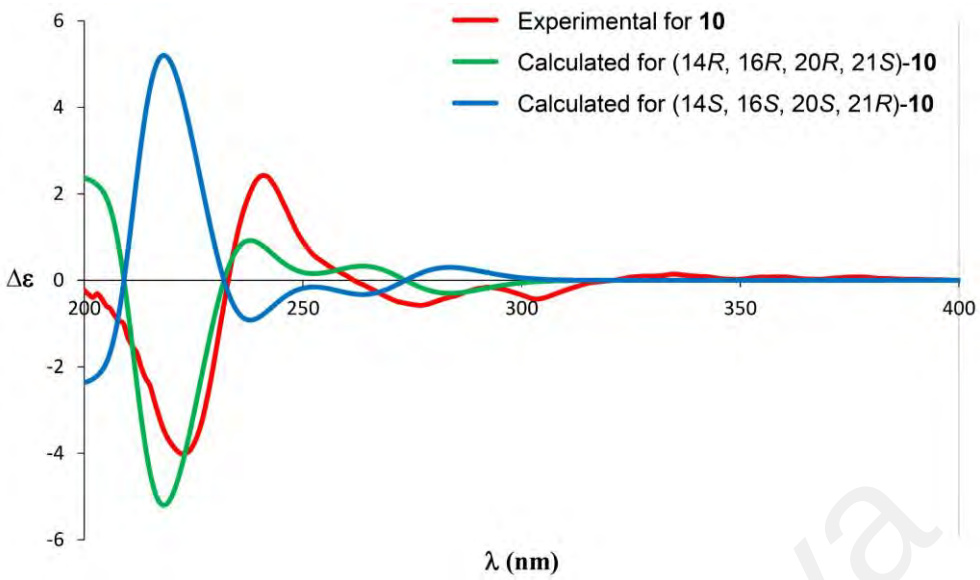


Figure 2.43: Experimental ECD spectrum of **10** and calculated ECD spectra of (14*R*, 16*R*, 20*R*, 21*S*)-**10** and (14*S*, 16*S*, 20*S*, 21*R*)-**10**

Table 2.11: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of Polyneurine K (**10**)[a]

H/C	δ_H (*J*/Hz)	δ_C	H/C	δ_H (*J*/Hz)	δ_C
2	-	140.8	14	1.96 m	25.9
3	3.01 m	49.2	15	1.63 m	27.6
3	3.06 m		15	1.72 m	
5α	3.16 m	53.4	16	3.06 m	41.0
5β	3.32 m		17	1.69 m	34.0
6α	2.76 m	20.0	17	2.13 m	
6β	3.31 m		18	3.61 m	58.3
7	-	108.8	18	3.85 m	
8	-	129.4	19	1.80 m	37.0
9	7.46 d (7.5)	117.9	19	1.90 m	
10	7.09 td (7.5, 1.3)	119.3	20	2.13 m	38.8
11	7.13 td (7.5, 1.3)	121.3	21	2.92 m	59.0
12	7.26 d (7.5)	110.2	N(1)-H	7.72 br s	-
13	-	134.7			

[a]$CDCl_3$, 600 (^{1}H) and 150 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and NOESY.

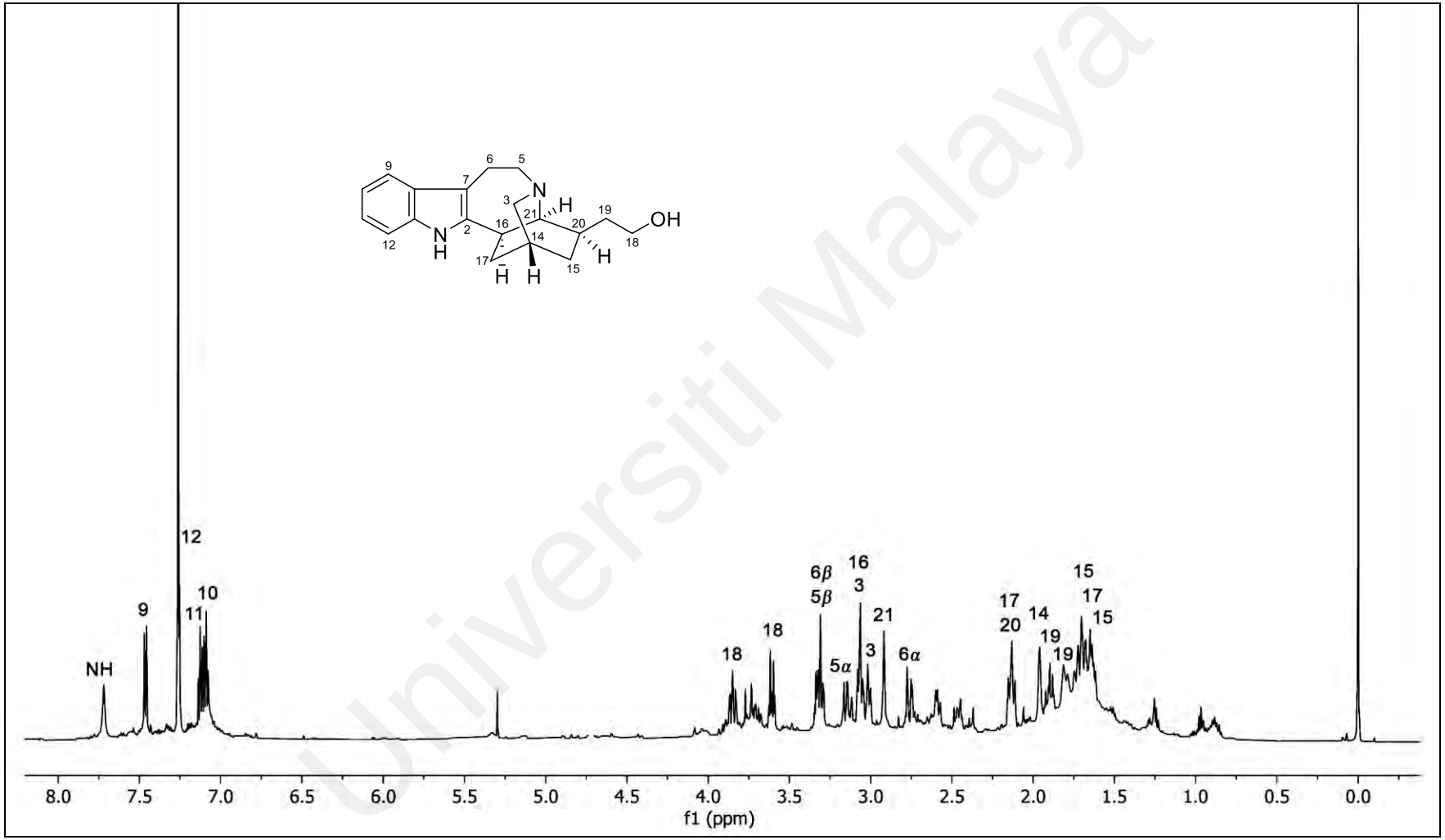


Figure 2.44: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Polyneurine K (**10**)

2.1.1.9 Ibogamine (11), 19(*S*)-Hydroxyibogamine (12), 19(*R*)-Hydroxyibogamine (13), Coronaridine (14), (–)-Albifloranine (15), (–)-Heyneanine (16), 19-*Epi*-heyneanine (17), 3-Oxo-19-*epi*-heyneanine (18), 3-Oxo-coronaridine (19), 3(*S*)-Cyanocoronaridine (20), Ervatamine G (21), 3-Hydroxy-3,4-*seco*coronaridine (22), Voacangine (23), Voacristine (24), Conopharyngine (25), 19(*S*)-Hydroxy-conopharyngine (26), Coronaridine pseudoindoxyl (27), Ibogamine 7(*S*)-hydroxyindolenine (28), Coronaridine-7-hydroxyindolenine (29)

Nineteen known iboga alkaloids including ibogamine (**11**) (Damak, Poupat *et al.*, 1976; Gorman *et al.*, 1960; Pereira *et al.*, 2008), 19(*S*)-hydroxyibogamine (**12**) (De Bellefon *et al.*, 1975; Kam & Sim, 2002a; Wenkert, Hagaman *et al.*, 1976), 19(*R*)-hydroxyibogamine (**13**) (Achenbach & Raffelsberger, 1980a; De Bellefon *et al.*, 1975; Hock & Borschberg, 2006), coronaridine (**14**) (Gorman *et al.*, 1960; Gunasekera *et al.*, 1980; Santos *et al.*, 2009), (–)-albifloranine (**15**) (Kan *et al.*, 1981a), (–)-heyneanine (**16**) (Govindachari *et al.*, 1965; Gunasekera *et al.*, 1980; Matos *et al.*, 1976), 19-*epi*-heyneanine (**17**) (Matos *et al.*, 1976), 3-oxo-19-*epi*-heyneanine (**18**) (Clivio, Richard, Hadi *et al.*, 1990), 3-oxo-coronaridine (**19**) (Feng *et al.*, 1982; Perera *et al.*, 1985), 3(*S*)-cyanocoronaridine (**20**) (Kam *et al.*, 2004), ervatamine G (**21**) (Zhang, Yu *et al.*, 2015), 3-hydroxy-3,4-*seco*coronaridine (**22**) (Clivio, Richard, Hadi *et al.*, 1990), voacangine (**23**) (Gorman *et al.*, 1960; Gunasekera *et al.*, 1979; Ladhar *et al.*, 1981; Santos *et al.*, 2009), voacristine (**24**) (Santos *et al.*, 2009), conopharyngine (**25**) (Renner *et al.*, 1959), 19(*S*)-hydroxy-conopharyngine (**26**) (Van Beek, Kuijlaars *et al.*, 1984), coronaridine pseudoindoxyl (**27**) (Husain *et al.*, 1997), ibogamine 7(*S*)-hydroxyindolenine (**28**) (Dickel *et al.*, 1958), and coronaridine-7-hydroxyindolenine (**29**) (Azoug *et al.*, 1995; Pereira *et al.*, 1999; Sharma & Cordell, 1988) were also isolated in the present study.

The absolute configuration of ibogamine 7(*S*)-hydroxyindolenine (**28**) was confirmed by the TDDFT-ECD (Figure 2.45). The ^{1}H NMR spectra of these compounds are shown in Figures 2.46–2.64, whereas the ^{1}H and ^{13}C NMR spectroscopic data are summarized in Tables 2.12–2.21. Other data are given in the Experimental Section.

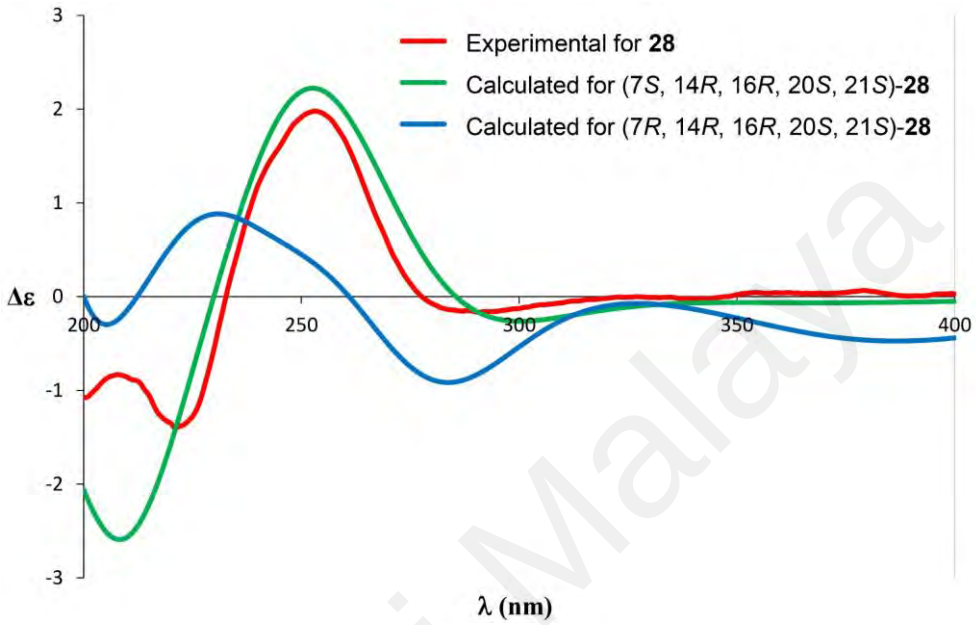


Figure 2.45: Experimental ECD spectrum of **28** and calculated ECD spectra of (7*S*, 14*R*, 16*R*, 20*S*, 21*S*)-**28** and (7*R*, 14*R*, 16*R*, 20*S*, 21*S*)-**28**

Table 2.12: ^{1}H NMR Spectroscopic Data (δ) of Ibogamine (**11**), 19(*S*)-Hydroxyibogamine (**12**), and 19(*R*)-Hydroxyibogamine (**13**)[a]

H	**11** (*J*/Hz)	**12** (*J*/Hz)	**13** (*J*/Hz)
3	2.98 dt (9, 3)	3.00 dt (10, 2)	3.06 m
3	3.07 dt (9, 2)	3.08 dt (10, 2)	3.06 m
5	3.16 m	3.20 ddd (15, 4, 1)	3.17 m
5	3.39 m	3.34 dt (15, 4)	3.31 m
6	2.68 m	2.75 ddd (16, 4, 1)	2.76 ddd (16, 4, 2)
6	3.33 m	3.31 dt (16, 4)	3.26 m
9	7.47 ddd (8, 2, 1)	7.46 br dd (8, 1)	7.46 br d (7)
10	7.08 td (8, 2)	7.09 td (8, 1)	7.09 td (7, 1)
11	7.11 td (8, 2)	7.12 td (8, 1)	7.13 td (7, 1)
12	7.24 ddd (8, 2, 1)	7.25 ddd (8, 1, 1)	7.25 dd (7, 1)
14	1.84 m	2.00 m	1.99 m
15	1.22 ddt (13, 8, 3)	1.64 dddd (13, 11, 4, 2)	1.84 td (13, 3)
15	1.79 m	1.98 ddt (13, 8, 3)	1.91 m
16	2.92 ddd (11, 4, 2)	3.01 ddd (12, 4, 2)	2.93 ddd (12, 4, 2)
17	1.64 ddd (13, 7, 4)	1.67 ddd (13, 7, 4)	1.68 dq (13, 3)
17	2.04 ddt (13, 11, 3)	2.08 ddt (13, 12, 3)	2.07 br t (13)
18	0.90 t (7)	1.12 d (7)	1.28 d (7)
19	1.49 m	4.17 qd (7, 2)	3.91 qd (7, 2)
19	1.55 m	-	-
20	1.55 m	1.58 ddt (11, 4, 2)	1.62 m
21	2.96 br s	3.13 t (2)	3.39 br s
N(1)-H	7.64 br s	7.79 br s	8.04 br s

[a]$CDCl_3$, 400 MHz; assignments based on COSY and HSQC.

Table 2.13: ^{13}C NMR Spectroscopic Data (δ) of Ibogamine (**11**), 19(*S*)-Hydroxyibogamine (**12**), and 19(*R*)-Hydroxyibogamine (**13**)[a]

C	11	12	13
2	141.8	140.7	141.0
3	49.9	49.3	49.2
5	54.1	52.9	53.0
6	20.6	20.2	20.3
7	109.1	108.4	108.5
8	129.7	129.5	129.5
9	117.8	118.0	118.1
10	119.0	119.2	119.3
11	120.9	121.3	121.4
12	110.1	110.2	110.4
13	134.6	134.8	134.9
14	26.4	25.9	26.1
15	32.1	23.0	29.2
16	41.3	40.2	40.0
17	34.1	34.3	34.3
18	11.9	20.1	23.0
19	27.8	71.5	71.7
20	41.9	42.2	42.5
21	57.5	60.9	54.8

[a]$CDCl_3$, 100 MHz; assignments based on HSQC and HMBC.

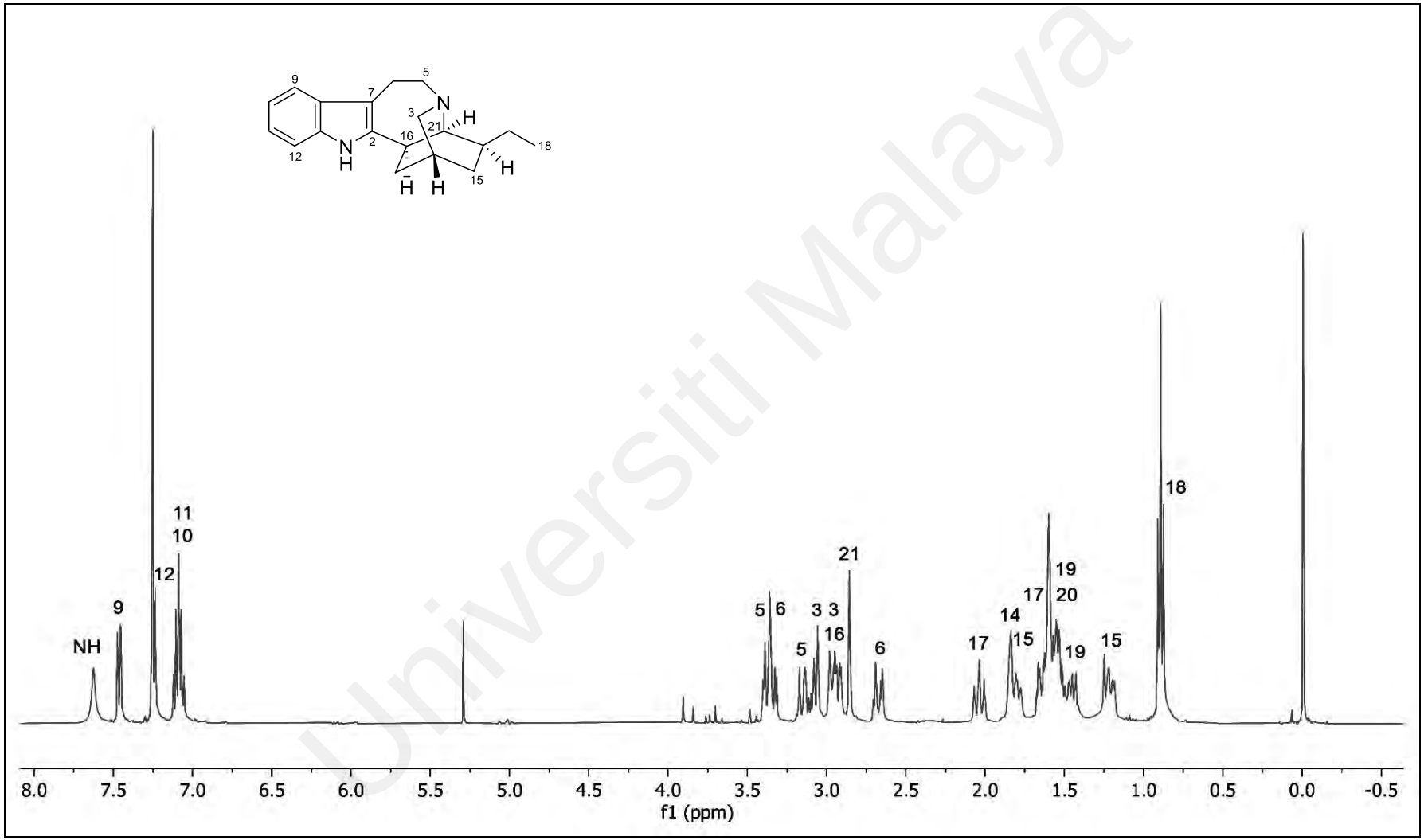


Figure 2.46: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Ibogamine (**11**)

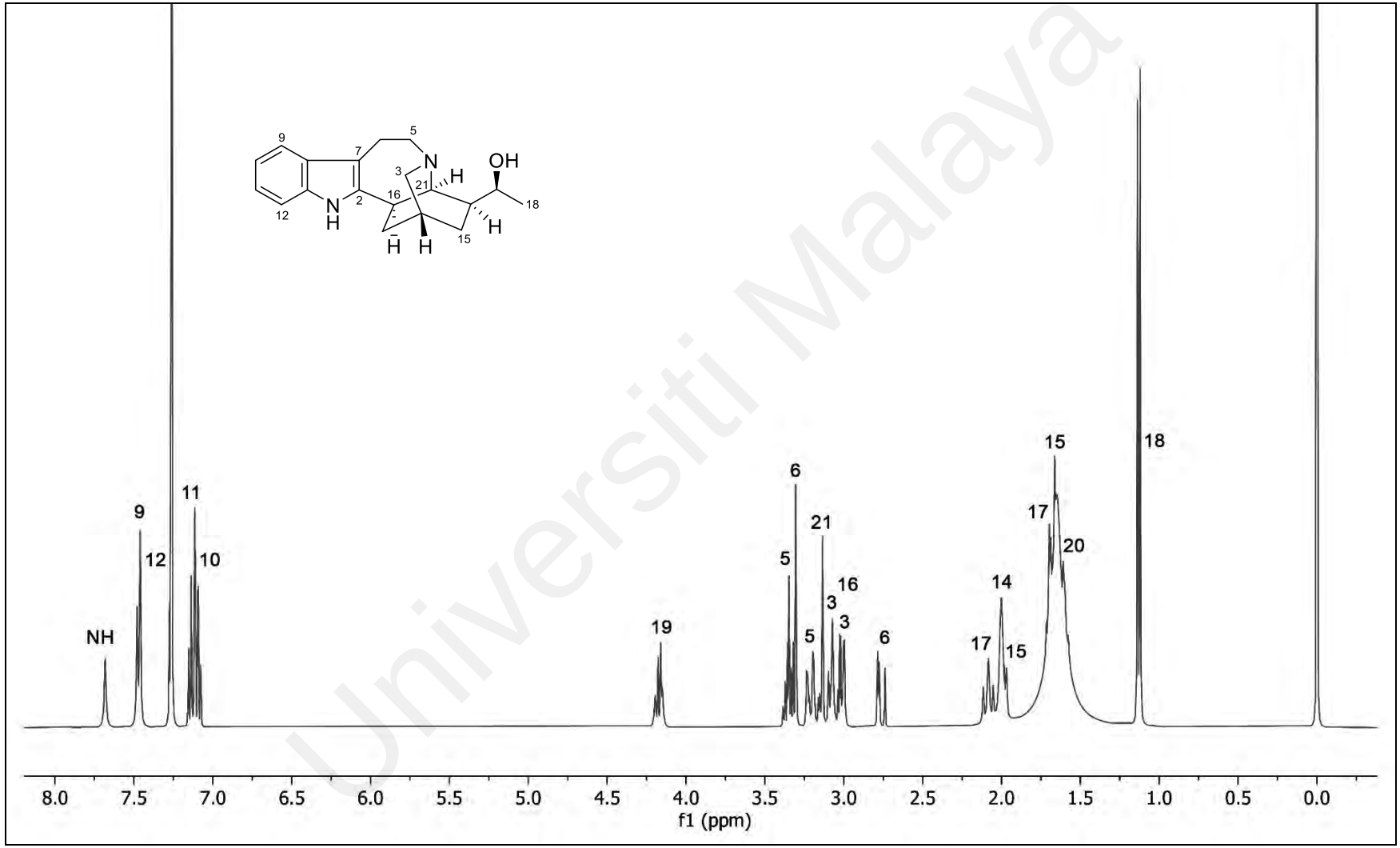


Figure 2.47: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 19(*S*)-Hydroxyibogamine (**12**)

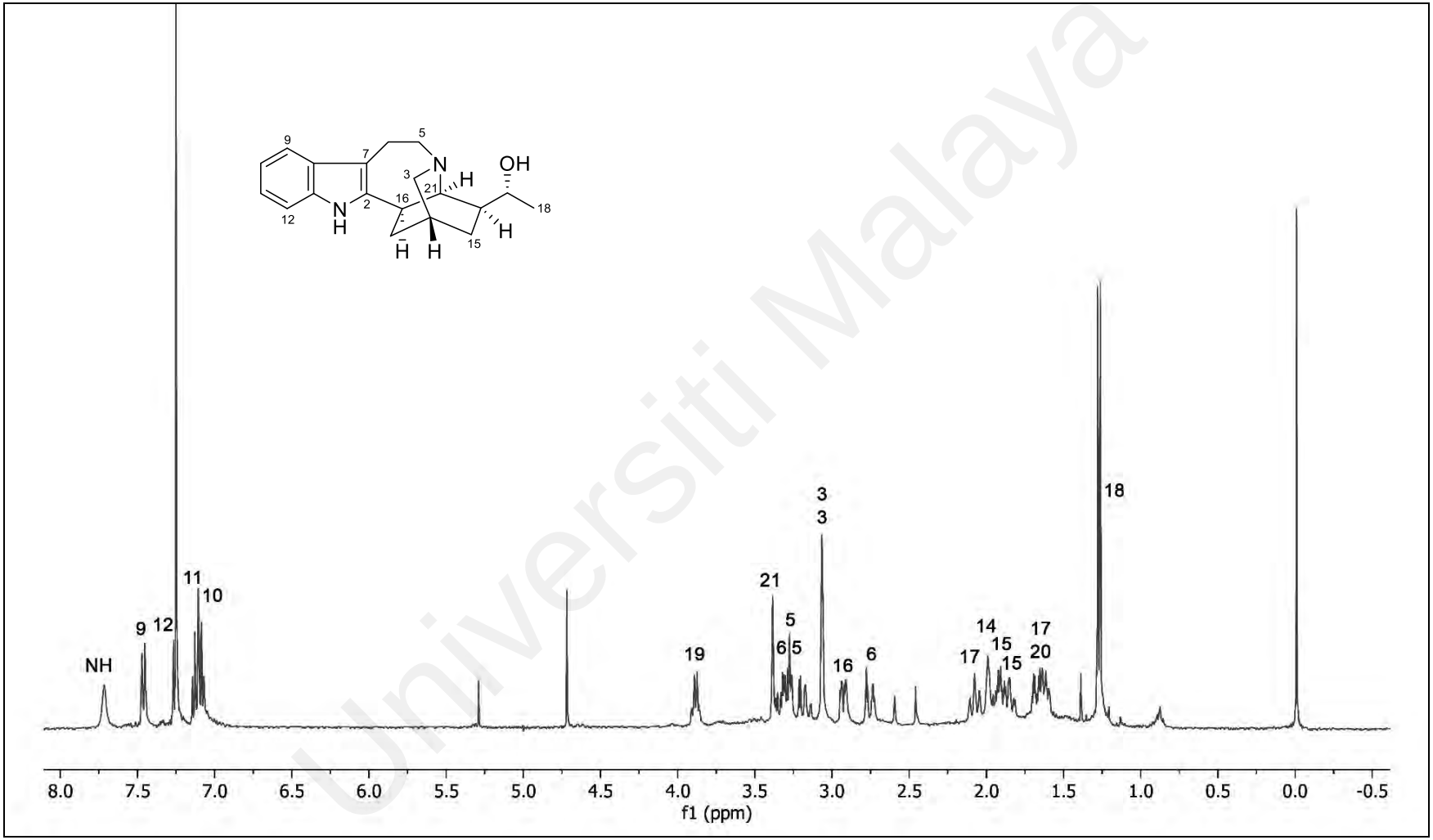


Figure 2.48: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 19(*R*)-Hydroxyibogamine (**13**)

Table 2.14: ^{1}H NMR Spectroscopic Data (δ) of Coronaridine (**14**), (−)-Albifloranine (**15**), (−)-Heyneanine (**16**), 19-*Epi*-heyneanine (**17**), and 3-Oxo-19-*epi*-heyneanine (**18**)[a]

H	**14** (*J*/Hz)	**15** (*J*/Hz)	**16** (*J*/Hz)	**17** (*J*/Hz)	**18** (*J*/Hz)
3	2.82 br d (9)	2.80 d (9)	2.81 dt (9, 2)	2.81 dt (9, 2)	-
3	2.90 br dd (9, 3)	2.97 dd (9, 4)	2.99 ddd (9, 4, 3)	3.00 ddd (9, 4, 3)	-
5	3.21 m	3.18 m	3.13 m	3.15 m	3.23 m
5	3.39 m	3.43 m	3.46 m	3.44 dt (13, 5)	4.43 m
6	3.00 m	3.12 m	3.13 m	3.15 m	3.23 m
6	3.19 m	3.12 m	3.13 m	3.15 m	3.23 m
9	7.48 br d (8)	7.47 d (8)	7.47 dd (8, 1)	7.47 dd (8, 1)	7.47 dd (8, 1)
10	7.08 td (8, 1)	7.10 td (8, 1)	7.10 td (8, 1)	7.10 td (8, 1)	7.08 td (8, 1)
11	7.15 td (8, 1)	7.16 td (8, 1)	7.17 td (8, 1)	7.17 td (8, 1)	7.14 td (8, 1)
12	7.25 dd (8, 1)	7.26 d (8)	7.25 dd (8, 1)	7.25 dd (8, 1)	7.25 dd (8, 1)
14	1.88 m	1.97 m	2.03 m	2.02 m	2.62 m
15	1.13 br dd (12, 8)	1.51 m	1.56 dddd (13, 10, 4, 2)	1.78 tdd (13, 8, 2)	1.32 ddt (13, 6, 2)
15	1.74 br td (11, 3)	1.69 m	1.91 ddt (13, 7, 2)	1.85 ddt (13, 8, 2)	1.89 ddd (13, 9, 3)
17	1.90 m	2.00 m	1.98 ddd (13, 4, 3)	1.97 ddd (13, 4, 3)	2.33 ddd (14, 4, 2)
17	2.58 br d (14)	2.61 dd (12, 2)	2.16 dt (13, 2)	2.60 dt (13, 2)	2.65 dd (14, 2)
18	0.90 t (8)	3.69 m	1.10 d (7)	1.29 d (6)	1.21 d (6)
18		3.80 m			
19	1.44 m	1.84 m	4.17 qd (7, 2)	-	-
19	1.57 m	1.84 m	-	3.90 qd (6, 3)	3.57 dq (9, 6)
20	1.33 m	1.84 m	1.46 ddt (10, 7, 2)	1.42 m	1.73 br td (9, 6)
21	3.56 s	3.66 s	3.86 br s	4.09 br s	5.07 br s
CO_2Me	3.71 s	3.73 s	3.74 s	3.73 s	3.71 s
19-OH	-	-	6.42 br s	6.39 br s	*n.o.*
N(1)-H	7.83 br s	7.90 br s	7.89 br s	7.93 br s	8.11 br s

[a]$CDCl_3$, 400 MHz; assignments based on COSY and HSQC.

Table 2.15: ^{13}C NMR Spectroscopic Data (δ) of Coronaridine (**14**), (−)-Albifloranine (**15**), (−)-Heyneanine (**16**), 19-*Epi*-heyneanine (**17**), and 3-Oxo-19-*epi*-heyneanine (**18**)[a]

C	14	15	16	17	18
2	136.4	135.5	135.8	135.7	135.7
3	51.6	51.4	51.2	50.7	172.9
5	53.1	52.9	52.1	51.9	42.4
6	21.9	21.5	21.2	21.5	20.9
7	110.0	110.1	109.5	109.7	109.4
8	128.6	128.5	128.2	128.5	127.7
9	118.3	118.4	118.2	118.4	118.3
10	119.0	119.4	119.1	119.3	119.5
11	121.7	122.2	121.9	122.1	122.2
12	110.3	110.5	110.3	110.4	110.6
13	135.5	135.7	135.5	135.5	133.9
14	27.2	27.0	26.6	26.9	37.9
15	31.8	28.8	22.8	28.6	27.9
16	54.9	54.6	53.9	53.9	55.1
17	36.3	36.4	36.6	36.6	35.7
18	11.6	59.2	20.2	22.2	21.0
19	26.6	36.2	71.2	70.7	68.9
20	39.9	35.0	39.3	39.9	41.7
21	57.3	58.2	59.5	54.1	52.9
*C*O$_2$Me	175.6	175.3	174.6	174.9	175.9
CO$_2$*Me*	52.5	52.9	52.7	52.7	53.1

[a]$CDCl_3$, 100 MHz; assignments based on HSQC and HMBC.

Table 2.16: ^{1}H NMR Spectroscopic Data (δ) of 3-Oxo-coronaridine (**19**), 3(*S*)-Cyanocoronaridine (**20**), Ervatamine G (**21**), and 3-Hydroxy-3,4-*seco*coronaridine (**22**)

H	**19**^{a} (*J*/Hz)	**20**^{a} (*J*/Hz)	**21**^{b} (*J*/Hz)	**22**^{a} (*J*/Hz)
3	-	3.84 t (2)	2.94 d (6)	3.48 d (6)
3	-	-	-	3.48 d (6)
5	3.21 m	3.32 ddd (14, 7, 6)	3.29 m	3.15 m
5	4.49 m	3.48 ddd (14, 7, 6)	3.36 m	3.41 m
6	3.21 m	3.10 dt (16, 7)	3.08 m	2.93 m
6	3.21 m	3.17 ddd (16, 7, 6)	3.15 m	3.15 m
9	7.47 dd (7, 1)	7.48 dd (8, 1)	7.48 d (8)	7.47 dd (8, 1)
10	7.11 td (7, 1)	7.11 td (8, 1)	7.10 t (8)	7.07 td (8, 1)
11	7.07 td (7, 1)	7.18 td (8, 1)	7.16 t (8)	7.13 td (8, 1)
12	7.21 dd (7, 1)	7.26 dd (8, 1)	7.26 d (8)	7.25 dd (8, 1)
14	2.59 m	2.19 tq (4, 2)	1.93 m	1.76 m
15	1.39 m	1.52 ddt (13, 7, 2)	1.49 m	0.98 m
15	1.97 ddd (13, 10, 3)	1.79 dddd (13, 10, 4, 2)	1.93 m	1.47 dt (15, 3)
17	2.29 ddd (14, 4, 3)	1.97 ddd (14, 4, 2)	2.00 dt (14, 3)	1.62 t (13)
17	2.63 dd (14, 2)	2.70 dd (14, 2)	2.65 dd (14, 2)	2.52 dt (13, 2)
18	0.98 t (7)	0.93 t (7)	0.92 t (7)	0.97 t (7)
19	1.39 m	1.55 br dq (14, 7)	1.45 m	1.38 m
19	1.52 m	1.65 br dq (14, 7)	1.60 m	1.56 m
20	1.73 m	1.40 dq (10, 7)	1.32 m	1.38 m
21	4.51 br s	3.67 br s	3.70 br s	3.90 d (2)
24	-	-	3.55 dd (11, 2)	-
24	-	-	3.66 dd (11, 7)	-
CO_2*Me*	3.70 s	3.73 s	3.72 s	3.71 s
N(1)-H	8.26 br s	7.82 br s	7.79 br s	8.27 br s

^{a}$CDCl_3$, 400 MHz; ^{b}$CDCl_3$, 600 MHz; assignments based on COSY and HSQC.

Table 2.17: ^{13}C NMR Spectroscopic Data (δ) of 3-Oxo-coronaridine (**19**), 3(*S*)-Cyanocoronaridine (**20**), Ervatamine G (**21**), and 3-Hydroxy-3,4-*seco*coronaridine (**22**)

C	**19**[a]	**20**[a]	**21**[b]	**22**[a]
2	133.9	135.3	136.3	134.0
3	172.9	53.3	59.9	67.4
5	42.7	51.9	51.6	49.1
6	21.0	21.5	21.8	24.0
7	109.2	109.9	110.1	110.2
8	127.7	128.3	128.6	128.3
9	118.3	118.5	118.4	118.2
10	119.5	119.6	119.4	119.2
11	122.2	122.5	122.2	122.0
12	110.6	110.5	110.4	110.6
13	135.7	135.5	135.6	135.3
14	38.1	31.3	30.9	37.1
15	30.9	28.5	27.7	28.5
16	55.5	54.3	55.0	56.0
17	35.8	35.7	38.2	33.4
18	11.3	11.5	11.8	11.7
19	27.5	26.6	26.5	25.7
20	35.4	38.3	38.4	40.9
21	56.1	56.1	58.0	57.6
24	-	-	62.4	-
CO_2Me	175.7	174.5	175.5	173.9
CO_2*Me*	52.9	52.9	52.7	52.6
*C*N	-	120.1	-	-

[a]$CDCl_3$, 100 MHz; [b]$CDCl_3$, 150 MHz; assignments based on HSQC and HMBC.

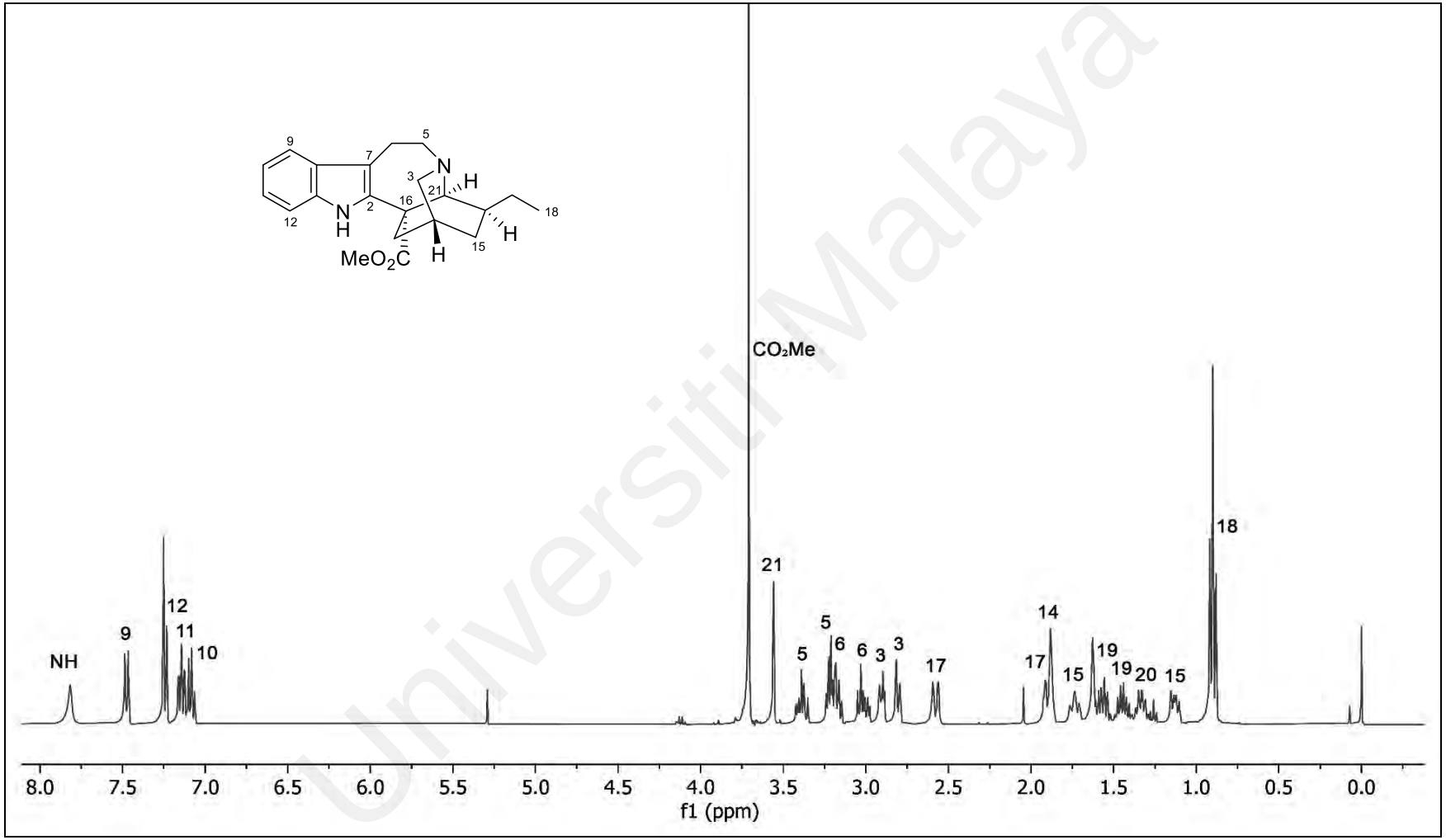


Figure 2.49: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Coronaridine (**14**)

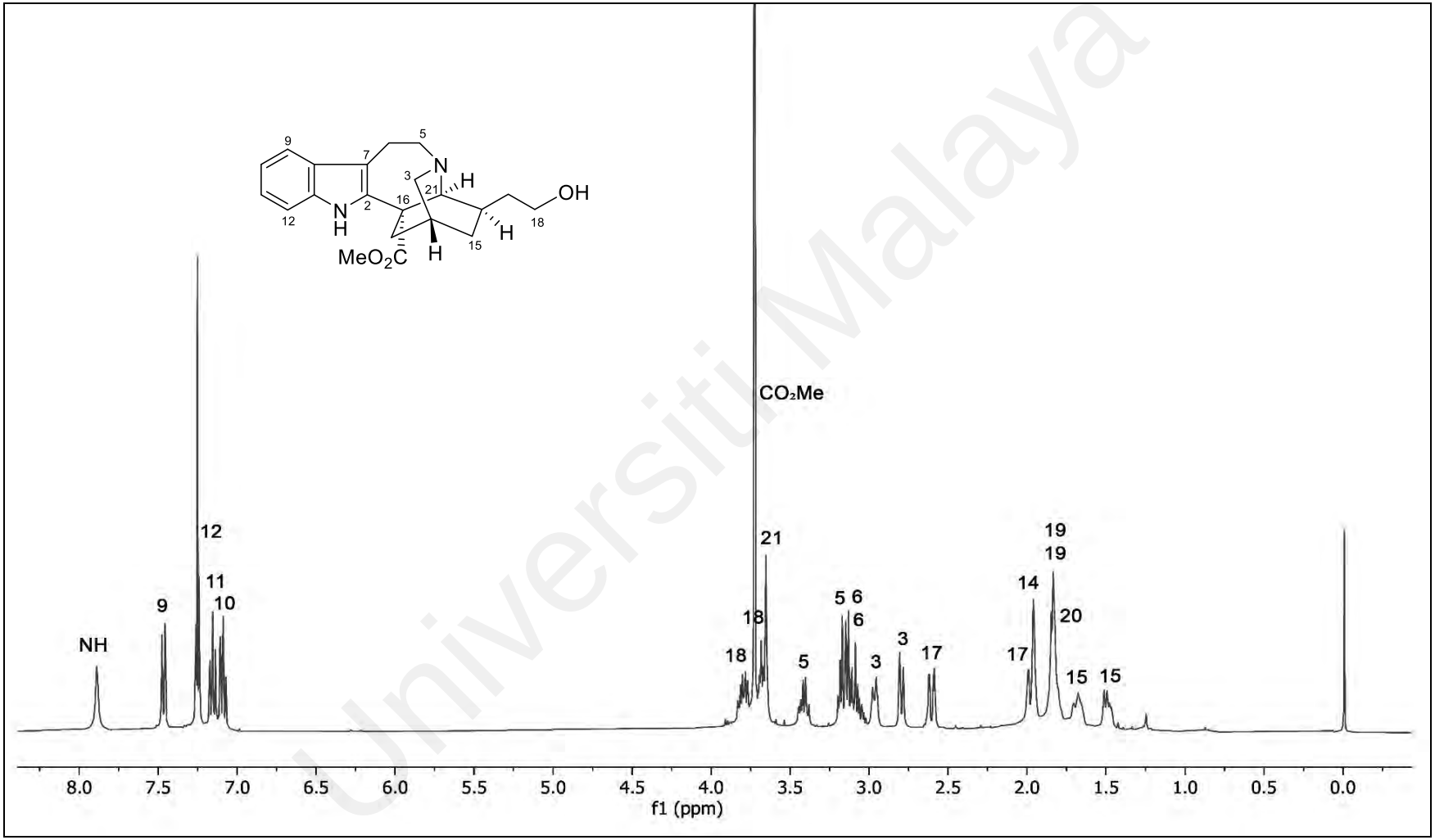


Figure 2.50: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of (–)-Albifloranine (**15**)

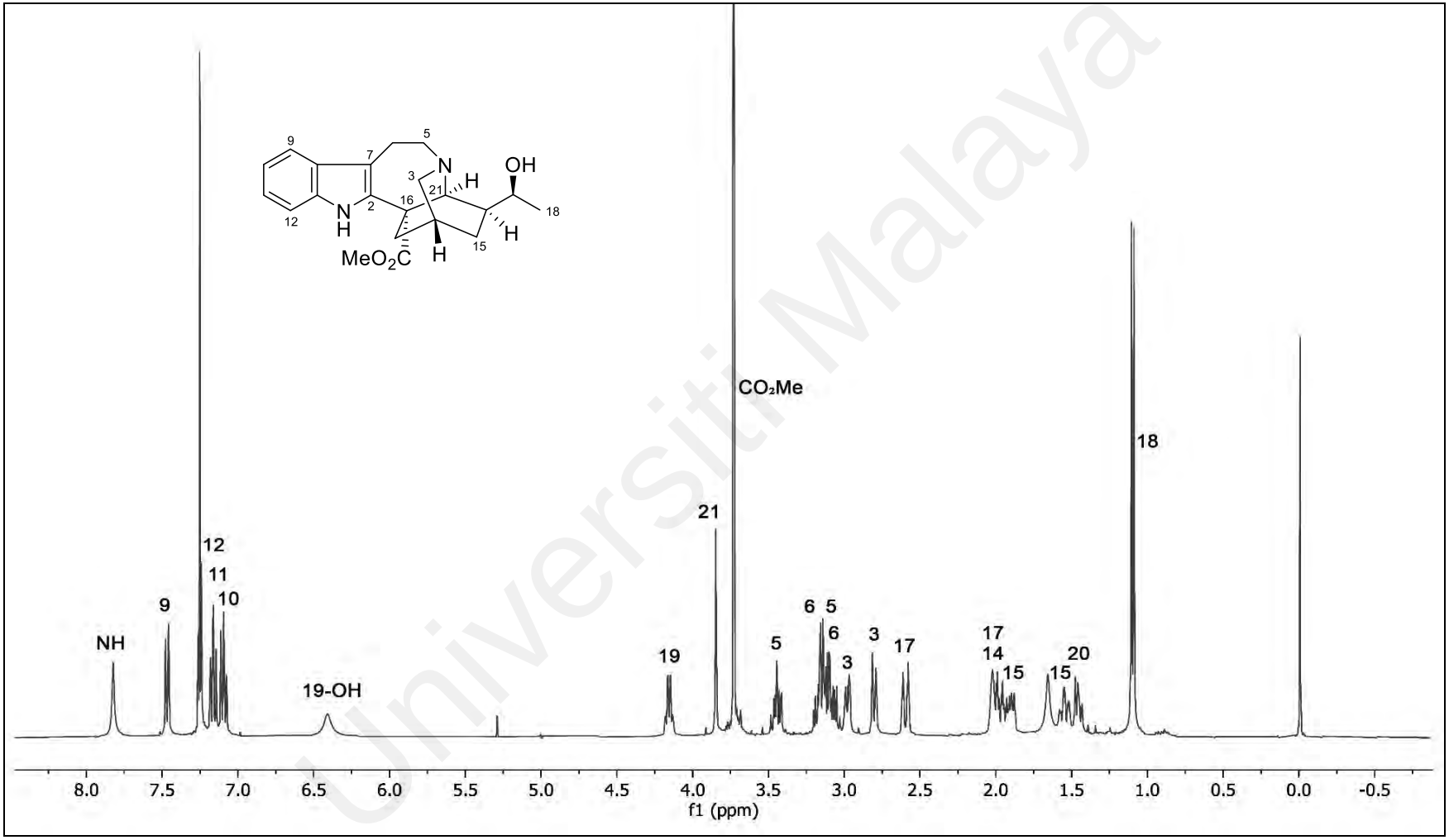


Figure 2.51: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of (–)-Heyneanine (**16**)

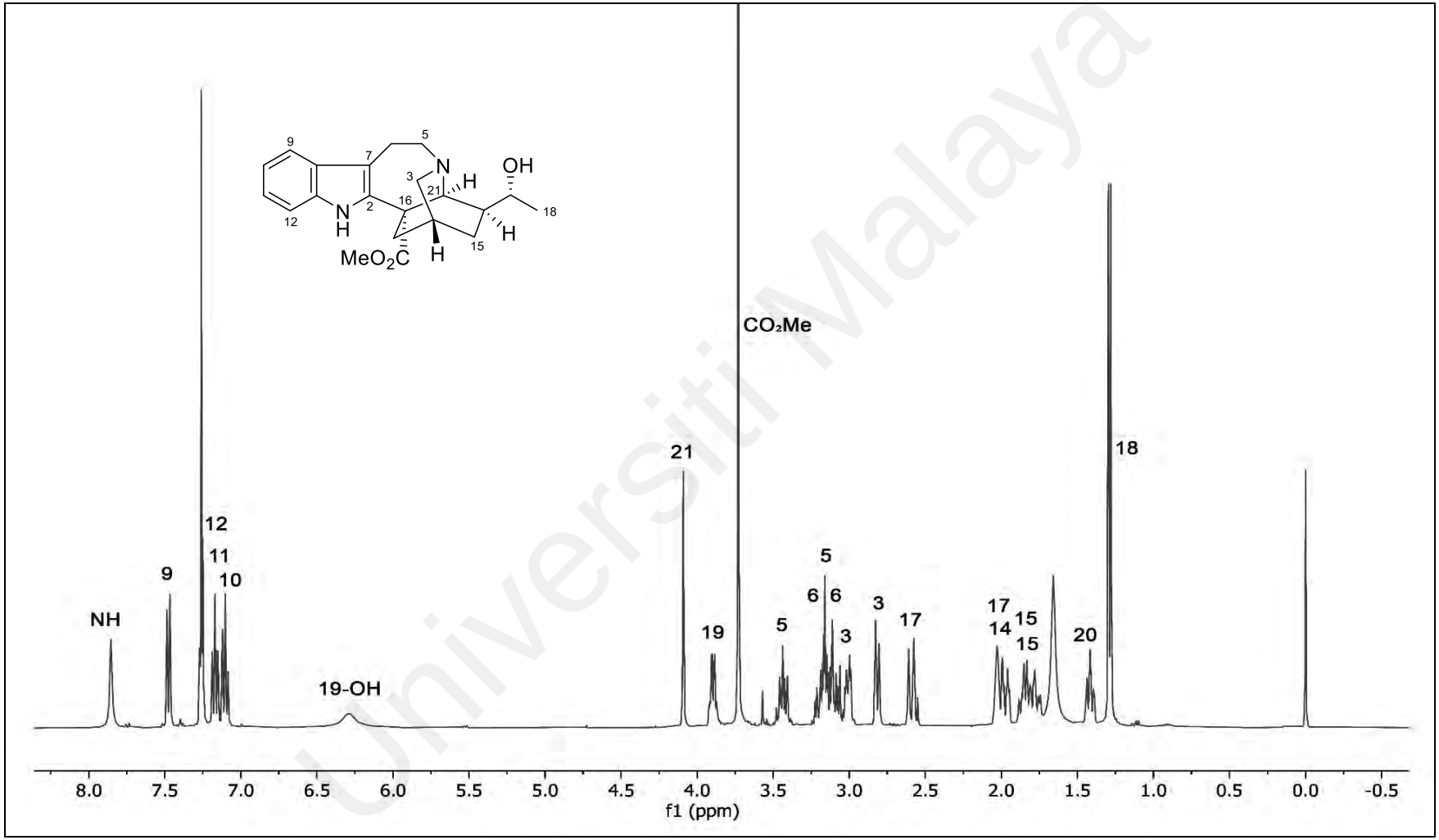


Figure 2.52: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 19-*Epi*-heyneanine (**17**)

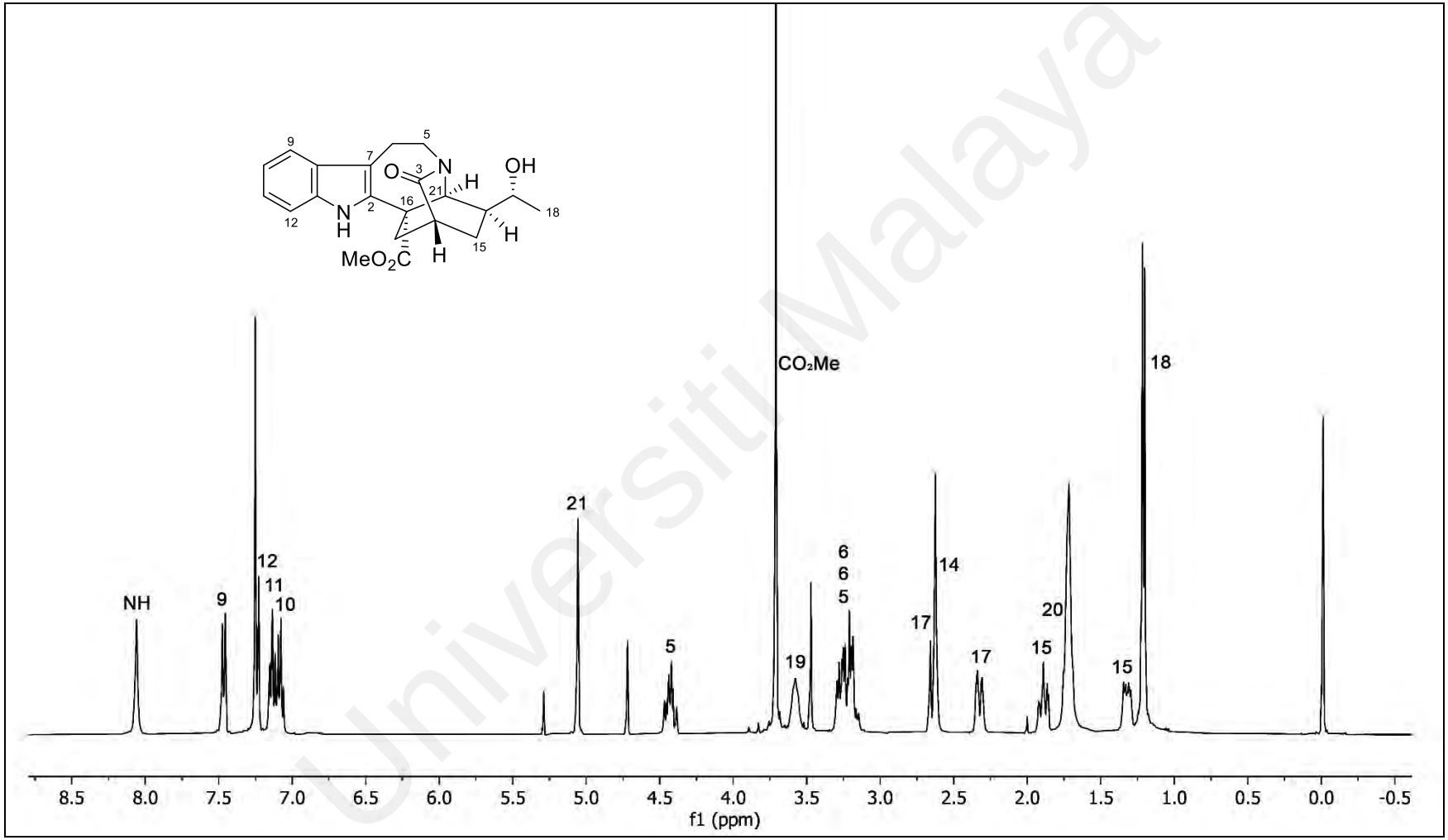


Figure 2.53: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 3-Oxo-19-*epi*-heyneanine (**18**)

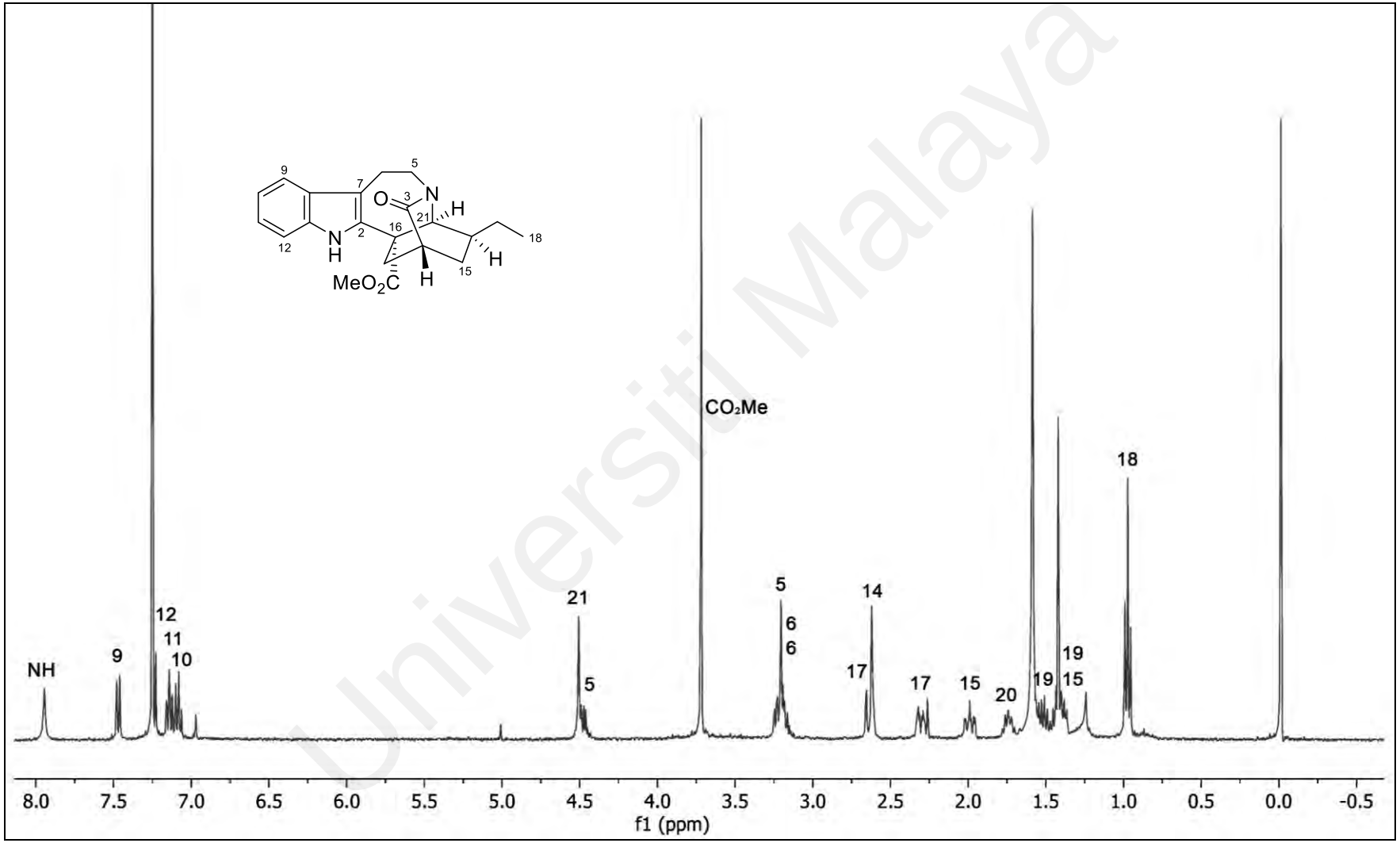


Figure 2.54: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 3-Oxo-coronaridine (**19**)

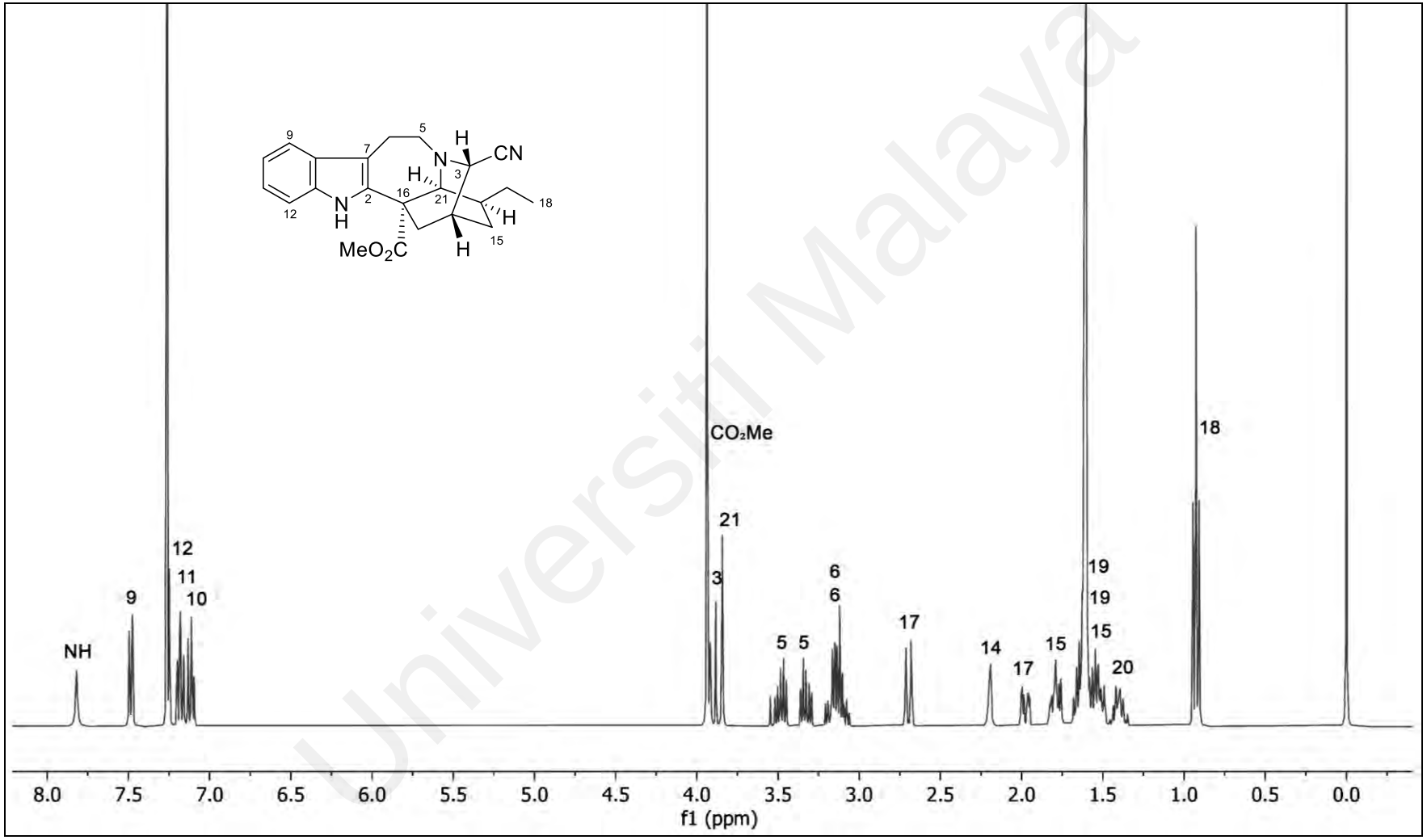


Figure 2.55: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 3(*S*)-Cyanocoronaridine (**20**)

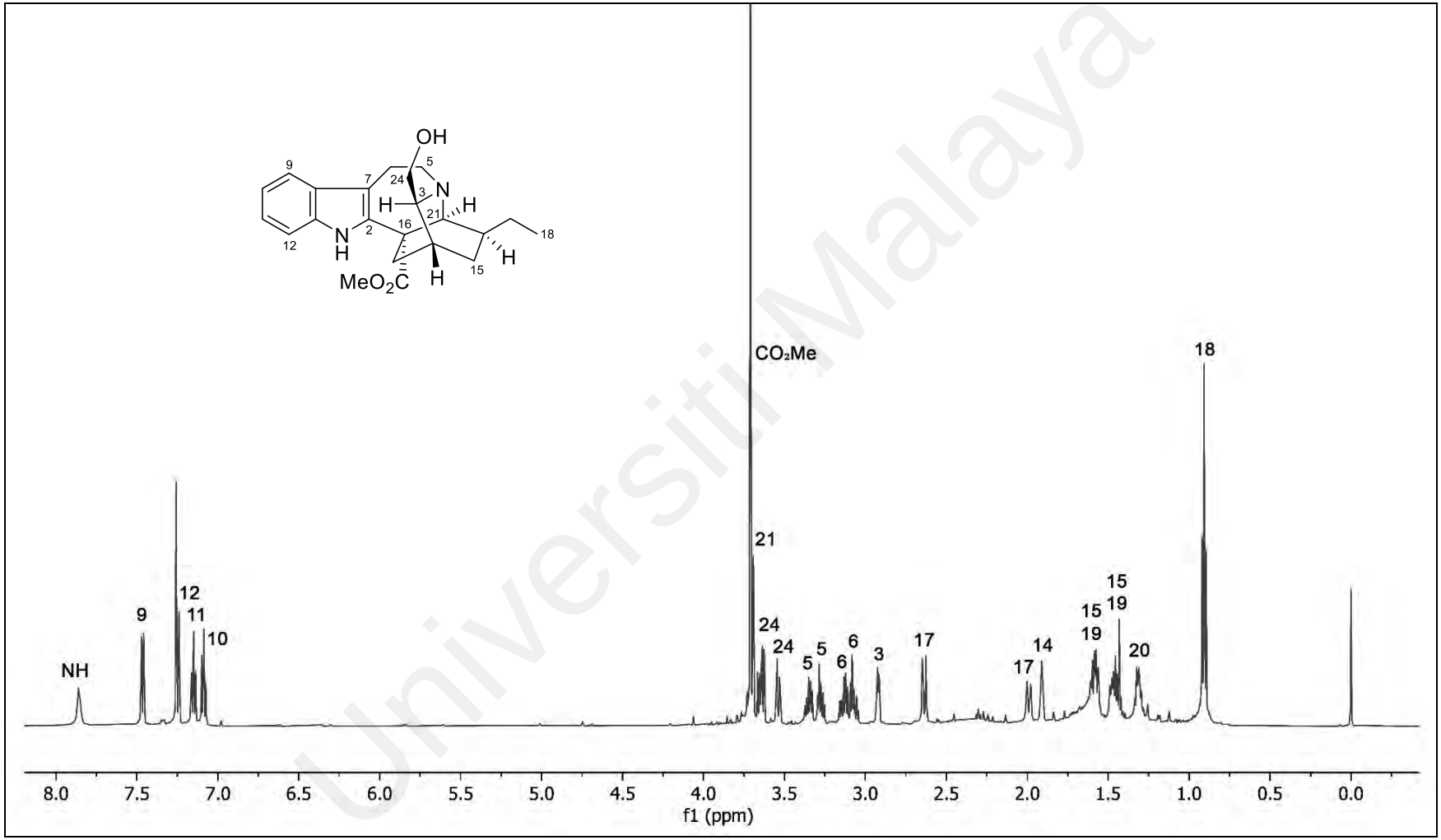


Figure 2.56: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Ervatamine G (**21**)

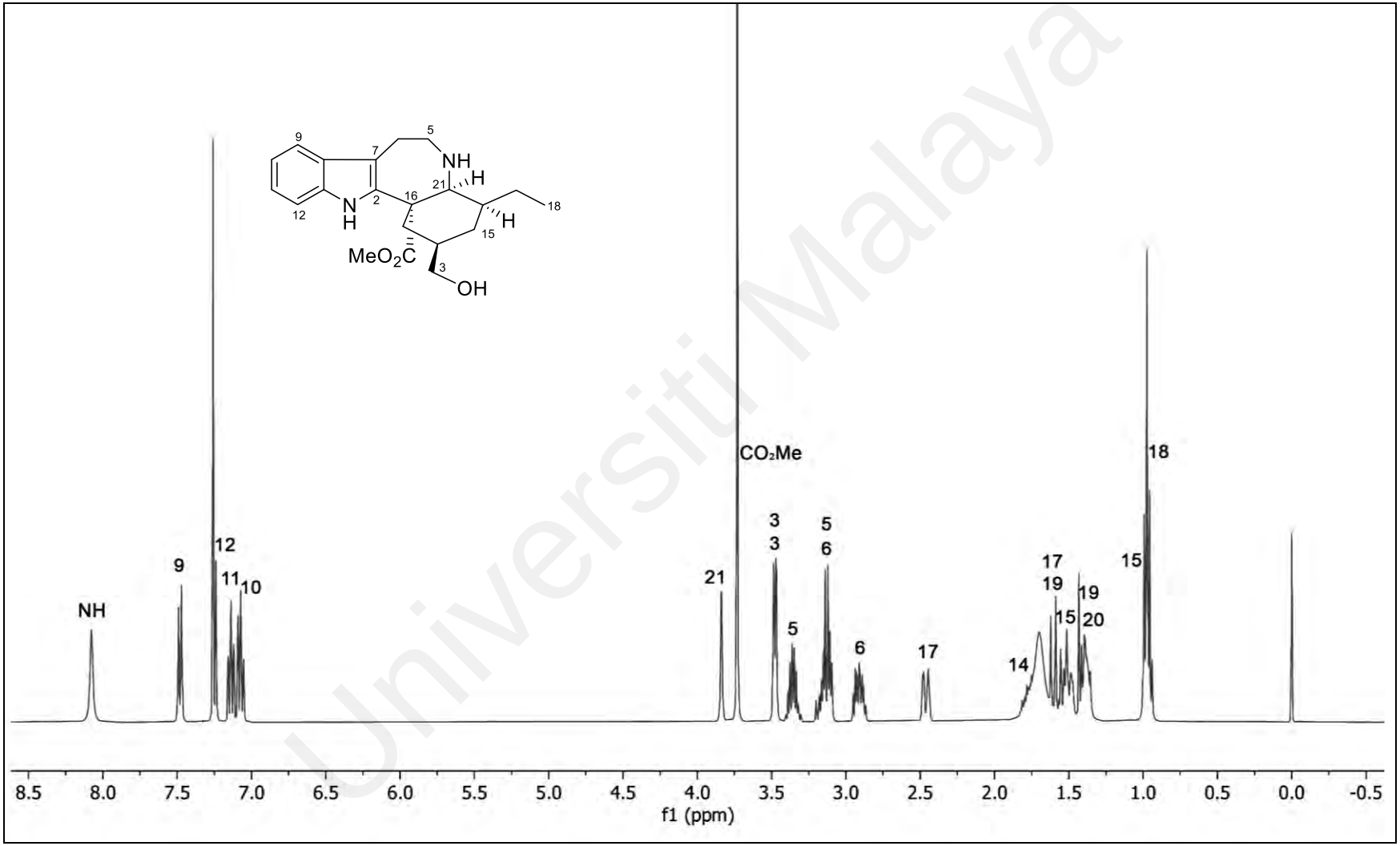


Figure 2.57: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 3-Hydroxy-3,4-*seco*coronaridine (**22**)

Table 2.18: ^{1}H NMR Spectroscopic Data (δ) of Voacangine (**23**), Voacristine (**24**), Conopharyngine (**25**), and 19(*S*)-Hydroxyconopharyngine (**26**)[a]

H	**23** (*J*/Hz)	**24** (*J*/Hz)	**25** (*J*/Hz)	**26** (*J*/Hz)
3	2.81 dt (9, 2)	2.79 br d (9)	2.82 d (8)	2.79 br d (9)
3	2.91 m	2.98 ddd (9, 5, 2)	2.91 m	2.98 ddd (9, 5, 2)
5	3.21 dt (13, 6)	3.10 m	2.97 m	3.10 m
5	3.37 dt (13, 5)	3.43 m	3.13 m	3.43 m
6	2.97 m	3.03 m	3.21 m	3.03 m
6	3.13 m	3.13 m	3.37 m	3.13 m
9	6.92 d (2)	6.90 d (2)	6.90 s	6.83 s
10	-	-	-	-
11	6.80 dd (9, 2)	6.81 dd (9, 2)	-	-
12	7.13 d (9)	7.13 d (9)	6.78 s	6.71 s
14	1.87 m	2.00 m	1.87 m	2.00 m
15	1.10 m	1.54 br ddd (13, 10, 2)	1.12 m	1.54 br ddd (13, 10, 2)
15	1.73 dddd (12, 10, 4, 2)	1.89 ddt (13, 7, 2)	1.71 m	1.89 ddt (13, 10, 2)
17	1.89 ddd (14, 4, 2)	1.95 ddd (13, 4, 2)	1.90 m	1.95 br d (13)
17	2.57 dt (14, 2)	2.59 br d (13)	2.54 m	2.59 ddd (13, 4, 2)
18	0.90 t (8)	1.09 d (7)	0.89 t (8)	1.09 d (7)
19	1.44 dqd (13, 8, 7)	-	1.44 m	-
19	1.56 dqd (13, 8, 7)	4.15 q (7)	1.55 m	4.23 q (7)
20	1.32 m	1.44 br dd (10, 7)	1.39 m	1.44 dd (10, 7)
21	3.55 br s	3.83 br s	3.53 br s	3.83 br s
CO_2*Me*	3.71 s	3.72 s	3.71 s	3.72 s
10-O*Me*	3.85 s	3.83 s	3.89 s	3.86 s
11-O*Me*	-	-	3.92 s	3.78 s
19-OH	-	-	-	-
N(1)-H	7.69 br s	7.83 br s	7.62 br s	7.83 br s

[a]$CDCl_3$, 400 MHz; assignments based on COSY and HSQC.

