ZIRCONIUM CATALYZED CEMOSELECTIVE SYNTHESIS OF NEW AMIDO-SUBSTITUTED BENZO[*b*]FURANS VIA A ONE-POT REACTION

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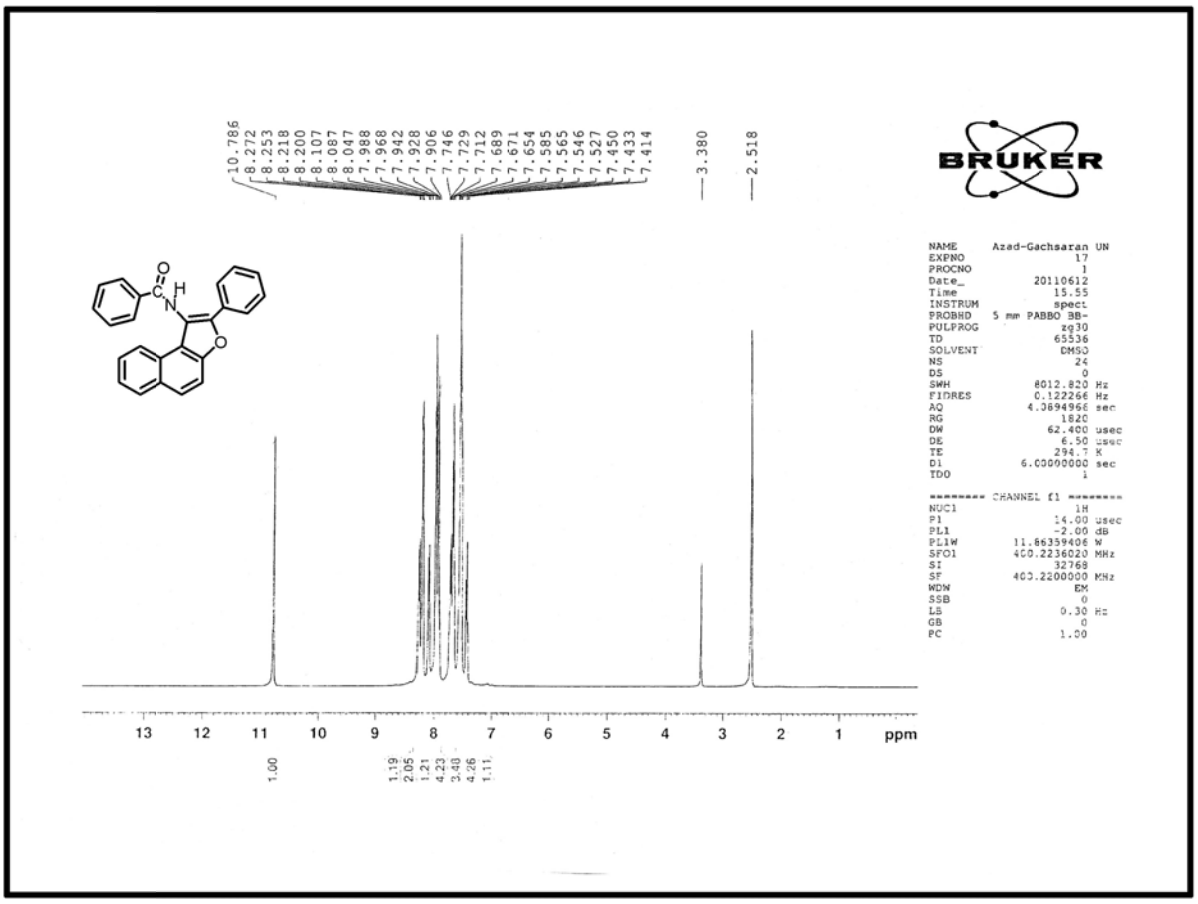
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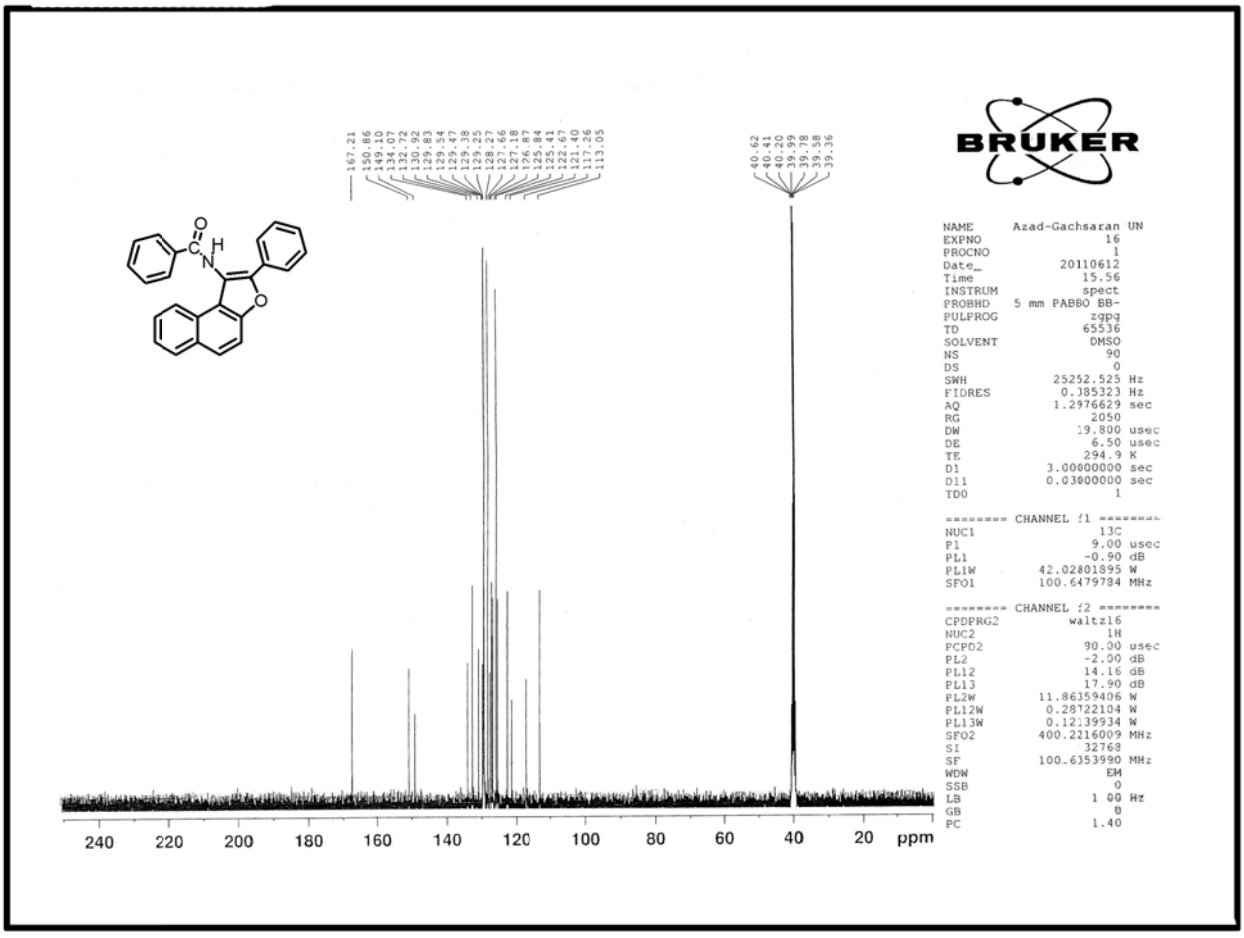
8.218
8.200
8.107
8.087
8.047
7.988
7.968
7.942
7.928
7.906
7.746
7.729
7.712
7.689
7.671
7.654
7.585
7.565
7.546
7.527
7.450
7.433
7.414
3.380
2.518
BRUKER
NAME Azad-Gachsaran UN
EXPNO 17
PROCNO 1
Date_ 20110612
Time 15.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 1820
DW 62.400 usec
DE 6.50 usec
TE 294.7 K
D1 6.00000000 sec
