

Supporting Information

Design, synthesis, molecular docking and molecular dynamic studies of novel benzimidazole-thiazole derivatives as potent and selective COX-2 inhibitors

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Copies of ¹H, ¹³C NMR and MS spectra of compounds (S1)

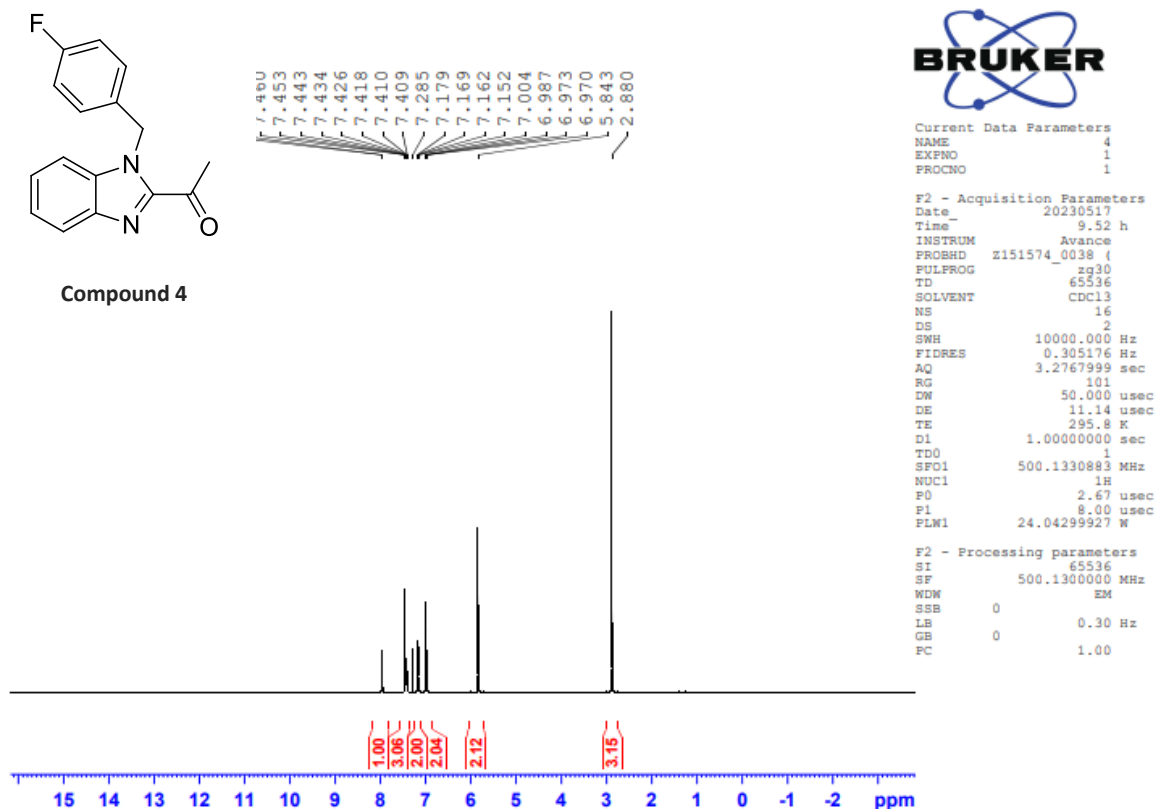


Figure S1-1. ¹H-NMR spectrum of compound 4

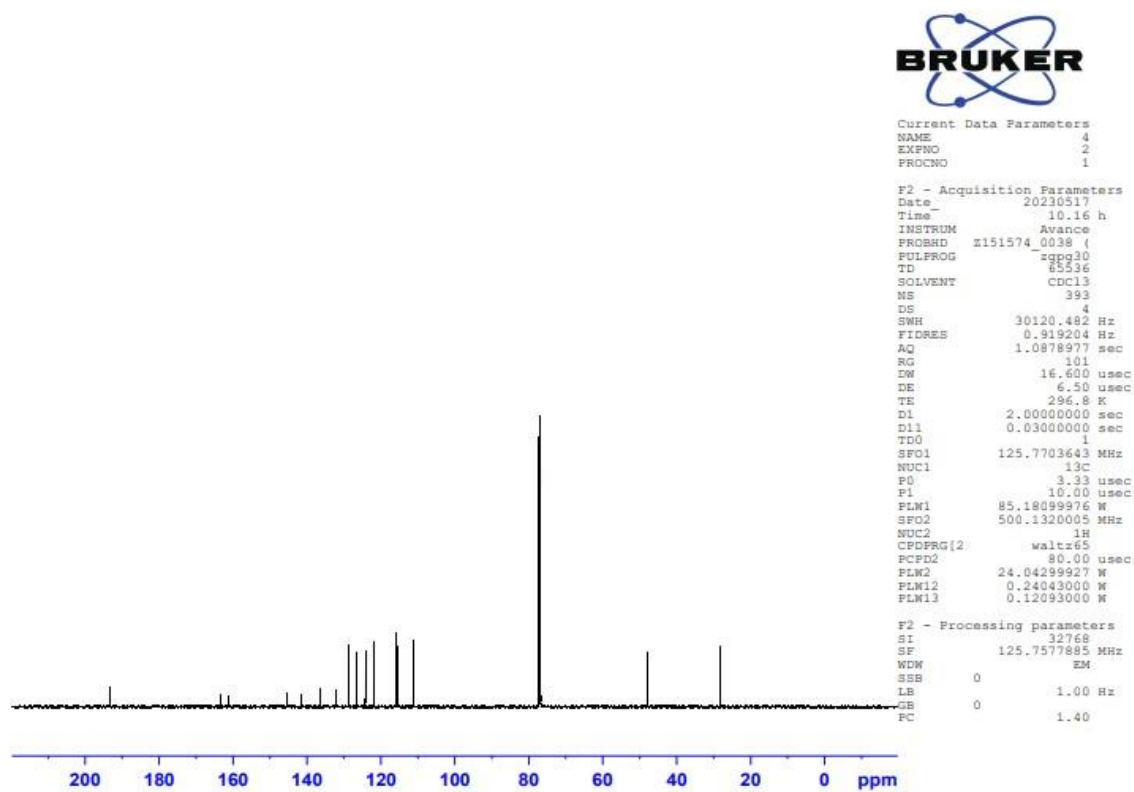


Figure S1-2. ¹³C-NMR spectrum of compound 4

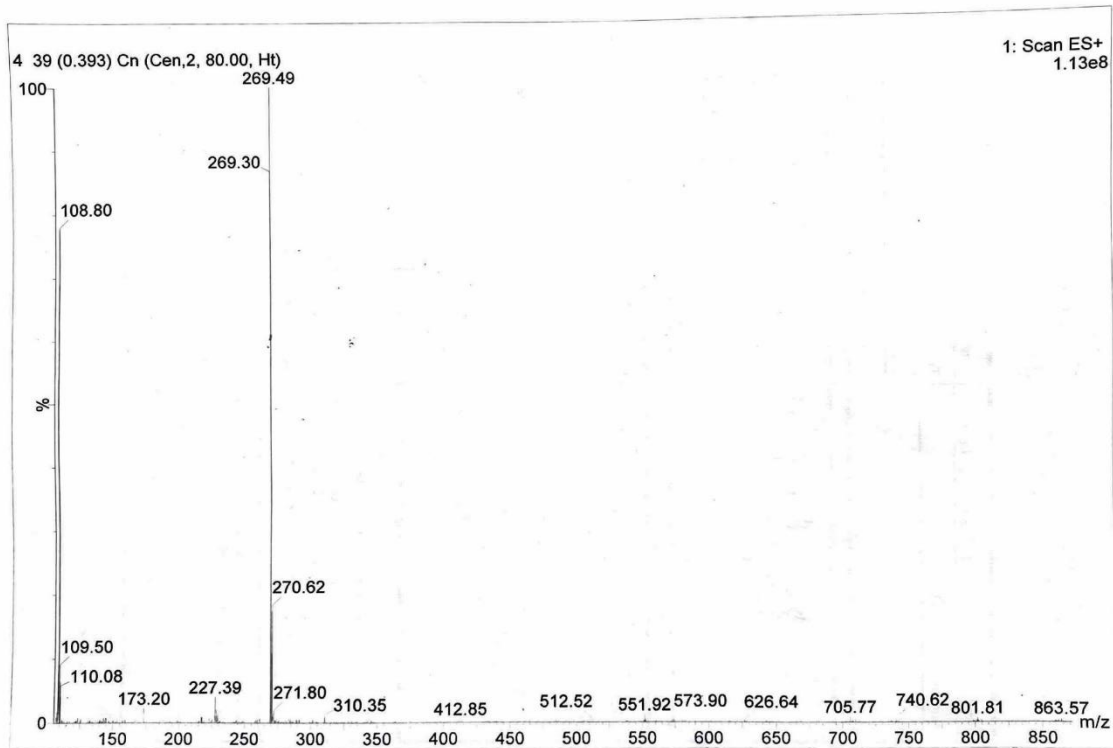
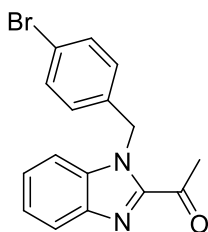
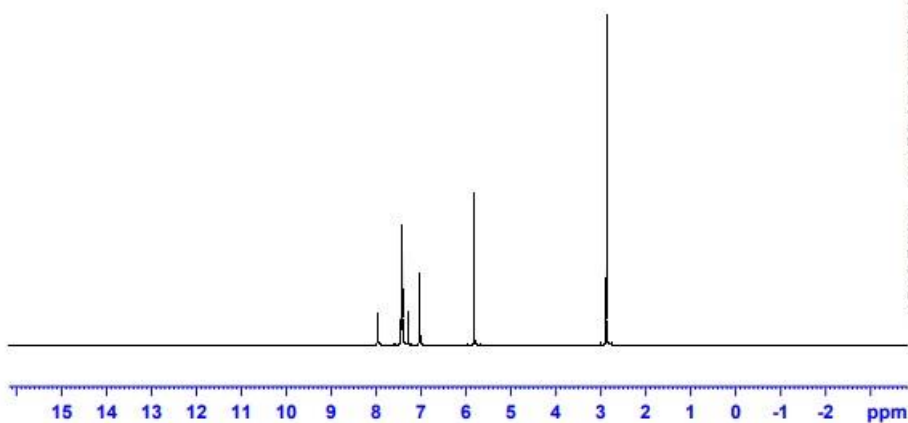


Figure S1-3. Mass spectrum of compound 4



Compound 5



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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DE 50.000 usec
TE 11.14 usec
TD0 295.8 K
D1 1.00000000 sec
SFO1 500.1330883 MHz
NUC1 1H
P0 2.67 usec
F1 8.00 usec
PLW1 24.04299927 W

F2 - Processing parameters
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WDW EM
SSB 0
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GB 0
PC 1.00

Figure S1-4. ¹H-NMR spectrum of compound 5

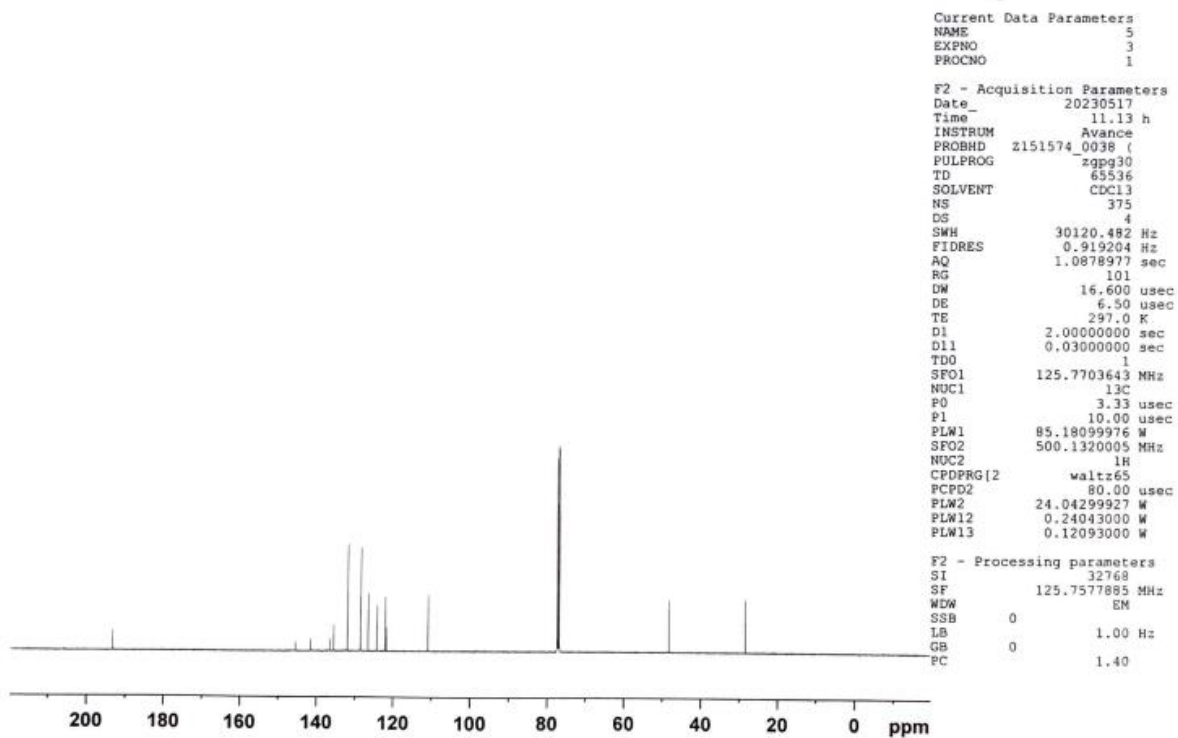


Figure S1-5. ¹³C-NMR spectrum of compound 5

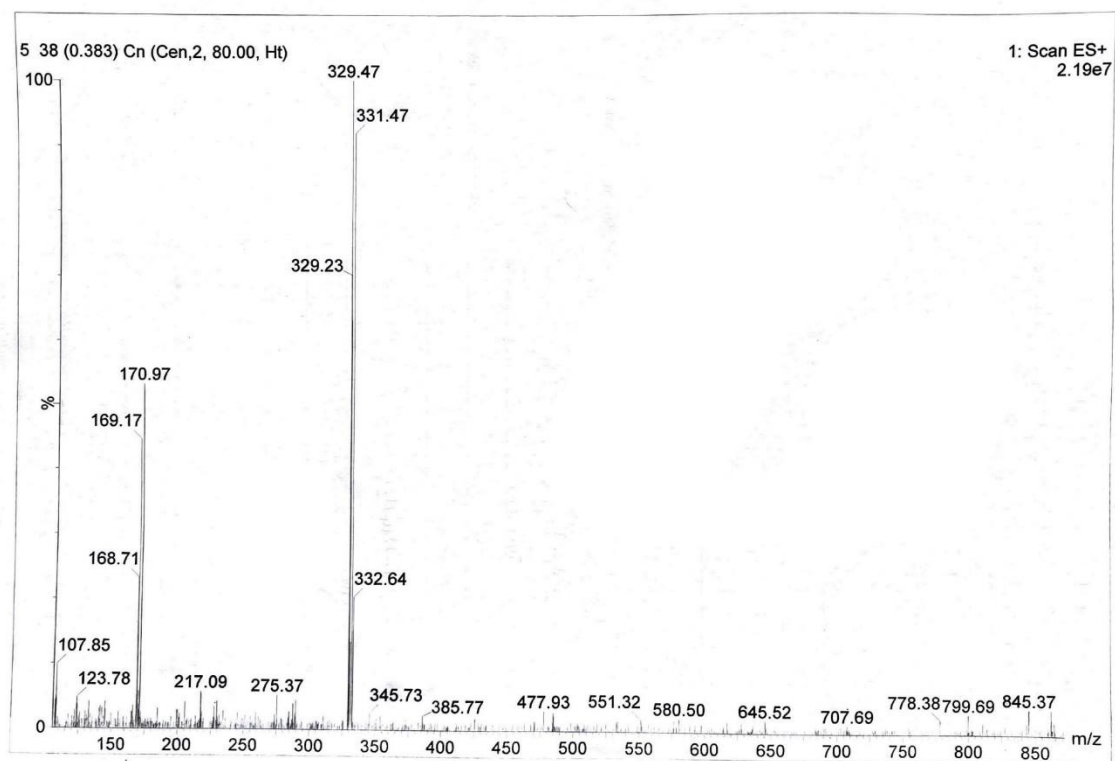
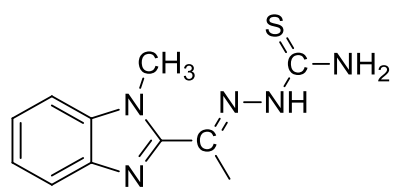


Figure S1-6. Mass spectrum of compound 5



Compound 6



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EXPNO        4
PROCNO       1

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Time_         10.18 h
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PULPROG      zg30
TD           65536
SOLVENT      DMSO
NS           16
DS           2
SWH          10000.000 Hz
FIDRES       0.305176 Hz
AQ           3.2767999 sec
RG           101
DW           50.000 usec
DE           11.14 usec
TE           302.7 K
D1           1.0000000 sec
TD0          1
SFO1         500.1330883 MHz
NUC1         1H
P0           2.67 usec
PL           8.00 usec
PLW1        24.04299927 W

F2 - Processing parameters
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PC           1.00
  
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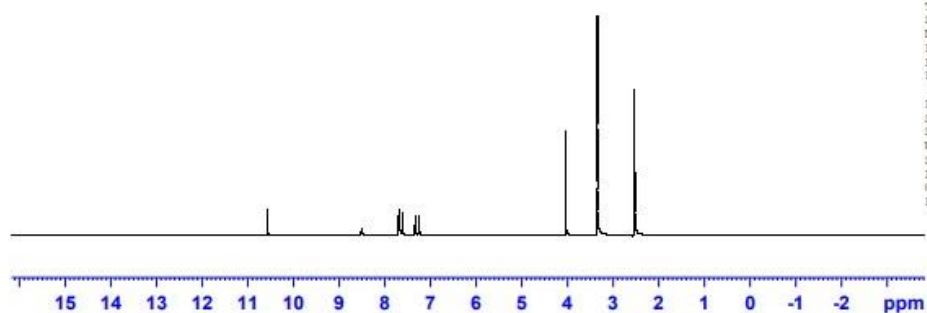


Figure S1-7. ¹H-NMR spectrum of compound 6-1

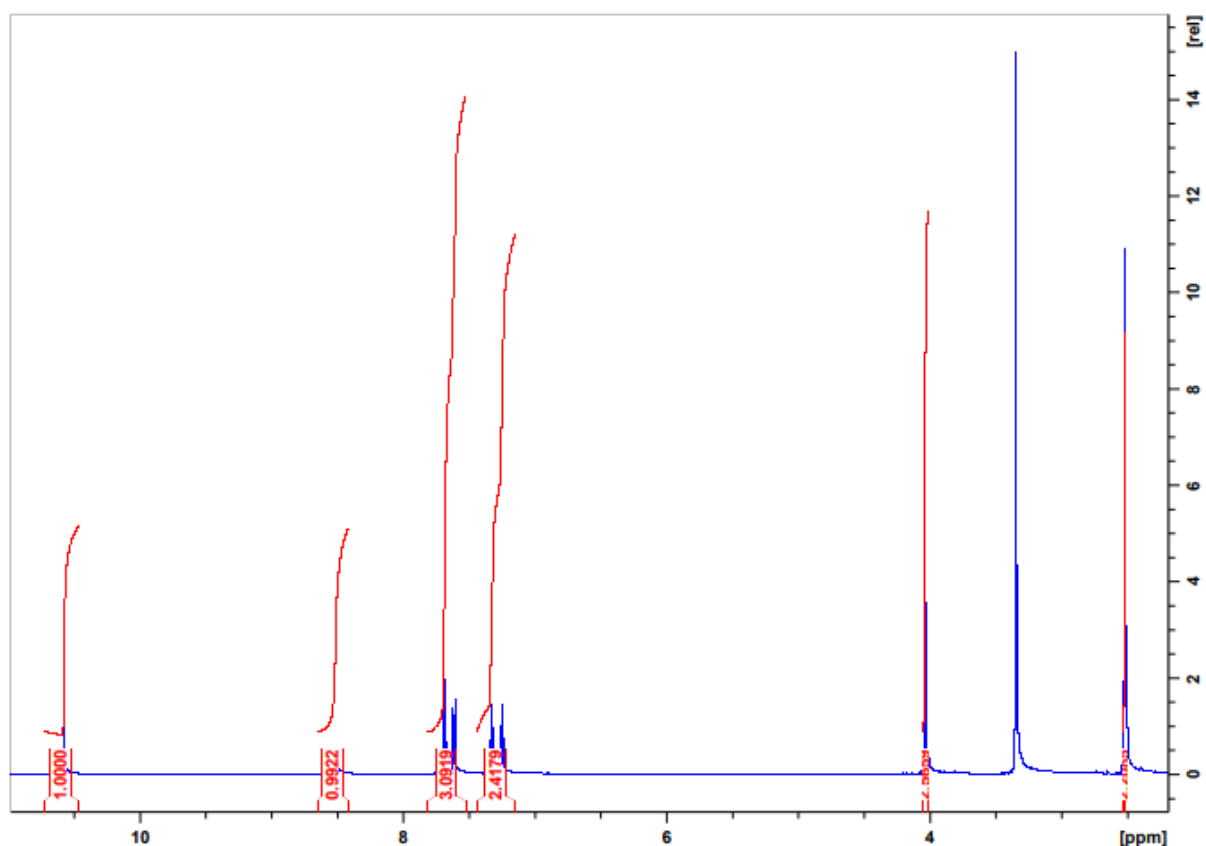


Figure S1-8. ¹H-NMR spectrum of compound 6-2

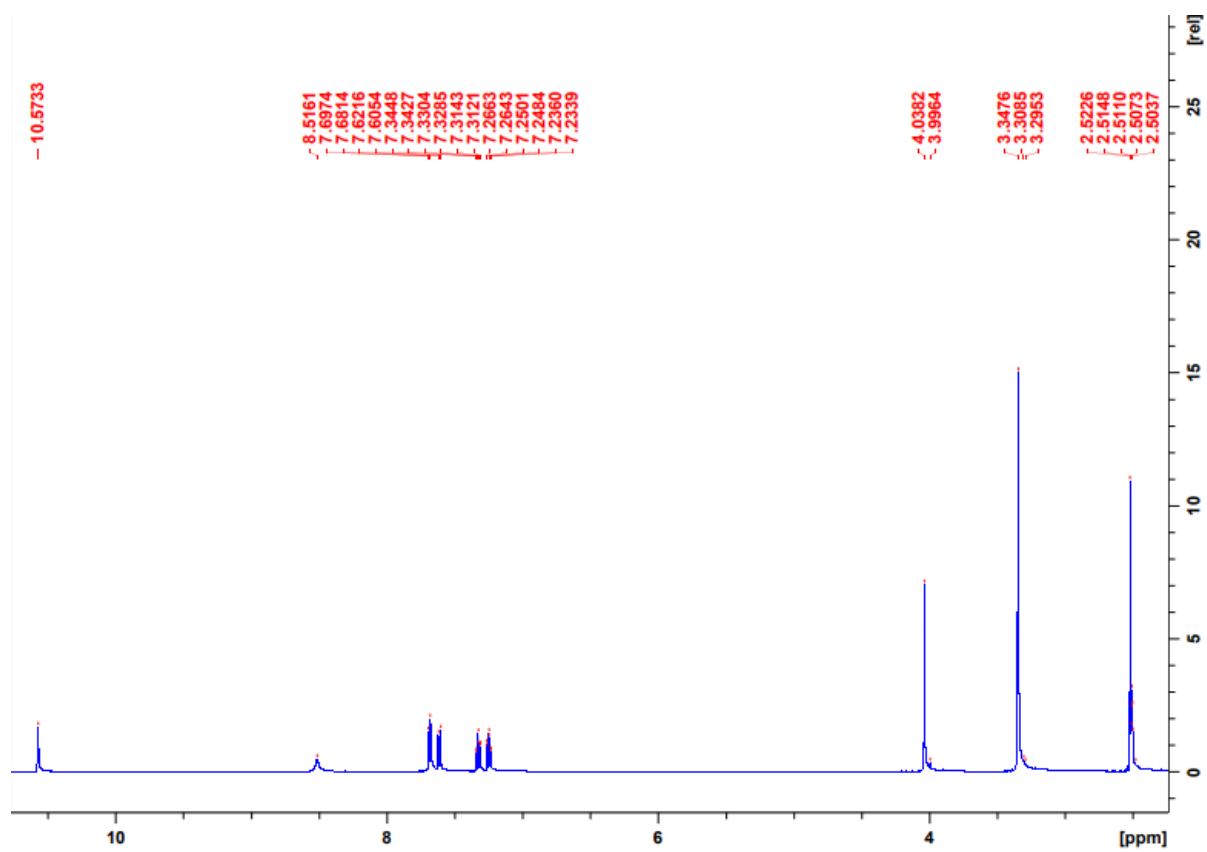


Figure S1-9. ^1H -NMR spectrum of compound 6-3

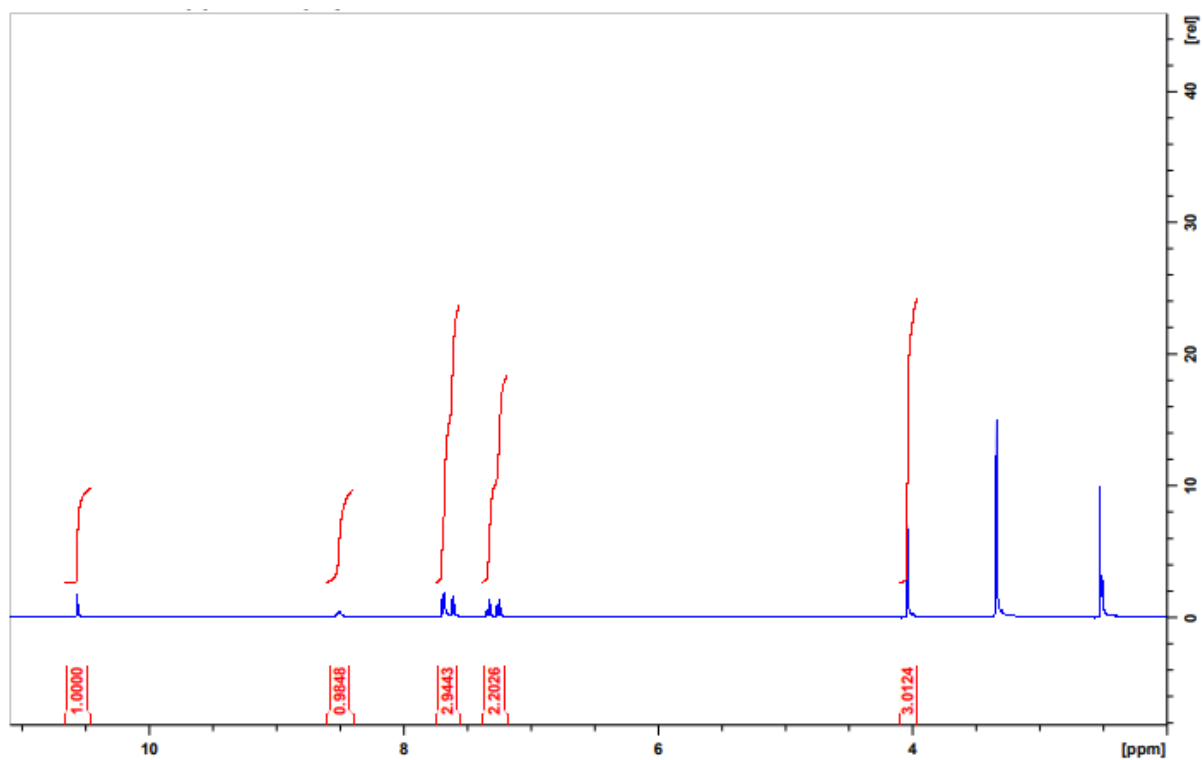


Figure S1-10. ^1H -NMR spectrum of compound 6-4

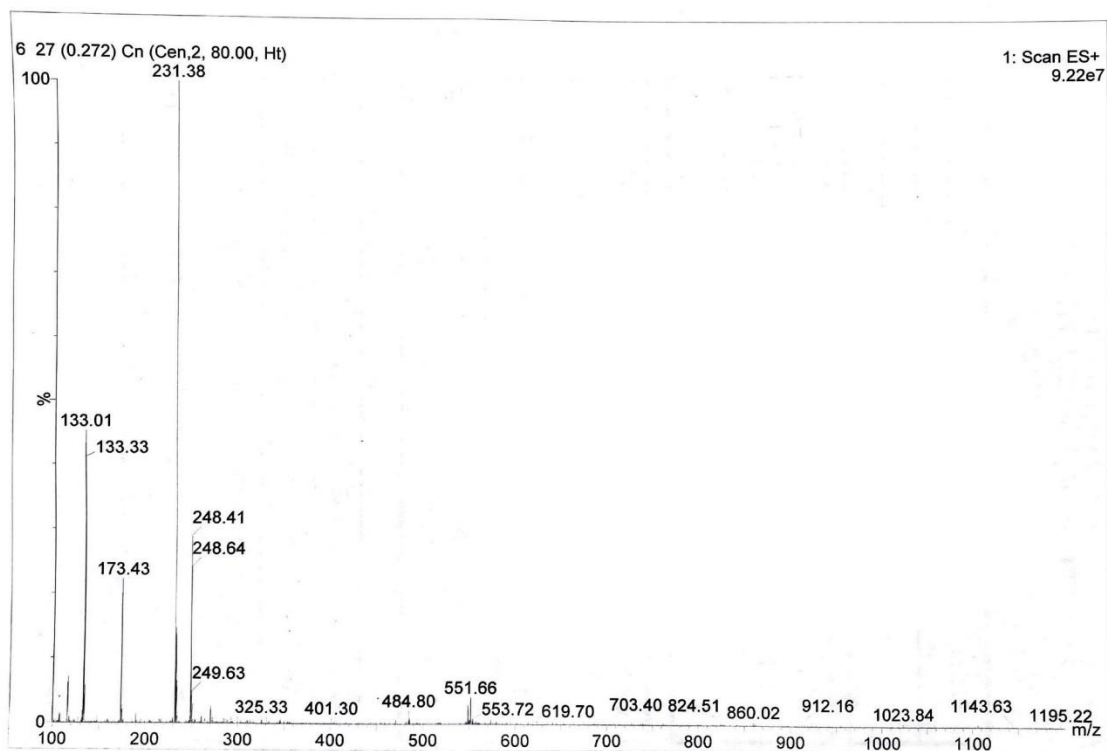
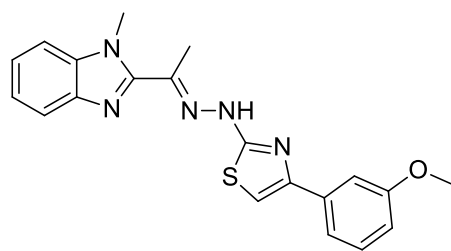


