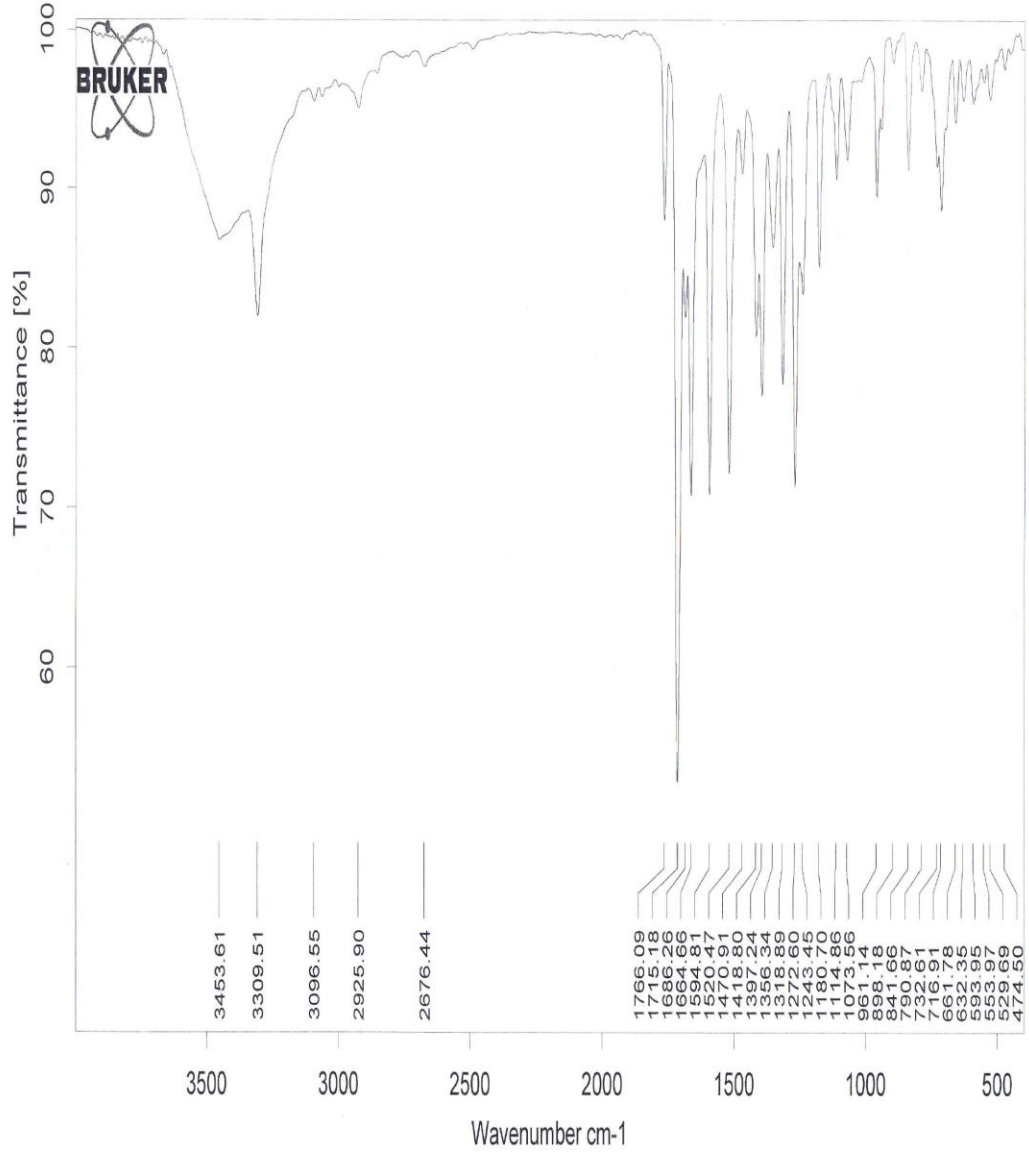
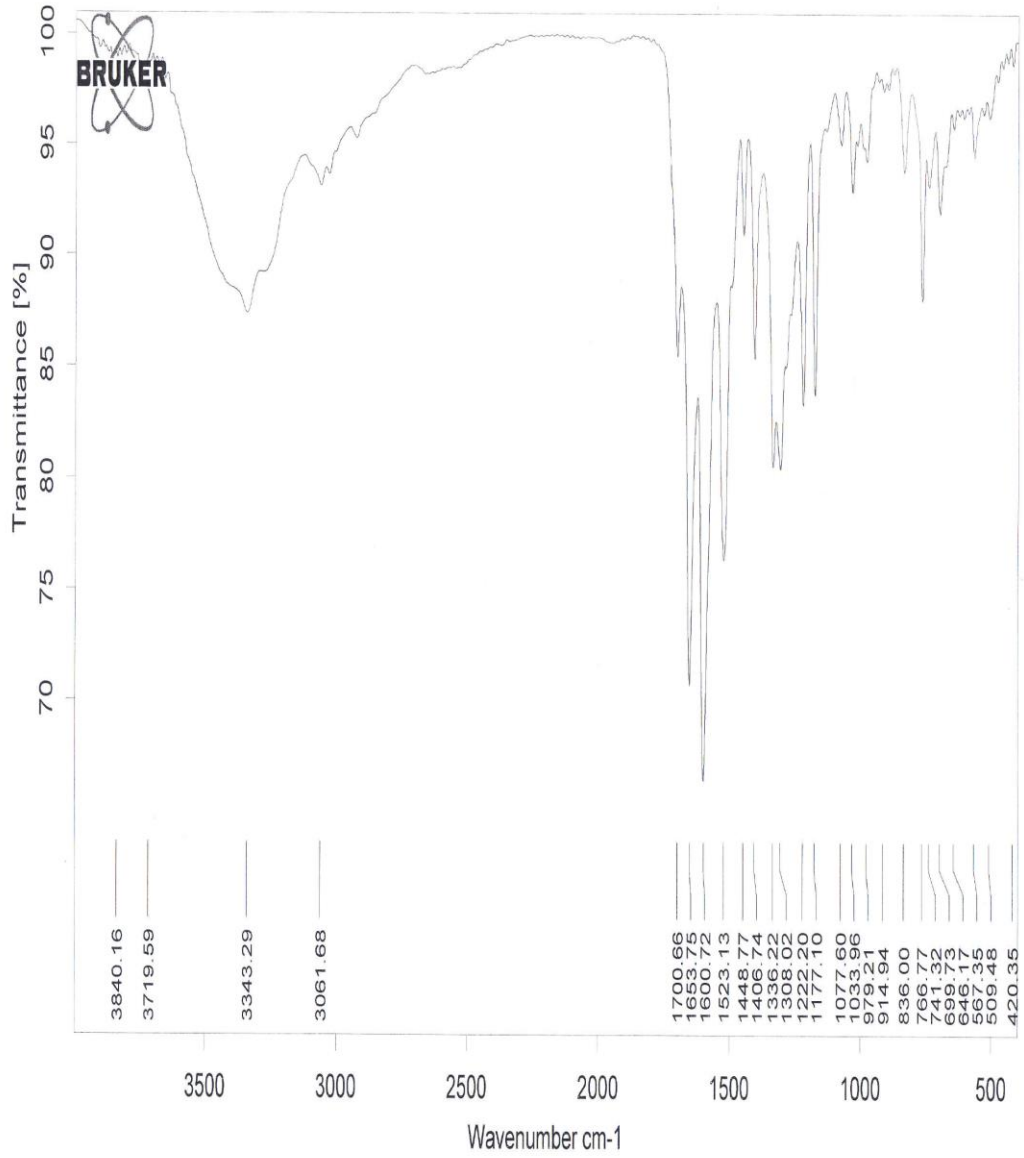


**Supplementary Data:**

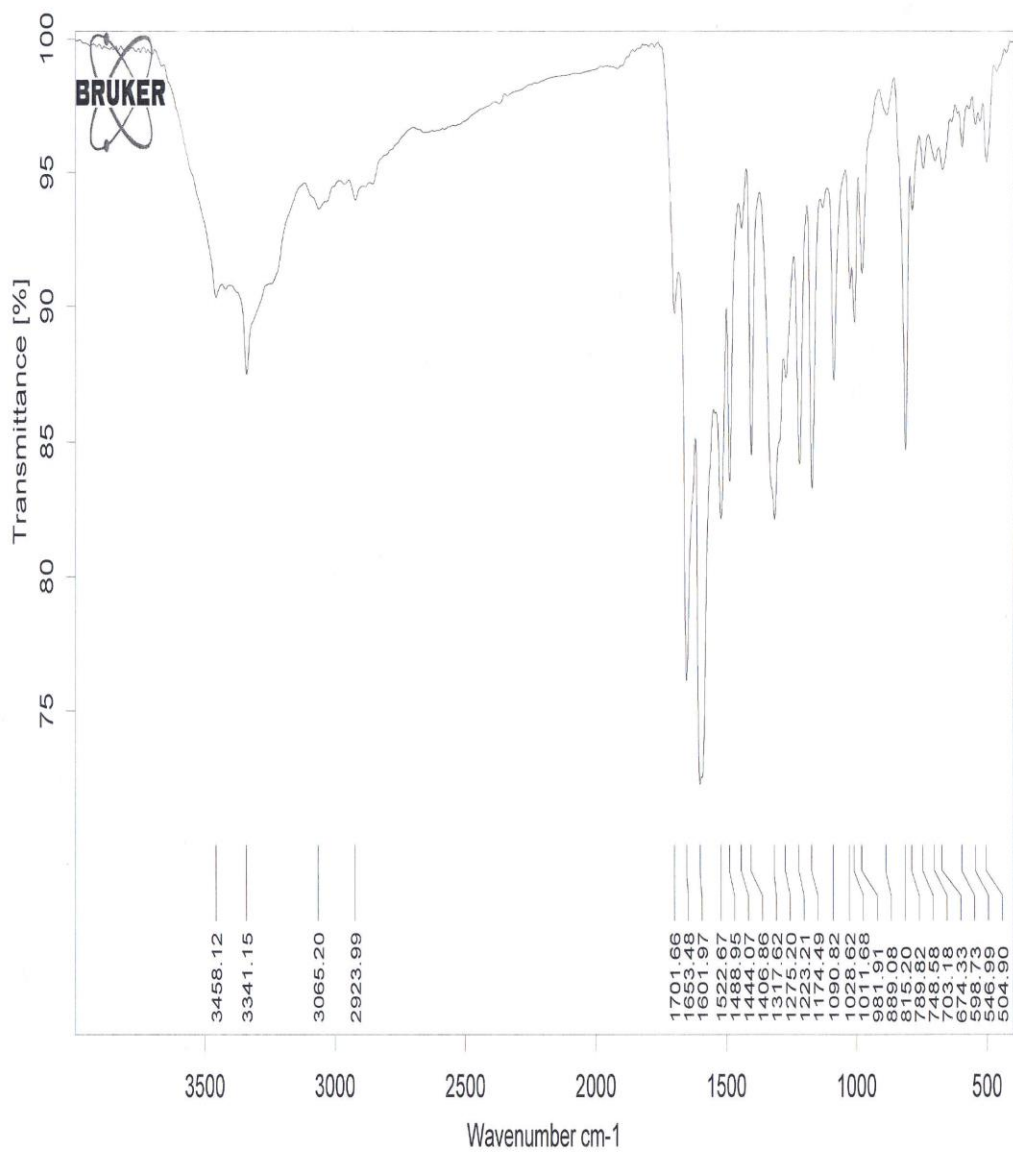
**IR spectroscopy:**



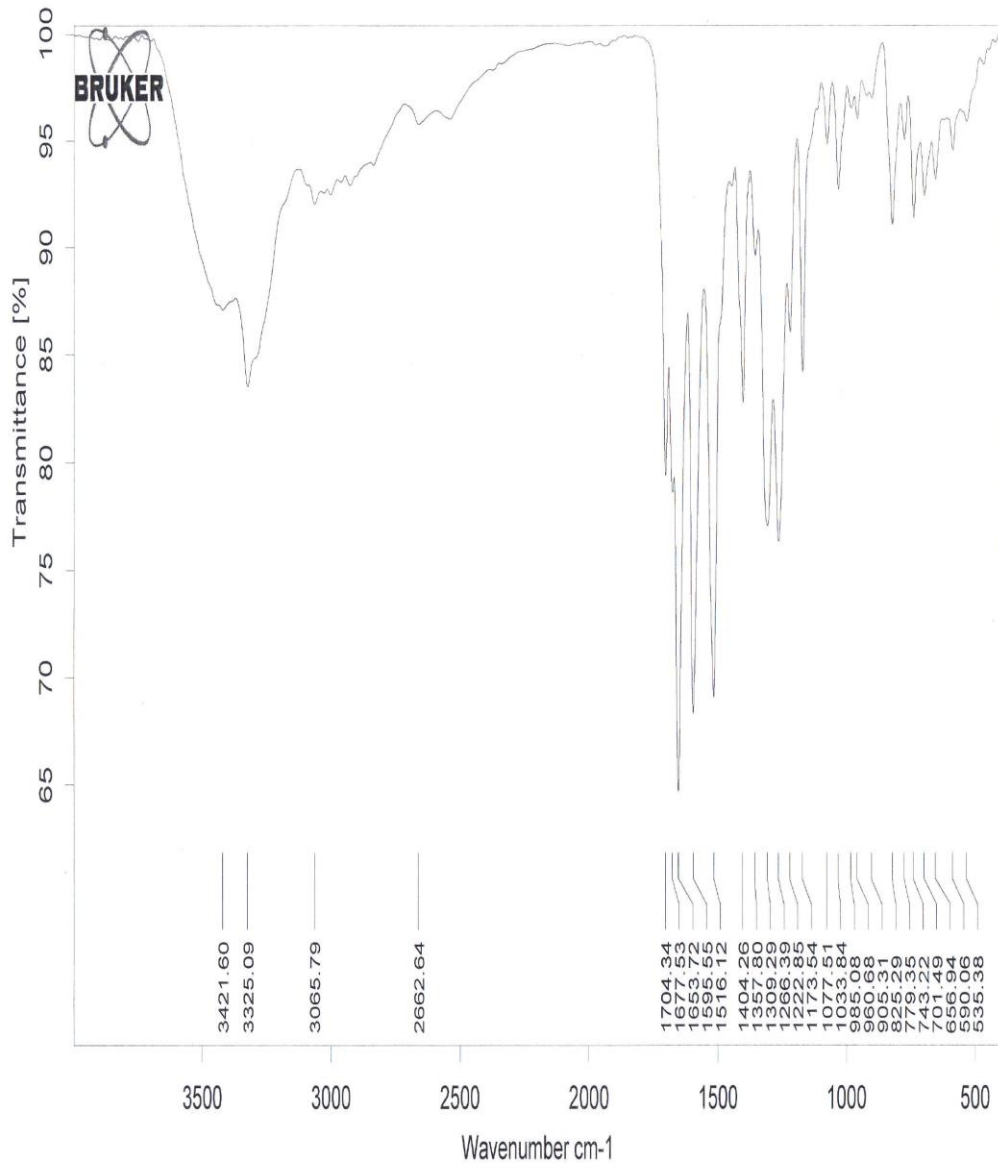
|                                       |   |                    |            |
|---------------------------------------|---|--------------------|------------|
| C:\Program Files\OPUS_65\MEAS\IMA 8.0 | 6 | Sample Compartment | 05/12/2018 |
|---------------------------------------|---|--------------------|------------|




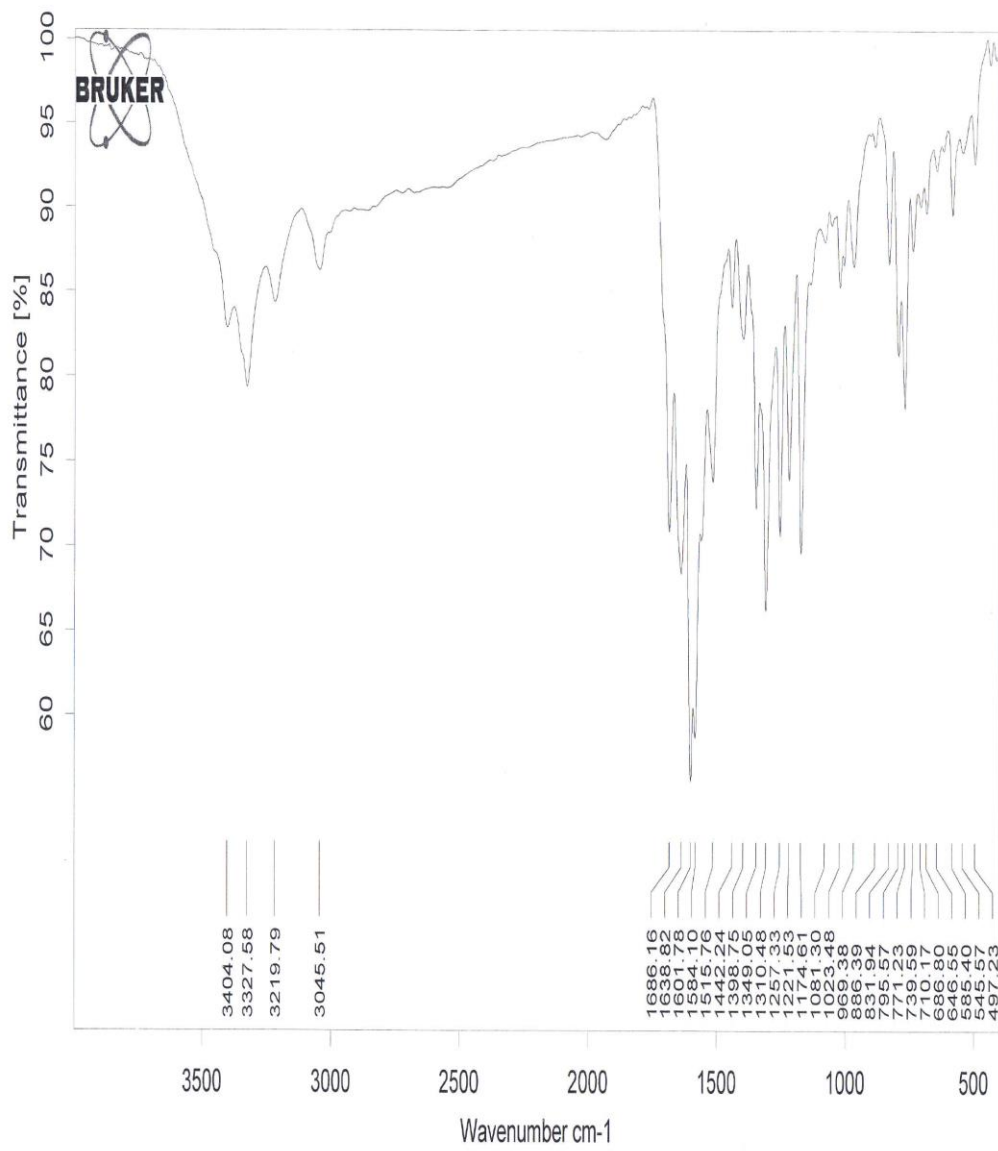
|                                       |    |                    |            |
|---------------------------------------|----|--------------------|------------|
| C:\Program Files\OPUS_65\MEAS\AM 11.0 | 7a | Sample Compartment | 12/12/2018 |
|---------------------------------------|----|--------------------|------------|



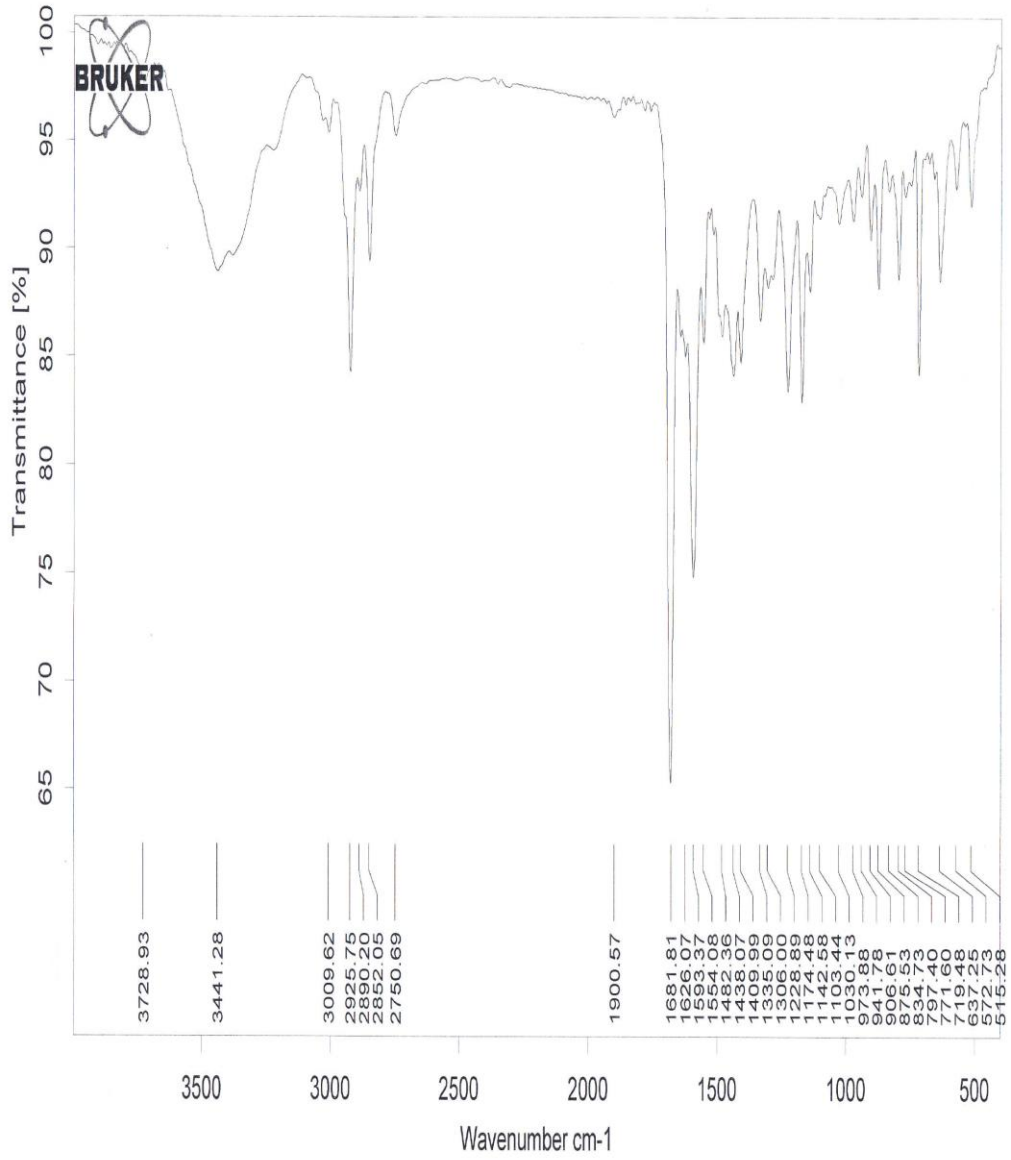
|                                      |                       |            |
|--------------------------------------|-----------------------|------------|
| C:\Program Files\OPUS_65\MEASIMA 9.0 | 7b Sample Compartment | 05/12/2018 |
|--------------------------------------|-----------------------|------------|



|  |   |            |
|--|---|------------|
| C:\Program Files\OPUS_65\MEAS\IMA 10.0 |  7c Sample Compartment | 05/12/2018 |
|--|---|------------|



|                                       |    |                    |            |
|---------------------------------------|----|--------------------|------------|
| C:\Program Files\OPUS_65\MEAS\AM 12.0 | 7d | Sample Compartment | 12/12/2018 |
|---------------------------------------|----|--------------------|------------|

