

Supplementary Information

Expanding the scope of fused pyrimidines as kinase inhibitor scaffolds: synthesis and modification of pyrido[3,4-*d*]pyrimidines

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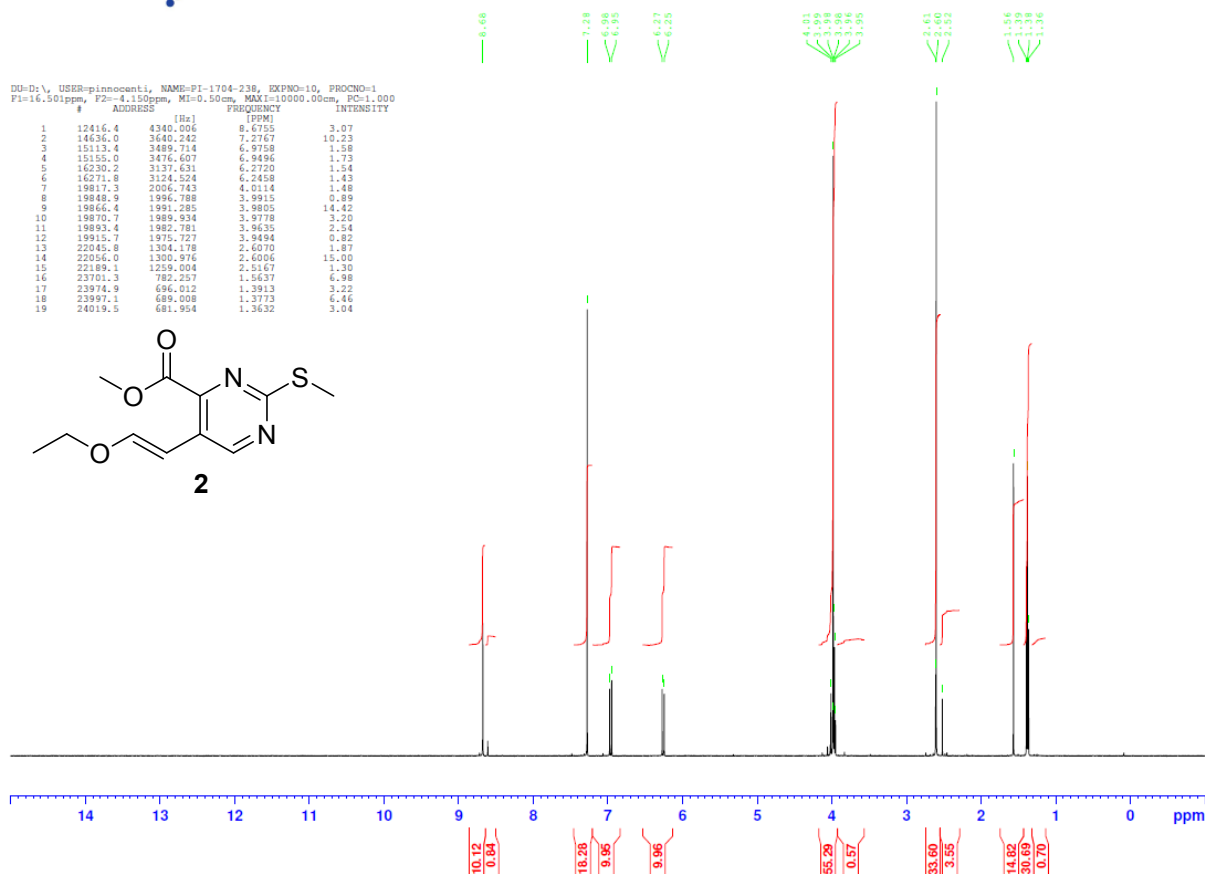
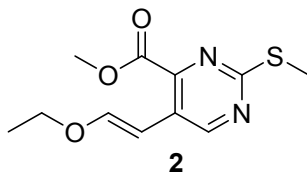
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S2 – S36

¹H and ¹³C spectra for compounds 2-7, 9, 11-37 and 39

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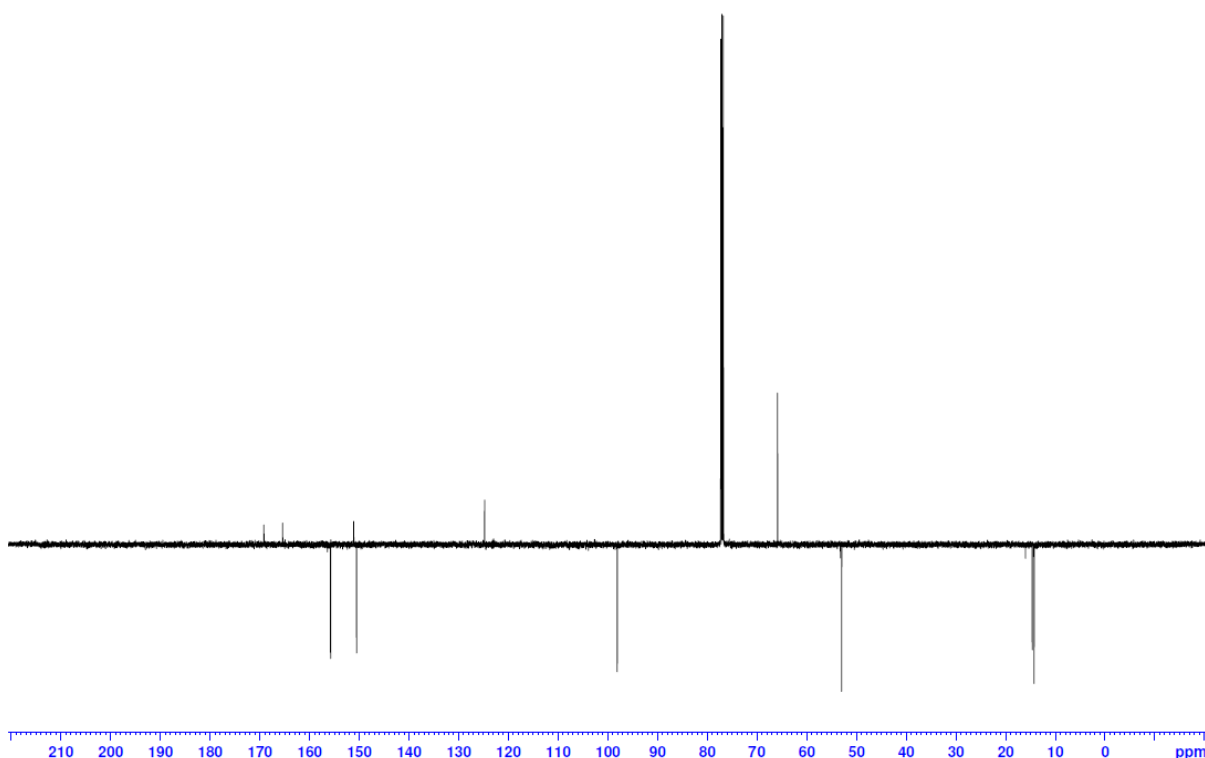
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1	12416.4	4340.006	8.6755	3.07	
2	14636.0	3640.242	7.2767	10.23	
3	15113.4	3489.714	6.9758	1.58	
4	15155.0	3476.507	6.9496	1.73	
5	16230.2	3137.631	6.2720	1.54	
6	16271.8	3124.524	6.2458	1.43	
7	19817.3	2006.743	4.0114	1.48	
8	19848.9	1996.788	3.9915	0.89	
9	19866.4	1991.285	3.9805	14.42	
10	19870.7	1989.534	3.9778	3.20	
11	19893.4	1982.781	3.9635	2.54	
12	19915.7	1975.727	3.9494	0.82	
13	22045.8	1304.178	2.6070	1.87	
14	22056.0	1300.976	2.6006	15.00	
15	22189.1	1259.004	2.5167	1.30	
16	23701.3	782.257	1.5637	6.98	
17	23974.9	696.012	1.3913	3.22	
18	23997.1	689.008	1.3773	6.46	
19	24019.5	681.954	1.3632	3.04	



NAME PI-1704-238
EXPNO 10
PROCNO 1
Date_ 20111018
Time 15.43
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1728407 s
RG 7290
EW 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 u
PL1 -3.00 d
PL1W 35.68453217 W
SFO1 500.2618193 M
SI 32768
SF 500.2600000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00

165.18	165.41	156.42	155.78	155.12	155.53	124.79	98.09	77.28	76.77	65.85	53.18	52.98	15.97	14.33	14.25
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EXPNO 10
PROCNO 1
Date_ 20110902
Time 1.50
INSTRUM spect
PROBHD 5 mm PABO BB-
PULPROG deptqqep.2
TD 65536
SOLVENT CDCl3
NS 2048
DS 8
SWH 30303.031 H
FIDRES 0.462388 H
AQ 1.0814105 s
RG 46300
EW 16.500 u
DE 6.00 u
TE 295.0 K
CNST2 145.0000000
CNST12 1.5000000
D1 4.00000000 s
D2 0.00344828 s
D12 0.00002000 s
D16 0.00020000 s
D28 2.00000000 s
TDO 1

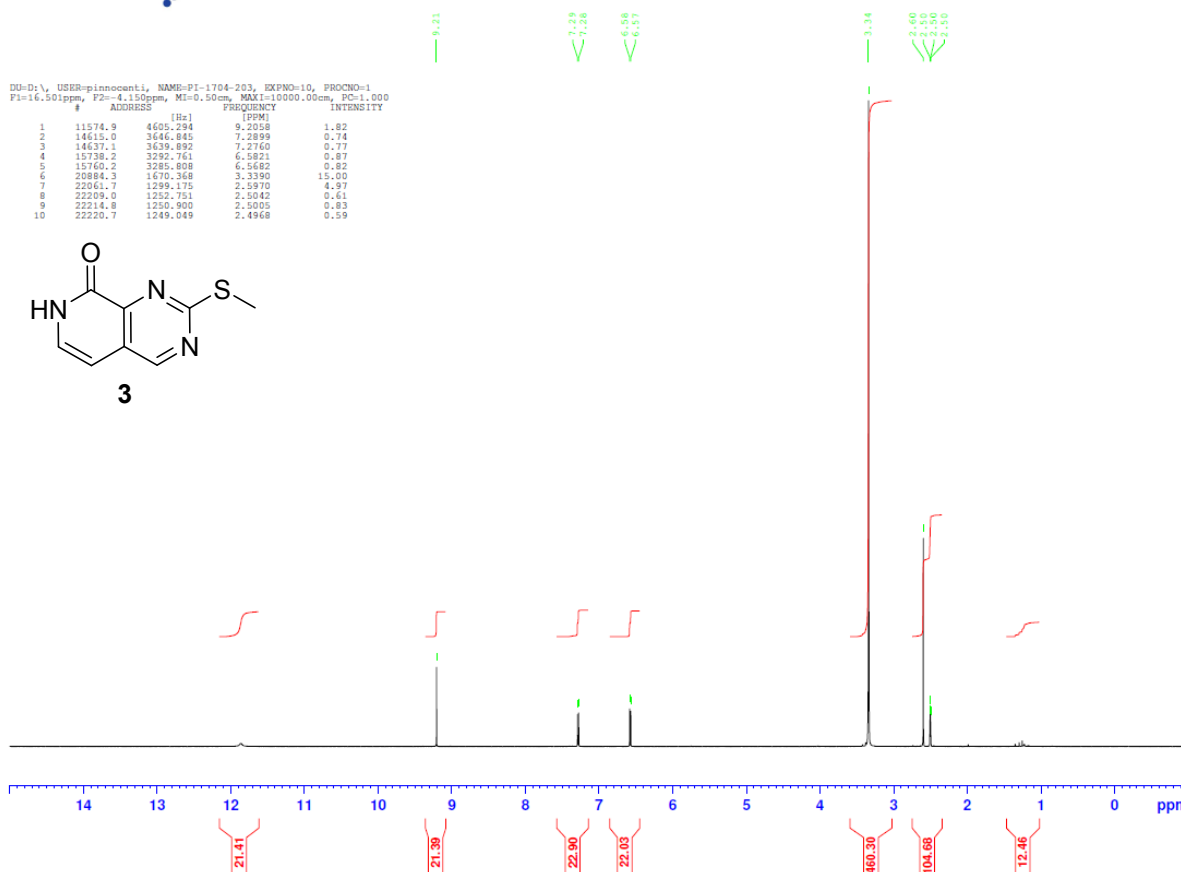
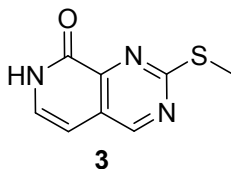
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NUC1 13C
P1 8.75 u
PL1 2000.00 u
PL2 120.00 d
PL1 1.00 d
PL1W 0.00000000 W
SFO1 125.7703643 M
SI 32768
SF 125.7577890 M
WDW EM
SSB 0
LB 1.00 H
GB 0
PC 1.40

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 15.54 u
PL2 10.36 u
PL3 20.72 u
PL4 80.00 u
PL2 0.00 d
PL1 17.90 d
PL3 18.00 d
PL2W 23.10935593 W
PL1W 0.37478989 W
PL1W 0.3625855 W
SFO2 500.1320005 M

===== GRADIENT CHANNEL =====
GPM1 SINE.100
GPM2 SINE.100
GPM3 SINE.100
GPR2 31.00 u
GPR3 31.00 u
P16 1000.00 u
SI 65536
SF 125.7577890 M
WDW EM
SSB 0
LB 1.00 H
GB 0
PC 1.40

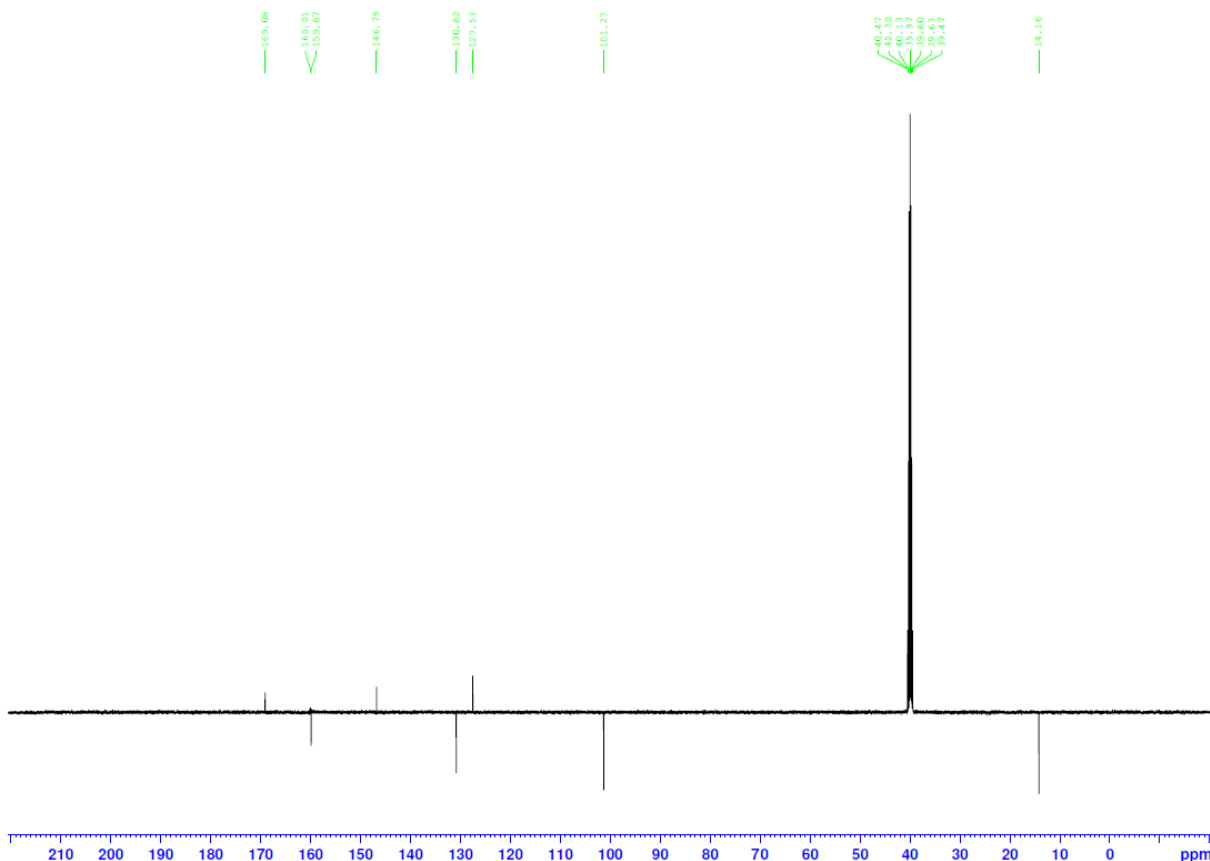
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#	ADDRESS	FREQUENCY	INTENSITY
1	11574.9	4695.294	1.82
2	14615.0	3646.845	0.74
3	14637.1	3639.892	0.77
4	15738.2	3292.761	0.87
5	15760.2	3285.808	0.82
6	20884.3	1670.368	15.00
7	22061.7	1299.175	2.5970
8	22209.0	1252.751	0.61
9	22214.8	1250.800	0.83
10	22220.7	1249.049	2.4968



NAME PI-1704-203
EXPNO 10
PROCNO 1
Date_ 20110905
Time 15.45
INSTRUM av500a
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 2050
CW 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 u
PL1 3.00 d
PL1W 35.6845317 M
SFO1 500.2630893 M
SI 32768
SF 500.2600000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00



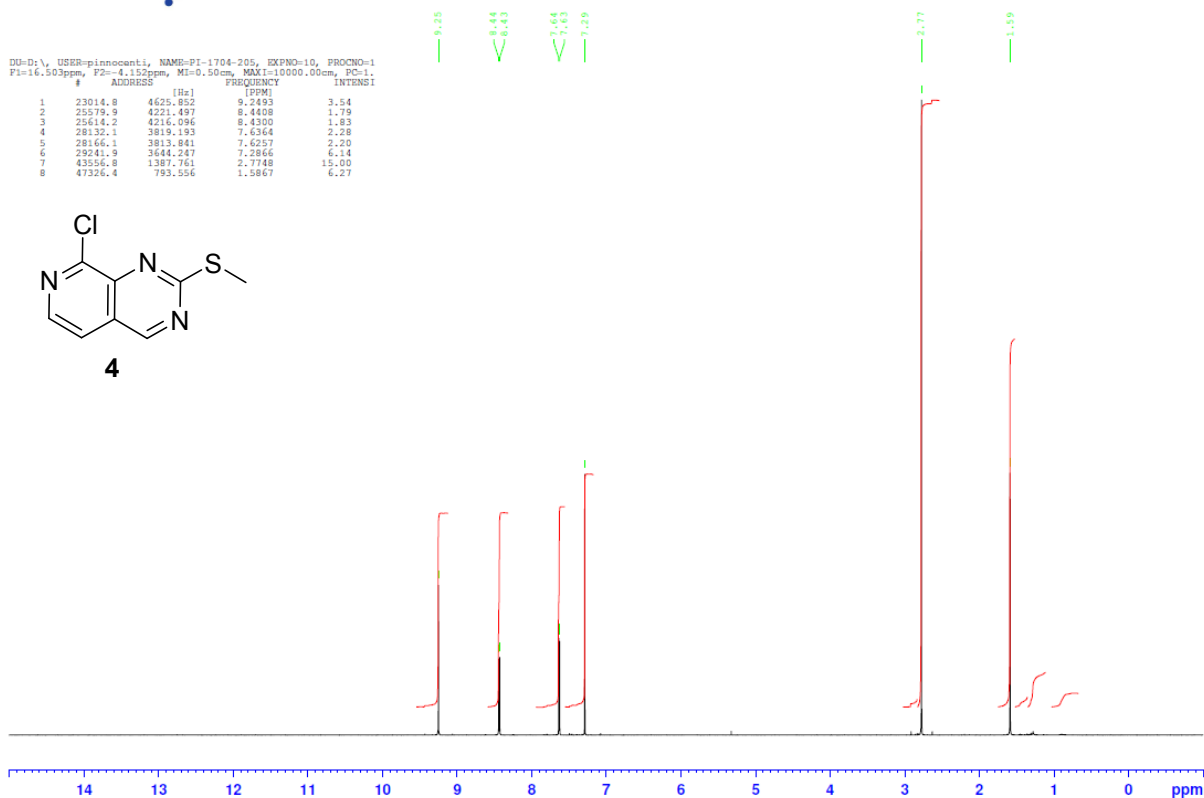
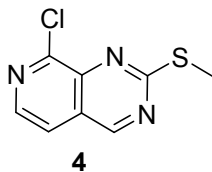
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PROCNO 1
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Time 21.05
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PROBHD 5 mm PABBO BB-
PULPROG deptqqep.2
TD 65536
SOLVENT DMSO
NS 2048
DS 8
SWH 30303.031 H
FIDRES 0.462388 H
AQ 1.0814105 s
RG 46300
CW 16.500 u
DE 6.00 u
TE 295.0 K
CNST2 145.0000000
CNST12 1.5000000
D1 4.0000000 s
D2 0.00344828 s
D12 0.00002000 s
D16 0.00020000 s
D28 2.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.75 u
PL1 2000.00 u
PL1W 1.00 d
PL1W 0.00000000 M
PL1W 65.24507804 M
SFO1 125.7703643 M
SF2 10.32 d
SFNAM2 Crp60comp.4
SFOAL2 0.500
SFOFF2 0.00 H

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 15.54 u
P3 10.36 u
P4 20.72 u
PCPD2 80.00 u
PL2 0.00 d
PL12 17.90 d
PL13 18.00 d
PL2W 23.10935593 M
PL12W 0.37478899 M
PL13W 0.3625859 M
SFO2 500.1320005 M

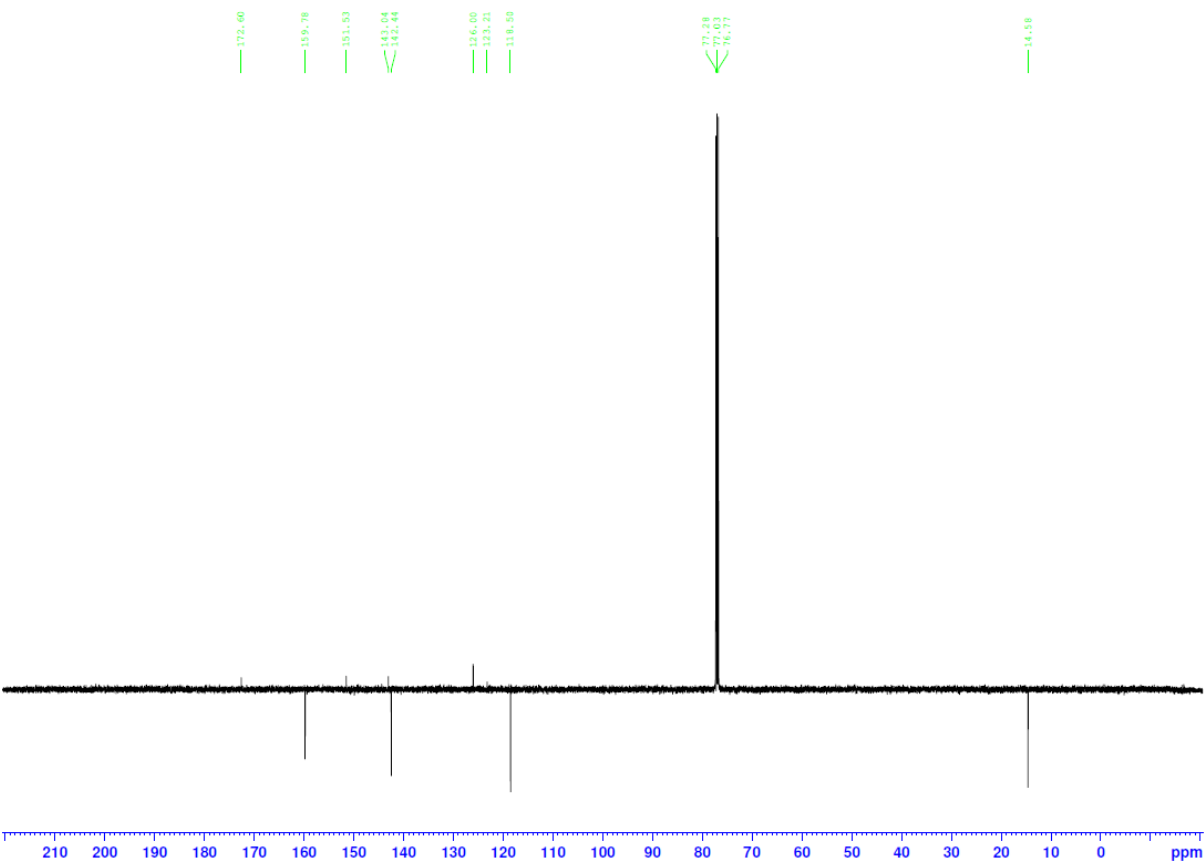
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GPNAM2 SINE.100
GPNAM3 SINE.100
GF1 31.00 %
GF2 31.00 %
GF3 31.00 %
P16 1000.00 u
SI 65536
SF 125.7577890 M
WDW EM
SSB 0
LB 1.00 H
GB 0
PC 1.40

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1 23014.8 4625.852 9.2493 3.54
2 23519.9 4221.497 8.4408 1.79
3 25614.2 4216.096 8.4300 1.83
4 28132.1 3819.193 7.6364 2.28
5 28166.1 3813.841 7.6257 2.20
6 29241.9 3644.247 7.2866 6.14
7 43556.8 1387.761 2.7748 15.00
8 47326.4 793.556 1.5867 6.27



NAME PI-1704-205
EXPNO 10
PROCNO 1
Date_ 20110906
Time 14.59
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.151632 H
AQ 3.1720407 s
RG 3250
DW 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.25 u
PL1 0.00 d
PL1W 23.10935593 W
SFO1 500.1330885 M
SI 65536
SF 500.1330005 M
WCM EM
SSB 0
LB 0.30 H
GB 0
PC 1.00



NAME PI-1704-205
EXPNO 11
PROCNO 1
Date_ 20110907
Time 4.40
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 8
SWH 30303.031 H
FIDRES 0.462388 H
AQ 1.0814103 s
RG 46300
DW 16.500 u
DE 6.00 u
TE 295.0 K
CNST1 145.000000
CNST12 1.5000000
D1 4.00000000 s
D2 0.00348820 s
D12 0.00002000 s
D16 0.00020000 s
D28 2.00000000 s
TD0 1

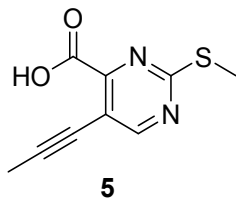
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NUC1 13C
P1 8.75 u
PL1 2000.00 u
PL1W 120.00 d
PL1 1.00 d
PL1W 0.00000000 W
PL1W 65.24507804 W
SFO1 125.7703643 M
SF2 10.32 d
SPNAM2 Crp60comp.f
SFOAL2 0.500
SFOFFS2 0.00 H

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 15.54 u
P3 10.34 u
P4 20.72 u
PCPD2 80.00 u
PL2 0.00 d
PL12 17.90 d
PL13 18.00 d
PL2W 23.10935593 W
PL12W 0.37478989 W
PL13W 0.3625853 W
SFO2 500.1320005 M

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 u
SI 65536
SF 125.7577890 M
WCM EM
SSB 0
LB 1.00 H
GB 0
PC 1.40

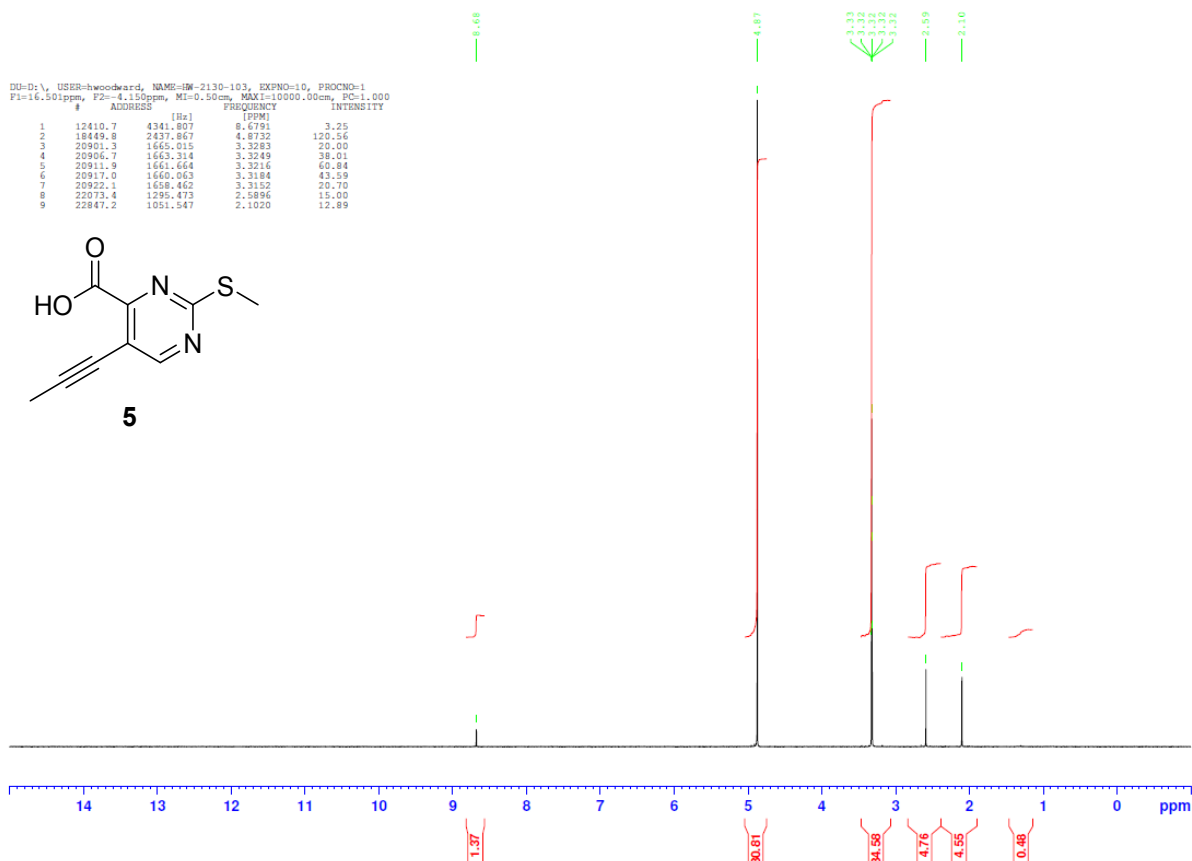
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1	12410.7	4341.807	8.6791	3.25	
2	18449.8	2437.867	4.8732	120.56	
3	20961.3	1665.015	3.3283	20.00	
4	20966.7	1663.314	3.3249	38.01	
5	20911.9	1661.664	3.3216	60.84	
6	20917.0	1660.063	3.3184	43.59	
7	20922.1	1658.462	3.3152	20.70	
8	22073.4	1295.473	2.5896	15.00	
9	22847.2	1051.547	2.1020	12.89	



NAME HW-2130-103
EXPNO 10
PROCNO 1
Date_ 20140415
Time 17:44
INSTRUM 5 mm QNP 1H/13
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 3200
DM 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.0000000 s
TDO 1

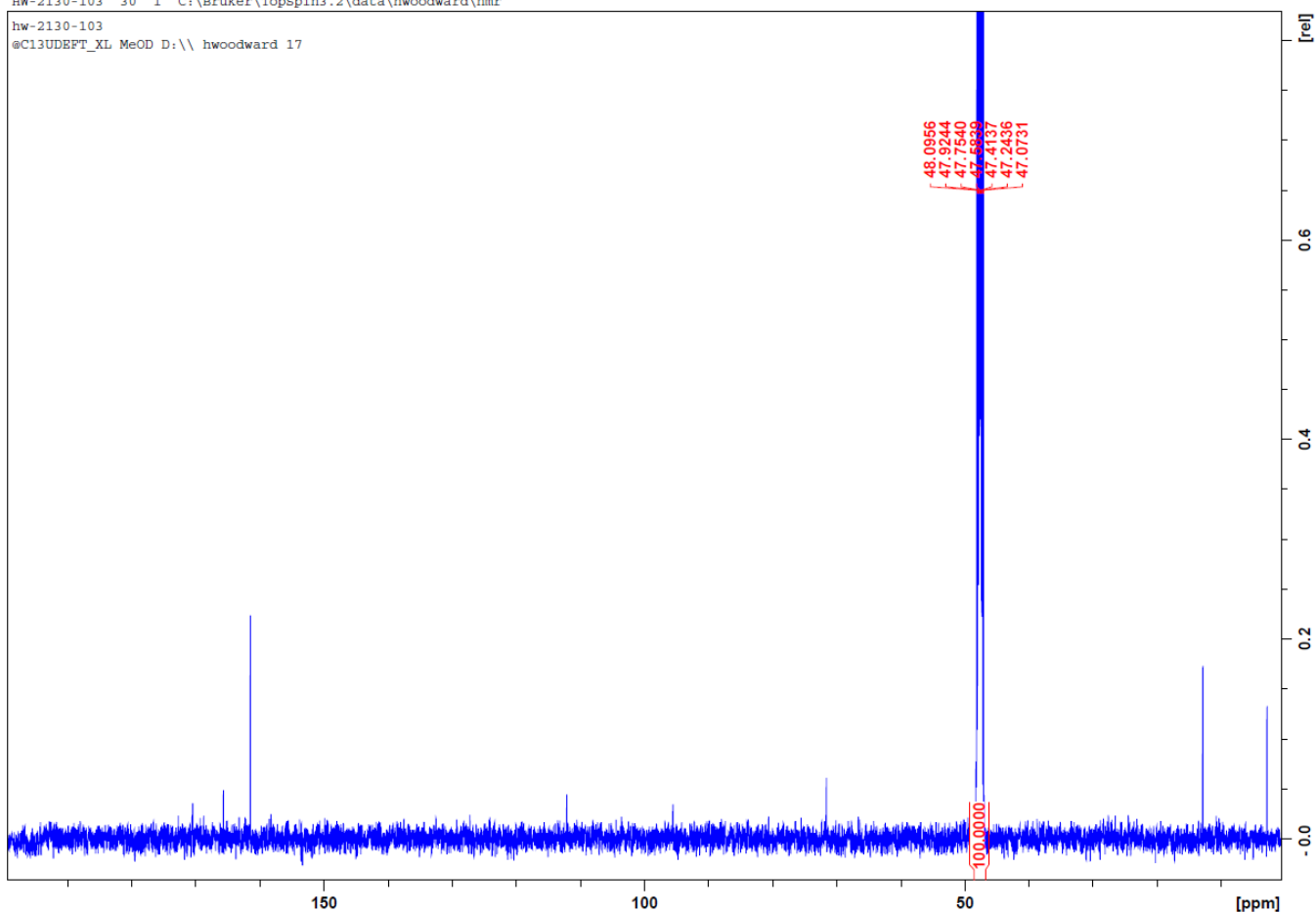
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P1 9.50 u
PL1 -3.00 dB
PL1W 35.68453217 W
SFO1 500.2630993 M
SI 32768
SF 500.2600000 M
WDM 0
SSB 0
LB 0.30 H
GB 0
PC 1.00



