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APPENDIX 1

DOCKING OUTPUT FILES

4-OH Panduratin A Docking Output file (extracted from *.dlg file)

```
Number of distinct conformational clusters found = 6,  out of 100 runs,
Using an rmsd-tolerance of 0.5 A


        CLUSTERING HISTOGRAM
        ____________________

_____|____________|_____|____________|_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|
     |            |     |            |     |
Clus | Lowest     | Run | Mean       | Num | Histogram
-ter | Docked     |     | Docked     | in  |
Rank | Energy     |     | Energy     | Clus|    5    10   15   20   25   30   35   40   45   50   55   60   65   70   75   80
_____|____________|_____|____________|_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|_____:_____|
   1 |    -10.23  |   9 |    -10.16  |   9 |#########
   2 |    -10.13  |  93 |    -10.02  |  30 |##############################
   3 |    -10.02  |  63 |     -9.93  |   9 |#########
   4 |     -9.99  |  21 |     -9.91  |   7 |#######
   5 |     -9.88  |  96 |     -9.84  |   8 |########
   6 |     -9.54  |  18 |     -9.48  |  37 |#####################################
_____|____________|_____|____________|_____|_____________________________________


MODEL        9
USER    Run = 9
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 9
USER
USER    RMSD from reference structure       = 2.977 A
USER
USER    Estimated Free Energy of Binding    =   -7.38 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +3.86e-06       [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.23 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =   -8.94 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -1.29 kcal/mol
USER    (3) Torsional Free Energy           =   +1.56 kcal/mol
USER
USER
USER    DPF = 10-4-oh-panduratin-ns2b3-b4-1-606060box-r.dpf
USER    NEWDPF move       10-4-oh-panduratin.pdbq
USER    NEWDPF about      21.343000 70.076698 35.802601
USER    NEWDPF tran0      22.738017 69.630442 37.963966
USER    NEWDPF quat0      0.155462 0.220579 -0.962900 -156.276329
USER    NEWDPF ndihe      8
USER    NEWDPF dihe0      -61.70 98.59 15.25 24.50 -32.20 -14.34 151.47 -25.14
USER
USER                             x       y       z     vdW   Elec       q     RMS
ATOM      1  C1_____ <1> d      22.625  66.413  34.750 -0.68 +0.01    +0.043  2.977
ATOM      2  C13____ <1> d      21.767  69.250  37.301 -0.36 -0.00    +0.078  2.977
ATOM      3  C14____ <1> d      20.532  69.874  36.583 -0.24 +0.00    +0.034  2.977
ATOM      4  C20____ <1> d      22.694  68.557  36.251 -0.52 +0.00    +0.029  2.977
ATOM      5  C21____ <1> d      21.896  67.556  35.424 -0.64 -0.01    -0.082  2.977
ATOM      6  C22____ <1> d      20.566  67.683  35.237 -0.38 +0.00    -0.023  2.977
ATOM      7  C23____ <1> d      19.716  68.758  35.875 -0.38 +0.00    +0.037  2.977
ATOM      8  C11____ <1> d      22.539  70.236  38.164 -0.27 -0.01    +0.170  2.977
ATOM      9  O12____ <1> d      22.926  71.311  37.703 +0.16 +0.00    -0.292  2.977
ATOM     10  A6_____ <1> d      23.007  69.846  39.505 -0.27 -0.01    +0.076  2.977
ATOM     11  A5_____ <1> d      24.145  69.138  39.664 -0.39 -0.03    +0.085  2.977
ATOM     12  A7_____ <1> d      22.216  70.232  40.692 -0.23 -0.01    +0.085  2.977
ATOM     13  A4_____ <1> d      24.598  68.767  41.015 -0.09 -0.03    +0.074  2.977
ATOM     14  A8_____ <1> d      23.882  69.125  42.097 -0.35 -0.03    +0.071  2.977
ATOM     15  A3_____ <1> d      22.639  69.889  41.924 -0.28 -0.01    +0.074  2.977
ATOM     16  O2_____ <1> d      24.279  68.796  43.351 -0.11 +0.17    -0.361  2.977
ATOM     17  H32____ <1> d      24.365  67.899  43.622 -0.18 -0.23    +0.217  2.977
ATOM     18  O10____ <1> d      21.066  70.936  40.531 +0.13 +0.02    -0.360  2.977
ATOM     19  H31____ <1> d      21.071  71.868  40.398 +0.11 -0.01    +0.217  2.977
ATOM     20  O9_____ <1> d      24.871  68.750  38.586 -0.44 +0.05    -0.360  2.977
ATOM     21  H30____ <1> d      25.534  68.086  38.653 -0.21 -0.05    +0.217  2.977
ATOM     22  C19____ <1> d      23.428  69.558  35.300 -0.34 +0.01    +0.037  2.977
ATOM     23  C18____ <1> d      24.925  69.566  35.521 -0.67 -0.01    -0.024  2.977
ATOM     24  C16____ <1> d      25.669  70.687  35.618 -0.60 -0.01    -0.091  2.977
ATOM     25  C15____ <1> d      25.091  72.081  35.500 -0.41 +0.00    +0.042  2.977
ATOM     26  C17____ <1> d      27.154  70.572  35.890 -0.62 +0.00    +0.042  2.977
ATOM     27  A27____ <1> d      19.634  70.657  37.532 -0.11 -0.00    -0.053  2.977
ATOM     28  A26____ <1> d      19.581  72.003  37.460 -0.04 +0.00    +0.007  2.977
ATOM     29  A28____ <1> d      18.821  69.965  38.555 -0.19 -0.00    +0.007  2.977
ATOM     30  A24____ <1> d      18.736  72.769  38.387 -0.02 +0.00    +0.001  2.977
ATOM     31  A25____ <1> d      18.007  72.132  39.320 -0.03 +0.00    +0.000  2.977
ATOM     32  A29____ <1> d      18.052  70.667  39.407 -0.11 -0.00    +0.001  2.977
TER
ENDMDL
```

Panduratin A Docking Output file (extracted from *.dlg file)

```
Number of distinct conformational clusters found = 9,  out of 100 runs,
Using an rmsd-tolerance of 0.5 A


        CLUSTERING HISTOGRAM
        ____________________

_____|___________|_____|___________|_____|
     |           |     |           |     |
Clus | Lowest    | Run | Mean      | Num | Histogram
-ter | Docked    |     | Docked    | in  |
Rank | Energy    |     | Energy    | Clus|    5    10   15   20   25   30   35
_____|___________|_____|___________|_____|____:____|____:____|____:____|____:___
   1 |    -10.20 |  32 |    -10.16 |   3 |###
   2 |    -10.11 |  14 |    -10.04 |  34 |##################################
   3 |    -10.03 |  46 |     -9.95 |  27 |###########################
   4 |    -10.01 |   9 |     -9.96 |   7 |#######
   5 |     -9.94 |  80 |     -9.85 |   4 |####
   6 |     -9.90 |  82 |     -9.86 |   2 |##
   7 |     -9.87 |  13 |     -9.86 |   2 |##
   8 |     -9.77 |  73 |     -9.77 |   1 |#
   9 |     -9.59 |  96 |     -9.52 |  20 |####################
_____|___________|_____|___________|_____|_____________________________________


MODEL       14
USER    Run = 14
USER    Cluster Rank = 2
USER    Number of conformations in this cluster = 34
USER
USER    RMSD from reference structure       = 3.674 A
USER
USER    Estimated Free Energy of Binding    =   -7.70 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +2.28e-06       [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.11 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =   -9.56 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.55 kcal/mol
USER    (3) Torsional Free Energy           =   +1.87 kcal/mol
USER
USER
USER    DPF = 10-panduratin-a-ns2b3-b4-1-606060box-r.dpf
USER    NEWDPF move       10-panduratin-a.pdbq
USER    NEWDPF about      21.245399 70.046204 35.711201
USER    NEWDPF tran0      24.146369 70.570682 38.992737
USER    NEWDPF quat0      0.188694 0.368220 -0.910389 176.863752
USER    NEWDPF ndihe      8
USER    NEWDPF dihe0      63.19 -88.38 65.15 -31.17 -0.94 -10.82 122.24 -51.81
USER
USER                                x       y       z    vdW   Elec       q     RMS
ATOM      1  C1_____ <1> d      26.036  68.609  35.407 -0.68 +0.01    +0.043  3.674
ATOM      2  C2_____ <1> d      23.513  69.966  38.073 -0.38 -0.00    +0.078  3.674
ATOM      3  C3_____ <1> d      22.281  70.214  37.150 -0.26 +0.00    +0.034  3.674
ATOM      4  C4_____ <1> d      24.827  70.049  37.227 -0.49 +0.00    +0.029  3.674
ATOM      5  C5_____ <1> d      24.750  69.101  36.037 -0.63 -0.02    -0.082  3.674
ATOM      6  C6_____ <1> d      23.572  68.723  35.500 -0.55 -0.01    -0.023  3.674
ATOM      7  C7_____ <1> d      22.220  69.118  36.049 -0.44 +0.00    +0.037  3.674
ATOM      8  C8_____ <1> d      23.570  70.881  39.287 -0.29 -0.02    +0.170  3.674
ATOM      9  O9_____ <1> d      23.912  72.060  39.170 +0.13 +0.03    -0.292  3.674
ATOM     10  A10____ <1> d      23.449  70.320  40.644 -0.31 -0.02    +0.076  3.674
ATOM     11  A11____ <1> d      24.317  69.295  41.070 -0.32 -0.03    +0.085  3.674
ATOM     12  A12____ <1> d      22.463  70.805  41.528 -0.22 -0.01    +0.085  3.674
ATOM     13  A13____ <1> d      24.208  68.776  42.372 -0.23 -0.03    +0.074  3.674
ATOM     14  A14____ <1> d      23.236  69.265  43.261 -0.34 -0.02    +0.073  3.674
ATOM     15  A15____ <1> d      22.363  70.280  42.829 -0.24 -0.01    +0.074  3.674
ATOM     16  O16____ <1> d      23.188  68.716  44.507 -0.05 +0.17    -0.356  3.674
ATOM     17  C17____ <1> d      22.126  68.000  45.058 -0.41 -0.11    +0.210  3.674
ATOM     18  O18____ <1> d      21.616  71.786  41.131 +0.18 +0.02    -0.360  3.674
ATOM     19  H19____ <1> d      20.781  71.592  40.743 +0.11 -0.01    +0.217  3.674
ATOM     20  O20____ <1> d      25.246  68.794  40.216 -0.12 +0.16    -0.360  3.674
ATOM     21  H21____ <1> d      25.210  67.904  39.914 -0.24 -0.21    +0.217  3.674
ATOM     22  C28____ <1> d      25.161  71.492  36.729 -0.39 +0.00    +0.037  3.674
ATOM     23  C29____ <1> d      26.651  71.766  36.729 -0.56 -0.00    -0.024  3.674
ATOM     24  C30____ <1> d      27.222  72.834  36.134 -0.59 -0.01    -0.091  3.674
ATOM     25  C32____ <1> d      28.720  73.031  36.241 -0.70 +0.01    +0.042  3.674
ATOM     26  C31____ <1> d      26.437  73.884  35.376 -0.49 +0.00    +0.042  3.674
ATOM     27  A22____ <1> d      20.967  70.258  37.916 -0.16 +0.00    -0.053  3.674
ATOM     28  A23____ <1> d      20.218  71.452  37.947 -0.06 +0.00    +0.007  3.674
ATOM     29  A24____ <1> d      20.467  69.125  38.591 -0.21 -0.00    +0.007  3.674
ATOM     30  A25____ <1> d      19.003  71.517  38.651 -0.06 +0.00    +0.001  3.674
ATOM     31  A26____ <1> d      18.521  70.386  39.328 -0.15 -0.00    +0.000  3.674
ATOM     32  A27____ <1> d      19.255  69.189  39.296 -0.31 -0.00    +0.001  3.674
TER
ENDMDL
```

Ester 3 Docking Output file (extracted from *.dlg file)

```
Number of distinct conformational clusters found = 10,  out of 100 runs,
Using an rmsd-tolerance of 1.5 A


        CLUSTERING HISTOGRAM
        ____________________

_____|____________|_____|____________|_____|_____________________________________________________
     |            |     |            |     |
Clus | Lowest     | Run | Mean       | Num | Histogram
-ter | Docked     |     | Docked     | in  |
Rank | Energy     |     | Energy     | Clus|    5    10   15   20   25   30   35
_____|____________|_____|____________|_____|____:____|____:____|____:____|____:___
   1 |     -9.23 |  63 |     -8.90 |  55 |##########################################################
   2 |     -9.13 |   2 |     -8.67 |  33 |#################################
   3 |     -8.33 |   5 |     -8.31 |   2 |##
   4 |     -8.22 |  25 |     -7.98 |   3 |###
   5 |     -8.22 |  36 |     -8.22 |   1 |#
   6 |     -8.20 |  15 |     -8.20 |   1 |#
   7 |     -8.17 |  32 |     -8.17 |   1 |#
   8 |     -8.16 |  81 |     -8.15 |   2 |##
   9 |     -7.85 |  59 |     -7.85 |   1 |#
  10 |     -7.68 |  97 |     -7.68 |   1 |#
_____|____________|_____|____________|_____|_____________________________________________________


MODEL       63
USER    Run = 63
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 7
USER
USER    RMSD from reference structure       = 4.493 A
USER
USER    Estimated Free Energy of Binding    =   -6.10 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +3.36e-05       [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =   -9.23 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =   -8.90 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.32 kcal/mol
USER    (3) Torsional Free Energy           =   +2.80 kcal/mol
USER
USER
USER    DPF = 7-compound4-12-757-ns2b3-b4-1.dpf
USER    NEWDPF move       7-compound4-12-757-rigid.pdbq
USER    NEWDPF about      23.575300 70.044998 37.007500
USER    NEWDPF tran0      26.786331 70.847130 37.669288
USER    NEWDPF quat0      0.645909 0.660907 0.382103 -166.895328
USER    NEWDPF ndihe      10
USER    NEWDPF dihe0      -53.71 -81.71 -47.56 -70.73 54.04 168.06 -4.25 -131.79 120.60 84.73
USER
USER                            x       y       z    vdW   Elec        q     RMS
ATOM      1  A7_____ <1> d      27.254  72.065  36.108 -0.52 +0.01    +0.102  4.493
ATOM      2  A8_____ <1> d      26.489  72.346  37.336 -0.37 -0.00    +0.104  4.493
ATOM      3  A9_____ <1> d      25.663  71.403  37.830 -0.33 -0.01    +0.076  4.493
ATOM      4  A10____ <1> d      25.531  70.087  37.180 -0.47 +0.00    +0.114  4.493
ATOM      5  A11____ <1> d      26.234  69.828  36.057 -0.61 +0.00    +0.001  4.493
ATOM      6  A12____ <1> d      27.124  70.867  35.504 -0.44 +0.01    +0.051  4.493
ATOM      7  O13____ <1> d      26.696  73.558  37.924 +0.02 +0.00    -0.348  4.493
ATOM      8  C22____ <1> d      27.672  73.931  38.853 -0.39 -0.01    +0.185  4.493
ATOM      9  C1_____ <1> d      27.142  75.028  39.813 -0.35 -0.00    +0.138  4.493
ATOM     10  C2_____ <1> d      27.970  75.120  41.068 -0.31 -0.02    +0.260  4.493
ATOM     11  O3_____ <1> d      27.607  74.521  42.083 -0.27 -0.03    -0.265  4.493
ATOM     12  O4_____ <1> d      29.100  75.875  41.065 -0.30 -0.01    -0.322  4.493
ATOM     13  C5_____ <1> d      29.285  77.027  41.834 -0.38 +0.00    +0.174  4.493
ATOM     14  C6_____ <1> d      30.382  76.774  42.891 -0.37 +0.00    +0.034  4.493
ATOM     15  O14____ <1> d      28.075  73.048  35.643 -0.19 -0.02    -0.353  4.493
ATOM     16  C15____ <1> d      29.443  73.181  35.878 -0.72 +0.04    +0.210  4.493
ATOM     17  N16____ <1> d      24.679  69.125  37.780 -0.39 +0.00    -0.115  4.493
ATOM     18  O18____ <1> d      25.010  68.576  38.885 -0.47 +0.12    -0.532  4.493
ATOM     19  O17____ <1> d      23.455  69.047  37.424 -0.03 -0.01    -0.532  4.493
ATOM     20  C19____ <1> d      26.139  68.508  35.325 -0.56 +0.05    +0.205  4.493
ATOM     21  O20____ <1> d      24.963  68.505  34.506 -0.49 -0.24    -0.396  4.493
ATOM     22  H21____ <1> d      25.250  68.181  33.625 -0.97 +0.11    +0.209  4.493
TER
ENDMDL
```

