Electronic Supplementary Material (ESI) for New Journal of Chemistry.
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Nano-MoO_3 mediated synthesis of bioactive thiazolidin-4-ones and their anti-bacterial mode-of-action analysis using *in silico* target prediction, docking and similarity searching.

Supplementary Information

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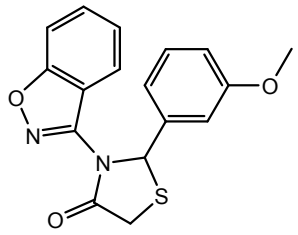
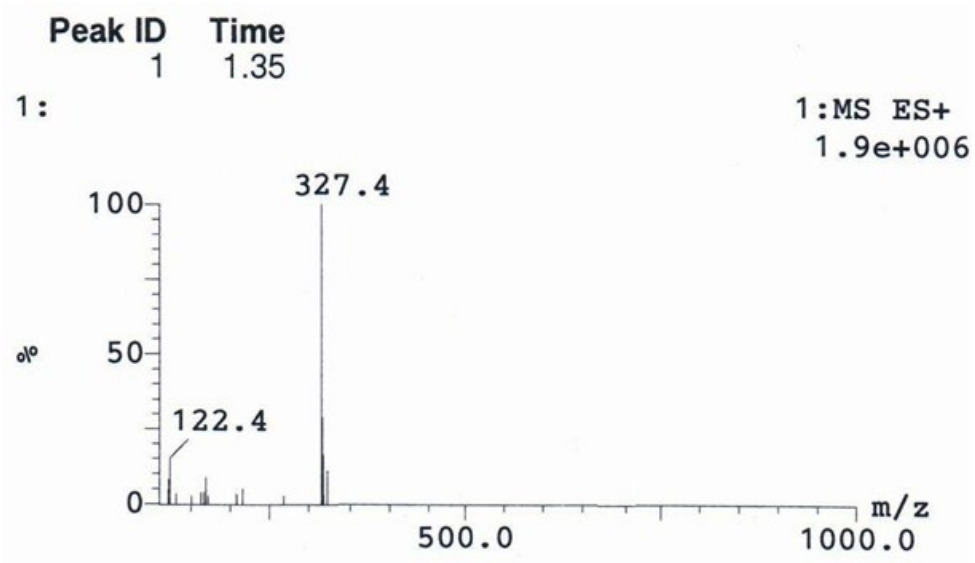

O
N
N
S
O
O

3b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1.9e+006
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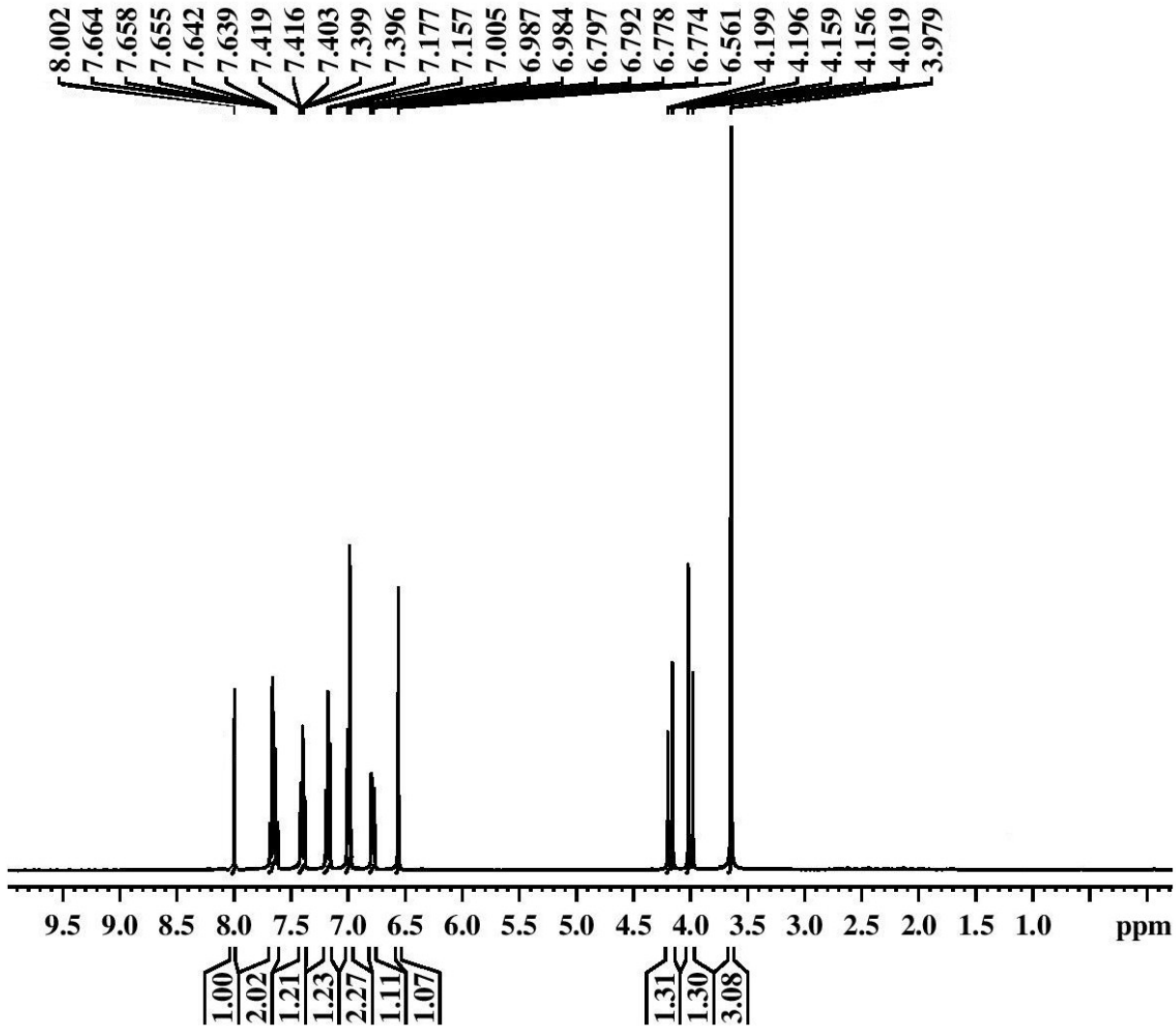
100
50
%
122.4
0
m/z
500.0
1000.0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7.664
7.658
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7.416
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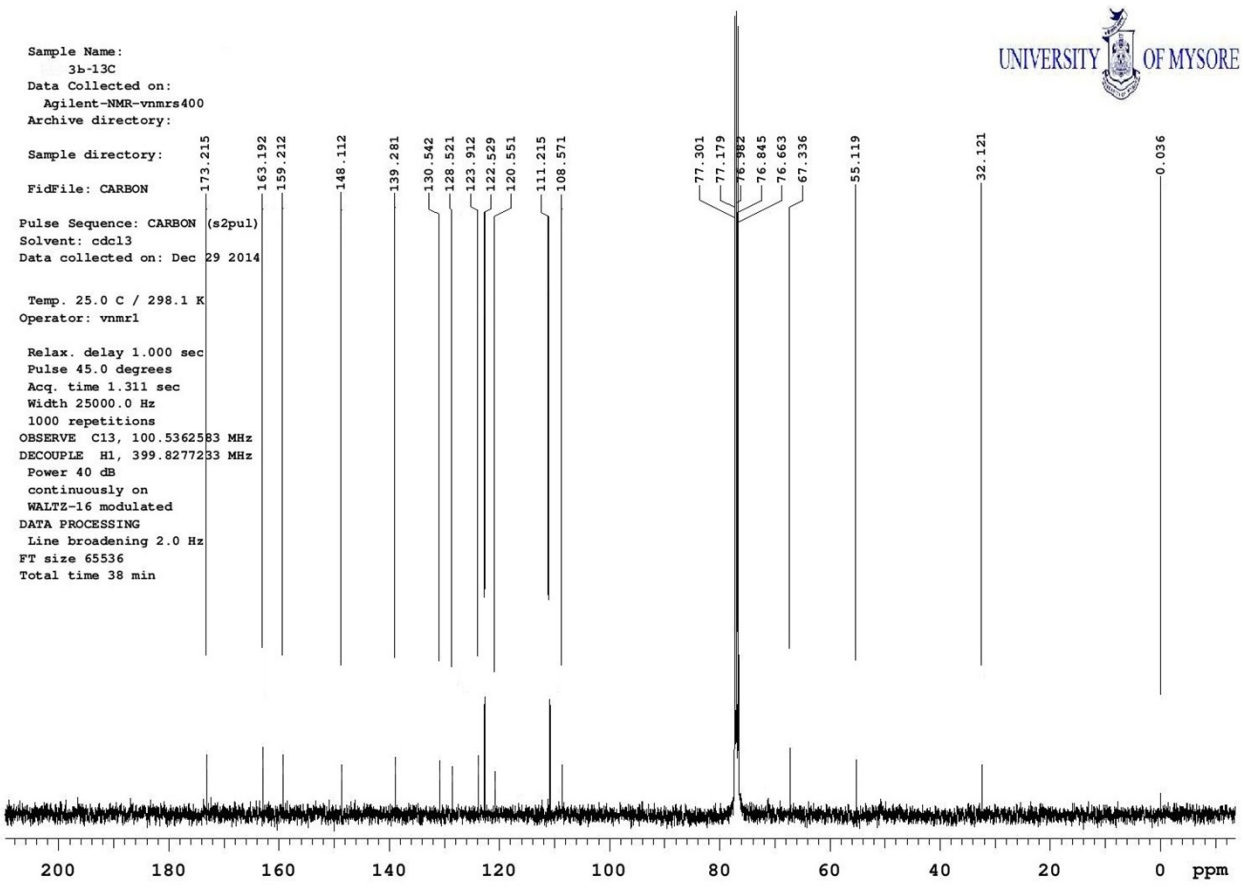
7.399
7.396
7.177
7.157
7.005
6.987
6.984
6.797
6.792
6.778
6.774
6.561
4.199
4.196
4.159
4.156
4.019
3.979
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
2.02
1.21
1.23
2.27
1.11
1.07
1.31
1.30
3.08


UNIVERSITY OF MYSORE
Sample Name:
3b-13C
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 29 2014
Temp. 25.0 C / 298.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5362583 MHz
DECOUPLE H1, 399.8277233 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min
173.215
163.192
159.212
148.112
139.281
130.542
128.521
123.912
122.529
120.551
111.215
108.571
77.301
77.179
76.982
76.845
76.663
67.336
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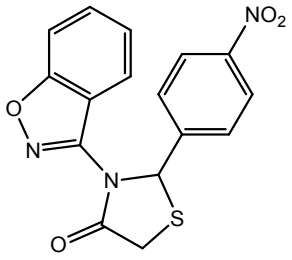
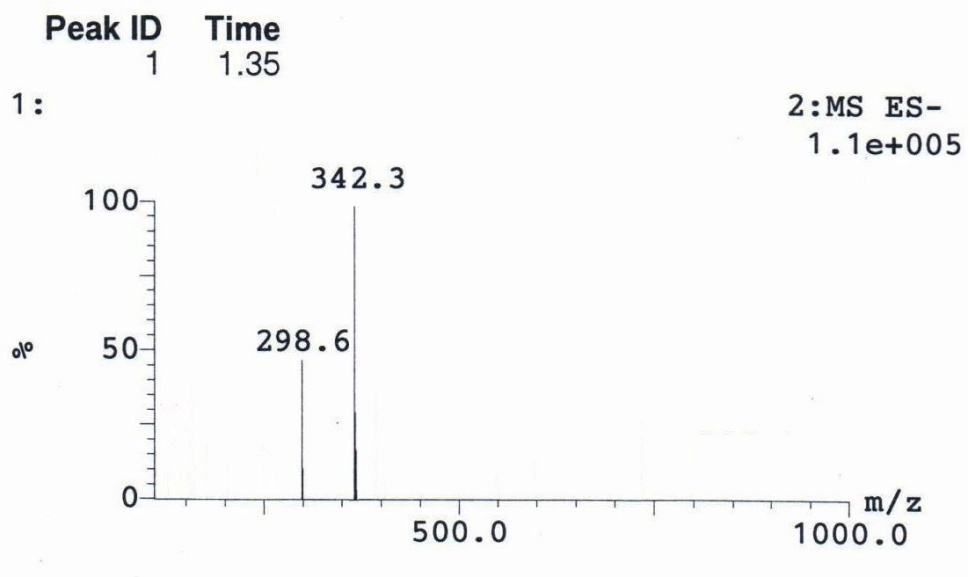
32.121
0.036
200
180
160
140
120
100
80
60
40
20
0
ppm