HW-2130-103 30 1 C:\Bruker\TopSpin3.2\data\hwoodward\nmr

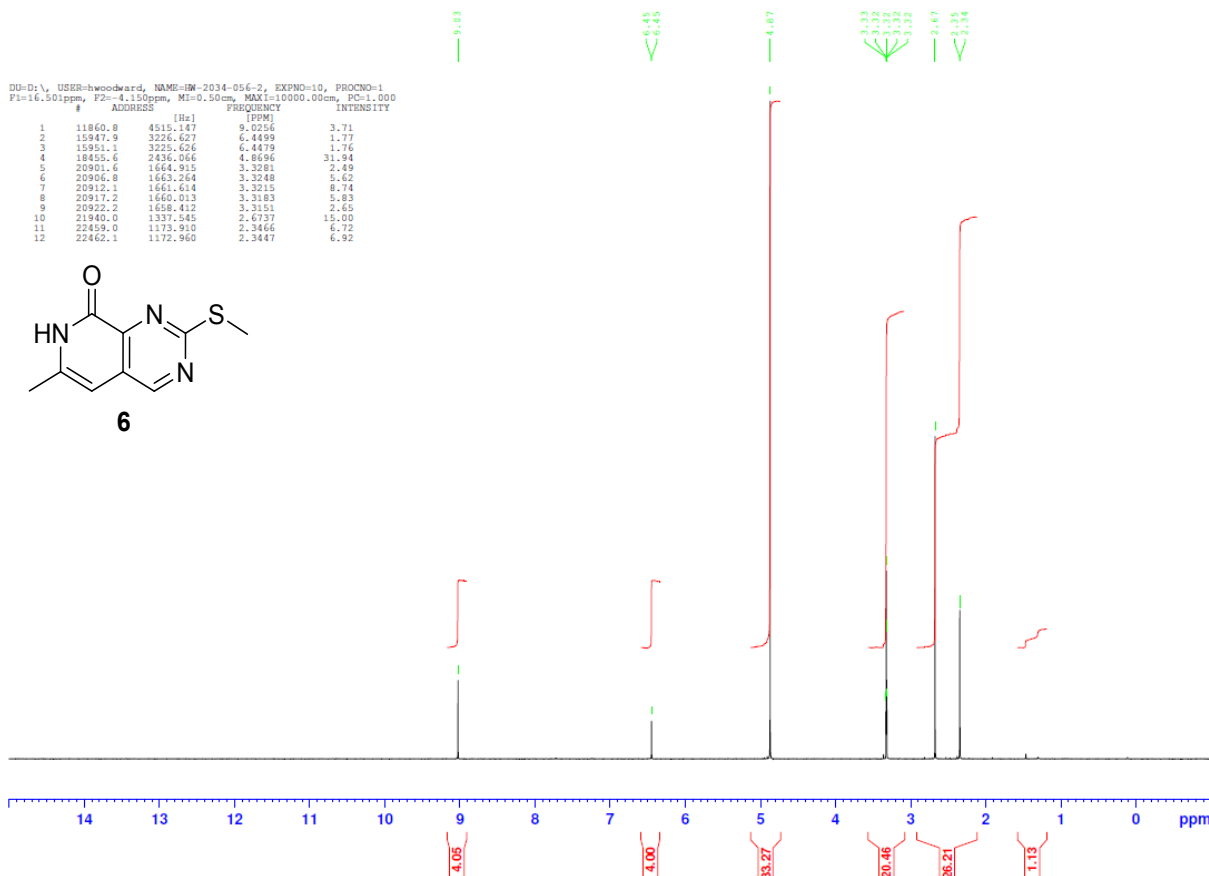
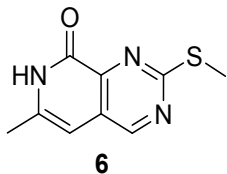
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1	11860.8	4515.147	3.71
2	15947.9	3226.627	1.77
3	15951.1	3225.626	1.76
4	18455.6	2436.066	31.84
5	20901.6	1664.915	2.49
6	20906.8	1663.264	5.62
7	20912.1	1661.614	8.74
8	20917.2	1660.013	3.3183
9	20922.2	1658.412	2.65
10	21940.0	1337.545	2.6737
11	22459.0	1173.910	2.3466
12	22462.1	1172.960	2.3447



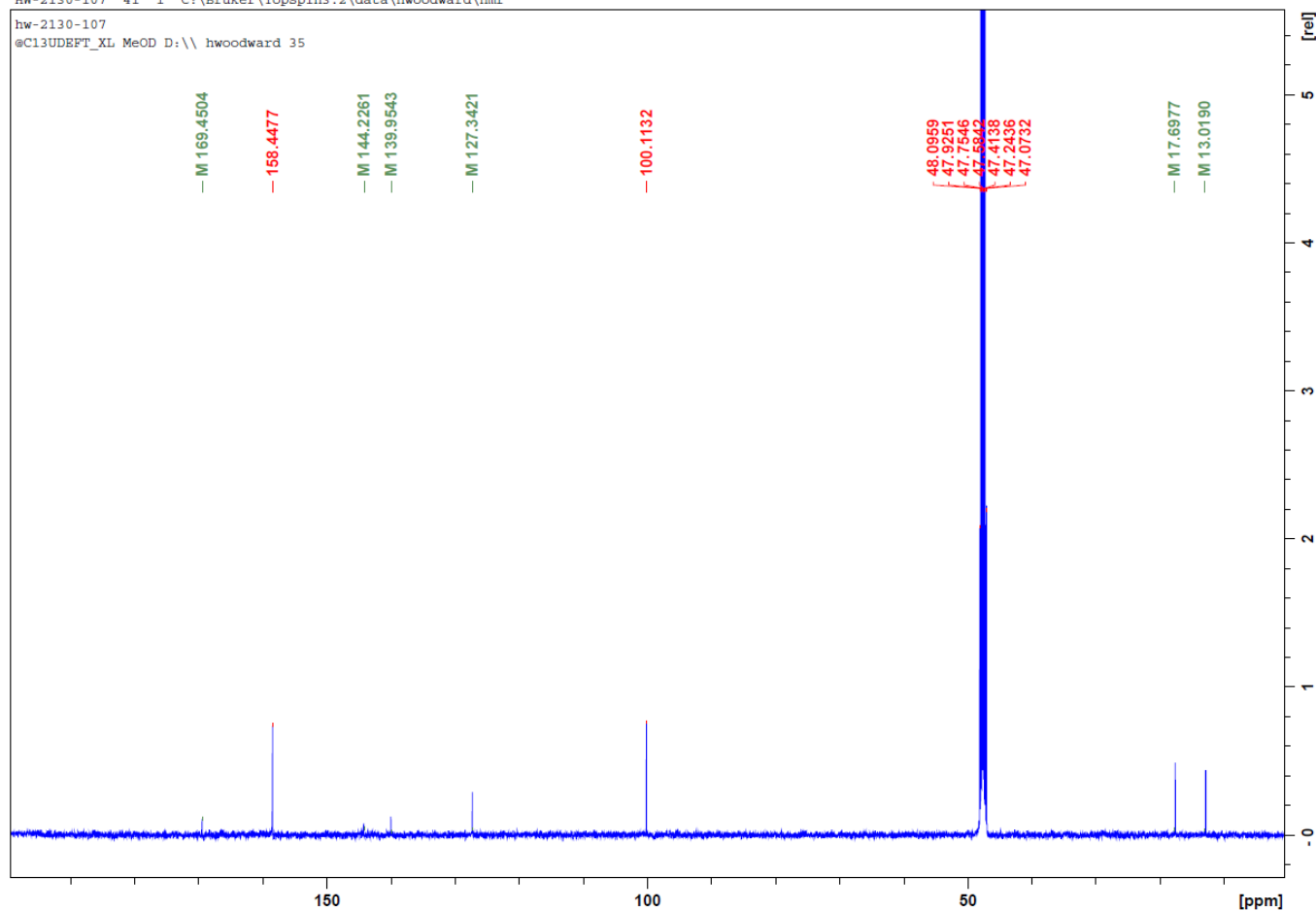
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PULPROG zg30
TD 65536
DO SOLVENT MeOD
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 8200
DM 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 u
PL1 3.00 dB
PLW 35.6843217 M
SFO1 500.2630893 M
SI 32768
SF 500.2600000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00

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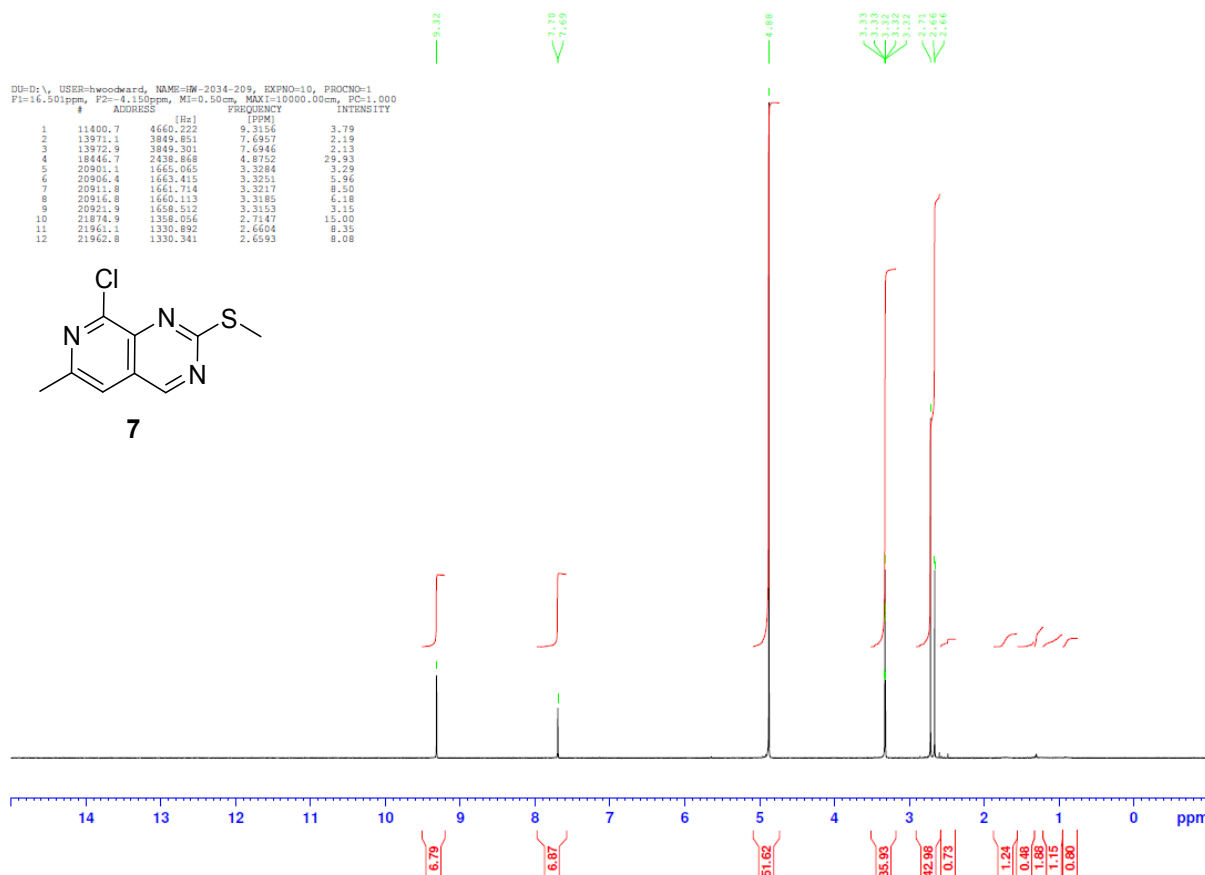
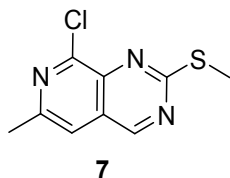
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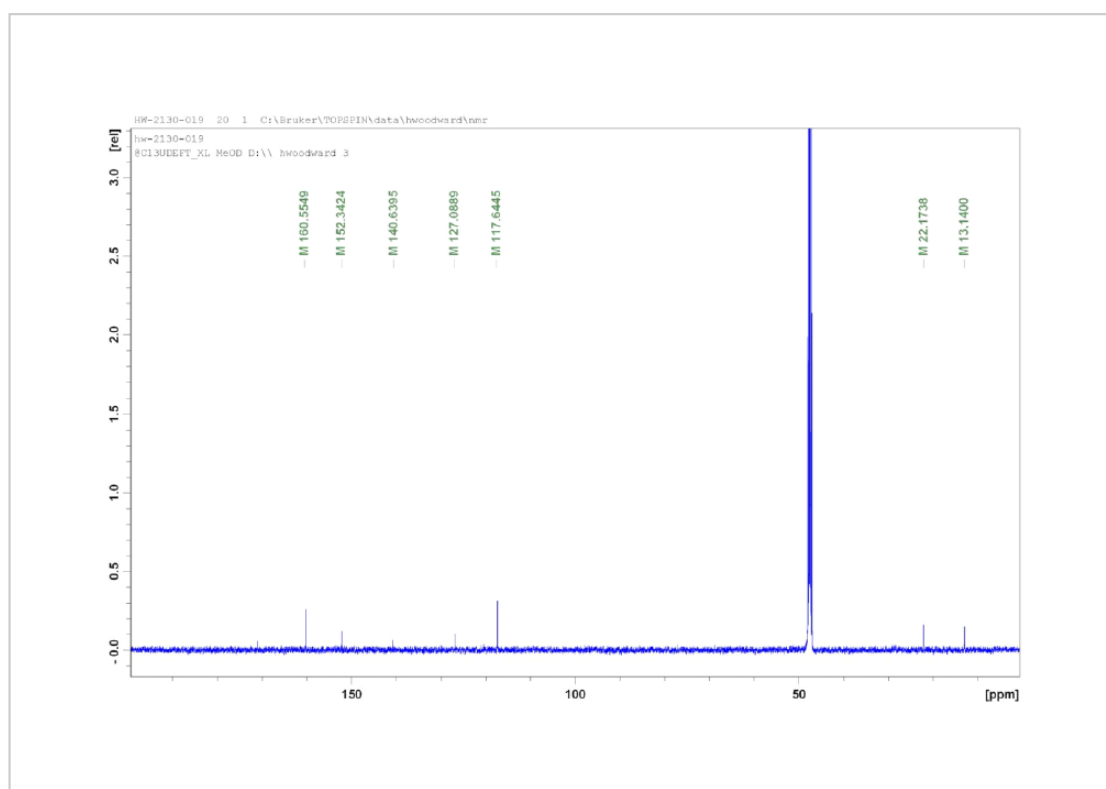


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1	11400.7	4660.222	3.79
2	13971.1	3849.851	2.19
3	13972.9	3849.301	2.13
4	18446.7	2438.868	29.93
5	20901.1	1665.065	3.29
6	20906.4	1663.415	5.96
7	20911.8	1661.714	8.50
8	20916.8	1660.113	6.18
9	20921.9	1658.512	3.15
10	21874.9	1358.056	15.00
11	21961.1	1330.892	8.35
12	21962.8	1330.341	8.08



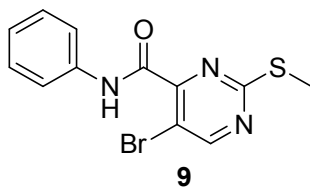
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PROCNO 1
Date_ 20131031
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PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 10330.378 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 6500
EW 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 9.50 u
PL1 -3.00 d
PL1W 35.6843217 M
SFO1 500.2630893 M
SI 32768
SF 500.2600000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00



18 March 2014
09:53

DU=D:\, USER=pinnocenti, NAME=PI-2029-140, EXPNO=10, PROCNO=1
F1=16.503ppm, F2=4.152ppm, M1=0.50cm, MAX1=10000.00cm, PC=1.

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1	24235.6	4433.402	8.8645	5.01
2	27745.7	3880.109	7.7882	1.45
3	27752.6	3879.008	7.7560	1.78
4	27764.7	3877.108	7.7522	0.50
5	27800.9	3871.405	7.7408	1.89
6	27806.6	3870.506	7.7390	1.64
7	28762.5	3719.817	7.4377	1.32
8	28810.4	3712.265	7.4226	1.91
9	28815.8	3711.415	7.4209	1.65
10	28852.6	3705.613	7.4093	0.51
11	28864.1	3703.813	7.4057	1.36
12	29241.3	3644.347	7.2868	18.03
13	29415.2	3616.940	7.2320	0.76
14	29462.4	3609.488	7.2171	1.25
15	29509.7	3602.036	7.2022	0.56
16	43907.4	1332.496	2.6643	15.00
17	47355.0	789.055	1.5777	13.87
18	47445.7	774.751	1.5491	1.13
19	47452.4	773.701	1.5470	1.22
20	47459.0	772.651	1.5449	1.10



NAME PI-2029-140
EXPNO 10
PROCNO 1
Date_ 20130930
Time 13:21
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 4100
DM 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.0000000 s
D11 1
D12 1
D20 1

CHANNEL f1
NUC1 1H
P1 10.25 u
PL1 0.00 d
PL1W 23.1093593 M
SFO1 500.1330885 M
SI 65536
SF 500.1330885 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00

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8304.57
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159.30
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NAME PI-2029-140
EXPNO 11
PROCNO 1
Date_ 20130930
Time 21:18
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 17996
SOLVENT CDCl3
NS 4096
DS 0
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AQ 0.35999500 s
RG 46300
DM 20.000 u
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TE 295.0 K
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D12 0.00002000 s
D20 60.00000000 s
D21 1

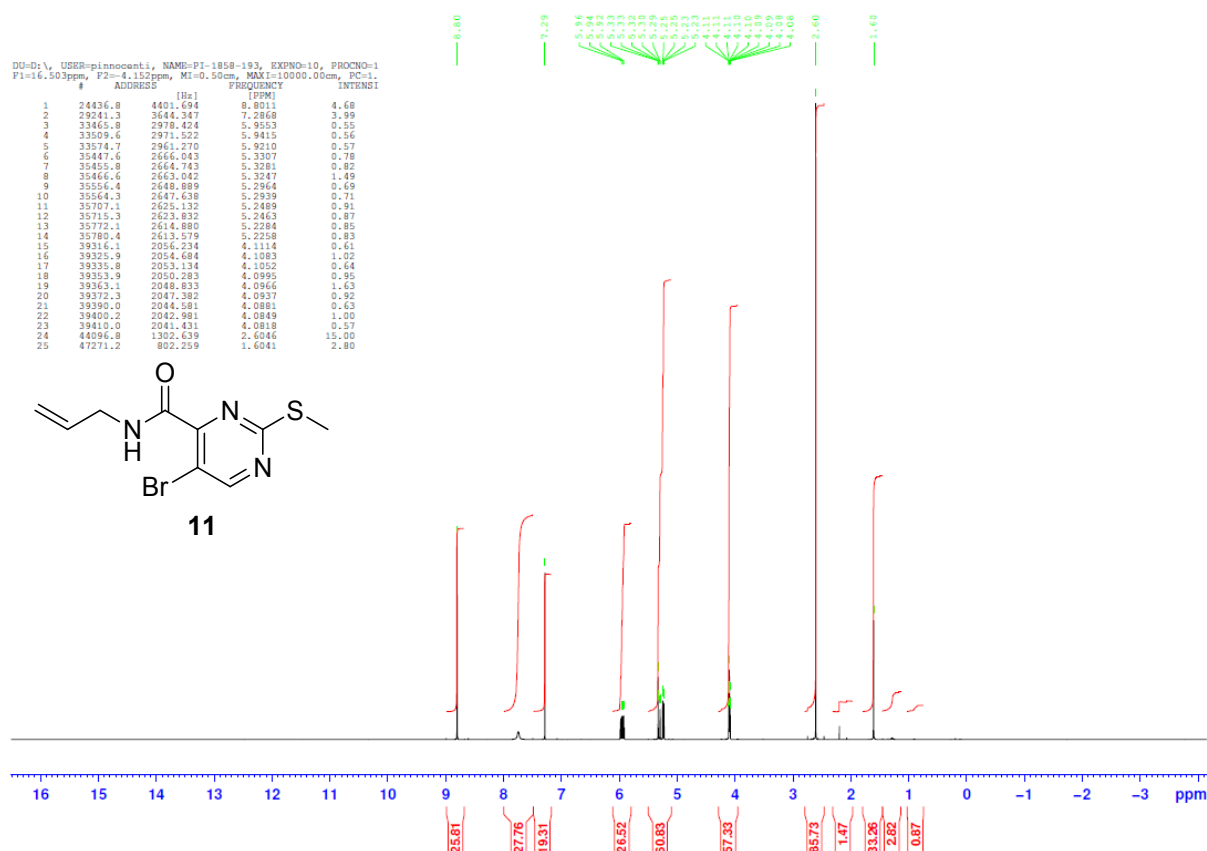
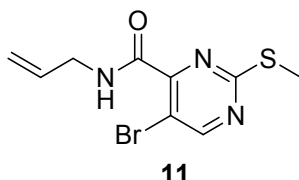
CHANNEL f1
NUC1 13C
P1 8.75 u
PL1 2000.00 u
PL2 500.00 u
PL1 1.00 d
PL1W 65.24507904 M
SFO1 125.7703643 M
SF2 10.32 d
SF8 10.32 d
SFO12 Crp60comp.4
SFO12 Crp60, 5, 5, 20, 1
SFOAL2 0.500
SFOAL8 0.500
SFOFFS2 0.00 H
SFOFFS8 0.00 H

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 0.00 d
PL12 17.90 d
PL12W 23.1093593 M
PL12W 0.37478989 M
SFO2 500.1320005 M
SI 32768
SF 125.7577890 M
WDW EM
SSB 0
LB 2.00 H
GB 0
PC 1.40

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

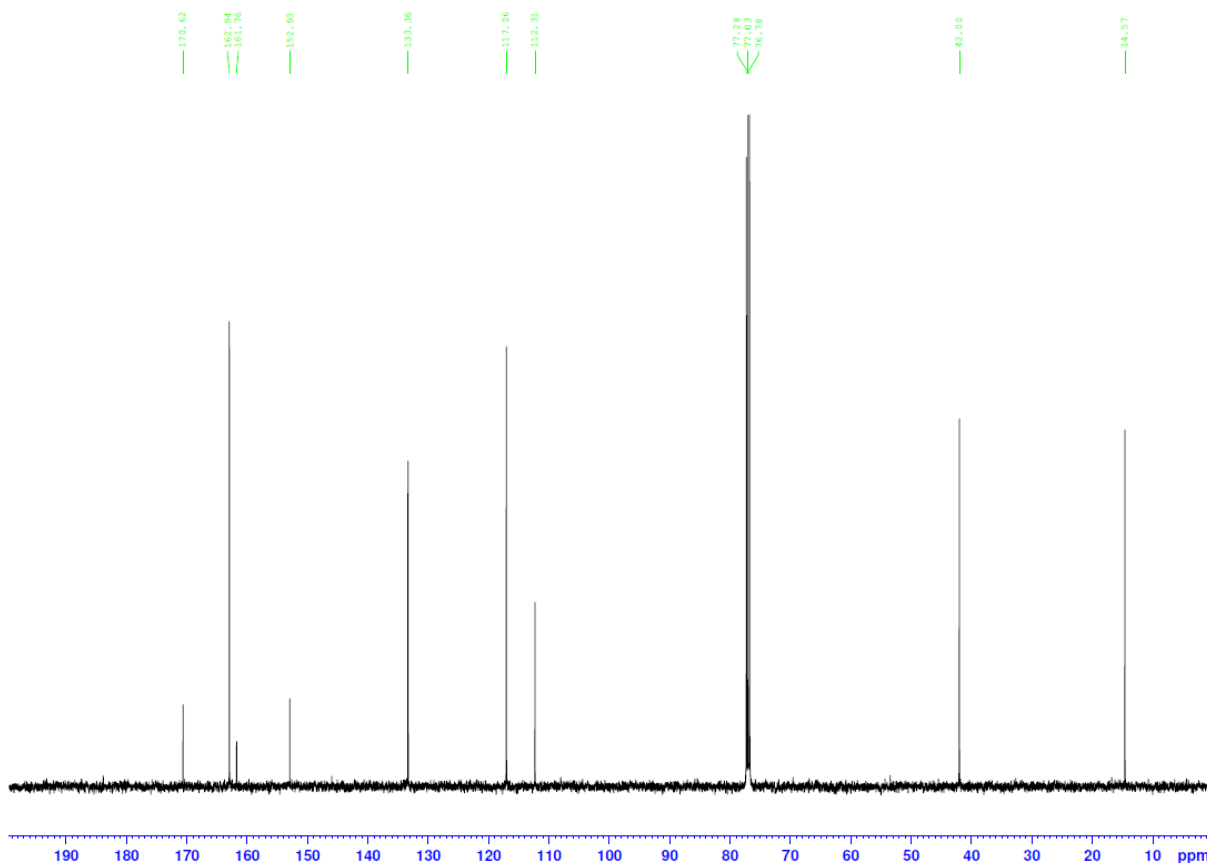

```
DU=D:\, USER=pinnocenti, NAME=PI-1858-193, EXPNO=10, PROCNO=1
F1=16.503ppm, F2=4.152ppm, MI=0.50cm, MAXI=10000.00cm, PC=1.
# ADDRESS FREQUENCY INTENS
```

Sample No.	P_{22} (1.52 ppm)	P_{33} (1.52 ppm)	P_{44} (1.52 ppm)	P_{55} (1.52 ppm)	P_{66} (1.52 ppm)	P_{77} (1.52 ppm)	P_{88} (1.52 ppm)	P_{99} (1.52 ppm)
1	24436.8	3644.674	5830.7	4.68				
2	22821.3	3644.674	7186.0	3.99				
3	33465.8	3644.674	5.9553	0.55				
4	33716.2	3644.674	5.9553	0.56				
5	33574.7	3644.674	5.9310	0.57				
6	35447.6	3644.604	8.3207	0.82				
7	35455.8	3644.743	5.3281	0.78				
8	34466.4	3644.674	7.1479	0.79				
9	35556.4	3644.689	5.2964	0.69				
10	35577.2	3644.689	5.2964	0.71				
11	35707.1	3625.132	5.2489	0.91				
12	35715.1	3625.132	5.2463	0.87				
13	35717.2	3625.132	5.2463	0.85				
14	35780.4	3631.579	5.2258	0.83				
15	39316.1	2056.234	4.1114	0.61				
16	39325.5	2056.234	4.1114	0.82				
17	39335.8	2053.134	4.1052	0.64				
18	39335.3	2053.283	4.0995	0.95				
19	39335.3	2053.283	4.0995	1.63				
20	39372.3	2047.382	4.0937	0.92				
21	39390.0	2044.581	4.0881	0.63				
22	39401.2	2044.581	4.0881	0.88				
23	39410.0	2041.431	4.0818	0.57				
24	40496.8	1302.339	2.6046	15.00				



NAME	PI-1858-193
EXPNO	10
PROCNO	1
Date_	20121101
Time	16.25
INSTRUM	av590b
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DSH	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 s
RG	2890
DW	48.4000 us
DE	6.00 us
TE	295.0 K
D1	1.00000000 s
TDO	1

```
===== CHANNEL f1 =====
NUC1              1H
P1                10.25 u
PL1              0.00 d
PLW              23.10935593 W
SFO1             500.1330885 M
SI               65536
SF              500.1300000 M
WDW              EM
SSB              0
LB              0.30 H
GB              0
PC              1.00
```



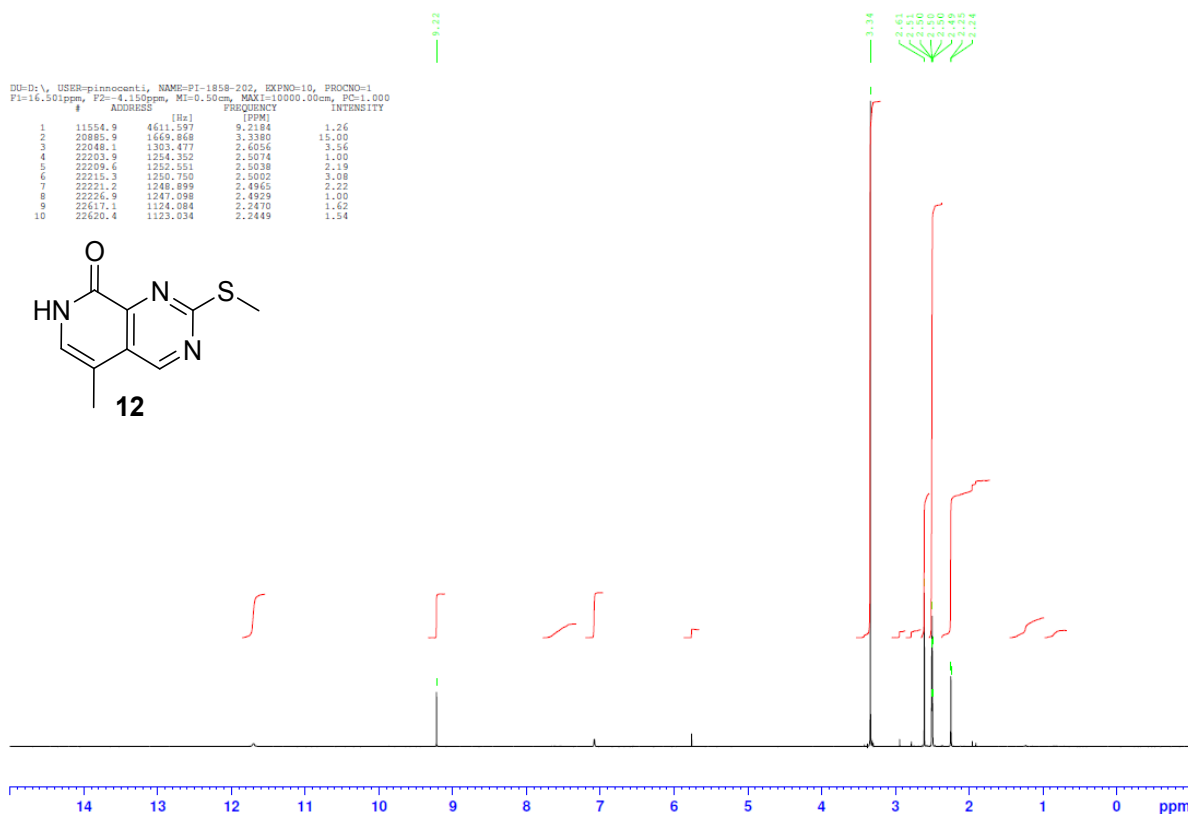
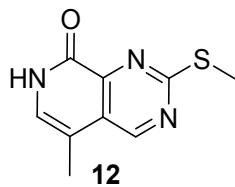
NAME	PI-1858-193
EXPNO	12
PROCNO	1
Date_	20121102
Time	4.37
INSTRUM	av500b
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	17996
SOLVENT	CDCl3
NS	4096
DS	0
SWH	25000.000 MHz
FIDRES	3891.98 Hz
AQ	0.3599900 s
RG	46300
DW	20.000 us
DE	6.00 us
TE	295.1 K
D1	2.00000000 s
D11	0.03000000 s
D12	0.00020000 s
D2	60.00000000 s
TD0	

```
===== CHANNEL f1 =====
MUC1      13C
P1         8.75 u
P12        2000.0 u
P26        500.0 u
PL1        1.00 u
PL1W       65.24507904 W
SF01       125.7703643 M
SF2        10.32 C
SP8        10.32 C
SPNAM2     Crp60comp.4
SPNAM8     Crp60, 0.5, 20.1
SPCAL2     0.500
SPCAL8     0.000
SPOFFS2    0.00 F
SPOFFS8    0.00 F
```

```
===== CHANNEL f2 =====
CPDPRG2          waltz16
NUC2             1H
PCPD2            80.00 u
PL2              0.00 d
PL12             17.90 d
PL2W             23.10935593 u
PL12W            0.37478989 M
SFO2             500.13200000 M
SI               32768
SF              125.7577890 M
WDM              EM
SSB              0
LB               2.00 F
GB               0
PC               1.40
```

DU-D:_USER-pinnocenti, NAME-PI-1858-202, EXPNO=10, PROCNO=1
F1=4.00ppm, F2=4.150ppm, MISO=0.50cm, MAXI=10000.00cm, PC=1.000