CP14 Docking Output file (extracted from *.dlg file)

```
Number of distinct conformational clusters found = 6, out of 100 runs,
Using an rmsd-tolerance of 0.5 A


        CLUSTERING HISTOGRAM
        ____________________

_____________________________________________________________________________
    |             |     |             |     |
Clus | Lowest     | Run | Mean        | Num | Histogram
-ter | Docked     |     | Docked      | in  |
Rank | Energy     |     | Energy      | Clus|    5    10   15   20   25   30   35
_____|____________|_____|_____________|_____|____:____|____:____|____:____|____:___
   1 |    -11.44 |  21 |    -11.30 |  92
|#############################################################################################
   2 |    -11.08 |  11 |    -10.95 |   4 |####
   3 |    -10.93 |  85 |    -10.93 |   1 |#
   4 |    -10.86 |  52 |    -10.86 |   1 |#
   5 |    -10.71 |  56 |    -10.71 |   1 |#
   6 |    -10.66 |   9 |    -10.66 |   1 |#
_____|____________|_____|_____________|_____|_____________________________________


MODEL       21
USER    Run = 21
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 92
USER
USER    RMSD from reference structure       = 1.231 A
USER
USER    Estimated Free Energy of Binding    =   -8.70 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +4.21e-07       [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.44 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.57 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.87 kcal/mol
USER    (3) Torsional Free Energy           =   +1.87 kcal/mol
USER
USER
USER    DPF = 46-ns2b3-b4-1-606060box-r.dpf
USER    NEWDPF move       46.pdbq
USER    NEWDPF about      22.728701 69.597504 38.105499
USER    NEWDPF tran0      23.590250 69.499526 37.958079
USER    NEWDPF quat0      -0.638436 -0.758282 -0.131936 13.346826
USER    NEWDPF ndihe      8
USER    NEWDPF dihe0      45.14 73.40 -110.44 -61.43 166.03 -7.51 29.08 2.59
USER
USER                            x       y       z    vdW   Elec        q     RMS
ATOM      1  C1_____ <1> d      23.104  69.135  36.942 -0.45 +0.01    +0.102  1.231
ATOM      2  C2_____ <1> d      21.726  69.276  36.217 -0.37 +0.00    +0.034  1.231
ATOM      3  C3_____ <1> d      24.235  68.751  35.920 -0.52 +0.07    +0.232  1.231
ATOM      4  N4_____ <1> d      23.684  67.993  34.758 -0.59 +0.06    +0.088  1.231
ATOM      5  C5_____ <1> d      22.567  67.098  35.125 -0.68 +0.06    +0.271  1.231
ATOM      6  C6_____ <1> d      21.326  67.935  35.530 -0.50 +0.00    +0.040  1.231
ATOM      7  H31____ <1> d      24.436  67.413  34.376 -0.46 +0.36    +0.316  1.231
ATOM      8  C7_____ <1> d      23.422  70.355  37.794 -0.31 -0.00    +0.169  1.231
ATOM      9  O8_____ <1> d      23.397  71.471  37.269 +0.15 -0.00    -0.292  1.231
ATOM     10  A9_____ <1> d      23.289  70.289  39.263 -0.28 -0.01    +0.046  1.231
ATOM     11  A11____ <1> d      22.347  71.210  39.931 -0.15 -0.00    +0.018  1.231
ATOM     12  A10____ <1> d      23.995  69.409  40.005 -0.37 -0.04    +0.112  1.231
ATOM     13  A14____ <1> d      22.180  71.165  41.263 -0.17 -0.00    +0.004  1.231
ATOM     14  A13____ <1> d      22.943  70.205  42.067 -0.29 -0.01    +0.039  1.231
ATOM     15  A12____ <1> d      23.813  69.366  41.472 -0.35 -0.03    +0.099  1.231
ATOM     16  O15____ <1> d      24.881  68.573  39.409 -0.44 +0.14    -0.357  1.231
ATOM     17  H16____ <1> d      24.929  67.659  39.626 -0.52 -0.17    +0.217  1.231
ATOM     18  O35____ <1> d      24.525  68.476  42.207 -0.06 +0.17    -0.358  1.231
ATOM     19  H51____ <1> d      24.126  67.710  42.581 -0.44 -0.21    +0.217  1.231
ATOM     20  A22____ <1> d      20.622  69.735  37.159 -0.20 -0.00    -0.053  1.231
ATOM     21  A23____ <1> d      20.049  70.945  36.999 -0.09 +0.00    +0.007  1.231
ATOM     22  A24____ <1> d      20.188  68.885  38.290 -0.19 -0.00    +0.007  1.231
ATOM     23  A25____ <1> d      19.014  71.414  37.932 -0.06 +0.00    +0.001  1.231
ATOM     24  A26____ <1> d      18.634  70.639  38.961 -0.12 -0.00    +0.000  1.231
ATOM     25  A27____ <1> d      19.247  69.318  39.148 -0.30 -0.00    +0.001  1.231
ATOM     26  C17____ <1> d      25.033  69.950  35.316 -0.55 +0.01    +0.039  1.231
ATOM     27  C18____ <1> d      26.521  70.033  35.769 -0.73 +0.00    +0.033  1.231
ATOM     28  C19____ <1> d      26.774  71.002  36.959 -0.62 -0.00    +0.114  1.231
ATOM     29  C20____ <1> d      27.903  72.028  36.677 -0.63 +0.00    +0.039  1.231
TER
ENDMDL
```

Blind Docking of CP14 Docking Output file (extracted from *.dlg file)

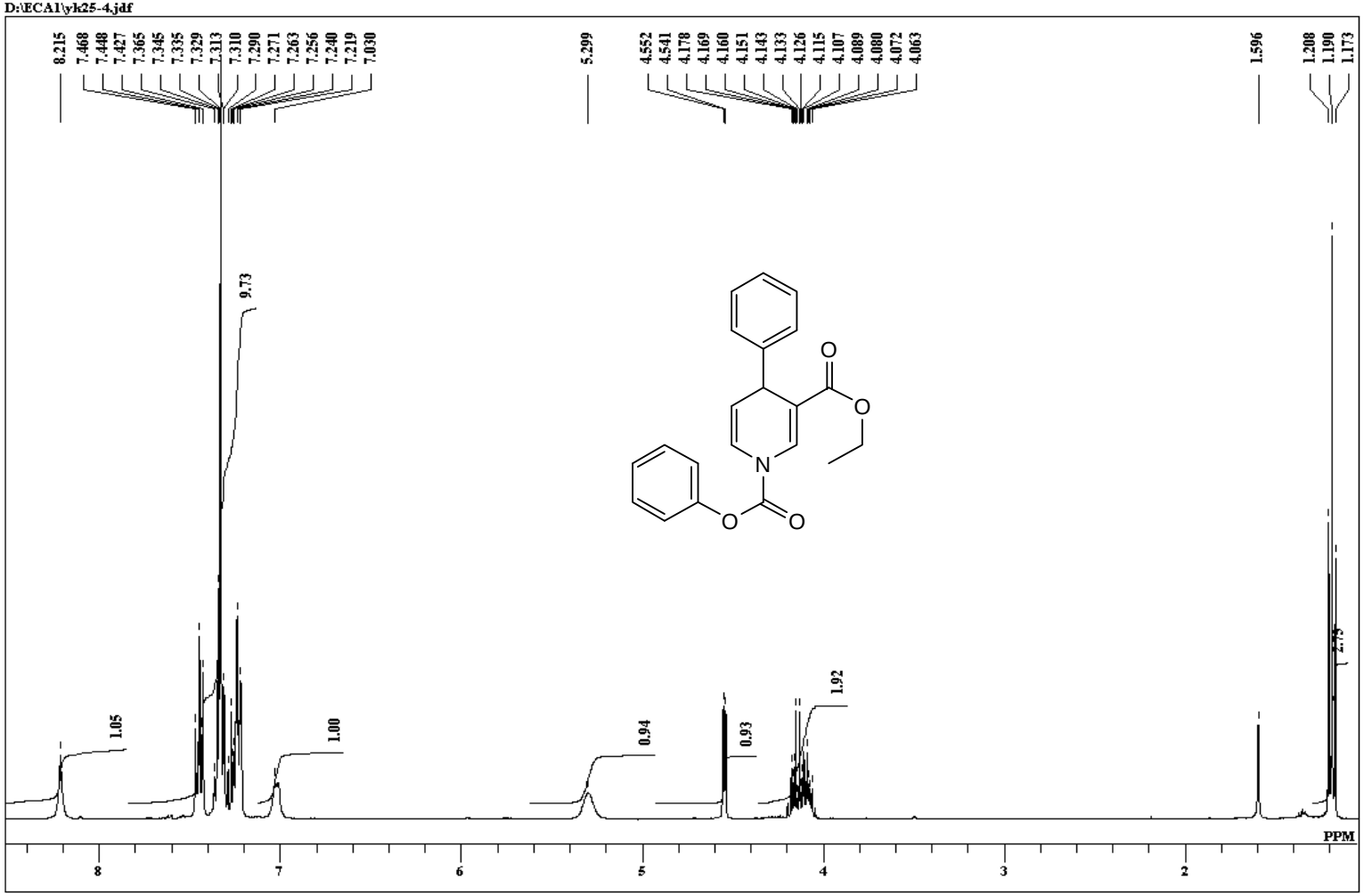
```
Number of distinct conformational clusters found = 5, out of 100 runs,
Using an rmsd-tolerance of 2.0 A


        CLUSTERING HISTOGRAM
        ____________________

_____________________________________________________________________________
     |            |     |            |     |
Clus | Lowest     | Run | Mean       | Num | Histogram
-ter | Docked     |     | Docked     | in  |
Rank | Energy     |     | Energy     | Clus|    5    10   15   20   25   30   35
_____|____________|_____|____________|_____|____:____|____:____|____:____|____:___
   1 |      -8.92 |  56 |      -8.92 |  65
|###################################################################
   2 |      -8.48 |  99 |      -8.48 |   5 |#####
   3 |      -8.31 |  27 |      -8.30 |   6 |######
   4 |      -7.98 |  43 |      -7.98 |  11 |###########
   5 |      -7.62 |  36 |      -7.62 |  13 |#############
_____|____________|_____|____________|_____|_____________________________________
Number of multi-member conformational clusters found = 5, out of 100 runs.

_
```

APPENDIX 2

^{1}H and ^{13}C NMR SPECTRUM OF SYNTHESISED MOLECULES

single_pulse-yk25

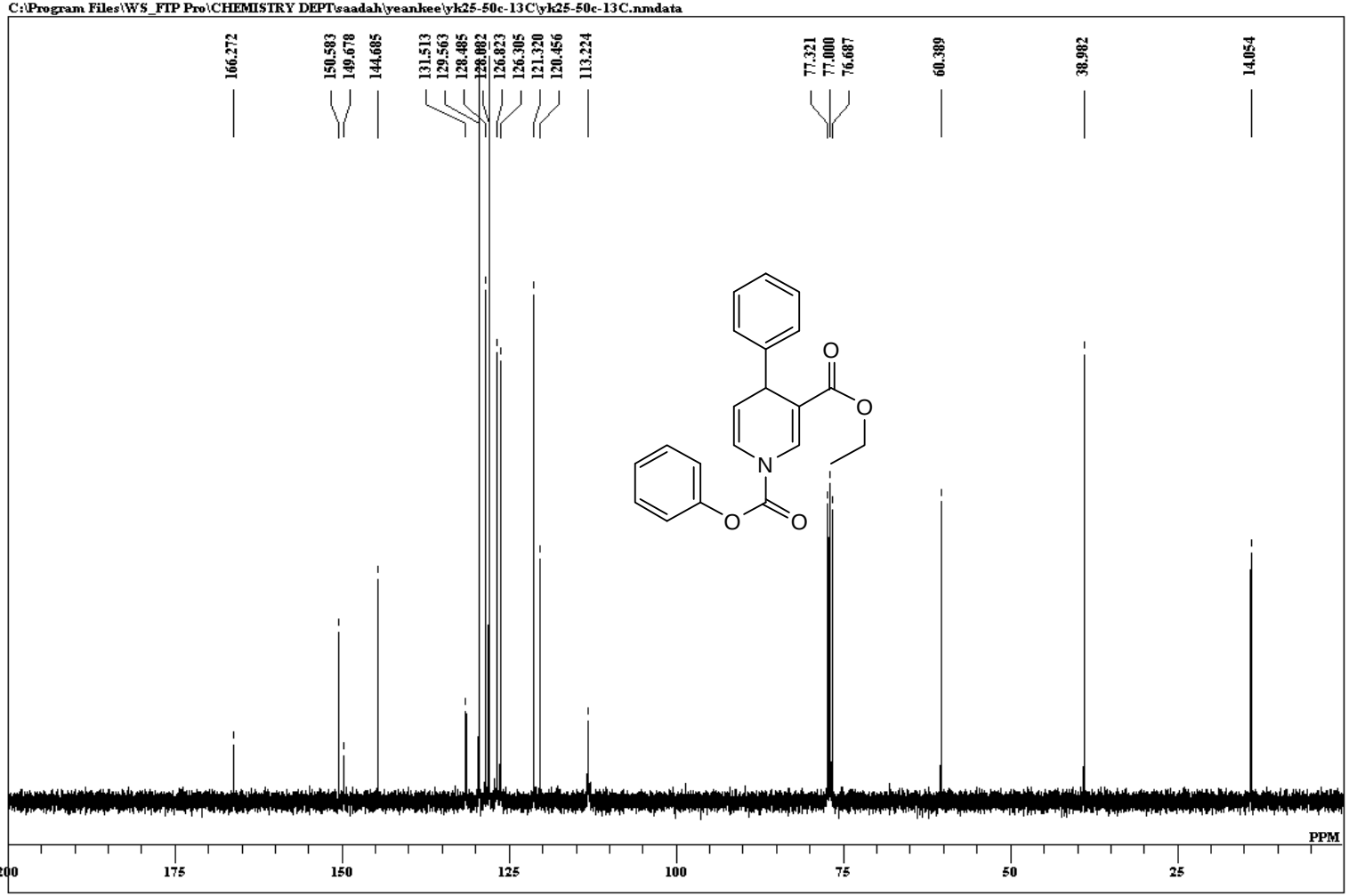
D:\ECA1\yk25-4.jdf



DFILE	yk25-4.jdf
COMNT	single_pulse-yk2
DATIM	09-04-2007 16:37
OBNUC	1H
EXMOD	single_pulse.ex2
OBFRQ	395.88 MHz
OBSET	6.28 KHz
OBFIN	0.87 Hz
POINT	16400
FREQU	7422.80 Hz
SCANS	8
ACQTM	2.2073 sec
PD	5.0000 sec
PW1	5.25 usec
IRNUC	1H
CTEMP	22.1 c
SLVNT	CDCL3
EXREF	7.24 ppm
BF	0.12 Hz
RGAIN	32