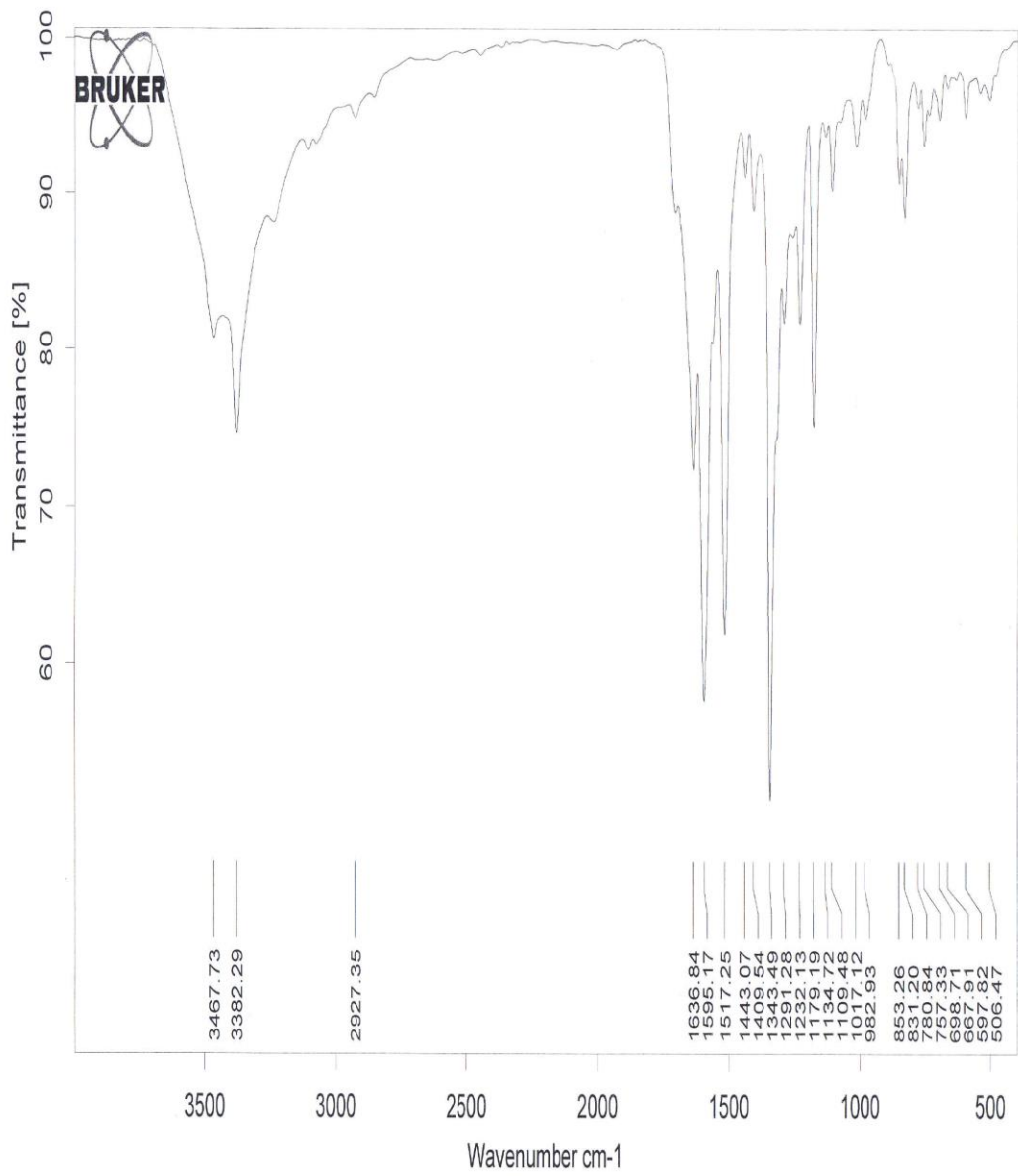


C:\Program Files\OPUS\_65\MEAS\AM 13.0

7c

Sample Compartment

12/12/2018

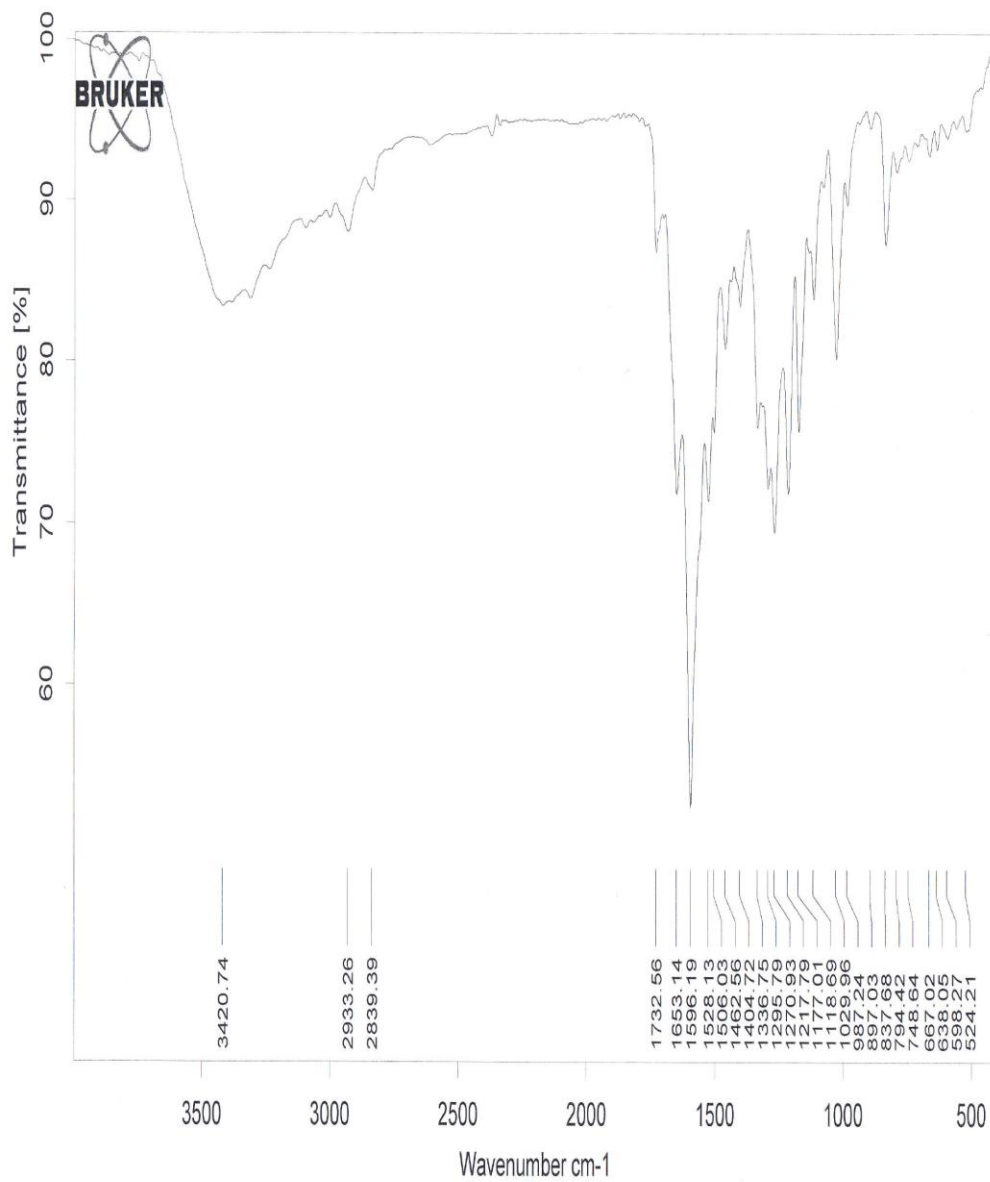


C:\Program Files\OPUS\_65\MEAS\AM 14.0

7f

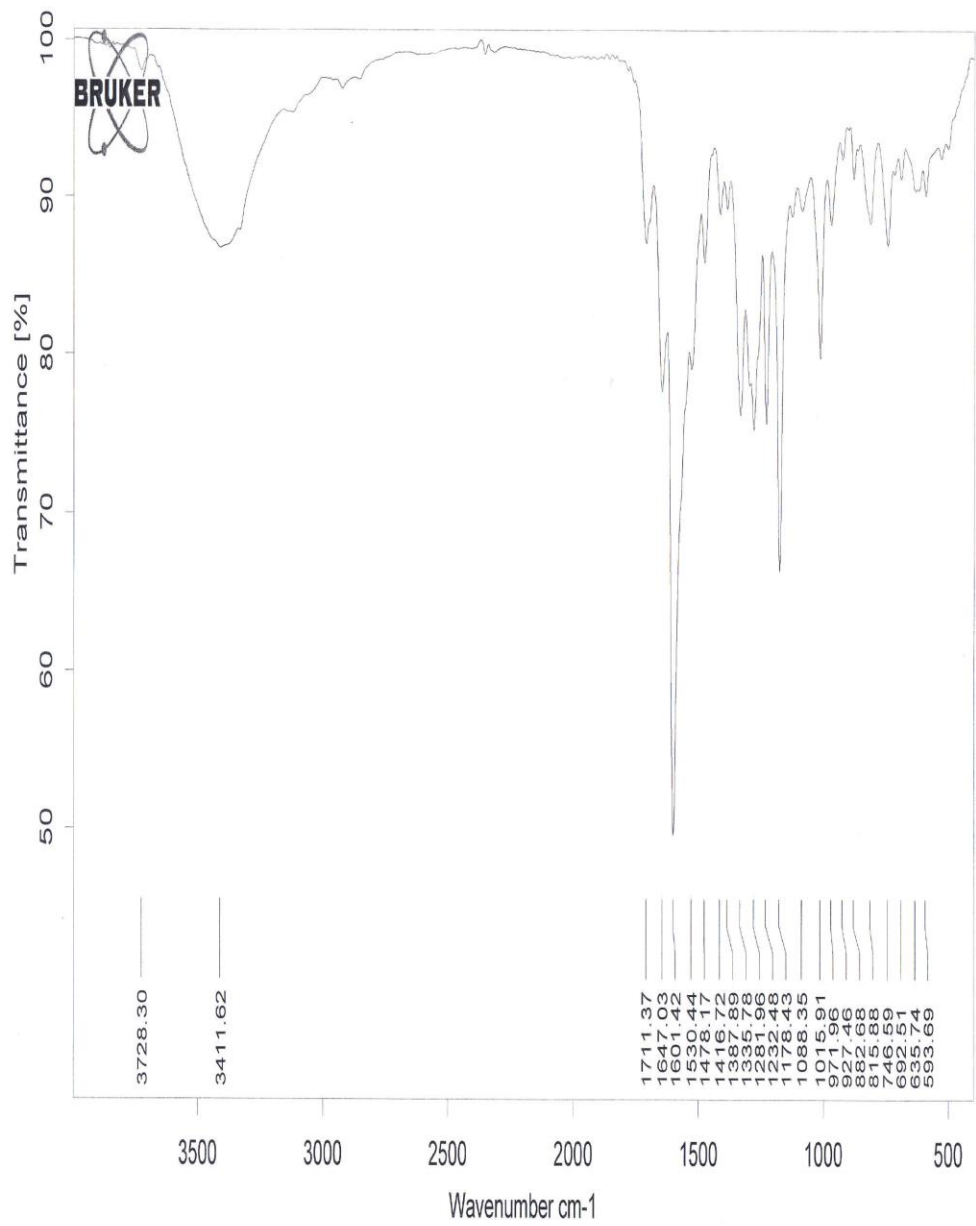
Sample Compartment

12/12/2018

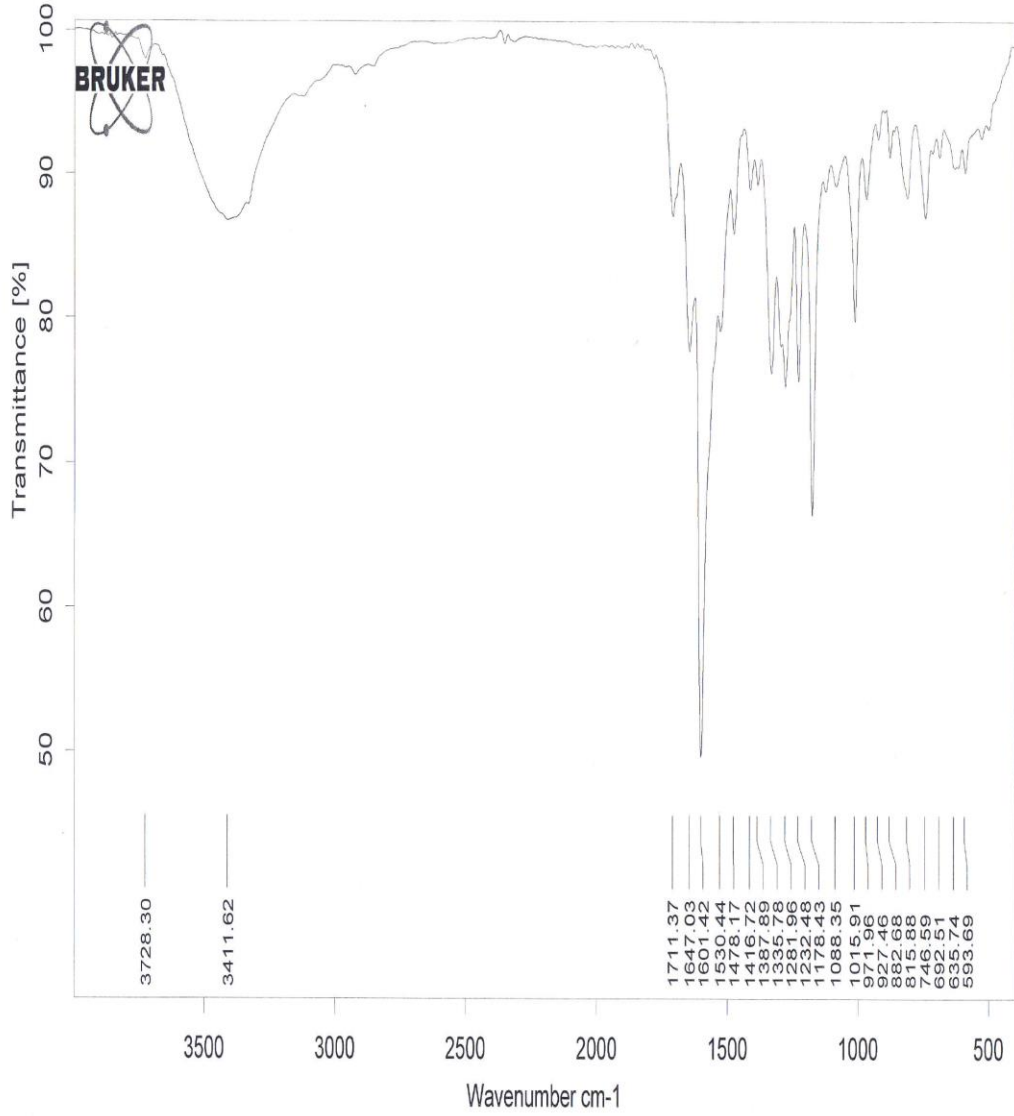


|                                       |    |                    |            |
|---------------------------------------|----|--------------------|------------|
| C:\Program Files\OPUS_65\MEAS\AM 15.0 | 7g | Sample Compartment | 12/12/2018 |
|---------------------------------------|----|--------------------|------------|





|                                       |    |                    |            |
|---------------------------------------|----|--------------------|------------|
| C:\Program Files\OPUS_65\MEAS\AM 16.0 | 7h | Sample Compartment | 12/12/2018 |
|---------------------------------------|----|--------------------|------------|

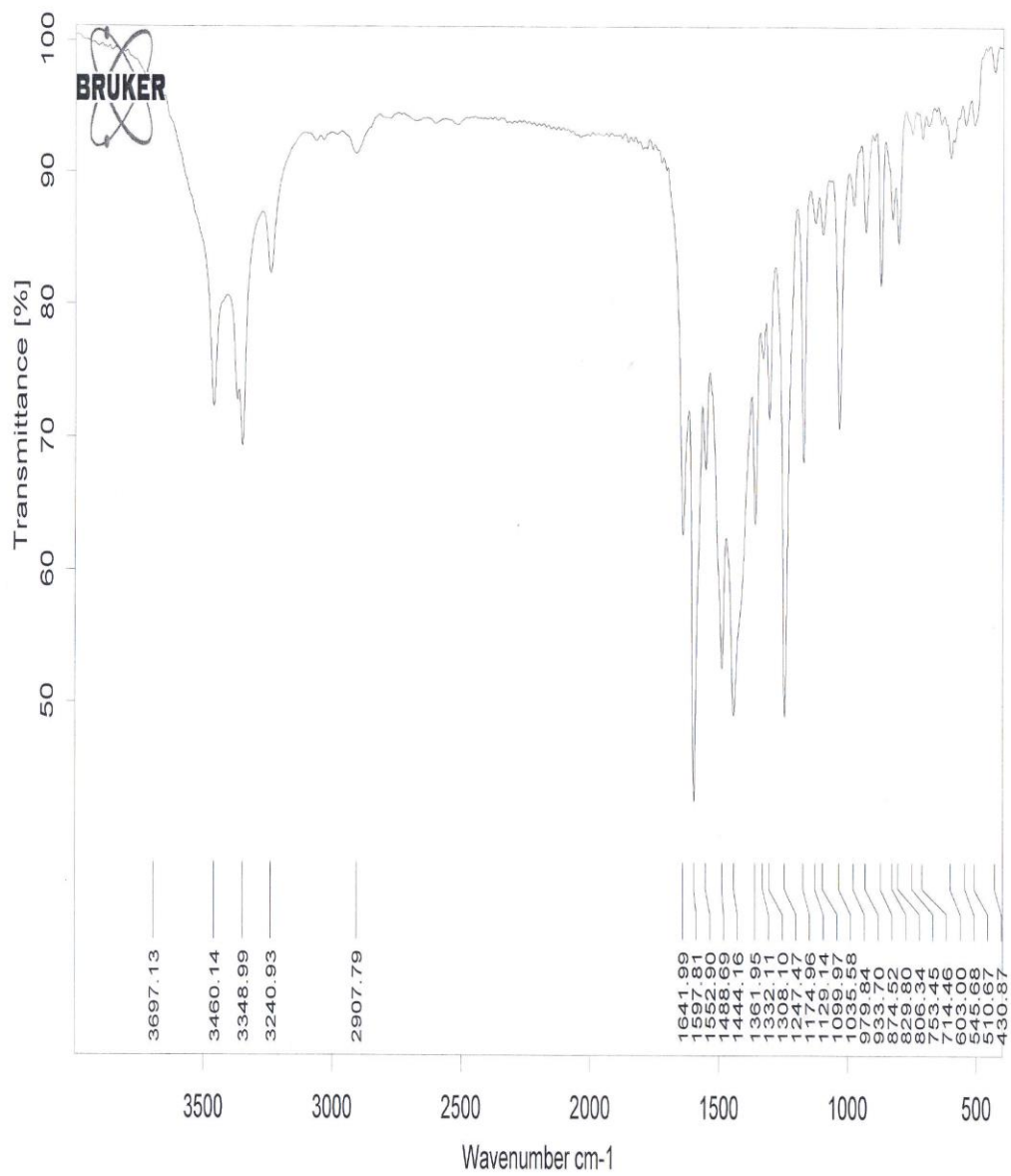


C:\Program Files\OPUS\_65\MEAS\AM 16.0

7h

Sample Compartment

12/12/2018

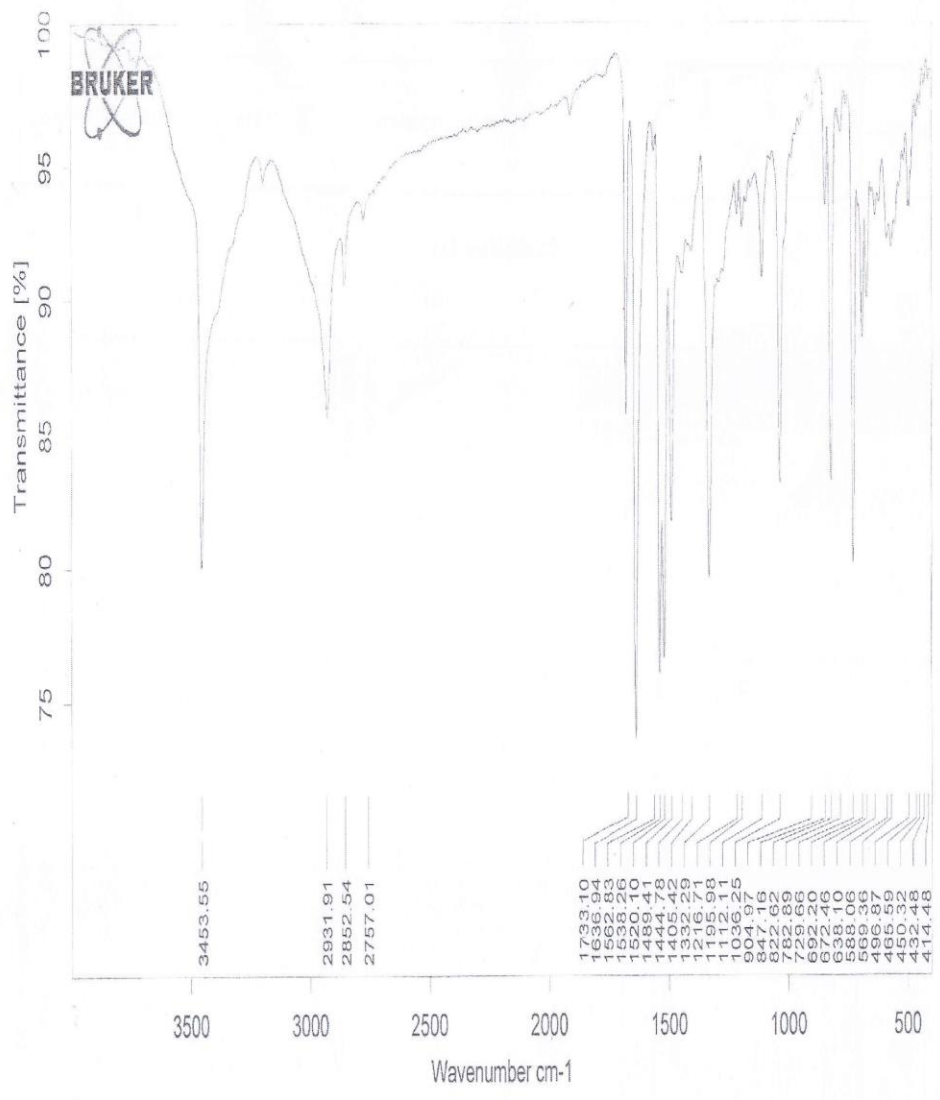


C:\Program Files\OPUS\_65\MEAS\AM 17.0

7i

Sample Compartment

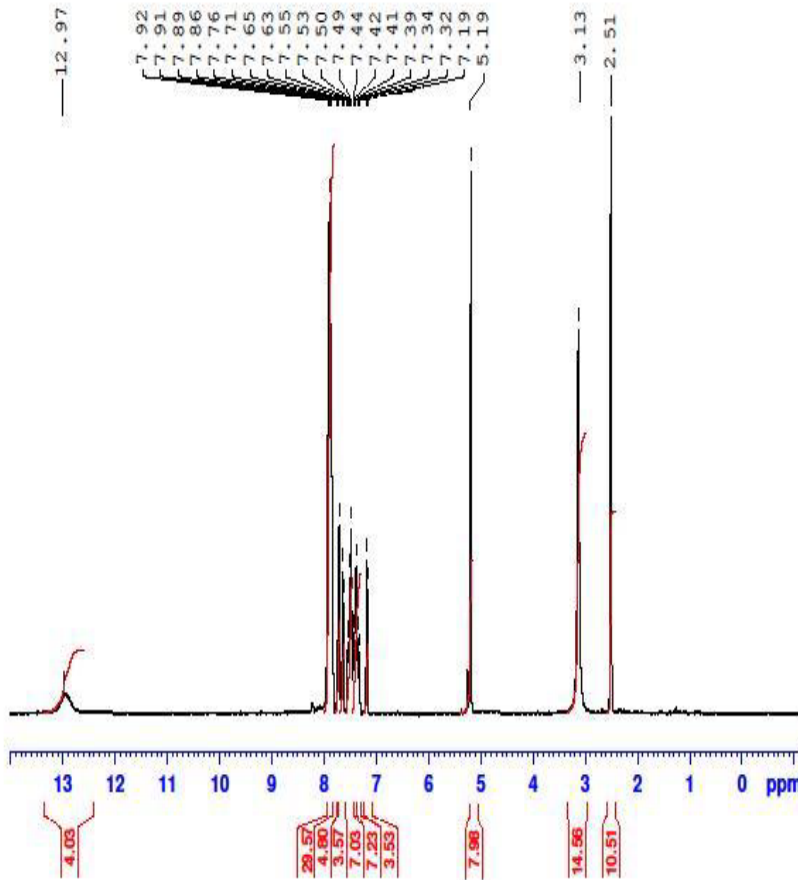
12/12/2018



|                                     |    |                    |            |
|-------------------------------------|----|--------------------|------------|
| C:\Program Files\OPUS_65\MEAS\AM16S | 7j | Sample Compartment | 14/05/2019 |
|-------------------------------------|----|--------------------|------------|