TDO 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.19
2.05
1.21
4.23
3.48
4.26
1.11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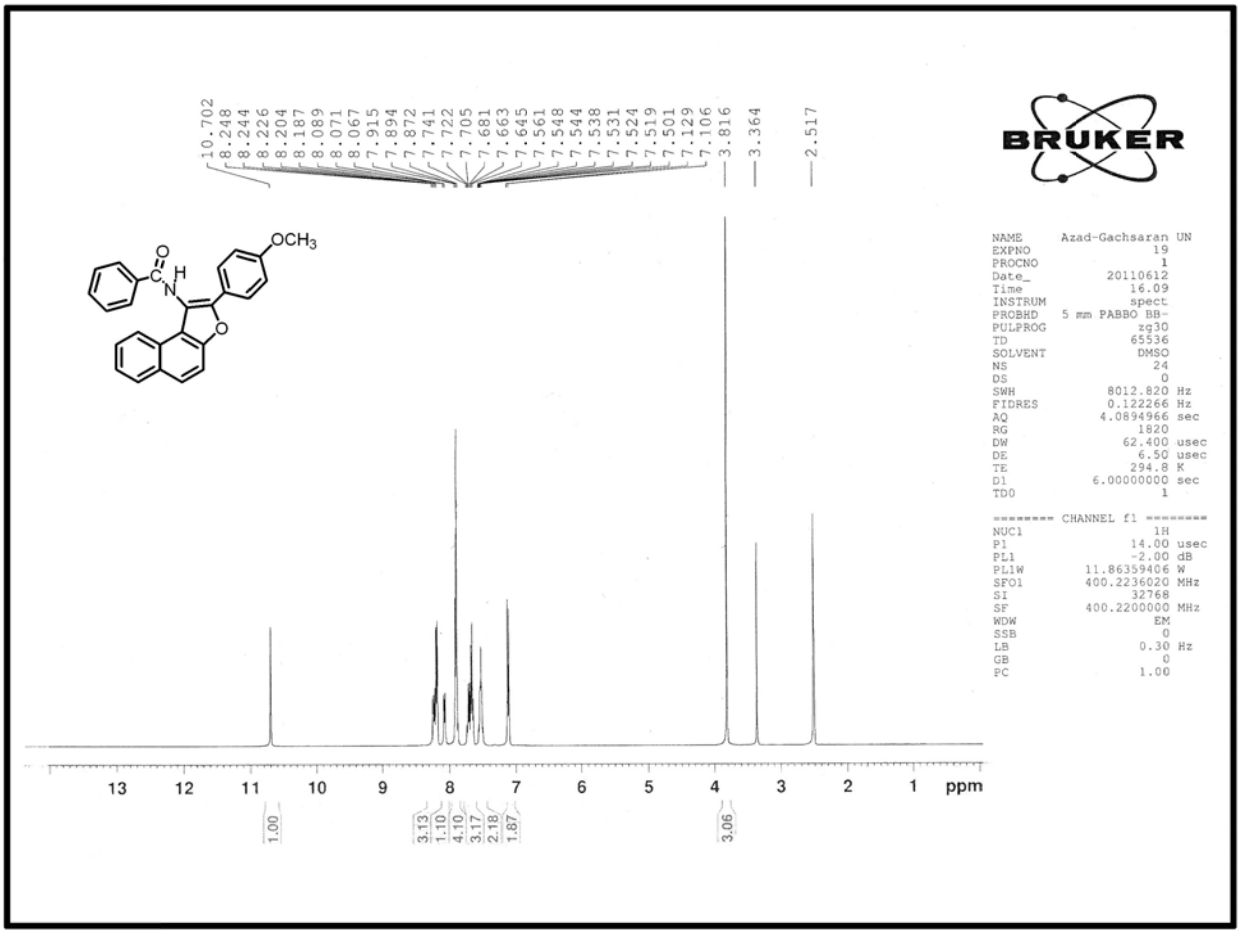
149.10
134.07
132.72
130.92
129.83
129.54
129.47
129.38
129.25
128.27
127.66
127.18
126.87
125.84
125.41
122.67
121.40
117.26
113.05
40.62
40.41
40.20
39.99
39.78
39.58
39.36
BRUKER
NAME Azad-Gachsaran UN
EXPNO 16
PROCNO 1
Date_ 20110612
Time 15.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 90
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 294.9 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
240
220
200
180
160
140
120
100
80
60
40
20
ppm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8.248
