

Supporting informations data

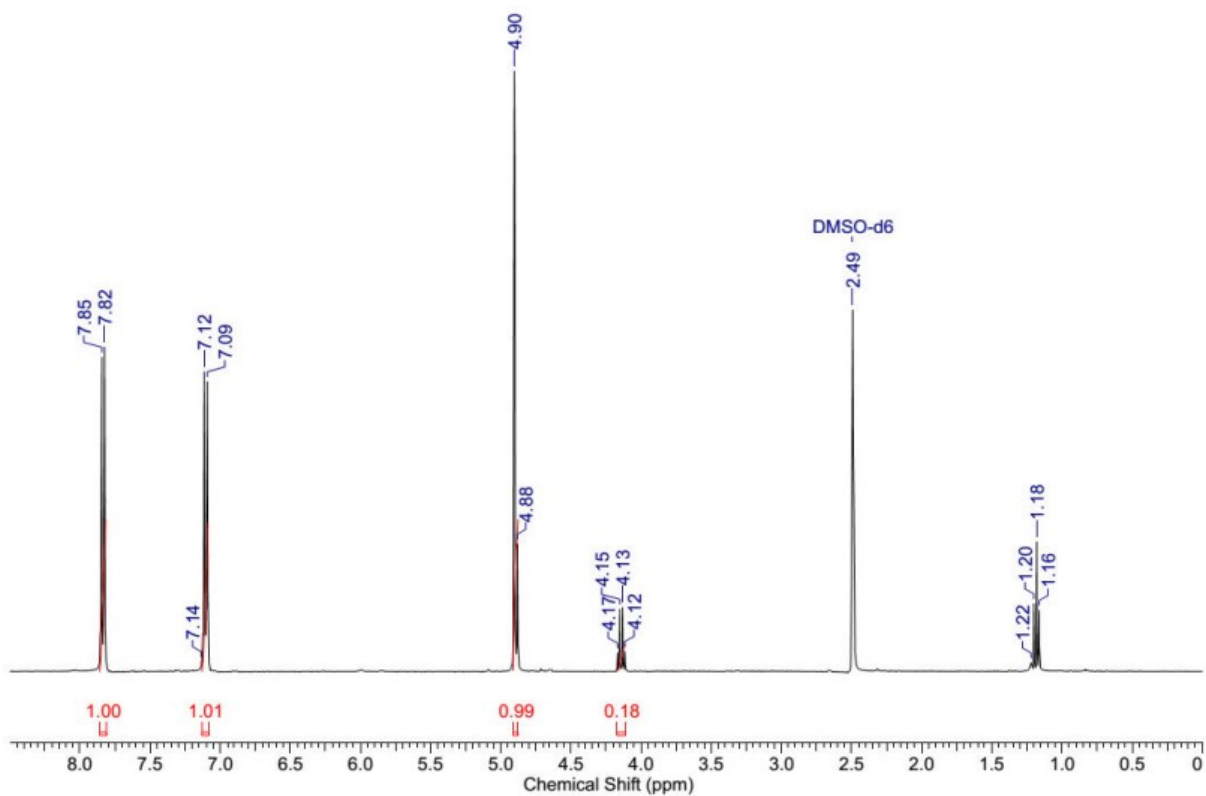


Figure S1: ^1H NMR OF COMPOUND SM2

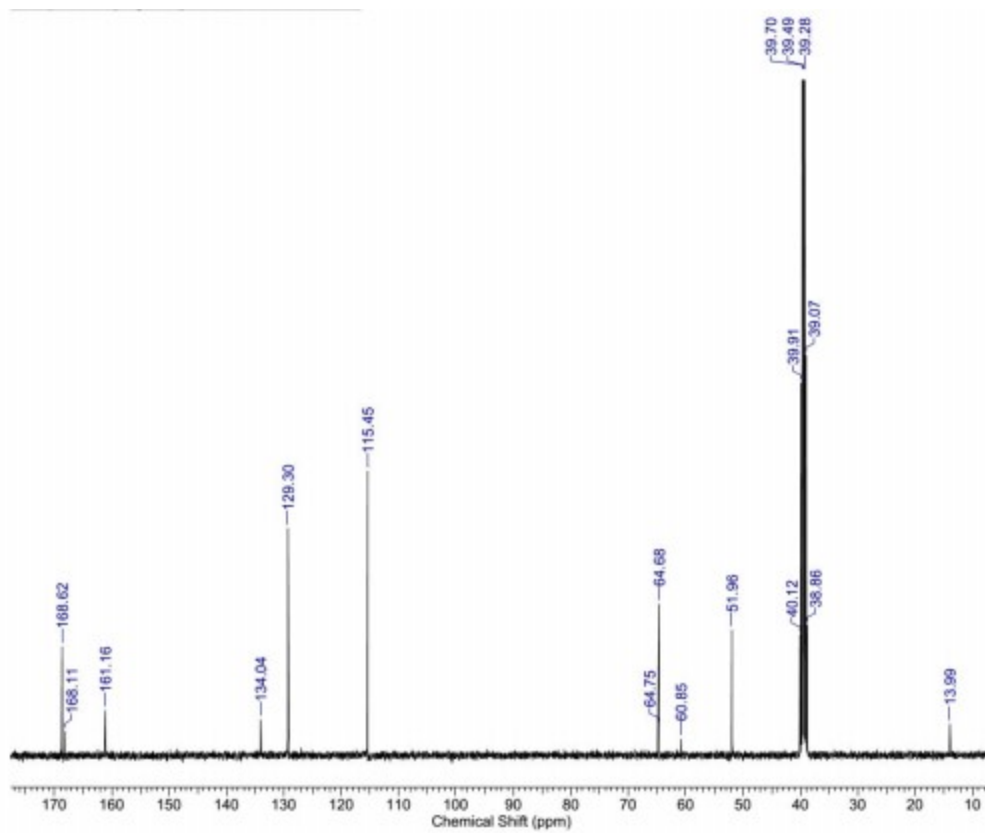


Figure S2: ¹³C NMR OF COMPOUND SM2

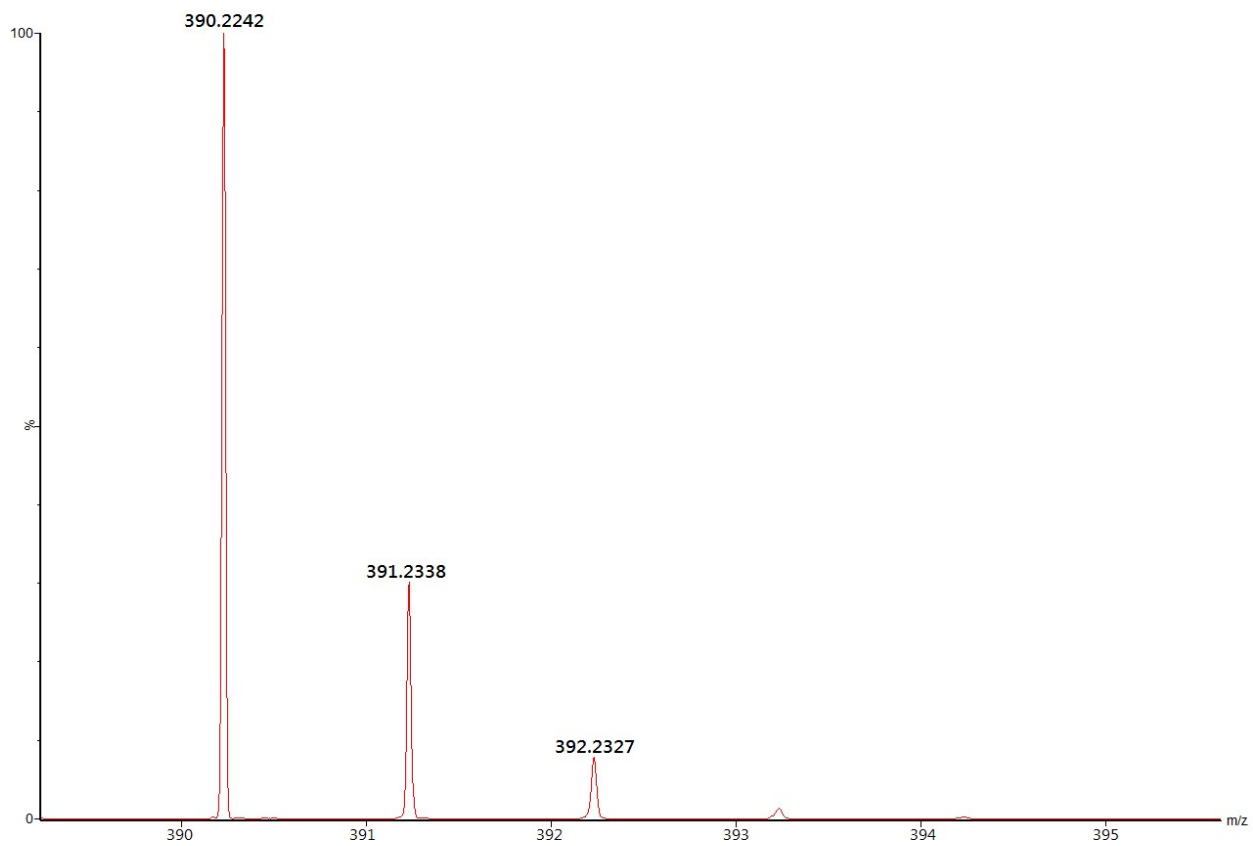


Figure S3: HR-MS OF COMPOUND SM2

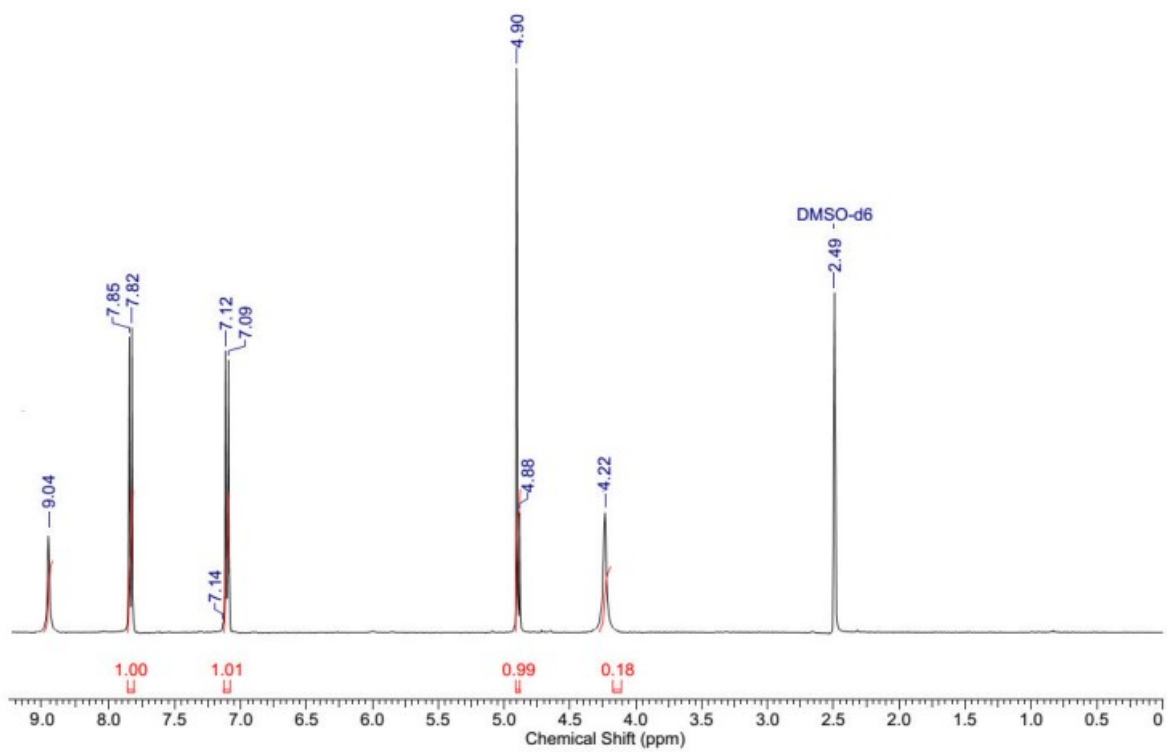


Figure S4: ^1H NMR OF COMPOUND SM3

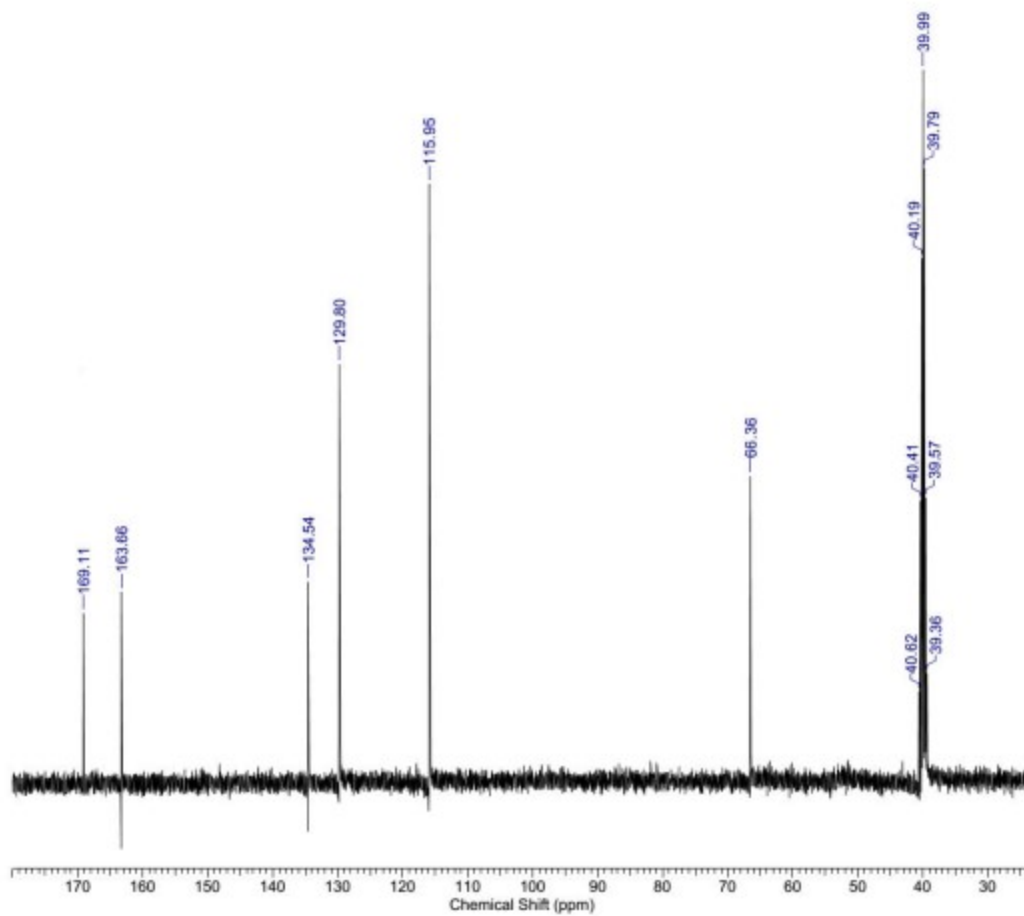


Figure S5: ¹³C NMR OF COMPOUND SM3

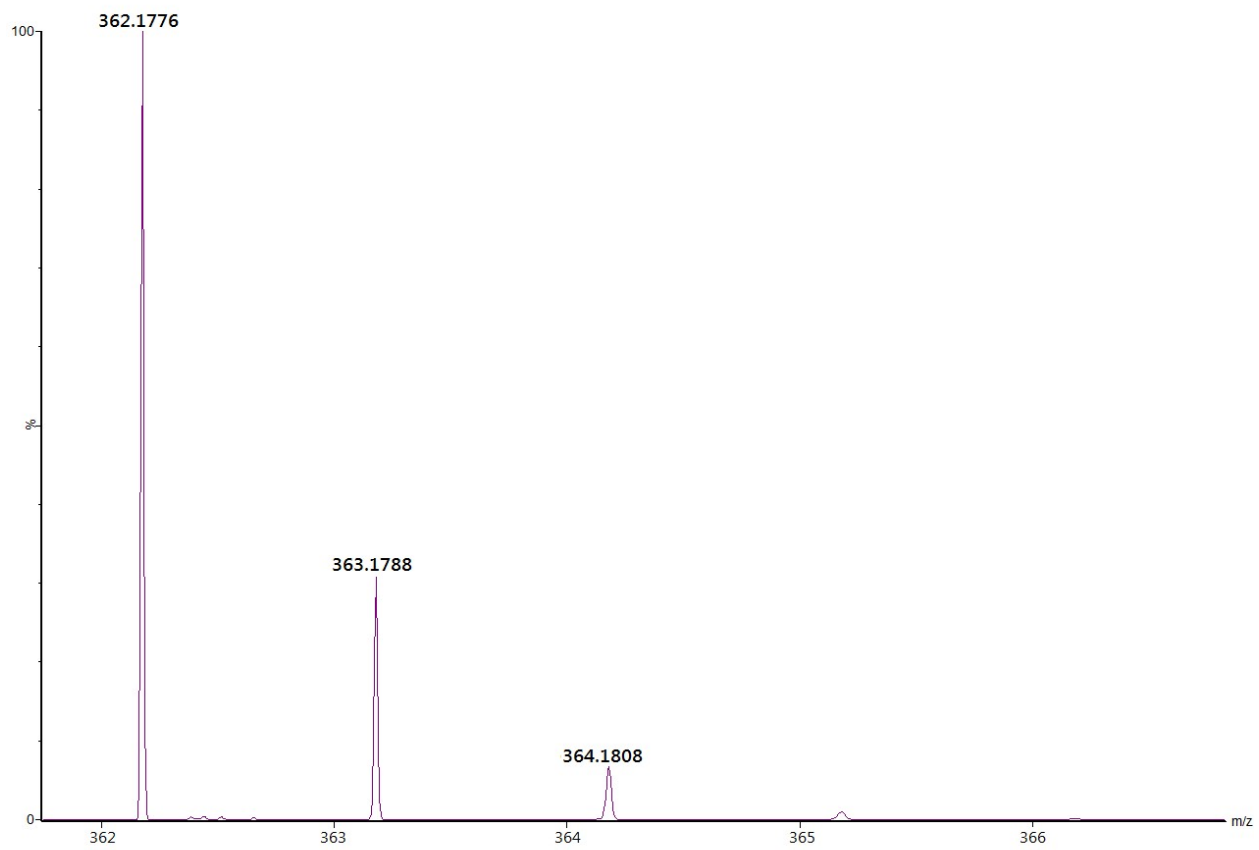


Figure S6: HR-MS OF COMPOUND SM3

Dr. Ajmal/Prof. Ahmed/M1M01/DMSO
PROTON

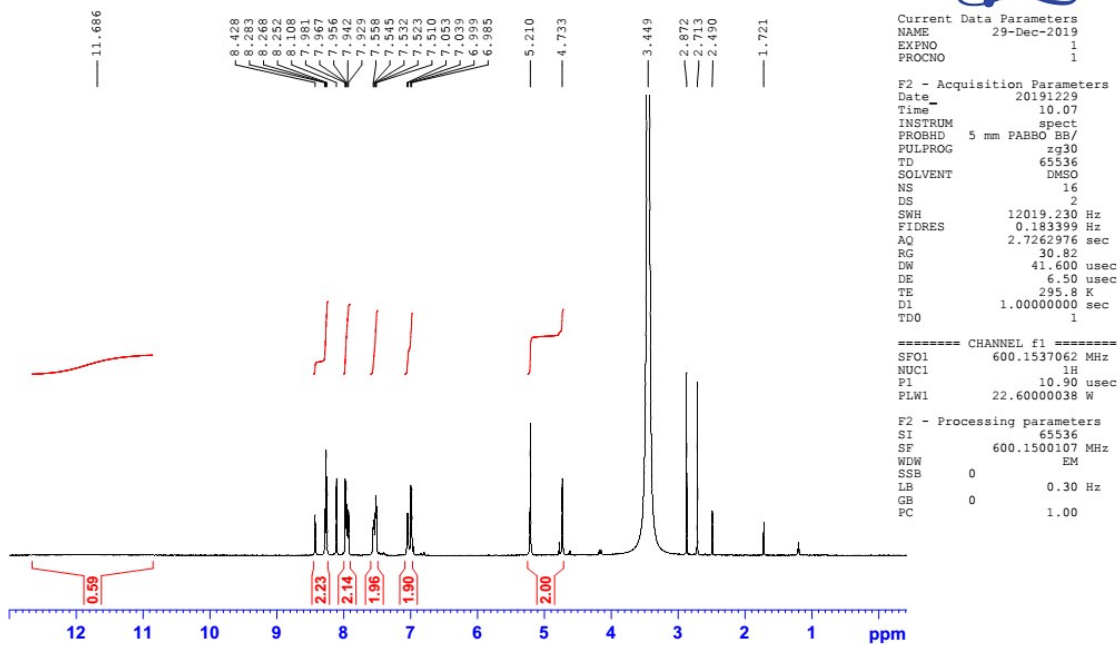
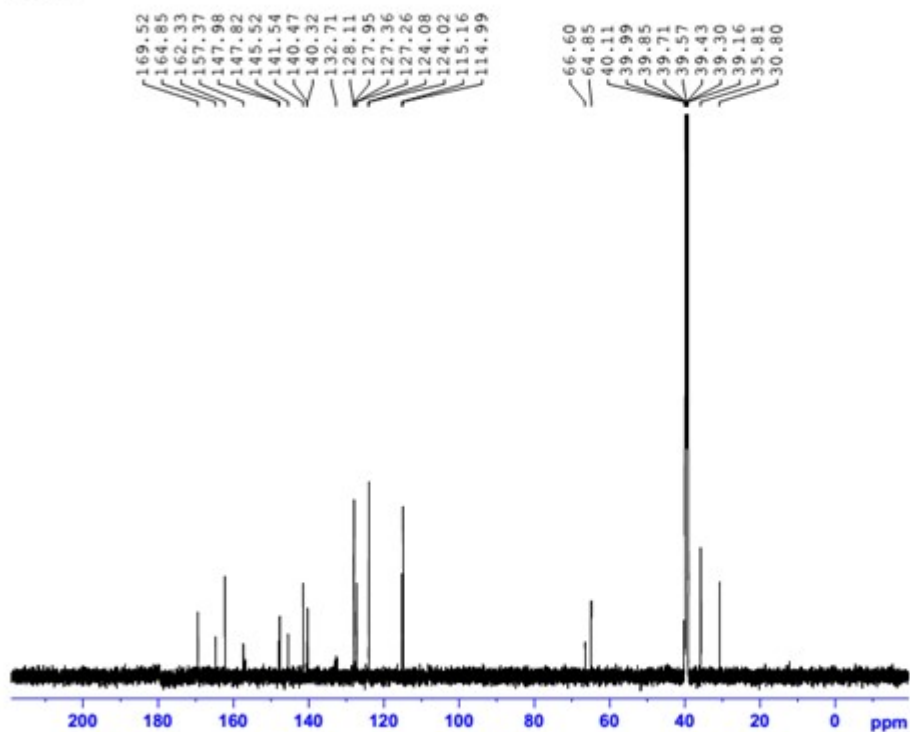


Figure S7: ^1H NMR OF COMPOUND 4a

Dr. Ajmal / MIM01 / DMSO
C13CPD



Current Data Parameters
NAME 25-Jan-2021
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210123
Time 22.23
INSTRUM spect
PROBHD 5 mm DSSBO 1H/1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.5087659 sec
RG 155.2
DM 13.947 usec
DE 6.30 usec
TE 294.6 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 150.9229276 MHz
MDC1 13C
P1 11.40 usec
PLW1 83.0000000 W

----- CHANNEL f2 -----
SFO2 400.1524006 MHz
MDC2 1H
CPCPRG2 waltz16
PCPD2 70.00 usec
PLW2 22.6000000 W
PLW3 0.5280400 W
PLW3 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9079041 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S8: ¹³C NMR OF COMPOUND 4a

Sample Name	MIM-01	Position	Vial 31	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-01_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 3:24:47 PM

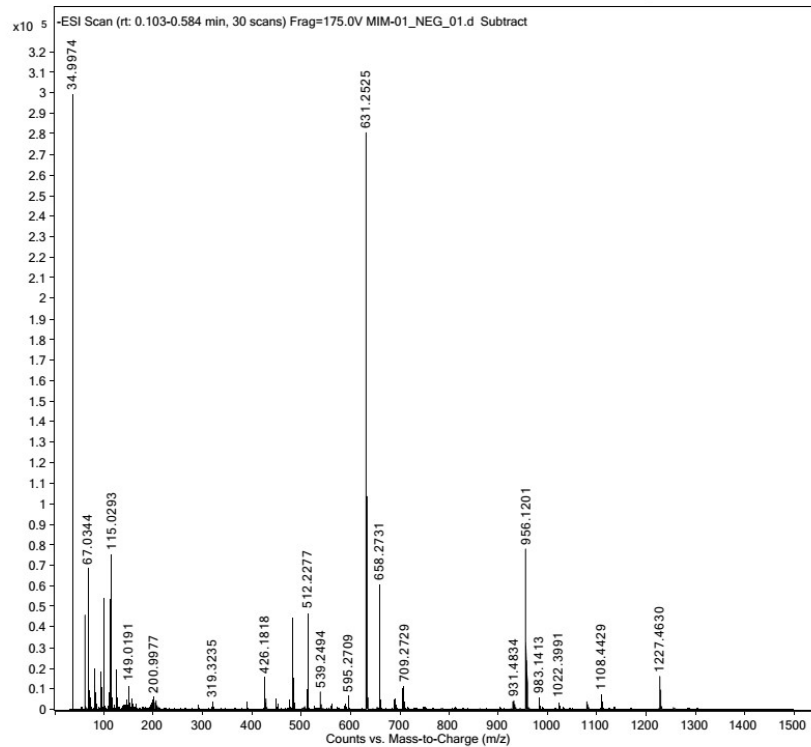


Figure S9: HR-MS OF COMPOUND 3a

Dr. Ajmal/Prof. Ahmed/M1M02/DMSO
PROTON

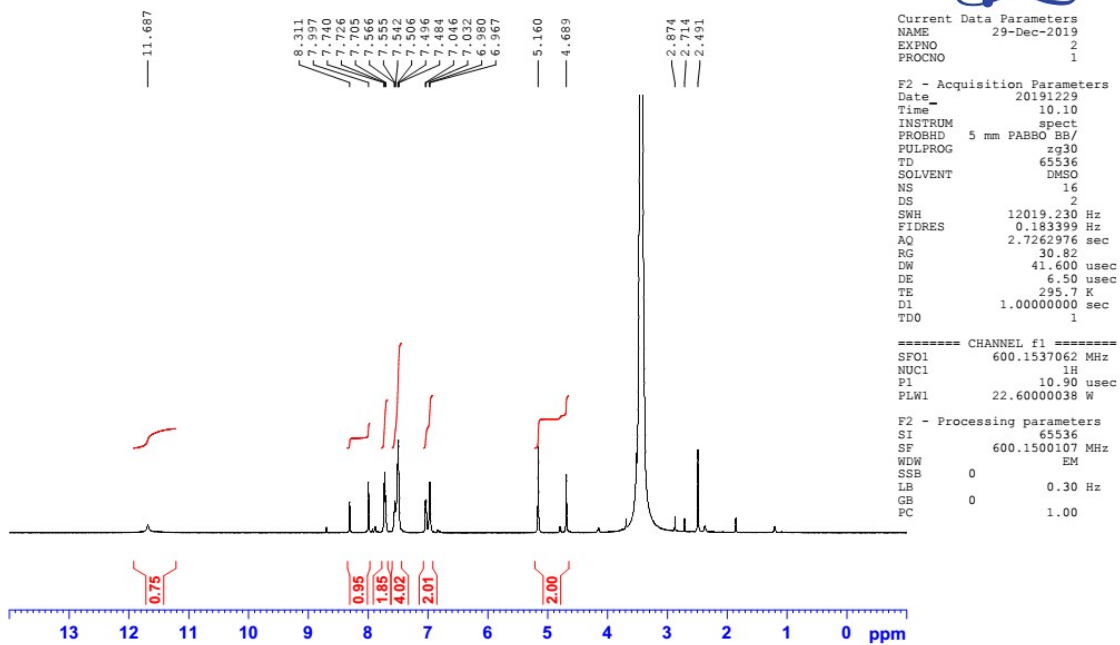
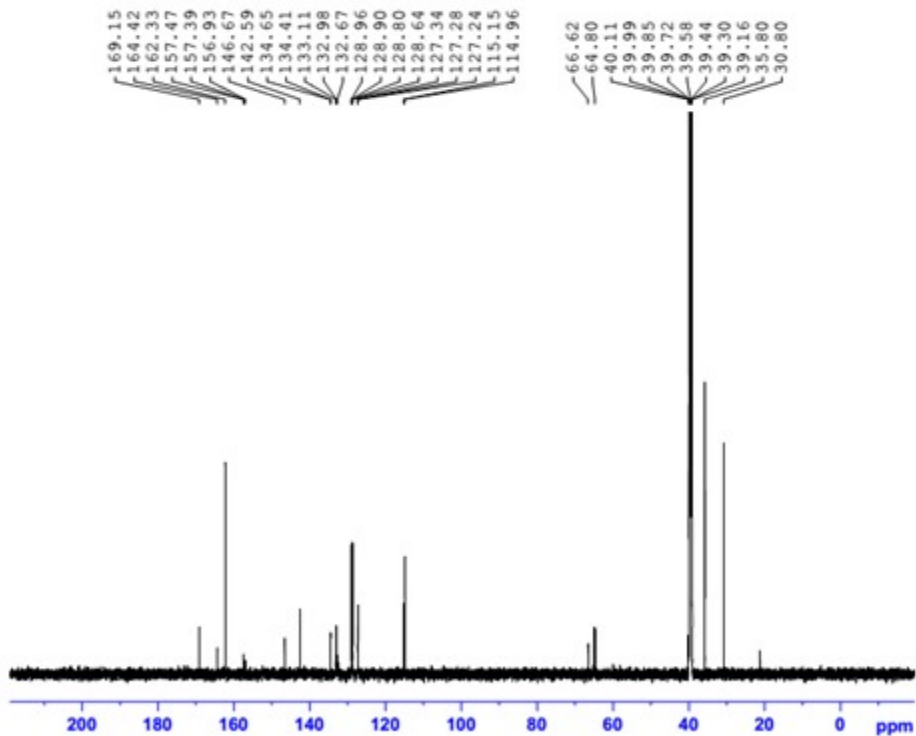


