Supporting information file for manuscript

Synthesis of Novel 2,3-Dihydro-1,5-Benzothiazepines as α-Glucosidase Inhibitors: *In Vitro*, *In Vivo*, Kinetic, SAR, Molecular Docking and QSAR Studies

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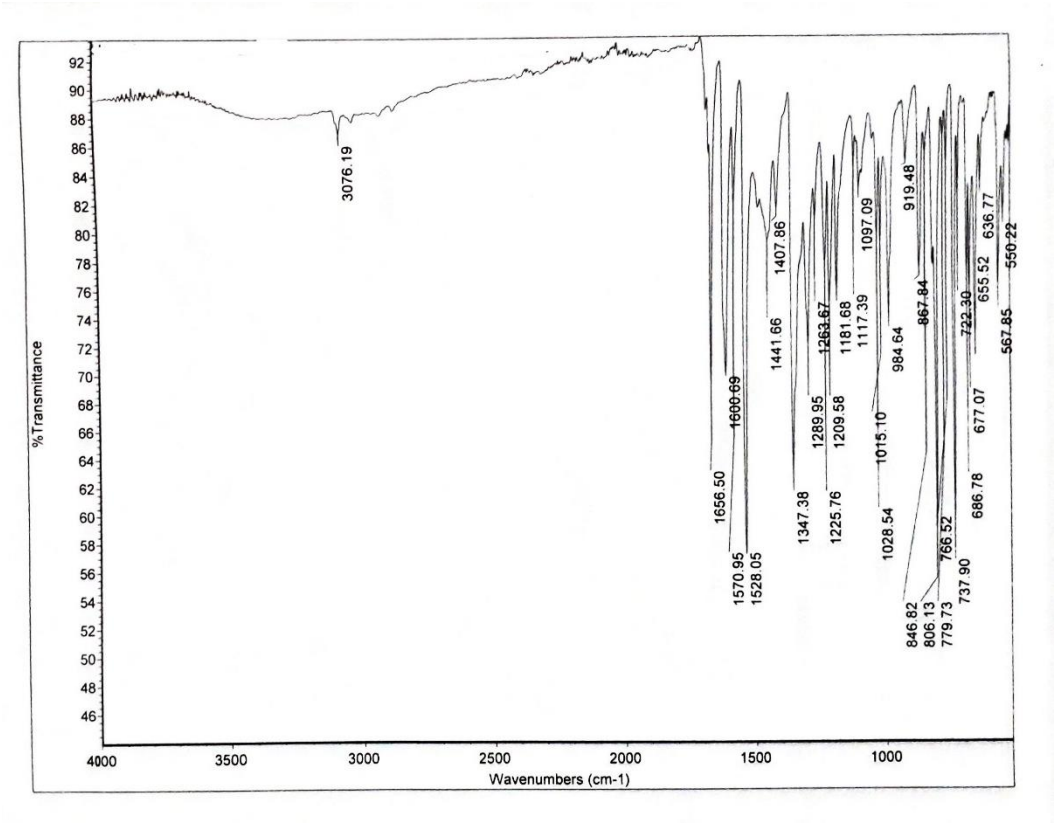