1H-yk25-50c-13C

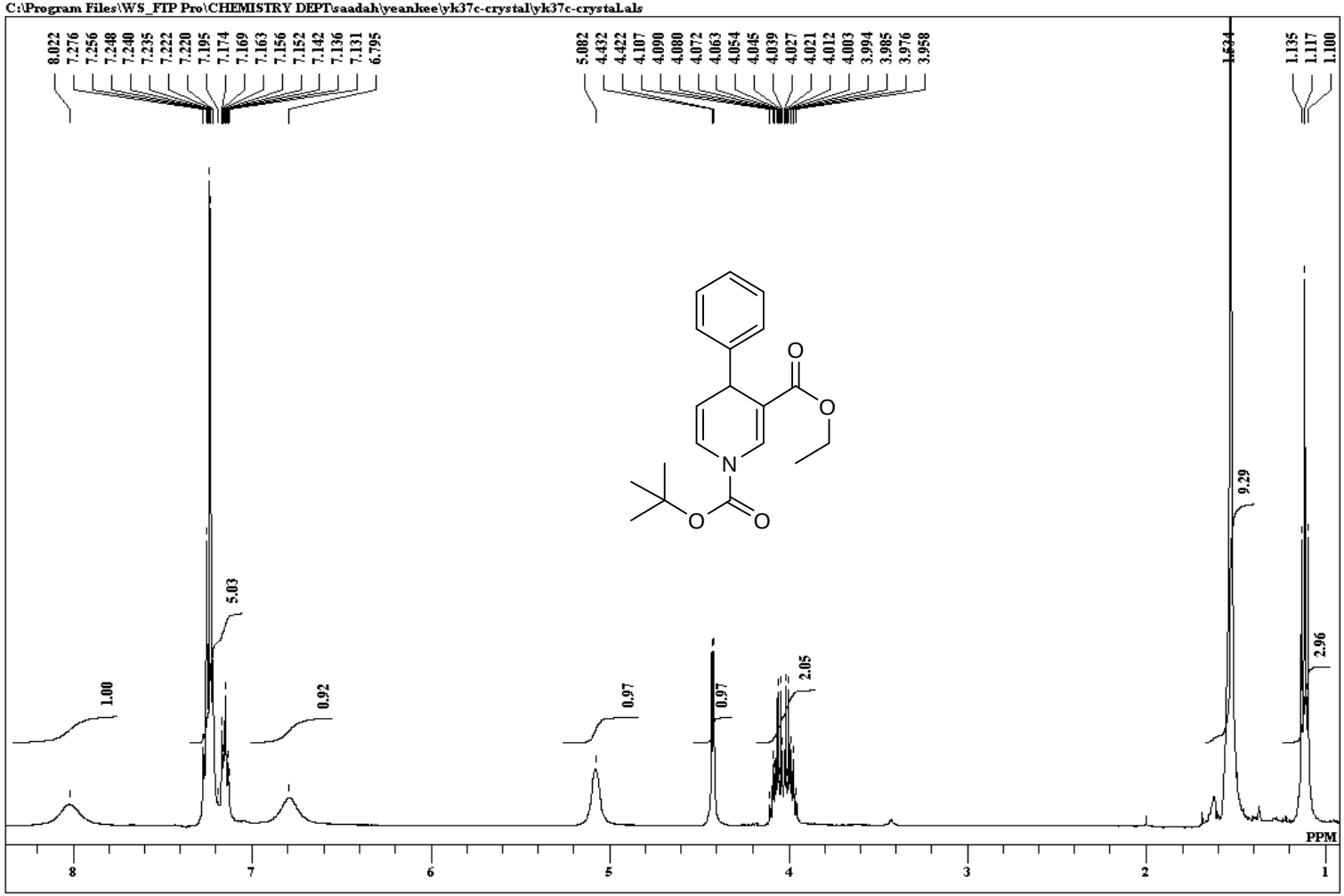
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk25-50c-13C\yk25-50c-13C.nmdata



DFILE	yk25-50c-13C.nm
COMNT	1H-yk25-50c-13C
DATIM	Mon Apr 23 14:5
OBNUC	13C
EXMOD	bcm
OBFRQ	100.40 MHz
OBSET	130.00 KHz
OBFIN	5500.00 Hz
POINT	32768
FREQU	27100.27 Hz
SCANS	400
ACQTM	1.2091 sec
PD	1.7909 sec
PW1	6.50 usec
IRNUC	1H
CTEMP	50.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	30

1H-yk37c-crystal

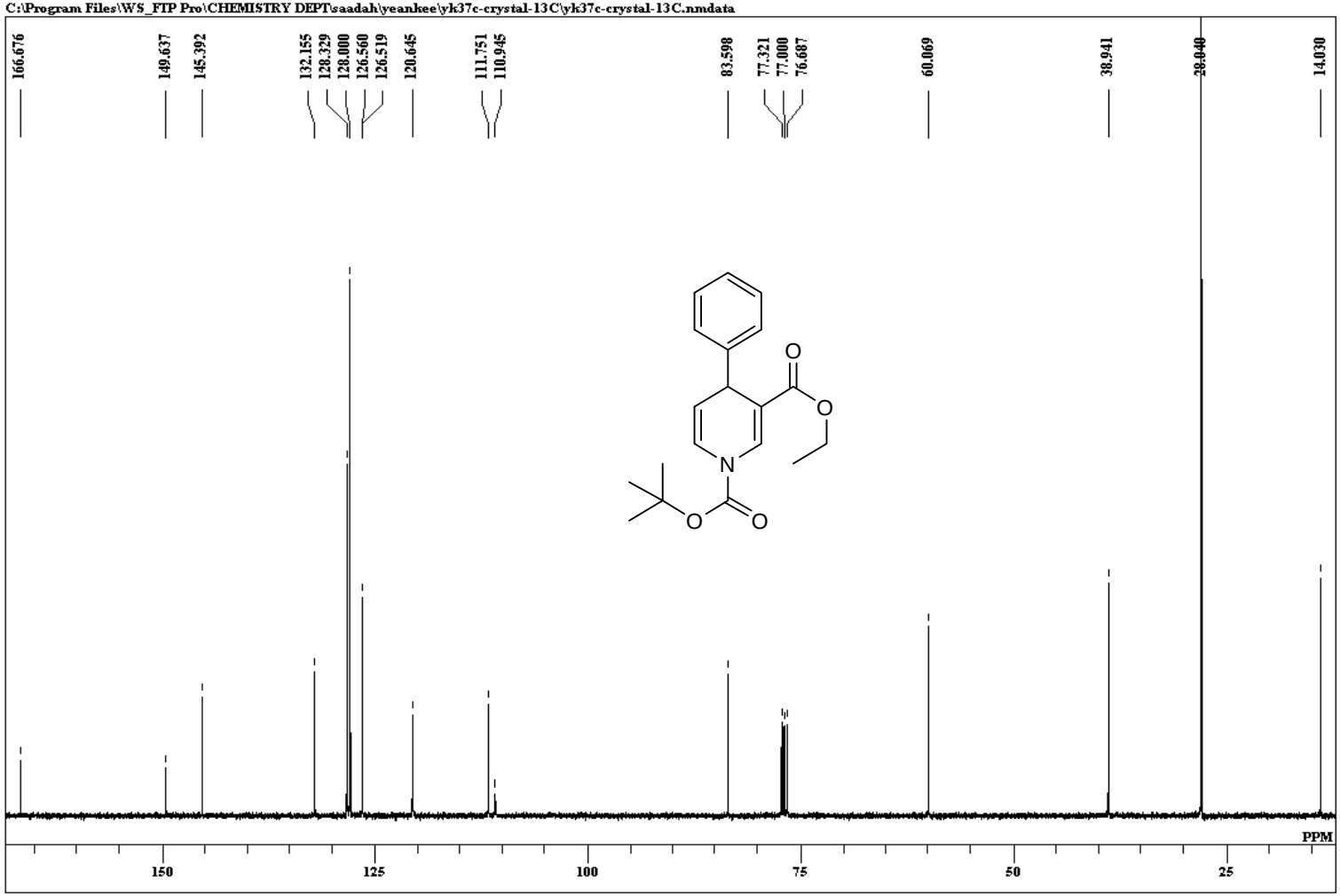
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk37c-crystal\yk37c-crystal.als



DFILE	yk37c-crystal.als
COMNT	1H-yk37c-crystal
DATIM	Fri May 4 15:09:
OBNUC	1H
EXMOD	non
OBFRQ	399.65 MHz
OBSET	130.00 KHz
OBFIN	4300.00 Hz
POINT	32768
FREQU	7993.60 Hz
SCANS	8
ACQTM	4.0993 sec
PD	2.9007 sec
PW1	6.95 usec
IRNUC	1H
CTEMP	24.3 c
SLVNT	CDCL3
EXREF	7.24 ppm
BF	0.12 Hz
RGAIN	15

13C-yk37c-crystal

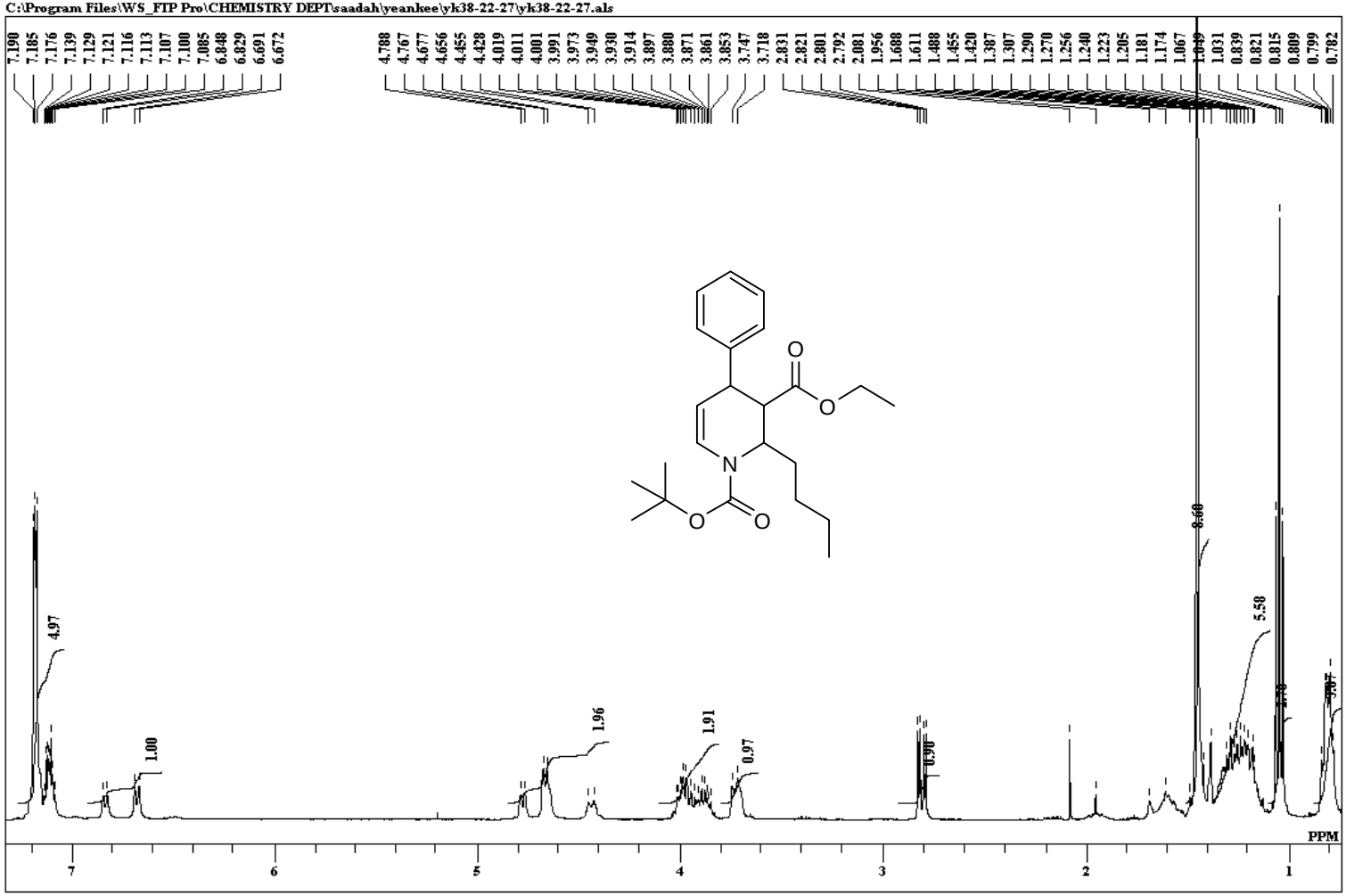
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk37c-crystal-13C\yk37c-crystal-13C.nmdata



DFILE	yk37c-crystal-13
COMNT	13C-yk37c-crystal
DATIM	Fri May 4 16:01:
OBNUC	13C
EXMOD	bcm
OBFRQ	100.40 MHz
OBSET	130.00 KHz
OBFIN	5500.00 Hz
POINT	32768
FREQU	27100.27 Hz
SCANS	881
ACQTM	1.2091 sec
PD	1.7909 sec
PW1	6.50 usec
IRNUC	1H
CTEMP	50.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	30

