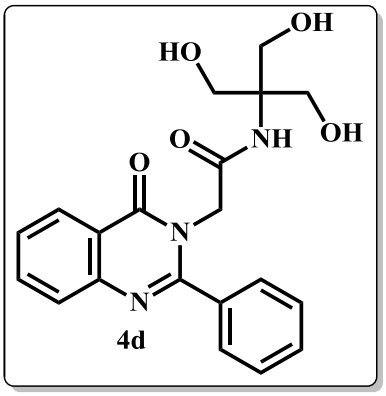
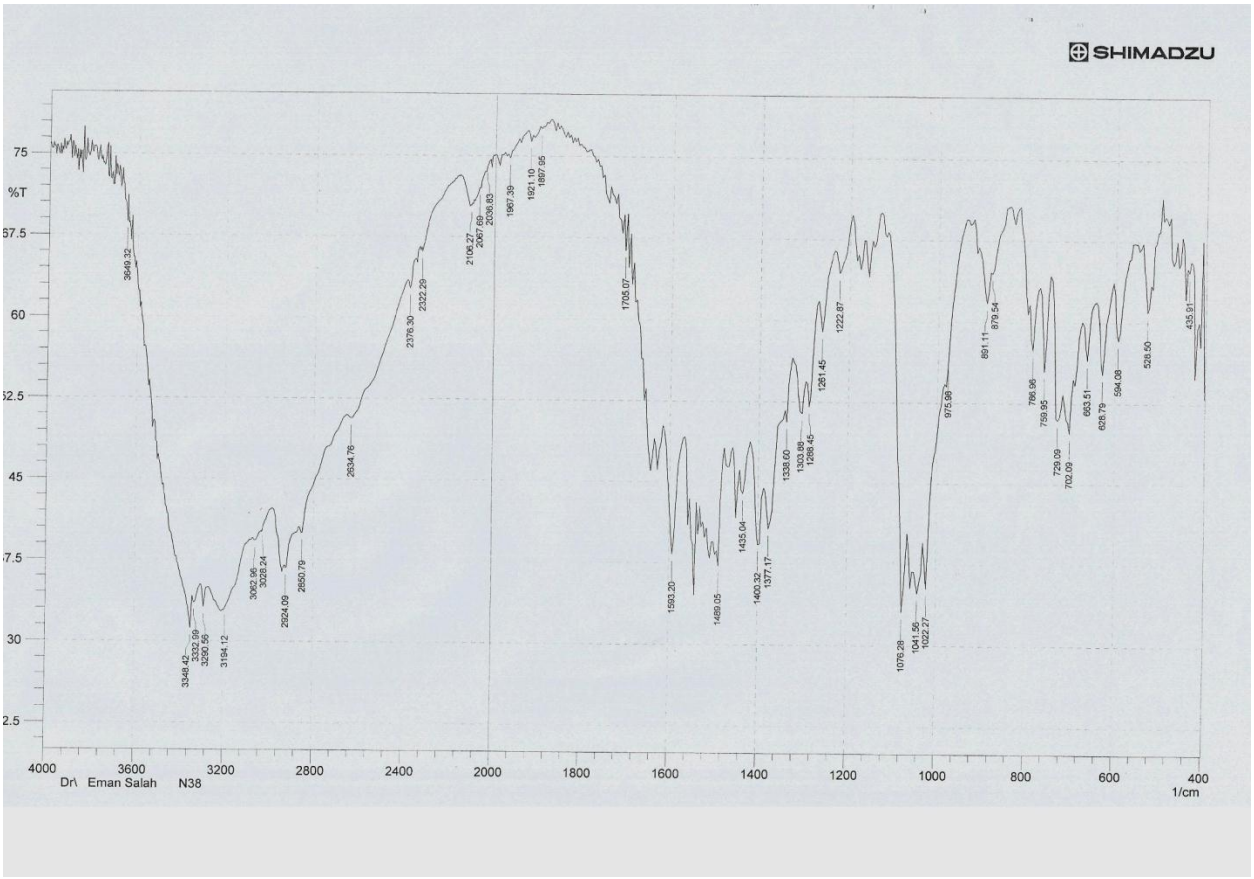
Compound 4d

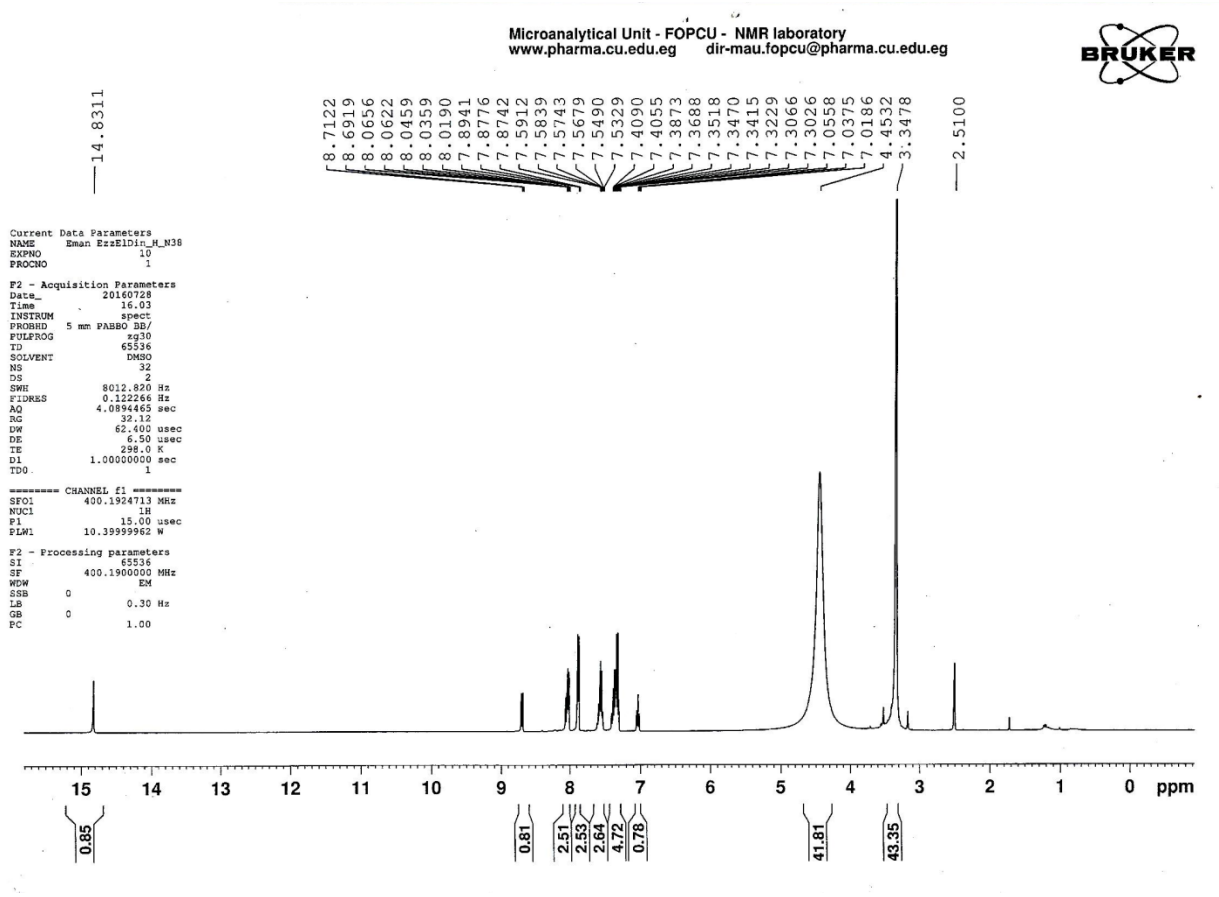
N-(1,3-dihydroxy-2-(hydroxymethyl)propan-2-yl)-2-(4-oxo-2-phenylquinazolin-3(4H)-yl)acetamide



IR of 4d



^{1}H NMR of 4d


Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
14.8311
8.7122
8.6919
8.0656
8.0622
8.0459
8.0359
8.0190
7.8941
7.8776
7.8742
7.5912
7.5839
7.5743
7.5679
7.5490
7.5329
7.4090
7.4055
7.3873
7.3688
7.3518
7.3470
7.3415
7.3229
7.3066
7.3026
7.0558
7.0375
7.0186
4.4532
3.3478
2.5100
Current Data Parameters
NAME Eman EzzElDin_H_N38
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160728
Time 16.03
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
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
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
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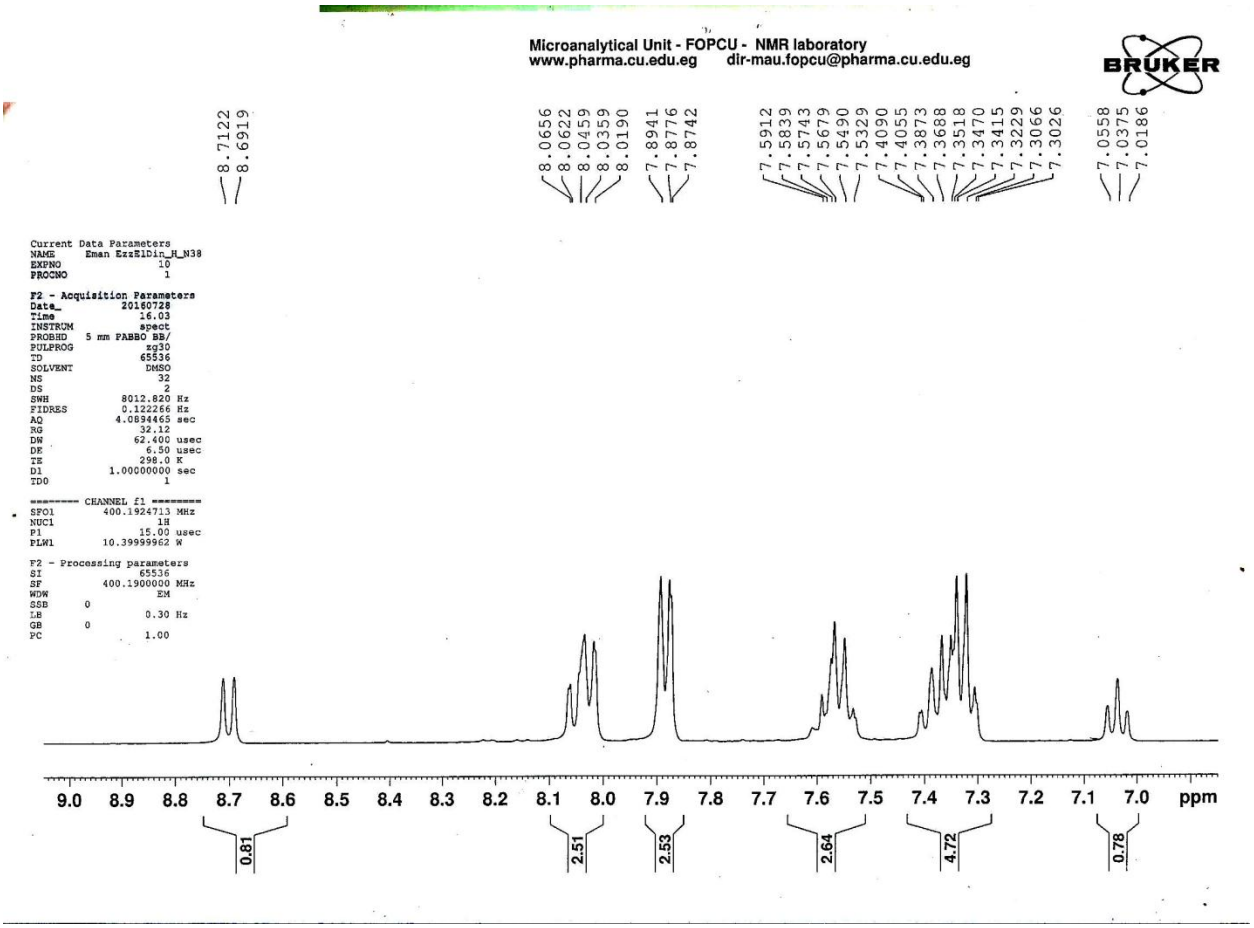
0.81
2.51
2.53
2.64
4.72
0.78
41.81
43.35


Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.7122
8.6919
8.0656
8.0622
8.0459
8.0359
8.0190
7.8941
7.8776
7.8742
7.5912
7.5839
7.5743
7.5679
7.5490
7.5329
7.4090
7.4055
7.3873
7.3688
7.3518
7.3470
7.3415
7.3229
7.3066
7.3026
7.0558
7.0375
7.0186
Current Data Parameters
NAME Eman EzzElDin_H_N38
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160728
Time 16.03
INSTRUM spect
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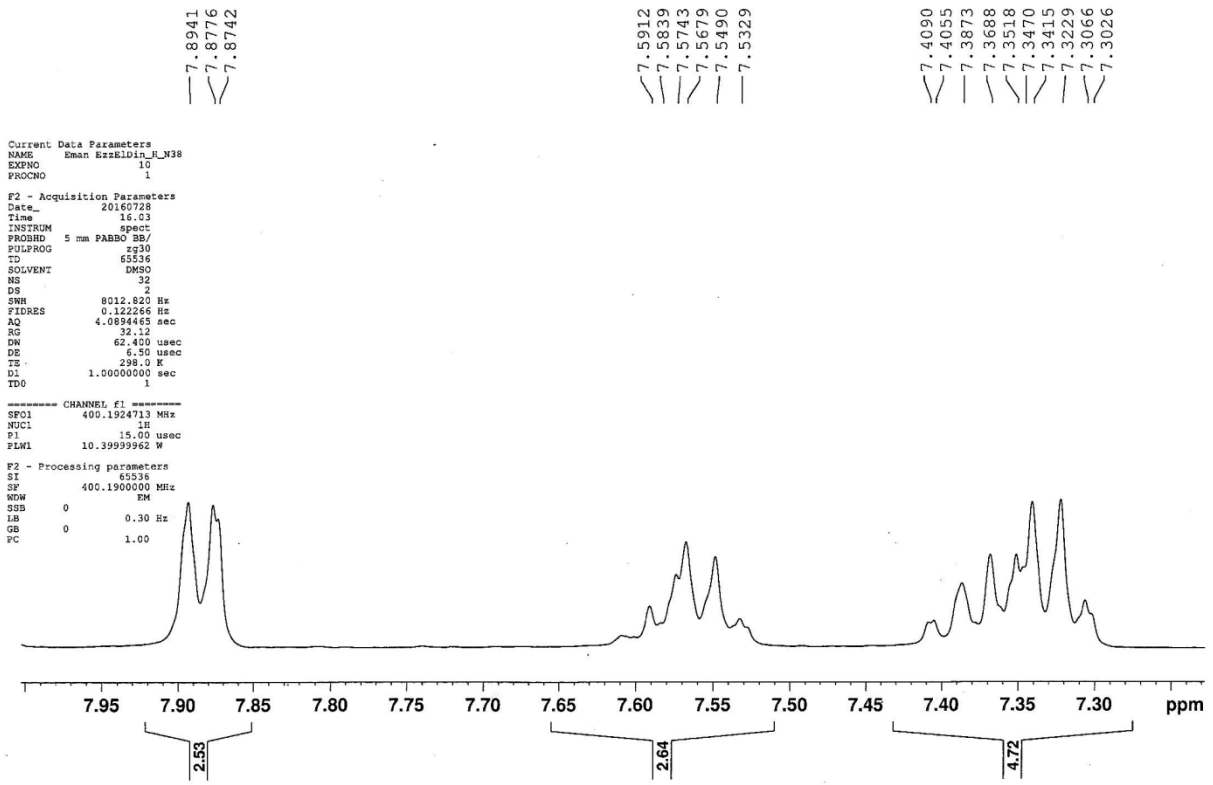
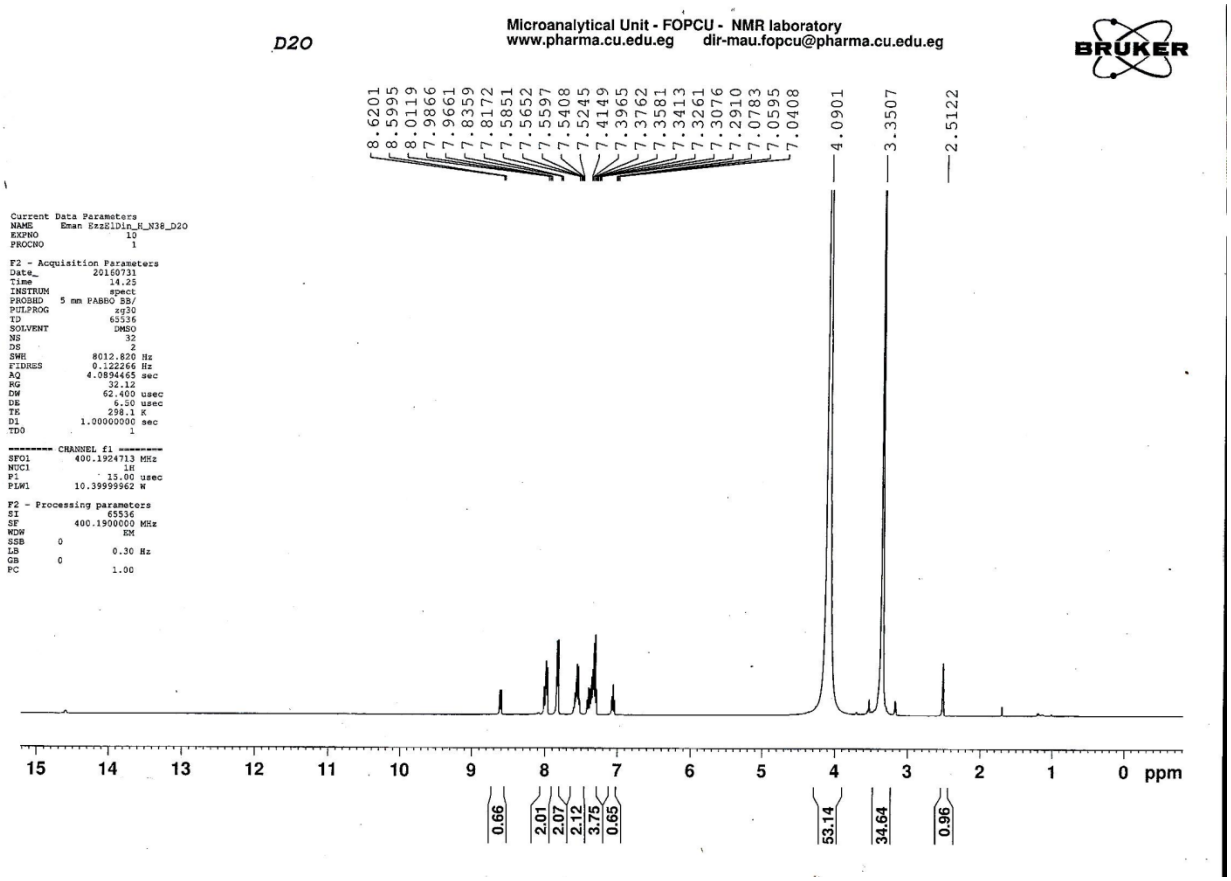
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 32.12
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
0.81
2.51
2.53
2.64
4.72
0.78


