

Synthesis and biological evaluation of novel pyrimidine amine derivatives bearing bicyclic monoterpene moieties

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Spectral Copies of HRMS, ¹H, ¹³C NMR Data Obtained in this Study

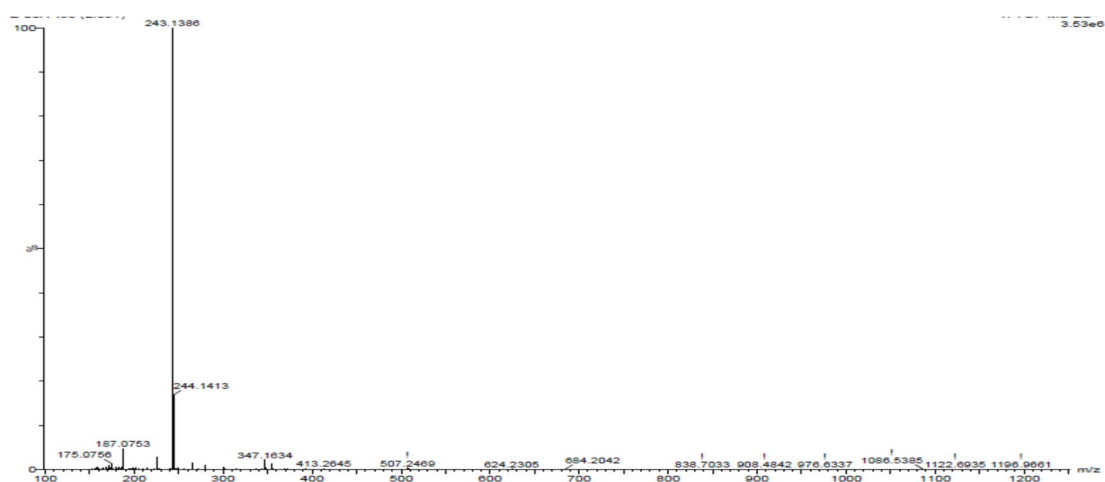


Figure S1. HRMS spectrum of compound 1a

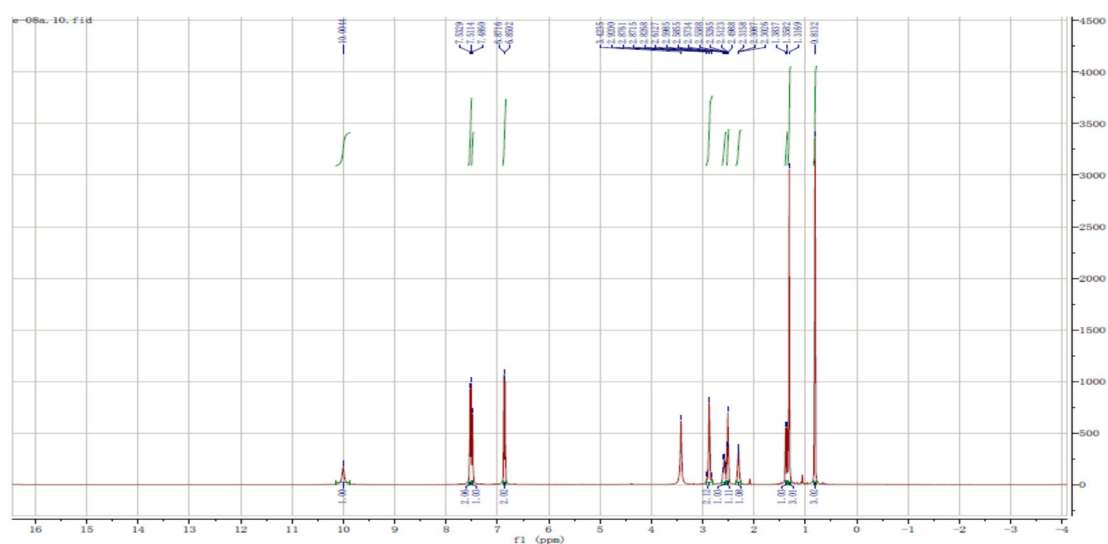


Figure S2. ¹H NMR spectrum of compound 1a

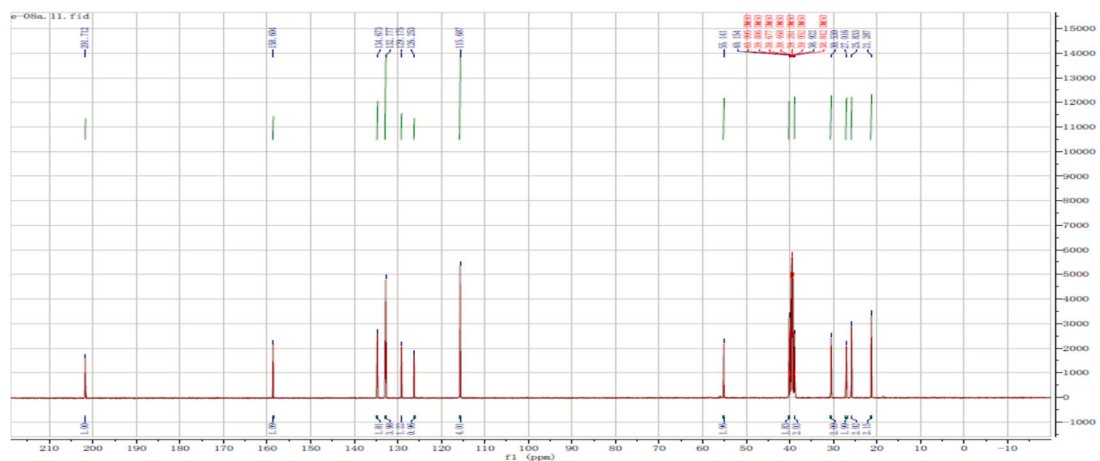


Figure S3. ¹³C NMR spectrum of compound **1a**

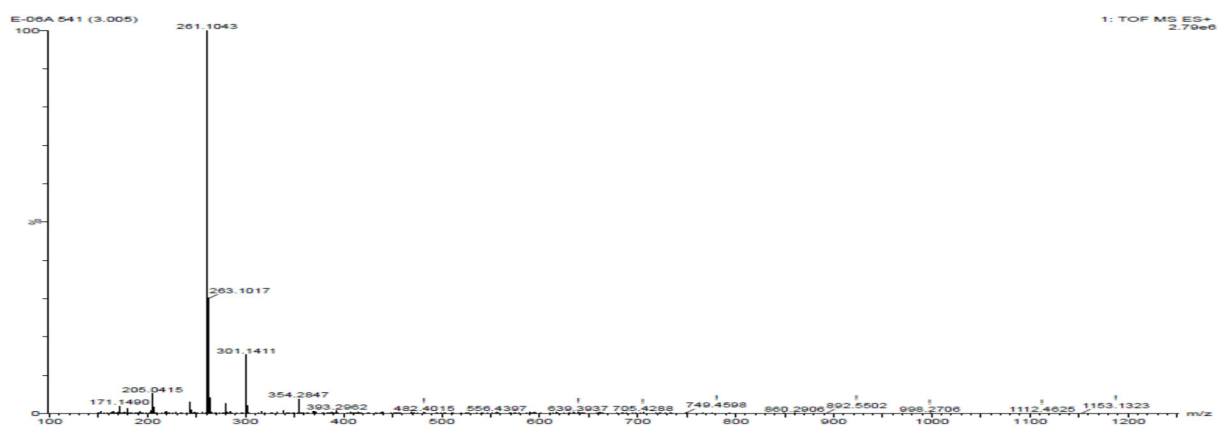