1H-yk38-22-27

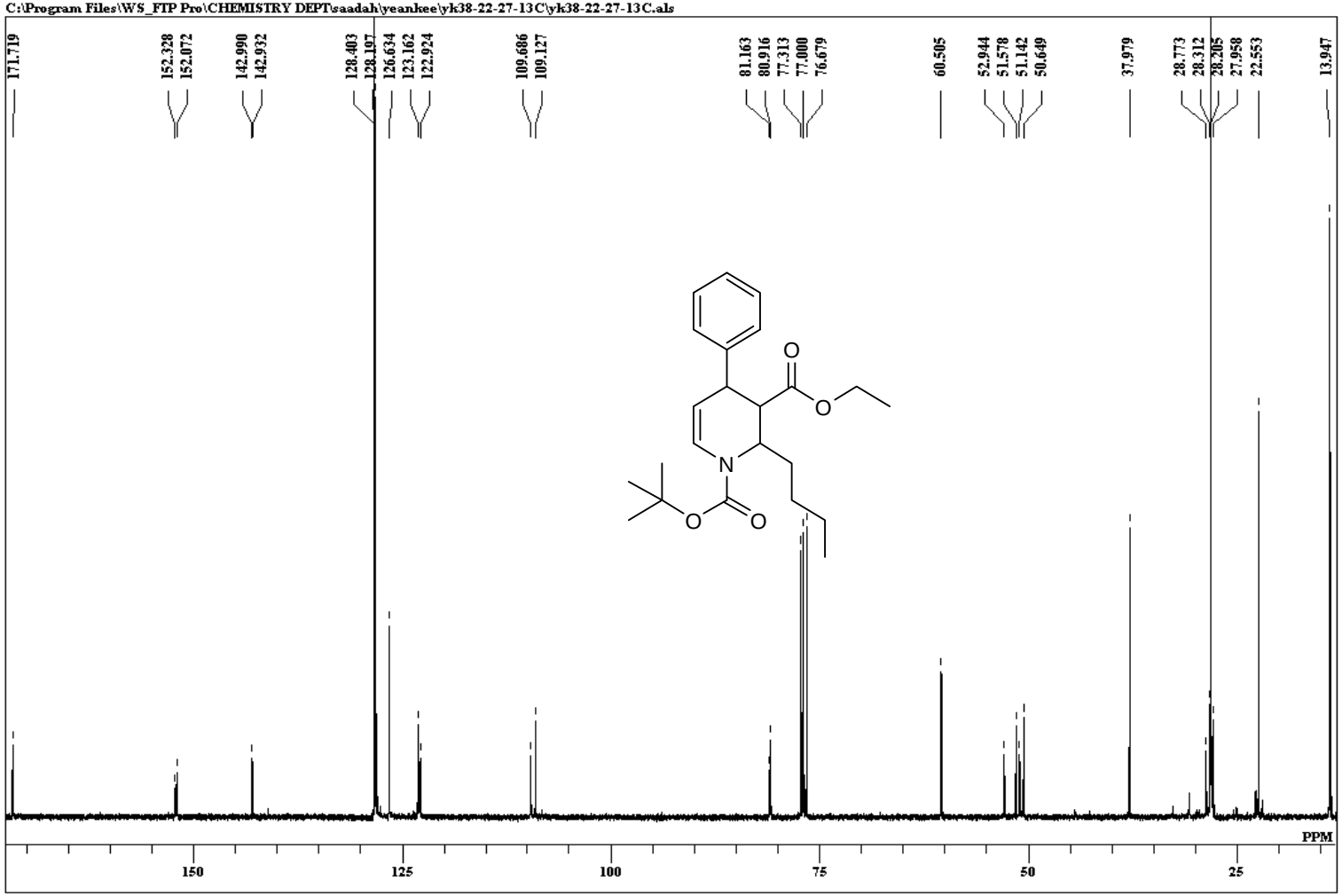
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk38-22-27\yk38-22-27.als



DFILE	yk38-22-27.als
COMNT	1H-yk38-22-27
DATIM	Tue Jan 16 17:30
OBNUC	1H
EXMOD	non
OBFRQ	399.65 MHz
OBSET	130.00 KHz
OBFIN	4300.00 Hz
POINT	32768
FREQU	8000.00 Hz
SCANS	8
ACQTM	4.0960 sec
PD	5.0000 sec
PW1	5.00 usec
IRNUC	1H
CTEMP	23.6 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	13

13C-yk38-22-27

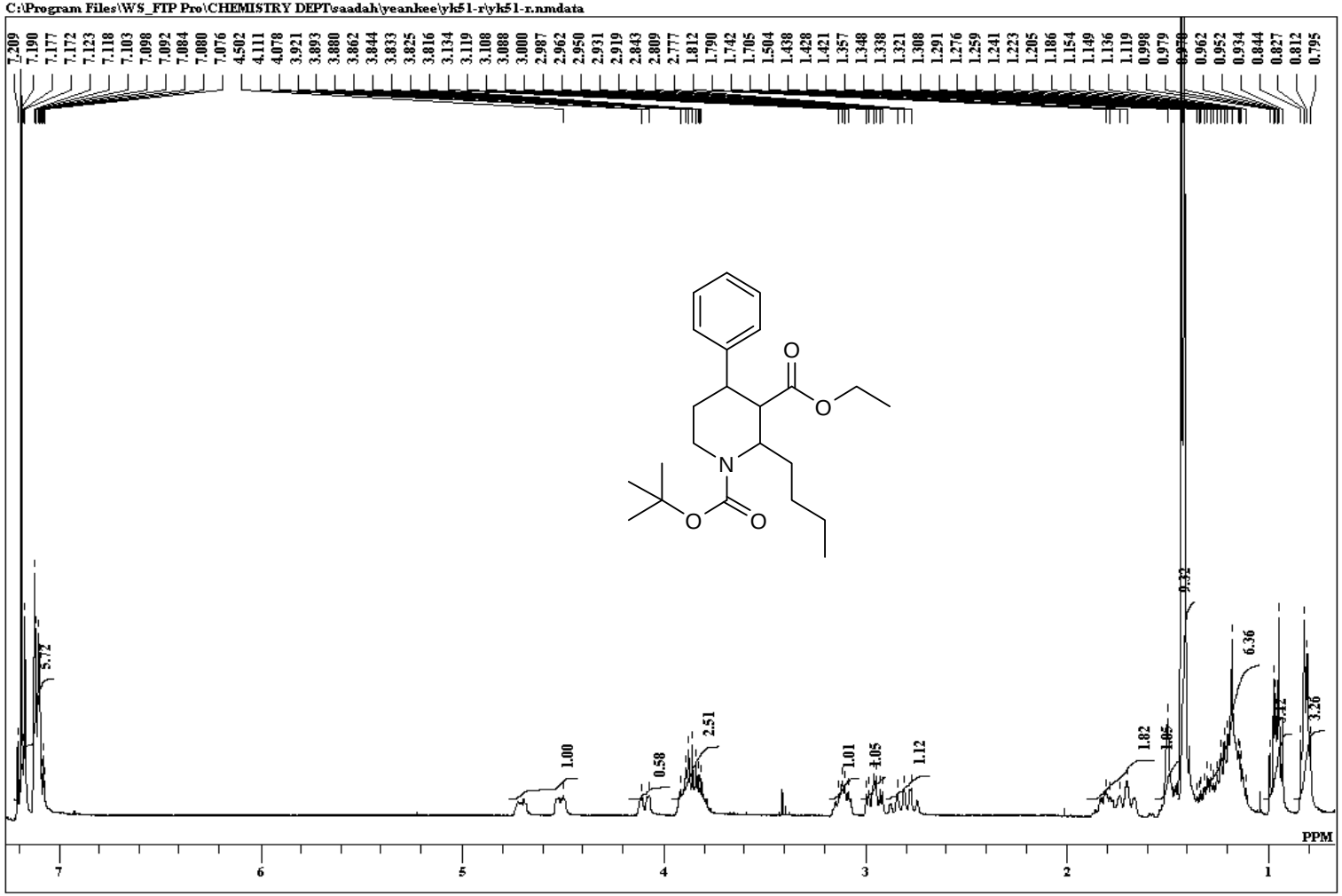
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk38-22-27-13C\yk38-22-27-13C.als



DFILE	yk38-22-27-13C.a
COMNT	13C-yk38-22-27
DATIM	Tue Jan 16 20:52
OBNUC	13C
EXMOD	bcm
OBFRQ	100.40 MHz
OBSET	130.00 KHz
OBFIN	5500.00 Hz
POINT	32768
FREQU	27100.27 Hz
SCANS	4000
ACQTM	1.2091 sec
PD	1.7909 sec
PW1	6.50 usec
IRNUC	1H
CTEMP	25.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	29

1H-yk51-r

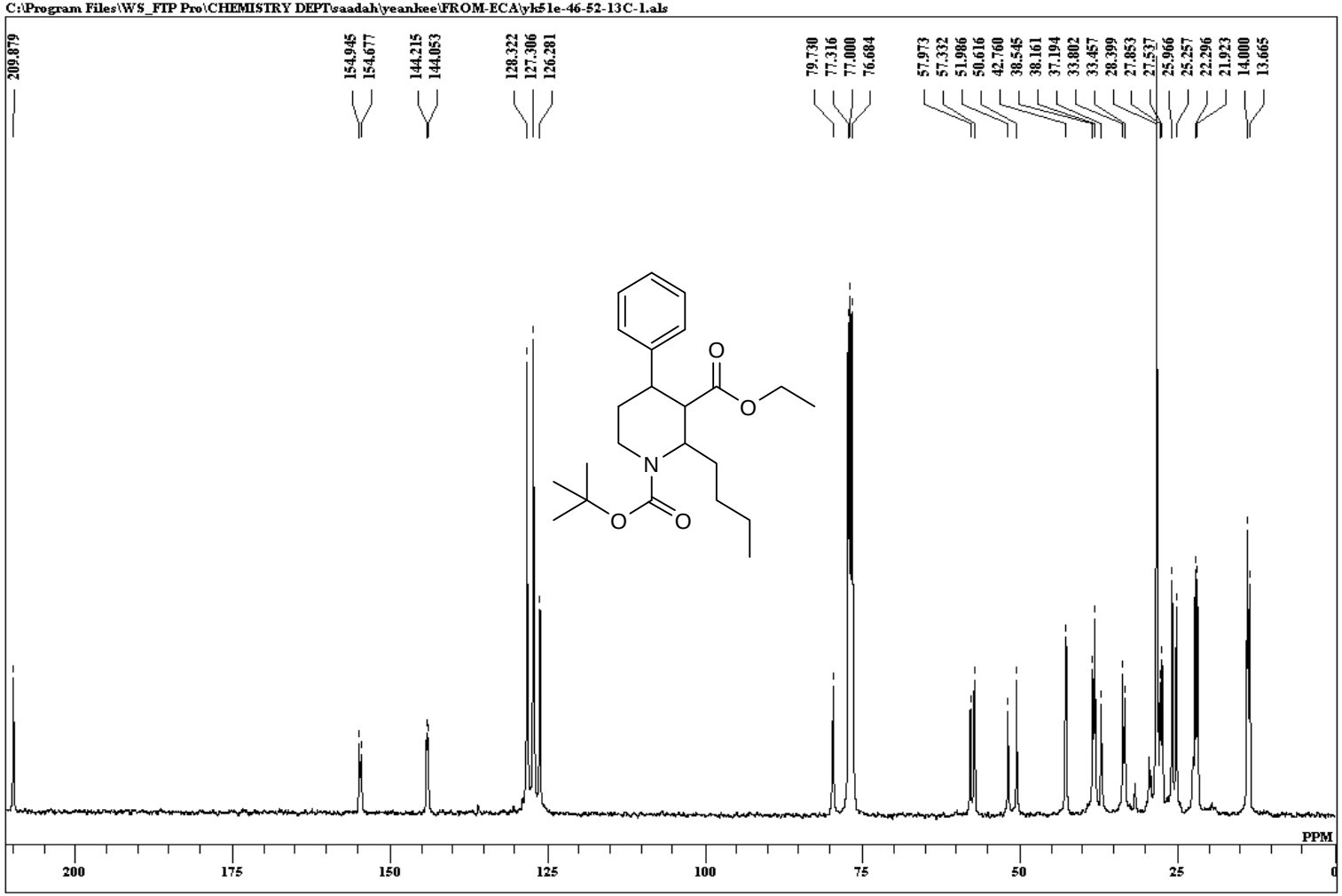
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk51-r\yk51-r.nmdata



DFILE	yk51-r.nmdata
COMNT	1H-yk51-r
DATIM	Thu Aug 7 17:22
OBNUC	1H
EXMOD	non
OBFRQ	399.65 MHz
OBSET	130.00 KHz
OBFIN	4300.00 Hz
POINT	32768
FREQU	7993.60 Hz
SCANS	8
ACQTM	4.0993 sec
PD	2.9007 sec
PW1	7.50 usec
IRNUC	1H
CTEMP	30.0 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	19

single pulse decoupled gated NOE-yk51e-46-52-13C

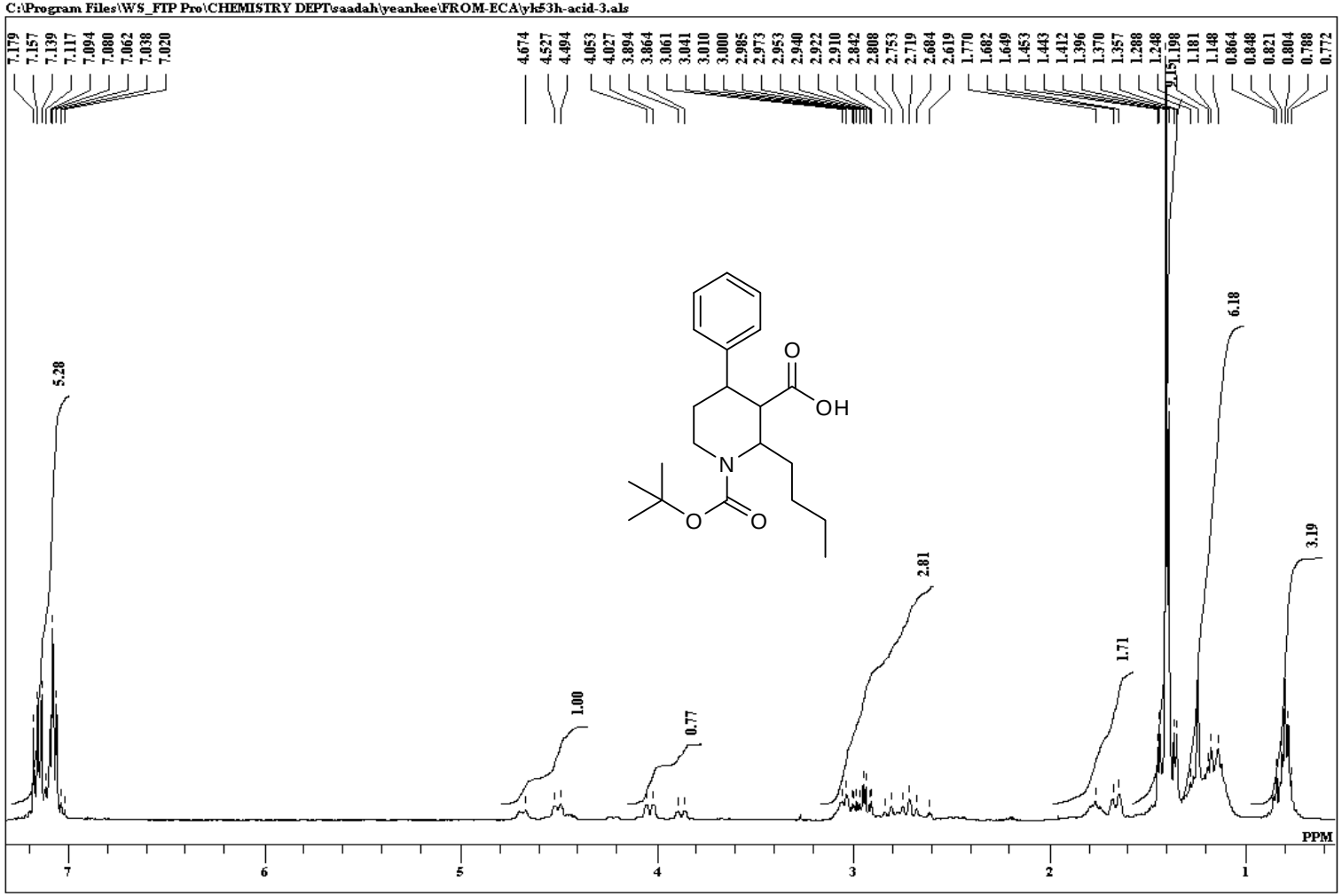
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\FROM-ECA\yk51e-46-52-13C-1.als