# <sup>1</sup>H NMR:

MA-6  
proton\_su DMSO (C:\nmr-data) Student 15



Current Data Parameters  
NAME Dec10-2018  
EXPNO 150  
PROCNO 1

F2 - Acquisition Parameters  
Data\_ 20181210  
Time 11.42  
INSTRUM spect  
PROBHD 5 mm PARBO HB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 25  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 199.04  
DW 62.400 usec  
DE 6.50 usec  
TE 333.2 K  
D1 1.00000000 sec  
TDO 1

----- CHANNEL f1 -----  
SF01 400.1324710 MHz  
NUC1 1H  
P1 12.00 usec  
P1M1 22.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

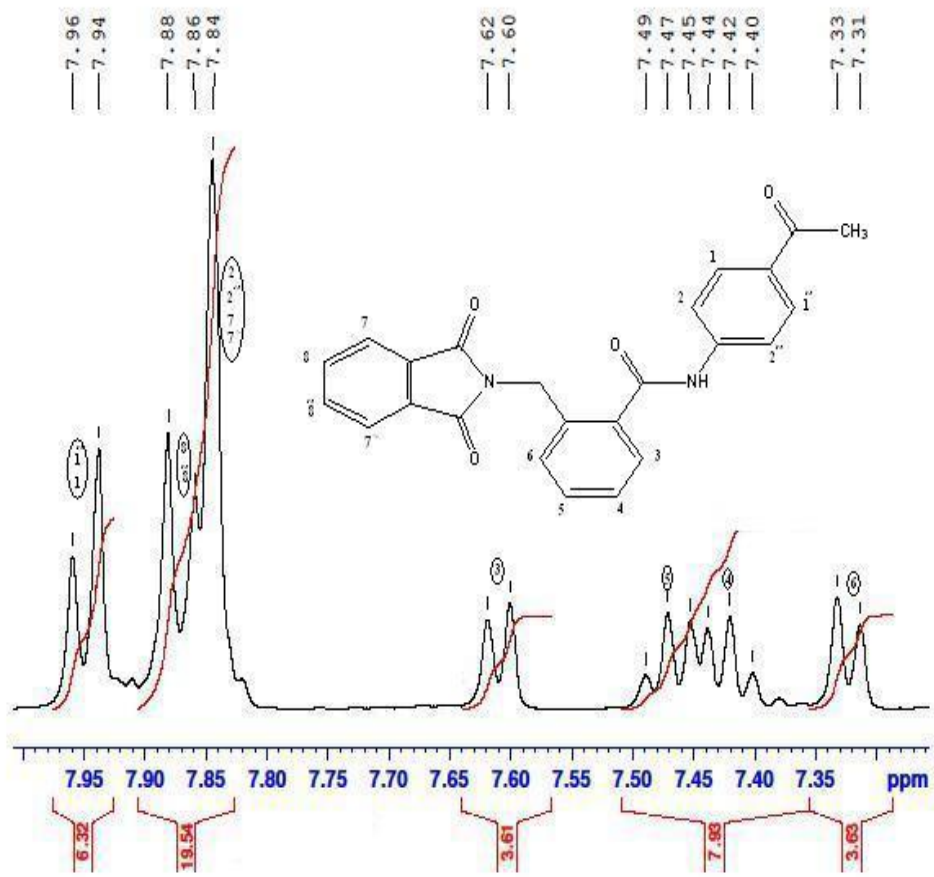
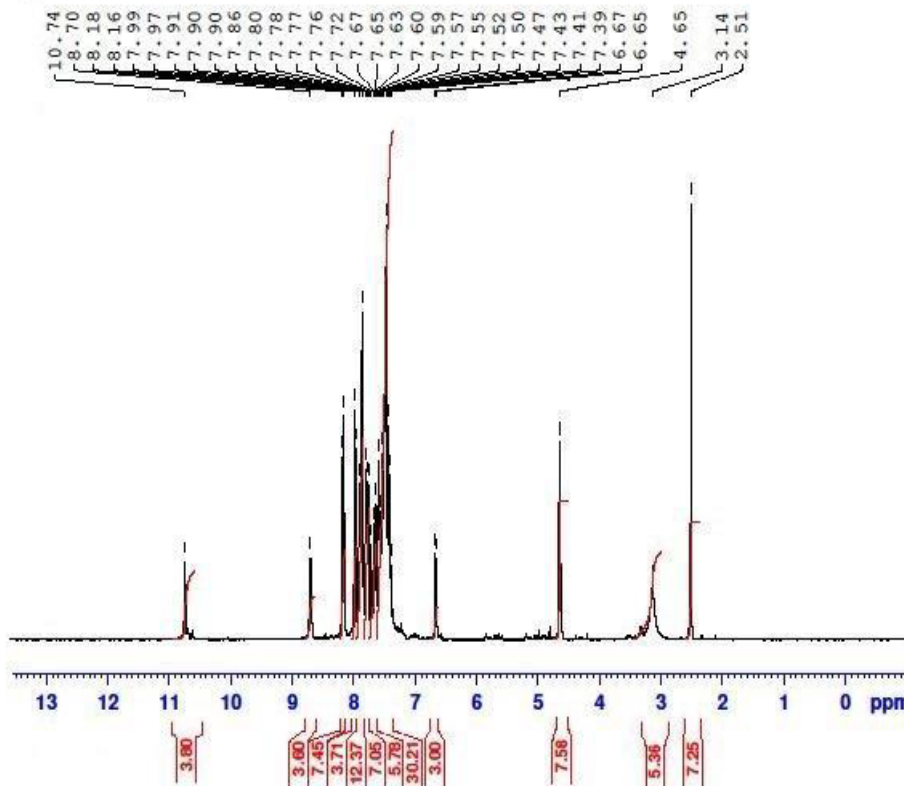


Fig. : Assignment of the aromatic protons in the  $^1\text{H}$  NMR for compound 6

AM-7a  
 proton\_su DMSO (C:\nmr-data) Student 5



```

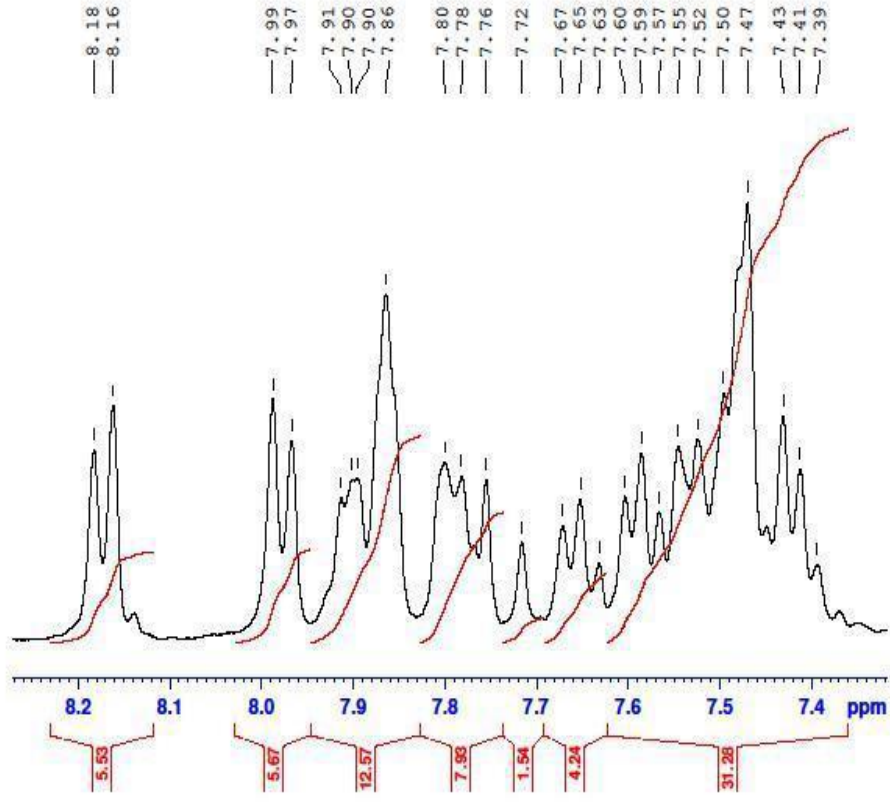
Current Data Parameters
NAME      Dacl0-2018
EXPNO    40
PROCNO   1

F2 - Acquisition Parameters
Date_    20181210
Time     10.44
INSTRUM  spect
PROBHD   5 mm PASBO BB/
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       25
DS       2
SWH      8012.820 Hz
FIDRES   0.122264 Hz
AQ       4.0894465 sec
RG       199.04
DW       62.400 usec
DE       6.50 usec
TE       333.2 K
D1       1.00000000 sec
TD0      1

----- CHANNEL f1 -----
SF01    400.1324710 MHz
NUC1     1H
P1       12.00 usec
P1M1    22.00000000 W

F2 - Processing parameters
SI       65536
SF       400.1300000 MHz
WEM      SM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```

AM-7a  
 proton\_su DMSO (C:\nmr-data) Student 5



8.18  
 8.16  
 7.99  
 7.97  
 7.91  
 7.90  
 7.90  
 7.86  
 7.80  
 7.78  
 7.76  
 7.72  
 7.67  
 7.65  
 7.63  
 7.60  
 7.59  
 7.57  
 7.55  
 7.52  
 7.50  
 7.47  
 7.43  
 7.41  
 7.39

```

Current Data Parameters
NAME      Dec10-2018
EXPNO    40
PROCNO   1

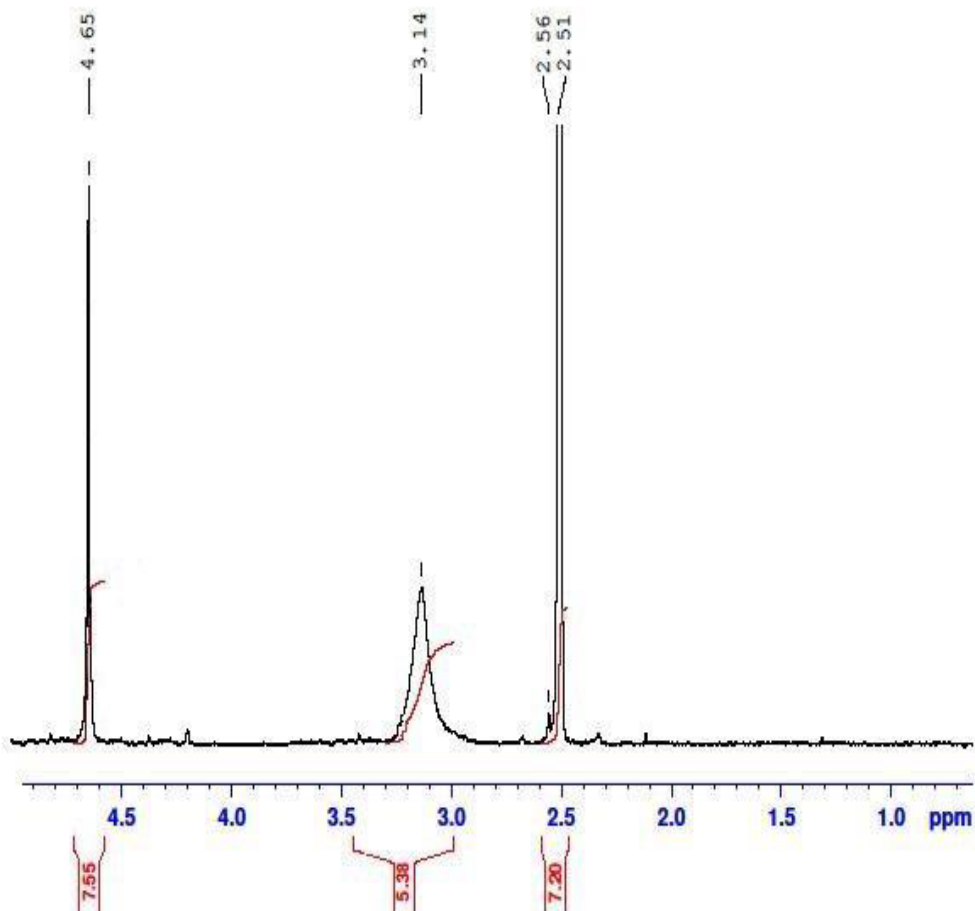
F2 - Acquisition Parameters
Date_    20181210
Time     10.44
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       25
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894465 sec
RG       199.04
DW       62.400 usec
DE       6.50 usec
TE       333.2 K
D1       1.00000000 sec
TD0      1

----- CHANNEL f1 -----
SF01    400.1324710 MHz
NUC1     1H
P1      12.00 usec
PLW1    22.00000000 W

