

Electronic Supplementary Information

Infrared and Raman screening of seized Novel Psychoactive Substances: A large scale study of >200 samples.

L. E. Jones, A. Stewart, K. L. Peters, M. McNaul, S. J. Speers and S. E. J. Bell

This supplement contains a list of the reference standards used in this study as well as NMR data for 33 compounds, listed below.

Reference Standards	2
5-MAPB	3
5-EAPB	4
5,6-MDAI	5
NM2AI	6
6-APB	7
5-IAP	8
Nitracaine	9
Etaqualone	10
Buphedrone	11
4-CMC	12 – 13
4-EMC	14 – 15
4-MBC	16 – 17
PV8	18 – 19
AH-7921	20
aMT	21
5-MeO-DALT	22
Ethylphenidate	23
n-Ethylketamine	24 – 25
Methoxphenidine	26
Diphenidine	27
DNP	28
Flubromazepam	29
Diclazepam	30
Etizolam	30
AB-FUBINACA	31
AM-1220	32
AM-2201	33 – 34
CB-13	35 – 36
2NE1	37
PB-22	38
RCS-4	39
UR-144	40
5-FUR-144	41

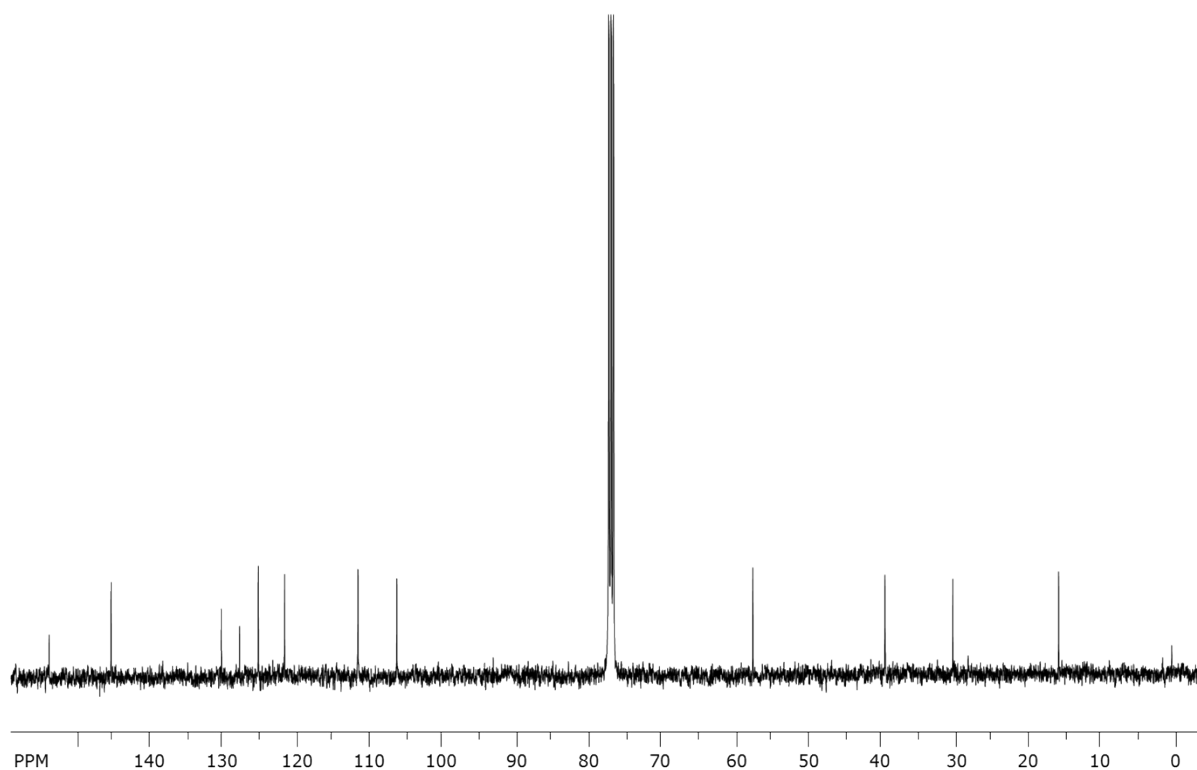
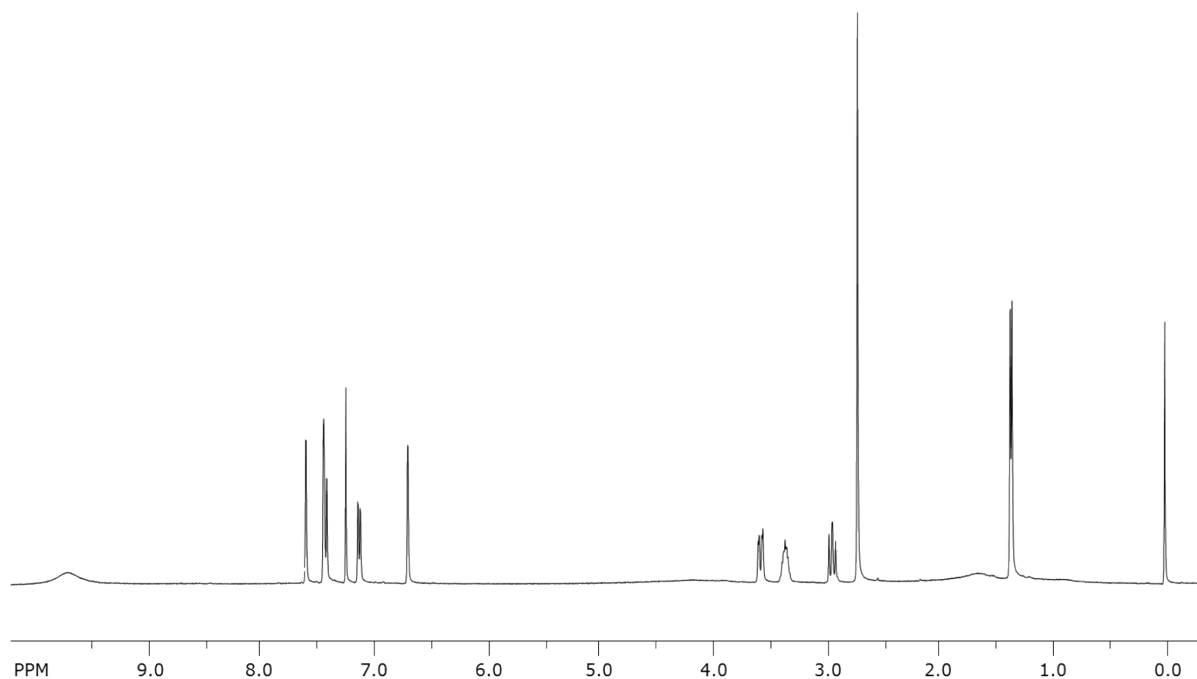
Reference Standards	IR	Raman
2-Fluoroamphetamine	X	X
3-Fluoroamphetamine	X	X
4-Fluoroamphetamine	X	X
2C-I	X	X
4-MEC	X	X
α -PVP	X	-
Alprazolam	X	X
BMDP	X	X
Butylone	X	X
Cathinone	X	X
Chlordiazepoxide	X	X
Cocaine HCl	X	-
Diazepam	X	X
Diethyltryptamine	X	X
Dihydrocodeine Bitartate	X	X
Dimethcathinone	X	X
D-proxyphene	X	X
Ethylone	X	X
Flephedrone	X	X
Ketamine	X	X
Lorazepam	X	X
Lormetazepam	X	X
MBDB	X	X
mCPP	X	X
MDEA	X	X
MDMA	X	X
MDPBP	X	X
MDPV	X	X
Mephedrone	X	X
Methadone	X	X
Methamphetamine	X	X
Methcathinone	X	X
Methedrone	X	X
Methiopropamine	X	X
Methoxetamine	X	X
Methylone	X	X
Methylphenidate	X	X
Naphyrone	X	X
N-ethylcathinone	X	X
N,N-dimethyltryptamine	X	X
oCPP	X	X
pCPP	X	X
PMMA	X	X

X = reference standard available

NMR Data of **5-MAPB**

δ_{H} (CDCl_3 , 400MHz) 9.73 (1H, bs) 7.61 (1H, d, J 2.1 Hz) 7.45 (1H, d, J 2.0 Hz) 7.43 (1H, s) 7.14 (1H, dd, J 8.5 Hz and J 1.4 Hz) 6.71 (1H, d, J 1.1 Hz) 3.58 (1H, dd, J 13.1 Hz and J 3.8 Hz) 3.32-3.42 (1H, m) 2.95 (1H, dd, J 12.8 Hz and J 10.9 Hz) 2.72 (3H, s) 1.36 (3H, d, J 6.4 Hz)

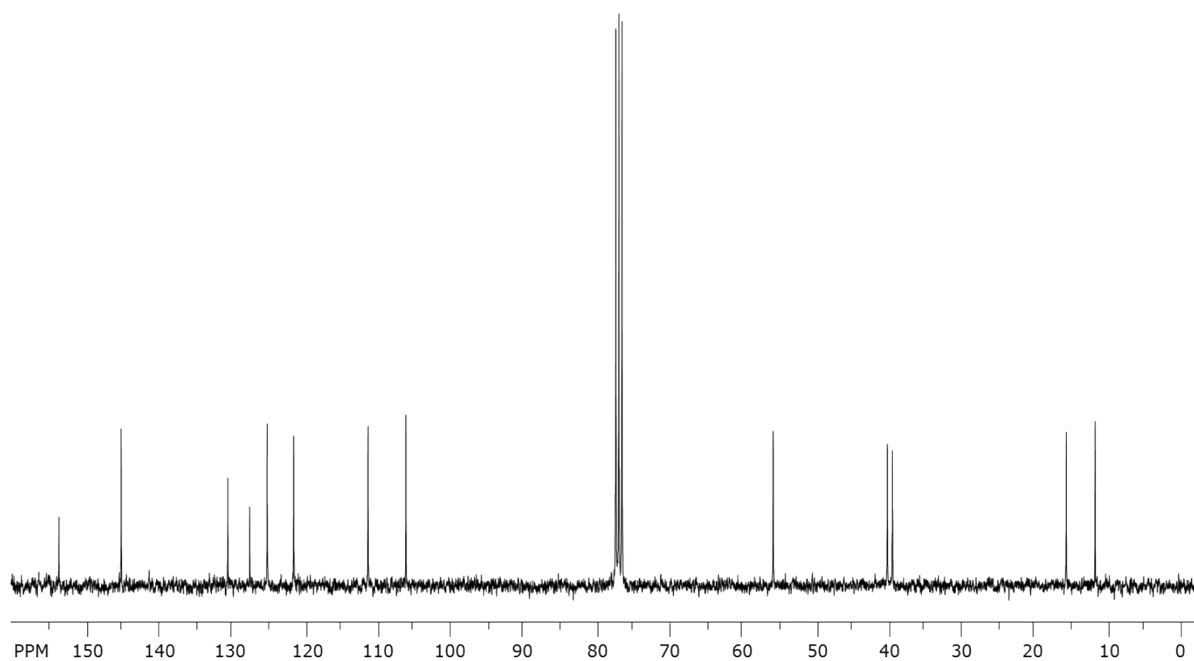
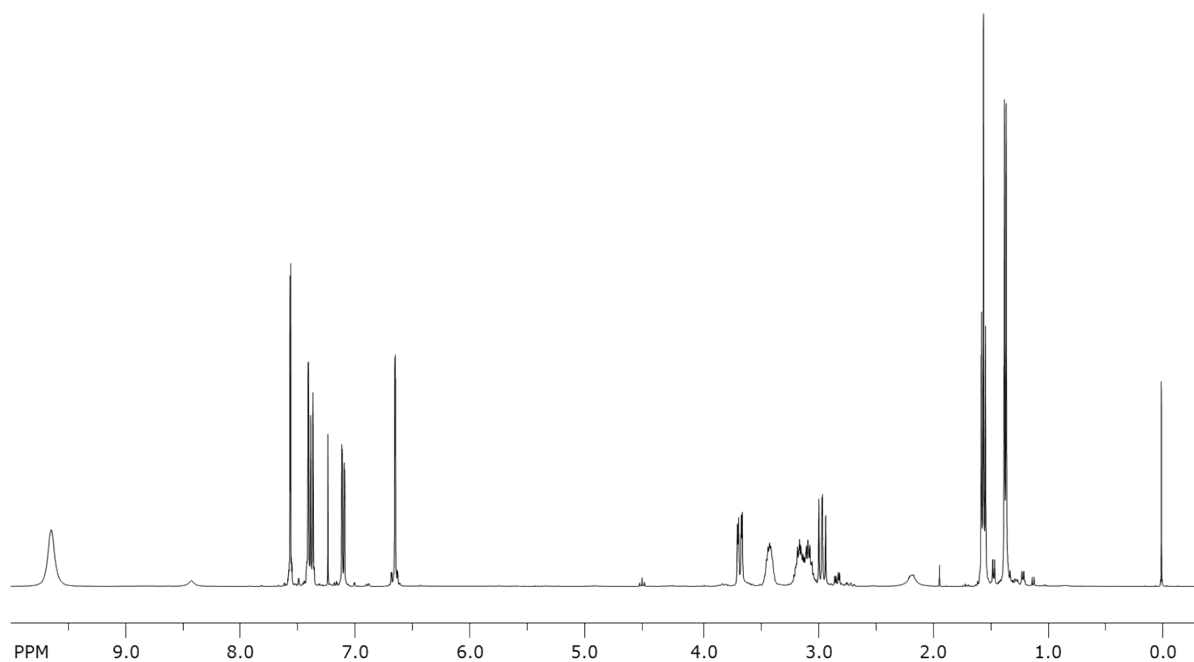
δ_{C} (CDCl_3 , 100MHz) 154.2, 145.6, 130.5, 128.0, 125.4, 121.8, 111.7, 106.4, 57.6, 39.4, 30.1, 15.5



NMR Data of **5-EAPB**

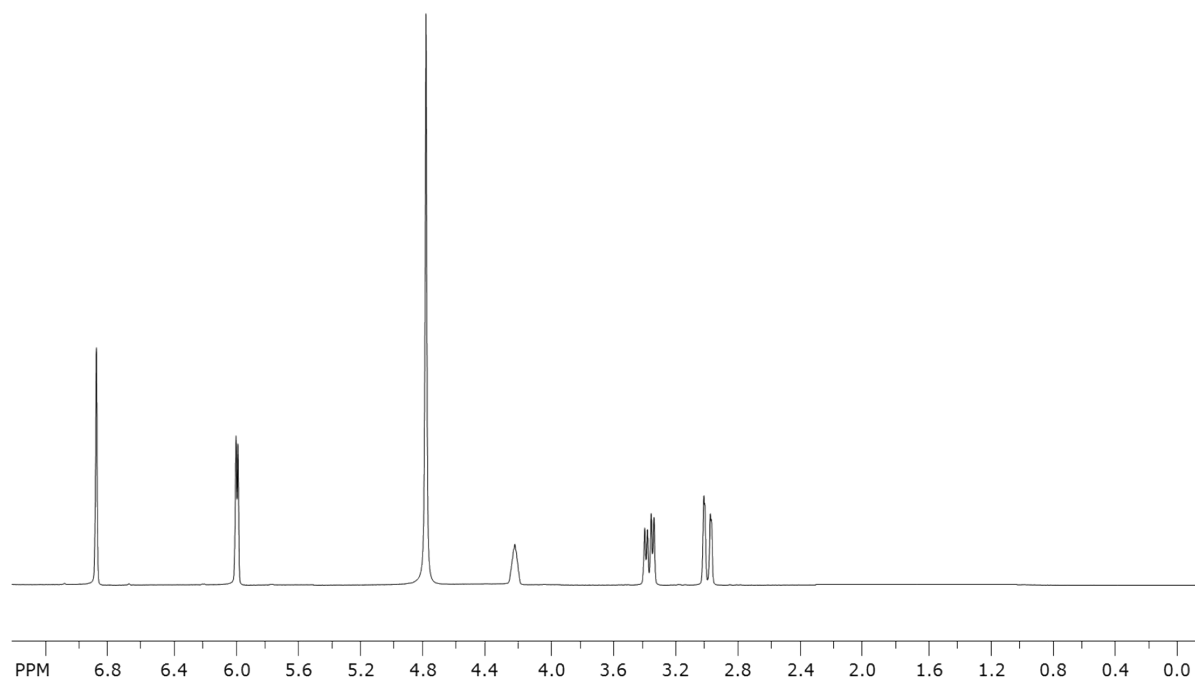
δ_{H} (CDCl₃, 400MHz) 9.67 (2H, bs) 7.59 (1H, d, J 2.4 Hz) 7.43 (1H, d, J 1.5 Hz) 7.40 (1H, d, J 8.4 Hz) 7.13 (1H, dd, J 8.5 Hz, and J 1.7 Hz) 6.68 (1H, dd, J 2.2 Hz and J 0.9 Hz) 3.66 (1H, dd, J 13.1 Hz and J 3.6 Hz) 3.36-3.46 (1H, m) 3.01-3.20 (2H, dm) 2.95 (1H, dd, J 13.0 Hz and J 10.9 Hz) 1.54 (3H, t, J 7.2 Hz) 1.35 (3H, d, J 6.5 Hz)

δ_{C} (CDCl₃, 75MHz) 154.5, 145.9, 131.3, 128.3, 125.8, 122.2, 112.0, 106.8, 56.3, 40.5, 39.8, 15.9, 12.0



NMR Data of **5,6-MDAI**

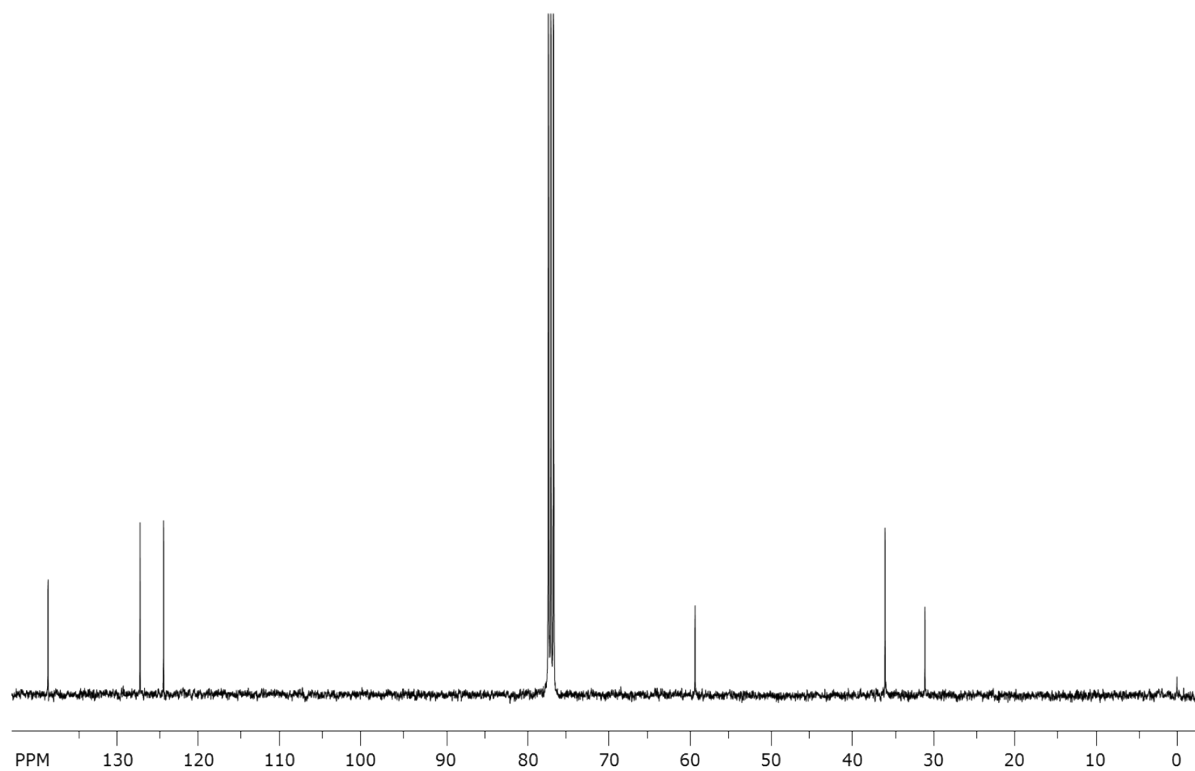
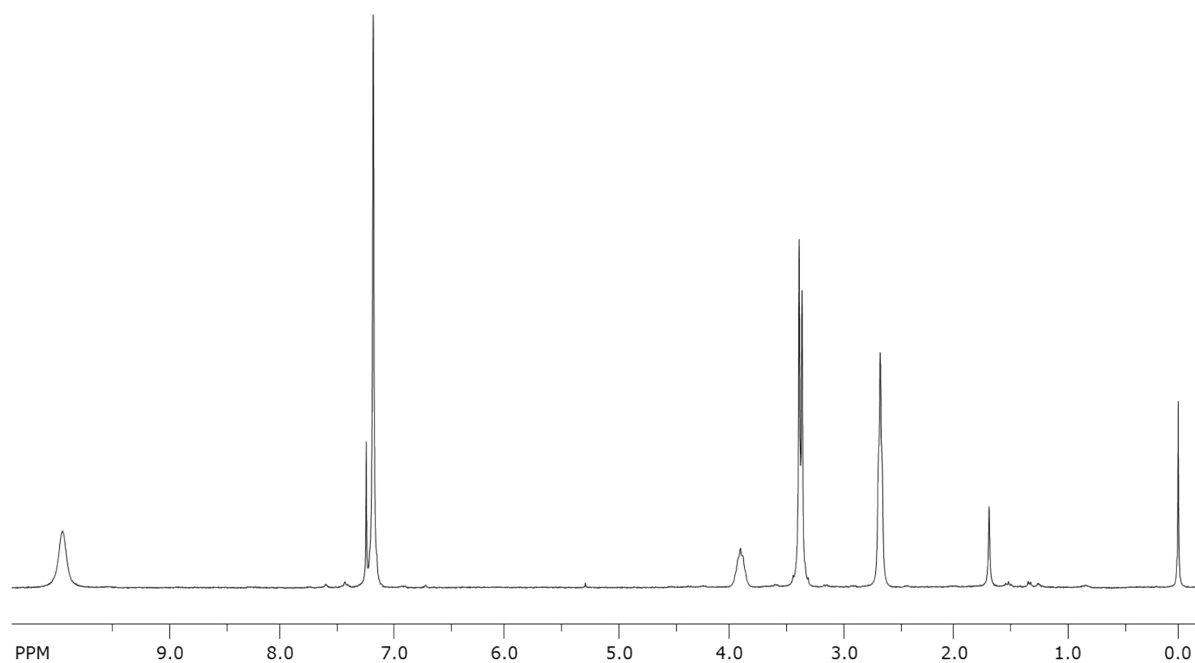
δ_{H} (D_2O , 400MHz) 6.90 (2H, s) 6.00 (2H, d, J 5.0 Hz) 4.19-4.25 (1H, m) 3.36 (2H, dd, J 16.7 Hz and J 7.1 Hz) 2.99 (2H, dd, J 16.6 Hz and J 2.9 Hz)



NMR Data of **N-Methyl-2-aminoindane**

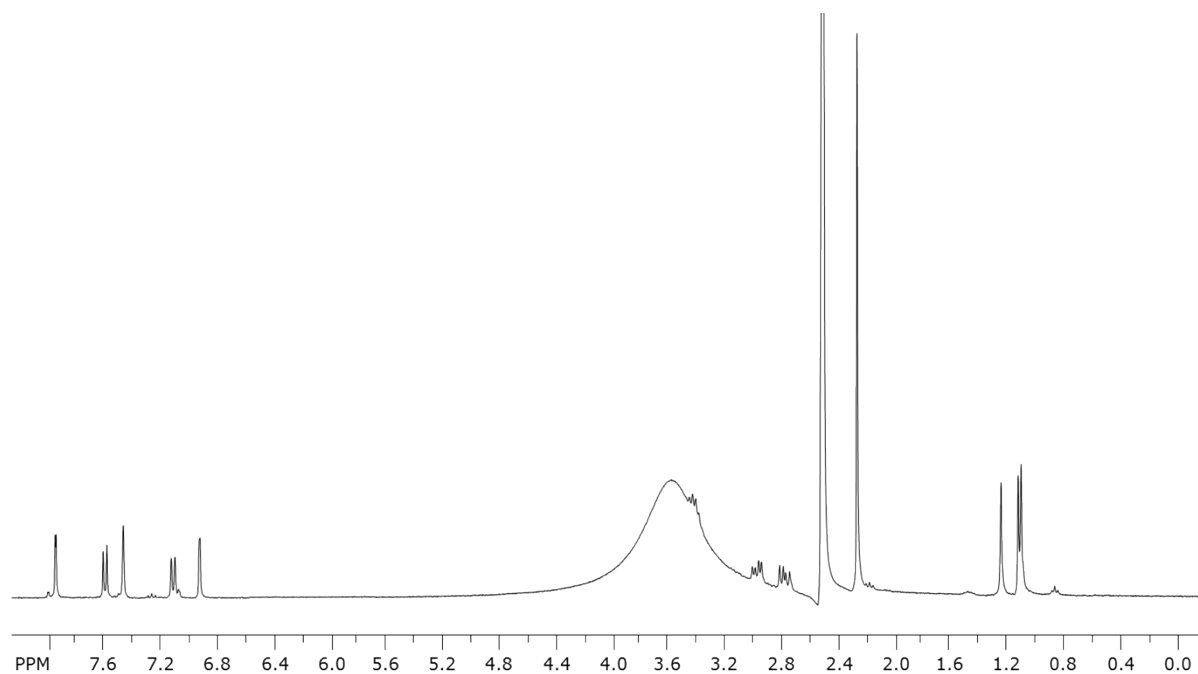
δ_{H} (CDCl_3 , 300MHz) 9.97 (2H, s) 7.20 (4H, s) 3.91 (1H, quin, J 6.5 Hz) 3.37 (4H, d, J 7.7 Hz) 2.66 (3H, t, J 4.8 Hz)