NO2
O
N
N
S
O

3c


Peak ID Time
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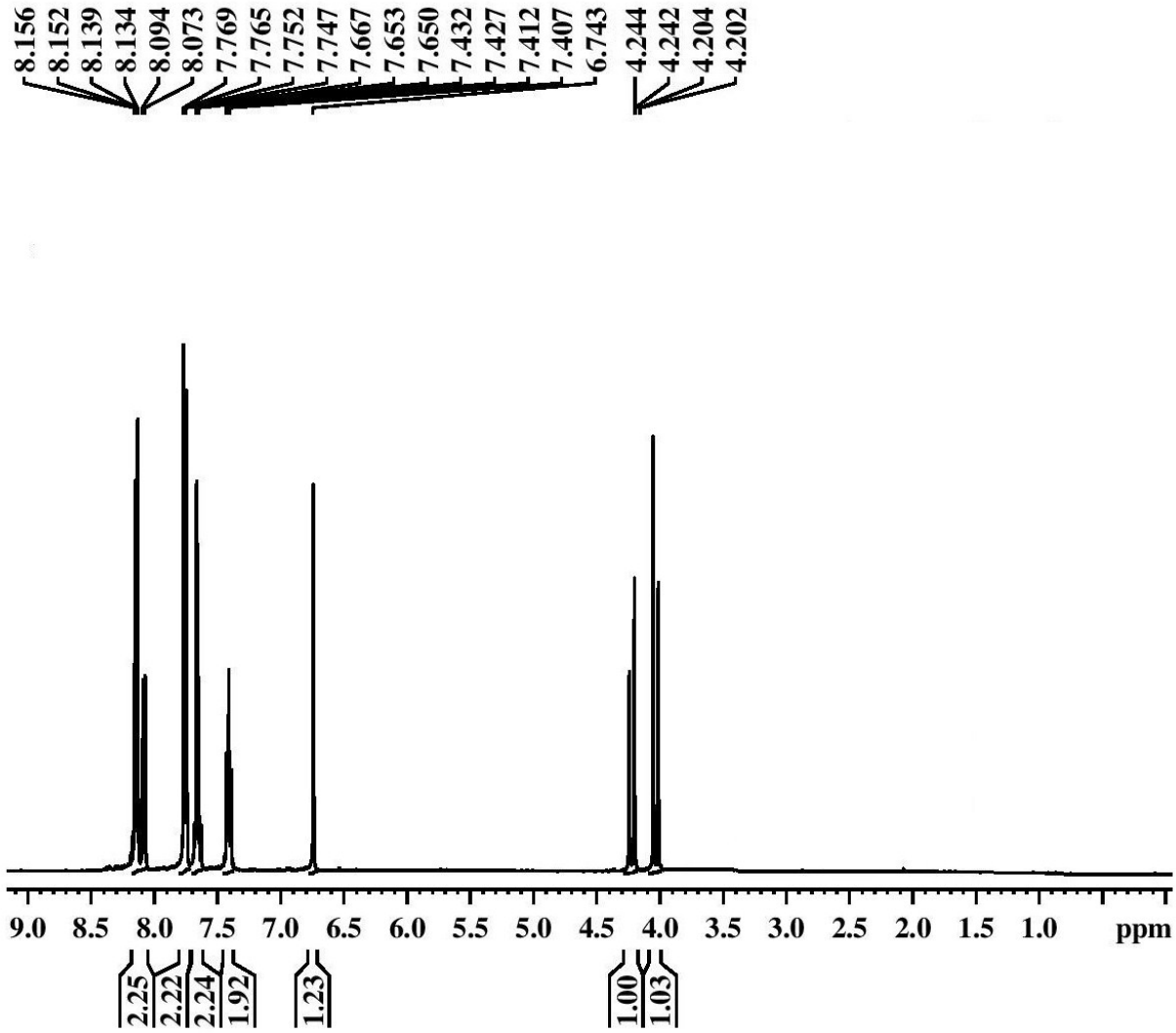
100
%
50
298.6
0
m/z
500.0
1000.0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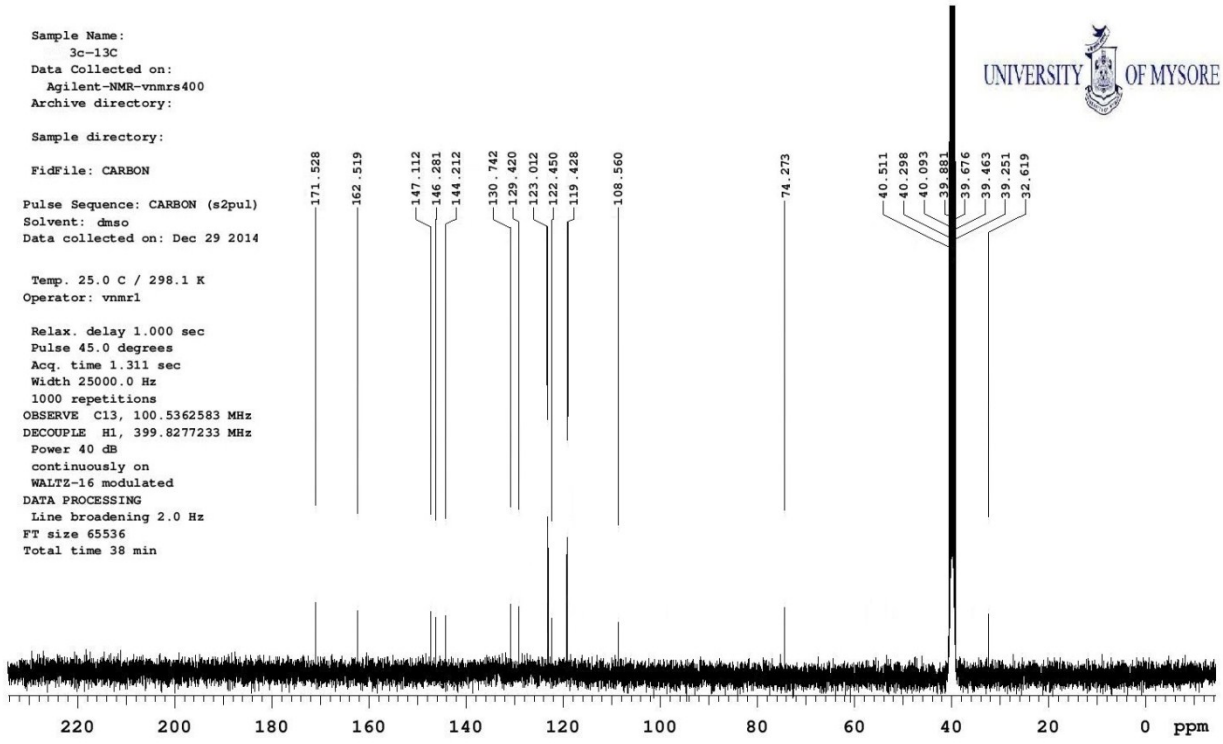
8.152
8.139
8.134
8.094
8.073
7.769
7.765
7.752
7.747
7.667
7.653
7.650
7.432
7.427
7.412
7.407
6.743
4.244
4.242
4.204
4.202
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.25
2.22
2.24
1.92
1.23
1.00
1.03


Sample Name:
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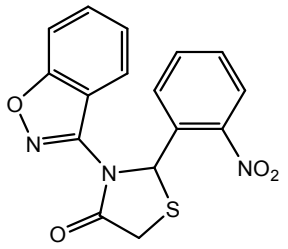
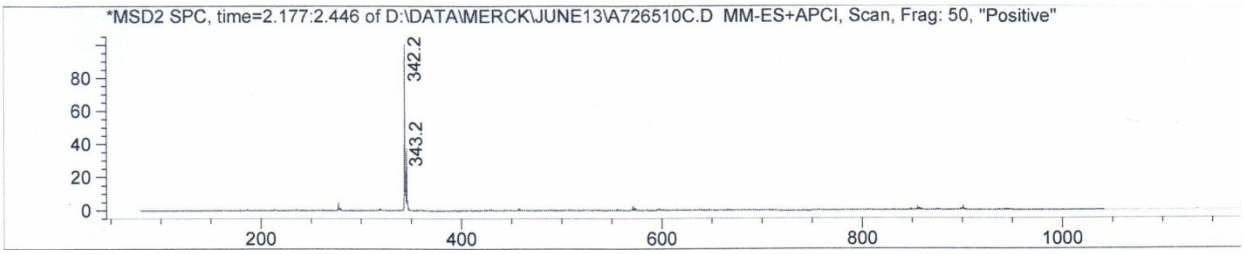
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Dec 29 2014
Temp. 25.0 C / 298.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5362583 MHz
DECOUPLE H1, 399.8277233 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min
171.528
162.519
147.112
146.281
144.212
130.742
129.420
123.012
122.450
119.428
108.560
74.273
40.511
40.298
40.093
39.881
39.676
39.463
39.251
32.619
220
200
180
160
140
120
100
80
60
40
20
0
ppm


O
N
N
S
O
NO2

3d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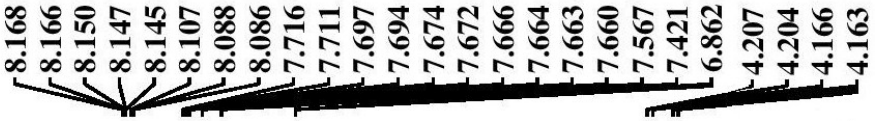
343.2
80
60
40
20
0
200
400
600
800
1000


8.168
8.166
8.150
8.147
8.145
8.107
8.088
8.086
7.716
7.711
7.697
7.694
7.674
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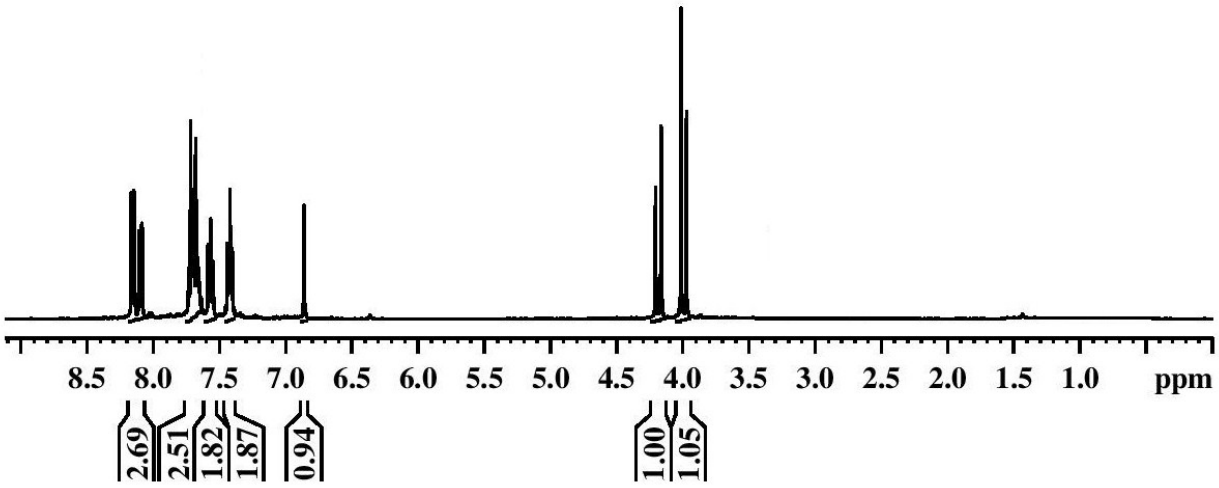
4.166
4.163


8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
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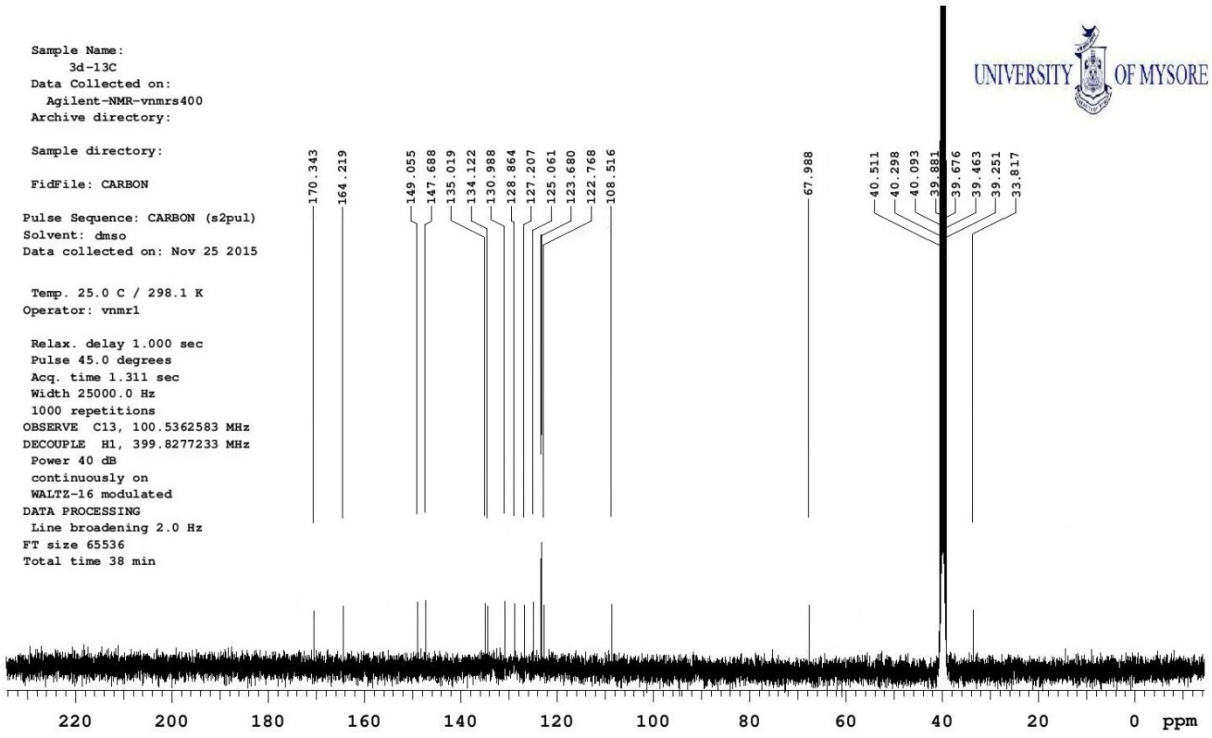
1.82
1.87
0.94
1.00
1.05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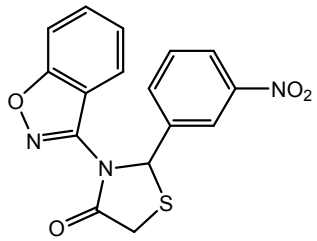
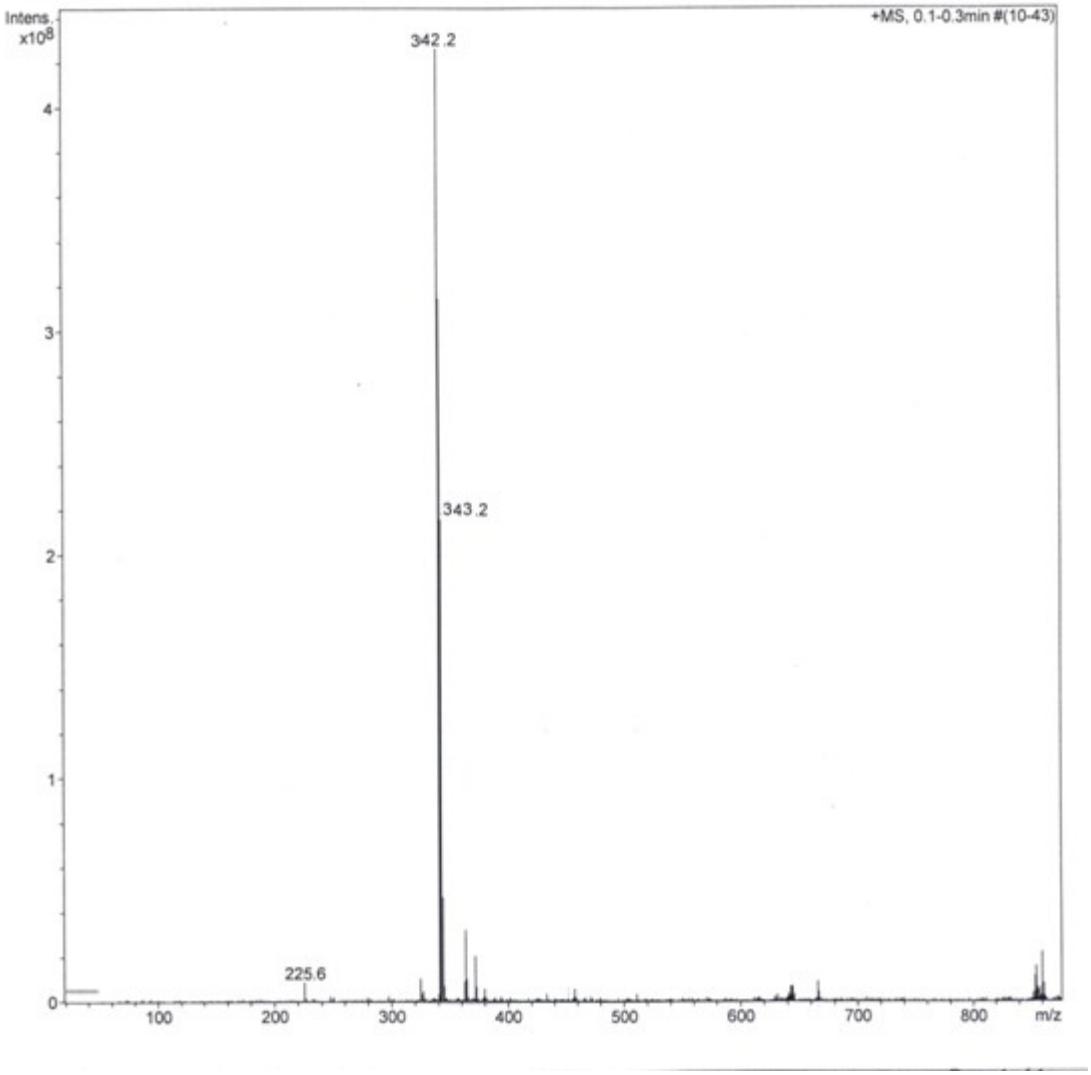
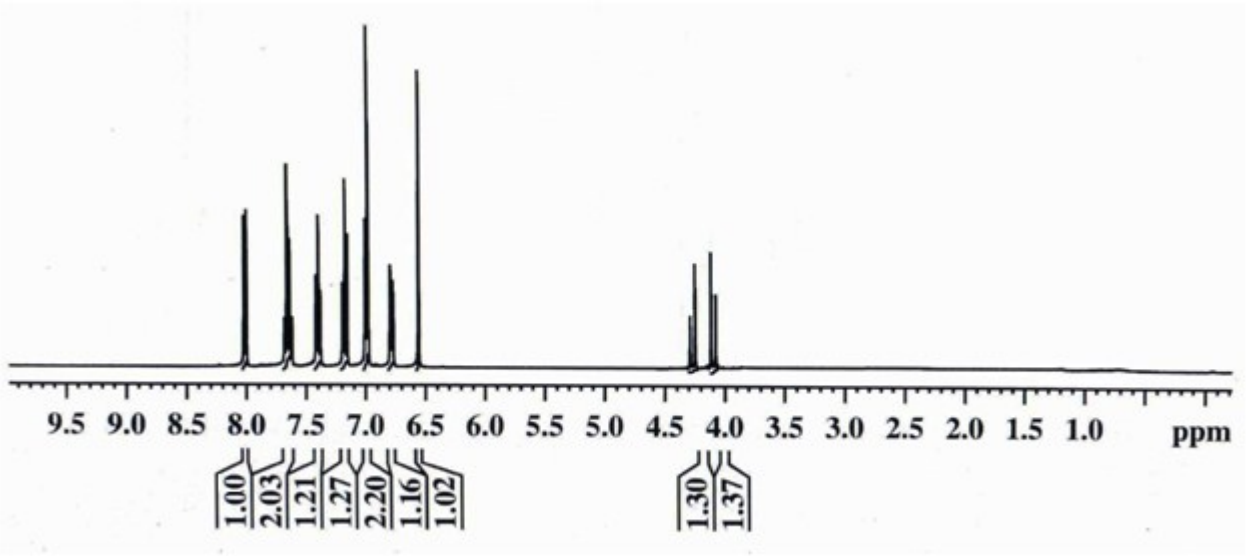
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Nov 25 2015
Temp. 25.0 C / 298.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5362583 MHz
DECOUPLE H1, 399.8277233 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min
170.343
164.219
149.055
147.688
135.019
134.122
130.988
128.864
127.207
125.061
123.680
122.768
108.516
67.988
40.511
40.298
40.093
39.881
39.676
39.463
39.251
33.817
220
200
180
160
140
120
100
80
60
40
20
0
ppm

