Supporting Information

Design and Synthesis of Pyrrolotriazepine Derivatives: An experimental and Computational Study

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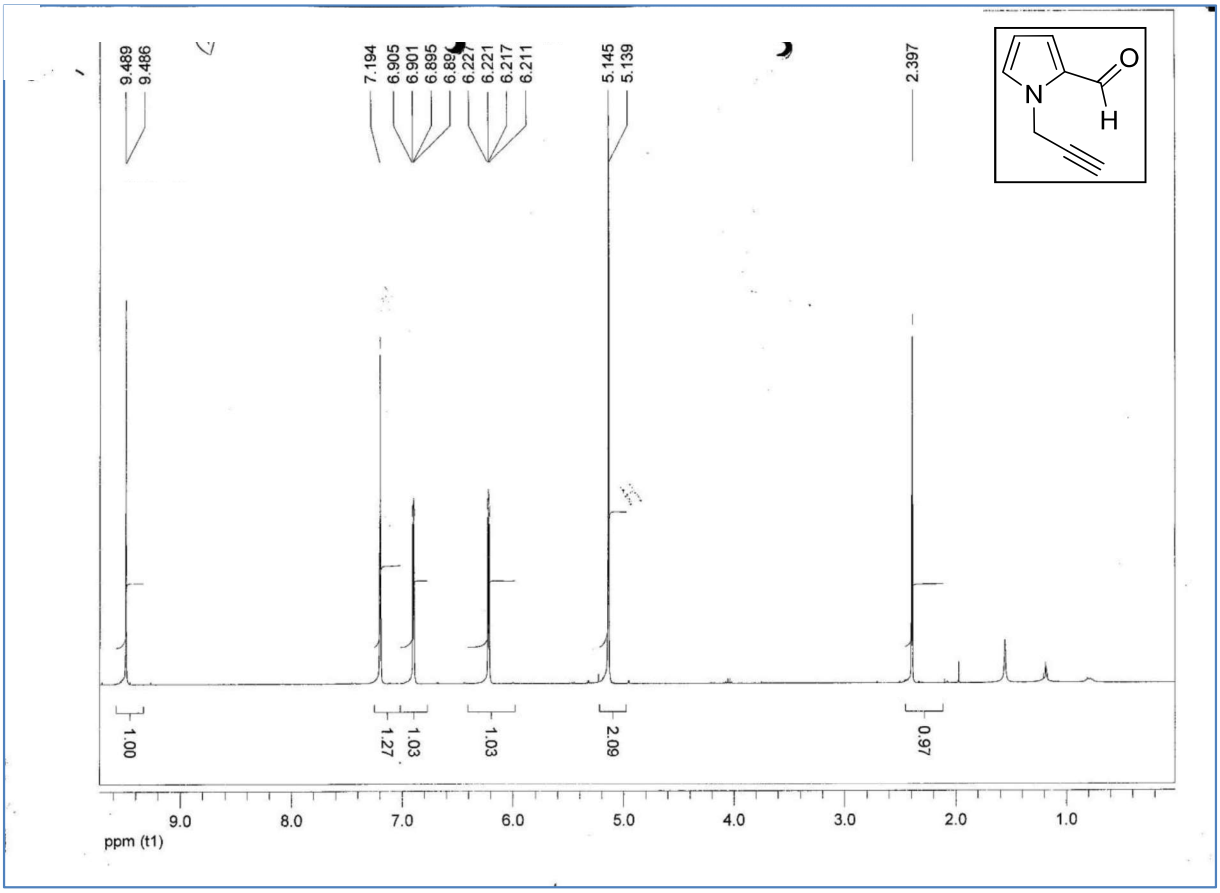
Experimental Section

General: The ^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz NMR spectrometer in $CDCl_3$ with solvent signal ($CHCl_3$: 7.26/77.0) using TMS as an internal standard. Chemical shifts (δ) are given in ppm and *J* values are given in Hz. ^{13}C NMR spectra were fully decoupled and were referenced to the middle peak of the solvent $CDCl_3$ at 77.00 ppm. Splitting pattern were designated as s, singlet; bs, broad singlet; d, doublet; dd, doublet of doublets; t, triplet; m, multiplet. Column chromatography was performed on silica gel (60-mesh,), TLC was carried out on Merck 0.2 mm silica gel 60 F_{254} analytical aluminum plates. High resolution Mass spectra were recorded by LC-MS TOF electrospray ionization technique. Mass spectrum was recorded by GC/MS electron impact (EI) technique using helium gas as carring gas. Chemicals and all solvents were commercially available and used without further purification. Infra-red (IR) spectra were recorded in the range 4000-600 cm^{-1} via ATR diamond. Melting points were measured using melting point apparatus and were uncorrected. Evaporation of solvents was performed at reduced pressure, using a rotary vacuum evaporator.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2.397
N
O
H
1.00
1.27
1.03
1.03
2.09
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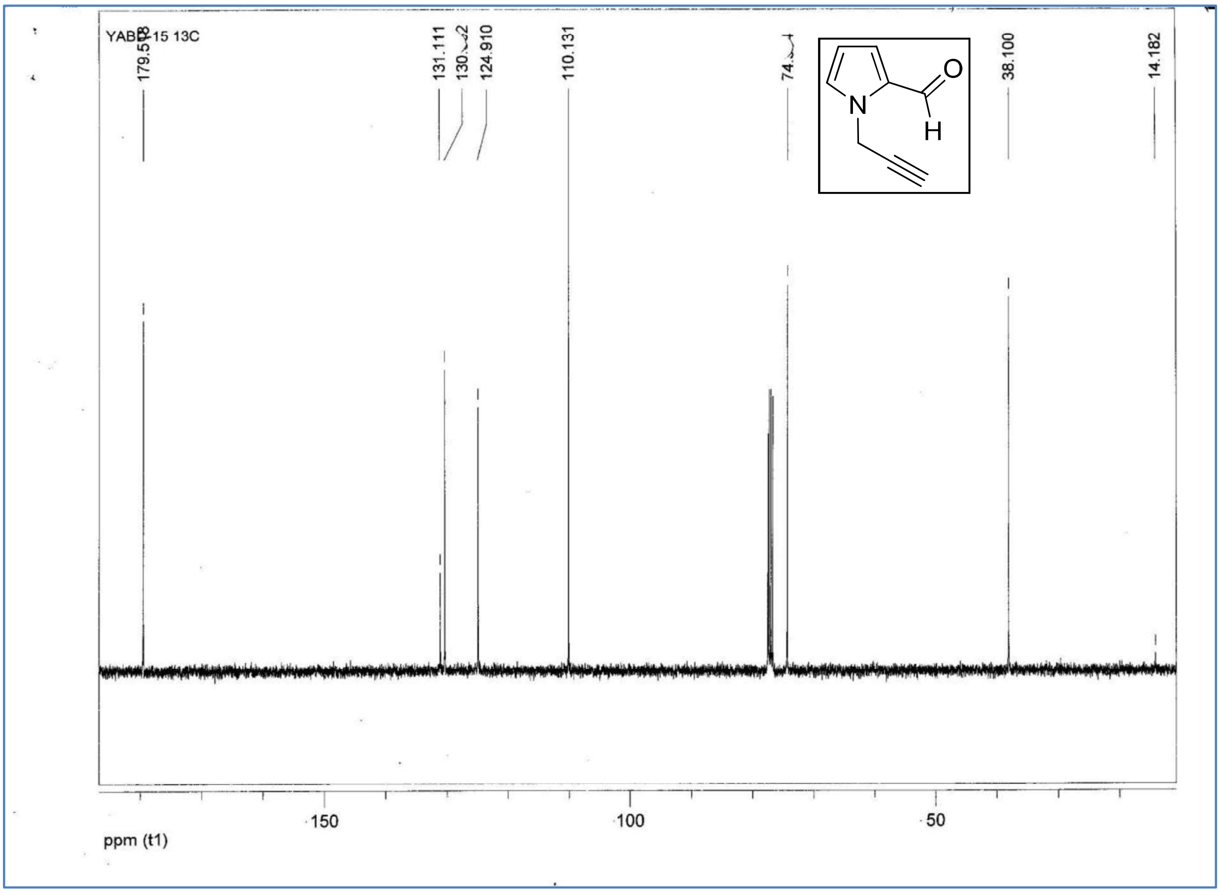
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)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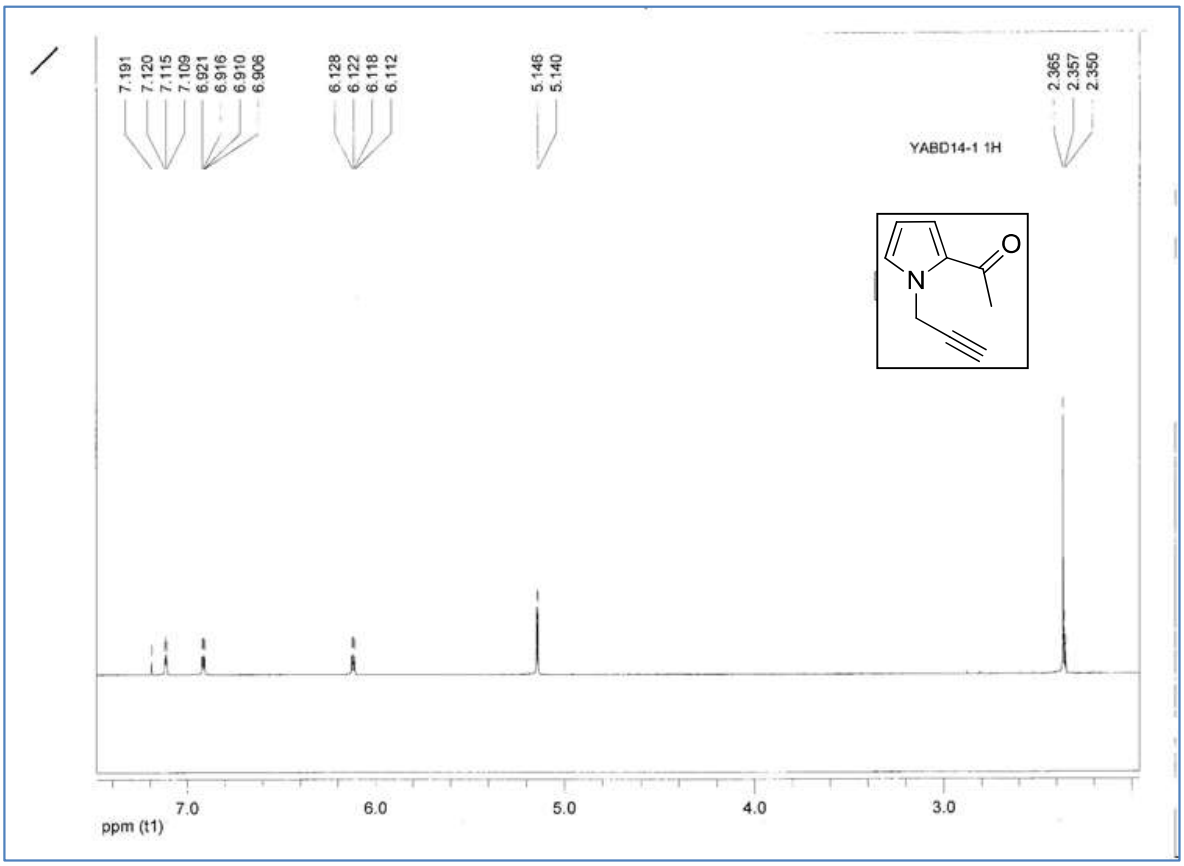
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6.916
6.910
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5.140
2.365
2.357
2.350
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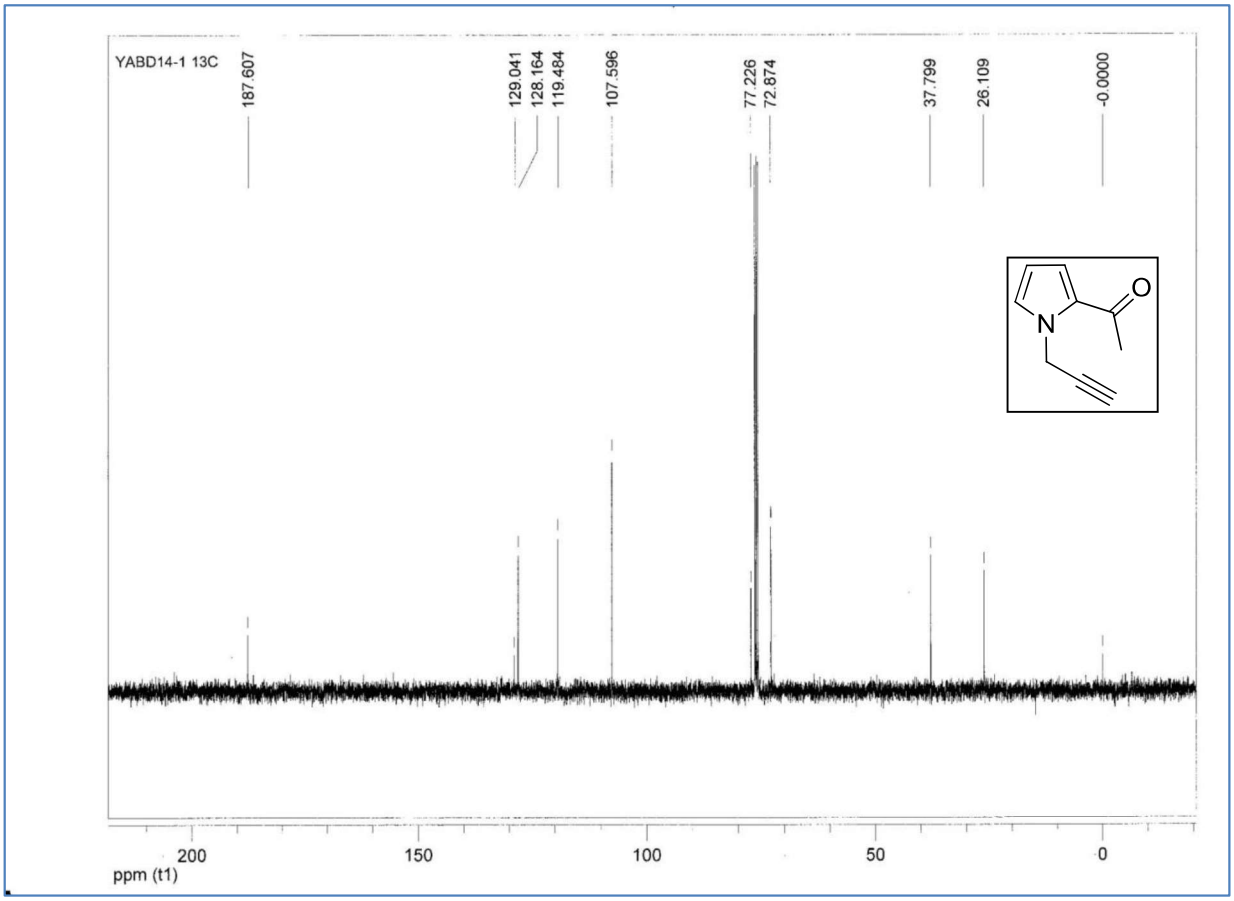
6.0
5.0
4.0
3.0
ppm (t1)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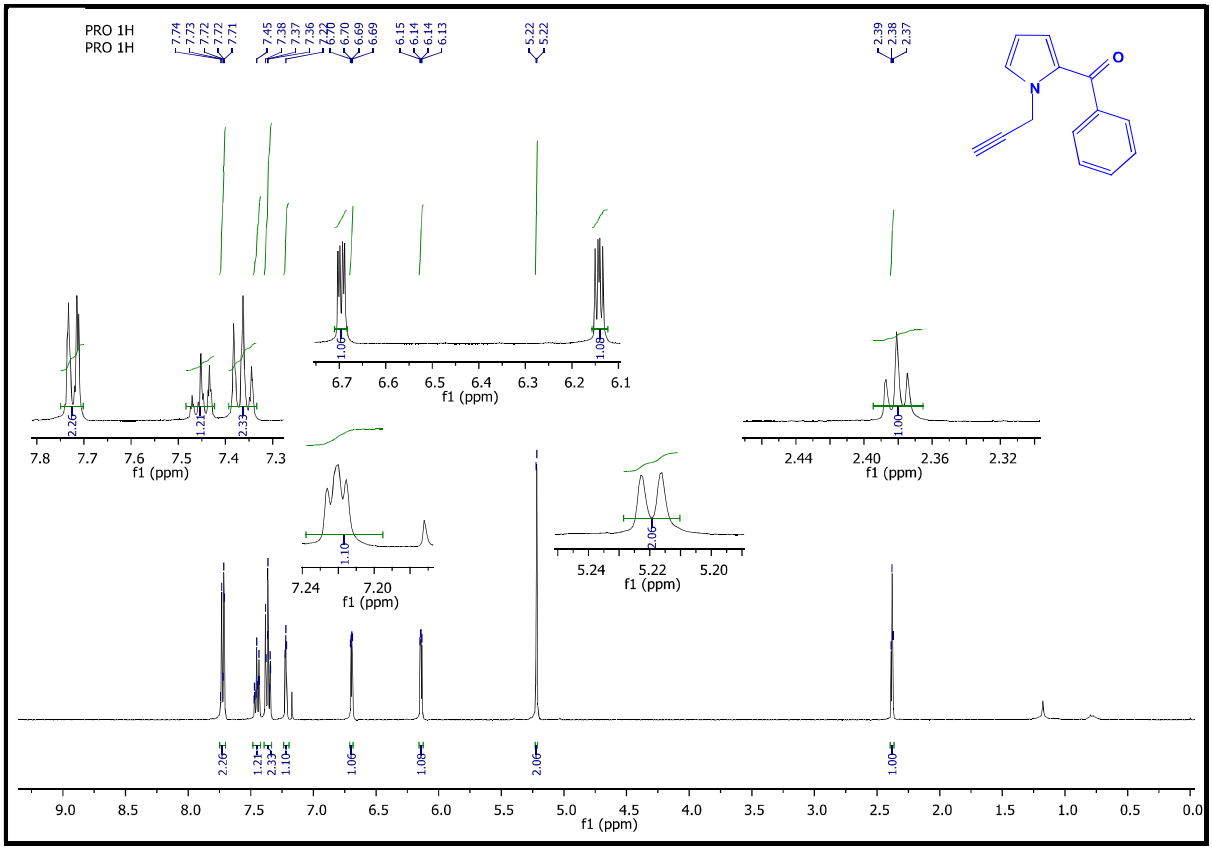
ppm (t1)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PRO 1H
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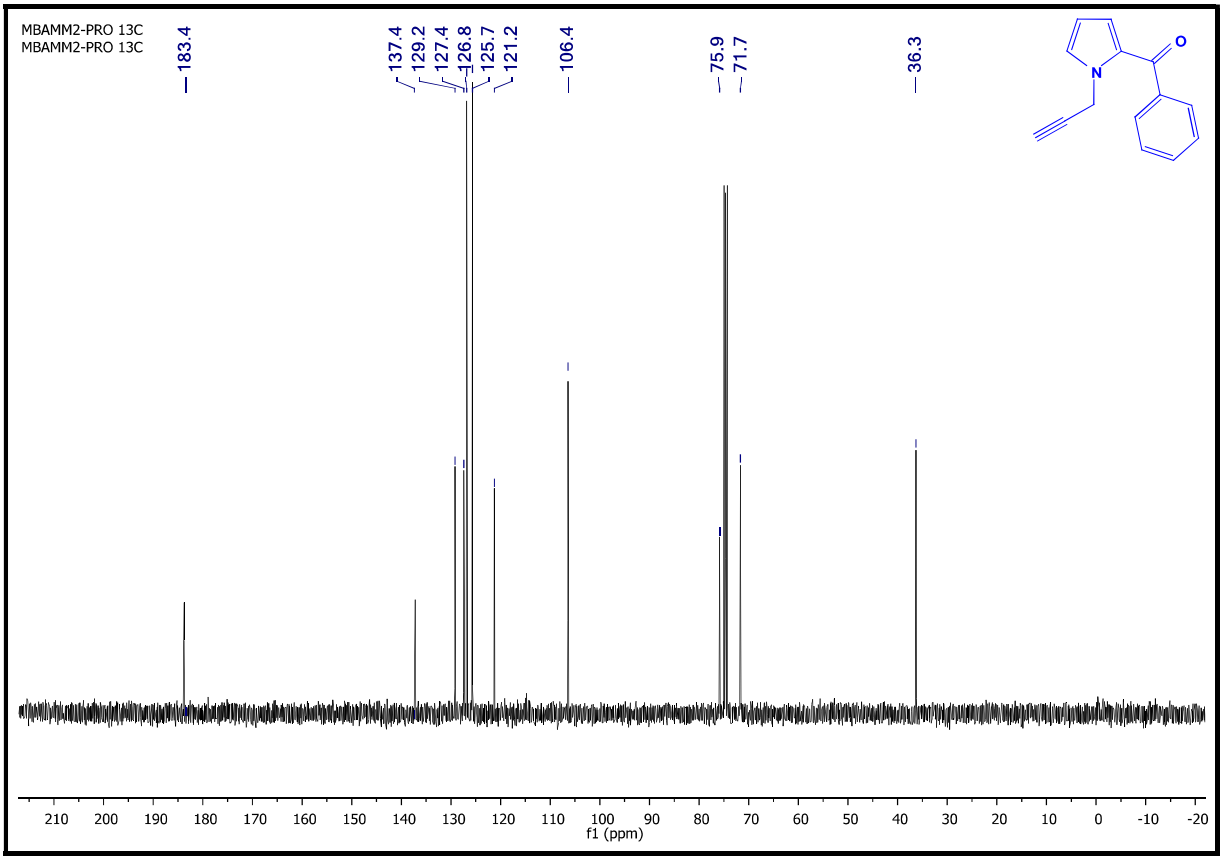
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MBAMM2-PRO 13C
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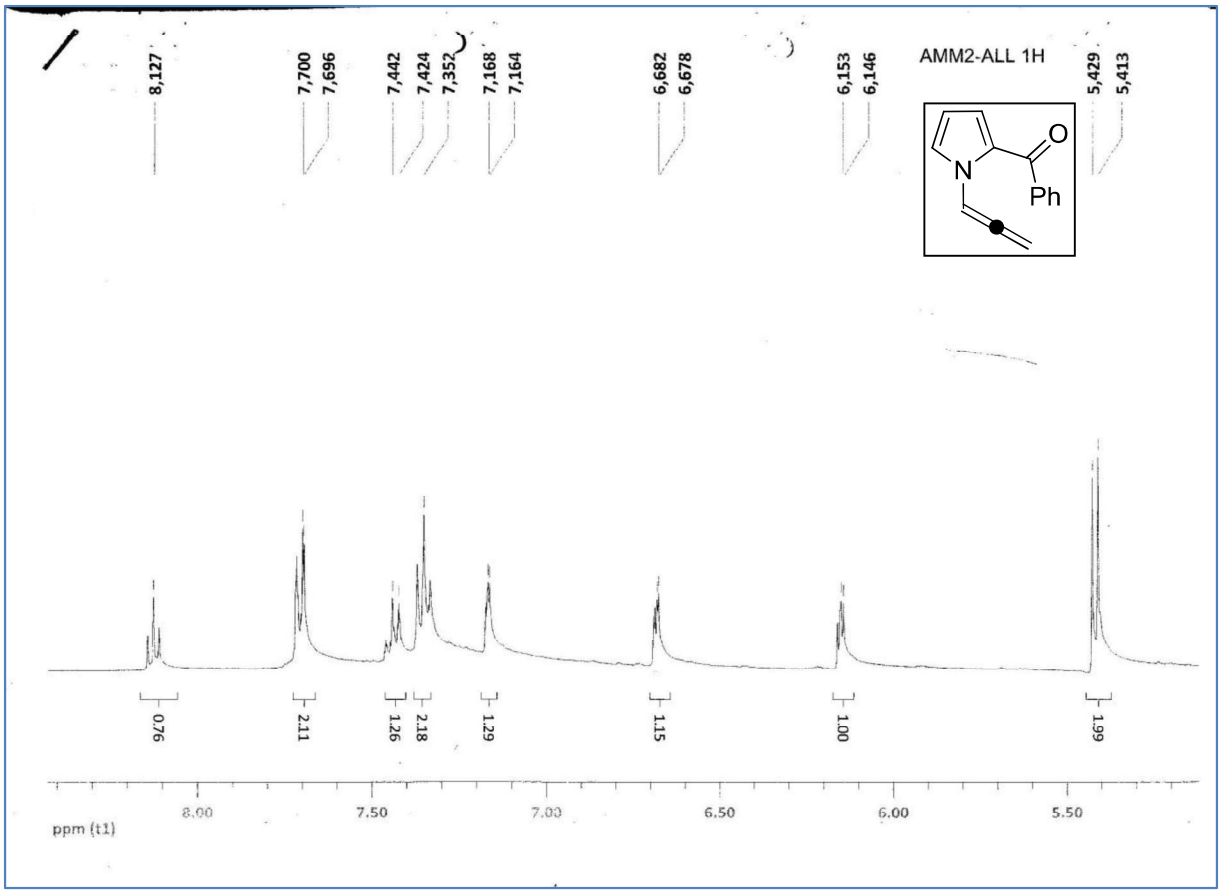
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5,429
5,413
O
N
Ph
0,76
2,11
1,26
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5,50
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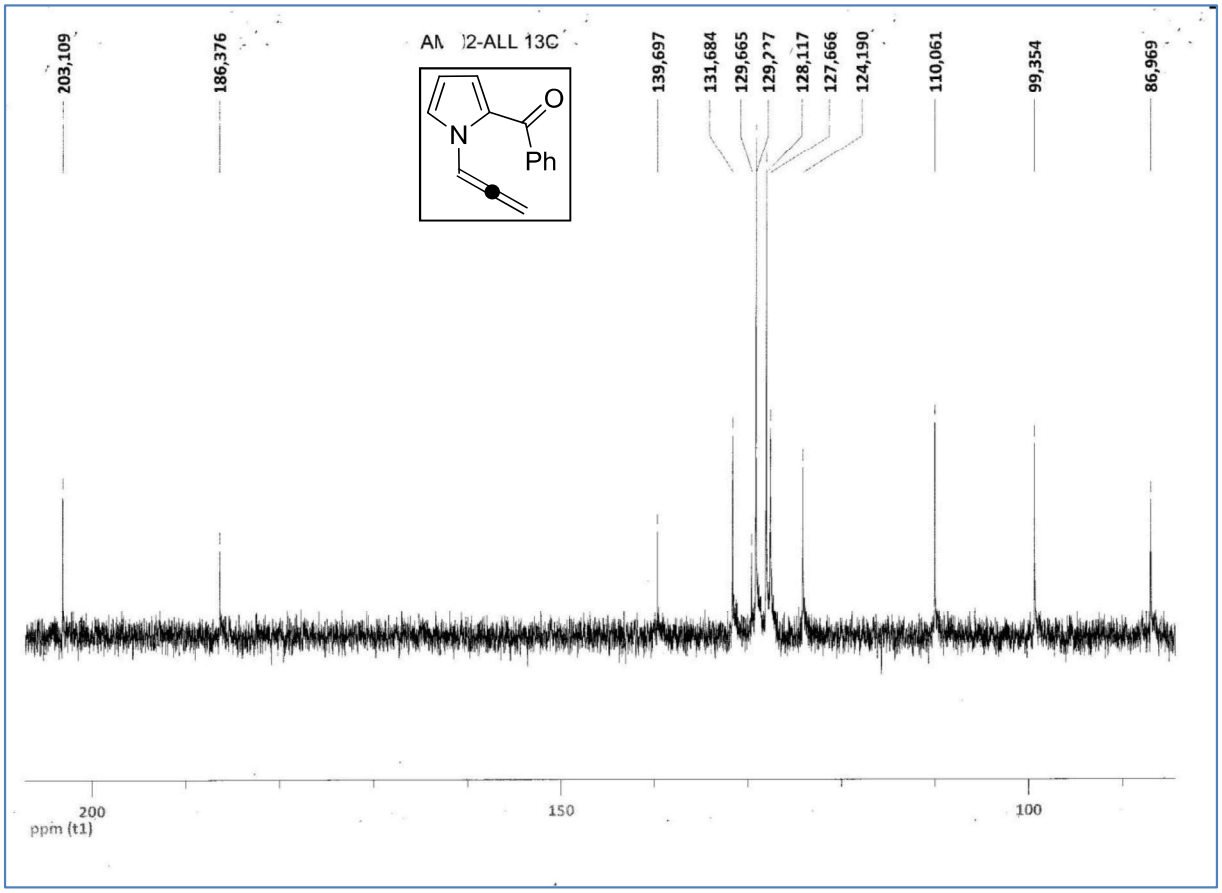
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N
Ph
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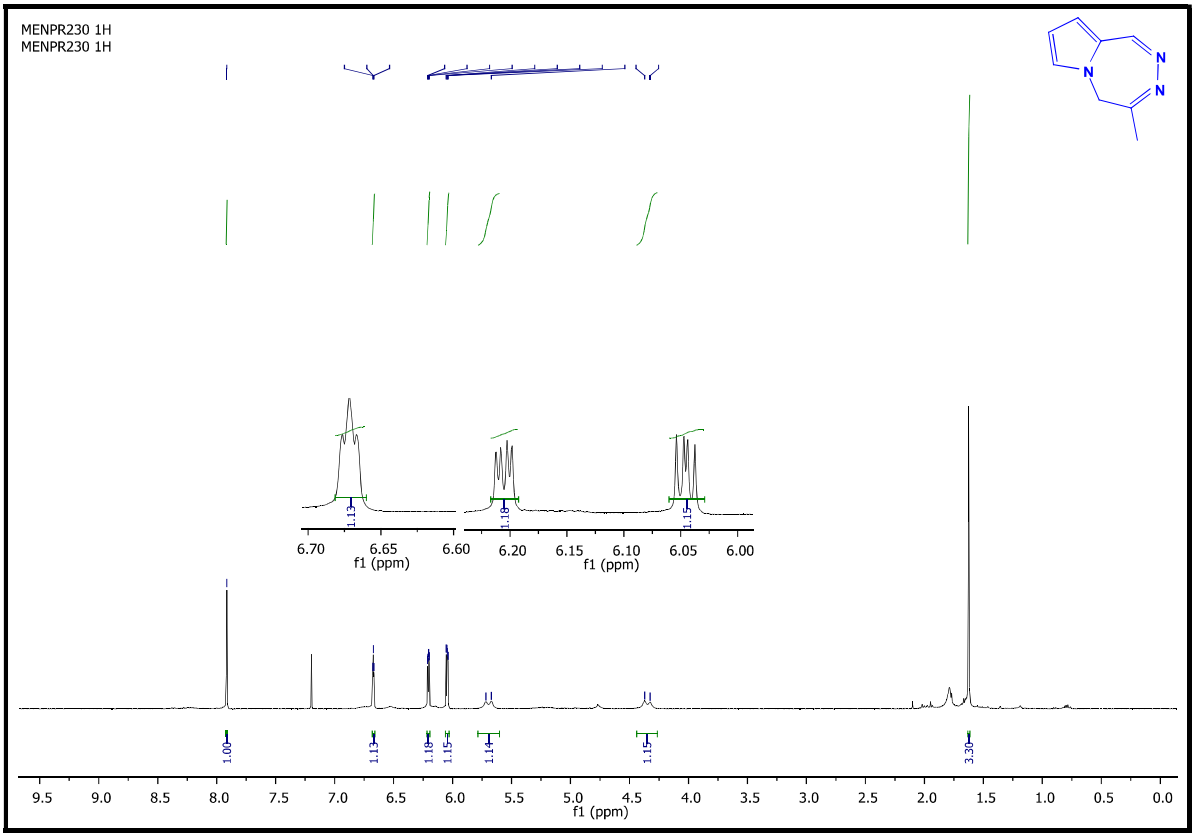
100
ppm (t1)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MENPR230 1H
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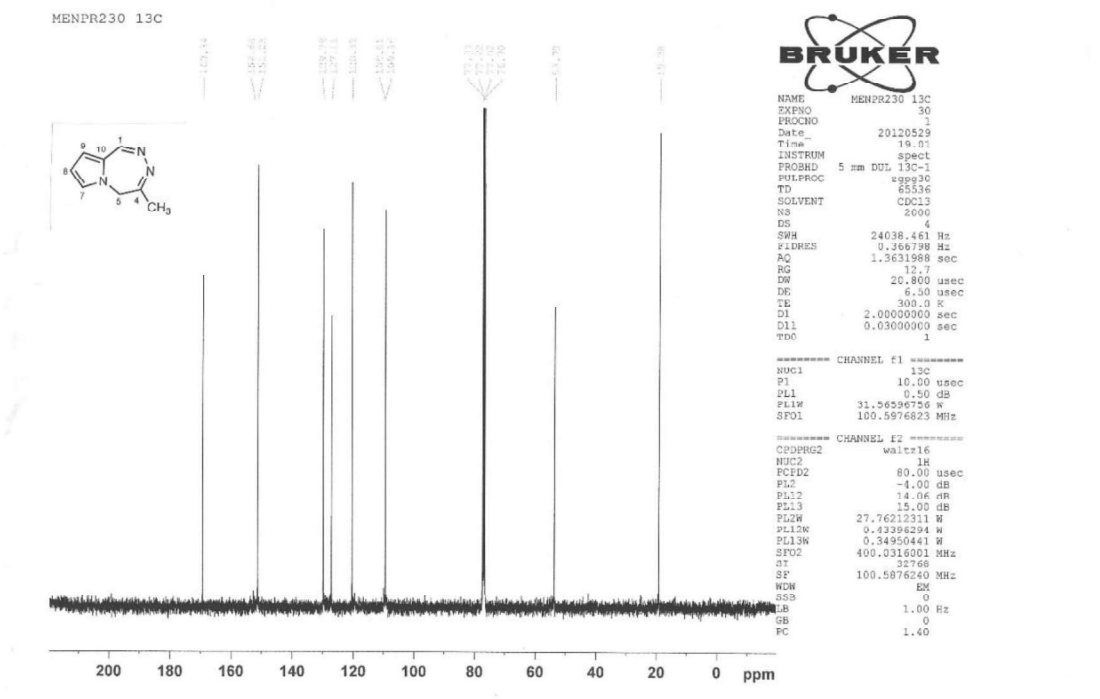
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SOLVENT CDCl3
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 12.7
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 0.50 dB
PL1W 31.56596756 W
SFO1 100.5976823 MHz
======== CHANNEL f2 ========
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NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.06 dB
PL13 15.00 dB
PL2W 27.76212311 W
PL12W 0.43396294 W
PL13W 0.34950441 W
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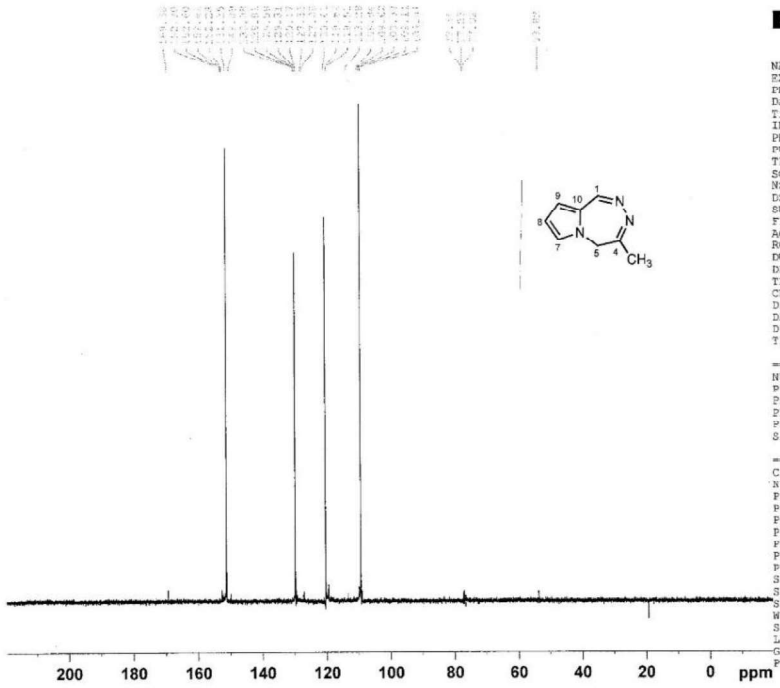
SI 32768
SF 100.5876240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm

MENPR230 DEPT90

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SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                 2050
DW              20.800 usec
DE               6.50 usec
TE              300.0 K
CNST2       145.0000000
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D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
P2                20.00 usec
PL1                0.50 dB
PL1W       31.56596756 W
SFO1       100.5976823 MHz

======== CHANNEL f2 ========
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NUC2                1H
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PL2               -4.00 dB
PL12              14.06 dB
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PL12W       0.43396294 W
SFO2       400.0316001 MHz
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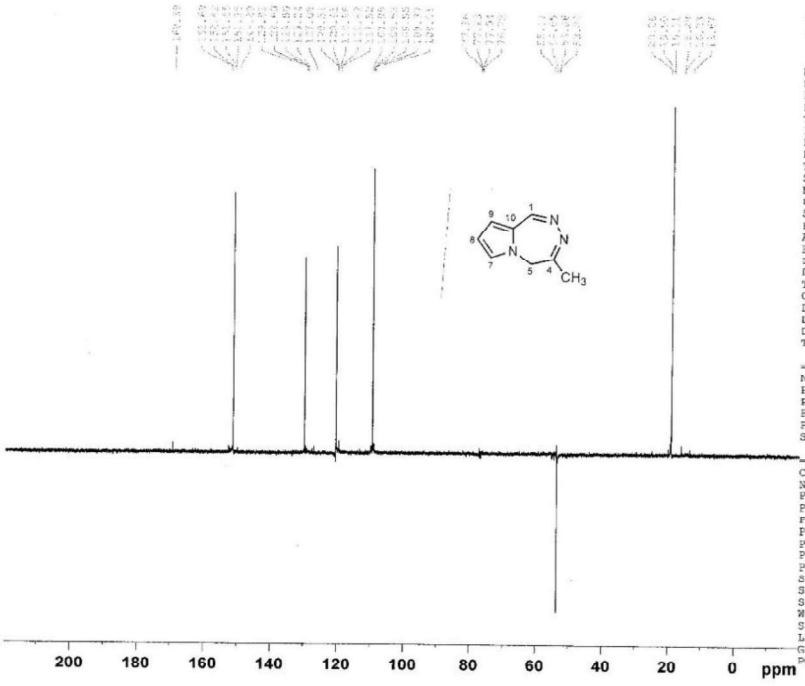

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FIDRES        0.366798 Hz
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RG                 2050
DW              20.800 usec
DE               6.50 usec
TE              300.0 K
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D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
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P2                20.00 usec
PL1                0.50 dB
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SFO1       100.5976823 MHz

======== CHANNEL f2 ========
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P4                20.00 usec
PCPD2             80.00 usec
PL2               -4.00 dB
PL12              14.06 dB
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PL12W       0.43396294 W
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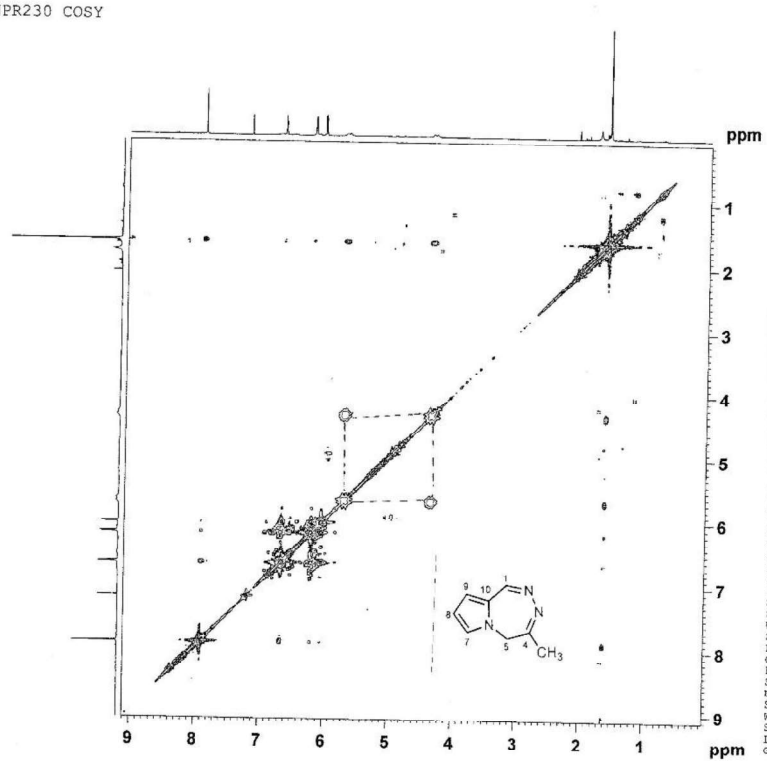
MENPR230 COSY



BRUKER

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DE	6.50 usec
TE	300.0 K
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D1	1.37056506 sec
D13	0.00000400 sec
D16	0.00010000 sec
IN0	0.00027600 sec
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P1	10.00 usec
PL1	-4.00 dB
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GPZ1	10.00 %
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FIDRES	14.153080 Hz
SW	9.057 ppm
FnMODE	QF
SI	1024
SF	400.0300351 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
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SSB	0
LB	0.00 Hz
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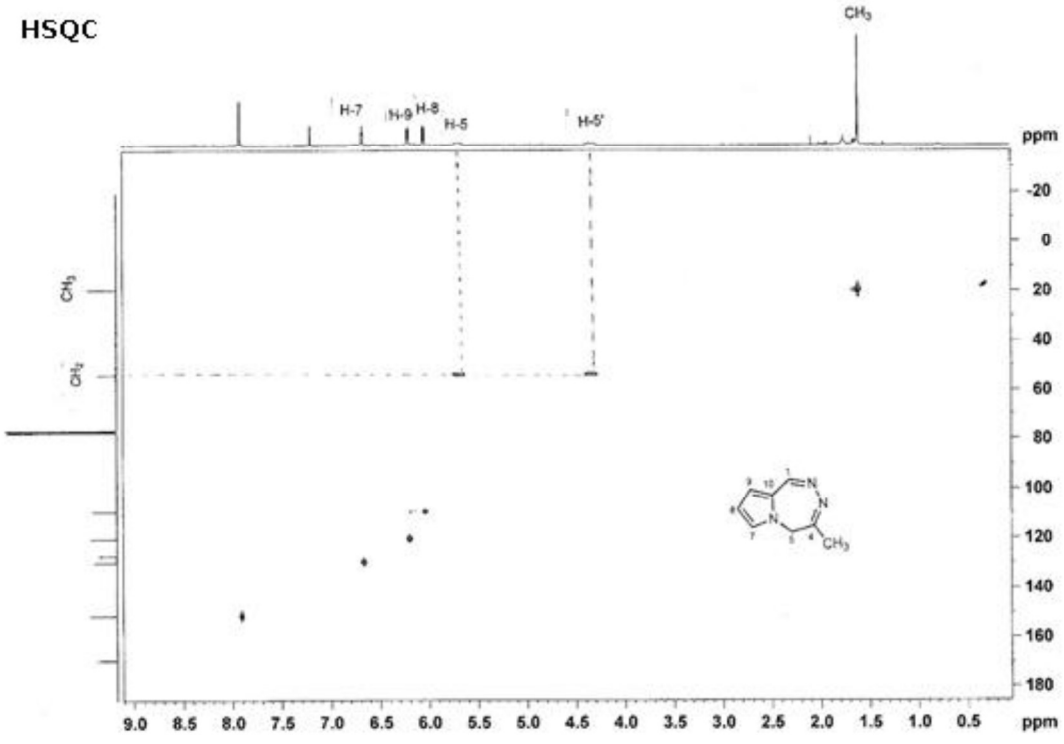

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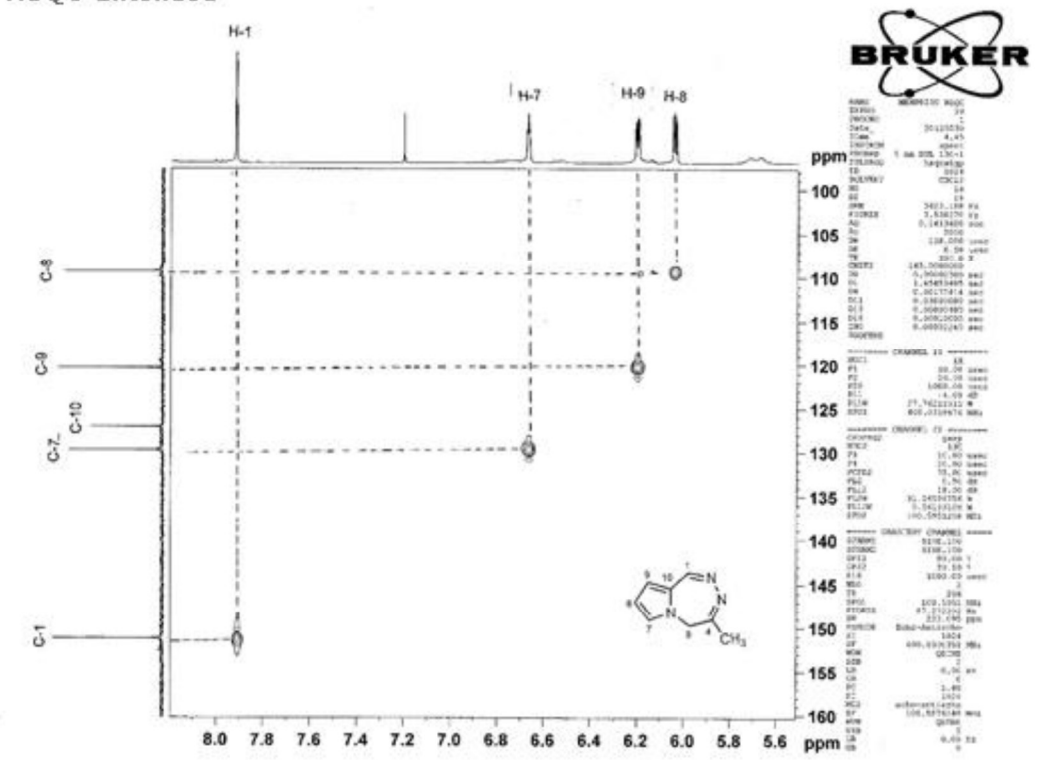

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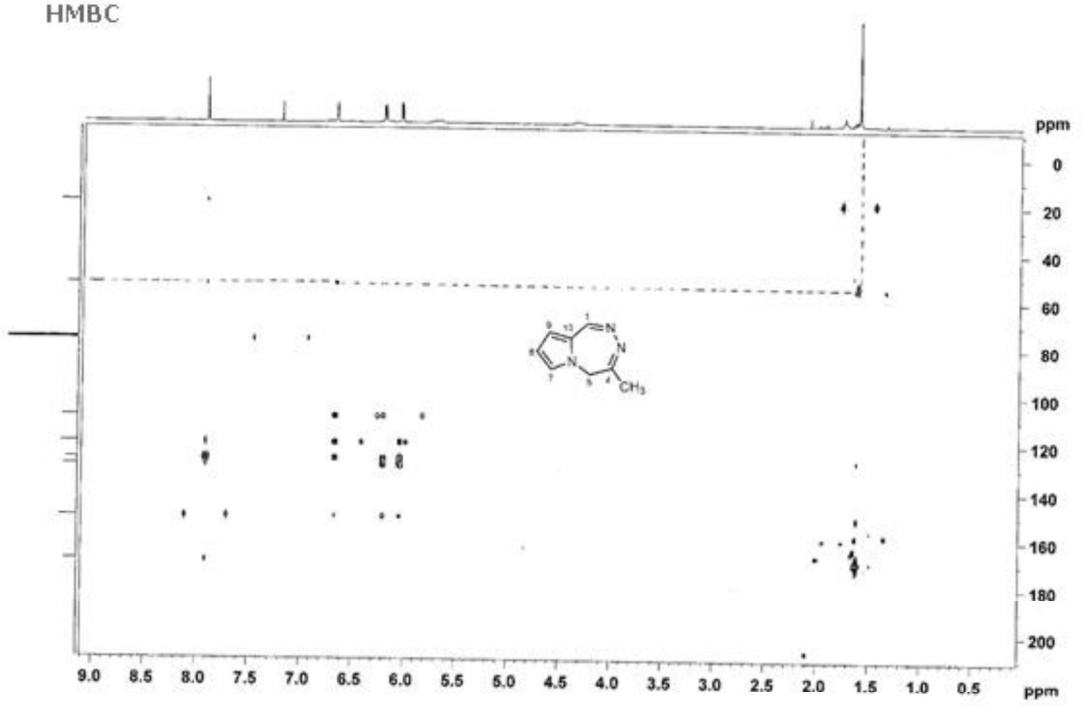

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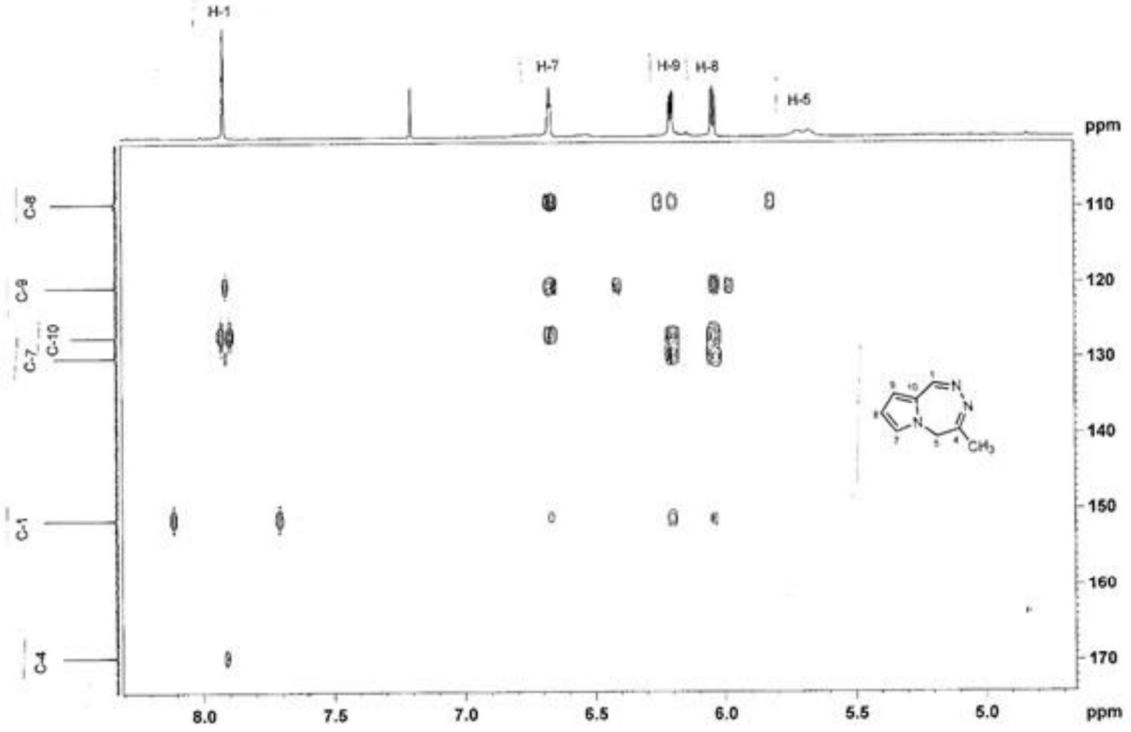