8.244
8.226
8.204
8.187
8.089
8.071
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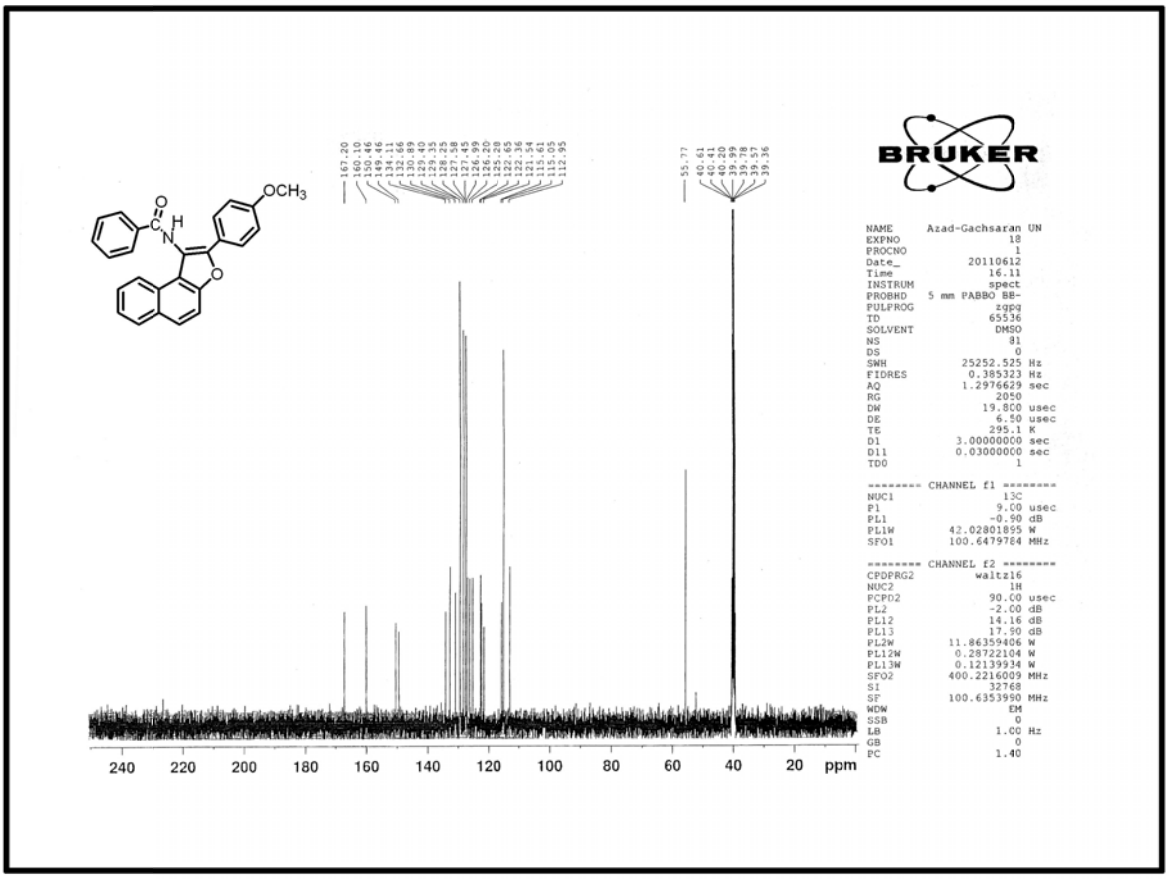
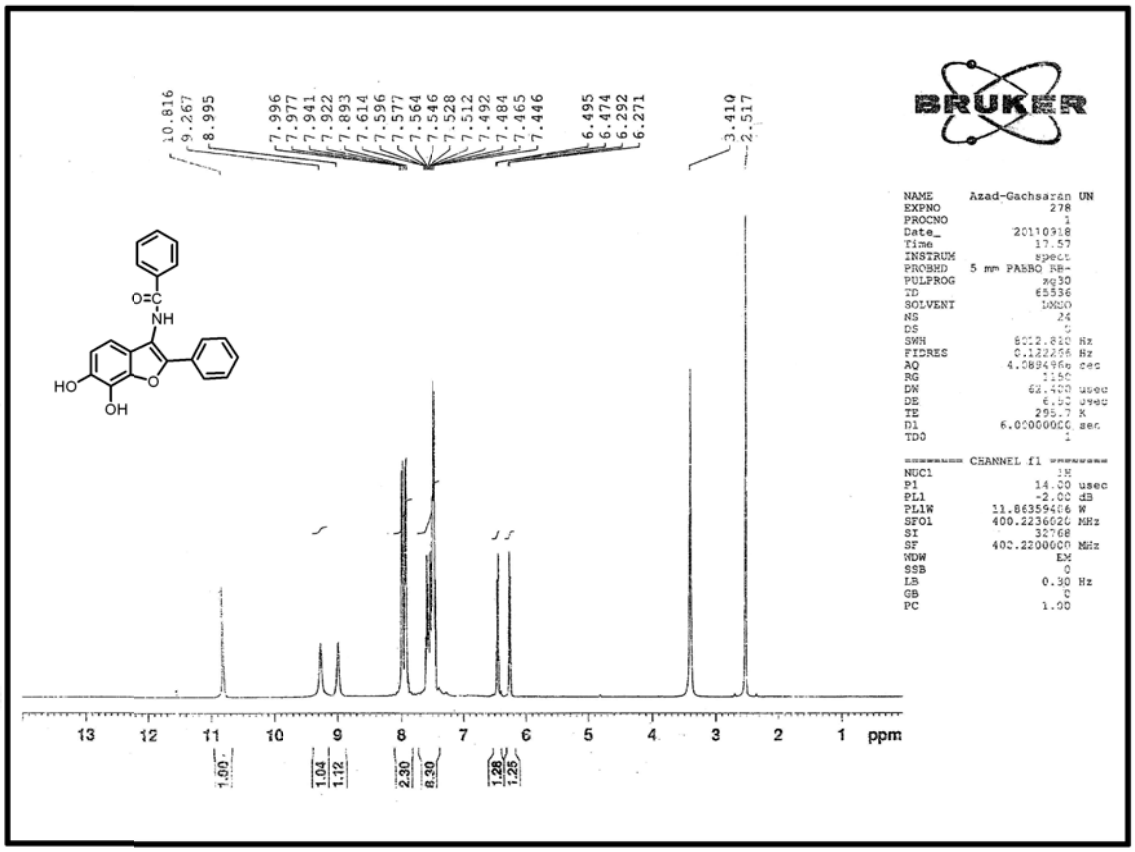
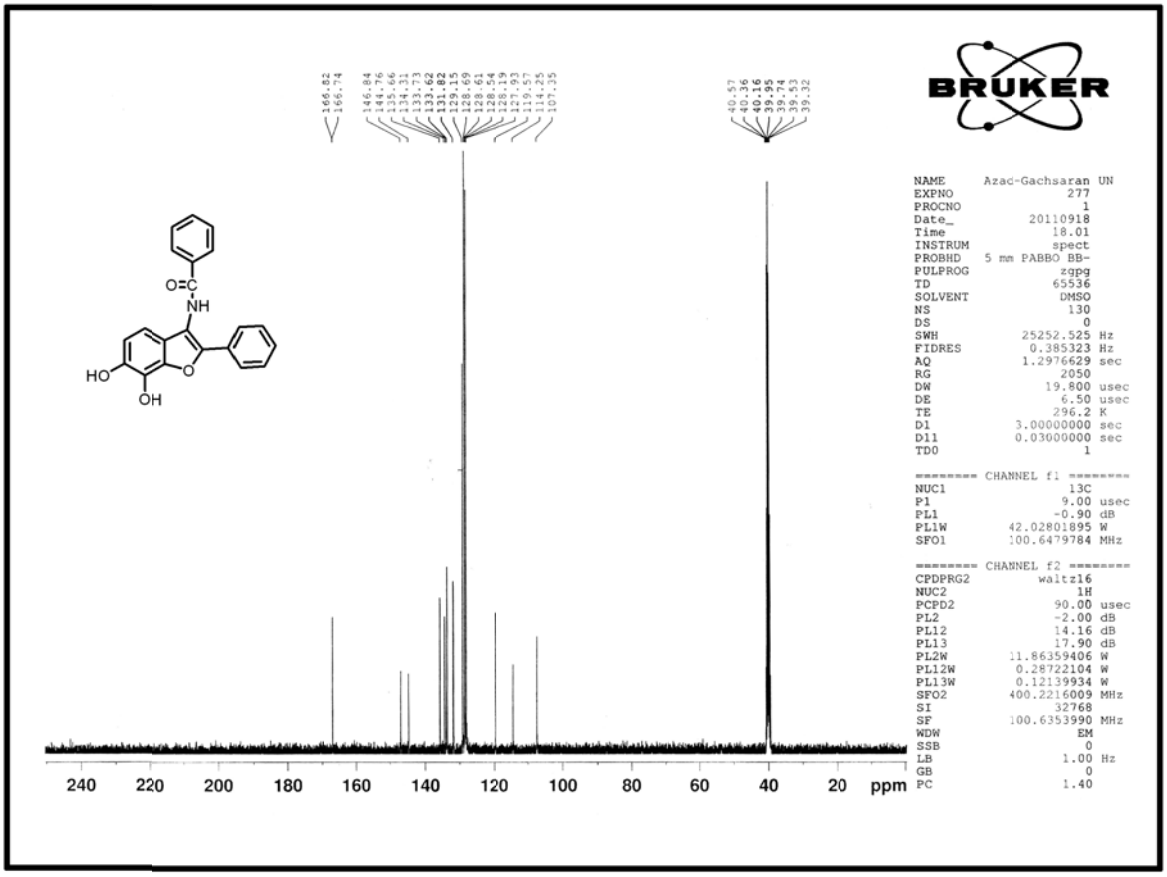
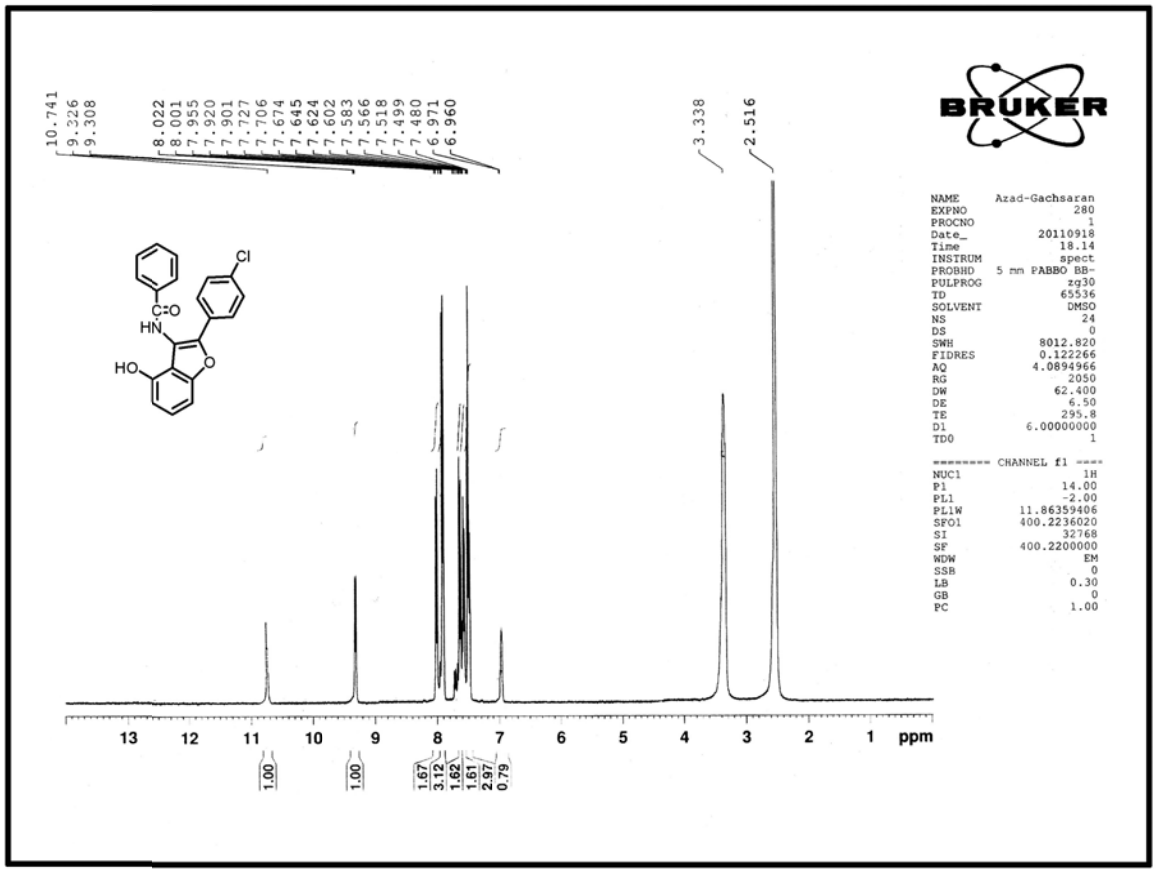
7.894
7.872
7.741
7.722
7.705
7.681
7.663
7.645
7.561
7.548
7.544
7.538
7.531
7.524
7.519
7.501
7.129
7.106
3.816
3.364
2.517
OCH3
O
H
N
O
BRUKER
NAME Azad-Gachsaran UN
EXPNO 19
PROCNO 1
Date_ 20110612
Time 16.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 1820
DW 62.400 usec
DE 6.50 usec
TE 294.8 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
3.13
1.10
4.10
3.17
2.18
1.87
3.06