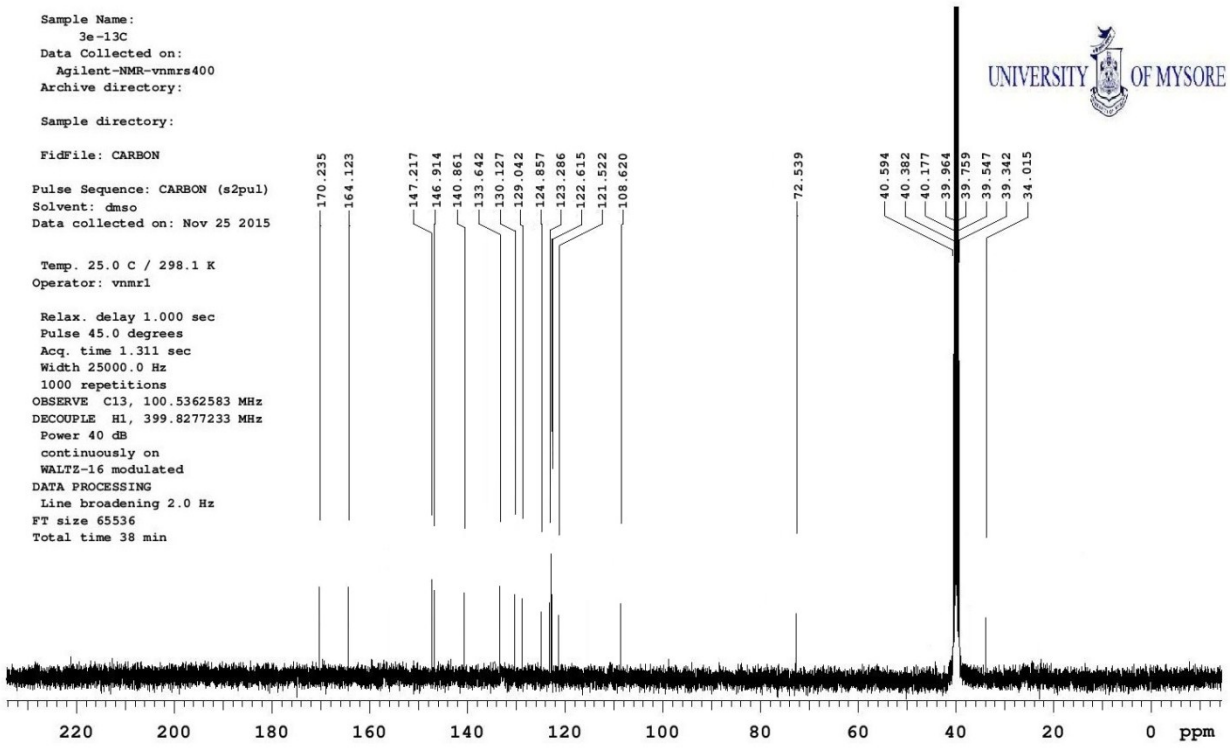


3e

Method	DEF_MS.M			Operator	MBU
Sample Name				Instrument	HCTultra ETD II
Acquisition Parameter					
Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	319 µs	Scan Begin	50 m/z	Scan End	1300 m/z
Capillary Exit	109.0 Volt	Skimmer	40.0 Volt	Trap Drive	49.6
Accumulation Time	Ultra Scan	Averages	5 Spectra	Auto MS/MS	off




9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
2.03
1.21
1.27
2.20
1.16
1.02
1.30
1.37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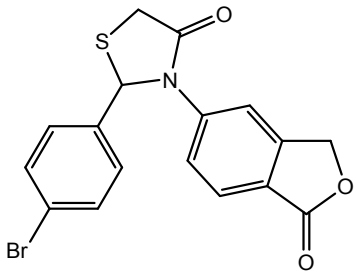
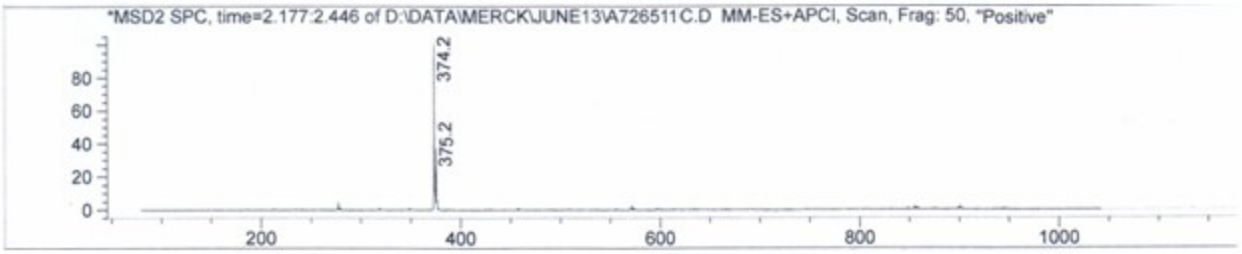
3e-13C
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Nov 25 2015
Temp. 25.0 C / 298.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5362583 MHz
DECOUPLE H1, 399.8277233 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min
UNIVERSITY OF MYSORE
170.235
164.123
147.217
146.914
140.861
133.642
130.127
129.042
124.857
123.286
122.615
121.522
108.620
72.539
40.594
40.382
40.177
39.964
39.759
39.547
39.342
34.015
220 200 180 160 140 120 100 80 60 40 20 0 ppm


S
O
N
Br
O
O

3f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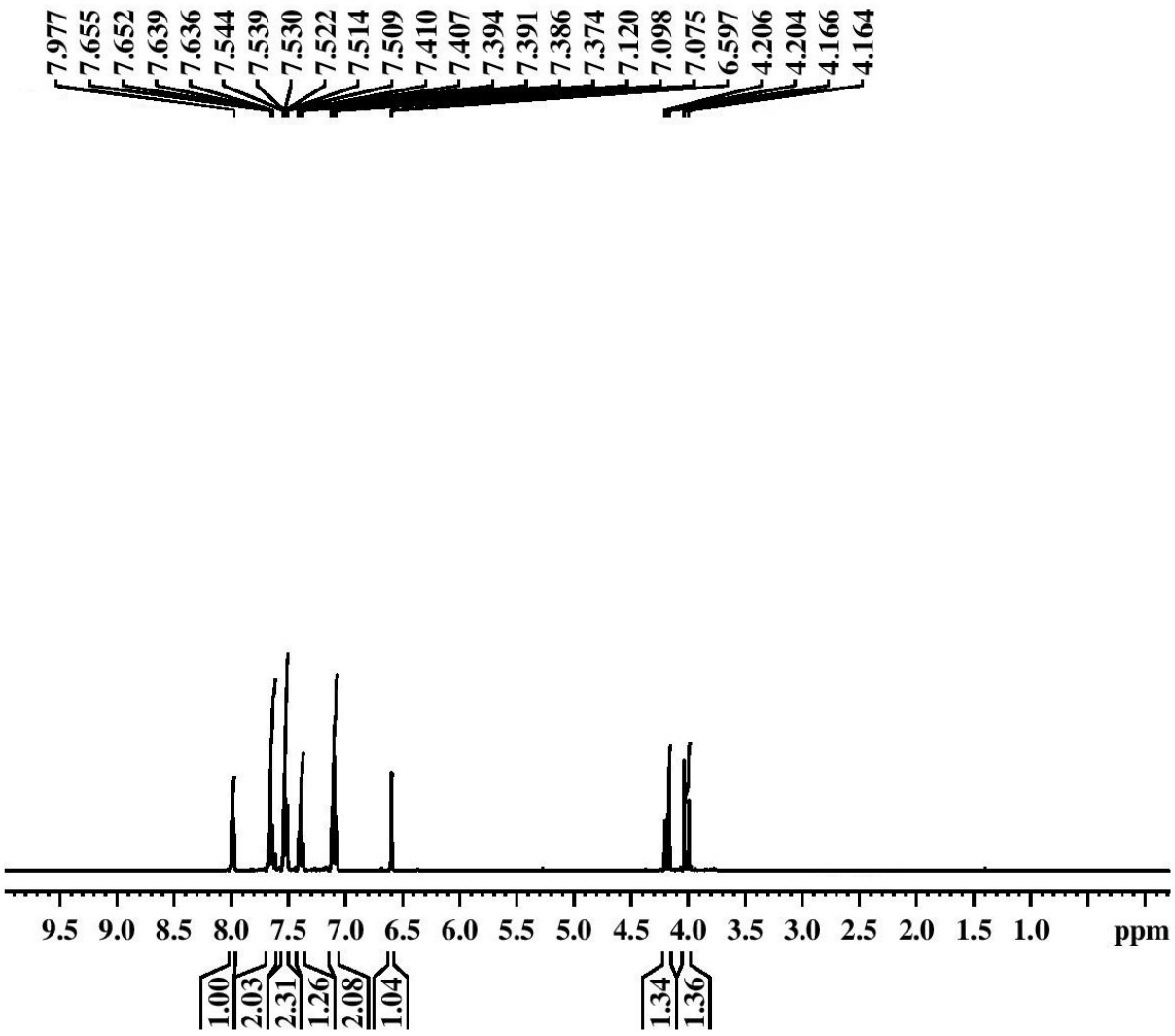
375.2
80
60
40
20
0
200
400
600
800
1000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7.636
7.544
7.539
7.530
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7.514
7.509
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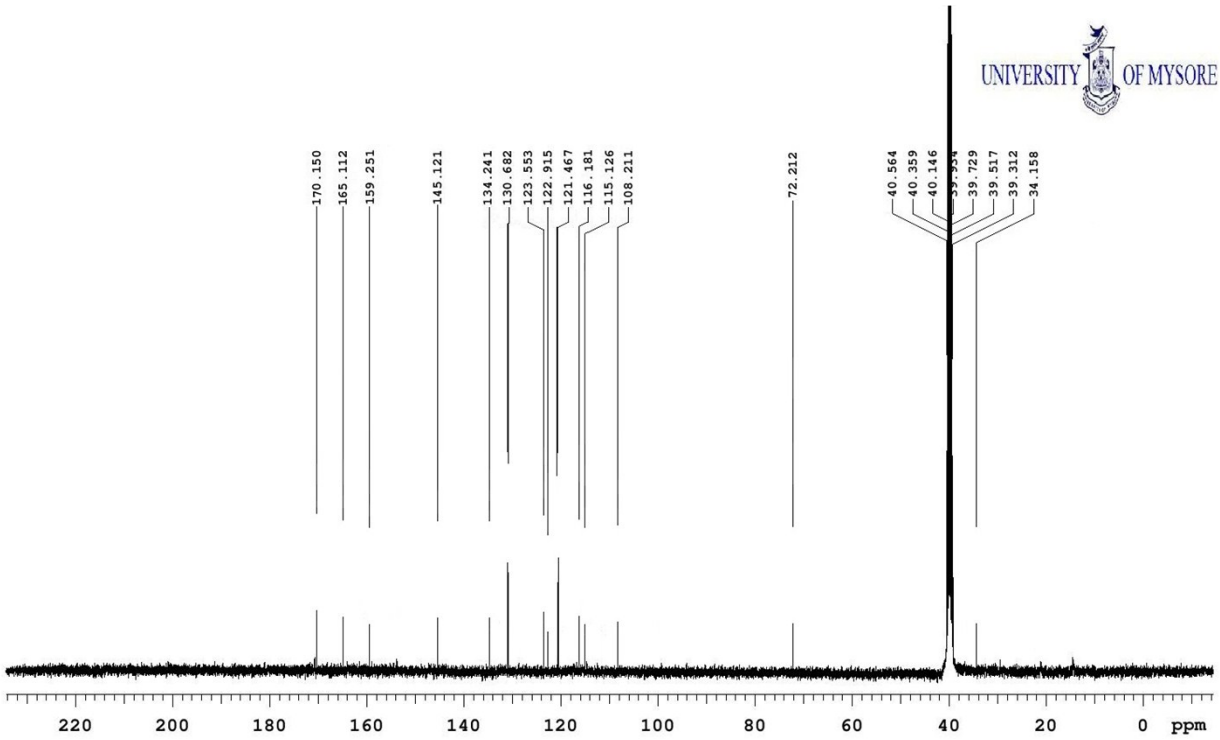
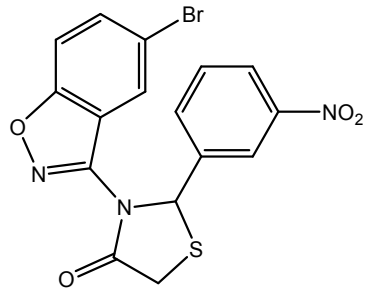
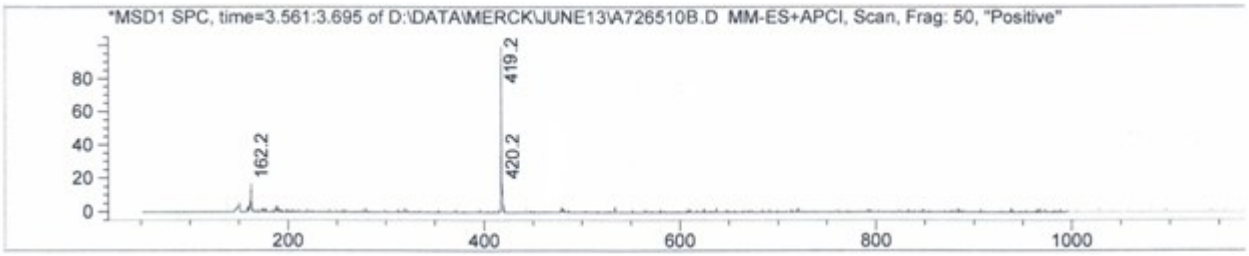
7.407
7.394
7.391
7.386
7.374
7.120
7.098
7.075
6.597
4.206
4.204
4.166
4.164
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
ppm
1.00
2.03
2.31
1.26
2.08
1.04
1.34
1.36



PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.311 sec Width 25000.0 Hz 3000 repetitions	OBSERVE C13, 100.5367359 DECOUPLE H1, 399.8296225 Power 40 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 115 minutes		1402373-3F-13C Solvent: dmso Ambient temperature Operator: vnmr1 File: 1402373-3F-13C VNMRS-400 "Agilent-NMR"


Br
O
N
N
S
O
NO2

3g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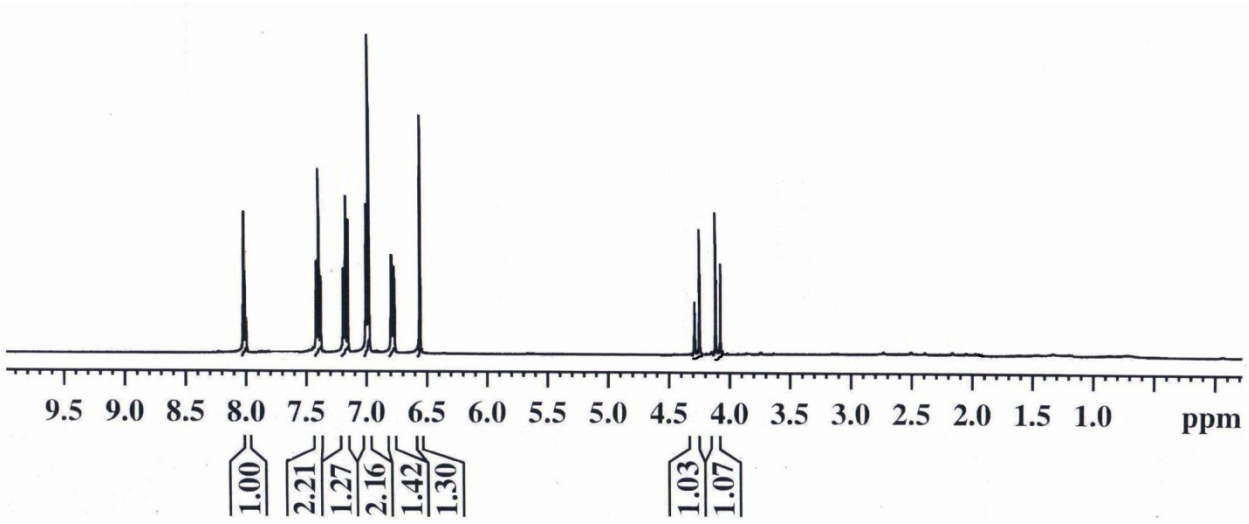
419.2
420.2
162.2
80
60
40
20
0
200
400
600
800
1000


9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
ppm
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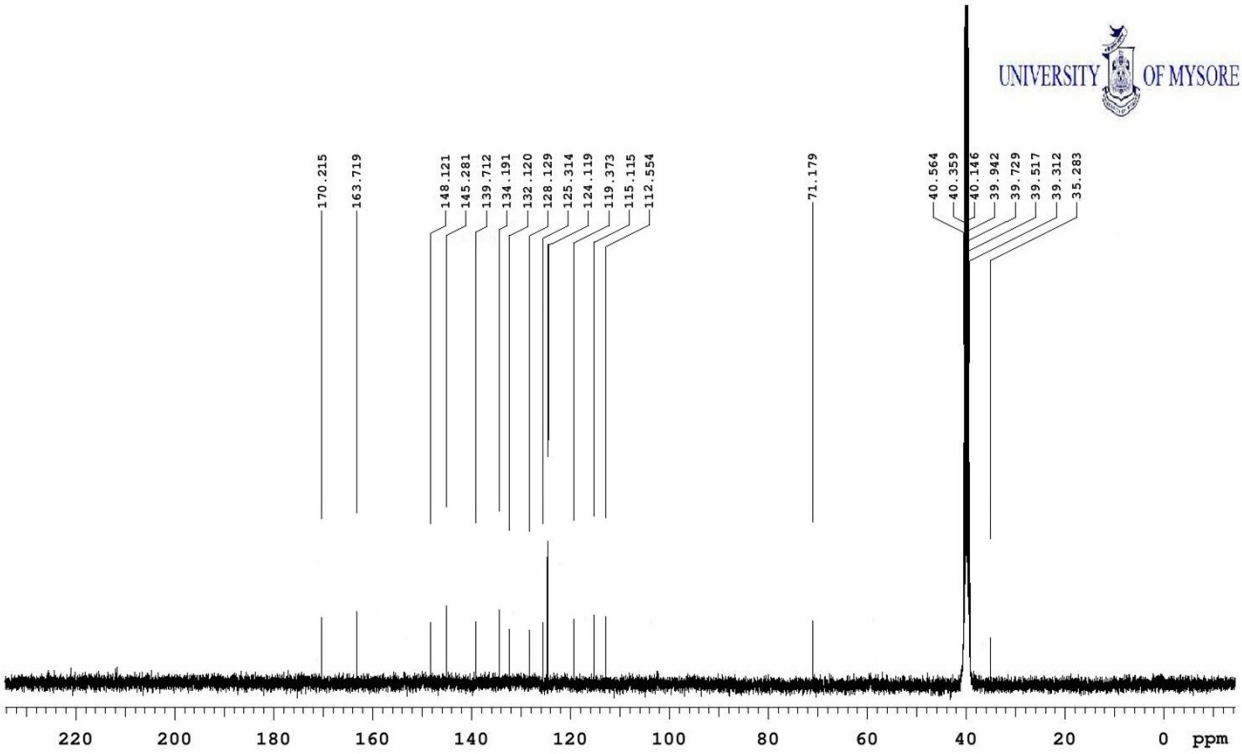
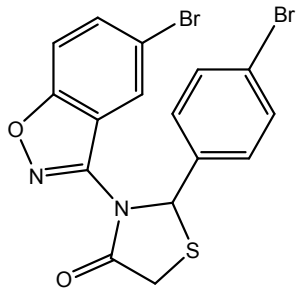
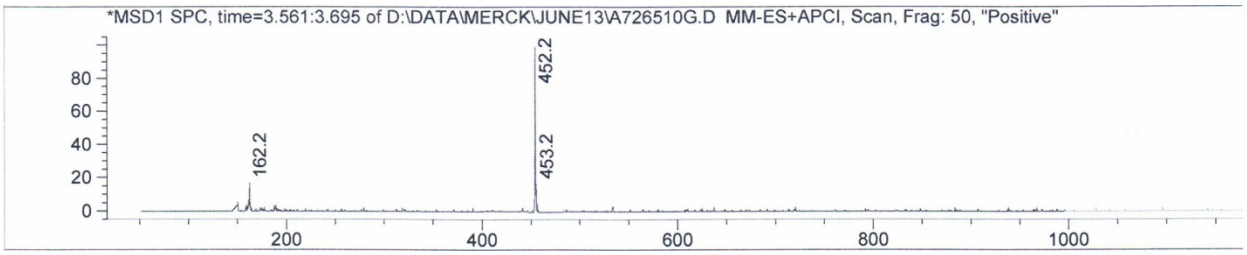
1.30
1.03
1.07

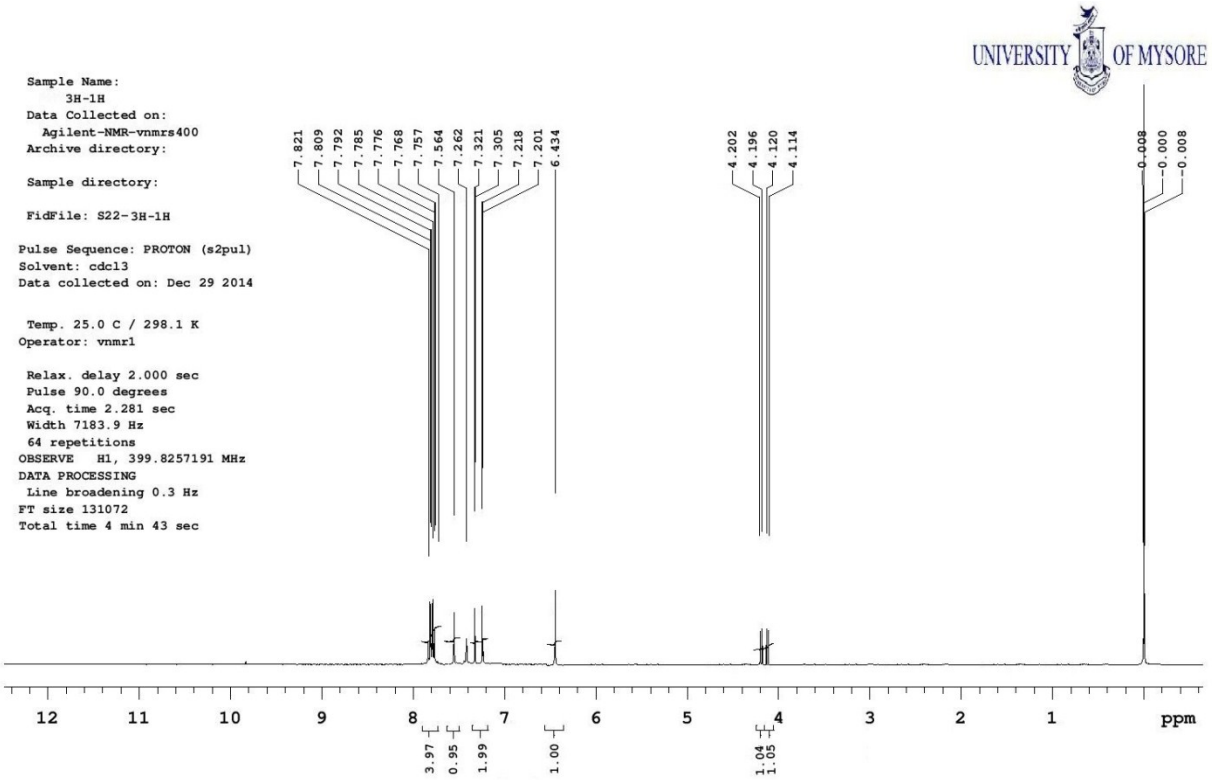


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.311 sec Width 25000.0 Hz 1650 repetitions	OBSERVE C13, 100.5367359 DECOUPLE H1, 399.8296225 Power 40 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 63 minutes		1402372-3G-13C Solvent: dmso Ambient temperature Operator: vnmr1 File: 1402372-3G-13C VNMRS-400 "Agilent-NMR"


Br
Br
O
N
N
S
O

3h


*MSD1 SPC, time=3.561:3.695 of D:\DATA\MERCK\JUNE13\A726510G.D MM-ES+APCI, Scan, Frag: 50, "Positive"
452.2
453.2
162.2
80
60
40
20
0
200
400
600
800
1000


UNIVERSITY OF MYSORE
Sample Name:
3H-1H
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: S22-3H-1H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 29 2014
Temp. 25.0 C / 298.1 K
Operator: vnmrl
Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 2.281 sec
Width 7183.9 Hz
64 repetitions
OBSERVE H1, 399.8257191 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 131072
Total time 4 min 43 sec
7.821
7.809
7.792
7.785
7.776
7.768
7.757
7.564
7.262
7.321
7.305
7.218
7.201
6.434
4.202
4.196
4.120
4.114
0.008
0.000
-0.008
12
11
10
9
8
7
6
5
4
3
2
1
ppm
3.97
0.95
1.99
1.00
1.04
1.05