7.8941
7.8776
7.8742
7.5912
7.5839
7.5743
7.5679
7.5490
7.5329
7.4090
7.4055
7.3873
7.3688
7.3518
7.3470
7.3415
7.3229
7.3066
7.3026
Current Data Parameters
NAME Eman EzzEldin_H_N38
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160728
Time 16.03
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
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
7.95
7.90
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
ppm
2.53
2.64
4.72

D_2O


D2O
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.6201
8.5995
8.0119
7.9866
7.9661
7.8359
7.8172
7.5851
7.5652
7.5597
7.5408
7.5245
7.4149
7.3965
7.3762
7.3581
7.3413
7.3261
7.3076
7.2910
7.0783
7.0595
7.0408
4.0901
3.3507
2.5122
Current Data Parameters
NAME Eman EzzElDin_H_N38_D2O
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160731
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 32.12
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
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
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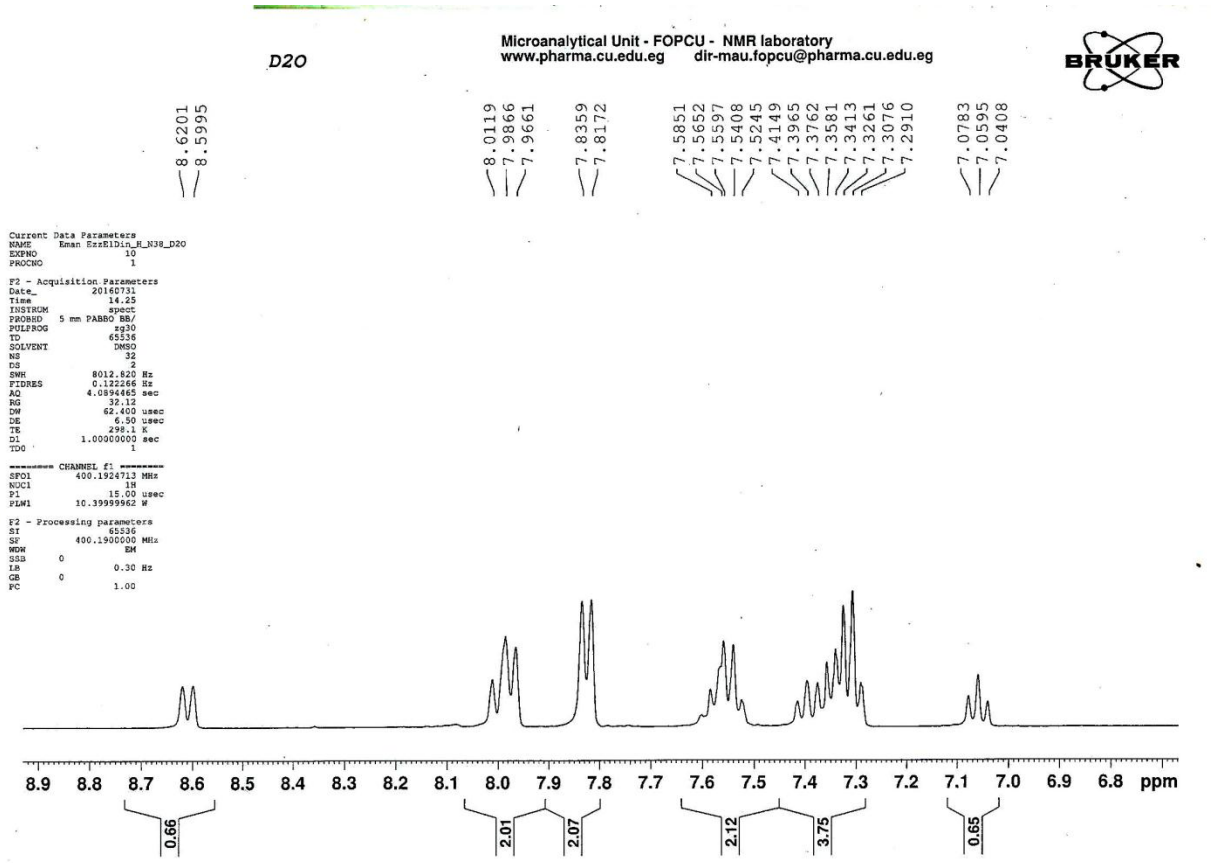
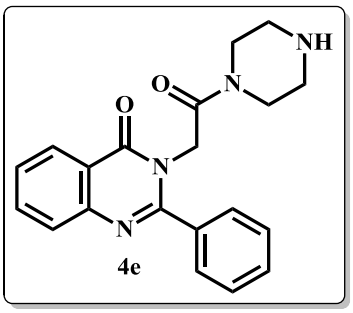
2.01
2.07
2.12
3.75
0.65
53.14
34.64
0.96


D2O
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.6201
8.5995
8.0119
7.9866
7.9661
7.8359
7.8172
7.5851
7.5652
7.5597
7.5408
7.5245
7.4149
7.3965
7.3762
7.3581
7.3413
7.3261
7.3076
7.2910
7.0783
7.0595
7.0408
Current Data Parameters
NAME Eman EzzElDin_H_N38_D2O
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160731
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 32.12
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
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 ppm
0.66
2.01
2.07
2.12
3.75
0.65