Table 2.19: ^{13}C NMR Spectroscopic Data (δ) of Voacangine (**23**), Voacristine (**24**), Conopharyngine (**25**), and 19(*S*)-Hydroxyconopharyngine (**26**)[a]

C	23	24	25	26
2	137.3	136.6	135.1	136.6
3	51.6	51.2	51.4	51.2
5	53.2	52.2	53.1	52.2
6	22.1	21.5	22.3	21.5
7	110.0	109.5	110.0	109.5
8	129.1	128.8	121.4	128.8
9	100.8	100.6	100.7	100.6
10	154.0	154.1	144.8	154.1
11	111.8	112.2	147.0	147.3
12	111.1	111.2	94.1	111.2
13	130.6	130.6	129.6	130.6
14	27.3	26.7	27.3	26.7
15	31.9	22.8	32.0	22.8
16	55.1	54.0	55.0	54.0
17	36.5	36.9	36.6	36.9
18	11.6	20.3	11.7	20.3
19	26.7	71.3	26.7	71.3
20	39.1	39.4	39.2	39.4
21	57.5	59.7	57.6	59.7
CO_2Me	175.8	174.8	175.9	174.8
CO_2*Me*	52.5	52.9	52.6	52.9
10-O*Me*	56.0	55.9	56.5	55.9
11-O*Me*	-	-	56.2	51.4

[a]$CDCl_3$, 100 MHz; assignments based on HSQC and HMBC.

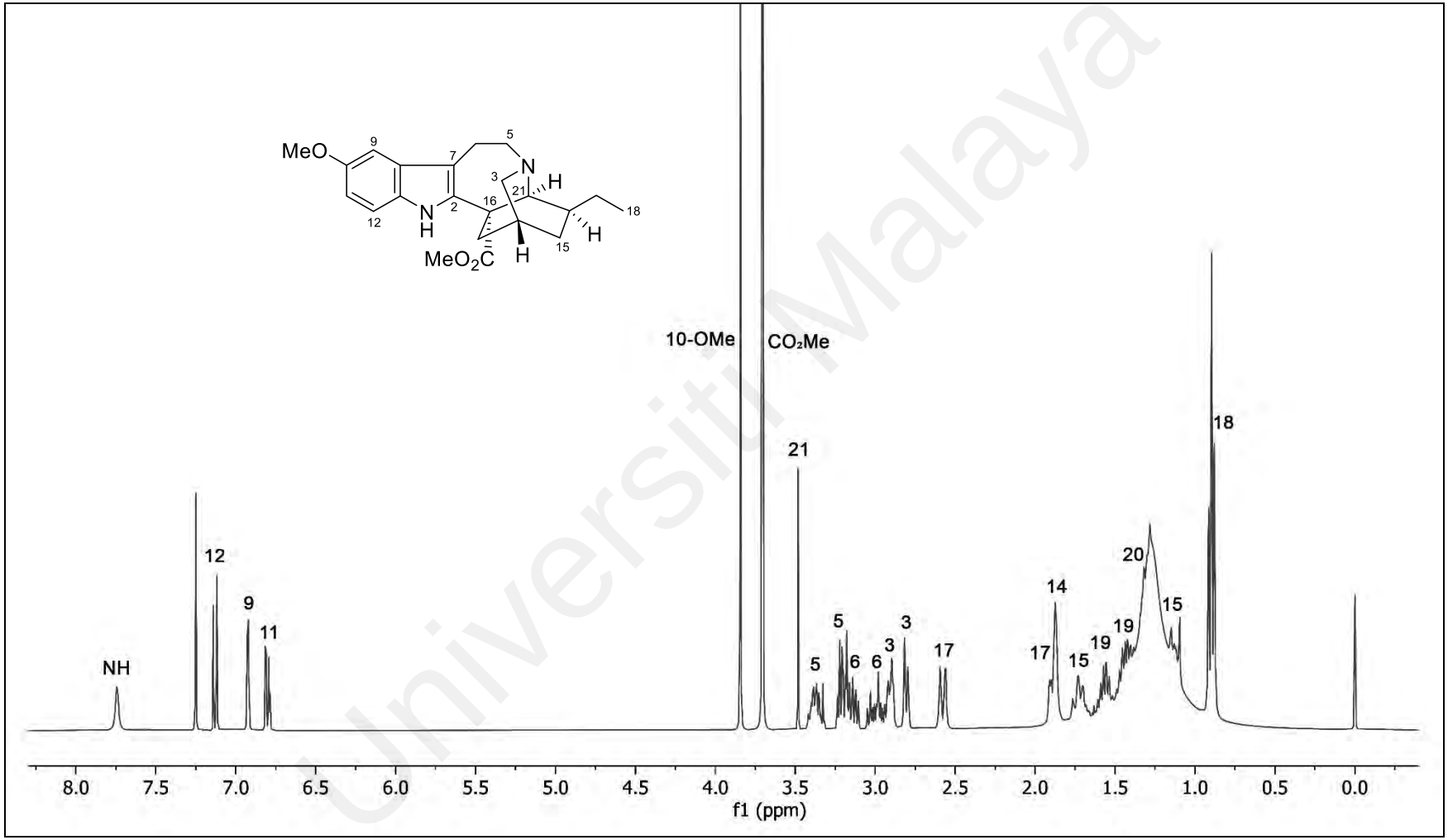


Figure 2.58: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Voacangine (**23**)

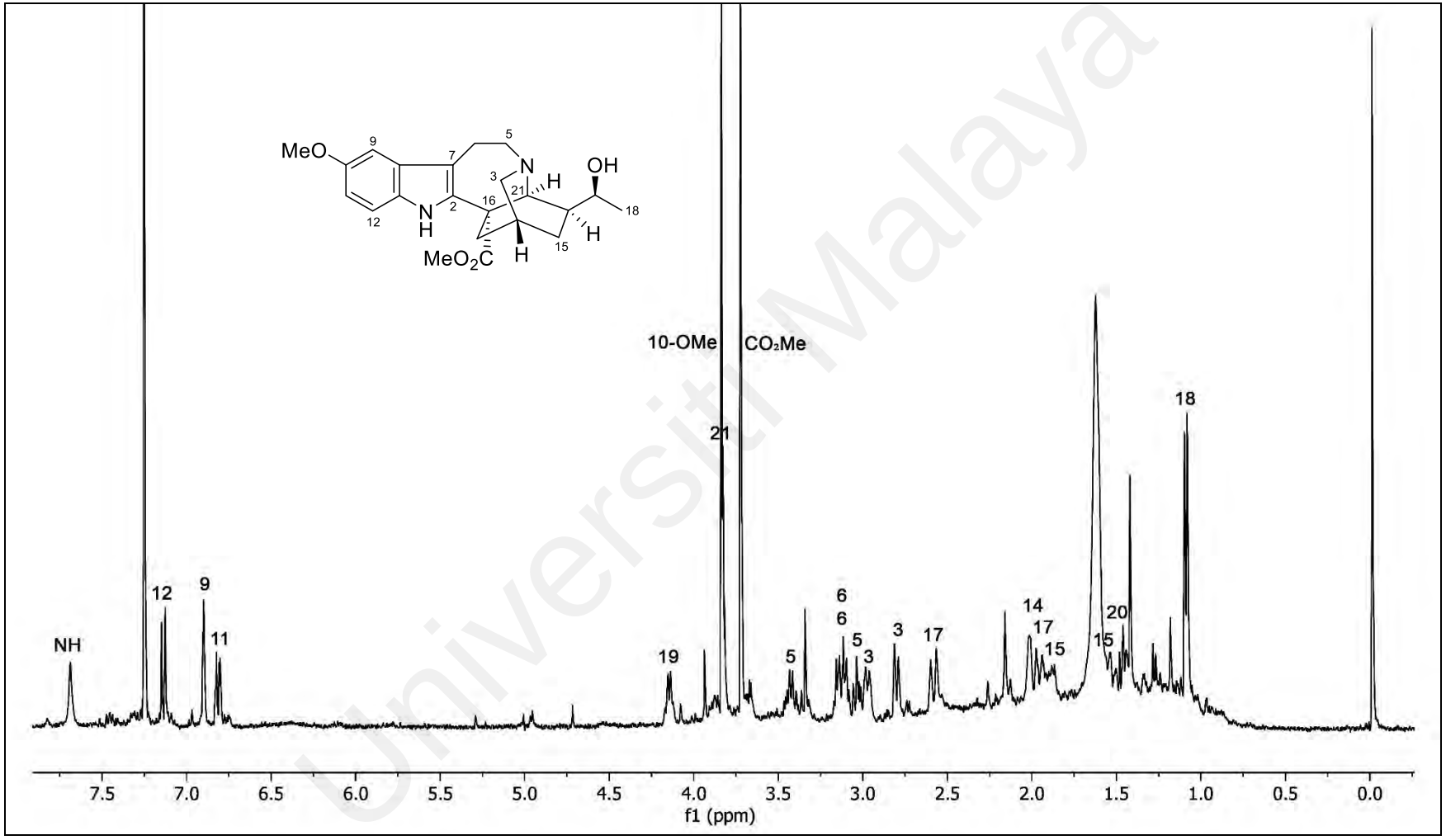


Figure 2.59: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Voacristine (**24**)

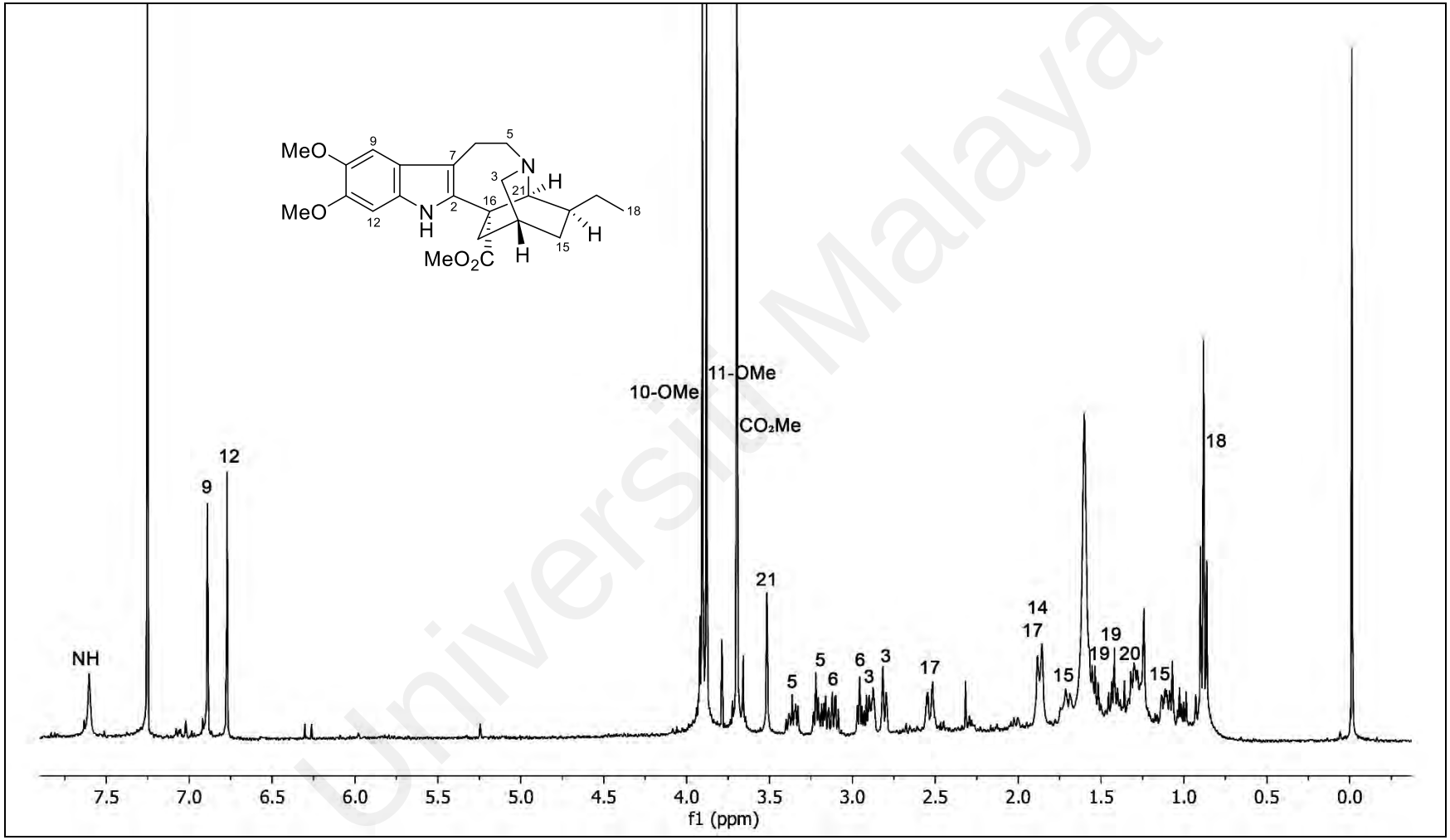


Figure 2.60: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Conopharyngine (**25**)

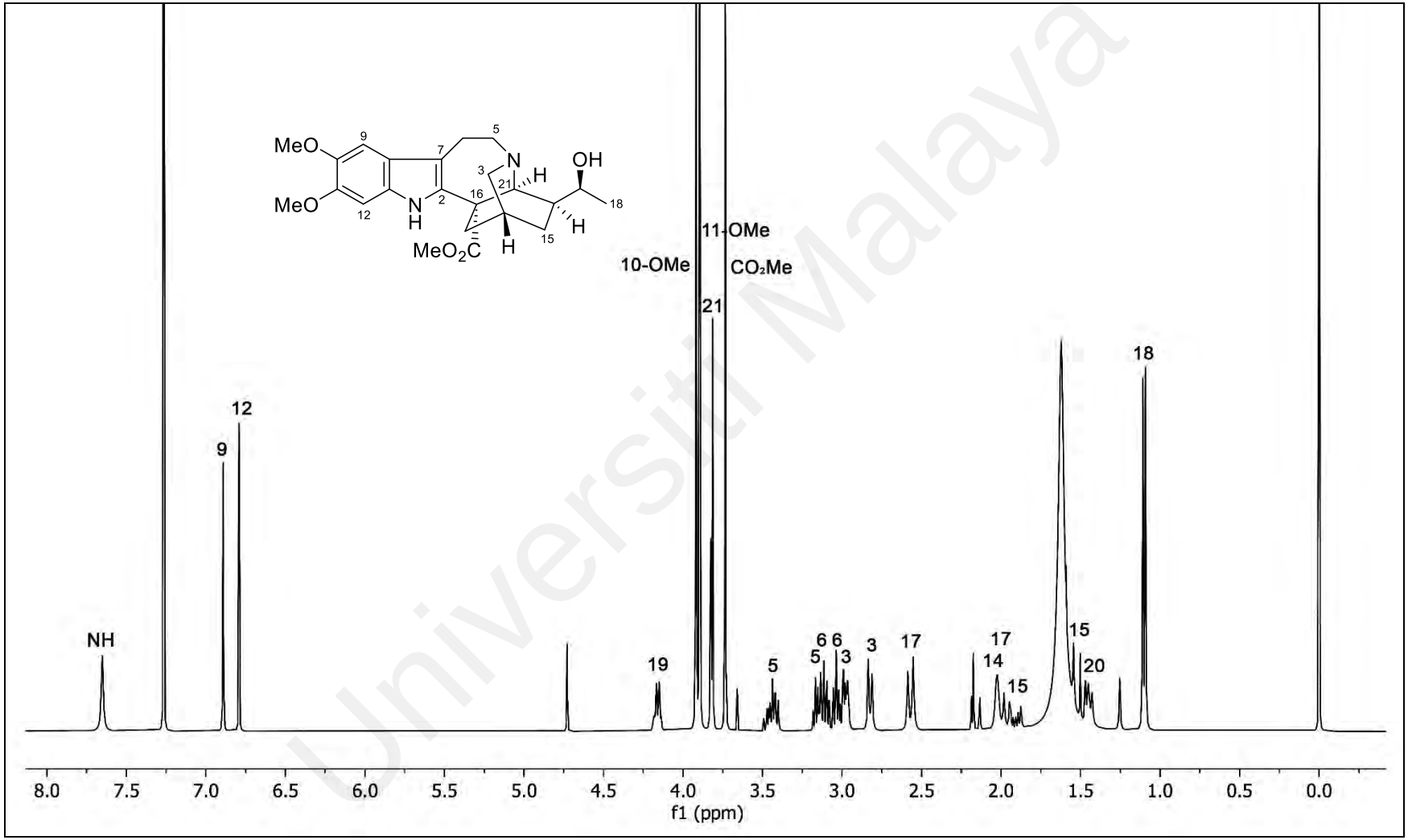


Figure 2.61: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 19(*S*)-Hydroxy-conopharyngine (**26**)

Table 2.20: ^{1}H NMR Spectroscopic Data (δ) of Coronaridine pseudoindoxyl (**27**), Ibogamine 7(*S*)-hydroxyindolenine (**28**), and Coronaridine-7-hydroxyindolenine (**29**)

H	**27**[a] (*J*/Hz)	**28**[b] (*J*/Hz)	**29**[a] (*J*/Hz)
3	2.62 m	2.71 d (9)	2.76 m
3	3.02 d (11)	2.80 m	2.76 m
5	2.73 dd (13, 4)	2.96 d (15)	2.97 ddd (15, 5, 2)
5	3.83 td (13, 3)	3.46 ddd (15, 13, 4)	3.51 m
6	1.48 m	1.92 m	1.86 ddd (15, 5, 2)
6	2.09 td (13, 4)	1.92 m	2.01 ddd (15, 3, 2)
9	7.57 d (8)	7.29 dd (8, 1)	7.46 dd (7, 1)
10	6.80 t (8)	7.17 td (8, 1)	7.34 td (7, 1)
11	7.38 td (8, 1)	7.22 td (8, 1)	7.31 td (7, 1)
12	6.77 d (8)	7.05 d (8)	7.24 dd (7, 1)
14	1.88 m	1.81 m	1.92 m
15	1.08 dq (13, 3)	1.16 m	1.10 ddt (11, 7, 2)
15	1.66 m	1.75 m	1.75 m
16	-	3.06 d (12)	-
17	1.66 m	2.03 m	2.48 ddd (14, 5, 3)
17	2.62 m	2.21 ddt (14, 12, 2)	2.74 m
18	0.91 t (8)	0.95 t (7)	0.87 t (7)
19	1.44 m	1.52 m	1.46 m
19	1.63 m	1.52 m	1.46 m
20	1.33 m	1.48 m	1.39 m
21	3.89 s	3.56 s	3.81 br s
CO_2*Me*	3.27 s	-	3.70 s
N(1)-H	4.55 br s	-	-

[a]$CDCl_3$, 400 MHz; [b]$CDCl_3$, 600 MHz; assignments based on COSY and HSQC.

Table 2.21: ^{13}C NMR Spectroscopic Data (δ) of Coronaridine pseudoindoxyl (**27**), Ibogamine 7(*S*)-hydroxyindolenine (**28**), and Coronaridine-7-hydroxyindolenine (**29**)

C	**27**[a]	**28**[b]	**29**[a]
2	67.8	193.1	189.3
3	52.2	49.6	48.7
5	47.7	49.1	49.0
6	25.8	31.8	33.8
7	202.9	87.2	88.3
8	121.5	141.7	142.6
9	124.5	121.3	120.8
10	119.4	126.0	111.4
11	136.7	129.5	129.1
12	112.3	120.0	116.7
13	158.6	152.1	151.3
14	26.4	27.2	27.0
15	31.3	31.8	32.0
16	52.2	43.7	55.8
17	31.0	34.1	34.8
18	12.2	11.8	11.5
19	28.9	27.3	26.5
20	36.1	40.6	37.5
21	51.3	53.6	58.3
CO_2Me	175.0	-	173.7
CO_2*Me*	51.9	-	53.1

[a]$CDCl_3$, 100 MHz; [b]$CDCl_3$, 150 MHz; assignments based on HSQC and HMBC.

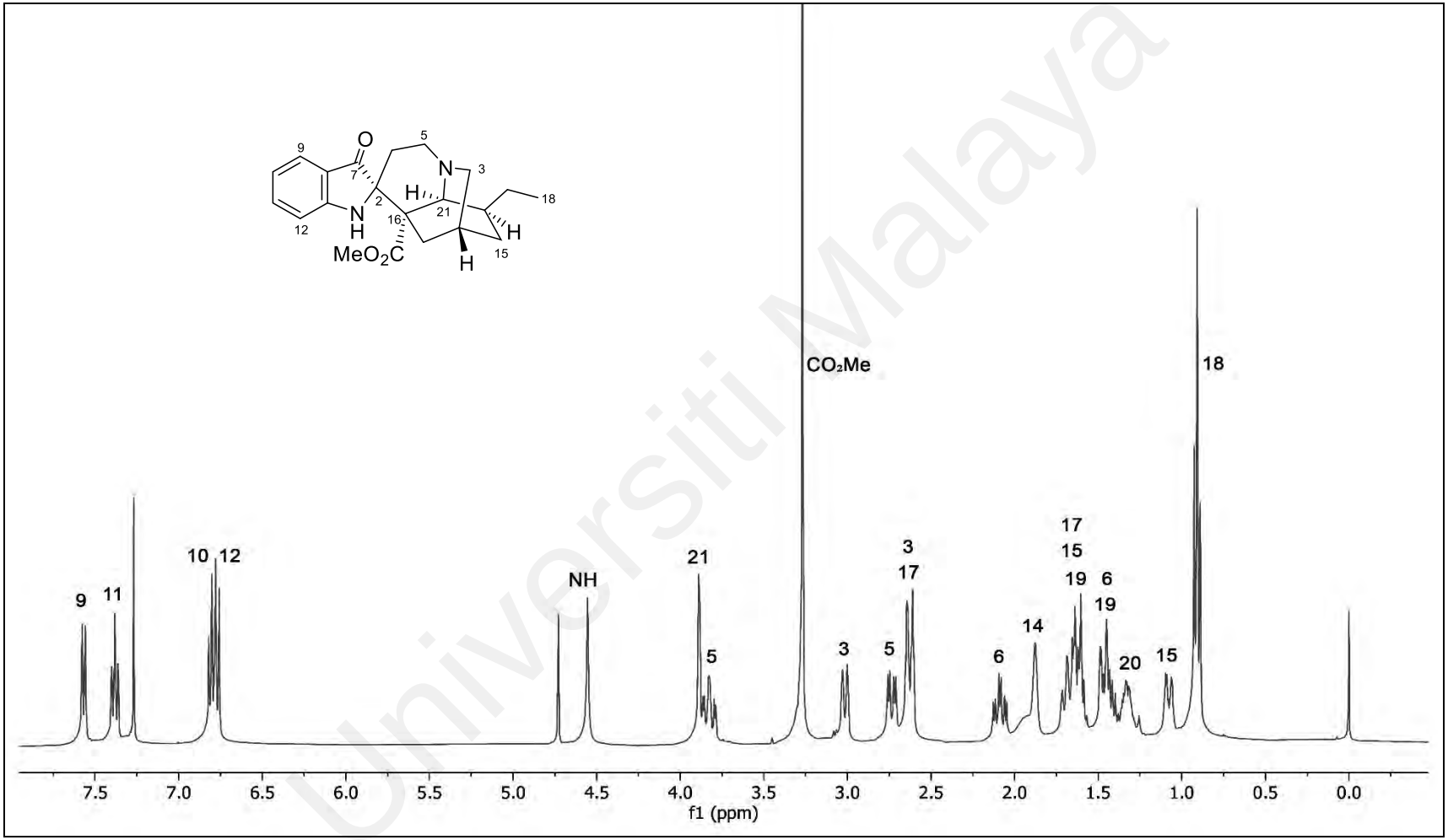


Figure 2.62: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Coronaridine pseudoindoxyl (**27**)

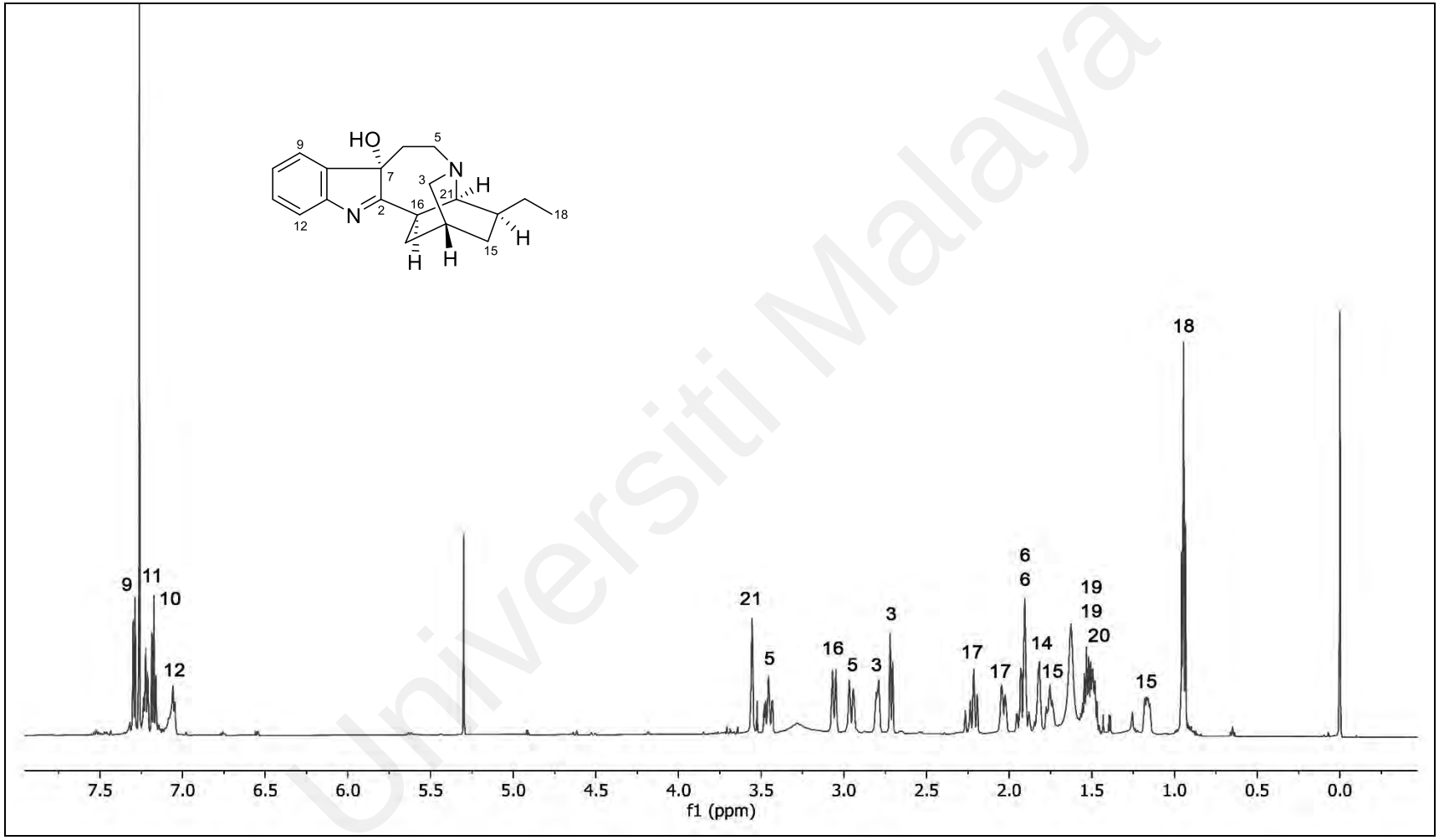


Figure 2.63: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Ibogamine 7(*S*)-hydroxyindolenine (**28**)

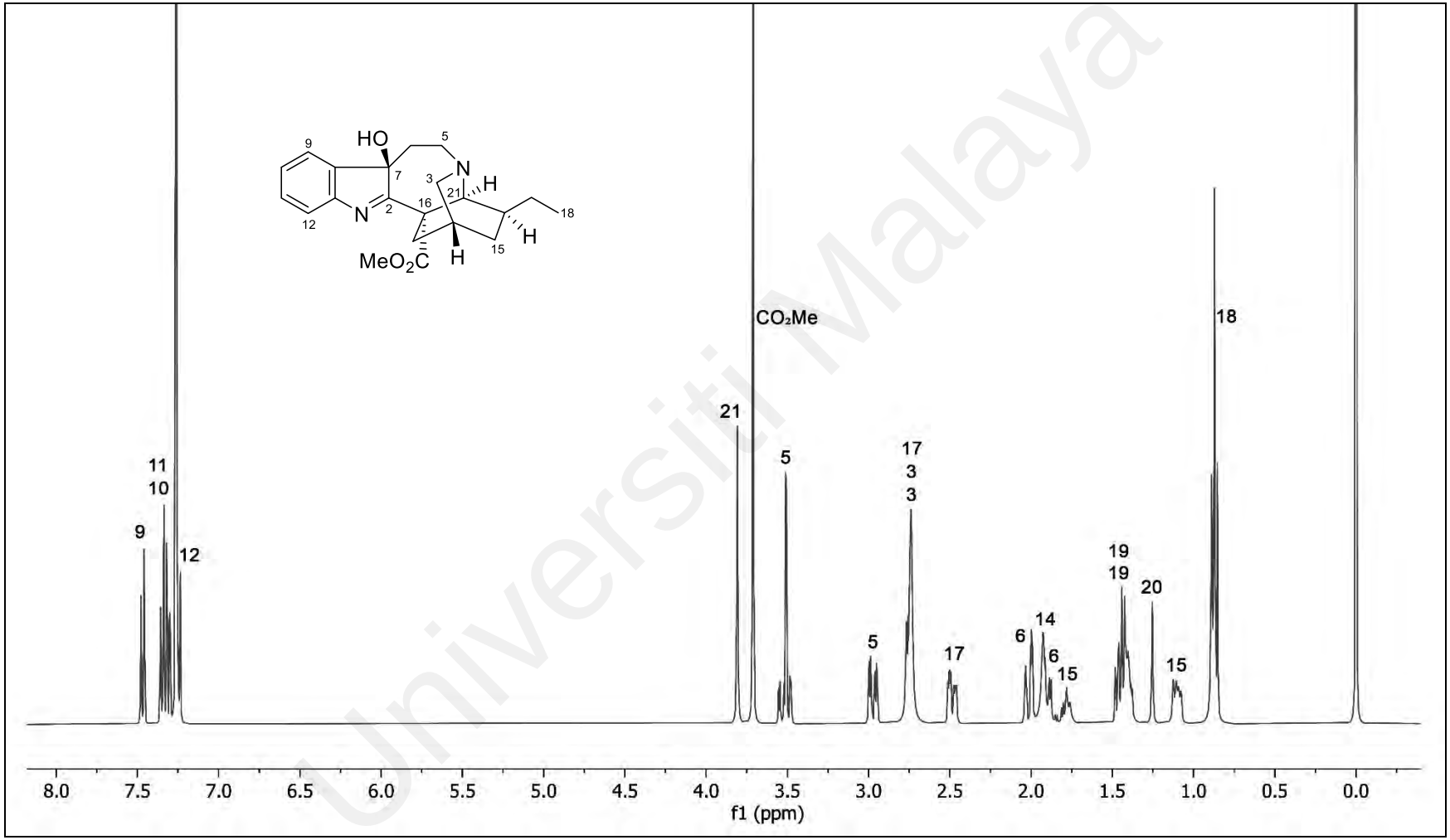


Figure 2.64: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Coronaridine-7-hydroxyindolenine (**29**)

2.1.2 Chippiine Alkaloids

2.1.2.1 Polyneurine I (30)

Polyneurine I (**30**) was obtained as a light yellowish oil, $[\alpha]^{25}_{D}$ −25 (*c* 0.1, $CHCl_3$). The UV spectrum showed absorption maxima at 223 and 285 nm, indicating the presence of an indole chromophore, while the IR spectrum showed absorption bands at 3384 and 1726 cm^{-1}, suggesting the presence of OH and ester carbonyl functions, respectively. The HRESIMS data showed an $[M + H]^+$ peak at *m/z* 353.1868, which corresponds to the molecular formula $C_{21}H_{24}N_2O_3$ + H (DBE = 11).

The ^{13}C NMR data (Table 2.22) accounted for a total of 21 carbon resonances comprising six methylenes, eight methines, one methyl ester, one ester carbonyl, two tertiary carbons bonded to indolic N, and three quaternary carbons. The ^{1}H NMR spectrum (Figure 2.68) showed the absence of an indolic NH, the presence of a methyl ester at δ_H 3.73, a deshielded doublet at δ_H 5.48 (*J* = 2.2 Hz, H-3), and an unusually shielded signal at δ_H 0.45 due to H-15α.

In addition to the contiguous aromatic hydrogens and the N–C-5–C-6 fragment, the COSY data revealed the presence of a $CHCH(CH_2)CH_2CH(CH)CH_2CH_2$ fragment in **30**, corresponding to C-3–C-14(C-17)–C-15–C-20(C-21)–C-19–C-18 (Figure 2.65). These structural features bear resemblance to the chippiine skeleton, *e.g.*, 10,11-demethoxychippiine (**31**) (Kam & Sim, 1999a; Nielsen *et al.*, 1994), except for the absence of the C-18 methyl triplet at δ_H 0.91 (δ_C 12.9), being replaced instead by a pair of methylene signals at δ_H 2.57 and 2.60 (δ_C 49.7) in **30**. The three-bond HMBC correlations observed from H-5 (δ_H 3.06, 3.20) to C-18 (δ_C 49.7) and from H-18 (δ_H 2.57, 2.60) to C-21 (δ_C 66.1) (Figure 2.65) showed that the methylene carbon at C-18 (δ_C 49.7) is linked to N-4 and thus forming an additional pyrrolidine ring. The presence

of an additional 5-membered ring is in agreement with the DBE number of **30** (DBE = 11), *cf.*, DBE number of **31** is 10.

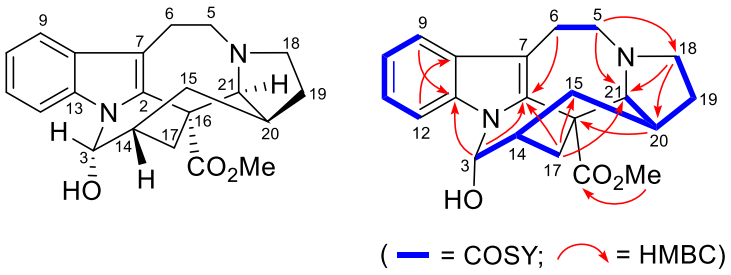


Figure 2.65: COSY and selected HMBCs of **30**

The relative configuration of **30** was deduced to resemble that of **31**, based on the NOE data (Figure 2.66). The configuration at C-3 (α-OH) was determined based on the observed H-3/H-12, H-15β NOEs (Figure 2.66), as well as the W coupling between H-3 and H-17β with J = 2.2 Hz, which was only possible for a β-oriented H-3. The assignment was further confirmed by the Gauge-Including Atomic Orbital (GIAO) NMR calculations and DP4+ probability analysis. The experimental NMR data were compared with the calculated ^{1}H and ^{13}C NMR shifts of **30** and its C-3 epimer using DP4+ probability analysis. The DP4+ results supported **30** with an α-OH function at C-3 as the correct relative configuration, with DP4+ probability score of 100% (based on all NMR data). The absolute configuration of **30** was eventually established as (3*S*, 14*R*, 16*S*, 20*R*, 21*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.67).

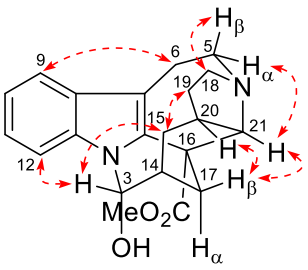


Figure 2.66: Selected NOEs of **30**

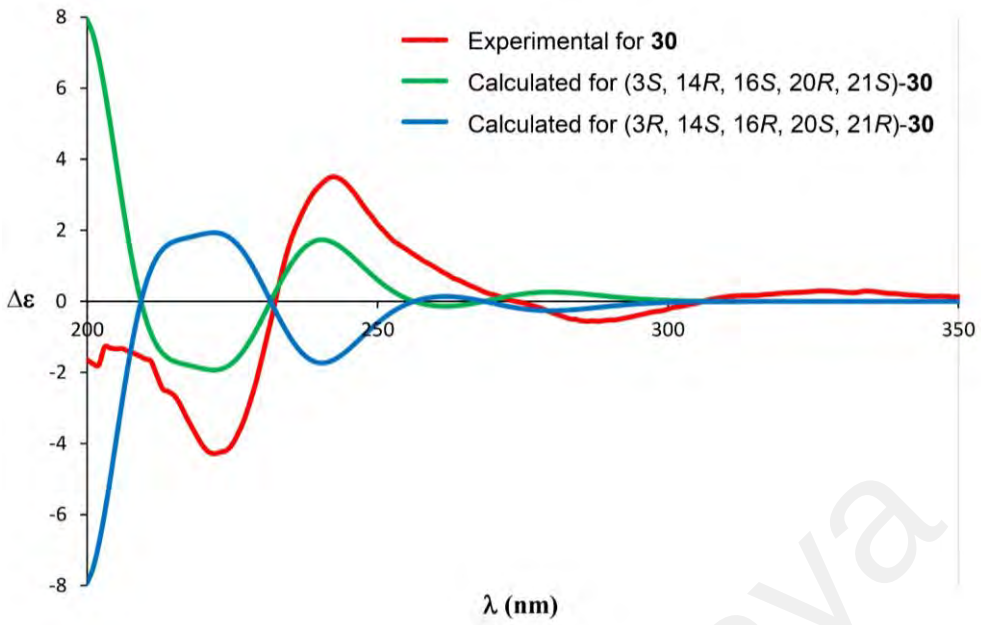
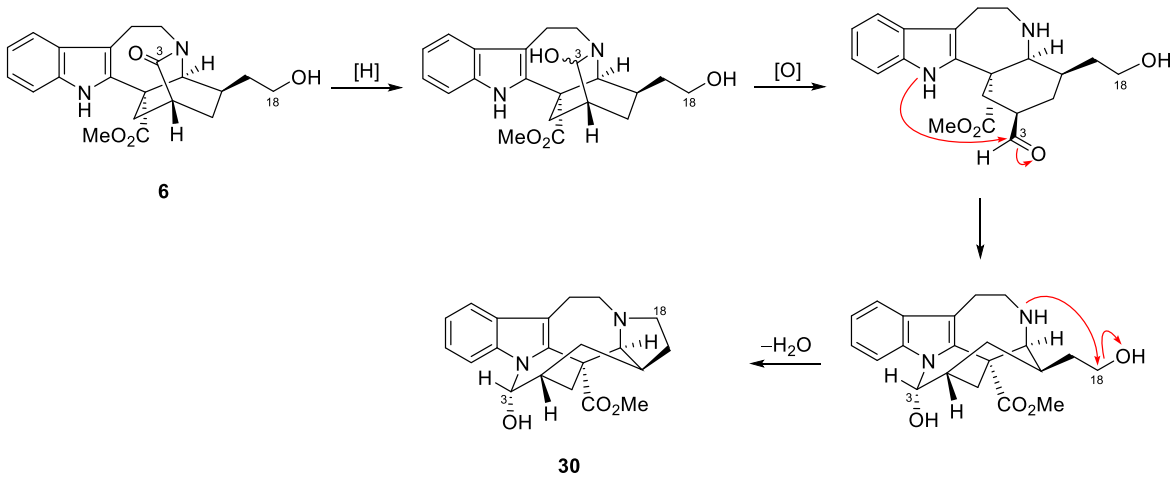


Figure 2.67: Experimental ECD spectrum of **30** and calculated ECD spectra of (3*S*, 14*R*, 16*S*, 20*R*, 21*S*)-**30** and (3*R*, 14*R*, 16*S*, 20*R*, 21*S*)-**30**

The biogenesis of chippiine-type alkaloids has been described previously and it arises biogenetically from the iboga class alkaloids (Taylor & Weinreb, 2021). We hypothesize that compound **30** may have arisen from the similar biosynthetic pathway. However, instead of (–)-catharantine, the precursor compound for **30** is polyneurine E (**6**), an iboga alkaloid also identified from the same system (Scheme 2.4). Reduction of **6** followed by a hemiaminal cleavage of C-3–N-4 bond leads to a a *seco*-coronaridine intermediate. Subsequent cyclization of the N-1 onto the C-3 aldehyde leads to a hypothetical chippiine derivative. Further cyclization between N-4 and C-18 leads to **30**.

Polyneurine I (**30**) represents a rare chippiine-type alkaloid. To date, only 14 members of this class have been isolated and characterized (Taylor & Weinreb, 2021). Compound **30** represents the first example of chippiine alkaloid that incorporates an additional pyrrolidine ring.



Scheme 2.4: Proposed biosynthetic pathway to **30**

Table 2.22: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of Polyneurine I (**30**)[a]

H/C	δ_H (J/Hz)	δ_C	H/C	δ_H (J/Hz)	δ_C
2	-	132.0	15α	0.45 td (13.4, 6.3)	27.7
3	5.48 d (2.2)	80.2	15β	1.76 m	
5α	3.06 m	43.2	16	-	46.8
5β	3.20 m		17β	1.89 m	25.3
6α	2.72 m	21.6	17α	2.43 m	
6β	3.14 m		18	2.57 m	49.7
7	-	110.7	18	2.60 m	
8	-	129.1	19β	0.97 m	29.5
9	7.51 d (8.0)	118.4	19α	1.85 m	
10	7.16 t (8.0)	120.4	20	2.44 m	34.1
11	7.22 t (8.0)	121.8	21	3.98 br s	66.1
12	7.44 d (8.0)	109.3	CO_2Me	3.73 s	52.8
13	-	138.0	CO_2Me	-	175.8
14	2.53 m	33.7			

[a]$CDCl_3$, 600 (^{1}H) and 150 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and NOESY.

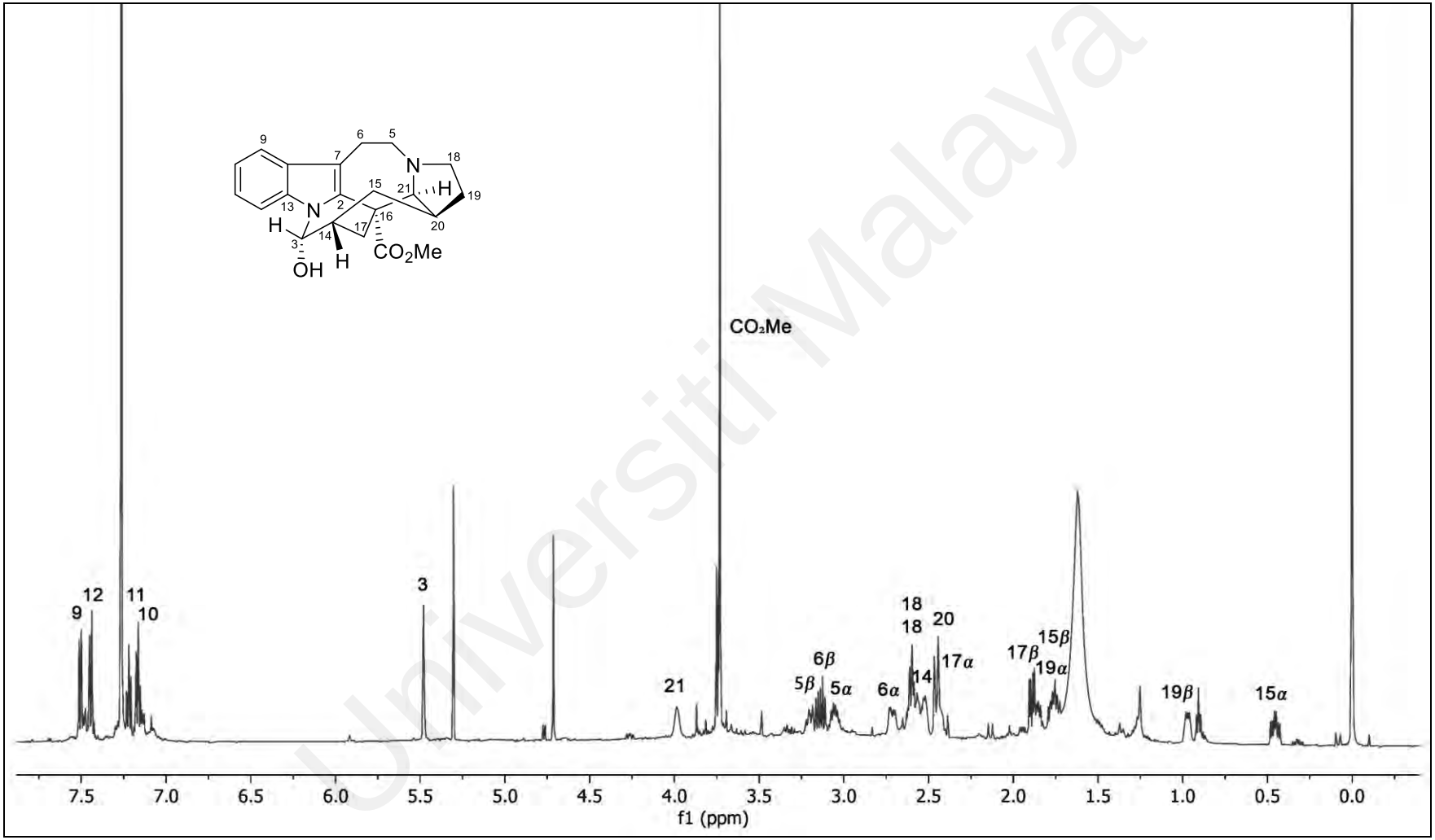


Figure 2.68: ^{1}H NMR Spectrum ($CDCl_3$, 600MHz) of Polyneurine I (**30**)

2.1.2.2 10,11-Demethoxychippiine (31) and 3-Methoxy-10,11-demethoxychippiine (32)

Two known alkaloids belonging to this group, *viz.*, 10,11-demethoxychippiine (**31**) (Kam & Sim, 1999a; Nielsen *et al.*, 1994) and 3-methoxy-10,11-demethoxychippiine (**32**) (Kitajima *et al.*, 2019; Shi *et al.*, 2019) were also isolated. The ^{1}H NMR spectra of these compounds are shown in Figures 2.69–2.70, while the ^{1}H and ^{13}C NMR spectroscopic data are summarized in Table 2.23. Other data are given in the Experimental Section.

Table 2.23: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of 10,11-Demethoxychippiine (**31**) and 3-Methoxy-10,11-demethoxychippiine (**32**)

H/C	**31**[a]		**32**[b]	
	δ_H (J/Hz)	δ_C	δ_H (J/Hz)	δ_C
2	-	137.7	-	131.8
3	5.48 d (2)	80.0	5.07 d (2)	86.9
5	2.68 m	40.9	2.70 m	40.3
5	3.18 td (10, 2)		3.18 td (11, 2)	
6	2.68 m	24.5	2.68 m	22.9
6	2.94 td (14, 10)		2.97 m	
7	-	110.1	-	109.6
8	-	129.5	-	129.1
9	7.51 br d (8)	118.8	7.51 br d (8)	118.2
10	7.17 td (8, 1)	120.9	7.16 td (8, 1)	120.2
11	7.22 td (8, 1)	122.2	7.21 td (8, 1)	121.6
12	7.46 br d (8)	109.9	7.41 br d (8)	109.7
13	-	132.0	-	138.0
14	2.53 m	34.9	2.63 m	31.6
15	0.34 td (14, 7)	23.5	0.30 ddd (14, 14, 7)	22.9
15	1.64 ddd (14, 11, 4)		1.60 m	
16	-	49.7	-	49.2
17	2.05 dd (14, 5)	24.4	2.00 dd (13, 5)	24.0
17	2.37 br d (14)		2.48 dd (13, 1)	
18	0.91 t (7)	12.9	0.91 t (7)	12.4
19	1.00 m	24.7	0.98 dqd (11, 7, 3)	24.2
19	1.38 dq (14, 7)		1.38 m	
20	1.85 dq (14, 7, 4)	36.4	1.86 m	36.0
21	3.94 d (7)	58.8	3.94 d (7)	58.6
CO_2Me	-	176.7	-	176.4
CO_2*Me*	3.72 s	53.2	3.72 s	52.7
3-O*Me*	-	-	3.62 s	56.1

[a]$CDCl_3$, 400 (^{1}H) and 100 MHz (^{13}C); [b]$CDCl_3$, 600 (^{1}H) and 150 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and NOESY.

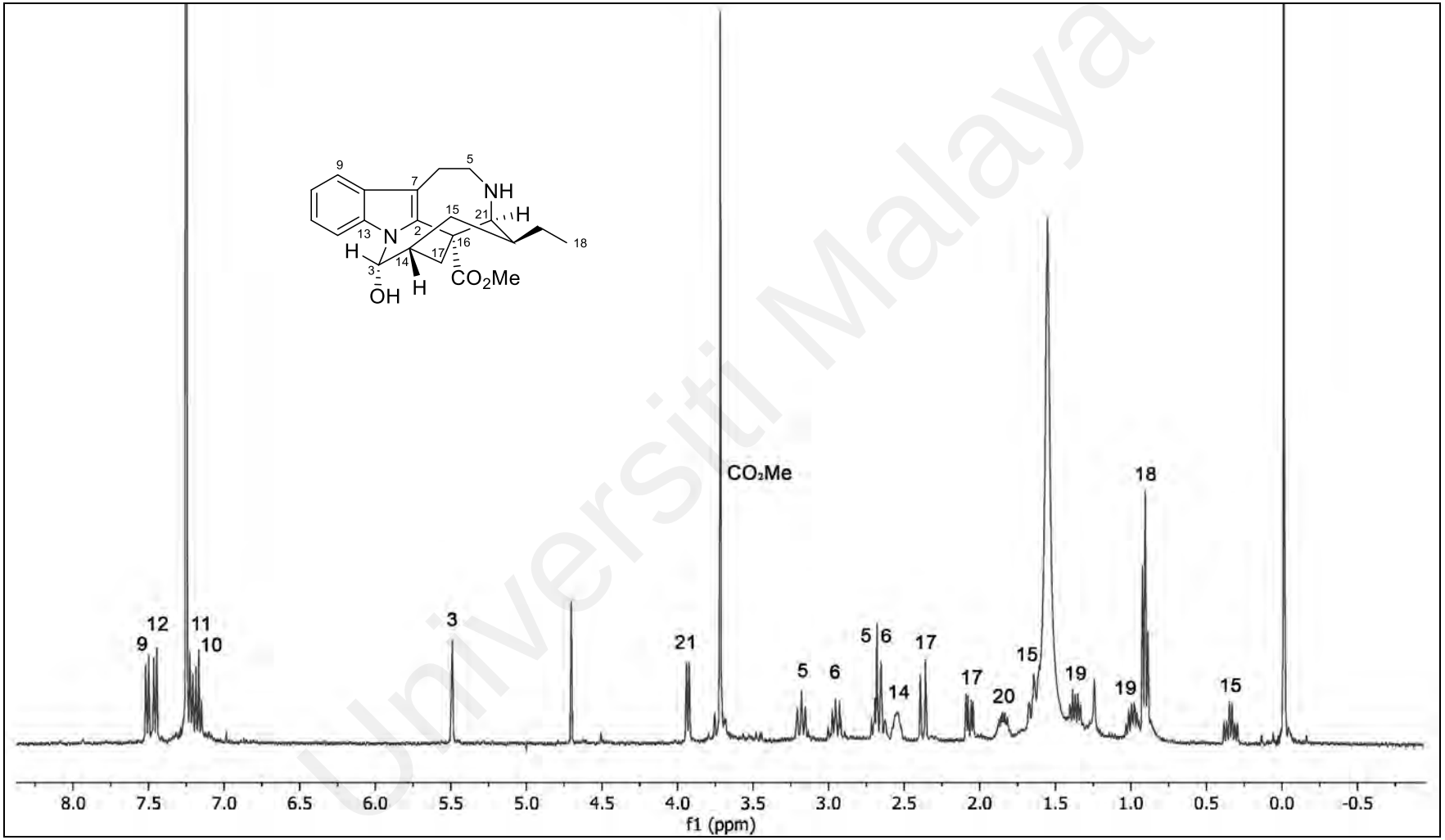


Figure 2.69: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 10,11-Demethoxychippiine (**31**)

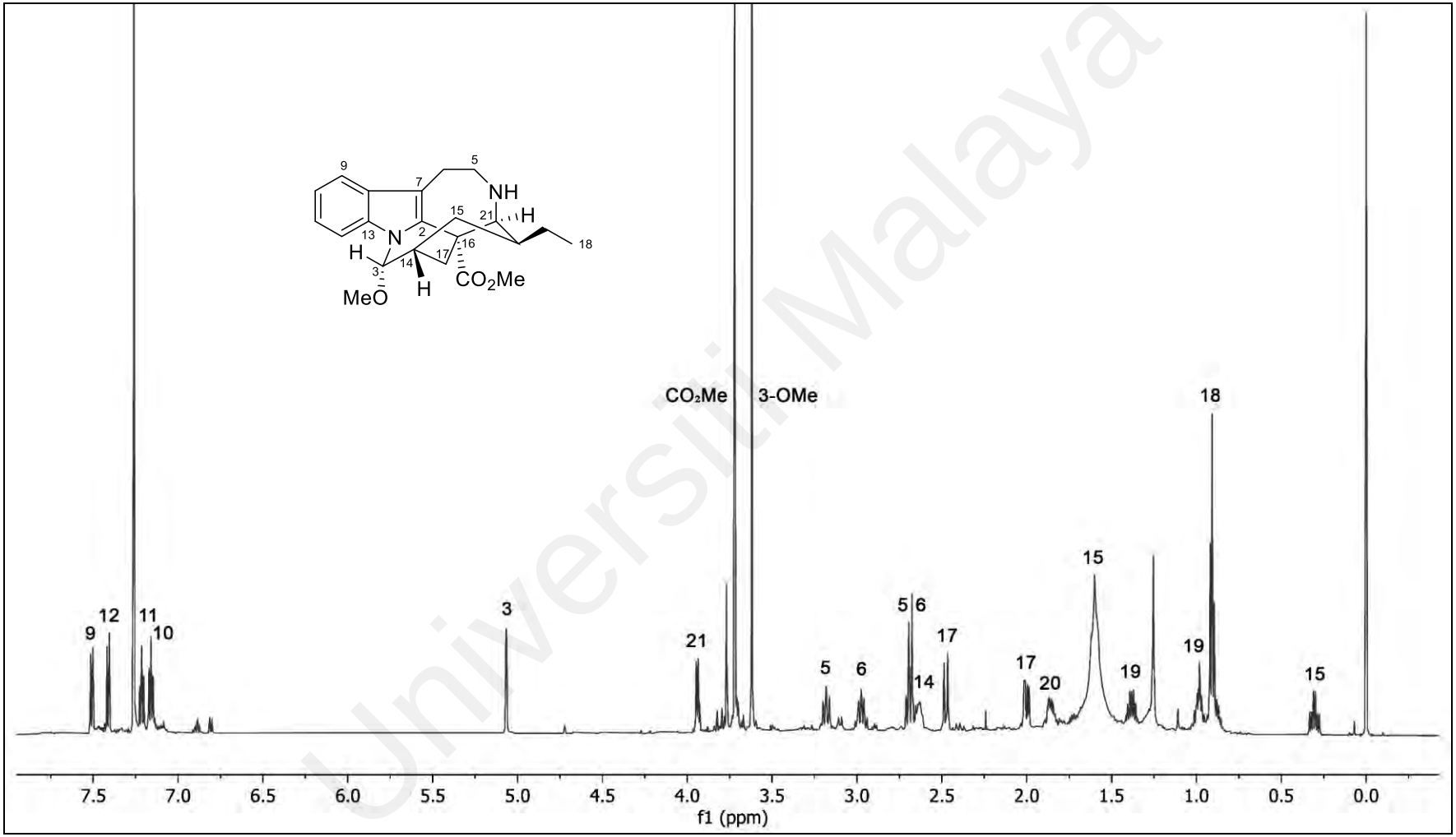


Figure 2.70: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of 3-Methoxy-10,11-demethoxychippiine (**32**)

2.1.3 Vobasine, Sarpagine, Ervatamine, and Corynantheine Alkaloids

2.1.3.1 Polyneurines M–O (33–35)

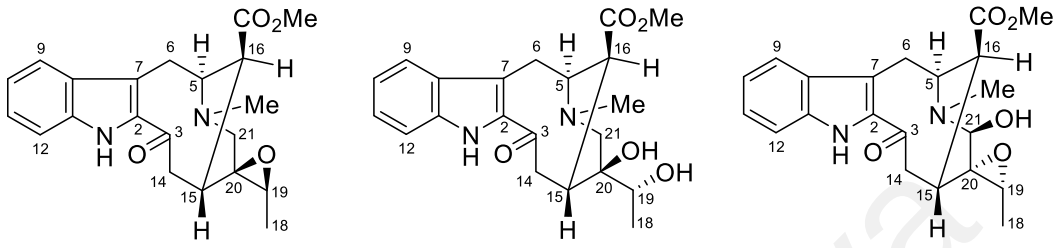


Figure 2.71: Structures of Polyneurines M–O

Polyneurine M (**33**) was obtained as a yellowish oil, $[\alpha]^{25}_{D}$ −51 (*c* 0.4, $CHCl_3$). The UV spectrum showed 2-acylindole absorption maxima at 227, 238, and 315 nm, while the IR spectrum showed absorption bands due to NH (3324 cm^{-1}), ester (1725 cm^{-1}), and conjugated carbonyl (1641 cm^{-1}) functions. The HRMS data ($[M + H]^+$ *m/z* 369.1811) established the molecular formula of **33** as $C_{21}H_{24}N_2O_4 + H$.

The ^1H NMR spectrum (Figure 2.82) showed the presence of an indolic NH (δ_H 9.04), four aromatic hydrogens (δ_H 7.17–7.73), an methyl ester group (δ_H 2.66), and an *N*(4)-methyl (δ_H 2.65). The ^{13}C NMR data (Table 2.25) displayed a total of 21 carbon resonances, including one methyl ester (δ_C 50.5), one ester carbonyl (δ_C 171.0), one conjugated ketone carbonyl (δ_C 189.0), an *N*(4)-methyl (δ_C 42.8), and an isolated aminomethylene (δ_C 51.3). The presence of an epoxide functionality was deduced based on the C-19 and C-20 resonances observed at δ_C 58.1 and 62.9, respectively. This was further supported by the $O–CHCH_3$ fragment revealed in the COSY spectrum, in addition to the $CH_2CHCHCHCH_2$ (C-6–C-5–C-16–C-15–C-14) partial structure which suggested a vobasine-type skeleton (Figure 2.72). The HMBC data confirmed the

proposed structure with the epoxide function at C-19, C-20 (^3J from H-14 and H-18 to C-20, from H-19 to C-21) (Figure 2.72).