F2 - Processing parameters
SI      65536
SF      400.1300000 MHz
WVW     RM
SSB     0
LB      0.30 Hz
CB      0
PC      1.00
  
```



AM-7a  
proton\_su DMSO (C:\nmr-data) Student 5



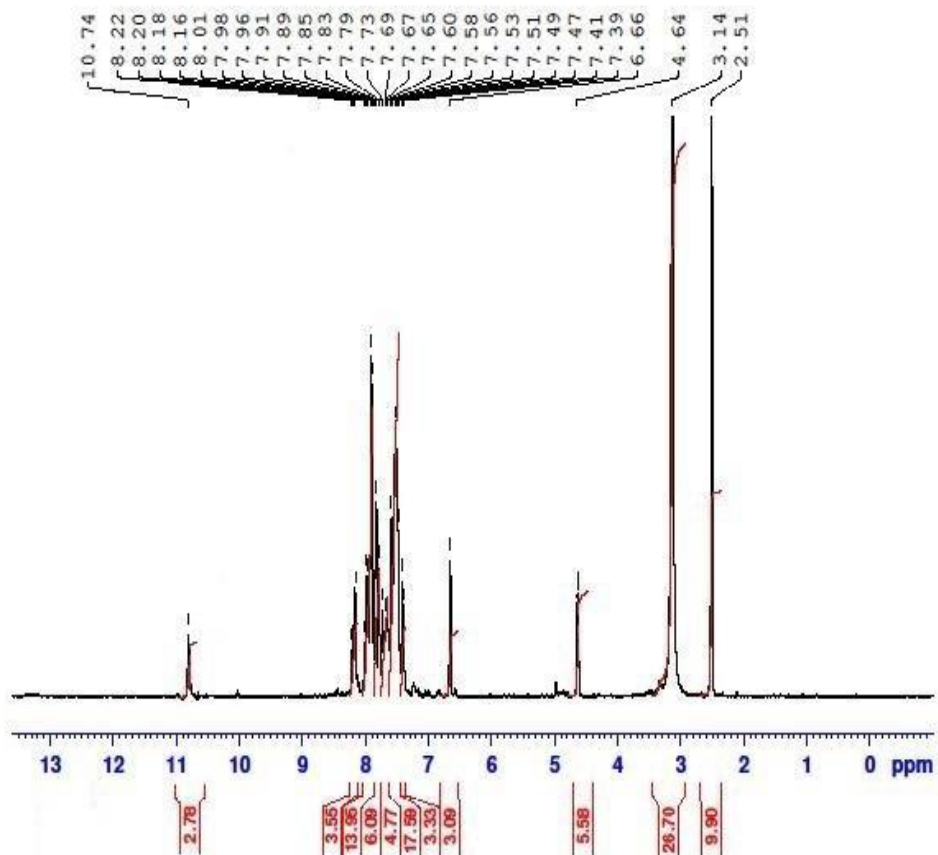
Current Data Parameters  
NAME Dec10-2018  
EXPNO 40  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20181210  
Time 10.44  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 25  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 199.04  
DW 62.400 usec  
DE 6.50 usec  
TE 333.2 K  
D1 1.00000000 sec  
TDO 1

----- CHANNEL f1 -----  
SF01 400.1324710 MHz  
NUC1 1H  
P1 12.00 usec  
PIW1 22.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AM-7b  
 proton\_su DMSO (C:\nmr-data) Student 10



Current Data Parameters  
 NAME Dec10-2018  
 EXPNO 100  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20181210  
 Time 11.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 ID 65536  
 SOLVENT DMSO  
 NS 25  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 199.04  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 333.2 K  
 D1 1.00000000 sec  
 ID0 1

----- CHANNEL f1 -----  
 SF01 400.1324710 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 22.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

AM-7b  
 proton\_su DMSO (C:\nmr-data) Student 10



8.22  
8.20  
8.18  
8.16

8.01  
7.98  
7.96

7.91  
7.89

7.85  
7.83  
7.79

7.73

7.69  
7.67  
7.65

7.60  
7.58  
7.56  
7.53  
7.51  
7.49  
7.47

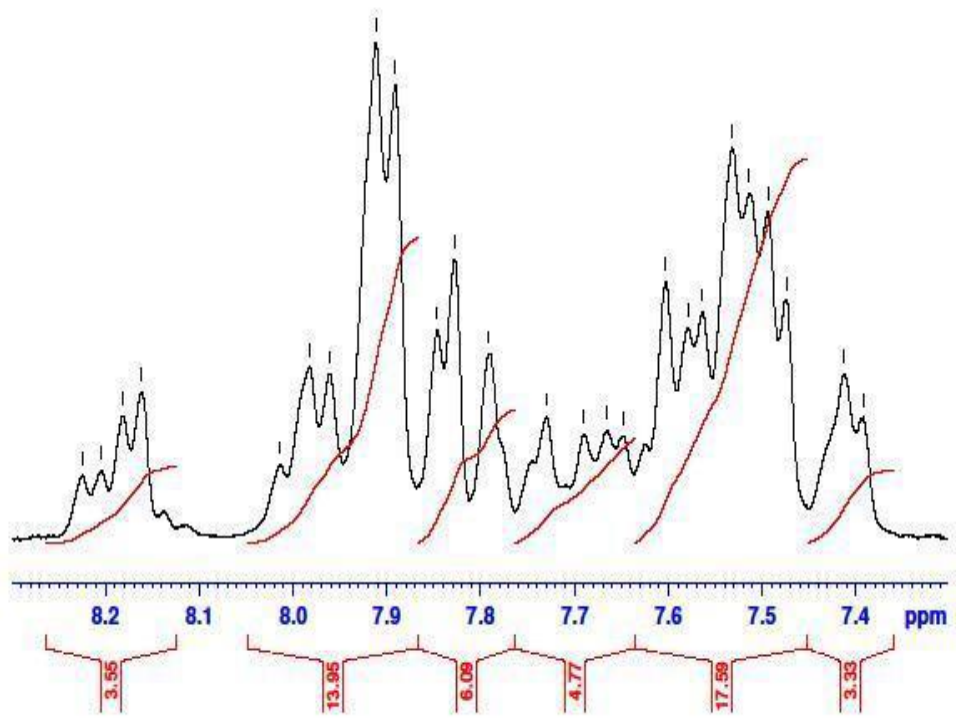
7.41  
7.39

Current Data Parameters  
 NAME Dec10-2018  
 EXPNO 100  
 PROCNO 1

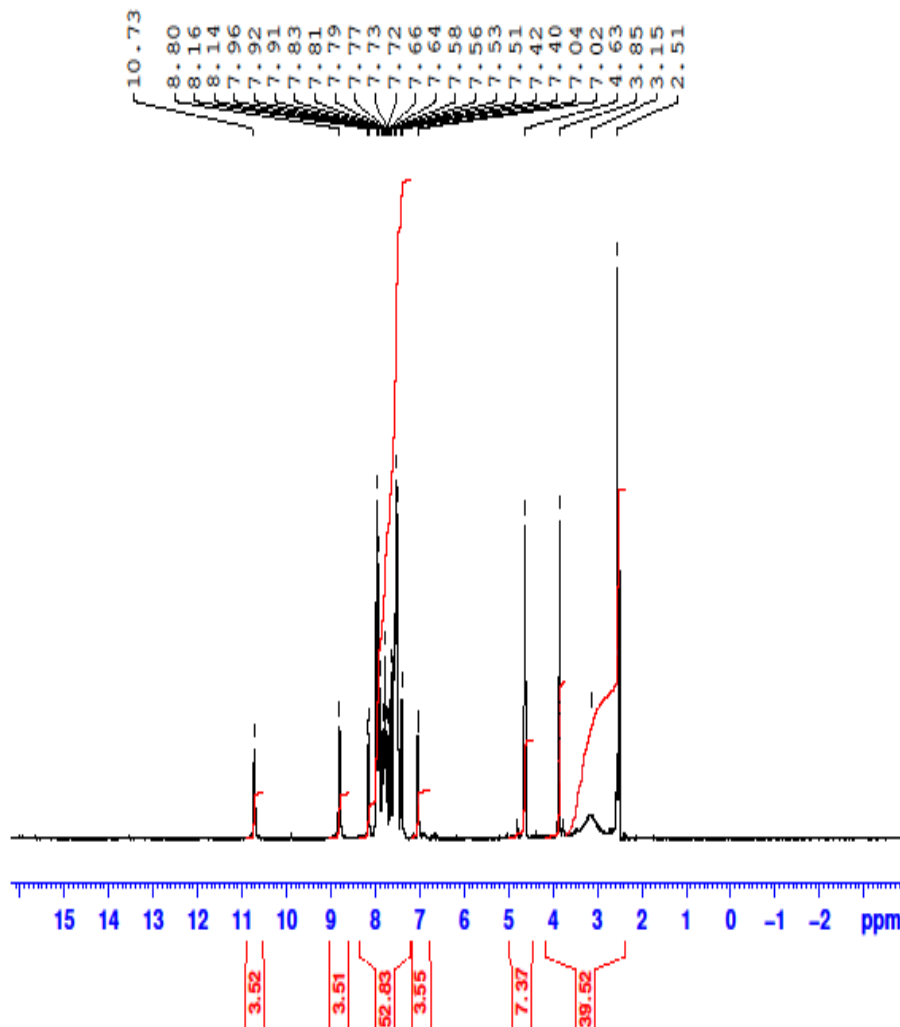
F2 - Acquisition Parameters  
 Date\_ 20181210  
 Time 11.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 25  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 199.04  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 333.2 K  
 D1 1.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 400.1324710 MHz  
 NUC1 1H  
 P1 12.00 usec  
 P1M1 22.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



AM-7c  
proton\_su DMSO (C:\nmr-data) Student 9



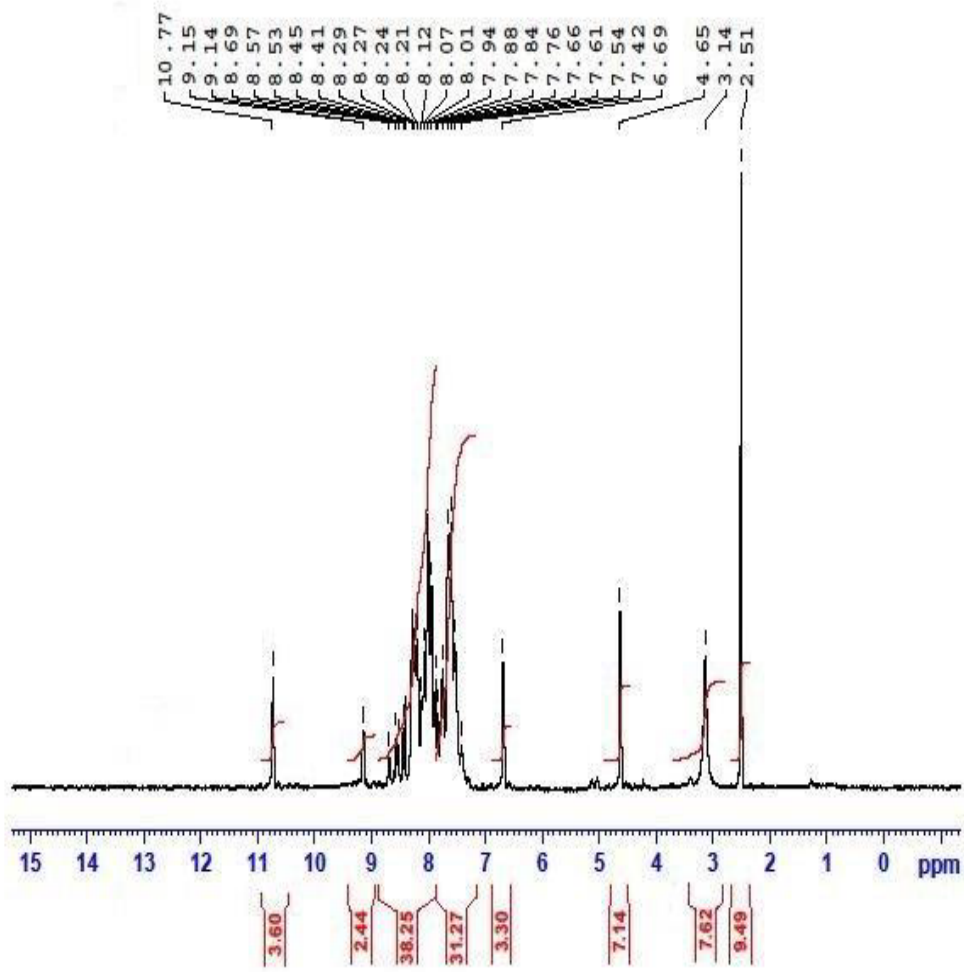
Current Data Parameters  
NAME Dacl0-2018  
EXPNO 90  
PROCNO 1

F2 - Acquisition Parameters  
Data\_ 20181210  
Time 11.08  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 25  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 199.04  
DW 62.400 usec  
DE 6.50 usec  
TE 333.2 K  
D1 1.00000000 sec  
TDO 1

----- CHANNEL f1 -----  
SF01 400.1324710 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 22.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AM-7d  
 proton\_su DMSO (C:\nmr-data) Student 20



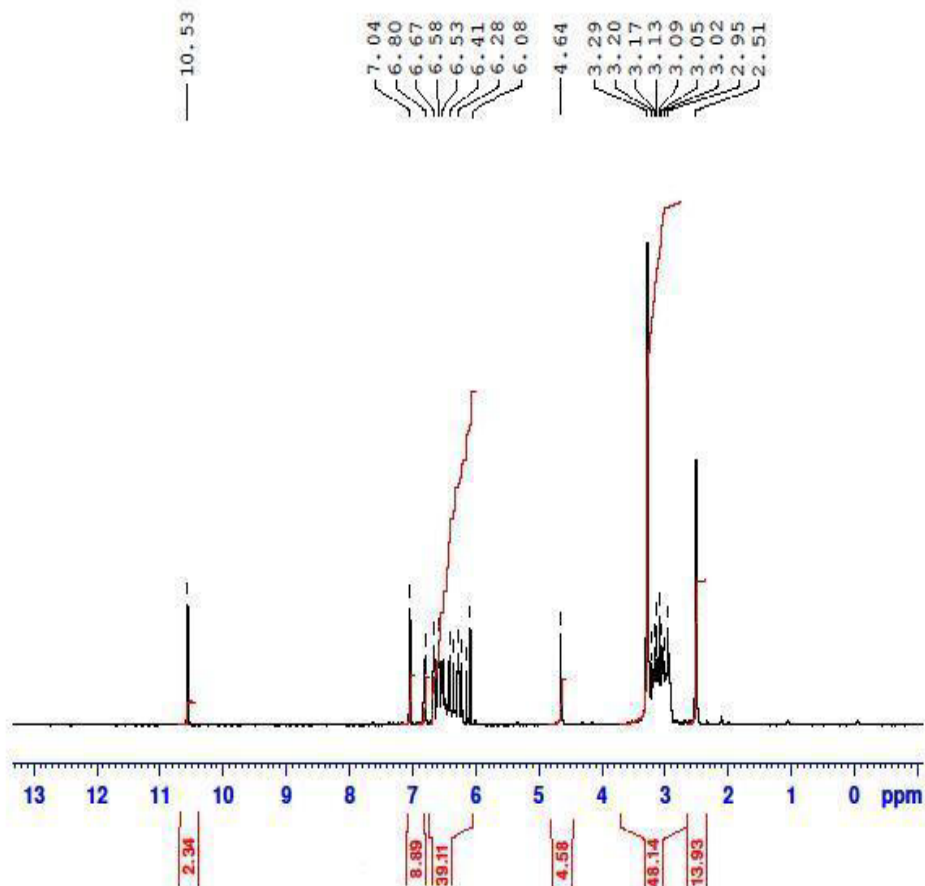
Current Data Parameters  
 NAME Dec10-2018  
 EXPNO 200  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20181210  
 Time 12.12  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 25  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 199.04  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 333.2 K  
 D1 1.00000000 sec  
 TD0 1

----- CHANNEL f1 -----  
 SP01 400.1324710 MHz  
 NUCL1 1H  
 P1 12.00 usec  
 PLW1 22.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

A-7e  
 proton\_su DMSO (C:\nmr-data) Student 15



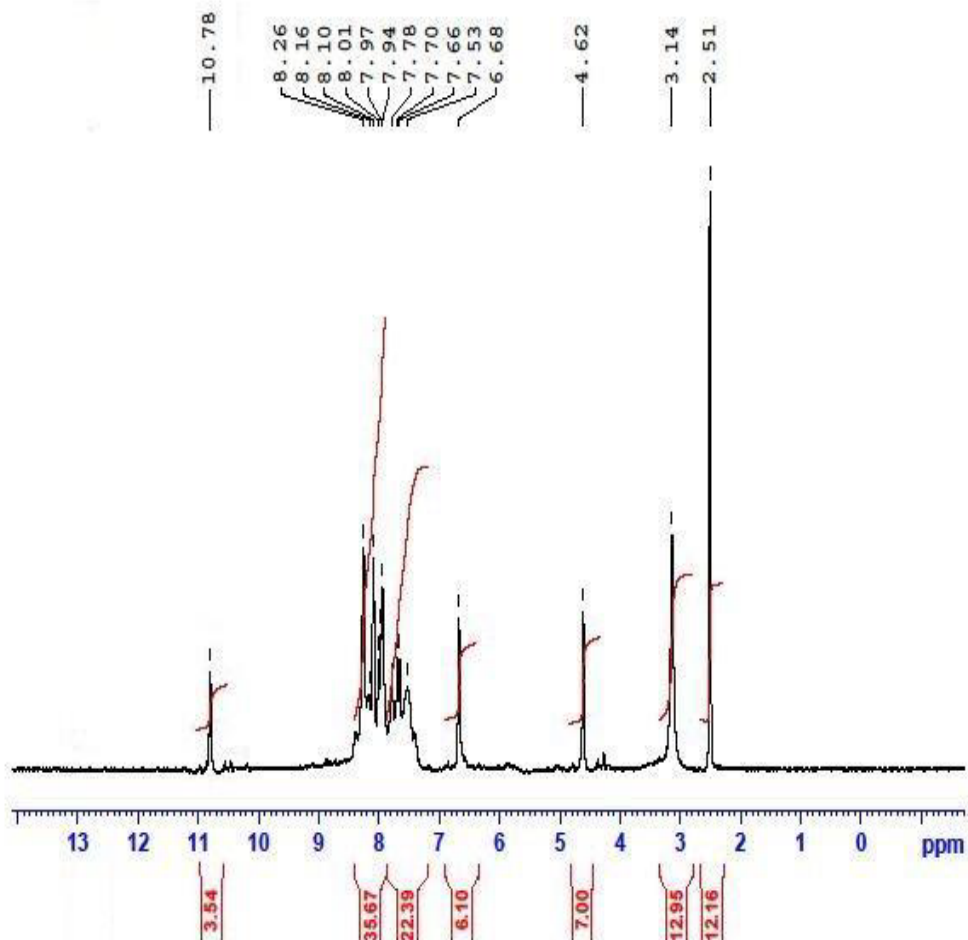
Current Data Parameters  
 NAME Apr02-2019  
 EXPNO 300  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20190402  
 Time 14.04  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 25  
 DS 2  
 SSB 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 199.04  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 308.1 K  
 D1 1.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 400.1324710 MHz  
 NUC1 1H  
 P1 12.00 usec  
 P1M1 22.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300000 MHz  
 WIN EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

AM-7f  
 proton\_su DMSO (C:\nmr-data) Student 3



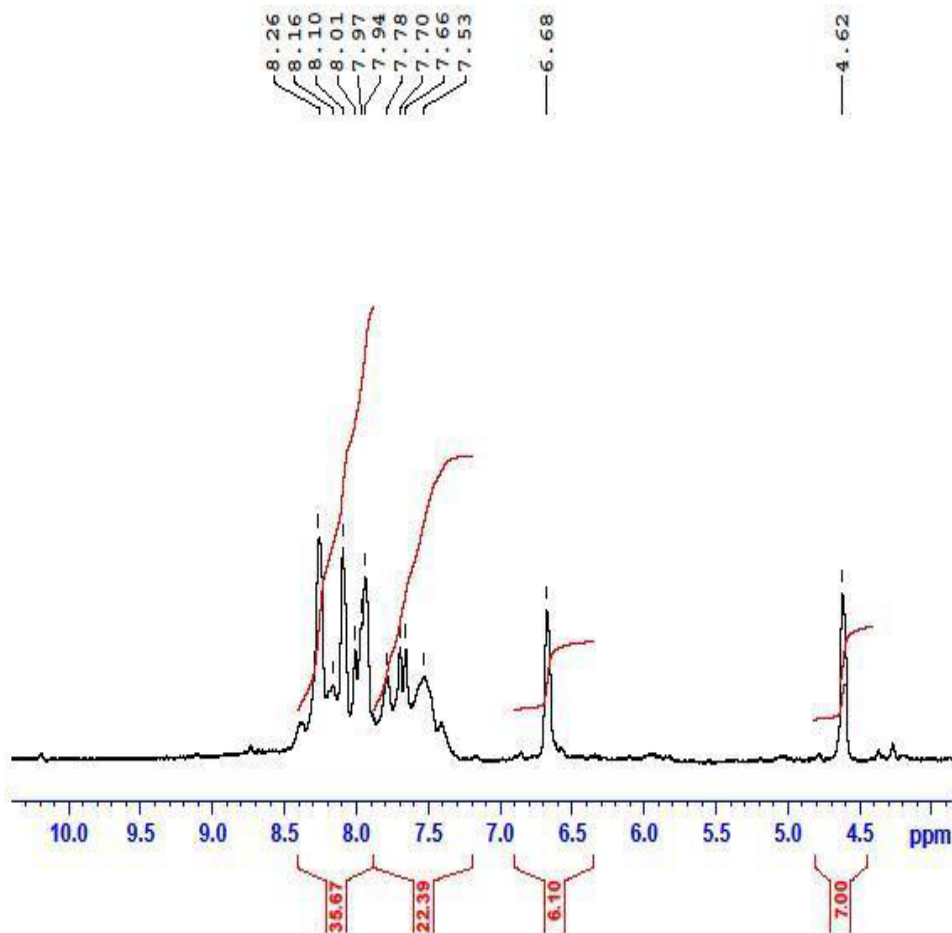
Current Data Parameters  
 NAME Dec10-2018  
 EXFNO 270  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20181210  
 Time 12.52  
 INSTRUM spect  
 PROBHD 5 mm DABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 25  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 199.04  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 333.2 K  
 D1 1.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SPOL 400.1324710 MHz  
 NUCL 1H  
 P1 12.00 usec  
 PLW1 22.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

AM-7f  
proton\_su DMSO {C:\nmr-data} student 3



Current Data Parameters  
NAME Dec10-2018  
EXNO 270  
PROCNO 1

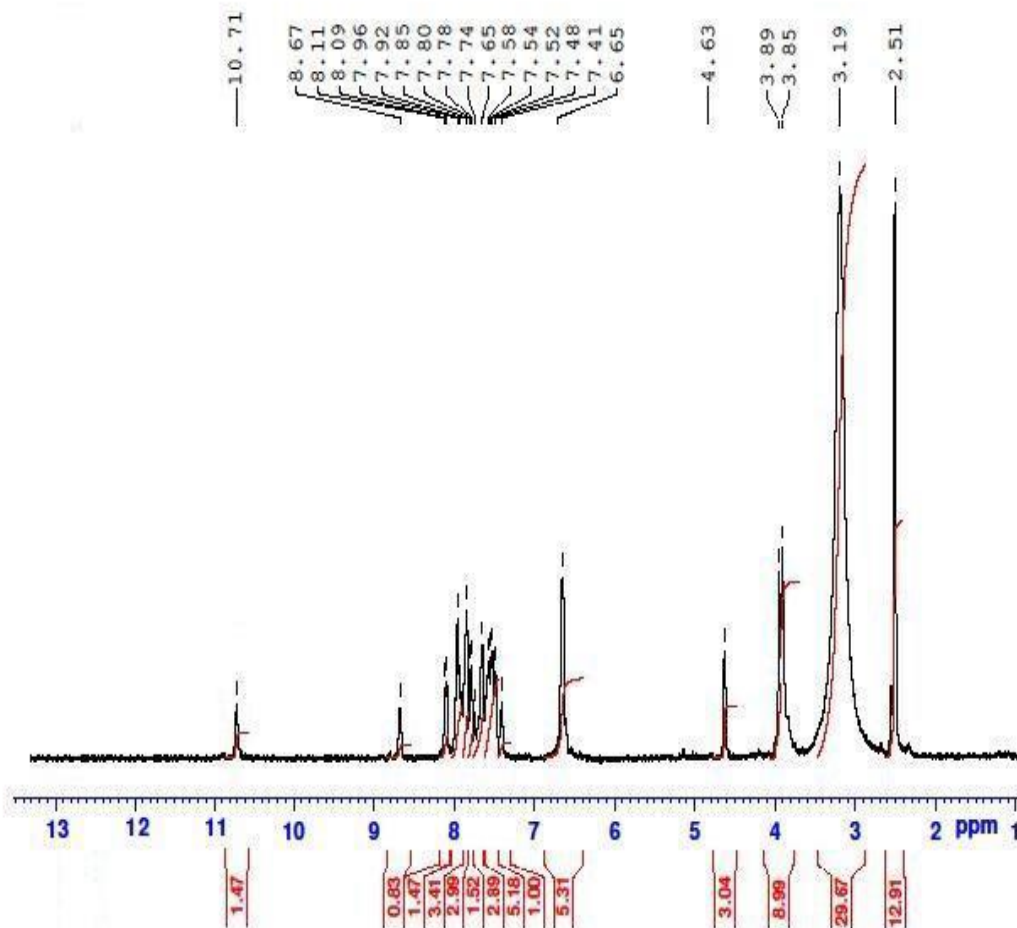
F2 - Acquisition Parameters  
Date\_ 20181210  
Time 12.52  
INSTRUM spect  
PROBHD 5 mm DABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 25  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 199.04  
DW 62.400 usec  
DE 6.50 usec  
TE 333.2 K  
D1 1.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
SF01 400.1324710 MHz  
NUC1 1H  
P1 12.00 usec  
PLM1 22.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



AM-7g  
 proton\_su DMSO (C:\nmr-data) Student 12



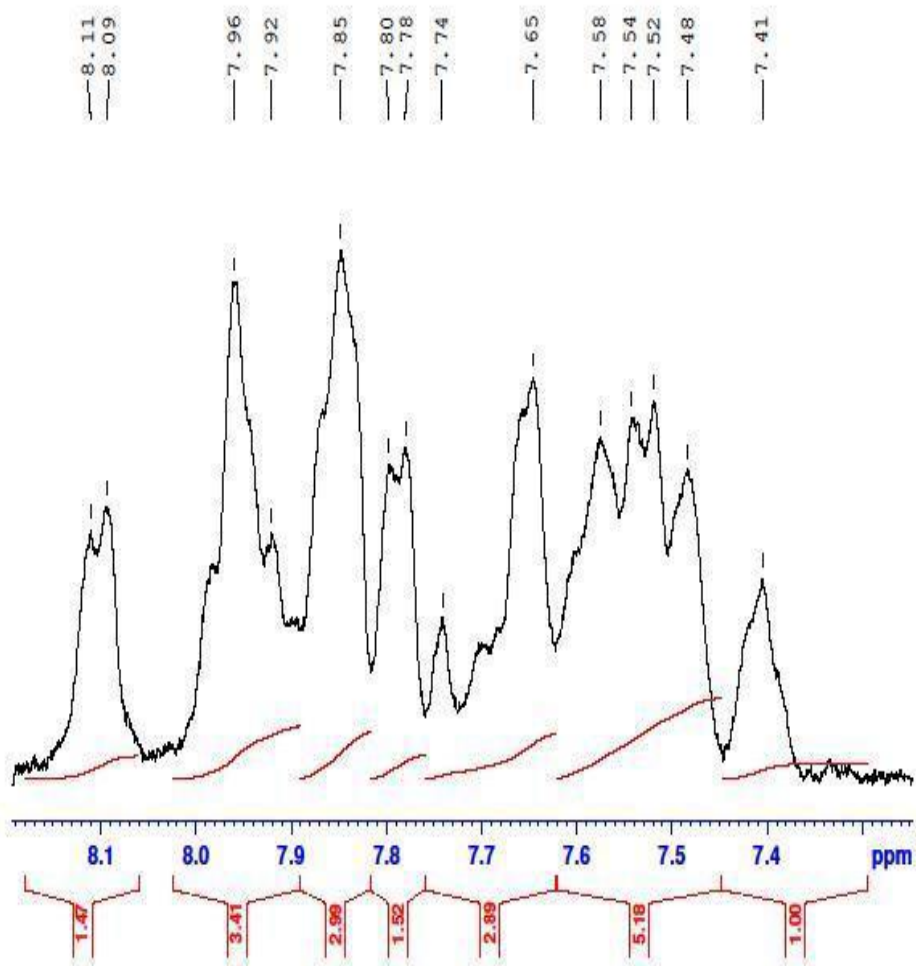
Current Data Parameters  
 NAME Dacl0-2018  
 EXPNO 120  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20181210  
 Time 11.25  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 25  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 199.04  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 333.2 K  
 D1 1.00000000 sec  
 ID0 1

CHANNEL f1  
 SF01 400.1324710 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 22.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

AM-7g  
proton\_su DMSO (C:\nmr-data) Student 12



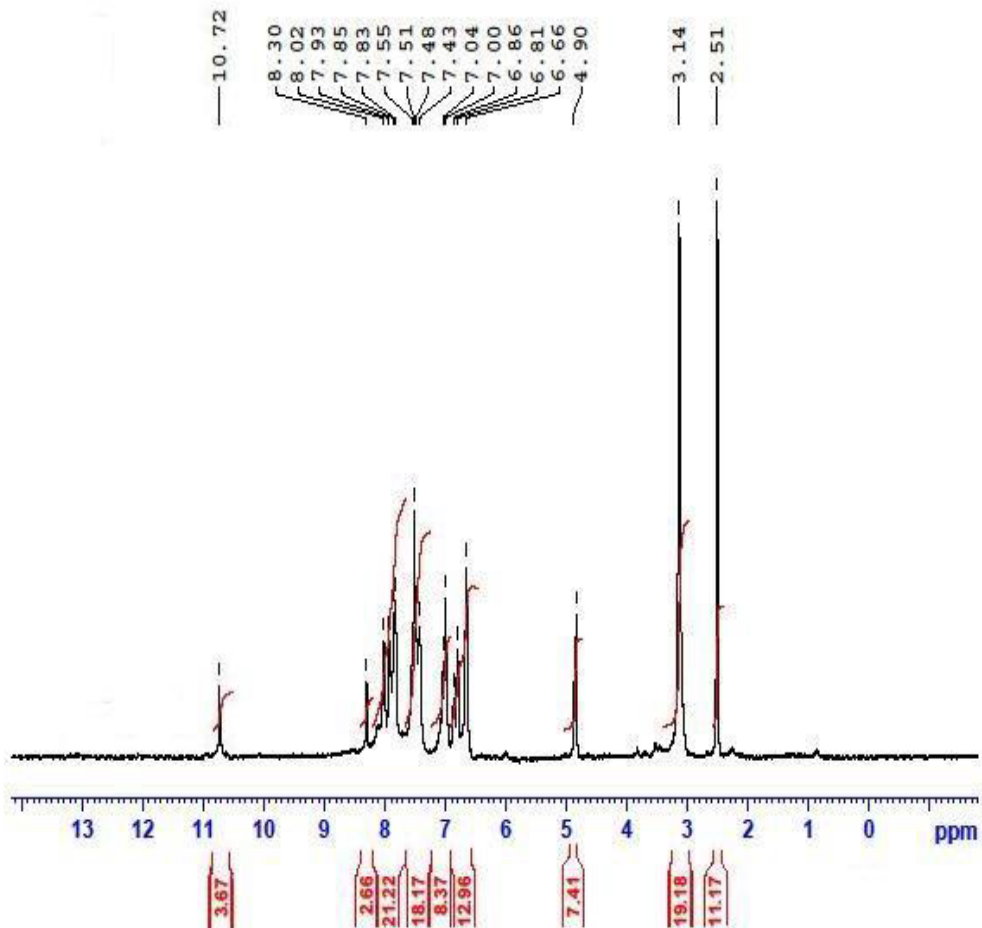
Current Data Parameters  
NAME Dec10-2018  
EXPNO 120  
PROCNO 1

F2 - Acquisition Parameters  
Data\_ 20181210  
Time 11.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 25  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 199.04  
DW 62.400 usec  
DE 6.50 usec  
TK 333.2 K  
D1 1.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
SF01 400.1324710 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 22.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AM-7h  
 proton\_su DMSO {C:\nmr-data} Student 17



Current Data Parameters  
 NAME Dec10-2018  
 EXPNO 170  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20181210  
 Time 11.54  
 INSTRUM spect  
 PROSHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 25  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 199.04  
 EC 62.400 usec  
 DE 6.50 usec  
 TE 333.2 K  
 D1 1.00000000 sec  
 TD0 1

----- CHANNEL f1 -----  
 SFO1 400.1324710 MHz  
 NUCL1 1H  
 P1 12.00 usec  
 PLN1 22.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

AM- 7h  
proton\_su DMSO (C:\nmr-data) Student 17



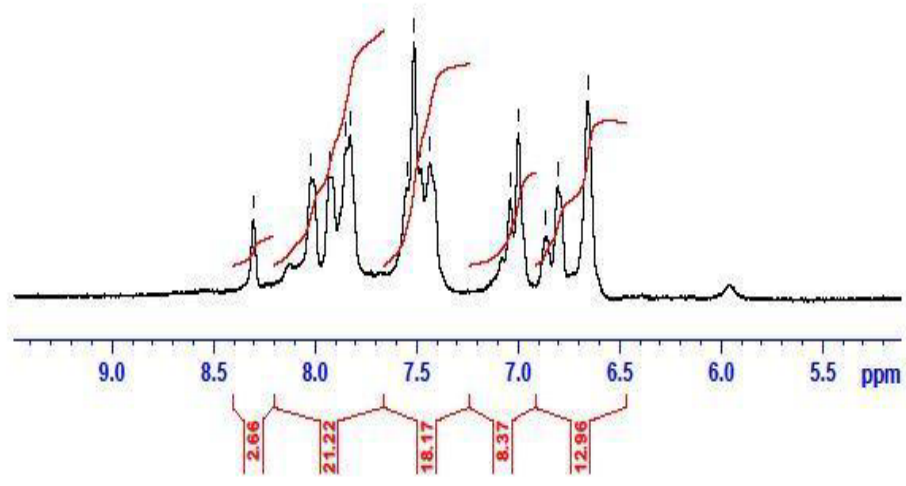
8.30  
8.02  
7.93  
7.85  
7.83  
7.55  
7.51  
7.48  
7.43  
7.04  
7.00  
6.86  
6.81  
6.66

Current Data Parameters  
NAME Dec10-2018  
EXPNO 170  
PROCNO 1

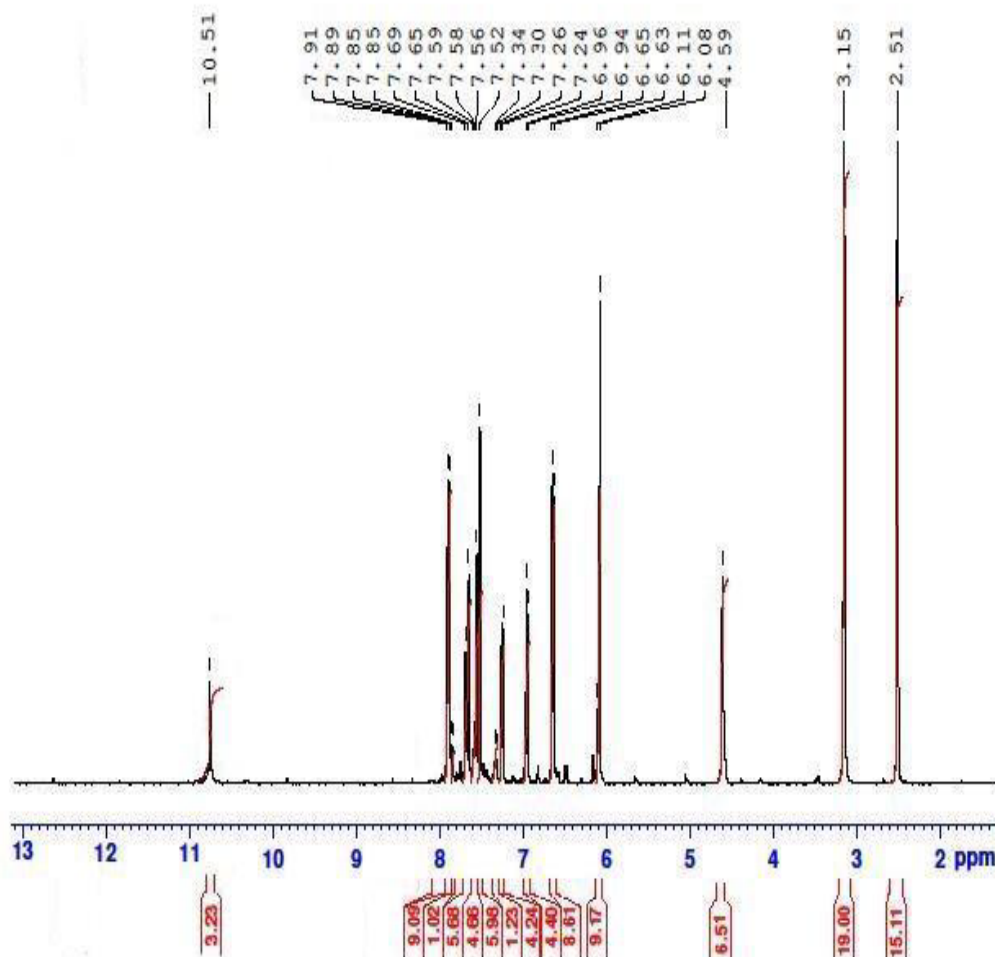
F2 - Acquisition Parameters  
Date\_ 20181210  
Time 11.54  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 25  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0804465 sec  
RG 199.04  
DM 62.400 usec  
DE 6.50 usec  
TE 333.2 K  
D1 1.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
SFO1 400.1324710 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 22.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
CB 0  
PC 1.00



AM-7i  
 proton\_su DMSO (C:\nmr-data) Student 3



