Design, Synthesis, In Vitro and In Silico Evaluation of Indole Based Tetrazole Derivatives as Putative Anti-Breast Cancer Agents

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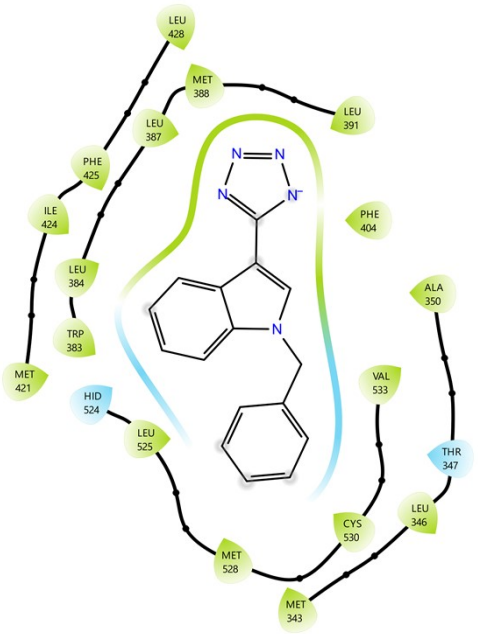
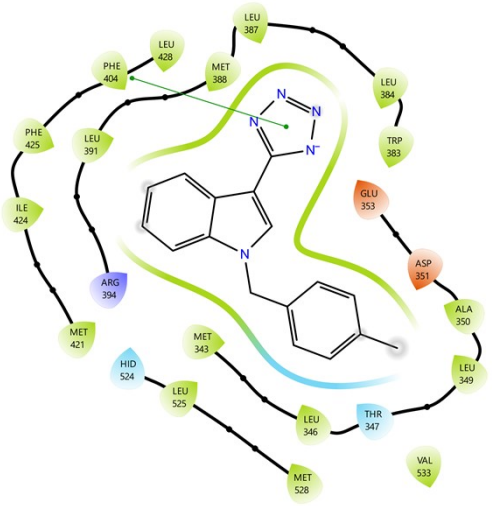
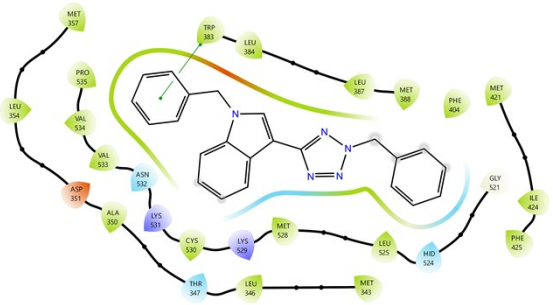
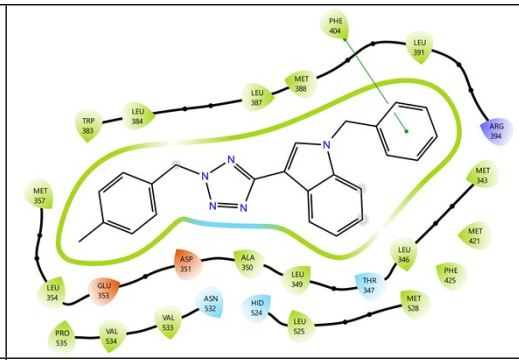
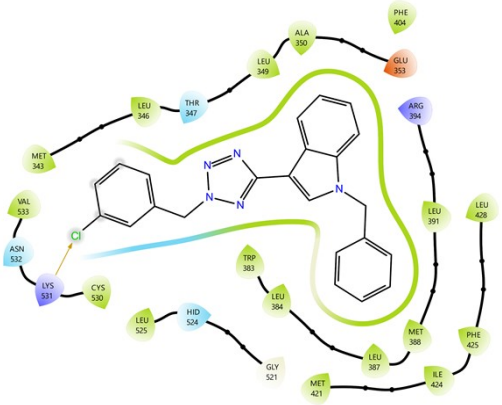
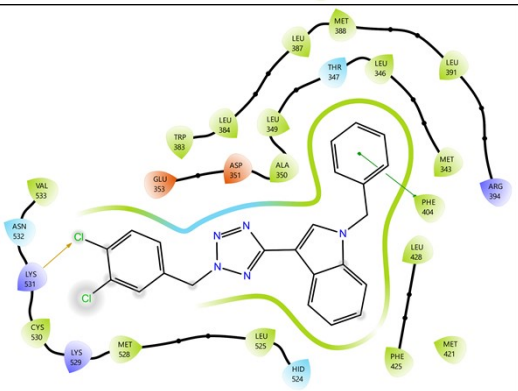
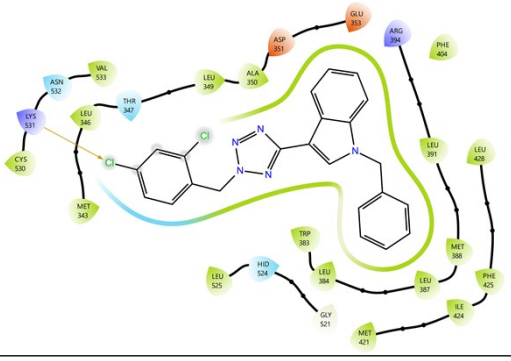
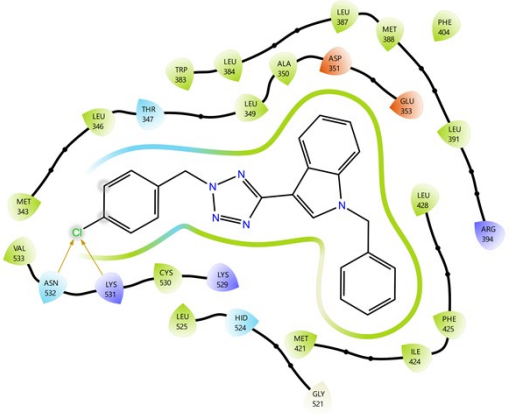
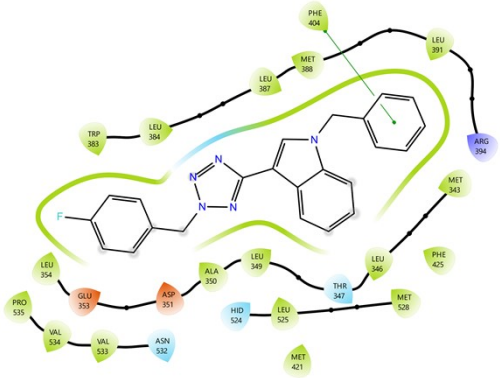
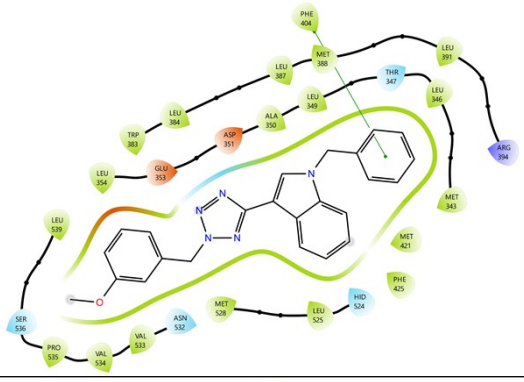
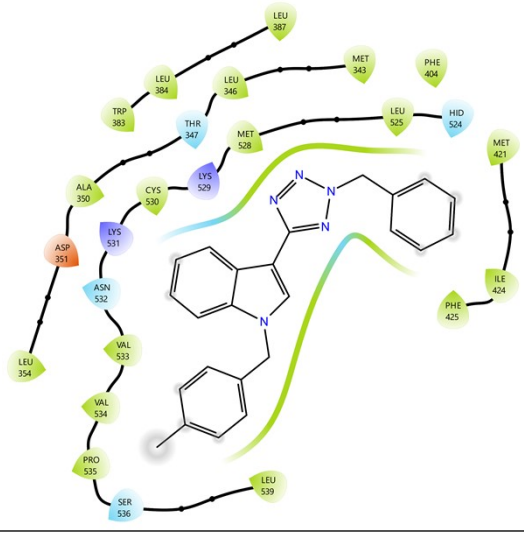
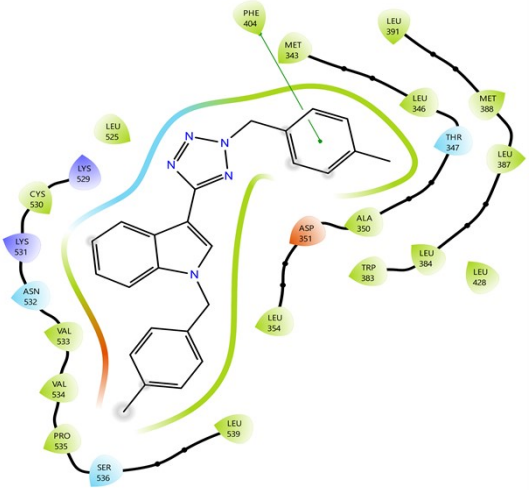
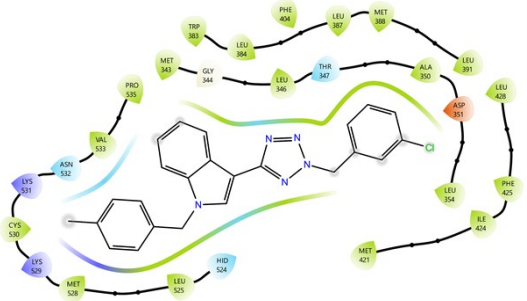
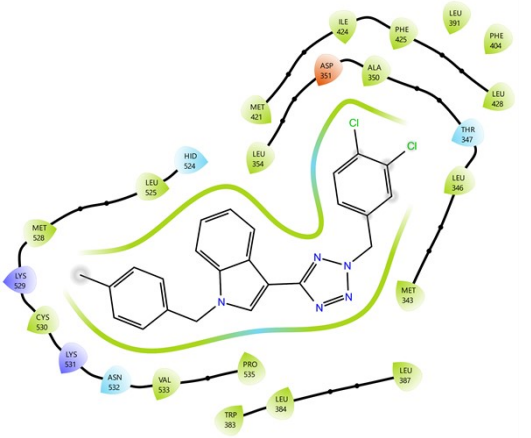
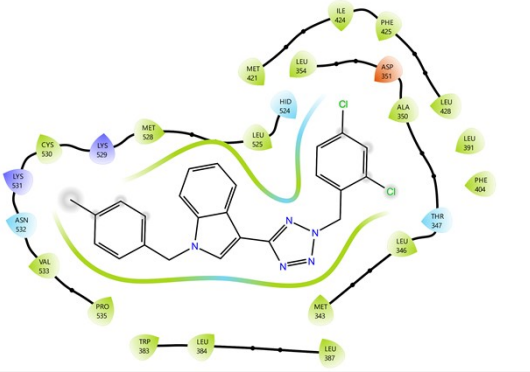
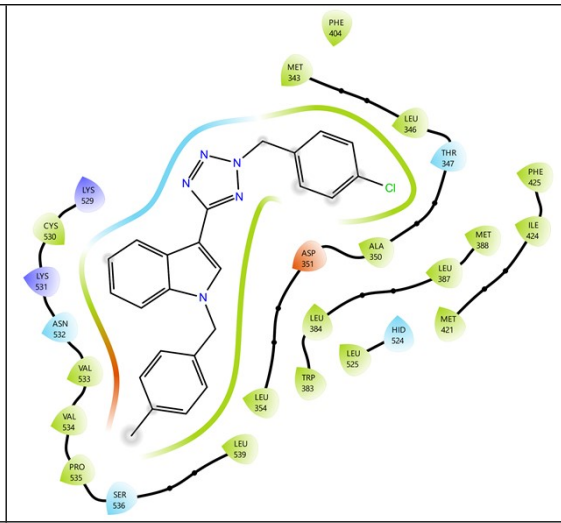
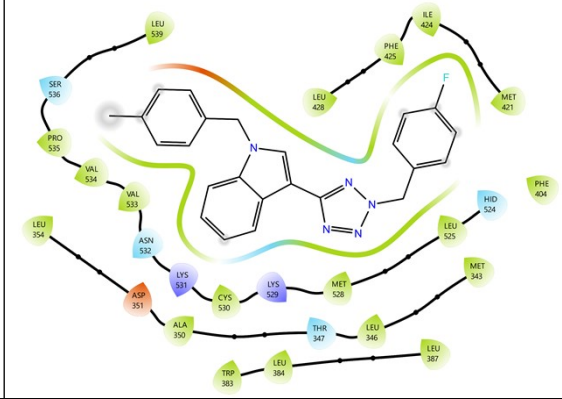
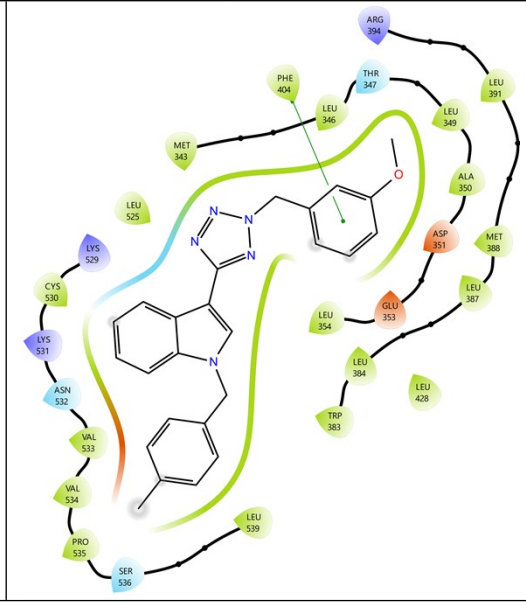
Supplementary Table 1. Docking score and binding poses of the synthesised indole-tetrazole derivatives.

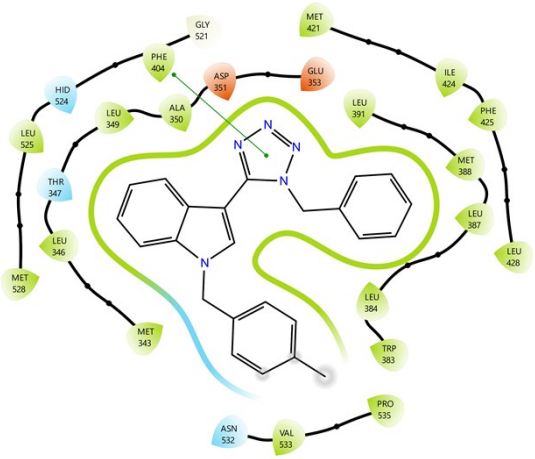
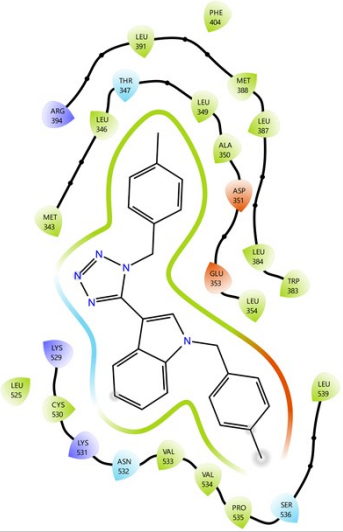
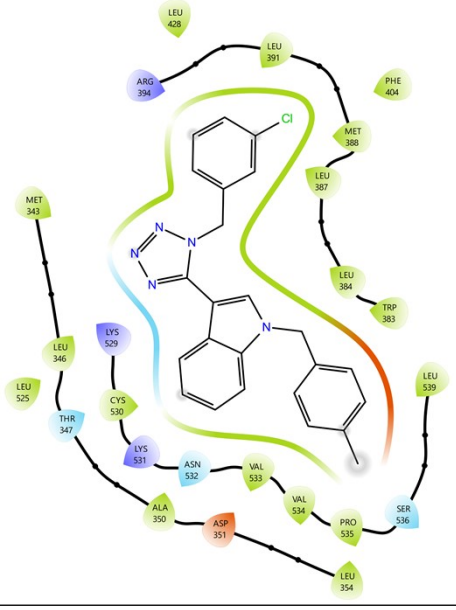
S. No.	Compound	Docking Score (Kcal/Mol)	Interaction Pose
1.	**4a**	-6.535	
2.	**4b**	-6.896	
3.	**5a**	-7.948	

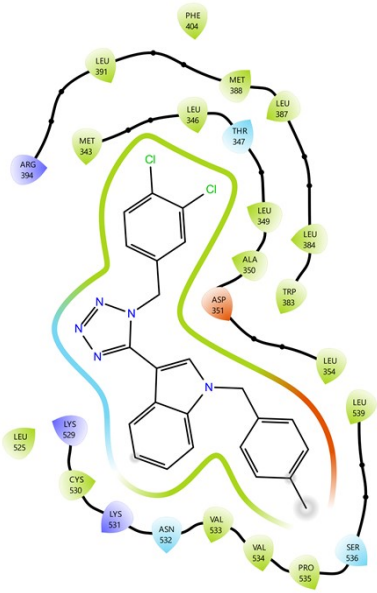
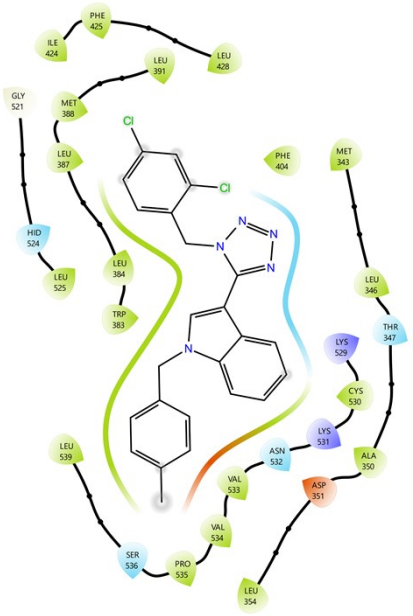
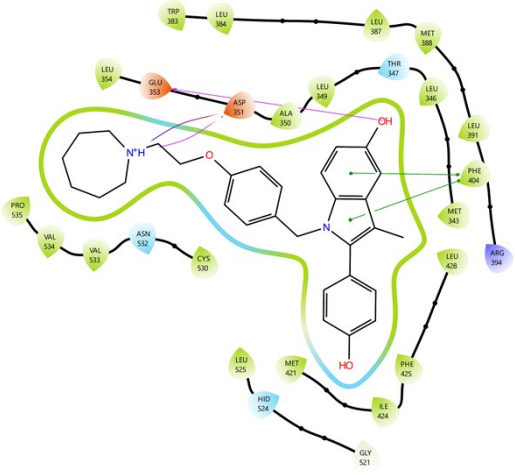
4.	**5b**	-8.614	
5.	**5c**	-8.575	
6.	**5d**	-7.877	
7.	**5e**	-7.735	

8.	**5f**	-7.871	
9.	**5g**	-7.575	
10.	**5h**	-8.342	
11.	**5i**	-6.335	

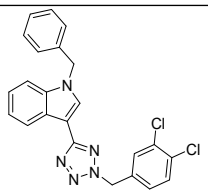
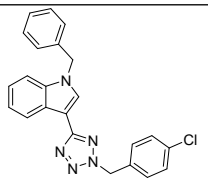
12.	**5j**	-7.3	
13.	**5k**	-7.172	
14.	**5l**	-7.739	
15.	**5m**	-7.272	

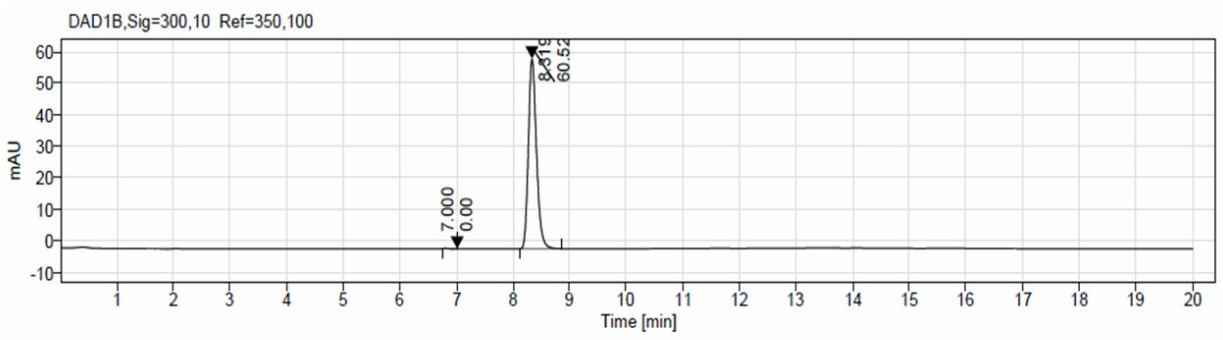
16.	**5n**	-6.742	
17.	**5o**	-6.708	
18.	**5p**	-6.543	

19.	**6i**	-8.323	
20.	**6j**	-6.873	
21.	**6k**	-7.574	

22.	**6l**	-7.284	
23.	**6m**	-7.35	
24.	**Bazedoxifene**	-9.482	

Supplementary Table S2. The SMILES strings of the active compounds.

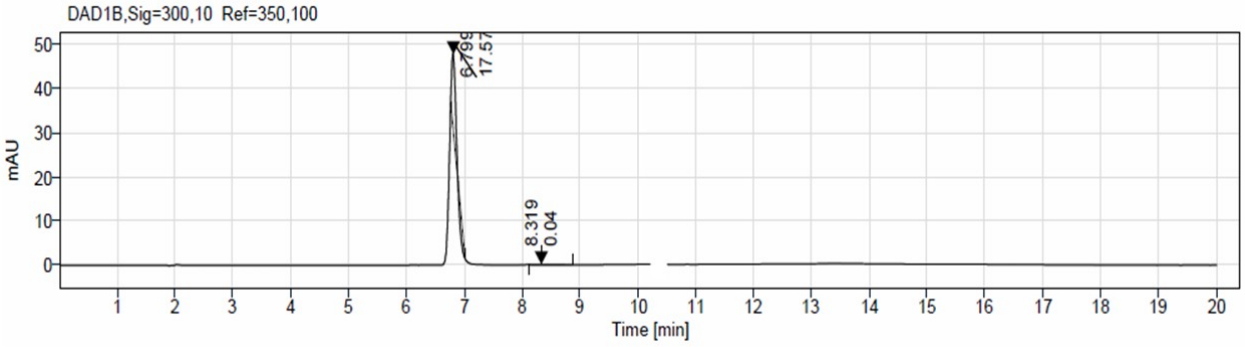
Compound	Structure	SMILES
5d		ClC1=CC(CN2N=NC(C3=CN(CC4=CC=CC=C4)C5=CC=CC=C53)=N2)=CC=C1Cl
5f		ClC(C=C1)=CC=C1CN2N=NC(C3=CN(CC4=CC=CC=C4)C5=CC=CC=C53)=N2



Signal: DAD1B, Sig=300,10 Ref=350,100

Name	RT [min]	Area	Area %	Height	Height %
1	7.000	0.309	0.05	0.000	0.00
2	8.319	601.990	99.95	60.517	100.00

Figure S1. HPLC spectrum and peak area of compound **5d**.



Signal: DAD1B,Sig=300,10 Ref=350,100

Name	RT [min]	Area	Area %	Height	Height %
1	6.799	55.768	97.97	17.572	99.76
2	8.319	1.156	2.03	0.043	0.24

Figure S2. HPLC spectrum and peak area of compound **5f**.

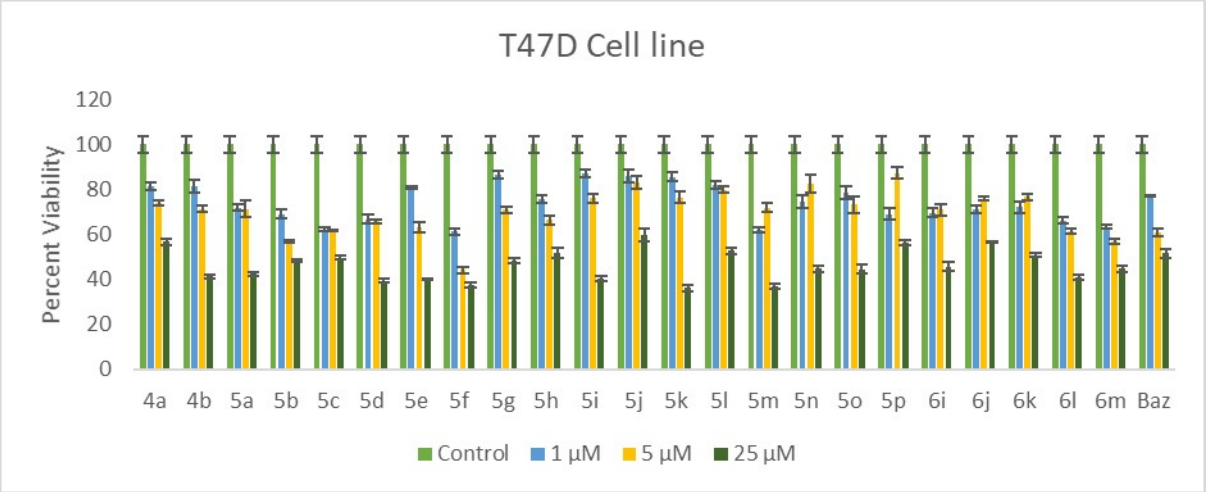


Figure S3. MTT assay results indicating dose-dependent response of test compounds in comparison to positive control bazedoxifene (Baz) on breast cancer cell line T-47D for 48 h.

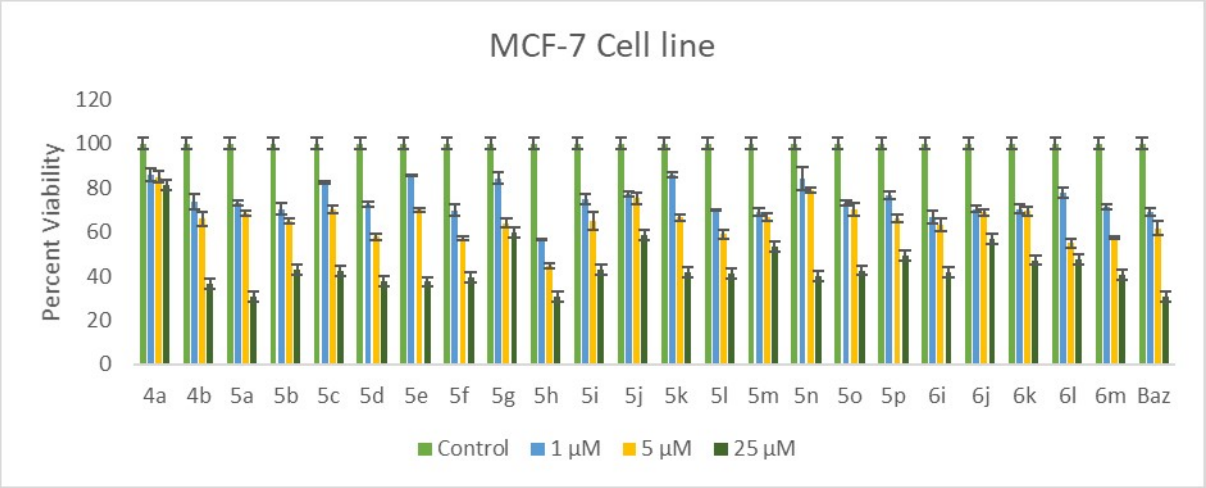


Figure S4. MTT assay results indicating dose-dependent response of test compounds in comparison to positive control bazedoxifene (Baz) on breast cancer cell line MCF-7 for 48 h.

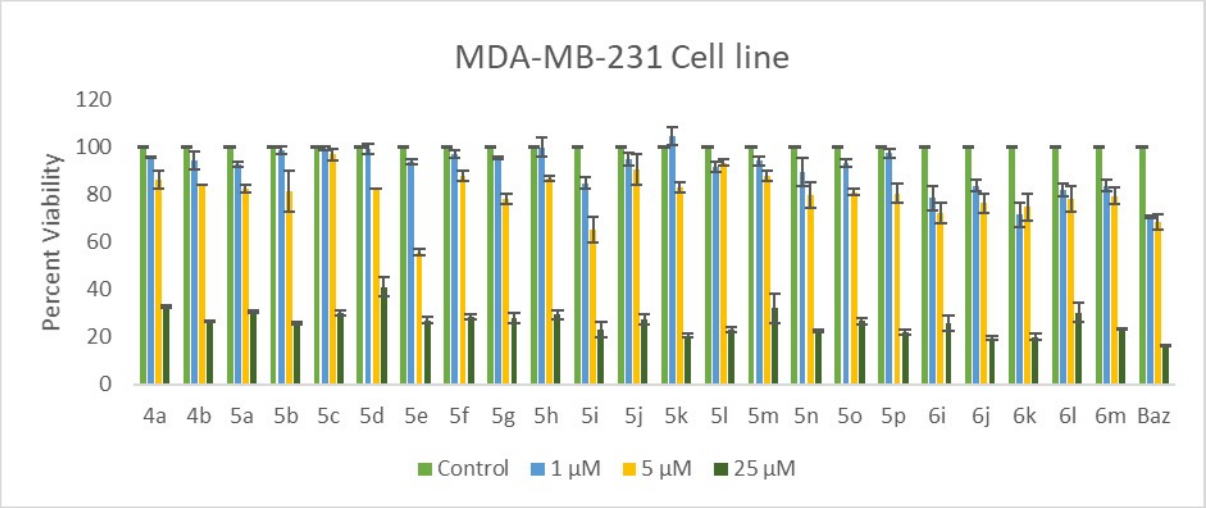


Figure S5. MTT assay results indicating dose-dependent response of test compounds in comparison to positive control bazedoxifene (Baz) on breast cancer cell line MDA-MB-231 for 48 h.

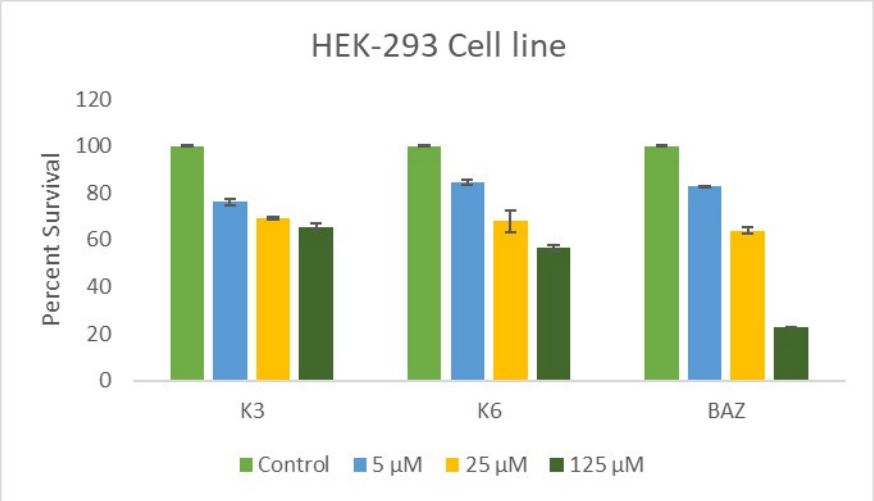


Figure S6. MTT assay results indicating dose-dependent response of selected test compounds in comparison to positive control bazedoxifene (Baz) on human embryonic kidney cells HEK-293 for 48 h.

^{1}H NMR, ^{13}C NMR, Mass Spectra and FT-IR of synthesized compounds.