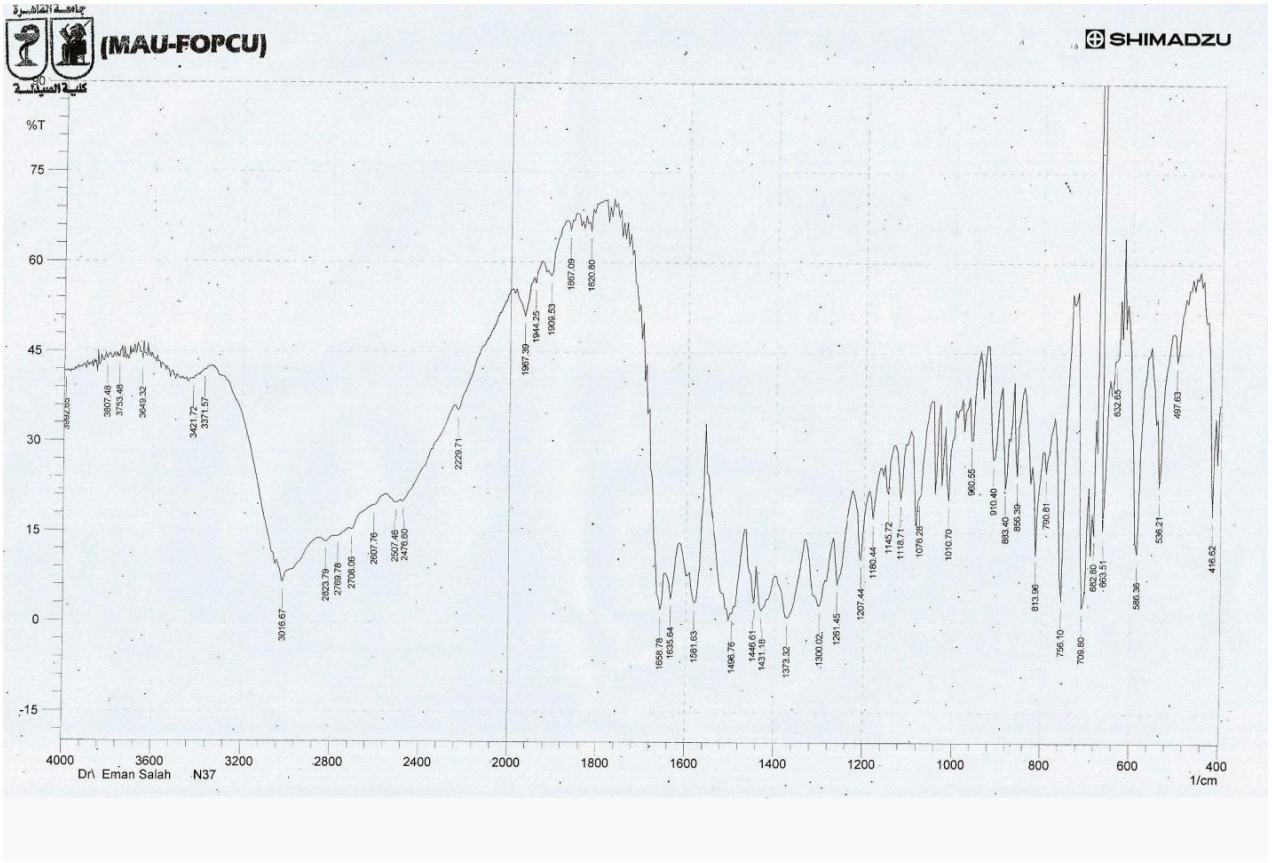
Compound 4e

3-(2-oxo-2-(piperazin-1-yl)ethyl)-2-phenylquinazolin-4(3H)-one

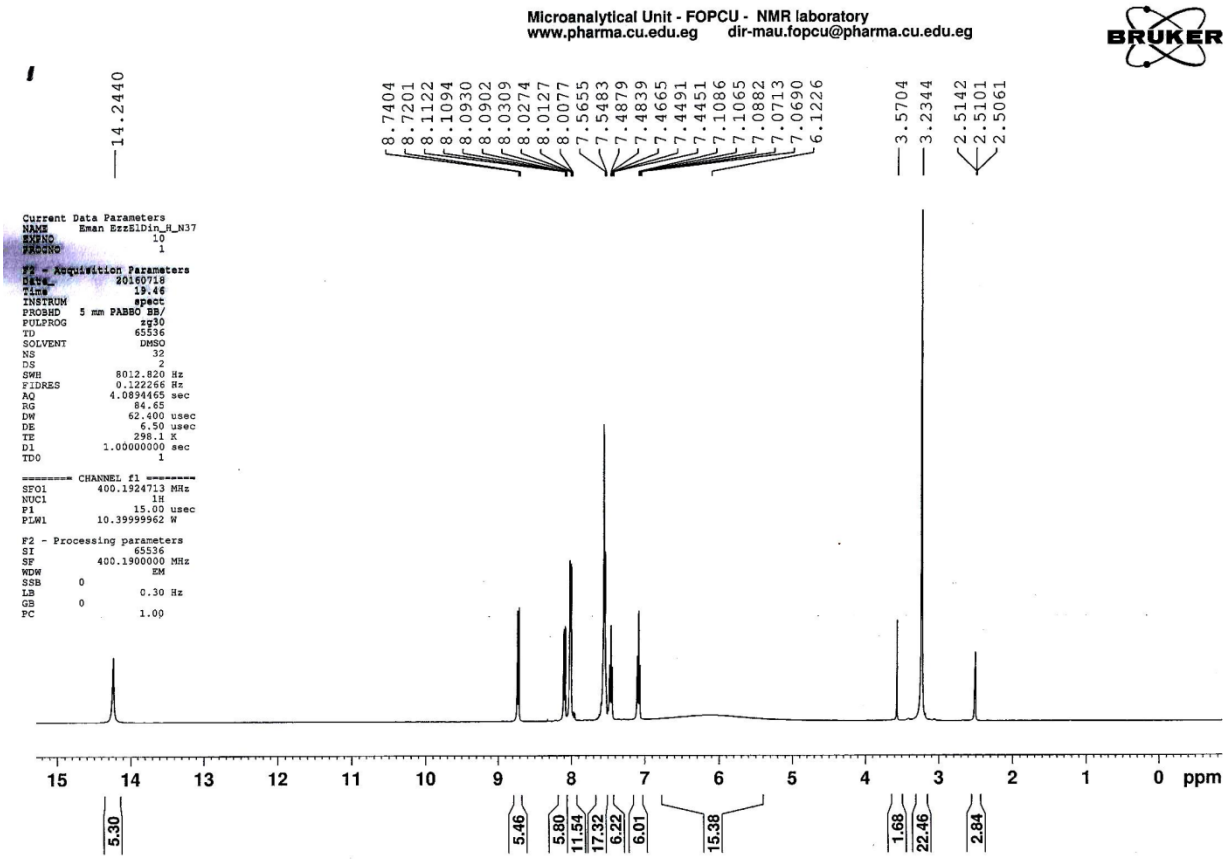


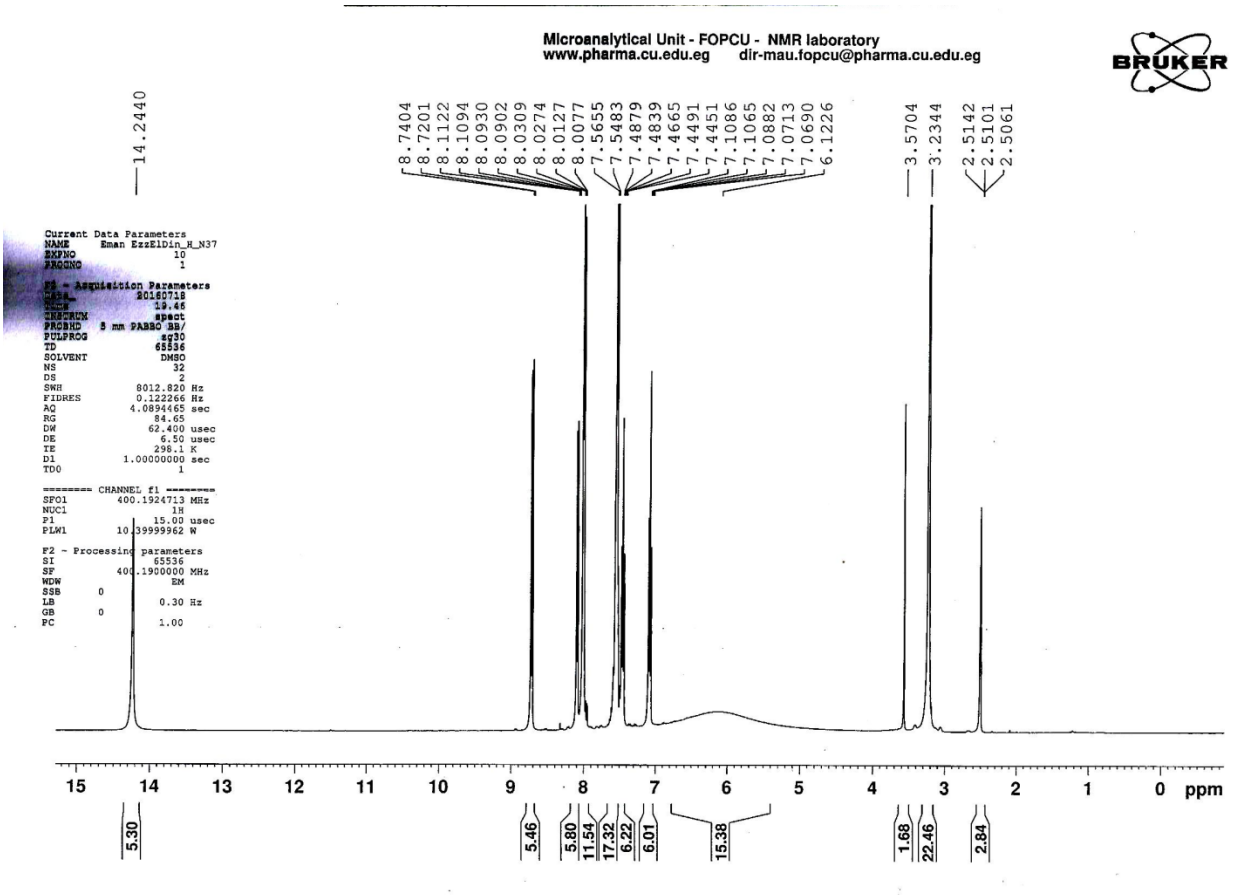
4e

IRof compound 4e



^{1}H NMR of compound 4e




Microanalytical Unit - FOPCU - NMR laboratory
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BRUKER
14.2440
8.7404
8.7201
8.1122
8.1094
8.0930
8.0902
8.0309
8.0274
8.0127
8.0077
7.5655
7.5483
7.4879
7.4839
7.4665
7.4491
7.4451
7.1086
7.1065
7.0882
7.0713
7.0690
6.1226
3.5704
3.2344
2.5142
2.5101
2.5061
Current Data Parameters
NAME Eman EzzElDin_H_N37
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
DATA 20160718
TIME 19.46
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 84.65
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
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
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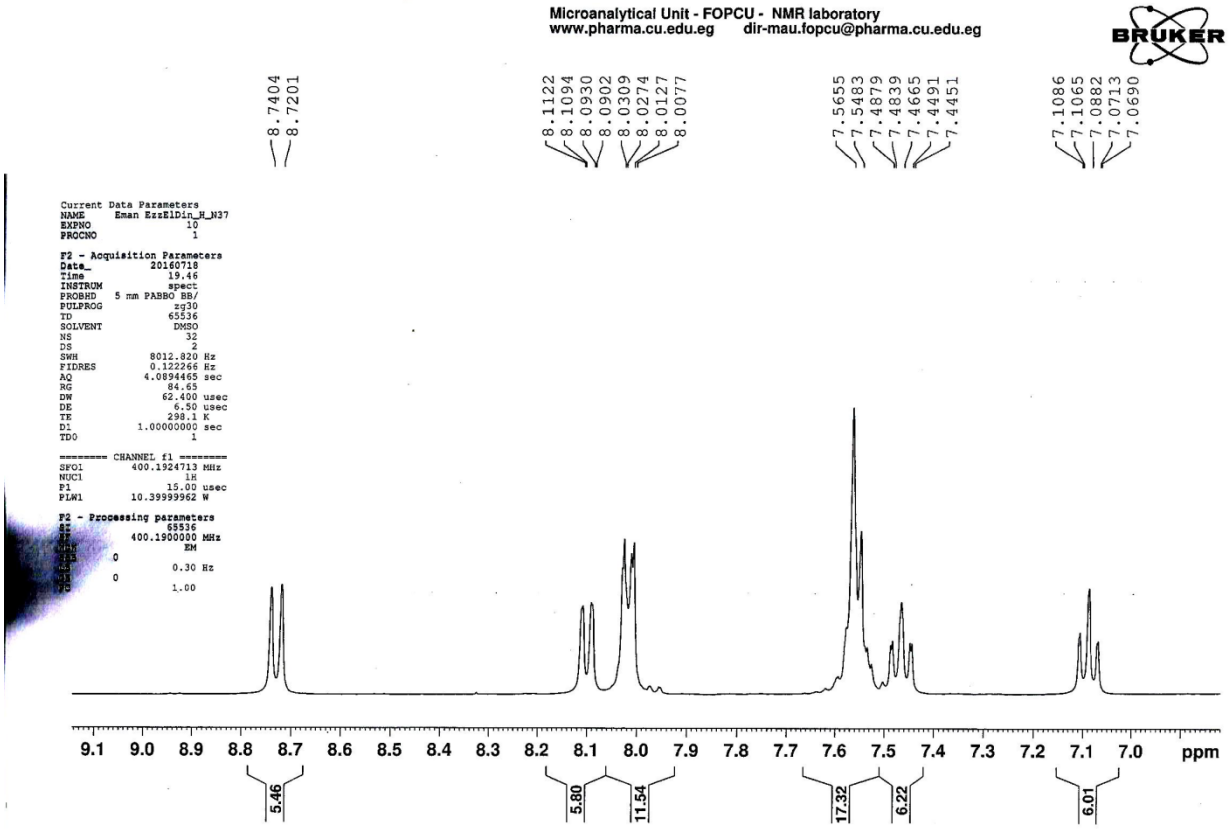
5.46
5.80
11.54
17.32
6.22
6.01
15.38
1.68
22.46
2.84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8.7201
8.1122
8.1094
8.0930
8.0902
8.0309
8.0274
8.0127
8.0077
7.5655
7.5483
7.4879
7.4839
7.4665
7.4491
7.4451
7.1086
7.1065
7.0882
7.0713
7.0690
Current Data Parameters
NAME Eman EzzElDin_H_N37
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160718
Time 19.46
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 84.65
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
WDW EM
0
0.30 Hz
0
1.00
9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
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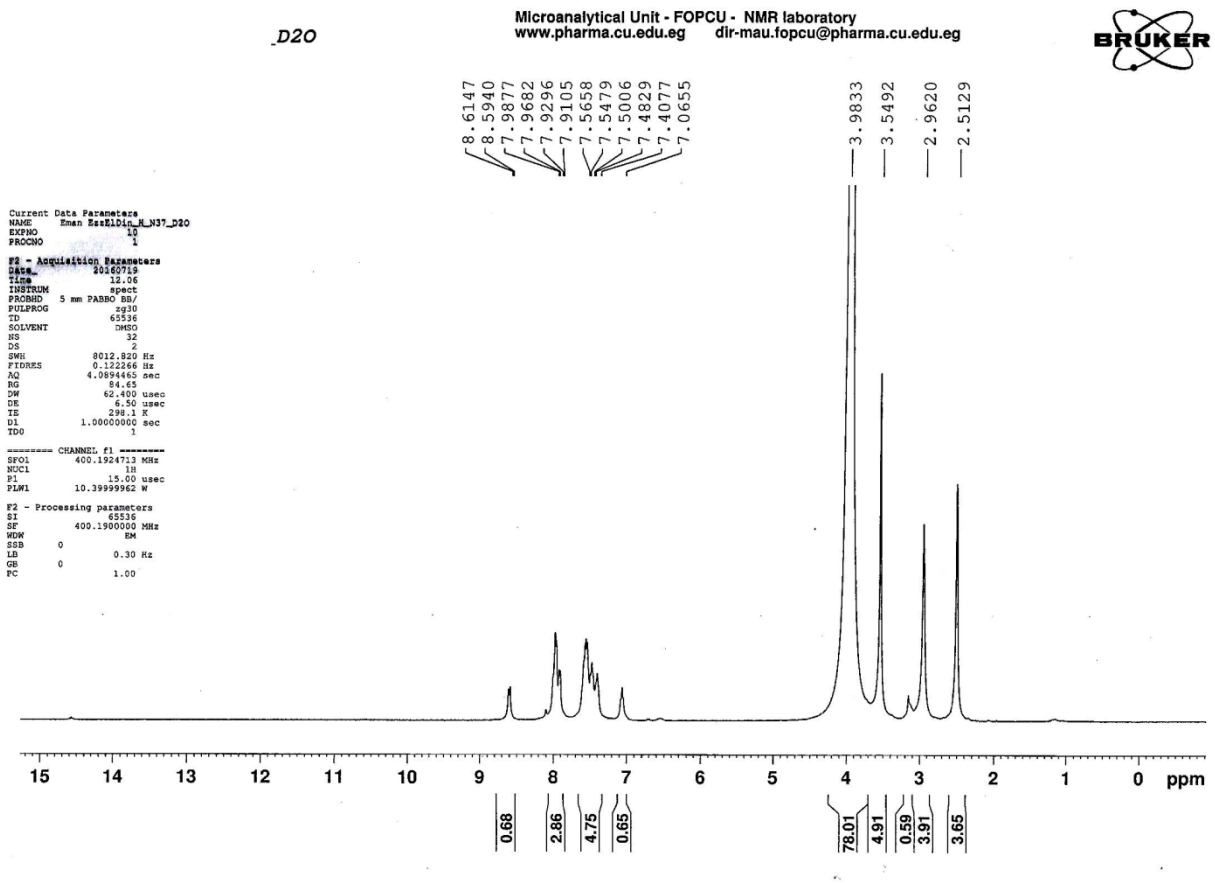
11.54
17.32
6.22
6.01

D_2O


D2O
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.6147
8.5940
7.9877
7.9682
7.9296
7.9105
7.5658
7.5479
7.5006
7.4829
7.4077
7.0655
3.9833
3.5492
2.9620
2.5129
Current Data Parameters
NAME Eman EzzElDin_R_N37_D2O
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160719
Time 12.06
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 84.65
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
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
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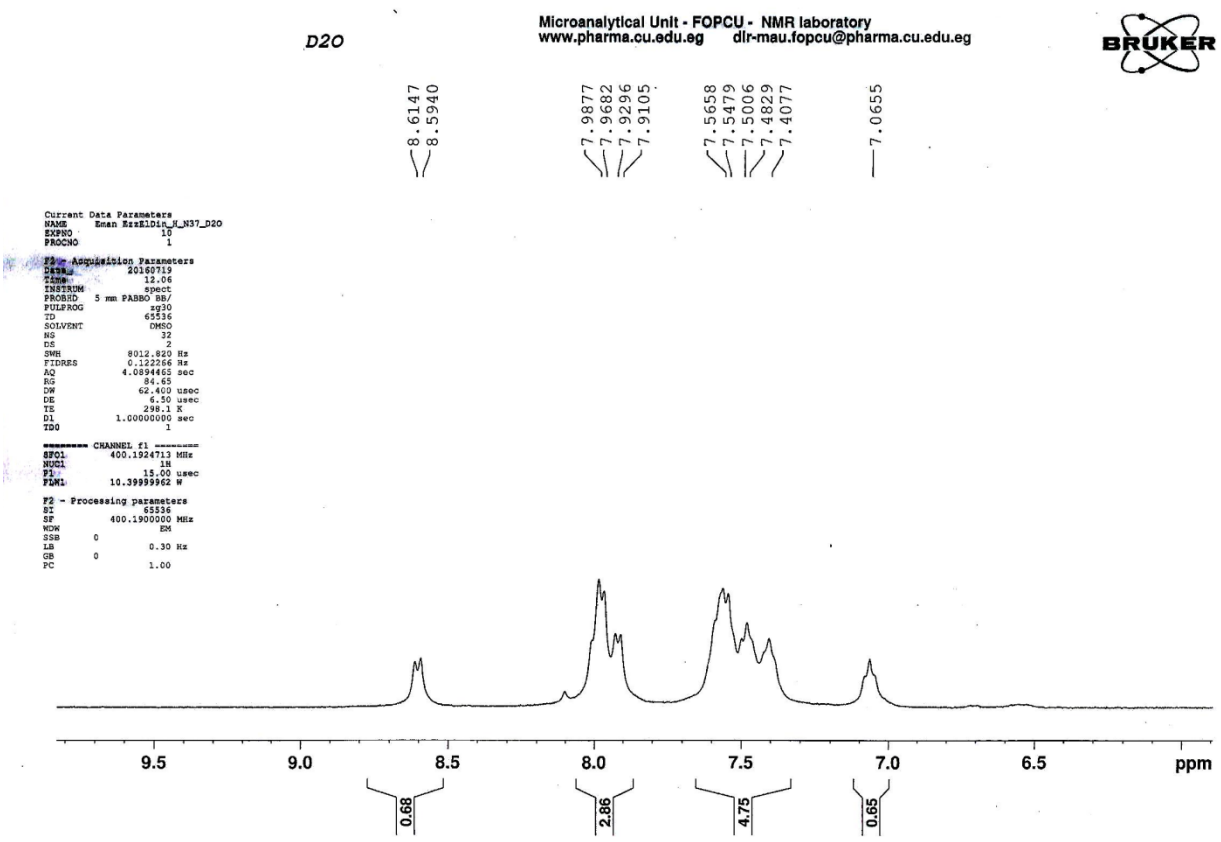
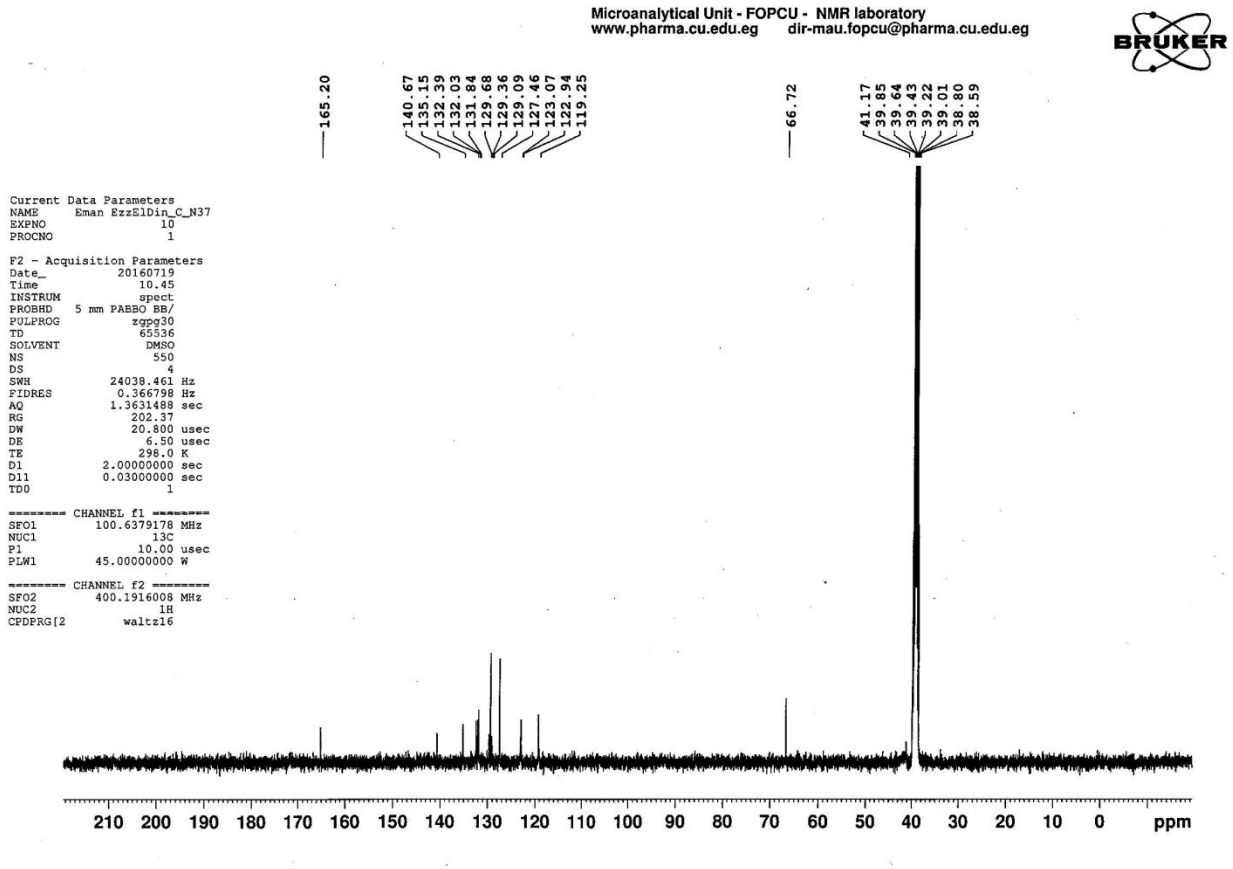
2.86
4.75
0.65
78.01
4.91
0.59
3.91
3.65


D2O
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.6147
8.5940
7.9877
7.9682
7.9296
7.9105
7.5658
7.5479
7.5006
7.4829
7.4077
7.0655
Current Data Parameters
NAME Eman ErrElDir_N_N37_D2O
EXPNO 10
PROCNO 1
F1 - Acquisition Parameters
Date_ 20160719
Time 12.06
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 84.65
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
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm
0.68
2.86
4.75
0.65

^{13}C NMR of 4e


Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
165.20
140.67
135.15
132.39
132.03
131.84
129.68
129.36
129.09
127.46
123.07
122.94
119.25
66.72
41.17
39.85
39.64
39.43
39.22
39.01
38.80
38.59
Current Data Parameters
NAME Eman EzzElDin_C_N37
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160719
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 550
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 ========
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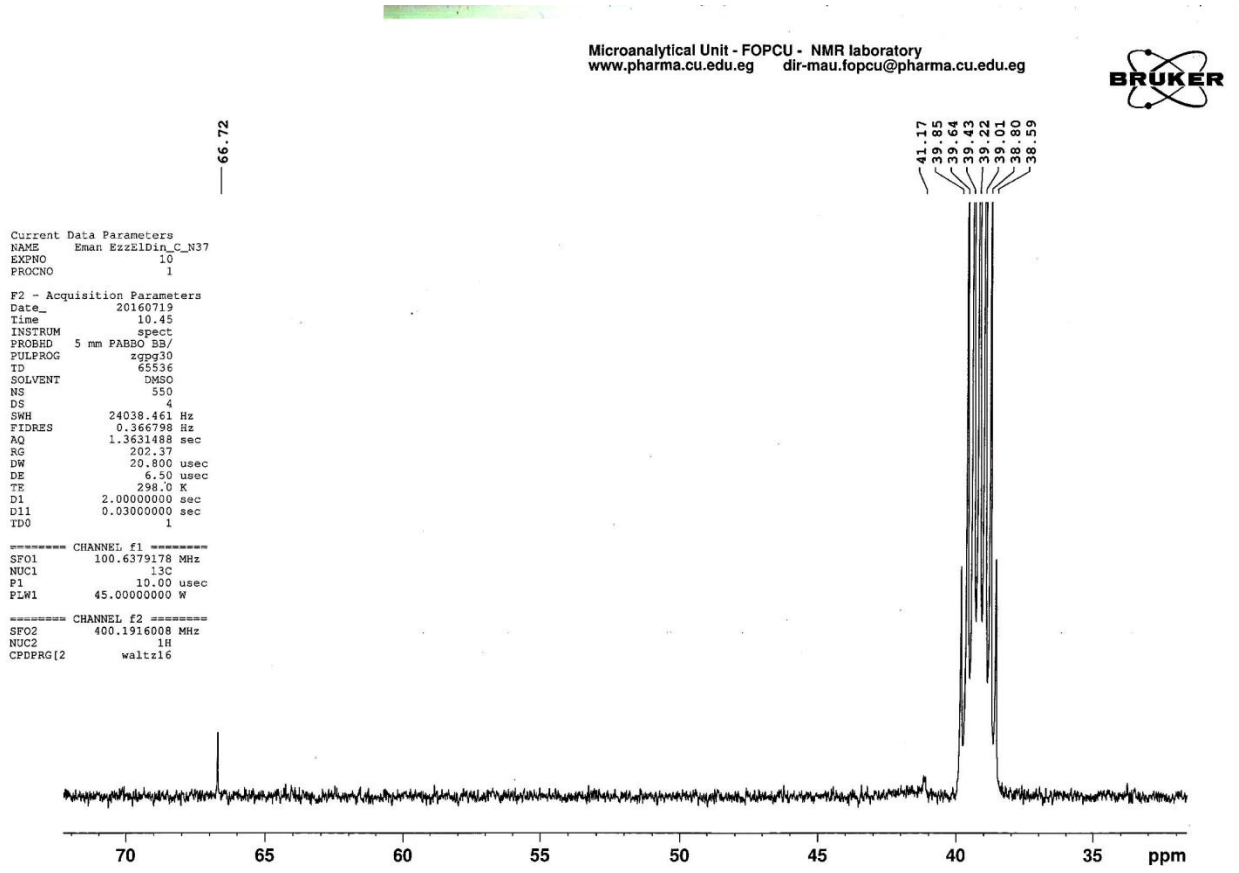
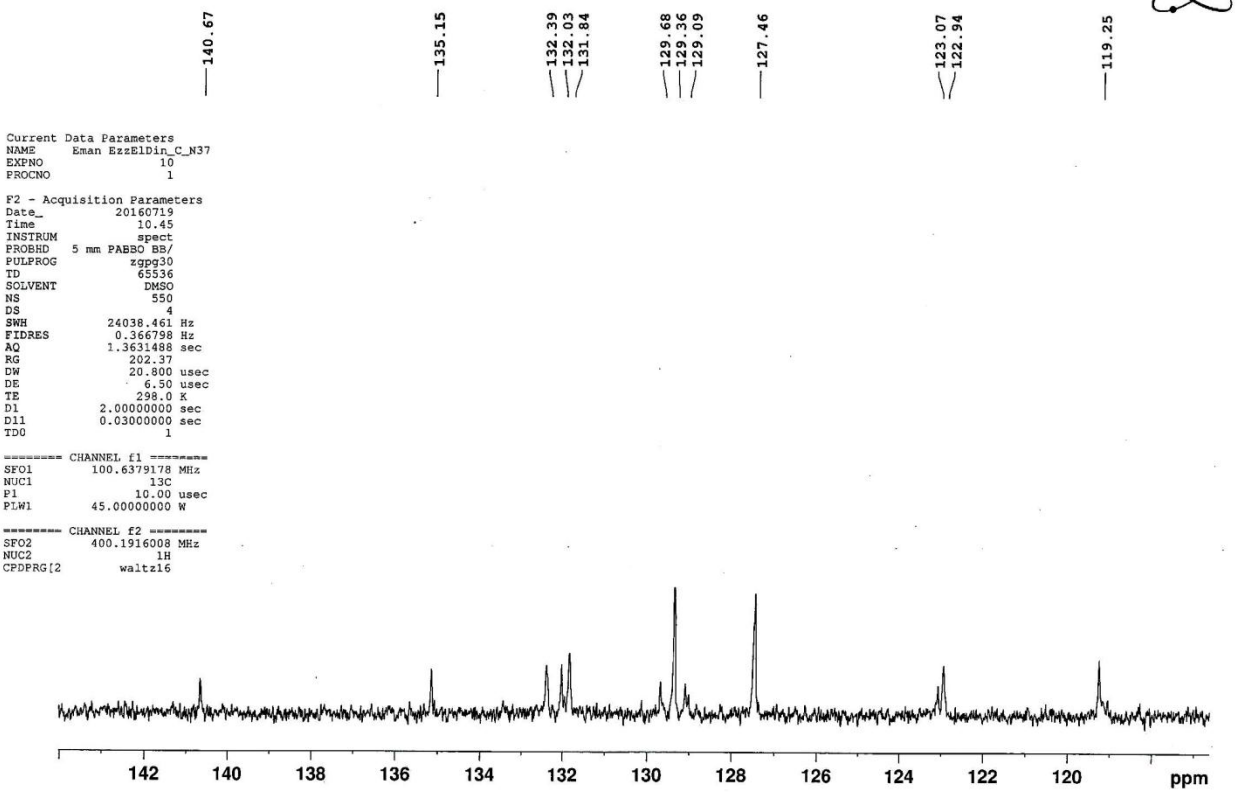
NUC2 1H
CPDPRG[2 waltz16
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