Figure S1-11. Mass spectrum of compound 6



Compound 6a

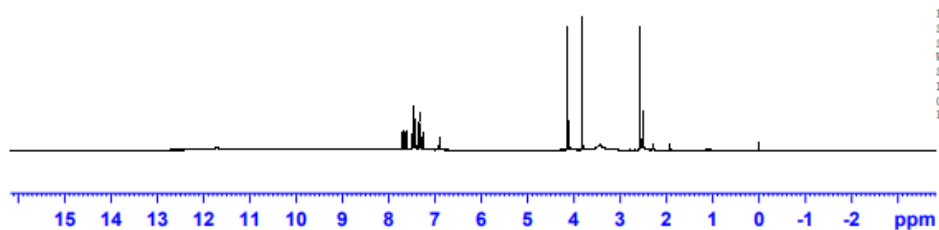


Figure S1-12. ¹H-NMR spectrum of compound 6a



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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SNH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 11.14 usec
TE 310.2 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330883 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.04299927 W

F2 - Processing parameters
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SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

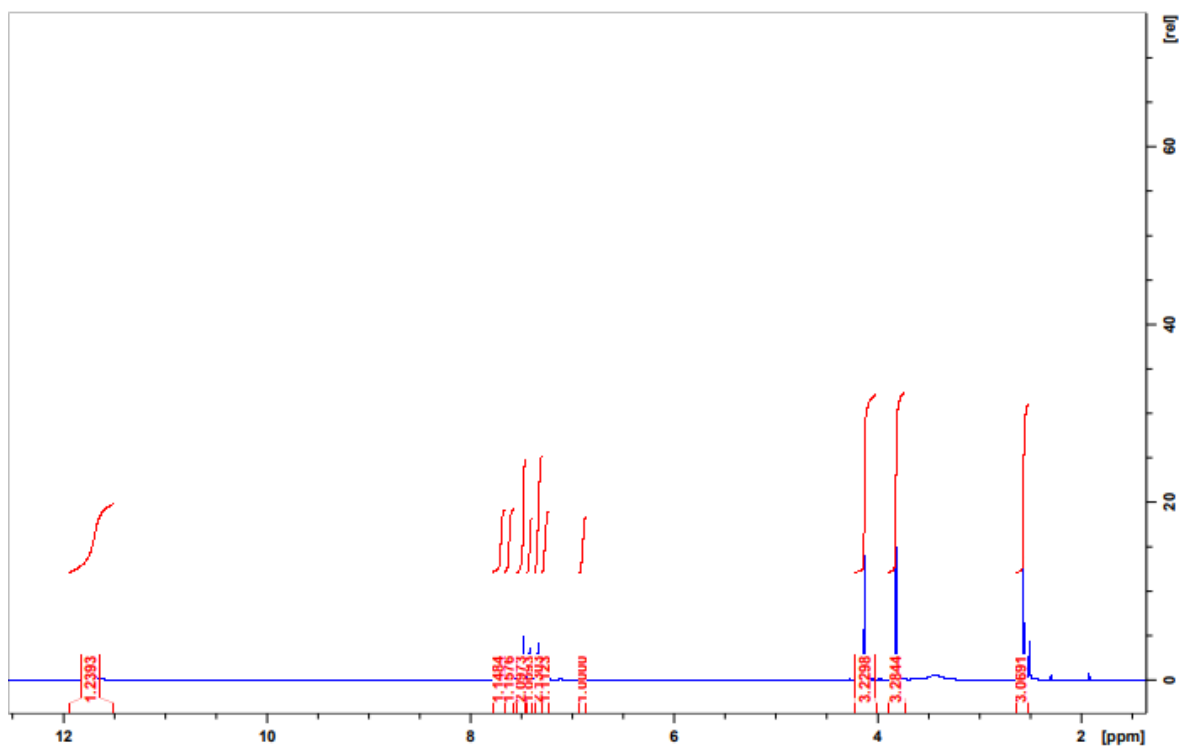


Figure S1-13. ^1H -NMR spectrum of compound **6a-1**

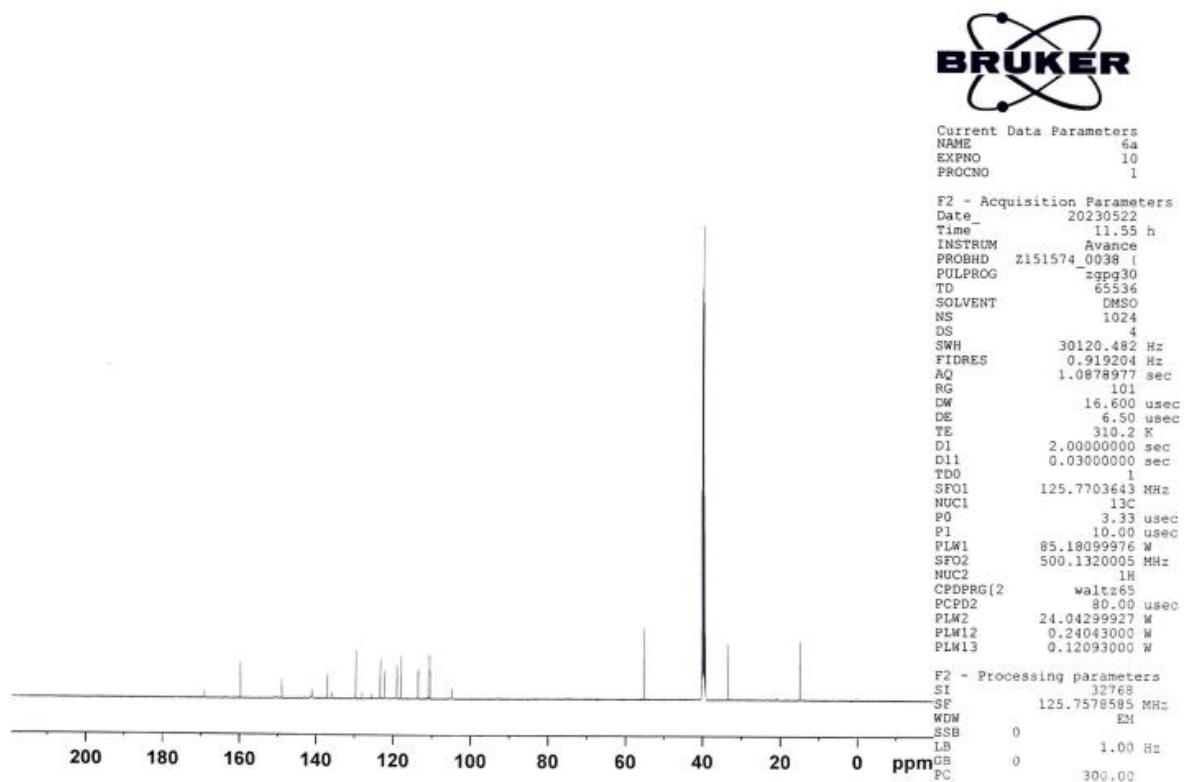


Figure S1-14. ^{13}C -NMR spectrum of compound **6a**

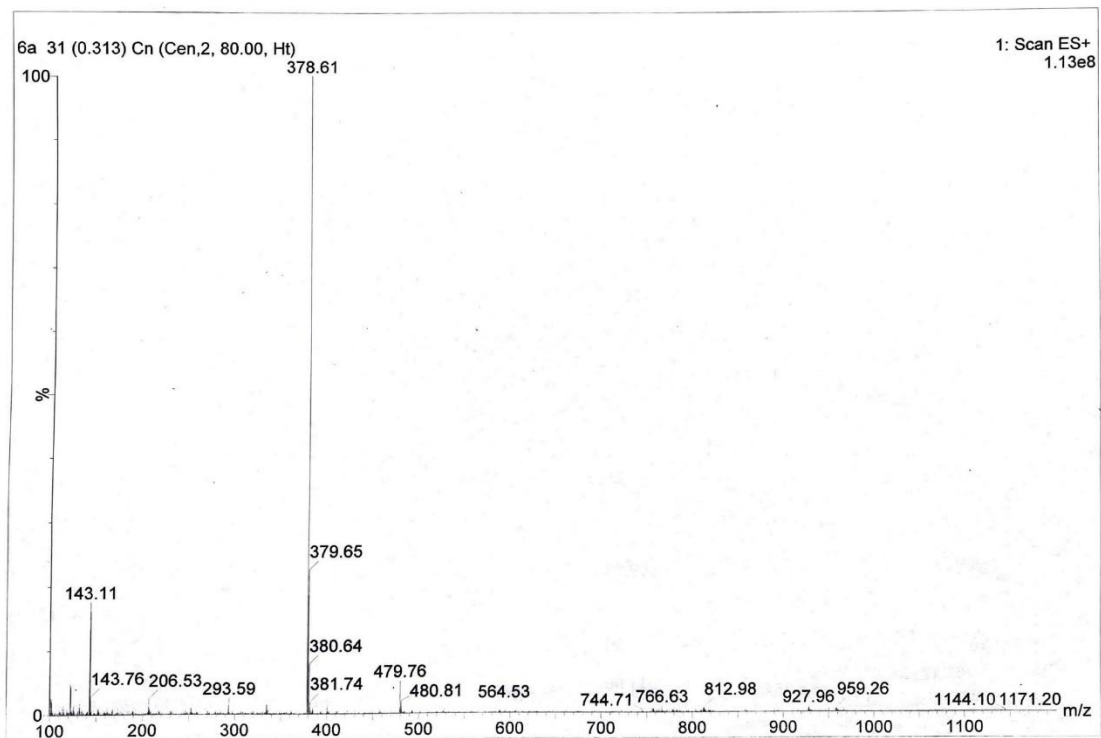


Figure S1-15. Mass spectrum of compound 6a

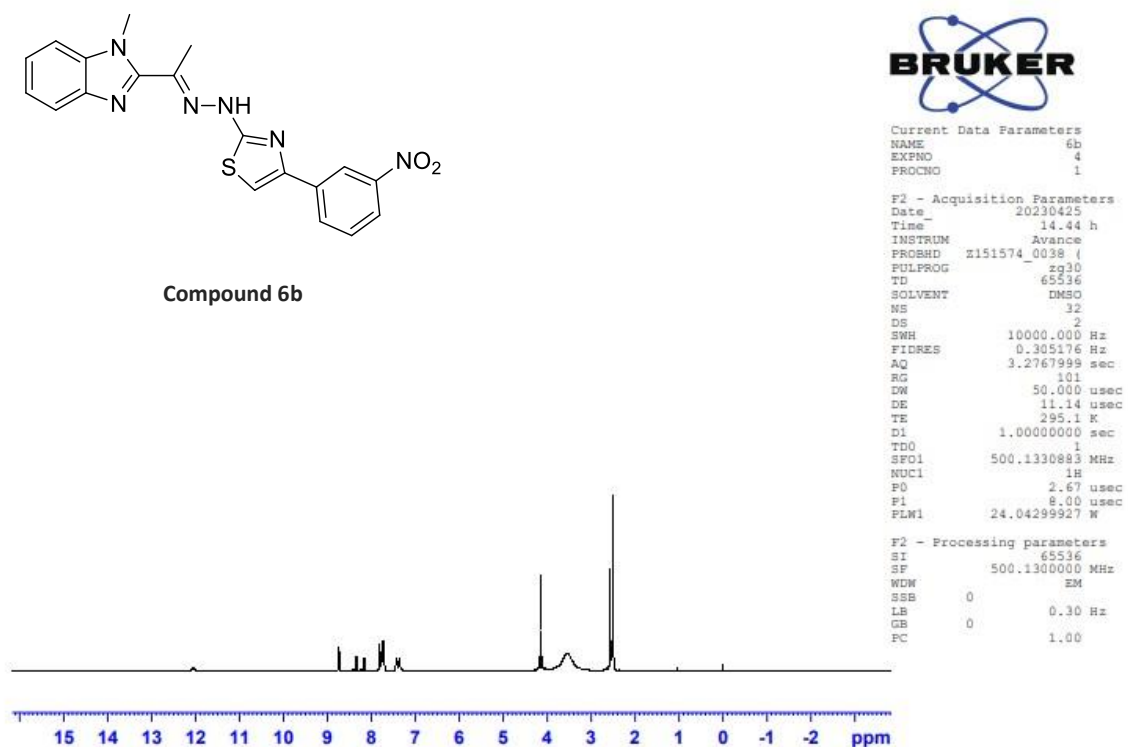


Figure S1-16. $^1\text{H-NMR}$ spectrum of compound 6b-1

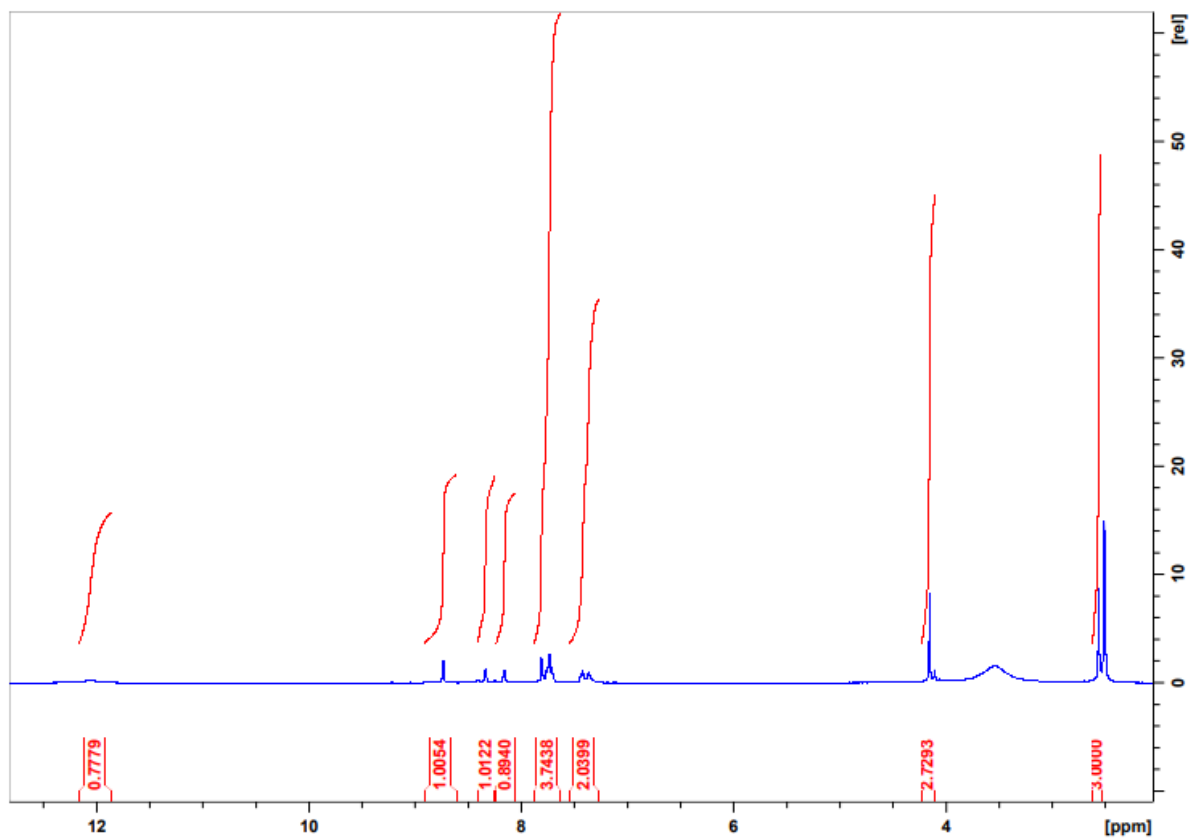


Figure S1-17. ^1H -NMR spectrum of compound 6b-2

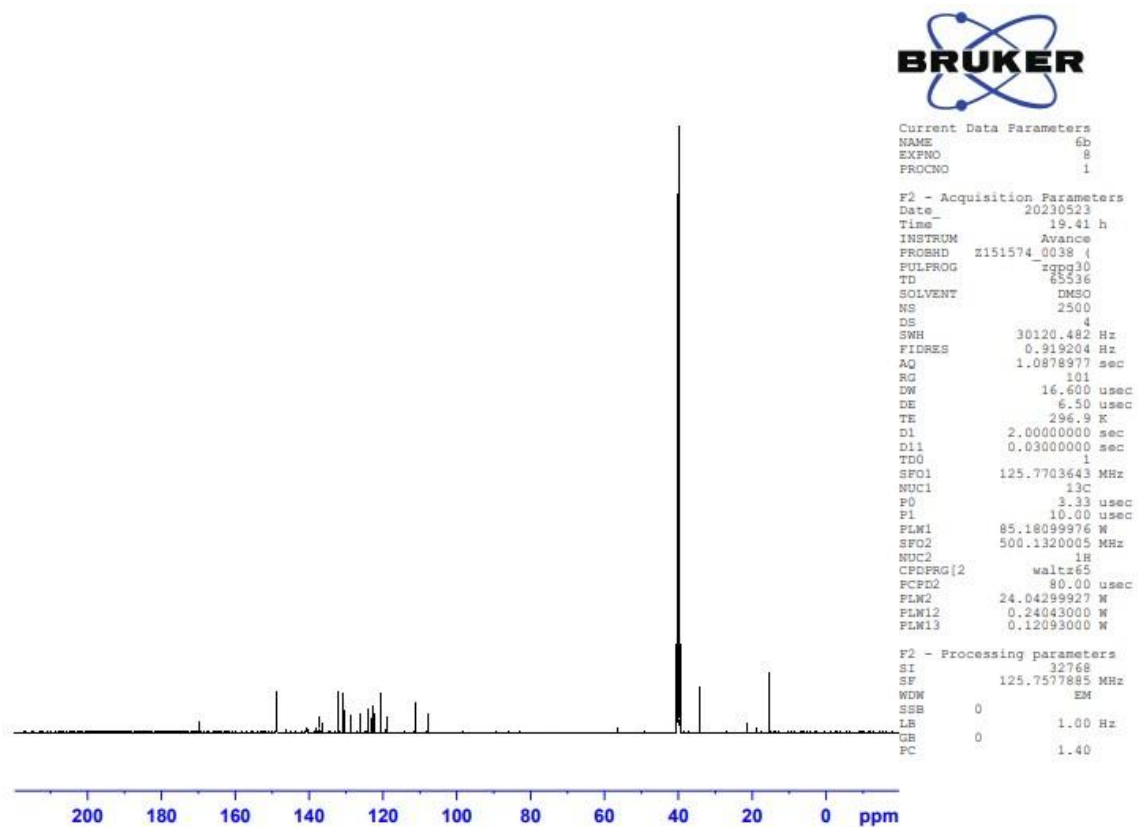


Figure S1-18. ^{13}C -NMR spectrum of compound 6b

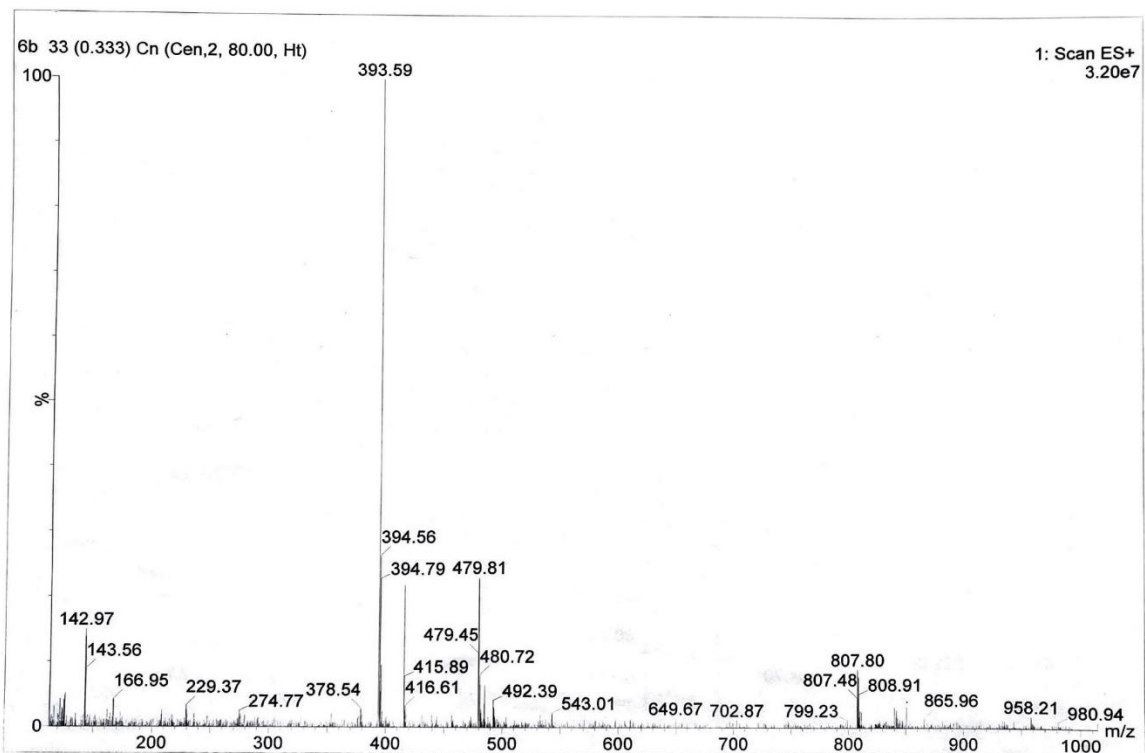


Figure S1-19. Mass spectrum of compound 6b

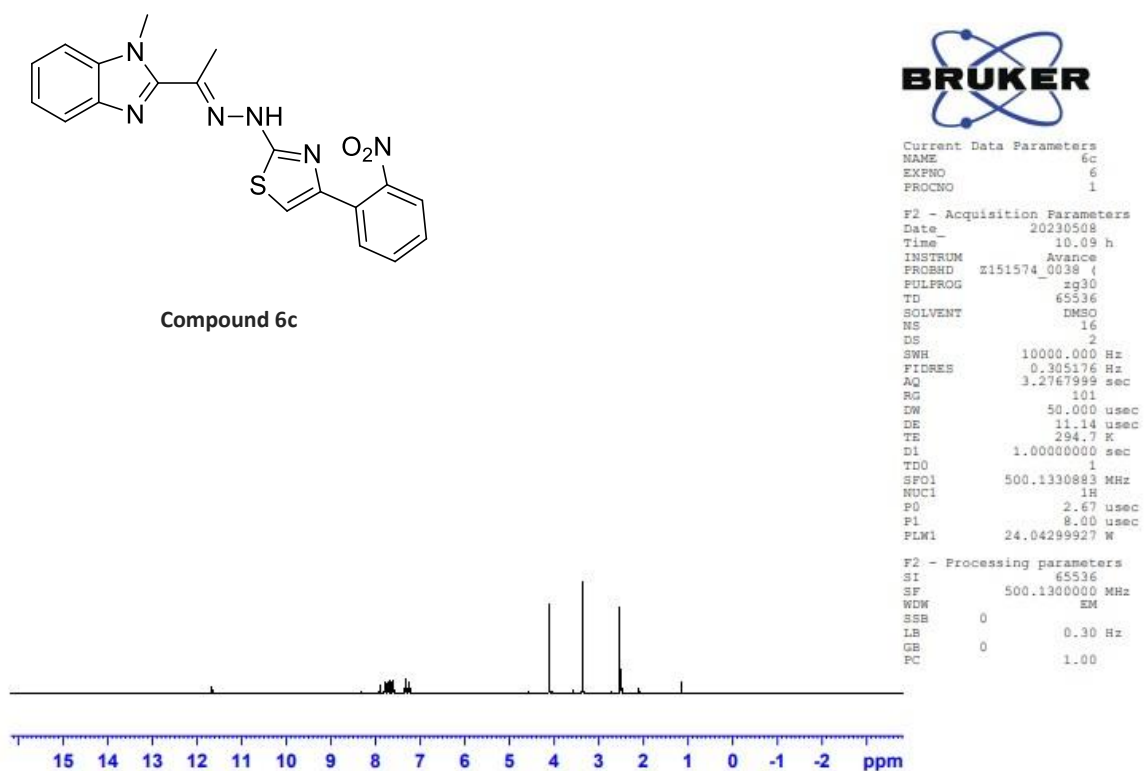


Figure S1-20. ¹H-NMR spectrum of compound 6c-1

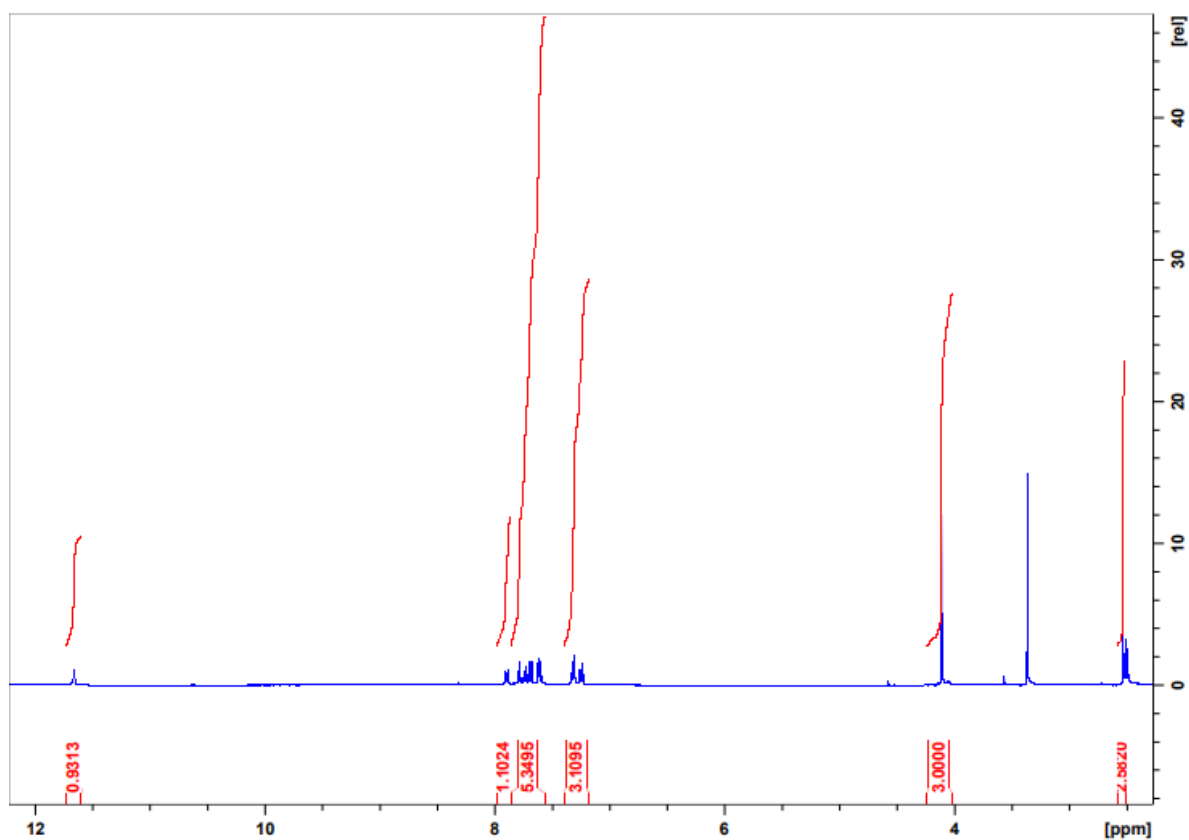


Figure S1-21. ¹H-NMR spectrum of compound 6c-2

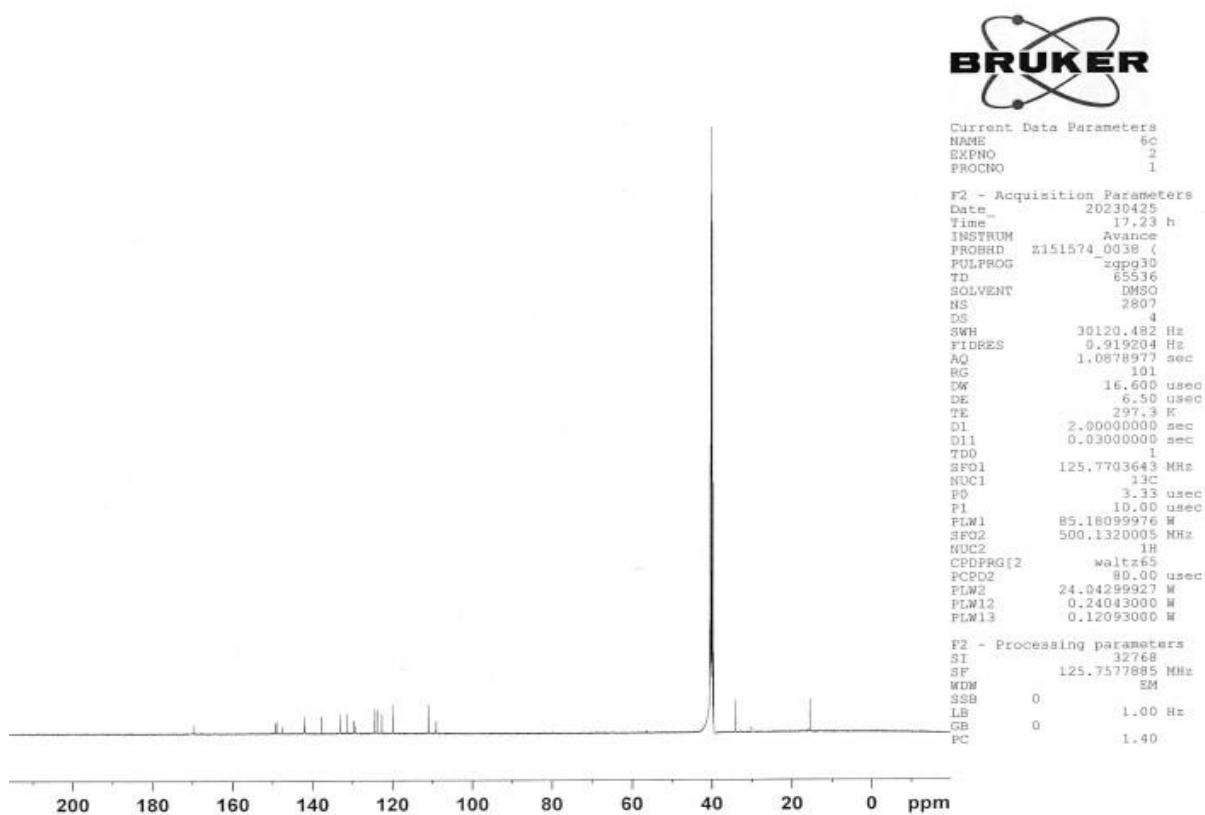


Figure S1-22. ¹³C-NMR spectrum of compound 6c

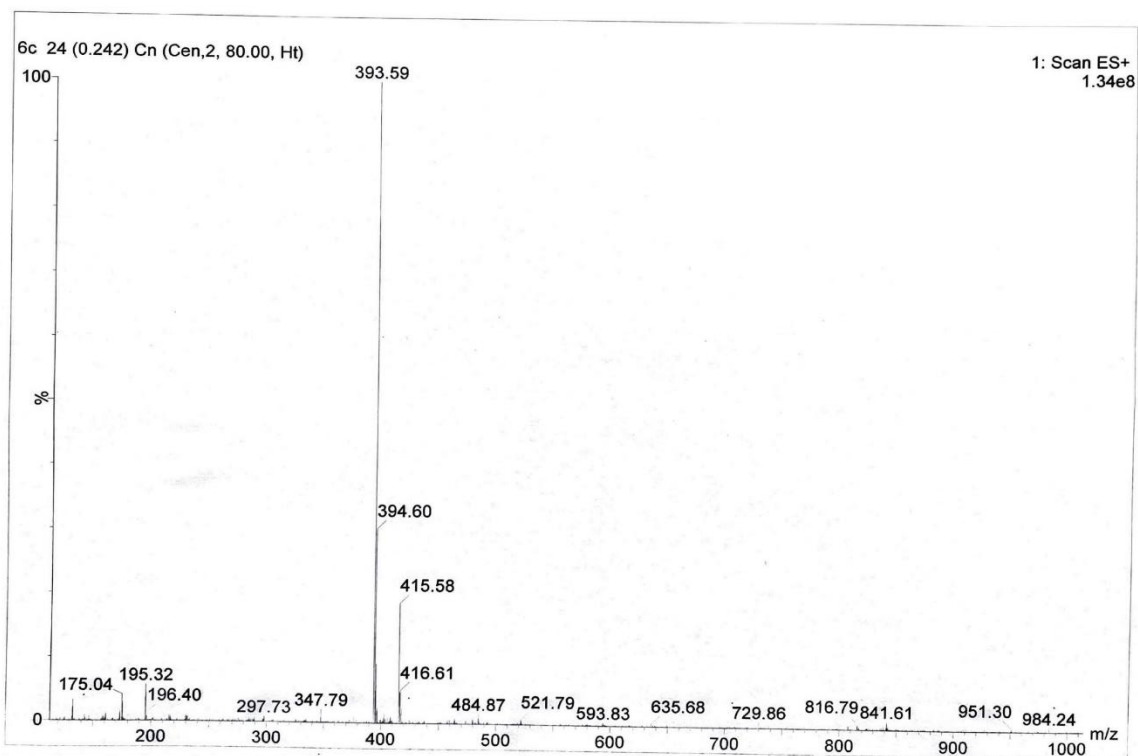
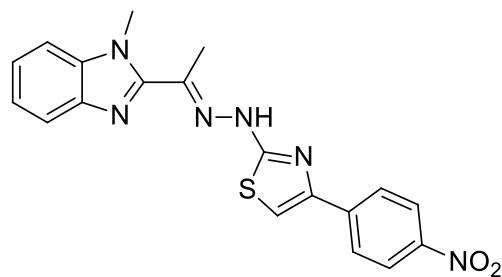
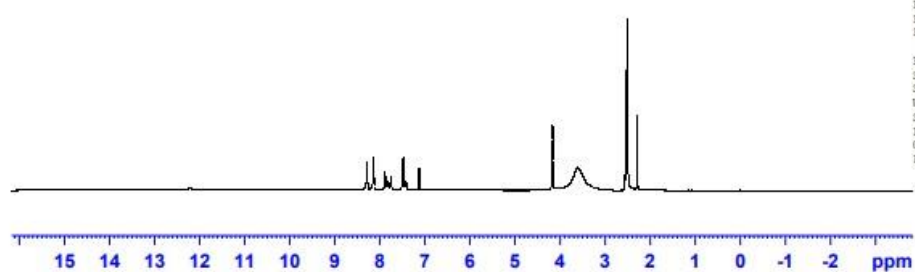


Figure S1-23. Mass spectrum of compound 6c



Compound 6d



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NAME 6d
EXPNO 1
PROCNO 1

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Time 15.11 h
INSTRUM Avance
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 11.14 usec
TE 294.9 K
D1 1.0000000 sec
TD0 1
SFO1 500.1330883 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.04299927 W

F2 - Processing parameters
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SF 500.1330000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S1-24. ¹H-NMR spectrum of compound 6d-1