Figure S10: ¹H NMR of compound 4b

Dr. Ajmal / MIM02 / DMSO
C13CPD



Current Data Parameters
NAME 23-Jun-2021
EXPRNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 2810126
Time 2.48
INSTRUM spect
PROBHD 5 mm PABBO 50/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 3657.692 Hz
FIDRES 0.580197 Hz
AQ 0.5087659 sec
RG 193.2
WE 11.847 usec
DE 4.50 usec
TE 296.2 K
D1 2.0000000 sec
D11 0.0100000 sec
TD 1

===== CHANNEL f1 =====
SFO1 150.921276 MHz
NUC1 13C
P1 11.40 usec
PLW1 83.0000000 W

===== CHANNEL f2 =====
SFO2 600.1324006 MHz
NUC2 1H
CFOFPG2 waltz16
PCPD2 70.00 usec
PLW2 22.6000000 W
PLW3 0.5200000 W
PLW4 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9079041 MHz
WDW EM
SSB 0
LA 1.00 Hz
GB 0
PC 1.40

Figure S11: ^{13}C NMR OF COMPOUND 4b

Sample Name	MIM-02	Position	Vial 32	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-02_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 3:31:54 PM

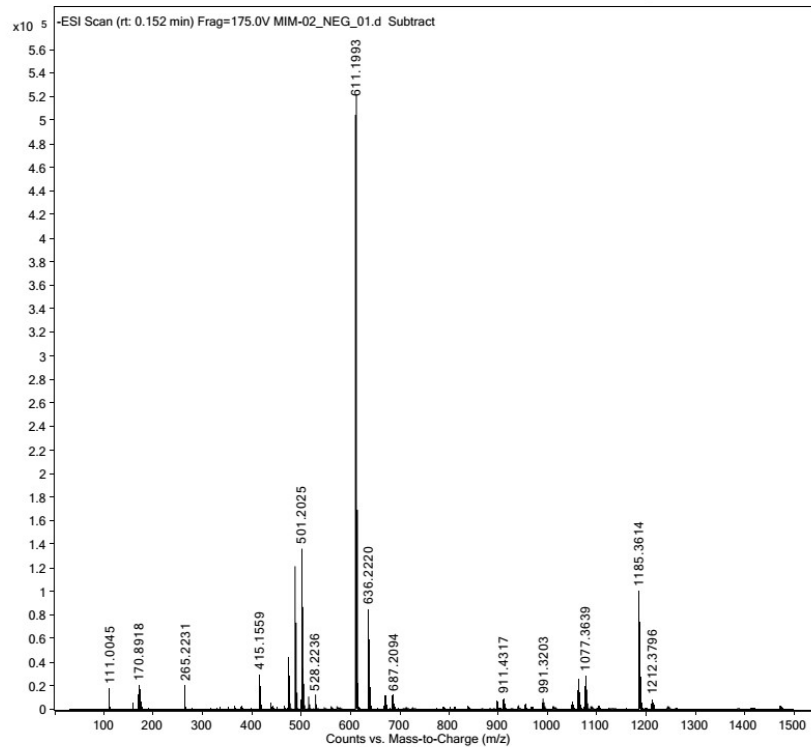


Figure S12: HR-MS OF COMPOUND 4b

Dr. Ajmal/Prof. Ahmed/M1M03/DMSO
PROTON

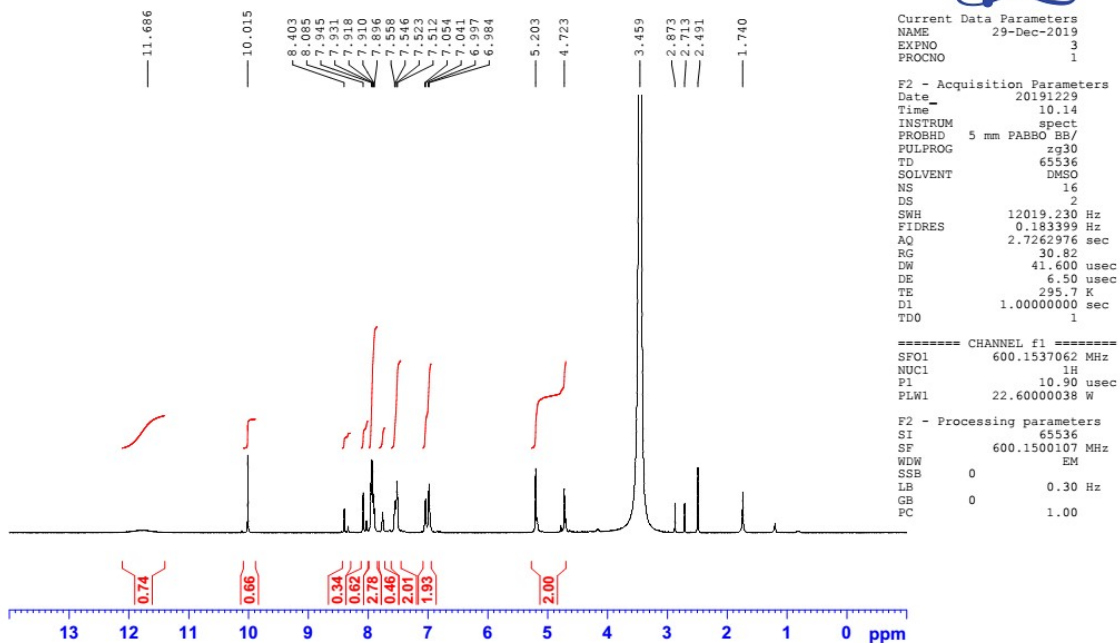
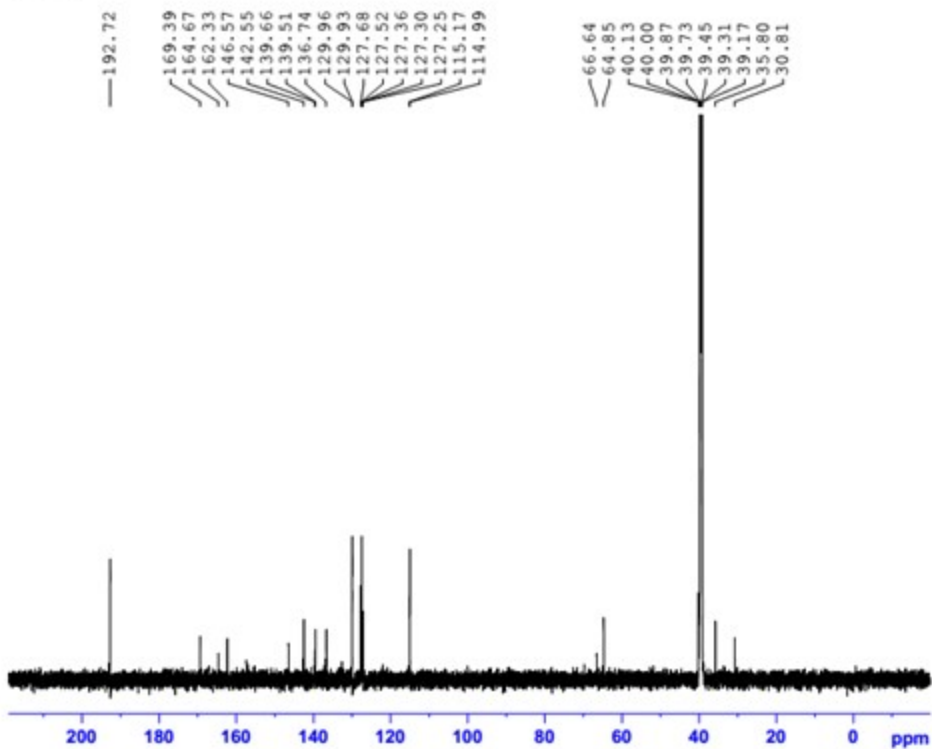


Figure S13: ^1H NMR OF COMPOUND 4c

Dr. Ajmal / MIM03 / DMSO
C13CPD



```
Current Data Parameters
NAME      28-Jan-2021
EXPRO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20210128
Time      22.46
INSTRUM   spect
PROBHD    5 mm VASBO 5B7
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         4096
DS         4
SWH        36057.691 Hz
FIDRES     0.550197 Hz
AQ         0.9087659 sec
RG         195.2
CW         11.567 usec
DE         6.50 usec
TE         296.4 K
D1         2.0000000 sec
d11        0.0300000 sec
TD0        1

----- CHANNEL f1 -----
SFO1      150.9229276 MHz
NUC1       13C
P1         11.60 usec
PLW1       83.0000000 W

----- CHANNEL f2 -----
SFO2      600.1524004 MHz
NUC2       1H
CPCPRG2   waltz16
PCPD2     70.00 usec
PLW2      22.6000000 W
PLW3      0.5280600 W
PLW4      0.25874999 W

F2 - Processing parameters
SI         32768
SF         150.9079041 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

Figure S14: ¹³C NMR OF COMPOUND 4c

Sample Name	MIM-03	Position	Vial 33	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-03_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 3:39:01 PM

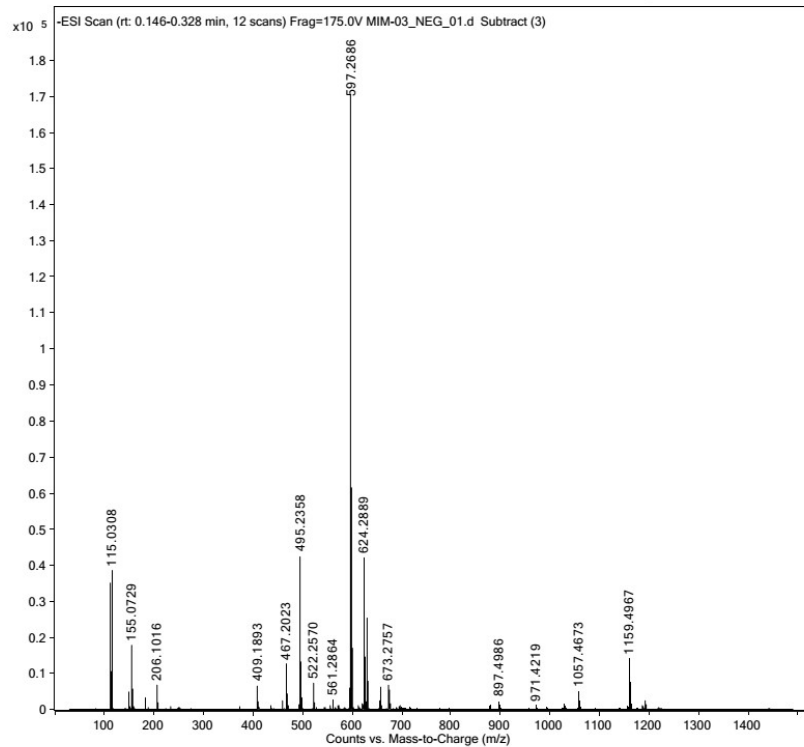


Figure S15: HR-MS OF COMPOUND 4c

Dr. Ajmal/Prof. Ahmed/M1M-04/DMSO
PROTON

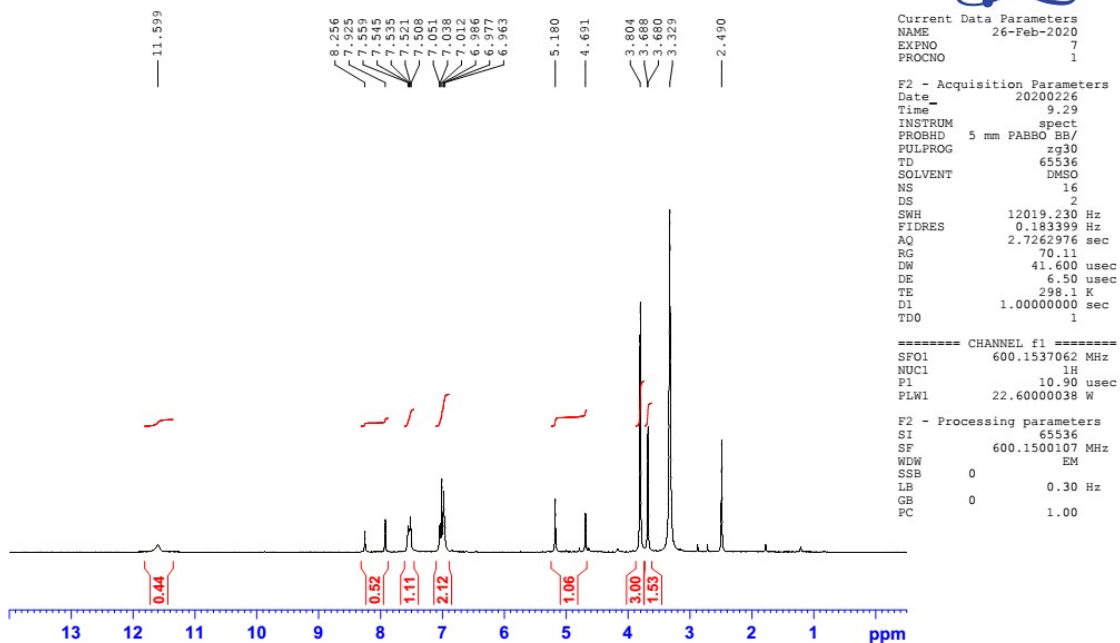
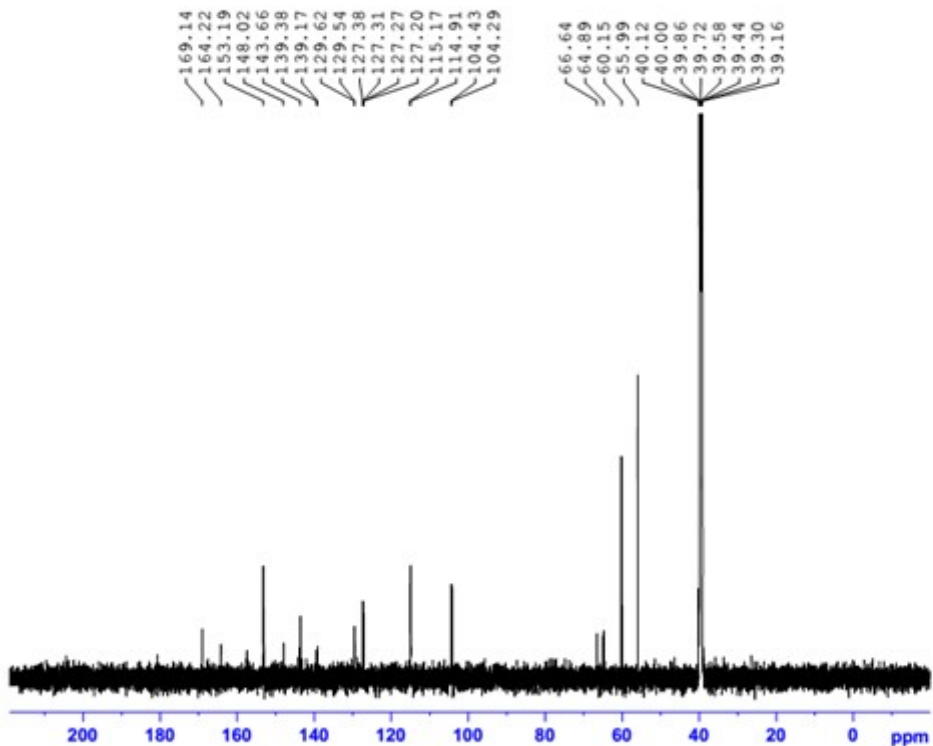


Figure S16: ^1H NMR OF COMPOUND 4d

Dr. Ajmal / MIM04 / DMSO
C13CPD



```
Current Data Parameters
NAME      28-Jan-2021
EXPNO    4
PROCNO   1

F2 - Acquisition Parameters
Date_    20210129
Time     4.20
INSTRUM  spect
PROBHD   5 mm BBOBO 1H/
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        2048
DS        4
SWH       34057.475 Hz
FIDRES    0.592197 Hz
AQ        0.9087659 sec
RG         195.2
DW        13.947 usec
DE         4.50 usec
TE        296.4 K
D1        2.0000000 sec
D11       0.0300000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     150.921776 MHz
MPC1     13C
P1        11.40 usec
PLA1     83.00000000 W

===== CHANNEL f2 =====
SFO2     400.1524006 MHz
MPC2     1H
CPDPRG2  waltz16
PCPD2    70.00 usec
PLA2     22.40000038 W
PLA22    0.52404002 W
PLA23    0.25874999 W

F2 - Processing parameters
SI        32768
SF        150.9079041 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

Figure S17: ^{13}C NMR OF COMPOUND 4d

Sample Name	MIM-04	Position	Vial 34	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-04_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 3:46:08 PM

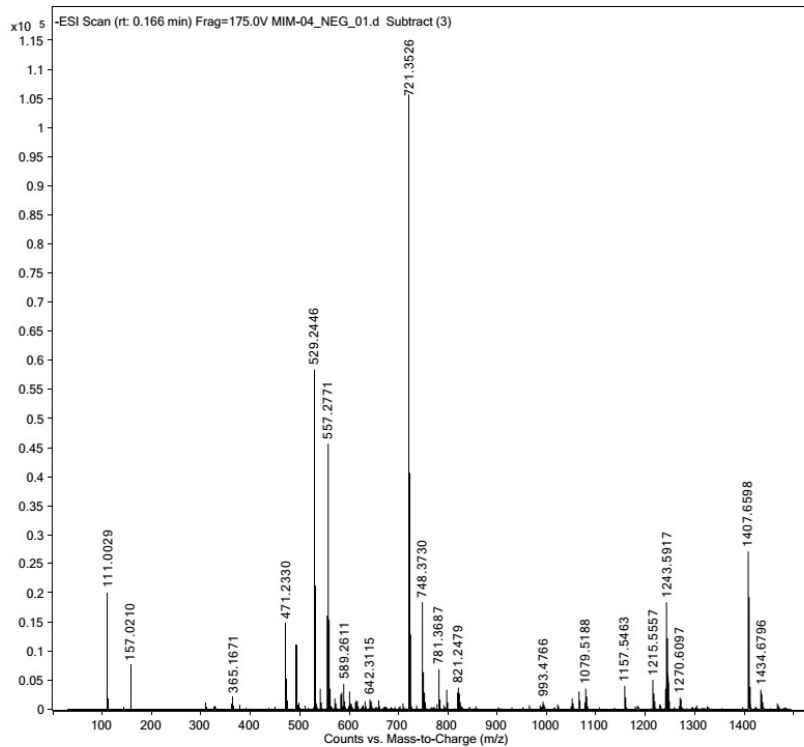


Figure S18: HR-MS OF COMPOUND 4d

Dr. Ajmal/Prof. Ahmed/M1M-05/DMSO
PROTON

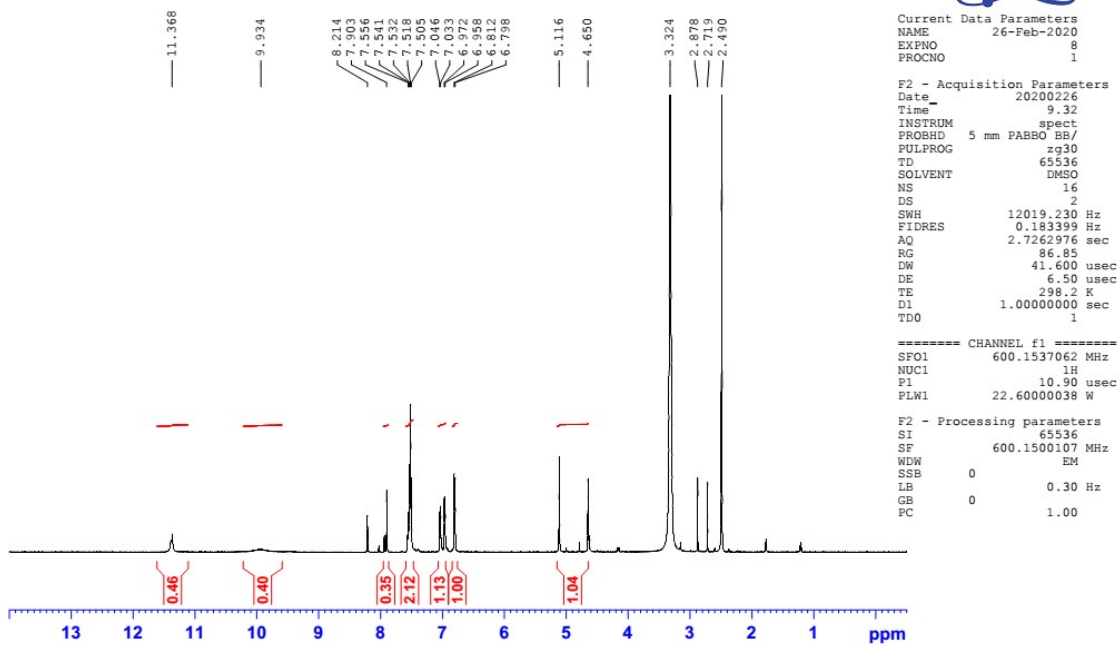
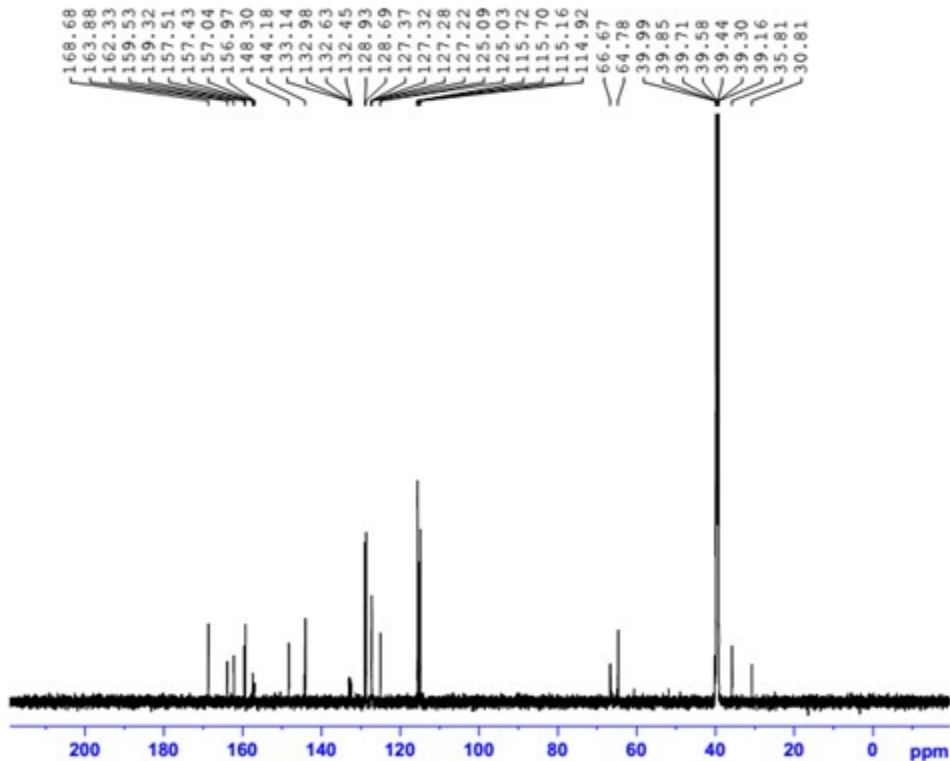


Figure S19: ^1H NMR OF COMPOUND 4e

Dr. Ajmal / MIM05 / DMSO
C13CPD



Current Data Parameters
NAME 25-Jan-2021
EXPNO 28
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210126
Time 6.24
INSTROM spect
PROBHD 5 mm BBOBO 507
PULPROG zgpg30
TD 65536
SOLVENT dmsd
NS 2048
DS 4
SWH 34057.491 Hz
FIDRES 0.550197 Hz
AQ 0.9097459 sec
RG 195.2
DM 13.867 usec
DE 6.50 usec
TE 296.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TUD 1

***** CHANNEL f1 *****
SFO1 150.9229274 MHz
NUC1 13C
P1 11.60 usec
PLW1 83.0000000 W

***** CHANNEL f2 *****
SFO2 600.1524006 MHz
NUC2 1H
PCPORG2 waix16
PCPD2 30.00 usec
PLW2 22.6000000 W
PLW3 0.52804002 W
PLW4 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9079041 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S20: ¹³C NMR OF COMPOUND 4e

Sample Name	MIM-05	Position	Vial 35	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-05_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 3:53:16 PM