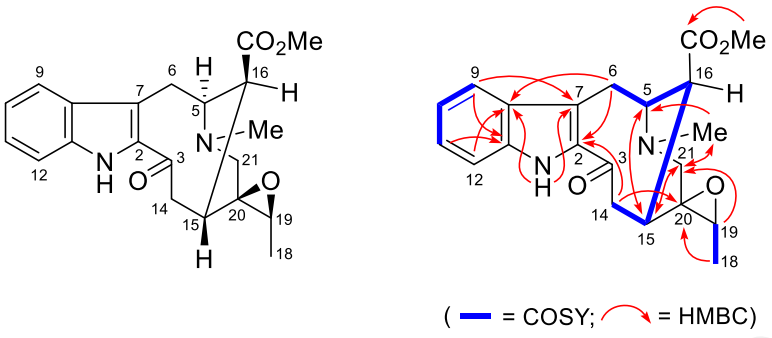
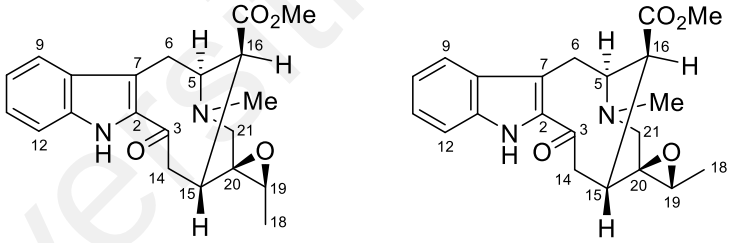


Figure 2.72: COSY and selected HMBCs of **33**

The proposed structure is similar to to vobasidine A (**196**), another vobasine-type alkaloid previously isolated from *T. corymbosa* (Sim *et al.*, 2014). The ^{1}H and ^{13}C NMR data of **33** were similar to **196**, except for the chemical shifts at H-15, H-18, H-21β, and H-21α, as well as C-15 and C-21, indicating that the epoxide function in **33** possesses a different configuration compared to **196** (Figure 2.73).



33 **196**

Figure 2.73: Structures of **33** and **196**

The relatively shielded ester methyl attached to C-16 at δ_H 2.66 indicates the placement of the methyl ester function within the shielding zone of the indole moiety (16*S*). The β-oriented epoxide moiety in **33** was deduced based on the chemical shift of H-16, in which the signal was observed downfield at δ_H 3.25 due to paramagnetic deshielding from the proximate epoxide moiety (compared to *ca.* δ_H 2.8–3.0 for an α-oriented epoxide) (Sim *et al.*, 2014). In addition, the NOE data of **33** also showed the presence of H-19/H-21β and Me-18/H-14β, H-15 enhancements (Figure 2.74) (*vs* H-

19/H-15, H-14β and Me-18/H-21β enhancements in **196**), enabling the assignment of the relative configuration of the epoxide moiety in **33** as 19*S*, 20*S*. The absolute configuration of **33** was eventually established as (5*S*, 15*R*, 16*S*, 19*S*, 20*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.75).

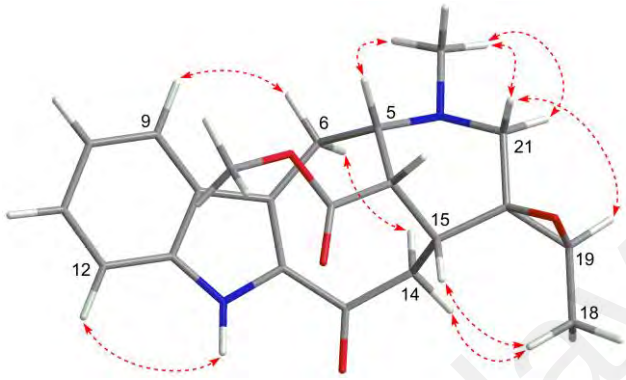


Figure 2.74: Selected NOEs of **33**

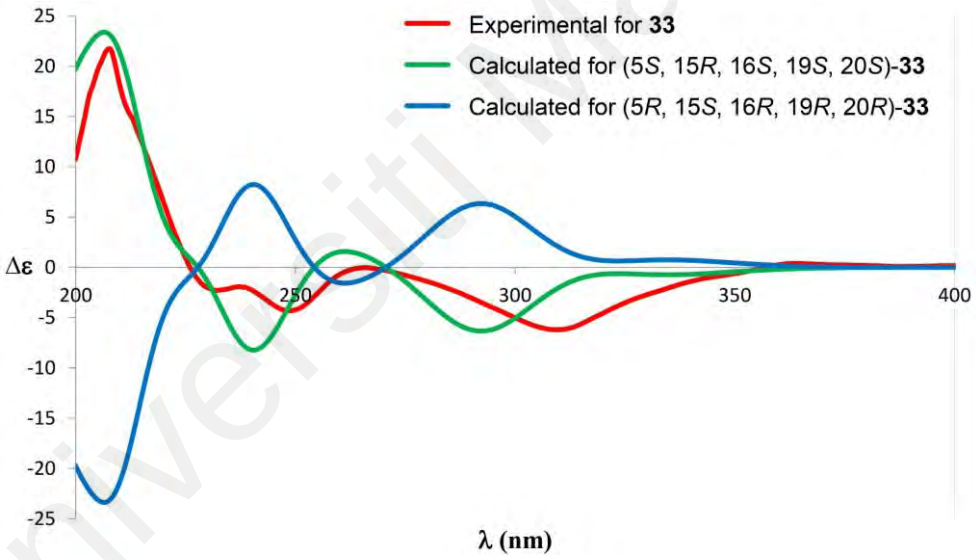


Figure 2.75: Experimental ECD spectrum of **33** and calculated ECD spectra of (5*S*, 15*R*, 16*S*, 19*S*, 20*S*)-**33** and (5*R*, 15*S*, 16*R*, 19*R*, 20*R*)-**33**

Polyneurine N (**34**) was isolated in minute amount as a light yellowish oil, $[\alpha]^{25}_{D}$ –31 (*c* 0.1, $CHCl_3$). The UV spectrum showed 2-acylindole absorption maxima at 221 and 315 nm, while the IR spectrum showed absorption bands due to NH/OH (3337 cm^{-1}), ester (1723 cm^{-1}), and conjugated carbonyl (1639 cm^{-1}) functions. The HRMS data ([M

+ H]$^+$ *m/z* 387.1925) established the molecular formula of **34** as $C_{21}H_{26}N_2O_5$ + H, 18 mass units higher than that of **33**, indicating the presence of an additional H_2O.

The ^{1}H NMR (Figure 2.83) and ^{13}C NMR data (Table 2.25) showed similarities with those of **33**, such as the presence of an indolic NH (δ_H 9.15), four aromatic hydrogens (δ_H 7.16–7.71), a methyl ester (δ_H 2.65; δ_C 50.5, 172.1), an *N*(4)-methyl (δ_H 2.62; δ_C 42.8), and an isolated aminomethylene (δ_H 2.45, 2.88; δ_C 50.1). The COSY data (Figure 2.76) indicated the presence of a $CH_2CHCHCH$ fragment, corresponding to C-6–C-5–C-16–C-15 of a vobasine-type alkaloid, in addition to a CH_3CHOH unit due to the C-18–C-19 side chain. Examination of the ^{13}C NMR data of **34** revealed a close resemblance to that of **33**, except for the resonances of C-19 and C-20 that were significantly shifted downfield from δ_C 58.1 and 62.9 in **33** to δ_C 67.7 and 75.2 in **34**, respectively, suggesting that the epoxide function at C-19 and C-20 has been converted into a diol. This suggestion was also reinforced by the additional of 18 mass units (H_2O) in the HRMS measurement.

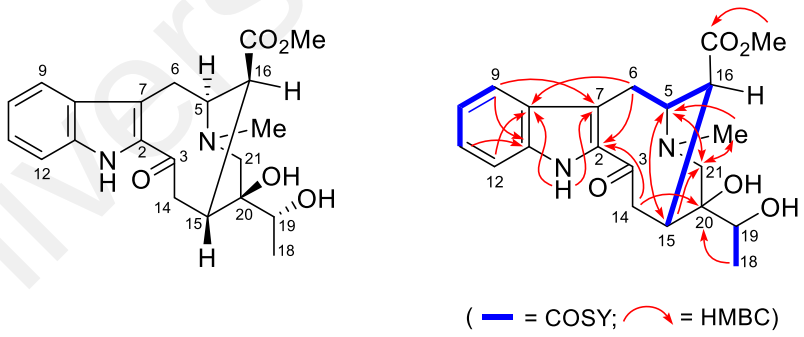


Figure 2.76: COSY and selected HMBCs of **34**

Similar to **33**, the relatively shielded ester methyl attached to C-16 at δ_H 2.65 for **34** indicated a 16*S* configuration. The β-orientation of the hydroxyl group at C-20 was assigned based on the observed Me-18/H-21β and H-19/H-14β NOE enhancements (Figure 2.77) (Sim *et al.*, 2022).

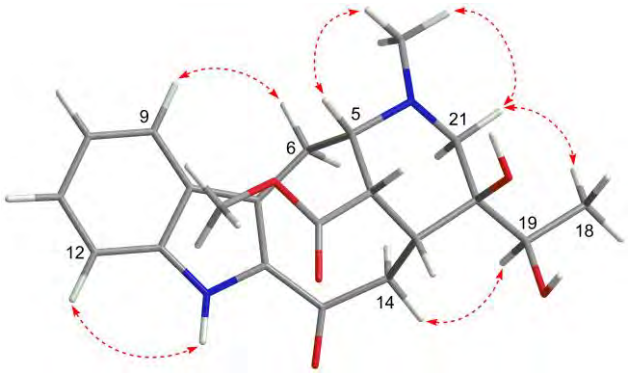


Figure 2.77: Selected NOEs of **34**

The remaining configuration at C-19 was determined using GIAO NMR calculations and DP4+ analysis. The experimental NMR data were compared with the calculated ^{1}H and ^{13}C NMR shifts of **34** and its C-19 epimer using DP4+ analysis. The DP4+ results supported **34** with 19*R* configuration as the correct relative configuration, with 100% DP4+ probability (all data). The absolute configuration of **34** was eventually established as (5*S*, 15*R*, 16*S*, 19*R*, 20*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.78).

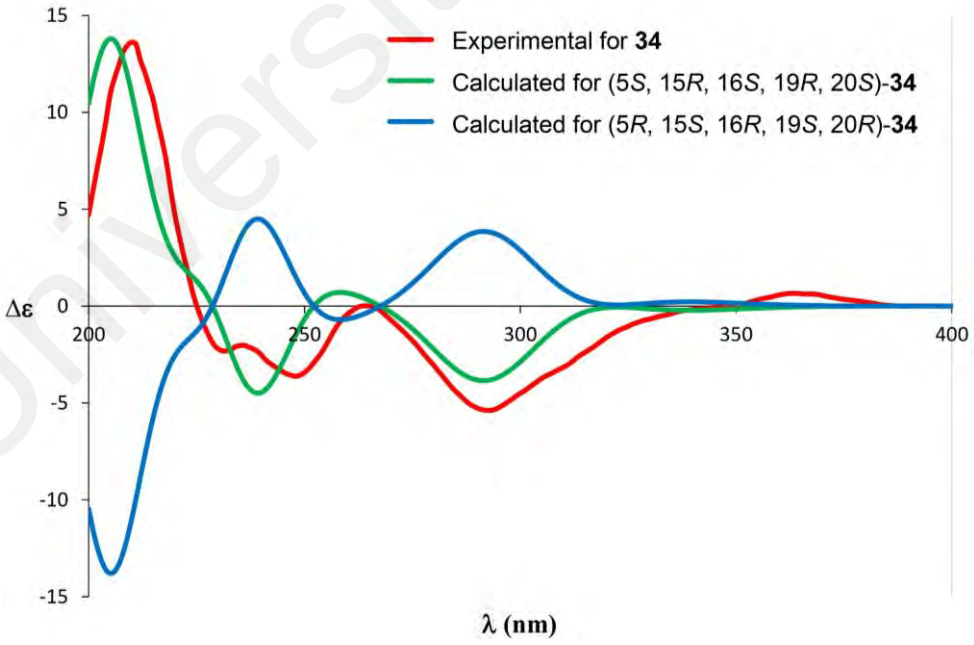


Figure 2.78: Experimental ECD spectrum of **34** and calculated ECD spectra of (5*S*, 15*R*, 16*S*, 19*R*, 20*S*)-**34** and (5*R*, 15*S*, 16*R*, 19*S*, 20*R*)-**34**

Polyneurine O (**35**) was obtained in minute amount as a light yellowish oil, $[\alpha]^{25}_{D}$ +11 (*c* 0.1, $CHCl_3$). The UV spectrum showed absorption maxima at 228, 240, and 315 nm, which were characteristic of a 2-acylindole chromophore, while the IR spectrum showed the presence of NH/OH (3166 cm^{-1}), ester (1726 cm^{-1}), and conjugated carbonyl (1637 cm^{-1}) functions. The HRMS data showed a $[M + H]^+$ peak at *m/z* 385.1762, which analyzed for $C_{21}H_{24}N_2O_5$ + H.

The ^{1}H NMR spectrum (Figure 2.84) of **35** showed the presence of an indolic NH (δ_H 8.93), an unsubstituted indole moiety (δ_H 7.15–7.73), a methyl ester (δ_H 2.63), and an *N*(4)-methyl (δ_H 2.89). The ^{13}C NMR data (Table 2.25) showed some common features with those of **33**, *viz.*, one methyl ester (δ_C 50.6), one ester carbonyl (δ_C 170.1), one conjugated ketone carbonyl (δ_C 190.9), and one *N*(4)-methyl (δ_C 38.8). Two contiguous carbons at δ_C 62.0 and 64.6 indicated the presence of an epoxide function in **35** (HMBCs: ^3J H-14, H-18/C-20 and H-21/C-19) (Figure 2.79). A notable difference is the replacement of the isolated aminomethylene group (δ_H 2.13, 3.68; δ_C 51.3) in **33** by a hemiaminal (δ_H 4.22; δ_C 90.0) in **35**. The presence of a hemiaminal group at C-21 was supported by the three-bond HMBCs from H-21 to C-5, C-15, and *N*(4)-Me, as well as from *N*(4)-Me to C-21 (Figure 2.79).

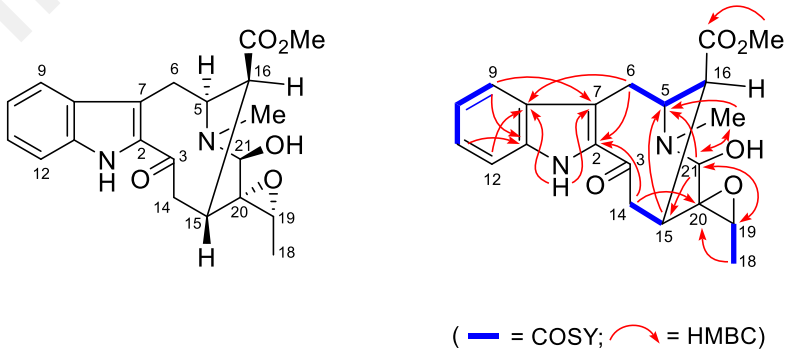


Figure 2.79: COSY and selected HMBCs of **35**

Similar to **33**, the relatively shielded ester methyl attached to C-16 at δ_H 2.63 indicates the placement of the methyl ester function within the shielding zone of the indole moiety (16*S*). In addition, the H-16 signal of **35** was shifted relatively upfield to δ_H 2.79 whereas the H-14α signal was shifted downfield to δ_H 4.33 (compared to H-16 and H-14α at δ_H 3.25 and 3.33, respectively, in **33**) (Sim *et al.*, 2014), suggesting the epoxide configuration is likely α. This suggestion was supported by the H-15/Me-18 NOE enhancement (Figure 2.80). The relative configuration at C-21 was deduced to be *S* based on the H-19/H-21 NOE enhancement.

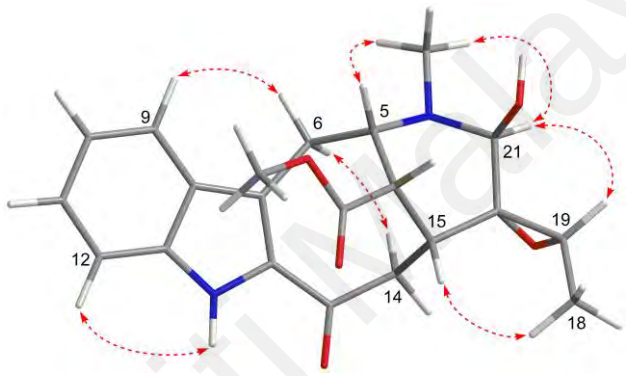


Figure 2.80: Selected NOEs of **35**

A GIAO NMR calculations and DP4+ analysis was carried out to verify the above configuration assignment. The experimental NMR data were compared with the calculated ^{1}H and ^{13}C NMR shifts of four possible diastereomers involving the C-19–C-20 epoxide and C-21 hemiaminal groups using DP4+ analysis. The DP4+ results supported **35** with an α-oriented epoxide and 21-OHβ as the correct relative configuration, with 100% DP4+ probability (all data). The absolute configuration of **35** was eventually established as (5*S*, 15*R*, 16*S*, 19*R*, 20*S*, 21*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.81).

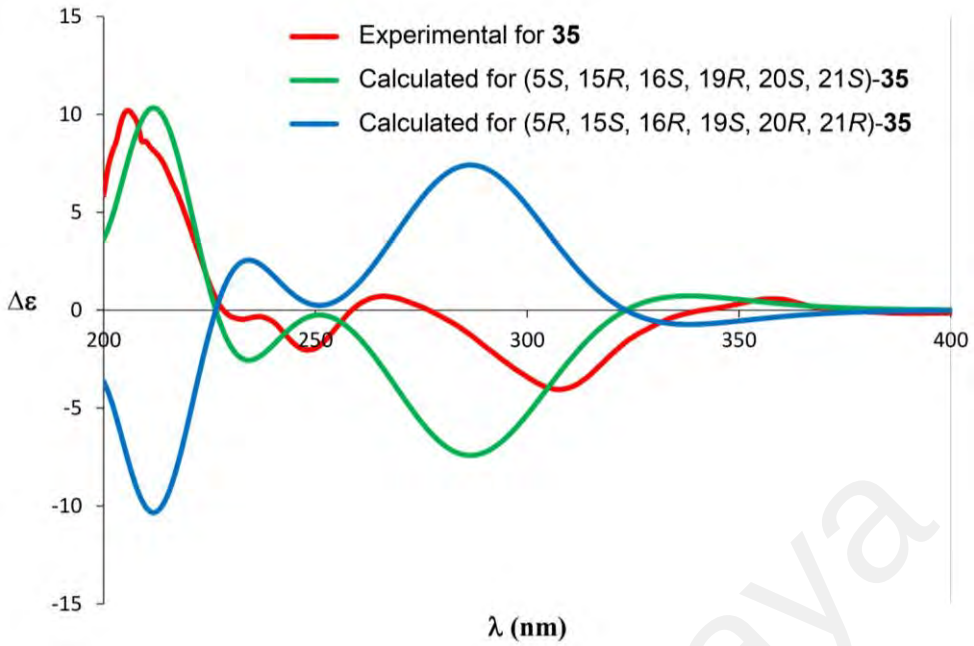


Figure 2.81: Experimental ECD spectrum of **35** and calculated ECD spectra of (5*S*, 15*R*, 16*S*, 19*R*, 20*S*, 21*S*)-**35** and (5*R*, 15*S*, 16*R*, 19*S*, 20*R*, 21*R*)-**35**

Table 2.24: ^{1}H NMR Spectroscopic Data (δ) of Polyneurines M (**33**), N (**34**), and O (**35**)

H	**33**[a] (*J*/Hz)	**34**[b] (*J*/Hz)	**35**[b] (*J*/Hz)
5	4.07 td (8.3, 3.3)	3.96 td (8.9, 3.1)	4.07 m
6	3.43 m	3.24 dd (14.3, 10.3) (α)	3.76 dd (13.6, 7.0) (β)
6	3.43 m	3.35 dd (14.6, 8.0) (β)	4.03 m (α)
9	7.73 d (8.0)	7.71 d (8.1)	7.73 d (8.1)
10	7.17 ddd (8.0, 6.1, 4.0)	7.16 ddd (8.1, 5.3, 2.7)	7.15 ddd (8.1, 4.9, 3.1)
11	7.35 m	7.35 m	7.33 m
12	7.35 m	7.35 m	7.33 m
14	2.79 dd (13.0, 7.0) (β)	2.96 dd (11.2, 11.3) (α)	2.92 dd (13.0, 6.8) (β)
14	3.33 t (13.0) (α)	3.07 dd (11.2, 6.2) (β)	4.33 t (13.0) (α)
15	2.62 m	3.01 m	2.75 m
16	3.25 t (3.3)	3.49 t (3.0)	2.79 t (3.0)
18	1.47 d (5.6)	1.28 d (6.2)	1.37 d (5.5)
19	3.05 q (5.6)	3.81 q (6.2)	3.16 q (5.5)
21	2.13 d (13.6) (β)	2.45 d (13.0) (β)	4.22 s
21	3.68 d (13.6) (α)	2.88 d (13.0) (α)	
CO_2*Me*	2.66 s	2.65 s	2.63 s
N(4)-*Me*	2.65 s	2.62 s	2.89 s
N(1)-H	9.04 br s	9.15 br s	8.93 br s

[a]$CDCl_3$, 400 MHz; [b]$CDCl_3$, 600 MHz; assignments based on COSY, HSQC, and NOESY.

Table 2.25: ^{13}C NMR Spectroscopic Data (δ) of Polyneurines M (**33**), N (**34**), and O (**35**)

C	**33**[a]	**34**[b]	**35**[b]
2	133.9	133.8	134.9
3	189.0	190.6	190.9
5	56.7	56.3	55.5
6	19.9	18.8	26.2
7	120.4	120.9	121.3
8	128.4	128.3	128.3
9	120.9	120.9	121.0
10	120.6	120.4	120.4
11	127.0	126.9	126.7
12	111.9	111.9	111.8
13	136.5	136.5	136.3
14	41.5	41.7	40.9
15	32.9	35.3	29.6
16	45.1	43.2	48.0
18	12.9	17.3	13.7
19	58.1	67.7	62.0
20	62.9	75.2	64.6
21	51.3	50.1	90.0
CO_2Me	171.0	172.1	170.1
CO_2*Me*	50.5	50.5	50.6
N(4)-*Me*	42.8	42.8	38.8

[a]$CDCl_3$, 100 MHz; [b]$CDCl_3$, 150 MHz; assignments based on HSQC and HMBC.

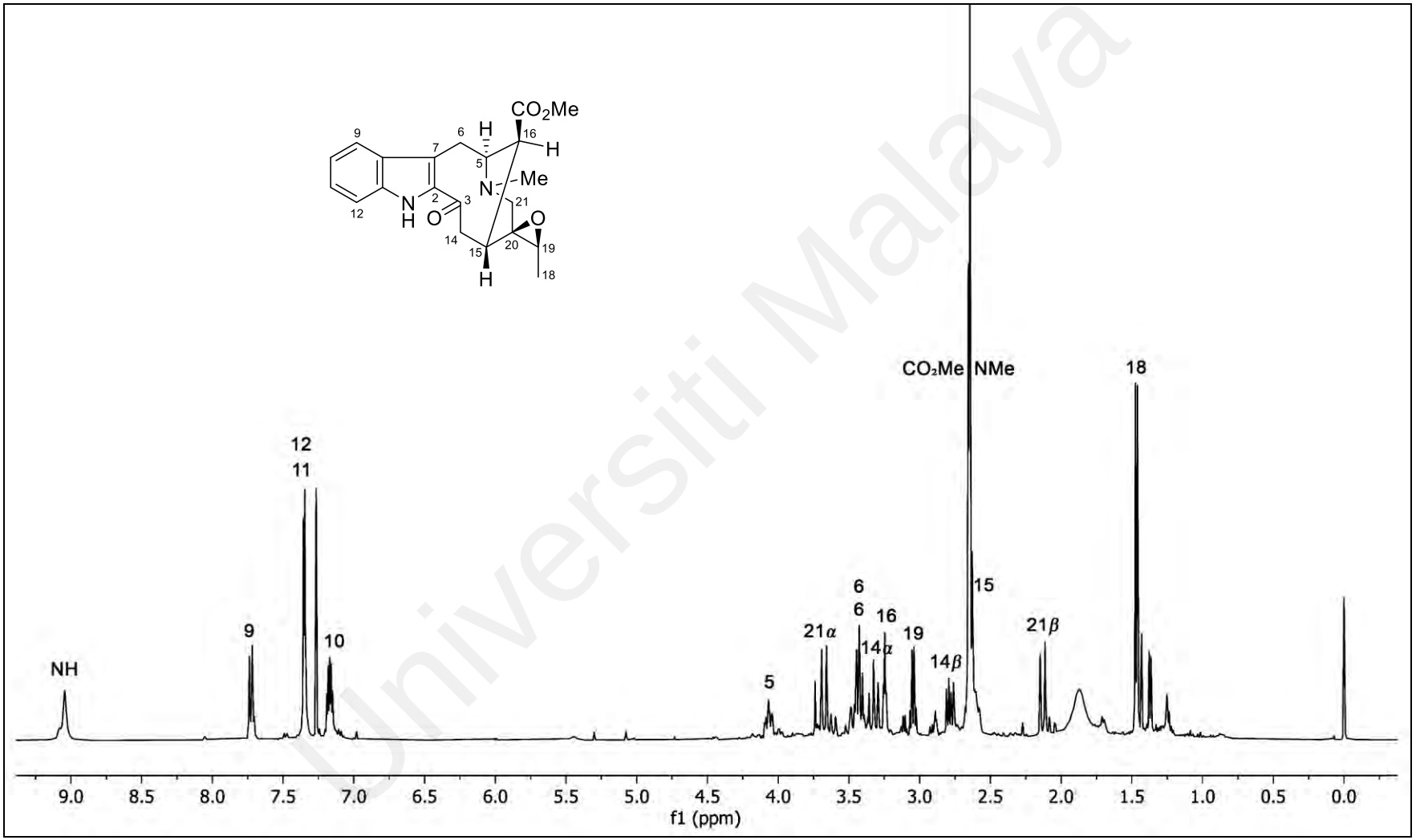


Figure 2.82: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Polyneurine M (**33**)

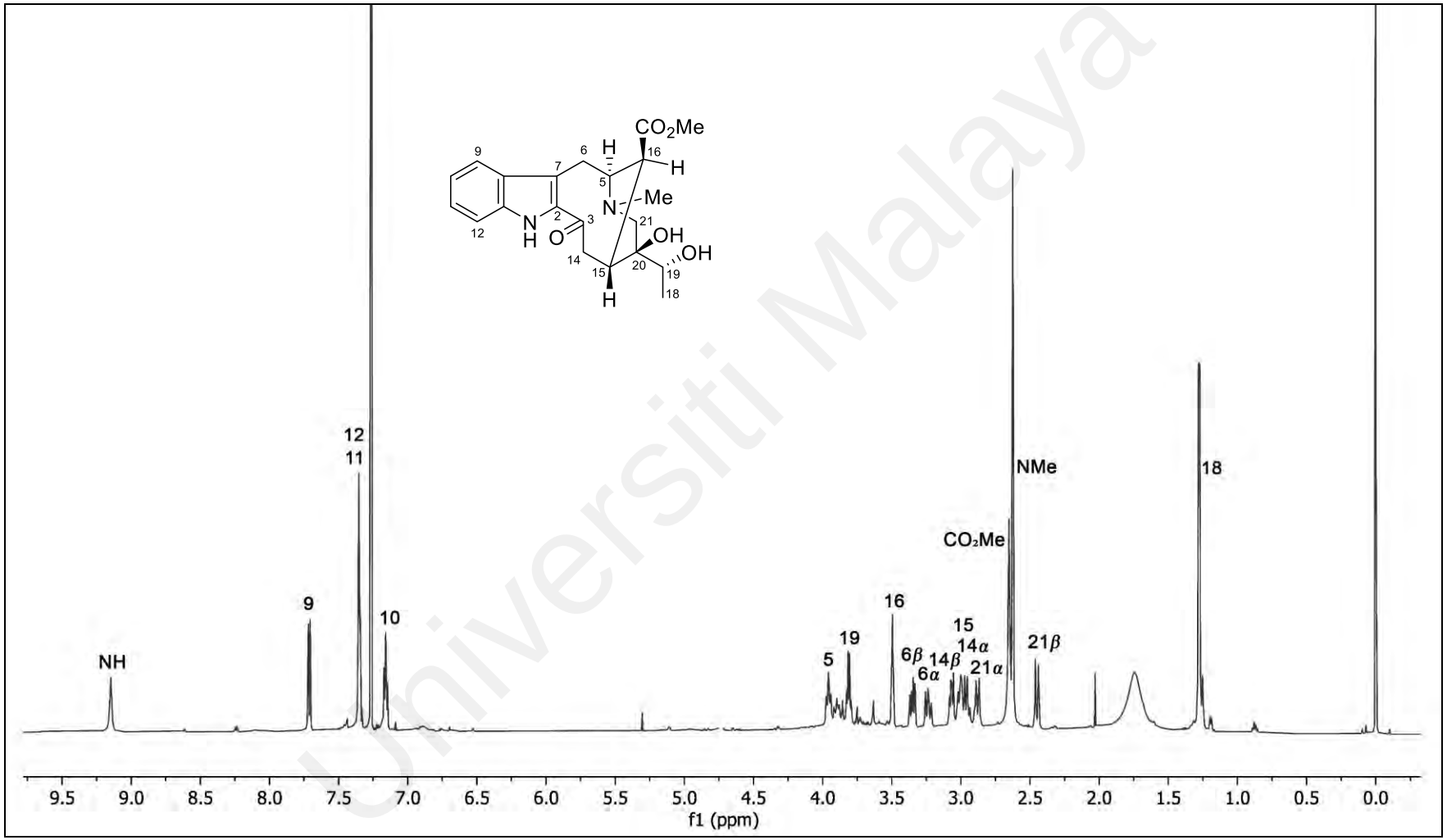


Figure 2.83: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Polyneurine N (**34**)

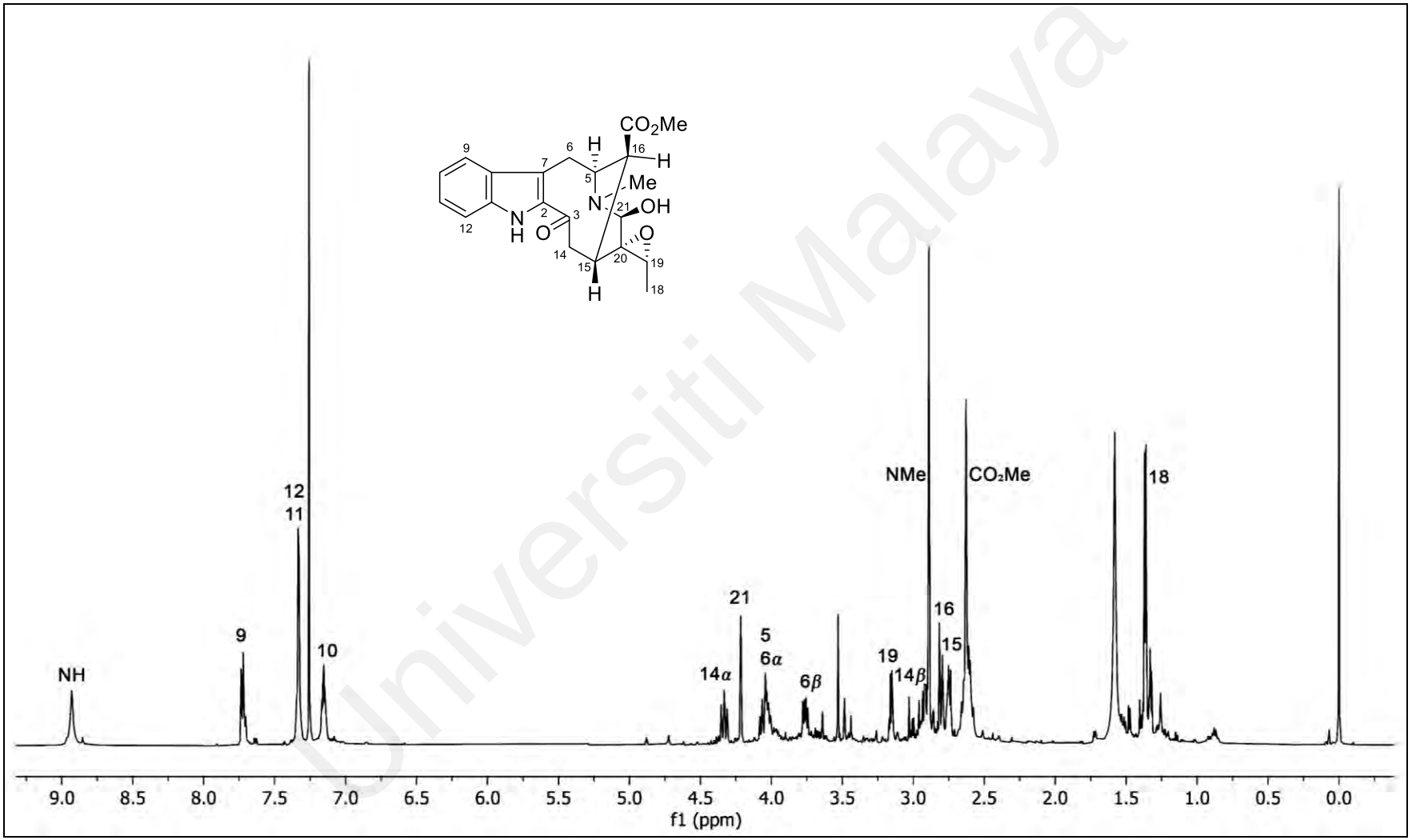


Figure 2.84: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Polyneurine O (**35**)

2.1.3.2 3-*Epi*-vobasinol (36), Vobasine (37), Vobasine *N*(4)-oxide (38), 16-*Epi*-vobasine (39), Perivine (40), Dregamine (41), Tabernaemontanine (42), Vobasenal (43), Vobasidine D (44), Vobasidine E (45), Vobasidine F (46), Pericyclivine (47), 16-*Epi*-voacarpine (48), 19,20-Dehydroervatamine (49), 16(*R*)-Sitsirikine (50), 16(*R*)-19,20-*E*-isositsirikine (51), 16(*R*)-19,20-*Z*-isositsirikine (52), and Fluorocarpamine (53)

A total of eighteen known monoterpenoid indole alkaloids belonging to the corynanthean-type alkaloids were isolated in this study. Of these, eleven alkaloids were identified as the vobasine-subtype, which include 3-*epi*-vobasinol (**36**) (Nugroho *et al.*, 2009), vobasine (**37**) (Ahond *et al.*, 1976; Van Beek, Kuijlaars *et al.*, 1984), vobasine *N*(4)-oxide (**38**) (Clivio, Richard, Hadi *et al.*, 1990), 16-*epi*-vobasine (**39**) (Clivio, Richard, Hadi *et al.*, 1990), perivine (**40**) (Agwada *et al.*, 1975; Tiong, 2014), dregamine (**41**) (Ahond *et al.*, 1976; Sim *et al.*, 2014), tabernaemontanine (**42**) (Ahond *et al.*, 1976; Cava *et al.*, 1963; Sim *et al.*, 2014), vobasenal (**43**) (Clivio, Richard, Hadi *et al.*, 1990), vobasidine D (**44**) (Sim *et al.*, 2014), vobasidine E (**45**) (Sim *et al.*, 2022), and vobasidine F (**46**) (Sim *et al.*, 2022). The sarpagine- and ervtamine-subtypes alkaloids were also isolated, *viz.*, pericyclivine (**47**) (Jokela & Lounasmaa, 1996; Lathuilliere *et al.*, 1966; Lounasmaa *et al.*, 1985; Mukhopadhyay & Cordell, 1981), 16-*epi*-voacarpine (**48**) (Kogure *et al.*, 2005; Lin & Cordell, 1990), and 19,20-dehydroervatamine (**49**) (Kam & Loh, 1993). Another four known alkaloids belonging to the corynantheine-subtype, *i.e.*, 16(*R*)-sitsirikine (**50**) (Brown & Leonard, 1979; Kitajima *et al.*, 2014; Kohl *et al.*, 1982; Kutney & Brown, 1966), 16(*R*)-19,20-*E*-isositsirikine (**51**) (Kutney & Brown, 1966; Lounasmaa *et al.*, 1994 & 1995), 16(*R*)-19,20-*Z*-isositsirikine (**52**) (Kan, Kan *et al.*, 1981; Kutney & Brown, 1966; Lounasmaa *et al.*, 1994), and fluorocarpamine (**53**) (Jacquier *et al.*, 1982), were also obtained. The

^{1}H NMR spectra of these compounds are shown in Figures 2.85–2.102, while the ^{1}H and ^{13}C NMR spectroscopic data are summarized in Tables 2.26–2.35. Other data are given in the Experimental Section.

Table 2.26: ^{1}H NMR Spectroscopic Data (δ) of 3-*Epi*-vobasinol (**36**), Vobasine (**37**), Vobasine *N*(4)-oxide (**38**), and 16-*Epi*-vobasine (**39**)

H	**36**^{b} (*J*/Hz)	**37**^{a} (*J*/Hz)	**38**^{b} (*J*/Hz)	**39**^{a} (*J*/Hz)
3	5.17 dd (12, 4)	-	-	-
5	3.93 td (9, 3)	3.98 ddd (10, 8, 3)	4.49 m	3.82 ddd (10, 9, 2)
6	3.15 dd (15, 8)	3.44 dd (15, 8)	3.44 m	3.44 dd (14, 9)
6	3.33 dd (15, 10)	3.53 dd (15, 10)	3.84 m	3.52 dd (14, 10)
9	7.55 d (8)	7.72 dd (8, 1)	7.72 d (8)	7.72 dd (8, 1)
10	7.09 t (8)	7.16 ddd (8, 5, 3)	7.22 ddd (8, 4, 4)	7.17 ddd (8, 7, 1)
11	7.17 t (8)	7.35 m	7.39 m	7.37 m
12	7.24 d (8)	7.35 m	7.39 m	7.37 m
14	2.12 ddd (15, 7, 4)	2.73 dd (14, 8)	2.82 dd (14, 8)	2.69 dd (13, 8)
14	2.61 m	3.32 dd (14, 12)	3.07 t (14)	3.35 t (13)
15	3.64 ddd (12, 7, 3)	3.76 ddd (12, 7, 3)	3.84 m	3.66 m
16	2.64 m	2.84 t (3)	4.38 s	2.81 t (2)
18	1.70 dd (7, 2)	1.72 dd (7, 2)	1.80 d (7)	1.74 dd (7, 2)
19	5.40 q (7)	5.48 qd (7, 2)	5.71 q (7)	5.50 br q (7)
21	2.94 d (14)	2.99 br d (14)	3.97 d (14)	2.97 br d (14)
21	3.72 d (14)	3.85 dt (14, 2)	4.49 m	3.66 m
CO_2*Me*	2.45 s	2.65 s	2.60 s	3.57 s
N(4)-Me	2.55 s	2.61 s	3.59 s	2.53 s
N(1)-H	8.20 br s	9.05 br s	9.24 br s	9.38 br s

^{a}$CDCl_3$, 400 MHz; ^{b}$CDCl_3$, 600 MHz; assignments based on COSY and HSQC.

Table 2.27: ^{13}C NMR Spectroscopic Data (δ) of 3-*Epi*-vobasinol (**36**), Vobasine (**37**), Vobasine *N*(4)-oxide (**38**), and 16-*Epi*-vobasine (**39**)

C	**36**[b]	**37**[a]	**38**[b]	**39**[a]
2	135.5	134.2	134.2	135.1
3	67.5	190.2	188.8	190.7
5	59.0	57.3	73.2	56.3
6	19.3	20.4	25.3	19.2
7	110.4	120.3	115.9	121.4
8	129.1	128.5	127.8	128.5
9	118.3	120.9	120.3	120.9
10	119.3	120.4	121.2	120.7
11	122.8	126.8	127.2	127.1
12	110.4	111.8	112.1	112.4
13	136.0	136.4	136.1	136.7
14	37.5	43.1	42.6	42.9
15	30.8	30.5	28.9	29.1
16	46.6	46.6	40.7	44.6
18	12.4	12.4	12.9	12.3
19	119.3	121.0	128.5	121.9
20	137.0	135.8	129.5	134.2
21	52.3	51.9	64.2	52.0
*C*O$_2$Me	171.9	171.3	170.3	173.6
CO$_2$*Me*	50.1	50.4	50.6	52.0
N(4)-Me	42.3	42.4	56.0	42.4

[a]$CDCl_3$, 100 MHz; [b]$CDCl_3$, 150 MHz; assignments based on HSQC and HMBC.

Table 2.28: ^{1}H NMR Spectroscopic Data (δ) of Perivine (**40**), Dregamine (**41**), and Tabernaemontanine (**42**)[a]

H	**40** (*J*/Hz)	**41** (*J*/Hz)	**42** (*J*/Hz)
5	4.16 m	3.95 ddd (10, 8, 3)	3.96 td (9, 3)
6	3.50 dd (15, 8)	3.32 dd (15, 10)	3.30 dd (15, 9)
6	3.67 dd (15, 10)	3.39 dd (15, 8)	3.44 dd (15, 9)
9	7.73 d (8)	7.70 dd (8, 1)	7.70 br d (8)
10	7.16 dd (8, 4)	7.16 ddd (8, 5, 3)	7.15 ddd (8, 5, 2)
11	7.34 m	7.33 m	7.33 m
12	7.34 m	7.33 m	7.33 m
14	3.39 dd (14, 12)	2.68 dd (12, 7)	2.76 dd (12, 7)
14	2.77 dd (14, 7)	3.11 t (12)	3.40 t (12)
15	3.86 m	2.90 m	2.70 m
16	2.68 t (2)	2.87 br s	3.03 t (3)
18	1.70 d (7)	1.02 t (8)	0.97 t (7)
19	5.44 br q (7)	1.35 m	1.54 m
19	-	1.35 m	1.73 m
20	-	1.91 m	1.54 m
21	3.25 d (15)	2.61 m	2.50 d (13)
21	4.16 br d (15)	2.78 t (13)	3.19 dd (13, 3)
CO_2*Me*	2.65 s	2.64 s	2.61 s
N(4)-Me	-	2.64 s	2.57 s
N(4)-H	*n.o.*	-	-
N(1)-H	8.97 br s	8.97 br s	8.87 br s

[a]$CDCl_3$, 400 MHz; assignments based on COSY and HSQC.

Table 2.29: ^{13}C NMR Spectroscopic Data (δ) of Perivine (**40**), Dregamine (**41**), and Tabernaemontanine (**42**)[a]

C	40	41	42
2	134.1	134.0	133.9
3	190.3	191.5	190.8
5	50.9	56.7	56.8
6	25.6	20.1	18.5
7	120.0	120.4	120.7
8	128.4	128.4	128.5
9	121.0	120.8	120.9
10	120.6	120.3	120.3
11	126.8	126.6	126.6
12	111.7	111.8	111.8
13	136.4	136.4	136.4
14	43.2	39.2	45.6
15	31.2	30.6	31.8
16	49.6	49.0	43.4
18	12.2	11.4	12.7
19	120.2	23.4	25.4
20	137.9	43.4	42.5
21	43.8	48.7	46.5
CO_2Me	171.0	171.3	172.0
CO_2*Me*	50.4	50.3	50.2
N(4)-Me	-	42.5	43.0

[a]$CDCl_3$, 100 MHz; assignments based on HSQC and HMBC.

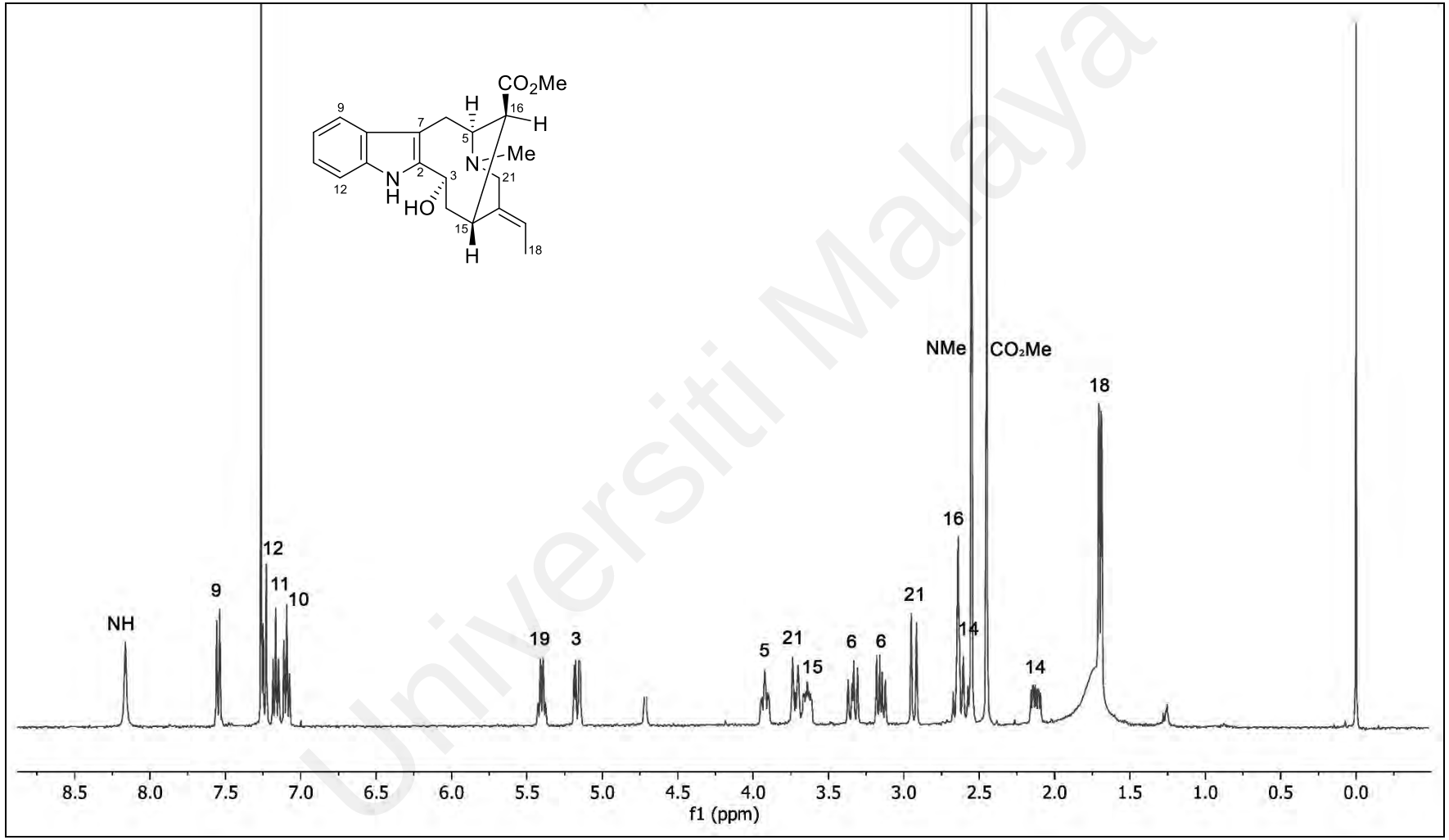


Figure 2.85: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of 3-*Epi*-vobasinol (**36**)

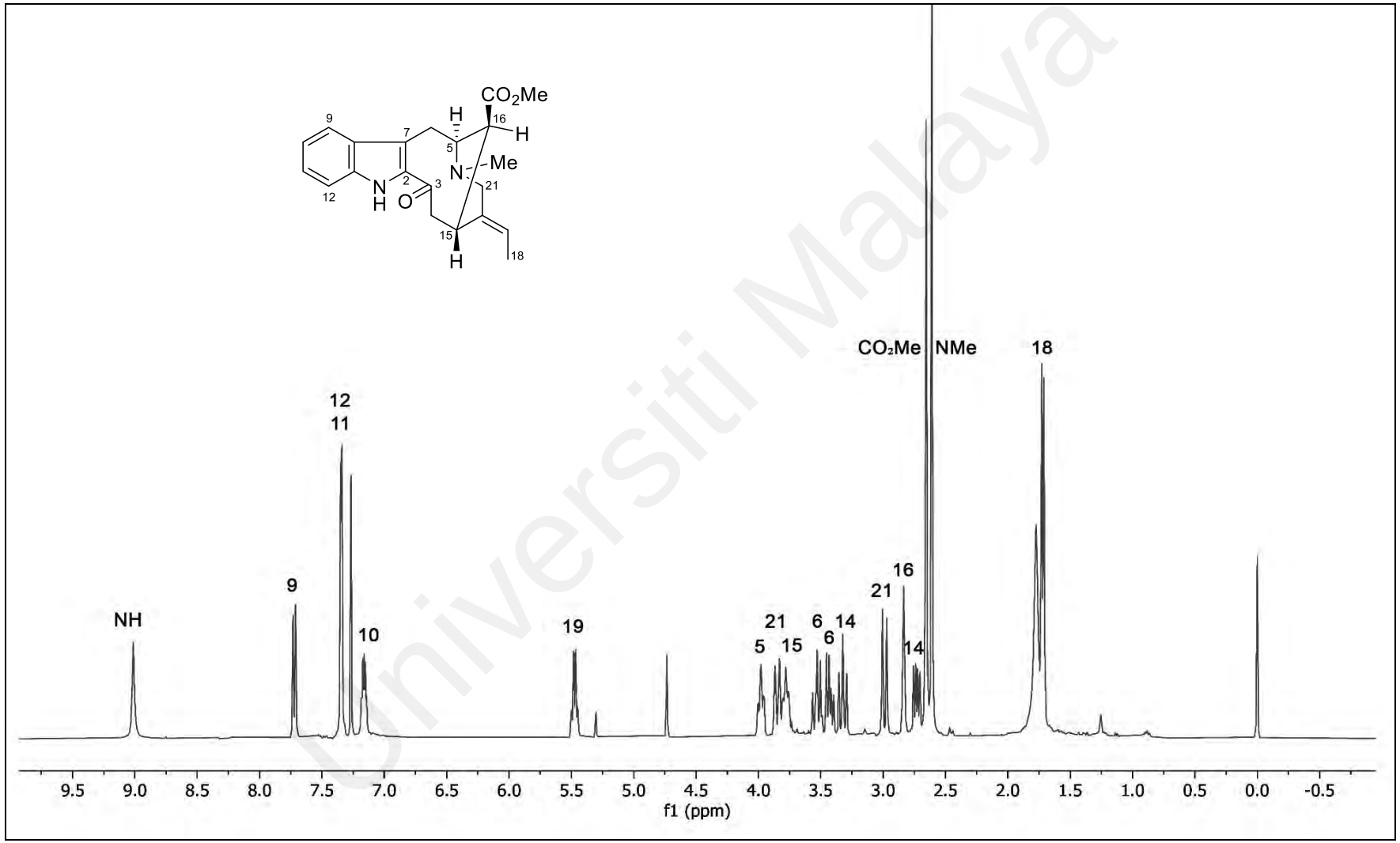


Figure 2.86: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Vobasine (**37**)

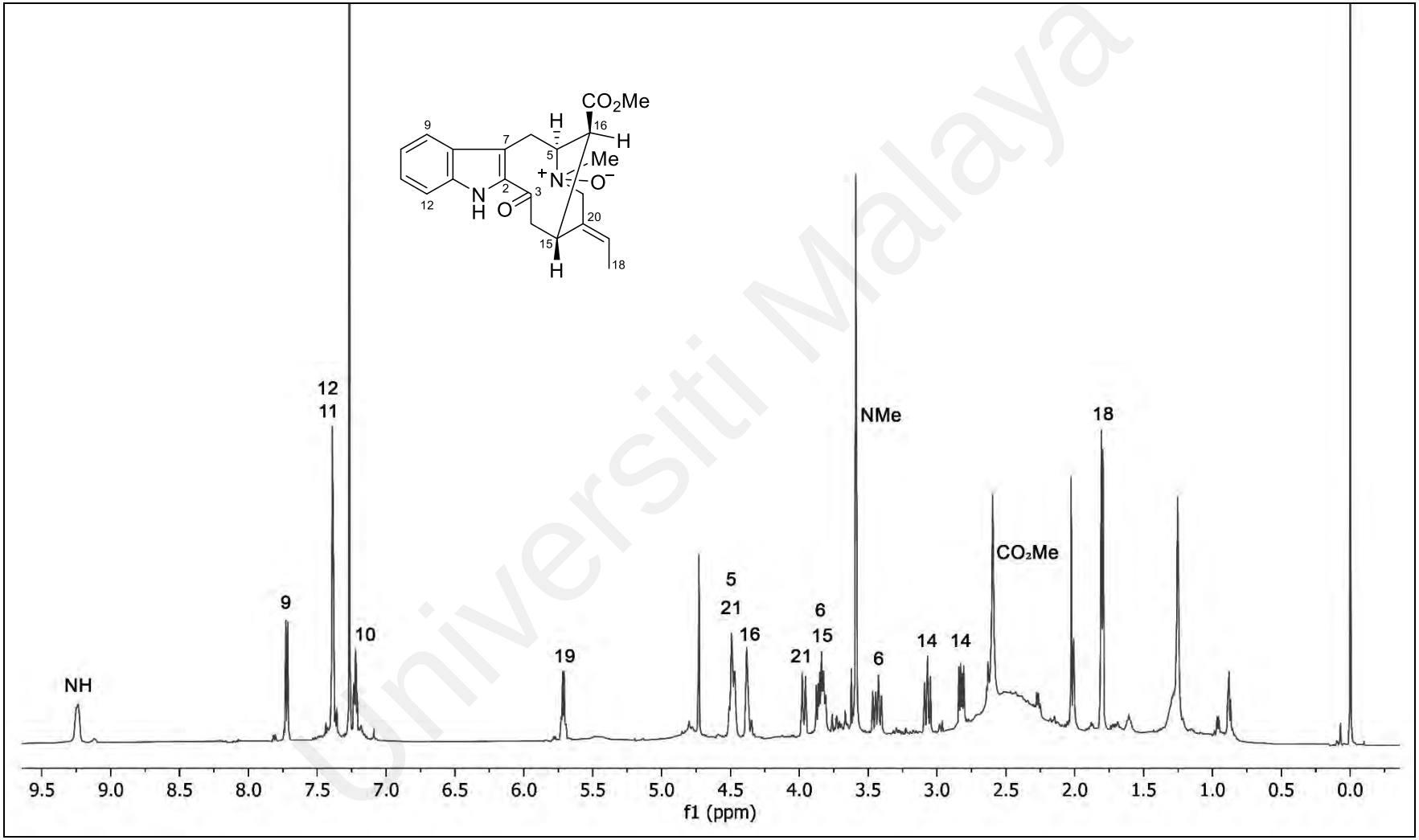


Figure 2.87: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Vobasine-*N*(4)-oxide (**38**)

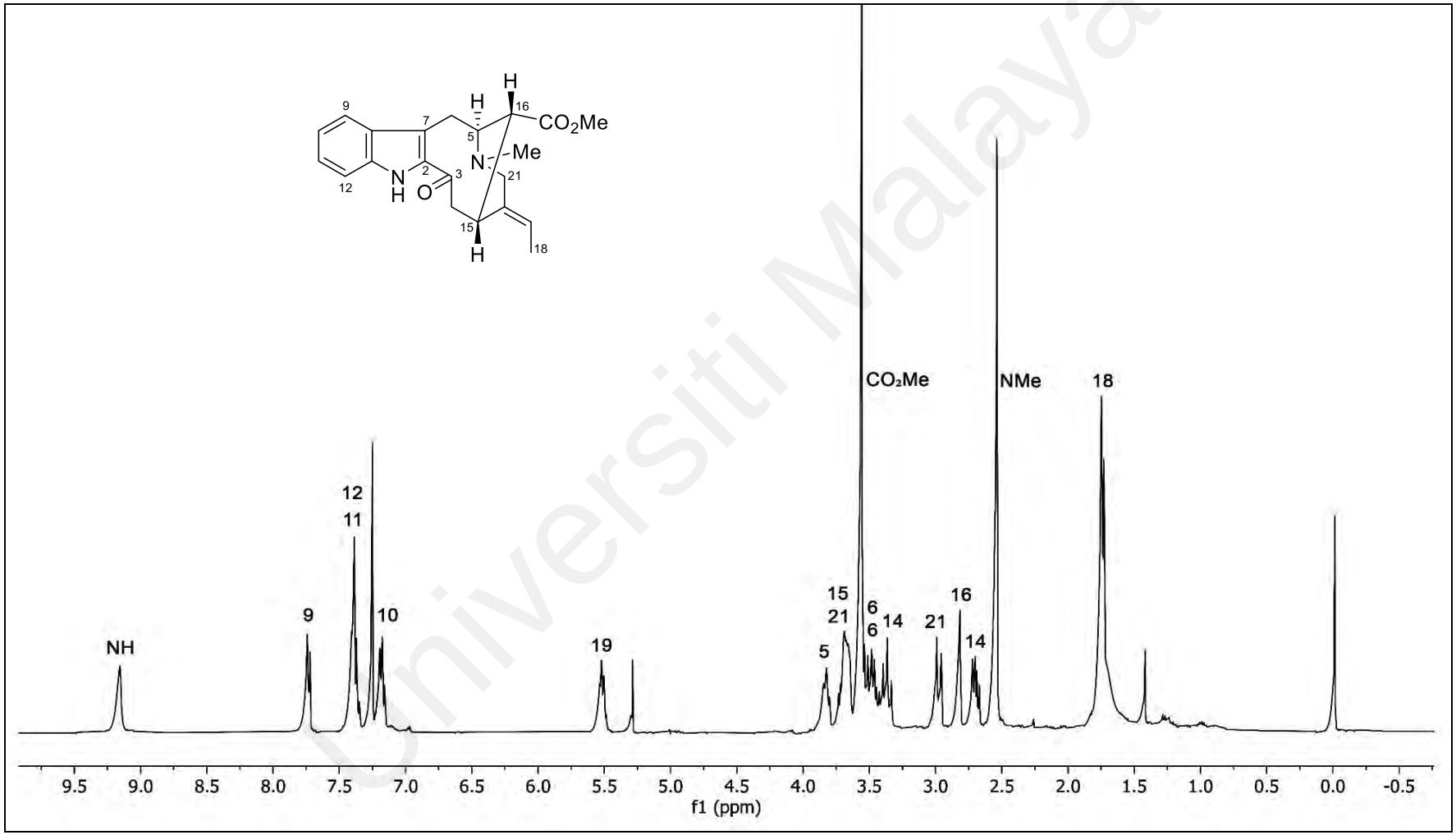


Figure 2.88: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 16-*Epi*-vobasine (**39**)

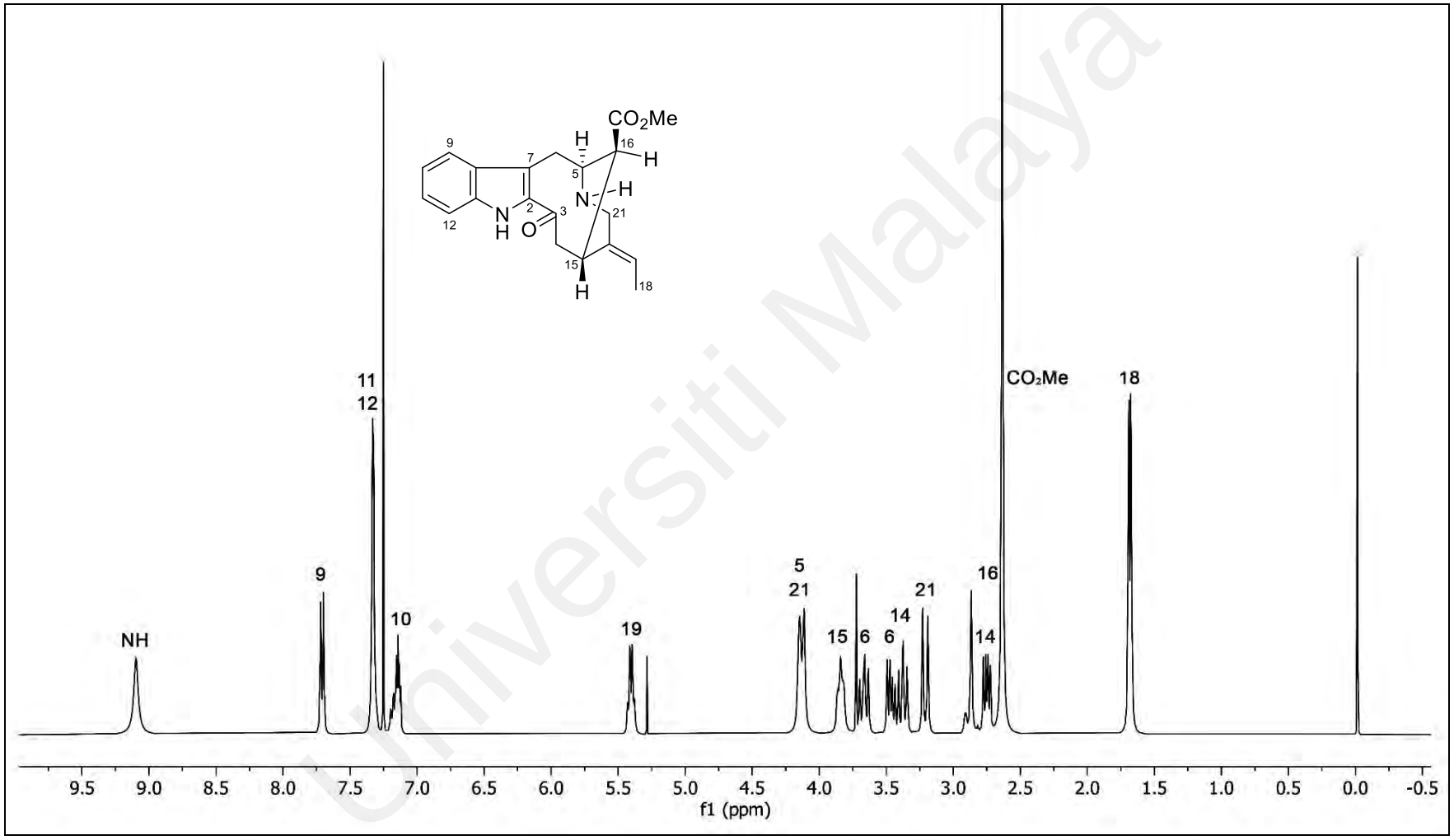


Figure 2.89: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Perivine (**40**)

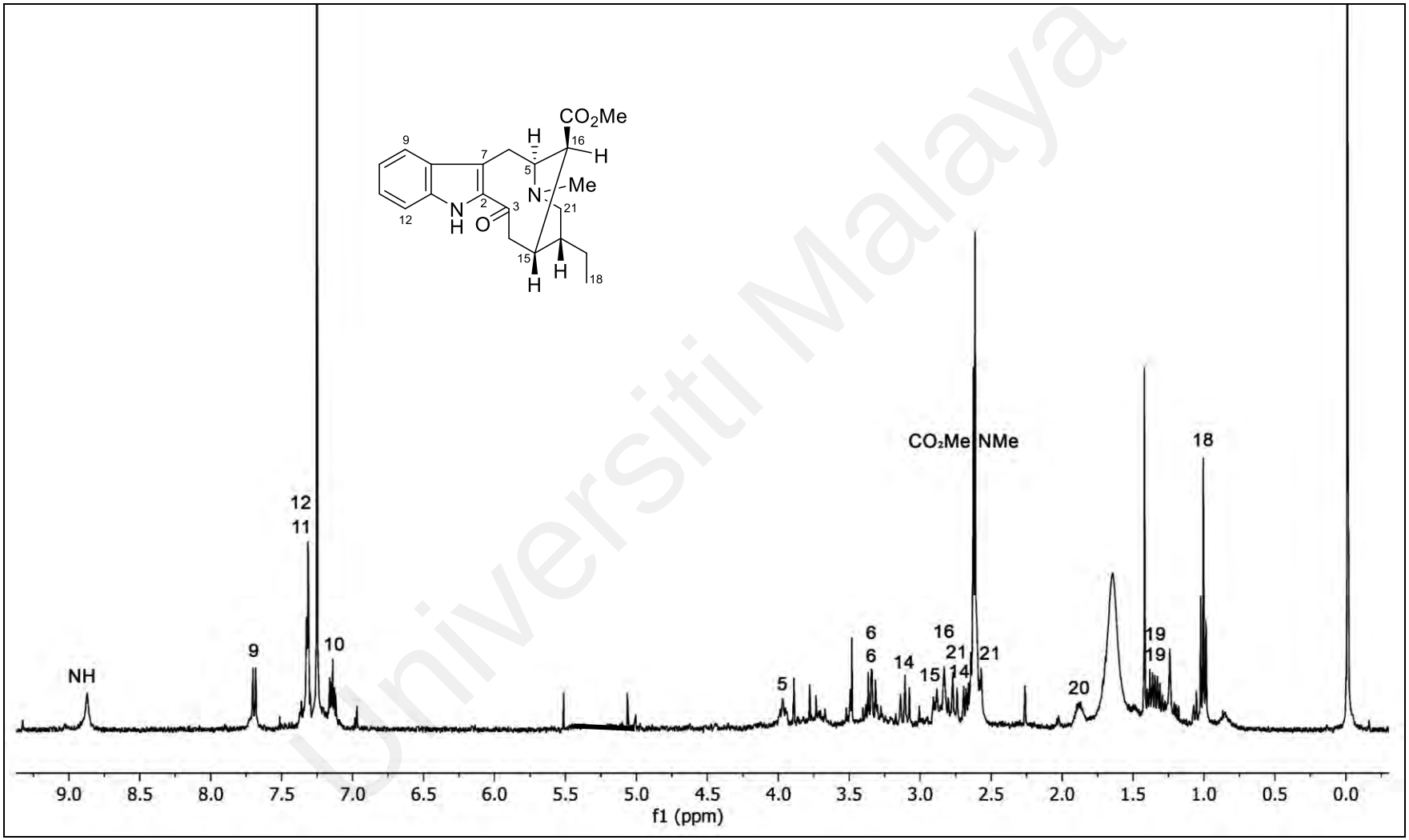


Figure 2.90: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Dregamine (**41**)

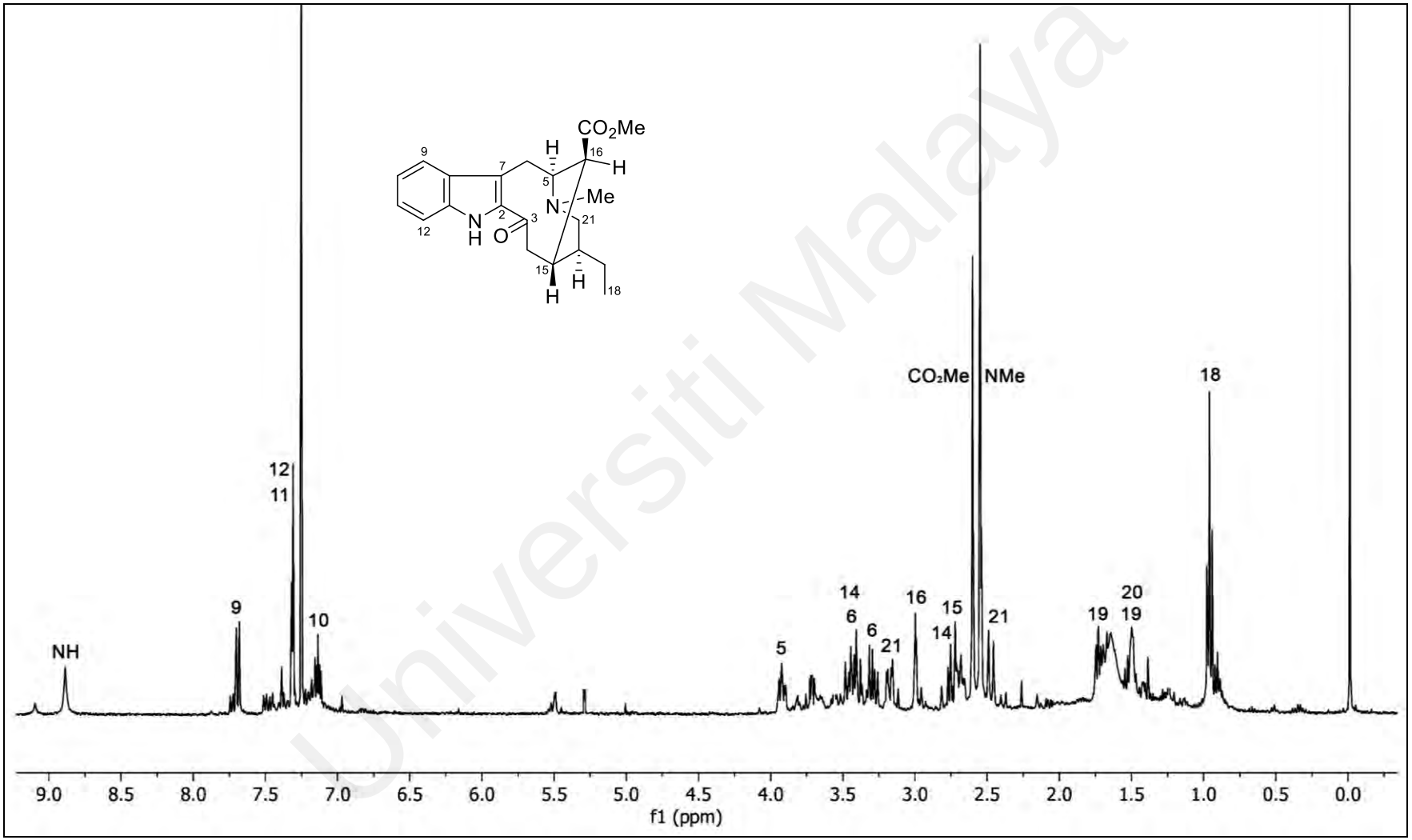


Figure 2.91: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Tabernaemontanine (**42**)

Table 2.30: ^{1}H NMR Spectroscopic Data (δ) of Vobasenal (**43**), Vobasidine D (**44**), Vobasidine E (**45**), and Vobasidine F (**46**)[a]

H	**43** (*J*/Hz)	**44** (*J*/Hz)	**45** (*J*/Hz)	**46** (*J*/Hz)
5	4.33 m	4.26 m	4.51 td (9, 4)	3.95 ddd (11, 8, 3)
6	2.96 t (12)	2.96 t (11)	3.10 dd (16, 9)	3.26 dd (15, 11)
6	3.92 m	3.91 m	4.05 dd (16, 9)	3.33 dd (15, 8)
9	7.73 d (8)	7.74 d (8)	7.70 d (8)	7.70 d (8)
10	7.17 t (8)	7.18 t (8)	7.19 td (8, 1)	7.15 ddd (8, 6, 2)
11	7.36 t (8)	7.36 t (8)	7.37 td (8, 1)	7.34 m
12	7.47 d (8)	7.39 d (8)	7.42 d (8)	7.34 m
14	2.63 br t (12)	2.59 m	2.84 t (13)	2.89 t (12)
14	3.59 m	3.57 dd (12, 7)	3.26 m	2.77 dd (12, 7)
15	3.87 m	3.93 m	3.37 m	2.72 m
16	2.59 br s	2.58 br s	3.01 dd (4, 2)	3.41 t (3)
18	-	2.24 s	-	1.06 t (8)
19	9.01 br s	-	-	1.53 m
19	-	-	-	1.53 m
20	-	-	4.24 d (6)	-
21	6.96 br s	7.32 br s	-	2.40 d (13)
21	-	-	-	3.03 d (13)
16-CO_2*Me*	2.83 s	2.85 s	2.58 s	2.67 br s
20-CO_2*Me*	-	-	3.24 s	
20-OH	-	-	-	*n.o.*
N(4)-Me	3.39 s	3.35 s	-	2.60 br s
N(1)-H	9.83 br s	9.41 br s	9.39 s	9.28 br s

[a]$CDCl_3$, 400 MHz; assignments based on COSY and HSQC.