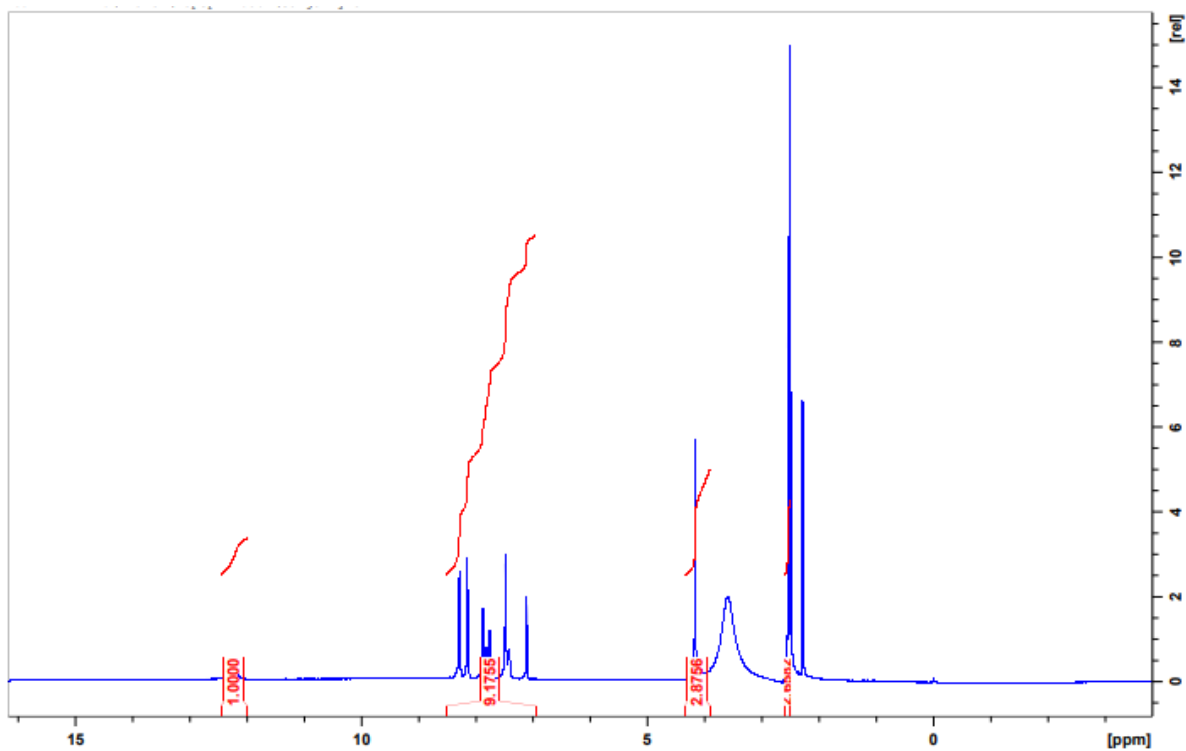


Figure S1-25. $^1\text{H-NMR}$ spectrum of compound **6d-2**

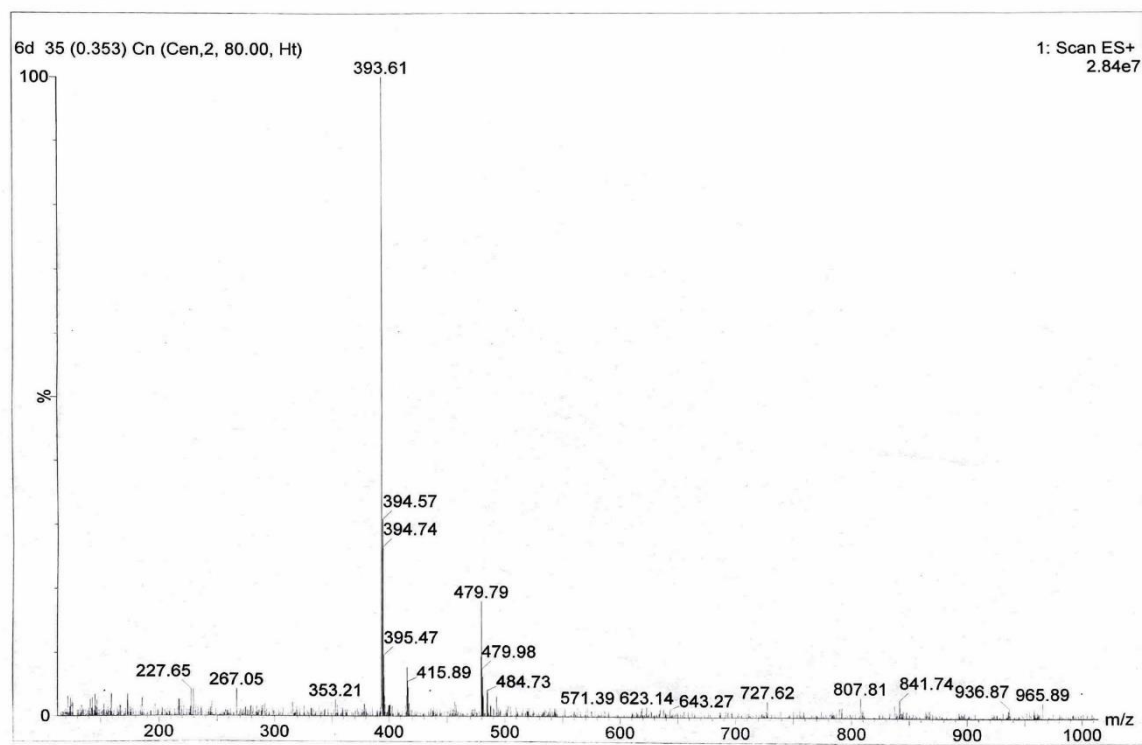


Figure S1-26. Mass spectrum of compound **6d**

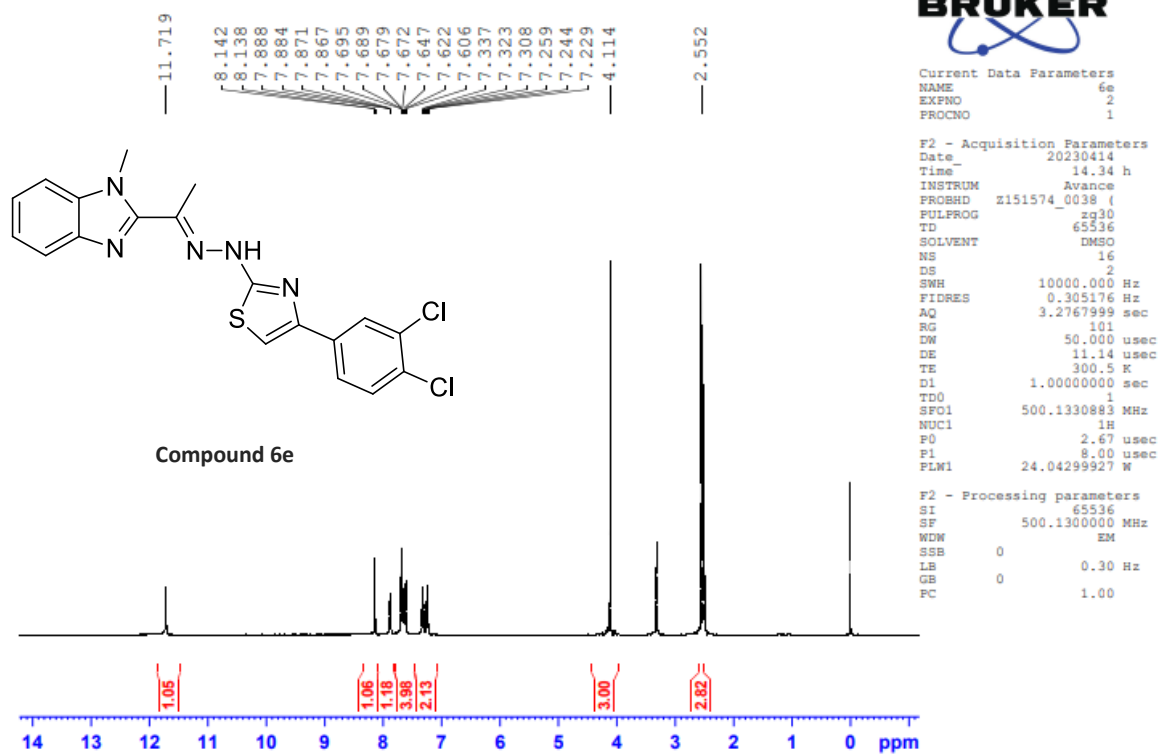


Figure S1-27. ¹H-NMR spectrum of compound 6e

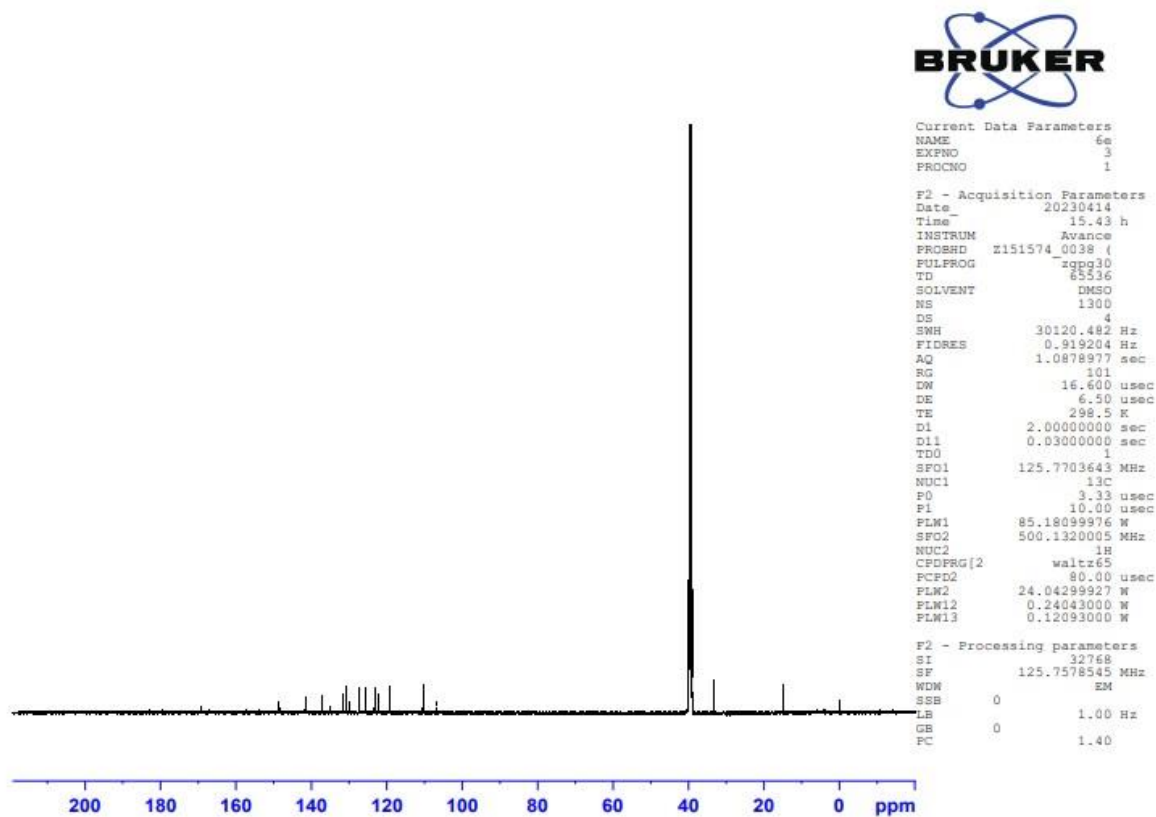


Figure S1-28. ¹³C-NMR spectrum of compound 6e

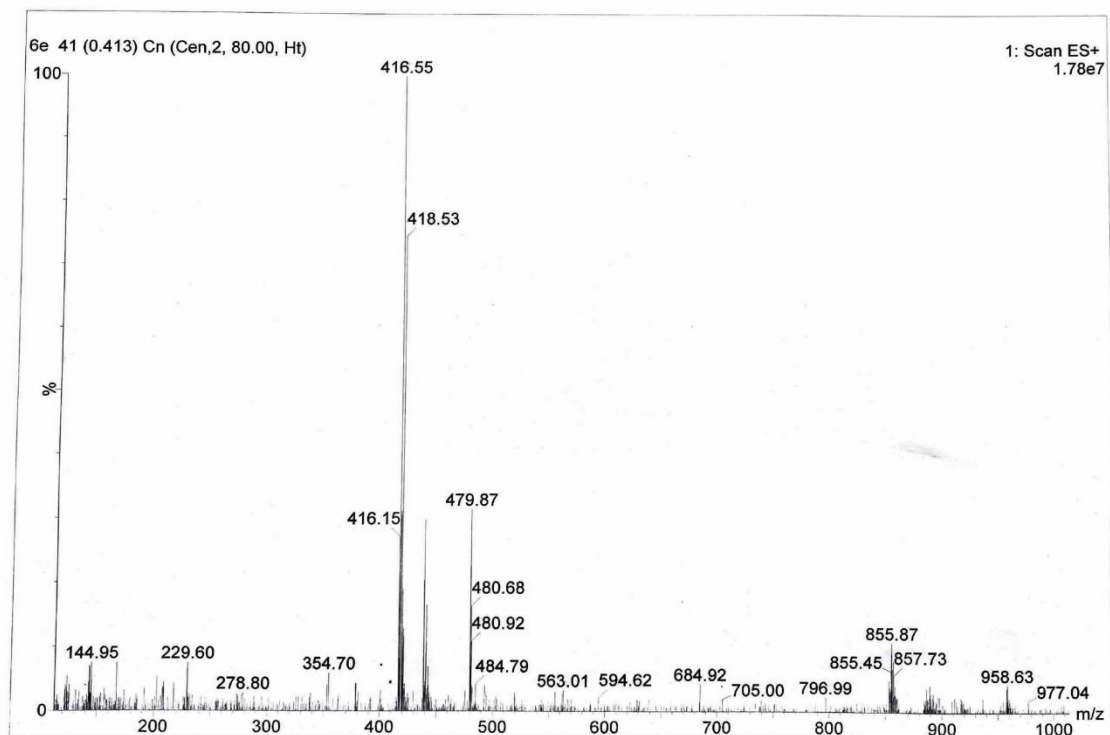


Figure S1-29. Mass spectrum of compound 6e

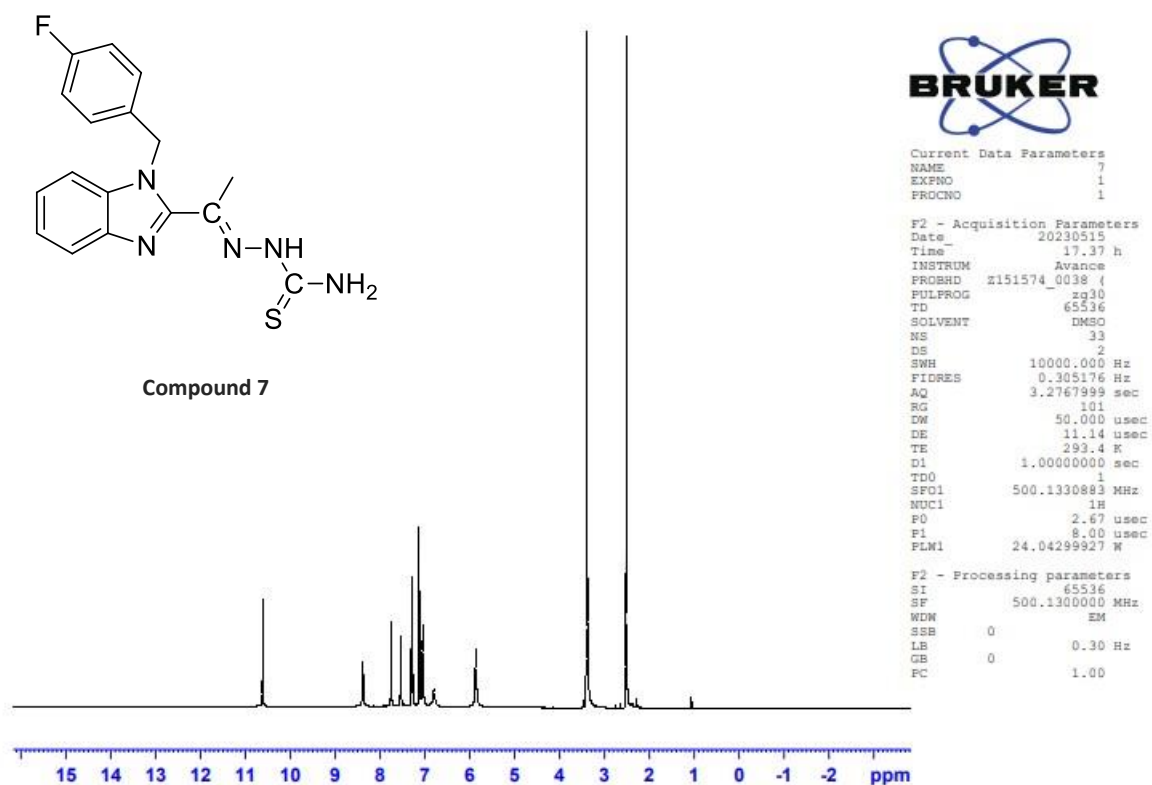


Figure S1-30. ¹H-NMR spectrum of compound 7-1

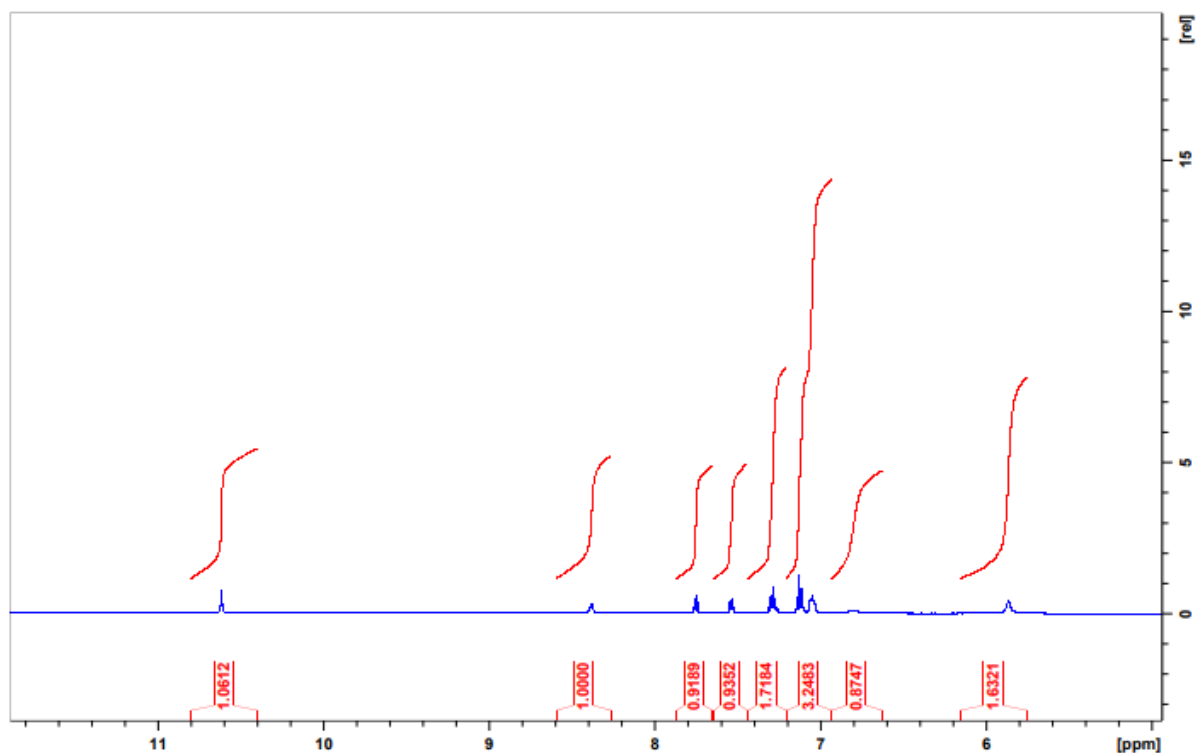


Figure S1-31. ¹H-NMR spectrum of compound 7-2

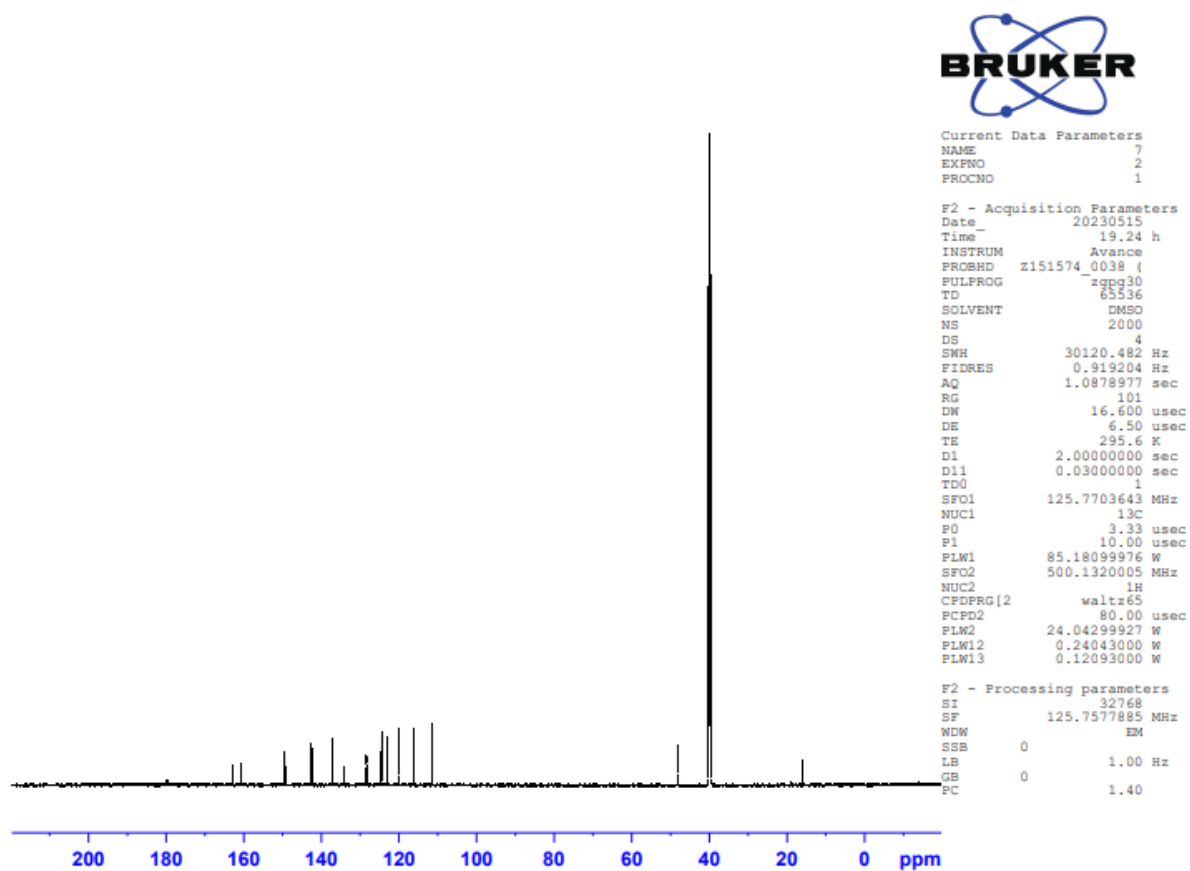


Figure S1-32. ¹³C-NMR spectrum of compound 7

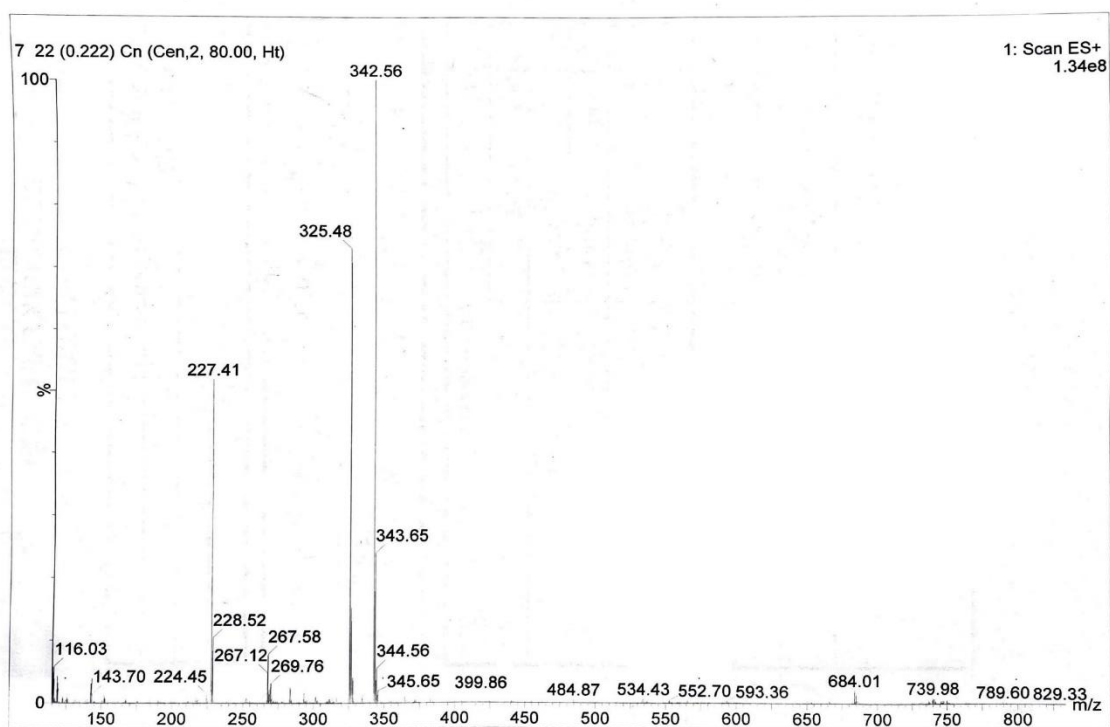
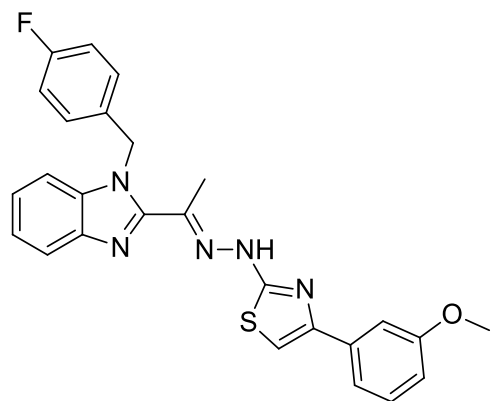


Figure S1-33. Mass spectrum of compound 7



Compound 7a



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PROCNO        1

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TD           65536
SOLVENT      DMSO
NS           16
DS           2
SWH          10000.000 Hz
FIDRES       0.305176 Hz
AQ           3.2767999 sec
RG           101
DW           50.000 usec
DE           11.14 usec
TE           291.8 K
D1           1.00000000 sec
TD0          1
SFO1         500.1330883 MHz
NUC1         1H
P0           2.67 usec
P1           8.00 usec
PLW1         24.04299927 W

F2 - Processing parameters
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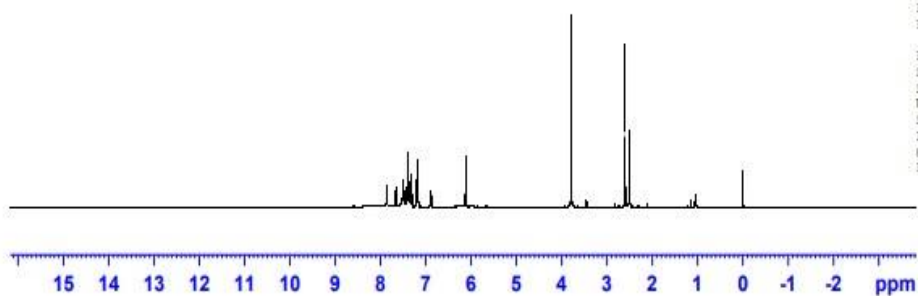