Figure S4. HRMS spectrum of compound **1b**

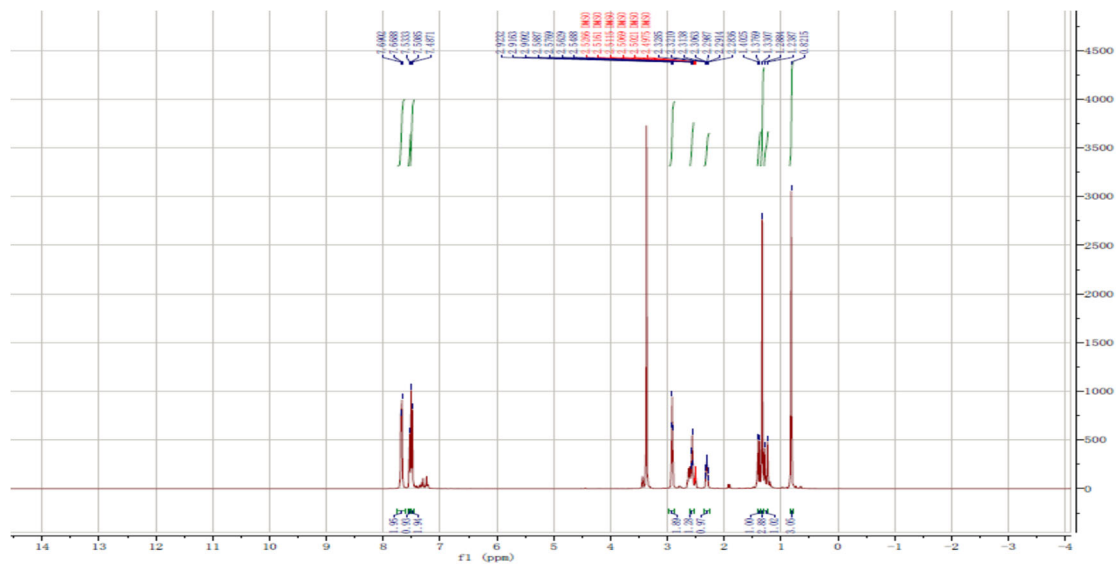


Figure S5. ¹H NMR spectrum of compound **1b**

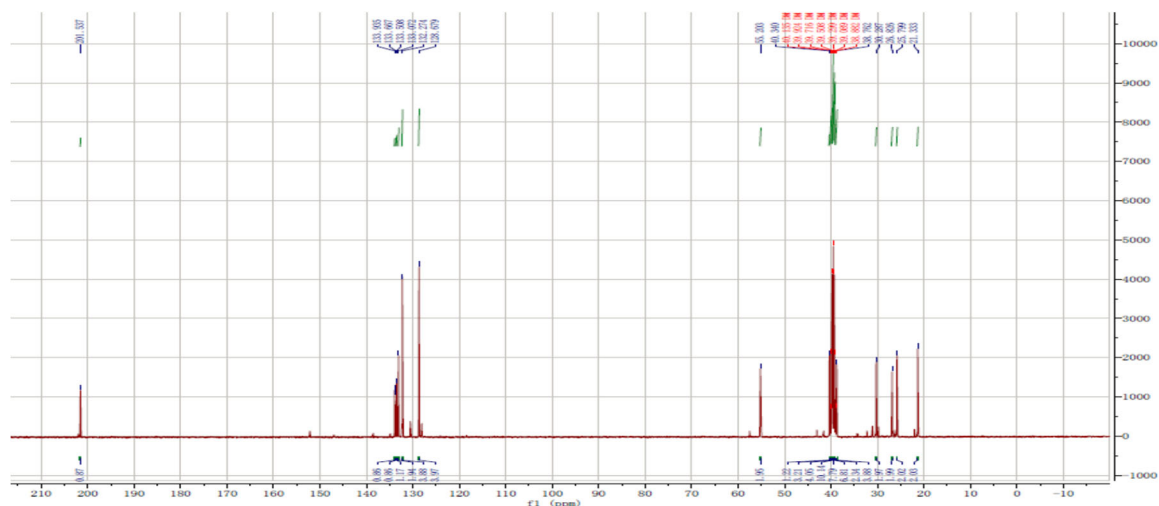


Figure S6. ¹³C NMR spectrum of compound **1b**

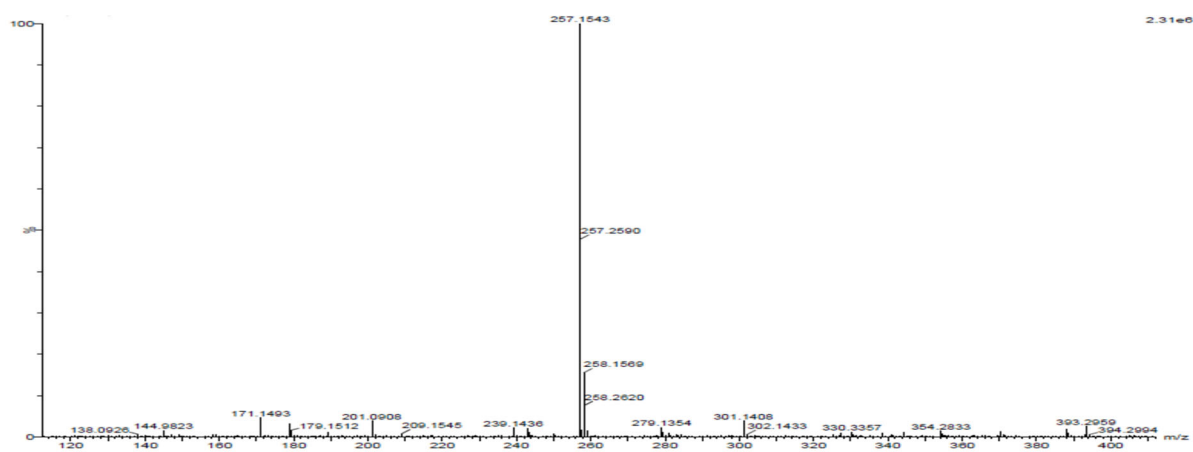


Figure S7. HRMS spectrum of compound **1c**

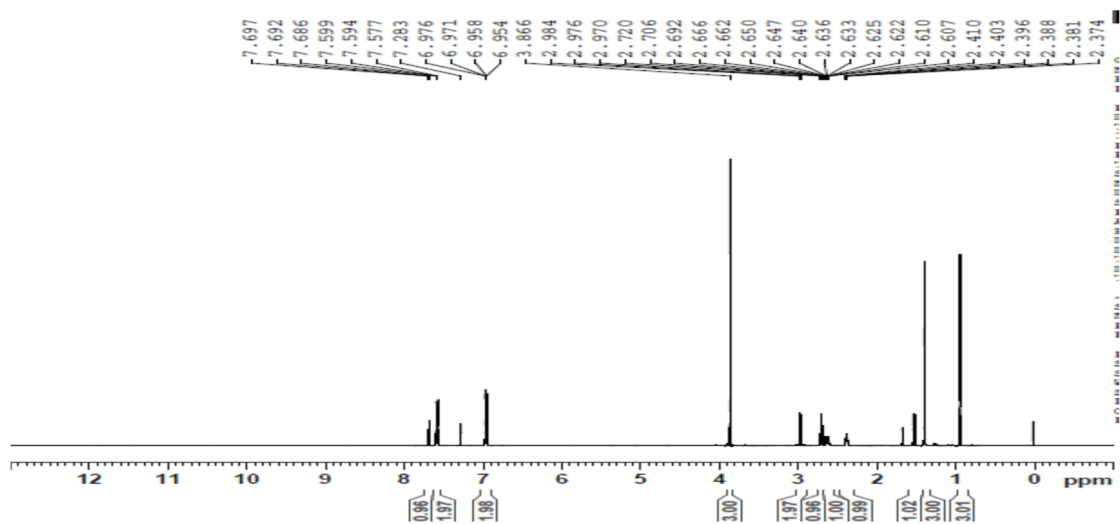


Figure S8. ¹H NMR spectrum of compound **1c**

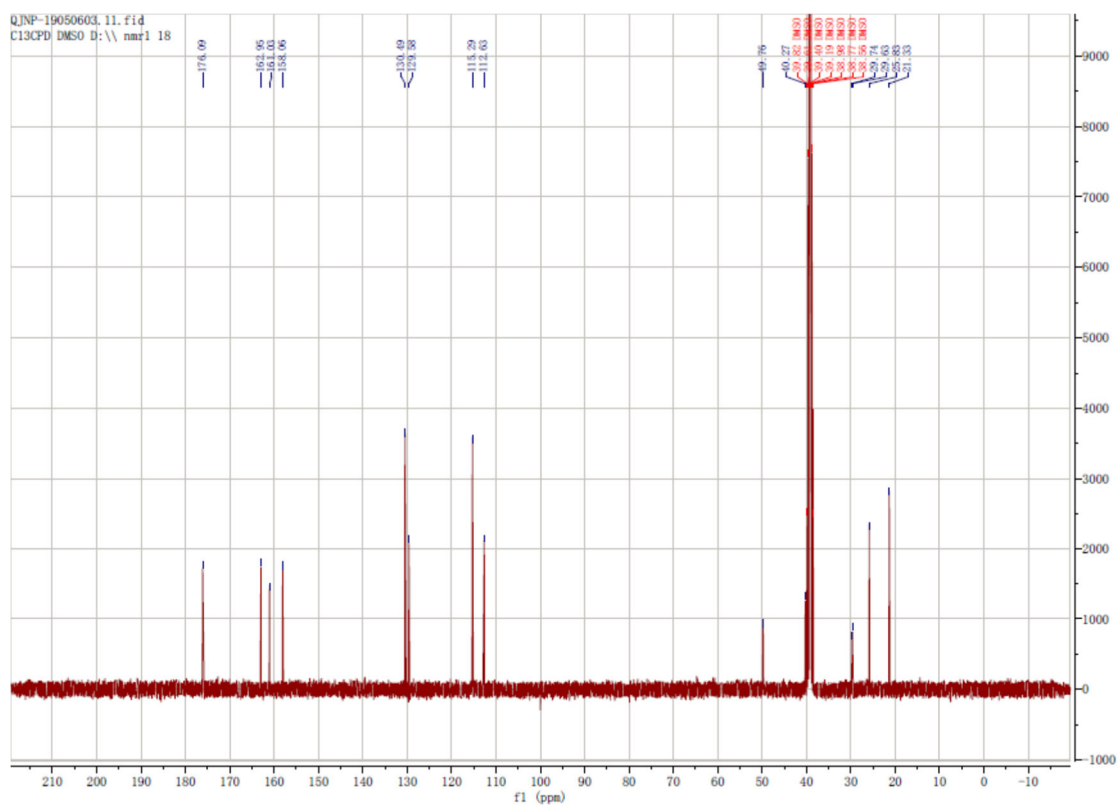


Figure S15. ^{13}C NMR spectrum of compound **1e**

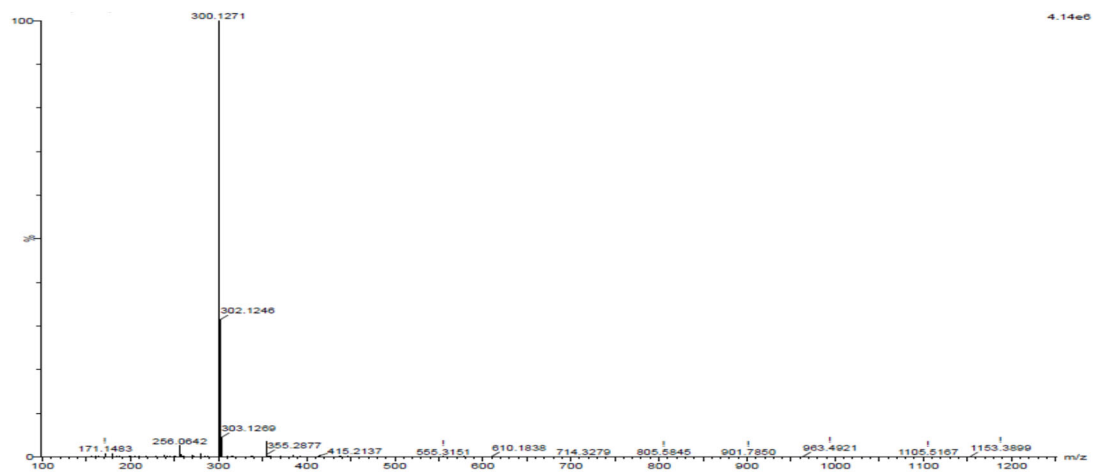