δ_{C} (CDCl_3 , 100MHz) 138.8, 127.5, 124.6, 59.2, 35.9, 31.0



NMR Data of **6-APB**

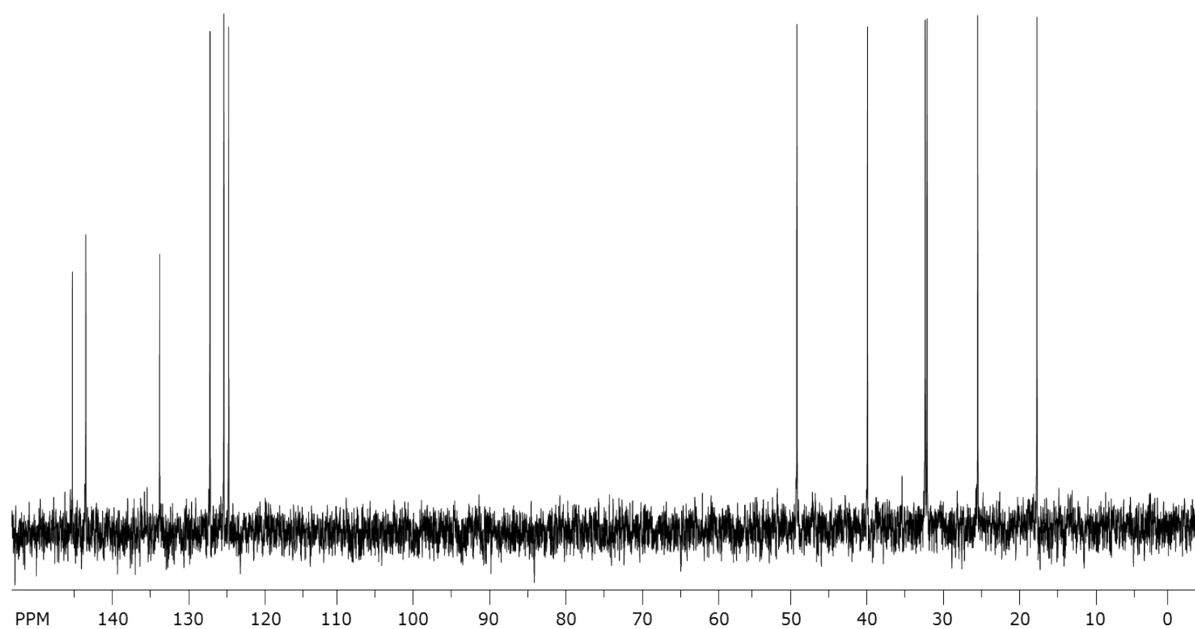
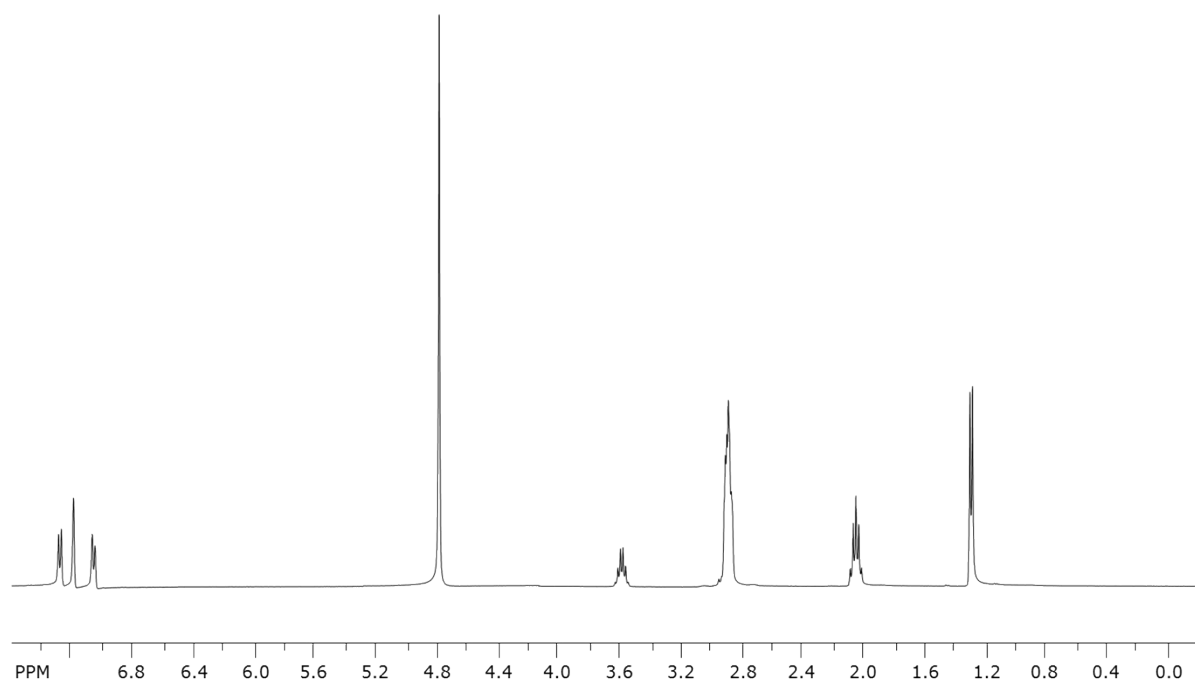
δ_{H} (DMSO- d_6 , 300MHz) 7.96 (1H, d, J 2.2 Hz) 7.61 (1H, d, J 8.0 Hz) 7.48 (1H, s) 7.13 (1H, d, J 7.7 Hz) 6.94 (1H, d, J 1.2 Hz) 3.42 (1H, q, J 6.8 Hz) 2.98 (1H, dd, J 13.3 Hz and J 6.1 Hz) 2.77 (1H, dd, J 13.5 Hz and J 8.1 Hz) 1.10 (3H, d, J 6.5 Hz)



NMR Data of **5-IAP**

δ_H (D_2O , 400MHz) 7.29 (1H, d, J 7.7 Hz) 7.20 (1H, s) 7.07 (1H, d, J 7.7 Hz) 3.59 (1H, tq, J 6.8 Hz and J 6.8 Hz) 2.85-2.92 (6H, m) 2.04 (2H, p, J 7.4 Hz) 1.28 (3H, d, J 6.5 Hz)

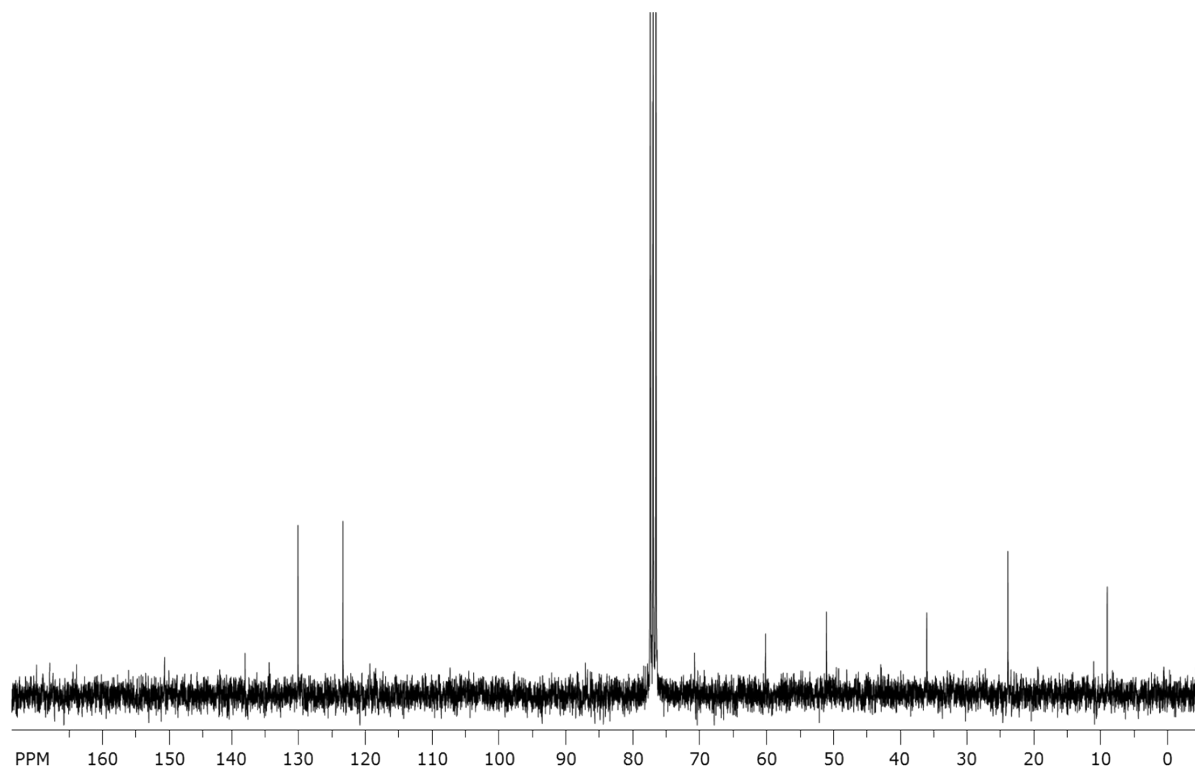
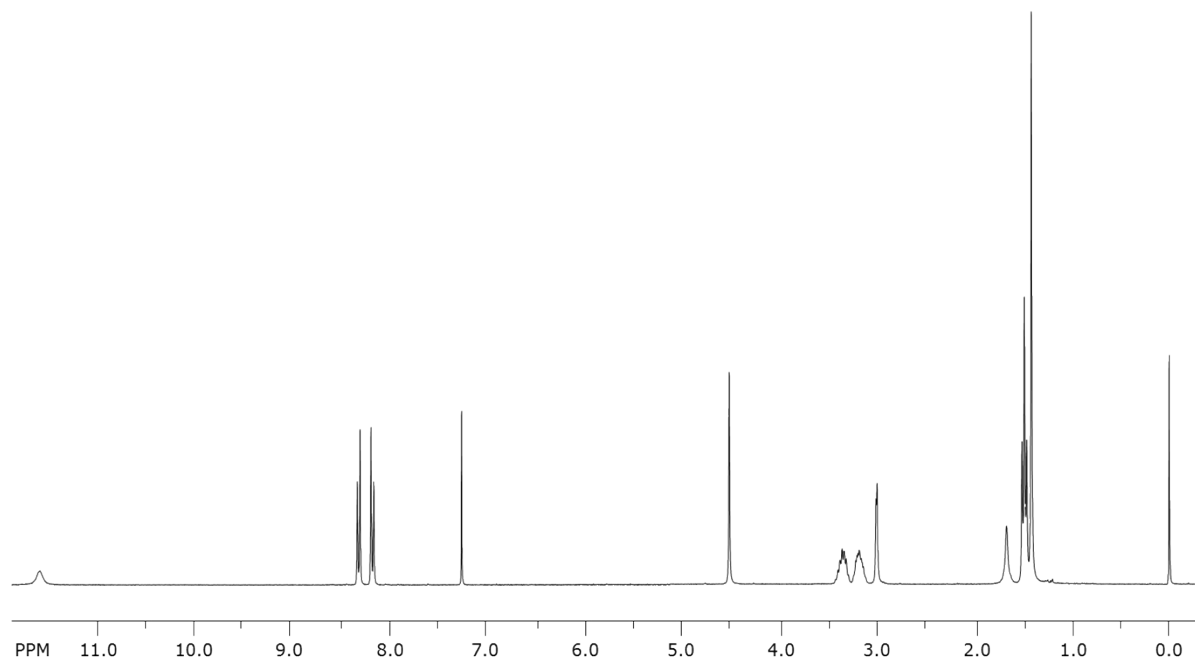
δ_C (D_2O , 100MHz) 145.6, 143.8, 133.9, 127.2, 125.4, 49.3, 39.9, 32.0, 31.9, 25.2, 17.4



NMR Data of Nitracaine

δ_H (CDCl₃, 300MHz) 11.60 (1H, s) 8.32 (2H, d, J 8.7 Hz) 8.18 (2H, d, J 8.7 Hz) 4.51 (2H, s) 3.27-3.43 (2H, m) 3.10-3.25 (2H, m) 2.98-3.01 (2H, m) 1.48 (6H, t, J 7.2 Hz) 1.41 (6H, s)

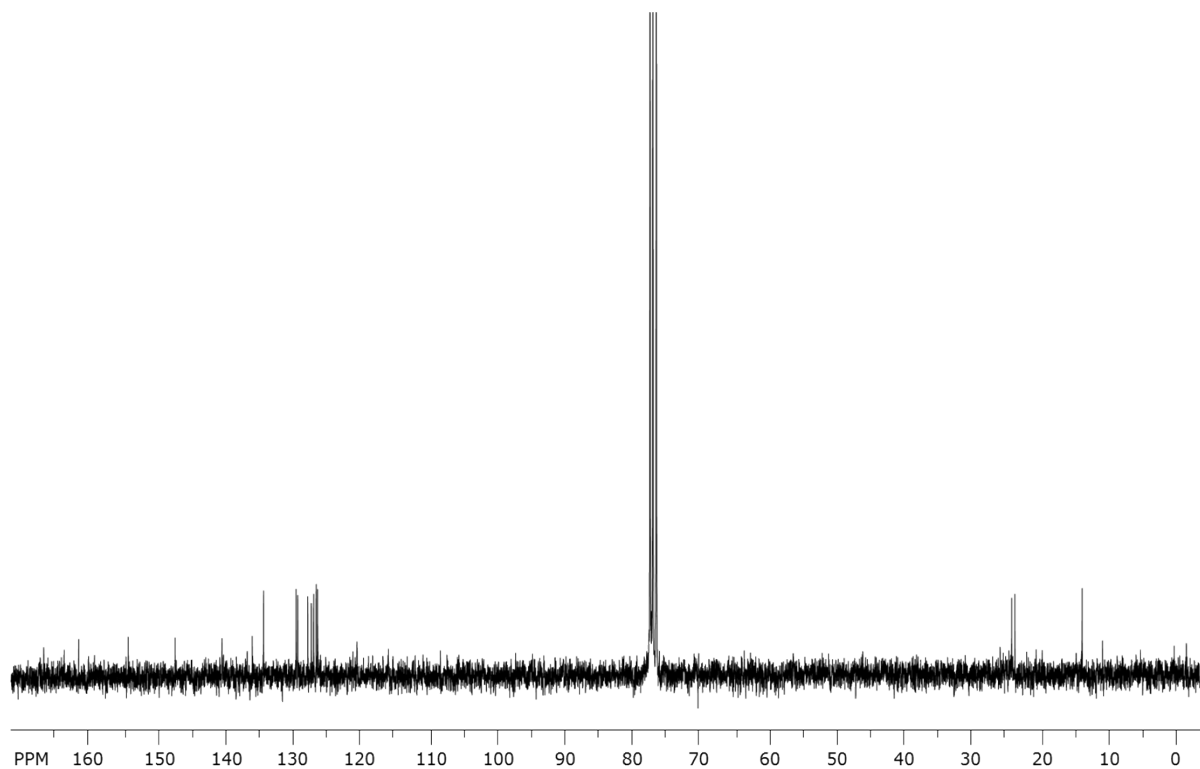
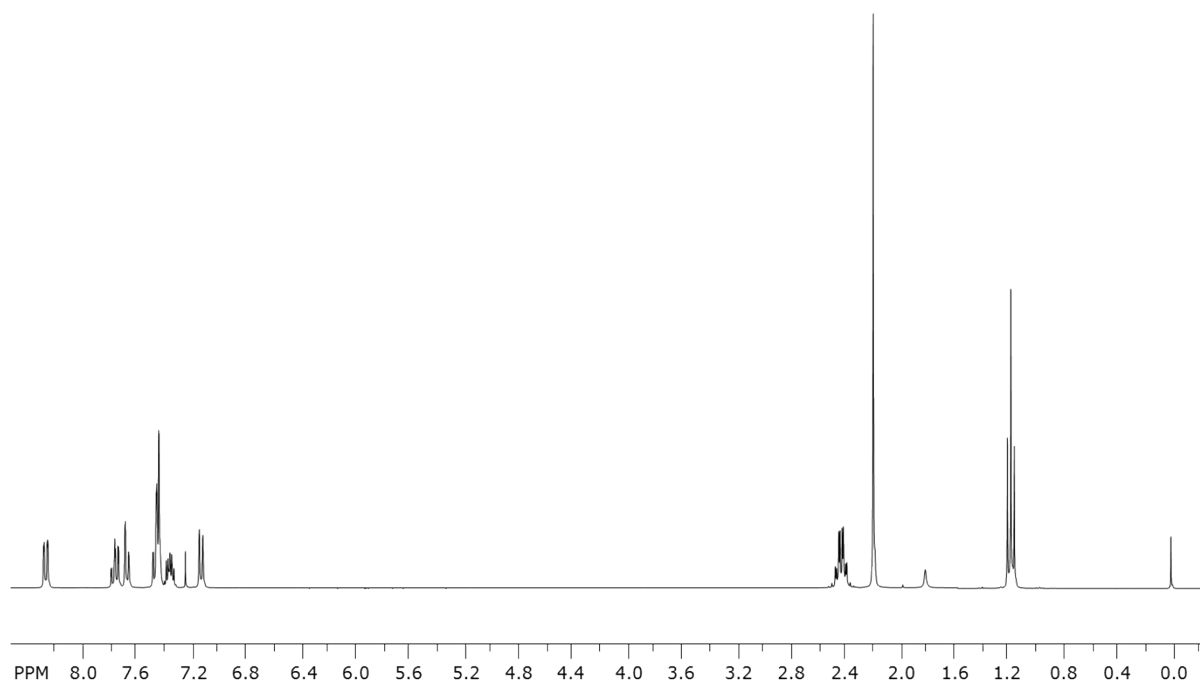
δ_C (CDCl₃, 75MHz) 164.4, 151.1, 139.1, 131.0, 124.2, 71.3, 60.6, 51.3, 36.2, 23.9, 8.9



NMR Data of **Etaqualone**

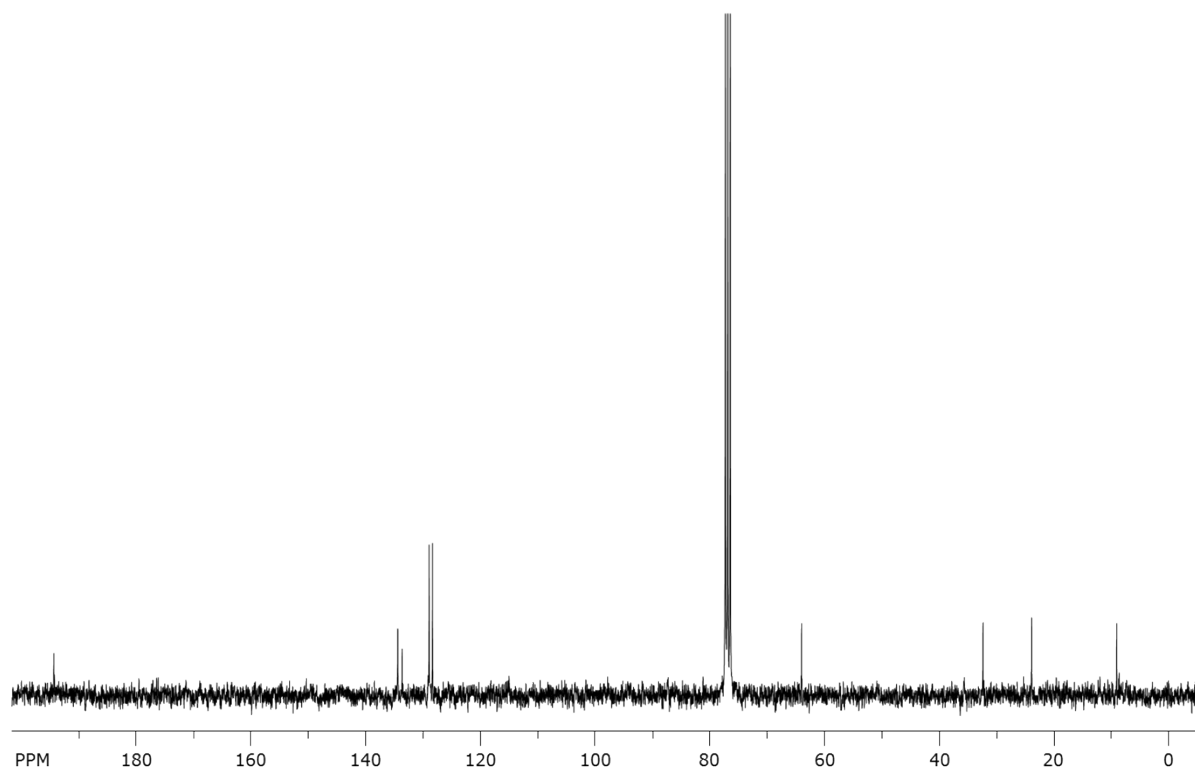
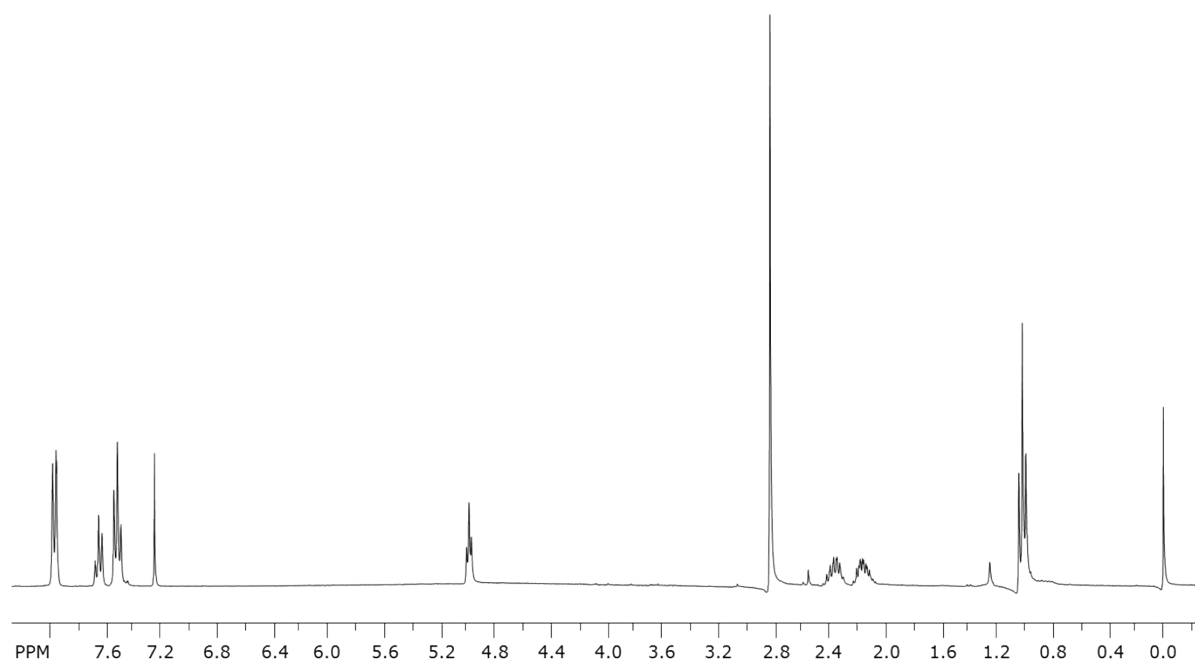
δ_{H} (CDCl_3 , 300MHz) 8.29 (1H, dd, J 8.0 Hz and J 1.3 Hz) 7.75-7.81 (1H, m) 7.69 (1H, dd, J 8.1 Hz and J 0.7 Hz) 7.44-7.51 (3H, m) 7.37-7.42 (1H, m) 7.14 (1H, d, J 7.7 Hz) 2.43 (2H, dq, J 7.6 Hz and J 2.7 Hz) 2.19 (3H, s) 1.18 (3H, t, J 7.6 Hz)

δ_{C} (CDCl_3 , 75MHz) 161.9, 154.5, 147.7, 140.7, 136.2, 134.6, 129.8, 129.5, 128.0, 127.5, 127.2, 126.8, 126.6, 120.8, 24.1, 23.6, 13.6



NMR Data of Buphedrone

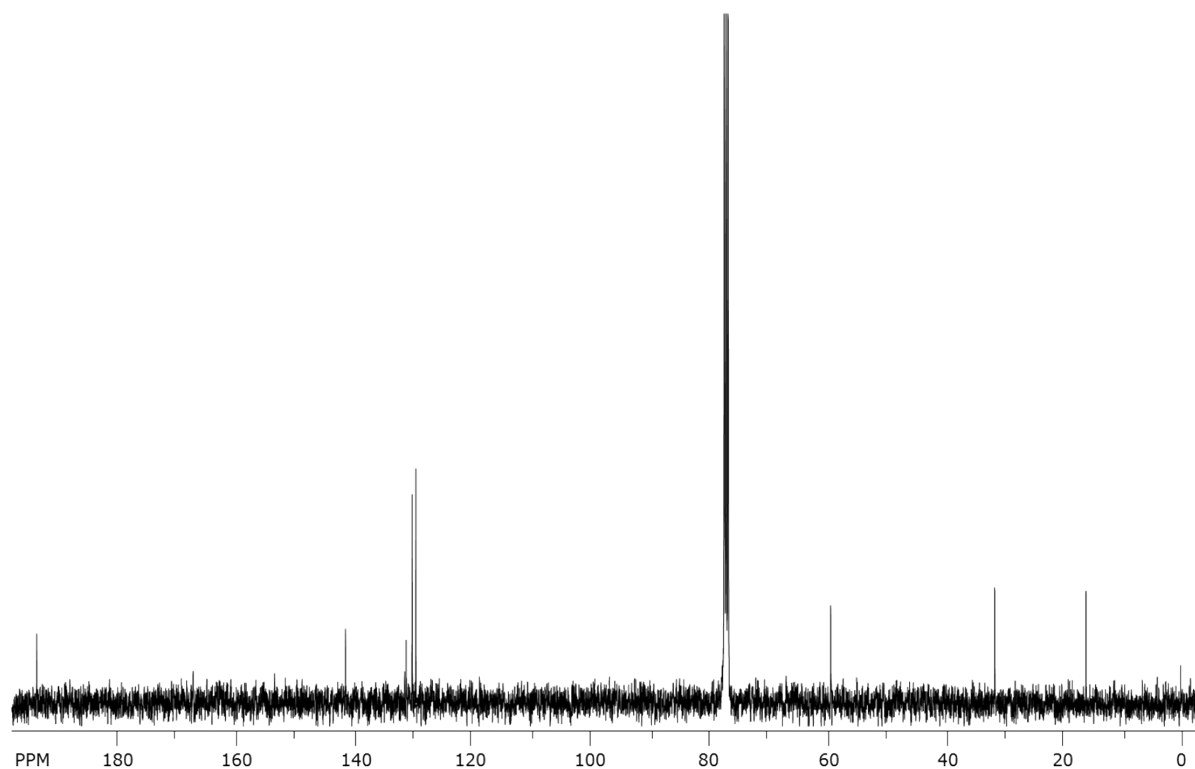
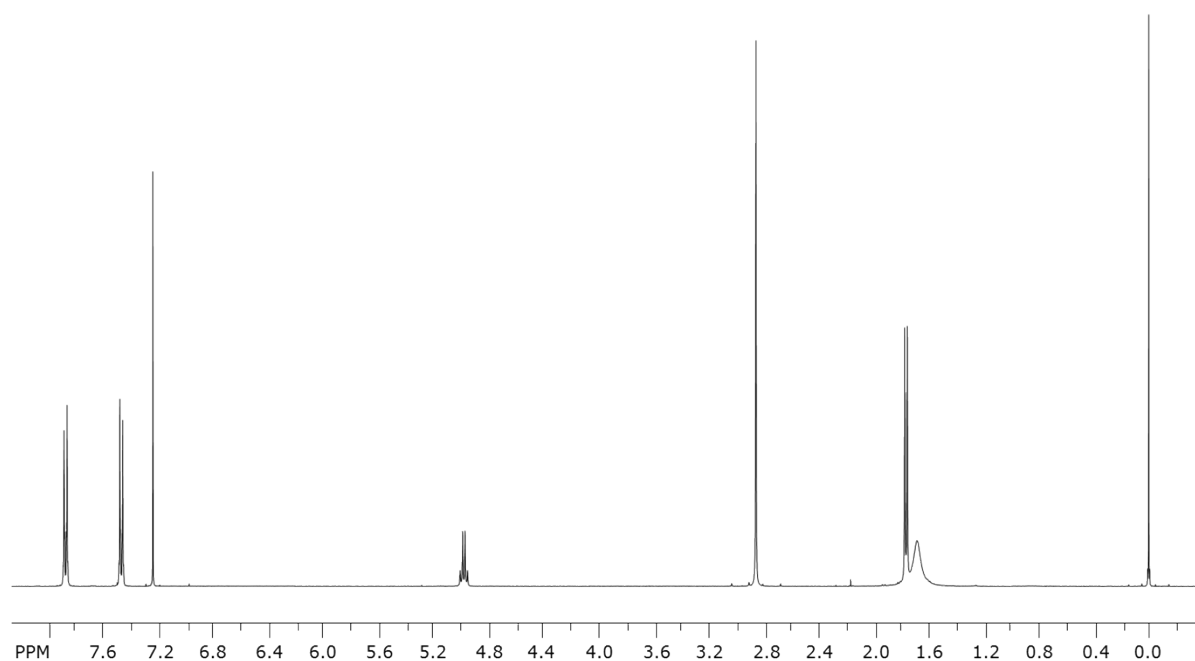
δ_H (CDCl₃, 300MHz) 7.95-8.00 (2H, m) 7.66 (1H, tt, J 7.4 Hz and J 1.4 Hz) 7.52 (2H, t, J 6.9 Hz) 4.99 (1H, t, J 5.2 Hz) 2.82 (3H, s) 2.29-2.44 (1H, m) 2.06-2.23 (1H, m) 1.01 (3H, t, J 7.6 Hz)
 δ_C (CDCl₃, 75MHz) 195.0, 134.9, 134.1, 129.4, 128.9, 64.2, 32.5, 24.0, 9.1