OCH3
O
H
N
O
167.20
160.10
150.46
149.46
134.11
132.66
130.89
129.40
129.35
128.25
127.68
127.45
126.99
126.20
125.28
125.05
122.36
121.54
115.61
115.55
112.95
55.77
40.61
40.41
40.20
39.99
39.78
39.57
39.36
BRUKER
NAME Azad-Gachsaran UN
EXPNO 18
PROCNO 1
Date_ 20110612
Time 16.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 81
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 295.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
240
220
200
180
160
140
120
100
80
60
40
20
ppm


10.816
9.267
8.995
7.996
7.977
7.941
7.922
7.893
7.614
7.596
7.577
7.564
7.546
7.528
7.512
7.492
7.484
7.465
7.446
6.495
6.474
6.292
6.271
3.410
2.517
BRUKER
NAME Azad-Gachsaran UN
EXPNO 278
PROCNO 1
Date_ 20110918
Time 17.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 24
DS 0
SWH 8012.810 Hz
FIDRES 0.122256 Hz
AQ 4.0894966 sec
RG 1150
DW 62.400 usec
DE 6.50 usec
TE 295.7 K
D1 6.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236026 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O=C
NH
HO
OH
O
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.04
1.12
2.30
8.30
1.26
1.25



NAME	Azac-Gachsaran UN	
EXPNO	277	
PROCNO	1	
Date_	20110918	
Time	18.01	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg	
TD	65536	
SOLVENT	DMSO	
NS	130	
DS	0	
SWH	25252.525	Hz
FIDRES	0.385323	Hz
AQ	1.2976629	sec
RG	2050	
DW	19.800	usec
DE	6.50	usec
TE	296.2	K
D1	3.00000000	sec
D11	0.03000000	sec
TD0	1	
========	CHANNEL f1 ========	
NUC1	13C	
P1	9.00	usec
PL1	-0.90	dB
PL1W	42.02801895	W
SFO1	100.6479784	MHz
========	CHANNEL f2 ========	
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-2.00	dB
PL12	14.16	dB
PL13	17.90	dB
PL2W	11.86359406	W
PL12W	0.28722104	W
PL13W	0.12139934	W
SFO2	400.2216009	MHz
SI	32768	
SF	100.6353990	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	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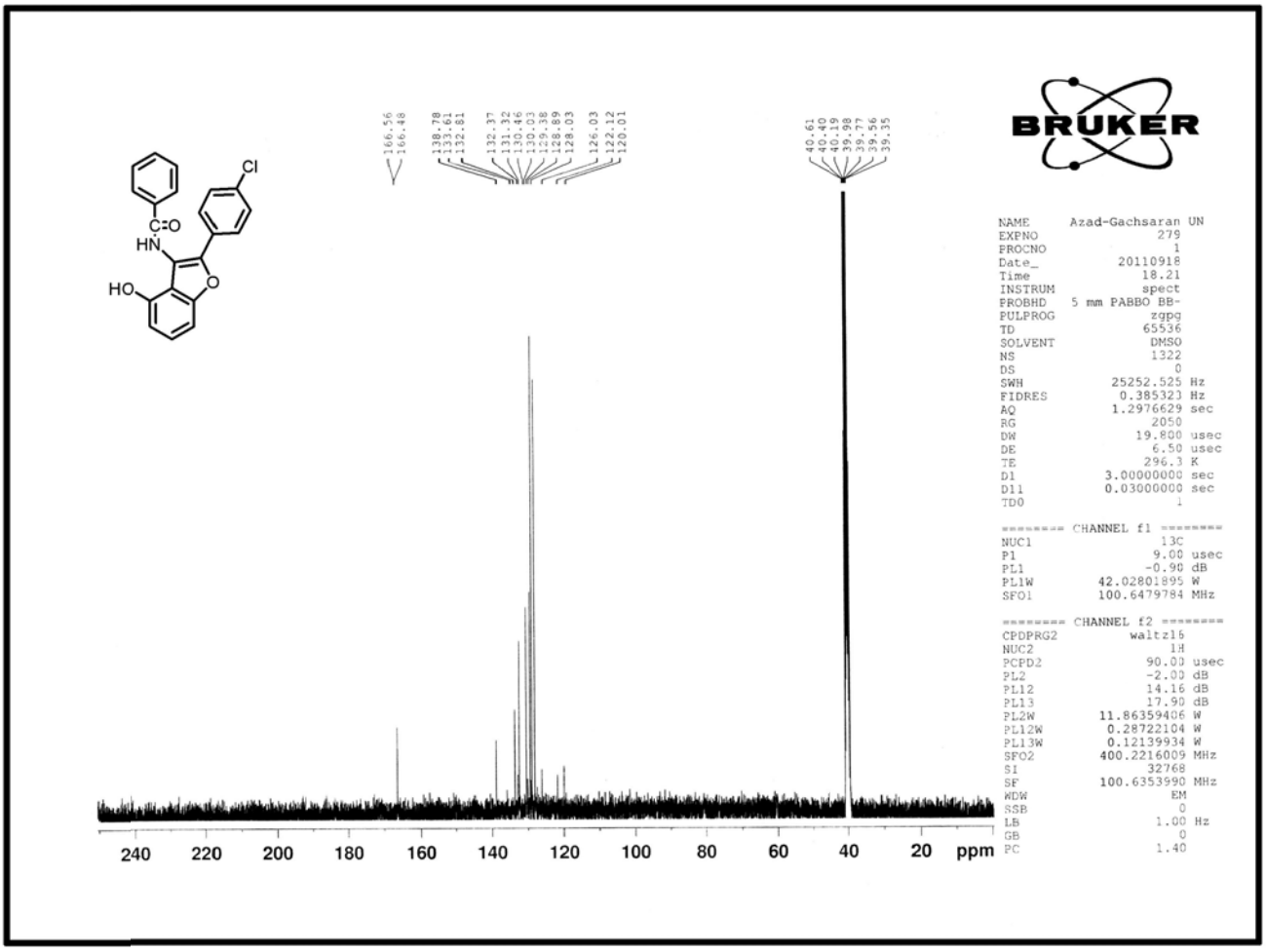
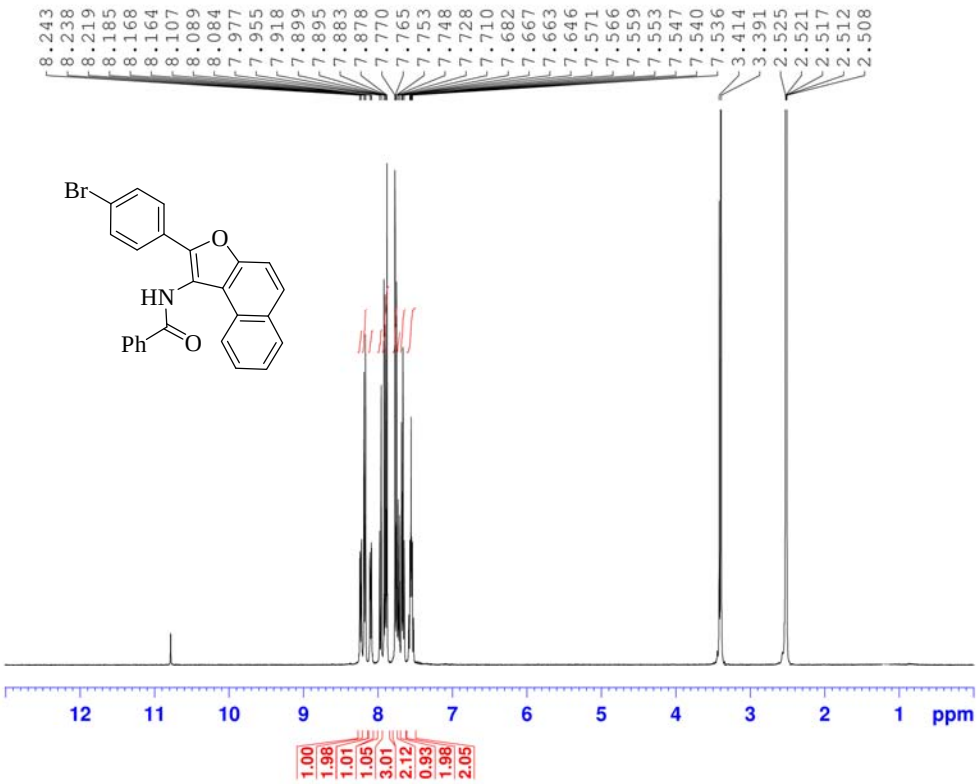
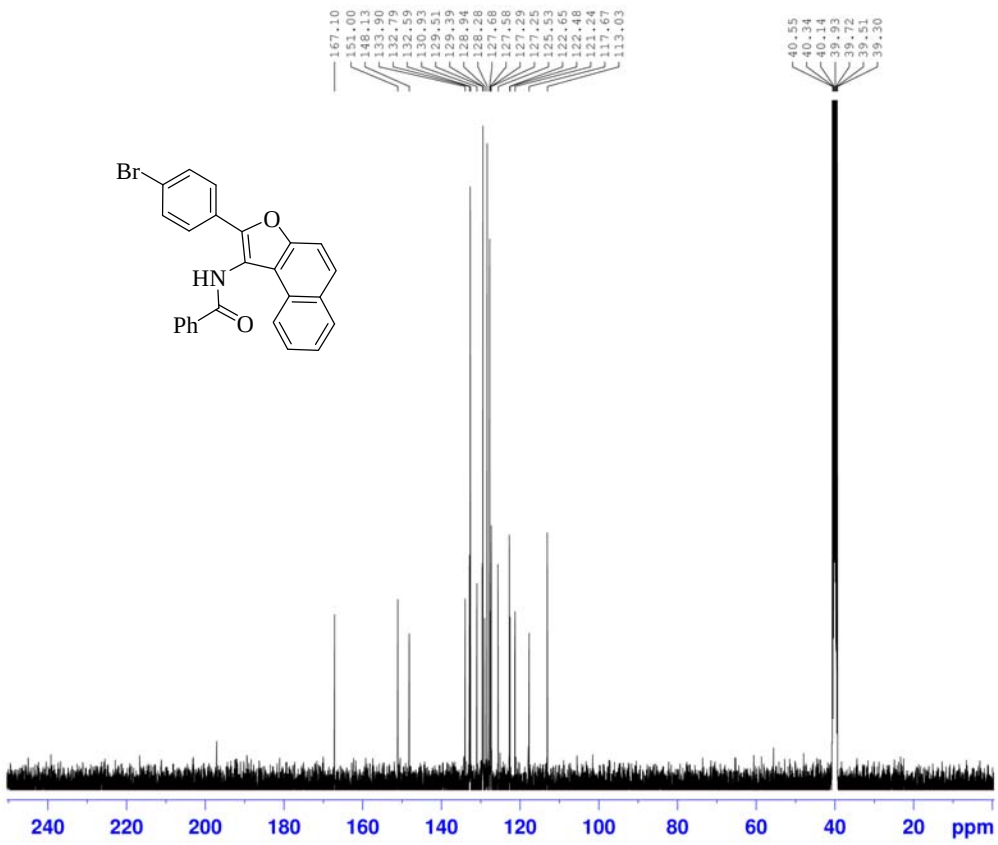
9.326
9.308
8.022
8.001
7.955
7.920
7.901
7.727
7.706
7.674
7.645
7.624
7.602
7.583
7.566
7.518
7.499
7.480
6.971
6.960
3.338
2.516
BRUKER
NAME Azad-Gachsaran
EXPNO 280
PROCNO 1
Date_ 20110918
Time 18.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 24
DS 0
SWH 8012.820
FIDRES 0.122266
AQ 4.0894966
RG 2050
DW 62.400
DE 6.50
TE 295.8
D1 6.00000000
TD0 1
======== CHANNEL f1 ====
NUC1 1H
P1 14.00
PL1 -2.00
PL1W 11.86359406
SFO1 400.2236020
SI 32768
SF 400.2200000
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
Cl
C=O
HN
HO
O
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.00
1.67
3.12
1.62
1.61
2.97
0.79