Table 2.31: ^{13}C NMR Spectroscopic Data (δ) of Vobasenal (**43**), Vobasidine D (**44**), Vobasidine E (**45**), and Vobasidine F (**46**)[a]

C	43	44	45	46
2	135.3	135.5	135.3	133.9
3	189.5	189.8	190.7	190.2
5	56.5	55.3	56.8	56.7
6	27.9	28.0	30.3	18.4
7	117.4	117.4	117.8	120.6
8	127.7	127.8	127.9	128.5
9	120.4	120.5	121.0	121.0
10	120.6	120.6	120.6	120.5
11	126.8	126.8	127.1	126.9
12	112.5	112.1	112.3	111.8
13	136.7	136.4	136.5	136.4
14	46.2	46.6	39.5	42.2
15	24.8	26.0	33.7	36.5
16	44.3	44.6	43.4	43.5
18	-	24.2	-	6.4
19	185.8	192.1	-	29.1
20	116.3	114.1	71.6	72.9
21	152.9	145.9	-	53.7
16-*C*O$_2$Me	169.5	169.9	168.9	171.9
16-CO$_2$*Me*	50.8	50.7	51.5	50.5
20-*C*O$_2$Me	-	-	171.3	-
20-CO$_2$*Me*	-	-	34.2	-
N(4)-Me	42.0	42.0	-	42.7

[a]$CDCl_3$, 100 MHz; assignments based on HSQC and HMBC.

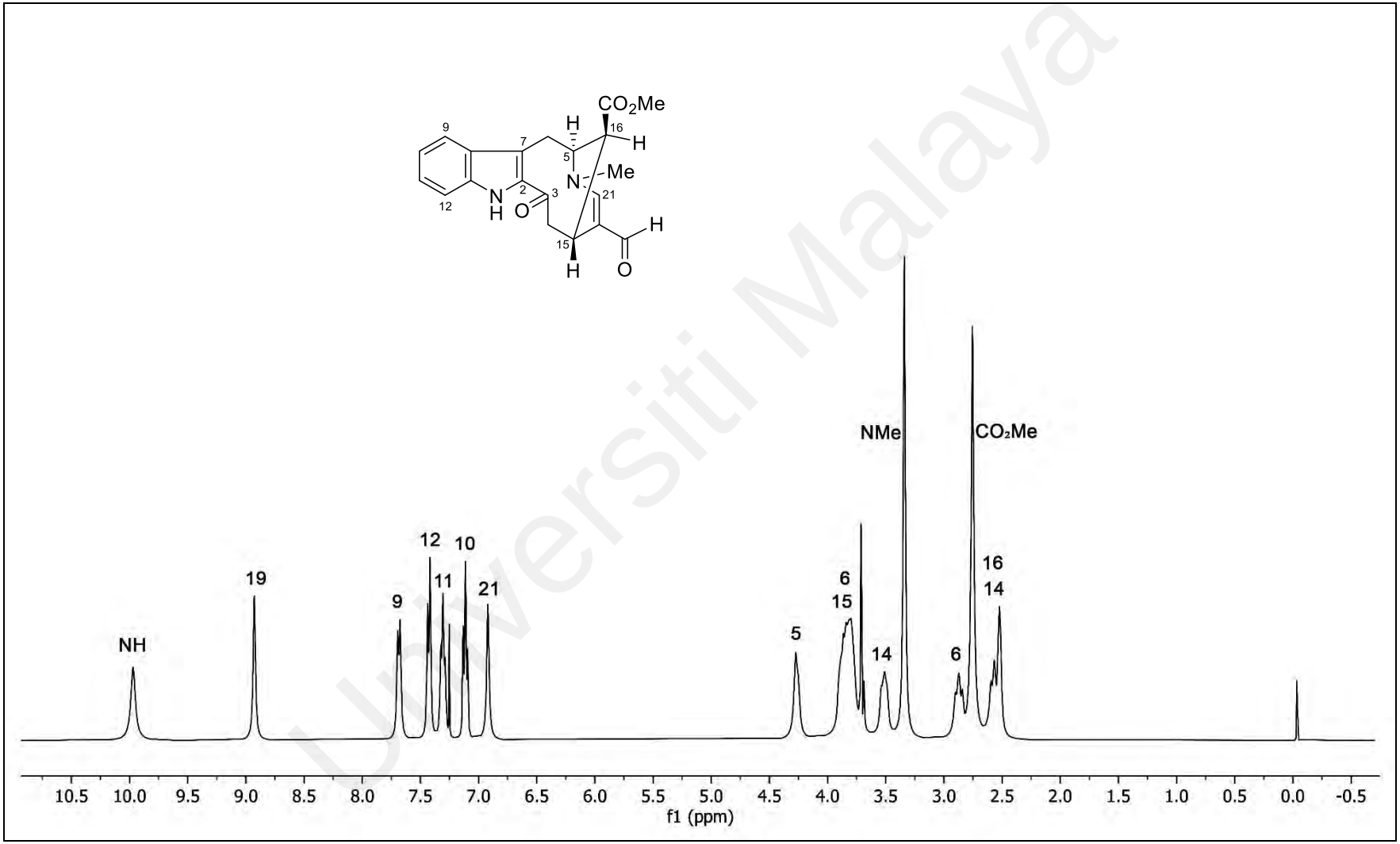


Figure 2.92: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Vobasenal (**43**)

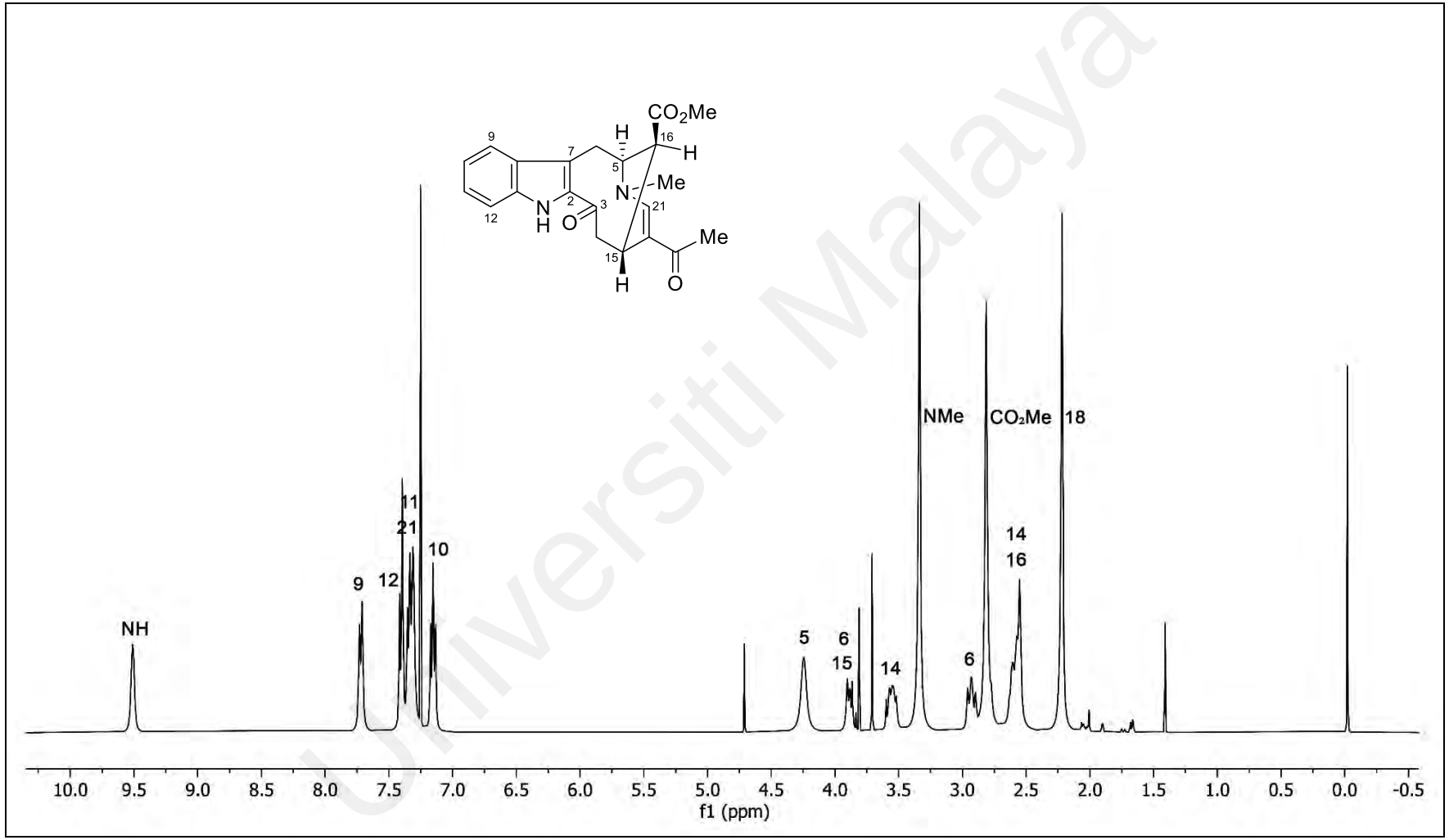


Figure 2.93: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Vobasidine D (**44**)

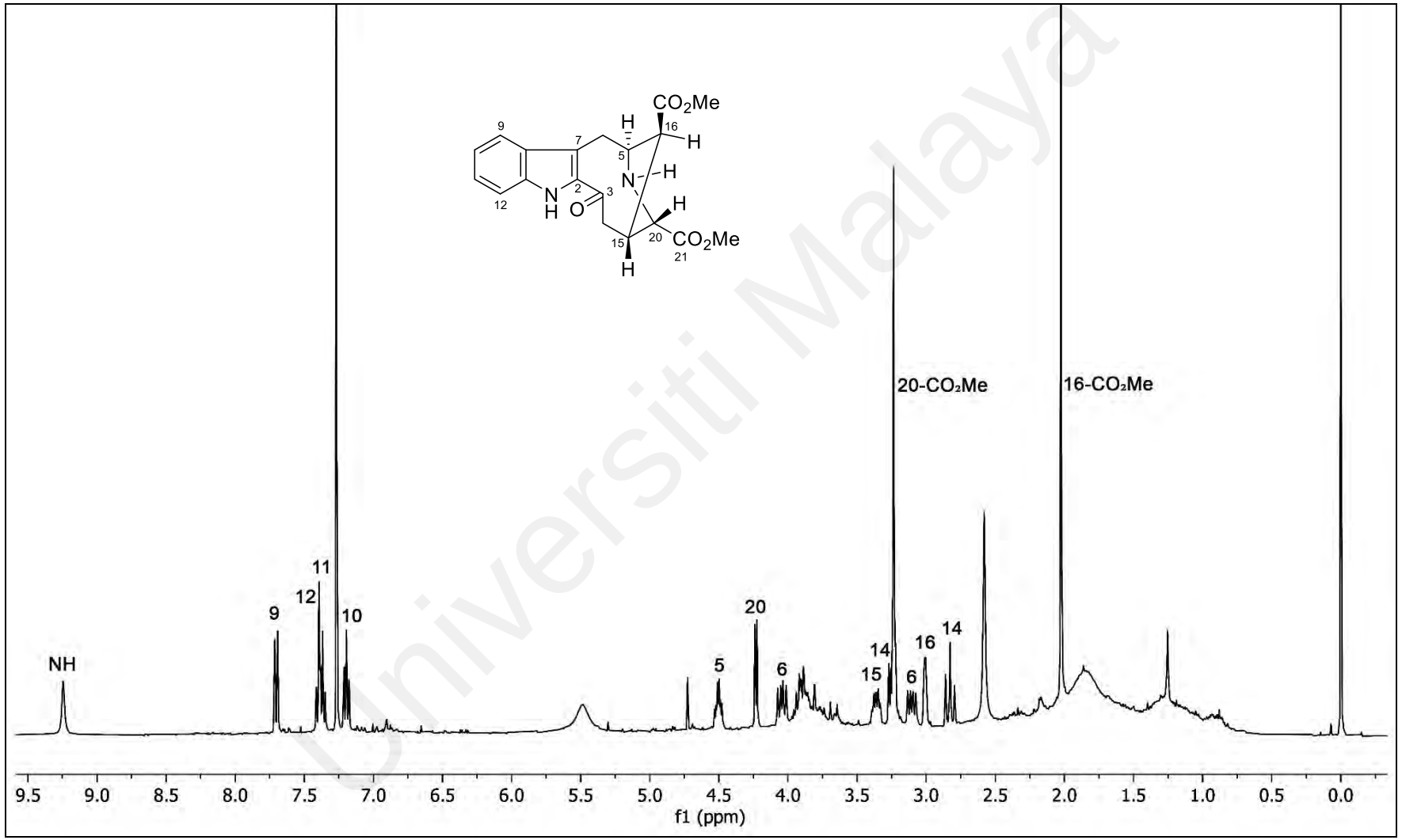


Figure 2.94: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Vobasidine E (**45**)

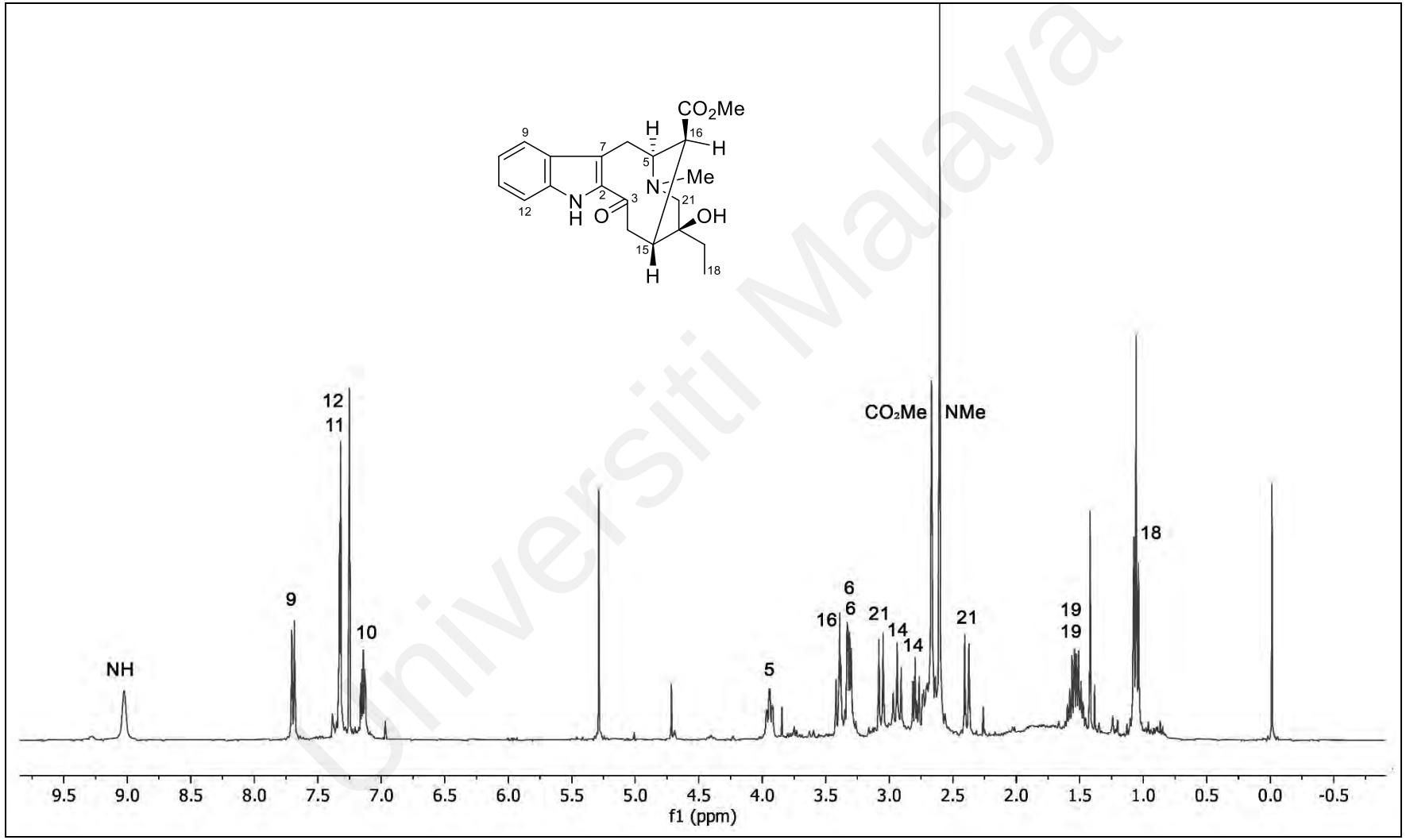


Figure 2.95: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Vobasidine F (**46**)

Table 2.32: ^{1}H NMR Spectroscopic Data (δ) of Pericyclivine (**47**), 16-*Epi*-voacarpine (**48**), and 19-20-Dehydroervatamine (**49**)

H	**47**[a] (*J*/Hz)	**48**[b] (*J*/Hz)	**49**[a] (*J*/Hz)
3	4.20 br d (10)	-	-
5	3.68 ddd (11, 5, 2)	4.42 d (6)	2.24 d (12)
5	-	-	3.44 br d (12)
6	2.91 ddd (16, 5, 1)	2.70 br d (15)	2.88 d (15.5)
6	3.23 dd (16, 2)	2.80 dd (15, 6)	3.62 d (15.5)
9	7.41 ddd (8, 1, 1)	6.98 d (7)	7.59 br d (8)
10	7.04 td (8, 1)	6.87 t (7)	7.14 ddd (8, 7, 1)
11	7.10 td (8, 1)	7.01 t (7)	7.34 ddd (8, 7, 1)
12	7.25 ddd (8, 1, 1)	7.05 d (7)	7.42 br d (8)
14	1.72 ddt (13, 10, 2)	1.76 br d (14)	2.45 d (16)
14	2.56 ddd (13, 4, 2)	2.06 dd (14, 4)	3.09 dd (16, 11)
15	2.97 m	3.15 m	3.53 d (11)
16	2.82 ddd (11, 3, 2)	-	-
17	-	3.42 m	-
17	-	3.42 m	-
18	1.62 dt (7, 2)	1.57 d (7)	1.59 dd (7, 2)
19	5.26 qt (7, 2)	5.26 q (7)	5.43 qd (7, 2)
19	-	-	-
21	3.61 dt (17, 2)	3.28 d (17)	2.58 dt (12, 2)
21	3.61 dt (17, 2)	4.17 d (17)	3.10 dd (12, 2)
CO_2*Me*	3.06 s	3.69 s	3.59 s
N(4)-*Me*	-	-	2.30 s
N(1)-H	7.85 br s	8.12 br s	9.16 br s

[a]$CDCl_3$, 400 MHz; [b]$CDCl_3$, 600 MHz; assignments based on COSY and HSQC.

Table 2.33: ^{13}C NMR Spectroscopic Data (δ) of Pericyclivine (**47**), 16-*Epi*-voacarpine (**48**), and 19-20-Dehydroervatamine (**49**)

C	**47**[a]	**48**[b]	**49**[a]
2	137.4	137.0	132.6
3	50.2	80.5	193.7
5	53.0	57.4	61.2
6	24.1	21.3	31.1
7	105.4	107.0	119.7
8	127.0	125.7	127.2
9	117.7	118.5	120.2
10	119.1	119.5	120.5
11	121.2	122.1	126.5
12	110.9	110.9	112.5
13	136.6	136.3	137.0
14	26.8	36.4	44.0
15	27.2	33.6	34.1
16	43.8	53.1	49.1
17	-	63.3	-
18	12.8	12.7	12.5
19	114.4	115.9	121.3
20	139.3	135.0	136.2
21	55.9	48.0	61.7
CO_2Me	172.9	175.7	175.2
CO_2*Me*	50.8	52.2	52.3
N(4)-*Me*	-	-	45.9

[a]$CDCl_3$, 100 MHz; [b]$CDCl_3$, 150 MHz; assignments based on HSQC and HMBC.

Table 2.34: ^{1}H NMR Spectroscopic Data (δ) of 16(*R*)-Sitsirikine (**50**), 16(*R*)-19,20-*E*-isositsirikine (**51**), 16(*R*)-19,20-*Z*-isositsirikine (**52**), and Fluorocarpamine (**53**)

H	**50**[a] (*J*/Hz)	**51**[a] (*J*/Hz)	**52**[b] (*J*/Hz)	**53**[a] (*J*/Hz)
3	3.26 br d (12)	4.33 br s	3.62 d (9)	3.51 br s
5	2.58 td (11, 5)	3.15 m	2.74 m	2.99 m
5	3.06 br dd (11, 6)	3.27 ddd (13, 6, 2)	3.18 m	2.99 m
6	2.73 dd (15, 5)	2.67 dd (16, 6)	2.74 m	2.21 dd (12, 6)
6	3.00 m	2.99 m	2.97 m	2.99 m
9	7.46 d (8)	7.47 br d (8)	7.38 d (8)	7.62 br d (8)
10	7.08 td (8, 1)	7.10 td (8, 1)	6.97 td (8, 1)	6.90 br t (8)
11	7.14 td (8, 1)	7.16 td (8, 1)	7.04 td (8, 1)	7.51 br t (8)
12	7.31 dd (8, 1)	7.39 br d (8)	7.29 d (8)	6.70 br d (8)
14	1.42 q (13)	2.24 m	1.55 q (12)	1.37 dt (13, 3)
14	2.20 ddd (13, 3, 3)	2.24 m	2.31 dt (12, 3)	1.91 dt (13, 3)
15	1.77 br t (12)	3.15 m	2.47 t (8)	3.64 br d (9)
16	2.61 m	2.52 ddd (11, 8, 5)	3.04 q (8)	4.56 d (9)
17	2.28 br t (11)	3.54 m	3.84 dd (7, 2)	-
17	3.00 dd (11, 4)	3.54 m	3.84 dd (7, 2)	-
18	5.19 dd (10, 2)	1.66 dd (7, 2)	1.75 d (7)	1.63 d (6)
19	5.25 ddd (17, 2, 1)	-	-	5.50 br q (6)
20	5.59 ddd (17, 10, 9)	5.65 br q (7)	5.58 q (7)	-
21	2.94 m	-	-	3.31 d (14)
21	3.76 dd (11, 5)	2.98 d (13)	2.84 d (12)	3.38 br d (14)
CO_2Me	3.98 dd (11, 8)	3.54 m	3.91 d (12)	3.72 s
N(1)-H	3.68 s	3.81 s	3.75 s	-

[a]$CDCl_3$, 400 MHz; [b]methanol-d_4, 600 MHz; assignments based on COSY and HSQC.

Table 2.35: ^{13}C NMR Spectroscopic Data (δ) of 16(*R*)-Sitsirikine (**50**), 16(*R*)-19,20-*E*-isositsirikine (**51**), 16(*R*)-19,20-*Z*-isositsirikine (**52**), and Fluorocarpamine (**53**)

C	**50**[a]	**51**[a]	**52**[b]	**53**[a]
2	134.3	133.8	135.2	76.0
3	59.7	52.8	61.5	61.8
5	52.8	51.3	53.5	55.0
6	21.6	17.7	22.2	39.0
7	108.1	107.7	107.9	205.2
8	127.3	127.6	128.4	120.4
9	118.2	118.0	118.8	124.1
10	119.5	119.5	119.9	119.5
11	121.5	121.6	122.2	137.2
12	111.1	111.3	112.1	111.1
13	136.2	136.2	138.2	163.6
14	31.9	30.2	35.0	24.9
15	40.5	32.6	42.4	30.5
16	48.2	49.6	51.0	63.0
17	61.0	62.1	63.6	-
18	118.4	13.3	13.3	12.3
19	138.4	123.7	119.4	121.0
20	44.8	133.7	136.0	133.9
21	62.1	52.5	56.3	53.4
*C*O$_2$Me	174.5	175.4	176.2	172.5
CO$_2$*Me*	51.9	52.2	52.3	51.8

[a]$CDCl_3$, 100 MHz; [b]methanol-d_4, 150 MHz; assignments based on HSQC and HMBC.

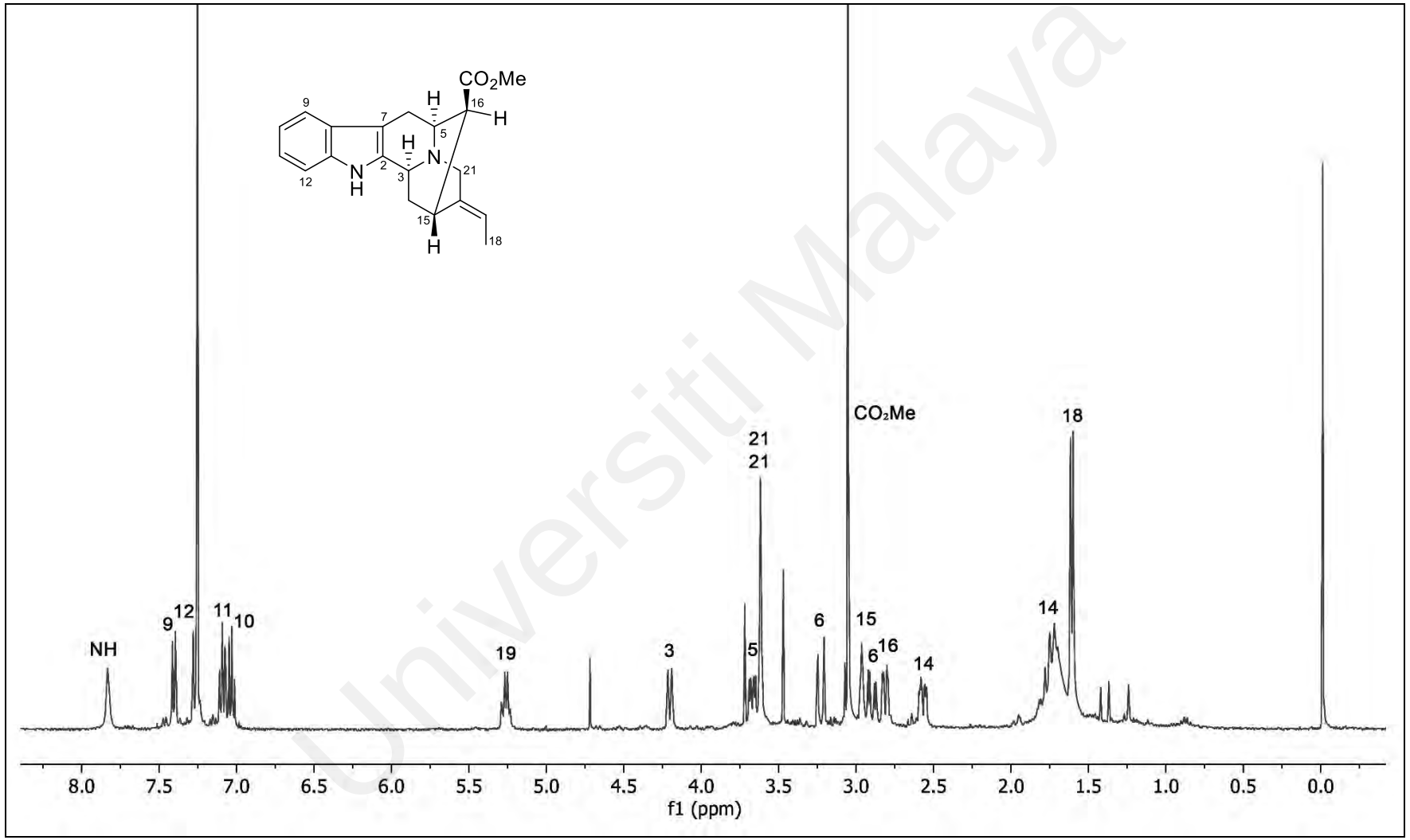


Figure 2.96: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Pericyclivine (**47**)

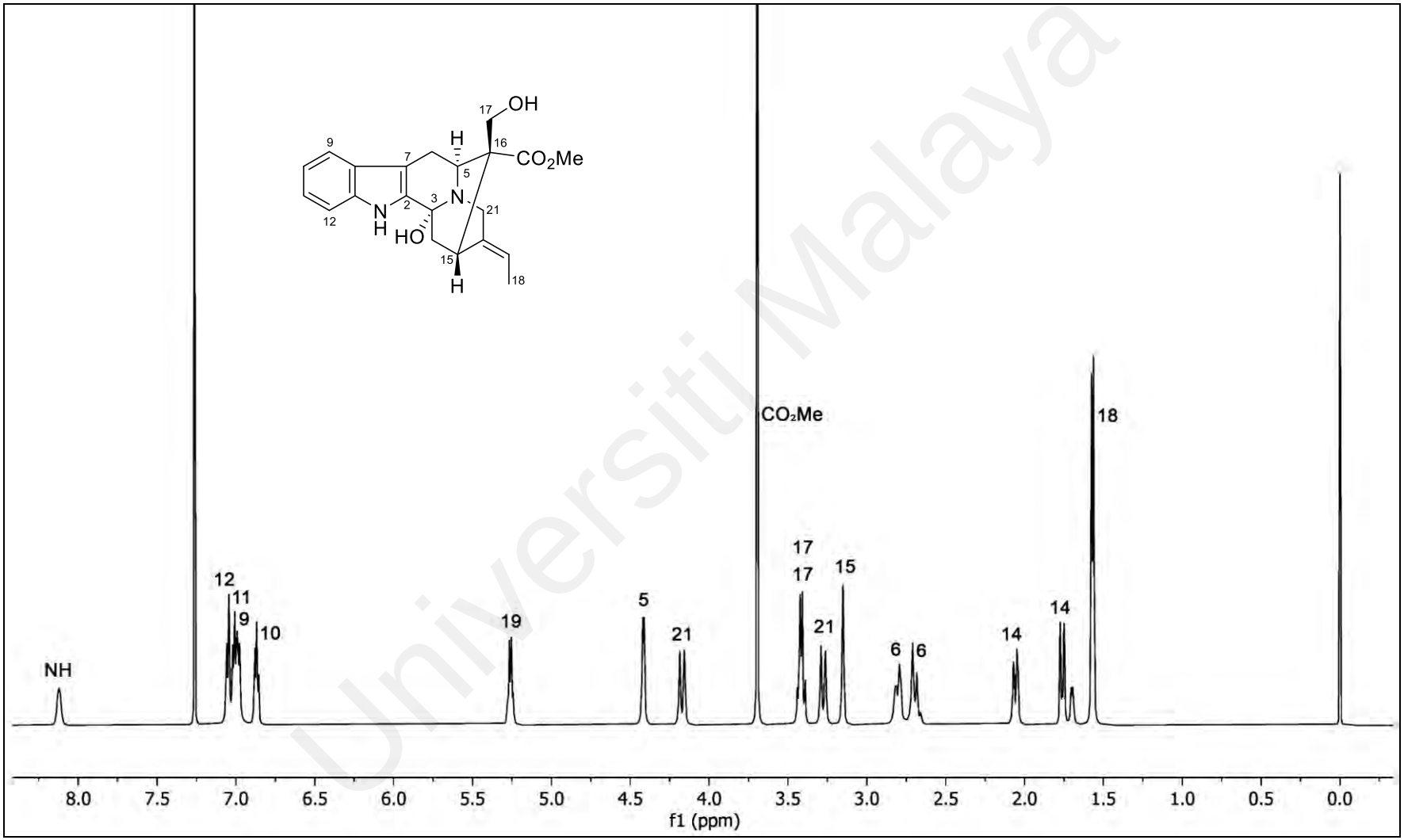


Figure 2.97: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of 16-*Epi*-voacarpine (**48**)

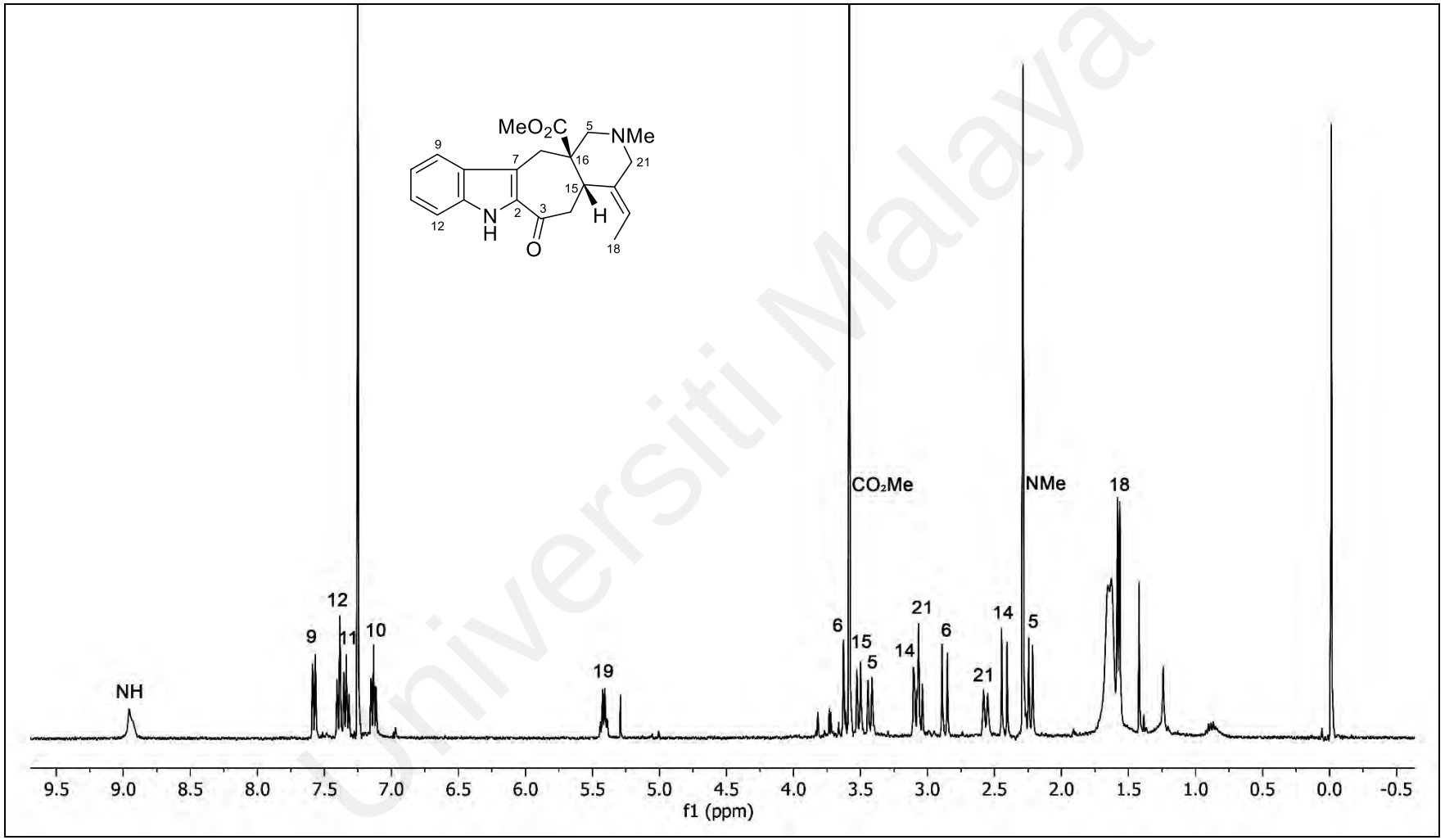


Figure 2.98: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 19,20-Dehydroervatamine (**49**)

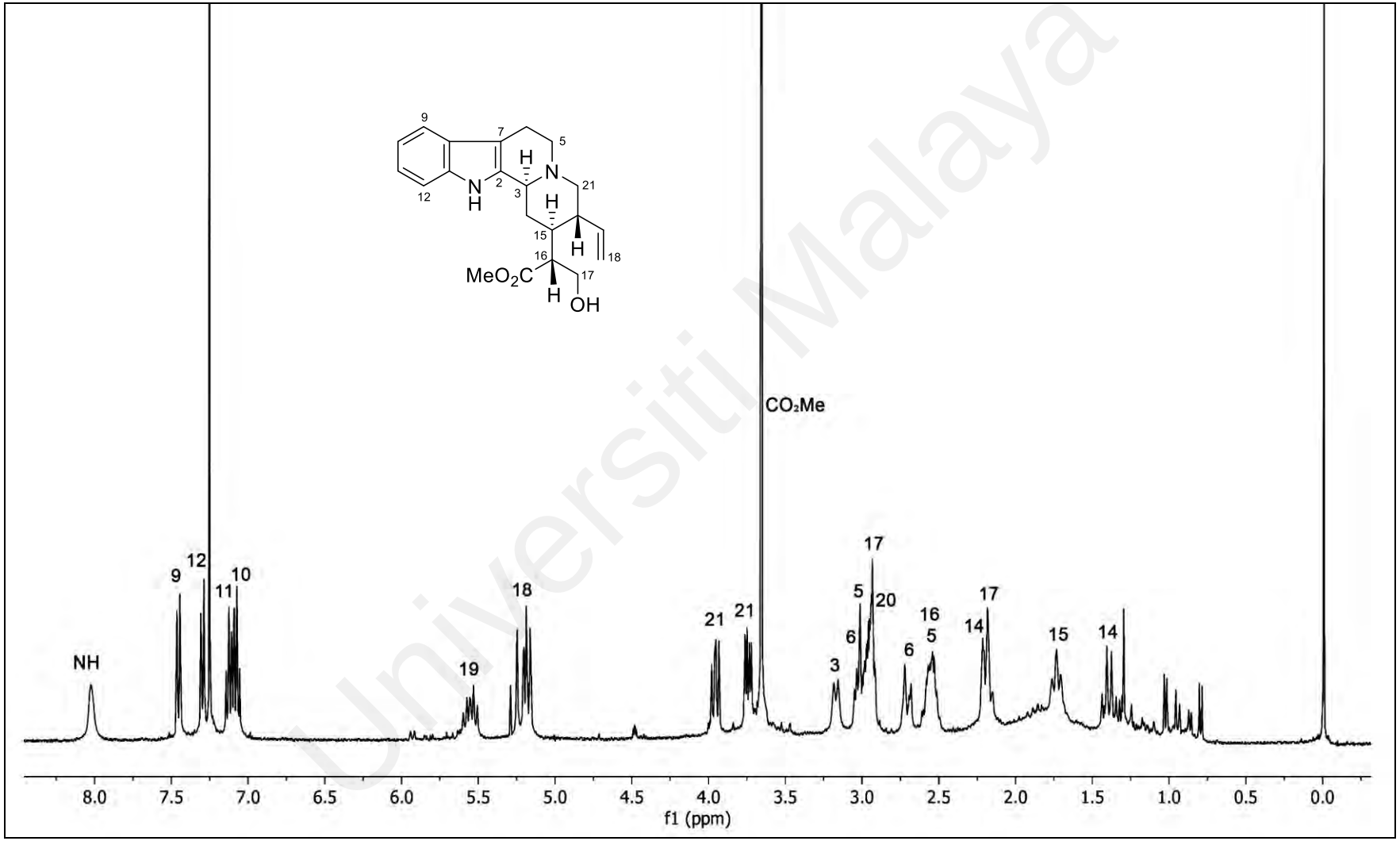


Figure 2.99: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 16(*R*)-Sitsirikine (**50**)

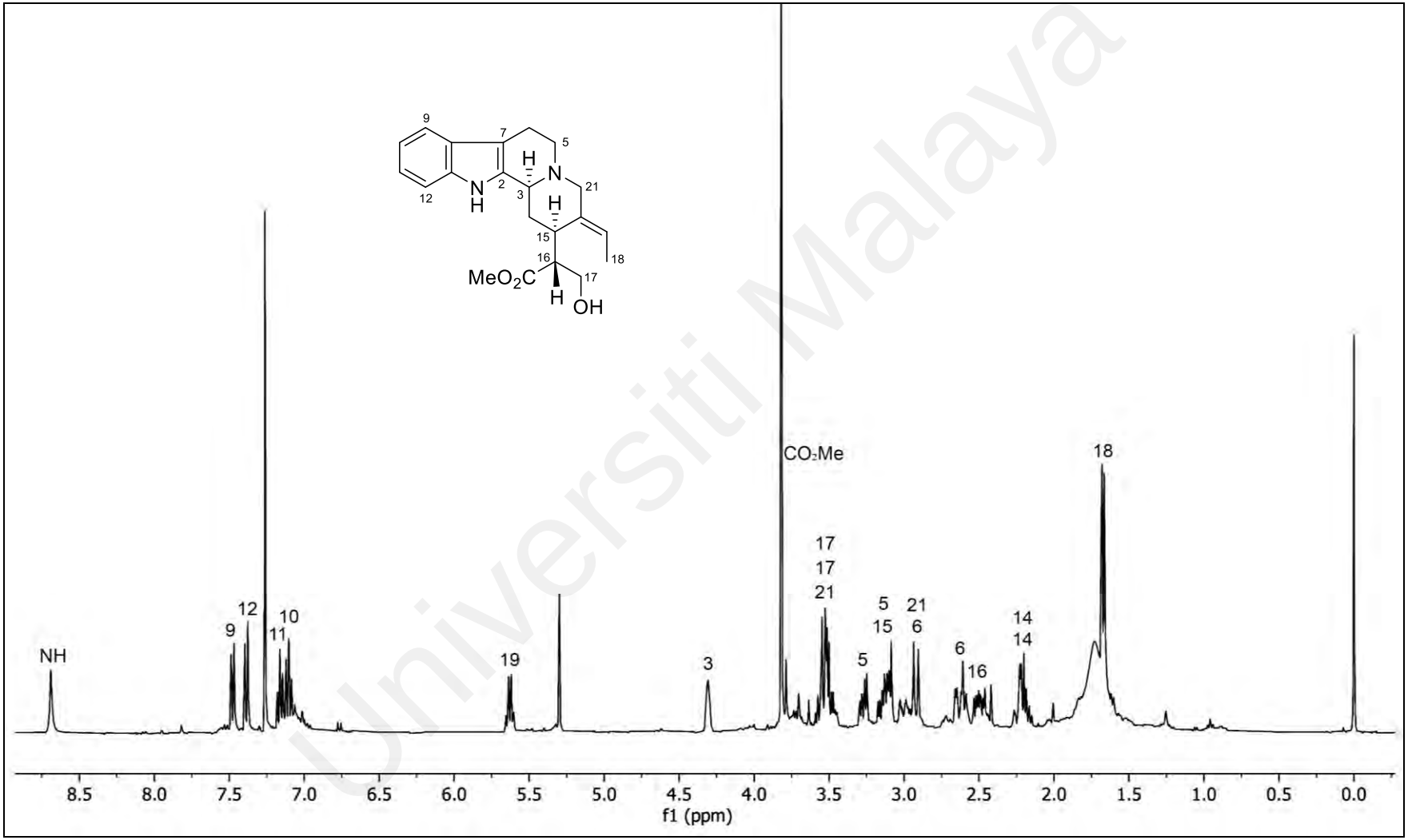


Figure 2.100: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 16(*R*)-19,20-*E*-isositsirikine (**51**)

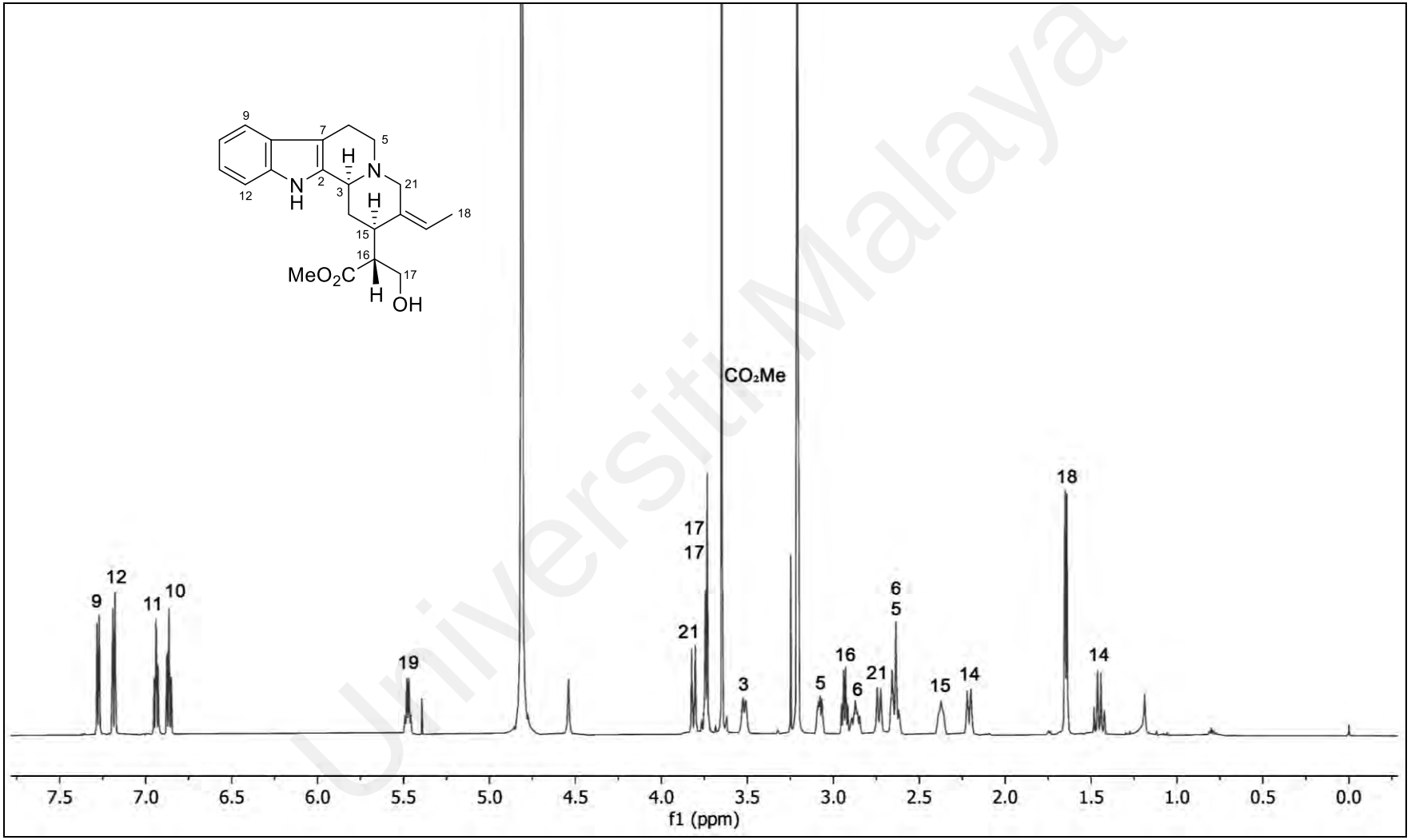


Figure 2.101: ^{1}H NMR Spectrum (CD_3OD, 600 MHz) of 16(*R*)-19,20-*Z*-isositsirikine (**52**)

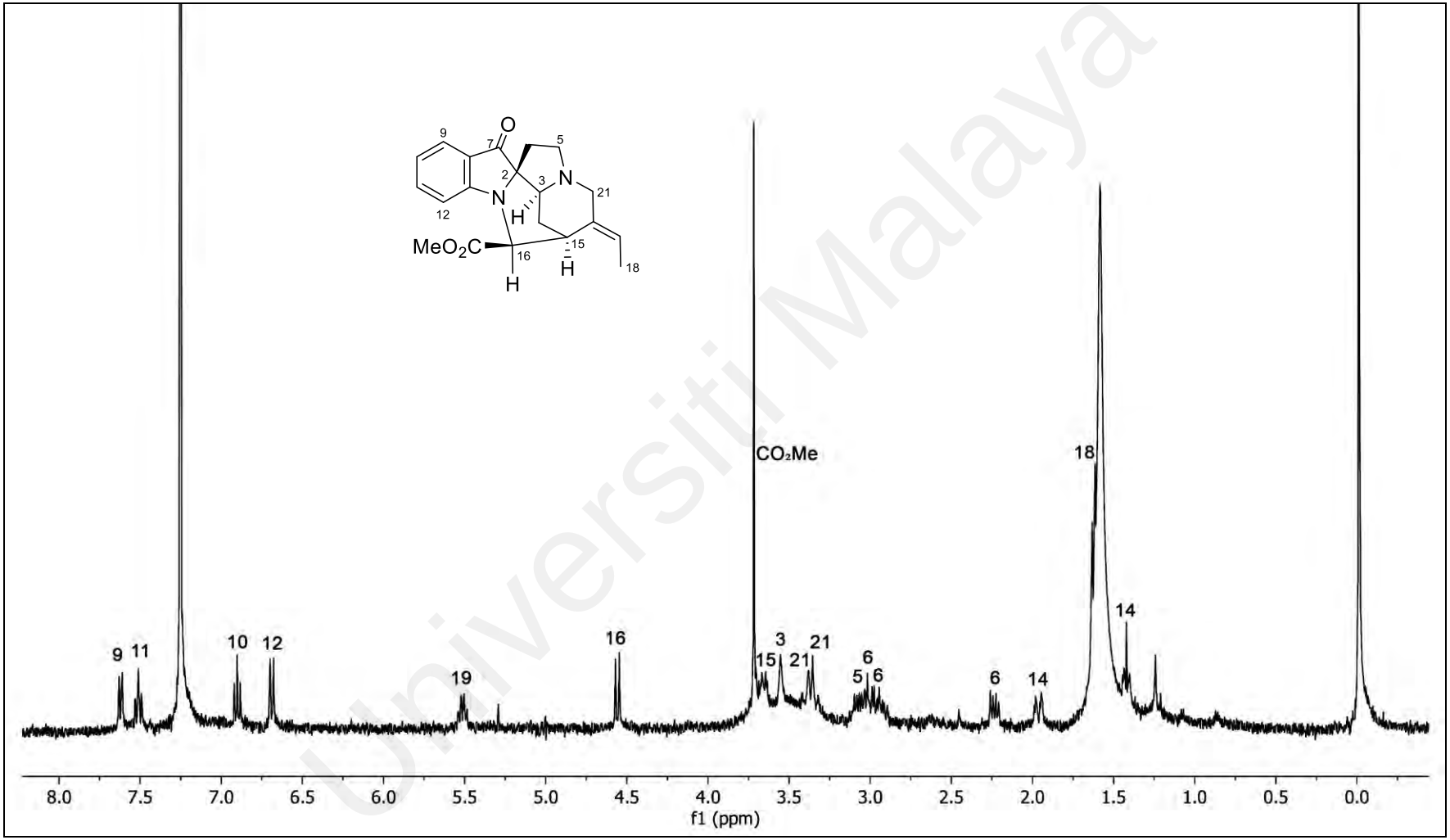


Figure 2.102: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Fluorocarpamine (**53**)

2.1.4 Cleavamine and Quebrachamine Alkaloids

2.1.4.1 Polyneurine L (54)

Polyneurine L (**54**) was obtained as a light yellowish oil, $[\alpha]^{25}_{D}$ −19 (*c* 0.3, $CHCl_3$). The UV spectrum showed absorption maxima at 219, 224, 283, and 292 nm, indicating the presence of an indole chromophore, while the IR spectrum showed absorption bands due to NH/OH (3369 cm^{-1}) and ester (1732 cm^{-1}) functions. The HRMS data showed an $[M + H]^+$ peak at *m/z* 373.2134, corresponding to the molecular formula $C_{21}H_{28}N_2O_4$ + H.

The ^1H NMR spectrum (Figure 2.107) showed the presence of an indolic NH (δ_H 8.25), four aromatic hydrogens (δ_H 7.11–7.52), a methyl ester group (δ_H 3.76), and an ethyl side chain (δ_H 0.81, 1.45). The ^{13}C NMR data (Table 2.36) showed a total of 21 carbon resonances, comprising one methyl, seven methylenes, five methines, two tertiary carbons bonded to indolic NH, four quaternary carbons, one methyl ester, and one ester carbonyl.

The COSY data showed three partial structures, *viz.*, NCH_2CH_2, $CH_2CH(CH_2)CH_2$, and CH_2CH_3 fragments, corresponding to C-5–C-6, C-3–C-14(C-17)–C-15, and C-19–C-18, respectively, while the HMBC data established the connectivity of these partial structures, which revealed a cleavamine-type alkaloid (Figure 2.103) (Bruneton *et al.*, 1976; Van Beek, Verpoorte *et al.*, 1984a; Wenkert, Hagaman *et al.*, 1976). The downfield quaternary carbon at δ_C 67.5 was assigned to C-16, a carbon bearing a hydroxy and methyl ester group, based on the HMBCs from H-17 to C-16 and the ester carbonyl, while the other downfield quaternary carbon at δ_C 74.7 was attributed to an OH substituent at C-20, based on the HMBC from H-18 to C-20. In addition, the

presence of C-20-OH was also confirmed by an acetylation reaction (Ac_2O, Pyr, cat. DMAP) to give an *O*-acetyl derivative **54a** (Figure 2.108).

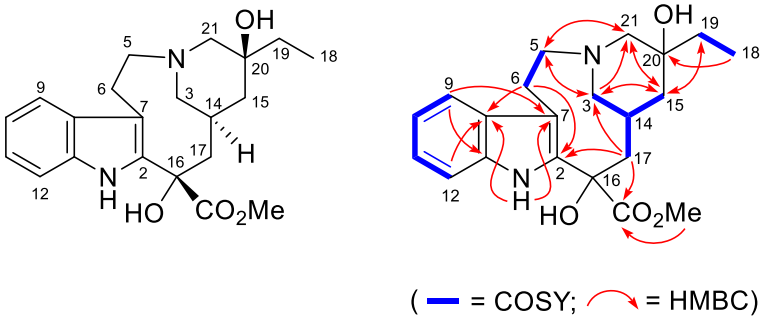


Figure 2.103: COSY and selected HMBCs of **54**

The NOE data revealed that both H-14 and the C-20 ethyl side chain were α oriented (C-14*S*, C-20*S*), based on the H-14/H-18, H-19 enhancements (Figure 2.104). The NOE data were however insufficient to determine the configuration at C-16, and thus a GIAO NMR calculations and DP4+ analysis was carried out to determine the configuration at this centre. The experimental NMR data of **54** were compared with the calculated ^{1}H and ^{13}C NMR shifts of **54** and its C-16 epimer using DP4+ analysis. The DP4+ results supported **54** with a 16β-CO_2Me (16*S*) as the most likely configuration with 93% DP4+ probability (all data). The GIAO NMR calculations and DP4+ analysis was also carried out on the *O*-acetyl derivative **54a**. The DP4+ results supported **54a** with a 16β-CO_2Me (16*S*) as the correct relative configuration, with 100% DP4+ probability (all data). The absolute configuration of **54** was eventually established as (14*S*, 16*S*, 20*S*) based on comparison of the experimental and calculated ECD spectra (Figures 2.105 and 2.106).

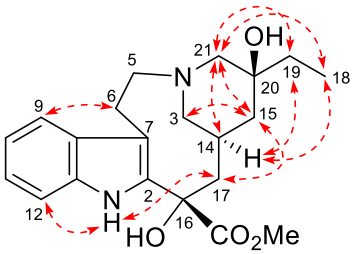


Figure 2.104: Selected NOEs of **54**

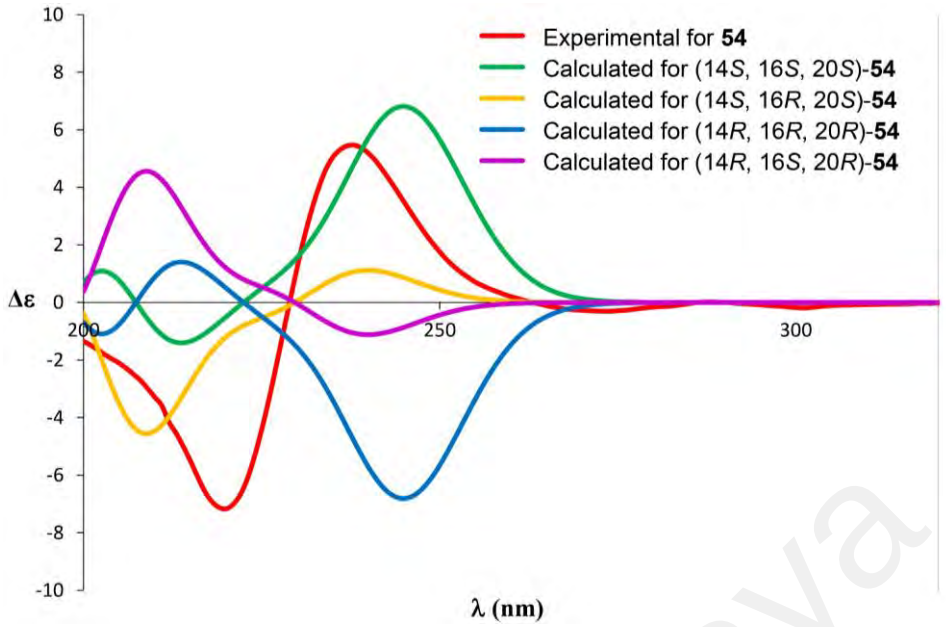


Figure 2.105: Experimental ECD spectrum of **54** and calculated ECD spectra of (14*S*, 16*S*, 20*S*)-**54**, (14*S*, 16*R*, 20*S*)-**54**, (14*R*, 16*R*, 20*R*)-**54**, and (14*R*, 16*S*, 20*R*)-**54**

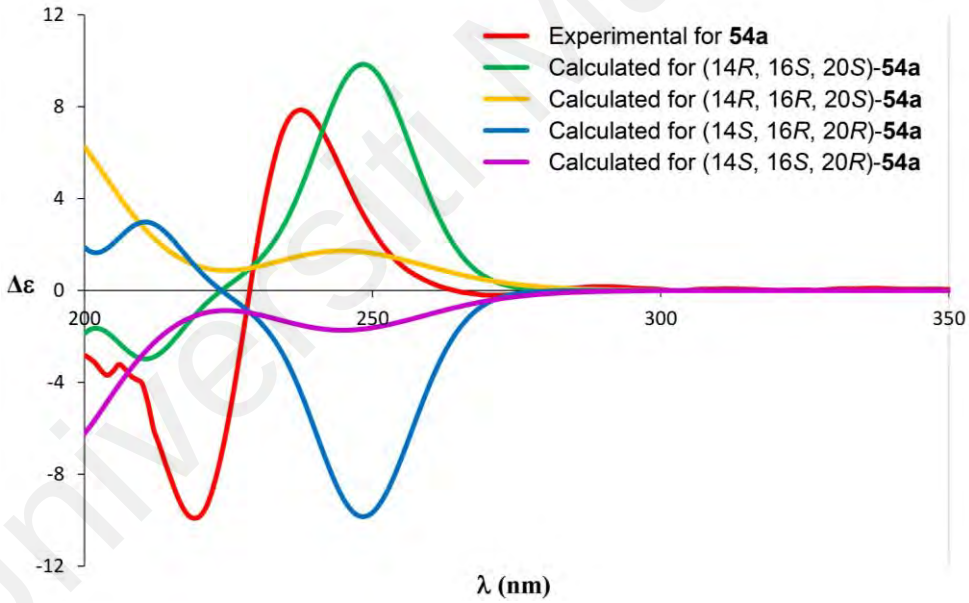


Figure 2.106: Experimental ECD spectrum of **54a** and calculated ECD spectra of (14*R*, 16*S*, 20*S*)-**54a**, (14*R*, 16*R*, 20*S*)-**54a**, (14*S*, 16*R*, 20*R*)-**54a**, and (14*S*, 16*S*, 20*R*)-**54a**

Table 2.36: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of Polyneurine L (**54**) and 20-*O*-Acetyl-polyneurine L (**54a**)[a]

H/C	**54**		**54a**	
	δ_H (*J*/Hz)	δ_C	δ_H (*J*/Hz)	δ_C
2	-	131.7	-	131.6
3	3.01 m	56.2	3.02 m	56.6
3	3.17 t (9.5)		3.18 t (9.2)	
5	3.29 m	43.9	3.32 m	44.2
5	3.29 m		3.32 m	
6α	2.53 ddd (16.3, 3.7, 1.7)	15.7	2.55 m	15.9
6β	2.99 m		2.99 m	
7	-	110.9	-	111.1
8	-	126.9	-	127.1
9	7.52 d (7.5)	118.4	7.50 d (8.0)	118.6
10	7.11 td (7.5, 1.0)	119.5	7.11 t (8.0)	119.7
11	7.20 td (7.5, 1.0)	122.3	7.19 t (8.0)	122.6
12	7.36 d (7.5)	111.1	7.35 d (8.0)	111.3
13	-	136.2	-	136.5
14	2.11 m	31.6	2.14 m	31.7
15	1.62 d (6.5)	40.0	1.65 dd (6.3, 1.6)	40.9
15	1.62 d (6.5)		1.65 dd (6.3, 1.6)	
16	-	67.5	-	67.8
17β	2.20 dd (12.0, 9.4)	44.6	2.20 dd (12.4, 9.6)	44.7
17α	2.58 dd (12.0, 7.1)		2.58 dd (12.4, 6.9)	
18	0.81 t (7.6)	8.1	0.83 t (7.6)	8.0
19	1.45 dq (14.0, 7.6)	29.1	1.29 m	30.0
19	1.45 dq (14.0, 7.6)		1.46 q (7.6)	
20	-	74.7	-	73.7
21α	3.37 d (10.9)	67.6	3.87 d (11.3)	69.4
21β	3.41 d (10.9)		3.94 d (11.3)	
CO_2Me	-	174.0	-	173.8
CO_2*Me*	3.76 s	52.8	3.76 s	52.9
20-OAc	-	-	-	171.2
20-OAc	-	-	2.04 s	21.0
N(1)-H	8.25 br s	-	8.18 br s	-

[a]$CDCl_3$, 600 (^{1}H) and 150 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and NOESY.