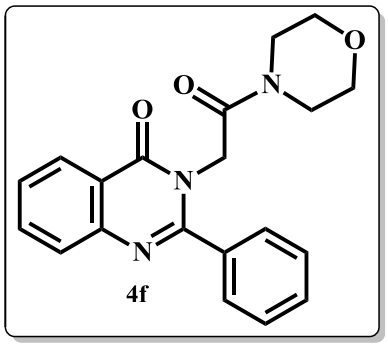

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
66.72
41.17
39.85
39.64
39.43
39.22
39.01
38.80
38.59
Current Data Parameters
NAME Eman EzzElDin_C_N37
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160719
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 550
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
70
65
60
55
50
45
40
35
ppm

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



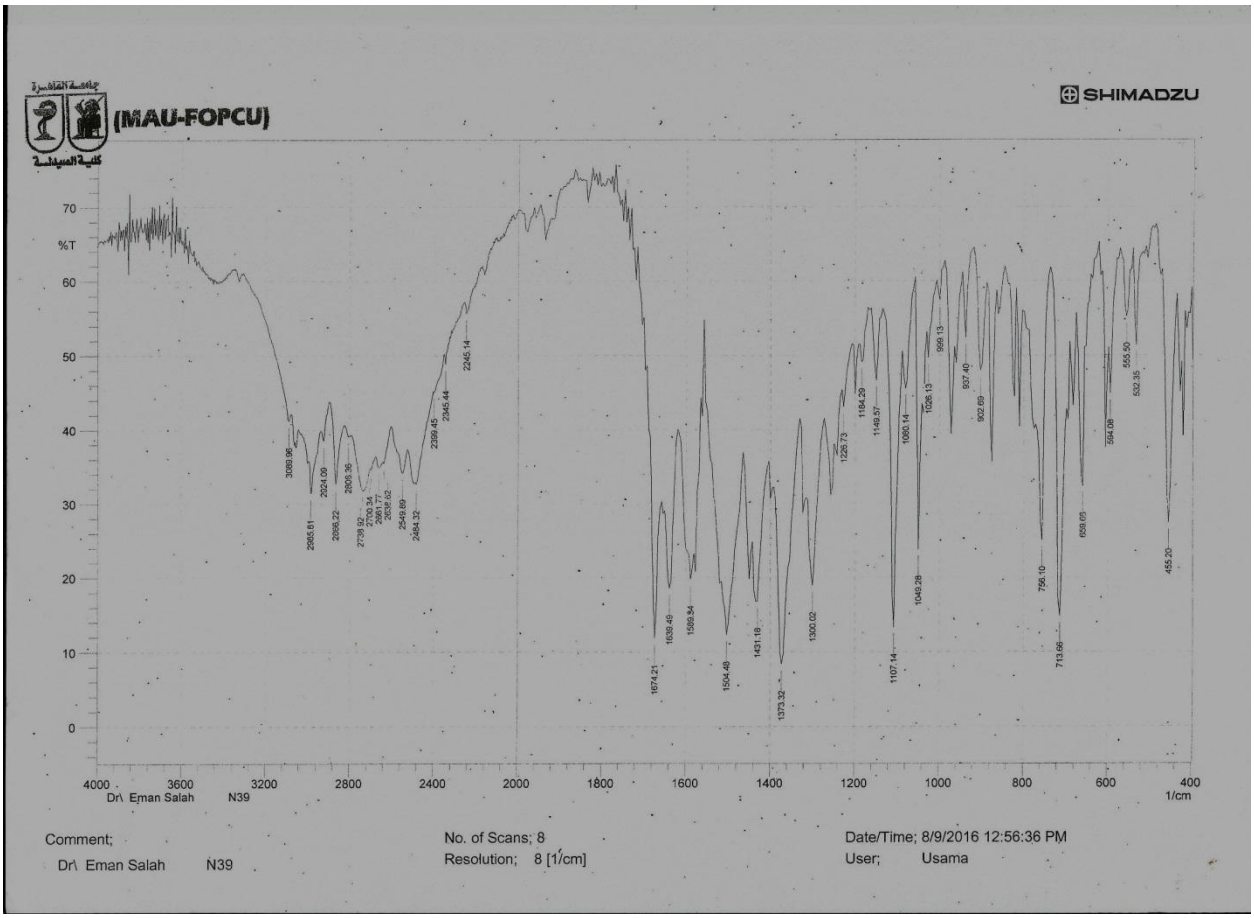
Compound 4f

3-(2-morpholino-2-oxoethyl)-2-phenylquinazolin-4(3H)-one

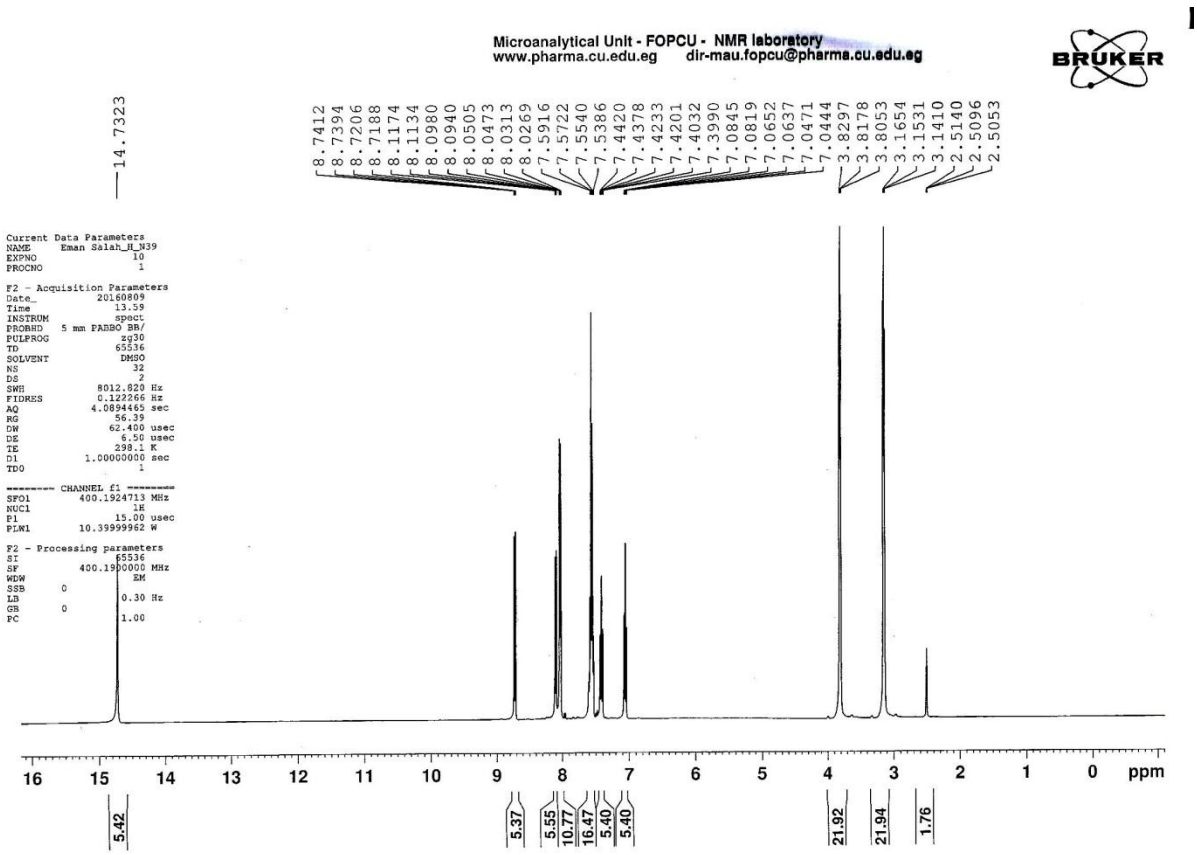


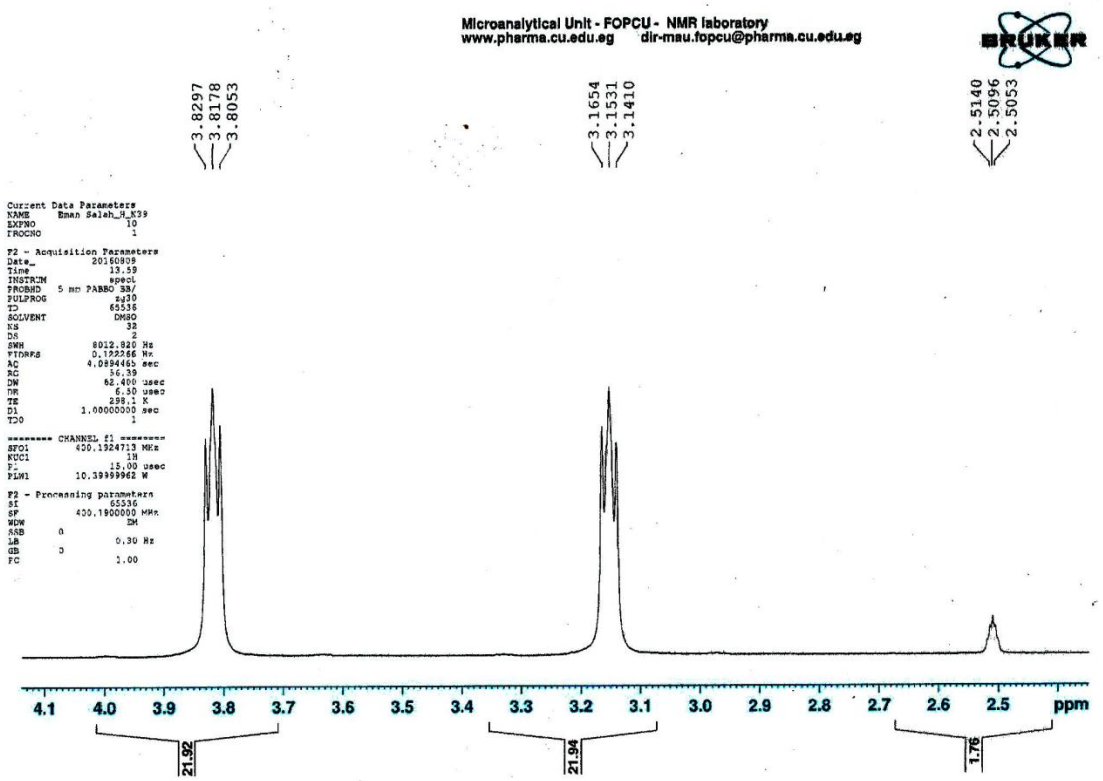
4f

IR of compound 4f



^{1}H NMR of 4f


Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
14.7323
8.7412
8.7394
8.7206
8.7188
8.1174
8.1134
8.0980
8.0940
8.0505
8.0473
8.0313
8.0269
7.5916
7.5722
7.5540
7.5386
7.4420
7.4378
7.4233
7.4201
7.4032
7.3990
7.0845
7.0819
7.0652
7.0637
7.0471
7.0444
3.8297
3.8178
3.8053
3.1654
3.1531
3.1410
2.5140
2.5096
2.5053
Current Data Parameters
NAME Eman Salah_H_N39
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160809
Time 13.59
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 56.39
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
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
5.42
5.37
5.55
10.77
16.47
5.40
5.40
21.92
21.94
1.76


Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
3.8297
3.8178
3.8053
3.1654
3.1531
3.1410
2.5140
2.5096
2.5053
Current Data Parameters
NAME Eman Saleh_H_K39
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160809
Time 13.59
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 36.39
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
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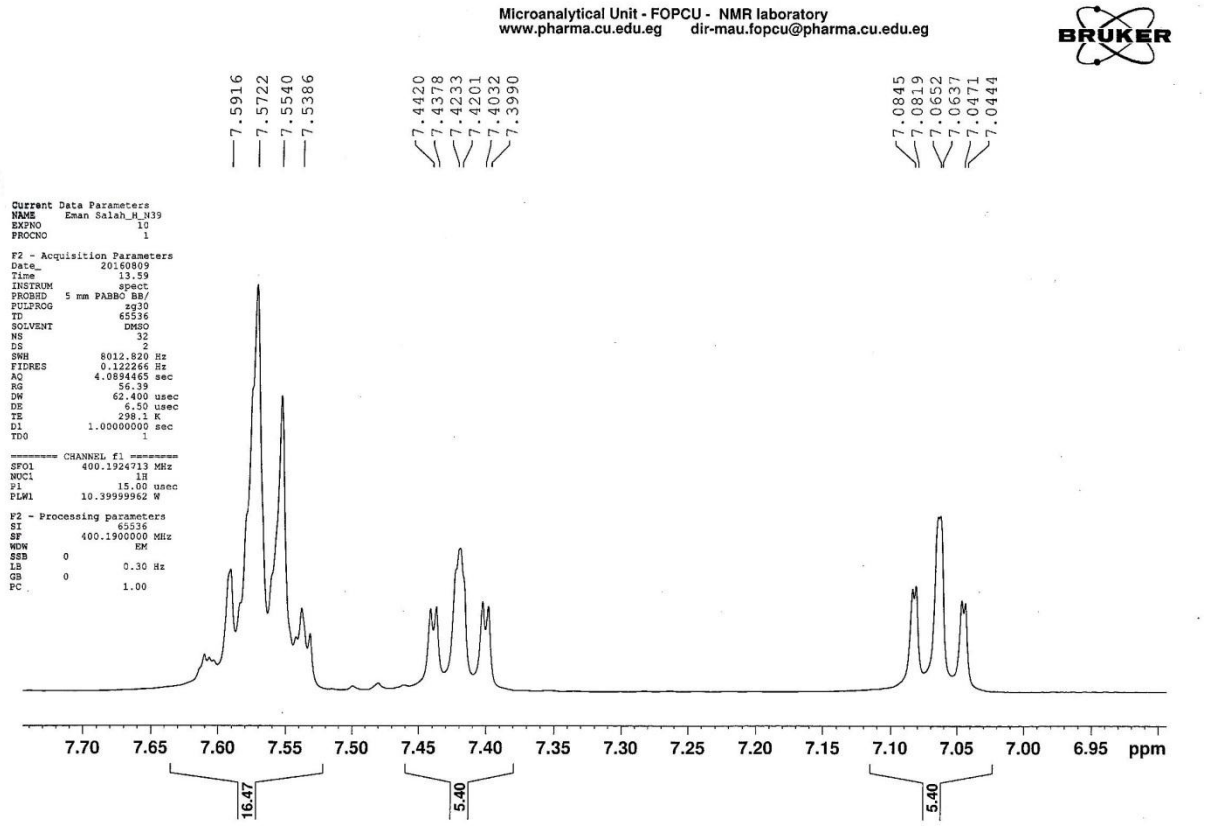
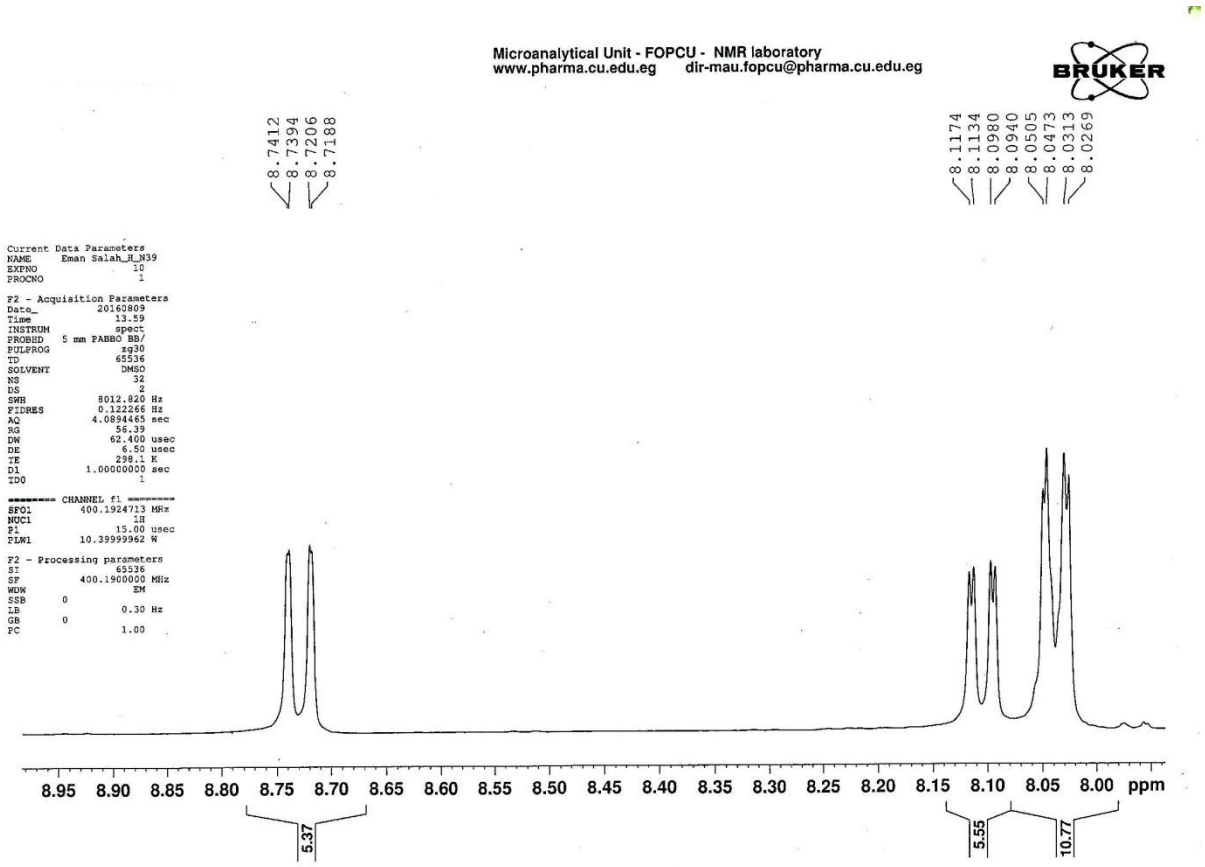
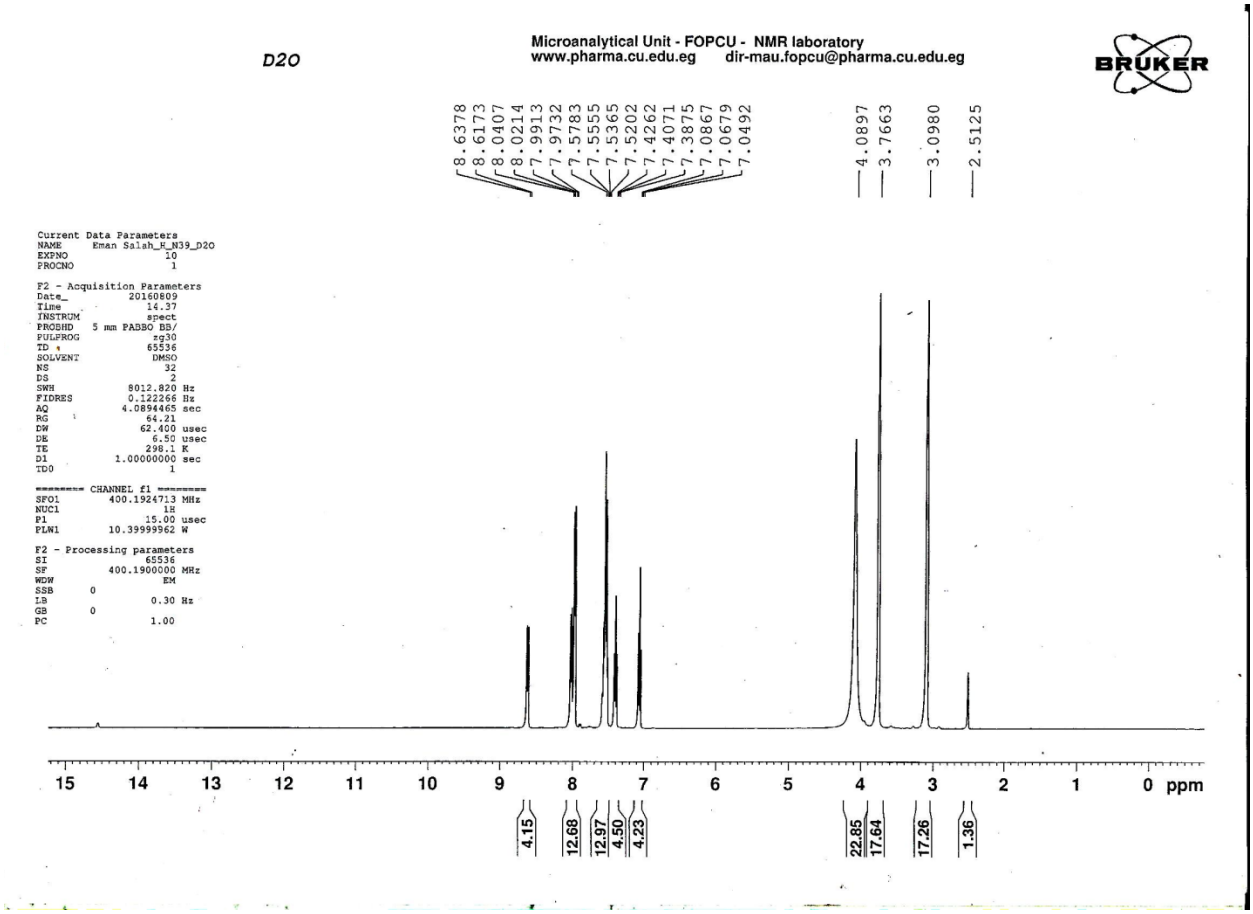
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 ppm
21.92
21.94
1.76


Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
7.5916
7.5722
7.5540
7.5386
7.4420
7.4378
7.4233
7.4201
7.4032
7.3990
7.0845
7.0819
7.0652
7.0637
7.0471
7.0444
Current Data Parameters
NAME Eman Salah_H_N39
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160809
Time 13.59
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 56.39
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
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.70
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
ppm
16.47
5.40
5.40


Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.7412
8.7394
8.7206
8.7188
8.1174
8.1134
8.0980
8.0940
8.0505
8.0473
8.0313
8.0269
Current Data Parameters
NAME Eman Salah_H_N39
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160809
Time 13.59
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 56.39
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
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.95 8.90 8.85 8.80 8.75 8.70 8.65 8.60 8.55 8.50 8.45 8.40 8.35 8.30 8.25 8.20 8.15 8.10 8.05 8.00 ppm
5.37
5.55
10.77

D_2O


D2O
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.6378
8.6173
8.0407
8.0214
7.9913
7.9732
7.5783
7.5555
7.5365
7.5202
7.4262
7.4071
7.3875
7.0867
7.0679
7.0492
4.0897
3.7663
3.0980
2.5125
Current Data Parameters
NAME Eman Salah_K_H39_D2O
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160809
Time 14.37
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
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
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
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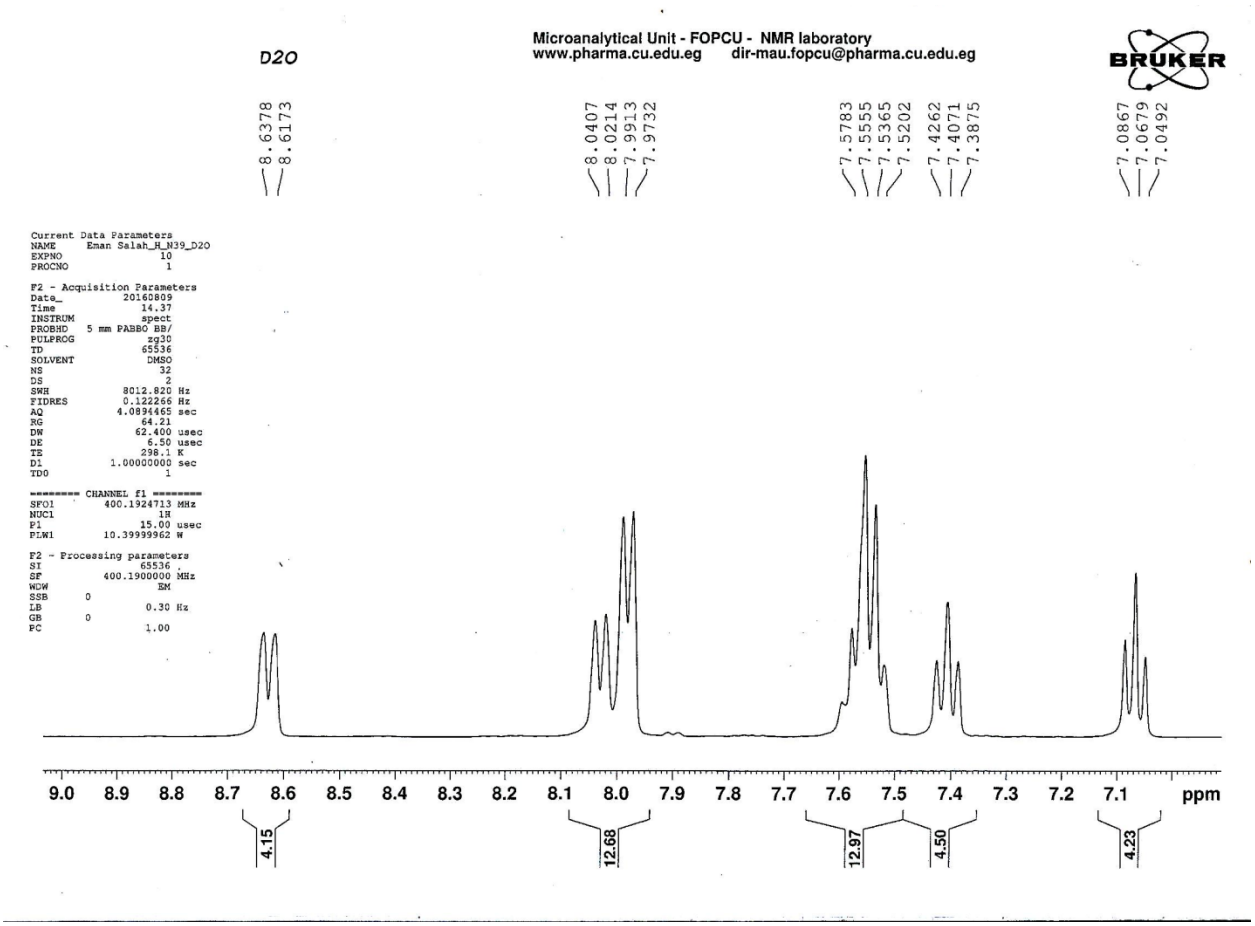
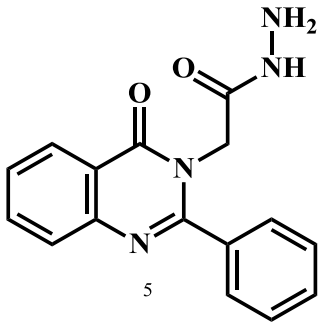
12.68
12.97
4.50
4.23
22.85
17.64
17.26
1.36

D_2O


D2O
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.6378
8.6173
8.0407
8.0214
7.9913
7.9732
7.5783
7.5555
7.5365
7.5202
7.4262
7.4071
7.3875
7.0867
7.0679
7.0492
Current Data Parameters
NAME Eman Salah_H_N39_D2O
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160809
Time 14.37
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
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
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
4.15
12.68
12.97
4.50
4.23

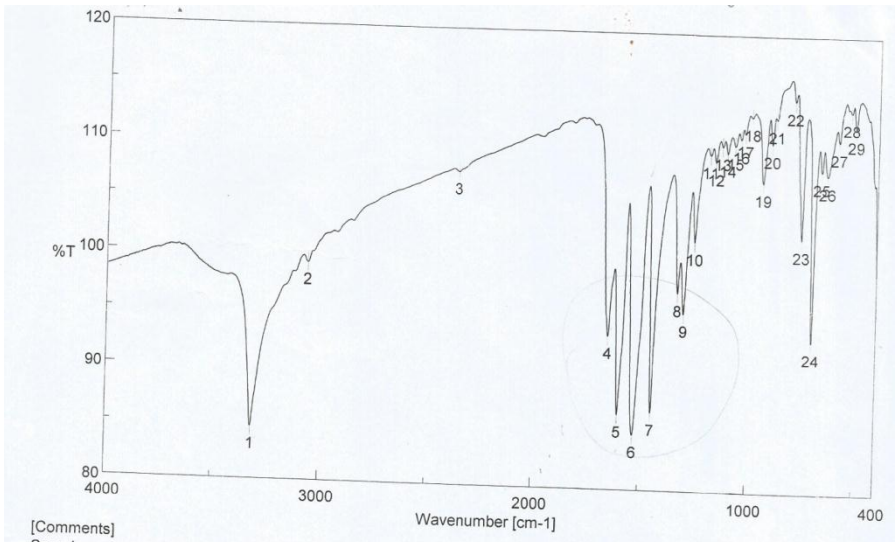
Compound 5

2-(4-oxo-2-phenylquinazolin-3(4H)-yl)acetohydrazide



5

IR of compound 5



[Comments]

Sample name	3
Comment	1/2/2015
User	IR
Division	IR
Company	MAC

[Result of Peak Picking]

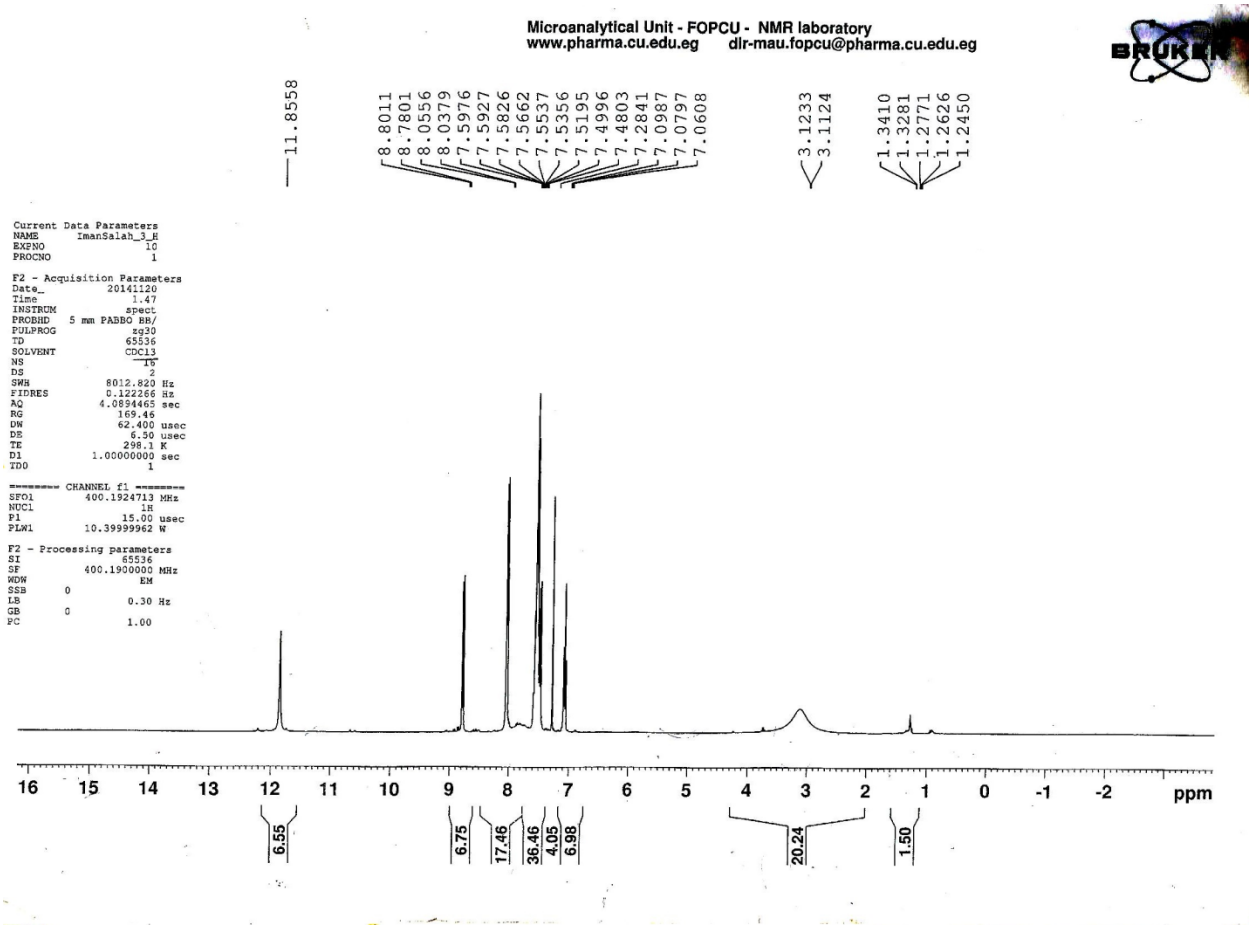
No.	Position	Intensity
1	3316.96	84.5929
4	1651.73	93.4305
7	1447.31	86.8308
10	1255.43	101.838
13	1133.94	110.243
16	1048.12	110.9
19	941.092	107.144
22	795.493	114.372
25	666.285	108.206
28	530.328	113.45

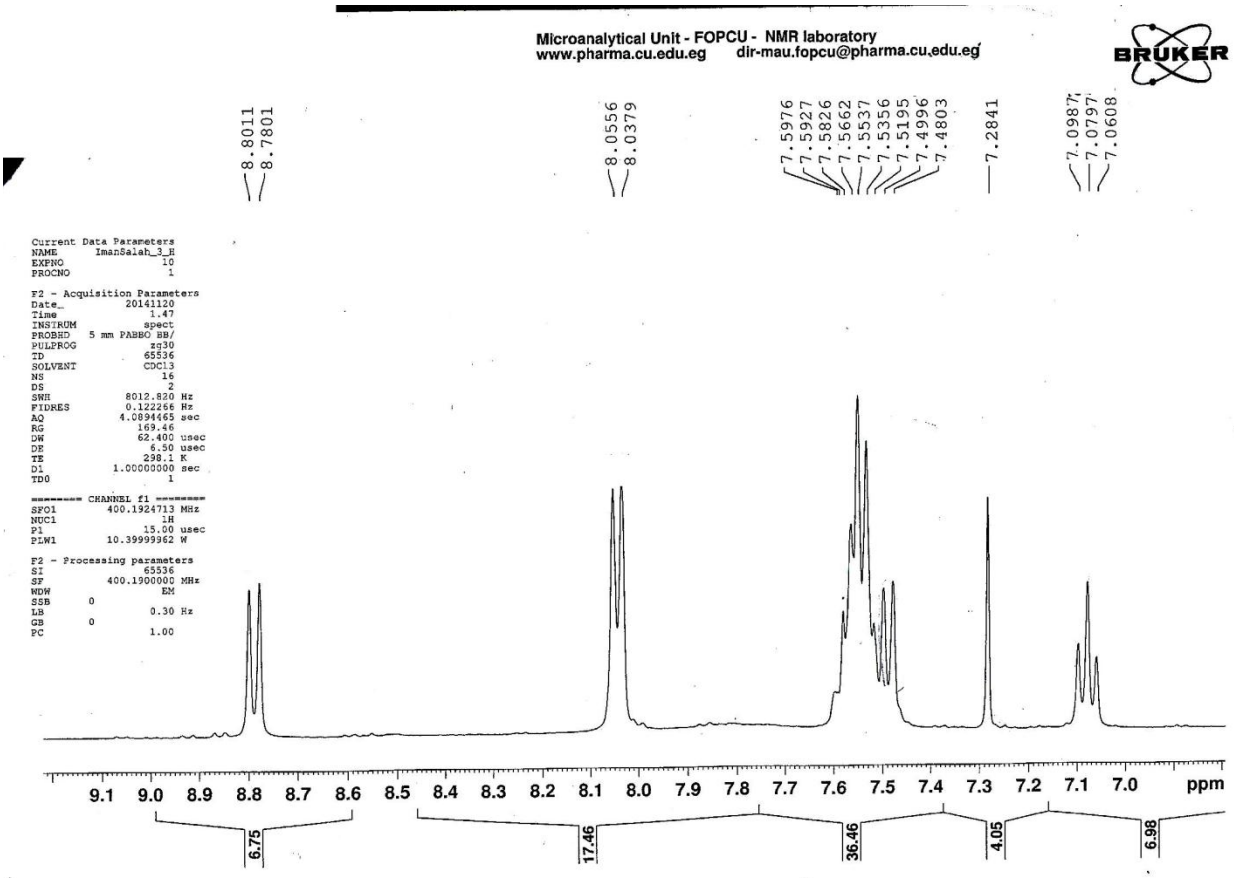
No.	Position	Intensity
2	3061.44	99.1221
5	1602.56	86.5978
8	1331.61	97.3051
11	1189.86	109.477
14	1110.8	109.68
17	1028.84	111.414
20	901.558	110.563
23	755.959	102.236
26	638.323	107.846
29	508.151	111.989

