Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Tetrazolopyrimidine Tethered Phenothiazine Molecular Hybrids: Synthesis, Biological and Molecular Docking Studies

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Supplementary Information

Table S1. Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for non-H atoms with esd's in parenthesis

Atom	x	y	z	Ueq
S(1)	867(1)	3839(1)	2100(1)	43(1)
O(1)	4411(1)	969(1)	3203(1)	60(1)
O(2)	3684(1)	1132(1)	4633(1)	47(1)
N(1)	4551(1)	4699(2)	3279(1)	42(1)
N(2)	4284(1)	6316(2)	4397(2)	45(1)
N(3)	3832(1)	6343(2)	5274(2)	48(1)
N(4)	3508(1)	5336(2)	5499(1)	42(1)
N(5)	3749(1)	4613(2)	4749(1)	33(1)
N(6)	-314(1)	3391(2)	3887(1)	32(1)
C(1)	3480(1)	3391(2)	4665(2)	30(1)
C(2)	4067(1)	2855(2)	3860(2)	33(1)
C(3)	4538(1)	3501(2)	3207(2)	38(1)
C(4)	4215(1)	5225(2)	4098(2)	34(1)
C(5)	5102(2)	3052(2)	2377(2)	62(1)
C(6)	4086(1)	1581(2)	3834(2)	36(1)
C(7)	3644(2)	-125(2)	4717(2)	52(1)
C(8)	3203(2)	-402(3)	5675(2)	82(1)
C(9)	2482(1)	3326(2)	4449(2)	28(1)
C(10)	1877(1)	3056(2)	5187(2)	32(1)
C(11)	961(1)	3086(2)	5008(2)	33(1)
C(12)	615(1)	3376(2)	4079(1)	28(1)
C(13)	1230(1)	3623(2)	3324(1)	29(1)
C(14)	2146(1)	3611(2)	3518(1)	30(1)
C(15)	-187(1)	4464(2)	2328(2)	35(1)
C(16)	-553(2)	5205(2)	1623(2)	47(1)
C(17)	-1427(2)	5586(2)	1697(2)	53(1)
C(18)	-1928(2)	5233(2)	2495(2)	49(1)
C(19)	-1565(1)	4533(2)	3219(2)	41(1)
C(20)	-685(1)	4126(2)	3157(2)	31(1)
C(21)	-914(1)	2807(2)	4590(2)	33(1)
C(22)	-1212(1)	3474(2)	5501(2)	36(1)
C(23)	-1827(2)	2719(2)	6127(2)	47(1)
C(24)	-2145(2)	3278(2)	7069(2)	60(1)

Table S2. Bond lengths (Å) and bond angles (°) with esd's in parenthesis

Atoms	Bond length	Atoms	Bond length
S(1)-C(13)	1.739(4)	C(20)-C(15)-S(1)	120.4(2)
S(1)-C(15)	1.748(4)	C(17)-C(16)-C(15)	120.9(2)
O(1)-C(6)	1.201(3)	C(18)-C(17)-C(16)	118.8(2)
O(2)-C(6)	1.332(3)	C(19)-C(18)-C(17)	121.0(3)
O(2)-C(7)	1.446(4)	C(18)-C(19)-C(20)	121.3(2)
N(1)-C(4)	1.350(3)	C(15)-C(20)-C(19)	117.3(2)
N(1)-C(3)	1.377(4)	C(15)-C(20)-N(6)	121.0(2)
N(1)-H(1)	0.8600	C(19)-C(20)-N(6)	121.7(2)
N(2)-C(4)	1.316(4)	N(6)-C(21)-C(22)	118.2(2)
N(2)-N(3)	1.358(4)	C(21)-C(22)-C(23)	109.8(2)
N(3)-N(4)	1.286(3)	C(24)-C(23)-C(22)	114.7(2)
N(4)-N(5)	1.351(3)	**Atoms**	**Bond angle**
N(5)-C(4)	1.319(3)	C(13)-S(1)-C(15)	99.5(1)
N(5)-C(1)	1.461(4)	C(6)-O(2)-C(7)	117.8(2)
N(6)-C(12)	1.399(4)	C(4)-N(1)-C(3)	119.8(2)
N(6)-C(20)	1.400(3)	C(4)-N(2)-N(3)	104.3(2)
N(6)-C(21)	1.463(3)	N(4)-N(3)-N(2)	111.7(2)
C(1)-C(9)	1.508(4)	N(3)-N(4)-N(5)	105.9(2)
C(1)-C(2)	1.521(3)	C(4)-N(5)-N(4)	108.0(2)
C(1)-H(1A)	0.9800	C(4)-N(5)-C(1)	127.1(2)
C(2)-C(3)	1.346(3)	N(4)-N(5)-C(1)	124.8(2)
C(2)-C(6)	1.461(4)	C(12)-N(6)-C(20)	121.1(2)
C(3)-C(5)	1.488(4)	C(12)-N(6)-C(21)	118.7(2)
C(7)-C(8)	1.480(4)	C(20)-N(6)-C(21)	119.1(2)
C(9)-C(10)	1.375(3)	N(5)-C(1)-C(9)	109.2(2)
C(9)-C(14)	1.379(4)	N(5)-C(1)-C(2)	106.5(2)
C(10)-C(11)	1.379(4)	C(9)-C(1)-C(2)	114.2(2)
C(11)-C(12)	1.383(4)	C(3)-C(2)-C(6)	121.6(2)
C(12)-C(13)	1.396(3)	C(3)-C(2)-C(1)	122.8(2)
C(13)-C(14)	1.380(4)	C(6)-C(2)-C(1)	115.6(2)
C(15)-C(16)	1.378(4)	C(2)-C(3)-N(1)	120.7(2)
C(15)-C(20)	1.393(4)	C(2)-C(3)-C(5)	126.3(2)
C(16)-C(17)	1.372(4)	N(1)-C(3)-C(5)	113.0(2)

C(17)-C(18)	1.367(4)	N(2)-C(4)-N(5)	110.1(2)
C(18)-C(19)	1.366(4)	N(2)-C(4)-N(1)	130.0(2)
C(19)-C(20)	1.390(4)	N(5)-C(4)-N(1)	119.9(2)
C(21)-C(22)	1.510(4)	O(1)-C(6)-O(2)	121.6(2)
C(22)-C(23)	1.515(3)	O(1)-C(6)-C(2)	127.4(2)
C(23)-C(24)	1.496(4)	O(2)-C(6)-C(2)	111.0(2)
C(11)-C(12)-C(13)	117.3(2)	O(2)-C(7)-C(8)	107.4(2)
C(11)-C(12)-N(6)	121.8(2)	O(2)-C(7)-H(7A)	110.2
C(13)-C(12)-N(6)	120.9(2)	C(8)-C(7)-H(7A)	110.2
C(14)-C(13)-C(12)	120.7(2)	O(2)-C(7)-H(7B)	110.2
C(14)-C(13)-S(1)	118.4(2)	C(10)-C(9)-C(14)	118.0(2)
C(12)-C(13)-S(1)	120.7(2)	C(10)-C(9)-C(1)	121.2(2)
C(9)-C(14)-C(13)	121.4(2)	C(14)-C(9)-C(1)	120.7(2)
C(16)-C(15)-C(20)	120.6(2)	C(9)-C(10)-C(11)	121.1(2)
C(16)-C(15)-S(1)	118.7(2)	C(10)-C(11)-C(12)	121.4(2)

Table S3. Torsion angles (º) with esd's in parenthesis

Atoms	Torsion angle	Atoms	Torsion angle
C(4)-N(2)-N(3)-N(4)	0.0(2)	C(9)-C(10)-C(11)-C(12)	0.8(3)
N(2)-N(3)-N(4)-N(5)	0.0(2)	C(10)-C(11)-C(12)-C(13)	0.8(3)
N(3)-N(4)-N(5)-C(4)	0.0(2)	C(10)-C(11)-C(12)-N(6)	178.9(2)
N(3)-N(4)-N(5)-C(1)	-176.4(2)	C(20)-N(6)-C(12)-C(11)	151.9(2)
C(4)-N(5)-C(1)-C(9)	-106.9(2)	C(21)-N(6)-C(12)-C(11)	-15.9(3)
N(4)-N(5)-C(1)-C(9)	68.8(3)	C(20)-N(6)-C(12)-C(13)	-30.1(3)
C(4)-N(5)-C(1)-C(2)	16.9(3)	C(21)-N(6)-C(12)-C(13)	162.2(2)
N(4)-N(5)-C(1)-C(2)	-167.4(2)	C(11)-C(12)-C(13)-C(14)	-2.0(3)
N(5)-C(1)-C(2)-C(3)	-16.0(3)	N(6)-C(12)-C(13)-C(14)	179.8(2)
C(9)-C(1)-C(2)-C(3)	104.7(2)	C(11)-C(12)-C(13)-S(1)	172.9(2)
N(5)-C(1)-C(2)-C(6)	164.3(2)	N(6)-C(12)-C(13)-S(1)	-5.2(3)
C(9)-C(1)-C(2)-C(6)	-75.1(2)	C(15)-S(1)-C(13)-C(14)	-152.9(2)
C(6)-C(2)-C(3)-N(1)	-176.4(2)	C(15)-S(1)-C(13)-C(12)	32.0(2)
C(1)-C(2)-C(3)-N(1)	3.9(3)	C(10)-C(9)-C(14)-C(13)	-0.2(3)
C(6)-C(2)-C(3)-C(5)	2.0(4)	C(1)-C(9)-C(14)-C(13)	-176.1(2)
C(1)-C(2)-C(3)-C(5)	-177.8(2)	C(12)-C(13)-C(14)-C(9)	1.8(3)
C(4)-N(1)-C(3)-C(2)	10.9(3)	S(1)-C(13)-C(14)-C(9)	-173.3(2)
C(4)-N(1)-C(3)-C(5)	-167.7(2)	C(13)-S(1)-C(15)-C(16)	153.2(2)
N(3)-N(2)-C(4)-N(5)	0.0(2)	C(13)-S(1)-C(15)-C(20)	-33.3(2)
N(3)-N(2)-C(4)-N(1)	-178.7(2)	C(20)-C(15)-C(16)-C(17)	-2.9(3)
N(4)-N(5)-C(4)-N(2)	0.0(2)	S(1)-C(15)-C(16)-C(17)	170.7(2)
C(1)-N(5)-C(4)-N(2)	176.3(2)	C(15)-C(16)-C(17)-C(18)	1.1(4)
N(4)-N(5)-C(4)-N(1)	178.9(2)	C(16)-C(17)-C(18)-C(19)	1.3(4)
C(1)-N(5)-C(4)-N(1)	-4.8(3)	C(17)-C(18)-C(19)-C(20)	-1.9(4)
C(3)-N(1)-C(4)-N(2)	167.9(2)	C(16)-C(15)-C(20)-C(19)	2.2(3)
C(3)-N(1)-C(4)-N(5)	-10.8(3)	S(1)-C(15)-C(20)-C(19)	-171.3(2)
C(7)-O(2)-C(6)-O(1)	-0.5(3)	C(16)-C(15)-C(20)-N(6)	-178.8(2)
C(7)-O(2)-C(6)-C(2)	179.8(2)	S(1)-C(15)-C(20)-N(6)	7.7(3)
C(3)-C(2)-C(6)-O(1)	-9.1(4)	C(18)-C(19)-C(20)-C(15)	0.1(3)
C(1)-C(2)-C(6)-O(1)	170.7(2)	C(18)-C(19)-C(20)-N(6)	-178.8(2)
C(3)-C(2)-C(6)-O(2)	170.6(2)	C(12)-N(6)-C(20)-C(15)	28.7(3)
C(1)-C(2)-C(6)-O(2)	-9.6(3)	C(21)-N(6)-C(20)-C(15)	-163.6(2)
C(6)-O(2)-C(7)-C(8)	177.9(2)	C(12)-N(6)-C(20)-C(19)	-152.4(2)
N(5)-C(1)-C(9)-C(10)	-102.1(2)	C(21)-N(6)-C(20)-C(19)	15.3(3)
C(2)-C(1)-C(9)-C(10)	138.7(2)	C(12)-N(6)-C(21)-C(22)	84.4(2)
N(5)-C(1)-C(9)-C(14)	73.6(2)	C(20)-N(6)-C(21)-C(22)	-83.6(3)
C(2)-C(1)-C(9)-C(14)	-45.5(3)	N(6)-C(21)-C(22)-C(23)	179.9(2)
C(14)-C(9)-C(10)-C(11)	-1.0(3)	C(21)-C(22)-C(23)-C(24)	178.3(2)
C(1)-C(9)-C(10)-C(11)	174.8(2)		

Table S4. Geometric details of hydrogen bond (Å,º)
(D-donor; A-acceptor; H-hydrogen)

Interactions	D-H	H…A	D…A	D-H…A
N1-H1...O1	0.86	2.07	2.912	167
C19-H19...N4	0.93	2.60	3.369	141
C11-H11…S1	0.93	2.94	3.570	126