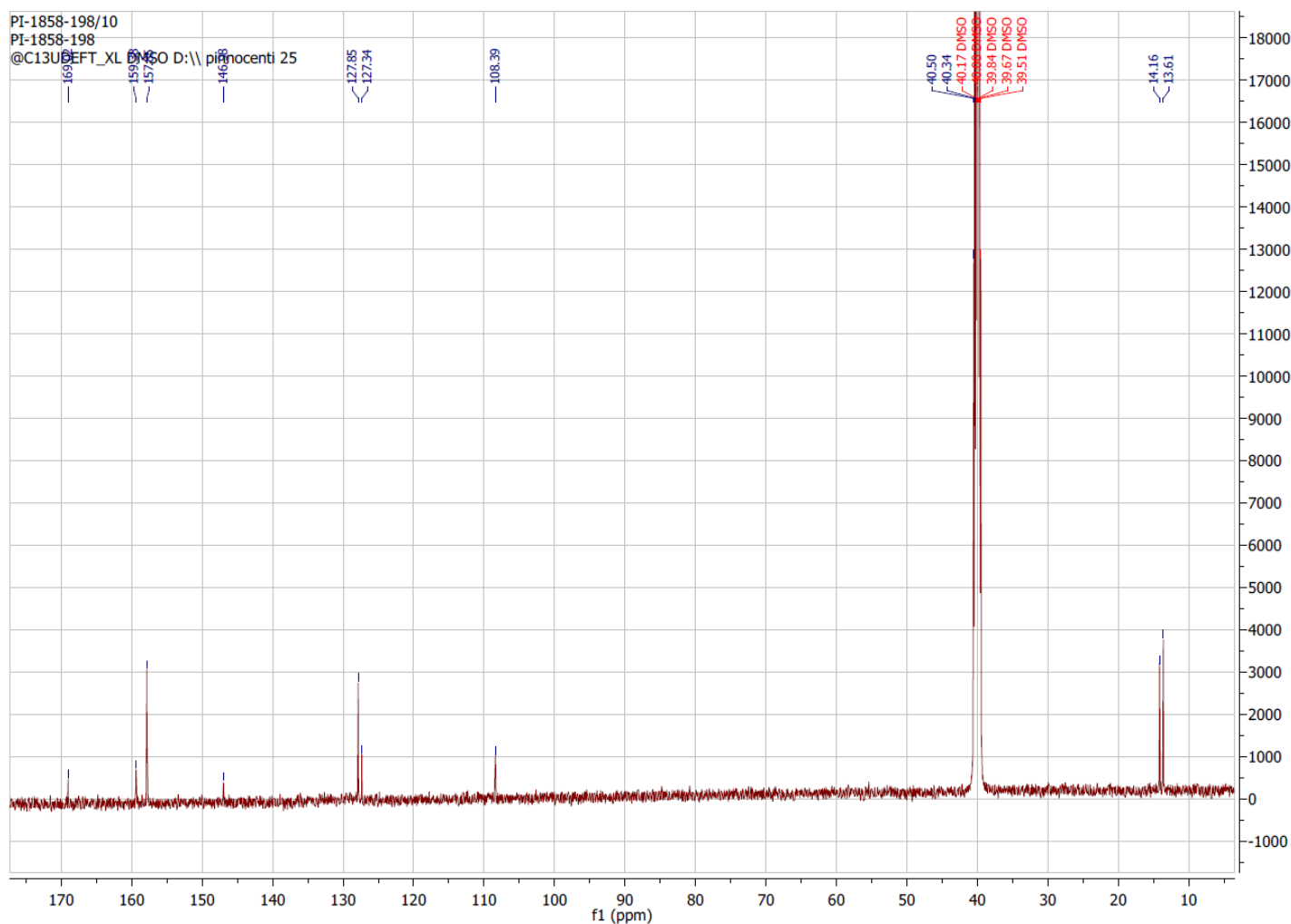
#	ADDRESS	[Hz]	[ppm]	FREQUENCY	INTENSITY
1	11554.9	4611.597	9.2184	1.26	
2	20885.9	1469.868	3.3380	15.00	
3	22048.1	1303.477	2.6056	3.56	
4	22203.9	1254.352	2.5074	1.00	
5	22209.6	1252.551	2.5038	2.19	
6	22215.3	1250.750	2.5002	3.08	
7	22221.2	1248.949	2.4965	2.22	
8	22226.9	1247.098	2.4929	1.00	
9	22617.1	1124.084	2.2470	1.62	
10	22620.4	1123.034	2.2449	1.54	



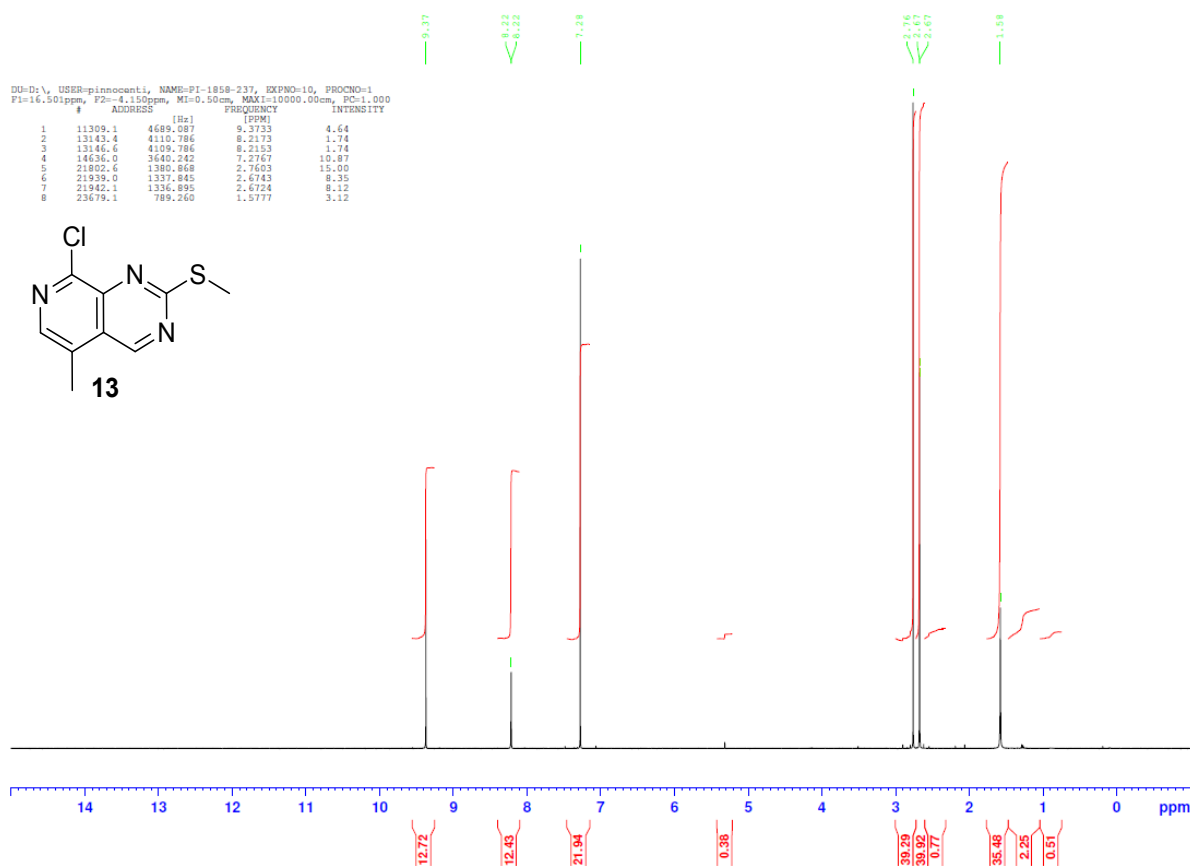
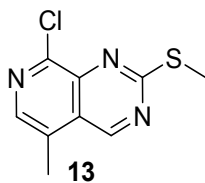
NAME PI-1858-202
EXPNO 10
PROCNO 1
Date_ 20121116
Time 10:14
INSTRUM av500a
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 8200
LW 48.400 u
DE 6.00 u
TE 292.7 K
D1 1.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 u
PL1 3.00 dB
PL1W 35.68453217 W
SFO1 500.2610893 M
S1 32768
SF 500.2600000 M
WDM 0
SSB 0
LB 0.30 H
GB 0
PC 1.00

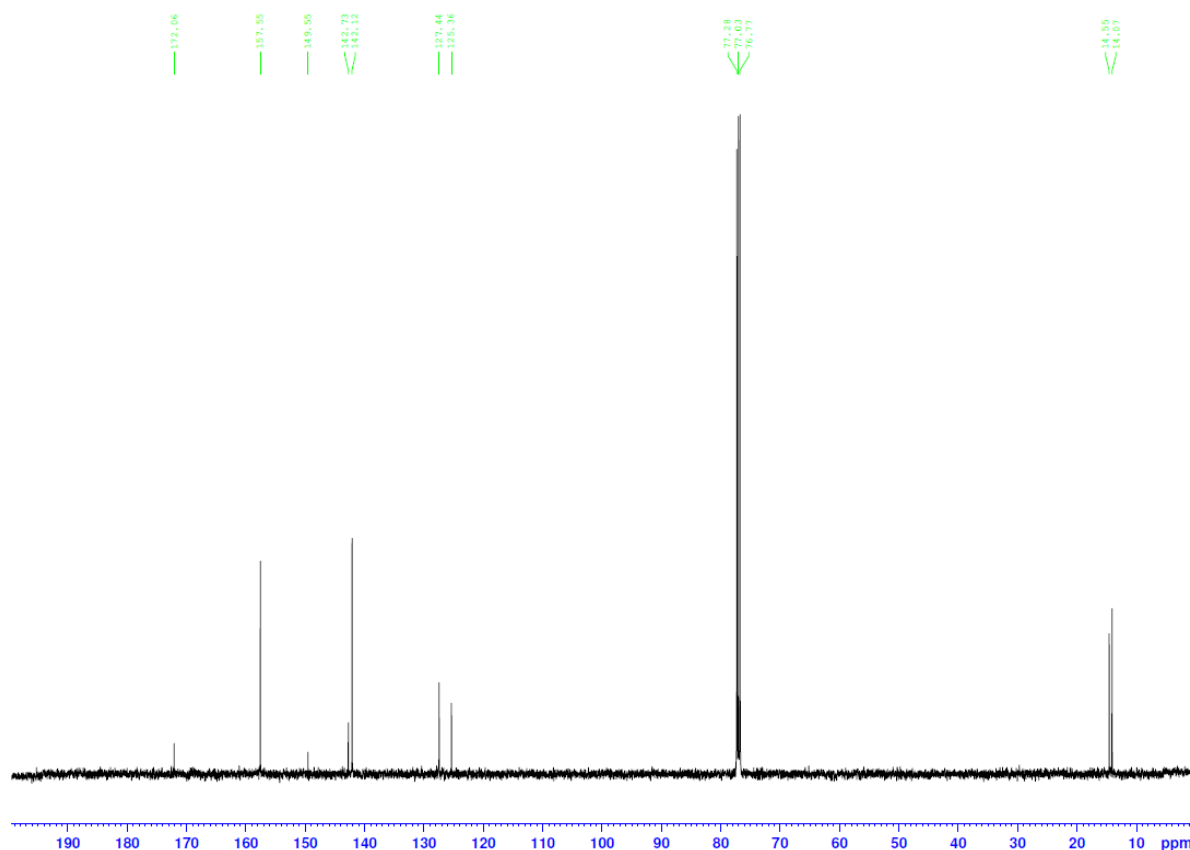
PI-1858-198/10
PI-1858-198
@C13UDEFT_XL DMSO D:



```
DU=D:\_USER-pinnocenti, NAME=P1-1858-237, EXPNO=10, PROCNO=1
F1=16.50ppm, F2=15.15ppm, M0=0.50mm, M1=0.0000, 0.00cm, P1=0.000
ADDRESS          FREQUENCY          INTENSITY
              [Hz]              [PPM]
1      11309.1      4699.087      9.2733      4.64
2      41343.4      4108.786      8.2173      1.74
3      13144.6      4019.086      8.1353      1.74
4      14636.0      3640.242      7.2767      10.87
5      21802.6      1380.686      2.7603      15.00
6      21939.0      1337.845      2.6743      8.35
7      21942.1      1336.995      2.6744      9.12
8      23672.1      789.260      1.5777      3.12
```



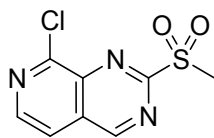
NAME	PI-1858-237
EXPNO	10
PROCNO	1
FILE	20130013
TIME	17:27
INSTRUM	av500a
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
TD SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
F2FIDRES	0.157532
AQ	3.1720407
RH	7290
TW	48.400 us
DE	6.00 us
TE	295.0 K
D1	1.00000000 s
TD0	1
===== CHANNEL f1 =====	
NUC1	13
F1	101.626119 MHz
PL1	-3.00 dB
SFO1	36.68430183 MHz
PL10	500.26230891 MHz
SI	321768
SWH	500.26000000 MHz
MUF	128
GB	0.30 Hz
LO	0.00
PC	1.00



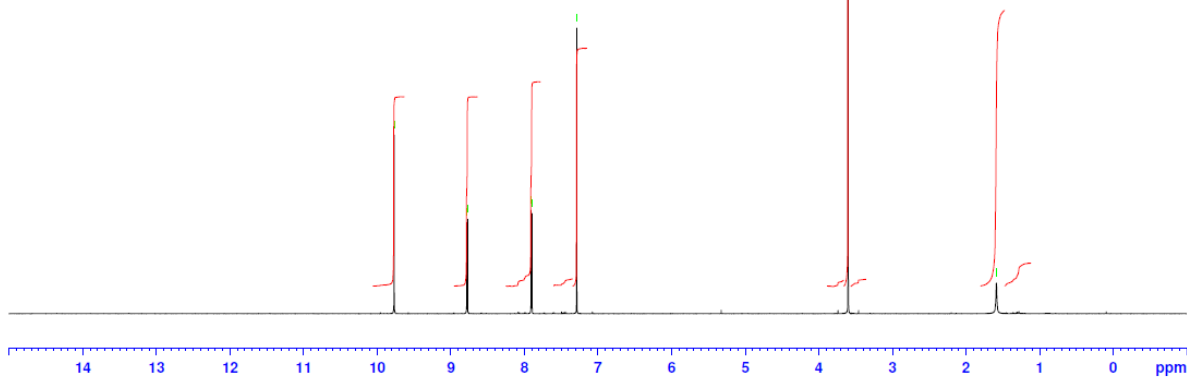
NAME	PI-1858-205
EXPNO	11
PROCNO	
Time	20121120
Time	5.25
INSTRUM	PROBHD
PROBHD	5 mm PABBO H-1
PROCPRG	ufdc ft
TD	1
SOLVENT	CDCl ₃
NS	409
DS	0
SWH	25000.000
FIDRES	1.3818358
RG	0.3599900
WE	6.300
WDW	4.000
SSB	0.000
LB	25.1
D1	2.00000000
D11	0.03000000
D2	0.03000000
D3	0.03000000
D4	60.00000000
D5	1
=====	CHANNEL F1 ==
NUC1	1
PI1	83C
P1	1.75
P2	200.000
P26	500.000
PL1	1.00
PLW	65.24500000
SF01	125.7703643
SF02	10.32
SF03	10.32
SPHARM2	Crp60comp.4
SPHARM3	Crp60 5, 5, 5, 5
SPHARM4	0.500
SPHARM5	0.500
SPHARM6	0.500
SPHARM7	0.500
=====	CHANNEL F2 ==
NUCPRG2	
NAME	HK walz13.6
PCF02	80.00
PCF03	80.00
PL12	17.90
PL2W	23.10935593
PL3W	0.37478990
PL4W	500.1320005
PL5W	1.00
SF	125.7571890
SP	0.500
KWM	EM
GC	0.00
PC	1.40

DU=D:\, USER=pinnocenti, NAME=PI-1858-057, EXPNO=10, PROCNO=1
F1=16.503ppm, F2=4.132ppm, M0=0.50cm, M1=15000.00cm, PC=1

#	ADDRESS	[Hz]	[ppm]	FREQUENCY	INTENSITY
1	21365.5	4885.820	9.7691	4.31	
2	24496.4	4392.292	8.7823	2.19	
3	24531.3	4386.790	8.7713	2.24	
4	27270.1	3955.078	7.9081	2.44	
5	27305.0	3949.577	7.8971	2.37	
6	29241.0	3644.397	7.2869	6.75	
7	40941.8	1799.968	3.5990	15.00	
8	47330.8	792.856	1.5893	0.72	

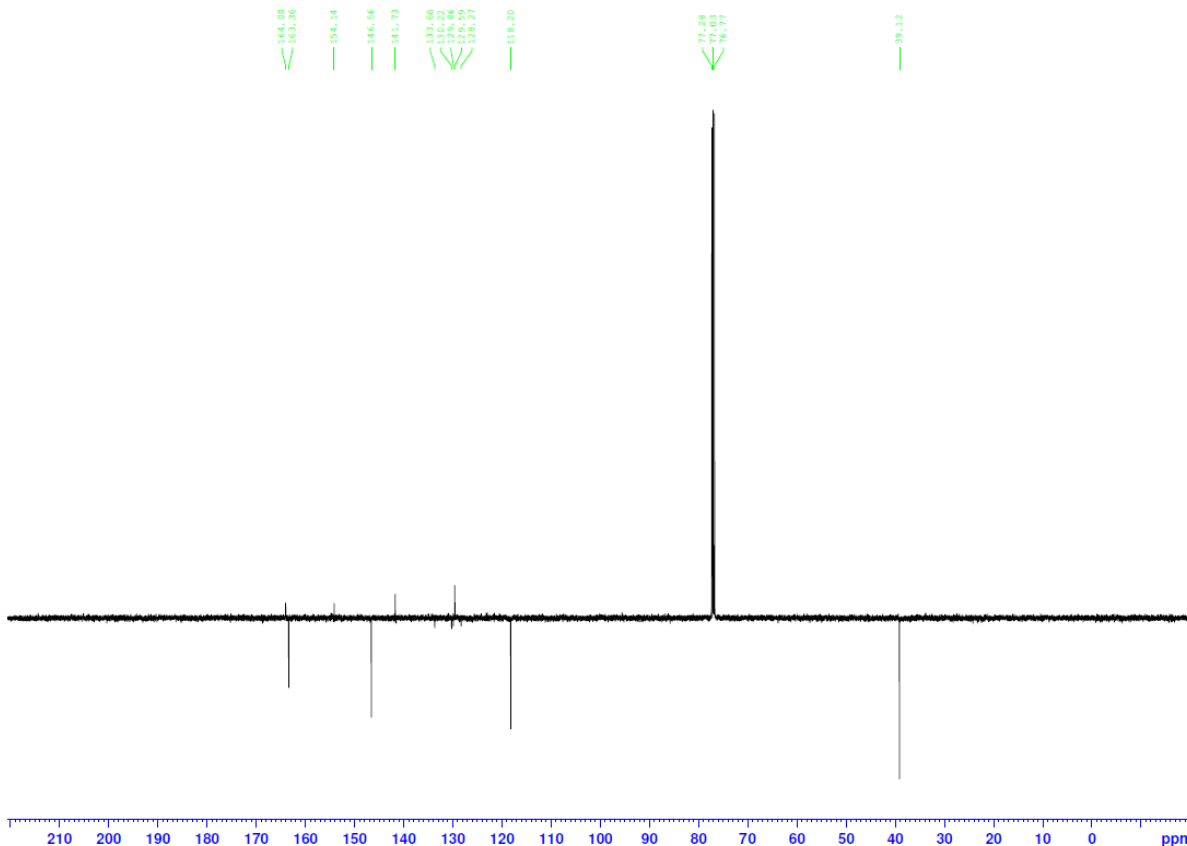


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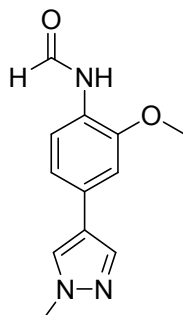
NAME PI-1858-057
EXPNO 10
PROCNO 1
Data_ 20120215
Time 13.27
INSTRUM mv500b
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720457 s
RG 3250
RW 46.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.25 u
P11 0.00 d
P1LW 23.10935593 M
SFO1 500.1330885 M
SI 65536
SF 500.1330000 M
NEW EM
SSB 0
LB 0.30 H
GB 0
PC 1.60

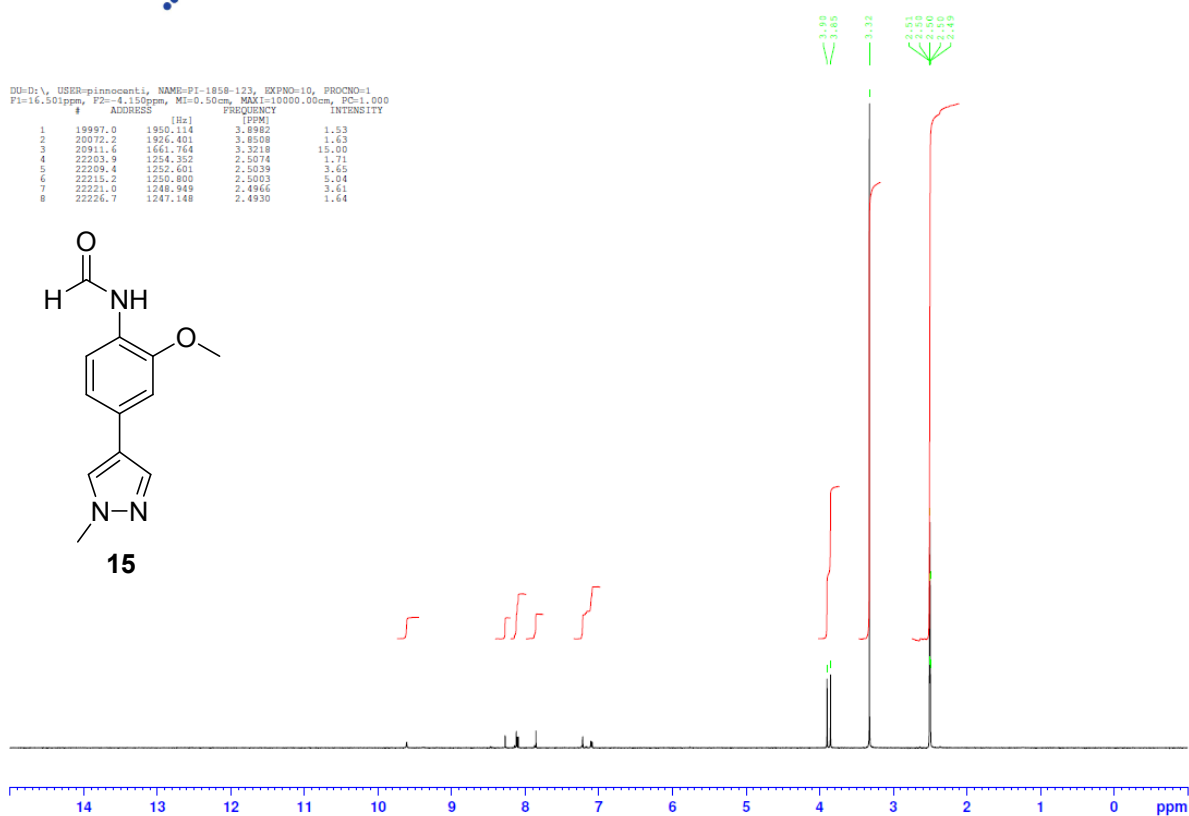


DU=Ds\, USER=pinnocenti, NAME=PI-1858-123, EXPNO=10, PROCNO=1
F1=16.501ppm, F2=4.150ppm, M1=0.50cm, NAXI=10000.00cm, PC=1.000

#	ADDRESS	FREQUENCY	INTENSITY
1	19997.0	1950.114	3.8982
2	20072.2	1926.401	3.8508
3	20911.6	1661.764	3.3218
4	22203.9	1254.352	1.71
5	22209.4	1252.601	2.5039
6	22215.2	1250.800	5.04
7	22221.0	1248.949	2.4966
8	22226.7	1247.148	1.64

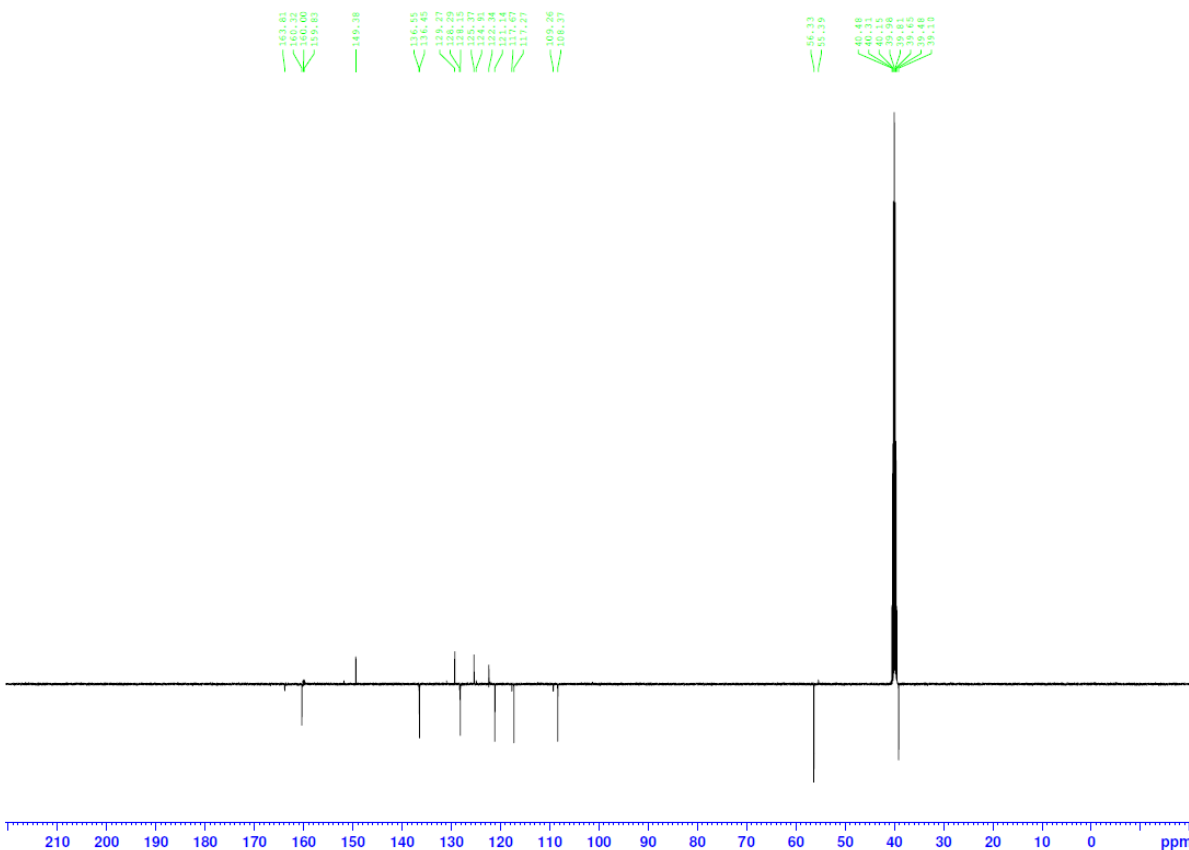


15



NAME PI-1858-123
EXPNO 10
PROCNO 1
Date_ 20120704
Time 10.01
INSTRUM mv500a
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.15732 H
AQ 3.1720407 s
RG 8200
DM 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 u
PL1 8.55 d
PL1W 35.6843217 W
SFO1 500.2630893 M
SI 32768
SF 500.2600000 M
WCH RM
SSB 0
LB 0.30 H
GB 0
PC 1.00



NAME PI-1858-033
EXPNO 10
PROCNO 1
Date_ 20120112
Time 8.54
INSTRUM mv500b
PROBHD 5 mm PABBO BB-
PULPROG deptqqep.2
TD 65536
SOLVENT DMSO
NS 4096
DS 2
SWH 30303.031 H
FIDRES 0.462388 H
AQ 1.0814105 s
RG 46300
DM 16.500 u
DE 6.00 u
TE 295.0 K
CNS12 145.000000
CNS12 1.5000000
D1 4.00000000 s
D2 0.00344828 s
D12 0.00020200 s
D16 0.00020200 s
D28 2.00000000 s
TDO 1

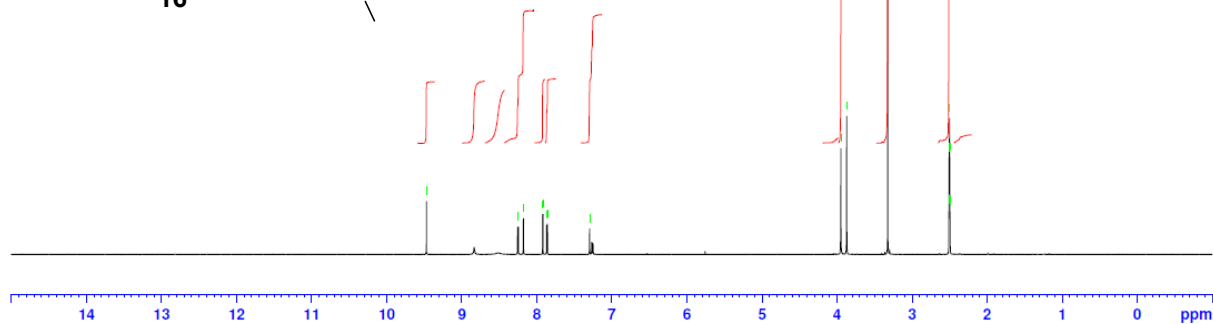
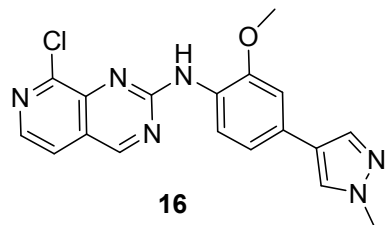
===== CHANNEL f1 =====
NUC1 13C
P1 8.75 u
PL1 2000.00 u
PL2 120.00 d
PL1 1.00 d
PL1W 0.00000000 W
PL1W 65.24507904 W
SFO1 125.7703643 M
SF2 10.32 d
SFO2 Cmp60comp.4
SFOAL2 0.500
SFOFFS2 0.00 H

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 15.54 u
P3 10.36 u
P4 20.72 u
PCPD2 80.00 u
PL2 0.00 d
PL12 17.90 d
PL13 18.00 d
PL1W 23.10935593 W
PL12W 0.37478989 W
PL13W 0.36258589 W
SFO2 500.1320005 M

===== GRADIENT CHANNEL =====
GRNAM1 SINE.100
GRNAM2 SINE.100
GRNAM3 SINE.100
GP21 31.00 %
GP22 31.00 %
GP23 31.00 %
P16 10000.00 u
SI 65536
SF 125.7577890 M
WCH RM
SSB 0
LB 1.00 H
GB 0
PC 1.40

DU=D:\, USER=pinnocenti, NAME=PI-1858-124, EXPNO=10, PROCNO=1
F1=16.501ppm, F2=4.150ppm, M1=0.50cm, MAX1=10000.00cm, PC=1.000

#	ADDRESS	[Hz]	FREQUENCY	INTENSITY
1	11155.0	4737.662	9.4704	1.20
2	13093.9	4129.546	8.2548	0.62
3	13100.3	4124.394	8.2445	0.65
4	13204.8	4091.426	8.1786	0.82
5	13616.9	3861.505	7.8189	0.88
6	13618.8	3860.909	7.9177	0.92
7	13697.5	3936.096	7.8681	0.70
8	13714.0	3930.893	7.8577	0.68
9	14600.2	3648.996	7.2942	0.58
10	19915.2	1974.626	3.9472	2.41
11	20041.6	1936.056	3.8701	3.26
12	20909.9	1662.314	3.3229	15.00
13	22031.6	1254.432	2.5076	1.02
14	22209.3	1252.651	2.5040	2.23
15	22215.2	1250.800	2.5003	3.10
16	22221.0	1248.949	2.4966	2.20
17	22226.7	1247.148	2.4930	0.98

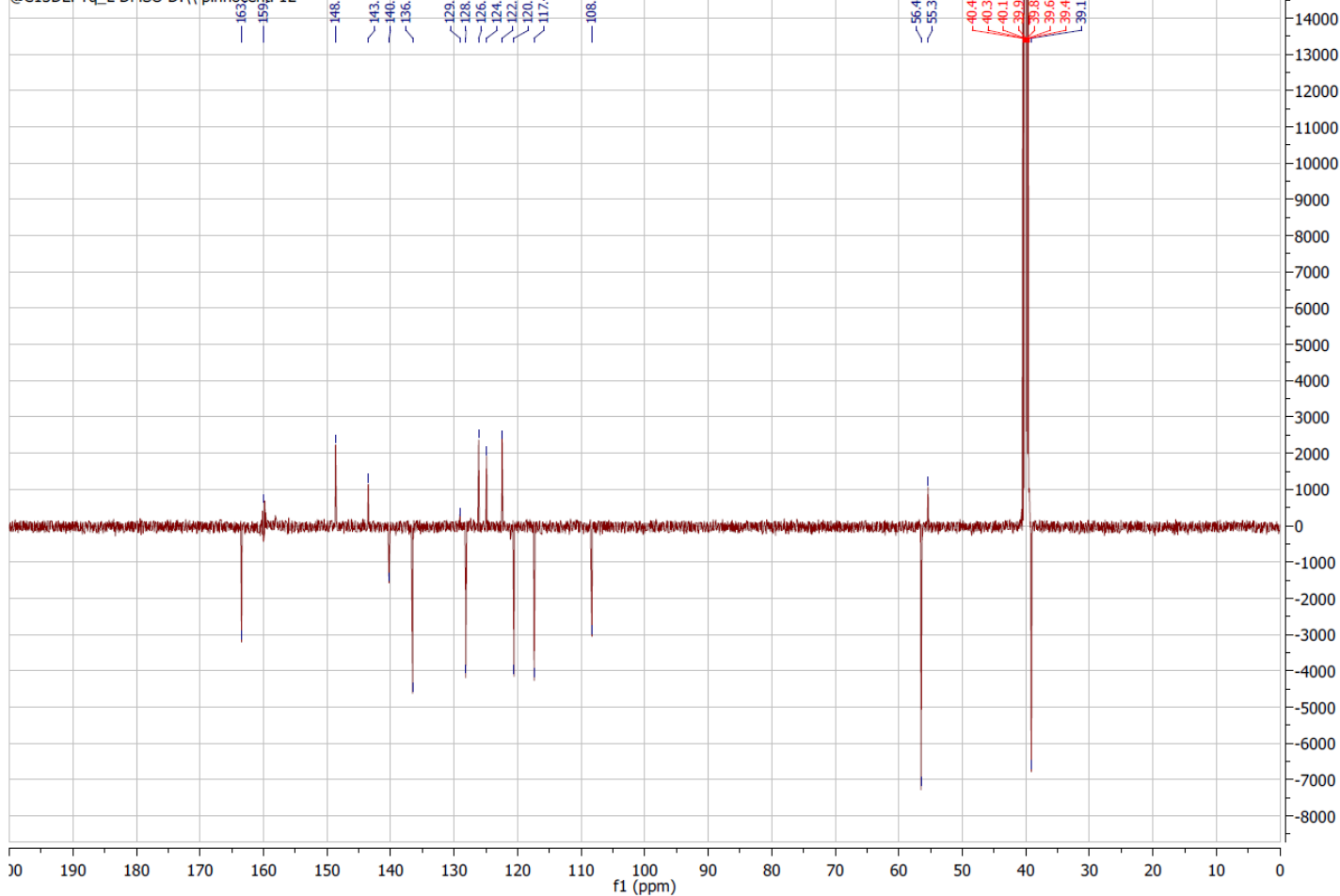


NAME: PI-1858-124
EXPNO: 10
PROCNO: 1
Date_: 20120706
Time: 9.48
INSTRUM: av500a
PROBHD: 5 mm QNP 1H/13
PULPROG: zg30
TD: 65536
SOLVENT: DMSO
DS: 2
NS: 16
SWH: 10330.578 Hz
FIDRES: 0.157632 Hz
AQ: 3.1725407 s
RG: 7290
DM: 48.400 u
DE: 6.00 u
TE: 295.0 K
D1: 1.00000000 s
TDO: 1

