

Design and synthesis of novel quinazolinones conjugated ibuprofen, indole acetamide or thioacetohydrazide as selective COX-2 inhibitors: Anti-inflammatory, analgesic and anti-cancer activities

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Keywords: COX-2 inhibition; quinazolinone; anti-inflammatory; molecular modeling; Anticancer.

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Asmaa Alaa_H_IN-1

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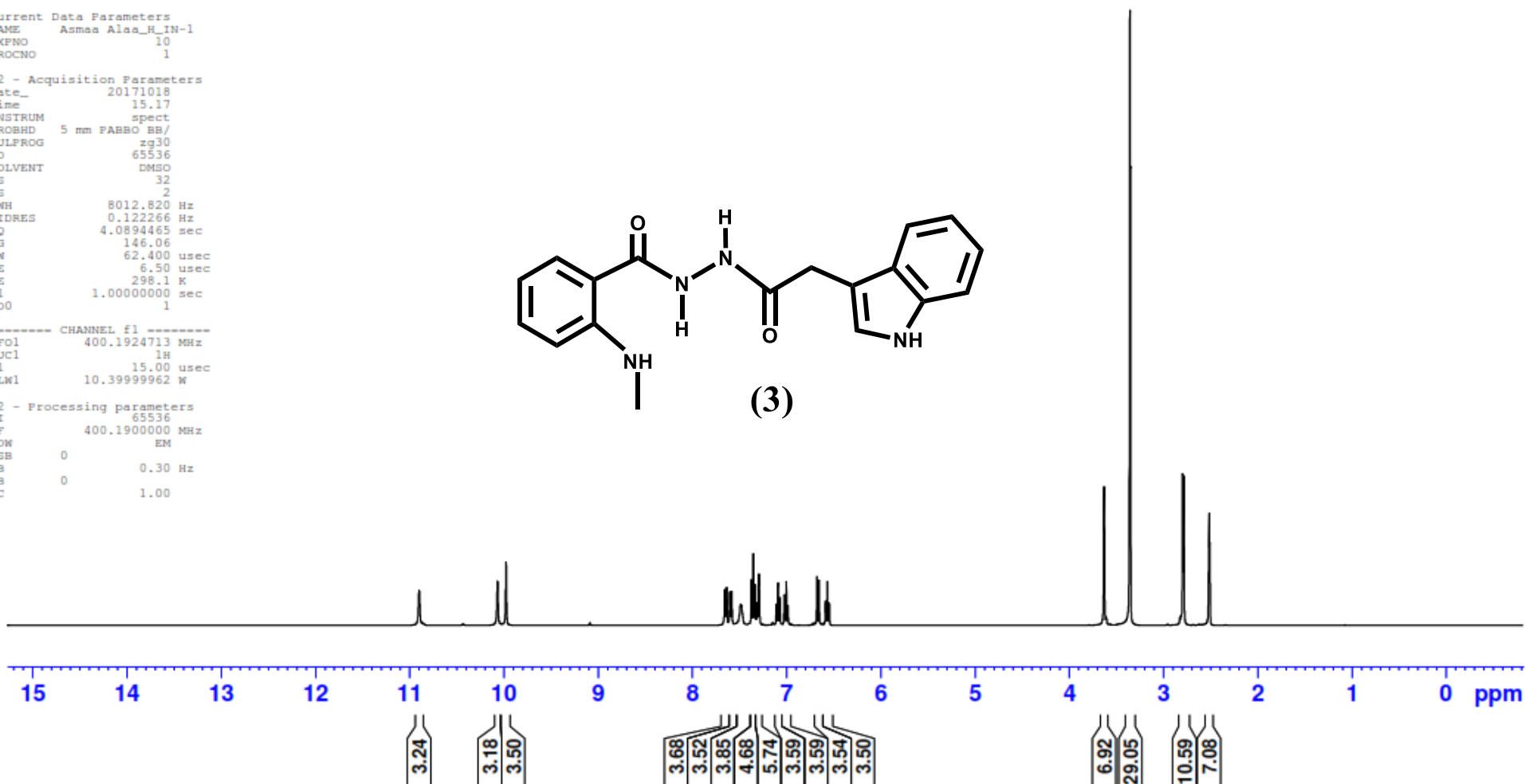
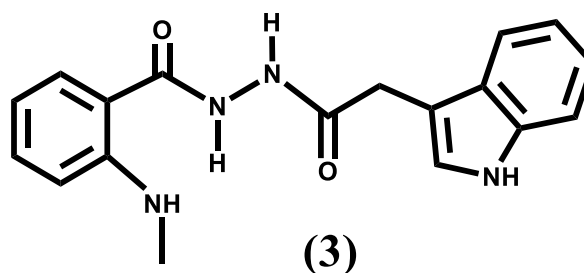
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2.5055

Current Data Parameters
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EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 146.06
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

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SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Asmaa Alaa_H_IN-1_D2O

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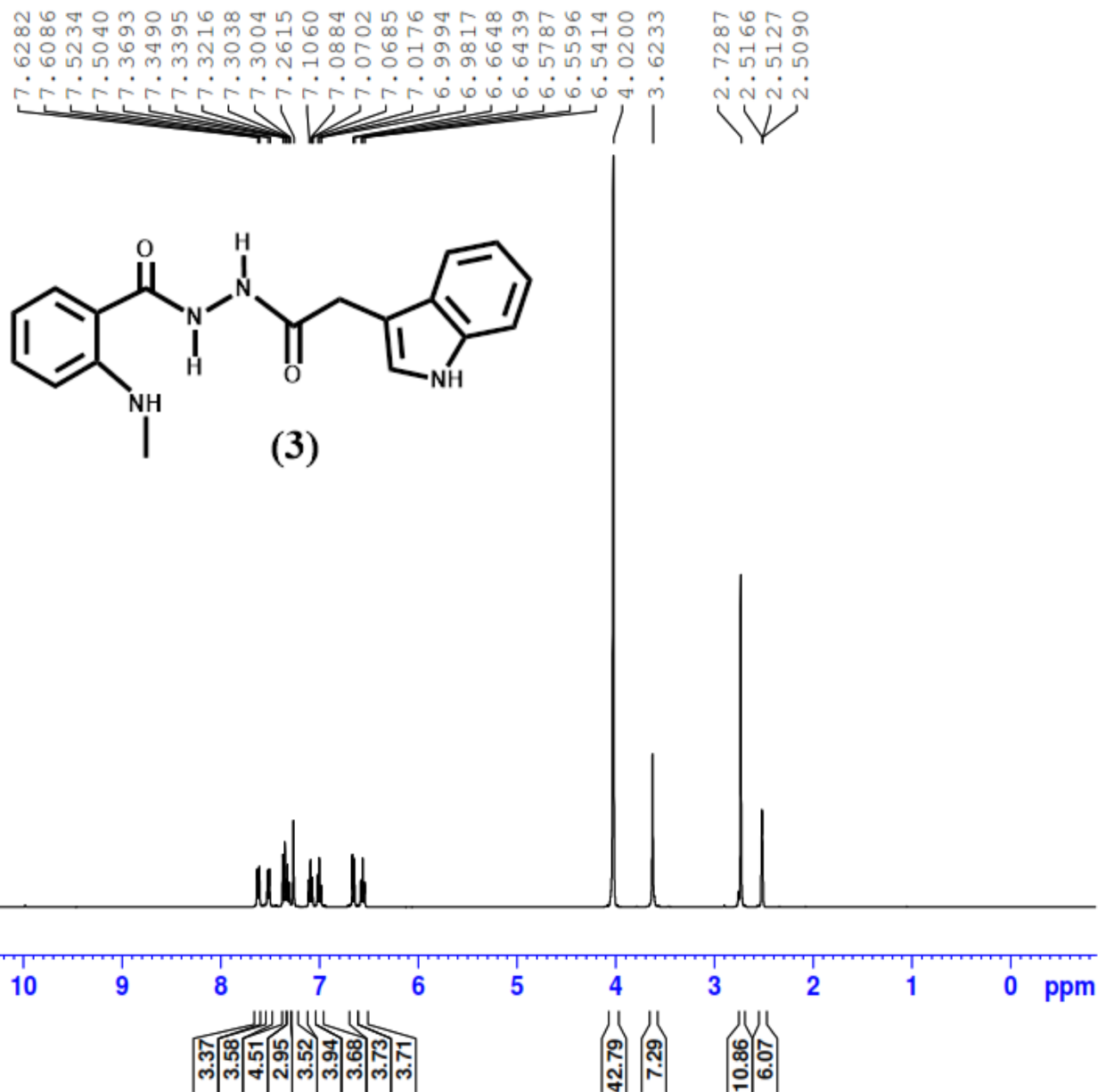


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EXPNO 10
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 129.43
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

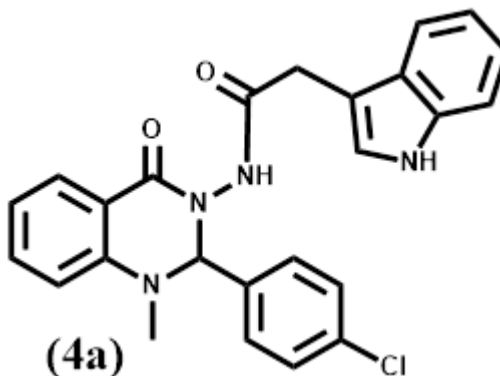




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 7.8125
 7.8097
 7.7935
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 7.4653
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 7.4444
 7.4264
 7.4229
 7.4084
 7.3874
 7.3736
 7.3533
 7.2391
 7.2180
 7.1116
 7.0932
 7.0746
 7.0012
 6.9822
 6.9642
 6.8820
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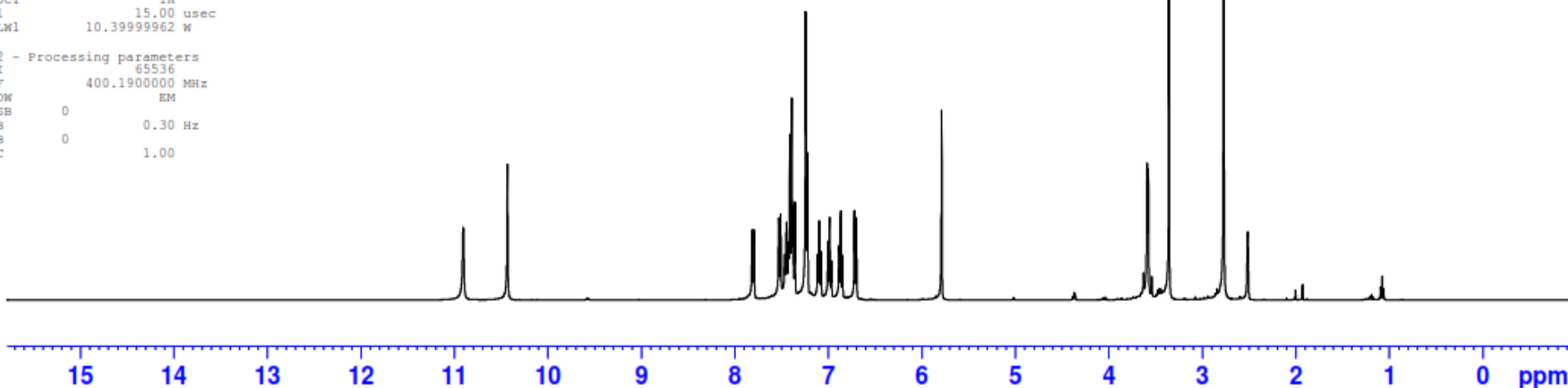
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 EXPNO 10
 PROCNO 1

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 Time 7.26
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 PROBHD 5 mm FAPBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 106.37
 DW 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1



----- CHANNEL f1 -----
 SFO1 400.1924713 MHz
 NUC1 1H
 F1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



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 3.71

4.07
 5.04
 18.62
 12.37
 4.32
 4.21
 4.27
 4.02
 3.93

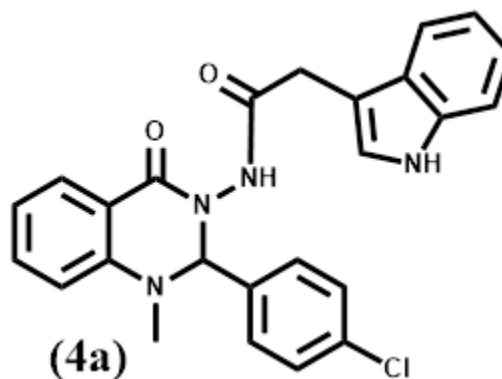
8.03
 9.50
 11.59
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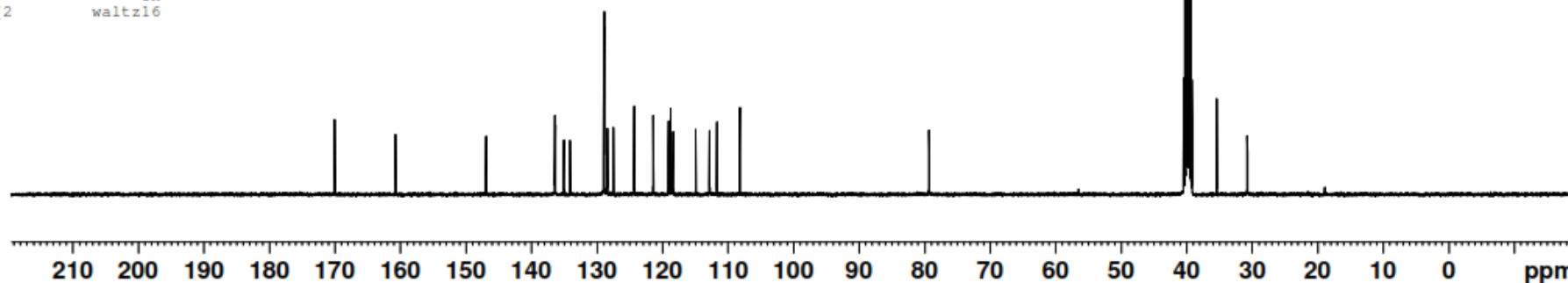
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 121.50
 119.17
 118.83
 118.46
 115.03
 112.90
 111.76
 108.28
 79.37
 40.50
 40.30
 40.09
 39.88
 39.67
 39.46
 39.25
 35.47
 30.80

Current Data Parameters
 NAME Asmaa Sakr_C_B-S30
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180510
 Time 2.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1200
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 202.37
 DW 20.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1



==== CHANNEL f1 =====
 SFO1 100.6379178 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 45.00000000 W
 ===== CHANNEL f2 =====
 SFO2 400.1916008 MHz
 NUC2 1H
 CPDPRG[2] waltz16



Asmaa Alaa_H_B-S11

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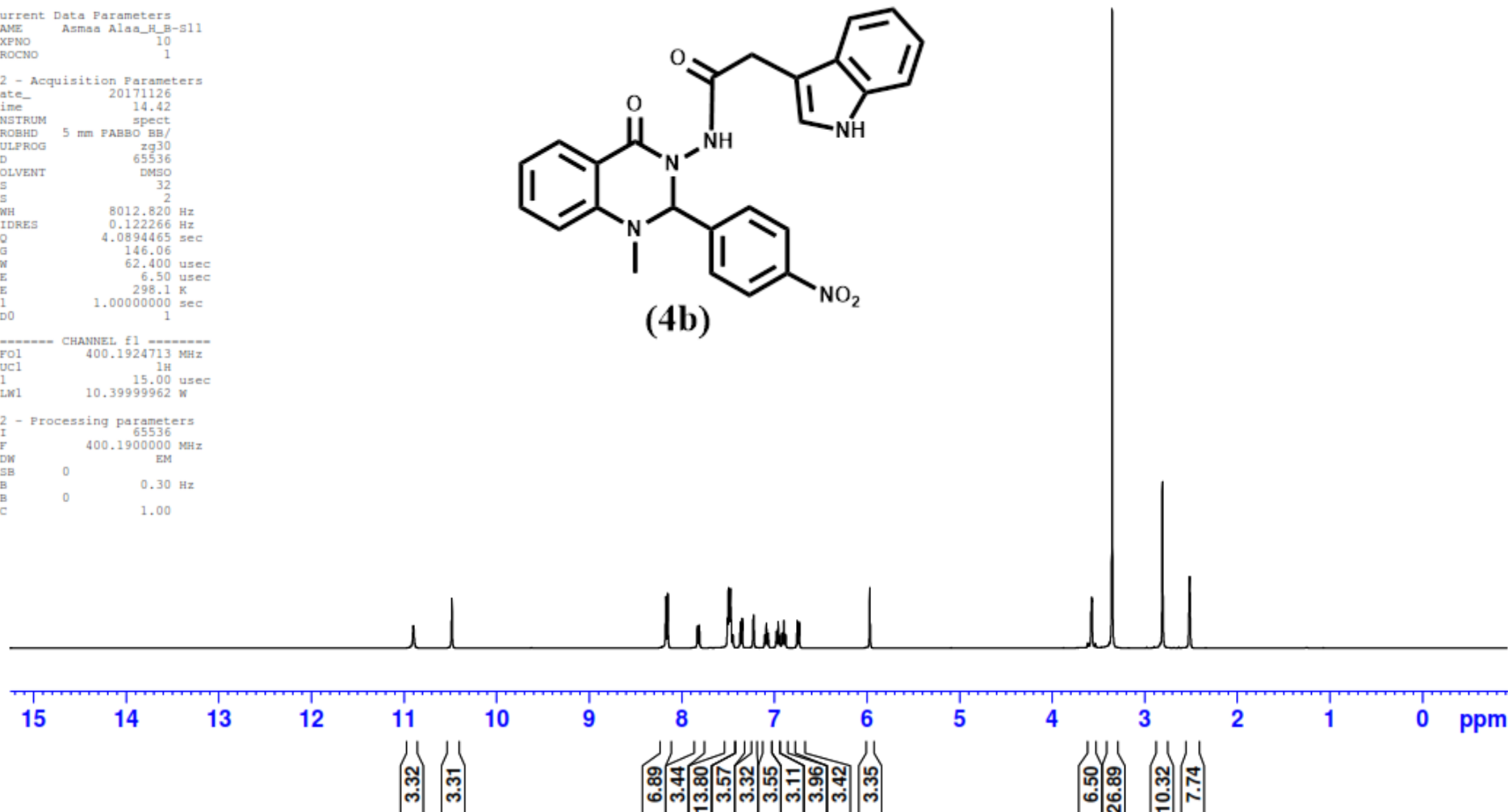
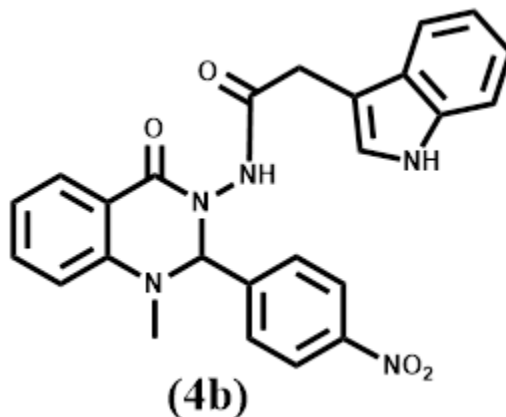
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7.3430
7.2238
7.2190
7.0995
7.0815
7.0633
6.9747
6.9558
6.9379
6.9118
6.8932
6.8749
6.7487
6.7280
5.9649
3.5715
3.5660
3.3479
2.8034
2.5139
2.5099
2.5060

Current Data Parameters
NAME Asmaa Alaa_H_B-S11
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171126
Time 14.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 146.06
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D10 1

----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLM1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

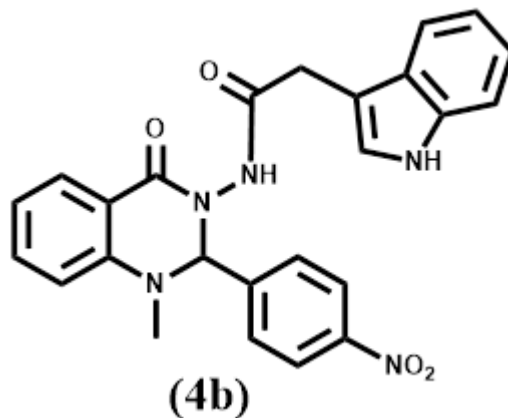




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 7.7715
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 7.3430
 7.3215
 7.1566
 7.0696
 7.0508
 7.0319
 6.9266
 6.9076
 6.8871
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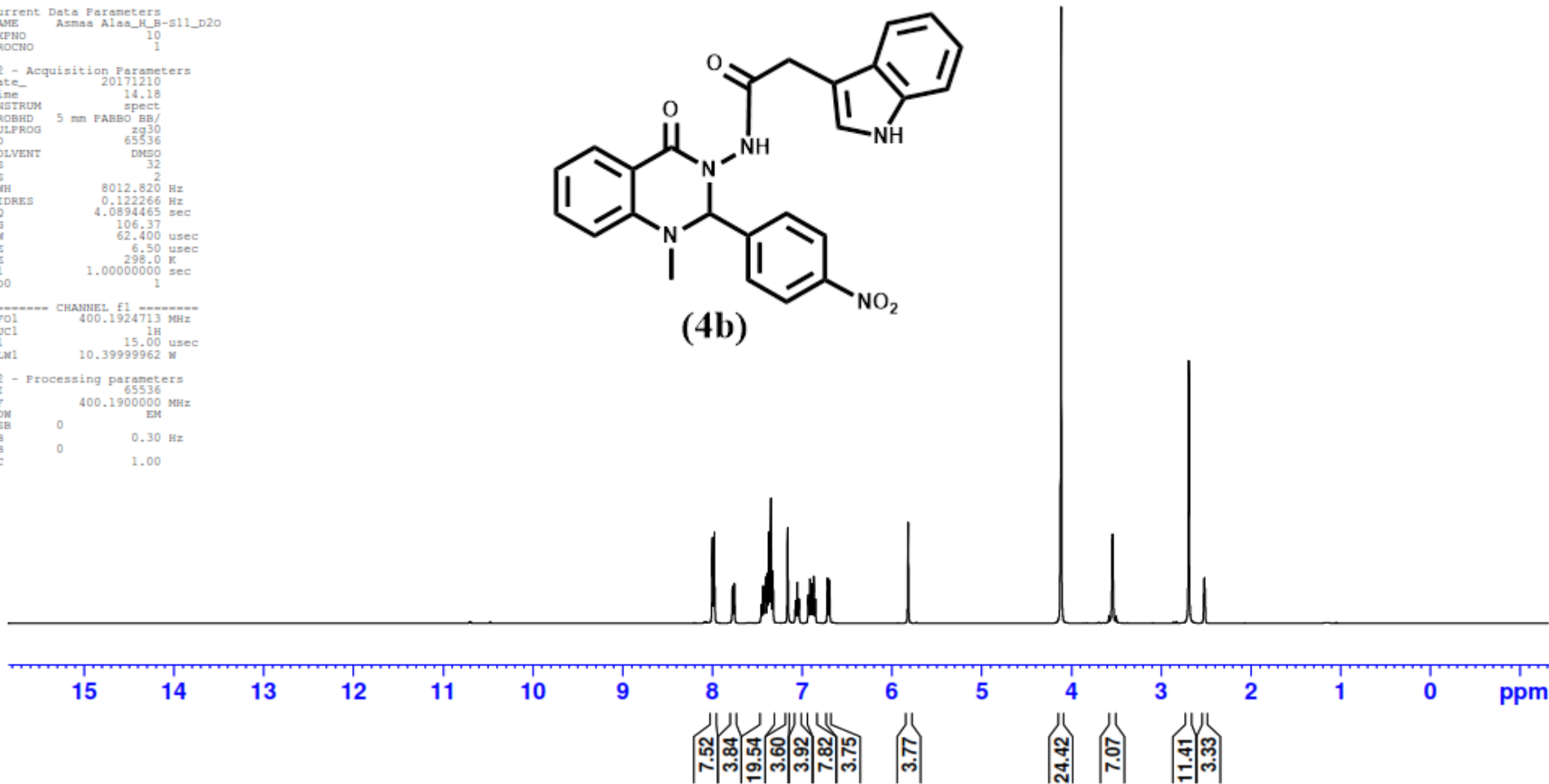
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 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171210
 Time 14.18
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 PROBHD 5 mm FAPBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 106.37
 DM 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1