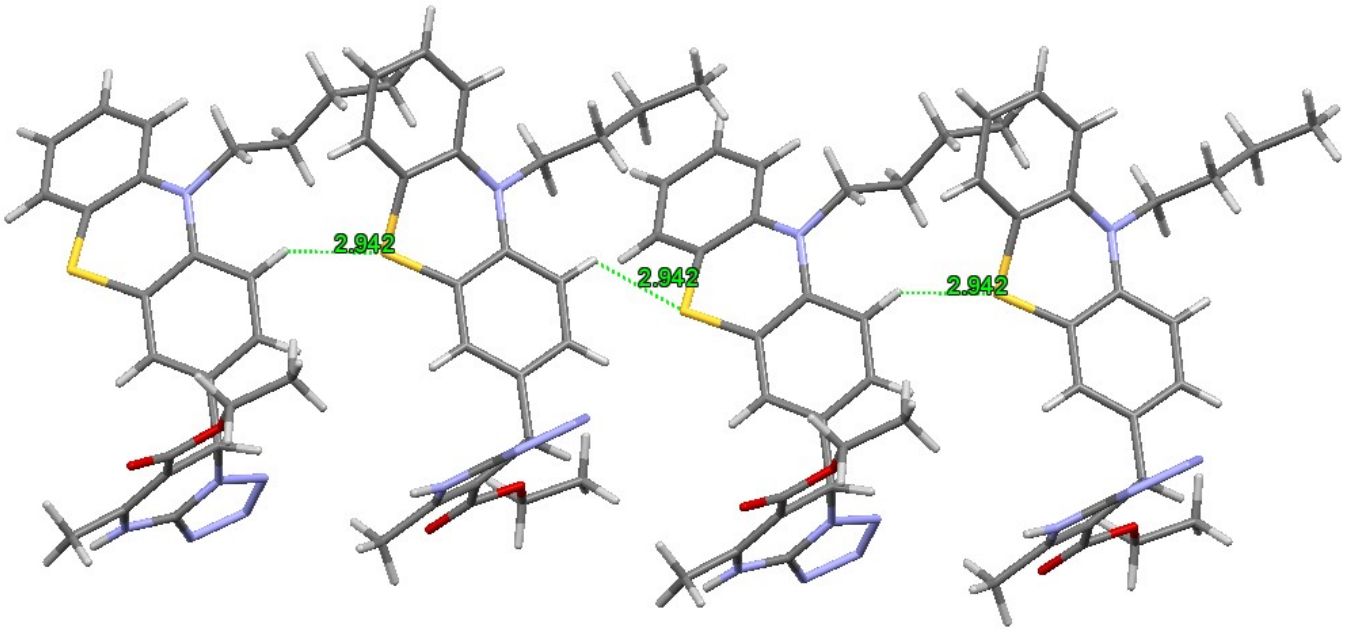


Fig S1. Intermolecular C11-H11…S1 interactions in compound **6b**.

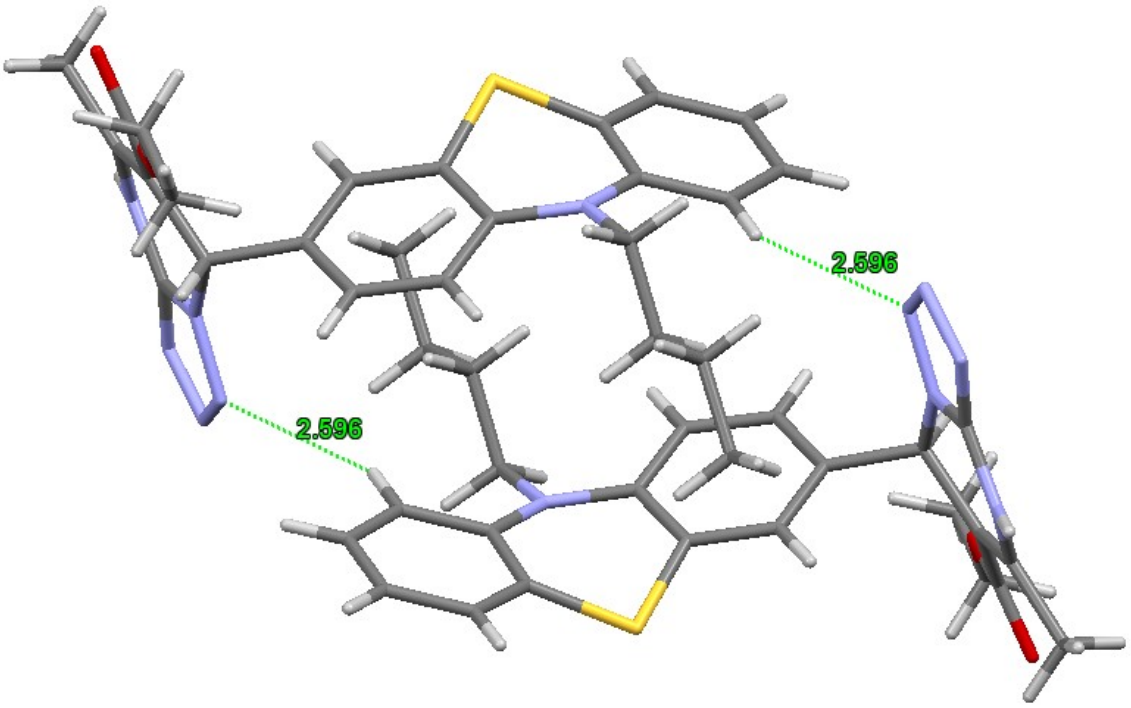
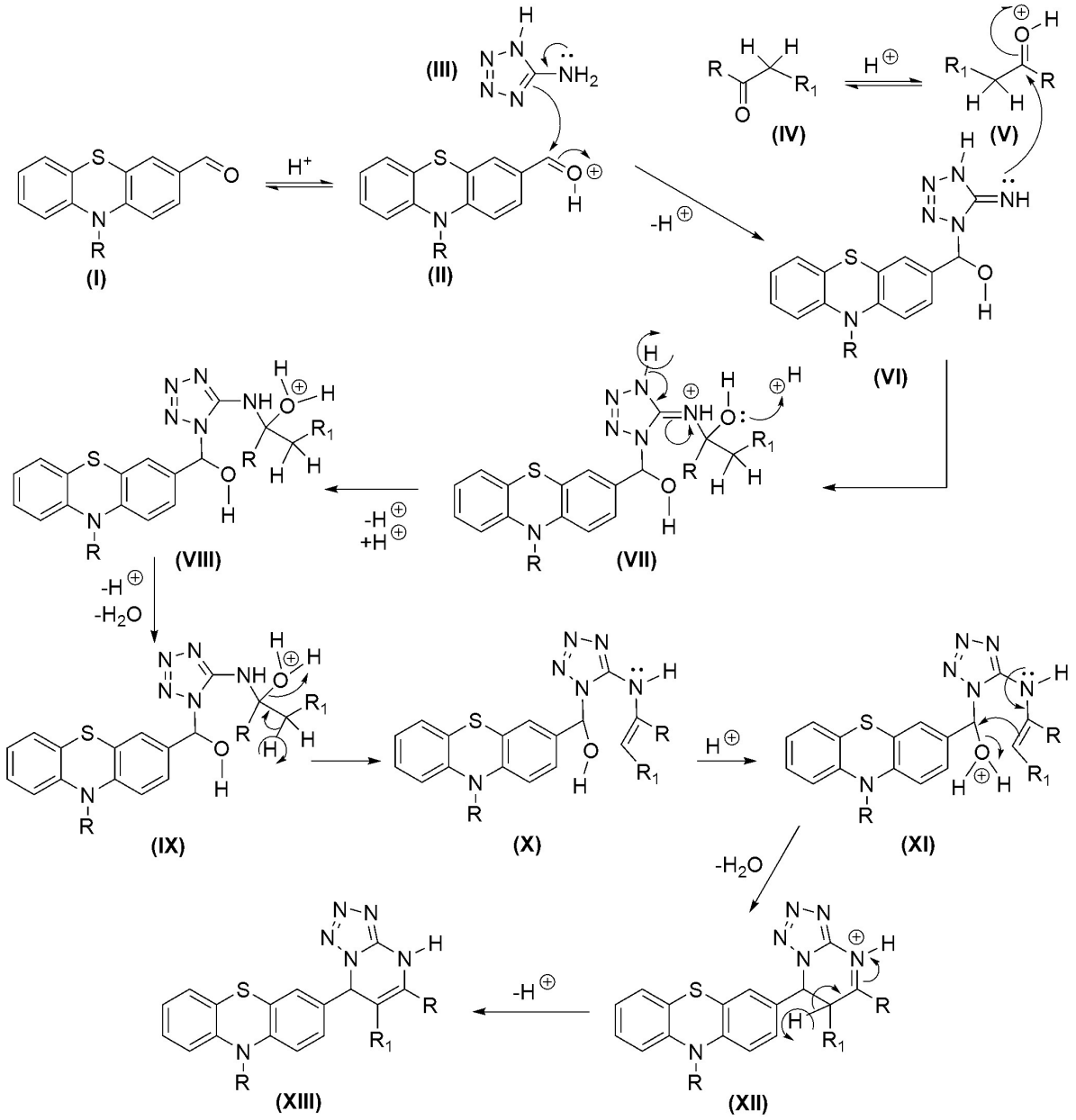
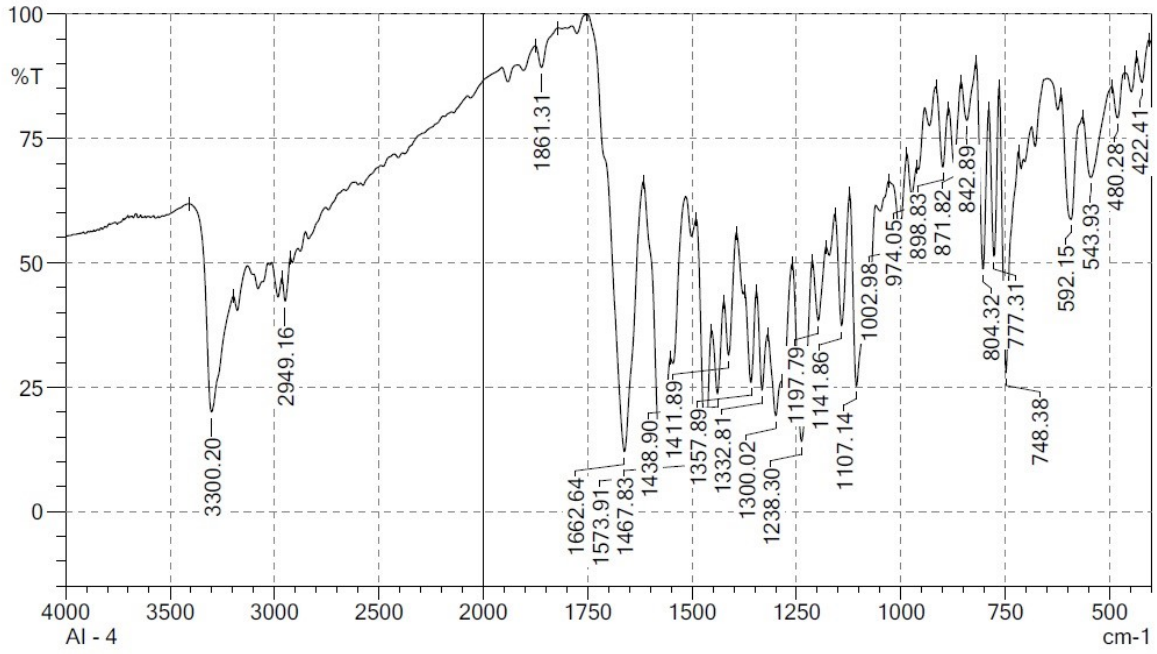


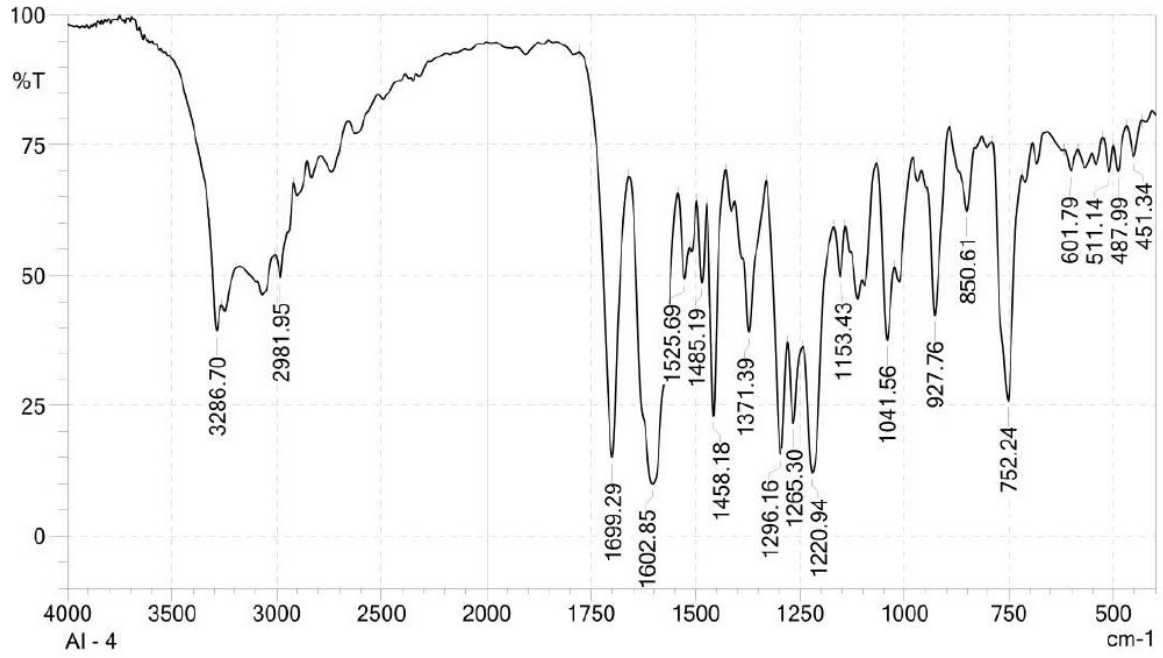
Fig S2. Intermolecular C19-H19...N4 interactions in compound. (22 number)