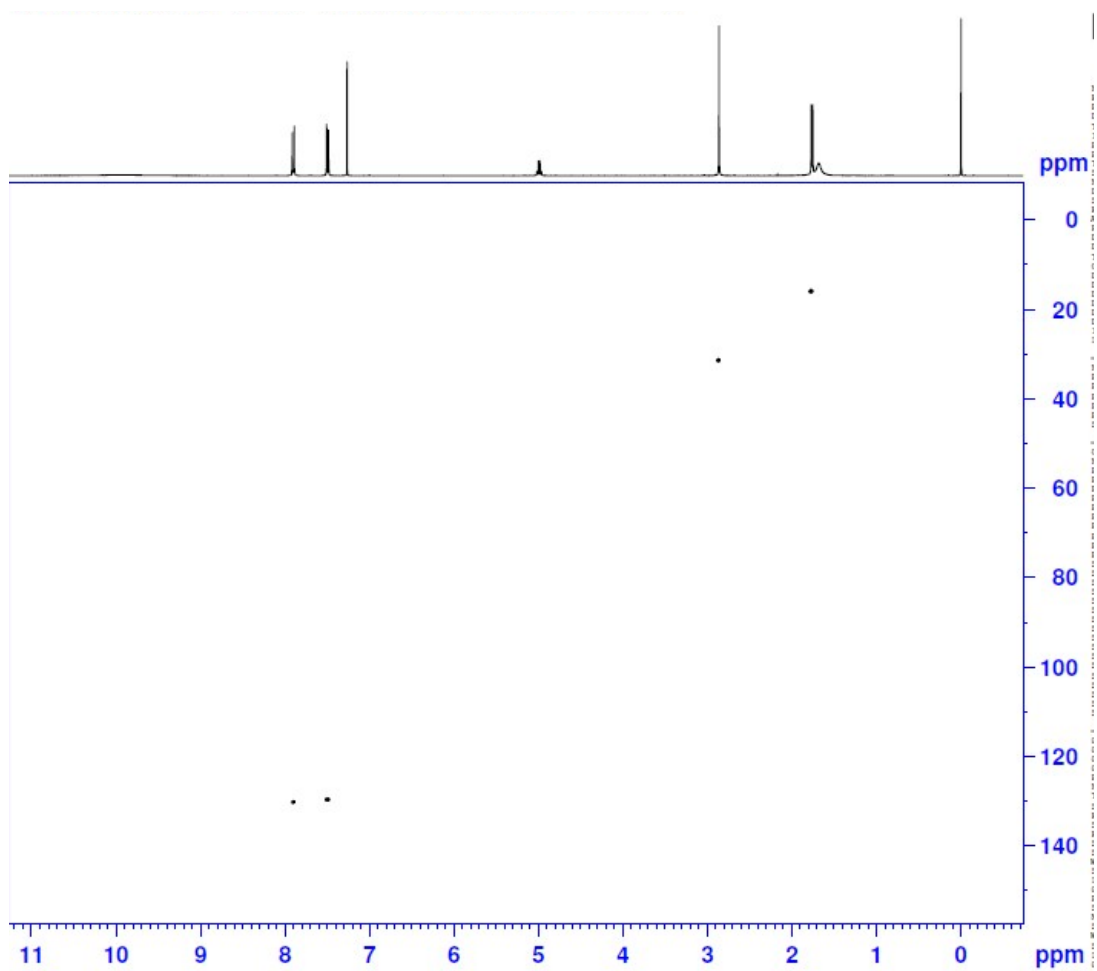
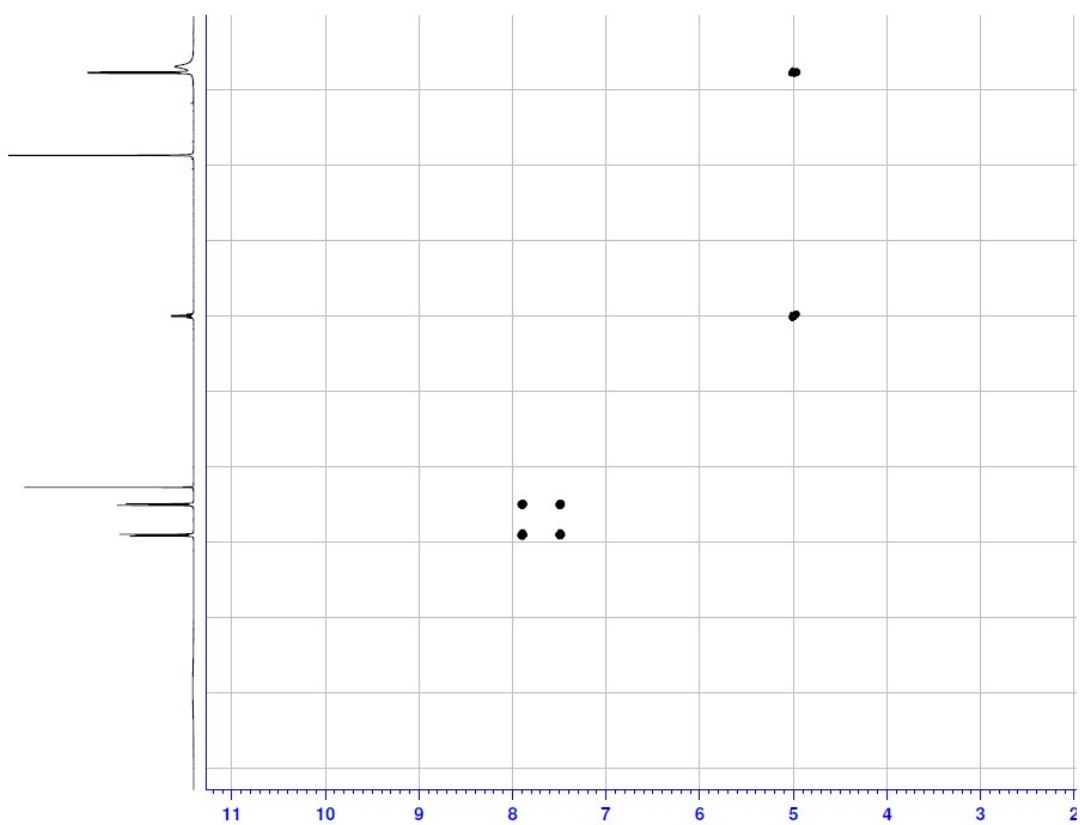


NMR Data of **4-Chloromethcathinone**

δ_{H} (CDCl_3 , 400MHz) 9.92 (2H, bs) 7.90 (2H, d, J 8.6 Hz) 7.49 (2H, d, J 8.6 Hz) 4.99 (1H, q, J 7.3 Hz) 2.86 (3H, s) 1.76 (3H, d, J 6.8 Hz)

δ_{C} (CDCl_3 , 100MHz) 193.9, 141.5, 131.3, 130.3, 129.6, 59.3, 31.5, 16.0

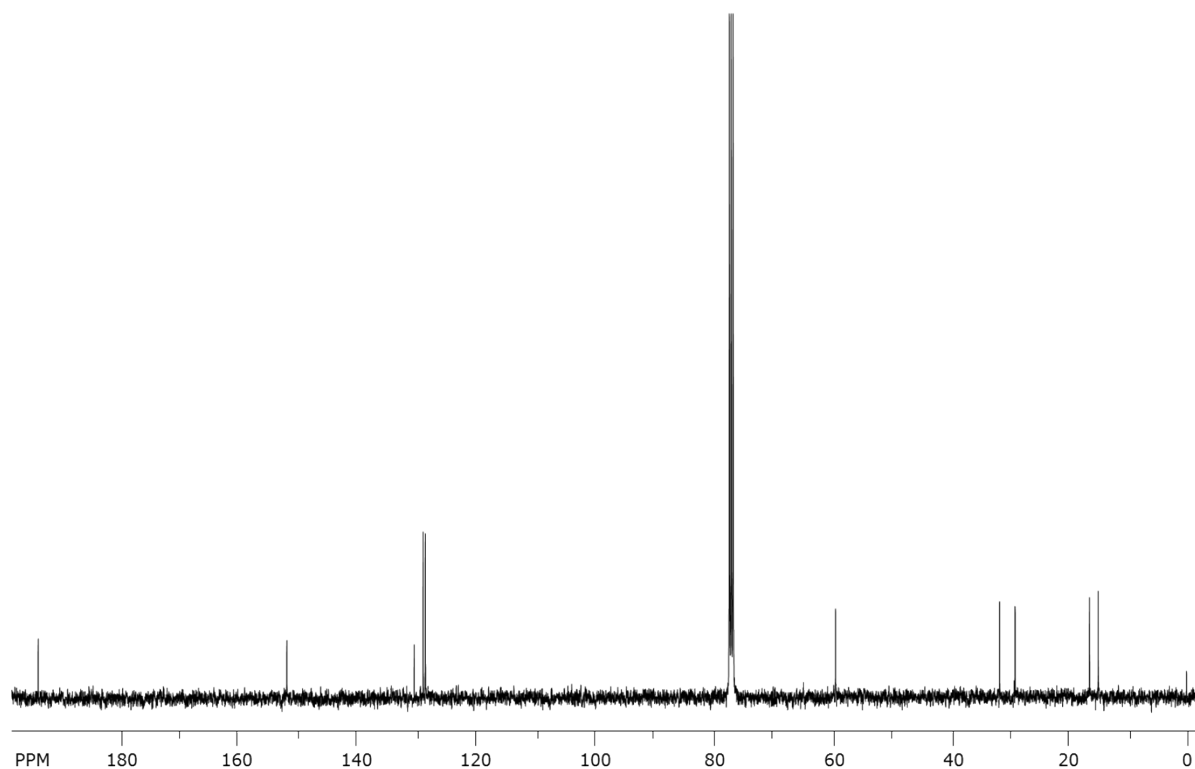
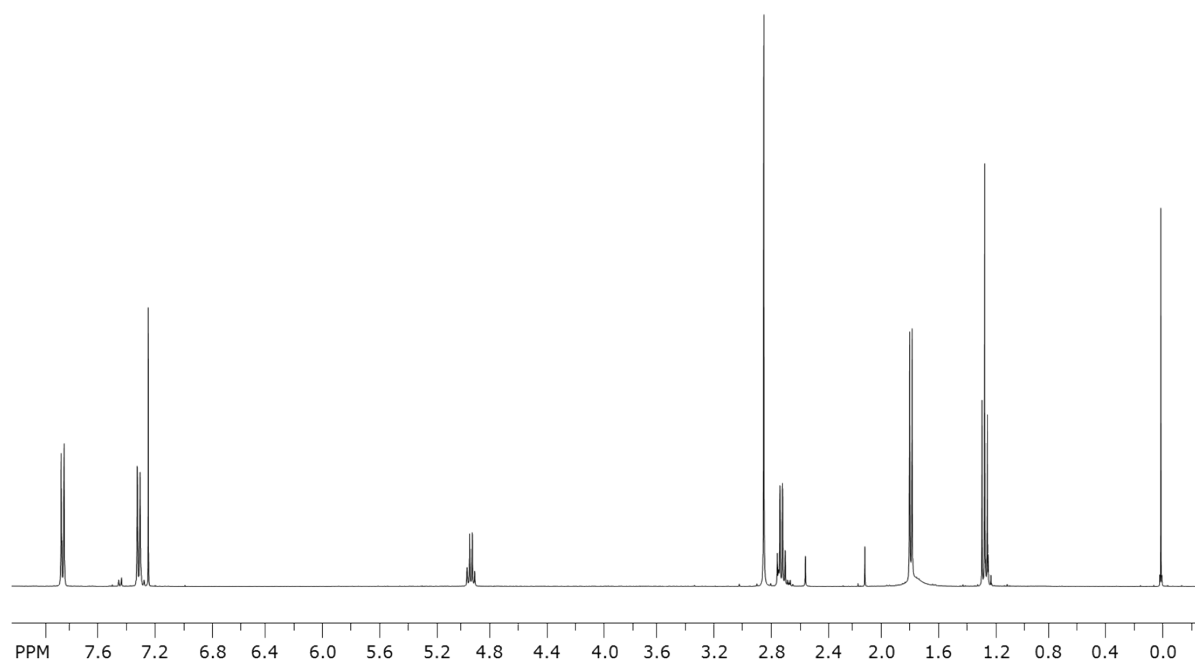


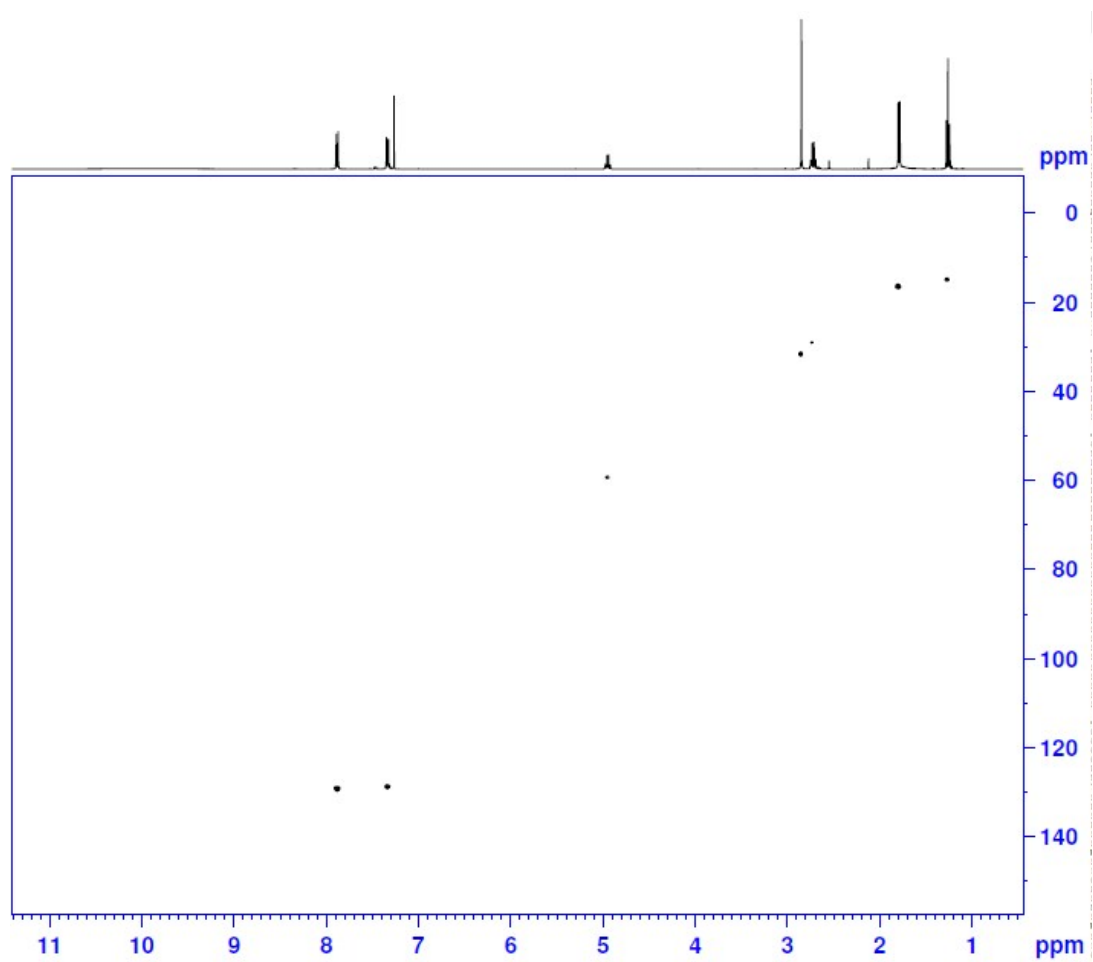
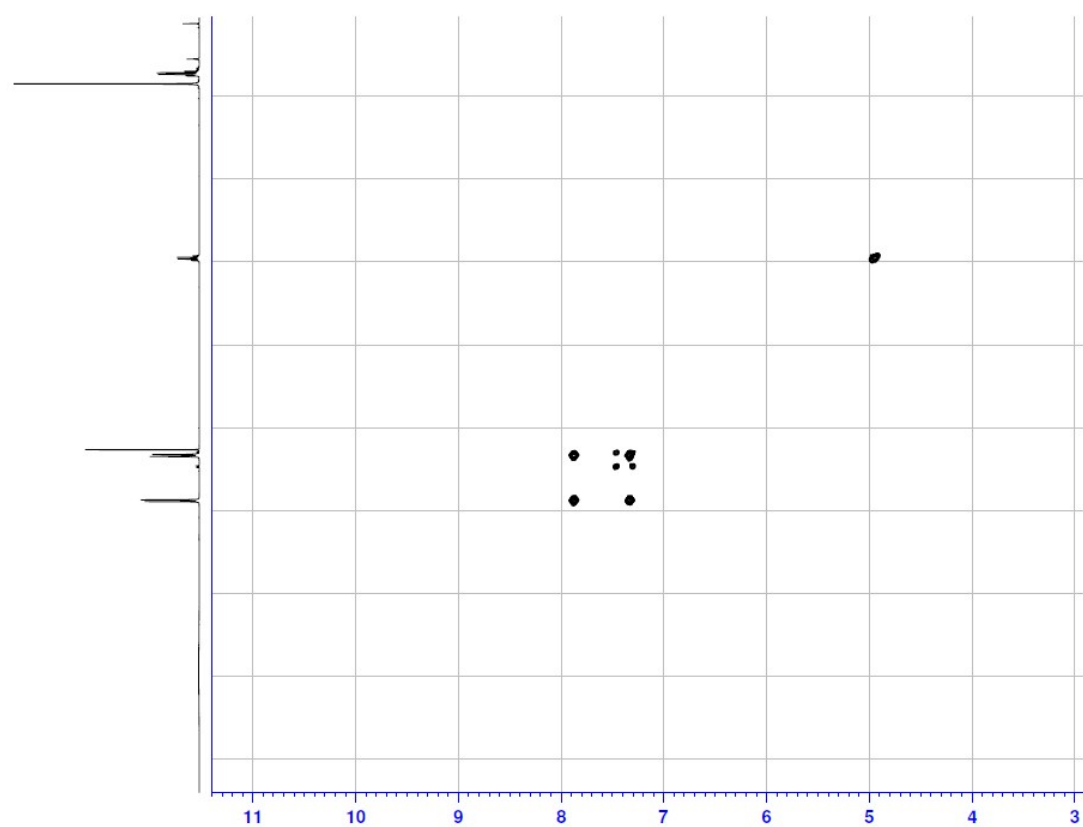


NMR Data of 4-Ethylmethcathinone

δ_{H} (CDCl₃, 400MHz) 7.87 (2H, d, J 8.4 Hz) 7.33 (2H, d, J 8.2 Hz) 4.95 (1H, q, J 7.3 Hz) 2.85 (3H, s) 2.72 (2H, q, J 7.5 Hz) 1.79 (3H, d, J 7.2 Hz) 1.26 (3H, t, J 7.6 Hz)

δ_{C} (CDCl₃, 100MHz) 194.3, 152.2, 130.6, 129.1, 128.7, 59.3, 31.7, 29.1, 16.5, 15.0



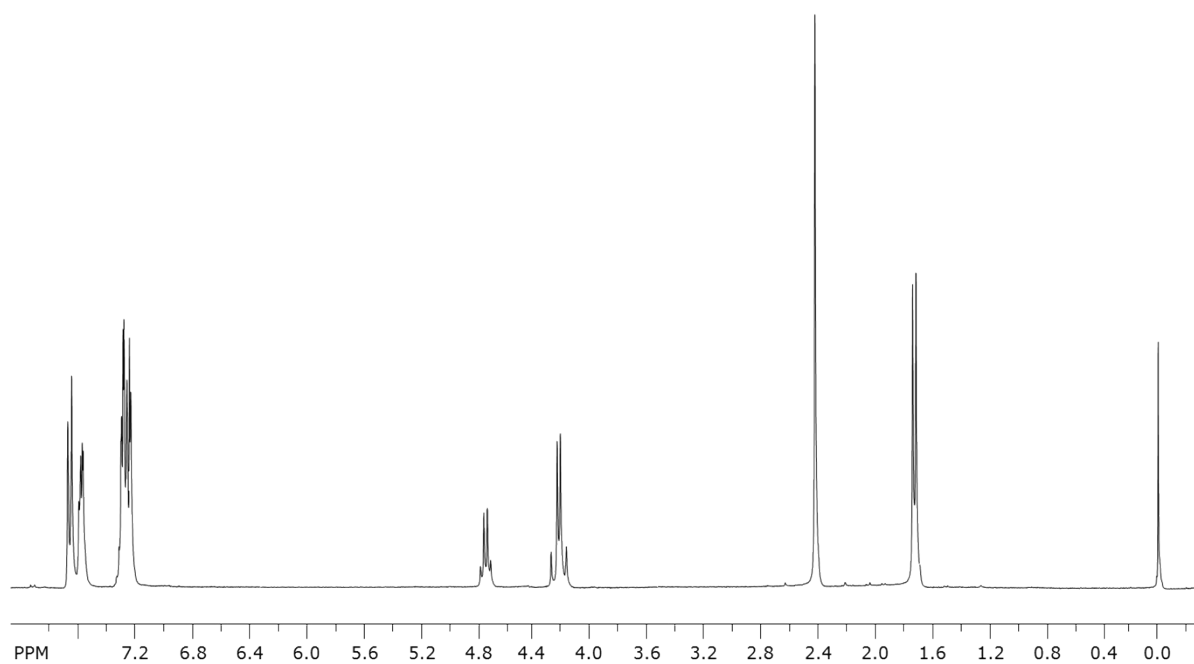
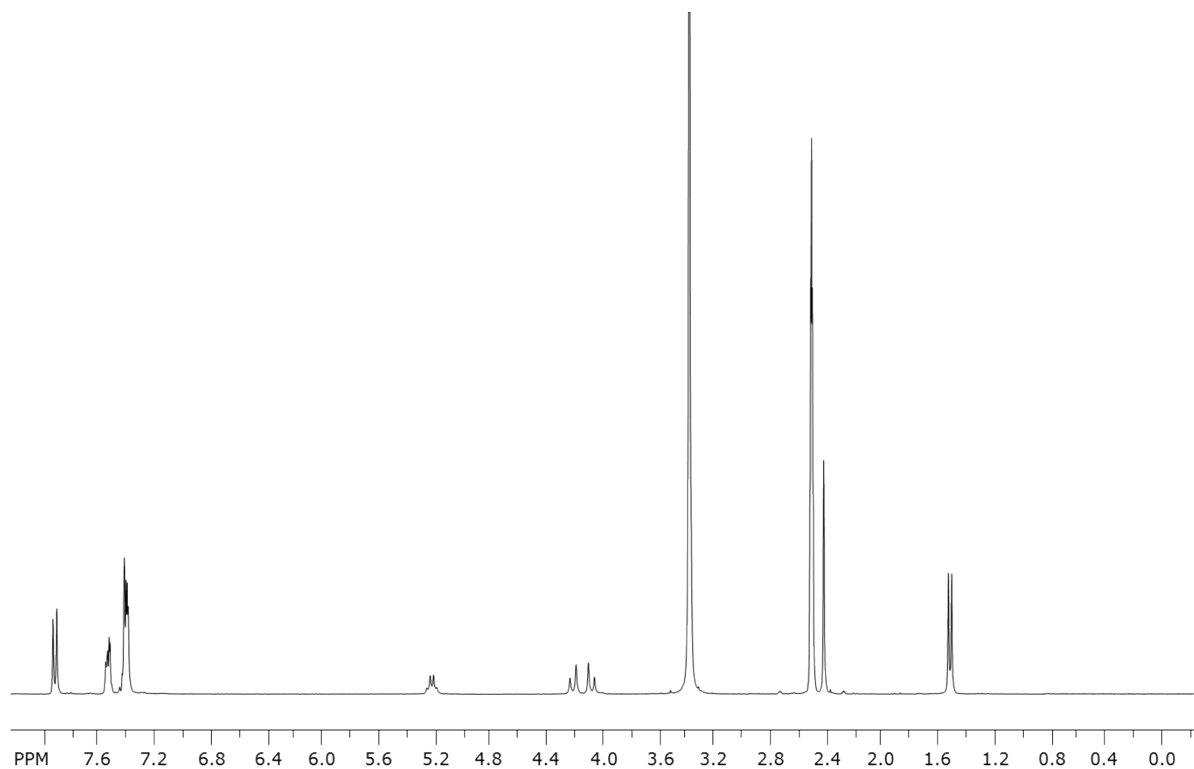


