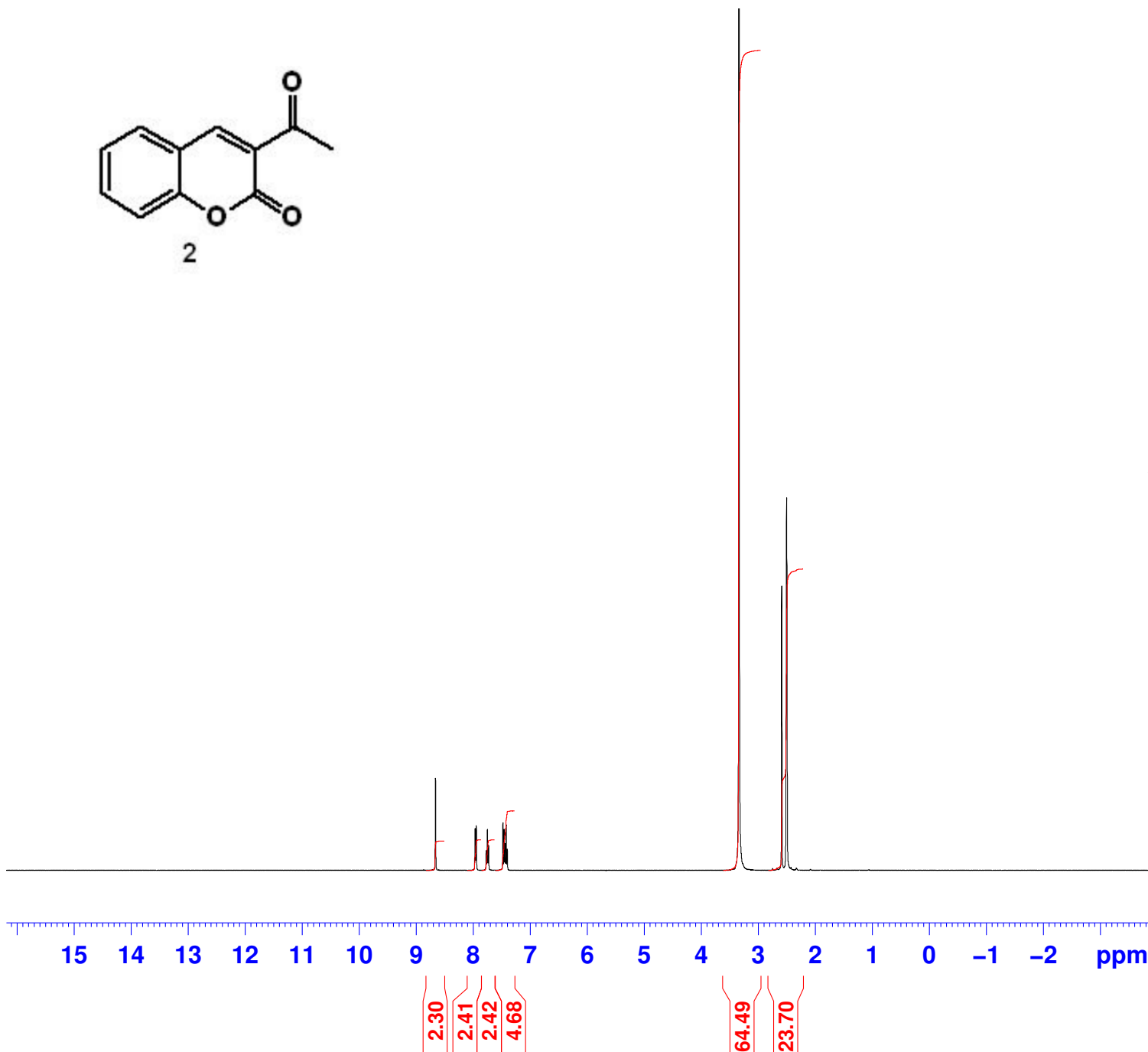


Current Data Parameters  
 NAME MG46  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130206  
 Time 17.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 181  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

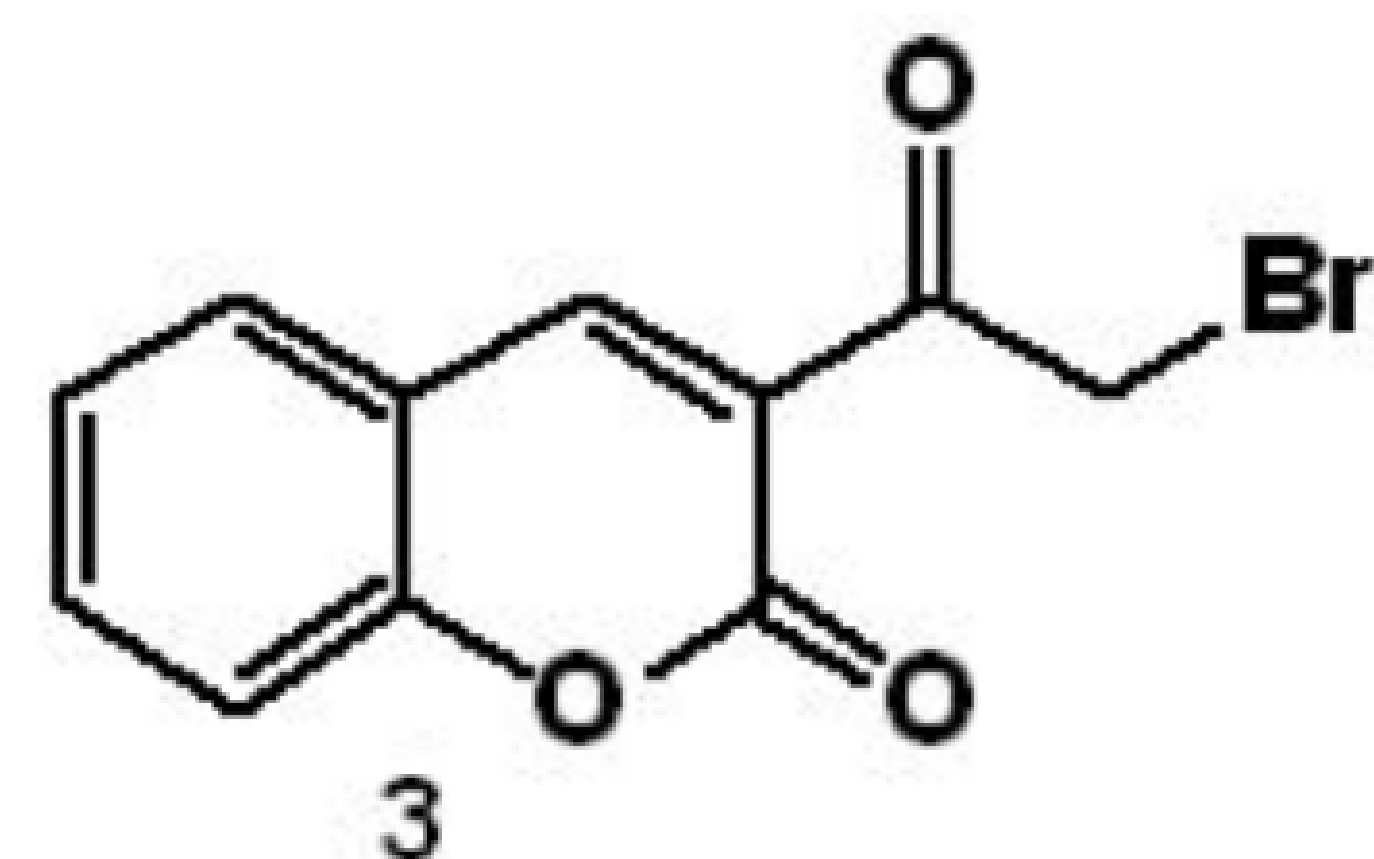
==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.40





test

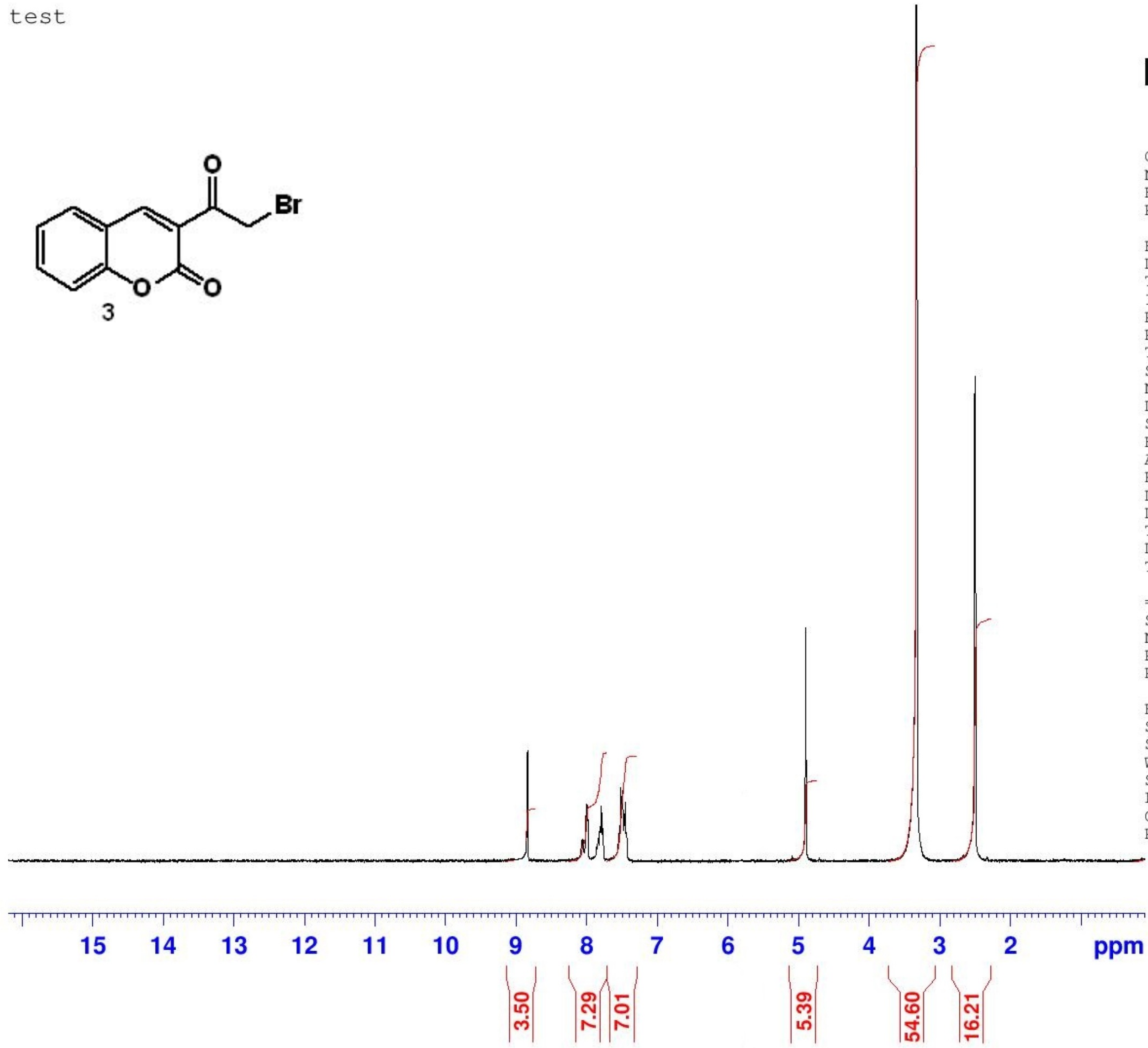


Current Data Parameters  
NAME MG53  
EXPNO 1  
PROCNO 1

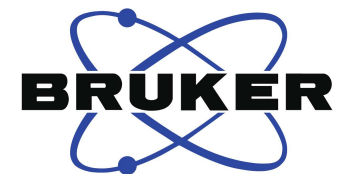
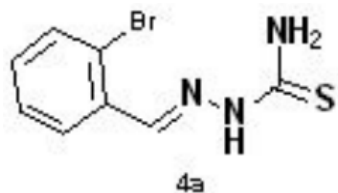
F2 - Acquisition Parameters  
Date\_ 20130220  
Time 14.18  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 400.1424710 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





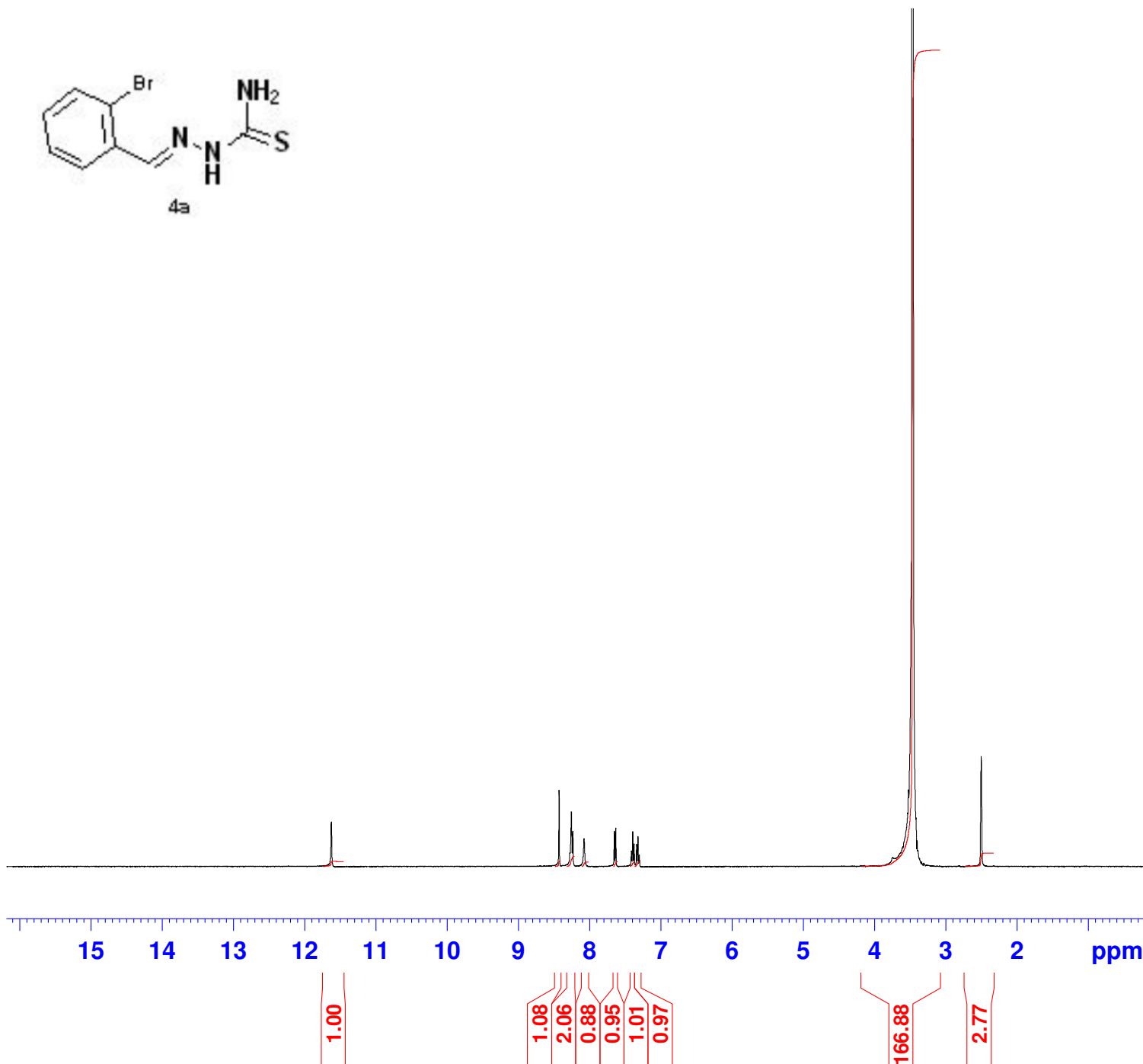


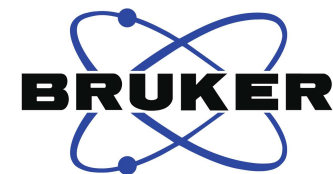
Current Data Parameters  
 NAME MG115  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130329  
 Time 18.27  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 3  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 64  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





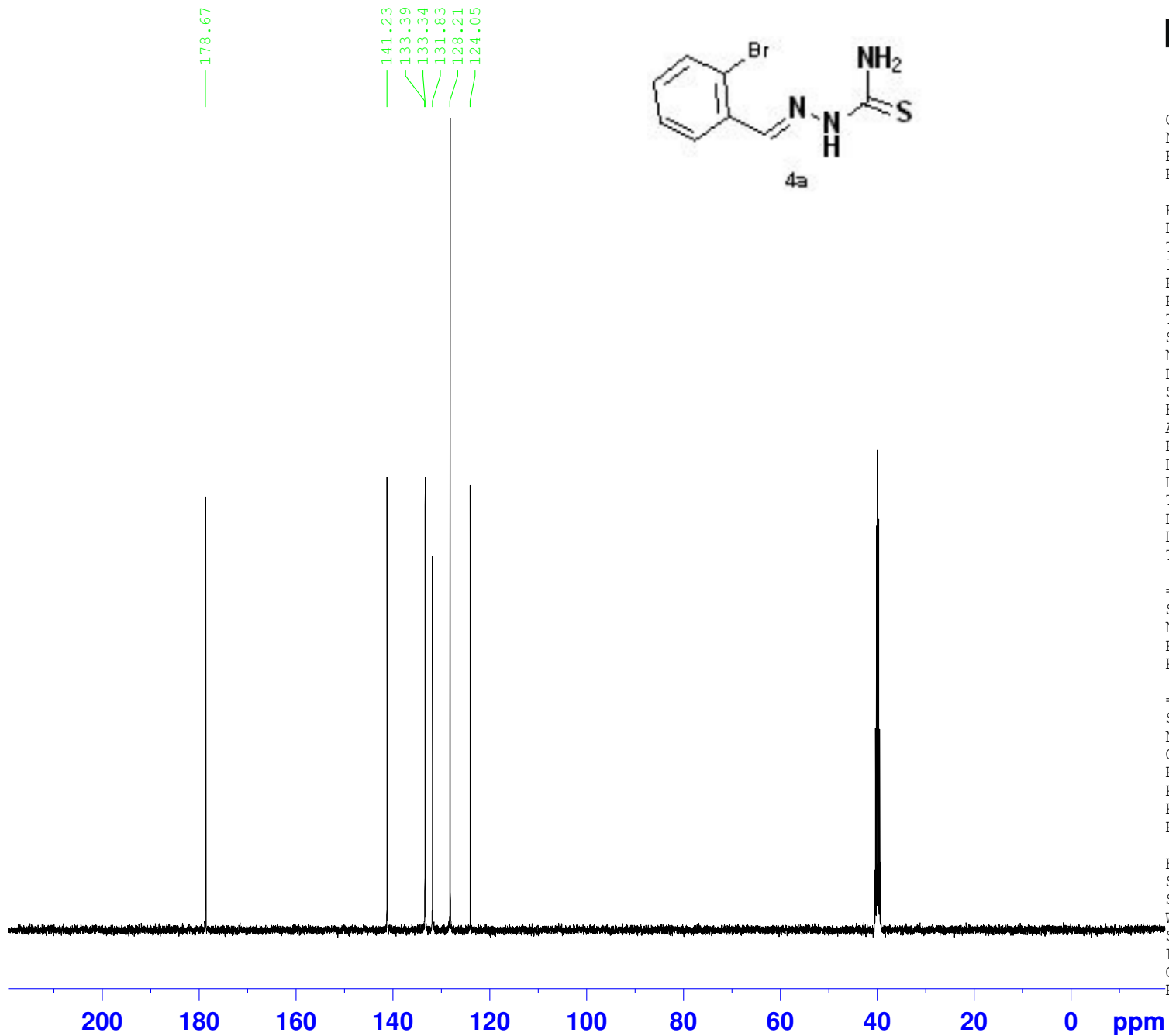
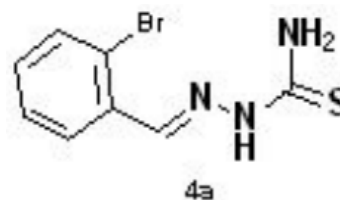
Current Data Parameters  
NAME MG-I-115c  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130524  
Time 16.29  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 61  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 181  
DW 20.800 usec  
DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

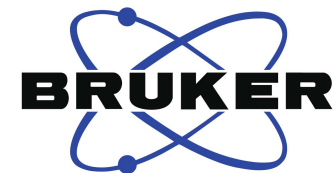
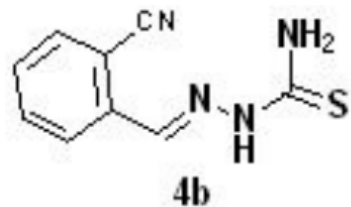
===== CHANNEL f1 =====  
SFO1 100.6253441 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1416006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



test

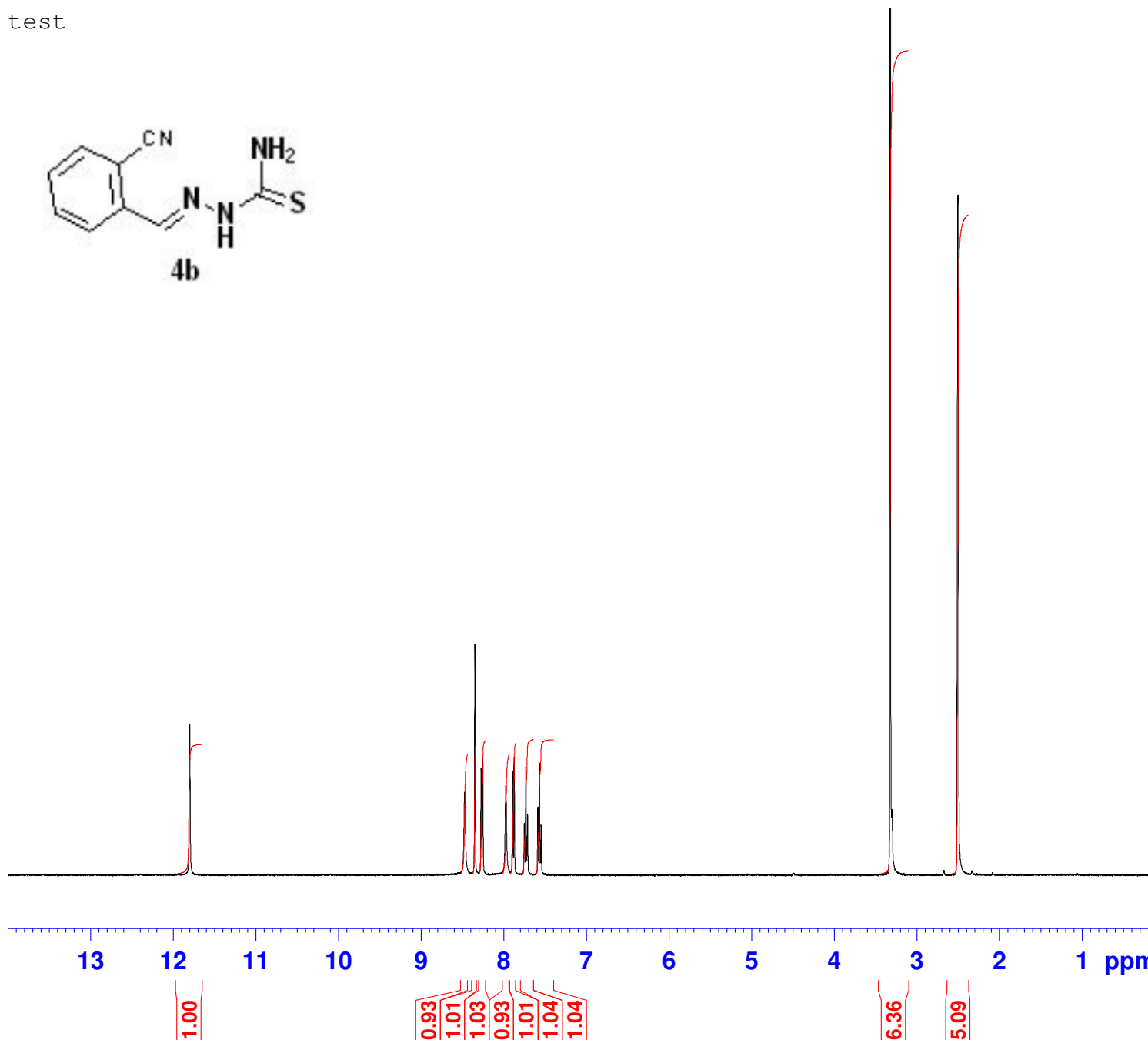


Current Data Parameters  
NAME MG-I-143  
EXPNO 1  
PROCNO 1

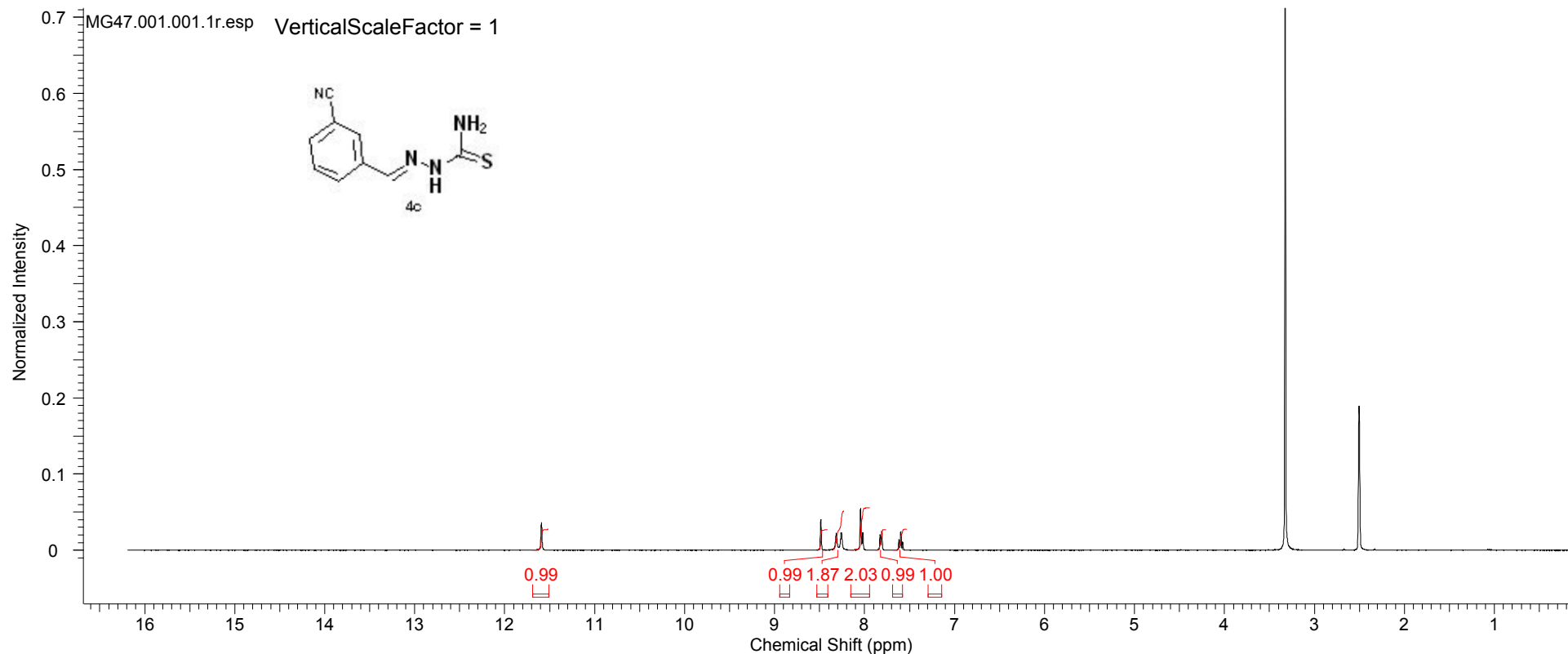
F2 - Acquisition Parameters  
Date\_ 20130510  
Time 16.02  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 400.1424710 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W

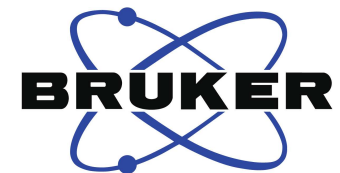
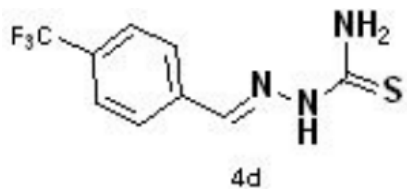
F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<b>Acquisition Time (sec)</b>	4.0894	<b>Comment</b>	5 mm PABBO BB-1H/D Z-GRD Z108618/0320		<b>Date</b>	08 Feb 2013 18:38:40	
<b>Date Stamp</b>	08 Feb 2013 18:38:40	<b>File Name</b>	C:\Users\moustafa\Desktop\NMR folder\MG47\1\data\1\1r				
<b>Frequency (MHz)</b>	400.14	<b>Nucleus</b>	1H	<b>Number of Transients</b>	16	<b>Origin</b>	spect
<b>Original Points Count</b>	32768	<b>Owner</b>	mgabr	<b>Points Count</b>	65536	<b>Pulse Sequence</b>	zg30
<b>Receiver Gain</b>	203.00	<b>SW(cyclical) (Hz)</b>	8012.82	<b>Solvent</b>	DMSO-d6	<b>Spectrum Offset (Hz)</b>	2471.0281
<b>Spectrum Type</b>	STANDARD	<b>Sweep Width (Hz)</b>	8012.70	<b>Temperature (degree C)</b>	25.048		



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[7.5317 .. 7.681]	0.00000000	2.74639300e+7	1.00000000
2	[7.7658 .. 7.870]	0.98532182	2.70608100e+7	0.98532182
3	[7.9448 .. 8.152]	0.02552295	5.56288200e+7	2.02552295
4	[8.2339 .. 8.351]	1.86501074	5.12205240e+7	1.86501074
5	[8.4129 .. 8.520]	0.98538440	2.70625280e+7	0.98538440
6	[11.5111 .. 11.60]	0.99302292	2.72723120e+7	0.99302292

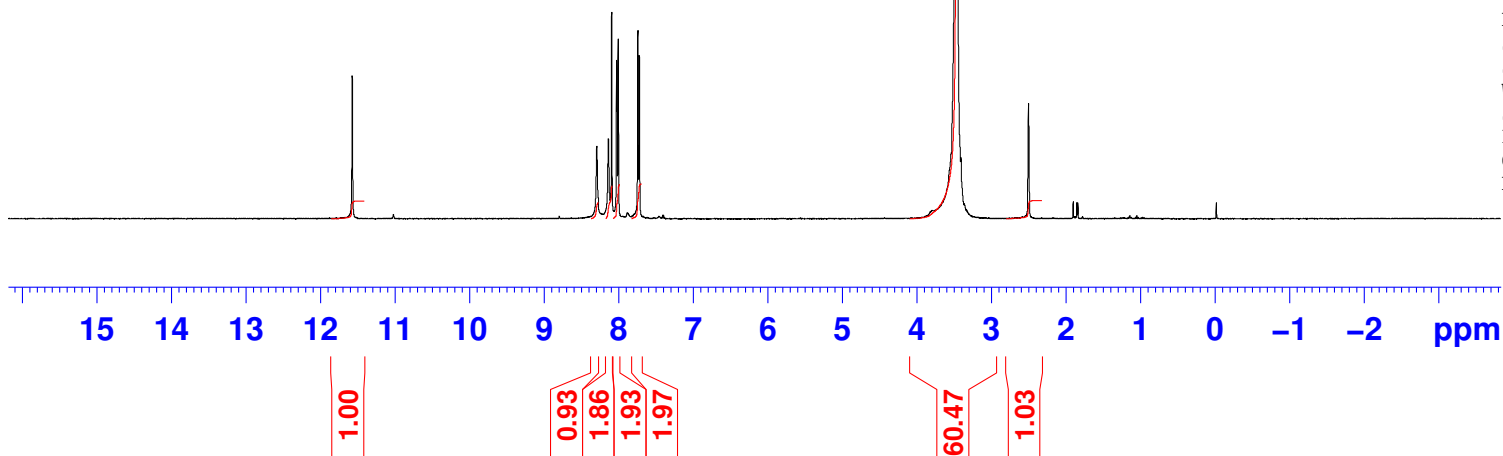


Current Data Parameters  
 NAME MG103  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130322  
 Time 18.23  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 3  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 57  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1

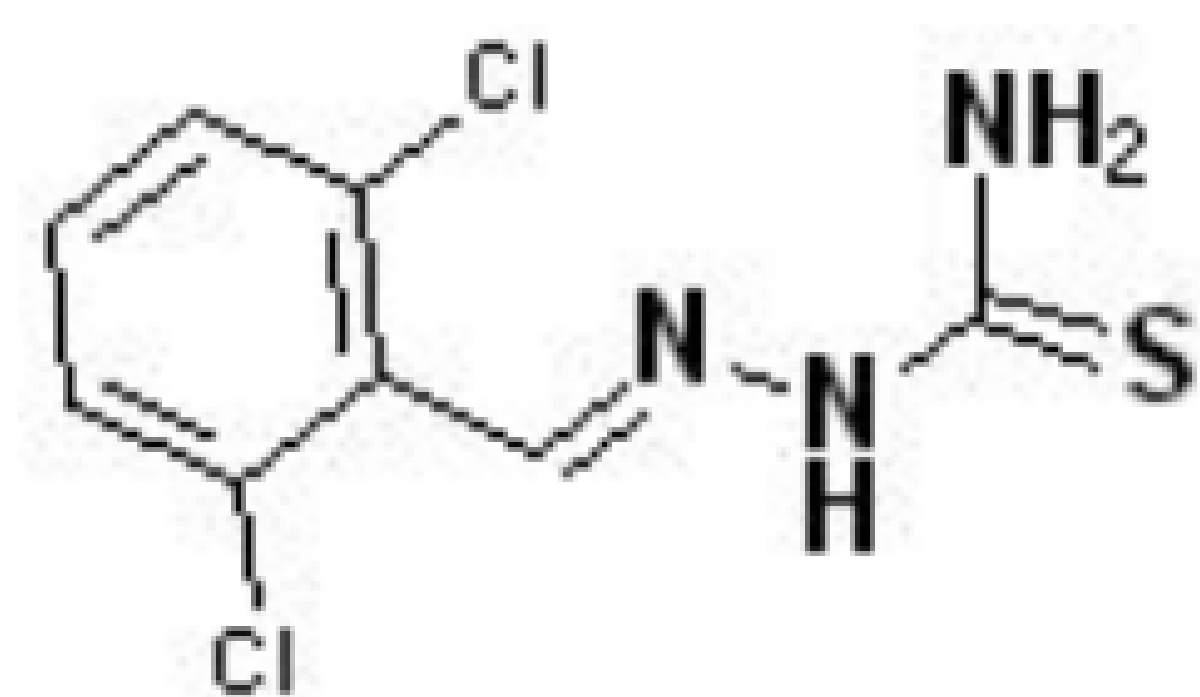
==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.40

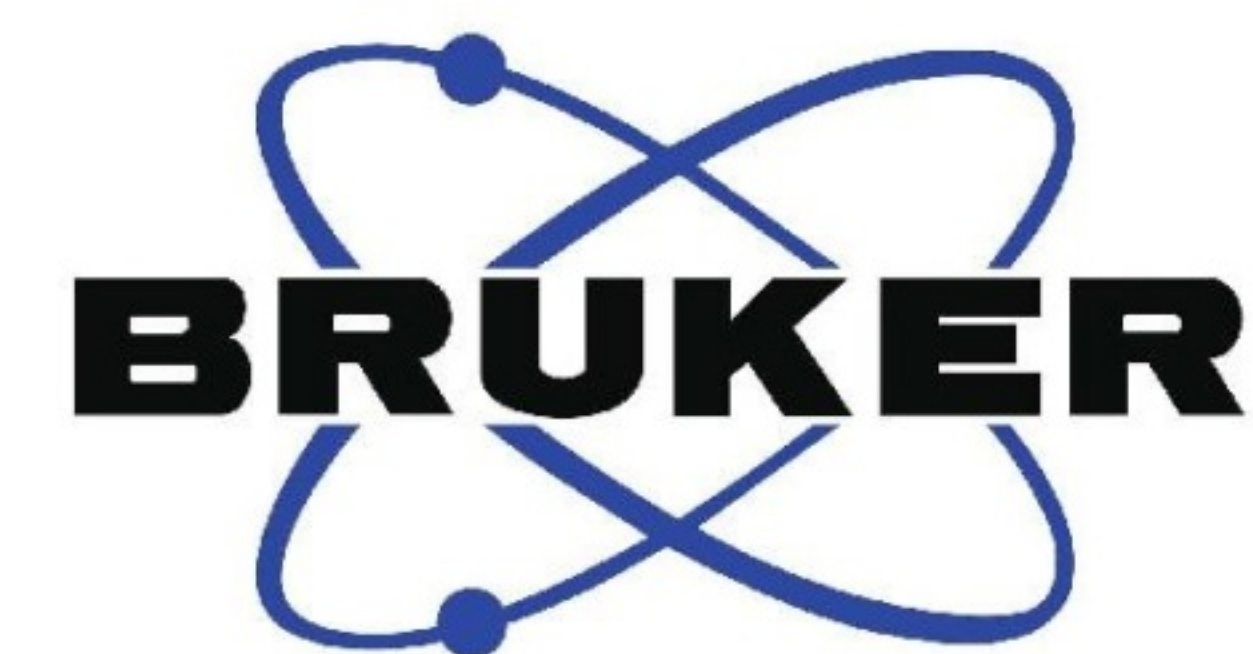




test



4f

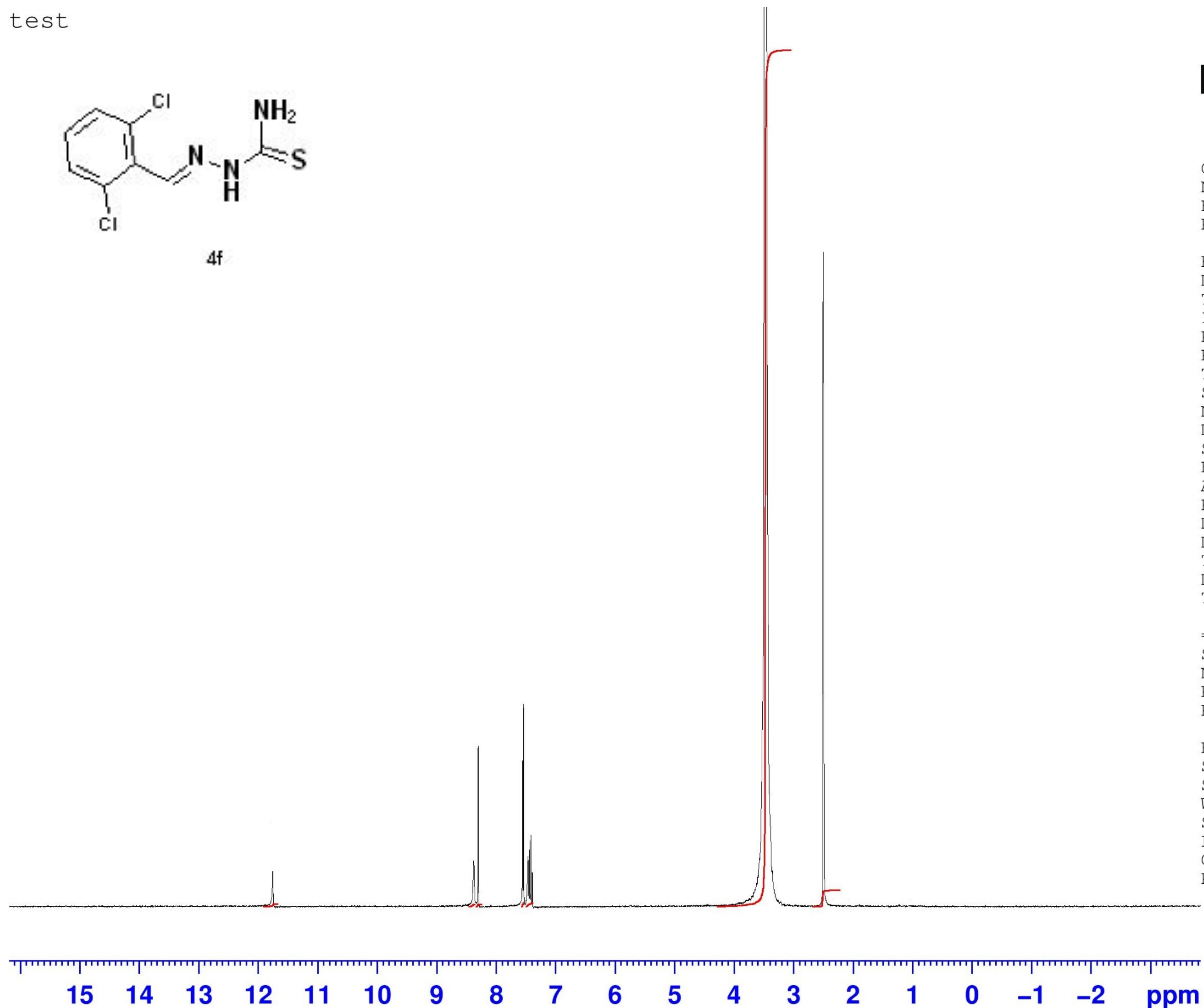


Current Data Parameters  
NAME MG72  
EXPNO 1  
PROCNO 1

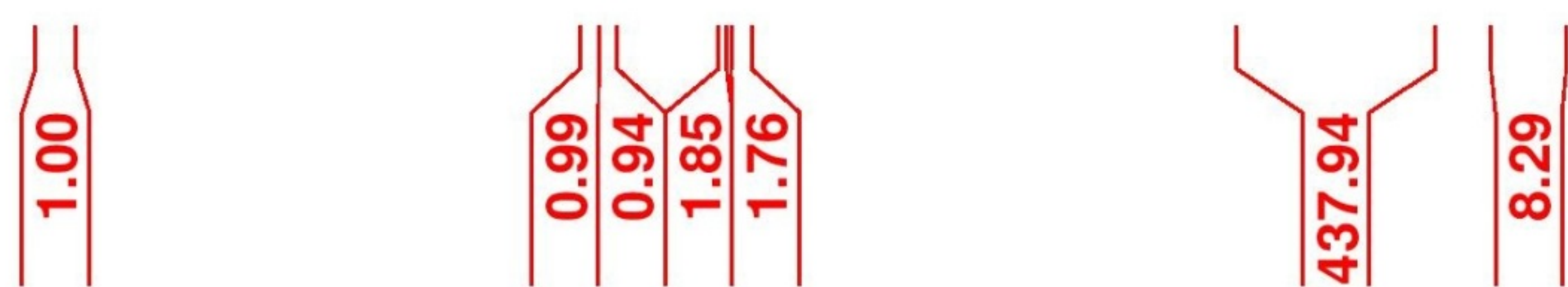
F2 - Acquisition Parameters  
Date\_ 20130308  
Time 17.40  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 71.8  
DW 62.400 usec  
DE 6.50 usec  
TE 293.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 400.1424710 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

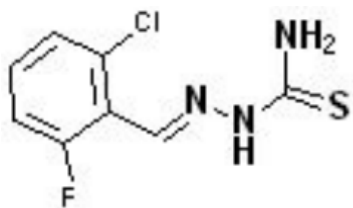


15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm

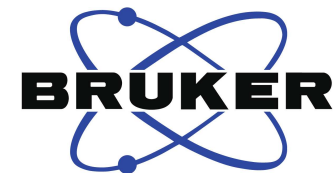




test



4g

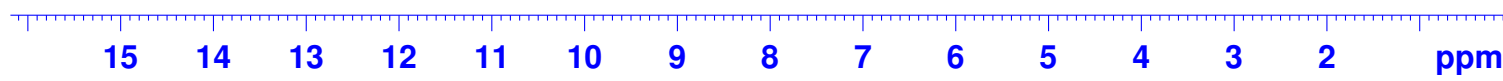
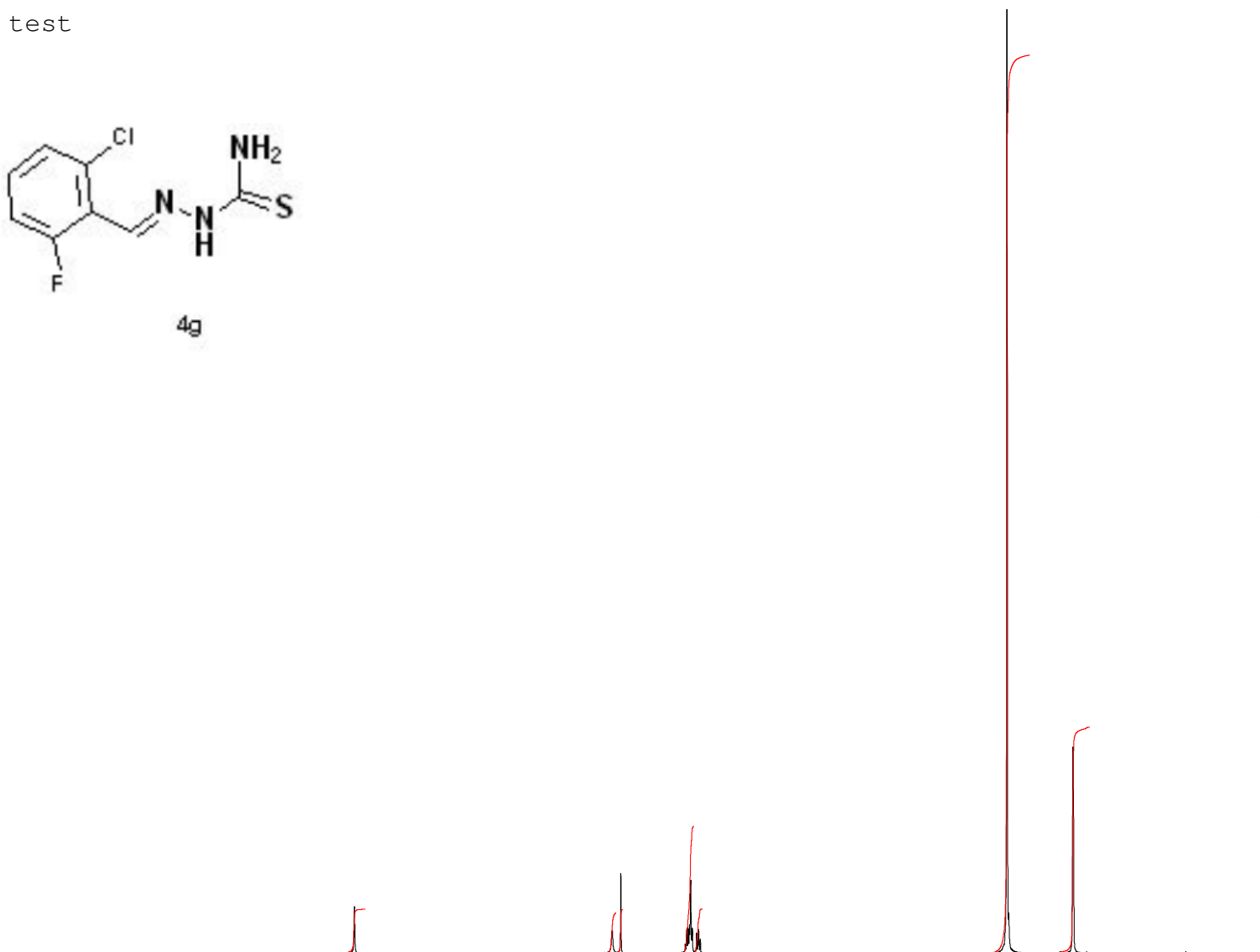