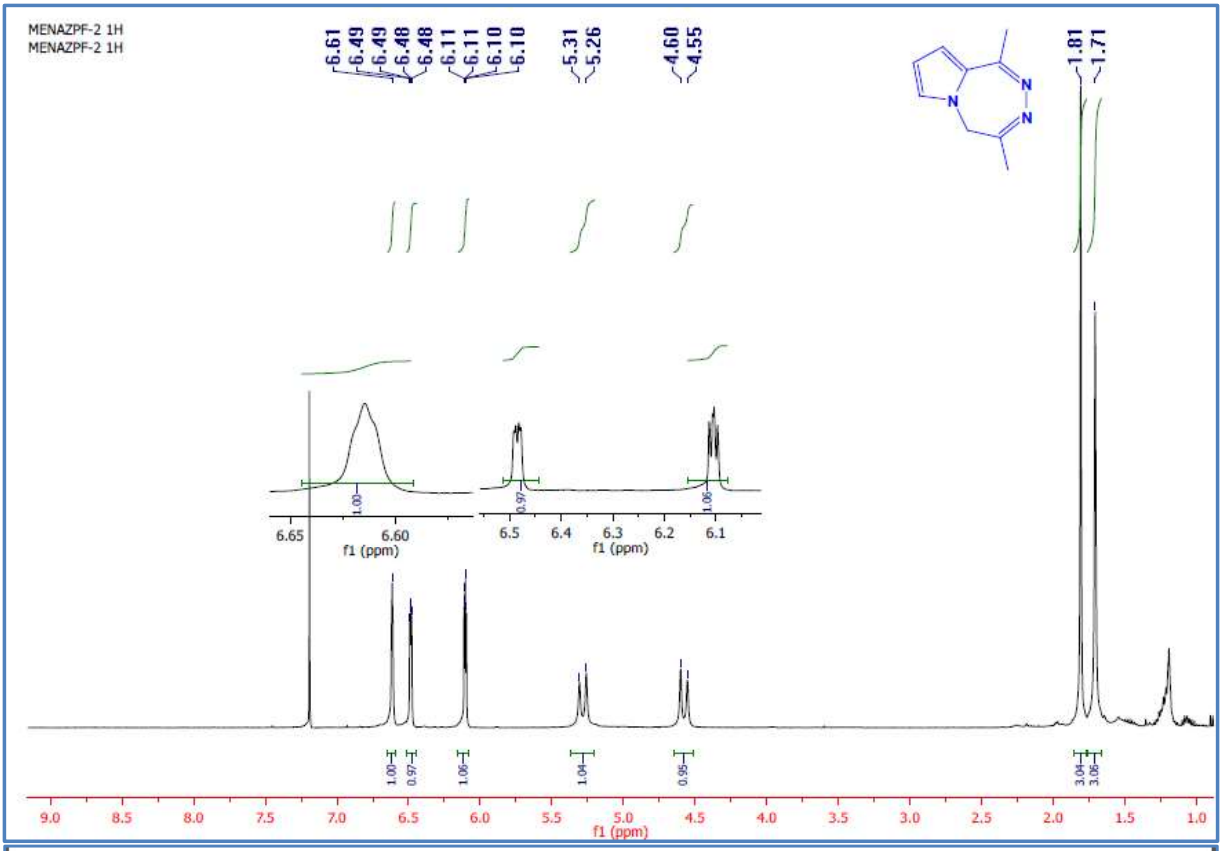
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MENAZPF-2 1H
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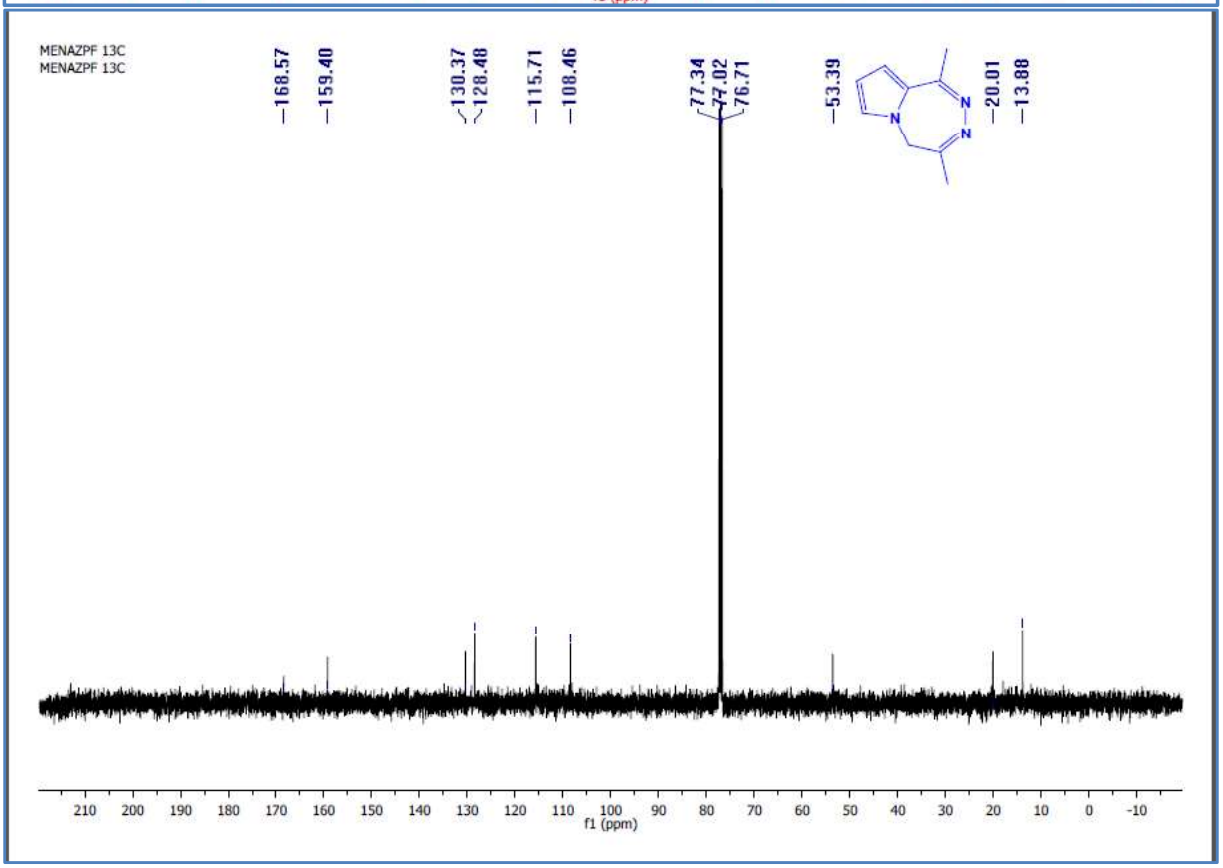
6.49
6.49
6.48
6.48
6.11
6.11
6.10
6.10
5.31
5.26
4.60
4.55
1.81
1.71
f1 (ppm)


MENAZPF 13C
MENAZPF 13C
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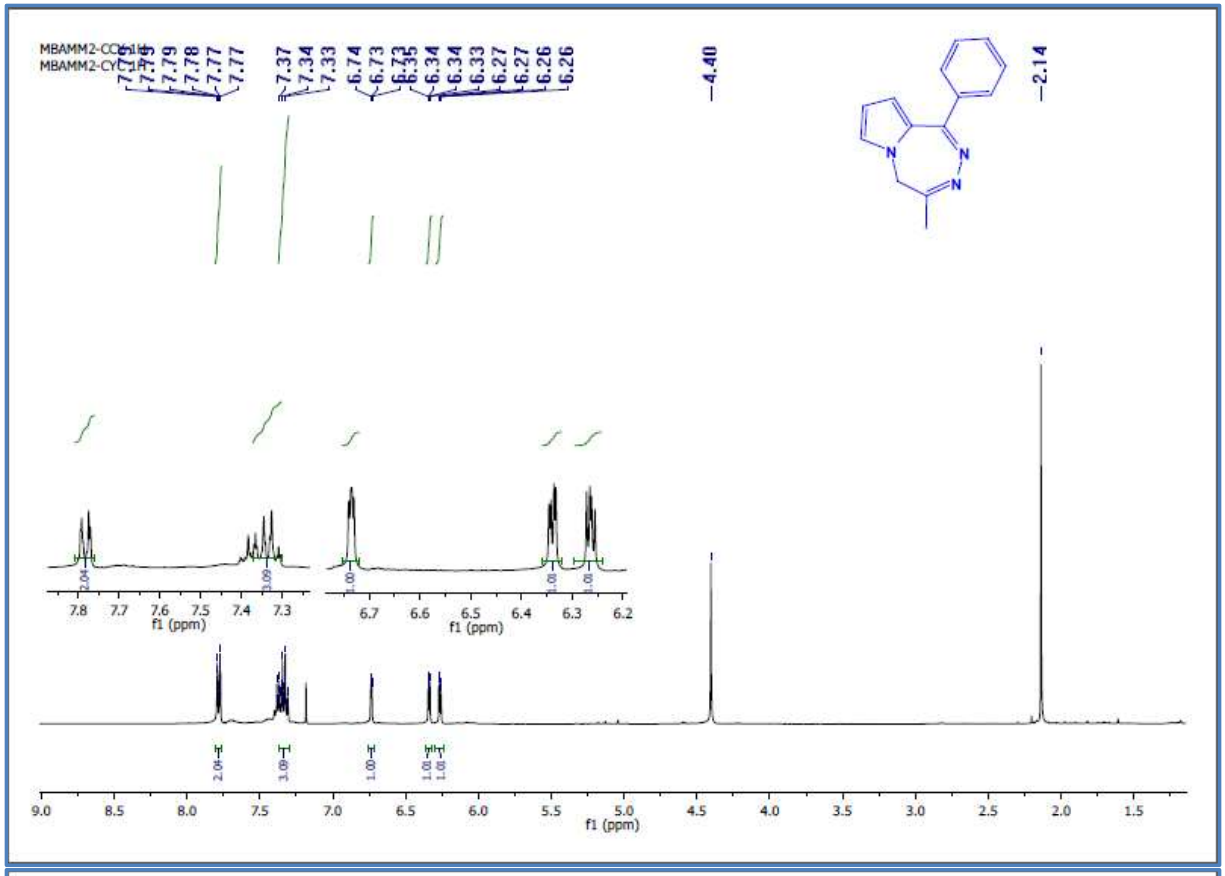
77.34
77.02
76.71
53.39
20.01
13.88
f1 (ppm)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7.77
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7.33
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6.27
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6.26
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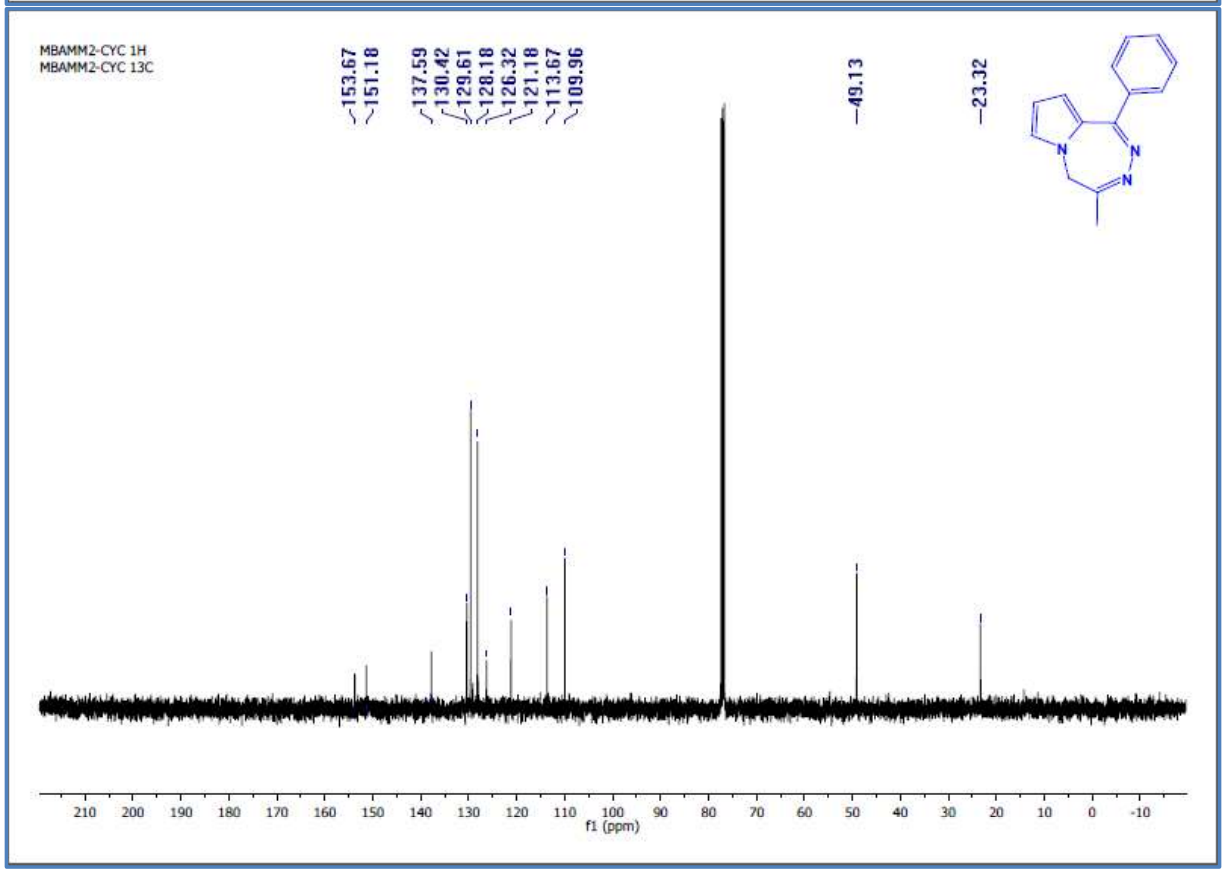
2.14
f1 (ppm)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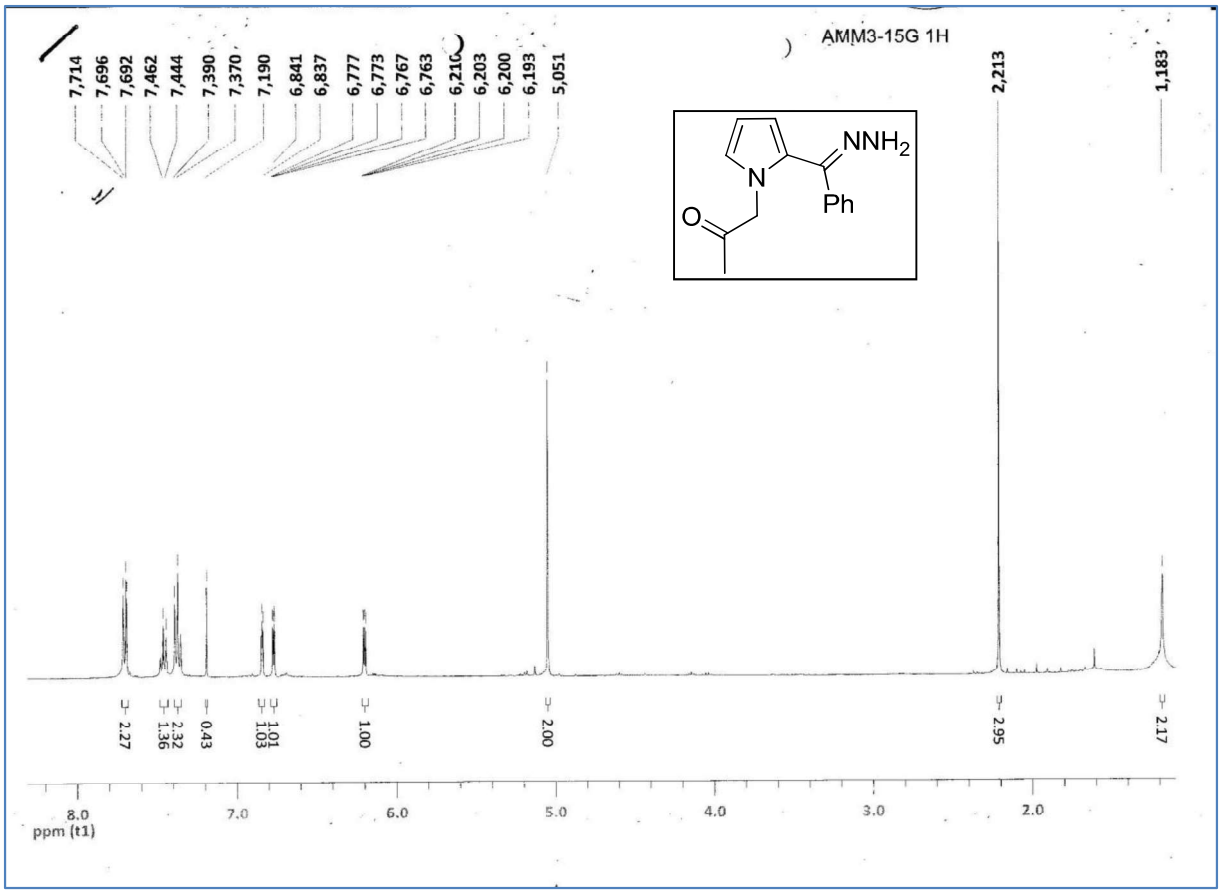
128.18
126.32
121.18
113.67
109.96
49.13
23.32
f1 (ppm)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6,777
6,773
6,767
6,763
6,216
6,203
6,200
6,193
5,051
2,213
1,183
NNH2
N
Ph
O
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2,32
1,36
0,43
1,01
1,03
1,00
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7,0
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4,0
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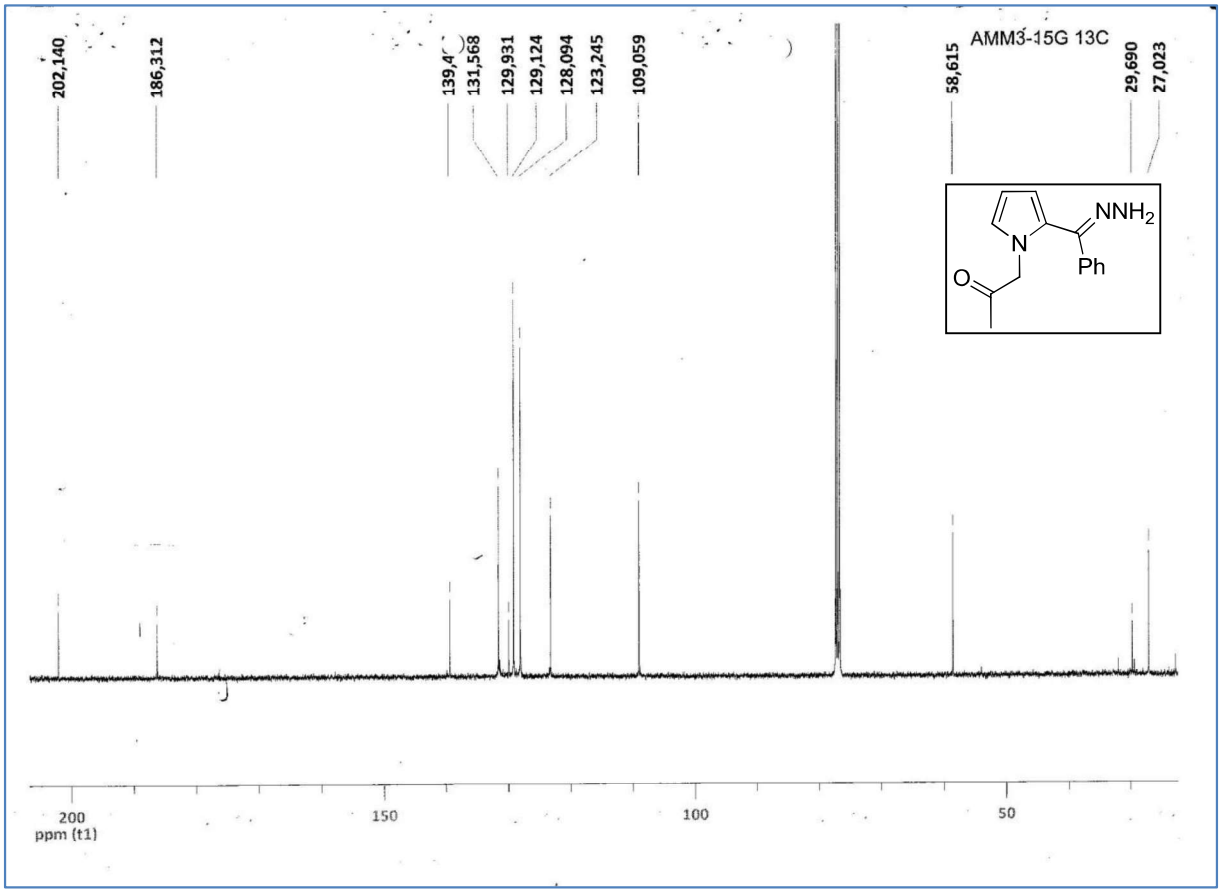
2,0
ppm (t1)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29,690
27,023
NNH2
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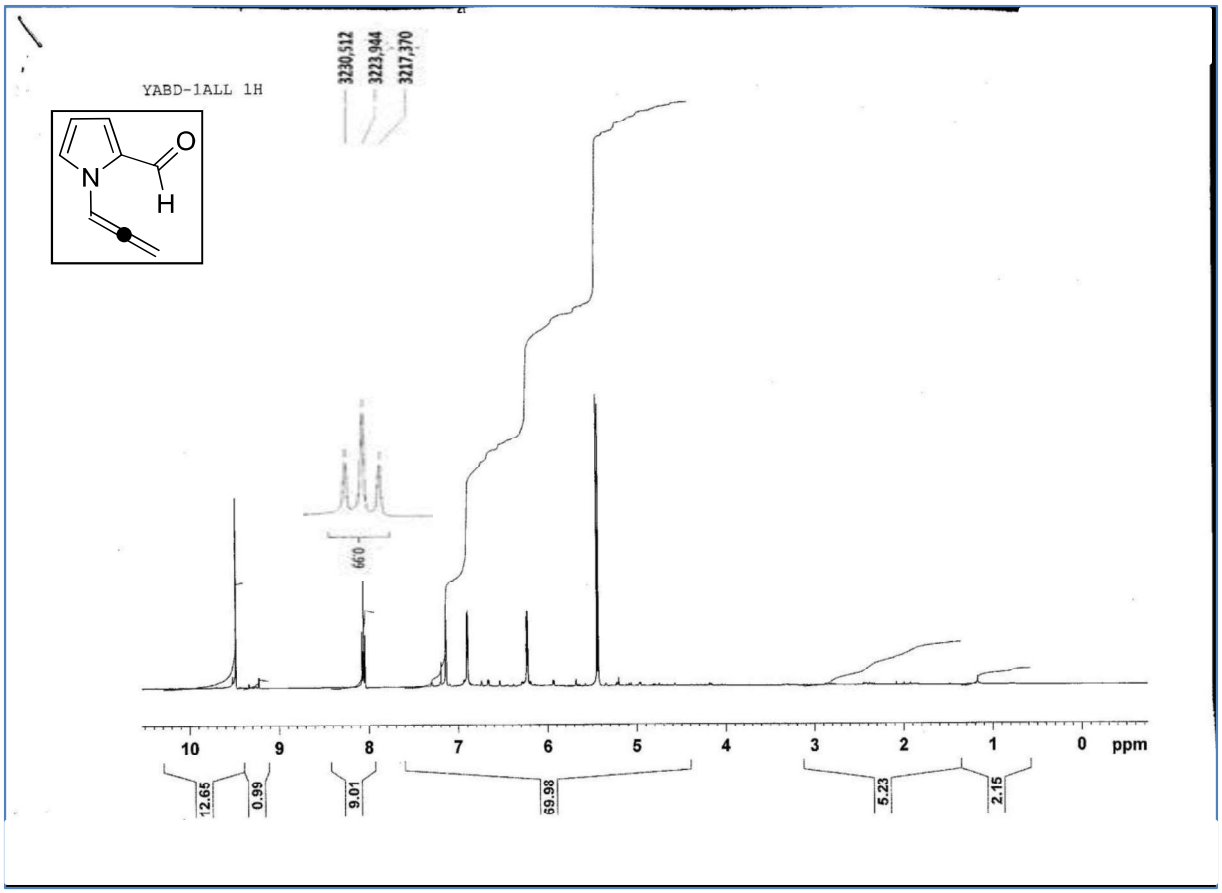
Ph
O
200
150
100
50
ppm (t1)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O
N
H
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10
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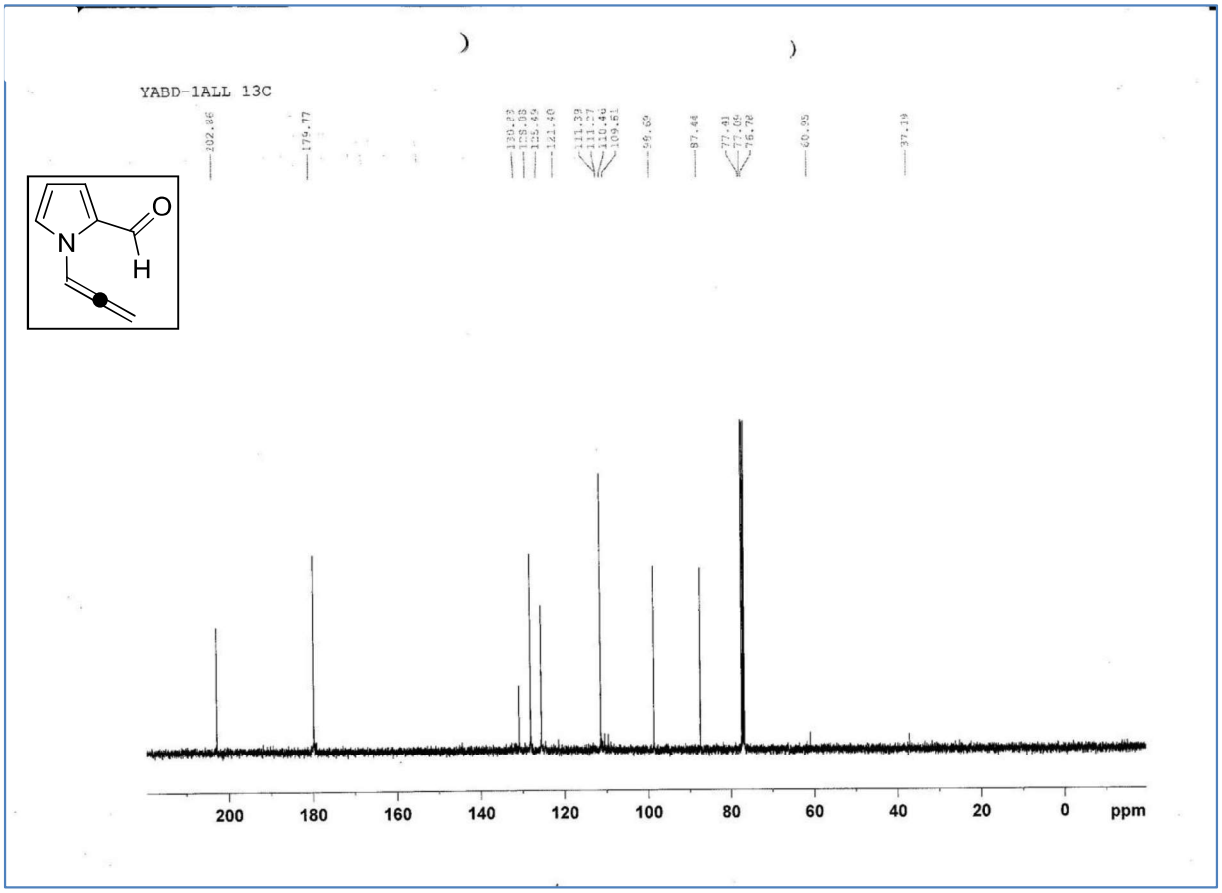
5.23
2.15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179.17
139.23
129.05
125.69
121.40
111.39
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110.46
109.61
96.89
87.44
77.41
77.06
76.70
60.95
37.19
O
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H
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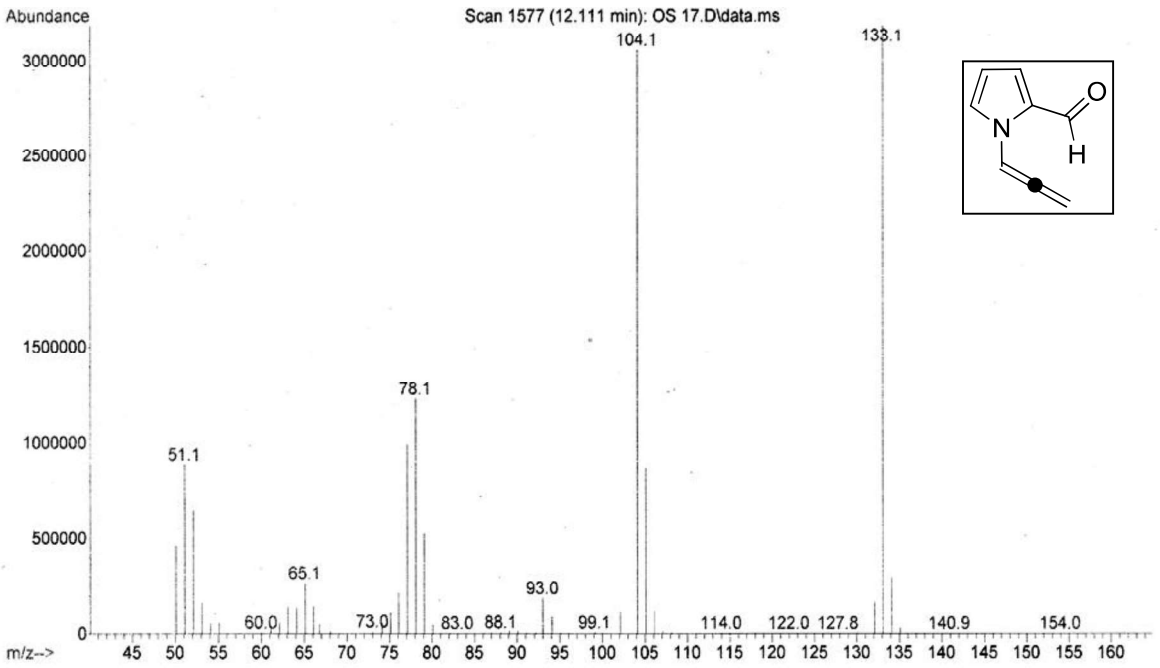
120
100
80
60
40
20
0
ppm