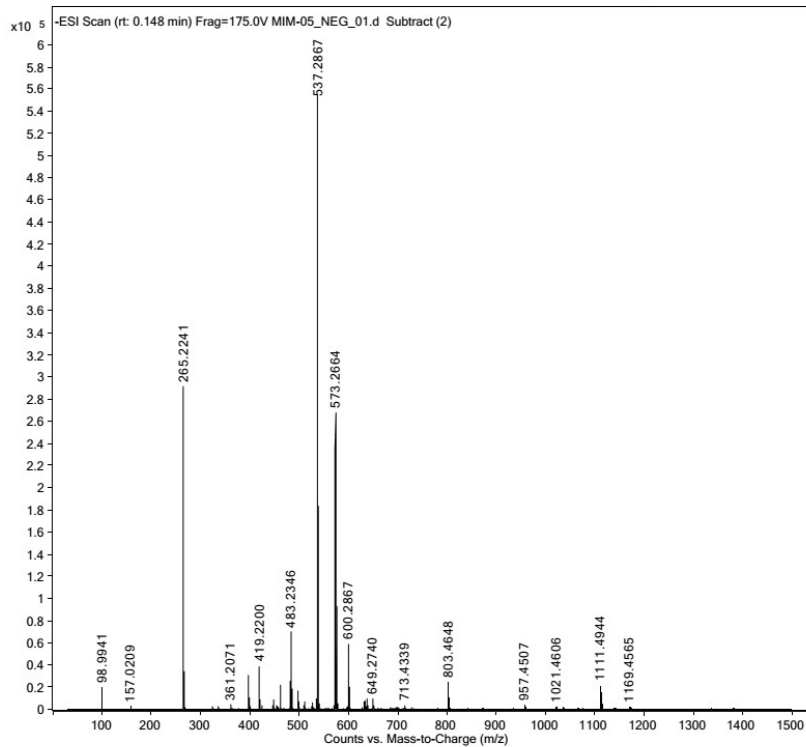


Figure S21: HR-MS OF COMPOUND 4e

Dr. Ajmal/Prof. Ahmed/M1M-06/DMSO
PROTON

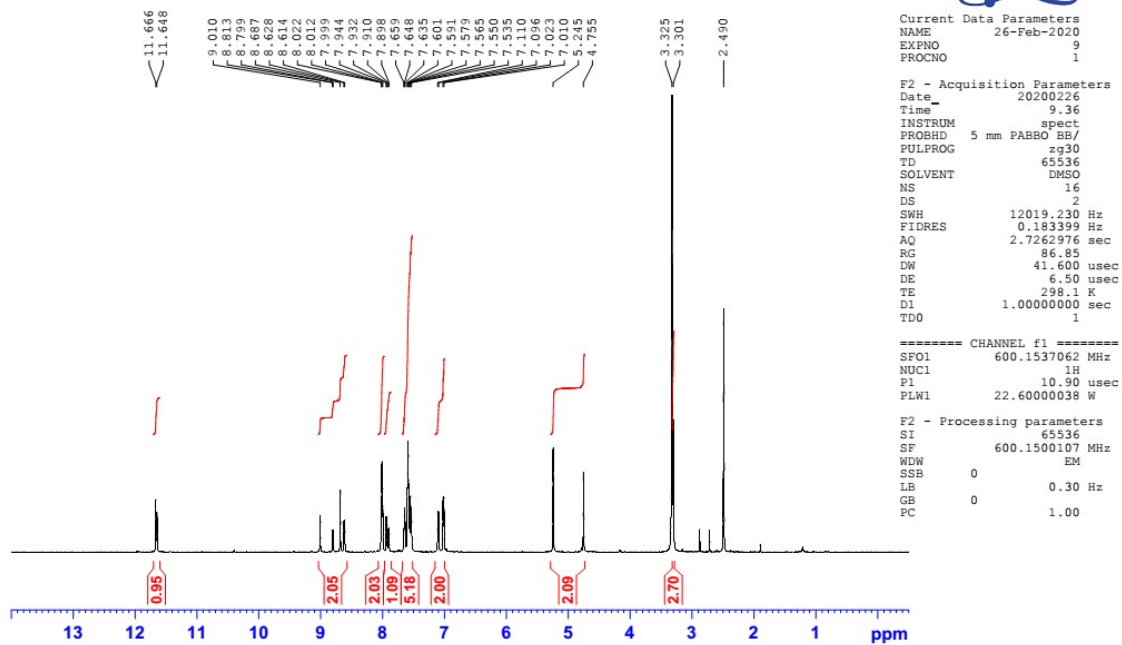
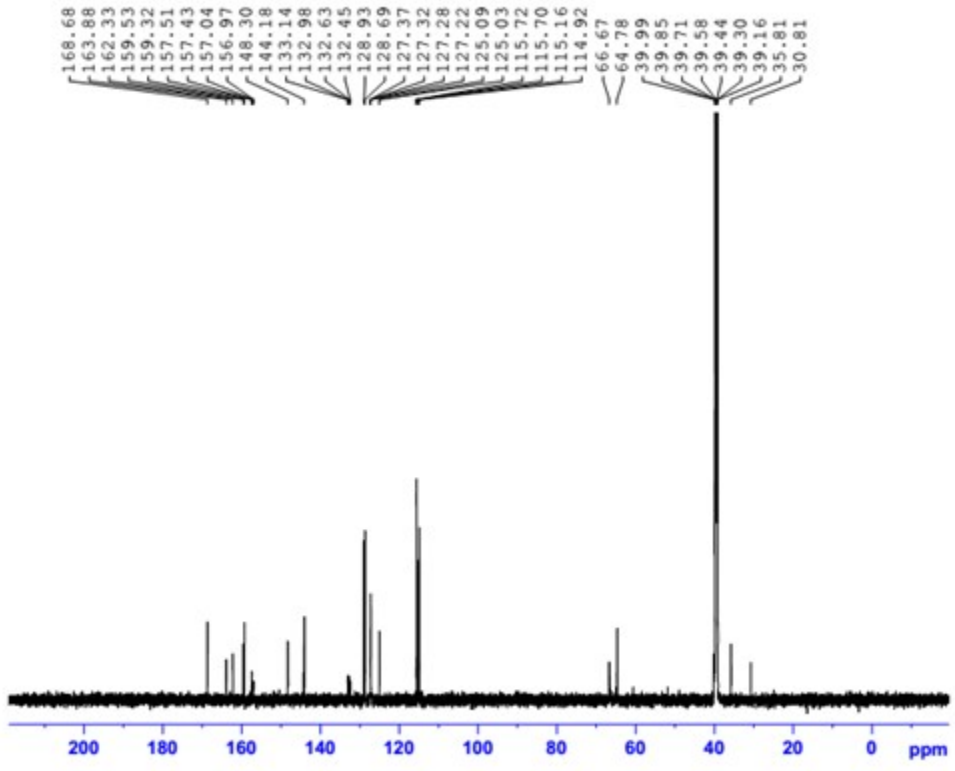


Figure S22: ¹H NMR OF COMPOUND 4f

Dr. Ajmal / MIM06 / DMSO
C13CPD



Current Data Parameters
NAME 25-Jan-2021
EXPRO 28
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210126
Time 6.24
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087450 sec
RG 195.2
DW 13.987 usec
DE 6.50 usec
TE 296.2 K
D1 2.0000000 sec
D11 0.3300000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 150.9229276 MHz
NUC1 13C
P1 11.60 usec
PL1 83.0000000 W

----- CHANNEL f2 -----
SFO2 400.1524004 MHz
NUC2 1H
CPCORR2 wait14
PCPD 70.00 usec
PLM2 22.6000000 W
PLM1 0.3280600 W
PLM3 0.35874999 W

F2 - Processing parameters
S1 32768
SF 150.9079041 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S23: ¹³C NMR OF COMPOUND 4f



Figure S24: HR-MS OF COMPOUND 4f

Dr. Ajmal/Prof. Ahmed/M1M-07/DMSO
PROTON

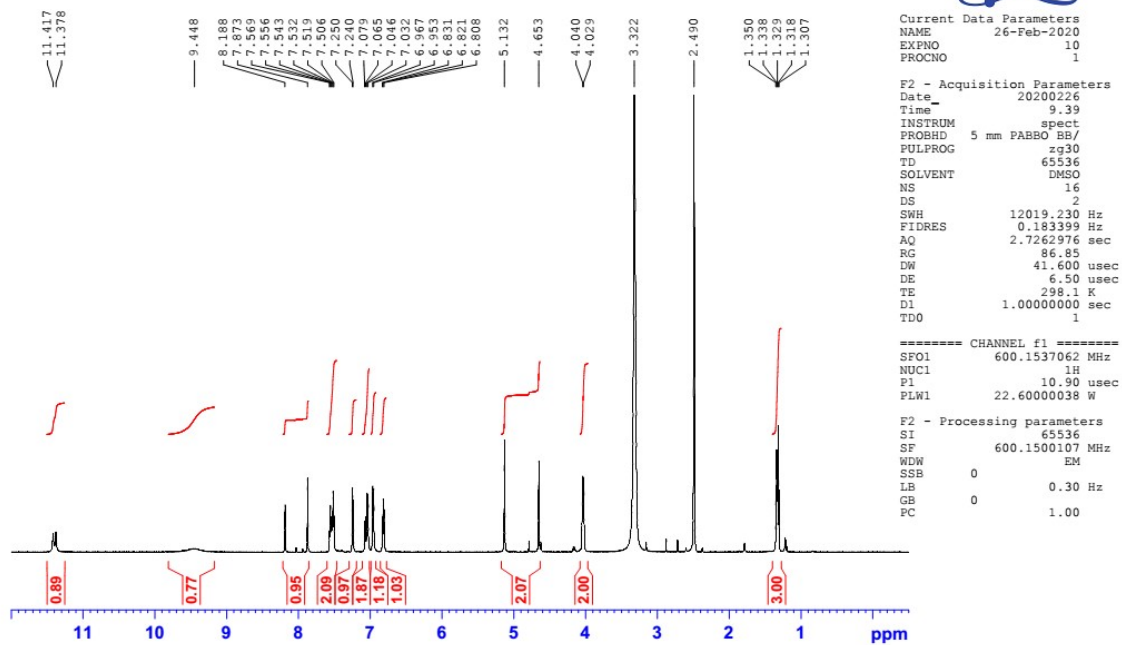
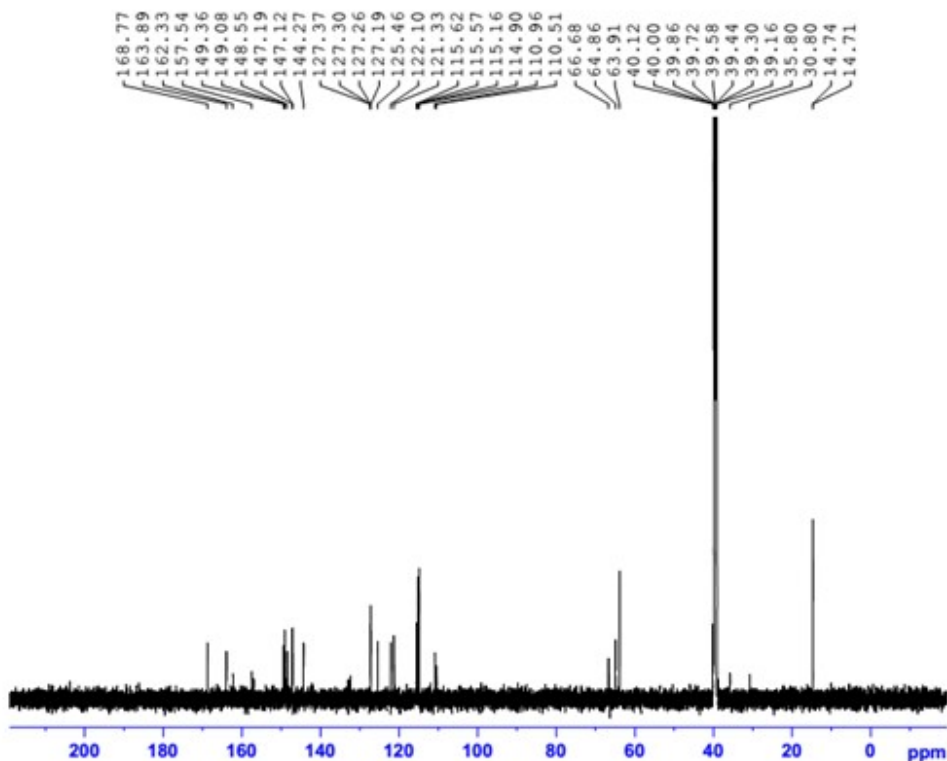


Figure S25: ^1H NMR OF COMPOUND 4g

Dr. Ajmal / MIM07 / DMSO
C13CPD



```
Current Data Parameters
NAME      28-Jan-2021
EXNO      26
PROCNO    1

F2 - Acquisition Parameters
Date_     20210130
Time      1.56
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         65534
SOLVENT   DMSO
NS         2048
DS         4
SWH        36057.691 Hz
FIDRES     0.550197 Hz
AQ         0.9087659 sec
RG         199.2
DM         13.867 usec
DE         6.50 usec
TE         296.4 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      150.9229276 MHz
MPC1      13C
PI         11.40 usec
PLM1      83.00000000 W

===== CHANNEL f2 =====
SFO2      600.1524006 MHz
MPC2      1H
CPCPRG2   waltz16
PCPD2     70.00 usec
PLM2      22.60000038 W
PLM12     0.82806002 W
PLM13     0.25874999 W

F2 - Processing parameters
SI         32768
SF         150.9079041 MHz
MSW        6M
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

Figure S26: ¹³C NMR OF COMPOUND 4g

Sample Name	MIM-07	Position	Vial 37	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-07_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 4:07:30 PM

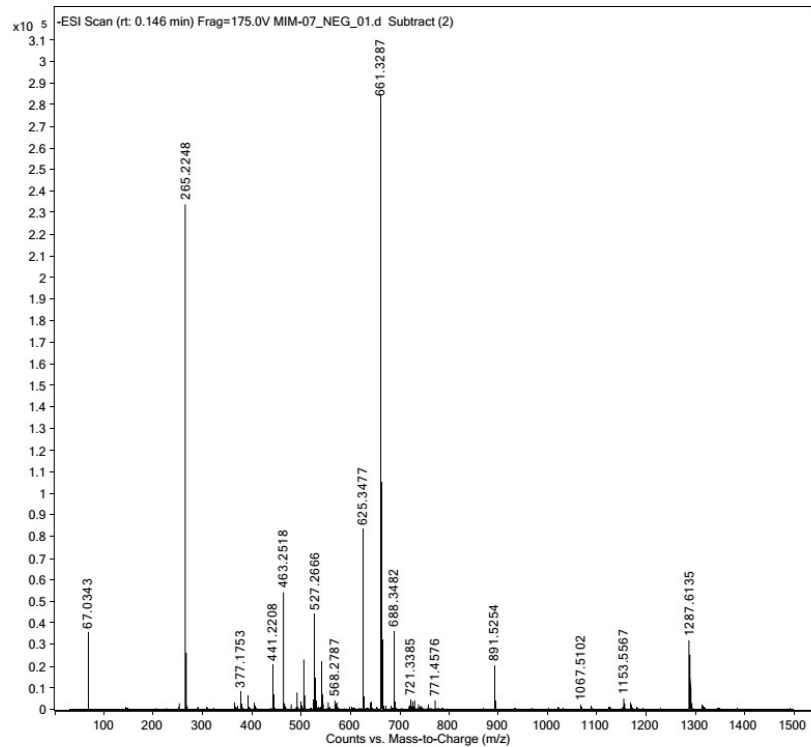


Figure S27: HR-MS OF COMPOUND 4g

Dr. Ajmal/Prof. Ahmed/M1M-08/DMSO
PROTON

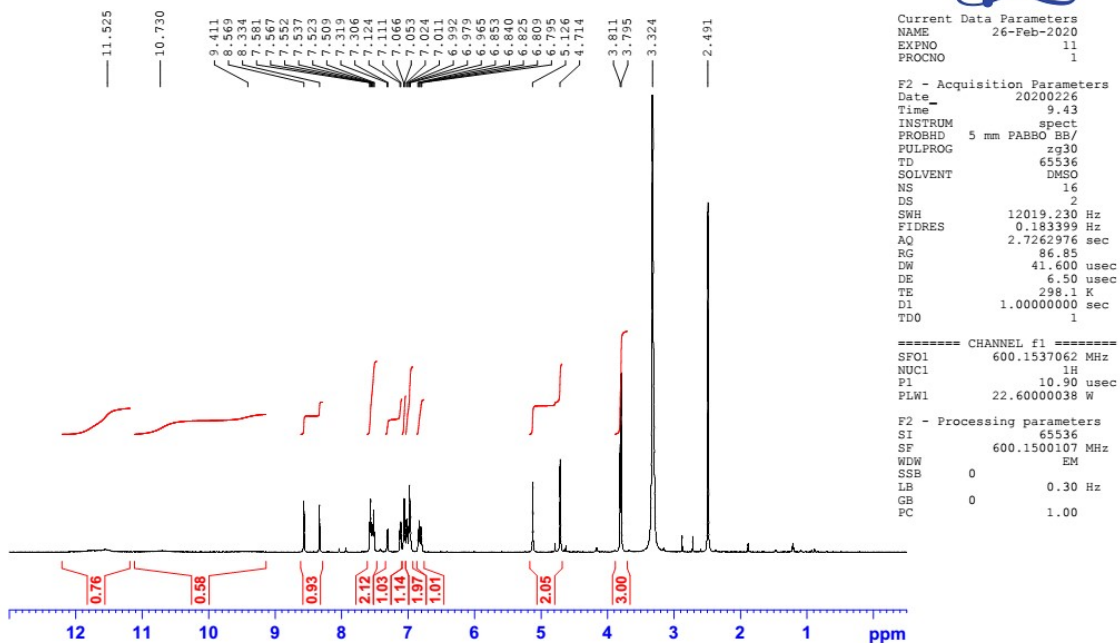
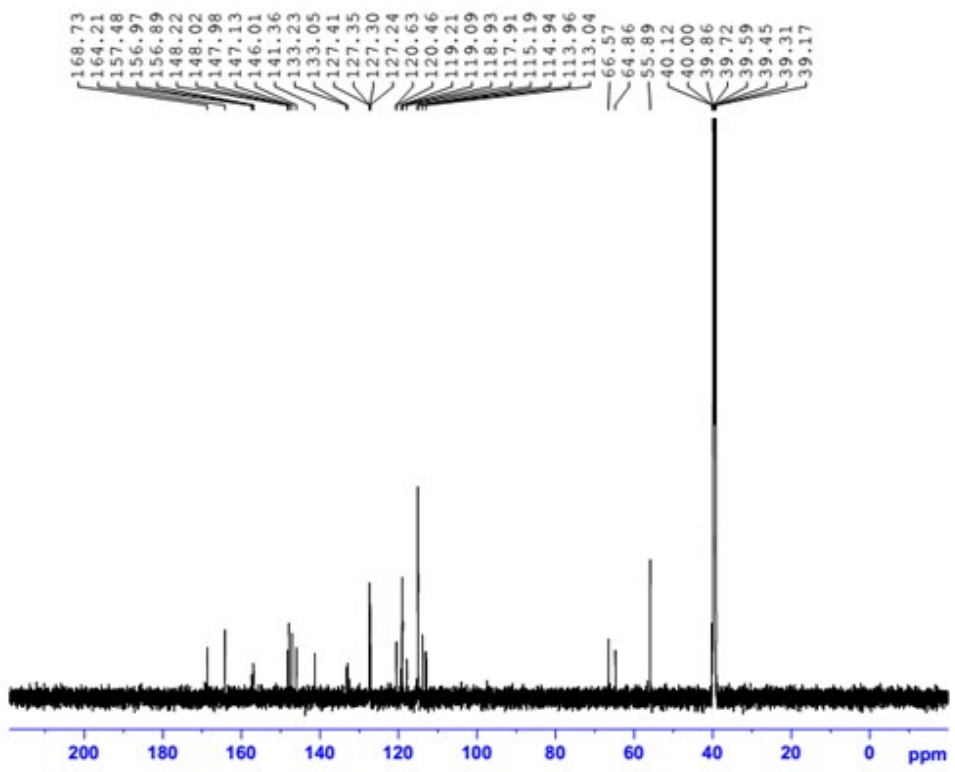


Figure S28: ^1H NMR OF COMPOUND 4h

Dr. Ajmal / MIM08 / DMSO
C13CPD



```
Current Data Parameters
NAME      19-Jan-2021
EXPNO    36
PROCNO   1

F2 - Acquisition Parameters
Data_    20210126
Time     12.34
INSTRUM  spect
PROBHD   5 mm PABBO 30P
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        2048
DS        4
SWH       34057.491 Hz
FIDRES    0.550197 Hz
AQ         0.9087499 sec
RG         195.2
DM         11.547 usec
DE         6.50 usec
TE         294.2 K
D1         2.0000000 sec
d11        0.0300000 sec
TD0        1

----- CHANNEL f1 -----
SF01      150.9229276 MHz
NUC1       13C
P1         11.60 usec
PLM1       83.0000000 W

----- CHANNEL f2 -----
SF02      600.1524006 MHz
NUC2       1H
CPCPRG2   waltz16
PCPD2     70.00 usec
PLM2      22.4000000 W
PLM3      0.25874999 W

F2 - Processing parameters
SI         32768
SF         150.9079041 MHz
WOW        DM
SFR        0
LA         1.00 Hz
GB         0
PC         1.40
```

Figure S29: ¹³C NMR OF COMPOUND 4h

Sample Name	MIM-08	Position	Vial 38	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-08_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 4:14:38 PM

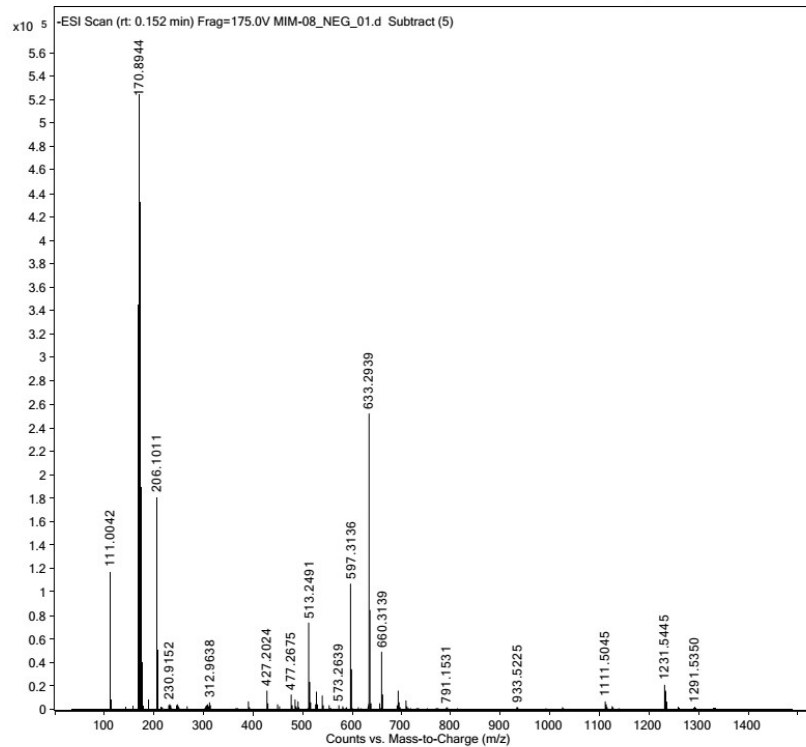


Figure S30: HR-MS OF COMPOUND 4h

Dr. Ajmal/Prof. Ahmed/M1M-09/DMSO
PROTON

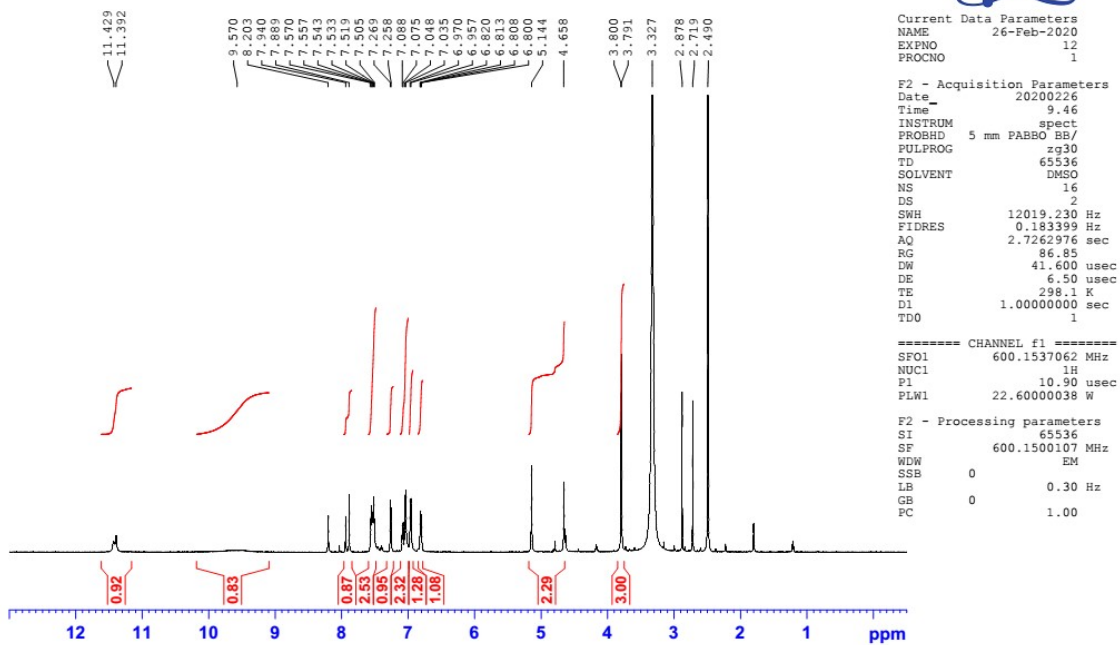
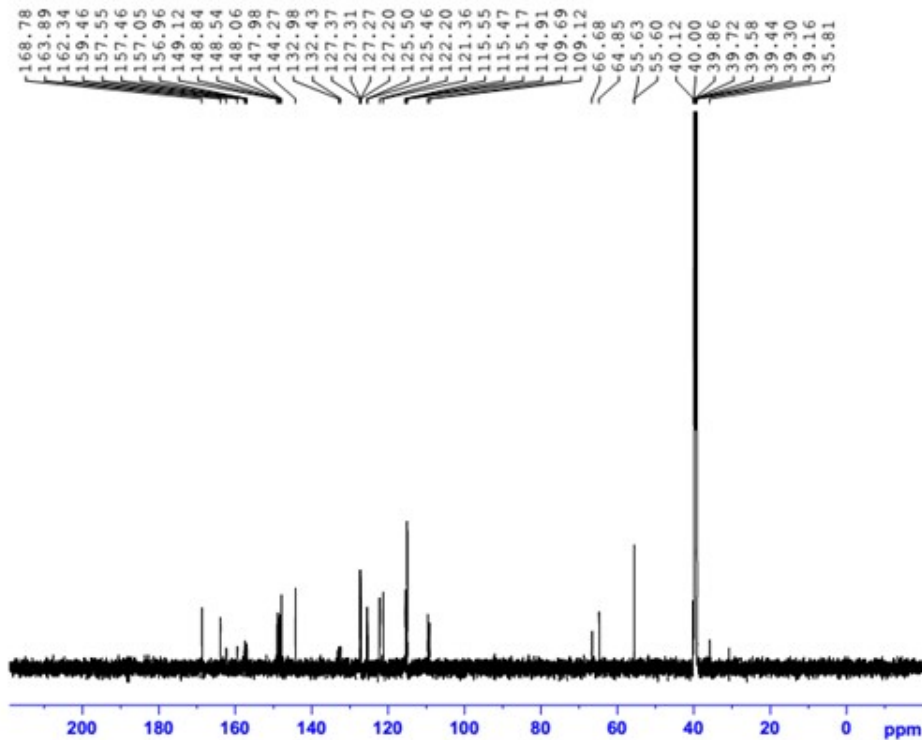


Figure S31: ^1H NMR OF COMPOUND 4i

Dr. Ajmal / MIM09 / DMSO
C13CPD



```
Current Data Parameters
NAME      28-Jan-2021
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20210129
Time      7.56
INSTRUM   spect
PROBHD    5 mm PABBO MM7
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         2048
DS         4
SWH        36057.691 Kz
FIDRES     0.550197 Kz
AQ         0.9087659 sec
RG         195.2
CW         13.867 usec
DE         6.50 usec
TE         294.4 K
D1         2.00000000 sec
d11        0.03000000 sec
TD0        1