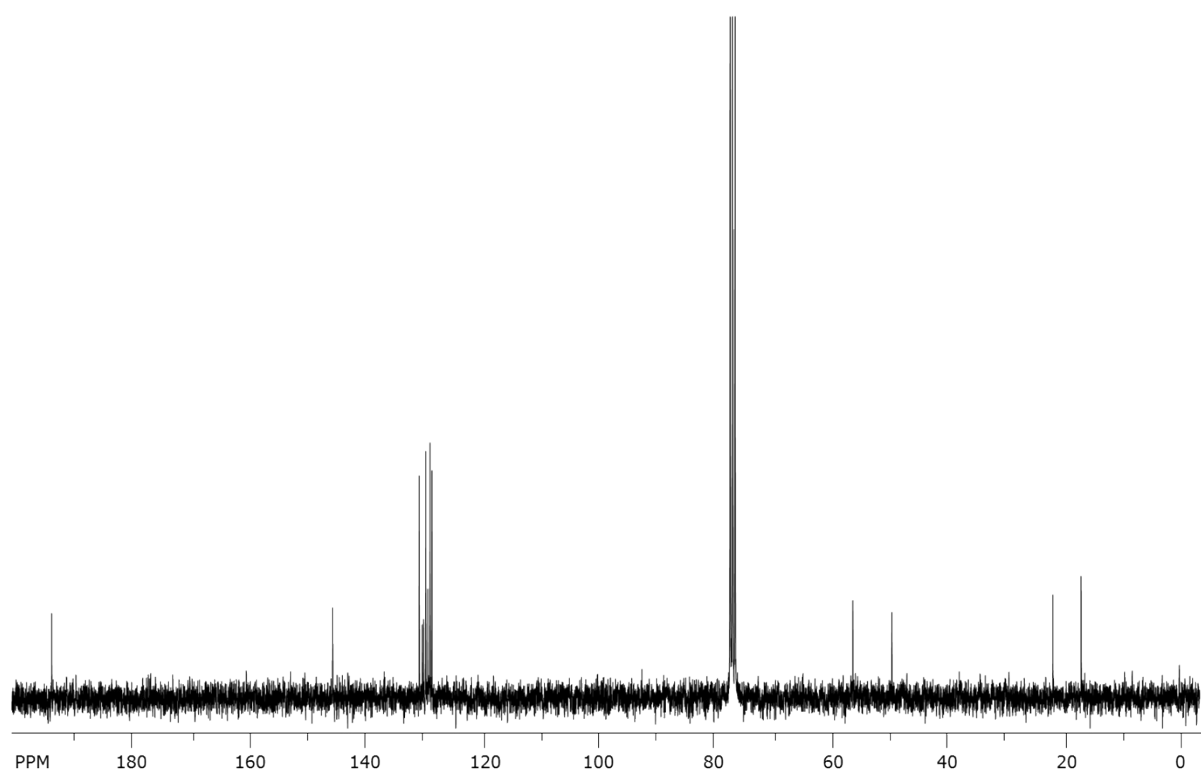
NMR Data of **4-Methylbenzylcathinone**

δ_{H} (DMSO- d_6 , 300MHz) 7.88 (2H, d, J 8.2 Hz) 7.48-7.53 (2H, m) 7.35-7.40 (5H, m) 5.18 (1H, q, J 7.0 Hz) 4.17 (1H, d, J 13.1 Hz) 4.03 (1H, d, J 12.9 Hz) 2.37 (3H, s) 1.46 (3H, d, J 7.2 Hz)

δ_{H} (CDCl_3 , 300MHz) 7.68 (2H, d, J 8.2 Hz) 7.57-7.62 (2H, m) 7.23-7.34 (5H, m) 4.74 (1H, q, J 7.2 Hz) 4.26 (1H, d, J 13.0 Hz) 4.19 (1H, d, J 12.9 Hz) 2.42 (3H, s) 1.71 (3H, d, J 7.2 Hz)

δ_{C} (CDCl_3 , 75MHz) 194.5, 146.1, 131.1, 130.6, 130.4, 130.0, 129.6, 129.2, 128.9, 56.5, 49.7, 22.0, 17.0

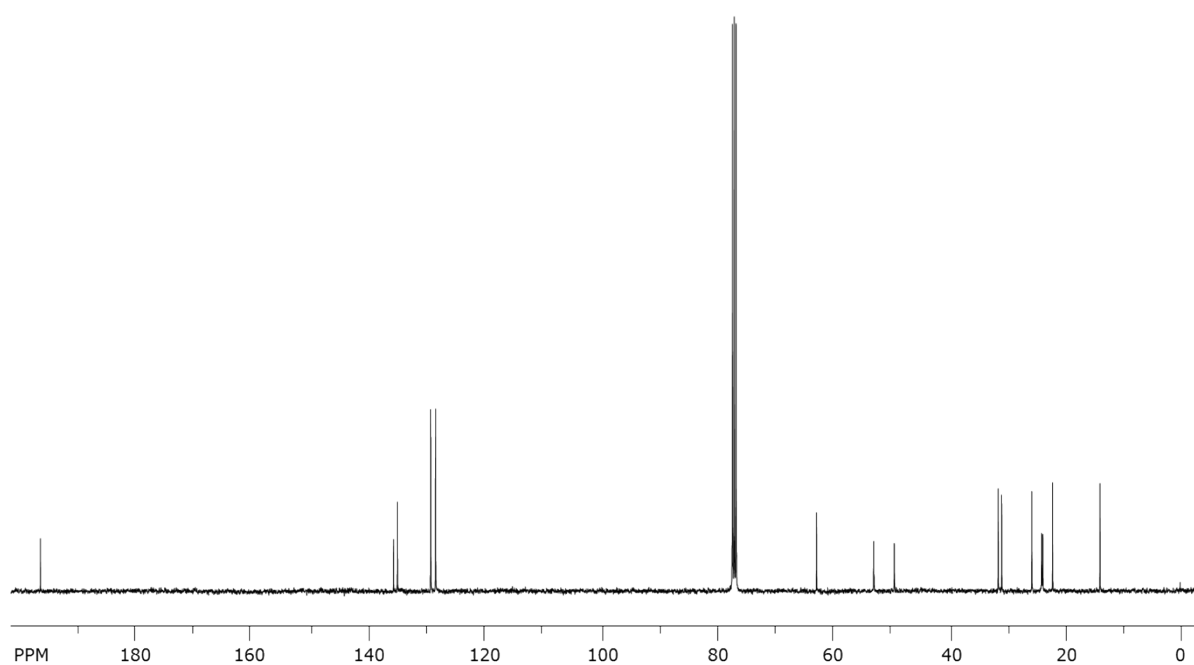
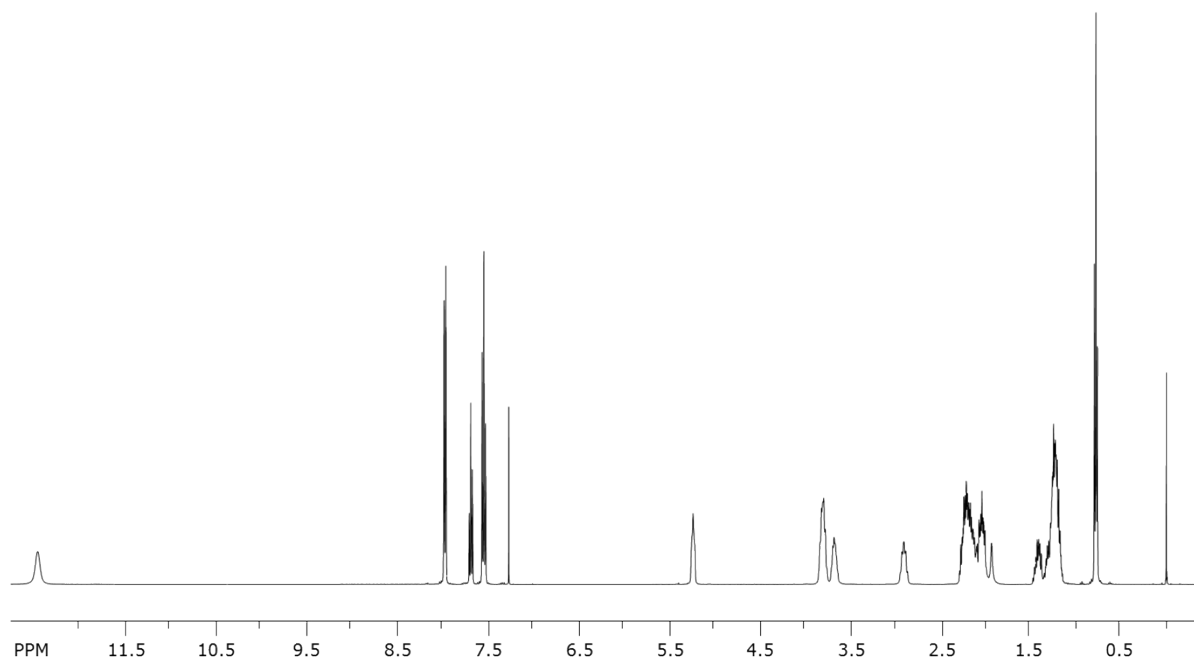


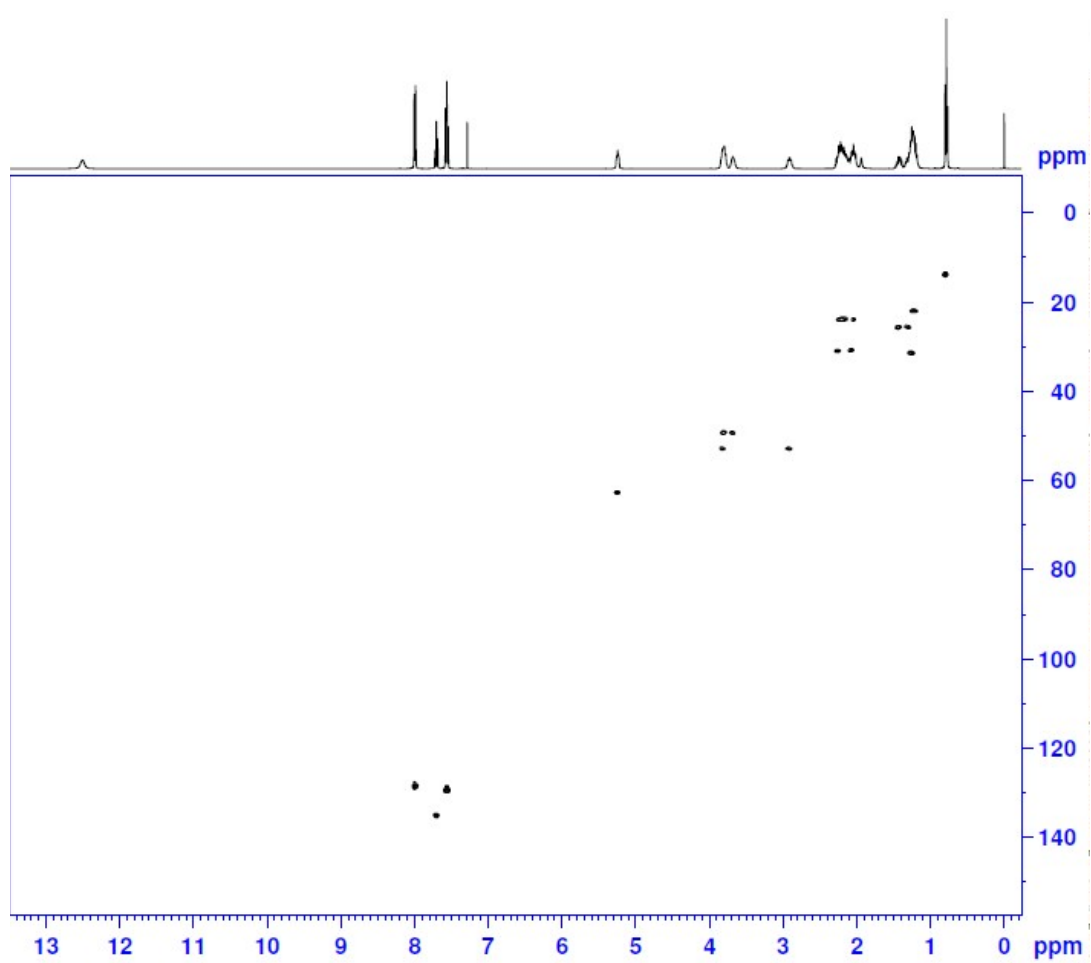
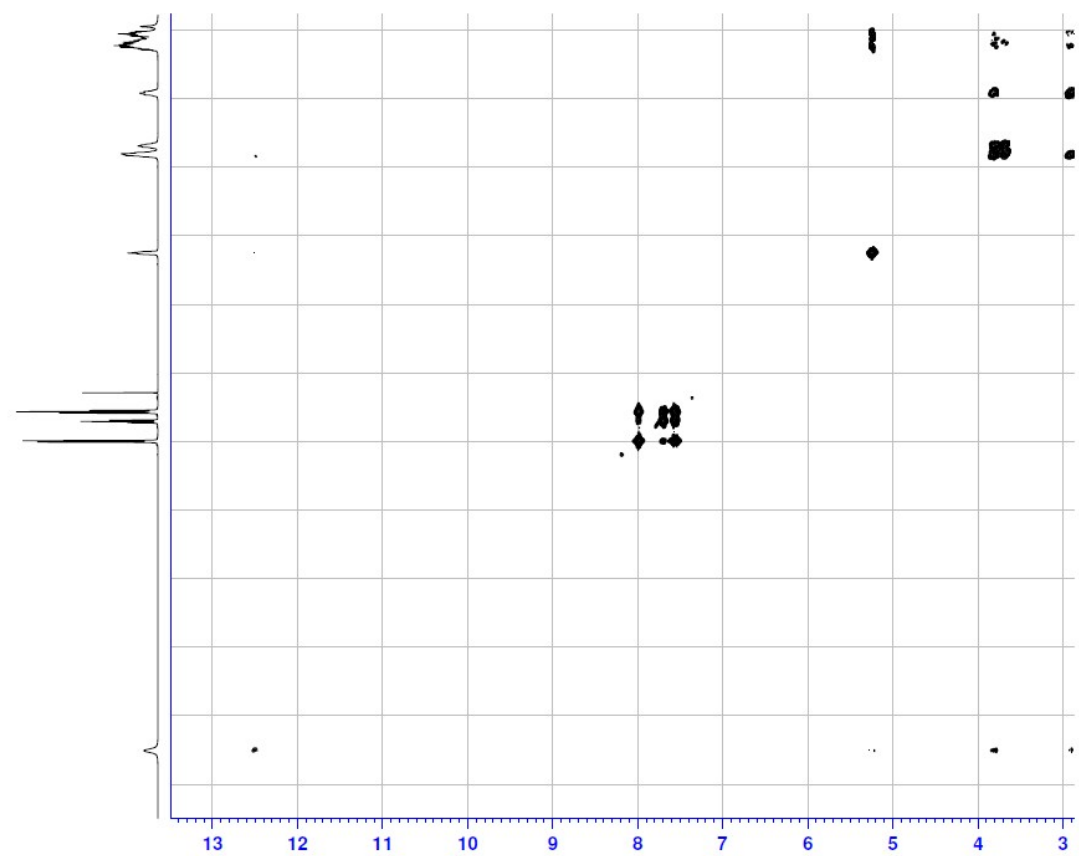


NMR Data of **PV8**

δ_{H} (CDCl_3 , 400MHz) 12.5 (1H, bs) 7.95-7.98 (2H, m) 7.68 (1H, tt, J 7.4 Hz and J 1.3 Hz) 7.53 (2H, t, J 7.8 Hz) 5.19-5.25 (1H, m) 3.73-3.83 (2H, m) 3.61-3.70 (1H, m) 2.84-2.93 (1H, m) 1.98-2.27 (6H, m) 1.35-1.46 (1H, m) 1.13-1.34 (5H, m) 0.76 (3H, t, J 7.1 Hz)

δ_{C} (CDCl_3 , 100MHz) 196.8, 135.8, 135.2, 129.4, 128.6, 62.7, 52.9, 49.3, 31.4, 30.9, 25.6, 24.0, 23.7, 22.0, 13.8

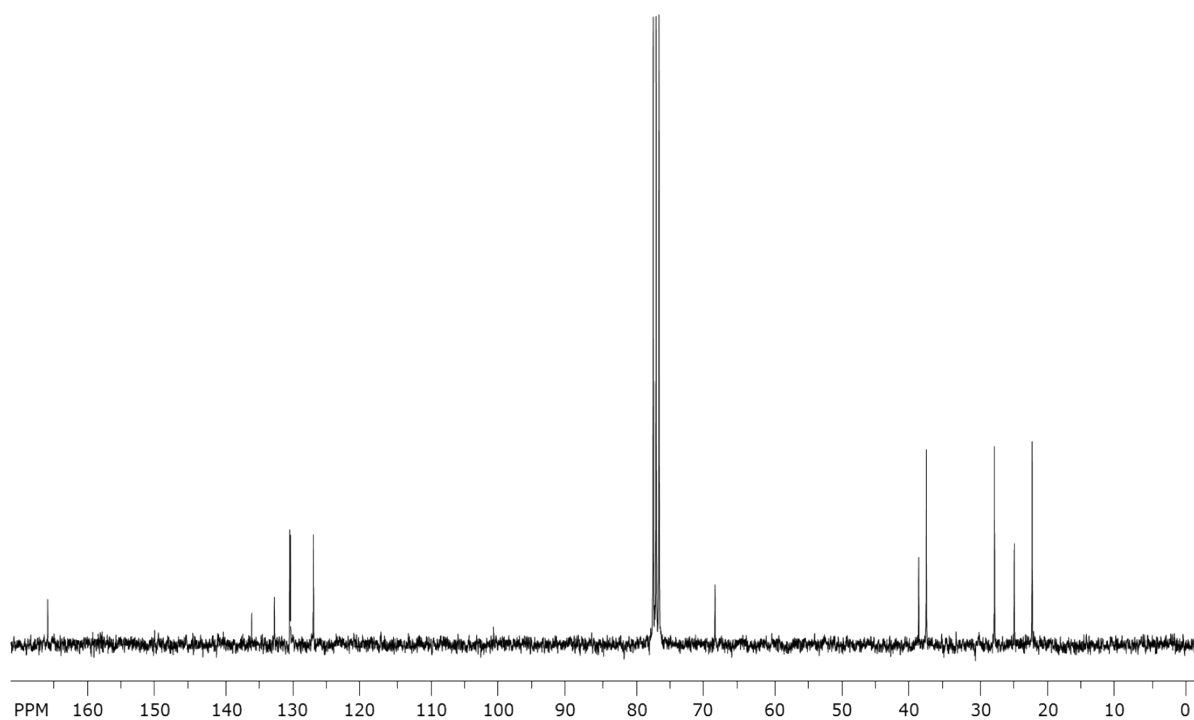
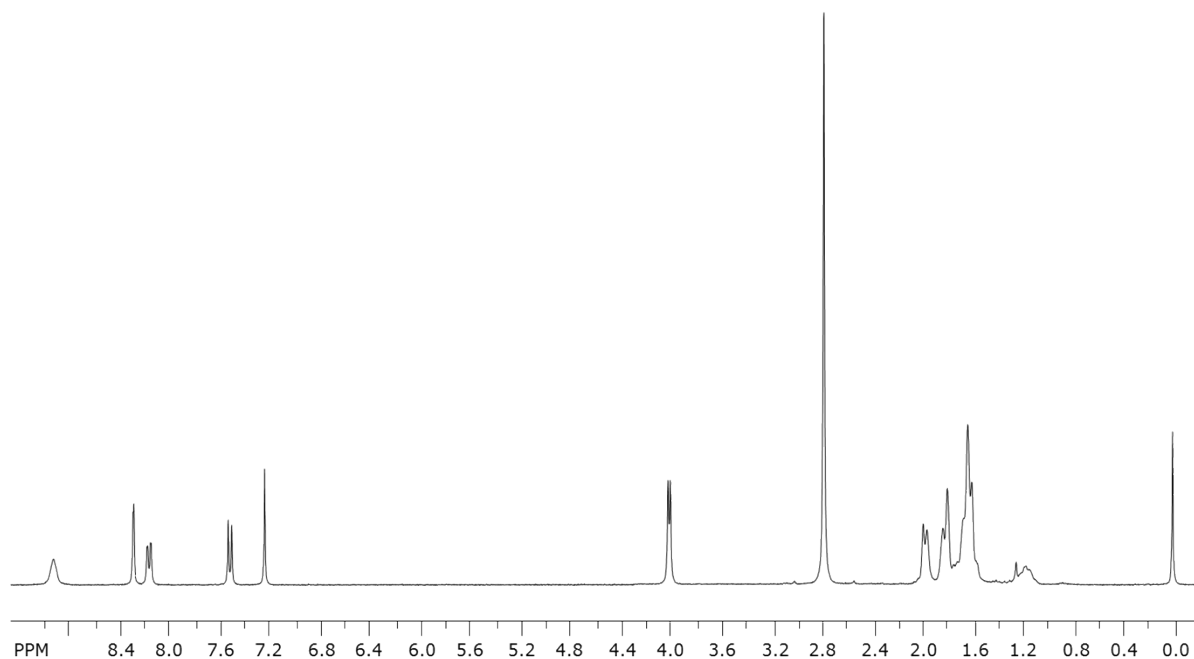




NMR Data of **AH-7921**

δ_{H} (CDCl₃, 300MHz) 8.95 (1H, s) 8.31 (1H, d, J 1.8 Hz) 8.18 (1H, dd, J 8.5 Hz and J 1.8 Hz) 7.54 (1H, d, J 8.4 Hz) 4.02 (2H, d, J 5.6 Hz) 2.79 (6H, s) 1.97 (2H, d, J 8.9 Hz) 1.77-1.86 (3H, m) 1.59-1.70 (4H, m) 1.10-1.25 (1H, m)

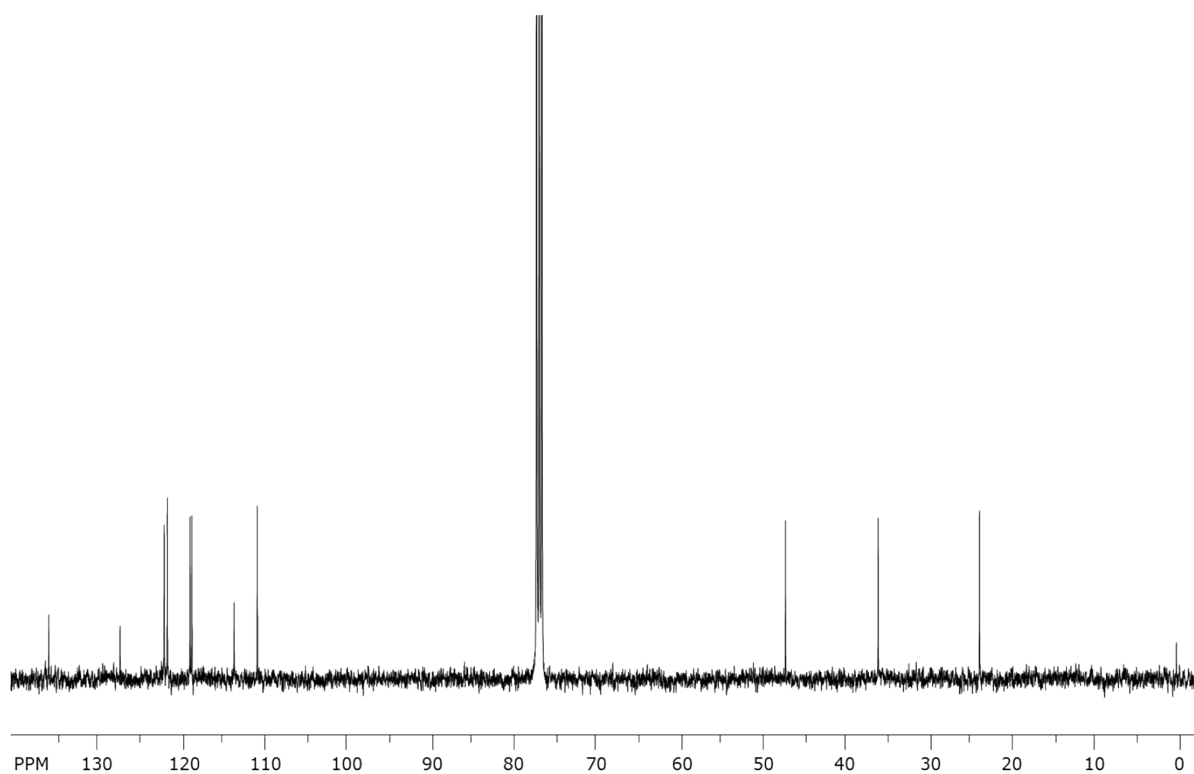
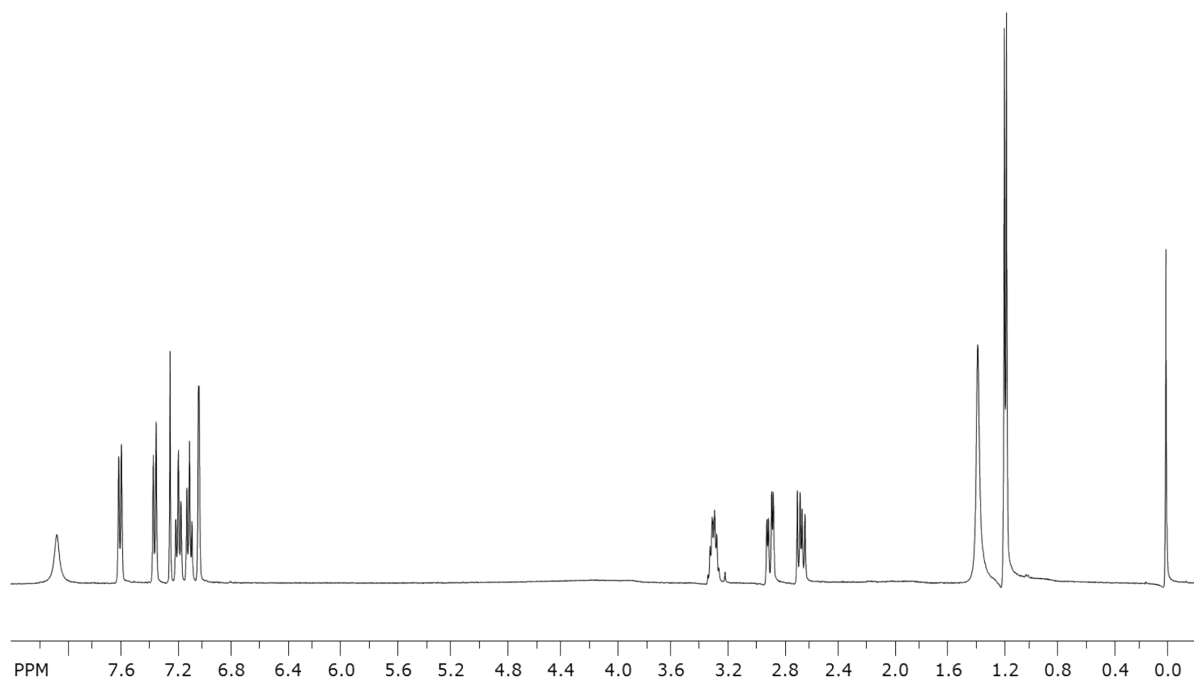
δ_{C} (CDCl₃, 75MHz) 166.5, 136.6, 133.3, 131.0, 130.9, 127.6, 68.9, 39.0, 37.9, 28.0, 25.1, 22.4



NMR Data of α -Methtryptamine

δ_H (CDCl₃, 400MHz) 8.08 (1H, bs) 7.62 (1H, d, J 8.0 Hz) 7.37 (1H, d, J 8.1 Hz) 7.20 (1H, dt, J 7.6 Hz and J 1.0 Hz) 7.12 (1H, dt, J 7.5 Hz and J 0.9 Hz) 7.05 (1H, s) 3.26-3.35 (1H, m) 2.89 (1H, dd, J 14.1 Hz and J 5.0 Hz) 2.66 (1H, dd, J 14.1 Hz and J 8.3 Hz) 1.38 (2H, s) 1.18 (3H, d, J 6.3 Hz)