Abundance
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78.1
51.1
65.1
93.0
60.0
73.0
83.0
88.1
99.1
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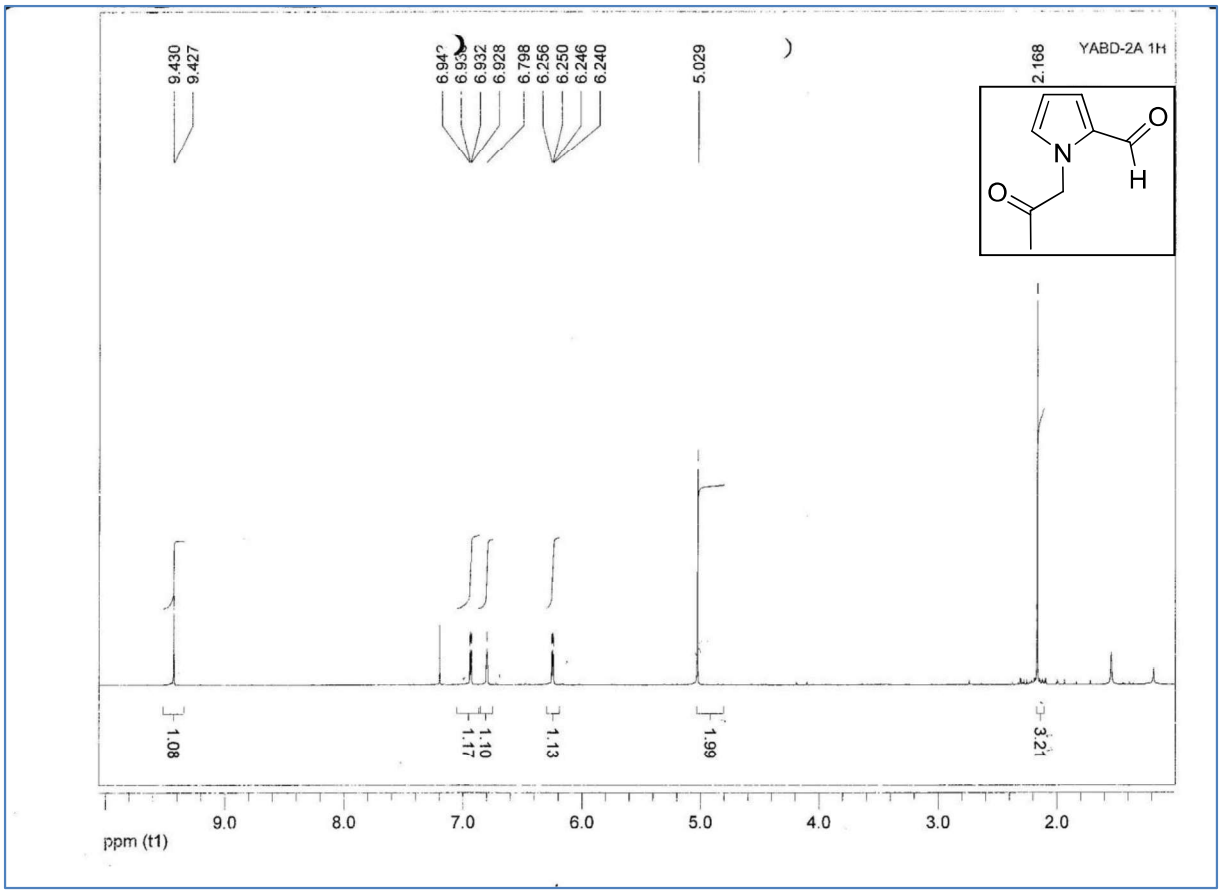
122.0
127.8
140.9
154.0
m/z-->
O
N
H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6.936
6.932
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6.246
6.240
5.029
2.168
1.08
1.17
1.10
1.13
1.99
3.21
9.0
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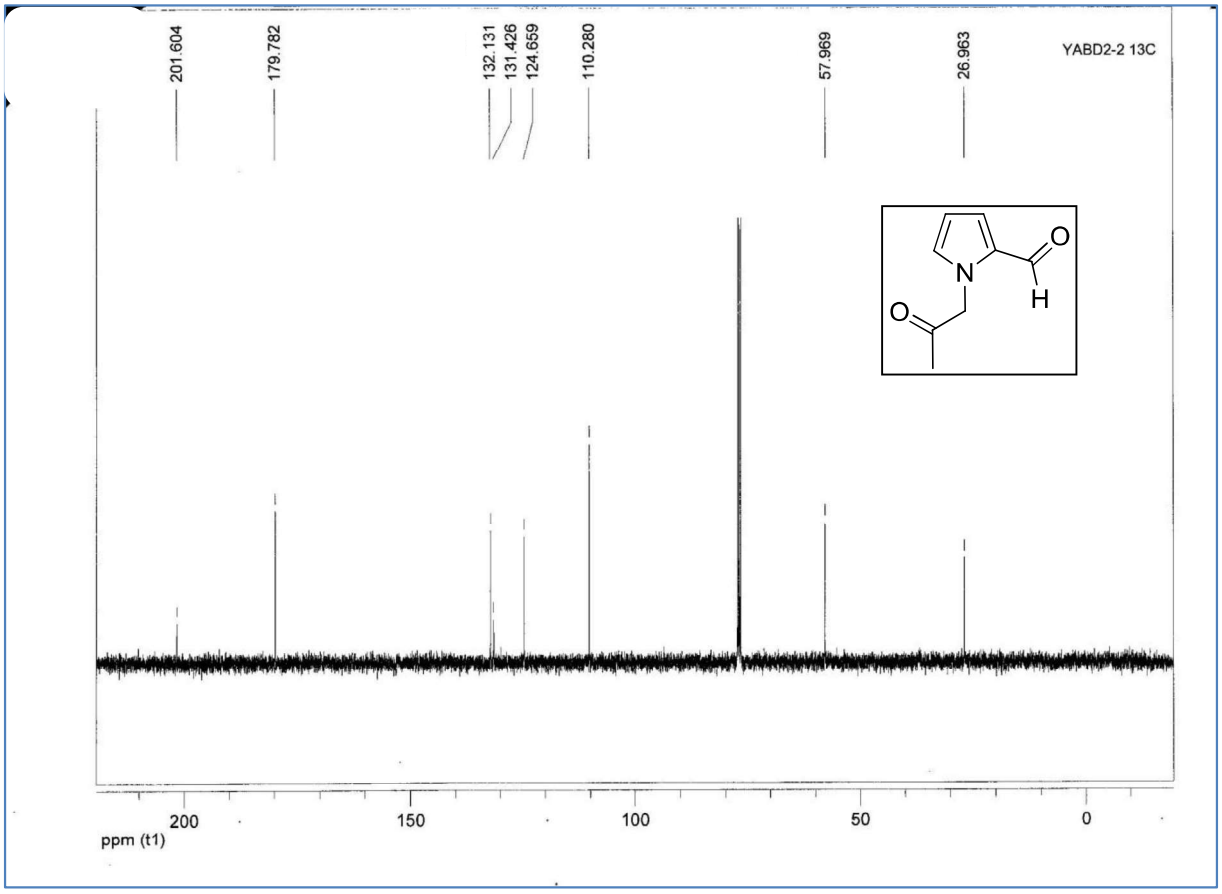
7.0
6.0
5.0
4.0
3.0
2.0
ppm (t1)
N
O
O
H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110.280
57.969
26.963
200
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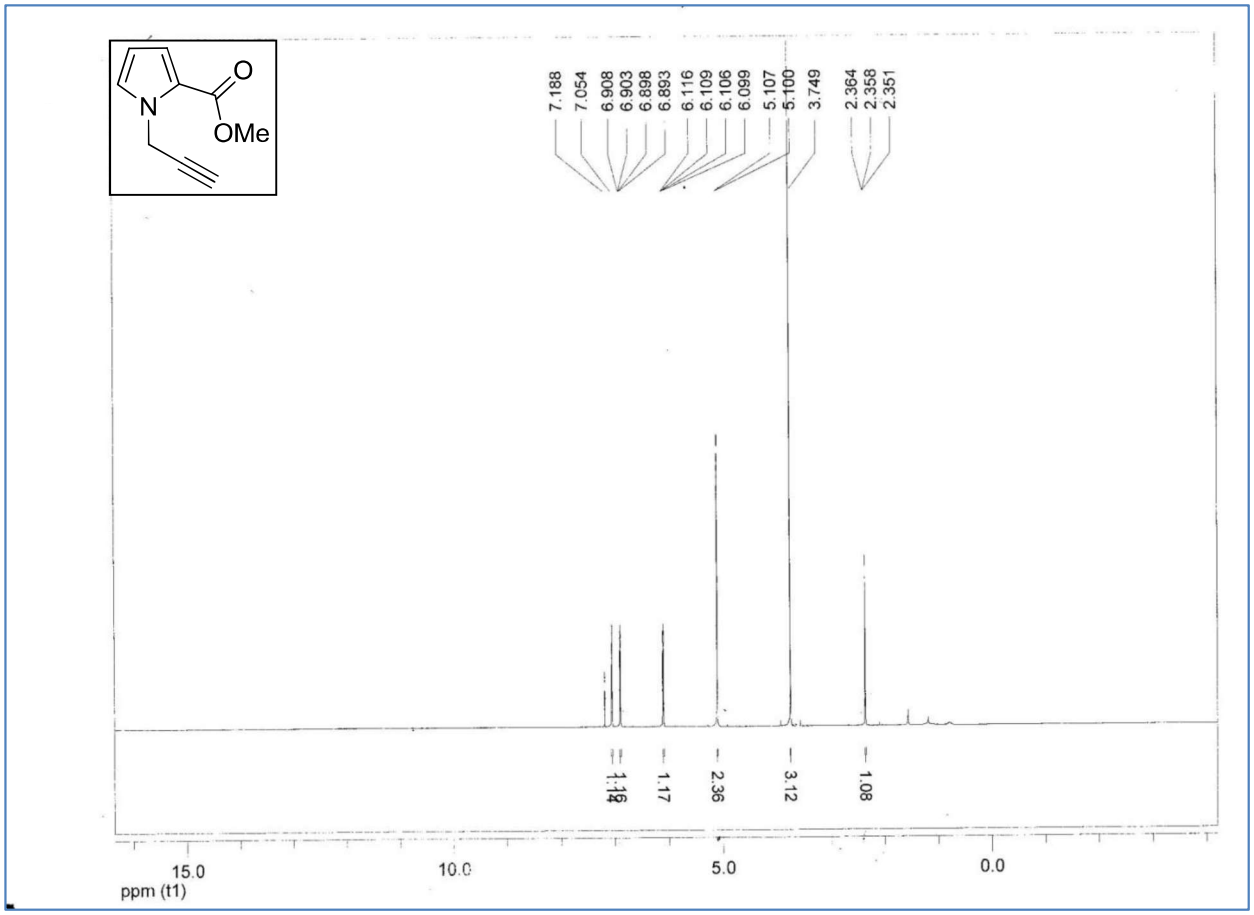
100
50
0
ppm (t1)
N
O
O
H


O
N
OMe
7.188
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6.908
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6.109
6.106
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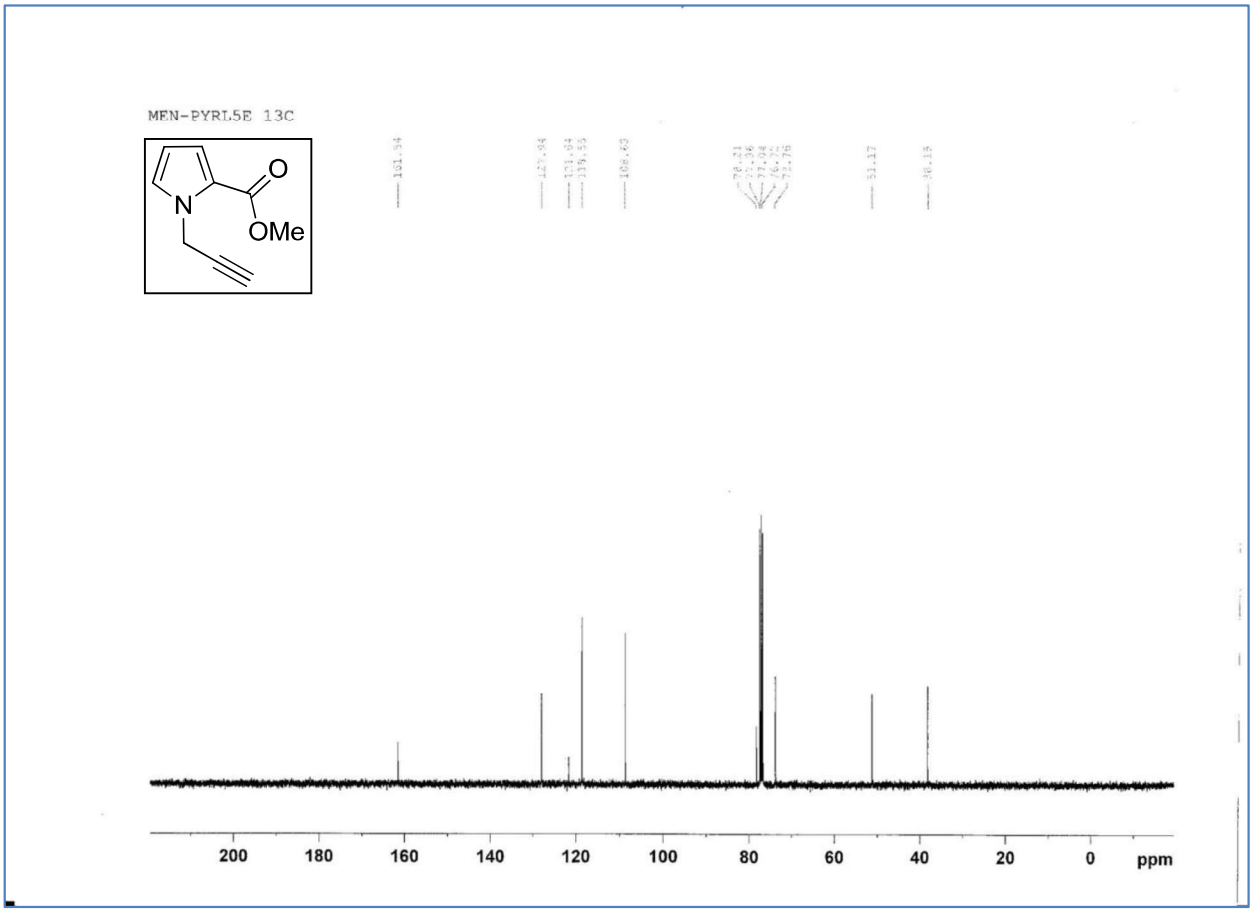
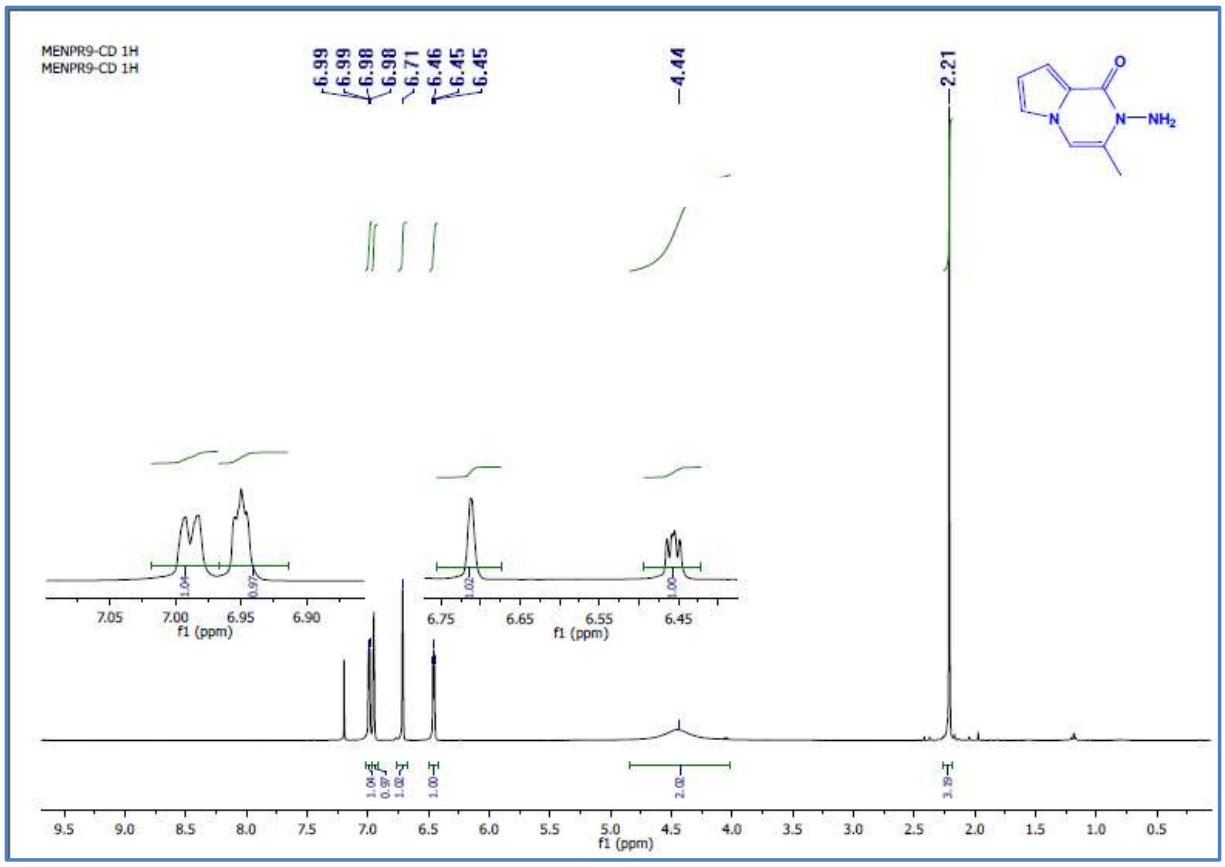
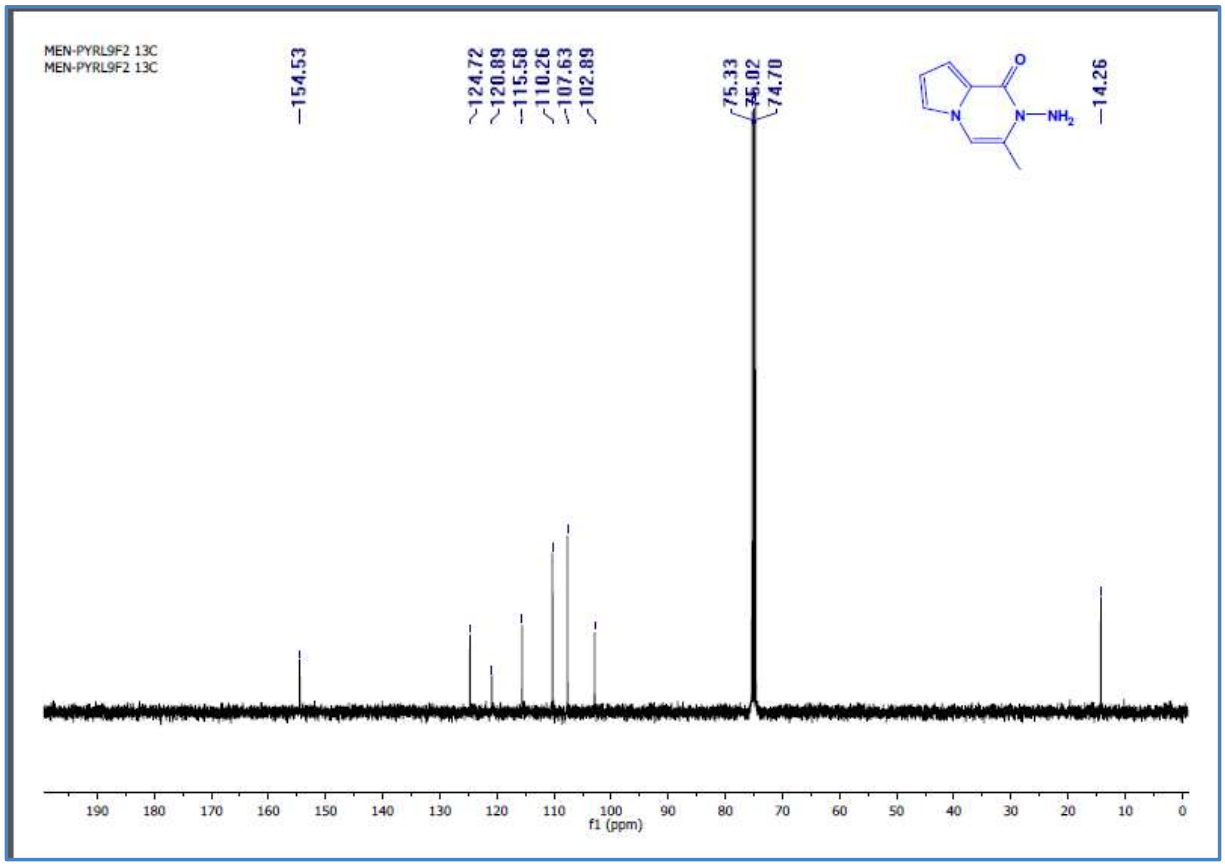
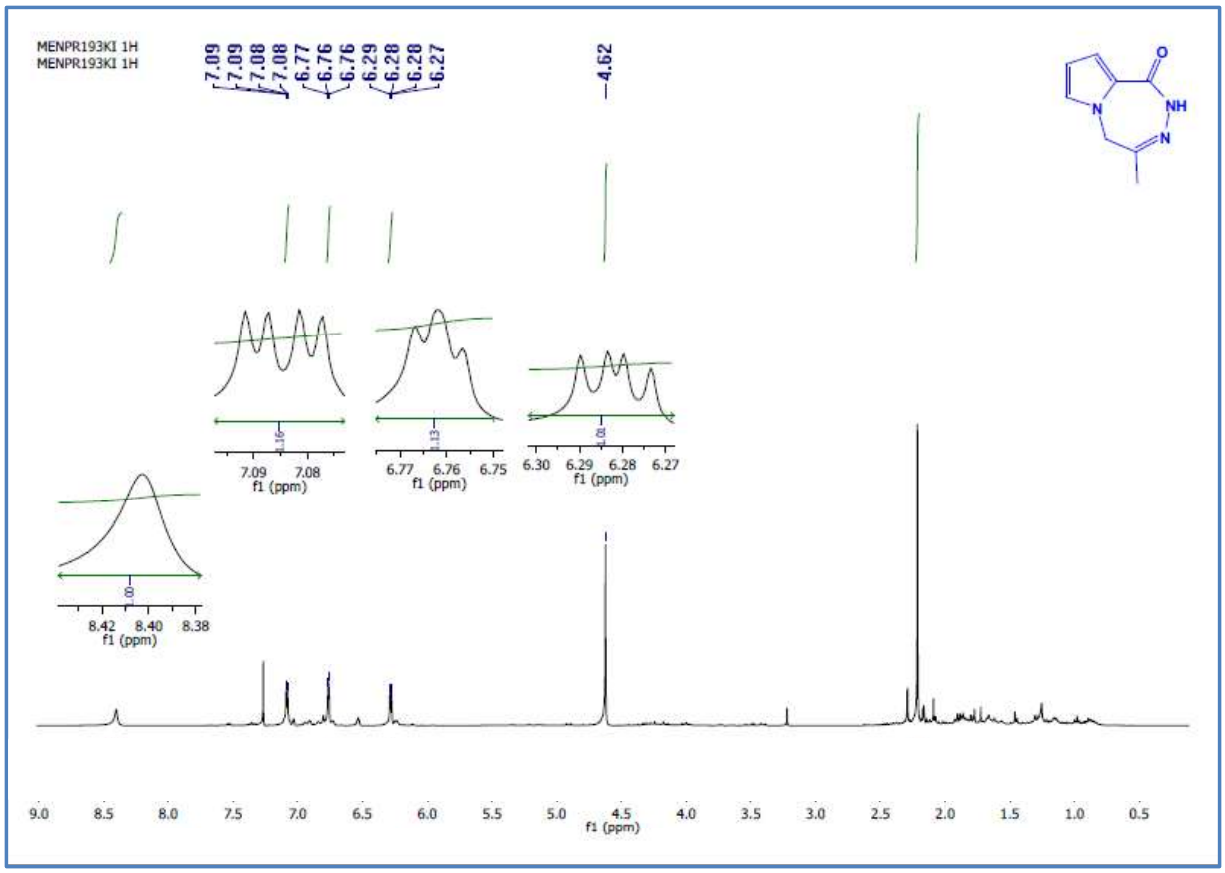
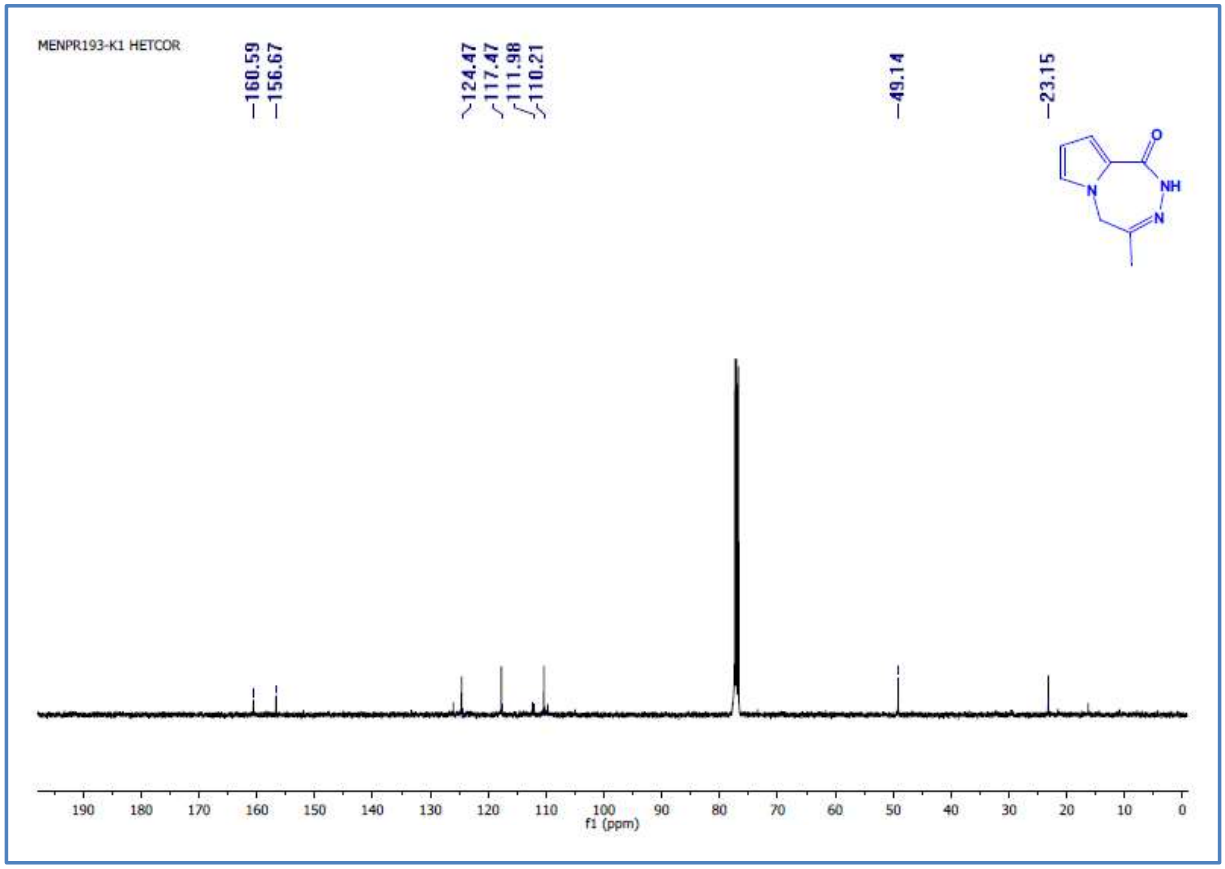
5.107
5.100
3.749
2.364
2.358
2.351
1.17
2.36
3.12
1.08
15.0
10.0
5.0
0.0
ppm (t1)