===== CHANNEL f1 =====
NUC1: 1H
P1: 9.40 u
PL1: -3.00 dB
PL1W: 35.68453217 W
SFO1: 500.2638893 MHz
SI: 32768
SF: 500.2600000 MHz
WFW: RM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

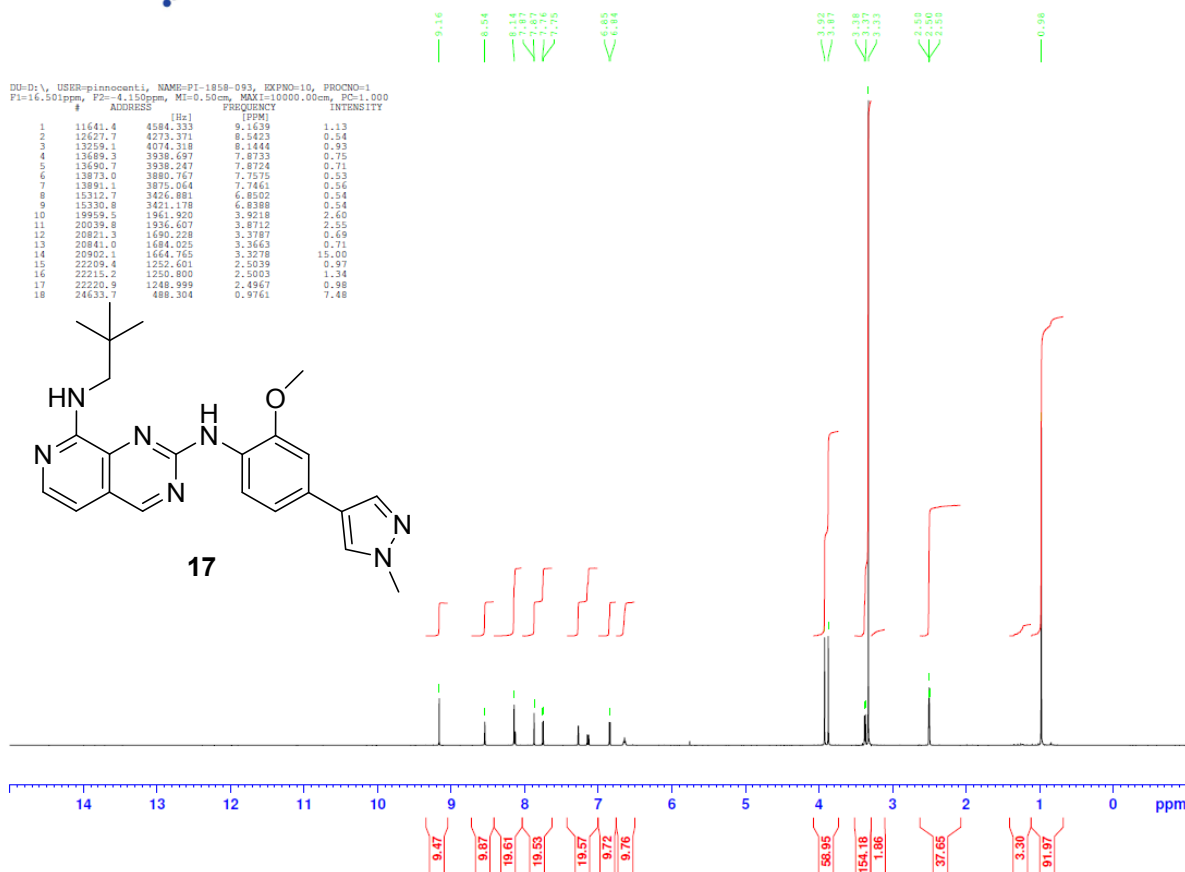
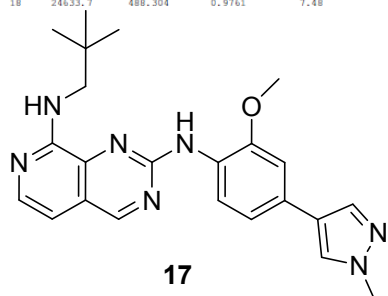
PI-1858-053/20
PI-1858-053

@C13DEPTq_L DMSO D:



DU=D:\, USER=pinnocenti, NAME=PI-1858-093, EXPNO=10, PROCNO=1
F1=16.501ppm, F2=4.150ppm, MI=0.50cm, MAXI=10000.00cm, PC=1.000

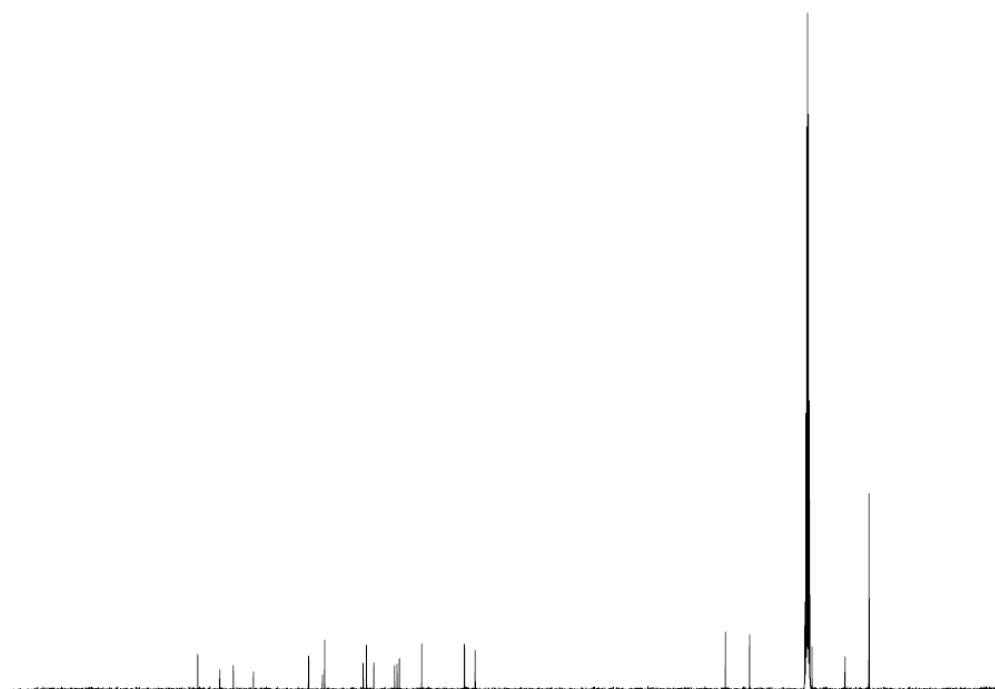
#	ADDRESS	FREQUENCY [Hz]	INTENSITY
1	11641.4	4584.333	1.13
2	12627.7	4273.371	0.54
3	13259.1	4074.318	0.93
4	13680.3	3938.697	0.75
5	13690.7	3938.247	0.71
6	13873.0	3880.767	0.53
7	13891.1	3875.064	0.56
8	15312.7	3426.881	0.54
9	15330.9	3421.178	0.54
10	19959.5	1961.920	2.60
11	20039.8	1936.607	2.55
12	20921.3	1680.208	0.69
13	20841.0	1684.025	0.71
14	20902.1	1664.765	15.00
15	22209.4	1252.601	0.97
16	22215.2	1250.800	1.34
17	22220.9	1248.999	0.98
18	24633.7	480.304	0.9761



NAME PI-1858-093
EXPNO 10
PROCNO 1
Data_ 20120411
Time 17.20
INSTRUM av500a
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 3640
DM 48.4000 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
D11 1
D12 1

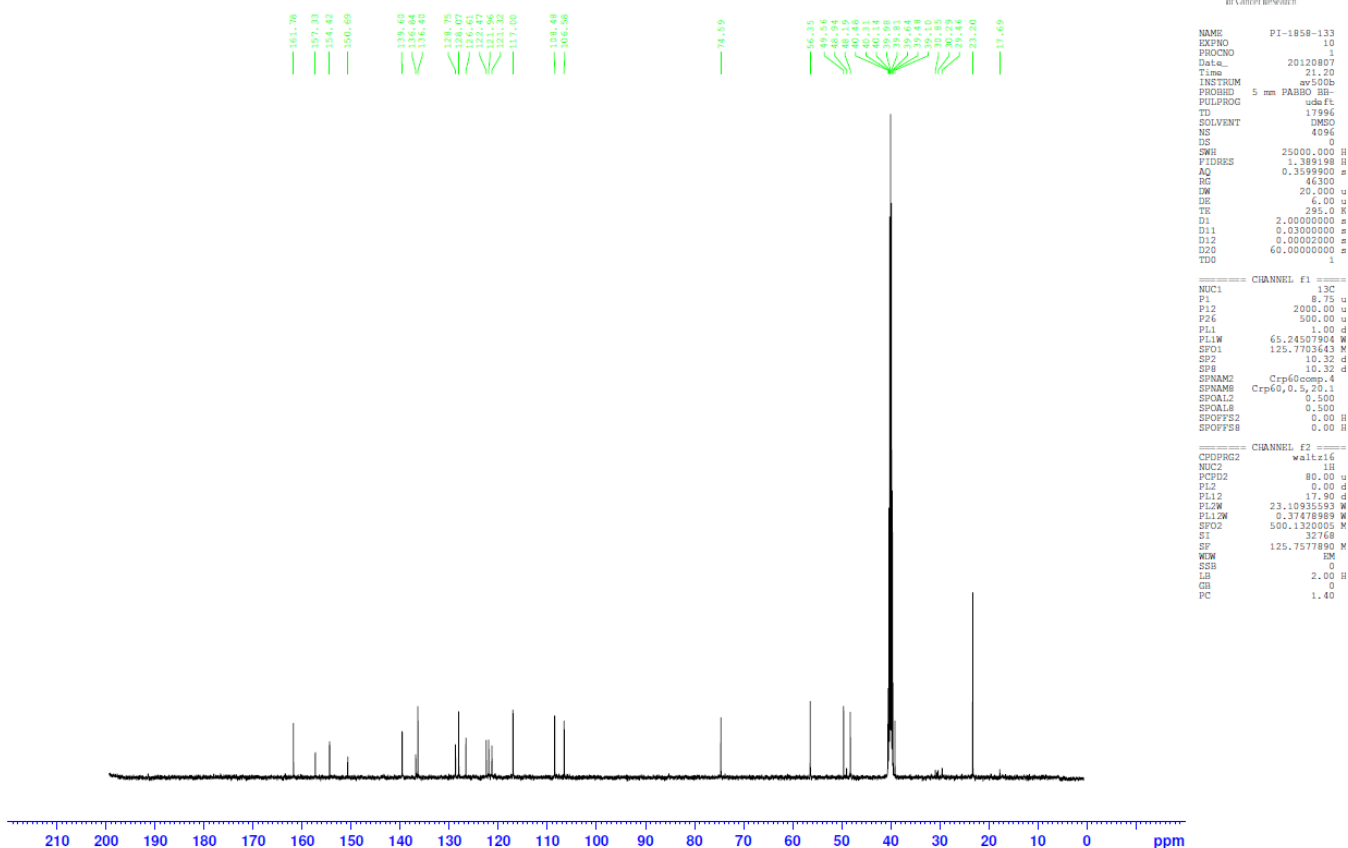
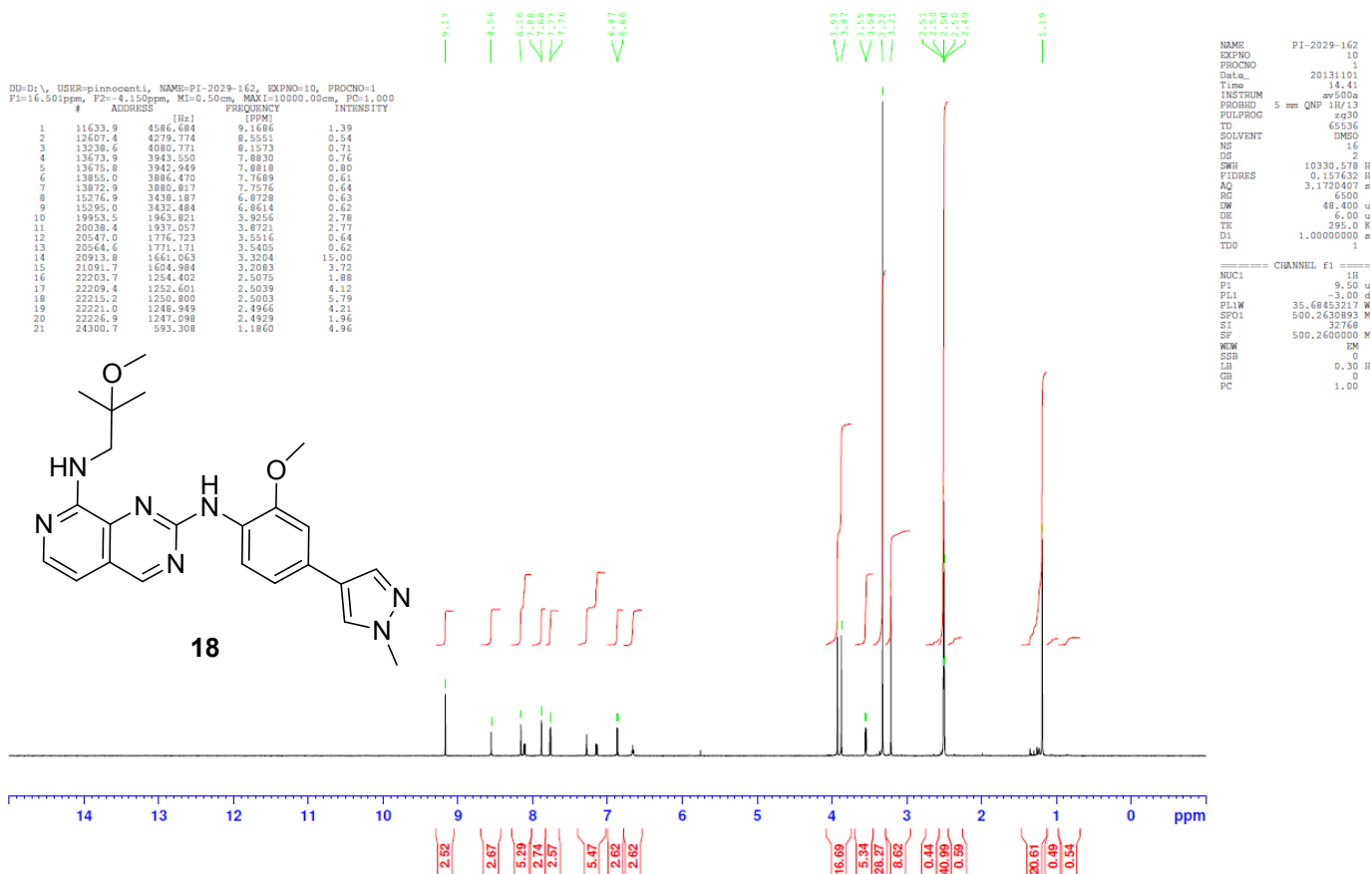
===== CHANNEL f1 =====
NUC1 13C
P1 9.40 u
PL1 3.00 d
PL1W 35.68453217 M
SFO1 500.2630893 M
SI 32768
SF 500.2630893 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00

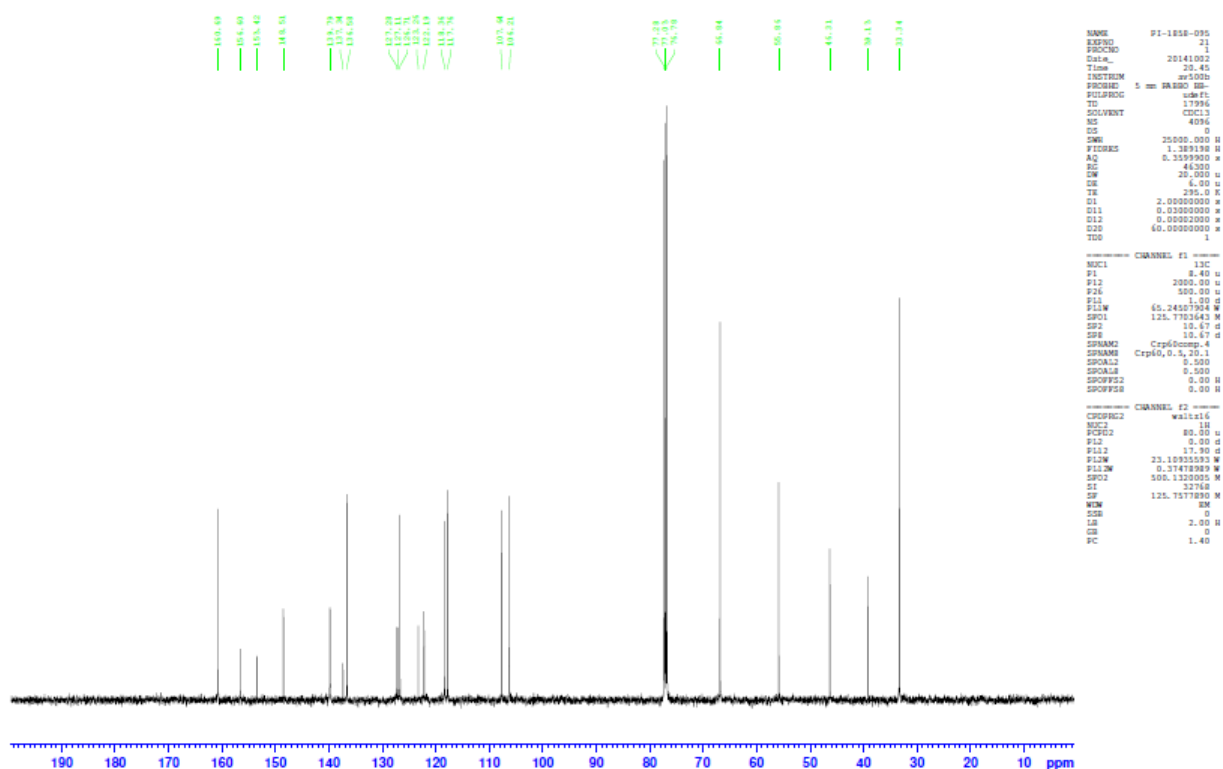
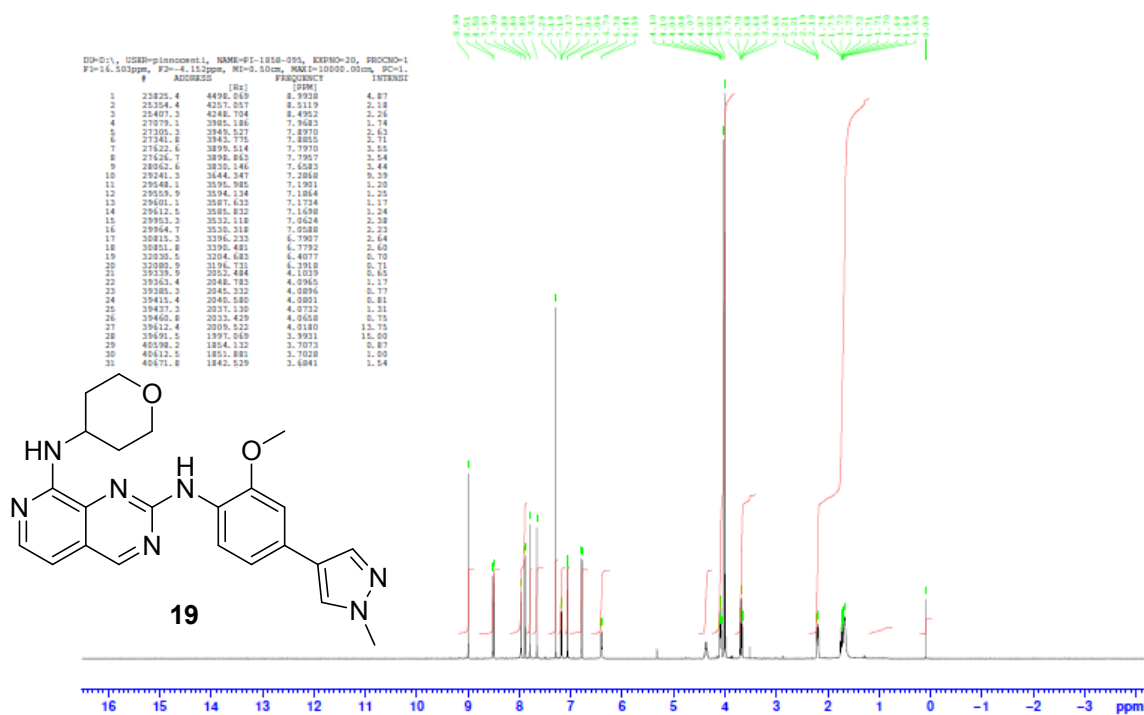
#	ADDRESS	FREQUENCY [Hz]	INTENSITY
1	161.77	161.77	1.13
2	157.97	157.97	0.54
3	154.66	154.66	0.93
4	151.64	151.64	0.75
5	139.61	139.61	0.71
6	136.86	136.86	0.53
7	136.41	136.41	0.56
8	128.75	128.75	0.54
9	128.07	128.07	0.54
10	122.48	122.48	2.60
11	121.96	121.96	2.55
12	121.06	121.06	0.69
13	117.04	117.04	0.71
14	108.49	108.49	15.00
15	106.35	106.35	0.97

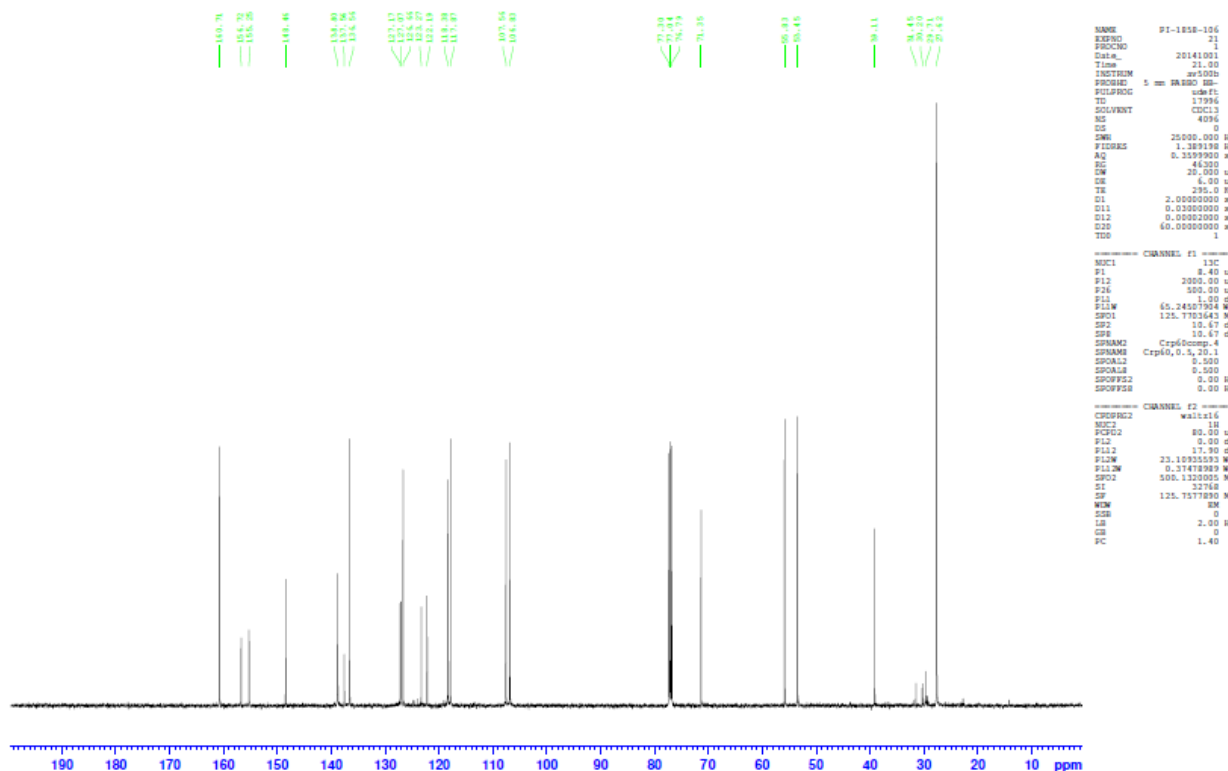
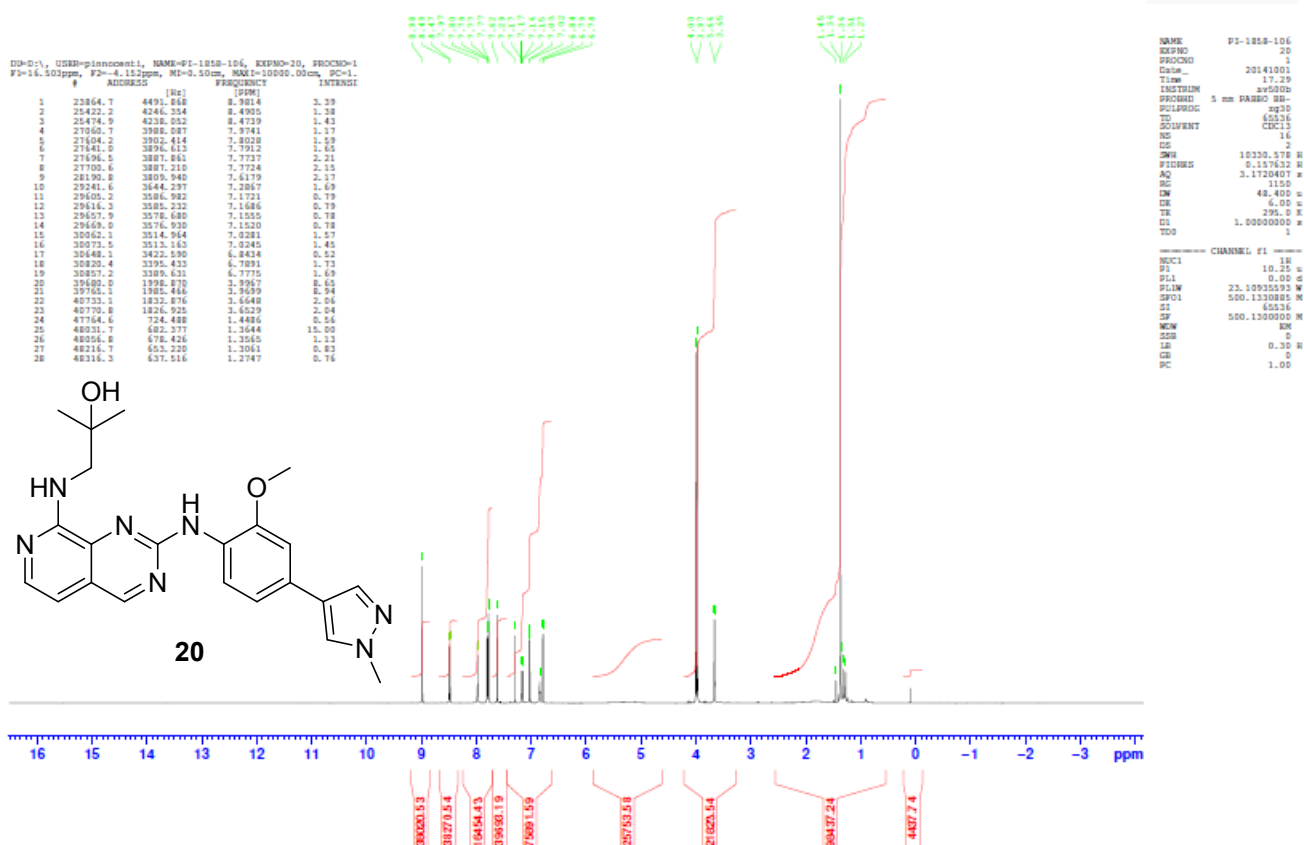


NAME PI-1858-093
EXPNO 10
PROCNO 1
Data_ 20120411
Time 22.12
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 17996
SOLVENT DMSO
NS 4096
DS 0
SWH 25000.000 H
FIDRES 1.389198 H
AQ 0.3599800 s
RG 46300
DM 20.000 u
DE 6.00 u
TE 295.1 K
D1 2.00000000 s
D11 0.00000000 s
D12 0.00002000 s
D20 60.00000000 s
D13 1
D14 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.75 u
PL1 2000.00 u
PL2 80.00 u
PL2W 17.90 d
PL1W 65.24507804 M
SFO1 125.7703643 M
SI 32768
SF 125.7703643 M
WDW EM
SSB 0
LB 2.00 H
GB 0
PC 1.40







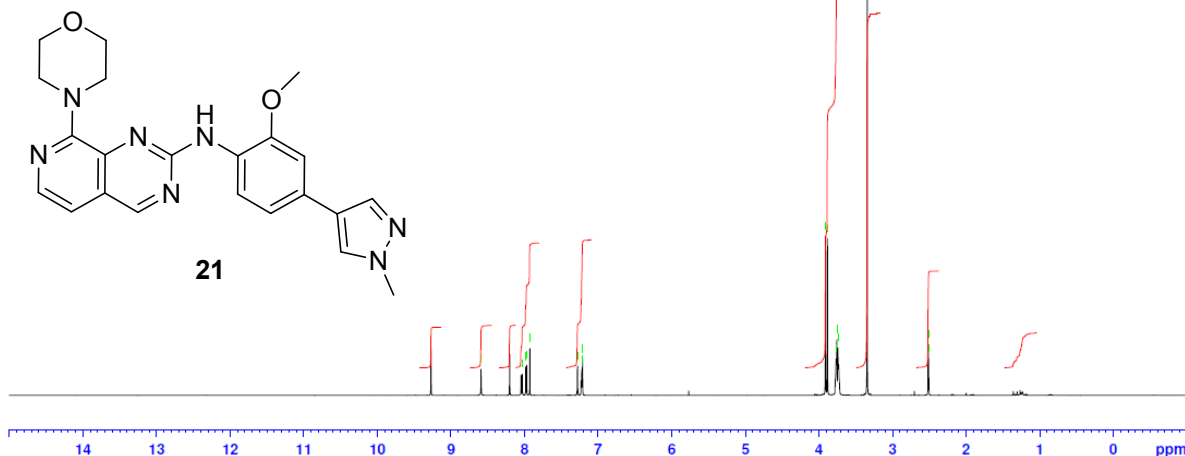


DU=D:\, USER=pinnocenti, NAME=PI-1858-065, EXPNO=10, PROCNO=1
 FI=16.503ppm, F2=4.152ppm, MI=0.50cm, MAX1=10000.00cm, PC=1.