```

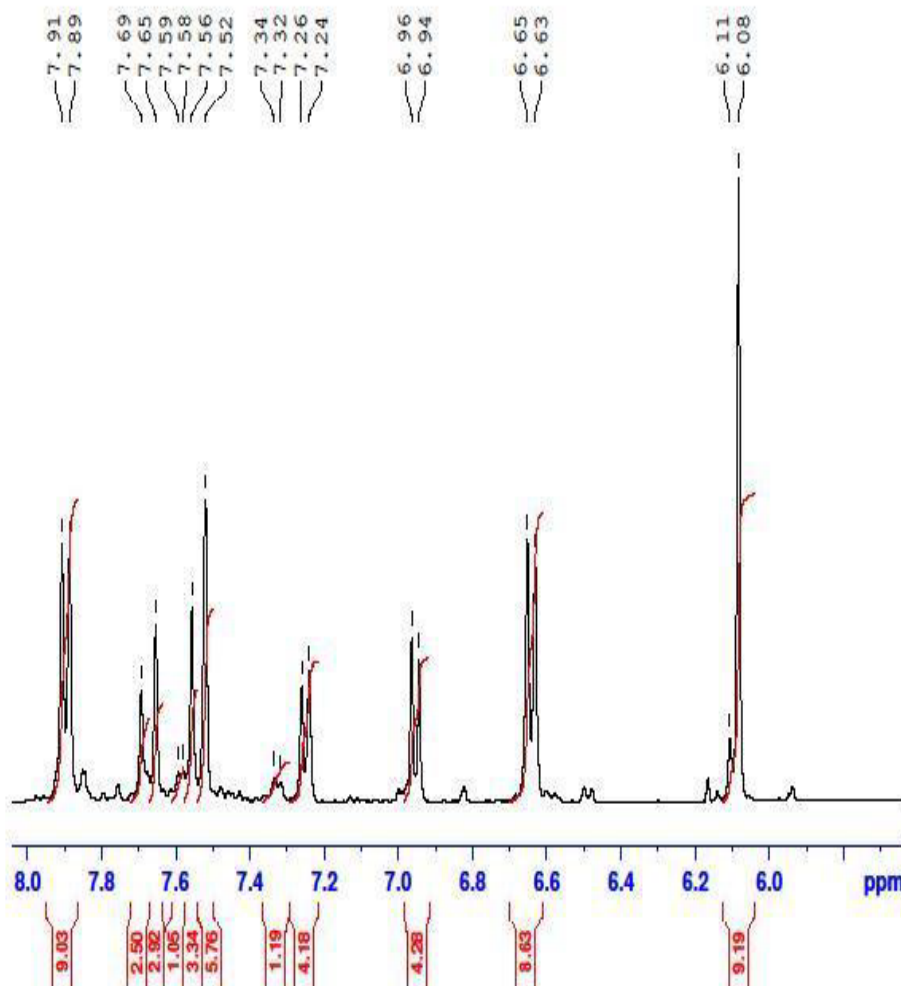
Current Data Parameters
NAME      Dec10-2018
EXPNO    20
PROCNO    1

F2 - Acquisition Parameters
Date_     20181210
Time      10.32
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         25
DS         2
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894465 sec
RG         199.04
DW         62.400 usec
DE         6.50 usec
TE         331.4 K
D1         1.00000000 sec
TD0        1

----- CHANNEL f1 -----
SF01      400.1324710 MHz
NUC1       1H
P1         12.00 usec
PLW1      22.00000000 W

F2 - Processing parameters
SI         65536
SF         400.1300000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

AM-7i  
 proton\_su DMSO (C:\nmr-data) Student 3



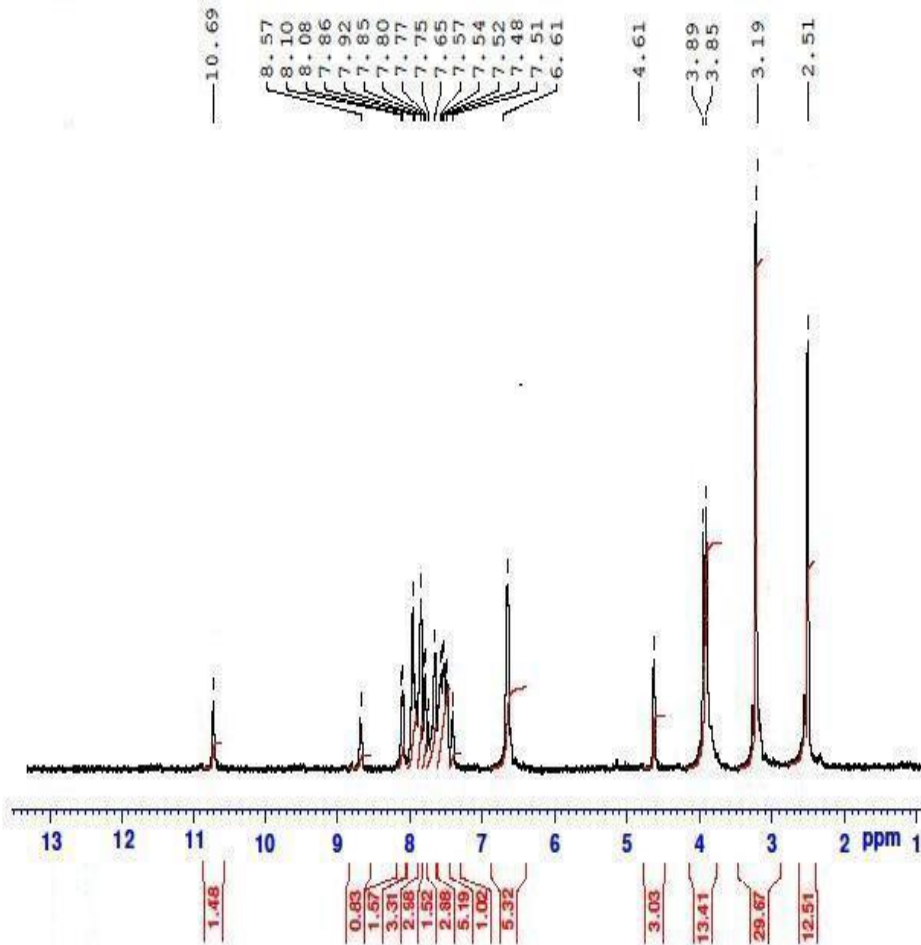
Current Data Parameters  
 NAME Dec10-2018  
 EXPNO 20  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20181210  
 Time 10.32  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 25  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 199.04  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 331.4 K  
 D1 1.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SF01 400.1324710 MHz  
 NUC1 1H  
 P1 12.00 usec  
 P1M1 22.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

AM-7j  
proton\_su DMSO (C:\nmr-data) Student 12



Current Data Parameters  
NAME Dec10-2018  
EXPNO 120  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20181210  
Time 11.25  
INSTRUM spect  
PROBHD 5 mm PARBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 25  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 199.04  
DW 62.400 usec  
DE 6.50 usec  
TE 333.2 K  
D1 1.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
SF01 400.1324710 MHz  
NUC1 1H  
P1 12.00 usec  
PIW1 22.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WVW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

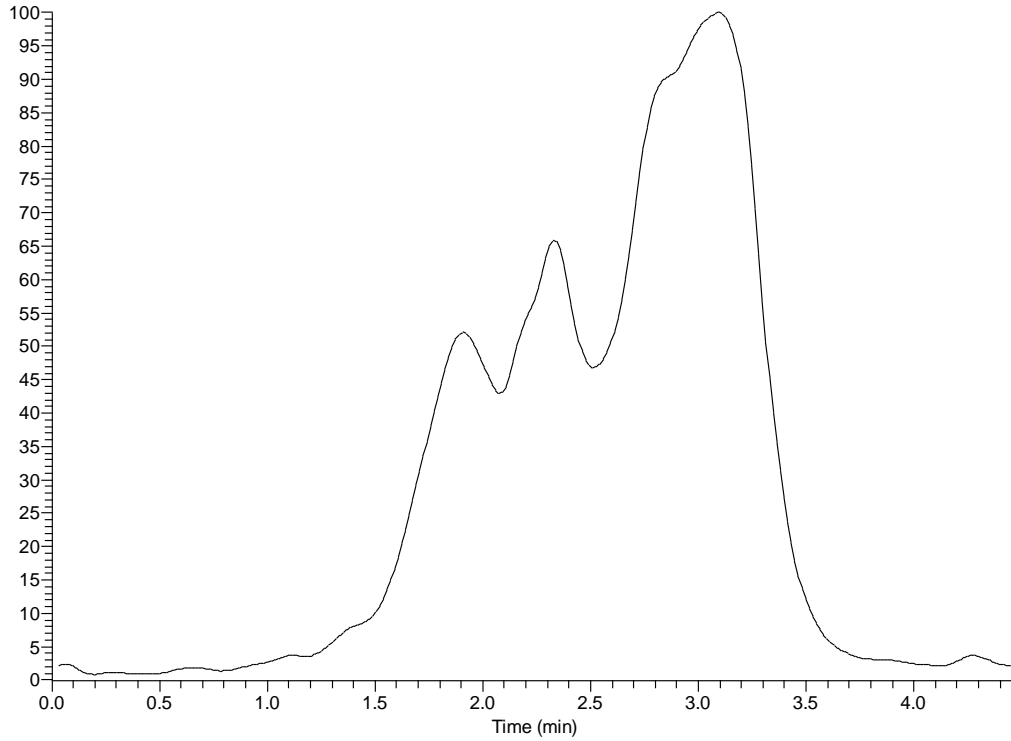
# Mass spectrometry

C:\xcalibur\data\SMAI-MORAD-6

13-May-19 1:51:15 PM  
THE  
AZH

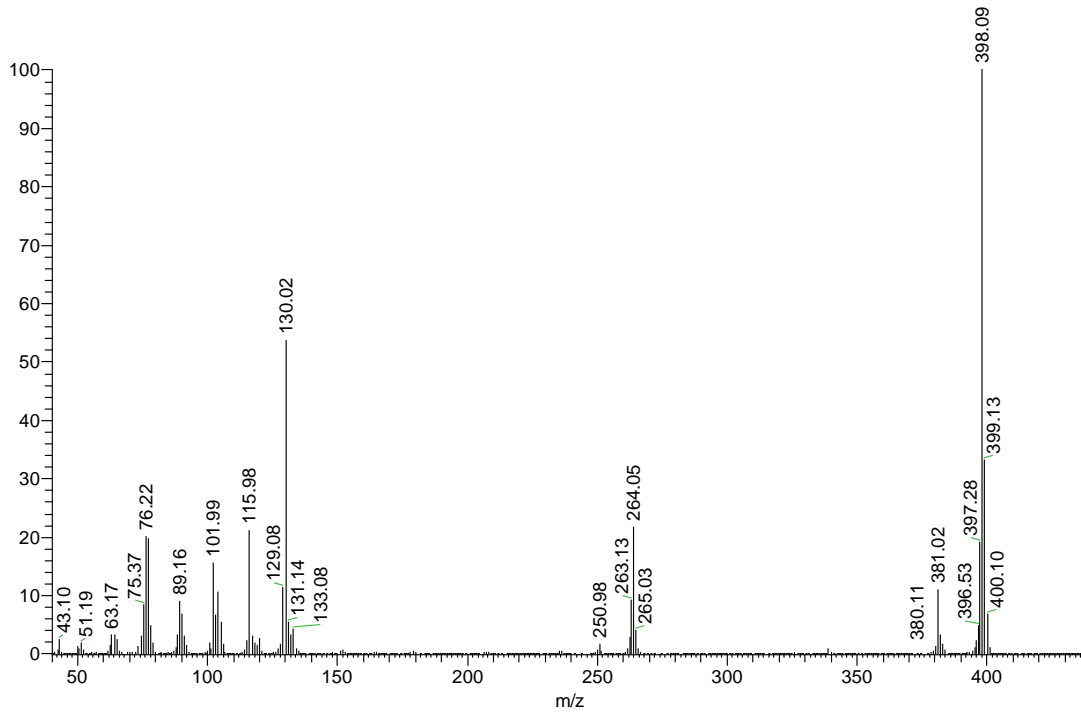
OGY AND BIOTECHNOLOGY

RT: 0.00 - 4.49 SM: 15G



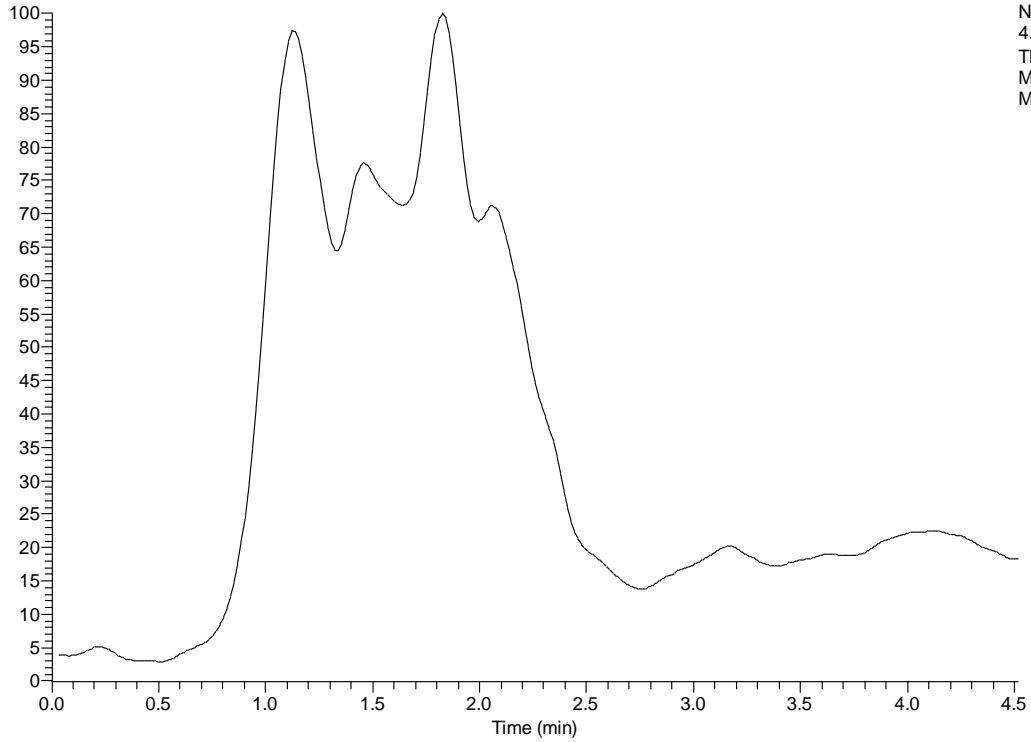
NL:  
6.21E5  
TIC MS  
MAI-  
MORAD-6

MAI-MORAD-6 #161-198 RT: 2.71-3.33 AV: 38 SB: 2 4.49, 4.49 NL: 9.69E4  
T: {0,0} + c EI Full ms [40.00-1000.00]