Current Data Parameters  
NAME MG80  
EXPNO 1  
PROCNO 1

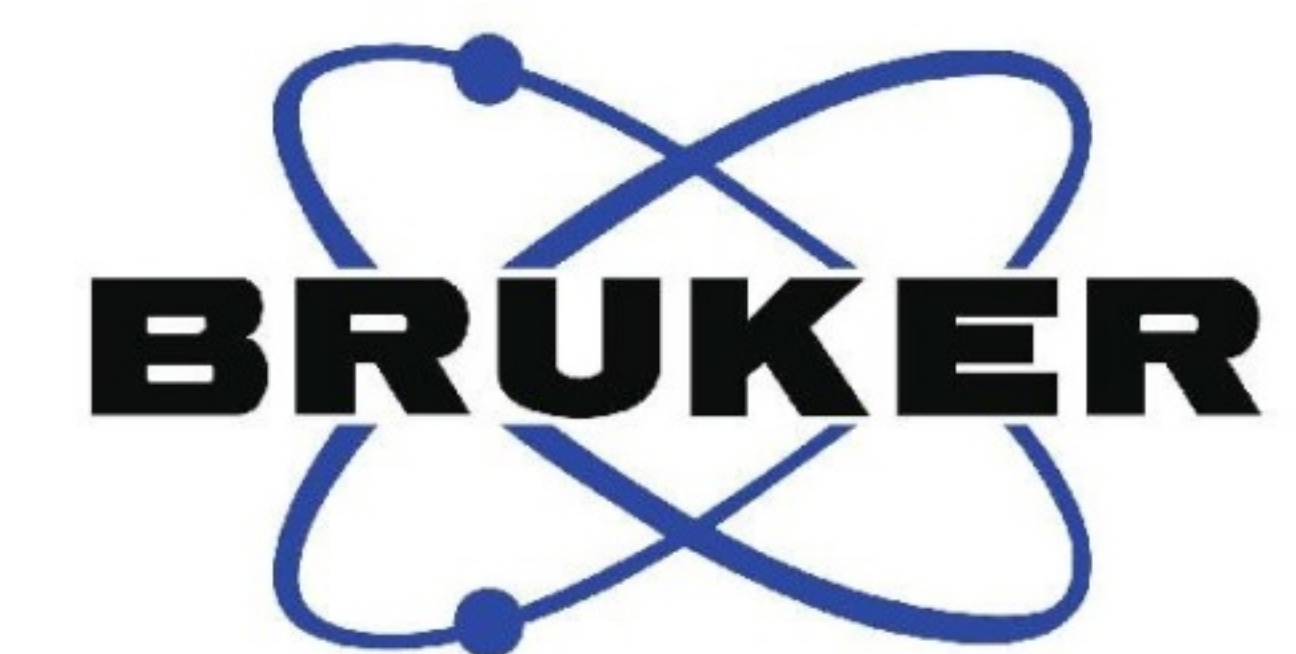
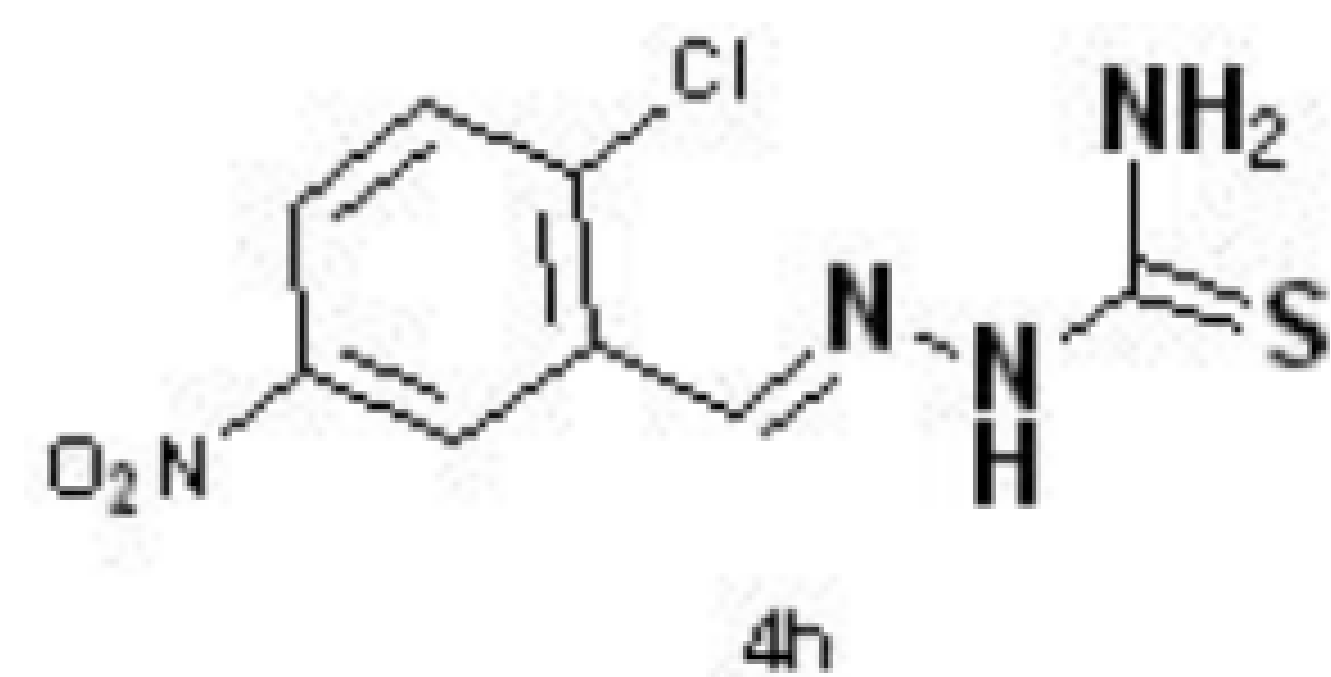
F2 - Acquisition Parameters  
Date\_ 20130314  
Time 18.23  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 293.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 400.1424710 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



test

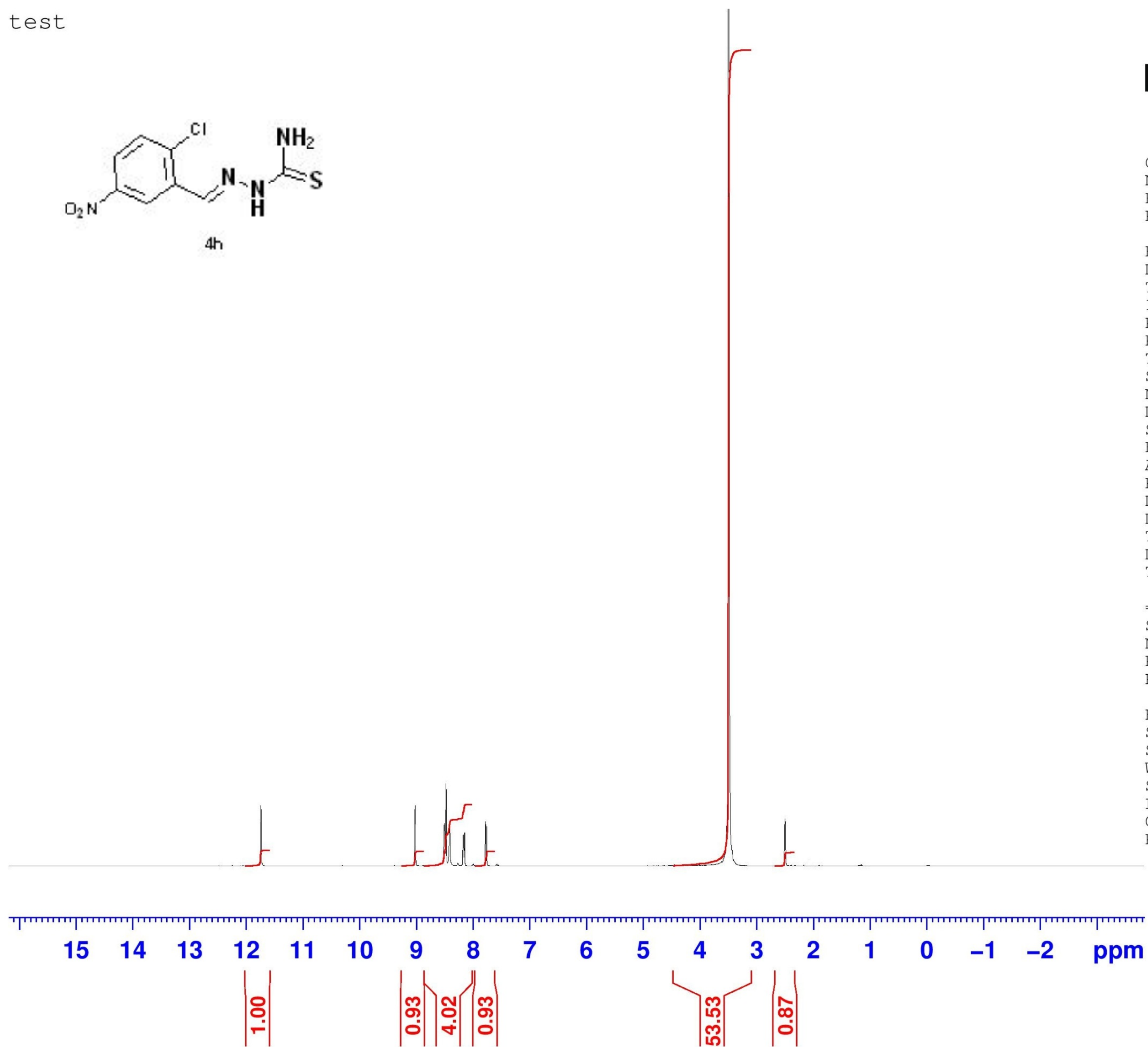


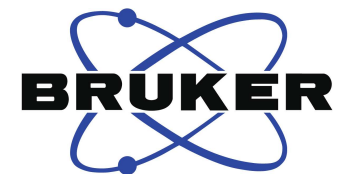
Current Data Parameters  
NAME MG73  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130307  
Time 12.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 57  
DW 62.400 usec  
DE 6.50 usec  
TE 292.6 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 400.1424710 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



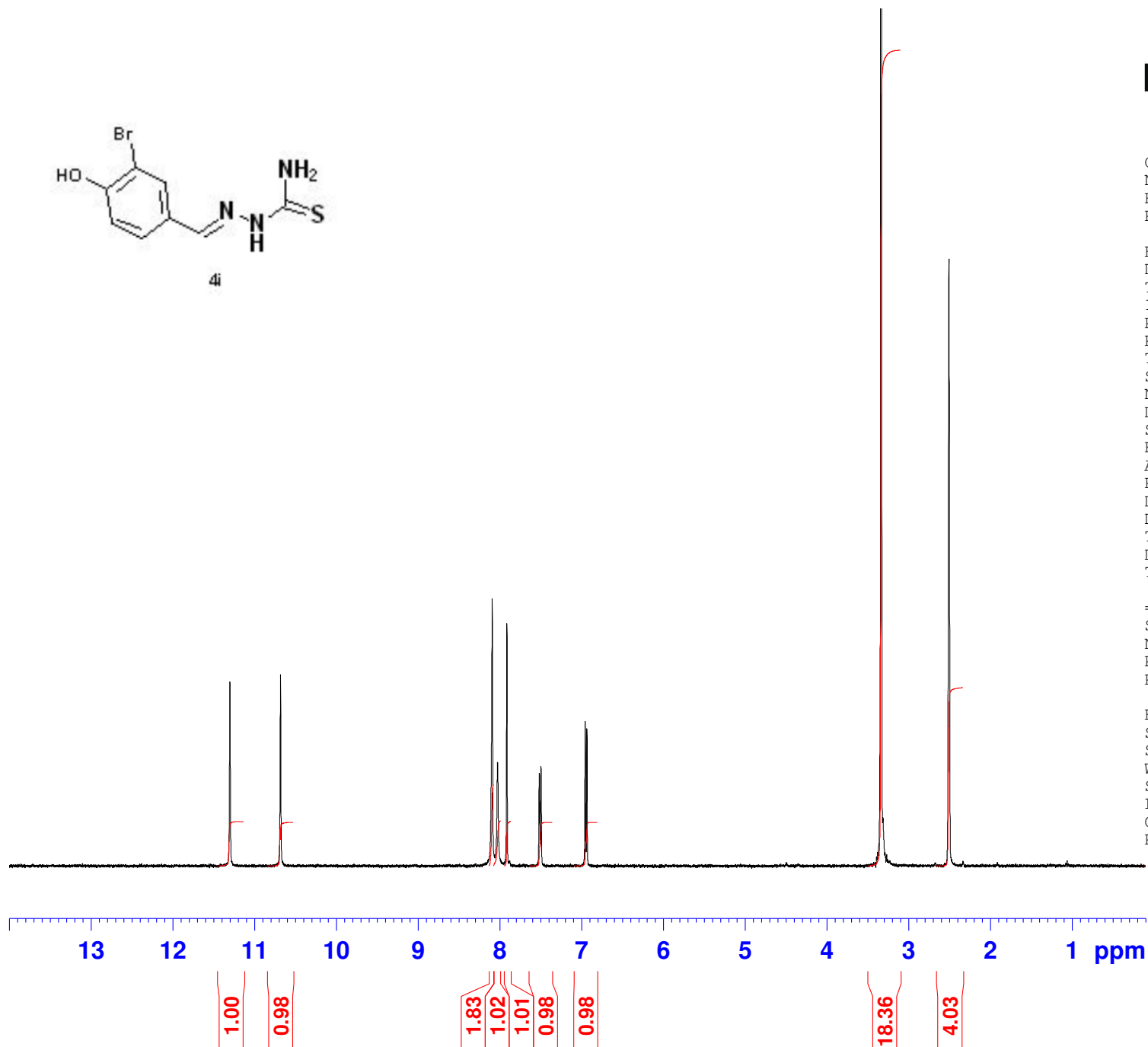
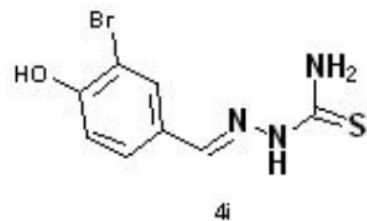


Current Data Parameters  
NAME MG-II-21  
EXPNO 1  
PROCNO 1

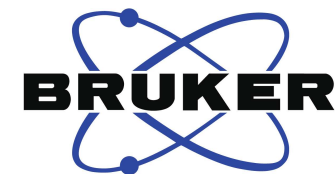
F2 - Acquisition Parameters  
Date\_ 20130509  
Time 18.23  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 3  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 400.1424710 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





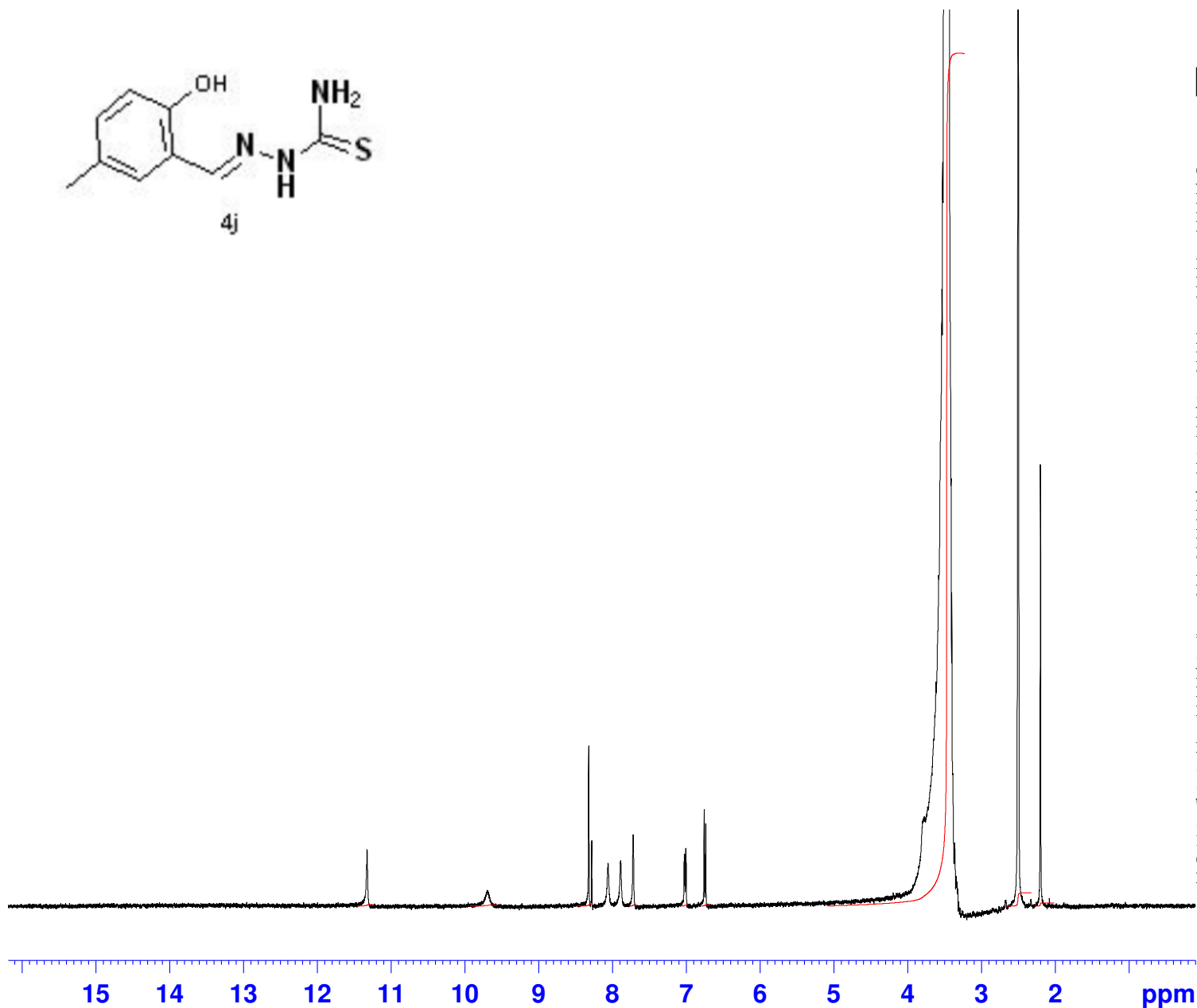
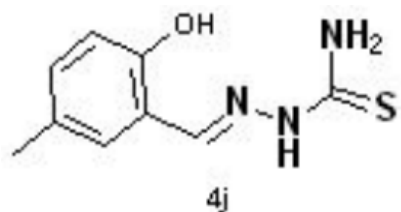


Current Data Parameters  
NAME MG108  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130329  
Time 18.06  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 64  
DW 62.400 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 400.1424710 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.40



1.02

0.81

1.43

0.89

1.05

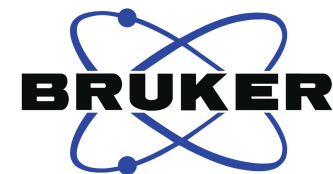
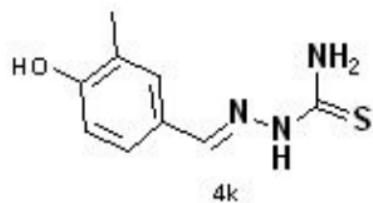
1.02

848.08

13.01

3.00

test

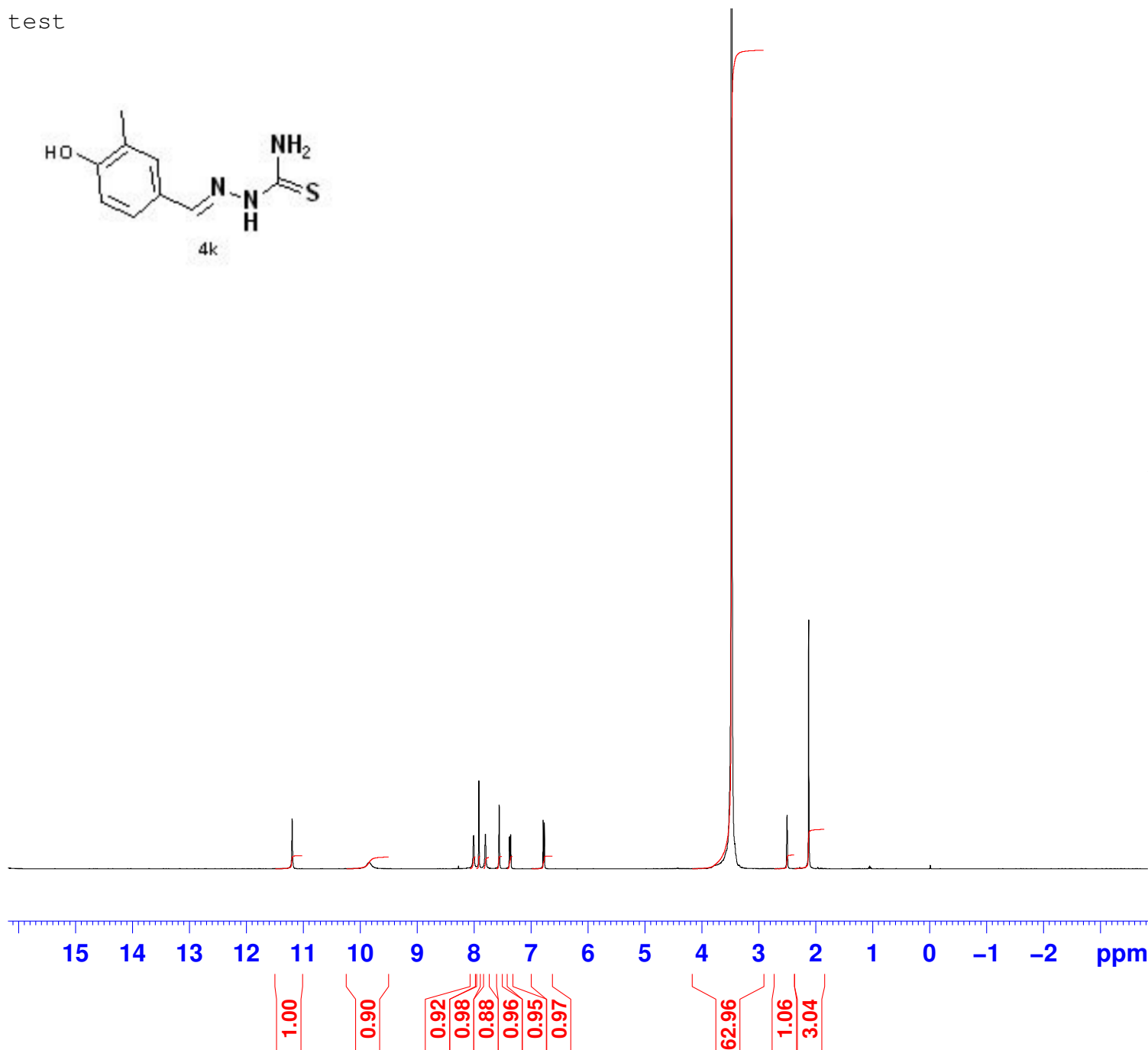


Current Data Parameters  
NAME MG83  
EXPNO 1  
PROCNO 1

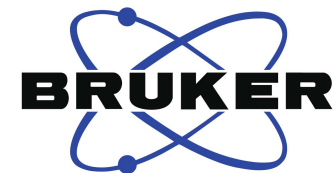
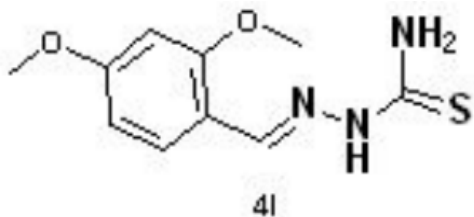
F2 - Acquisition Parameters  
Date\_ 20130327  
Time 16.33  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 4  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 57  
DW 62.400 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 400.1424710 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.40



test

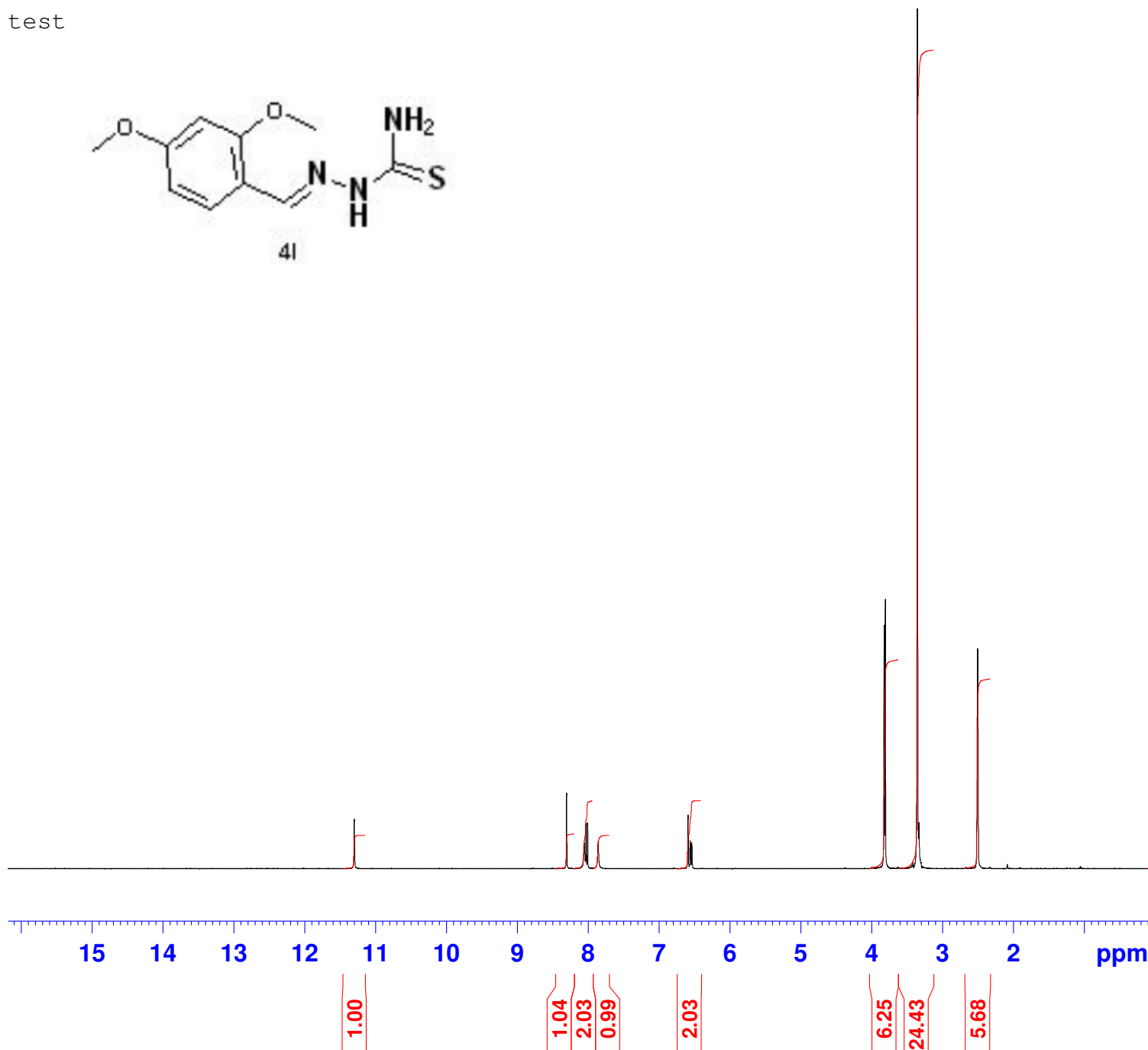


Current Data Parameters  
NAME MG64p  
EXPNO 1  
PROCNO 1

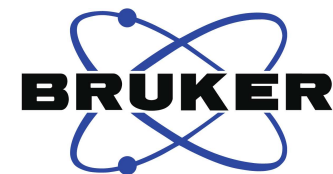
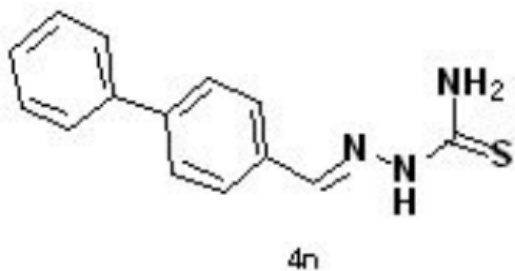
F2 - Acquisition Parameters  
Date\_ 20130314  
Time 18.18  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 293.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 400.1424710 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





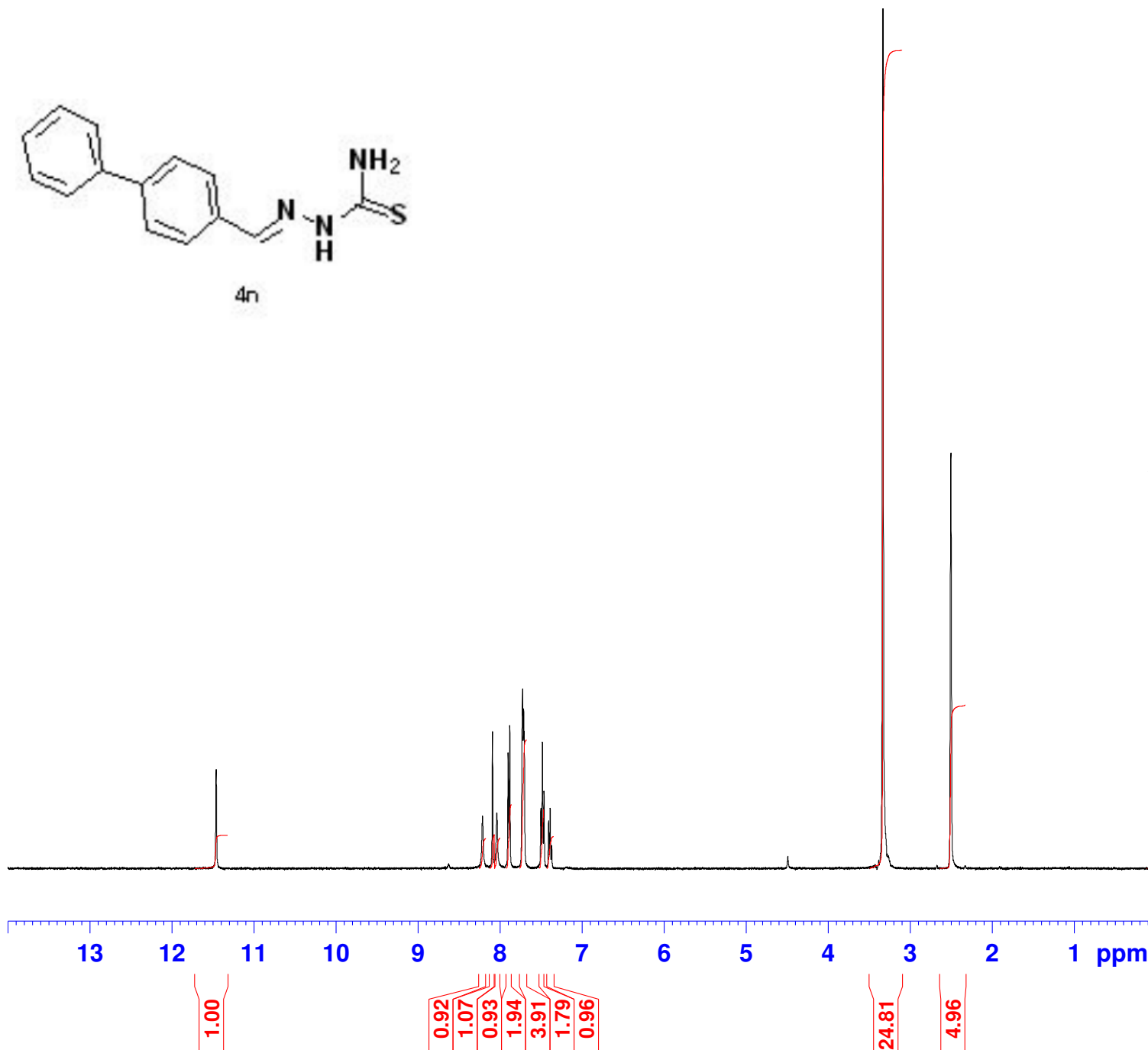


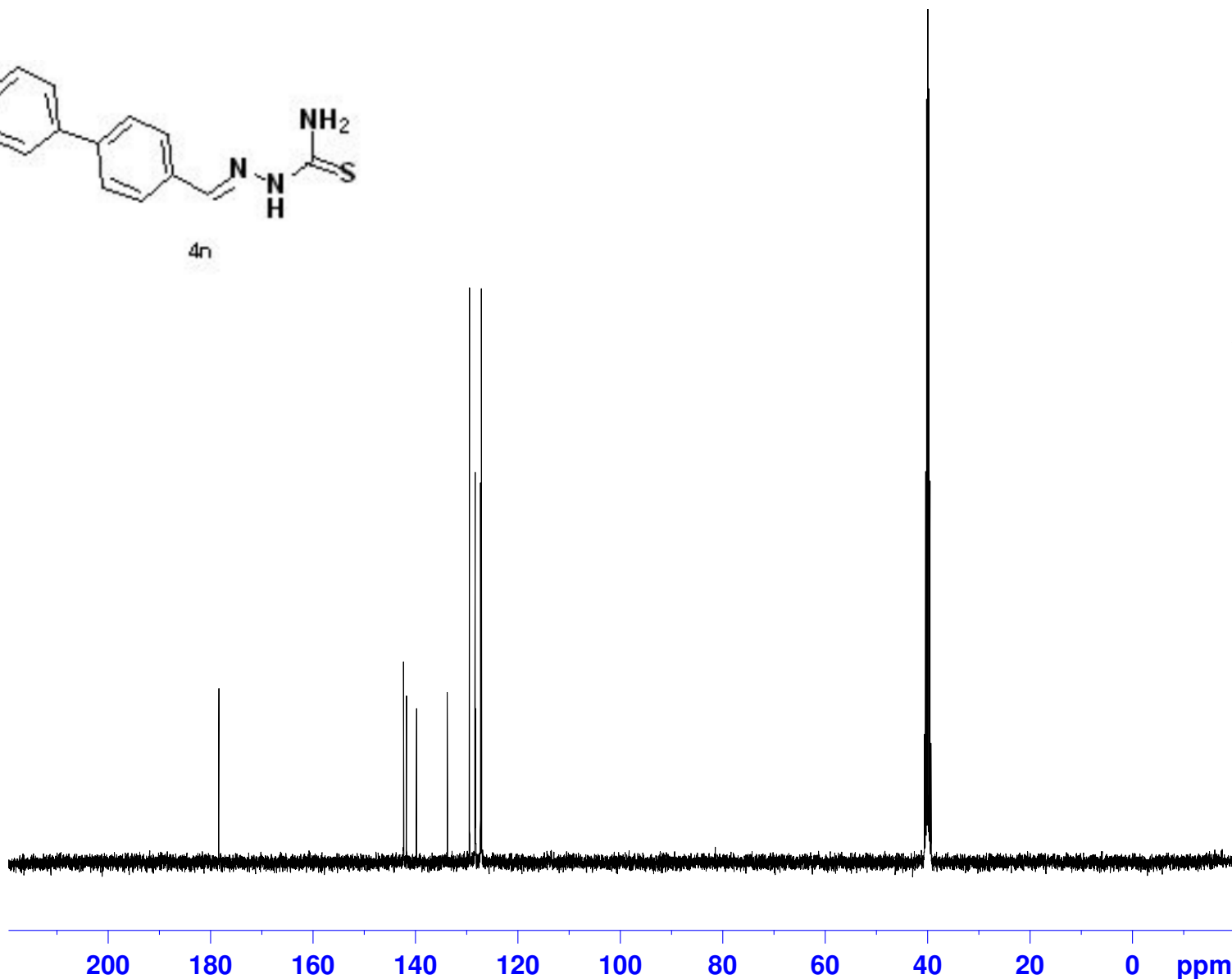
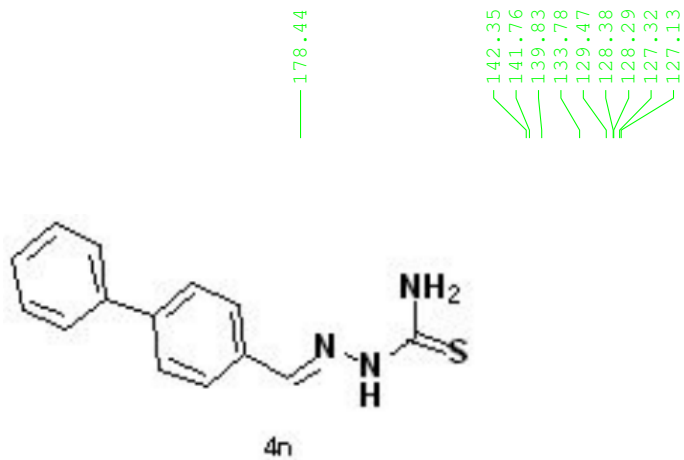
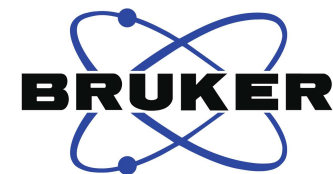
Current Data Parameters  
 NAME MG-I-141  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130509  
 Time 18.03  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 3  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





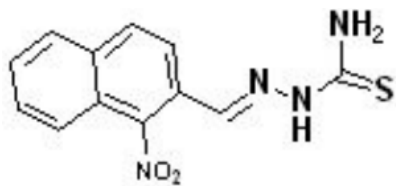
Current Data Parameters  
NAME MG-I-141c  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130515  
Time 18.00  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 70  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 144  
DW 20.800 usec  
DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

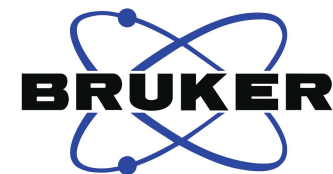
===== CHANNEL f1 =====  
SFO1 100.6253441 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1416006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



4p

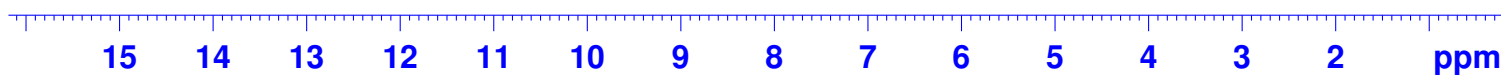
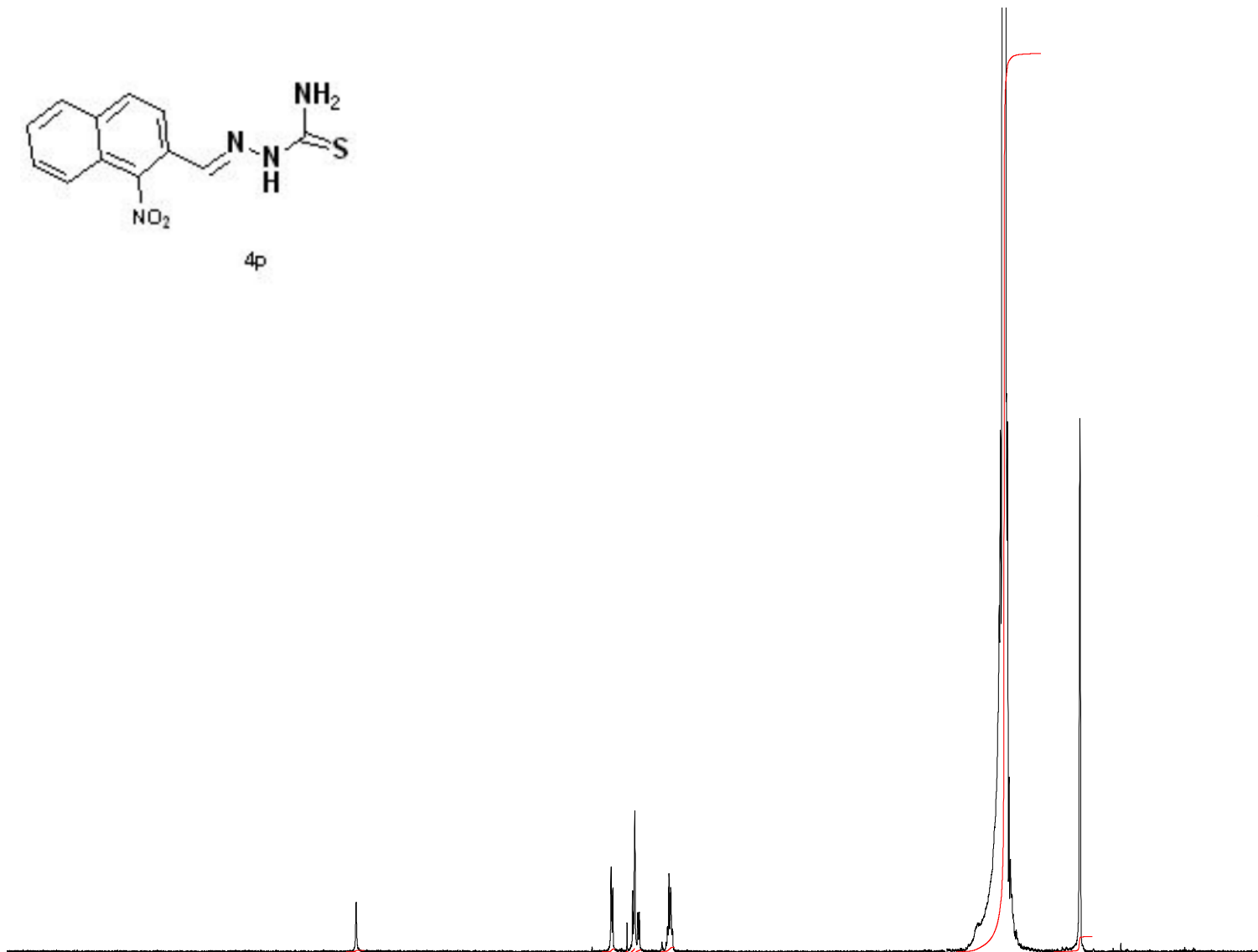


Current Data Parameters  
 NAME MG100  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130329  
 Time 18.19  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 4  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 64  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



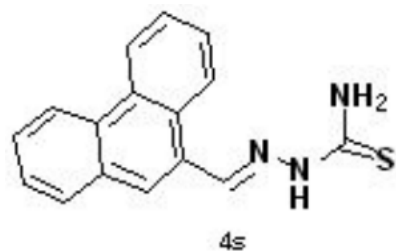
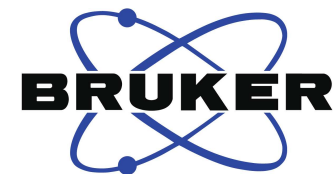
1.00

1.89  
 0.24  
 2.54  
 1.23  
 3.08

609.18

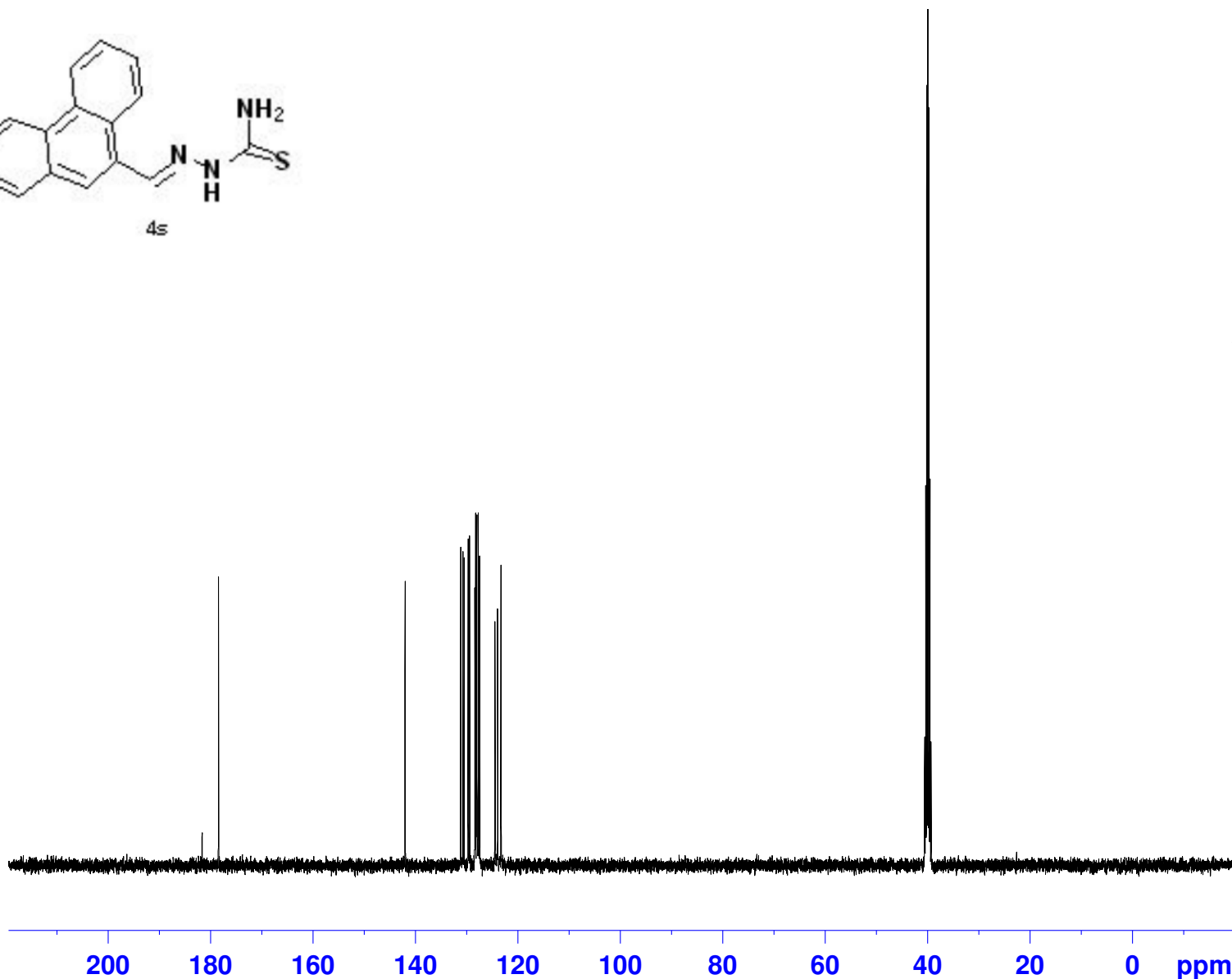
10.22





181.70  
178.48

142.06  
131.20  
130.78  
130.52  
129.72  
129.43  
128.41  
128.28  
128.07  
127.99  
127.73  
127.48  
124.48  
123.98  
123.31



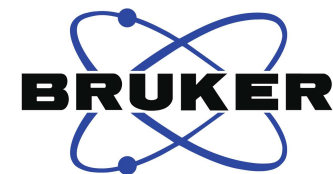
Current Data Parameters  
NAME MG-I-146c  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130524  
Time 16.23  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 84  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 161  
DW 20.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 100.6253441 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1416006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