#	ADDRESS	FREQUENCY (PPM)	INTENSITY
1	22945.0	4636.855	9.2713
2	25105.6	4296.267	0.62
3	26344.6	4100.966	0.98
4	26886.5	4015.544	0.50
5	27036.2	3991.938	0.68
6	27070.5	3986.536	0.71
7	27211.1	3964.380	1.11
8	29258.4	3641.647	0.61
9	29269.2	3639.946	0.69
10	29451.0	3611.289	0.61
11	29484.7	3605.987	0.86
12	39959.2	1954.858	3.9087
13	40043.0	1941.655	3.72
14	40416.4	1882.789	0.86
15	40444.3	1878.388	1.32
16	40494.5	1870.486	1.13
17	41755.3	1671.735	15.00
18	44384.0	1257.377	0.88
19	44395.4	1255.576	1.21
20	44406.8	1253.776	0.88

NAME PI-1858-065
 EXPNO 10
 PROCNO 1
 Date_ 20120301
 Time 8.53
 INSTRUM av500b
 PROBRD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10330.578 H
 FIDRES 0.157632 H
 AQ 3.1720407 s
 RG 2050
 DM 48.400 u
 DE 6.00 u
 TE 295.0 K
 D1 1.00000000 s
 D11 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 u
 PL1 0.00 d
 PL1W 23.10935583 M
 SFO1 500.1330885 M
 SI 65536
 SF 500.1300000 M
 WGM RM
 SSB 0
 LB 0.30 H
 GB 0
 PC 1.00

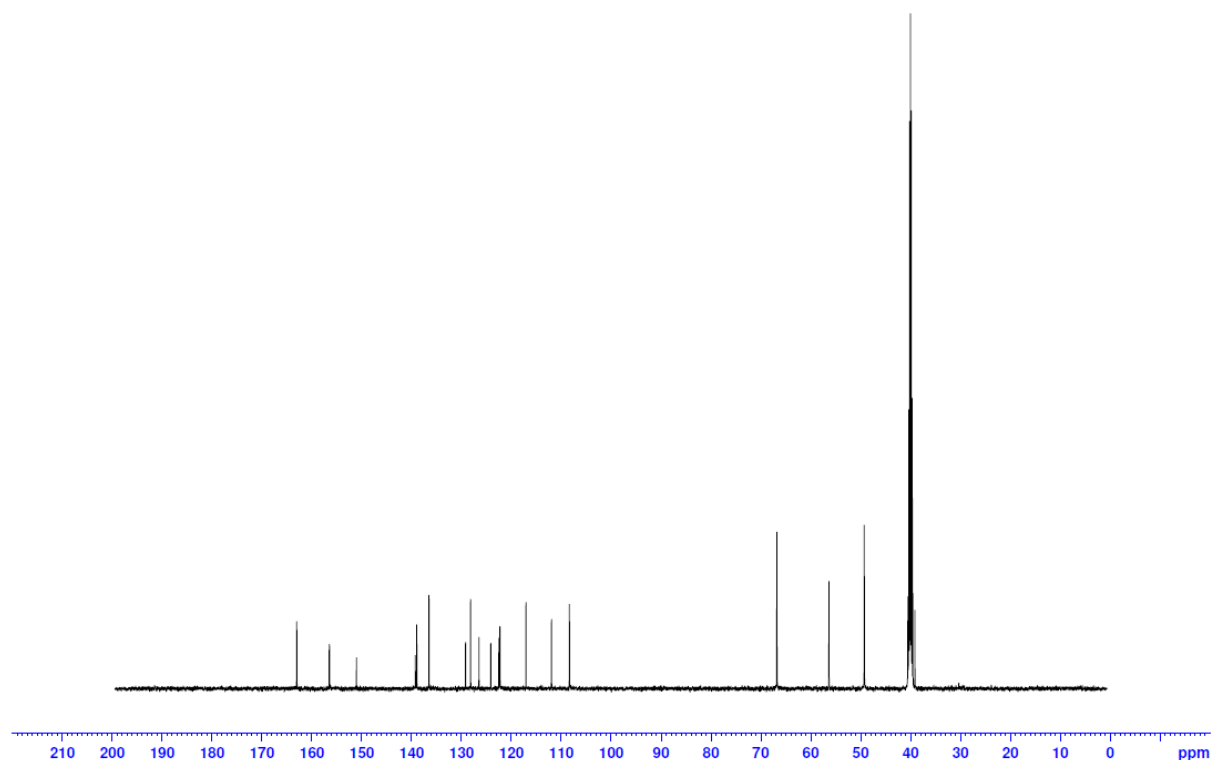


163.01	156.48	156.43	151.03
136.25	136.56	136.49	128.72
128.38	128.38	128.46	126.46
122.43	122.43	122.26	117.86
111.85	108.35	66.75	56.31
49.25	40.48	40.15	39.98
39.45	39.45	39.46	39.10

NAME PI-1858-065
 EXPNO 11
 PROCNO 1
 Date_ 20120302
 Time 21.35
 INSTRUM av500b
 PROBRD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 17996
 SOLVENT DMSO
 NS 4096
 DS 0
 SWH 25000.000 H
 FIDRES 1.389198 H
 AQ 0.3599900 s
 RG 46300
 DM 30.000 u
 DE 6.00 u
 TE 295.0 K
 D1 2.00000000 s
 D11 0.03000000 s
 D12 0.00000000 s
 D20 60.00000000 s
 TD0 1

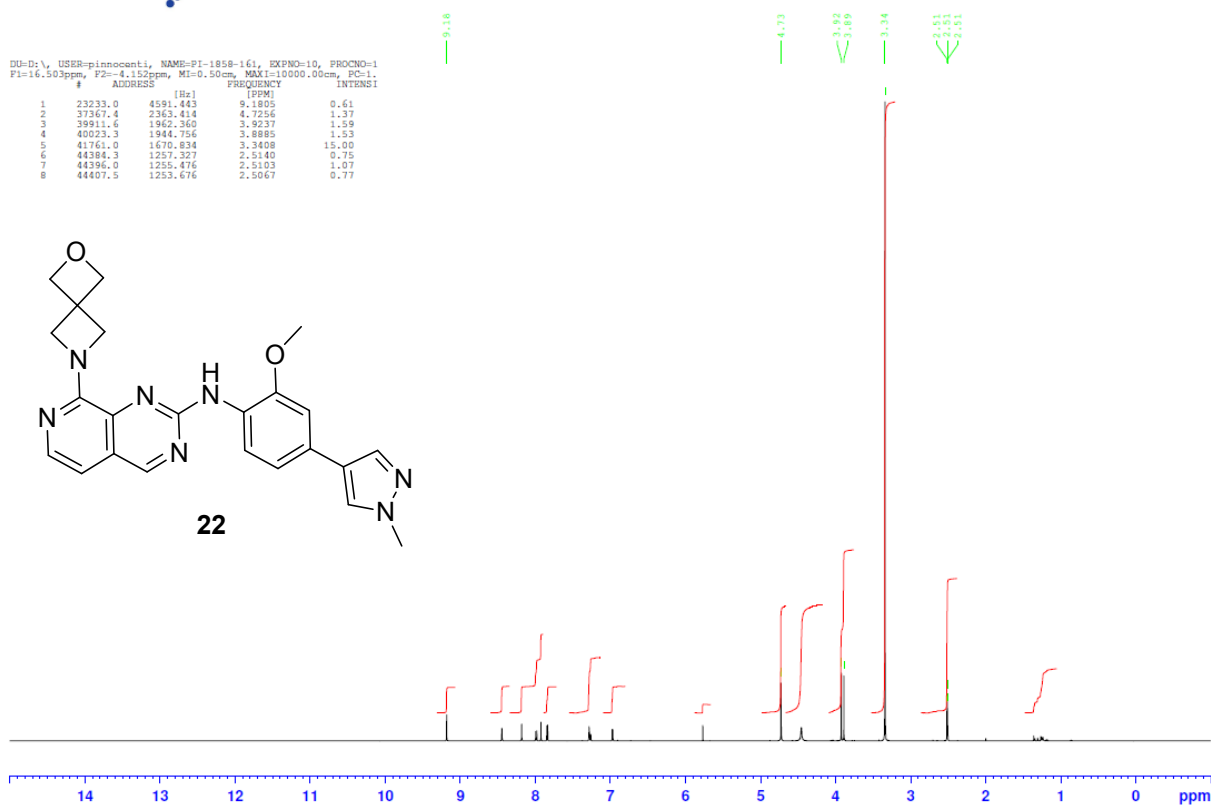
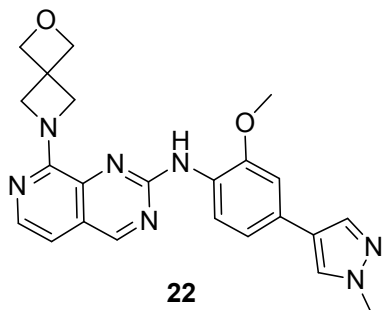
===== CHANNEL f1 =====
 NUC1 13C
 P1 8.75 u
 PL1 2000.00 u
 PL1W 1.00 d
 PL1Z 65.24507904 M
 SFO1 125.7703643 M
 SP2 10.32 d
 SP8 10.32 d
 SPNAM2 Crp60comp-4
 SPNAM8 Crp60,0.5,20.1
 SPOAL2 0.500
 SPOAL8 0.500
 SPOFFS2 0.00 H
 SPOFFS8 0.00 H

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 u
 PL2 0.00 d
 PL2W 17.90 d
 PL2Z 23.10935583 M
 PL1Z 0.37478989 M
 SFO2 500.1320000 M
 SI 32768
 SF 125.7577890 M
 WGM RM
 SSB 0
 LB 2.00 H
 GB 0
 PC 1.40



DU=D:\, USER=pinnocenti, NAME=PI-1858-161, EXPNO=10, PROCNO=1
F1=16.503ppm, F2=-4.152ppm, MI=0.50cm, MAXI=10000.00cm, PC=1.

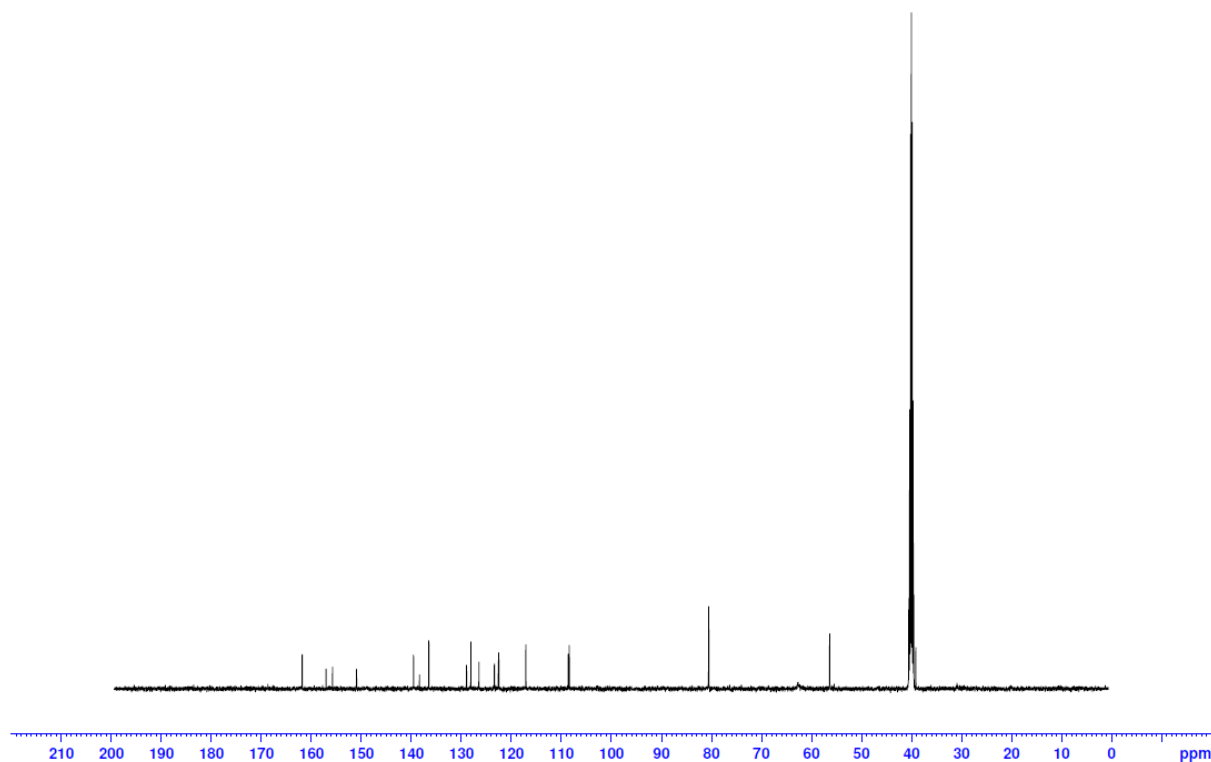
#	ADDRESS	[Hz]	FREQUENCY	INTENSITY
1	23233.0	4591.443	9.1805	0.61
2	37367.4	2363.414	4.7256	1.37
3	39911.6	1962.360	3.9237	1.59
4	40023.3	1944.756	3.8885	1.53
5	41761.0	1670.836	3.3408	15.00
6	44384.3	1257.327	2.5140	0.75
7	44396.0	1255.476	2.5103	1.07
8	44407.5	1253.676	2.5067	0.77



NAME PI-1858-161
EXPNO 10
PROCNO 1
Date_ 20120924
Time 14.36
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 2880
DM 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.25 u
PL1 0.00 d
PL1W 23.10935593 M
SFO1 500.1330885 M
SI 65536
SF 500.1300000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00

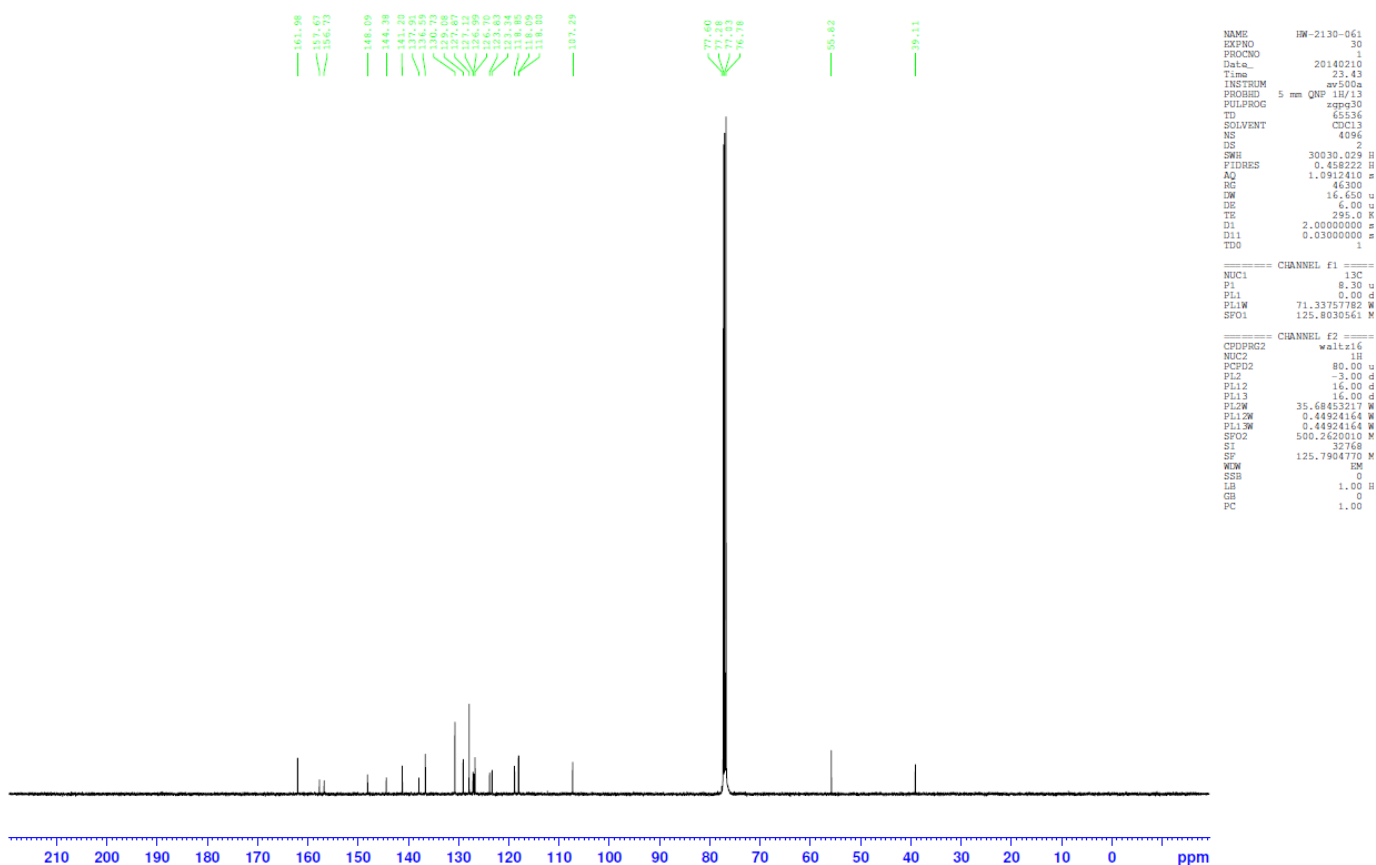
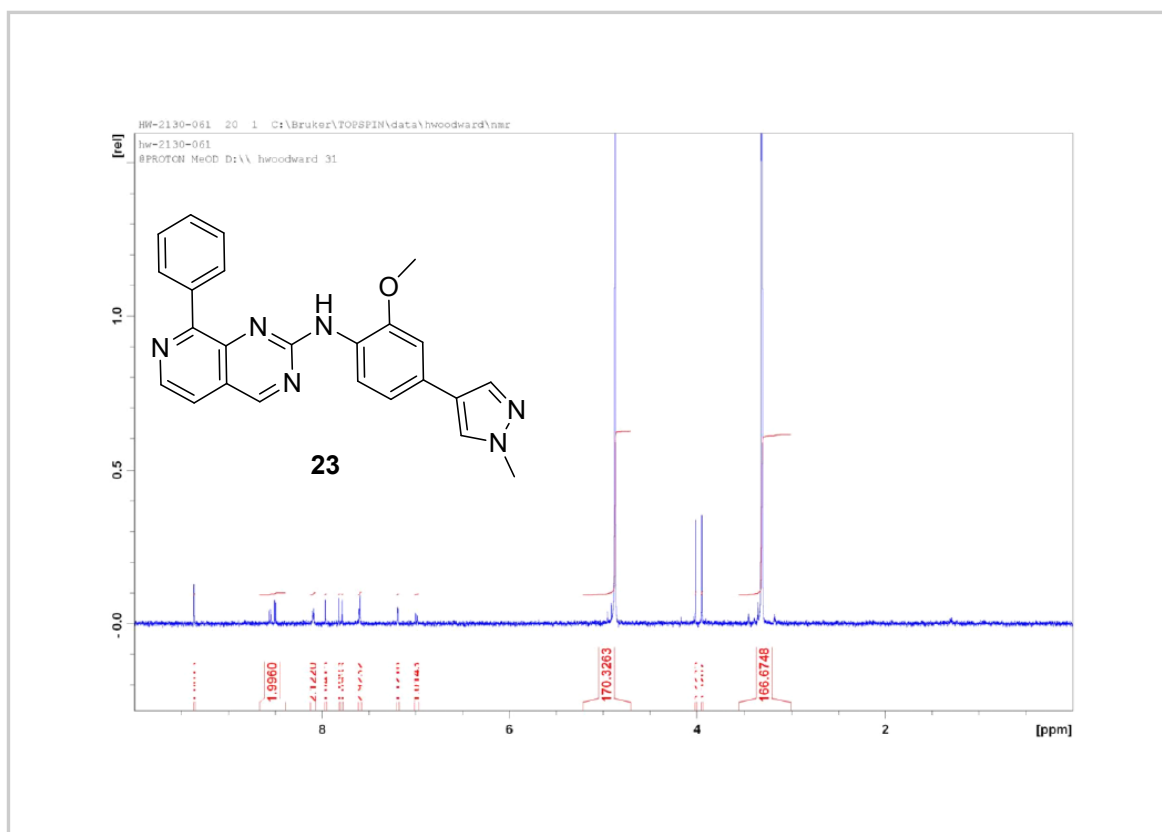
161.85	139.95	139.52	62.64	40.49
157.04	138.36	60.52	56.32	40.32
156.77	136.90			39.99
150.96	128.95			38.82
	128.10			38.55
	127.44			38.49
	123.39			38.49
	122.59			38.49
	122.51			38.49
	117.11			38.49
	106.61			38.49
	106.40			38.49



NAME PI-1858-161
EXPNO 11
PROCNO 1
Date_ 20120925
Time 1.46
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 17996
SOLVENT DMSO
NS 4096
DS 0
SWH 25000.000 H
FIDRES 1.388198 H
AQ 0.3599900 s
RG 46300
DM 20.000 u
DE 6.00 u
TE 295.3 K
D1 2.00000000 s
D11 0.03000000 s
D12 0.00002000 s
D20 60.00000000 s
TD0 1

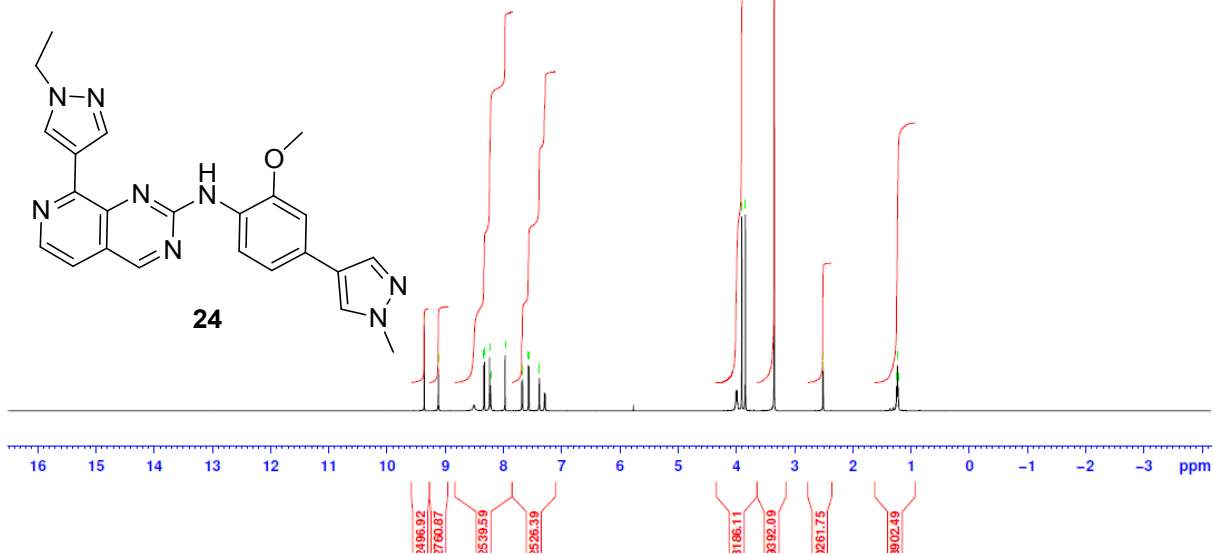
===== CHANNEL f1 =====
NUC1 13C
P1 8.75 u
PL1 2000.00 u
PL2 500.00 u
PL1 1.00 d
PL1W 65.24807804 M
SFO1 125.7733643 M
SP2 10.32 d
SP8 10.32 d
SPNAM2 Crp60comp.4
SPNAM8 Crp60,0.5,20.1
SFOAL2 0.500
SFOAL8 0.500
SFOFFS2 0.00 H
SFOFFS8 0.00 H

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 0.00 d
PL12 17.90 d
PL1W 23.10935593 M
PL12W 0.37478889 M
SFO2 500.1320005 M
SI 32768
SF 125.7577890 M
WDW EM
SSB 0
LB 2.00 H
GB 0
PC 1.40



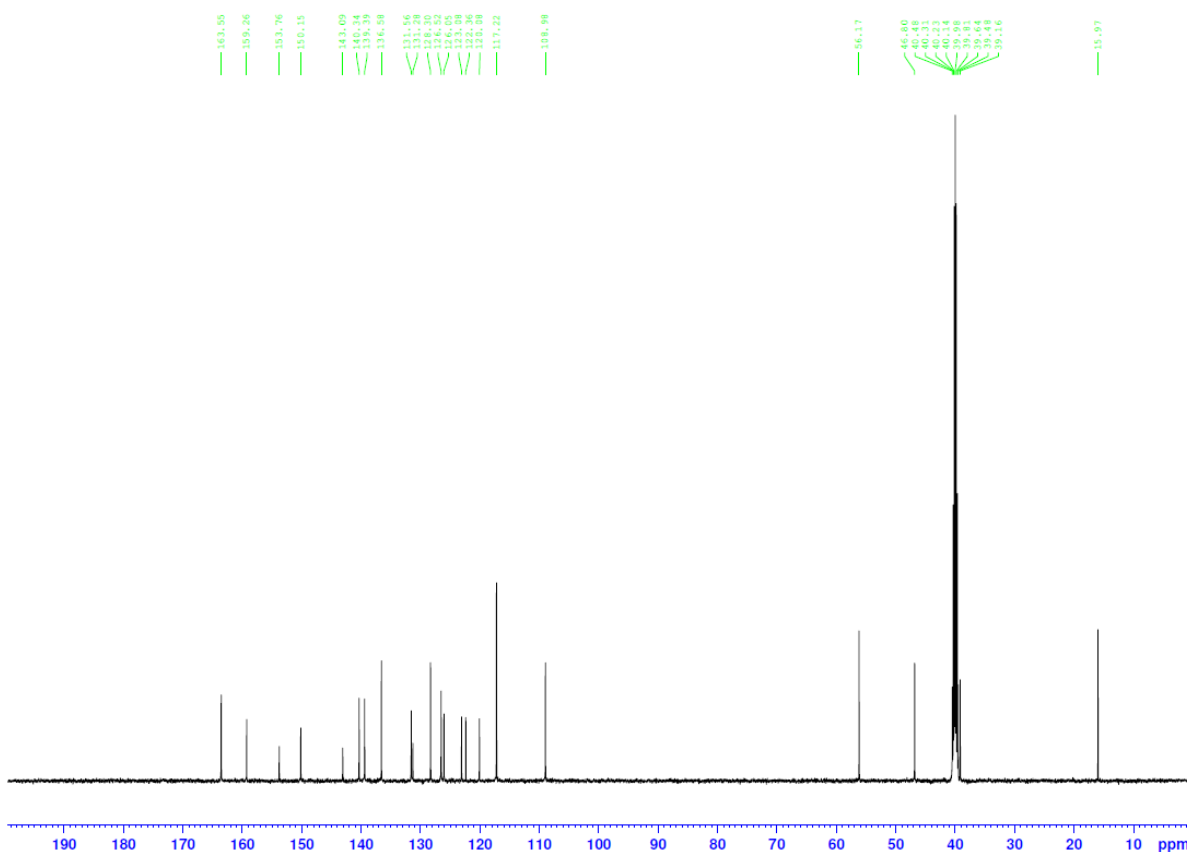
DU=D:\, USER=pinnocenti, NAME=PI-1858-083, EXPNO=10, PROCNO=1
F1=16.503ppm, F2=4.152ppm, M1=0.50cm, MM1=10000.00cm, PC=1.

#	ADDRESS	FREQUENCY	INTENSITY
1	22663.8	4681.167	2.01
2	23432.3	4560.035	0.97
3	25904.5	4170.334	1.07
4	25937.8	4165.083	1.14
5	26218.0	4120.921	1.24
6	26282.1	4110.819	0.59
7	27064.8	3987.436	1.29
8	27977.9	3843.499	0.68
9	28029.0	3835.447	0.73
10	28335.2	3787.184	1.07
11	28368.8	3781.883	1.03
12	28928.2	3693.710	0.73
13	28938.6	3692.060	0.76
14	39966.8	1953.658	4.53
15	40162.3	1922.850	4.60
16	41735.7	1674.835	3.488
17	44385.2	1257.177	0.78
18	44396.7	1255.376	1.05
19	44408.1	1253.576	0.76
20	48402.9	623.862	0.57
21	48448.6	616.660	1.06
22	48494.0	609.508	0.53



NAME PI-1858-083
EXPNO 10
PROCNO 1
Date_ 20140317
Time 14.45
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 2050
DM 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
D11
TD0 1

CHANNEL F1
NUC1 1H
P1 10.25 u
PL1 0.00 d
PL1W 23.10935993 M
SFO1 500.1320885 M
S1 65536
SF 500.1300000 M
WDM 0
SSB 0
LB 0.30 H
GB 0
PC 1.00



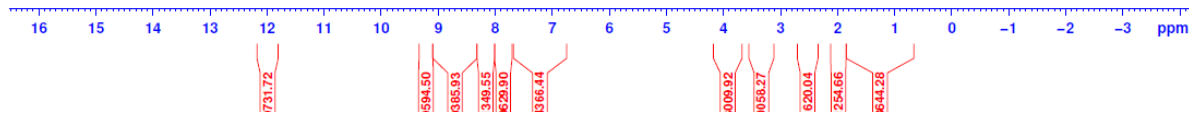
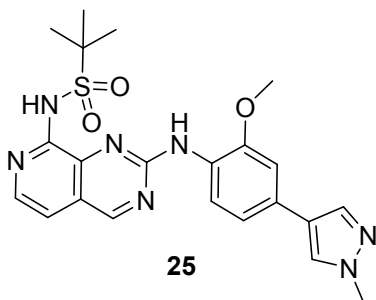
NAME PI-1858-083
EXPNO 11
PROCNO 1
Date_ 20140317
Time 20.20
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 17896
SOLVENT DMSO
NS 4096
DS 0
SWH 25000.000 H
FIDRES 1.389198 H
AQ 0.3599900 s
RG 46300
DM 20.000 u
DE 6.00 u
TE 295.0 K
D1 2.00000000 s
D11 0.13000000 s
D12 0.00002000 s
D20 60.00000000 s
TD0 1

CHANNEL F1
NUC1 13C
P1 8.75 u
PL1 2000.00 u
P2 500.00 u
PL1 1.00 d
PL1W 65.24507904 M
SFO1 125.7703643 M
S2 10.32 d
SF 10.32 d
SFO2 Cmp60comp.4
SFOAL2 Crp60, 0.5, 25.1
SFOAL2 0.500
SFOAL2 0.500
SFOFFS2 0.00 H
SFOFFS2 0.00 H

CHANNEL F2
NUC2 waltz16
PCPD2 80.00 u
PL2 0.00 d
PL12 17.90 d
PL1W 23.10935993 M
SFO2 500.1320005 M
S1 32168
SF 125.7577890 M
WDM 0
SSB 0
LB 2.00 H
GB 0
PC 1.40

DU=D₂O, USER=pinnocenti, NAME=PI-1858-148, EXPNO=10, PROCNO=1
F1=16.503ppm, F2=4.152ppm, MI=0.50cm, MUX=10000.00cm, PC=1.
ADDRESS FREQUENCY INTENS1

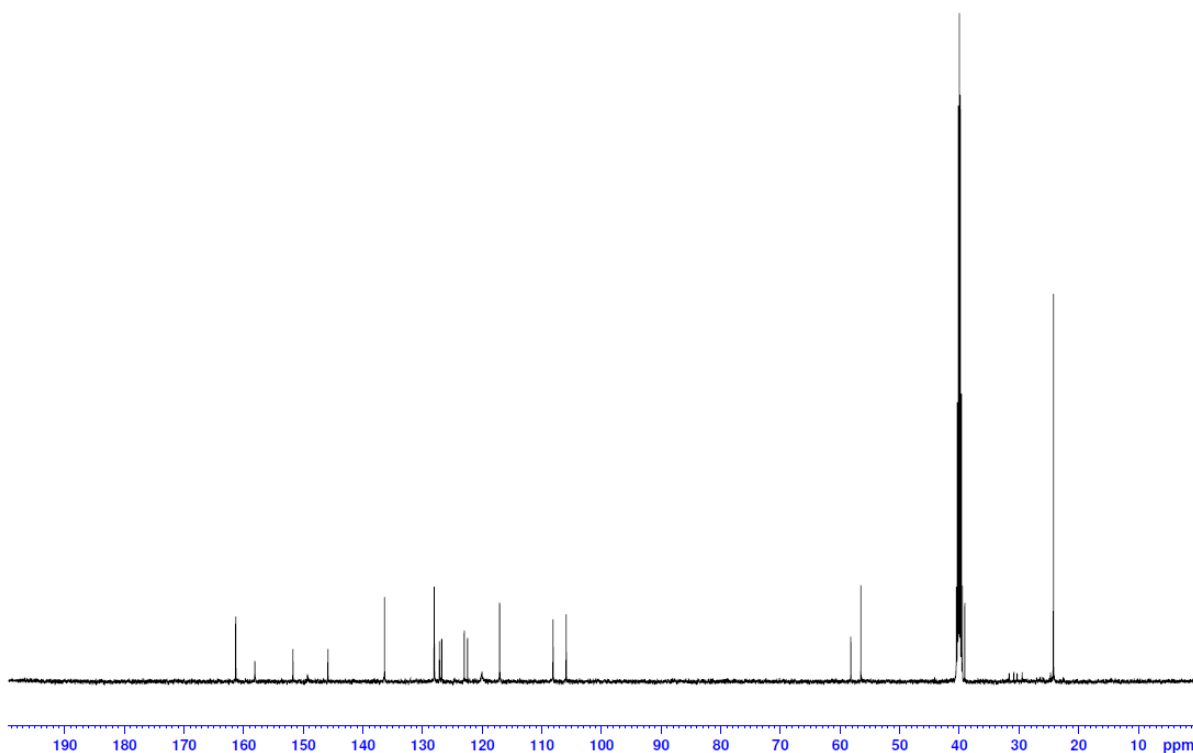
		[Hz]	[ppm]	
1	23276.8	4584.542	9.1667	1.28
2	26490.2	4078.010	8.1539	0.88
3	27249.1	3942.625	7.9832	0.93
4	27352.9	3942.025	7.9820	0.94
5	29292.4	3636.295	7.2707	0.59
6	29303.8	3634.495	7.2671	0.59
7	30475.8	3449.747	6.8977	0.53
8	39784.4	1982.415	3.9638	2.78
9	40058.2	1939.254	3.8775	3.30
10	41748.4	1672.835	3.3448	15.00
11	44385.2	1257.177	2.5137	0.73
12	44397.0	1255.326	2.5100	1.00
13	44408.4	1253.526	2.5064	0.71
14	47650.3	742.493	1.4846	7.84



NAME PI-1858-148
EXPNO 10
PROCNO 1
Data 20140317
Time 14.59
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 s
AQ 3.1720407 s
RG 1820
INW 46.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.25 u
PL1 0.00 d
PL1W 23.10935593 M
SFO1 500.1300885 M
SI 65536
SF 500.1300000 M
WFW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00