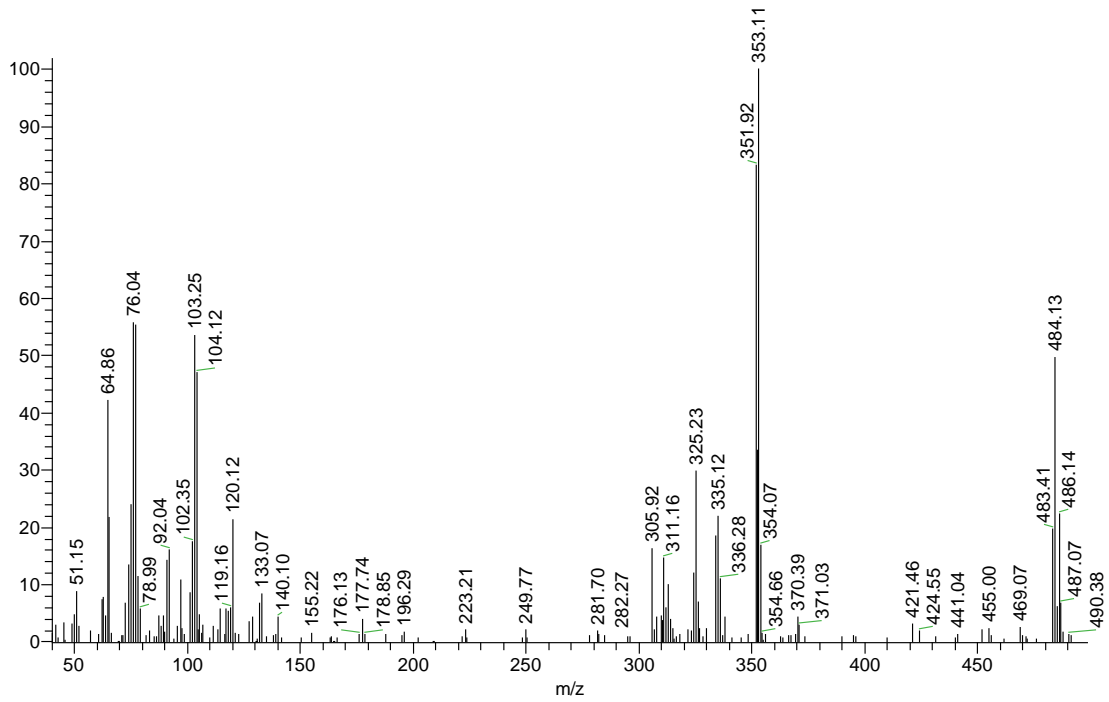


RT: 0.00 - 4.52 SM: 15G

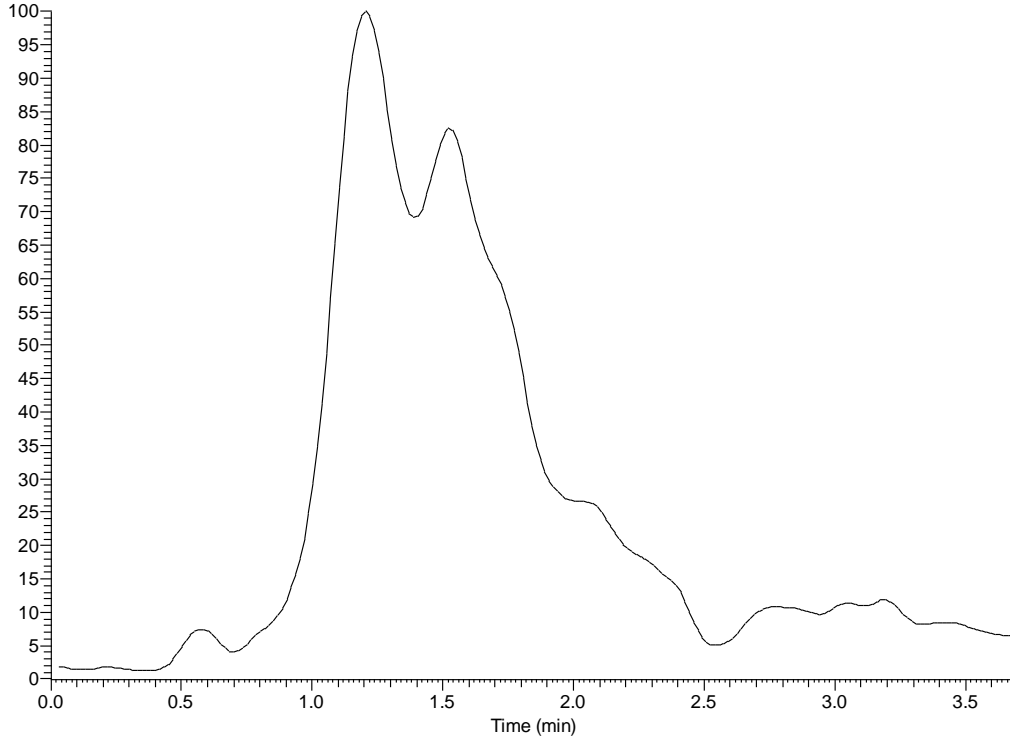


NL:  
4.64E5  
TIC MS  
MAI-  
MORAD-7a

MAI-MORAD-7a #123 RT: 2.08 AV: 1 SB: 2 4.52, 4.52 NL: 1.79E4  
T: (0,0) +c EI Full ms [40.00-1000.00]

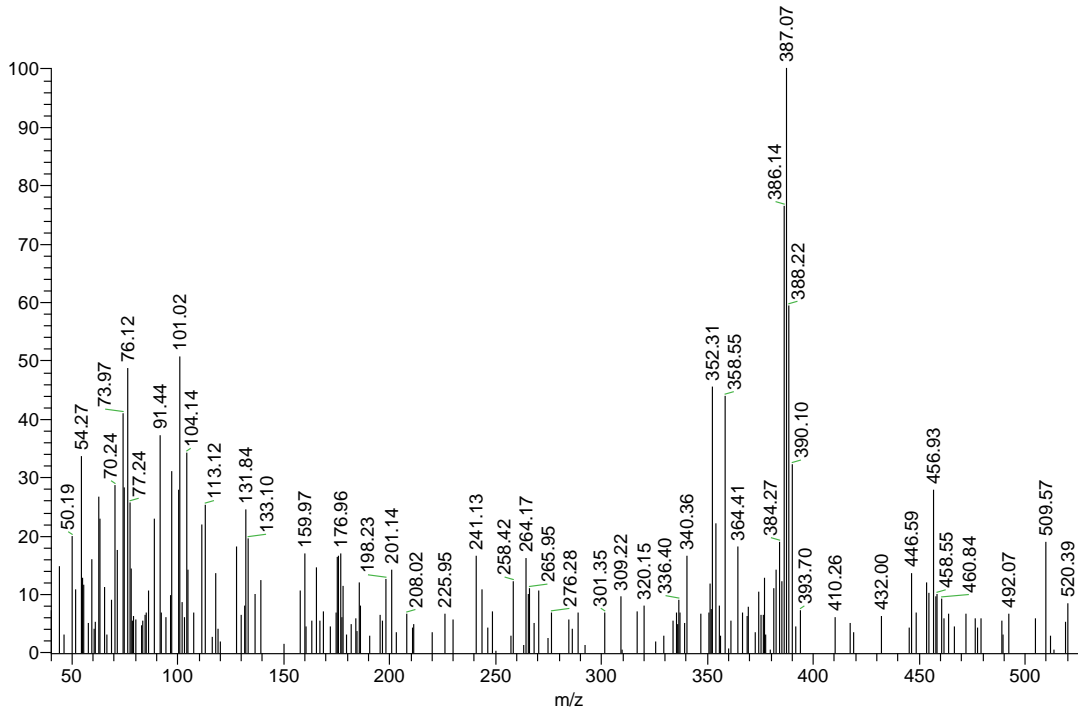


RT: 0.00 - 3.70 SM: 15G

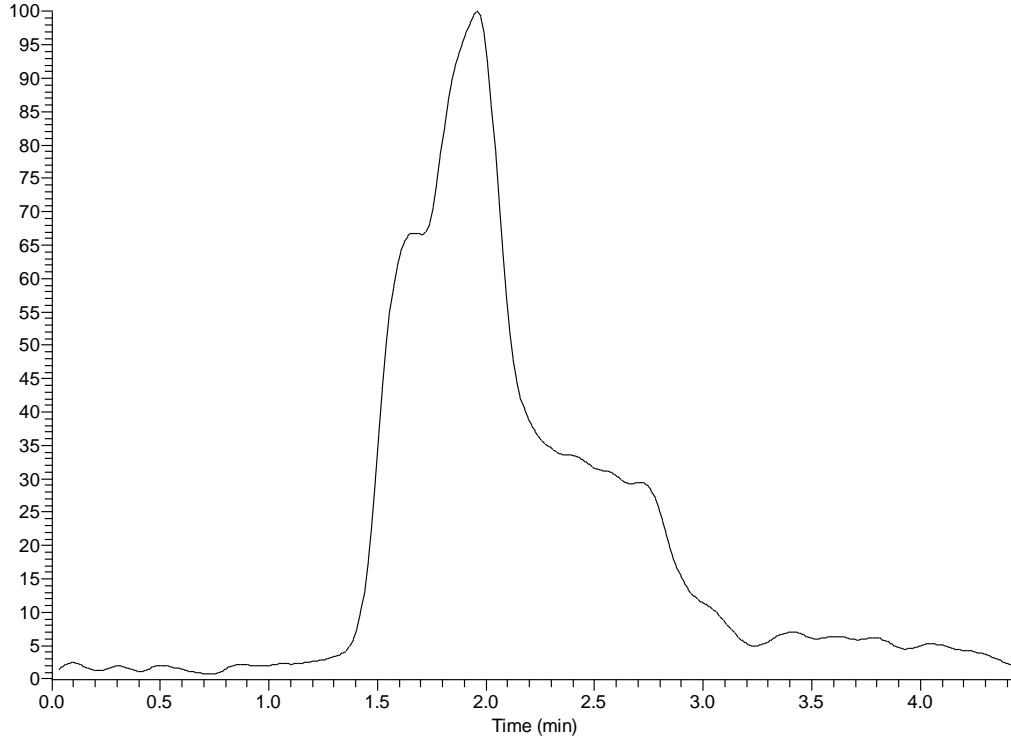


NL:  
3.40E5  
TIC MS  
MAI-  
MORAD-7B

MAI-MORAD-7B #142 RT: 2.39 AV: 1 SB: 2 3.70, 3.70 NL: 1.81E3  
T: (0,0) + c EI Full ms [40.00-1000.00]

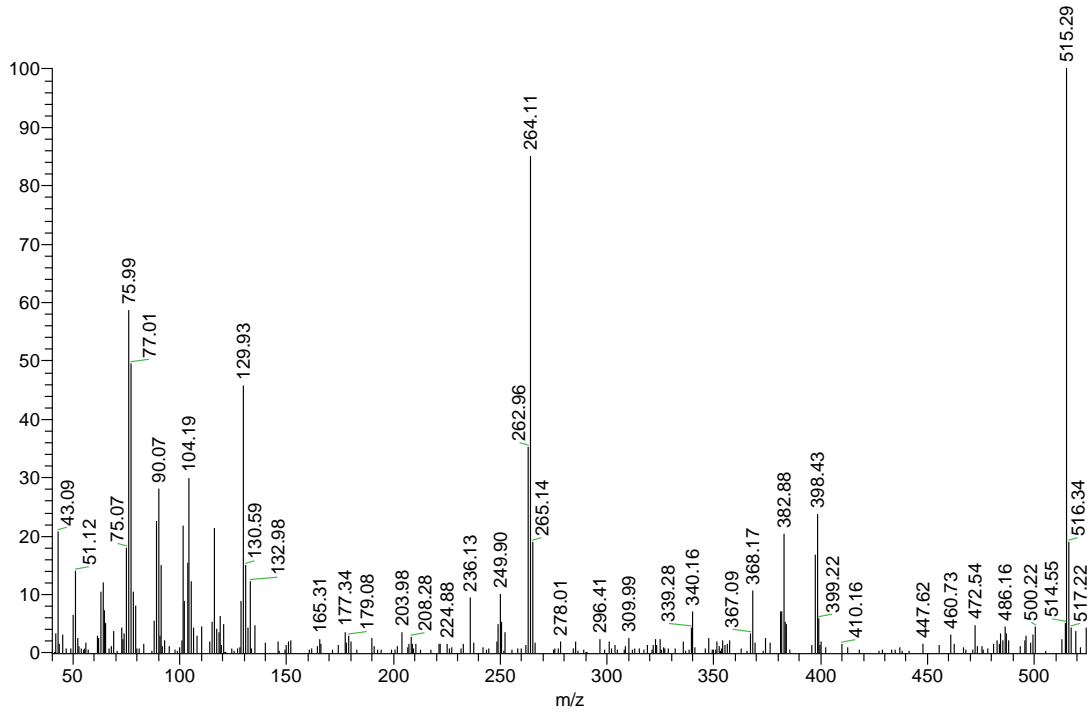


RT: 0.00 - 4.45 SM: 15G

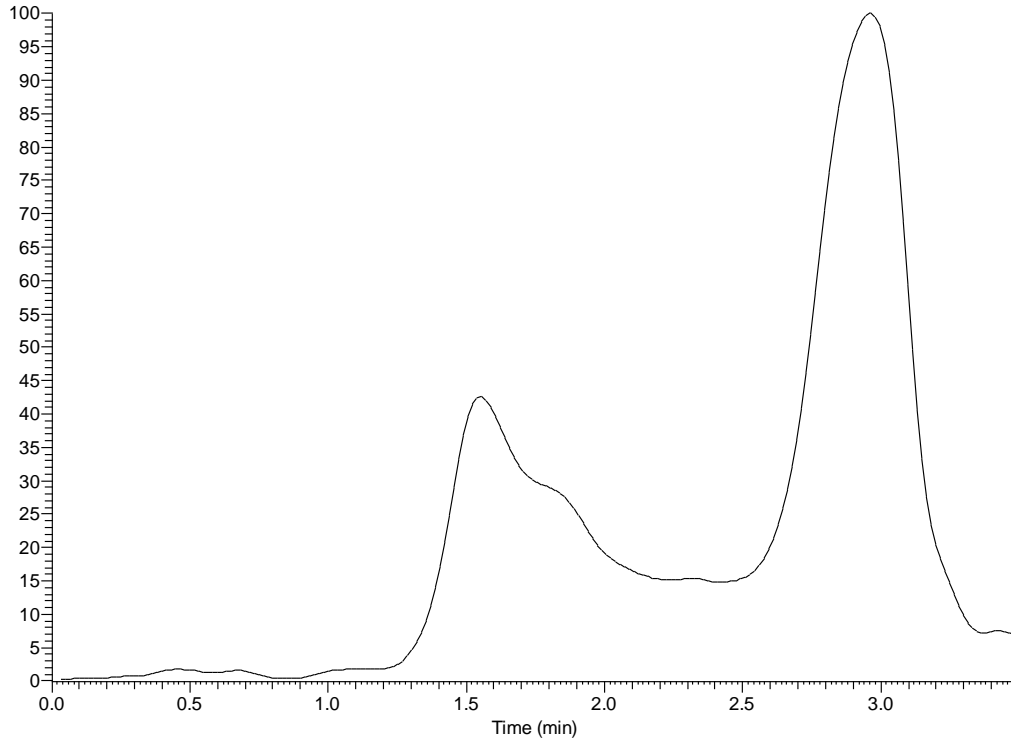


NL:  
7.76E5  
TIC MS  
MAI-  
MORAD-  
7C

MAI-MORAD-7C #153 RT: 2.58 AV: 1 SB: 2 4.45, 4.45 NL: 1.75E4  
T: {0,0} +c EI Full ms [40.00-1000.00]

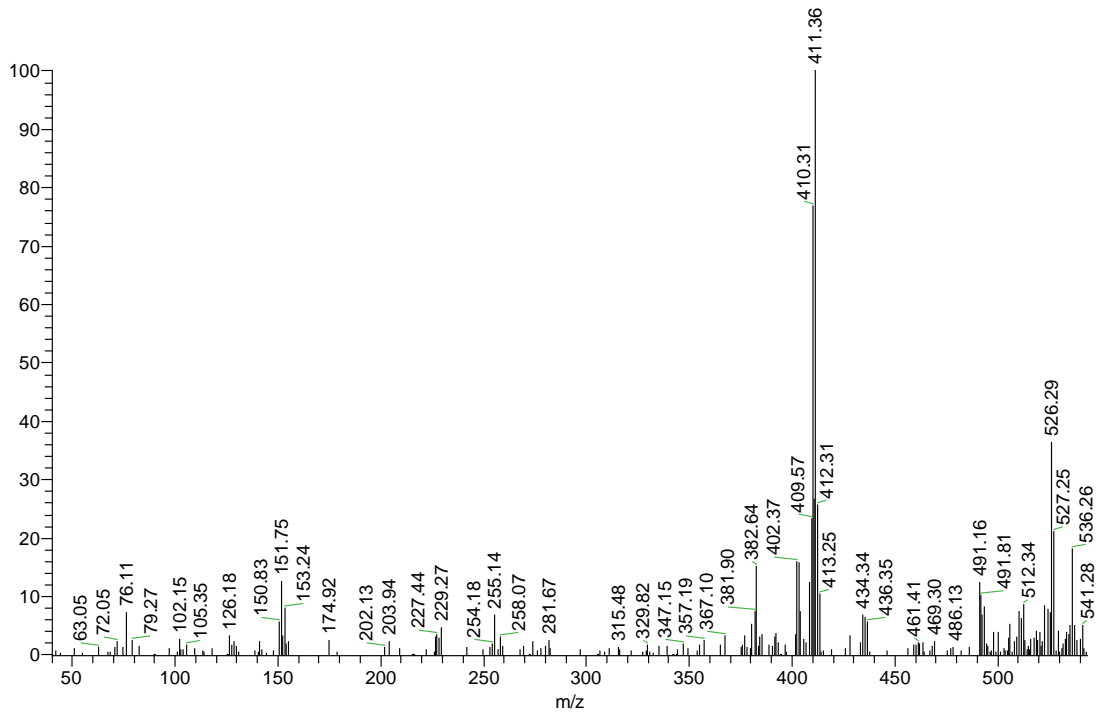


RT: 0.00 - 3.50 SM: 15G

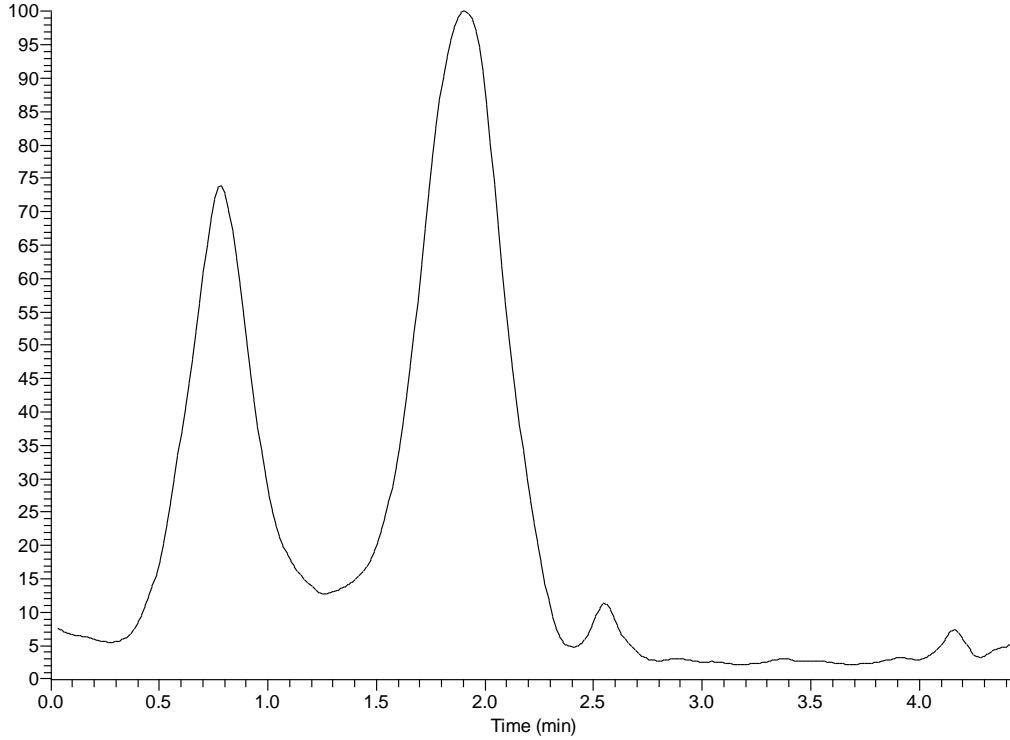


NL:  
1.35E6  
TIC MS  
MAI-  
MORAD-  
7D

MAI-MORAD-7D #192 RT: 3.23 AV: 1 SB: 2 3.50, 3.50 NL: 2.19E4  
T: (0,0) +c EI Full ms [40.00-1000.00]

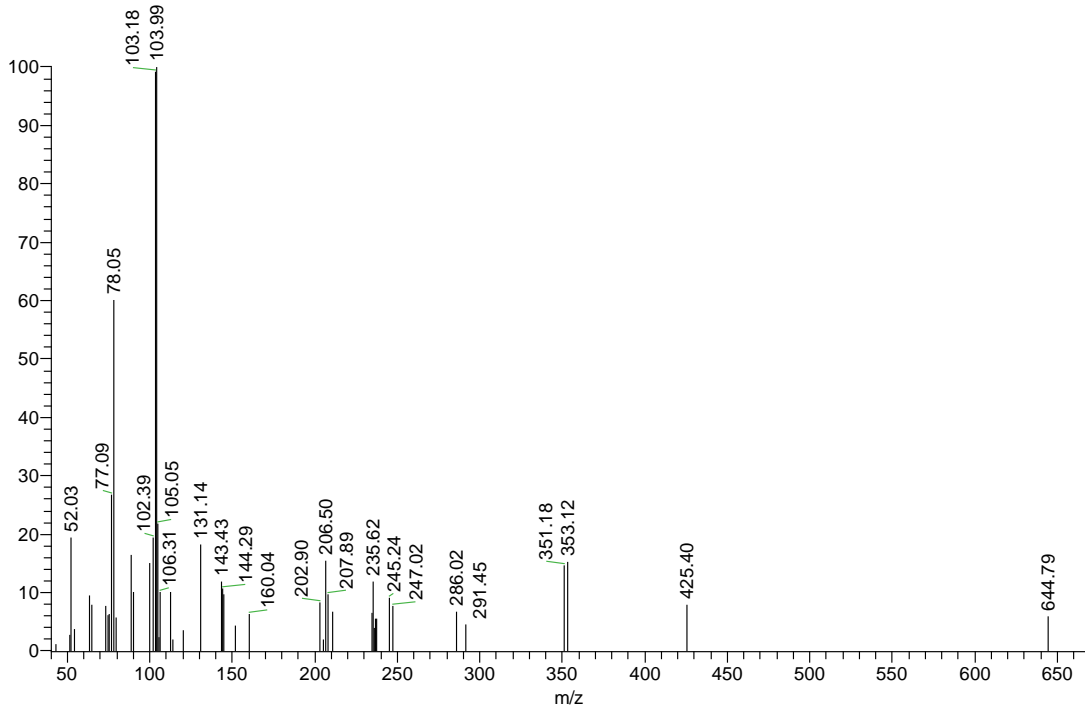


RT: 0.00 - 4.45 SM: 15G

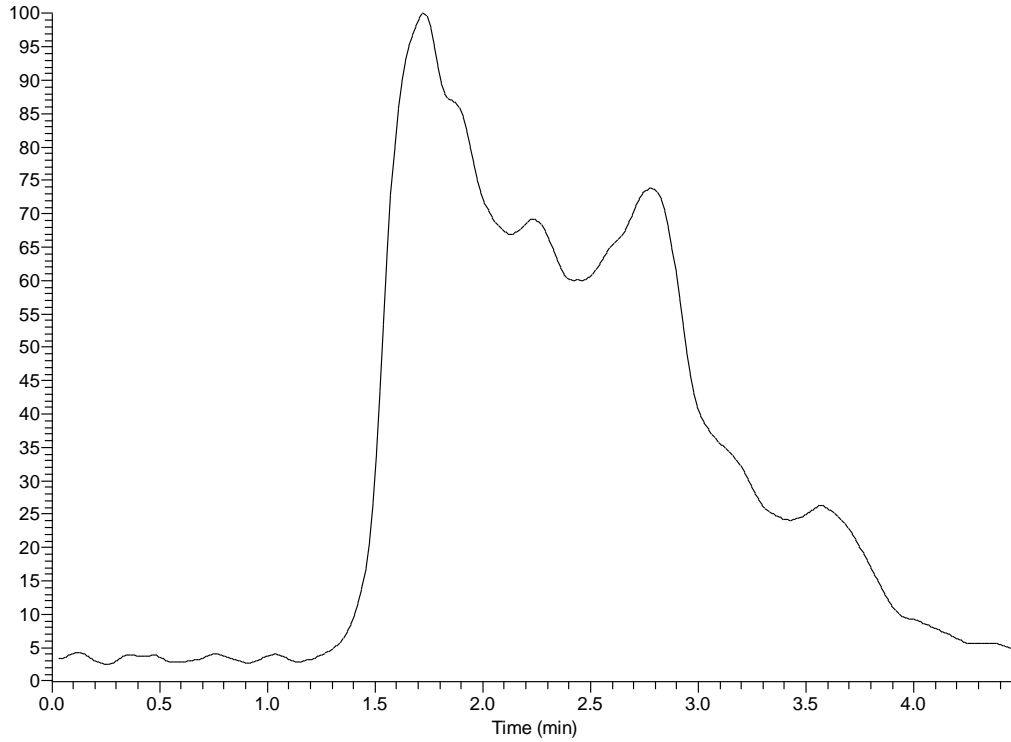


NL:  
1.82E5  
TIC MS  
MAI-  
MORAD-7e

MAI-MORAD-7e #77 RT: 1.31 AV: 1 SB: 2 4.45, 4.45 NL: 2.26E3  
T: (0,0) + c EI Full ms [40.00-1000.00]