----- CHANNEL f1 -----
 SF01 400.1924713 MHz
 NUC1 1H
 F1 15.00 usec
 PLM1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 MDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

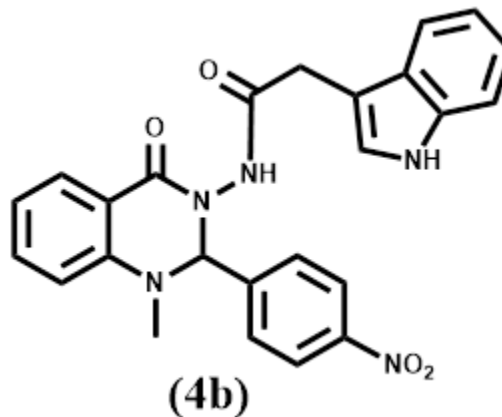




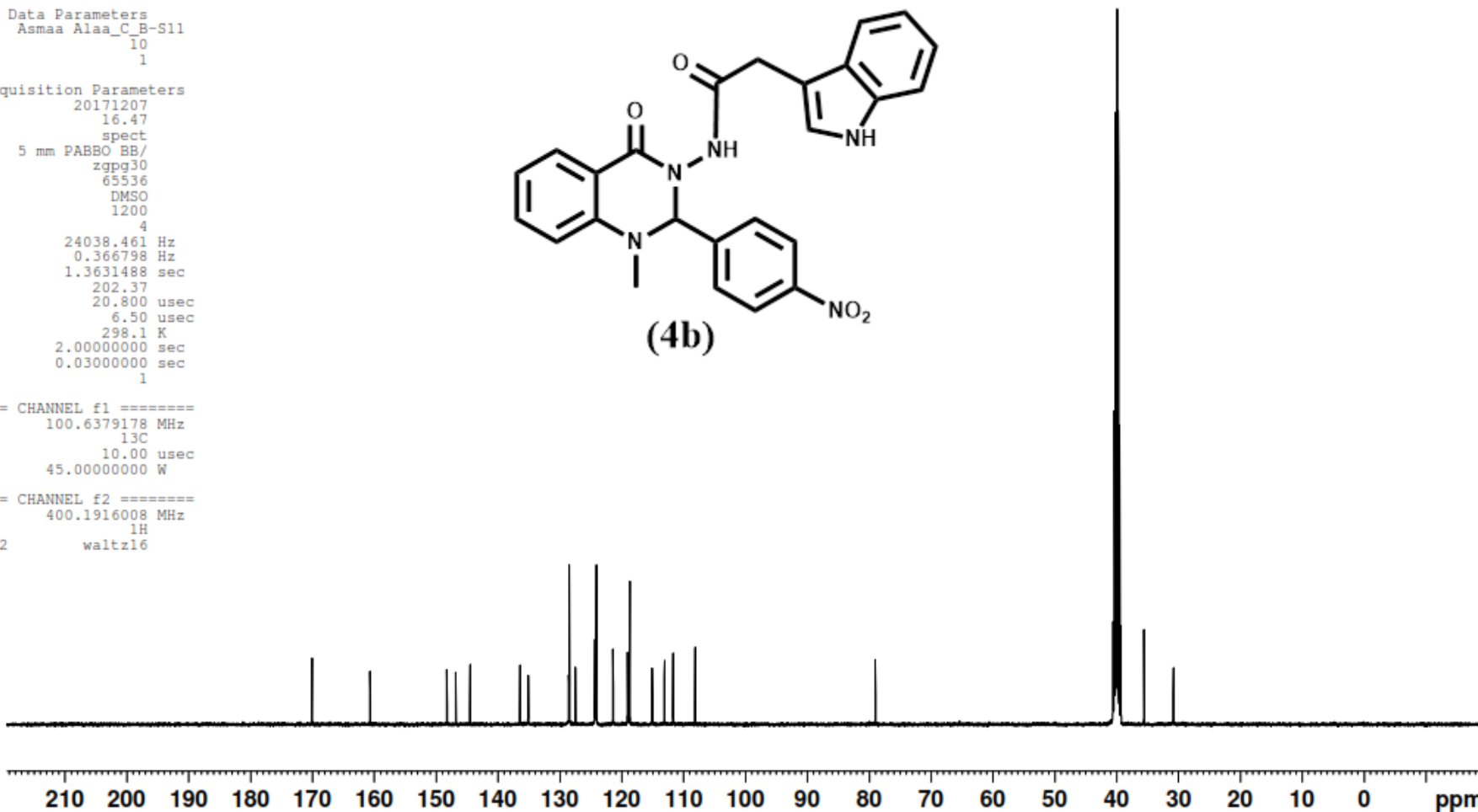
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Current Data Parameters
 NAME Asmaa Alaa_C_B-S11
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171207
 Time_ 16.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1200
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 202.37
 DW 20.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1



==== CHANNEL f1 =====
 SFO1 100.6379178 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 45.00000000 W
 ===== CHANNEL f2 =====
 SFO2 400.1916008 MHz
 NUC2 1H
 CPDPRG[2] waltz16



Asmaa Alaa_H_B-S31

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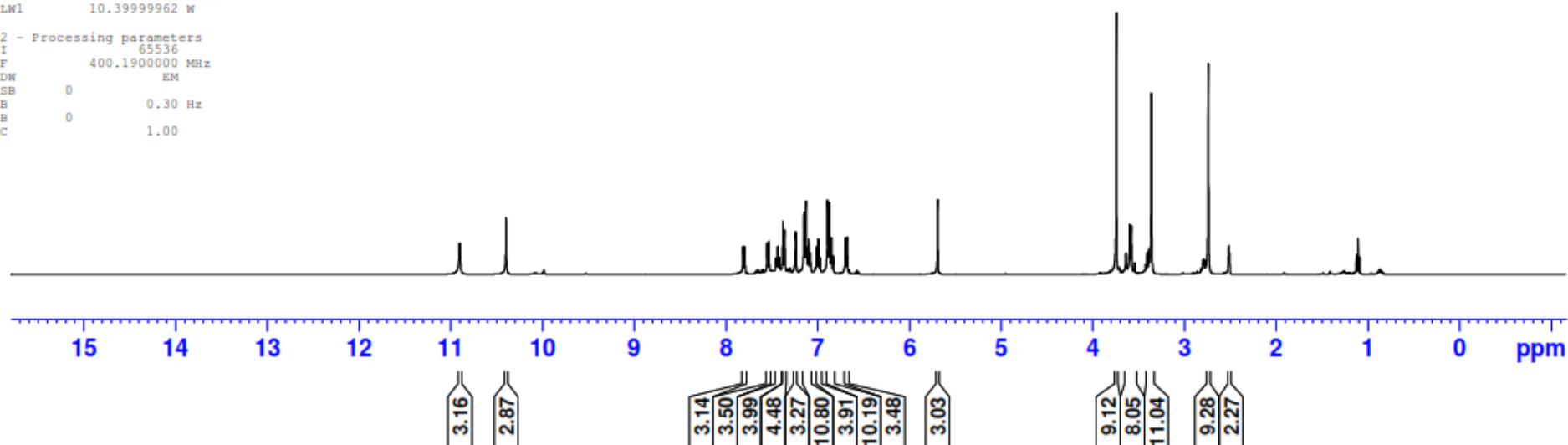
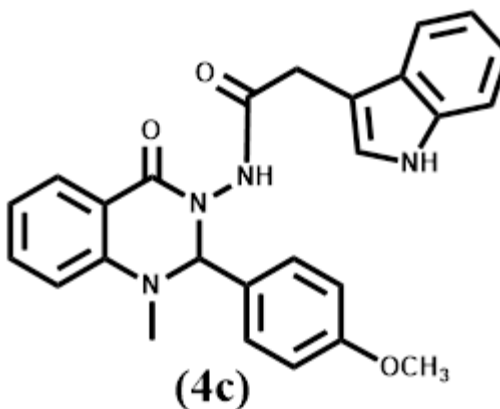
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7.4121
7.4084
7.3753
7.3545
7.2369
7.2320
7.1448
7.1232
7.0946
7.0751
7.0062
6.9878
6.9694
6.8879
6.8660
6.8440
6.8253
6.6947
6.6740
5.6871
3.7393
3.5928
3.5746
3.3552
2.7354
2.5095

Current Data Parameters
NAME Asmaa Alaa_H_B-S31
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180423
Time 7.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SMH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.58
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



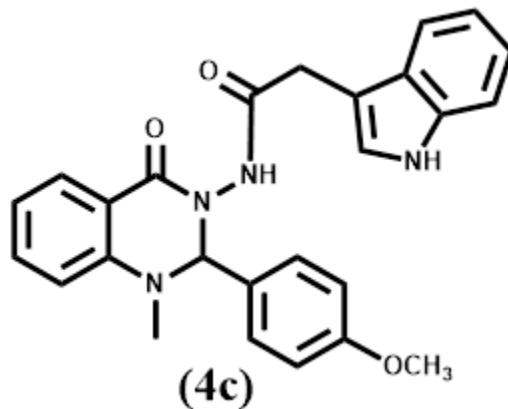


Current Data Parameters
 NAME Asmaa Sakr_H_B-S31_D20
 EXPNO 10
 PROCNO 1

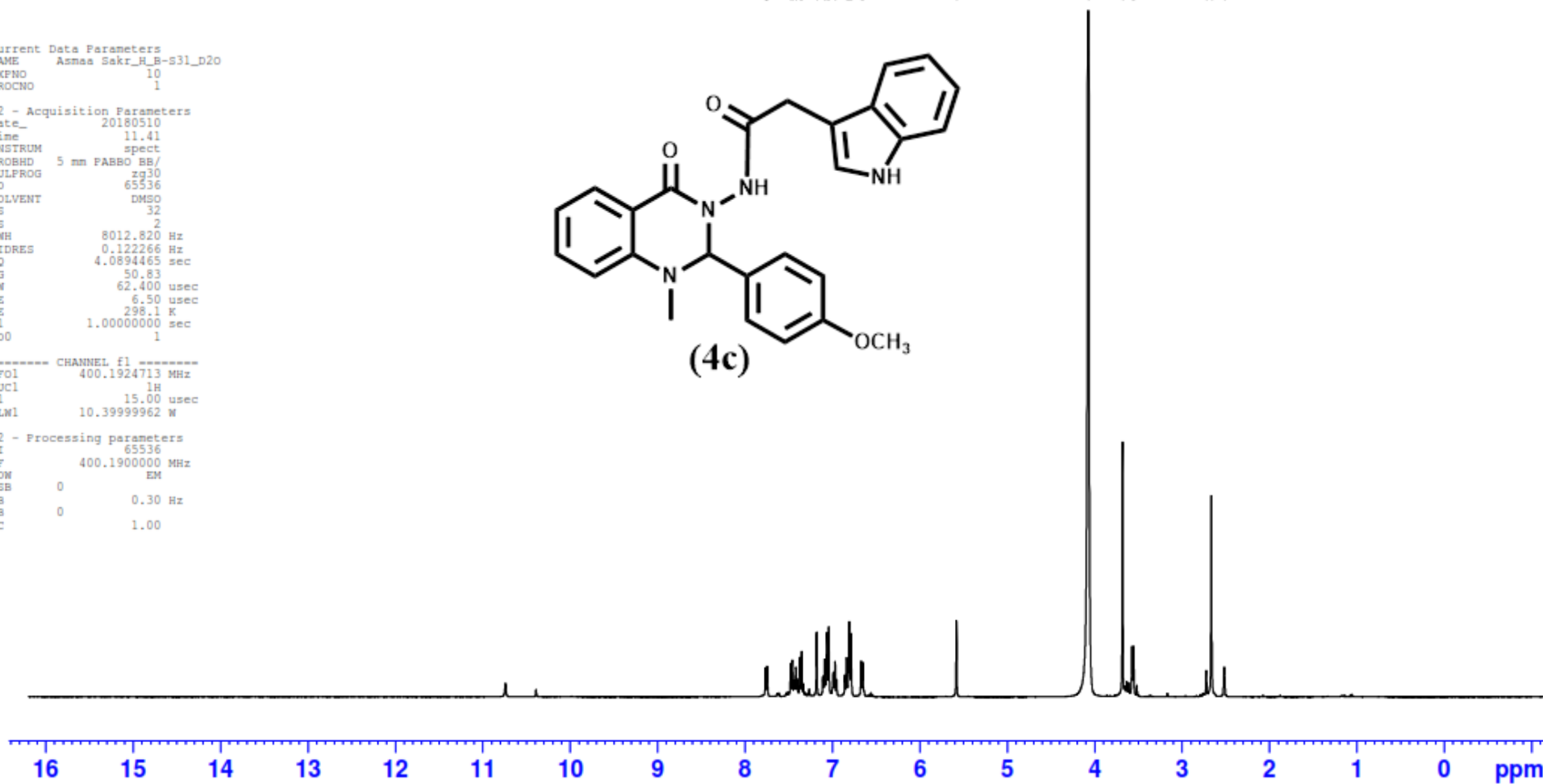
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 Date_ 20180510
 Time 11.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 50.83
 DM 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 S1 65536
 SF 400.1900000 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



7.7620
 7.7596
 7.7429
 7.4742
 7.4545
 7.4146
 7.3674
 7.3472
 7.1771
 7.0859
 7.0596
 7.0380
 6.9659
 6.8340
 6.8146
 6.8035
 6.7820
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 5.5771
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 3.5676
 3.5498
 2.7177
 2.6599
 2.5121



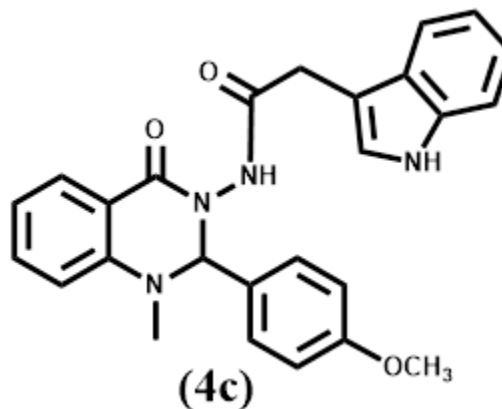
1.64
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 7.23
 5.59
 1.28
 67.86
 4.58
 2.43
 4.30



170.07
 161.00
 160.23
 147.24
 136.51
 135.00
 129.53
 128.79
 128.44
 127.61
 124.39
 121.49
 119.21
 118.82
 118.15
 115.07
 114.34
 112.71
 111.75
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 30.76

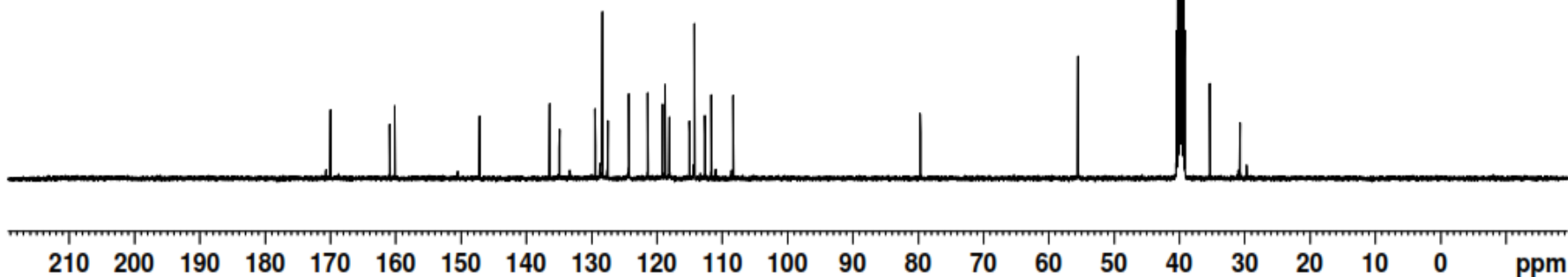
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 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
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 Time 1.20
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 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1200
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 202.37
 DW 20.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1



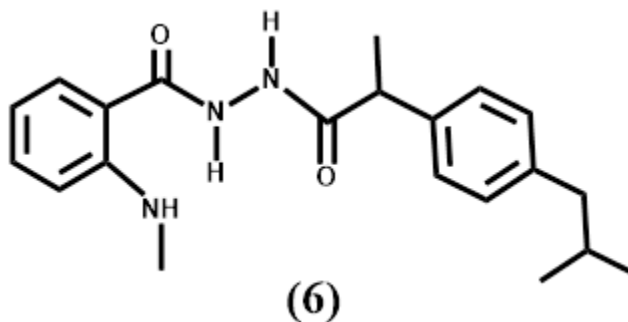
==== CHANNEL f1 =====
 SFO1 100.6379178 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 45.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1916008 MHz
 NUC2 1H
 CPDPRG[2] waltz16





10.0481
 9.9730
 7.5902
 7.5715
 7.5105
 7.4990
 7.3436
 7.3234
 7.3050
 7.2852
 7.1191
 7.0991
 6.6696
 6.6487
 6.5682
 6.5496
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 3.7400
 3.7228
 3.7052
 3.6879
 3.3379
 2.7902
 2.7780
 2.5137
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 2.5060
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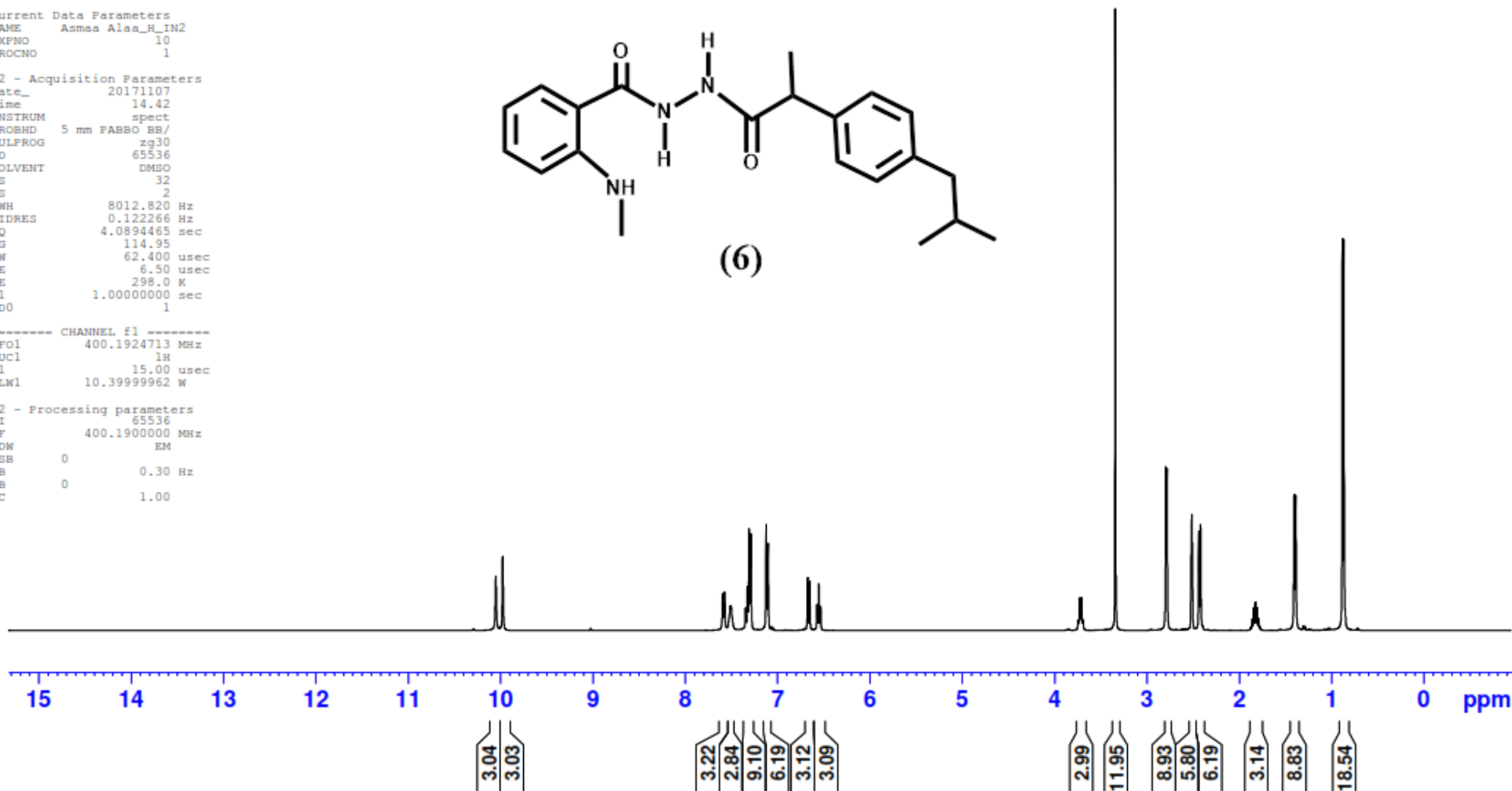


Current Data Parameters
 NAME Asmaa Alaa_H_IN2
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171107
 Time 14.42
 INSTRUM spect
 PROBHD 5 mm FAPBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SMH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 114.95
 DM 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SF01 400.1924713 MHz
 NUCL 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



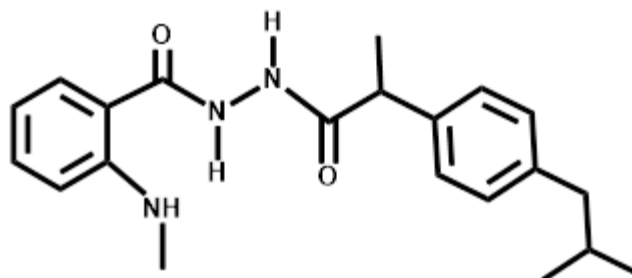


Current Data Parameters
 NAME Asmaa Alaa_H_IN2_D2O
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171108
 Time 12.33
 INSTRUM spect
 PROBHD 5 mm FAPBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 129.43
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

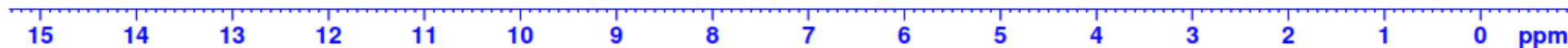
----- CHANNEL f1 -----
 SF01 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



(6)

7.4933
 7.4743
 7.3363
 7.3168
 7.2980
 7.2588
 7.2401
 7.0823
 7.0632
 6.6631
 6.6423
 6.5712
 6.5527
 6.5344
 4.1421
 3.6822
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 2.5141
 2.3799
 2.3627
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 1.7314
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 0.8168
 0.8006