Figure S1-34. ¹H-NMR spectrum of compound 7a-1

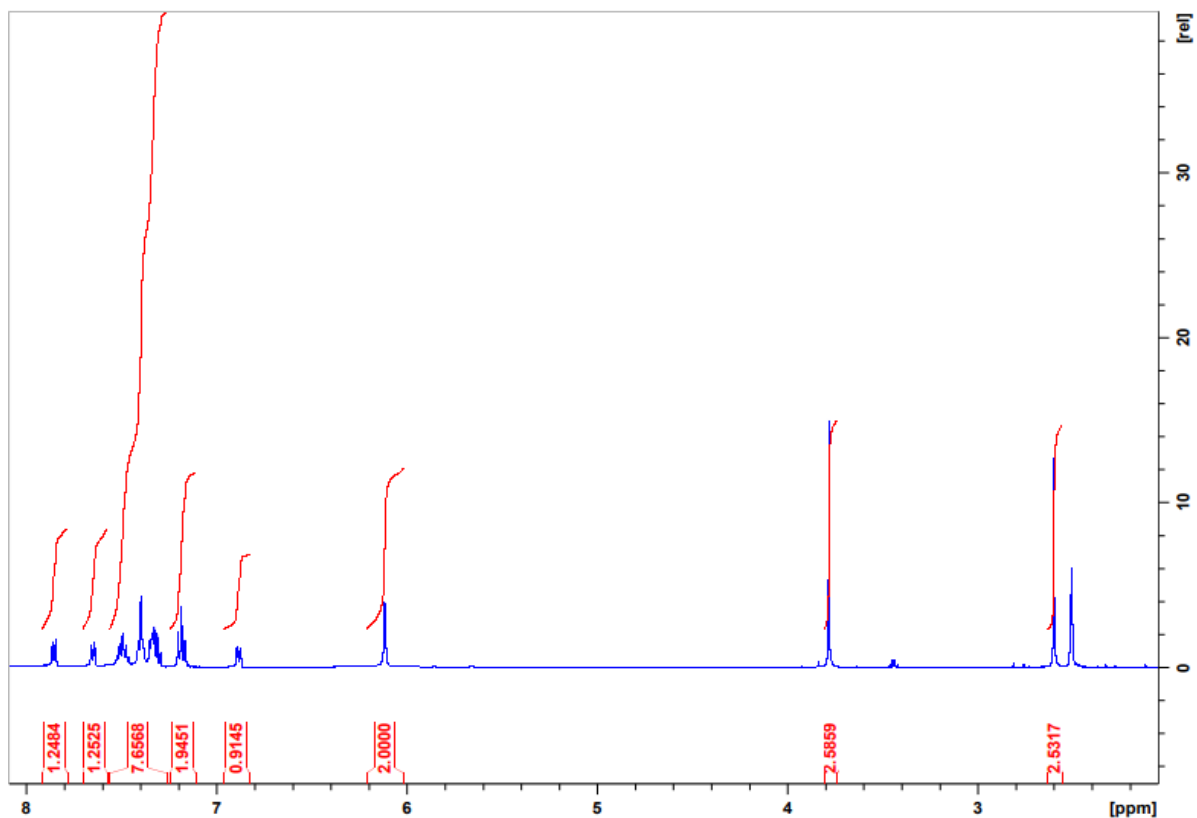


Figure S1-35. ¹H-NMR spectrum of compound 7a-2

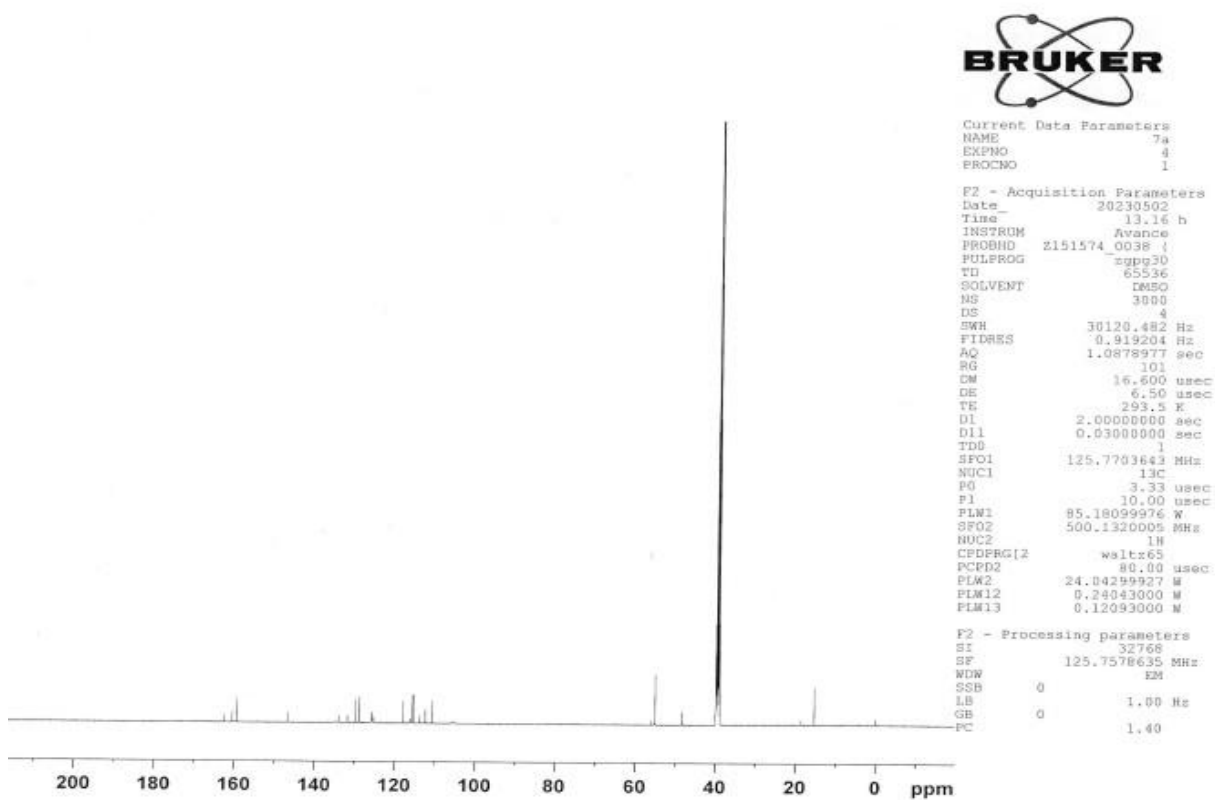


Figure S1-36. ¹³C-NMR spectrum of compound 7a

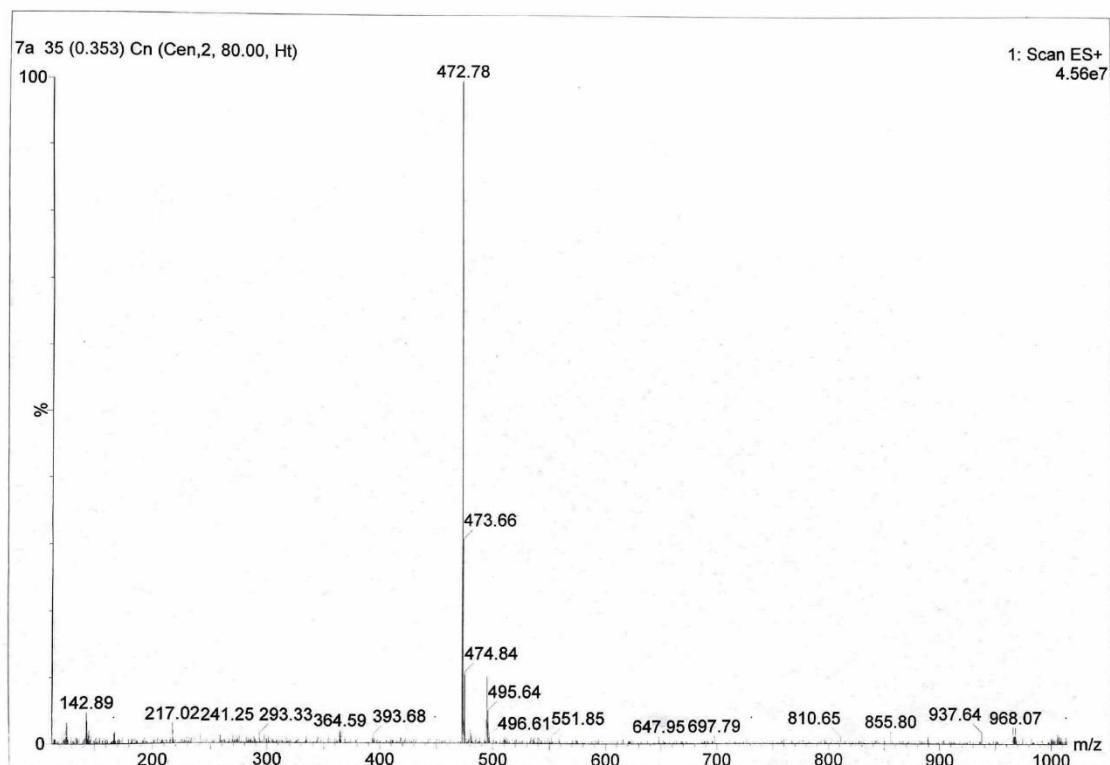


Figure S1-37. Mass spectrum of compound 7a

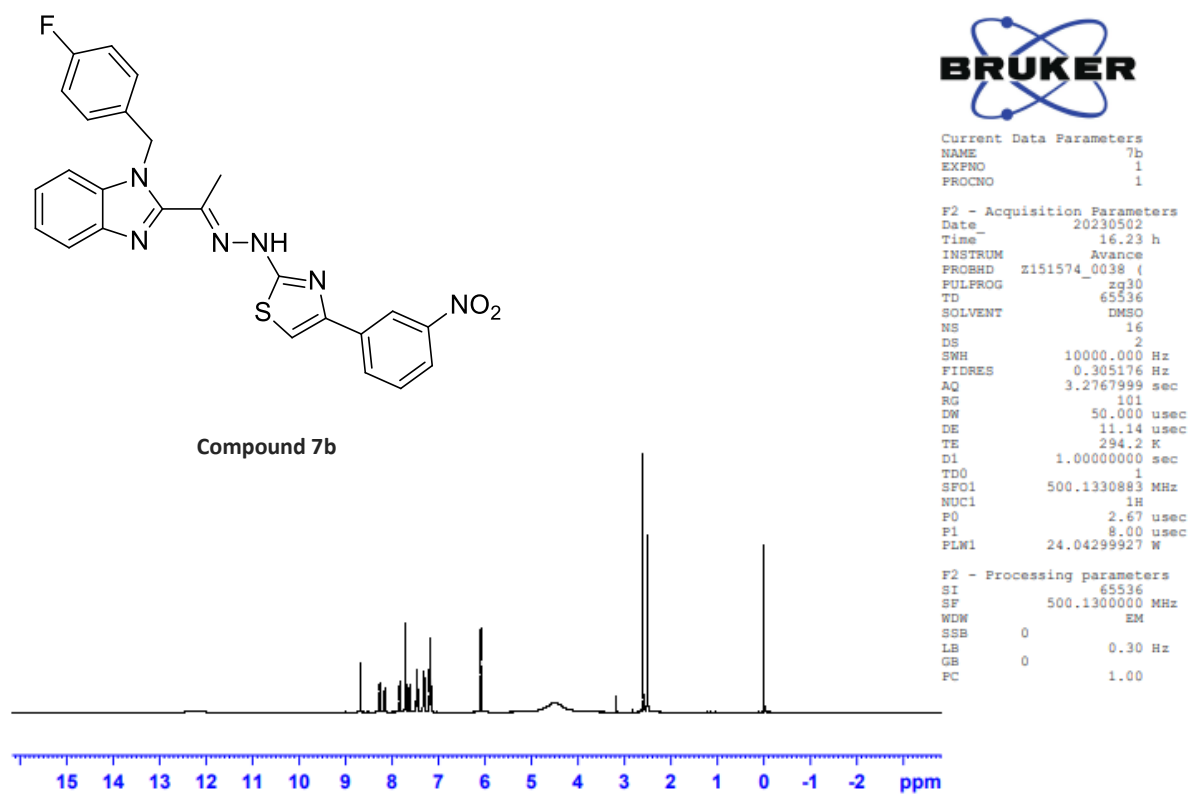


Figure S1-38. $^1\text{H-NMR}$ spectrum of compound 7b-1

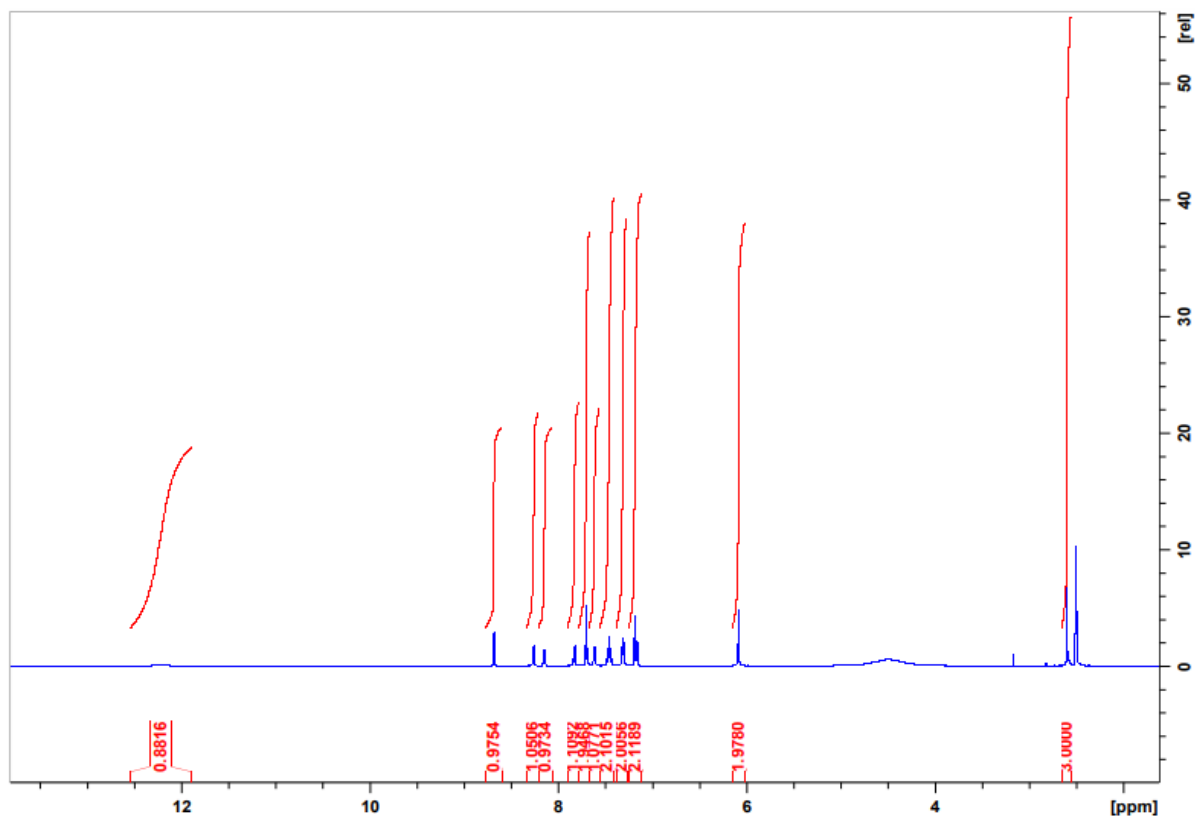


Figure S1-39. ^1H -NMR spectrum of compound **7b-2**

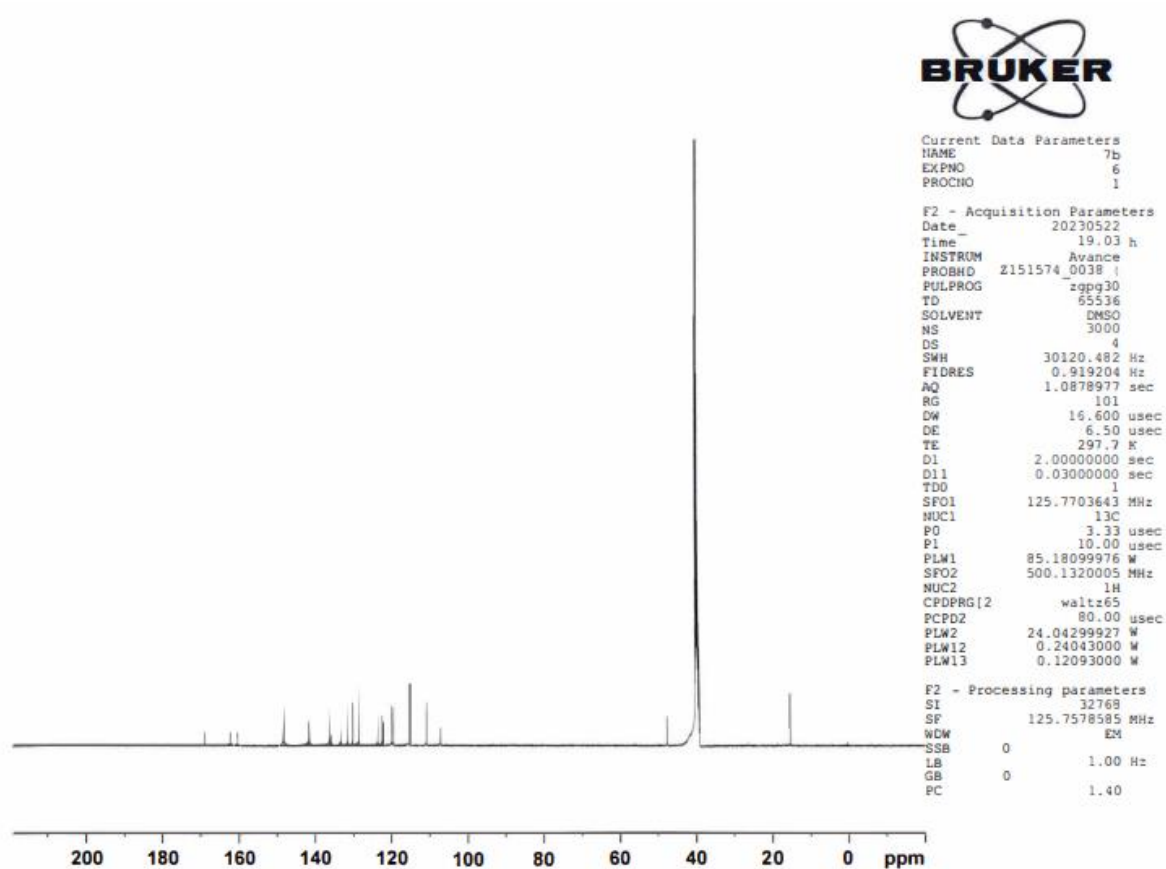


Figure S1-40. ^{13}C -NMR spectrum of compound **7b**

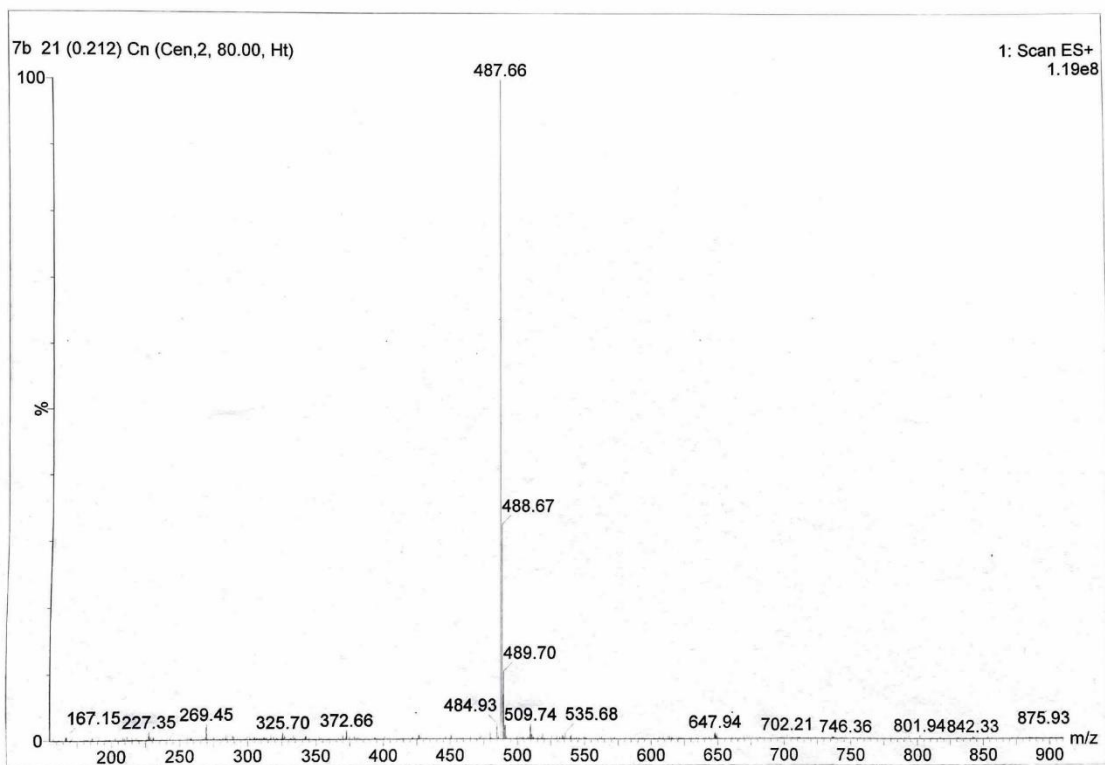


Figure S1-41. Mass spectrum of compound 7b

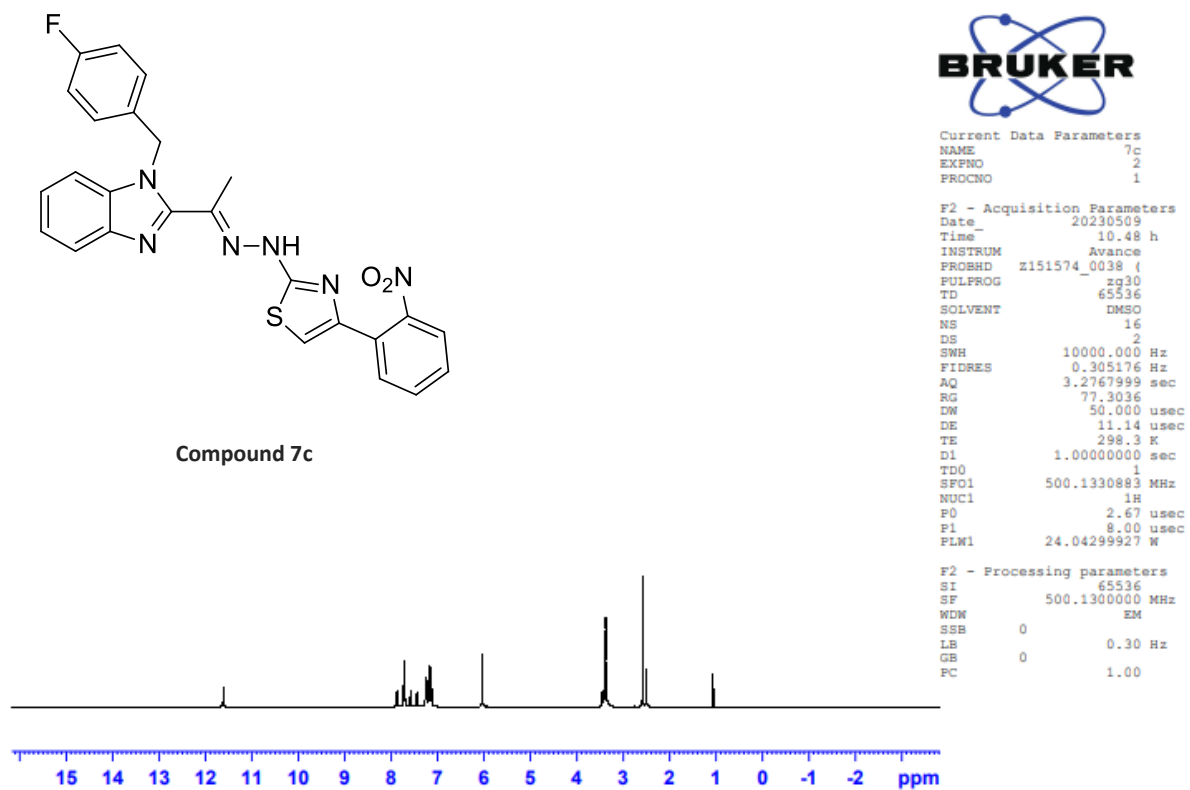


Figure S1-42. ¹H-NMR spectrum of compound 7c-1

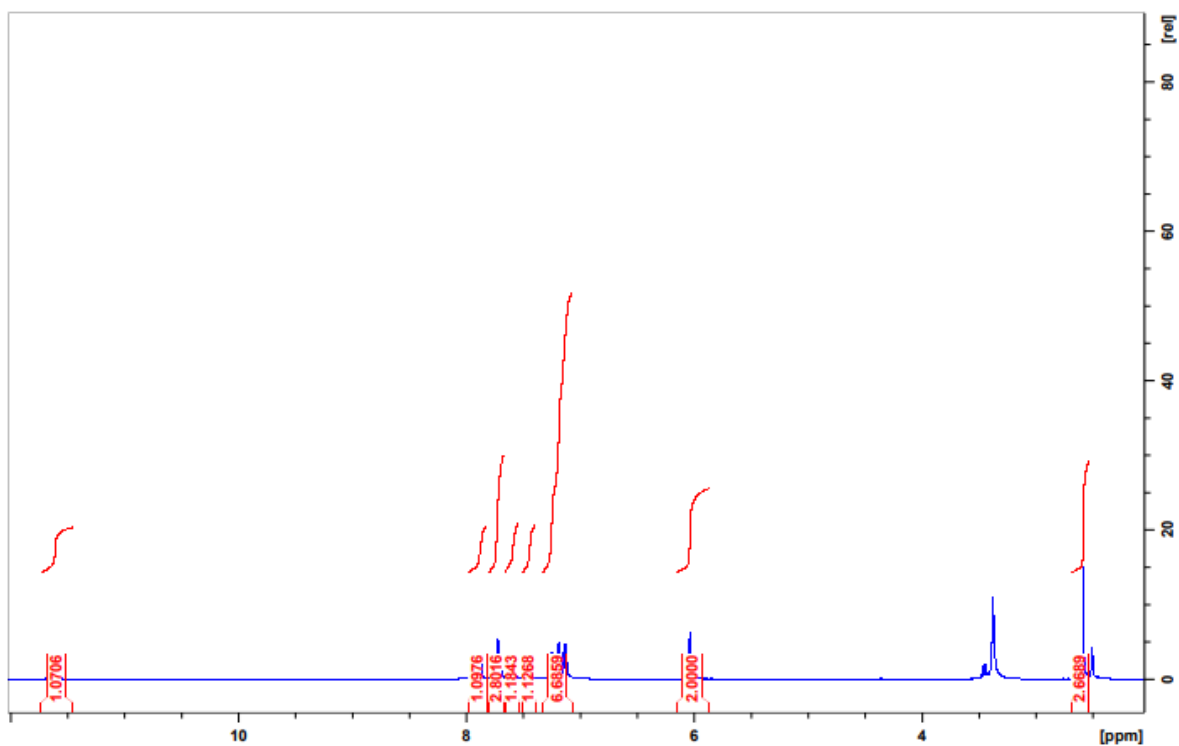