166.56
166.48
138.78
133.61
132.81
132.37
131.32
131.16
130.03
129.38
128.89
128.03
126.03
122.12
120.01
40.61
40.40
40.19
39.98
39.77
39.56
39.35
Cl
C=O
HN
HO
O
240
220
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
NAME Azad-Gachsaran UN
EXPNO 279
PROCNO 1
Date_ 20110918
Time 18.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 1322
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 296.3 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



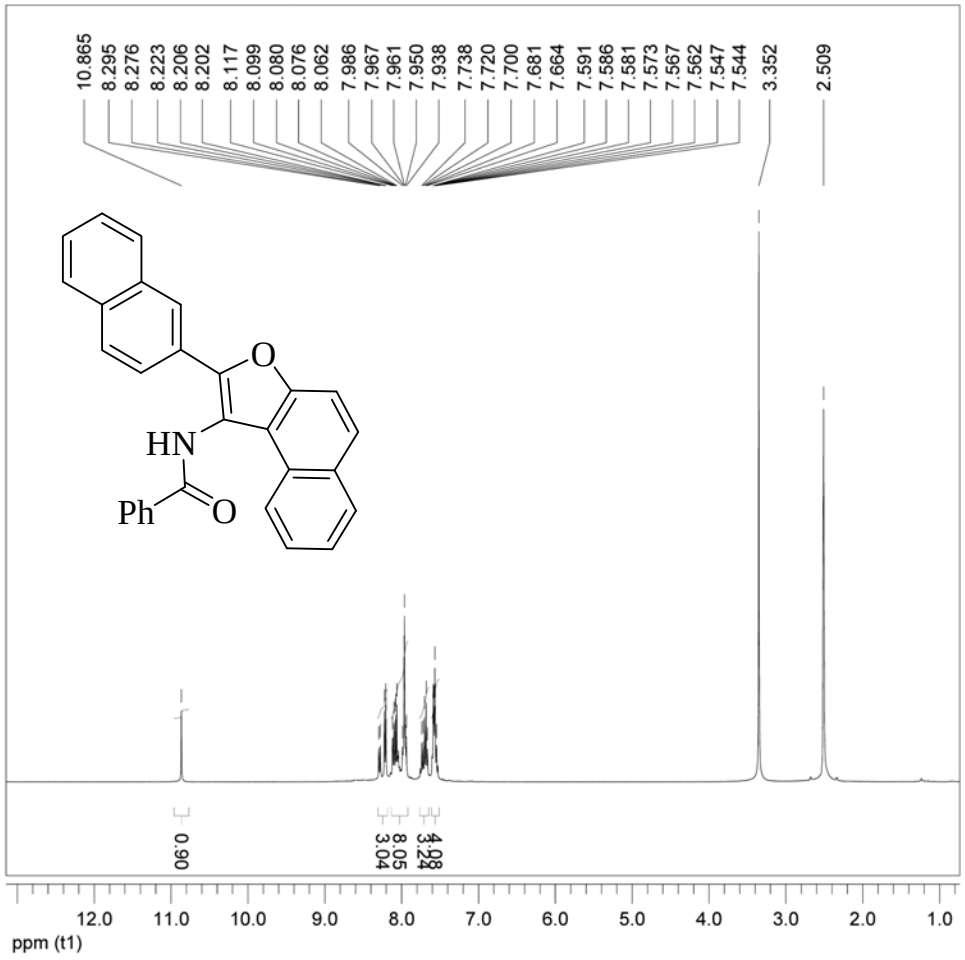
BRUKER

NAME	ilam UN
EXPNO	537
PROCNO	1
Date_	20120701
Time	14.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	20
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	2050
DW	62.400 usec
DE	6.50 usec
TE	295.1 K
D1	6.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
PL1	-2.00 dB
PL1W	11.86359406 W
SFO1	400.2236020 MHz
SI	32768
SF	400.2200000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	ilam UN
EXPNO	536
PROCNO	1
Date_	20120701
Time	15.06
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	701
DS	0
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	6.50 usec
TE	295.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	-0.90 dB
PL1W	42.02801895 W
SFO1	100.6479784 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	14.48 dB
PL13	17.90 dB
PL2W	11.86359406 W
PL12W	0.26681873 W
PL13W	0.12139934 W
SFO2	400.2216009 MHz
SI	32768
SF	100.6353990 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