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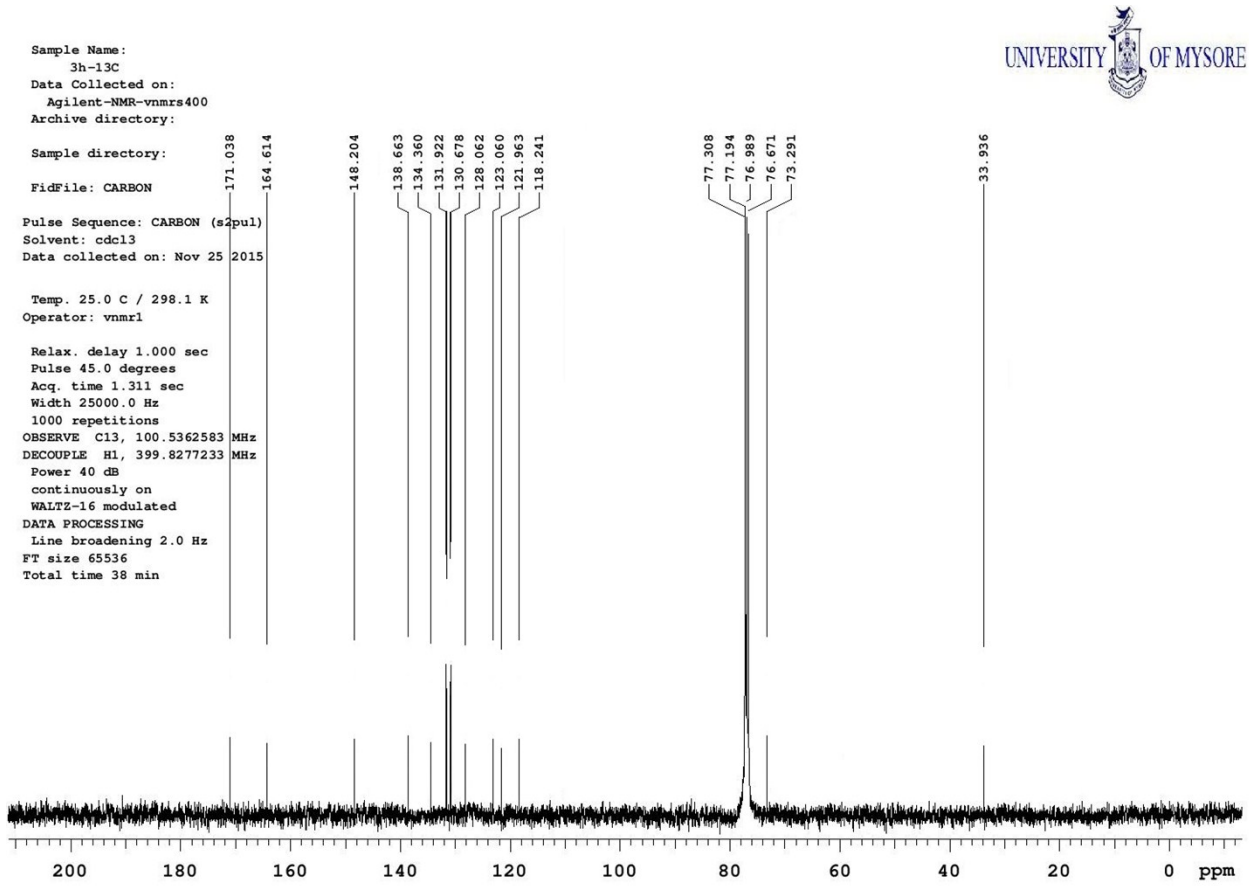
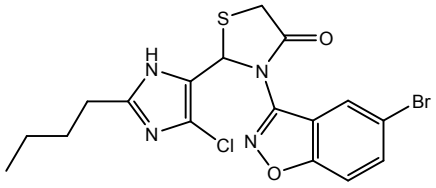
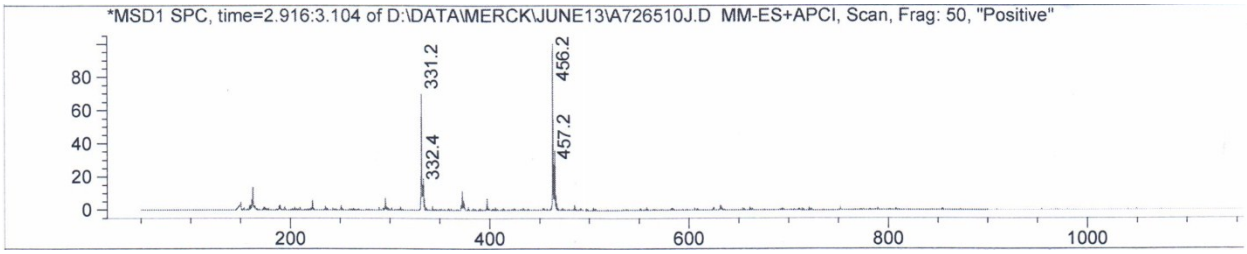
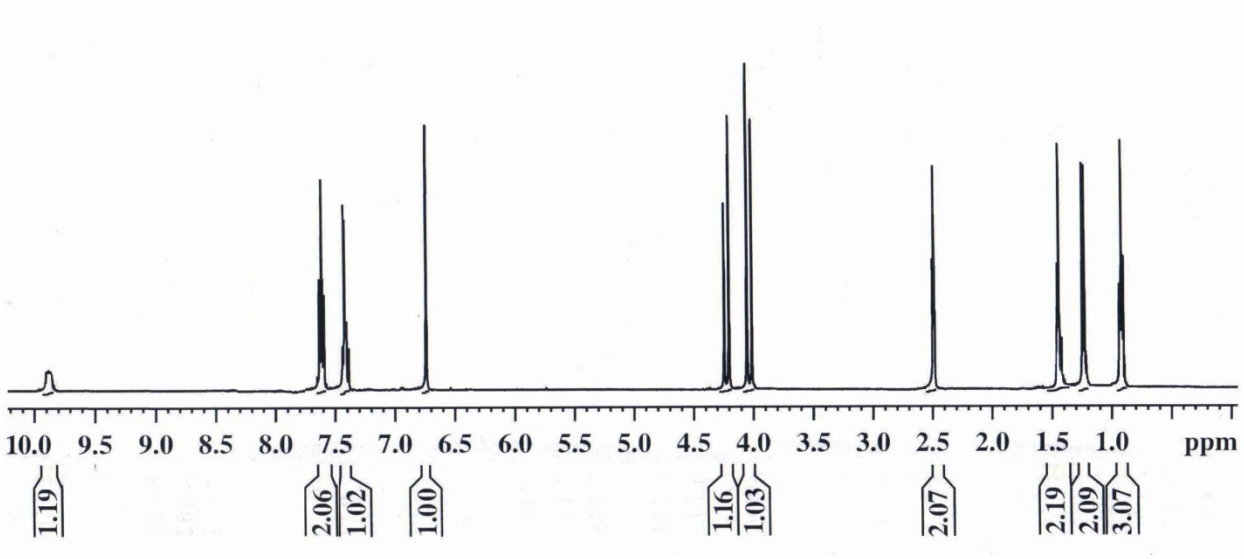
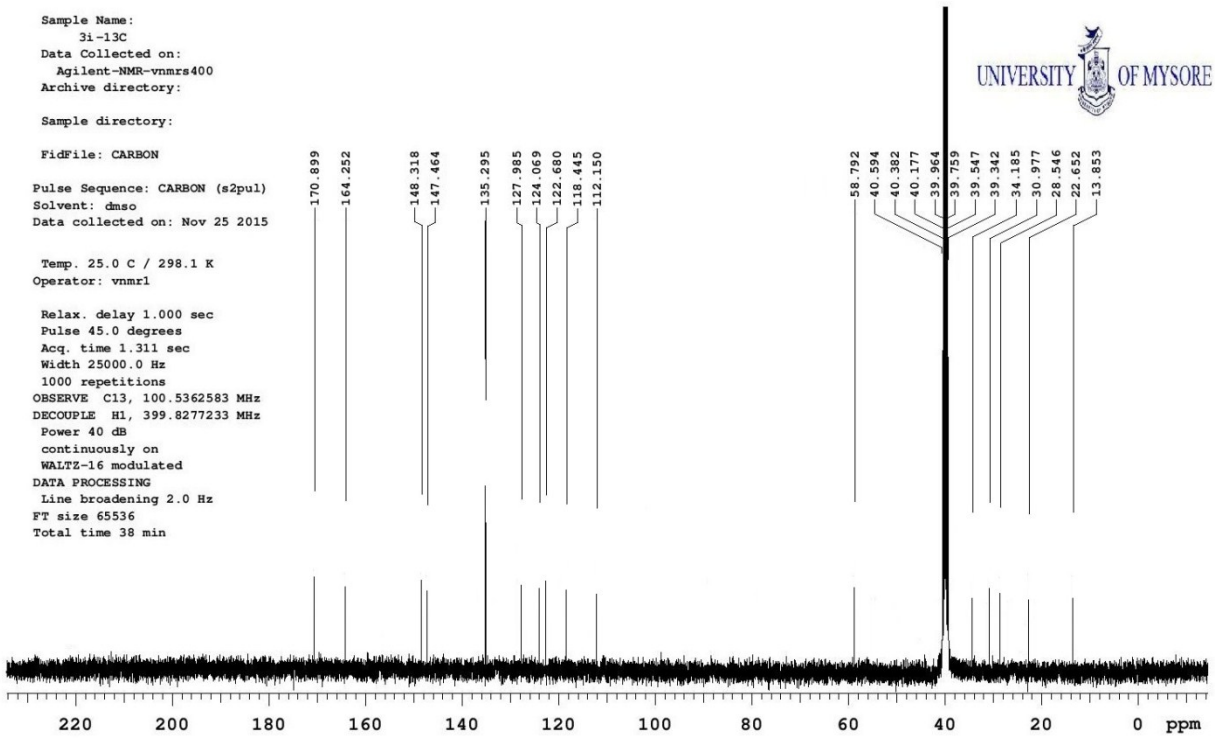


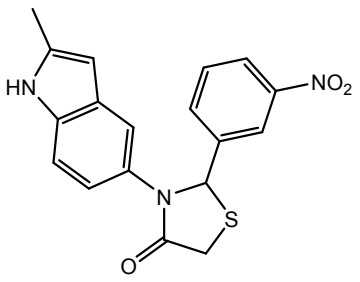

S
O
H
N
N
N
Br
Cl
N
O

3i

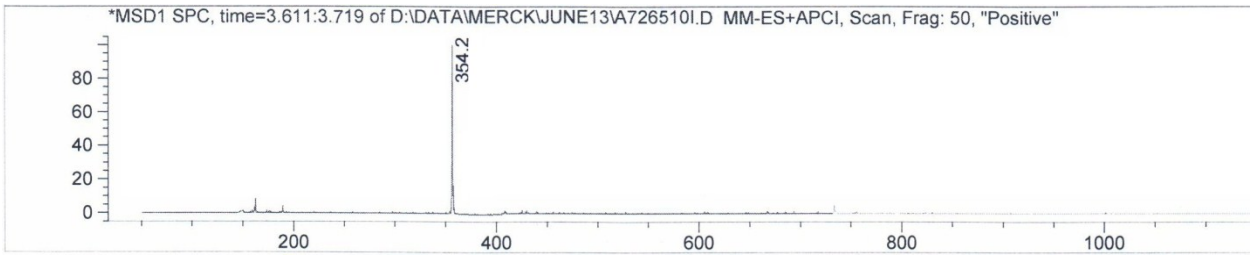

*MSD1 SPC, time=2.916:3.104 of D:\DATA\MERCK\JUNE13\A726510J.D MM-ES+APCI, Scan, Frag: 50, "Positive"
331.2
332.4
456.2
457.2
80
60
40
20
0
200
400
600
800
1000

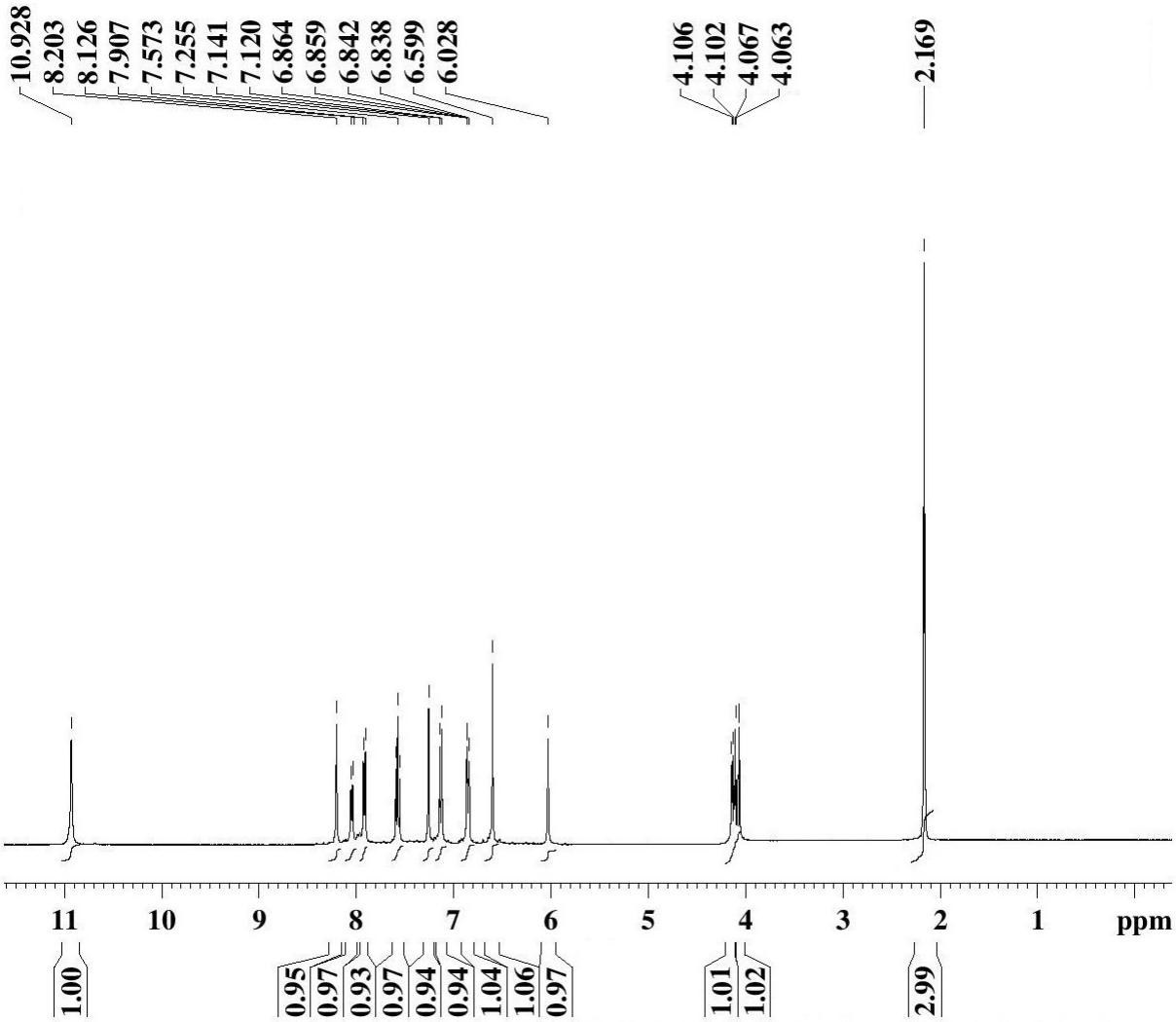

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.19
2.06
1.02
1.00
1.16
1.03
2.07
2.19
2.09
3.07