Figure S1-43. ¹H-NMR spectrum of compound 7c-2

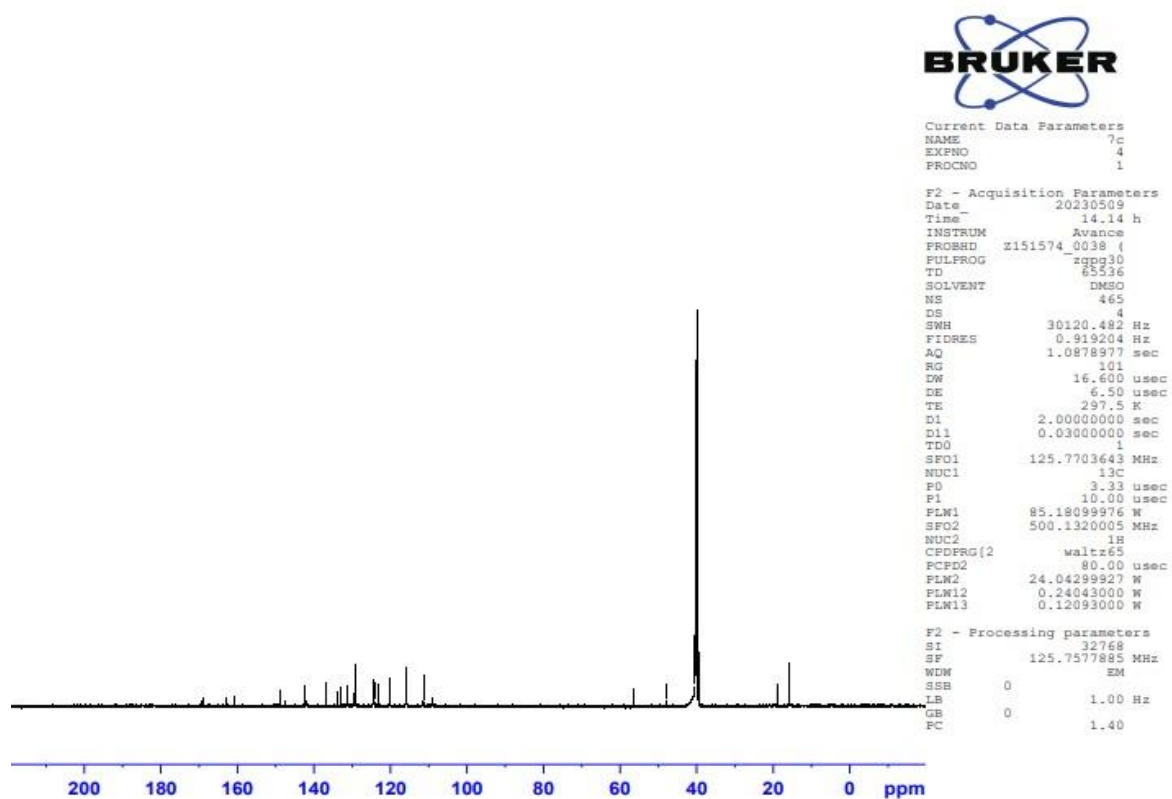


Figure S1-44. ¹³C-NMR spectrum of compound 7c

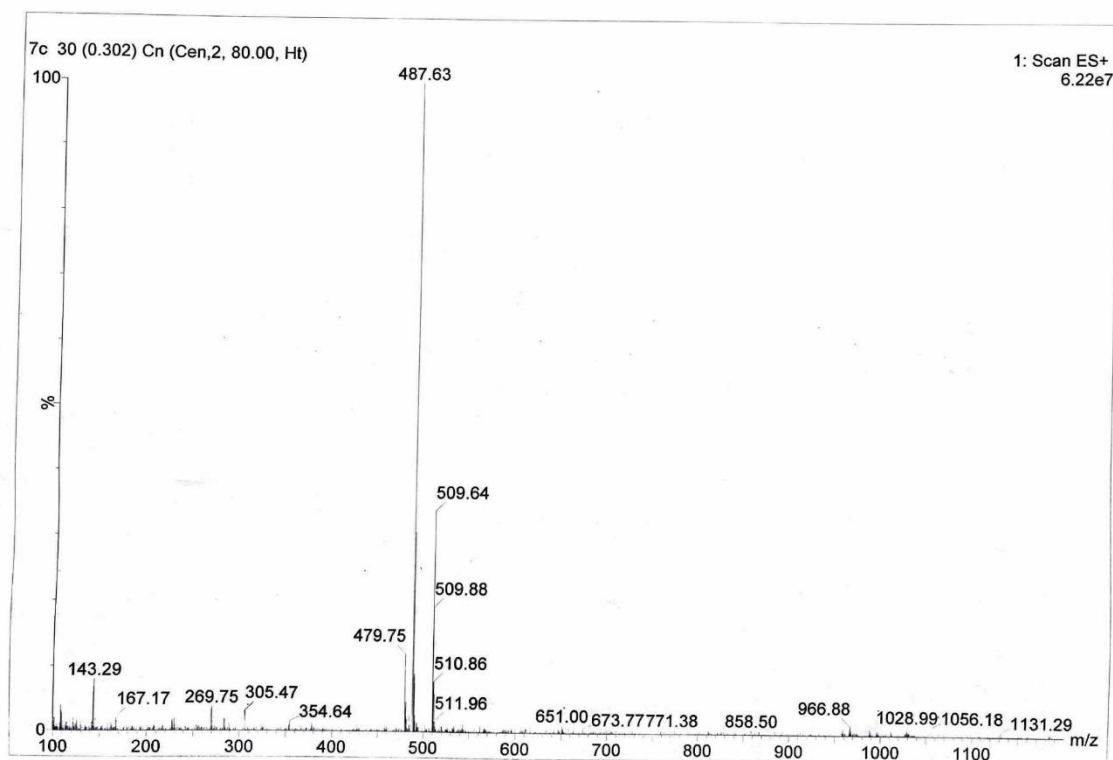
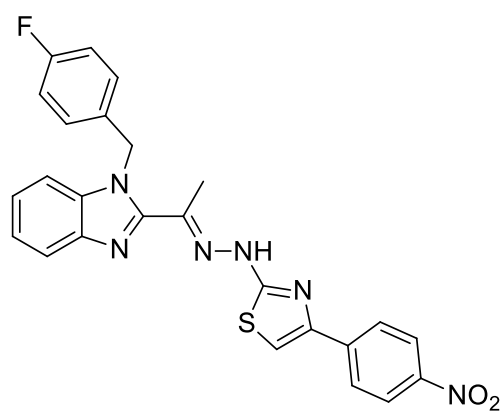


Figure S1-45. Mass spectrum of compound 7c



Compound 7d

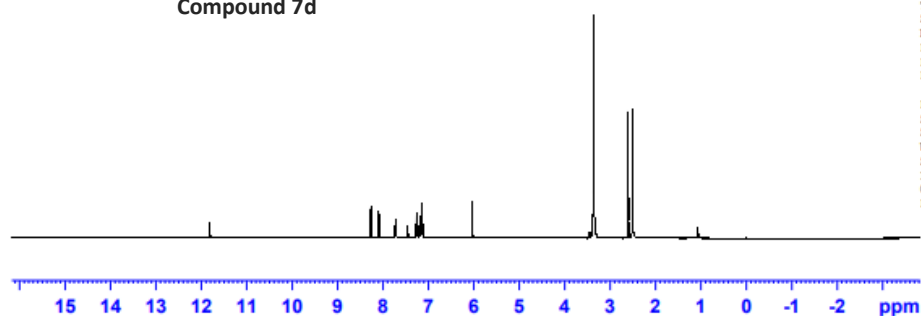


Figure S1-46. ¹H-NMR spectrum of compound 7d-1



Current Data Parameters
NAME 7d
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230508
Time 10.24 h
INSTRUM Avance
PROBHD z151574_0038 (zq30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 11.14 usec
TE 294.9 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330893 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLM1 24.04299927 W

F2 - Processing parameters
SI 65536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