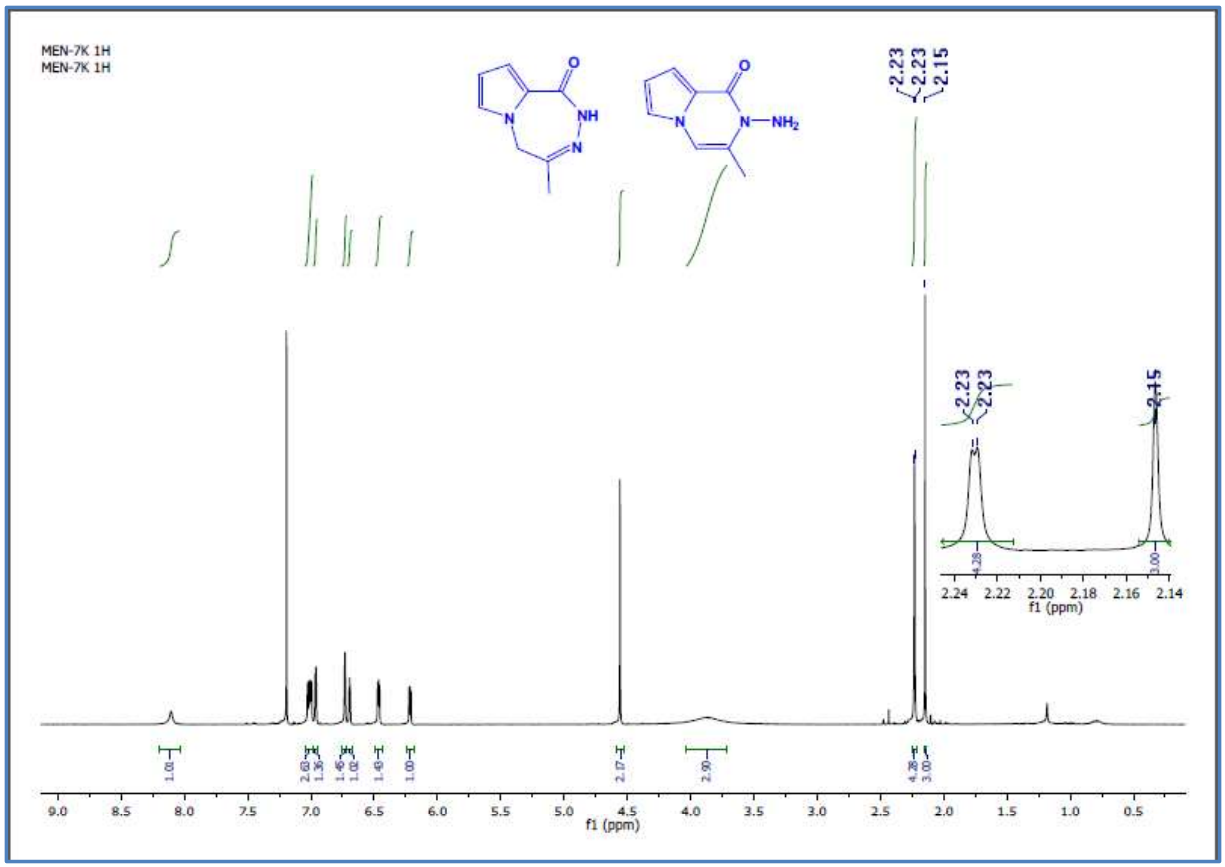

MEN-PYRL5E 13C
O
N
OMe
200
180
160
140
120
100
80
60
40
20
0
ppm


MENPR9-CD 1H
MENPR9-CD 1H
6.99
6.99
6.98
6.98
6.71
6.46
6.45
6.45
4.44
2.21
O
N
N—NH2
f1 (ppm)

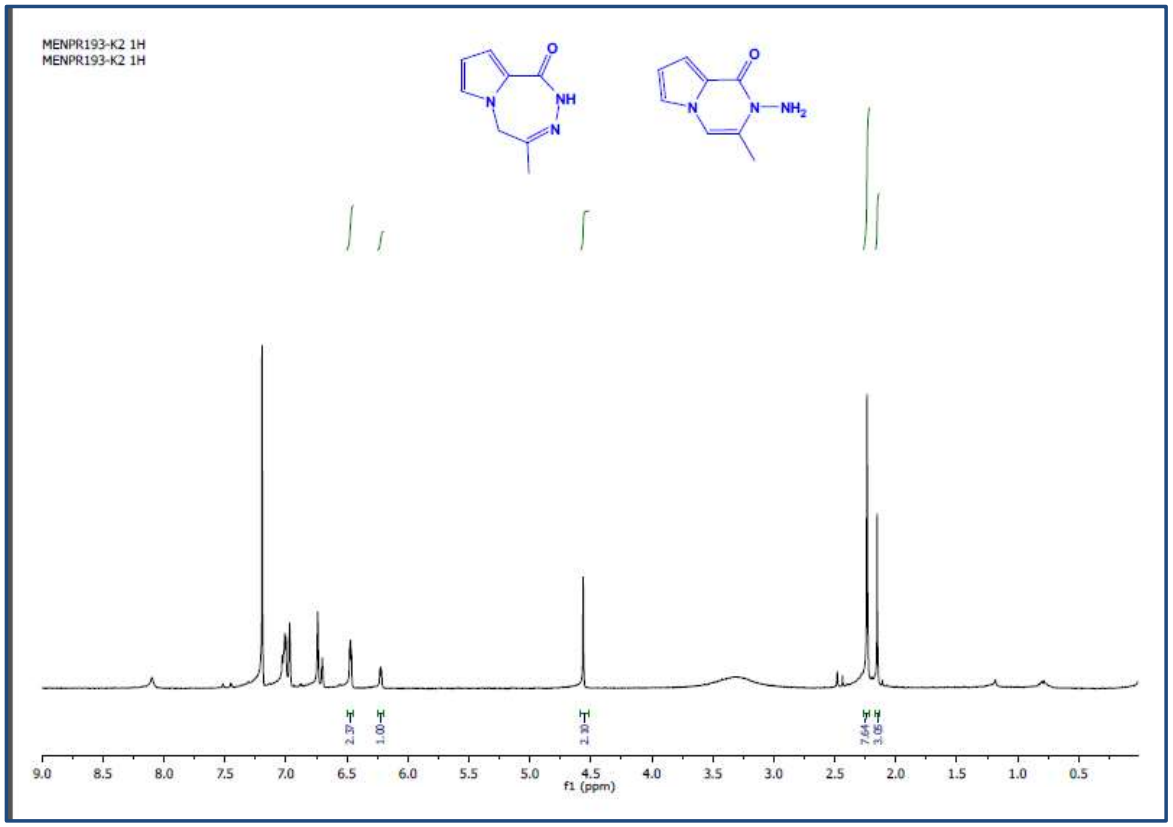

MEN-PYRL9F2 13C
MEN-PYRL9F2 13C
154.53
124.72
120.89
115.58
110.26
107.63
102.89
75.33
75.02
74.70
14.26
O
N
N—NH2
f1 (ppm)


MENPR193KI 1H
MENPR193KI 1H
7.09
7.09
7.08
7.08
6.77
6.76
6.76
6.29
6.28
6.28
6.27
4.62
O
NH
N
N
7.09 7.08
f1 (ppm)
6.77 6.76 6.75
f1 (ppm)
6.30 6.29 6.28 6.27
f1 (ppm)
8.42 8.40 8.38
f1 (ppm)
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

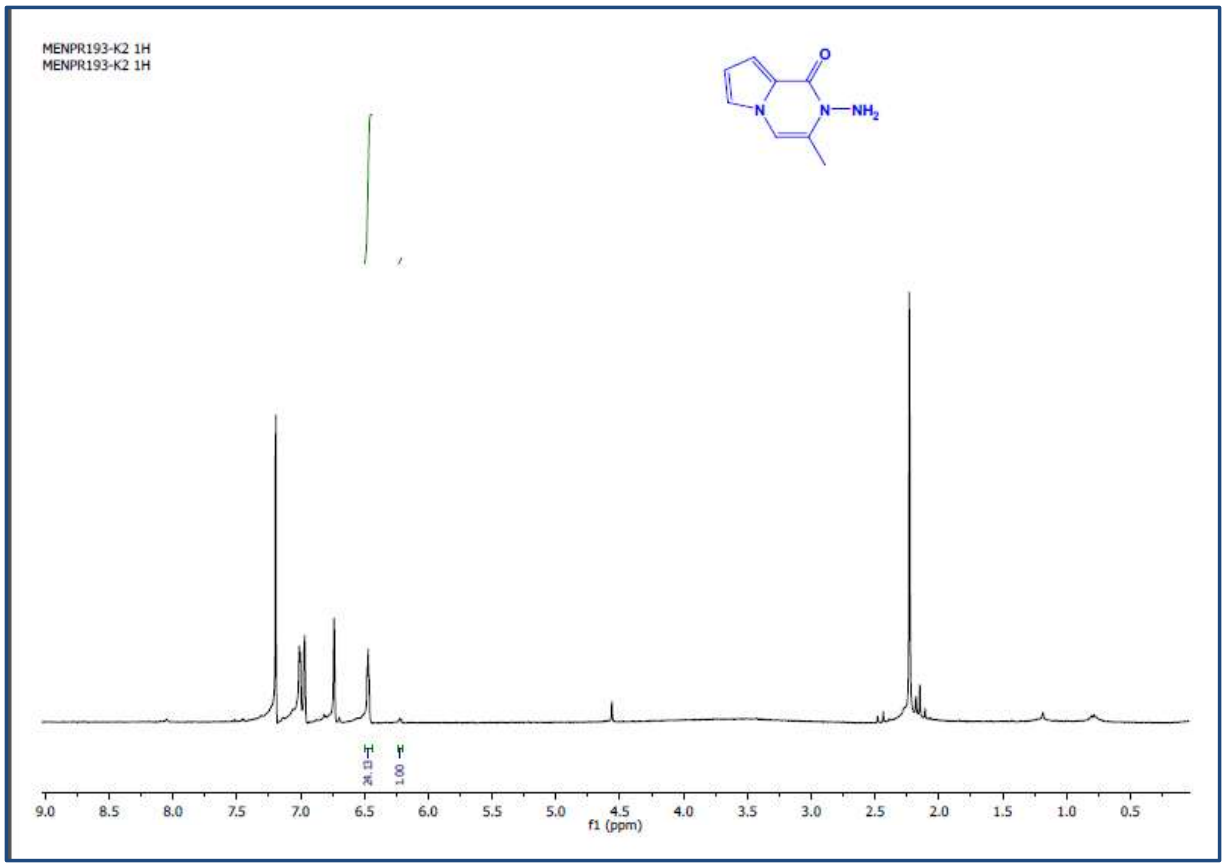

MENPR193-K1 HETCOR
160.59
156.67
124.47
117.47
111.98
110.21
49.14
23.15
O
NH
N
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



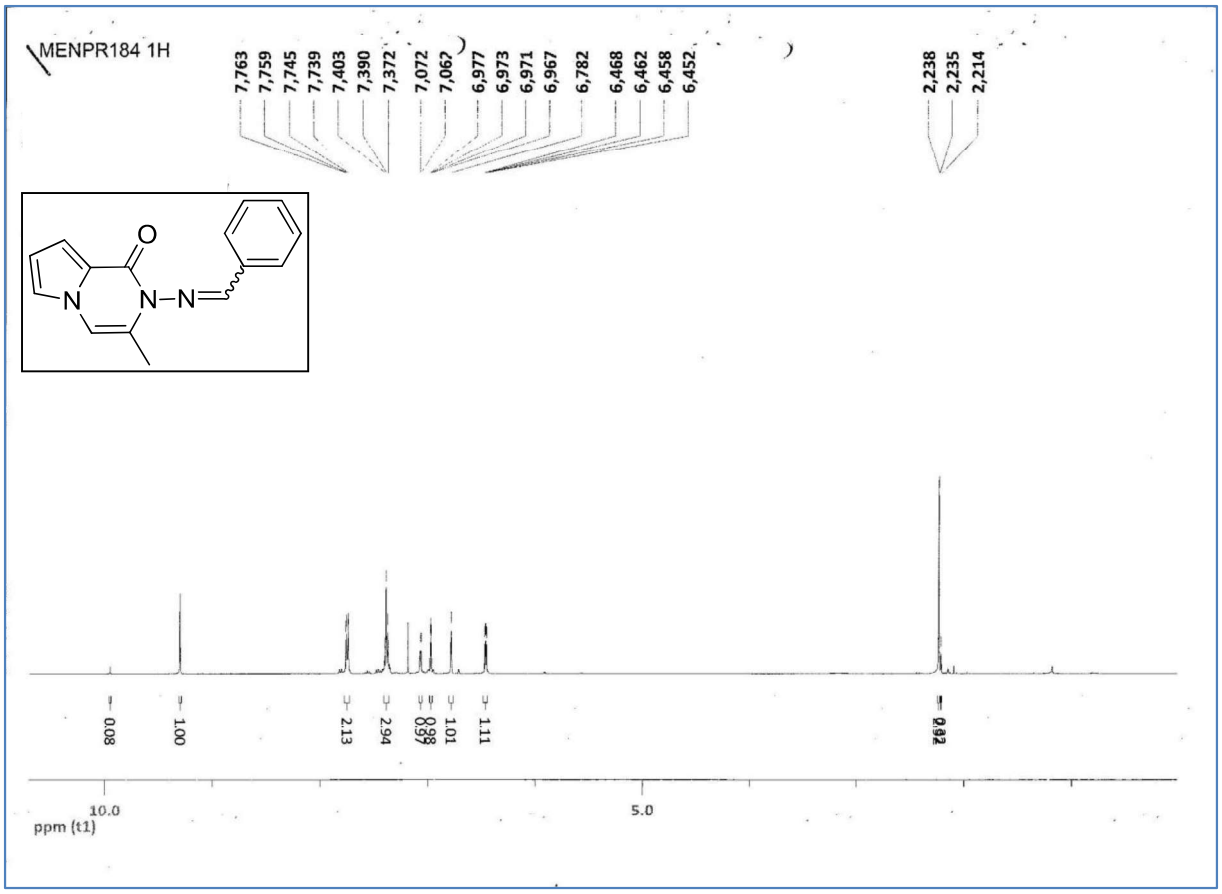
This spectrum was taken after 1 day from making the seven-membered product solution in $CDCl_3$.

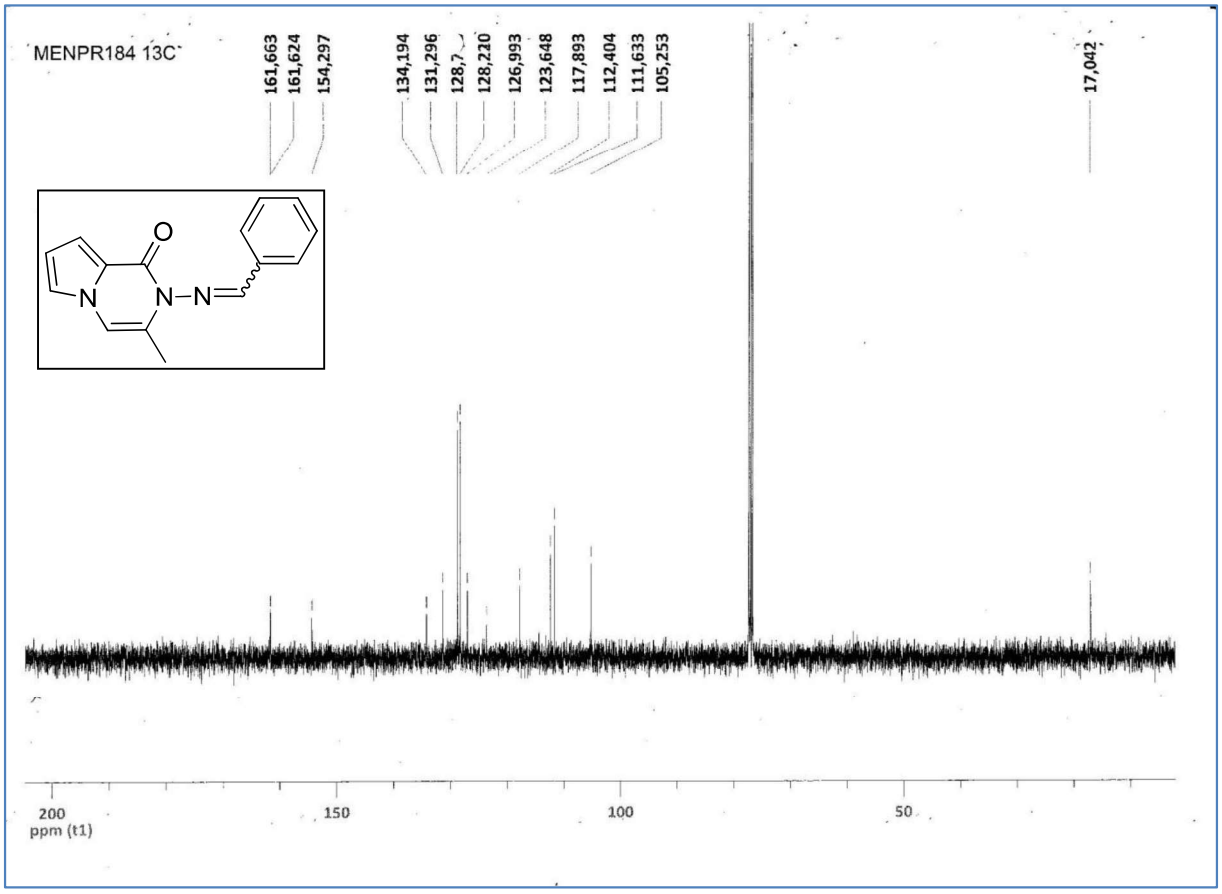


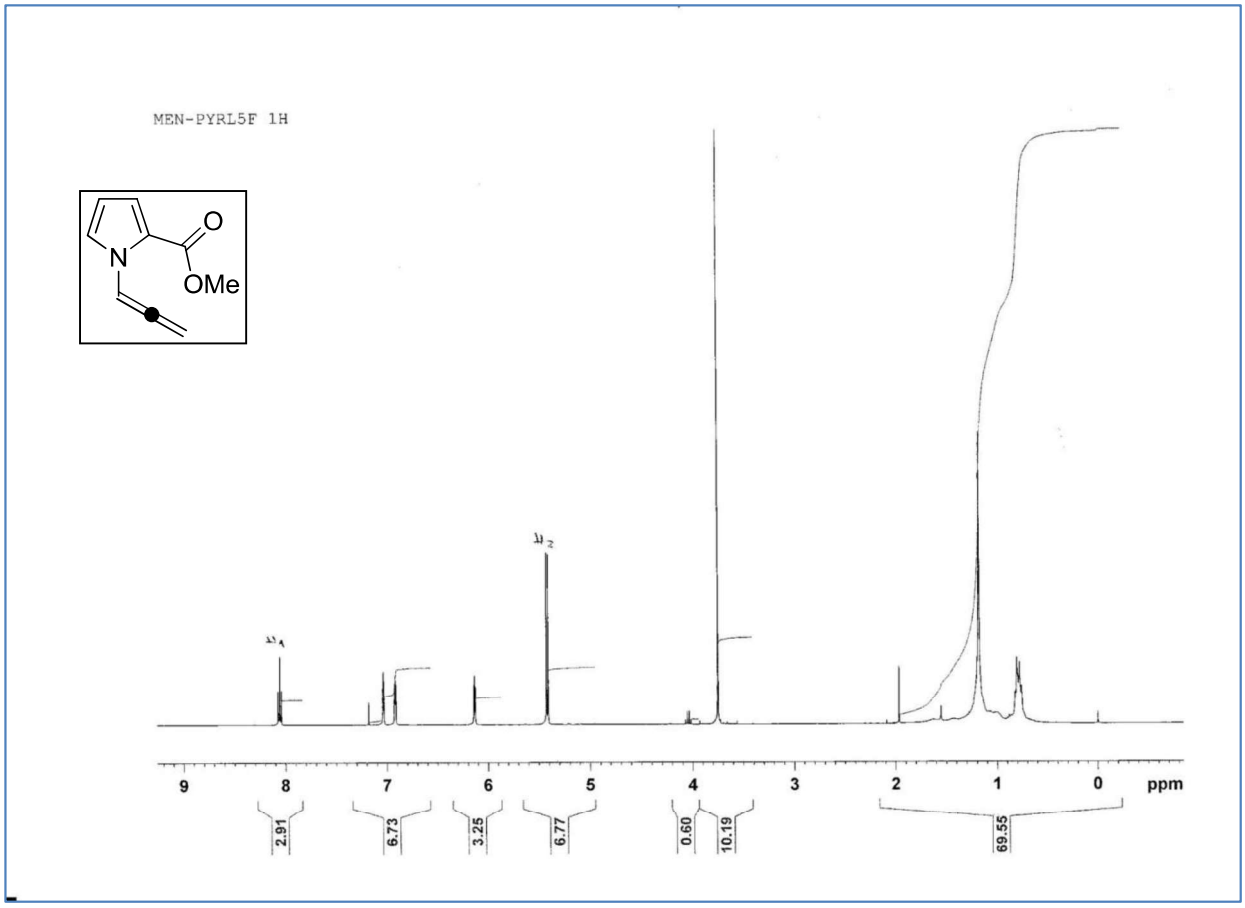
This spectrum was taken after 2 days from making the seven-membered product solution in $CDCl_3$.

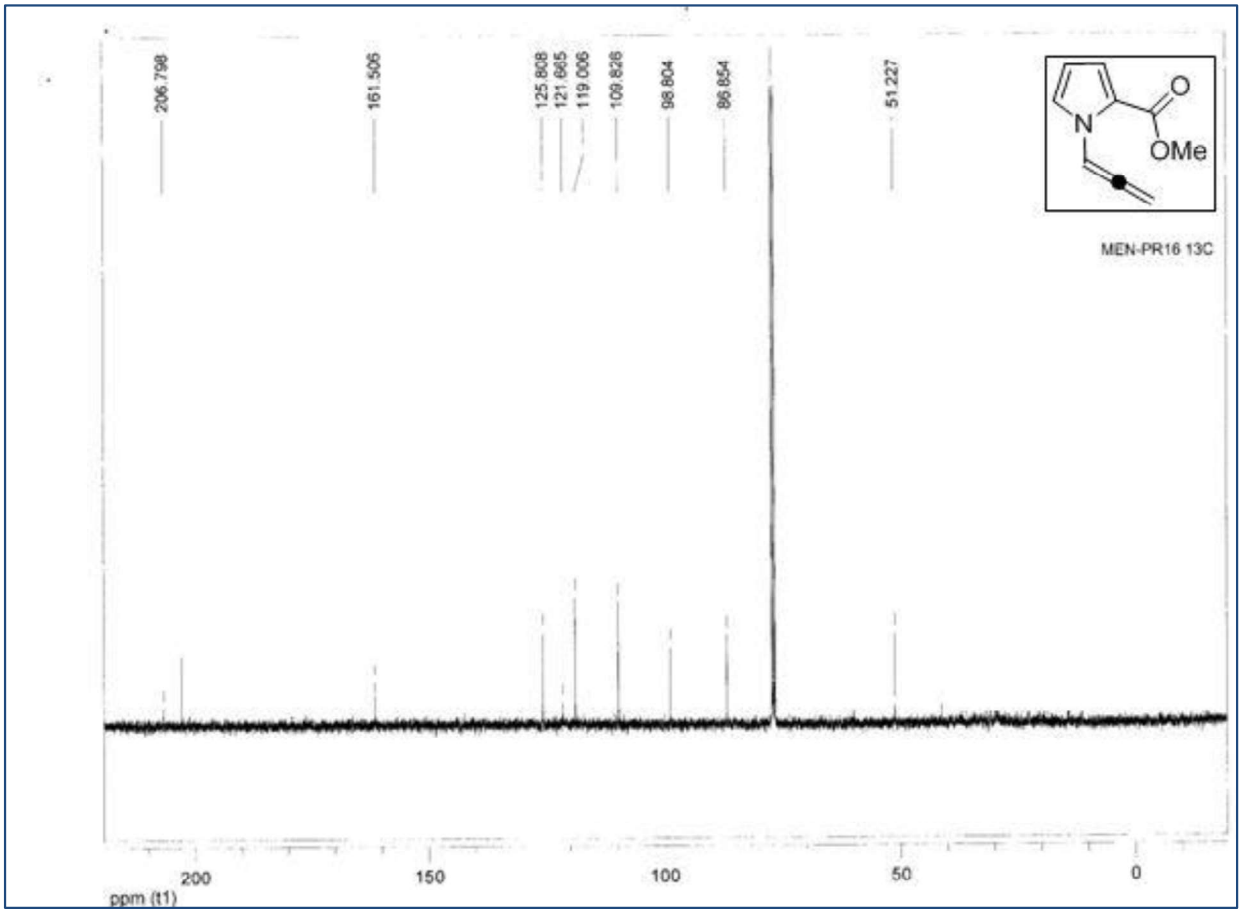


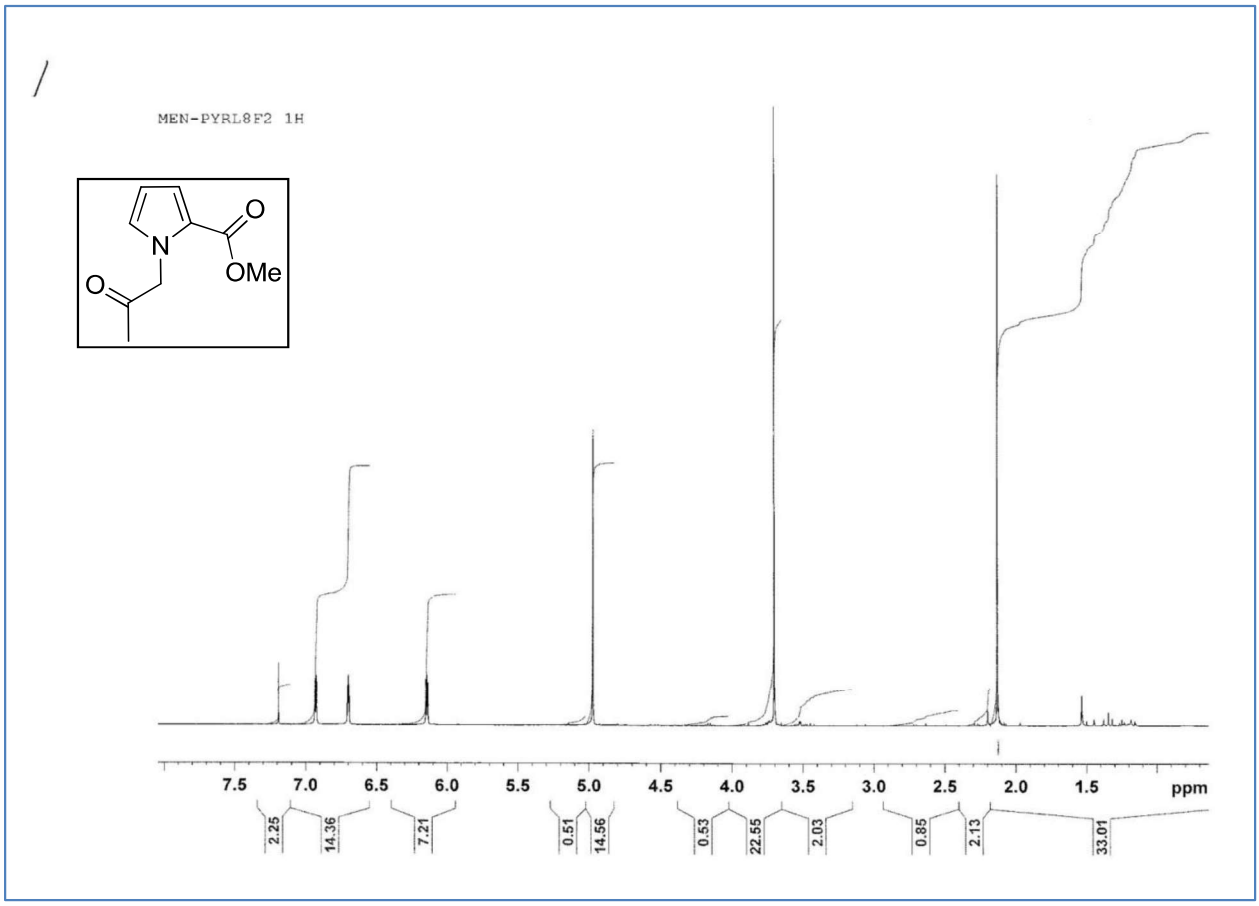
This spectrum was taken after 3 days from making the seven-membered product solution in $CDCl_3$.