Figure S1. FTIR Spectrum of Compound 4C

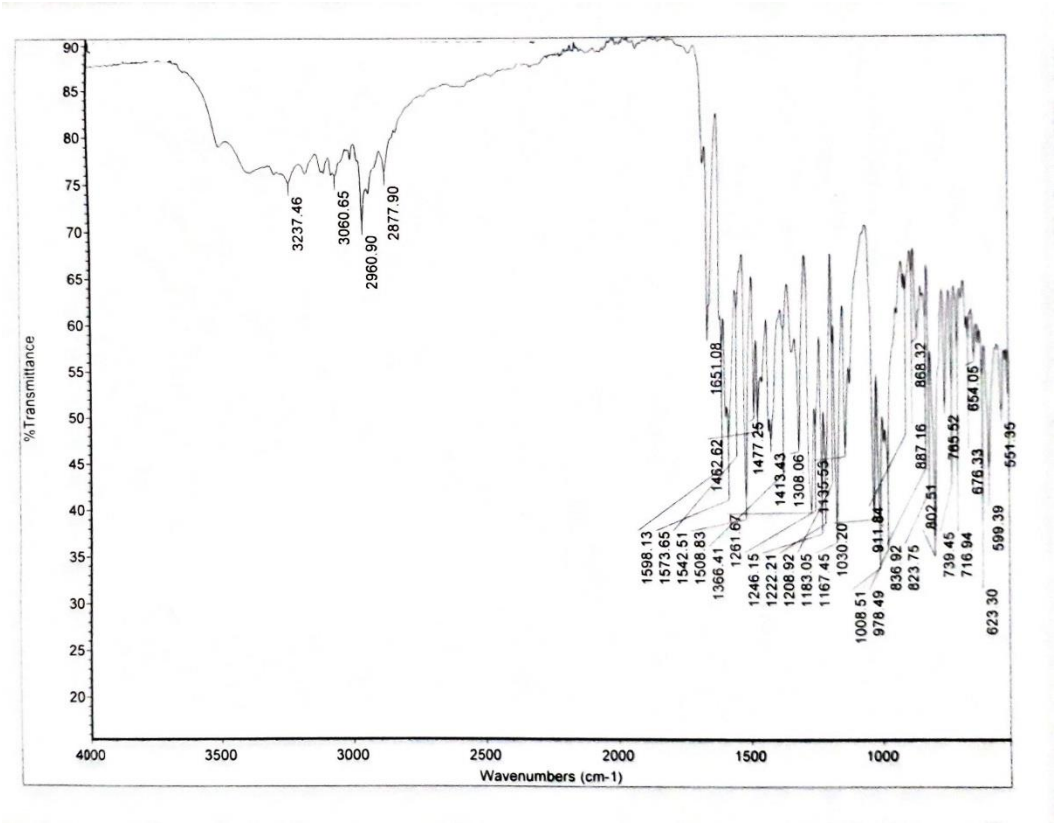

Figure S2. FTIR Spectrum of Compound 5C

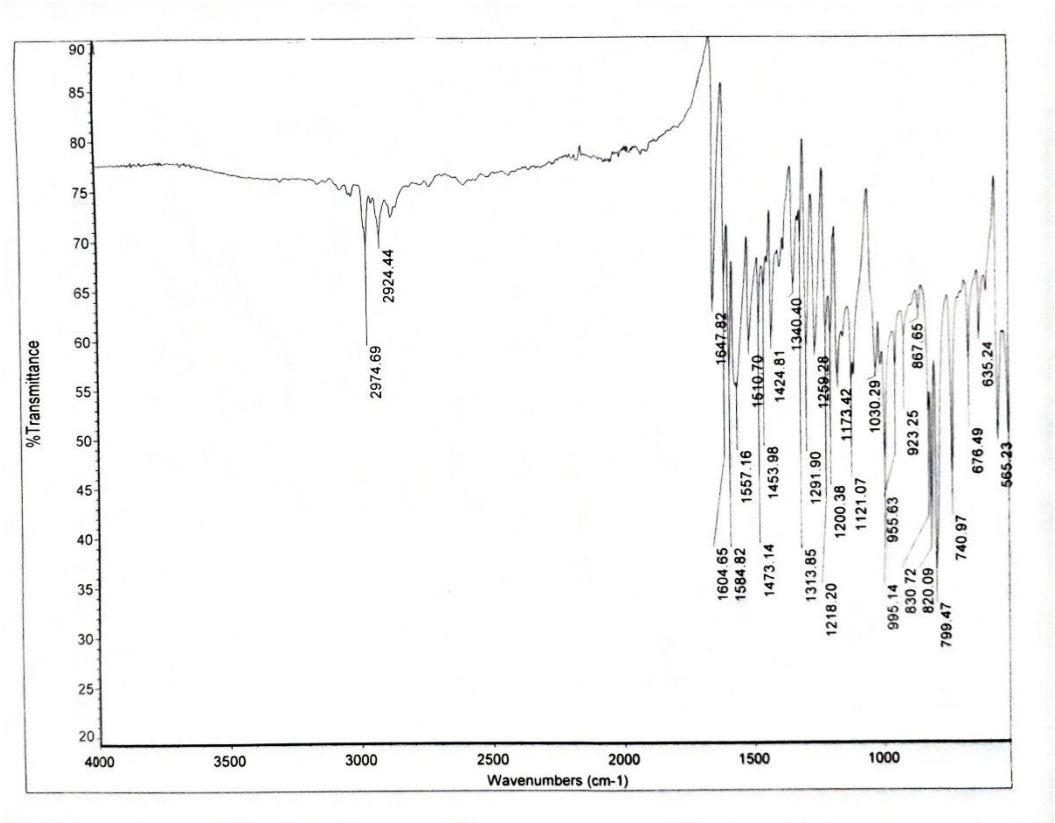

Figure S3. FTIR Spectrum of Compound 9C

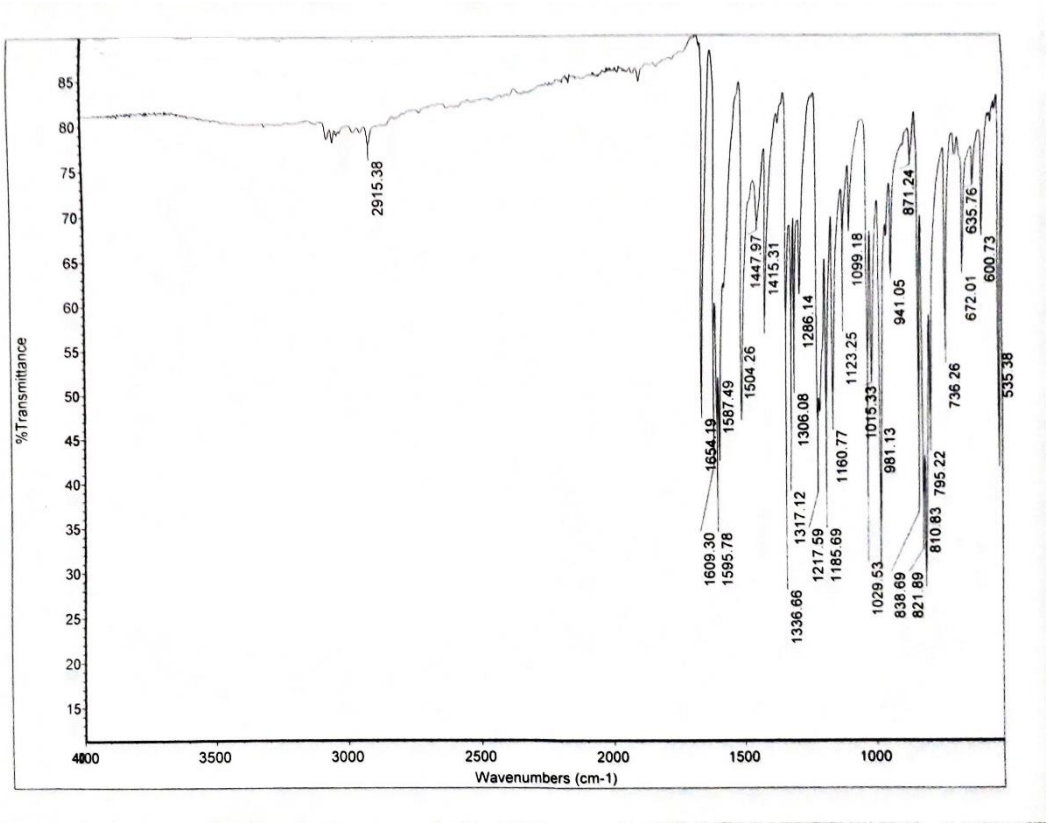

Figure S4. FTIR Spectrum of Compound 12C