No.	Position	Intensity
3	2363.34	107.423
6	1529.27	84.8541
9	1302.68	95.5283
12	1163.83	108.862
15	1075.12	110.324
18	997.017	112.866
21	881.309	112.723
24	701.962	93.3053
27	587.218	110.827

i

^{1}H NMR of compound 5




Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.8011
8.7801
8.0556
8.0379
7.5976
7.5927
7.5826
7.5662
7.5537
7.5356
7.5195
7.4996
7.4803
7.2841
7.0987
7.0797
7.0608
Current Data Parameters
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EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141120
Time 1.47
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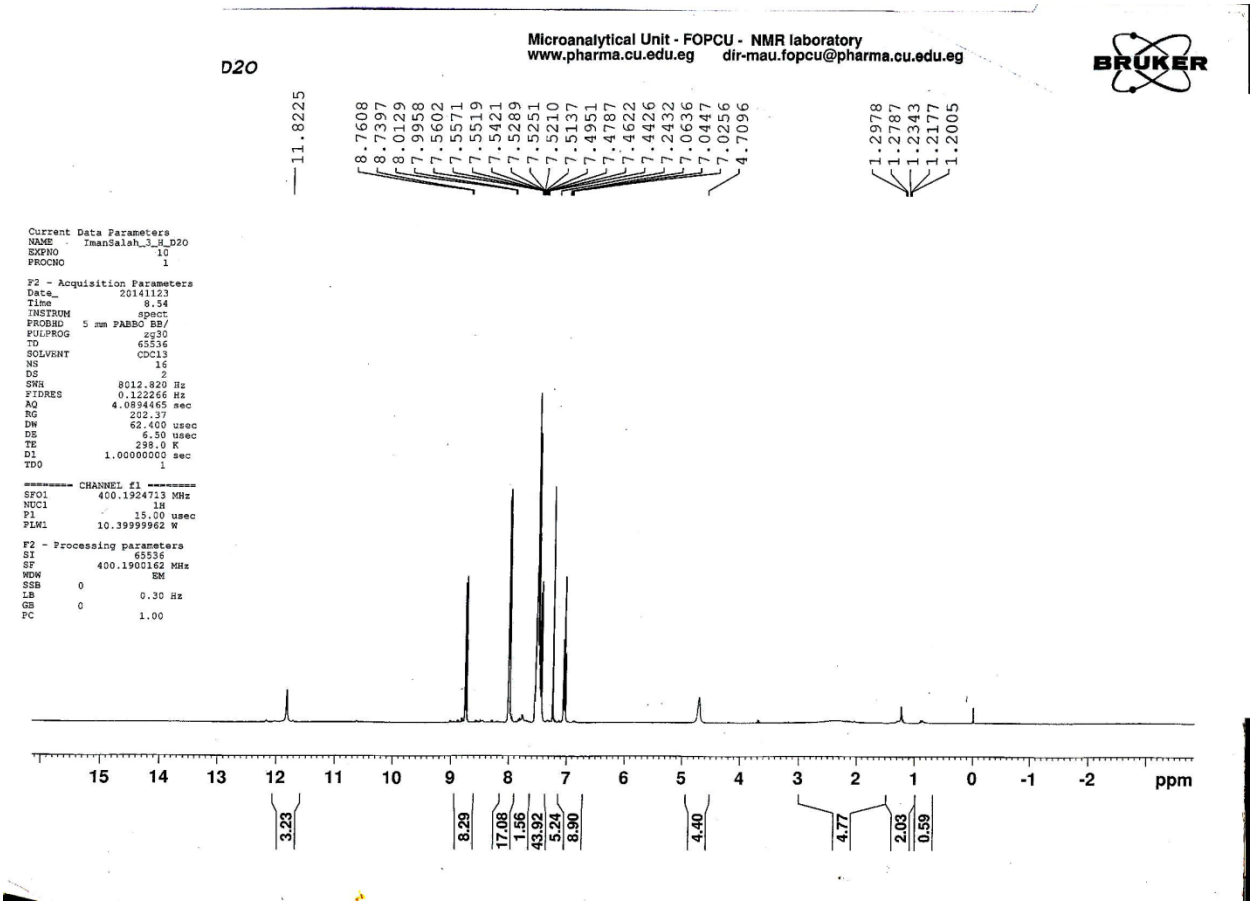
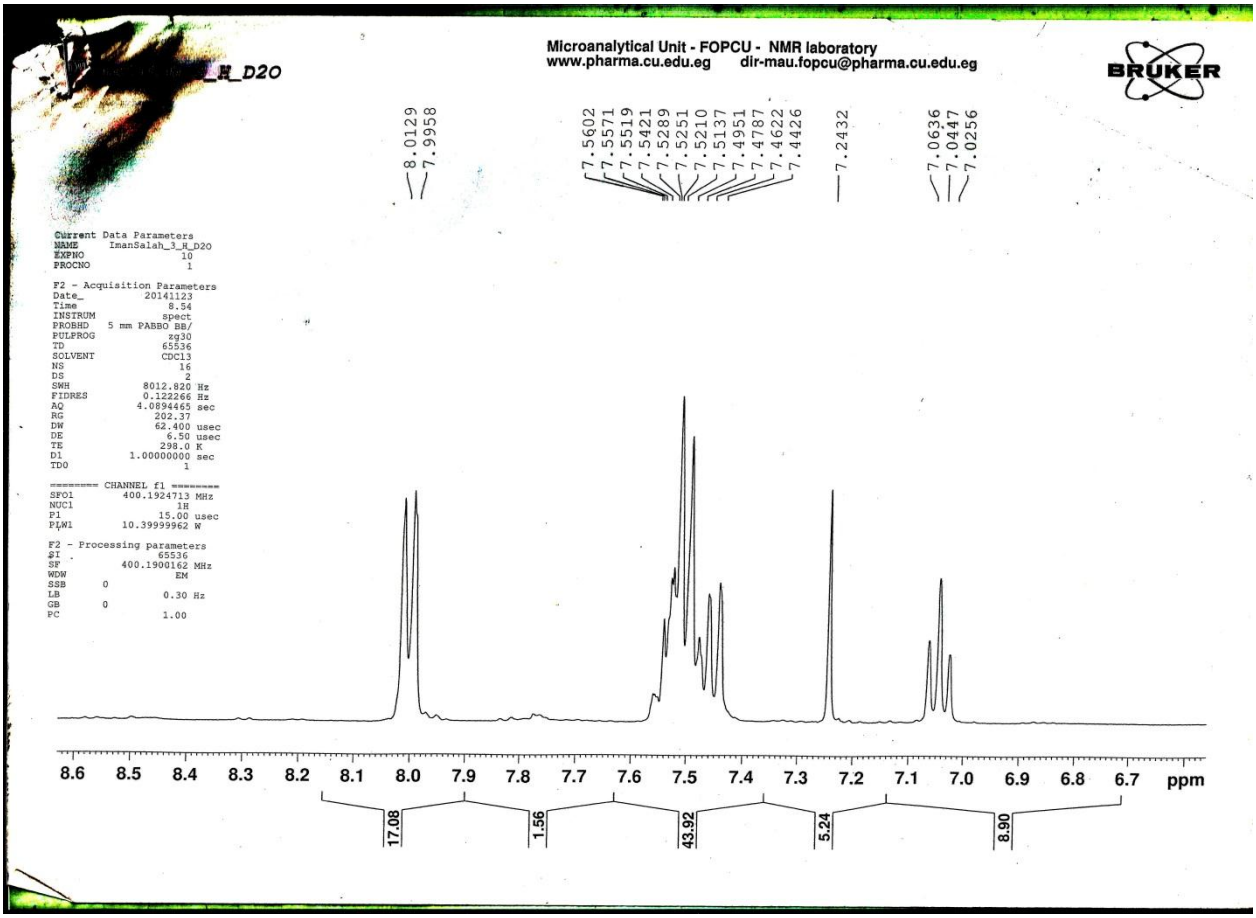
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
6.75
17.46
36.46
4.05
6.98

D_2O


Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
D2O
BRUKER
11.8225
8.7608
8.7397
8.0129
7.9958
7.5602
7.5571
7.5519
7.5421
7.5289
7.5251
7.5210
7.5137
7.4951
7.4787
7.4622
7.4426
7.2432
7.0636
7.0447
7.0256
4.7096
1.2978
1.2787
1.2343
1.2177
1.2005
Current Data Parameters
NAME ImanSalah_3_H_D2O
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141123
Time 8.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 202.37
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 400.1900162 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
3.23
8.29
17.08
1.56
43.92
5.24
8.90
4.40
4.77
2.03
0.59


_H_D2O
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.0129
7.9958
7.5602
7.5571
7.5519
7.5421
7.5289
7.5251
7.5210
7.5137
7.4951
7.4787
7.4622
7.4426
7.2432
7.0636
7.0447
7.0256
Current Data Parameters
NAME ImanSalah_3_H_D2O
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141123
Time 8.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 202.37
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 400.1900162 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm
17.08
1.56
43.92
5.24
8.90

EI-MS of compound 5

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

Analyzed by	: N.Bagato
Analyzed	: 17/02/2015 04:40:16 م
Sample Name	: sample 3
Sample ID	:
Customer Name	: صيدلة دمنهور - ايمان صلاح
Data File	: C:\GCMSsolution\Data\Project1\sample 3.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\sample 3.QGD
Method File	: C:\GCMSsolution\Data\Project1\A.GABR.qgm
Org Method File	: C:\GCMSsolution\Data\Project1\A.GABR.qgm
Report File	:
Tuning File	: C:\GCMSsolution\System\Tune1_default1.qgt
$EndIf$Modified by	: N.Bagato
Modified	: 17/02/2015 04:45:03 م

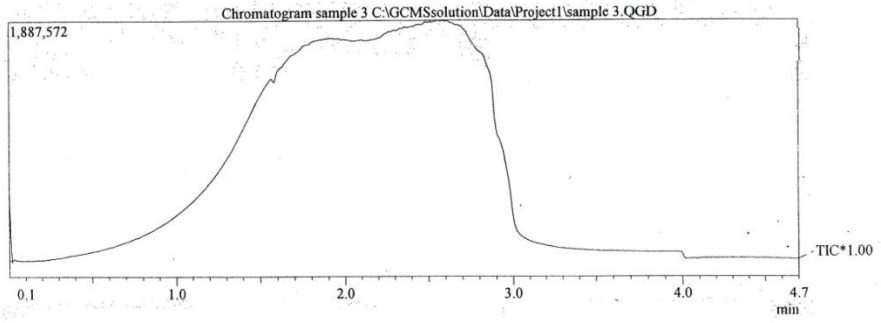
Method

Analytical Line 1

IonSourceTemp	:250.00 °C
[MS Table]	
--Group 1 - Event 1--	
Start Time	:0.00min
End Time	:10.00min
ACQ Mode	:Scan
Event Time	:0.50sec
Scan Speed	: 769
Start m/z	:50.00
End m/z	:400.00
Electron Voltage	: 70 eV
Ionization Mode	: EI

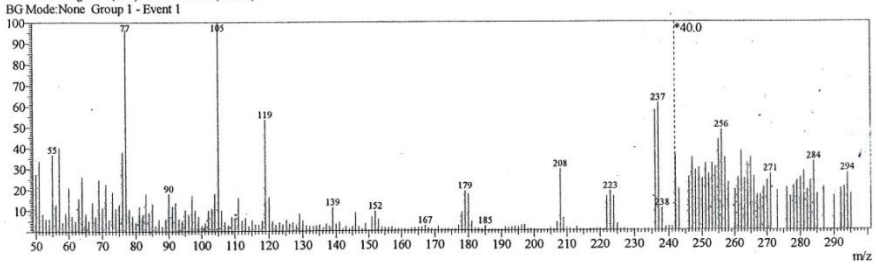
C:\GCMSsolution\Data\Project1\sample 3.QGD

Chromatogram sample 3 C:\GCMSsolution\Data\Project1\sample 3.QGD



Spectrum

Line#:1 R.Time:3.4(Scan#:406)
MassPeaks:232
RawMode:Single 3.4(406) BasePeak:105(12731)
BG Mode:None Group 1 - Event 1



Mass Table

Line#:1 R.Time:3.4(Scan#:406)
MassPeaks:232
RawMode:Single 3.4(406) BasePeak:105(12731)
BG Mode:None Group 1 - Event 1

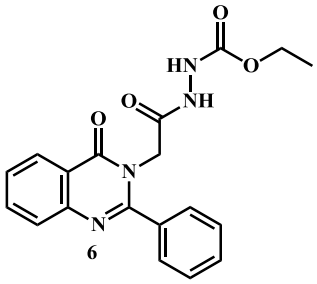
#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	3502	27.51	4	53.00	754	5.92	7	56.05	1622	12.74
2	51.00	4284	33.65	5	54.05	762	5.99	8	57.05	5134	40.33
3	52.05	1071	8.41	6	55.05	4677	36.74	9	58.05	576	4.52

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	59.00	1105	8.68	79	128.10	374	2.94	148	198.00	100	0.79
11	60.00	2668	20.96	80	129.10	1058	8.31	149	199.00	130	1.02
12	61.00	961	7.55	81	130.10	654	5.14	150	200.00	110	0.86
13	62.00	618	4.85	82	131.10	353	2.77	151	201.00	71	0.56
14	63.00	2007	15.76	83	132.10	308	2.42	152	202.00	65	0.51
15	63.95	3350	26.31	84	133.10	303	2.38	153	203.00	79	0.62
16	65.00	1087	8.54	85	134.10	327	2.57	154	204.00	70	0.55
17	65.95	639	5.02	86	135.10	388	3.05	155	205.00	172	1.35
18	67.00	1764	13.86	87	136.10	223	1.75	156	206.00	97	0.76
19	68.00	908	7.13	88	137.10	433	3.40	157	207.00	532	4.18
20	69.00	3161	24.83	89	138.05	315	2.47	158	208.05	3737	29.35
21	70.05	1452	11.41	90	139.05	1427	11.21	159	209.00	778	6.11
22	71.05	2863	22.49	91	140.05	442	3.47	160	210.00	196	1.54
23	72.00	714	5.61	92	141.05	553	4.34	161	211.00	138	1.08
24	73.00	2398	18.84	93	142.10	166	1.30	162	212.00	74	0.58
25	74.00	1380	10.84	94	143.10	308	2.42	163	213.00	226	1.78
26	75.00	1636	12.85	95	144.10	156	1.23	164	214.00	95	0.75
27	76.00	4831	37.95	96	145.05	290	2.28	165	215.00	97	0.76
28	77.00	12298	96.60	97	146.00	1121	8.81	166	216.00	82	0.64
29	78.00	1362	10.70	98	147.00	290	2.28	167	217.00	110	0.86
30	79.00	930	7.31	99	148.00	154	1.21	168	218.00	105	0.82
31	80.00	556	4.37	100	149.05	457	3.59	169	219.00	153	1.20
32	81.05	1507	11.84	101	151.05	877	6.89	170	220.00	127	1.00
33	82.05	1024	8.04	102	152.05	1204	9.46	171	222.00	2082	16.35
34	83.05	2293	18.01	103	153.05	720	5.66	172	223.00	2383	18.72
35	84.05	1147	9.01	104	154.10	258	2.03	173	224.00	2071	16.27
36	85.05	1680	13.20	105	155.10	212	1.67	174	225.05	430	3.38
37	86.05	331	2.60	106	156.10	194	1.52	175	226.00	111	0.87
38	87.00	714	5.61	107	157.10	268	2.11	176	227.00	126	0.99
39	88.00	311	2.44	108	158.10	137	1.08	177	228.00	62	0.49
40	89.05	734	5.77	109	159.10	142	1.12	178	229.00	62	0.49
41	90.00	2273	17.85	110	160.10	129	1.01	179	230.00	71	0.56
42	91.05	1512	11.88	111	161.10	143	1.12	180	231.00	66	0.52
43	92.00	1735	13.63	112	162.10	86	0.68	181	233.00	79	0.62
44	93.05	756	5.94	113	163.10	167	1.31	182	234.00	79	0.62
45	94.05	662	5.20	114	164.10	196	1.54	183	236.05	7346	57.70
46	95.05	1291	10.14	115	165.10	230	1.81	184	237.05	7776	61.08
47	96.05	1042	8.18	116	166.10	239	1.88	185	238.05	1339	10.52
48	97.10	2174	17.08	117	167.10	319	2.51	186	239.10	231	1.81
49	98.05	1296	10.18	118	168.10	178	1.40	187	240.10	242	1.90
50	99.10	905	7.11	119	169.10	153	1.20	188	241.10	226	1.78
51	100.05	349	2.74	120	170.10	110	0.86	189	242.10	114	0.90
52	101.05	518	4.07	121	171.10	257	2.02	190	243.10	63	0.49
53	102.05	1266	9.94	122	172.10	132	1.04	191	246.10	82	0.64
54	103.05	1390	10.92	123	173.10	126	0.99	192	247.10	111	0.87
55	103.95	2278	17.89	124	174.10	132	1.04	193	248.10	92	0.72
56	105.05	12731	100.00	125	175.10	100	0.79	194	249.10	95	0.75
57	106.05	1267	9.95	126	176.10	113	0.89	195	250.10	79	0.62
58	107.05	592	4.65	127	177.05	322	2.53	196	251.10	102	0.80
59	108.10	358	2.81	128	178.05	1135	8.92	197	252.10	86	0.68
60	109.10	882	6.93	129	179.05	2405	18.89	198	253.10	102	0.80
61	110.10	754	5.92	130	180.05	2252	17.69	199	254.10	97	0.76
62	111.05	2048	16.09	131	181.05	592	4.65	200	255.10	138	1.08
63	112.10	652	5.12	132	182.10	154	1.21	201	256.10	153	1.20
64	113.10	796	6.25	133	183.10	151	1.19	202	257.10	111	0.87
65	114.10	306	2.40	134	184.10	122	0.96	203	258.10	73	0.57
66	115.10	686	5.39	135	185.10	298	2.34	204	260.10	62	0.49
67	116.05	415	3.26	136	186.10	73	0.57	205	261.10	81	0.64
68	117.05	398	3.13	137	187.10	84	0.66	206	262.10	121	0.95
69	118.05	658	5.17	138	188.10	63	0.49	207	263.10	79	0.62
70	119.05	6803	53.44	139	189.10	66	0.52	208	264.10	103	0.81
71	120.05	2088	16.40	140	190.10	63	0.49	209	265.10	111	0.87
72	121.10	615	4.83	141	191.10	222	1.74	210	266.10	82	0.64
73	122.10	385	3.02	142	192.10	204	1.60	211	267.10	54	0.42
74	123.10	532	4.18	143	193.10	214	1.68	212	268.10	54	0.42
75	124.10	414	3.25	144	194.10	247	1.94	213	269.10	66	0.52
76	125.15	688	5.40	145	195.10	230	1.81	214	270.10	76	0.60
77	126.10	454	3.57	146	196.05	340	2.67	215	271.10	86	0.68
78	127.10	550	4.32	147	197.05	369	2.90	216	273.10	60	0.47

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
217	276.10	65	0.51	223	282.10	62	0.49	229	292.10	63	0.49
218	277.10	52	0.41	224	283.10	76	0.60	230	293.10	66	0.52
219	278.10	68	0.53	225	284.10	105	0.82	231	294.10	87	0.68
220	279.10	76	0.60	226	285.10	55	0.43	232	295.10	55	0.43
221	280.10	81	0.64	227	287.10	66	0.52				
222	281.10	90	0.71	228	290.10	52	0.41				