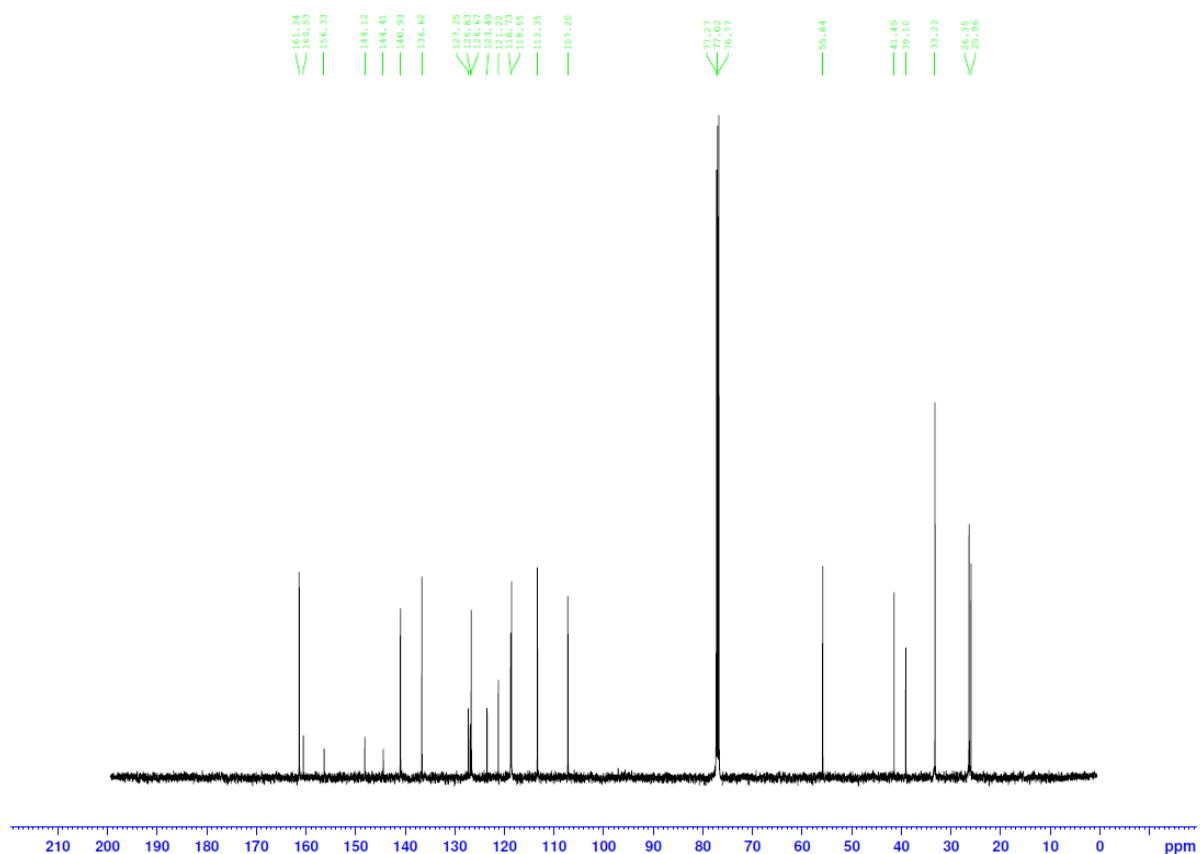
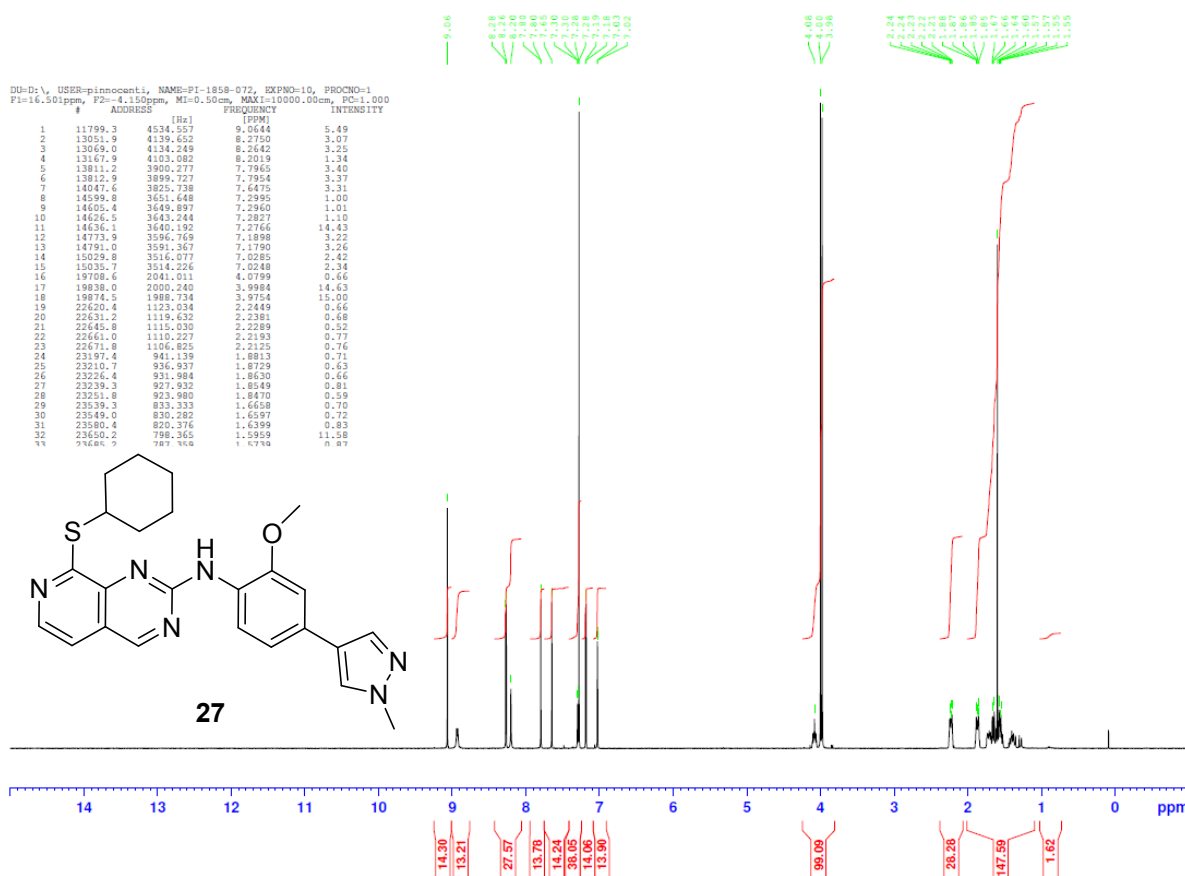
161.34
158.11
151.74
145.86
131.38
128.03
127.16
126.80
122.47
117.96
106.13
105.92
58.18
56.50
40.48
40.31
40.14
39.98
39.84
39.64
39.48
39.09
24.21



NAME PI-1858-148
EXPNO 11
PROCNO 1
Data 20140317
Time 23.39
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG udeft
TD 17896
SOLVENT DMSO
NS 0
DS 0
SWH 25000.000 H
FIDRES 1.389198 H
AQ 0.3599900 s
RG 46300
INW 20.000 u
DE 6.00 u
TE 295.0 K
D1 2.00000000 s
D11 0.03000000 s
D12 0.00000000 s
D20 60.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.75 u
PL1 2000.00 u
PL2 500.00 u
PL12 1.00 d
PL1W 65.24507904 M
SFO1 125.7703643 M
SP2 10.32 d
SFB 10.32 d
SPNAM2 Crp60comp.4
SPNAM9 Crp60,0.5,20.1
SFOAL2 0.500
SFOAL8 0.500
SFOFFS2 0.00 H
SFOFFS8 0.00 H

===== CHANNEL f2 =====
CPDPRG2 waitz16
NUC2 1H
PCPD2 80.00 u
PL2 0.00 d
PL12 17.90 d
PL1W 23.10935593 M
PL12W 0.37478989 M
SFO2 500.1300000 M
SI 32768
SF 125.7577890 M
WFW EM
SSB 0
LB 2.00 H
GB 0
PC 1.40

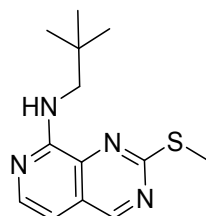


DU=D:\v, USB=hwoodward, NAME=HW-2130-0083, EXPNO=11, PROCNO=1
F1=16.501ppm, F2=4.150ppm, M1=0.50cm, MAX1=10000.00cm, PC=1.000

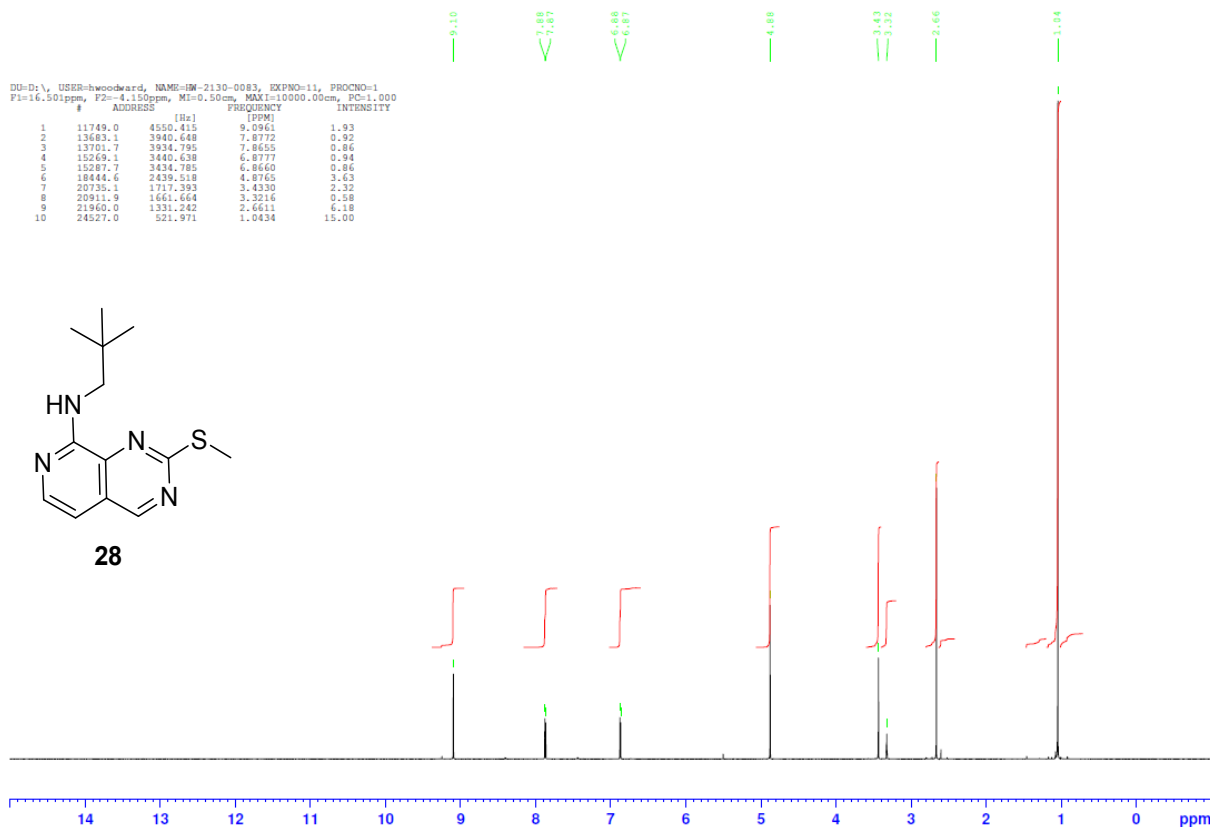
#	ADDRESS	FREQUENCY (PPM)	INTENSITY
1	11749.0	4550.415	9.0961
2	13683.1	3940.648	7.8772
3	13701.7	3934.795	7.8655
4	15269.1	3440.638	6.8777
5	15287.7	3434.785	6.8660
6	18444.6	2439.518	4.8765
7	20735.1	1717.393	3.4330
8	20811.9	1661.664	3.3216
9	21960.0	1331.242	2.6611
10	24527.0	521.971	1.0434

NAME HW-2130-0083
EXPNO 11
PROCNO 1
Date_ 20140318
Time 11.37
INSTRUM av500a
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 1820
RW 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 u
PL1 3.00 d
PL1W 35.68453217 W
SFO1 500.26130893 M
SI 32768
SF 500.26000000 M
MCH 1M
SSB 0
LB 0.30 H
GB 0
PC 1.00



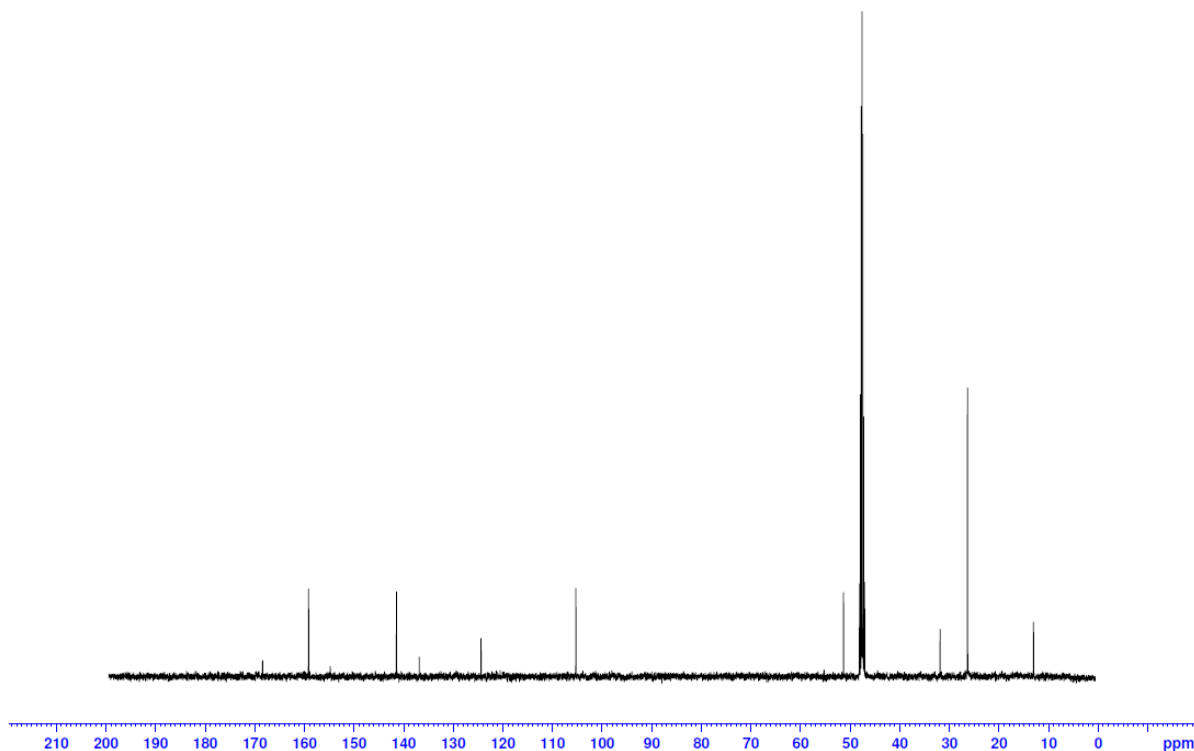
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159.14	141.42	124.39	105.26	51.32	48.10	47.52	47.59	47.52	47.58	31.86	26.35	13.03
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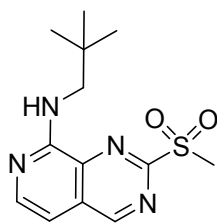
NAME HW-2130-0083
EXPNO 10
PROCNO 1
Date_ 20140318
Time 10.36
INSTRUM av500a
PROBHD 5 mm QNP 1H/13
PULPROG udeft
TD 17996
SOLVENT MeOD
NS 128
DS 0
SWH 25000.000 H
FIDRES 1.389198 H
AQ 0.3599800 s
RG 46300
RW 26.000 u
DE 6.00 u
TE 295.0 K
D1 2.00000000 s
D11 0.03000000 s
D12 0.00002000 s
D20 60.00000000 s
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.30 u
PL1 2000.00 u
P2 500.00 u
PL2 0.00 d
PL1W 71.33757782 W
SFO1 125.8030561 M
SF2 9.83 d
SF8 9.83 d
SFO2 125.7904770 M
MCH 1M
SSB 0
LB 2.00 H
GB 0
PC 1.00

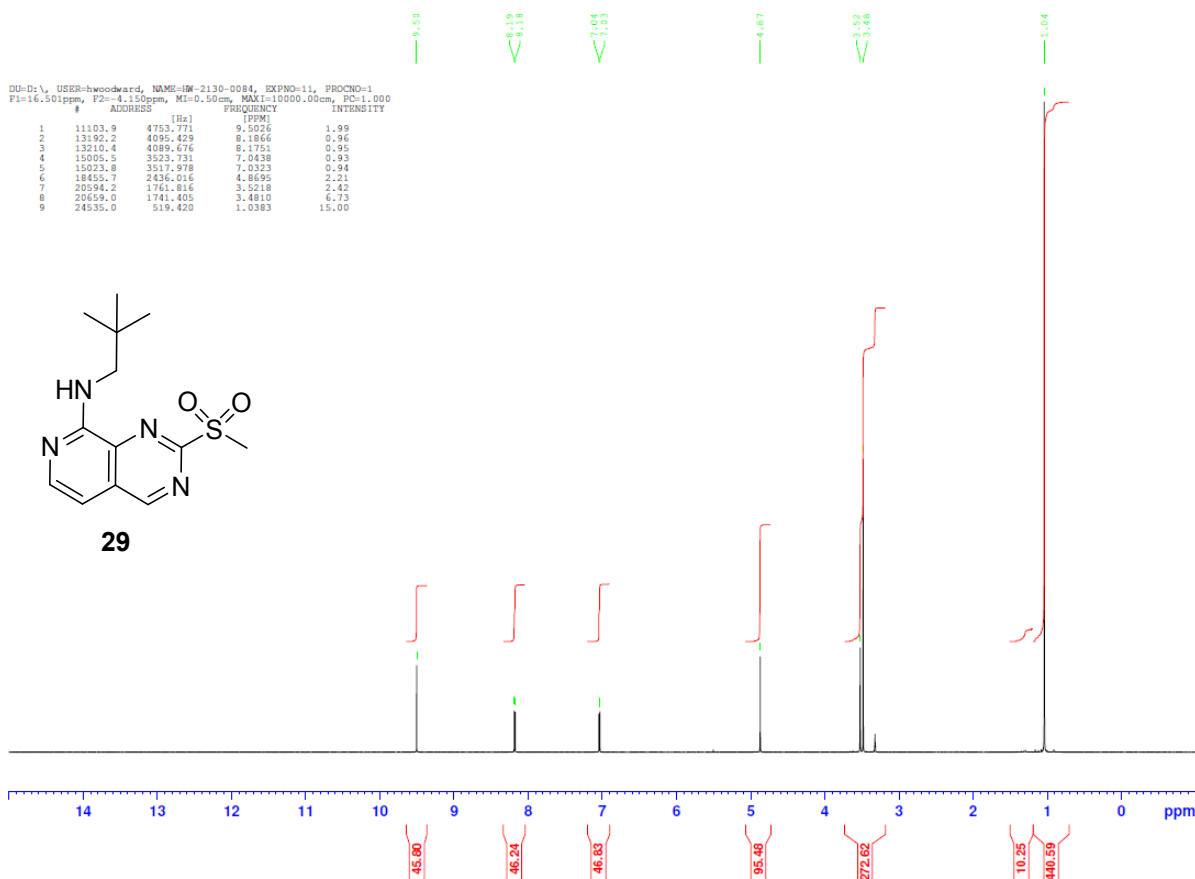


DU=D:\, USER=hwoodward, NAME=HW-2130-0084, EXPNO=11, PROCNO=1
F1=16.501ppm, F2=4.150ppm, M1=0.50cm, M2=1.0000.00cm, PC=1.000

#	ADDRESS	FREQUENCY	INTENSITY
1	11103.9	4753.771	1.99
2	13192.2	4095.429	0.96
3	13210.4	4089.676	0.95
4	15005.5	3523.731	0.93
5	15023.8	3517.978	0.94
6	18455.7	2436.016	2.21
7	20594.2	1761.816	2.42
8	20659.0	1741.405	6.73
9	24535.0	519.420	15.00

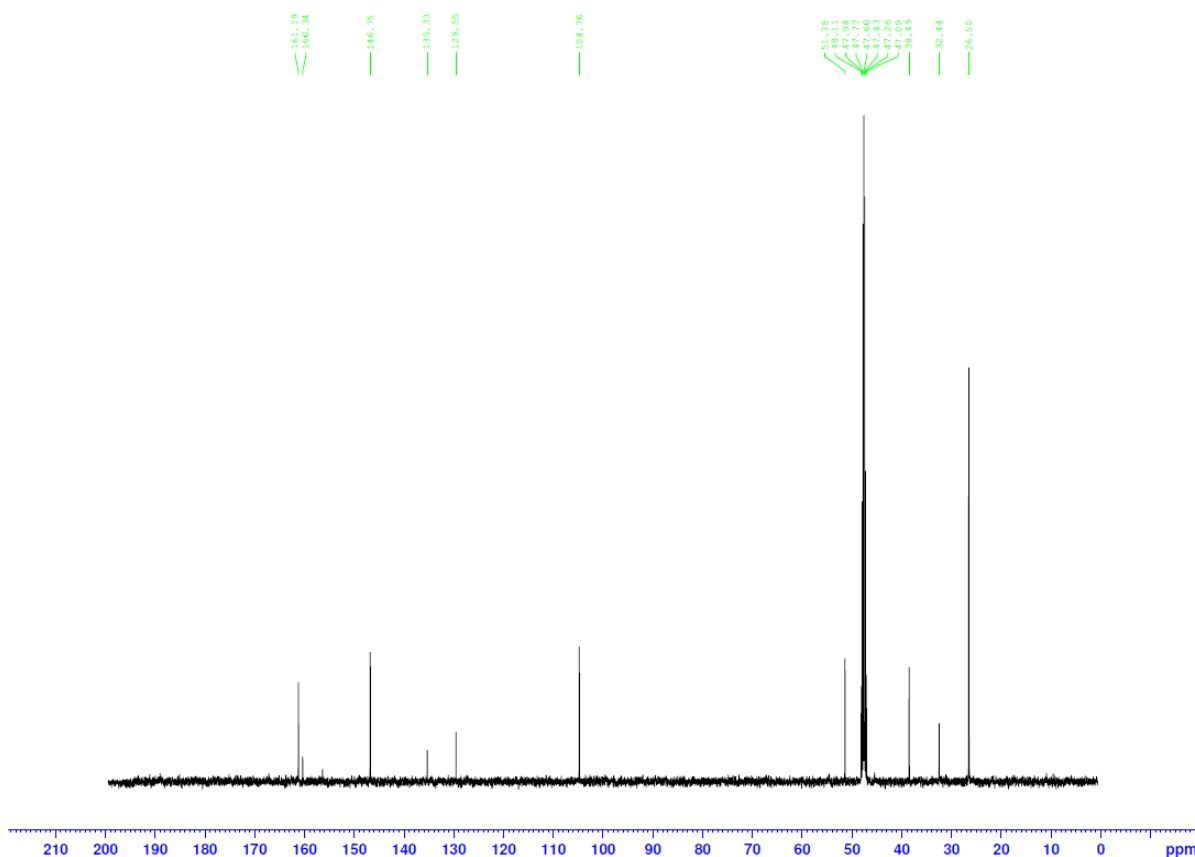


29



NAME HW-2130-0084
EXPNO 11
PROCNO 1
Date_ 20140318
Time 11.44
INSTRUM av500a
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 1820
DM 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 u
PL1 10.49
PL1W 35.68453217 M
SFO1 500.2630893 M
SI 32768
SF 500.2600000 M
MCW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00

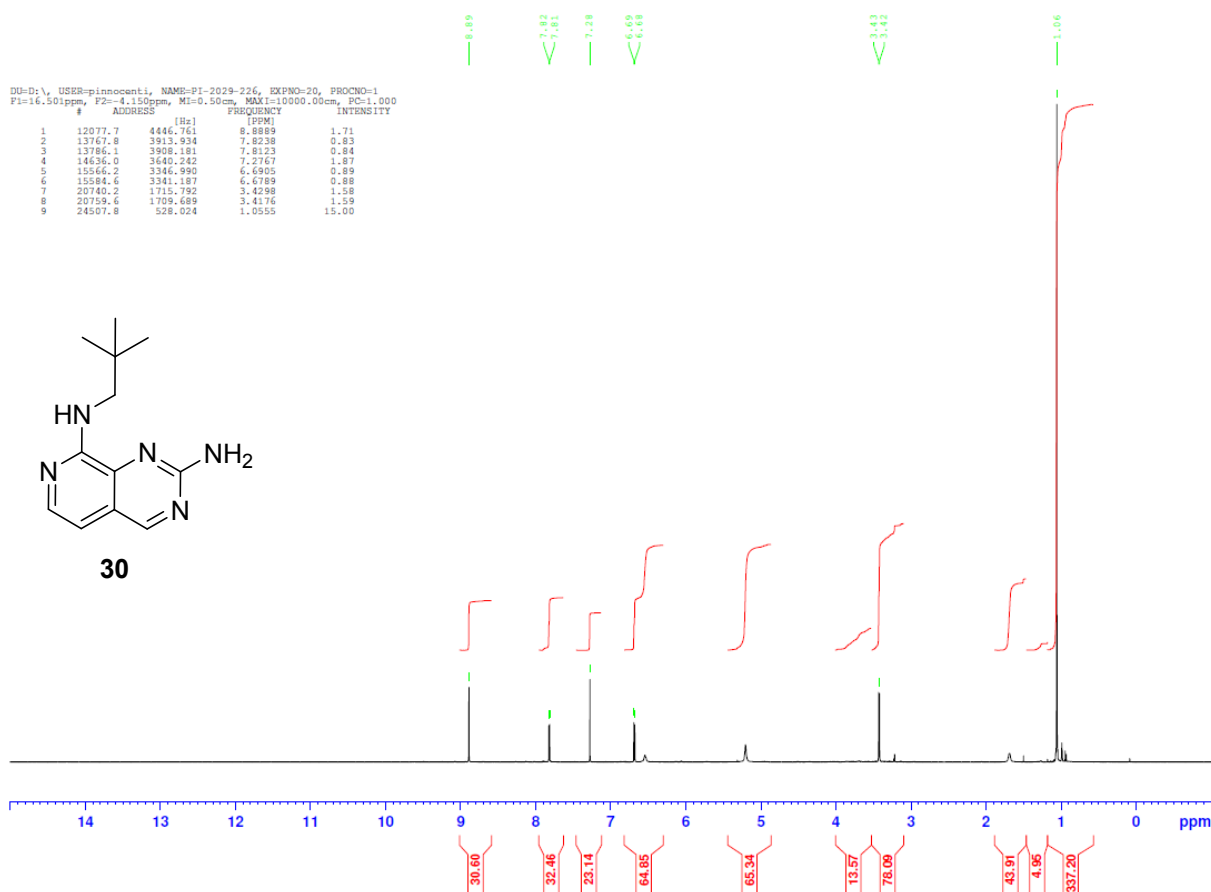
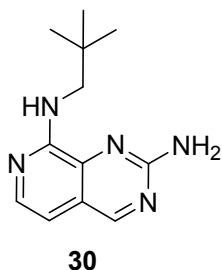


NAME HW-2130-0084
EXPNO 10
PROCNO 1
Date_ 20140318
Time 10.49
INSTRUM av500a
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 17996
SOLVENT MeOD
NS 128
DS 0
SWH 25000.000 H
FIDRES 1.389198 H
AQ 0.3599900 s
RG 46300
DM 20.000 u
DE 6.00 u
TE 295.0 K
D1 2.00000000 s
D11 0.03000000 s
D12 0.00002000 s
D20 60.00000000 s
TD0 1

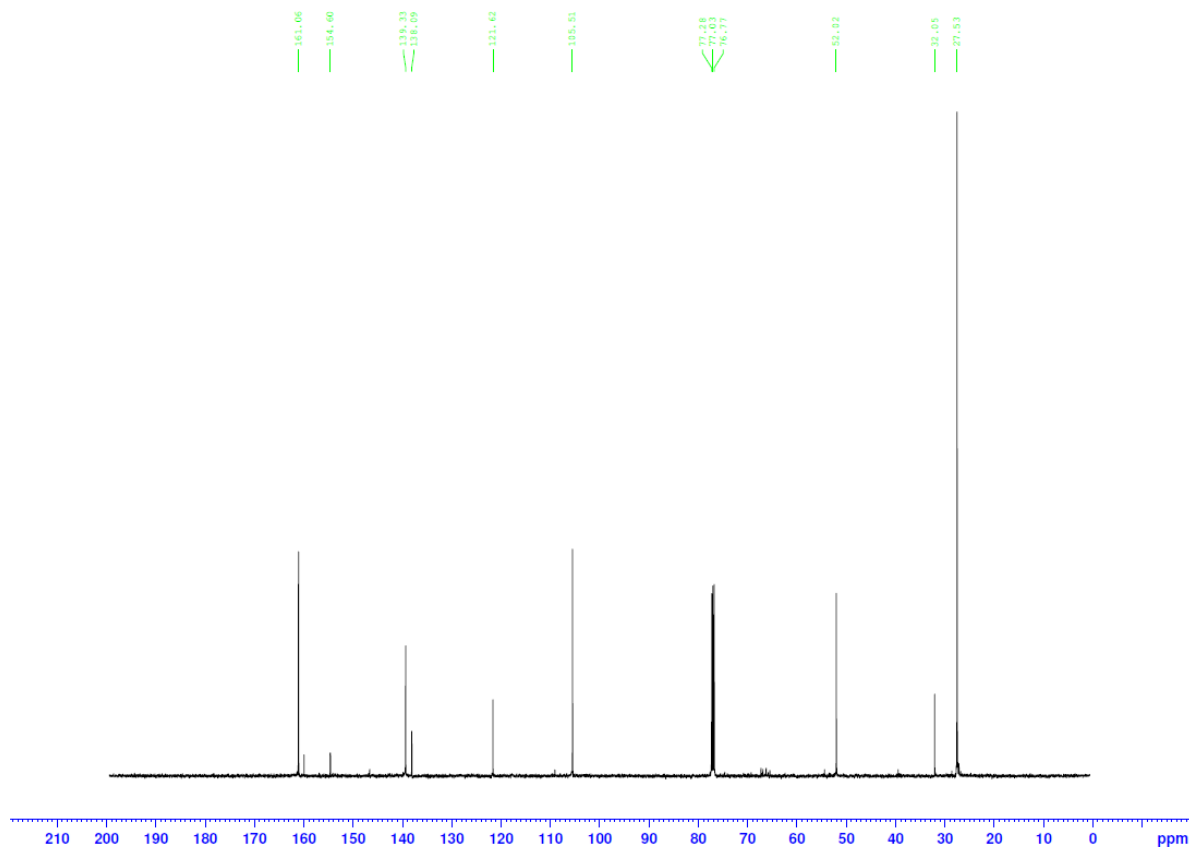
===== CHANNEL f1 =====
NUC1 13C
P1 8.30 u
PL1 2000.00 u
P2 500.00 u
PL2 0.00 d
PL1W 71.33757782 M
SFO1 125.8030561 M
SI 9.83 d
SF 9.83 d
SPRAME Crp60comp.4
SFOAL2 Crp60, 0.5, 25.1
SFOAL2 0.500
SFOAL2 0.500
SFOAL2 0.00 H
SFOAL2 0.00 H

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 -3.00 d
PL12 16.00 d
PL2W 35.68453217 M
PL12W 0.44594164 M
SFO2 500.2620010 M
SI 32768
SF 125.7564770 M
MCW EM
SSB 0
LB 2.00 H
GB 0
PC 1.00

#	ADDRESS	FREQUENCY	INTENSITY
1	1277.7	4446.181	1.71
2	13767.8	3913.934	0.83
3	13786.1	3908.181	0.84
4	14636.0	3640.242	1.87
5	15566.6	3348.990	0.85
6	15584.6	3341.187	0.88
7	20740.2	1715.792	3.4298
8	20759.6	1681.688	3.156
9	24507.0	528.021	10.055
			15.00



NAME	PI-2029-226
EXPNO	20
PROCN0	1
Date_	20140402
Time	17.32
INSTRUM	av5000a
PULPROG	zgpg30
PRGFM	5 mm QNP 1H/13
TD	2630
TD	6536
TD	CD13
TD	16
TD	16
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 s
RG	48
FW	48.1820
WDW	48.400 u
SSB	6.00 u
DE	295.0 K
TE	1.00000000 s
TD0	1
===== CHANNEL f1 =====	
NUC1	1H
P1	9.50
PL1	-3.00 dB
PL1W	35.664552317 W
SFO1	36.4630893 MHz
SP1	321768
SF	500.2600000 MHz
NUC2	13C
LB	0.30 Hz
GB	0
PC	1.90