----- CHANNEL f1 -----
SF01      150.9229274 MHz
WDW01     1.30
SSB01     11.60 usec
PLM01     83.00000000 W

----- CHANNEL f2 -----
SF02      600.1524004 MHz
WDW02     18
SSB02     wait:16
PCPD02    70.00 usec
PLM02     22.60000038 W
PLM03     0.25806001 W
PLM03     0.25874999 W

F2 - Processing parameters
SI         32768
SF         150.9079041 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

Figure S32: ¹³C NMR OF COMPOUND 4i

Sample Name	MIM-09	Position	Vial 39	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-09_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 4:21:48 PM

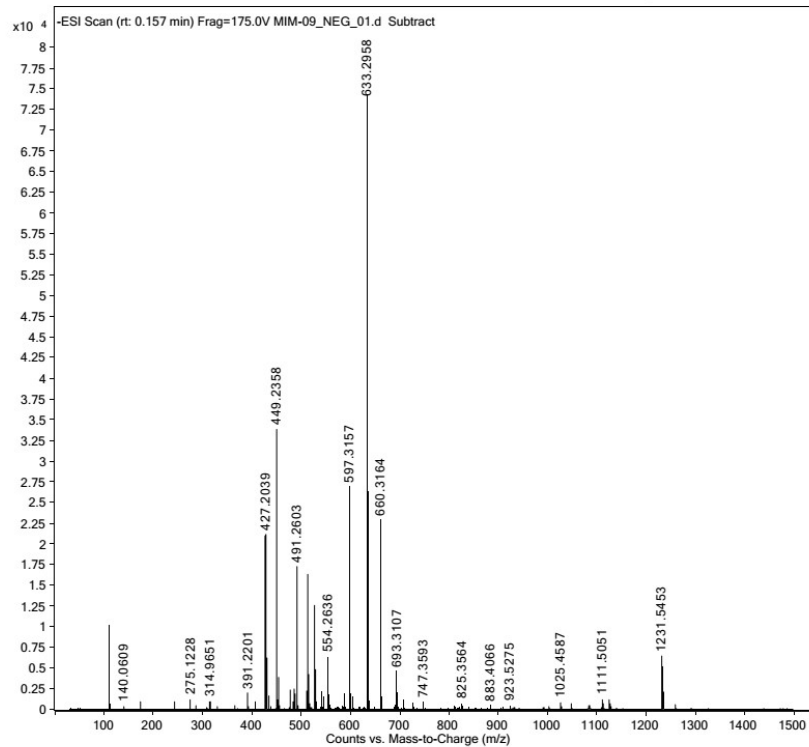


Figure S33: HR-MS OF COMPOUND 4i

Dr. Ajmal/Prof. Ahmed/M1M-10/DMSO
PROTON

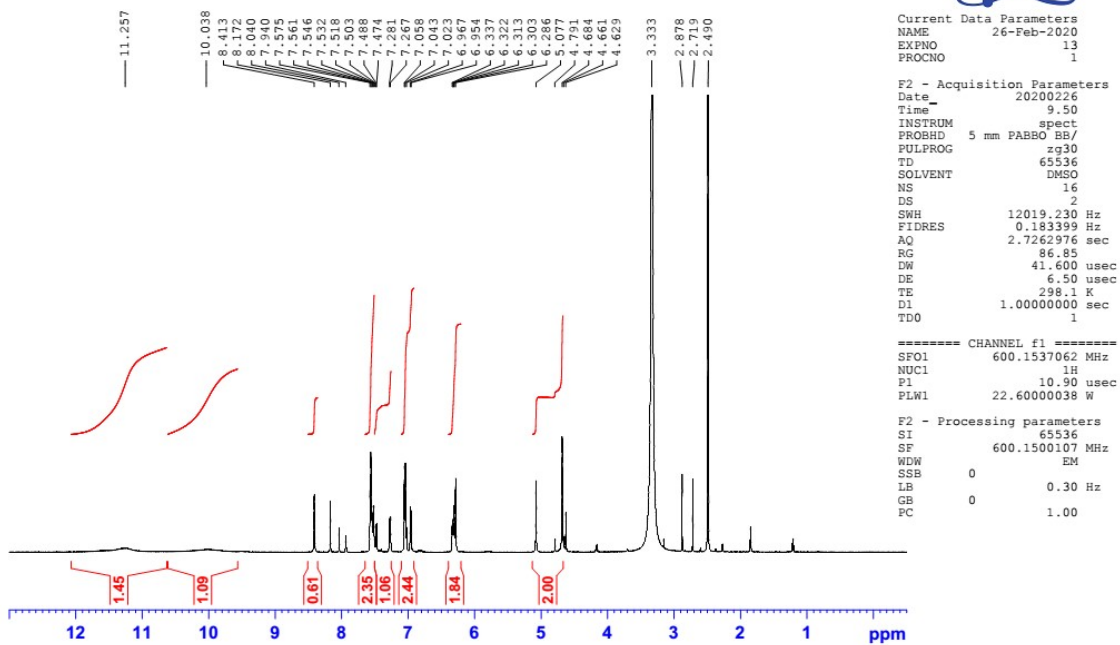
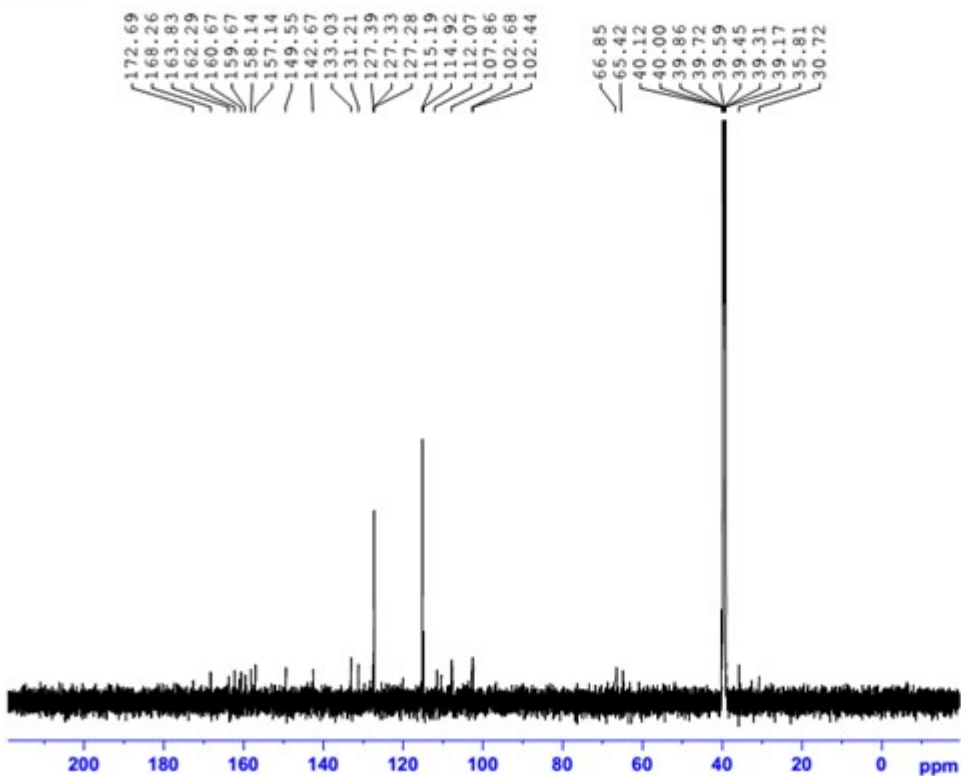


Figure S34: ^1H NMR OF COMPOUND 4j

Dr. Ajmal / MIM10 / DMSO
C13CPD



```
Current Data Parameters
NAME      28-Jan-2021
EXPRO     22
PROCNO    1

F2 = Acquisition Parameters
Data_     20210129
Time      22.20
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         2048
DS         4
SWH        36057.491 Hz
FIDRES     0.550197 Hz
AQ         0.9027459 sec
RG         195.2
DN         11.867 usec
DE         4.50 usec
TE         298.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

----- CHANNEL f1 -----
SFO1      150.9219276 MHz
NUC1       13C
P1         11.60 usec
PLA1       03.00000000 W

----- CHANNEL f2 -----
SFO2      400.1524006 MHz
NUC2       1H
CFPPROG[2]  waltz16
PCPD[2]    70.00 usec
PLA2       22.40000000 W
PLA3       0.52000000 W
PLA4       0.25874999 W

F2 = Processing parameters
SI         32768
SF         150.9079041 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

Figure S35: ^{13}C NMR OF COMPOUND 4j

Sample Name	MIM-10	Position	Vial 40	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-10_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 4:29:00 PM

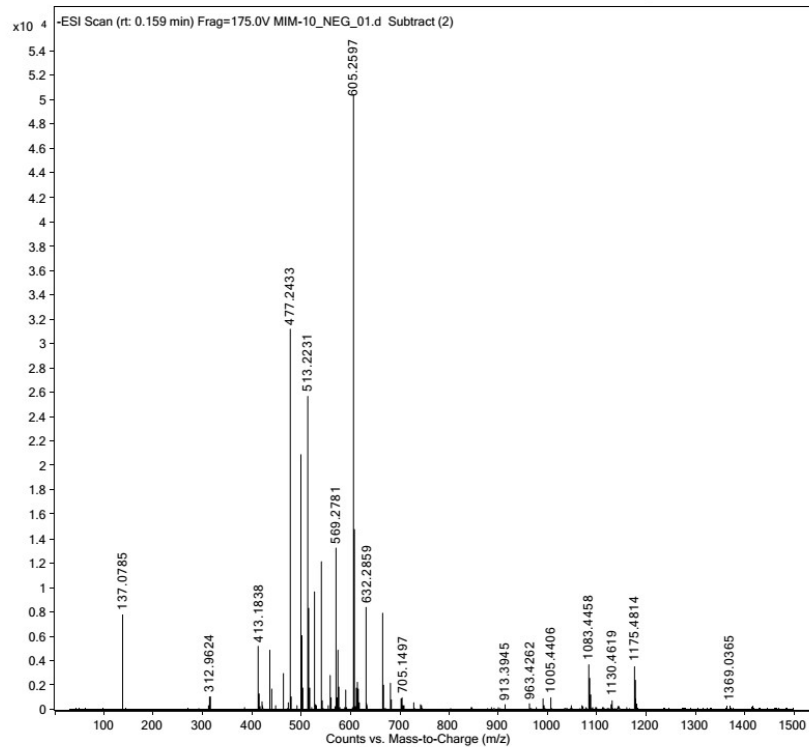


Figure S36: HR-MS OF COMPOUND 4j

Dr. Ajmal/Prof. Ahmed/M1M-11/DMSO
PROTON

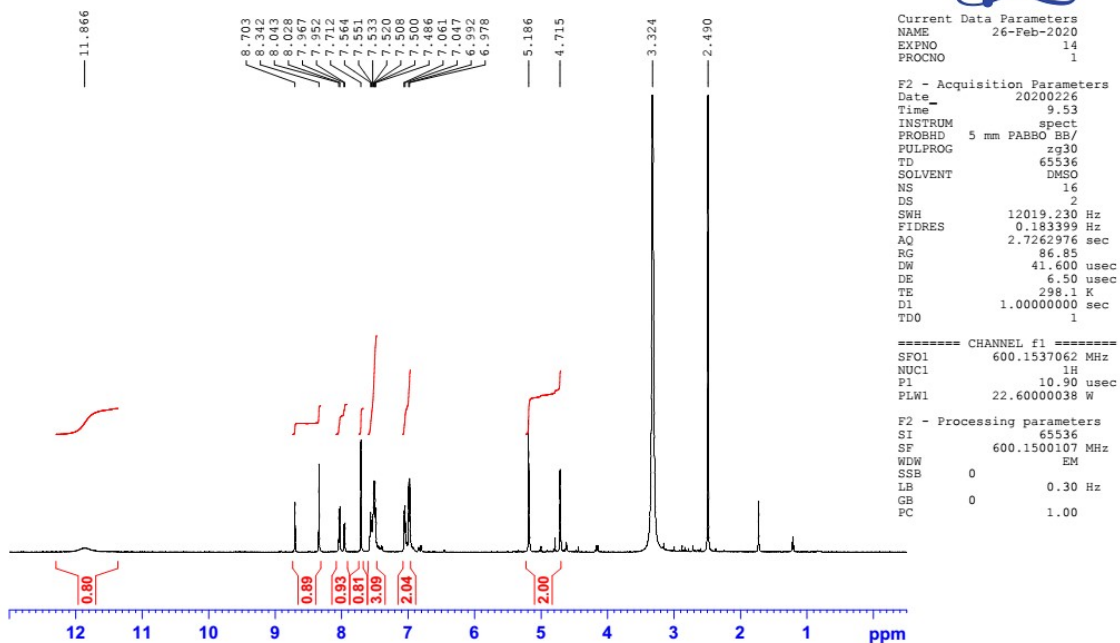


Figure S37: ^1H NMR OF COMPOUND 4k

Dr. Ajmal / MIM11 / DMSO
C13CPD

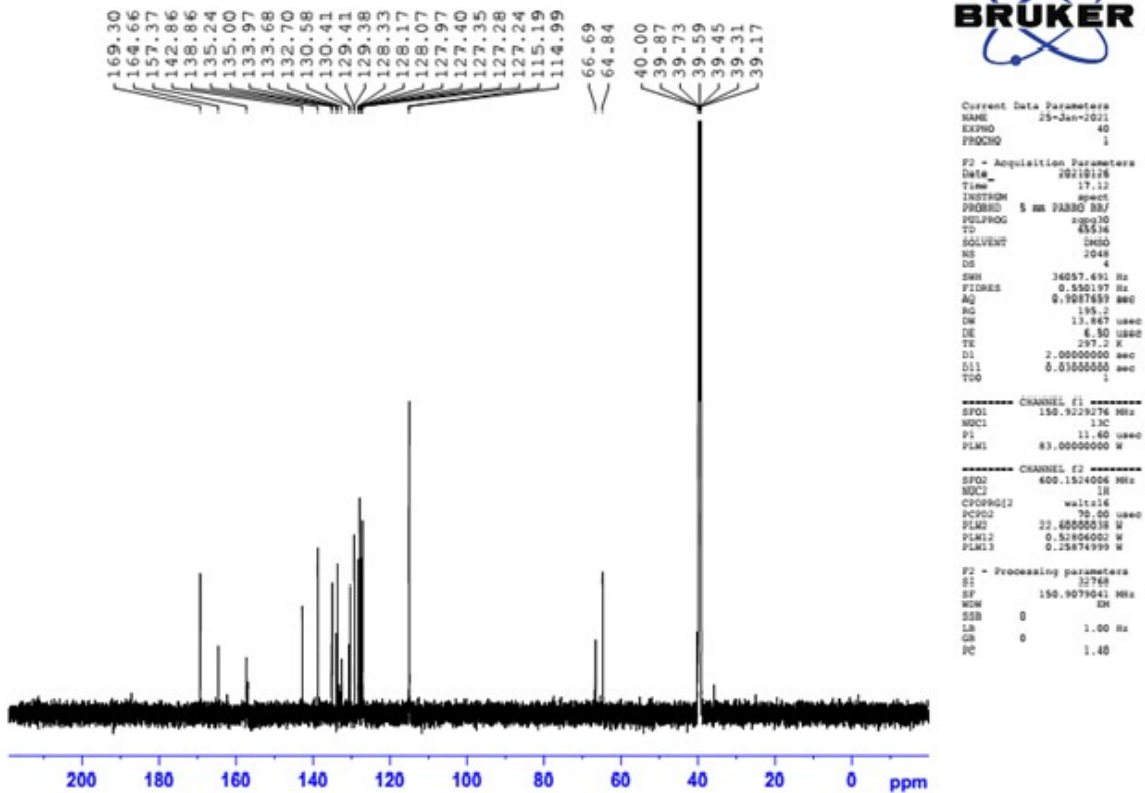


Figure S38: ¹³C NMR OF COMPOUND 4k

Sample Name	MIM-11	Position	Vial 41	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-11_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 4:36:11 PM

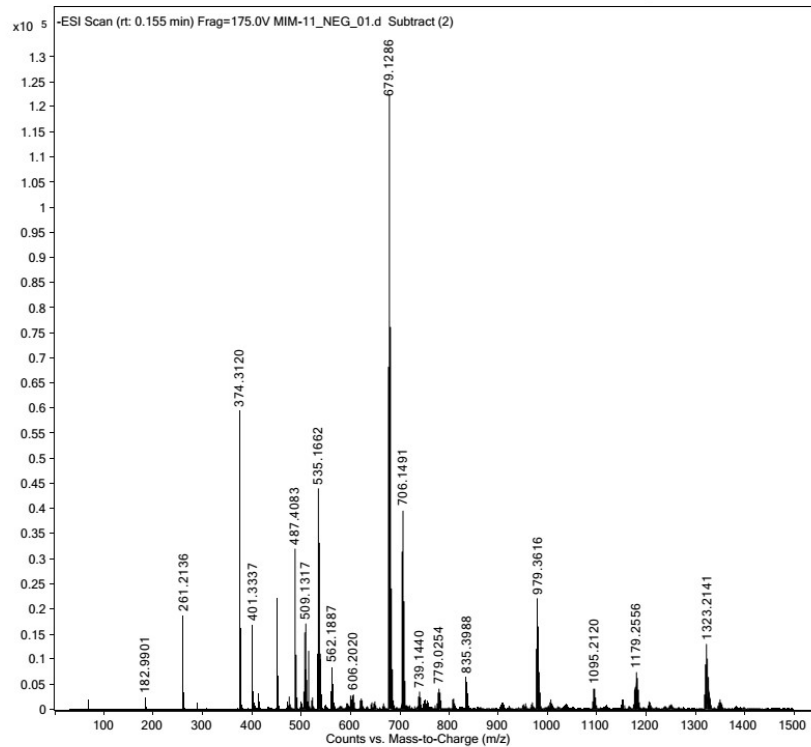


Figure S39: HR-MS OF COMPOUND 4k

Dr. Ajmal/Prof. Ahmed/M1M-12/DMSO
PROTON

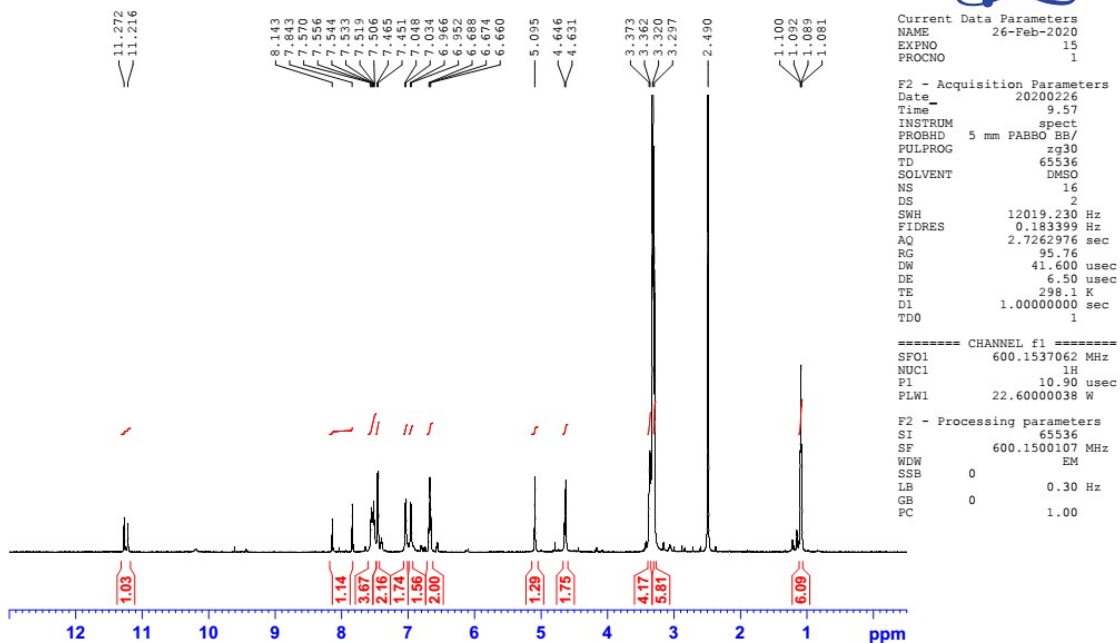
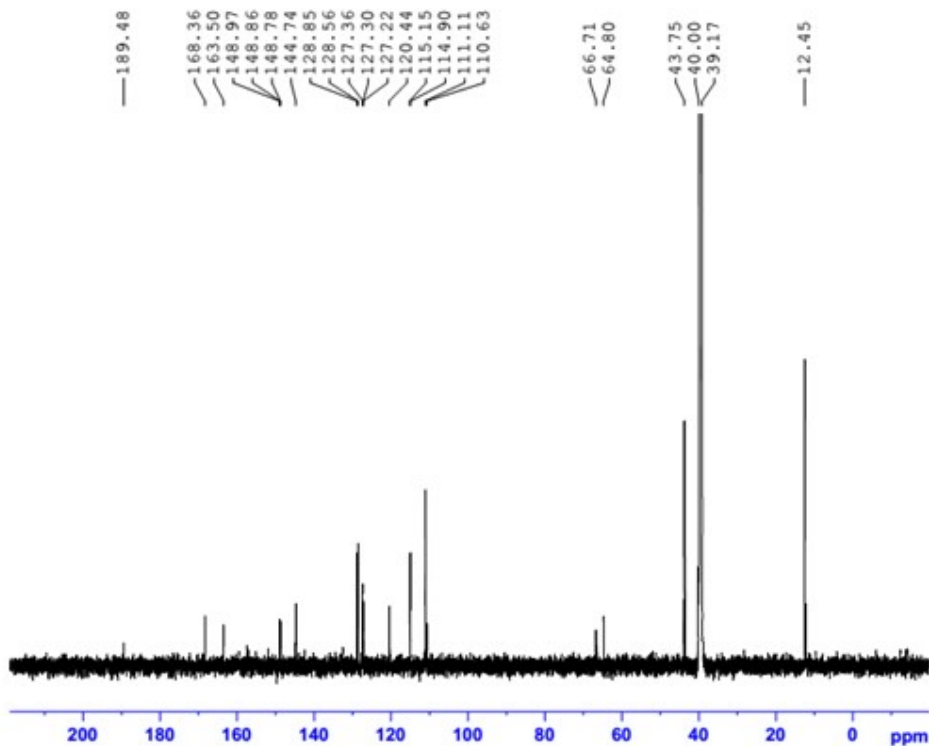


Figure S40: ¹H NMR OF COMPOUND 41

Dr. Ajmal / MIM12 / DMSO
C13CPD



```
Current Data Parameters
NAME      25-Jan-2021
EXPNO    32
PROCNO   1

F2 - Acquisition Parameters
Date_    20210126
Time     9.39
INSTRUM spect
PROBHD   5 mm PABBO BBI
PULPROG zgpg30
TD       65536
SOLVENT  DMSO
NS       2048
DS       4
SWS     36051.491 Hz
FIDRES  0.550197 Hz
AQ      0.9087459 sec
RG      193.2
DM      11.867 usec
DE      6.50 usec
TE      296.3 K
D1      2.0000000 sec
D11     0.0300000 sec
TD0     1

===== CHANNEL f1 =====
SFO1   150.9229276 MHz
NUC1    13C
P1      11.60 usec
PLM1   83.0000000 W

===== CHANNEL f2 =====
SFO2   600.1524006 MHz
NUC2    1H
CPOPRG[2]  waltz16
PCYCL2  30.00 usec
PLM2   22.6000000 W
PLM12  0.52806002 W
PLM13  0.25874999 W

F2 - Processing parameters
SI      32768
SF      150.9079041 MHz
WDW     EM
SSB     0
LB      2.00 Hz
GB      0
PC      1.40
```

Figure S41: ^{13}C NMR OF COMPOUND 41

Sample Name	MIM-12	Position	Vial 42	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-12_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 4:43:20 PM

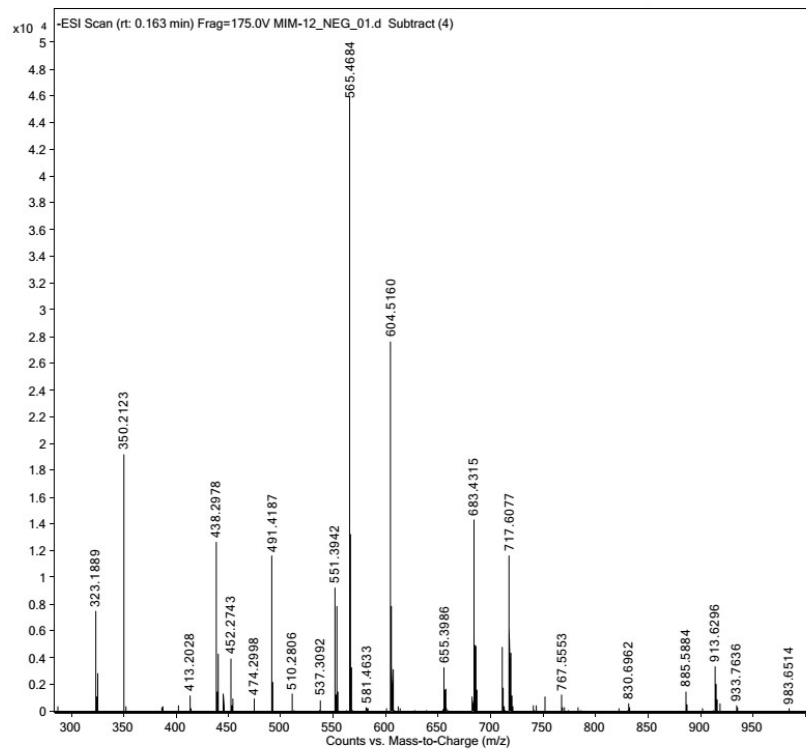


Figure S42: HR-MS OF COMPOUND 41

Dr. Ajmal/Prof. Ahmed/M1M-13/DMSO
PROTON

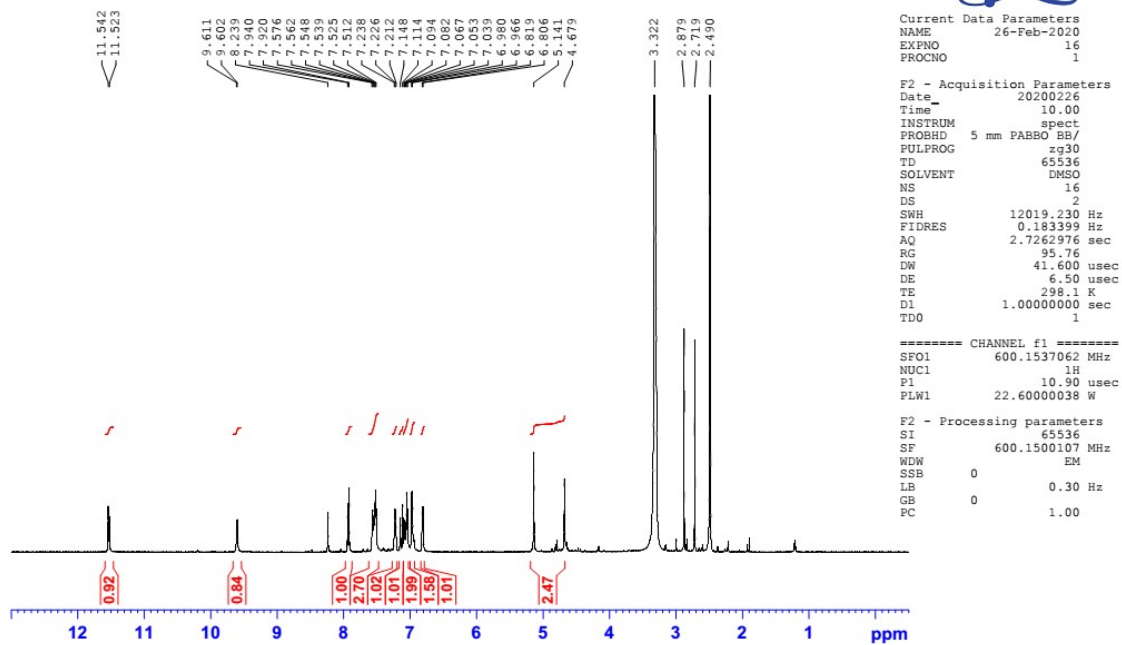
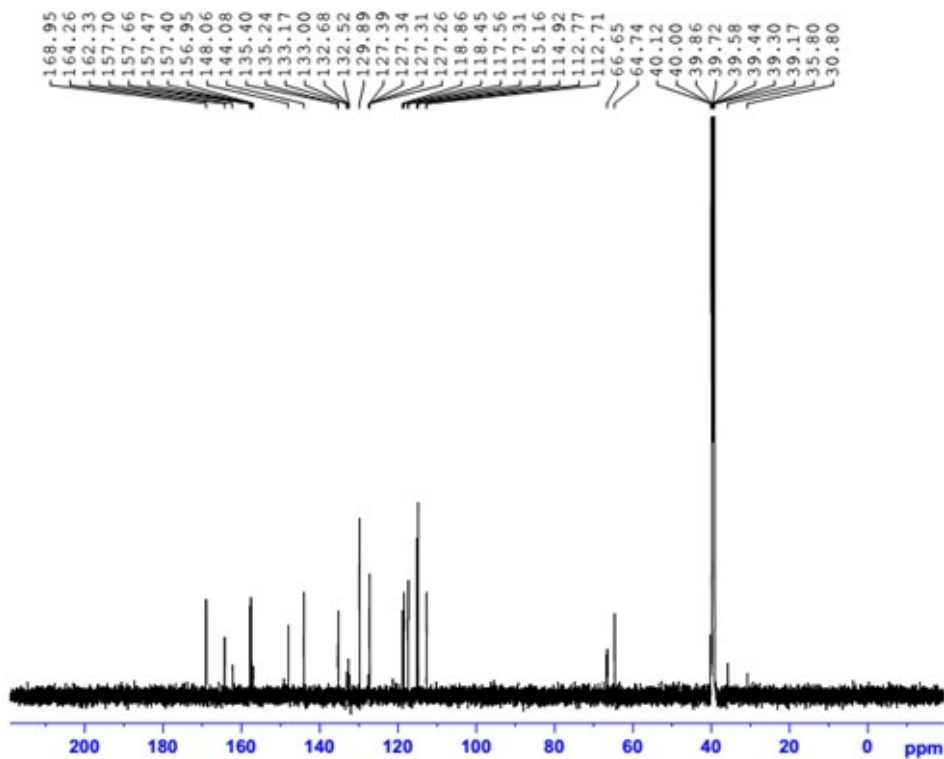


Figure S43: ^1H NMR OF COMPOUND 4m

Dr. Ajmal / M1M13 / DMSO
C13CPD