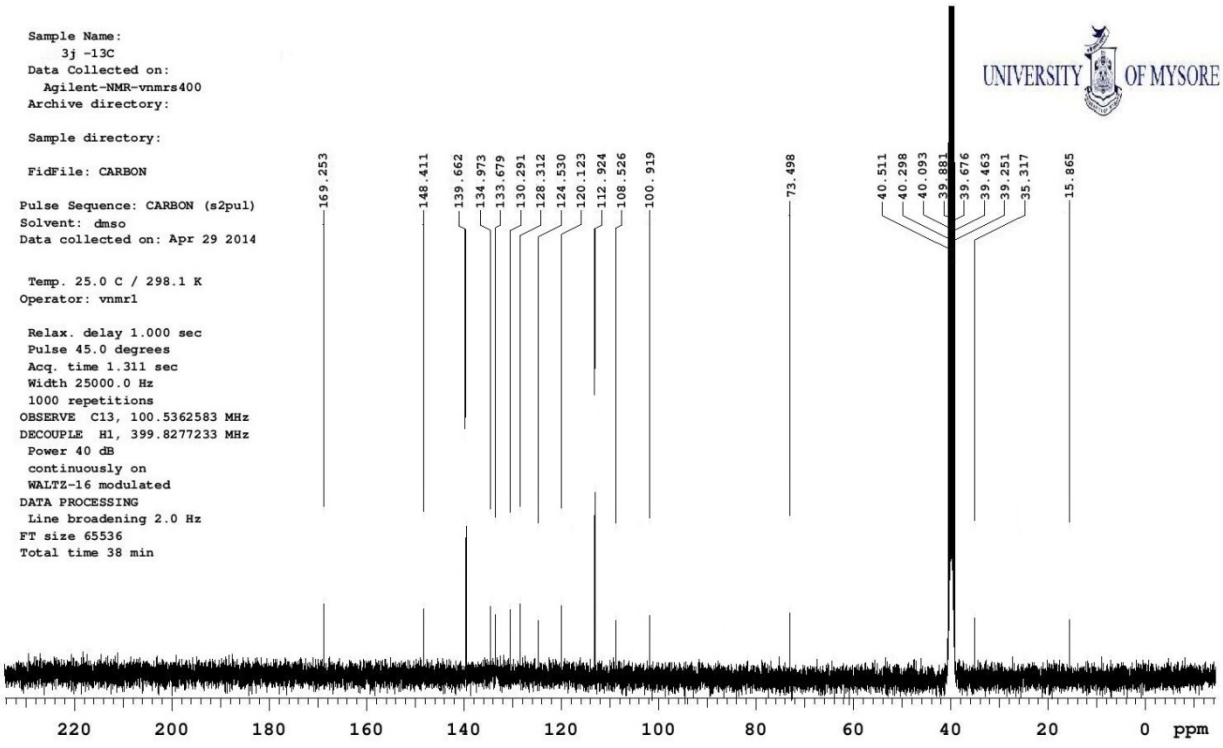

Sample Name:
3i-13C
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Nov 25 2015
Temp. 25.0 C / 298.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5362583 MHz
DECOUPLE H1, 399.8277233 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min
170.899
164.252
148.318
147.464
135.295
127.985
124.069
122.680
118.445
112.150
58.792
40.594
40.382
40.177
39.964
39.759
39.547
39.342
34.185
30.977
28.546
22.652
13.853
220
200
180
160
140
120
100
80
60
40
20
0
ppm

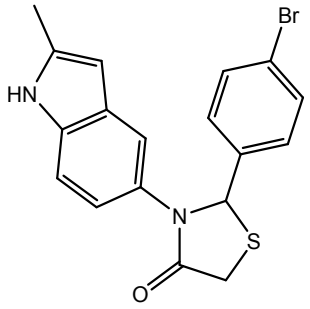

HN
NO2
N
S
O

3j

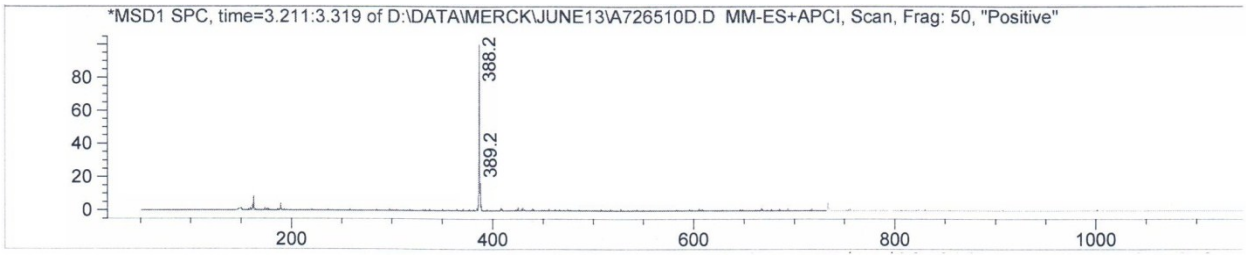

*MSD1 SPC, time=3.611:3.719 of D:\DATA\MERCK\JUNE13\A726510I.D MM-ES+APCI, Scan, Frag: 50, "Positive"
354.2
80
60
40
20
0
200
400
600
800
1000

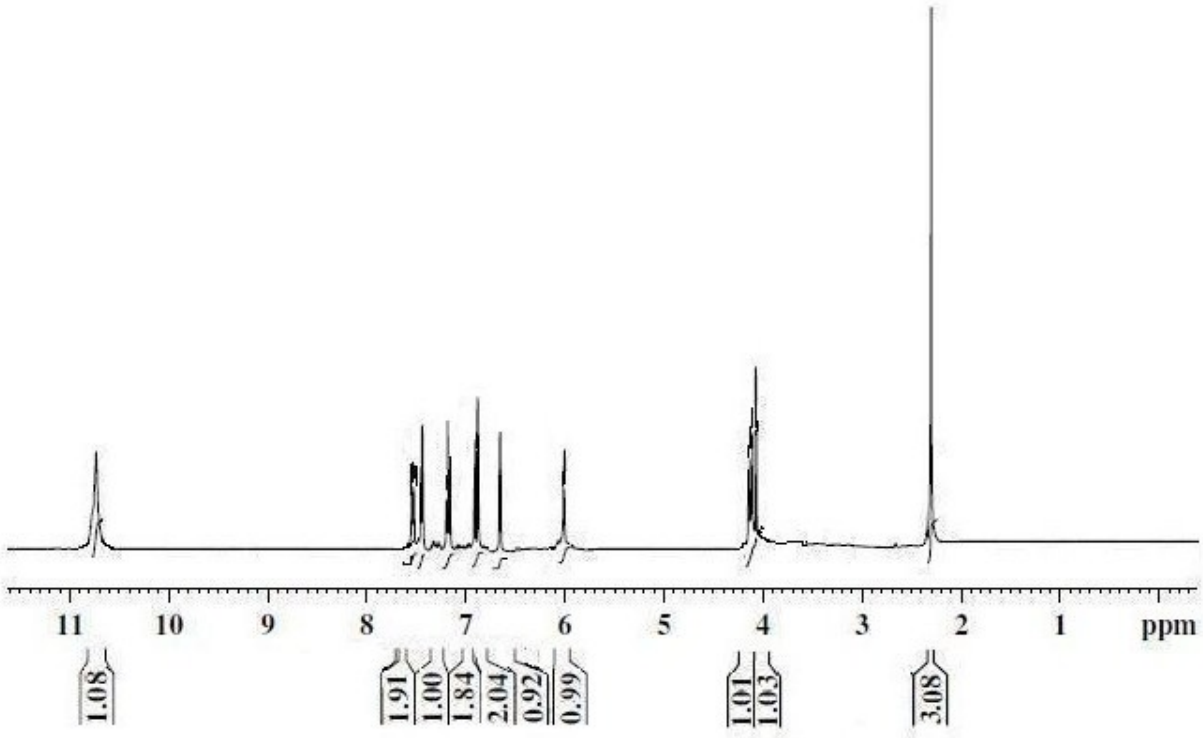

10.928
8.203
8.126
7.907
7.573
7.255
7.141
7.120
6.864
6.859
6.842
6.838
6.599
6.028
4.106
4.102
4.067
4.063
2.169
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.95
0.97
0.93
0.97
0.94
0.94
1.04
1.06
0.97
1.01
1.02
2.99

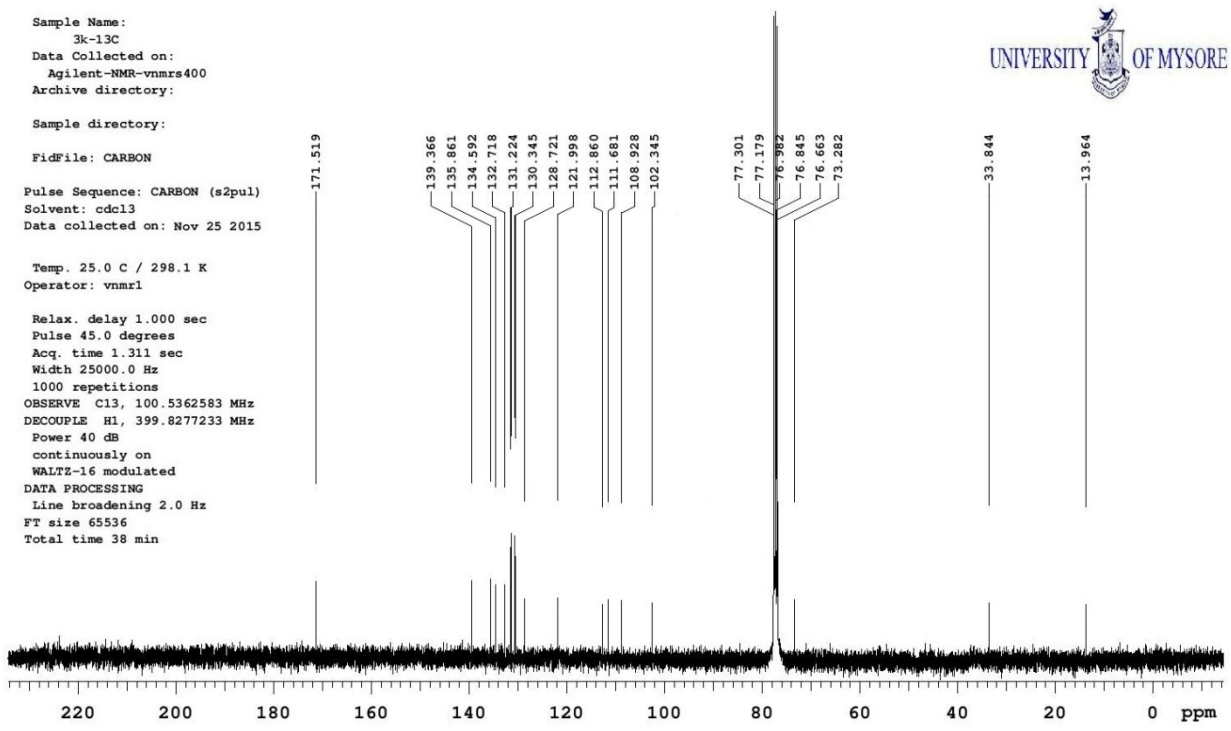

Sample Name:
3j -13C
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Apr 29 2014
Temp. 25.0 C / 298.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5362583 MHz
DECOUPLE H1, 399.8277233 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min
169.253
148.411
139.662
134.973
133.679
130.291
128.312
124.530
120.123
112.924
108.526
100.919
73.498
40.511
40.298
40.093
39.881
39.676
39.463
39.251
35.317
15.865
220
200
180
160
140
120
100
80
60
40
20
0
ppm

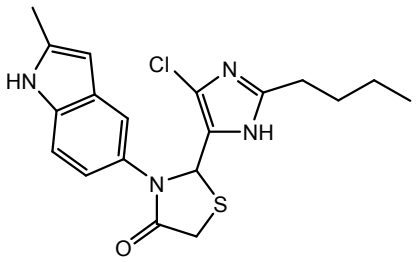

Br
HN
N
S
O

3k

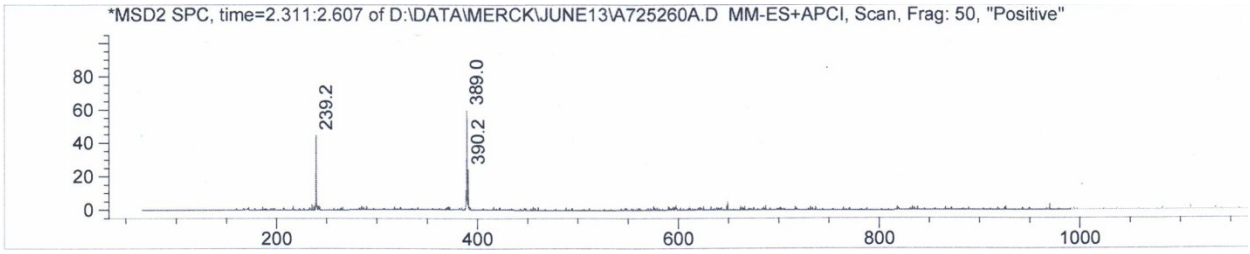

*MSD1 SPC, time=3.211:3.319 of D:\DATA\MERCK\JUNE13\A726510D.D MM-ES+APCI, Scan, Frag: 50, "Positive"
388.2
389.2
80
60
40
20
0
200
400
600
800
1000