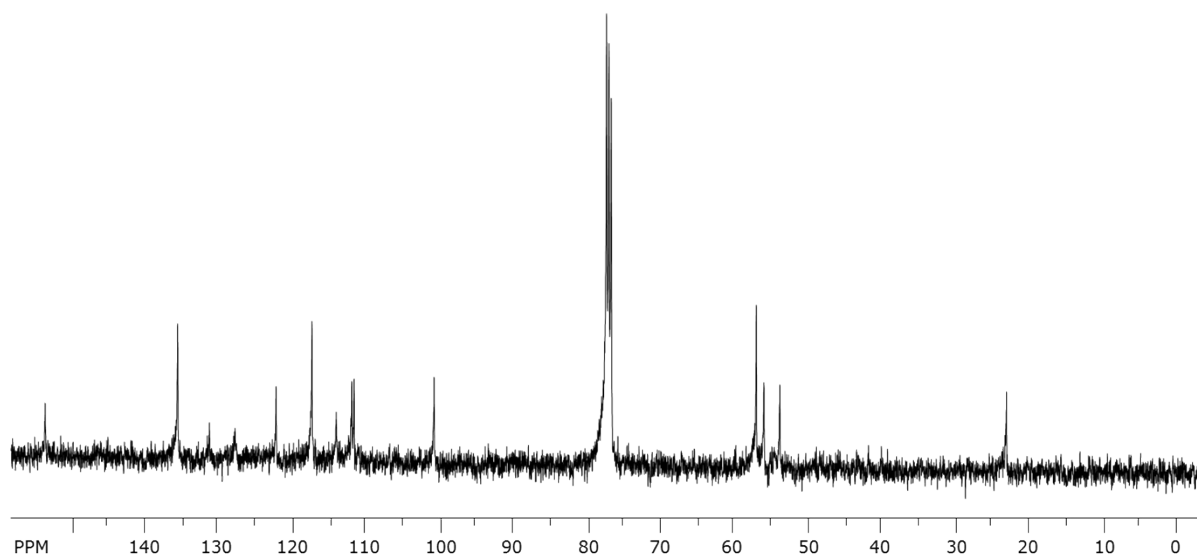
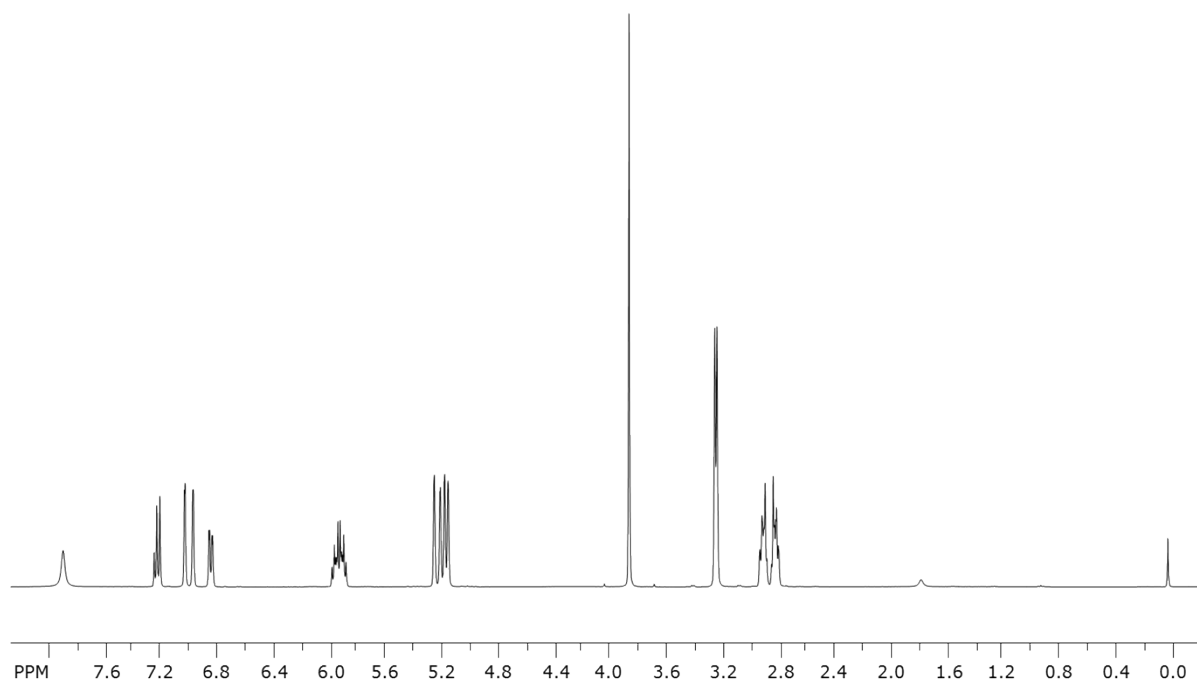
δ_C (CDCl₃, 100MHz) 136.4, 127.8, 122.4, 122.0, 119.3, 119.1, 113.9, 111.1, 47.3, 36.1, 23.8



NMR Data of **5-MeO-DALT**

δ_{H} (CDCl_3 , 400MHz) 7.91 (1H, bs) 7.23 (1H, d, J 8.7 Hz) 7.04 (1H, d, J 1.9 Hz) 6.98 (1H, d, J 1.7 Hz) 6.85 (1H, dd, J 8.8 Hz and J 2.2 Hz) 5.88-6.00 (2H, m) 5.24 (2H, dd, J 17.1 Hz and J 1.3 Hz) 5.17 (2H, dd, J 10.2 Hz and J 0.8 Hz) 3.87 (3H, s) 3.24 (4H, d, J 6.5 Hz) 2.78-2.94 (4H, m)

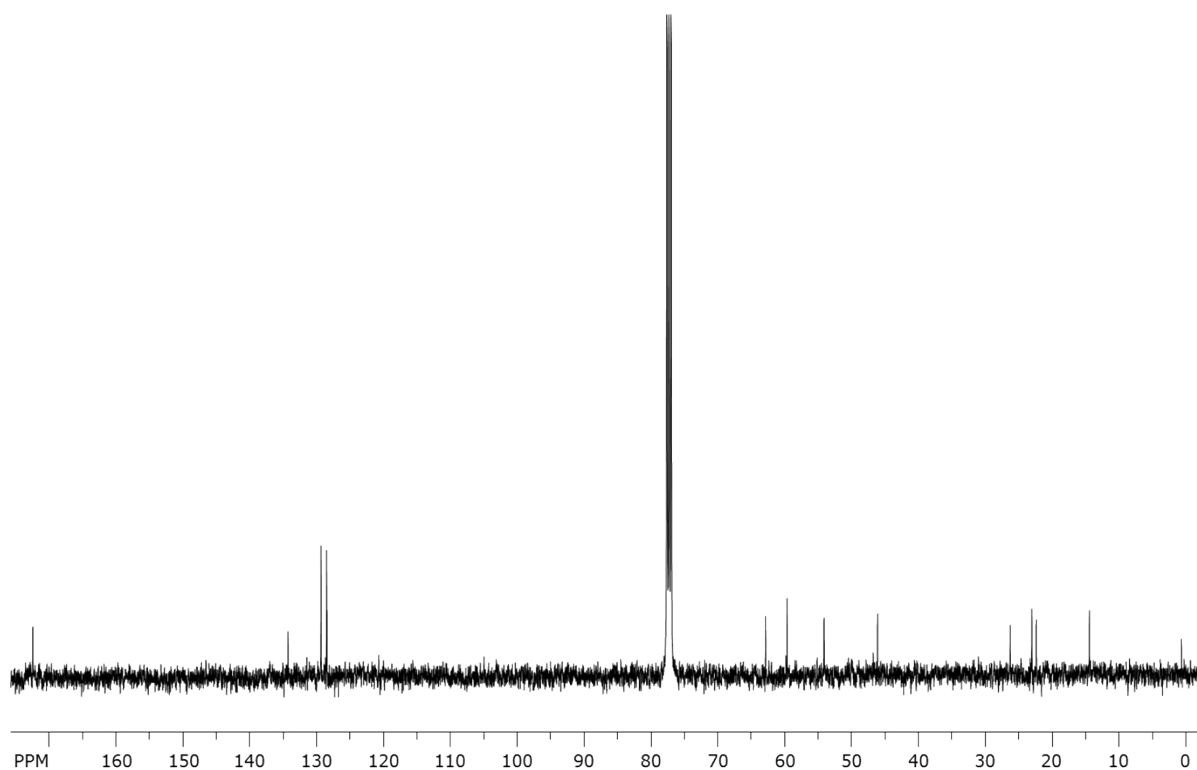
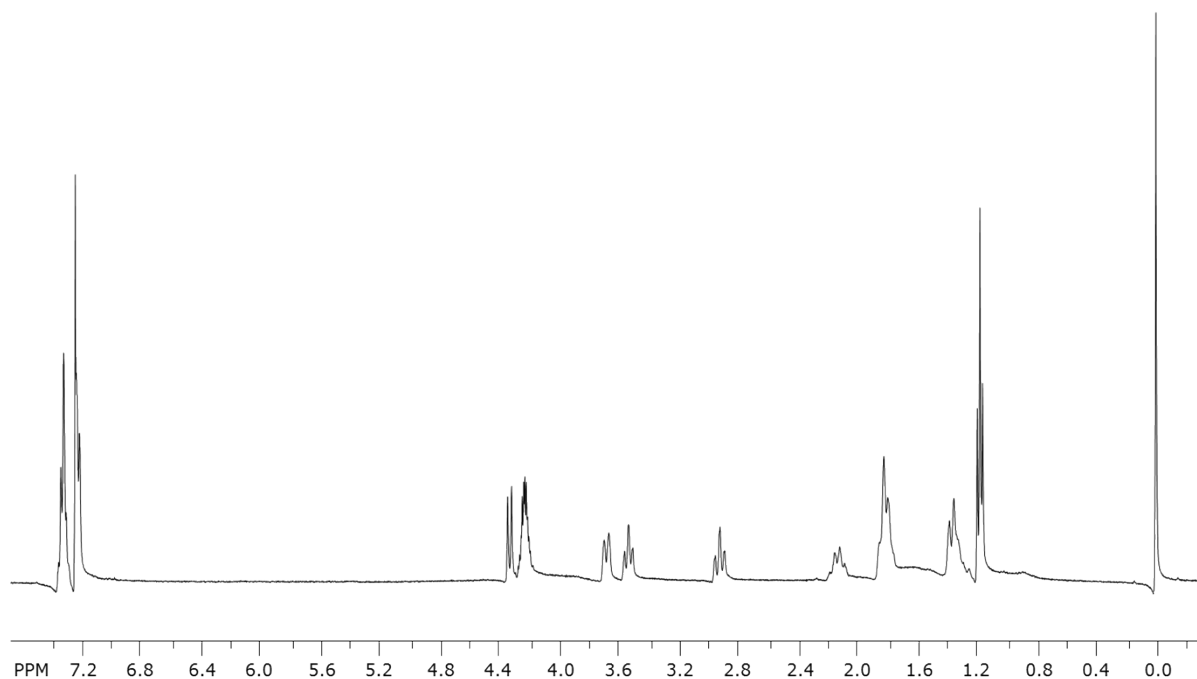
δ_{C} (CDCl_3 , 100MHz) 153.8, 135.7, 131.4, 127.9, 122.3, 117.5, 114.2, 112.1, 111.8, 100.8, 56.9, 55.9, 53.7, 22.8



NMR Data of Ethylphenidate

δ_H (CDCl₃, 400MHz) 7.31-7.36 (3H, m) 7.24 (2H, dd, J 7.8 Hz and J 1.5 Hz) 4.34 (1H, d, J 10.4 Hz) 4.24 (2H, m) 3.69 (1H, d, J 12.6 Hz) 3.54 (1H, t, J 10.8 Hz) 2.93 (1H, dt, J 12.7 Hz and J 2.4 Hz) 2.07-2.20 (1H, m) 1.75-1.87 (3H, m) 1.32-1.40 (2H, m) 1.18 (3H, t, J 7.1 Hz)

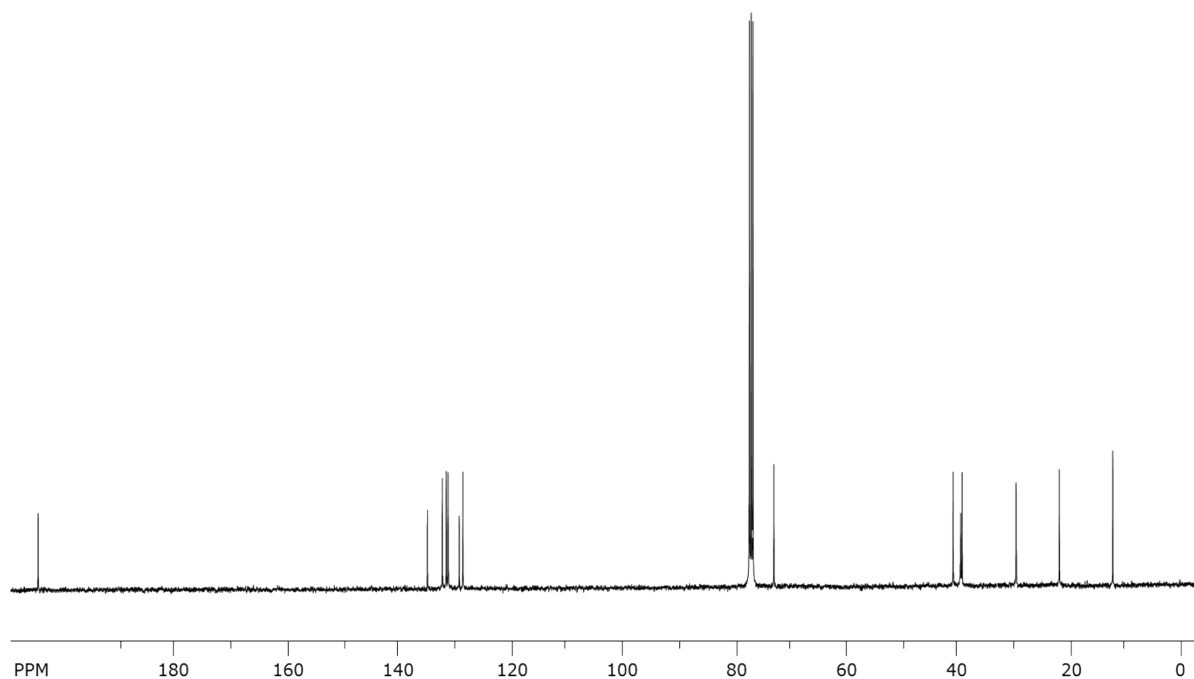
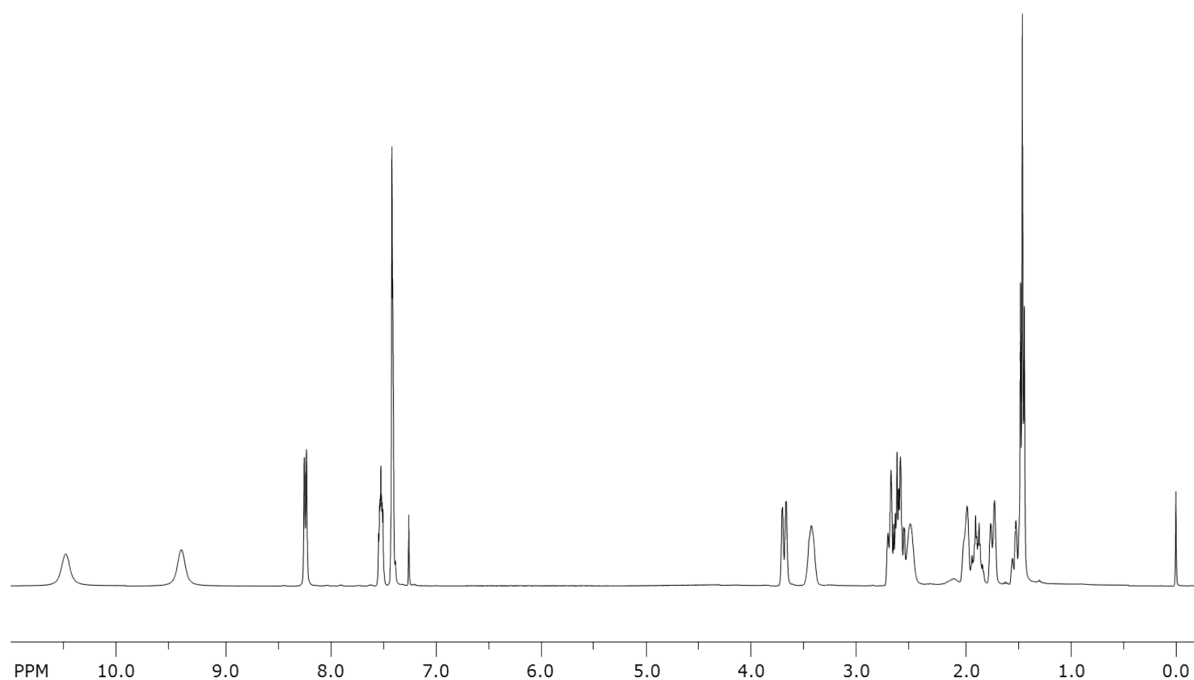
δ_C (CDCl₃, 100MHz) 172.5, 134.2, 129.3, 128.4, 128.4, 62.4, 59.2, 53.7, 45.7, 25.8, 22.5, 21.9, 13.8

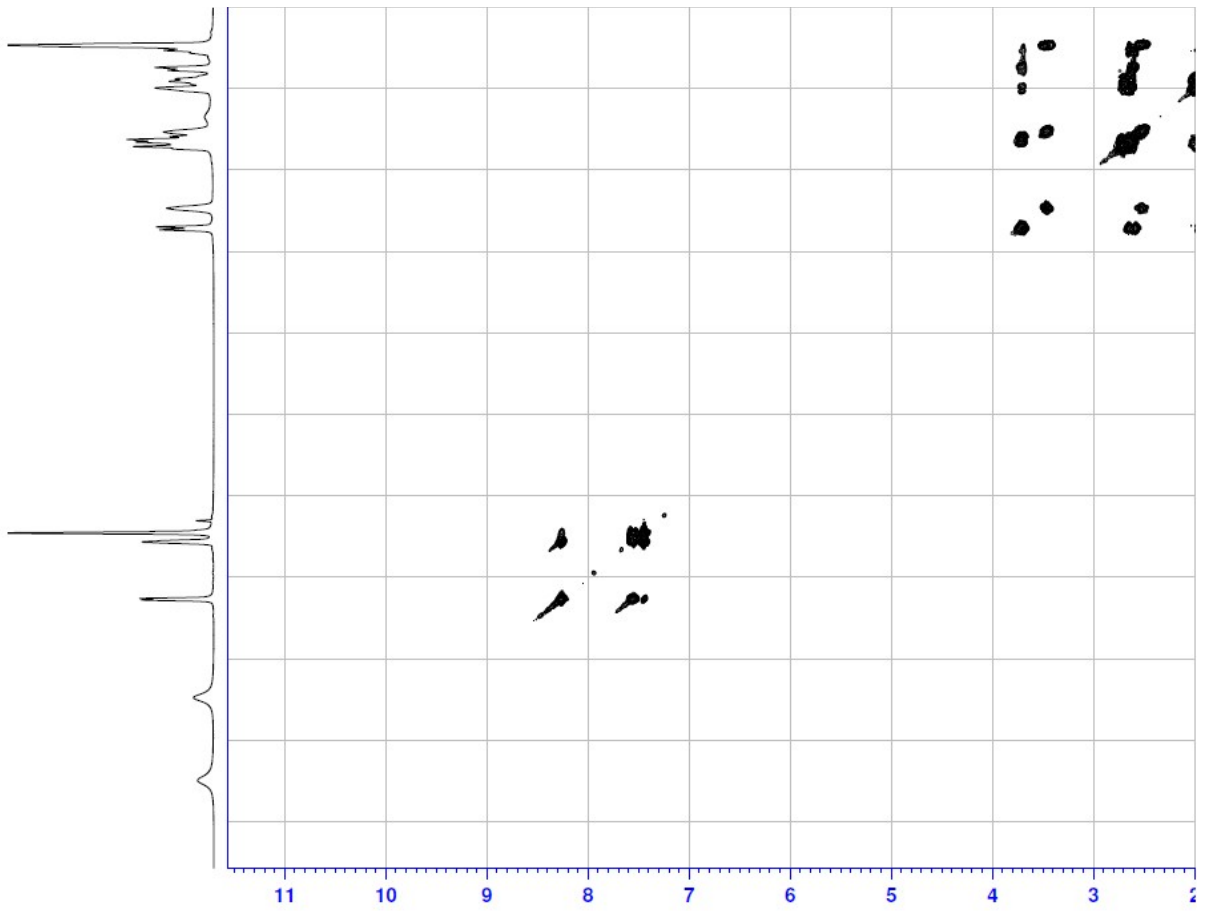


NMR Data of **N-Ethylketamine**

δ_{H} (CDCl_3 , 400MHz) 10.51 (1H, bs) 9.42 (1H, bs) 8.24 (1H, d, J 8.0 Hz) 7.50-7.55 (1H, m) 7.40-7.43 (2H, m) 3.69 (1H, dd, J 14.4 Hz and J 1.8 Hz) 3.43 (1H, bs) 2.54-2.73 (3H, m) 2.49 (1H, bs) 1.93-2.00 (1H, m) 1.86 (1H, qt, J 13.1 Hz and J 4.3 Hz) 1.72 (1H, d, J 14.0 Hz) 1.50 (1H, m) 1.44 (3H, t, J 7.2 Hz)

δ_{C} (CDCl_3 , 100MHz) 205.0, 135.1, 132.4, 131.7, 131.4, 129.4, 128.7, 72.9, 40.6, 39.3, 39.0, 29.4, 21.6, 12.0

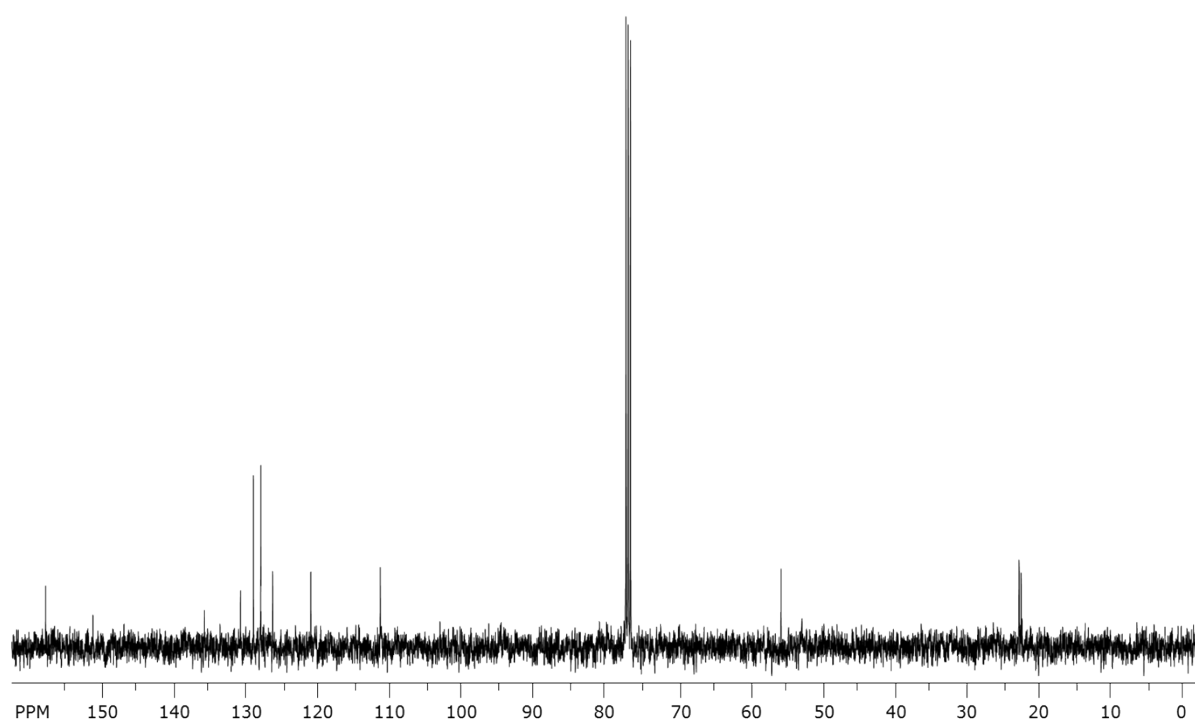
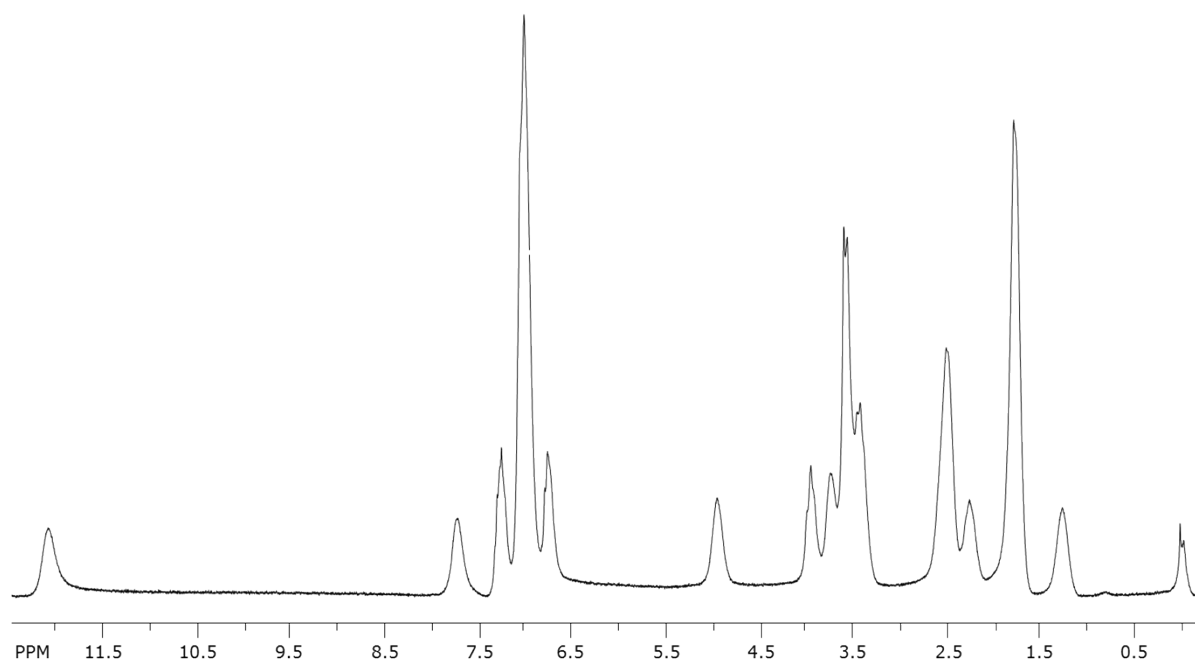




NMR Data of **Methoxyphenidine**

δ_H (CDCl₃, 300MHz) 12.14 (1H, s) 7.75 (1H) 7.28 (1H) 7.03 (6H) 6.78 (1H) 4.97 (1H) 3.96 (1H) 3.74 (1H) 3.61 (3H) 3.44 (2H) 2.51 (3H) 2.26 (1H) 1.78 (3H) 1.27 (1H)