```
Current Data Parameters
NAME      28-Jan-2021
EXPRO    30
PROCNO   1

F2 - Acquisition Parameters
Date_    20210130
Time     5.32
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       2048
DS       4
SWH      34057.491 Hz
FIDRES   0.550197 Hz
AQ       0.9057639 sec
RG       199.2
DM       13.847 usec
DE       6.50 usec
TE       294.4 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1

----- CHANNEL f1 -----
SF01    150.9229276 MHz
MPC1    13C
P1      11.40 usec
PLM1    83.0000000 W

----- CHANNEL f2 -----
SF02    400.1524004 MHz
MPC2    1H
CPCPRG2 waltz16
PCPROG  70.00 usec
PLM2    22.6000000 W
PLM12   0.5240400 W
PLM13   0.15874999 W

F2 - Processing parameters
SI      32768
SF      150.9079041 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
```

Figure S44: ¹³C NMR OF COMPOUND 4m

Sample Name	MIM-13	Position	Vial 43	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-13_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 4:50:26 PM

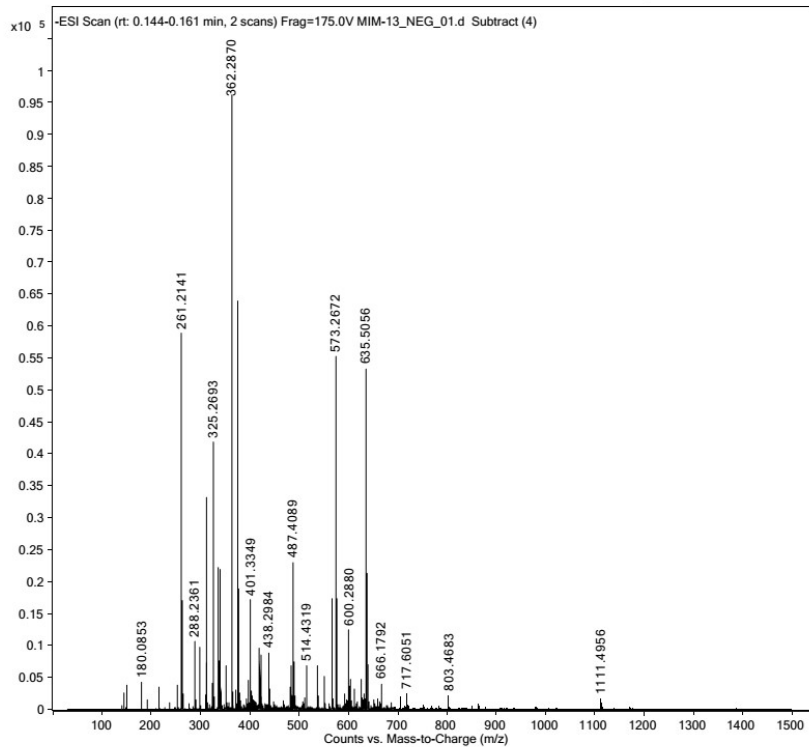


Figure S45: HR-MS OF COMPOUND 4m

Dr. Ajmal/Prof. Ahmed/M1M-14/DMSO
PROTON

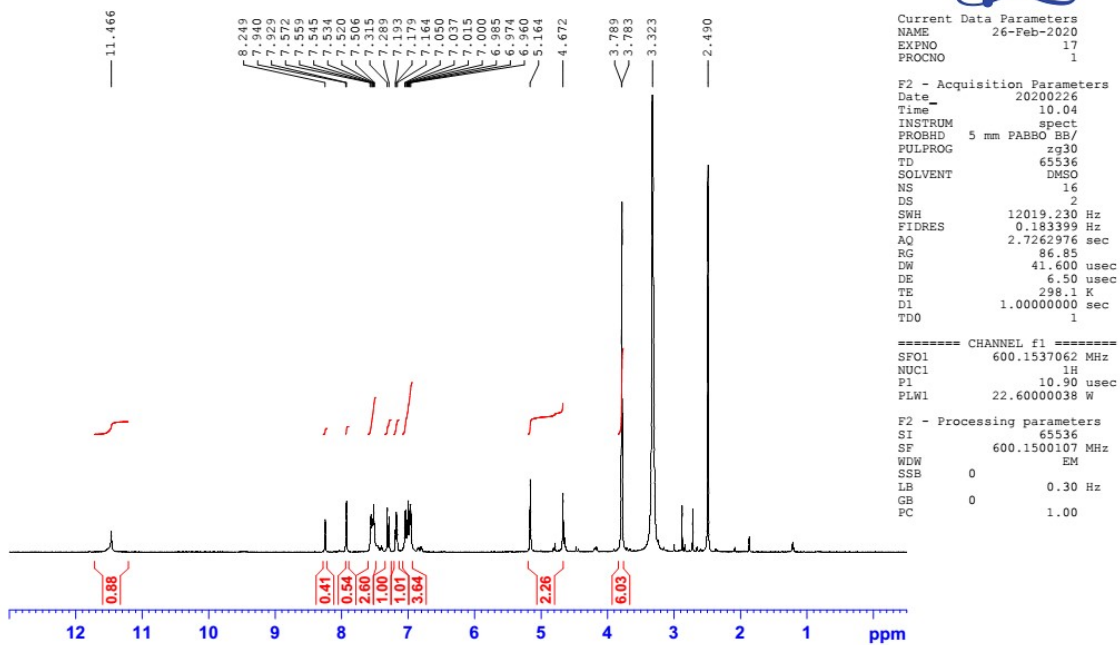
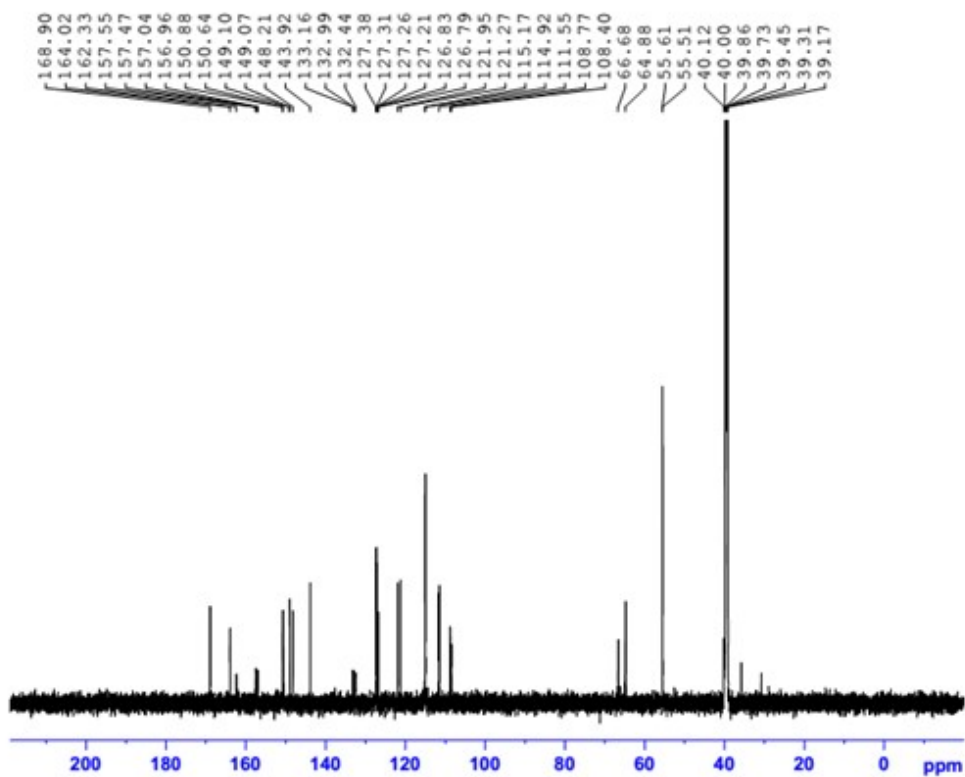


Figure S46: ^1H NMR OF COMPOUND 4n

Dr. Ajmal / MIM14 / DMSO
C13CPD



```
Current Data Parameters
NAME      28-Jan-2021
EXPRO    14
PROCNO   1

F2 - Acquisition Parameters
Date_    20181129
Time     15.08
INSTRUM  spect
PROBHD   5 mm BBOBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       2048
DS       4
SWH      34057.691 Hz
FIDRES   0.552197 Hz
AQ       0.9087659 sec
RG       195.2
OW       13.847 usec
SE       6.50 usec
TE       296.8 K
SI       2.0000000 sec
SII      0.0300000 sec
TDD      1

----- CHANNEL f1 -----
SFO1    150.9229276 MHz
NUC1     13C
P1      11.60 usec
PLM1    83.0000000 W

----- CHANNEL f2 -----
SFO2    600.1524004 MHz
NUC2     1H
CROSSPC2  wait1816
PCPD2    70.00 usec
PLM2    22.6000000 W
PLM12   0.52306002 W
PLM13   0.25874999 W

F2 - Processing parameters
SI       32768
SF       150.9079041 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```

Figure S47: ^{13}C NMR OF COMPOUND 4n



Figure S48: HR-MS OF COMPOUND 4n

Dr. Ajmal/Prof. Ahmed/M1M-15/DMSO
PROTON

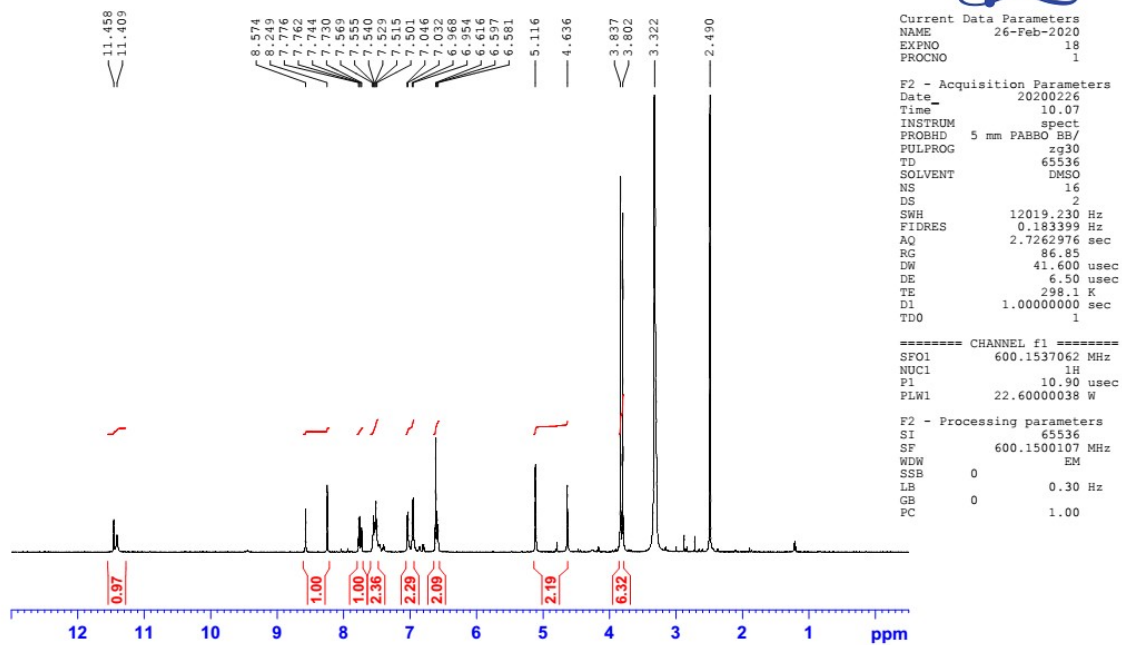
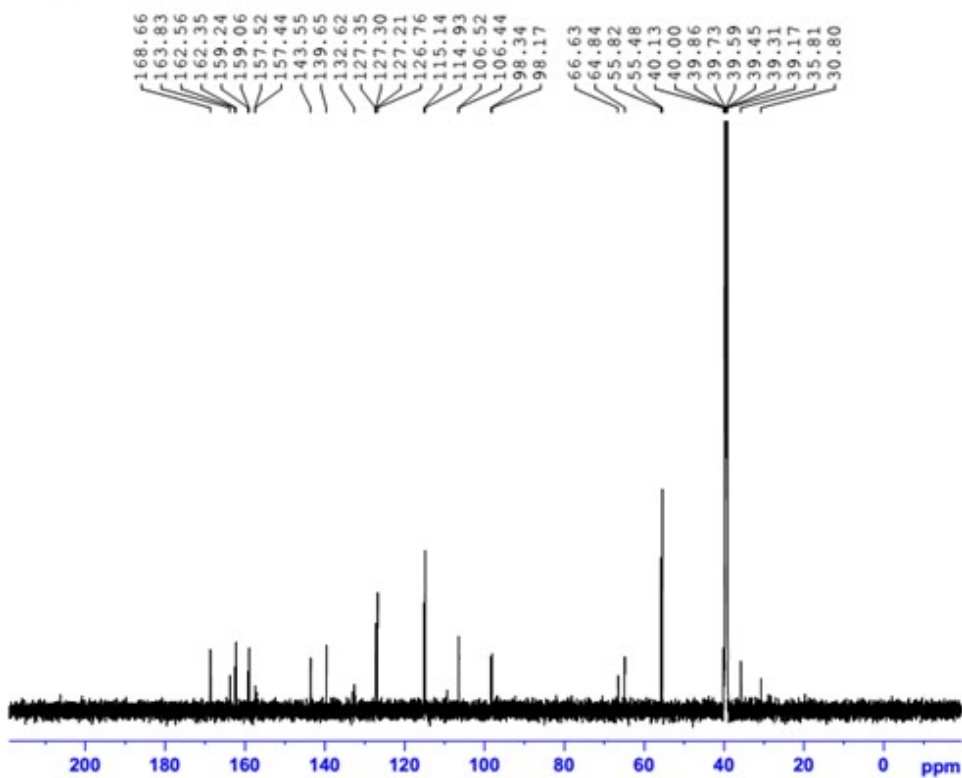


Figure S49: ¹H NMR OF COMPOUND 4o

Dr. Ajmal / MIM15 / DMSO
C13CPD



Current Data Parameters
NAME 28-Jan-2021
EXPRD 18
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210129
Time 18.44
INSTRM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 34057.491 Hz
FIDRES 0.590197 Hz
AQ 0.9087659 sec
RG 195.2
DW 13.867 usec
DE 6.50 usec
TE 296.3 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 150.9229274 MHz
NUC1 13C
P1 11.60 usec
PLM1 83.0000000 W

----- CHANNEL f2 -----
SFO2 600.1524004 MHz
NUC2 1H
CPCPRG2 waitx16
PCPD2 70.00 usec
PLM2 22.6000000 W
PLM3 0.5204000 W
PLM3 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9079041 MHz
WOW 0
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S50: ¹³C NMR OF COMPOUND 4o

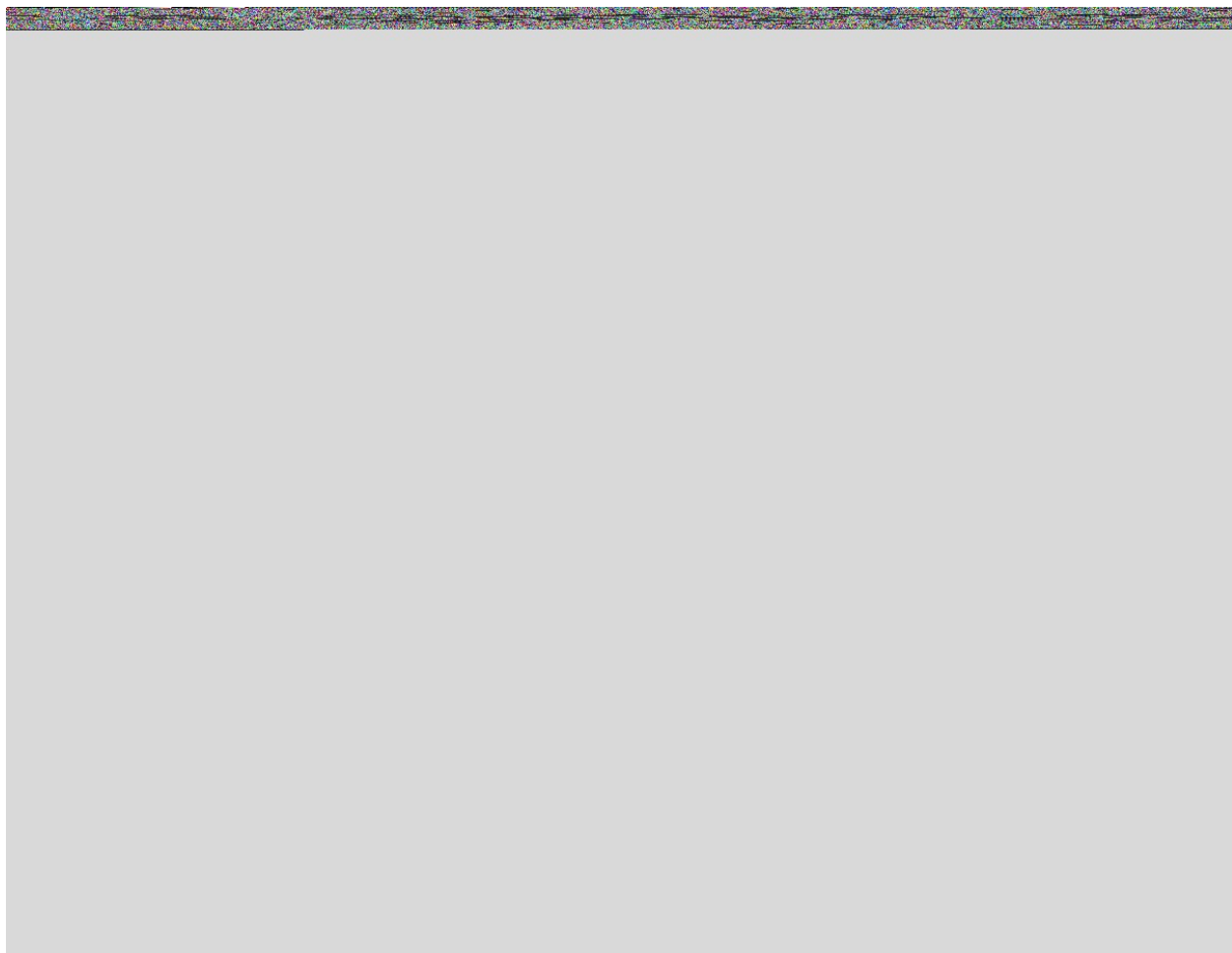


Figure S51: HR-MS OF COMPOUND 4n

Dr. Ajmal/Prof. Ahmed/M1M-16/DMSO
PROTON

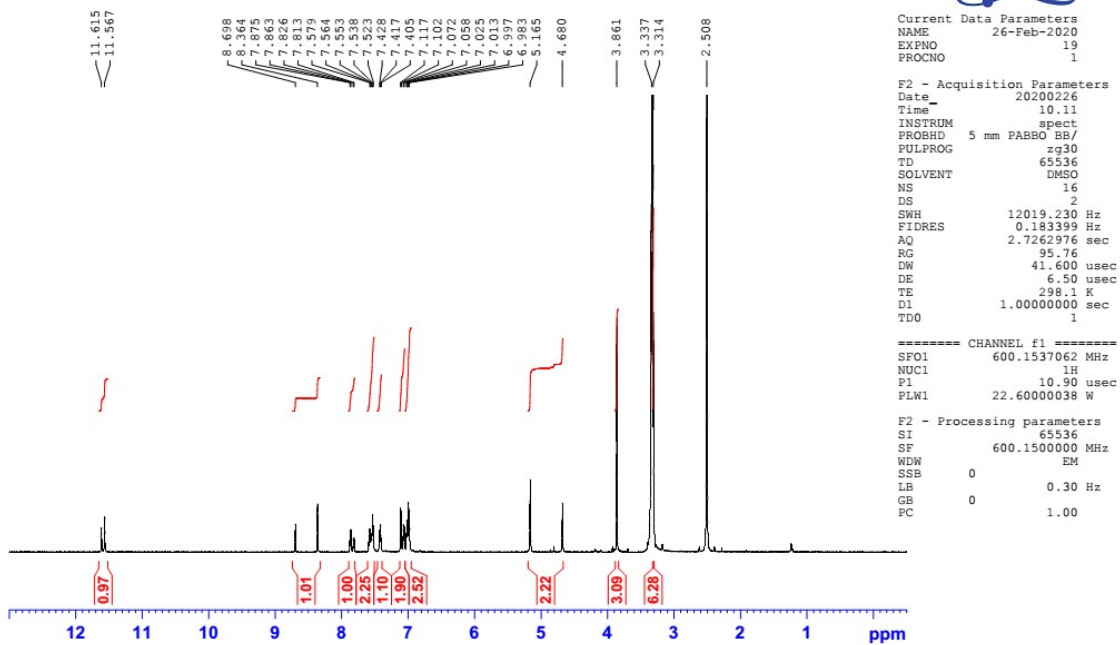
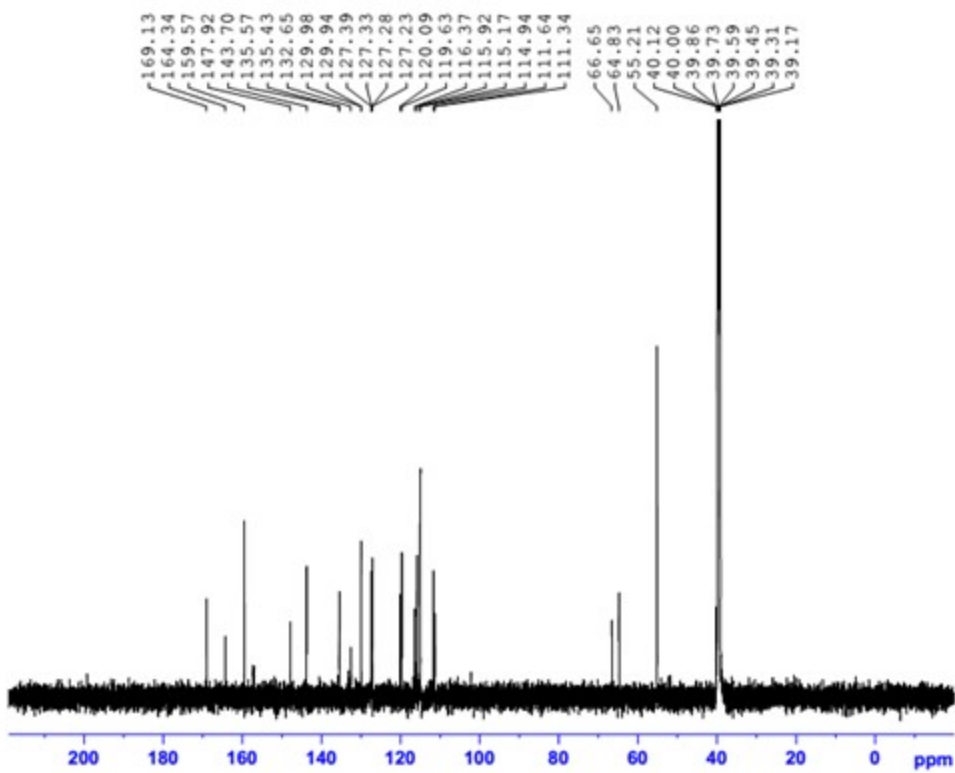


Figure S52: ^1H NMR OF COMPOUND 4p

Dr. Ajmal / M1M16 / DMSO
C13CPD



```
Current Data Parameters
NAME      28-Jan-2021
EXPNO    36
PROCNO    1

F2 - Acquisition Parameters
Date_     20210130
Time      12.44
INSTRUM   spect
PROBHD    5 mm QNP300
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         2048
DS         4
SWH        36057.491 Hz
FIDRES    0.550197 Hz
AQ         0.9087459 sec
RG         198.2
DW         13.847 usec
DE         6.50 usec
TE         296.4 K
D1         2.0000000 sec
D11        0.0300000 sec
TOD        1

----- CHANNEL f1 -----
SFO1      150.9229276 MHz
MPC1      13C
P1         11.60 usec
PLW1      83.0000000 W

----- CHANNEL f2 -----
SFO2      400.1524004 MHz
MPC2      1H
CPOPRG[2] waltz16
PCPD2     70.00 usec
PLW2      22.6000000 W
PLW3      0.5280600 W
PLW4      0.25874999 W

F2 - Processing parameters
SI         32768
SF         150.9079041 MHz
WDW        EM
SSB        0
LA         0
GB         0
PC         1.40
```

Figure S53: ¹³C NMR OF COMPOUND 4p

Sample Name	MIM-16	Position	Vial 46	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-16_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 5:11:48 PM

