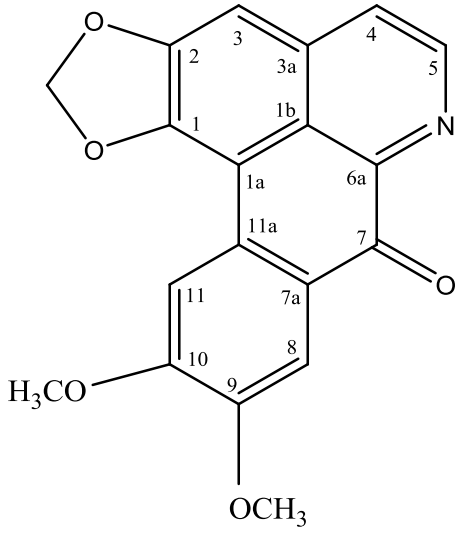
3.2.7 Alkaloid CD7: Dicentrinone 67



67

Alkaloid **CD7** was afforded as a yellow solid from the bark of *C. densiflora*. The UV spectrum showed absorption at 295 nm, indicated that it possessed an oxoaphorpine skeleton[67]. The IR spectrum showed a strong absorption at 1644 cm^{-1} which indicated the presence of a conjugated carbonyl group. The presence of a methylenedioxyl group was proven by its characteristic absorptions at 1262 and 983 cm^{-1} which indicated asymmetric O-C-O stretching. The ESIMS (positive mode) spectrum revealed a molecular ion peak at m/z 336.08 corresponding to a possible molecular formula of $C_{19}H_{13}NO_5$, with fourteen degrees of unsaturation.

The ^{1}H-NMR spectrum (Table 3.7 and Figure 3.34) revealed the characteristic of AB *dd*, typical of an oxoaporphinic H-4 and H-5 coupling pattern. A coupling constant of 5.36 Hz for H-4 and H-5 was small compared to the normal *cis* pattern coupling. This is due to the fact that H-5 is adjacent to *N* atom. H-5 resonated more downfield at δ 8.87 compared to H-4 at δ 7.76. A singlet peak was observed at δ 7.18 attributed to H-3 indicating that, C-1 and C-2 could be substituted by methylenedioxy group. This group

was observed as a singlet at δ 6.13. Two distinct methoxyl signals appeared as singlet at δ 3.99 and 4.08 which most probably attached to C-9 and C-10, respectively. Two other aromatic protons were observed at δ 8.67 (*s*, H-11) and 7.99 (*s*, H-8). H-11 has the highest chemical shift due the deshielding effect caused by ring A and most probably forming the hydrogen bonding with the methylenedioxy group. Due to the limitation of the sample amount, we were unable to get its 2D NMR spectrum including HMBC spectrum.

Comparison of the empirical data obtained with the literature values of the known compound [102-106] confirmed that alkaloid **CD7** is dicentrinone **67**.

Table 3.7: ^{1}H NMR (in $CDCl_3$, 400 MHz) of **67** and ^{1}H NMR of dicentrinone[105].

Position	δ_H, ppm (J in Hz)	δ_H, ppm (J in Hz) dicentrnone[105]
3	7.18, *s*	7.16, *s*
4	7.76, *d*, *J* = 5.36	7.74, *d*, *J* = 5.49
5	8.87, *d*, *J* = 5.36	8.86, *d*, *J* = 5.49
8	7.99, *s*	7.97 *s*
11	8.67, *s*	8.64 *s*
1,2-OCH_2O	6.13, *s*	6.13, *s*
9-OMe	3.99, *s*	3.99, s
10-OMe	4.08, *s*	4.08, *s*