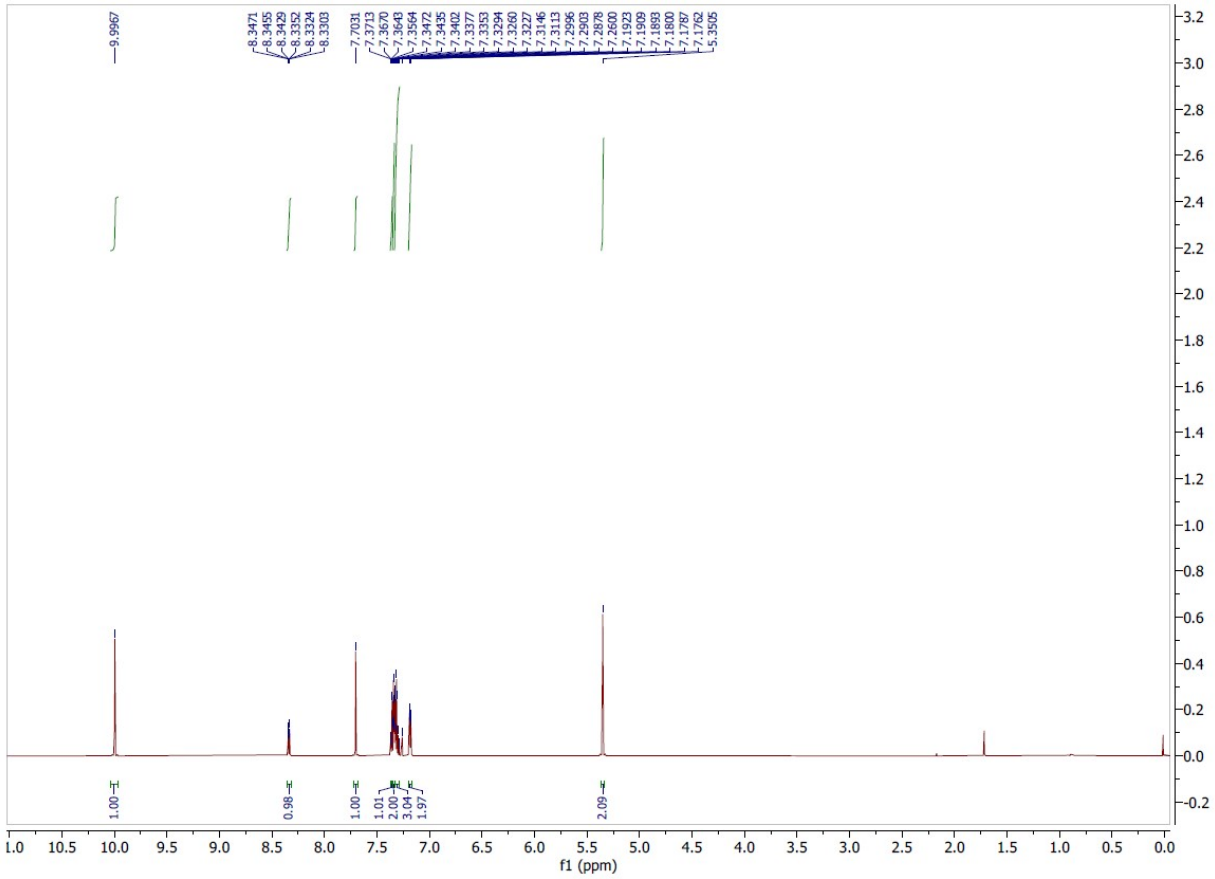


Figure S7. ^{1}H NMR spectrum of compound 2a

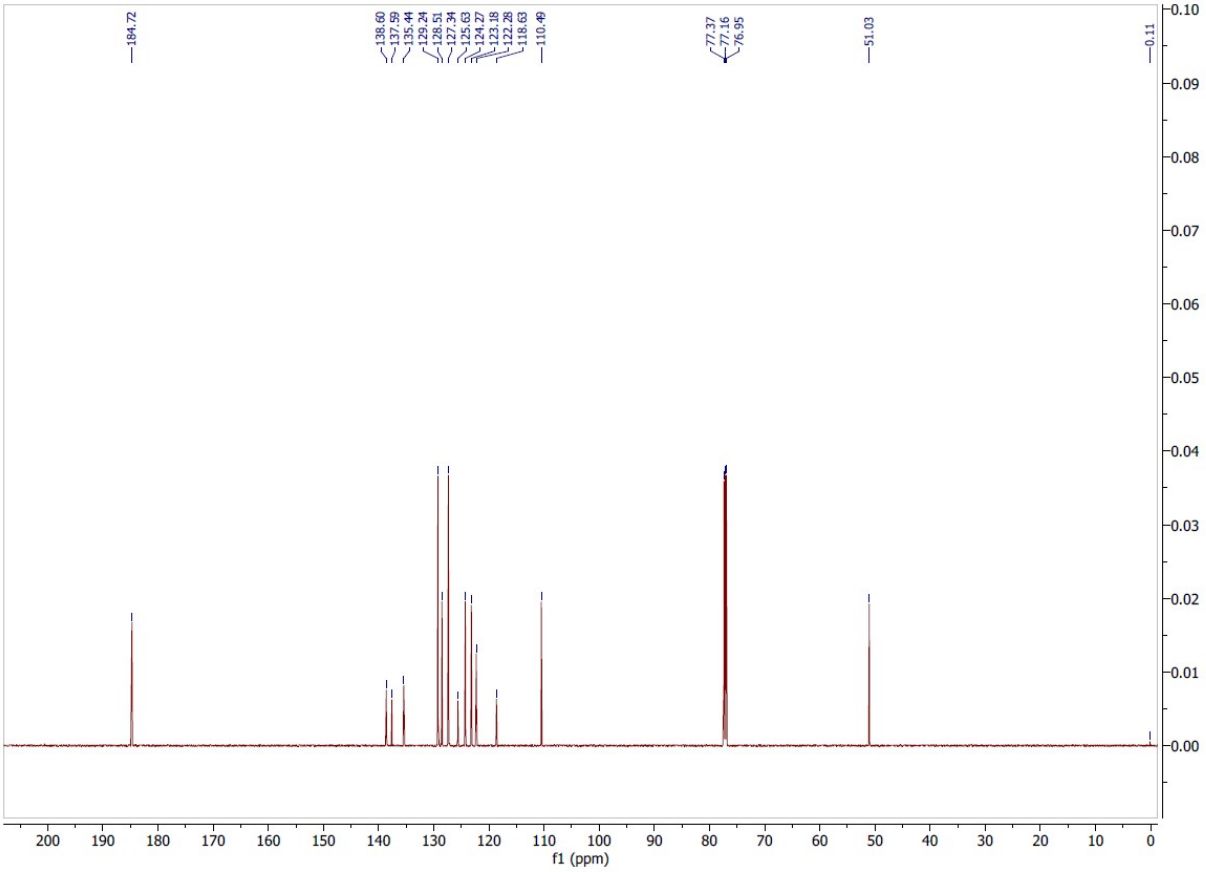


Figure S8. ^{13}C NMR spectrum of compound 2a

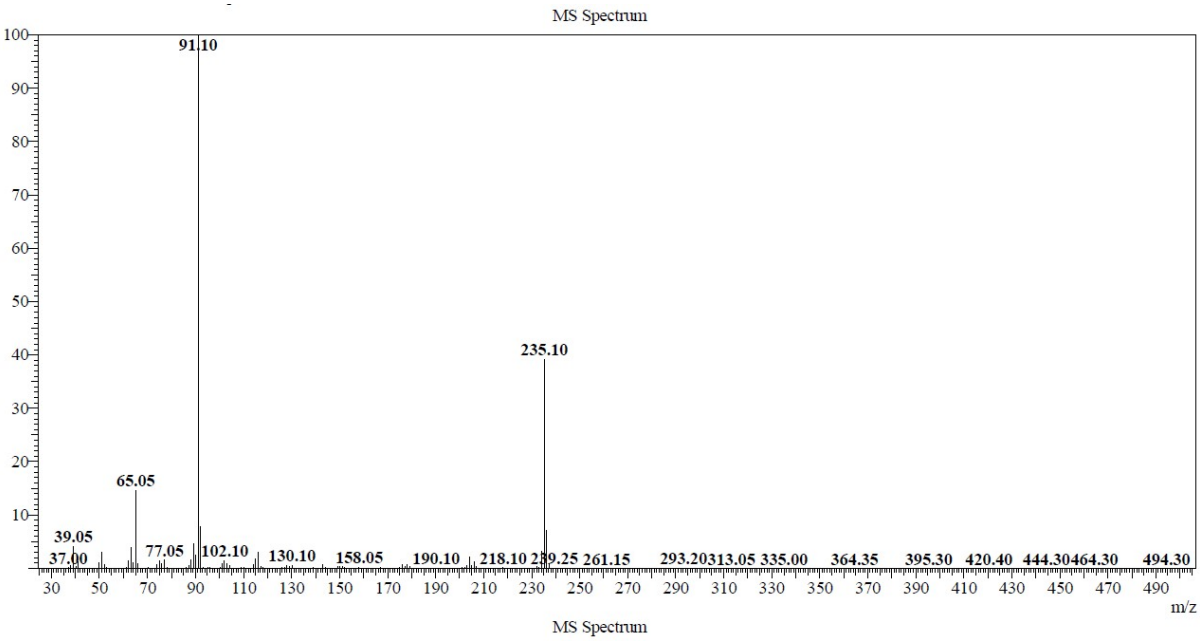


Figure S9. Mass spectrum (ESI-MS) of compound 2a

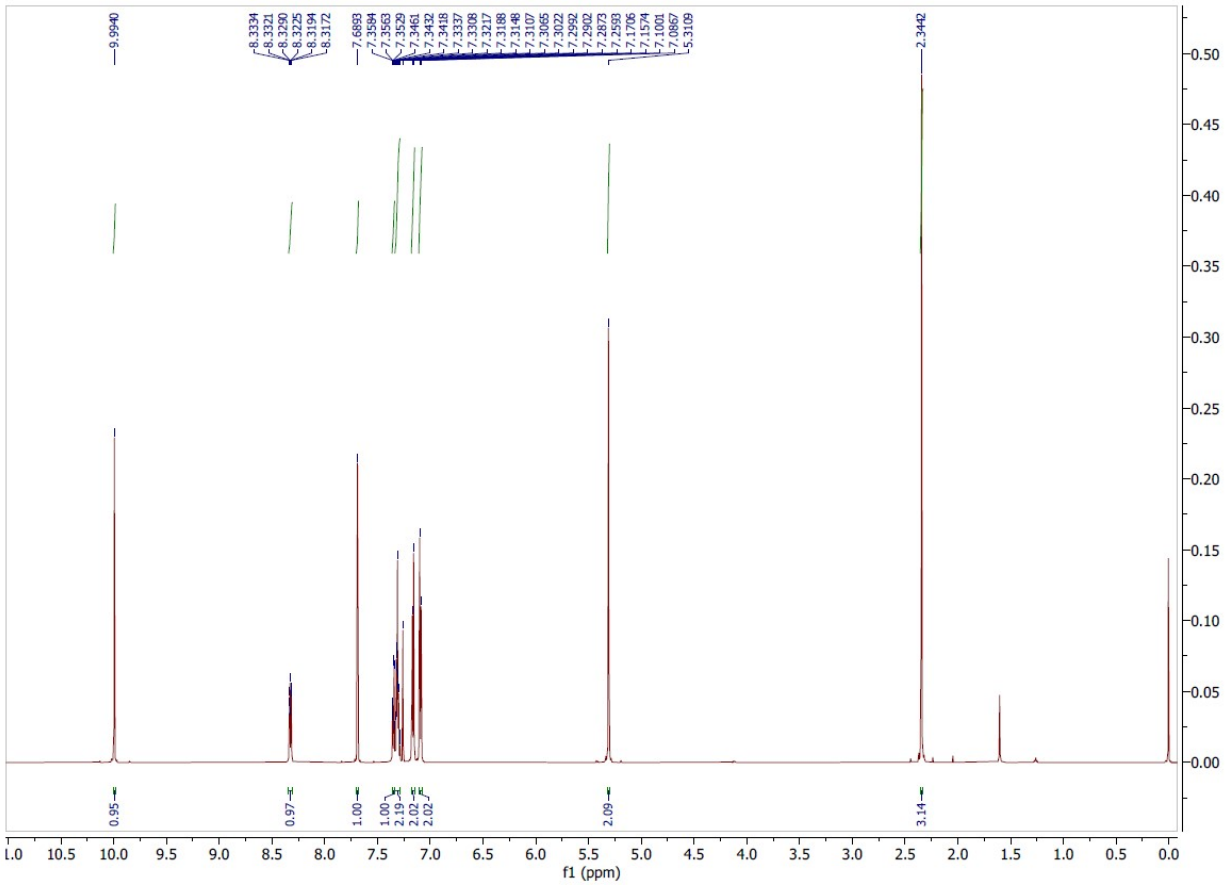


Figure S10. ^{1}H NMR spectrum of compound 2b

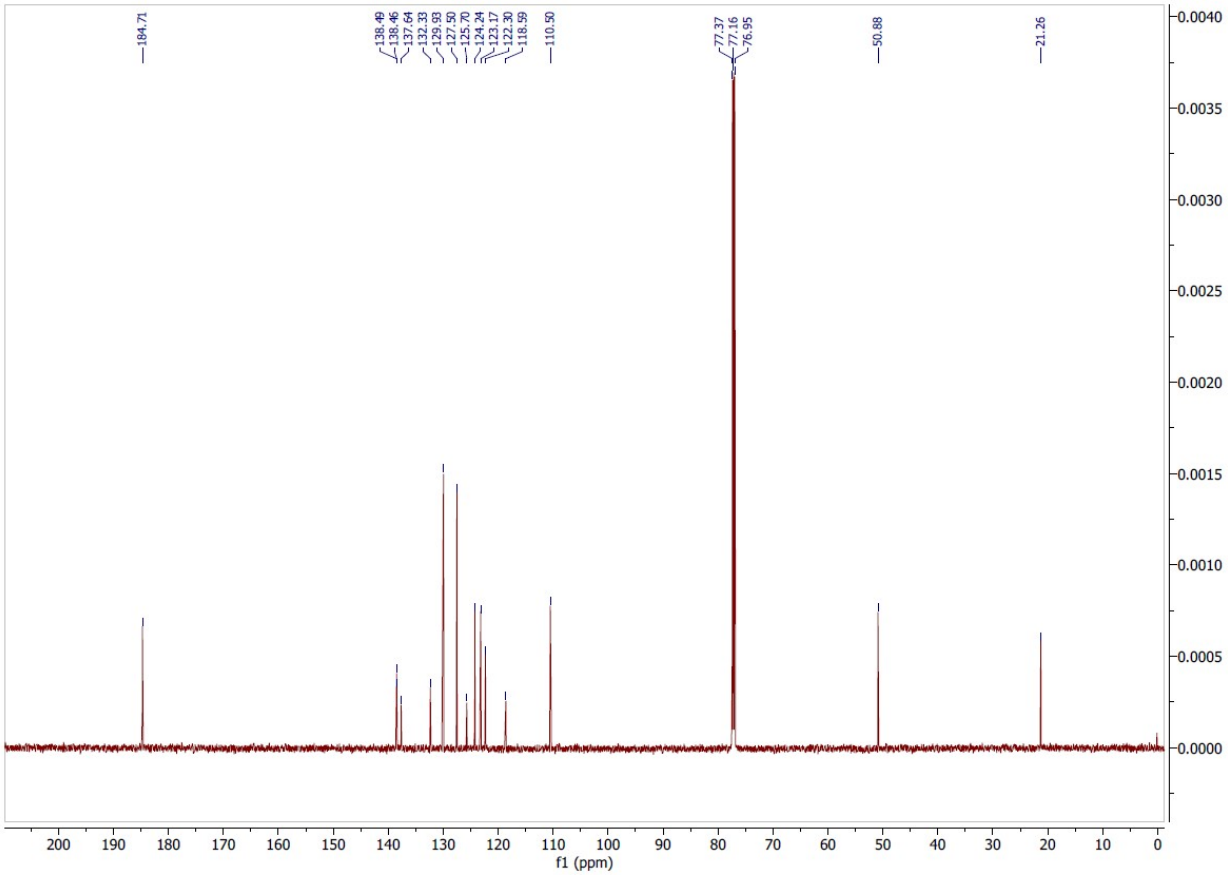


Figure S11. ^{13}C NMR spectrum of compound 2b

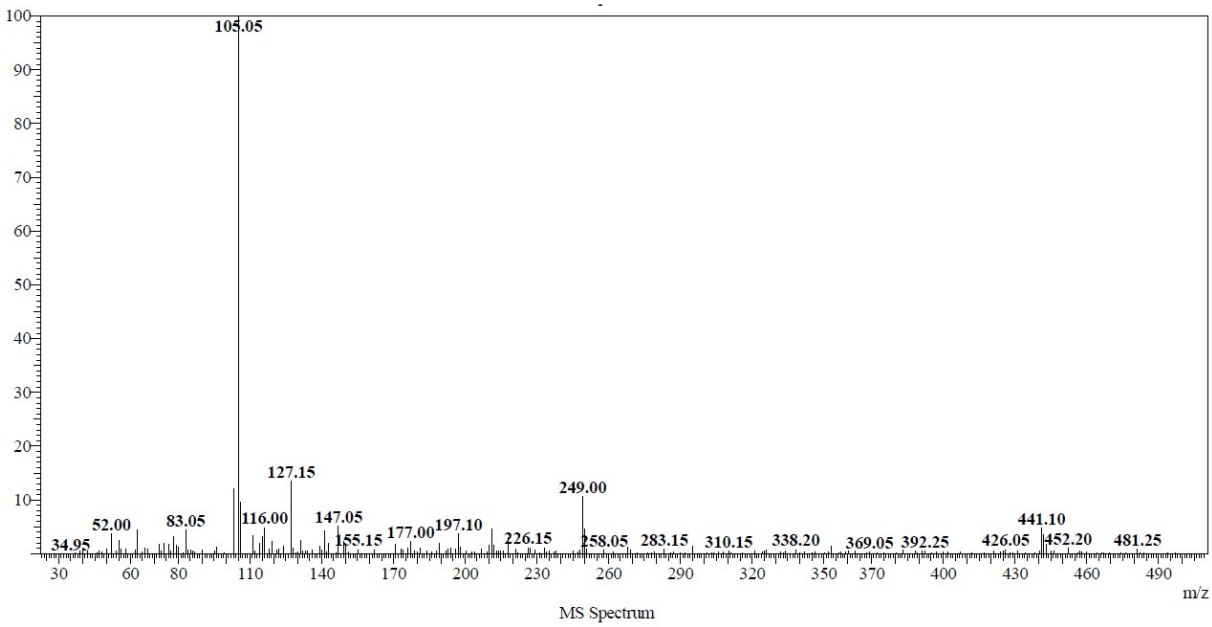


Figure S12. Mass spectrum (ESI-MS) of compound 2b

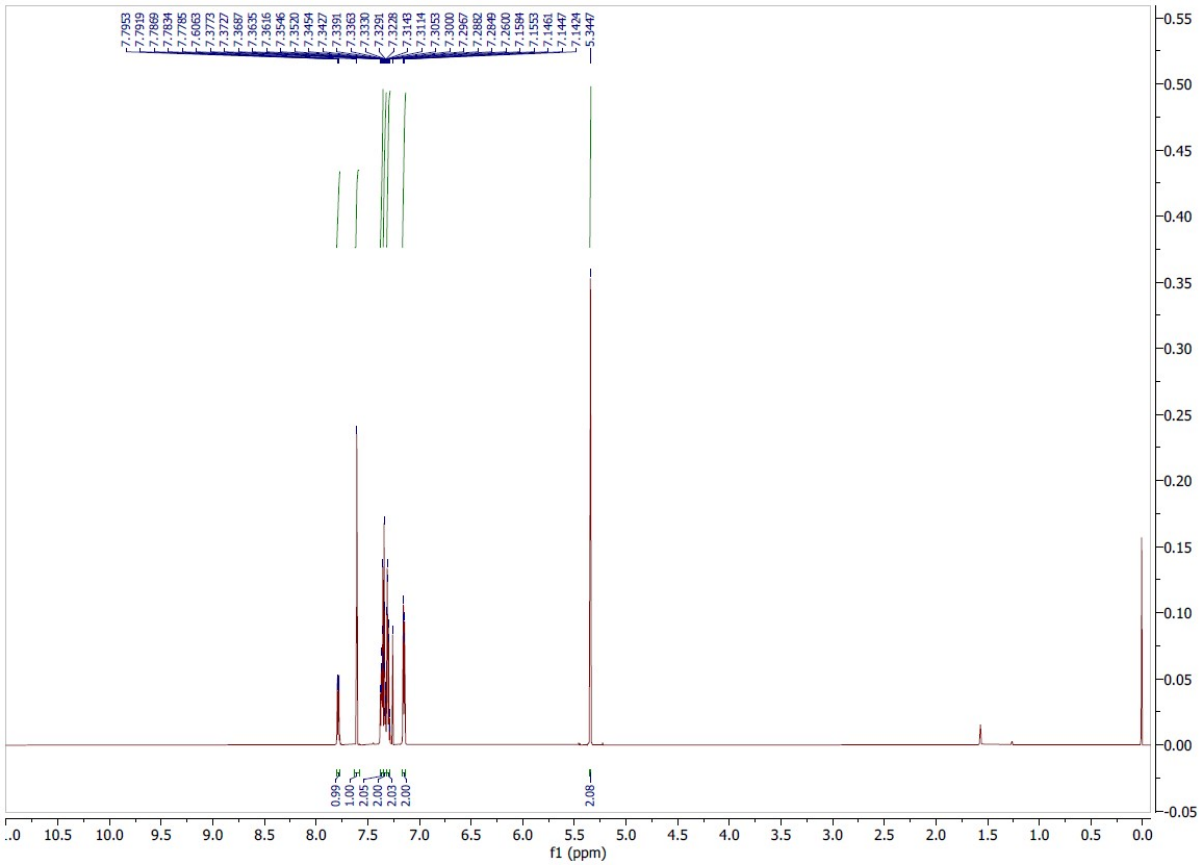


Figure S13. ^{1}H NMR spectrum of compound 3a

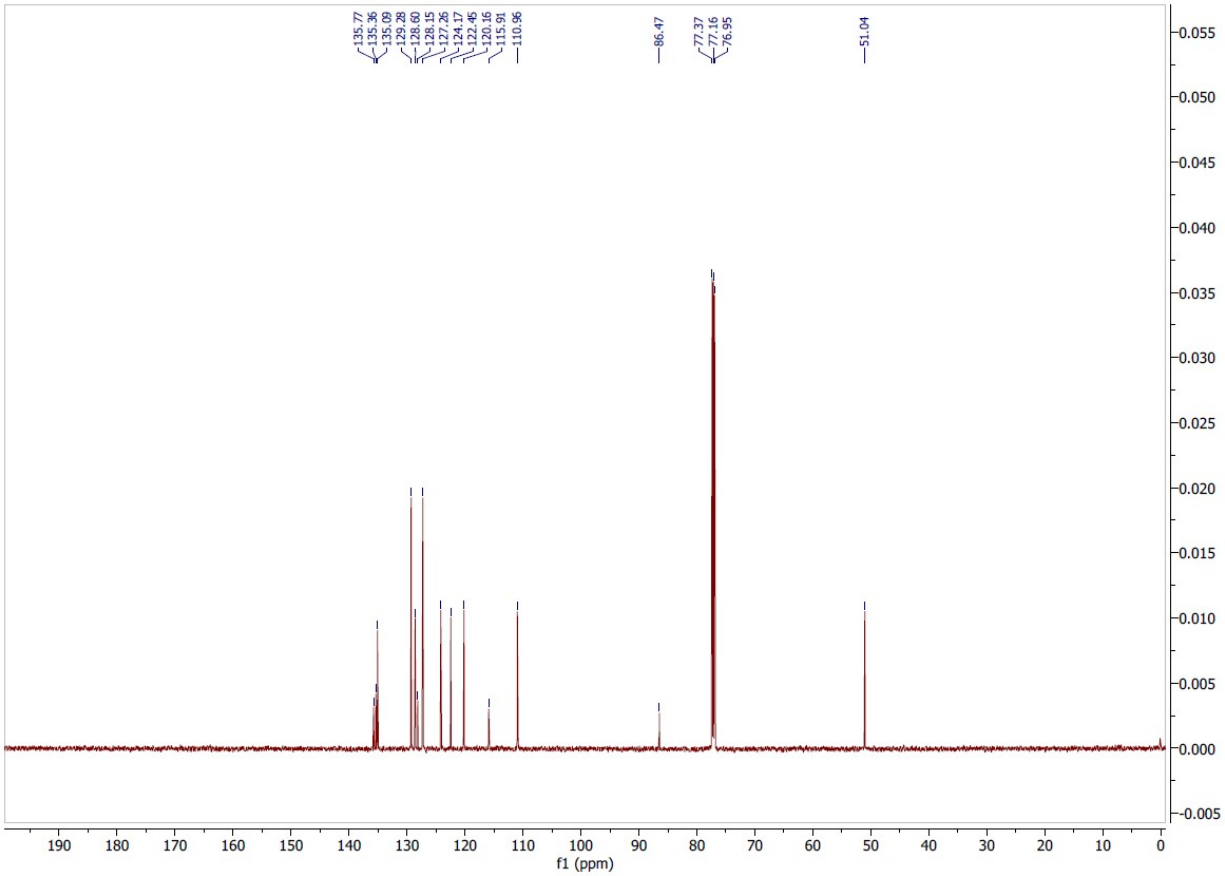


Figure S14. ^{13}C NMR spectrum of compound 3a

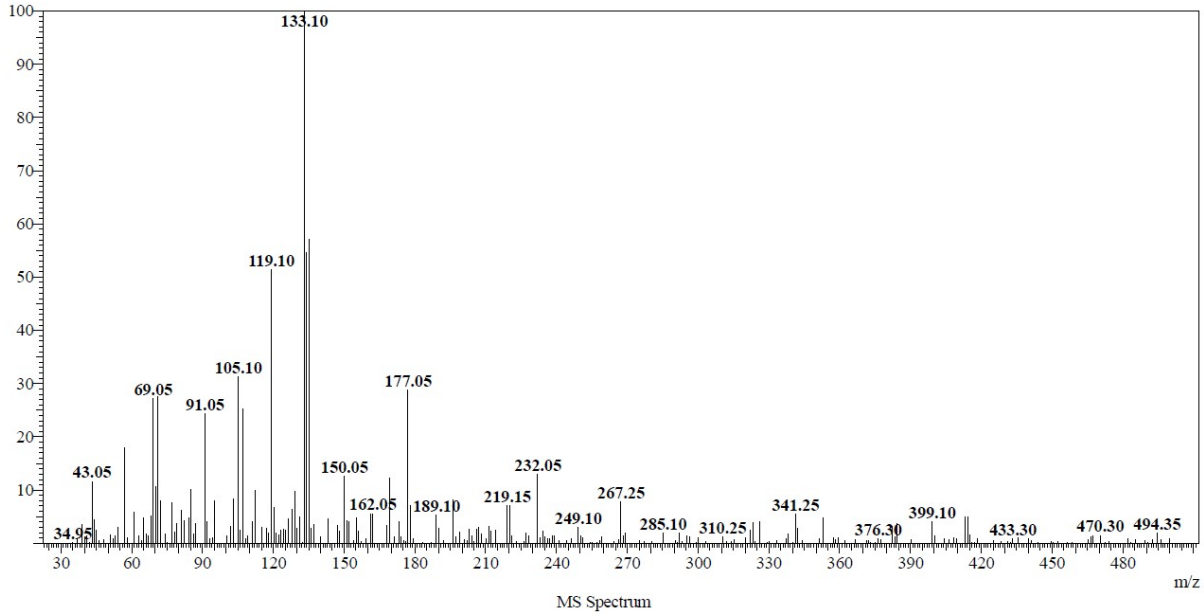


Figure S15. Mass spectrum (ESI-MS) of compound 3a

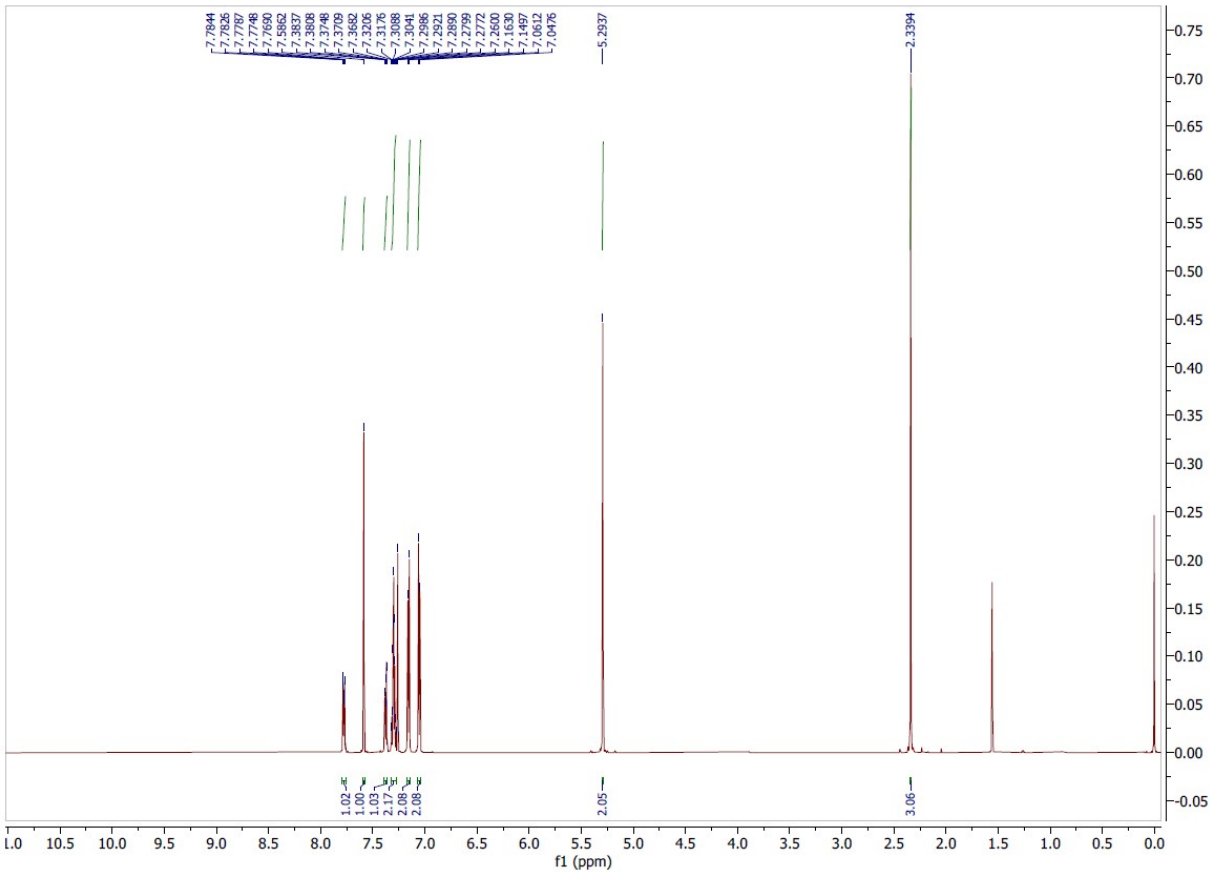


Figure S16. ^{1}H NMR spectrum of compound 3b

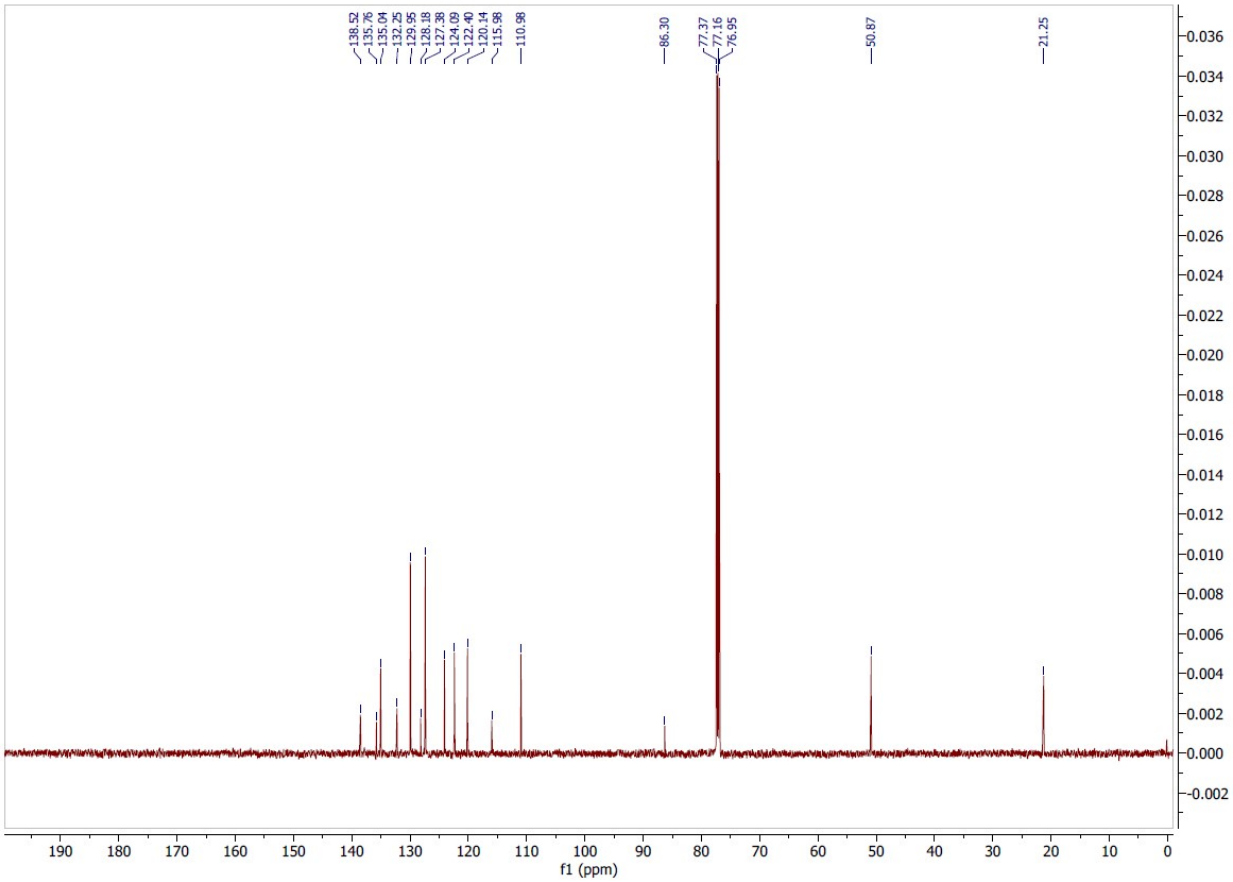


Figure S17. ^{13}C NMR spectrum of compound 3b

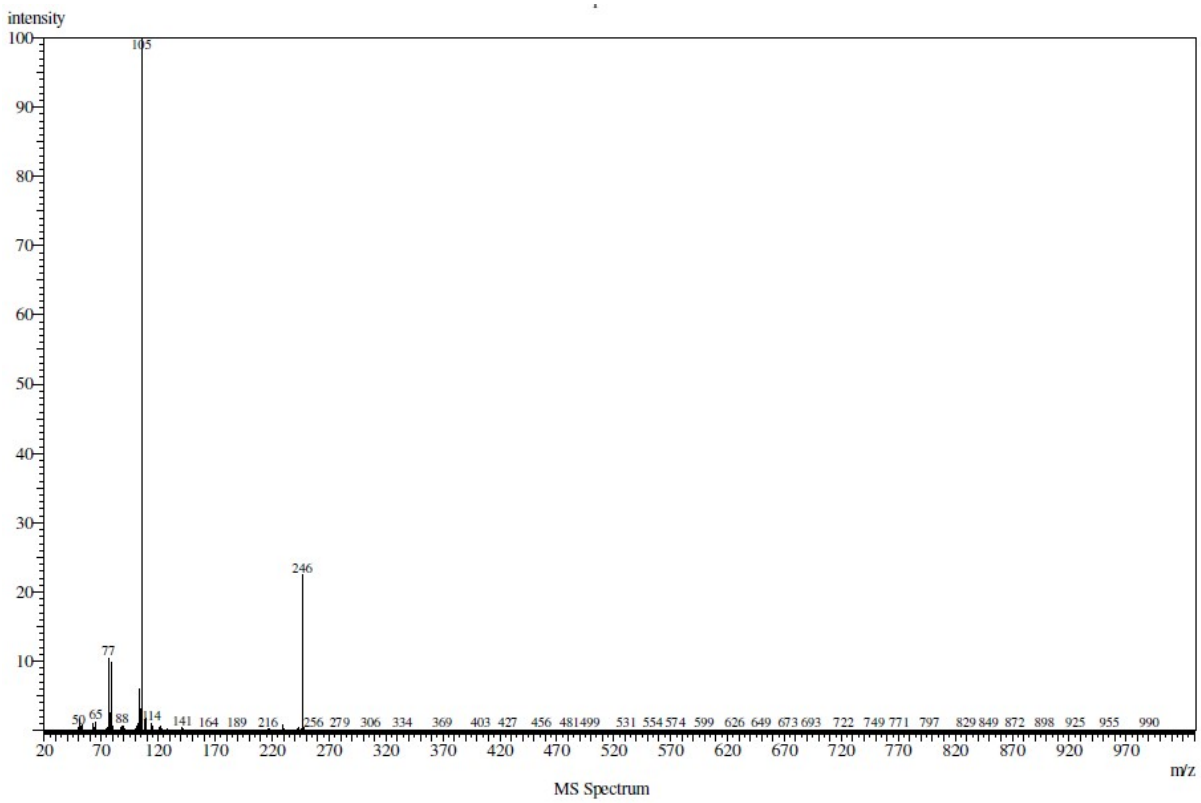