Figure S16. HRMS spectrum of compound **1f**

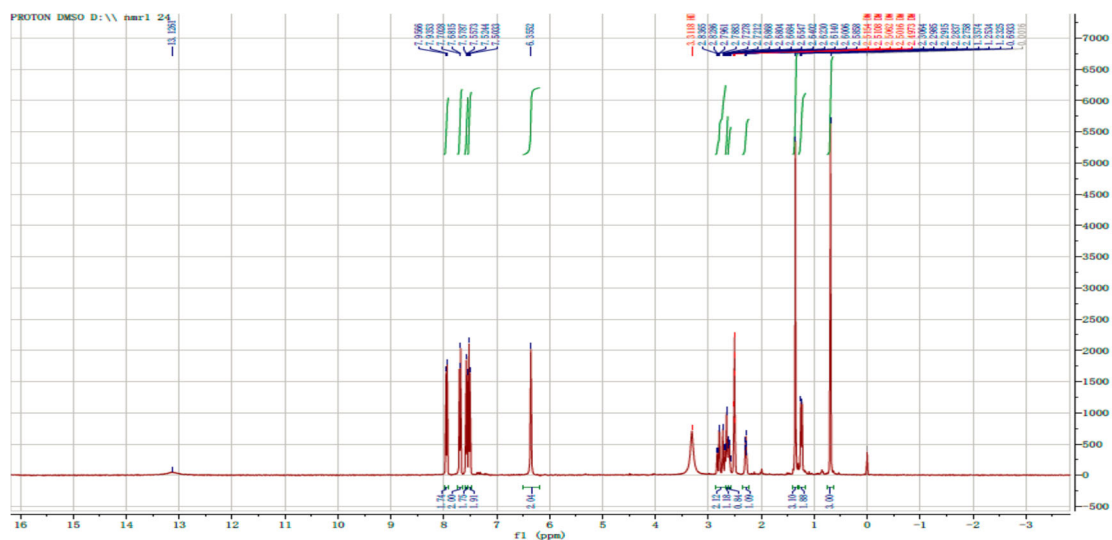


Figure S17. ^1H NMR spectrum of compound **1f**

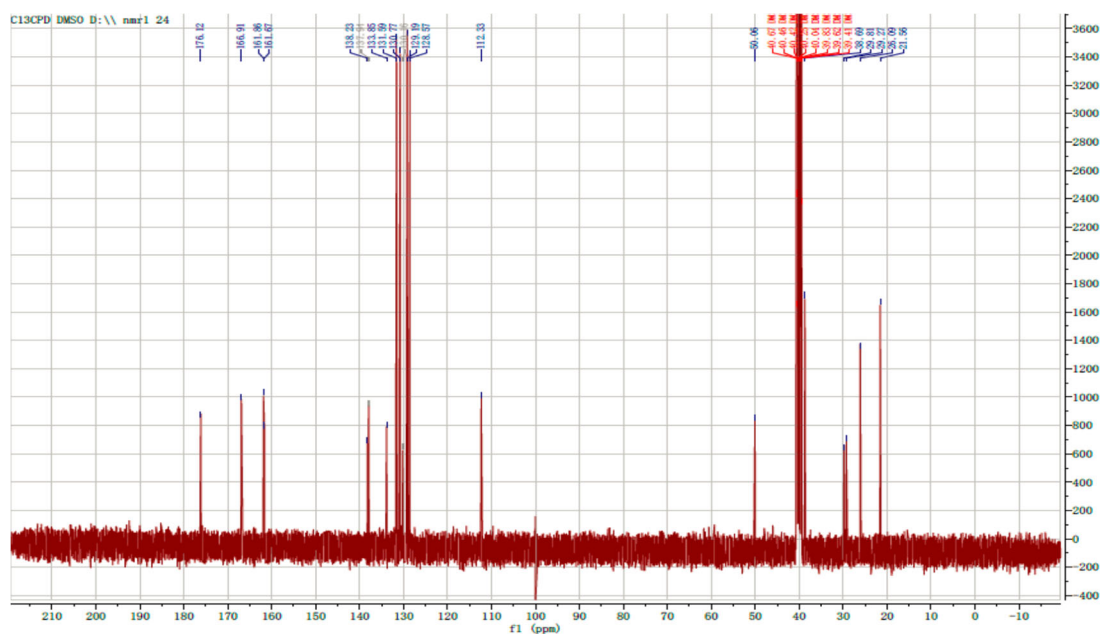


Figure S18. ^{13}C NMR spectrum of compound **1f**

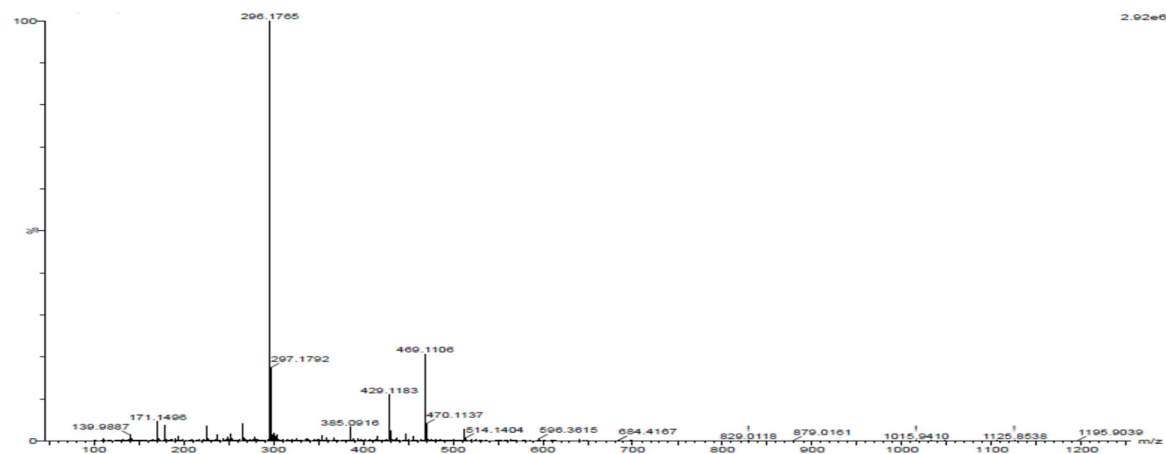


Figure S19. HRMS spectrum of compound **1g**

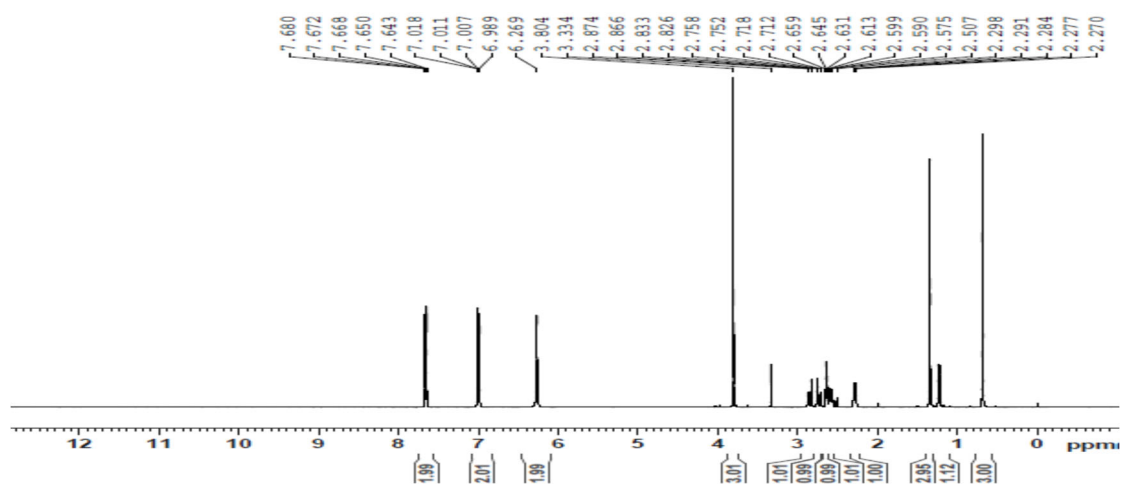


Figure S20. ¹H NMR spectrum of compound **1g**

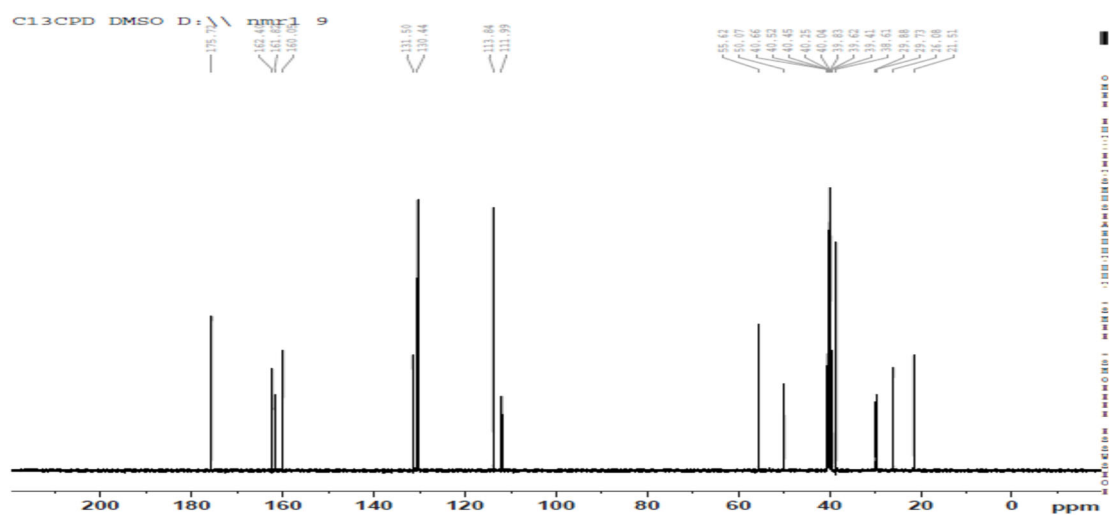


Figure S21. ¹³C NMR spectrum of compound **1g**

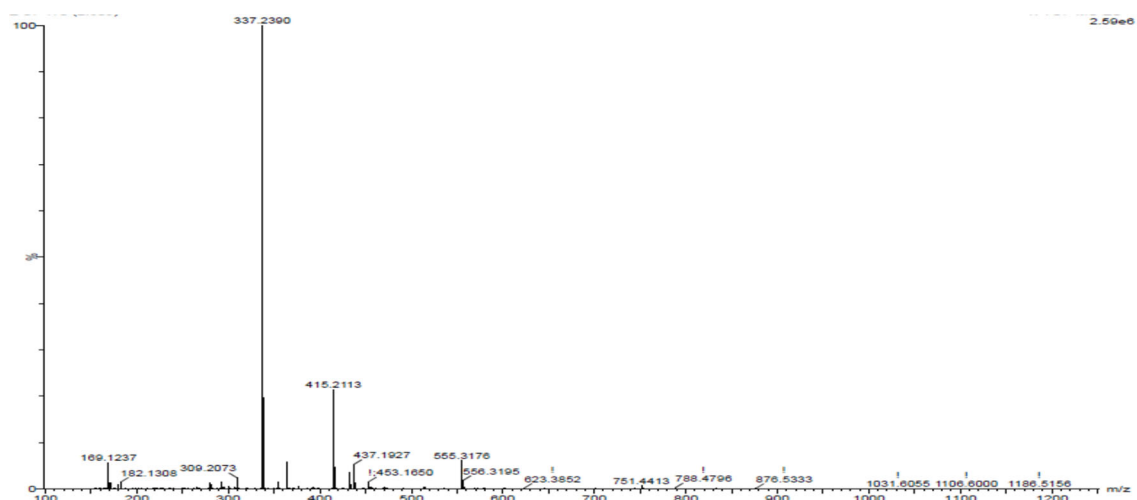