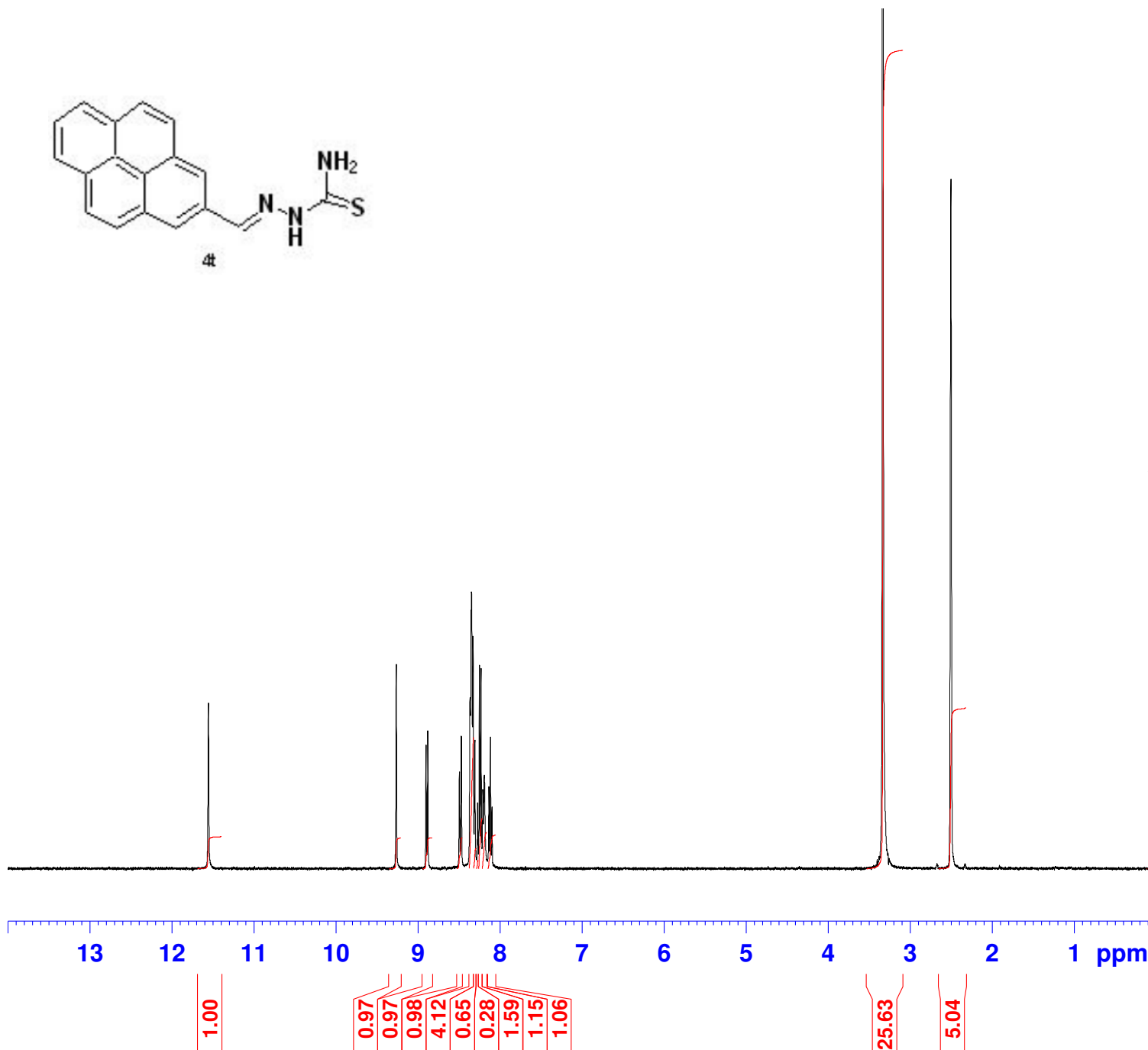
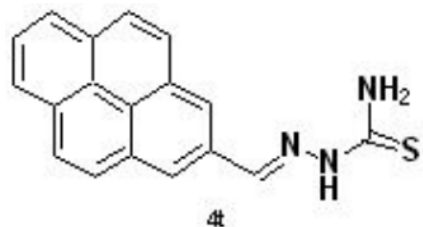


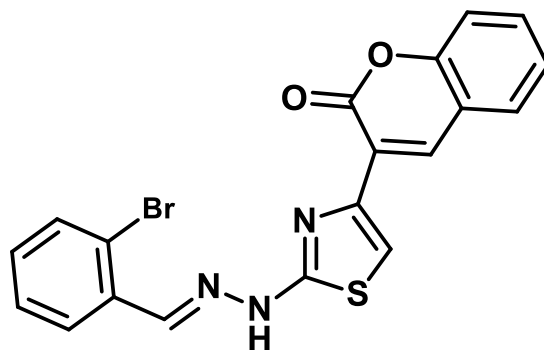
Current Data Parameters  
NAME MG-I-149  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130509  
Time 18.27  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 6  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 400.1424710 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

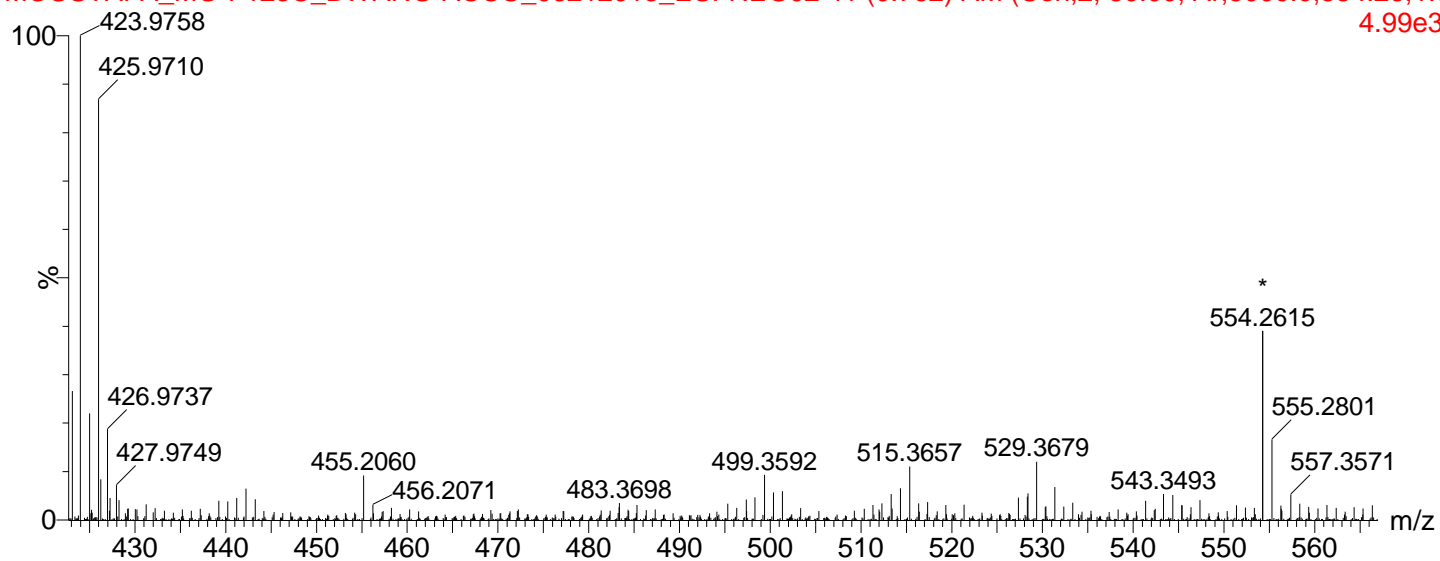




5a

21-Jun-2013 15:09:29

MOUSTAFA\_MG-I-123C\_BWANG-ACCU\_06212013\_ESI-NEG02 41 (0.762) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.0  
4.99e3



Elemental Composition Report



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

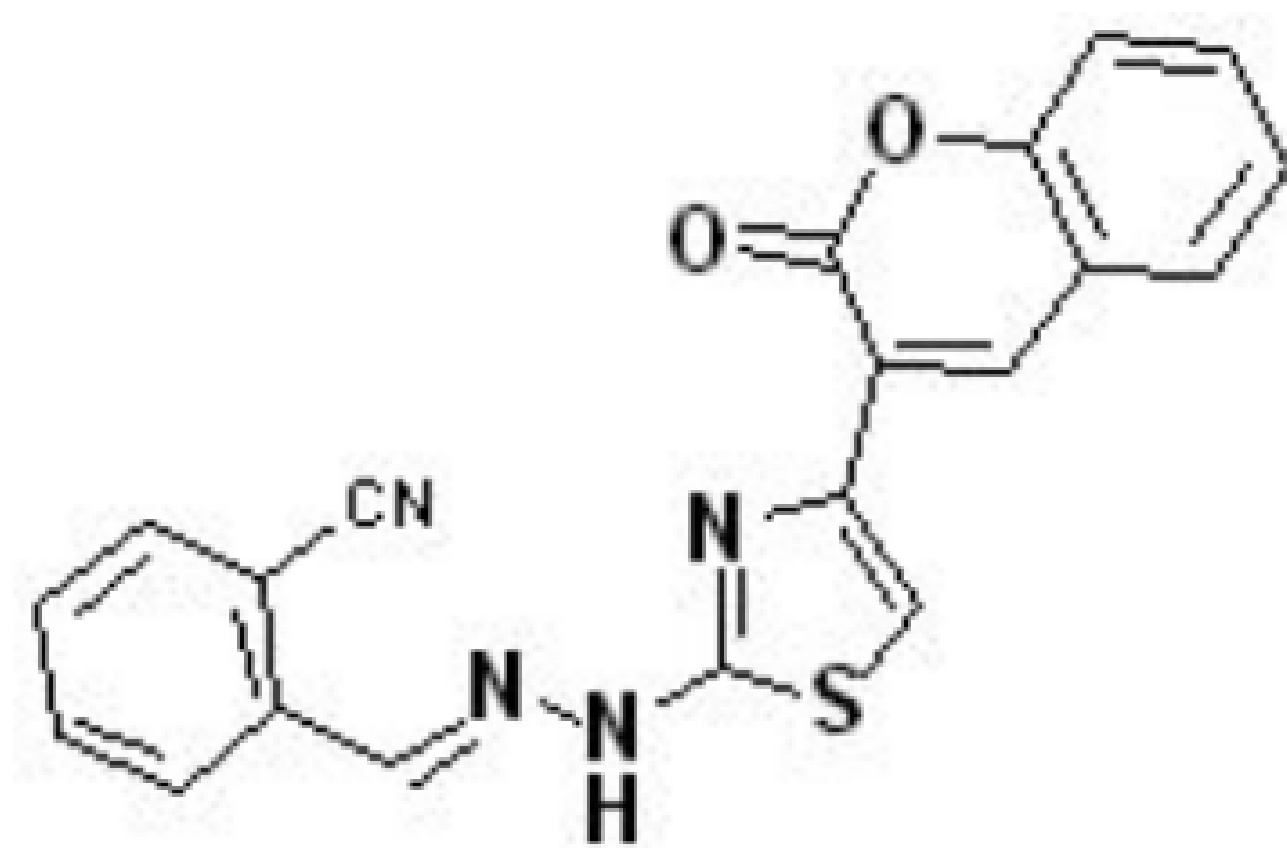
1136 formula(e) evaluated with 13 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-2 Br: 1-2

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
423.9758	423.9749	0.9	2.1	6.5	121.5	C11 H15 N5 O4 S2 Br
	423.9762	-0.4	-0.9	6.0	106.9	C13 H17 N2 O5 S2 Br
	423.9776	-1.8	-4.2	11.0	79.7	C14 H13 N6 O S2 Br
	423.9742	1.6	3.8	16.0	43.3	C17 H9 N6 O S Br
	423.9755	0.3	0.7	15.5	42.1	C19 H11 N3 O2 S Br
	423.9747	1.1	2.6	9.0	222.5	C2 H5 N18 O2 S Br
	423.9747	1.1	2.6	3.5	260.5	C3 H11 N11 O7 S Br
	423.9760	-0.2	-0.5	8.5	192.6	C4 H7 N15 O3 S Br
	423.9760	-0.2	-0.5	3.0	227.9	C5 H13 N8 O8 S Br
	423.9752	0.6	1.4	1.0	959.5	C5 H18 N10 O S Br2
	423.9774	-1.6	-3.8	8.0	166.6	C6 H9 N12 O4 S Br
	423.9774	-1.6	-3.8	2.5	199.2	C7 H15 N5 O9 S Br
	423.9766	-0.8	-1.9	0.5	938.7	C7 H20 N7 O2 S Br2





5b

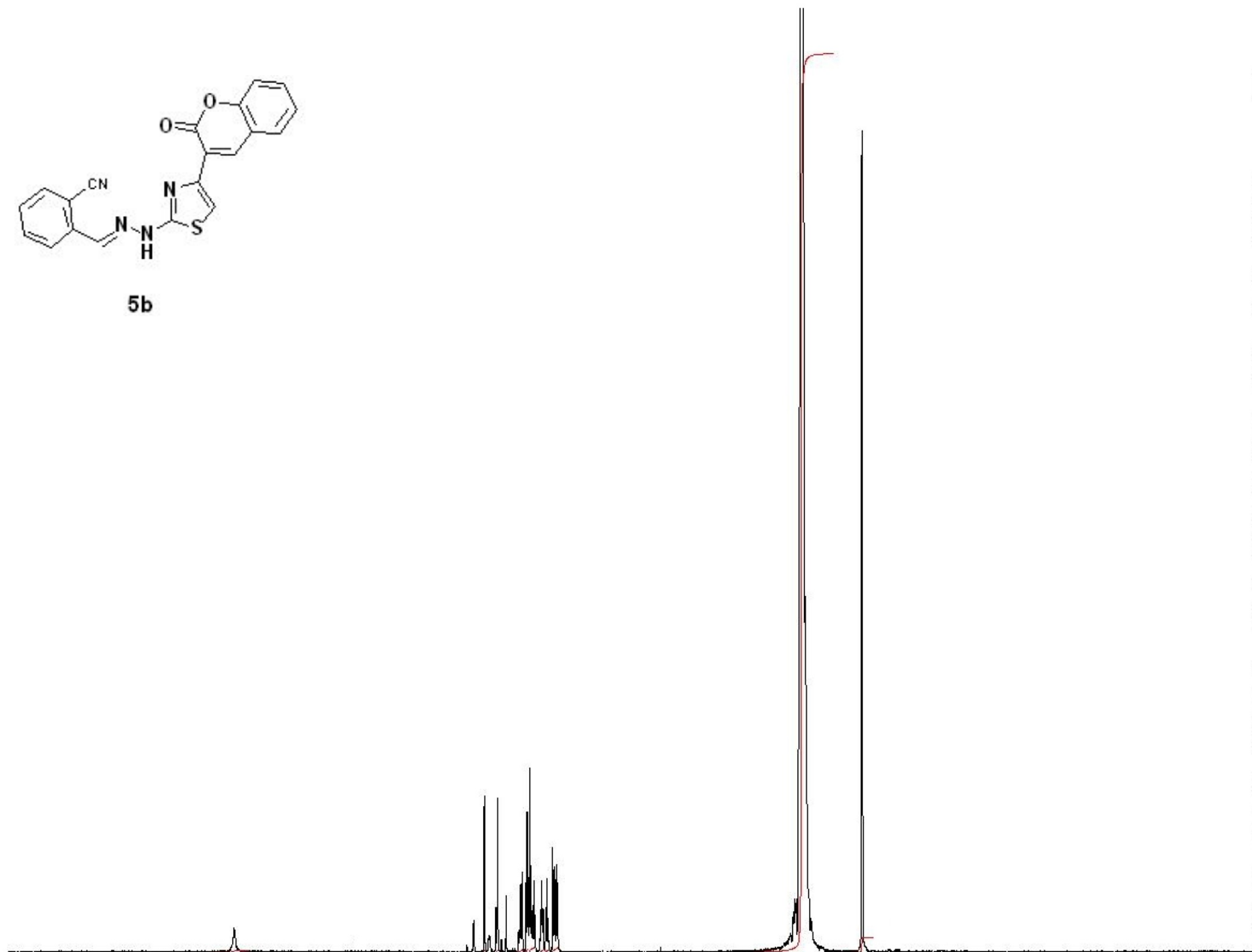


Current Data Parameters  
 NAME MG150  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130418  
 Time 17.54  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 64  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.40



15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm

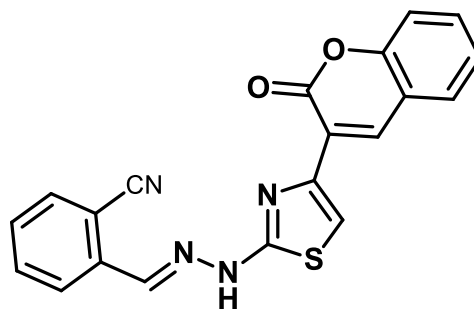
1.00

0.95  
1.30  
1.37  
2.00  
2.73  
1.31  
1.01  
2.74

567.05

9.36

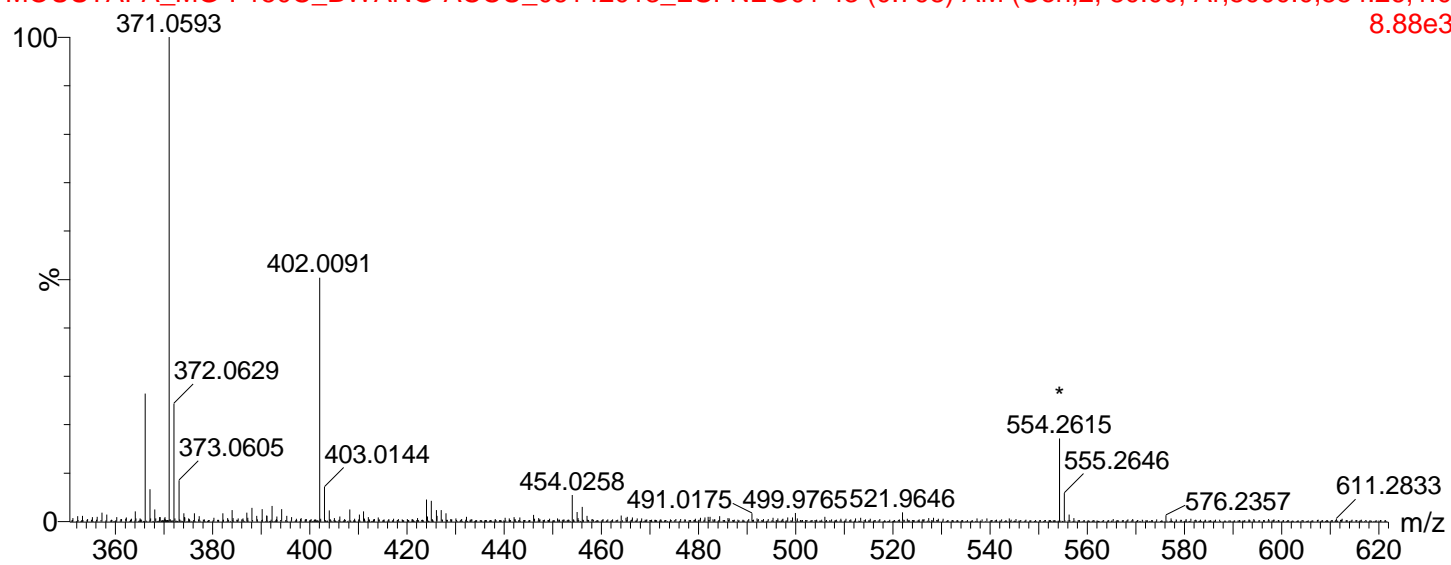




5b

14-Jun-2013 17:16:23

MOUSTAFI\_MG-I-150C\_BWANG-ACCU\_06142013\_ESI-NEG01 43 (0.798) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.00) 8.88e3



Elemental Composition Report

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

### Monoisotopic Mass, Even Electron Ions

1064 formula(e) evaluated with 8 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-2

Minimum:

-1.5

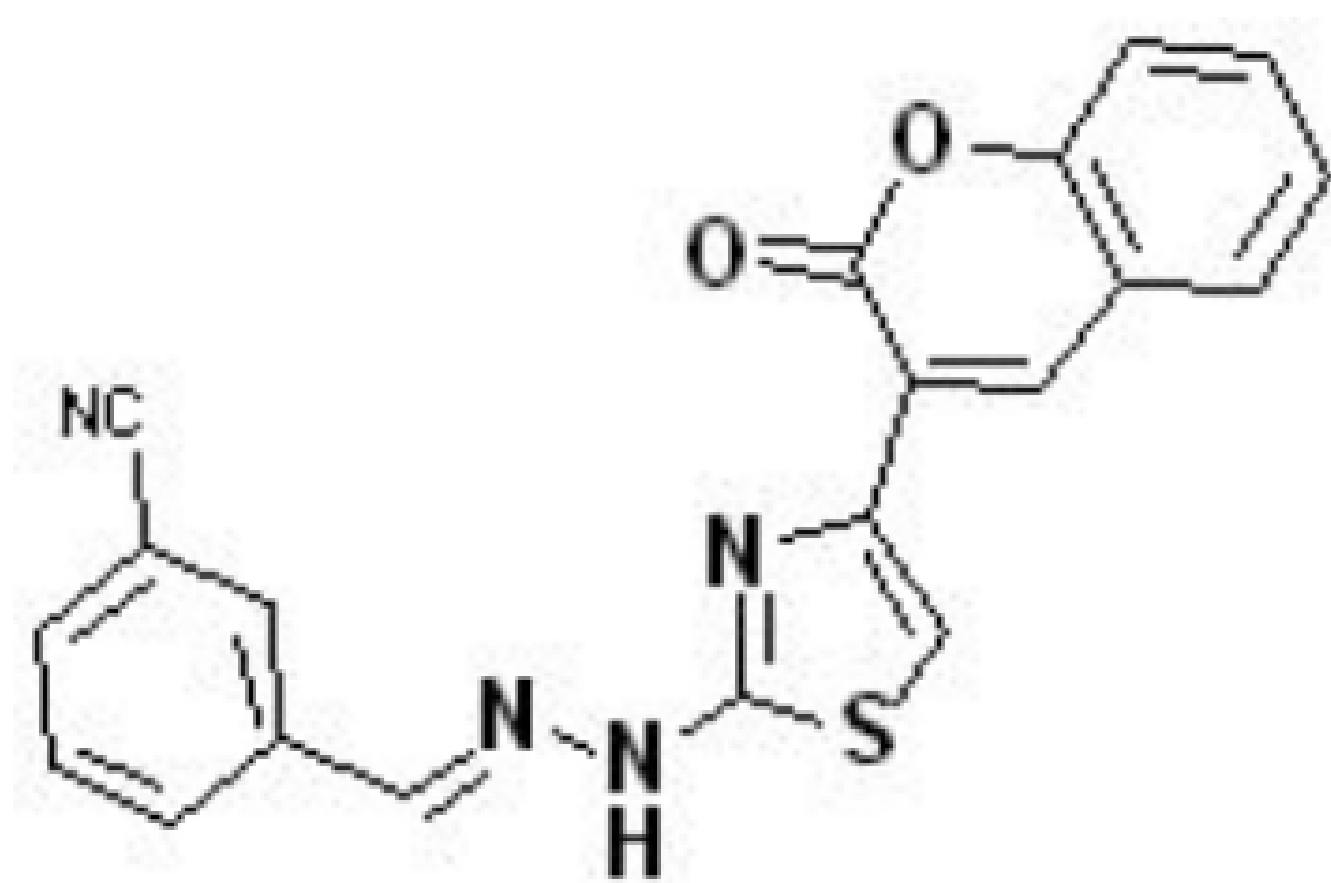
Maximum:

5.0

5.0

100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
371.0593	371.0581	1.2	3.2	11.5	406.0	C H3 N22 O S
	371.0583	1.0	2.7	3.5	203.4	C11 H19 N2 O8 S2
	371.0596	-0.3	-0.8	8.5	121.2	C12 H15 N6 O4 S2
	371.0603	-1.0	-2.7	17.5	3.0	C20 H11 N4 O2 S
	371.0581	1.2	3.2	0.5	499.5	C3 H15 N8 O11 S
	371.0594	-0.1	-0.3	5.5	371.7	C4 H11 N12 O7 S
	371.0608	-1.5	-4.0	10.5	270.4	C5 H7 N16 O3 S
	371.0608	-1.5	-4.0	-0.5	356.2	C7 H19 N2 O13 S



5c

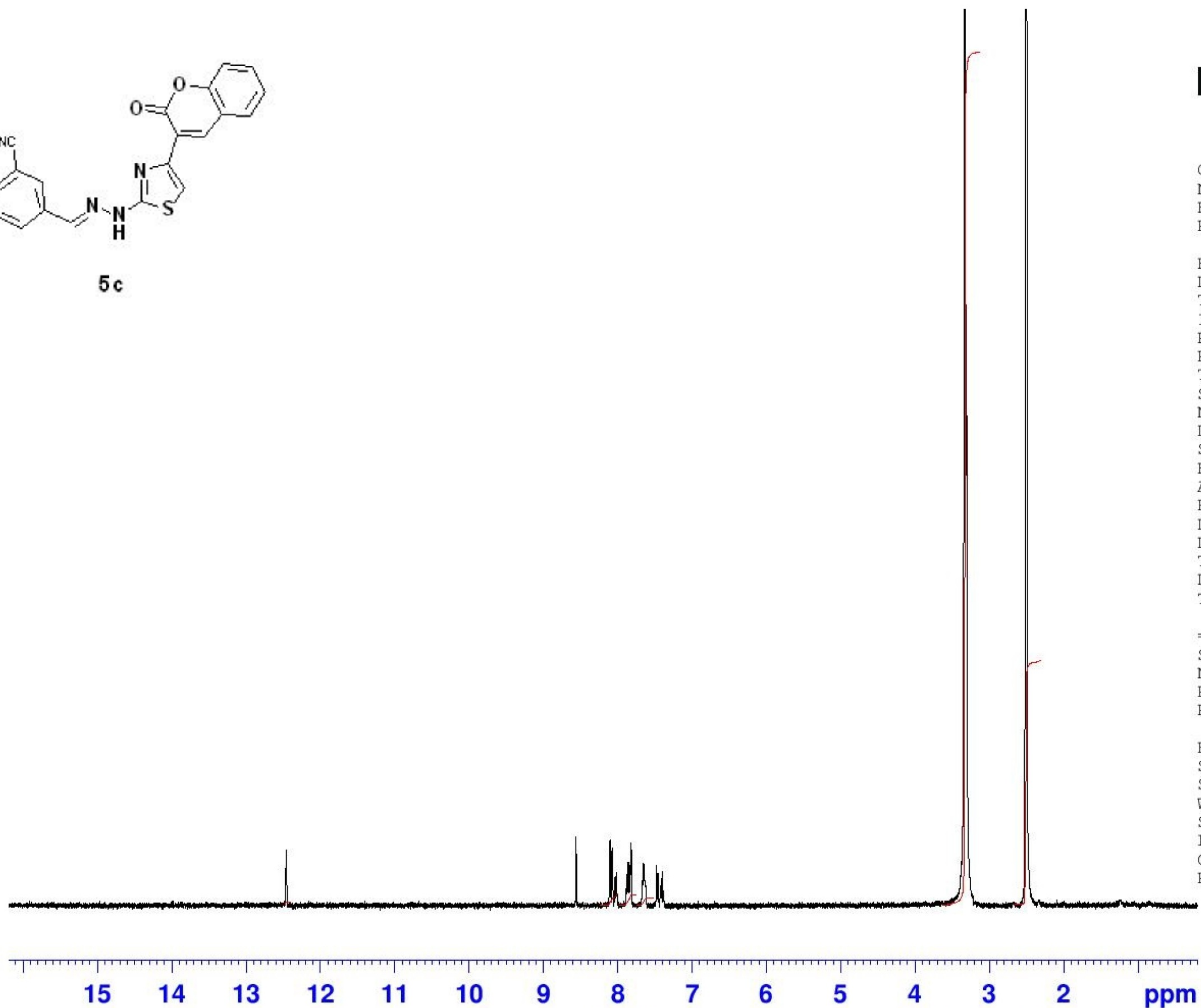


Current Data Parameters  
 NAME MG58  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130214  
 Time 16.08  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

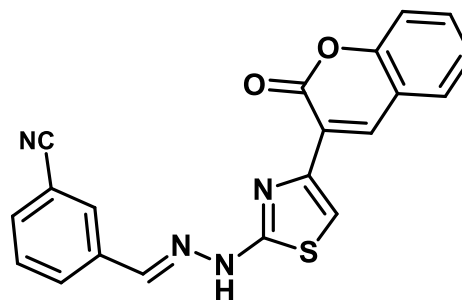
F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



0.91  
 0.88  
 0.58

71.25  
 20.43



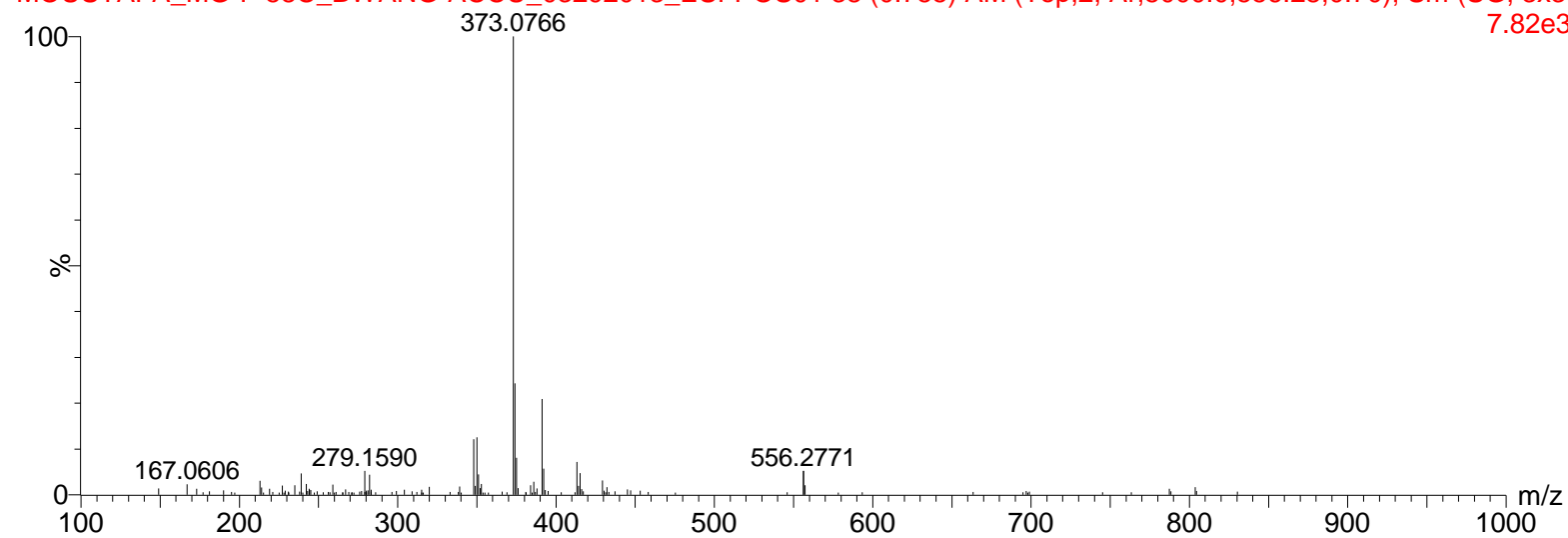


5c

80% ACN

15:58:00 29-Mar-2013

MOUSTAFA\_MG-I--58C\_BWANG-ACCU\_03292013\_ESI-POS01 38 (0.755) AM (Top,2, Ar,5000.0,556.28,0.70); Sm (SG, 3x3.l  
7.82e3



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

2006 formula(e) evaluated with 17 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-10

Minimum:

-1.5

Maximum:

5.0

5.0

50.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

373.0766

373.0785

-1.9

-5.1

-0.5

477.7

C H17 N12 O7 S2

373.0753

1.3

3.5

7.5

120.1

C12 H17 N6 O4 S2

373.0748

1.8

4.8

1.5

600.1

C12 H25 N2 O3 S4

373.0766

0.0

0.0

7.0

110.0

C14 H19 N3 O5 S2

373.0780

-1.4

-3.8

12.0

66.0

C15 H15 N7 O S2

373.0759

0.7

1.9

16.5

2.6

C20 H13 N4 O2 S

373.0773

-0.7

-1.9

16.0

6.5

C22 H15 N O3 S

373.0751

1.5

4.0

10.0

284.2

C3 H7 N19 O2 S

373.0751

1.5

4.0

4.5

320.4

C4 H13 N12 O7 S

373.0760

0.6

1.6

3.5

407.8

C5 H17 N12 O2 S3

373.0751

1.5

4.0

-1.0

370.0

C5 H19 N5 O12 S

373.0764

0.2

0.5

9.5

229.8

C5 H9 N16 O3 S

373.0764

0.2

0.5

4.0

264.5

C6 H15 N9 O8 S

373.0778

-1.2

-3.2

9.0

182.6

C7 H11 N13 O4 S

373.0773

-0.7

-1.9

3.0

385.2

C7 H19 N9 O3 S3

373.0764

0.2

0.5

-1.5

312.2

C7 H21 N2 O13 S

373.0778

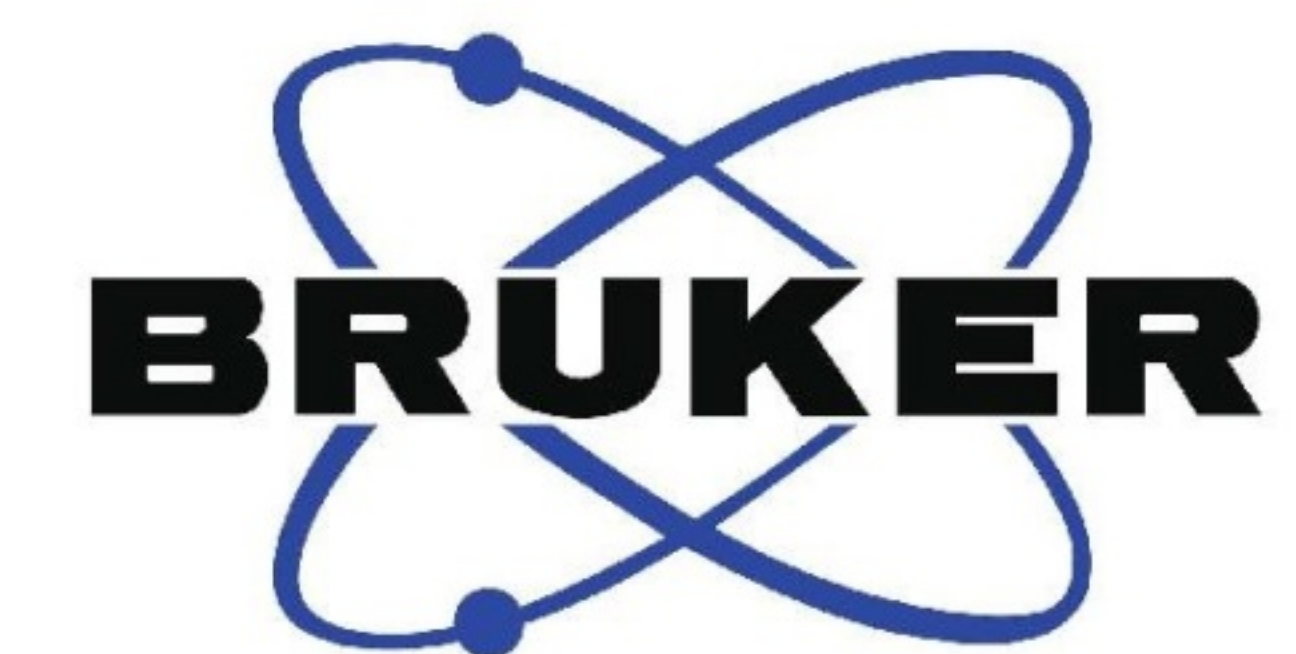
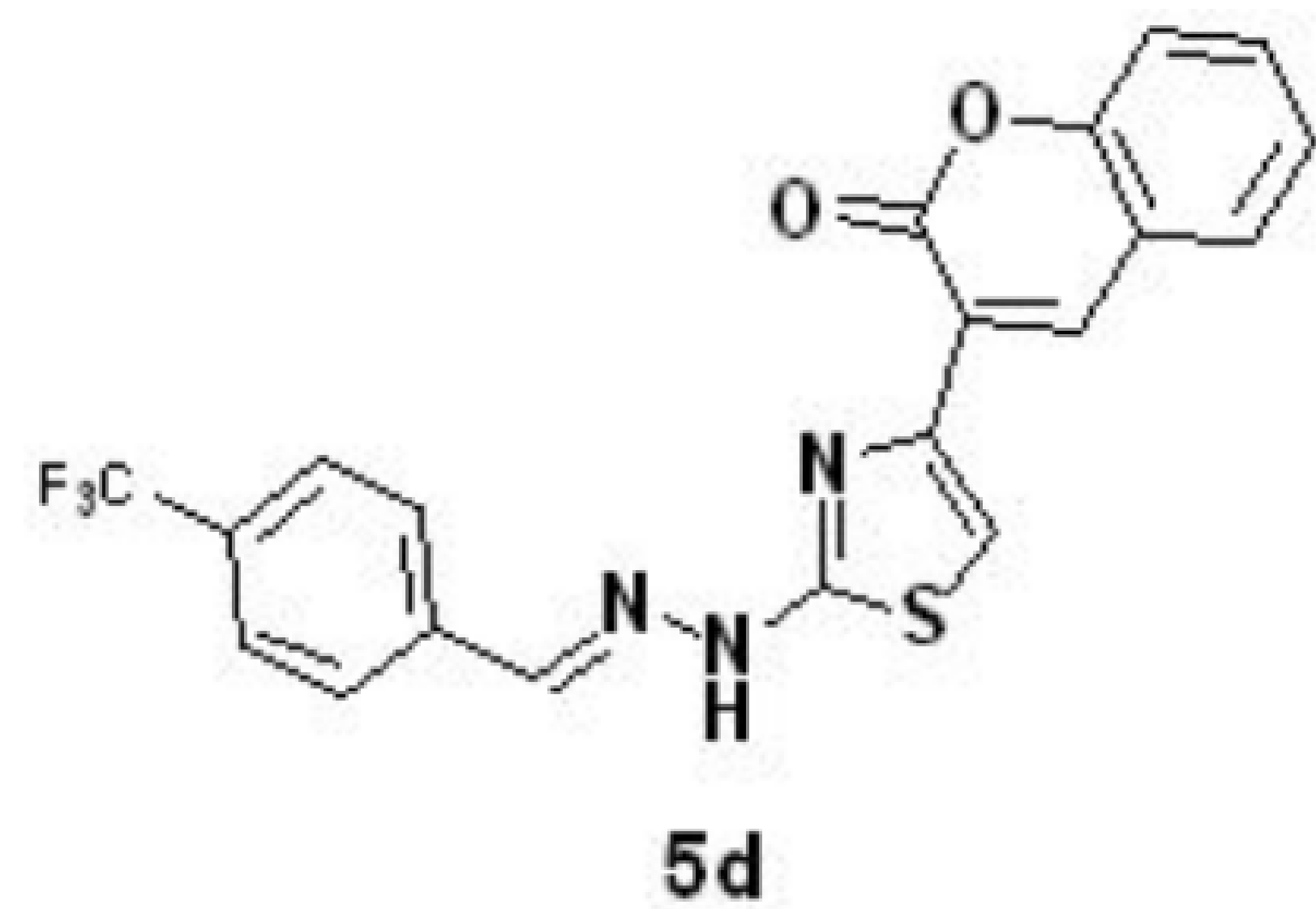
-1.2

-3.2

3.5

215.7

C8 H17 N6 O9 S

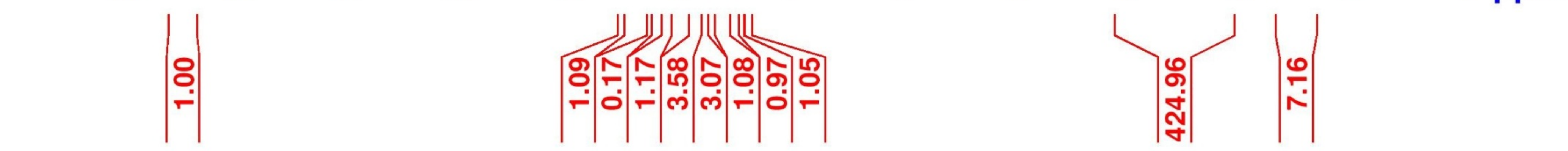
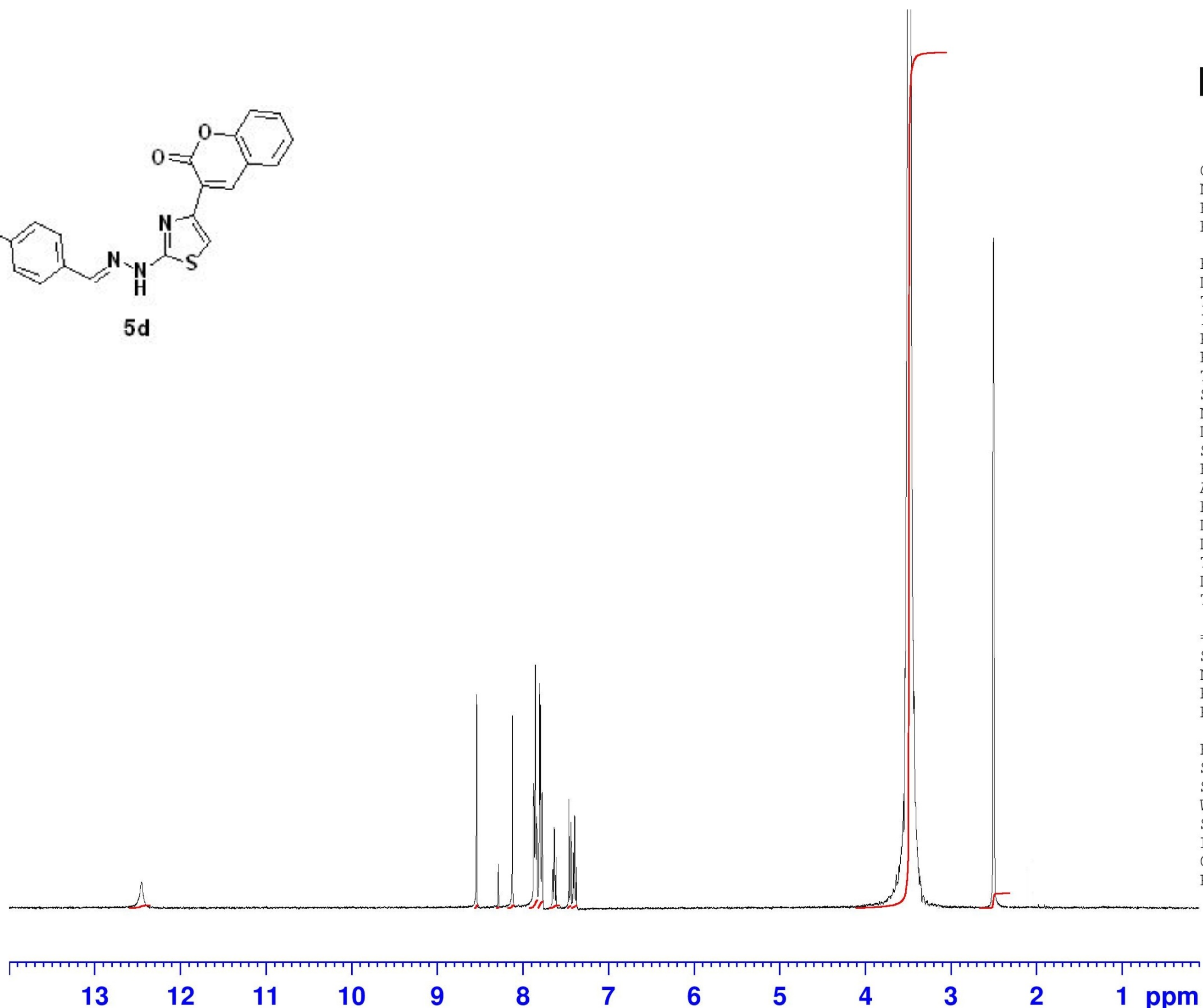


Current Data Parameters  
 NAME MG111  
 EXPNO 1  
 PROCNO 1

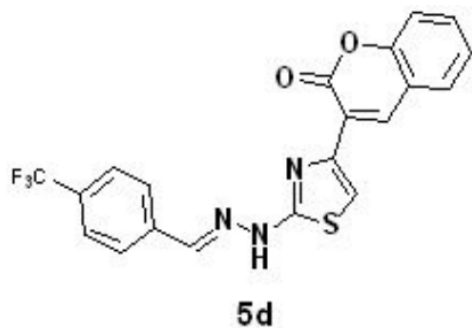
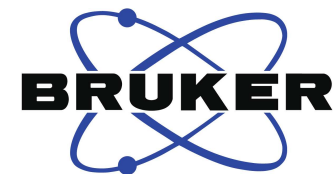
F2 - Acquisition Parameters  
 Date\_ 20130321  
 Time 18.48  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 64  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 293.9 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

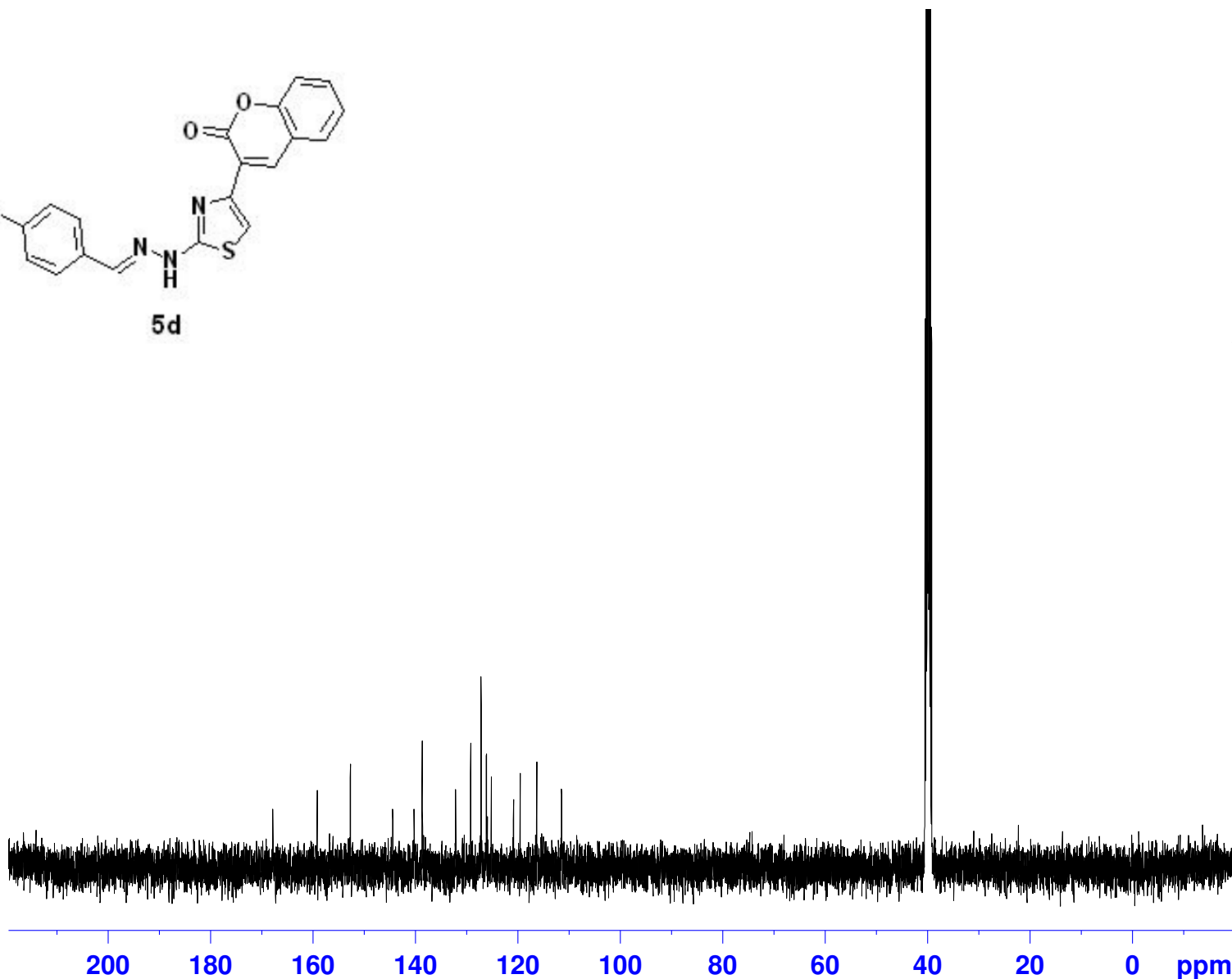
F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.40