Figure S18. Mass spectrum (ESI-MS) of compound 3b

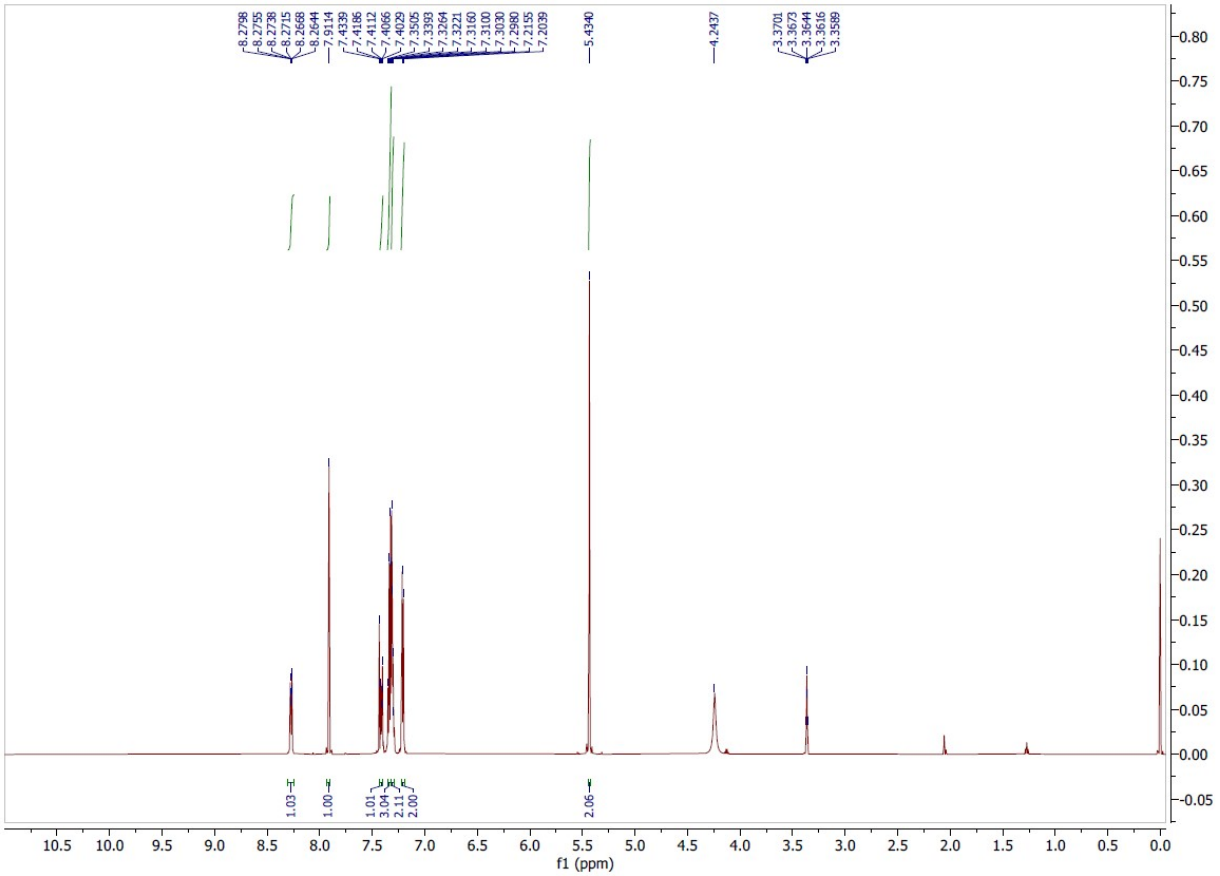


Figure S19. ^{1}H NMR spectrum of compound 4a

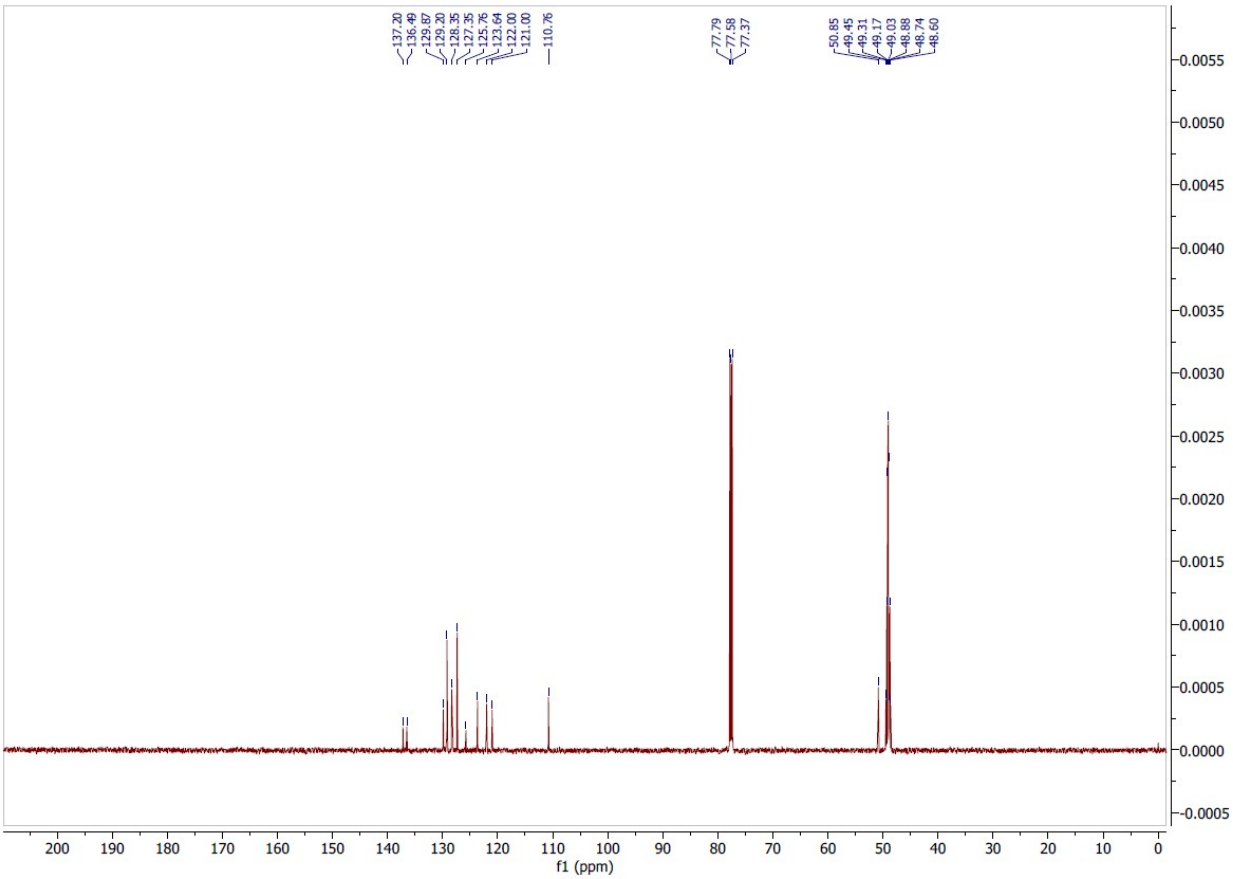


Figure S20. ^{13}C NMR spectrum of compound 4a

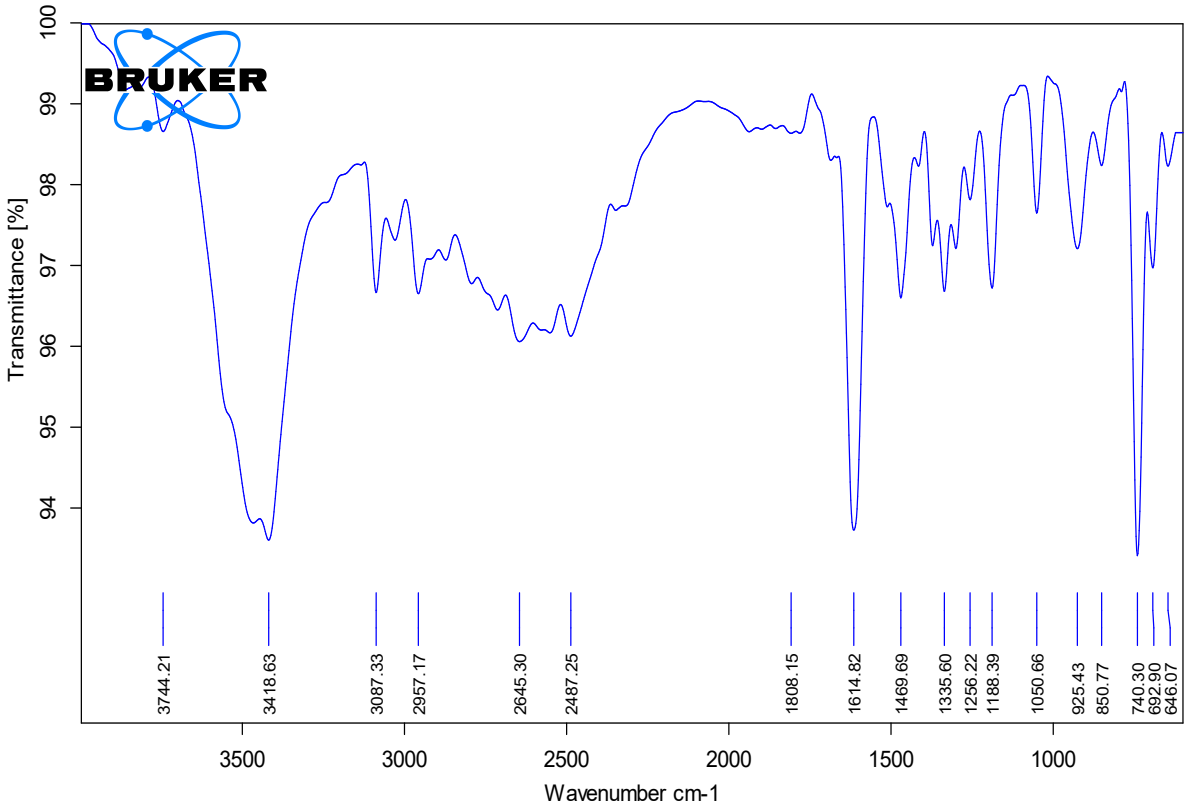


Figure S21. FT-IR spectrum of compound 4a

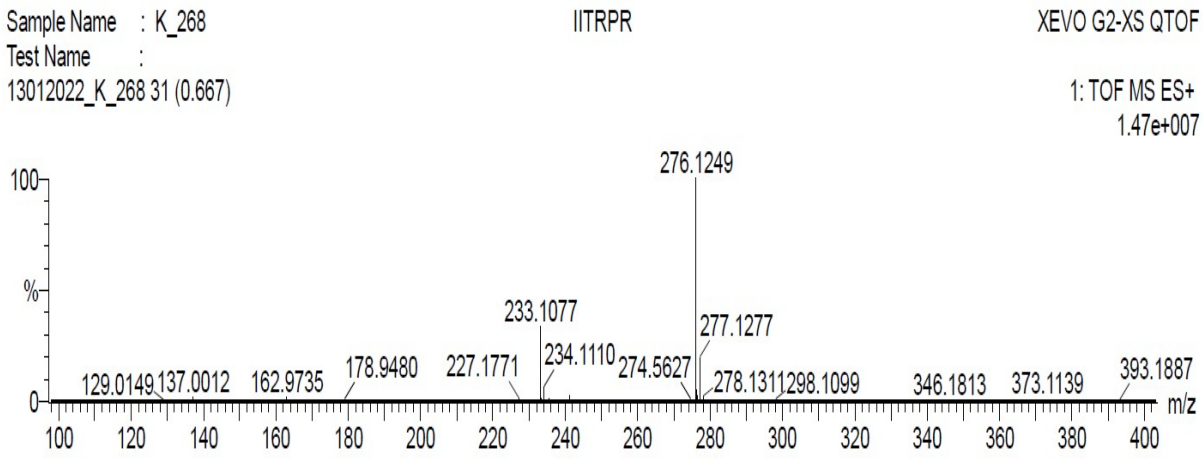


Figure S22. HRMS spectrum of compound 4a

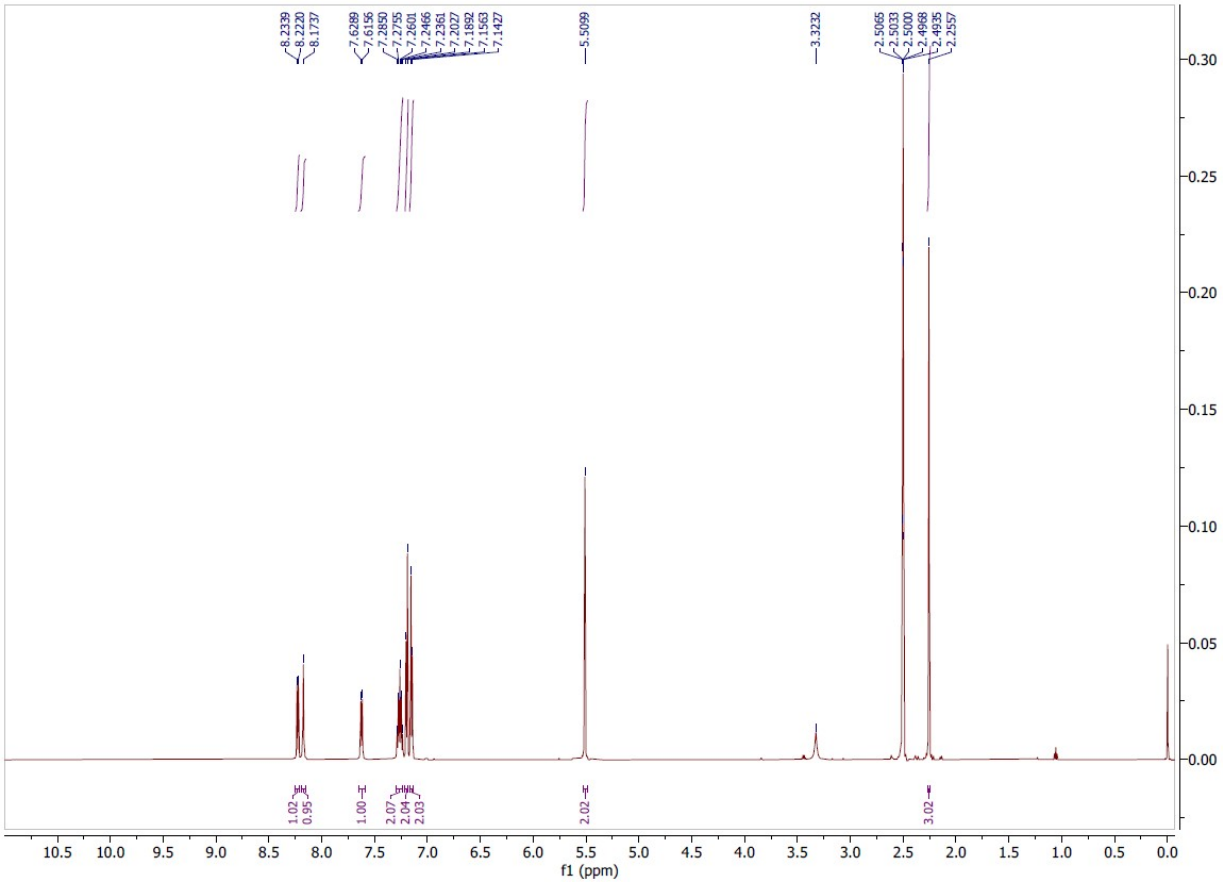


Figure S23. ^{1}H NMR spectrum of compound 4b

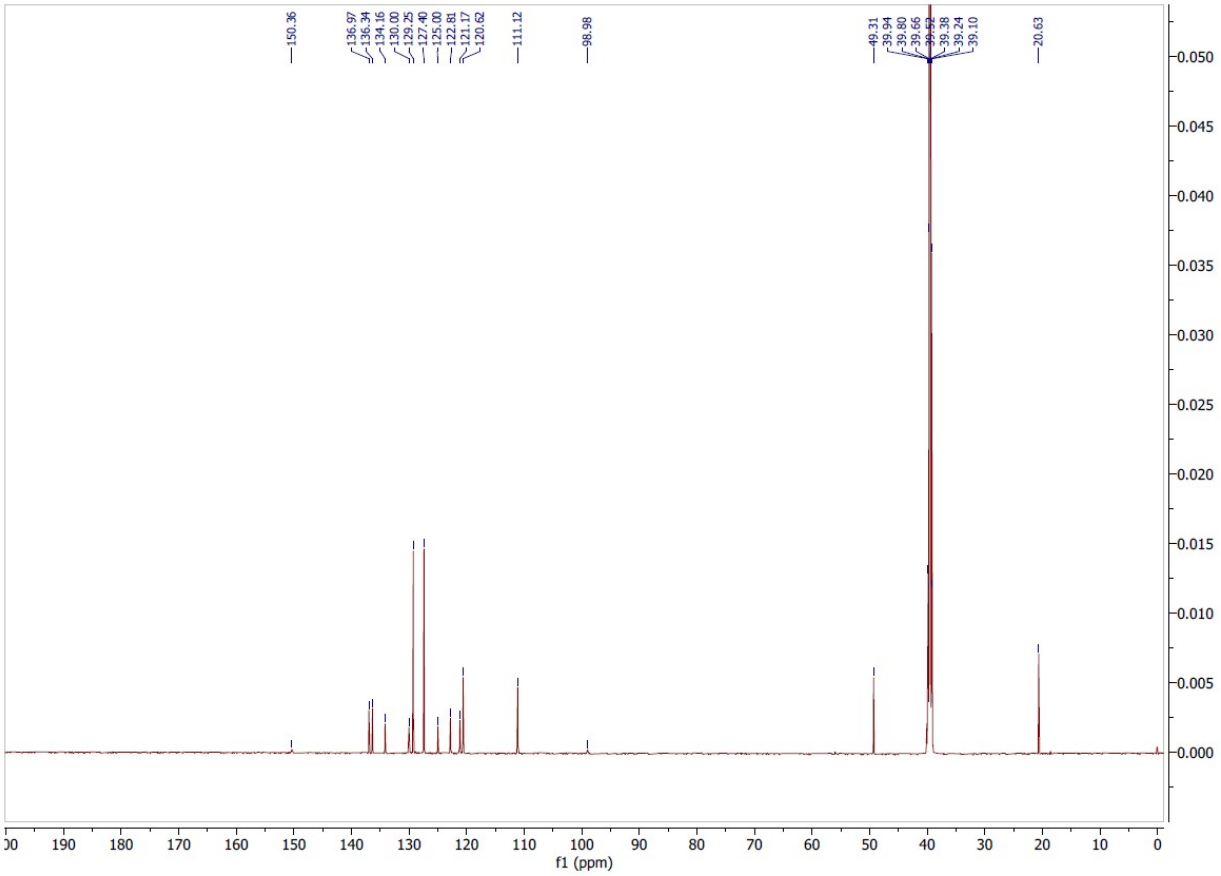


Figure S24. ^{13}C NMR spectrum of compound 4b

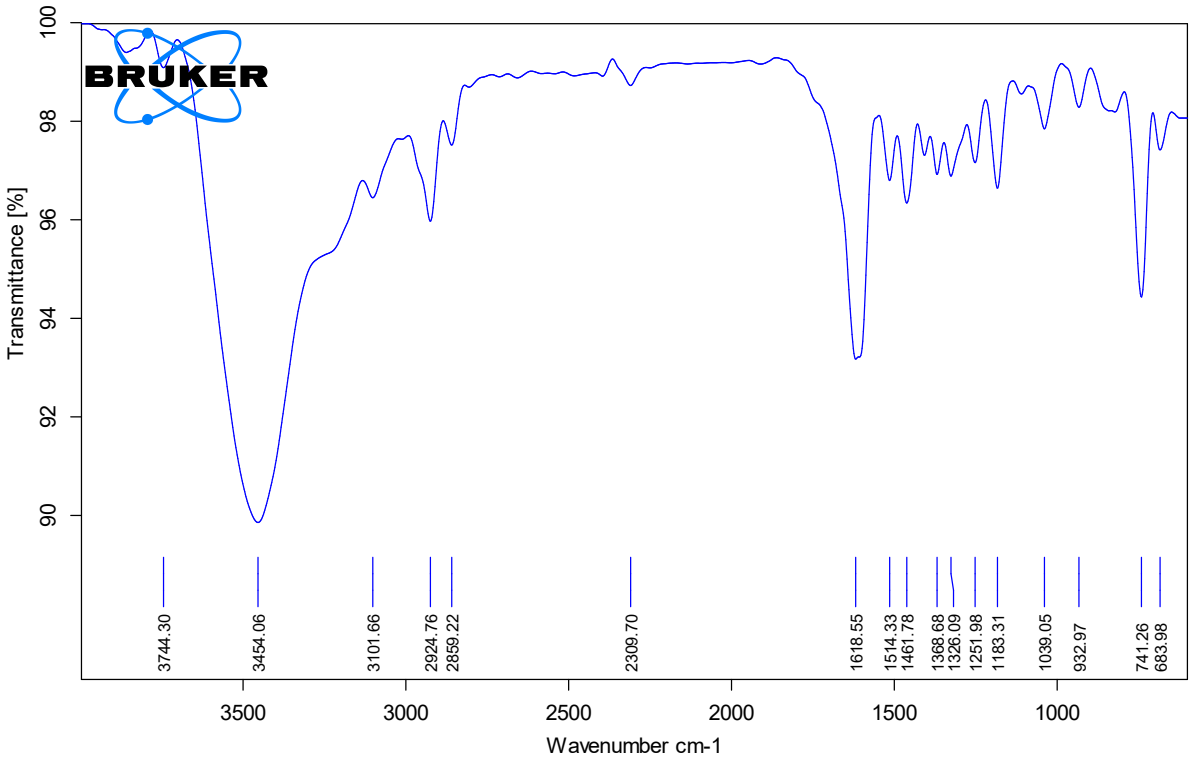


Figure S25. FT-IR spectrum of compound 4b

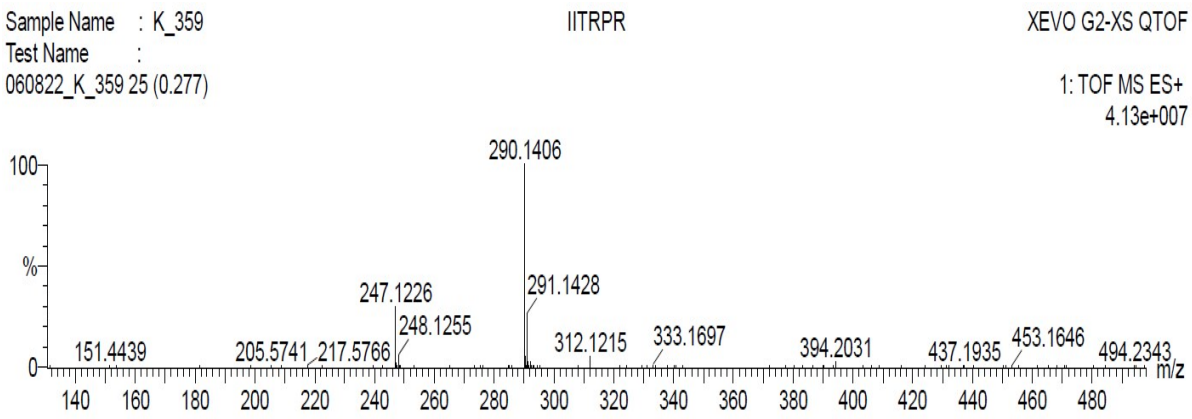


Figure S26. HRMS spectrum of compound 4b

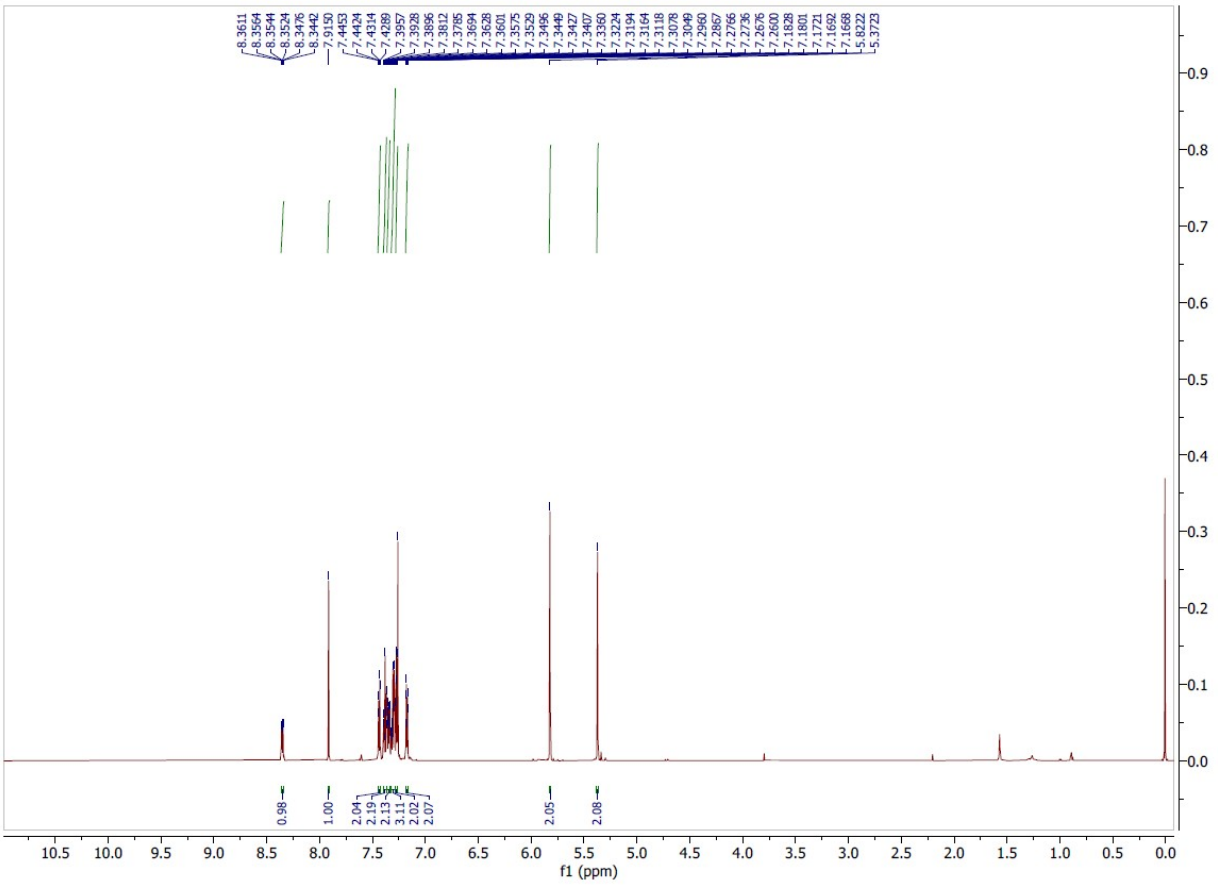


Figure S27. ^{1}H NMR spectrum of compound 5a

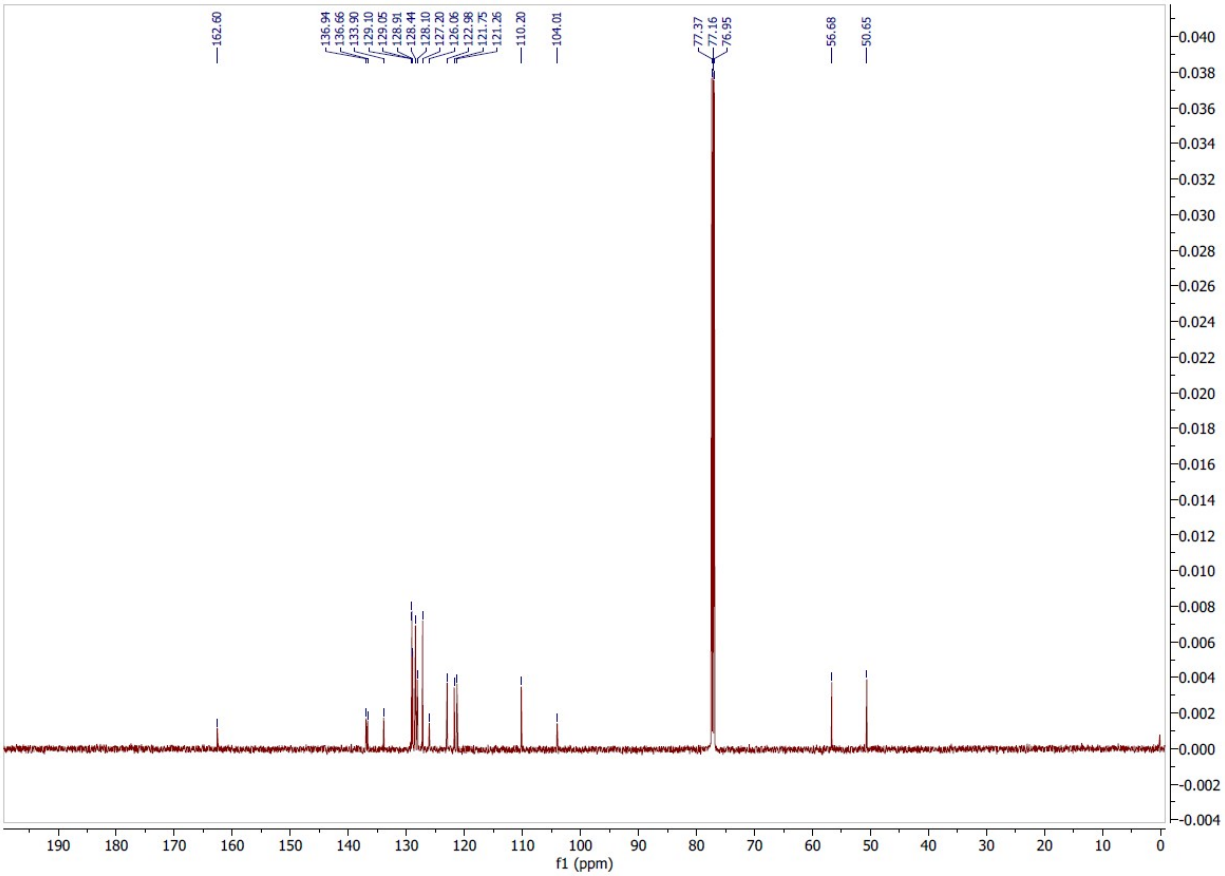


Figure S28. ^{13}C NMR spectrum of compound 5a

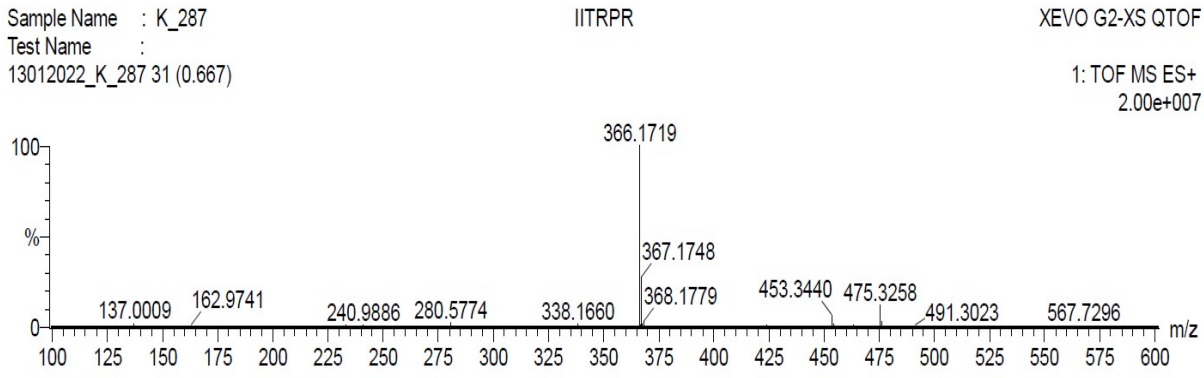


Figure S29. HRMS spectrum of compound 5a

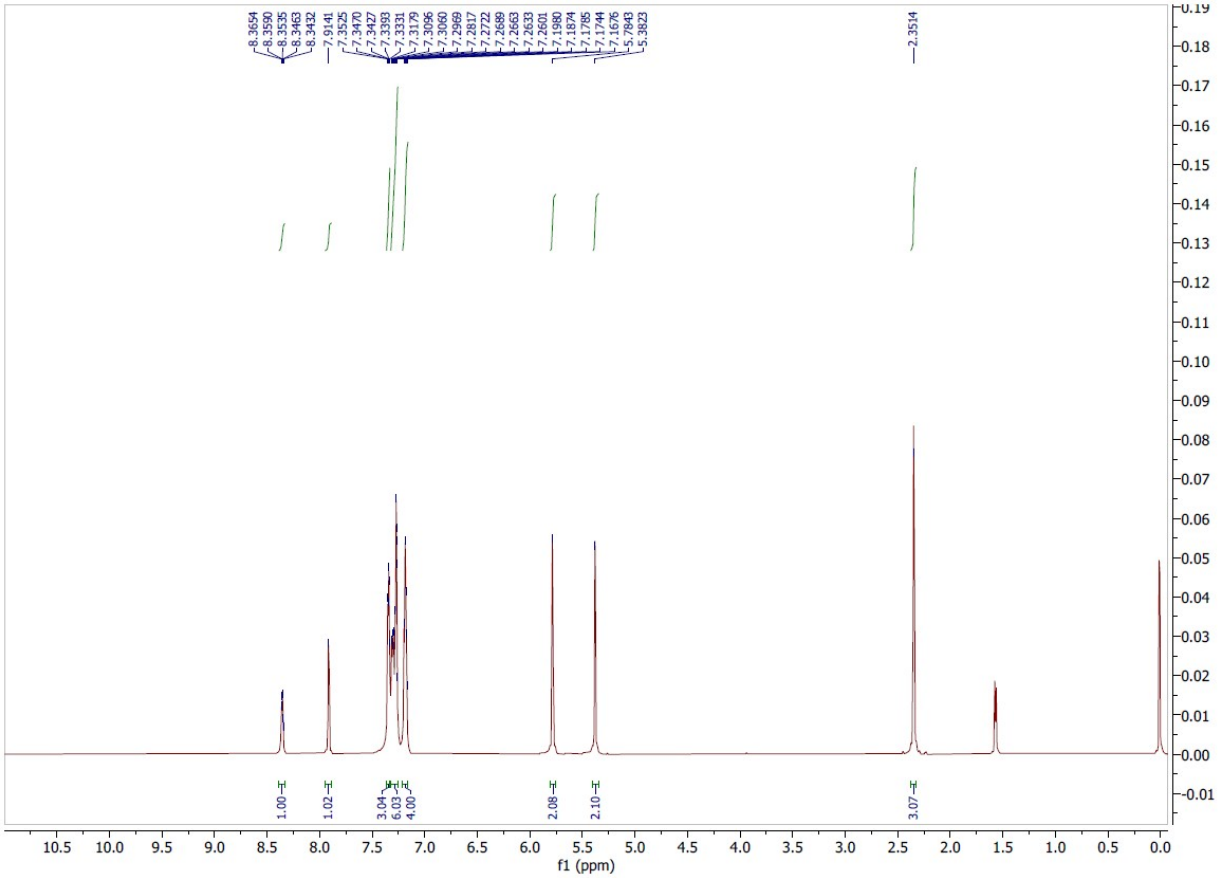