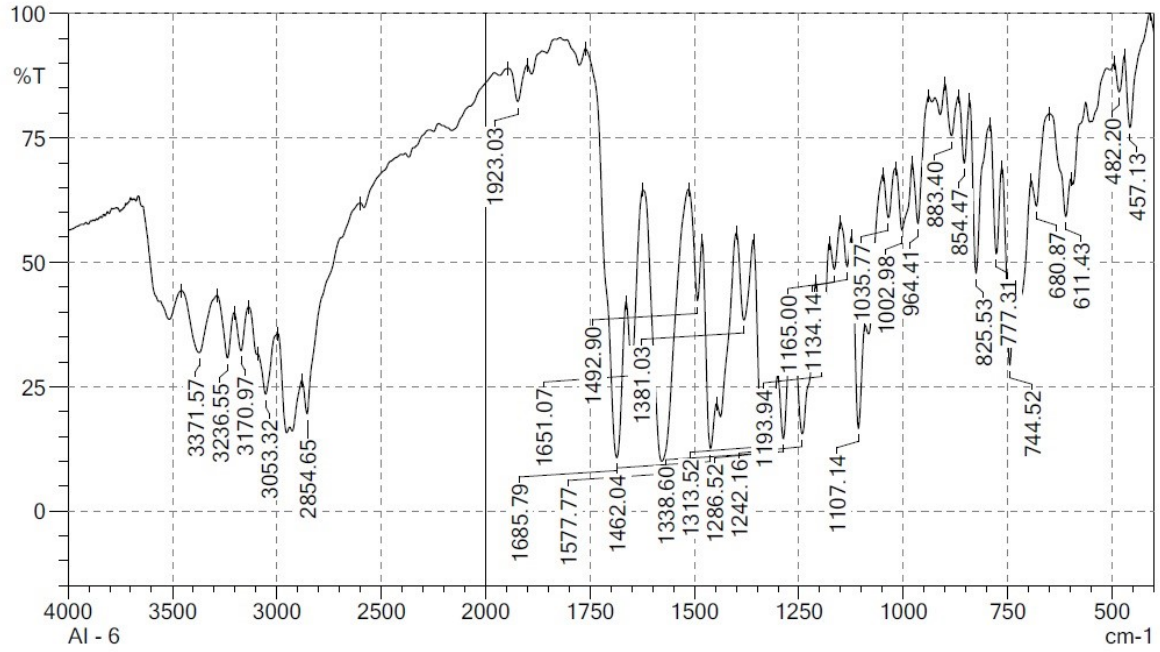
Scheme S1. Plausible mechanism for the synthesis of tetrazolopyrimidine tethered phenothiazine molecular hybrids