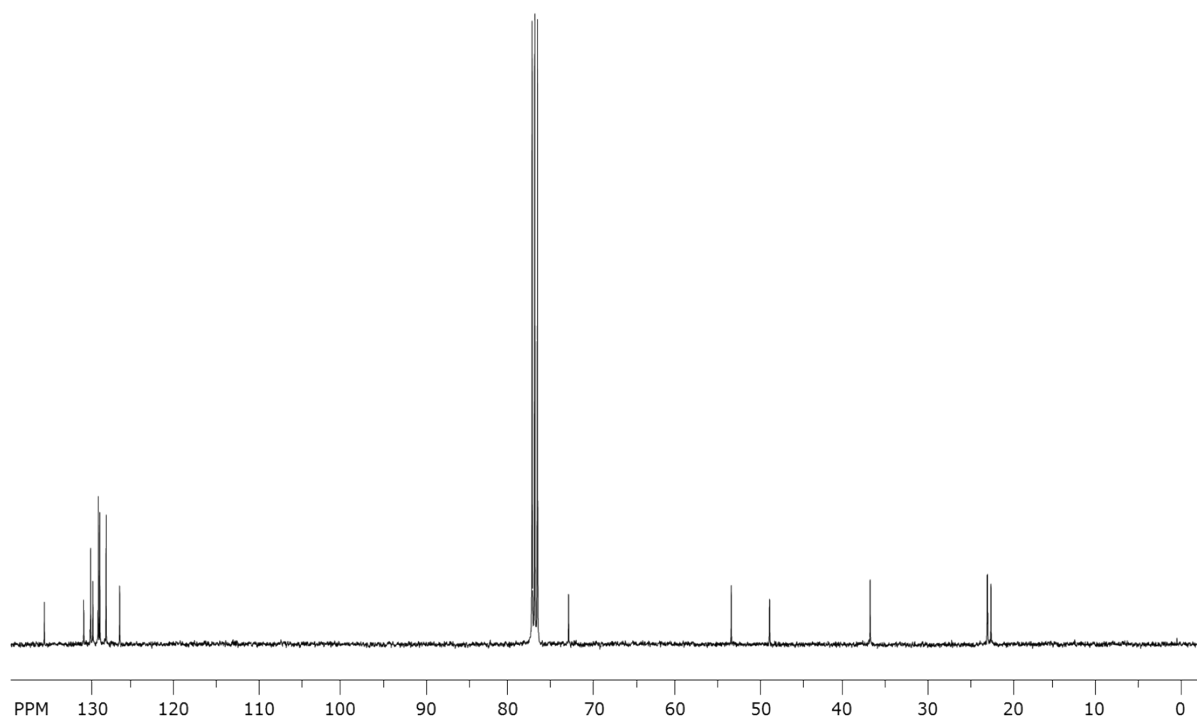
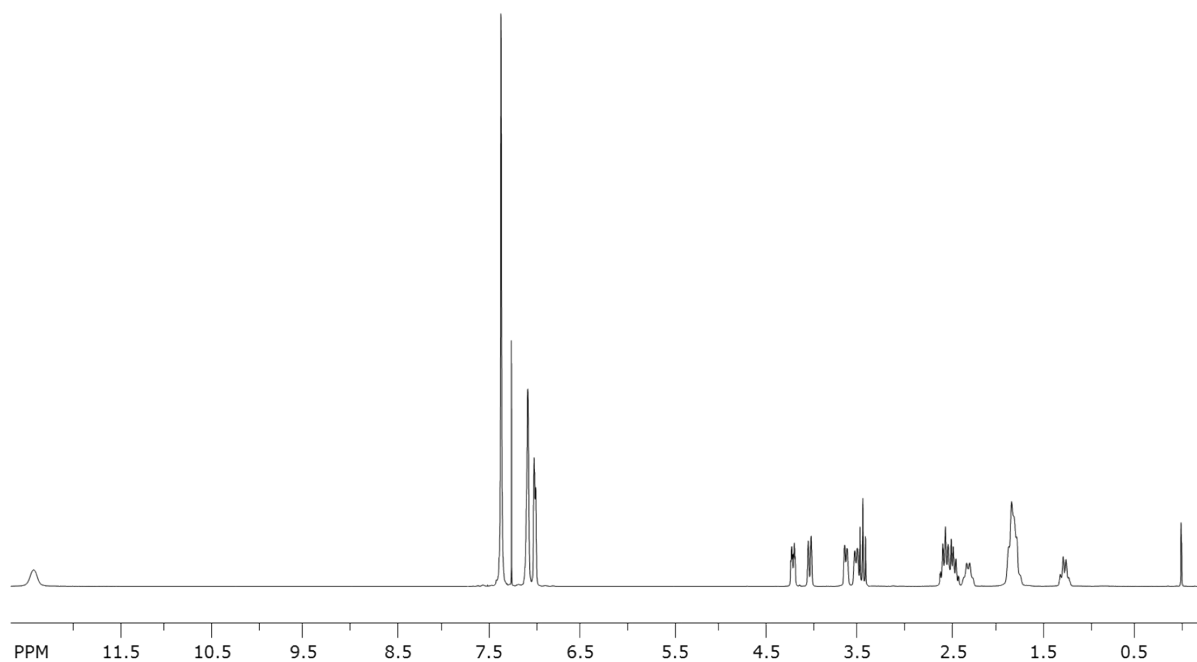
δ_C (CDCl₃, 100MHz) 158.2, 151.6, 136.1, 131.0, 129.2, 128.2, 126.6, 123.4, 121.3, 111.6, 55.8, 52.9, 36.3, 22.6, 22.3, 22.2



NMR Data of Diphenidine

δ_{H} (CDCl_3 , 400MHz) 12.45 (1H, bs) 7.37 (5H, s) 7.08 (3H, s) 7.00 (2H, m) 4.20 (1H, dt, J 11.7 Hz and J 3.6 Hz) 4.02 (1H, d, J 12.8 Hz) 3.62 (1H, d, J 10.6 Hz) 3.51 (1H, d, J 11.3 Hz) 3.44 (1H, t, J 12.2 Hz) 2.40-2.61 (3H, m) 2.30 (1H, q, J 13.2 Hz) 1.73-1.88 (3H, m) 1.25 (1H, q, J 12.6 Hz)

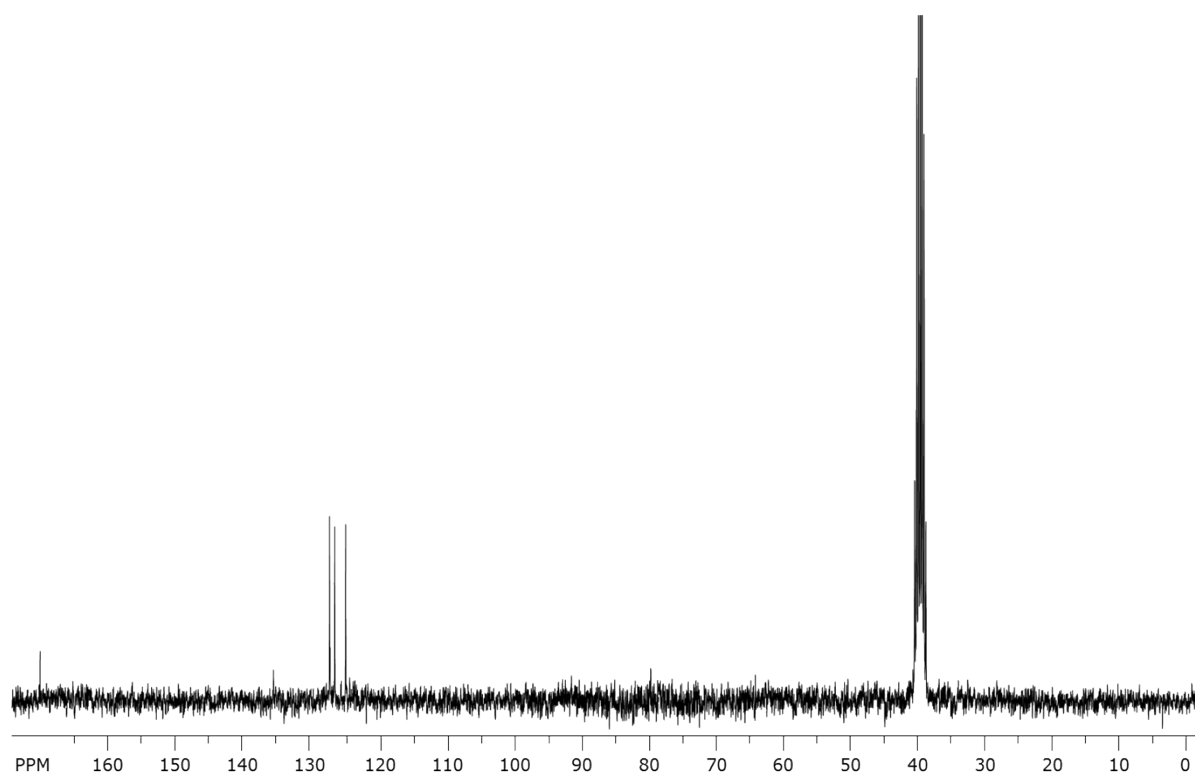
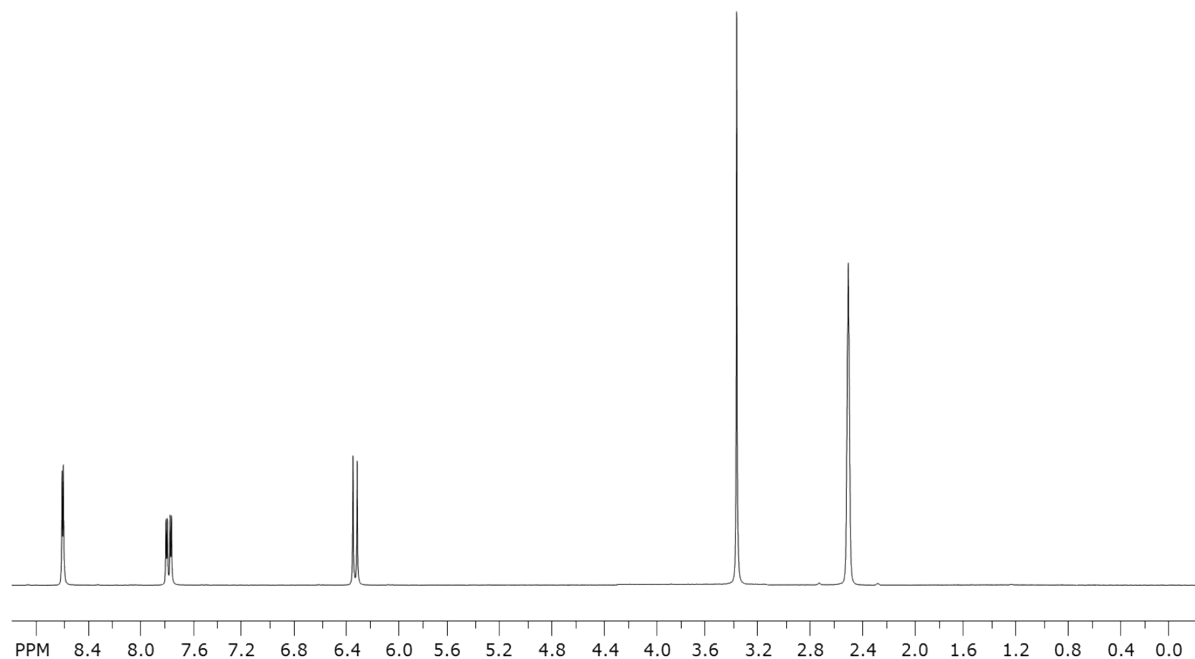
δ_{C} (CDCl_3 , 100MHz) 135.8, 131.1, 130.3, 130.0, 129.4, 129.2, 128.4, 126.8, 73.0, 53.5, 48.9, 36.8, 22.8, 22.7, 22.3



NMR Data of **Dintrophenol**

δ_H (DMSO- d_6 , 300MHz) 8.61 (1H, d, J 3.2 Hz) 7.79 (1H, dd, J 9.8 Hz and J 3.2 Hz) 6.34 (1H, d, J 9.8 Hz)

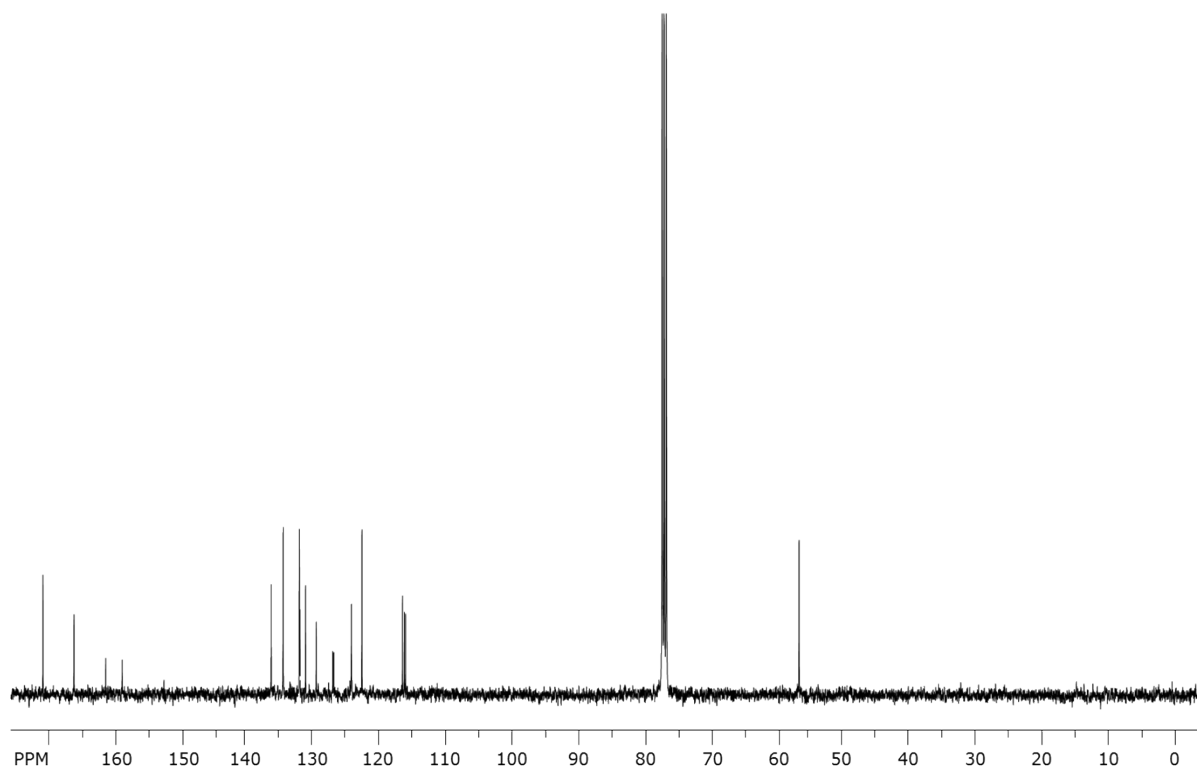
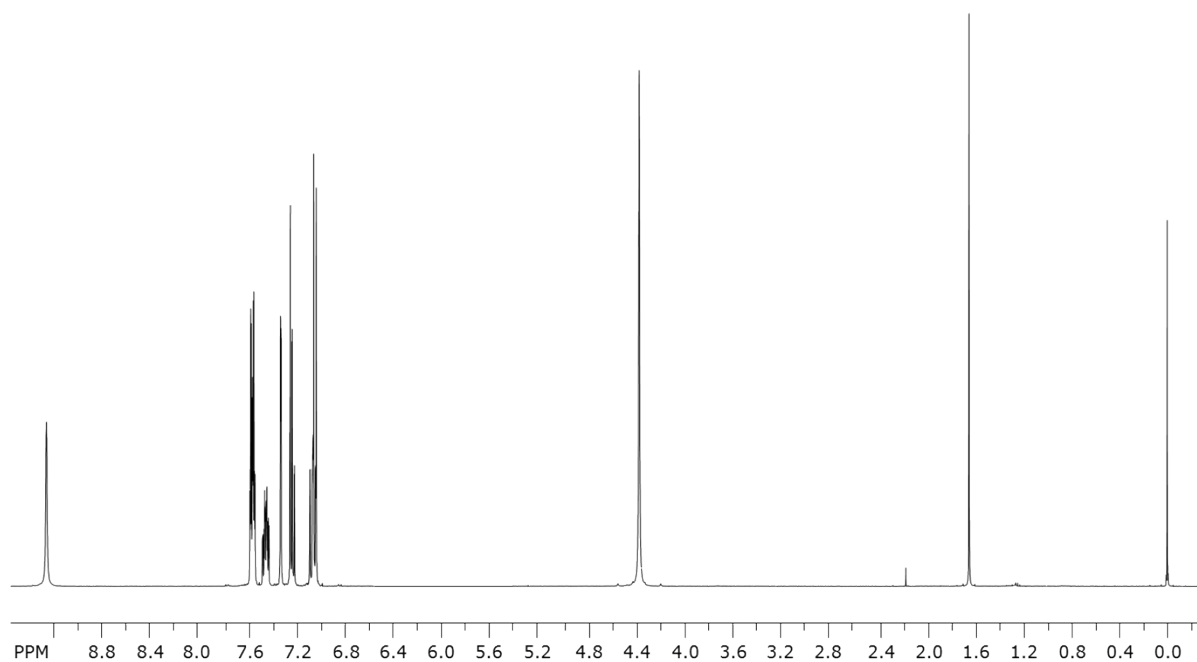
δ_C (DMSO- d_6 , 75MHz) 170.6, 135.9, 127.5, 127.4, 126.8, 125.1



NMR Data of **Flubromazepam**

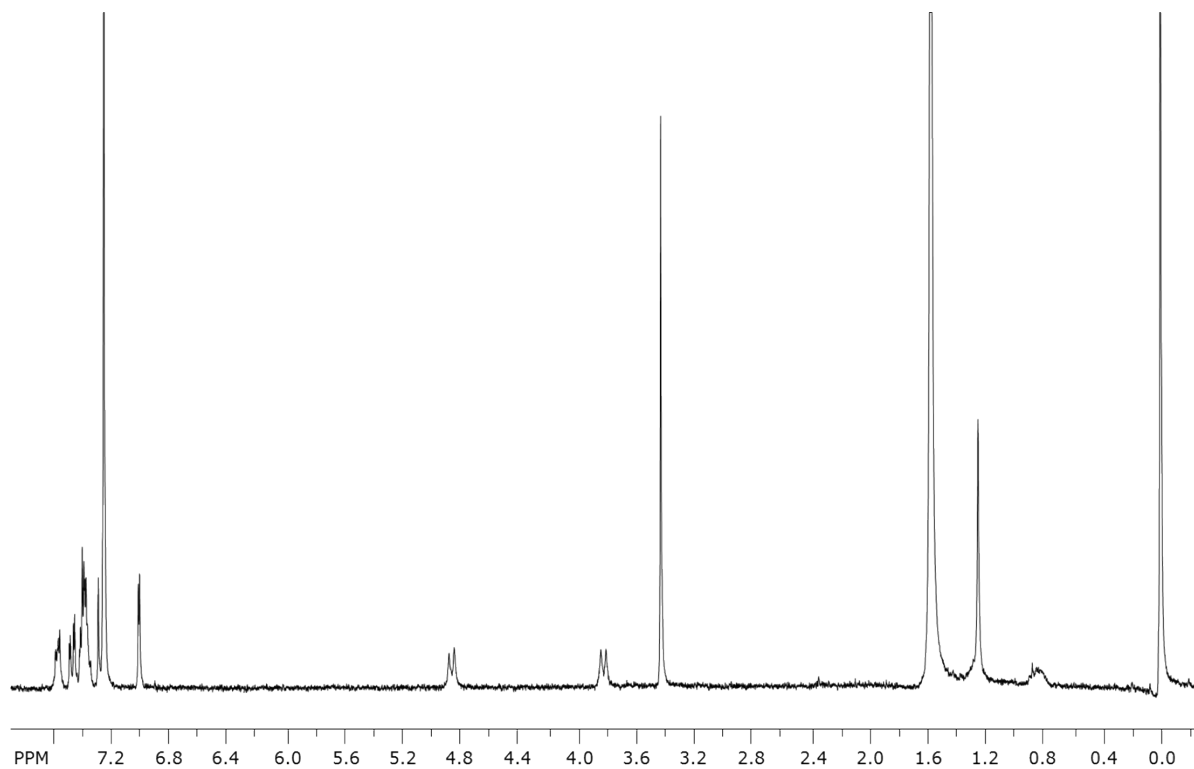
δ_H (CDCl₃, 400MHz) 9.28 (1H, s) 7.55-7.60 (2H, m) 7.43-7.50 (1H, m) 7.34 (1H, d, J 2.0 Hz) 7.24 (1H, td, J 7.6 Hz and J 1.2 Hz) 7.07 (1H, ddd, J 10.4 Hz, J 8.4 Hz and J 1.1 Hz) 7.06 (1H, d, J 8.6 Hz) 4.37 (2H, s)

δ_C (CDCl₃, 100MHz) 171.2, 166.5, 160.5, 136.6, 134.8, 132.4, 132.3, 131.4, 129.8, 127.2, 124.4, 122.9, 116.7, 116.3, 56.6



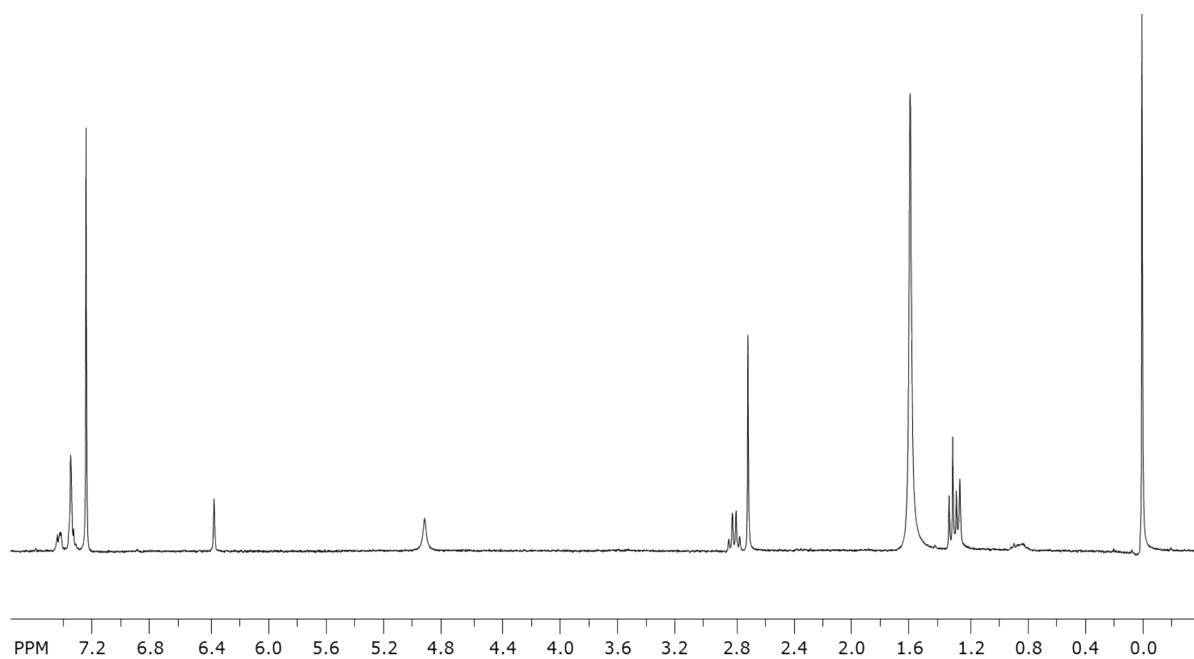
NMR Data of **Diclazepam**

δ_{H} (CDCl₃, 300MHz) 7.55-7.60 (1H, m) 7.48 (1H, dd, J 8.7 Hz and J 2.5 Hz) 7.35-7.43 (3H, m) 7.28 (1H, d, J 9.0 Hz) 7.02 (1H, d, J 2.4 Hz) 4.87 (1H, d, J 10.7 Hz) 3.82 (1H, d, J 10.7 Hz) 3.43 (3H, s)



NMR Data of **Etizolam**

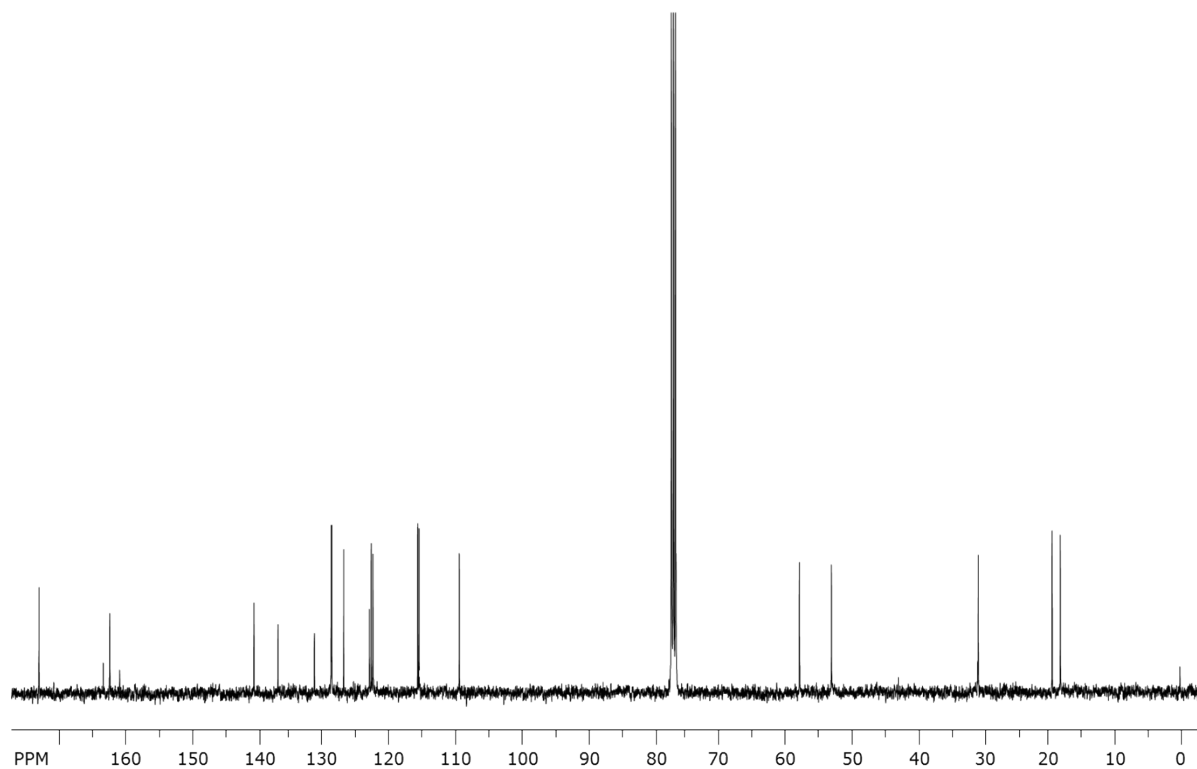
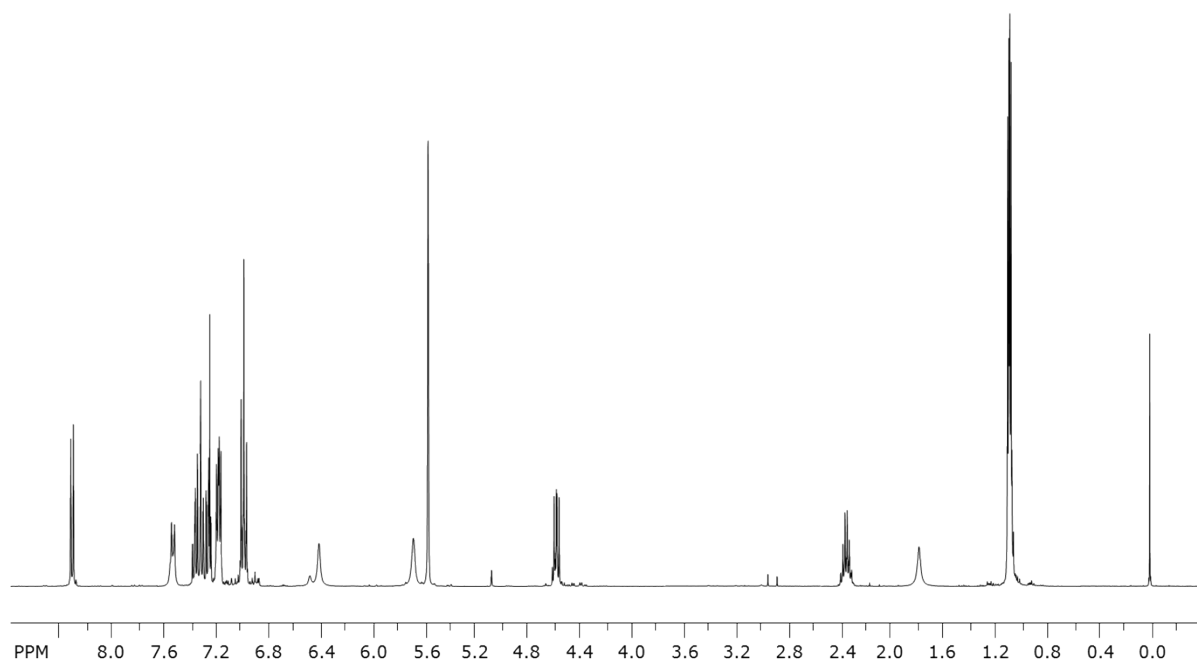
δ_{H} (CDCl₃, 300MHz) 7.42-7.47 (1H, m) 7.33-7.39 (3H, m) 6.38 (1H, s) 4.93 (2H, s) 2.80 (2H, q, J 7.5 Hz) 2.71 (3H, s) 1.30 (3H, t, J 7.5 Hz)