Figure S30. ^{1}H NMR spectrum of compound 5b

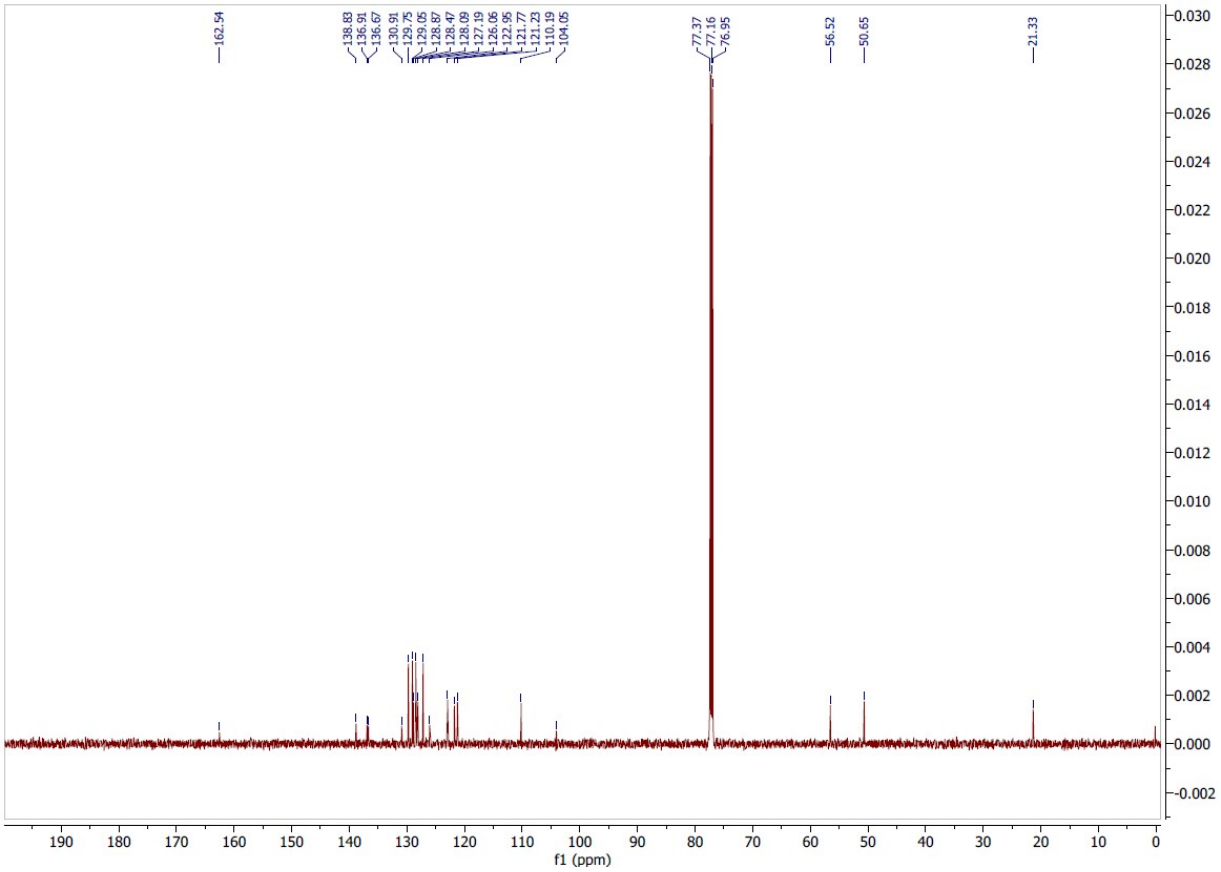


Figure S31. ^{13}C NMR spectrum of compound 5b

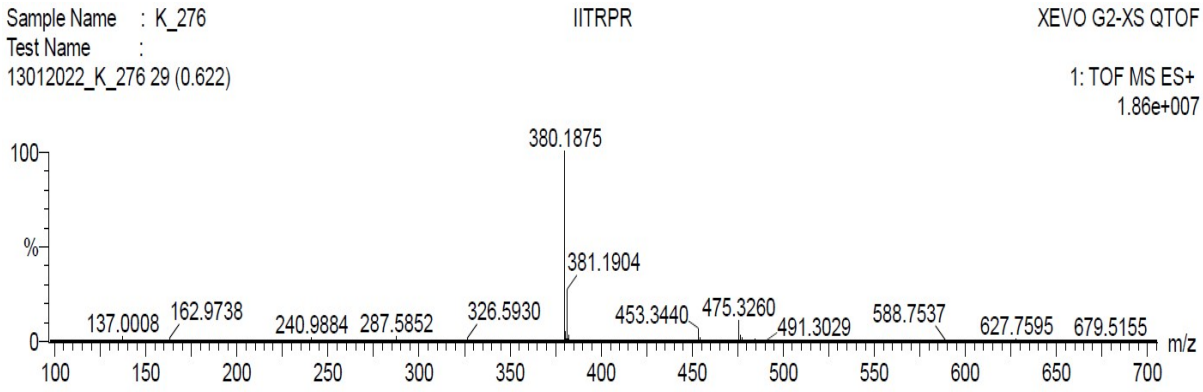


Figure S32. HRMS spectrum of compound 5b

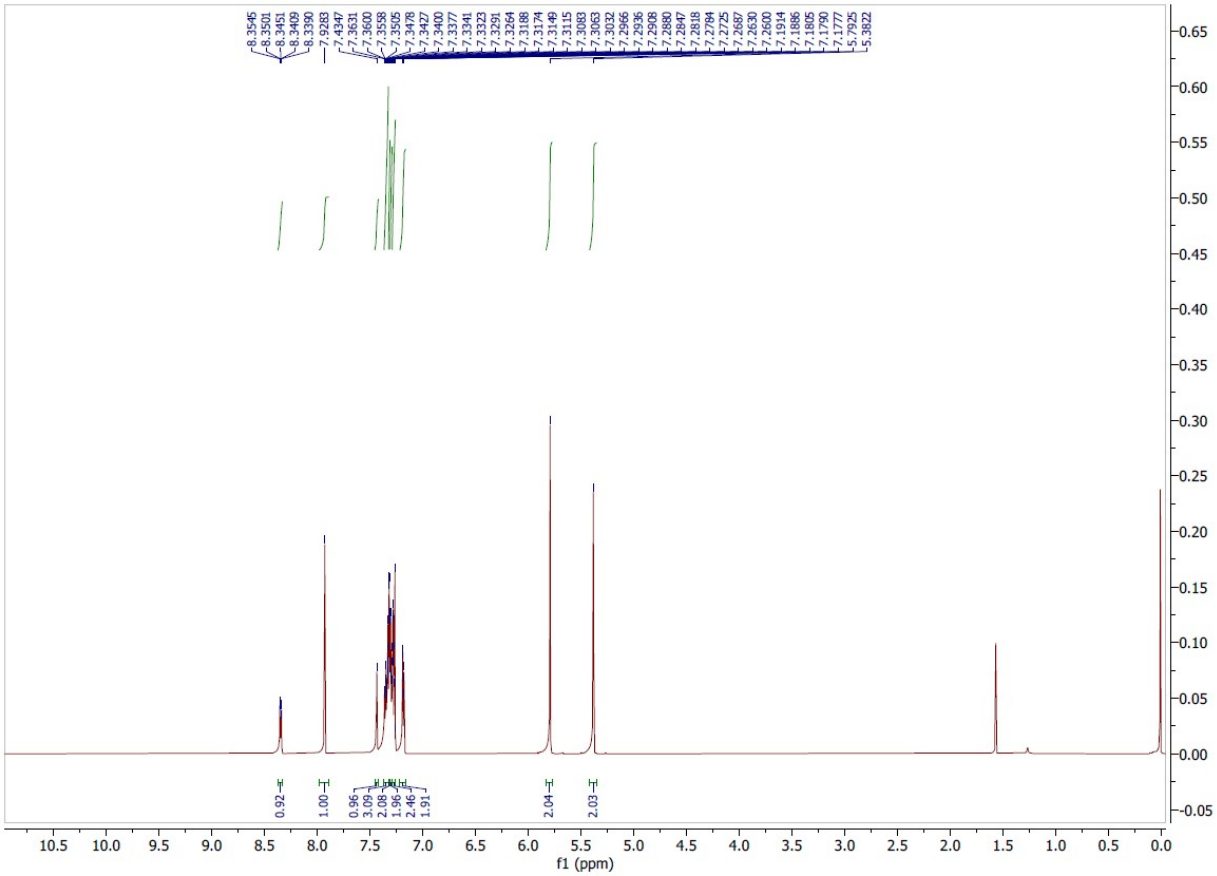


Figure S33. ^{1}H NMR spectrum of compound 5c

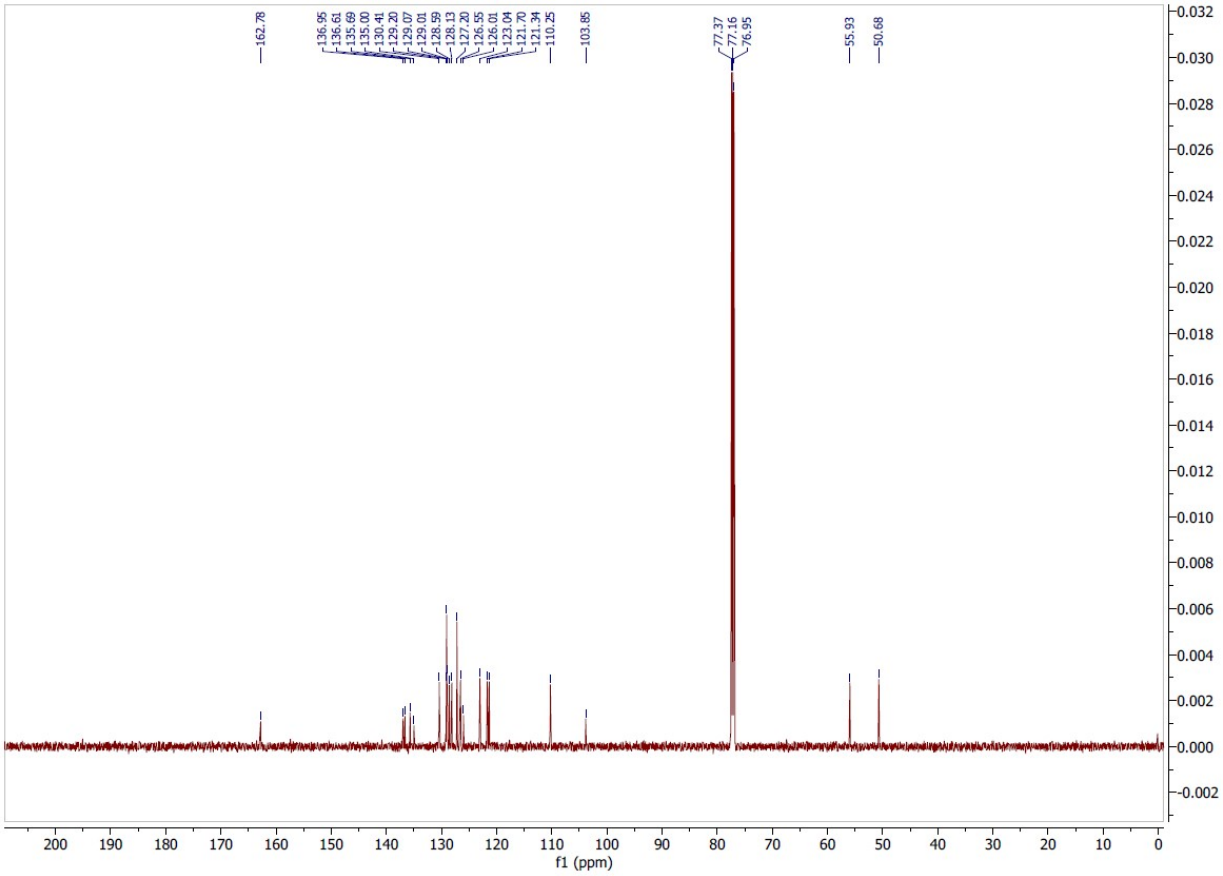


Figure S34. ^{13}C NMR spectrum of compound 5c

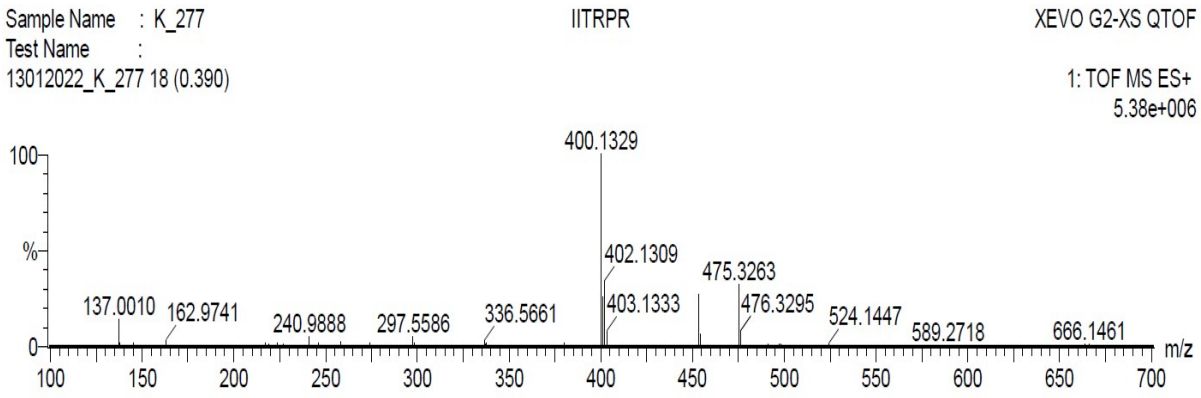


Figure S35. HRMS spectrum of compound 5c

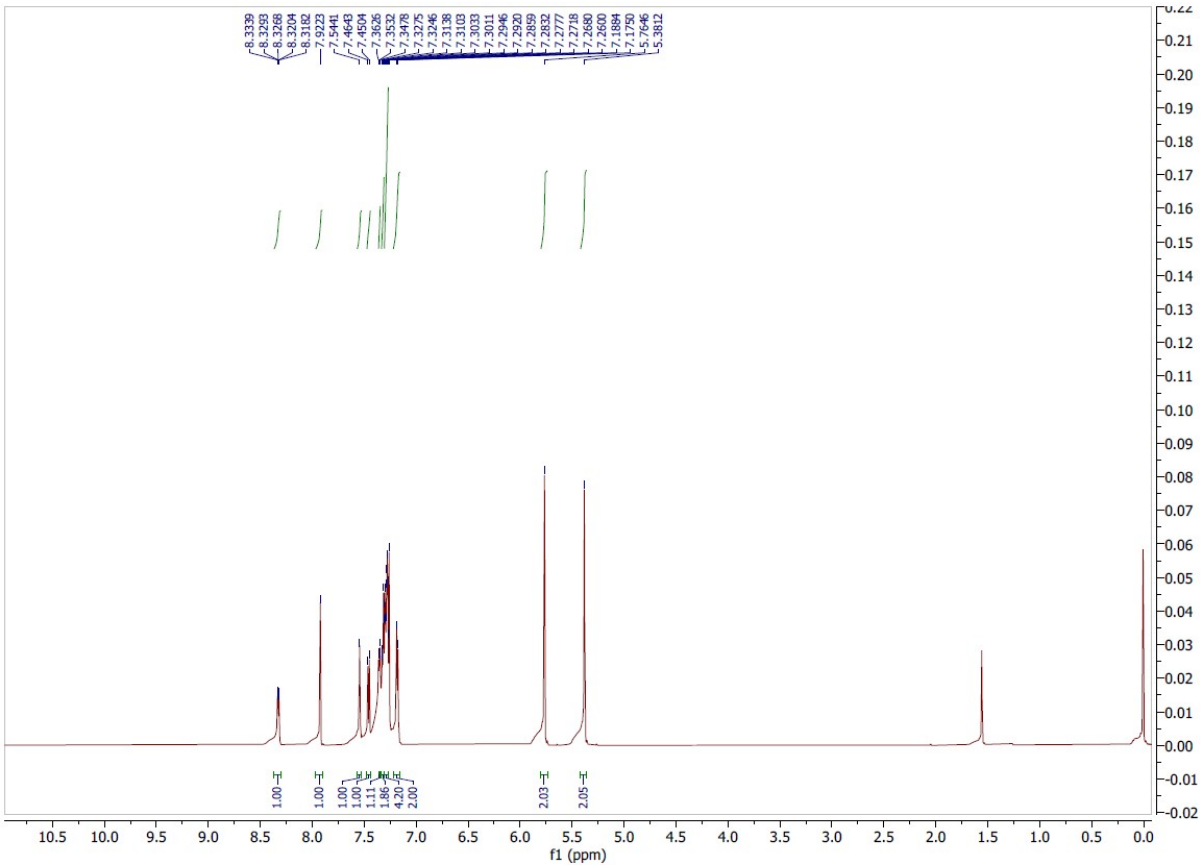


Figure S36. ^{1}H NMR spectrum of compound 5d

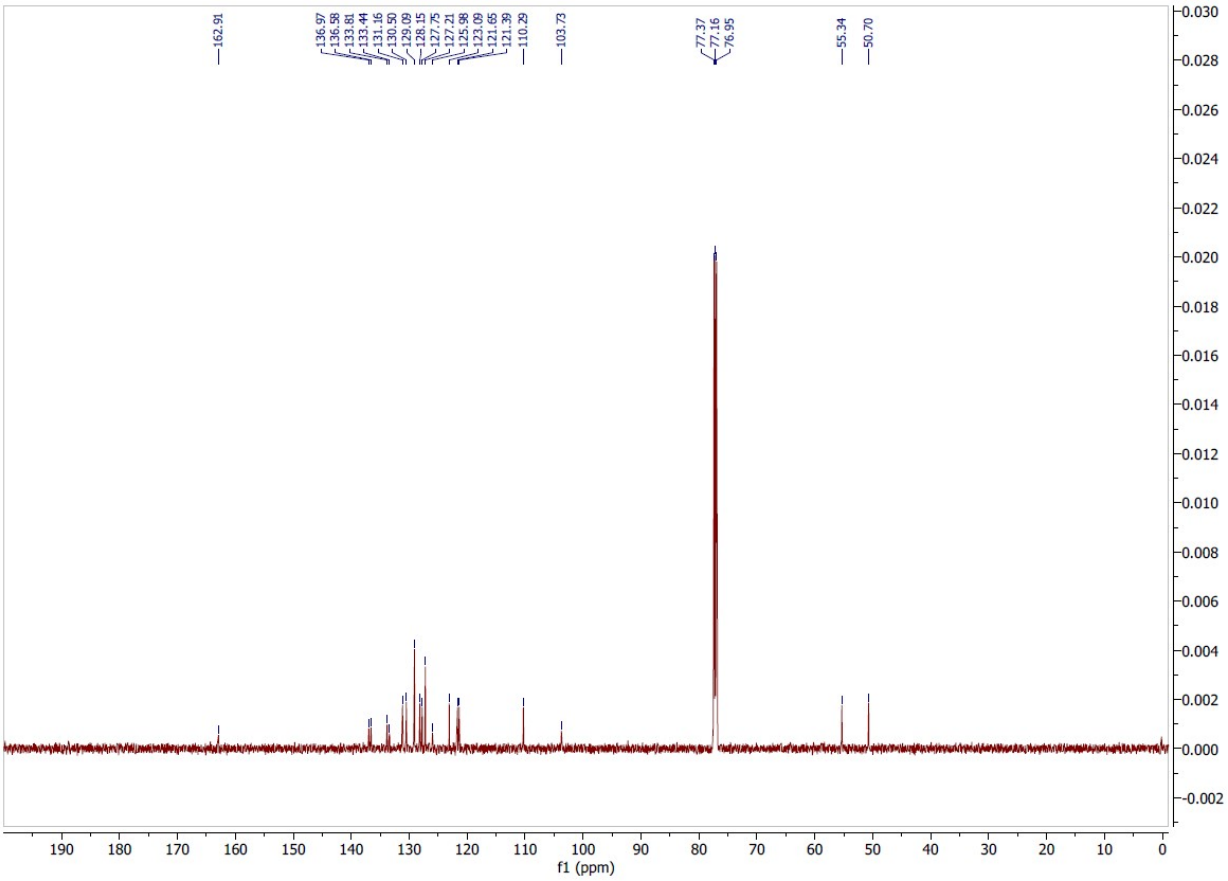


Figure S37. ^{13}C NMR spectrum of compound 5d

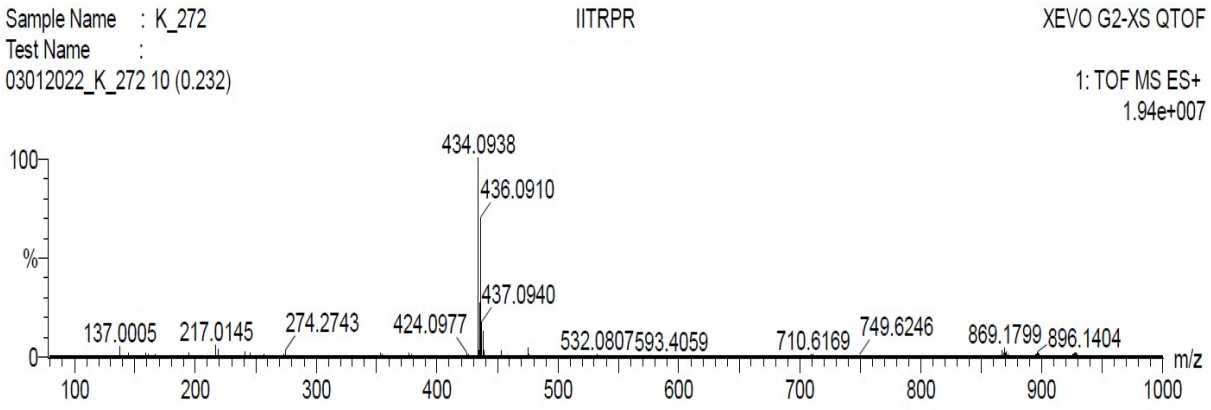


Figure S38. HRMS spectrum of compound 5d

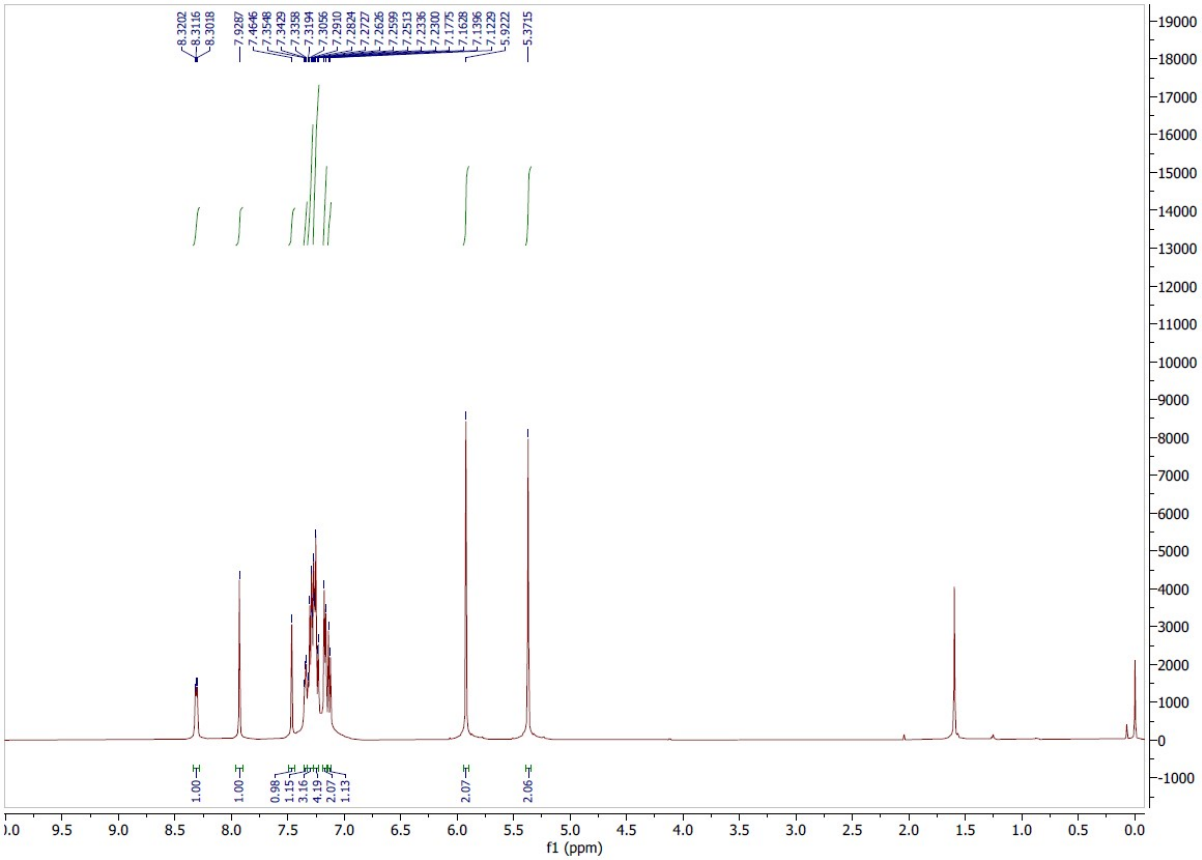


Figure S39. ^{1}H NMR spectrum of compound 5e

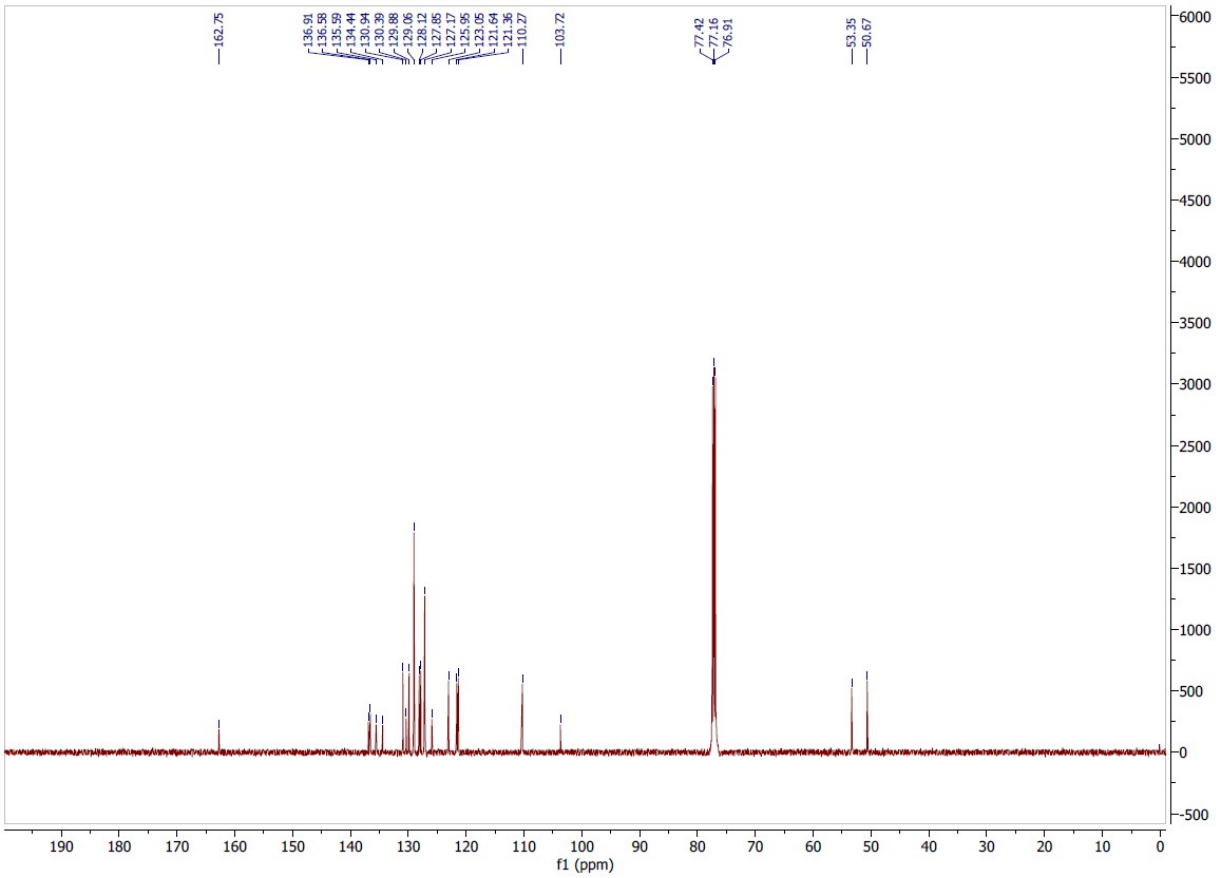


Figure S40. ^{13}C NMR spectrum of compound 5e

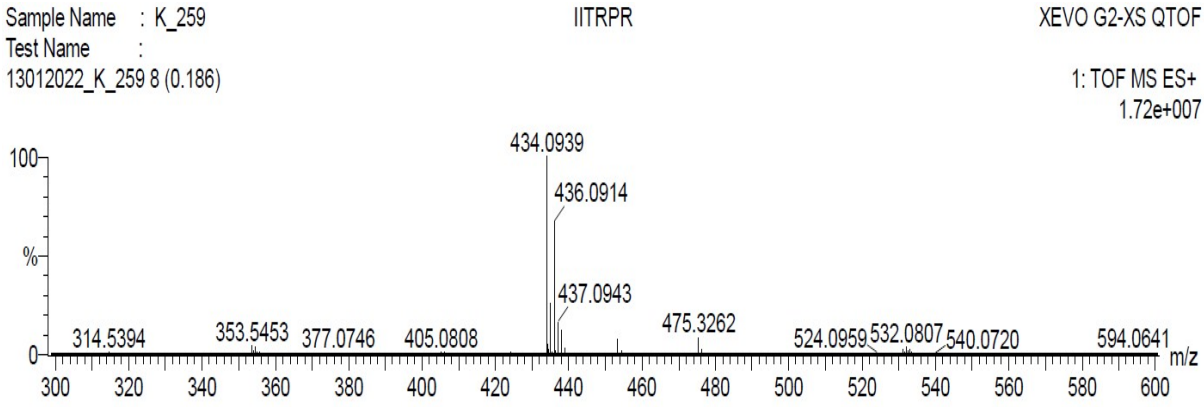


Figure S41. HRMS spectrum of compound 5e

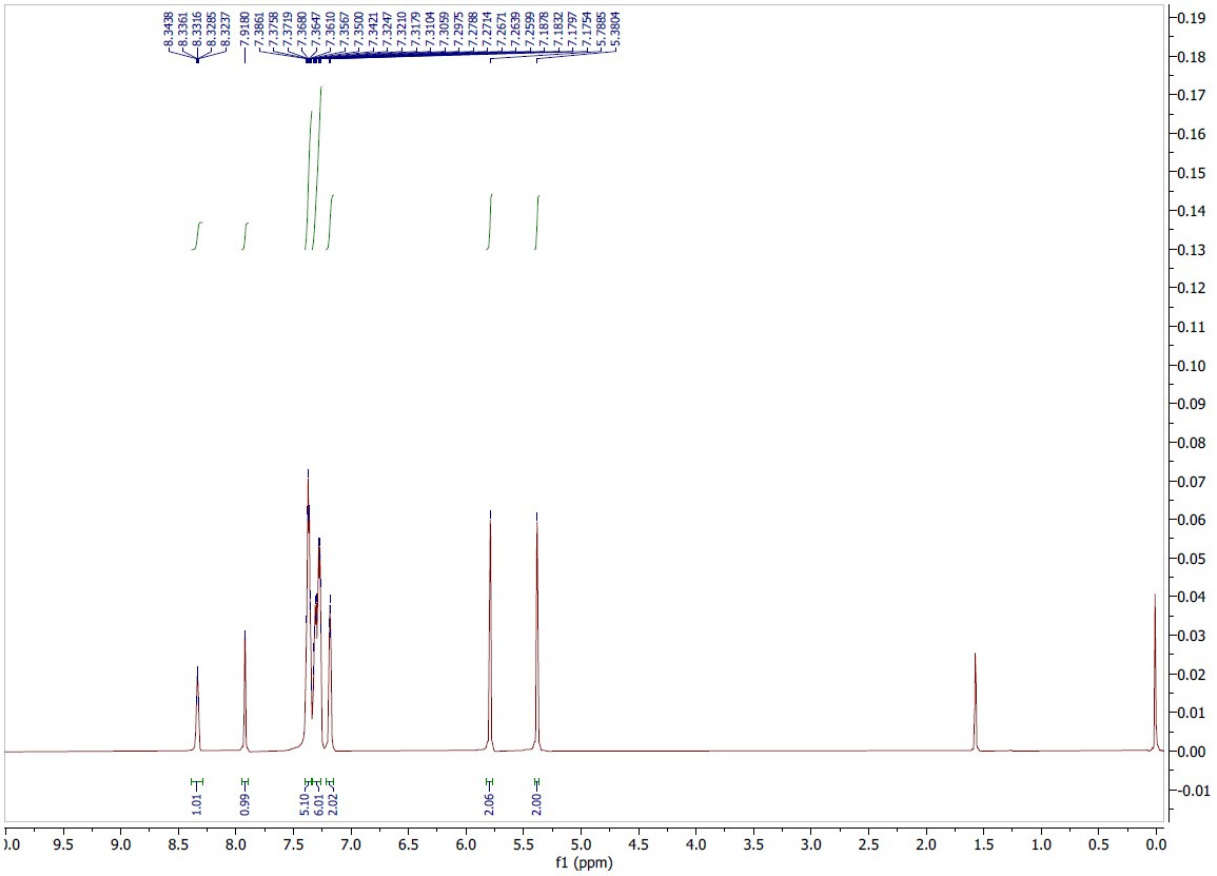