167.89  
159.21  
152.73  
144.47  
140.28  
138.67  
132.18  
129.24  
126.13  
125.20  
120.86  
119.56  
116.33  
111.48



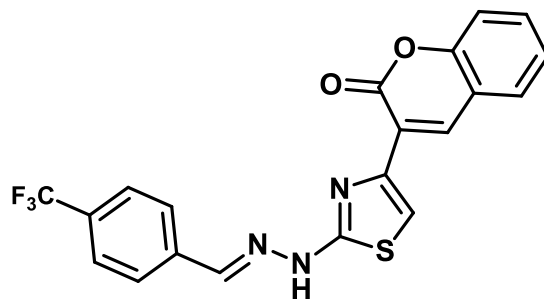
Current Data Parameters  
NAME MG111c  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130325  
Time 13.24  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 223  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

=====  
CHANNEL f1  
SFO1 100.6253441 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W

=====  
CHANNEL f2  
SFO2 400.1416006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W

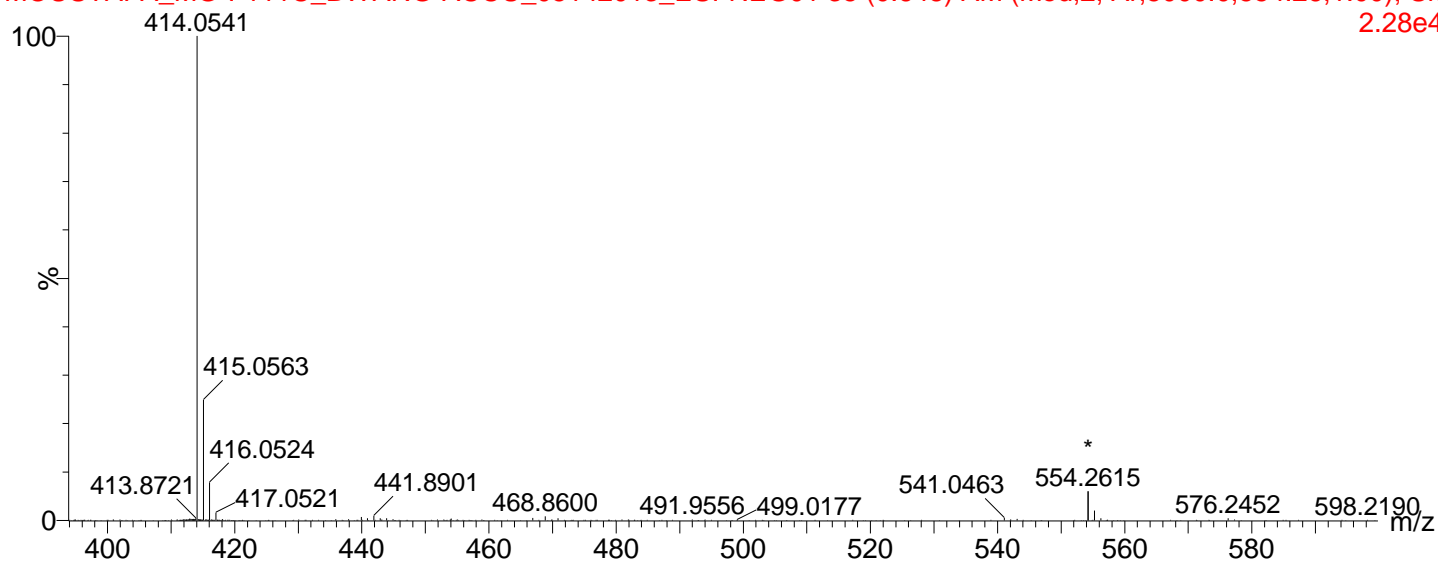
F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



5d

15-May-2013 12:59:09

MOUSTAFA\_MG-I-111C\_BWANG-ACCU\_05142013\_ESI-NEG01 35 (0.648) AM (Med,2, Ar,5000.0,554.26,1.00); Sm  
2.28e4



Elemental Composition Report

Single Mass Analysis



Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

7294 formula(e) evaluated with 79 results within limits (all results (up to 1000) for each mass)

Elements Used:

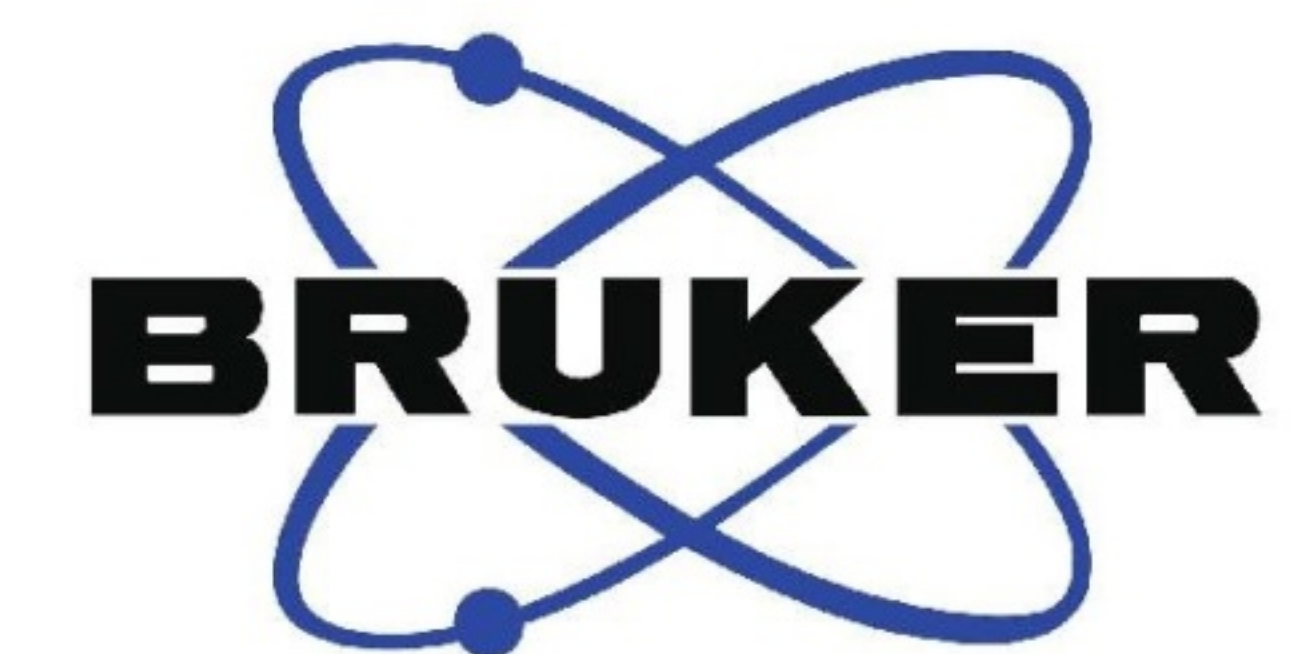
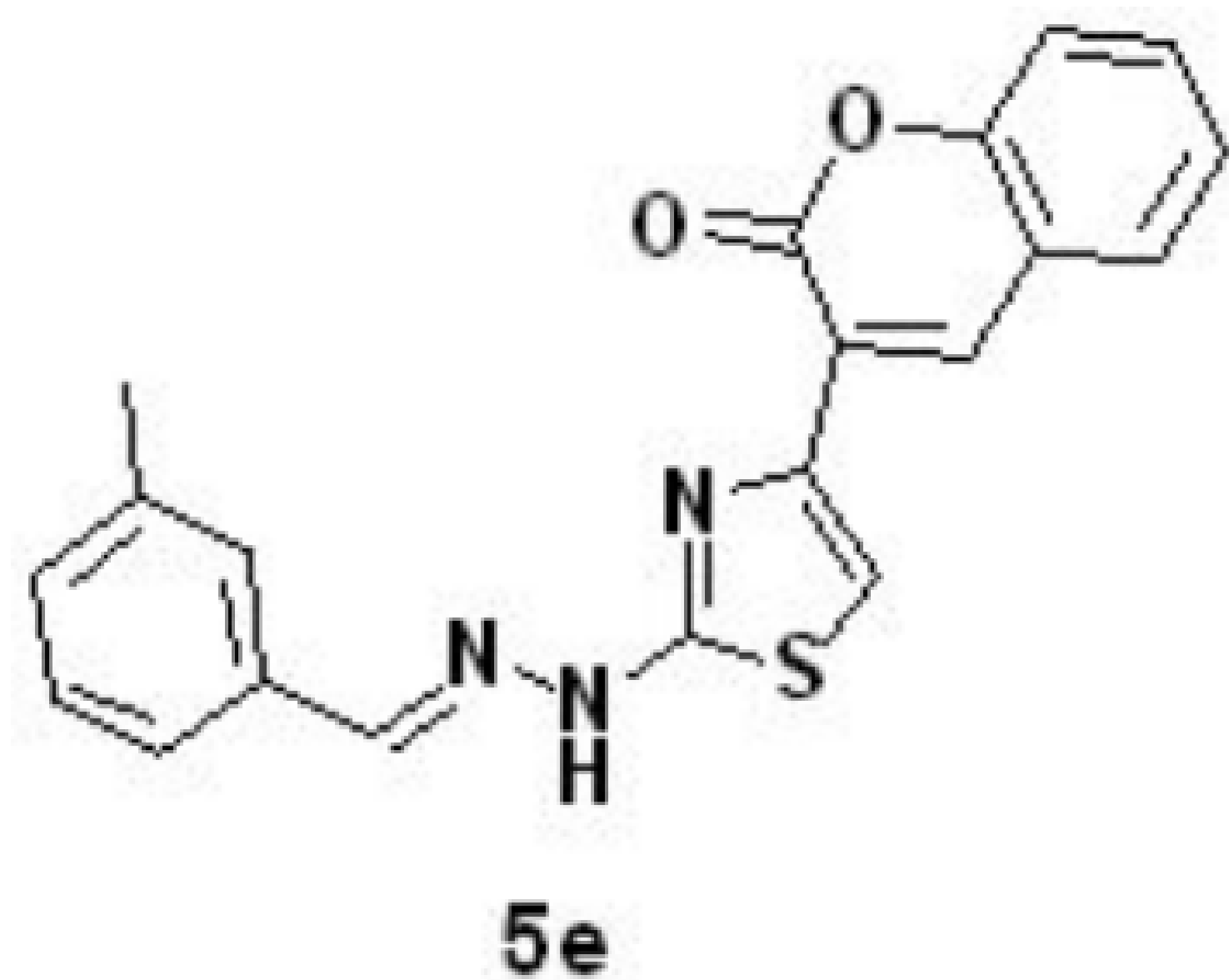
C: 1-150 H: 1-150 N: 1-30 O: 1-60 F: 1-6 S: 1-4

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
414.0541	414.0535	0.6	1.4	0.0	2094.2	C9 H23 N4 O5 F S4
	414.0551	-1.0	-2.4	1.5	1194.6	C9 H19 N5 O4 F3 S3
	414.0529	1.2	2.9	2.5	676.1	C9 H16 N5 O5 F4 S2
	414.0540	0.1	0.2	6.0	602.5	C9 H15 N8 O6 F S2
	414.0545	-0.4	-1.0	4.0	592.8	C9 H12 N6 O4 F6 S
	414.0556	-1.5	-3.6	7.5	471.4	C9 H11 N9 O5 F3 S
	414.0540	0.1	0.2	11.5	430.8	C8 H9 N15 O F S2
	414.0527	1.4	3.4	1.0	895.0	C8 H19 N4 O10 F S2
	414.0532	0.9	2.2	-1.0	851.2	C8 H16 N2 O8 F6 S
	414.0543	-0.2	-0.5	2.5	707.0	C8 H15 N5 O9 F3 S
	414.0543	-0.2	-0.5	8.0	599.7	C7 H9 N12 O4 F3 S
	414.0522	1.9	4.6	0.5	2134.6	C7 H21 N7 O4 F S4
	414.0560	-1.9	-4.6	1.0	2025.0	C7 H20 N8 O2 F2 S4
	414.0527	1.4	3.4	-1.5	1319.0	C7 H18 N5 O2 F6 S3
	414.0538	0.3	0.7	2.0	1253.3	C7 H17 N8 O3 F3 S3
	414.0554	-1.3	-3.1	3.5	711.5	C7 H13 N9 O2 F5 S2
	414.0527	1.4	3.4	6.5	682.5	C7 H13 N11 O5 F S2
	414.0532	0.9	2.2	4.5	741.6	C7 H10 N9 O3 F6 S
	414.0540	0.1	0.2	-1.5	1038.7	C6 H17 N5 O6 F5 S2
	414.0551	-1.0	-2.4	2.0	927.2	C6 H16 N8 O7 F2 S2

414.0529	1.2	2.9	3.0	860.2	C6 H13 N8 O8 F3 S
414.0529	1.2	2.9	8.5	748.8	C5 H7 N15 O3 F3 S
414.0547	-0.6	-1.4	1.5	2070.7	C5 H18 N11 O F2 S4
414.0554	-1.3	-3.1	-1.5	1148.6	C5 H16 N5 O10 F4 S
414.0524	1.7	4.1	2.5	1328.6	C5 H15 N11 O2 F3 S3
414.0540	0.1	0.2	4.0	823.3	C5 H11 N12 O F5 S2
414.0551	-1.0	-2.4	7.5	717.6	C5 H10 N15 O2 F2 S2
414.0560	-1.9	-4.6	1.5	1524.9	C4 H17 N11 O5 F S3
414.0527	1.4	3.4	-1.0	1177.5	C4 H15 N8 O5 F5 S2
414.0538	0.3	0.7	2.5	1048.0	C4 H14 N11 O6 F2 S2
414.0554	-1.3	-3.1	4.0	1007.3	C4 H10 N12 O5 F4 S
414.0538	0.3	0.7	8.0	831.9	C3 H8 N18 O F2 S2
414.0541	0.0	0.0	-1.0	1341.5	C3 H14 N8 O9 F4 S
414.0552	-1.1	-2.7	2.5	1158.2	C3 H13 N11 O10 F S
414.0546	-0.5	-1.2	14.5	229.9	C20 H14 N3 O F2 S2
414.0524	1.7	4.1	15.5	2.1	C20 H11 N3 O2 F3 S
414.0541	0.0	0.0	4.5	1195.9	C2 H8 N15 O4 F4 S
414.0552	-1.1	-2.7	8.0	1016.3	C2 H7 N18 O5 F S
414.0536	0.5	1.2	-1.5	1727.4	C2 H16 N11 O3 F4 S3
414.0547	-0.6	-1.4	2.0	1622.1	C2 H15 N14 O4 F S3
414.0525	1.6	3.9	3.0	1188.7	C2 H12 N14 O5 F2 S2
414.0552	-1.1	-2.7	0.0	1263.7	C2 H12 N12 O2 F6 S2
414.0560	-1.9	-4.6	14.5	11.5	C19 H13 N3 O5 F S
414.0542	-0.1	-0.2	9.0	896.8	C17 H19 N2 O3 F S3
414.0558	-1.7	-4.1	10.5	237.2	C17 H15 N3 O2 F3 S2
414.0536	0.5	1.2	11.5	57.7	C17 H12 N3 O3 F4 S
414.0547	-0.6	-1.4	15.0	26.6	C17 H11 N6 O4 F S
414.0533	0.8	1.9	10.0	100.2	C16 H15 N2 O8 F S
414.0533	0.8	1.9	15.5	59.7	C15 H9 N9 O3 F S
414.0528	1.3	3.1	9.5	867.8	C15 H17 N5 O2 F S3
414.0544	-0.3	-0.7	11.0	234.8	C15 H13 N6 O F3 S2

414.0522	1.9	4.6	12.0	108.6	C15 H10 N6 O2 F4 S
414.0553	-1.2	-2.9	5.0	976.8	C14 H20 N2 O4 F2 S3
414.0531	1.0	2.4	6.0	386.9	C14 H17 N2 O5 F3 S2
414.0547	-0.6	-1.4	7.5	209.8	C14 H13 N3 O4 F5 S
414.0558	-1.7	-4.1	11.0	143.2	C14 H12 N6 O5 F2 S
414.0545	-0.4	-1.0	6.0	283.0	C13 H16 N2 O9 F2 S
414.0551	-1.0	-2.4	1.0	1796.9	C12 H22 N2 O F4 S4
414.0529	1.2	2.9	2.0	996.4	C12 H19 N2 O2 F5 S3
414.0540	0.1	0.2	5.5	981.0	C12 H18 N5 O3 F2 S3
414.0556	-1.5	-3.6	7.0	372.8	C12 H14 N6 O2 F4 S2
414.0534	0.7	1.7	8.0	297.8	C12 H11 N6 O3 F5 S
414.0545	-0.4	-1.0	11.5	213.1	C12 H10 N9 O4 F2 S
414.0549	-0.8	-1.9	-0.5	2074.3	C11 H25 N O6 F S4
414.0526	1.5	3.6	0.5	1242.9	C11 H22 N O7 F2 S3
414.0542	-0.1	-0.2	2.0	597.4	C11 H18 N2 O6 F4 S2
414.0553	-1.2	-2.9	5.5	542.4	C11 H17 N5 O7 F S2
414.0531	1.0	2.4	6.5	375.7	C11 H14 N5 O8 F2 S
414.0558	-1.7	-4.1	3.5	465.8	C11 H14 N3 O5 F6 S
414.0531	1.0	2.4	12.0	303.2	C10 H8 N12 O3 F2 S
414.0540	0.1	0.2	0.5	808.0	C10 H21 N O11 F S2
414.0549	-0.8	-1.9	5.0	1799.4	C10 H19 N8 O F S4
414.0556	-1.5	-3.6	2.0	573.5	C10 H17 N2 O10 F3 S
414.0526	1.5	3.6	6.0	1000.3	C10 H16 N8 O2 F2 S3
414.0542	-0.1	-0.2	7.5	425.0	C10 H12 N9 O F4 S2
414.0553	-1.2	-2.9	11.0	376.2	C10 H11 N12 O2 F S2
414.0549	-0.8	-1.9	-1.5	1526.1	C H15 N11 O7 F3 S2
414.0527	1.4	3.4	-0.5	1554.2	C H12 N11 O8 F4 S
414.0538	0.3	0.7	3.0	1353.0	C H11 N14 O9 F S



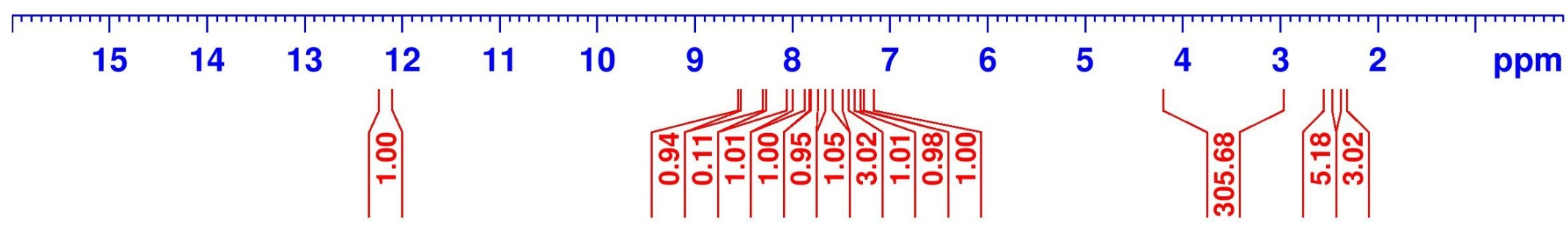
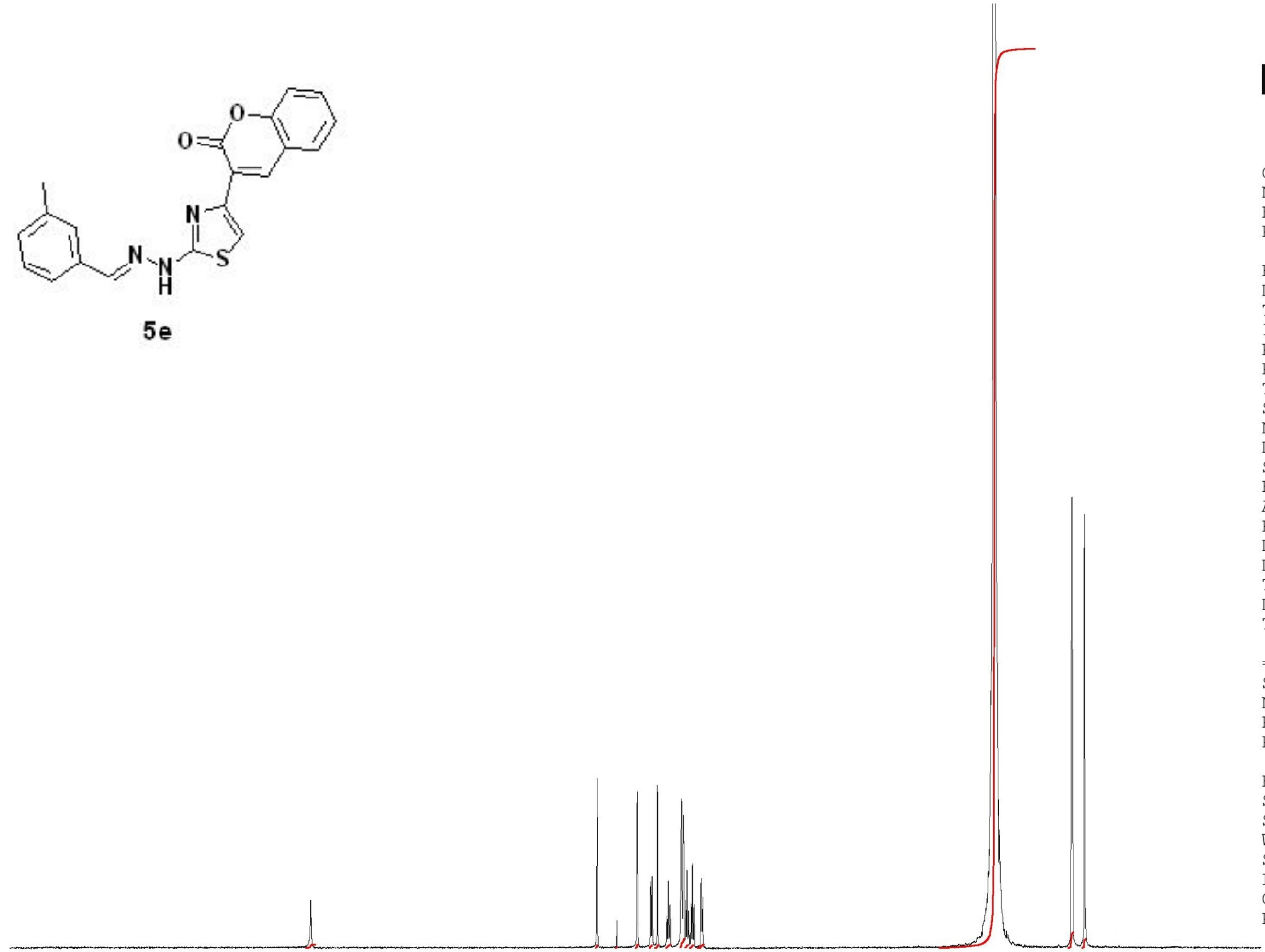


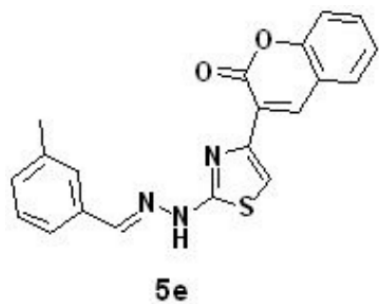
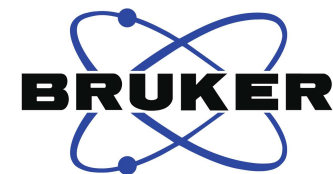
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 SOLVENT DMSO  
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 DS 2  
 SWH 8012.820 Hz  
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 TE 293.9 K  
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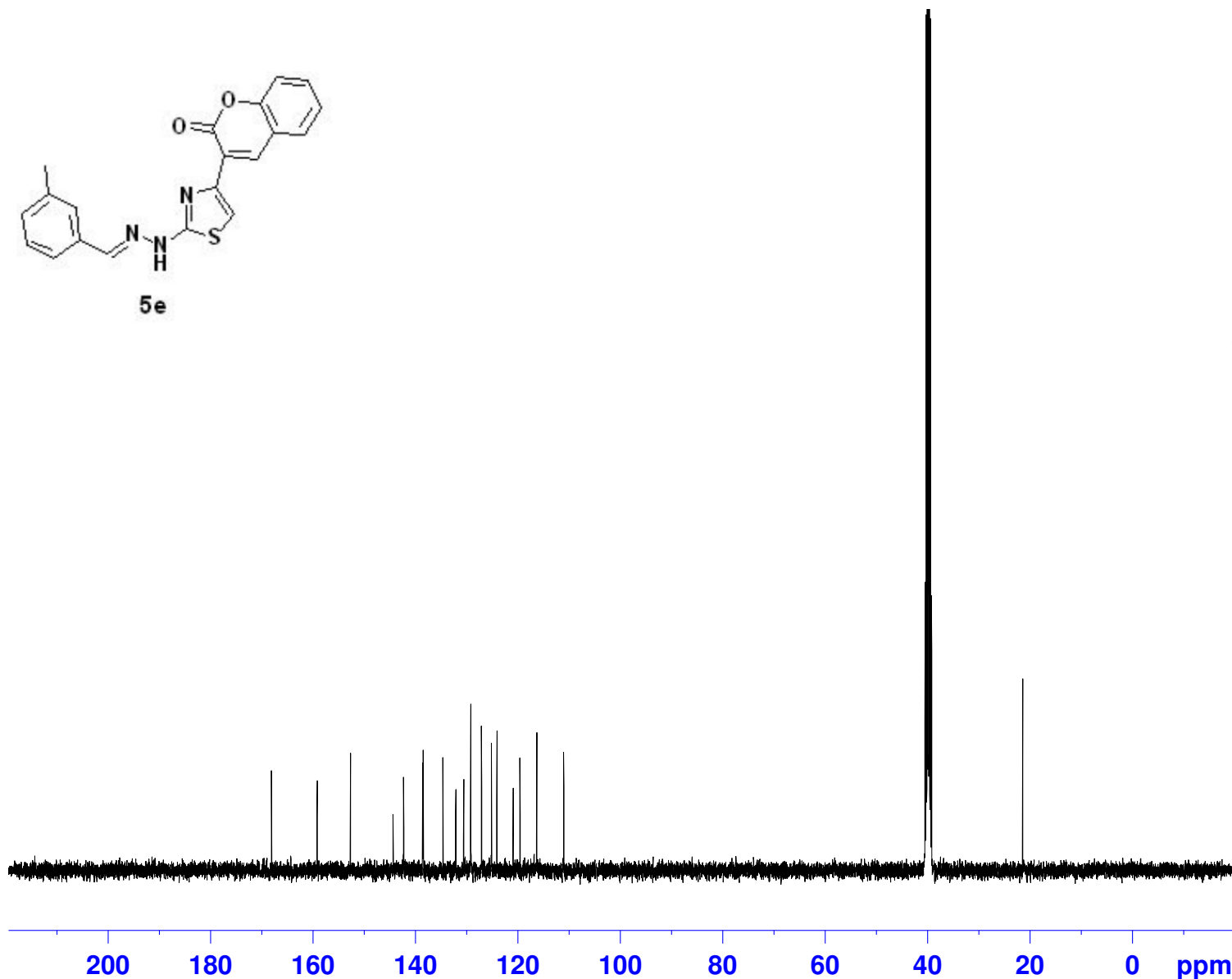
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168.14  
159.22  
152.72  
144.40  
142.34  
138.60  
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132.14  
130.59  
129.22  
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21.41



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EXPNO 1  
PROCNO 1

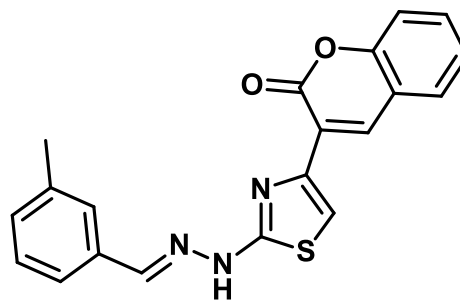
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TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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P1 9.00 usec  
PLW1 62.00000000 W

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NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
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PC 1.40

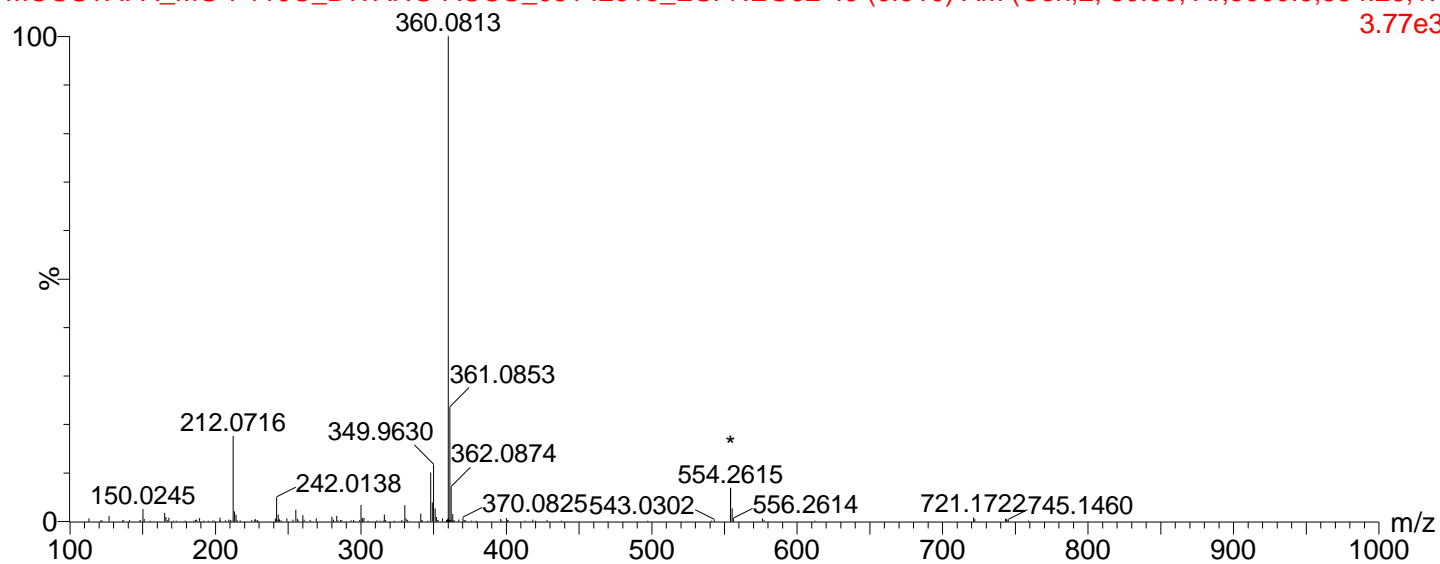




5e

15-May-2013 12:31:46

MOUSTAFA\_MG-I-110C\_BWANG-ACCU\_05142013\_ESI-NEG02 49 (0.910) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.0  
3.77e3



Elemental Composition Report

Single Mass Analysis



Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

1424 formula(e) evaluated with 13 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-4

Minimum:

-1.5

Maximum:

5.0

5.0

50.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

360.0813

360.0800

1.3

3.6

6.5

74.3

C12 H18 N5 O4 S2

360.0796

1.7

4.7

0.5

351.2

C12 H26 N O3 S4

360.0814

-0.1

-0.3

6.0

70.9

C14 H20 N2 O5 S2

360.0827

-1.4

-3.9

11.0

47.4

C15 H16 N6 O S2

360.0807

0.6

1.7

15.5

1.6

C20 H14 N3 O2 S

360.0798

1.5

4.2

9.0

127.4

C3 H8 N18 O2 S

360.0798

1.5

4.2

3.5

147.6

C4 H14 N11 O7 S

360.0812

0.1

0.3

8.5

101.5

C5 H10 N15 O3 S

360.0807

0.6

1.7

2.5

232.5

C5 H18 N11 O2 S3

360.0812

0.1

0.3

3.0

121.1

C6 H16 N8 O8 S

360.0825

-1.2

-3.3

8.0

79.3

C7 H12 N12 O4 S

360.0821

-0.8

-2.2

2.0

222.7

C7 H20 N8 O3 S3

360.0825

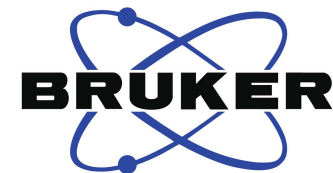
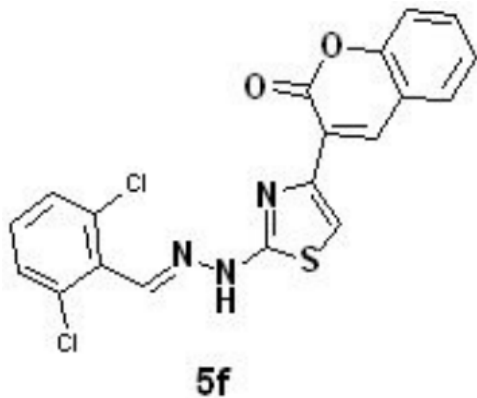
-1.2

-3.3

2.5

98.1

C8 H18 N5 O9 S

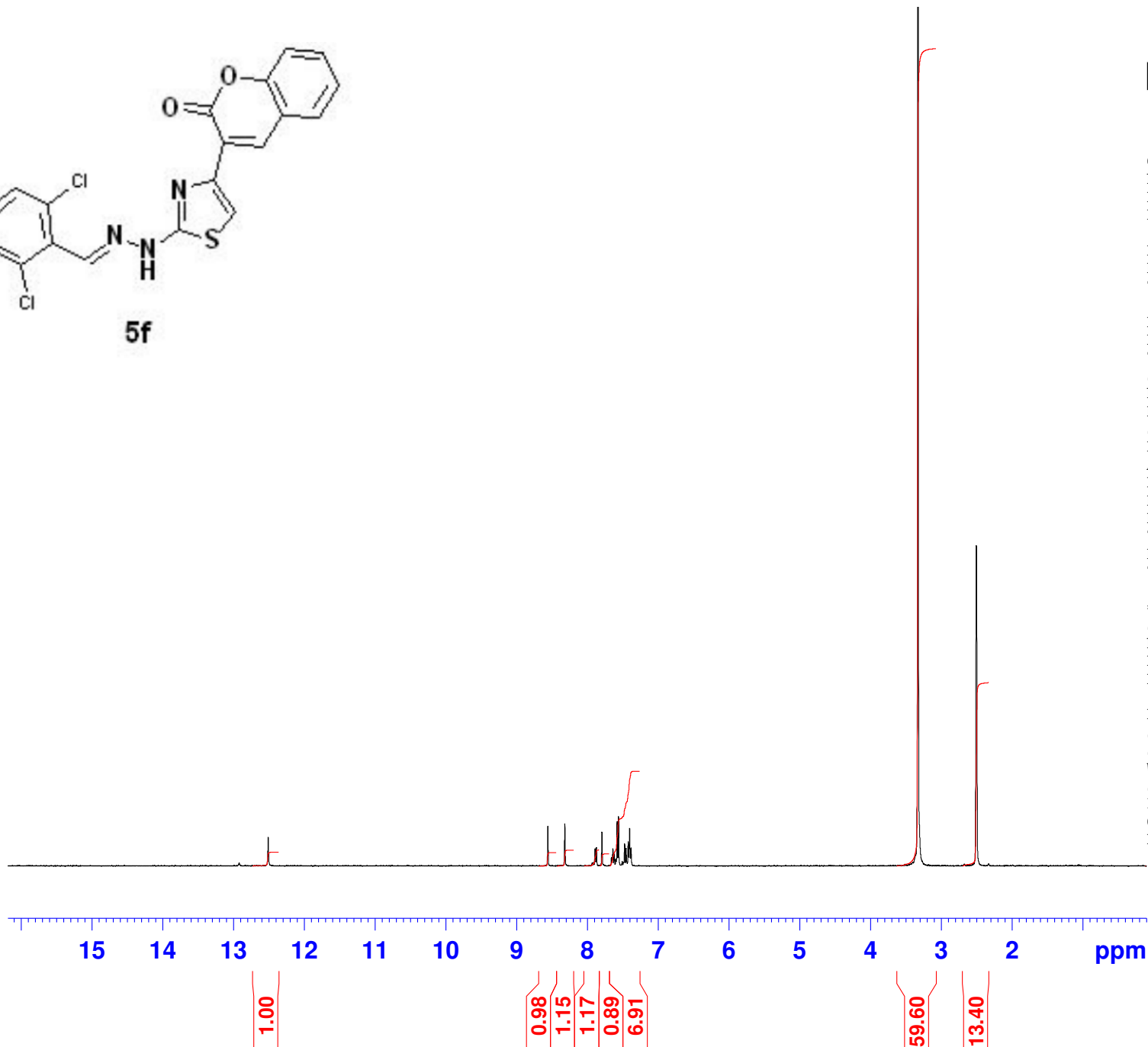


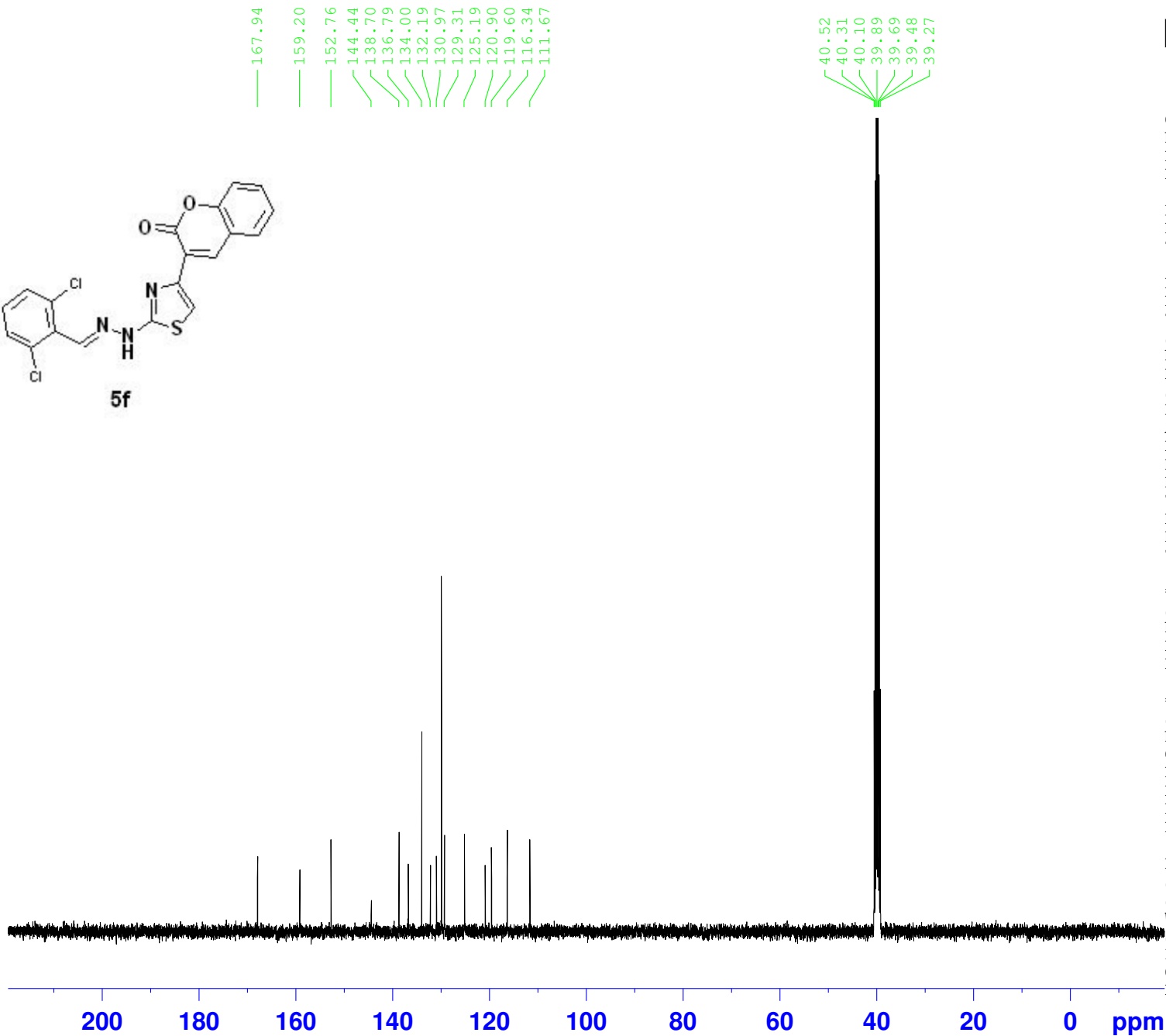
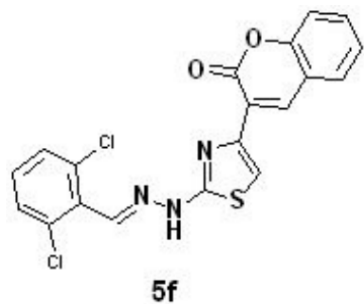
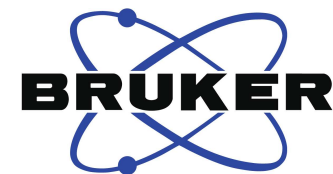
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 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 203  
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 TE 298.0 K  
 D1 1.00000000 sec  
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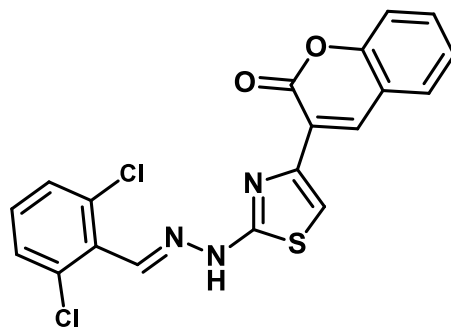
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RG 161  
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DE 6.50 usec  
TE 293.8 K  
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TD0 1

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PLW1 62.00000000 W

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NUC2 1H  
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PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W

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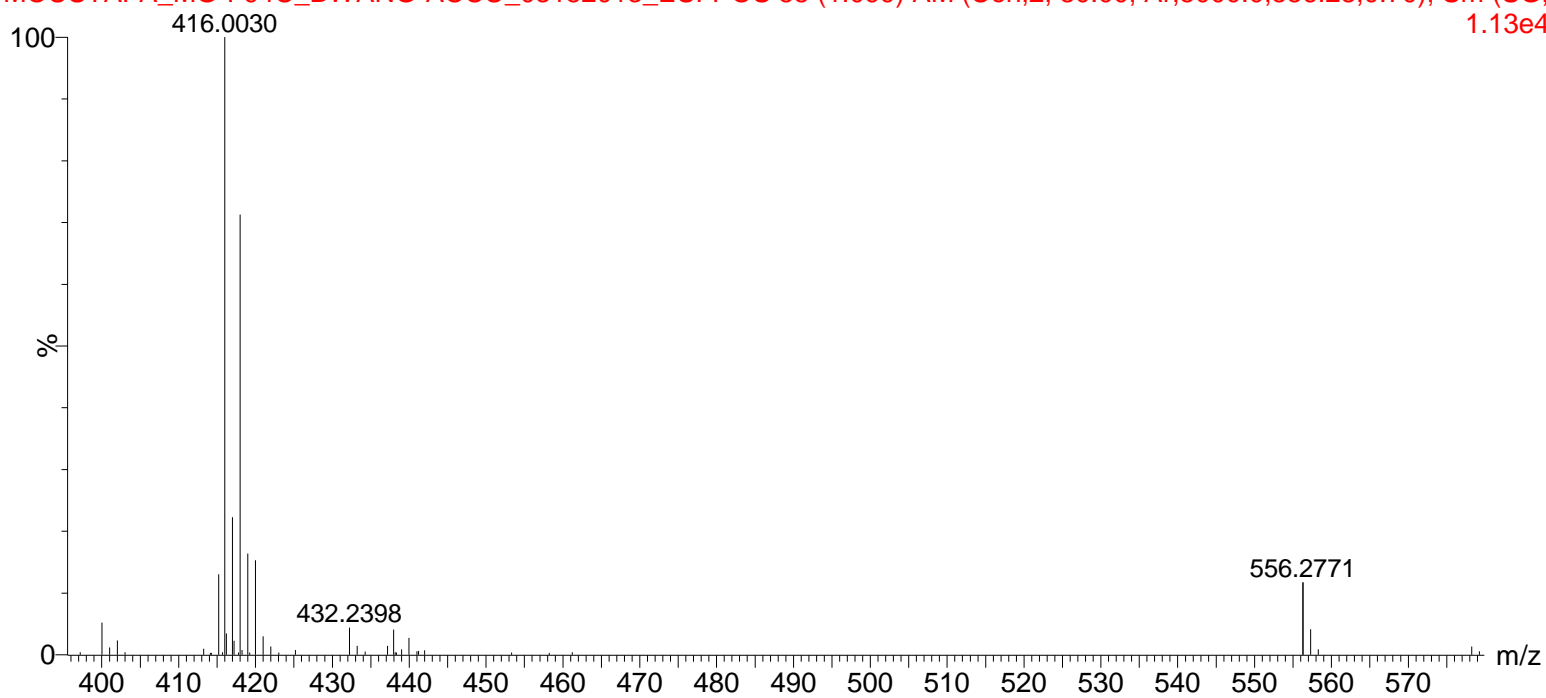


5f

80%MeOH

16:42:23 15-Mar-2013

MOUSTAFA\_MG-I-94C\_BWANG-ACCU\_03152013\_ESI-POS 55 (1.099) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 1.13e4



## Elemental Composition Report

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

### Monoisotopic Mass, Odd and Even Electron Ions

3532 formula(e) evaluated with 40 results within limits (up to 100 closest results for each mass)

Elements Used:

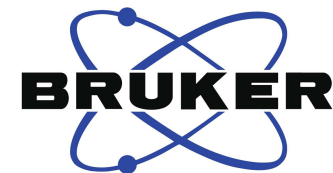
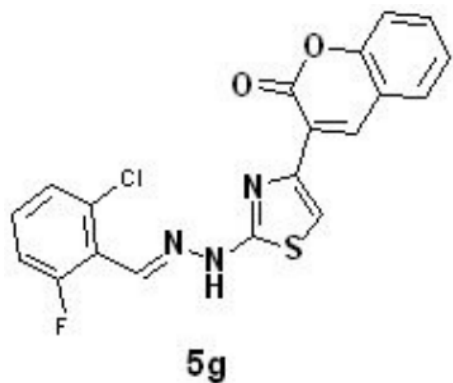
C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-10 Cl: 1-2

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			mDa	PPM			
416.0030	416.0034	-0.4	-1.0	2.5	957.0	C H11 N13 O7 S2 Cl	
	416.0041	-1.1	-2.6	6.0	755.8	C10 H13 N4 O10 S Cl	
	416.0021	0.9	2.2	5.5	108.0	C11 H16 N5 O4 S2 Cl2	
	416.0050	-2.0	-4.8	5.0	370.8	C11 H17 N4 O5 S3 Cl	
	416.0016	1.4	3.4	-0.5	184.1	C11 H24 N O3 S4 Cl2	
	416.0034	-0.4	-1.0	5.0	76.3	C13 H18 N2 O5 S2 Cl2	
	416.0016	1.4	3.4	10.0	481.1	C14 H13 N4 O5 S2 Cl	
	416.0048	-1.8	-4.3	10.0	28.7	C14 H14 N6 O S2 Cl2	
	416.0029	0.1	0.2	15.0	501.2	C15 H9 N8 O S2 Cl	
	416.0029	0.1	0.2	9.5	463.6	C16 H15 N O6 S2 Cl	
	416.0014	1.6	3.8	15.0	1.1	C17 H10 N6 O S Cl2	
	416.0043	-1.3	-3.1	14.5	498.8	C17 H11 N5 O2 S2 Cl	
	416.0038	-0.8	-1.9	8.5	220.5	C17 H19 N O S4 Cl	
	416.0027	0.3	0.7	14.5	2.4	C19 H12 N3 O2 S Cl2	
	416.0014	1.6	3.8	2.0	417.1	C2 H14 N14 O S3 Cl2	
	416.0043	-1.3	-3.1	1.5	526.7	C2 H15 N13 O2 S4 Cl	
	416.0019	1.1	2.6	8.0	379.7	C2 H6 N18 O2 S Cl2	