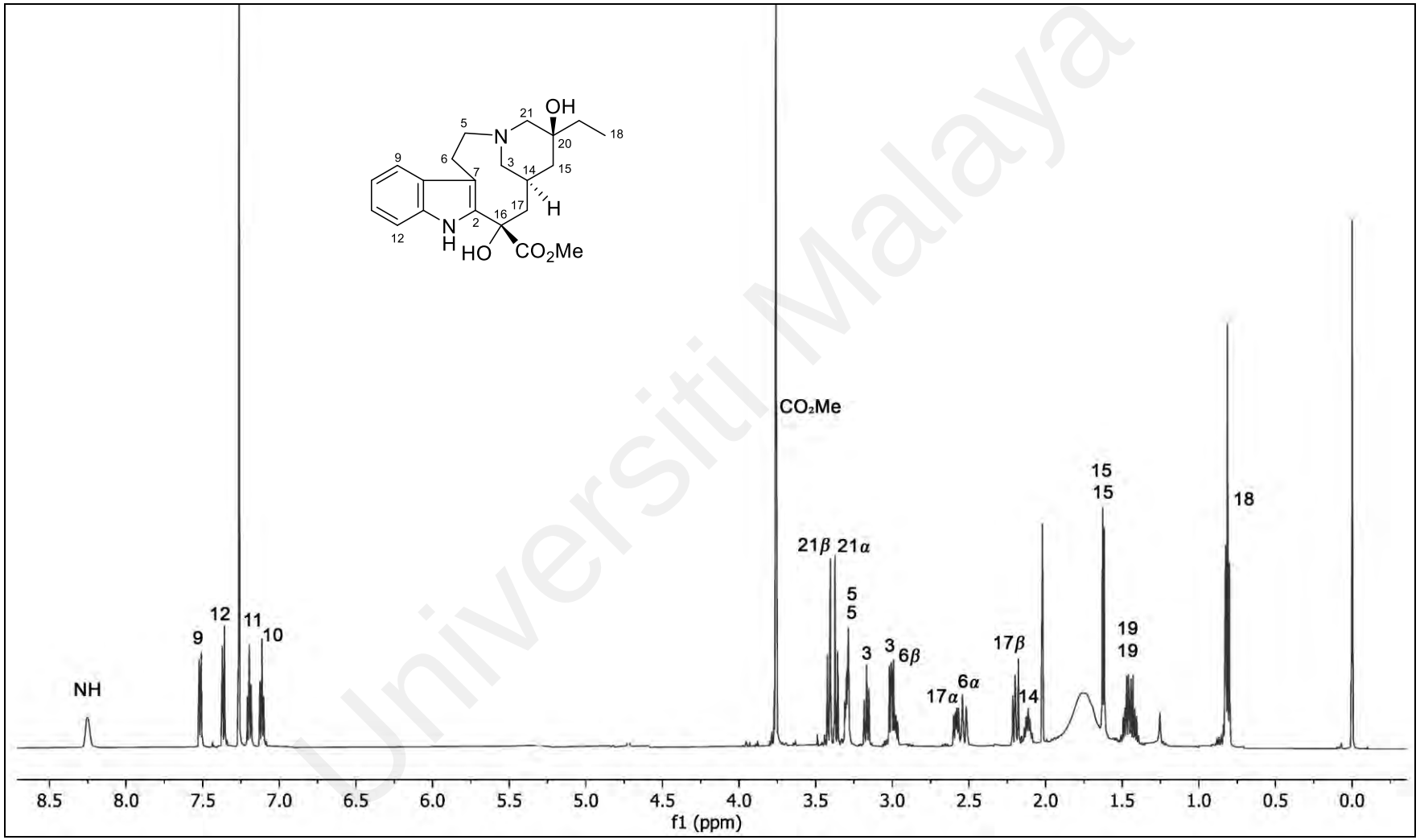


Figure 2.107: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Polyneurine L (**54**)

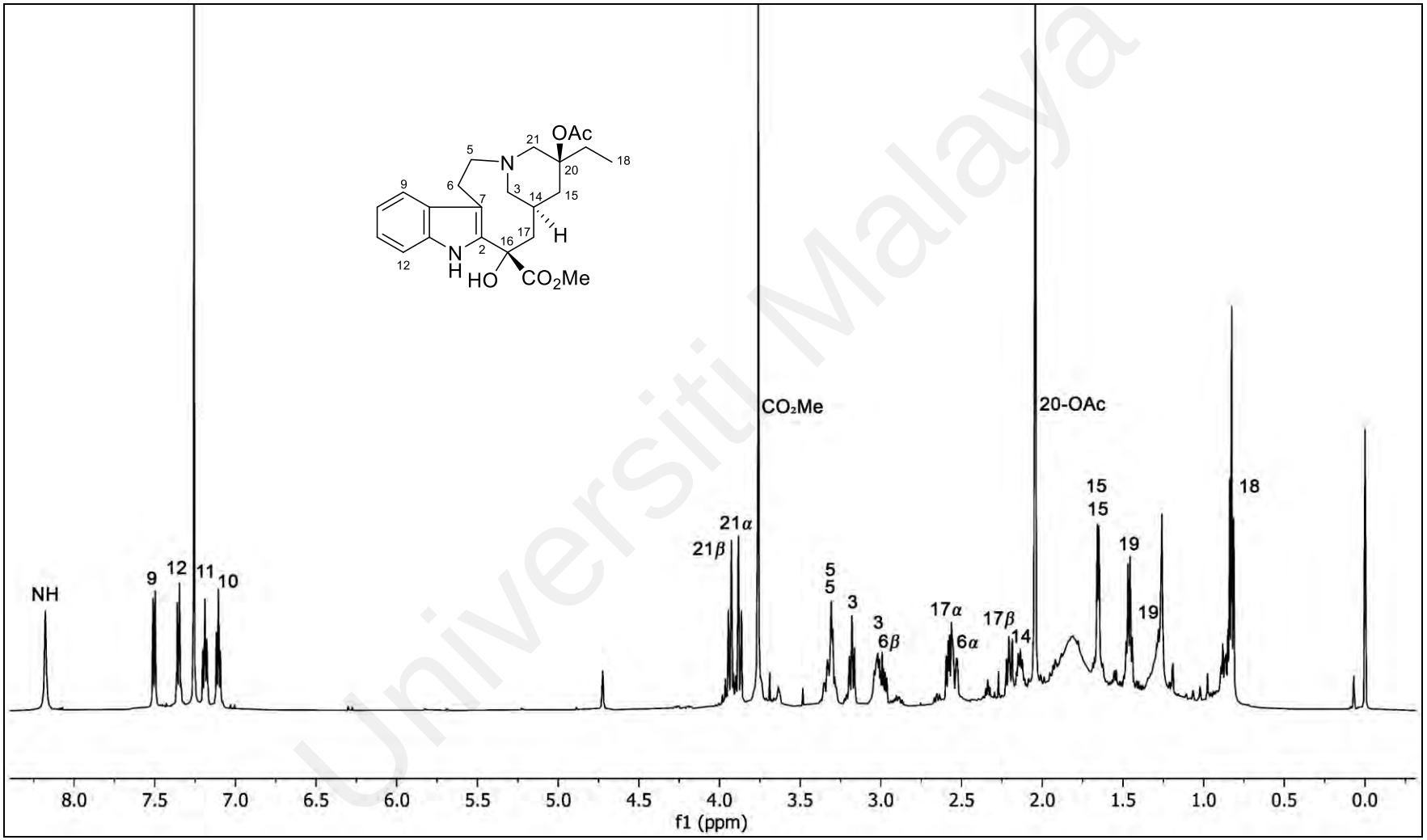


Figure 2.108: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of 20-*O*-Acetyl-polyneurine L (**54a**)

2.1.4.2 Voaphylline (55), Voaphylline-7-hydroxyindolenine (56), and Voaphyllinediol (57)

Three known quebrachamine-type alkaloids including voaphylline (**55**) (Perera *et al.*, 1983; Robinson *et al.*, 1967), voaphylline-7-hydroxyindolenine (**56**) (Azoug *et al.*, 1995; Perera *et al.*, 1983), and voaphyllinediol (**57**) (Van Beek, Verpoorte, Baerheim Svendsen *et al.*, 1985) were also isolated in the present study. The absolute configuration of voaphylline-7-hydroxyindolenine (**56**) was confirmed by the TDDFT-ECD (Figure 2.109). The ^{1}H NMR spectra of these compounds are shown in Figures 2.110–2.112, while the ^{1}H and ^{13}C NMR spectroscopic data are summarized in Tables 2.37 and 2.38. Other data are given in the Experimental Section.

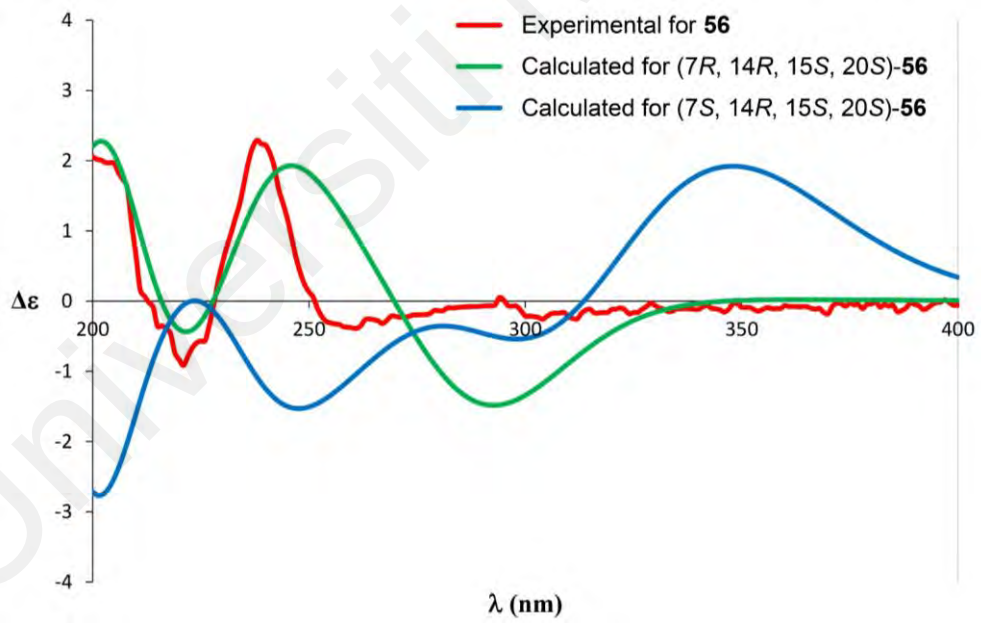


Figure 2.109: Experimental ECD spectrum of **56** and calculated ECD spectra of (7*R*, 14*R*, 15*S*, 20*S*)-**56** and (7*S*, 14*R*, 15*S*, 20*S*)-**56**

Table 2.37: ^{1}H Spectroscopic Data (δ) of Voaphylline (**55**), Voaphylline-7-hydroxyindolenine (**56**), and Voaphyllinediol (**57**)

H	**55**^{a} (*J*/Hz)	**56**^{b} (*J*/Hz)	**57**^{a} (*J*/Hz)
3	2.67 br d (13)	2.55 d (13)	2.42 d (13)
3	3.29 dt (13, 1)	3.23 d (13)	2.94 m
5	2.31 ddd (13, 10, 4)	1.61 m	2.33 m
5	2.60 dt (13, 4)	2.42 m	2.54 dt (12, 4)
6	2.83 ddd (14, 10, 4)	2.07 dd (13, 6)	2.94 m
6	2.85 dt (14, 4)	2.21 m	2.94 m
9	7.46 dd (7, 1)	7.40 d (8)	7.45 d (8)
10	7.06 td (7, 1)	7.14 t (8)	7.06 td (8, 1)
11	7.10 td (7, 1)	7.28 t (8)	7.09 td (8, 1)
12	7.29 dd (7, 1)	7.30 d (8)	7.26 d (8)
14	3.15 dt (4, 1)	3.08 d (4)	3.55 br s
15	2.93 dd (4, 1)	2.98 d (4)	3.55 br s
16	2.72 ddd (14, 8, 1)	2.42 m	2.75 dd (15, 8)
16	4.17 br dd (14, 13)	3.95 t (14)	2.94 m
17	1.73 ddd (14, 13, 1)	2.17 m	1.84 dd (14, 10)
17	2.23 ddt (14, 8, 1)	2.42 m	2.18 dd (15, 9)
18	0.74 t (8)	0.93 t (7)	0.86 t (7)
19	1.12 m	1.30 m	1.26 m
19	1.12 m	1.30 m	1.26 m
21	1.71 dd (12, 1)	1.94 d (12)	1.93 d (13)
21	2.37 br d (12)	2.51 d (12)	3.02 d (12)
N(1)-H	7.81 br s	-	7.84 br s

^{a}$CDCl_3$, 400 MHz; ^{b}$CDCl_3$, 600 MHz; assignments based on COSY and HSQC.

Table 2.38: ^{13}C Spectroscopic Data (δ) of Voaphylline (**55**), Voaphylline-7-hydroxyindolenine (**56**), and Voaphyllinediol (**57**)

C	**55**[a]	**56**[b]	**57**[a]
2	139.2	192.1	138.8
3	53.4	52.3	58.7
5	53.2	50.3	52.6
6	25.8	40.8	23.1
7	108.8	87.6	108.9
8	128.1	140.9	128.1
9	117.2	122.2	117.5
10	118.2	125.7	119.0
11	120.0	129.7	120.8
12	110.0	119.7	110.4
13	135.3	153.5	135.2
14	52.1	51.6	71.1
15	59.2	59.5	73.6
16	22.8	27.4	21.5
17	36.1	33.5	32.0
18	7.1	7.5	7.4
19	31.9	31.7	28.0
20	33.1	33.0	40.2
21	57.9	59.0	53.4

[a]$CDCl_3$, 100 MHz; [b]$CDCl_3$, 150 MHz; assignments based on HSQC and HMBC.

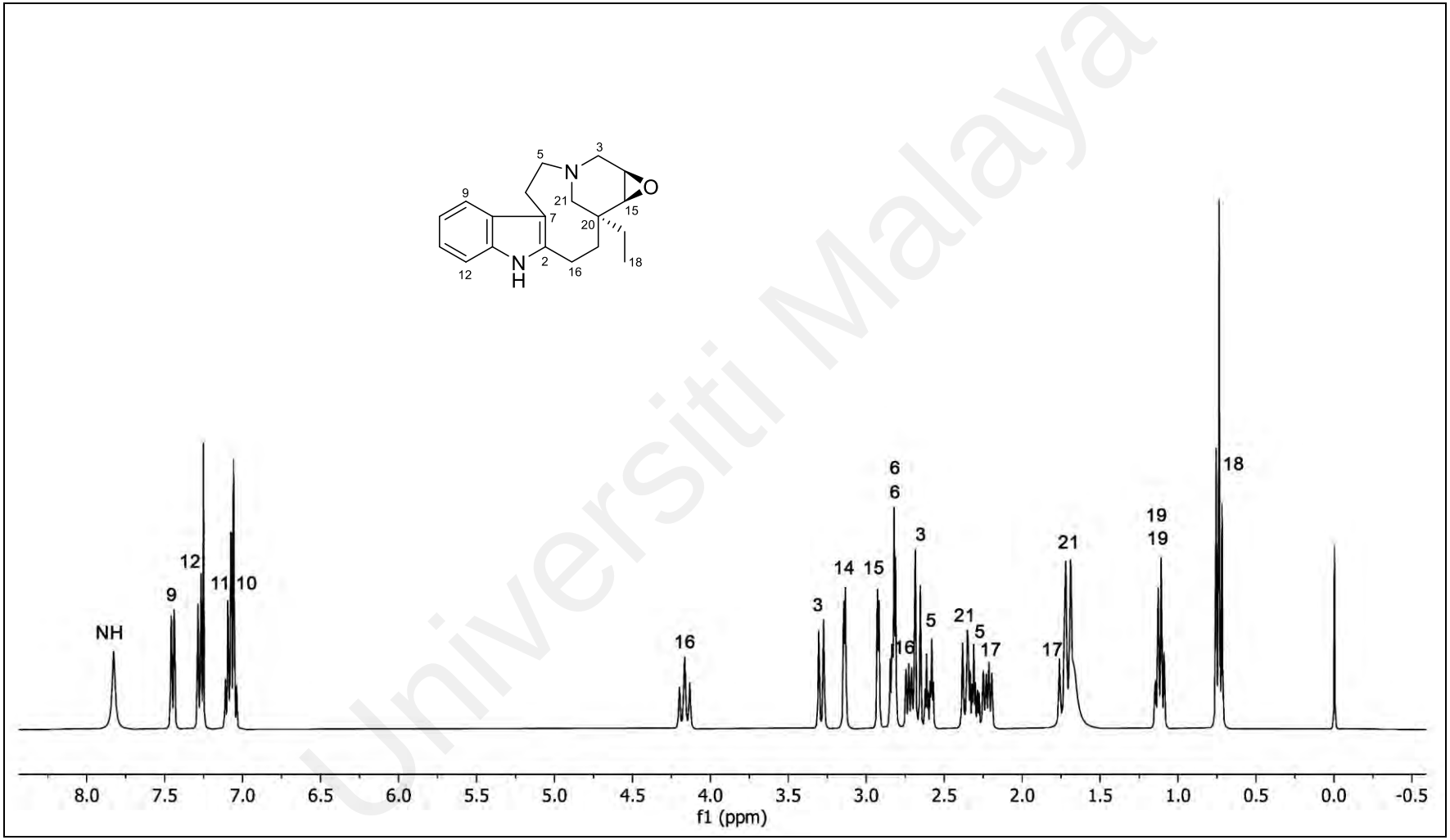


Figure 2.110: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Voaphylline (**55**)

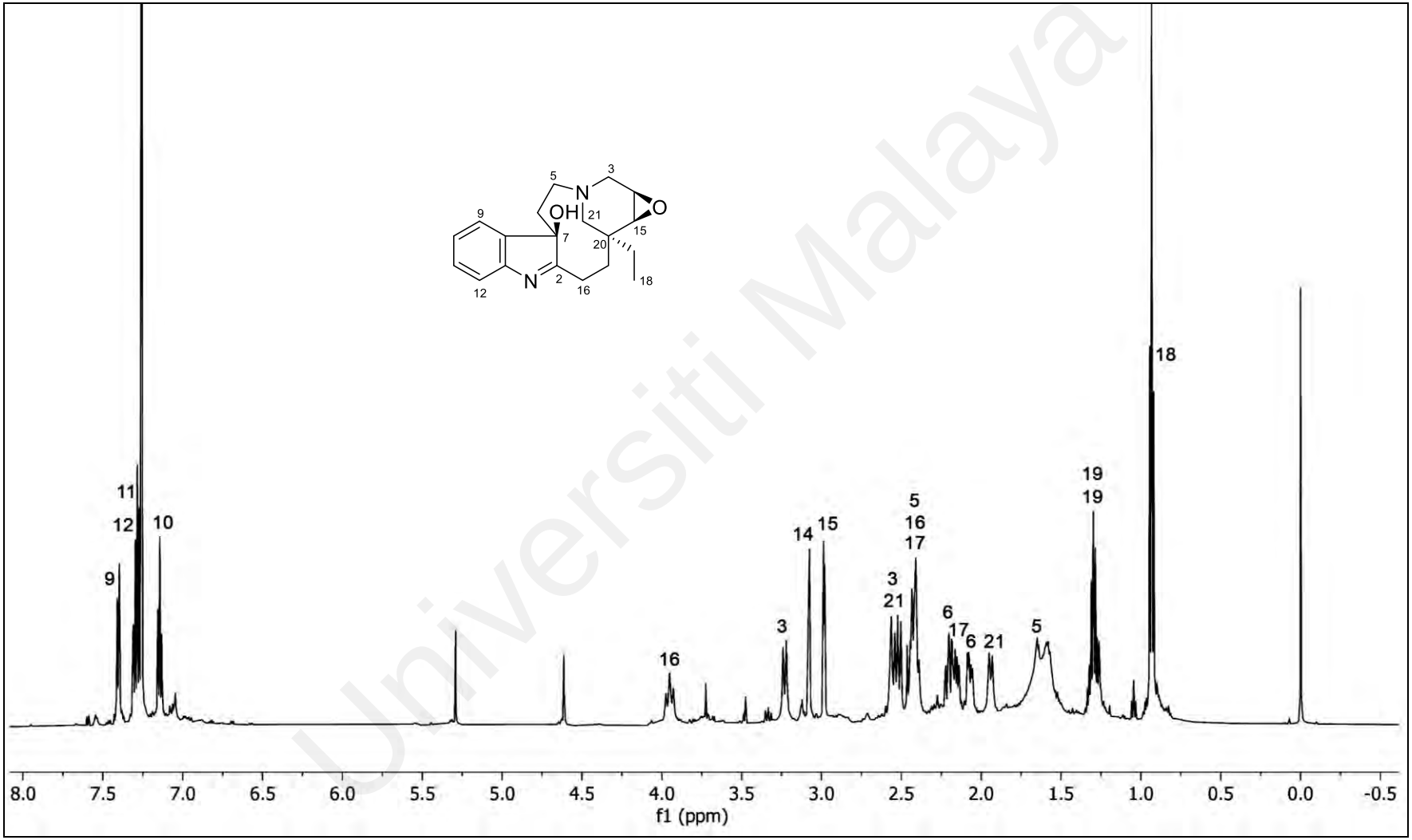


Figure 2.111: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Voaphylline-7-hydroxyindolenine (**56**)

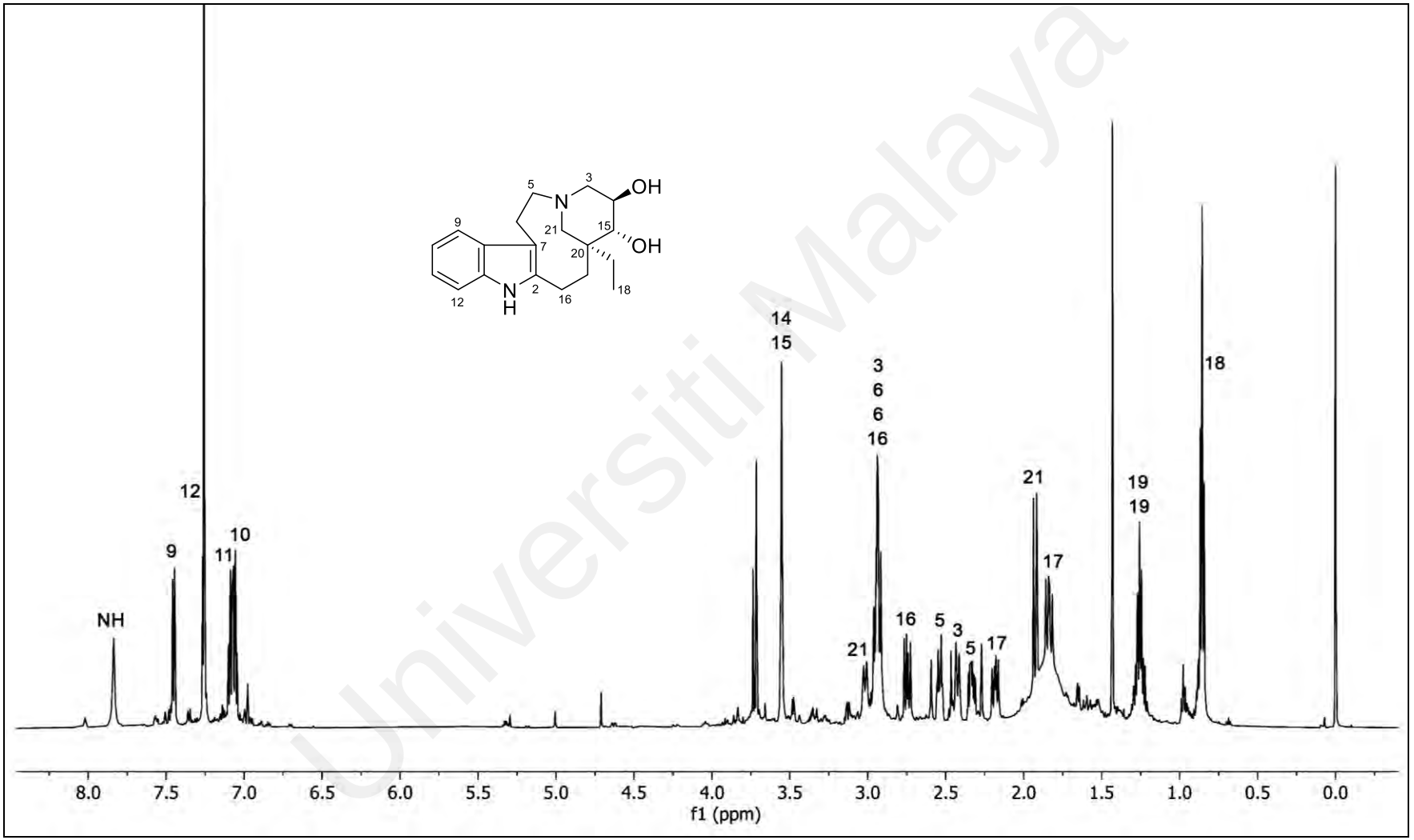


Figure 2.112: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Voaphyllinediol (**57**)

2.1.5 Vallesiachotamine, Vincamine, Aspidospermatan, and Other Alkaloids

2.1.5.1 Antirhine (58)

One known alkaloid belonging to the vallesiachotamine-subtype, *viz.*, antirhine (**58**) (Johns *et al.*, 1967), was isolated. The ^{1}H NMR spectrum is shown in Figure 2.113, while the ^{1}H and ^{13}C NMR spectroscopic data are summarized in Table 2.39. Other data are given in the Experimental Section.

Table 2.39: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of Antirhine (**58**)[a]

H/C	δ_H (*J*/Hz)	δ_C	H/C	δ_H (*J*/Hz)	δ_C
2	-	133.2	15	1.54 m	31.1
3	4.15 br s	54.2	16	1.47 m	28.6
5	3.03 m	51.5	16	1.72 m	
5	3.21 m		17	2.62 m	46.6
6	2.64 m	18.0	17	2.76 ddd (12, 9, 4)	
6	3.03 m		18	5.16 dd (17, 2)	117.7
7	-	107.0	18	5.22 dd (10, 2)	
8	-	127.2	19	5.60 ddd (17, 10, 9)	138.3
9	7.47 d (8)	117.7	20	2.24 m	49.6
10	7.09 td (8, 1)	119.0	21	3.59 dd (11, 7)	63.3
11	7.14 td (8, 1)	121.0	21	3.74 dd (10, 4)	
12	7.33 d (8)	110.9	*C*O$_2$Me	-	-
13	-	135.8	CO$_2$*Me*	-	-
14	1.90 m	31.2	N(1)-H	8.22 br s	-
14	2.05 m				

[a]$CDCl_3$, 400 (^{1}H) and 100 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and NOESY.

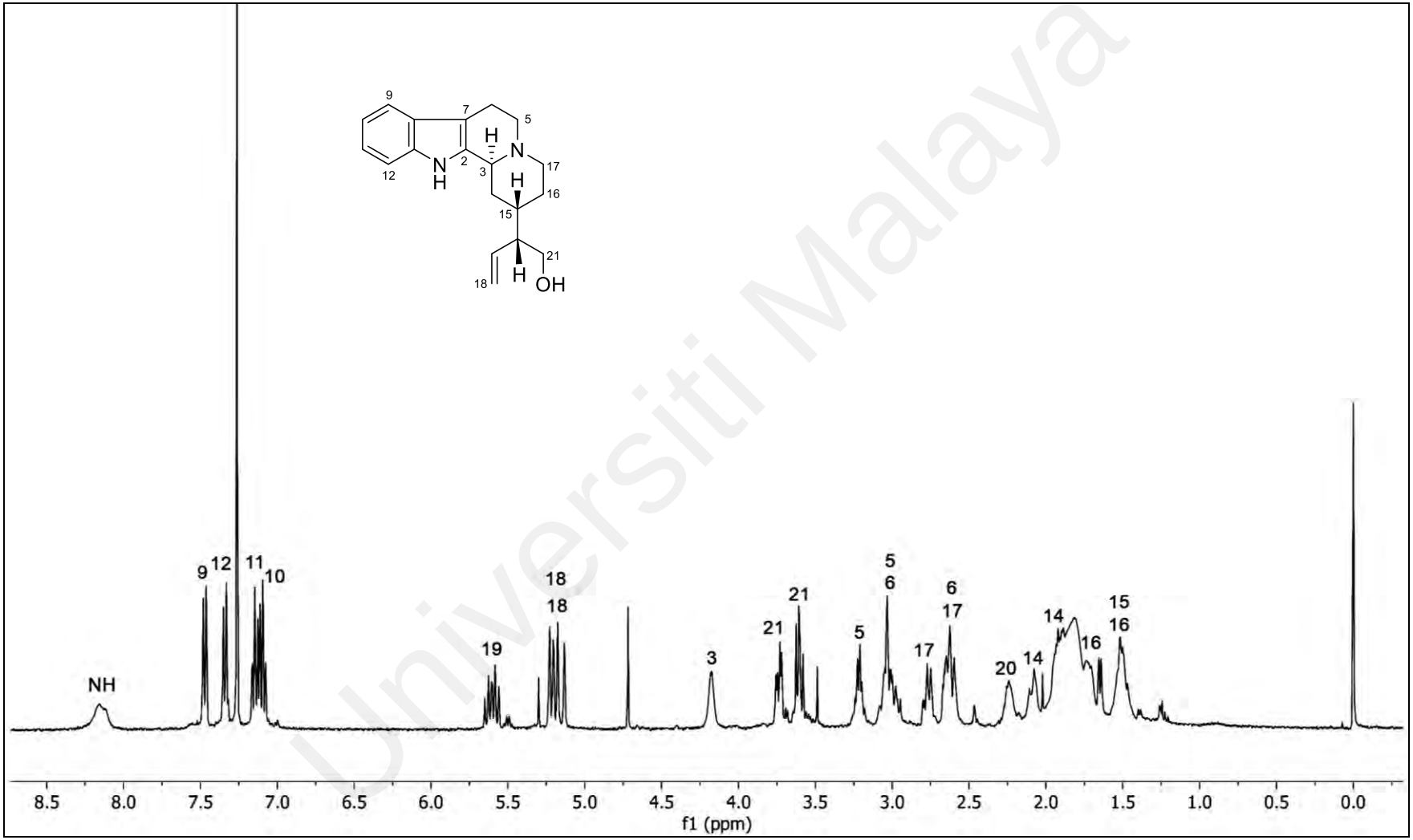


Figure 2.113: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Antirhine (**58**)

2.1.5.2 14,15-Dehydro-16-*epi*-vincamine (59)

One known alkaloid belonging to the vincamine group, *viz.*, 14,15-dehydro-16-*epi*-vincamine (**59**) (Aimi *et al.*, 1978; Kitajima *et al.*, 2014; Panas *et al.*, 1974; Zhang *et al.*, 2003), was isolated. The ^{1}H NMR spectrum is shown in Figure 2.114, while the ^{1}H and ^{13}C NMR spectroscopic data are summarized in Table 2.40. Other data are given in the Experimental Section.

Table 2.40: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of 14,15-Dehydro-16-*epi*-vincamine (**59**)[a]

H/C	δ_H (*J*/Hz)	δ_C	H/C	δ_H (*J*/Hz)	δ_C
2	-	132.8	13	-	136.7
3	3.00 m	43.9	14	5.46 dt (10, 3)	125.8
3	3.00 m		15	5.24 br d (10)	126.8
5	3.24 m	49.8	16	-	83.9
5	3.37 dd (14, 8)		17	2.02 d (14)	46.0
6	2.51 ddd (16, 6, 2)	16.7	17	2.56 d (14)	
6	3.09 m		18	0.92 t (8)	8.5
7	-	106.5	19	1.45 dq (15, 8)	35.4
8	-	129.0	19	1.78 dq (15, 8)	
9	7.43 m	118.1	20	-	38.5
10	7.10 m	120.3	21	3.79 br s	57.1
11	7.09 m	121.7	*C*O_2Me	-	172.3
12	7.45 m	112.7	CO_2*Me*	3.46 s	52.7

[a]$CDCl_3$, 400 (^{1}H) and 100 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and NOESY.

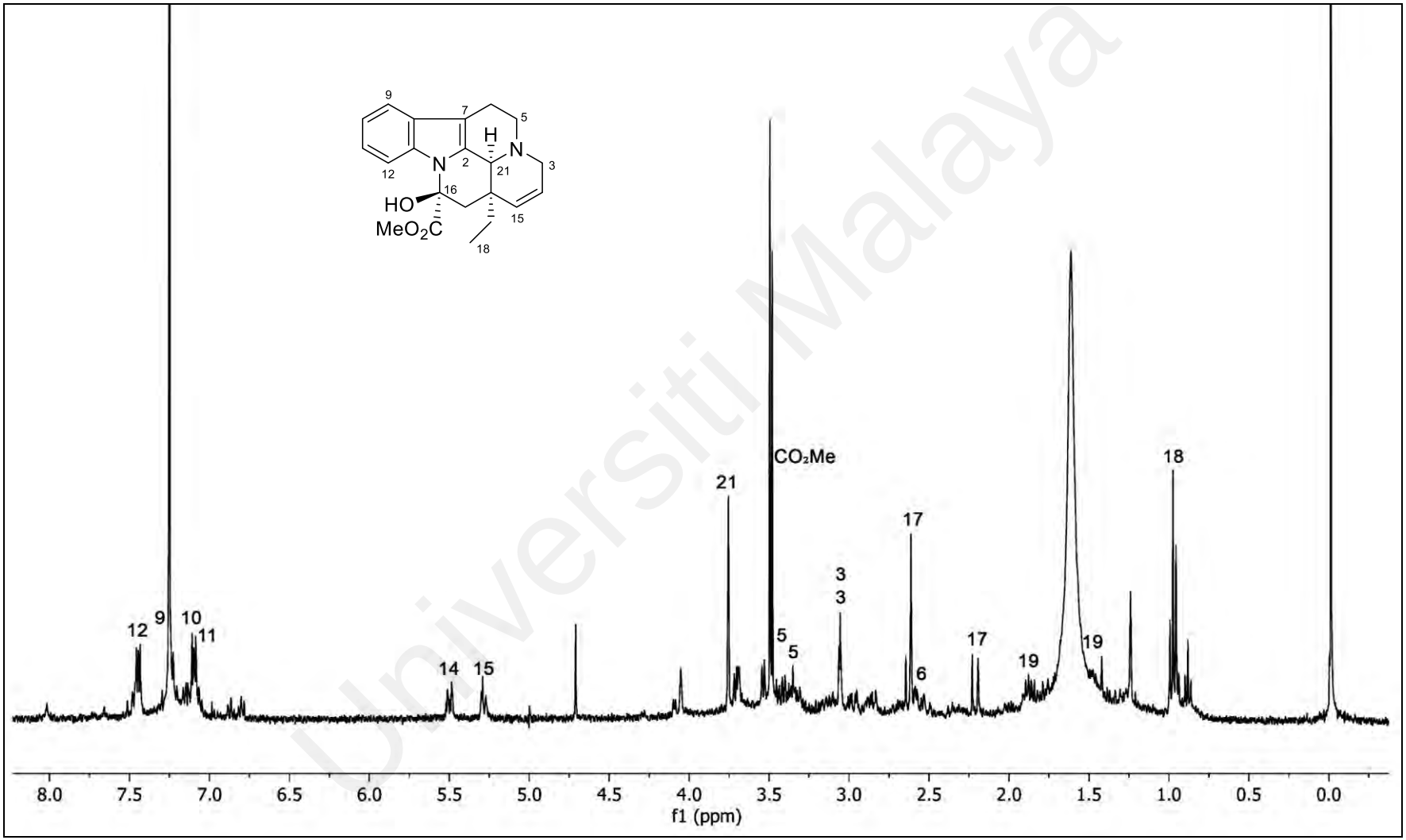


Figure 2.114: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 14,15-Dehydro-16-*epi*-vincamine (**59**)

2.1.5.3 Tubotaiwine (60), Tubotaiwine *N*(4)-oxide (61), *N*(4)-Chloromethyl-tubotaiwine chloride (62), and Janetine (63)

Four known aspidospermatan-type alkaloids including tubotaiwine (**60**) (Lounasmaa *et al.*, 1986; Pinar *et al.*, 1972; Schripsema *et al.*, 1987), tubotaiwine *N*(4)-oxide (**61**) (Pinar *et al.*, 1972), *N*(4)-chloromethyl-tubotaiwine chloride (**62**) (Besselievre *et al.*, 1972), and janetine (**63**) (Azoug *et al.*, 1995) were also isolated in the present study. The ^{1}H NMR spectra of these compounds are shown in Figures 2.115–2.118, while the ^{1}H and ^{13}C NMR spectroscopic data are summarized in Tables 2.41 and 2.42. Other data are given in the Experimental Section.

Table 2.41: ^{1}H NMR Spectroscopic Data (δ) of Tubotaiwine (**60**), Tubotaiwine *N*(4)-oxide (**61**), *N*(4)-Chloromethyl-tubotaiwine chloride (**62**), and Janetine (**63**)[a]

H	**60** (*J*/Hz)	**61** (*J*/Hz)	**62** (*J*/Hz)	**63** (*J*/Hz)
3	2.45 dt (12, 9)	3.49 m	3.39 td (14, 4)	3.07 ddd (13, 9, 6)
3	2.95 dt (12, 4)	3.49 m	4.09 dd (14, 4)	3.35 dt (13, 6)
5	2.83 dd (11, 7)	3.62 dd (11, 8)	3.80 m	-
5	2.89 m	3.73 td (12, 8)	4.44 td (12, 8)	-
6	1.80 m	2.10 dd (15, 8)	2.26 dd (14, 8)	-
6	2.92 m	2.60 td (14, 8)	2.89 ddd (14, 12, 8)	-
9	7.13 dd (8, 1)	7.26 d (8)	8.00 br d (8)	8.00 d (8)
10	6.87 td (8, 1)	6.94 t (8)	6.99 td (8, 1)	7.18 td (8)
11	7.10 td (8, 1)	7.17 t (8)	7.18 td (8, 1)	7.36 t (8)
12	6.80 dd (8, 1)	6.85 d (8)	6.87 br d (8)	7.40 d (8)
14	1.80 m	1.78 br d (13)	1.98 br d (14)	2.84 m
14	1.80 m	2.38 m	2.30 m	2.84 m
15	3.04 m	3.20 m	3.33 m	-
17	-	-	-	2.34 s
18	0.70 t (7)	0.73 t (7)	0.77 t (7)	1.59 d (6)
19	0.81 m	0.87 m	0.88 dq (14, 7)	4.28 q (6)
19	0.81 m	0.87 m	1.01 dq (14, 7)	-
20	1.96 tt (7, 3)	2.51 m	2.30 m	-
21	3.79 m	4.25 m	5.51 m	7.71 s
22	-	-	5.97 d (10)	-
22	-	-	6.60 d (10)	-
CO_2*Me*	3.76 s	3.79 s	3.81 s	-
N(1)-H	8.86 s	8.77 s	8.81 s	8.53 s

[a]$CDCl_3$, 400 MHz; assignments based on COSY and HSQC.

Table 2.42: ^{13}C NMR Spectroscopic Data (δ) of Tubotaiwine (**60**), Tubotaiwine *N*(4)-oxide (**61**), *N*(4)-Chloromethyl-tubotaiwine chloride (**62**), and Janetine (**63**)[a]

C	60	61	62	63
2	170.8	166.7	166.7	138.0
3	45.3	59.9	50.2	41.6
5	54.1	67.6	59.5	-
6	44.1	39.3	38.9	-
7	55.2	51.3	53.6	120.9
8	137.3	134.5	133.2	123.7
9	119.6	119.6	121.8	120.1
10	121.1	121.9	122.6	119.0
11	127.2	128.5	128.7	125.4
12	109.7	110.5	110.2	110.6
13	143.7	143.1	142.3	139.9
14	28.6	24.8	24.4	27.6
15	31.0	29.6	29.0	130.3
16	95.7	95.8	95.0	117.3
17	-	-	-	12.9
18	11.7	11.2	10.9	23.2
19	24.0	22.5	22.5	52.2
20	41.3	36.8	37.3	131.7
21	65.6	78.7	73.6	114.7
22	-	-	65.2	-
*C*O$_2$Me	168.9	168.0	167.5	-
CO$_2$*Me*	51.2	51.5	50.2	-

[a]$CDCl_3$, 100 MHz; assignments based on HSQC and HMBC.

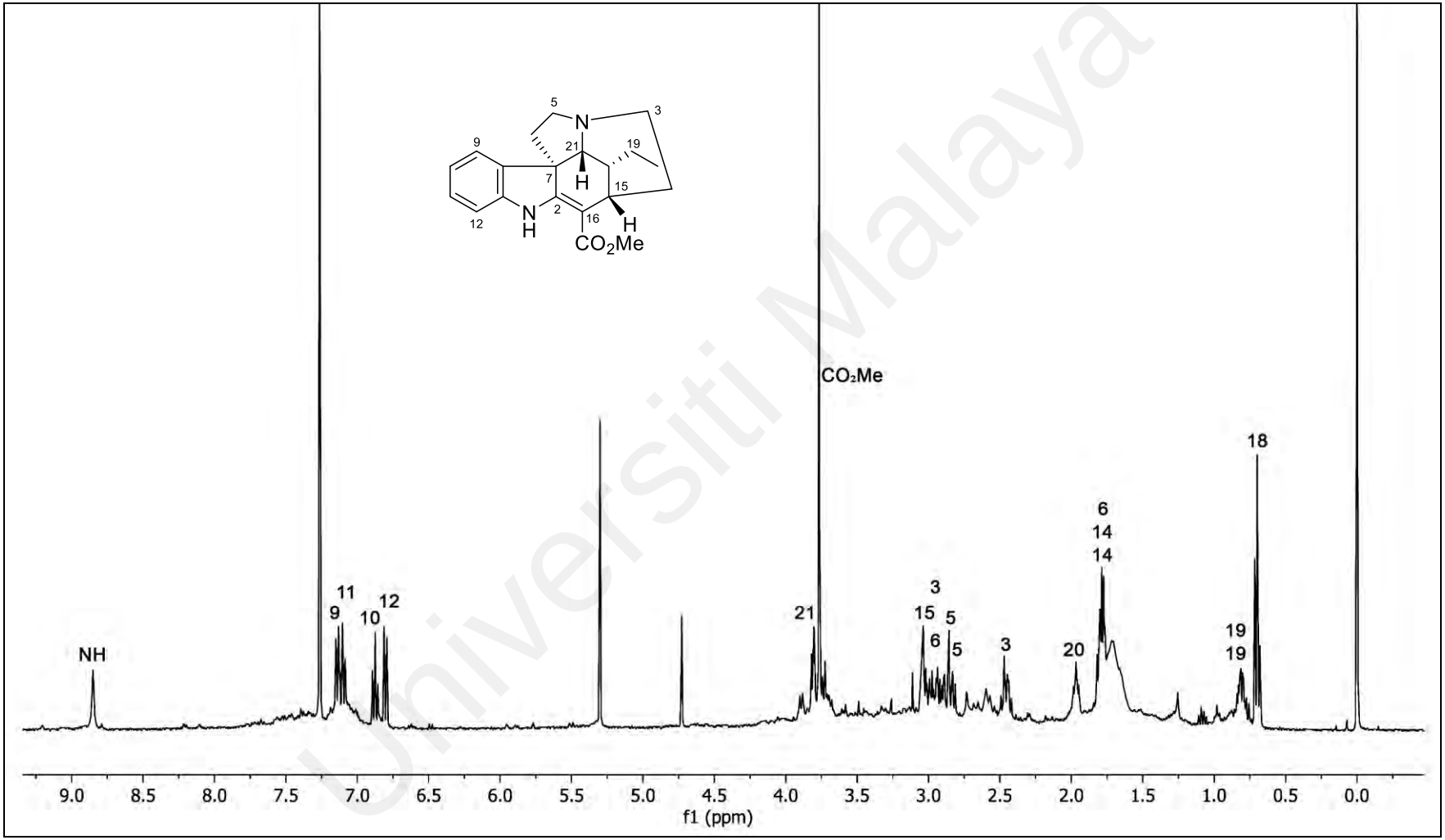


Figure 2.115: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Tubotaiwine (**60**)

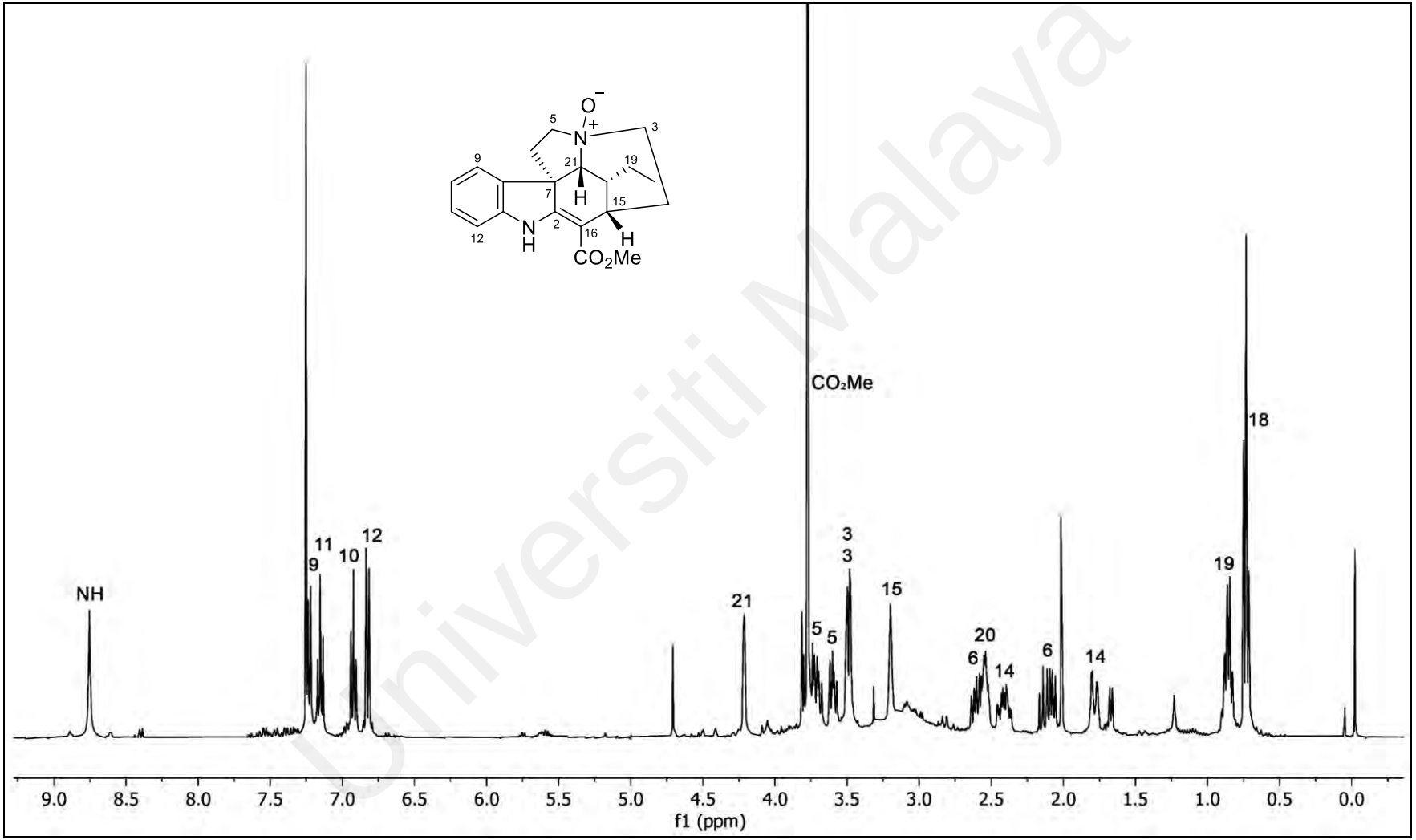


Figure 2.116: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Tubotaiwine *N*(4)-oxide (**61**)

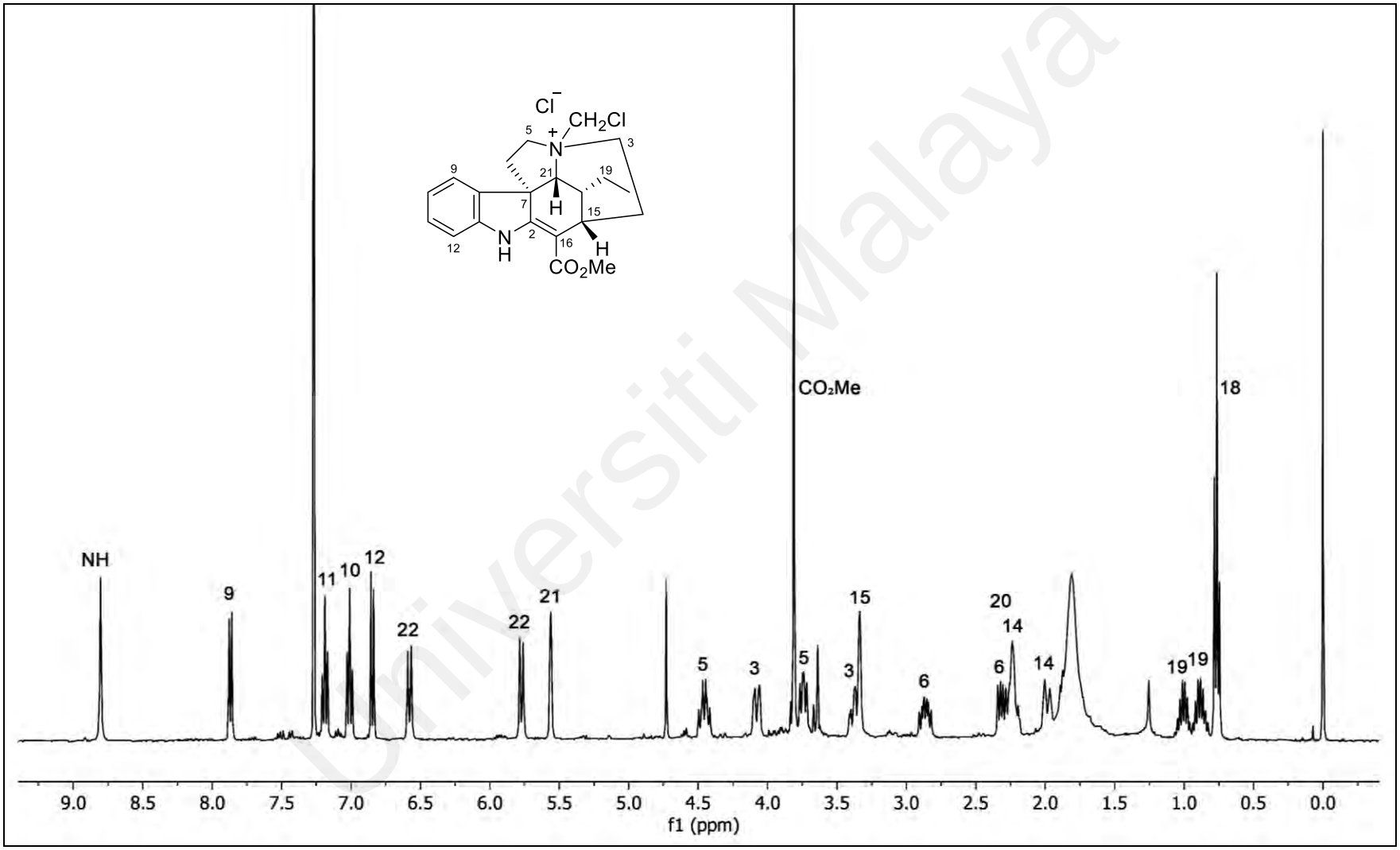


Figure 2.117: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of *N*(4)-Chloromethyl-tubotaiwine chloride (**62**)

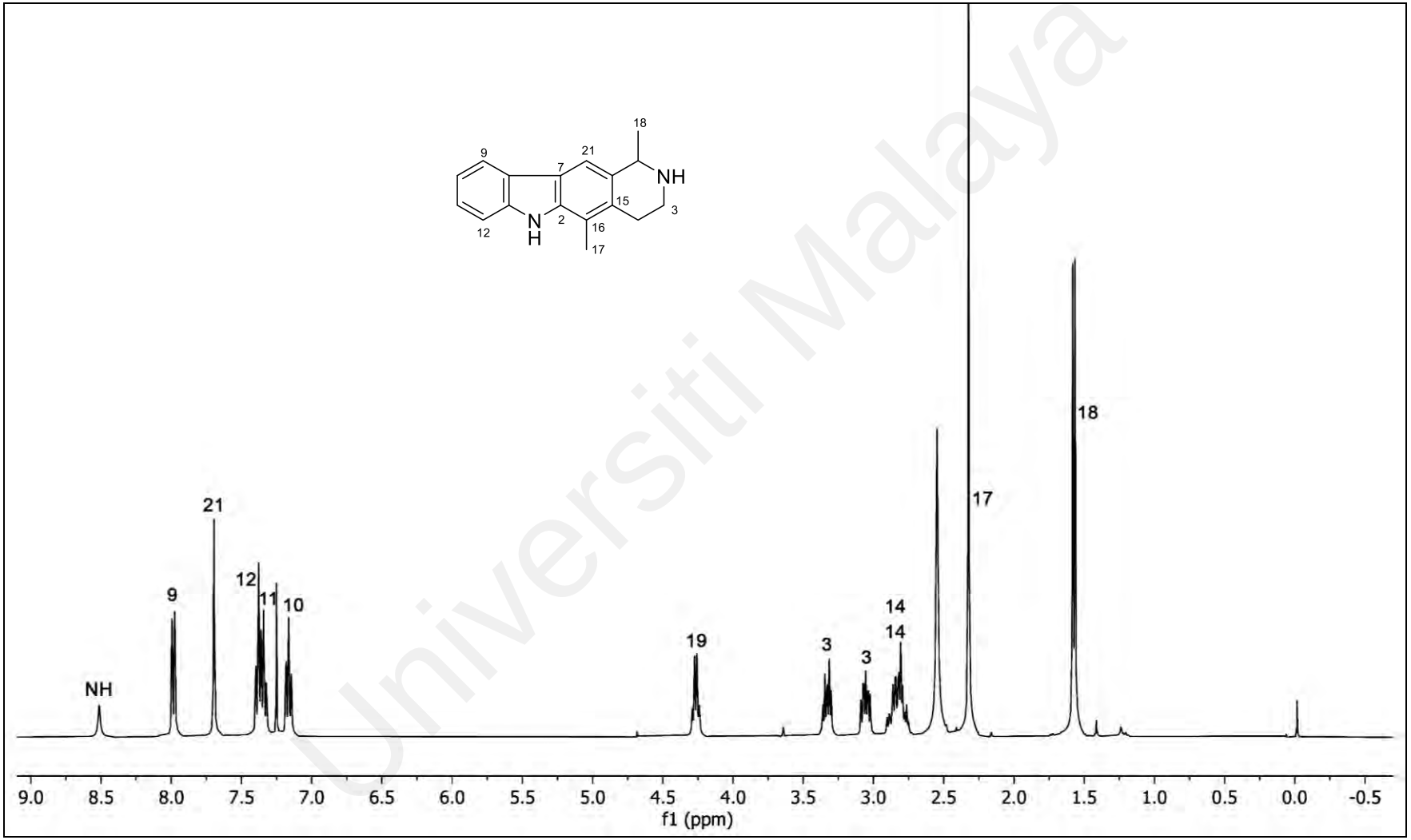


Figure 2.118: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Janetine (**63**)

2.1.5.4 Harmane (64) and Taberdivamine B (65)

Other types of alkaloids including harmane (**64**) (Coune *et al.*, 1980; Omar *et al.*, 2010) and taberdivamine B (**65**) (Zhu *et al.*, 2020) were also isolated and identified. The ^{1}H NMR spectra of these compounds are shown in Figures 2.119–2.120, while the ^{1}H and ^{13}C NMR spectroscopic data are summarized in Table 2.43. Other data are given in the Experimental Section.

Table 2.43: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of Harmane (**64**) and Taberdivamine B (**65**)[a]

H/C	64		65	
	δ_H (J/Hz)	δ_C	δ_H (J/Hz)	δ_C
2	-	134.5	-	133.2
3	-	141.7	3.11 d (10)	60.3
3	-		3.86 dd (10, 5)	
5	8.36 d (6)	138.6	3.50 dd (12, 6)	54.3
5	-		5.14 td (12, 6)	
6	7.83 d (6)	112.9	3.04 ddd (17, 13, 6)	17.2
6	-		3.15 dd (17, 6)	
7	-	128.3	-	101.5
8	-	122.1	-	125.5
9	8.12 br d (8)	111.6	7.39 d (8)	117.8
10	7.29 m	128.4	7.07 td (8, 1)	119.8
11	7.41 m	120.2	7.14 td (8, 1)	122.7
12	7.41 m	122.1	7.36 d (8)	111.9
13	-	140.1	-	137.0
14	2.84 s	20.3	2.66 s	29.6
15	-	-	2.10 m	36.4
15	-	-	2.47 d (18)	
16	-	-	-	86.6
17	-	-	2.92 m	40.7
17	-	-	2.92 m	
18	-	-	1.08 t (7)	11.6
19	-	-	2.10 m	26.8
19	-	-	2.10 m	
20	-	-	-	136.8
21	-	-	6.54 s	132.2
*C*OO$^-$	-	-	-	167.7
N(1)-H	8.50 br s	-	9.65 br s	-

[a]$CDCl_3$, 400 (^{1}H) and 100 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and NOESY.

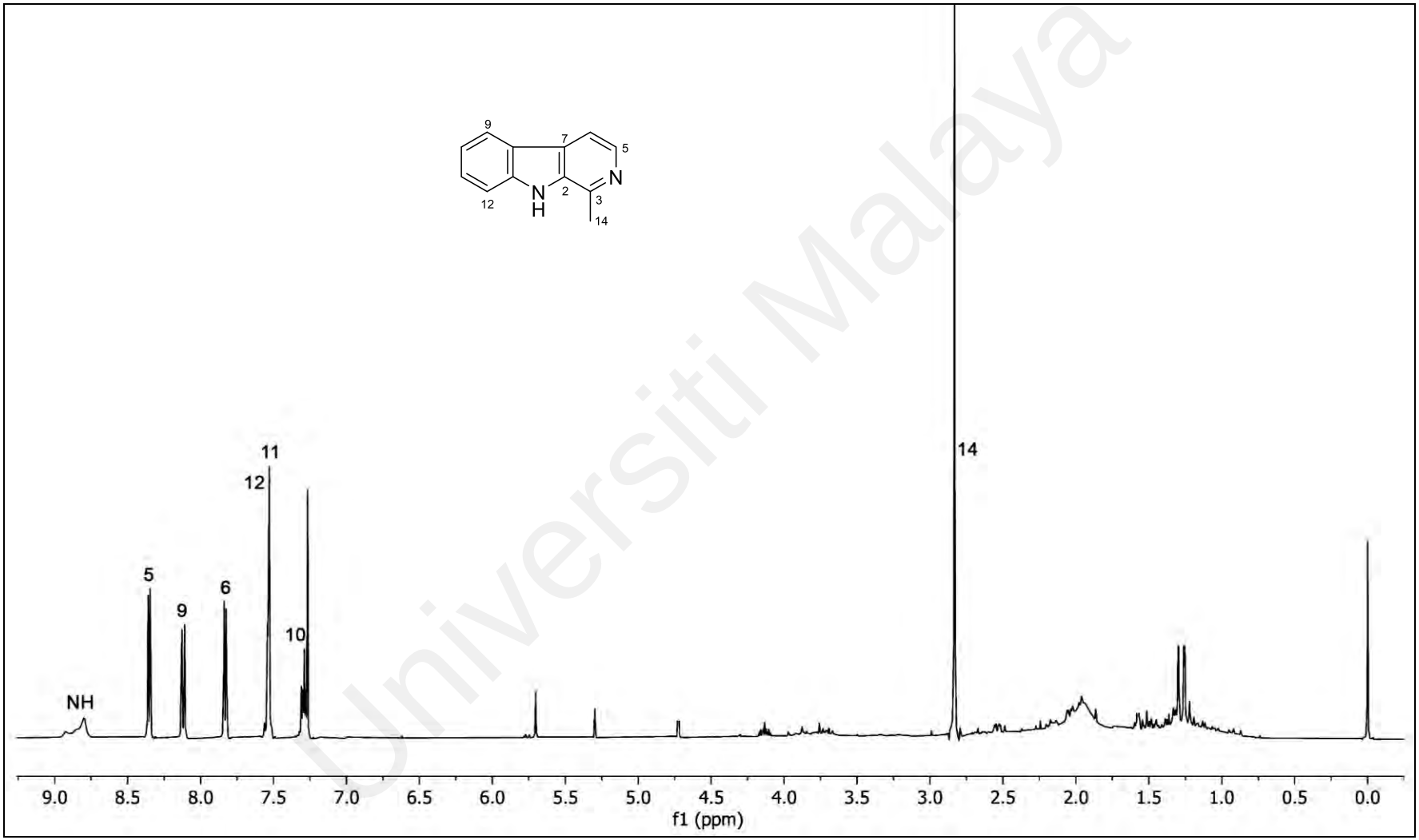


Figure 2.119: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Harmane (**64**)

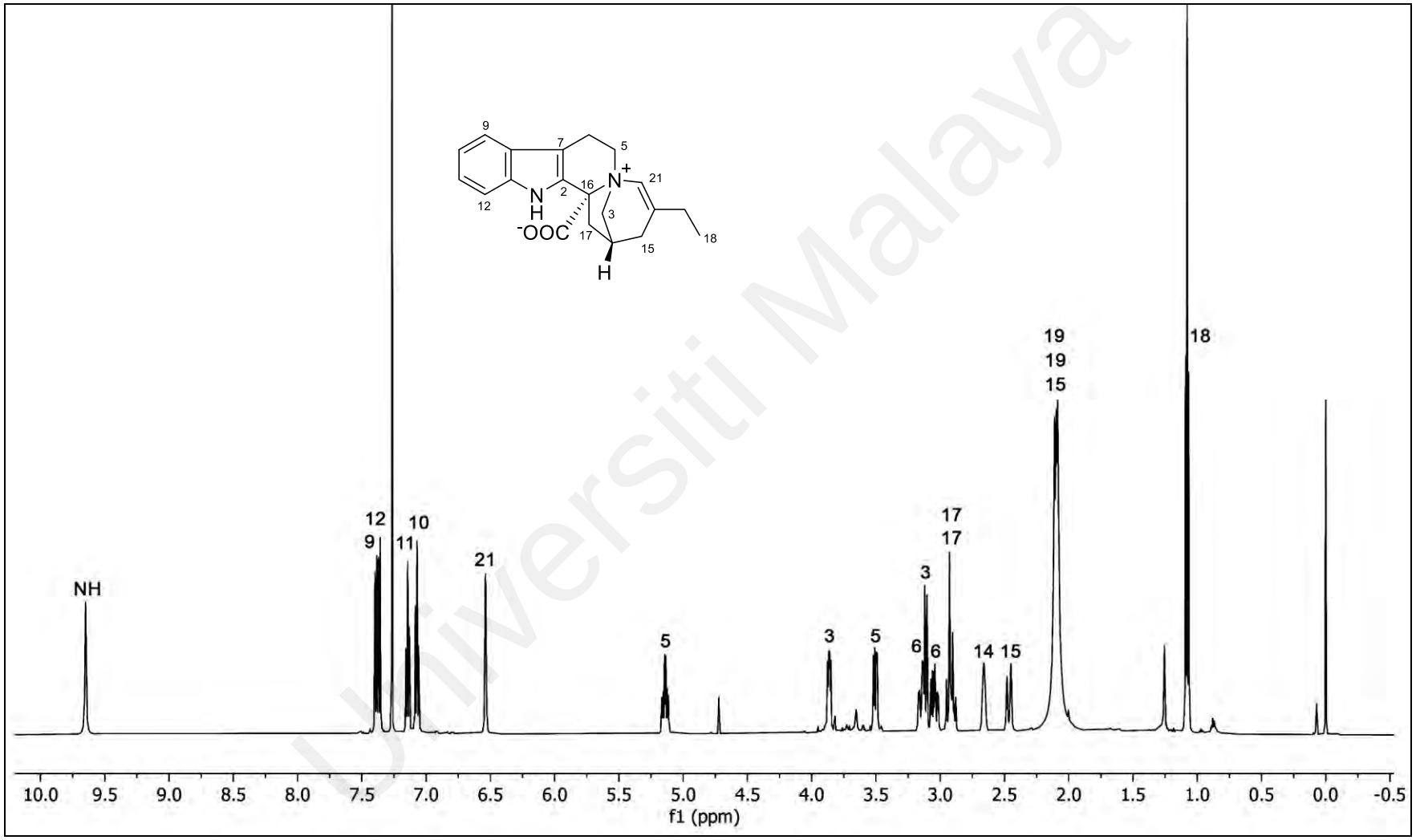


Figure 2.120: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Taberdivamine B (**65**)

2.1.6 Bisindole Alkaloids

2.1.6.1 Polyneurine P (66)

Polyneurine P (**66**) was obtained as a light yellowish oil, $[\alpha]^{25}_{D}$ −103 (*c* 0.5, $CHCl_3$). The UV spectrum exhibited absorption maxima indicative of an indole chromophore at 225 and 288 nm, while the IR spectrum showed the presence of NH/OH and ester carbonyl groups at 3373 and 1714 cm^{-1}, respectively. The HRMS data ($[M + H]^+$ *m/z* 691.3870) established the molecular formula of **66** as $C_{42}H_{50}N_4O_5$ + H.