Figure S42. ^{1}H NMR spectrum of compound 5f

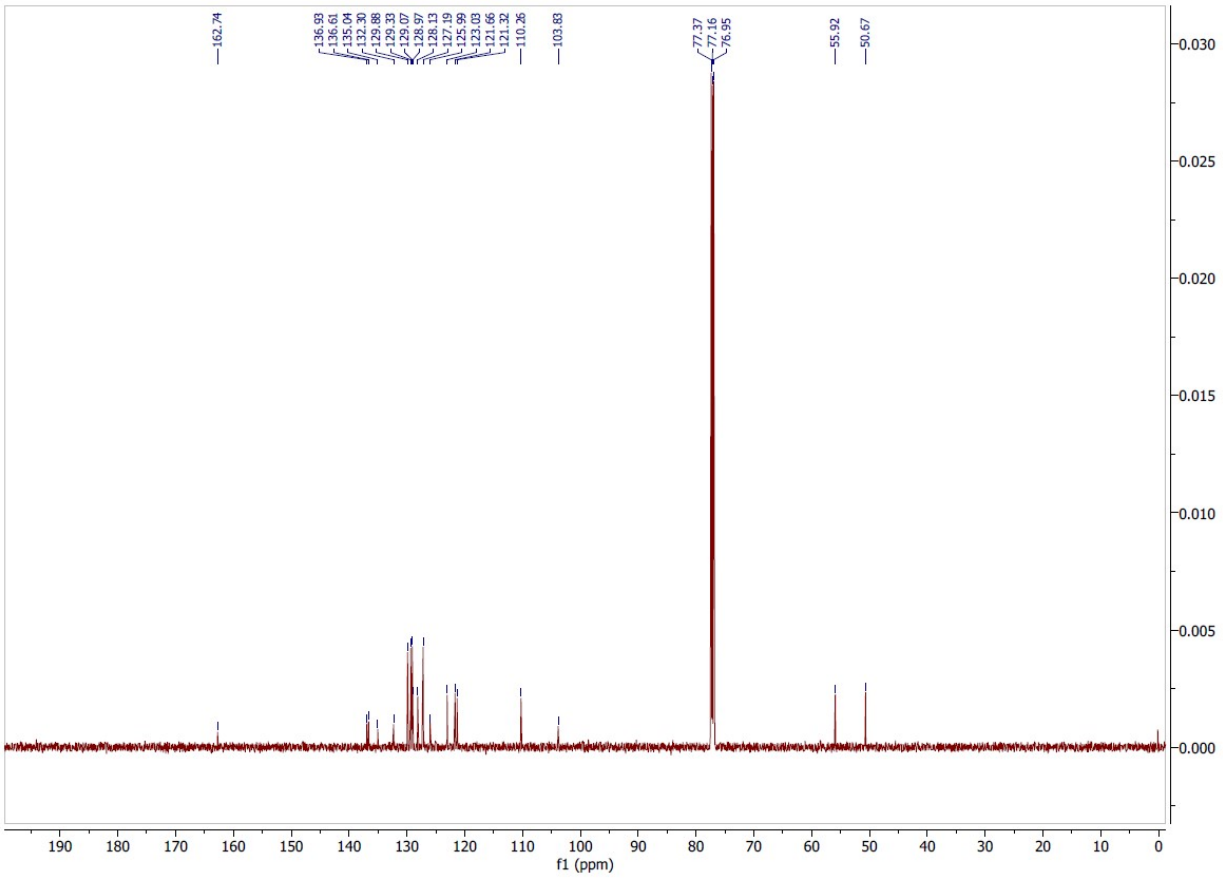


Figure S43. ^{13}C NMR spectrum of compound 5f

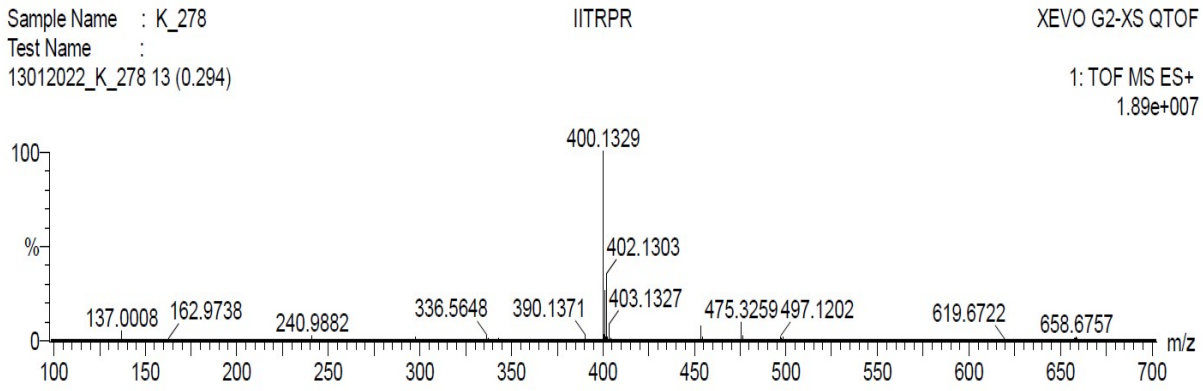


Figure S44. HRMS spectrum of compound 5f

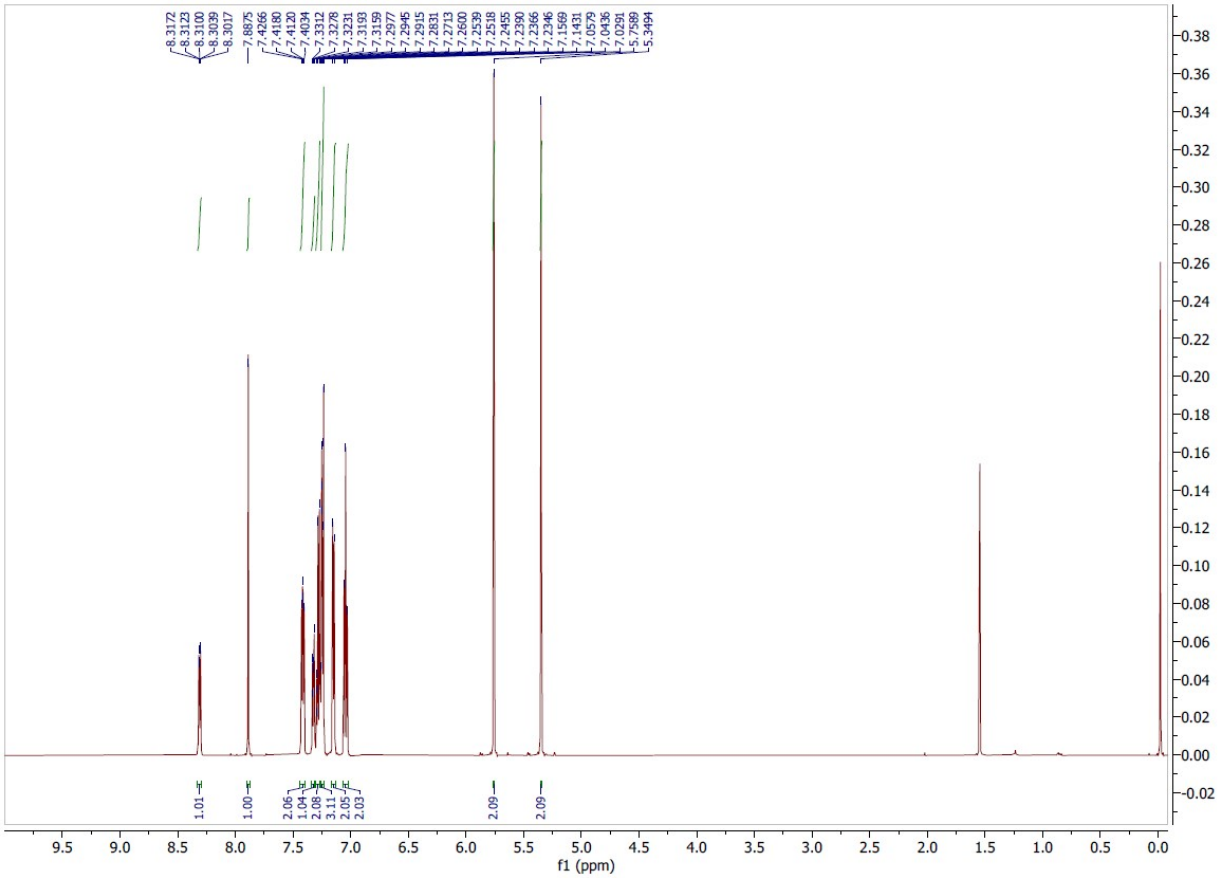


Figure S45. ^{1}H NMR spectrum of compound 5g

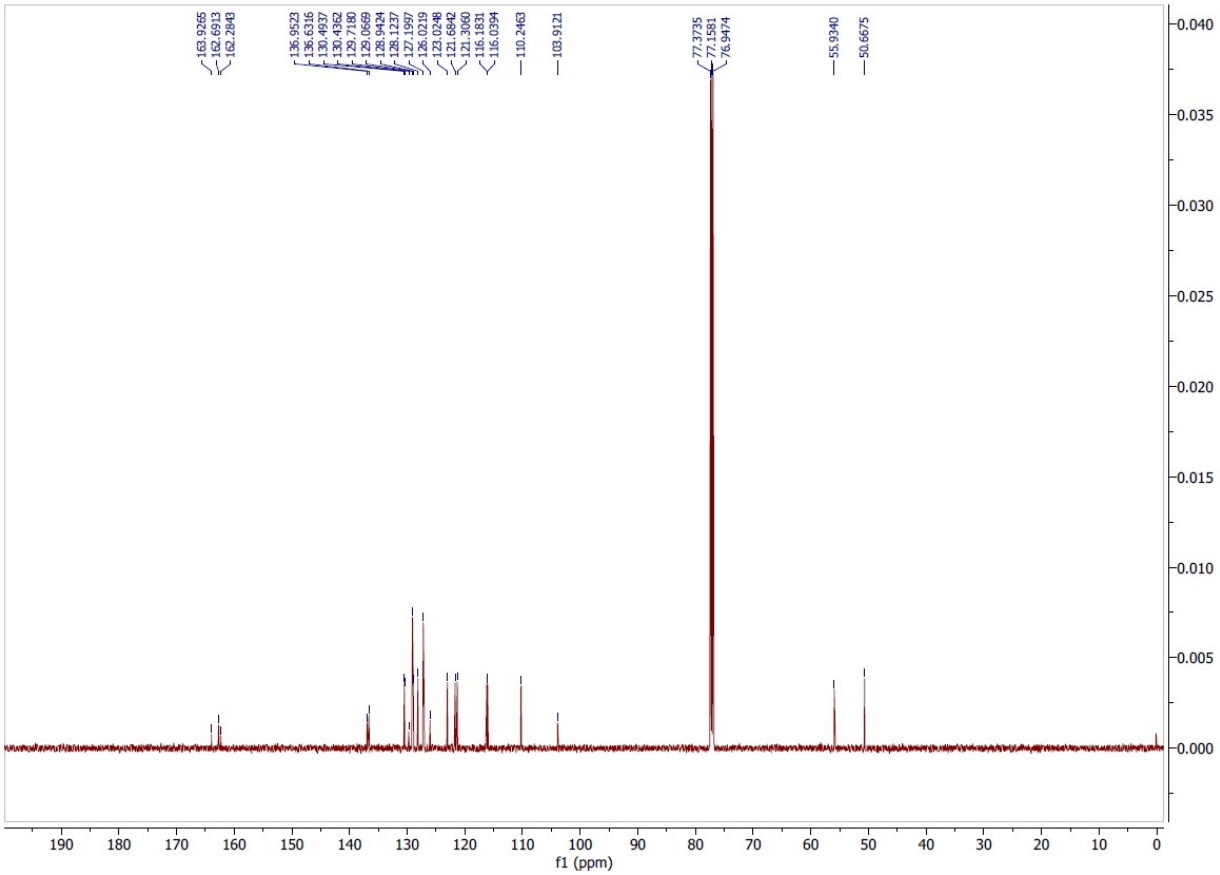


Figure S46. ^{13}C NMR spectrum of compound 5g

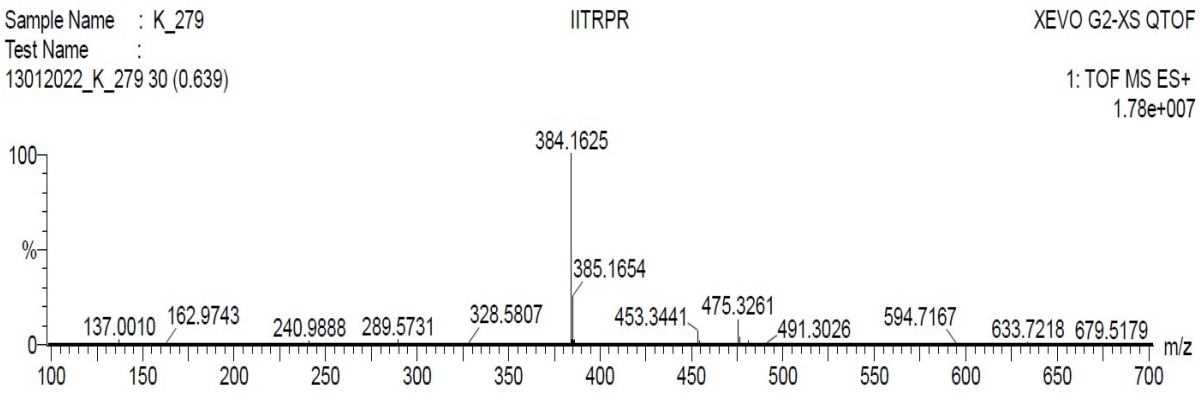


Figure S47. HRMS spectrum of compound 5g

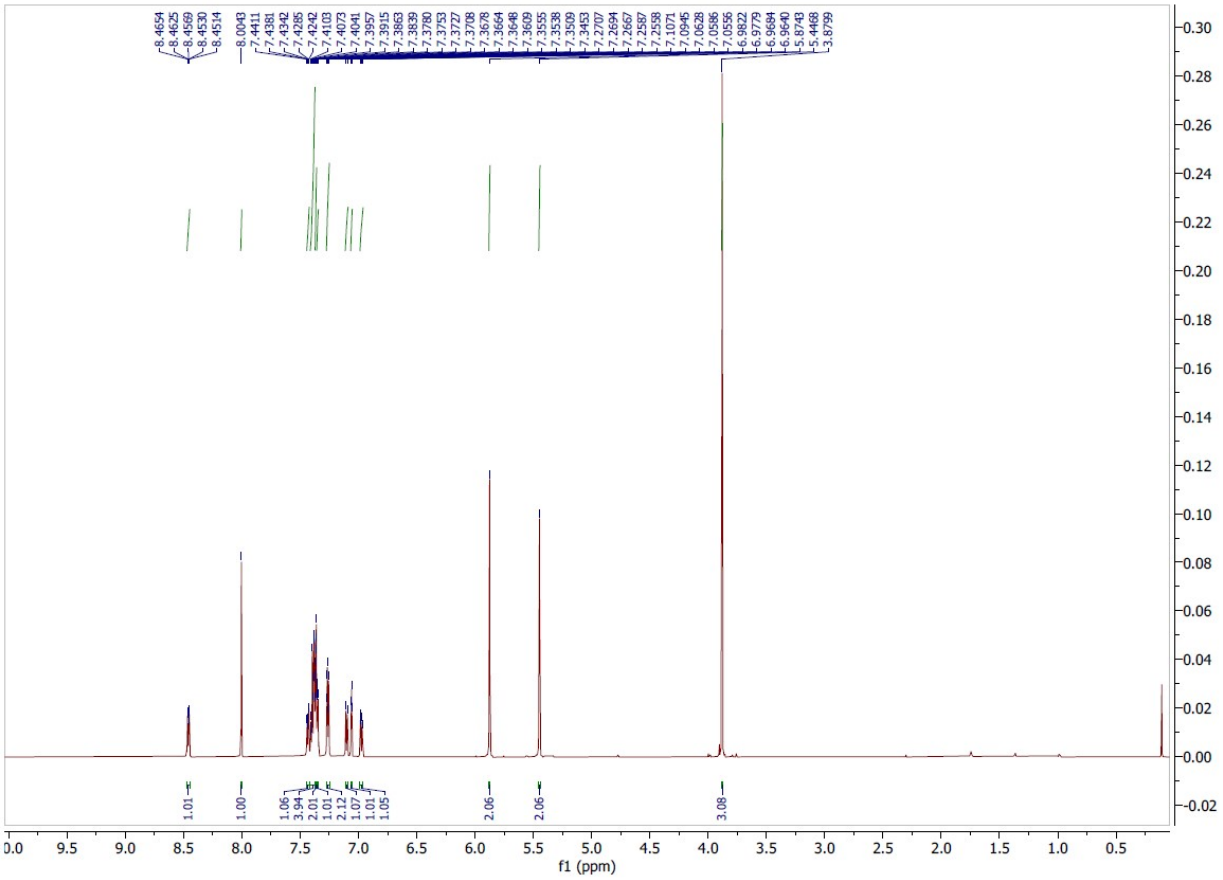


Figure S48. ^{1}H NMR spectrum of compound 5h

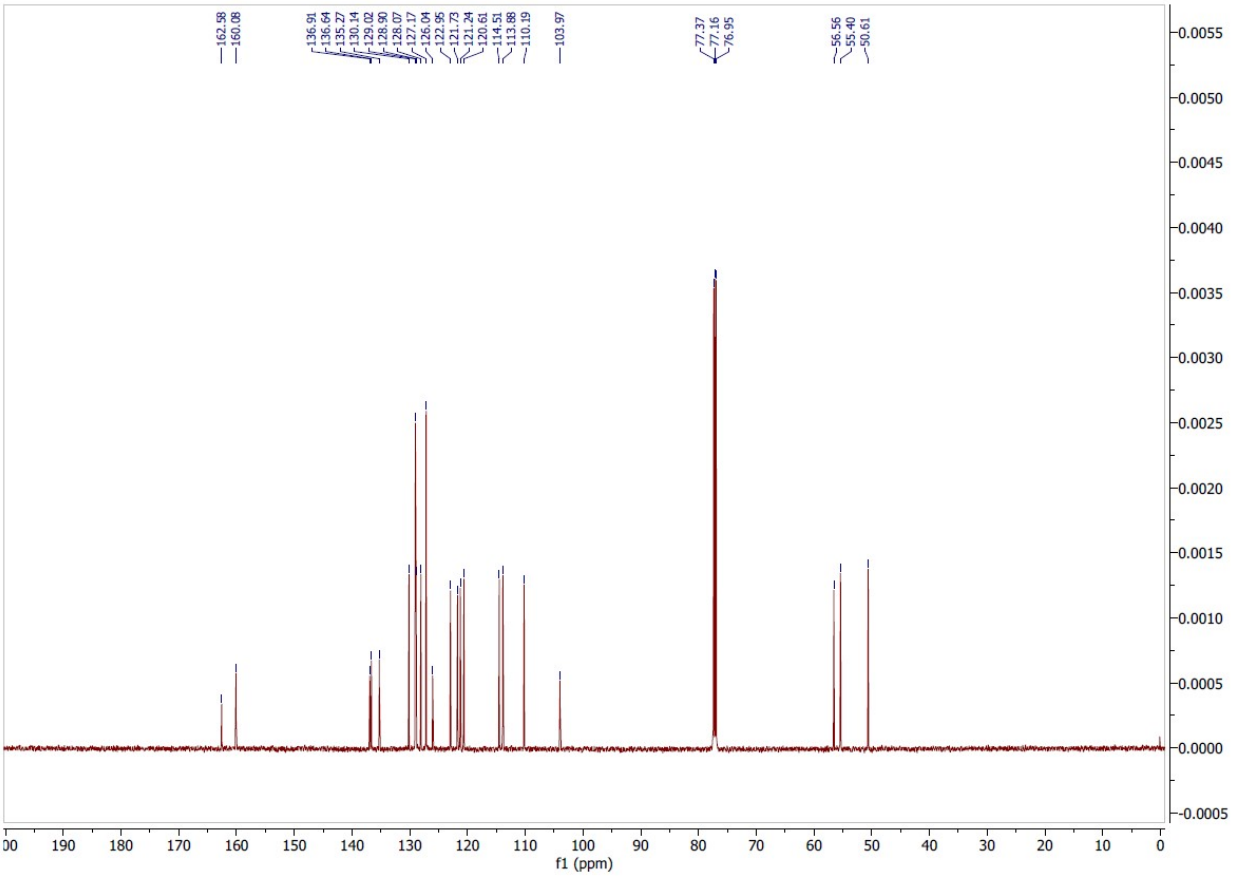


Figure S49. ^{13}C NMR spectrum of compound 5h

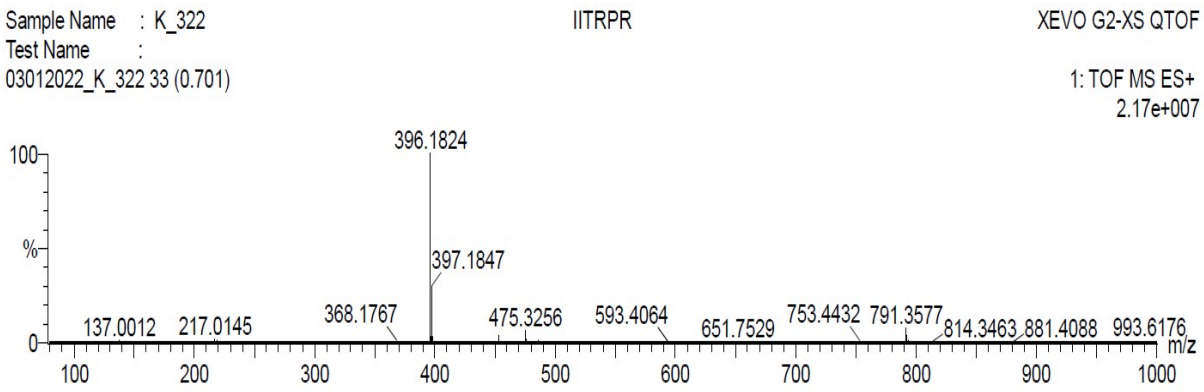


Figure S50. HRMS spectrum of compound 5h

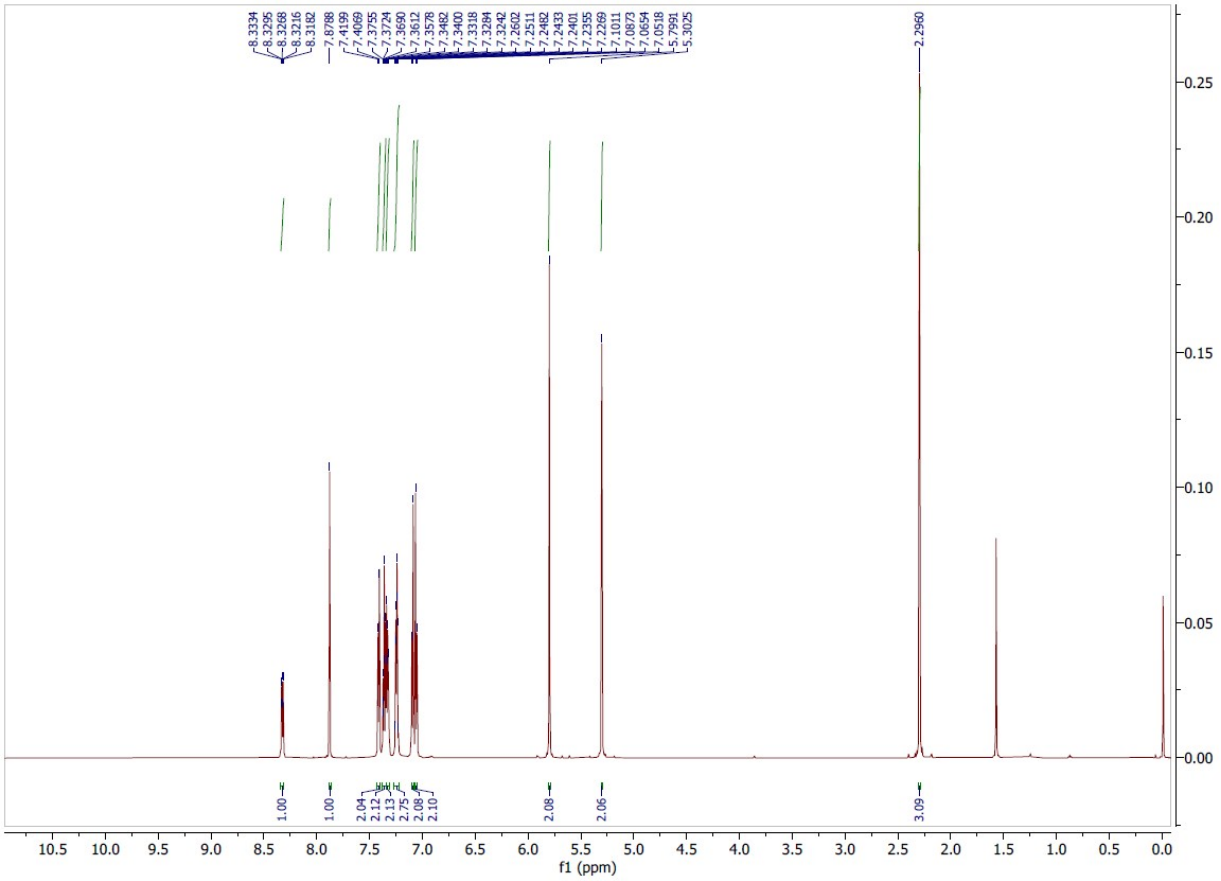


Figure S51. ^{1}H NMR spectrum of compound 5i

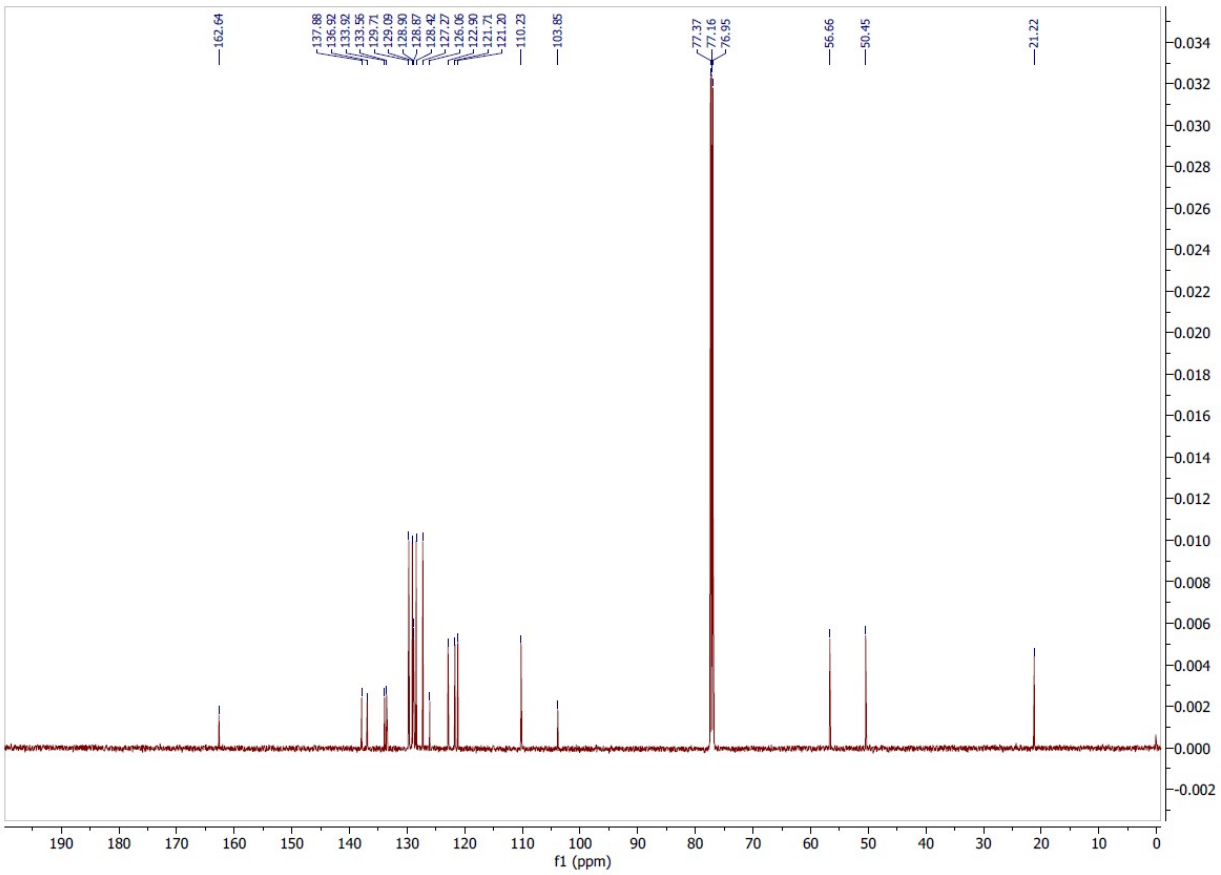


Figure S52. ^{13}C NMR spectrum of compound 5i

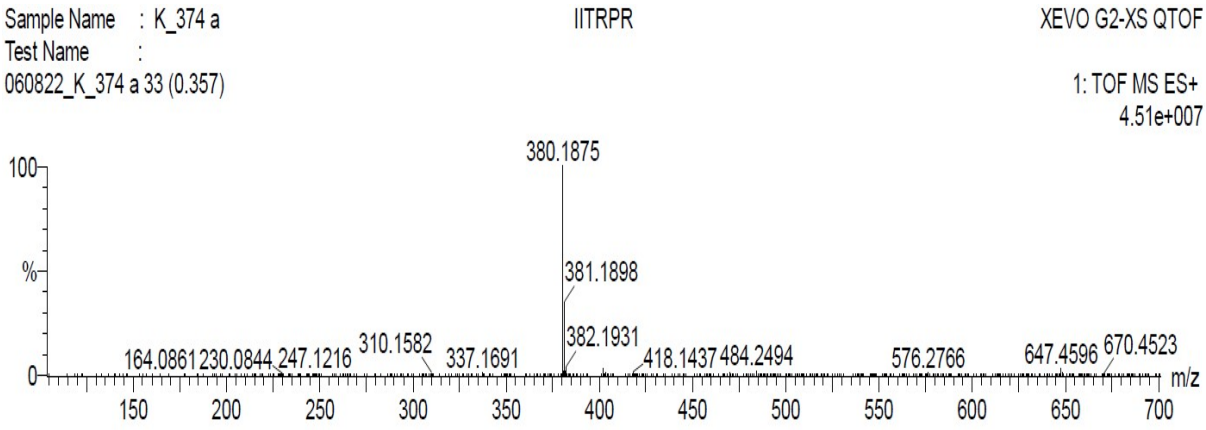


Figure S53. HRMS spectrum of compound 5i

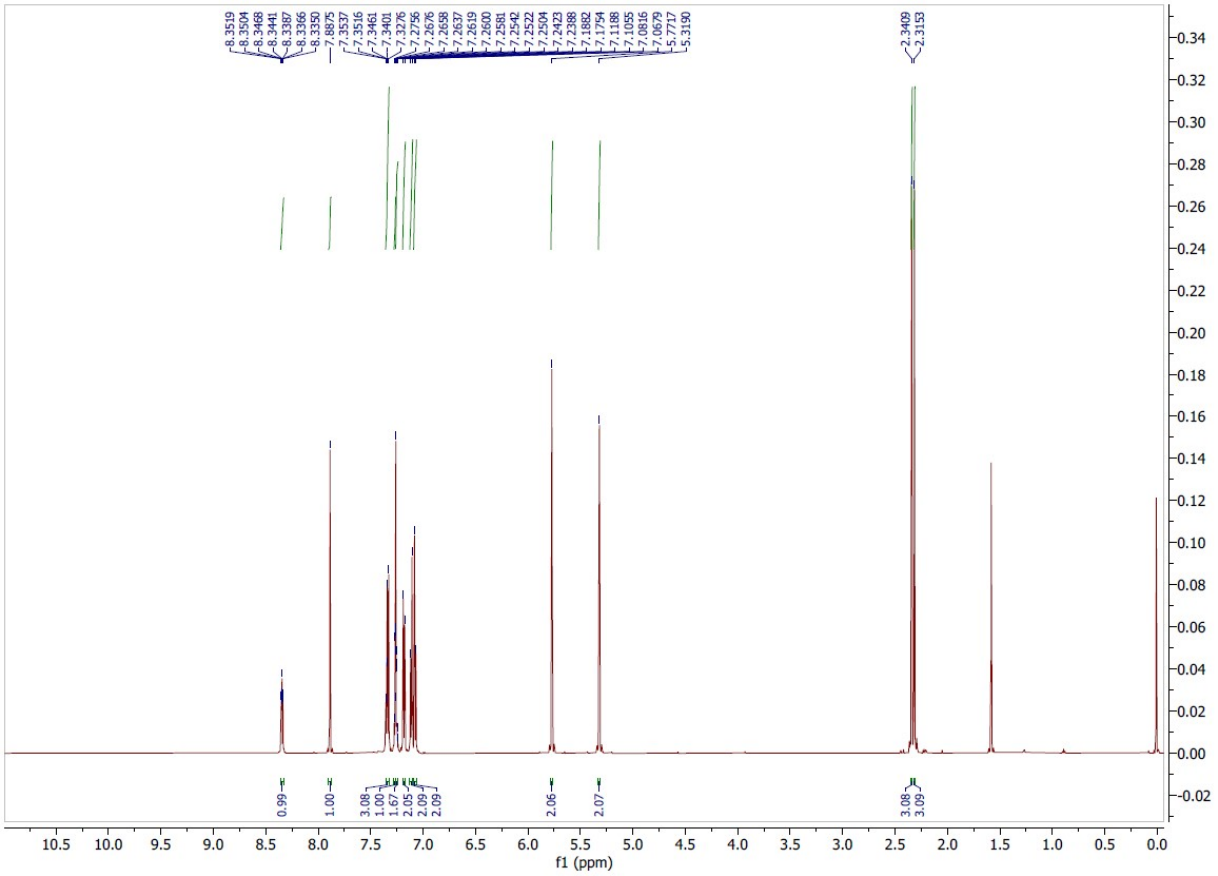