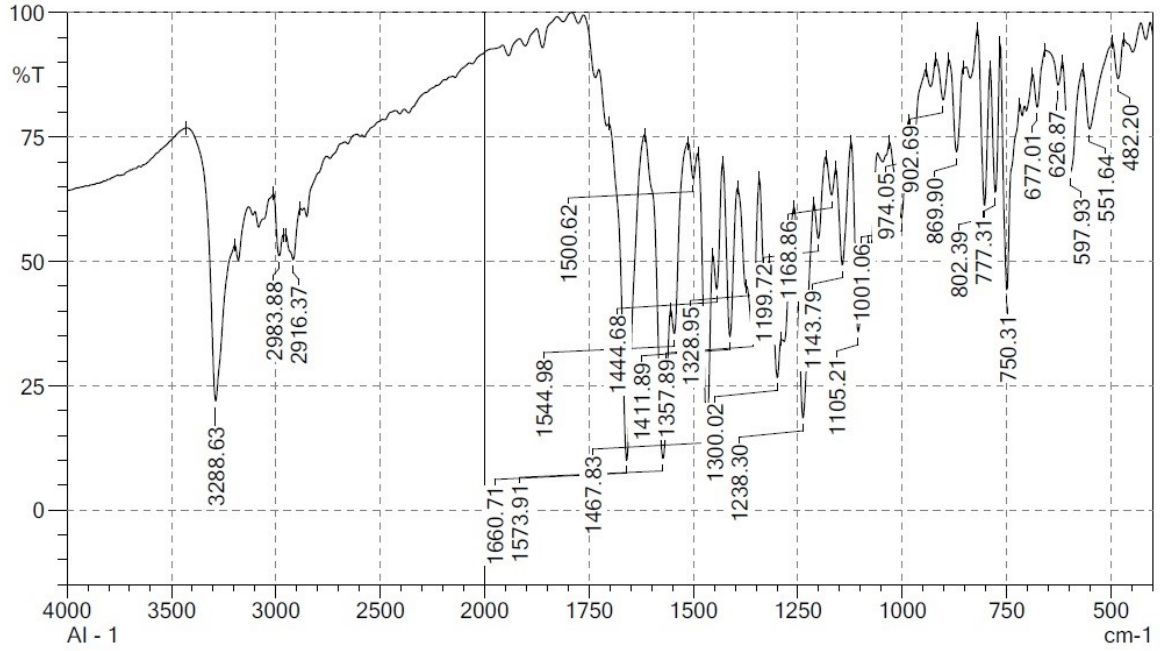
FT-IR Spectrum of **5a**



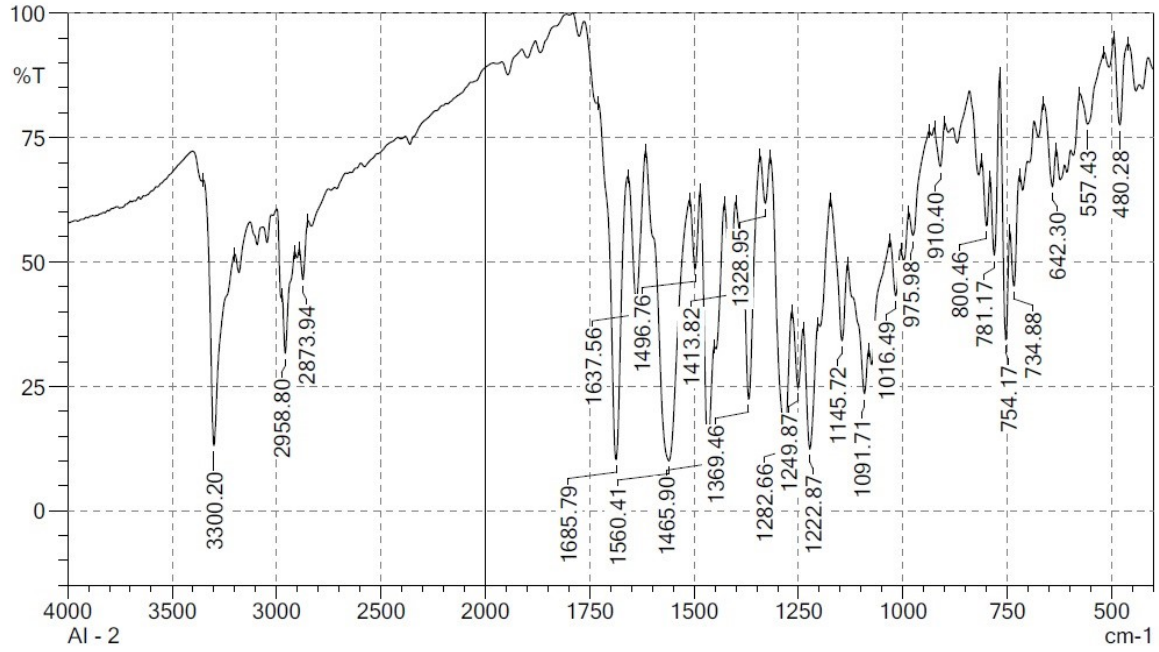
FT-IR Spectrum of **5b**



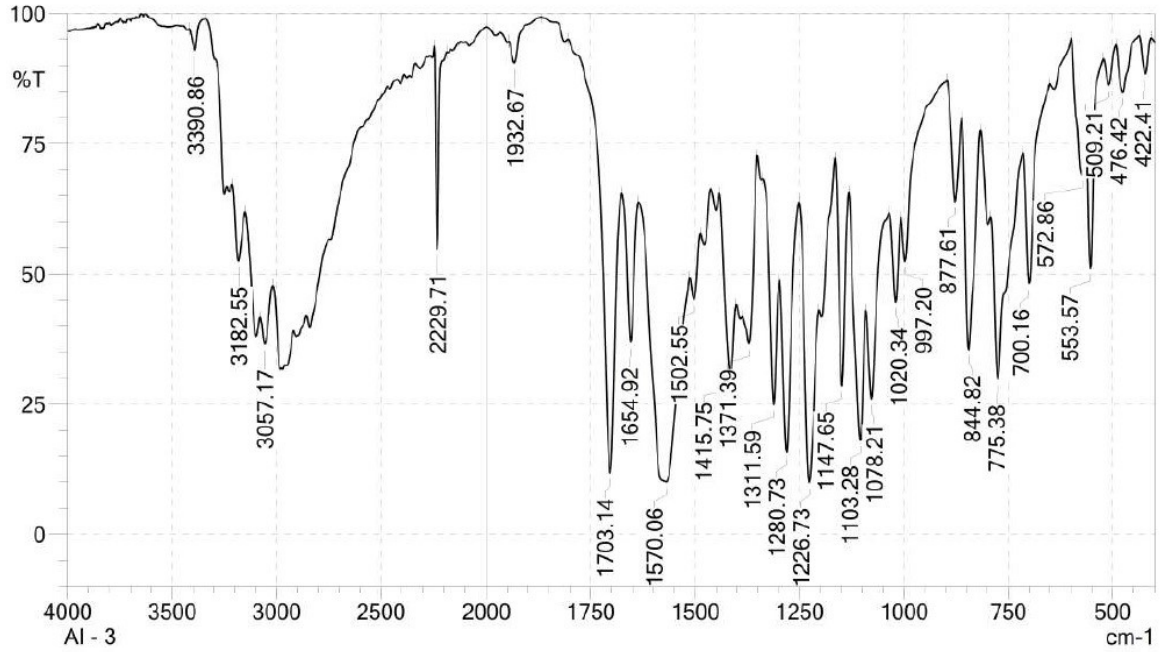
FT-IR Spectrum of **5c**



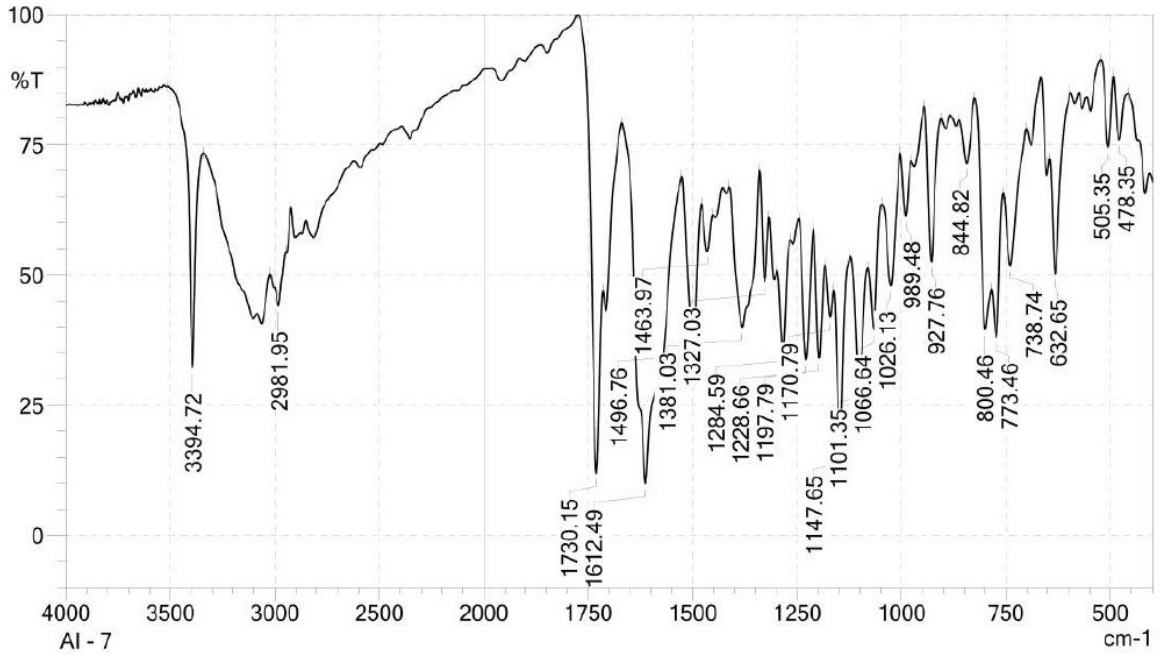
FT-IR Spectrum of **6a**



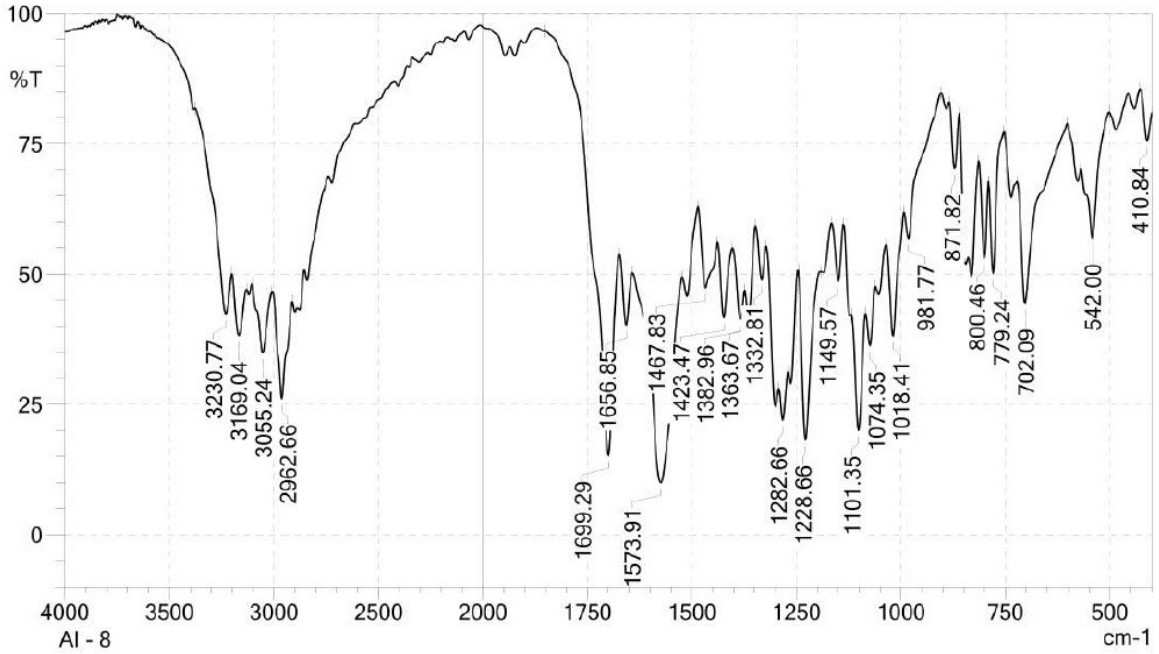
FT-IR Spectrum of **6b**



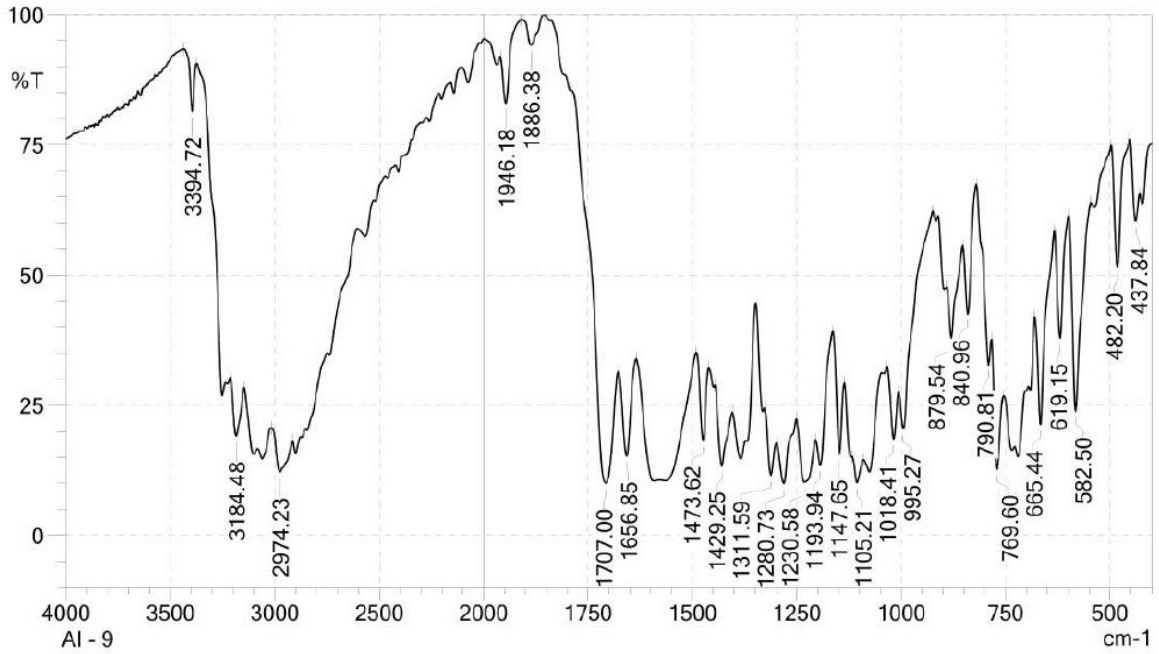
FT-IR Spectrum of **6c**



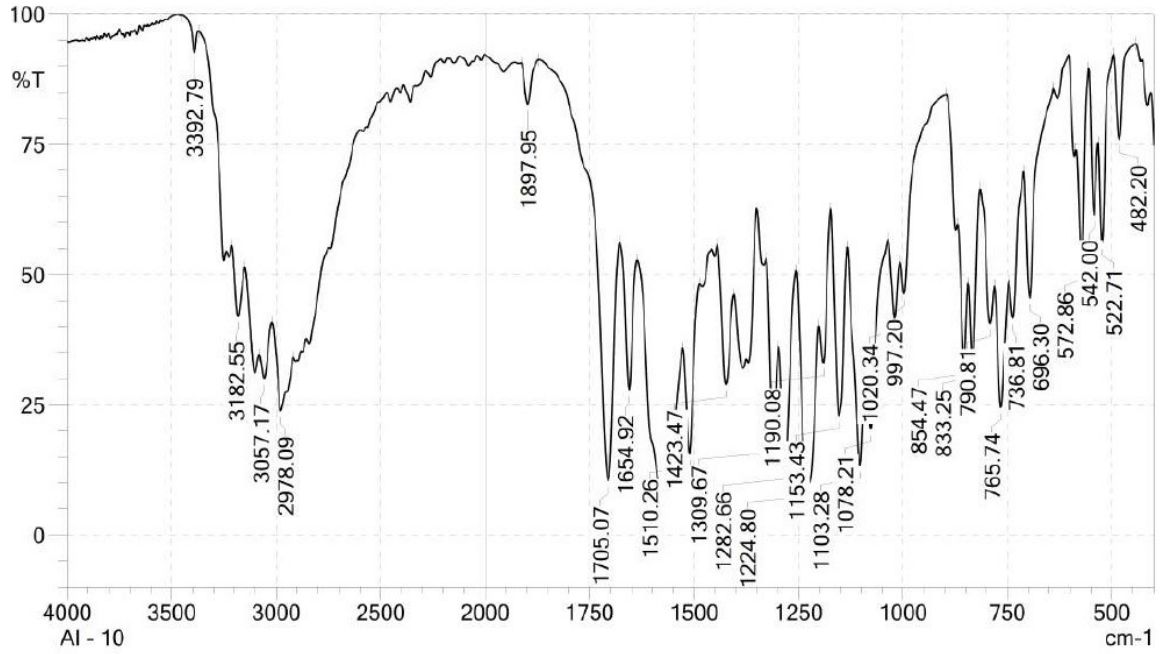
FT-IR Spectrum of **7a**



FT-IR Spectrum of **7b**



FT-IR Spectrum of **8a**



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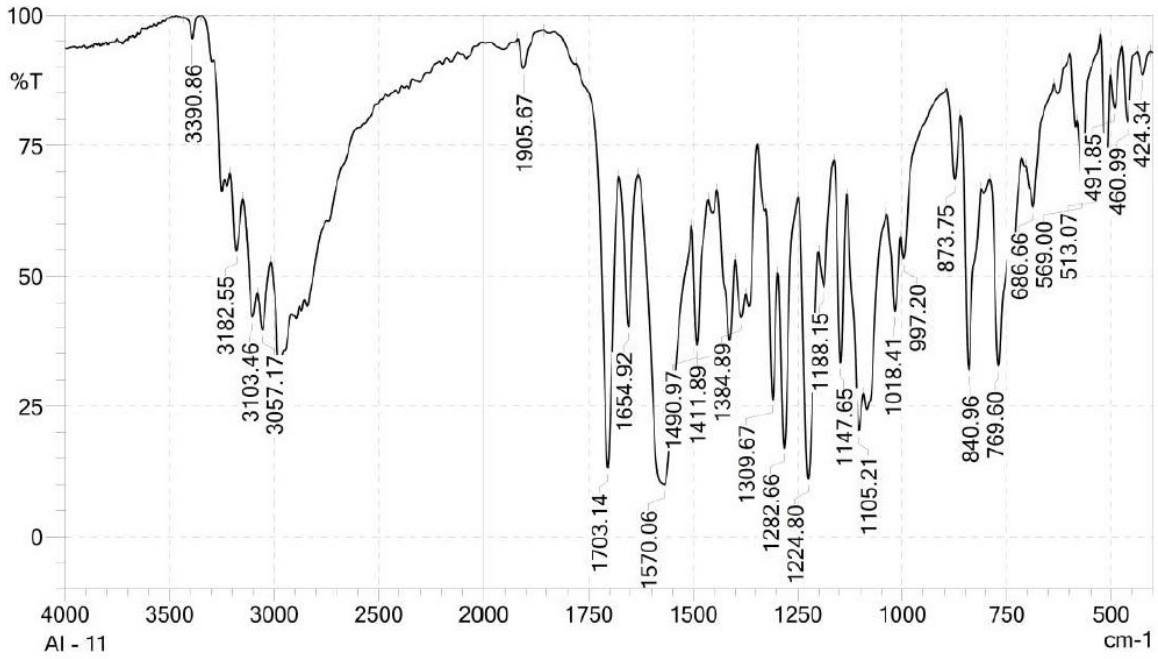
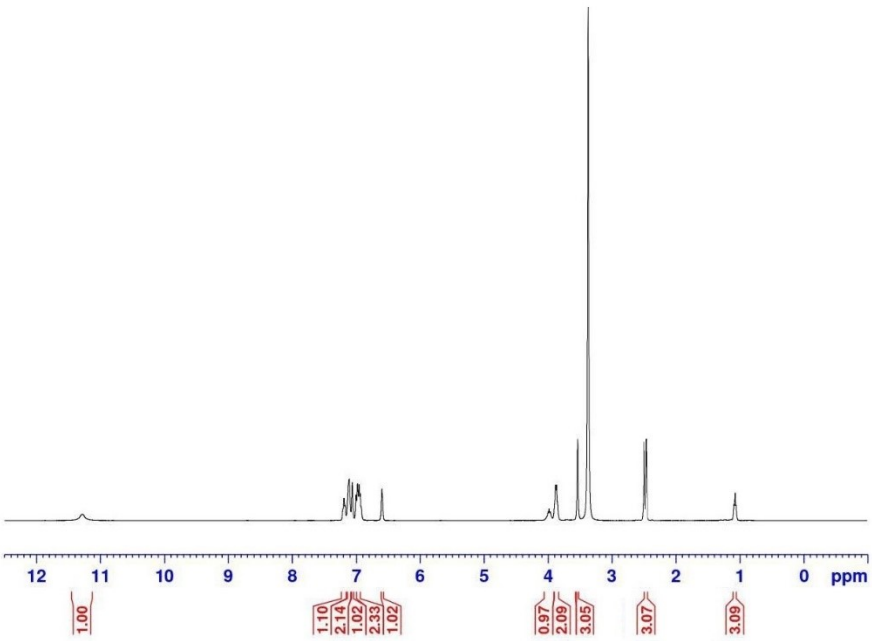


FT-IR Spectrum of **9b**



BRUKER

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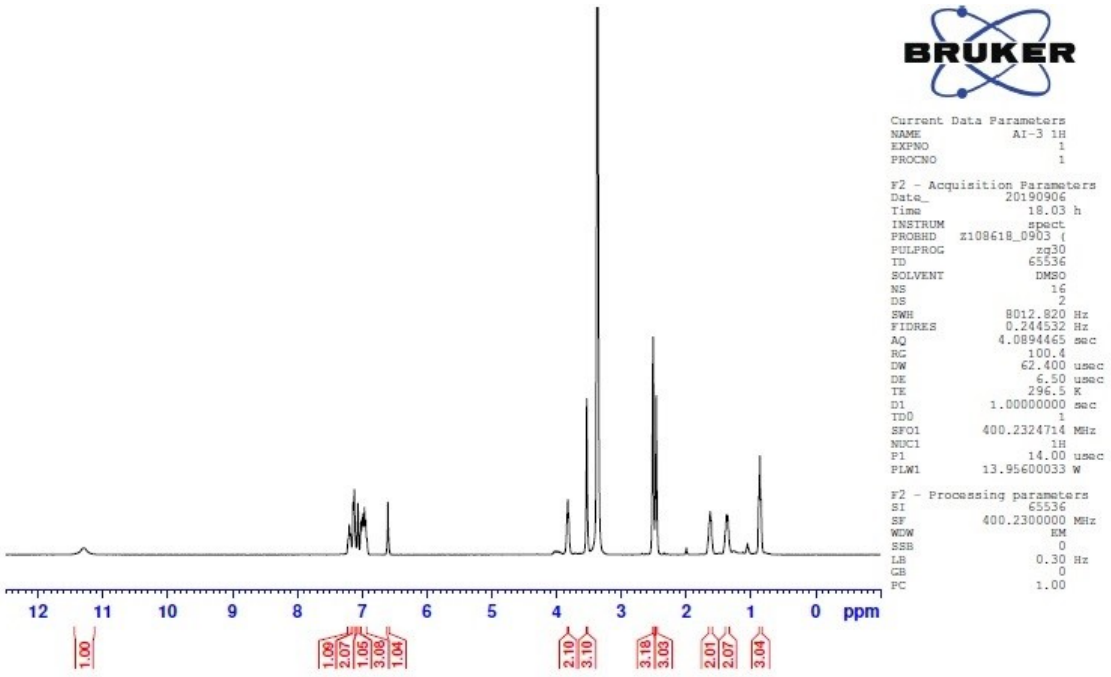
^{1}H NMR Spectrum of **5a**