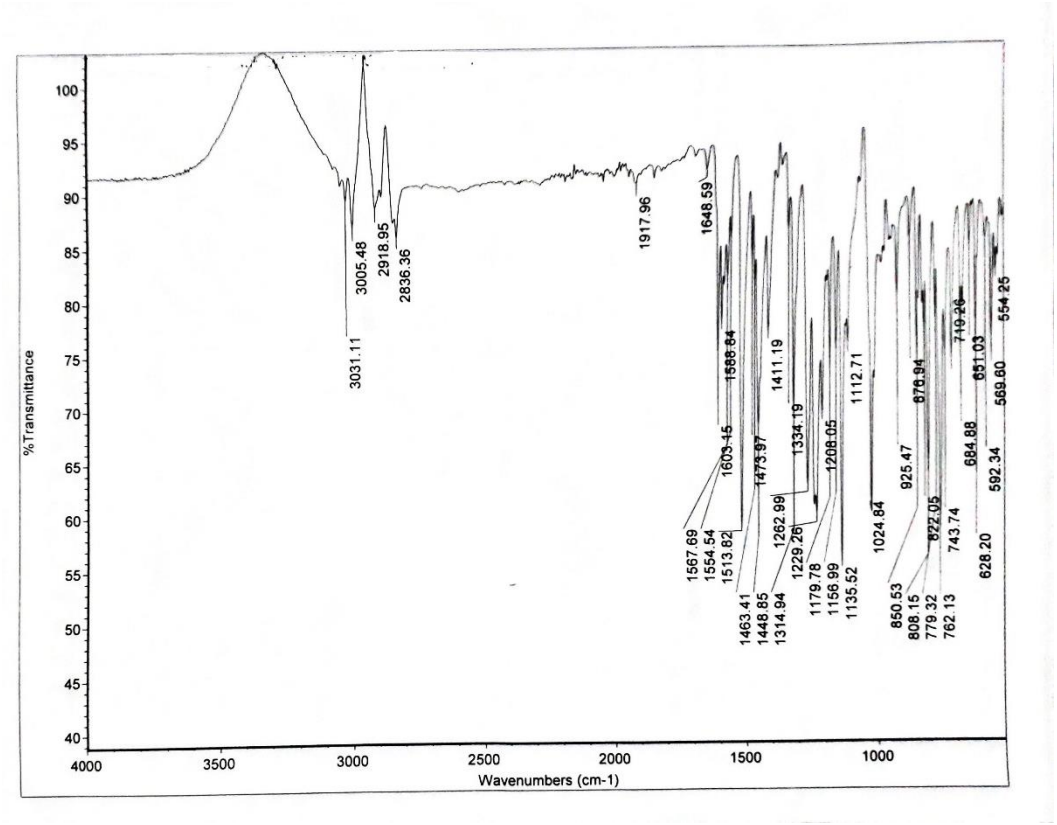

Figure S5. FTIR Spectrum of Compound 4B

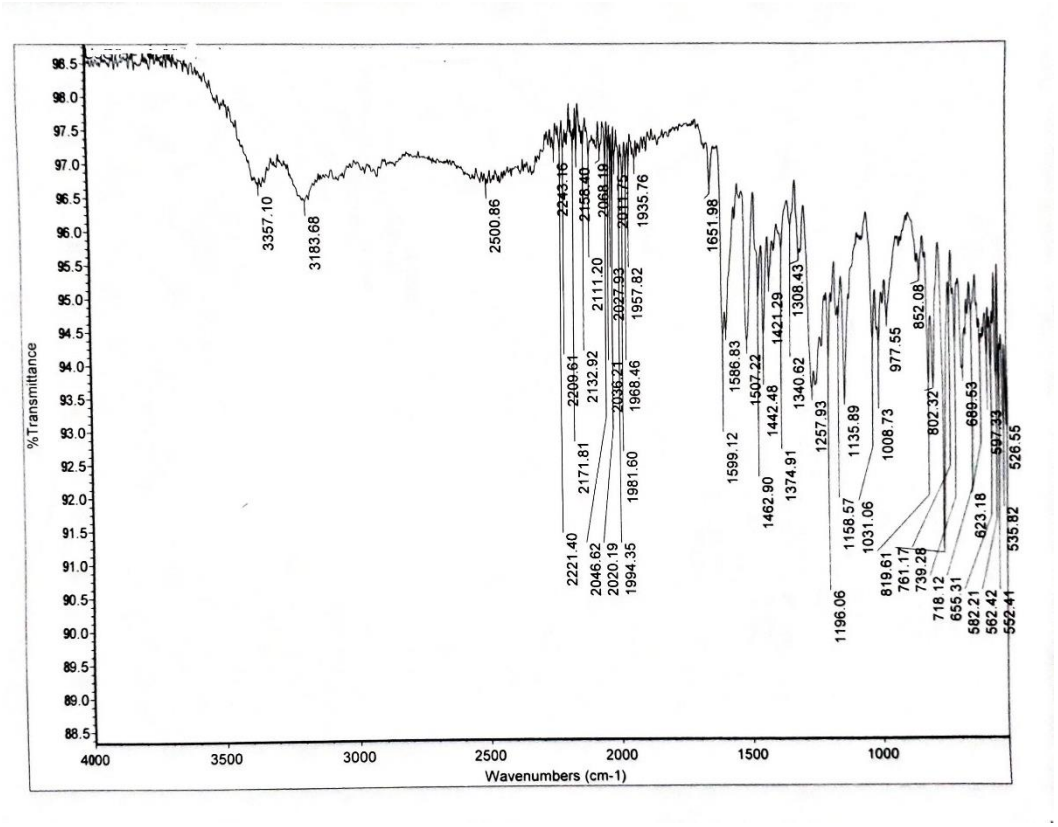

Figure S6. FTIR Spectrum of Compound 5B

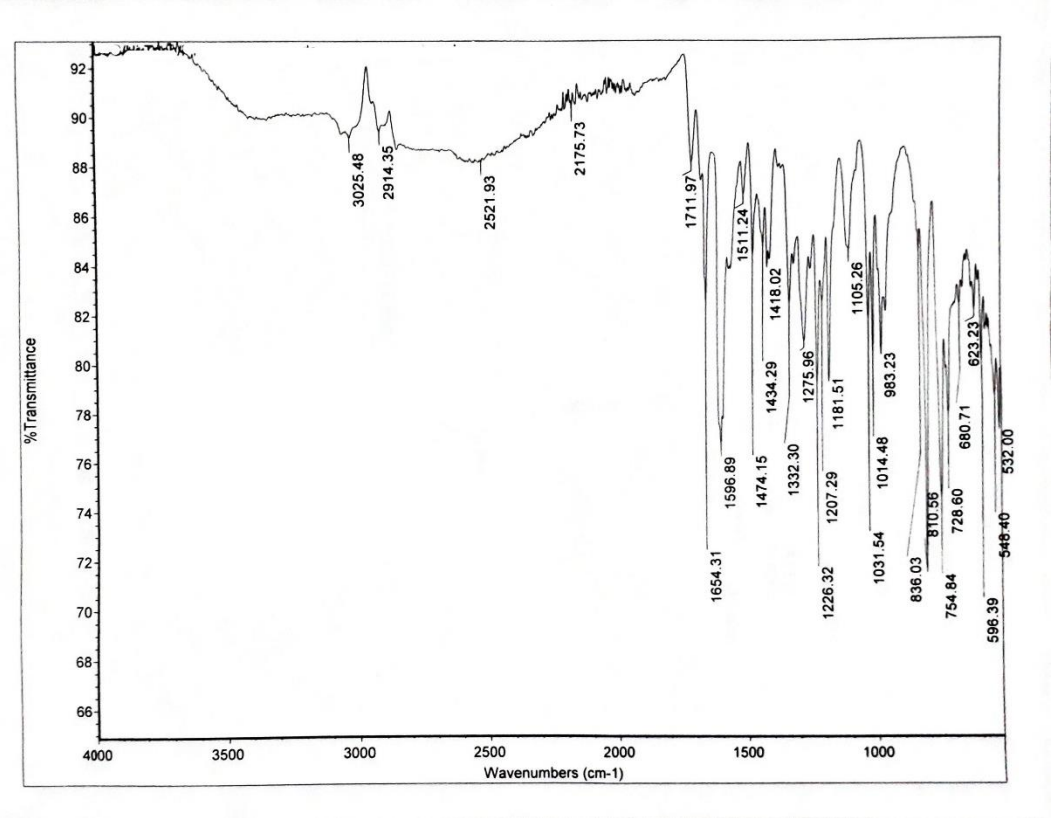

Figure S7. FTIR Spectrum of Compound 6B

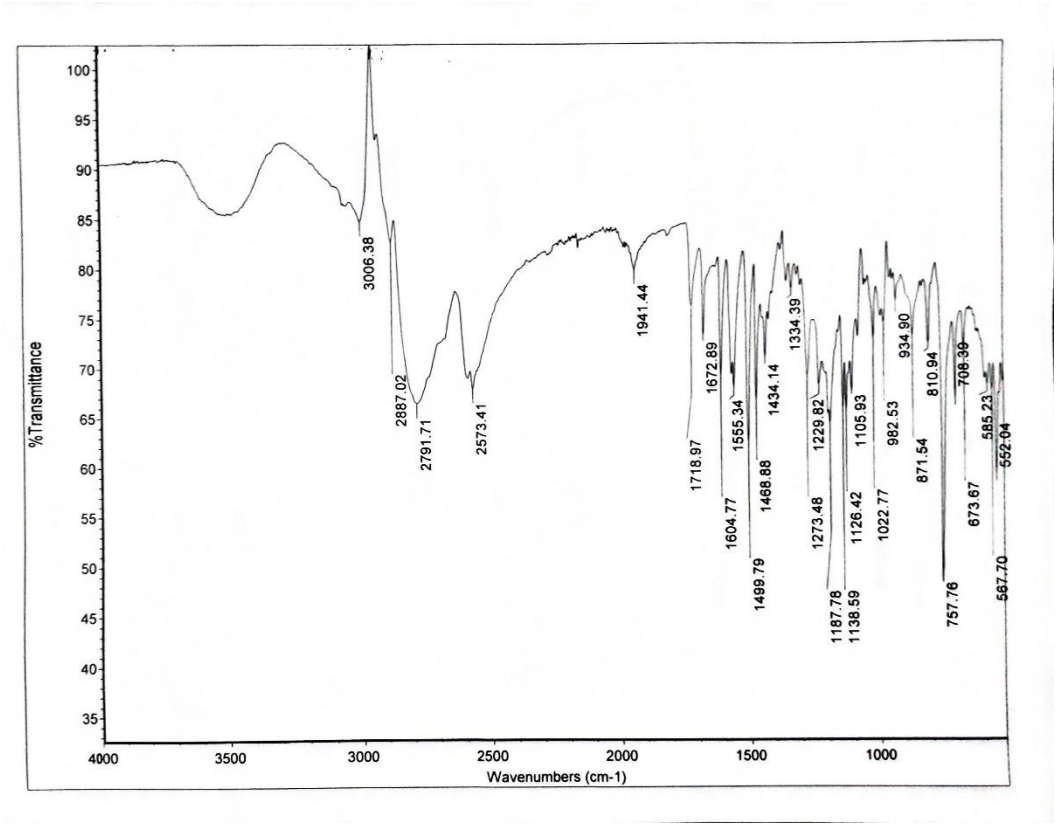

Figure S8. FTIR Spectrum of Compound 7B