The ^{1}H NMR spectrum (Figure 2.125) showed signals for two indolic NH (δ_H 7.47, 7.83), an unsubstituted indole moiety (δ_H 7.03−7.57), another indole ring substituted at C-10' (δ_H 7.00−7.29), two methyl ester groups (δ_H 2.46, 3.69), an *N*(4)-methyl (δ_H 2.60), an ethylidene side chain (δ_H 1.65, 5.32), and a hydroxyethyl side chain (δ_H 1.26, 3.88). The ^{13}C NMR data (Table 2.44) revealed resonances for all 42 carbon atoms, including two ester carbonyls (δ_C 171.7, 174.9), two ester methyls (δ_C 50.0, 52.8), an *N*(4)-methyl (δ_C 42.3), two olefinic carbons (δ_C 119.1, 137.2), and a hydroxyethyl side chain (δ_C 22.2, 70.8). All the data mentioned earlier confirmed the dimeric nature of compound **66** which is constituted from the union of two monomeric units (A and B).

The gross structure of unit A (vobasinyl half) was elucidated based on the presence of a characteristic $CH_2CHCHCHCH_2CH$ (C-6–C-5–C-16–C-15–C-14–C-3) partial structure (Figure 2.122), which was further confirmed by the HMBC data (Figure 2.122). The 16*S* configuration was deduced from the high-field signal of the methyl ester at δ_H 2.46, indicating the orientation of the ester function within the shielding zone of the indole ring, whereas the observed NOEs H-15/H-18 and H-19/H-21 (Figure 2.123) determined the *E* geometry of the 19,20-double bond. The remaining COSY fragments, *viz.*, CHCH (C-11'–C-12'), CH_2CH_2 (C-5'–C-6'),

$CH_2CH(CH_2)CH_2CH(CH)CHCH_3$ (C-17'–C-14'(C-3')–C-15'–C-20'(C-21')–C-19'–C-18'), corresponded to those in unit B (Figure 2.122). Examination of the HMBC data (Figure 2.122) indicated that unit B possessed an iboga-type framework, corresponding to that of 19'(*R*)-hydroxyconoduramine (**685**), as evident from the similarity of the NMR data (Takayama *et al.*, 1994), except for changes involving the aromatic signals (Figure 2.121).

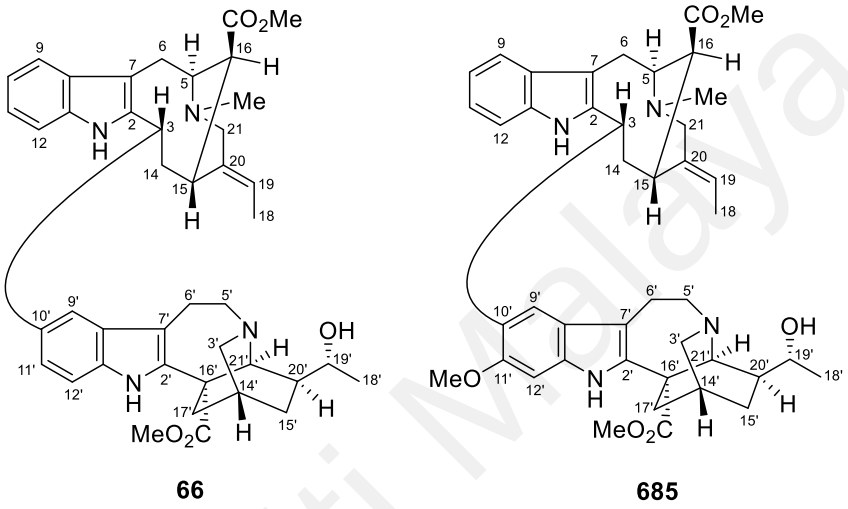


Figure 2.121: Structures of **66** and **685**

In unit B, an isolated aromatic hydrogen at δ_H 7.29 was attributed to H-9' from the observed three-bond correlations from this proton to C-7', C-11', and C-13' in the HMBC spectrum (Figure 2.122), as well as the NOE observed between H-9' and H-6' (Figure 2.123). This suggested C-10' as the branching point of the bisindole from the iboga half as H-11' and H-12' were observed as a pair of AB doublet at δ_H 7.00 and 7.16 with J = 8.0 Hz. In unit A, the H-3 resonance was observed as a 1H doublet of doublet at δ_H 4.65 (J = 13.1, 3.3 Hz), indicating that the branching of the bisindole is from C-3 of the vobasinyl half. The observed three-bond correlations H-9', H-11'/C-3 and H-3/C-9', C-11' in the HMBC spectrum (Figure 2.122) provided confirmation for the linkage between the two monomeric units of the bisindole *via* C-3–C-10' bond. The H-3β configuration was assigned based on the observed NH/H-3 NOE and $J_{3\beta-14\alpha}$ coupling value of 13.1 Hz. Other NOEs, such as H-3/H-9', H-11' were also consistent with the

proposed structure. In unit B, the 20'*S* configuration was determined based on the H-15'α/H-20' NOE enhancement (Figure 2.123) and the observed $J_{15'\alpha-20'}$ coupling value of 9.0 Hz, which requires the H-20'α/H-15'α dihedral angle to be ~0° (Nge, Chong *et al.*, 2016). The 19'*R* configuration was assigned based on the carbon shifts of C-15' (δ_C 28.6) and C-21' (δ_C 54.1), which correspond to those of the 19*R* series of iboga alkaloids with a β-substituted hydroxyethyl side chain at C-20 (Sim *et al.*, 2016; Takayama *et al.*, 1994; Wenkert, Cochran *et al.*, 1976). The 19'*R* configuration was further confirmed by GIAO NMR calculations and DP4+ analysis. The experimental NMR data were compared with the calculated ^{1}H and ^{13}C NMR shifts of **66** and its C-19' epimer using DP4+ analysis. The DP4+ results supported **66** with 19'*R* configuration as the correct relative configuration, with 100% DP4+ probability (all data). The absolute configuration of **66** was eventually established as (3*R*, 5*S*, 15*R*, 16*S*, 14'*R*, 16'*S*, 19'*R*, 20'*S*, 21'*S*) based on comparison of the experimental and calculated ECD spectra (Figure 2.124).

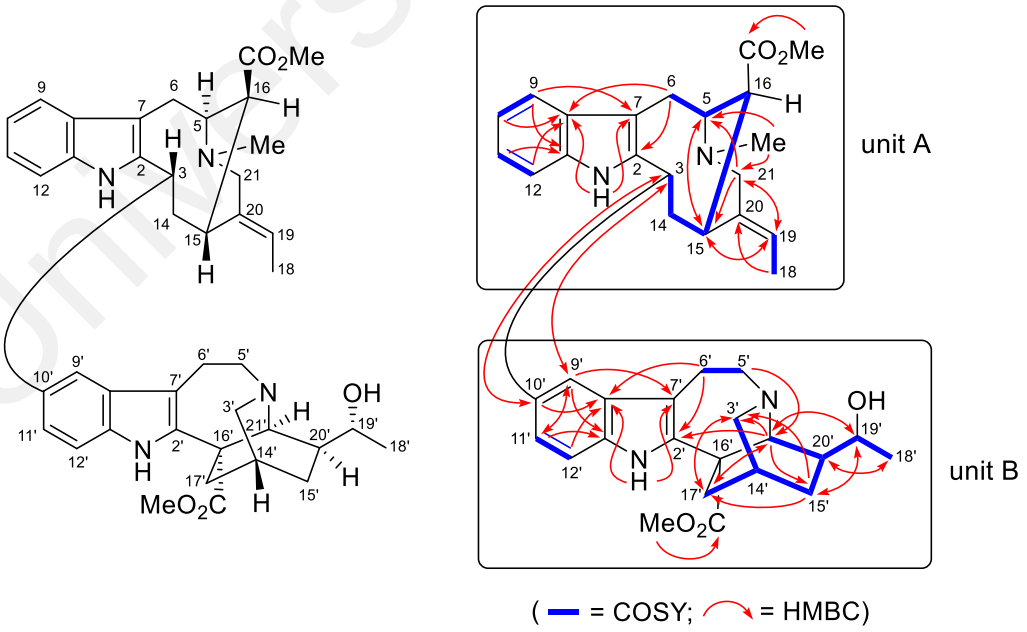


Figure 2.122: COSY and selected HMBCs of **66**

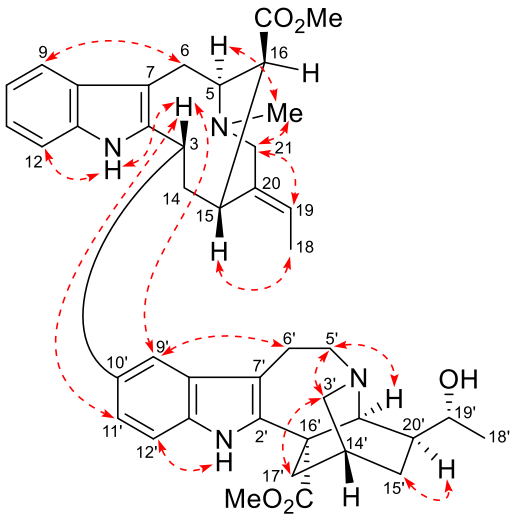


Figure 2.123: Selected NOEs of **66**

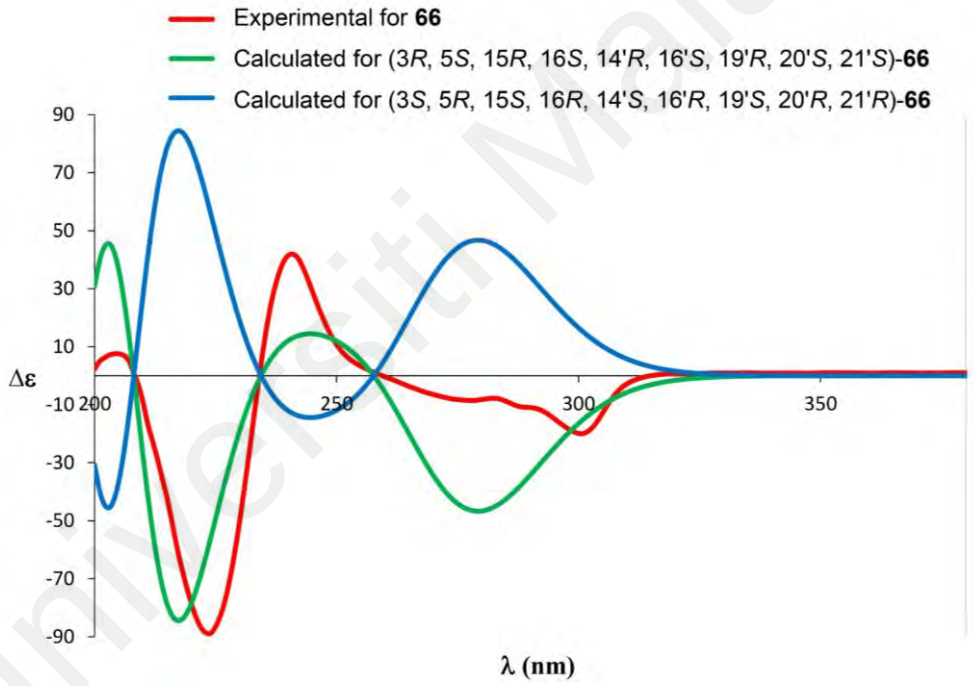


Figure 2.124: Experimental ECD spectrum of **66** and calculated ECD spectra of (3*R*, 5*S*, 15*R*, 16*S*, 14'*R*, 16'*S*, 19'*R*, 20'*S*, 21'*S*)-**66** and (3*S*, 5*R*, 15*S*, 16*R*, 14'*S*, 16'*R*, 19'*S*, 20'*R*, 21'*R*)-**66**

Table 2.44: ^{1}H and ^{13}C NMR Spectroscopic Data (δ) of Polyneurine P (**66**)[a]

H/C	δ_H (J/Hz)	δ_C	H/C	δ_H (J/Hz)	δ_C
2	-	137.3	2'	-	136.4
3	4.65 dd (13.1, 3.3)	45.3	3'	2.80 d (9.0)	50.7
			3'	3.01 m	
5	4.04 m	59.7	5'β	3.12 m	51.9
			5'α	3.38 m	
6β	3.26 dd (14.6, 8.0)	19.4	6'	3.01 m	21.6
6α	3.52 dd (14.6, 10.4)		6'	3.12 m	
7	-	110.1	7'	-	109.8
8	-	129.8	8'	-	128.7
9	7.57 d (8.0)	117.6	9'	7.29 s	117.1
10	7.07 m	119.0	10'	-	137.4
11	7.07 m	121.7	11'	7.00 dd (8.0, 1.0)	122.4
12	7.03 m	109.9	12'	7.16 d (8.0)	110.9
13	-	136.0	13'	-	134.3
14	1.94 m	39.1	14'	2.01 br s	26.9
14	2.66 m				
15	3.75 m	33.5	15'	1.76 m	28.6
			15'	1.84 m	
16	2.72 t (3.3)	47.0	16'	-	53.9
17	-	-	17'β	1.91 m	36.6
			17'α	2.57 d (13.3)	
18	1.65 d (6.8)	12.4	18'	1.26 d (6.4)	22.2
19	5.32 q (6.8)	119.1	19'	3.88 qd (6.4, 2.3)	70.8
20	-	137.2	20'	1.38 t (9.0)	39.9
21	2.91 d (13.8)	52.3	21'	4.04 br s	54.1
21	3.73 m				
N(4)-Me	2.60 s	42.3	N(4)-Me'	-	-
*C*O$_2$Me	-	171.7	*C*O$_2$Me'	-	174.9
CO$_2$*Me*	2.46 s	50.0	CO$_2$*Me*'	3.69 s	52.8
N(1)-H	7.47 br s	-	N(1)-H'	7.83 br s	-

[a]$CDCl_3$, 400 (^{1}H) and 100 MHz (^{13}C); assignments based on COSY, HSQC, HMBC, and 1D/2D NOESY.

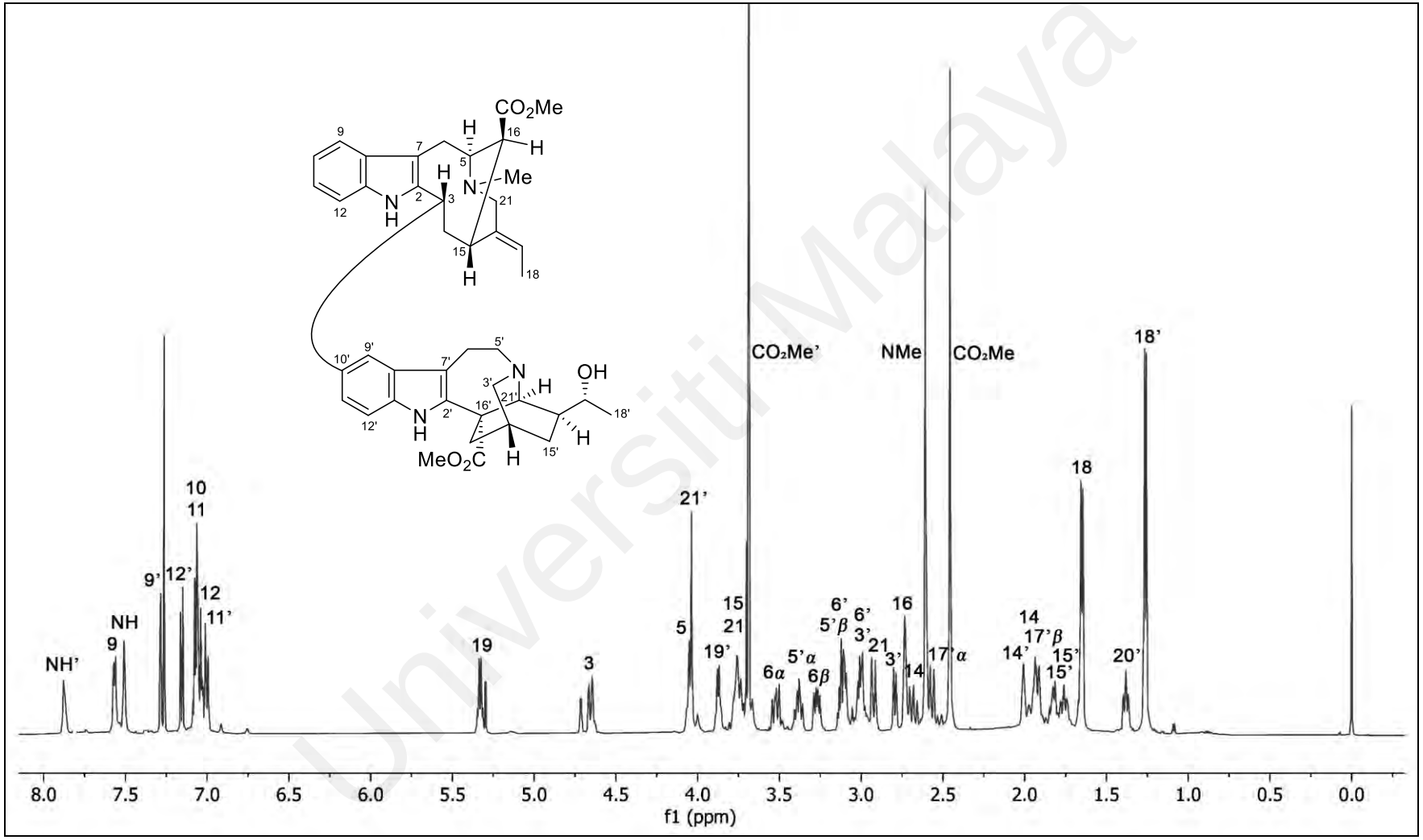


Figure 2.125: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Polyneurine P (**66**)

2.1.6.2 Tabernamine (67), 19'(*R*)-Hydroxytabernamine (68), Ervahaimine A (69), Ervahaimine B (70), Conophylline (71), and Conophylline quinone (72)

Four known vobasinyl-iboga alkaloids, *viz.*, tabernamine (**67**) (Kam & Sim, 2002b; Perera *et al.*, 1985), 19'(*R*)-hydroxytabernamine (**68**) (Kam & Sim, 2002b), and ervahaimines A (**69**) and B (**70**) (Feng *et al.*, 1989) were isolated in the present study. Another two known bisindole alkaloids belonging to the Aspidosperma-aspidosperma type, *viz.*, conophylline (**71**) (Kam, Loh *et al.*, 1992 & 1993) and conophylline quinone (**72**) (Kam, Pang *et al.*, 2003), were also obtained. The ^{1}H NMR spectra of these compounds are shown in Figures 2.126–2.131, while the ^{1}H and ^{13}C NMR spectroscopic data are summarized in Tables 2.45–2.50. Other data are given in the Experimental Section.

Table 2.45: ^{1}H NMR Spectroscopic Data (δ) of Tabernamine (**67**) and 19'(*R*)-Hydroxytabernamine (**68**)[a]

H	**67** (*J*/Hz)	**68** (*J*/Hz)	**H**	**67** (*J*/Hz)	**68** (*J*/Hz)
3	4.63 dd (13, 3)	4.64 dd (13, 3)	3'	2.93 dt (9, 3)	3.01 m
			3'	3.01 dt (9, 2)	3.01 m
5	4.05 ddd (10, 8, 3)	4.03 ddd (10, 8, 3)	5'	3.09 m	3.12 m
			5'	3.33 m	3.24 m
6	3.25 dd (15, 8)	3.24 m	6'	2.64 m	2.69 m
6	3.50 dd (15, 10)	3.50 dd (15, 10)	6'	3.33 m	3.24 m
9	7.56 dd (7, 1)	7.56 dd (8, 2)	9'	7.35 d (7)	7.36 d (9)
10	7.05 m	7.05 m	10'	6.96 dd (7, 1)	6.99 dd (9, 2)
11	7.05 m	7.05 m	11'	-	-
12	7.05 m	7.05 m	12'	7.01 d (1)	6.97 d (1)
14	1.97 m	1.93 m	14'	1.80 m	1.93 m
14	2.64 m	2.65 m			
15	3.77 dt (8, 3)	3.77 m	15'	1.18 tdd (12, 4, 2)	1.81 td (14, 4)
			15'	1.76 m	1.87 m
16	2.71 t (3)	2.72 t (3)	16'	2.85 ddd (12, 4, 2)	2.84 ddd (12, 4, 2)
17	-	-	17'	1.50 m	1.56 m
			17'	1.97 m	2.00 m
18	1.65 dd (7, 2)	1.65 dd (7, 1)	18'	0.88 d (7)	1.25 d (6)
19	5.31 qd (7, 1)	5.32 q (7)	19'	1.50 m	3.86 qd (6, 3)
			19'	1.50 m	
20	-	-	20'	1.50 m	1.56 m
21	2.89 d (14)	2.89 d (14)	21'	2.79 t (2)	3.31 t (2)
21	3.72 dd (14, 2)	3.72 br d (14)			
N(4)-Me	2.59 s	2.59 s	N(4)-Me'	-	-
CO_2*Me*	2.47 s	3.46 s	CO_2*Me*'	-	-
N(1)-H	7.51 br s	7.52 br s	N(1)-H'	7.47 br s	7.57 br s

[a]$CDCl_3$, 400 MHz; assignment based on COSY, HSQC, and NOESY.

Table 2.46: ^{13}C NMR Spectroscopic Data (δ) of Tabernamine (**67**) and 19'(*R*)-Hydroxytabernamine (**68**)[a]

C	67	68	C	67	68
2	137.4	137.4	2'	142.0	141.1
3	45.1	45.2	3'	49.7	49.0
5	59.6	59.7	5'	54.0	52.7
6	19.2	19.4	6'	20.5	20.2
7	110.1	110.3	7'	108.8	108.5
8	129.6	129.7	8'	128.2	128.2
9	117.4	117.5	9'	117.9	118.2
10	118.9	119.0	10'	119.2	119.5
11	121.6	121.7	11'	138.6	139.3
12	109.8	109.9	12'	109.1	109.2
13	135.9	136.0	13'	134.6	134.9
14	38.9	38.9	14'	26.3	26.0
15	33.5	33.6	15'	31.9	29.0
16	47.0	47.0	16'	41.2	40.0
17	-	-	17'	34.0	34.1
18	12.2	12.3	18'	11.8	22.7
19	118.6	118.8	19'	27.7	71.5
20	137.6	137.6	20'	41.8	42.5
21	52.3	52.4	21'	57.5	54.6
N(4)-Me	42.2	42.4	N(4)-Me'	-	-
CO_2Me	171.7	171.8	*C*O_2Me'	-	-
CO_2*Me*	49.8	49.9	CO_2*Me*'	-	-

[a]$CDCl_3$, 100 MHz; assignments based on HSQC and HMBC.

Table 2.47: ^{1}H NMR Spectroscopic Data (δ) of Ervahaimines A (**69**) and B (**70**)

H	**69**^{a} (*J*/Hz)	**70**^{b} (*J*/Hz)	**H**	**69**^{a} (*J*/Hz)	**70**^{b} (*J*/Hz)
3	4.64 dd (13, 3)	4.64 dd (13, 3)	3'	-	-
			3'	-	-
5	4.12 t (7)	4.06 t (9)	5'	3.18 m	3.24 m
			5'	4.45 m	4.50 m
6	3.26 dd (15, 8)	3.24 m	6'	3.15 m	3.12 m
6	3.49 m	3.53 dd (14, 11)	6'	3.15 m	3.12 m
9	7.56 m	7.56 m	9'	7.38 d (8)	7.31 s
10	7.09 m	7.07 m	10'	7.00 dd (8, 2)	-
11	7.09 m	7.07 m	11'	-	6.95 dd (8, 1)
12	7.09 m	7.07 m	12'	6.99 s	7.13 d (8)
14	1.94 m	1.93 m	14'	2.55 m	2.56 m
14	2.66 m	2.56 m			
15	3.78 m	3.77 m	15'	1.34 m	1.35 m
			15'	1.94 m	1.93 m
16	2.73 dd (2)	2.74 m	16'	-	-
17	-	-	17'	2.18 dt (13, 4)	2.22 dt (14, 2)
			17'	2.58 m	2.56 m
18	1.66 dd (7, 2)	1.65 d (7)	18'	0.96 t (7)	0.96 t (7)
19	5.33 q (7)	5.33 q (7)	19'	1.41 m	1.41 m
			19'	1.50 dq (14, 7)	1.51 m
20	-	-	20'	1.73 m	1.71 m
21	2.92 d (14)	2.93 d (14)	21'	4.61 s	4.47 s
21	3.78 m	3.77 m			
N(4)-Me	2.60 s	2.62 s	N(4)-Me'	-	-
CO_2*Me*	2.47 s	2.47 s	CO_2*Me*'	3.73 s	3.69 s
N(1)-H	7.49 s	7.60 s	N(1)-H'	7.90 s	8.09 s

^{a}$CDCl_3$, 600 MHz; ^{b}$CDCl_3$, 400 MHz; assignment based on COSY, HSQC, and NOESY.

Table 2.48: ^{13}C NMR Spectroscopic Data (δ) of Ervahaimines A (**69**) and B (**70**)

C	**69**[a]	**70**[b]	**C**	**69**[a]	**70**[b]
2	137.1	137.2	2'	134.0	134.5
3	45.2	45.3	3'	175.7	175.8
5	59.8	59.7	5'	42.6	42.5
6	19.4	19.3	6'	21.1	21.1
7	110.3	110.0	7'	109.3	109.3
8	129.7	129.8	8'	126.6	127.9
9	117.6	117.5	9'	118.7	117.0
10	119.1	118.9	10'	119.9	137.4
11	121.8	121.6	11'	140.4	122.4
12	110.0	110.0	12'	109.5	111.1
13	136.0	136.1	13'	135.9	134.6
14	38.9	38.8	14'	38.1	38.0
15	33.6	33.5	15'	30.9	31.0
16	46.9	47.0	16'	55.5	55.6
17	-	-	17'	35.8	35.9
18	12.4	12.4	18'	11.3	11.3
19	118.9	119.0	19'	27.6	27.6
20	137.6	137.4	20'	35.4	35.4
21	52.3	52.4	21'	56.1	56.1
N(4)-Me	42.3	42.3	N(4)-Me'	-	-
CO_2Me	171.7	171.7	*C*O_2Me'	172.9	172.9
CO_2*Me*	50.0	50.0	CO_2*Me*'	53.0	53.0

[a]$CDCl_3$, 150 MHz; [b]$CDCl_3$, 100 MHz; assignments based on HSQC and HMBC.

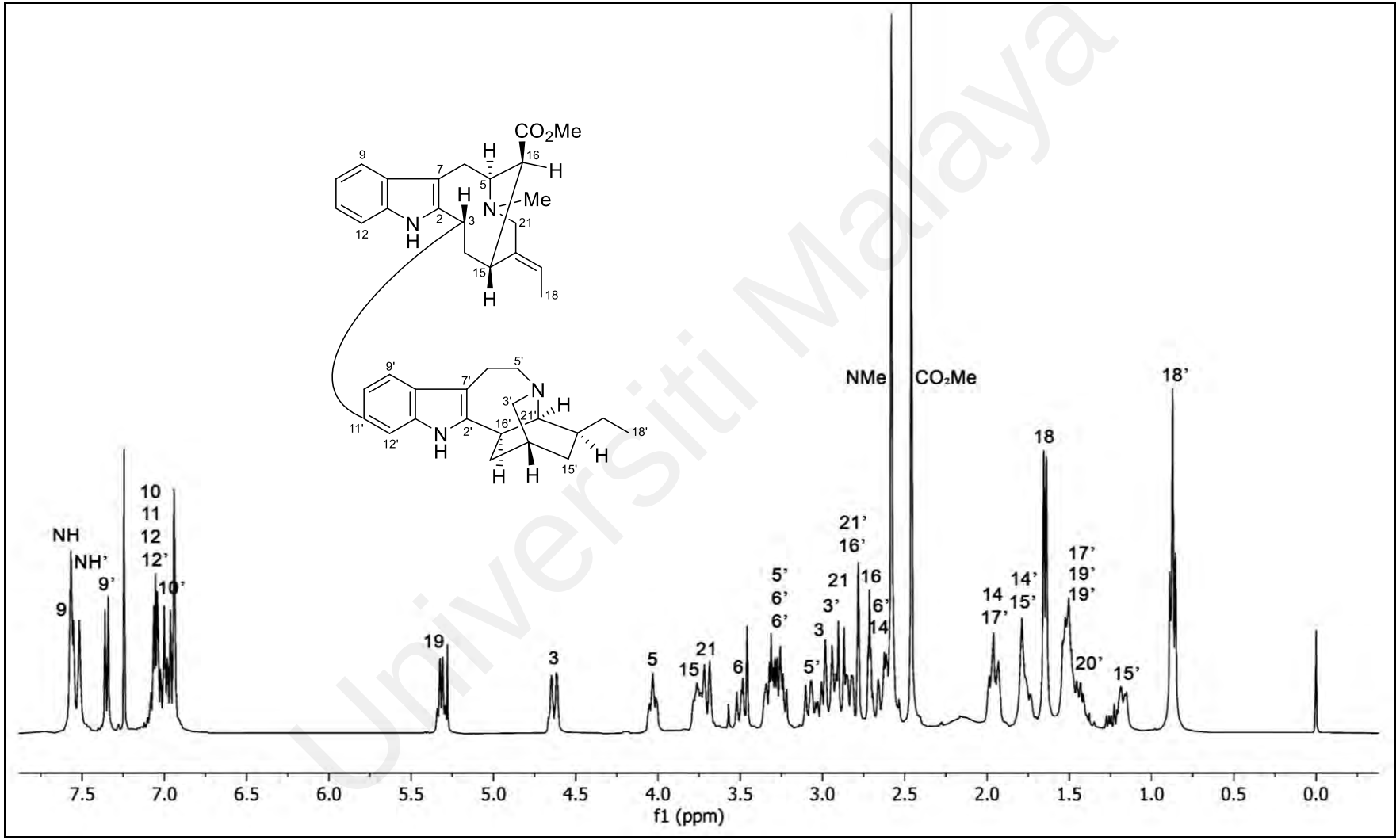


Figure 2.126: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Tabernamine (**67**)

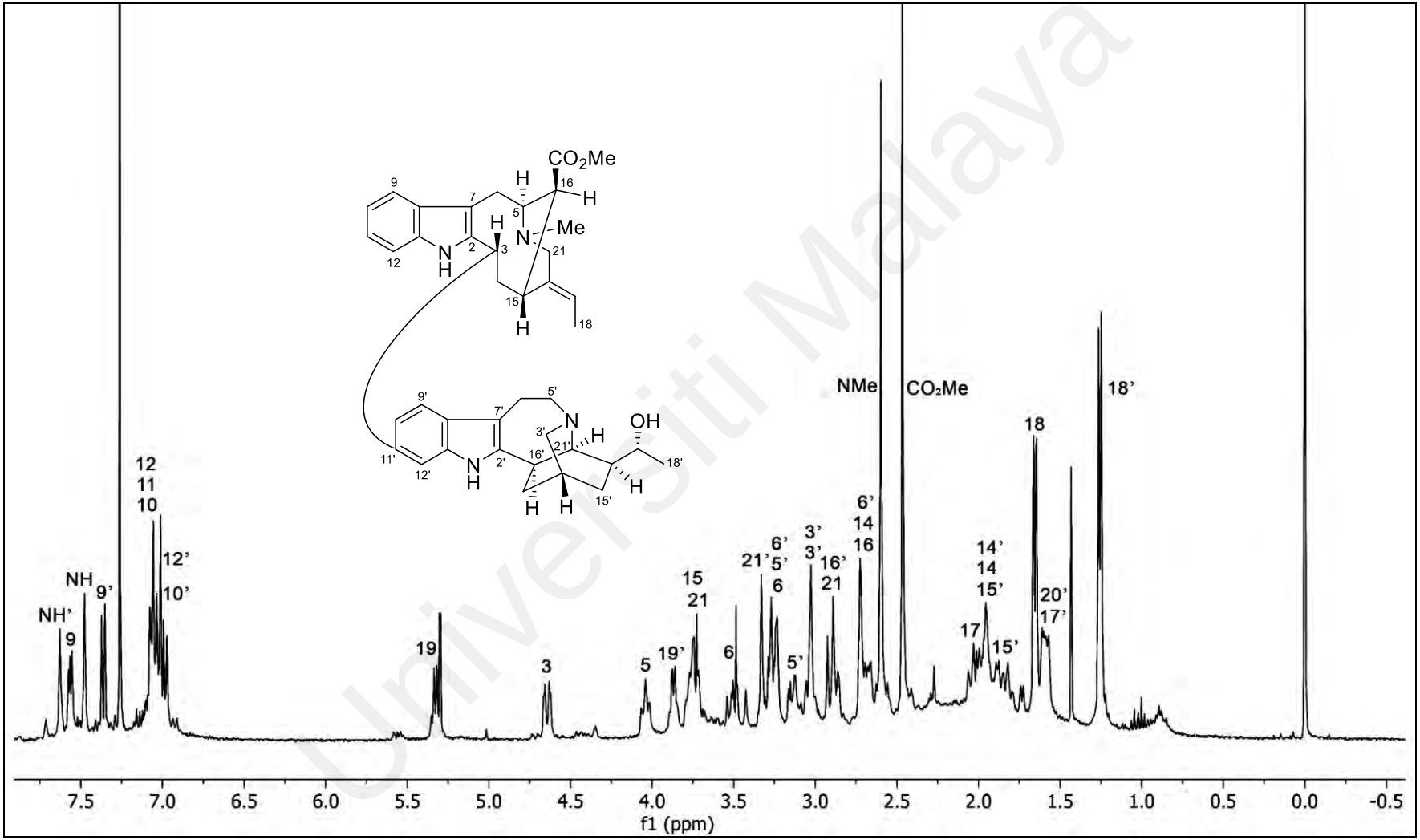


Figure 2.127: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of 19'(*R*)-Hydroxytabernamine (**68**)

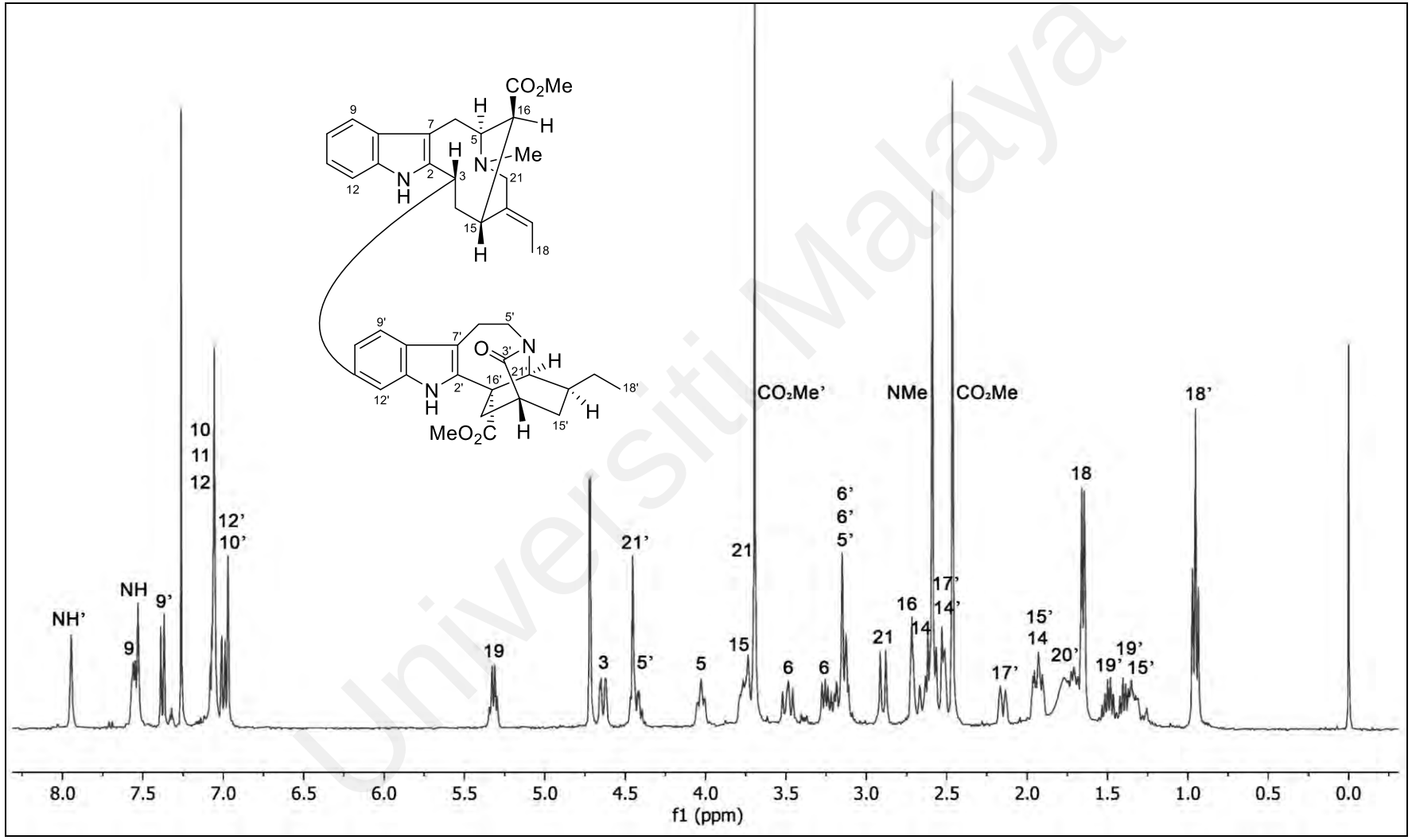


Figure 2.128: ^{1}H NMR Spectrum ($CDCl_3$, 600 MHz) of Ervahaimine A (**69**)

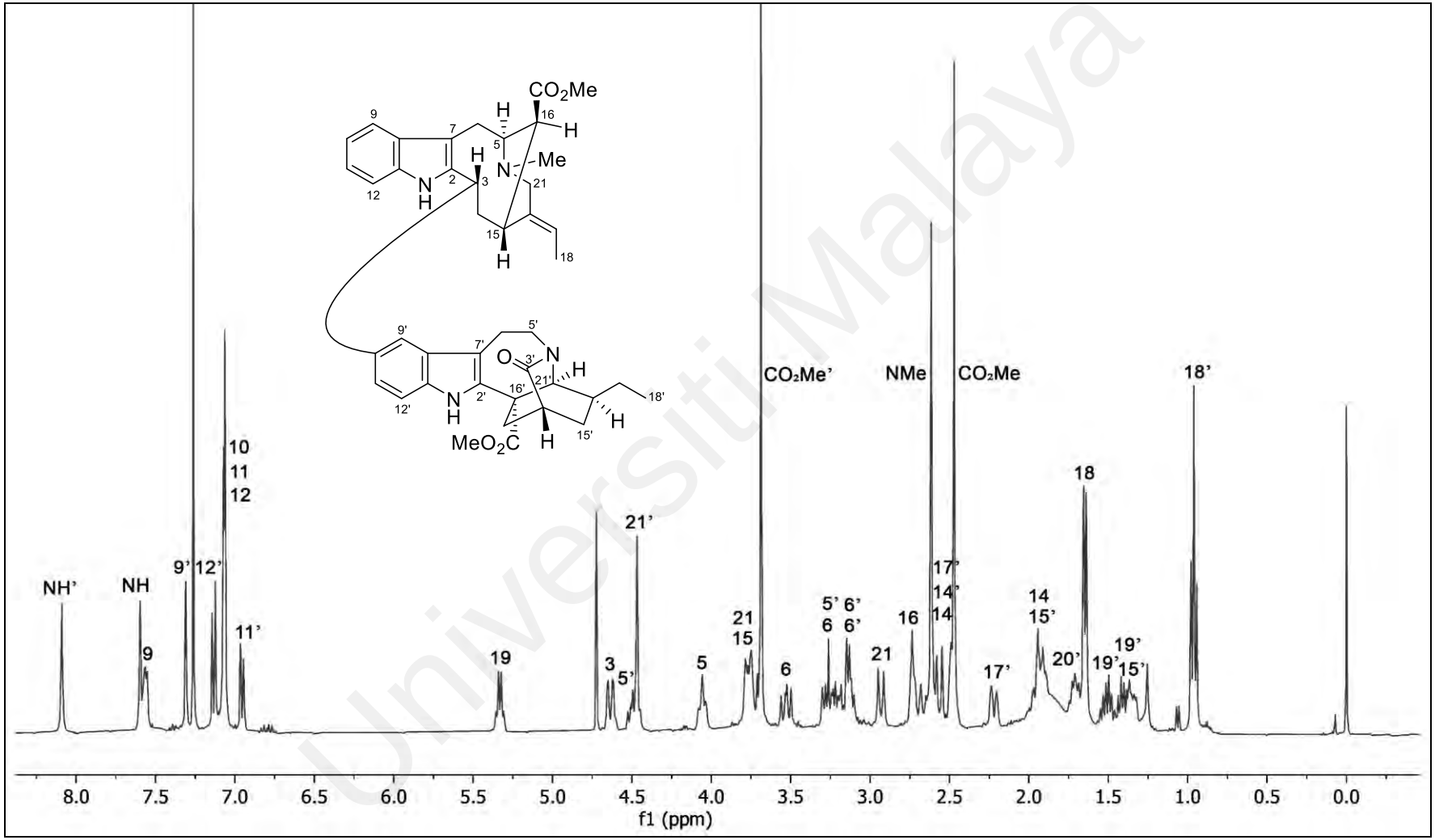


Figure 2.129: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Ervahaimine B (**70**)

Table 2.49: ^{1}H NMR Spectroscopic Data (δ) of Conophylline (**71**) and Conophylline quinone (**72**)[a]

H	**71** (*J*/Hz)	**72** (*J*/Hz)	**H**	**71** (*J*/Hz)	**72** (*J*/Hz)
3	4.81 d (8)	4.82 d (8)	3'	2.98 d (13)	2.93 d (13)
			3'	3.60 d (13)	3.59 d (13)
5	2.88 m	2.72 m	5'	2.88 m	2.72 m
5	2.99 m	3.07 m	5'	3.07 m	3.07 m
6	1.68 m	1.73 dd (12, 4)	6'	1.68 m	1.68 dd (12, 4)
6	2.00 td (12, 6)	2.08 m	6'	2.09 td (12, 7)	2.06 m
9	5.55 s	4.99 s	9'	7.14 s	7.06 s
12	-	-	12'	6.34 s	6.33 s
14	5.06 dd (8, 4)	5.06 dd (8, 4)	14'	3.26 d (4)	3.25 d (4)
15	4.15 dd (11, 4)	4.14 d (4)	15'	3.11 d (4)	3.13 d (4)
17	2.40 d (16)	2.69 d (16)	17'	2.53 d (16)	2.51 d (16)
17	2.74 br d (16)	2.97 br d (16)	17'	2.74 d (16)	2.75 br d (16)
18	0.71 t (8)	0.81 t (8)	18'	0.79 t (8)	0.90 t (8)
19	0.85 dq (14, 8)	0.81 m	19'	1.18 m	1.26 m
19	1.18 m	1.16 dq (14, 8)	19'	1.18 m	1.28 m
21	2.56 br s	2.37 br s	21'	2.60 br s	2.47 br s
10-OH	5.26 s	-	-	-	-
11-OMe	3.83 s	4.17 s	-	-	-
12-OMe	3.86 s	3.87 s	-	-	-
CO_2*Me*	3.78 s	3.89 s	CO_2*Me*'	3.79 s	3.78 s
N(1)-H	8.79 br s	-	N(1)-H'	9.00 br s	9.02 br s

[a]$CDCl_3$, 400 MHz; assignment based on COSY, HSQC, and NOESY.

Table 2.50: ^{13}C NMR Spectroscopic Data (δ) of Conophylline (**71**) and Conophylline quinone (**72**)[a]

C	71	72	C	71	72
2	164.3	164.6	2'	165.1	163.6
3	59.4	59.4	3'	49.2	49.5
5	45.8	45.8	5'	50.9	51.1
6	41.7	40.1	6'	44.2	44.4
7	54.7	53.1	7'	54.3	54.1
8	133.4	154.3	8'	130.8	131.1
9	104.0	118.0	9'	119.2	119.1
10	143.5	182.8	10'	113.7	112.7
11	138.7	145.3	11'	160.9	161.0
12	136.7	144.0	12'	93.0	92.9
13	128.6	166.4	13'	144.9	145.9
14	85.0	84.7	14'	52.0	52.3
15	69.4	69.1	15'	56.2	56.3
16	90.5	121.6	16'	91.2	92.0
17	22.1	27.1	17'	23.3	23.3
18	7.3	7.6	18'	7.3	7.4
19	26.3	27.1	19'	26.6	26.9
20	44.7	48.8	20'	36.9	37.1
21	65.1	65.6	21'	71.6	72.1
11-OMe	60.8	61.1	-	-	-
12-OMe	60.3	61.3	-	-	-
CO_2Me	168.7	166.4	*C*O_2Me'	168.6	168.8
CO_2*Me*	51.0	53.1	CO_2*Me*'	50.8	51.1

[a]$CDCl_3$, 100 MHz; assignments based on HSQC and HMBC.

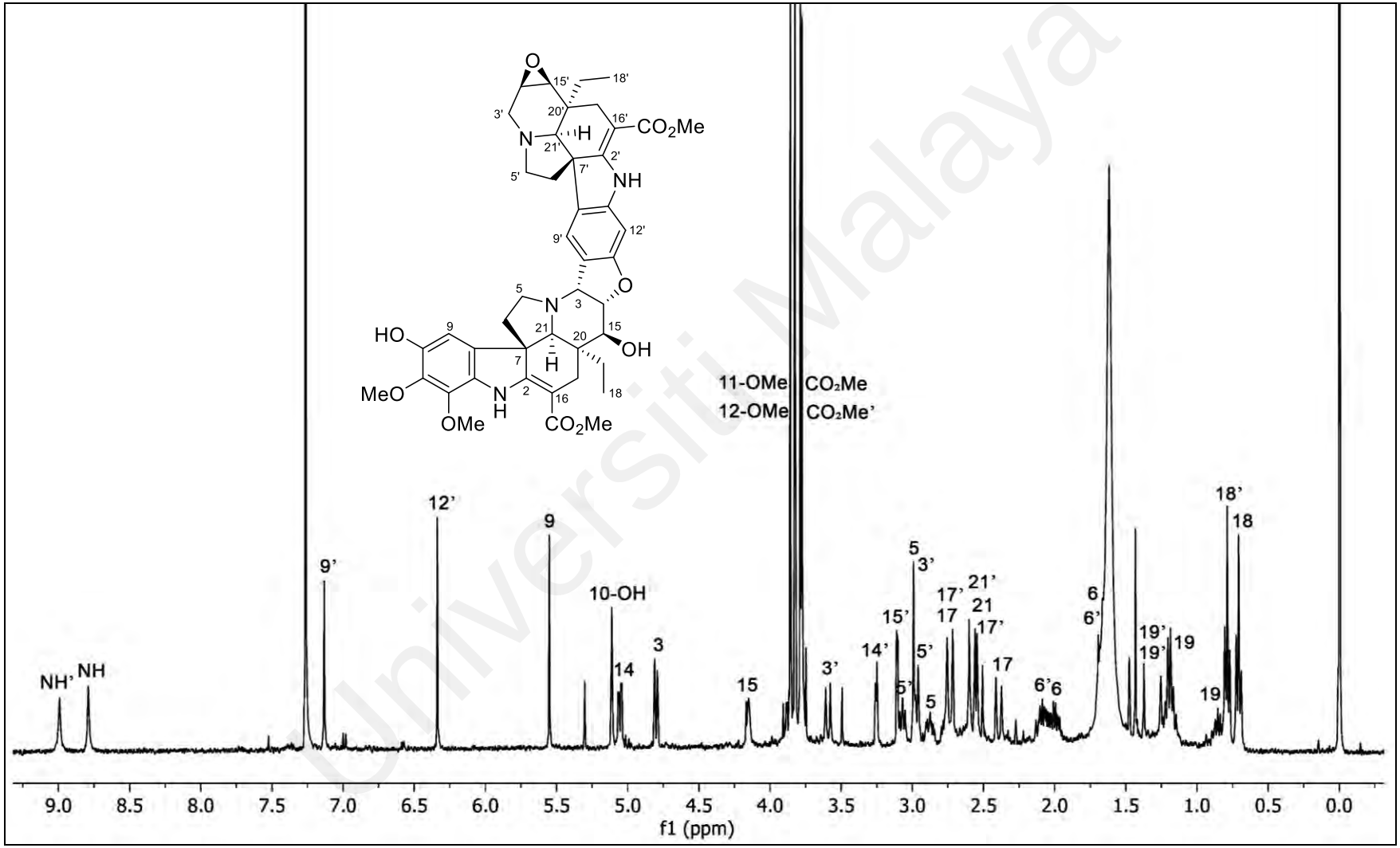


Figure 2.130: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Conophylline (**71**)

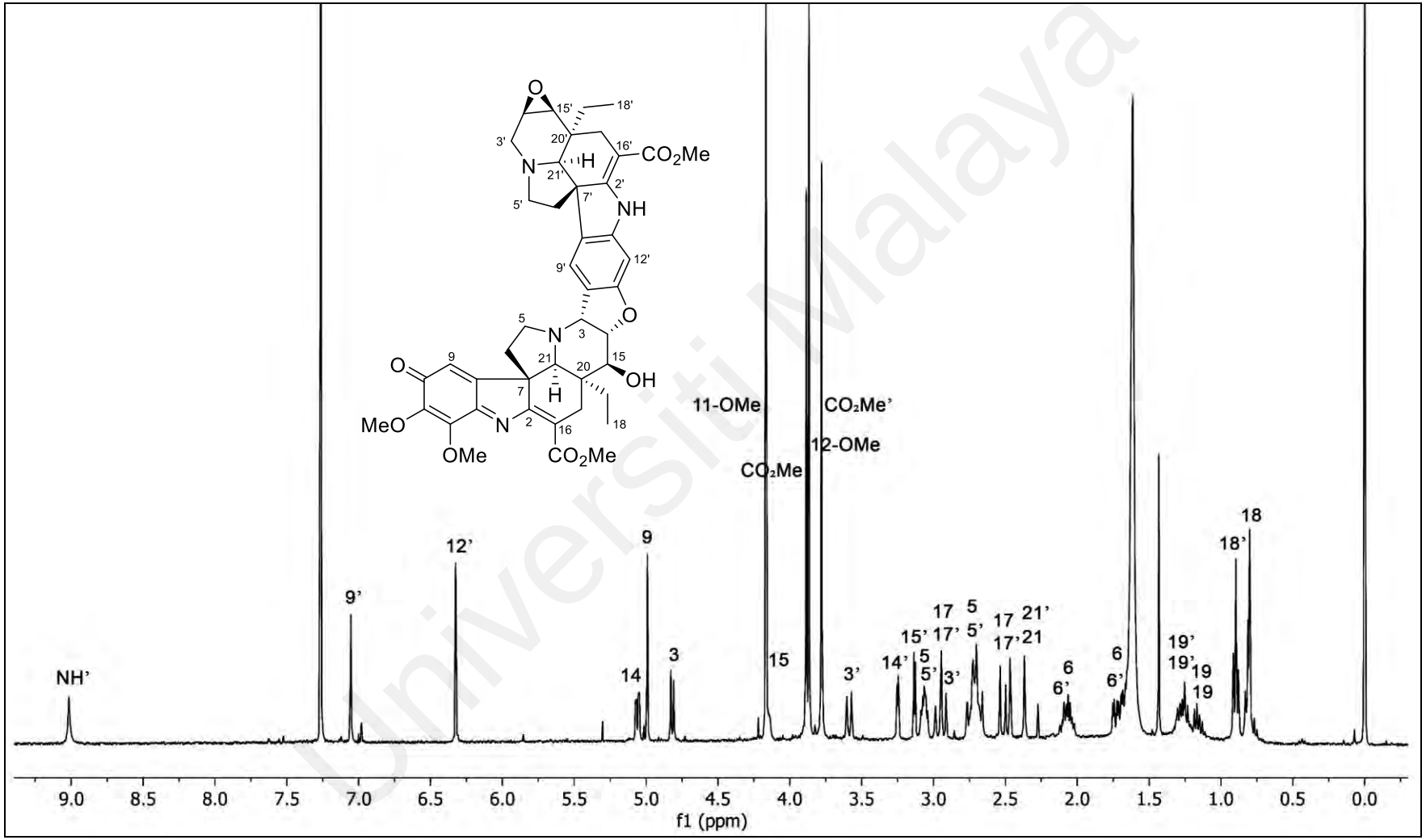


Figure 2.131: ^{1}H NMR Spectrum ($CDCl_3$, 400 MHz) of Conophylline quinone (**72**)

2.2 Comparison of Alkaloid Composition of *T. polyneura* from Fraser's Hill, Pahang (Sample A) and from Genting Sempah, Selangor (Sample B)

The present investigation of the bark and leaves of *T. polyneura* yielded a total of 72 alkaloids, of which 16 are new (**1**–**10**, **30**, **33**–**35**, **54**, **66**). The monomeric alkaloids are constituted of 10 different skeletal types, which include twenty nine iboga (**1**–**29**), three chippiine (**30**–**32**), twenty one corynanthean (**33**–**53**), one cleavamine (**54**), three quebrachamine (**55**–**57**), one vallesiachotaman (**58**), one vincamine (**59**), four aspidospermatan (**60**–**63**), one simple *β*-carboline (**64**), and one other skeleton (**65**), as well as five vobasinyl-iboga bisindole (**66**–**70**) and two aspidosperma-aspidosperma bisindole (**71**–**72**) alkaloids. Among the alkaloids obtained, two alkaloids, *viz.*, coronaridine (**14**) and vobasine (**37**), were isolated in both the bark and leaves extracts of *T. polyneura*.

A comparison of the alkaloids isolated from the results (Sample A, Fraser's Hill, Pahang, Peninsular Malaysia) with those from a previous sample collected from a different location (Sample B, Genting Sempah, Selangor, Peninsular Malaysia) revealed a significant variation in alkaloid composition. Both sets of samples primarily yielded monomeric indole alkaloids of the iboga- and vobasine-types. Vobasine was found to be the major compound in both samples, despite their different locations and collection years.

The alkaloids which were found common in both studies include eight iboga (**14**, **16**–**19**, **22**, **23**, **29**), seven corynanthean (**37**–**41**, **43**, **47**), one quebrachamine (**55**), one aspidospermatan (**60**), and one aspidosperma-aspidosperma bisindole (**71**) alkaloids. Some compounds, such as eglandine (**432**), vobasinol (**209**), 16-*epi*-vobasenal (**198**), anhydrovobasindiol (**212**), 3,14-dihydroellipticine (**76**), apparicine (**272**), and polyervinine (**859**), were present in Sample B but absent in Sample A. Conversely, a

total of 54 alkaloids (48 monomeric and 6 bisindole alkaloids) were obtained in Sample A but not found in Sample B. In terms of the new alkaloids, the bark extract of the present sample yielded a variety of skeletal types (**1**–**10**, **30**, **33**–**35**, **54**, **66**) (Tang *et al.*, 2023), whereas the stem bark extract of the previous sample only yielded two new vobasine (**43**, **198**) and two new iboga alkaloids (**18**, **22**) (Clivio, Richard, Hadi *et al.*, 1990).

Table 2.51: Comparison of the alkaloid composition of *T. polyneura* from Peninsular Malaysia (Sample A, Fraser's Hill, Pahang) and *E. polyneura* from an earlier study (Sample B, Genting Sempah, Selangor)

Alkaloids	**Sample A**		**Sample B** (Clivio, Richard, Hadi *et al.*, 1990; Clivio, Guillaume *et al.*, 1995)	
	Bark	**Leaves**	**Stem-bark**	**Leaves**
Iboga				
Polyneurine A (**1**) (new)	+			
Polyneurine B (**2**) (new)	+			
Polyneurine C (**3**) (new)	+			
Polyneurine D (**4**) (new)	+			
Polyneurine E (**5**) (new)	+			
Polyneurine F (**6**) (new)	+			
Polyneurine G (**7**) (new)	+			
Polyneurine H (**8**) (new)	+			
Polyneurine J (**9**) (new)	+			
Polyneurine K (**10**) (new)	+			
Ibogamine (**11**)	+			
19(*S*)-Hydroxyibogamine (**12**)	+			
19(*R*)-Hydroxyibogamine (**13**)	+			
Coronaridine (**14**)	+	+	+	
(–)-Albifloranine (**15**)	+			
(–)-Heyneanine (**16**)	+		+	
19-*Epi*-heyneanine (**17**)	+		+	
3-Oxo-19-*epi*-heyneanine (**18**)	+		+	
3-Oxo-coronaridine (**19**)	+		+	
3(*S*)-Cyanocoronaridine (**20**)	+			
Ervatamine G (**21**)	+			
3-Hydroxy-3,4-*seco*coronaridine (**22**)	+		+	
Voacangine (**23**)	+		+	
Voacristine (**24**)		+		
Conopharyngine (**25**)		+		
19(*S*)-Hydroxy-conopharyngine (**26**)		+		

Table 2.51, continued

Alkaloids	**Sample A**		**Sample B** (Clivio, Richard, Hadi *et al.*, 1990; Clivio, Guillaume *et al.*, 1995)	
	Bark	**Leaves**	**Stem-bark**	**Leaves**
Coronaridine pseudoindoxyl (**27**)	+			
Ibogamine 7(*S*)-hydroxyindolenine (**28**)	+			
Coronaridine-7-hydroxyindolenine (**29**)	+		+	
Eglandine (**432**)			+	
Chippiine				
Polyneurine I (**30**) (new)	+			
10,11-Demethoxychippiine (**31**)	+			
3-Methoxy-10,11-demethoxychippiine (**32**)	+			
Corynanthean				
Vobasine-subtype				
Polyneurine M (**33**) (new)	+			
Polyneurine N (**34**) (new)	+			
Polyneurine O (**35**) (new)	+			
3-*Epi*-vobasinol (**36**)	+			
Vobasine (**37**)	+	+	+	+
Vobasine *N*(4)-oxide (**38**)	+			+
16-*Epi*-vobasine (**39**)	+		+	
Perivine (**40**)	+		+	
Dregamine (**41**)	+		+	+
Tabernaemontanine (**42**)	+			
Vobasenal (**43**)	+		+	+
Vobasidine D (**44**)	+			
Vobasidine E (**45**)		+		
Vobasidine F (**46**)	+			
Vobasinol (**209**)			+	
16-*Epi*-vobasenal (**198**)			+	
Anhydrovobasindiol (**212**)			+	
Sarpagine-subtype				
Pericyclivine (**47**)	+		+	
16-*Epi*-voacarpine (**48**)	+			
Ervatamine-subtype				
19,20-Dehydroervatamine (**49**)	+			
Corynantheine-subtype				
16(*R*)-Sitsirikine (**50**)	+			
16(*R*)-19,20-*E*-isositsirikine (**51**)	+			
16(*R*)-19,20-*Z*-isositsirikine (**52**)	+			
Fluorocarpamine (**53**)	+			
Cleavamine				
Polyneurine L (**54**) (new)	+			

Table 2.51, continued

Alkaloids	**Sample A**		**Sample B** (Clivio, Richard, Hadi *et al.*, 1990; Clivio, Guillaume *et al.*, 1995)	
	Bark	**Leaves**	**Stem-bark**	**Leaves**
Quebrachamine				
Voaphylline (**55**)	+		+	
Voaphylline-7-hydroxyindolenine (**56**)	+			
Voaphyllinediol (**57**)	+			
Vallesiachotamine				
Antirhine (**58**)	+			
Vincamine				
14,15-Dehydro-16-*epi*-vincamine (**59**)	+			
Aspidospermatan				
Tubotaiwine (**60**)	+		+	
Tubotaiwine *N*(4)-oxide (**61**)		+		
N(4)-Chloromethyl-tubotaiwine chloride (**62**)	+			
Janetine (**63**)		+		
3,14-Dihydroellipticine (**76**)			+	
Simple β-carboline				
Harmane (**64**)		+		
Others				
Taberdivamine B (**65**)	+			
Apparicine (**272**)			+	
Bisindole				
Polyneurine P (**66**) (new)	+			
Tabernamine (**67**)	+			
19'(*R*)-Hydroxytabernamine (**68**)	+			
Ervahaimine A (**69**)	+			
Ervahaimine B (**70**)	+			
Conophylline (= polyervine) (**71**)		+		+
Conophylline quinone (**72**)		+		
Polyervinine (**859**)				+

The observed variations in alkaloid composition may be attributed to several factors as follows.

(i) Variation in sample sizes can be a significant factor. In the earlier study (Clivio, Richard, Hadi *et al.*, 1990), 5.0 kg of dried stem-bark and 2.2 kg of dried leaves were collected, whereas the present study employed 11.9 kg of dried bark and 11.1

kg of dried leaves. The larger sample sizes in the present investigation enable a more thorough assessment of alkaloid content within the plant species. Conversely, the smaller sample sizes in the earlier study may have yielded less representative data.

(ii) While both specimens underwent alkaloid extraction, variations in solvent choice and extraction protocols can contribute to differences in alkaloid profiles. In the earlier study (Clivio, Richard, Hadi *et al.*, 1990), the stem-bark and leaves were initially wetted with ammonium hydroxide, followed by maceration in ethyl acetate, and subsequently lixiviation before extraction with 2% sulfuric acid in the usual manner. Conversely, in the present study, the dried bark and leaves underwent direct extraction with methanol, followed by partitioning the methanol extract with 3% tartaric acid in the standard manner.

(iii) Geographic variation encompasses diverse environmental conditions, including sunlight exposure, temperature, and soil composition, which can modulate the alkaloid biosynthesis in plant (Yang *et al.*, 2018).

(iv) The growth and developmental stage of the plant at the time of collection can also influence alkaloid content (Li *et al.*, 2020).

2.3 Biological Activity

2.3.1 Cytotoxicity

Cancer is an important health-care issue. It is one of the leading causes of human morbidity and mortality that can be caused by external factors (radiations, smoking, infectious agents *etc.*) and internal factors (genetic mutations, hormonal disorders *etc.*) (Iqbal *et al.*, 2017). Cancers are characterized by the growth of uncontrolled proliferation of abnormal cells, and are usually treated by surgery, radiotherapy, chemotherapy or combination thereof (Iqbal *et al.*, 2017). However, it remains challenging as treatment methods or chemotherapeutic agents often impose harmful side effects to human body due to high toxicity and low specificity (Iqbal *et al.*, 2017). Therefore, the discovery of phytochemicals and development of new anticancer drugs with minimal side effects as well as better selectivity and efficacy are of great importance in the cancer research.

As part of our ongoing search of bioactive compounds from plants, the alkaloids obtained from this study were screened for their cytotoxic effects against several human cancer cell lines (HT-29, HCT 116, MDA-MB-231, A549, PC-3, and MCF7), as well as normal human colon fibroblast (CCD-18Co). The results are summarized in Table 2.52.