2.76
 2.92
 5.51
 5.55
 2.80
 2.81
 27.37
 2.69
 8.49
 5.11
 5.71
 2.88
 8.13
 17.25

Asmaa Alaa_H_B-S17

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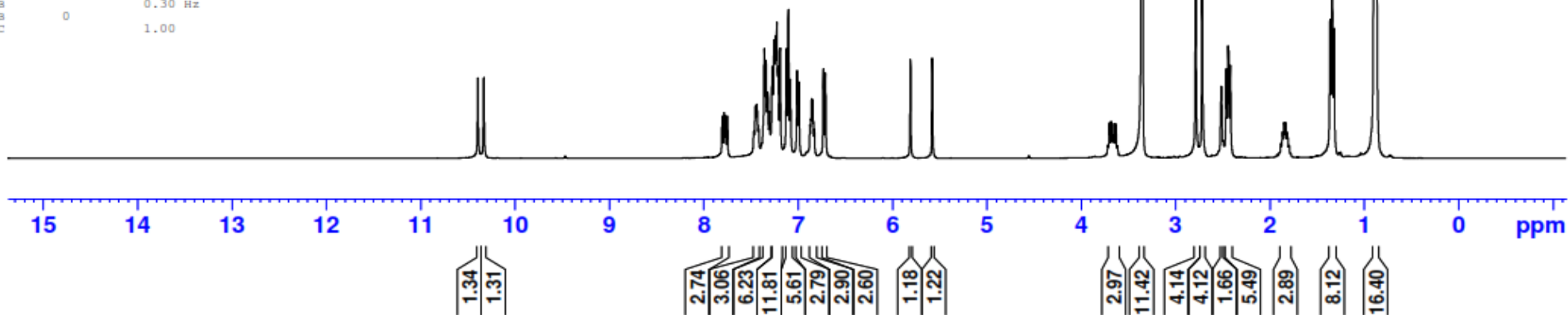
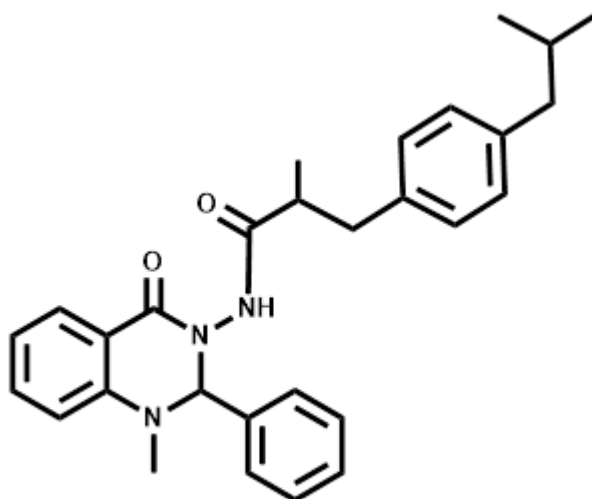
10.3905
10.3281
7.8013
7.7824
7.7666
7.7475
7.4674
7.4642
7.4472
7.4342
7.4170
7.3545
7.3376
7.3179
7.2994
7.2697
7.2512
7.2409
7.2326
7.2215
7.2071
7.1868
7.1204
7.0989
7.0780
7.0074
6.9889
6.8710
6.8526
6.8426
6.8243
6.7277
6.7070
5.8057
5.5746
3.6956
3.6780
3.6616
3.6455
3.6280
3.3596
3.3461
2.7821
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2.5095
2.4577
2.4395
2.4327
2.4145
1.8625
1.8454
1.8250

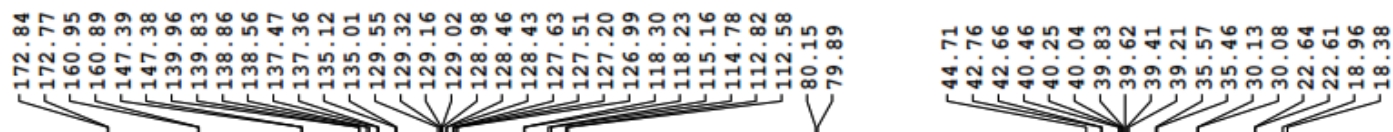
Current Data Parameters
NAME Asmaa Alaa_H_B-S17
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180423
Time 7.15
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 84.65
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



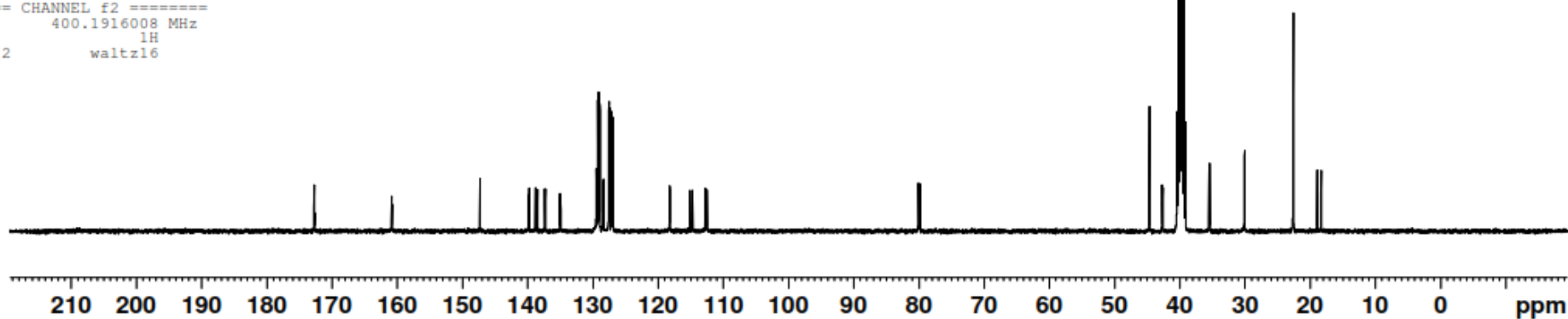
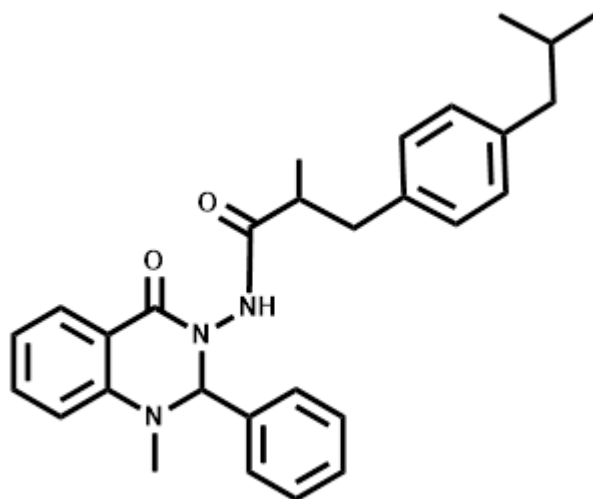


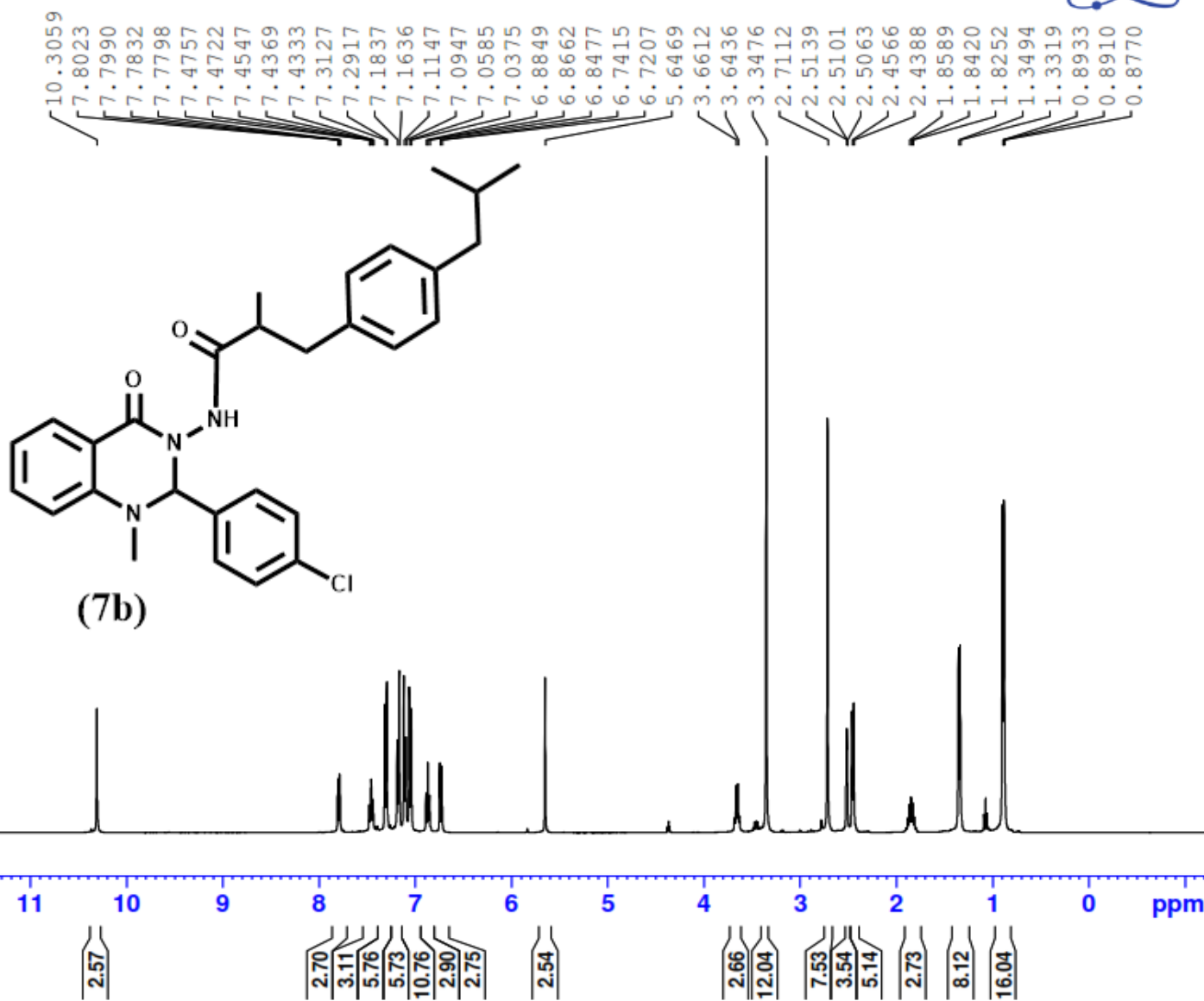
Current Data Parameters
NAME Asmaa Sakr_C_B-S17
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180510
Time 0.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16





Current Data Parameters
 NAME Asmaa Alaa_H_B-S13
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171207
 Time 14.42
 INSTRUM spect
 PROBHD 5 mm FAPBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 91.58
 DN 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

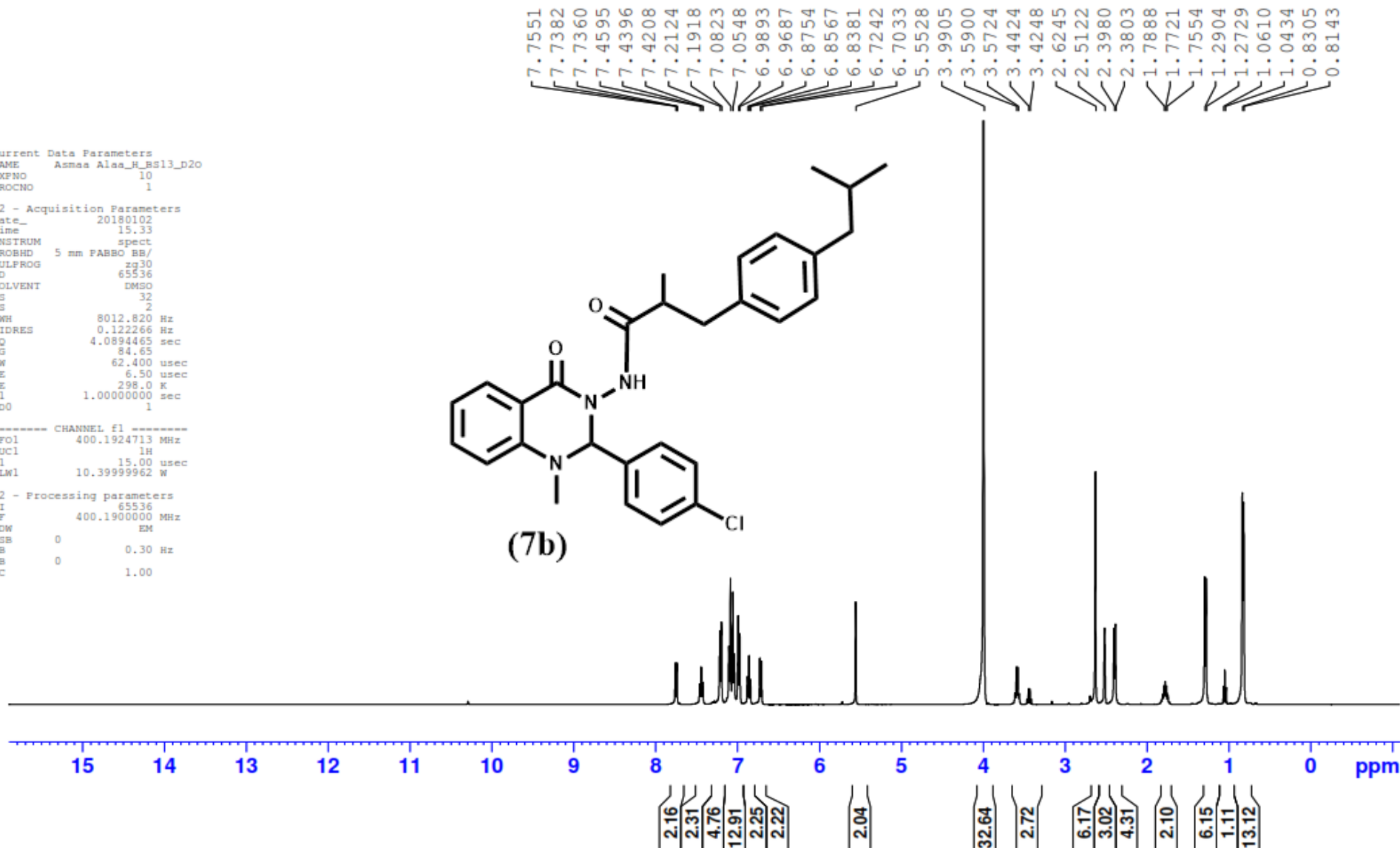
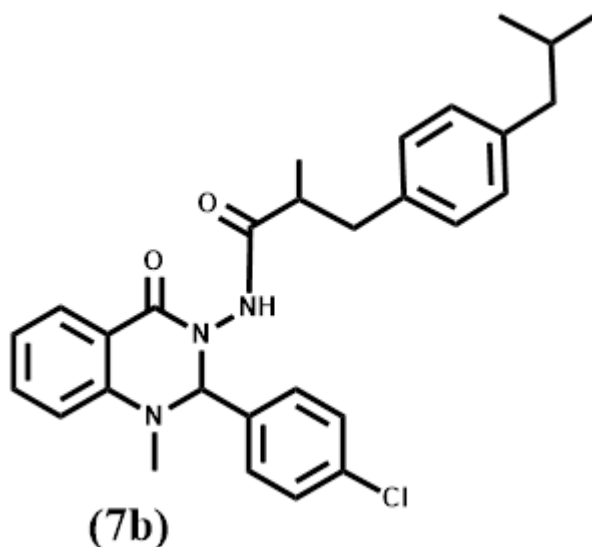


Current Data Parameters
 NAME Asmaa Alaa_H_BS13_D20
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180102
 Time 15.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 FULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 84.65
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SF01 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLM1 10.39999962 W

F2 - Processing parameters
 S1 65536
 SF 400.1900000 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





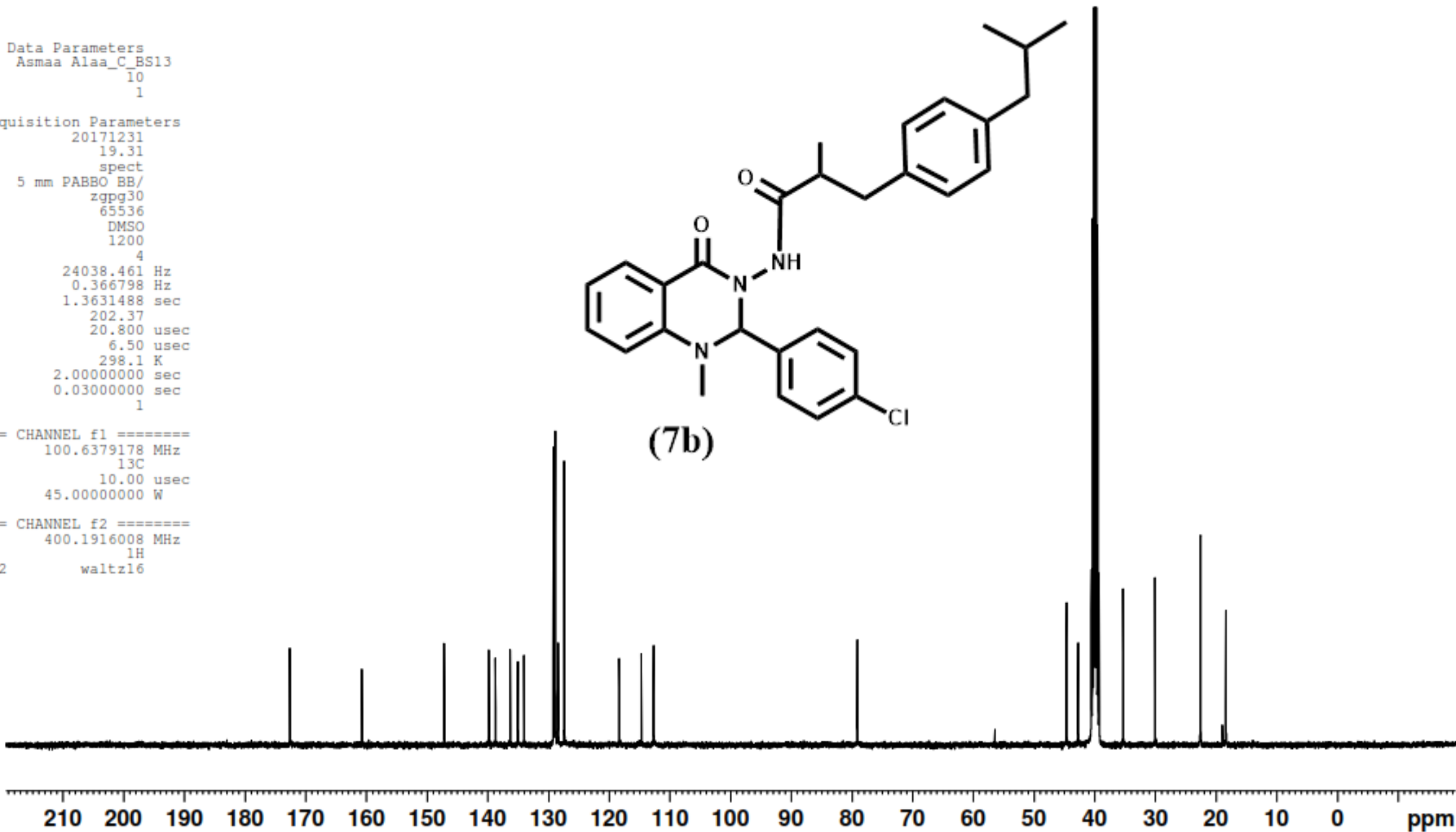
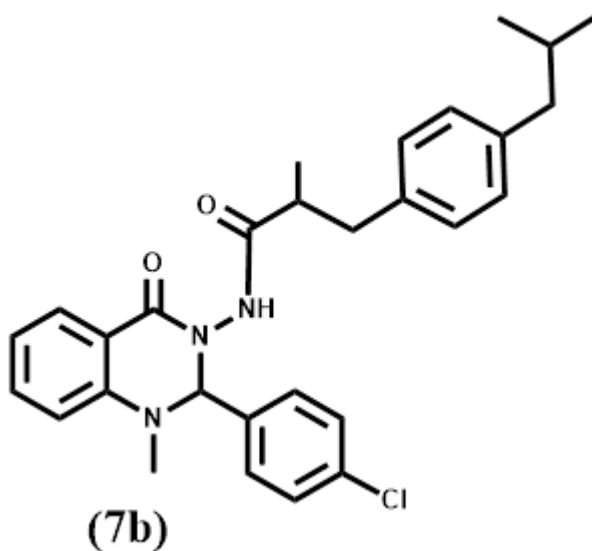
— 172.73 — 160.84 — 147.27 — 139.93 — 138.83 — 136.40 — 135.13 — 134.13 — 129.29 — 128.99 — 128.96 — 128.51 — 127.50 — 118.42 — 114.78 — 112.77 — 79.18 — 44.72 — 42.81 — 40.60 — 40.40 — 40.19 — 39.98 — 39.77 — 39.56 — 39.35 — 35.36 — 30.12 — 22.67 — 22.64 — 18.44

Current Data Parameters
 NAME Asmaa Alaa_C_BS13
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171231
 Time_ 19.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1200
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 202.37
 DW 20.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 100.6379178 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 45.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1916008 MHz
 NUC2 1H
 CPDPRG[2] waltz16





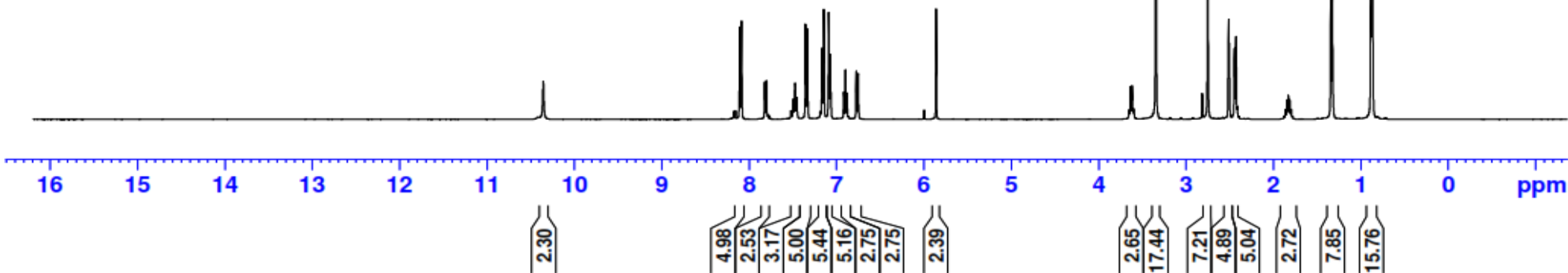
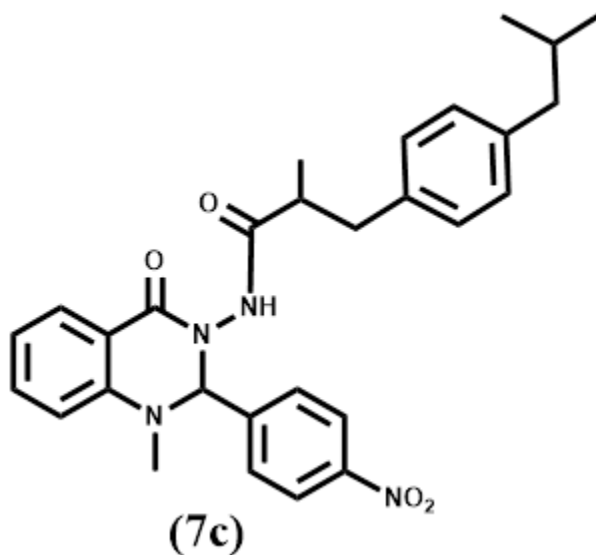
10.3562
8.1080
8.0863
7.8227
7.8193
7.8035
7.8000
7.4956
7.4919
7.4743
7.4567
7.4529
7.3549
7.3332
7.1657
7.1454
7.0894
7.0694
6.9167
6.8981
6.8797
6.7735
6.7527
5.8601
3.6521
3.6347
3.6171
3.5996
3.3454
2.8143
2.7511
2.5142
2.5102
2.5062
2.4444
2.4269
1.8461
1.8293
1.8125
1.3423
1.3248
0.8854
0.8808