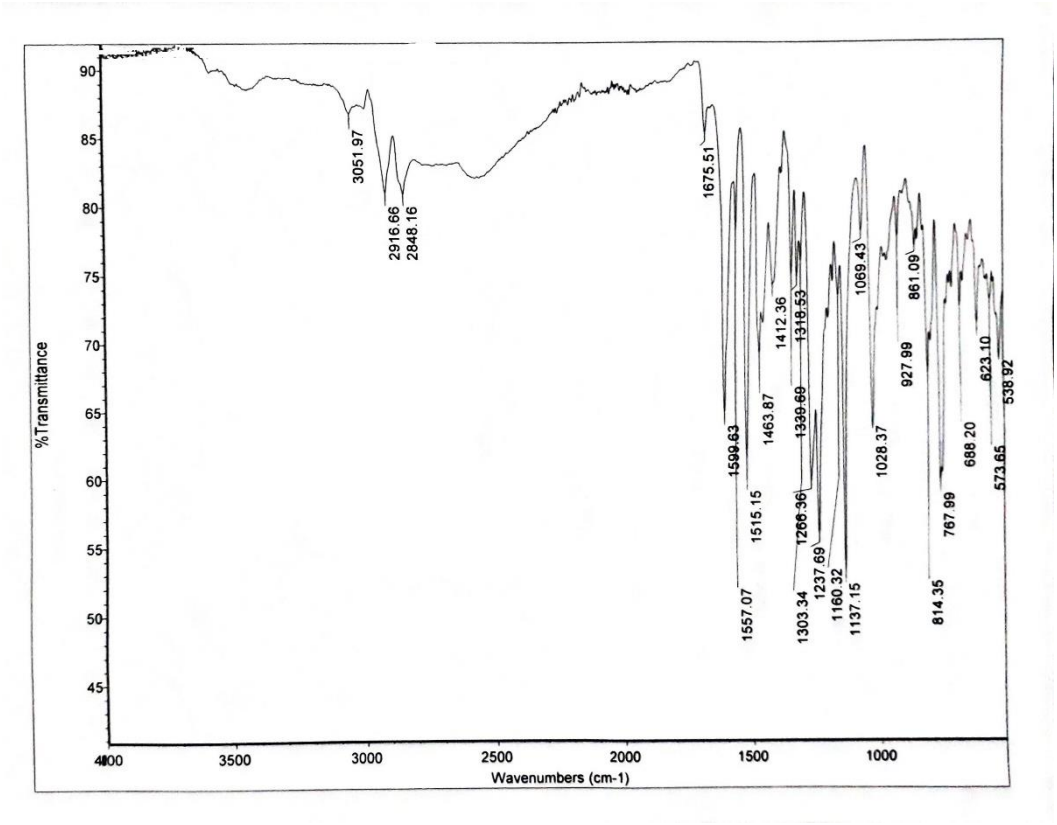

Figure S9. FTIR Spectrum of Compound 8B

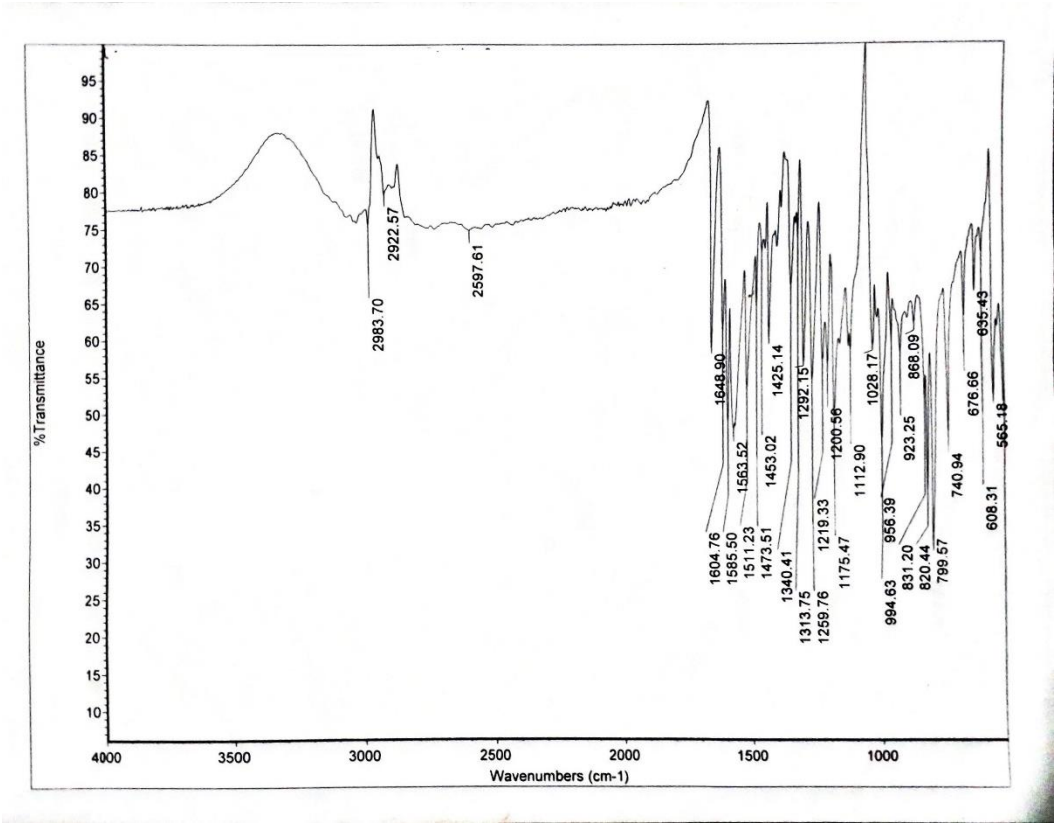

Figure S10. FTIR Spectrum of Compound 9B

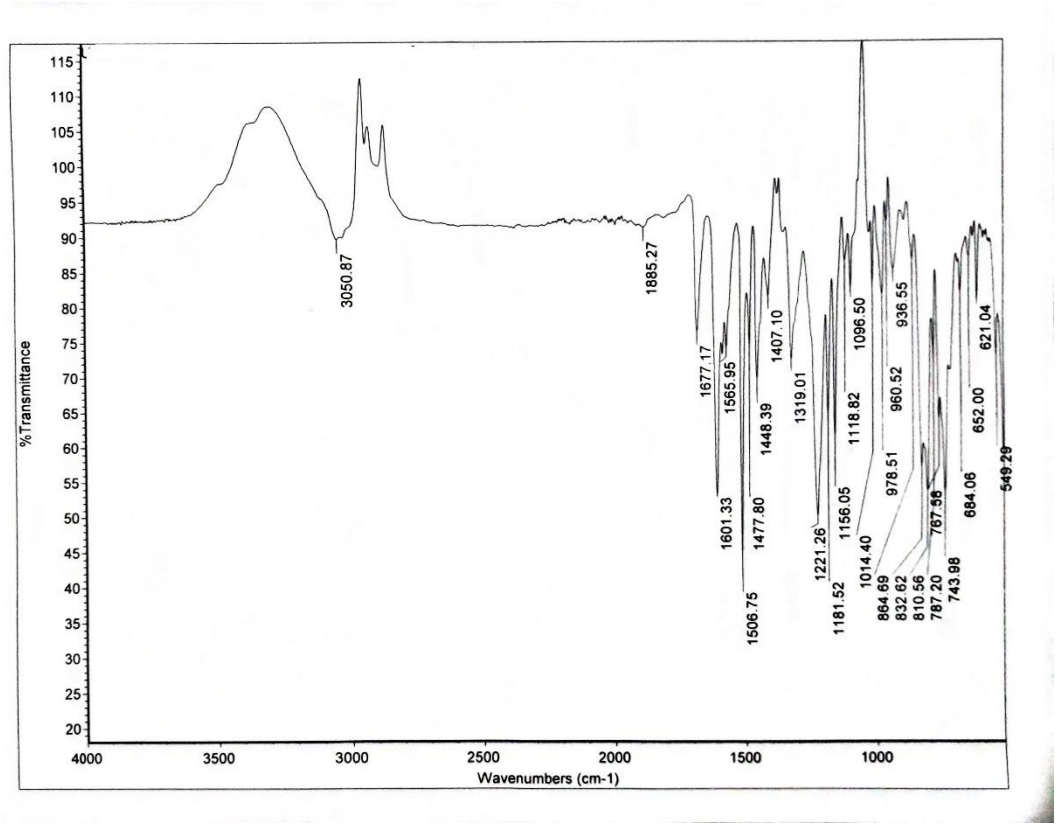

Figure S11. FTIR Spectrum of Compound 12B

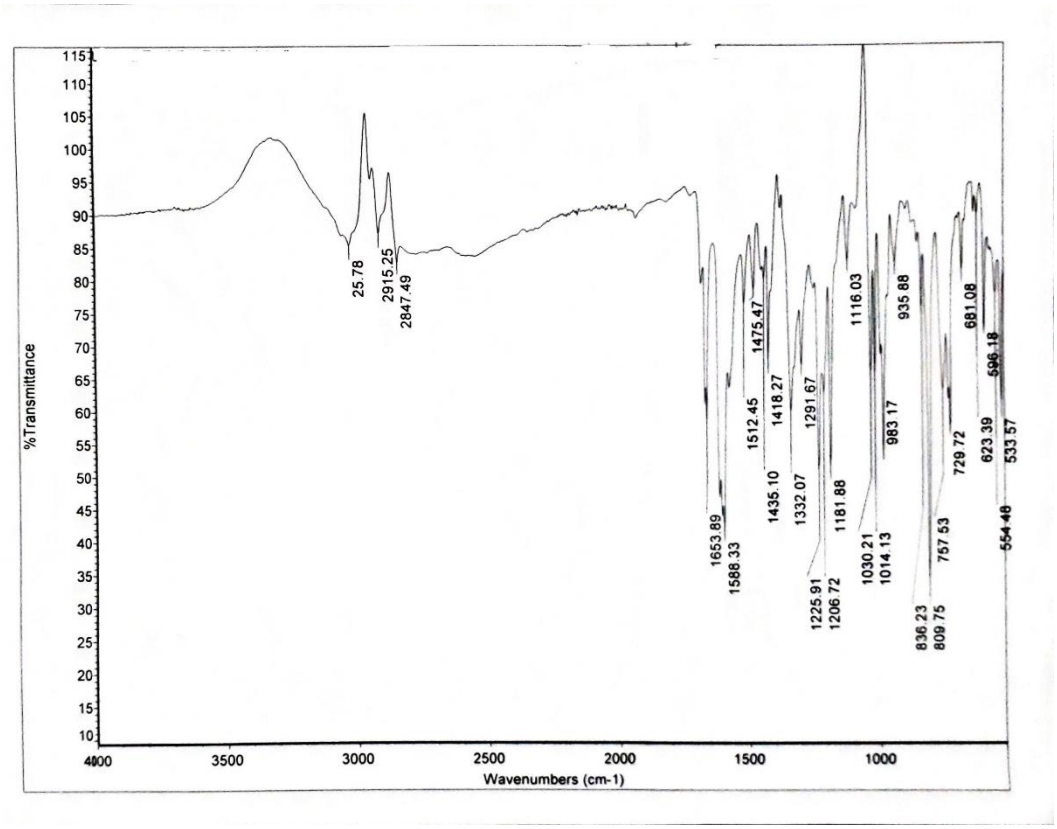