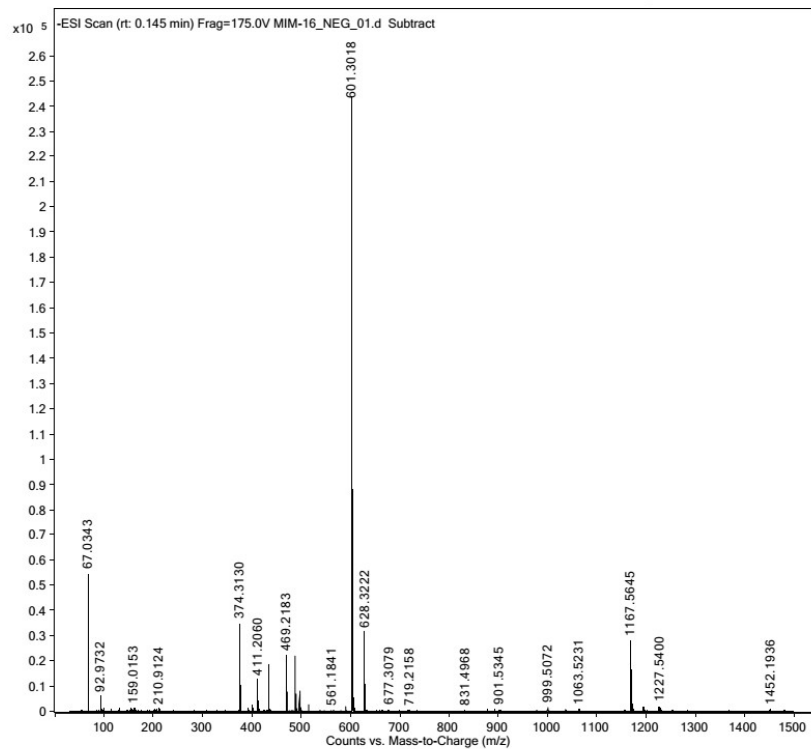


Figure S54: HR-MS OF COMPOUND 4p

Dr. Ajmal/Prof. Ahmed/M1M-17/DMSO
PROTON

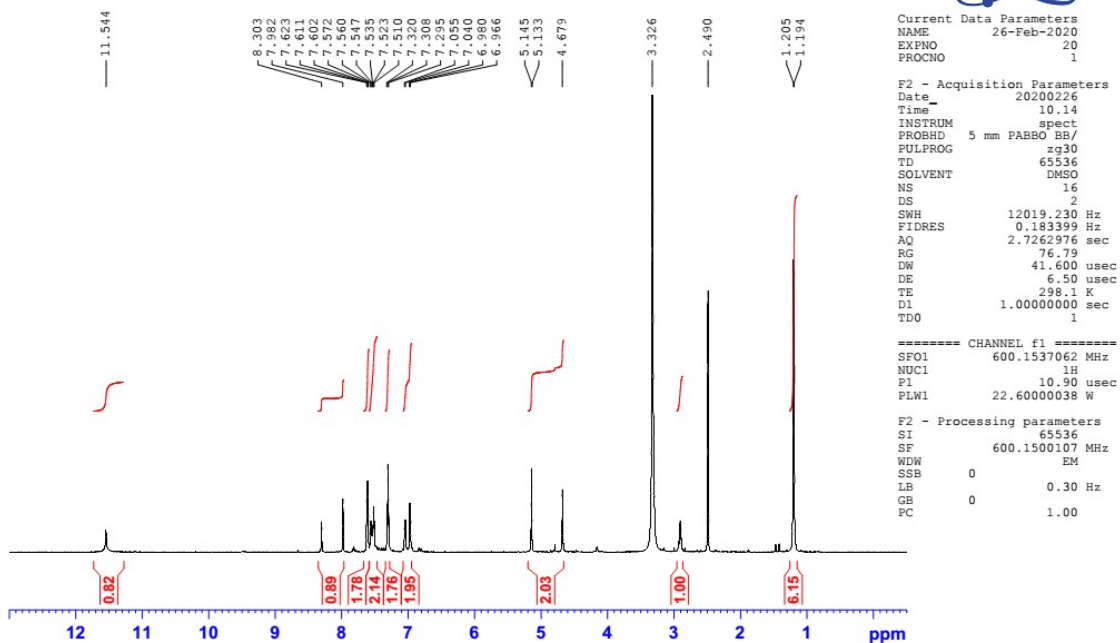
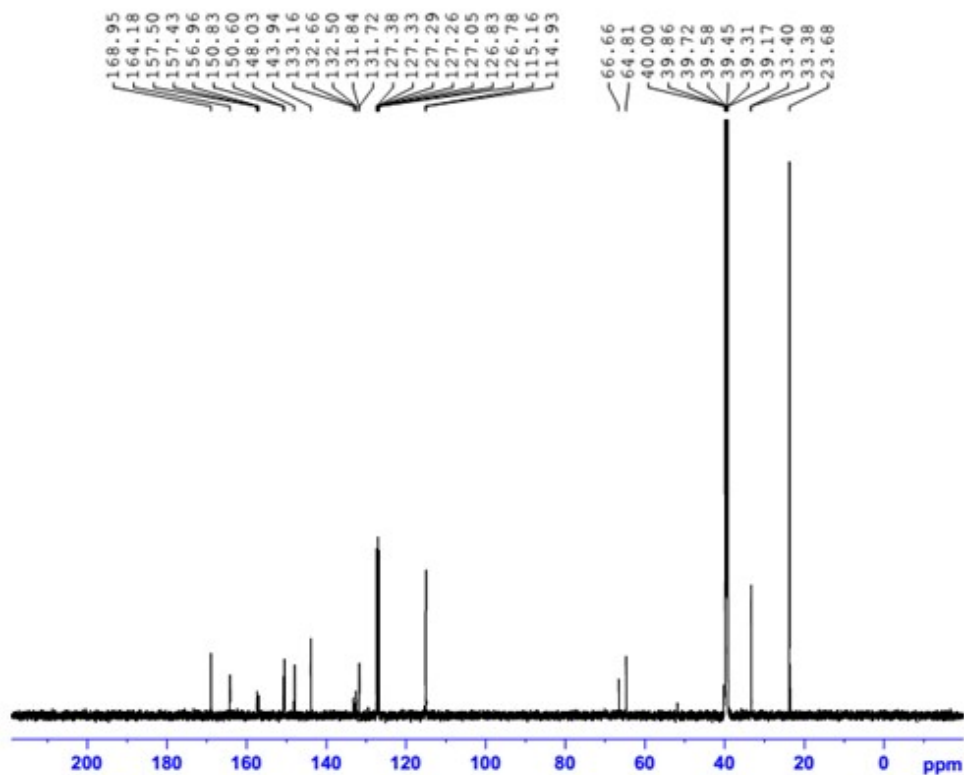


Figure S55: ^1H NMR OF COMPOUND 4q

Dr. Ajmal / MIM17 / DMSO
C13CPD



Current Data Parameters
NAME J8-Jan-2021
EXPRO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210128
Time_ 0.26
INSTRUM spect
PROBHD 5 mm PABBO BBO
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36057.491 Kz
FIDRES 0.550197 Kz
AQ 0.9087459 sec
RG 199.2
IN 11.947 usec
DE 6.50 usec
TE 294.6 K
D1 2.0000000 sec
D11 0.0100000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 150.9229276 MHz
MPC1 13C
P1 11.60 usec
PLM1 83.0000000 W

----- CHANNEL f2 -----
SFO2 400.1524006 MHz
MPC2 1H
CPCPG2 waltz16
PCPD2 70.00 usec
PLM2 22.6000038 W
PLM2 0.51806002 W
PLM3 0.2874999 W

F2 - Processing parameters
SI 32768
SF 150.9079041 MHz
WDW EM
SSB 0
LB 1.00 Kz
GB 0
PC 1.40

Figure S56: ¹³C NMR OF COMPOUND 4q

Sample Name	MIM-17	Position	Vial 47	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-17_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 5:19:00 PM

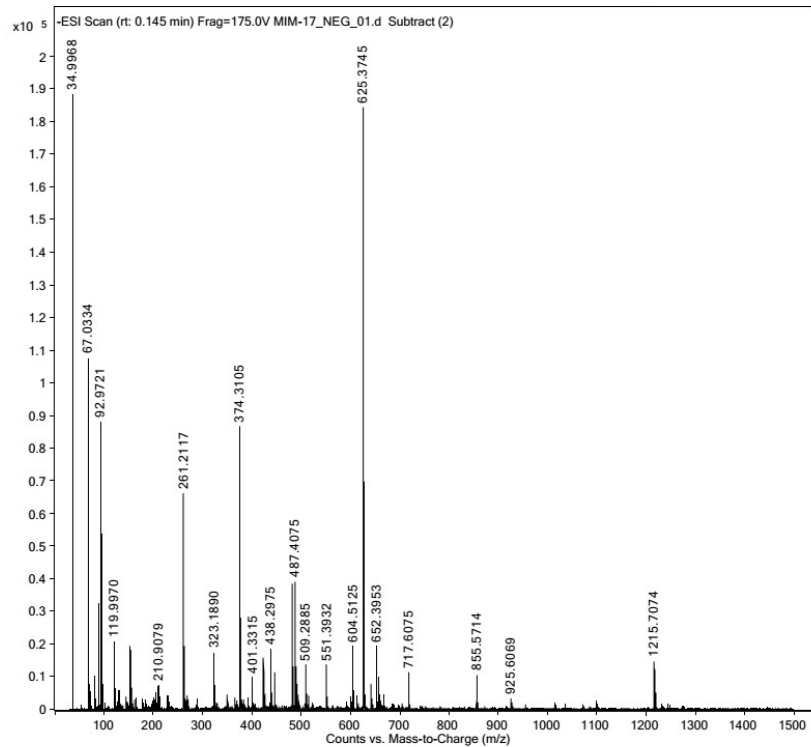


Figure S57: HR-MS OF COMPOUND 4q

Dr. Ajmal/Prof. Ahmed/M1M-18/DMSO
PROTON

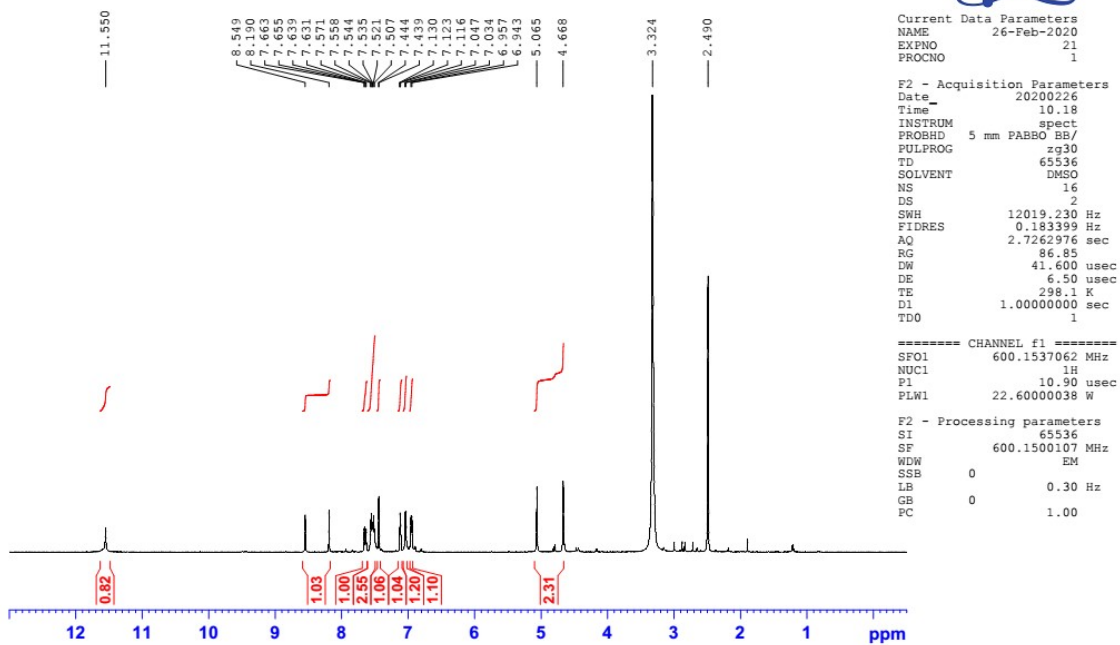
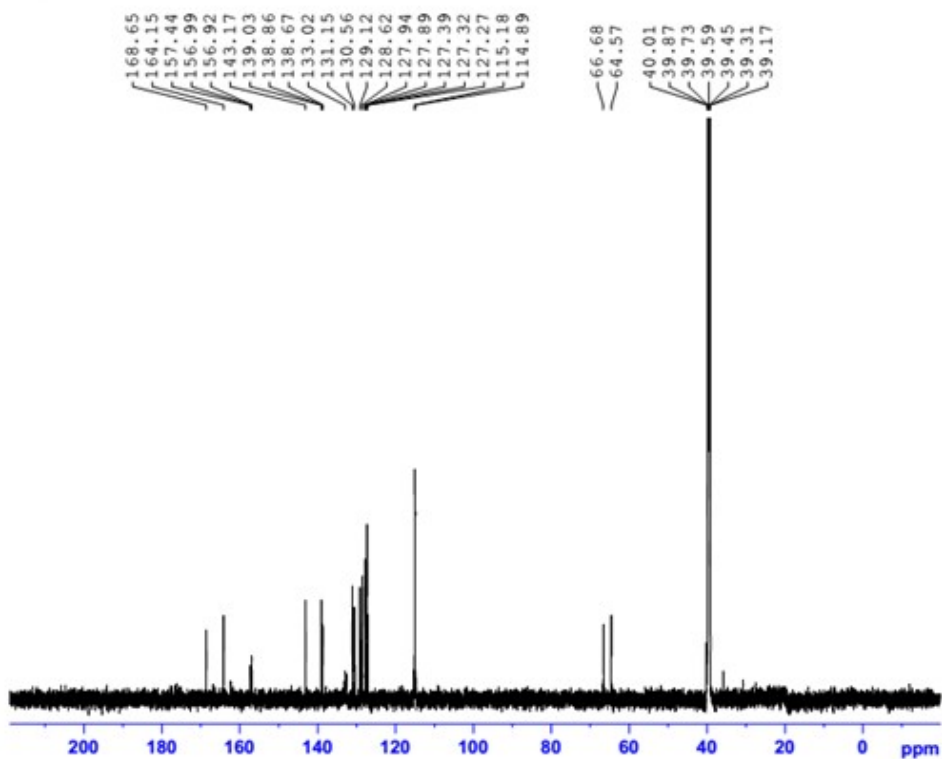


Figure S58: ¹H NMR OF COMPOUND 4r

Dr. Ajmal / MIM18 / DMSO
C13CPD



```
Current Data Parameters
NAME      28-Jan-2021
EXPNO    70
PROCNO   1

F2 - Acquisition Parameters
Date_    20210118
Time     14.50
INSTRUM  spect
PROBHD   5 mm PABBO BBI/
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        2048
DS        4
SWH       36057.491 Hz
FIDRES    0.550197 Hz
AQ         0.9087659 sec
RG         195.2
DW         13.867 usec
DE         6.50 usec
TE         304.2 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

----- CHANNEL f1 -----
SFO1     150.9229276 MHz
NUC1      13C
P1         11.60 usec
PLW1      83.0000000 W

----- CHANNEL f2 -----
SFO2     600.1524056 MHz
NUC2      1H
CPDPRG2  waltz16
PCPD2     70.00 usec
PLW2      22.6000000 W
PLW12     0.52804002 W
PLW13     0.25874999 W

F2 - Processing parameters
SI         32768
SF         150.9079041 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

Figure S59: ¹³C NMR OF COMPOUND 4r

Sample Name	MIM-18	Position	Vial 48	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-18_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 5:26:11 PM

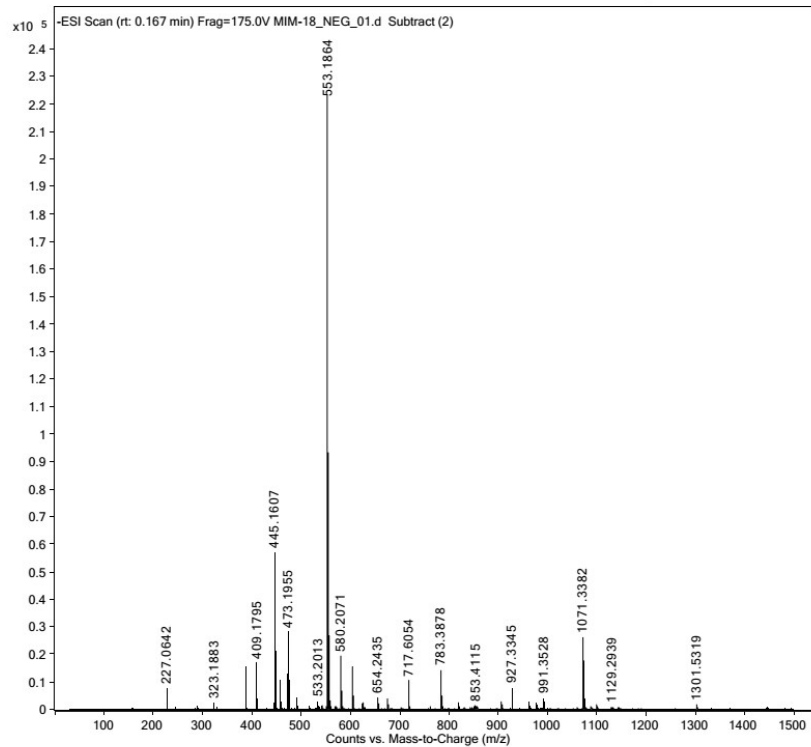


Figure S60: HR-MS OF COMPOUND 4r

Dr. Ajmal/Prof. Ahmed/M1M-19/DMSO
PROTON

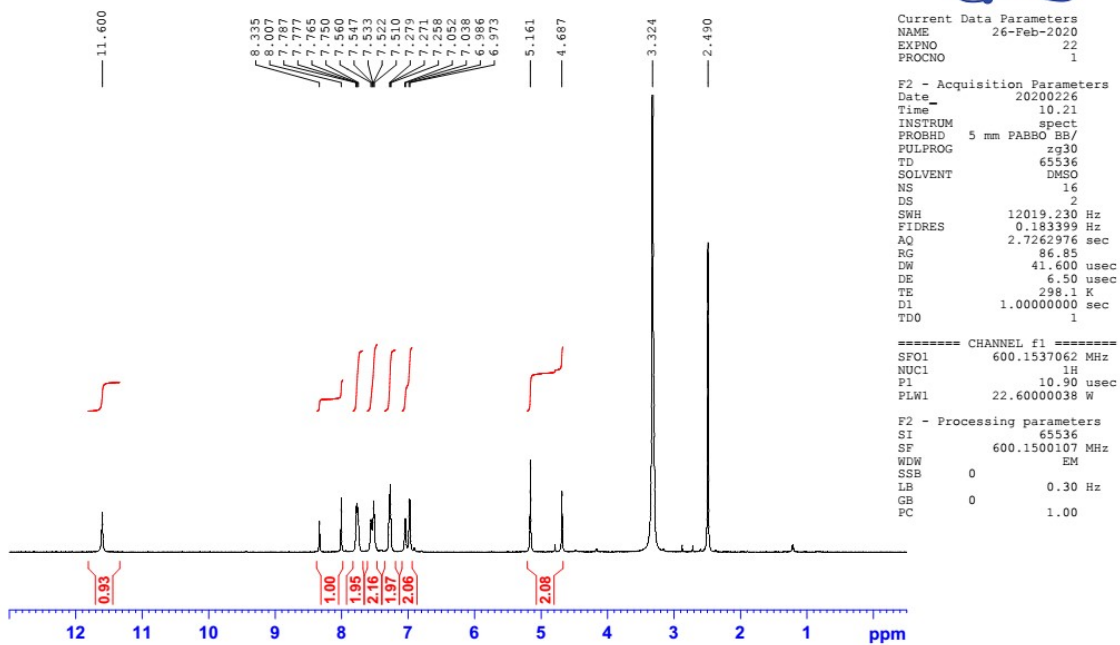
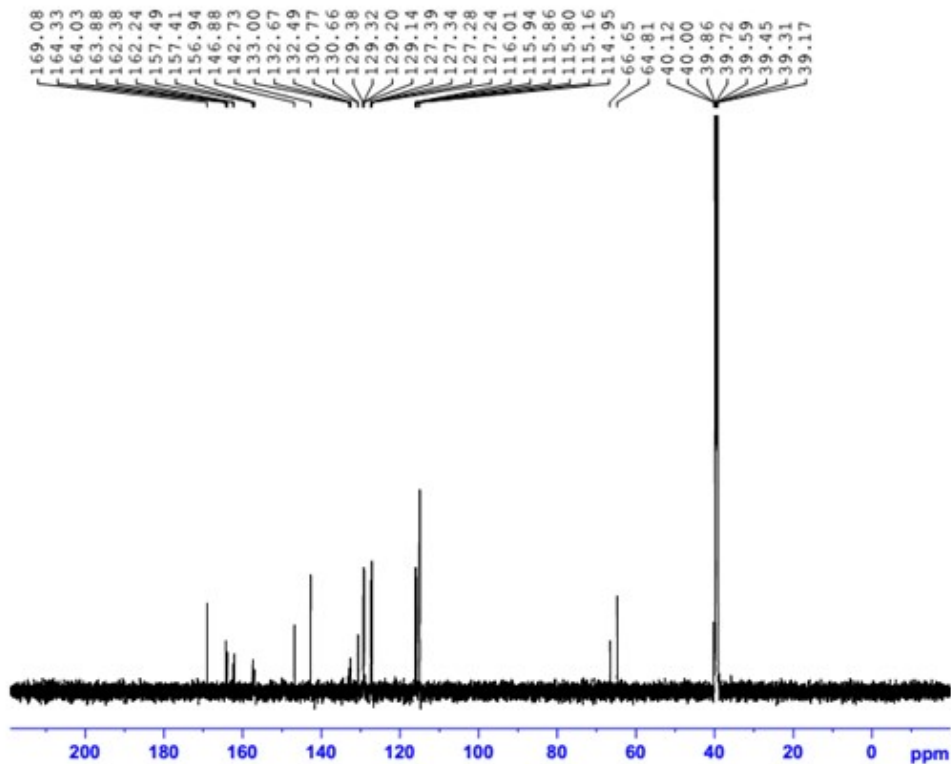


Figure S61: ^1H NMR OF COMPOUND 4s

Dr. Ajmal / MIM19 / DMSO
C13CPD



Current Data Parameters
NAME 28-Jan-2021
EXNO 78
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210129
Time 11.32
INSTNM spect
PROBHD 5 mm PABBO 507
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 34057.491 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 195.2
DM 13.847 usec
DE 4.50 usec
TE 296.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 150.9229276 MHz
NUC1 13C
P1 11.60 usec
PLW1 83.0000000 W

----- CHANNEL f2 -----
SFO2 600.1524006 MHz
NUC2 1H
CPCPRG[2] waltz16
PCPD2 70.00 usec
PLW2 22.4000000 W
PLW3 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9079041 MHz
WEW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S62: ^{13}C NMR OF COMPOUND 4s

Sample Name	MIM-19	Position	Vial 49	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-19_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 5:33:21 PM

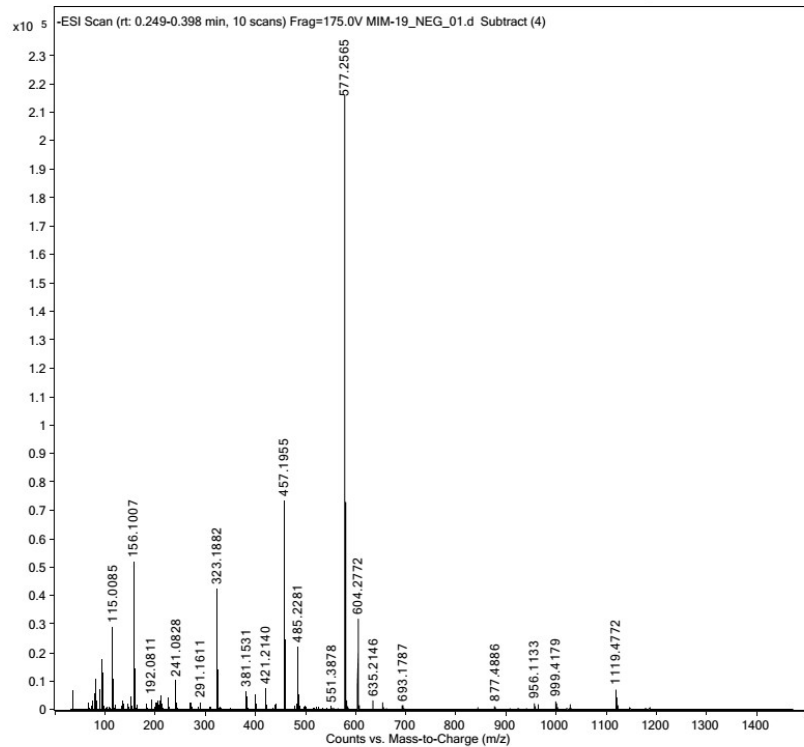


Figure S63: HR-MS OF COMPOUND 4s

Dr. Ajmal/Prof. Ahmed/M1M-20/DMSO
PROTON

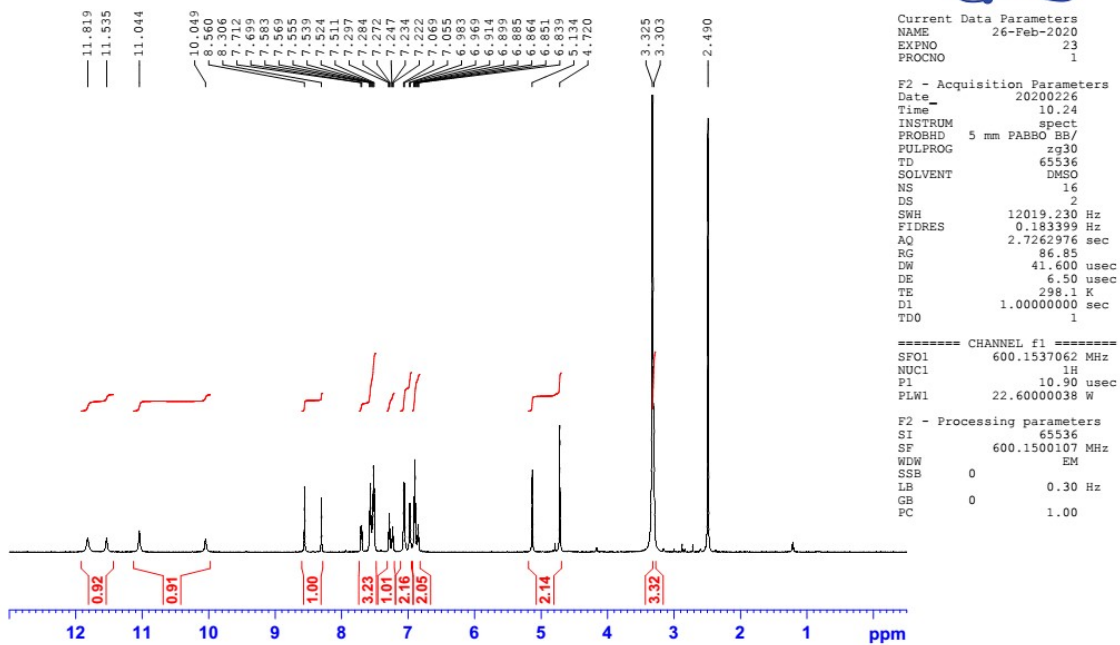
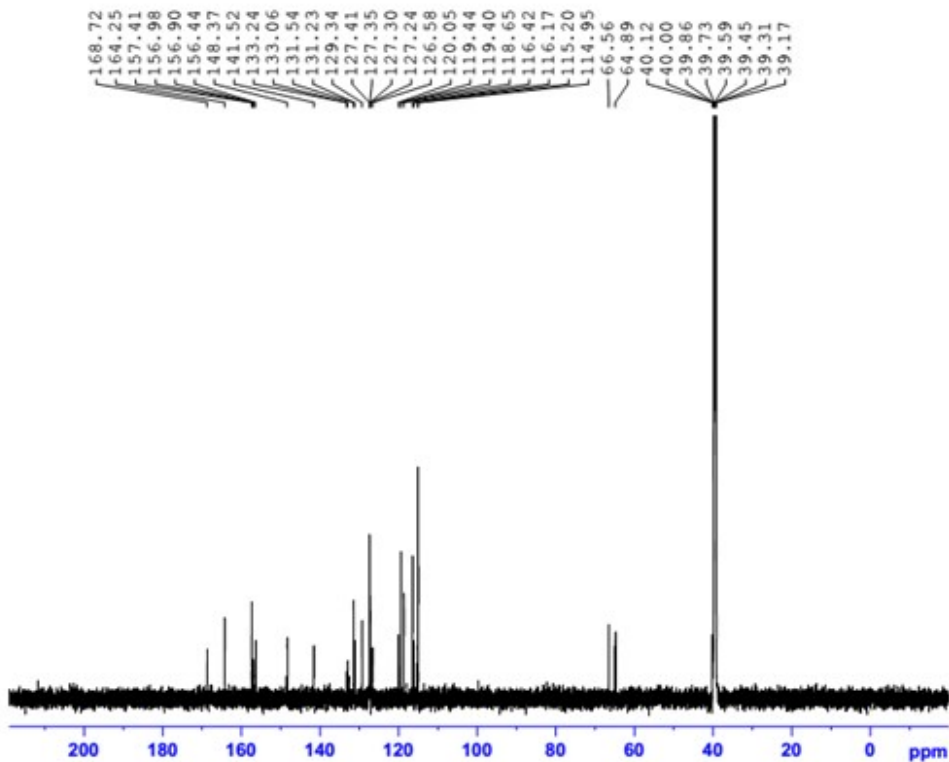


Figure S64: ^1H NMR OF COMPOUND 4t

Dr. Ajmal / MIM20 / DMSO
C13CPD