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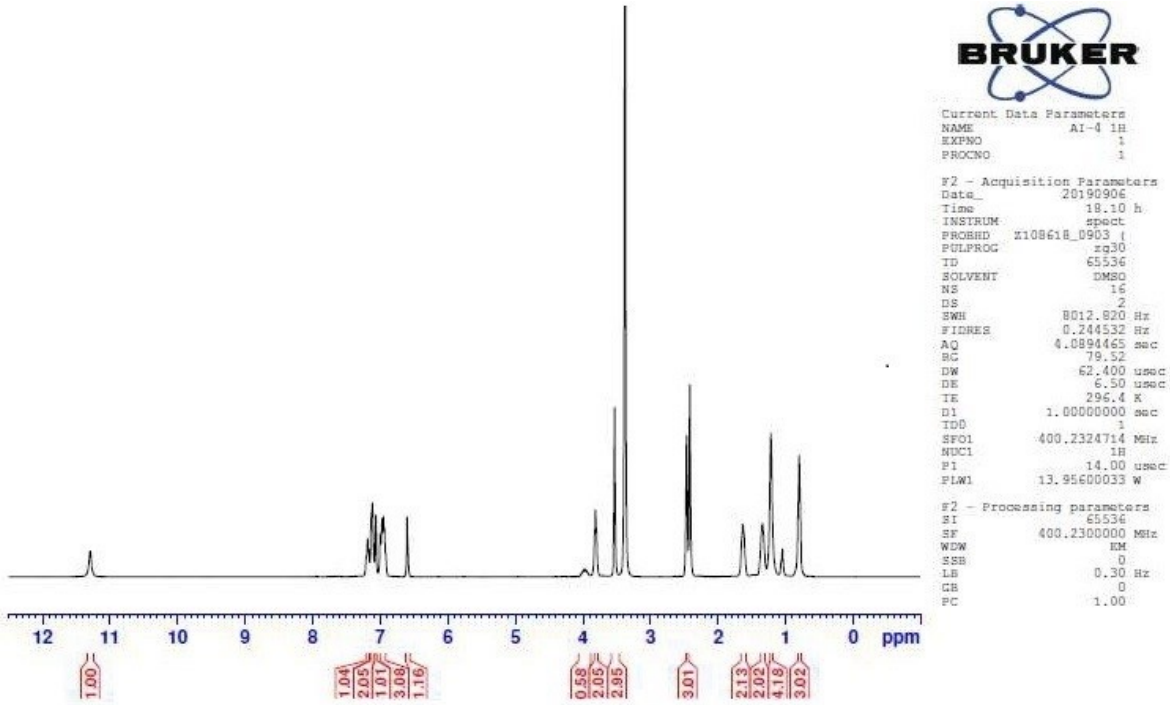

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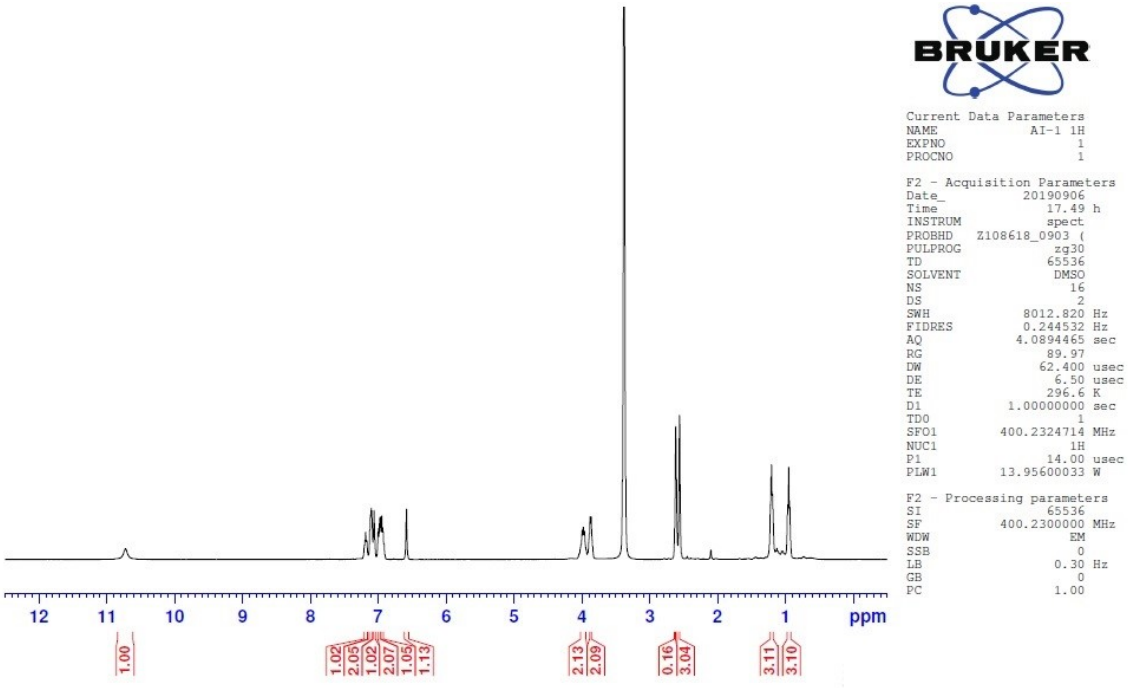
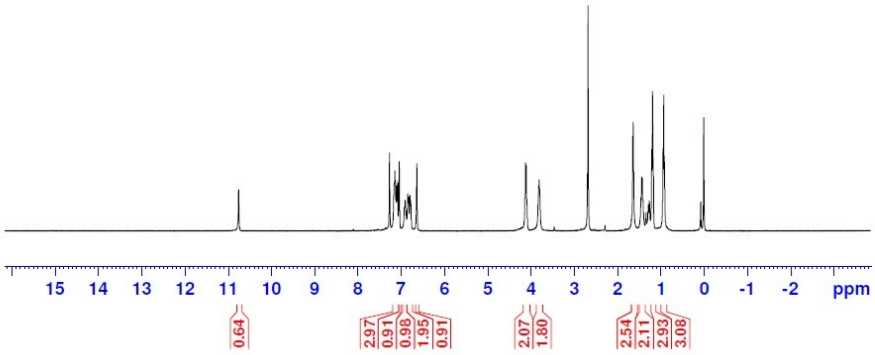


^{1}H NMR Spectrum of **6a**

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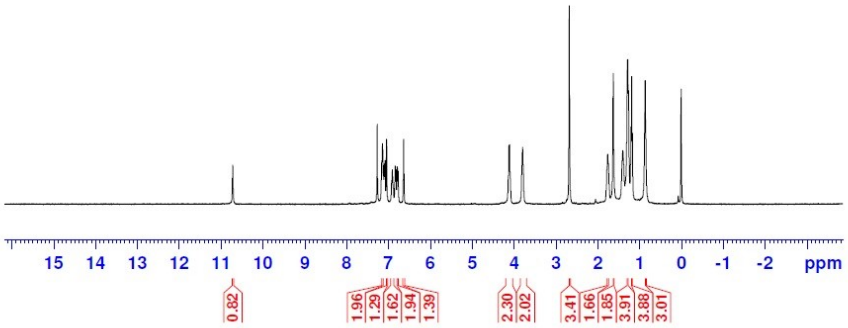
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20190202
Time              16.48 h
INSTRUM           spect
PROBHD   Z108618_0903 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH            8012.820 Hz
FIDRES            0.244532 Hz
AQ             4.0894465 sec
RG                199.04
DW                62.400 usec
DE                 6.50 usec
TE                295.2 K
D1             1.00000000 sec
TD0                  1
SFO1          400.2324714 MHz
NUC1                 1H
P1                14.00 usec
PLW1          13.95600033 W

F2 - Processing parameters
SI               65536
SF            400.2300085 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

^{1}H NMR Spectrum of **6b**



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Current Data Parameters
NAME       AI  12.9  1H
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20190202
Time              16.54 h
INSTRUM             spect
PROBHD   Z108618_0903 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                199.04
DW                62.400 usec
DE                 6.50 usec
TE                295.2 K
D1           1.00000000 sec
TD0                    1
SFO1         400.2324714 MHz
NUC1                  1H
P1                14.00 usec
PLW1         13.95600033 W

F2 - Processing parameters
SI                 65536
SF           400.2300085 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```
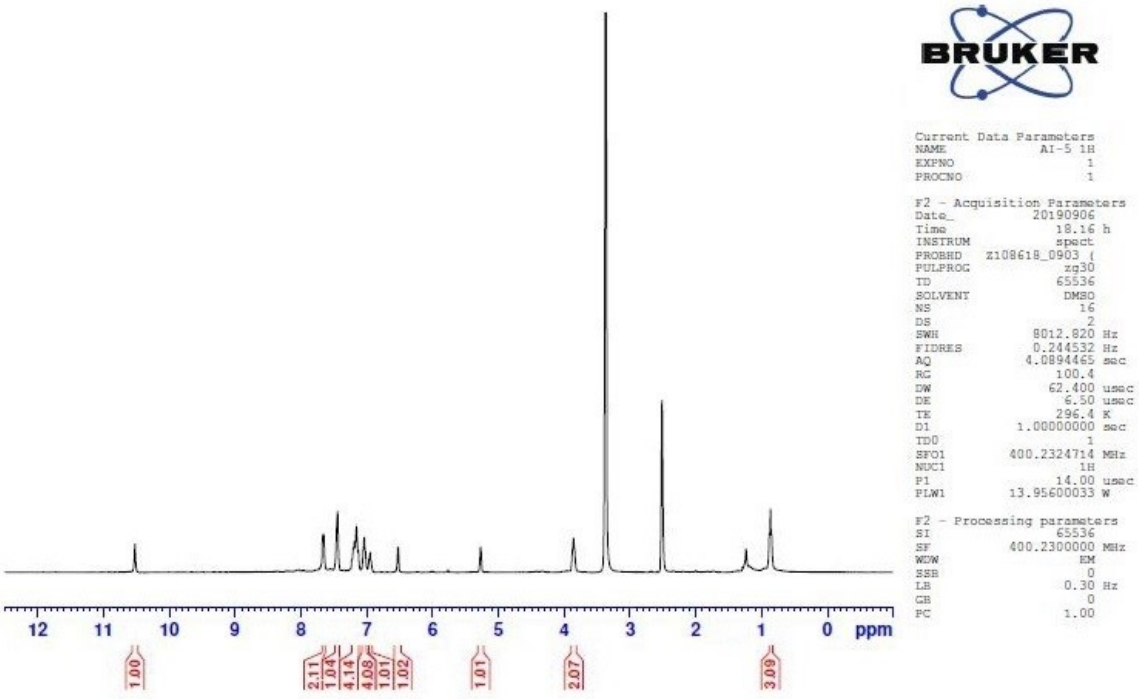
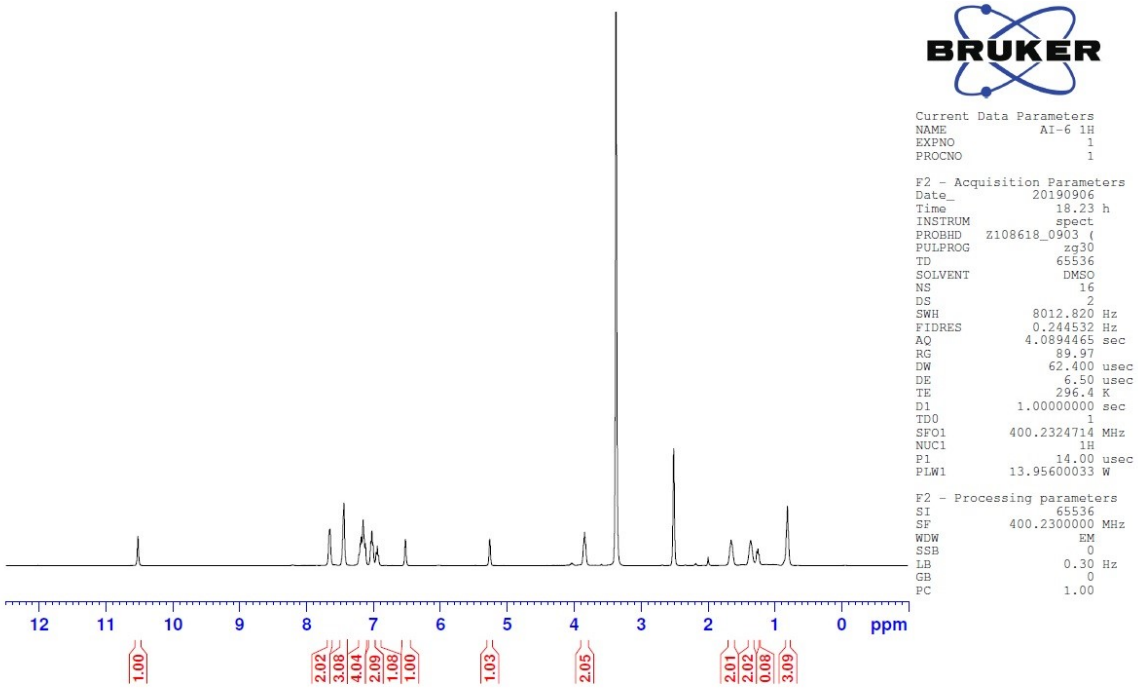
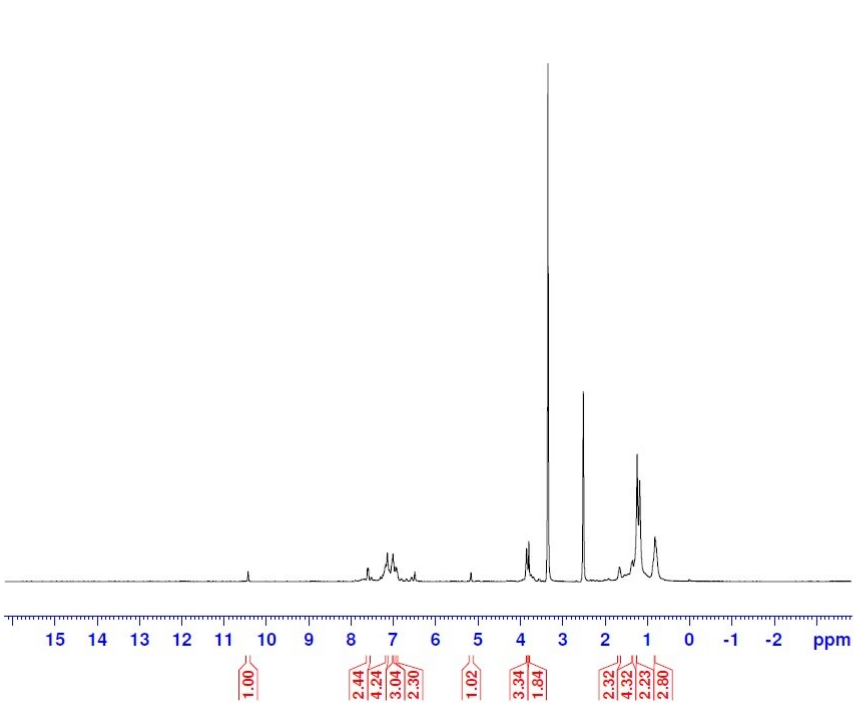