416.0048	-1.8	-4.3	7.5	818.7	C2 H7 N17 O3 S2 Cl
416.0022	0.8	1.9	19.0	736.6	C22 H9 N2 O3 S Cl
416.0019	1.1	2.6	2.5	459.5	C3 H12 N11 O7 S Cl2
416.0048	-1.8	-4.3	2.0	859.2	C3 H13 N10 O8 S2 Cl
416.0028	0.2	0.5	1.5	348.1	C4 H16 N11 O2 S3 Cl2
416.0032	-0.2	-0.5	7.5	307.4	C4 H8 N15 O3 S Cl2
416.0009	2.1	5.0	6.5	517.5	C5 H11 N13 O2 S3 Cl
416.0032	-0.2	-0.5	2.0	380.2	C5 H14 N8 O8 S Cl2
416.0014	1.6	3.8	12.5	877.5	C5 H3 N17 O3 S Cl
416.0046	-1.6	-3.8	7.0	244.6	C6 H10 N12 O4 S Cl2
416.0009	2.1	5.0	1.0	544.9	C6 H17 N6 O7 S3 Cl
416.0041	-1.1	-2.6	1.0	288.2	C6 H18 N8 O3 S3 Cl2
416.0014	1.6	3.8	7.0	890.9	C6 H9 N10 O8 S Cl
416.0023	0.7	1.7	6.0	458.4	C7 H13 N10 O3 S3 Cl
416.0014	1.6	3.8	1.5	914.7	C7 H15 N3 O13 S Cl
416.0046	-1.6	-3.8	1.5	310.1	C7 H16 N5 O9 S Cl2
416.0018	1.2	2.9	0.0	244.7	C7 H21 N6 O2 S5 Cl
416.0027	0.3	0.7	12.0	812.7	C7 H5 N14 O4 S Cl
416.0027	0.3	0.7	6.5	817.8	C8 H11 N7 O9 S Cl
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416.0036	-0.6	-1.4	5.5	409.6	C9 H15 N7 O4 S3 Cl
416.0032	-0.2	-0.5	-0.5	199.7	C9 H23 N3 O3 S5 Cl
416.0041	-1.1	-2.6	11.5	759.2	C9 H7 N11 O5 S Cl

test

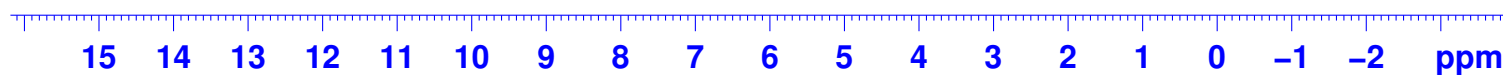
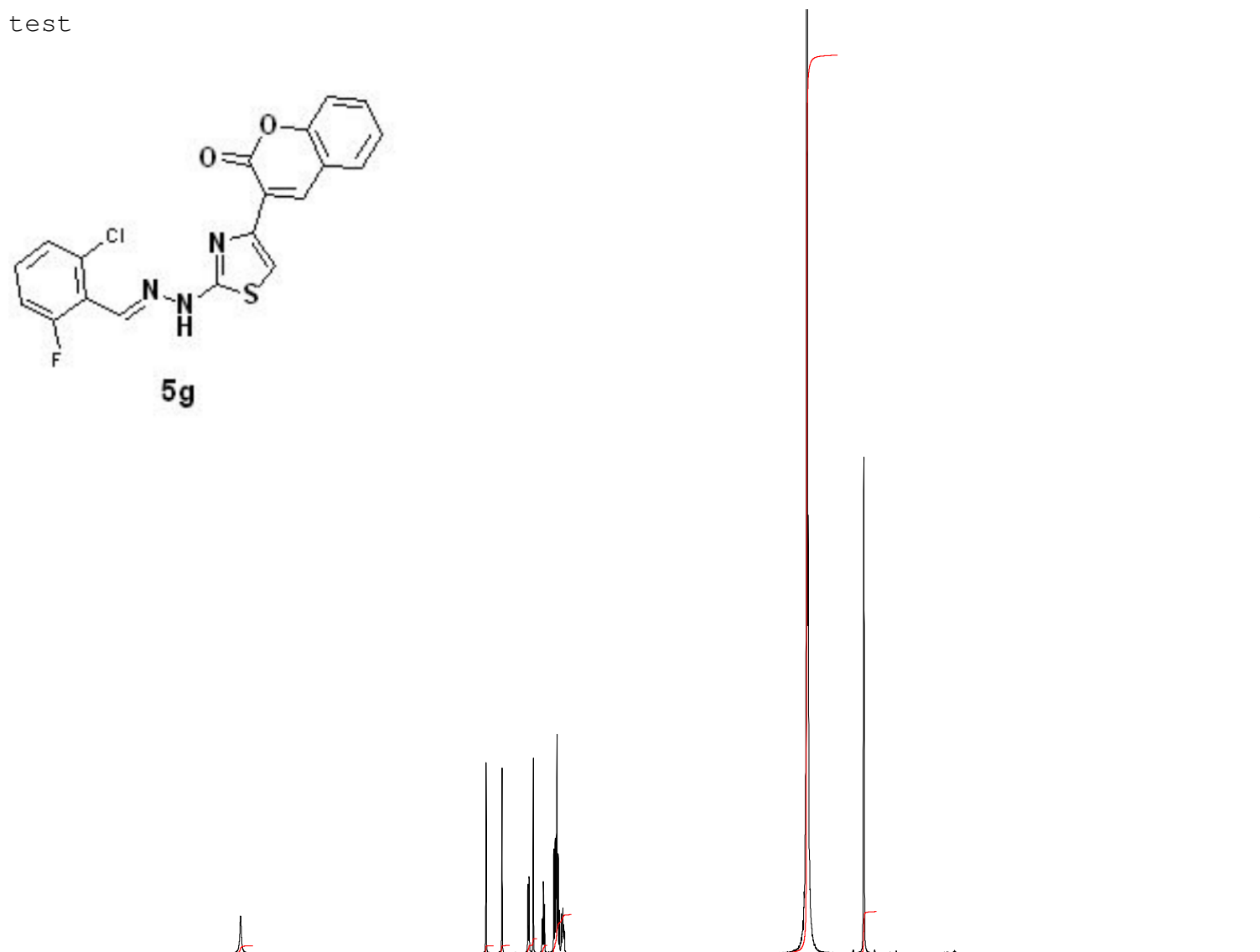


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EXPNO 1  
PROCNO 1

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Time 18.12  
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PULPROG zg30  
TD 65536  
SOLVENT DMSO  
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DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
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RG 101  
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DE 6.50 usec  
TE 293.6 K  
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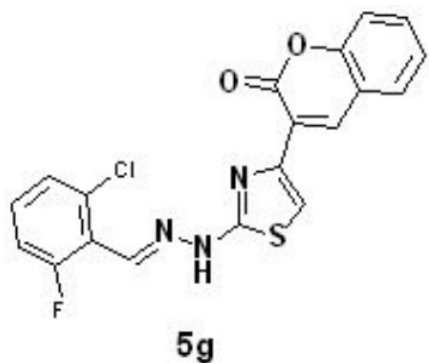
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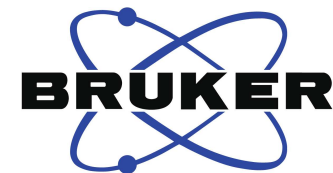
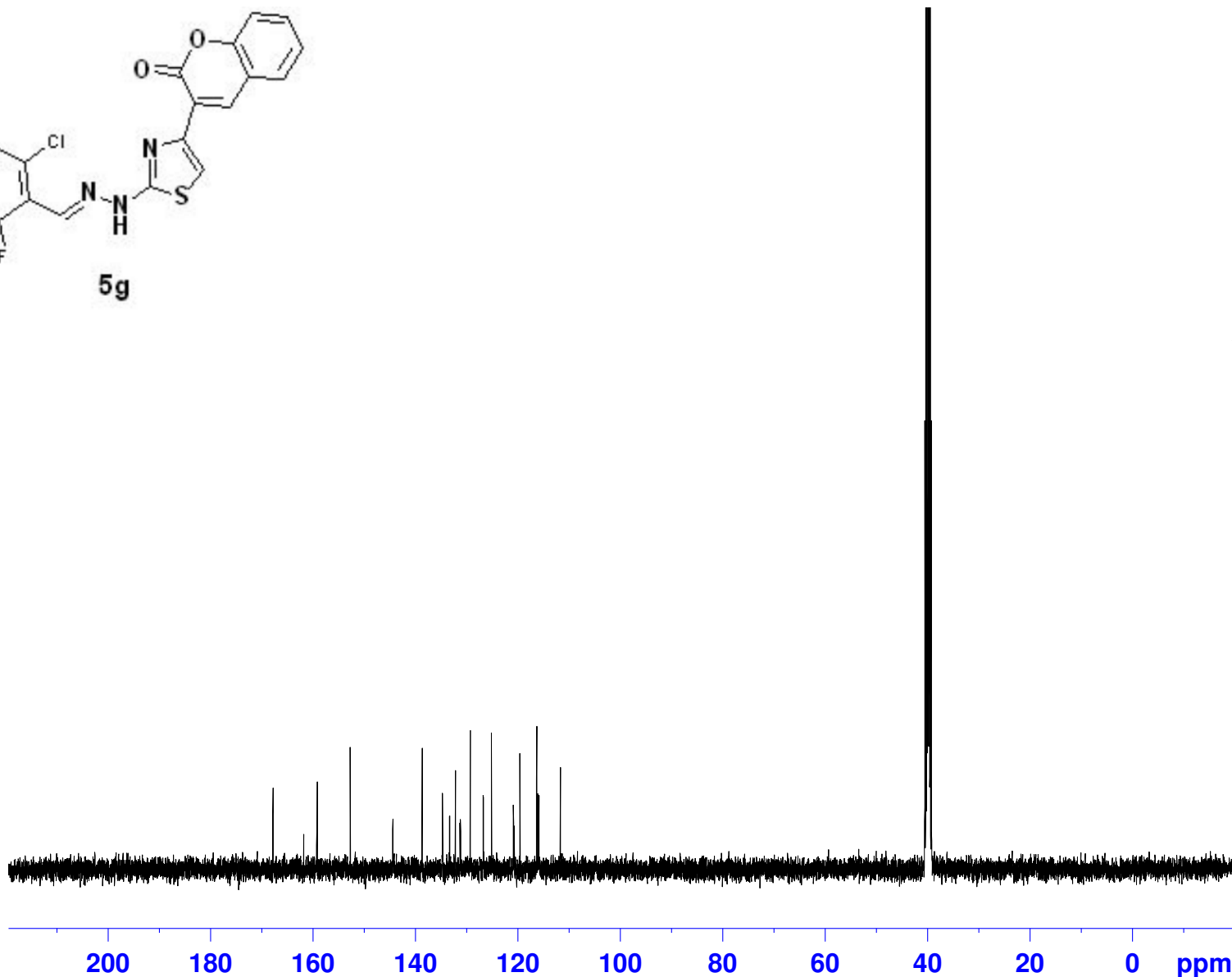


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1.02  
1.93  
1.06  
5.05  
117.27  
5.47

test



167.86  
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152.77  
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134.75  
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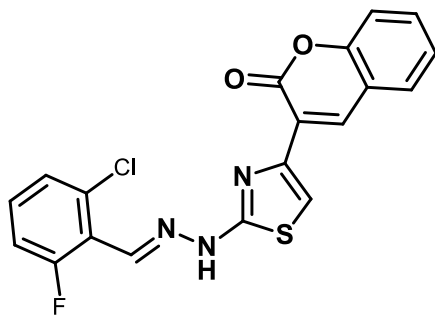
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EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
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TD 65536  
SOLVENT DMSO  
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D1 2.00000000 sec  
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PLW12 0.36000001 W  
PLW13 0.29159999 W

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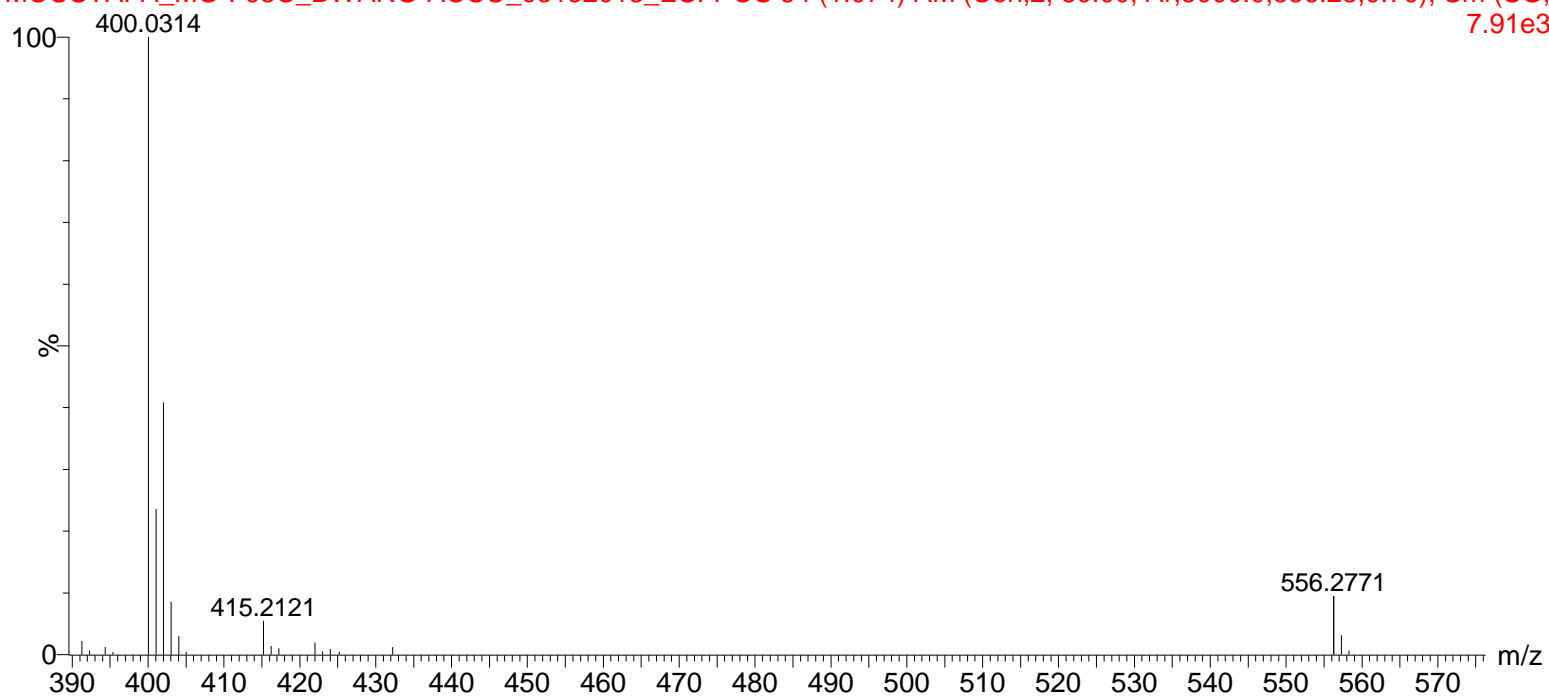


5g

80%MeOH

16:38:18 15-Mar-2013

MOUSTAFA\_MG-I-93C\_BWANG-ACCU\_03152013\_ESI-POS 54 (1.074) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 7.91e3



## Elemental Composition Report

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

### Monoisotopic Mass, Odd and Even Electron Ions

8125 formula(e) evaluated with 61 results within limits (up to 100 closest results for each mass)

Elements Used:

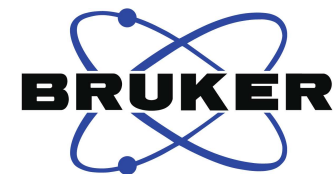
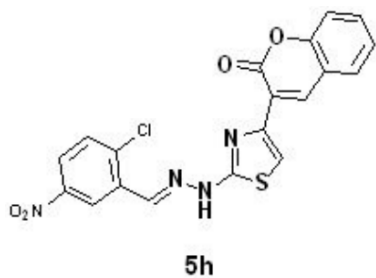
C: 1-150 H: 1-150 N: 1-30 O: 1-60 F: 1-12 S: 1-10 Cl: 1-2

Mass	Calc. Mass	5.0	5.0	50.0	DBE	i-FIT	Formula
			mDa	PPM			
400.0314	400.0328	-1.4	-3.5	0.0	476.4	C H10 N12 O3 F5 S Cl	
	400.0301	1.3	3.2	3.0	427.8	C H10 N14 O6 F S Cl	
	400.0333	-1.9	-4.7	3.0	852.5	C H11 N16 O2 F S Cl2	
	400.0322	-0.8	-2.0	-0.5	899.0	C H12 N13 O F4 S Cl2	
	400.0312	0.2	0.5	-1.5	450.8	C H14 N11 O4 F3 S2 Cl	
	400.0319	-0.5	-1.2	2.0	167.8	C10 H16 N2 O7 F3 S Cl	
	400.0312	0.2	0.5	1.5	659.3	C10 H18 N3 O5 F2 S Cl2	
	400.0303	1.1	2.7	0.5	166.7	C10 H20 N O8 F S2 Cl	
	400.0332	-1.8	-4.5	7.0	98.1	C11 H12 N6 O3 F3 S Cl	
	400.0321	-0.7	-1.7	3.5	129.1	C11 H13 N3 O2 F6 S Cl	
	400.0326	-1.2	-3.0	6.5	573.1	C11 H14 N7 O F2 S Cl2	
	400.0316	-0.2	-0.5	5.5	95.5	C11 H16 N5 O4 F S2 Cl	
	400.0305	0.9	2.2	2.0	123.7	C11 H17 N2 O3 F4 S2 Cl	
	400.0299	1.5	3.7	1.5	698.4	C11 H19 N3 O F3 S2 Cl2	
	400.0328	-1.4	-3.5	1.0	136.6	C11 H20 N2 O2 F3 S3 Cl	
	400.0312	0.2	0.5	-0.5	184.2	C11 H24 N O3 F S4 Cl	
	400.0307	0.7	1.7	11.5	53.0	C12 H9 N9 O F2 S Cl	

400.0307	0.7	1.7	6.0	75.5	C13 H15 N2 O6 F2 S Cl
400.0328	-1.4	-3.5	2.5	571.2	C13 H17 N O F5 S Cl2
400.0301	1.3	3.2	5.5	565.7	C13 H17 N3 O4 F S Cl2
400.0330	-1.6	-4.0	5.0	71.1	C13 H18 N2 O5 F S2 Cl
400.0321	-0.7	-1.7	11.0	33.2	C14 H11 N6 O2 F2 S Cl
400.0310	0.4	1.0	7.5	51.7	C14 H12 N3 O F5 S Cl
400.0316	-0.2	-0.5	5.0	70.2	C14 H19 N2 O F2 S3 Cl
400.0296	1.8	4.5	10.0	22.0	C16 H14 N2 O5 F S Cl
400.0328	-1.4	-3.5	10.0	483.4	C16 H15 N4 O F S Cl2
400.0309	0.5	1.2	15.0	4.6	C17 H10 N6 O F S Cl
400.0323	-0.9	-2.2	14.5	1.5	C19 H12 N3 O2 F S Cl
400.0310	0.4	1.0	2.0	333.9	C2 H14 N14 O F S3 Cl
400.0314	0.0	0.0	8.0	306.3	C2 H6 N18 O2 F S Cl
400.0303	1.1	2.7	4.5	362.9	C2 H7 N15 O F4 S Cl
400.0314	0.0	0.0	2.5	362.2	C3 H12 N11 O7 F S Cl
400.0303	1.1	2.7	-1.0	423.1	C3 H13 N8 O6 F4 S Cl
400.0297	1.7	4.2	-1.5	871.5	C3 H15 N9 O4 F3 S Cl2
400.0306	0.8	2.0	0.5	358.9	C4 H10 N9 O F7 S Cl
400.0301	1.3	3.2	2.5	286.6	C4 H13 N11 O3 F2 S2 Cl
400.0294	2.0	5.0	2.0	845.2	C4 H15 N12 O F S2 Cl2
400.0323	-0.9	-2.2	1.5	284.6	C4 H16 N11 O2 F S3 Cl
400.0328	-1.4	-3.5	7.5	252.1	C4 H8 N15 O3 F S Cl
400.0317	-0.3	-0.7	4.0	302.7	C4 H9 N12 O2 F4 S Cl
400.0328	-1.4	-3.5	2.0	303.5	C5 H14 N8 O8 F S Cl
400.0317	-0.3	-0.7	-1.5	358.5	C5 H15 N5 O7 F4 S Cl
400.0330	-1.6	-4.0	3.5	249.3	C6 H11 N9 O3 F4 S Cl
400.0319	-0.5	-1.2	0.0	299.4	C6 H12 N6 O2 F7 S Cl
400.0324	-1.0	-2.5	3.0	711.1	C6 H13 N10 O F3 S Cl2
400.0314	0.0	0.0	2.0	236.9	C6 H15 N8 O4 F2 S2 Cl
400.0303	1.1	2.7	-1.5	283.1	C6 H16 N5 O3 F5 S2 Cl
400.0308	0.6	1.5	1.5	806.1	C6 H17 N9 O2 F S2 Cl2



400.0305	0.9	2.2	8.0	170.5	C7 H8 N12 O F3 S Cl
400.0333	-1.9	-4.7	-0.5	246.7	C8 H14 N3 O3 F7 S Cl
400.0305	0.9	2.2	2.5	211.8	C8 H14 N5 O6 F3 S Cl
400.0294	2.0	5.0	-1.0	258.8	C8 H15 N2 O5 F6 S Cl
400.0326	-1.2	-3.0	-1.0	708.5	C8 H16 N4 O F6 S Cl2
400.0299	1.5	3.7	2.0	694.1	C8 H16 N6 O4 F2 S Cl2
400.0328	-1.4	-3.5	1.5	193.3	C8 H17 N5 O5 F2 S2 Cl
400.0321	-0.7	-1.7	1.0	770.9	C8 H19 N6 O3 F S2 Cl2
400.0319	-0.5	-1.2	7.5	131.1	C9 H10 N9 O2 F3 S Cl
400.0308	0.6	1.5	4.0	167.8	C9 H11 N6 O F6 S Cl
400.0303	1.1	2.7	6.0	125.8	C9 H14 N8 O3 F S2 Cl
400.0314	0.0	0.0	1.5	166.4	C9 H18 N5 O F3 S3 Cl
400.0298	1.6	4.0	0.0	212.4	C9 H22 N4 O2 F S4 Cl

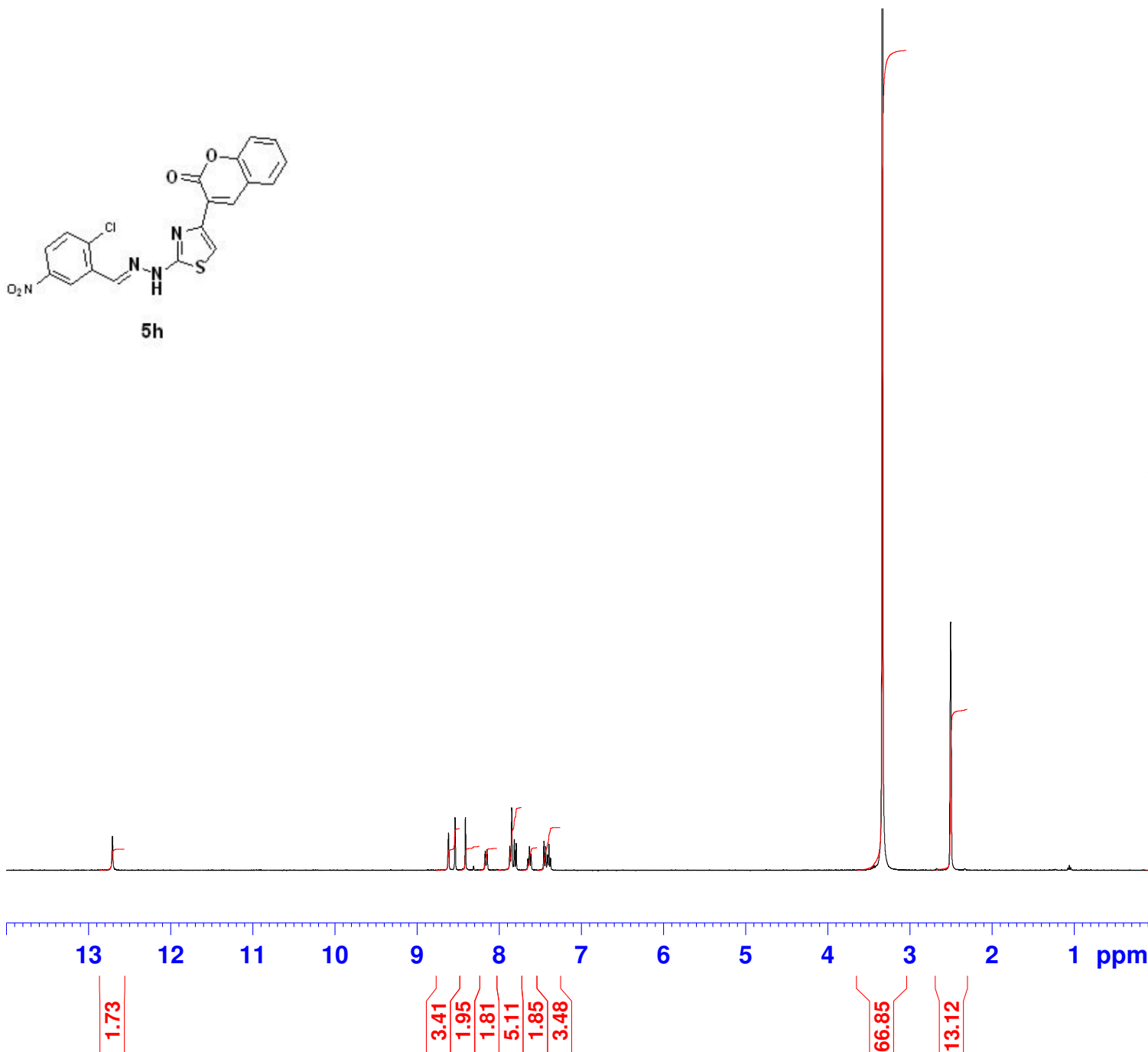


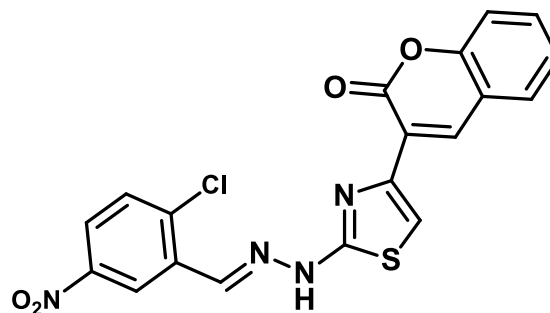
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 PULPROG zg30  
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 SOLVENT DMSO  
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 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 203  
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 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1

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 P1 13.50 usec  
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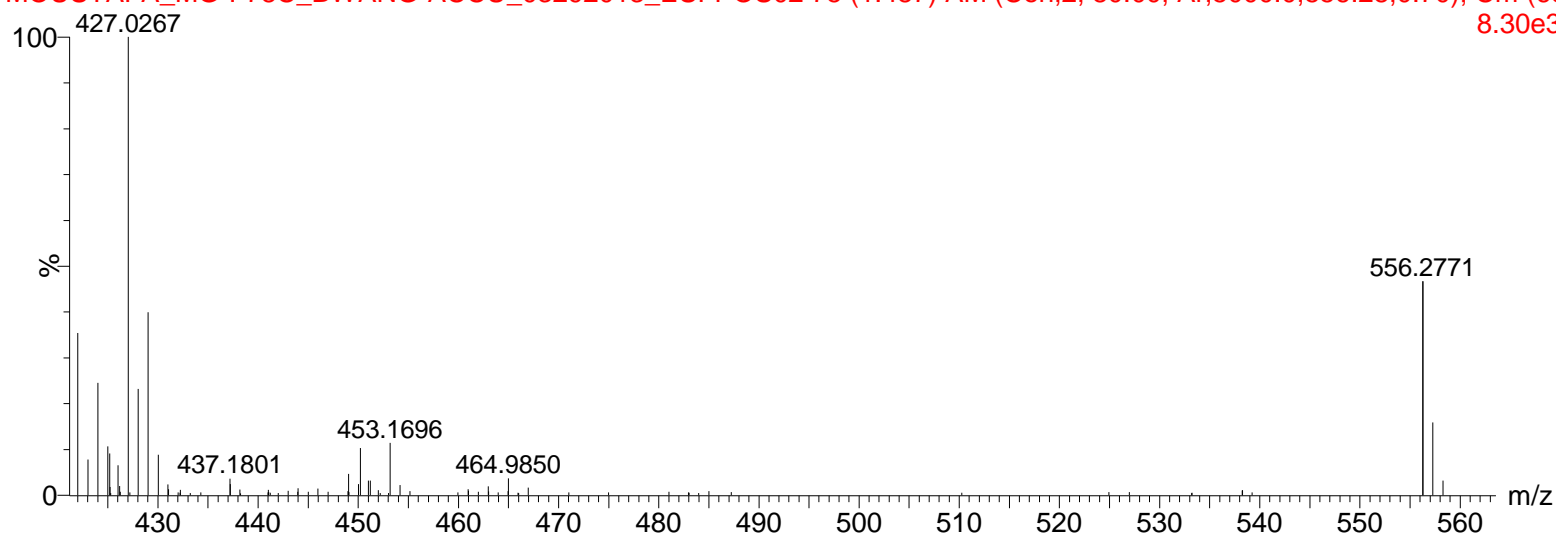


5h

80% ACN

16:34:25 29-Mar-2013

MOUSTAFA\_MG-I-78C\_BWANG-ACCU\_03292013\_ESI-POS02 75 (1.487) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Cm (69  
8.30e3



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

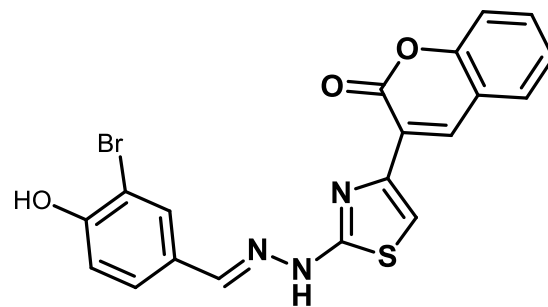
3911 formula(e) evaluated with 41 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-10 Cl: 1-2

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
427.0267	427.0246	2.1	4.9	4.0	411.9	C H10 N15 O8 S Cl
	427.0278	-1.1	-2.6	4.0	906.8	C H11 N17 O4 S Cl2
	427.0261	0.6	1.4	12.0	61.8	C10 H10 N13 O S2 Cl
	427.0248	1.9	4.4	1.5	163.8	C10 H20 N2 O10 S2 Cl
	427.0280	-1.3	-3.0	1.5	803.5	C10 H21 N4 O6 S2 Cl2
	427.0261	0.6	1.4	6.5	92.9	C11 H16 N6 O6 S2 Cl
	427.0257	1.0	2.3	0.5	201.0	C11 H24 N2 O5 S4 Cl
	427.0288	-2.1	-4.9	0.5	947.8	C11 H25 N4 O S4 Cl2
	427.0246	2.1	4.9	12.0	572.0	C12 H11 N11 O S Cl2
	427.0275	-0.8	-1.9	11.5	43.3	C12 H12 N10 O2 S2 Cl
	427.0270	-0.3	-0.7	5.5	143.0	C12 H20 N6 O S4 Cl
	427.0246	2.1	4.9	6.5	622.8	C13 H17 N4 O6 S Cl2
	427.0275	-0.8	-1.9	6.0	69.8	C13 H18 N3 O7 S2 Cl
	427.0259	0.8	1.9	11.5	553.6	C14 H13 N8 O2 S Cl2
	427.0288	-2.1	-4.9	11.0	30.6	C14 H14 N7 O3 S2 Cl
	427.0255	1.2	2.8	5.5	778.9	C14 H21 N4 O S3 Cl2
	427.0283	-1.6	-3.7	5.0	130.8	C14 H22 N3 O2 S4 Cl
	427.0259	0.8	1.9	6.0	601.2	C15 H19 N O7 S Cl2
	427.0273	-0.6	-1.4	11.0	540.0	C16 H15 N5 O3 S Cl2
	427.0268	-0.1	-0.2	5.0	762.9	C16 H23 N O2 S3 Cl2

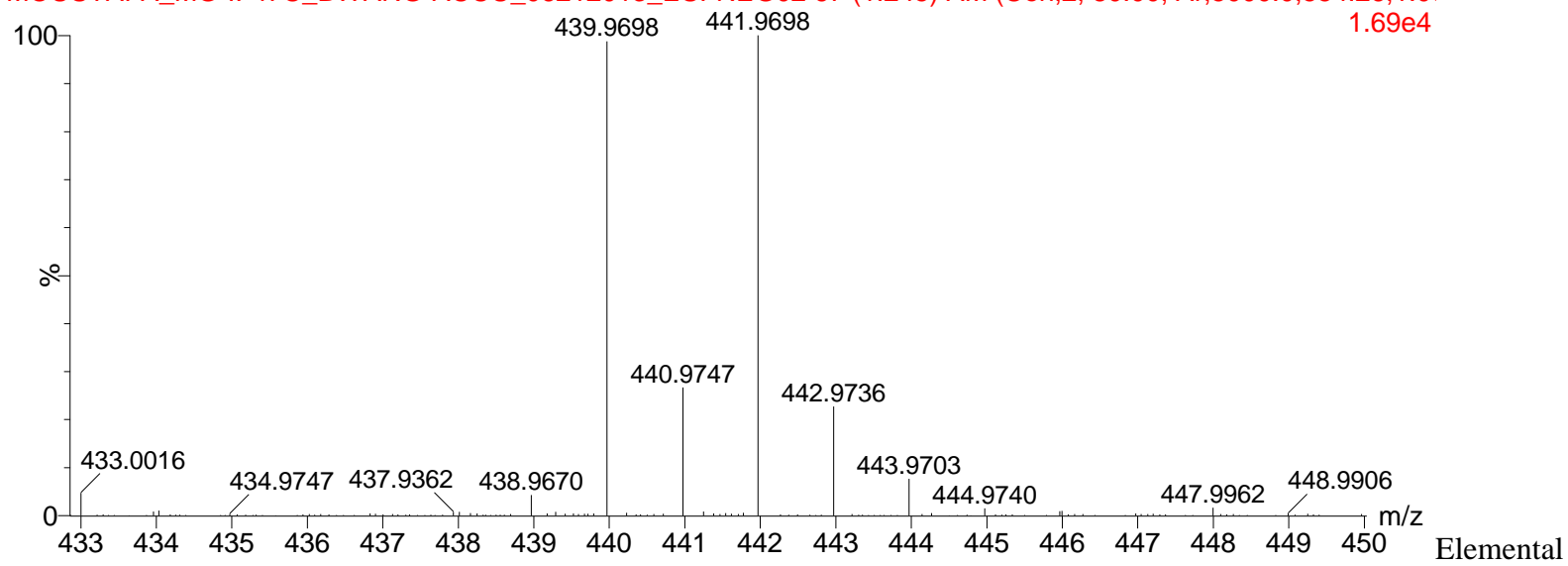
427.0254	1.3	3.0	16.0	1.3	C17 H10 N7 O3 S Cl
427.0250	1.7	4.0	10.0	51.5	C17 H18 N3 O2 S3 Cl
427.0286	-1.9	-4.4	10.5	530.0	C18 H17 N2 O4 S Cl2
427.0268	-0.1	-0.2	15.5	0.5	C19 H12 N4 O4 S Cl
427.0255	1.2	2.8	3.0	336.3	C2 H14 N15 O3 S3 Cl
427.0246	2.1	4.9	-1.5	481.1	C2 H16 N8 O13 S Cl
427.0278	-1.1	-2.6	-1.5	986.0	C2 H17 N10 O9 S Cl2
427.0259	0.8	1.9	9.0	288.5	C2 H6 N19 O4 S Cl
427.0281	-1.4	-3.3	15.0	4.5	C21 H14 N O5 S Cl
427.0259	0.8	1.9	3.5	346.4	C3 H12 N12 O9 S Cl
427.0268	-0.1	-0.2	2.5	287.4	C4 H16 N12 O4 S3 Cl
427.0273	-0.6	-1.4	8.5	234.8	C4 H8 N16 O5 S Cl
427.0273	-0.6	-1.4	3.0	287.8	C5 H14 N9 O10 S Cl
427.0286	-1.9	-4.4	13.5	146.6	C5 H4 N20 O S Cl
427.0286	-1.9	-4.4	8.0	187.8	C6 H10 N13 O6 S Cl
427.0253	1.4	3.3	2.5	869.4	C6 H17 N10 O4 S2 Cl2
427.0282	-1.5	-3.5	2.0	244.6	C6 H18 N9 O5 S3 Cl
427.0286	-1.9	-4.4	2.5	236.0	C7 H16 N6 O11 S Cl
427.0266	0.1	0.2	2.0	834.4	C8 H19 N7 O5 S2 Cl2
427.0248	1.9	4.4	7.0	121.7	C9 H14 N9 O5 S2 Cl
427.0280	-1.3	-3.0	7.0	744.5	C9 H15 N11 O S2 Cl2



5i

21-Jun-2013 15:20:04

MOUSTAFA\_MG-II-47C\_BWANG-ACCU\_06212013\_ESI-NEG02 67 (1.245) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.00  
1.69e4



Elemental  
Composition Report

Single Mass Analysis



Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

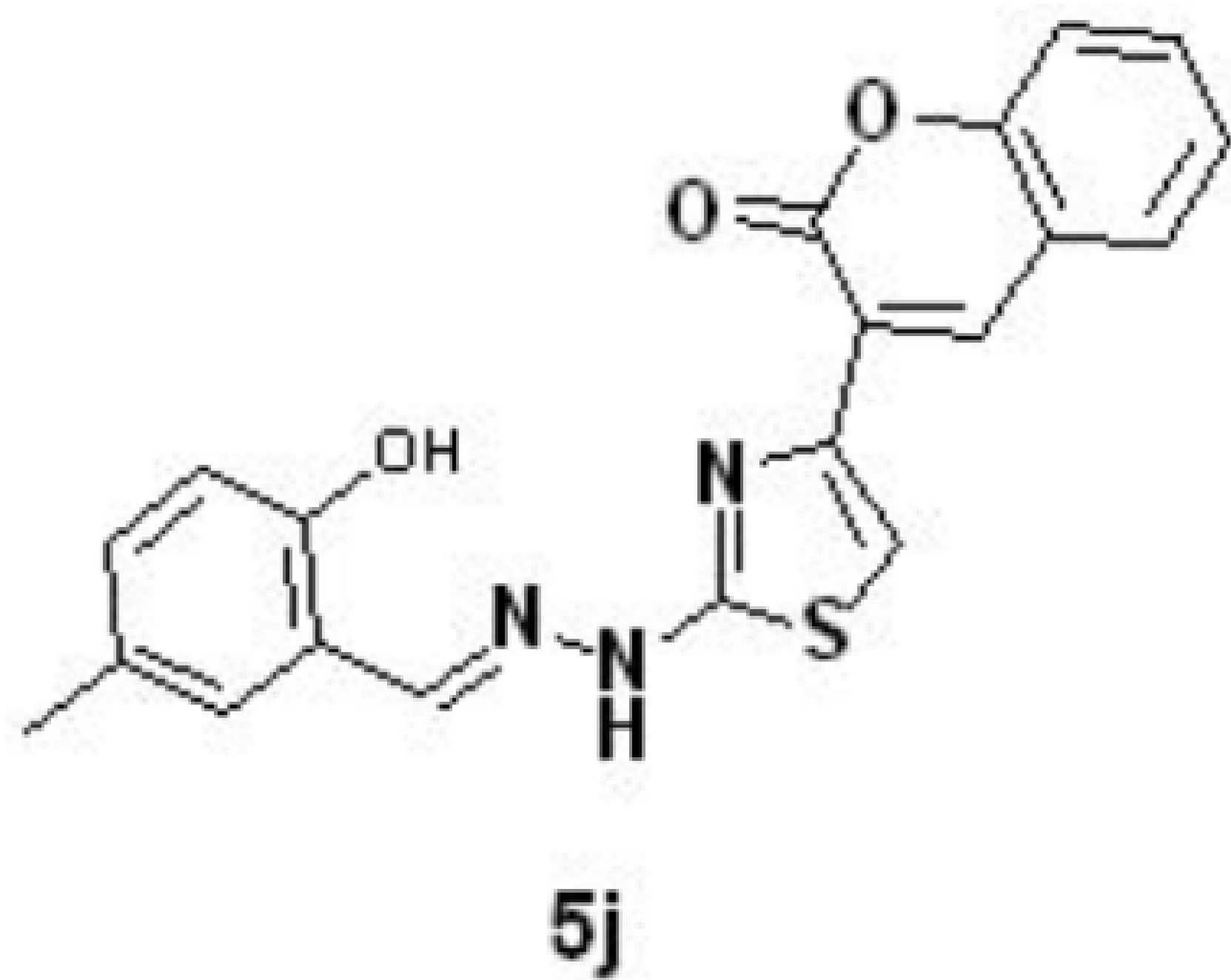
Monoisotopic Mass, Even Electron Ions

1335 formula(e) evaluated with 11 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-2 Br: 1-2

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
439.9698	439.9685	1.3	3.0	1.5	598.0	C10 H19 N O9 S2 Br
	439.9677	2.1	4.8	-0.5	2775.7	C10 H24 N3 O2 S2 Br2
	439.9698	0.0	0.0	6.5	412.5	C11 H15 N5 O5 S2 Br
	439.9711	-1.3	-3.0	11.5	263.7	C12 H11 N9 O S2 Br
	439.9678	2.0	4.5	16.5	125.2	C15 H7 N9 O S Br
	439.9704	-0.6	-1.4	15.5	53.6	C19 H11 N3 O3 S Br
	439.9683	1.5	3.4	-1.5	1343.1	C2 H15 N7 O12 S Br
	439.9696	0.2	0.5	3.5	1046.8	C3 H11 N11 O8 S Br
	439.9688	1.0	2.3	1.5	3033.5	C3 H16 N13 O S Br2
	439.9710	-1.2	-2.7	8.5	787.3	C4 H7 N15 O4 S Br
	439.9715	-1.7	-3.9	0.5	2855.8	C7 H20 N7 O3 S Br2

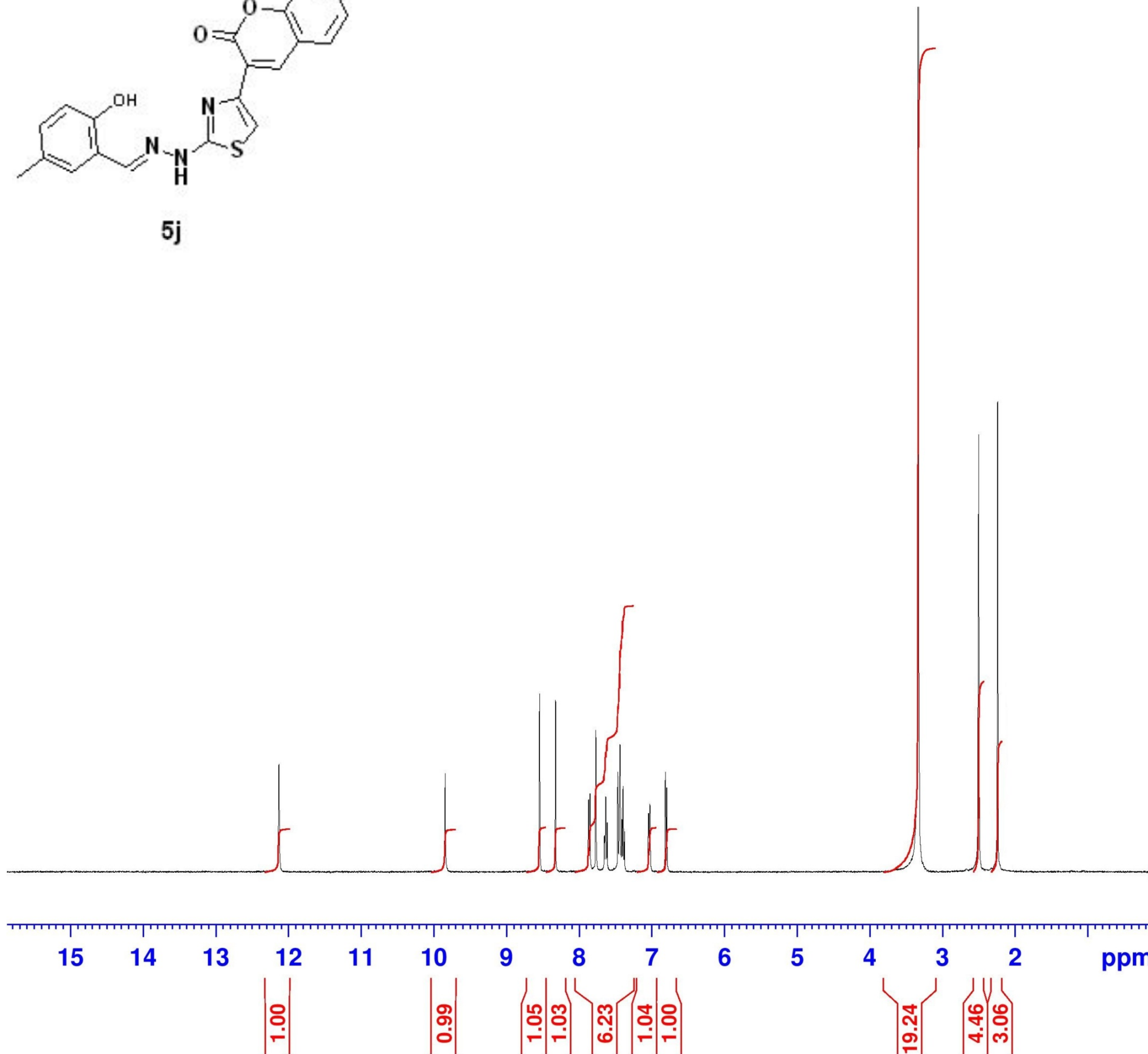


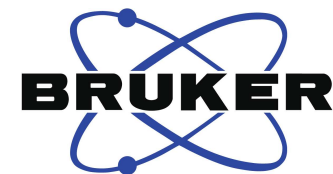
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 PROCNO 1

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 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 181  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
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 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
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 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
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EXPNO 1  
PROCNO 1