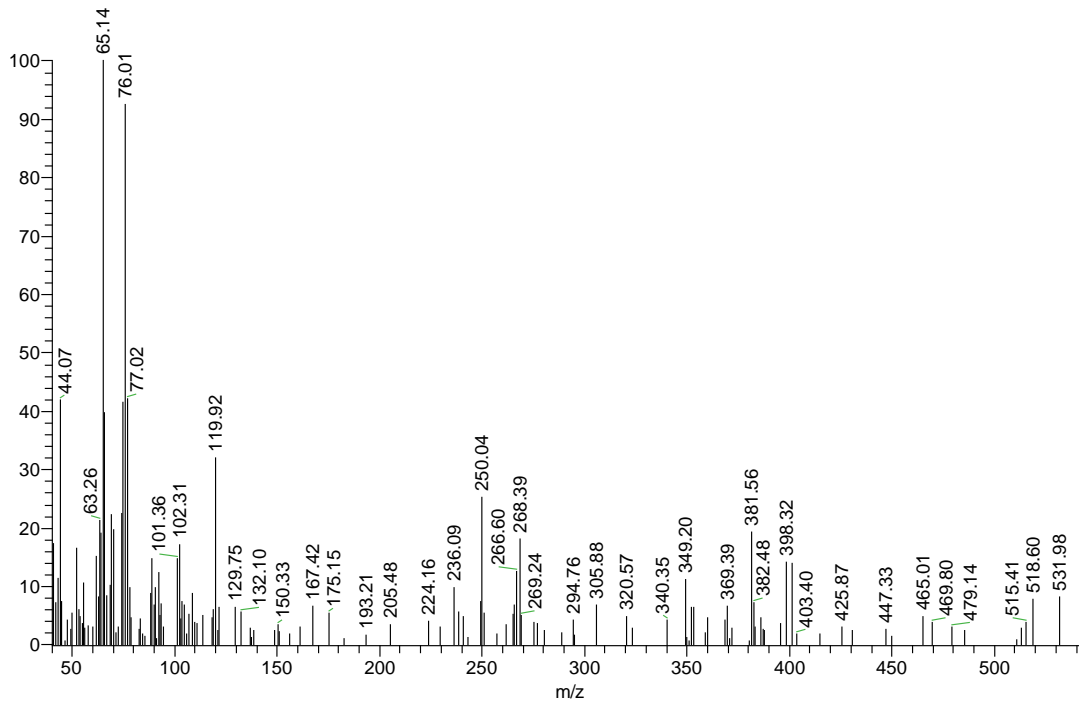


RT: 0.00 - 4.49 SM: 15G

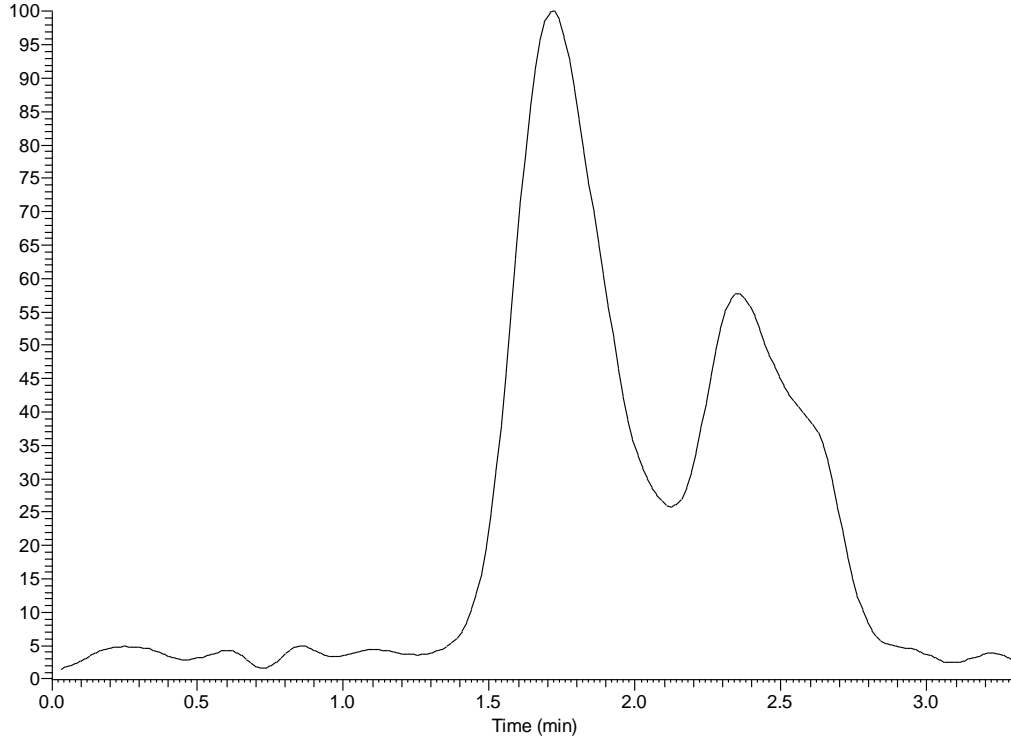


NL:  
4.29E5  
TIC MS  
MAI-  
MORAD-7F

MAI-MORAD-7F #223 RT: 3.75 AV: 1 SB: 2 4.49, 4.49 NL: 5.06E3  
T: (0,0) +c EI Full ms [40.00-1000.00]

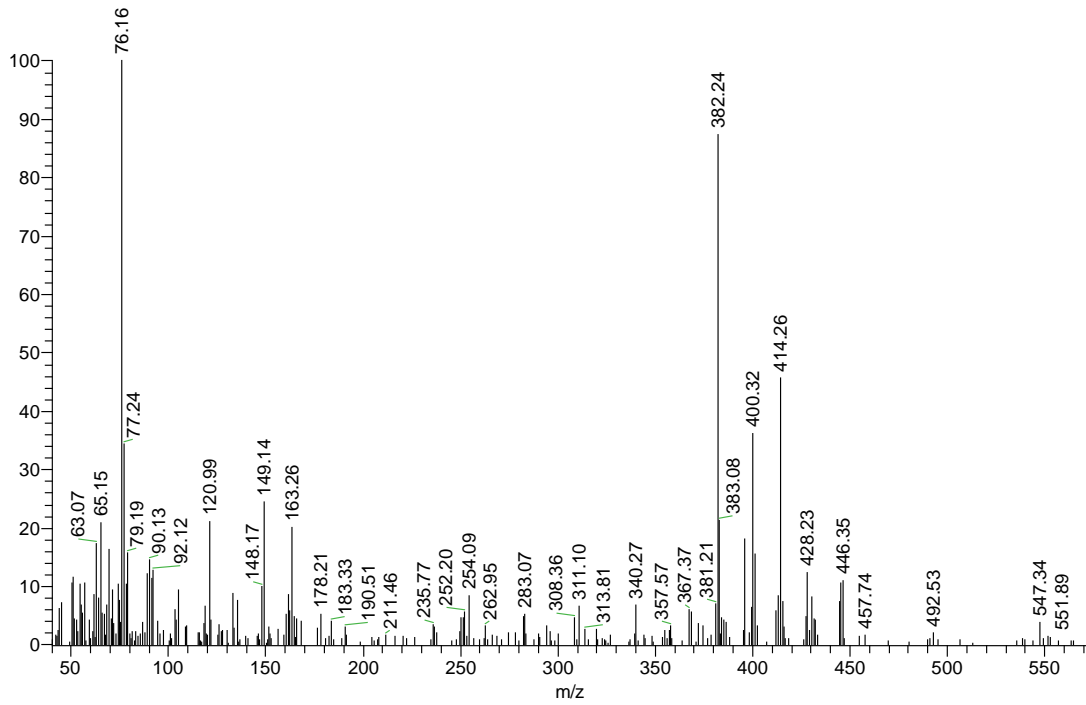


RT: 0.00 - 3.31 SM: 15G

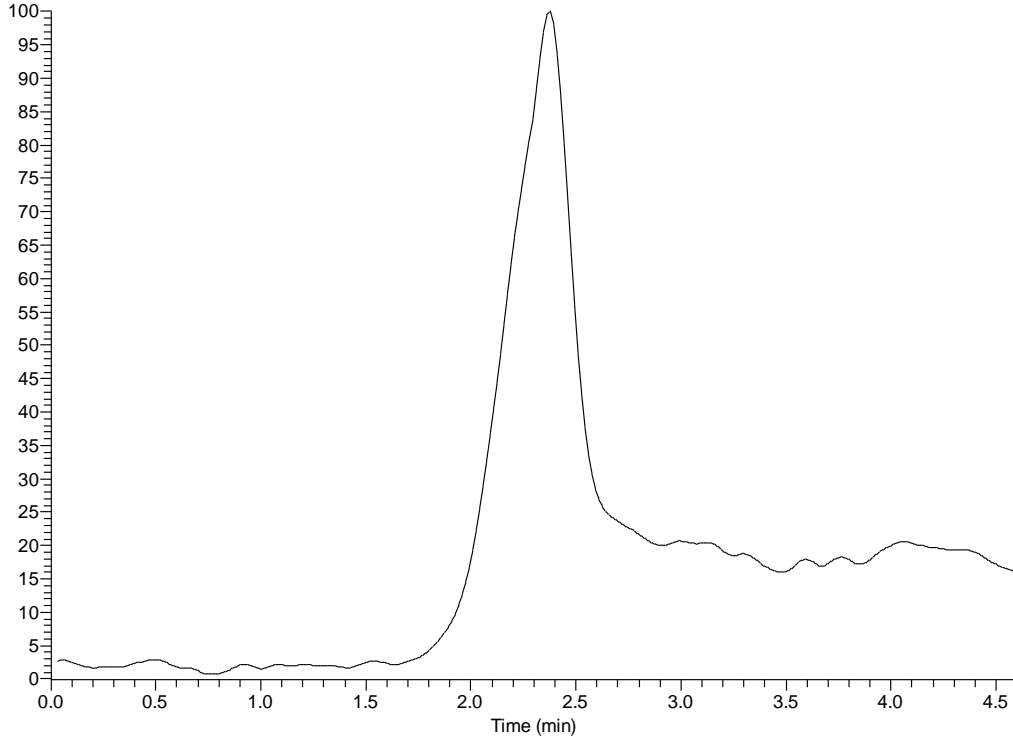


NL:  
5.08E5  
TIC MS  
MAI-  
MORAD-  
7G

MAI-MORAD-7G #156 RT: 2.63 AV: 1 SB: 2 3.31, 3.31 NL: 1.39E4  
T: (0,0) + c EI Full ms [40.00-1000.00]

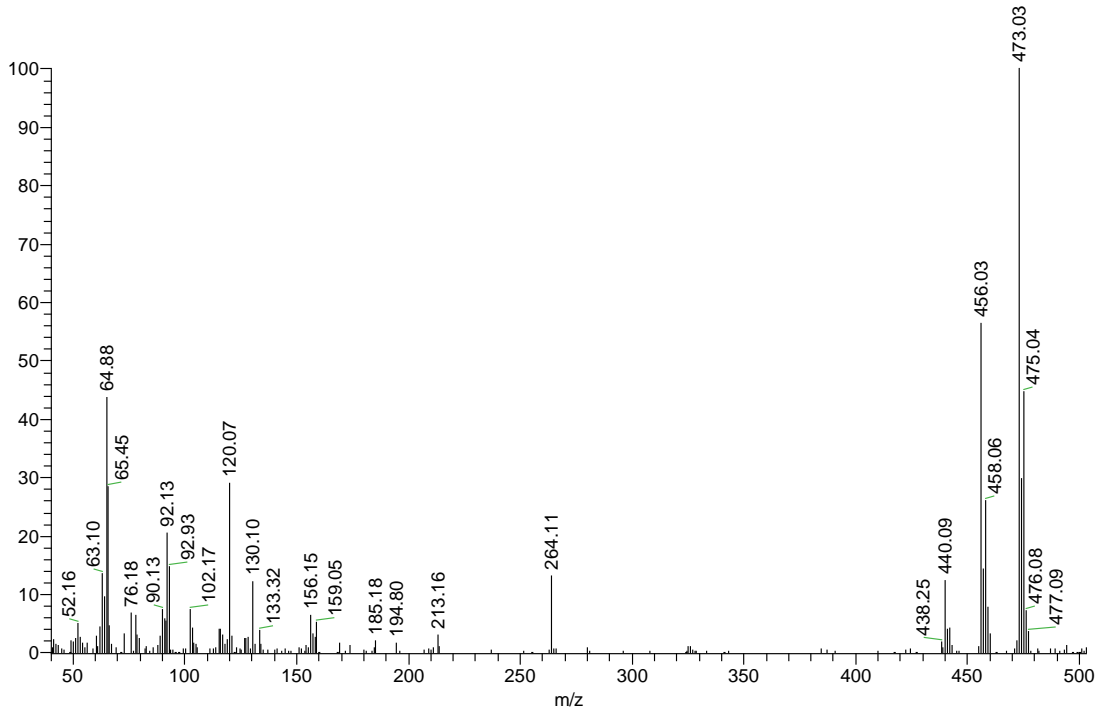


RT: 0.00 - 4.60 SM: 15G



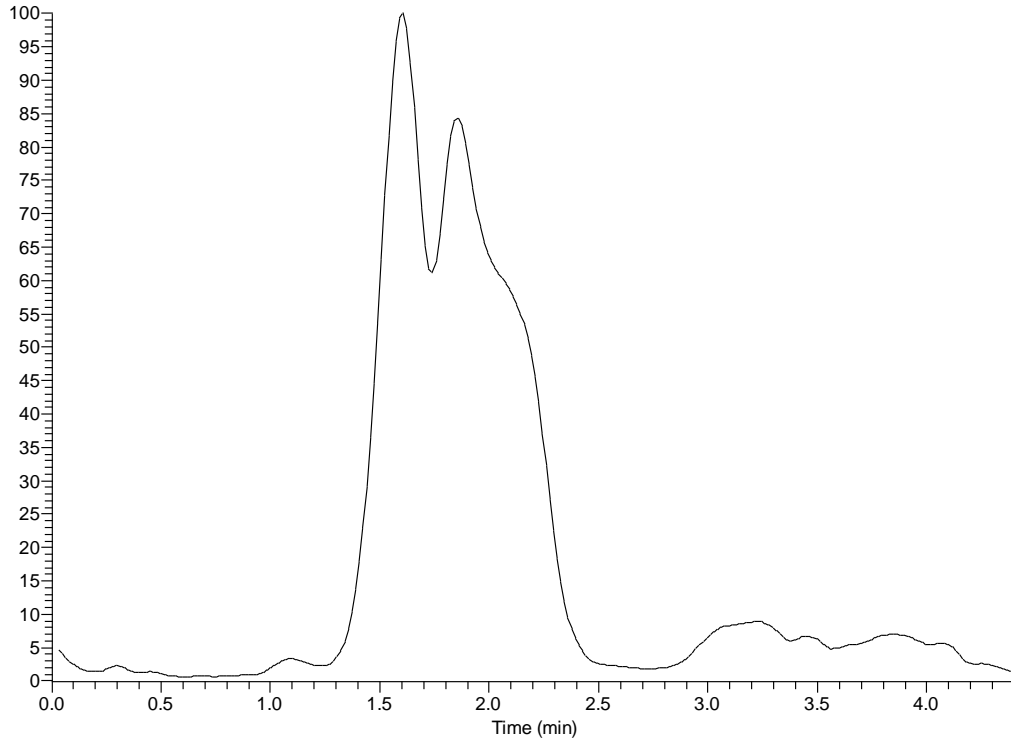
NL:  
7.64E5  
TIC MS  
MAI-  
MORAD-7h

MAI-MORAD-7h #142 RT: 2.39 AV: 1 SB: 2 4.55, 4.59 NL: 5.41E4  
T: (0,0) + c EI Full ms [40.00-1000.00]



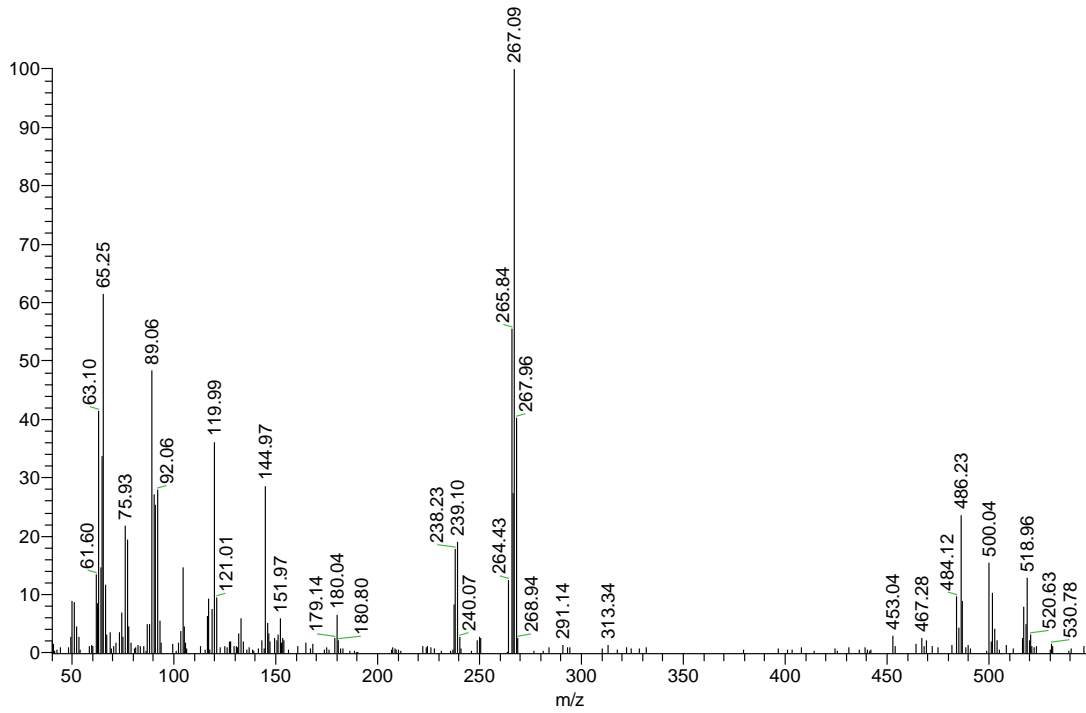


RT: 0.00 - 4.42 SM: 15G

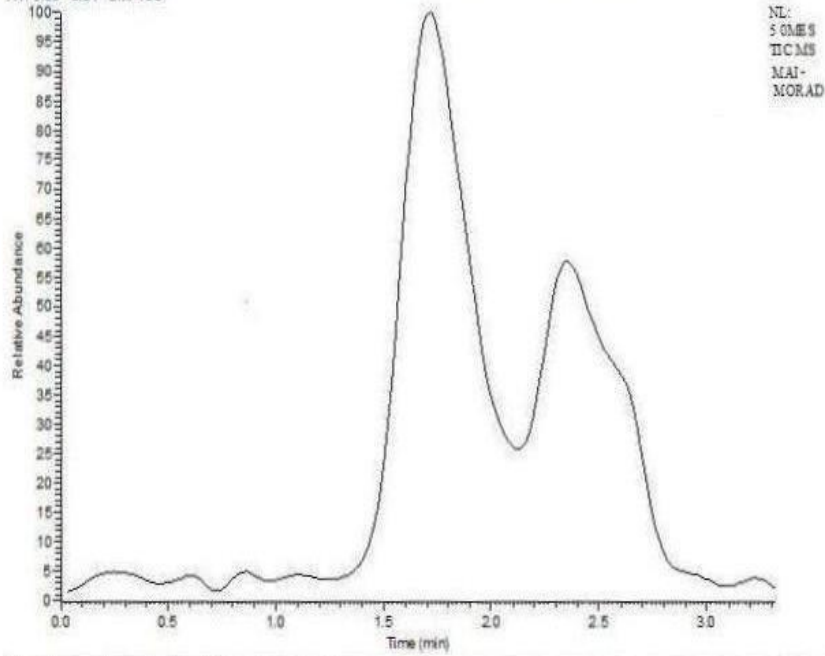


NL:  
4.88E5  
TIC MS  
MAI-  
MORAD-7i

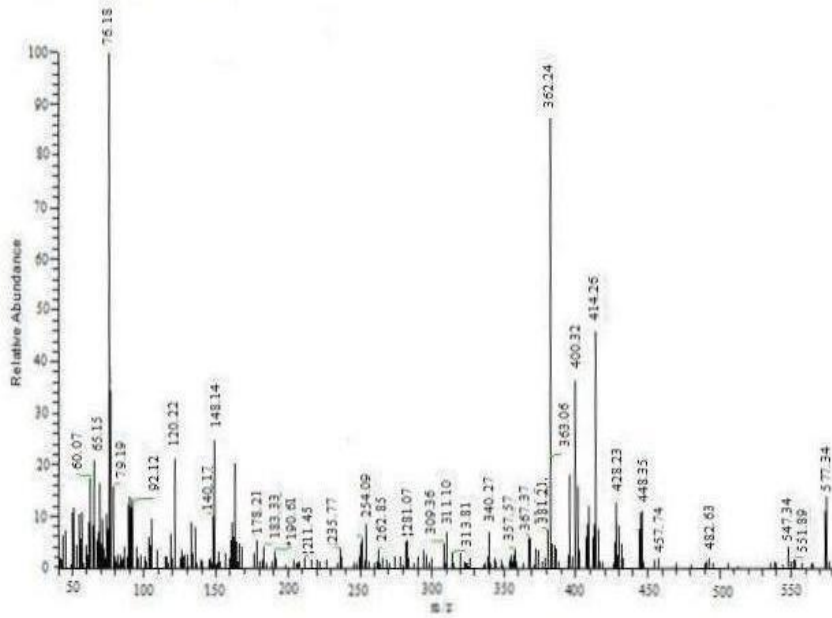
MAI-MORAD-7i #118 RT: 1.99 AV: 1 SB: 2 4.42, 4.42 NL: 2.60E4  
T: (0,0) + c EI Full ms [40.00-1000.00]