```
Current Data Parameters
NAME      28-Jan-2021
EXPRO    34
PROBHD    1
F2 - Acquisition Parameters
Date_    20210128
Time     18.26
INSTRUM  spect
PROBHD   5 mm PABBO 50/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       2048
DS       4
SRR      36057.691 Hz
FIDRES   0.550197 Hz
AQ       0.9087659 sec
RG       195.2
IR       11.847 sec
DE       6.50 sec
TE       294.2 K
D1       2.0000000 sec
d11      0.0300000 sec
TD0      1
----- CHANNEL f1 -----
SFO1    150.9229276 MHz
NUC1     13C
P1       11.60 sec
PLW1     83.00000000 W
----- CHANNEL f2 -----
SFO2    600.1524004 MHz
NUC2     1H
PCPD212  wait:16
PCPD2    70.00 sec
PLW2     22.60000038 W
PLW3     0.25874999 W
-----
F2 - Processing parameters
SI       32768
SF       150.9079041 MHz
WDW      DM
SSB      0
LA       1.00 Hz
GB       0
PC       1.40
```

Figure S65: ^{13}C NMR OF COMPOUND 4t

Sample Name	MIM-20	Position	Vial 50	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-20_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 5:40:31 PM

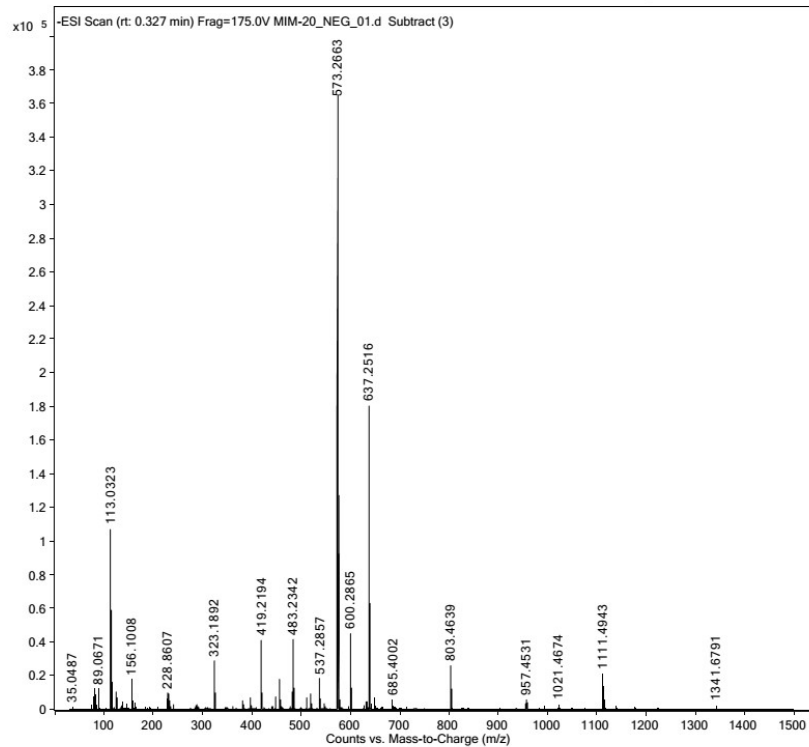


Figure S66: HR-MS OF COMPOUND 4t

Dr. Ajmal/Prof. Ahmed/M1M-21/DMSO
PROTON

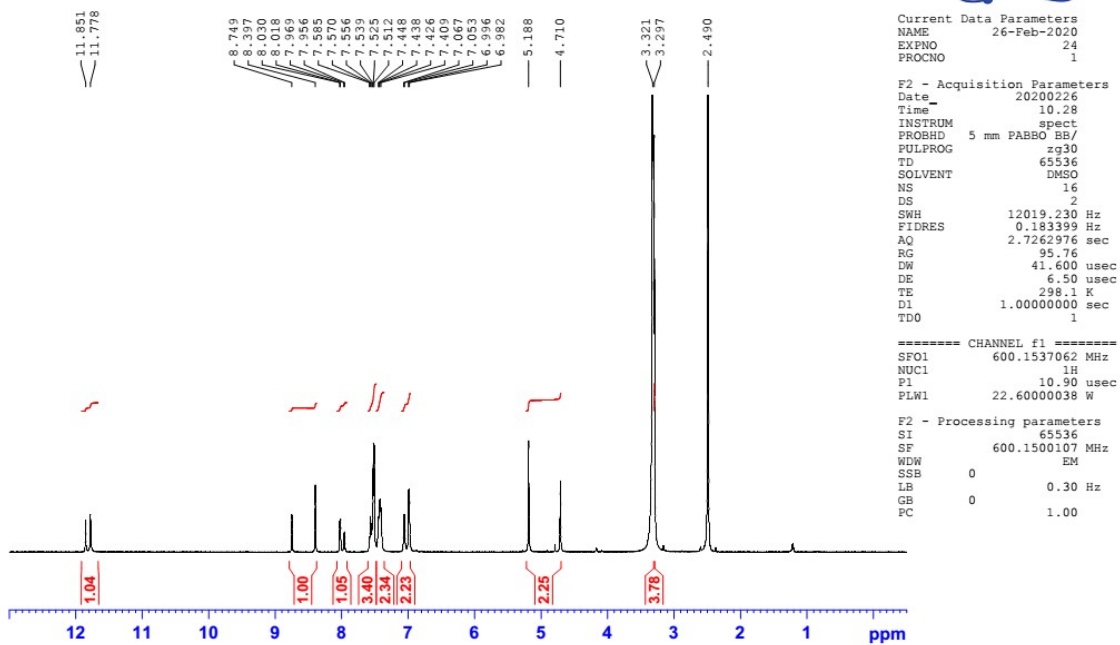
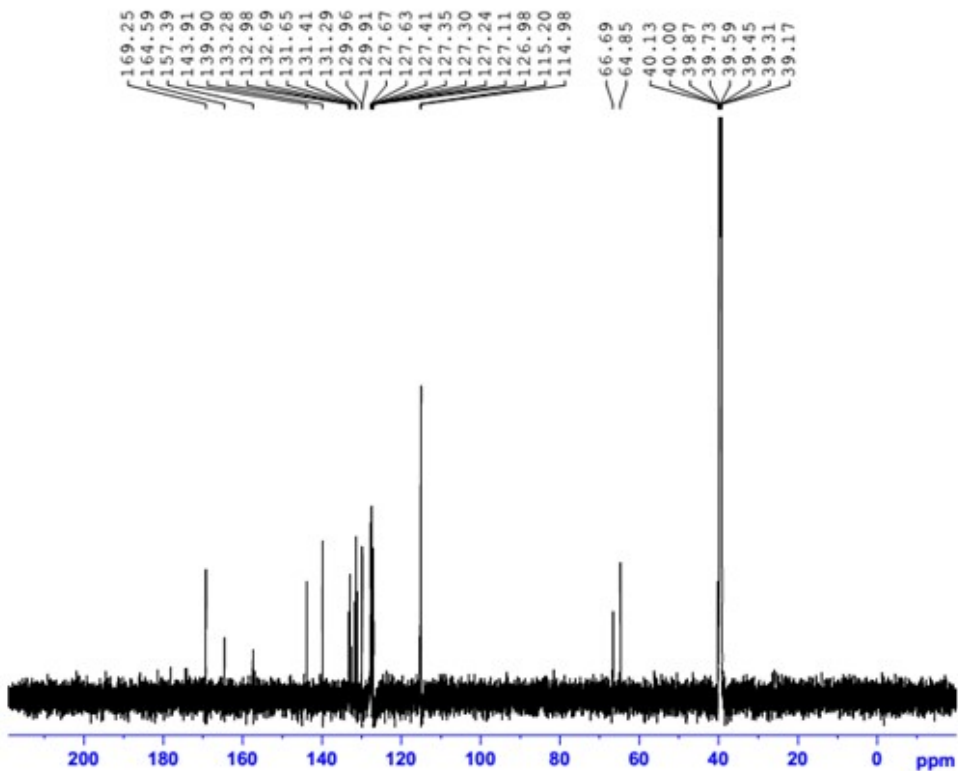


Figure S67: ^1H NMR OF COMPOUND 4u

Dr. Ajmal / MIM21 / DMSO
C13CPD



Current Data Parameters
NAME 28-Jan-2021
EXNO 66
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210128
Time 11.14
INSTRUM spect
PROBHD 5 mm DABBO 50/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 34057.491 Hz
FIDRES 0.550197 Hz
AQ 0.9097659 sec
RG 199.2
DM 13.847 usec
DE 6.50 usec
TE 296.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

----- CHANNEL f1 -----
SF01 150.9229276 MHz
NUC1 13C
P1 11.60 usec
PLM1 83.0000000 W

----- CHANNEL f2 -----
SF02 600.1524006 MHz
NUC2 1H
CPOPRG[2] waltz16
PCPD2 70.00 usec
PLM2 22.6000000 W
PLM3 0.5200000 W
PLM3 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9079041 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S68: ¹³C NMR OF COMPOUND 4u

Sample Name	MIM-21	Position	Vial 51	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-21_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 5:47:39 PM

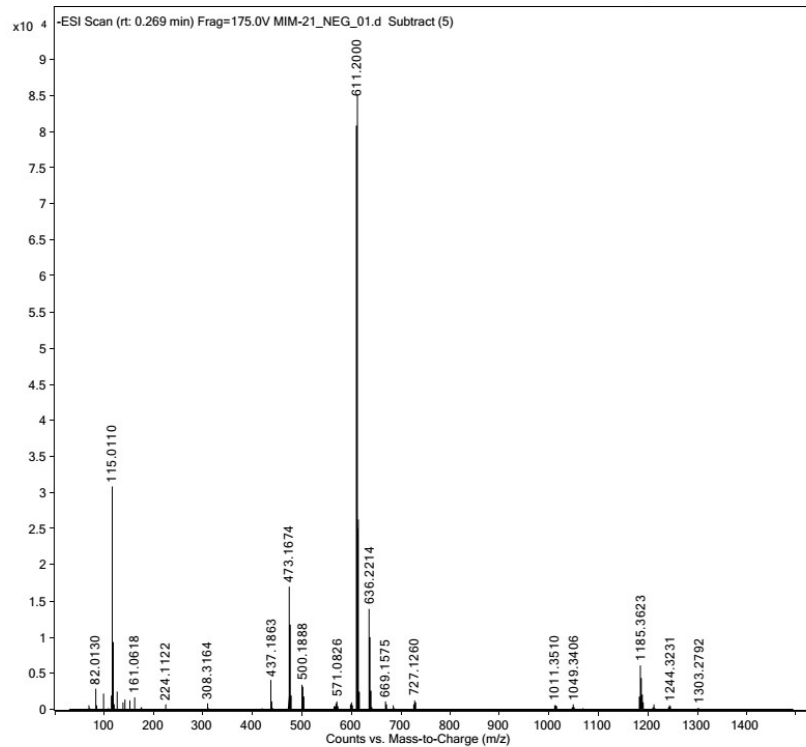


Figure S69: HR-MS OF COMPOUND 4u

Dr. Ajmal/Prof. Ahmed/M1M-22/DMSO
PROTON

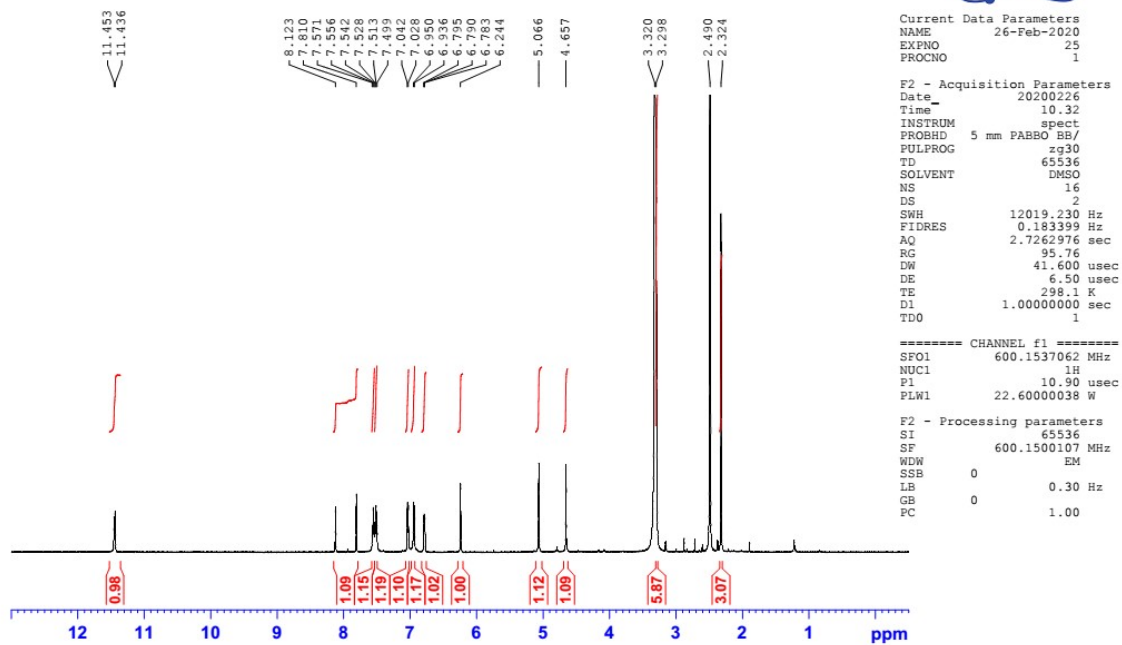
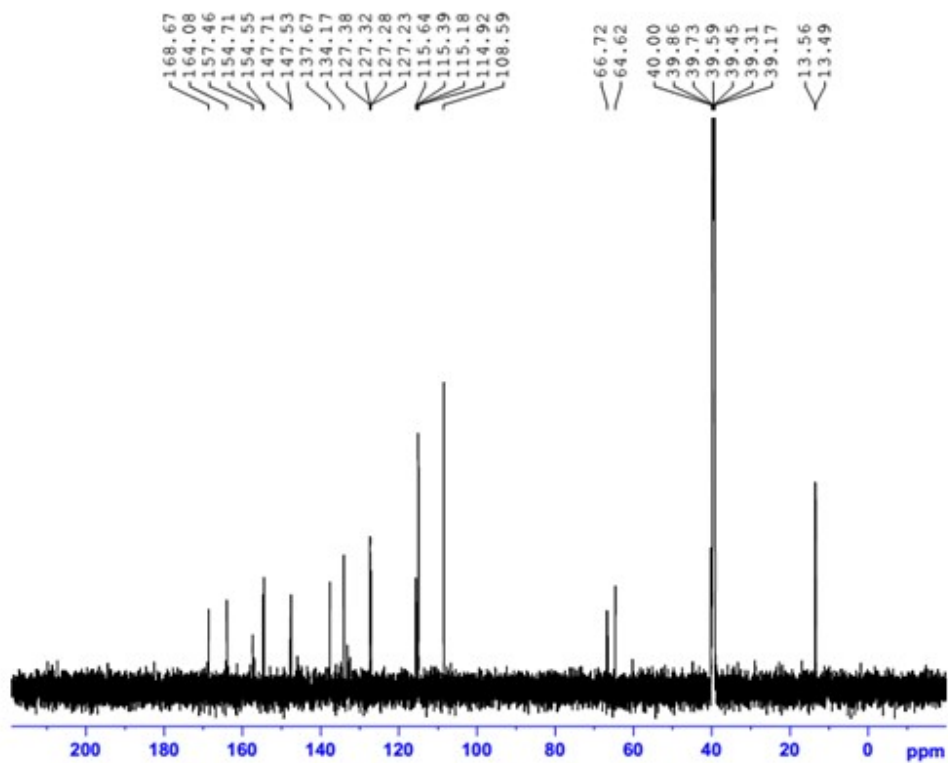


Figure S70: ^1H NMR OF COMPOUND 4v

Dr. Ajmal / MIM22 / DMSO
C13CPD



Current Data Parameters
NAME 28-Jun-2021
EXPNO 62
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210128
Time 7.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65534
SOLVENT DMSO
NS 2048
DS 4
SWH 36057.491 Hz
FIDRES 0.550197 Hz
AQ 0.5087459 sec
RG 195.2
DM 13.867 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 150.923276 MHz
NUC1 13C
P1 11.60 usec
PLM1 83.00000000 W

----- CHANNEL f2 -----
SFO2 600.1524006 MHz
NUC2 1H
CPOPRG12 waltz16
PCPD2 70.00 usec
PLM2 22.60000038 W
PLM12 0.52804002 W
PLM13 0.35874999 W

F2 - Processing parameters
SI 32768
SF 150.9079041 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S71: ¹³C NMR OF COMPOUND 4v



Figure S72: HR-MS OF COMPOUND 4v

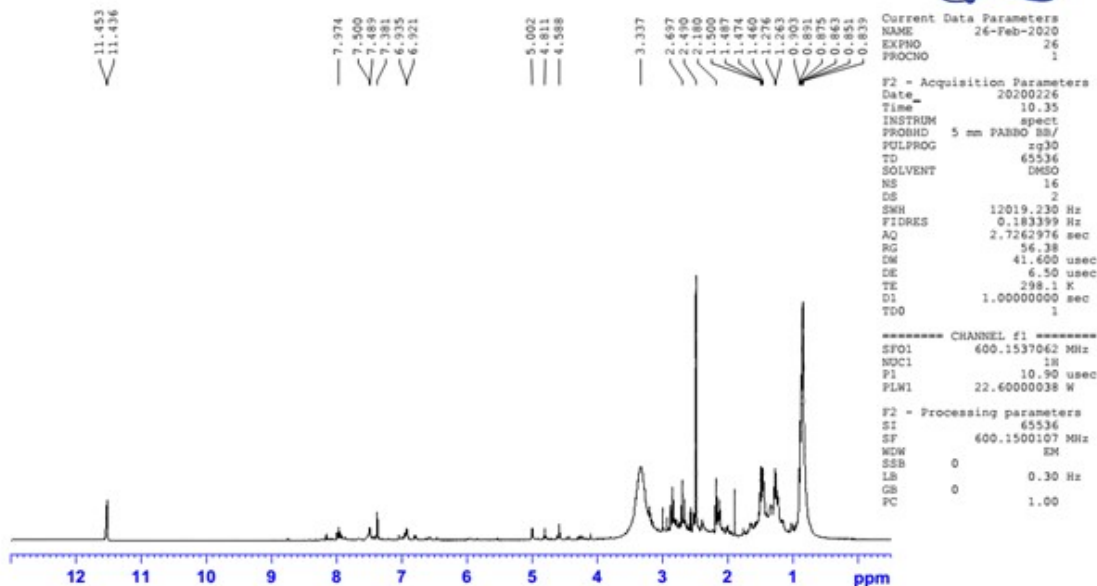
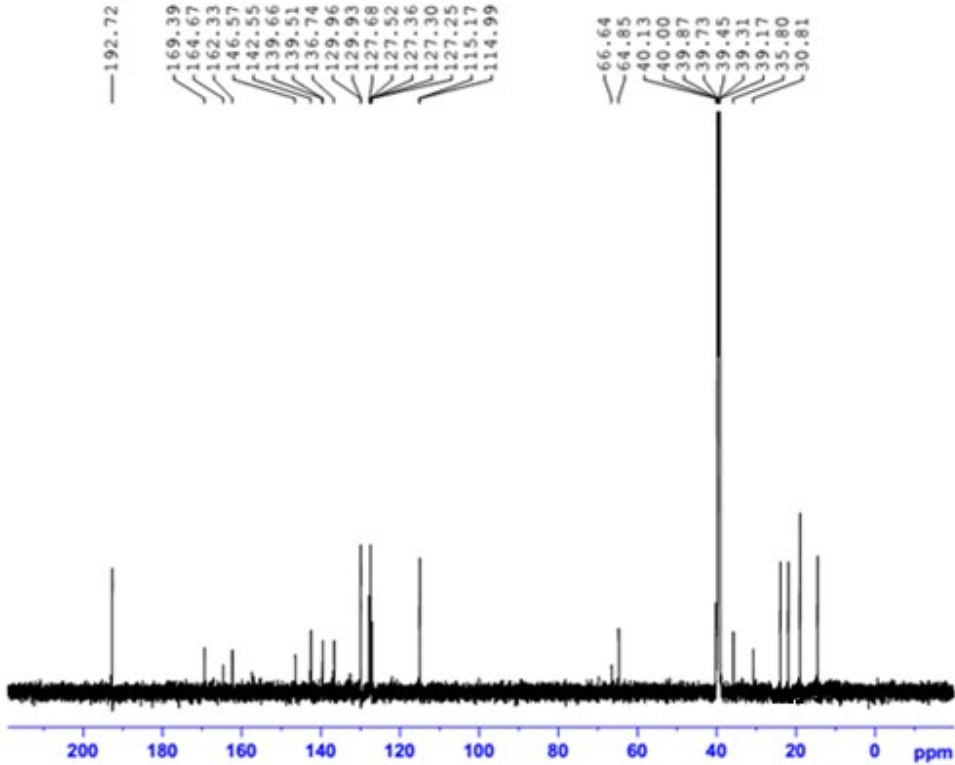


Figure S73: ^1H NMR OF COMPOUND 4w

Dr. Ajmal / MIN23 / DMSO
C13CPD



Current Date Parameters
NAME 28-Jan-2021
EXFNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210128
Time 23.46
INSTRUM spect
PROBHD 5 mm PABBO 1H/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 34057.491 Hz
FIDRES 0.180197 Hz
AQ 0.9087659 sec
RG 199.2
SW 13.645 used
DE 6.50 used
TE 296.6 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL F1 =====
SFO1 150.9229276 MHz
NUC1 13C
P1 11.60 used
PLM1 83.0000000 W

==== CHANNEL F2 =====
SFO2 400.1524006 MHz
NUC2 1H
CFOFREQ2 waltz16
PCPO2 70.00 used
PLM2 22.6000000 W
PLM3 0.5000000 W
PLM3 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9079041 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S74: ¹³C NMR OF COMPOUND 4w

Sample Name	MIM-15	Position	Vial 45	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	MIM-15_NEG_01.d
ACQ Method	NEG ION METHOD MS.m	Comment		Acquired Time	10-Mar-20 5:04:41 PM

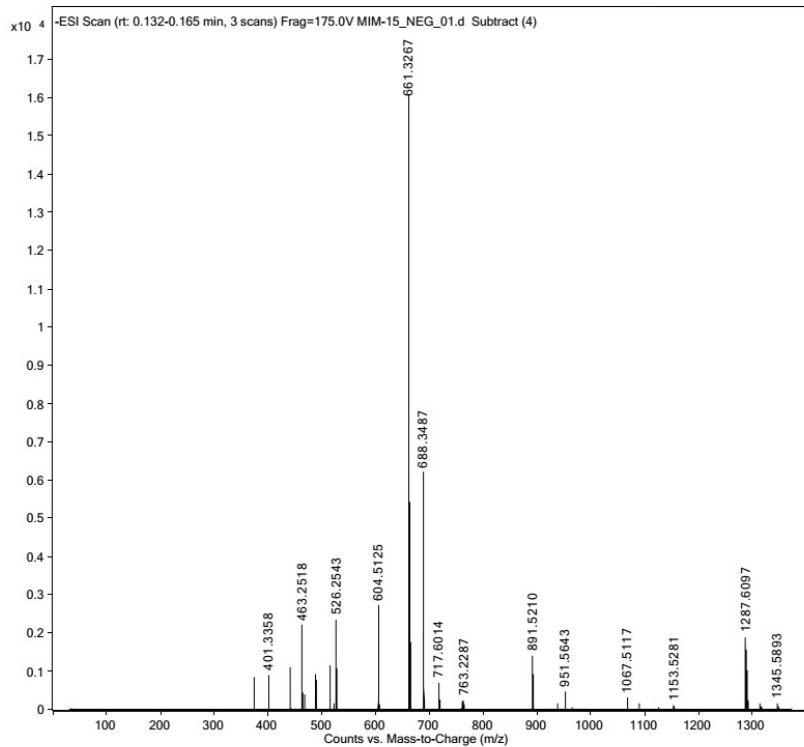


Figure S75: HR-MS OF COMPOUND 4w

Dr. Ajmal/Prof. Ahmed/M1M-24/DMSO
PROTON

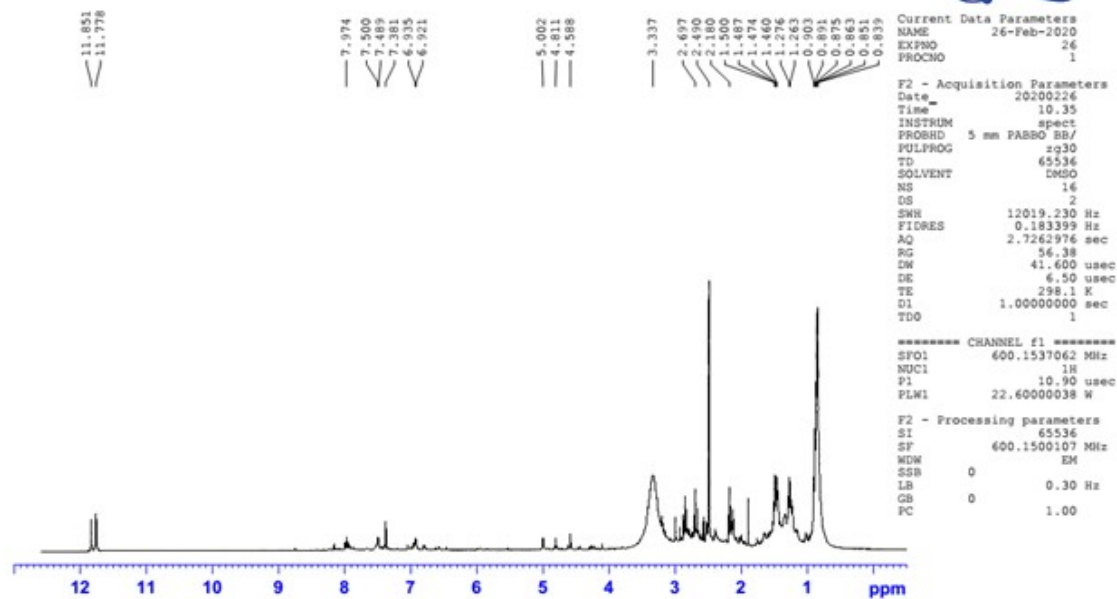
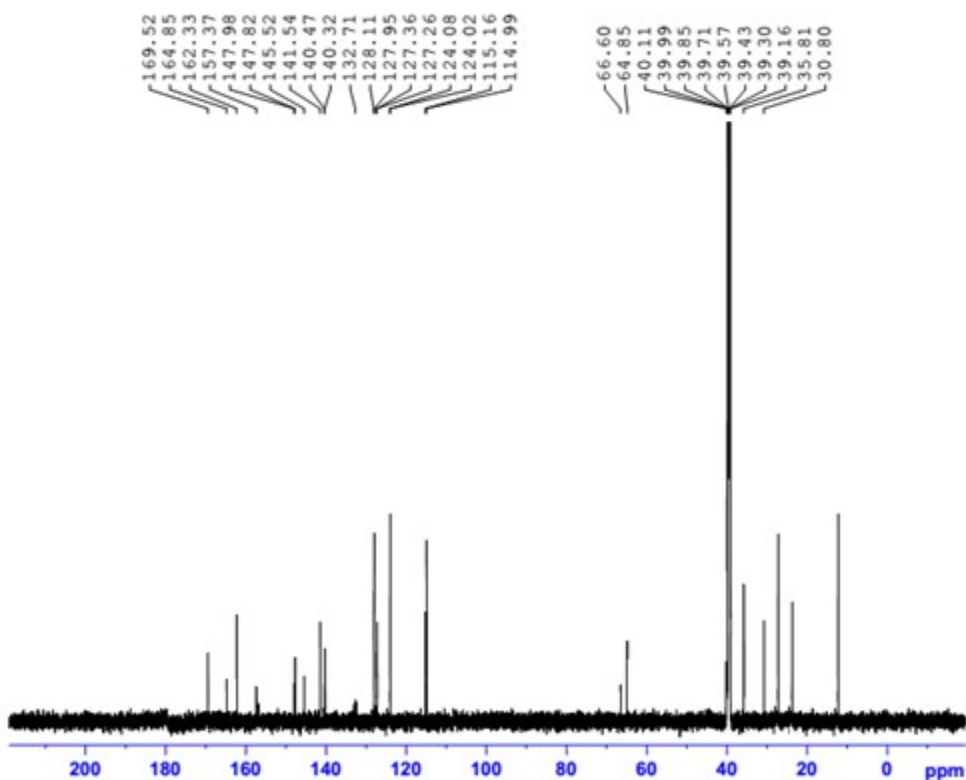


Figure S76: ^1H NMR OF COMPOUND 4x

Dr. Ajmal / MIM24 / DMSO
C13CPD