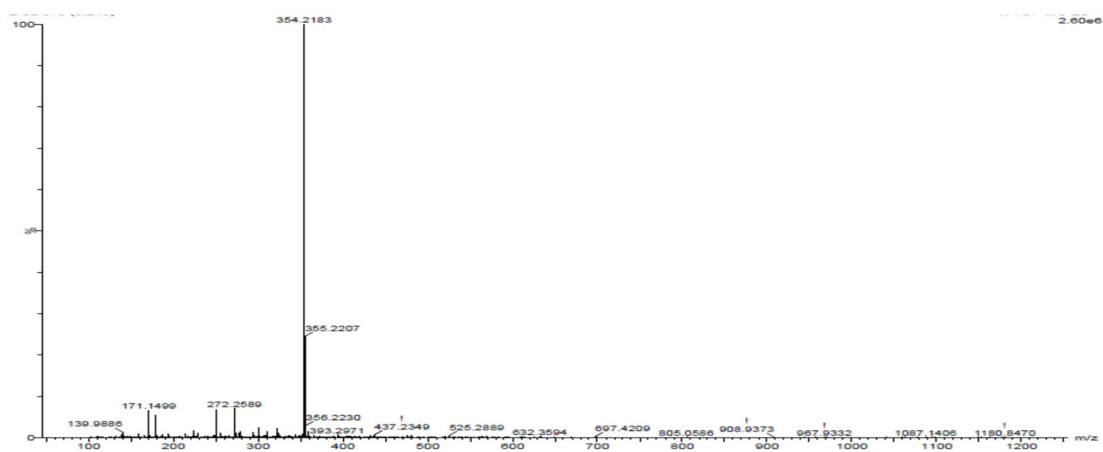
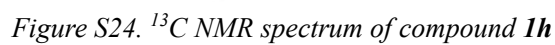
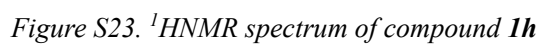


Figure S22. HRMS spectrum of compound **1h**



C13CPD DMSO D:C1=CC=C(C=C1)C2=CC=CC=C2 nmr 1 44

175.62
160.40
160.11
131.65
130.48
113.93
111.88
71.20
58.35
55.66
50.25
40.73
40.66
40.53
40.45
40.25
40.04
39.83
31.62
31.41
28.81
28.77
25.78
21.07
21.55
0.57

ppm

Figure S27. ^{13}C NMR spectrum of compound **1i**

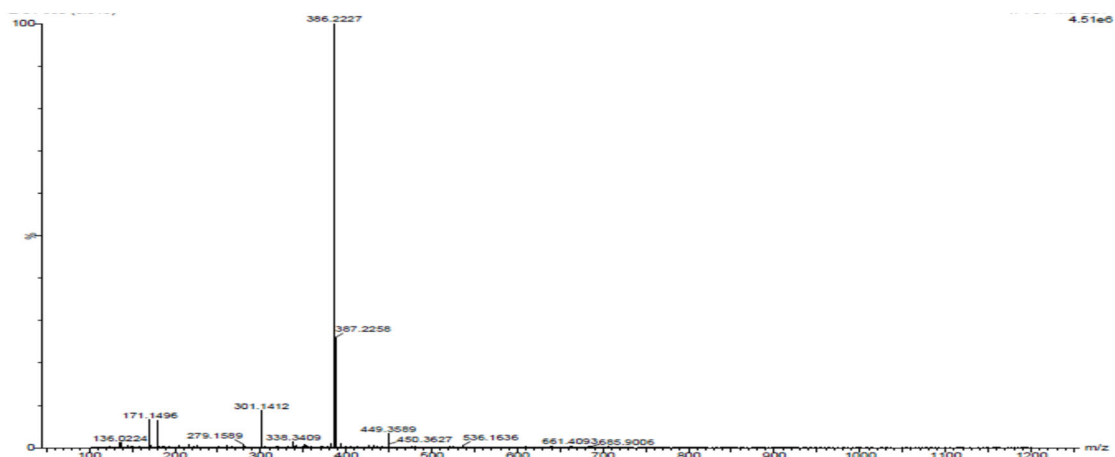
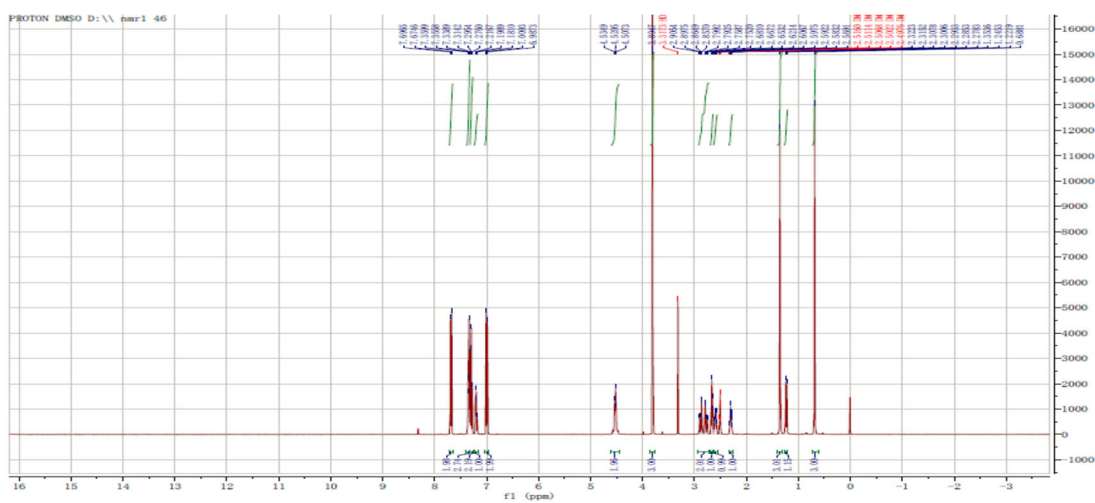