RT: 0.00 - 3.31 SM 15G

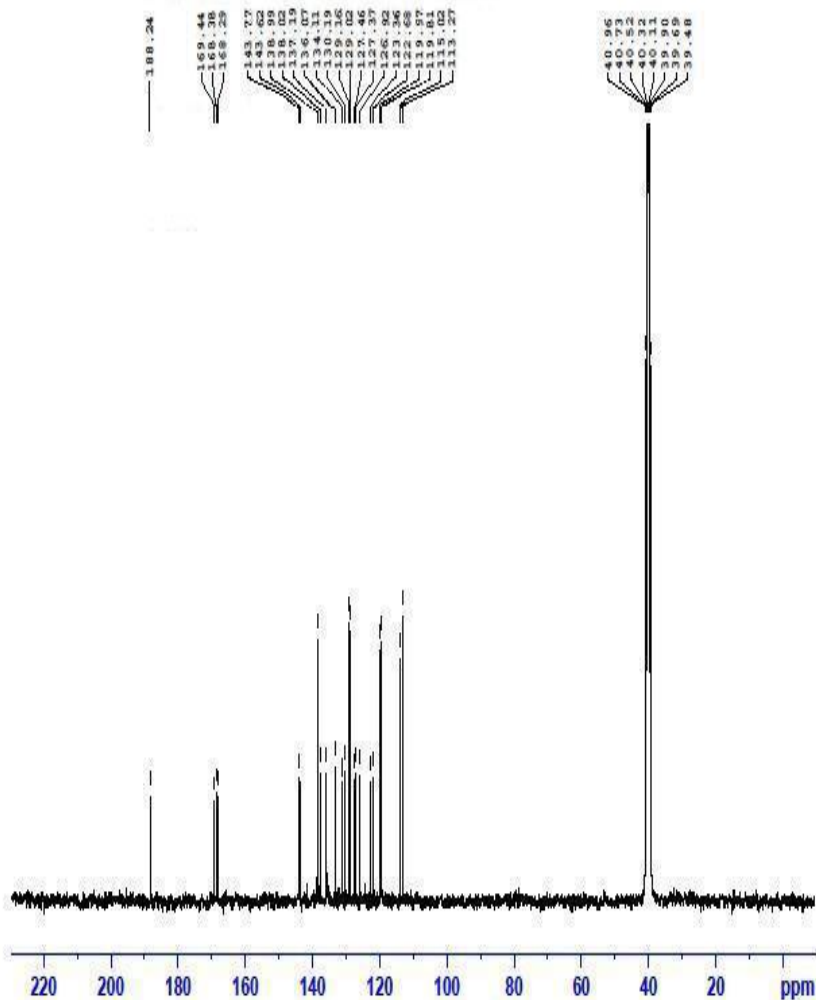


MAI-MORAD-7) 156RT,263 AV, 1 SB 2 331,331 NL :339  
T:(0.0)-:r:EFd ms [40.00-1000.00]



# <sup>13</sup>C NMR:

AM-7a  
c13\_su DMSO (c:\nmr-data) Student 12



Current Data Parameters  
NAME Jan08-2019  
EXPNO 330  
PROCNO 1

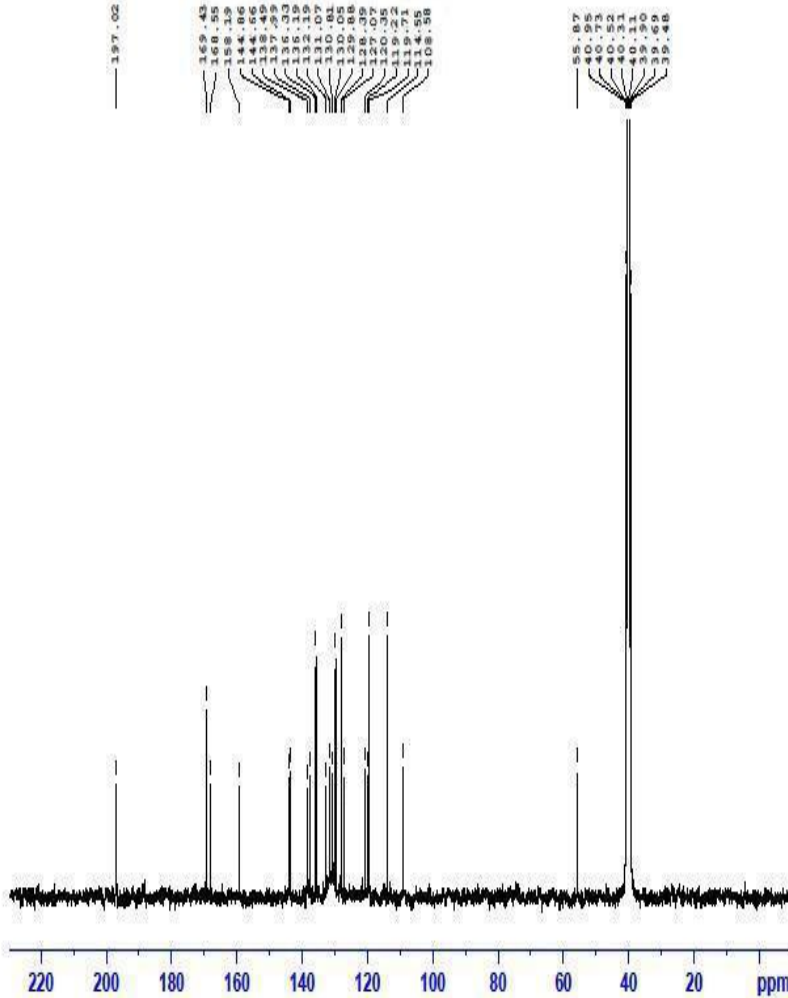
F2 - Acquisition Parameters  
Date\_ 20190109  
Time 3.11  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1200  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 175.84  
DW 20.800 usec  
DE 6.50 usec  
TE 313.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

----- CHANNEL f1 -----  
SFO1 100.6238364 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 56.00000000 W

----- CHANNEL f2 -----  
SFO2 400.1316005 MHz  
NUC2 <sup>1</sup>H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 22.00000000 W  
PLW12 0.41091001 W  
PLW13 0.33284000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 6.00 Hz  
GB 0  
PC 1.40

AM-7c  
 c13\_su DMSO {C:\nmr-data} Student 10



Current Data Parameters  
 NAME Jan08-2019  
 EXPNO 310  
 PROCNO 1

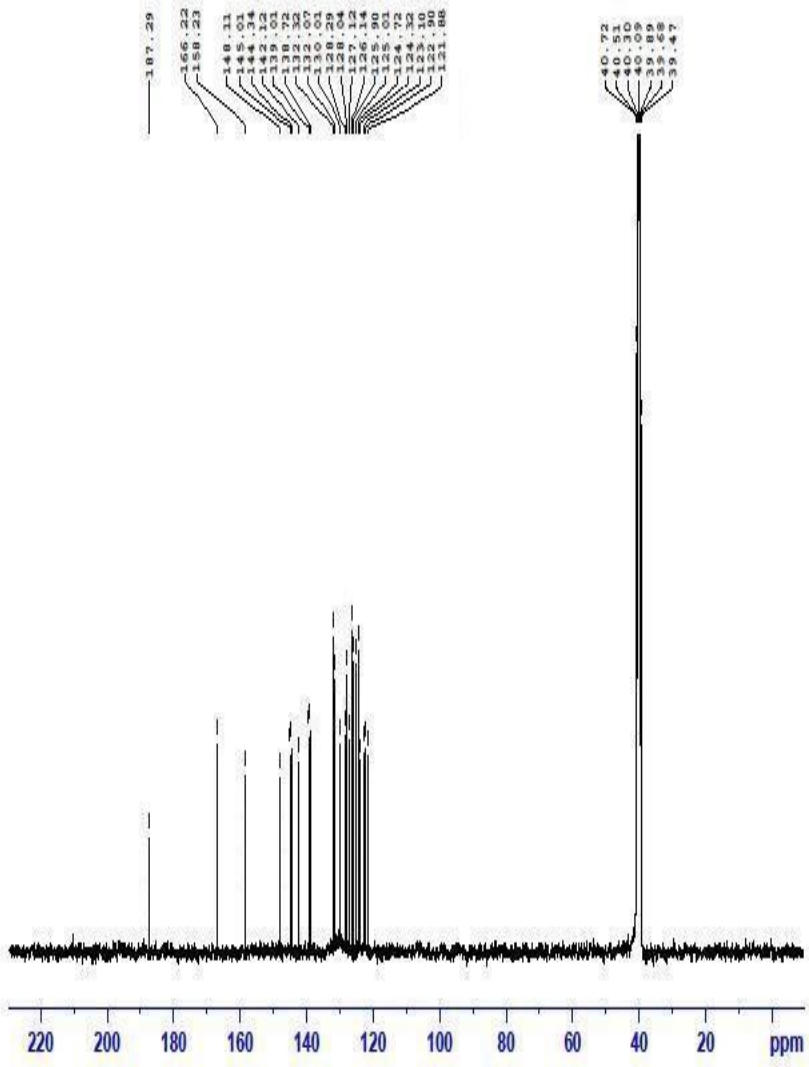
F2 - Acquisition Parameters  
 Date\_ 20190109  
 Time 0.48  
 INSTRUM spect  
 PROHD 5 mm PARBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1200  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 175.84  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 313.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 100.6238364 MHz  
 NUC1 13C  
 P1 9.50 usec  
 PLW1 56.00000000 W

----- CHANNEL f2 -----  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 22.00000000 W  
 PLW12 0.41091001 W  
 PLW13 0.33284000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127690 MHz  
 WDW EM  
 SSB 0  
 LB 6.00 Hz  
 GB 0  
 PC 1.40

AM-7f  
 c13\_su DMSO (C:\nmr-data} Student 11



Current Data Parameters  
 NAME Jan08-2019  
 EXPNO 320  
 PROCNO 1

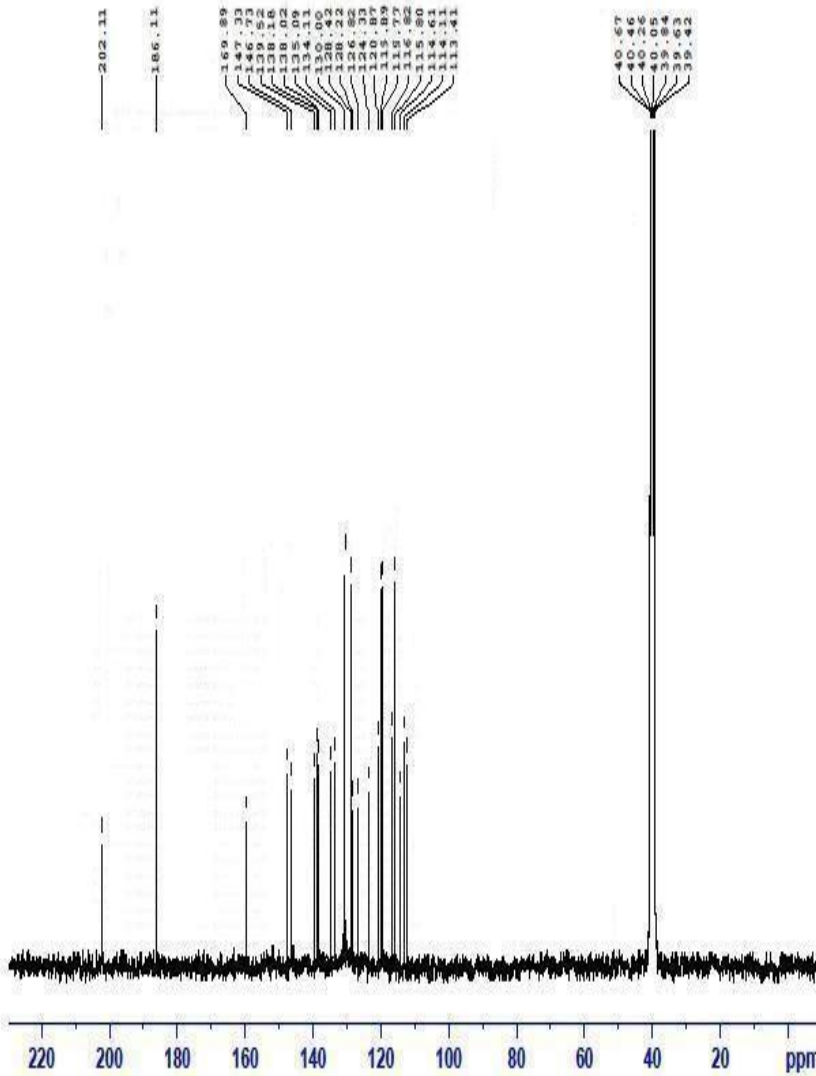
F2 - Acquisition Parameters  
 Date\_ 20190109  
 Time 1.59  
 INSTRUM spect  
 PROBRD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1200  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 106.18  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 313.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 100.6238364 MHz  
 NUC1 13C  
 P1 9.50 usec  
 PLW1 56.00000000 W

----- CHANNEL f2 -----  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CFPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 22.00000000 W  
 PLW12 0.41091001 W  
 PLW13 0.33284000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127690 MHz  
 WDW EM  
 SSB 0  
 LB 6.00 Hz  
 GB 0  
 PC 1.40

AM-7h  
 c13\_su DMSO (C:\nmr-data) Student 5



```

Current Data Parameters
NAME       Jan08-2019
EXPNO     260
PROCNO    1

F2 - Acquisition Parameters
Date_     20190108
Time     18.49
INSTRUM  spect
PROBHD   5 mm FAPBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       1200
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       175.84
DW       20.800 usec
DE       6.50 usec
TE       313.2 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
  
```

```

----- CHANNEL f1 -----
SFO1    100.6238364 MHz
NUC1     13C
P1       9.50 usec
PLW1    56.00000000 W
  
```

```

----- CHANNEL f2 -----
SFO2    400.1316005 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLW2    22.00000000 W
PLW12   0.41091001 W
PLW13   0.33284000 W
  
```

```

F2 - Processing parameters
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       6.00 Hz
GB       0
PC       1.40
  
```

## X-ray structure determination of compound 6

**Table S1. Crystallographic data for compound 6**

| Compound                                   | <b>6</b>  |
|--|---|
| Formula                                    | C <sub>24</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub> |
| <i>M<sub>r</sub></i>                       | 398.40  |
| Temperature (K)                            | 100   |
| Crystal habit                              | colourless plate  |
| Crystal size (mm)                          | 0.15 × 0.10 × 0.04  |
| Crystal system                             | Monoclinic  |
| Space group                                | <i>P</i> 2 <sub>1</sub> / <i>c</i>                            |
| Cell dimensions:                           |   |
| <i>a</i> (Å)                               | 6.5120(3)   |
| <i>b</i> (Å)                               | 33.6736(13)   |
| <i>c</i> (Å)                               | 8.5409(3)   |
| β (°)                                      | 95.237(4)   |
| Cell volume (Å <sup>3</sup> )              | 1865.06   |
| <i>Z</i>                                   | 4   |
| <i>D<sub>x</sub></i> (g cm <sup>-3</sup> ) | 1.419   |
| Radiation, wavelength (Å)                  | Cu <i>K</i> α, 1.54184 Å                                      |
| μ (mm <sup>-1</sup> )                      | 0.80  |
| 2θ(max) (°)                                | 154.8   |
| Reflections collected                      | 39381   |
| Independent reflections                    | 3927  |
| R(int)                                     | 0.031   |
| Transmissions                              | 0.728 – 1.000   |
| No. of parameters                          | 276   |
| Goodness-of-fit on <i>F</i> <sup>2</sup>   | 1.04  |
| <i>wR</i> 2 (all reflections)              | 0.092   |
| <i>R</i> 1 ( <i>F</i> > 4σ( <i>F</i> ))    | 0.036   |
| Max. Δρ (e Å <sup>-3</sup> )               | 0.22  |

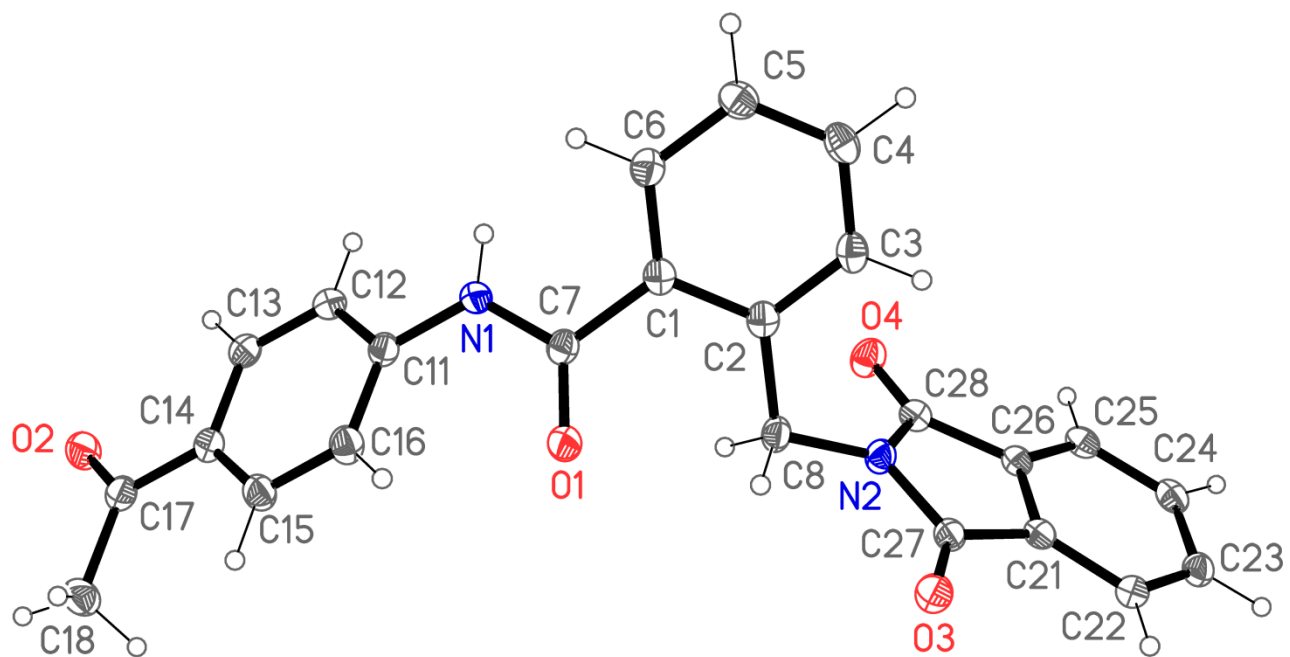


Fig. S1. The structure of compound **6** in the crystal. Ellipsoids represent 50% probability levels.



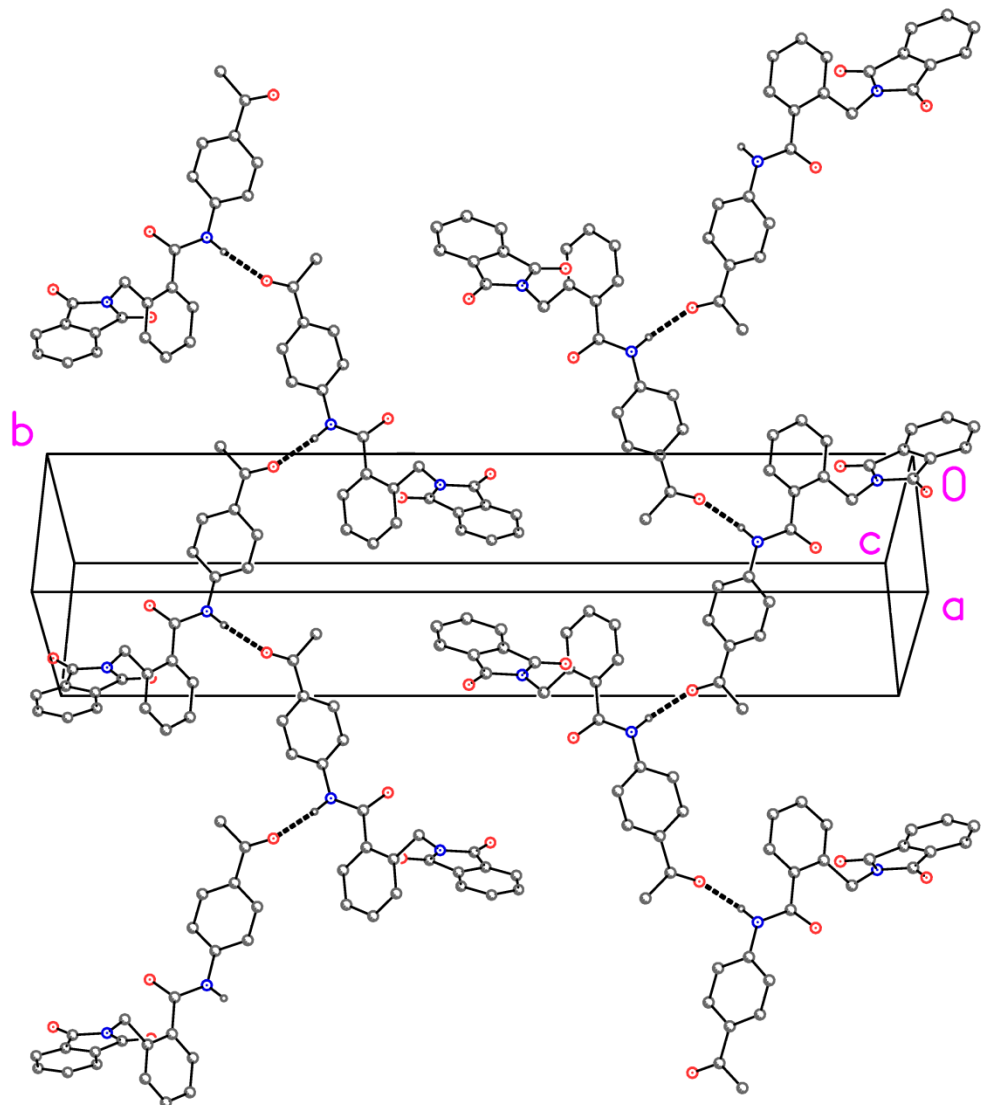


Fig. S2. Packing diagram of compound **6**. Thick dashed lines indicate classical hydrogen bonds N1–H01...O2 via the *c* glide plane. Molecules are linked to form chains parallel to [201]. View direction is perpendicular to  $(10\bar{2})$ . Hydrogen atoms not involved in hydrogen bonding are omitted for clarity.