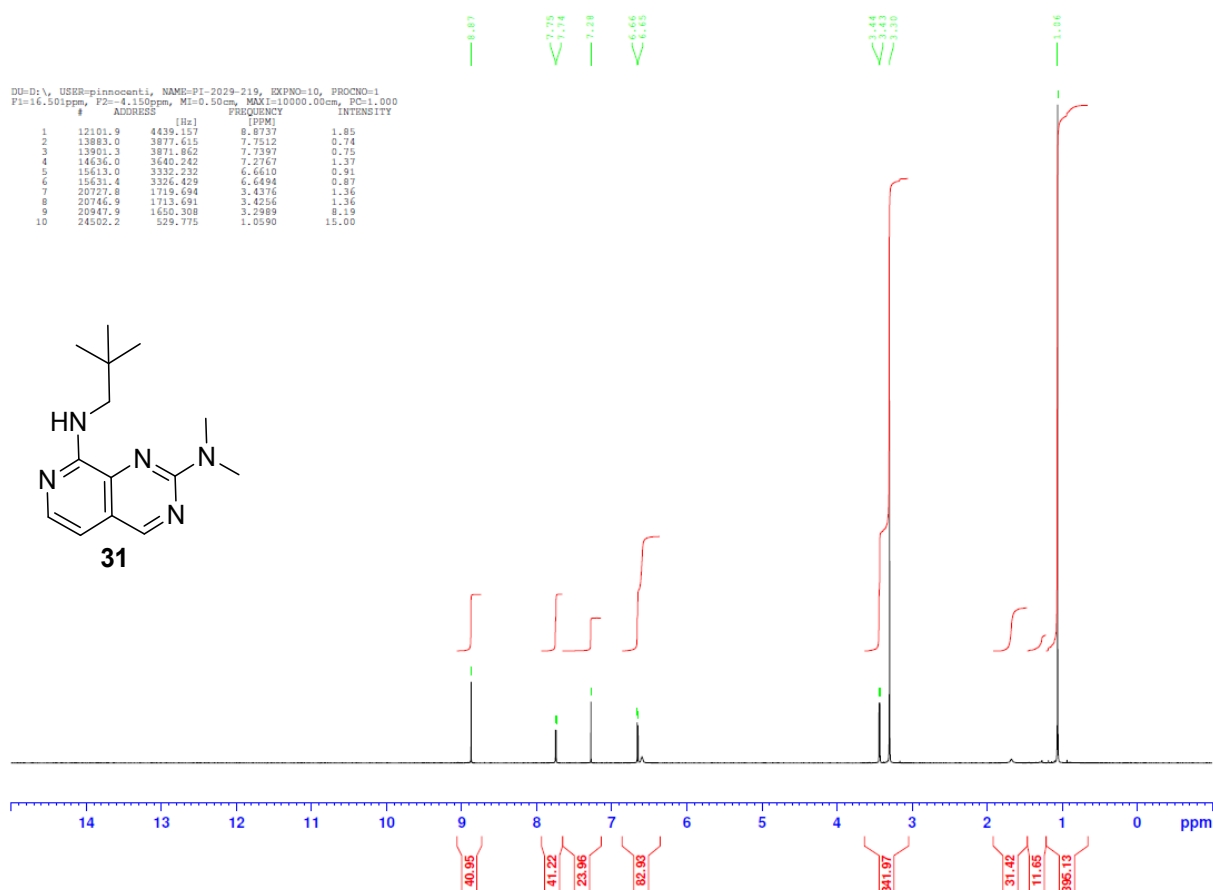
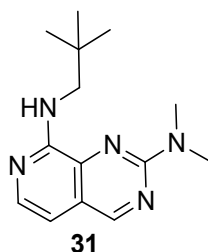


```
NAME          PI-2029-226
EXPNO         11
PROCNO        1
Date_         2014.04.02
Time          1.29
INSTRUM       5 mm QNP 1H/13
PROBHD        zgpg30
PULPROG       zgpg30
AQ            500.00
RG            327.68
SI            1
SOLVENT       CDCl3
NS            4096
DS            5
SWH            25000.00 MHz
F2            1.388125000
F1            0.135990000
DE            46.300
RG            25.000
WDW            6.000
SSB            0.000
LB             0.500
GB            0.000000000
D1            2.000000000
D11            0.030000000
D2            0.000000000
D20            60.000000000
D21            1
===== CHANNEL f1 =====
NUC1           13C
P1            1.300
PCPD2         2008.000
P2            500.000
PL1W          71.337575000
SF01          125.830365000
SP01          9.830
SP02          9.830
SPRPM02       Crp60comp.4
SPR02         Crp60.5-12.0
SP01A2        0.500
SP01A1        0.500
SP01B2        0.000
SP01B1        0.000
SP01F22       0.000
===== CHANNEL f2 =====
PCPR02        NUC2
NUC2          waltzi16
P1            80.000
PCPD2         2008.000
P2            16.000
PL1W          35.684532100
PL2W          0.444700000
SF02          125.926260000
SF01          125.799477000
SP01          EM
SP02          EM
LB            2.000
GB            1.000
PC            0
```

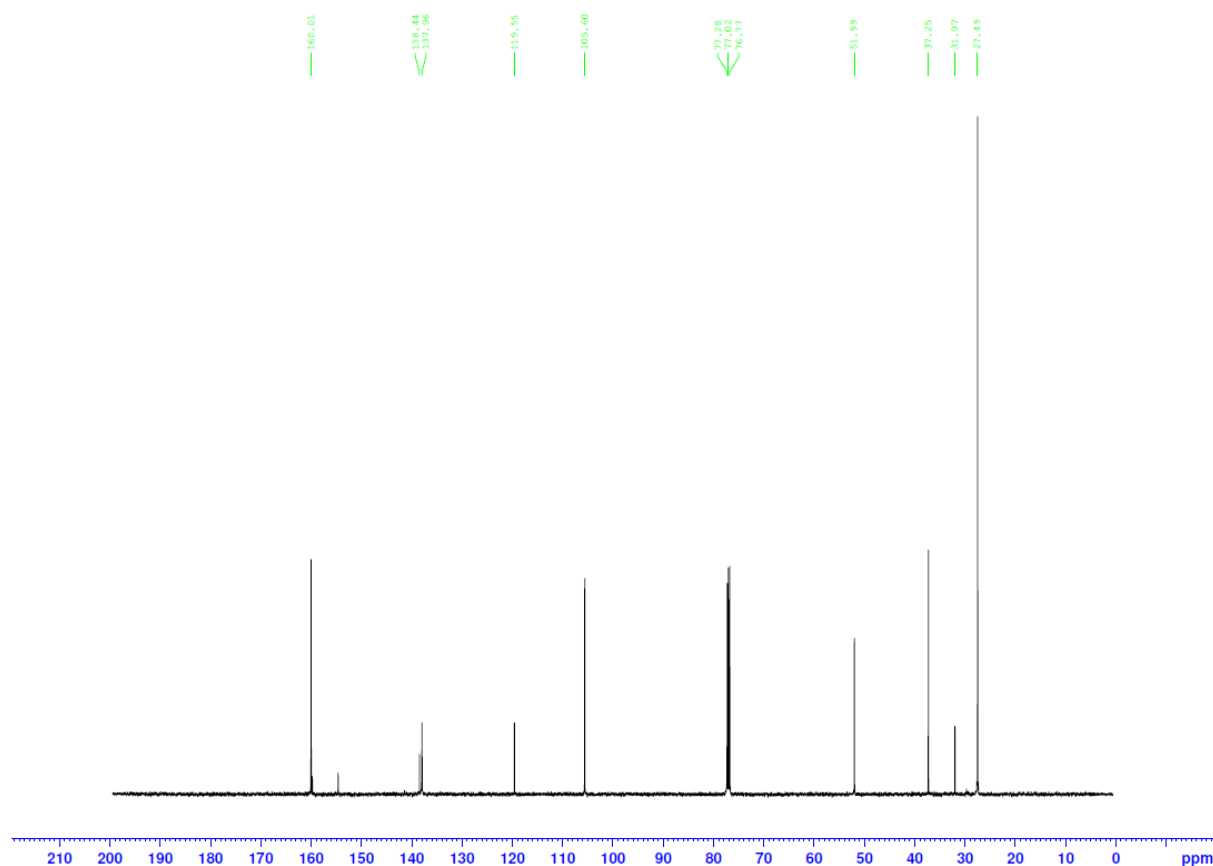
```

GNU-D, USER=pi@centos1, NAME=PI-2029-219, EXPNO=10, PROCN=1
F1=16.501ppm, F2=4.150ppm, M1=0.50cm, MAX1=10000.00cm, PC1=1.000
# ADDRESS      FREQUENCY      INTENSITY
1      12101.9      4439.157      8.8737      1.85
2      13803.0      3877.615      7.5152      0.74
3      13901.3      3871.662      7.4707      0.75
4      14636.0      3376.342      7.2767      1.37
5      15613.0      3332.322      6.6101      0.91
6      16531.4      3326.429      6.4494      0.87
7      20777.8      1311.894      2.7466      1.36
8      20746.9      1173.691      3.4256      1.36
9      20947.9      1650.308      3.2989      1.19
10     24469.2      1775.775      3.6000      1.00

```



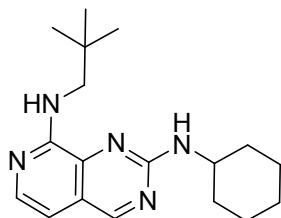
NAME	PI-2029-219
EXPNO	10
PROCNO	1
Date_	20140318
Time	12:57
INSTRUM	av500a
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	6536
TD SOLVENT	CDCl3
NS	16
DS	4
SWH	10330.378 Hz
FIDRES	0.157632 Hz
AQ	3.1720400 s
RG	1620
DW	48.400 us
DE	6.000 us
TE	295.0 K
D1	1.00000000 s
TD0	1
===== CHANNEL f1 =====	
NUC1	1H
PL1	9.50 u
PL1	-3.00 dB
PL1W	35.68453217 W
SFO1	500.2630893 MHz
CF	312768
SF	500.2600000 MHz
MCH	EM
LB	0.30 Hz
PC	0
GC	1.00



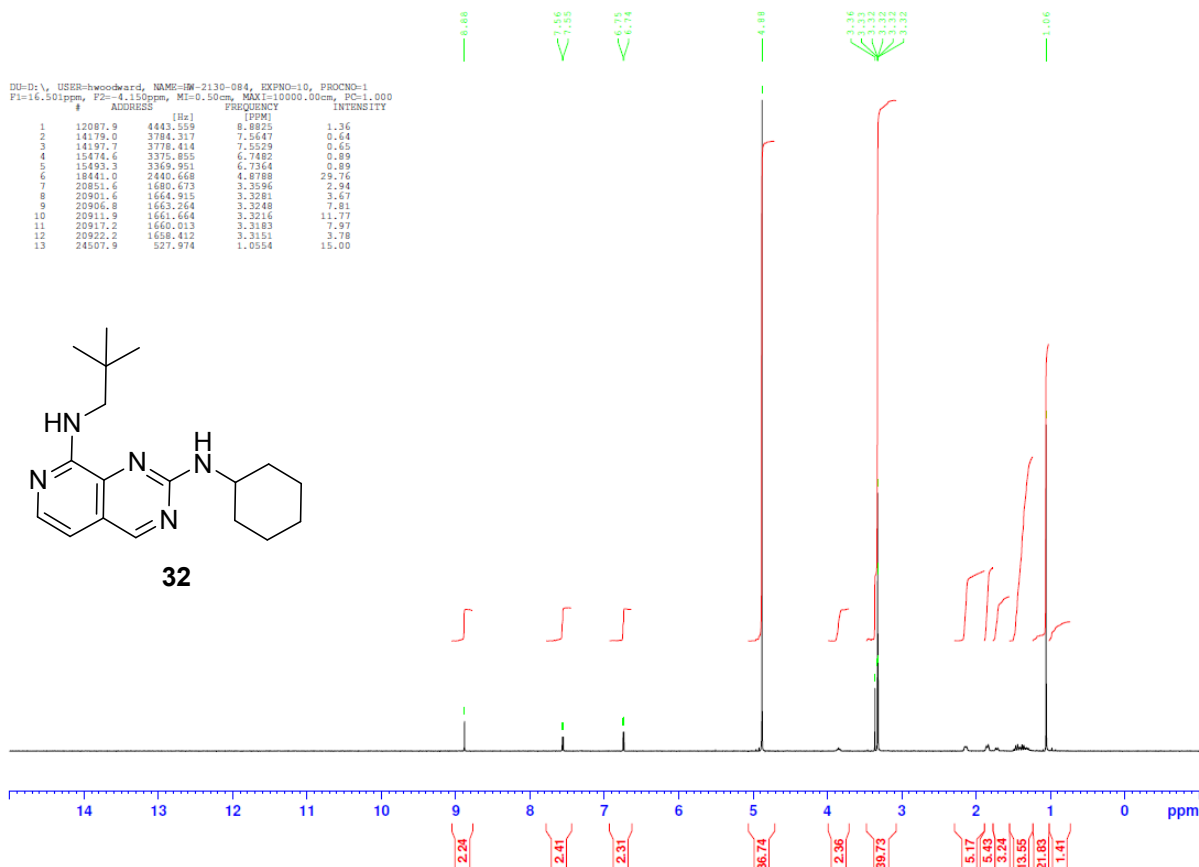
```
NAME          PI-2029-219
EXPNO          20
PROCNO        1
PROC          1
TIME          20140319
Time          6.26
INSTRUM       MPR
PROBHD        5 mm QNP 1H/1
PULPROG       zgpg30
DECO          udecfg
AQ            0.00100000
SOLVENT       CDCl3
NS            4096
DS            4
SWH            25000.000 MHz
F2            1.3881333 GHz
AQRES         0.03359900 Hz
RG            4K
DECO          0.00100000
PC            20.000000
DC            6.00 uV
D1            0.00100000
D11           2.000000000 s
D12           0.030000000 s
D13           0.001000000 s
D14           0.001000000 s
D15           60.000000000 s
D16           1.000000000 s
D17           1.000000000 s
D18           1.000000000 s
D19           1.000000000 s
D20           1.000000000 s
===== CHANNEL f1 =====
NUC1           13C
P1            0.30 uS
PC1           2000.000000
PL1           500.00 uV
PL2           500.00 uV
PL12          71.33757500 MHz
SPF1          125.80396400 MHz
SFO1          8.83 MHz
SFB           8.83 MHz
SFPM2         Cmp66.0 comp. 4
SFO2          8.83 MHz
SFB2          8.83 MHz
SFOAL2        0.5000
SFOAL4        0.5000
SFOAL8        0.5000
SFOAL16       0.5000
SFOFFB8       0.00 Hz
SFOFFB16      0.00 Hz
===== CHANNEL f2 =====
NUC2           1H
PCPD2         16.00 uS
PCPD2         80.00 uV
PL2           16.00 uV
PL12          35.68453210 MHz
PL12          9.44646790 MHz
SFO2          500.2626010 MHz
SFB           500.2626010 MHz
SF           125.7904770 MHz
SF           0.00 MHz
SGS           0.00 MHz
LB            2.00 MHz
PCPD          1.00 MHz
PCPD          1.00 MHz
```

DU=D:\, USER=hwoodward, NAME=HW-2130-084, EXPNO=10, PROCNO=1
PI=16.501ppm, F2=-4.150ppm, MI=0.50cm, MAXI=10000.00cm, PC=1.000

#	ADDRESS	[Hz]	FREQUENCY	INTENSITY
1	12087.9	4443.559	8.8025	1.36
2	14179.0	3784.317	7.5647	0.64
3	14197.7	3778.414	7.5529	0.65
4	15474.6	3375.855	6.7462	0.89
5	15493.3	3365.951	6.7364	0.89
6	18441.0	2440.668	4.8788	29.76
7	20851.6	1690.473	3.3596	2.94
8	20901.6	1664.915	3.3281	3.67
9	20906.8	1663.264	3.3248	7.81
10	20911.9	1661.664	3.3216	11.77
11	20917.2	1660.013	3.3183	7.97
12	20922.2	1658.412	3.3151	3.78
13	24507.9	521.974	1.0554	15.00

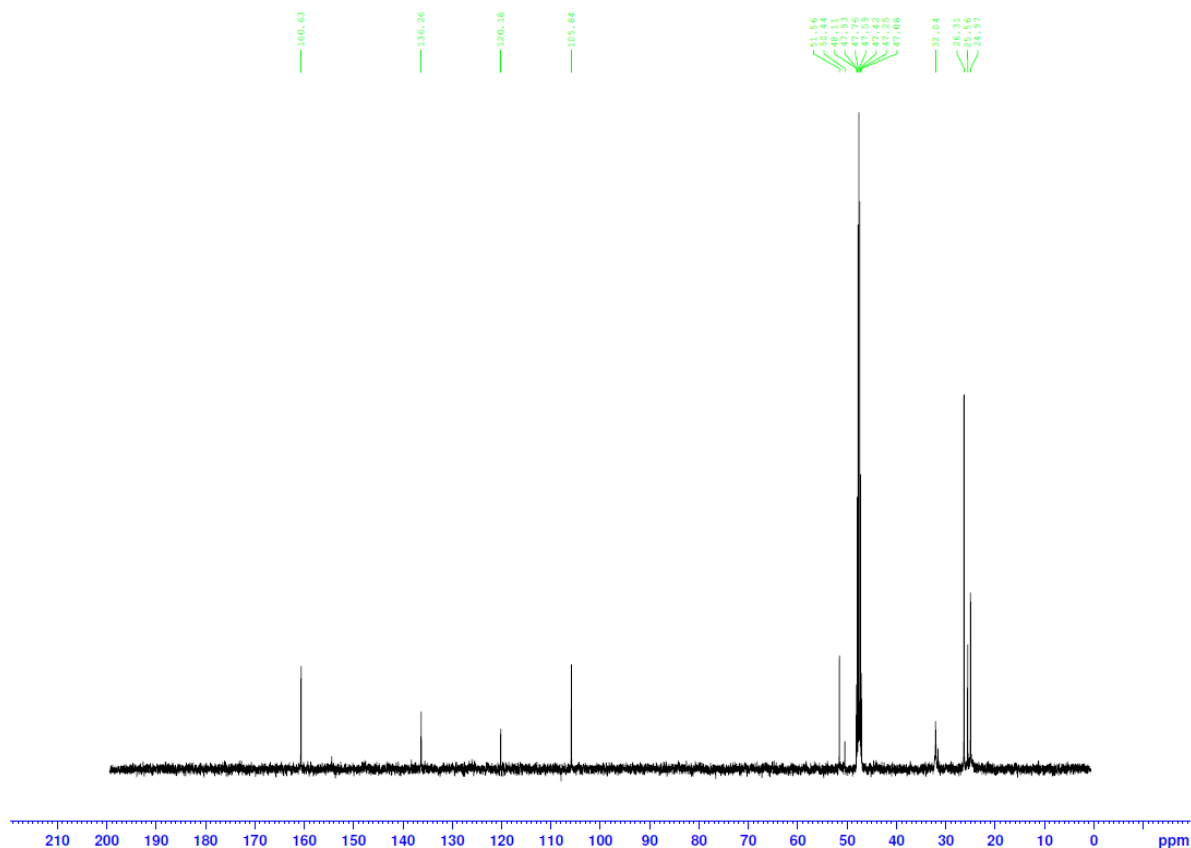


32



NAME HW-2130-084
EXPNO 10
PROCNO 1
Data_ 20140324
Time 11.13
INSTRUM av500a
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.157632 H
AQ 3.1720407 s
RG 9200
DM 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 u
PL1 -3.00 d
PL1W 35.68453217 M
SFO1 500.2620893 M
S1 32768
SF 500.2600000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00



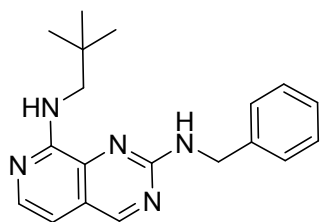
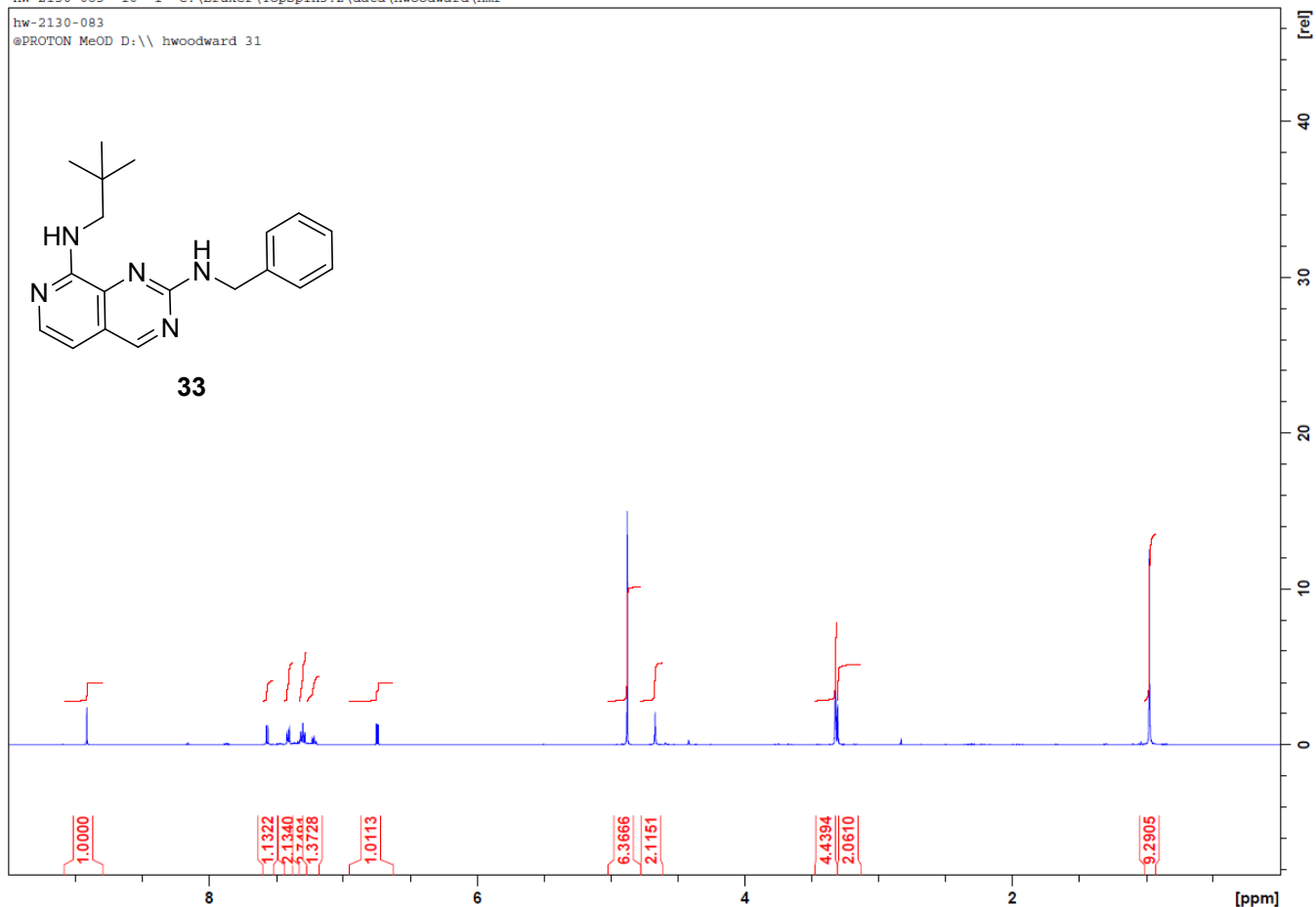
NAME HW-2130-084
EXPNO 11
PROCNO 1
Data_ 20140324
Time 12.06
INSTRUM av500a
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 17996
SOLVENT MeOD
NS 128
DS 0
SWH 25000.000 H
FIDRES 1.389198 H
AQ 0.3599900 s
RG 46300
DM 20.000 u
DE 6.00 u
TE 295.0 K
D1 2.00000000 s
D11 0.03000000 s
D12 0.00002000 s
D20 60.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.30 u
PL1 2000.00 u
PL2 500.00 u
PL1 0.00 d
PL1W 71.33757782 M
SFO1 125.8030561 M
SFO2 9.83 d
SFO 9.83 d
SPH2 Crp60comp.4
SPH2 Crp60,0.5,20.1
SFOAL2 0.500
SFOALS 0.500
SPOFFS2 0.00 H
SPOFFS8 0.00 H

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 -3.00 d
PL12 16.00 d
PL1W 35.68453217 M
PL12W 0.44924164 M
SFO2 500.2620810 M
S1 32768
SF 125.7904770 M
WDW EM
SSB 0
LB 2.00 H
GB 0
PC 1.00

hw-2130-083

@PROTON MeOD D:\ hwoodward 31

**33**

162.72

128.29
128.04
126.73
126.45

135.74

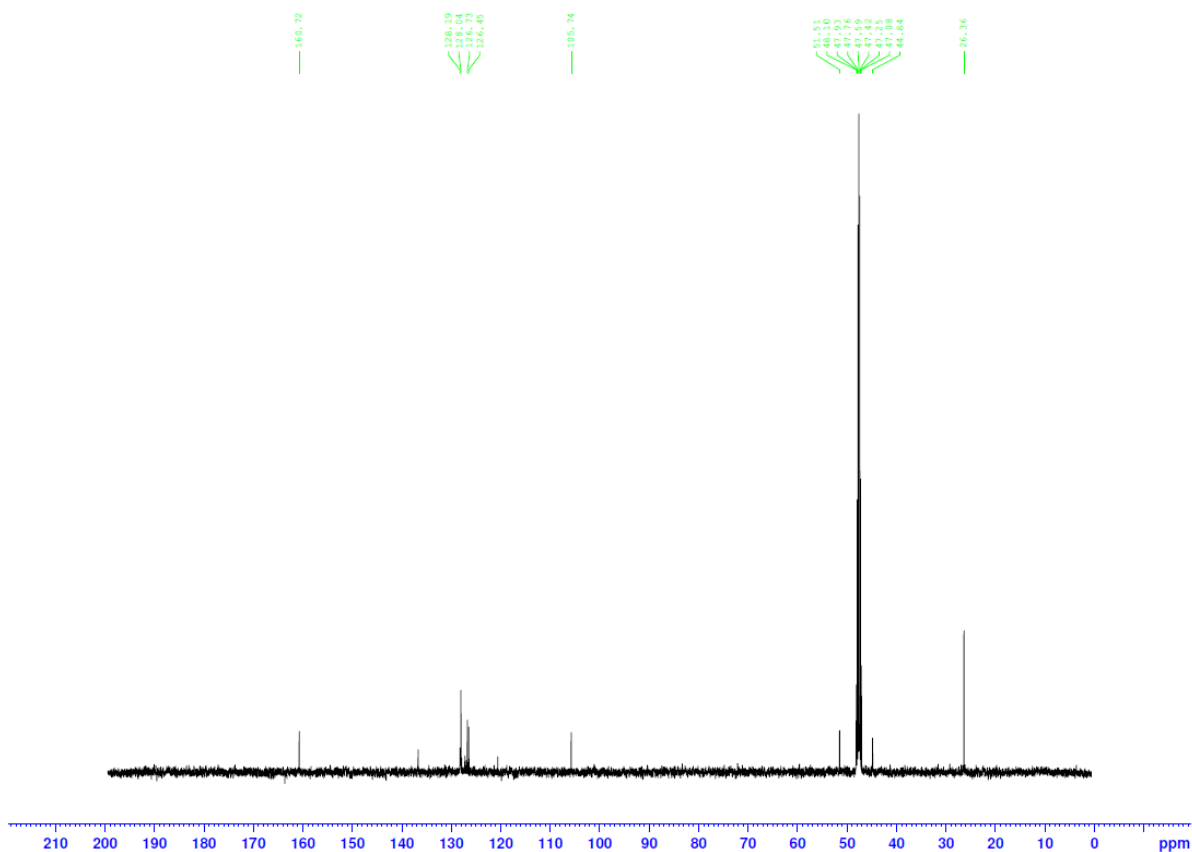
51.51
47.93
47.76
47.42
47.35
47.25
44.86

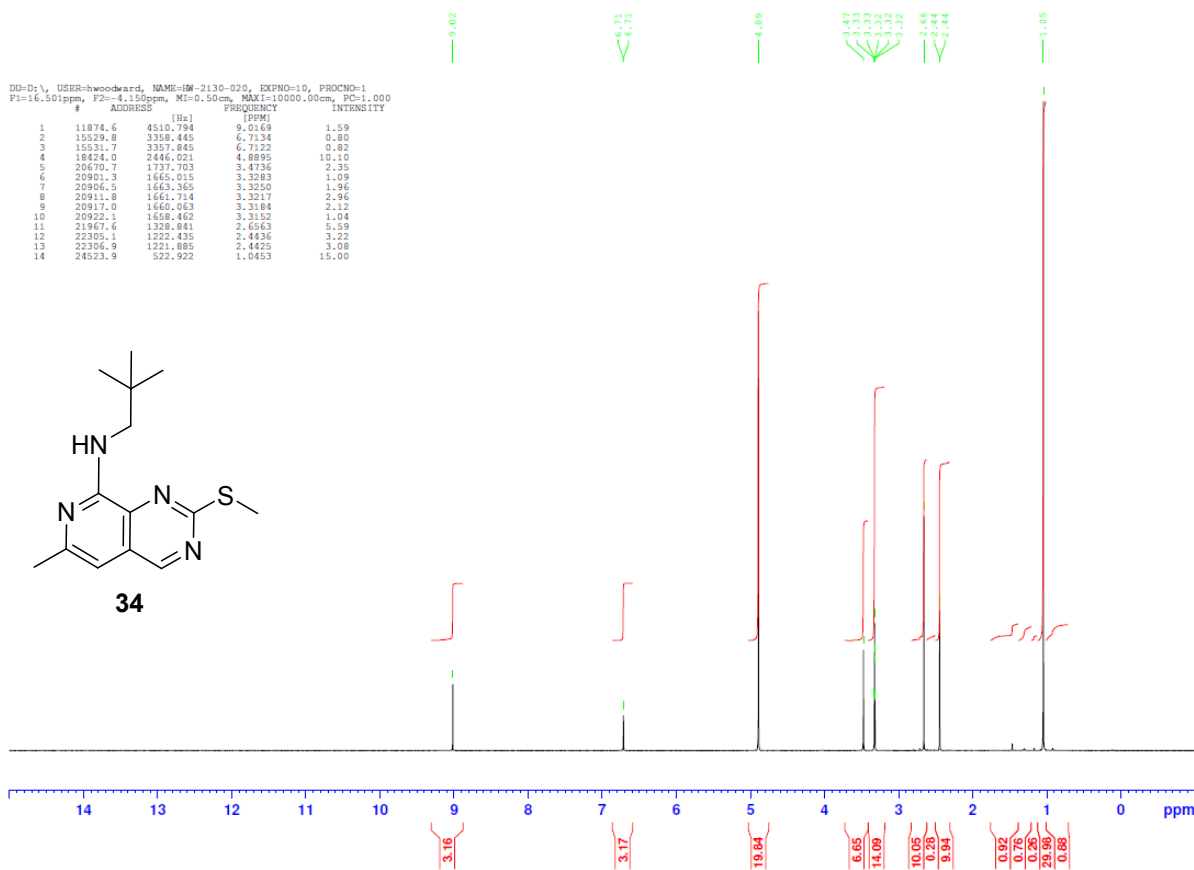
26.36

NAME HW-2130-083
EXPNO 11
PROCNO 1
Data_ 20140324
Time 11.44
av500a
INSTRUM 5 mm QNP 1H/13
PROBHD 17996
TD 128
SOLVENT MeOD
NS 0
DS 0
SWH 25000.000 Hz
FIDRES 1.38198 Hz
AQ 0.3599900 s
RG 46300
PC 20.000 u
DE 6.00 u
TE 295.0 K
D1 2.00000000 s
D11 0.03000000 s
D12 0.00000000 s
D20 60.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 0.30 u
P12 2000.00 u
P26 500.00 u
PL1 0.00 d
PL1W 71.3375782 MHz
SFO1 125.8030561 MHz
SF2 9.83 d
SFB 9.83 d
SPNAM2 Crp60comp.4
SPNAM6 Crp60, 0.5, 20.1
SFOAL2 0.500
SFOAL6 0.500
SFOFF2 0.00 Hz
SFOFF6 0.00 Hz

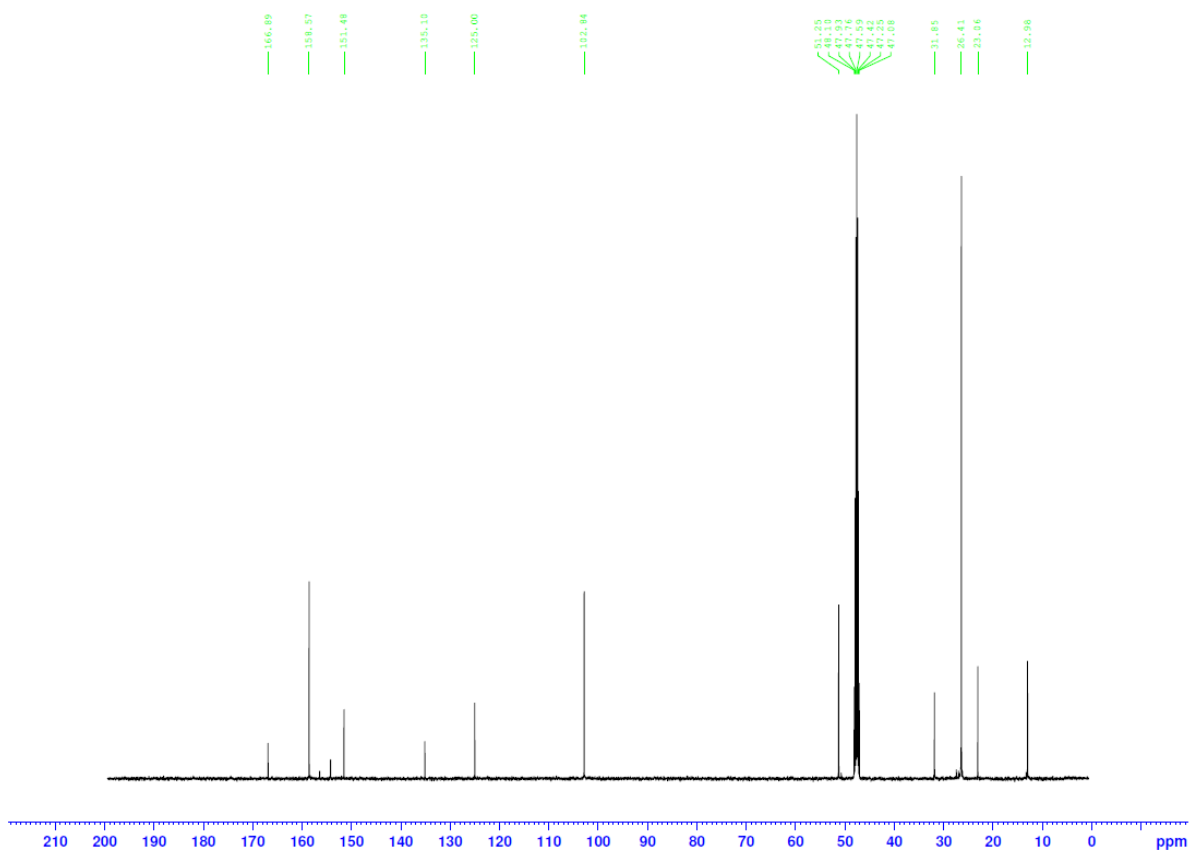
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 -3.00 d
PL12 16.00 d
PL2W 35.68453217 MHz
PL1W 9.44924164 MHz
SFO2 500.2620010 MHz
S1 32768
SF 125.7904770 MHz
WUW EM
SFB 0
LB 2.00 Hz
GB 0
PC 1.00