Figure S31. HRMS spectrum of compound **1k**



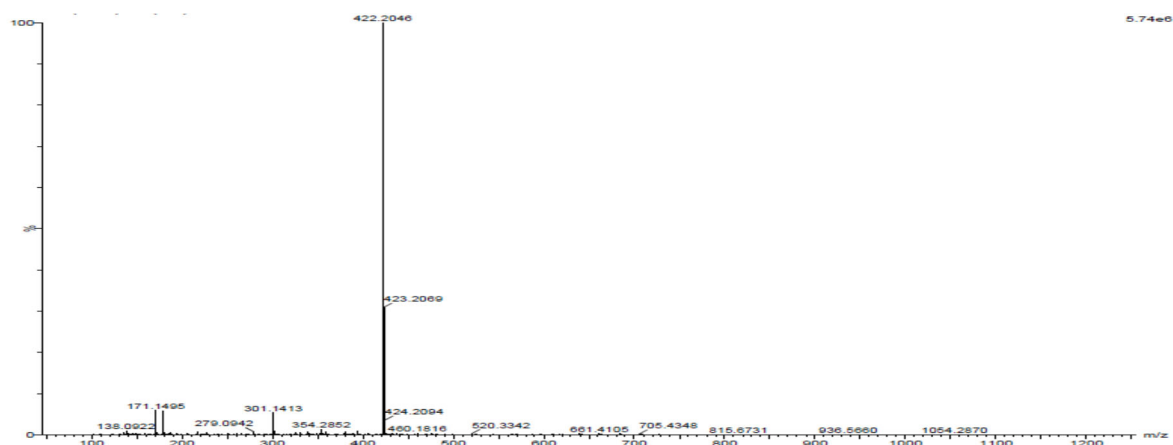


Figure S34. HRMS spectrum of compound 11

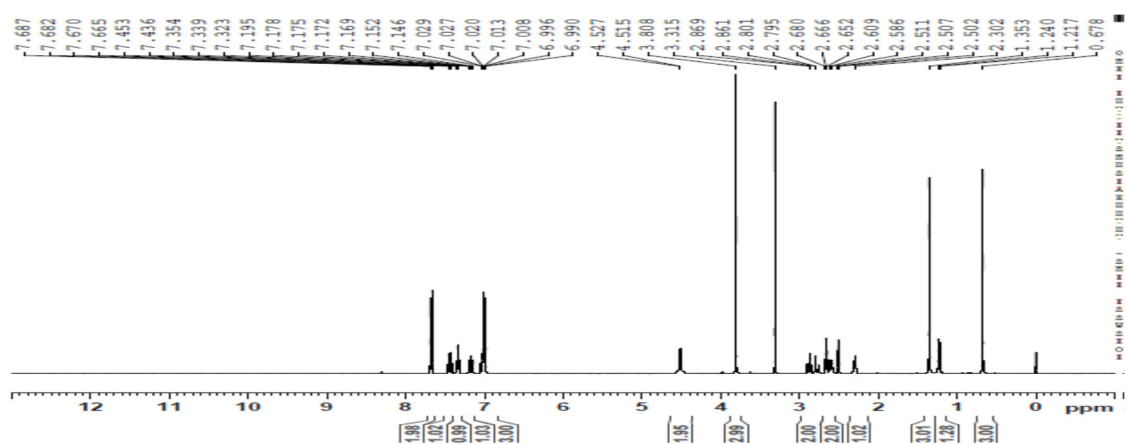


Figure S35. ¹H NMR spectrum of compound 11

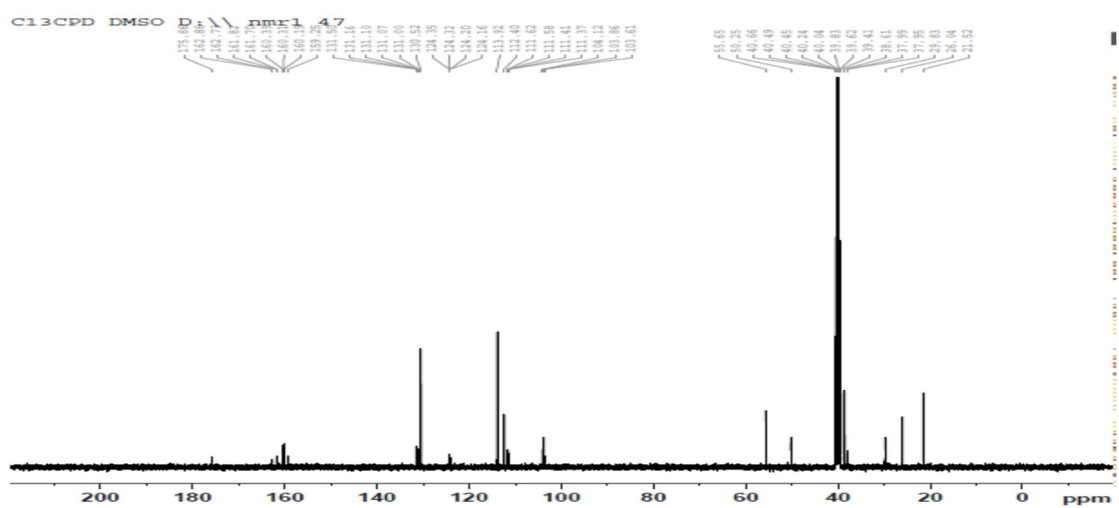


Figure S36. ¹³C NMR spectrum of compound 11

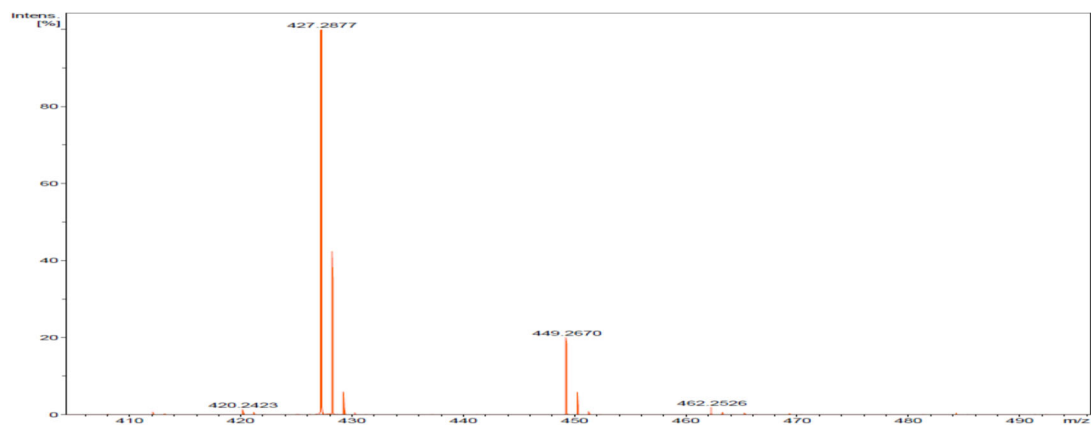


Figure S37. HRMS spectrum of compound **1m**

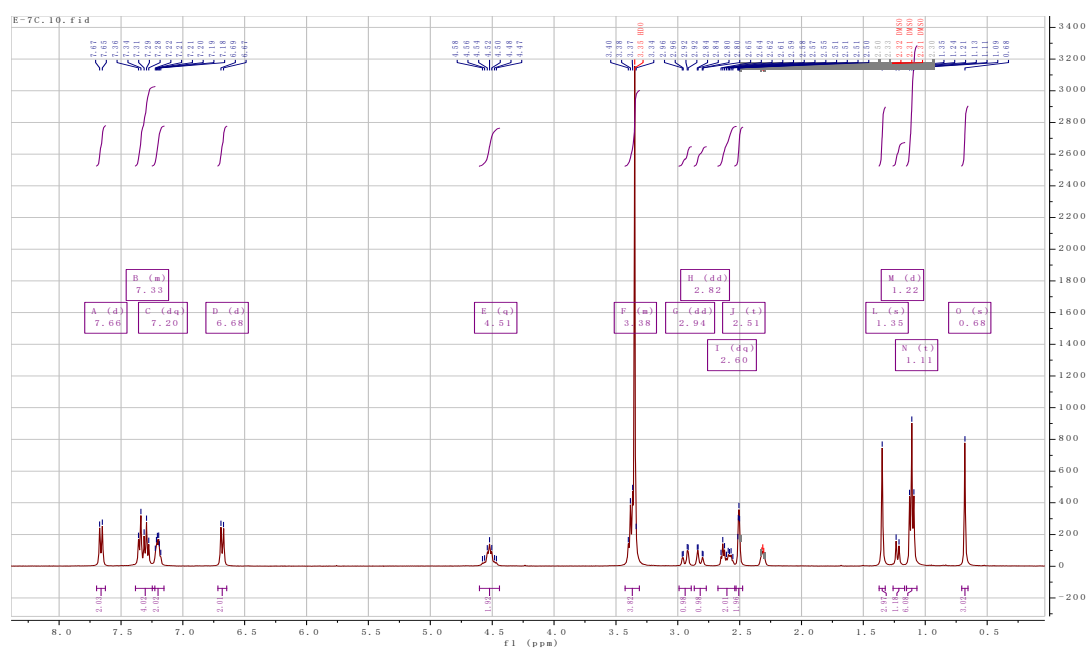


Figure S38. ¹H NMR spectrum of compound **1m**

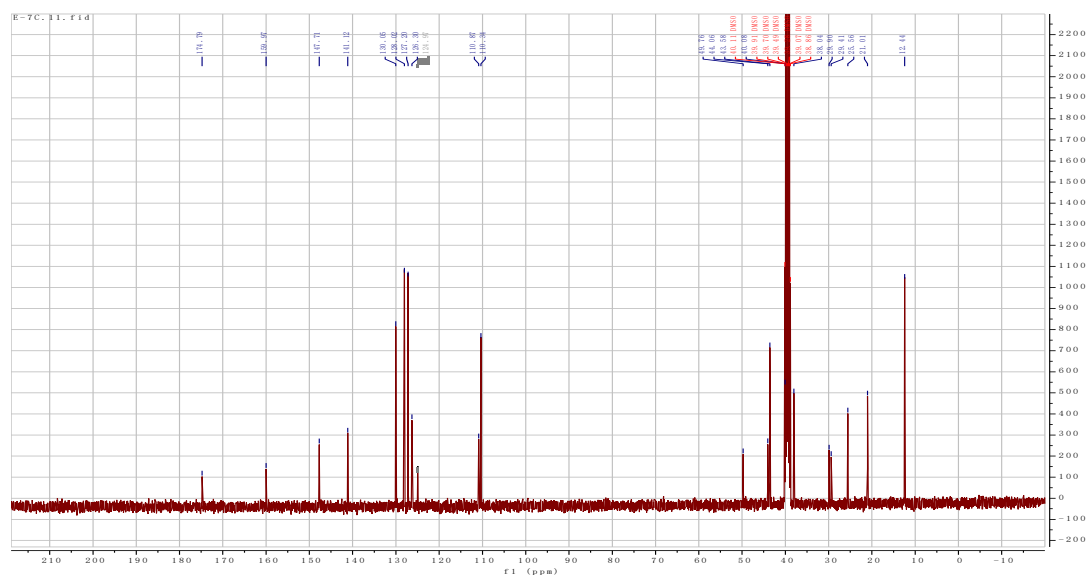


Figure S39. ^{13}C NMR spectrum of compound **1m**

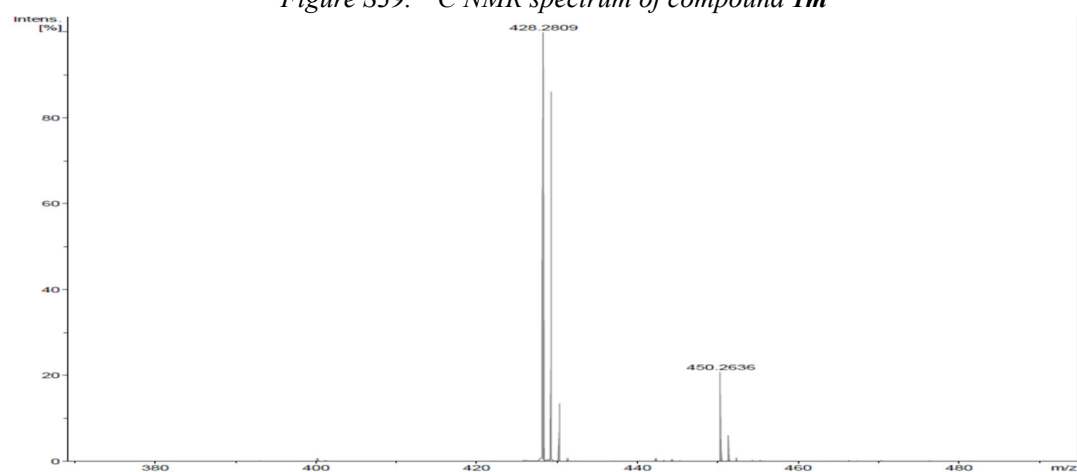


Figure S40. HRMS spectrum of compound **1n**

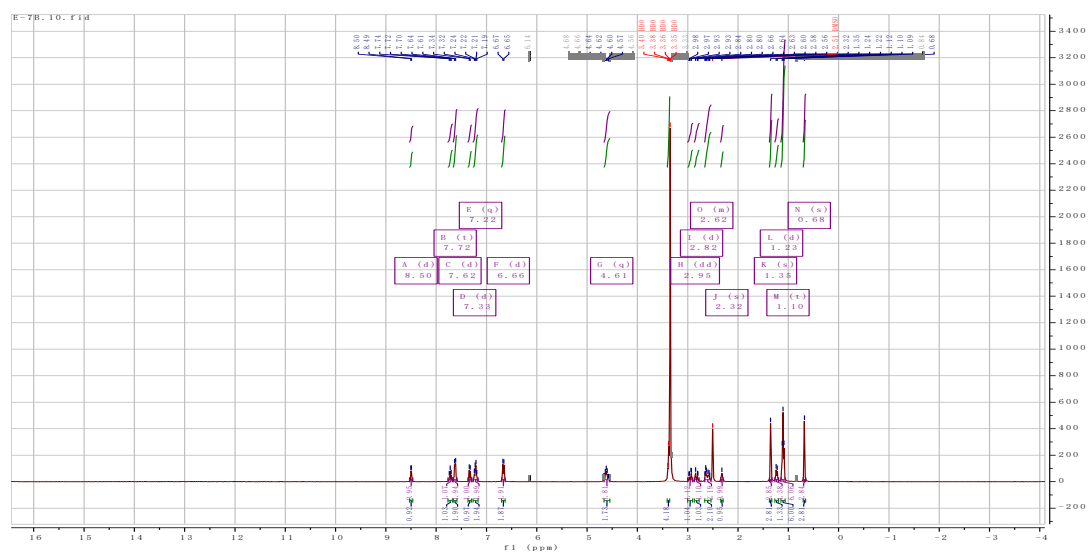
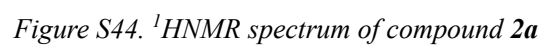
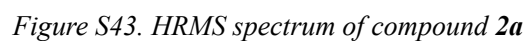
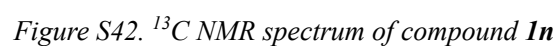