Figure S12. FTIR Spectrum of Compound 13B

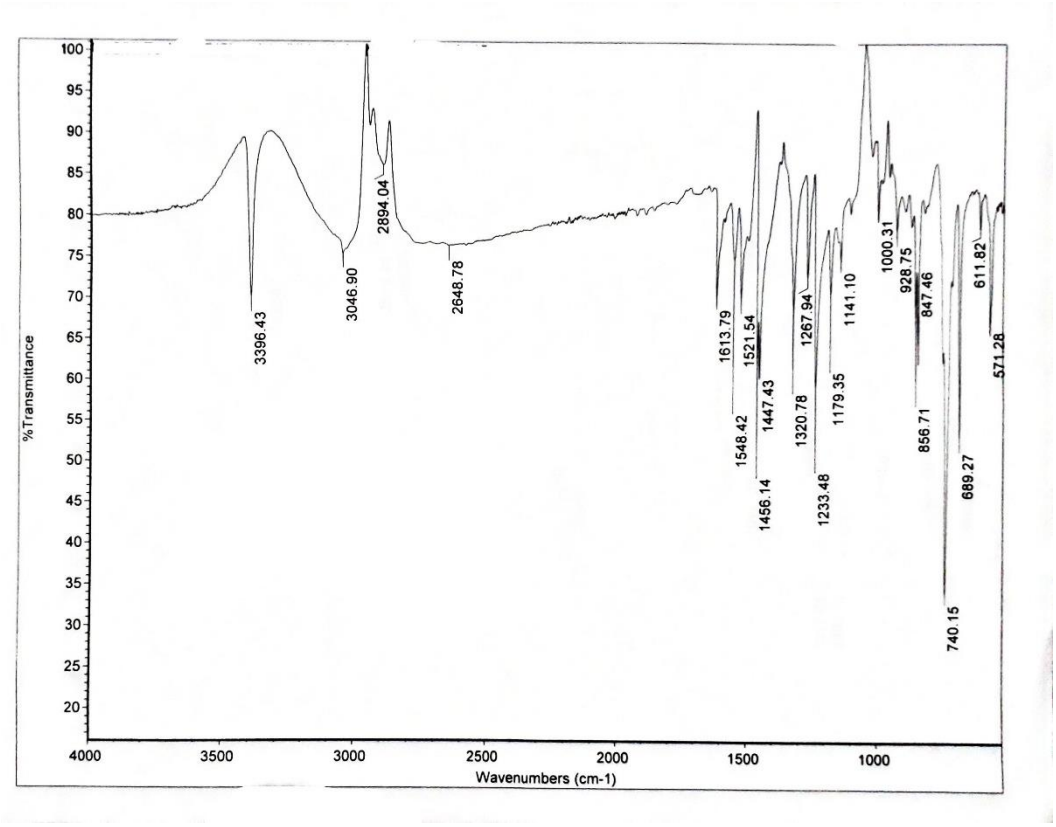

Figure S13. FTIR Spectrum of Compound 14B

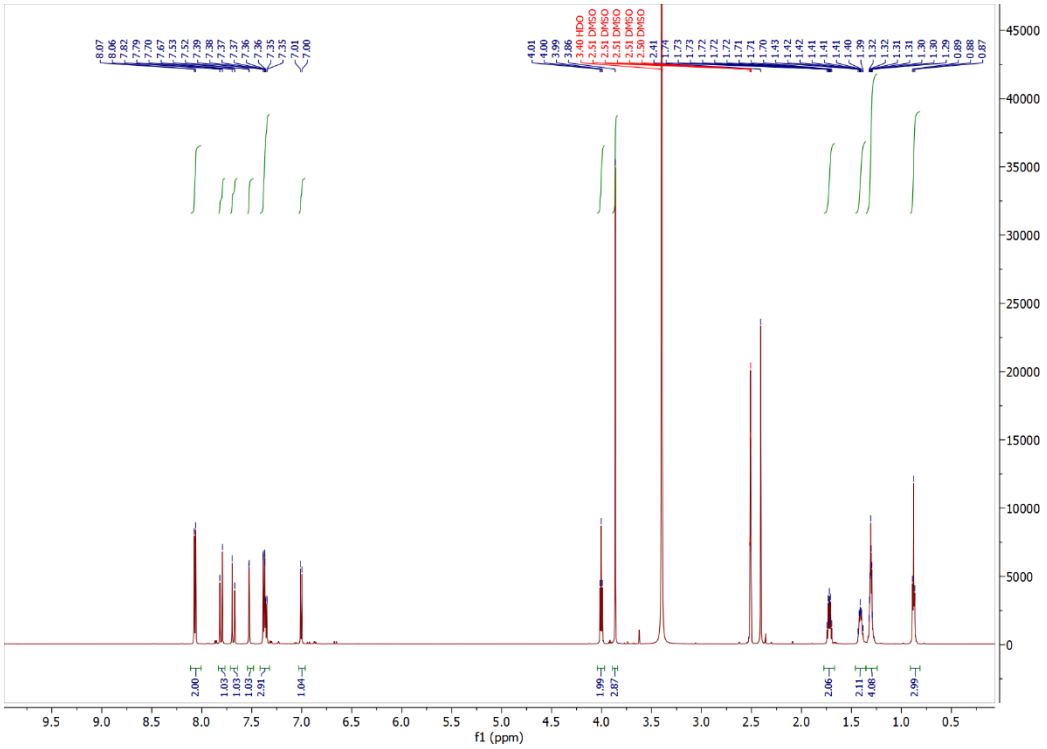

Figure S14. ^{1}H-NMR Spectrum of Compound (4C)

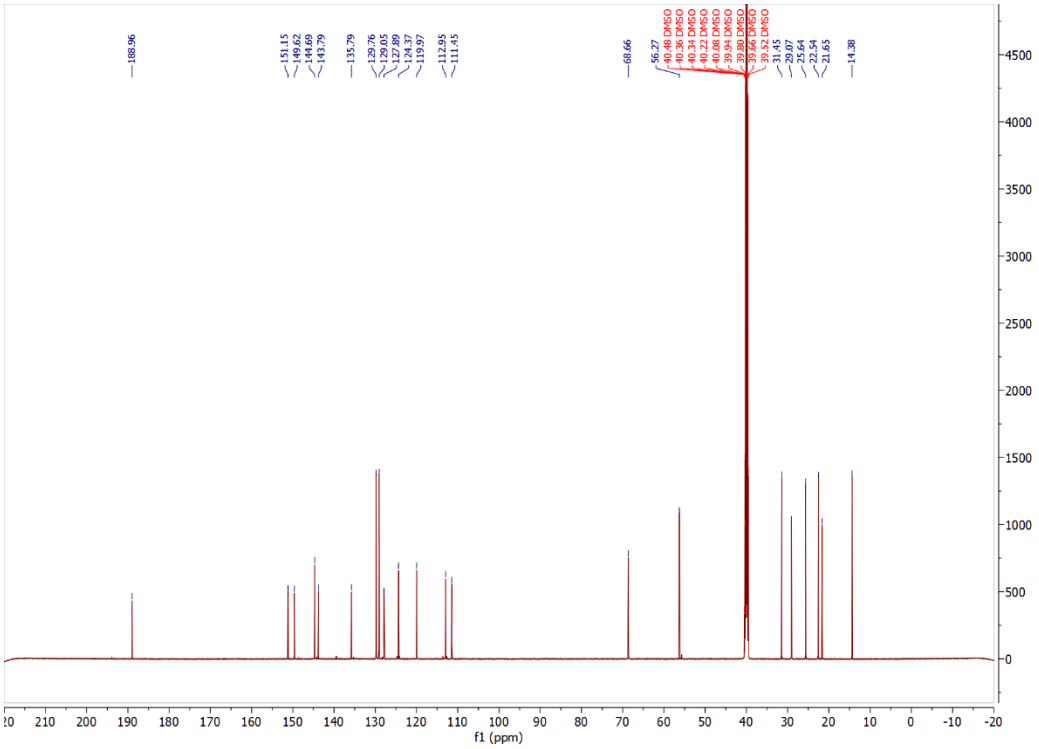

Figure S15. ^{13}C-NMR Spectrum of Compound (4C)