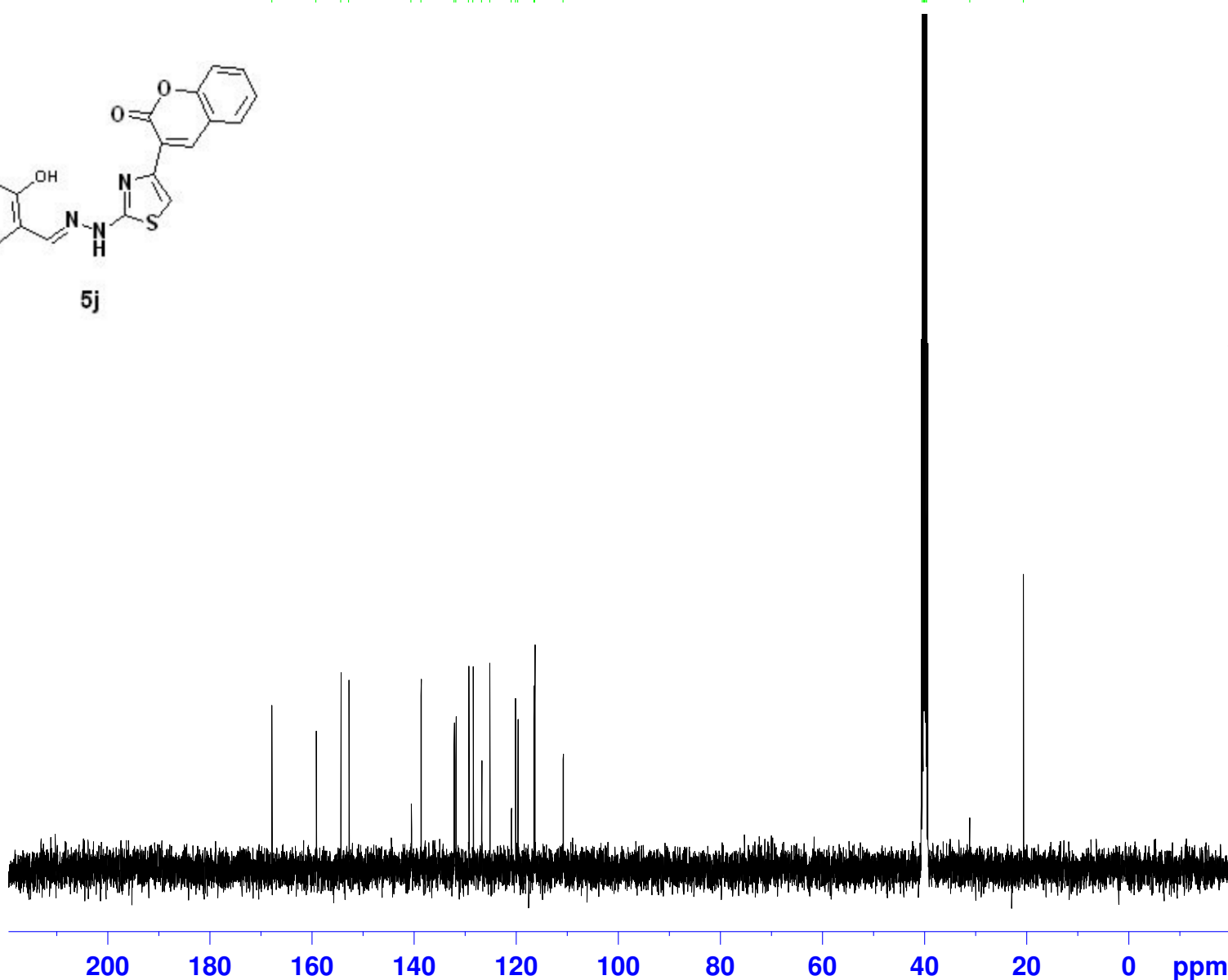
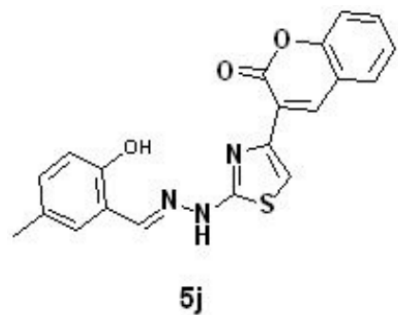
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PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 187  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 161  
DW 20.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
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PLW1 62.00000000 W

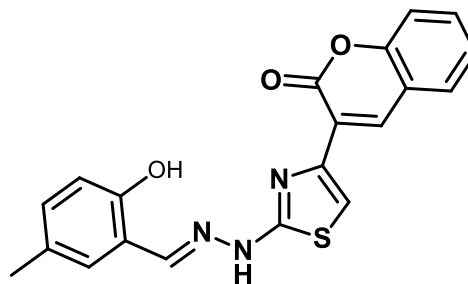
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NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

167.88  
159.20  
154.36  
152.77  
140.57  
138.64  
132.15  
131.81  
129.28  
128.43  
126.74  
125.17  
120.96  
120.14  
119.64  
116.52  
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40.40  
40.19  
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39.77  
39.57  
31.15  
20.62



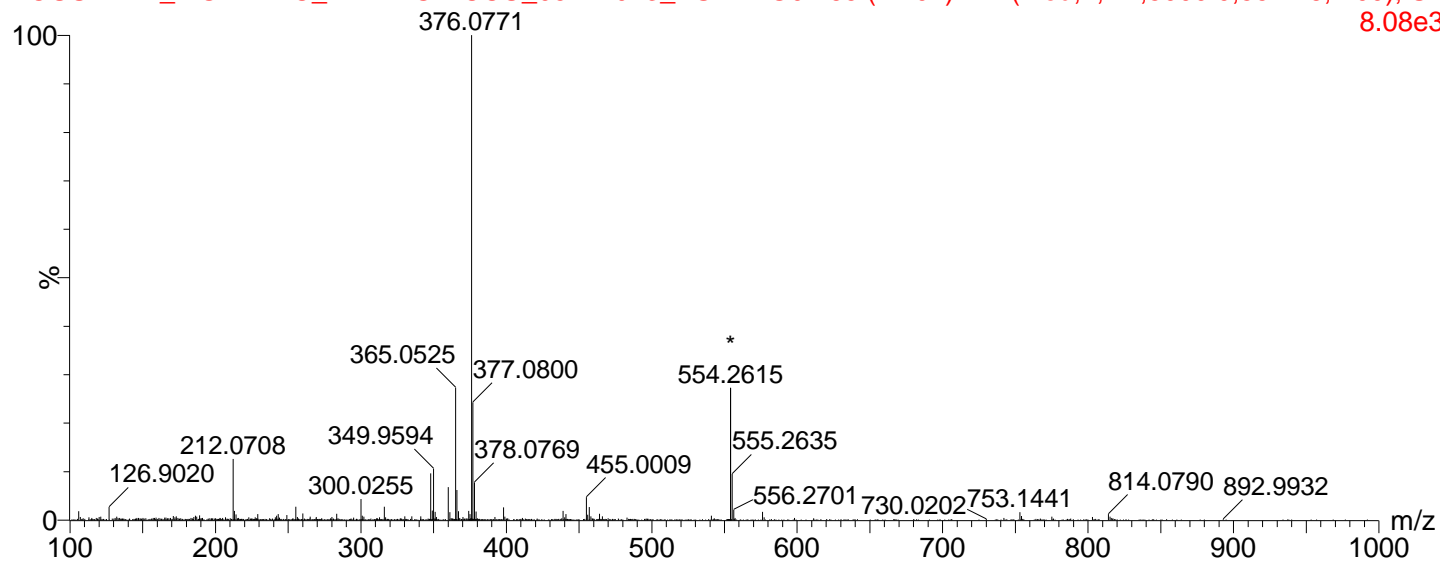




5j

15-May-2013 12:45:47

MOUSTAF A\_MG-I-121C\_BWANG-ACCU\_05142013\_ESI-NEG01 65 (1.204) AM (Med,2, Ar,5000.0,554.26,1.00); Sm  
8.08e3



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1659 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-4

Minimum:

-1.5

Maximum:

5.0

5.0

50.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

376.0771

376.0781

-1.0

-2.7

-1.5

525.5

C H18 N11 O8 S2

376.0763

0.8

2.1

11.5

88.8

C13 H14 N9 O S2

376.0790

-1.9

-5.1

10.5

89.9

C17 H18 N3 O3 S2

376.0756

1.5

4.0

15.5

0.6

C20 H14 N3 O3 S

376.0761

1.0

2.7

8.5

240.8

C5 H10 N15 O4 S

376.0756

1.5

4.0

2.5

470.8

C5 H18 N11 O3 S3

376.0774

-0.3

-0.8

2.5

229.5

C8 H18 N5 O10 S

376.0788

-1.7

-4.5

7.5

147.6

C9 H14 N9 O6 S

376.0783

-1.2

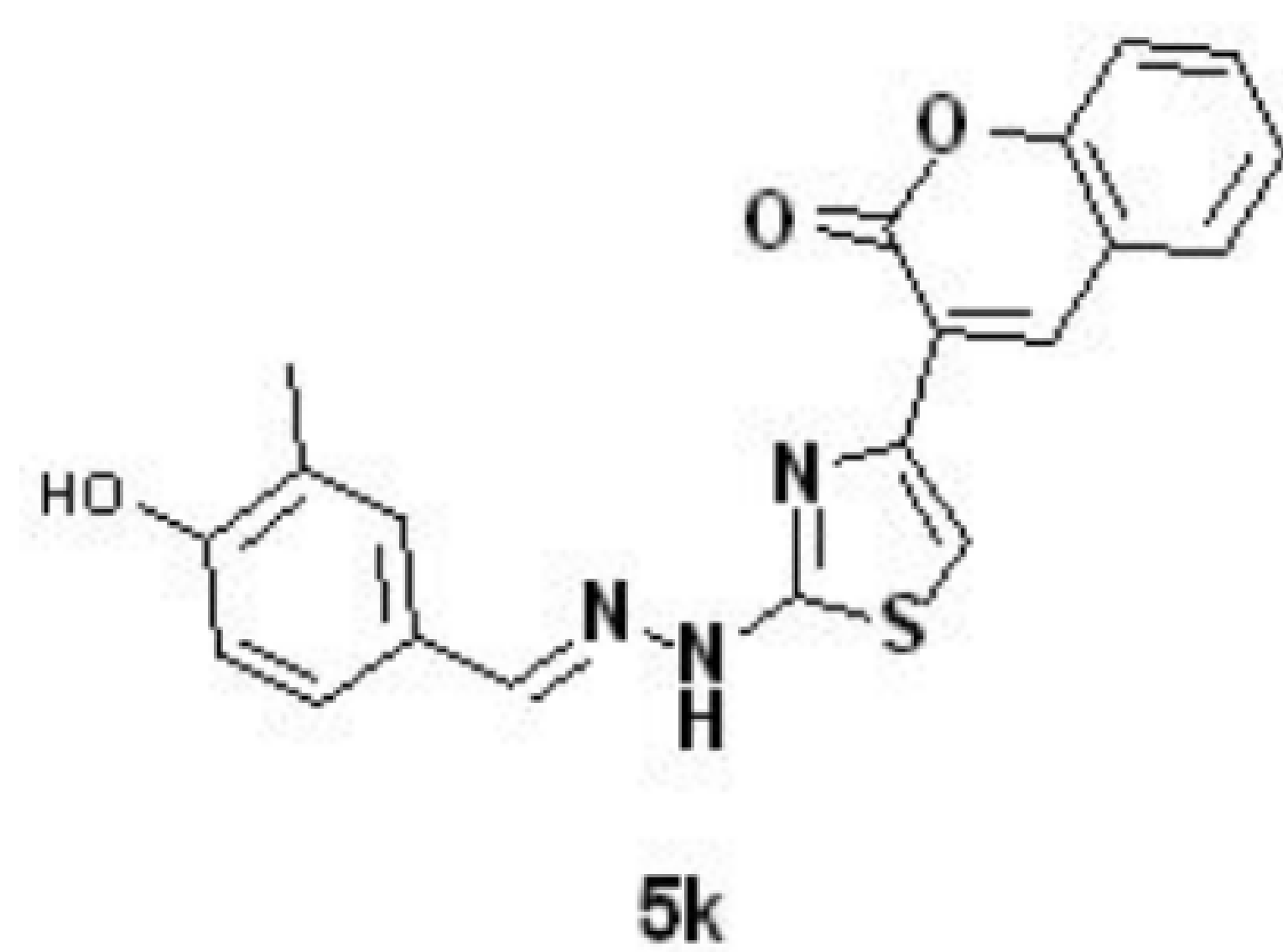
-3.2

1.5

427.7

C9 H22 N5 O5 S3



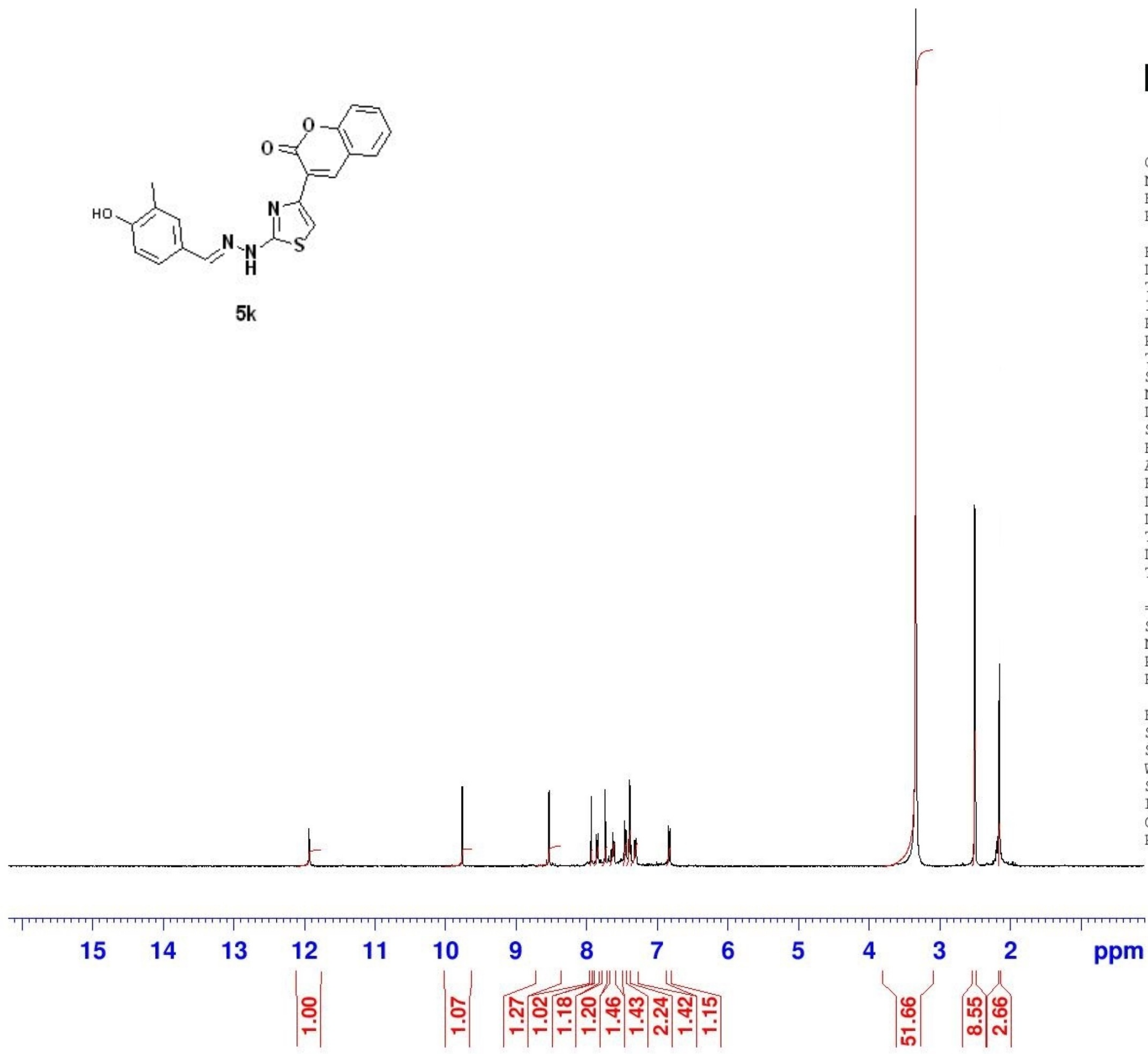


Current Data Parameters  
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 EXPNO 1  
 PROCNO 1

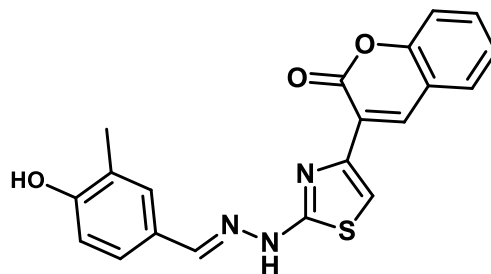
F2 - Acquisition Parameters  
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 Time 18.27  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 181  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
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 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.40



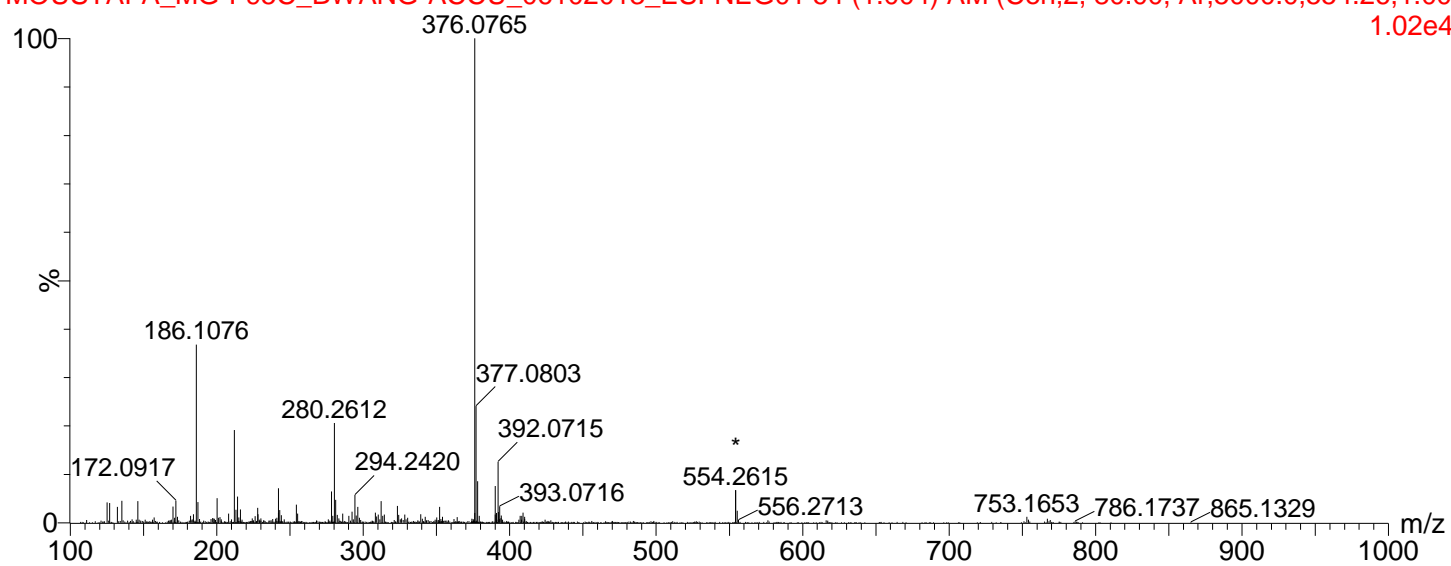




5k

10-Jun-2013 16:46:36

MOUSTAFA\_MG-I-95C\_BWANG-ACCU\_06102013\_ESI-NEG01 54 (1.004) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.00)  
1.02e4



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

1078 formula(e) evaluated with 12 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-2

Minimum:

-1.5

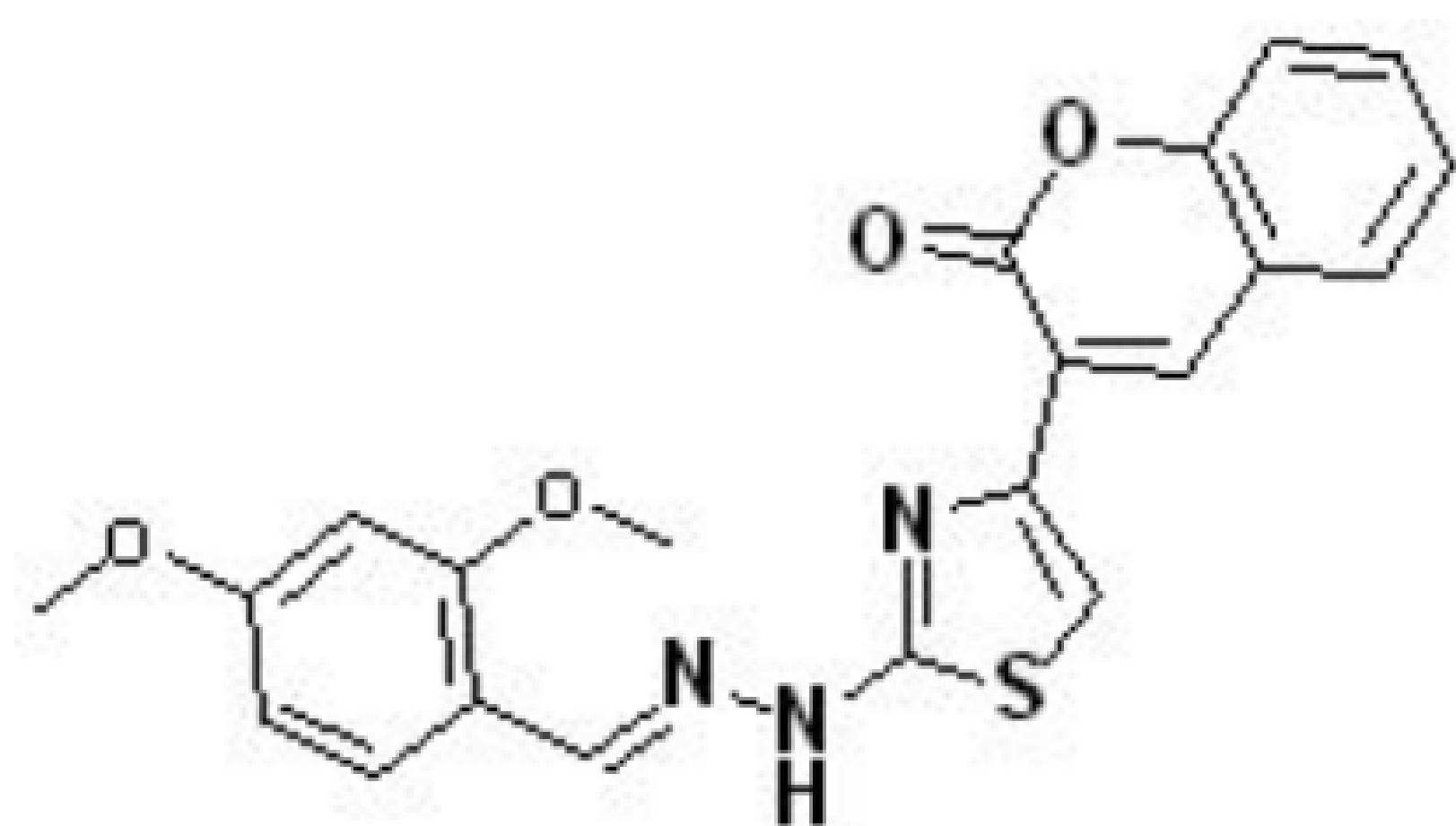
Maximum: 5.0

5.0

100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
376.0765	376.0781	-1.6	-4.3	-1.5	620.9	C H18 N11 O8 S2
	376.0749	1.6	4.3	6.5	144.3	C12 H18 N5 O5 S2
	376.0763	0.2	0.5	11.5	76.0	C13 H14 N9 O S2
	376.0763	0.2	0.5	6.0	127.1	C14 H20 N2 O6 S2
	376.0776	-1.1	-2.9	11.0	69.7	C15 H16 N6 O2 S2
	376.0756	0.9	2.4	15.5	2.9	C20 H14 N3 O3 S
	376.0747	1.8	4.8	9.0	386.1	C3 H8 N18 O3 S
	376.0748	1.7	4.5	3.5	431.3	C4 H14 N11 O8 S
	376.0761	0.4	1.1	8.5	311.2	C5 H10 N15 O4 S
	376.0761	0.4	1.1	3.0	354.3	C6 H16 N8 O9 S
	376.0774	-0.9	-2.4	8.0	246.4	C7 H12 N12 O5 S
	376.0774	-0.9	-2.4	2.5	287.0	C8 H18 N5 O10 S





5I

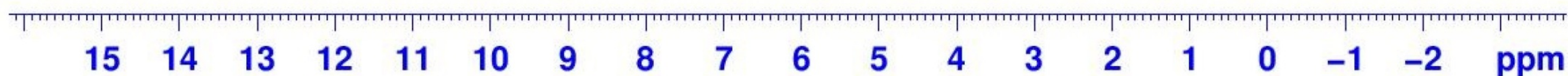
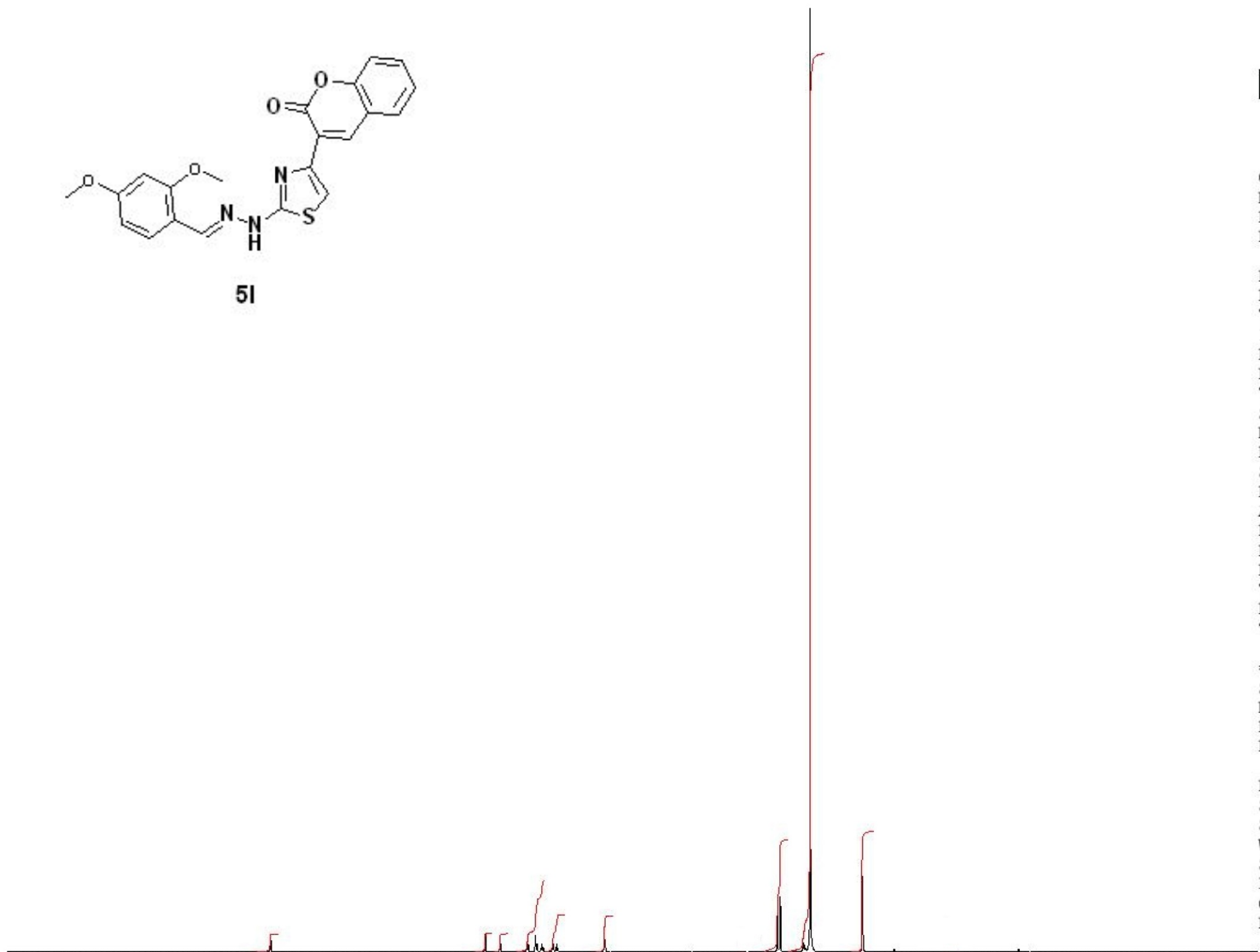


Current Data Parameters  
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 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130227  
 Time 18.41  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 181  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

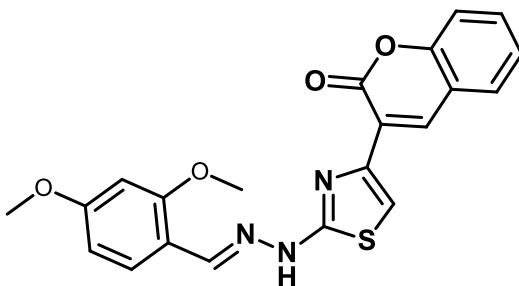
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 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.40



1.00  
 1.05  
 1.02  
 4.05  
 2.09  
 2.00  
 6.33  
 50.65  
 6.83



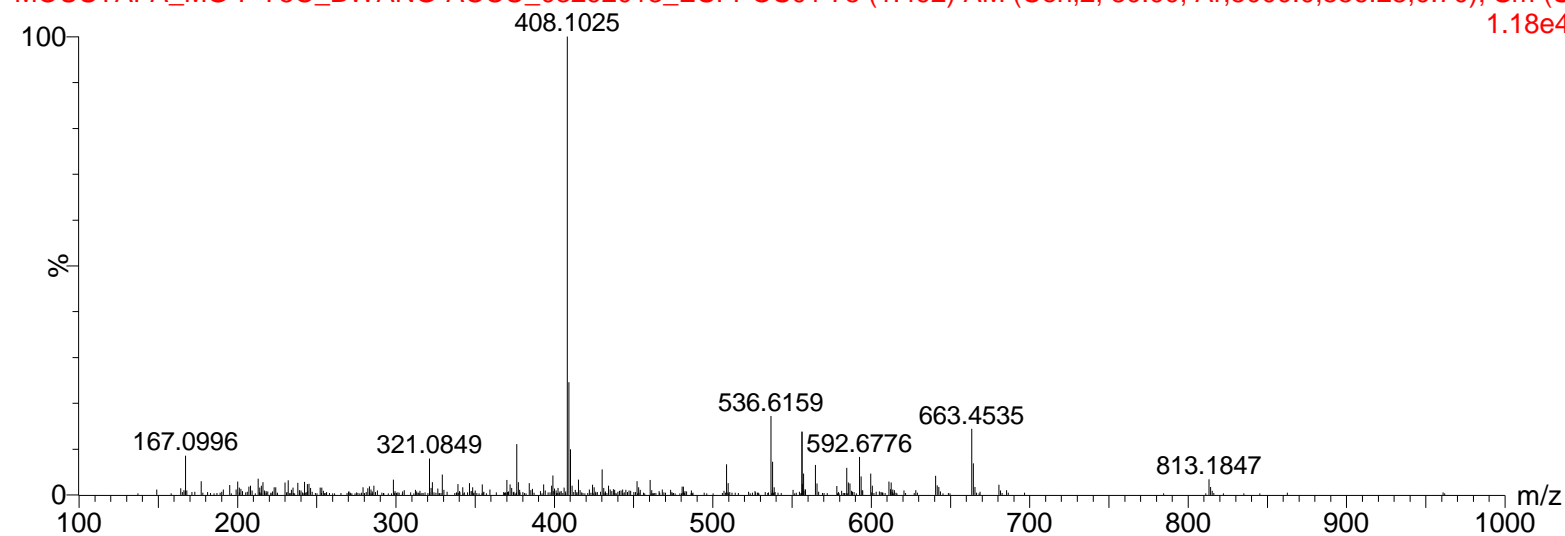


5I

80% ACN

16:09:16 29-Mar-2013

MOUSTAFA\_MG-I--75C\_BWANG-ACCU\_03292013\_ESI-POS01 75 (1.492) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (Si) 1.18e4



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

2791 formula(e) evaluated with 24 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-10

Minimum:

-1.5

Maximum:

5.0

5.0

50.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

408.1025

408.1037

-1.2

-2.9

1.5

303.6

C9 H22 N5 O11 S

408.1045

-2.0

-4.9

6.0

279.4

C9 H20 N12 O S3

408.1032

-0.7

-1.7

1.0

403.6

C8 H24 N8 O5 S3

408.1036

-1.1

-2.7

7.0

270.6

C8 H16 N12 O6 S

408.1023

0.2

0.5

2.0

379.2

C7 H20 N8 O10 S

408.1036

-1.1

-2.7

12.5

254.1

C7 H10 N19 O S

408.1018

0.7

1.7

1.5

443.0

C6 H22 N11 O4 S3

408.1023

0.2

0.5

7.5

343.0

C6 H14 N15 O5 S

408.1010

1.5

3.7

2.5

464.9

C5 H18 N11 O9 S

408.1005

2.0

4.9

2.0

491.8

C4 H20 N14 O3 S3

408.1010

1.5

3.7

8.0

425.6

C4 H12 N18 O4 S

408.1045

-2.0

-4.9

19.0

52.7

C24 H16 N4 O S

408.1018

0.7

1.7

14.5

16.6

C21 H18 N3 O4 S

408.1005

2.0

4.9

15.0

23.7

C19 H16 N6 O3 S

408.1034

-0.9

-2.2

4.0

538.8

C16 H28 N2 O2 S4

408.1038

-1.3

-3.2

10.0

37.2

C16 H20 N6 O3 S2

408.1025

0.0

0.0

5.0

86.7

C15 H24 N2 O7 S2

408.1020

0.5

1.2

4.5

528.1

C14 H26 N5 O S4

408.1025

0.0

0.0

10.5

45.3

C14 H18 N9 O2 S2

408.1007

1.8

4.4

-0.5

628.3

C13 H30 N O5 S4

408.1012

1.3

3.2

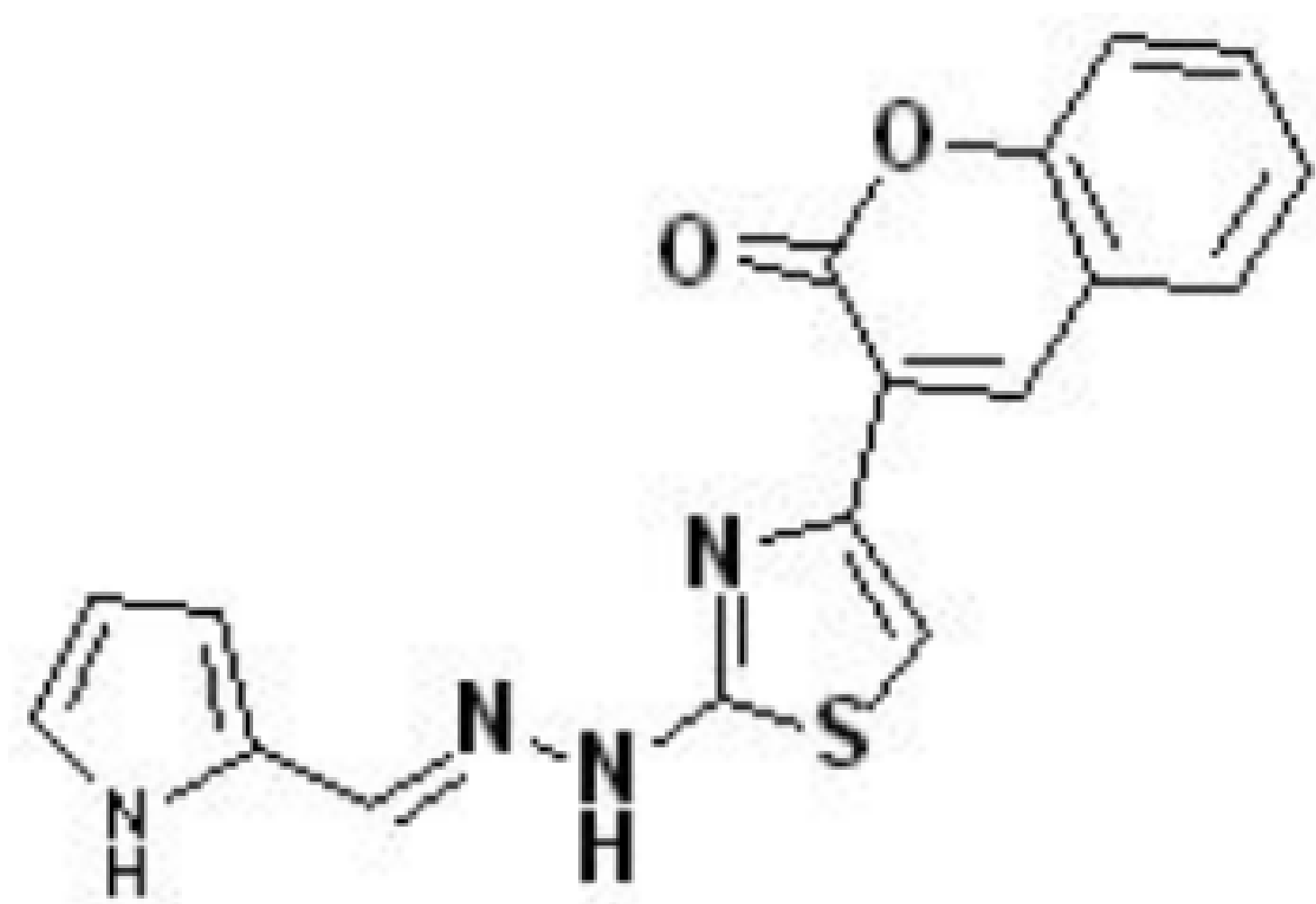
5.5

106.9

C13 H22 N5 O6 S2

408.1011	1.4	3.4	11.0	62.2	C12 H16 N12 O S2
408.1045	-2.0	-4.9	0.5	373.7	C10 H26 N5 O6 S3
408.1043	-1.8	-4.4	3.0	516.6	C H16 N18 O4 S2





5m

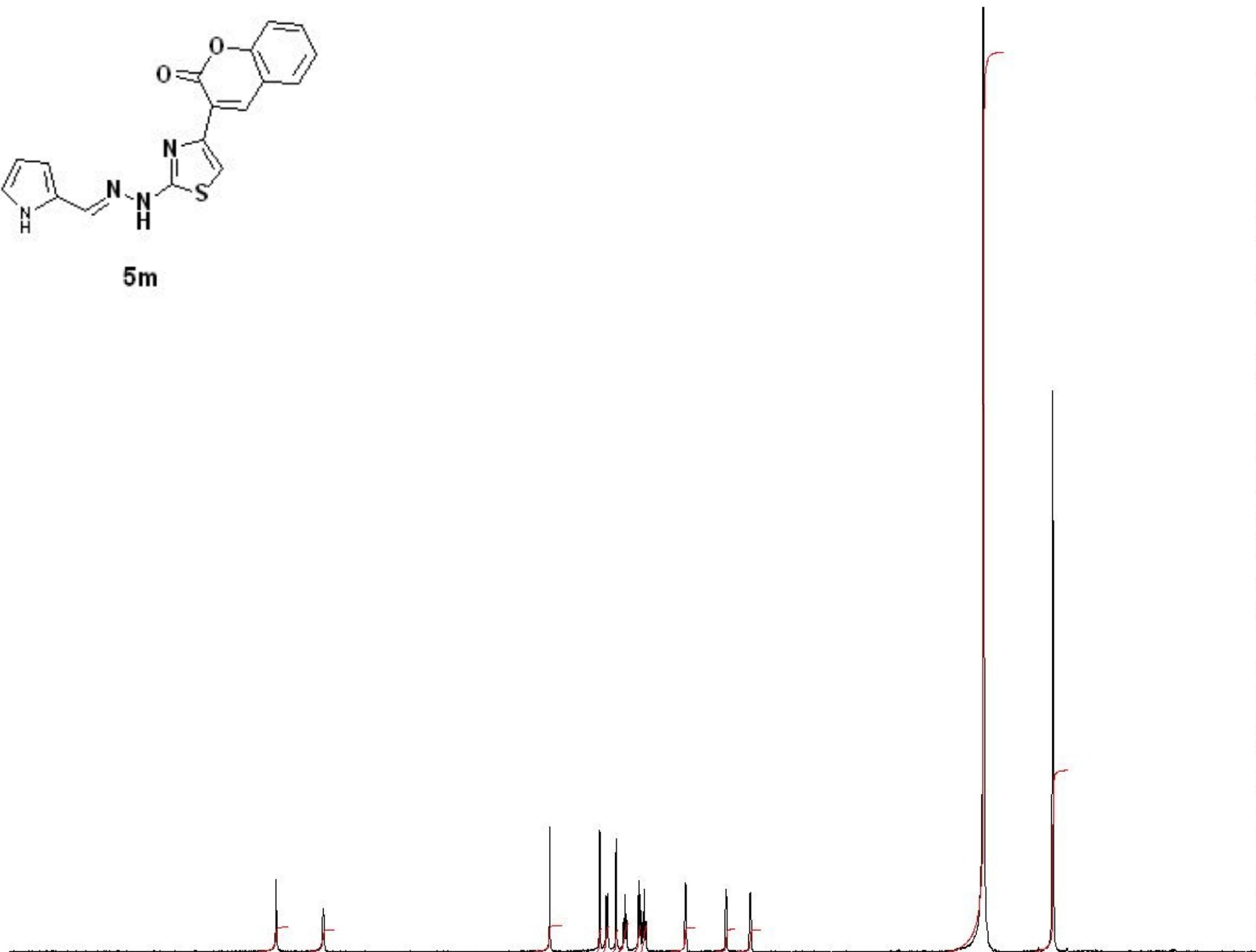


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 PROCNO 1

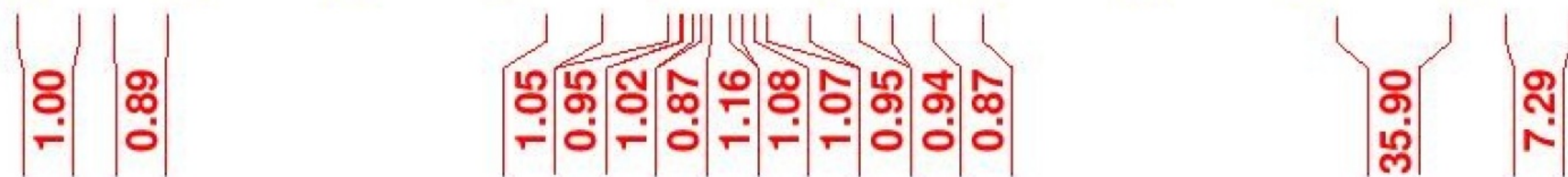
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 PULPROG zg30  
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 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 181  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 297.9 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
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 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

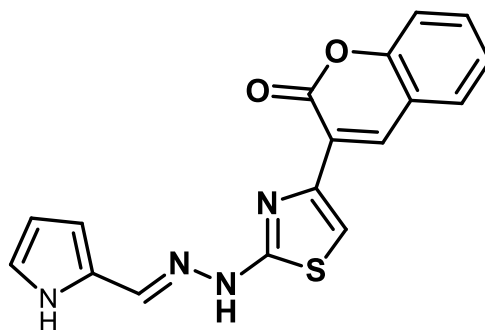
F2 - Processing parameters  
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 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm



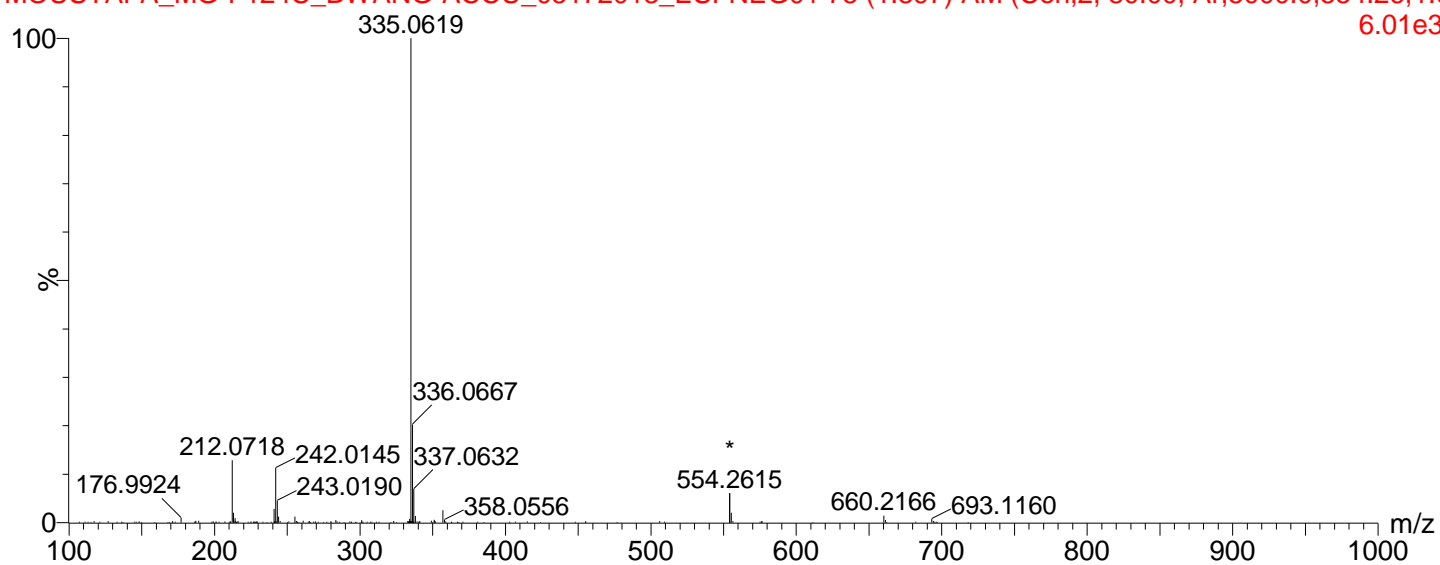




5m

17-May-2013 15:20:56

MOUSTAFA\_MG-I-124C\_BWANG-ACCU\_05172013\_ESI-NEG01 75 (1.397) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.0  
6.01e3



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

1139 formula(e) evaluated with 13 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-4

Minimum:

-1.5

Maximum:

5.0

5.0

50.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

335.0619

335.0610

0.9

2.7

5.0

106.0

C11 H17 N3 O5 S2

335.0623

-0.4

-1.2

10.0

65.0

C12 H13 N7 O S2

335.0603

1.6

4.8

14.5

2.6

C17 H11 N4 O2 S

335.0616

0.3

0.9

14.0

7.6

C19 H13 N O3 S

335.0603

1.6

4.8

1.5

383.9

C2 H15 N12 O2 S3

335.0608

1.1

3.3

7.5

184.1

C2 H7 N16 O3 S

335.0608

1.1

3.3

2.0

219.0

C3 H13 N9 O8 S

335.0617

0.2

0.6

1.0

362.0

C4 H17 N9 O3 S3

335.0621

-0.2

-0.6

7.0

142.8

C4 H9 N13 O4 S

335.0621

-0.2

-0.6

1.5

175.9

C5 H15 N6 O9 S

335.0635

-1.6

-4.8

6.5

107.9

C6 H11 N10 O5 S

335.0630

-1.1

-3.3

0.5

345.4

C6 H19 N6 O4 S3

335.0635

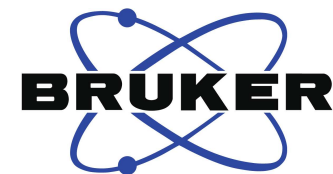
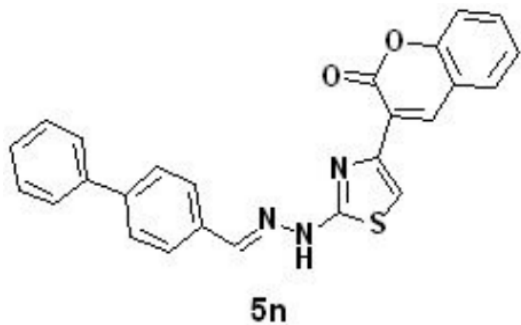
-1.6