Figure S41. ^1H NMR spectrum of compound **1n**



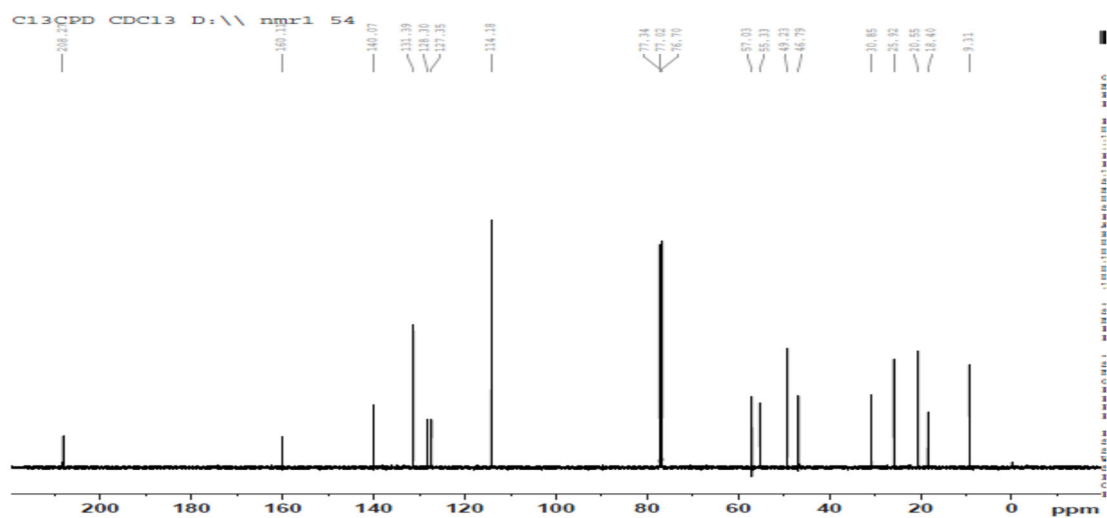


Figure S45. ^{13}C NMR spectrum of compound **2a**

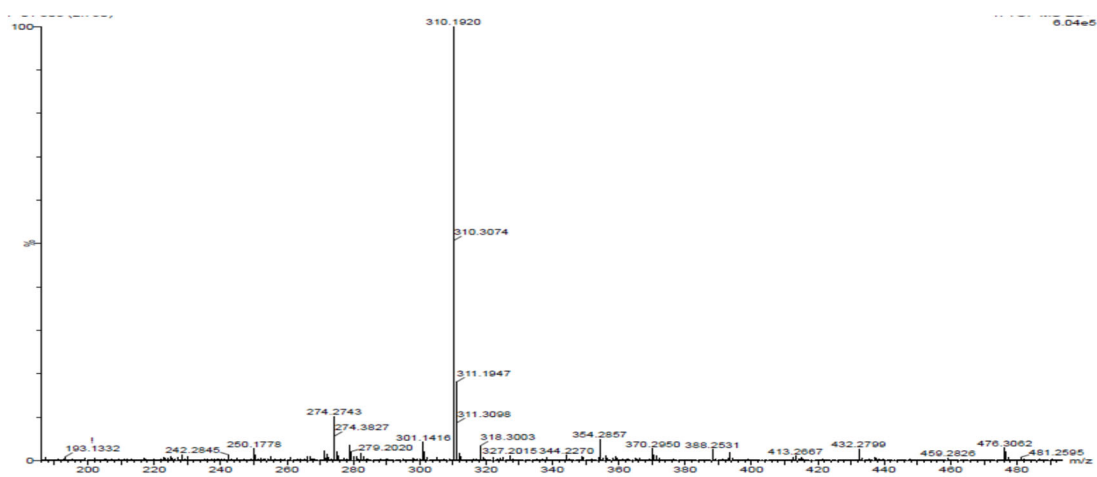


Figure S46. HRMS spectrum of compound **2b**

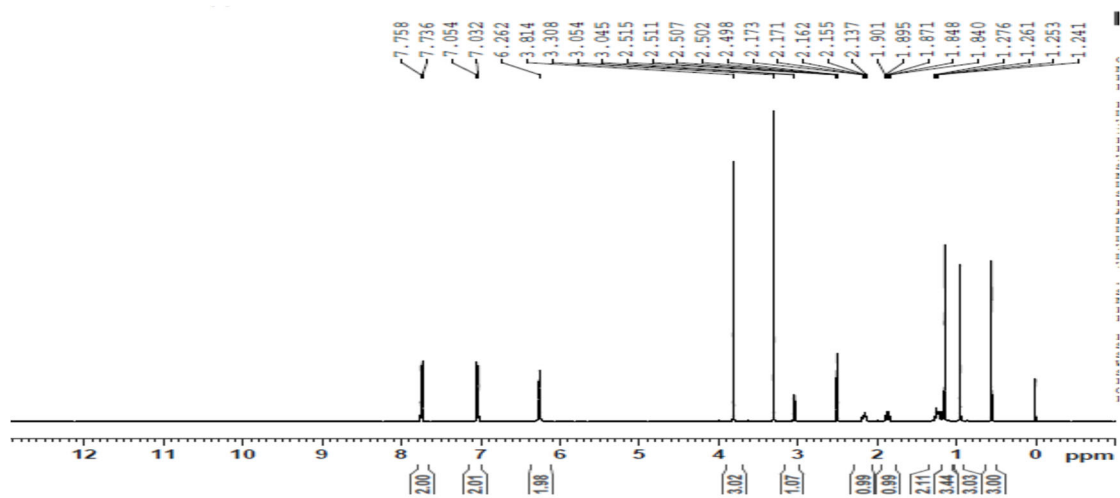


Figure S47. ^1H NMR spectrum of compound **2b**

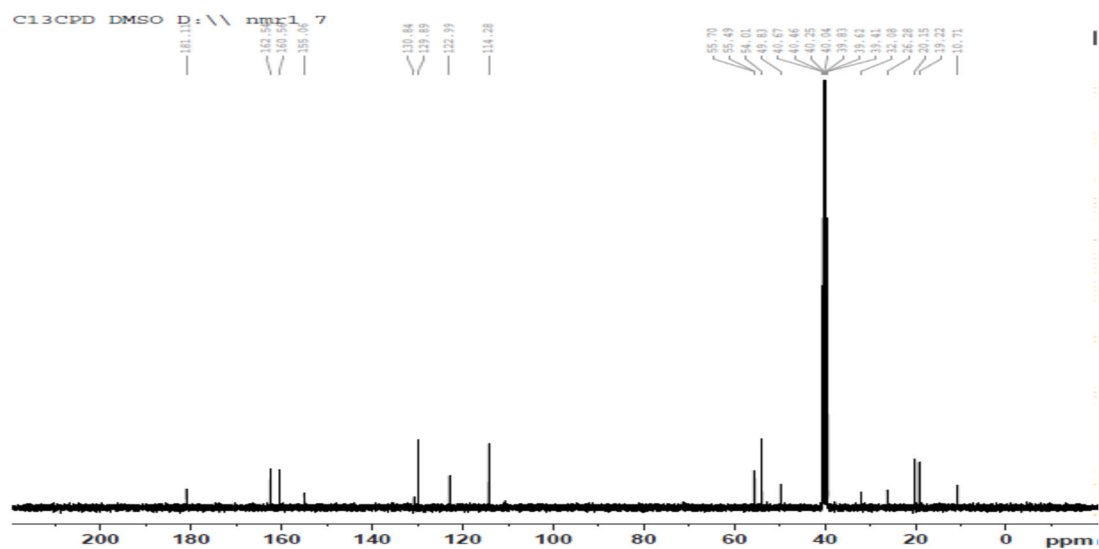


Figure S48. ^{13}C NMR spectrum of compound **2b**

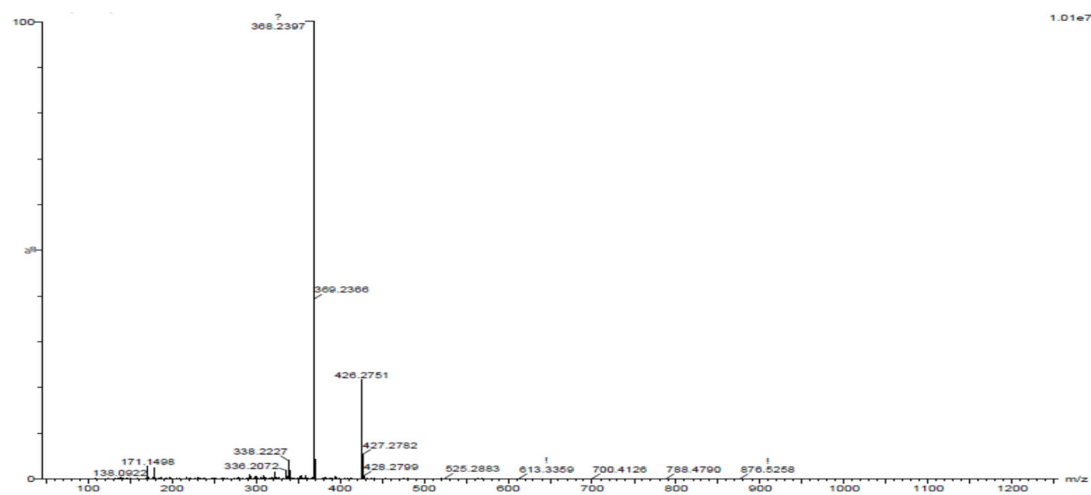


Figure S49. HRMS spectrum of compound **2c**

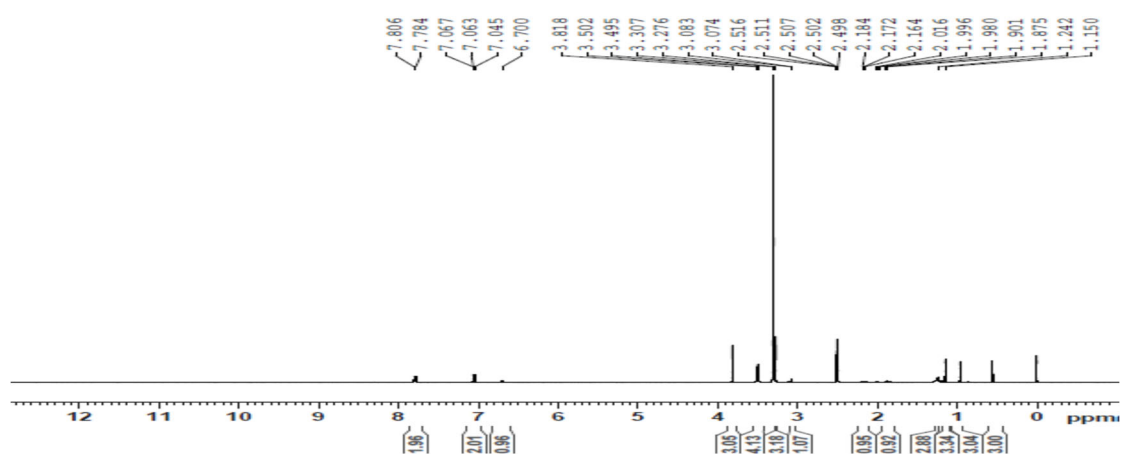


Figure S50. ^1H NMR spectrum of compound **2c**