NAME HW-2130-020
EXPNO 10
PROCNO 1
Date_ 20131127
Time 17.48
INSTRUM av500a
PROBHD 5 mm PABBI 1H/
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 10330.578 H
FIDRES 0.151622 H
AQ 3.1720407 s
RG 2580
DW 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.0000000 s
TD0 1

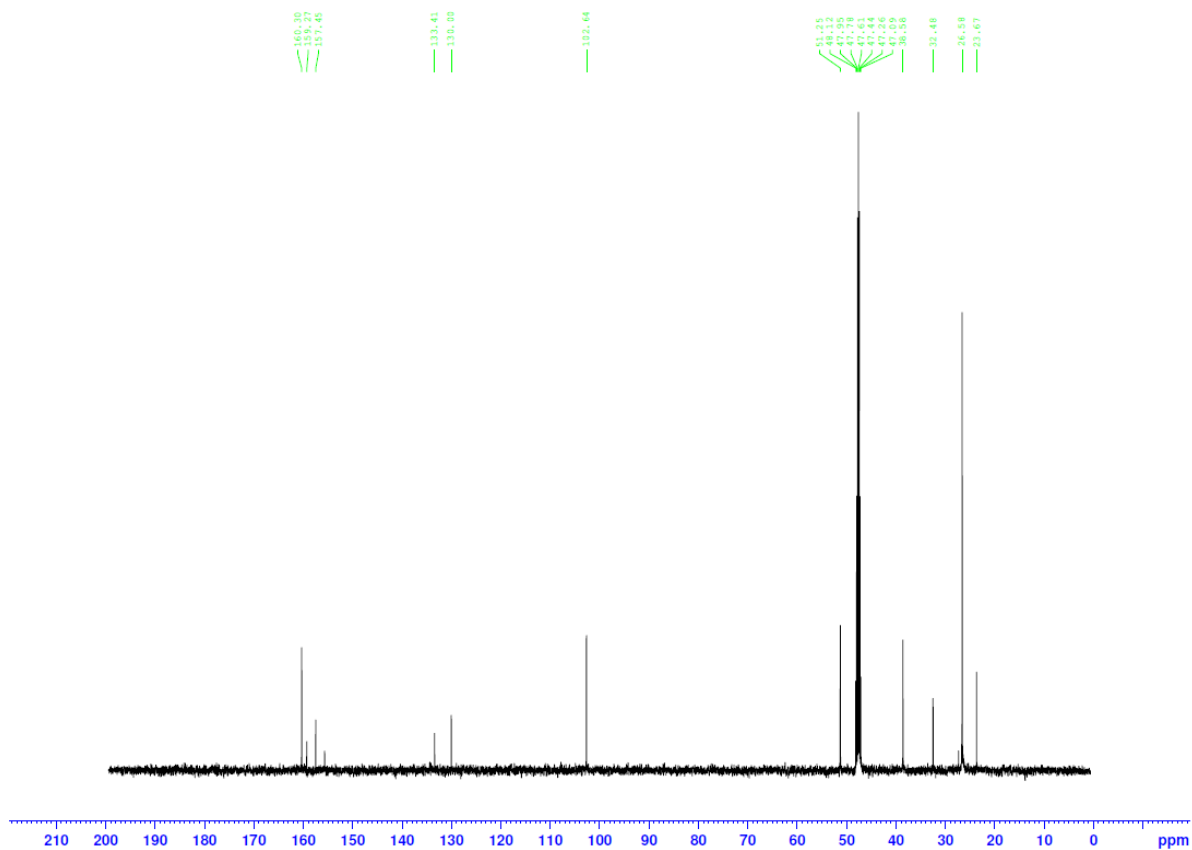
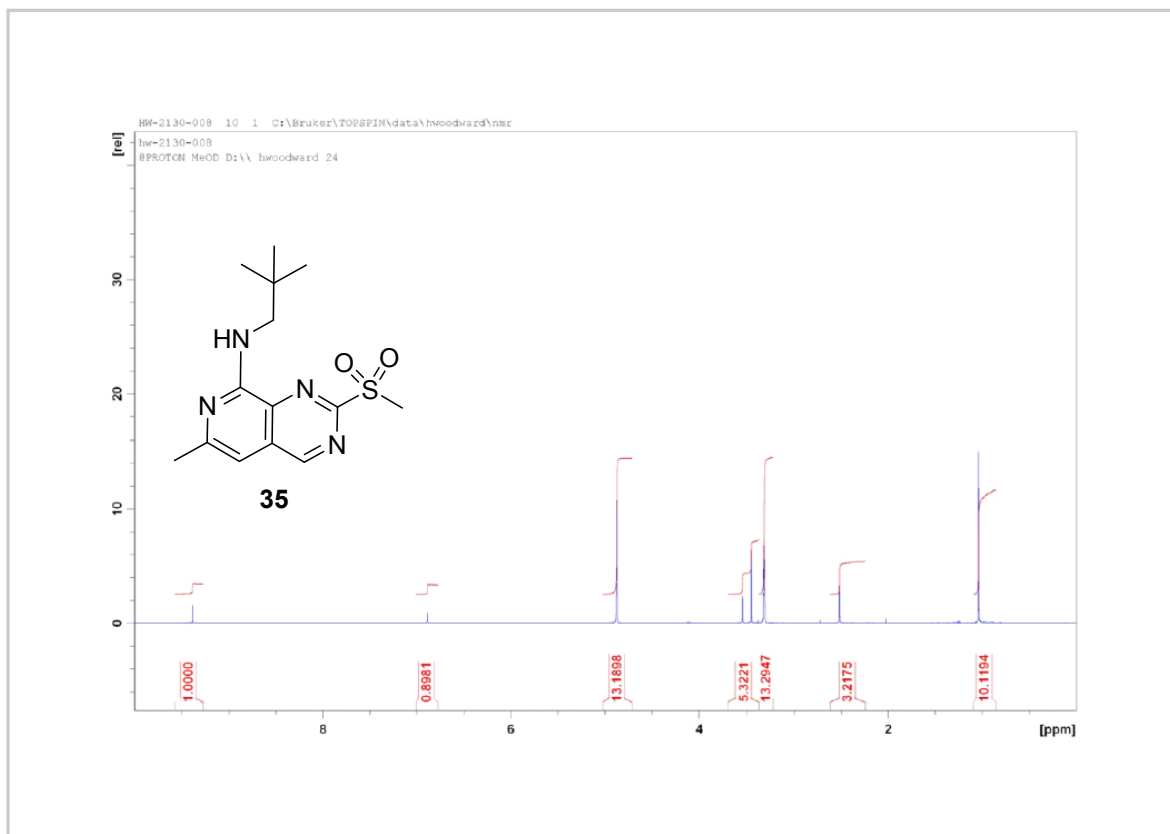
===== CHANNEL f1 =====
NUC1 1H
P1 7.70 u
PL1 0.50 d
PL1W 15.93969440 M
SFO1 500.2630893 M
SI 32768
SF 500.2600000 M
WDM EM
SSB 0
LB 0.30 H
GB 0
PC 1.00



NAME PI-2029-233
EXPNO 20
PROCNO 1
Date_ 20140417
Time 4.42
INSTRUM av500a
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 17996
SOLVENT MeOD
NS 4096
DS 0
SWH 25000.000 H
FIDRES 1.389198 H
AQ 0.3599960 s
RG 46300
DW 20.000 u
DE 6.00 u
TE 295.0 K
D1 2.0000000 s
D11 0.0100000 s
D12 0.0000200 s
D20 60.0000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.30 u
PL1 2000.00 u
P26 500.00 u
PL1 0.00 d
PL1W 71.33757782 M
SFO1 125.8030561 M
SF2 9.83 d
SF2W 9.83 d
SPNAM2 Crp60comp.4
SPNAM2 Crp60,0.5,20.1
SFOAL2 0.500
SFOAL6 0.500
SPOFFS2 0.00 H
SPOFFS8 0.00 H

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 -3.00 d
PL12 16.00 d
PL1W 35.6843217 M
PL12W 0.44924164 M
SFO2 500.2620010 M
SI 32768
SF 125.7904770 M
WDM EM
SSB 0
LB 2.00 H
GB 0
PC 1.00



```

NAME      HW-2130-025
EXPNO     10
PROCNO    1
Date_     20140317
Time      10.49
INSTRUM    av500a
PROBHD     5 mm QNP
PULPROG    zgpg30
TD         17996
SOLVENT    MeOD
NS         128
DS         0
SWH         25000.000 H
FIDRES     1.389198 H
AQ         0.359900 s
RG         46300
BW         20.000 u
DE         6.00 u
TE         295.0 K
D1         2.00000000 s
D11        0.03000000 s
D12        0.00002000 s
D20        60.00000000 s
TDO        1

===== CHANNEL f1 =====
NUC1       13C
P1         8.30 u
P12        2000.00 u
P24        500.00 u
PL1        0.00 d
PL1W       71.33757782 W
SFO1       125.8030461 M
SP2        9.83 d
SP8        9.83 d
SFOAM2     Crp60,0.5,20.1
SFOAM8     Crp60,0.5,20.1
SFOAL2     0.500
SFOAL8     0.500
SFOFFS2    0.00 H
SFOFFS8    0.00 H

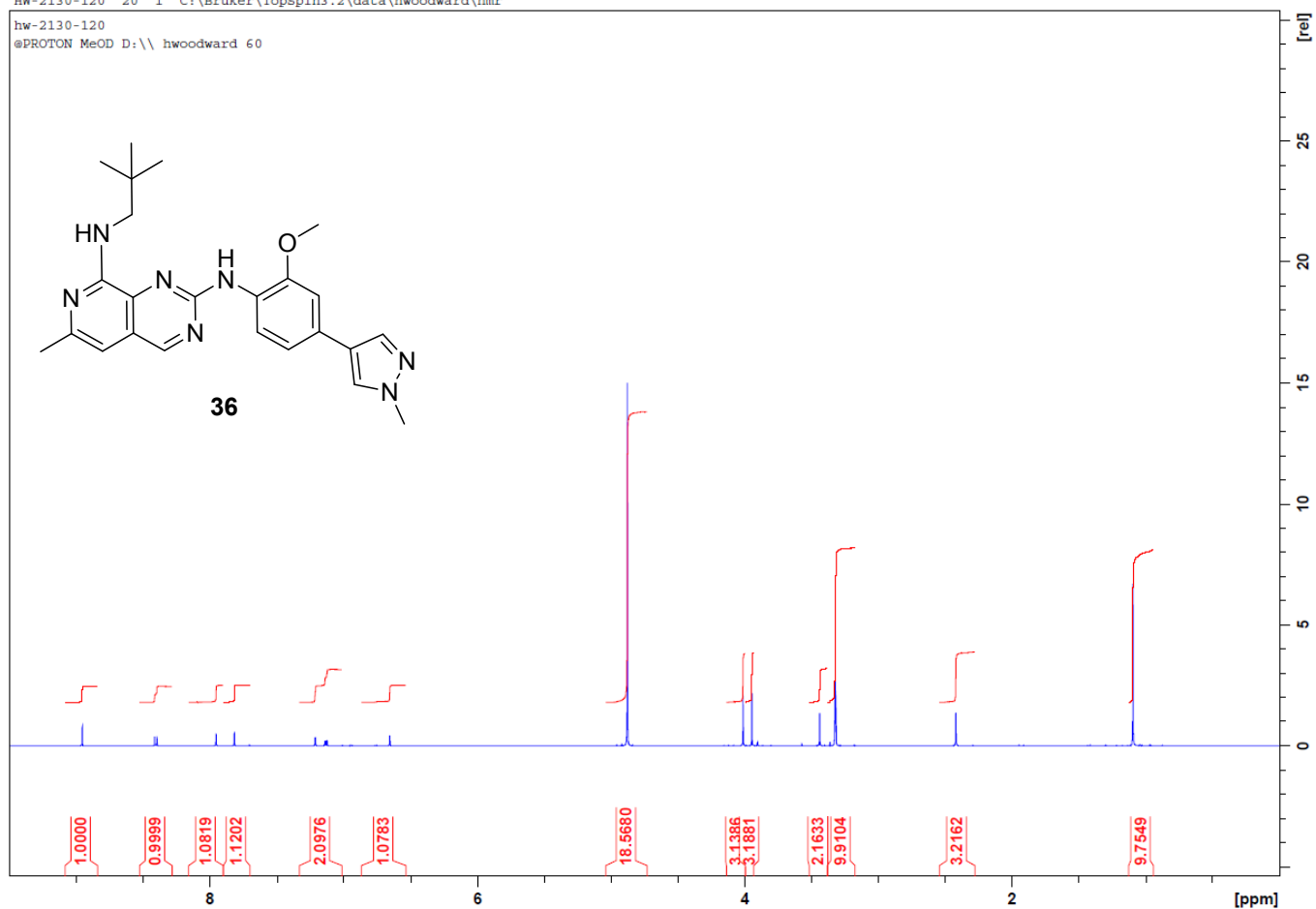
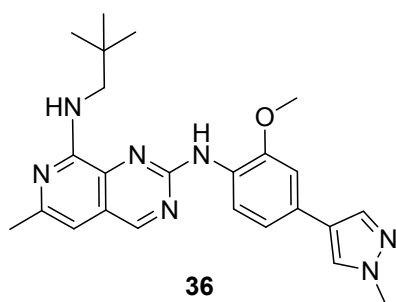
===== CHANNEL f2 =====
CHOPROG2   waltz16
NUC2       1H
PCPD2      80.00 u
PL2        -3.00 d
PL12       16.00 d
PL12W     35.68433217 W
PL12W     0.44924164 W
SFO2       500.2620010 M
ST         32768
SF         125.7904770 M
NEW        1H
SSB        0
LB         2.00 H
GB         0
PC         1.00

```

HW-2130-120 20 1 C:\Bruker\TopSpin3.2\data\hwoodward\nmr

hw-2130-120

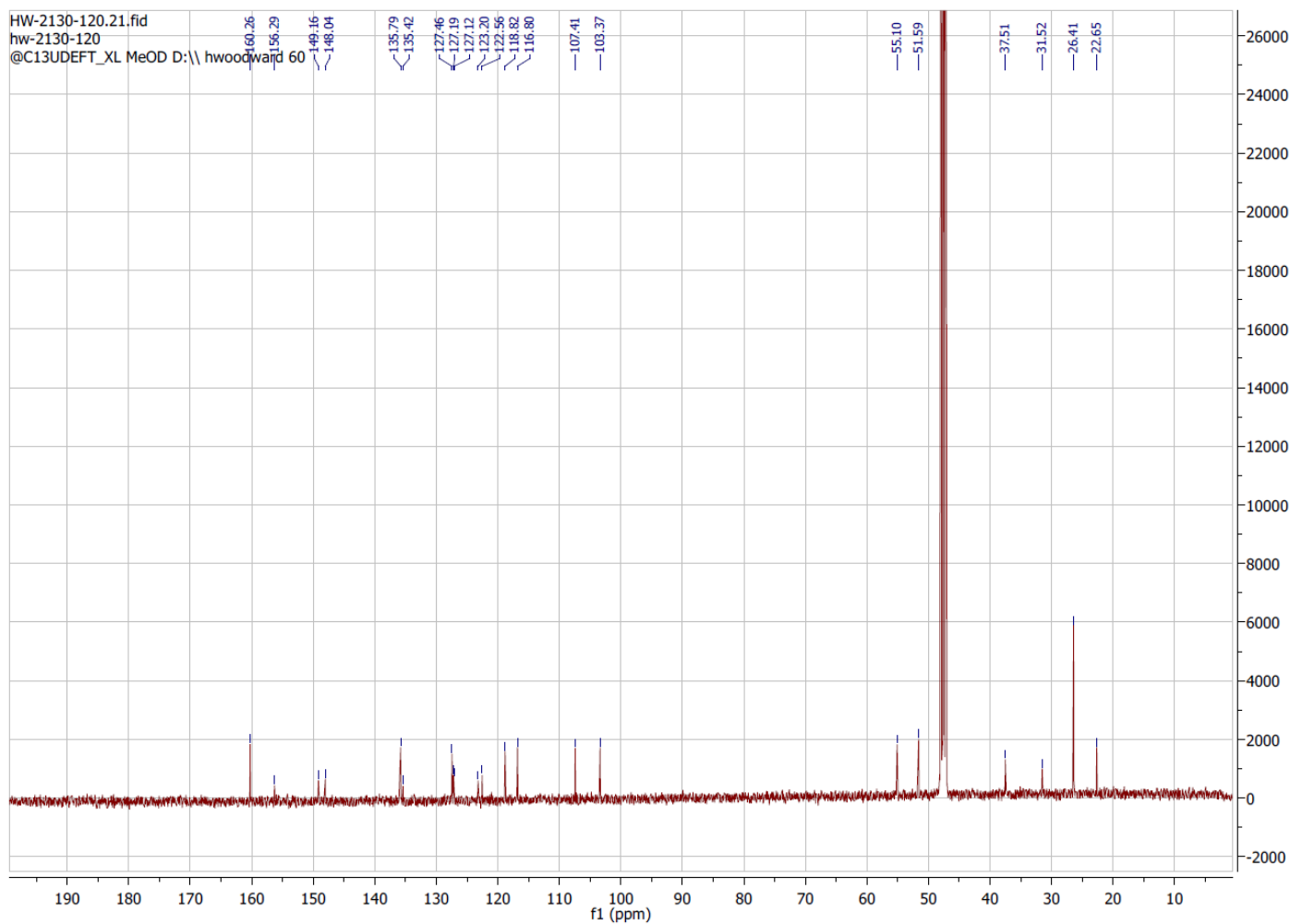
@PROTON MeOD D:\ hwoodward 60



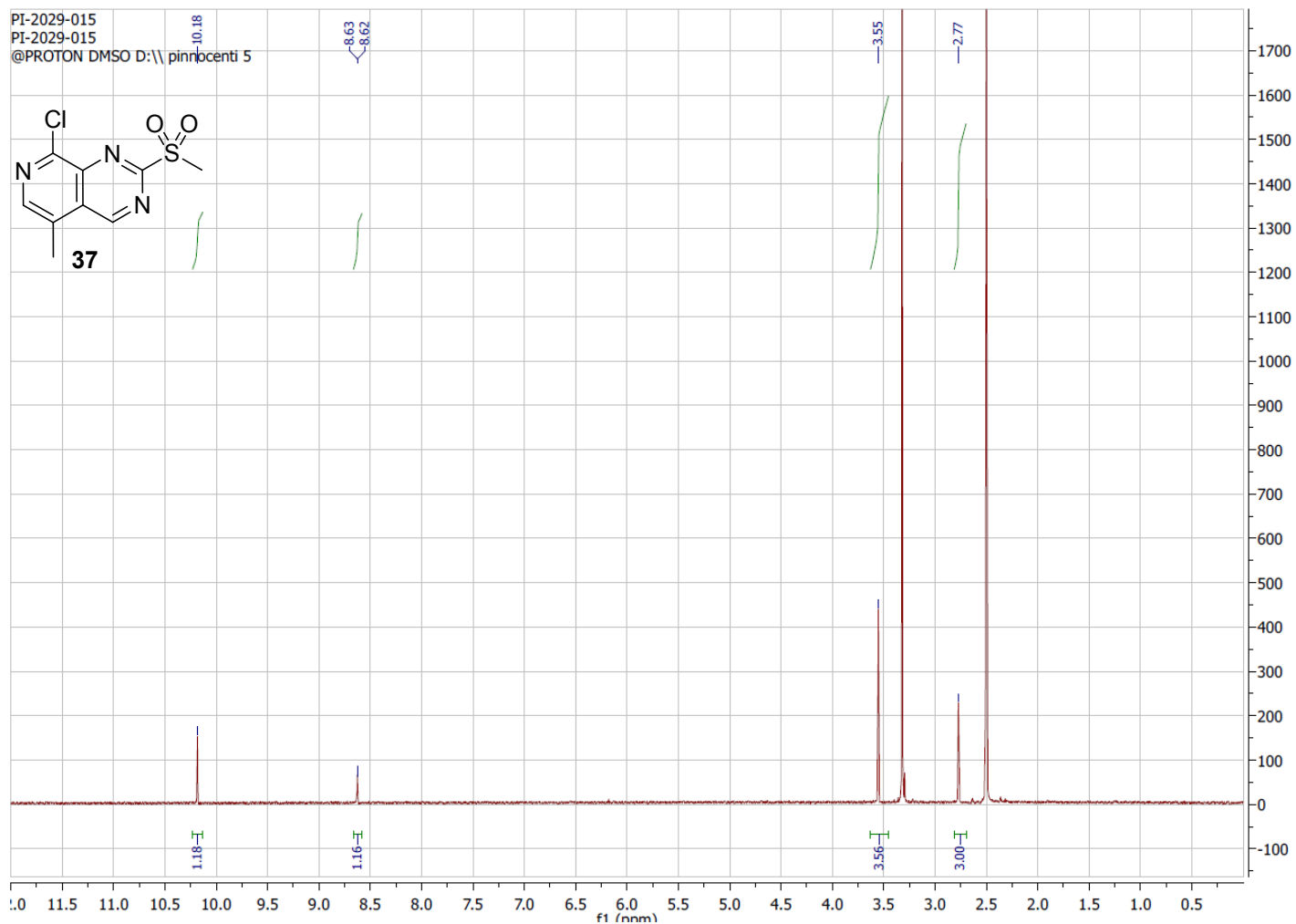
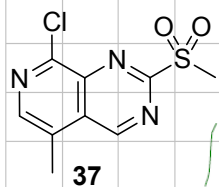
HW-2130-120.21.fid

hw-2130-120

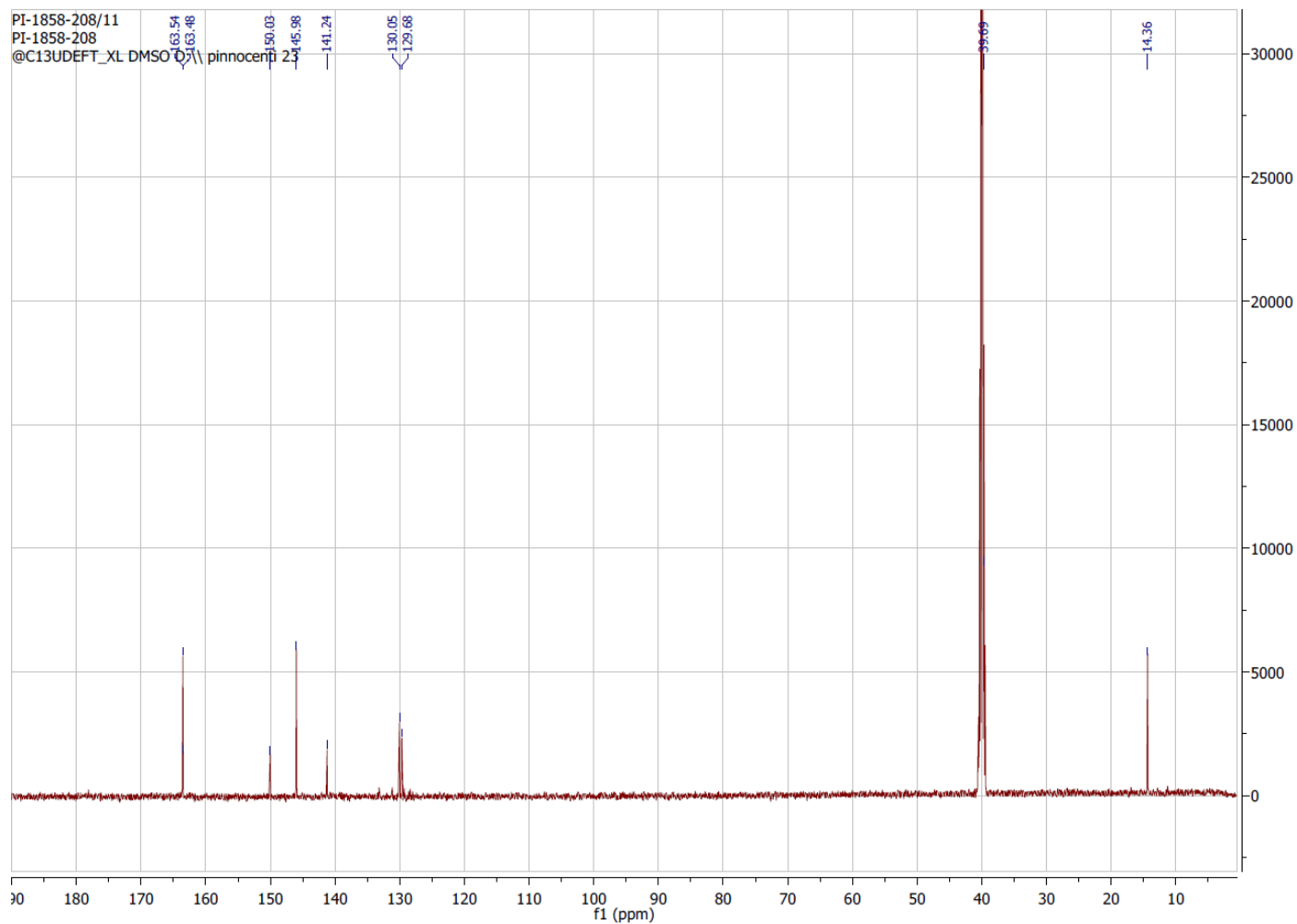
@C13UDEFT_XL MeOD D:\ hwoodward 60

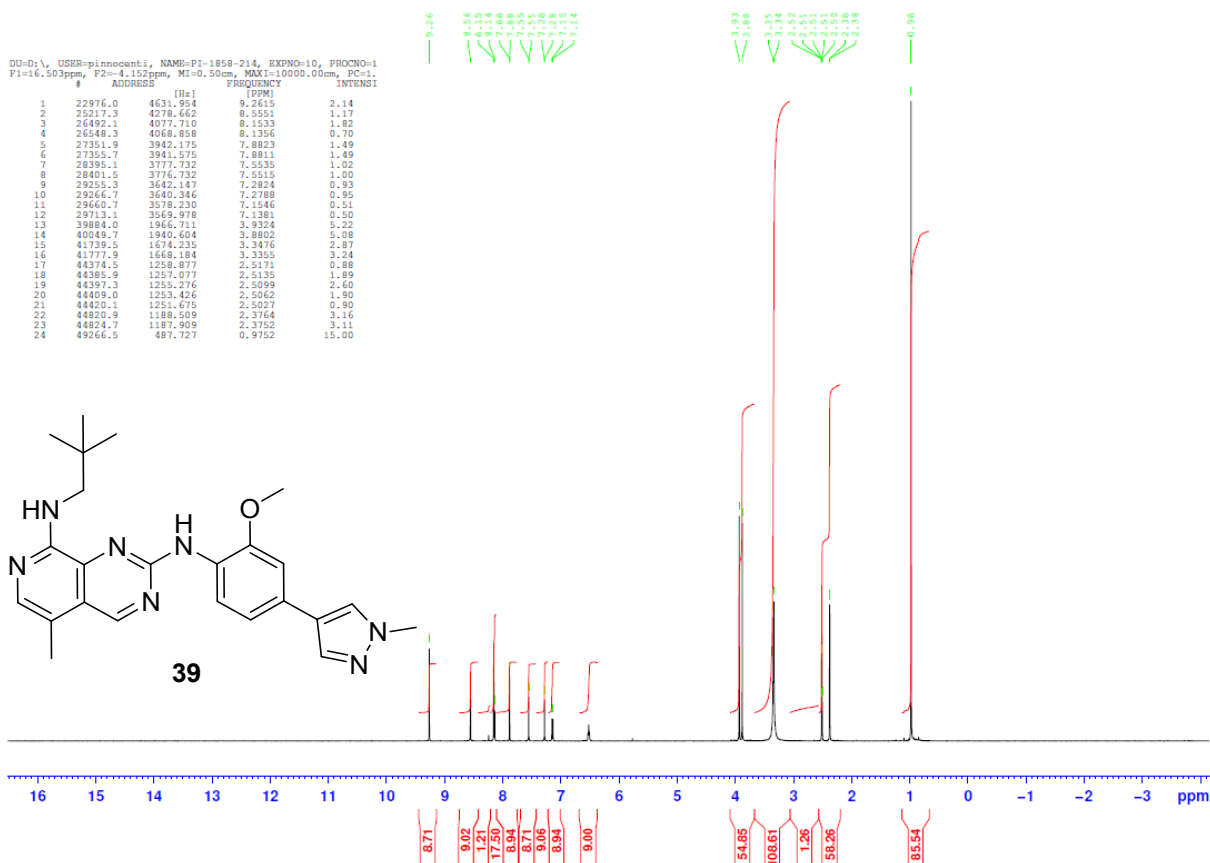


PI-2029-015
PI-2029-015
@PROTON DMSO D₂ pinnocenti 5



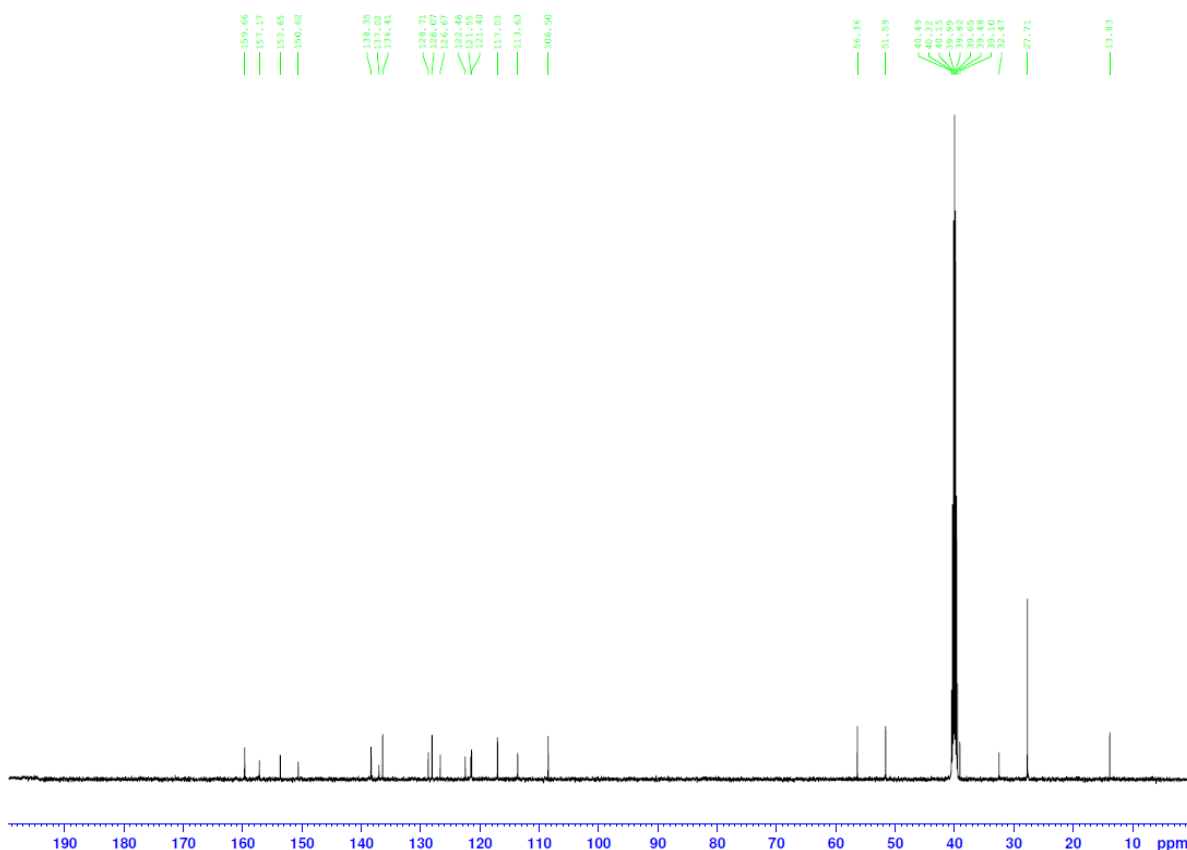
PI-1858-208/11
PI-1858-208
@C13UDEFT_XL DMSO D₂ pinnocenti 23





NAME PI-1858-214
EXPNO 10
PROCNO 1
Date_ 20121206
Time 14.56
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 s
RG 2580
DM 48.400 u
DE 6.00 u
TE 295.0 K
D1 1.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.25 u
PL1 0.00 d
PL1W 23.10935593 W
SFO1 500.1300885 M
SI 65536
SF 500.1300000 M
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME PI-1858-214
EXPNO 11
PROCNO 1
Date_ 20121207
Time 21.45
INSTRUM av500b
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 17996
SOLVENT DMSO
NS 4096
DS 0
SWH 25000.000 Hz
FIDRES 1.389198 Hz
AQ 0.3589860 s
RG 46300
DM 20.000 u
DE 6.00 u
TE 295.0 K
D1 2.00000000 s
D11 0.03000000 s
D12 0.00020000 s
D20 60.00000000 s
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.75 u
PL1 2000.00 u
PL2 500.00 u
PL1 1.00 d
PL1W 65.24507904 W
SFO1 125.7703644 M
SF2 10.32 d
SF 10.32 d
SPNAM2 Crp60comp-4
SPNAM8 Crp60,0.5,20.1
SFOAL2 0.500
SFOAL8 0.500
SFOF22 0.00 Hz
SFOF28 0.00 Hz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 0.00 d
PL12 17.90 d
PL2W 23.10935593 W
PL12W 0.37478989 W
SFO2 500.1300000 M
SI 32768
SF 125.7577890 M
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40