Figure S54. ^{1}H NMR spectrum of compound 5j

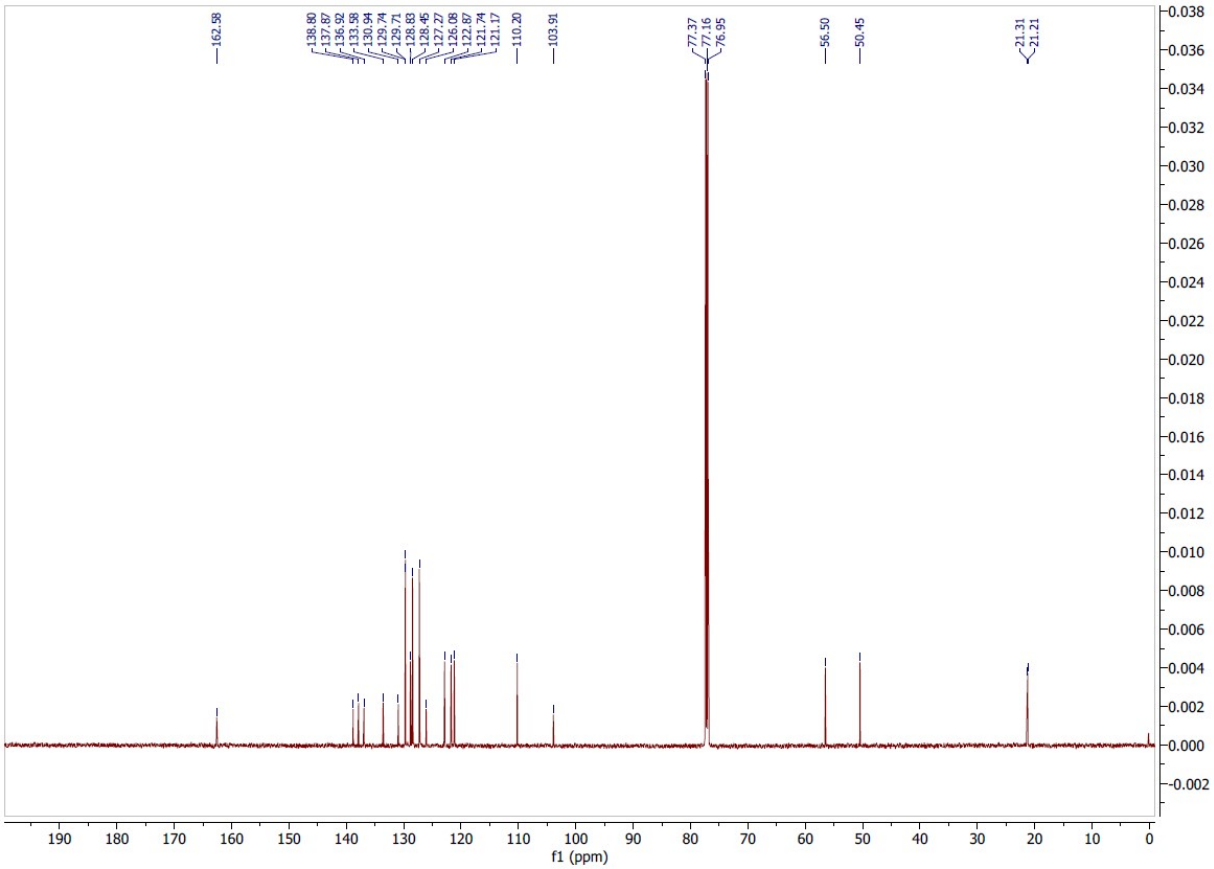


Figure S55. ^{13}C NMR spectrum of compound 5j

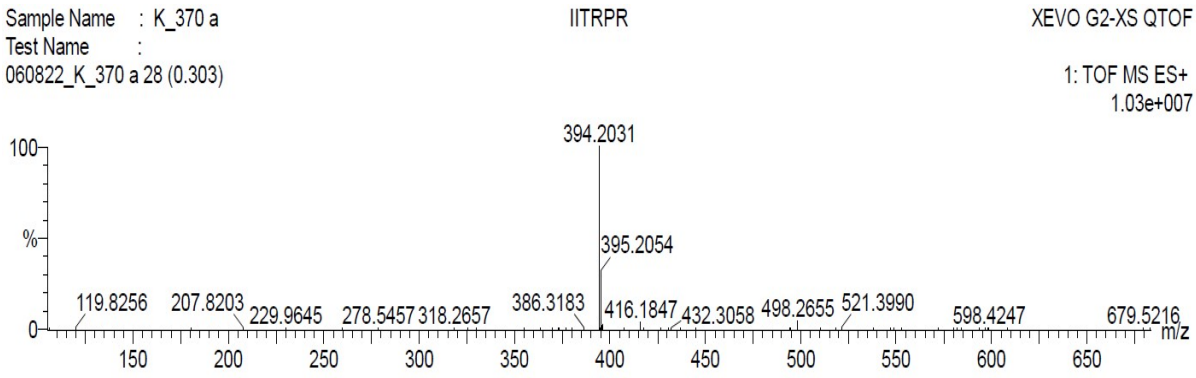


Figure S56. HRMS spectrum of compound 5j

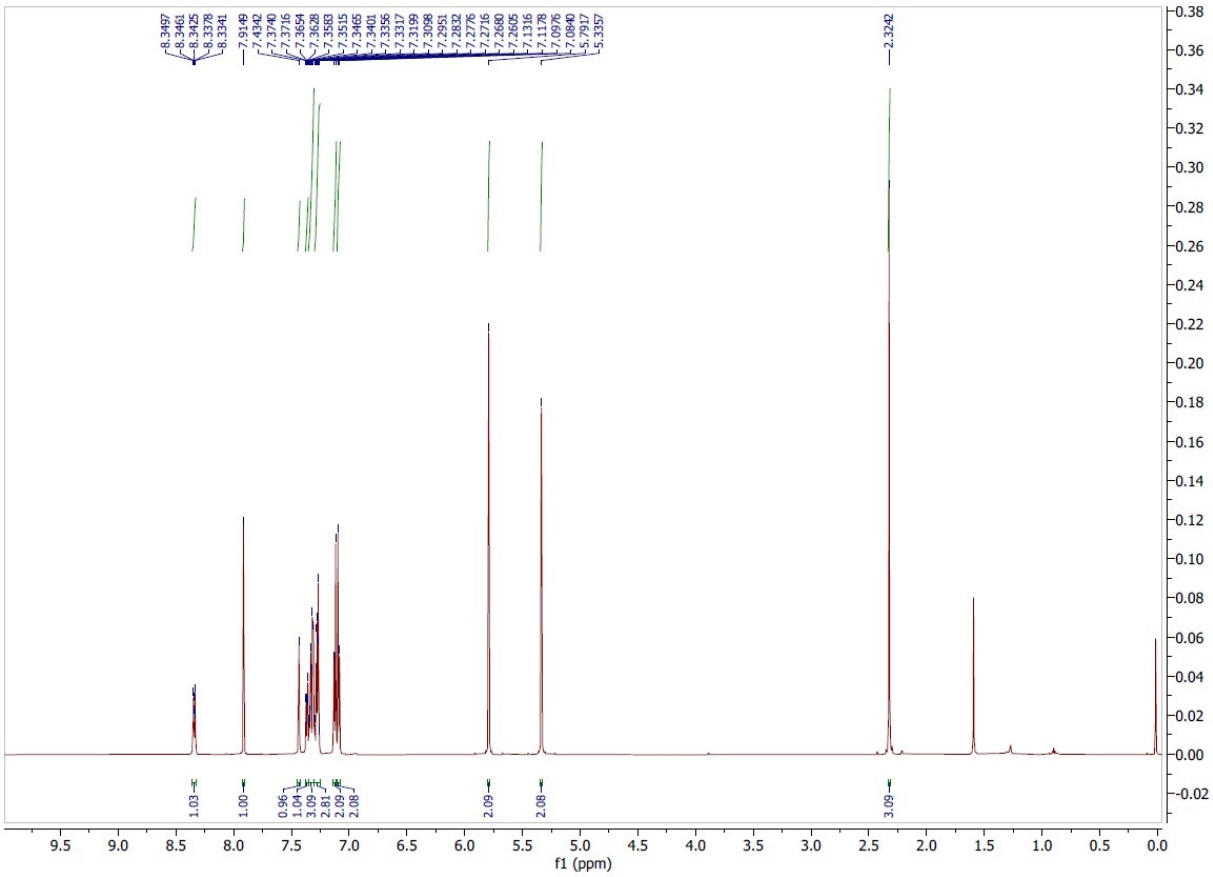


Figure S57. ^{1}H NMR spectrum of compound 5k

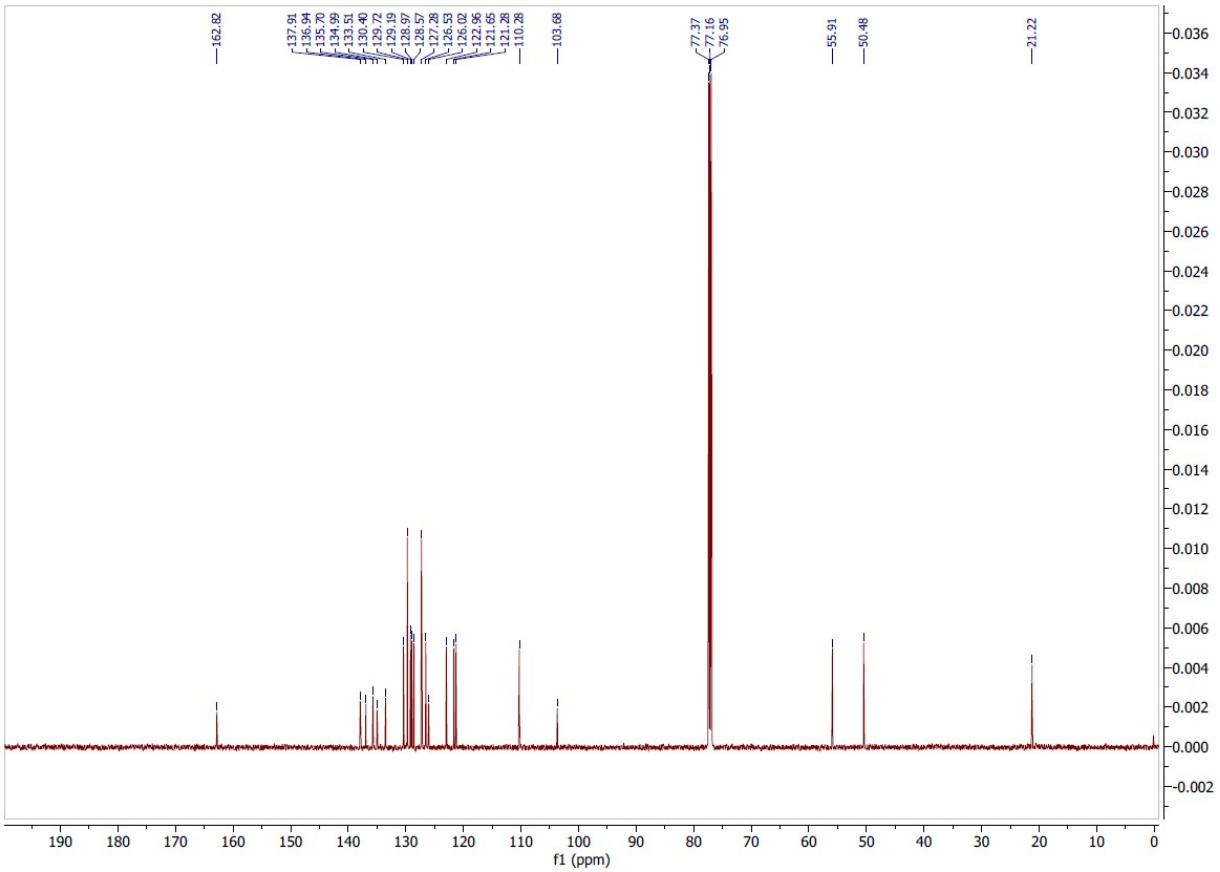


Figure S58. ^{13}C NMR spectrum of compound 5k

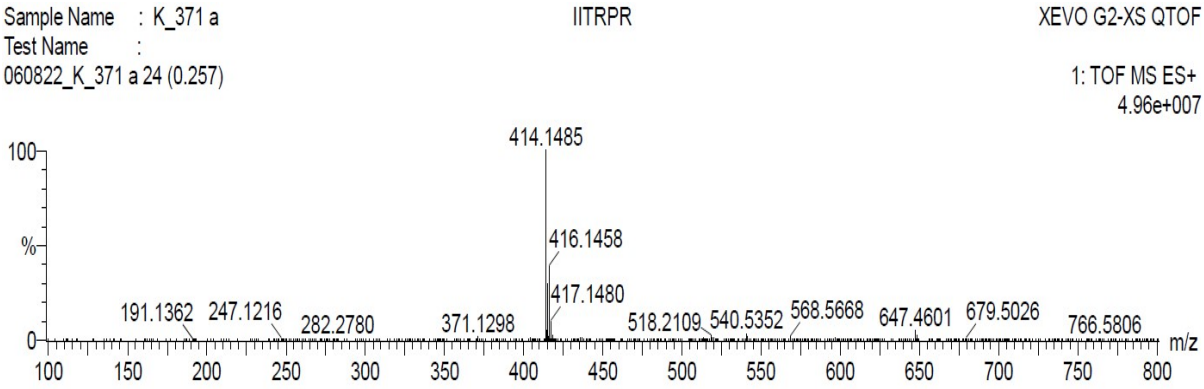


Figure S59. HRMS spectrum of compound 5k

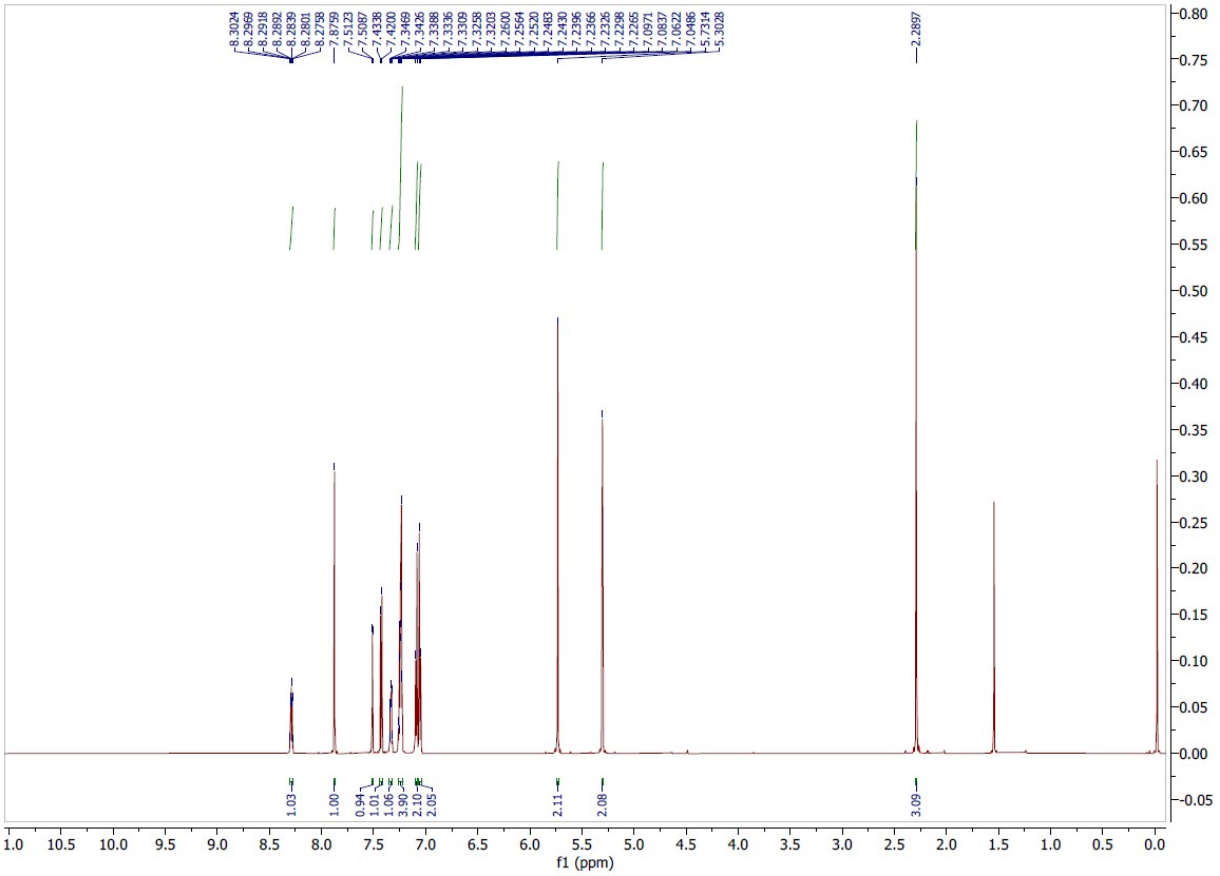


Figure S60. ^{1}H NMR spectrum of compound 5l

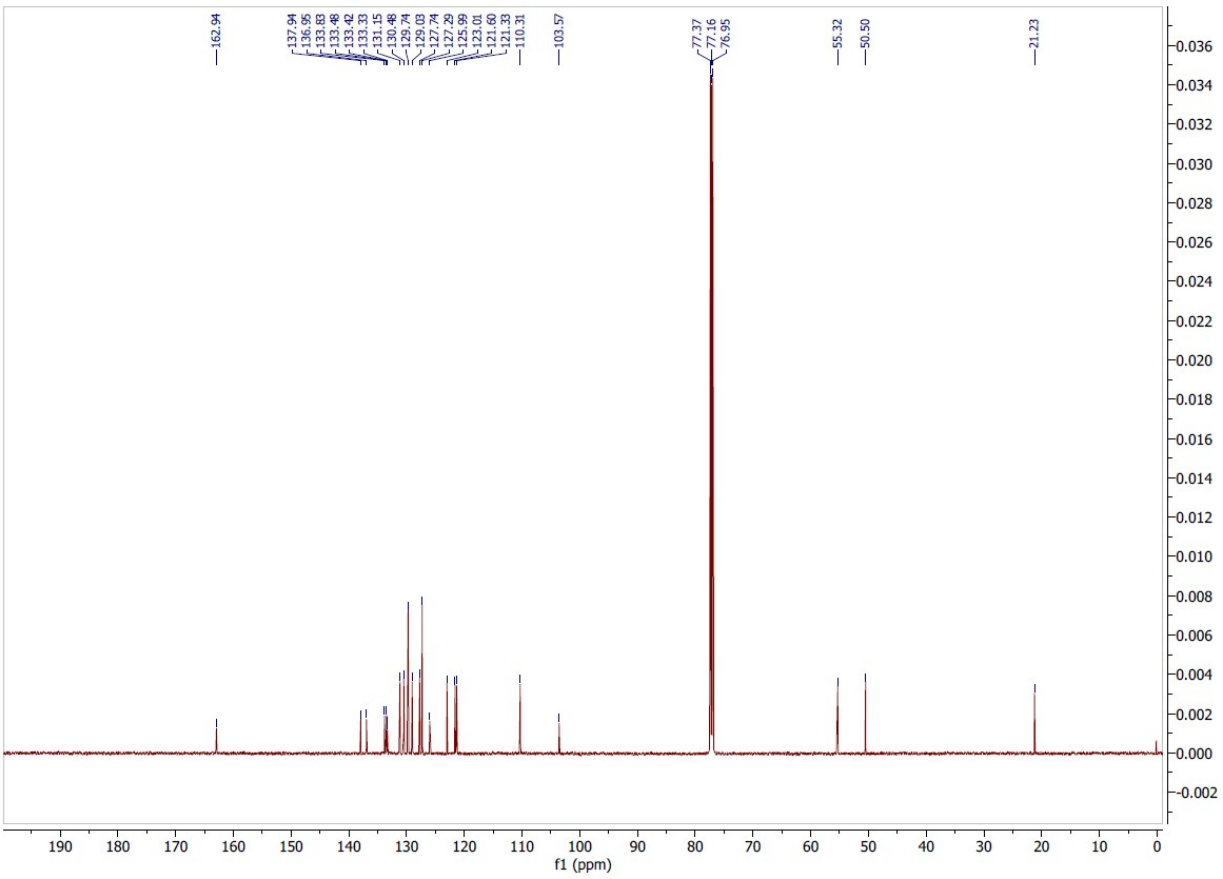


Figure S61. ^{13}C NMR spectrum of compound 5l

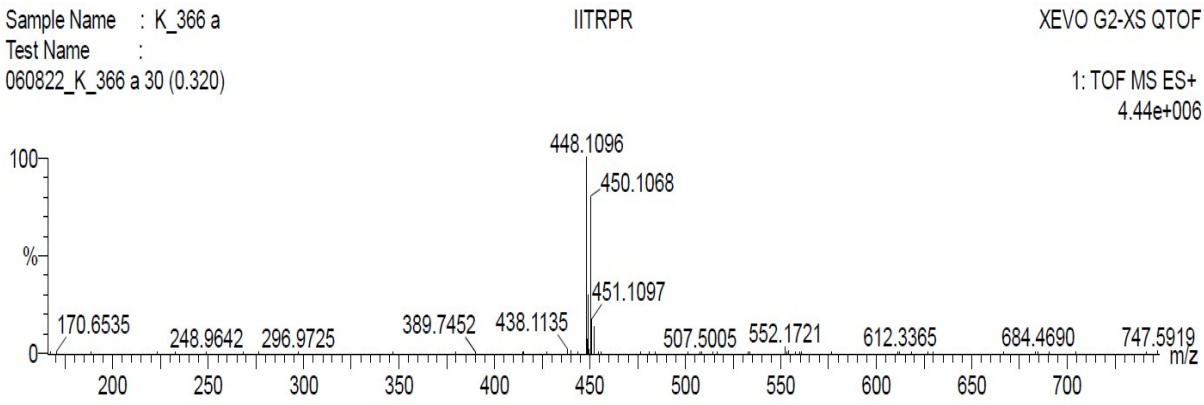


Figure S62. HRMS spectrum of compound 5l

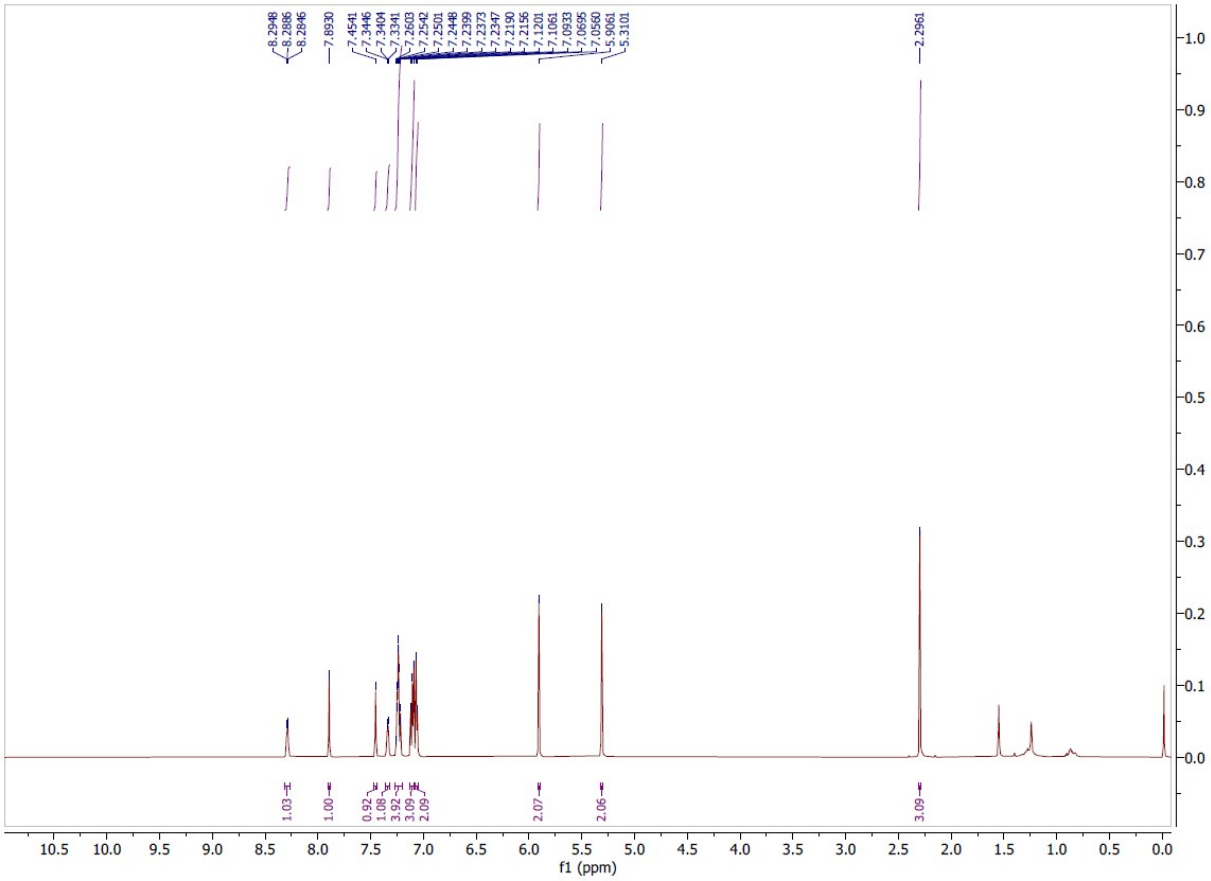


Figure S63. ^{1}H NMR spectrum of compound 5m

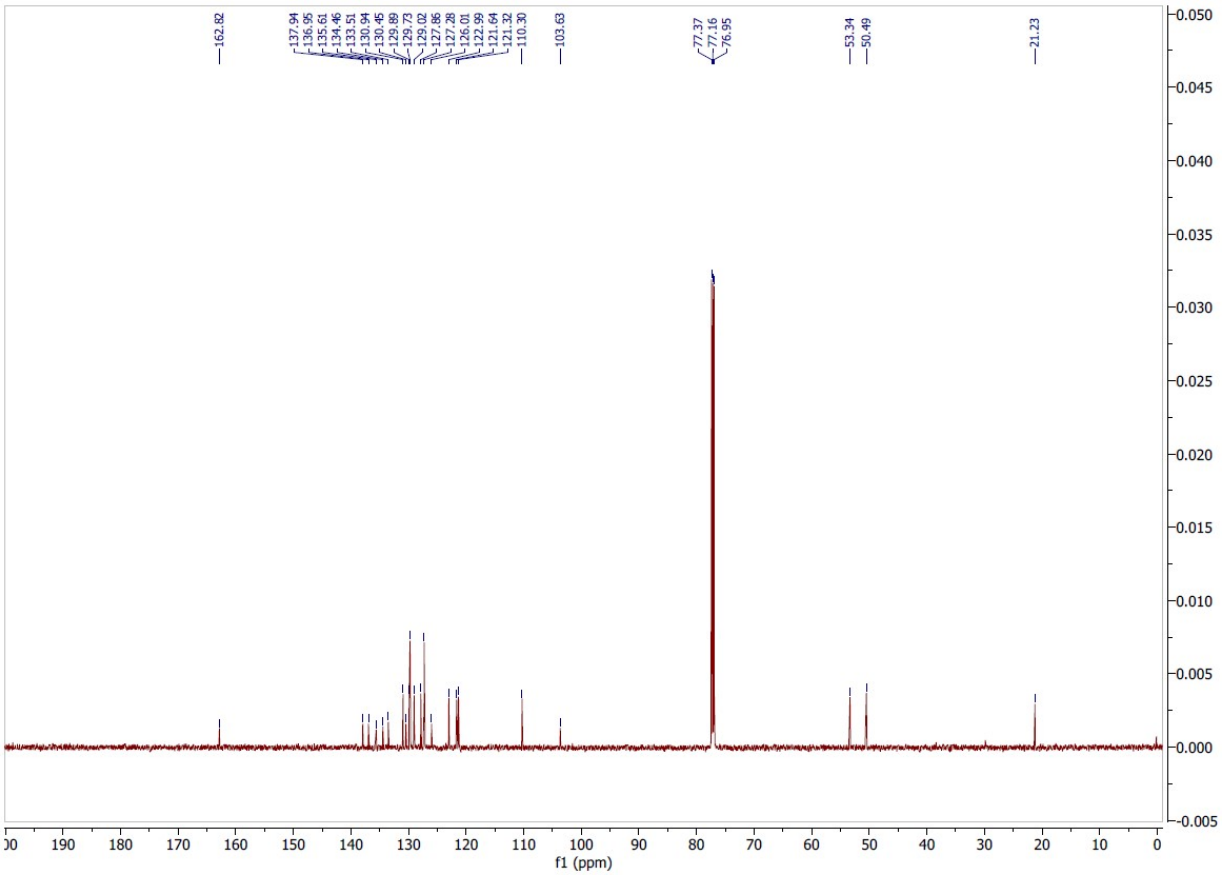


Figure S64. ^{13}C NMR spectrum of compound 5m

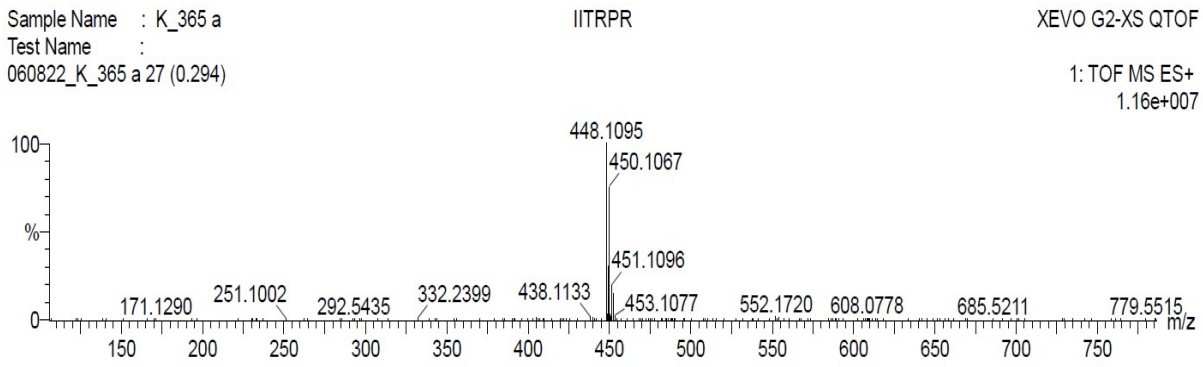


Figure S65. HRMS spectrum of compound 5m