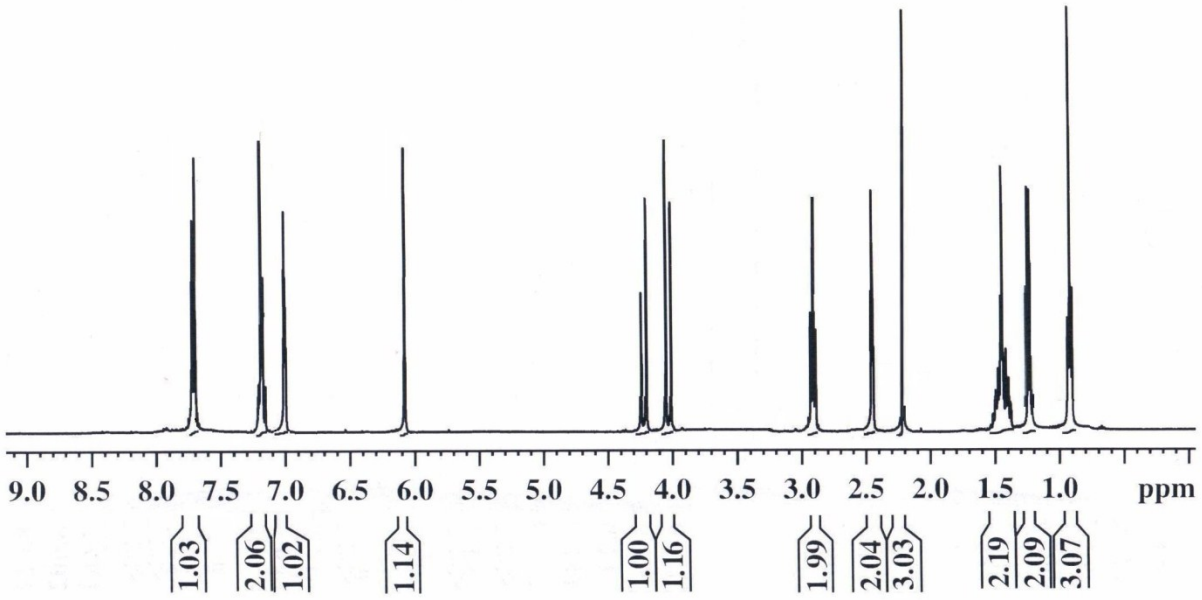

11
10
9
8
7
6
5
4
3
2
1
ppm
1.08
1.91
1.00
1.84
2.04
0.92
0.99
1.01
1.03
3.08

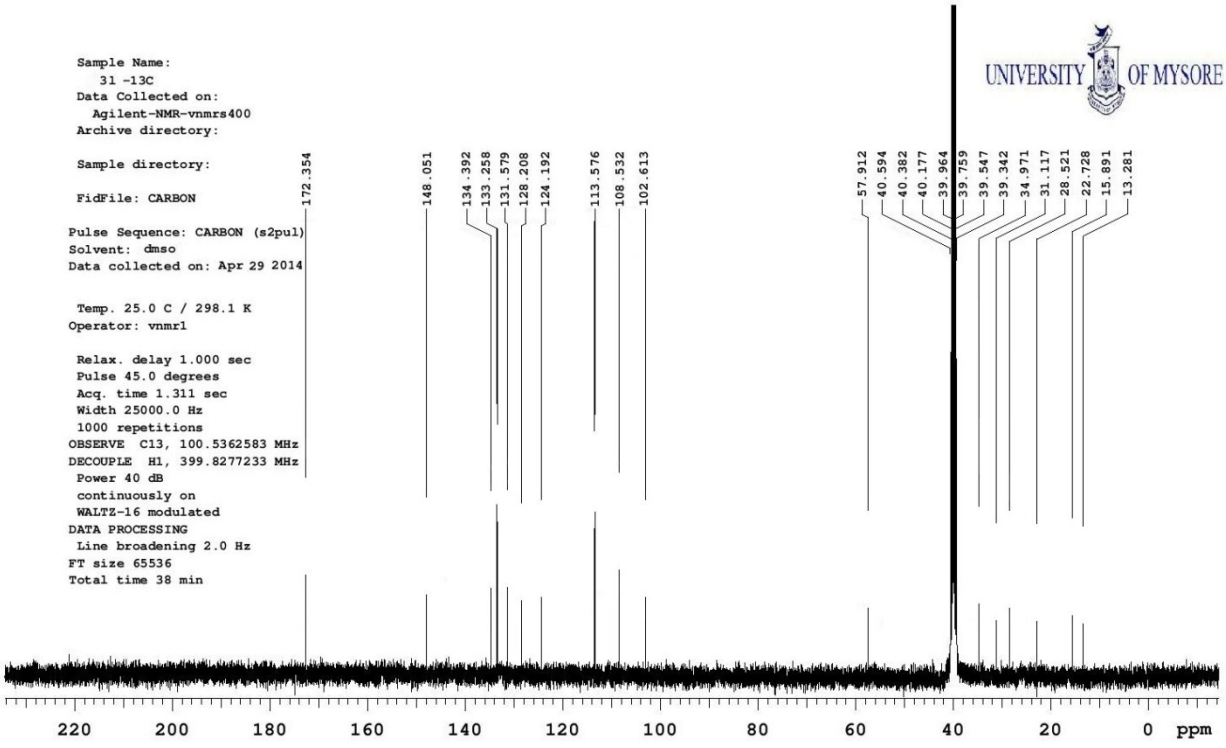

Sample Name:
3k-13C
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 25 2015
Temp. 25.0 C / 298.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5362583 MHz
DECOUPLE H1, 399.8277233 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min
171.519
139.366
135.861
134.592
132.718
131.224
130.345
128.721
121.998
112.860
111.681
108.928
102.345
77.301
77.179
76.982
76.845
76.663
73.282
33.844
13.964
220
200
180
160
140
120
100
80
60
40
20
0
ppm

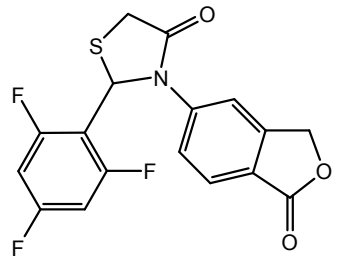

HN
Cl
N
NH
N
S
O

3l

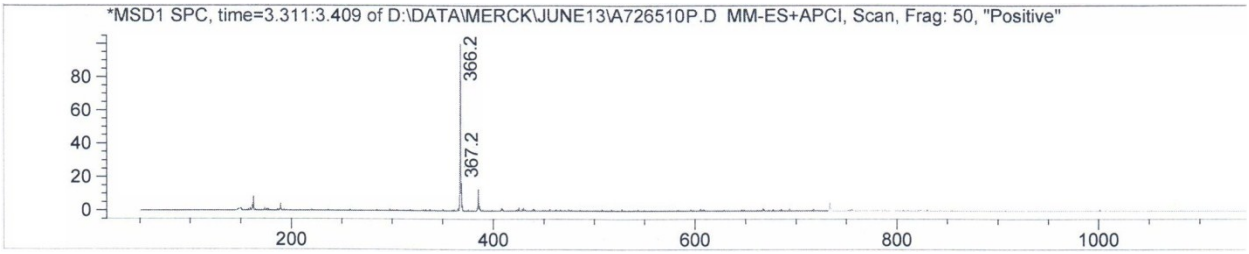

*MSD2 SPC, time=2.311:2.607 of D:\DATA\MERCK\JUNE13\A725260A.D MM-ES+APCI, Scan, Frag: 50, "Positive"
239.2
389.0
390.2
80
60
40
20
0
200
400
600
800
1000

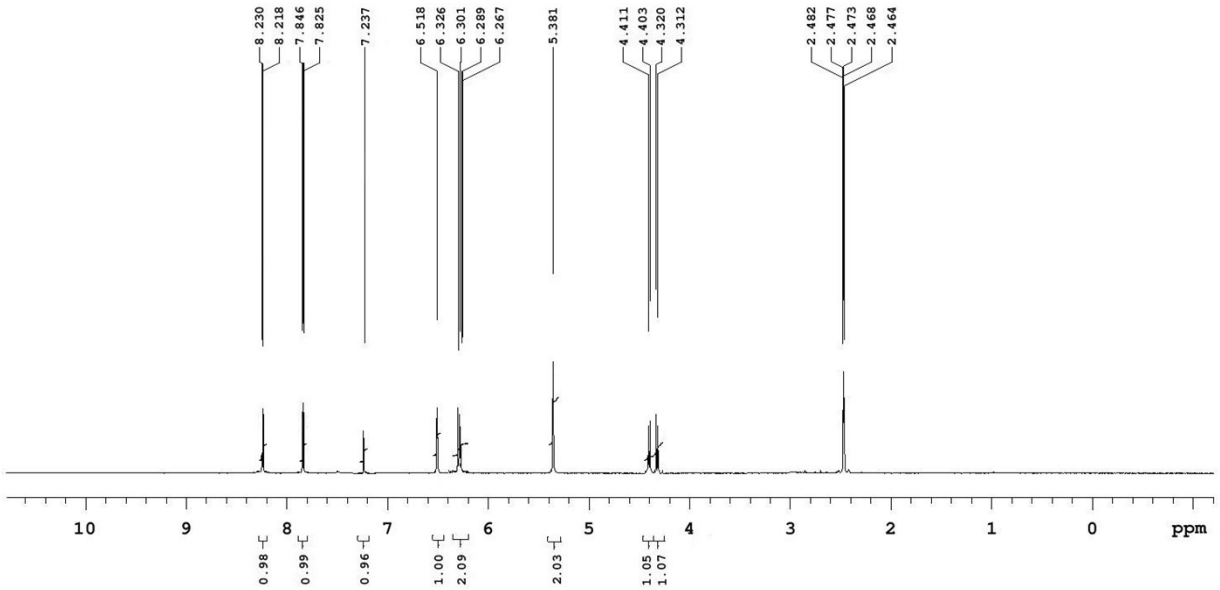

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.03
2.06
1.02
1.14
1.00
1.16
1.99
2.04
3.03
2.19
2.09
3.07

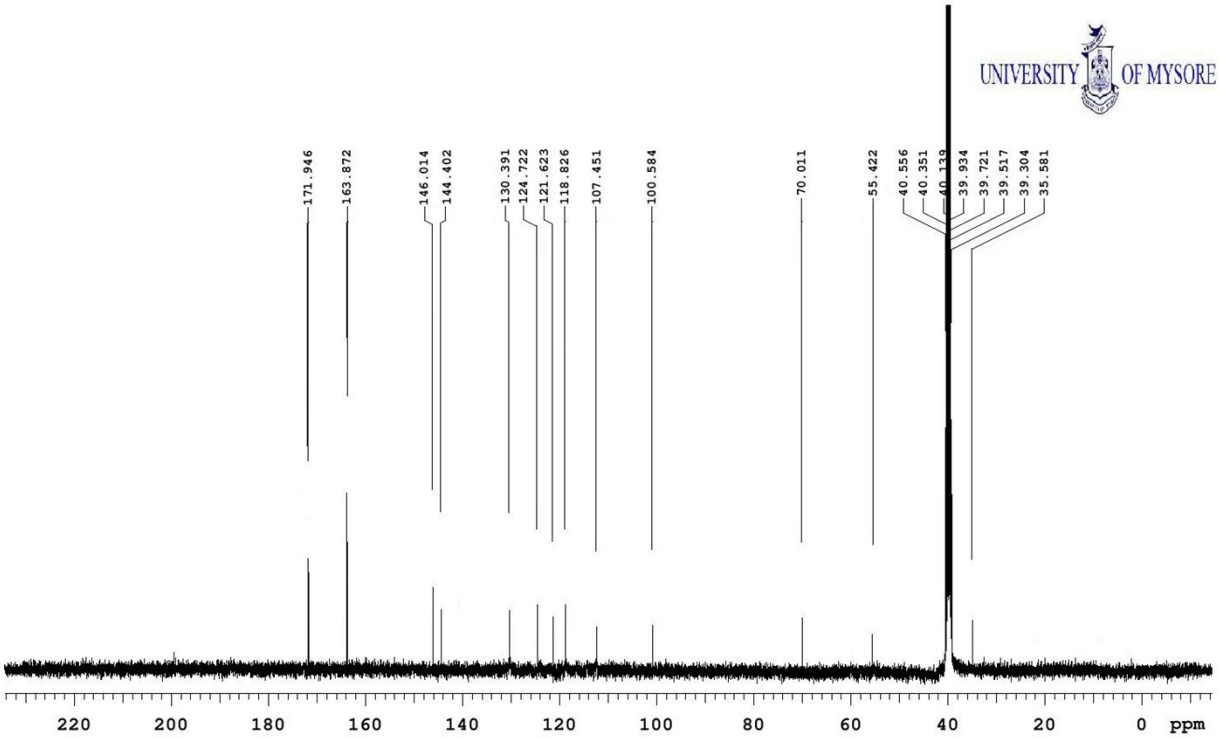

UNIVERSITY OF MYSORE
Sample Name:
31 -13C
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Apr 29 2014
Temp. 25.0 C / 298.1 K
Operator: vnmrl
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5362583 MHz
DECOUPLE H1, 399.8277233 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min
172.354
148.051
134.392
133.258
131.579
128.208
124.192
113.576
108.532
102.613
57.912
40.594
40.382
40.177
39.964
39.759
39.547
39.342
34.971
31.117
28.521
22.728
15.891
13.281
220
200
180
160
140
120
100
80
60
40
20
0
ppm


O
S
N
F
F
F
O
O

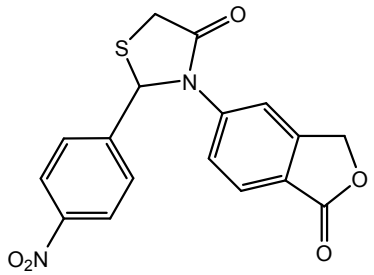
3m


*MSD1 SPC, time=3.311:3.409 of D:\DATA\MERCK\JUNE13\A726510P.D MM-ES+APCI, Scan, Frag: 50, "Positive"
366.2
367.2
80
60
40
20
0
200
400
600
800
1000

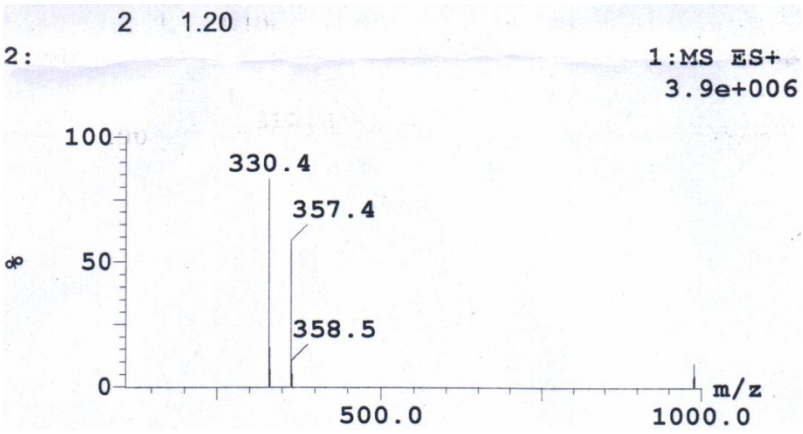

8.230
8.218
7.846
7.825
7.237
6.518
6.326
6.301
6.289
6.267
5.381
4.411
4.403
4.320
4.312
2.482
2.477
2.473
2.468
2.464
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
0.99
0.96
1.00
2.09
2.03
1.05
1.07