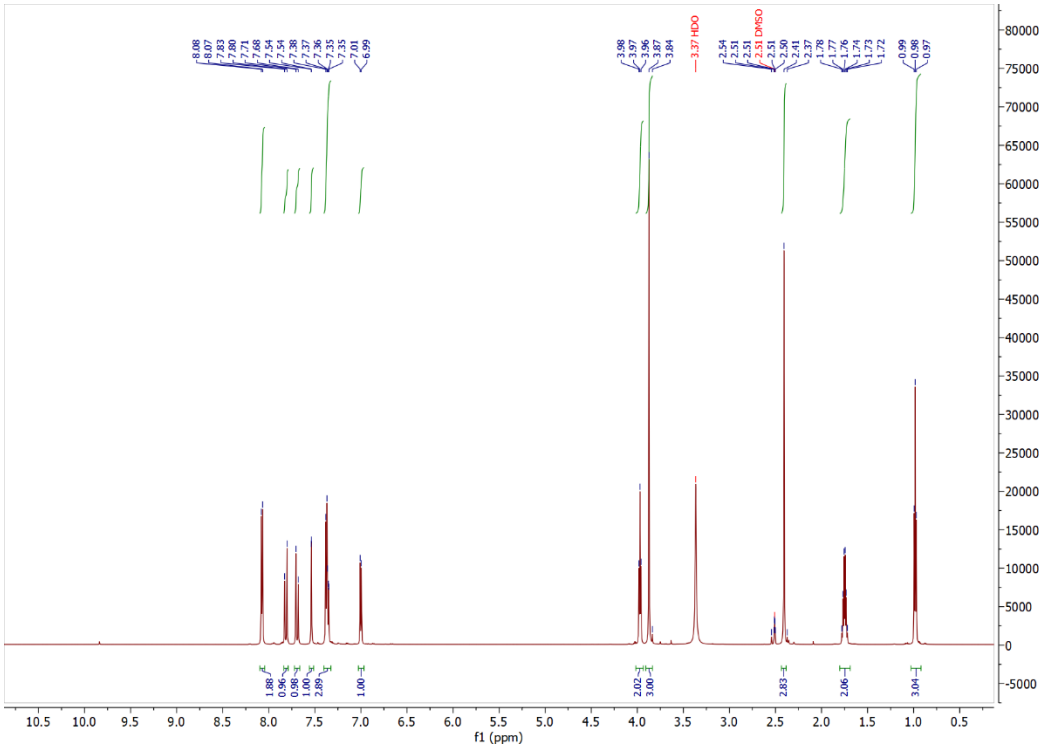

Figure S16. ^{1}H-NMR Spectrum of Compound (5C)

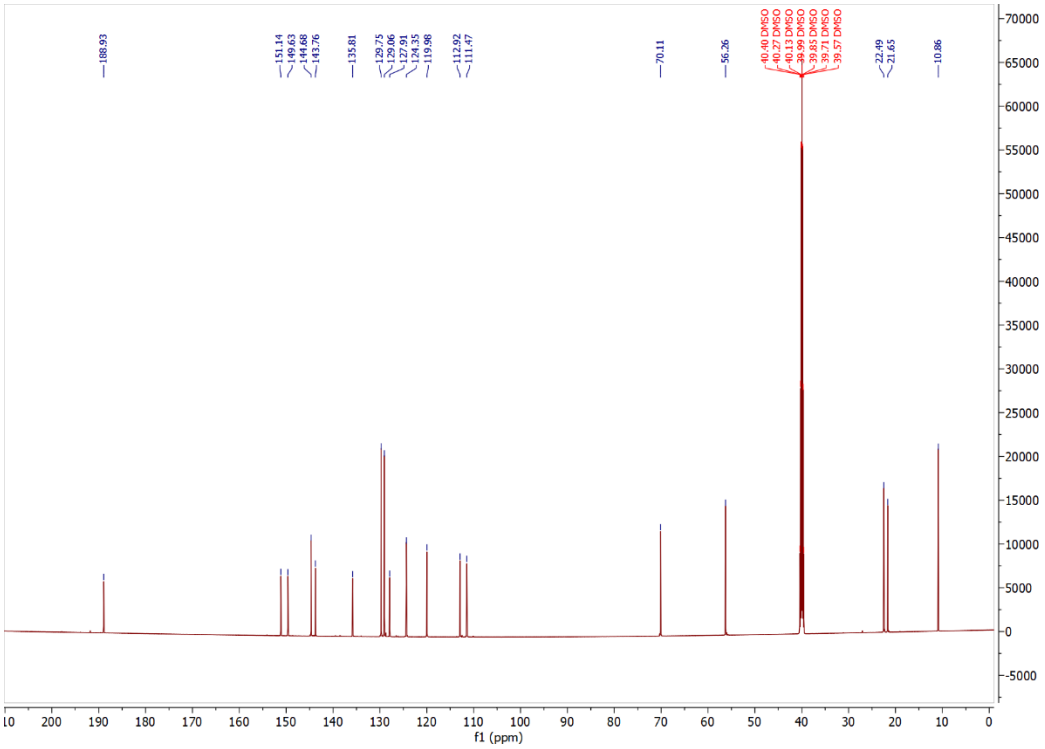

Figure S17. ^{13}C-NMR Spectrum of Compound (5C)

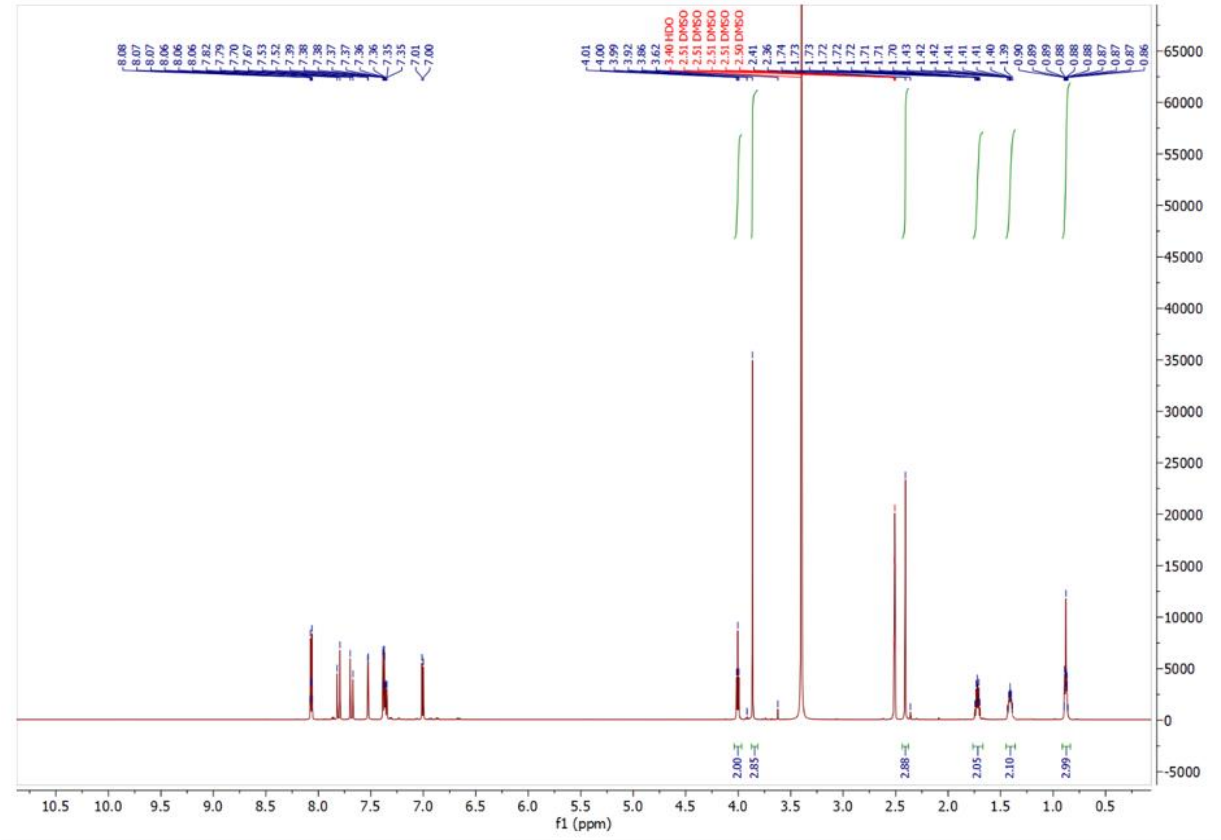

Figure S18. ^{1}H-NMR Spectrum of Compound (9C)