The monomeric indole alkaloids tested were found to be inactive against the human cancer cell lines (IC_{50} > 10 μM). Only the bisindole alkaloids (**66**–**70**) displayed pronounced growth inhibitory activity (IC_{50} 0.34–9.02 μM) against HT-29, HCT 116, MDA-MB-231, A549, and MCF7 cancer cells. While prior investigations assessed the effects of tabernamine (**67**) and 19'(*R*)-hydroxytabernamine (**68**) on KB cells (Nge, Chong *et al.*, 2016), as well as examining tabernamine (**67**)'s impact on A549 and MCF7 cancer cells (Cai *et al.*, 2018). Notably, the current cytotoxic screening presents

novel findings as it encompasses a broader spectrum of human cancer cell lines, thereby advancing the evidence supporting the therapeutic potential of these compounds. Furthermore, bisindoles **66**–**70** exhibited substantial selectivity, as evident from their strong cytotoxicity towards the human colorectal cancer cell line (HT-29) without appreciable effects in the normal human colon fibroblast (CCD-18Co).

Table 2.52: Cytotoxic Effects of Alkaloids Isolated from *T. polyneura*[a]

Compound	IC_{50}, μM						
	HT-29	**HCT 116**	**MDA-MB-231**	**A549**	**PC-3**	**MCF7**	**CCD-18Co**
Iboga							
Polyneurine A (**1**) (new)	>10	>10	>10	>10	>10	>10	>10
Polyneurine B (**2**) (new)	>10	>10	>10	>10	>10	>10	>10
Polyneurine F (**6**) (new)	>10	>10	>10	>10	>10	>10	>10
Polyneurine G (**7**) (new)	>10	>10	>10	>10	>10	>10	>10
Polyneurine H (**8**) (new)	>10	>10	>10	>10	>10	>10	>10
Polyneurine J (**9**) (new)	>10	>10	-	-	-	-	>10
(–)-Albifloranine (**15**)	>10	>10	-	-	-	>10	-
Vobasine							
Polyneurine M (**33**) (new)	>10	>10	-	-	-	-	>10
Sarpagine							
16-*Epi*-voacarpine (**48**)	>10	>10	-	-	-	>10	-
Other							
Taberdivamine B (**65**)	>10	>10	-	-	-	-	>10
Bisindole							
Polyneurine P (**66**) (new)	1.95	8.63	>10	>10	>10	>10	>10
Tabernamine (**67**)	0.34	4.18	5.58	-	>10	-	>10
19'(*R*)-Hydroxytabernamine (**68**)	1.09	4.31	3.18	7.22	>10	-	>10
Ervahaimine A (**69**)	0.96	9.02	>10	>10	>10	8.59	>10
Ervahaimine B (**70**)	0.57	>10	>10	>10	>10	-	>10

Table 2.52, continued

Compound	IC_{50}, μM						
	HT-29	**HCT 116**	**MDA-MB-231**	**A549**	**PC-3**	**MCF7**	**CCD-18Co**
Control							
Doxorubicin	0.57	0.31	1.16	8.35		3.24	
Cisplatin					9.07		9.30

[a]HT-29: human colorectal adenocarcinoma; HCT 116: human colorectal carcinoma; MCF7 and MDA-MB-231: human breast adenocarcinoma; A549: human lung carcinoma; PC-3: human prostate adenocarcinoma; CCD-18Co: normal human colon fibroblast.

CHAPTER 3: EXPERIMENTAL

3.1 Source and Authentication of Plant Materials

The bark and leaves of *T. polyneura* (King & Gamble) D.J.Middleton (Apocynaceae) were collected in June 2016 in Fraser's Hill, Pahang, Malaysia (3.7249° N, 101.7143° E). The plant was identified by Dr. Kien-Thai Yong (Institute of Biological Sciences, Universiti Malaya). A voucher specimen (KLU49438) was deposited at the Herbarium, Universiti Malaya.

3.2 General

Melting points were determined on an Electrothermal IA9100 digital melting point apparatus and were uncorrected. Optical rotations were measured on a JASCO P-1020 automatic digital polarimeter. UV spectra were obtained on a Shimadzu UV-2600 spectrophotometer. IR spectra were recorded on a Perkin-Elmer RX1 FT-IR, Spectrum 400 FT-IR/FT-FIR or Perkin-Elmer Frontier FT-IR spectrophotometer. HRDART-MS was recorded on a JEOL Accu TOF-DART mass spectrometer, and HRESIMS were obtained on an Agilent LC HR QTOF System Model G6530A or Agilent Technologies 6550 iFunnel Q-TOF LC/MS. 1D and 2D NMR spectra were recorded in $CDCl_3$ using tetramethylsilane (TMS) as internal standard on JEOL JNM (ECA 400 MHz) or Bruker Avance III (400 or 600 MHz) spectrometers and using a 1.7 mm microprobe for compound **5**. Coupling constants (J) are reported in Hz and chemical shifts (δ) in ppm. ECD spectra were obtained using a JASCO J-810 or JASCO J-815 circular dichroism spectrometer. All solvents used (chloroform, dichloromethane, ethyl acetate, methanol, ethanol, hexane, and petroleum ether) were distilled prior to use except diethyl ether.

The acetylation reaction was carried out under N_2, in oven-dried glassware. Dichloromethane and pyridine were distilled from CaH_2 and stored in 4Å molecular sieves, while acetic anhydride was distilled and stored in 4Å molecular sieves, prior to use.

3.3 X-ray Diffraction Analysis

X-ray diffraction analyses were carried out on a Rigaku Oxford (formerly Agilent Technologies) SuperNova Dual diffractometer with Cu Kα (λ = 1.54184 Å) or Mo Kα (λ = 0.71073 Å) radiation at room temperature. Using Olex2, the structures were solved by SHELXT-2018/2 structure solution program using Intrinsic Phasing and refined with SHELXT-2018/3 refinement package using Least Square minimization. All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were placed in idealized positions and refined as riding atoms with the relative isotropic parameters. The absolute configurations were determined on the basis of Flack parameter (Flack, 1983; Flack & Bernardinelli, 2000; Parsons *et al.*, 2013) and corroborated by use of the Hooft parameter (Hooft *et al.*, 2008 & 2010). Crystallographic data for compounds **2** and **6** had been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained, free of charge, on application to the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [fax: +44 (0)1223-336033, or e-mail: deposit@ccdc.cam.ac.uk].

3.4 Computational Method

A conformational search was performed by Spartan'14 software (*Spartan'14*, 2014) using the MMFF94 force field. Conformers occurring within a 5 kcal mol^{-1} energy window from the global minimum were then imported into the Gaussian 09 software (Frisch *et al.*, 2010) for geometry optimization and frequency calculation at DFT level using B3LYP/6-31G(d) or *ω*B97X-D/def2-TZVP (imported from Basis Set Exchange) (Bruhn *et al.*, 2017). TDDFT ECD calculations were performed on the optimized conformers at the B3LYP/6-311G++(d,p), *ω*B97X-D/6-311G++(d,p) or *ω*B97X-D/def2-TZVP (imported from Basis Set Exchange) (Bruhn *et al.*, 2017) level using a PCM solvation model for MeOH. The ECD spectrum for each optimized conformer was weighted by Boltzmann distribution, and the overall ECD curves were produced by SpecDis (version 1.64) software (Bruhn *et al.*, 2015) after UV correction. Gauge-Including Atomic Orbital (GIAO) NMR calculations were performed on the B3LYP/6-31G(d)-optimized conformers at the mPW1PW91/6-31+G(d,p) level with PCM solvation model for $CHCl_3$. The Boltzmann-averaged magnetic shielding tensors were converted into chemical shifts (ppm) with TMS as the reference standard (Willoughby *et al.*, 2014 & 2020). The DP4+ calculations were carried out using the Excel spreadsheet provided by the Sarotti group (Grimblat *et al.*, 2015).

3.5 Chromatographic Methods

3.5.1 Column Chromatography

Fractionation and isolation of alkaloids were carried out by flash column chromatrography. It was done using silica gel (Merck 9385, 230–400 mesh ASTM or Friendemann Schmidt silica gel 60, 0.04–0.06 mm). For crude samples, the ratio of silica gel to sample was approximately 30:1, whereas for semi-pure fractions, the ratio was around 100:1. The gel was made into a slurry with the chosen starting solvent before it was packed onto the column. Then the column was allowed to equilibrate. Next, the sample was loaded either by wet or dry packing method. For wet loading, the sample was directly dissolved and loaded onto the column. For dry packing, the sample was pre-adsorbed on silica prior to being loaded onto the column (the weight of silica gel is approximately three times the weight of the sample). During elution, the polarity of the mobile phase was gradually increased. The process was monitored by thin layer chromatography (TLC), and fractions showing a similar profile were combined. The combined fractions were subjected to further separation by re-chromatography or preparative radial chromatography (Chromatotron) where necessary.

3.5.2 Gel Permeation Chromatography

Sephadex LH-20 or G-75 dried powder was allowed to swell overnight in methanol. The slurry was then poured onto the column and equilibrated for at least one hour at room temperature before use. To ensure a longer column lifespan, the sample was filtered through a 0.45 μm nylon membrane prior to use. The column can be

reconstituted by flushing and washing the gel with 2–3 column volumes of MeOH followed by re-equilibration.

3.5.3 Thin Layer Chromatography (TLC)

Thin layer chromatography (TLC) was routinely used: (i) for preliminary detection of alkaloids, (ii) to test and select a suitable solvent system for isolation, (iii) to monitor the isolation of alkaloids, and (iv) to check the purity of a compound. TLC was done on pre-coated 5 × 10 cm aluminium plates with 0.25 mm thickness of silica gel 60 F_{254} (Merck, Darmstadt, G.F.R.). The samples were loaded on the TLC plates using a fine glass capillary tube and subsequently developed in chromatographic tanks saturated with appropriate solvent system at room temperature. The alkaloidal spots were visualized by examining the TLC plates under UV light (short wave 254 nm), followed by spraying with Dragendorff's reagent that shows orange spots in the presence of alkaloids. The hR_f values of the alkaloids are tabulated in Table 3.1.

Table 3.1: The hR_f Values of Alkaloids Isolated from *Tabernaemontana polyneura*

Alkaloid	$CHCl_3$	EtOAc	Et_2O	$CHCl_3$/ MeOH (10:1)	EtOAc/ MeOH (10:1)
Polyneurine A (**1**)	52	58	64	79	60
Polyneurine B (**2**)	0	13	3	28	34
Polyneurine C (**3**)	0	43	4	45	54
Polyneurine D (**4**)	9	54	24	58	59
Polyneurine E (**5**)	0	54	59	78	67
Polyneurine F (**6**)	0	16	0	36	39
Polyneurine G (**7**)	0	26	7	41	45

Table 3.1, continued

Alkaloid	$CHCl_3$	EtOAc	Et_2O	$CHCl_3$/ MeOH (10:1)	EtOAc/ MeOH (10:1)
Polyneurine H (**8**)	4	53	22	62	59
Polyneurine J (**9**)	3	15	12	33	26
Polyneurine K (**10**)	1	8	4	22	12
Ibogamine (**11**)	8	48	60	46	55
19(*S*)-Hydroxyibogamine (**12**)	7	35	17	43	31
19(*R*)-Hydroxyibogamine (**13**)	6	19	18	29	28
Coronaridine (**14**)	57	75	83	93	79
(−)-Albifloranine (**15**)	9	47	33	63	54
(−)-Heyneanine (**16**)	20	53	43	86	64
19-*Epi*-heyneanine (**17**)	13	49	42	80	60
3-Oxo-19-*epi*-heyneanine (**18**)	3	23	3	42	51
3-Oxo-coronaridine (**19**)	0	60	44	82	52
3(*S*)-Cyanocoronaridine (**20**)	61	75	81	83	76
Ervatamine G (**21**)	22	64	66	71	65
3-Hydroxy-3,4-*seco*coronaridine (**22**)	4	53	51	49	57
Voacangine (**23**)	40	72	83	94	77
Voacristine (**24**)	14	49	26	70	60
Conopharyngine (**25**)	16	65	54	76	67
19(*R*)-Hydroxy-conopharyngine (**26**)	8	48	26	77	50
Coronaridine pseudoindoxyl (**27**)	5	26	14	36	36
Ibogamine 7(*S*)-hydroxyindolenine (**28**)	3	38	39	46	55
Coronaridine-7-hydroxyindolenine (**29**)	39	64	89	93	67
Polyneurine I (**30**)	0	14	9	36	27

Table 3.1, continued

Alkaloid	$CHCl_3$	EtOAc	Et_2O	$CHCl_3$/ MeOH (10:1)	EtOAc/ MeOH (10:1)
10,11-Demethoxychippiine (**31**)	8	22	15	49	27
3-Methoxy-10,11-demethoxychippiine (**32**)	5	35	34	66	49
Polyneurine M (**33**)	5	27	11	66	46
Polyneurine N (**34**)	0	7	0	17	22
Polyneurine O (**35**)	8	33	16	75	61
3-*Epi*-vobasinol (**36**)	0	12	7	29	29
Vobasine (**37**)	6	25	18	68	30
Vobasine *N*(4)-oxide (**38**)	0	0	0	7	0
16-*Epi*-vobasine (**39**)	13	42	39	73	46
Perivine (**40**)	1	11	6	39	16
Dregamine (**41**)	5	21	12	64	27
Tabernaemontanine (**42**)	11	42	37	73	49
Vobasenal (**43**)	1	12	0	46	21
Vobasidine D (**44**)	1	17	2	46	31
Vobasidine E (**45**)	0	35	6	51	45
Vobasidine F (**46**)	3	13	5	46	26
Pericyclivine (**47**)	1	31	19	32	38
16-*Epi*-voacarpine (**48**)	3	53	36	47	57
19,20-Dehydroervatamine (**49**)	4	22	16	54	40
16(*R*)-Sitsirikine (**50**)	1	49	23	55	51
16(*R*)-19,20-*E*-isositsirikine (**51**)	0	8	5	33	16
16(*R*)-19,20-*Z*-isositsirikine (**52**)	0	27	14	31	46
Fluorocarpamine (**53**)	3	8	5	60	28
Polyneurine L (**54**)	0	9	3	24	31
Voaphylline (**55**)	40	60	72	72	69

Table 3.1, continued

Alkaloid	$CHCl_3$	EtOAc	Et_2O	$CHCl_3$/ MeOH (10:1)	EtOAc/ MeOH (10:1)
Voaphylline-7-hydroxyindolenine (**56**)	1	8	7	25	15
Voaphyllinediol (**57**)	1	21	14	22	36
Antirhine (**58**)	0	3	0	14	7
14,15-Dehydro-16-*epi*-vincamine (**59**)	5	40	32	56	48
Tubotaiwine (**60**)	0	5	4	46	9
Tubotaiwine *N*(4)-oxide (**61**)	0	3	0	29	4
N(4)-Chloromethyl-tubotaiwine chloride (**62**)	0	0	0	15	0
Janetine (**63**)	0	3	1	8	4
Harmane (**64**)	0	32	26	46	44
Taberdivamine B (**65**)	0	0	0	24	3
Polyneurine P (**66**)	0	16	5	51	29
Tabernamine (**67**)	0	3	0	31	10
19'(*R*)-Hydroxytabernamine (**68**)	0	30	1	33	47
Ervahaimine A (**69**)	0	11	3	50	28
Ervahaimine B (**70**)	0	11	3	50	28
Conophylline (**71**)	5	53	14	76	63
Conophylline quinone (**72**)	3	28	3	8	29

3.5.4 Preparative Radial Chromatography (Chromatotron)

Preparative radial chromatography (PRC) (Chromatotron) was carried out using a circular glass plate measuring 24 cm in diameter. Different ratios of silica and water were formulated for preparation of different sorbent thickness. For example, approximately 50 g of silica gel (Merck 7749 Kieselgel 60 PF_{254}) was added to 80–100

mL of cold distilled water to make a slurry for the preparation of a 1 mm sorbent layer. The slurry was then shaken and quickly poured onto the circular disc, which had been taped to the edges with cellophane tape. The slurry formed an even surface covering the entire glass plate. It was left to air-dry before putting it into the oven (80 ^{o}C) overnight.

PRC is a chromatographic method that uses centrifugal force to separate a multi-component fraction. The sample was first dissolved in a minimum amount of solvent. It was then loaded near the center of the spinning rotor. The dissolved sample adsorbed to the sorbent. The mobile phase was introduced in gradient elution. Concentric bands of separated compounds were visualized under UV. The eluents were then collected, concentrated with a rotary evaporator, and finally analyzed by TLC. Fractions showing similar TLC profiles were combined, while unresolved fractions were re-chromatographed. The solvent systems commonly used for PRC are chloroform/petroleum ether, chloroform, chloroform/methanol, dichloromethane/petroleum ether, dichloromethane, ethyl acetate, ethyl acetate/methanol, diethyl ether/petroleum ether, diethyl ether, and diethyl ether/methanol. All solvent systems were ammonia-saturated.

3.6 Spray Reagent (Dragendorff's Reagent)

Solution A: 0.85 g of bismuth nitrate was dissolved in a mixture of 10 mL glacial acetic acid and 40 mL of distilled water.

Solution B: 8 g of potassium iodide was dissolved in 20 mL of distilled water.

The stock solution was prepared by mixing equal volumes (1:1) of solutions A and B. The Dragendorff's reagent was prepared by mixing 1 mL of stock solution with 2 mL of glacial acetic acid and 10 mL of distilled water. The orange spots on the TLC plates appear to indicate compounds likely to be alkaloids.

3.7 Extraction of Alkaloids

3.7.1 Soaking

11.9 kg of bark was dried, ground, and weighed before soaking in distilled methanol for 2–3 days at room temperature. The methanol extract was then filtered, and the plant material was re-extracted with a fresh portion of methanol. The procedures were repeated four times. The combined extract was then concentrated by evaporation under reduced pressure using a rotary evaporator. Finally, the plant material was soaked twice in distilled ethanol to maximize the yield of extracted alkaloids.

Given that leaves might contain higher levels of non-polar or lipophilic compounds, 11.1 kg of dried, ground leaves were first soaked in hexane to defat. The plant material was then soaked in distilled methanol for 2–3 days at room temperature. The methanol extract was filtered, and the leaves were re-extracted with a fresh portion of methanol. The procedures were repeated four times. The extract was then concentrated by evaporation under reduced pressure using a rotary evaporator.

3.7.2 Acid-Base Extraction

The viscous extract was acidified with 3% tartaric acid with constant stirring. It was then filtered through Kieselguhr to remove non-alkaloidal material. The filtrate was basified with sodium carbonate to pH 11 or 12 with cooling, and the liberated alkaloids were extracted exhaustively with chloroform. The chloroform extract was then washed with distilled water and dried over anhydrous sodium sulfate. Finally, the solvent was

removed *in vacuo* to furnish the crude alkaloidal mixture (60 g from bark, 14.7 g from leaves).

3.8 Isolation of Alkaloids

3.8.1 General Procedure

The crude alkaloidal mixture was first fractionated by column chromatography over silica gel. The column was eluted with dichloromethane, followed by a progressive increase of the methanol concentration. Fractions were combined based on TLC profiles and further fractionated by flash column chromatography, preparative radial chromatography, or gel permeation chromatography (Sephadex LH-20/G-75) until pure compounds were obtained.

3.8.2 Isolation of Alkaloids from the Bark of *T. polyneura*

Extraction of 11.9 kg of the bark of *T. polyneura* yielded 60 g of crude alkaloidal mixture. It was repeatedly chromatographed, and 63 alkaloids were obtained as summarized in the flow diagram as shown in Figure 3.1.

3.8.3 Isolation of Alkaloids from the Leaves of *T. polyneura*

Extraction of 11.1 kg of the leaves of *T. polyneura* yielded 14.7 g of crude alkaloidal mixture. It was repeatedly chromatographed, and 11 alkaloids were obtained as summarized in the flow diagram as shown in Figure 3.2.

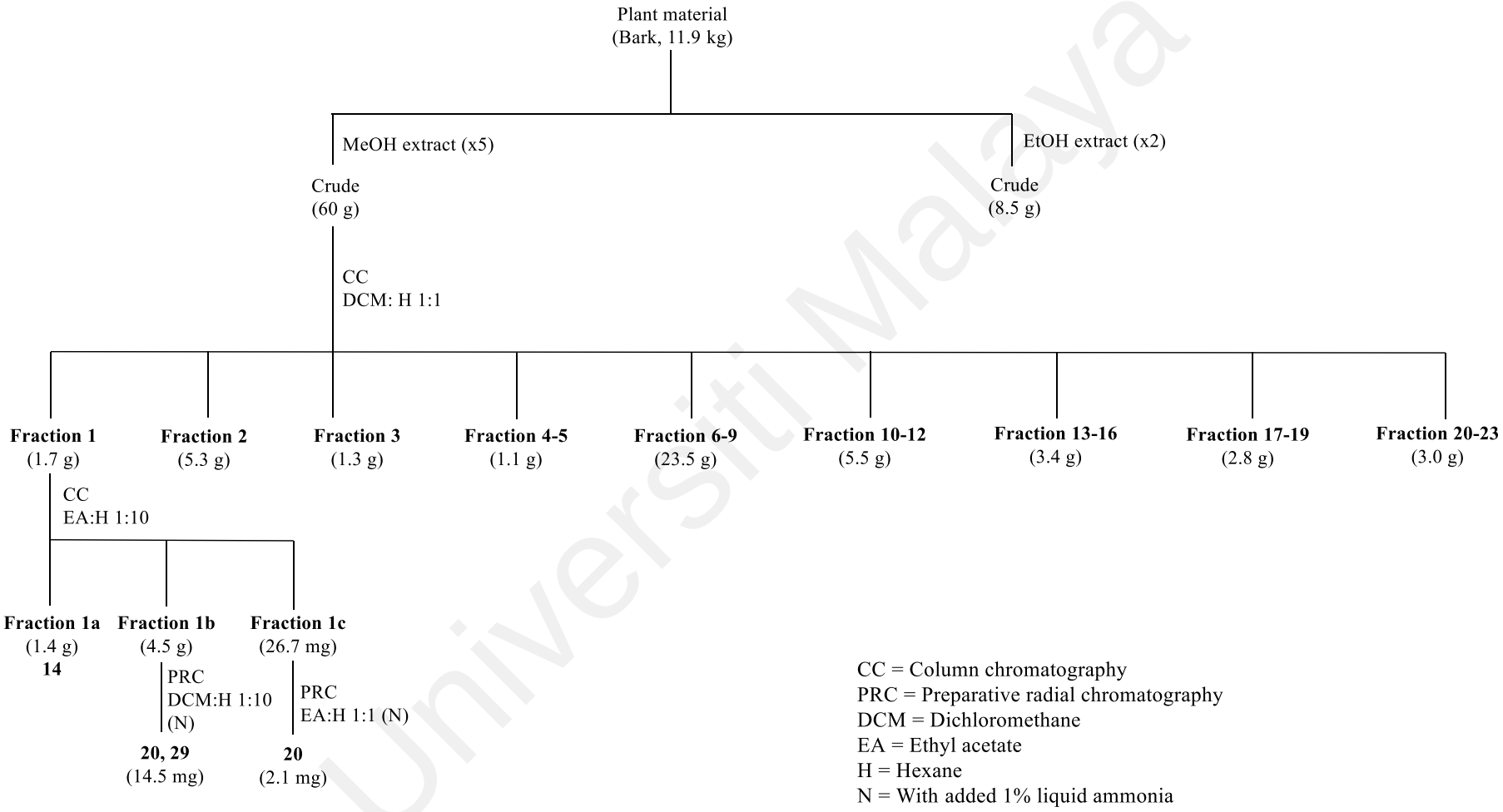


Figure 3.1: Isolation of alkaloids from the bark extract of *T. polyneura*

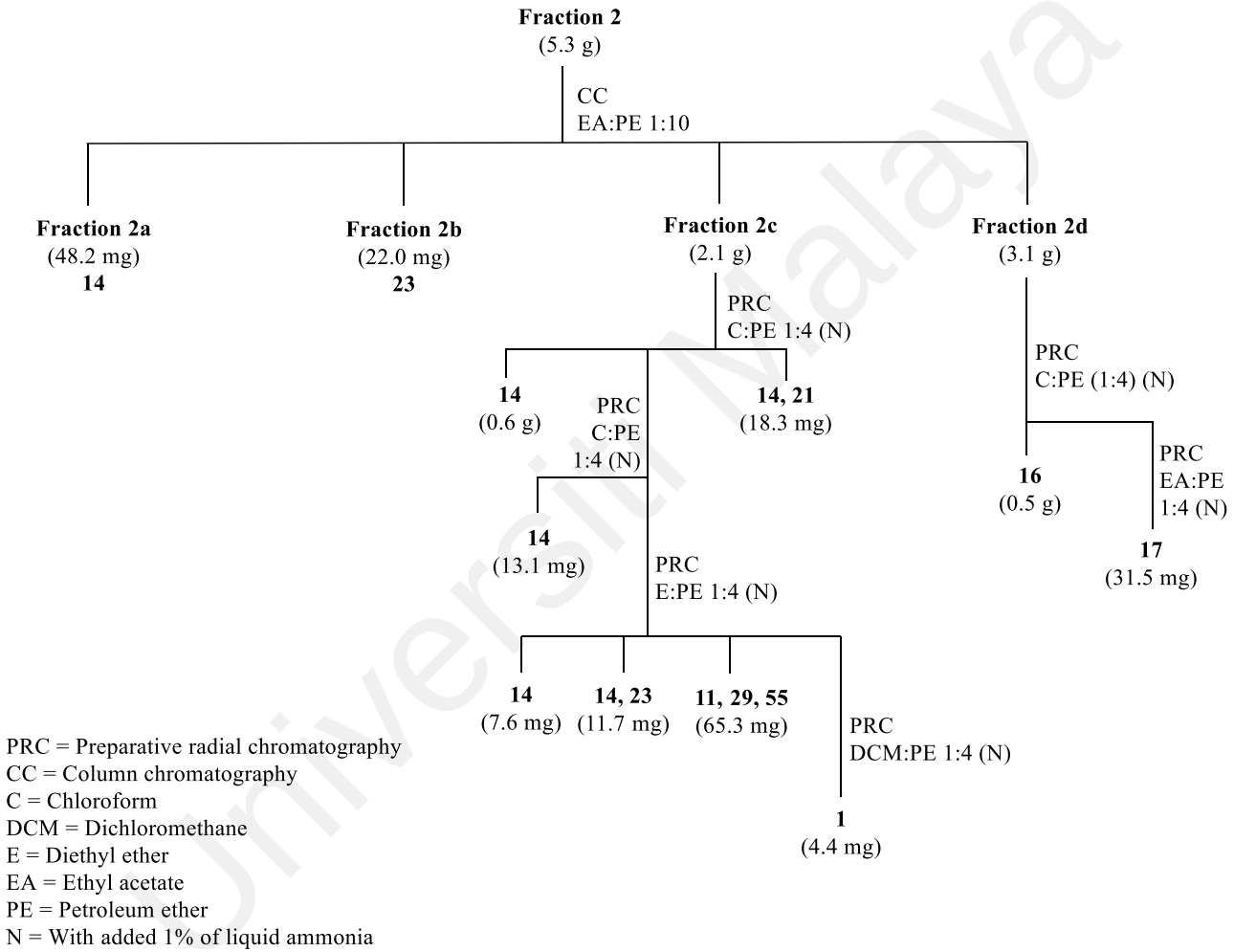


Figure 3.1, continued

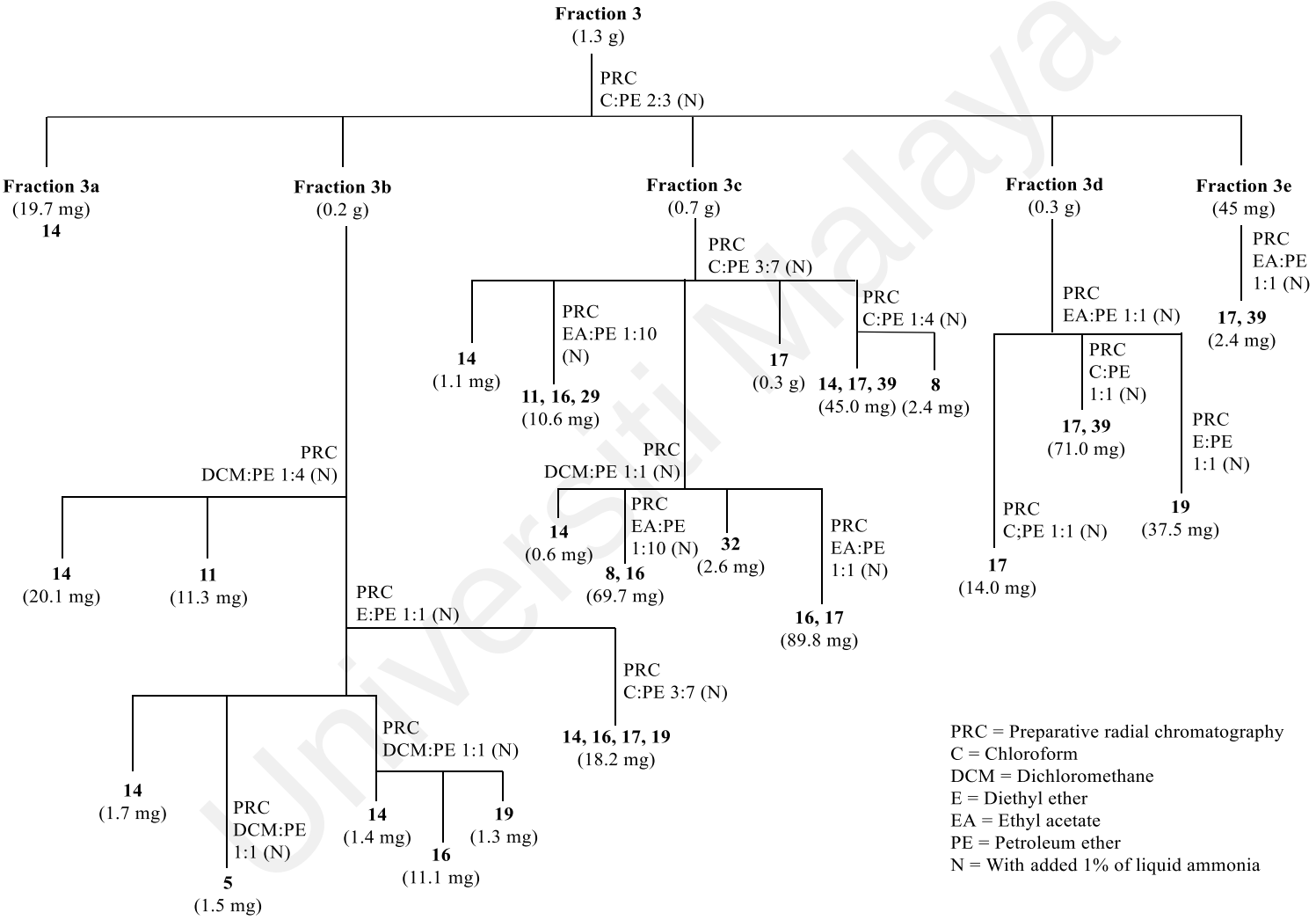


Figure 3.1, continued

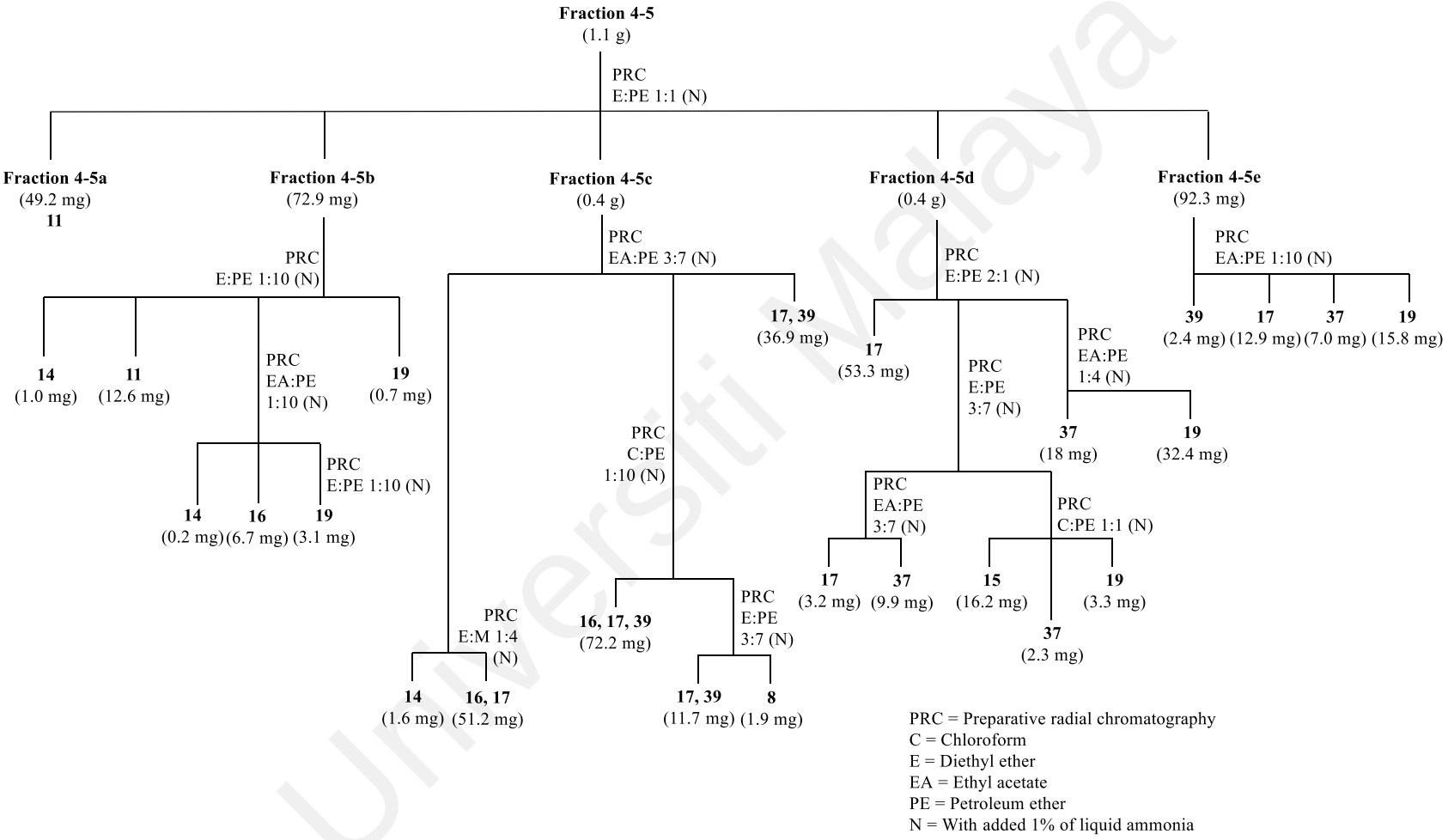


Figure 3.1, continued

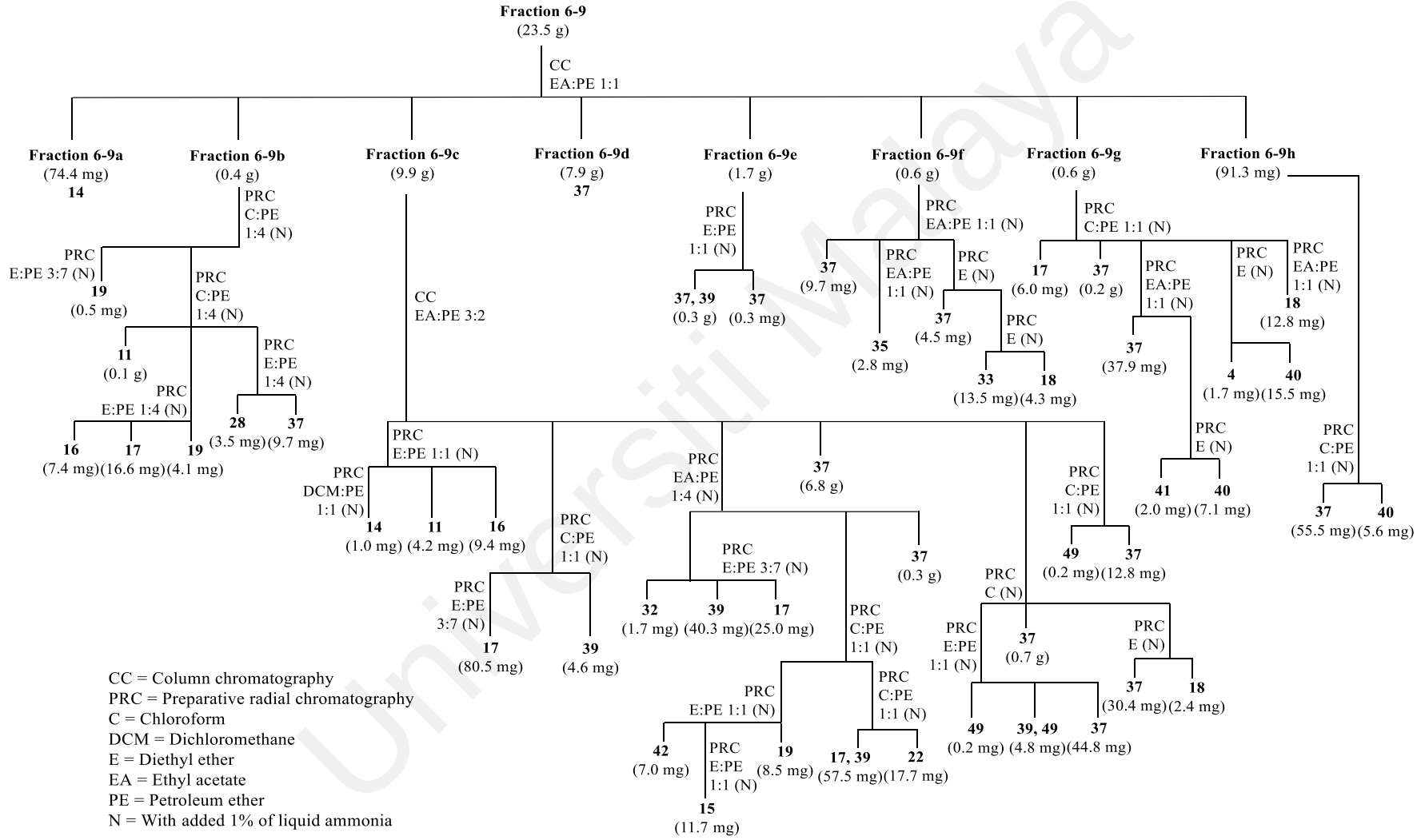


Figure 3.1, continued

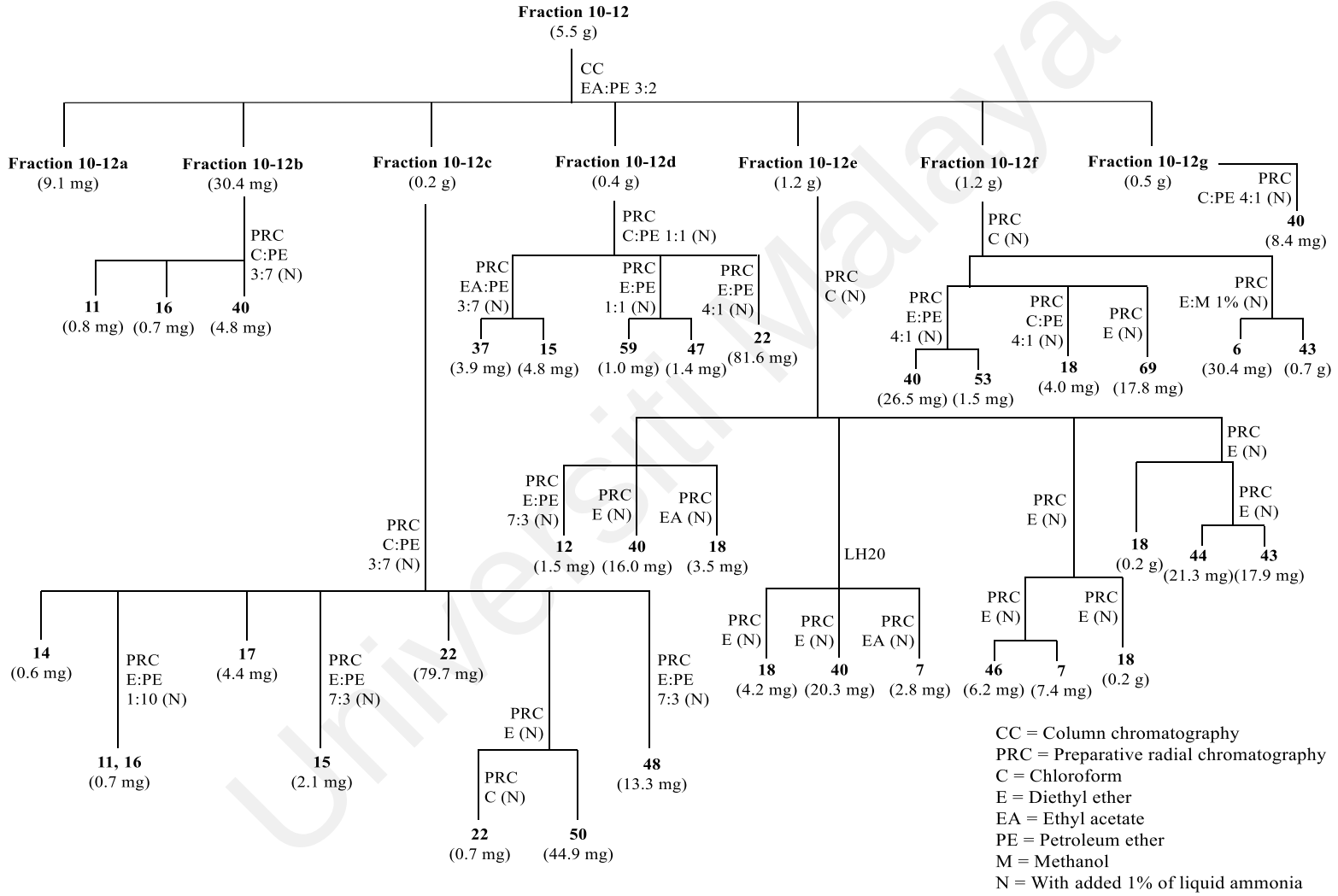


Figure 3.1, continued

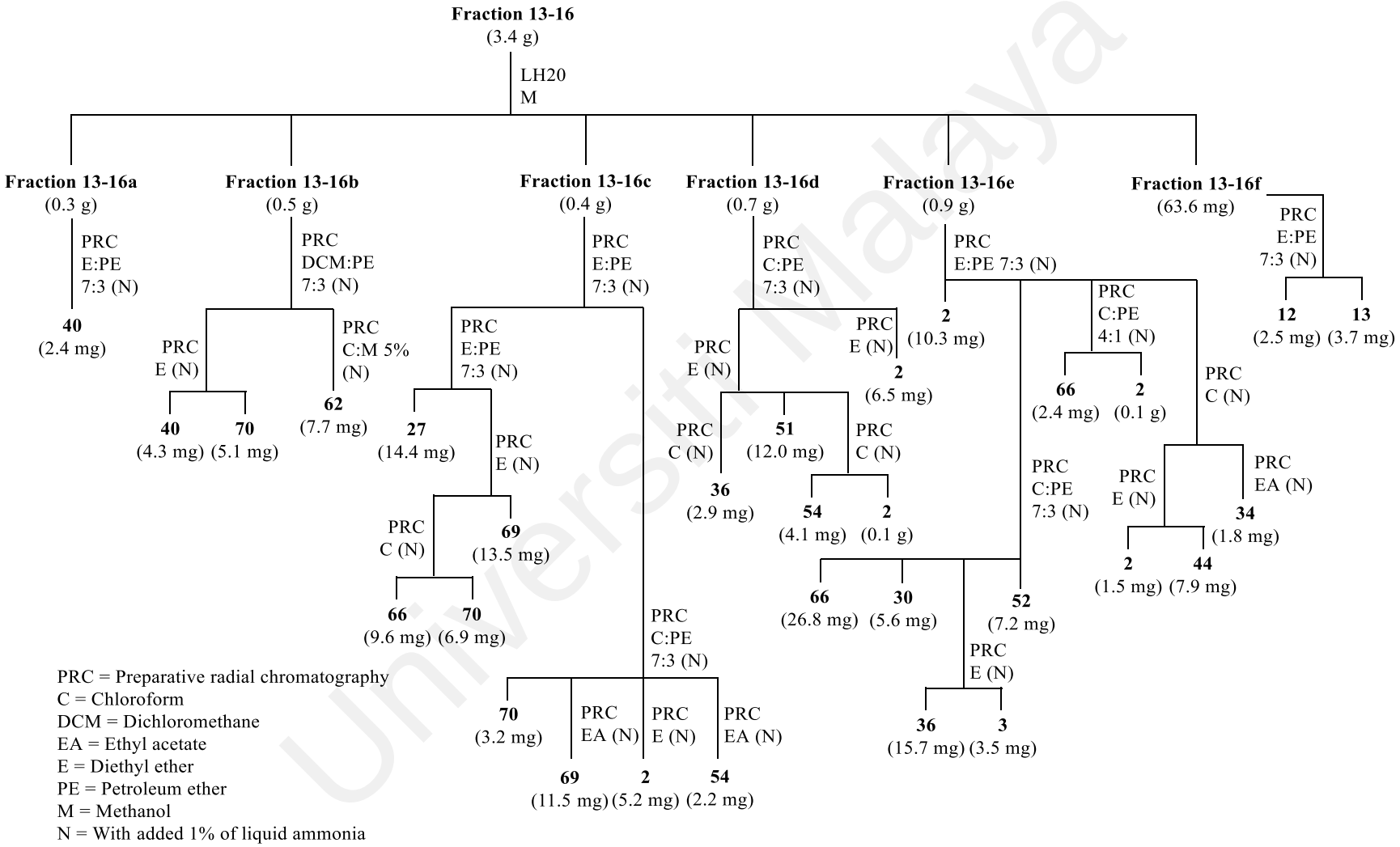


Figure 3.1, continued

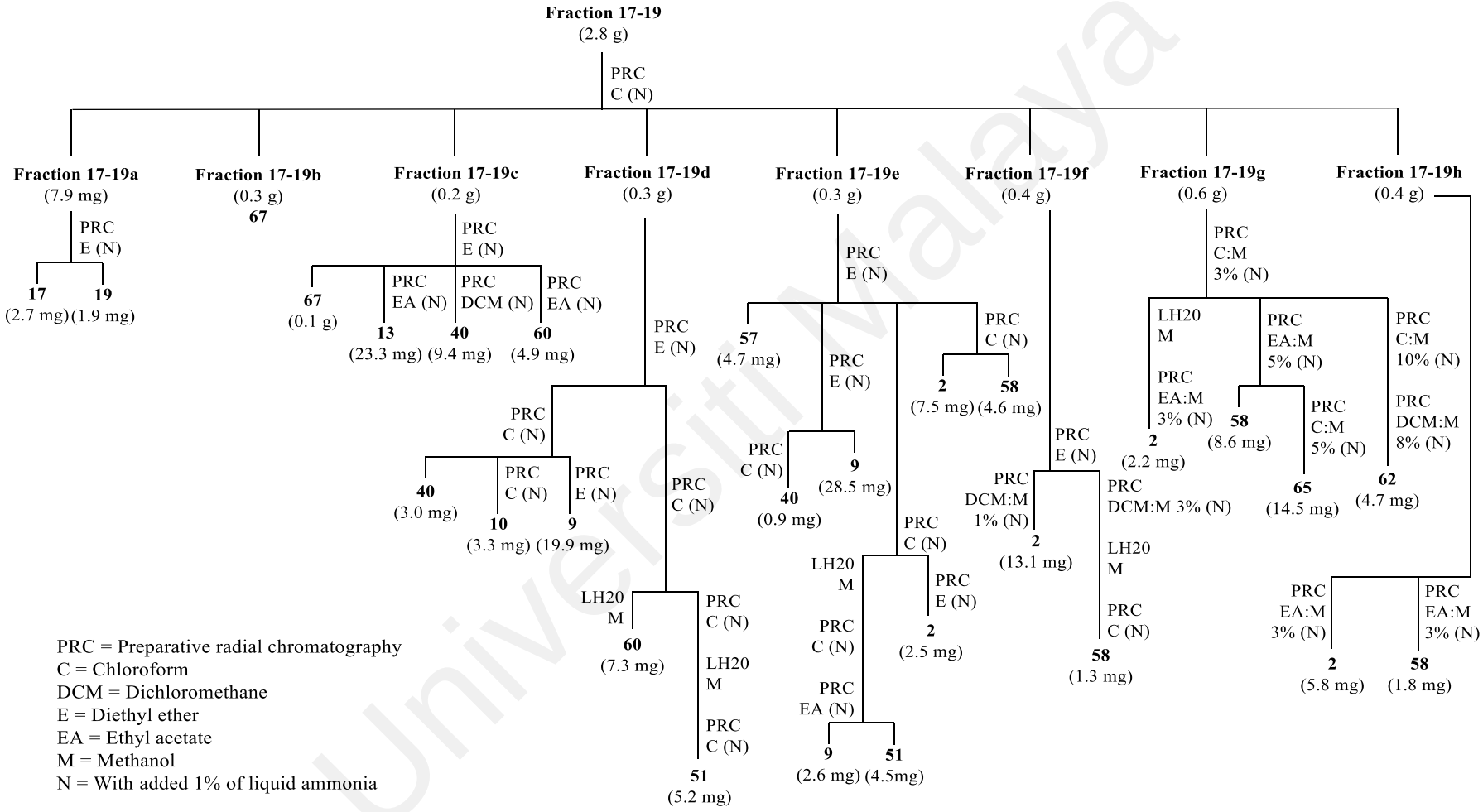


Figure 3.1, continued

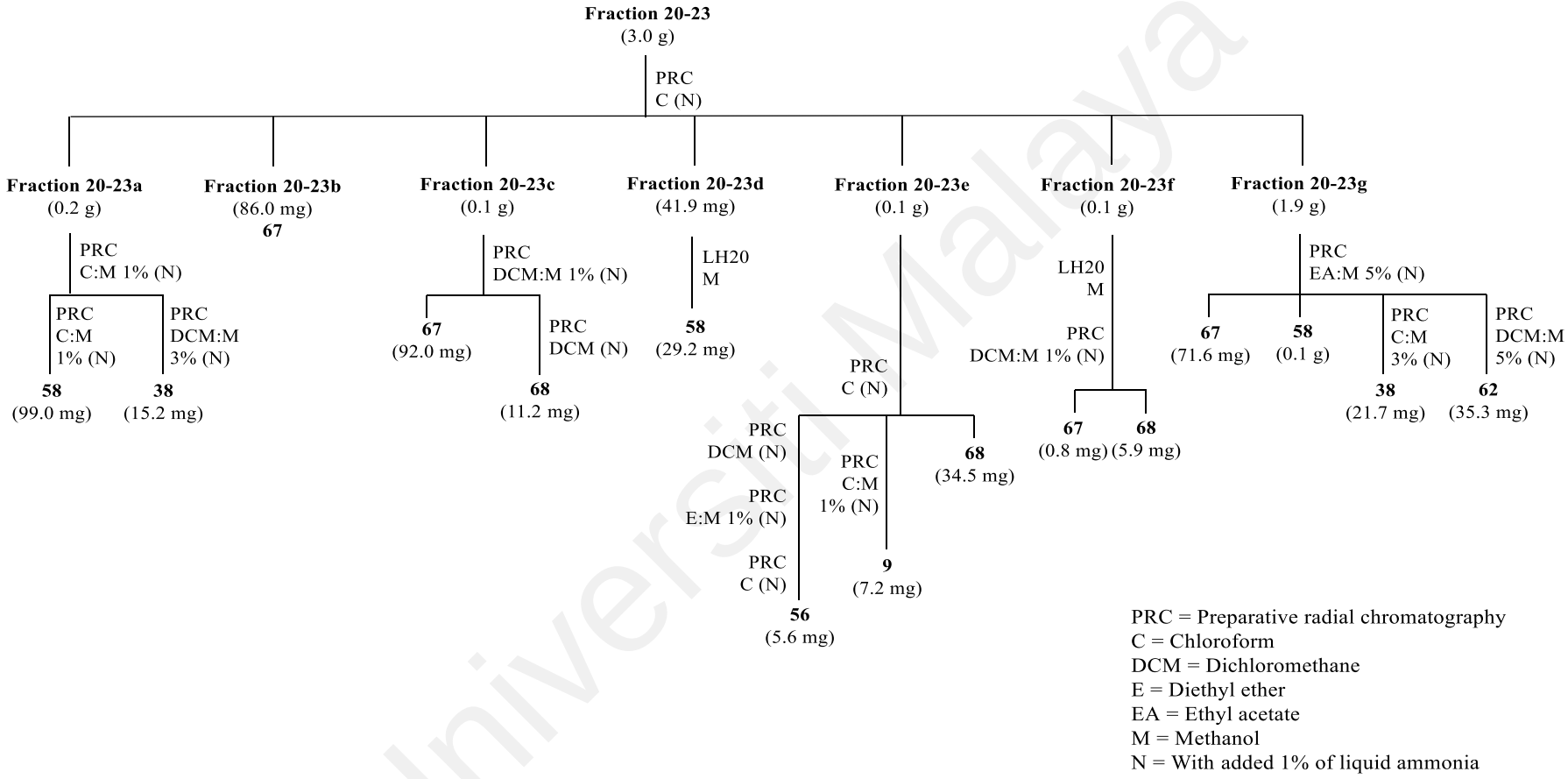


Figure 3.1, continued

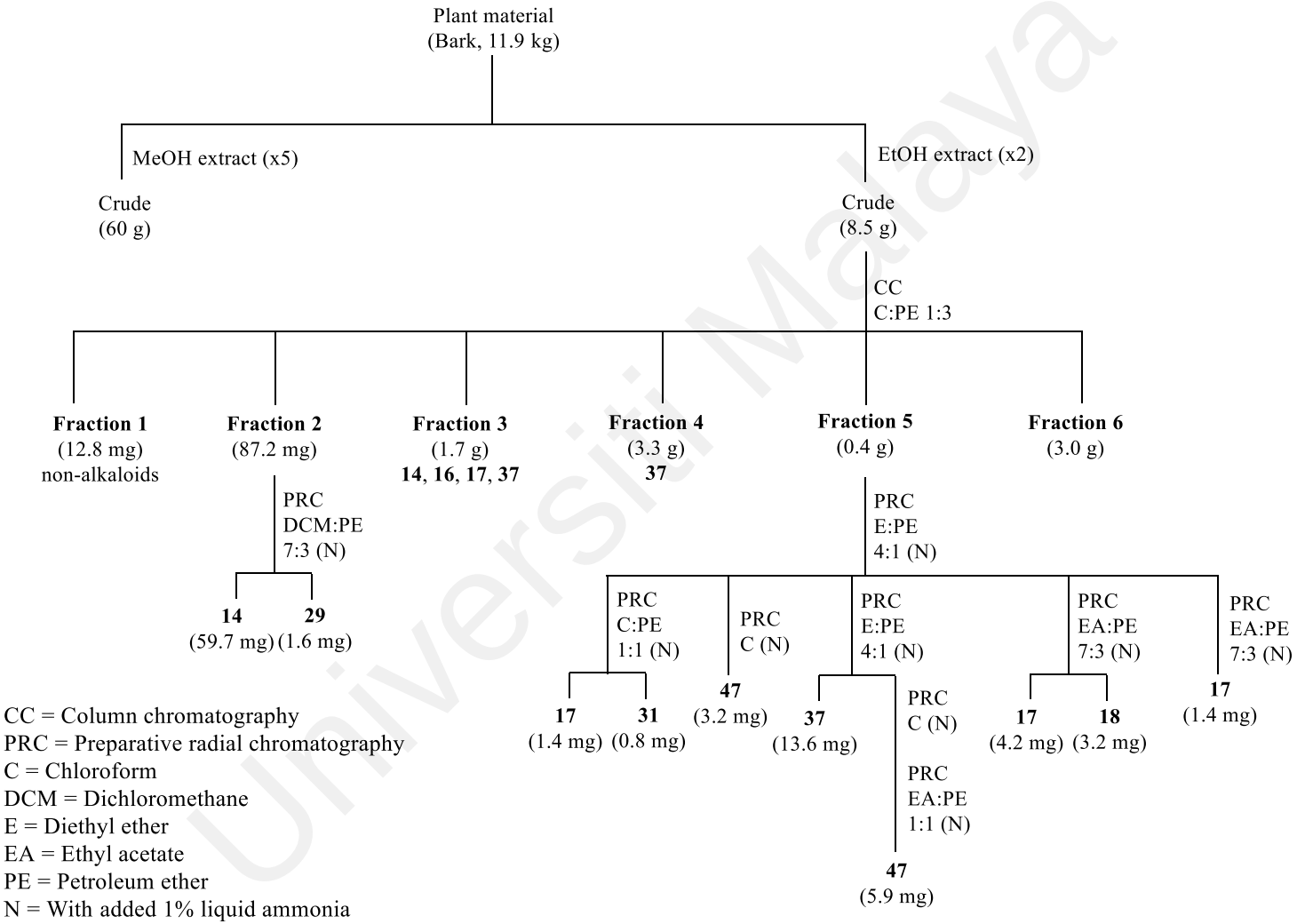


Figure 3.1, continued

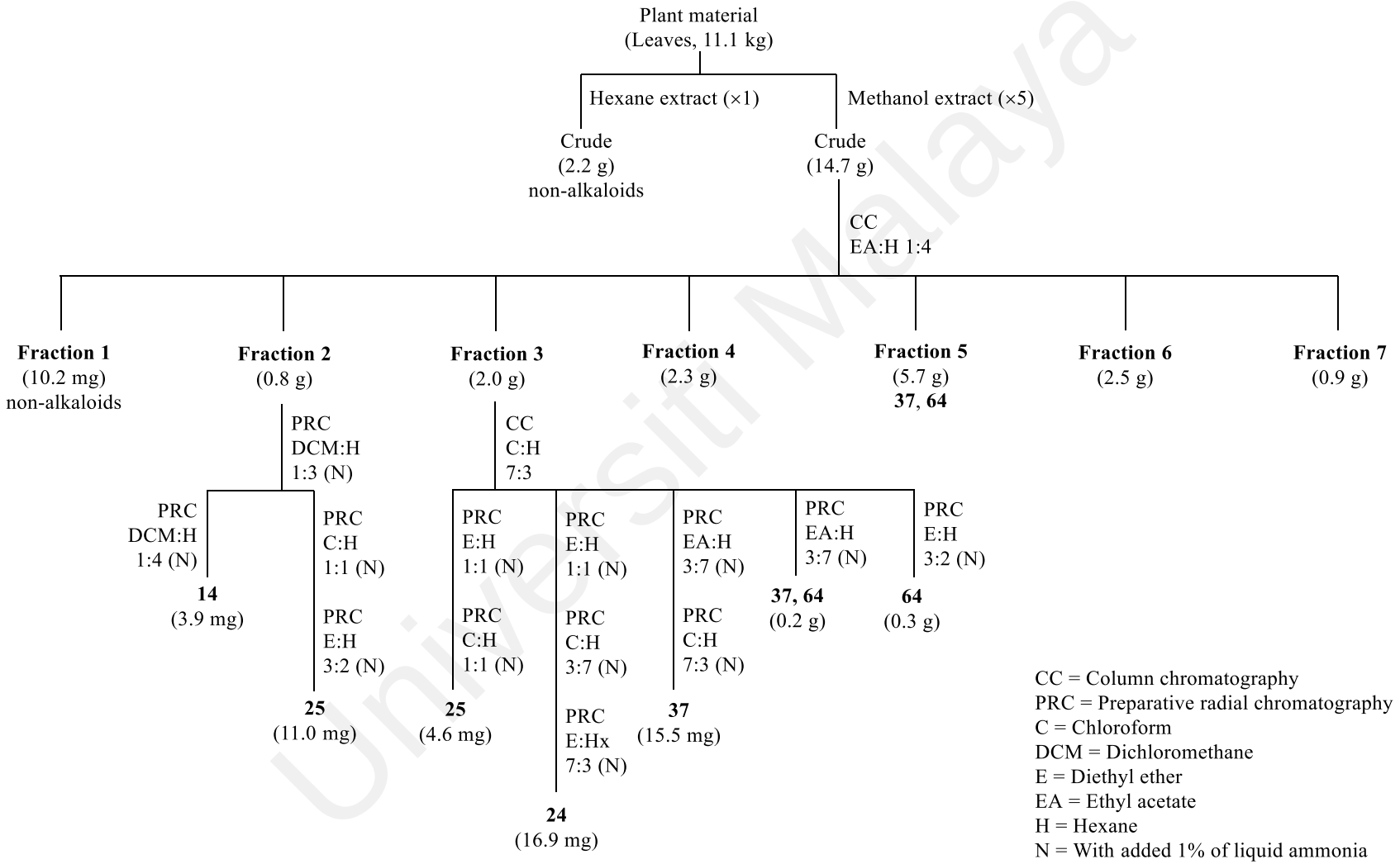


Figure 3.2: Isolation of alkaloids from the leaf extract of *T. polyneura*

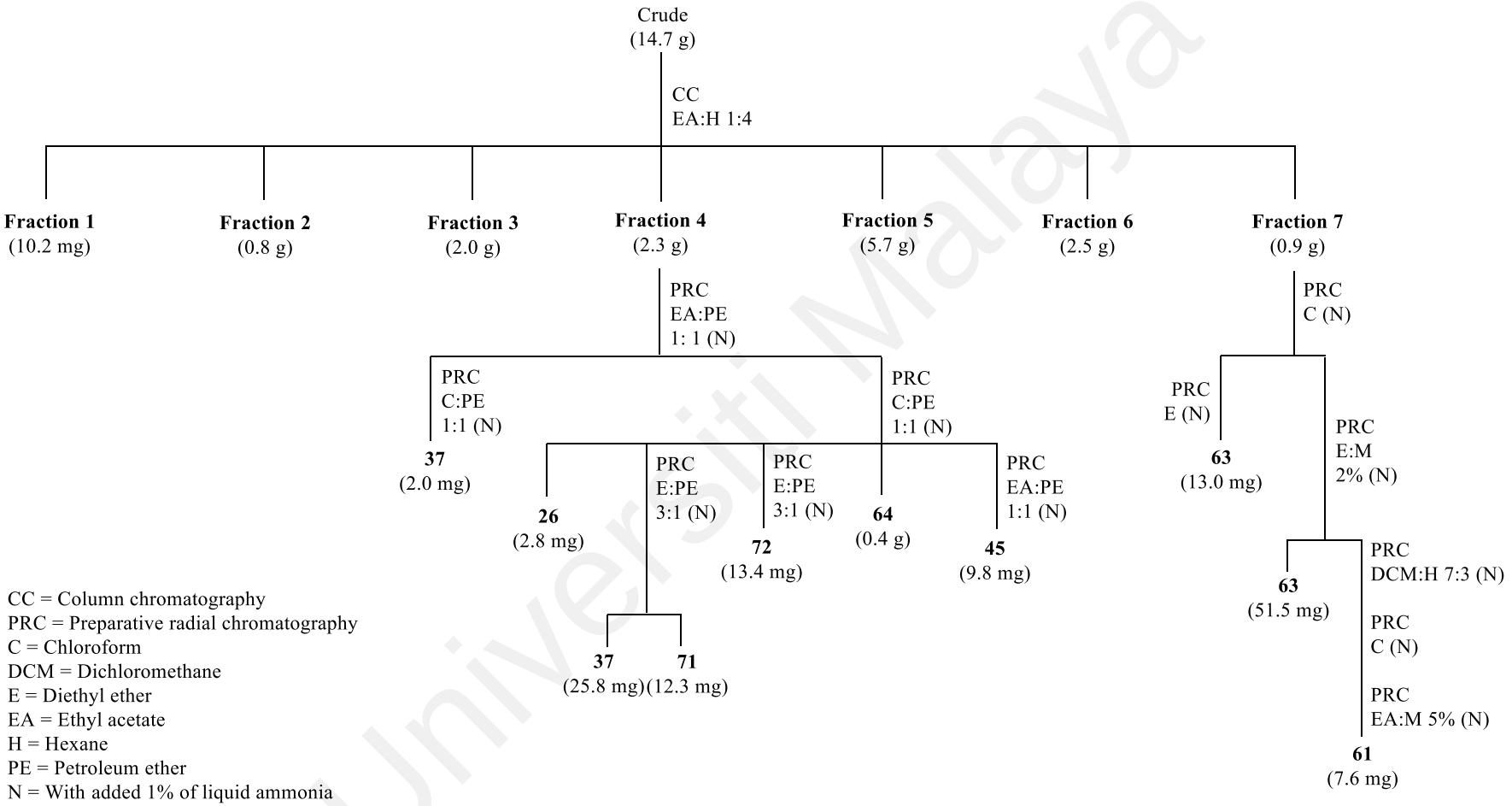


Figure 3.2, continued

3.9 Compound Data

Alkaloids from T. polyneura (bark and leaves)

Polyneurine A (1): light orange oil; $[\alpha]^{25}_{D}$ –44 (*c* 0.22, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 220 (–6.18), 233 (+1.66), 245 (–3.27), 288 (+0.83) nm; UV (EtOH) λ_{max} (log ε) 226 (3.93), 284 (3.31), 291 (3.31) nm; IR (dry film) ν_{max} 3427, 1756 cm^{-1}; HRDARTMS *m/z* 323.1761 $[M + H]^+$ (calcd for $C_{20}H_{22}N_2O_2$ + H, 323.1760). ^{1}H NMR and ^{13}C NMR data, see Table 2.2. HMBC: ^2J H-3 to C-14; H-5 to C-6; H-6 to C-5, C-7; H-9 to C-8; H-10 to C-9; H-11 to C-12; H-15 to C-14, C-20; H-17 to C-2, C-14, C-16; H-18 to C-19; H-19 to C-18, C-20; H-21 to C-16, C-20; N(1)-H to C-13. ^3J H-3 to C-5, C-15, C-17, C-21; H-5 to C-3, C-7, C-21; H-6 to C-2, C-8; H-9 to C-7, C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-14 to C-16, C-20; H-15 to C-3, C-17, C-19; H-17 to C-3, C-15, *C*OO; H-18 to C-20; H-19 to C-15, C-21; H-21 to C-2, C-3, C-5, C-15, C-17, C-19; N(1)-H to C-7, C-8. 1D/2D NOESY: H-3a/H-14, H-15β; H-3b/H3a, H-14, H-17β; H-5α/H-6α; H-5β/H-5α, H-6α; H-6β/H-3b, H-6α, H-17β; H-9/H-6α, H-10; H-12/H-11; H-14/H-15α, H-15β, H-17β; H-15β/H-18; H-15α/H-18, H-19a, H-19b; H-17α/H-15α; H-19a/H-18; H-19b/H-15β, H-18; H-21/H-5α, H-19a, H-19b; N(1)-H/H-12.