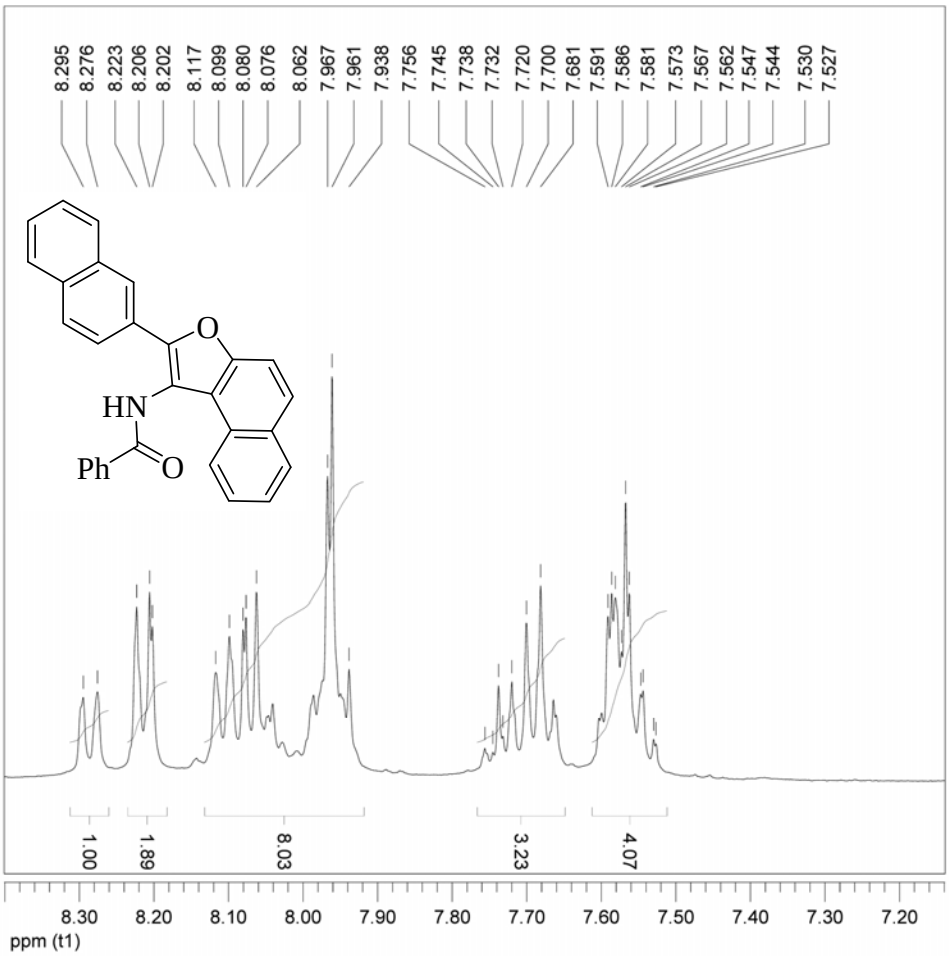


Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:
16 Sep 2012
Document's Title:
HNMR

Spectrum Title:
H1 DMSO-2-naphthyl gly

Frequency (MHz):
(f1) 400.130
Original Points Count:
(f1) 32768
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 3.8928
Spectral Width (ppm):
(f1) 21.037
Pulse Program:
Unknown

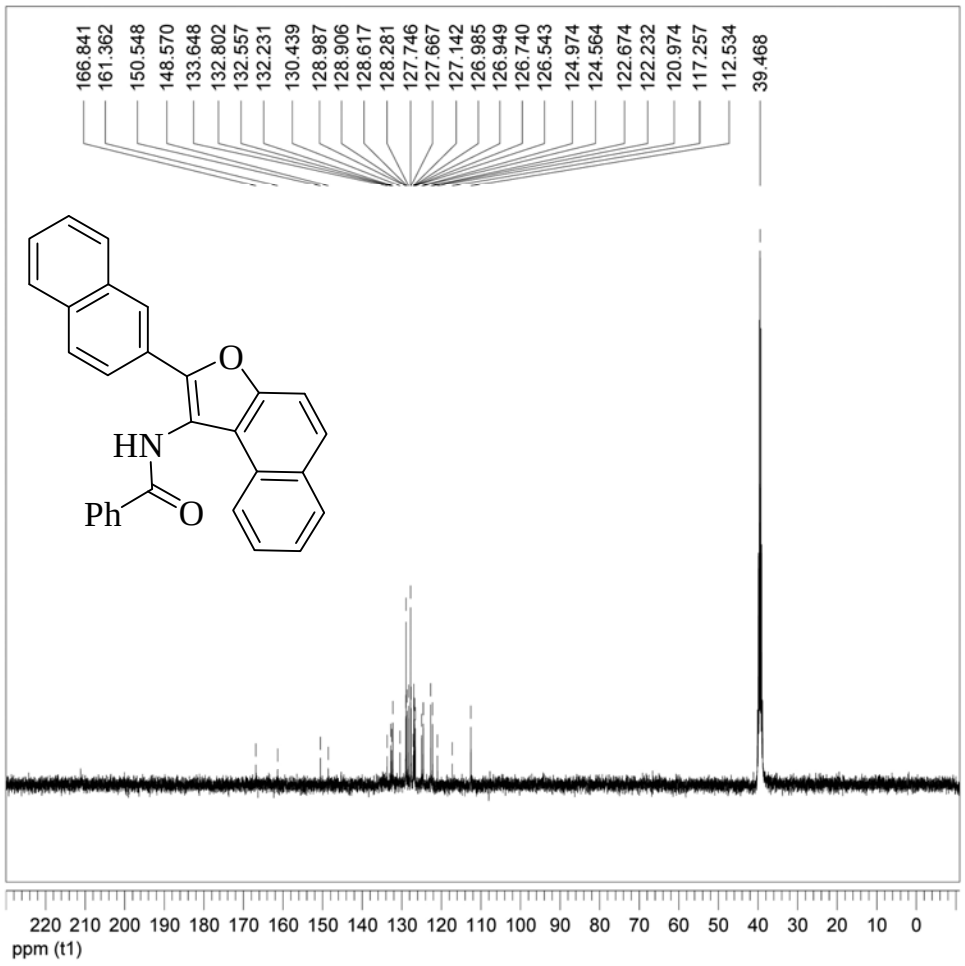


Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:
16 Sep 2012
Document's Title:
Extended-HNMR

Spectrum Title:
H1 DMSO-2-Naphthl-Extended

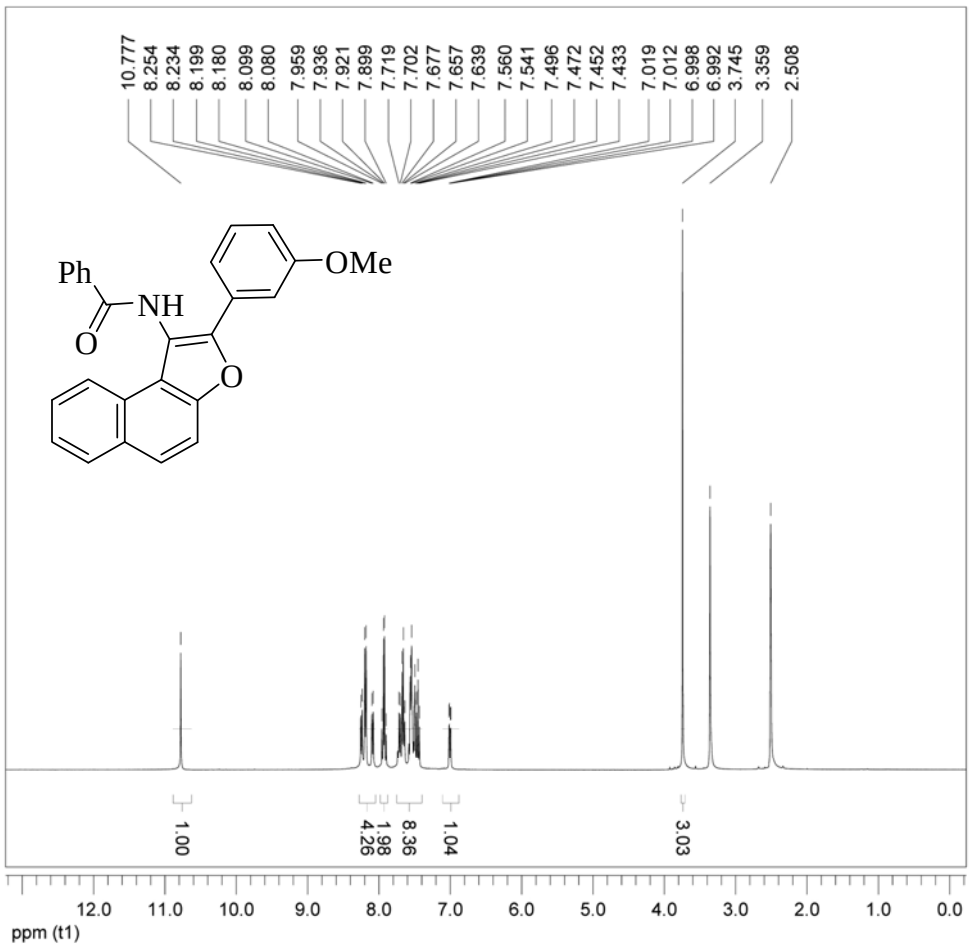
Frequency (MHz):
(f1) 400.130
Original Points Count:
(f1) 32768
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 3.8928
Spectral Width (ppm):
(f1) 21.037
Pulse Program:
Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:
16 Sep 2012
Spectrum Title:
13C DMSO-2-Naphthyl gly