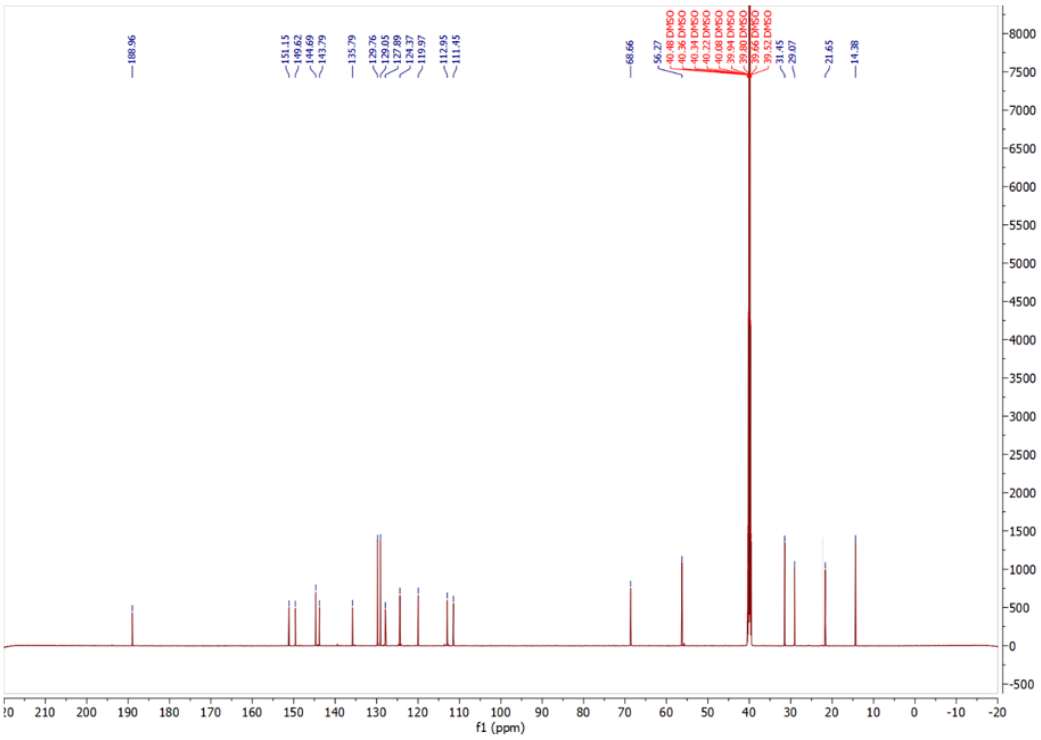

Figure S19. ^{13}C-NMR Spectrum of Compound (9C)

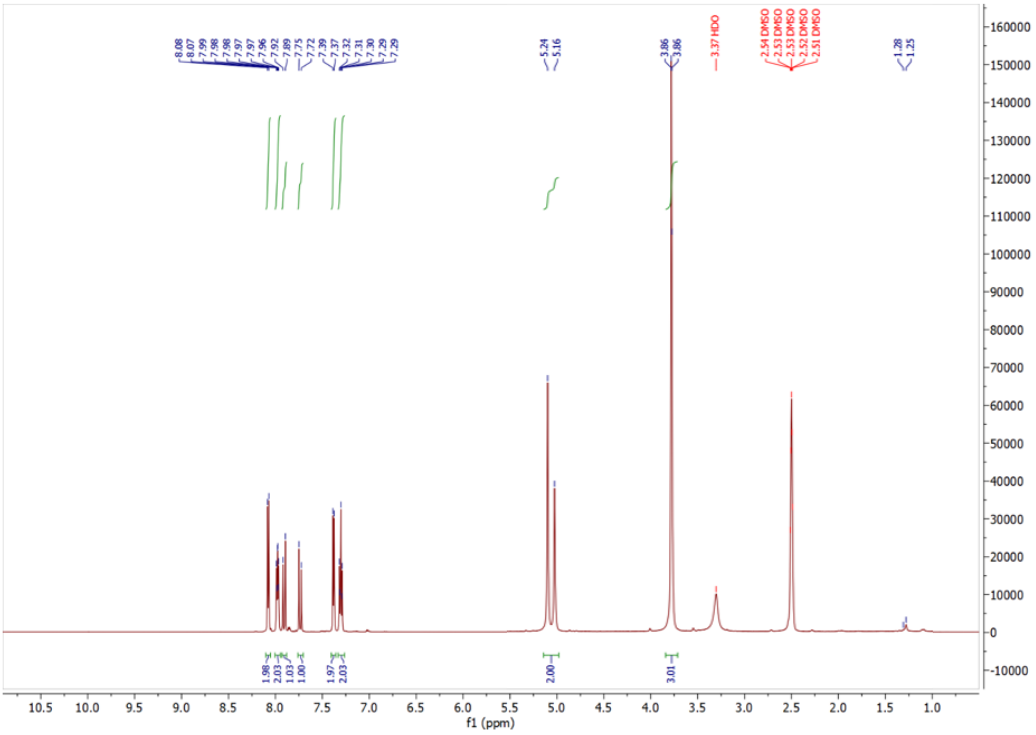

Figure S20. ^{1}H-NMR Spectrum of Compound (12C)

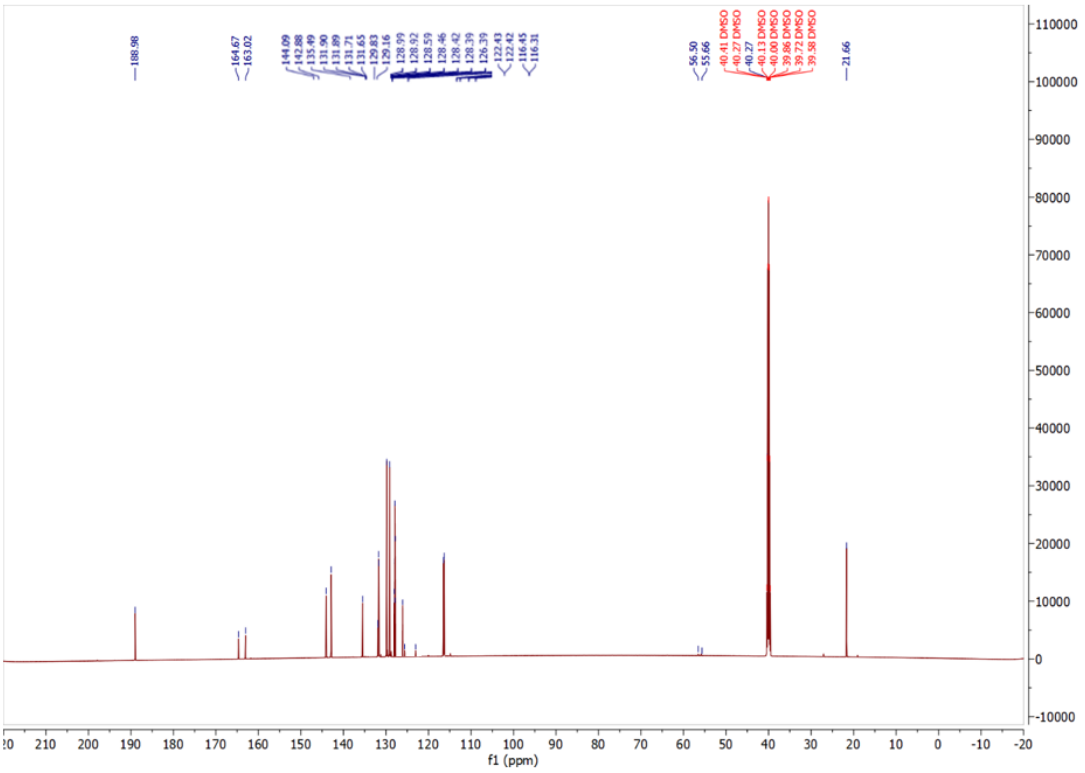

Figure S21. ^{13}C-NMR Spectrum of Compound (12C)