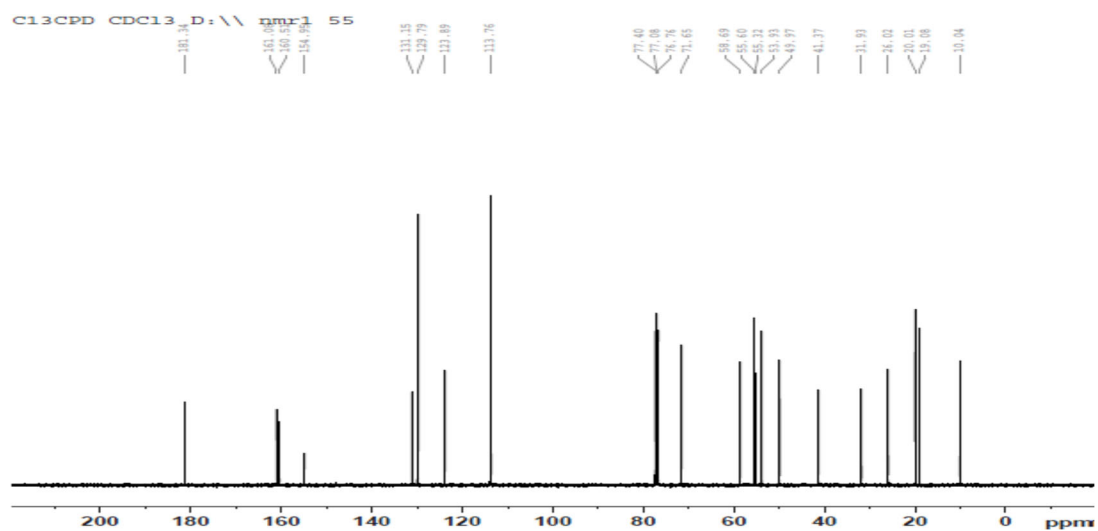


Figure S51. ^{13}C NMR spectrum of compound **2c**

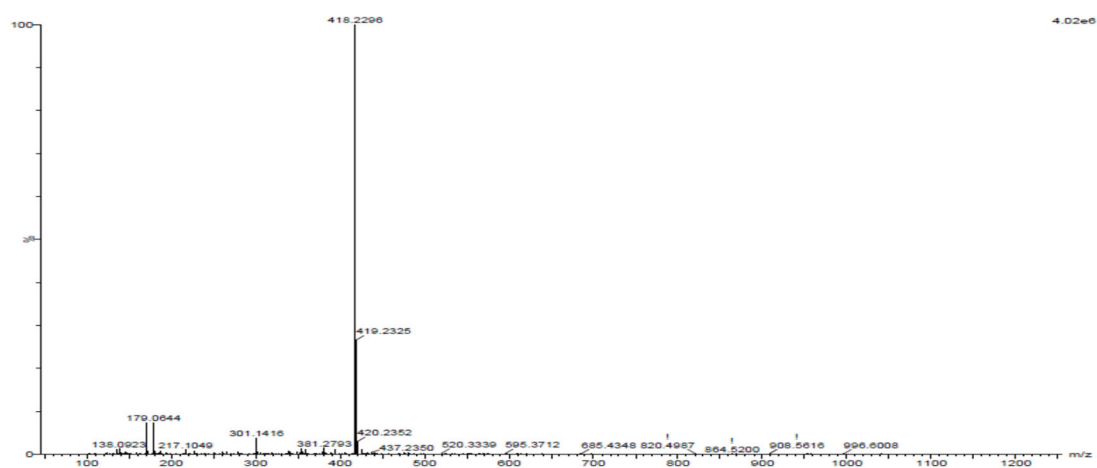


Figure S52. HRMS spectrum of compound **2d**

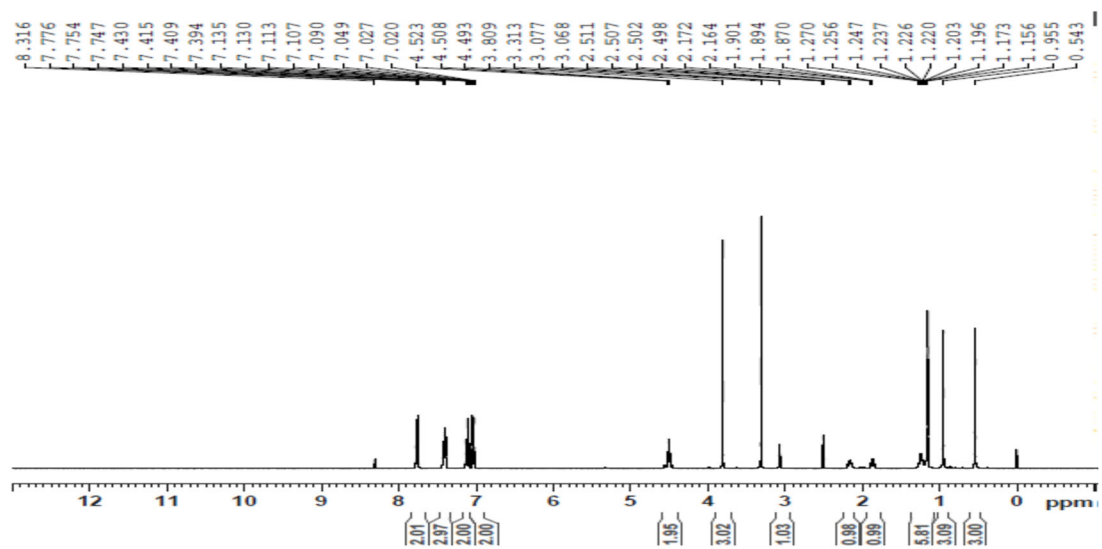


Figure S53. ^1H NMR spectrum of compound **2d**

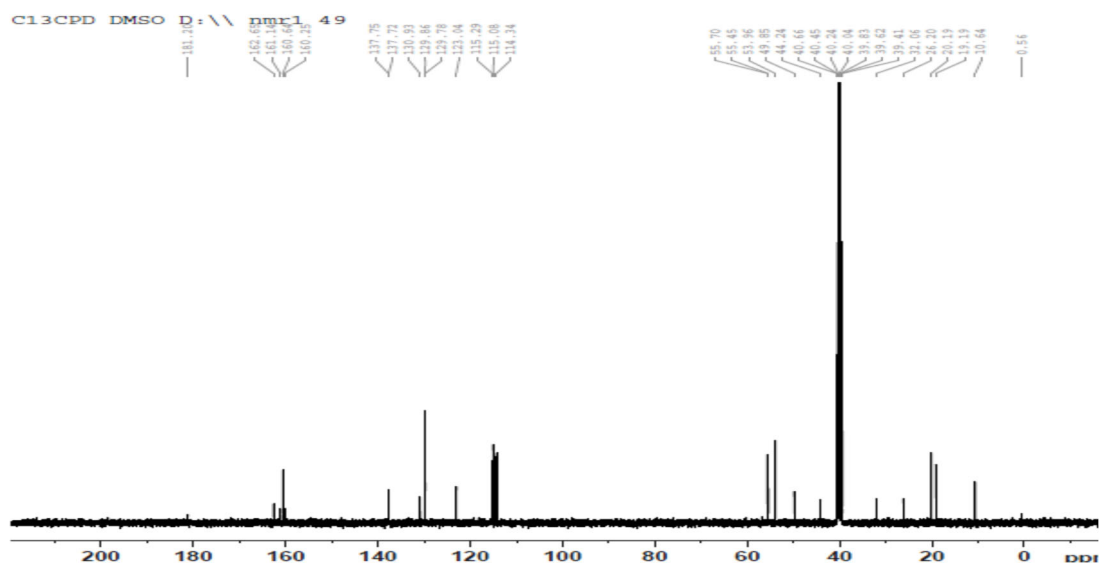


Figure S54. ^{13}C NMR spectrum of compound **2d**



Figure S55. HRMS spectrum of compound **2e**

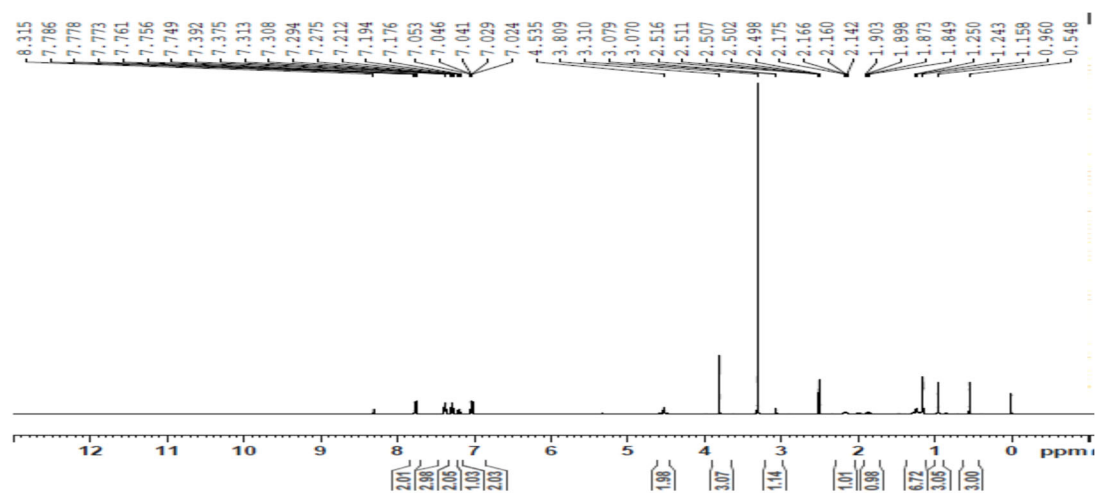


Figure S56. ^1H NMR spectrum of compound **2e**

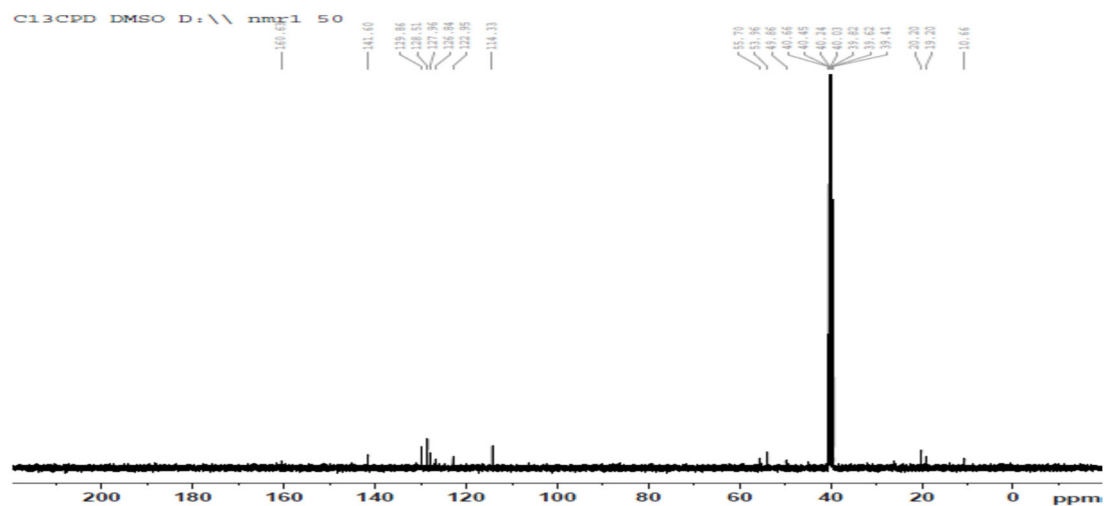