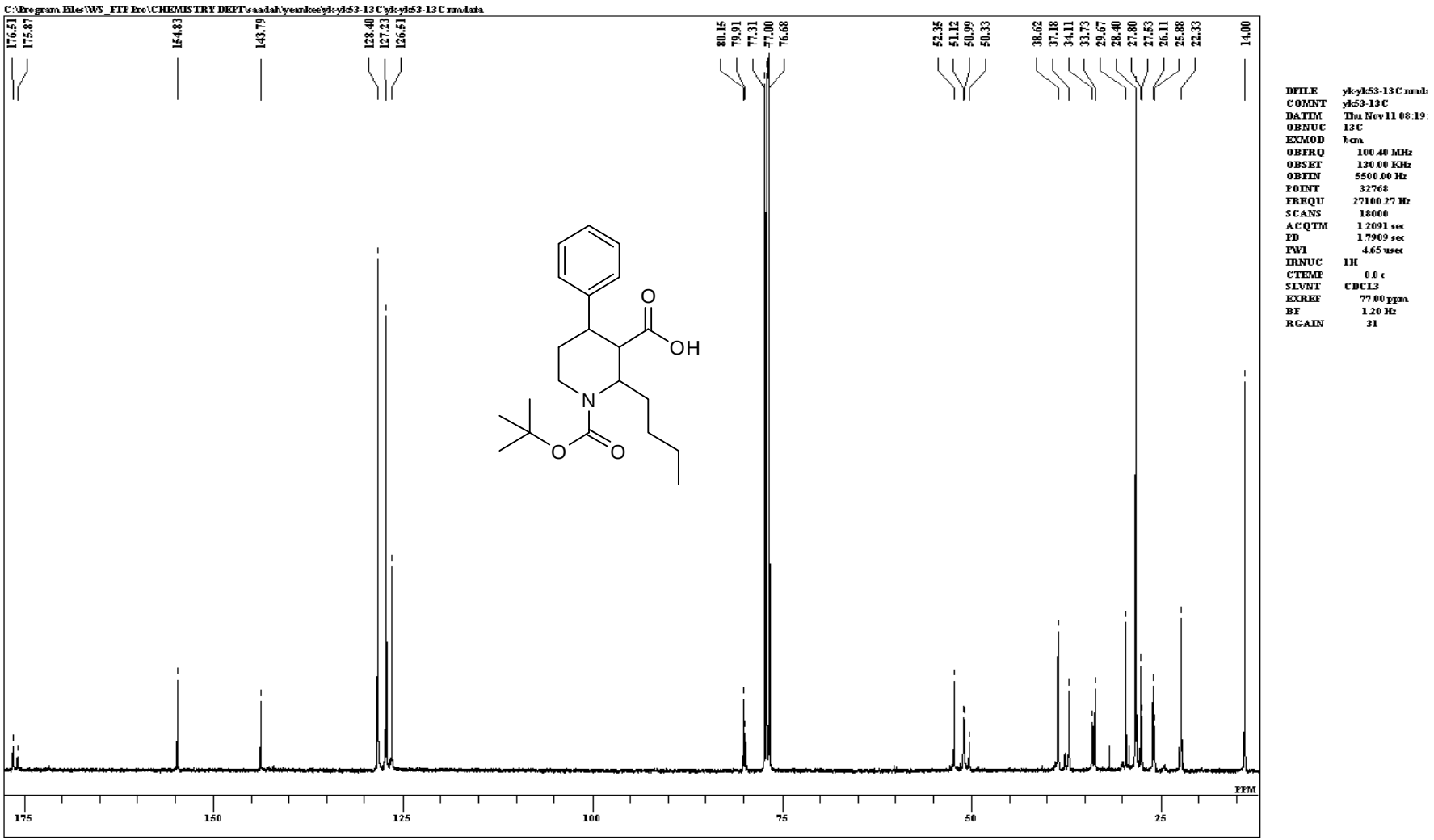
DFILE	yk51e-46-52-13C
COMNT	single pulse decc
DATIM	22-12-2007 01:49
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	99.55 MHz
OBSET	5.13 KHz
OBFIN	0.98 Hz
POINT	26214
FREQU	24999.62 Hz
SCANS	3000
ACQTM	1.0486 sec
PD	2.0000 sec
PW1	3.07 usec
IRNUC	1H
CTEMP	20.9 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	10.00 Hz
RGAIN	54

single_pulse-yk53h-acid

C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\FROM-ECA\yk53h-acid-3.als

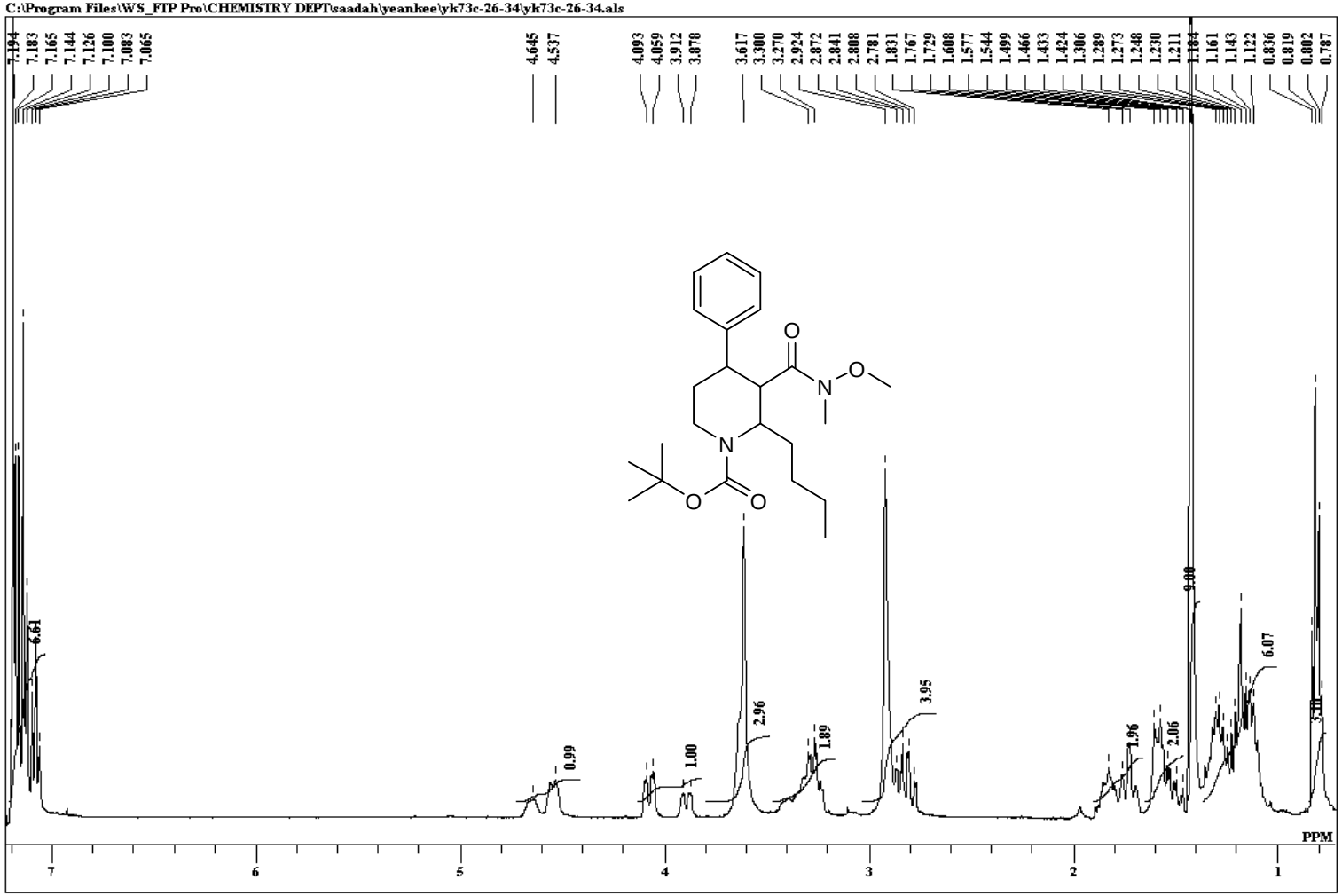


DFILE	yk53h-acid-3.als
COMNT	single_pulse-yk5
DATIM	04-12-2007 13:32
OBNUC	1H
EXMOD	single_pulse.ex2
OBFRQ	395.88 MHz
OBSET	6.28 KHz
OBFIN	0.87 Hz
POINT	16400
FREQU	7422.80 Hz
SCANS	8
ACQTM	2.2073 sec
PD	5.0000 sec
PW1	5.75 usec
IRNUC	1H
CTEMP	21.0 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	10.00 Hz
RGAIN	26


C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk-yk53-13C\yk-yk53-13C.nmrdata
176.51
175.87
154.83
143.79
128.40
127.23
126.51
80.15
79.91
77.31
77.00
76.68
52.35
51.12
50.99
50.33
38.62
37.18
34.11
33.73
29.67
28.40
27.80
27.53
26.11
25.88
22.33
14.00
O
OH
N
O
O
PPM
175
150
125
100
75
50
25
DFILE yk-yk53-13C.nmrda
COMNT yk53-13C
DATIM Thu Nov 11 08:19:
OBNUC 13C
EXMOD bcm
OBFRQ 100.40 MHz
OBSET 130.00 KHz
OBFIN 5500.00 Hz
POINT 32768
FREQU 27100.27 Hz
SCANS 18000
ACQTM 1.2091 sec
PD 1.7909 sec
PW1 4.65 usec
IRNUC 1H
CTEMP 0.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 31

1H-yk73c-26-34

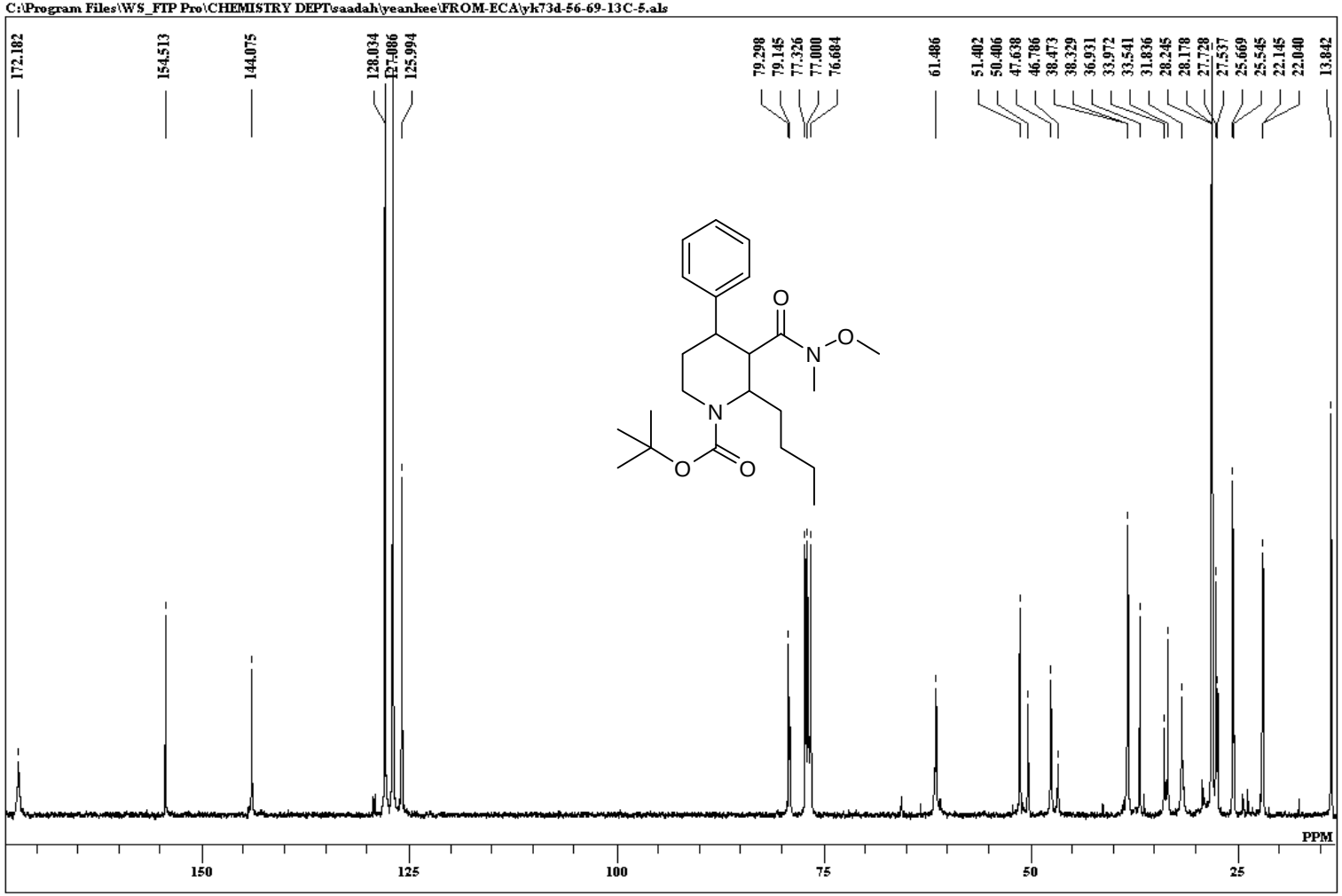
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk73c-26-34\yk73c-26-34.als