^{1}H NMR Spectrum of **6c**



^{1}H NMR Spectrum of **7a**

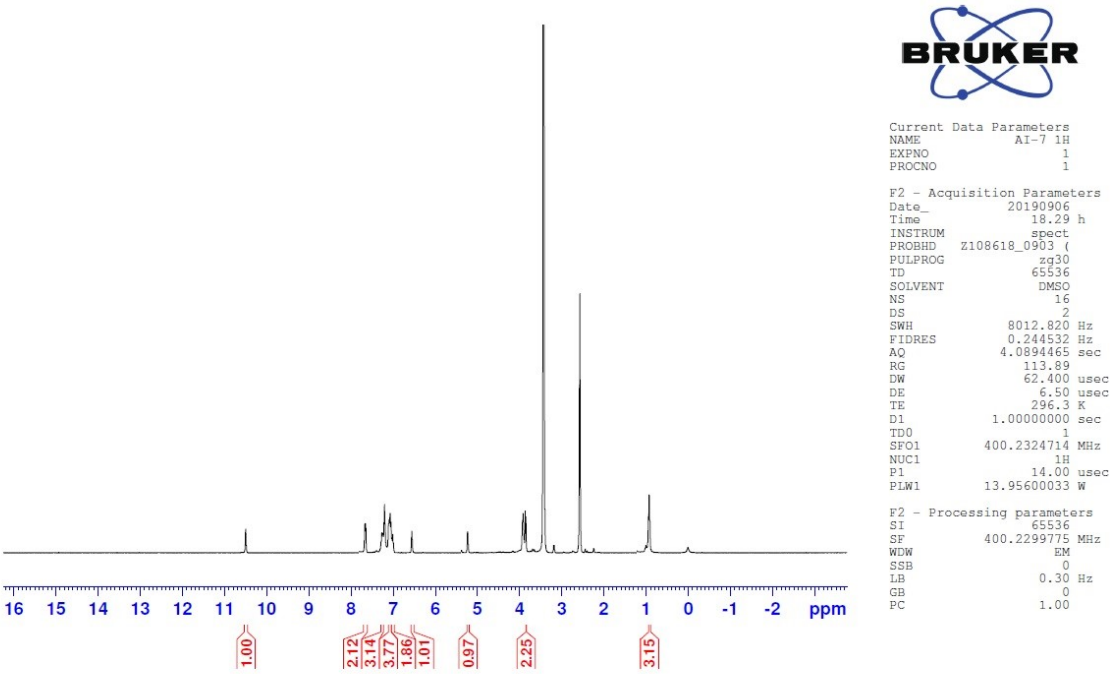


^{1}H NMR Spectrum of **7b**



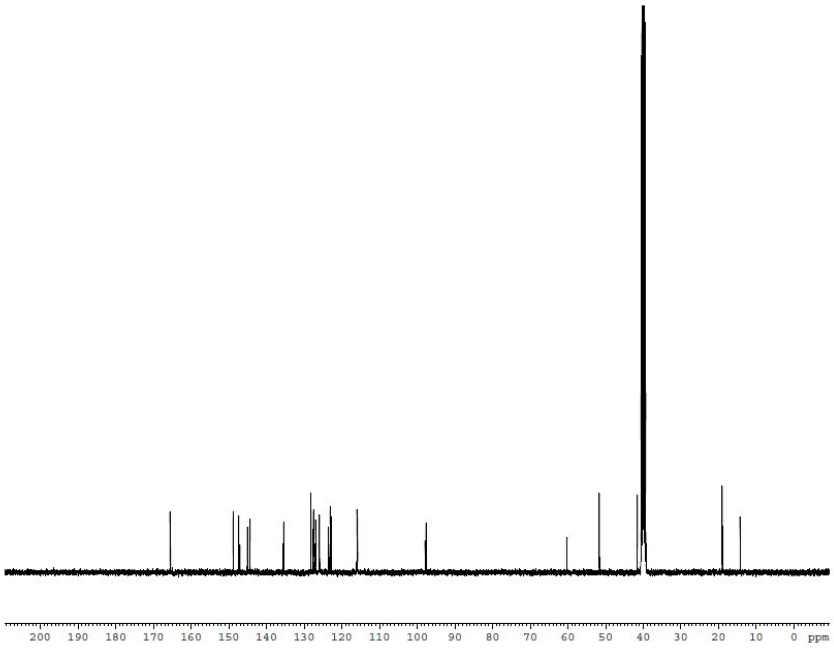

```
Current Data Parameters
NAME                  AI-9 1H
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190907
Time                  15.38 h
INSTRUM                spect
PROBHD    Z108618_0903 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH               8012.820 Hz
FIDRES               0.244532 Hz
AQ                4.0894465 sec
RG                   113.89
DW                   62.400 usec
DE                    6.50 usec
TE                   296.7 K
D1             1.00000000 sec
TD0                        1
SFO1           400.2324714 MHz
NUC1                      1H
P1                   14.00 usec
PLW1           13.95600033 W

F2 - Processing parameters
SI                    65536
SF             400.2300009 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                    1.00
```

^{1}H NMR Spectrum of **8a**



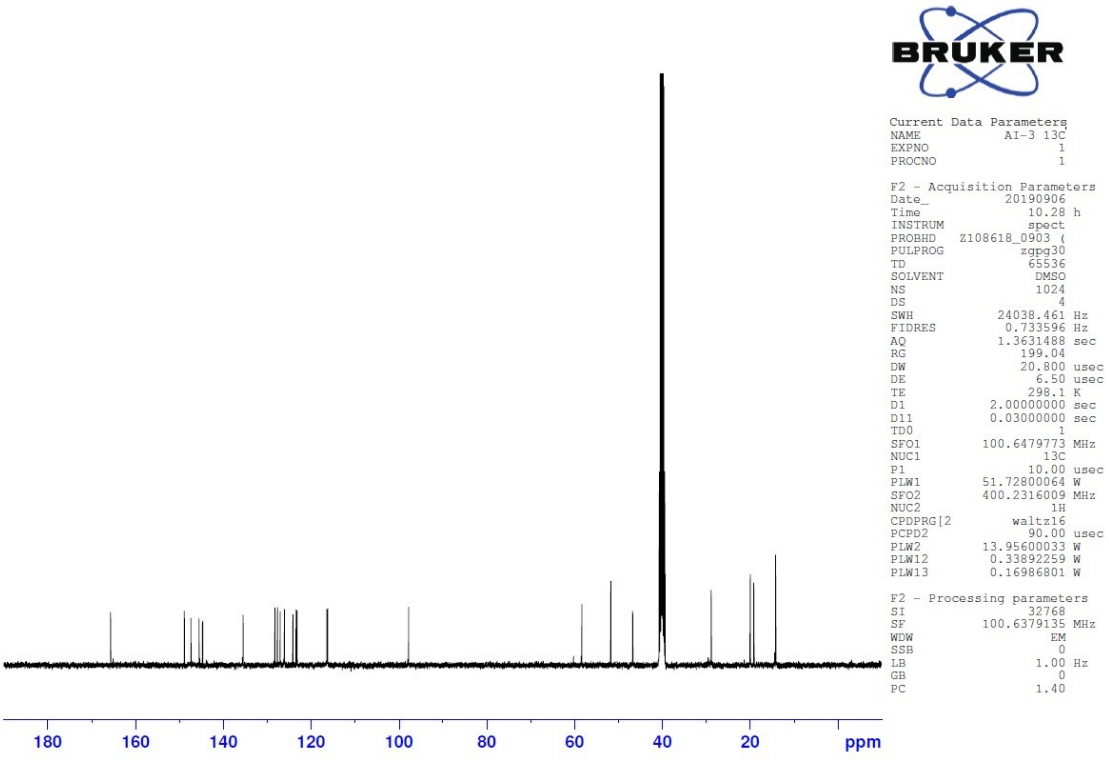

```
Current Data Parameters
NAME                  AI-7 1H
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190906
Time                   18.29 h
INSTRUM                spect
PROBHD    Z108618_0903 (
PULPROG                 zq30
TD                     65536
SOLVENT                 DMSO
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  4.0894465 sec
RG                     113.89
DW                     62.400 usec
DE                      6.50 usec
TE                     296.3 K
D1                  1.00000000 sec
TD0                         1
SFO1               400.2324714 MHz
NUC1                       1H
P1                     14.00 usec
PLW1               13.95600033 W

F2 - Processing parameters
SI                     65536
SF                 400.2299775 MHz
WDW                        EM
SSB                         0
LB                      0.30 Hz
GB                          0
PC                      1.00
```