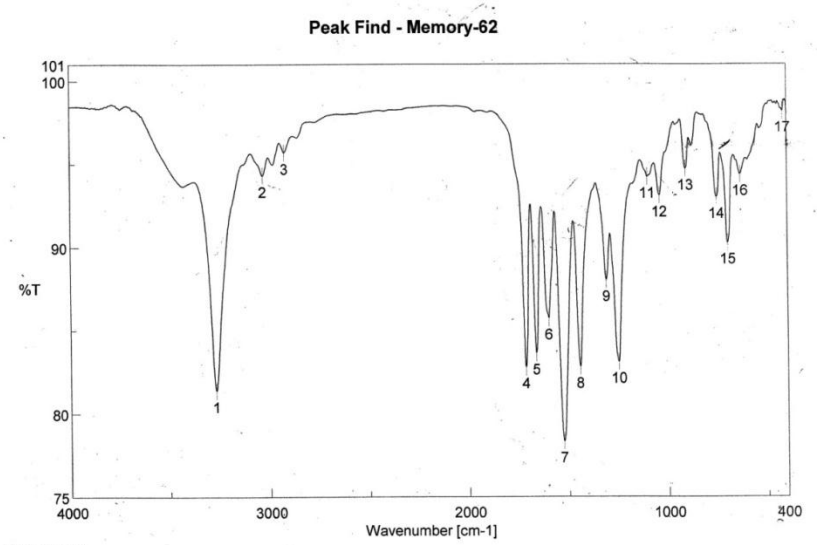
Compound 6

ethyl 2-(2-(4-oxo-2-phenylquinazolin-3(4H)-yl)acetyl)hydrazinecarboxylate



6

IR of compound 6



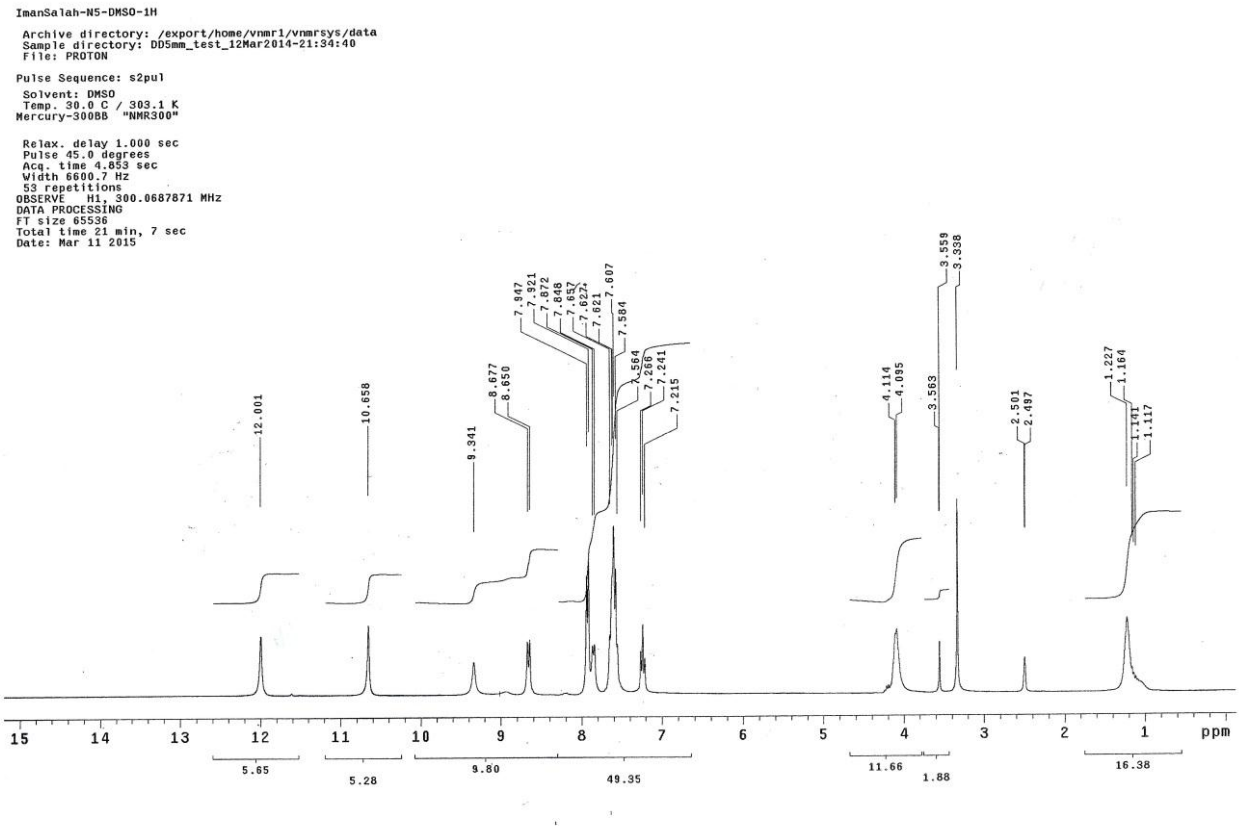
[Comments]

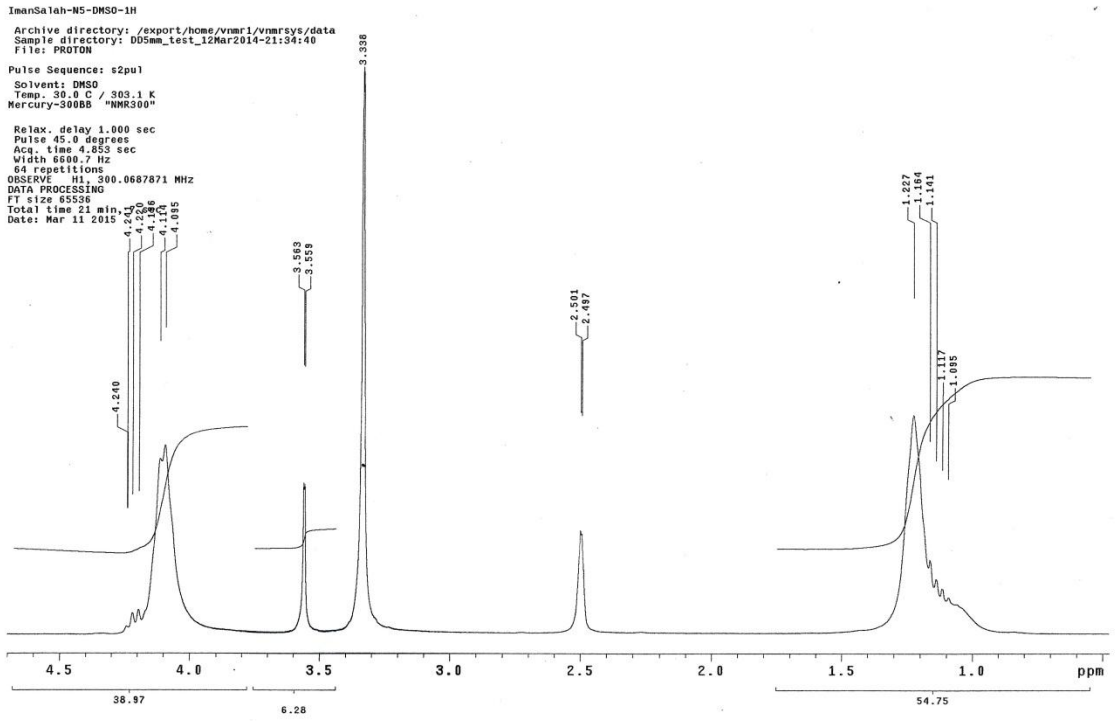
Sample name	N5
Comment	9/3/2015
User	IR
Division	RD
Company	MAC

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3270.68	81.3959	2	3032.51	94.3123	3	2924.52	95.6873
4	1715.37	82.7756	5	1663.3	83.6129	6	1599.66	85.6961
7	1527.35	78.3095	8	1444.42	82.7871	9	1311.36	87.9941
10	1250.61	83.0798	11	1102.12	94.2055	12	1041.37	93.0817
13	909.272	94.6975	14	754.031	92.9911	15	698.105	90.2389
16	634.466	94.3554	17	420.406	98.1776			

^{1}H NMR spectrum of compound 6

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Solvent: DMSO
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Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
64 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 21 min,
Date: Mar 11 2015
4.241
4.220
4.198
4.176
4.155
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4.240
3.583
3.559
3.338
2.501
2.497
1.227
1.164
1.141
1.117
1.095
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3.0
2.5
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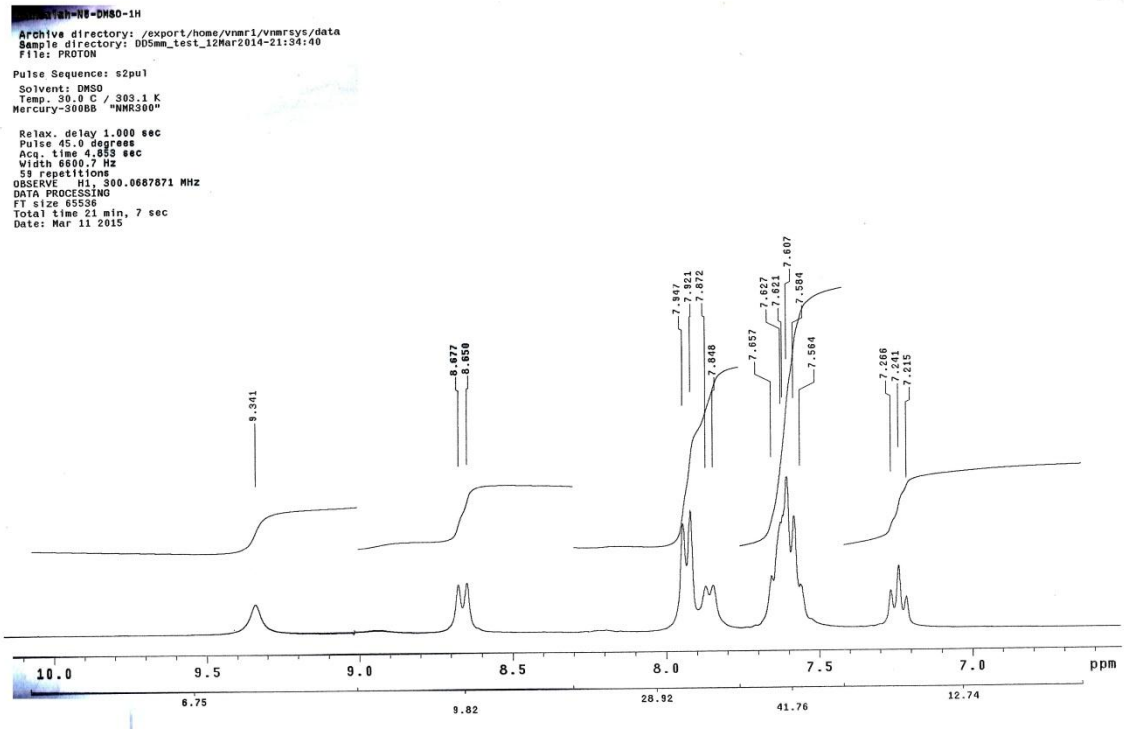
1.5
1.0
ppm
38.97
6.28
54.75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Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
59 repetitions
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Total time 21 min, 7 sec
Date: Mar 11 2015
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7.921
7.872
7.848
7.657
7.627
7.621
7.607
7.584
7.564
7.266
7.241
7.215
10.0
9.5
9.0
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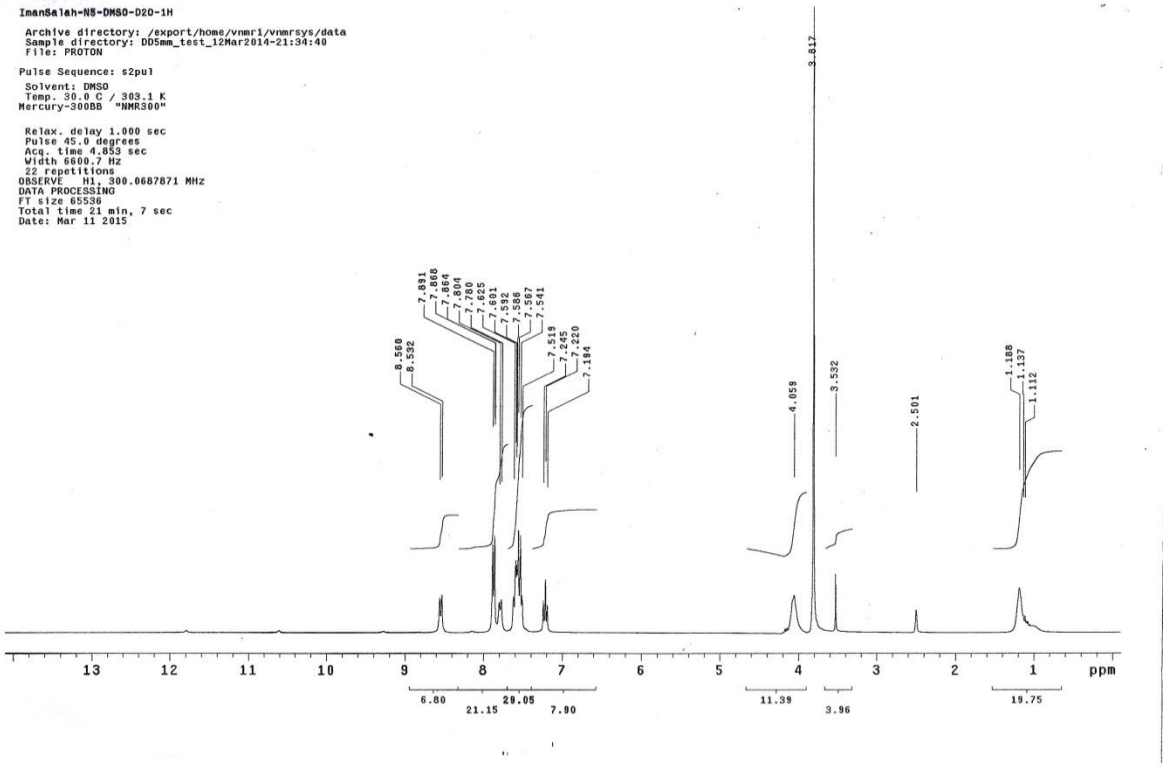
8.0
7.5
7.0
ppm
6.75
9.82
28.92
41.76
12.74

D_2O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File: PROTON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMRS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
22 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 21 min, 7 sec
Date: Mar 11 2015
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8.532
7.891
7.866
7.864
7.804
7.780
7.625
7.601
7.592
7.586
7.567
7.541
7.519
7.495
7.220
7.194
4.059
3.817
3.532
2.501
1.168
1.137
1.112
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
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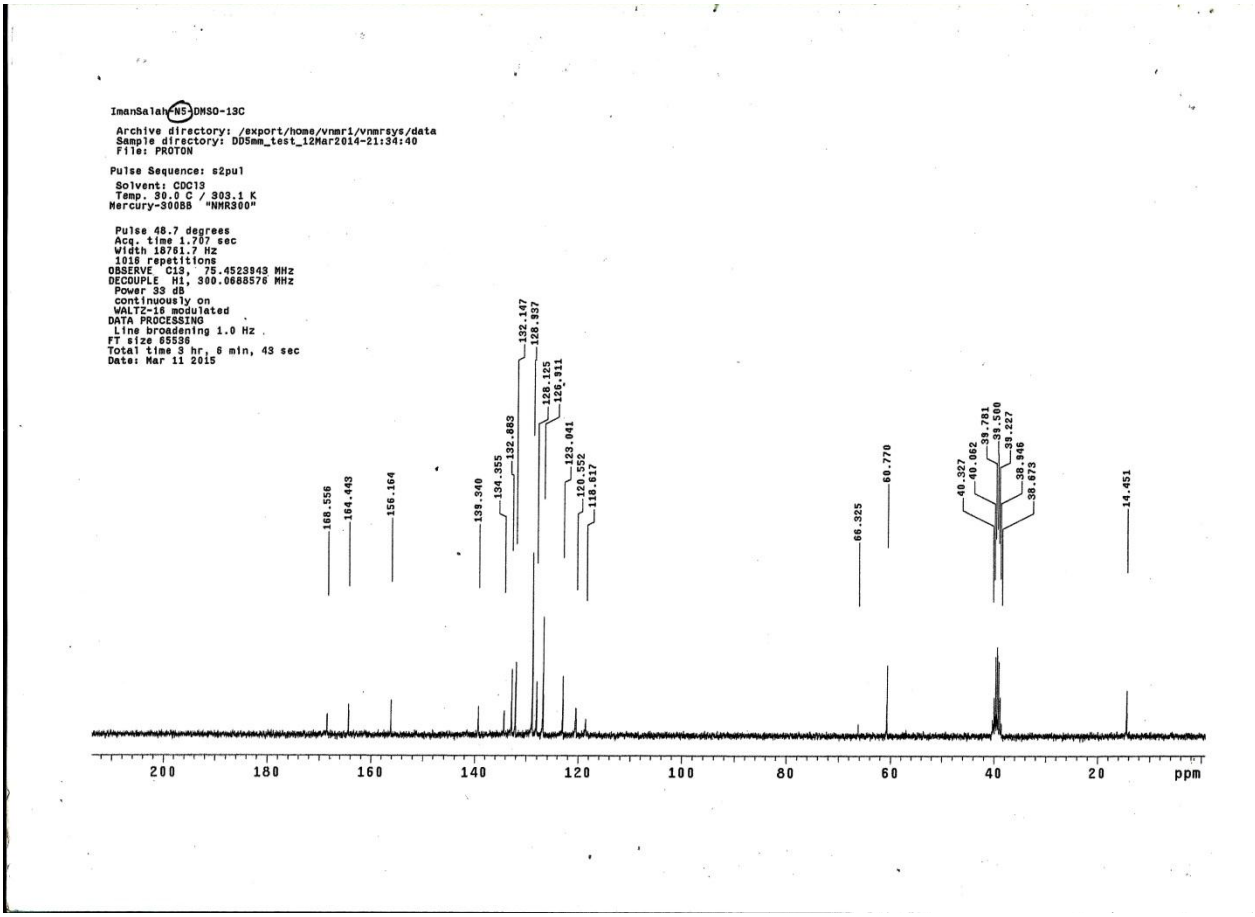
29.05
7.90
11.39
3.96
19.75

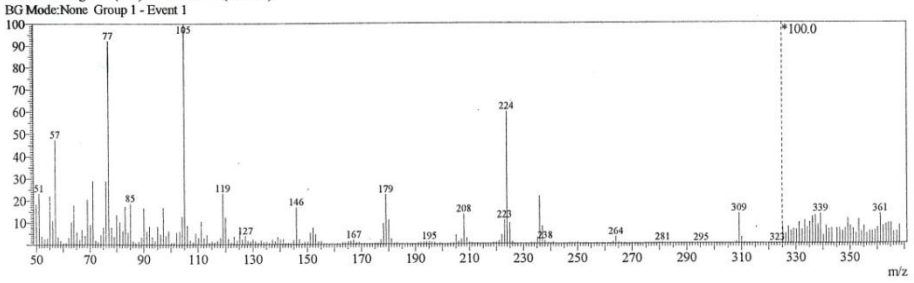
^{13}C NMR spectrum of compound 6



Mass spectrum of compound 6

10-Jun-15 17:17:06

Line#:2 R.Time:3.1(Scan#:377)
MassPeaks:315
RawMode:Single 3.1(377) BasePeak:105(142912)
BG Mode:None Group 1 - Event 1



Mass Table
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MassPeaks:311
RawMode:Single 1.5(179) BasePeak:57(387394)
BG Mode:None Group 1 - Event 1