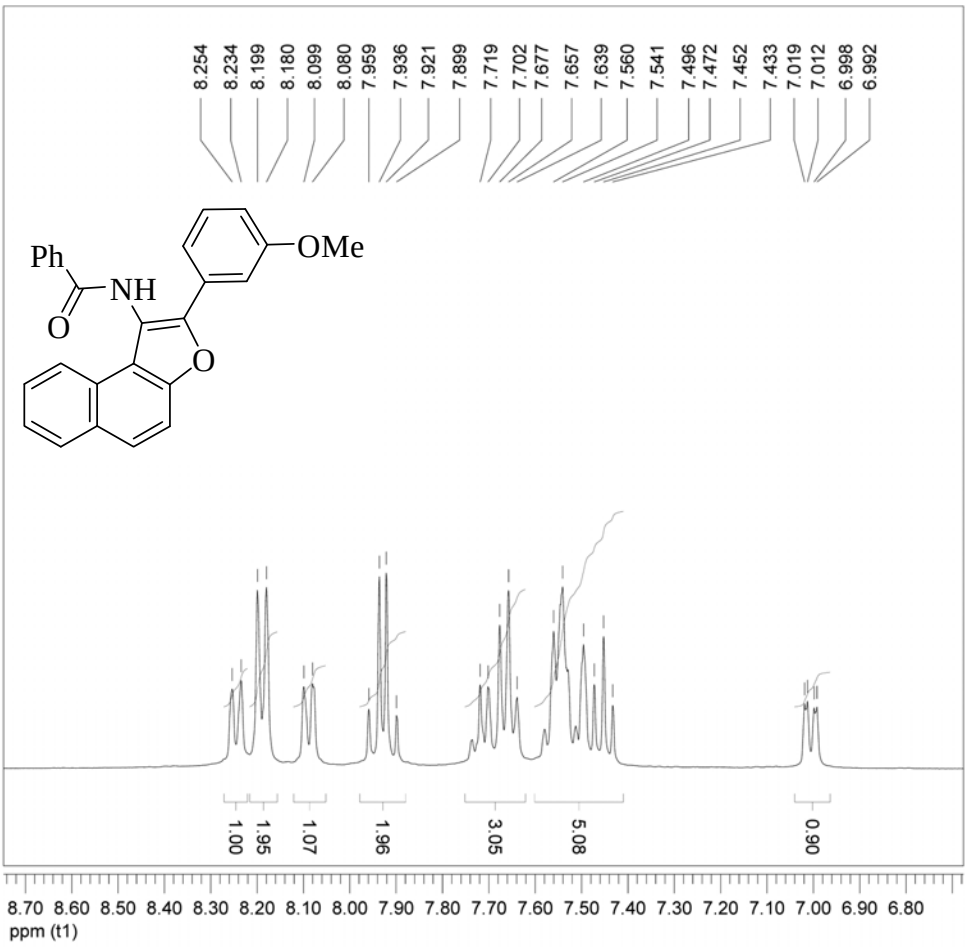
Frequency (MHz):
(f1) 100.613
Original Points Count:
(f1) 32768
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 1.2976
Spectral Width (ppm):
(f1) 250.987
Pulse Program:
Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:
16 Sep 2012
Spectrum Title:
H1 DMSO-3-Methoxy gly

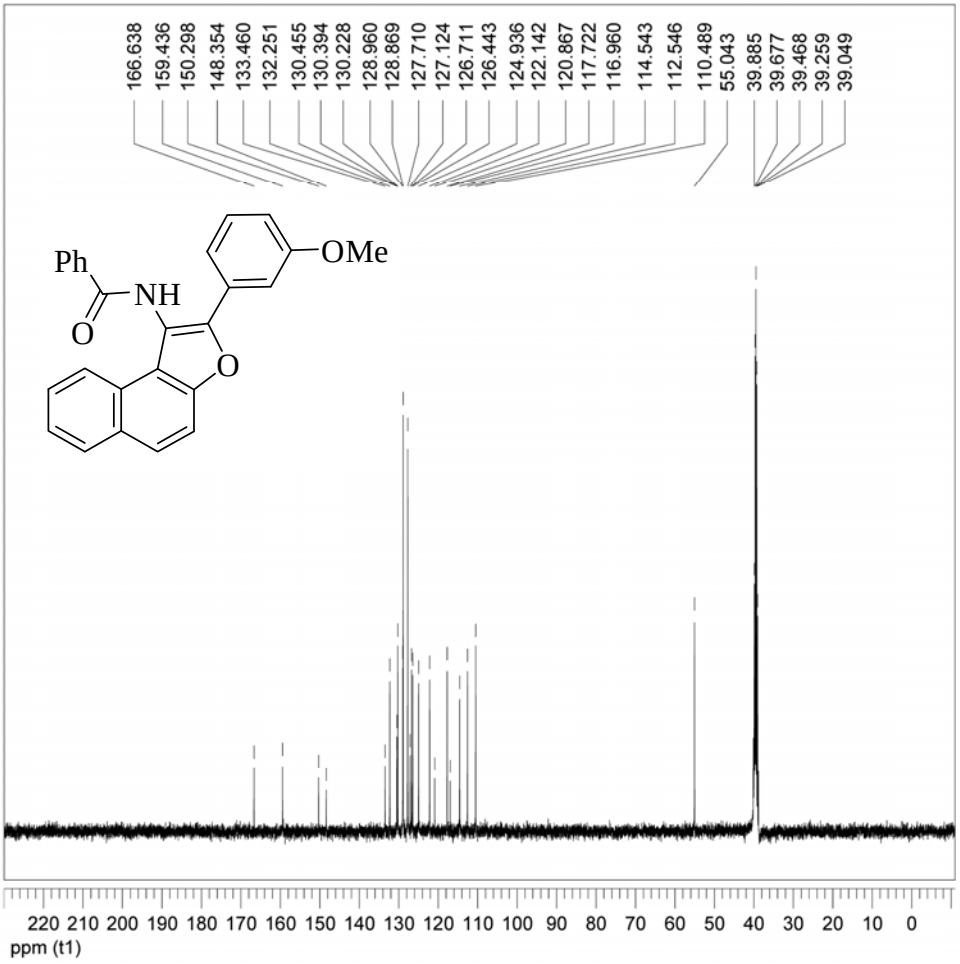
Frequency (MHz):
(f1) 400.130
Original Points Count:
(f1) 32768
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 3.8928
Spectral Width (ppm):
(f1) 21.037
Pulse Program:
Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:
16 Sep 2012
Spectrum Title:
H1 DMSO-Extended-3-MeO

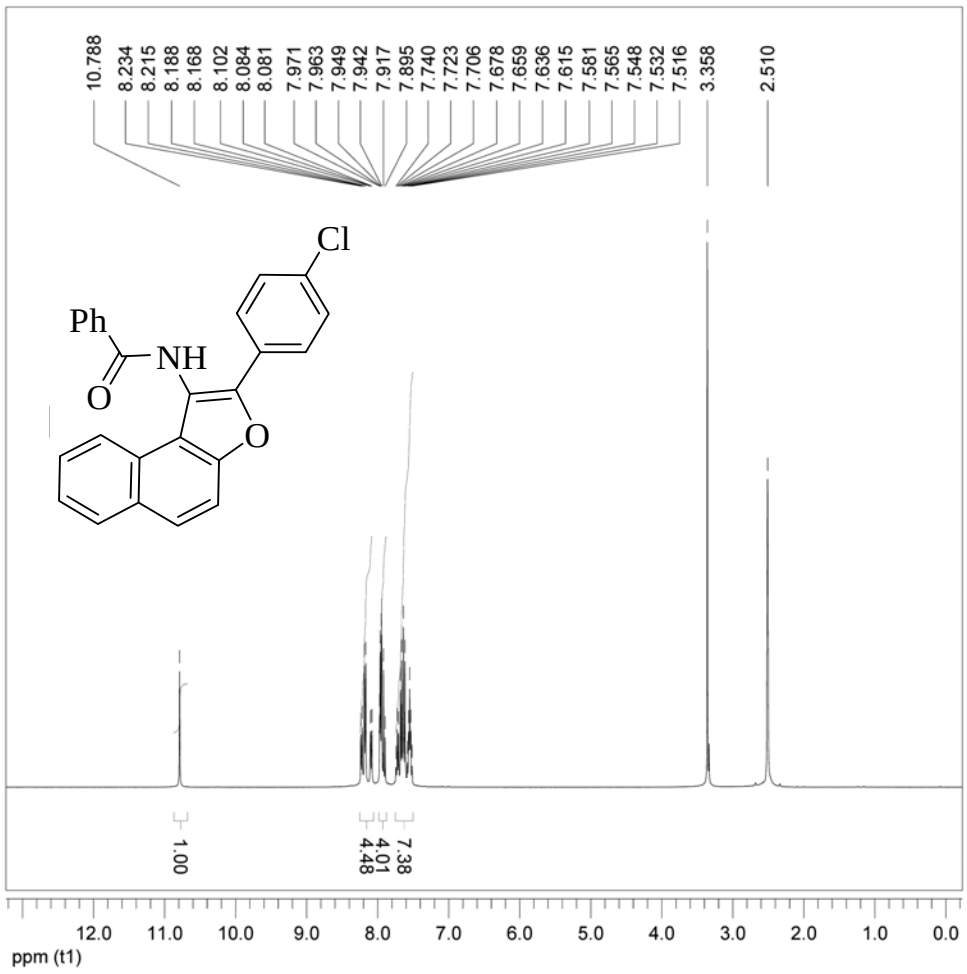
Frequency (MHz):
(f1) 400.130
Original Points Count:
(f1) 32768
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 3.8928
Spectral Width (ppm):
(f1) 21.037
Pulse Program:
Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:
16 Sep 2012
Spectrum Title:
13C DMSO-3-MeO