Current Data Parameters
NAME Asmaa Alaa_H_B-S14
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171207
Time 14.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 106.37
DM 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLM1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





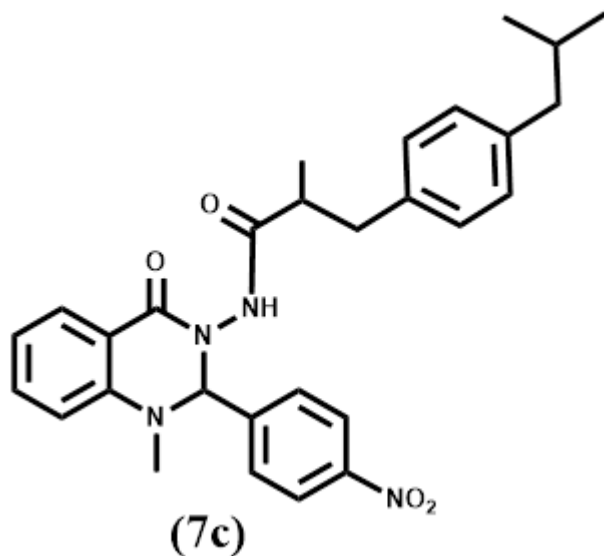
Current Data Parameters
NAME Asmaa Alaa_H_BS14_D20-
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

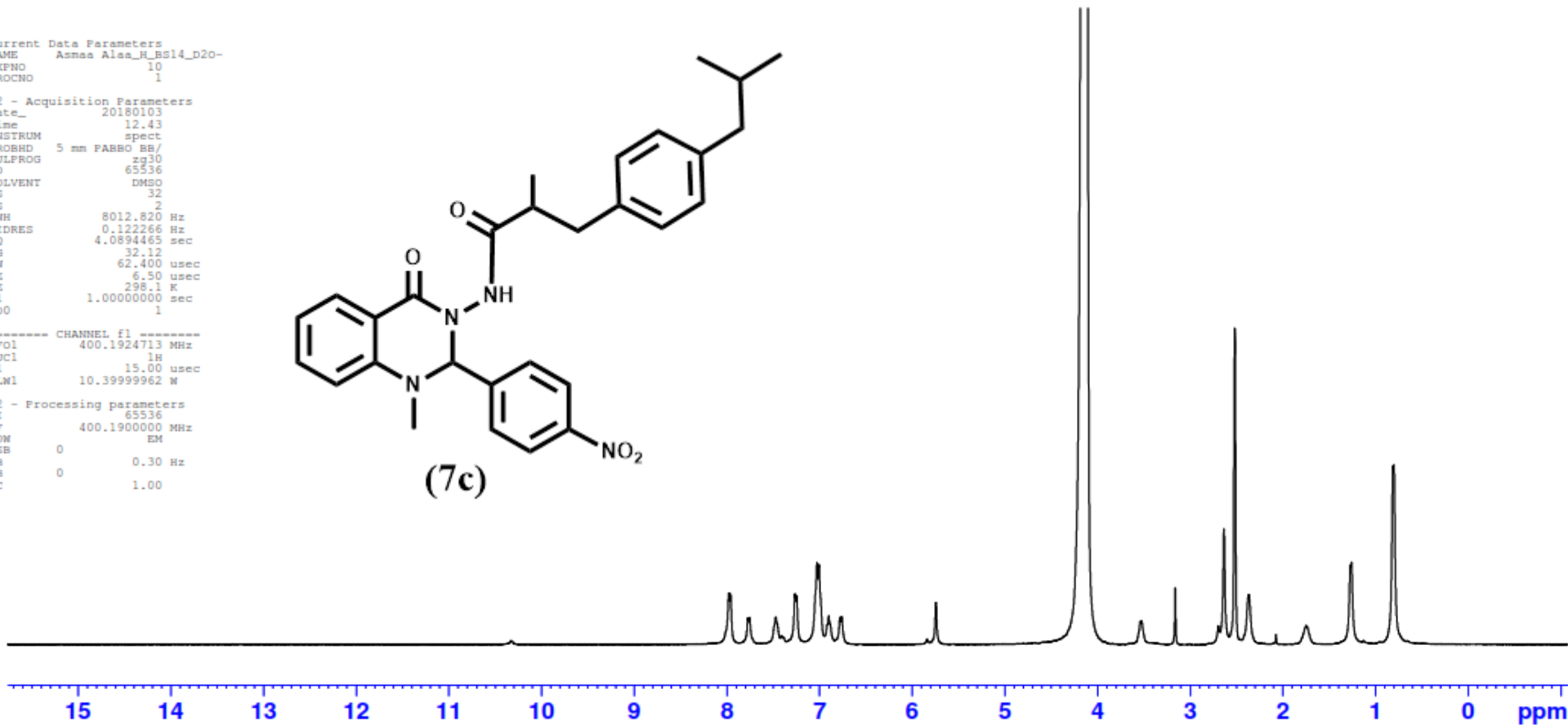
Date_ 20180103
Time 12.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 32.12
DM 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

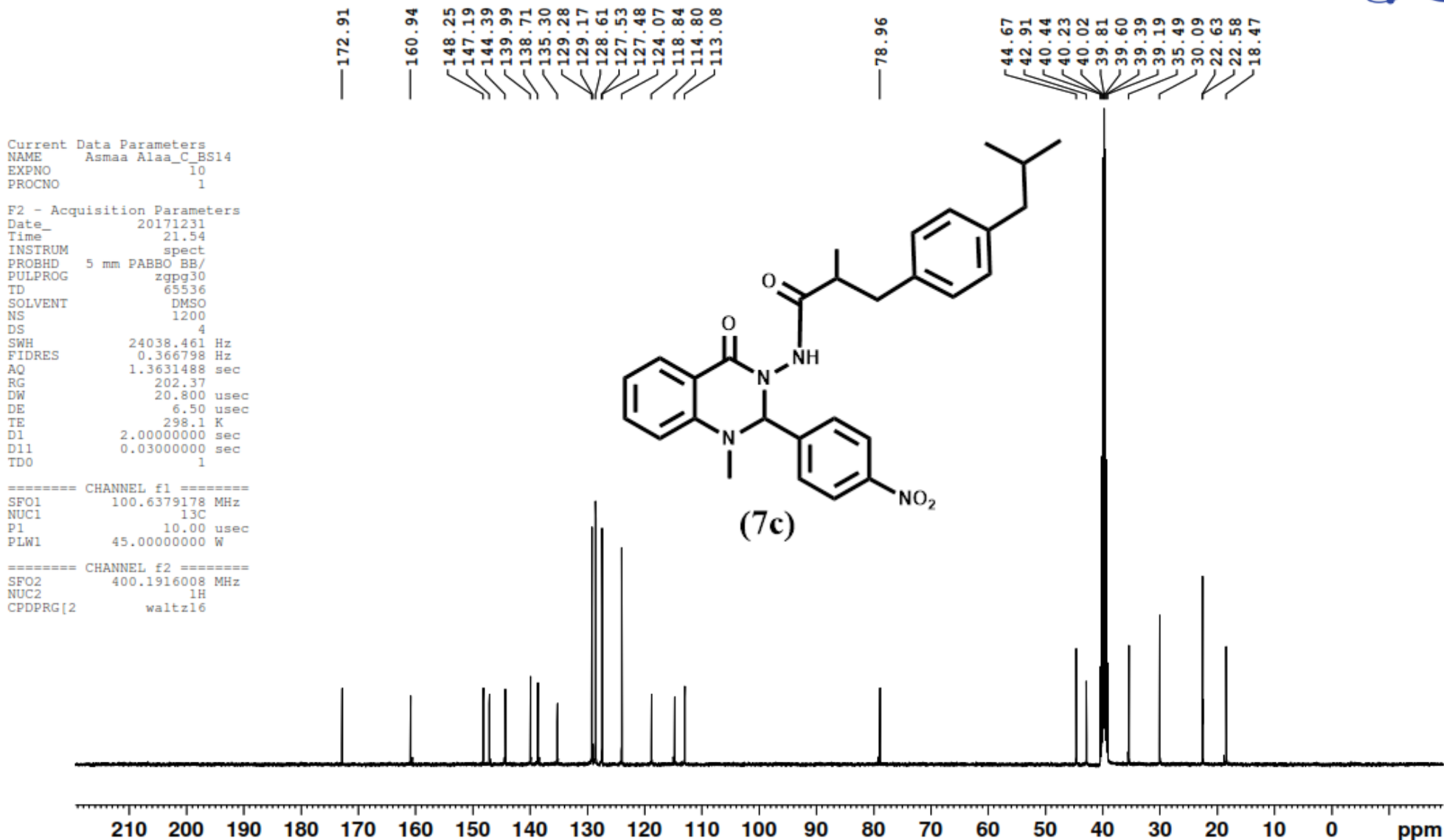
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7.9756
7.9562
7.7690
7.7518
7.4683
7.2616
7.2434
7.0229
7.0026
6.8962
6.7750
6.7564
5.7394
4.1494
3.1567
2.6300
2.5141
2.3629
1.2668
1.2536
0.8062
0.7958



1.06
1.16
2.04
89.31
3.28
3.15

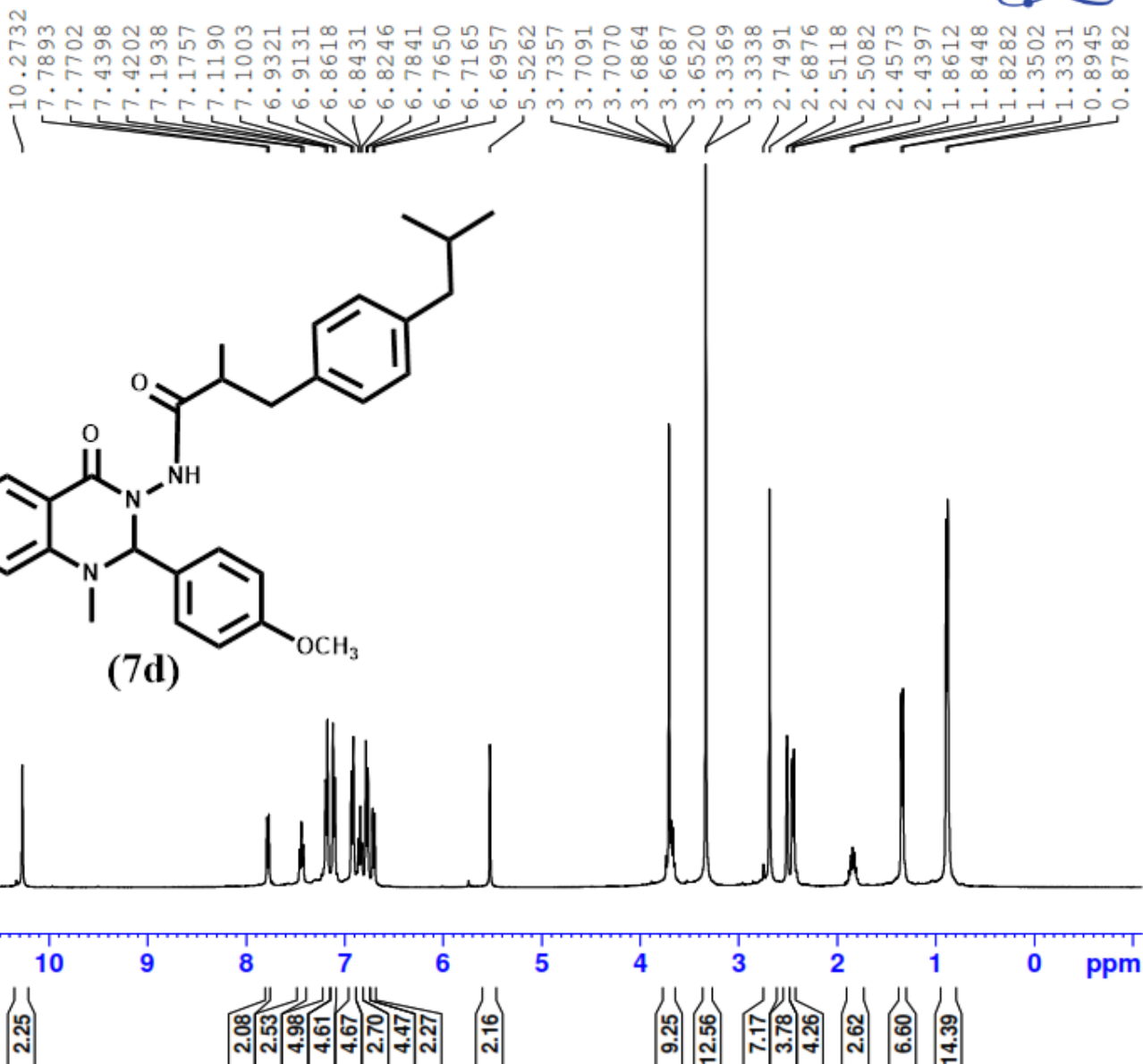
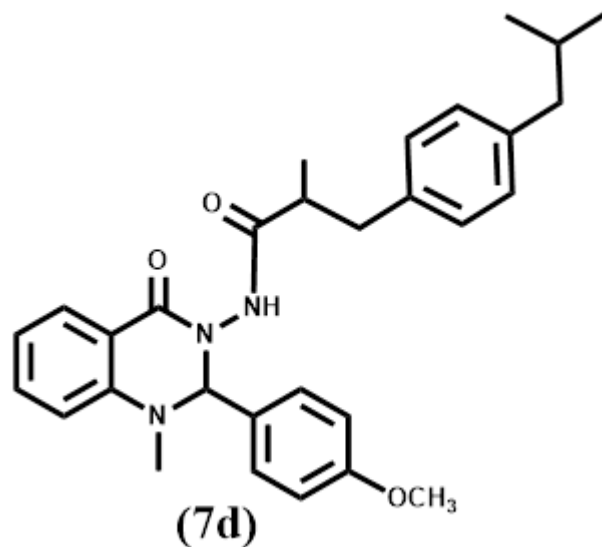


Current Data Parameters
 NAME Asmaa Alaa_H_B-S15
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180102
 Time 18.04
 INSTRUM spect
 PROBHD 5 mm FAPBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 129.43
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PL1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



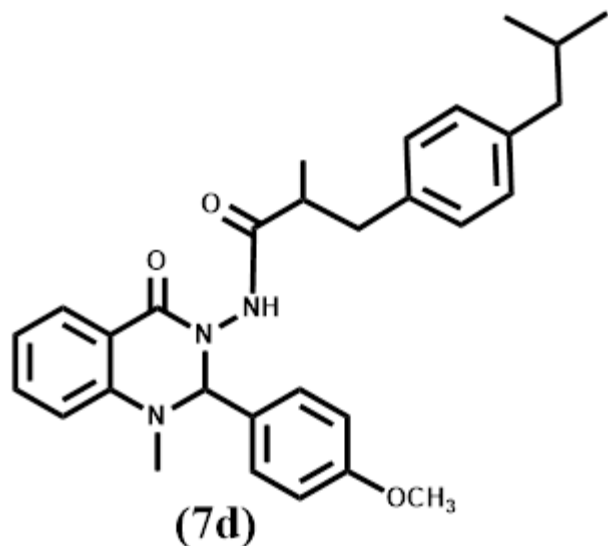


Current Data Parameters
 NAME Asmaa Alaa_H_BS-15_D2O
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180114
 Time 13.07
 INSTRUM spect
 PROBHD 5 mm FAPBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 129.43
 DW 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

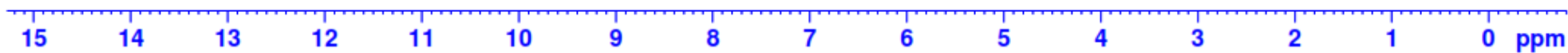
----- CHANNEL f1 -----
 SFO1 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLM1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



7.7435
 7.7260
 7.4540
 7.4356
 7.4174
 7.1222
 7.1023
 7.0734
 7.0532
 6.8690
 6.8475
 6.8230
 6.7188
 6.7058
 6.6976
 6.6861
 5.4357
 4.0605
 3.6829
 3.6536
 3.6141
 3.5965
 2.6804
 2.6209
 2.5127
 2.4035
 2.3859
 1.7754
 1.7585
 1.3006
 1.2830
 0.8368
 0.8310
 0.8210
 0.8152

1.56
 1.69
 6.98
 4.89
 4.50
 1.32
 42.83
 6.43
 0.70
 4.12
 3.57
 3.49
 1.75
 4.62
 10.25





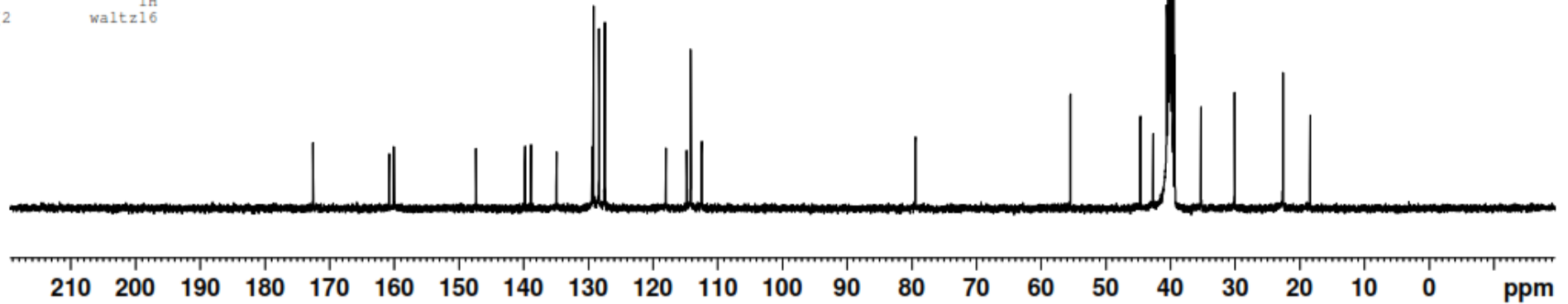
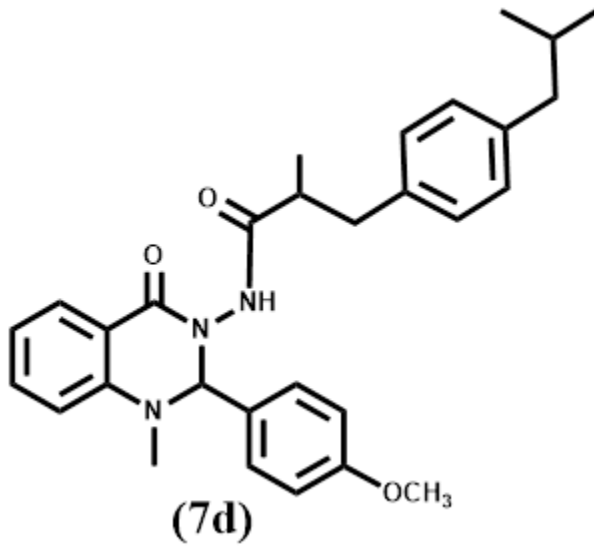
— 172.64
 < 160.89
 < 160.16
 — 147.44
 < 139.88
 < 138.95
 < 134.99
 < 129.51
 < 129.29
 < 128.39
 < 127.52
 < 118.08
 < 114.84
 < 114.25
 < 112.55
 — 79.51
 < 55.54
 < 44.72
 < 42.72
 < 40.62
 < 40.41
 < 40.20
 < 39.99
 < 39.78
 < 39.57
 < 39.36
 < 35.32
 < 30.14
 < 22.68
 < 22.63
 < 18.44

Current Data Parameters
 NAME Asmaa Alaa_C_B-S15
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180111
 Time_ 21.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1200
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 202.37
 DW 20.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6379178 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 45.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1916008 MHz
 NUC2 1H
 CPDPRG[2] waltz16



Asmaa Alaa_H_B-S16

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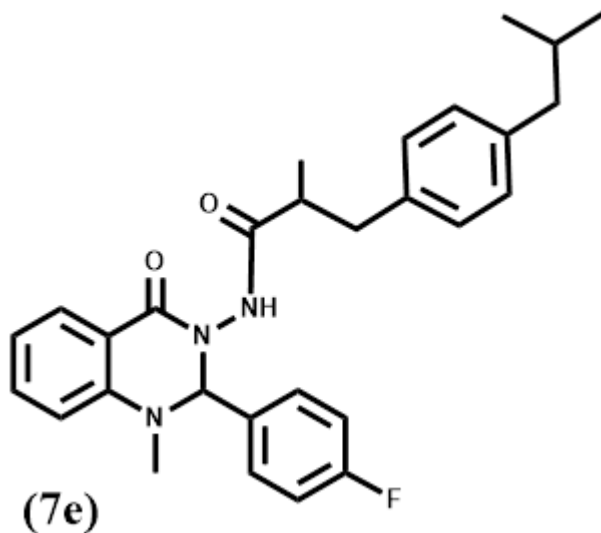
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7.7966
7.7809
7.7774
7.4753
7.4716
7.4541
7.4364
7.4326
7.1834
7.1633
7.1129
7.0928
7.0757
7.0576
6.8811
6.8625
6.8440
6.7405
6.7198
5.6330
3.6614
3.6438
3.3343
2.7036
2.5136
2.5095
2.5054
2.4532
2.4354
1.8568
1.8400
1.8232
1.3459
1.3283
0.8896
0.8736

Current Data Parameters
NAME Asmaa Alaa_H_B-S16
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180423
Time 7.09
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 146.06
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