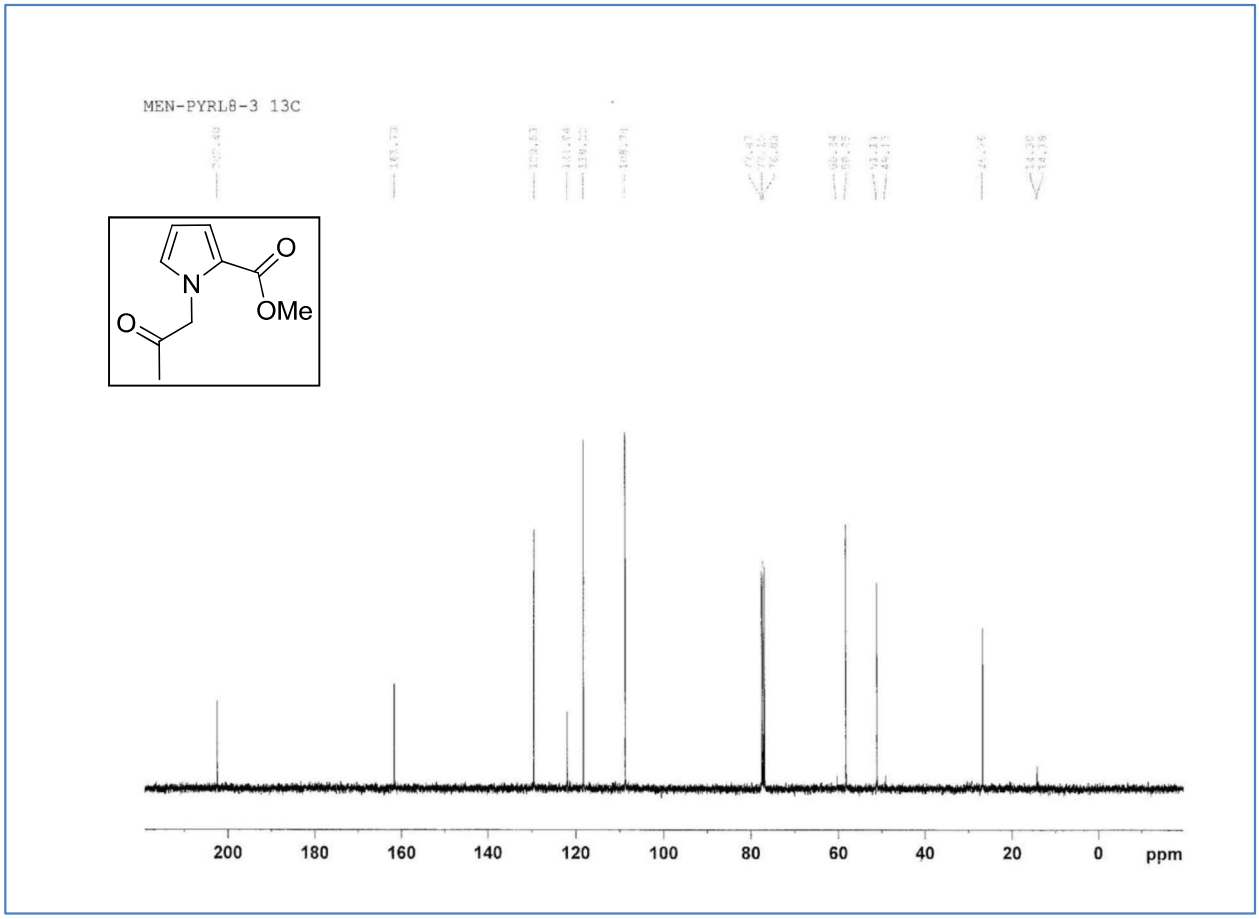

MENPR184 1H
7,763
7,759
7,745
7,739
7,403
7,390
7,372
7,072
7,067
6,977
6,973
6,971
6,967
6,782
6,468
6,462
6,458
6,452
2,238
2,235
2,214
O
N
N–N
0,08
1,00
2,13
2,94
0,88
1,01
1,11
3,02
10.0
5.0
ppm (t1)

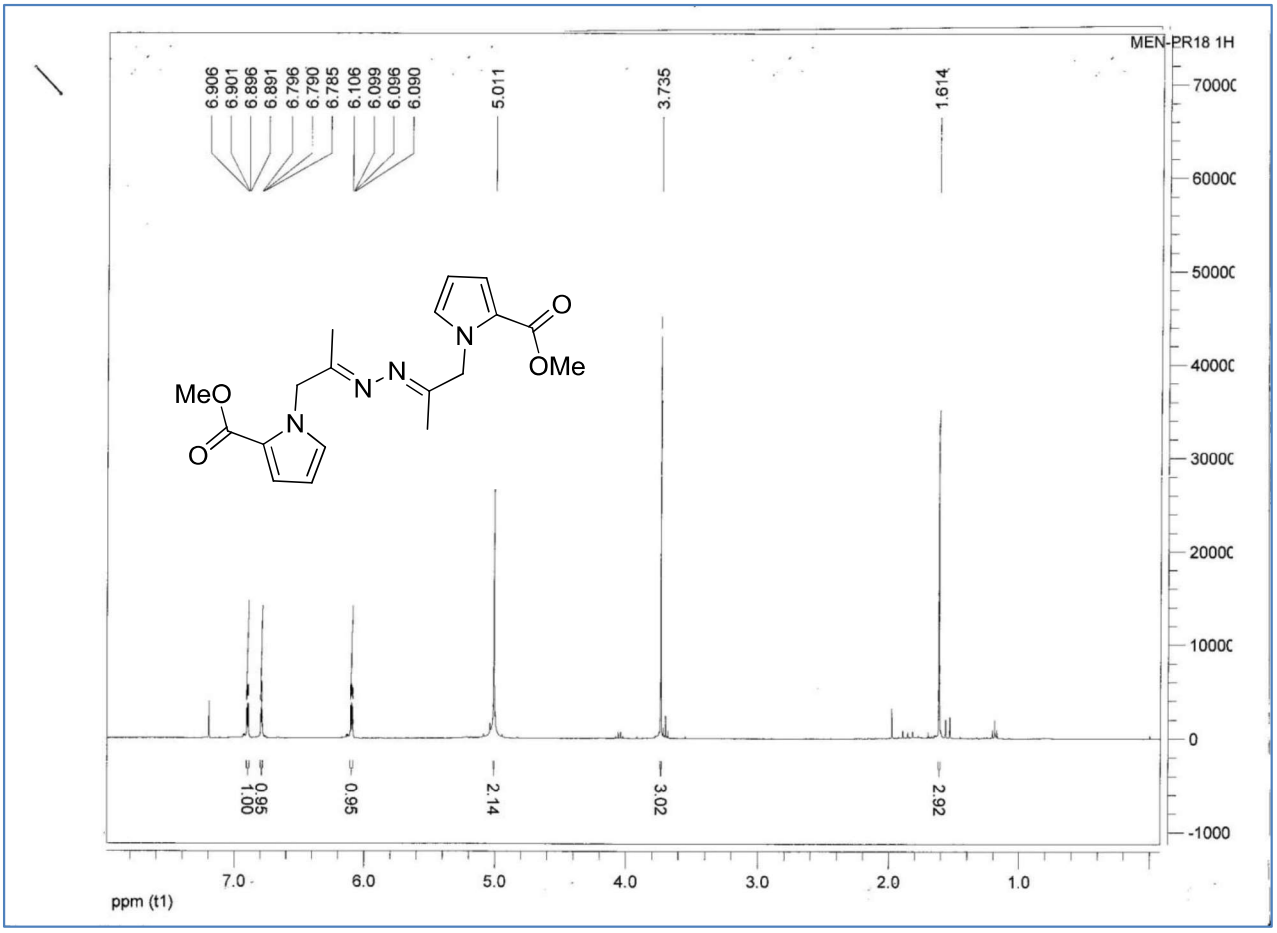

MENPR184 13C
161,663
161,624
154,297
134,194
131,296
128,220
126,993
123,648
117,893
112,404
111,633
105,253
17,042
O
N
N–N
200
150
100
50
ppm (t1)

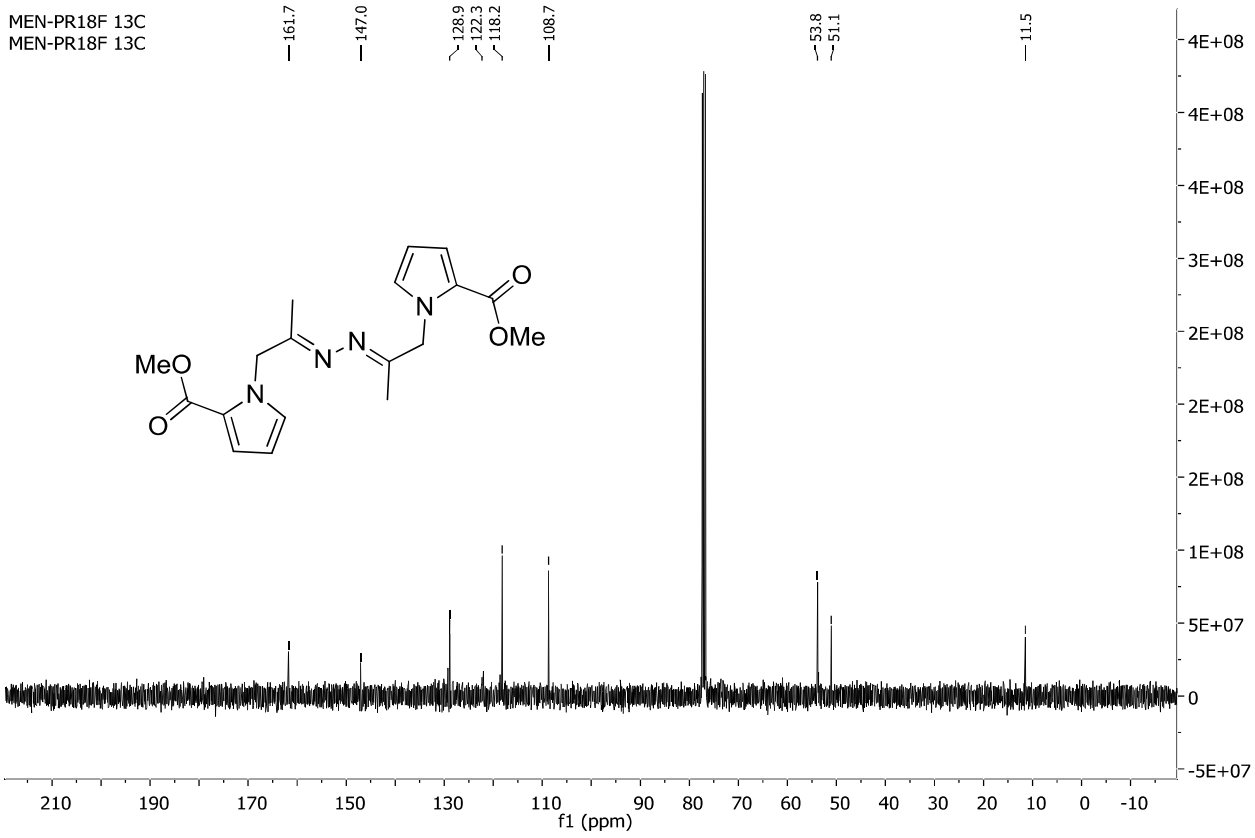

MEN-PYRL5F 1H
O
N
OMe
9
8
7
6
5
4
3
2
1
0
ppm
2.91
6.73
3.25
6.77
0.60
10.19
69.55


206.798
161.506
125.808
121.665
119.006
109.826
98.804
86.854
51.227
O
N
OMe
MEN-PR16 13C
200
150
100
50
0
ppm (t1)


MEN-PYRL8F2 1H
O
N
OMe
O
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
2.25
14.36
7.21
0.51
14.56
0.53
22.55
2.03
0.85
2.13
33.01


MEN-PYRL8-3 13C
O
N
OMe
O
200
180
160
140
120
100
80
60
40
20
0
ppm


MEN-PR18 1H
6.906
6.901
6.896
6.891
6.796
6.790
6.785
6.106
6.099
6.096
6.090
5.011
3.735
1.614
MeO
O
N
N
N
O
OMe
1.00
0.95
0.95
2.14
3.02
2.92
ppm (t1)


MEN-PR18F 13C
MEN-PR18F 13C
161.7
147.0
128.9
122.3
118.2
108.7
53.8
51.1
11.5
MeO
O
N
N
N
O
OMe
f1 (ppm)

THEORETICAL CALCULATIONS

1. Methodology

Geometrical parameters of reactants, intermediates, transition states (TS) and products were fully optimized at the hybrid density functional B3LYP[1,2] (Becke-3-parameter-Lee-Yang-Parr) method using 6-31+G(d,p) basis set implemented in Gaussian 09[3], as a good compromise between accuracy and computational cost. Hybrid DFT methods are quite reliable in predicting the activation barriers for a variety of reactions.[4] The 6-31+G(d,p) basis set is also recommended for calculating transition state geometries and barrier heights.[5] In order to characterize local minima (positive frequencies) and transition states (one imaginary frequency), harmonic vibrational frequencies were calculated using analytical second derivatives at 25 °C and 1 atm. The intrinsic reaction coordinates[6] (IRC) was followed to make sure that each transition state connects the corresponding reactant and the product . The total electronic energies including zero point energy corrections, enthalpy corrections and Gibbs free energy corrections were extracted from the output of the frequency calculations. Theoretical background for calculating electronic energies and performances of various basis sets can be found in ref.7. In order to account for the polarization effects of the solvent, single point energy calculations with polarizable continuum model[8] (PCM) were carried out at the PCM/B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) level with methanol solvent since it was used in the experimental study. PCM is a common method to compute the polarization effect of the solvent implicitly as a dielectric continuum. Theoretical background of PCM and related solvation methodologies was recently reviewed in detail by Tomasi et al[9]. Gibbs free energy corrections extracted from the corresponding frequency calculations of the gas phase stationary points were added to single point PCM energies in order to compute Gibbs free energy values in the solution phase. This approach is well-established and widely used in attaining Gibbs free energy in solvent.[10,11] The estimated error of this approach for the Gibbs free activation energy of the nucleophilic attack of N8 on the C2 atom via TS3 was calculated to be -0.64 kcal/mol. Unless otherwise specified, energies were discussed at the B3LYP/6-31+G(d,p) method throughout the manuscript.

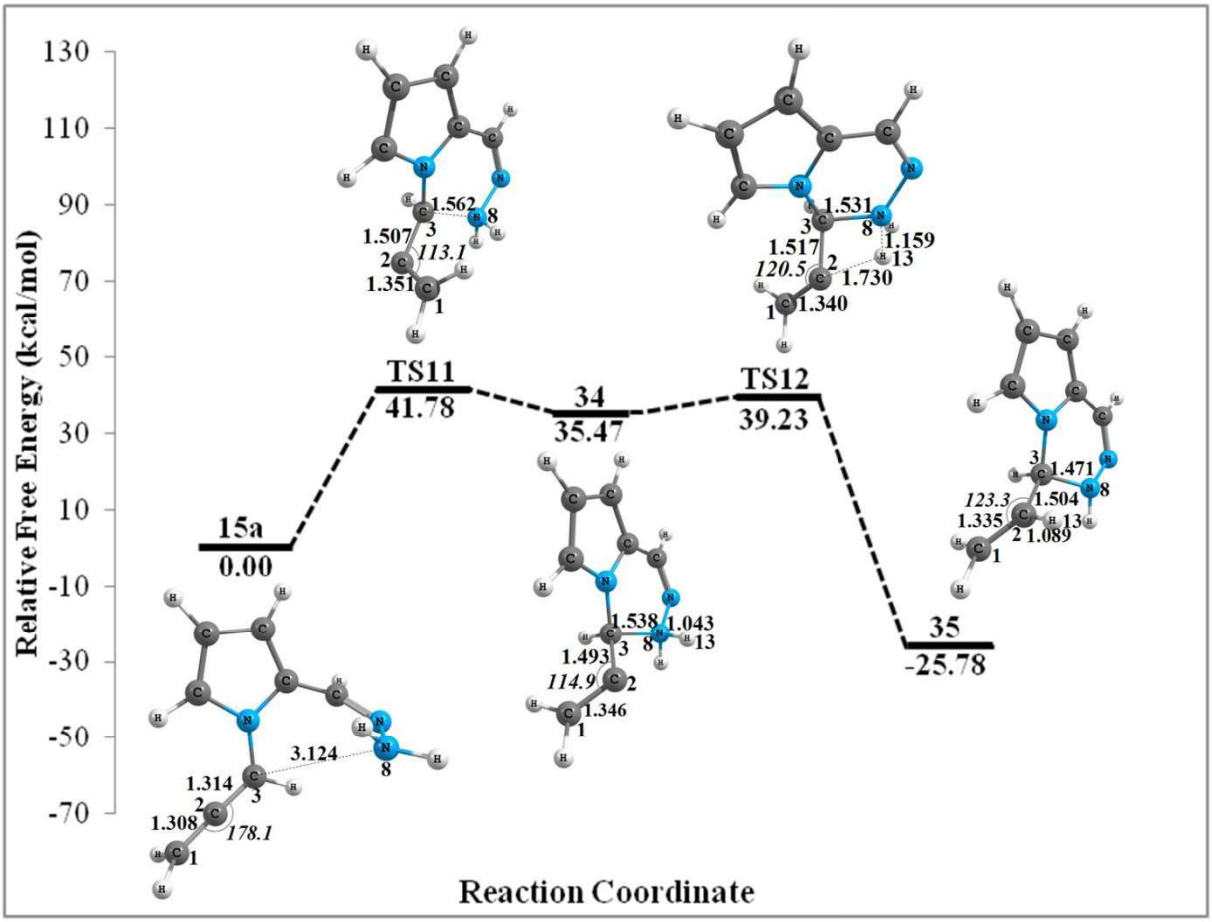


Figure S1. The potential energy profile related to the formation of a six-membered heterocyclic structure **35** starting from N-allene pyrrolehydrazone **15a** at the PCM/B3LYP/6-31+G (d,p)//B3LYP/6-31+G(d,p) level in methanol. (Polarization effect of the solvent was considered implicitly).

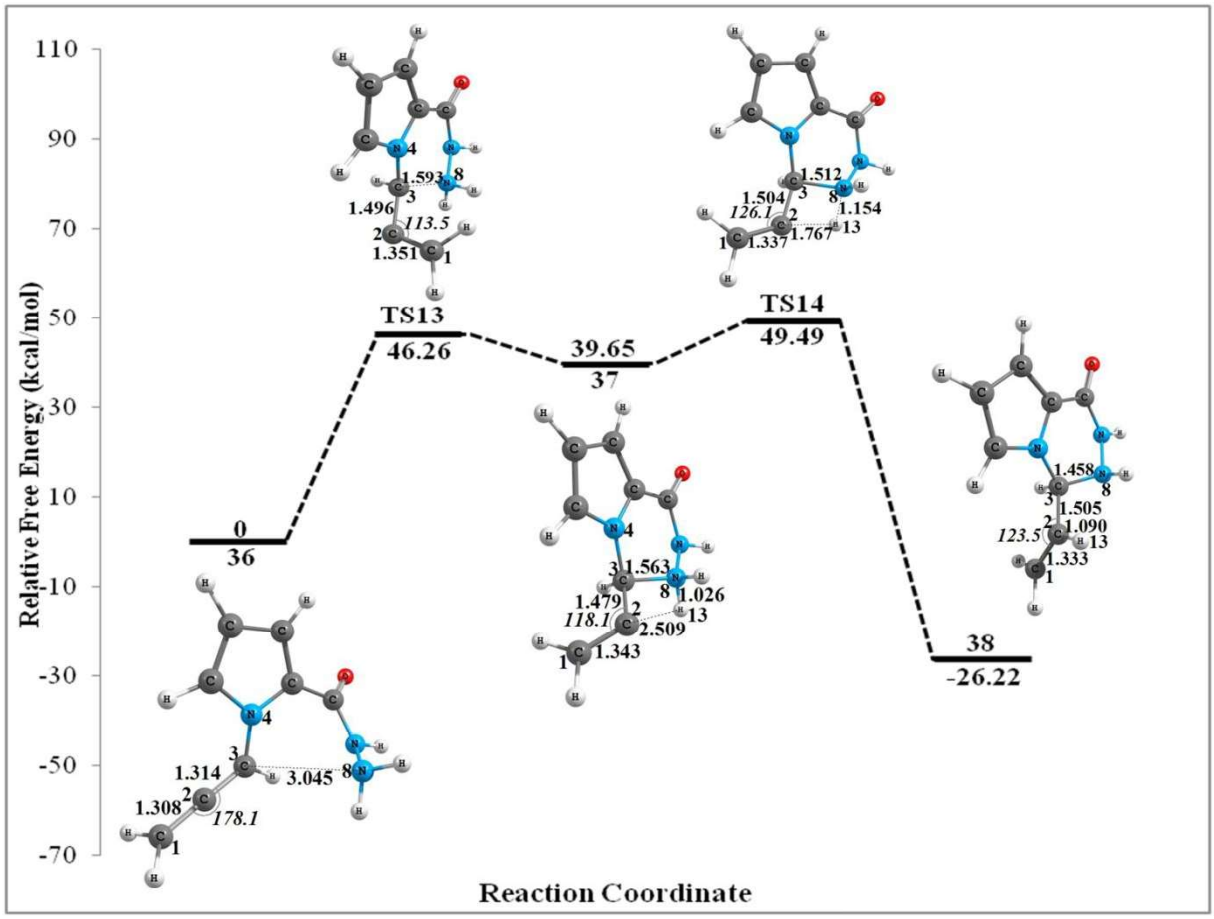


Figure S2. Potential energy profile related to formation of **38** starting from **36** at the PCM/B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) level in methanol. (Polarization effect of the solvent was considered implicitly).

2. Absolute Energies of the Structures

Energies are given in terms of ZPE-corrected total energy (Eel+ZPE), enthalpy (Eel+H) and Gibbs free-energy (Eel+G) as extracted from Gaussian output of each structure.

Table S1. Absolute energies of optimized structures in gas phase **(**RHF/6-31+G(d))

Compound No	Eel[a]+ZPE[b] (au)	Eel+H[c] (au)	Eel+G[d] (au)	Imaginary Frequency (*i*)
RC (11a+OH^-)	-546.629055	-546.615484	-546.668613	—
TS1	-546.623966	-546.610898	-546.663521	-1616.9
PC (33a+H_2O)	-546.638944	-546.624833	-546.680548	—
RC (33a′+H_2O)	-546.651214	-546.637018	-546.694440	—
TS2	-546.628378	-546.615127	-546.669226	-1351.8
PC (15a+OH^-)	-546.627991	-546.614014	-546.669680	—

[a]Eel = Total electronic energy
[b]ZPE = Zero point energy correction
[c]H = Enthalpy correction
[d]G = Gibbs free energy correction

Table S2. Single point energies in methanol (PCM/RHF/6-31+G(d)//RHF/6-31+G(d))

Compound No	Eel[a] (au)	Eel+G[b] (au)
RC (11a+OH^-)	-546.913239	-546.768882
TS1	-546.892538	-546.754434
PC (33a+H_2O)	-546.899865	-546.759745
RC (33a'+H_2O)	-546.914658	-546.776186
TS2	-546.901582	-546.765489
PC (15a+OH^-)	-546.918899	-546.779170

[a]Eel = Total electronic energy
[b]G = Gibbs free energy correction extractedfrom the corresponding gas phase frequency calculation and added to single point energy Eel.