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1	50.05	7152	1.85	46	95.10	45162	11.66	91	140.25	9214	2.38
2	51.05	10390	2.68	47	96.15	29589	7.64	92	141.20	18833	4.86
3	52.15	2426	0.63	48	97.10	113639	29.33	93	142.20	2393	0.62
4	53.10	8137	2.10	49	98.15	28697	7.41	94	143.15	900	0.23
5	54.15	15807	4.08	50	99.10	64246	16.58	95	144.15	622	0.16
6	55.10	161994	41.82	51	100.10	5327	1.38	96	145.15	2077	0.54
7	56.15	83300	21.50	52	101.15	834	0.22	97	146.10	3825	0.99
8	57.10	387394	100.00	53	102.05	2748	0.71	98	147.10	2052	0.53
9	58.10	19431	5.02	54	103.10	3449	0.89	99	148.15	1336	0.34
10	59.10	1329	0.34	55	104.15	6808	1.76	100	149.10	5761	1.49
11	60.05	991	0.26	56	105.05	52392	13.52	101	150.25	2097	0.54
12	61.05	544	0.14	57	106.05	7185	1.85	102	151.15	7615	1.97
13	62.05	1363	0.35	58	107.10	5914	1.53	103	152.15	6104	1.58
14	63.05	4602	1.19	59	108.15	4387	1.13	104	153.15	9196	2.37
15	64.00	7292	1.88	60	109.10	28191	7.28	105	154.20	6001	1.55
16	65.05	5407	1.40	61	110.15	18228	4.71	106	155.20	12034	3.11
17	66.15	4677	1.21	62	111.15	69829	18.03	107	156.20	1564	0.40
18	67.05	39216	10.12	63	112.25	22284	5.75	108	157.15	604	0.16
19	68.15	23412	6.04	64	113.15	42111	10.87	109	159.15	946	0.24
20	69.05	135862	35.07	65	114.20	4076	1.05	110	160.10	518	0.13
21	70.15	71106	18.35	66	115.10	1644	0.42	111	161.10	1210	0.31
22	71.10	263250	67.95	67	116.15	912	0.24	112	162.15	879	0.23
23	72.05	15212	3.93	68	117.10	2505	0.65	113	163.15	2569	0.66
24	73.05	1575	0.41	69	118.15	2450	0.63	114	164.25	1401	0.36
25	74.05	1995	0.51	70	119.10	17489	4.51	115	165.20	3870	1.00
26	75.05	3287	0.85	71	120.10	4759	1.23	116	166.20	2532	0.65
27	76.05	11426	2.95	72	121.10	5121	1.32	117	167.15	5862	1.51
28	77.05	36455	9.41	73	122.25	3754	0.97	118	168.20	3927	1.01
29	78.15	4650	1.20	74	123.15	17081	4.41	119	169.20	8071	2.08
30	79.10	12076	3.12	75	124.25	11047	2.85	120	170.20	1246	0.32
31	80.15	11853	3.06	76	125.20	35666	9.21	121	171.20	446	0.12
32	81.10	53454	13.80	77	126.25	14711	3.80	122	172.10	260	0.07
33	82.15	35550	9.18	78	127.20	27463	7.09	123	173.10	596	0.15
34	83.10	116854	30.16	79	128.15	4214	1.09	124	175.15	869	0.22
35	84.15	45201	11.67	80	129.15	2034	0.53	125	176.15	677	0.17
36	85.10	189042	48.80	81	130.10	1382	0.36	126	177.15	2344	0.61
37	86.10	12852	3.32	82	131.15	2479	0.64	127	178.15	4357	1.12
38	87.10	1017	0.26	83	132.15	1404	0.36	128	179.05	9950	2.57
39	88.10	724	0.19	84	133.15	3194	0.82	129	180.10	6206	1.60
40	89.15	1662	0.43	85	134.25	1945	0.50	130	181.15	4076	1.05
41	90.05	6728	1.74	86	135.15	4681	1.21	131	182.20	3262	0.84
42	91.10	8815	2.28	87	136.25	2729	0.70	132	183.20	5962	1.54
43	92.10	4929	1.27	88	137.20	10463	2.70	133	184.25	1113	0.29
44	93.10	8972	2.32	89	138.25	6213	1.60	134	185.20	386	0.10
45	94.15	6518	1.68	90	139.20	16047	4.14	135	186.20	234	0.06

2 / 5

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
136	187.15	458	0.12	195	249.25	1141	0.29	254	311.20	337	0.09
137	188.15	338	0.09	196	250.30	1034	0.27	255	312.20	94	0.02
138	189.10	791	0.20	197	251.25	1059	0.27	256	313.20	174	0.04
139	190.25	485	0.13	198	252.30	1194	0.31	257	314.20	119	0.03
140	191.15	2008	0.52	199	253.30	2564	0.66	258	315.20	236	0.06
141	192.10	929	0.24	200	254.25	529	0.14	259	316.20	239	0.06
142	193.15	2297	0.59	201	255.20	206	0.05	260	317.20	305	0.08
143	194.15	1552	0.40	202	256.20	215	0.06	261	318.20	286	0.07
144	195.15	2625	0.68	203	257.20	314	0.08	262	319.35	522	0.13
145	196.20	2697	0.70	204	258.20	246	0.06	263	320.30	518	0.13
146	197.20	5060	1.31	205	259.30	489	0.13	264	321.30	474	0.12
147	198.20	897	0.23	206	261.30	620	0.16	265	322.35	635	0.16
148	199.20	239	0.06	207	262.25	474	0.12	266	323.35	1035	0.27
149	200.20	150	0.04	208	263.25	1241	0.32	267	324.30	268	0.07
150	201.20	255	0.07	209	264.15	2027	0.52	268	325.30	135	0.03
151	203.15	764	0.20	210	265.25	1281	0.33	269	326.30	102	0.03
152	204.15	513	0.13	211	266.25	1274	0.33	270	327.30	140	0.04
153	205.05	2990	0.77	212	267.30	2017	0.52	271	328.30	137	0.04
154	206.05	893	0.23	213	268.40	500	0.13	272	329.30	175	0.05
155	207.15	2635	0.68	214	269.10	218	0.06	273	330.30	196	0.05
156	208.05	7559	1.95	215	270.15	449	0.12	274	331.30	295	0.08
157	209.10	2932	0.76	216	271.10	359	0.09	275	332.30	218	0.06
158	210.15	2283	0.59	217	272.10	322	0.08	276	333.35	523	0.14
159	211.20	3889	1.00	218	273.10	386	0.10	277	334.40	415	0.11
160	212.15	771	0.20	219	274.10	217	0.06	278	335.45	394	0.10
161	213.20	247	0.06	220	275.30	447	0.12	279	336.45	727	0.19
162	214.20	135	0.03	221	276.30	314	0.08	280	337.45	1051	0.27
163	215.20	282	0.07	222	277.30	574	0.15	281	338.35	475	0.12
164	217.15	752	0.19	223	278.30	674	0.17	282	339.40	121	0.03
165	218.15	533	0.14	224	279.35	800	0.21	283	340.40	105	0.03
166	219.15	1291	0.33	225	280.30	1097	0.28	284	341.40	145	0.04
167	220.20	775	0.20	226	281.30	1834	0.47	285	342.40	170	0.04
168	221.20	1759	0.45	227	282.25	410	0.11	286	343.40	193	0.05
169	222.15	2914	0.75	228	283.30	193	0.05	287	344.40	193	0.05
170	223.15	2994	0.77	229	284.30	161	0.04	288	345.40	204	0.05
171	224.15	3611	0.93	230	285.30	178	0.05	289	346.40	177	0.05
172	225.20	3799	0.98	231	286.30	116	0.03	290	347.35	452	0.12
173	226.25	717	0.19	232	287.30	308	0.08	291	348.40	478	0.12
174	227.30	199	0.05	233	288.30	202	0.05	292	349.20	348	0.09
175	228.30	113	0.03	234	289.20	465	0.12	293	350.35	752	0.19
176	229.30	273	0.07	235	291.35	525	0.14	294	351.40	1138	0.29
177	231.20	630	0.16	236	292.35	534	0.14	295	352.45	439	0.11
178	232.20	460	0.12	237	293.35	617	0.16	296	353.40	262	0.07
179	233.15	960	0.25	238	294.35	949	0.24	297	354.40	126	0.03
180	234.05	650	0.17	239	295.40	1422	0.37	298	355.40	146	0.04
181	235.05	2147	0.55	240	296.40	374	0.10	299	356.40	114	0.03
182	236.05	11265	2.91	241	297.40	161	0.04	300	357.40	193	0.05
183	237.05	4976	1.28	242	298.40	134	0.03	301	358.40	188	0.05
184	238.25	2034	0.53	243	299.40	132	0.03	302	359.40	295	0.08
185	239.25	3146	0.81	244	300.40	129	0.03	303	360.40	177	0.05
186	240.15	821	0.21	245	301.40	217	0.06	304	361.40	406	0.10
187	241.05	4109	1.06	246	302.40	190	0.05	305	362.40	390	0.10
188	242.10	801	0.21	247	303.40	359	0.09	306	363.45	366	0.09
189	243.15	385	0.10	248	305.25	548	0.14	307	364.40	729	0.19
190	244.20	244	0.06	249	306.25	493	0.13	308	365.35	1066	0.28
191	245.20	610	0.16	250	307.25	506	0.13	309	366.40	409	0.11
192	246.25	484	0.12	251	308.25	1230	0.32	310	367.40	178	0.05
193	247.25	818	0.21	252	309.15	7388	1.91	311	368.40	71	0.02
194	248.25	505	0.13	253	310.15	1562	0.40				

Line#:2 R.Time:3.1(Scan#:377)
MassPeaks:315
RawMode:Single 3.1(377) BasePeak:105(142912)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	26115	18.27	5	54.15	4243	2.97	9	58.10	5074	3.55
2	51.05	33101	23.16	6	55.10	31598	22.11	10	59.05	2557	1.79
3	52.05	5456	3.82	7	56.15	15548	10.88	11	60.05	1090	0.76
4	53.05	3566	2.50	8	57.10	67569	47.28	12	61.05	1213	0.85

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
13	62.05	4547	3.18	82	131.10	2260	1.58	151	200.10	114	0.08
14	63.05	14800	10.36	83	132.15	1197	0.84	152	201.10	191	0.13
15	64.00	25409	17.78	84	133.10	2730	1.91	153	202.10	204	0.14
16	65.05	8177	5.72	85	134.10	1454	1.02	154	203.10	402	0.28
17	66.15	3146	2.20	86	135.15	2009	1.41	155	204.15	619	0.43
18	67.05	9732	6.81	87	136.25	995	0.70	156	205.05	5875	4.11
19	68.15	5850	4.09	88	137.20	3282	2.30	157	206.05	1646	1.15
20	69.05	29277	20.49	89	138.25	1982	1.39	158	207.05	3113	2.18
21	70.15	13062	9.14	90	139.20	4879	3.41	159	208.05	19253	13.47
22	71.10	41284	28.89	91	140.15	3323	2.33	160	209.00	3788	2.65
23	72.10	2729	1.91	92	141.20	3303	2.31	161	210.05	996	0.70
24	73.05	1747	1.22	93	142.15	705	0.49	162	211.05	784	0.55
25	74.05	6313	4.42	94	143.05	836	0.58	163	212.00	196	0.14
26	75.05	11241	7.87	95	144.05	718	0.50	164	213.00	374	0.26
27	76.05	41322	28.91	96	145.05	2750	1.92	165	214.00	190	0.13
28	77.05	131527	92.03	97	146.05	24049	16.83	166	215.00	233	0.16
29	78.05	11274	7.89	98	147.10	3394	2.37	167	216.00	121	0.08
30	79.05	5149	3.60	99	148.15	670	0.47	168	217.00	257	0.18
31	80.00	19450	13.61	100	149.10	1562	1.09	169	219.05	762	0.53
32	81.10	14729	10.31	101	150.15	1653	1.16	170	220.05	842	0.59
33	82.15	8898	6.23	102	151.10	7540	5.28	171	221.05	1753	1.23
34	83.10	24622	17.23	103	152.10	10946	7.66	172	222.05	5997	4.20
35	84.15	7879	5.51	104	153.10	6588	4.61	173	223.05	15557	10.89
36	85.10	26585	18.60	105	154.10	1945	1.36	174	224.05	85296	59.68
37	86.10	2265	1.58	106	155.15	1890	1.32	175	225.00	13751	9.62
38	87.05	1307	0.91	107	156.15	532	0.37	176	226.00	1567	1.10
39	88.10	1937	1.36	108	157.15	526	0.37	177	227.00	310	0.22
40	89.15	4835	3.38	109	158.10	246	0.17	178	228.00	118	0.08
41	90.05	23762	16.63	110	159.10	734	0.51	179	229.00	231	0.16
42	91.10	8593	6.01	111	160.15	330	0.23	180	230.00	129	0.09
43	92.10	11930	8.35	112	161.15	821	0.57	181	231.00	231	0.16
44	93.10	4966	3.47	113	162.10	503	0.35	182	233.00	794	0.56
45	94.15	2371	1.66	114	163.15	1132	0.79	183	234.15	669	0.47
46	95.10	11774	8.24	115	164.10	975	0.68	184	235.15	4212	2.95
47	96.15	6818	4.77	116	165.15	1864	1.30	185	236.05	31091	21.76
48	97.15	23981	16.78	117	166.10	2070	1.45	186	237.05	11484	8.04
49	98.10	5902	4.13	118	167.10	2666	1.87	187	238.10	1974	1.38
50	99.10	8910	6.23	119	168.15	1052	0.74	188	239.20	788	0.55
51	100.10	1262	0.88	120	169.15	1264	0.88	189	240.15	381	0.27
52	101.15	1241	0.87	121	170.05	391	0.27	190	241.10	1052	0.74
53	102.05	7760	5.43	122	171.10	580	0.41	191	242.10	332	0.23
54	103.15	8557	5.99	123	172.10	242	0.17	192	243.10	146	0.10
55	104.15	18330	12.83	124	173.00	458	0.32	193	244.10	164	0.11
56	105.05	142912	100.00	125	174.00	230	0.16	194	245.10	297	0.21
57	106.05	12449	8.71	126	175.15	683	0.48	195	246.15	358	0.25
58	107.10	2902	2.03	127	176.15	778	0.54	196	247.10	956	0.67
59	108.15	1531	1.07	128	177.15	3006	2.10	197	248.15	611	0.43
60	109.10	7398	5.18	129	178.15	13582	9.50	198	249.15	625	0.44
61	110.15	4338	3.04	130	179.05	32090	22.45	199	250.10	1031	0.72
62	111.15	15093	10.56	131	180.05	15852	11.09	200	251.20	434	0.30
63	112.15	4188	2.93	132	181.10	3494	2.44	201	252.35	330	0.23
64	113.15	6358	4.45	133	182.20	817	0.57	202	253.30	489	0.34
65	114.15	1175	0.82	134	183.20	1004	0.70	203	254.30	114	0.08
66	115.10	1950	1.36	135	184.15	370	0.26	204	255.30	199	0.14
67	116.10	1356	0.95	136	185.05	436	0.31	205	256.30	167	0.12
68	117.10	2450	1.71	137	186.00	178	0.12	206	257.30	358	0.25
69	118.15	4249	2.97	138	186.90	383	0.27	207	258.30	193	0.14
70	119.10	33103	23.16	139	187.90	228	0.16	208	259.30	263	0.18
71	120.05	17757	12.43	140	188.90	289	0.20	209	260.30	188	0.13
72	121.10	3754	2.63	141	190.10	354	0.25	210	261.30	351	0.25
73	122.15	1376	0.96	142	191.10	743	0.52	211	262.15	346	0.24
74	123.15	5032	3.52	143	192.05	879	0.62	212	263.15	1315	0.92
75	124.25	2589	1.81	144	193.10	1292	0.90	213	264.10	4529	3.17
76	125.20	8402	5.88	145	194.05	1168	0.82	214	265.10	1086	0.76
77	126.20	3489	2.44	146	195.10	1575	1.10	215	266.10	324	0.23
78	127.20	5602	3.92	147	196.10	1170	0.82	216	267.30	476	0.33
79	128.15	2469	1.73	148	197.15	962	0.67	217	268.30	73	0.05
80	129.15	1852	1.30	149	198.10	209	0.15	218	269.00	186	0.13
81	130.10	3366	2.36	150	199.10	236	0.17	219	270.05	424	0.30

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
220	271.00	222	0.16	252	303.20	121	0.08	284	336.20	175	0.12
221	272.00	180	0.13	253	304.20	92	0.06	285	337.20	182	0.13
222	273.00	198	0.14	254	305.20	170	0.12	286	338.20	121	0.08
223	274.00	183	0.13	255	306.20	170	0.12	287	339.20	191	0.13
224	275.00	174	0.12	256	308.15	1127	0.79	288	340.20	52	0.04
225	276.00	113	0.08	257	309.15	19383	13.56	289	341.20	114	0.08
226	277.00	185	0.13	258	310.10	4092	2.86	290	342.20	92	0.06
227	278.00	228	0.16	259	311.20	596	0.42	291	343.20	100	0.07
228	279.00	212	0.15	260	312.20	127	0.09	292	345.20	97	0.07
229	280.25	414	0.29	261	313.20	140	0.10	293	346.20	97	0.07
230	281.20	663	0.46	262	314.20	63	0.04	294	347.20	79	0.06
231	282.20	167	0.12	263	315.20	84	0.06	295	348.20	97	0.07
232	283.20	94	0.07	264	316.20	114	0.08	296	349.20	162	0.11
233	284.20	97	0.07	265	317.20	151	0.11	297	350.20	114	0.08
234	285.20	162	0.11	266	318.20	116	0.08	298	351.20	94	0.07
235	286.20	132	0.09	267	319.20	127	0.09	299	352.20	66	0.05
236	287.20	89	0.06	268	320.20	129	0.09	300	353.20	156	0.11
237	288.20	156	0.11	269	321.20	182	0.13	301	354.20	78	0.05
238	289.20	186	0.13	270	322.20	110	0.08	302	355.20	114	0.08
239	290.20	148	0.10	271	323.20	217	0.15	303	356.20	65	0.05
240	291.20	196	0.14	272	324.20	66	0.05	304	357.20	79	0.06
241	292.20	178	0.12	273	325.20	113	0.08	305	358.20	78	0.05
242	293.20	135	0.09	274	326.20	63	0.04	306	359.20	84	0.06
243	294.20	174	0.12	275	327.20	108	0.08	307	360.20	103	0.07
244	295.20	231	0.16	276	328.20	79	0.06	308	361.20	191	0.13
245	296.20	153	0.11	277	329.20	94	0.07	309	362.20	113	0.08
246	297.20	153	0.11	278	330.20	90	0.06	310	363.20	124	0.09
247	298.20	127	0.09	279	331.20	134	0.09	311	364.20	132	0.09
248	299.20	134	0.09	280	332.20	89	0.06	312	365.20	132	0.09
249	300.20	119	0.08	281	333.20	148	0.10	313	366.20	73	0.05
250	301.20	145	0.10	282	334.20	103	0.07	314	367.20	76	0.05
251	302.20	126	0.09	283	335.20	138	0.10	315	368.20	116	0.08