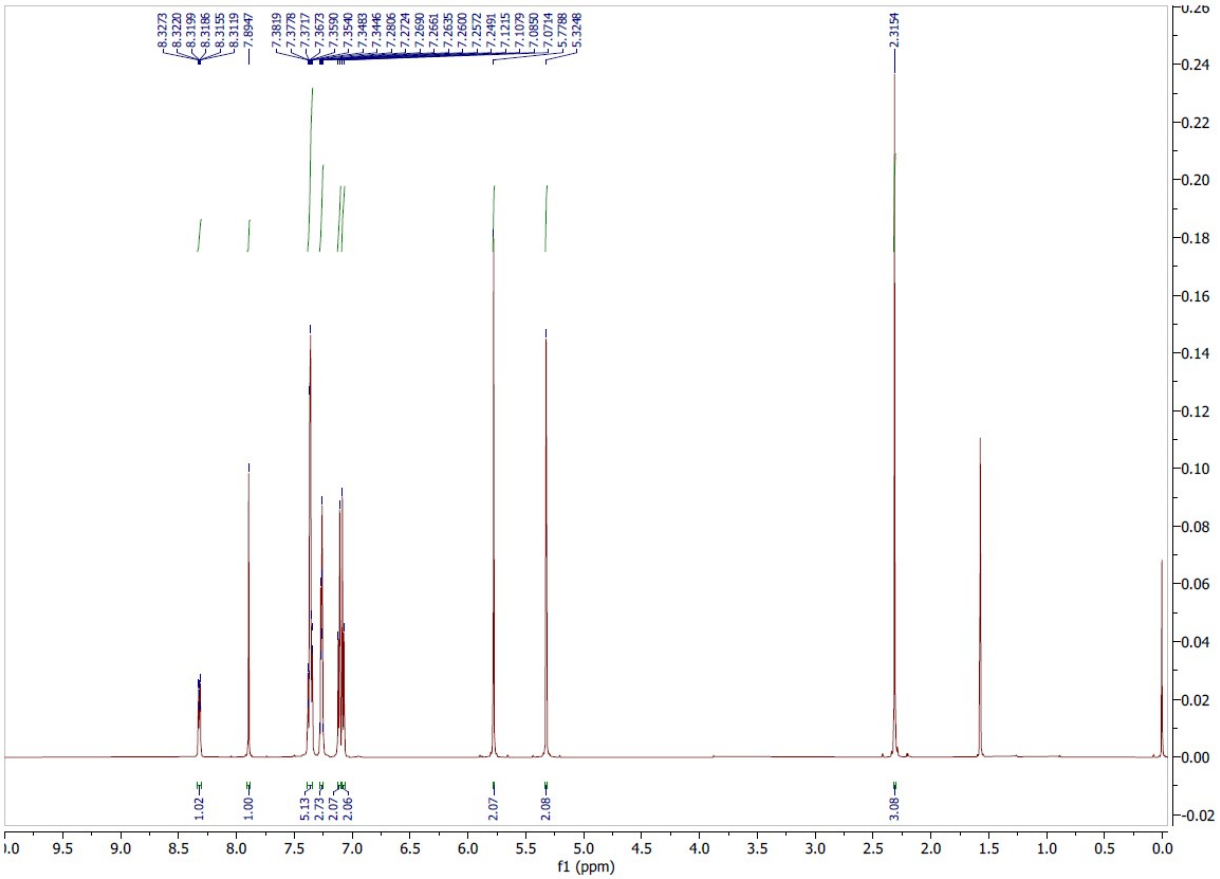


Figure S66. ^{1}H NMR spectrum of compound 5n

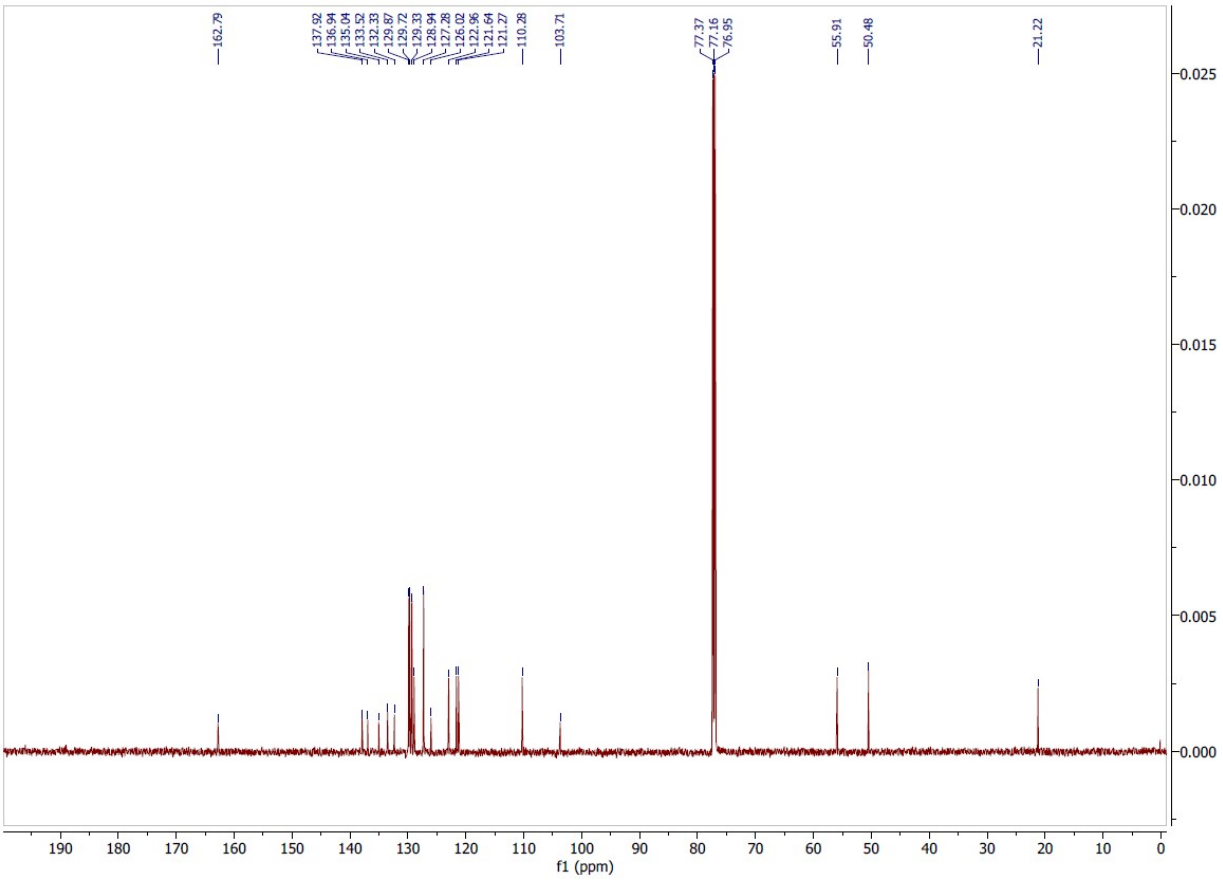


Figure S67. ^{13}C NMR spectrum of compound 5n

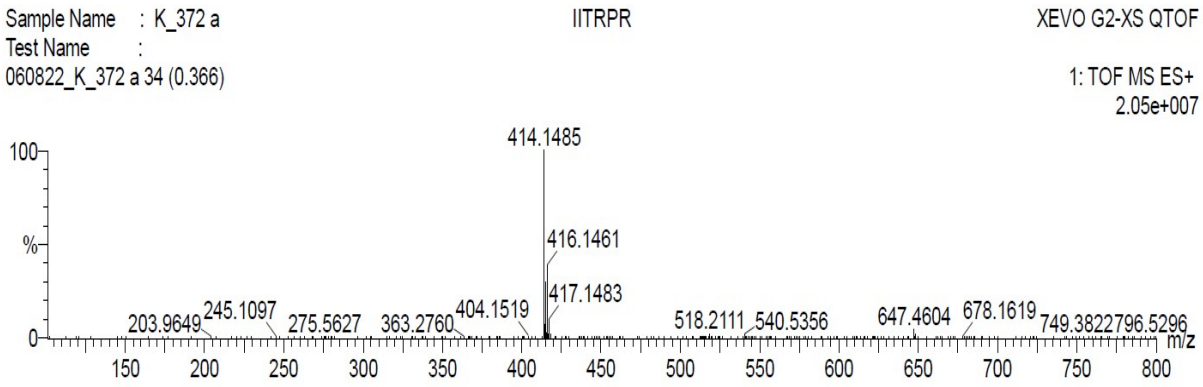


Figure S68. HRMS spectrum of compound 5n

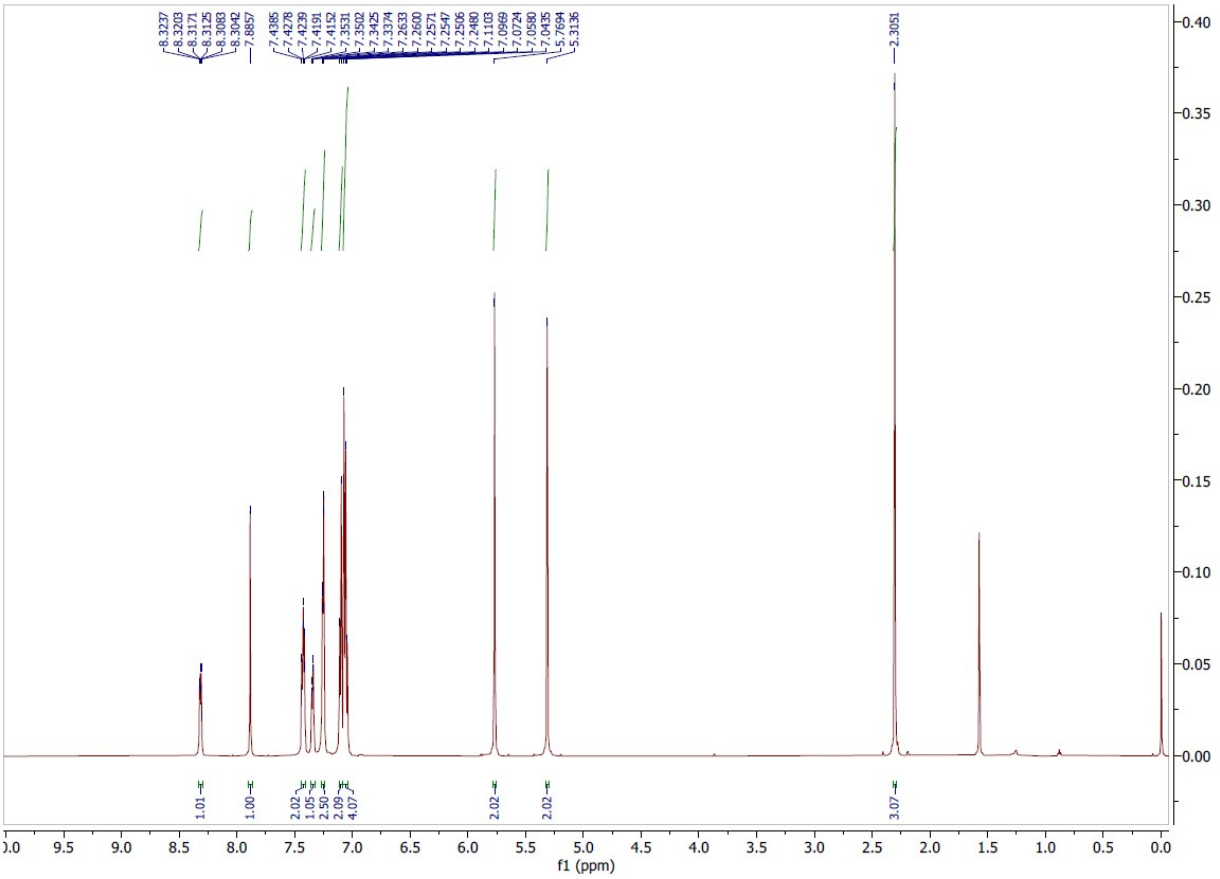


Figure S69. ^{1}H NMR spectrum of compound 5o

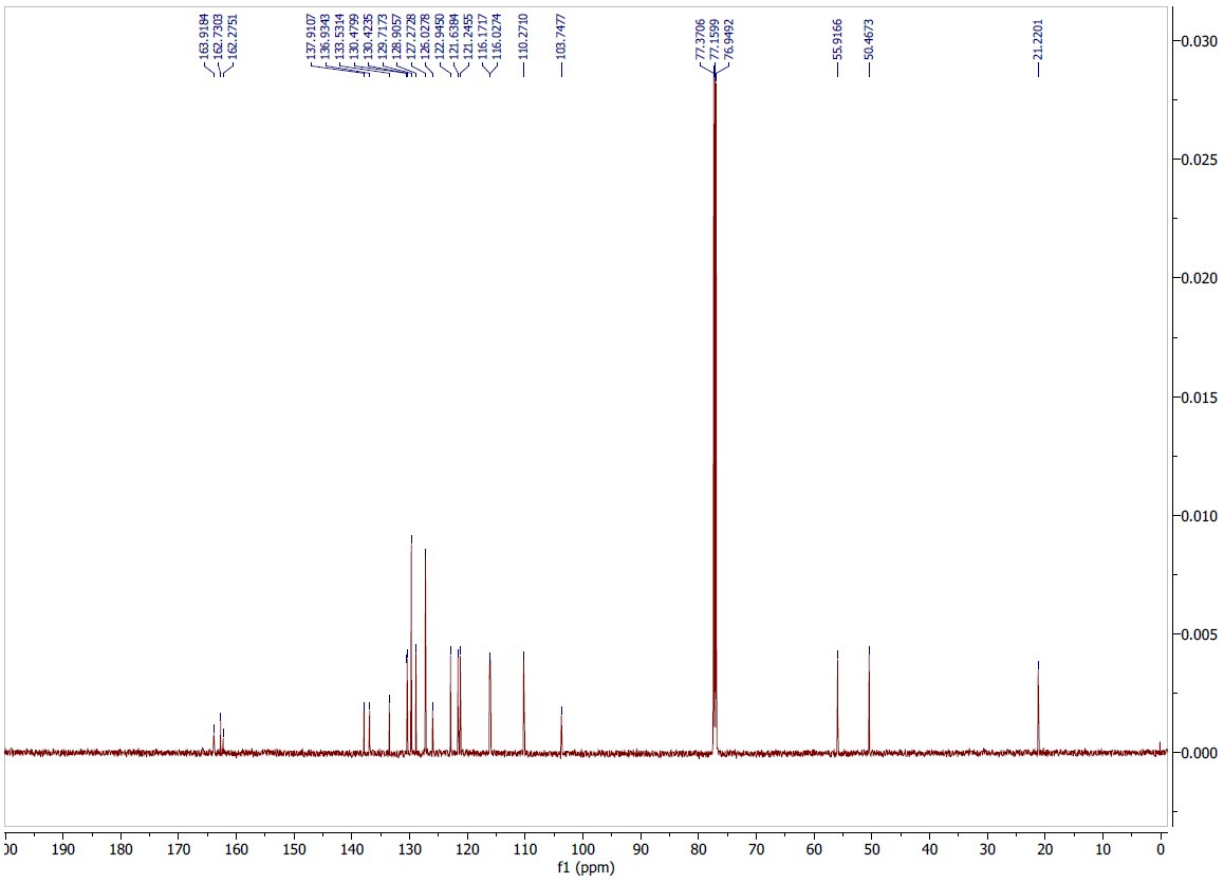


Figure S70. ^{13}C NMR spectrum of compound 5o

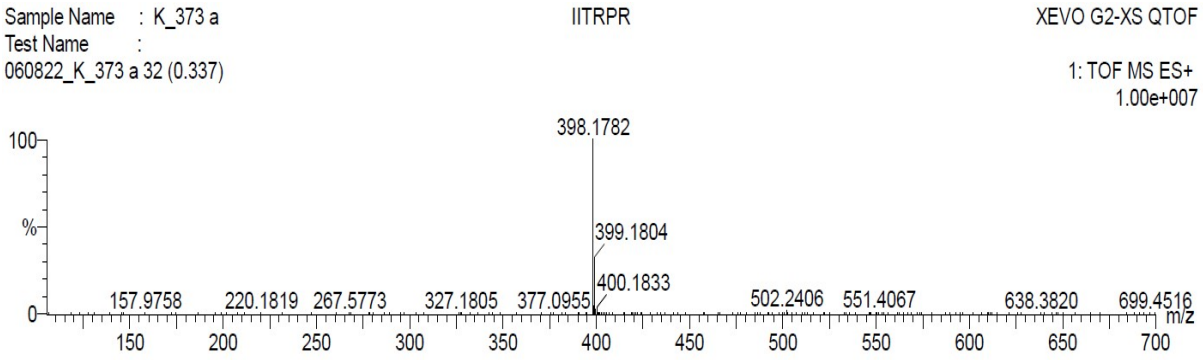


Figure S71. HRMS spectrum of compound 5o

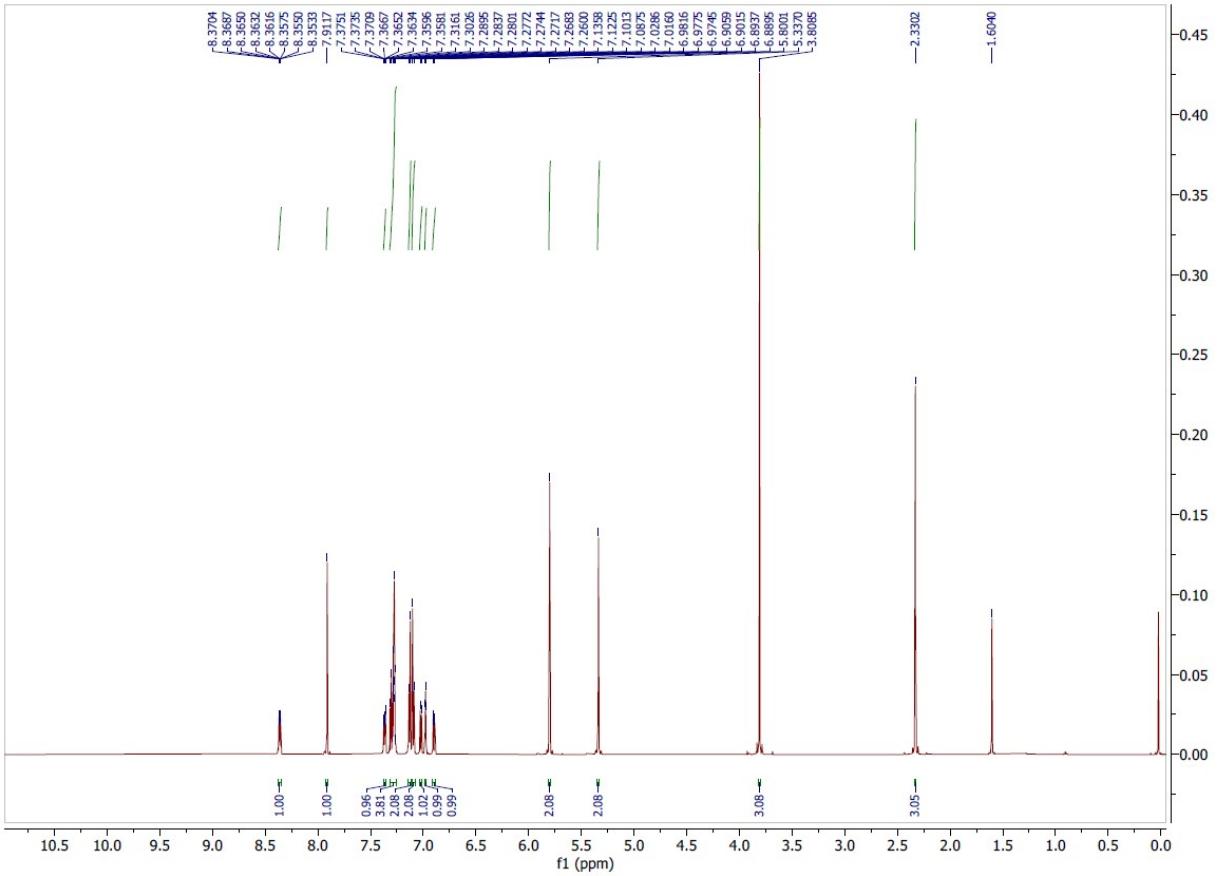


Figure S72. ^{1}H NMR spectrum of compound 5p

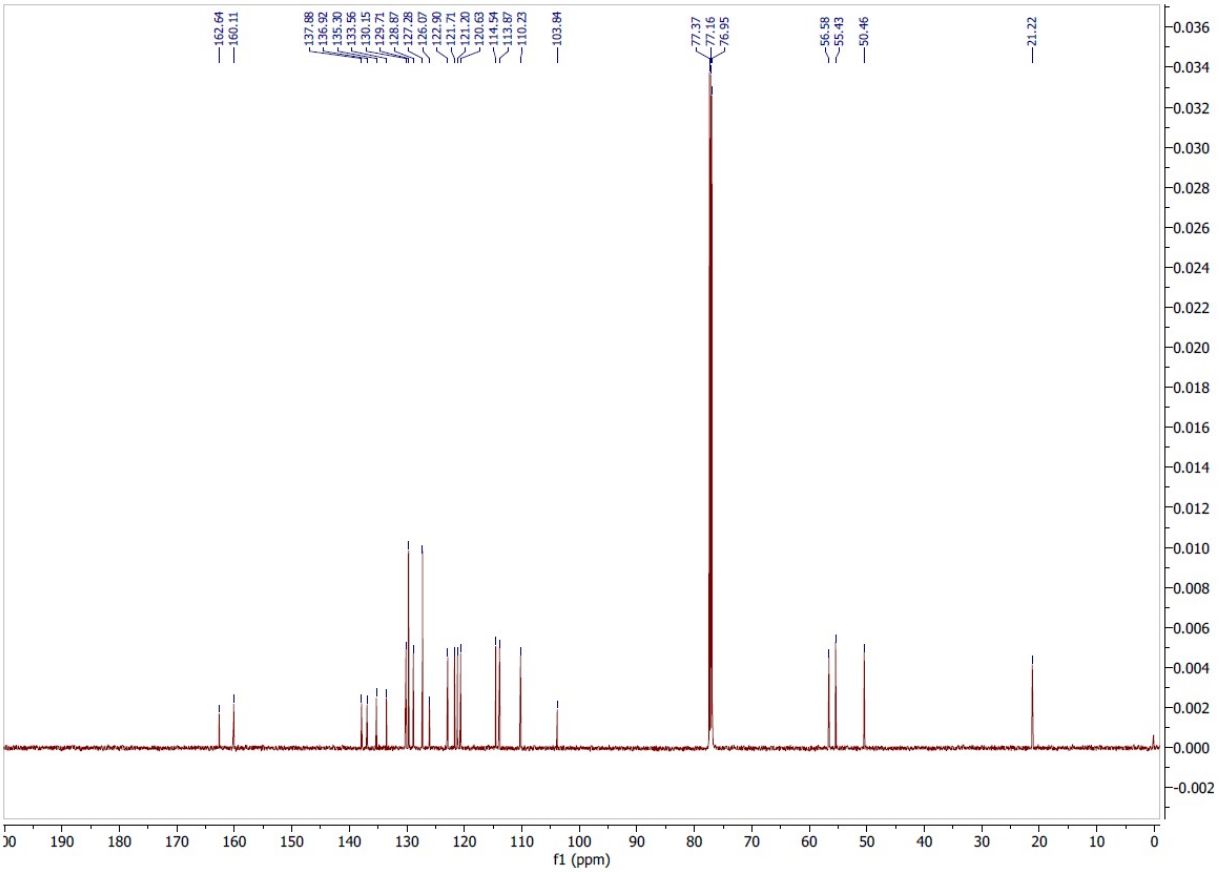


Figure S73. ^{13}C NMR spectrum of compound 5p

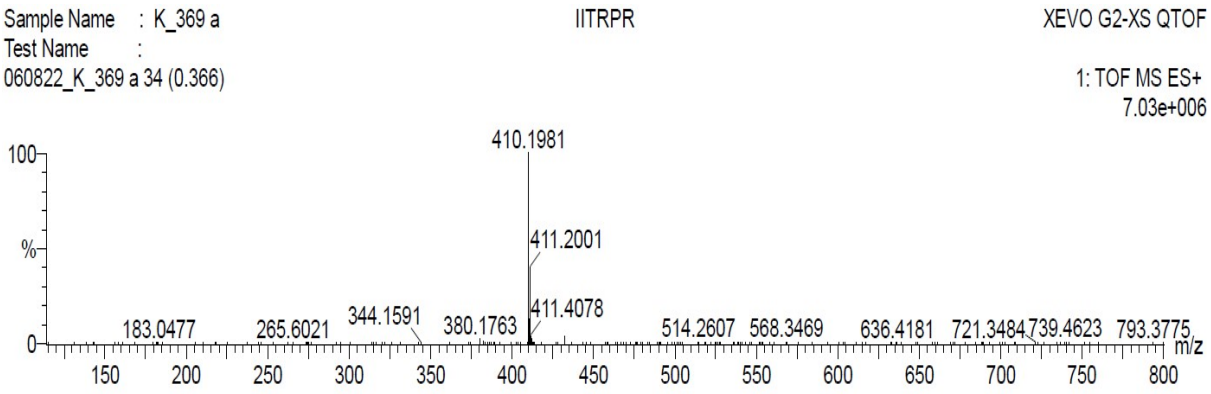


Figure S74. HRMS spectrum of compound 5p

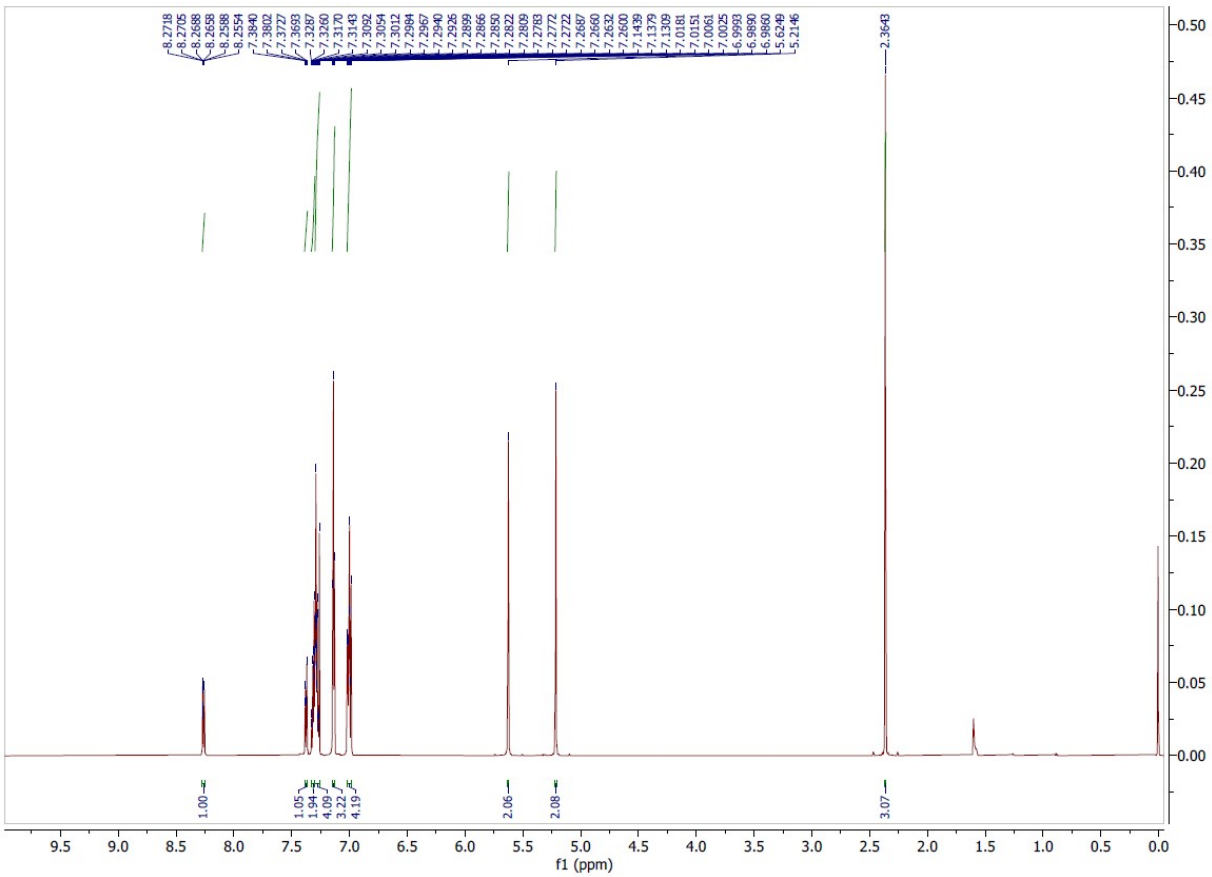


Figure S75. ^{1}H NMR spectrum of compound 6i

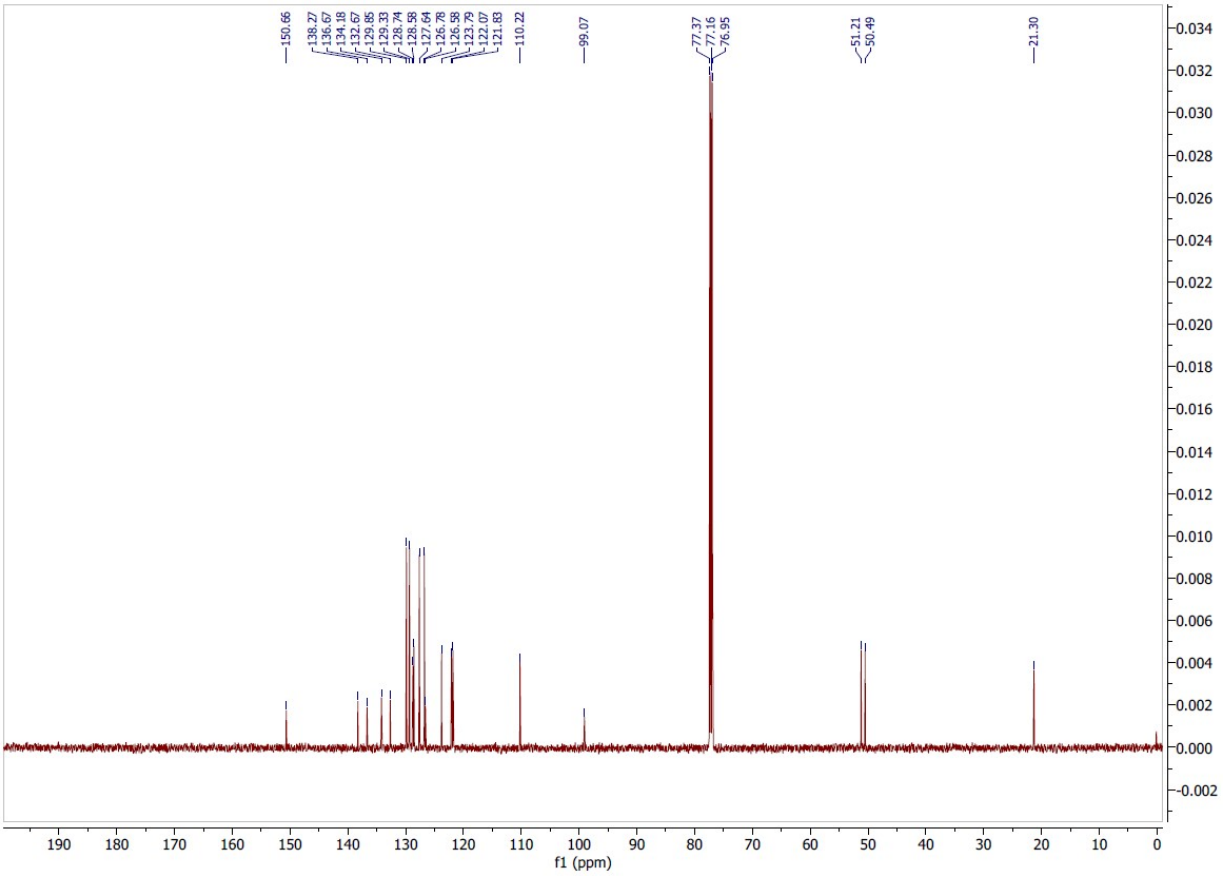


Figure S76. ^{13}C NMR spectrum of compound 6i

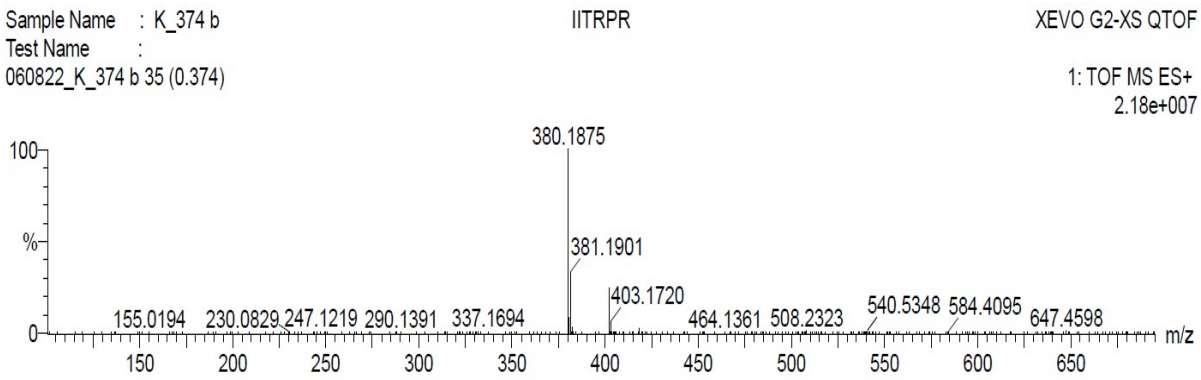


Figure S77. HRMS spectrum of compound 6i