-4.8

1.0

139.2

C7 H17 N3 O10 S

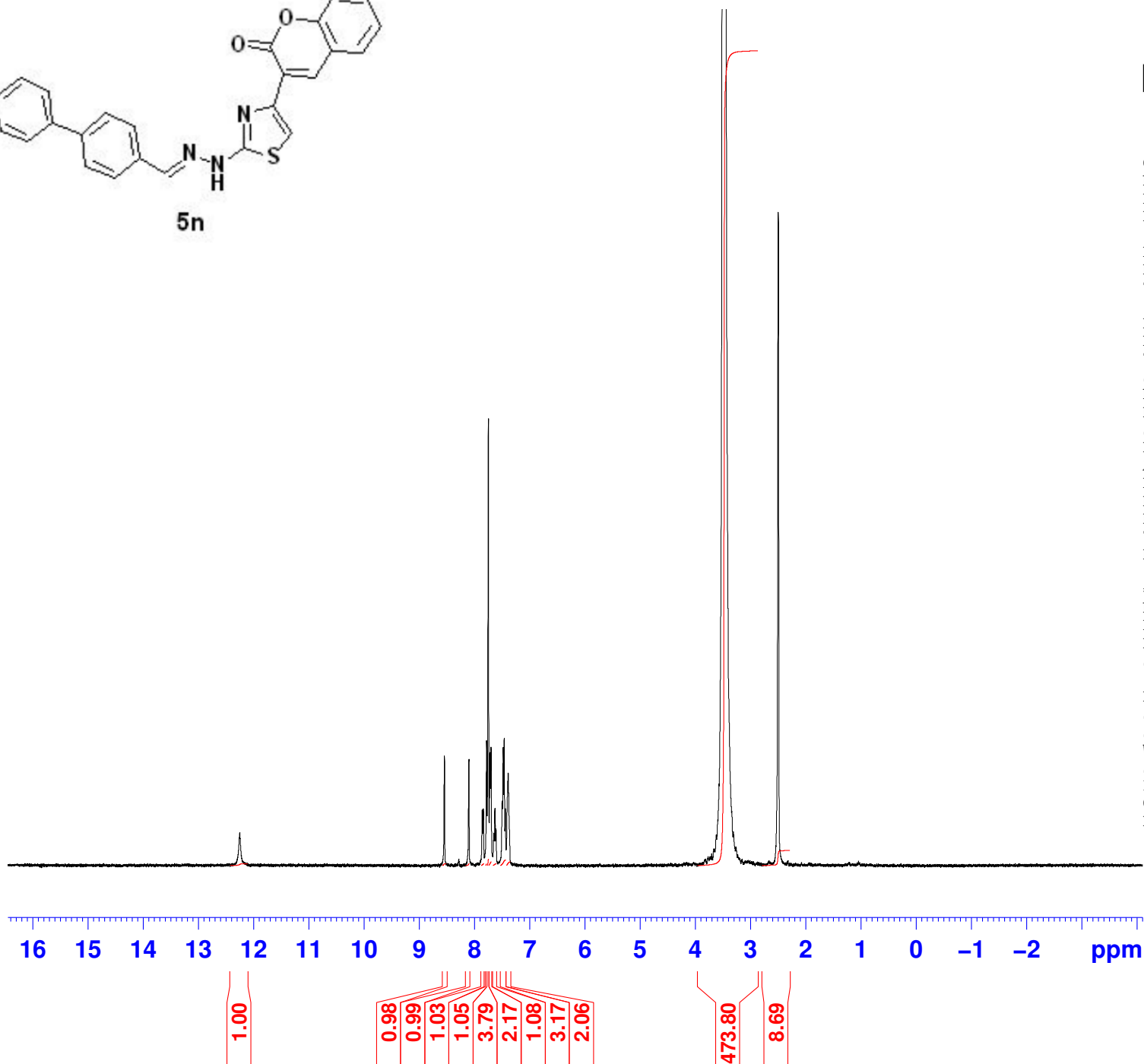


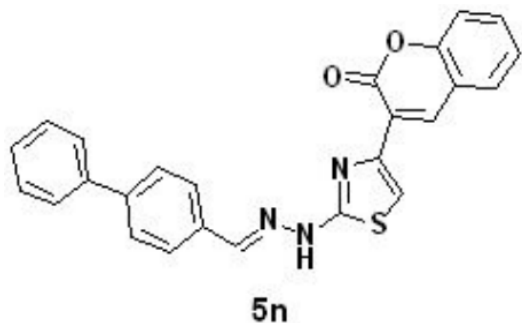
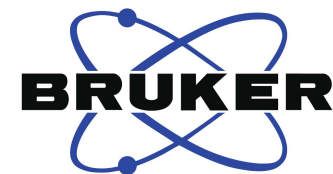
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 PROCNO 1

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 Time 18.27  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 64  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 294.4 K  
 D1 1.00000000 sec

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 P1 13.50 usec  
 PLW1 16.00000000 W  
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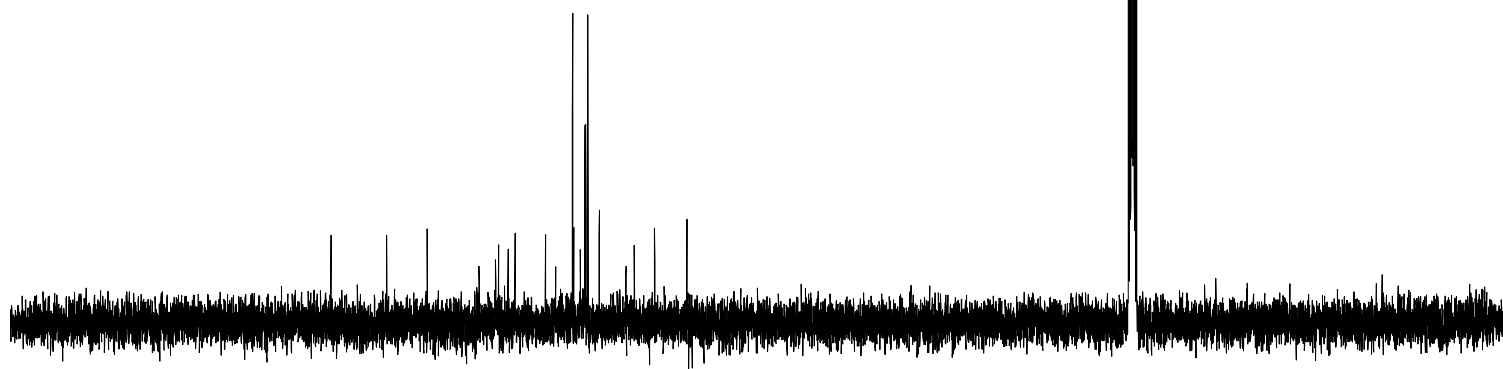
F2 - Processing parameters  
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 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





168.15  
159.26  
152.76  
144.47  
141.82  
141.33  
139.83  
138.68  
133.84  
132.20  
129.50  
129.27  
128.26  
127.53  
127.38  
127.06  
125.23  
120.96  
119.61  
116.36  
111.18

40.07  
39.86  
39.65



200 180 160 140 120 100 80 60 40 20 0 ppm

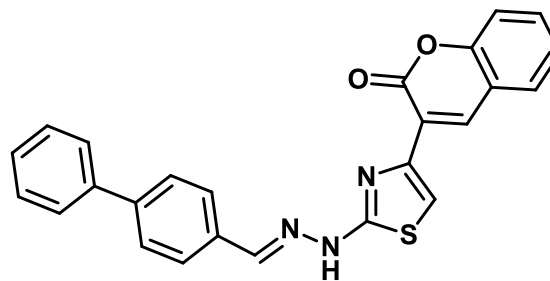
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PROCNO 1

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INSTRUM spect  
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PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 157  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 181  
DW 20.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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SFO1 100.6253441 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W

==== CHANNEL f2 =====  
SFO2 400.1416006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
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PLW12 0.36000001 W  
PLW13 0.29159999 W

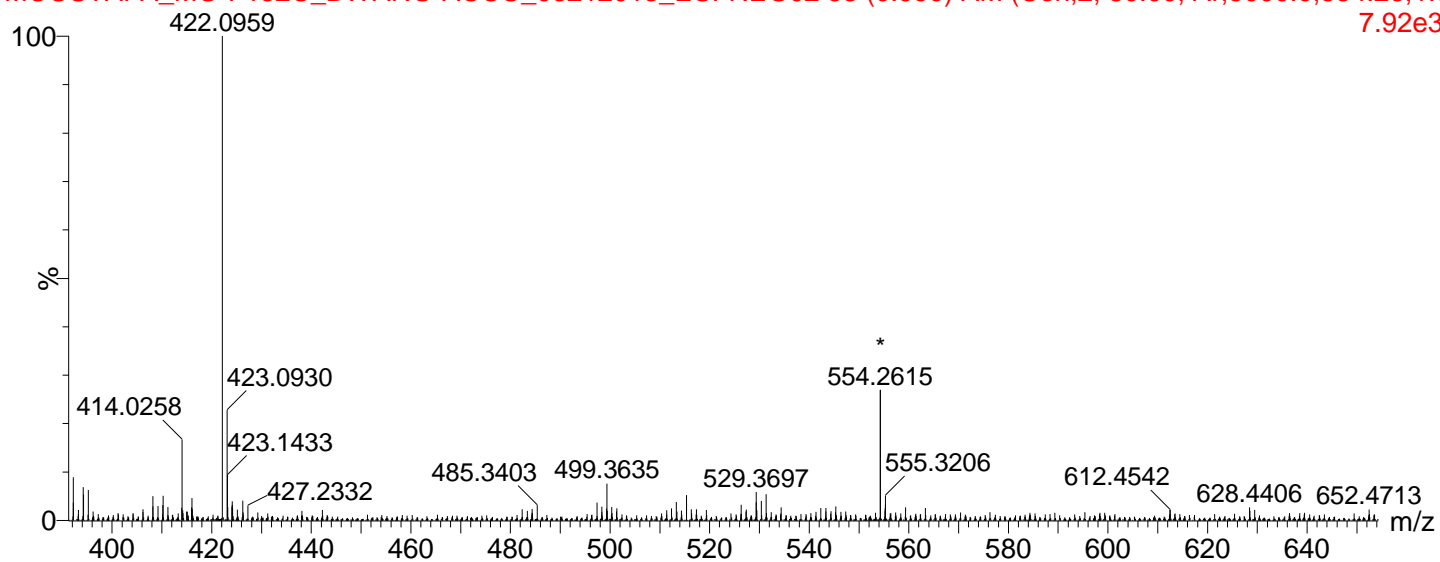
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SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



5n

21-Jun-2013 15:03:59

MOUSTAFA\_MG-I-152C\_BWANG-ACCU\_06212013\_ESI-NEG02 53 (0.990) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.0  
7.92e3



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

1556 formula(e) evaluated with 19 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-2

Minimum:

-1.5

Maximum:

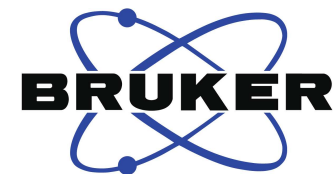
5.0

5.0

100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
422.0959	422.0955	0.4	0.9	7.5	187.9	C9 H16 N11 O7 S
	422.0942	1.7	4.0	2.5	290.0	C8 H20 N7 O11 S
	422.0955	0.4	0.9	13.0	116.6	C8 H10 N18 O2 S
	422.0941	1.8	4.3	8.0	200.0	C7 H14 N14 O6 S
	422.0941	1.8	4.3	13.5	128.1	C6 H8 N21 O S
	422.0975	-1.6	-3.8	3.0	630.3	C4 H18 N14 O6 S2
	422.0975	-1.6	-3.8	8.5	499.4	C3 H12 N21 O S2
	422.0963	-0.4	-0.9	19.5	253.7	C25 H16 N3 O2 S
	422.0950	0.9	2.1	20.0	205.7	C23 H14 N6 O S
	422.0962	-0.3	-0.7	3.5	643.9	C2 H16 N17 O5 S2
	422.0970	-1.1	-2.6	10.0	561.7	C19 H22 N2 O5 S2
	422.0957	0.2	0.5	10.5	522.1	C17 H20 N5 O4 S2
	422.0943	1.6	3.8	5.5	586.3	C16 H24 N O8 S2
	422.0943	1.6	3.8	11.0	487.3	C15 H18 N8 O3 S2
	422.0968	-0.9	-2.1	1.5	271.4	C12 H24 N O13 S
	422.0968	-0.9	-2.1	7.0	183.9	C11 H18 N8 O8 S
	422.0955	0.4	0.9	2.0	276.8	C10 H22 N4 O12 S
	422.0968	-0.9	-2.1	12.5	113.1	C10 H12 N15 O3 S
	422.0948	1.1	2.6	-1.5	812.3	C H20 N13 O9 S2



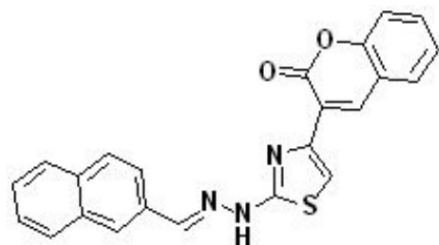


Current Data Parameters  
NAME MG151  
EXPNO 1  
PROCNO 1

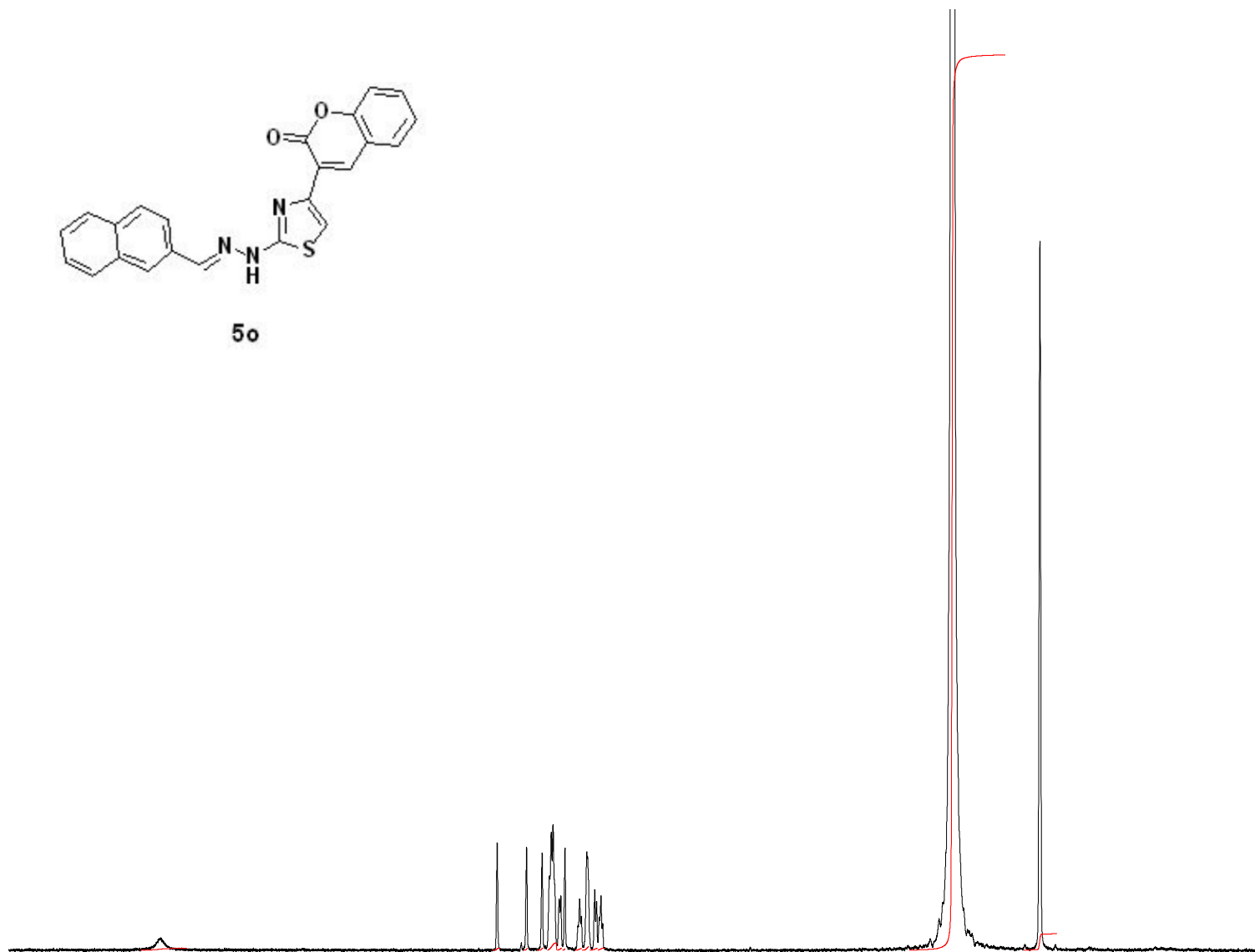
F2 - Acquisition Parameters  
Date\_ 20130417  
Time 18.22  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 64  
DW 60.800 usec  
DE 6.50 usec  
TE 294.4 K  
D1 1.00000000 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SFO1 400.1424710 MHz

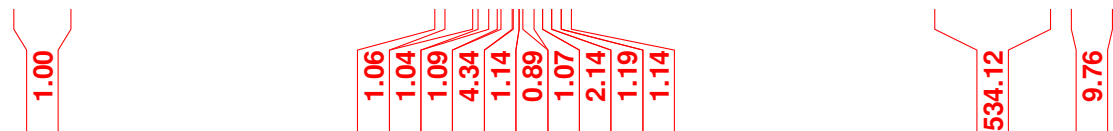
F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

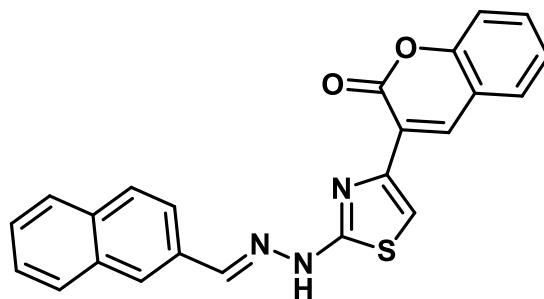


5o



13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

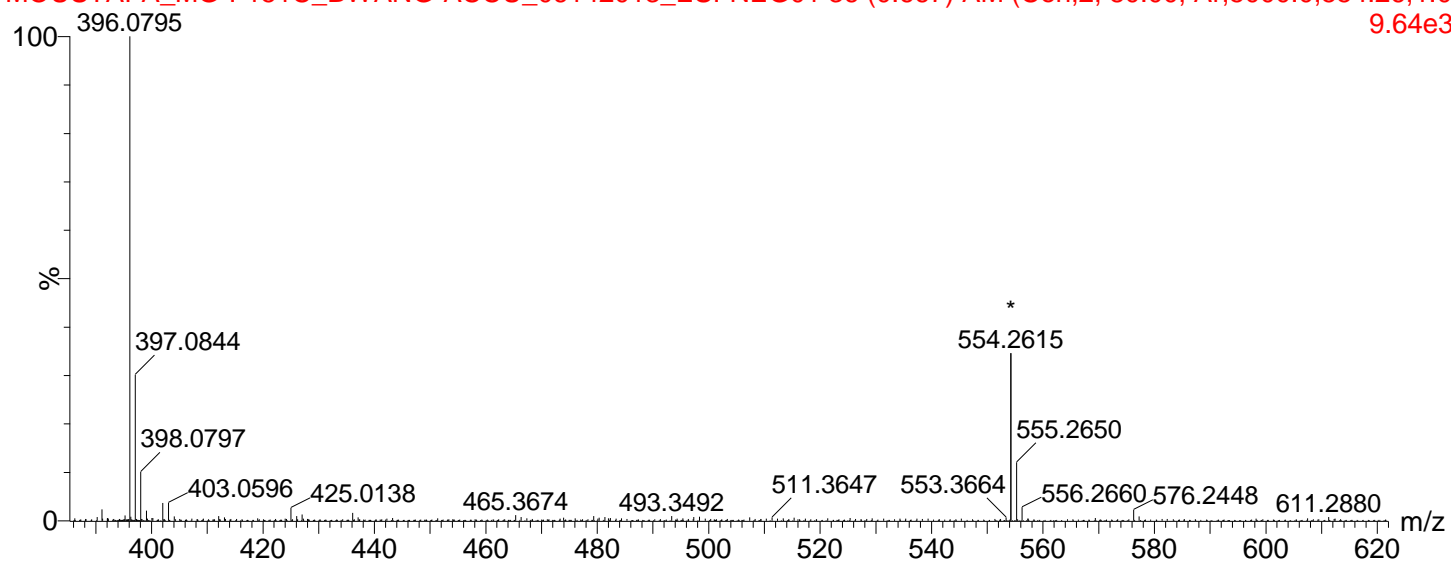




5o

14-Jun-2013 17:23:25

MOUSTAFA\_MG-I-151C\_BWANG-ACCU\_06142013\_ESI-NEG01 36 (0.667) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.0(9.64e3



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1275 formula(e) evaluated with 8 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-2

Minimum:

-1.5

Maximum:

5.0

5.0

100.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

396.0795

396.0812

-1.7

-4.3

0.5

452.2

C10 H22 N O13 S

396.0787

0.8

2.0

4.5

239.5

C14 H22 N O8 S2

396.0800

-0.5

-1.3

9.5

152.3

C15 H18 N5 O4 S2

396.0807

-1.2

-3.0

18.5

16.0

C23 H14 N3 O2 S

396.0785

1.0

2.5

12.5

526.4

C4 H6 N21 O S

396.0785

1.0

2.5

1.5

608.3

C6 H18 N7 O11 S

396.0798

-0.3

-0.8

6.5

480.4

C7 H14 N11 O7 S

396.0812

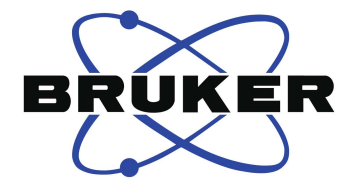
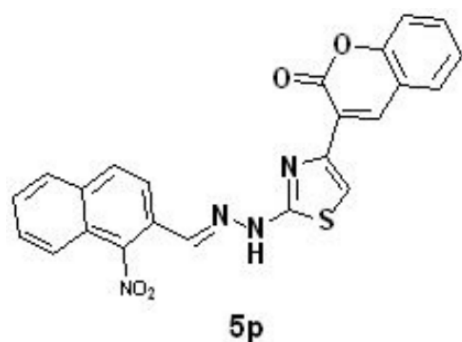
-1.7

-4.3

11.5

375.1

C8 H10 N15 O3 S

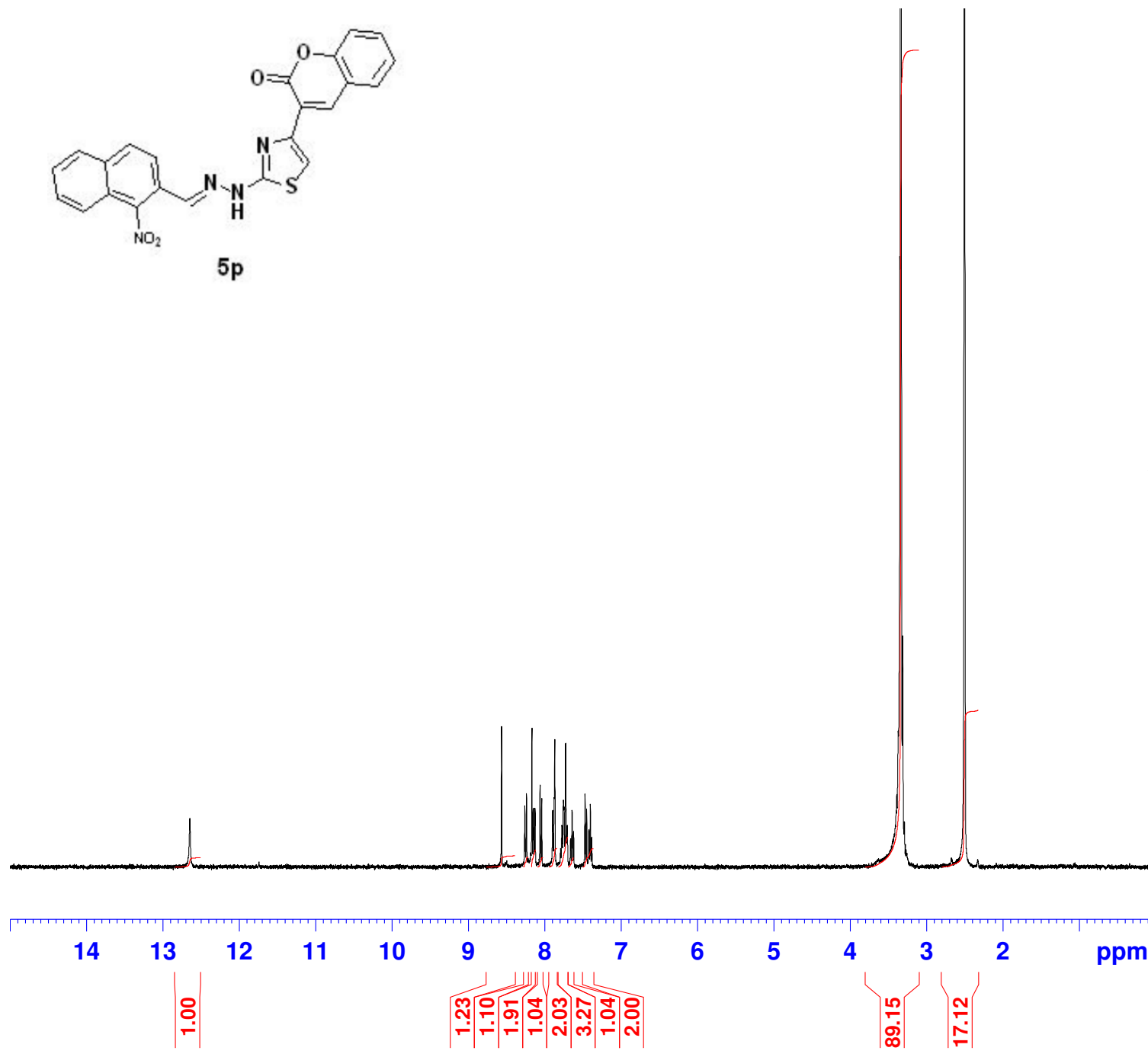


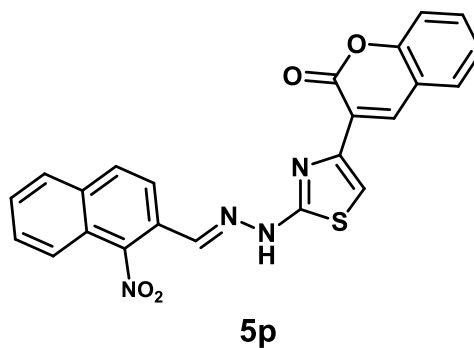
Current Data Parameters  
 NAME MG122p  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130328  
 Time 18.22  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 4  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

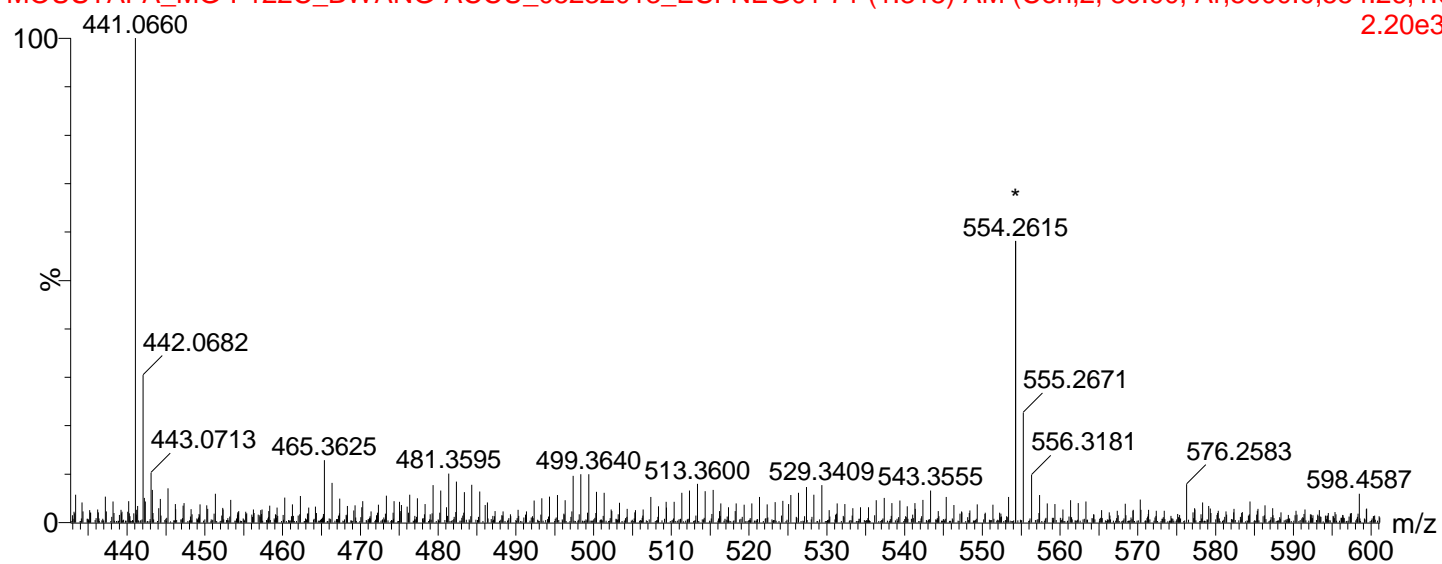
F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.40





23-May-2013 12:33:09

MOUSTAFA\_MG-I-122C\_BWANG-ACCU\_05232013\_ESI-NEG01 71 (1.315) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.0  
2.20e3



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

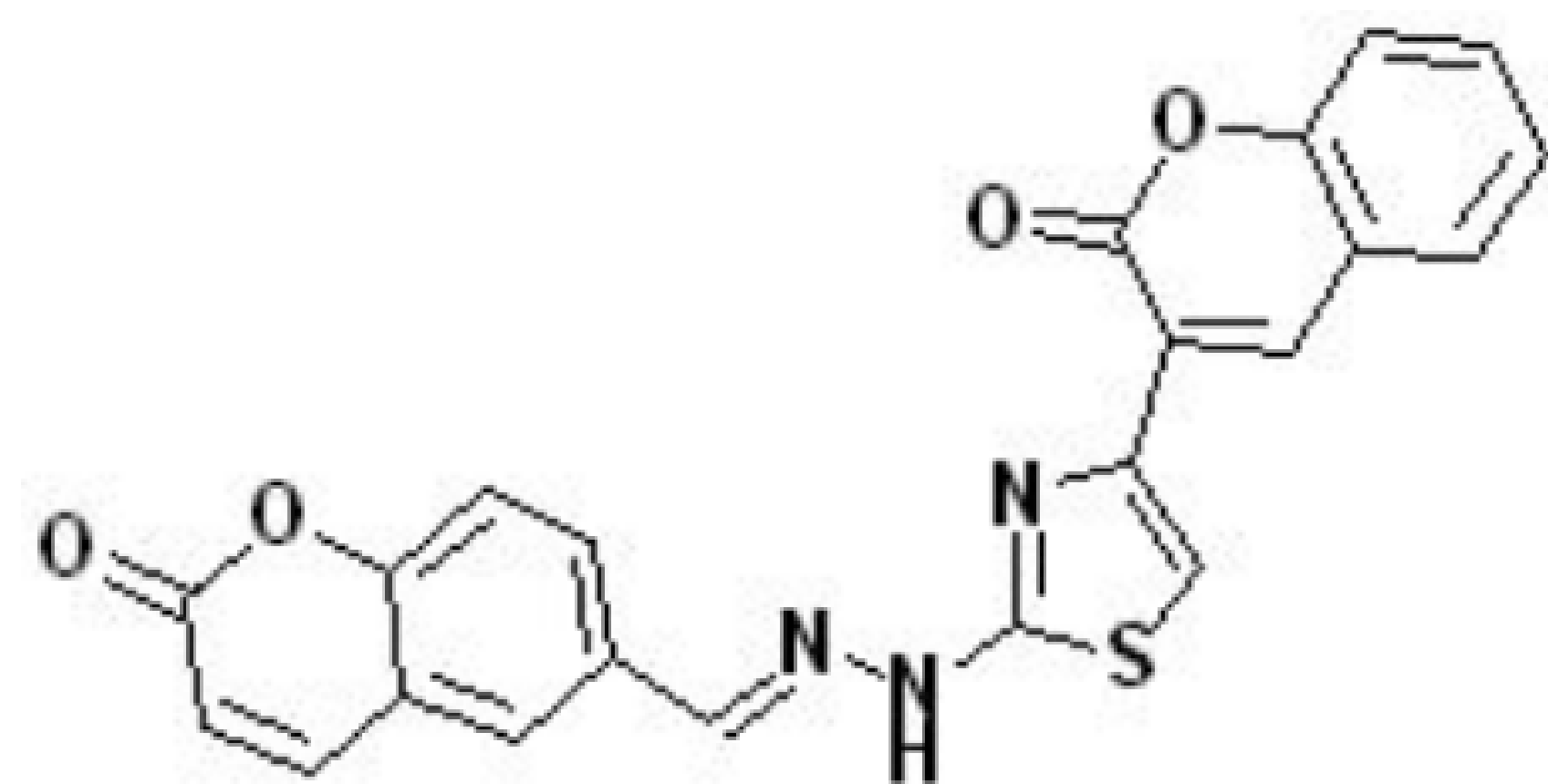
1035 formula(e) evaluated with 6 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-1

Mass	Calc. Mass	mDa	PPM	DBE	Formula
441.0660	441.0663	-0.3	-0.7	1.5	C10 H21 N2 O15 S
	441.0676	-1.6	-3.6	6.5	C11 H17 N6 O11 S
	441.0658	0.2	0.5	19.5	C23 H13 N4 O4 S
	441.0649	1.1	2.5	7.5	C7 H13 N12 O9 S
	441.0663	-0.3	-0.7	12.5	C8 H9 N16 O5 S
	441.0676	-1.6	-3.6	17.5	C9 H5 N20 O S





5q

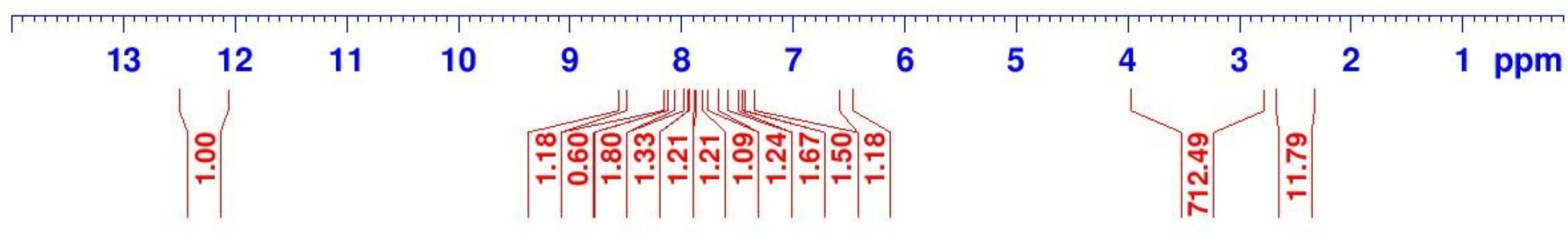
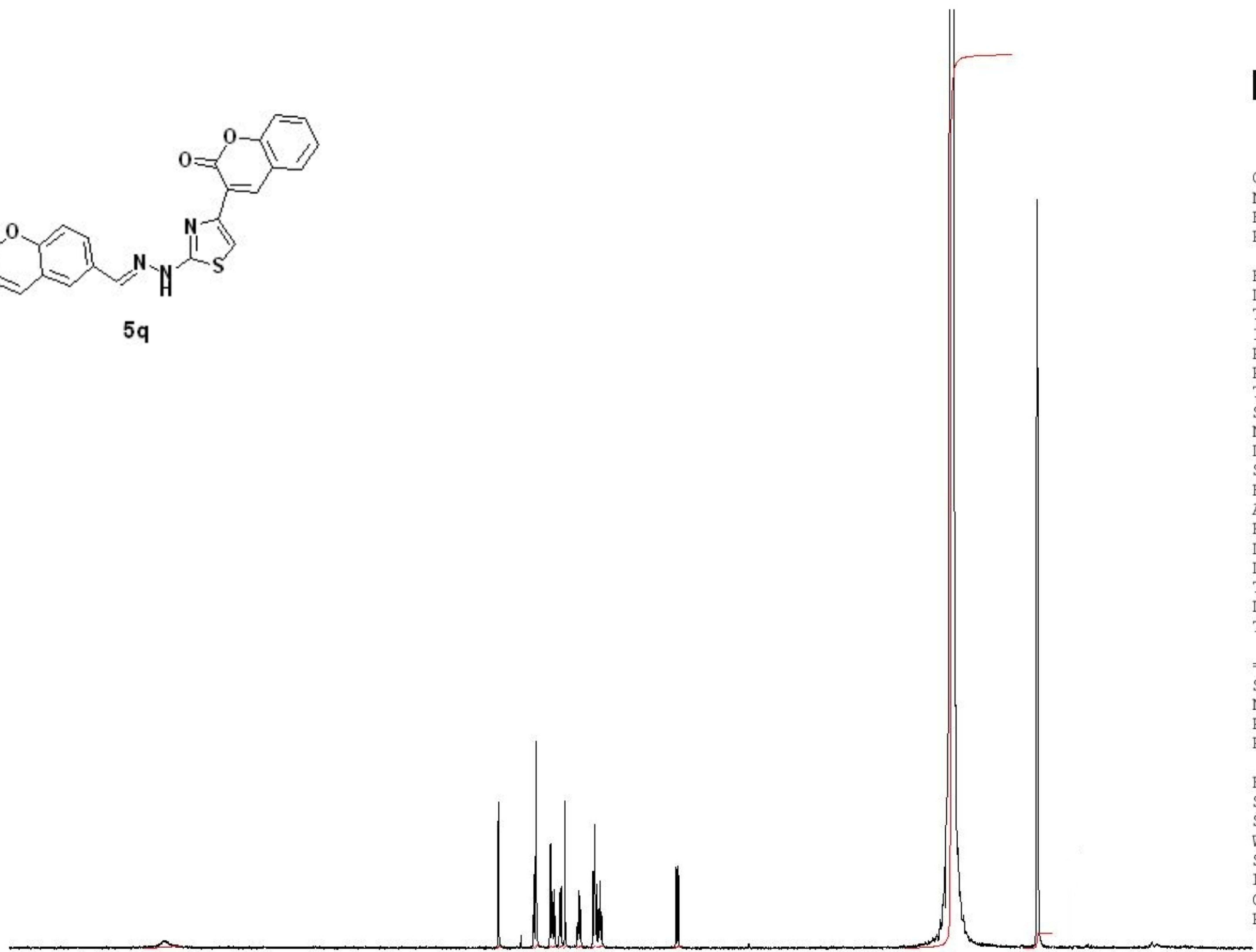


Current Data Parameters  
 NAME MG153  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130418  
 Time 18.09  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 64  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.40



1.00

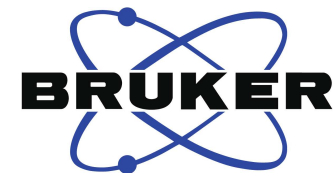
1.18  
 0.60  
 1.80  
 1.33  
 1.21  
 1.21  
 1.09  
 1.24  
 1.67  
 1.50  
 1.18

712.49

11.79



test



168.00  
160.16  
159.21  
154.37  
152.74  
144.56  
140.63  
138.63  
131.28  
129.69  
129.26  
126.77  
125.21  
120.92  
119.59  
119.50  
117.54  
117.21  
116.34  
111.20

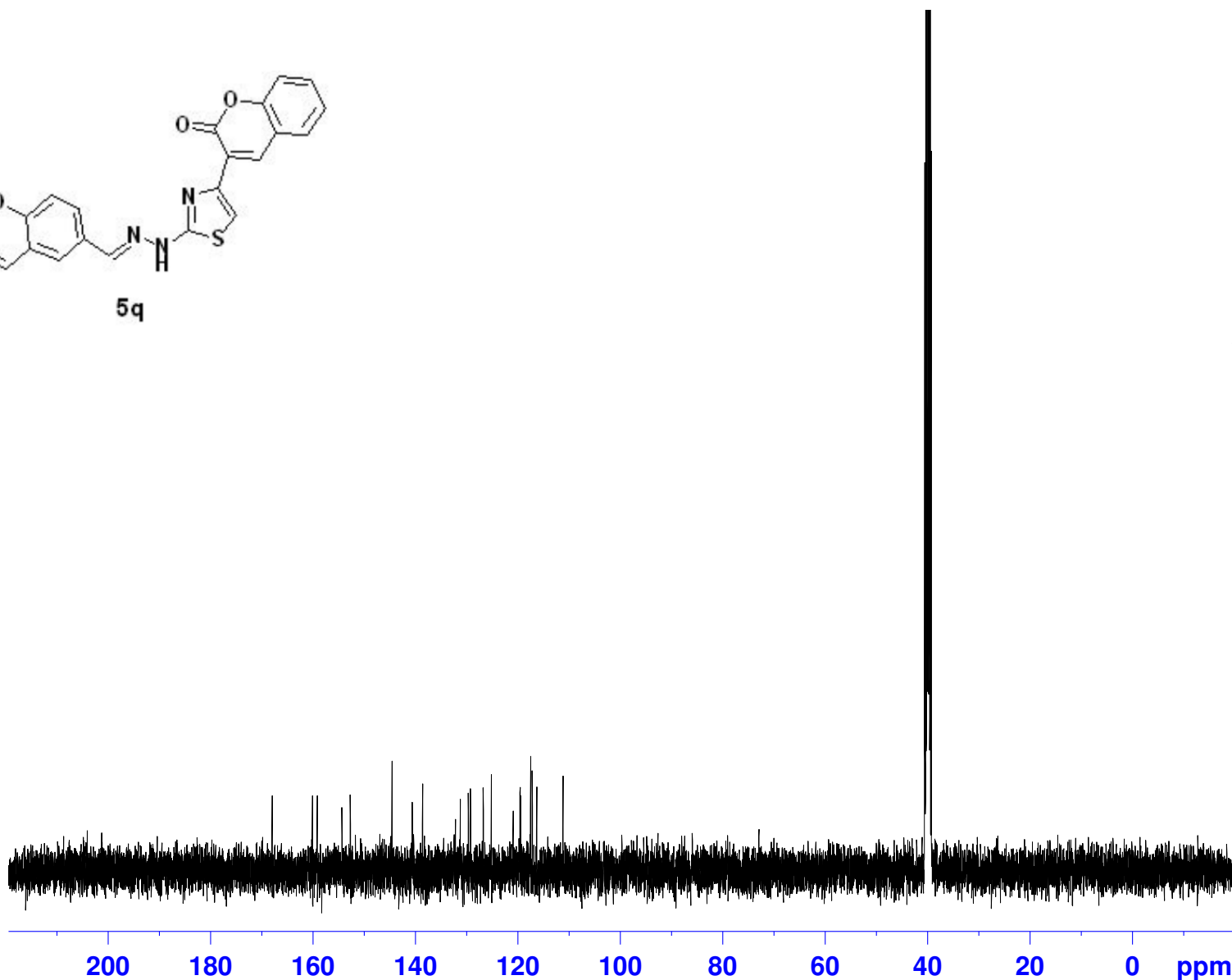
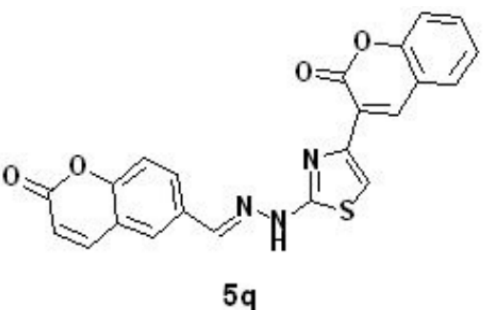
Current Data Parameters  
NAME MG153cc  
EXPNO 1  
PROCNO 1

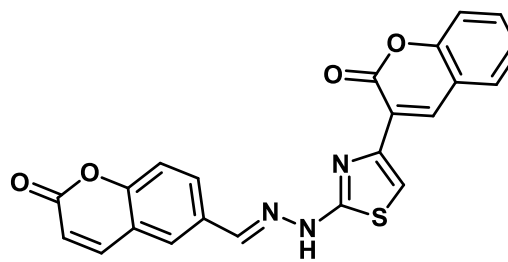
F2 - Acquisition Parameters  
Date\_ 20130429  
Time 12.17  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 215  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 114  
DW 20.800 usec  
DE 6.50 usec  
TE 298.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 100.6253441 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W

==== CHANNEL f2 =====  
SFO2 400.1416006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

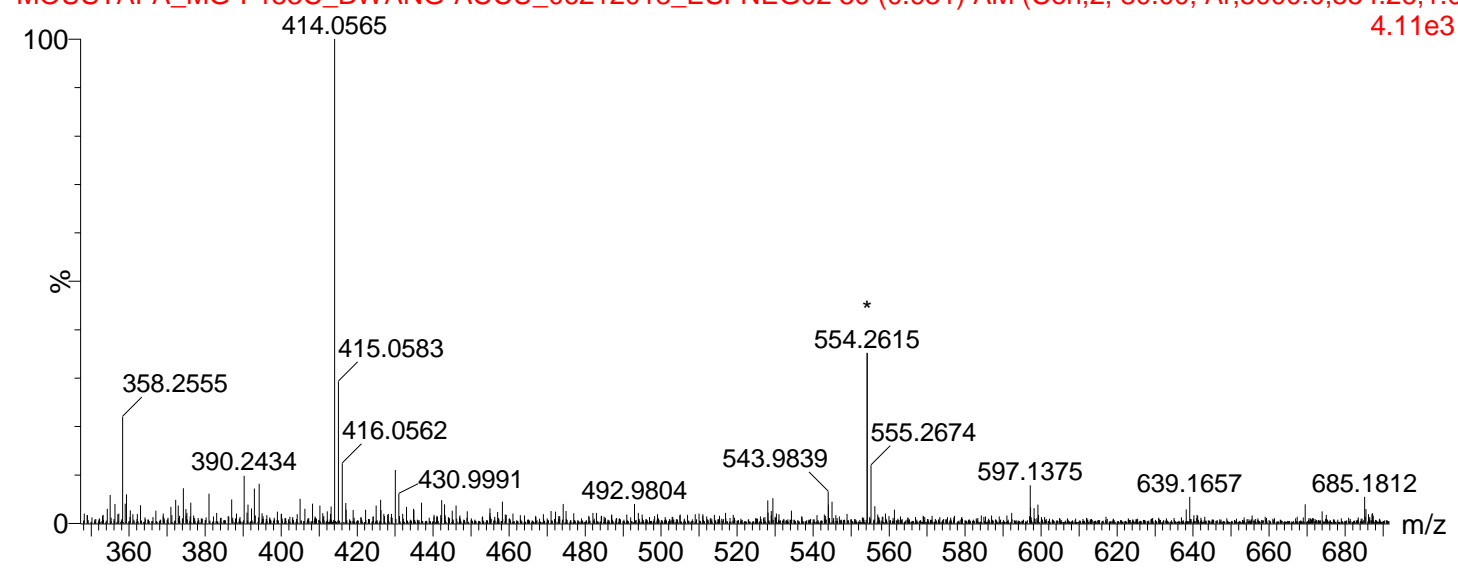




5q

21-Jun-2013 14:51:41

MOUSTAFA\_MG-I-153C\_BWANG-ACCU\_06212013\_ESI-NEG02 50 (0.931) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.0 4.11e3



Elemental Composition Report

Single Mass Analysis  
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0  
Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