```
Current Data Parameters
NAME      25-Jan-2011
EXPNO    20
PROCNO    1

F2 = Acquisition Parameters
Date_     20110125
Time      22.23
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         2048
DS         4
SWH        36057.491 Hz
FIDRES     0.550197 Hz
AQ         0.9087459 sec
RG         195.2
DM         13.867 usec
DE         6.50 usec
TE         296.6 K
D1         2.0000000 sec
d11        0.0100000 sec
TDO        1

----- CHANNEL f1 -----
SFO1      150.922976 MHz
NUC1       13C
P1         11.60 usec
PLM1       83.0000000 W

----- CHANNEL f2 -----
SFO2      400.1524006 MHz
NUC2       1H
CPOPRG[2] waltz16
PCPD1      70.00 usec
PLM2       22.6000000 W
PLM12      0.52806002 W
PLM13      0.25874999 W

F2 = Processing parameters
SI         32768
SF         150.9079041 MHz
WDW        EM
SSB        0
LA         1.00 Hz
GB         0
PC         1.40
```

Figure S77: ^{13}C NMR OF COMPOUND 4x



Figure S78: HR-MS OF COMPOUND 4x

Dr. Ajmal/Prof. Ahmed/M1M-25/DMSO
PROTON

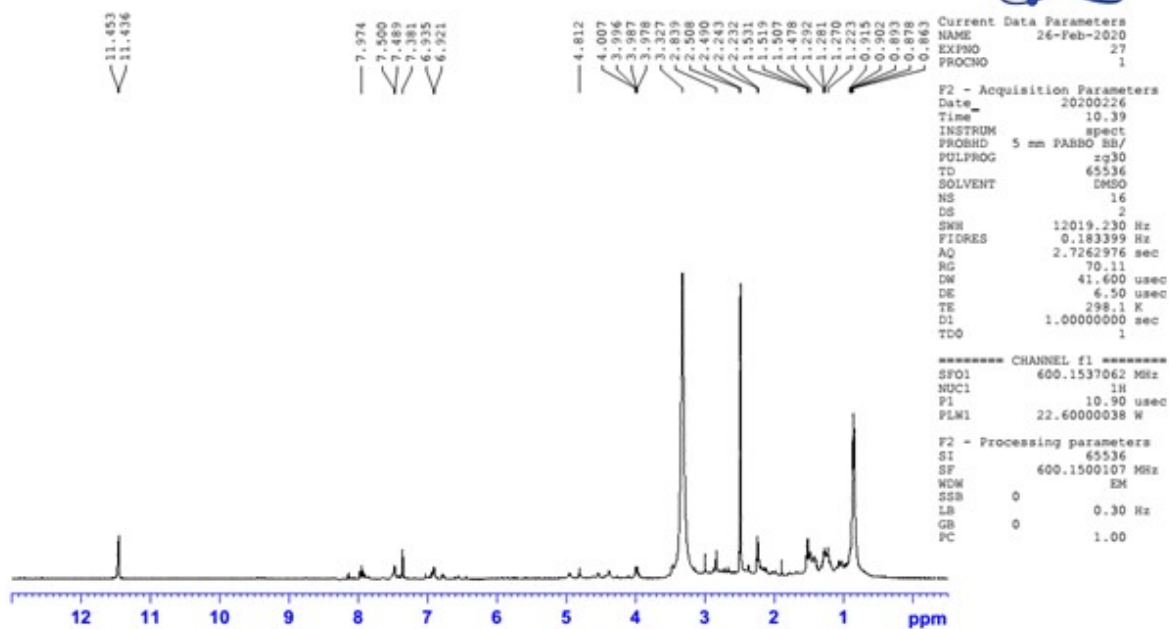
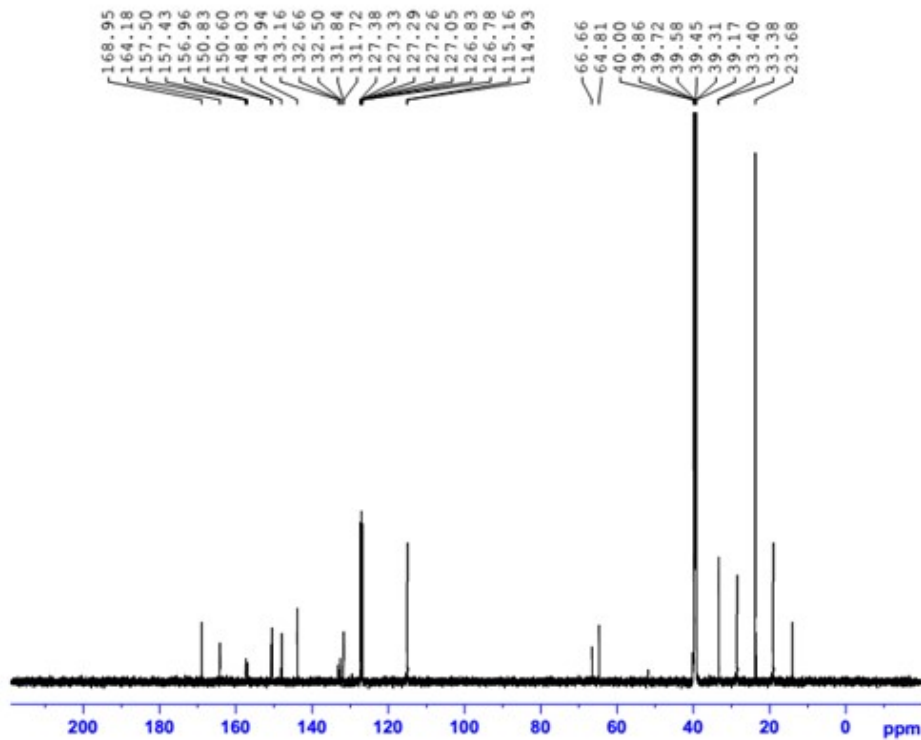


Figure S79: ^1H NMR OF COMPOUND 4y

Dr. Ajmal / MIM25 / DMSO
C13CPD



```
Current Data Parameters
NAME      28-Jun-2021
EXPNO    50
PROCNO    1

F2 - Acquisition Parameters
Date_     20210128
Time      0.24
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        2048
DS        4
SWH        34057.691 Hz
FIDRES    0.550197 Hz
AQ         0.3087459 sec
RG         195.2
DE         13.867 usec
TE         296.4 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

----- CHANNEL f1 -----
SF01      150.9229276 MHz
NUC1       13C
P1         11.60 usec
PLW1       83.0000000 W

----- CHANNEL f2 -----
SF02      600.1524006 MHz
NUC2       1H
CPCORR[2]  wait:16
PCPD2     70.00 usec
PLW2     22.6000000 W
PLW12     0.52806002 W
PLW13     0.25874999 W

F2 - Processing parameters
SI         32768
SF         150.9079041 MHz
WDW        EM
SSB        0
GB         0
PC         1.40
```

Figure S80: ^{13}C NMR OF COMPOUND 4y

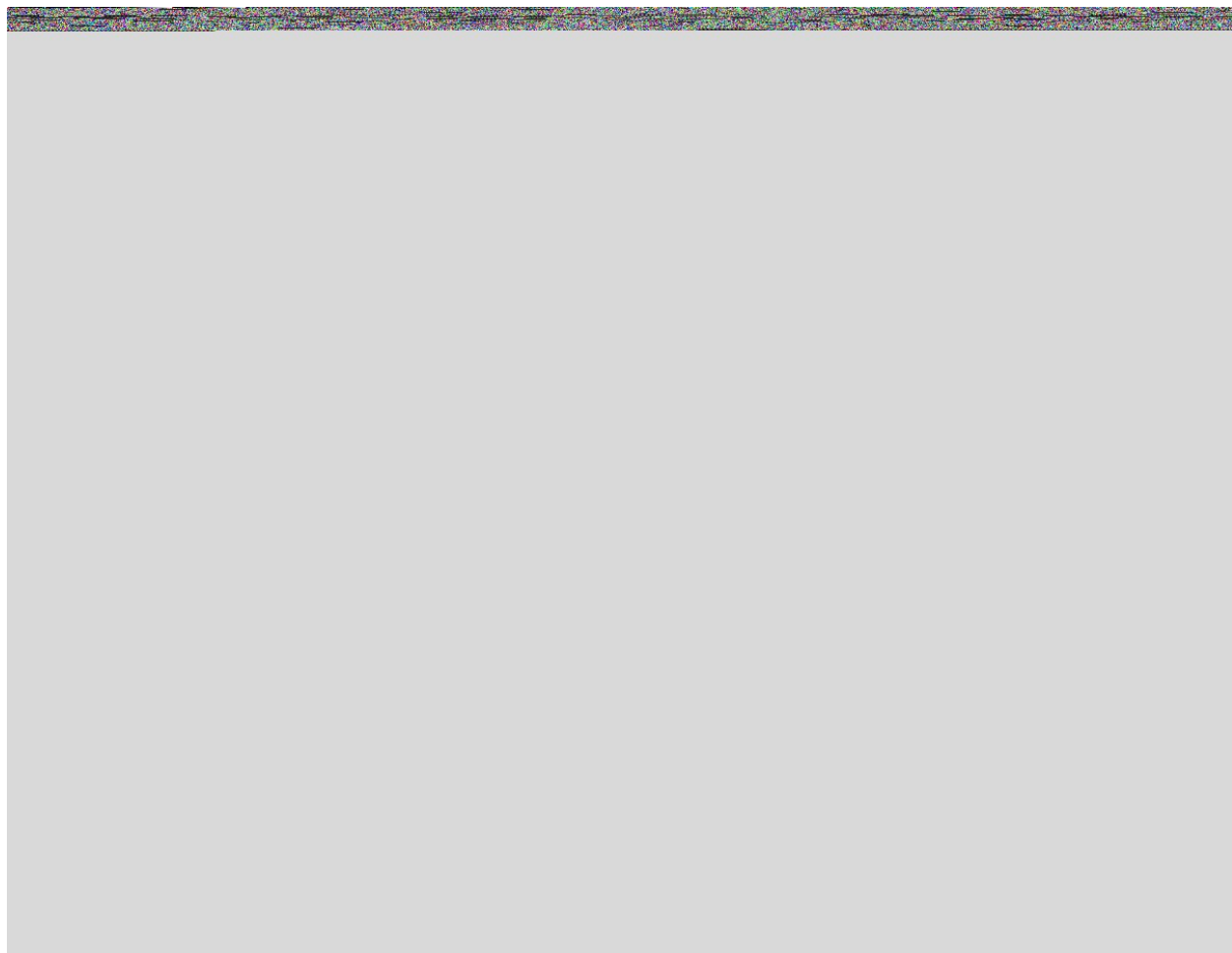
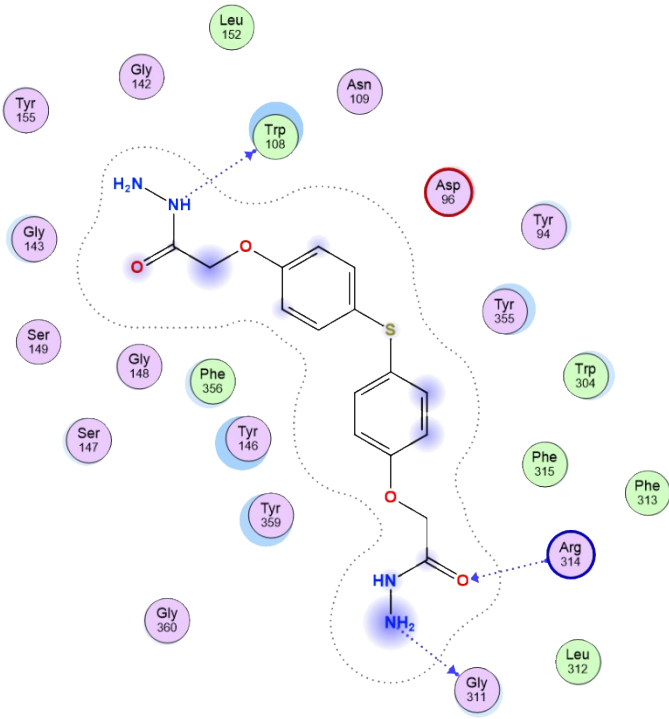
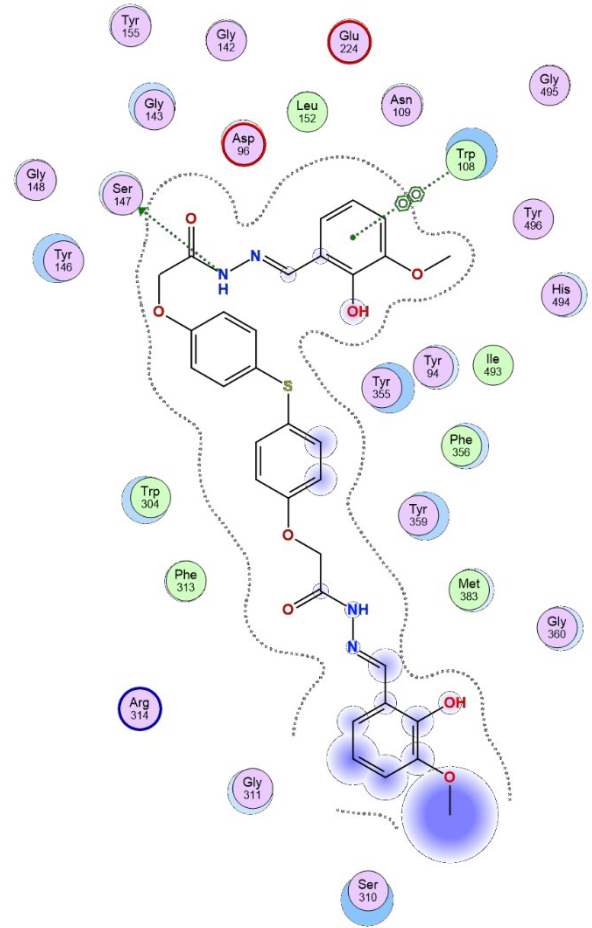


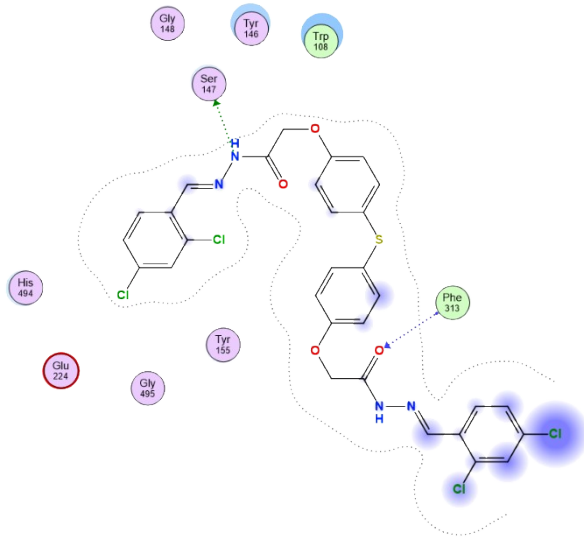
Figure S81: HR-MS OF COMPOUND 4y



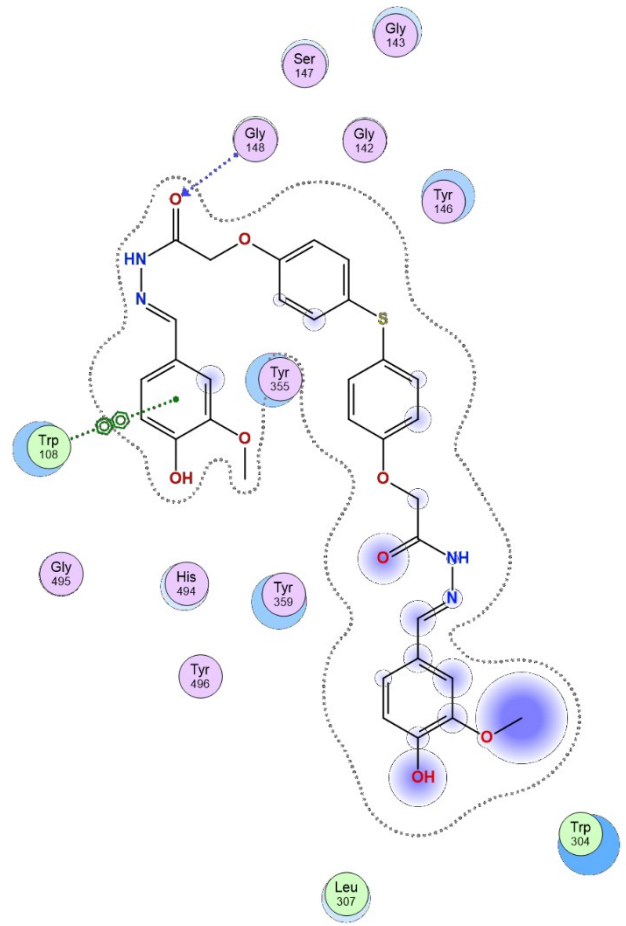
SM3



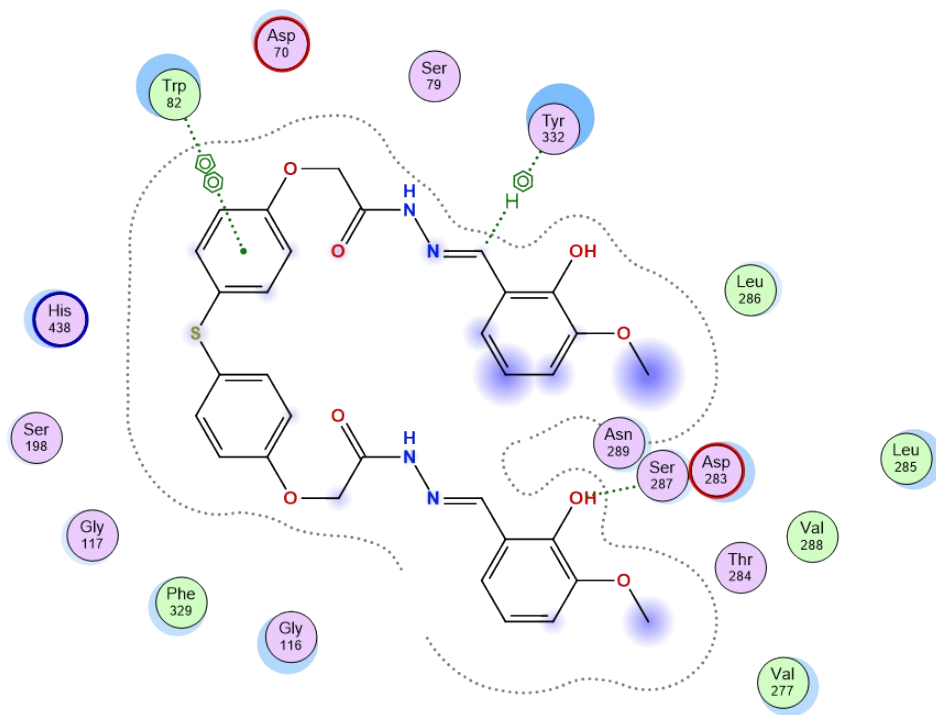
4h



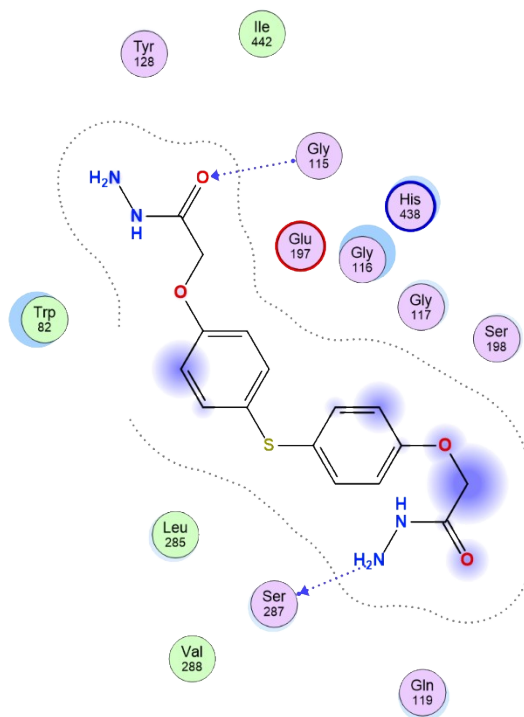
4k



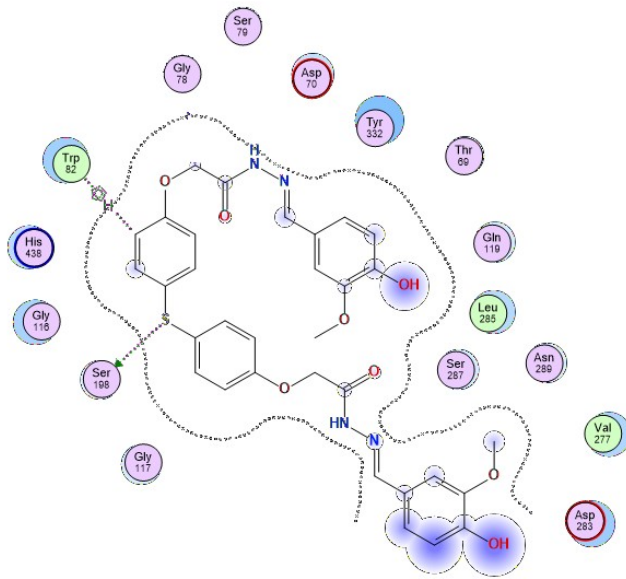
4i



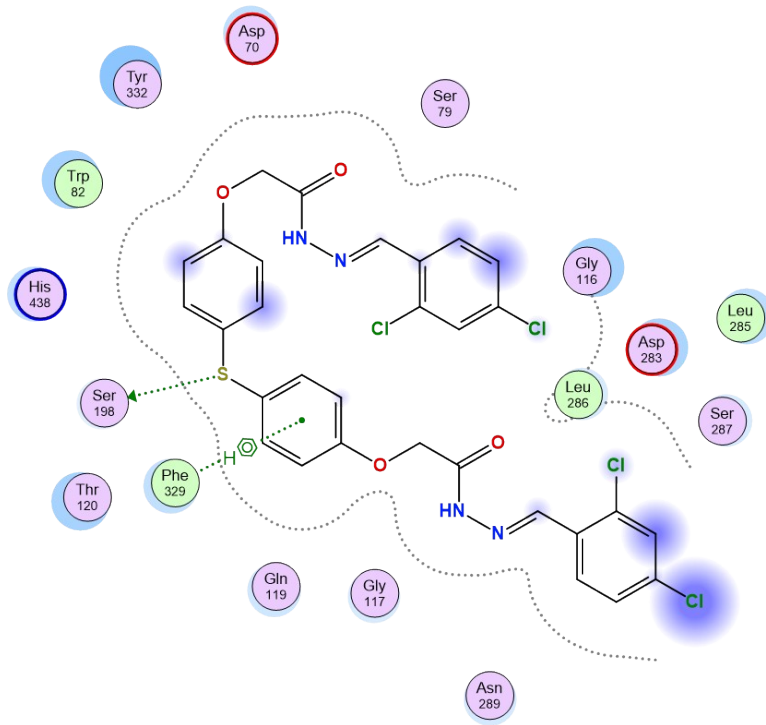
4h



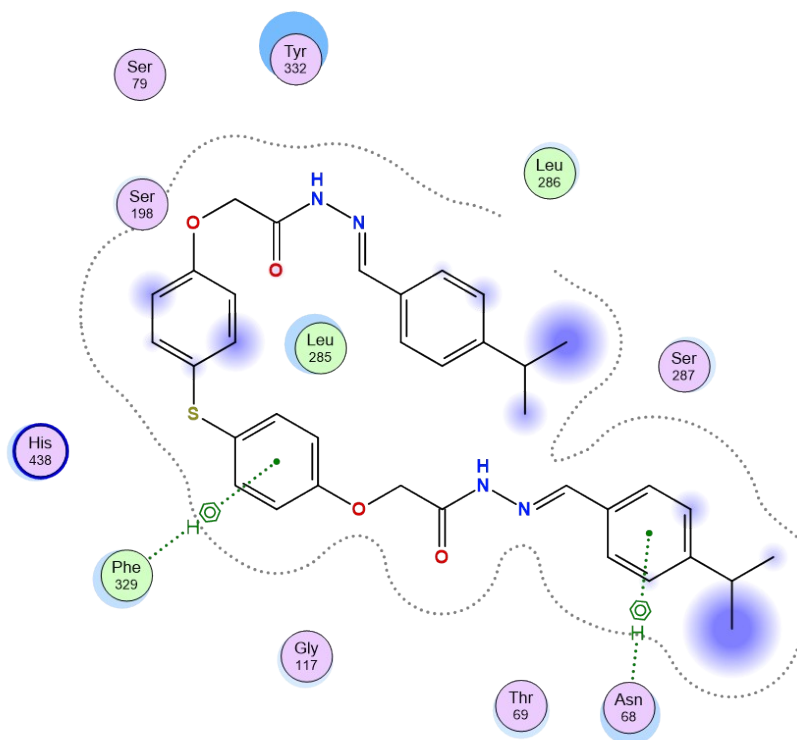
SM3



4i



4k



4q

Figure S83. 2D interactions of docked compounds with the active site residues of BuChE