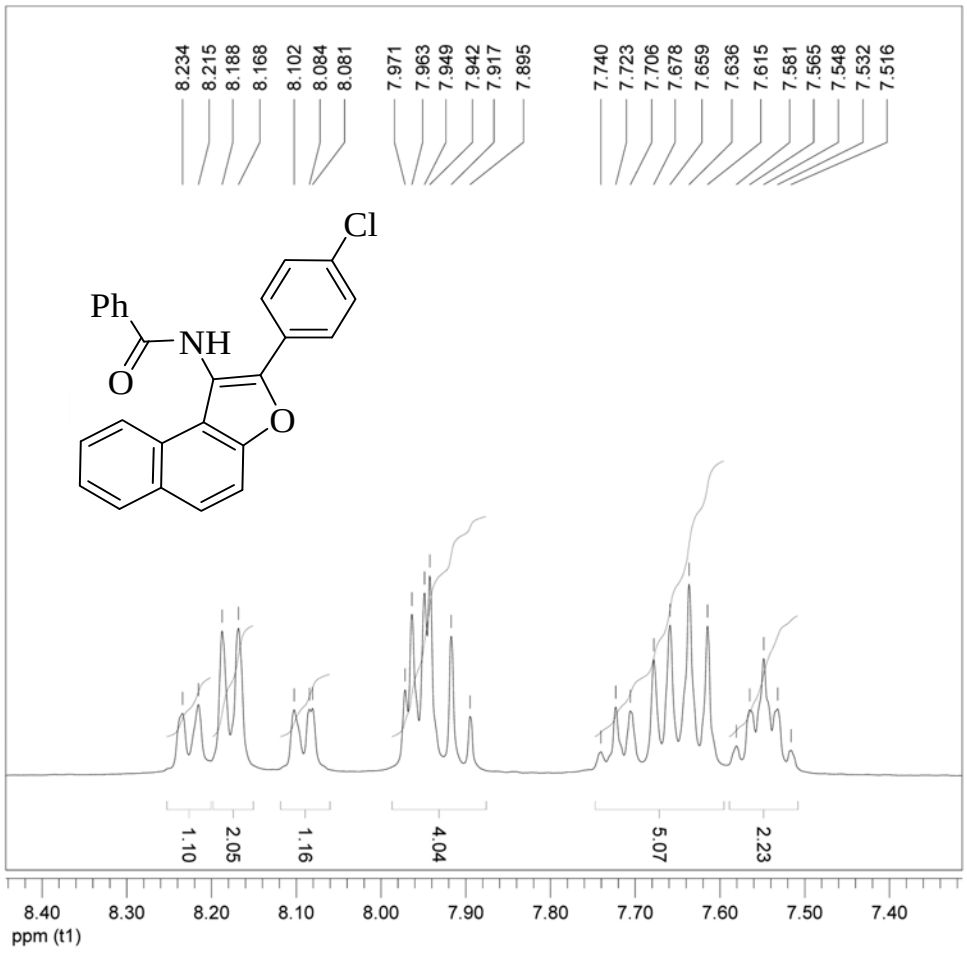
Frequency (MHz):
(f1) 100.613
Original Points Count:
(f1) 32768
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 1.2976
Spectral Width (ppm):
(f1) 250.987
Pulse Program:
Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:
16 Sep 2012
Spectrum Title:
H1 DMSO D-4-Chloro gly

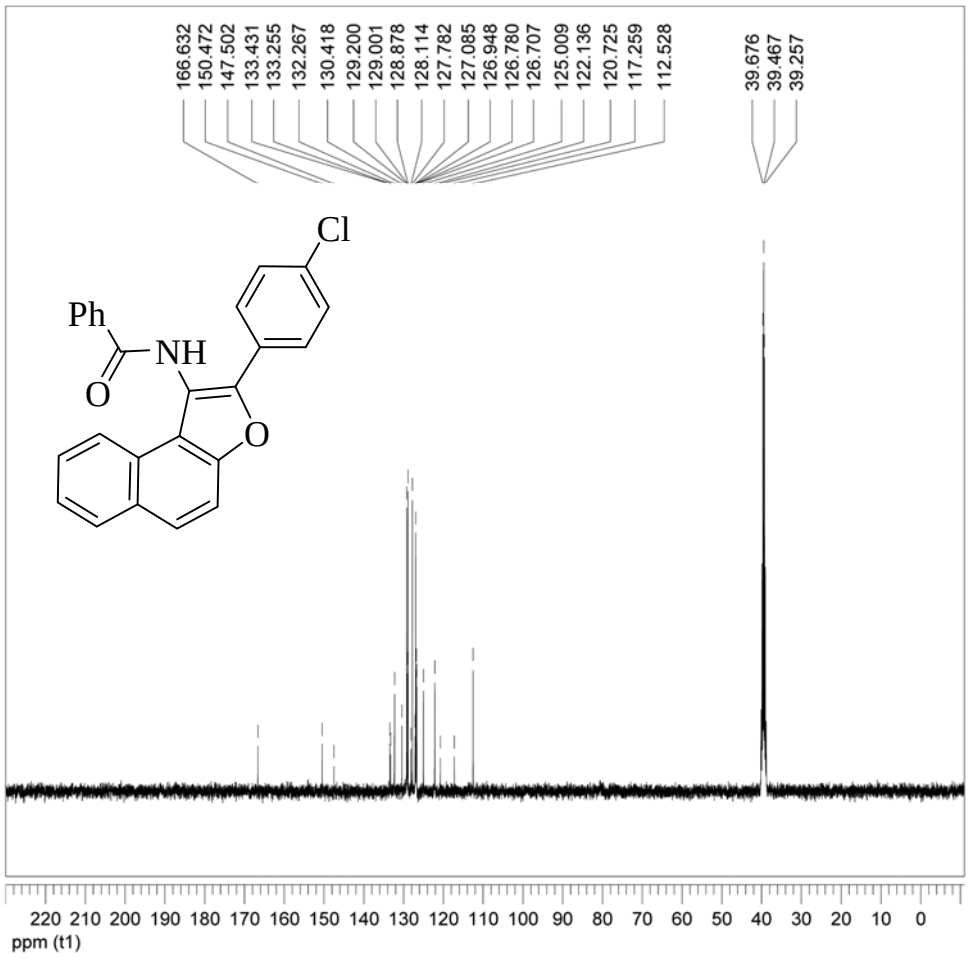
Frequency (MHz):
(f1) 400.130
Original Points Count:
(f1) 32768
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 3.8928
Spectral Width (ppm):
(f1) 21.037
Pulse Program:
Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:
16 Sep 2012
Spectrum Title:
H1 DMSO -Extended-4-Cl

Frequency (MHz):
(f1) 400.130
Original Points Count:
(f1) 32768
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 3.8928
Spectral Width (ppm):
(f1) 21.037
Pulse Program:
Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:
16 Sep 2012
Spectrum Title:
13C DMSO-4-Chloro gly

Frequency (MHz):
(f1) 100.613
Original Points Count:
(f1) 32768
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 1.2976
Spectral Width (ppm):
(f1) 250.987
Pulse Program:
Unknown