Figure S57. ^{13}C NMR spectrum of compound **2e**

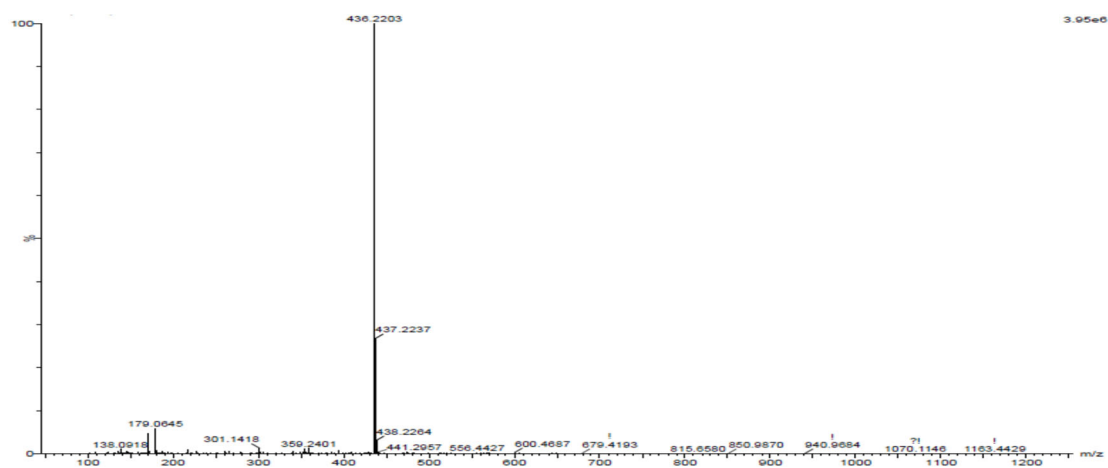


Figure S58. HRMS spectrum of compound **2f**

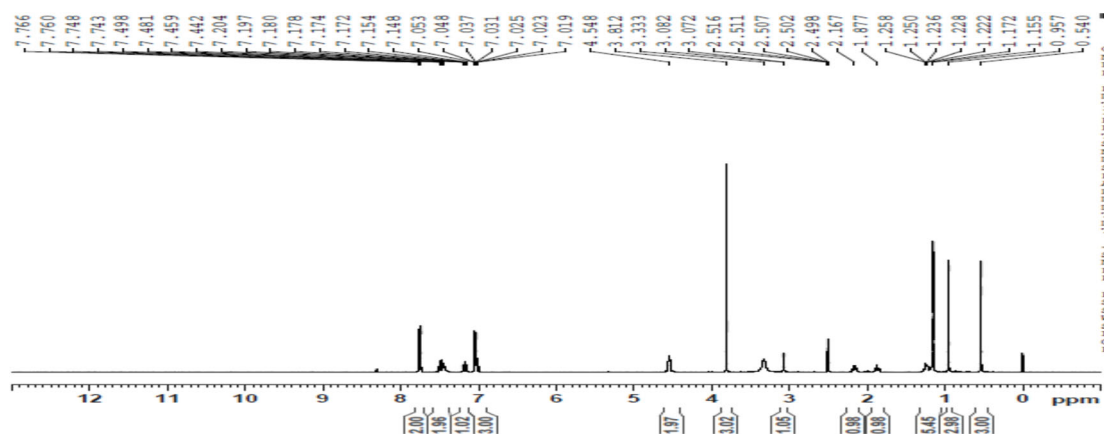


Figure S59. ^1H NMR spectrum of compound **2f**

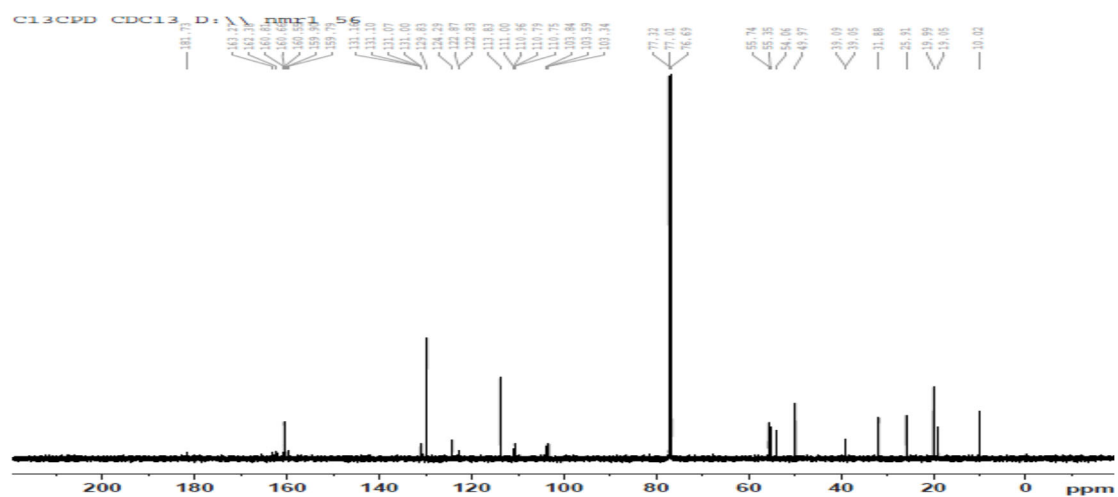


Figure S60. ^{13}C NMR spectrum of compound 2f

Table S1 Flexible docking result of 1f and the standard compound (PDB ID:2AZ5)

| Compound | PDB | Binding Residues | Docking Score |
|----------|------|------------------|---------------|
| 1f | 2AZ5 | Ser60, Try59 | -7.964 |
| Aspirin | 2AZ5 | Ser60, Try59 | -8.143 |