Polyneurine B (2): colorless oil and subsequently colorless plates (CCl_4/MeOH); mp 175–177 °C; $[\alpha]^{25}_{D}$ –44 (*c* 0.46, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 217 (4.15), 220 (4.14), 285 (3.66), 292 (3.61) nm; IR (ATR) ν_{max} 3259, 1716 cm^{-1}; HRESIMS *m/z* 373.2139 $[M + H]^+$ (calcd for $C_{21}H_{28}N_2O_4$ + H, 373.2122). ^{1}H NMR and ^{13}C NMR data, see Table 2.3. HMBC: ^2J H-3 to C-14; H-5 to C-6; H-6 to C-5, C-7; H-9 to C-8; H-10 to C-9, C-11; H-15 to C-14, C-20; H-17 to C-2, C-14, C-16; H-18 to C-19; H-19 to C-20; H-20 to

C-15; H-21 to C-16, C-20; N(1)-H to C-2. ^{3}J H-3 to C-15, C-17; H-5 to C-7, C-21; H-6 to C-2, C-8; H-9 to C-7, C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-15 to C-3, C-17, C-19, C-21; H-17 to C-2, C-3, C-15, C-21, *C*O_2Me; H-18 to C-20; H-19 to C-15, C-21; H-21 to C-2, C-5, C-15, C-17, C-19, *C*O_2Me; CO_2*Me* to *C*O_2Me; N(1)-H to C-7, C-8. NOESY: H-3/H-14; H-5β/H-6; H-5α/H-6; H-9/H-6, H-10; H-12/H-11; H-14/H-15α; H-17α/H-14, H-17β, N(1)-H; H-19/H-15α, H-18, H-20; H-21/H-5α, H-18, H-20; N(1)-H/H-12, H-17α.

Crystallographic data of polyneurine B (2): Colorless plates (CCl_4/MeOH), mp 175–177 °C, $C_{21}H_{28}N_2O_4.CCl_4$, *M*r = 526.26, monoclinic, space group $P2_1$, a = 9.7036(3) Å, b = 9.7698(3) Å, c = 13.5325(5) Å, β = 100.585(3)°, V = 1261.08(7) Å^3, Z = 2, D_{calcd} = 1.386 g cm^{-3}, crystal size 0.5 x 0.4 x 0.01 mm^3, F(000) = 548, Mo Kα radiation (λ = 0.71073 Å), T = 293(2) K. The final R_1 value is 0.0930 (wR_2 = 0.2790) for 6472 reflections [$I>2\sigma(I)$], while the Flack, Hooft, and Parson's parameters were x = 0.02(3), y = 0.05(2), and z = 0.01(3), respectively. For the inverted structure, the R_1 value is 0.0932 (wR_2 = 0.2796) for 6472 reflections [$I>2\sigma(I)$], while the Flack, Hooft, and Parson's parameters were x = 0.98(3), y = 0.95(2), and z = 0.99(3), respectively, from which it follows the correct enantiomer is the one depicted in Figure 2.7 (14*R*, 16*S*, 19*R*, 20*S*, 21*S*). CCDC number 2169029.

Polyneurine C (3): light yellowish oil; $[\alpha]^{25}_{D}$ –28 (*c* 0.19, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 205 (+2.95), 225 (–1.33), 244 (+1.26), 275 (–0.73) nm; UV (EtOH) λ_{max} (log ε) 223 (4.22), 286 (3.76) nm; IR (ATR) ν_{max} 3374, 1726 cm^{-1}; HRESIMS *m/z* 385.2130 $[M + H]^+$ (calcd for $C_{22}H_{28}N_2O_4$ + H, 385.2122). ^{1}H NMR and ^{13}C NMR data, see Tables 2.5 and 2.6, respectively. HMBC: ^{2}J H-3 to C-14, C-24; H-5 to C-6; H-6 to C-5,

C-7; H-9 to C-8; H-10 to C-11; H-11 to C-10; H-12 to C-11; H-15 to C-14, C-20; H-17 to C-14, C-16; H-18 to C-19; H-19 to C-20; H-21 to C-16, C-20; H-24 to C-3; N(1)-H to C-2, C-13. ^{3}J H-3 to C-5, C-15, C-17; H-5 to C-3, C-7, C-21; H-6 to C-2, C-8; H-9 to C-7, C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-14 to C-16, C-20; H-15 to C-3, C-17, C-19, C-21; H-17 to C-2, C-3, C-15, *C*O_2Me; H-18 to C-20; H-19 to C-15, C-21; H-20 to C-18; H-21 to C-3, C-5, C-15, C-17, C-19, *C*O_2Me; H-24 to C-14; CO_2*Me* to *C*O_2Me; N(1)-H to C-7, C-8. NOESY: H-3/H-14, H-17*β*; H-5*β*/H-3, H-6; H-5*α*/H-5*β*, H-6; H-6/H-3; H-9/H-6; H-14/H-15*α*, H-15*β*; H-15*α*/H-20; H-15*β*/H-15*α*; H-17*α*/H-14, H-15*α*, H-17*β*; H-19/H-15*β*, H-18, H-20; H-20/H-18; H-21/H-5*α*, H-6, H-18, H-20; H-24/H-3, H-5*β*, H-14, H-15*β*; N(1)-H/H-12, H-17*β*.

Polyneurine D (4): light yellowish oil; $[\alpha]^{25}_{D}$ –36 (*c* 0.09, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 206 (+0.33), 214 (+10.49), 230 (–4.89), 246 (+17.61), 280 (–31.27) nm; UV (EtOH) λ_{max} (log ε) 225 (4.10), 285 (3.50), 293 (3.47) nm; IR (dry film) ν_{max} 3376, 1725, 1718 cm^{-1}; HRESIMS *m/z* 397.2126 $[M + H]^+$ (calcd for $C_{23}H_{28}N_2O_4$ + H, 397.2122). ^{1}H NMR and ^{13}C NMR data, see Tables 2.5 and 2.6, respectively. HMBC: ^{2}J H-3 to C-14; H-5 to C-6; H-6 to C-2, C-5, C-7; H-9 to C-8; H-14 to C-17; H-15 to C-14; H-17 to C-14, C-16; H-18 to C-19; H-21 to C-16, C-20; H-24 to C-3, *C*HO; C*H*O to C-24; N(1)-H to C-2, C-13. ^{3}J H-3 to C-5, C-15, C-17, *C*HO; H-5 to C-2, C-3, C-7, C-21; H-6 to C-8; H-9 to C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-14 to C-16; H-15 to C-3, C-17, C-19; H-17 to C-2, C-15, *C*O_2Me; H-18 to C-20; H-19 to C-21; H-20 to C-16; H-21 to C-5, C-15, C-17, C-19, *C*O_2Me; H-24 to C-14; CO_2*Me* to *C*O_2Me; C*H*O to C-3; N(1)-H to C-7, C-8. NOESY: H-3/H-5*β*, H-14, H-17*β*, H-24; H-5*β*/H-24; H-5*α*/H-5*β*, H-6; H-9/H-6, H-10; H-14/H-15*α*; H-15*α*/H-20; H-15*β*/H-15*α*; H-17*β*/H-14; H-17*α*/H-14, H-15*α*, H-17*β*; H-19/H-15*β*, H-18, H-20; H-

21/H-5α, H-6, H-18, H-20; H-24/H-14, H-15β; C*H*O/H-3, H-14, H-15β, H-24; N(1)-H/H-12, H-17β.

Polyneurine E (5): light orange oil; $[\alpha]^{25}_{D}$ –29 (*c* 0.09, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 203 (+5.56), 221 (–1.06), 246 (+5.03), 279 (–7.62), 315 (+0.62) nm; UV (EtOH) λ_{max} (log ε) 227 (4.18), 286 (3.66), 293 (3.63) nm; IR (dry film) ν_{max} 3378, 1726, 1717 cm^{-1}; HRESIMS *m/z* 381.2174 $[M + H]^+$ (calcd for $C_{23}H_{28}N_2O_3$ + H, 381.2173). ^{1}H NMR and ^{13}C NMR data, see Tables 2.5 and 2.6, respectively. HMBC: ^2J H-3 to C-14; H-5 to C-6; H-6 to C-5, C-7; H-9 to C-8; H-10 to C-9, C-11; H-12 to C-11; H-14 to C-15; H-15 to C-14; H-17 to C-14, C-16; H-18 to C-19; H-19 to C-18, C-20; H-20 to C-19; H-21 to C-16; H-24 to C-3, *C*HO; C*H*O to C-24; N(1)-H to C-2, C-13. ^3J H-3 to C-5, C-15, C-17, *C*HO; H-5 to C-3, C-7, C-21; H-6 to C-2, C-8; H-9 to C-7, C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-14 to C-16, C-20; H-15 to C-3, C-19, C-21; H-17 to C-2, C-15, *C*O_2Me; H-18 to C-20; H-19 to C-15, C-21; H-20 to C-14, C-16, C-18; H-21 to C-2, C-3, C-5, C-17, C-19; H-24 to C-14; CO_2*Me* to *C*O_2Me; C*H*O to C-3; N(1)-H to C-7, C-8. NOESY: H-3/H-5β, H-14, H-17β, H-24b; H-5β/H-6α, H-24; H-5α/H-5β, H-6α; H-6β/H-6α; H-9/H-6β, H-6α, H-10; H-11/H-10; H-14/H-15β; H-15β/H-18; H-15α/H-15β, H-18, H-19a, H-20; H-17β/H-14; H-17α/H-15α, H-17β, H-20; H-19a/H-18, H-20; H-19b/H-15β, H-18, H-19a, H-20; H-20/H-18; H-21/H-5α, H-6α, H-18, H-19b, H-20; H-24a/H-14; H-24b/H-14, H-15β, H-24a; N(1)-H/H-12, H-17β.

Polyneurine F (6): light yellowish oil and subsequently light yellowish block crystals (EtOH); mp 153–154 °C; $[\alpha]^{25}_{D}$ –43 (*c* 0.35, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 223 (4.13), 285 (3.61), 293 (3.58) nm; IR (dry film) ν_{max} 3331, 1732, 1657 cm^{-1}; HRESIMS

m/z 369.1817 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_4$ + H, 369.1809). ^{1}H NMR and ^{13}C NMR data, see Table 2.7. HMBC: ^2J H-5 to C-6; H-6 to C-5, C-7; H-14 to C-15; H-15 to C-14, C-20; H-17 to C-14, C-16; H-18 to C-19; H-19 to C-18; H-20 to C-15, C-19; H-21 to C-16. ^3J H-5 to C-3, C-7, C-21; H-6 to C-8; H-9 to C-7, C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-14 to C-16; H-15 to C-2, C-3; H-17 to C-3, C-15, *C*O_2Me; H-18 to C-20; H-19 to C-15, C-21; H-20 to C-18; H-21 to C-2, C-3, C-5, C-15, C-17; CO_2*Me* to *C*O_2Me; N(1)-H to C-2, C-7, C-8. 1D/2D NOESY: H-5β/H-5α, H-6; H-9/H-6, H-10; H-12/H-11; H-14/H-15a, H-15b, H-17β; H-15b/H-15a; H-17β/H-14, H-17α, N(1)-H; H-17α/H-15α, H-17β; H-18a/H-19b, H-20; H-18b/H-19b; H-19b/H-19a; H-20/H-19a, H-19b; H-21/H-6, H-18, H-19b, H-20; N(1)-H/H-12, H-17β.

Crystallographic data of polyneurine F (6): light yellowish block crystals (EtOH), mp 153–154 °C, $C_{21}H_{24}N_2O_4.H_2O$, *M*r = 386.44, triclinic, space group *P*1, *a* = 7.8152(6) Å, *b* = 9.4777(9) Å, *c* = 13.9307(12) Å, α = 77.234(7)°, β = 79.526(7)°, γ = 89.595(7)°, *V* = 988.98(15) Å^3, *Z* = 2, D_{calcd} = 1.298 g cm^{-3}, crystal size 0.2 x 0.1 x 0.03 mm^3, *F*(000) = 412, Cu Kα radiation (λ = 1.54184 Å), *T* = 293(2) K. The final R_1 value is 0.0507 (wR_2 = 0.1071) for 7405 reflections [$I>2\sigma(I)$], while the Flack, Hooft, and Parson's parameters were *x* = –0.09(19), *y* = –0.10(18), and *z* = –0.1(2), respectively. For the inverted structure, the R_1 value is 0.0508 (wR_2 = 0.1070) for 7405 reflections [$I>2\sigma(I)$], while the Flack, Hooft, and Parson's parameters were *x* = 1.08(19), *y* = 1.10(18), and *z* = 1.1(2), respectively, from which it follows the correct enantiomer is the one depicted in Figure 2.23 (14*R*, 16*S*, 20*R*, 21*S*). CCDC number 2169030.

Polyneurine G (7): orange oil; $[\alpha]^{25}_{D}$ –25 (*c* 0.46, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 203 (+7.32), 221 (+0.72), 243 (+4.84), 281 (–5.92) nm; UV (EtOH) λ_{max} (log ε) 225 (4.69), 285 (4.11), 293 (4.07) nm; IR (dry film) ν_{max} 3376, 1728 cm^{-1}; HRESIMS *m/z* 371.1984 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_4$ + H, 371.1965). ^{1}H NMR and ^{13}C NMR data, see Table 2.7. HMBC: ^2J H-3 to C-14; H-5 to C-6; H-6 to C-5; H-9 to C-8; H-10 to C-9; H-14 to C-15; H-15 to C-14; H-17 to C-14, C-16; H-18 to C-19; H-19 to C-18, C-20; H-20 to C-15, C-19; H-21 to C-16, C-20; N(1)-H to C-2, C-13. ^3J H-3 to C-5, C-15, C-17, C-21; H-5 to C-2, C-3, C-7, C-21; H-6 to C-2, C-8; H-9 to C-11, C-13; H-10 to C-8; H-11 to C-9, C-13; H-12 to C-8, C-10; H-15 to C-3, C-17, C-19; H-17 to C-2, C-3, C-15, *C*O_2Me; H-18 to C-20; H-19 to C-15, C-21; H-20 to C-16, C-18; H-21 to C-2, C-3, C-15, C-17, C-19, *C*O_2Me; CO_2*Me* to *C*O_2Me; N(1)-H to C-7, C-8. NOESY: H-3a/H-14, H-17β; H-3b/H-3a, H-14, H-15β; H-5β/H-3α; H-5α/H-5β, H-6; H-6β/H-3a; H-9/H-6β, H-10; H-11/H-10; H-12/H-11; H-14/H-15α, H-15β; H-15α/H-20; H-17α/H-14, H-15α, H-17β, H-20; H-18a/H-20; H-18b/H-18a; H-19/ H-15α, H-15β, H-18a, H-20; H-21/H-5α, H-6α, H-18, H-20; N(1)-H/H-12, H-17β.

Polyneurine H (8): yellowish oil; $[\alpha]^{25}_{D}$ –30 (*c* 0.12, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 207 (–8.68), 257 (+11.07), 293 (–3.63) nm; UV (EtOH) λ_{max} (log ε) 223 (3.52), 232 sh (3.36), 266 (2.91), 292 (2.84) nm; IR (dry film) ν_{max} 3301, 1732 cm^{-1}; HRESIMS *m/z* 371.1952 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_4$ + H, 371.1965). ^{1}H NMR and ^{13}C NMR data, see Table 2.9. HMBC: ^2J H-3 to C-14; H-6 to C-5, C-7; H-15 to C-14, C-20; H-17 to C-14, C-16; H-18 to C-19; H-20 to C-15; H-21 to C-16, C-20. ^3J H-3 to C-5, C-15, C-17, C-21; H-5 to C-3, C-7, C-21; H-6 to C-2; H-9 to C-7, C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-15 to C-3, C-17, C-19; H-17 to C-2, C-3, C-15, *C*O_2Me; H-18 to C-20; H-19 to C-21; H-21 to C-2, C-3, C-15, C-17, C-19, *C*O_2Me;

CO_2*Me* to *C*O_2Me; 7-OH to C-6. NOESY: H-3a/H-6*β*, H-14, H-17*β*; H-3b/H-3a, H-14, H-15; H-5*β*/H-6*β*, H-6*α*; H-5*α*/H-5*β*, H-6*α*; H-6*α*/H-6*β*; H-9/H-6*α*, H-10; H-12/H-11; H-14/H-15; H-15/H-18; H-15*α*/H-20; H-17*β*/H-14; H-17*α*/H-14, H-15*α*, H-17*β*, H-20; H-19/H-15, H-18, H-20; H-20/H-18; H-21/H-5*α*, H-18, H-19, H-20, 7-OH.

Polyneurine J (9): light yellowish oil; $[\alpha]^{25}_{D}$ −14 (*c* 0.21, $CHCl_3$); ECD (MeOH), λ_{max} (Δε) 216 (−2.91), 239 (+5.61), 273 (−1.58) nm; UV (EtOH) λ_{max} (log ε) 221 (4.40), 284 (3.90) nm; IR (ATR) ν_{max} 3384, 1719 cm^{-1}; HRDARTMS *m/z* 355.2024 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_3$ + H, 355.2022). ^{1}H NMR and ^{13}C NMR data, see Table 2.10. HMBC: ^2J H-3 to C-14; H-5 to C-6; H-6 to C-5, C-7; H-9 to C-8; H-10 to C-9, C-11; H-14 to C-17; H-15 to C-14; H-17 to C-16; H-18 to C-19; H-19 to C-18; H-20 to C-19; H-21 to C-16, C-20; N(1)-H to C-2, C-13. ^3J H-3 to C-15, C-17; H-5 to C-7, C-18, C-21; H-6 to C-2, C-8; H-9 to C-7, C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-14 to C-16; H-15 to C-3, C-17, C-21; H-17 to C-2, C-3, C-21, *C*O_2Me; H-18 to C-5, C-20, C-21; H-19 to C-21; H-20 to C-18; H-21 to C-2, C-5, C-15, C-17, *C*O_2Me; CO_2*Me* to *C*O_2Me; N(1)-H to C-7, C-8. 1D/2D NOESY: H-3/H-14, H-15*β*, H-15*α*, H-17*β*, H-17*α*; H-5*α*/H-5*β*, H-6*β*, H-6*α*; H-5*β*/H-5*α*, H-6*β*, H-6*α*, H-18*α*; H-6*β*/H-5*α*; H-6*α*/H-5*α*, H-6*β*; H-9/H-6*α*, H-10, H-11; H-14/H-15*α*; H-15*β*/H-3, H-14, H-15*α*, H-17*β*, H-18*β*, H-19*β*; H-15*α*/H-15*β*; H-17*β*/H-15*β*, H-17*α*; H-17*α*/H-14; H-18*α*/H-19*α*; H-18*β*/H-5*β*, H-15*β*, H-18*α*, H-19*β*; H-19*β*/H-15*α*, H-15*β*, H-18*β*, H-19*α*, H-20; H-19*α*/H-18*α*, H-19*β*, H-20, H-21; H-20/H-14, H-15*α*, H-19*β*; H-21/H-5*α*, H-18*α*, H-19*α*, H-20; N(1)-H/H-12, H-17*α*.

Polyneurine K (10): yellowish oil; $[\alpha]^{25}_{D}$ –39 (*c* 0.18, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 222 (–4.00), 241 (+2.43), 277 (–0.58), 292 (–0.16), 304 (–0.43) nm; UV (EtOH) λ_{max} (log ε) 220 (4.51), 286 (4.00) nm; IR (ATR) ν_{max} 3267 cm^{-1}; HRDARTMS *m/z* 297.1974 $[M + H]^+$ (calcd for $C_{19}H_{24}N_2O$ + H, 297.1967). ^1H NMR and ^{13}C NMR data, see Table 2.11. HMBC: ^2J H-6 to C-5, C-7; H-10 to C-9; H-11 to C-12; H-15 to C-14, C-20; H-16 to C-2; H-17 to C-14, C-16; H-19 to C-18, C-20; H-20 to C-15, C-19; H-21 to C-16; N(1)-H to C-2, C-13. ^3J H-3 to C-5, C-15, C-17, C-21; H-5 to C-3, C-7, C-21; H-6 to C-2, C-8; H-9 to C-7, C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-15 to C-3, C-17, C-19; H-16 to C-7, C-20; H-17 to C-3, C-15; H-18 to C-20; H-19 to C-15, C-21; H-20 to C-16, C-18; H-21 to C-2, C-3, C-5, C-15, C-17, C-19; N(1)-H to C-7, C-8. NOESY: H-3a/H-14, H-15β; H-3b/H-14, H-17β; H-5α/H-6α, H-21; H-5β/H-3b, H-5α, H-6α; H-9/H-6α, H-10; H-12/H-11; H-14/H-17; H-16/H-17, H-20; H-18/H-15, H-19; H-20/H-15α, H-17α; H-21/H-19, H-20; N(1)-H/H-12, H-16.

Ibogamine (11): colorless oil; $[\alpha]^{25}_{D}$ –33 (*c* 0.85, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 227 (4.28), 285 (3.68), 291 (3.67) nm; IR (dry film) ν_{max} 3399 cm^{-1}; HRESIMS *m/z* 281.2019 $[M + H]^+$ (calcd for $C_{19}H_{24}N_2$ + H, 281.2012). ^1H NMR and ^{13}C NMR data, see Tables 2.12 and 2.13, respectively.

19(*S*)-Hydroxyibogamine (12): colorless oil; $[\alpha]^{25}_{D}$ –12 (*c* 0.10, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 226 (4.54), 283 (3.90), 291 (3.85) nm; IR (dry film) ν_{max} 3399, 3227 cm^{-1}; HRESIMS *m/z* 297.1967 $[M + H]^+$ (calcd for $C_{19}H_{24}N_2O$ + H, 297.1961). ^1H NMR and ^{13}C NMR data, see Tables 2.12 and 2.13, respectively.

19(*R*)-Hydroxyibogamine (13): light yellowish oil; $[\alpha]^{25}_{D}$ –22 (*c* 0.52, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 227 (4.30), 283 (3.67) nm; IR (dry film) ν_{max} 3347 cm^{-1}; HRESIMS *m/z* 297.1967 $[M + H]^+$ (calcd for $C_{19}H_{24}N_2O$ + H, 297.1961). ^1H NMR and ^{13}C NMR data, see Tables 2.12 and 2.13, respectively.

Coronaridine (14): colorless oil; $[\alpha]^{25}_{D}$ –32 (*c* 1.39, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 224 (3.90), 286 (4.24), 292 (4.21) nm; IR (dry film) ν_{max} 3380, 1719 cm^{-1}; HRESIMS *m/z* 339.2069 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_2$ + H, 339.2067). ^1H NMR and ^{13}C NMR data, see Tables 2.14 and 2.15, respectively.

(–)-Albifloranine (15): colorless oil; $[\alpha]^{25}_{D}$ –210 (*c* 1.00, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 230 (4.43), 288 (3.82), 294 (3.63) nm; IR (dry film) ν_{max} 3500, 1705 cm^{-1}; HRESIMS *m/z* 355.2022 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_3$ + H, 355.2025). ^1H NMR and ^{13}C NMR data, see Tables 2.14 and 2.15, respectively.

(–)-Heyneanine (16): light yellowish oil; $[\alpha]^{25}_{D}$ –24 (*c* 0.82, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 225 (4.51), 285 (3.89), 292 (3.81) nm; IR (dry film) ν_{max} 3380, 3232, 1725 cm^{-1}; HRESIMS *m/z* 355.2025 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_3$ + H, 355.2016). ^1H NMR and ^{13}C NMR data, see Tables 2.14 and 2.15, respectively.

19-*Epi*-heyneanine (17): light yellowish oil; $[\alpha]^{25}_{D}$ –38 (*c* 0.09, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 226 (4.36), 285 (3.77), 294 (3.72) nm; IR (dry film) ν_{max} 3378, 3245, 1728 cm^{-1}; ESIMS *m/z* 355 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_3$ + H). ^1H NMR and ^{13}C NMR data, see Tables 2.14 and 2.15, respectively.

3-Oxo-19-*epi*-heyneanine (18): yellowish oil; $[\alpha]^{25}_{D}$ –49 (*c* 0.59, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 224 (4.45), 285 (3.89), 293 (3.82) nm; IR (dry film) ν_{max} 3321, 1721, 1650 cm^{-1}; ESIMS *m/z* 369 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_4$ + H). ^1H NMR and ^{13}C NMR data, see Tables 2.14 and 2.15, respectively.

3-Oxo-coronaridine (19): light yellowish oil; $[\alpha]^{25}_{D}$ –60 (*c* 0.40, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 224 (4.32), 285 (3.69), 293 (3.61) nm; IR (dry film) ν_{max} 3255, 1732, 1663 cm^{-1}; ESIMS *m/z* 353 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_3$ + H). ^1H NMR and ^{13}C NMR data, see Tables 2.16 and 2.17, respectively.

3(*S*)-Cyanocoronaridine (20): light yellowish oil; $[\alpha]^{25}_{D}$ –64 (*c* 0.30, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 225 (4.68), 276 (4.06), 293 (4.01) nm; IR (dry film) ν_{max} 3375, 2235, 1728 cm^{-1}; HRESIMS *m/z* 363.1945 $[M]^+$ (calcd for $C_{22}H_{25}N_3O_2$, 363.1947). ^1H NMR and ^{13}C NMR data, see Tables 2.16 and 2.17, respectively.

Ervatamine G (21): colorless oil; $[\alpha]^{25}_{D}$ –23 (*c* 0.65, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 225 (4.48), 284 (3.96), 290 (3.94) nm; IR (dry film) ν_{max} 3378, 1729 cm^{-1}; HRESIMS *m/z* 369.2182 $[M + H]^+$ (calcd for $C_{22}H_{28}N_2O_3$ + H, 369.2173). ^1H NMR and ^{13}C NMR data, see Tables 2.16 and 2.17, respectively.

3-Hydroxy-3,4-*seco*coronaridine (22): light yellowish oil; $[\alpha]^{25}_{D}$ –46 (*c* 0.17, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 225 (4.28), 286 (3.62), 294 (3.56) nm; IR (dry film) ν_{max} 3361, 1721 cm^{-1}; HRESIMS *m/z* 357.2195 $[M + H]^+$ (calcd for $C_{21}H_{28}N_2O_3$ + H, 357.2193). ^1H NMR and ^{13}C NMR data, see Tables 2.16 and 2.17, respectively.

Voacangine (23): light yellowish oil; $[\alpha]^{25}_{D}$ –33 (*c* 0.21, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 220 (4.38), 286 (3.93), 299 sh (3.87) nm; IR (dry film) ν_{max} 3376, 1724 cm^{-1}; HRESIMS *m/z* 369.2180 $[M + H]^+$ (calcd for $C_{22}H_{28}N_2O_3$ + H, 369.2173). ^1H NMR and ^{13}C NMR data, see Tables 2.18 and 2.19, respectively.

Voacristine (24): light yellowish oil; $[\alpha]^{25}_{D}$ –67 (*c* 0.02, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 223 (4.28), 283 (3.98), 300 (3.90) nm; IR (dry film) ν_{max} 3246, 1725 cm^{-1}; HRESIMS *m/z* 385.2130 $[M + H]^+$ (calcd for $C_{22}H_{29}N_2O_4$ + H, 385.2122). ^1H NMR and ^{13}C NMR data, see Tables 2.18 and 2.19, respectively.

Conopharyngine (25): colorless oil; $[\alpha]^{25}_{D}$ –17 (*c* 0.23, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 223 (3.50), 282 (2.98), 300 (2.99) nm; IR (dry film) ν_{max} 3371, 1728 cm^{-1}; HRESIMS *m/z* 399.2297 $[M + H]^+$ (calcd for $C_{23}H_{30}N_2O_4$ + H, 399.2278). ^1H NMR and ^{13}C NMR data, see Tables 2.18 and 2.19, respectively.

19(*S*)-Hydroxy-conopharyngine (26): orange oil; $[\alpha]^{25}_{D}$ –28 (*c* 0.06, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 227 (3.88), 305 (3.46) nm; IR (dry film) ν_{max} 3375, 1727 cm^{-1}; ESIMS *m/z* 415 $[M + H]^+$ (calcd for $C_{23}H_{30}N_2O_5$ + H). ^1H NMR and ^{13}C NMR data, see Tables 2.18 and 2.19, respectively.

Coronaridine pseudoindoxyl (27): fluorescent yellowish oil; $[\alpha]^{25}_{D}$ –110 (*c* 0.41, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 231 (4.25), 255 (3.64), 388 (3.29) nm; IR (ATR) ν_{max} 3345, 1688 cm^{-1}; ESIMS *m/z* 355 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_3$ + H). ^1H NMR and ^{13}C NMR data, see Tables 2.20 and 2.21, respectively.

Ibogamine 7(*S*)-hydroxyindolenine (28): yellowish oil; $[\alpha]^{25}_{D}$ +46 (*c* 0.16, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 208 (–0.83), 221 (–1.40), 253 (+1.98), 291 (–0.17) nm; UV (EtOH) λ_{max} (log ε) 225 (4.32), 284 (3.71) nm; IR (ATR) ν_{max} 3438 cm^{-1}; HRESIMS *m/z* 297.1977 $[M + H]^+$ (calcd for $C_{19}H_{24}N_2O$ + H, 297.1961). ^1H NMR and ^{13}C NMR data, see Tables 2.20 and 2.21, respectively.

Coronaridine-7-hydroxyindolenine (29): light yellowish oil; $[\alpha]^{25}_{D}$ –7 (*c* 0.19, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 223 (4.25), 260 (3.48), 293 (3.47) nm; IR (dry film) ν_{max} 3377, 1733 cm^{-1}; ESIMS *m/z* 355 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_3$ + H). ^1H NMR and ^{13}C NMR data, see Tables 2.20 and 2.21, respectively.

Polyneurine I (30): light yellowish oil; $[\alpha]^{25}_{D}$ –25 (*c* 0.06, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 203 (–1.29), 222 (–4.29), 242 (+3.50), 288 (–0.56), 327 (+0.29) nm; UV (EtOH) λ_{max} (log ε) 223 (4.43), 285 (3.93) nm; IR (ATR) ν_{max} 3384, 1726 cm^{-1}; HRESIMS *m/z* 353.1868 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_3$ + H, 353.1860). ^1H NMR and ^{13}C NMR data, see Table 2.22. HMBC: ^2J H-5 to C-6; H-6 to C-5, C-7; H-9 to C-8; H-10 to C-9; H-15 to C-20; H-17 to C-14, C-16; H-18 to C-19; H-20 to C-15, C-21. ^3J H-3 to C-2, C-13, C-15, C-17; H-5 to C-18, C-21; H-6 to C-2; H-9 to C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-15 to C-3, C-19, C-21; H-17 to C-2, C-3, C-15, C-21; H-18 to C-20, C-21; H-19 to C-15; H-20 to C-14, C-16; CO_2Me to CO_2Me. NOESY: H-3β/H-14, H-15α; H-5α/H-6α, H-21; H-5β/H-5α, H-6α, H-18; H-6β/H-6α, H-18; H-9/H-6β, H-10; H-12/H-3, H-11; H-14/H-15β, H-17β, H-17α; H-15β/H-15α, H-19β; H-17α/H-17β; H-18/H-15β, H-19β, H-19α; H-19β/H-15α; H-19α/H-19β; H-20/H-15α, H-17β, H-19α; H-21/H-5α, H-17β, H-20.

10,11-Demethoxychippiine (31): light yellowish oil; $[\alpha]^{25}_{D}$ +926 (*c* 0.03, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 228 (4.28), 278 (3.71), 285 (3.75), 293 (3.70) nm; IR (dry film) ν_{max} 3328, 1724 cm^{-1}; ESIMS *m/z* 355 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_3$ + H). ^1H NMR and ^{13}C NMR data, see Table 2.23.

3-Methoxy-10,11-demethoxychippiine (32): colorless oil; $[\alpha]^{25}_{D}$ –7 (*c* 0.07, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 226 (3.73), 283 (3.20) nm; IR (dry film) ν_{max} 3437, 1715 cm^{-1}; HRESIMS *m/z* 369.2175 $[M + H]^+$ (calcd for $C_{22}H_{28}N_2O_3$ + H, 369.2173). ^1H NMR and ^{13}C NMR data, see Table 2.23.

Polyneurine M (33): yellowish oil; $[\alpha]^{25}_{D}$ –51 (*c* 0.44, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 208 (+21.67), 232 (–2.31), 237 (–1.92), 249 (–4.32), 266 (–0.04), 309 (–6.20), 364 (+0.40) nm; UV (EtOH) λ_{max} (log ε) 227 (4.05), 238 (4.00), 315 (4.03) nm; IR (ATR) ν_{max} 3324, 1725, 1641 cm^{-1}; HRDARTMS *m/z* 369.1811 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_4$ + H, 369.1814). ^1H NMR and ^{13}C NMR data, see Tables 2.24 and 2.25, respectively. HMBC: ^2J H-5 to C-6, C-16; H-6 to C-5, C-7; H-9 to C-10; H-10 to C-9; H-12 to C-13; H-14 to C-3, C-15; H-15 to C-14, C-20; H-16 to C-5, *C*O_2Me; H-18 to C-19; H-19 to C-18, C-20; H-21 to C-20; N(1)-H to C-2, C-13. ^3J H-5 to C-15, C-21; H-6 to C-2, C-8, C-16; H-9 to C-7, C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8; H-14 to C-2, C-16, C-20; H-15 to C-5, C-21; H-16 to C-6, C-14, C-20; H-18 to C-20; H-19 to C-21; H-21 to C-5, C-15, N(4)-Me; CO_2Me to *C*O_2Me; N(4)-Me to C-5, C-21; N(1)-H to C-7, C-8. NOESY: H-5/H-6, H-16, N(4)-Me; H-6/H-14α, H-21α, N(4)-Me; H-9/H-6, H-10; H-14β/H-14α, H-18; H-14α/H-14β, H-21α; H-15/H-16, H-18; H-16/H-5, H-15; H-18/H-14β, H-15, H-19; H-19/H-18, H-21β; H-21β/H-19, H-

21α; H-21α/H-6, H-14α, H-21β, N(4)-Me; N(4)-Me/H-5, H-6, H-21α, H-21β; N(1)-H/H-12.

Polyneurine N (34): light yellowish oil; $[\alpha]^{25}_{D}$ –31 (*c* 0.10, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 210 (+13.61), 232 (–2.31), 236 (–2.03), 248 (–3.62), 264 (+0.01), 293 (–5.38), 364 (+0.66) nm; UV (EtOH) λ_{max} (log ε) 221 (3.61), 315 (3.56) nm; IR (ATR) ν_{max} 3337, 1723, 1639 cm^{-1}; HRESIMS *m/z* 387.1925 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_5$ + H, 387.1914). ^{1}H NMR and ^{13}C NMR data, see Tables 2.24 and 2.25, respectively. HMBC: ^2J H-5 to C-16; H-6 to C-5, C-7; H-9 to C-10; H-10 to C-9, C-11; H-14 to C-3, C-15; H-15 to C-14; H-16 to C-5, C-15, *C*O_2Me; H-18 to C-19; H-19 to C-18; H-21 to C-20; N(1)-H to C-2, C-13. ^3J H-5 to C-15 to C-21; H-6 to C-2, C-8, C-16; H-9 to C-11, C-13; H-10 to C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-14 to C-2, C-16, C-20; H-15 to C-5, C-20, C-21; H-16 to C-6, C-14; H-18 to C-20; H-21 to C-5, N(4)-Me; CO_2Me to *C*O_2Me; N(4)-Me to C-5, C-21; N(1)-H to C-7, C-8. NOESY: H-5/H-6β, H-16, N(4)-Me; H-9/H-6β, H-10; H-11/H-10; H-14β/H-19; H-16/H-15; H-19/H-14β, H-18; H-21β/H-18; H-21α/H-21β; N(4)-Me/H-5, H-6α, H-6β, H-21β; N(1)-H/H-12.

Polyneurine O (35): light yellowish oil; $[\alpha]^{25}_{D}$ +11 (*c* 0.14, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 206 (+10.18), 233 (–0.46), 237 (–0.33), 248 (–2.03), 266 (+0.72), 308 (–4.05), 358 (+0.58) nm; UV (EtOH) λ_{max} (log ε) 228 (3.91), 240 (3.95), 315 (4.01) nm; IR (ATR) ν_{max} 3166, 1726, 1637 cm^{-1}; HRESIMS *m/z* 385.1762 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_5$ + H, 385.1764). ^{1}H NMR and ^{13}C NMR data, see Tables 2.24 and 2.25, respectively. HMBC: ^2J H-6 to C-5, C-7; H-9 to C-10; H-10 to C-9, C-11; H-11 to C-10; H-12 to C-13; H-14 to C-3, C-15; H-16 to C-5, C-15, *C*O_2Me; H-18 to C-19; H-19 to C-18; H-21 to C-20; N(1)-H to C-13. ^3J H-5 to C-7; H-6 to C-2, C-8, C-16; H-9 to C-

11, C-13; H-10 to C-12; H-11 to C-13; H-12 to C-8, C-10; H-14 to C-2, C-16, C-20; H-15 to C-5, *C*O_2Me; H-16 to C-6, C-14; H-18 to C-20; H-19 to C-21; H-21 to C-5, C-15, C-19, N(4)-Me; CO_2*Me* to *C*O_2Me; N(4)-Me to C-5, C-21; N(1)-H to C-7, C-8. NOESY: H-5/H-6*β*, H-16, N(4)-Me; H-6*β*/H-5, H-6*α*; H-6*α*/H-14*α*; H-9/H-6*β*, H-10; H-14*β*/H-14*α*, H-15; H-14*α*/H-6*α*, H-14*β*; H-15/H-18; H-16/H-5, H-18; H-18/H-15, H-19; H-19/H-18, H-21; H-21/H-19, N(4)-Me; N(1)-H/H-12.

3-*Epi*-vobasinol (36): light yellowish oil; $[\alpha]^{22}_D$ +17 (*c* 0.19, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 225 (3.98), 285 (3.48) nm; IR (dry film) ν_{max} 3400, 1730 cm^{-1}; HRESIMS *m/z* 355.2002 $[M + H]^+$ (calcd for $C_{21}H_{27}N_2O_3$ + H, 355.2022). ^{1}H NMR and ^{13}C NMR data, see Tables 2.26 and 2.27, respectively.

Vobasine (37): light yellowish oil; $[\alpha]^{25}_D$ –130 (*c* 1.93, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 208 (4.26), 240 (4.16), 316 (4.22) nm; IR (dry film) ν_{max} 3301, 1719, 1637 cm^{-1}; HRESIMS *m/z* 353.1862 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_3$ + H, 353.1865). ^{1}H NMR and ^{13}C NMR data, see Tables 2.26 and 2.27, respectively.

Vobasine *N*(4)-oxide (38): light yellowish oil; $[\alpha]^{25}_D$ –147 (*c* 0.42, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 211 (4.18), 239 (4.06), 314 (4.11) nm; IR (dry film) ν_{max} 3315, 1721, 1647 cm^{-1}; HRESIMS *m/z* 369.1815 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_4$ + H, 369.1814). ^{1}H NMR and ^{13}C NMR data, see Tables 2.26 and 2.27, respectively.

16-*Epi*-vobasine (39): light yellowish oil; $[\alpha]^{25}_D$ –127 (*c* 0.25, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 212 (4.34), 227 sh (4.19), 237 (4.16), 320 (4.20) nm; IR (dry film) ν_{max}

3308, 1720, 1642 cm^{-1}; HRESIMS *m/z* 353.1861 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_3$ + H, 353.1865). ^1H NMR and ^{13}C NMR data, see Tables 2.26 and 2.27, respectively.

Perivine (40): light yellowish oil; $[\alpha]^{25}_D$ –83 (*c* 0.12, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 226 (4.39), 242 (4.21), 314 (4.19) nm; IR (dry film) ν_{max} 3310, 1717, 1640 cm^{-1}; HRESIMS *m/z* 339.1715 $[M + H]^+$ (calcd for $C_{20}H_{22}N_2O_3$ + H, 339.1709). ^1H NMR and ^{13}C NMR data, see Tables 2.28 and 2.29, respectively.

Dregamine (41): light yellowish oil; $[\alpha]^{25}_D$ –81 (*c* 0.10, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 213 (4.06), 240 (4.03), 316 (4.09) nm; IR (dry film) ν_{max} 3301, 1719, 1637 cm^{-1}; HRESIMS *m/z* 355.2017 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_3$ + H, 355.2022). ^1H NMR and ^{13}C NMR data, see Tables 2.28 and 2.29, respectively.

Tabernaemontanine (42): light yellowish oil; $[\alpha]^{25}_D$ –53 (*c* 0.15, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 228 (4.28), 311 (3.98) nm; IR (dry film) ν_{max} 3312, 1727, 1640 cm^{-1}; HRESIMS *m/z* 355.2013 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_3$ + H, 353.2022). ^1H NMR and ^{13}C NMR data, see Tables 2.28 and 2.29, respectively.

Vobasenal (43): light yellowish oil; $[\alpha]^{25}_D$ –89 (*c* 0.08, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 211 (4.28), 239 (4.17), 293 (4.63) nm; HRESIMS *m/z* 353.1489 $[M + H]^+$ (calcd for $C_{20}H_{20}N_2O_4$ + H, 353.1501). ^1H NMR and ^{13}C NMR data, see Tables 2.30 and 2.31, respectively.

Vobasidine D (44): light yellowish oil; $[\alpha]^{25}_{D}$ −70 (*c* 0.26, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 207 (4.04), 236 (3.84), 297 (4.13) nm; IR (dry film) ν_{max} 3304, 1727, 1639 cm^{-1}; HRESIMS *m/z* 367.1654 $[M + H]^+$ (calcd for $C_{21}H_{22}N_2O_4$ + H, 367.1652). ^1H NMR and ^{13}C NMR data, see Tables 2.30 and 2.31, respectively.

Vobasidine E (45): light yellowish oil; $[\alpha]^{25}_{D}$ −17 (*c* 0.49, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 210 (4.37), 239 (4.24), 313 (4.26) nm; IR (dry film) ν_{max} 3307, 1730, 1640 cm^{-1}; HRESIMS *m/z* 357.1461 $[M + H]^+$ (calcd for $C_{19}H_{20}N_2O_5$ + H, 357.1450). ^1H NMR and ^{13}C NMR data, see Tables 2.30 and 2.31, respectively.

Vobasidine F (46): light yellowish oil; $[\alpha]^{25}_{D}$ −29 (*c* 0.09, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 224 (4.08), 239 (4.20), 315 (4.27) nm; IR (dry film) ν_{max} 3308, 1723, 1648 cm^{-1}; HRESIMS *m/z* 371.1959 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_4$ + H, 371.1971). ^1H NMR and ^{13}C NMR data, see Tables 2.30 and 2.31, respectively.

Pericyclivine (47): light yellowish oil; $[\alpha]^{25}_{D}$ −7 (*c* 0.19, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 226 (4.37), 282 (3.67), 291 (3.54) nm; IR (dry film) ν_{max} 3360, 1721 cm^{-1}; HRESIMS *m/z* 323.1765 $[M + H]^+$ (calcd for $C_{20}H_{23}N_2O_2$ + H, 323.1760). ^1H NMR and ^{13}C NMR data, see Tables 2.32 and 2.33, respectively.

16-*Epi*-voacarpine (48): colorless oil; $[\alpha]^{25}_{D}$ +42 (*c* 0.20, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 226 (4.49), 283 (3.79), 291 (3.71) nm; IR (dry film) ν_{max} 3330, 1731 cm^{-1}; HRESIMS *m/z* 369.1812 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_4$ + H, 369.1814). ^1H NMR and ^{13}C NMR data, see Tables 2.32 and 2.33, respectively.

19,20-Dehydroervatamine (49): colorless oil; $[\alpha]^{25}_{D}$ +65 (*c* 0.05, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 209 (4.33), 236 (4.08), 311 (4.22) nm; IR (dry film) ν_{max} 3298, 1731, 1641 cm^{-1}; ESIMS *m/z* 353 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_3$ + H). ^1H NMR and ^{13}C NMR data, see Tables 2.32 and 2.33, respectively.

16(*R*)-Sitsirikine (50): light yellowish oil; $[\alpha]^{25}_{D}$ –33 (*c* 0.14, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 226 (4.47), 272 (3.72), 283 (3.80), 290 (3.73) nm; IR (dry film) ν_{max} 3375, 2813, 2766, 1708 cm^{-1}; HRESIMS *m/z* 353.1868 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_3$ + H, 353.1860). ^1H NMR and ^{13}C NMR data, see Tables 2.34 and 2.35, respectively.

16(*R*)-19,20-*E*-isositsirikine (51): yellowish oil; $[\alpha]^{25}_{D}$ +10 (*c* 0.33, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 225 (4.27), 286 (3.96), 295 (3.65) nm; HRDARTMS *m/z* 355.2024 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_3$ + H, 355.2022). ^1H NMR and ^{13}C NMR data, see Tables 2.34 and 2.35, respectively.

16(*R*)-19,20-*Z*-isositsirikine (52): yellowish oil; $[\alpha]^{25}_{D}$ –45 (*c* 0.08, MeOH); UV (EtOH) λ_{max} (log ε) 226 (4.05), 282 (3.39), 290 (3.33) nm; IR (ATR) ν_{max} 3353, 2980, 2797, 1727 cm^{-1}; HRESIMS *m/z* 355.2033 $[M + H]^+$ (calcd for $C_{21}H_{26}N_2O_3$ + H, 355.2016). ^1H NMR and ^{13}C NMR data, see Tables 2.34 and 2.35, respectively.

Fluorocarpamine (53): yellowish oil; $[\alpha]^{25}_{D}$ +163 (*c* 0.07, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 232 (4.15), 260 (3.59), 289 (3.20) nm; IR (dry film) ν_{max} 1748, 1696 cm^{-1}; HRDARTMS *m/z* 339.1693 $[M + H]^+$ (calcd for $C_{20}H_{22}N_2O_3$ + H, 339.1709). ^1H NMR and ^{13}C NMR data, see Tables 2.34 and 2.35, respectively.

Polyneurine L (54): light yellowish oil; $[\alpha]^{25}_{D}$ −19 (*c* 0.30, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 220 (−7.17), 238 (+5.46) nm; UV (EtOH) λ_{max} (log ε) 219 (3.50), 224 (3.90), 283 (3.34), 292 (3.27) nm; IR (ATR) ν_{max} 3369, 1732 cm^{-1}; HRESIMS *m/z* 373.2140 $[M + H]^+$ (calcd for $C_{21}H_{28}N_2O_4$ + H, 373.2122). ^{1}H NMR and ^{13}C NMR data, see Table 2.36. HMBC: ^2J H-3 to C-14; H-5 to C-6; H-6 to C-5, C-7; H-9 to C-8; H-10 to C-9, C-11; H-11 to C-12; H-12 to C-11; H-14 to C-3, C-15, C-17; H-15 to C-14, C-20; H-17 to C-14, C-16; H-18 to C-19; H-19 to C-18, C-20; H-21 to C-20; N(1)-H to C-2, C-13. ^3J H-3 to C-5, C-15, C-21; H-5 to C-3, C-7, C-21; H-6 to C-2, C-8; H-9 to C-7, C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-15 to C-3, C-17, C-19, C-21; H-17 to C-2, C-3, C-15, *C*O_2Me; H-18 to C-20; H-19 to C-15, C-21; H-21 to C-5, C-15, C-19; CO_2*Me* to *C*O_2Me; N(1)-H to C-7, C-8. NOESY: H-3β/H-14, H-15, H-17β; H-3α/H-3β, H-14; H-5/H-6α, H-6β; H-9/H-6α, H-10; H-14/H-15, H-18, H-19; H-15/H-18, H-19; H-17β/H-15; H-17α/H-14, H-17β; H-19/H-18; H-21α/H-14, H-15, H-18, H-19; H-21β/H-15, H-18, H-19; N(1)-H/H-6α, H-12, H-17α.

Acetylation of polyneurine L (54): To a solution of **54** (3.5 mg, 0.0094 mmol) in CH_2Cl_2 (2 mL) and pyridine (25 μL) was added 4-dimethylaminopyridine (0.2 mg, 0.0016 mmol) and acetic anhydride (15 μL, 0.16 mmol), and the mixture was stirred at room temperature. The progress of the reaction was monitored by TLC. When the TLC showed ca. 95% completion, the reaction was quenched with 5% Na_2CO_3 and extracted with CH_2Cl_2 (3 x 10 mL). The combined organic phase was washed with water, dried (anhydrous Na_2SO_4), the solvent evaporated, and the residue was purified via preparative radial chromatography (SiO_2, $CHCl_3$–MeOH, 0–5%, NH_3-saturated) to give 20-*O*-acetyl-polyneurine L **54a** (3 mg, 86%).

20-*O*-Acetyl-polyneurine L (54a): light yellowish oil; $[\alpha]^{25}_{D}$ –13 (*c* 0.14, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 219 (–9.91), 238 (+7.84) nm; UV (EtOH) λ_{max} (log ε) 226 (4.68), 283 (3.89), 292 (3.78) nm; IR (ATR) ν_{max} 3366, 1734 cm^{-1}; HRESIMS *m/z* 415.2231 $[M + H]^+$ (calcd for $C_{23}H_{30}N_2O_5$ + H, 415.2233). ^1H NMR and ^{13}C NMR data, see Table 2.36. HMBC: ^2J H-3 to C-14; H-6 to C-7; H-11 to C-12; H-14 to C-17; H-15 to C-20; H-17 to C-14, C-16; H-18 to C-19; H-19 to C-18, C-20; H-21 to C-20; N(1)-H to C-13. ^3J H-3 to C-5, C-15, C-17; H-5 to C-7; H-6 to C-2; H-9 to C-7, C-11, C-13; H-10 to C-8, C-12; H-11 to C-9, C-13; H-12 to C-8, C-10; H-15 to C-17, C-19, C-21; H-17 to C-2, C-3, C-15; H-18 to C-20; H-19 to C-15, C-21; H-20 to C-15, C-19; CO_2Me to CO_2Me; 20-OCO*Me* to 20-O*C*OMe; N(1)-H to C-7, C-8. NOESY: H-3β/H-15; H-3α/H-3β, H-14; H-5/H-6α, H-6β; H-6β/H-6α; H-9/H-6α, H-10; H-14/H-15, H-19; H-15/H-18, H-19; H-17β/H-15; H-17α/H-14, H-17β; H-19/H-18; H-21α/H-14, H-15, H-18, H-19; H-21β/H-15, H-18, H-19; N(1)-H/H-6α, H-12, H-17α.

Voaphylline (55): light yellowish oil; $[\alpha]^{25}_{D}$ +21 (*c* 0.71, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 229 (4.38), 285 (3.79), 293 (3.77) nm; IR (dry film) ν_{max} 3402 cm^{-1}; ESIMS *m/z* 297 $[M + H]^+$ (calcd for $C_{19}H_{24}N_2O$ + H). ^1H NMR and ^{13}C NMR data, see Tables 2.37 and 2.38, respectively.

Voaphylline-7-hydroxyindolenine (56): light yellowish oil; $[\alpha]^{25}_{D}$ –87 (*c* 0.22, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 200 (+2.06), 221 (–0.92), 238 (+2.29), 261 (–0.39) nm; UV (EtOH) λ_{max} (log ε) 225 (3.70), 231 (3.65), 263 (2.95), 288 (3.18) nm; IR (dry film) ν_{max} 3400 cm^{-1}; ESIMS *m/z* 312 $[M]^+$ (calcd for $C_{19}H_{24}N_2O_2$). ^1H NMR and ^{13}C NMR data, see Tables 2.37 and 2.38, respectively.

Voaphyllinediol (57): yellowish oil; $[\alpha]^{25}_{D}$ +10 (*c* 0.21, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 228 (4.51), 285 (3.94), 292 (3.91) nm; IR (ATR) ν_{max} 3554 cm^{-1}; HRDARTMS *m/z* 315.2074 $[M + H]^+$ (calcd for $C_{19}H_{26}N_2O_2$ + H, 315.2073). ^1H NMR and ^{13}C NMR data, see Tables 2.37 and 2.38, respectively.

Antirhine (58): colorless oil; $[\alpha]^{25}_{D}$ –25 (*c* 0.32, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 225 (4.41), 282 (3.80), 289 (3.68) nm; HRESIMS *m/z* 297.1972 $[M + H]^+$ (calcd for $C_{19}H_{24}N_2O$ + H, 297.1967). ^1H NMR and ^{13}C NMR data, see Table 2.39.

14,15-Dehydro-16-*epi*-vincamine (59): light yellowish oil; $[\alpha]^{25}_{D}$ +9 (*c* 0.05, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 226 (4.57), 275 (4.01), 291 (3.89) nm; IR (dry film) ν_{max} 3344, 1737 cm^{-1}; HRDARTMS *m/z* 353.1866 $[M + H]^+$ (calcd for $C_{21}H_{24}N_2O_3$ + H, 353.1860). ^1H NMR and ^{13}C NMR data, see Table 2.40.

Tubotaiwine (60): light yellowish oil; $[\alpha]^{25}_{D}$ +609 (*c* 0.19, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 210 (4.43), 231 (3.82), 295 (3.57) nm; IR (dry film) ν_{max} 3361, 1673 cm^{-1}; ESIMS *m/z* 325 $[M + H]^+$ (calcd for $C_{20}H_{24}N_2O_2$ + H). ^1H NMR and ^{13}C NMR data, see Tables 2.41 and 2.42, respectively.

Tubotaiwine *N*(4)-oxide (61): light yellowish oil; $[\alpha]^{25}_{D}$ +360 (*c* 0.04, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 229 (4.03), 294 (3.76), 327 (3.81) nm; IR (dry film) ν_{max} 3373, 1679 cm^{-1}; HRESIMS *m/z* 341.1867 $[M + H]^+$ (calcd for $C_{20}H_{24}N_2O_3$ + H, 341.1860). ^1H NMR and ^{13}C NMR data, see Tables 2.41 and 2.42, respectively.

***N*(4)-Chloromethyl-tubotaiwine chloride (62):** light yellowish oil; $[\alpha]^{25}_{D}$ +323 (*c* 0.08, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 229 (3.89), 293 (3.75), 329 (3.84) nm; IR (dry film) ν_{max} 3353, 1681 cm^{-1}; HRESIMS *m/z* 373.1677 $[M]^+$ (calcd for $C_{21}H_{26}ClN_2O_2^+$). ^1H NMR and ^{13}C NMR data, see Tables 2.41 and 2.42, respectively.

Janetine (63): yellowish oil; UV (EtOH) λ_{max} (log ε) 240 (4.75), 250 (4.62), 262 (4.48), 289 (4.21), 299 (4.39), 328 (3.76), 342 (3.65) nm; HRESIMS *m/z* 251.1547 $[M + H]^+$ (calcd for $C_{17}H_{18}N_2$ + H, 251.1543). ^1H NMR and ^{13}C NMR data, see Tables 2.41 and 2.42, respectively.

Harmane (64): yellowish oil; UV (EtOH) λ_{max} (log ε) 213 (3.98), 235 (4.27), 250 (4.07), 289 (3.29), 335 (3.39) nm; IR (dry film) ν_{max} 3420 cm^{-1}; ESIMS *m/z* 182 $[M]^+$ (calcd for $C_{12}H_{10}N_2$). ^1H NMR and ^{13}C NMR data, see Table 2.43.

Taberdivamine B (65): brownish oil; $[\alpha]^{25}_{D}$ −118 (*c* 0.16, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 220 (4.42), 276 (3.98) nm; IR (dry film) ν_{max} 3405, 1640 cm^{-1}; HRESIMS *m/z* 323.1759 $[M + H]^+$ (calcd for $C_{20}H_{22}N_2O_2$ + H, 323.1754). ^1H NMR and ^{13}C NMR data, see Table 2.43.

Polyneurine P (66): light yellowish oil; $[\alpha]^{25}_{D}$ −103 (*c* 0.45, $CHCl_3$); ECD (MeOH), λ_{max} ($\Delta\varepsilon$) 205 (+7.57), 224 (−88.76), 241 (+41.89), 301 (−19.93) nm; UV (EtOH) λ_{max} (log ε) 225 (4.20), 288 (4.68) nm; IR (dry film) ν_{max} 3373, 1714 cm^{-1}; HRESIMS *m/z* 691.3870 $[M + H]^+$ (calcd for $C_{42}H_{50}N_4O_5$ + H, 691.3854). ^1H NMR and ^{13}C NMR data, see Table 2.44. HMBC: ^2J H-3 to C-2, C-14, C-10'; H-5 to C-16; H-6 to C-5, C-7; H-9 to C-8; H-10 to C-9, C-11; H-11 to C-12; H-12 to C-13; H-14 to C-3, C-15; H-15 to C-

20; H-16 to C-5, C-15, *C*O_2Me; H-18 to C-19; H-19 to C-18; H-21 to C-20; N(1)-H to C-2; H-3' to C-14'; H-5' to C-6'; H-6' to C-5', C-7'; H-11' to C-12'; H-12' to C-13'; H-15' to C-14'; H-17' to C-14'; H-18' to C-19'; H-19' to C-20'; H-20' to C-15'; N(1)-H' to C-2'. ^3J H-3 to C-7, C-9', C-11'; H-6 to C-2, C-8, C-16; H-9 to C-11, C-13; H-10 to C-8, C-12; H-11 to C-13; H-12 to C-8, C-10; H-14 to C-10'; H-15 to C-5, C-19; H-18 to C-20; H-19 to C-15, C-21; H-21 to C-5, C-15, C-19; CO_2*Me* to *C*O_2Me; N(4)-Me to C-5, C-21; N(1)-H to C-7, C-8; H-3' to C-5', C-17'; H-5' to C-3', C-7', C-21'; H-6' to C-2', C-8'; H-9' to C-3, C-7', C-11', C-13'; H-11' to C-3, C-9', C-13'; H-12' to C-8', C-10'; H-15' to C-3', C-17', C-19'; H-17' to C-2', C-3', C-21', *C*O_2Me'; H-18' to C-20'; H-19' to C-15', C-21'; H-20' to C-16', C-18'; H-21' to C-2', C-3', C-15', C-17', C-19', *C*O_2Me'; CO_2*Me*' to *C*O_2Me'; N(1)-H' to C-7', C-8'. 1D/2D NOESY: H-3β/H-14, H-15, N(1)-H, H-9', H-11'; H-5/H-16, N(4)-Me; H-9/H-6β, H-10; H-15/H-16, H-18; H-19/H-18, H-21; N(1)-H/H-3β, H-12; H-3'a/H-3'b, H-5'β, H-14', H-17'β; H-5'β/H-6'a; H-5'α/H-6'b; H-9'/H-3β, H-6'a, H-6'b; H-11'/H-3β; H-12'/H-11'; H-19'/H-15', H-18', H-20'; H-20'/H-15'α, H-18', H-19', H-21'; H-21'/H-5'α, H-18', H-19', H-20'; N(1)-H'/H-12', H-17'β, H-17'α.

Tabernamine (67): light yellowish oil; $[\alpha]^{25}_D$ –20 (*c* 0.09, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 234 (4.56), 287 (4.01), 294 (4.00) nm; IR (dry film) ν_{max} 3396, 1720 cm^{-1}; HRESIMS *m/z* 617.3846 $[M + H]^+$ (calcd for $C_{40}H_{48}N_4O_2$ + H, 617.3851). ^{1}H NMR and ^{13}C NMR data, see Tables 2.45 and 2.46, respectively.

19'(*R*)-Hydroxytabernamine (68): light yellowish oil; $[\alpha]^{25}_D$ –139 (*c* 0.13, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 231 (4.59), 286 (4.07), 295 (4.02) nm; IR (dry film) ν_{max} 3391, 1721 cm^{-1}; HRESIMS *m/z* 632.3732 $[M]^+$ (calcd for $C_{40}H_{48}N_4O_3$, 632.3726). ^{1}H NMR and ^{13}C NMR data, see Tables 2.45 and 2.46, respectively.

Ervahaimine A (69): light yellowish oil; $[\alpha]^{25}_{D}$ –58 (*c* 0.31, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 233 (4.55), 289 (4.13), 296 (4.02) nm; IR (dry film) ν_{max} 3320, 1724 cm^{-1}; HRESIMS *m/z* 689.3717 $[M + H]^+$ (calcd for $C_{42}H_{48}N_4O_5$ + H, 689.3697). ^1H NMR and ^{13}C NMR data, see Tables 2.47 and 2.48, respectively.

Ervahaimine B (70): light yellowish oil; $[\alpha]^{25}_{D}$ –103 (*c* 0.24, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 233 (4.56), 289 (4.00), 296 (3.90) nm; IR (dry film) ν_{max} 3380, 1730 cm^{-1}; HRESIMS *m/z* 689.3717 $[M + H]^+$ (calcd for $C_{42}H_{48}N_4O_5$ + H, 689.3698). ^1H NMR and ^{13}C NMR data, see Tables 2.47 and 2.48, respectively.

Conophylline (71): light yellowish oil; $[\alpha]^{25}_{D}$ –117 (*c* 0.45, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 206 (4.59), 240 (4.45), 310 (4.48), 334 (4.59) nm; IR (dry film) ν_{max} 3382, 1673 cm^{-1}; HRESIMS *m/z* 795.3600 $[M + H]^+$ (calcd for $C_{44}H_{50}N_4O_{10}$ + H, 795.3605). ^1H NMR and ^{13}C NMR data, see Tables 2.49 and 2.50, respectively.

Conophylline quinone (72): reddish-orange amorphous solid; $[\alpha]^{25}_{D}$ –138 (*c* 0.25, $CHCl_3$); UV (EtOH) λ_{max} (log ε) 202 (4.63), 248 (4.46), 329 (4.56), 393 (4.17) nm; IR (dry film) ν_{max} 3373, 1679 cm^{-1}; ESIMS *m/z* 793 $[M + H]^+$ (calcd for $C_{44}H_{48}N_4O_{10}$ + H). ^1H NMR and ^{13}C NMR data, see Tables 2.49 and 2.50, respectively.

3.10 Cytotoxicity Assays

The human cancer cell lines (HT-29, HCT 116, MCF7, MDA-MB-231, A549, and PC-3) were purchased from American Type Culture Collection (ATCC), USA. The MCF7, PC-3, and A549 cells were cultured in RPMI 1650 medium. MDA-MB-231

cells were cultured in Eagle's medium (DMEM). HT-29 and HCT 116 cells were cultured in McCoy's 5A medium. Cytotoxicity assays were carried out based on the same procedures as in previous publications (Lim *et al.*, 2014). All media were supplemented with 10% fetal bovine serum, 2% penicillin/streptomycin, and 1% amphotericin. The cells were cultured at 37 °C under a humidified atmosphere in a CO_2 incubator, which were then seeded in a 96-well microtiter plate (Nunc, Germany) at a concentration of approximate 70,000 cells/mL and incubated again in a CO_2 incubator at 37 °C for 24 hours prior to treatment with samples at six different concentrations (0.1, 0.3, 1, 3, 10, and 30 μg/mL). The treated cells were incubated for 72 hours. The wells containing untreated cells (without addition of sample) were regarded as negative control whereas cells treated with doxorubicin or cisplatin served as positive control. The samples were diluted with DMSO. To avoid any adverse effect resulting from excess DMSO, the final concentration of DMSO in each well shall not exceed 0.5% (v/v). At the end of the incubation, 20 μL of MTT working solution (5 mg MTT in 1 mL phosphate-buffered saline) was added into each well, and the 96-well microtiter plate was incubated at 37 °C for another three hours. The medium was then gently aspirated from each well, followed by addition of 200 μL of DMSO to solubilize the formazan crystals. After 15 minutes of agitation, the absorbance of each well was measured from 540 to 650 nm using a microplate reader (Emax, Molecular Devices, USA). The cytotoxic activity of each sample was expressed as IC_{50} value, which indicates the sample concentration that causes 50% inhibition of cell growth. All samples were assayed in three independent experiments.

CHAPTER 4: CONCLUSION

A total of 72 alkaloids were isolated and characterized from the bark and leaf extracts of *Tabernaemontana polyneura*. The bark extract yielded 16 new alkaloids of various skeletal types. The biosynthetic pathways towards several new alkaloids were also proposed. Additionally, the present study substantiated the medicinal potential of *T. polyneura* as highlighted by the observed cytotoxic effects of the bisindole alkaloids.

This comprehensive study represents a significant advancement in our understanding of the chemical composition and biological aspect of *T. polyneura*, effectively bridging a notable gap in prior research. Moreover, the observed disparity in alkaloid content between specimens from different geographical locations suggested variability in alkaloid composition within the same species.

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