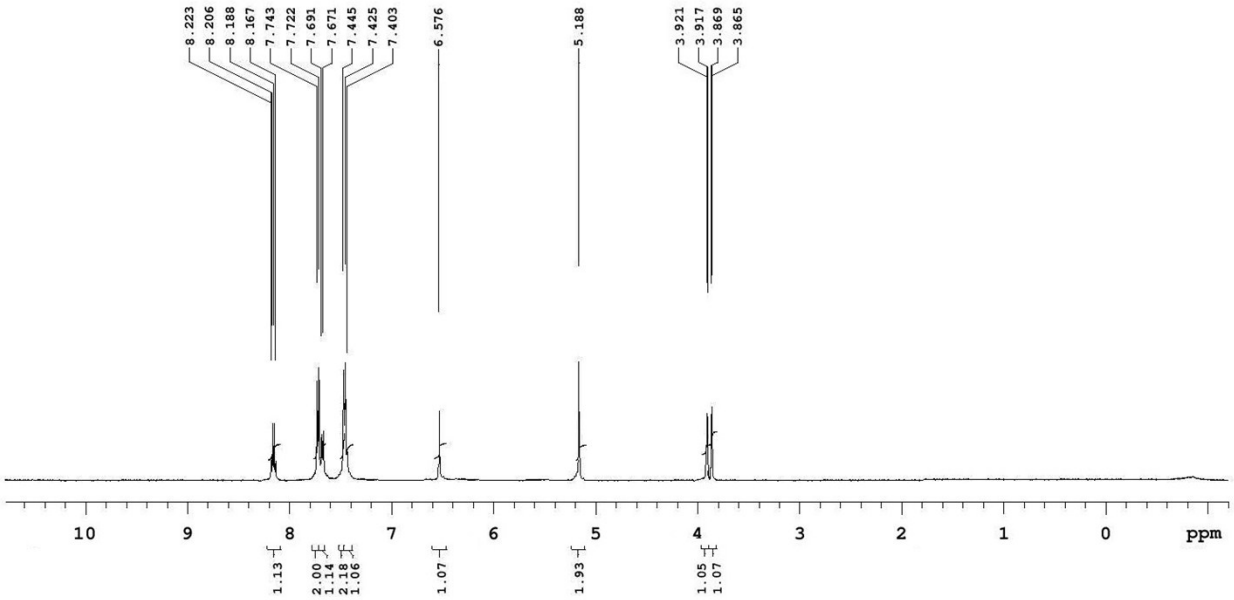


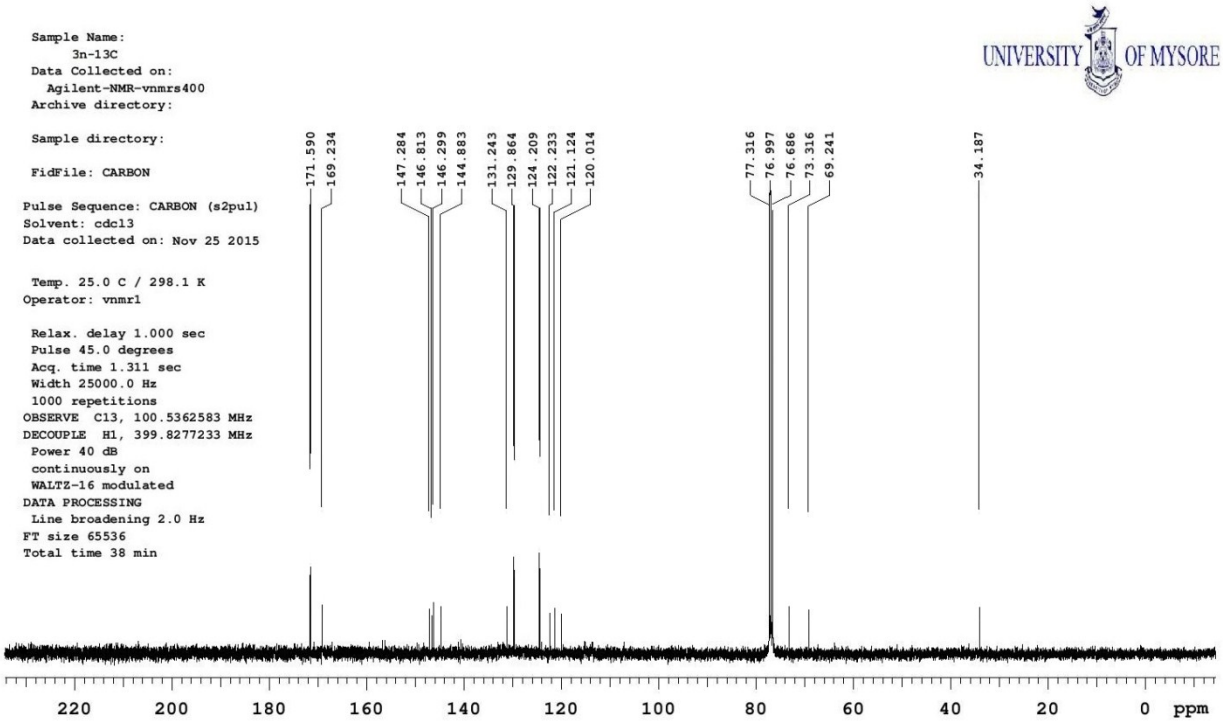
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.311 sec Width 25000.0 Hz 2282 repetitions	OBSERVE C13, 100.5367359 DECOUPLE H1, 399.8296225 Power 40 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 87 minutes		1402374-3M-13C Solvent: dmso Ambient temperature Operator: vnmr1 VNMRS-400 "Agilent-NMR"

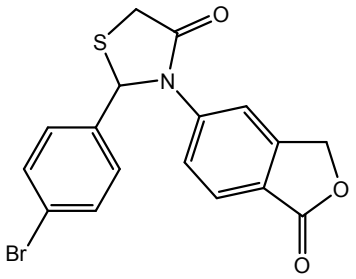

O
S
N
O
O
O2N

3n

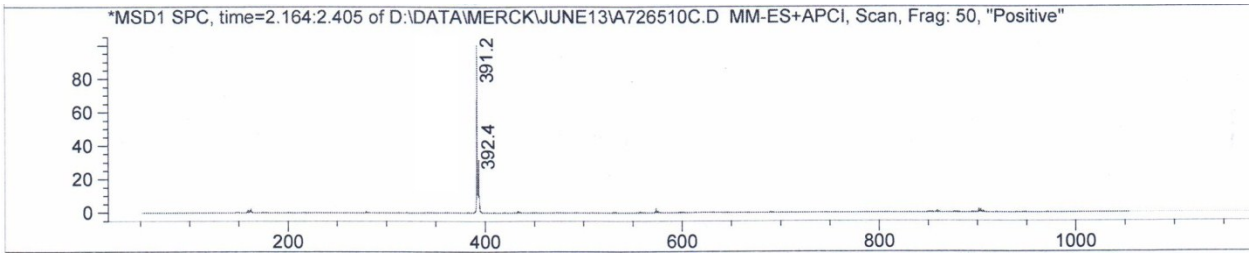

2 1.20
2:
1:MS ES+
3.9e+006
100
50
0
%
330.4
357.4
358.5
m/z
500.0
1000.0

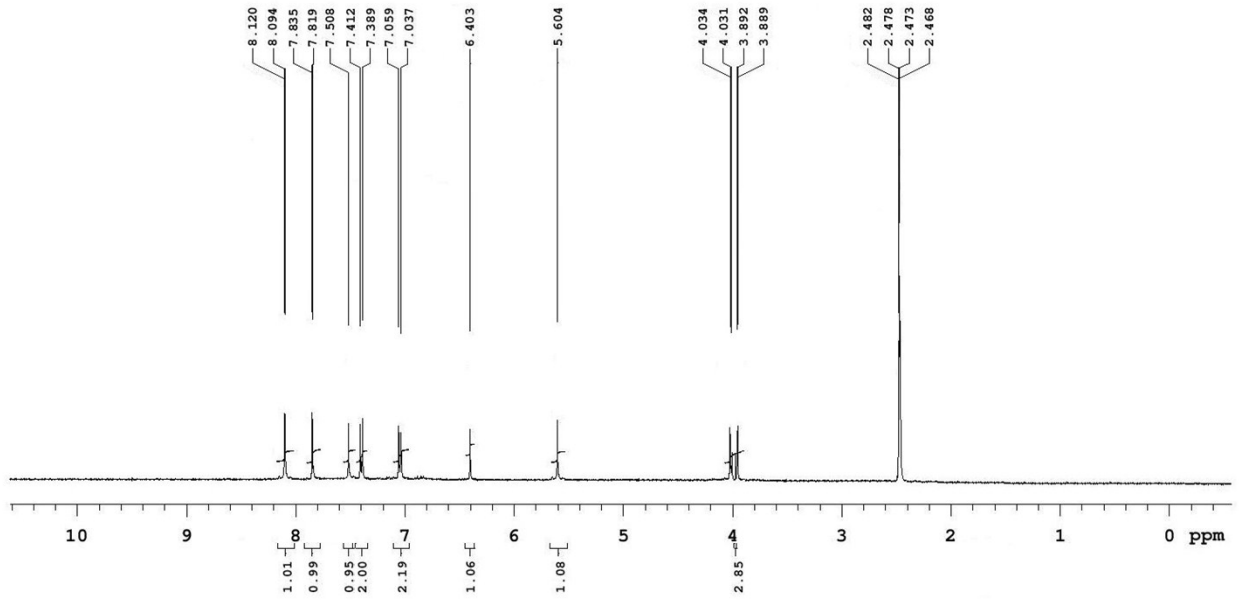

8.223
8.206
8.188
8.167
7.743
7.722
7.691
7.671
7.445
7.425
7.403
6.576
5.188
3.921
3.917
3.869
3.865
10
9
8
7
6
5
4
3
2
1
0
ppm
1.13
2.00
1.14
2.18
1.06
1.07
1.93
1.05
1.07

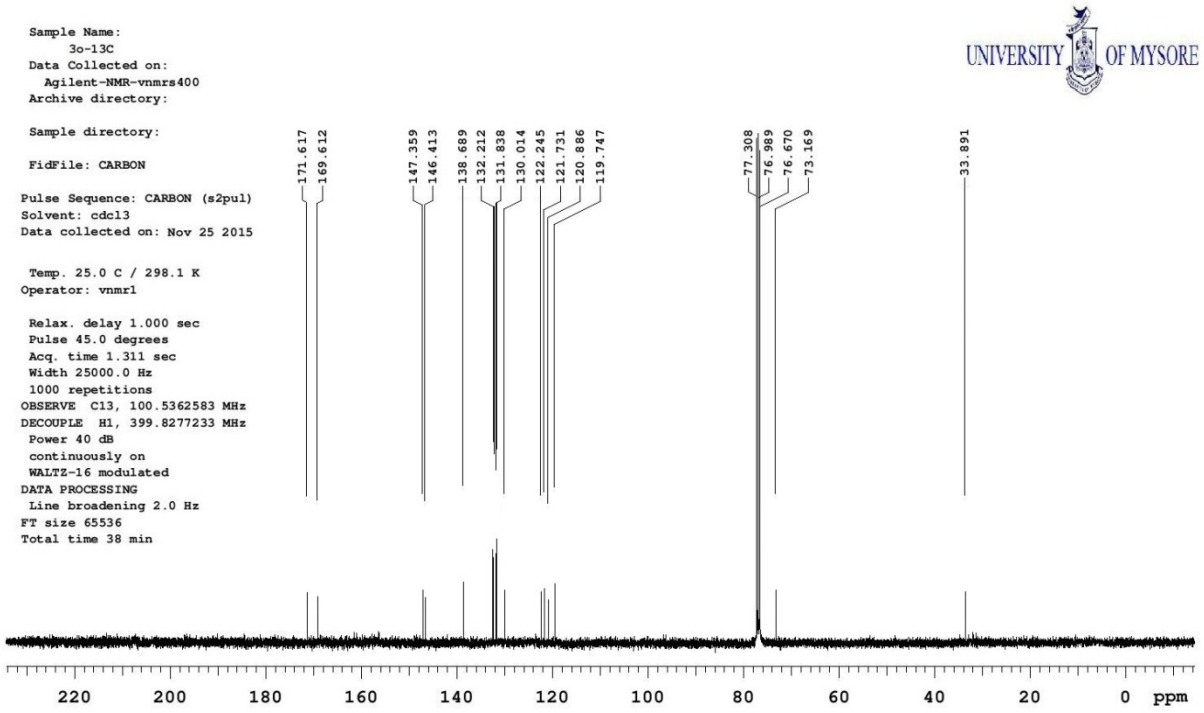

Sample Name:
3n-13C
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 25 2015
Temp. 25.0 C / 298.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5362583 MHz
DECOUPLE H1, 399.8277233 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min
171.590
169.234
147.284
146.813
146.299
144.883
131.243
129.864
124.209
122.233
121.124
120.014
77.316
76.997
76.686
73.316
69.241
34.187
220
200
180
160
140
120
100
80
60
40
20
0
ppm


S
O
N
Br
O
O

3o


*MSD1 SPC, time=2.164:2.405 of D:\DATA\MERCK\JUNE13\A726510C.D MM-ES+APCI, Scan, Frag: 50, "Positive"
391.2
392.4
80
60
40
20
0
200
400
600
800
1000


8.120
8.094
7.835
7.819
7.508
7.412
7.389
7.059
7.037
6.403
5.604
4.034
4.031
3.892
3.889
2.482
2.478
2.473
2.468
10
9
8
7
6
5
4
3
2
1
0 ppm
1.01
0.99
0.95
2.00
2.19
1.06
1.08
2.85


Sample Name:
3o-13C
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 25 2015
Temp. 25.0 C / 298.1 K
Operator: vnmrl
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5362583 MHz
DECOUPLE H1, 399.8277233 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min
171.617
169.612
147.359
146.413
138.689
132.212
131.838
130.014
122.245
121.731
120.886
119.747
77.308
76.989
76.670
73.169
33.891
220
200
180
160
140
120
100
80
60
40
20
0
ppm