DFILE	yk73c-26-34.als
COMNT	1H-yk73c-26-34
DATIM	Wed Jun 6 12:4
OBNUC	1H
EXMOD	non
OBFRQ	399.65 MHz
OBSET	130.00 KHz
OBFIN	4300.00 Hz
POINT	32768
FREQU	7993.60 Hz
SCANS	8
ACQTM	4.0993 sec
PD	2.9007 sec
PW1	6.95 usec
IRNUC	1H
CTEMP	22.8 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	10.00 Hz
RGAIN	18

single pulse decoupled gated NOE-yk73d-56-69-13C

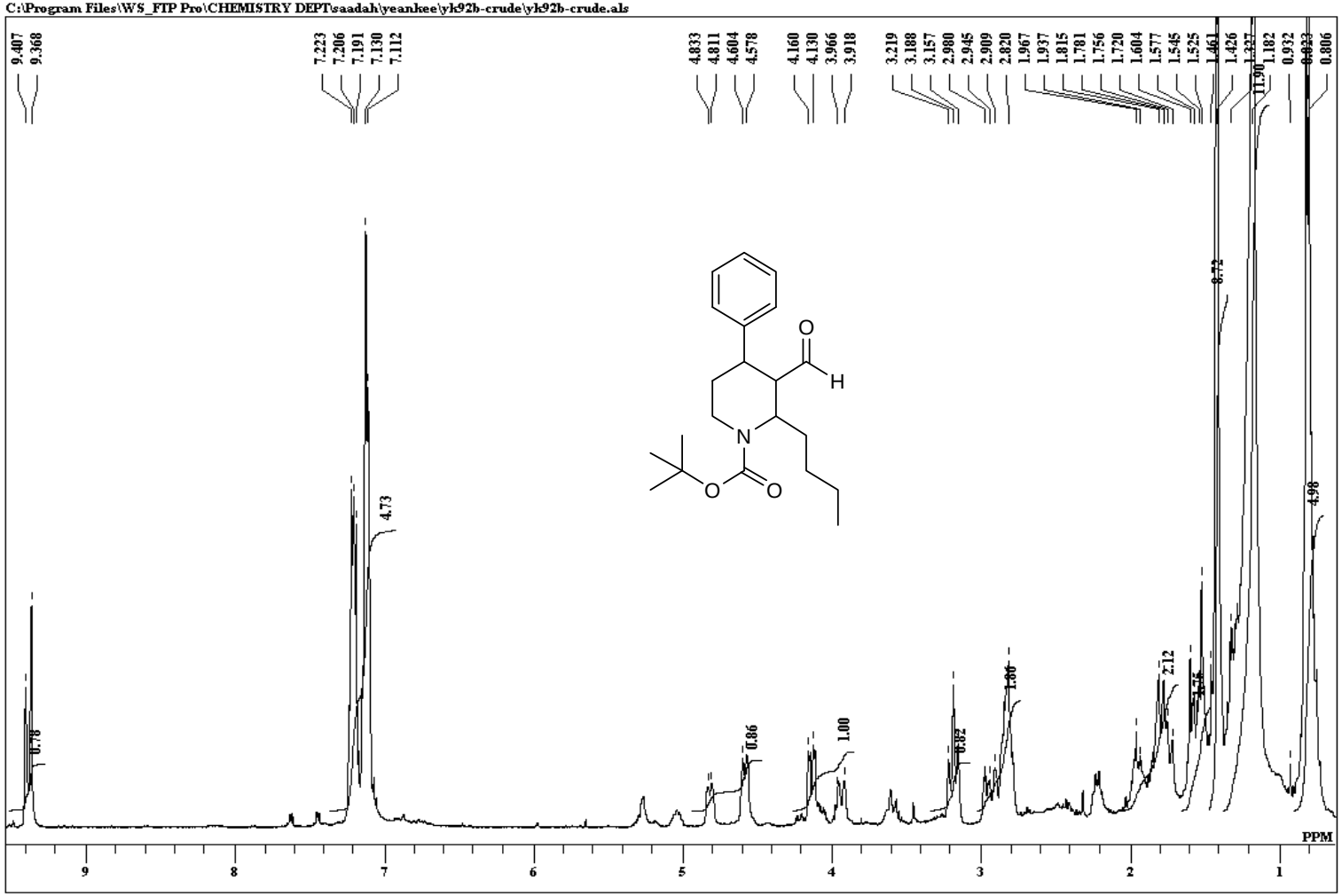
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\FROM-ECA\yk73d-56-69-13C-5.als



DFILE	yk73d-56-69-13C
COMNT	single pulse decc
DATIM	28-06-2007 03:29
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	99.55 MHz
OBSET	5.13 KHz
OBFIN	0.98 Hz
POINT	32781
FREQU	31250.00 Hz
SCANS	2000
ACQTM	1.0486 sec
PD	2.0000 sec
PW1	2.92 usec
IRNUC	1H
CTEMP	23.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	50

1H-yk92b-crude

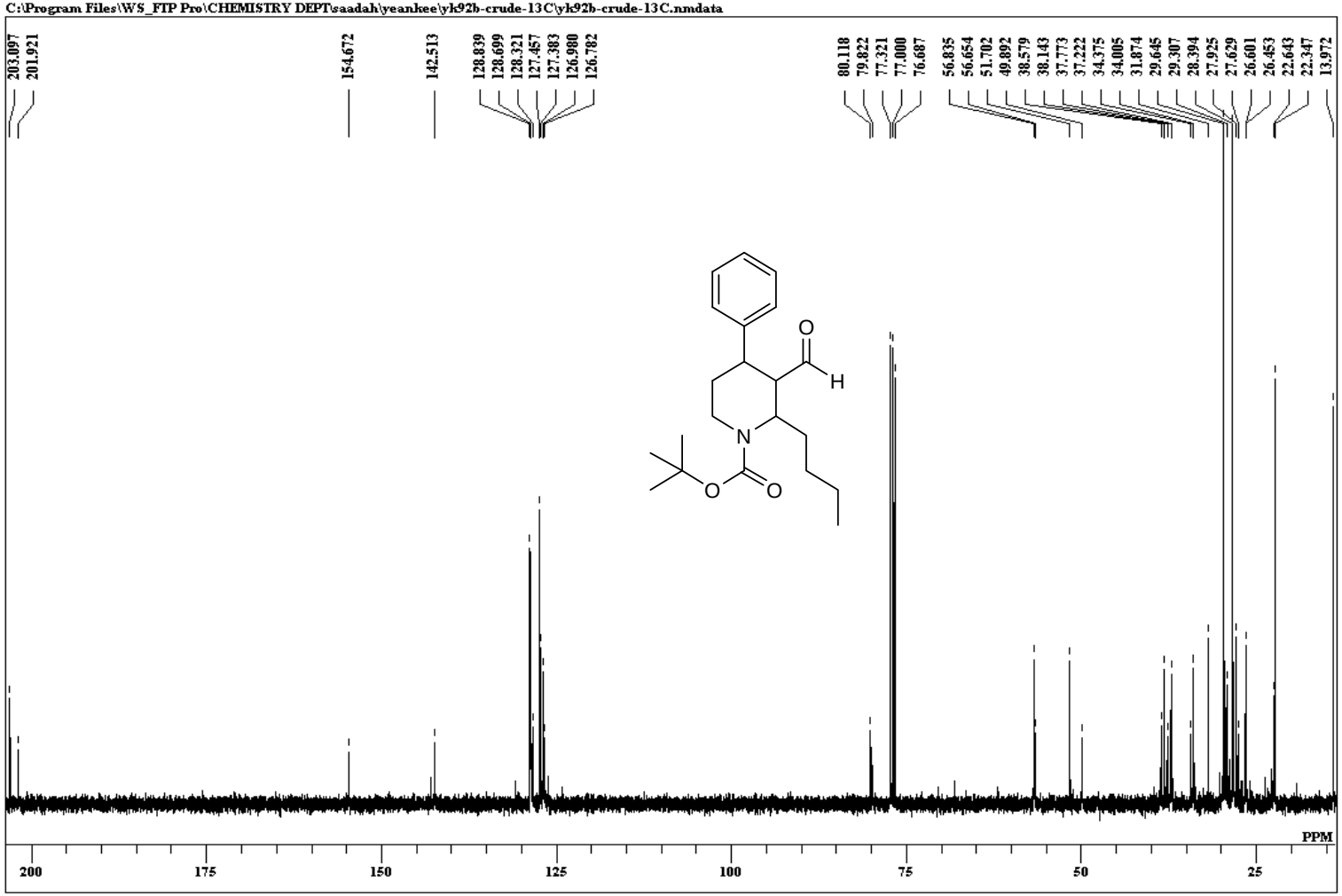
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk92b-crude\yk92b-crude.als



DFILE	yk92b-crude.als
COMNT	1H-yk92b-crude
DATIM	Fri Jan 11 11:13:
OBNUC	1H
EXMOD	non
OBFRQ	399.65 MHz
OBSET	130.00 KHz
OBFIN	4300.00 Hz
POINT	32768
FREQU	7993.60 Hz
SCANS	8
ACQTM	4.0993 sec
PD	2.9007 sec
PW1	6.95 usec
IRNUC	1H
CTEMP	22.7 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.00 Hz
RGAIN	13

13C-yk92b-crude

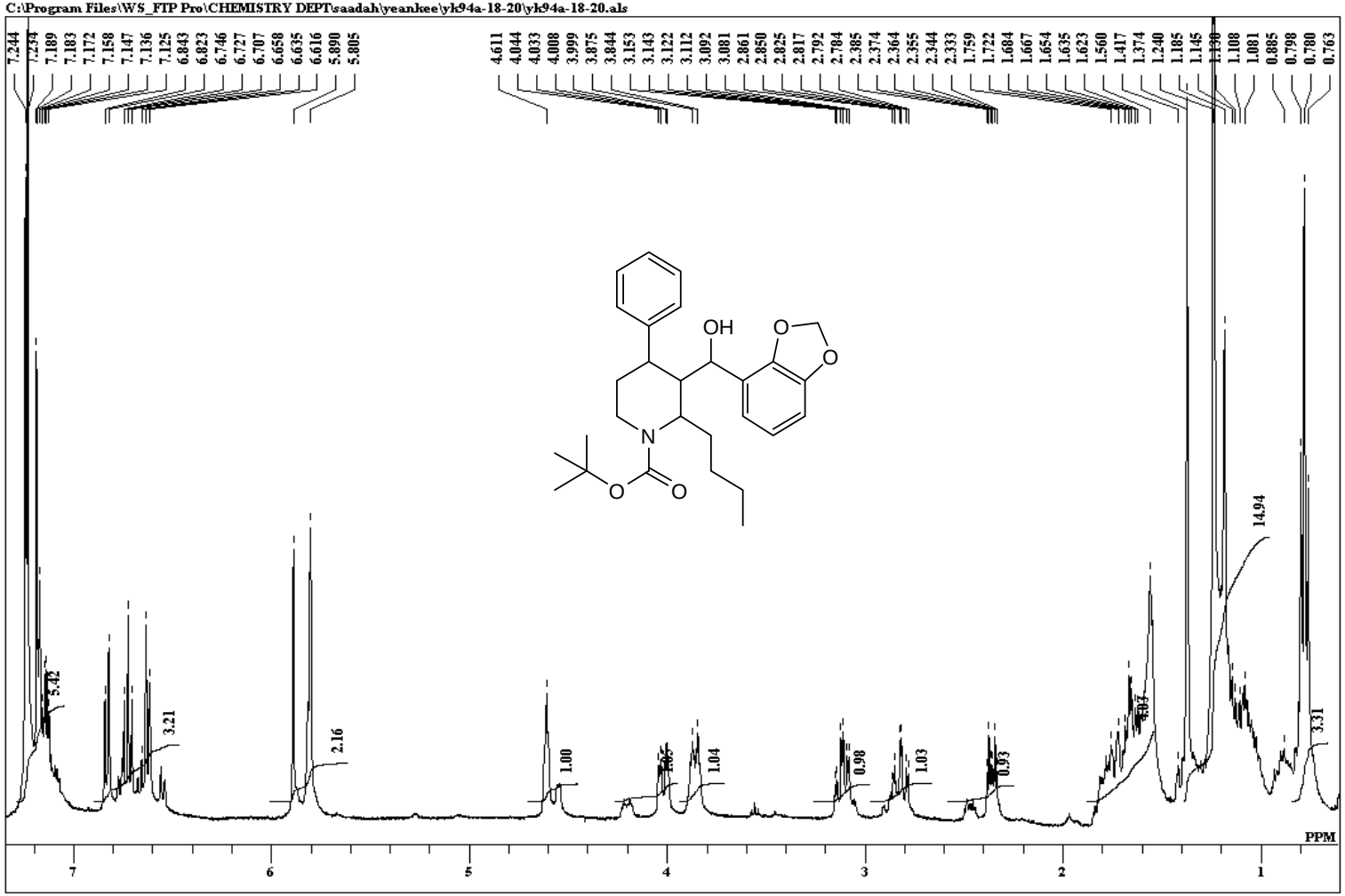
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk92b-crude-13C\yk92b-crude-13C.nmdata



DFILE	yk92b-crude-13C
COMNT	13C-yk92b-crude
DATIM	Fri Jan 11 14:13:
OBNUC	13C
EXMOD	bcm
OBFRQ	100.40 MHz
OBSET	130.00 KHz
OBFIN	5500.00 Hz
POINT	32768
FREQU	27100.27 Hz
SCANS	1442
ACQTM	1.2091 sec
PD	1.7909 sec
PW1	6.50 usec
IRNUC	1H
CTEMP	24.5 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.00 Hz
RGAIN	30