2.48

2.61

2.79

5.86

15.18

2.89

2.68

2.44

2.75

17.07

7.61

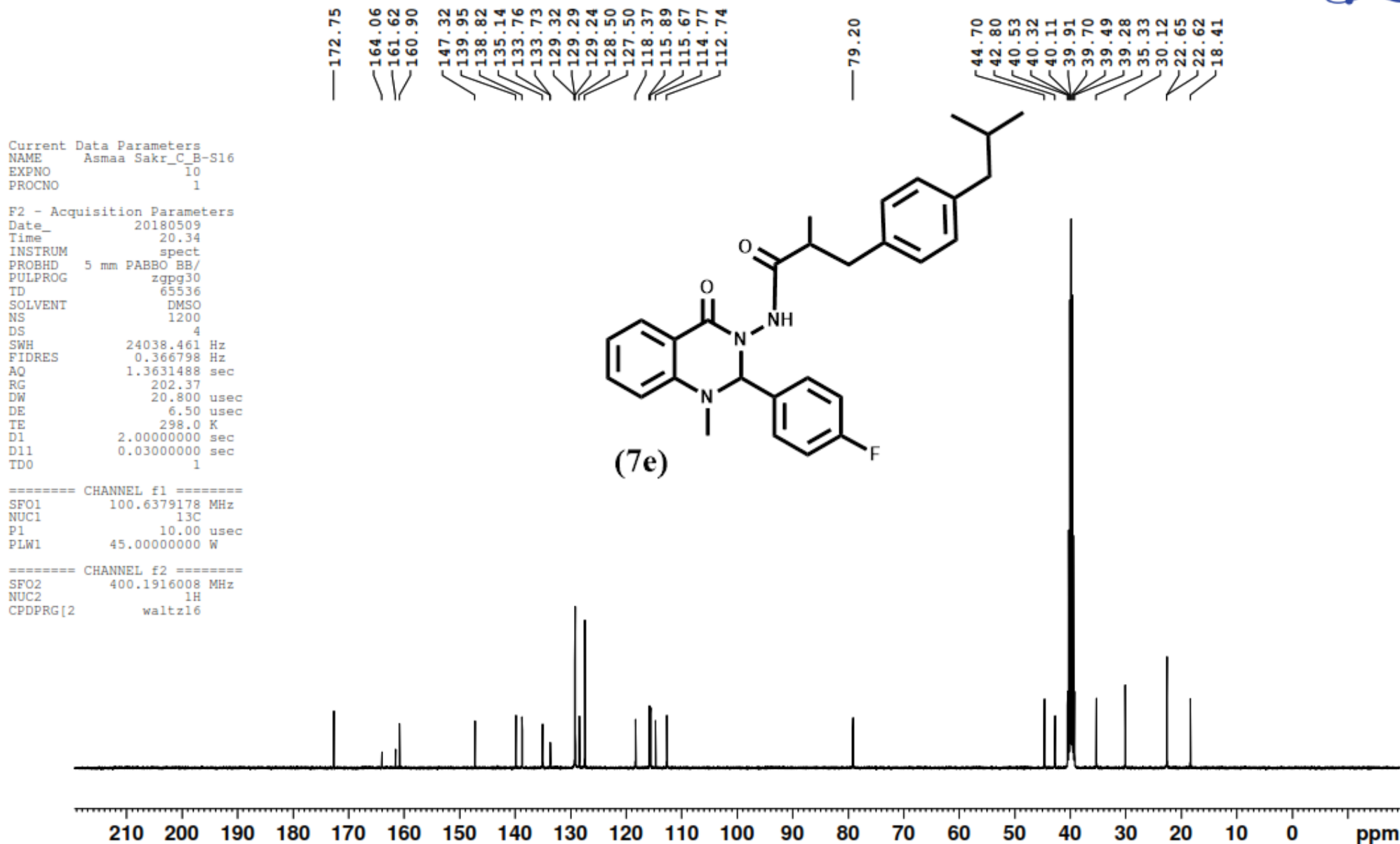
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4.93

2.69

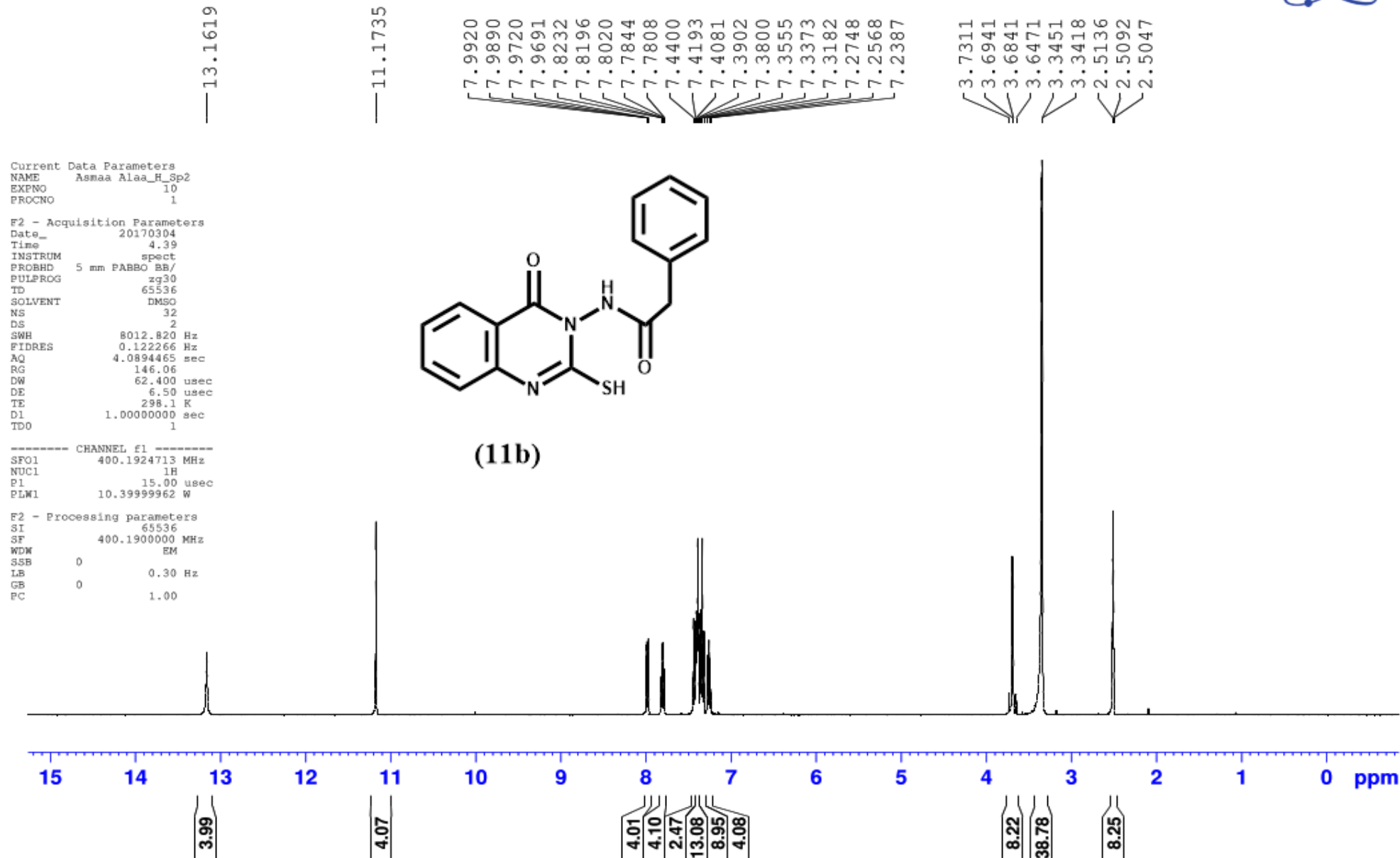
7.87

15.79



Asmaa Alaa_H_Sp2

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```

Current Data Parameters
NAME      Asmaa Alaa_H_Sp2_D20
EXPNO    10
PROCNO    1

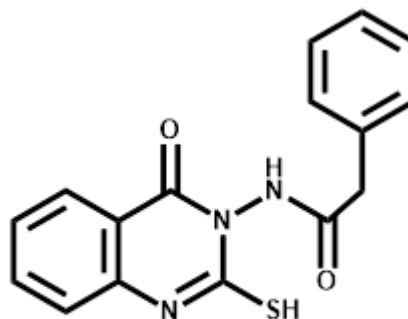
F2 - Acquisition Parameters
Date_     20170305
Time      20.07
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        65536
SOLVENT   DMSO
NS        32
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894465 sec
RG        146.06
DW        62.400 usec
DE        6.50 usec
TE        298.0 K
D1        1.00000000 sec
TDO       1

----- CHANNEL f1 -----
SF01      400.1924713 MHz
NUC1      1H
P1        15.00 usec
PLW1      10.39999962 W

F2 - Processing parameters
SI        65536
SF        400.1900000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

7.9706
 7.9671
 7.9499
 7.9469
 7.7916
 7.7882
 7.7709
 7.7527
 7.7493
 7.3828
 7.3712
 7.3601
 7.3329
 7.3151
 7.2961
 7.2641
 7.2462
 7.2283

3.9201
 3.6581
 3.6522
 2.5152
 2.5109
 2.5066

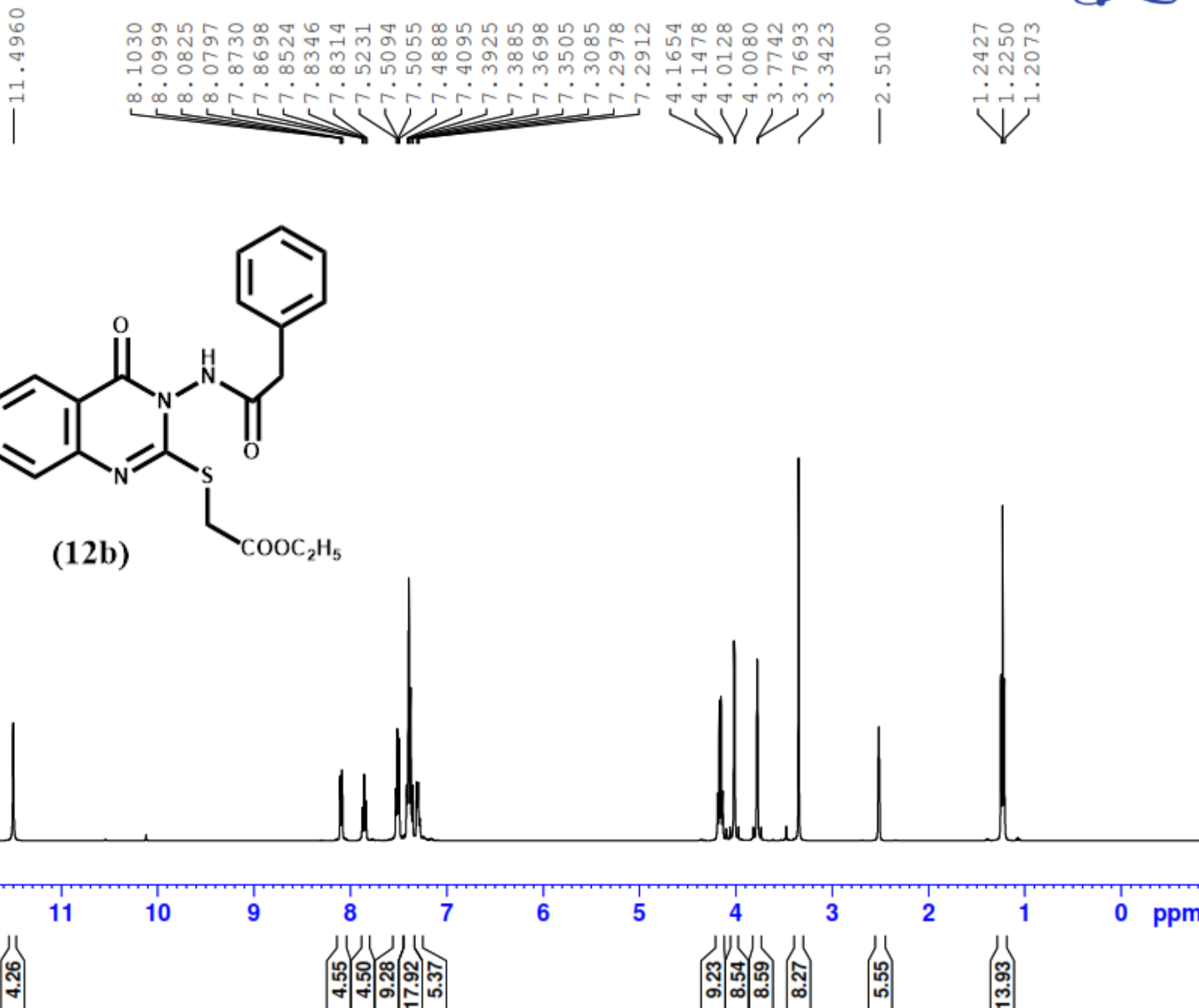


(11b)



2.54
 2.66
 10.40
 5.69
 2.50

65.61
 5.22
 5.37



Current Data Parameters
 NAME Asmaa Alaa_H_PH2
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170605
 Time 12.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 114.95
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SP01 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

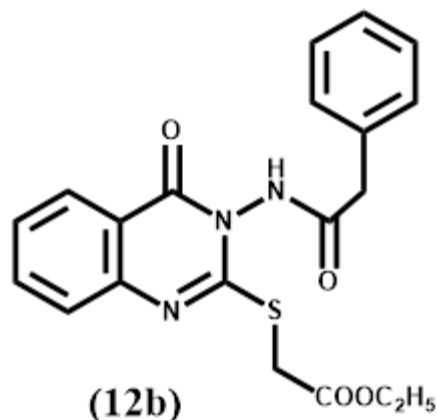
F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



8.0724
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7.8327
7.8161
7.8126
7.5102
7.4895
7.4675
7.3836
7.3673
7.3502
7.3305
7.2942
7.2855
7.2767
4.1533
4.1357
4.1180
4.1004
3.9486
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3.7419
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2.5077
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1.1726

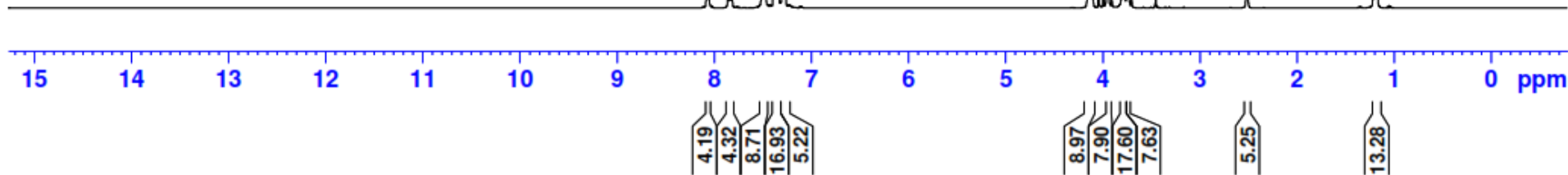
Current Data Parameters
 NAME Asmaa Alaa_H_PH2_D2O
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170605
 Time 14.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 114.95
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1



----- CHANNEL f1 -----
 SF01 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.399999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Asmaa Alaa_H_PO3#

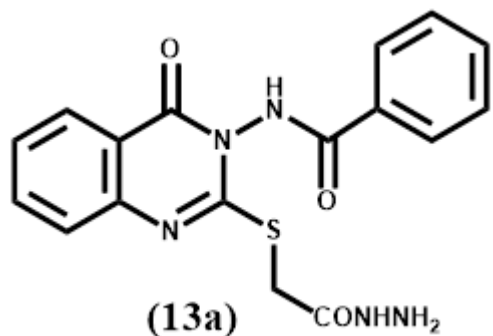
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg



11.4310
11.4219
11.4117
11.1511
9.3835
8.1296
8.1272
8.1099
8.1075
8.0104
7.9922
7.8965
7.8789
7.8755
7.7185
7.7001
7.6757
7.6552
7.6449
7.6255
7.6071
7.5524
7.5330
4.3401
3.9887
3.9459
3.9098
3.8540
3.8179
3.3369
2.5137
2.5097
2.5057

Current Data Parameters
NAME Asmaa Alaa_H_PO3#
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180102
Time 17.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DN 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1



----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

3.51
4.57
5.79
10.16
5.20
20.74
5.18
9.16
10.69
17.53
7.49

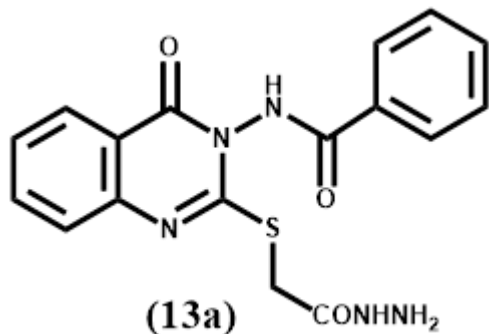


Current Data Parameters
 NAME Asmaa Alaa_H_PO3#_D20
 EXPNO 10
 PROCNO 1

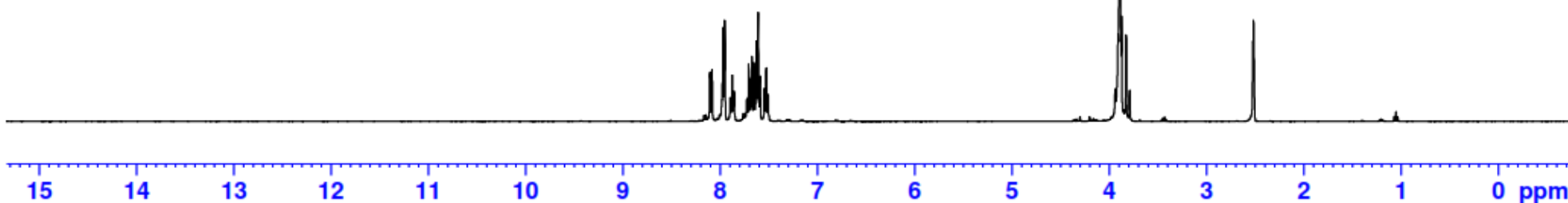
F2 - Acquisition Parameters
 Date_ 20180103
 Time 13.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 169.46
 DW 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



8.1022
 8.0995
 8.0824
 8.0798
 7.9683
 7.9503
 7.9471
 7.8938
 7.8903
 7.8729
 7.8553
 7.8518
 7.7225
 7.7041
 7.6855
 7.6705
 7.6502
 7.6248
 7.6053
 7.5868
 7.5416
 7.5220
 7.5040
 3.9345
 3.9047
 3.8854
 3.8685
 3.8218
 3.7851
 2.5156
 2.5115
 2.5074



4.22
 8.67
 4.59
 9.19
 8.90
 4.45
 48.93
 3.70
 1.25
 6.10

Asmaa Alaa_C_Po3

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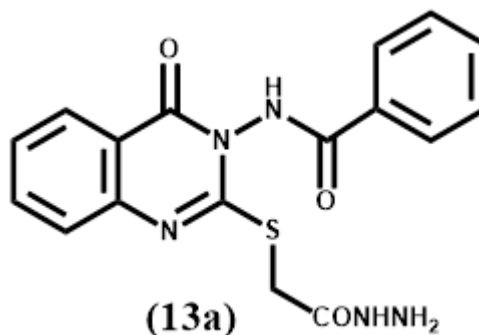
166.74
166.32
159.12
158.92
147.15
135.87
133.50
131.47
129.37
128.32
127.14
126.90
126.86
119.74

40.61
40.40
40.19
39.98
39.77
39.56
39.35
33.95

Current Data Parameters
NAME Asmaa Alaa_C_Po3
EXPNO 10
PROCNO 1

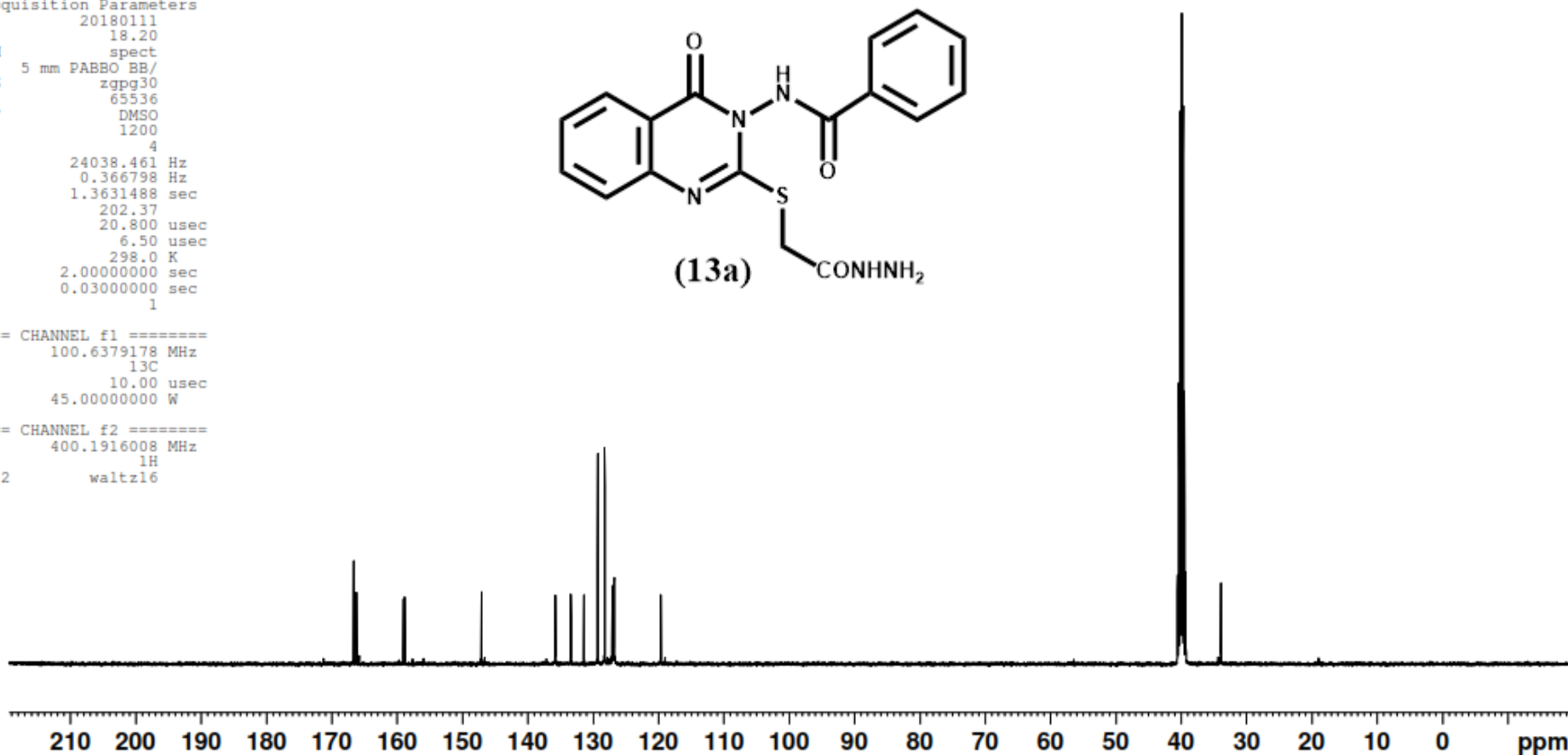
F2 - Acquisition Parameters

Date_ 20180111
Time 18.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1



==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16





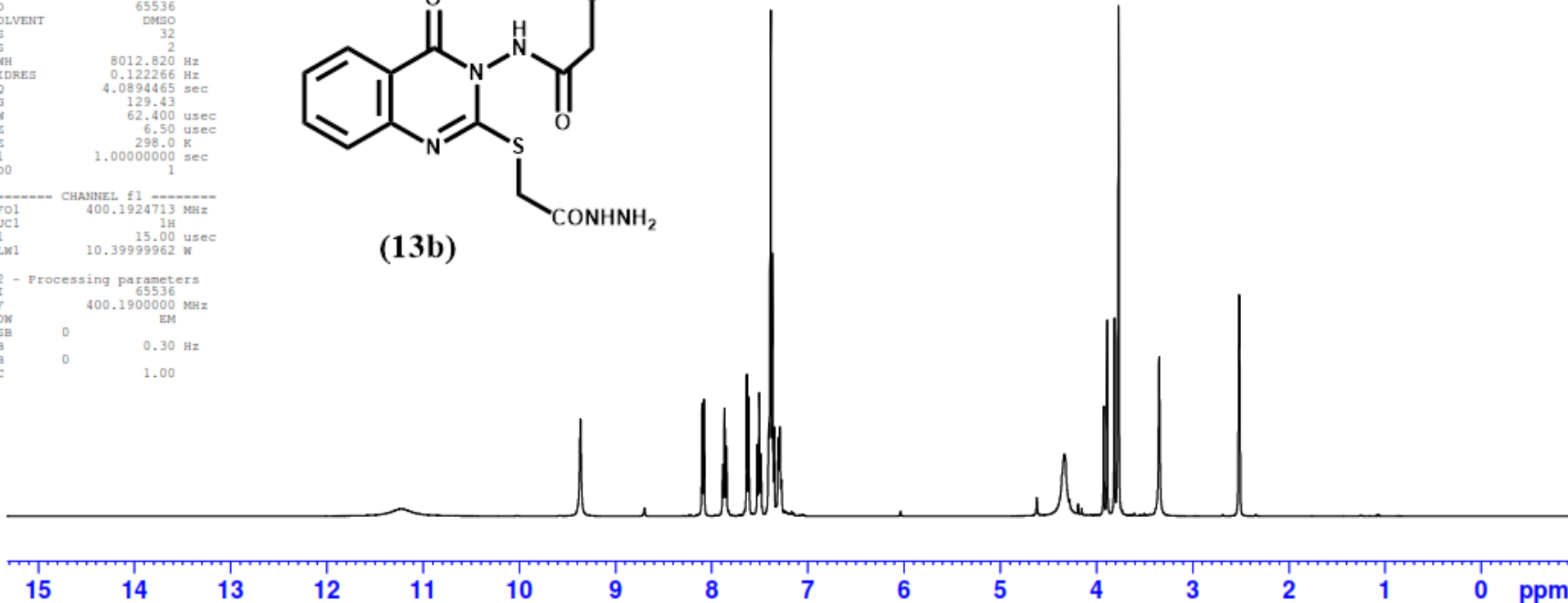
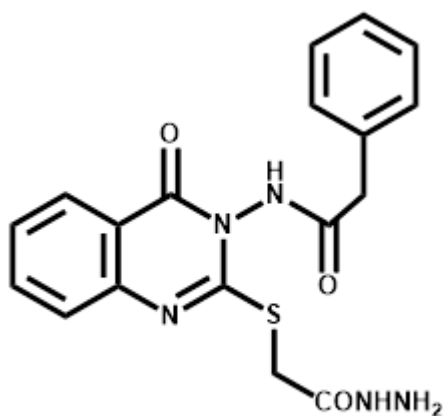
— 11.2293
 9.3610
 8.0937
 8.0762
 8.0740
 7.8788
 7.8613
 7.8437
 7.8404
 7.6309
 7.6107
 7.5197
 7.5015
 7.4834
 7.3455
 7.3041
 7.2873
 4.3303
 4.3165
 3.9191
 3.8827
 3.8088
 3.7657
 3.3427
 — 2.5098