Table S3. Absolute energies of optimized structures in gas phase (B3LYP/6-31+G(d,p))

Compound No	Eel+ZPE (au)	Eel+H (au)	Eel+G (au)	Imaginary Frequency (*i*)
11a	-474.264934	-474.253578	-474.301576	—
15a (Fig.2)	-474.277952	-474.266549	-474.314694	—
TS3	-474.198804	-474.189528	-474.232119	-191.6
34	-474.212432	-474.202530	-474.246835	—
TS4	-474.212392	-474.202809	-474.246341	-886.7
35	-474.320443	-474.310656	-474.354577	—
15a (Fig.3)	-474.277951	-474.266548	-474.314694	—
TS5	-474.232388	-474.222476	-474.266154	-431.9
MeOH	-115.683636	-115.679355	-115.706401	—
16a	-474.242452	-474.232504	-474.276259	—
RC(16a+MeOH)	-589.941018	-589.926985	-589.981479	—
TS6	-589.941430	-589.928302	-589.980711	-1047.2
PC(17a+MeOH)	-590.011104	-589.996579	-590.054058	—
17a	-474.322505	-474.312817	-474.356413	—
RC (17a+MeOH)	-590.012959	-589.998114	-590.056371	—
TS7	-589.966099	-589.953094	-590.004819	-1410.4
10a	-474.327677	-474.317896	-474.361392	—
PC(10a+MeOH)	-590.020342	-590.005697	-590.064080	—

36 (Fig.4)	-549.517748	-549.505311	-549.555628	—
TS8	-549.430683	-549.420272	-549.465418	-228.8
37	-549.445705	-549.434648	-549.481409	—
TS9	-549.438104	-549.427466	-549.473258	-1151.0
38	-549.561898	-549.550894	-549.597774	—
36 (Fig.5)	-549.517748	-549.505309	-549.555635	—
TS10	-549.466089	-549.454982	-549.501397	-373.5

Table S3 continues

Compound No	Eel+ZPE (au)	Eel+H (au)	Eel+G (au)	Imaginary Frequency (*i*)
39	-549.469676	-549.458668	-549.504826	—
RC(39+MeOH)	-665,170580	-665,155449	-665,211868	—
40	-549.567408	-549.556440	-549.602832	—
TS11	-665.167181	-665.152929	-665.207771	-1141.3
41	-549.561935	-549.551234	-549.597088	—
PC(41+MeOH)	-665.253790	-665.238310	-665.297411	—
RC(41+MeOH)	-665.252650	-665.236827	-665.296130	—
TS12	-665.208768	-665.194636	-665.249019	-1711.0
26	-549.582996	-549.572211	-549.618182	—
PC(26+MeOH)	-665.273464	-665.257750	-665.318524	—
36 (Fig.6)	-549.516305	-549.503813	-549.553972	—
TS13	-549.468480	-549.457391	-549.503831	-420.7
42	-549.478449	-549.466985	-549.514086	—
RC(42+MeOH)	-665.175175	-665.158978	-665.218834	—
TS14	-665.171034	-665.156330	-665.211864	-903.7
PC(25+MeOH)	-665.286768	-665.271199	-665.329712	—

25	-549.591719	-549.580445	-549.627266	—

Table S4. Single point energies in methanol (PCM/B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p))

Compound No	Eel (au)	Eel+G (au)
11a	-474.432730	-474.310359
15a (Fig.2)	-474.443875	-474.322208
TS3	-474.382965	-474.255631
34	-474.392306	-474.265686
TS4	-474.382761	-474.259687
35	-474.491211	-474.363291
15a (Fig.3)	-474.443875	-474.322208
TS5	-474.401282	-474.276552
16a	-474.416981	-474.290062
MeOH	-115.740785	-115.712311
RC(16a+MeOH)	-590.166954	-589.992791
TS6	-590.163074	-589.992566
PC(17a+MeOH)	-590.237688	-590.064956
RC (17a+MeOH)	-590.238615	-590.066859
17a	-474.493556	-474.364959
TS7	-590.188922	-590.019099
10a	-474.500751	-474.373212
PC(10a+MeOH)	-590,248614	-590,077960
36 (Fig.4)	-549.696448	-549.570434

TS8	-549.627258	-549.496715
37	-549.637140	-549.507252
TS9	-549.618217	-549.491564
38	-549.743322	-549.612216
36 (Fig.5)	-549.696452	-549.570443
TS10	-549.647934	-549.520041
39	-549.656593	-549.526189

Table S4 continues

Compound No	Eel (au)	Eel+G (au)
RC(39+MeOH)	-665.408234	-665.230111
40	-549.746933	-549.615550
TS11	-665.401646	-665.228567
41	-549.742347	-549.610149
PC(41+MeOH)	-665.487674	-665.310630
RC(41+MeOH)	-665.487652	-665.311407
TS12	-665.436535	-665.263745
26	-549.763811	-549.631898
PC(26+MeOH)	-665.510456	-665.335421
36 (Fig.6)	-549.6944675	-549.568376
TS13	-549.6437598	-549.515960
42	-549.656646	-549.527553
RC(42+MeOH)	-665.407182	-665.232825
TS14	-665.398795	-665.226982
PC(25+MeOH)	-665.517729	-665.340069
25	-549.769934	-549.638719

3. Cartesian Coordinates for the Optimized Structures Given in Paths

Structure No: RC (11a+OH^-) (RHF/6-31+G(d))

	X	Y	Z
C	0.626644	-1.052326	-0.445479
H	1.686592	-1.222045	-0.665351
C	0.227941	-1.920786	0.682592
C	-0.104382	-2.640550	1.572369
H	-0.367600	-3.272157	2.377547
O	3.550601	-0.923855	-0.799917
H	4.335578	-1.427078	-0.972548
H	0.037358	-1.297187	-1.315621
C	1.596624	1.110514	0.067923
C	1.229995	2.380687	0.431159
C	-0.177876	2.396037	0.454332
C	-0.638192	1.146205	0.100526
N	0.483561	0.364415	-0.130634
H	2.560748	0.650517	-0.089609
H	1.896063	3.193237	0.642425
H	-0.810268	3.232538	0.684376
C	-2.087136	0.936962	-0.009853
H	-2.596689	1.822971	0.334427
N	-2.900410	0.059085	-0.412532
N	-2.441681	-1.149842	-0.933892
H	-1.918248	-1.658607	-0.246931
H	-3.260344	-1.687413	-1.131389

Structure No: TS1 (RHF/6-31+G(d))

	X	Y	Z
C	0.971123	-0.659739	-0.494170
H	2.163211	-0.270783	-0.946631
C	1.184877	-1.623960	0.579840
C	1.422669	-2.412708	1.449321
H	1.664814	-3.097552	2.216215
O	3.293519	0.204578	-1.323857
H	3.943953	-0.481437	-1.238002
H	0.402318	-1.105454	-1.297154
C	0.969728	1.581786	0.493719
C	0.117772	2.609918	0.799874
C	-1.170300	2.177690	0.415693
C	-1.056075	0.895617	-0.073482
N	0.272587	0.543584	-0.017310
H	2.036194	1.514894	0.548505
H	0.392094	3.560621	1.212950

H	-2.087079	2.733731	0.474494
C	-2.225973	0.186115	-0.633274
H	-2.935020	0.866151	-1.077447
N	-2.625102	-1.009574	-0.635009
N	-1.861976	-2.020356	-0.112575
H	-1.235303	-1.742048	0.618332
H	-2.474816	-2.738629	0.208715

Structure No: PC (33a+H_2O) (RHF/6-31+G(d))

	X	Y	Z
C	0.961277	-0.424349	-0.486458
H	2.985355	0.261314	-1.081769
C	1.435527	-1.237042	0.568991
C	1.890773	-1.919224	1.458789
H	2.361273	-2.471474	2.225977
O	3.941048	0.404521	-1.097172
H	4.251746	-0.145853	-0.391034
H	0.584456	-0.955301	-1.342735
C	0.502394	1.834950	0.356786
C	-0.544192	2.684214	0.610751
C	-1.710925	1.963768	0.282544
C	-1.325546	0.699769	-0.117247
N	0.045897	0.640352	-0.073876
H	1.557317	1.996516	0.427952
H	-0.474515	3.694941	0.962955
H	-2.725282	2.313177	0.328796
C	-2.343161	-0.281611	-0.550570
H	-3.230144	0.217443	-0.908338
N	-2.474771	-1.535539	-0.523257
N	-1.476891	-2.377551	-0.114637
H	-0.796720	-1.977344	0.501897
H	-1.898398	-3.183272	0.294556

Structure No: RC (33a'+H_2O) (RHF/6-31+G(d))

	X	Y	Z
C	-0.902246	-0.851349	-0.365404
C	-2.016715	-1.096585	0.323436
C	-3.146494	-1.258385	0.896742
H	-3.195339	-1.917072	1.755337
H	-0.597896	-1.419474	-1.224408
C	-0.453403	1.557611	0.003589
C	0.619252	2.359792	0.293274
C	1.743145	1.505946	0.391060
C	1.299289	0.220011	0.169438
N	-0.047943	0.272046	-0.060466
H	-1.482231	1.800070	-0.160223

H	0.601473	3.424564	0.418626
H	2.741117	1.802368	0.650417
C	1.978190	-1.082973	0.276725
H	1.388442	-1.872138	0.708046
N	3.147677	-1.418592	-0.056717
N	3.962523	-0.534073	-0.733390
H	3.752341	0.429264	-0.578452
H	4.909674	-0.732543	-0.492961
O	-5.334546	0.260684	-0.686150
H	-4.752151	-0.202326	-0.066031
H	-4.850976	0.241735	-1.500299

Structure No: TS2 (RHF/6-31+G(d))

	X	Y	Z
C	0.595710	-0.782516	-0.138159
C	1.829699	-0.736596	-0.582691
C	3.071469	-0.669842	-0.932243
H	3.293987	-0.816832	-1.982961
H	0.122892	-1.681277	0.206314
C	0.232793	1.618285	0.356573
C	-0.790445	2.521773	0.280407
C	-1.930193	1.805520	-0.170376
C	-1.545306	0.501630	-0.344012
N	-0.220300	0.397061	-0.018563
H	1.257927	1.743619	0.635940
H	-0.732324	3.564502	0.522096
H	-2.916709	2.192023	-0.340595
C	-2.379467	-0.632574	-0.812965
H	-2.730258	-0.608213	-1.830982
N	-2.776997	-1.616961	-0.136575
N	-2.355329	-1.748217	1.162115
H	-2.150450	-0.873724	1.610666
H	-3.043819	-2.259773	1.670930
O	5.103880	-0.155948	0.644161
H	4.036203	-0.434237	-0.131239
H	4.994335	-0.555776	1.498495

Structure No: PC (15a+OH^-) (RHF/6-31+G(d))

	X	Y	Z
C	0.529030	-0.795669	-0.193158
C	1.767127	-0.763357	-0.601856
C	3.014061	-0.716333	-0.951767
H	3.259068	-0.817711	-1.998680
H	0.031036	-1.701500	0.091649
C	0.231998	1.604445	0.328240
C	-0.774329	2.525291	0.281623

C	-1.942016	1.832382	-0.136318
C	-1.593809	0.521525	-0.318393
N	-0.259092	0.390339	-0.031639
H	1.266443	1.709671	0.580950
H	-0.688979	3.565707	0.523839
H	-2.924412	2.240175	-0.276805
C	-2.467690	-0.591936	-0.761912
H	-2.894383	-0.525551	-1.748364
N	-2.820431	-1.600096	-0.095550
N	-2.310420	-1.781147	1.163934
H	-2.090198	-0.924778	1.639485
H	-2.952945	-2.330046	1.693440
O	5.330895	-0.136647	0.635376
H	3.848215	-0.558505	-0.236451
H	5.642374	-0.326036	1.511959

Structure No: 11a (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.103434	0.518159	0.210768
C	1.497720	1.803871	-0.137879
C	0.328229	2.567382	-0.390526
C	-0.754039	1.738989	-0.171108
N	-0.290453	0.489601	0.174307
H	2.524082	2.131472	-0.234394
H	0.280564	3.599321	-0.709054
H	-1.814822	1.930358	-0.231372
C	1.961710	-0.622649	0.566409
H	2.759344	-0.432170	1.281882
N	1.950242	-1.823032	0.093603
N	0.994085	-2.156809	-0.841345
C	-1.117200	-0.556940	0.794048
H	-1.210262	-0.359256	1.870294
C	-2.451050	-0.650732	0.199525
C	-3.564259	-0.751061	-0.261107
H	0.702594	-1.394803	-1.456863
H	1.299807	-2.969686	-1.360887
H	-0.603009	-1.513865	0.669265
H	-4.542690	-0.841797	-0.675602

Structure No: 15a (Fig.S1) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.056927	0.544564	-0.317127
C	1.422699	1.861766	-0.092783
C	0.269140	2.570667	0.345231
C	-0.778863	1.677253	0.364205

N	-0.309553	0.441215	-0.033948
H	2.422664	2.255553	-0.212815
H	0.214216	3.614557	0.620669
H	-1.820501	1.809692	0.614053
C	-1.102312	-0.705084	-0.281278
C	-2.411677	-0.747929	-0.184557
C	-3.714064	-0.832038	-0.097260
H	-4.357346	-0.637213	-0.954427
H	-0.536437	-1.590405	-0.549642
H	-4.208268	-1.100511	0.835673
C	1.891798	-0.570168	-0.800323
N	2.106862	-1.707754	-0.231080
N	1.465476	-1.993542	0.946709
H	1.964650	-2.716815	1.447140
H	1.233718	-1.191851	1.534943
H	2.445921	-0.416630	-1.724011

Structure No: TS11 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-1.218096	0.557374	0.049513
C	-2.450854	-0.074238	0.255868
C	-2.243275	-1.454595	0.075429
C	-0.897313	-1.641940	-0.246465
N	-0.284605	-0.430760	-0.242059
H	-3.371092	0.416989	0.542063
H	-2.978527	-2.240176	0.174312
H	-0.340129	-2.536277	-0.480068
C	1.060917	-0.083956	-0.725398
C	2.171771	-1.082128	-0.523797
C	2.349504	-1.421060	0.771414
H	3.135598	-2.113047	1.073698
H	0.967308	0.285203	-1.753738
H	1.733061	-1.080079	1.634358
C	-0.792585	1.916407	0.085347
N	0.441308	2.338776	0.065068
N	1.373607	1.209570	0.093133
H	2.279854	1.548380	-0.238969
H	1.520421	0.894154	1.064096
H	-1.539078	2.706574	0.119789

Structure No: 34 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.390666	0.266178	0.067661
C	2.439848	-0.656794	-0.024599
C	1.858765	-1.935984	-0.101005
C	0.472399	-1.773783	-0.048501

N	0.202151	-0.449274	0.047159
H	3.492665	-0.411838	-0.062621
H	2.375717	-2.879572	-0.200085
H	-0.331189	-2.494232	-0.077743
C	-1.096180	0.177268	0.299768
C	-2.226151	-0.376280	-0.504552
C	-3.108820	-1.115909	0.192579
H	-3.981134	-1.557344	-0.290112
H	-1.229915	0.301803	1.390478
H	-3.032067	-1.335134	1.270652
C	1.334870	1.685417	0.141903
N	0.260598	2.415256	0.044034
N	-0.913989	1.597104	-0.263893
H	-1.737223	2.133284	0.020248
H	-1.041917	1.432441	-1.285352
H	2.251345	2.248304	0.303904

Structure No: TS12 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.382906	0.308827	-0.004020
C	2.453364	-0.577320	-0.153613
C	1.927328	-1.882726	-0.072676
C	0.552420	-1.768987	0.121122
N	0.235041	-0.446817	0.165763
H	3.482052	-0.295274	-0.331866
H	2.473071	-2.810744	-0.164643
H	-0.213273	-2.524106	0.215635
C	-1.071086	0.129094	0.462912
C	-2.169669	-0.314565	-0.484157
C	-3.073565	-1.225750	-0.097923
H	-3.885463	-1.521655	-0.760787
H	-1.253613	0.110596	1.546433
H	-3.069025	-1.730313	0.876885
C	1.280002	1.730866	-0.034353
N	0.172464	2.408500	-0.006123
N	-1.001671	1.574131	-0.037738
H	-1.744425	2.100517	0.425063
H	-1.507090	1.194257	-1.009180
H	2.186728	2.329383	-0.074607

Structure No: 35 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.423261	0.332659	0.048102
C	2.505097	-0.540973	0.011842
C	1.979675	-1.857286	-0.049481
C	0.595911	-1.758558	-0.040419

N	0.269584	-0.427506	-0.012724
H	3.547702	-0.254097	0.009761
H	2.543058	-2.778085	-0.105878
H	-0.167579	-2.521530	-0.062487
C	-1.025915	0.196578	0.250584
C	-2.164242	-0.546318	-0.393898
C	-3.224200	-0.994188	0.282067
H	-4.043937	-1.499607	-0.219173
H	-1.177954	0.235485	1.346093
H	-3.307259	-0.871480	1.359597
C	1.269518	1.762371	0.145206
N	0.131484	2.361601	-0.009986
N	-0.942536	1.542652	-0.336399
H	-1.802613	2.060762	-0.202079
H	-2.086949	-0.668743	-1.472756
H	2.131186	2.394351	0.336673

Structure No: 15a (Fig.2) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-1.056996	0.544499	-0.316973
C	-1.422961	1.861625	-0.092355
C	-0.269372	2.570658	0.345273
C	0.778784	1.677382	0.363819
N	0.309537	0.441350	-0.034390
H	-2.423054	2.255184	-0.212033
H	-0.214448	3.614516	0.620827
H	1.820527	1.810002	0.613102
C	-1.891894	-0.570237	-0.800148
H	-2.445961	-0.416738	-1.723886
N	-2.106678	-1.707929	-0.231054
N	-1.464852	-1.993741	0.946646
C	1.102295	-0.705061	-0.281491
H	0.536317	-1.590315	-0.549788
C	2.411636	-0.747792	-0.184701
C	3.713981	-0.831800	-0.096920
H	4.207925	-1.100074	0.836181
H	4.357507	-0.636997	-0.953903
H	-1.233687	-1.191929	1.534989
H	-1.964013	-2.717050	1.447080

Structure No: TS3 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.086076	0.635897	-0.173685
C	2.456090	0.624338	0.097727
C	2.830793	-0.717741	0.321194
C	1.686040	-1.490412	0.160325

N	0.626418	-0.678795	-0.130176
H	3.091257	1.498474	0.152761
H	3.815850	-1.087431	0.568329
H	1.549869	-2.561569	0.200855
C	0.222232	1.765872	-0.442129
H	0.673078	2.620292	-0.945779
N	-1.017330	1.953574	-0.121488
N	-1.591985	0.888499	0.641251
C	-0.650871	-1.126912	-0.624643
H	-0.622672	-1.776479	-1.489782
C	-1.827700	-0.729722	-0.081492
C	-3.104673	-1.136325	0.097046
H	-3.952905	-0.460278	0.032911
H	-3.312994	-2.194779	0.204504
H	-1.029714	0.687047	1.476368
H	-2.519409	1.181801	0.946675

Structure No: 16a (B3LYP/6-31+G(d,p))

	X	Y	Z
C	0.997852	0.660272	-0.143569
C	2.411426	0.787410	-0.166165
C	2.950353	-0.477066	0.043305
C	1.881328	-1.373408	0.179634
N	0.696120	-0.706539	0.062215
H	2.942594	1.722688	-0.277846
H	3.996837	-0.740907	0.105398
H	1.884448	-2.444748	0.316835
C	-0.553966	-1.345244	0.004396
C	-1.775870	-0.674742	-0.007984
C	-3.014876	-1.027044	-0.467335
H	-3.914451	-0.517415	-0.135866
C	0.067652	1.708399	-0.325473
N	-1.207352	1.829344	-0.051777
N	-1.723720	0.674796	0.689612
H	-1.188665	0.570793	1.561412
H	-2.679840	0.935046	0.932856
H	-0.518564	-2.402374	-0.213953
H	-3.135573	-1.876718	-1.126481
H	0.474492	2.618970	-0.763548

Structure No: RC (16a+MeOH) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.534403	-0.372591	-0.459902
C	2.837565	0.141949	-0.663360
C	3.067040	1.104936	0.317005
C	1.914617	1.162405	1.111153

N	0.991540	0.274608	0.655371
H	3.500781	-0.158979	-1.462901
H	3.955007	1.705449	0.454874
H	1.701859	1.762888	1.983967
C	-0.279120	0.056871	1.284215
C	-1.090444	-1.041633	0.892266
C	-1.827309	-1.899962	1.643342
H	-2.633608	-2.494186	1.222292
C	0.921783	-1.358716	-1.277668
N	-0.285009	-1.828509	-1.418030
N	-1.300551	-1.156092	-0.598135
H	-1.490679	-0.194216	-0.966615
H	-2.138344	-1.716197	-0.754070
H	-0.238987	0.241649	2.352631
H	-1.670225	-1.965190	2.712907
O	-1.685830	1.581464	-0.724443
H	-1.290809	1.397064	0.172590
C	-2.804624	2.457741	-0.615532
H	-3.580502	2.051828	0.047674
H	-2.499084	3.443728	-0.243711
H	-3.224860	2.579993	-1.616910
H	1.610774	-1.841581	-1.970740

Structure No: TS4 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.484792	-0.391954	-0.486708
C	2.834858	-0.039071	-0.702873
C	3.172335	0.937729	0.236486
C	2.030966	1.159225	1.015143
N	1.021291	0.360659	0.587530
H	3.467514	-0.462352	-1.471308
H	4.124845	1.433379	0.358641
H	1.878986	1.826695	1.851490
C	-0.325158	0.369612	1.151383
C	-1.070956	-0.874121	0.963459
C	-1.636614	-1.679682	1.876476
H	-2.359444	-2.446465	1.609693
C	0.769898	-1.349942	-1.266815
N	-0.456669	-1.771662	-1.341186
N	-1.422842	-1.104095	-0.469961
H	-1.668794	-0.086670	-0.853435
H	-2.248823	-1.698111	-0.528266
H	-0.268305	0.655098	2.200829
H	-1.402802	-1.564308	2.928607
O	-1.645575	1.409687	-0.823011
H	-1.093900	1.221925	0.179668
C	-2.806511	2.206536	-0.662612
H	-3.334009	1.985164	0.279410

H	-2.546605	3.273795	-0.665153
H	-3.499409	2.025181	-1.493505
H	1.401227	-1.865136	-1.990895

Structure No: PC (17a+MeOH) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.348453	-0.652135	0.573849
C	2.589170	-1.295414	0.609710
C	3.317428	-0.892497	-0.530477
C	2.505517	-0.021372	-1.242138
N	1.320903	0.121735	-0.571617
H	2.919934	-1.960670	1.395710
H	4.317498	-1.193975	-0.807939
H	2.674234	0.492631	-2.177629
C	0.162663	0.866830	-1.056890
C	-0.506923	1.663283	0.037794
C	-0.529153	3.005631	0.040699
H	-1.023263	3.567648	0.827848
C	0.306407	-0.747894	1.571671
N	-0.795366	-0.109450	1.794966
N	-1.261633	0.912535	0.972916
H	-2.544181	-0.253809	-0.232938
H	-1.887913	1.484742	1.526894
H	0.513868	1.547901	-1.833475
H	-0.078967	3.573551	-0.765432
O	-2.857692	-0.703835	-1.035843
H	-0.562458	0.173696	-1.500408
C	-3.494301	-1.925000	-0.676742
H	-4.386827	-1.757485	-0.057754
H	-3.806021	-2.408658	-1.605996
H	-2.814643	-2.601703	-0.141017
H	0.497379	-1.515520	2.320170

Structure No: 17a (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-0.999150	0.718761	0.006476
C	-2.353450	0.779592	-0.329565
C	-2.864858	-0.538257	-0.298284
C	-1.820643	-1.372638	0.069024
N	-0.696862	-0.607931	0.249089
H	-2.888408	1.681829	-0.592874
H	-3.875489	-0.851294	-0.519427
H	-1.793147	-2.440799	0.229888
C	0.577465	-1.075943	0.775074
H	0.562818	-2.166340	0.757963
H	0.680984	-0.748626	1.817836

C	1.757968	-0.581646	-0.028412
C	2.566501	-1.428099	-0.694303
H	2.412079	-2.499351	-0.645141
C	-0.056540	1.814862	0.063154
N	1.237094	1.876636	0.088822
N	2.055715	0.780957	0.086908
H	3.413598	-1.072974	-1.273335
H	2.993287	1.051316	-0.172748
H	-0.521123	2.798803	0.045119

Structure No: RC (17a+MeOH) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.624793	-0.946822	0.030339
C	2.812392	-1.566487	-0.365394
C	3.817873	-0.573037	-0.422798
C	3.230547	0.625229	-0.047651
N	1.906161	0.391783	0.222413
H	2.915315	-2.614841	-0.610308
H	4.851968	-0.707496	-0.707531
H	3.650276	1.614814	0.062091
C	0.965165	1.348968	0.785975
H	1.426849	2.335959	0.737145
H	0.789715	1.102698	1.841523
C	-0.353212	1.377962	0.046900
C	-0.769881	2.481904	-0.605605
H	-0.182494	3.392293	-0.587824
C	0.319281	-1.550541	0.191592
N	-0.880671	-1.062358	0.259647
N	-1.181214	0.264266	0.197988
H	-4.846670	0.758210	-0.040395
H	-1.713077	2.502331	-1.141961
C	-4.516399	-1.193380	-0.032057
H	-5.307544	-1.499258	-0.727570
H	-4.856505	-1.341996	0.999993
H	-3.628051	-1.803997	-0.198504
O	-4.119215	0.165446	-0.264764
H	-2.173493	0.397343	0.019142
H	0.334151	-2.638243	0.224167

Structure No: TS5 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.881389	0.769700	0.009706
C	3.148840	0.895325	0.584553
C	3.690641	-0.401847	0.708572
C	2.762516	-1.292501	0.182909
N	1.672144	-0.580695	-0.230771

H	3.599030	1.824373	0.905889
H	4.651127	-0.668734	1.125957
H	2.807702	-2.364371	0.054330
C	0.524449	-1.067551	-0.979303
H	0.592910	-2.152205	-1.059191
H	0.537730	-0.638462	-1.990718
C	-0.752646	-0.681695	-0.266312
C	-1.746936	-1.633492	0.165821
H	-1.574309	-2.655244	-0.169574
C	0.917482	1.784067	-0.331792
N	-0.377345	1.734170	-0.454388
N	-1.080665	0.598084	-0.153560
H	-2.820233	-0.987684	-0.189207
H	-1.950246	-1.600798	1.241971
C	-4.433816	0.214039	0.813039
H	-4.020110	-0.260088	1.725424
H	-5.376865	-0.302324	0.576282
H	-4.676315	1.255291	1.072570
O	-3.542758	0.161455	-0.272960
H	-2.200523	0.698424	-0.074916
H	1.321721	2.782993	-0.487254

Structure No: 10a (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-1.046505	0.707813	-0.023425
C	-2.363169	0.597890	-0.469166
C	-2.732170	-0.763922	-0.374190
C	-1.648186	-1.454759	0.152223
N	-0.633213	-0.562000	0.357905
H	-2.967888	1.412633	-0.842774
H	-3.681676	-1.200742	-0.649877
H	-1.533300	-2.497852	0.410109
C	0.667670	-0.786063	0.975589
H	0.764278	-1.846974	1.213347
H	0.734041	-0.211837	1.908893
C	1.738147	-0.332982	-0.006289
C	2.630903	-1.370585	-0.624928
H	3.221725	-1.886203	0.143469
C	-0.184721	1.853421	0.185001
N	1.113471	1.922451	0.148447
N	1.866187	0.892369	-0.366334
H	3.309139	-0.904028	-1.341000
H	2.033312	-2.134692	-1.138626
H	-0.676563	2.795071	0.427440