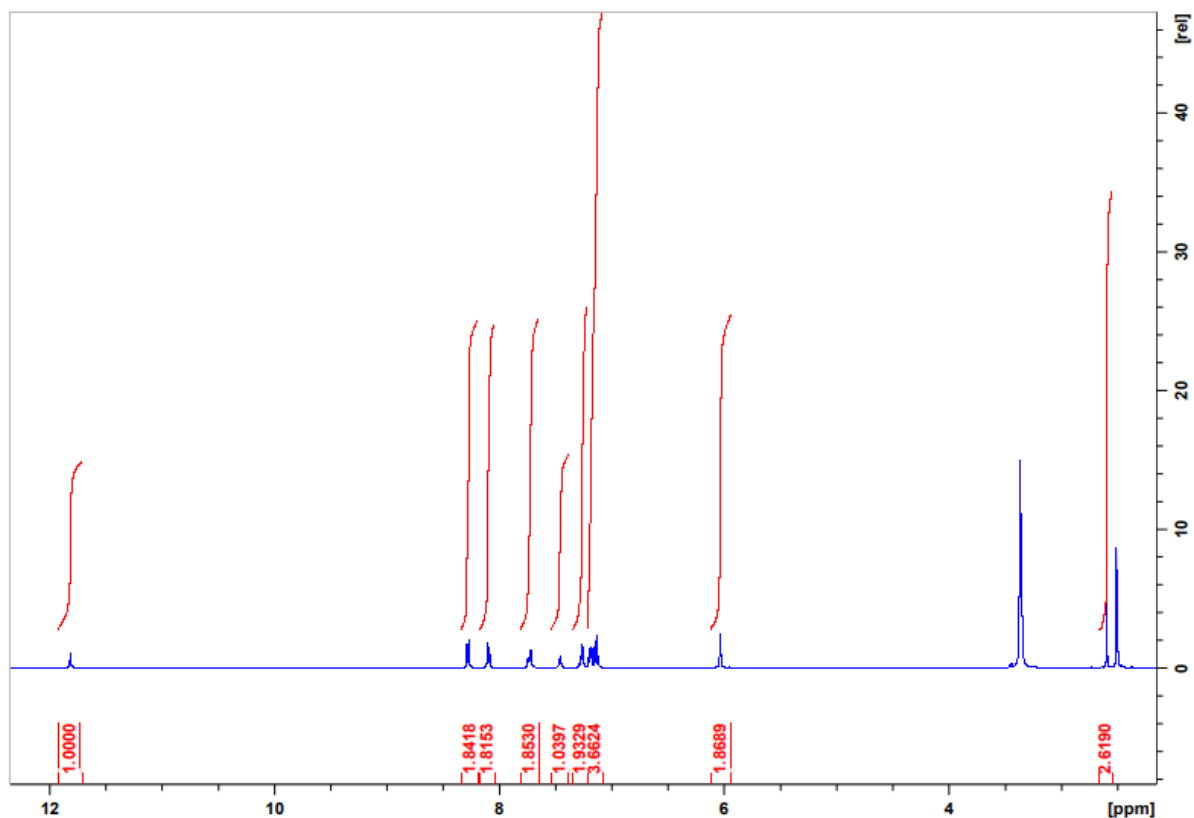


Figure S1-47. ¹H-NMR spectrum of compound 7d-2

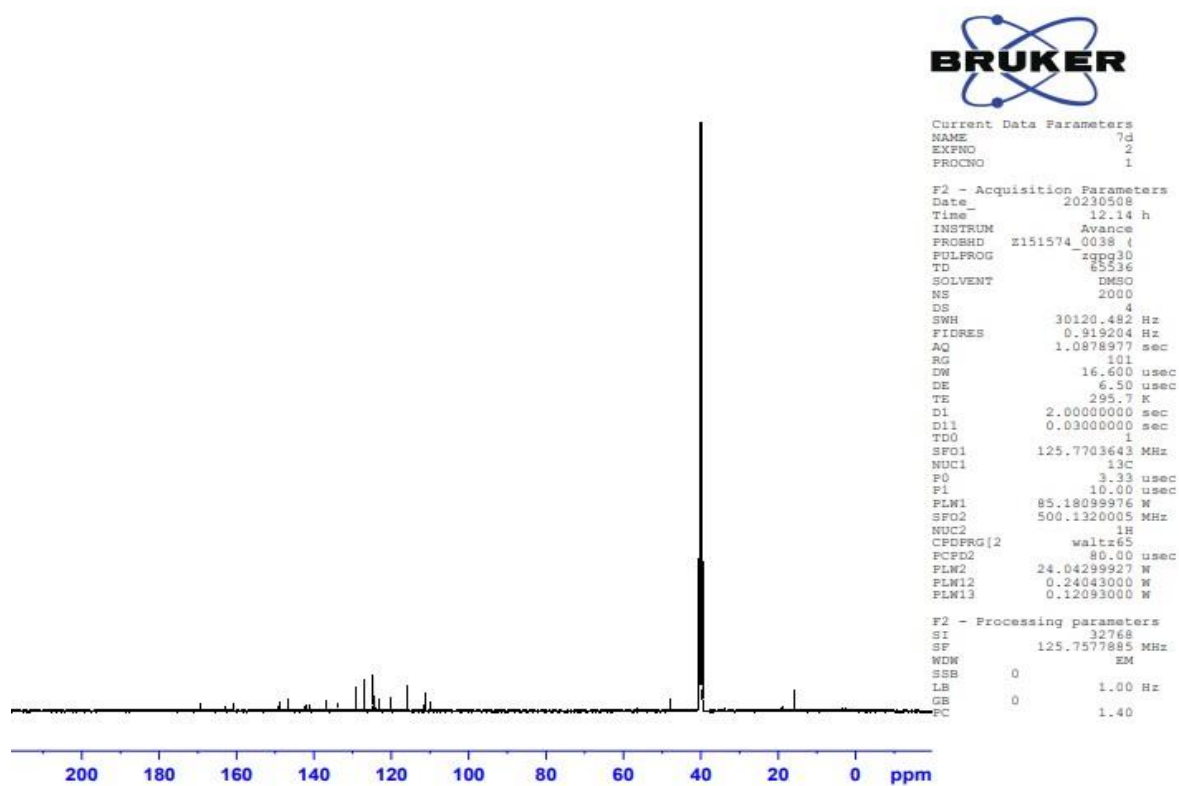


Figure S1-48. ¹³C-NMR spectrum of compound 7d

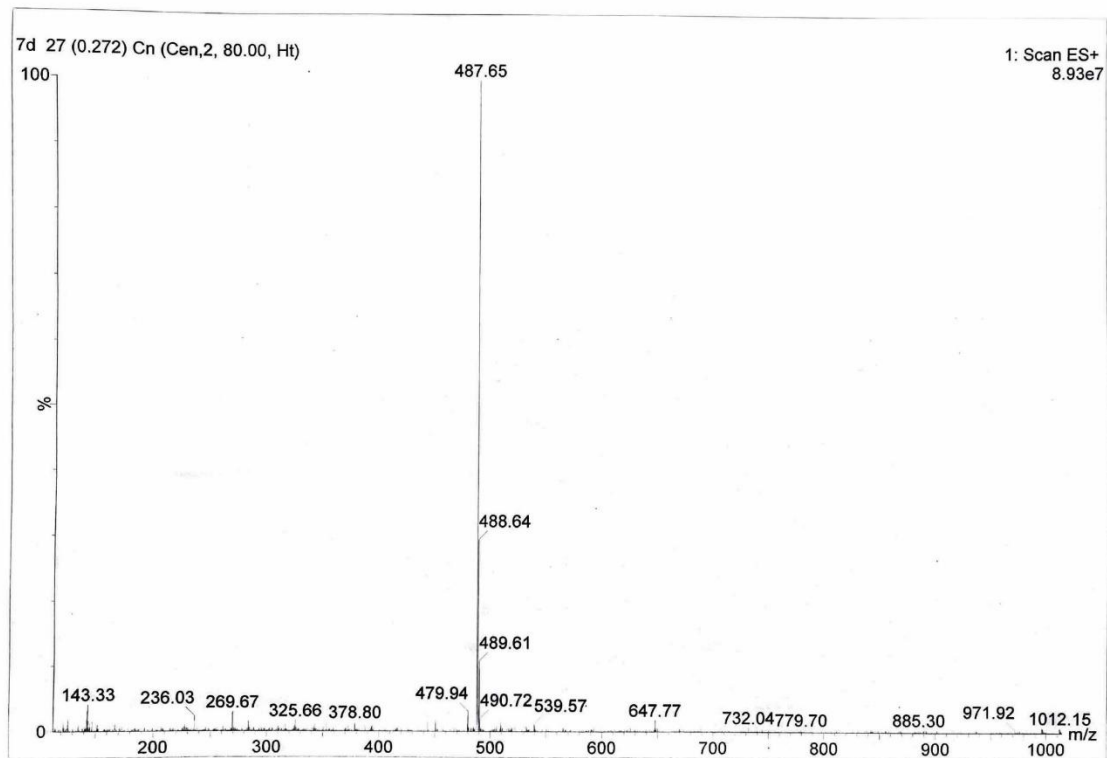


Figure S1-49. Mass spectrum of compound 7d

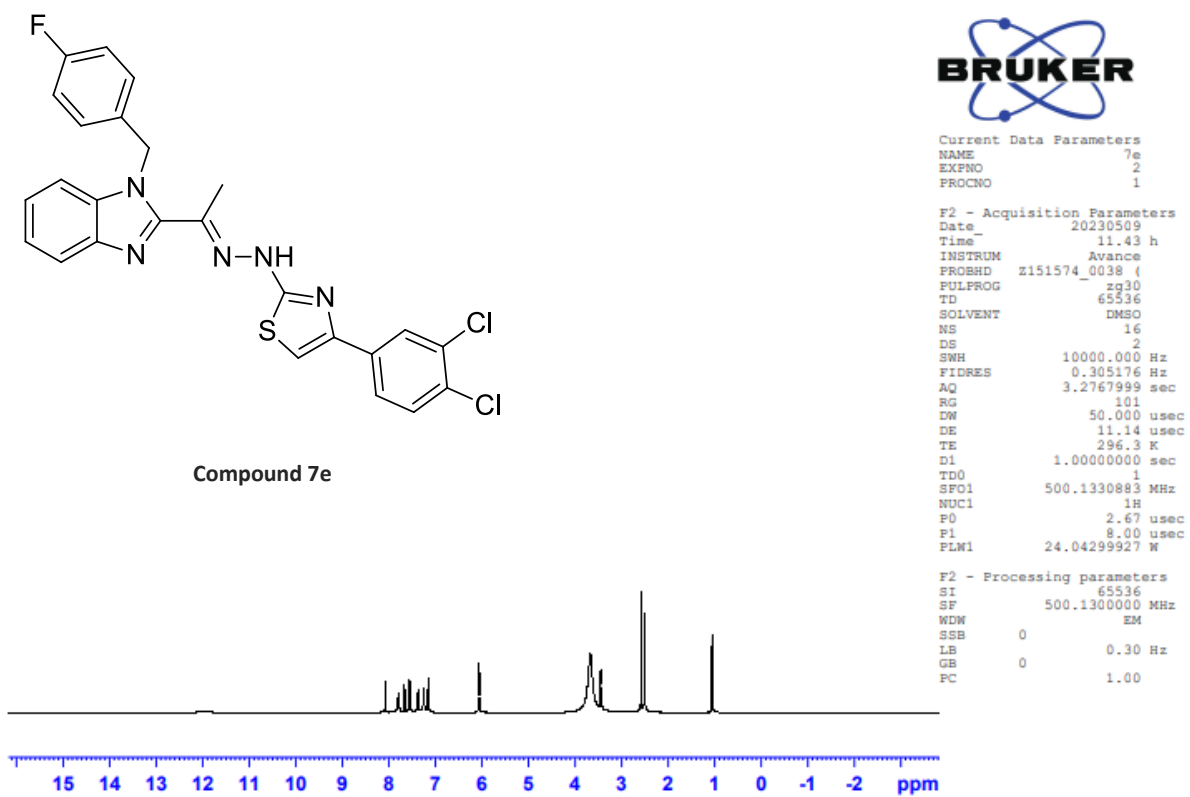


Figure S1-50. ¹H-NMR spectrum of compound 7e-1

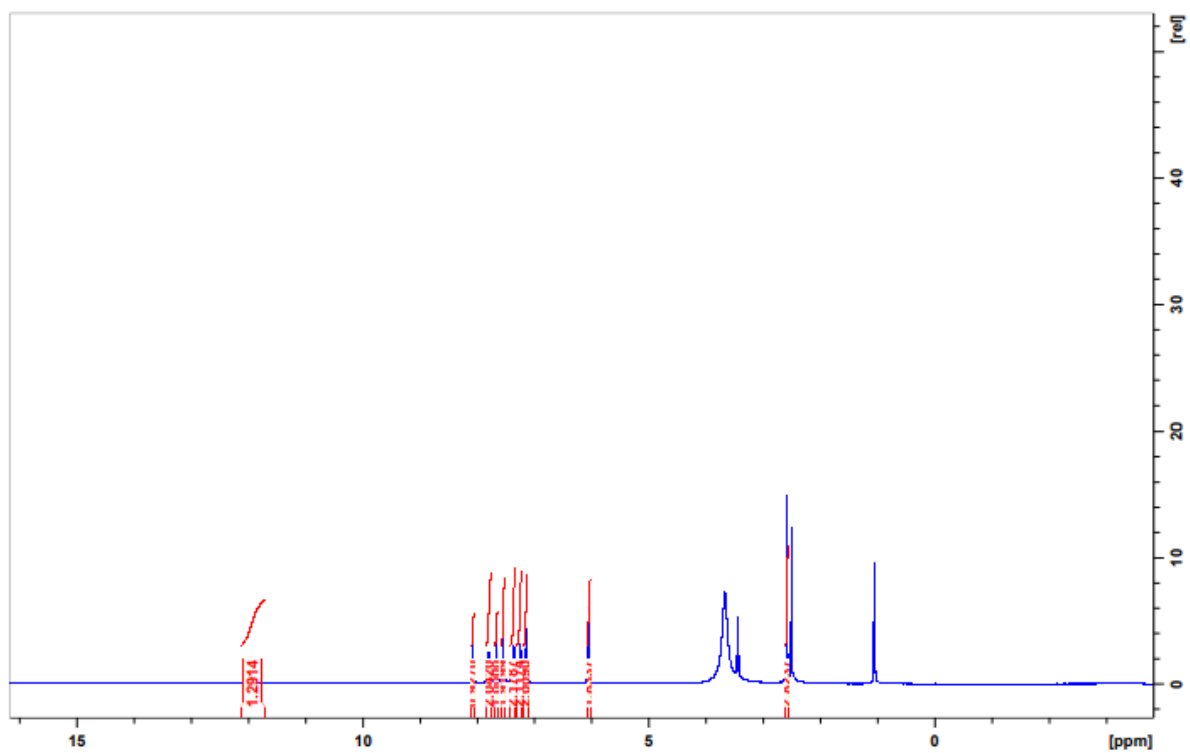


Figure S1-51. ¹H-NMR spectrum of compound 7e-2

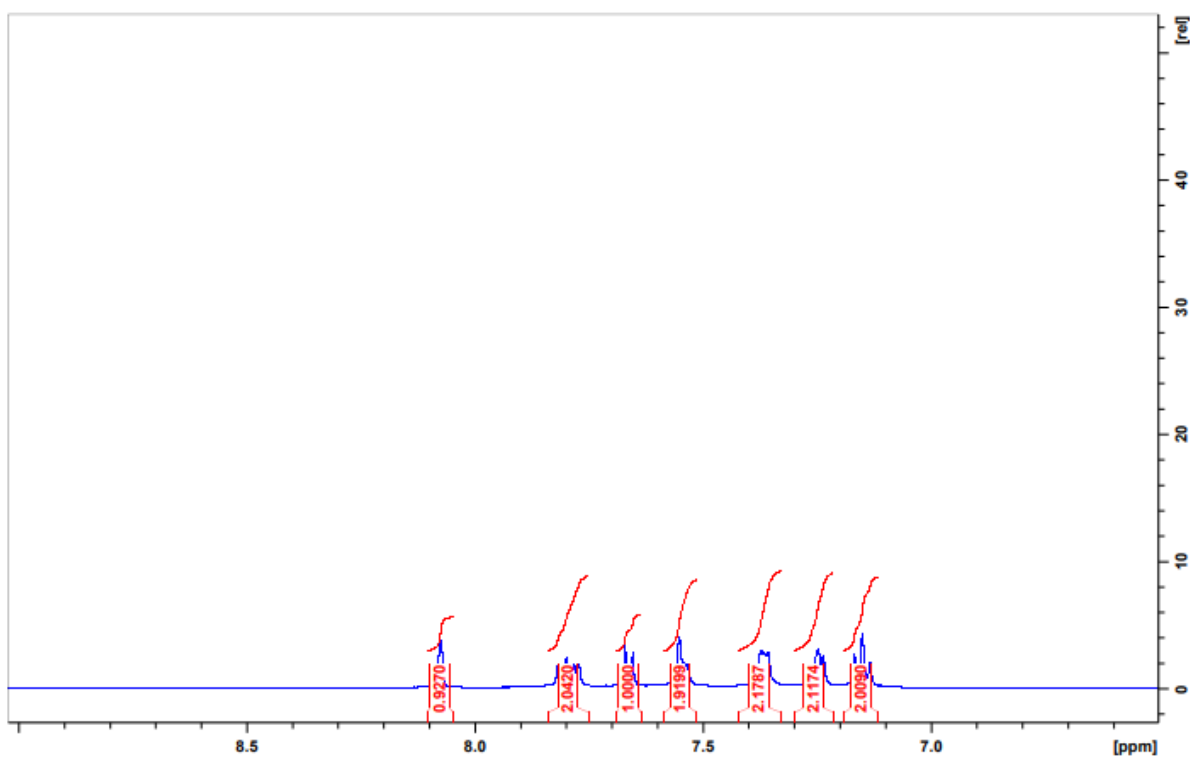


Figure S1-52. ¹H-NMR spectrum of compound 7e-3

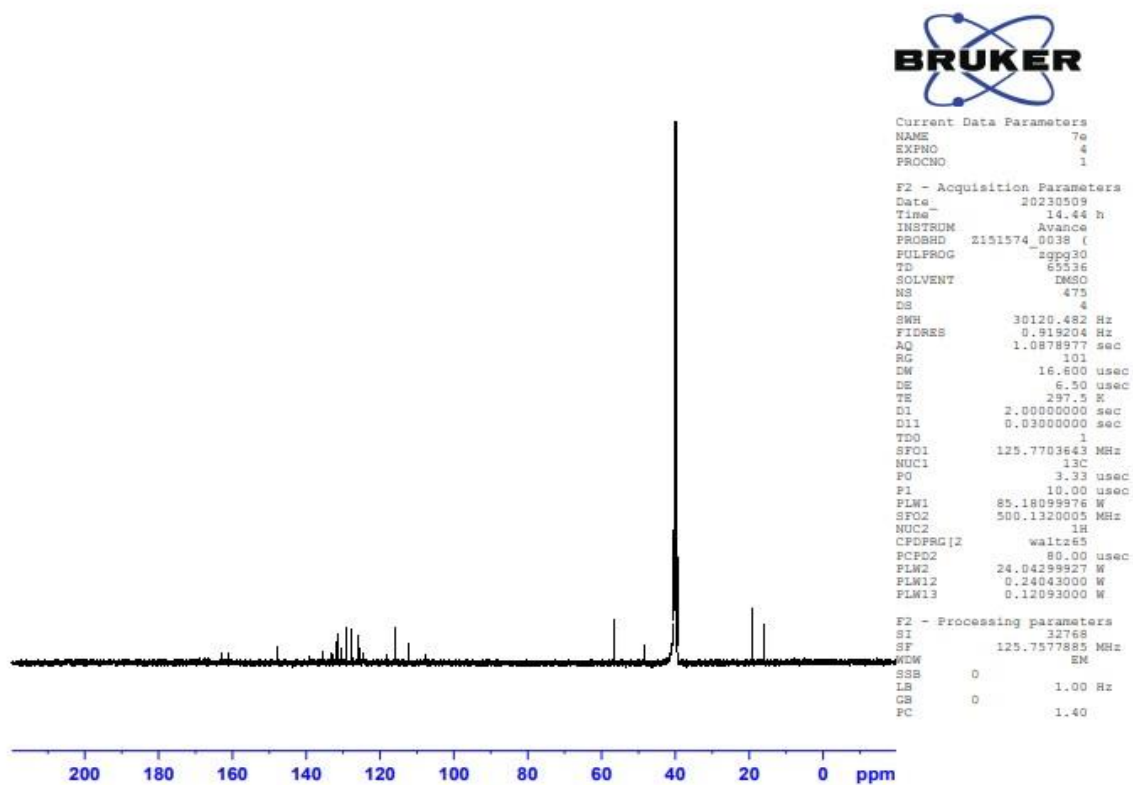


Figure S1-53. ^{13}C -NMR spectrum of compound 7e

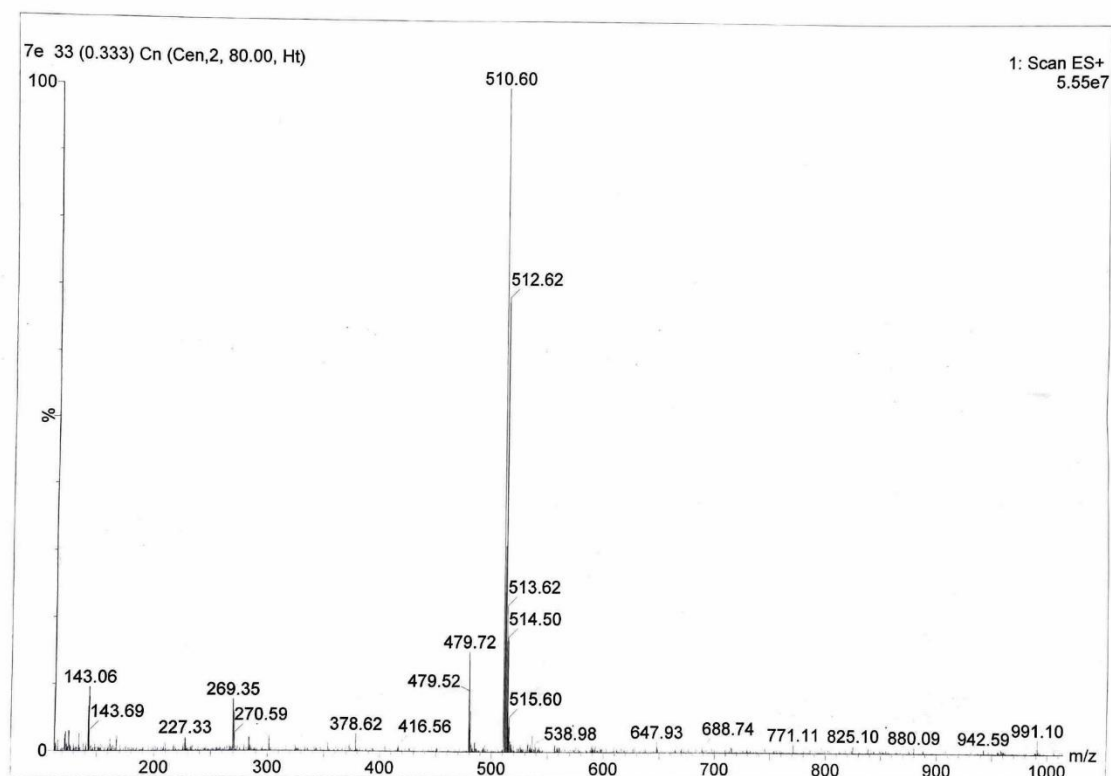
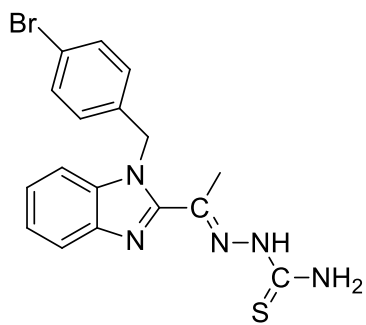


Figure S1-54. Mass spectrum of compound 7e



Compound 8



```

Current Data Parameters
NAME          8
EXPNO        4
PROCNO       1

F2 - Acquisition Parameters
Date_         20230517
Time_        14.14 h
INSTRUM      Avance
PROBHD       Z151574_0038 (
PULPROG      zg30
TD           65536
SOLVENT      DMSO
NS           16
DS           2
SWH          10000.000 Hz
FIDRES       0.305176 Hz
AQ           3.2767999 sec
RG           101
DW           50.000 usec
DE           11.14 usec
TE           295.4 K
D1           1.0000000 sec
TDO          1
SF01         500.1330883 MHz
NUC1         1H
P0           2.67 usec
P1           8.00 usec
PLW1         24.04299927 W

F2 - Processing parameters
SI           65536
SF           500.1300000 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```

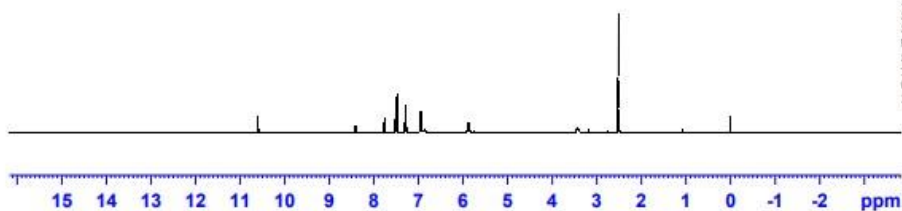


Figure S1-55. ¹H-NMR spectrum of compound 8-1

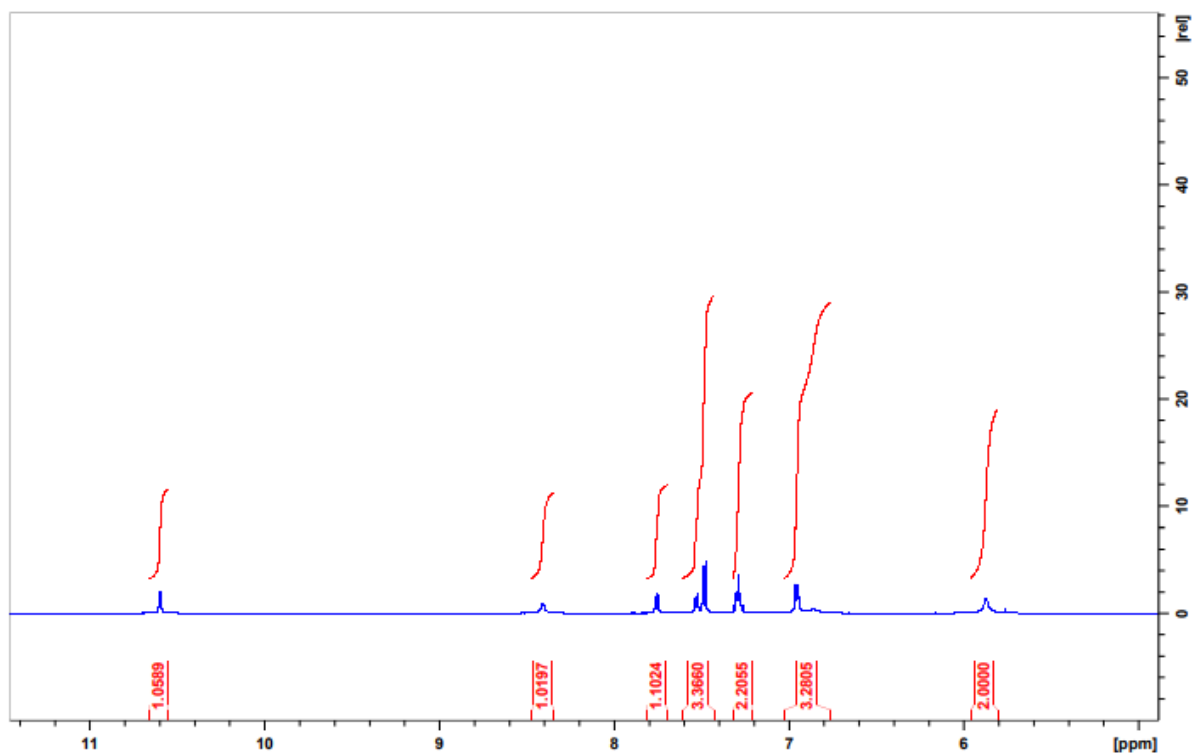


Figure S1-56. ¹H-NMR spectrum of compound 8-2



Current Data Parameters
NAME 8
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230517
Time 13.38 h
INSTRUM Avance
PROBHD z151574_0038 (4
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1225
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
FO 3.33 usec
P1 10.00 usec
PLW1 85.18099976 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 24.04299927 W
PLW12 0.24043000 W
PLW13 0.12093000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

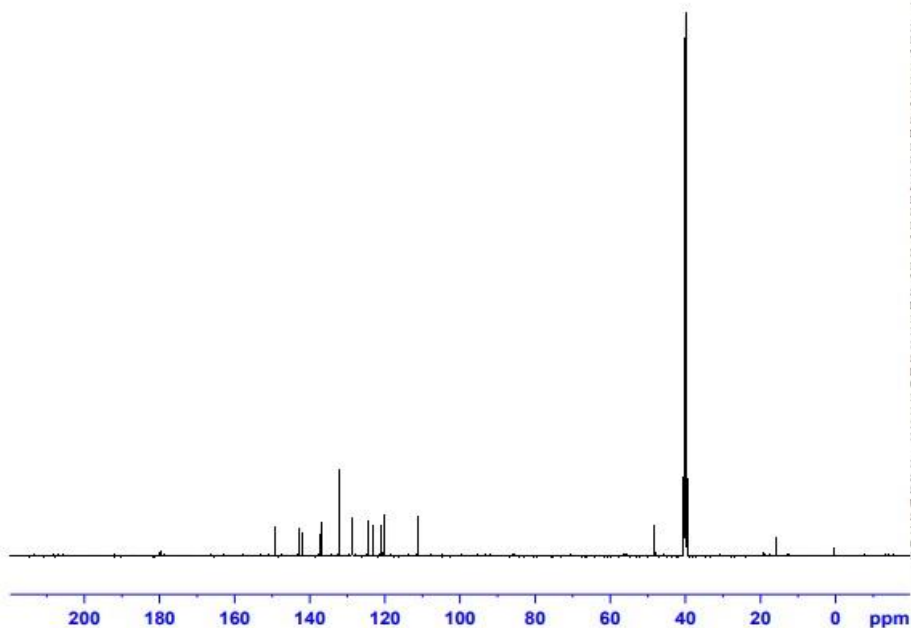


Figure S1-57. ¹³C-NMR spectrum of compound 8

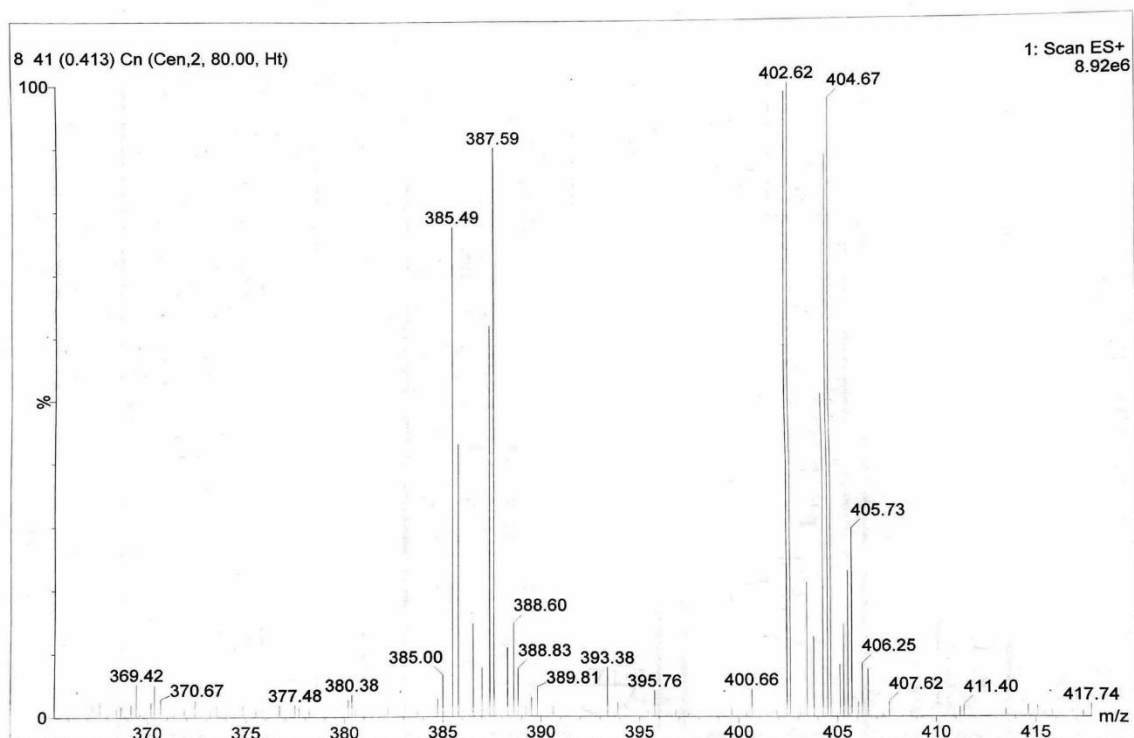
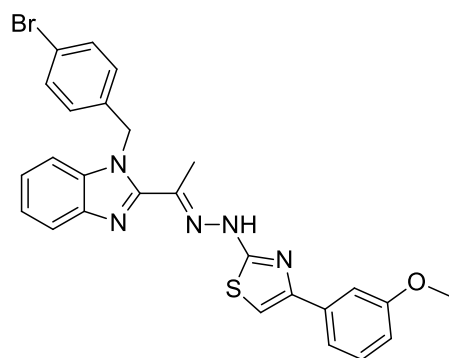


Figure S1-58. Mass spectrum of compound 8



Compound 8a



```

Current Data Parameters
NAME          8a
EXPNO        2
PROCNO       1

F2 - Acquisition Parameters
Date_        20230508
Time         16.21 h
INSTRUM      Avance
PROBHD       z151574_0038 (
FULPROG      zg30
TD           65536
SOLVENT      DMSO
NS           16
DS           2
SWH          10000.000 Hz
FIDRES       0.305176 Hz
AQ           3.2767999 sec
RG           101
DM           50.000 usec
DE           11.14 usec
TE           295.4 K
D1           1.0000000 sec
TD0          1
SFO1         500.1330883 MHz
NUC1         1H
P0           2.67 usec
F1           8.00 usec
FLM1         24.04299927 W