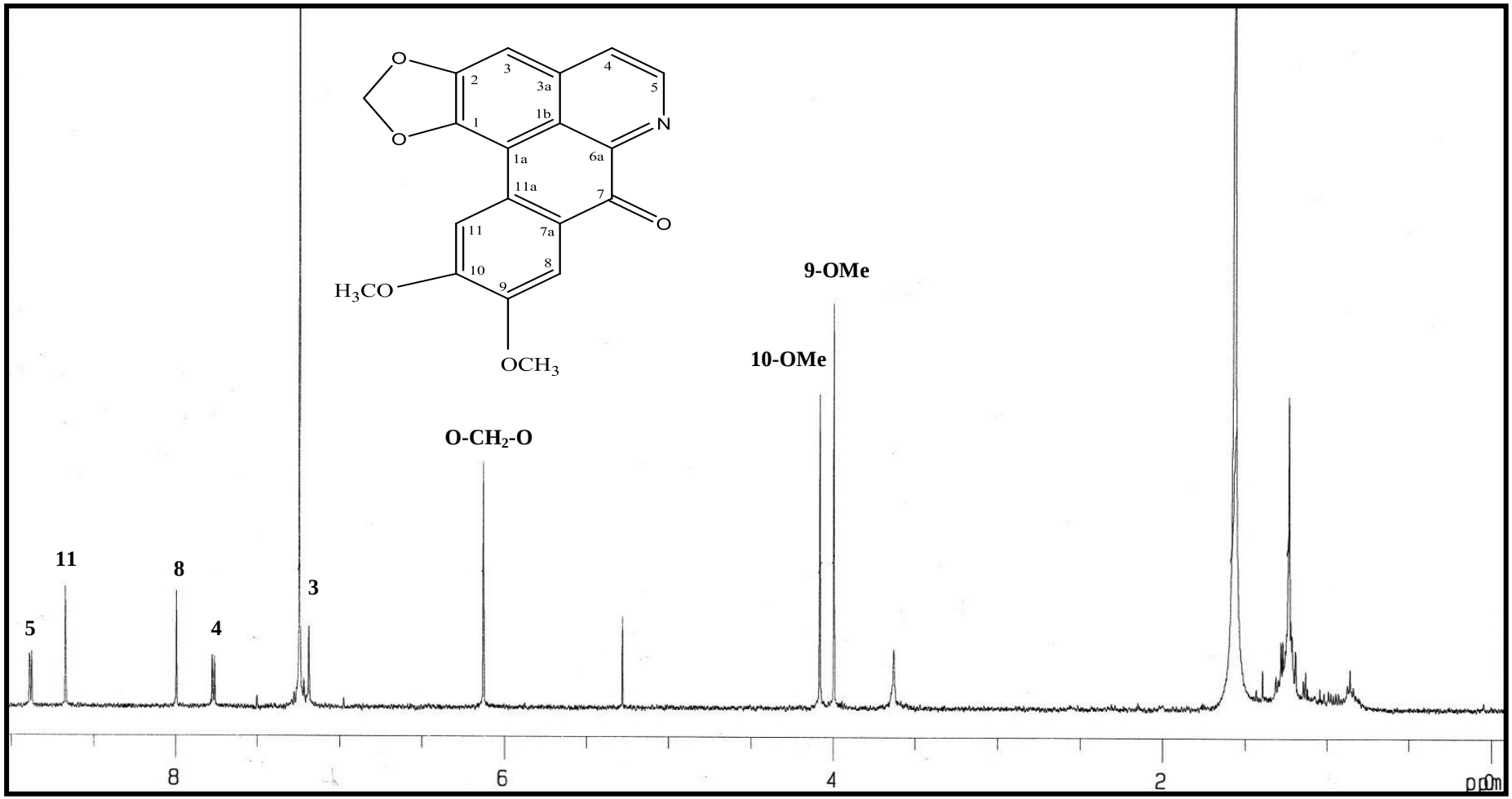


Figure 3.34: ^{1}H NMR Spectrum of Dicentrinone **67**