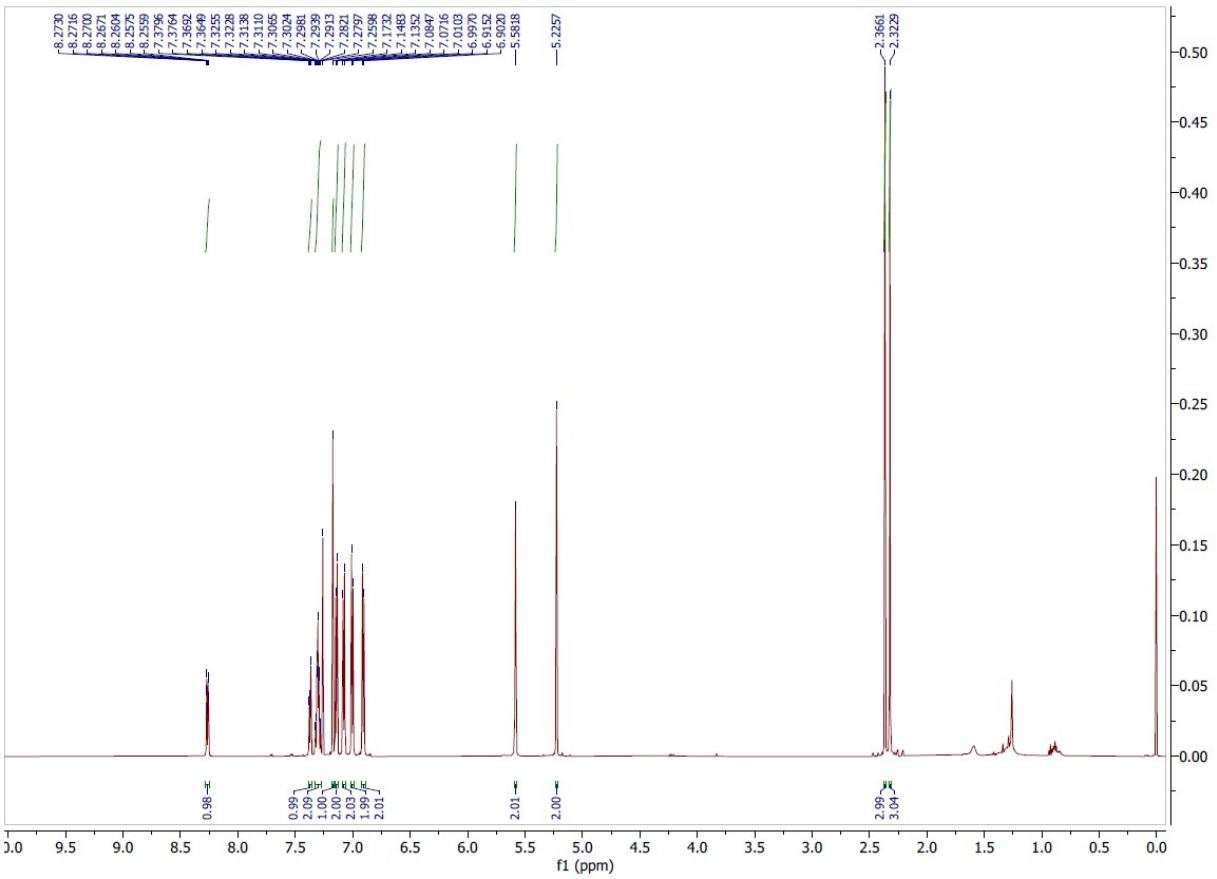


Figure S78. ^{1}H NMR spectrum of compound 6j

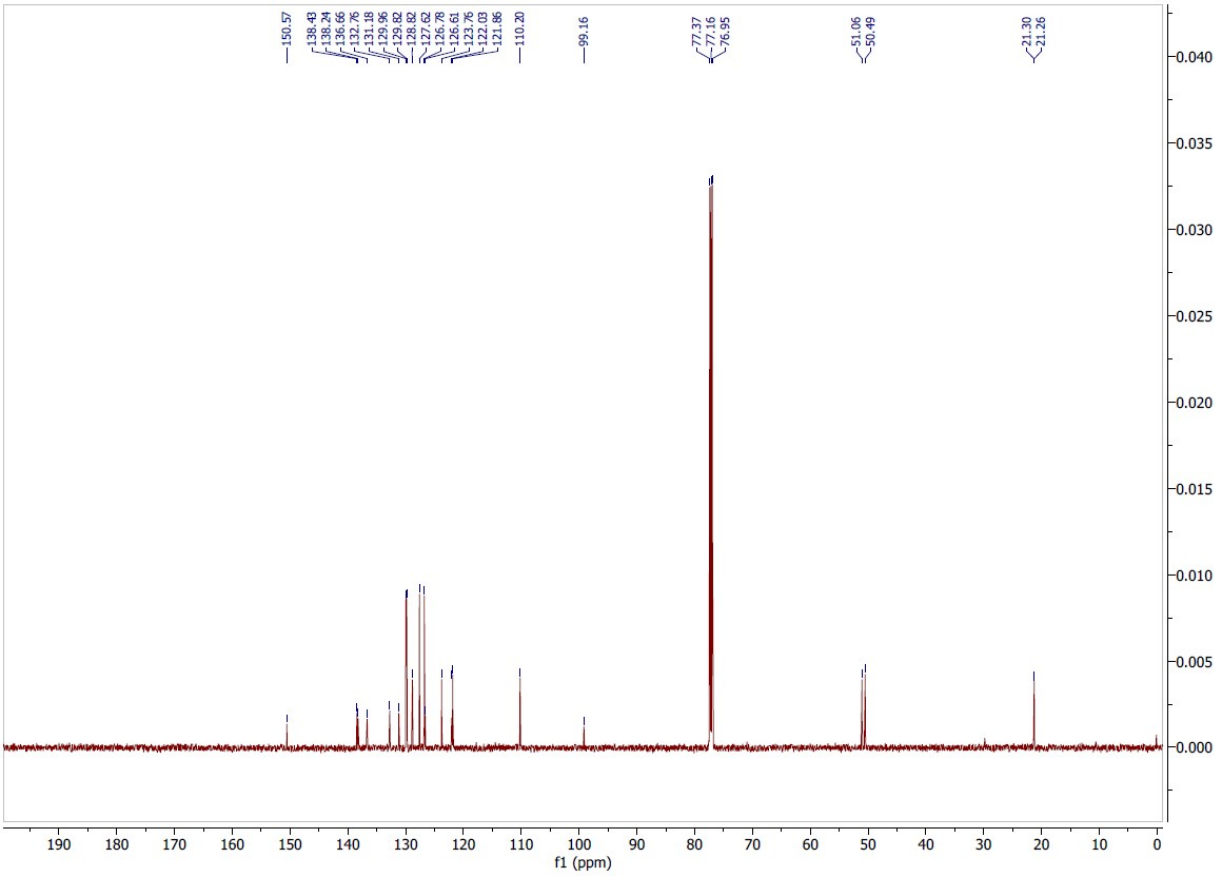


Figure S79. ^{13}C NMR spectrum of compound 6j

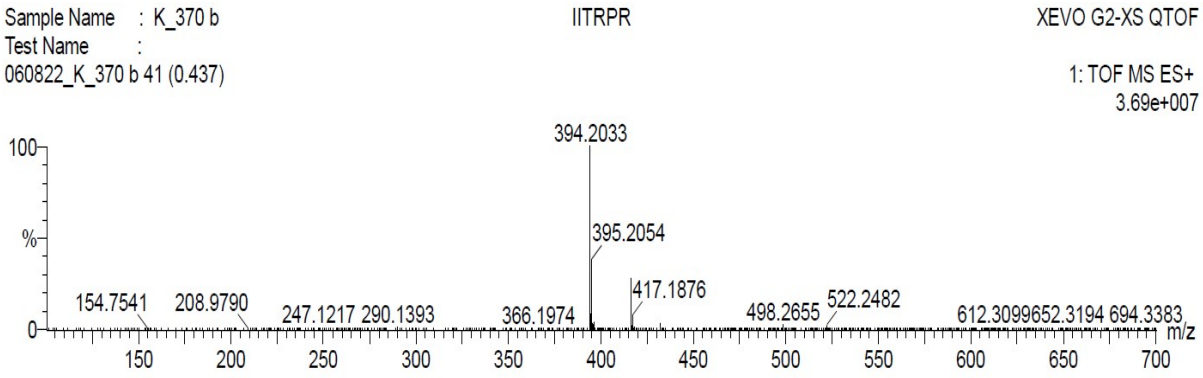


Figure S80. HRMS spectrum of compound 6j

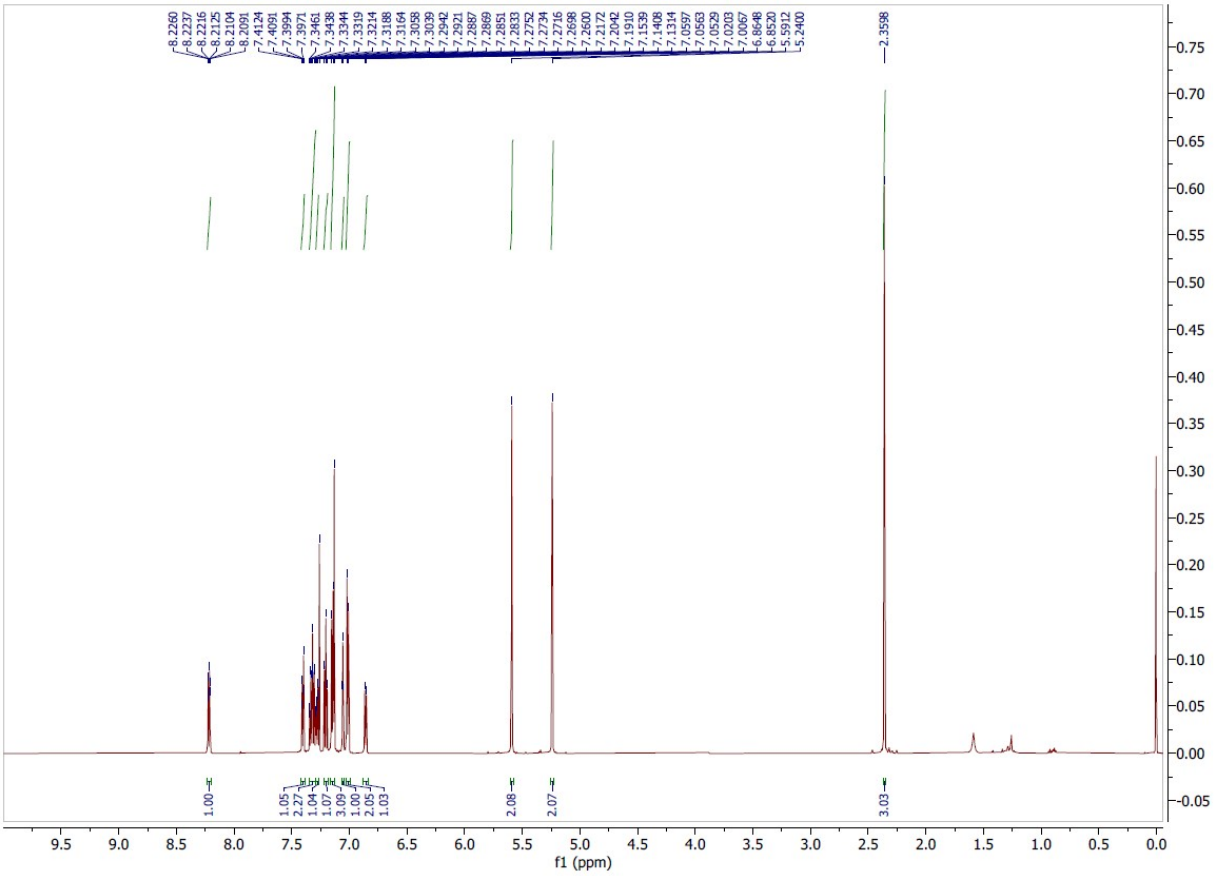


Figure S81. ^{1}H NMR spectrum of compound 6k

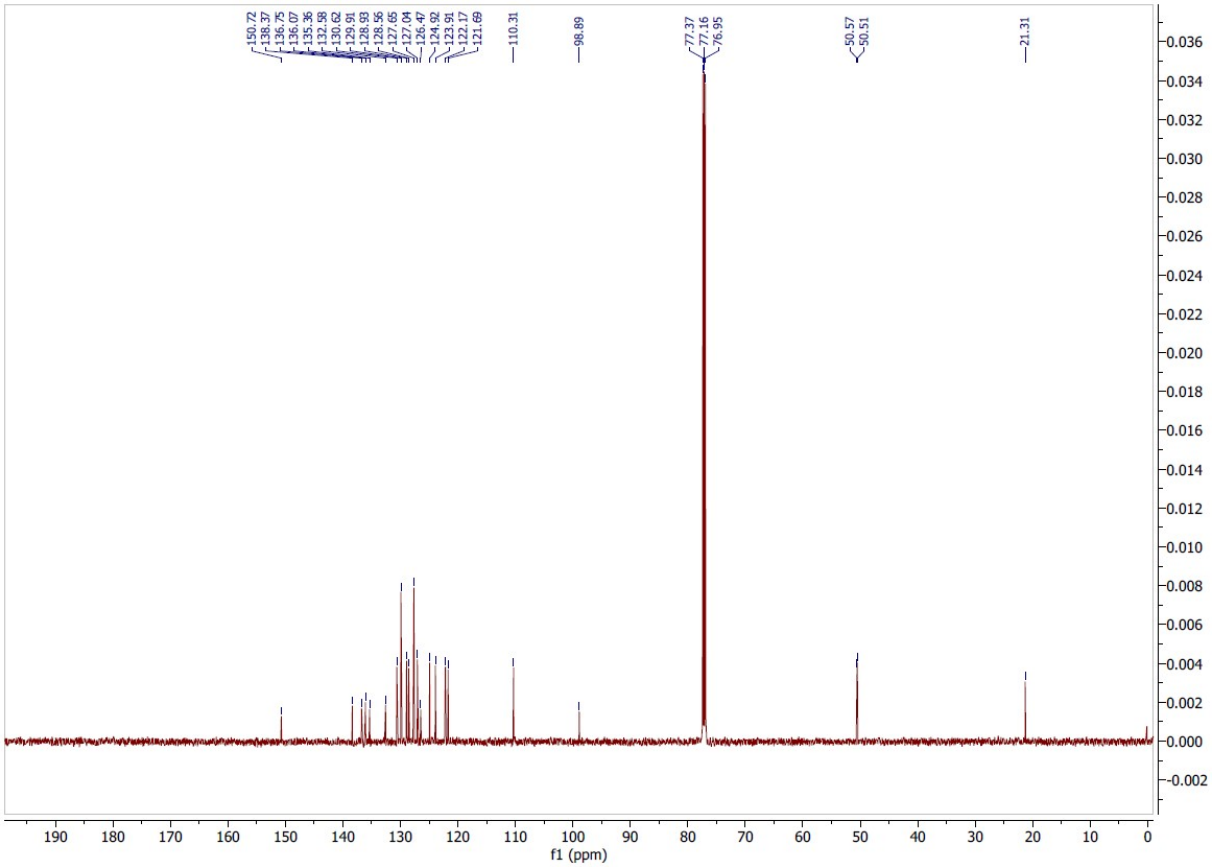


Figure S82. ^{13}C NMR spectrum of compound 6k

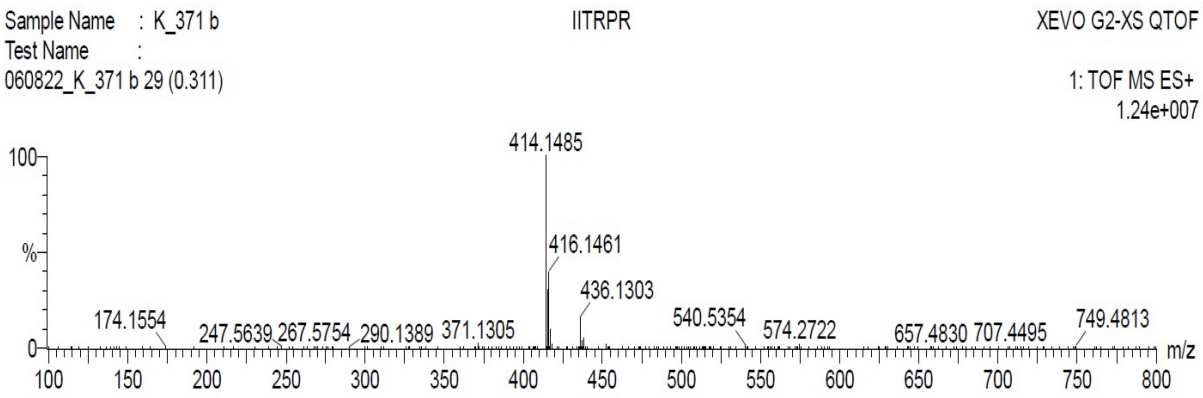


Figure S83. HRMS spectrum of compound 6k

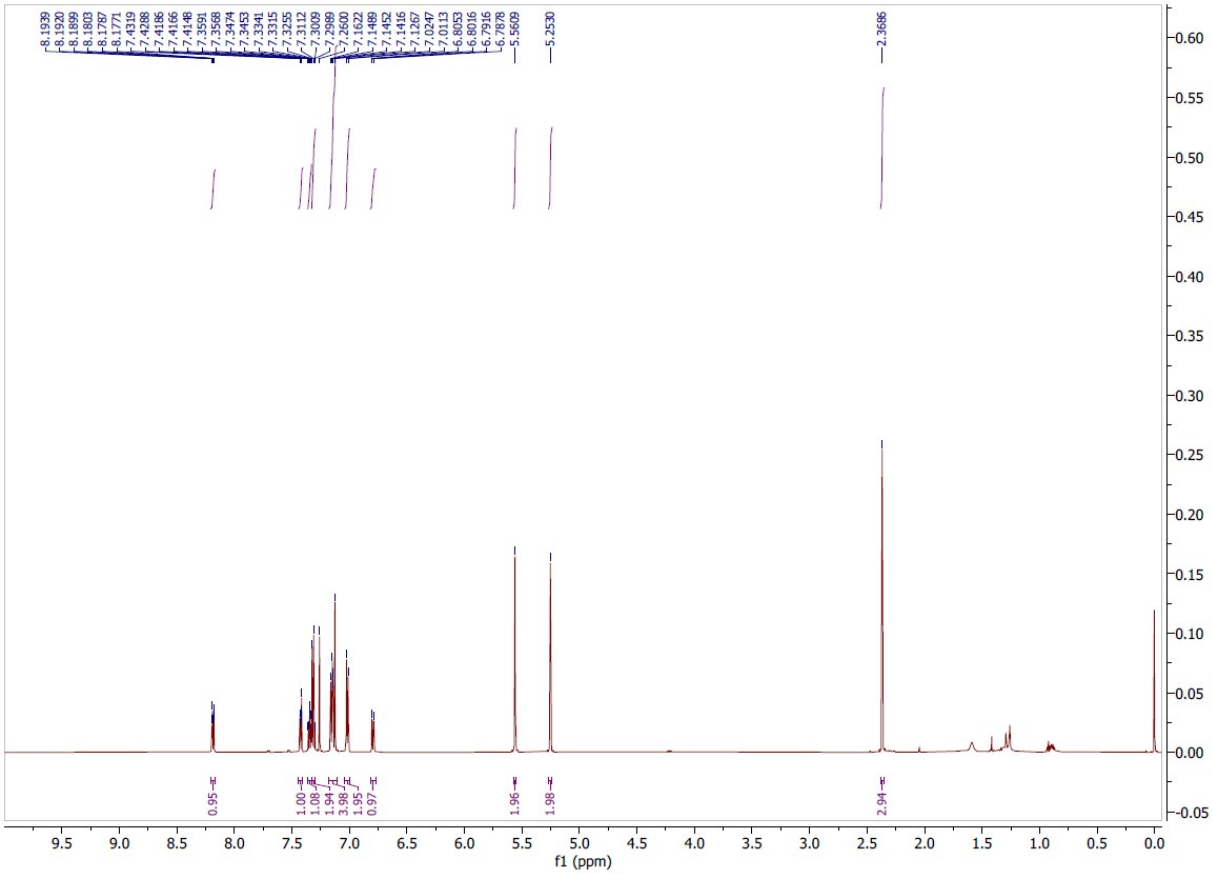


Figure S84. ^{1}H NMR spectrum of compound 6l

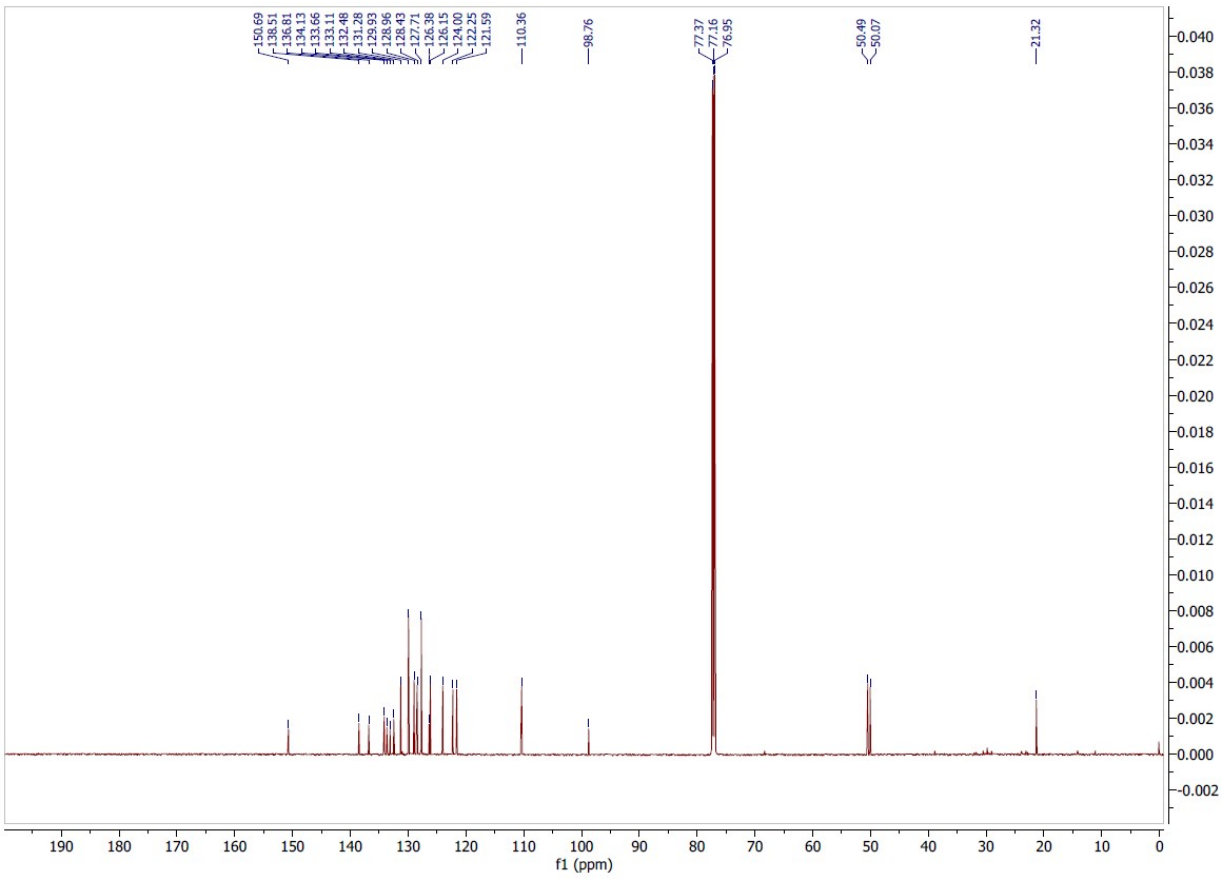


Figure S85. ^{13}C NMR spectrum of compound 6l

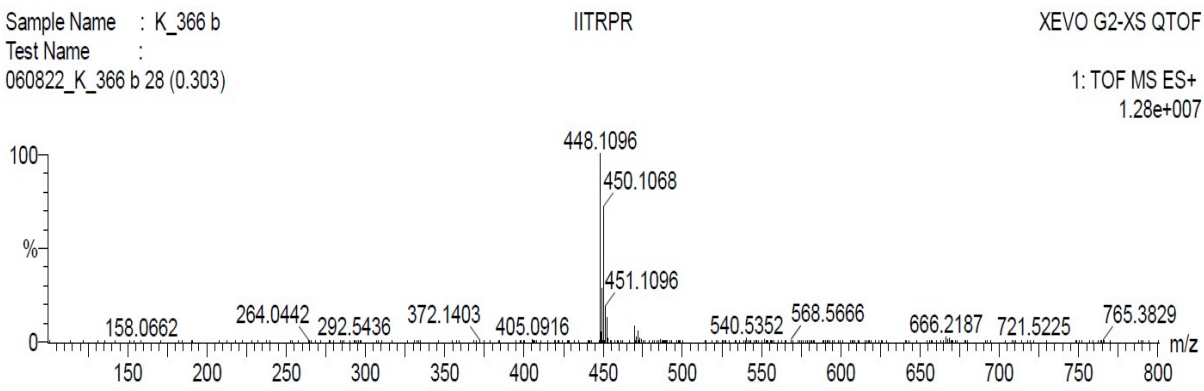


Figure S86. HRMS spectrum of compound 6l

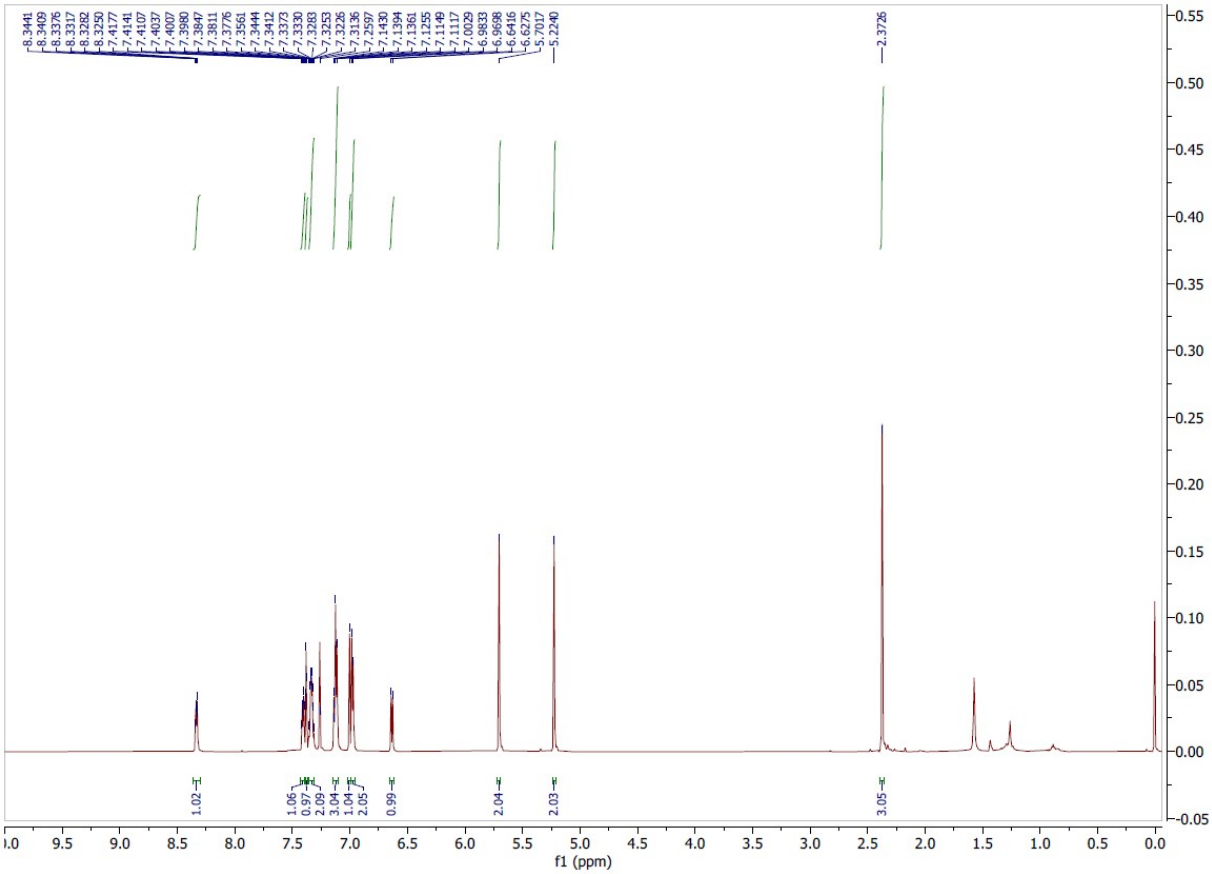


Figure S87. ^{1}H NMR spectrum of compound 6m

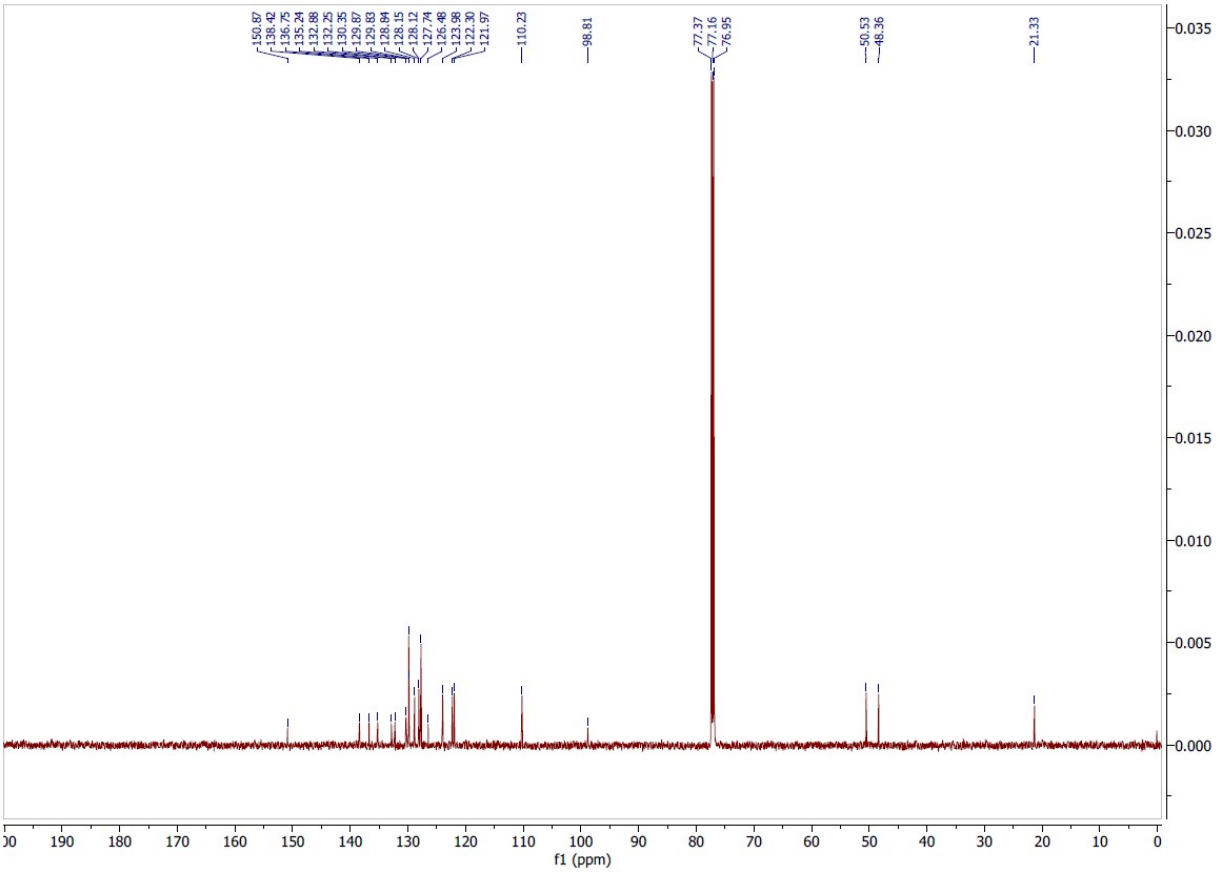


Figure S88. ^{13}C NMR spectrum of compound 6m

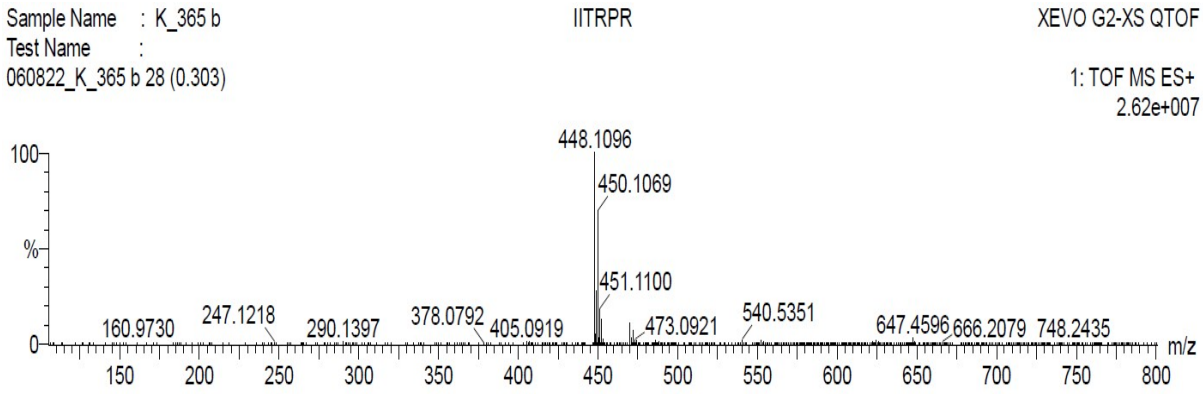


Figure S89. HRMS spectrum of compound 6m