F2 - Processing parameters
SI           65536
SF           500.1300000 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
FC           1.00
  
```

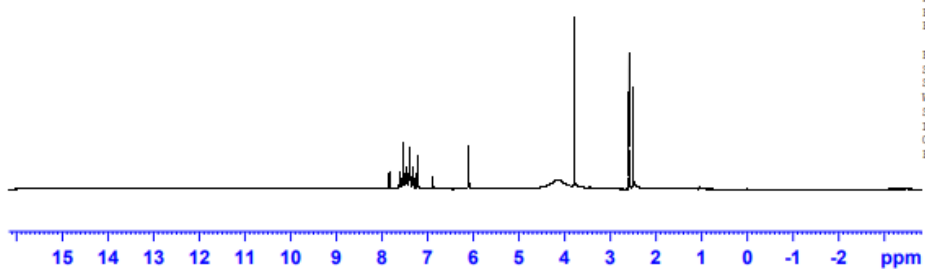


Figure S1-59. ¹H-NMR spectrum of compound 8a-1

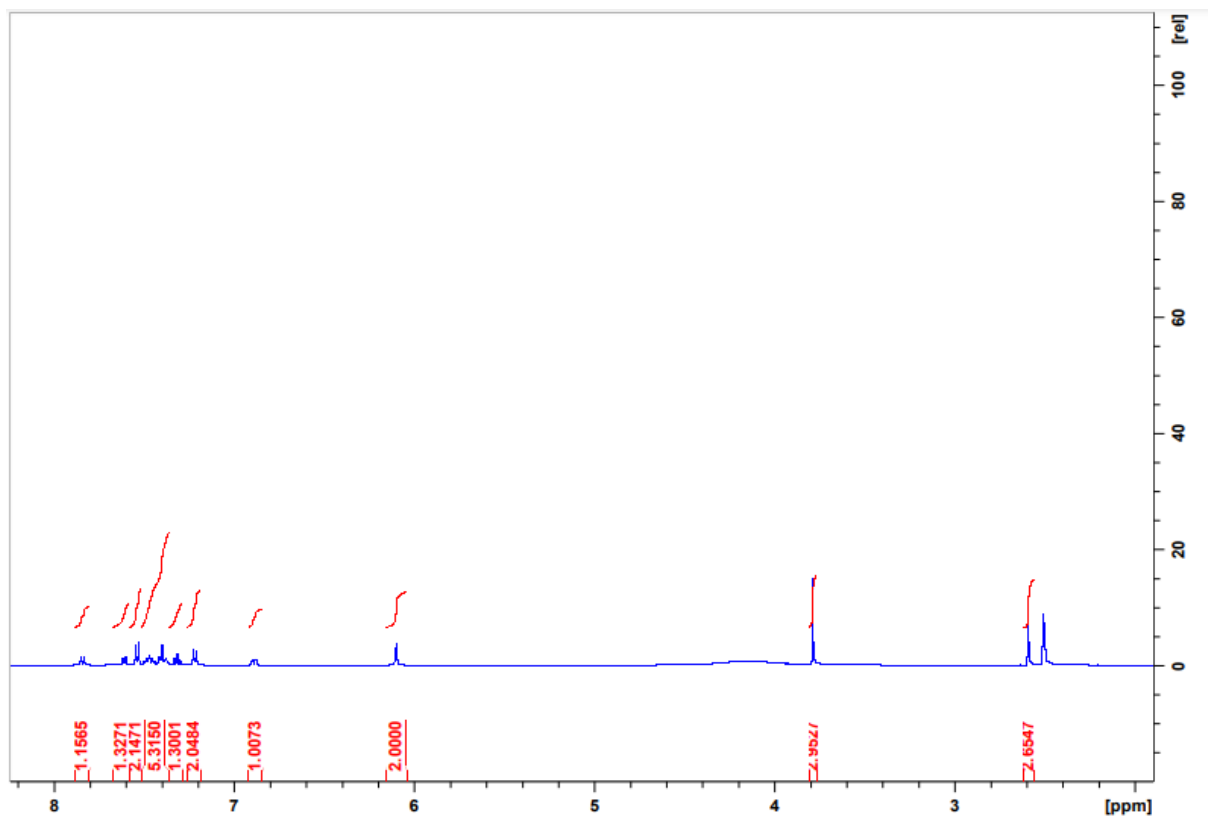


Figure S1-60. ¹H-NMR spectrum of compound 8a-2



Current Data Parameters
NAME 8a
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230508
Time_ 18.45 h
INSTRUM Avance
PROBHD Z151574_0038 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2500
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 6.50 usec
TE 303.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
PO 3.33 usec
P1 10.00 usec
PLW1 85.18099976 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 24.04299927 W
PLW12 0.24043000 W
PLW13 0.12093000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SBB 0
LB 1.00 Hz
GB 0
PC 1.40

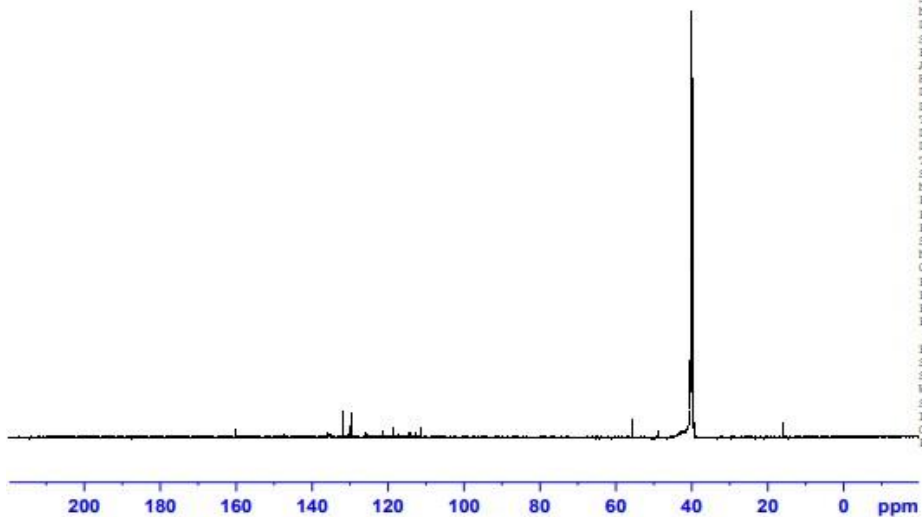


Figure S1-61. ¹³C-NMR spectrum of compound 8a

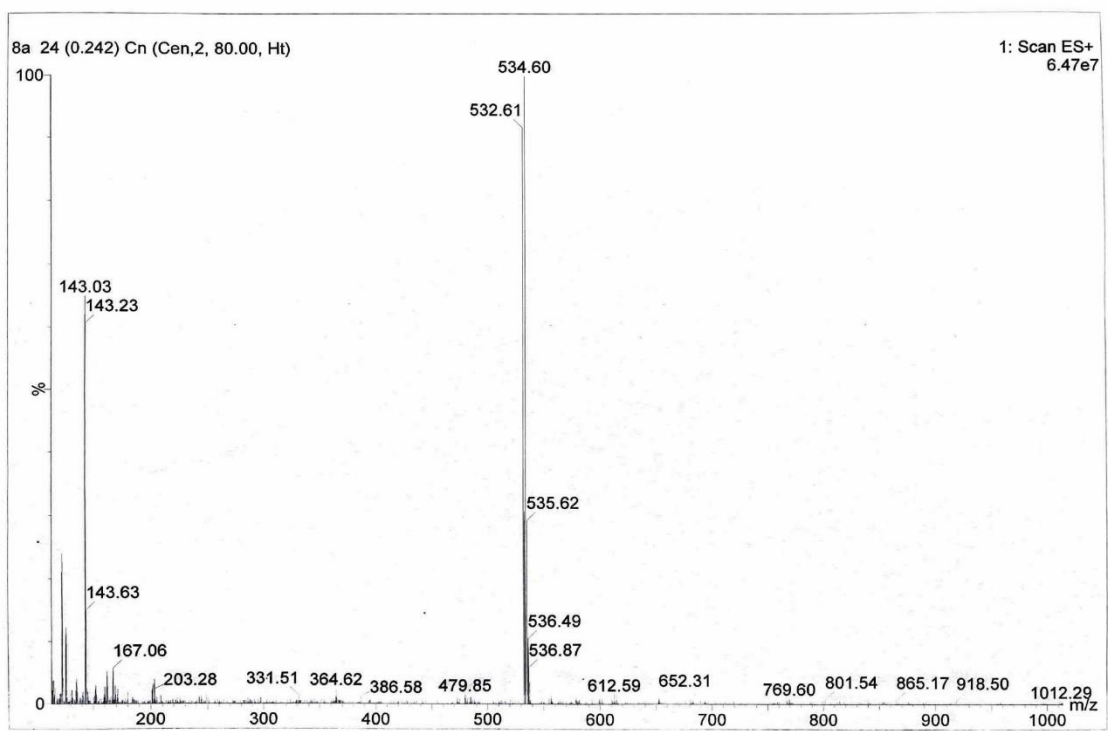


Figure S1-62. Mass spectrum of compound 8a

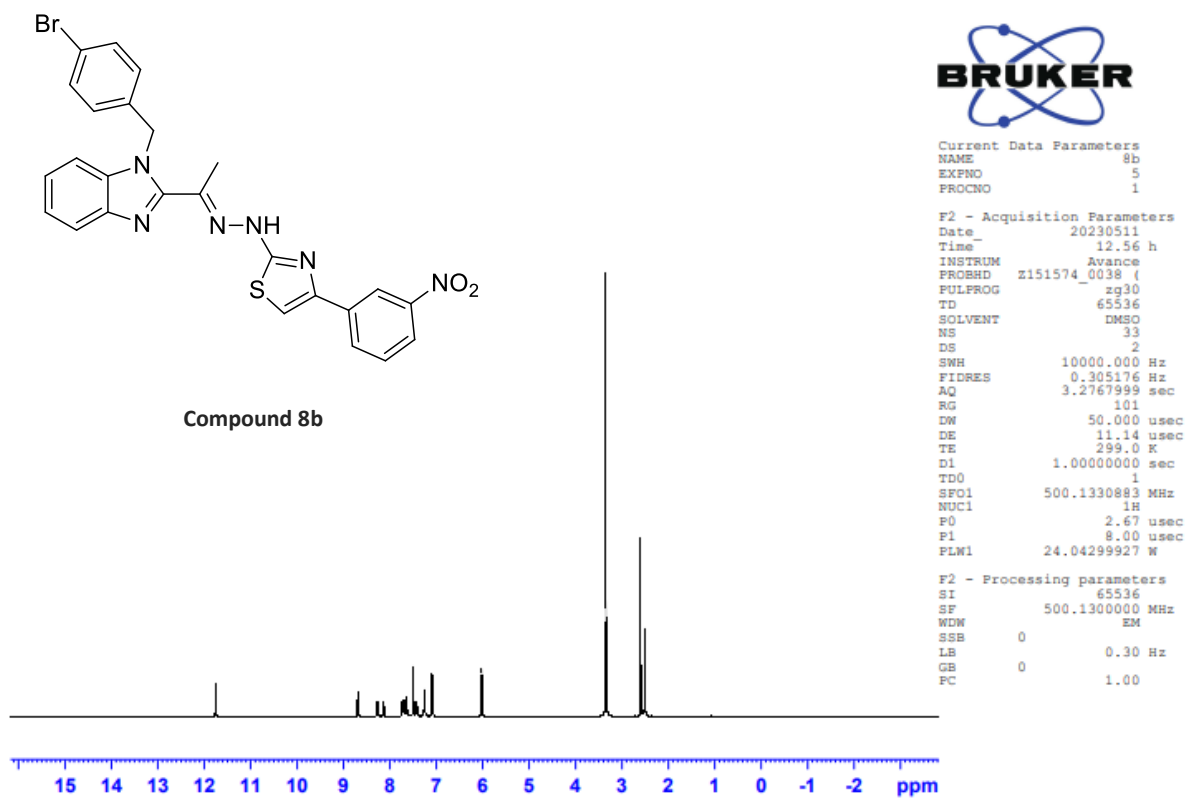


Figure S1-63. ¹H-NMR spectrum of compound 8b-1

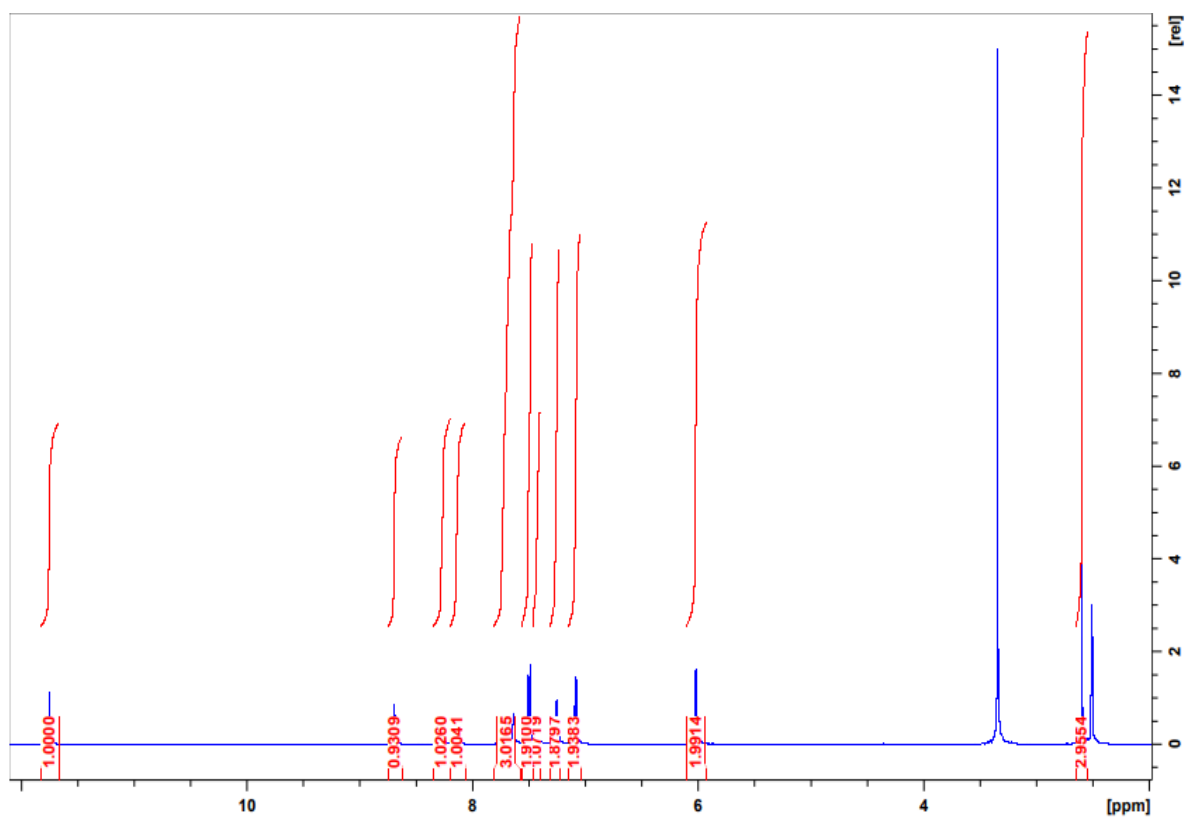


Figure S1-64. ¹H-NMR spectrum of compound 8b-2

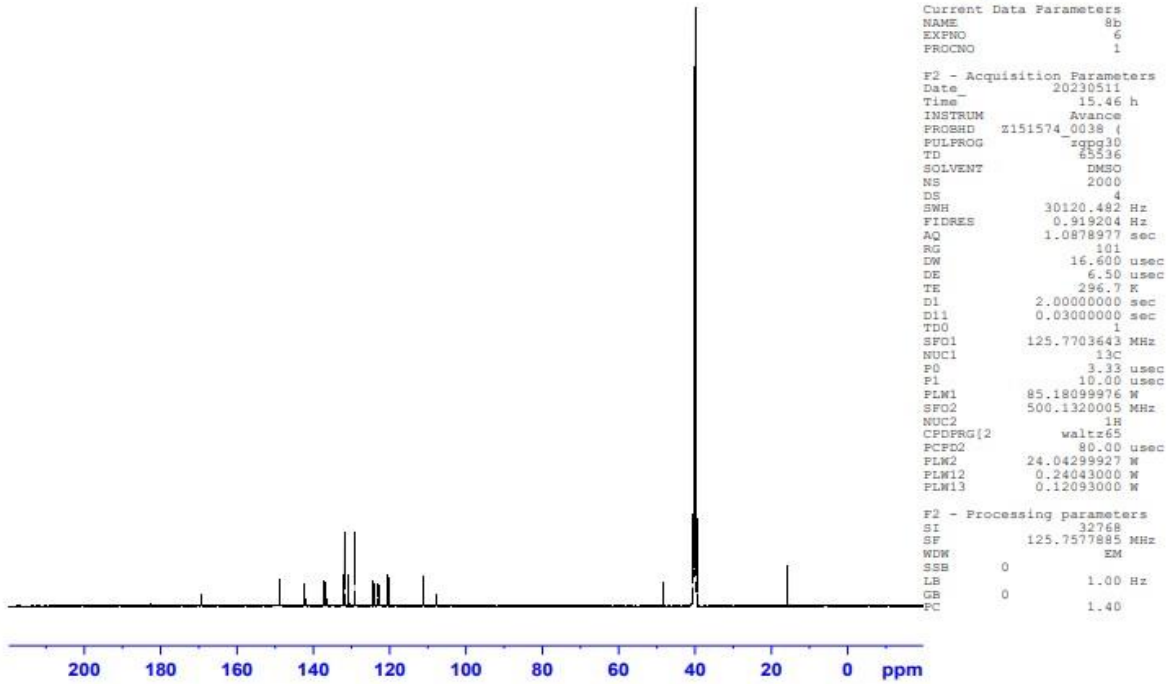


Figure S1-65. ¹³C-NMR spectrum of compound 8b

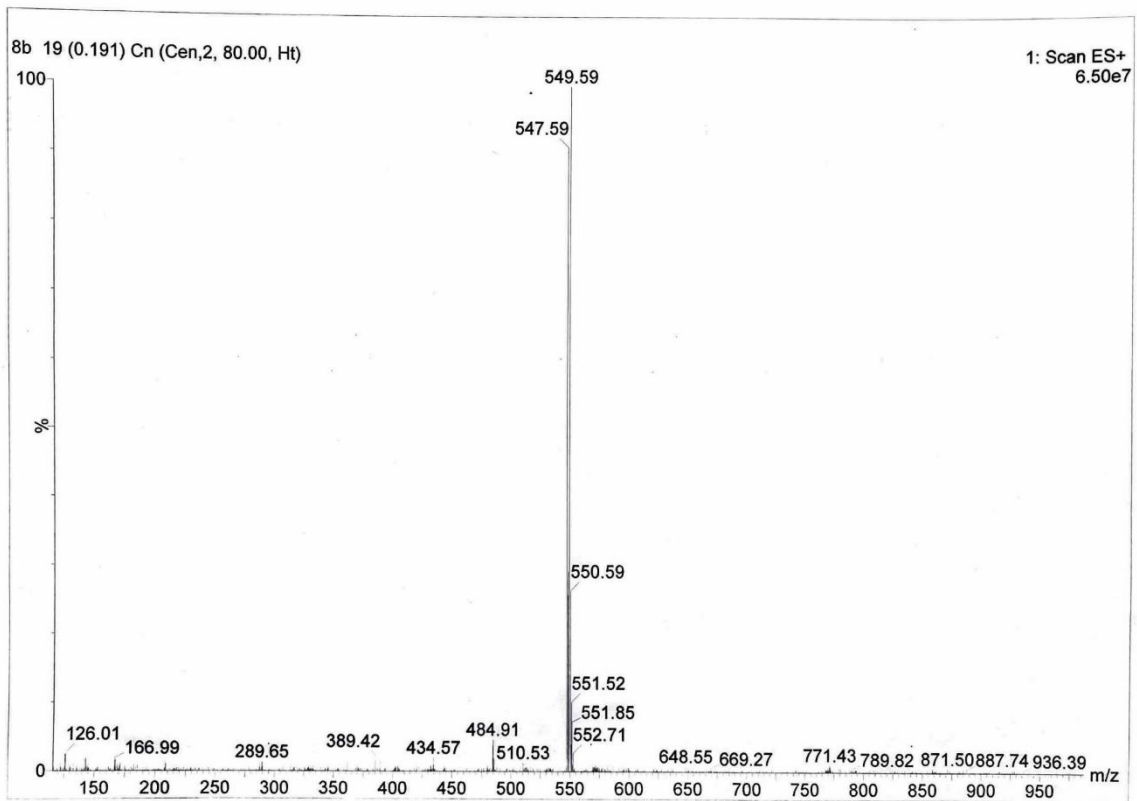
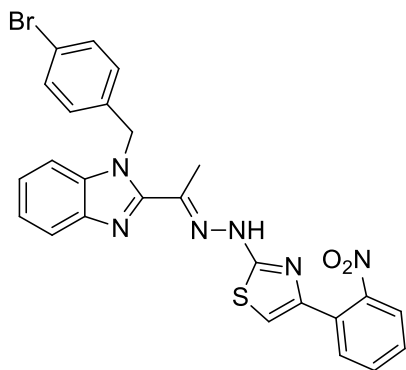


Figure S1-66. Mass spectrum of compound 8b



Compound 8c



```

Current Data Parameters
NAME      8c
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20230511
Time     15.53 h
INSTRUM  Avance
PROBHD   z151574_0038 (
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      10000.000 Hz
FIDRES   0.305176 Hz
AQ       3.2767999 sec
RG       101
MW       50.000 usec
DE       11.14 usec
TE       295.7 K
D1       1.00000000 sec
TD0      1
SFO1     500.1330883 MHz
NUC1     1H
P0       2.67 usec
P1       8.00 usec
PLW1     24.04299927 W

F2 - Processing parameters
SI       65536
SF       500.1300000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```