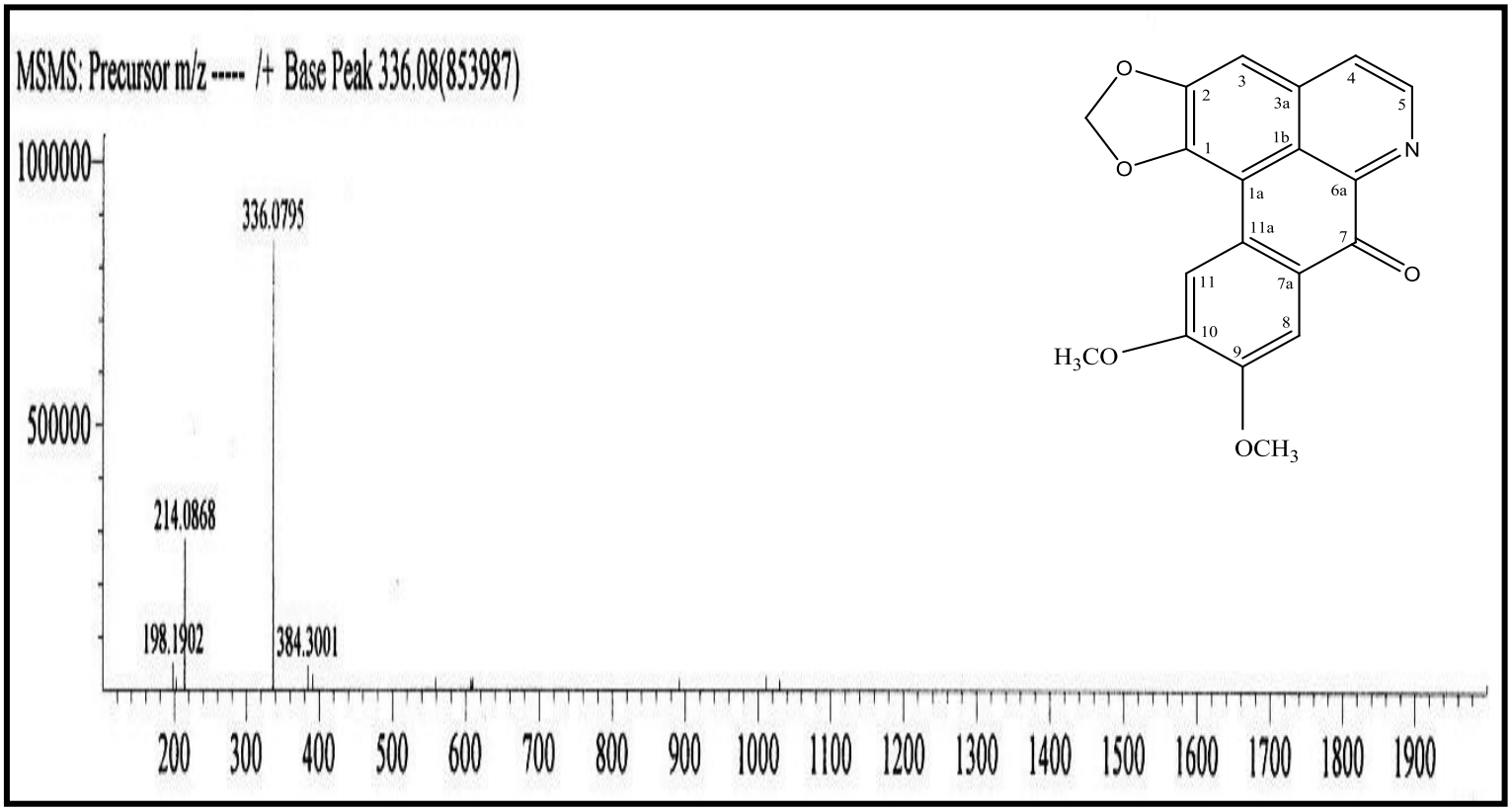


Figure 3.35: LCMS Spectrum of Dicentrinone **67**