NMR Data of **AB-FUBINACA**

δ_{H} (CDCl_3 , 400MHz) 8.33 (1H, dt, J 8.2 Hz and J 0.9 Hz) 7.55 (1H, d, J 8.8 Hz) 7.25-7.40 (3H, m) 7.20 (1H, d, J 8.8 Hz) 7.19 (1H, d, J 8.6 Hz) 7.00 (2H, t, J 8.7 Hz) 5.57 (2H, s) 4.58 (1H, dd, J 8.9 Hz and J 6.7 Hz) 2.35 (1H, octet, J 6.7 Hz) 1.09 (3H, d, J 6.8 Hz) 1.08 (3H, d, J 6.8 Hz)

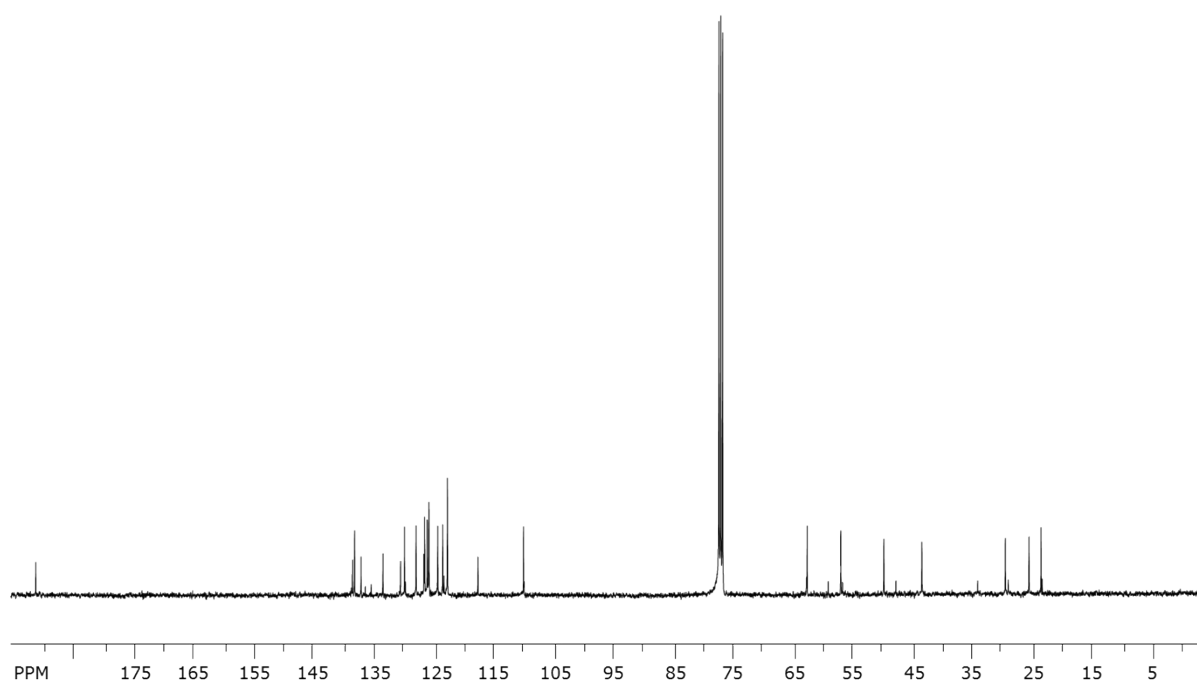
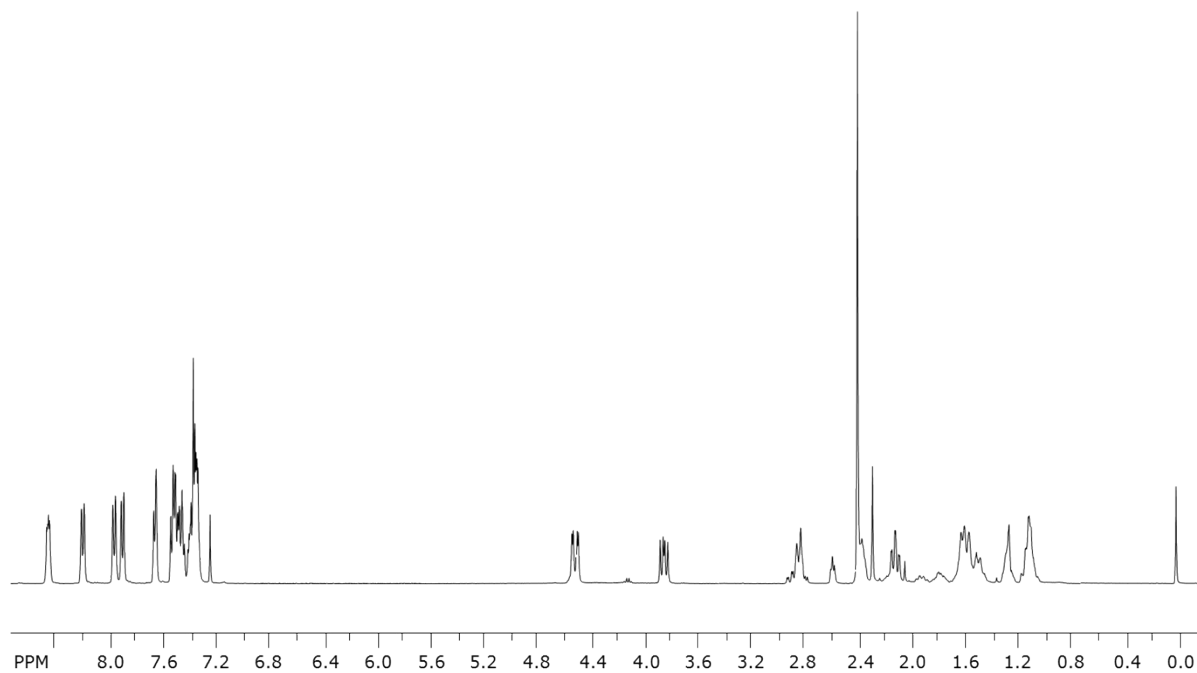
δ_{C} (CDCl_3 , 100MHz) 173.5, 163.7, 162.8, 140.8, 137.1, 131.6, 129.1, 127.1, 123.3, 123.0, 122.7, 115.8, 109.5, 57.8, 53.0, 30.7, 19.5, 18.2



NMR Data of **AM-1220**

δ_{H} (CDCl_3 , 400MHz) 8.45-8.49 (1H, m) 8.22 (1H, d, J 8.3 Hz) 7.98 (1H, d, J 8.4 Hz) 7.92 (1H, d, J 8.0 Hz) 7.68 (1H, dd, J 7.1 Hz and J 1.1 Hz) 7.44-7.55 (3H, m) 7.33-7.42 (4H, m) 4.52 (1H, dd, J 14.1 Hz and 4.1 Hz) 3.85 (1H, dd, J 14.0 Hz and J 9.1 Hz) 2.81-2.88 (1H, m) 2.40 (3H, s) 2.33-2.40 (1H, m) 2.12 (1H, dt, J 11.6 Hz and J 2.6 Hz) 1.44-1.66 (3H, m) 1.24-1.32 (1H, m) 1.05-1.18 (2H, m)

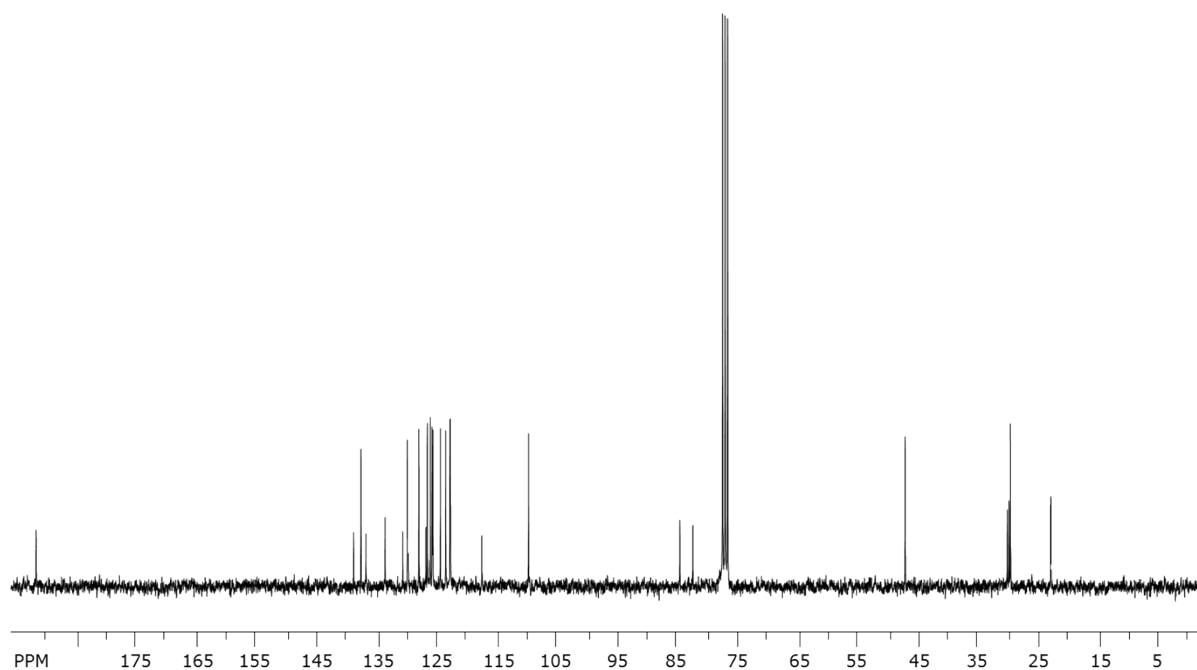
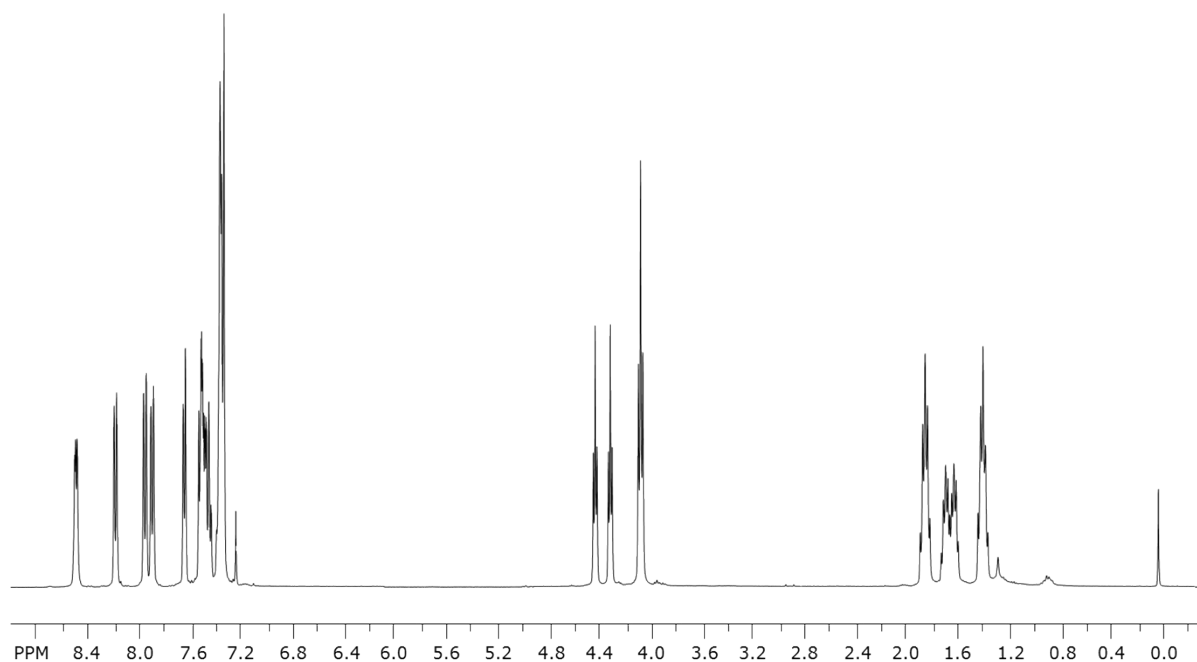
δ_{C} (CDCl_3 , 75MHz) 192.4, 139.5, 138.2, 137.4, 134.2, 131.2, 130.4, 128.6, 127.4, 127.2, 126.7, 126.4, 126.3, 125.0, 124.1, 123.4, 123.3, 118.1, 110.3, 85.1, 82.9, 47.4, 30.4, 30.1, 29.9, 23.2, 23.2

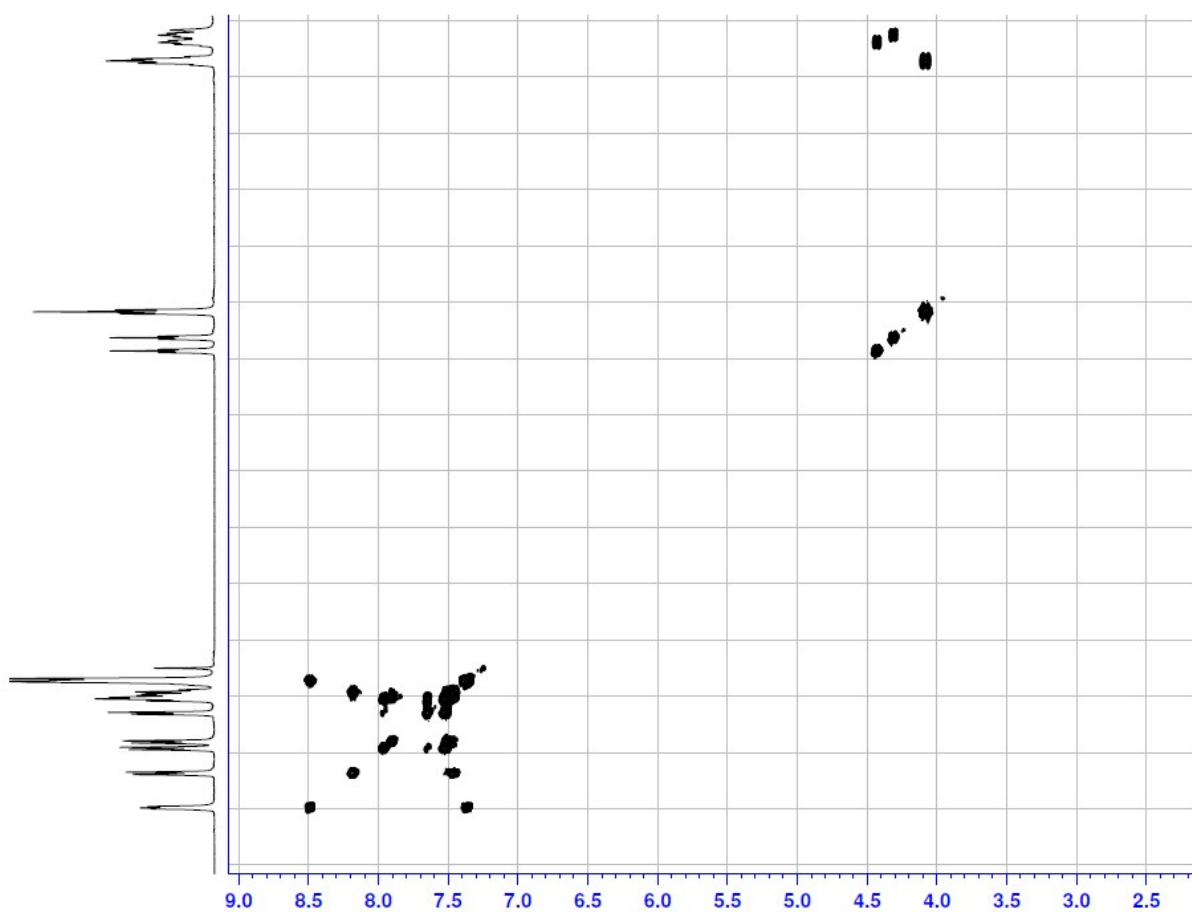


NMR Data of **AM-2201**

δ_{H} (CDCl₃, 400MHz) 8.49-8.53 (1H, m) 8.20 (1H, d, J 8.3 Hz) 7.97 (1H, d, J 8.2 Hz) 7.91 (1H, d, J 8.0 Hz) 7.66 (1H, dd, J 6.9 Hz and J 0.9 Hz) 7.45-7.56 (3H, m) 7.34-7.40 (4H, m) 4.44 (1H, t, J 5.9 Hz) 4.32 (1H, t, J 5.9 Hz) 4.08 (2H, t, J 7.2 Hz) 1.86 (2H, p, J 7.5 Hz) 1.59-1.73 (2H, m) 1.36-1.45 (2H, m)

δ_{C} (CDCl₃, 75MHz) 192.4, 139.5, 138.2, 137.4, 134.2, 131.2, 130.4, 128.6, 127.4, 127.2, 126.7, 126.4, 126.3, 125.0, 124.1, 123.4, 123.3, 118.1, 110.3, 85.1, 82.9, 47.4, 30.4, 30.1, 29.9, 23.2, 23.2

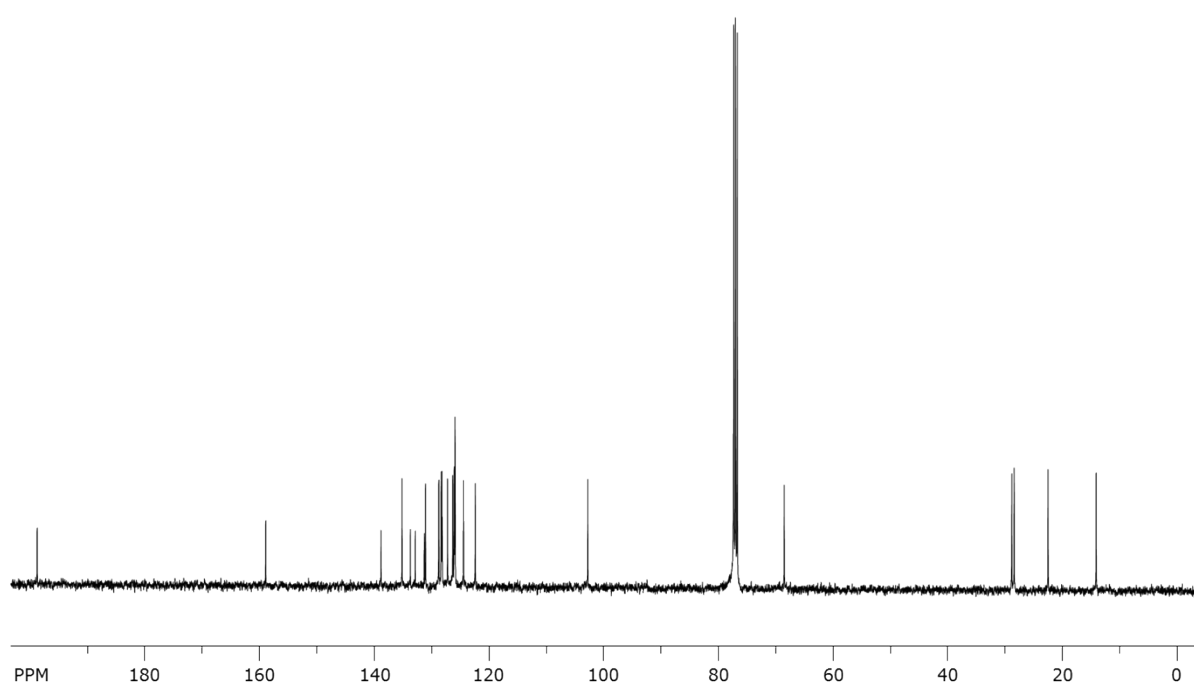
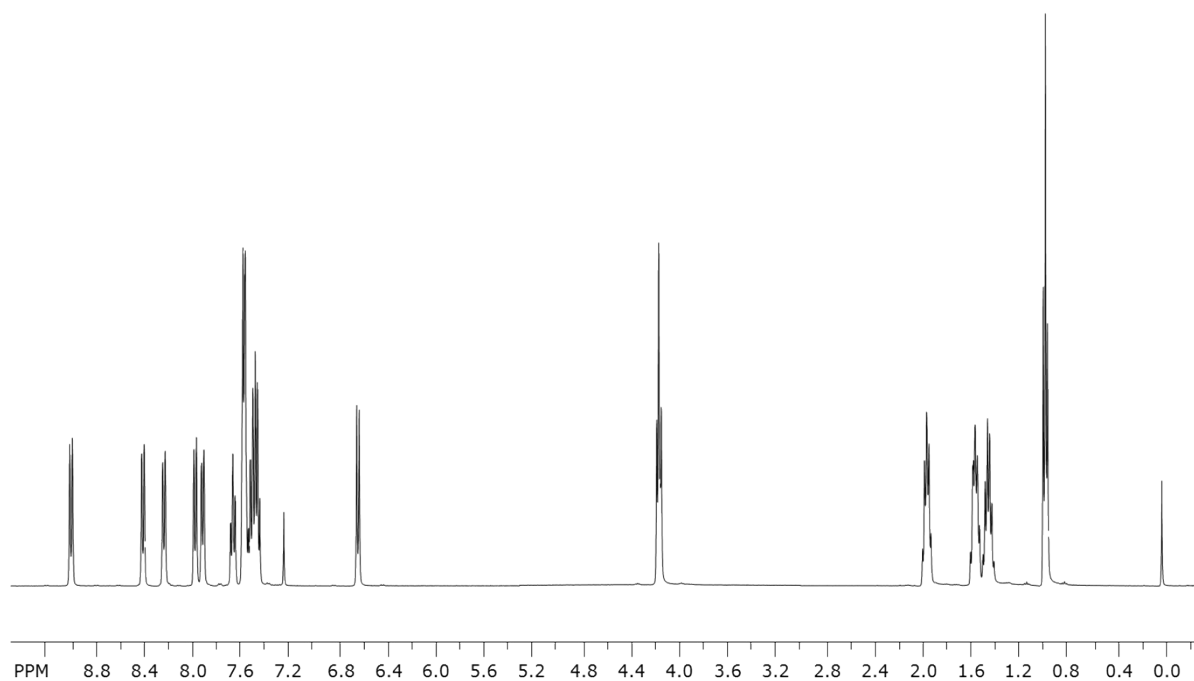


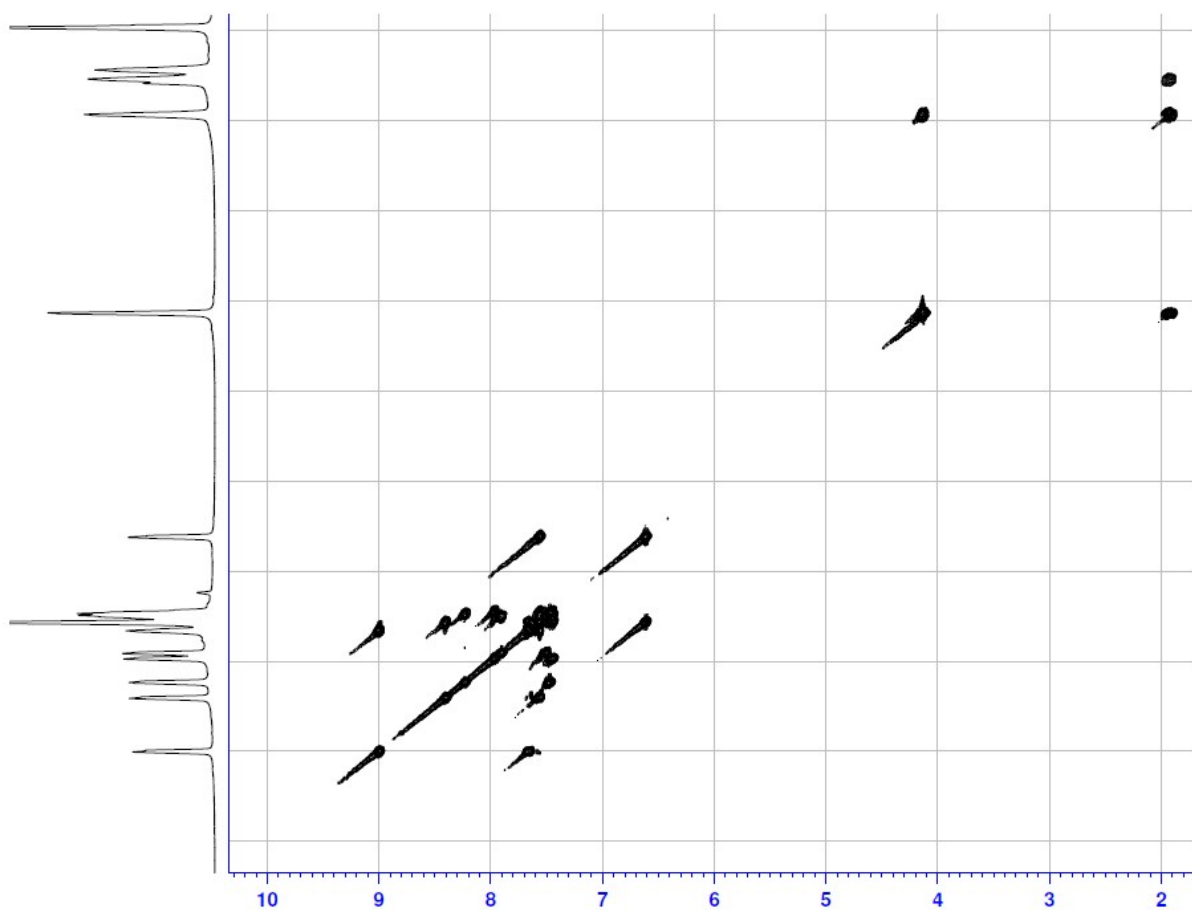


NMR Data of **CB-13**

δ_{H} (CDCl₃, 400MHz) 9.01 (1H, d, J 8.6 Hz) 8.42 (1H, d, J 8.6 Hz) 8.25 (1H, d, J 8.2 Hz) 7.99 (1H, d, J 8.2 Hz) 7.93 (1H, d, J 7.9 Hz) 7.65-7.71 (1H, m) 7.56-7.62 (3H, m) 7.45-7.56 (3H, m) 6.65 (1H, d, J 8.1 Hz) 4.16 (2H, t, J 6.4 Hz) 1.95 (2H, tt, J 7.4 Hz and J 6.9 Hz) 1.51-1.61 (2H, m) 1.39-1.50 (2H, m) 0.98 (3H, t, J 7.3 Hz)