Current Data Parameters
 NAME Asmaa Alaa_H_PH1
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170605
 Time 12.30
 INSTRUM spect
 PROBHD 5 mm FAPBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SMH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 129.43
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SF01 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



4.13
 4.68
 5.18
 5.28
 5.32
 5.48
 21.18
 5.51
 8.46
 5.36
 15.44
 6.56
 7.43

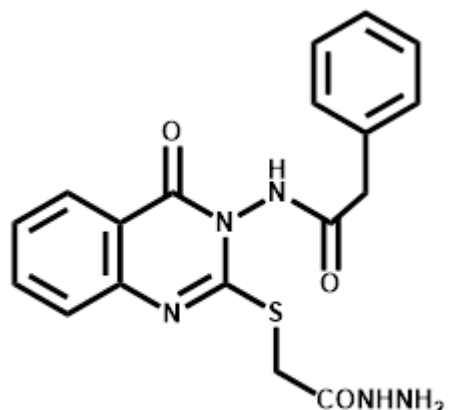


Current Data Parameters
 NAME Asmaa Alaa_R_PH1_D2O
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170618
 Time 15.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 64.21
 DN 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

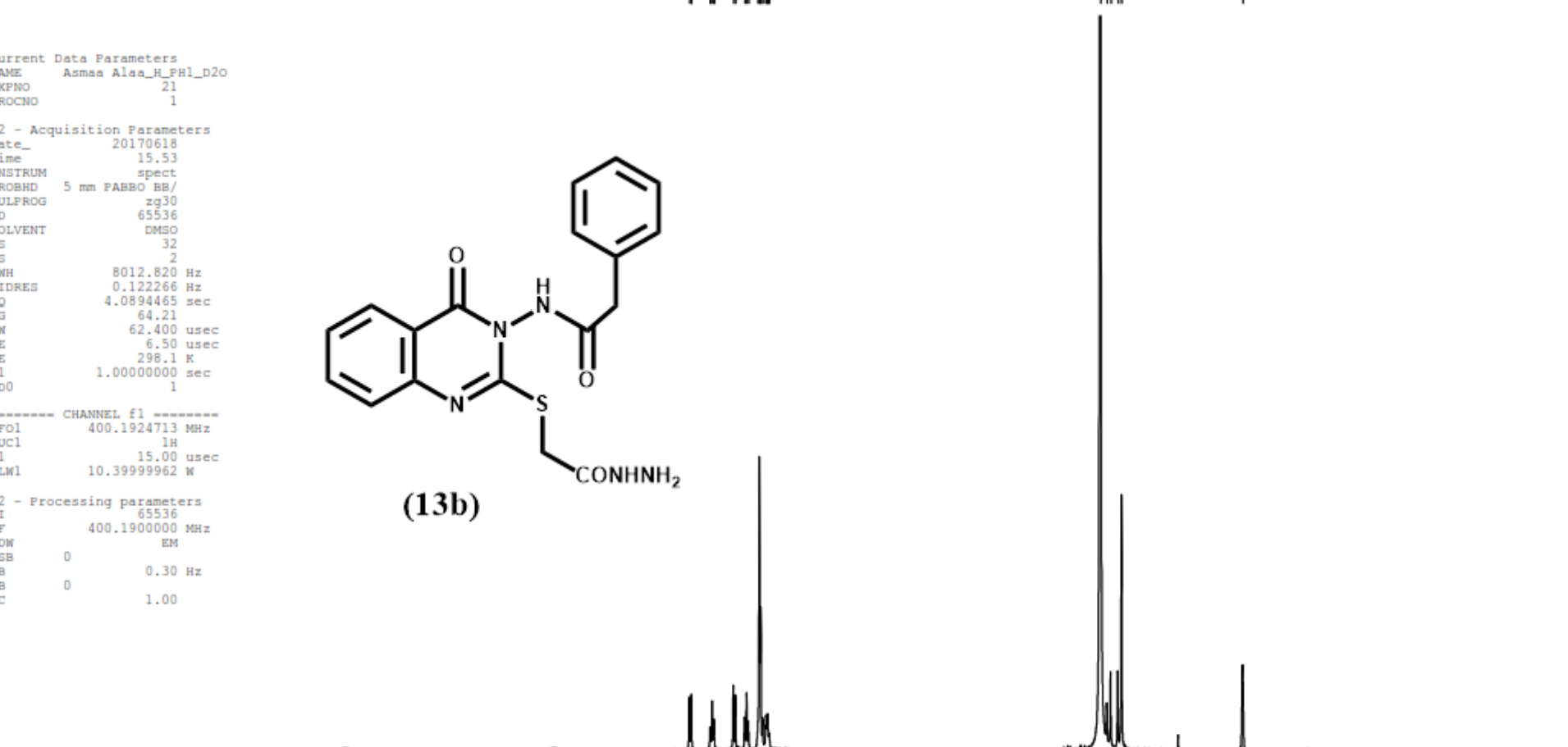
----- CHANNEL f1 -----
 SFO1 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



(13b)

8.0574
 8.0398
 8.0376
 7.8511
 7.8479
 7.8303
 7.8127
 7.8095
 7.6178
 7.5974
 7.5035
 7.4848
 7.4665
 7.3706
 7.3573
 7.3514
 7.3422
 7.3222
 7.2936
 7.2876
 7.2803
 7.2722
 7.2636
 7.2572
 3.9389
 3.8732
 3.8362
 3.7639
 3.7265
 — 2.5122



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

2.02
 2.08
 2.05
 2.10
 7.98
 2.12

73.38
 5.94

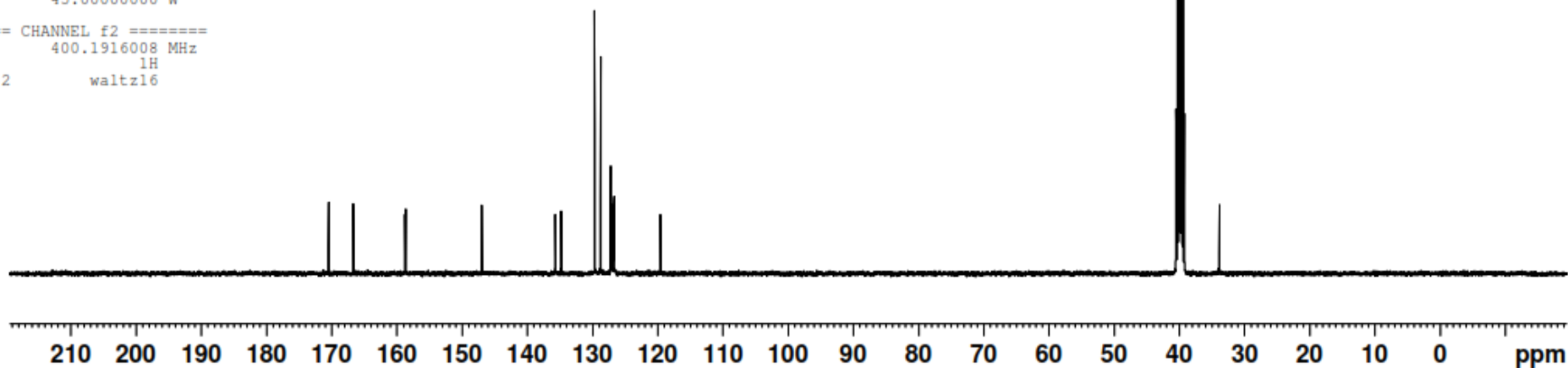
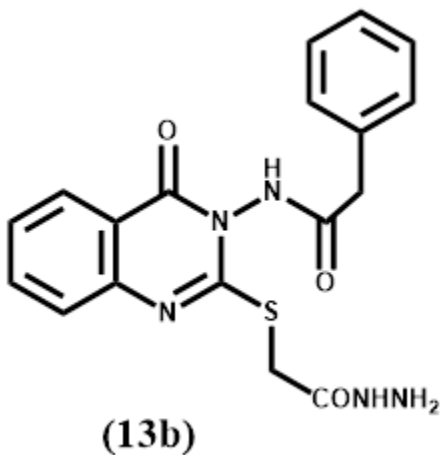
2.34



170.55
 166.77
 158.85
 158.72
 147.05
 135.79
 134.90
 129.76
 128.84
 127.29
 127.10
 126.83
 126.78
 119.67
 40.55
 40.34
 40.13
 39.92
 39.71
 39.50
 39.29
 33.89

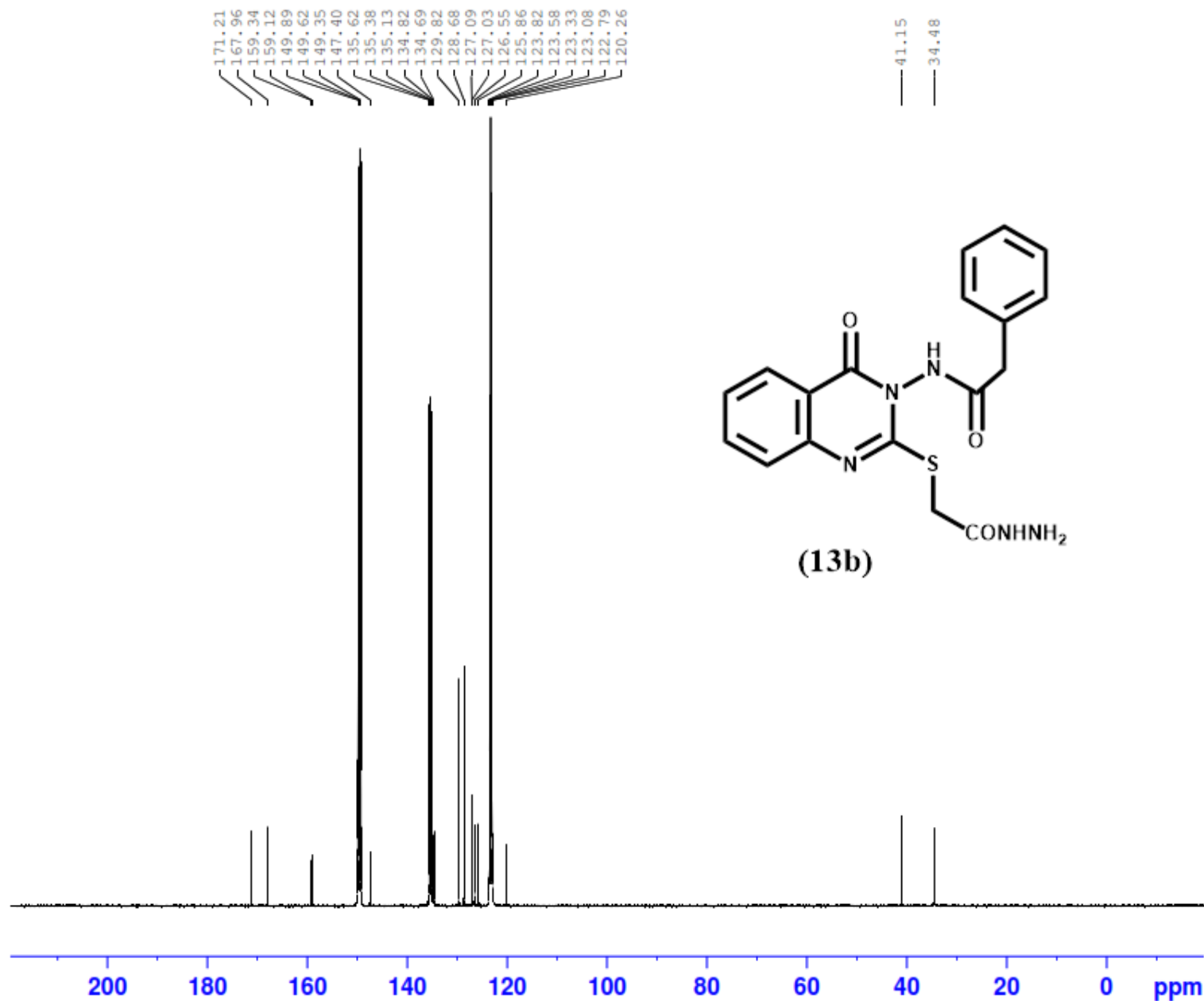
Current Data Parameters
 NAME Asmaa Alaa_C_PH1
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170616
 Time 8.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1200
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 202.37
 DW 20.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1



===== CHANNEL f1 =====
 SFO1 100.6379178 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 45.00000000 W
 ===== CHANNEL f2 =====
 SFO2 400.1916008 MHz
 NUC2 1H
 CPDPRG[2] waltz16

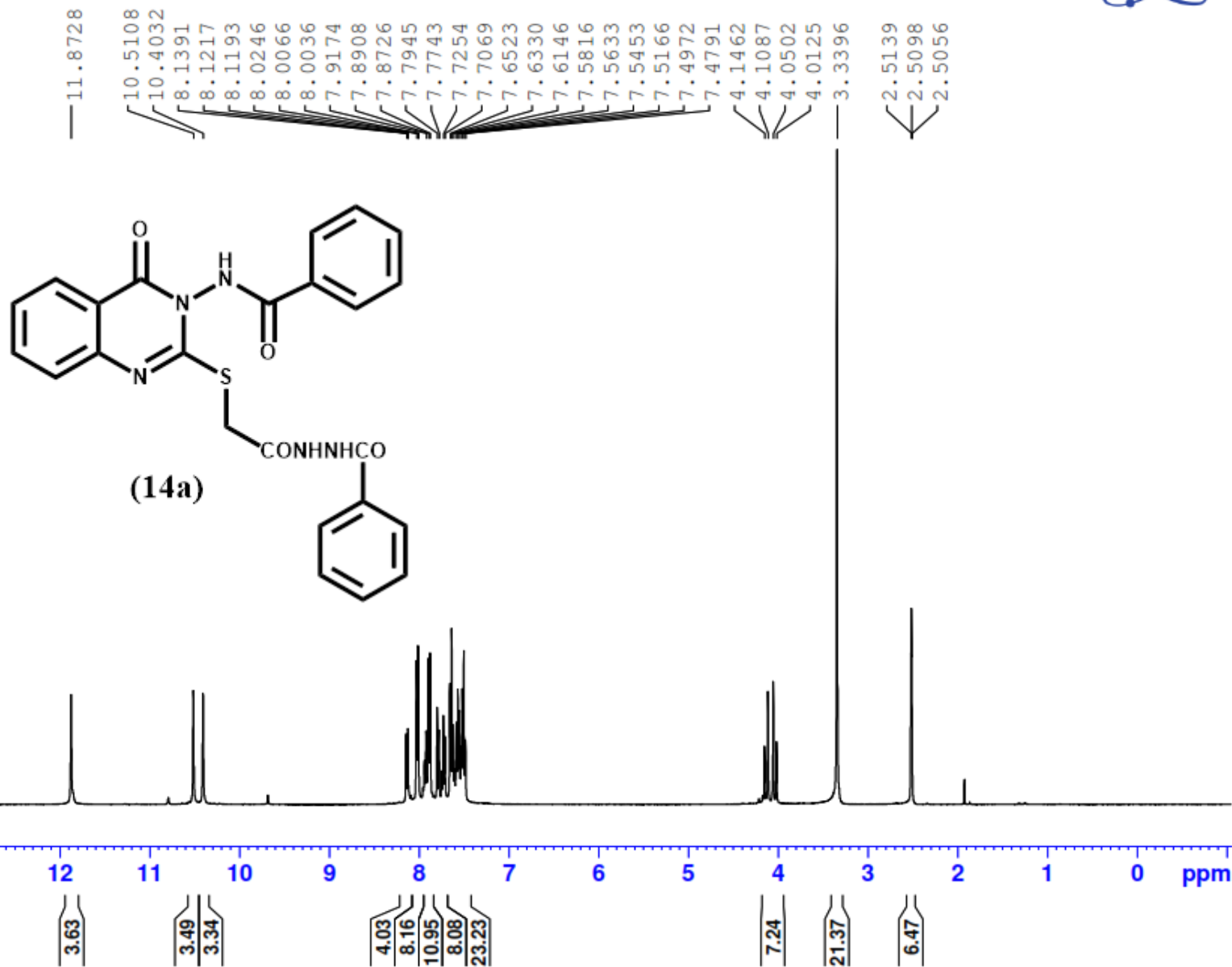
asmaa alaa Ph1-M-carbon



Current Data Parameters
NAME asmaa alaa Ph1-M
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180507
Time 21.32 h
INSTRUM spect
PROBHD Z108618_0945 (
PULPROG zgpg30
TD 65536
SOLVENT Pyr
NS 2100
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 197.77
DW 20.800 usec
DE 6.50 usec
TE 293.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6404331 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W
SFO2 400.2016008 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.29249999 W
PLW13 0.14713000 W

F2 - Processing parameters
SI 32768
SF 100.6303700 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME Asmaa Alaa_H_PO4
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180102
 Time 17.58
 INSTRUM spect
 PROBHD 5 mm FAPBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 169.46
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SF01 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 MDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

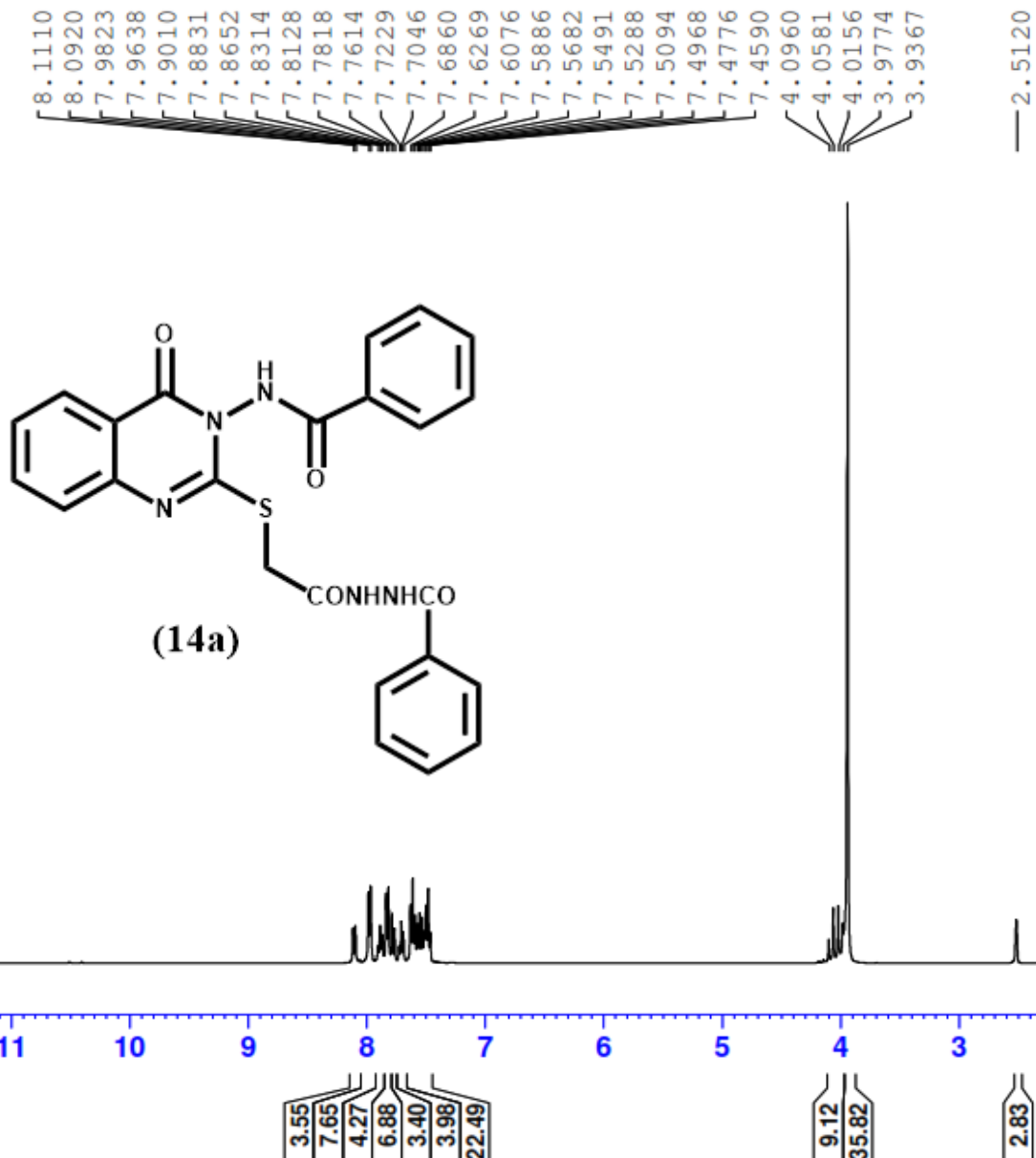


Current Data Parameters
 NAME Asmaa Alaa_H_PO4_D2O
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180114
 Time 13.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 114.95
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFOL 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