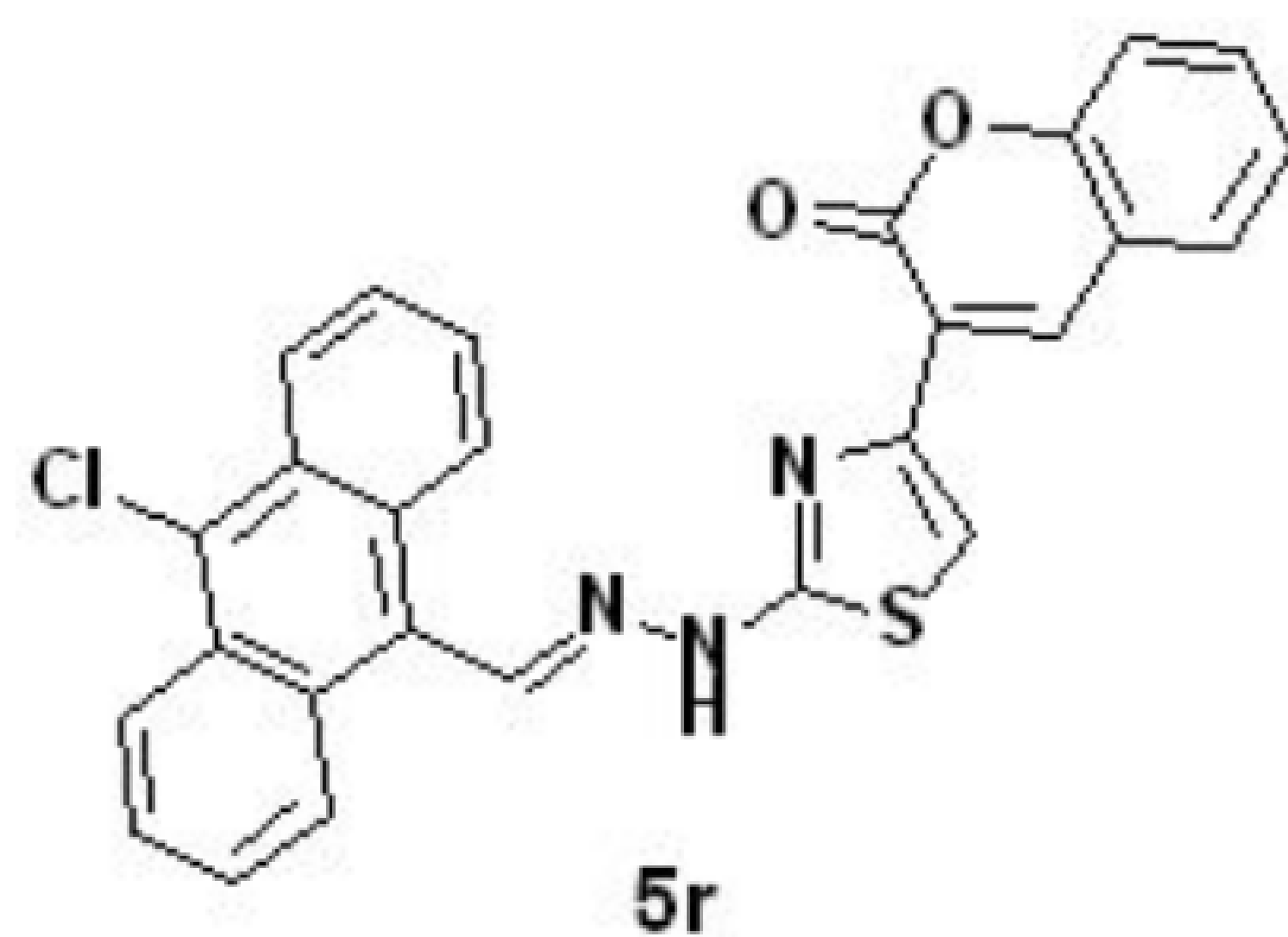
1476 formula(e) evaluated with 18 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-2

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
		5.0	5.0	100.0		
				-1.5		
414.0565	414.0560	0.5	1.2	2.0	301.6	C H14 N14 O8 S2
	414.0567	-0.2	-0.5	5.5	173.7	C10 H16 N5 O11 S
	414.0580	-1.5	-3.6	16.0	132.0	C10 H6 N16 O2 S
	414.0580	-1.5	-3.6	10.5	136.1	C11 H12 N9 O7 S
	414.0580	-1.5	-3.6	5.0	145.1	C12 H18 N2 O12 S
	414.0555	1.0	2.4	14.5	33.8	C15 H12 N9 O2 S2
	414.0555	1.0	2.4	9.0	46.0	C16 H18 N2 O7 S2
	414.0569	-0.4	-1.0	14.0	23.3	C17 H14 N6 O3 S2
	414.0582	-1.7	-4.1	13.5	15.7	C19 H16 N3 O4 S2
	414.0574	-0.9	-2.2	7.0	236.0	C2 H10 N18 O4 S2
	414.0549	1.6	3.9	18.5	24.1	C22 H12 N3 O4 S
	414.0575	-1.0	-2.4	23.0	19.1	C25 H10 N4 O S
	414.0574	-0.9	-2.2	1.5	265.5	C3 H16 N11 O9 S2
	414.0554	1.1	2.7	11.5	194.3	C7 H8 N15 O5 S
	414.0554	1.1	2.7	6.0	205.0	C8 H14 N8 O10 S
	414.0567	-0.2	-0.5	16.5	158.8	C8 H4 N19 O S
	414.0567	-0.2	-0.5	11.0	163.7	C9 H10 N12 O6 S
	414.0554	1.1	2.7	0.5	220.5	C9 H20 N O15 S



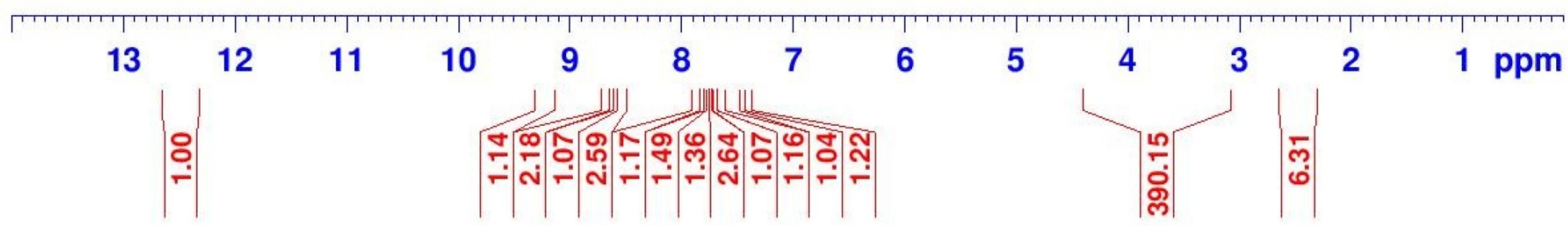
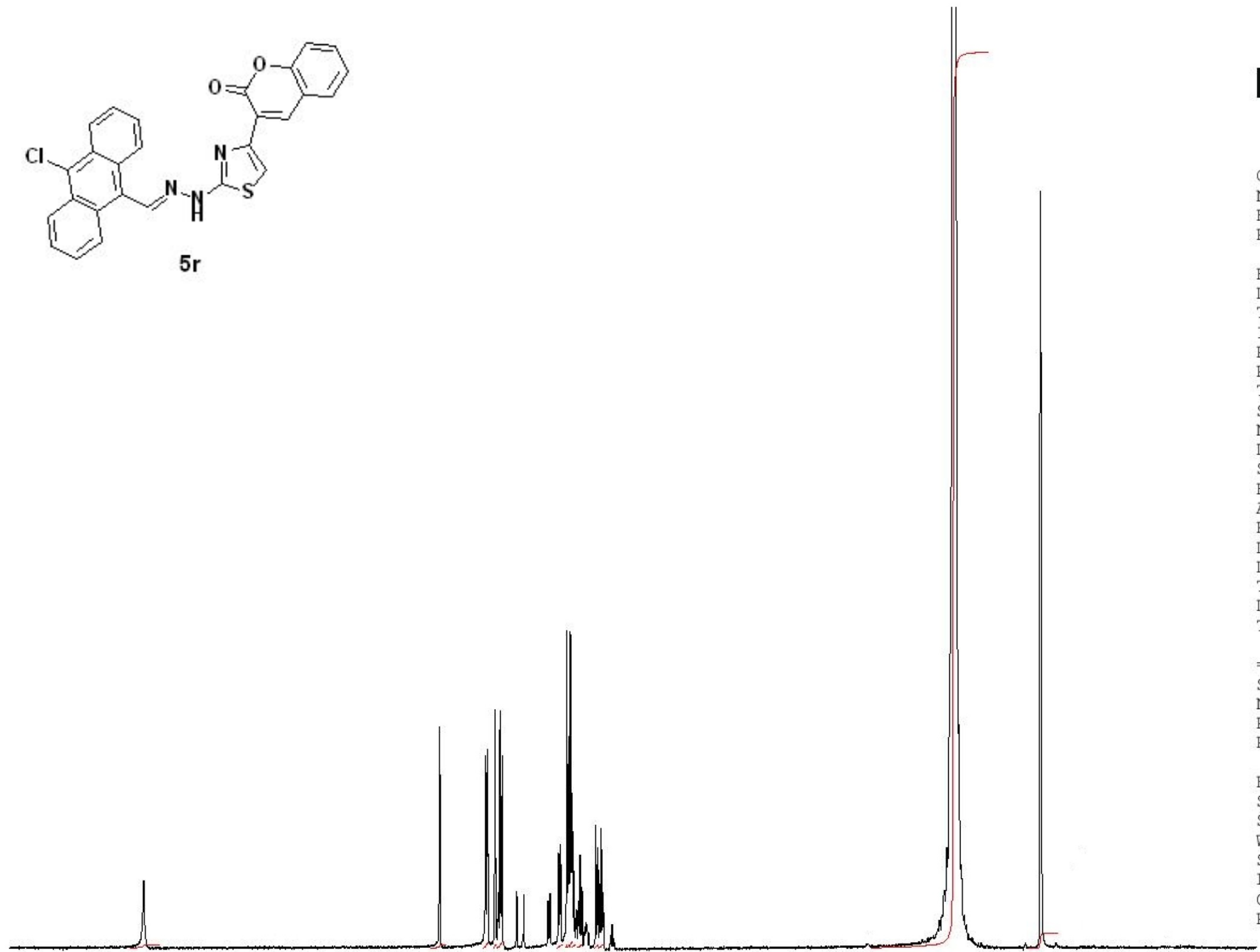


Current Data Parameters  
 NAME MG155  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130418  
 Time 18.14  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 64  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.40



1.00

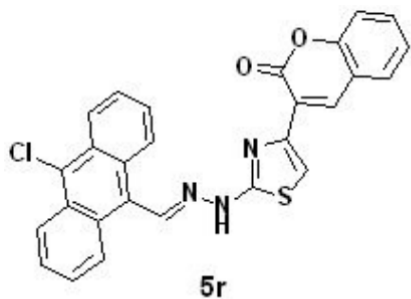
1.14  
 2.18  
 1.07  
 2.59  
 1.17  
 1.49  
 1.36  
 2.64  
 1.07  
 1.16  
 1.04  
 1.22

390.15

6.31

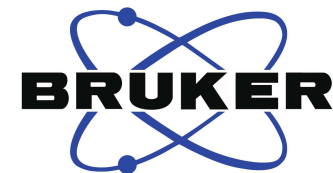
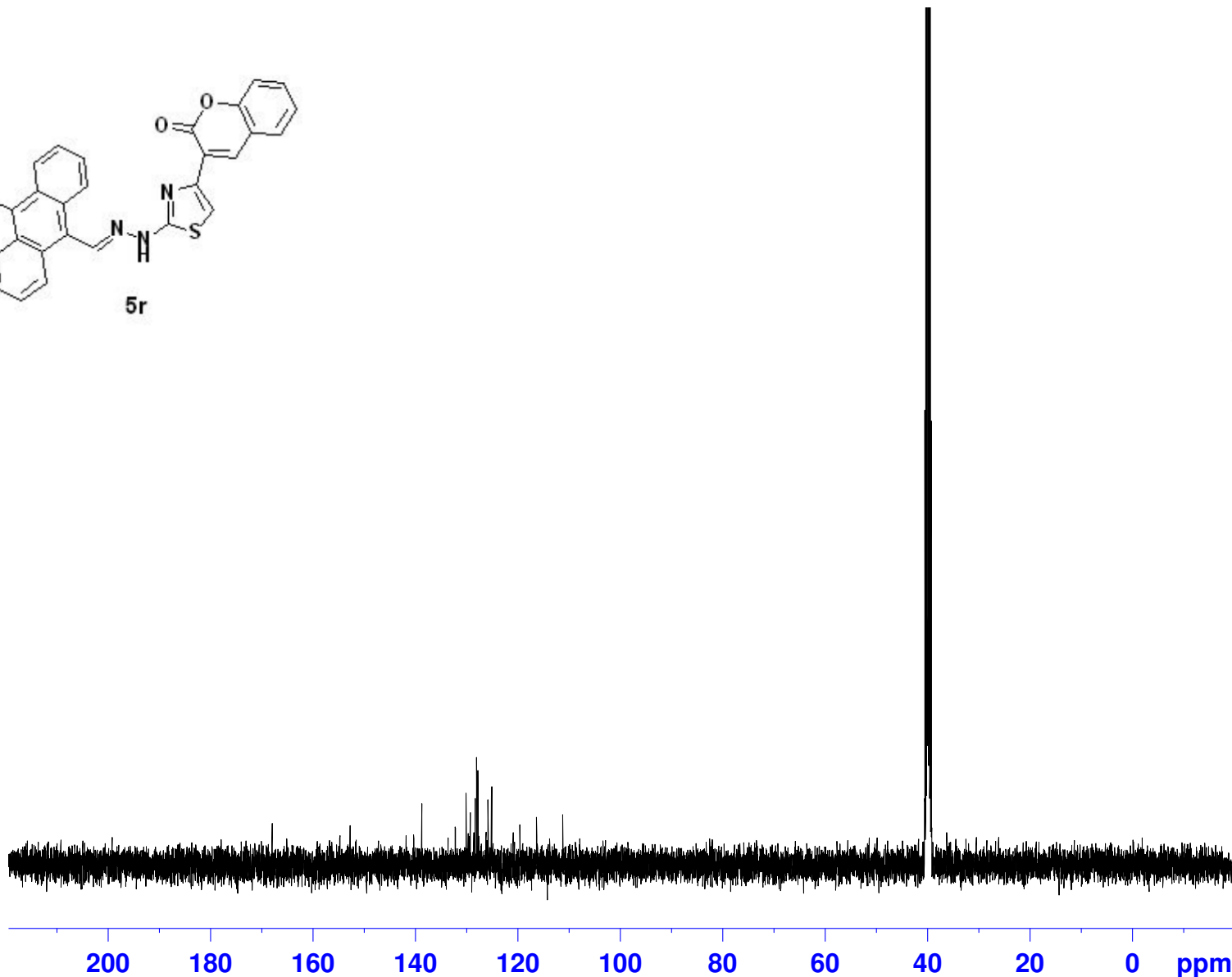


test



168.02

138.79  
130.11  
129.33  
128.38  
128.08  
127.81  
125.85  
125.22  
125.15  
116.36  
111.25



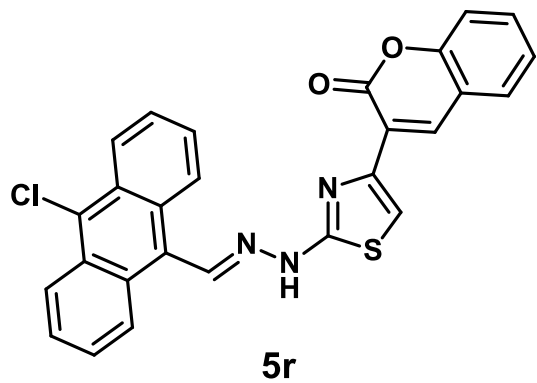
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NAME MG155c  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130422  
Time 17.55  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 164  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 181  
DW 20.800 usec  
DE 6.50 usec  
TE 297.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 100.6253441 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W

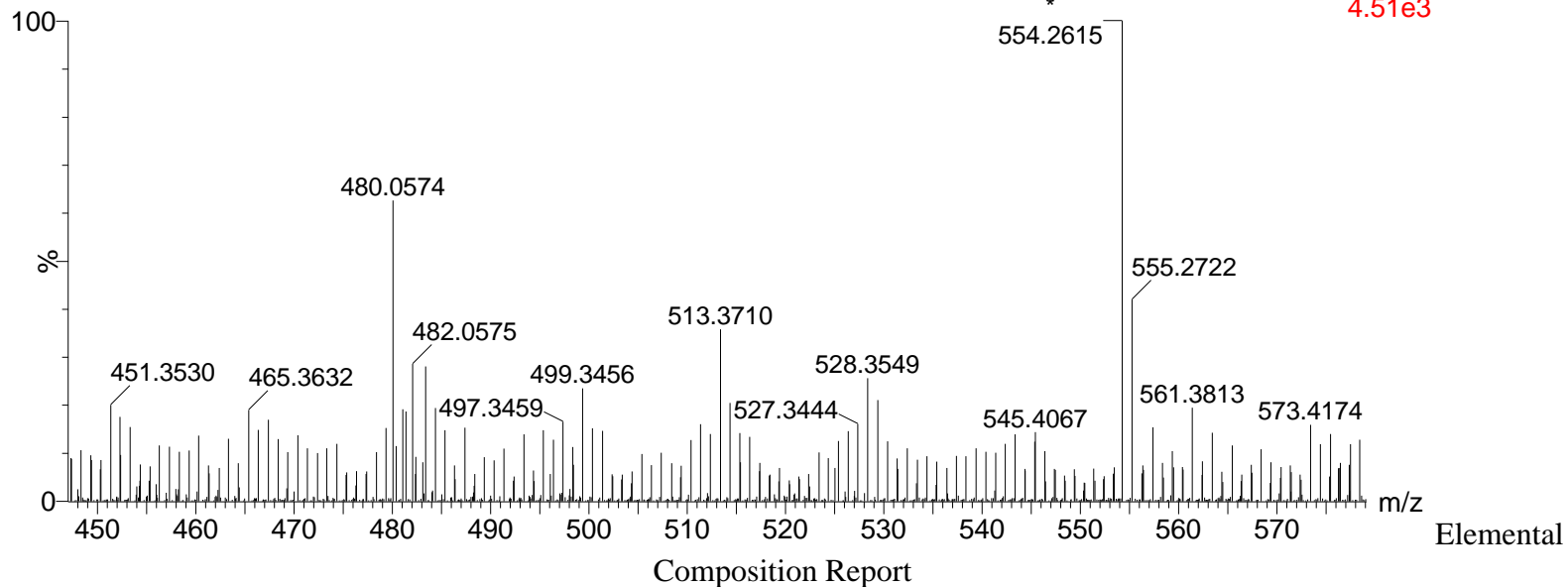
===== CHANNEL f2 =====  
SFO2 400.1416006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



21-Jun-2013 15:40:27

MOUSTAFA\_MG-I-155C\_BWANG\_06212013\_ESI-NEG 42 (0.780) AM (Top,2, Ar,5000.0,554.26,1.00); Sm (SG, 2x3, 4.51e3



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

3218 formula(e) evaluated with 44 results within limits (all results (up to 1000) for each mass)

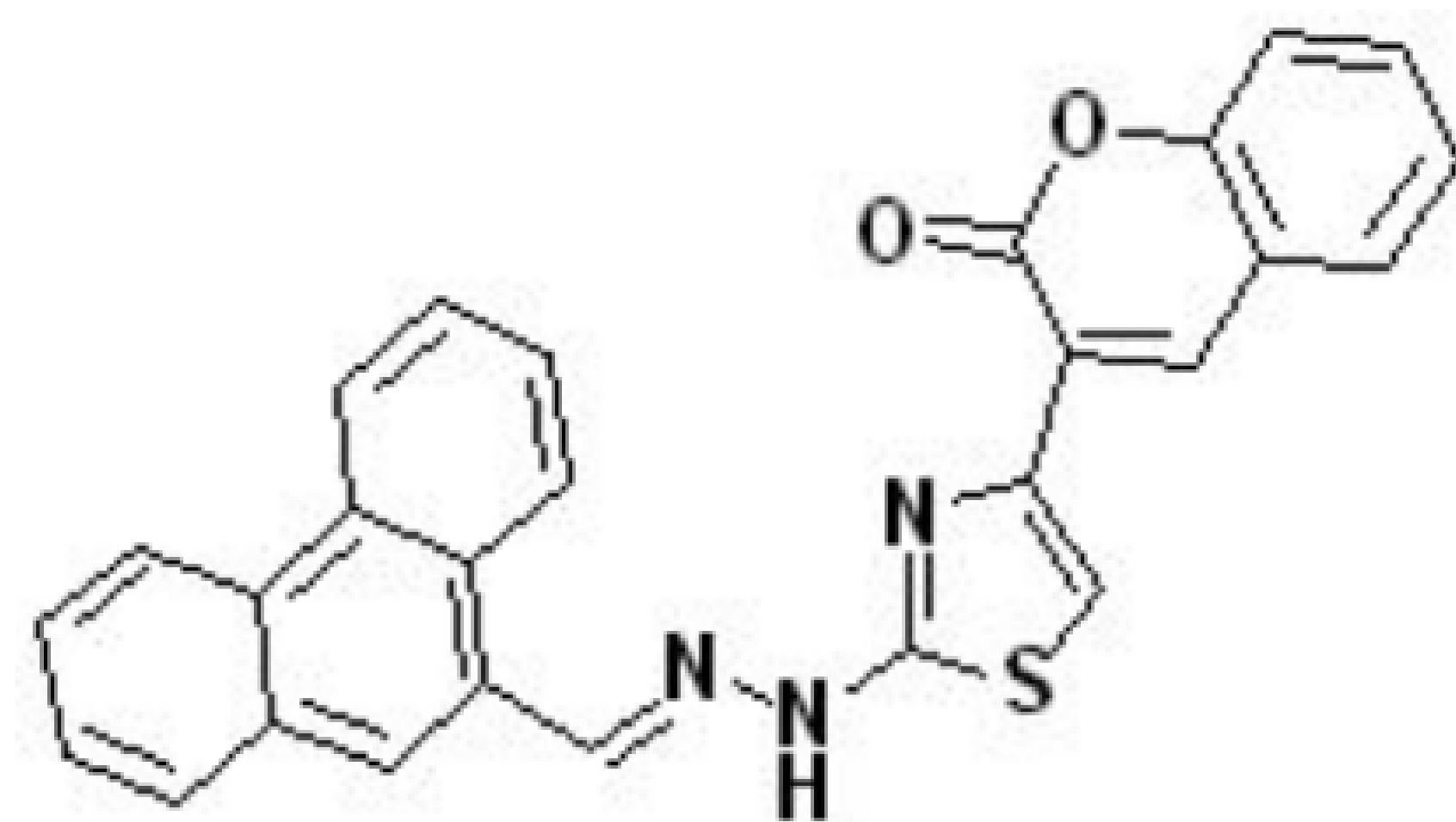
Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-2 Cl: 1-2

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
480.0574	480.0574	0.0	0.0	21.5	6.3	C27 H15 N3 O2 S Cl
	480.0572	0.2	0.4	5.5	141.0	C4 H15 N17 O5 S2 Cl
	480.0572	0.2	0.4	0.0	161.3	C5 H21 N10 O10 S2 Cl
	480.0572	0.2	0.4	8.0	202.9	C16 H22 N6 O3 S2 Cl2
	480.0577	-0.3	-0.6	1.0	353.2	C H18 N18 O4 S2 Cl2
	480.0570	0.4	0.8	10.5	226.4	C7 H12 N19 O S Cl2
	480.0570	0.4	0.8	-0.5	272.6	C9 H24 N5 O11 S Cl2
	480.0570	0.4	0.8	5.0	248.8	C8 H18 N12 O6 S Cl2
	480.0578	-0.4	-0.8	17.0	126.9	C24 H18 N4 O S Cl2
	480.0579	-0.5	-1.0	14.5	51.1	C12 H11 N15 O3 S Cl
	480.0579	-0.5	-1.0	3.5	72.2	C14 H23 N O13 S Cl
	480.0579	-0.5	-1.0	9.0	60.7	C13 H17 N8 O8 S Cl
	480.0580	-0.6	-1.2	12.0	7.9	C21 H21 N2 O5 S2 Cl
	480.0567	0.7	1.5	12.5	12.9	C19 H19 N5 O4 S2 Cl
	480.0565	0.9	1.9	9.5	74.8	C11 H15 N11 O7 S Cl
	480.0583	-0.9	-1.9	4.5	234.9	C10 H20 N9 O7 S Cl2
	480.0565	0.9	1.9	4.0	87.6	C12 H21 N4 O12 S Cl
	480.0583	-0.9	-1.9	10.0	213.3	C9 H14 N16 O2 S Cl2
	480.0565	0.9	1.9	15.0	63.9	C10 H9 N18 O2 S Cl
	480.0584	-1.0	-2.1	-1.0	257.5	C11 H26 N2 O12 S Cl2

480.0585	-1.1	-2.3	7.5	195.5	C18 H24 N3 O4 S2 Cl2
480.0585	-1.1	-2.3	10.5	103.9	C5 H11 N21 O S2 Cl
480.0585	-1.1	-2.3	5.0	121.3	C6 H17 N14 O6 S2 Cl
480.0586	-1.2	-2.5	-0.5	140.4	C7 H23 N7 O11 S2 Cl
480.0560	1.4	2.9	22.0	6.2	C25 H13 N6 O S Cl
480.0559	1.5	3.1	3.0	230.2	C15 H26 N2 O7 S2 Cl2
480.0559	1.5	3.1	0.5	184.2	C3 H19 N13 O9 S2 Cl
480.0559	1.5	3.1	6.0	162.6	C2 H13 N20 O4 S2 Cl
480.0590	-1.6	-3.3	0.5	335.3	C3 H20 N15 O5 S2 Cl2
480.0558	1.6	3.3	8.5	211.4	C14 H20 N9 O2 S2 Cl2
480.0557	1.7	3.5	0.0	288.8	C7 H22 N8 O10 S Cl2
480.0557	1.7	3.5	5.5	264.3	C6 H16 N15 O5 S Cl2
480.0592	-1.8	-3.7	8.5	48.4	C15 H19 N5 O9 S Cl
480.0592	-1.8	-3.7	14.0	40.1	C14 H13 N12 O4 S Cl
480.0592	-1.8	-3.7	16.5	125.6	C26 H20 N O2 S Cl2
480.0554	2.0	4.2	7.5	26.7	C18 H23 N O8 S2 Cl
480.0594	-2.0	-4.2	17.0	2.0	C22 H17 N6 O S2 Cl
480.0554	2.0	4.2	13.0	19.4	C17 H17 N8 O3 S2 Cl
480.0552	2.2	4.6	4.5	104.8	C10 H19 N7 O11 S Cl
480.0552	2.2	4.6	12.5	146.0	C21 H20 N3 O4 S Cl2
480.0552	2.2	4.6	15.5	78.6	C8 H7 N21 O S Cl
480.0552	2.2	4.6	10.0	90.8	C9 H13 N14 O6 S Cl
480.0597	-2.3	-4.8	4.0	222.3	C12 H22 N6 O8 S Cl2
480.0597	-2.3	-4.8	9.5	201.6	C11 H16 N13 O3 S Cl2





5s

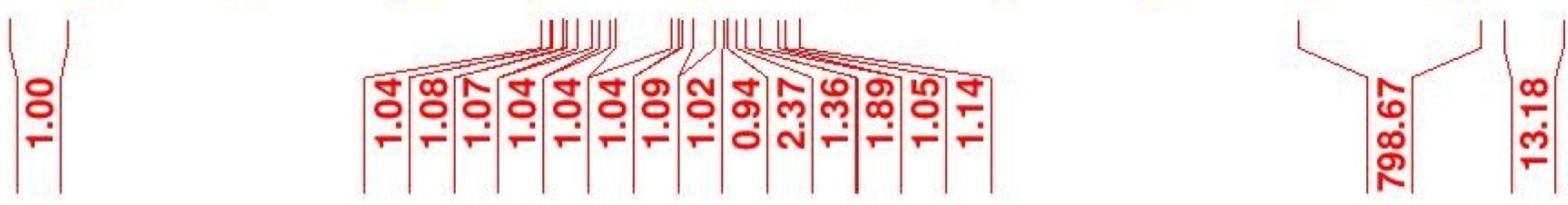
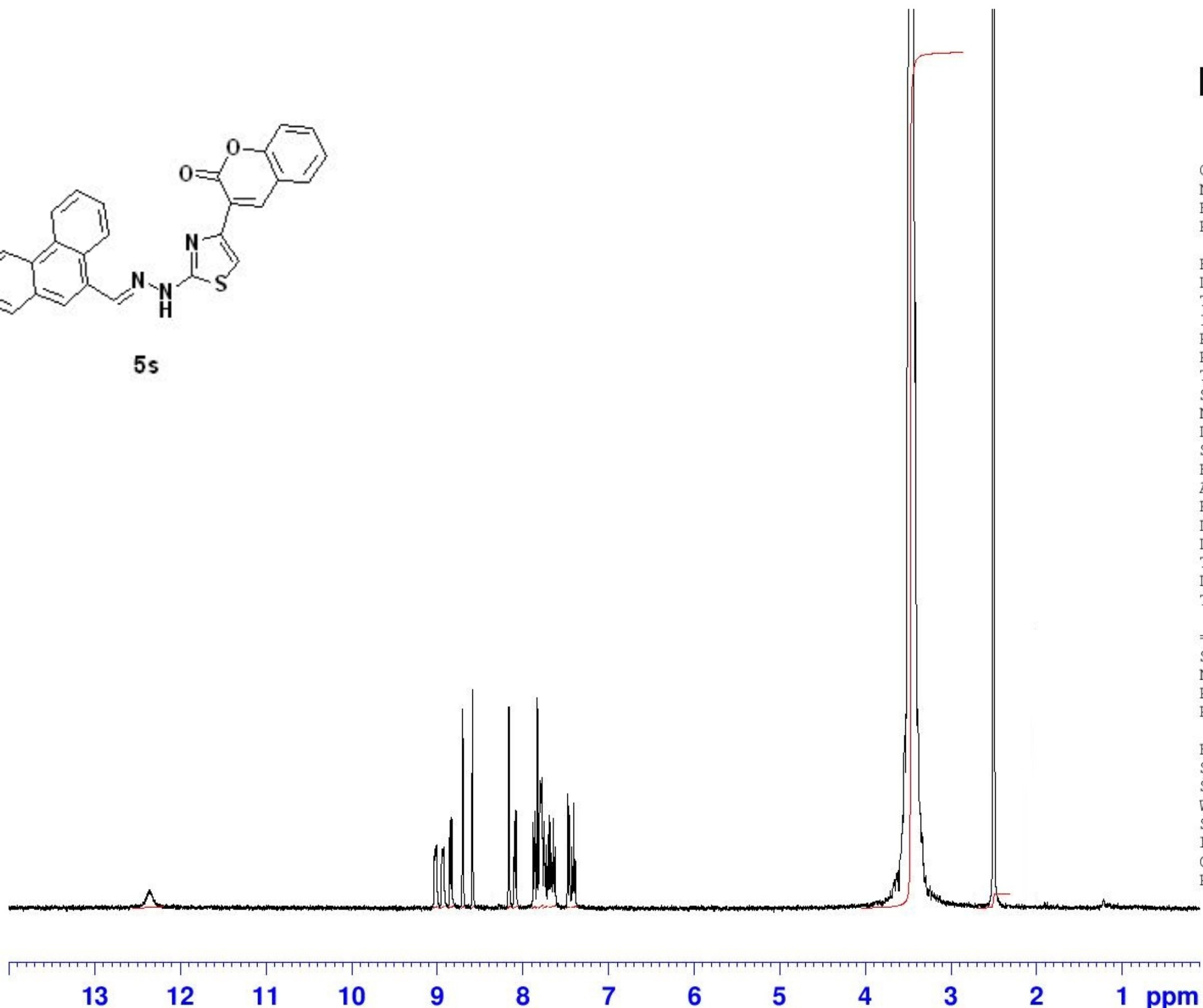


Current Data Parameters  
 NAME MG154  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130418  
 Time 18.04  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 64  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.40



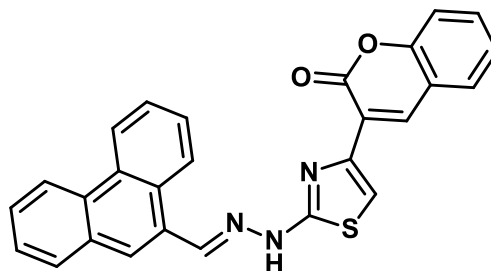
1.00

1.04  
 1.08  
 1.07  
 1.04  
 1.04  
 1.04  
 1.09  
 1.02  
 0.94  
 2.37  
 1.36  
 1.89  
 1.05  
 1.14

798.67

13.18

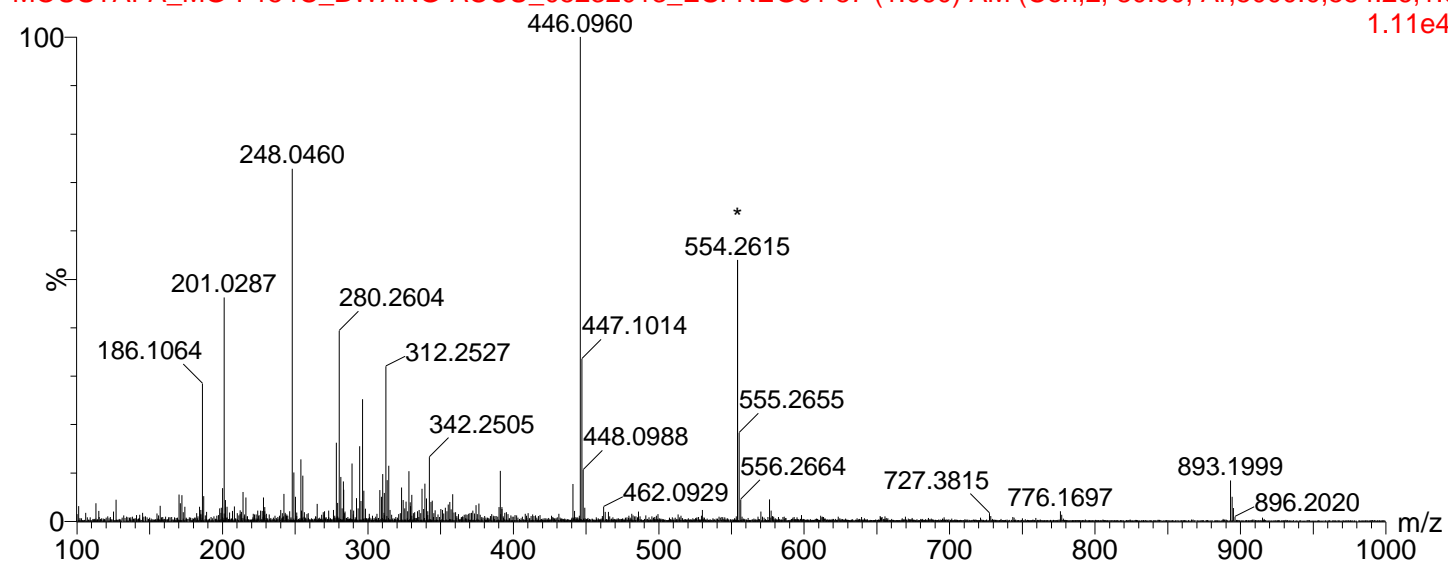




5s

23-May-2013 12:37:11

MOUSTAFA\_MG-I-154C\_BWANG-ACCU\_05232013\_ESI-NEG01 57 (1.060) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.C  
1.11e4



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1042 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-1

Minimum:

-1.5

Maximum:

5.0

5.0

100.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

446.0960

446.0941

1.9

4.3

15.5

470.5

C8 H8 N21 O S

446.0963

-0.3

-0.7

21.5

4.4

C27 H16 N3 O2 S

446.0982

-2.2

-4.9

8.5

289.7

C15 H20 N5 O9 S

446.0968

-0.8

-1.8

3.5

394.5

C14 H24 N O13 S

446.0968

-0.8

-1.8

14.5

323.1

C12 H12 N15 O3 S

446.0955

0.5

1.1

9.5

422.9

C11 H16 N11 O7 S

446.0942

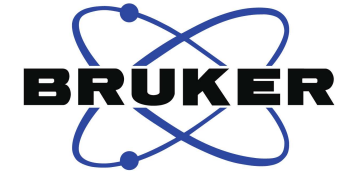
1.8

4.0

4.5

546.0

C10 H20 N7 O11 S

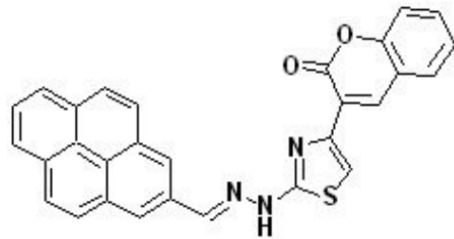


Current Data Parameters  
NAME MG156  
EXPNO 1  
PROCNO 1

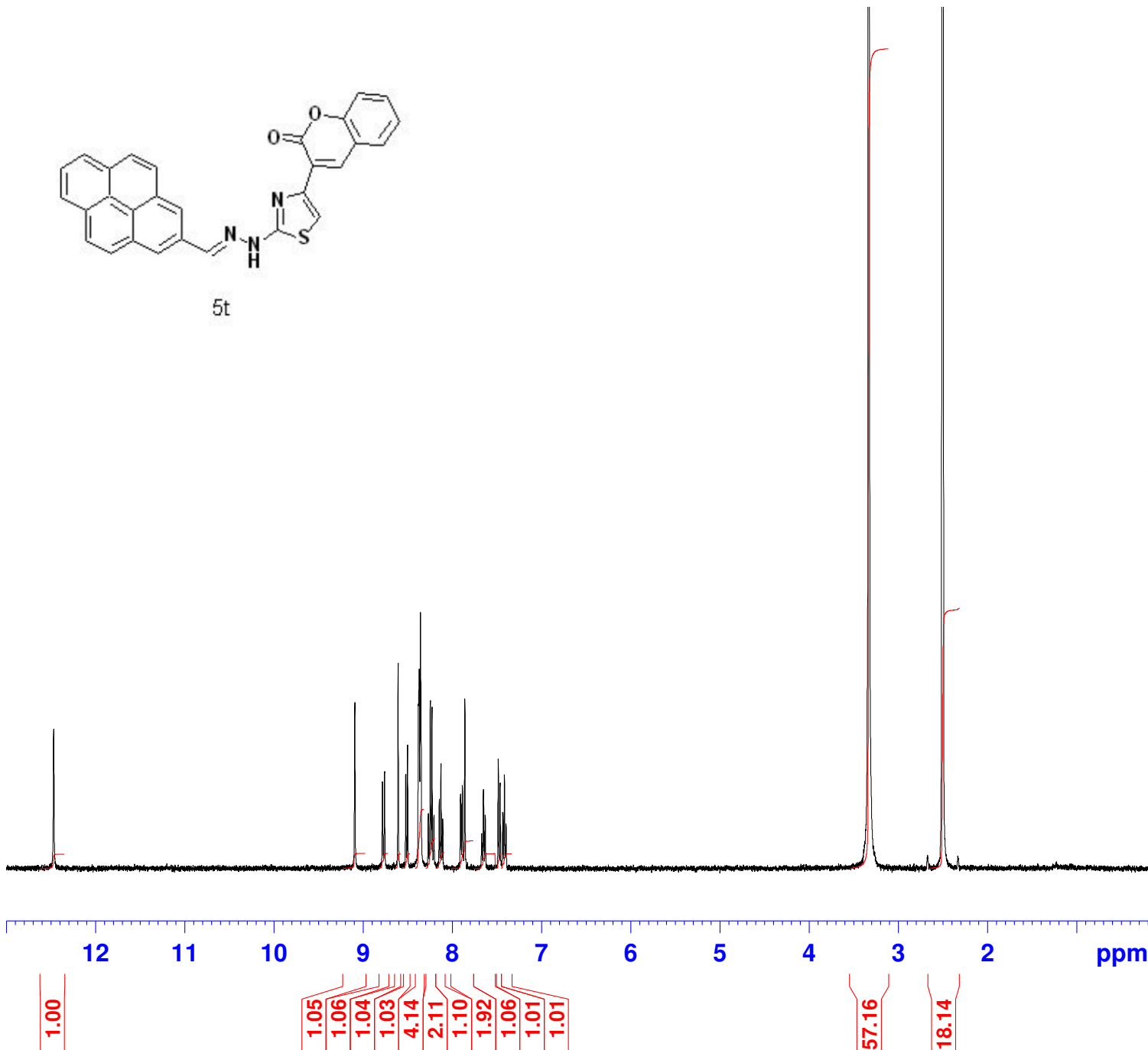
F2 - Acquisition Parameters  
Date\_ 20130419  
Time 18.11  
INSTRUM spect  
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PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 5  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 297.9 K  
D1 1.00000000 sec  
TD0 1

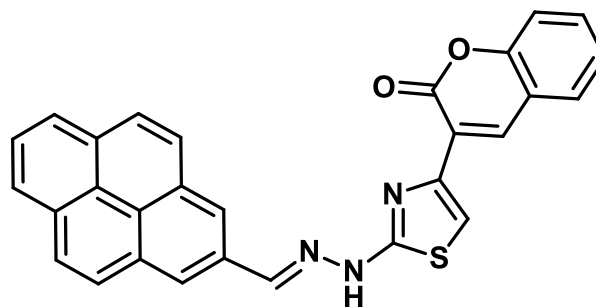
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NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.40



5t

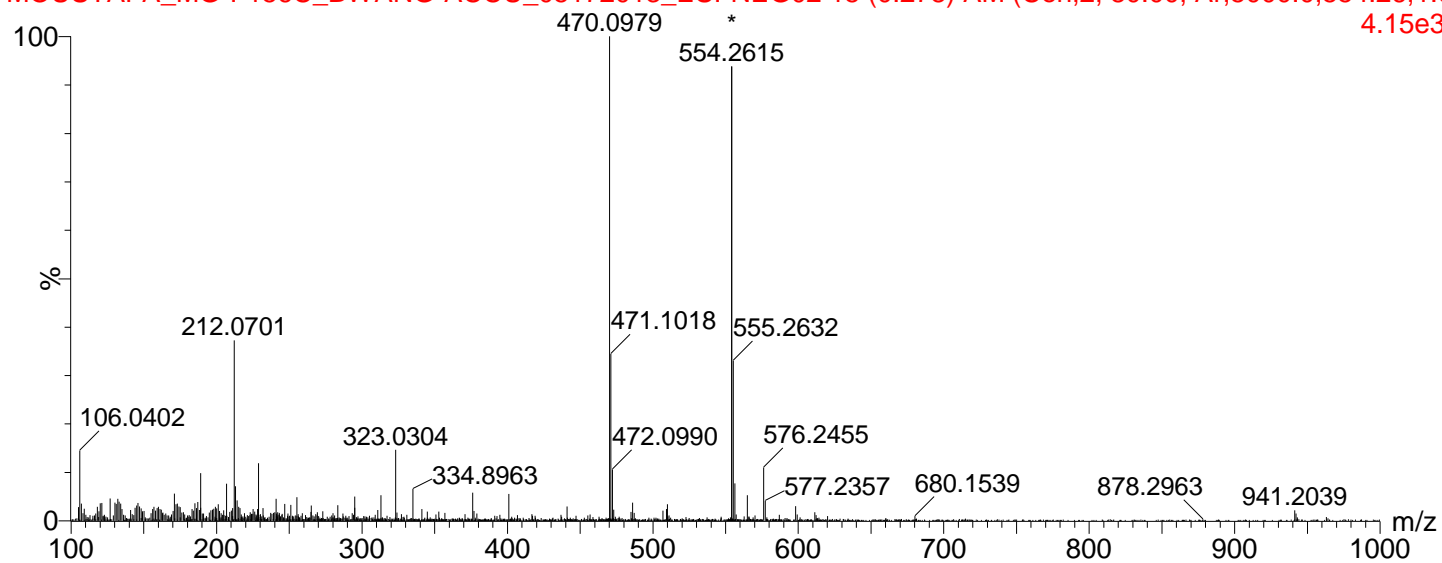




5t

17-May-2013 15:46:21

MOUSTAFA\_MG-I-156C\_BWANG-ACCU\_05172013\_ESI-NEG02 15 (0.278) AM (Cen,2, 80.00, Ar,5000.0,554.26,1.0  
4.15e3



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

3573 formula(e) evaluated with 42 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-4

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
470.0979	470.0975	0.4	0.9	1.5	225.8	C9 H24 N7 O11 S2
	470.0984	-0.5	-1.1	6.0	299.3	C9 H22 N14 O S4
	470.0989	-1.0	-2.1	12.0	141.8	C9 H14 N18 O2 S2
	470.0971	0.8	1.7	1.0	359.2	C8 H26 N10 O5 S4
	470.0975	0.4	0.9	7.0	192.6	C8 H18 N14 O6 S2
	470.0962	1.7	3.6	2.0	252.4	C7 H22 N10 O10 S2
	470.0975	0.4	0.9	12.5	164.0	C7 H12 N21 O S2
	470.0957	2.2	4.7	1.5	375.6	C6 H24 N13 O4 S4
	470.0962	1.7	3.6	7.5	218.6	C6 H16 N17 O5 S2
	470.1000	-2.1	-4.5	3.0	332.8	C4 H18 N14 O11 S
	470.0995	-1.6	-3.4	2.5	329.9	C3 H20 N17 O5 S3
	470.1000	-2.1	-4.5	8.5	310.9	C3 H12 N21 O6 S
	470.0963	1.6	3.4	23.5	0.2	C29 H16 N3 O2 S
	470.0997	-1.8	-3.8	18.5	28.5	C26 H20 N3 O2 S2
	470.0984	-0.5	-1.1	19.0	26.3	C24 H18 N6 O S2
	470.0970	0.9	1.9	14.0	41.4	C23 H22 N2 O5 S2
	470.0957	2.2	4.7	14.5	44.7	C21 H20 N5 O4 S2
	470.1000	-2.1	-4.5	14.0	294.2	C2 H6 N28 O S
	470.0987	-0.8	-1.7	3.5	372.7	C2 H16 N17 O10 S
	470.0995	-1.6	-3.4	10.0	65.3	C19 H22 N2 O10 S



470.0990	-1.1	-2.3	9.5	136.3	C18 H24 N5 O4 S3
470.0995	-1.6	-3.4	15.5	55.9	C18 H16 N9 O5 S
470.0977	0.2	0.4	4.5	174.1	C17 H28 N O8 S3
470.0982	-0.3	-0.6	10.5	82.8	C17 H20 N5 O9 S
470.0968	1.1	2.3	5.5	117.5	C16 H24 N O13 S
470.0977	0.2	0.4	10.0	140.7	C16 H22 N8 O3 S3
470.0982	-0.3	-0.6	16.0	73.0	C16 H14 N12 O4 S
470.0964	1.5	3.2	5.0	182.1	C15 H26 N4 O7 S3
470.0968	1.1	2.3	11.0	103.1	C15 H18 N8 O8 S
470.0964	1.5	3.2	10.5	147.6	C14 H20 N11 O2 S3
470.0968	1.1	2.3	16.5	93.2	C14 H12 N15 O3 S
470.1002	-2.3	-4.9	0.5	181.2	C13 H28 N O13 S2
470.0997	-1.8	-3.8	0.0	334.9	C12 H30 N4 O7 S4
470.1002	-2.3	-4.9	6.0	149.7	C12 H22 N8 O8 S2
470.0989	-1.0	-2.1	1.0	202.1	C11 H26 N4 O12 S2
470.0997	-1.8	-3.8	5.5	289.7	C11 H24 N11 O2 S4
470.1002	-2.3	-4.9	11.5	122.5	C11 H16 N15 O3 S2
470.0984	-0.5	-1.1	0.5	345.9	C10 H28 N7 O6 S4
470.0989	-1.0	-2.1	6.5	169.6	C10 H20 N11 O7 S2
470.0973	0.6	1.3	-1.5	443.1	C H20 N13 O14 S
470.0982	-0.3	-0.6	3.0	356.8	C H18 N20 O4 S3
470.0987	-0.8	-1.7	9.0	350.6	C H10 N24 O5 S