^{1}H NMR Spectrum of **9a**

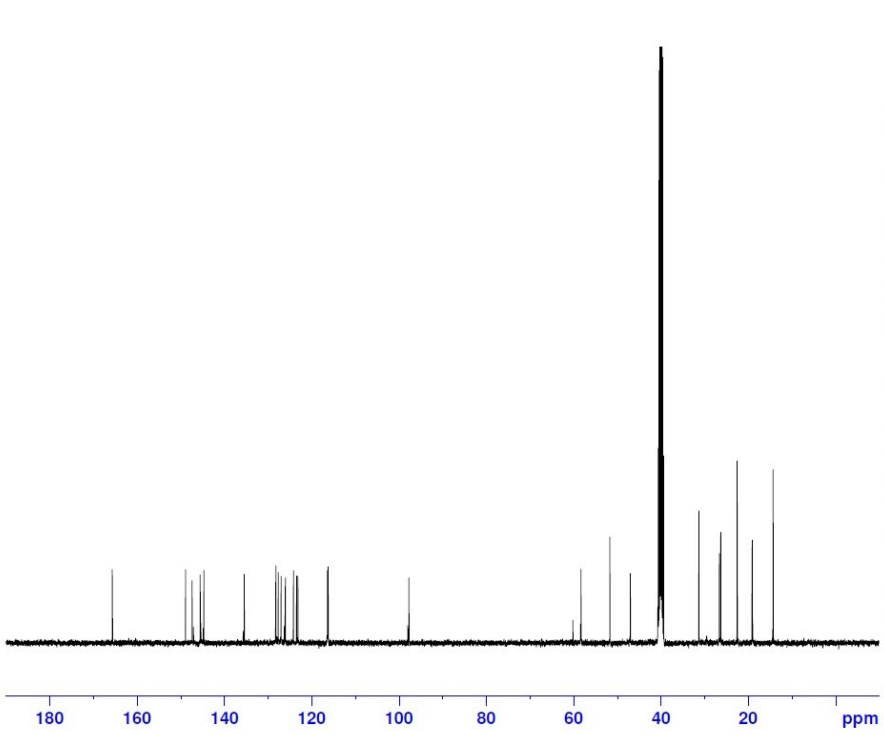



```
Current Data Parameters
NAME                  AI2 13C
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190903
Time                   14.03 h
INSTRUM                spect
PROBHD    Z108618_0903 (
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                      1024
DS                         4
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                1.3631488 sec
RG                    199.04
DW                   20.800 usec
DE                    6.50 usec
TE                   297.4 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1           100.6479773 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           51.72800064 W
SFO2           400.2316009 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2           13.95600033 W
PLW12           0.33892259 W
PLW13           0.16986801 W

F2 - Processing parameters
SI                     32768
SF             100.6379135 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

^{13}C NMR Spectrum of **5a**

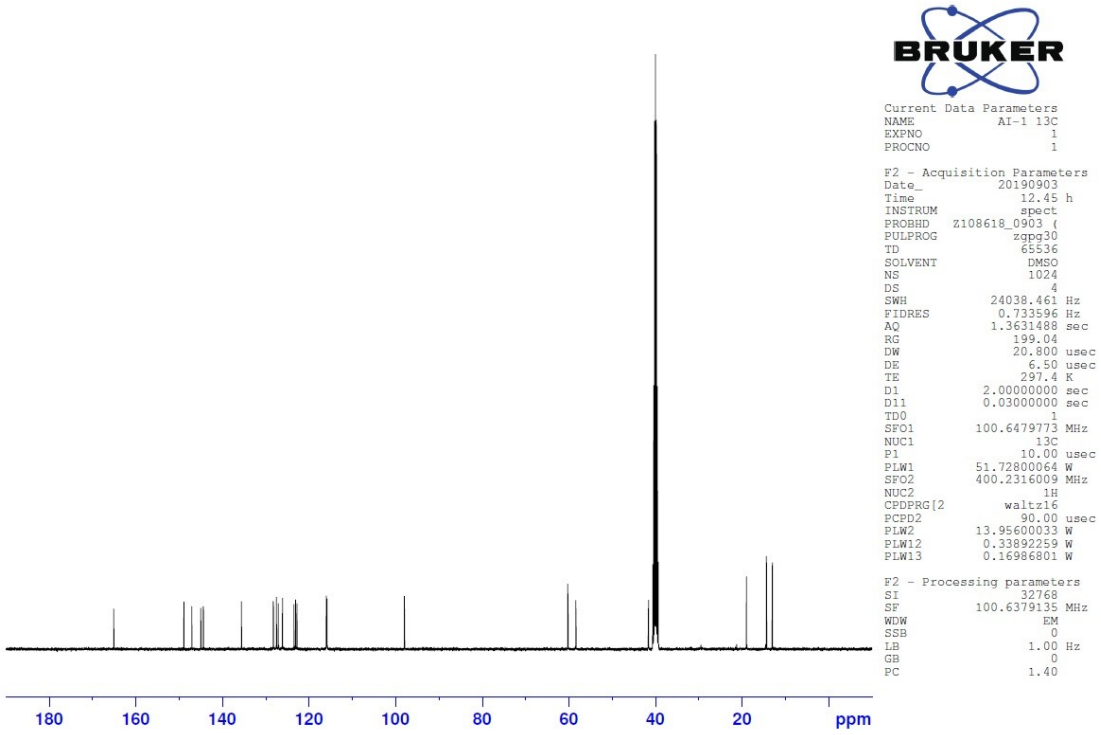


^{13}C NMR Spectrum of **5b**

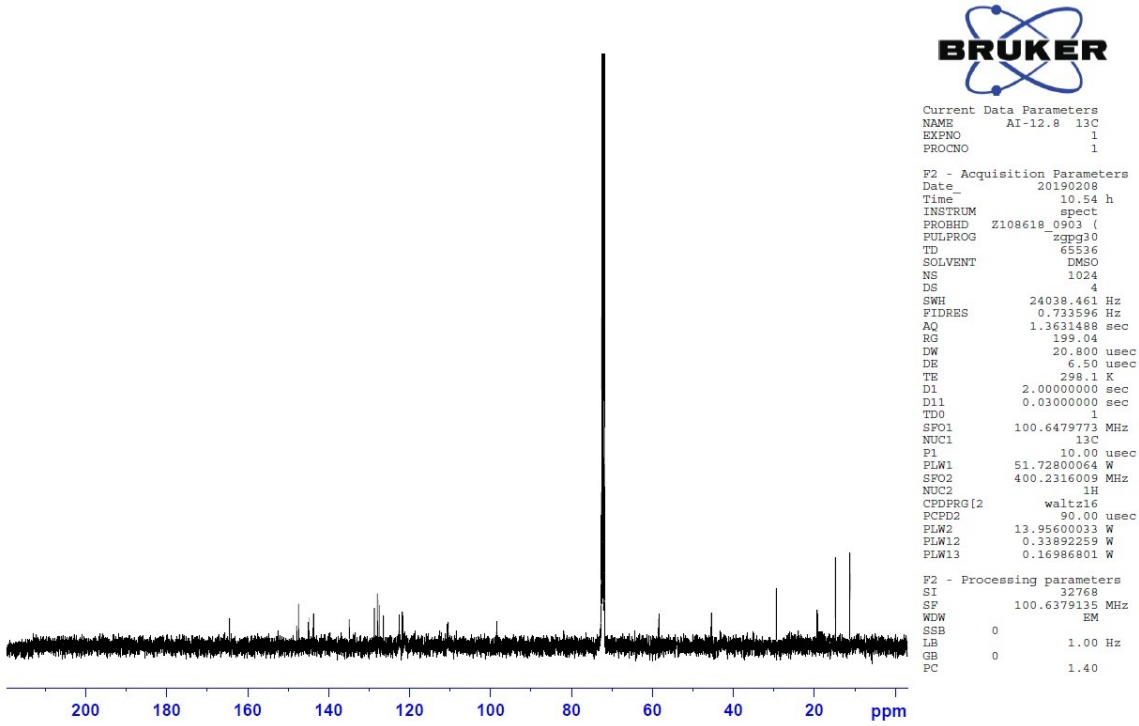



```
Current Data Parameters
NAME            AI-4 13C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190906
Time               12.12 h
INSTRUM             spect
PROBHD   Z108618_0903 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                 199.04
DW                 20.800 usec
DE                  6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6479773 MHz
NUC1                 13C
P1                 10.00 usec
PLW1          51.72800064 W
SFO2          400.2316009 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2          13.95600033 W
PLW12          0.33892259 W
PLW13          0.16986801 W

F2 - Processing parameters
SI                 32768
SF            100.6379135 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