δ_{C} (CDCl₃, 100MHz) 198.8, 158.9, 138.8, 135.1, 133.7, 132.8, 131.2, 131.0, 128.7, 128.3, 128.2, 128.1, 127.2, 126.3, 126.0, 125.9, 125.9, 124.4, 122.4, 102.7, 68.5, 28.7, 28.3, 22.4, 14.0

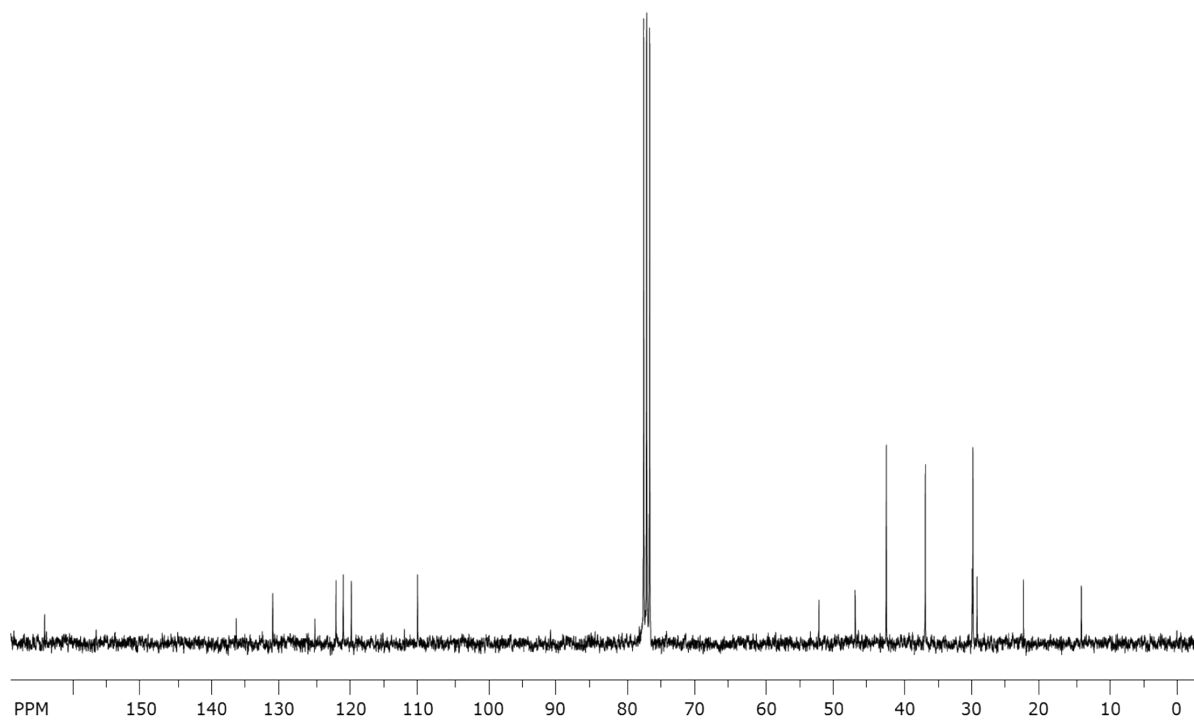
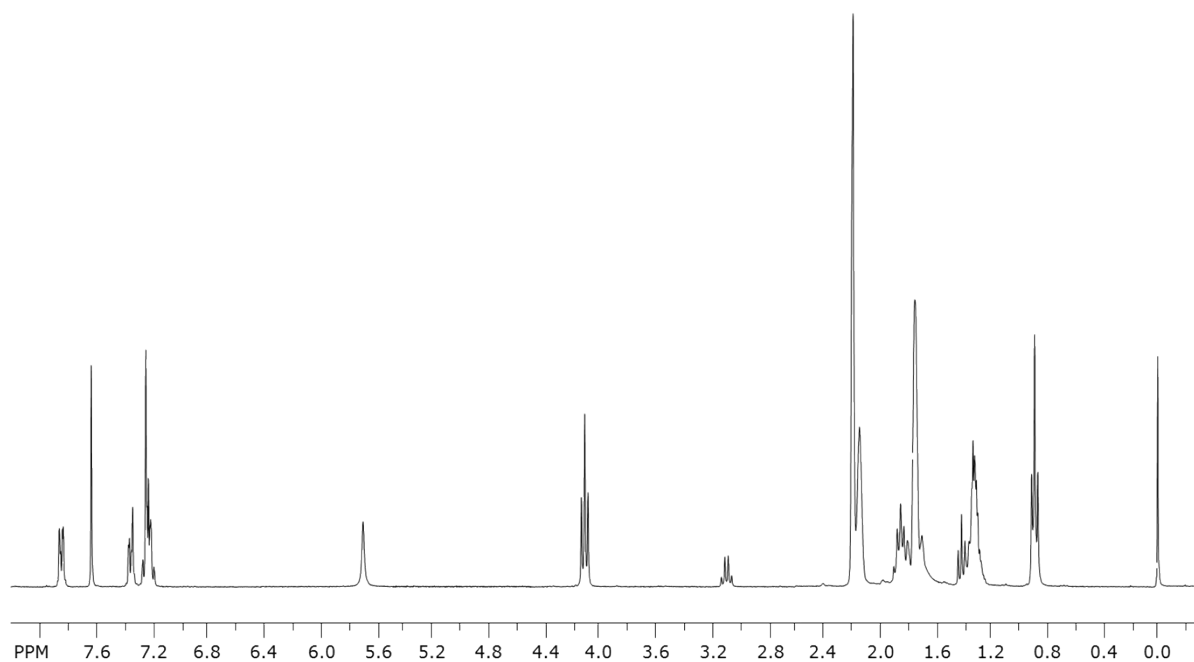




NMR Data of **2NE1**

δ_{H} (CDCl₃, 300MHz) 7.87 (1H, dd, J 6.3 Hz and J 2.4 Hz) 7.65 (1H, s) 7.34-7.39 (1H, m) 7.19-1.29 (2H, m) 4.11 (2H, t, J 7.1 Hz) 2.17-2.20 (6H, s) 2.11-2.16 (3H, s) 1.84 (2H, quin, J 7.2 Hz) 1.70-1.77 (6H, s) 1.26-1.36 (4H, m) 0.88 (3H, t, J 6.8 Hz)

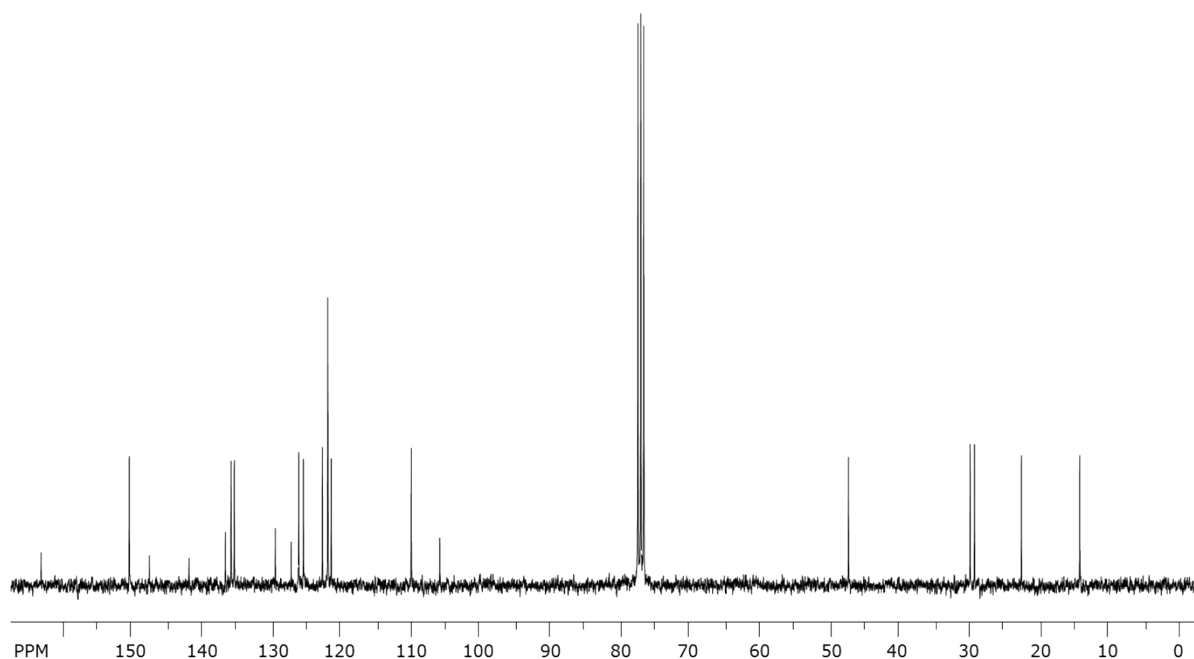
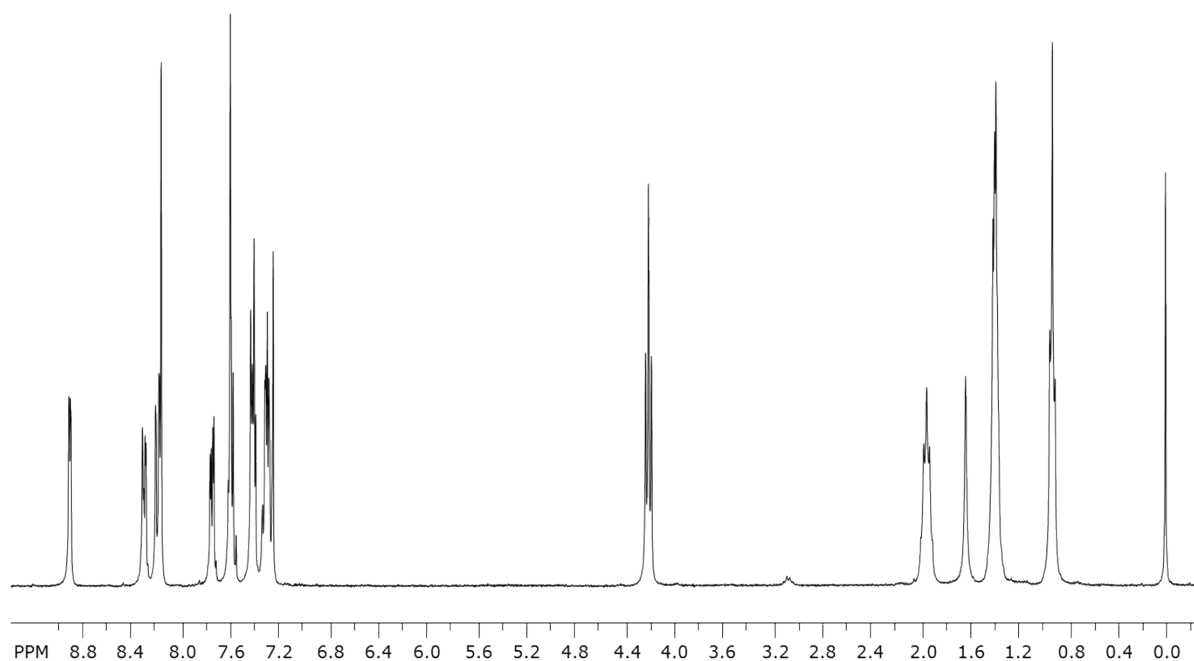
δ_{C} (CDCl₃, 75MHz) 164.9, 137.0, 131.8, 125.6, 122.6, 121.5, 120.3, 112.6, 110.7, 52.5, 47.2, 42.6, 36.9, 30.1, 30.0, 29.4, 22.7, 14.3



NMR Data of **PB-22**

δ_{H} (CDCl_3 , 300MHz) 8.92 (1H, dd, J 4.1 Hz and J 1.2 Hz) 8.28-8.34 (1H, m) 8.20 (1H, dd, J 8.5 Hz and J 1.2 Hz) 8.17 (1H, s) 7.76 (1H, dd, J 6.8 Hz and J 2.6 Hz) 7.58-7.64 (2H, m) 7.42 (2H, dd, J 8.3 Hz and J 4.3 Hz) 7.28-7.36 (2H, m) 4.21 (2H, t, J 7.2 Hz) 1.95 (2H, quin, J 7.2 Hz) 1.35-1.43 (4H, m) 0.92 (3H, t, J 6.6 Hz)

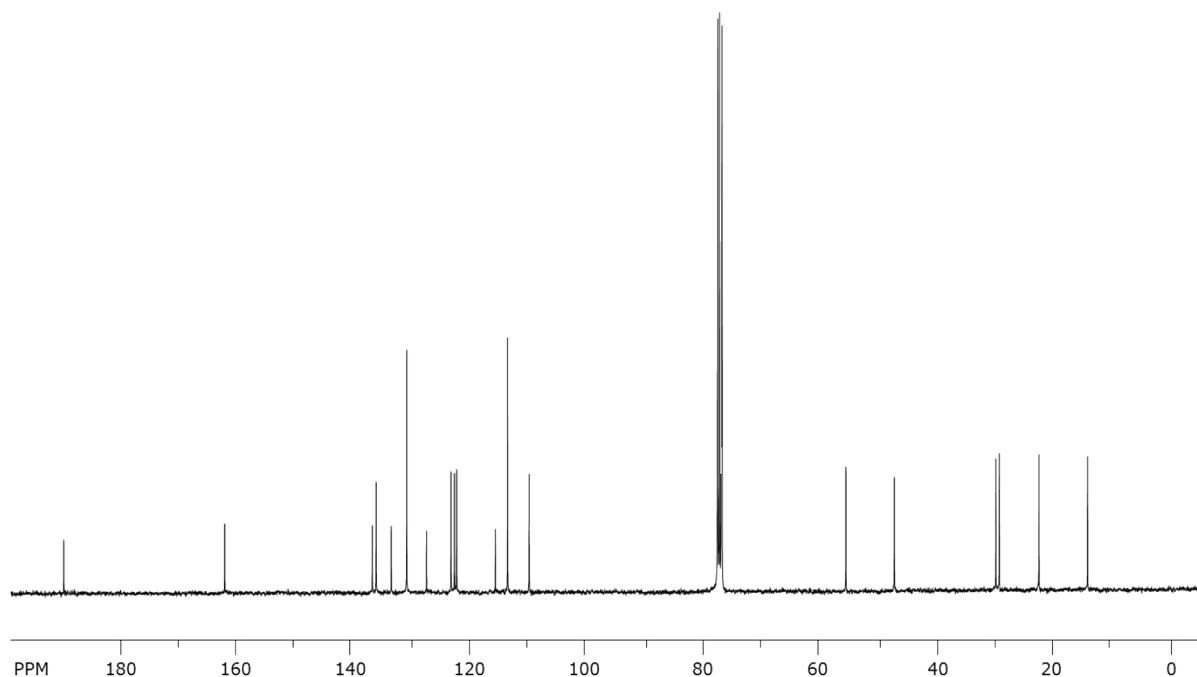
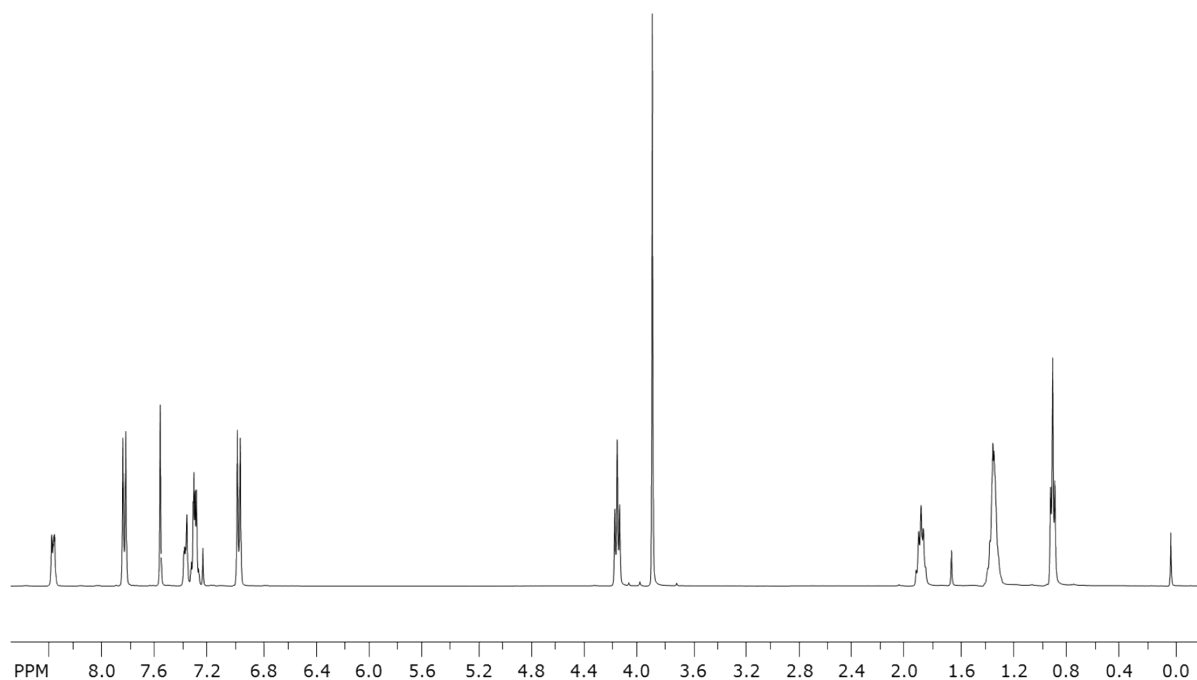
δ_{C} (CDCl_3 , 75MHz) 163.7, 151.0, 148.2, 142.5, 137.2, 136.4, 135.9, 130.0, 127.8, 126.7, 126.0, 123.3, 122.5, 122.5, 122.0, 110.5, 106.4, 47.6, 30.1, 29.5, 22.7, 14.3



NMR Data of **RCS-4**

δ_{H} (CDCl_3 , 400MHz) 8.36-8.40 (1H, m) 7.85 (2H, d, J 8.8 Hz) 7.58 (1H, s) 7.37-7.41 (1H, m) 7.30-7.34 (2H, m) 6.99 (2H, d, J 8.8 Hz) 4.16 (2H, t, 7.2 Hz) 3.89 (3H, s) 1.88 (2H, tt, J 7.2 Hz and J 7.2 Hz) 1.28-1.38 (4H, m) 0.90 (3H, t, J 6.8 Hz)

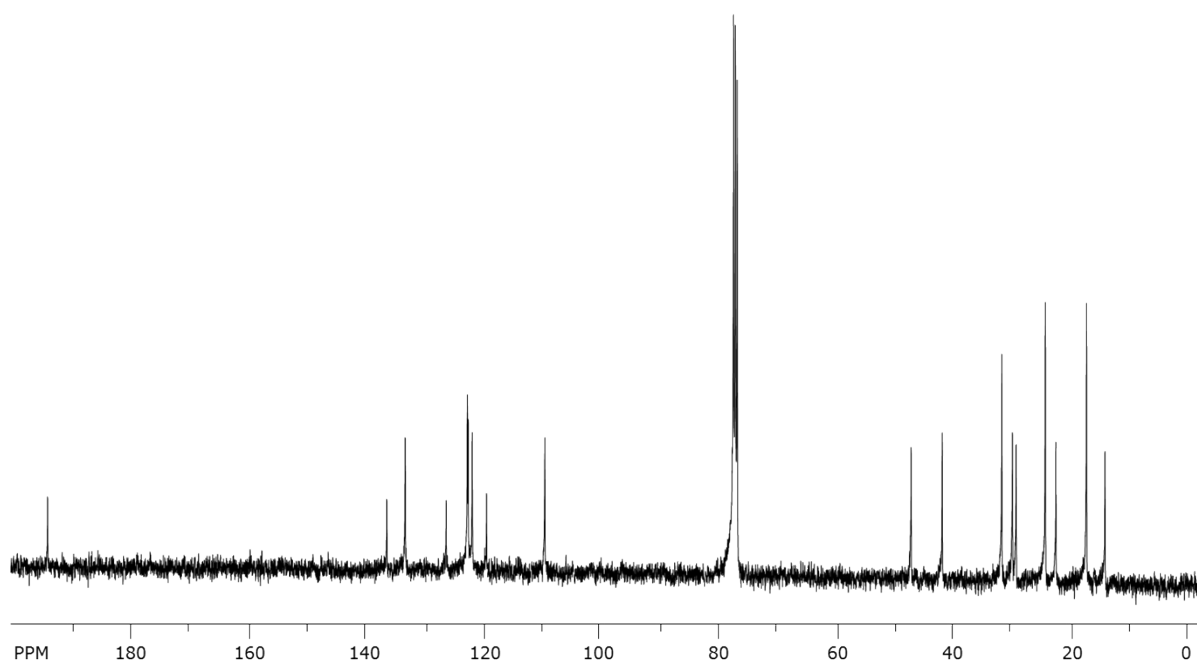
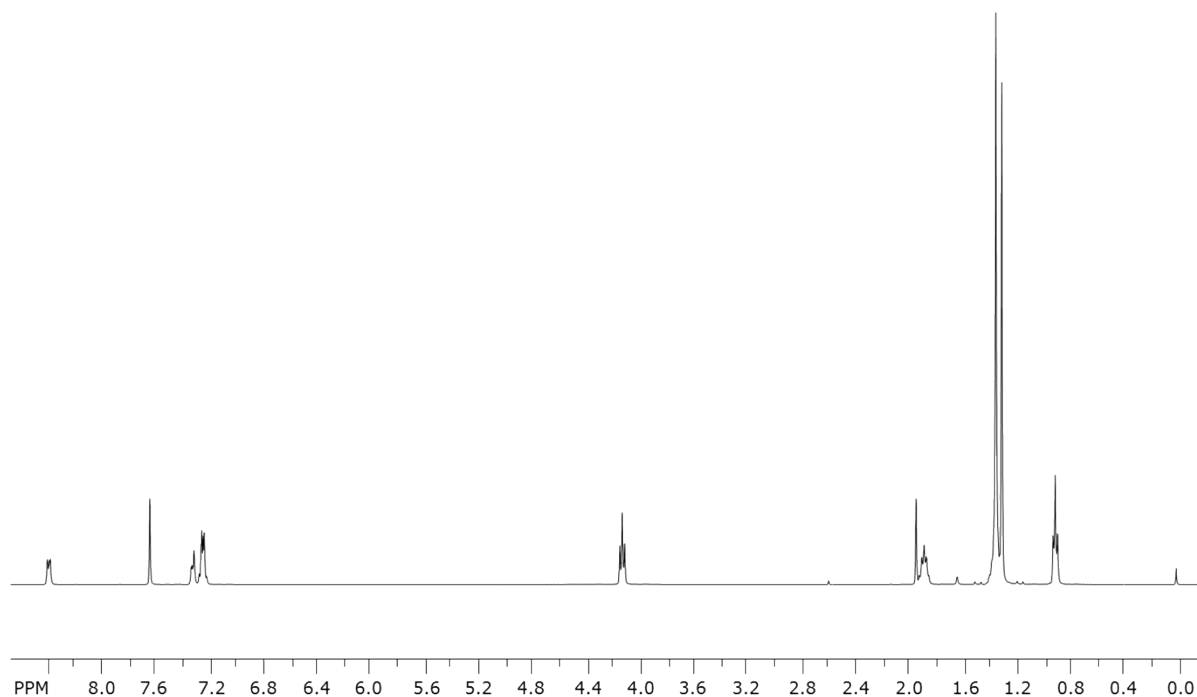
δ_{C} (CDCl_3 , 100MHz) 189.7, 162.1, 136.7, 136.1, 133.5, 130.1, 127.5, 123.3, 122.7, 122.3, 115.6, 113.5, 109.8, 55.4, 47.0, 29.6, 29.0, 22.2, 13.8



NMR Data of **UR-144**

δ_{H} (CDCl_3 , 400MHz) 8.40 (1H, m) 7.65 (1H, s) 7.31-7.35 (1H, m) 7.22-7.29 (2H, m) 4.13 (2H, t, J 7.2 Hz) 1.94 (1H, s) 1.88 (2H, quin, J 7.2 Hz) 1.35 (10H, s) 1.30 (6H, s) 0.90 (3H, t, J 6.8 Hz)

δ_{C} (CDCl_3 , 100MHz) 194.5, 136.6, 133.4, 126.4, 122.8, 122.7, 122.0, 119.6, 109.6, 46.9, 41.6, 31.4, 29.6, 29.0, 24.0, 22.2, 17.0, 13.9



NMR Data of **5-FUR-144**

δ_{H} (CDCl_3 , 300MHz) 8.39-8.44 (1H, m) 7.66 (1H, s) 7.30-7.37 (1H, m) 7.25-7.30 (2H, m) 4.44 (2H, dt, J 47.3 Hz and J 5.9 Hz) 4.18 (2H, t, J 7.2 Hz) 1.95 (2H, quin, J 7.4 Hz) 1.95 (1H, s) 1.62-1.83 (2H, dm) 1.43-1.57 (2H, m) 1.35 (6H, s) 1.31 (6H, s)

δ_{C} (CDCl_3 , 75MHz) 195.0, 137.0, 133.8, 126.8, 123.4, 123.2, 122.5, 120.2, 110.0, 84.1 (J = 164.4 Hz), 47.3, 42.1, 32.1, 30.4 (J = 20.2 Hz), 30.1, 24.5, 23.3 (J = 4.8 Hz), 17.4