166.83
 166.33
 165.82
 158.94
 158.87
 147.19
 135.85
 133.53
 132.82
 132.32
 131.43
 129.39
 128.92
 128.32
 127.94
 127.16
 127.10
 126.90
 119.75

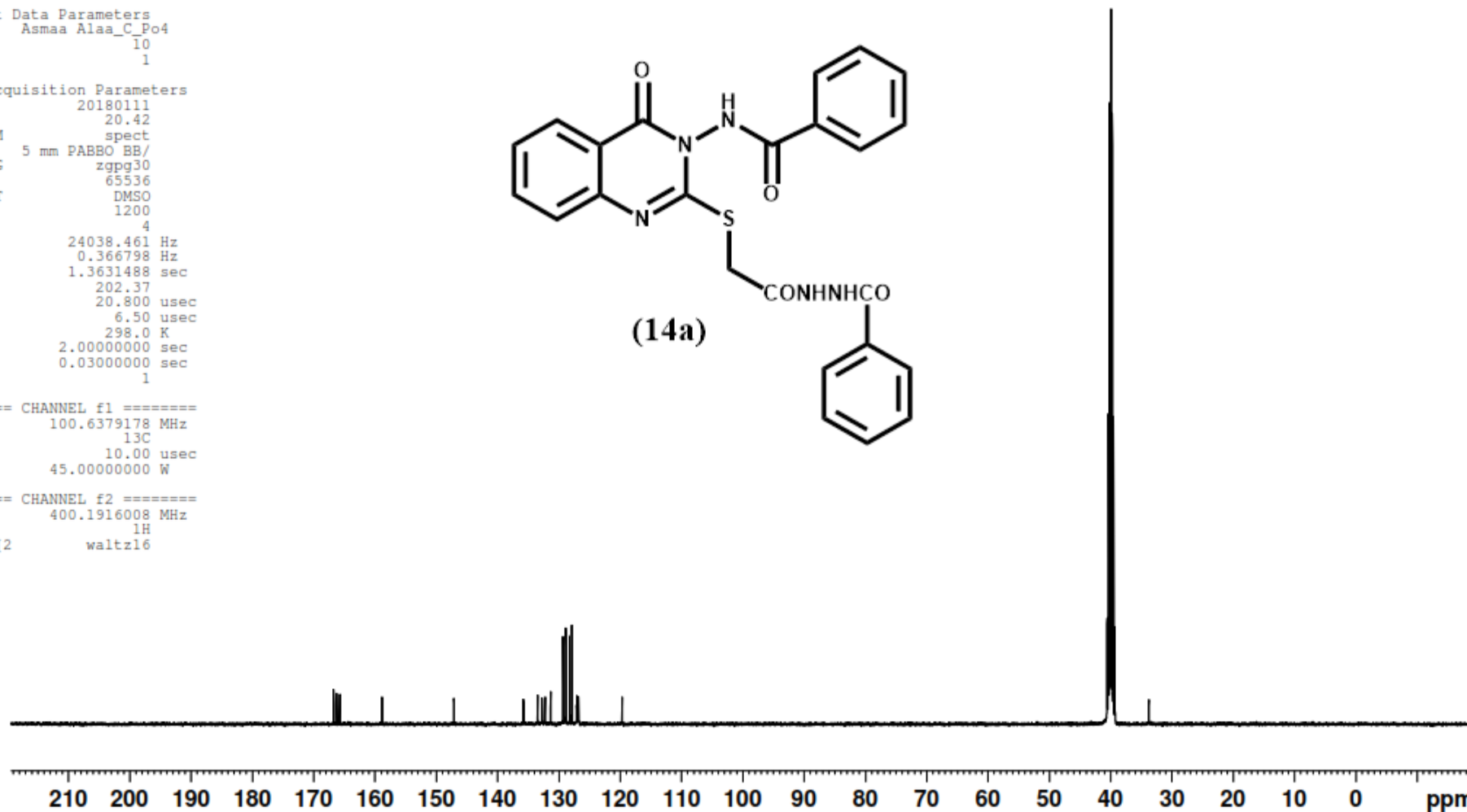
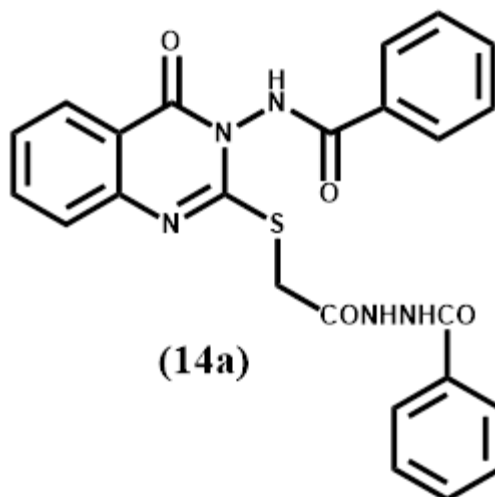
40.61
 40.40
 40.19
 39.98
 39.78
 39.57
 39.36
 33.83

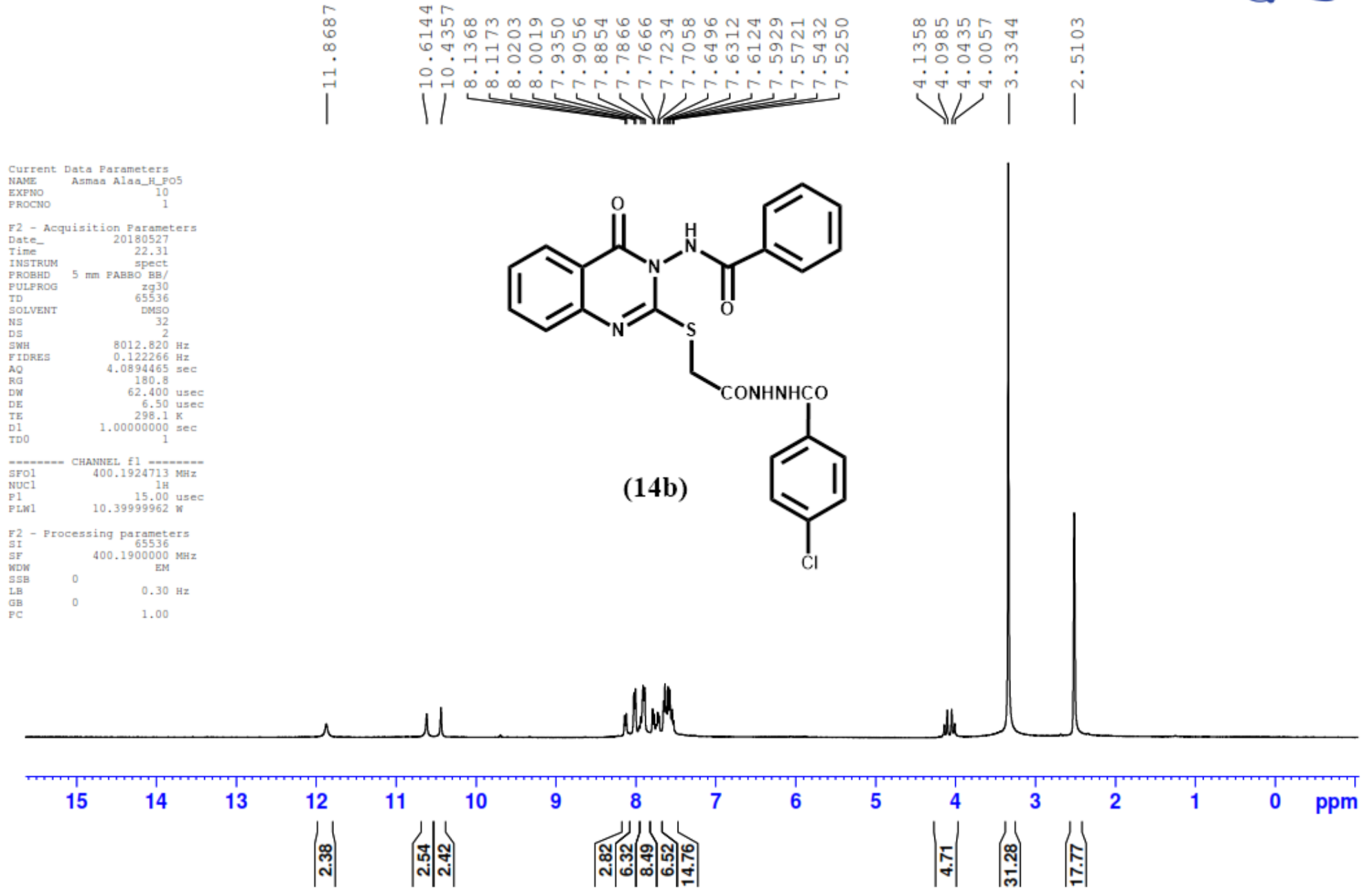
Current Data Parameters
 NAME Asmaa Alaa_C_Po4
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180111
 Time 20.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1200
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 202.37
 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 100.6379178 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 45.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1916008 MHz
 NUC2 1H
 CPDPRG[2] waltz16

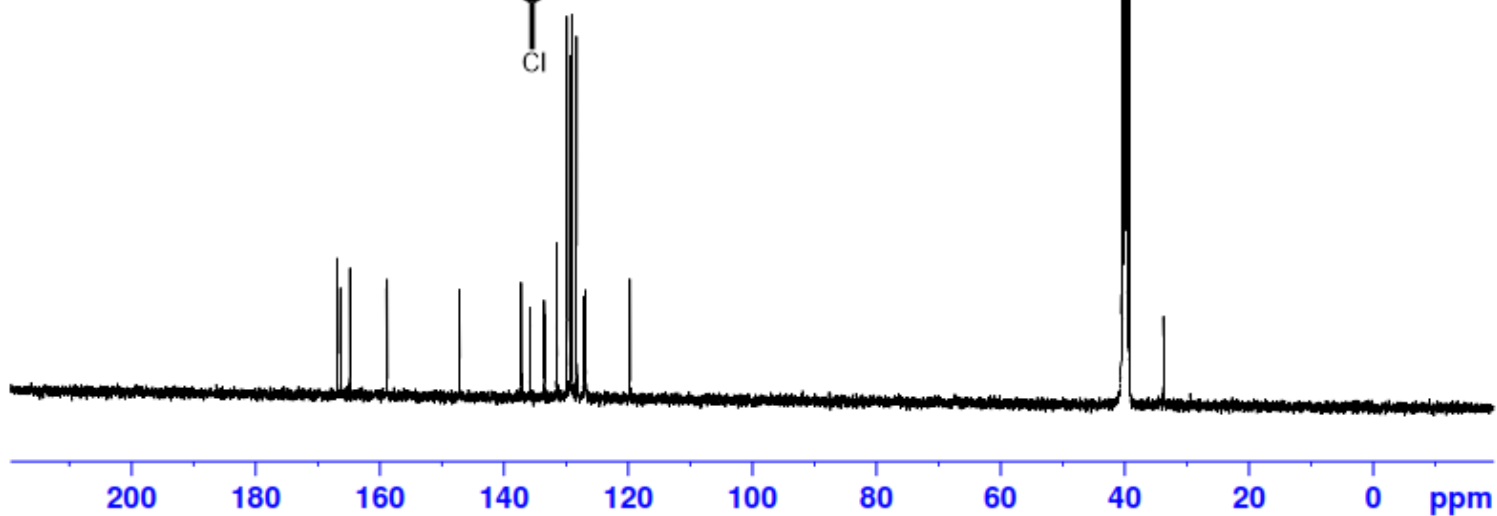
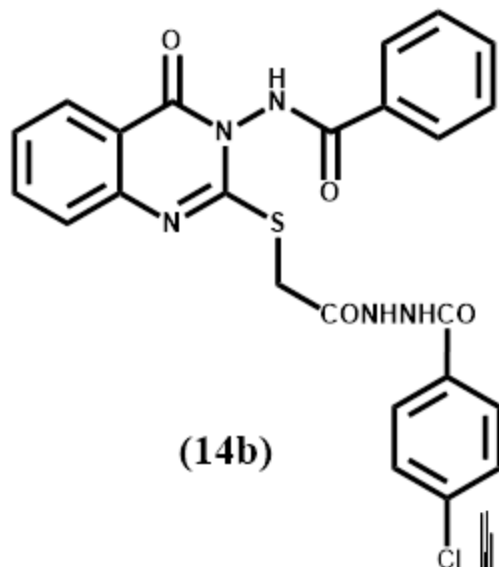




asmaa sakr-po5- carbon

166.89
166.40
164.86
158.95
158.86
147.18
137.20
135.82
133.50
131.52
129.88
129.38
129.24
129.18
129.09
128.33
127.15
127.09
126.89
119.74

40.32
40.11
39.90
39.69
39.49
33.79



Current Data Parameters
NAME asmaa sakr-PO5-SS
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180505
Time 12.57 h
INSTRUM spect
PROBHD Z108618_0945 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 197.77
DW 20.800 usec
DE 6.50 usec
TE 294.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6404331 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W
SFO2 400.2016008 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.29249999 W
PLW13 0.14713000 W

F2 - Processing parameters
SI 32768
SF 100.6303700 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Asmaa Alaa_H_PF2a

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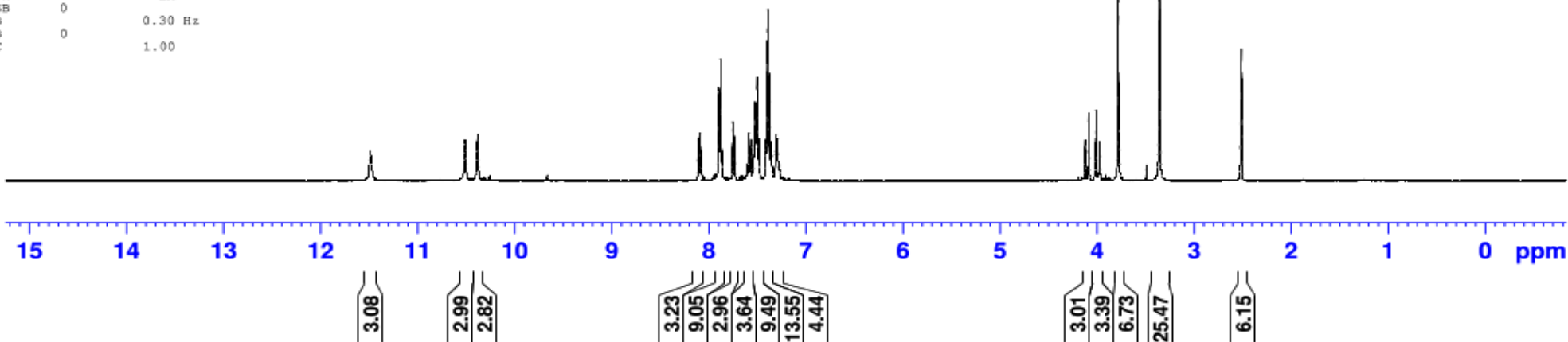
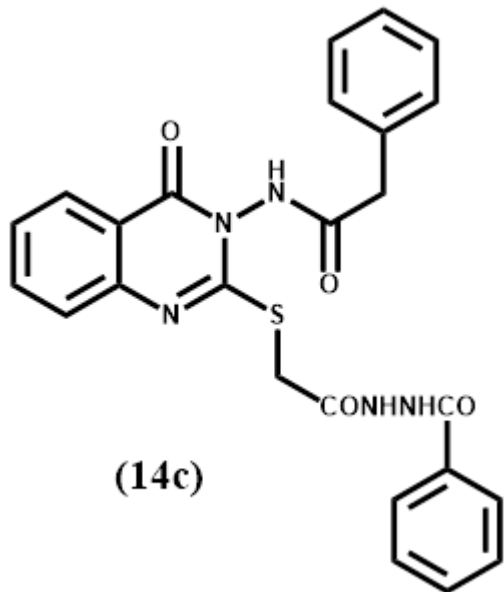
11.4856
10.5089
10.3815
8.1068
8.1044
8.0871
8.0846
7.8954
7.8771
7.8631
7.8595
7.7512
7.7311
7.6021
7.5838
7.5654
7.5305
7.5192
7.5152
7.5002
7.4821
7.4111
7.3944
7.3893
7.3703
7.3510
7.3109
7.3060
7.3032
7.2953
7.2893
7.2723
4.1193
4.0818
4.0075
3.9700
3.7782
3.7683
3.3515
2.5135
2.5092
2.5050

Current Data Parameters
NAME Asmaa Alaa_H_PF2a
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170215
Time 15.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 129.43
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





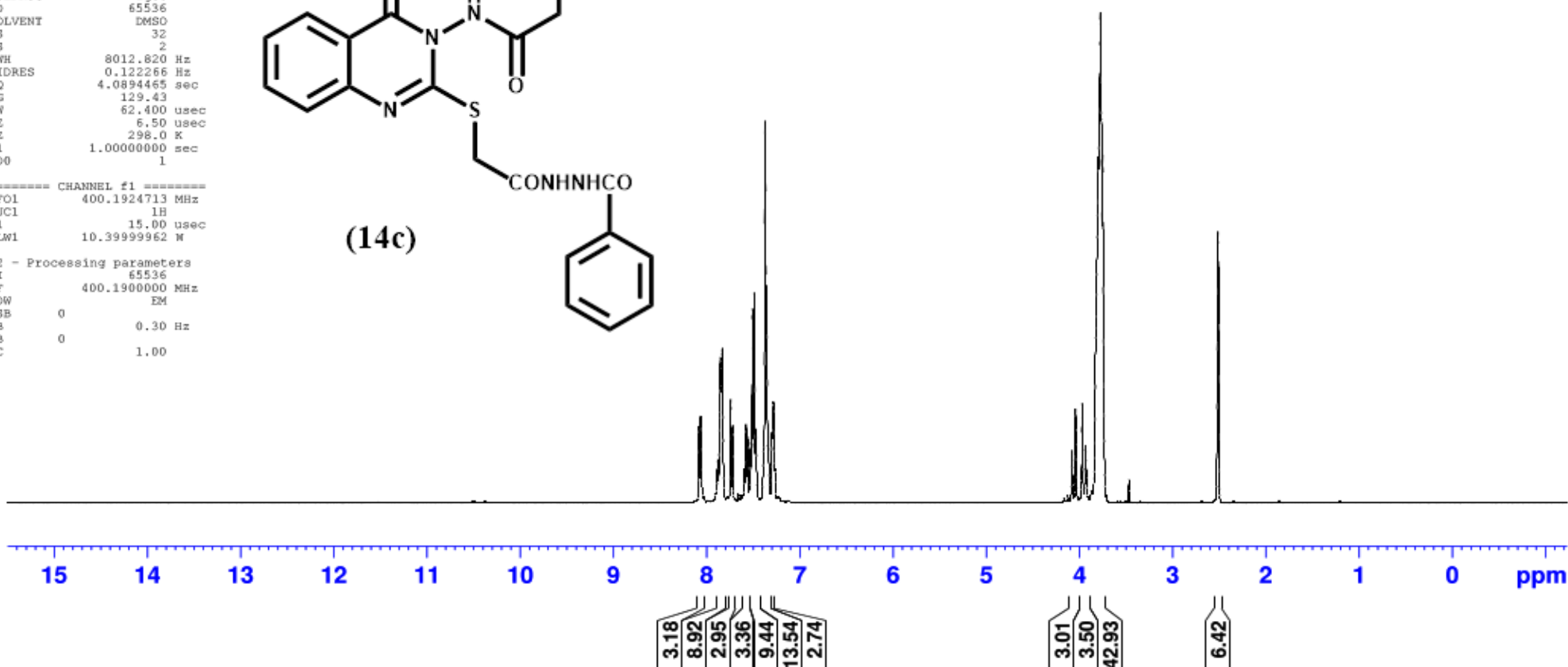
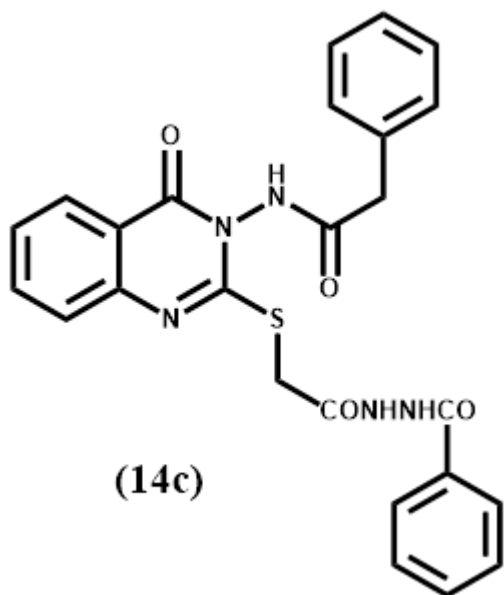
8.0819
 8.0622
 7.8788
 7.8503
 7.8325
 7.8296
 7.7409
 7.7205
 7.5940
 7.5766
 7.5583
 7.5240
 7.5060
 7.4875
 7.4689
 7.3707
 7.3556
 7.2813
 4.0793
 4.0411
 3.9697
 3.9320
 3.7728
 2.5119

Current Data Parameters
 NAME Asmaa Alaa_H_PF2a_D20
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170216
 Time 14.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 129.43
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