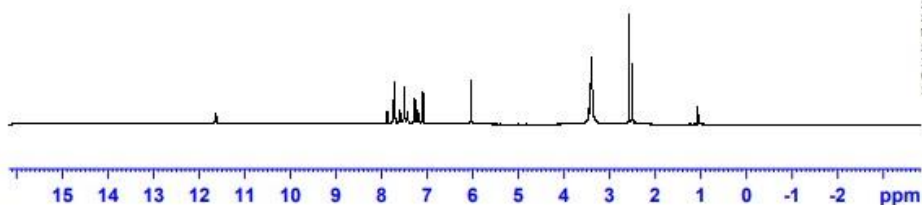


Figure S1-67. ¹H-NMR spectrum of compound 8c-1

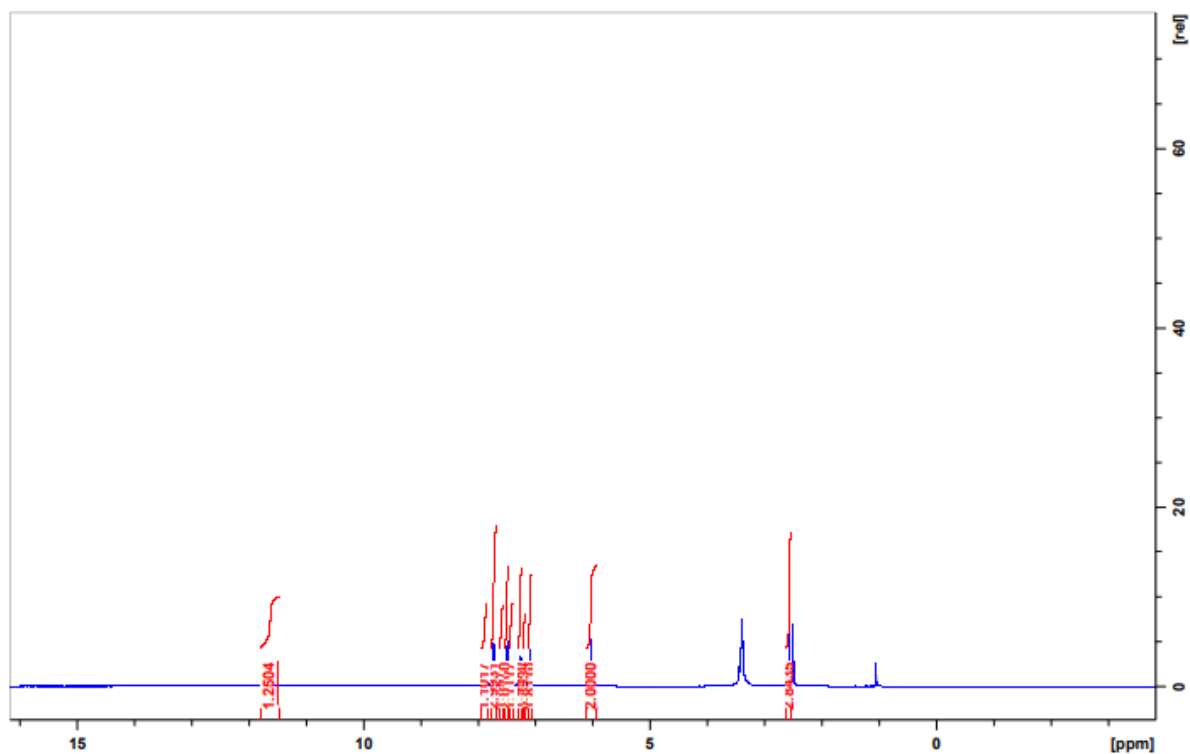


Figure S1-68. ¹H-NMR spectrum of compound 8c-2

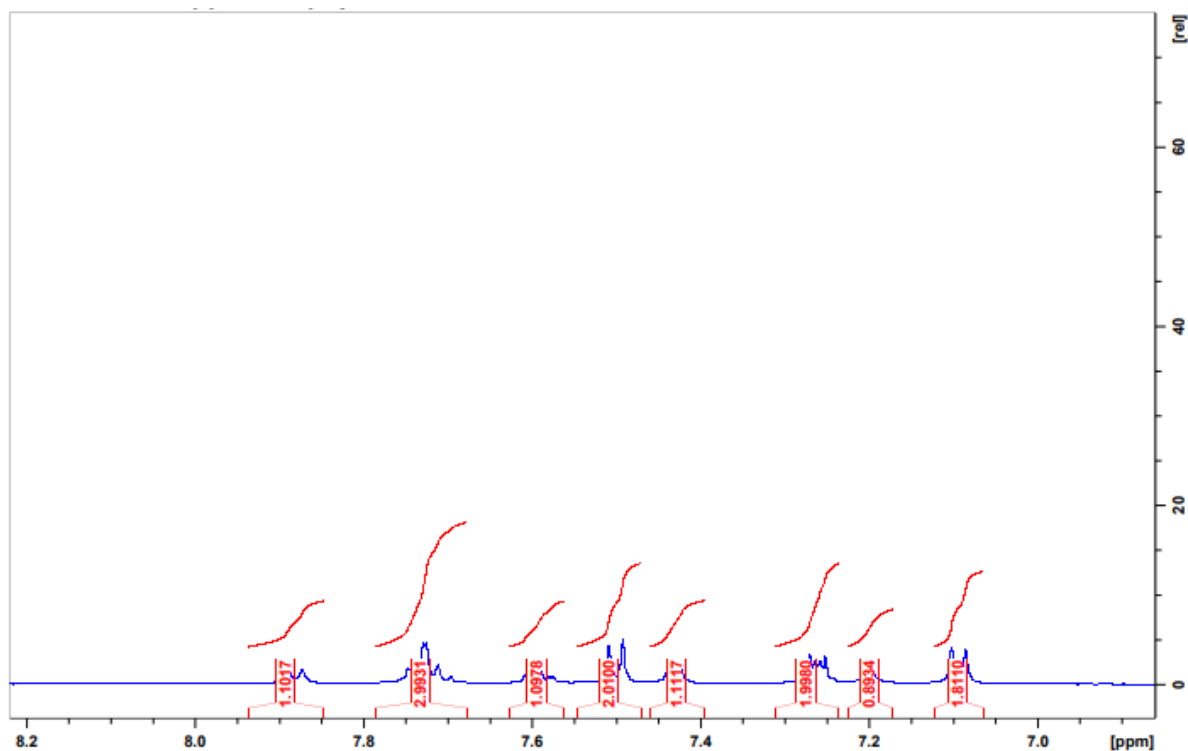


Figure S1-69. ^1H -NMR spectrum of compound **8c-3**

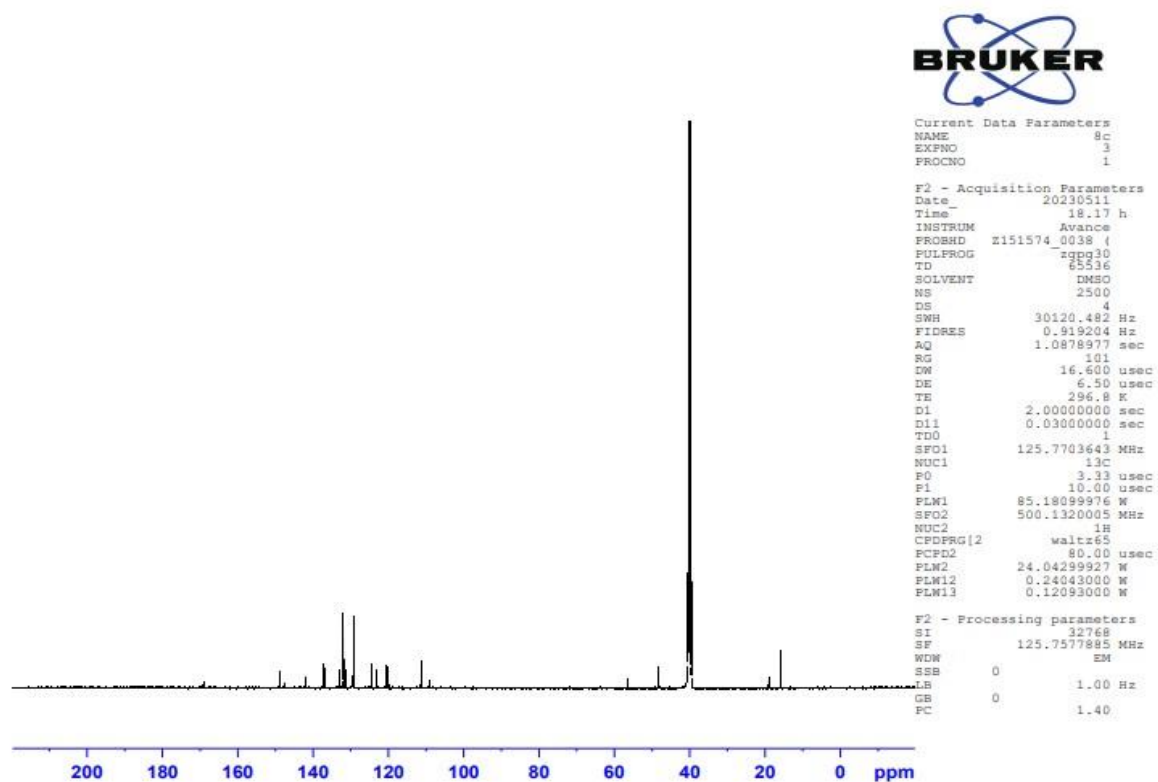


Figure S1-70. ^{13}C -NMR spectrum of compound **8c**

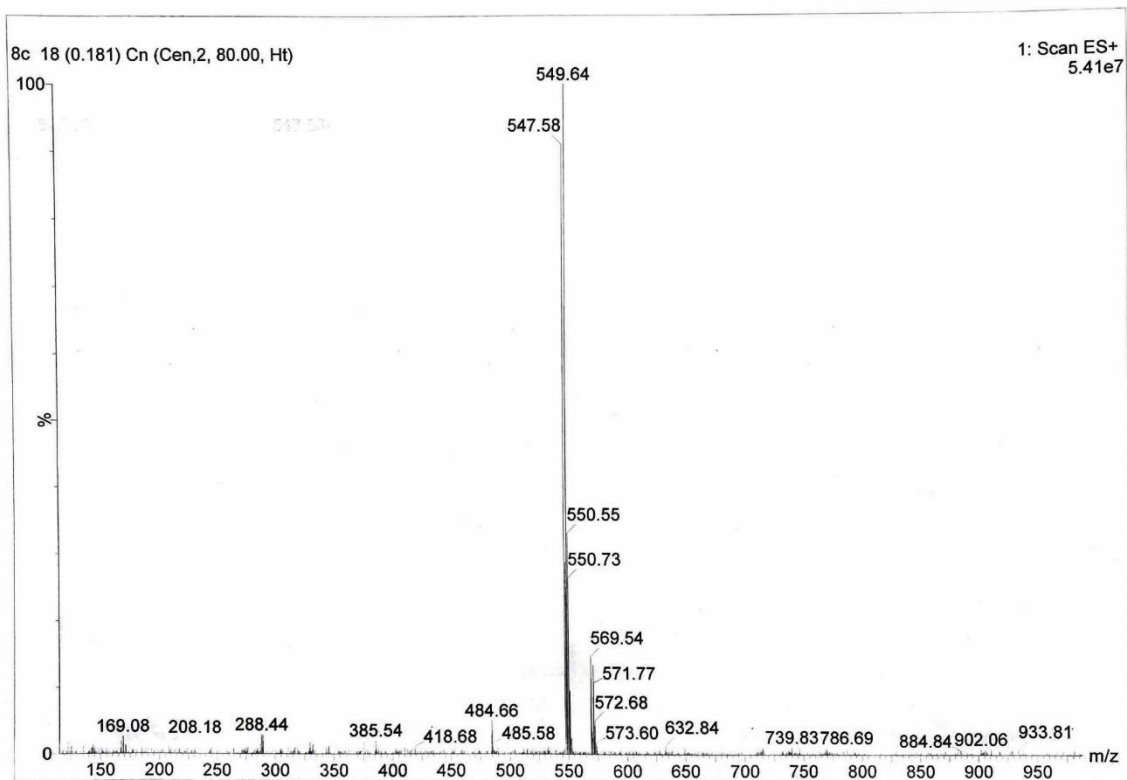


Figure S1-71. Mass spectrum of compound 8c

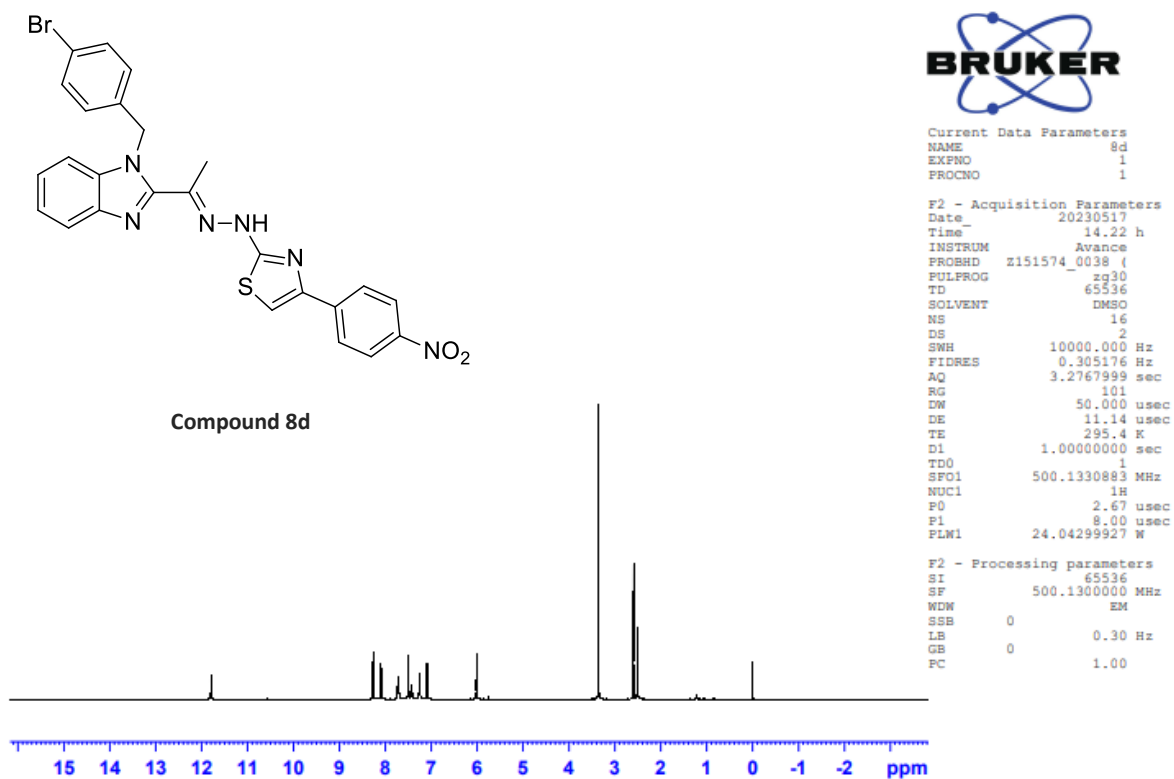


Figure S1-72. $^1\text{H-NMR}$ spectrum of compound 8d-1

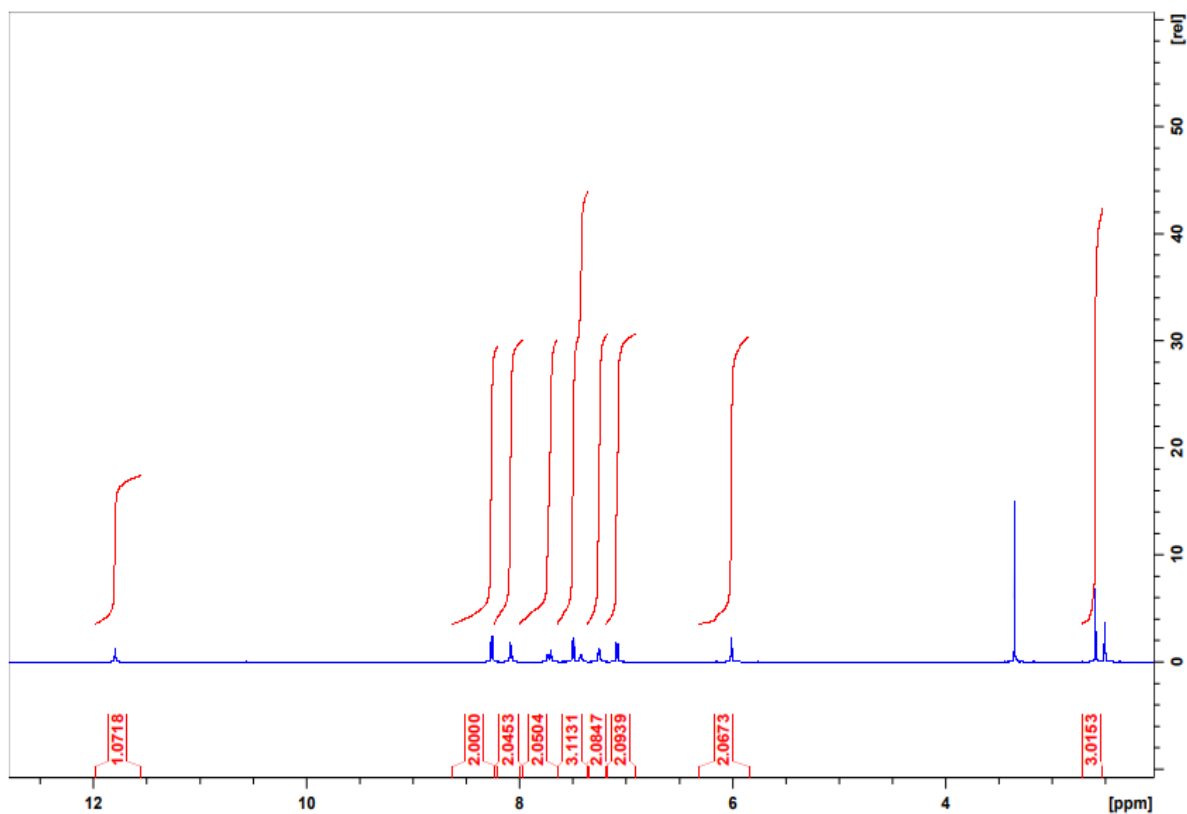


Figure S1-73. ¹H-NMR spectrum of compound 8d-2

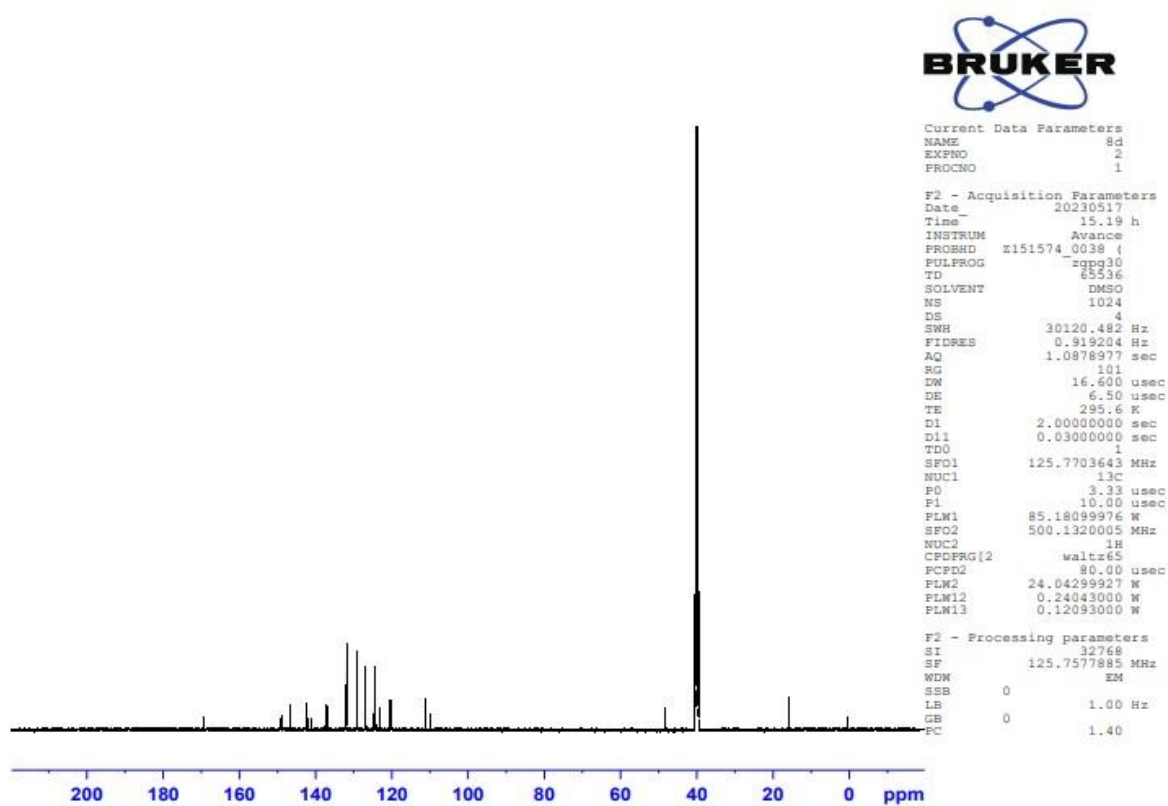


Figure S1-74. ¹³C-NMR spectrum of compound 8d

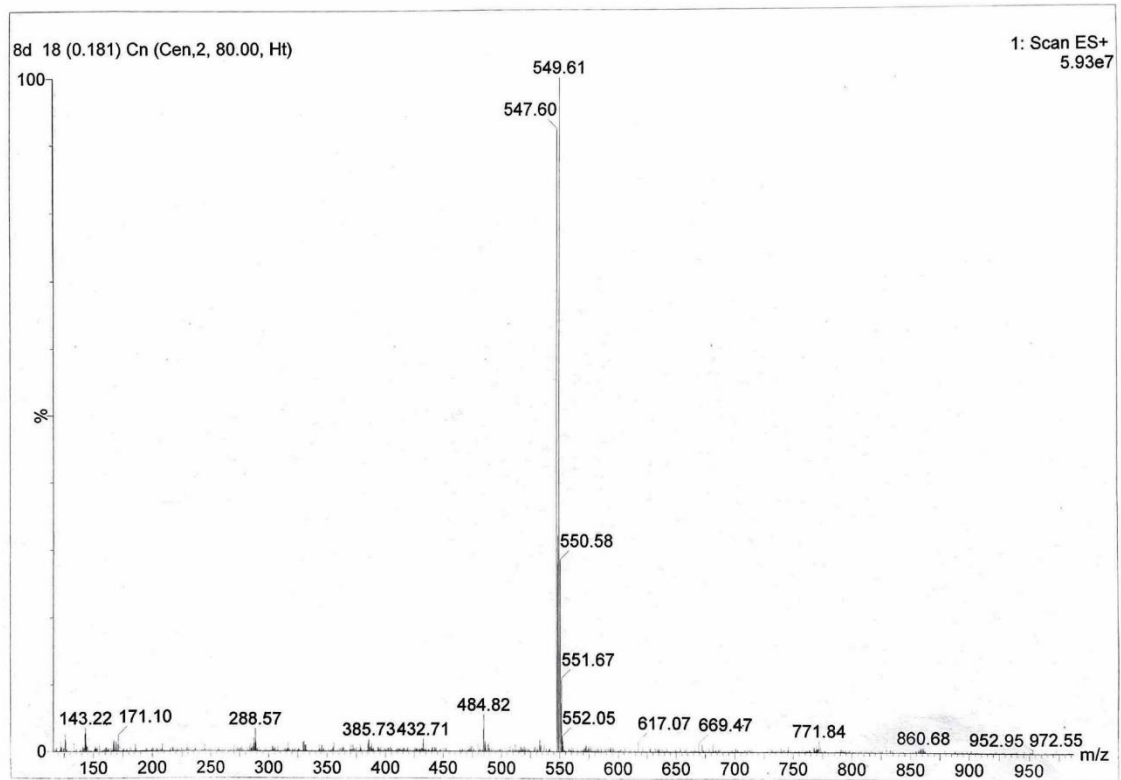
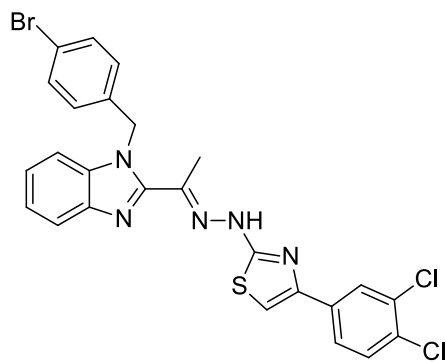


Figure S1-75. Mass spectrum of compound **8d**



Compound **8e**



Current Data Parameters
NAME 8e
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230508
Time 12.29 h
INSTRUM Avance
PROBHD z151574_0038 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 11.14 usec
TE 295.5 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330883 MHz
NUC1 1H
P0 2.67 usec
F1 0.00 usec
PLM1 24.04299927 W

F2 - Processing parameters
SI 65536
SF 500.1330000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

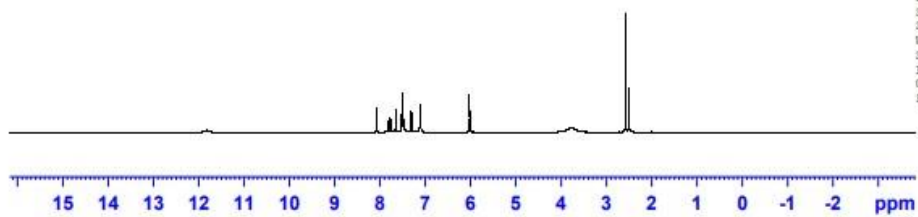


Figure S1-76. ¹H-NMR spectrum of compound **8e-1**

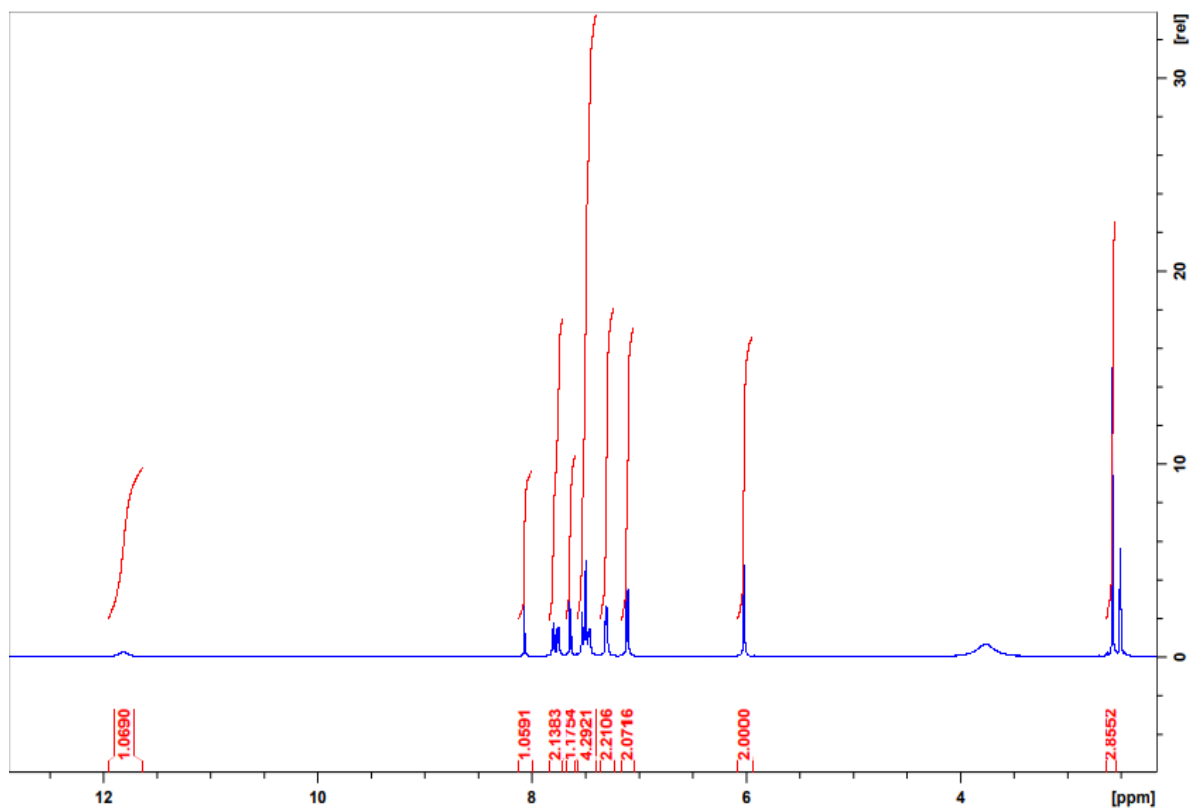


Figure S1-77. ^1H -NMR spectrum of compound **8e-2**

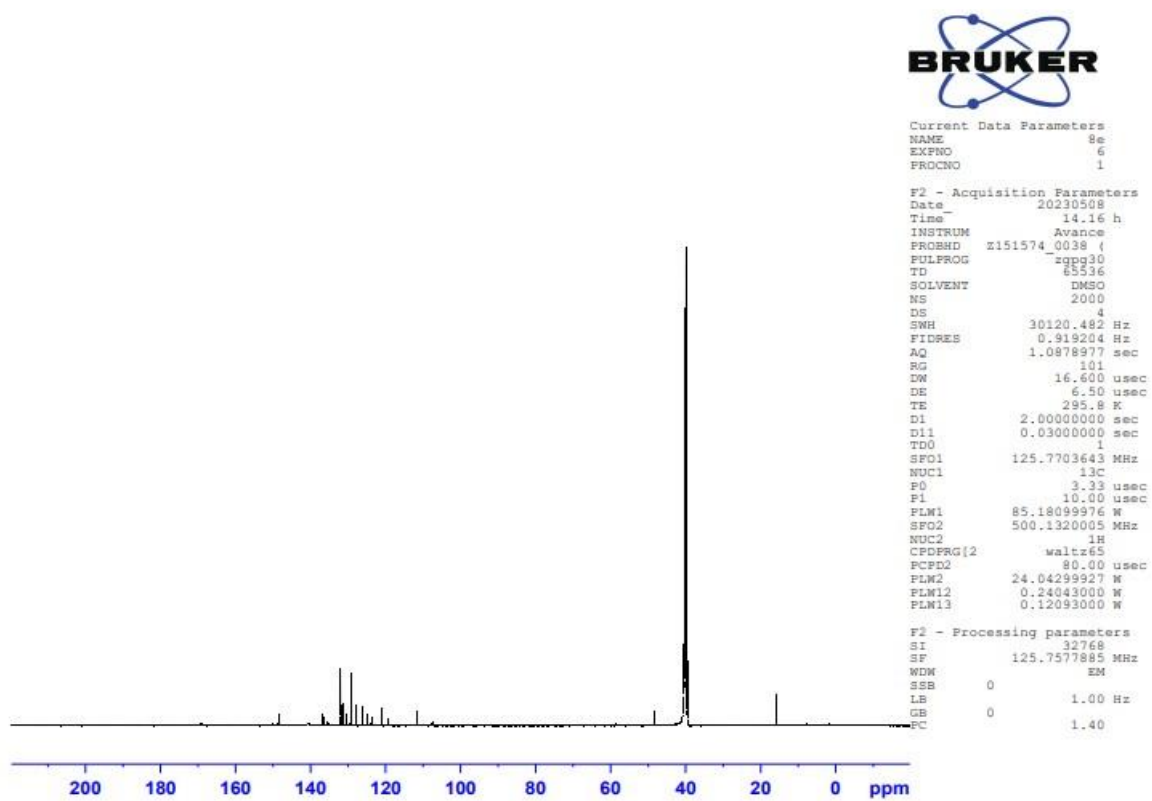


Figure S1-78. ^{13}C -NMR spectrum of compound **8e**

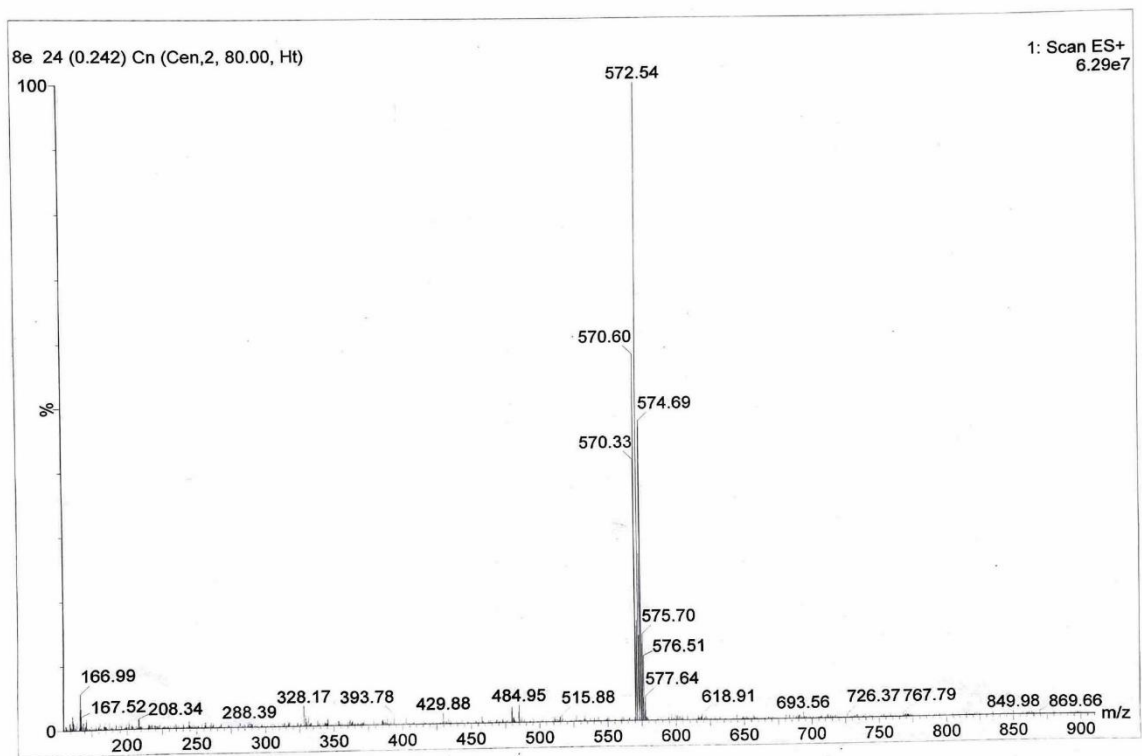


Figure S1-79. Mass spectrum of compound **8e**