1H-yk94a-18-20

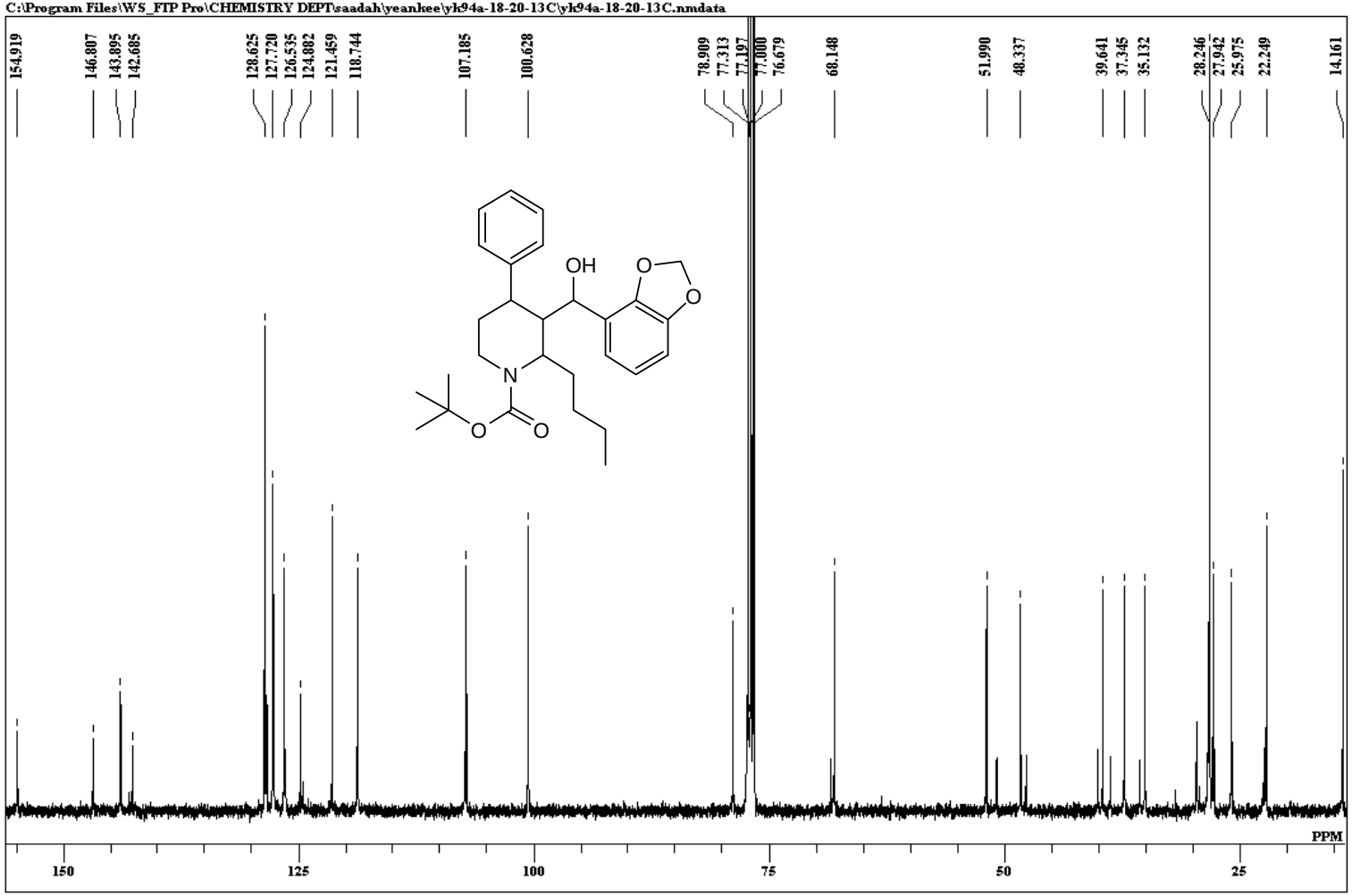
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk94a-18-20\yk94a-18-20.als



DFILE	yk94a-18-20.als
COMNT	1H-yk94a-18-20
DATIM	Wed Jan 30 17:1
OBNUC	1H
EXMOD	non
OBFRQ	399.65 MHz
OBSET	130.00 KHz
OBFIN	4300.00 Hz
POINT	32768
FREQU	7993.60 Hz
SCANS	4
ACQTM	4.0993 sec
PD	2.9007 sec
PW1	6.95 usec
IRNUC	1H
CTEMP	23.9 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.00 Hz
RGAIN	18

13C-yk94a-18-20

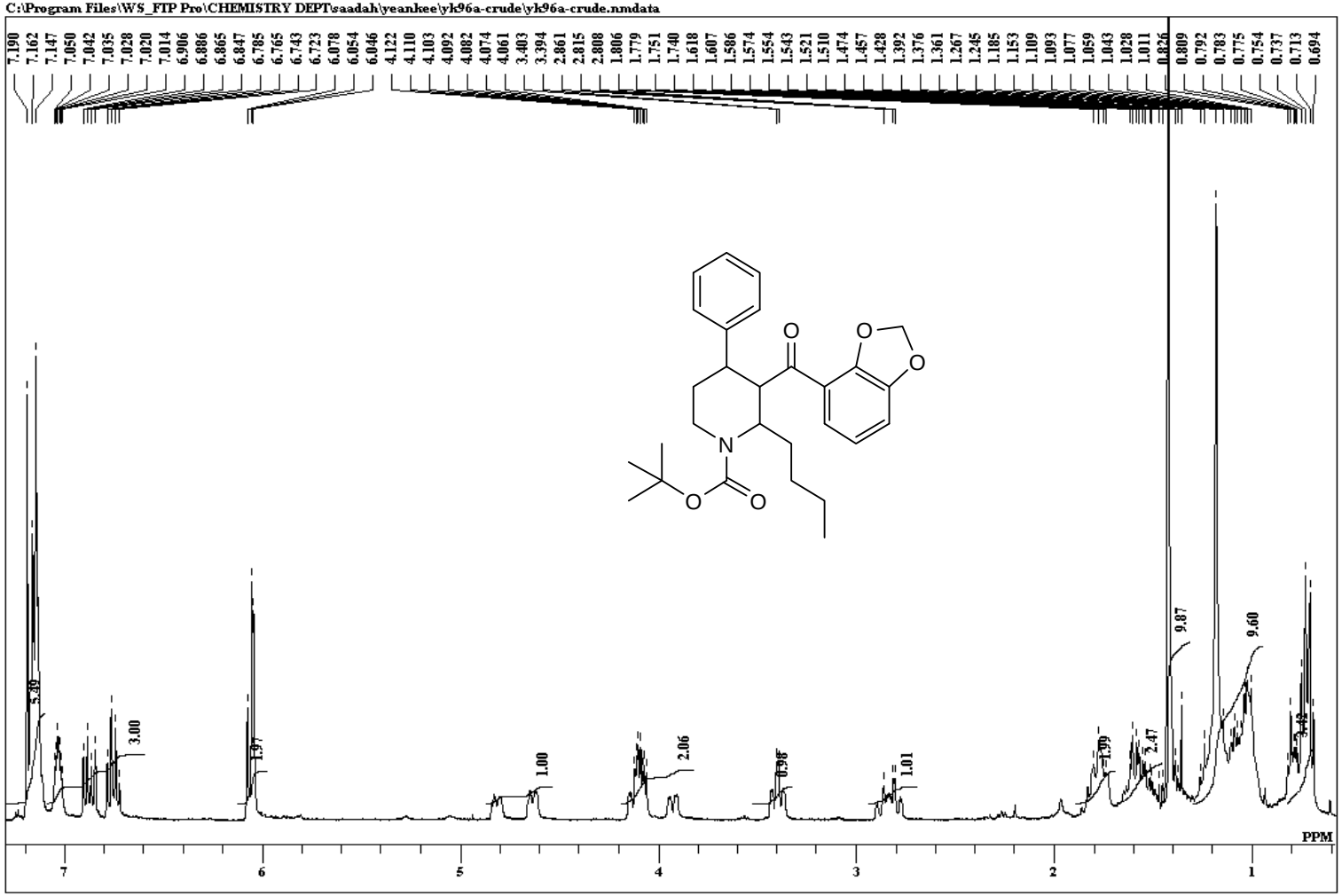
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk94a-18-20-13C\yk94a-18-20-13C.nmdata



DFILE	yk94a-18-20-13C
COMNT	13C-yk94a-18-20
DATIM	Thu Jan 31 08:45
OBNUC	13C
EXMOD	bcm
OBFRQ	100.40 MHz
OBSET	130.00 KHz
OBFIN	5500.00 Hz
POINT	32768
FREQU	27100.27 Hz
SCANS	7000
ACQTM	1.2091 sec
PD	1.7909 sec
PW1	6.90 usec
IRNUC	1H
CTEMP	25.4 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.00 Hz
RGAIN	29

1H-yk96a-crude

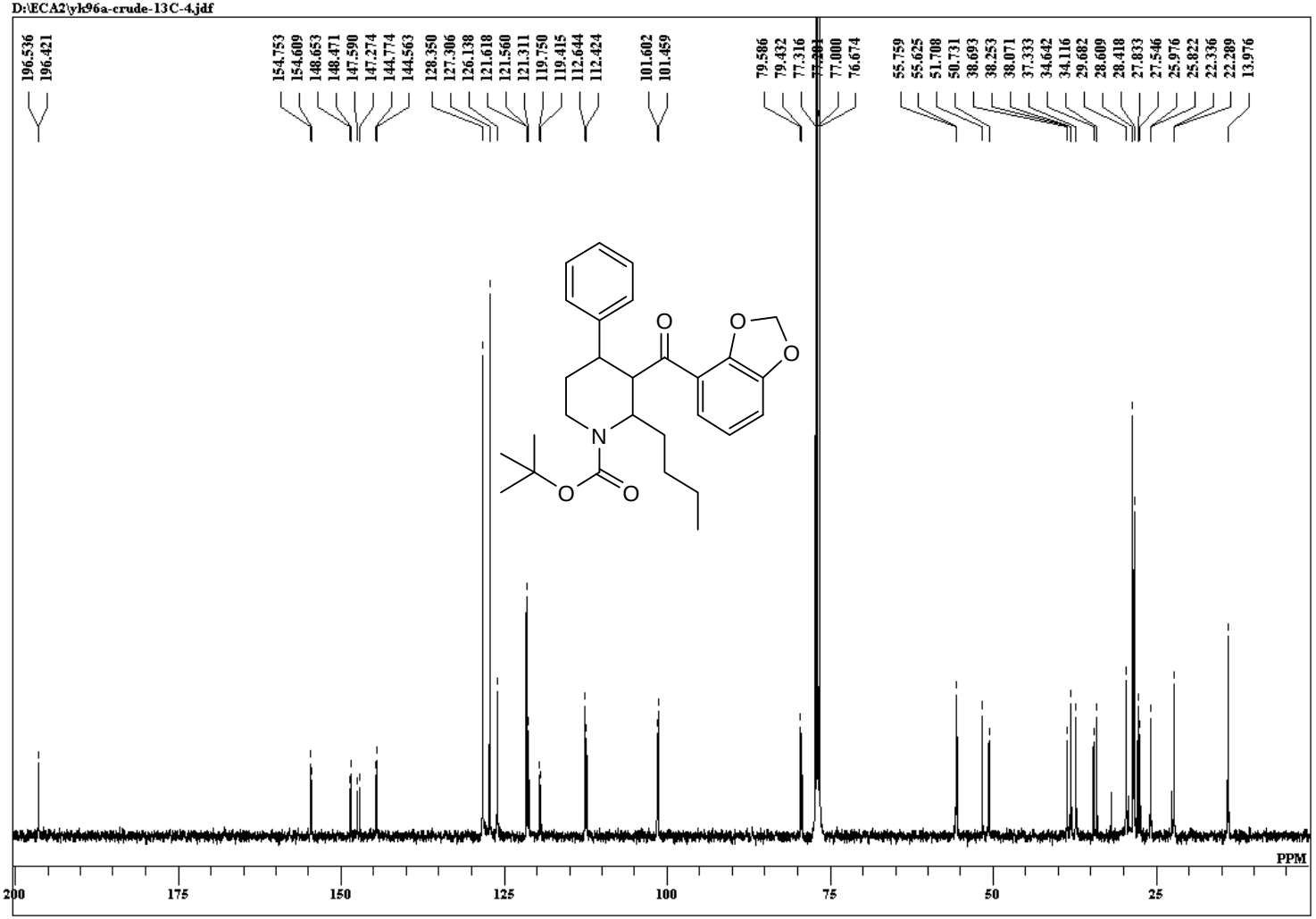
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk96a-crude\yk96a-crude.nmdata



DFILE	yk96a-crude.nmr
COMNT	1H-yk96a-crude
DATIM	Fri Feb 22 10:43:
OBNUC	1H
EXMOD	non
OBFRQ	399.65 MHz
OBSET	130.00 KHz
OBFIN	4300.00 Hz
POINT	32768
FREQU	7993.60 Hz
SCANS	8
ACQTM	4.0993 sec
PD	2.9007 sec
PW1	6.95 usec
IRNUC	1H
CTEMP	24.2 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	18

single pulse decoupled gated NOE-yk96a-crude-13C

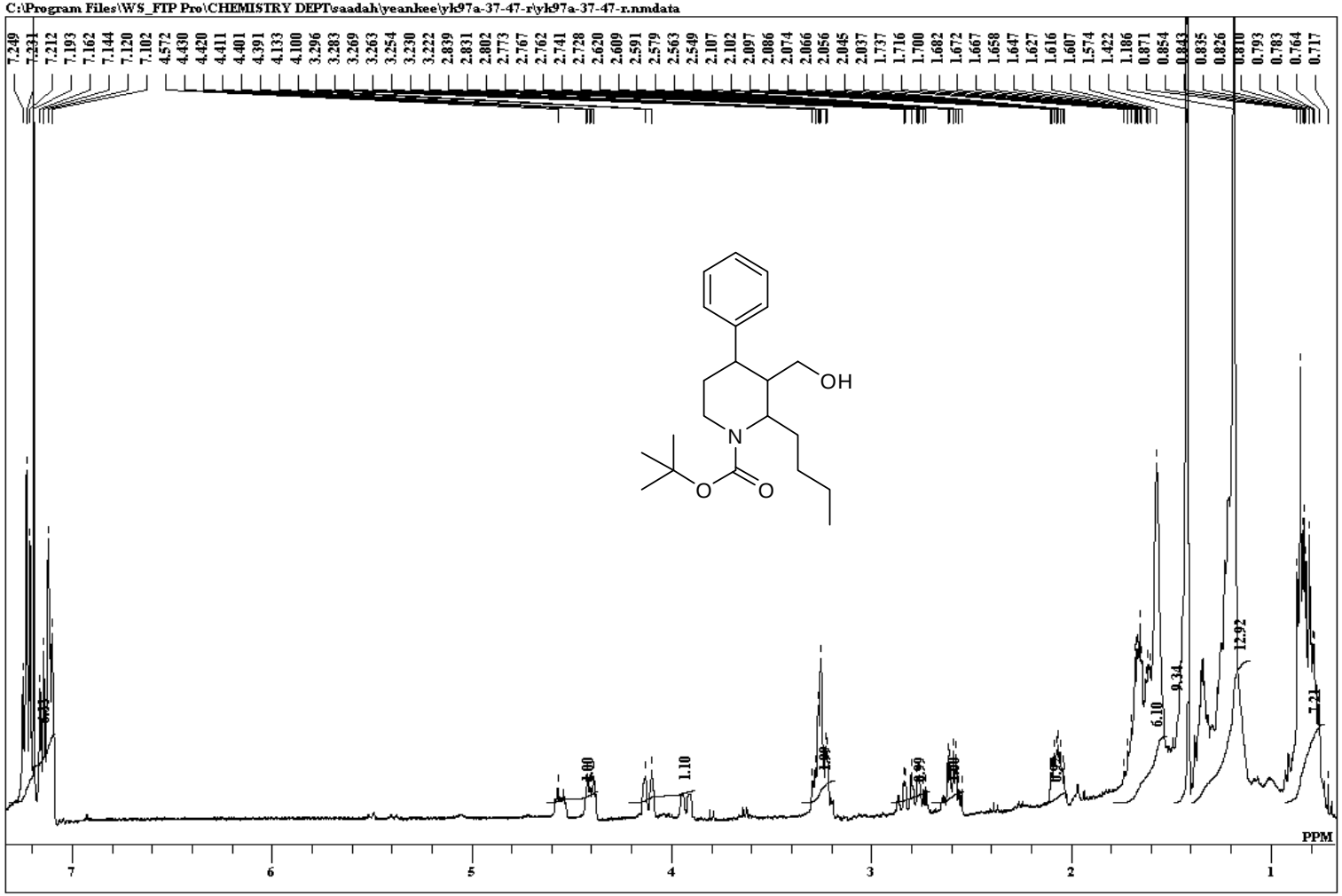
D:\ECA2\yk96a-crude-13C-4.jdf



DFILE	yk96a-crude-13C
COMNT	single pulse decc
DATIM	02-03-2008 04:08
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	99.55 MHz
OBSET	5.13 KHz
OBFIN	0.98 Hz
POINT	32781
FREQU	31250.00 Hz
SCANS	5000
ACQTM	1.0486 sec
PD	2.0000 sec
PW1	3.07 usec
IRNUC	1H
CTEMP	21.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	56