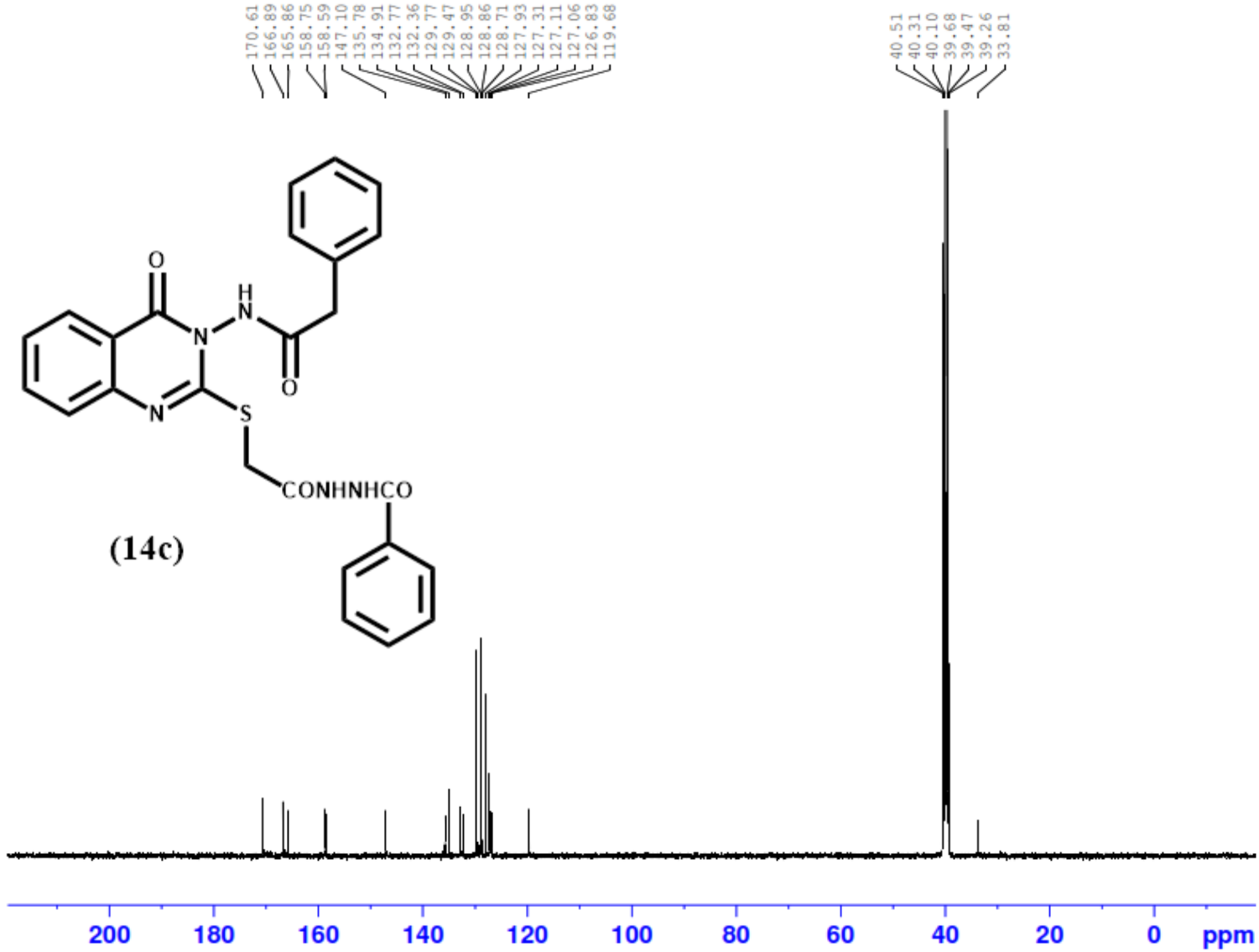
asmaa sakr- pf2a- carbon



Current Data Parameters
NAME asmaa sakr-pf2a-SS
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180428
Time 12.47 h
INSTRUM spect
PROBHD Z108618_0945 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 197.77
DW 20.800 usec
DE 6.50 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6404331 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W
SFO2 400.2016008 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.29249999 W
PLW13 0.14713000 W

F2 - Processing parameters
SI 32768
SF 100.6303700 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

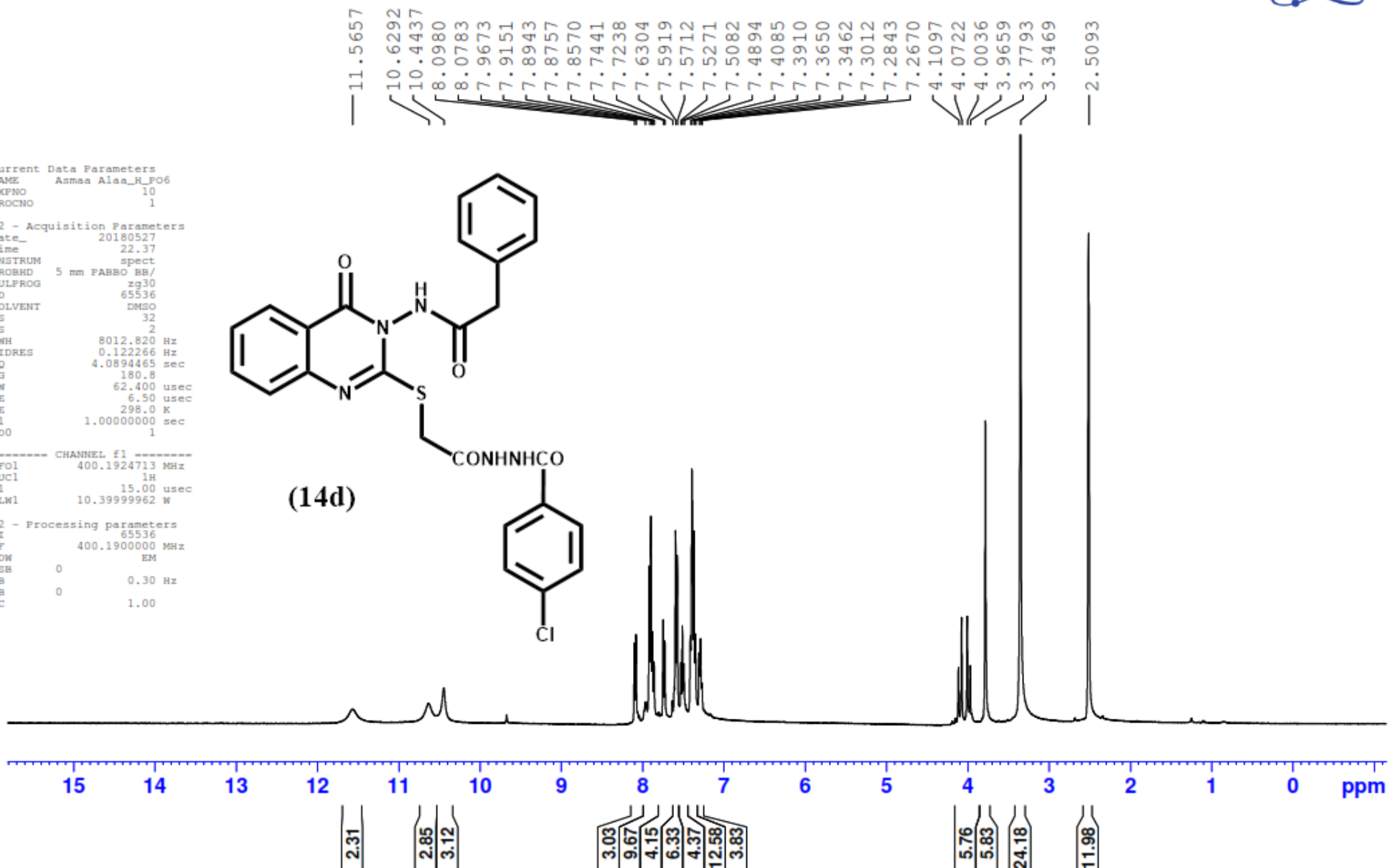
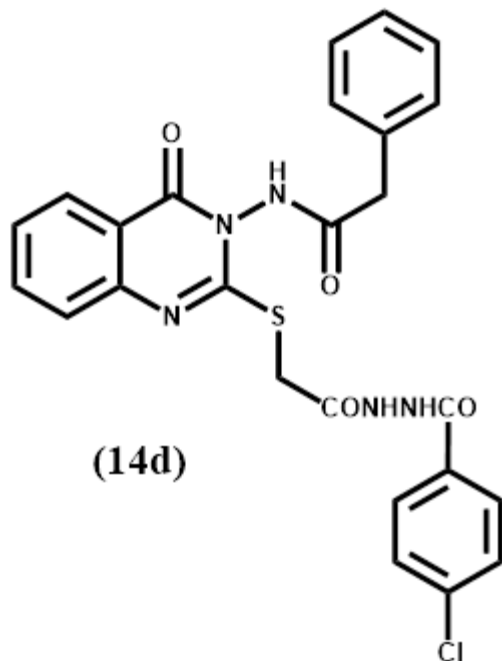


Current Data Parameters
NAME Asmaa Alaa_H_PO6
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180527
Time 22.37
INSTRUM spect
PROBHD 5 mm F4001 QNP
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 801.220 MHz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 180.8
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



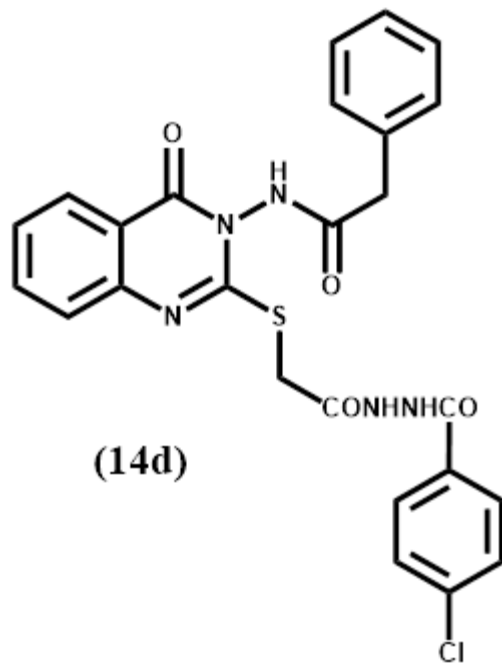


Current Data Parameters
NAME Asmaa Alaa_H_PO6_D2O
EXPNO 10
PROCNO 1

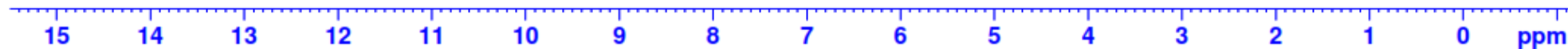
F2 - Acquisition Parameters
Date_ 20180529
Time 12.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 180.8
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDM EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



8.0647
8.0448
7.8642
7.8426
7.8303
7.8096
7.7273
7.7070
7.5444
7.5233
7.4961
7.4771
7.3578
7.3435
7.3247
7.2869
7.2727
3.9908
3.9412
3.7312
2.5123



2.70
8.25
3.02
9.01
13.98

46.61
5.70

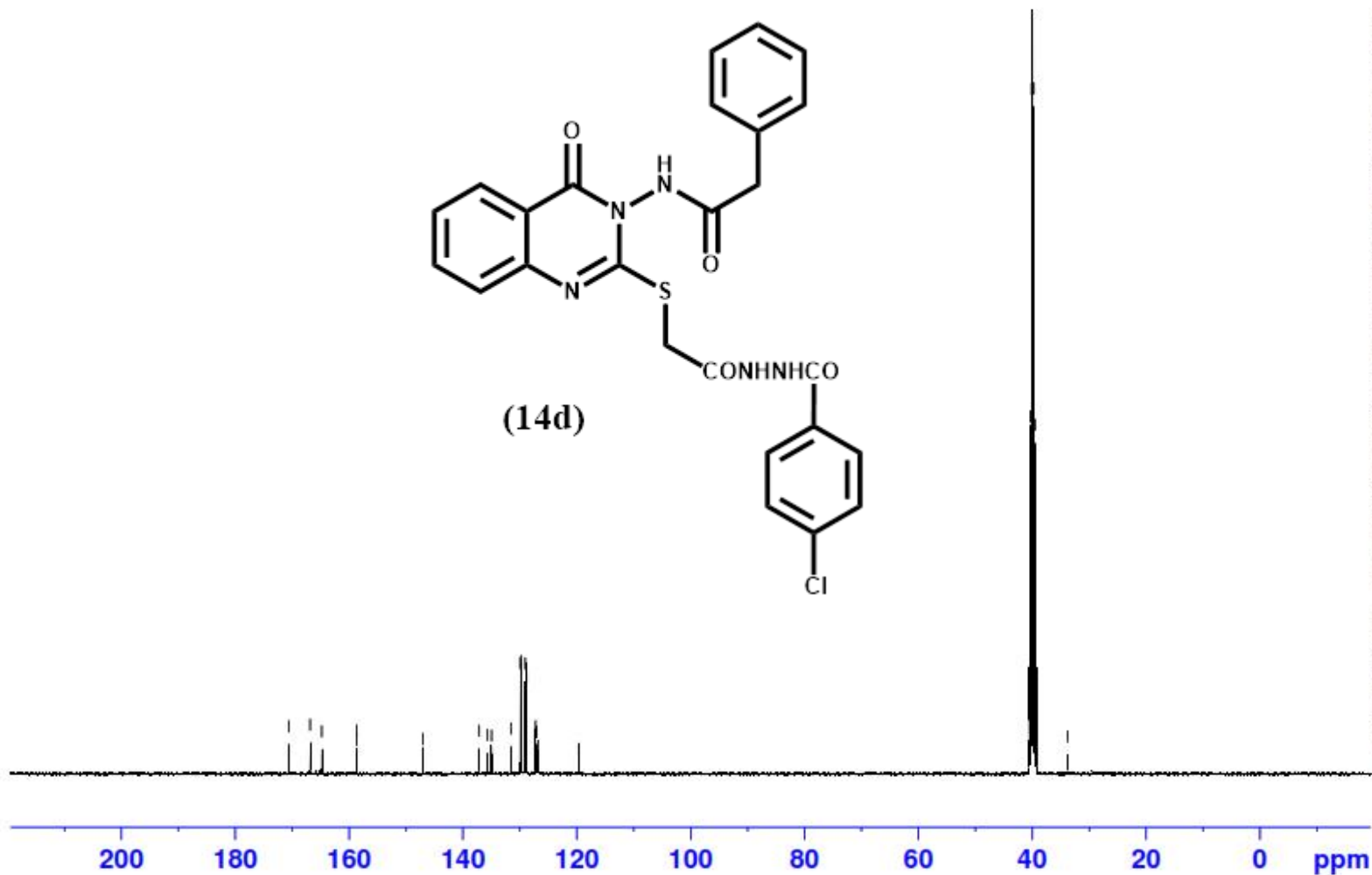
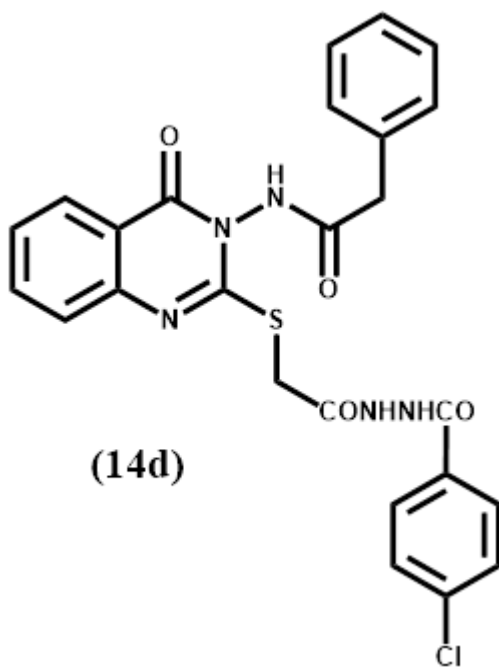
10.74

asmaa sakr- po6-carbon



170.59
166.85
164.81
158.70
158.63
147.09
137.16
135.74
134.99
131.54
129.91
129.79
129.15
129.07
128.83
127.27
127.11
127.04
126.80
119.69

40.54
40.33
40.12
39.92
39.71
39.50
39.29
33.80



Current Data Parameters
NAME asmaasakr-po6-SS
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180505
Time 11.55 h
INSTRUM spect
PROBHD Z108618_0945 (
PULPROG zgpg30
ID 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 197.77
DW 20.800 usec
DE 6.50 usec
TE 294.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6404331 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W
SFO2 400.2016008 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.29249999 W
PLW13 0.14713000 W

F2 - Processing parameters
SI 32768
SF 100.6303700 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

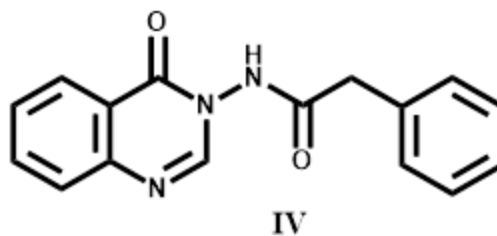


— 11.2257
 8.9501
 8.9289
 8.1274
 8.1241
 8.1079
 8.1046
 7.8831
 7.8793
 7.8614
 7.8434
 7.8396
 7.5393
 7.5200
 7.5016
 7.4029
 7.3824
 7.3644
 7.3451
 7.3016
 7.2847
 7.2677
 5.8476
 3.7470
 3.5727
 3.3448
 2.5132
 2.5092

Current Data Parameters
 NAME Asmaa Alaa_H_PF2
 EXPNO 10
 PROCNO 1

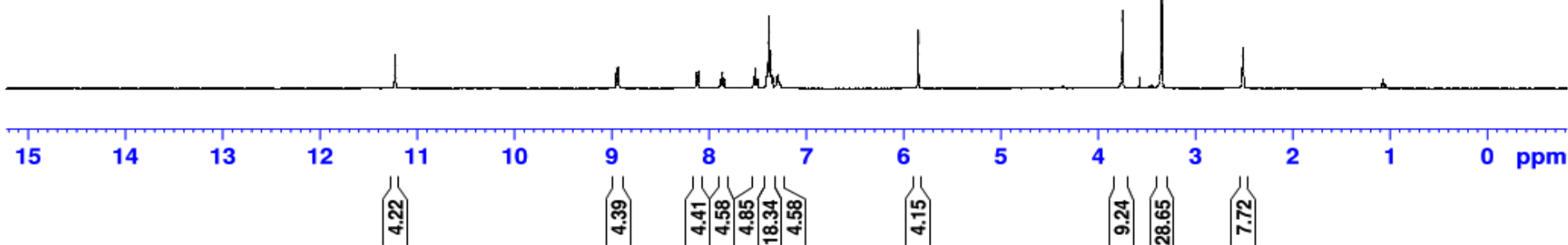
F2 - Acquisition Parameters
 Date_ 20170215
 Time 14.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 146.06
 DW 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TDO 1

Unexpected compound



----- CHANNEL f1 -----
 SFO1 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
 NAME Asmaa Alaa_H_PF2_D2O
 EXPNO 10
 PROCNO 1

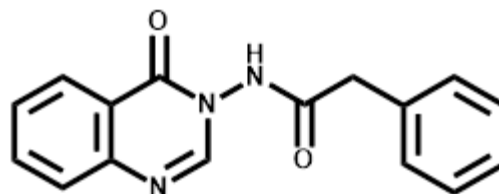
F2 - Acquisition Parameters
 Date_ 20170216
 Time 14.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 146.06
 DE 62.400 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 400.1924713 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.39999962 W

F2 - Processing parameters
 SI 65536
 SF 400.1900000 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.9201
 8.1017
 7.8483
 7.5149
 7.3650
 5.8060
 3.7896
 3.5584
 3.4365
 2.5159
 1.0551

Unexpected compound



IV

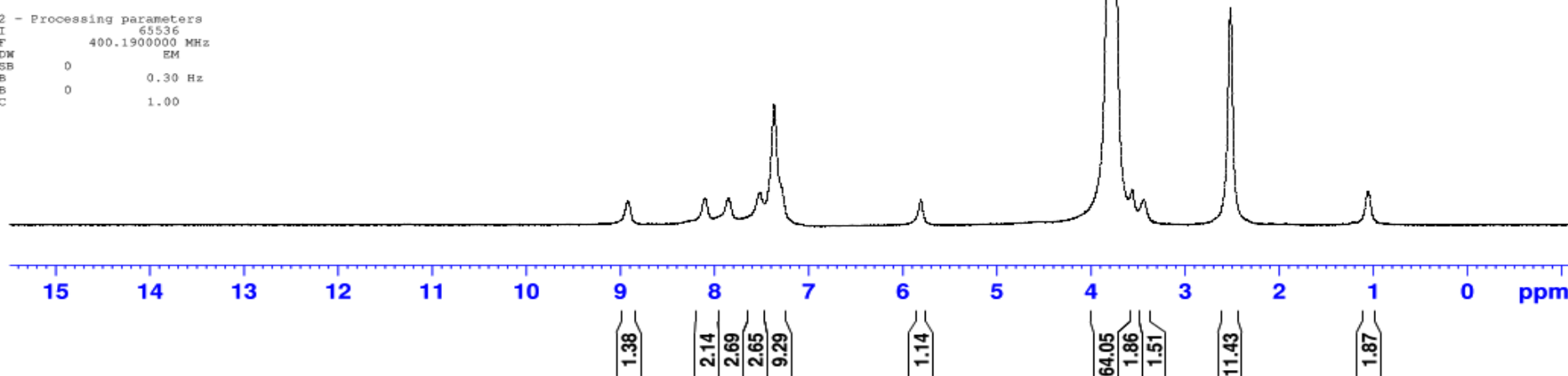


Table.1: Molecular docking details of target compounds with both (1CX2 and 1EQG):

Code	Docking of target compounds and 1CX2				Docking of target compounds and 1EQG			
	Number of bonds	Type of bond	Docking scores (Kcal/mol)	Amino acid interactions	Number of bonds	Type of bond	Docking scores (Kcal/mol)	Amino acid interactions
4a	1	1 HB ^a	-6.2604	Ala527	1	1 HB ^a	-5.9148	Arg120
4b	1	1 arene-H ^b	-7.0540	Ser353	2	2 HB ^a	-4.2701	Tyr355, Val116
7c	1	2 HB ^a	-6.9140	Val523, Arg120	-	-	-6.4143	-
13b	1	1 HB ^a	-8.4080	Arg120	2	1 HB ^a , 1 arene-H ^b	-2.0562	Arg120, Tyr355

14c	3	3 HB ^a	-8.5355	Arg513, Gly354, Ser353	1	1HB ^a	-6.3893	Arg120
SC-558	5	4 HB ^a , 1 arene- H ^b	-9.3983	Ty355, Arg120, Arg513, His90, ser353	-	-	-1.3609	-
Ibuprofen					3	HB ^a		Arg120, Tyr355

* ^a (HB) is symbol for hydrogen bond, ^b (arene-H); arene group attached with hydrogen bond.

Table.2: predict bioavailability using online website (MOLINSPIRATION): www.molinspiration.com

Code	Log p	M.WT	nON (HBA)	nOHNH (HBD)	LIPINSK'S VIOLATION	TPSA	%ABS	VOLUMES	NROTB
4a	4.57	444.92	6	2	0	68.44	85.39	384.66	4
4b	3.85	455.47	9	2	0	114.26	69.58	394.46	5
7c	5.80	486.57	8	1	1	98.47	75.03	448.82	7
13b	0.51	383.43	8	4	0	119.12	41.09	325.43	6
14c	2.75	487.54	9	3	0	122.19	66.84	416.94	8
Celecoxib	3.61	381.38	5	2	0	77.99	82.09	298.65	4
Ibuprofen	3.46	206.28	2	1	0	37.30	96.13	211.19	4
indomethacin	3.99	357.79	5	1	0	68.54	85.35	303.24	4

7c Lipinski violation was Log p which must be <5 or equal and in this compound it >5 log p= 5.80

Reference for equation:

<https://www.ncbi.nlm.nih.gov/pubmed/12425461>

The values of TPSA are used to calculate the percentage of oral absorption (%ABS) using the following equation:

$$\%ABS = 109 - 0.345 \text{ TPSA}$$

Table.3: Results of prediction of drug cell permeability, intestinal, BBB and PPB using Pre-ADMET calculator.

code	Caco2	MDCK	HIA	BBB	PPB
4a	34.04	0.42	93.96	4.07	90.25
4b	19.75	0.08	92.79	0.31	90.57
7c	21.15	0.06	96.97	0.05	90.37
13b	12.58	1.79	91.51	0.08	88.69
14c	11.24	0.07	93.56	0.03	100.00
Celecoxib	0.499	45.05	96.69	0.03	91.07
Ibuprofen	21.21	136.48	98.38	1.27	88.25
indomethacin	20.14	3.81*	98.44	0.03	78.06

All compounds showed the same results as 3 reference drugs (Celecoxib, Ibuprofen and indomethacin) as **non**-inhibitor activity for (CYP2D6 enzyme),so they will be expected to not included in any Drug-Drug interaction for both inhibitors and/or inducers of that enzyme.