Structure No: PC (10a+MeOH) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.685538	-0.935233	0.085554
C	2.779582	-1.429562	-0.624795
C	3.578055	-0.324816	-0.997585
C	2.976111	0.817629	-0.484961
N	1.832296	0.443379	0.162474
H	2.952731	-2.469596	-0.864350
H	4.494404	-0.348986	-1.570194
H	3.284854	1.852705	-0.516797
C	0.921499	1.264709	0.948420
H	1.246648	2.304553	0.887296
H	0.956126	0.950329	1.999883
C	-0.481737	1.092163	0.388623
C	-1.139600	2.270744	-0.269224
H	-1.243809	3.097908	0.445048
C	0.598216	-1.601826	0.766958
N	-0.604931	-1.178232	1.020649
N	-1.099237	-0.034818	0.426335
H	-2.125995	2.007738	-0.653947
H	-0.514738	2.636490	-1.094321
C	-4.661441	-1.009124	-0.561966
H	-4.251098	-1.830164	-1.168407
H	-5.626600	-0.719080	-0.987348
H	-4.832402	-1.381320	0.458805
O	-3.828075	0.138582	-0.580486
H	-2.952961	-0.085211	-0.205635
H	0.803209	-2.604424	1.141508

Structure No: 36 (Fig.S2) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	0.839548	0.637328	-0.094106
C	1.156119	1.953372	0.201541
C	-0.054812	2.642280	0.464651
C	-1.083854	1.737920	0.298023
N	-0.549991	0.513499	-0.035310
H	2.162107	2.345714	0.235919
H	-0.166469	3.682365	0.736554
H	-2.154201	1.865746	0.357000
C	-1.296446	-0.619351	-0.431395
C	-2.601797	-0.733579	-0.340287
C	-3.900556	-0.878258	-0.279268
H	-4.549022	-0.566191	-1.097327

H	-0.699835	-1.420536	-0.852297
H	-4.387378	-1.314122	0.592360
C	1.826067	-0.416979	-0.399047
O	2.848284	-0.176982	-1.038017
N	1.595090	-1.718228	0.045435
H	2.394760	-2.316793	-0.150637
N	0.879283	-1.938302	1.241174
H	0.330182	-2.788200	1.163241
H	1.507286	-2.007311	2.039557

Structure No: TS13 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.077881	0.415753	-0.035174
C	1.685391	1.646822	0.202302
C	0.687522	2.634761	0.080322
C	-0.510932	1.992374	-0.217644
N	-0.276946	0.651503	-0.275928
H	2.726313	1.782633	0.458711
H	0.811423	3.700869	0.205491
H	-1.503430	2.379063	-0.390743
C	-1.205200	-0.385773	-0.724793
C	-2.668840	-0.211627	-0.471170
C	-2.979042	-0.099989	0.839192
H	-4.012528	-0.002753	1.171707
H	-0.944442	-0.670363	-1.750704
H	-2.258688	-0.054216	1.687428
C	1.620306	-0.923279	0.037255
N	2.788937	-1.229233	0.220046
N	0.675801	-1.979909	-0.157182
H	0.976264	-2.860309	0.254471
N	-0.699577	-1.664058	0.080944
H	-1.303479	-2.418323	-0.262311
H	-0.940392	-1.489749	1.069002

Structure No: 37 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-1.073611	0.525981	0.056041
C	-1.520978	1.838617	-0.074623
C	-0.380675	2.664997	-0.121879
C	0.740160	1.844821	-0.029709
N	0.322211	0.553939	0.074448
H	-2.558488	2.132281	-0.145228
H	-0.361821	3.740130	-0.228390
H	1.794401	2.074927	-0.046491
C	1.168555	-0.612120	0.323076

C	2.450383	-0.682582	-0.410512
C	3.542175	-0.160153	0.172231
H	4.514568	-0.209955	-0.317952
H	1.155587	-0.864235	1.397022
H	3.560106	0.341324	1.152220
C	-1.813487	-0.715928	0.081999
O	-3.029083	-0.843556	0.084792
N	-1.010547	-1.893911	0.142860
H	-1.488849	-2.715689	-0.217022
N	0.342953	-1.767935	-0.330260
H	0.878135	-2.615630	-0.113886
H	0.481571	-1.601153	-1.347694

Structure No: TS14 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-1.106613	0.464918	0.013493
C	-1.661545	1.733759	-0.119721
C	-0.598426	2.661201	-0.094458
C	0.585479	1.944343	0.051266
N	0.281232	0.617879	0.100315
H	-2.716467	1.938198	-0.233417
H	-0.672573	3.735568	-0.184033
H	1.607819	2.283023	0.109047
C	1.132748	-0.532044	0.407959
C	2.539545	-0.819430	-0.041177
C	3.552489	0.052610	-0.067849
H	4.541828	-0.270082	-0.388442
H	1.012441	-0.791422	1.469441
H	3.495540	1.105851	0.225809
C	-1.745968	-0.846011	0.046346
O	-2.950222	-1.053494	0.034086
N	-0.847240	-1.949403	0.134822
H	-1.232630	-2.829031	-0.195632
N	0.479857	-1.676021	-0.333826
H	1.487378	-2.227293	-0.225245
H	0.495238	-1.420124	-1.334559

Structure No: 38 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.166979	0.400571	0.022949
C	1.788621	1.639797	0.083836
C	0.769730	2.621314	0.052681
C	-0.449078	1.960121	-0.031830
N	-0.206481	0.613652	-0.033002
H	2.856383	1.793862	0.141461
H	0.899875	3.693616	0.094002

H	-1.456782	2.345217	-0.080109
C	-1.146158	-0.514851	-0.221843
C	-2.496866	-0.207121	0.365081
C	-3.619785	-0.163988	-0.352583
H	-4.578655	0.048191	0.110058
H	-1.230426	-0.726361	-1.294138
H	-3.619735	-0.343103	-1.424912
C	1.712353	-0.957184	-0.066870
O	2.901023	-1.230541	-0.207968
N	0.731777	-1.938647	-0.058788
H	1.018519	-2.907388	-0.101882
N	-0.579776	-1.698368	0.412902
H	-2.518024	-0.016976	1.437928
H	-0.552754	-1.551143	1.425017

Structure No: 36 (Fig.3) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-0.839980	0.637020	-0.094000
C	-1.157360	1.952916	0.201640
C	0.053124	2.642602	0.464519
C	1.082748	1.738954	0.297413
N	0.549655	0.514132	-0.035535
H	-2.163645	2.344447	0.236402
H	0.164140	3.682774	0.736345
H	2.153018	1.867529	0.355893
C	1.296718	-0.618066	-0.432592
C	2.602330	-0.731160	-0.342704
C	3.900678	-0.877477	-0.277281
H	4.383370	-1.314786	0.595937
C	-1.826177	-0.417830	-0.398050
N	-1.594009	-1.719128	0.045179
H	-2.393563	-2.317986	-0.150420
N	-0.876135	-1.940160	1.239370
H	-1.502719	-2.010044	2.038787
H	-0.327042	-2.789887	1.159736
O	-2.849497	-0.177894	-1.035280
H	0.700555	-1.418895	-0.854822
H	4.552801	-0.565659	-1.092391

Structure No: TS6 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.111426	0.267342	-0.008755
C	2.429386	-0.005196	0.342620
C	2.578178	-1.409678	0.359771
C	1.351319	-1.955435	0.006319
N	0.451557	-0.946394	-0.208978

H	3.175706	0.742521	0.570677
H	3.472257	-1.966174	0.603149
H	1.049205	-2.984086	-0.127694
C	-0.849608	-1.115205	-0.802389
C	-1.983474	-0.731545	-0.166267
C	-3.295716	-1.022916	-0.023126
H	-4.062508	-0.260825	0.092077
C	0.479617	1.576867	-0.202327
N	-0.824953	1.763080	0.304431
H	-1.398988	2.401152	-0.235685
N	-1.557851	0.670729	0.856992
H	-1.003260	0.284420	1.626391
H	-2.425967	1.020782	1.269998
O	1.036600	2.545840	-0.699119
H	-0.880022	-1.592886	-1.773305
H	-3.627257	-2.048934	-0.134847

Structure No: 39 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.011302	0.389996	-0.038539
C	2.409814	0.450666	0.047586
C	2.888630	-0.863570	0.117529
C	1.781056	-1.708060	0.069727
N	0.634862	-0.969625	-0.027570
H	2.975370	1.370416	0.085963
H	3.917707	-1.180338	0.210867
H	1.721664	-2.786799	0.078279
C	-0.637343	-1.563262	-0.270248
C	-1.822946	-0.882202	-0.056486
C	-3.104432	-0.952917	-0.555218
H	-3.951959	-0.585258	0.018654
C	0.144175	1.545382	-0.162681
N	-1.172549	1.509811	0.414753
H	-1.877876	1.899508	-0.207223
N	-1.633241	0.243638	0.938723
H	-0.957825	-0.036413	1.661273
H	-2.526655	0.428106	1.402662
O	0.477299	2.618451	-0.645592
H	-0.622953	-2.467702	-0.861226
H	-3.320905	-1.572084	-1.415878

Structure No: 40 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.099649	0.273154	0.018099
C	2.464372	0.070251	0.152568
C	2.704795	-1.324670	0.145894

C	1.482988	-1.947293	-0.009824
N	0.493705	-0.989252	-0.077264
H	3.188424	0.868232	0.227239
H	3.659781	-1.821995	0.238349
H	1.227993	-2.995688	-0.069308
C	-0.860086	-1.309632	-0.292772
C	-1.896102	-0.535106	0.060557
C	-3.326686	-0.889377	-0.218166
H	-3.784763	-0.137506	-0.872161
C	0.448321	1.586274	-0.140438
N	-0.926170	1.647767	-0.000021
H	-1.320121	2.580087	-0.044331
N	-1.682547	0.718227	0.741126
H	-1.265553	0.574948	1.660972
H	-3.906454	-0.896589	0.712426
O	1.091606	2.597945	-0.414414
H	-1.012487	-2.265036	-0.783728
H	-3.418089	-1.868807	-0.696530

Structure No: RC (39+MeOH) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-0.212658	1.114280	0.428055
C	0.007891	2.356861	-0.159791
C	-1.092460	2.628629	-1.005157
C	-1.962526	1.552664	-0.901443
N	-1.431095	0.636116	-0.036781
H	0.867958	2.982571	0.032644
H	-1.244765	3.506861	-1.616368
H	-2.920238	1.376487	-1.370370
C	-2.063678	-0.623215	0.370672
C	-1.219162	-1.808447	-0.038491
C	-1.672670	-2.787677	-0.832658
H	-1.052578	-3.643383	-1.077591
C	0.629314	0.406585	1.404148
N	0.408693	-0.964821	1.521620
H	1.008235	-1.411889	2.206216
N	0.123341	-1.785642	0.410550
H	1.654476	0.338866	-1.444393
H	0.805263	-1.640665	-0.337945
O	1.445385	0.980504	2.122189
H	-2.201788	-0.610060	1.457534
H	-2.663228	-2.736991	-1.270298
O	2.078874	-0.531530	-1.460125
H	-3.047766	-0.676145	-0.096634
C	3.478789	-0.374631	-1.203011
H	3.912843	-1.376525	-1.211847
H	3.963016	0.223410	-1.984735
H	3.660868	0.085808	-0.224392

Structure No: TS7 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-1.477489	0.044233	-0.118325
C	-2.696136	-0.603390	-0.369311
C	-2.627098	-1.878187	0.206238
C	-1.373653	-1.982365	0.805894
N	-0.676938	-0.827393	0.623894
H	-3.509738	-0.162837	-0.926263
H	-3.387909	-2.645730	0.195171
H	-0.931749	-2.796420	1.362836
C	0.675167	-0.659675	1.159876
C	1.223263	0.681577	1.115718
C	1.838691	1.415839	2.061469
H	2.438102	2.290212	1.820207
C	-1.204832	1.398829	-0.569829
N	0.115814	1.887084	-0.768266
H	0.161044	2.881483	-0.566287
N	1.277024	1.180375	-0.294107
H	1.525734	0.242585	-0.915200
H	2.058871	1.826664	-0.408426
O	-2.093153	2.188318	-0.878748
H	0.735670	-1.103371	2.152271
H	1.789126	1.122602	3.103478
O	1.789042	-1.130225	-1.122635
H	1.451321	-1.223731	-0.024209
C	3.098516	-1.629239	-1.360194
H	3.084031	-2.724933	-1.403795
H	3.461304	-1.254035	-2.323682
H	3.807196	-1.323435	-0.574910

Structure No: 41 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-1.088091	0.226173	-0.029068
C	-2.345579	-0.173444	-0.468537
C	-2.401874	-1.581457	-0.376022
C	-1.182086	-2.007650	0.130618
N	-0.384555	-0.916638	0.338310
H	-3.115803	0.500131	-0.815393
H	-3.231535	-2.220382	-0.643388
H	-0.828065	-3.001417	0.366052

C	0.956337	-0.942989	0.927918
H	1.195088	-1.974960	1.187689
H	0.949450	-0.352570	1.851271
C	1.983806	-0.397559	-0.035466
C	3.035163	-1.107281	-0.467370
H	3.158855	-2.145527	-0.182539
C	-0.564220	1.588875	0.104922
N	0.827555	1.710811	0.207238
H	1.141872	2.666951	0.329076
N	1.729991	0.911104	-0.510123
H	3.778603	-0.672218	-1.127325
O	-1.278450	2.582893	0.197567
H	1.607465	0.971886	-1.515935

Structure No: PC (41+MeOH) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-0.212658	1.114280	0.428055
C	0.007891	2.356861	-0.159791
C	-1.092460	2.628629	-1.005157
C	-1.962526	1.552664	-0.901443
N	-1.431095	0.636116	-0.036781
H	0.867958	2.982571	0.032644
H	-1.244765	3.506861	-1.616368
H	-2.920238	1.376487	-1.370370
C	-2.063678	-0.623215	0.370672
C	-1.219162	-1.808447	-0.038491
C	-1.672670	-2.787677	-0.832658
H	-1.052578	-3.643383	-1.077591
C	0.629314	0.406585	1.404148
N	0.408693	-0.964821	1.521620
H	1.008235	-1.411889	2.206216
N	0.123341	-1.785642	0.410550
H	1.654476	0.338866	-1.444393
H	0.805263	-1.640665	-0.337945
O	1.445385	0.980504	2.122189
H	-2.201788	-0.610060	1.457534
H	-2.663228	-2.736991	-1.270298
O	2.078874	-0.531530	-1.460125
H	-3.047766	-0.676145	-0.096634
C	3.478789	-0.374631	-1.203011
H	3.912843	-1.376525	-1.211847
H	3.963016	0.223410	-1.984735
H	3.660868	0.085808	-0.224392

Structure No: RC (41+MeOH) (B3LYP/6-31+G(d,p))

	X	Y	Z

C	1.008216	-1.076081	-0.049139
C	1.791669	-2.158877	-0.426996
C	3.145682	-1.777489	-0.286284
C	3.155670	-0.474773	0.189474
N	1.863935	-0.044815	0.328458
H	1.402213	-3.105601	-0.772519
H	4.018629	-2.376284	-0.504546
H	3.982037	0.172137	0.448368
C	1.461424	1.237196	0.912398
H	2.361439	1.772131	1.217214
H	0.864396	1.039890	1.811019
C	0.658690	2.080617	-0.053752
C	0.932748	3.369799	-0.318039
H	1.812992	3.845919	0.096674
C	-0.457580	-0.981631	0.001420
N	-0.977031	0.302824	-0.012349
H	-1.989727	0.401358	0.087107
N	-0.315868	1.331598	-0.705030
H	-4.560612	1.096121	0.324717
H	0.308802	3.962991	-0.979653
O	-1.193468	-1.960492	0.141754
C	-4.471079	-0.876629	0.137906
H	-4.846950	-1.057373	1.151721
H	-3.652751	-1.570113	-0.062402
H	-5.278670	-1.029672	-0.587755
O	-3.917719	0.446492	0.016067
H	-0.882185	1.780445	-1.412001

Structure No: TS8 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.837548	0.440527	0.099134
C	3.061064	0.382641	0.758981
C	3.483200	-0.963770	0.757557
C	2.514907	-1.699105	0.087771
N	1.519654	-0.851007	-0.310218
H	3.564843	1.236351	1.188046
H	4.389739	-1.362960	1.189576
H	2.465140	-2.753883	-0.142362
C	0.337780	-1.215990	-1.081487
H	0.362867	-2.290066	-1.261926
H	0.351105	-0.687831	-2.044085
C	-0.911414	-0.843120	-0.311936
C	-1.907802	-1.773973	0.140799
H	-1.763280	-2.796901	-0.201556
C	1.026093	1.625190	-0.164719
N	-0.301674	1.441009	-0.601880
H	-0.783707	2.331867	-0.662201

N	-1.157629	0.438583	-0.127214
H	-3.017350	-0.980396	-0.179620
H	-2.107667	-1.739835	1.215207
O	1.463728	2.769211	-0.087822
C	-4.497124	0.236964	0.879242
H	-5.424725	-0.301149	0.644408
H	-4.748807	1.287402	1.070005
H	-4.081824	-0.186352	1.809647
O	-3.587195	0.143834	-0.202020
H	-2.306569	0.603106	-0.023272

Structure No: 26 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-1.103525	0.242029	-0.020434
C	-2.382737	-0.112132	-0.438423
C	-2.488304	-1.516361	-0.338624
C	-1.276982	-1.987815	0.149706
N	-0.440397	-0.922584	0.335363
H	-3.130638	0.587953	-0.780383
H	-3.345780	-2.124769	-0.588887
H	-0.954961	-2.991622	0.388376
C	0.899400	-0.955370	0.898992
H	1.165604	-1.997945	1.080825
H	0.903692	-0.423361	1.861183
C	1.907072	-0.293522	-0.022184
C	3.011347	-1.126501	-0.607399
H	3.575787	-1.634907	0.184782
C	-0.535202	1.584473	0.069058
N	0.856273	1.747781	0.225983
H	1.086037	2.729193	0.112741
N	1.881985	0.959347	-0.296090
H	3.691572	-0.499491	-1.186182
H	2.602549	-1.905752	-1.263168
O	-1.233165	2.595010	0.023721

Structure No: PC (26+MeOH) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.716428	0.641681	0.066117
C	2.810176	0.976914	0.858481
C	3.500845	-0.217598	1.155476
C	2.821752	-1.254406	0.529298
N	1.740641	-0.732412	-0.124351
H	3.050941	1.980513	1.176703
H	4.394195	-0.321777	1.754627

H	3.032674	-2.313786	0.490917
C	0.795513	-1.455557	-0.959610
H	1.052967	-2.515162	-0.926395
H	0.882807	-1.107715	-1.998721
C	-0.631933	-1.234652	-0.495909
C	-1.415581	-2.404528	0.023814
H	-1.430537	-3.210581	-0.720788
C	0.720818	1.541261	-0.507073
N	-0.475115	1.009084	-1.038721
H	-1.103986	1.773198	-1.262065
N	-1.201584	-0.085647	-0.563761
H	-2.441636	-2.118126	0.261326
H	-0.939415	-2.810179	0.925645
O	0.885584	2.756450	-0.566638
C	-4.440386	0.853616	1.177340
H	-5.468736	0.624606	1.469411
H	-4.415145	1.883171	0.791063
H	-3.807571	0.801382	2.075524
O	-4.059480	-0.098037	0.194232
H	-3.128769	0.049593	-0.057776

Structure No: 36 (Fig.4) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-0.751307	-0.458341	-0.250797
C	-2.065543	-0.839238	-0.460371
C	-2.900542	0.260860	-0.127809
C	-2.075186	1.293563	0.260219
N	-0.762854	0.862986	0.195803
H	-2.370802	-1.822863	-0.787633
H	-3.980071	0.293972	-0.167440
H	-2.298844	2.313905	0.536484
C	0.329247	1.760020	0.332499
C	1.467954	1.679229	-0.318219
C	2.598473	1.617126	-0.969138
H	2.729718	2.130841	-1.919607
C	0.432333	-1.347336	-0.392012
N	1.354683	-1.373793	0.635119
H	2.068485	-2.084231	0.526899
N	1.132169	-0.973971	1.966500
H	1.198364	0.038027	2.036614
H	0.210312	-1.268901	2.281054
O	0.572362	-2.077051	-1.371040
H	0.141743	2.574012	1.028965
H	3.441639	1.039798	-0.595214

Structure No: TS9 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.001894	0.471206	-0.038657
C	2.369170	0.727936	0.140664
C	3.010111	-0.510472	0.268342
C	2.035167	-1.504202	0.142121
N	0.818093	-0.920856	-0.036837
H	2.807527	1.713825	0.194436
H	4.061987	-0.684922	0.444894
H	2.128322	-2.580478	0.157532
C	-0.366738	-1.588120	-0.425704
C	-1.598166	-1.042024	-0.324747
C	-2.902602	-1.391852	-0.202459
H	-3.701252	-0.848219	-0.700600
C	-0.077340	1.361561	-0.326838
N	-1.406906	0.753847	-0.051204
H	-2.077756	1.245967	-0.646582
N	-1.824541	1.010079	1.314548
H	-2.501620	0.251715	1.492426
H	-1.009139	0.815980	1.899598
O	-0.031819	2.491036	-0.783413
H	-0.224247	-2.570724	-0.855586
H	-3.164776	-2.317130	0.299318

Structure No: 42 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	0.975982	0.487439	-0.160496
C	2.360759	0.811955	-0.162619
C	3.046704	-0.369211	0.071603
C	2.097857	-1.407490	0.201673
N	0.848813	-0.899148	0.057150
H	2.759353	1.807764	-0.287027
H	4.117298	-0.495878	0.151407
H	2.242347	-2.466348	0.358586
C	-0.362699	-1.597907	0.026492
C	-1.543461	-0.909675	-0.270808
C	-2.765772	-1.316416	-0.739249
C	-0.146051	1.310697	-0.321047
N	-1.478982	0.541773	0.083106
H	-2.206669	1.053259	-0.422316
N	-1.704182	0.821875	1.503602
H	-2.457420	0.187841	1.778629
H	-0.863076	0.494679	1.981121
O	-0.299183	2.471316	-0.632952
H	-0.293778	-2.671146	-0.067617
H	-2.928891	-2.345764	-1.032517

H	-3.615165	-0.642779	-0.776953

Structure No: RC (42+MeOH) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-1.386892	-0.752453	-0.106130
C	-2.444471	-1.698830	-0.189464
C	-3.628169	-0.976537	-0.179924
C	-3.301730	0.395719	-0.104765
N	-1.952936	0.535895	-0.065127
H	-2.311218	-2.770146	-0.213072
H	-4.633564	-1.372559	-0.214466
H	-3.942678	1.265158	-0.103194
C	-1.209403	1.720465	-0.071456
C	0.185285	1.651069	-0.177110
C	1.120717	2.566806	-0.585724
C	0.001626	-0.942592	-0.042369
N	0.759735	0.373281	0.346445
H	1.726084	0.233432	-0.022191
N	0.897349	0.349434	1.806192
H	1.414843	1.202866	2.027401
H	-0.047727	0.493281	2.166449
O	0.696984	-1.932454	-0.173862
H	-1.750912	2.622913	-0.313509
O	3.419158	-0.026100	-0.522077
H	3.504459	0.072498	-1.479631
C	3.974086	-1.295106	-0.121783
H	5.032573	-1.353806	-0.396970
H	3.880776	-1.341648	0.963655
H	3.412138	-2.125103	-0.558695
H	0.808767	3.529015	-0.973377
H	2.182001	2.391015	-0.455116

Structure No: TS10 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	-1.604624	-0.591212	-0.077743
C	-2.858342	-1.156836	-0.359715
C	-3.753871	-0.096641	-0.547128
C	-3.036390	1.094443	-0.384242
N	-1.742176	0.793105	-0.100443
H	-3.061165	-2.216673	-0.407462
H	-4.807090	-0.166025	-0.778345
H	-3.358436	2.122935	-0.461608
C	-0.675964	1.682822	0.115305
C	0.588890	1.252931	0.353653
C	1.836057	1.970279	0.262638

C	-0.356368	-1.207321	0.223604
N	0.780036	-0.226087	0.555541
H	1.618157	-0.448218	-0.172440
N	1.287401	-0.565426	1.875596
H	2.286421	-0.370547	1.865128
H	0.852561	0.080828	2.533201
O	-0.082915	-2.384307	0.249765
H	-0.904312	2.732326	-0.007673
O	2.649404	-0.094785	-1.122356
H	2.513535	0.948622	-0.725628
C	3.990715	-0.561378	-1.089935
H	4.536746	-0.170399	-0.217722
H	3.995214	-1.655445	-1.042735
H	4.523102	-0.249882	-1.997055
H	1.716026	3.013252	-0.029933
H	2.499892	1.878303	1.129513

Structure No: PC (25+MeOH) (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.044347	-0.975688	0.281253
C	1.502045	-2.288248	0.342526
C	2.825632	-2.285713	-0.147156
C	3.152853	-0.979839	-0.497780
N	2.070664	-0.185098	-0.236626
H	0.928760	-3.128804	0.703711
H	3.482433	-3.139295	-0.239760
H	4.061337	-0.562953	-0.907279
C	1.909304	1.186781	-0.417484
C	0.740061	1.781352	-0.085270
C	0.512039	3.253720	-0.256338
C	-0.218371	-0.376765	0.641286
N	-0.308013	1.004815	0.432203
H	-2.894458	-0.760687	0.445587
N	-1.498797	1.676749	0.795528
H	-2.269904	1.286991	0.246582
H	-1.697754	1.437061	1.766131
O	-1.173801	-1.013531	1.113156
H	2.747724	1.732244	-0.826114
O	-3.620464	-0.276575	0.005090
H	0.270006	3.730673	0.697442
C	-4.384885	-1.159832	-0.804675
H	-3.770932	-1.647616	-1.574755
H	-4.880994	-1.935188	-0.204916
H	-5.154249	-0.562736	-1.301211
H	1.412179	3.716574	-0.668231
H	-0.327941	3.450063	-0.928959

Structure No: 25 (B3LYP/6-31+G(d,p))

	X	Y	Z
C	1.040501	0.531830	-0.000502
C	2.357443	0.977440	-0.000243
C	3.181358	-0.169716	0.000211
C	2.357955	-1.289983	0.000426
N	1.057397	-0.863226	-0.000026
H	2.660985	2.013645	-0.000480
H	4.262184	-0.189690	0.000384
H	2.595520	-2.343782	0.000771
C	-0.120190	-1.610725	0.000015
C	-1.320110	-0.985702	-0.000130
C	-2.619057	-1.735440	-0.000125
C	-0.220454	1.241621	-0.000275
N	-1.361426	0.414966	-0.000542
N	-2.626958	1.043409	0.000604
H	-2.653220	1.663562	0.810188
H	-2.654358	1.664071	-0.808540
O	-0.344207	2.467471	0.000183
H	-0.020682	-2.686604	0.000017
H	-3.222349	-1.485973	-0.877953
H	-2.420447	-2.809891	-0.000834
H	-3.221742	-1.487089	0.878460

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