1H-yk97a-37-47-r

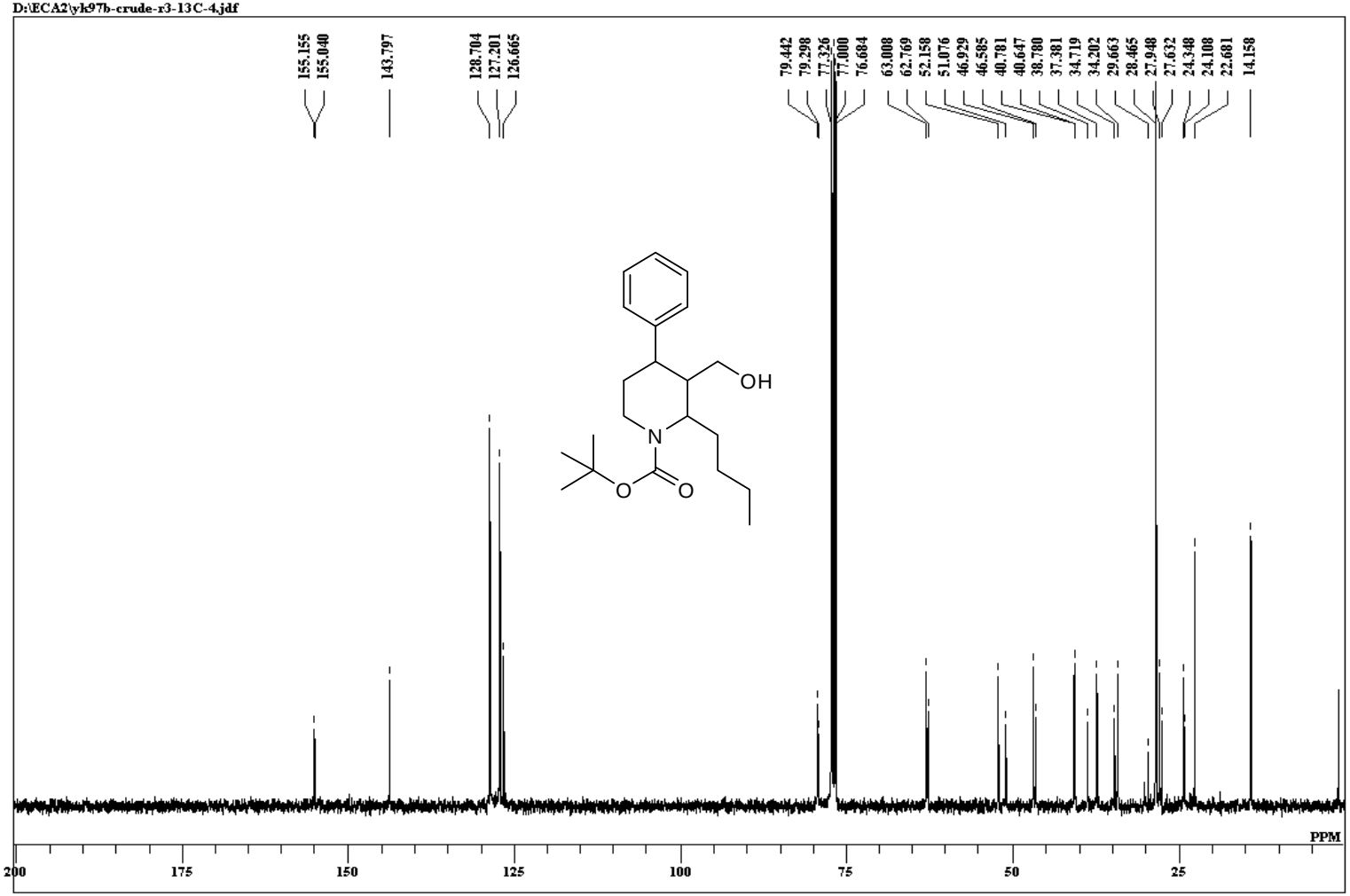
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk97a-37-47-r\yk97a-37-47-r.nmdata



DFILE	yk97a-37-47-r.nr
COMNT	1H-yk97a-37-47-
DATIM	Fri Mar 14 10:59
OBNUC	1H
EXMOD	non
OBFRQ	399.65 MHz
OBSET	130.00 KHz
OBFIN	4300.00 Hz
POINT	32768
FREQU	7993.60 Hz
SCANS	8
ACQTM	4.0993 sec
PD	2.9007 sec
PW1	6.95 usec
IRNUC	1H
CTEMP	23.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	19

single pulse decoupled gated NOE-yk97b-crude-r3-13C

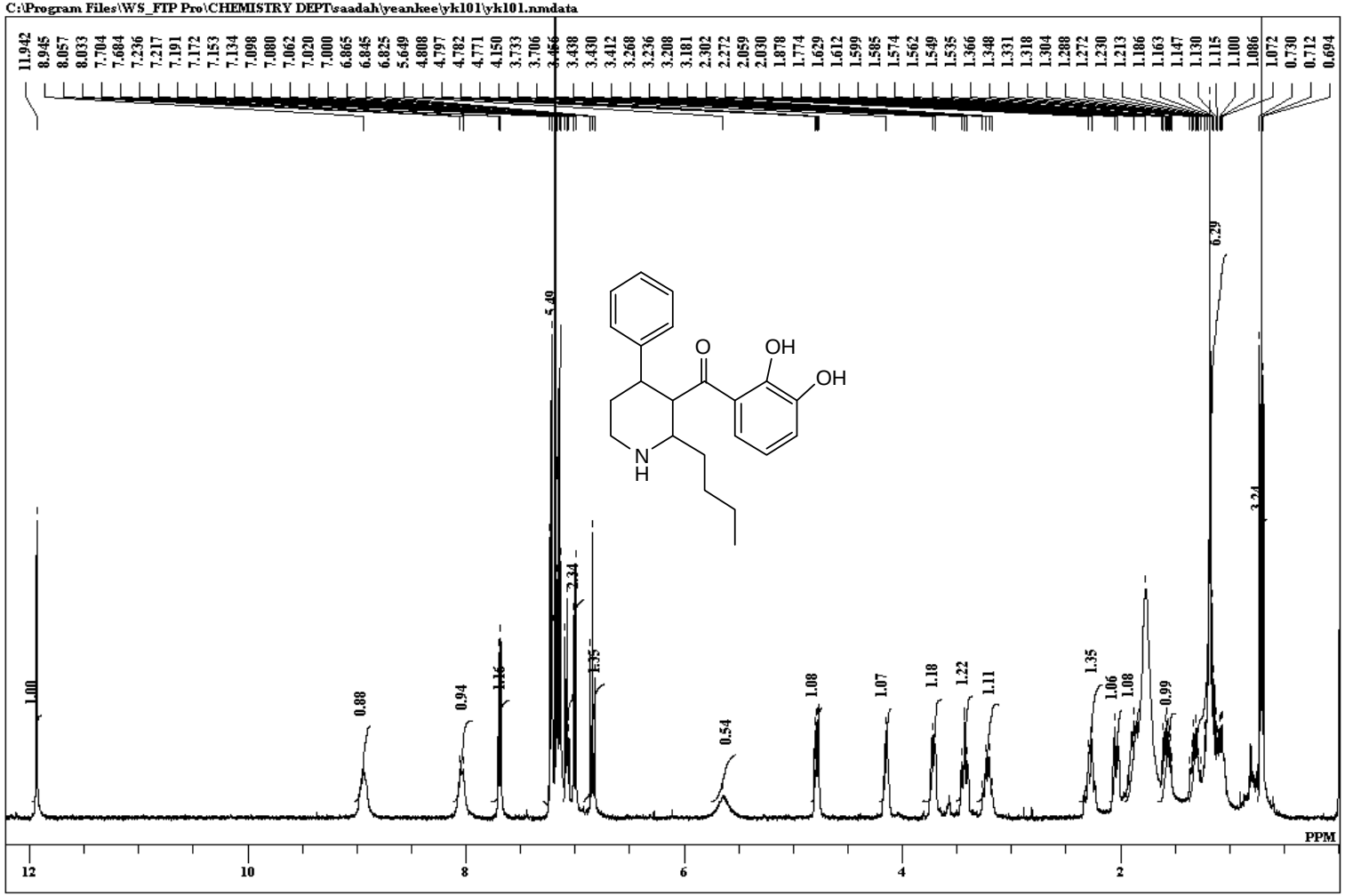
D:\ECA2\yk97b-crude-r3-13C-4.jdf



DFILE	yk97b-crude-r3-1
COMNT	single pulse decc
DATIM	18-03-2008 20:09
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	99.55 MHz
OBSET	5.13 KHz
OBFIN	0.98 Hz
POINT	32781
FREQU	31250.00 Hz
SCANS	2000
ACQTM	1.0486 sec
PD	2.0000 sec
PW1	4.42 usec
IRNUC	1H
CTEMP	21.8 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	54

1H-yk101

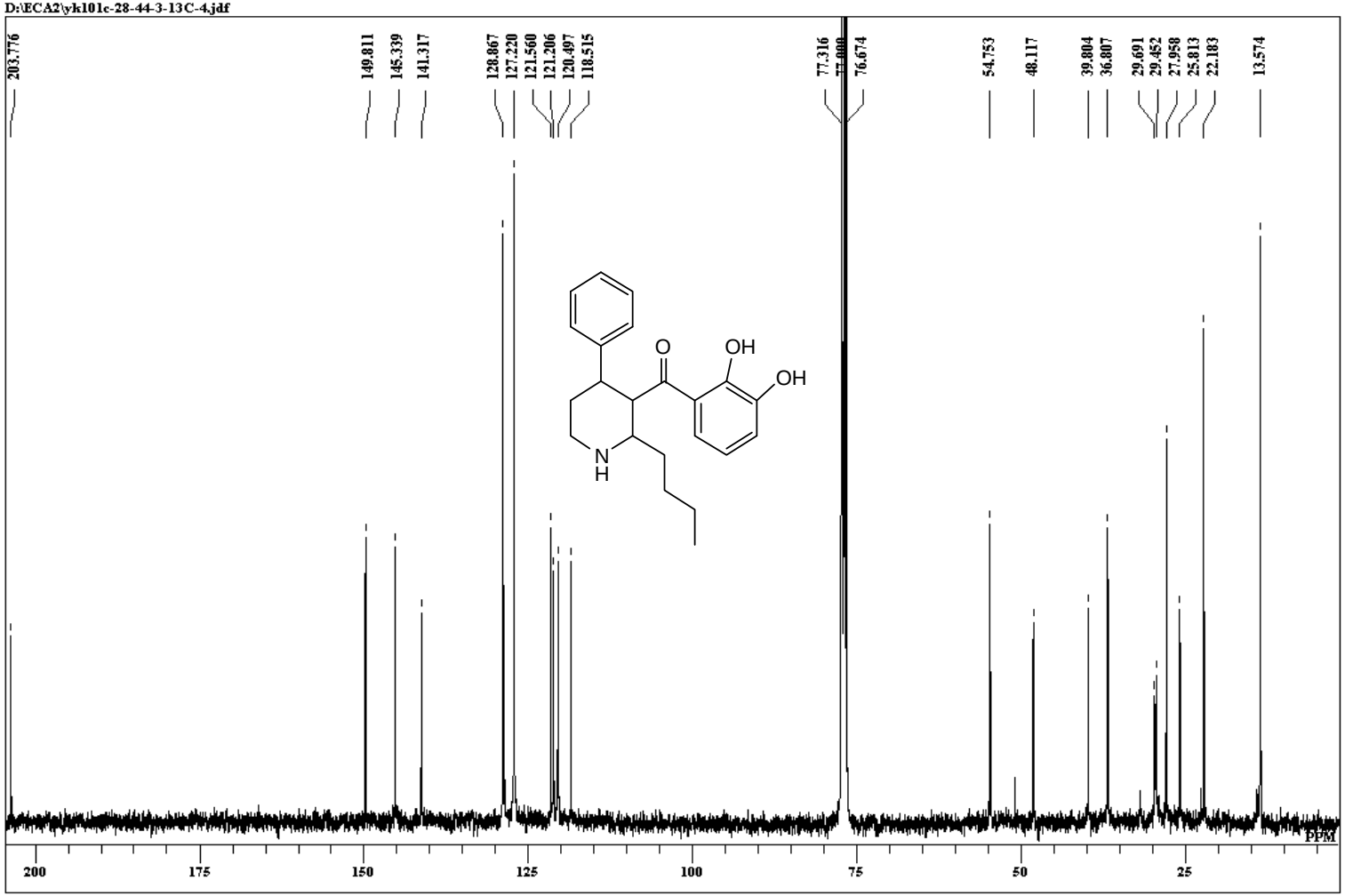
C:\Program Files\WS_FTP Pro\CHEMISTRY DEPT\saadah\yeankee\yk101\yk101.nmdata



DFILE	yk101.nmdata
COMNT	1H-yk101
DATIM	Mon Jun 16 15:3
OBNUC	1H
EXMOD	non
OBFRQ	399.65 MHz
OBSET	130.00 KHz
OBFIN	4300.00 Hz
POINT	32768
FREQU	7993.60 Hz
SCANS	4
ACQTM	4.0993 sec
PD	1.0500 sec
PW1	13.00 usec
IRNUC	1H
CTEMP	30.0 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.00 Hz
RGAIN	21

single pulse decoupled gated NOE-ykl01c-28-44-3-13C

D:\ECA2\ykl01c-28-44-3-13C-4.jdf



DFILE	ykl01c-28-44-3-1
COMNT	single pulse decc
DATIM	27-04-2008 02:23
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	99.55 MHz
OBSET	5.13 KHz
OBFIN	0.98 Hz
POINT	32781
FREQU	31250.00 Hz
SCANS	10000
ACQTM	1.0486 sec
PD	2.0000 sec
PW1	3.07 usec
IRNUC	1H
CTEMP	20.1 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.00 Hz
RGAIN	60