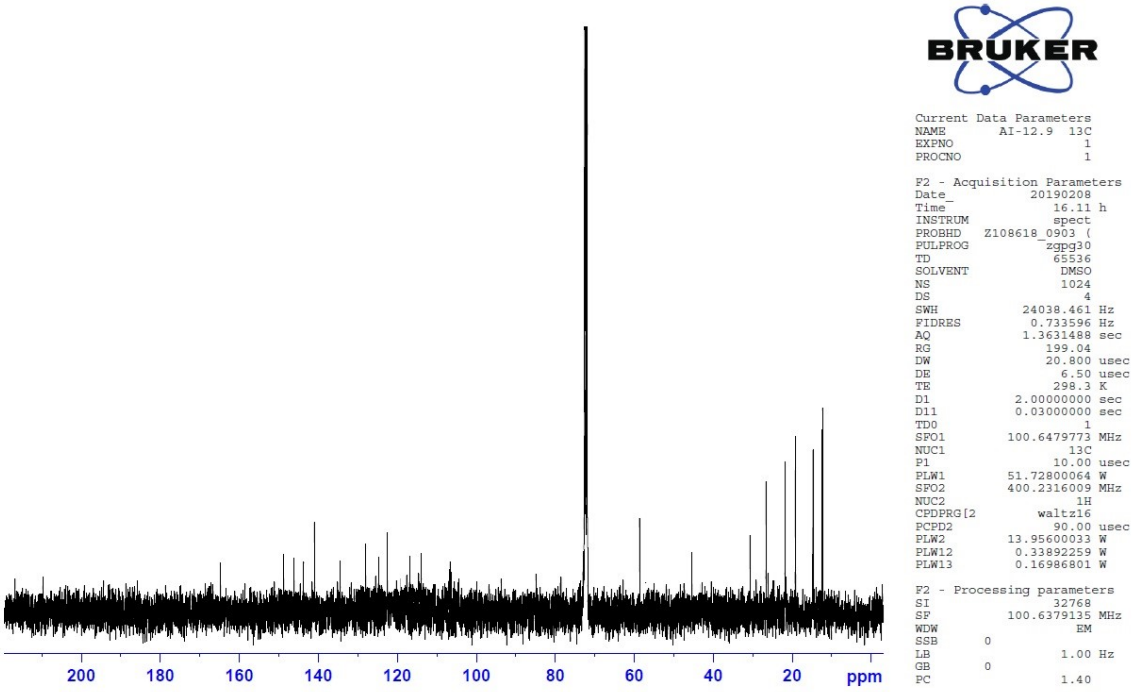
^{13}C NMR Spectrum of **5c**



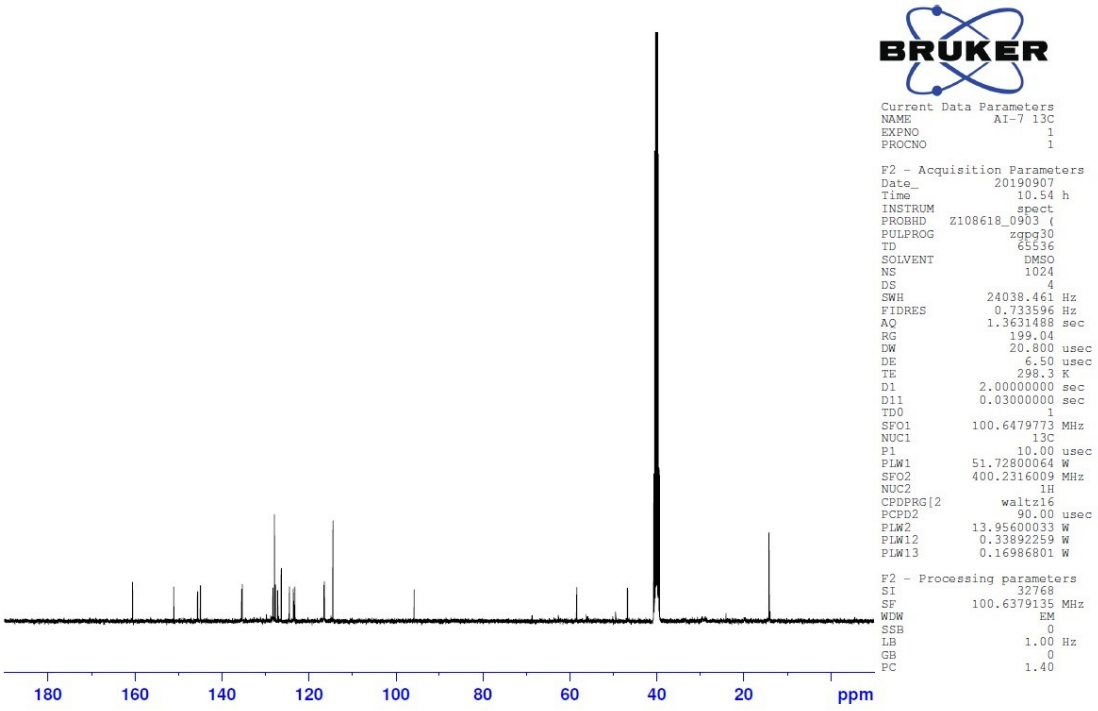
^{13}C NMR Spectrum of **6a**



^{13}C NMR Spectrum of **6b**

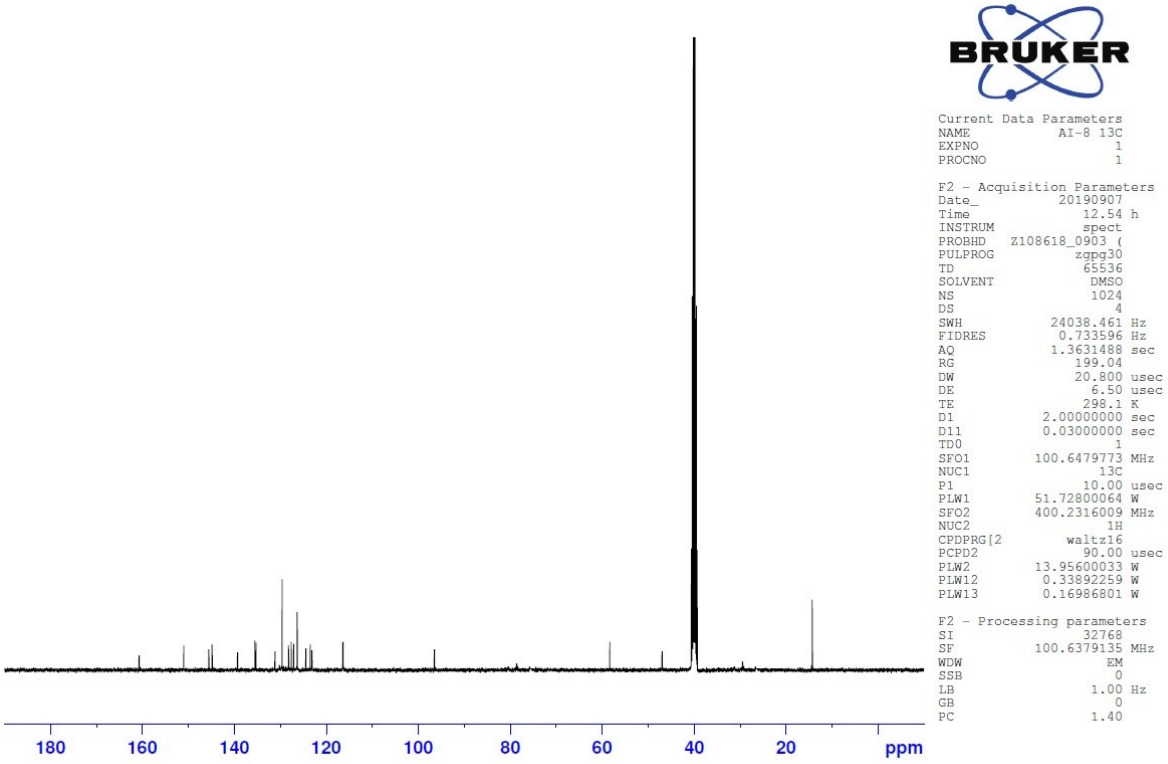


^{13}C NMR Spectrum of **6c**



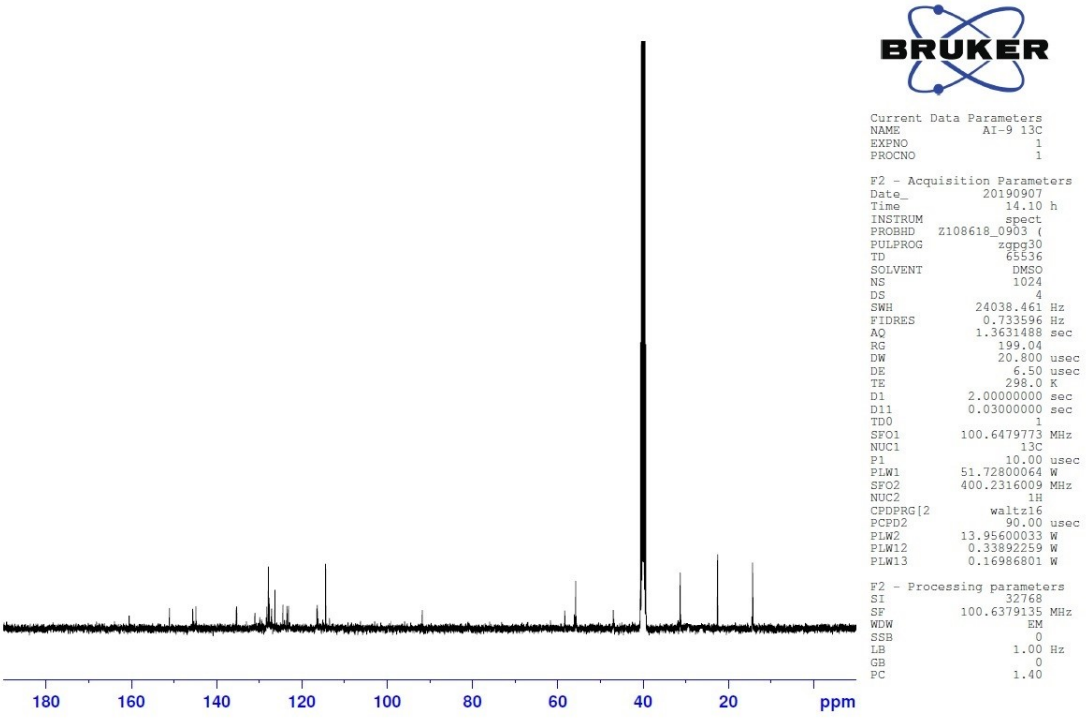

```
Current Data Parameters
NAME                  AI-7 13C
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190907
Time                 10.54 h
INSTRUM                spect
PROBHD    Z108618_0903 (
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                      1024
DS                         4
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                1.3631488 sec
RG                    199.04
DW                    20.800 usec
DE                     6.50 usec
TE                   298.3 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1           100.6479773 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           51.72800064 W
SFO2           400.2316009 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2           13.95600033 W
PLW12           0.33892259 W
PLW13           0.16986801 W

F2 - Processing parameters
SI                     32768
SF             100.6379135 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

^{13}C NMR Spectrum of **7a**

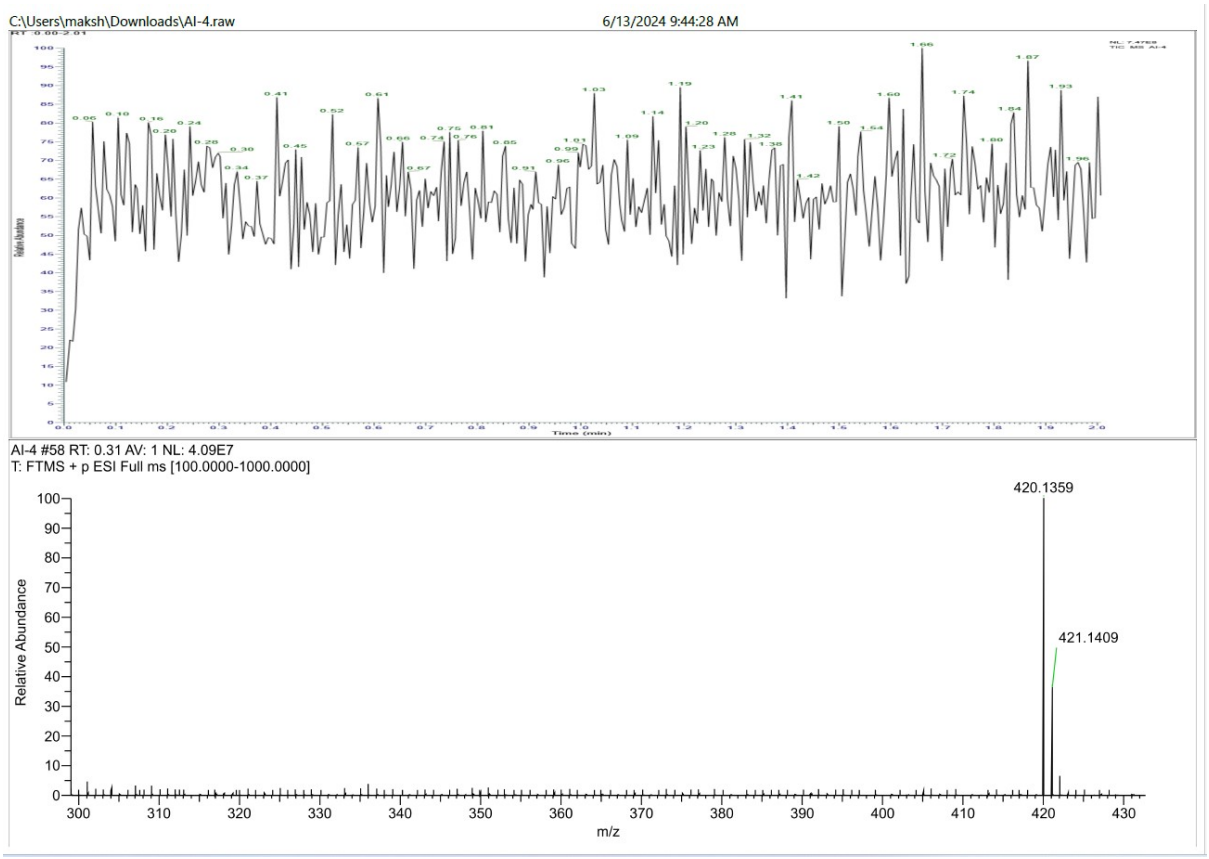



```
Current Data Parameters
NAME                  AI-8 13C
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20190907
Time                   12.54 h
INSTRUM                spect
PROBHD    Z108618_0903 (
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  1.3631488 sec
RG                     199.04
DW                     20.800 usec
DE                      6.50 usec
TE                     298.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1               100.6479773 MHz
NUC1                      13C
P1                     10.00 usec
PLW1               51.72800064 W
SFO2               400.2316009 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2               13.95600033 W
PLW12               0.33892259 W
PLW13               0.16986801 W

F2 - Processing parameters
SI                         32768
SF                 100.6379135 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

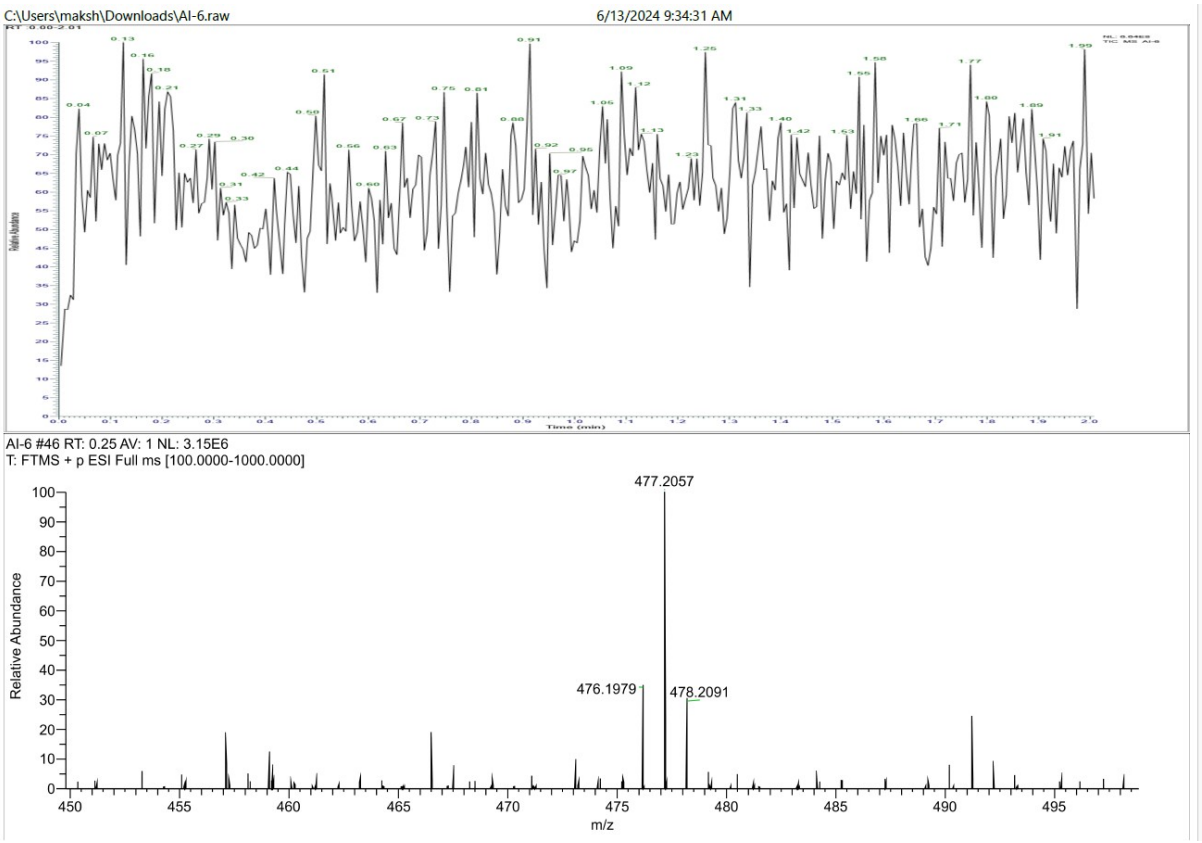
^{13}C NMR Spectrum of **9a**



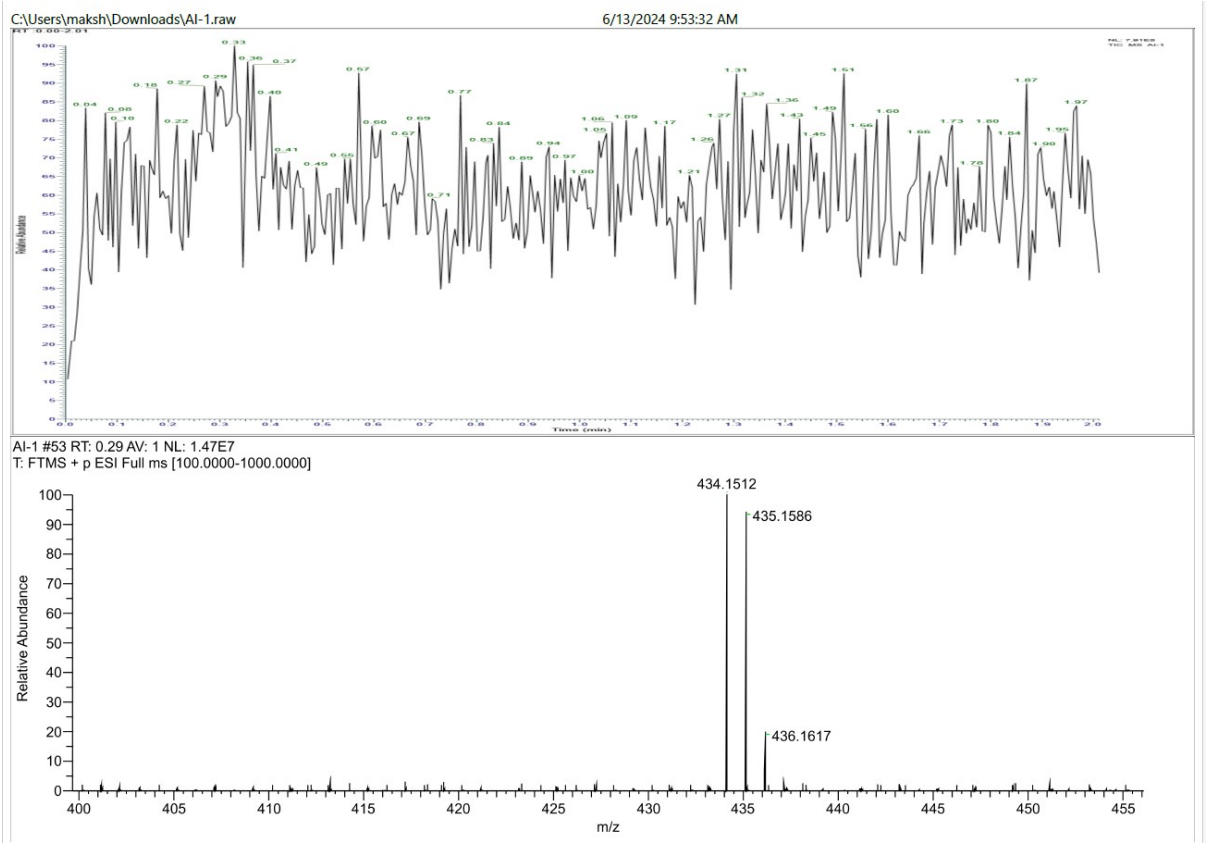
^{13}C NMR Spectrum of **9b**



HRMS spectrum of **5a**



HRMS spectrum of **5c**



HRMS spectrum of **6a**