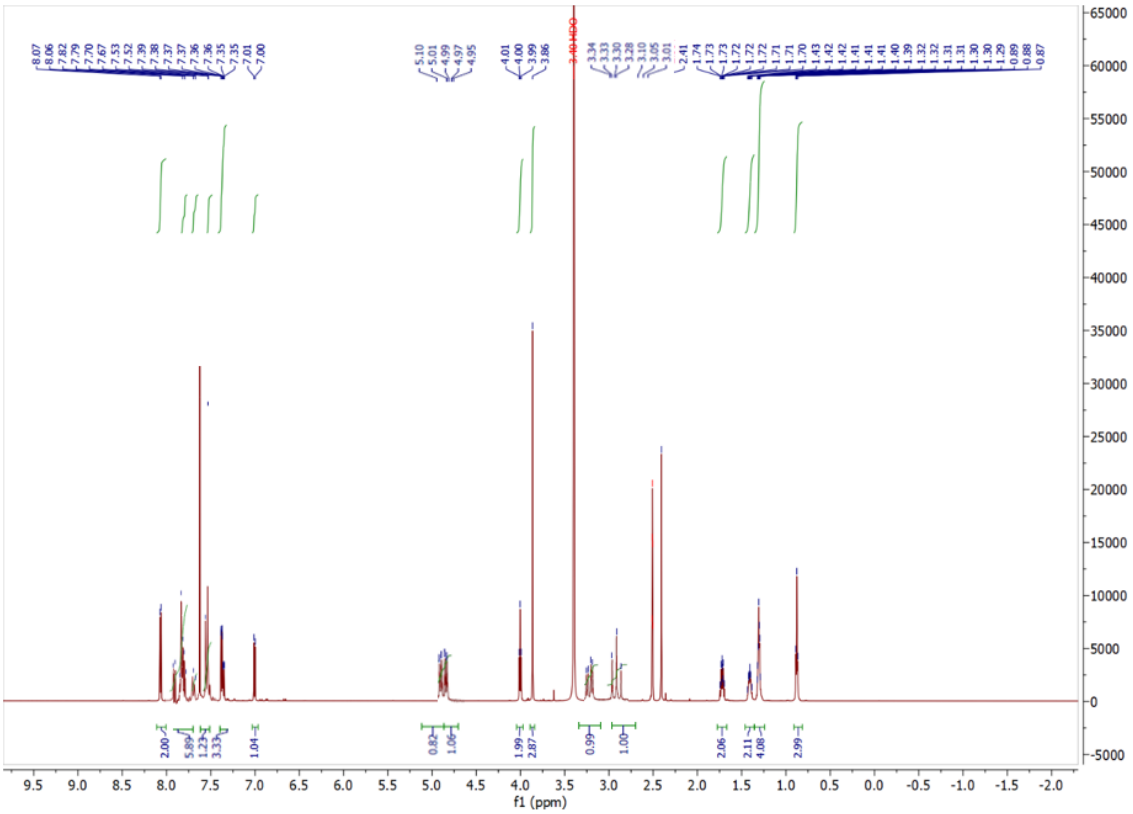

Figure S22. ^{1}H-NMR Spectrum of Compound (4B)

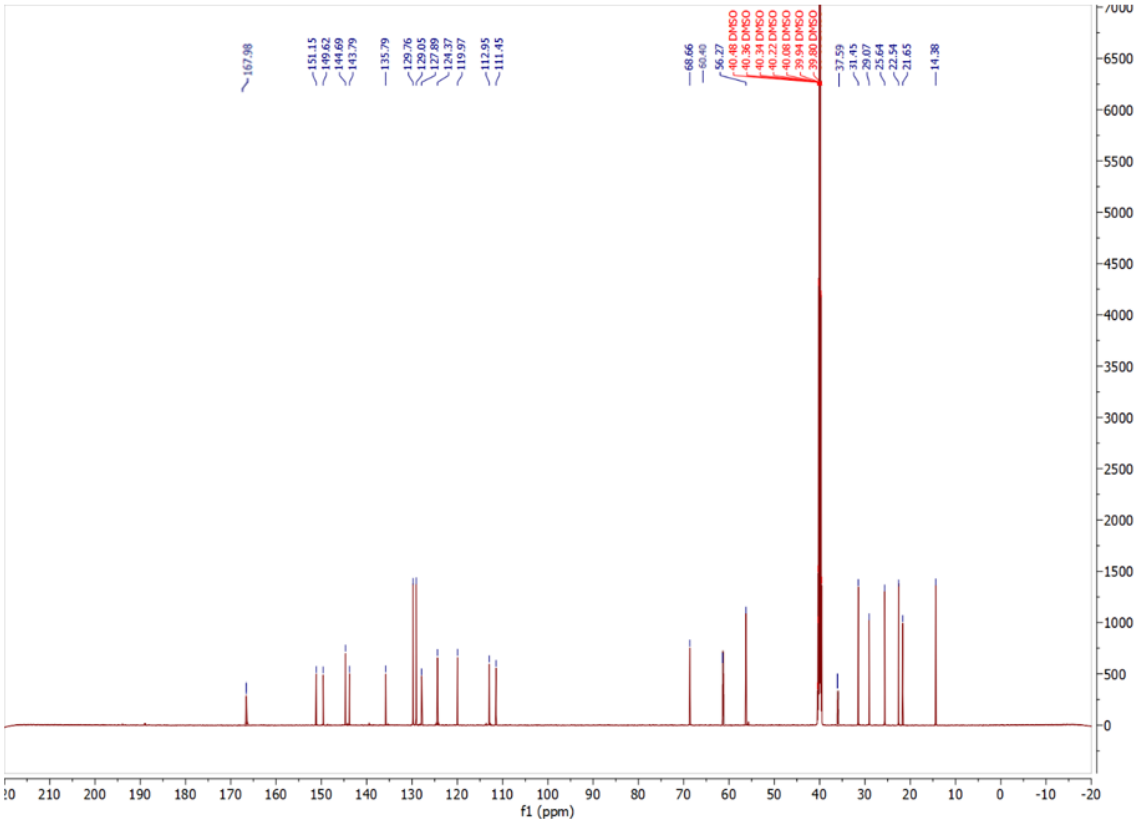

Figure S23. ^{13}C-NMR Spectrum of Compound (4B)

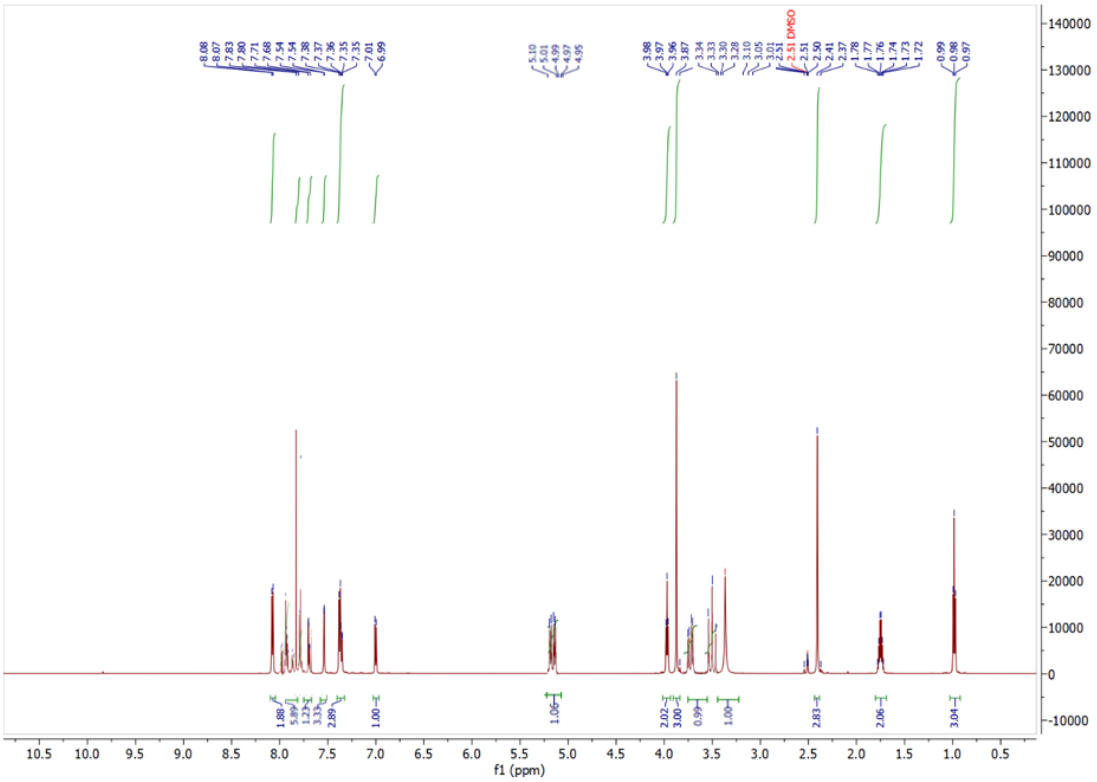

Figure S24. ^{1}H-NMR Spectrum of Compound (5B)

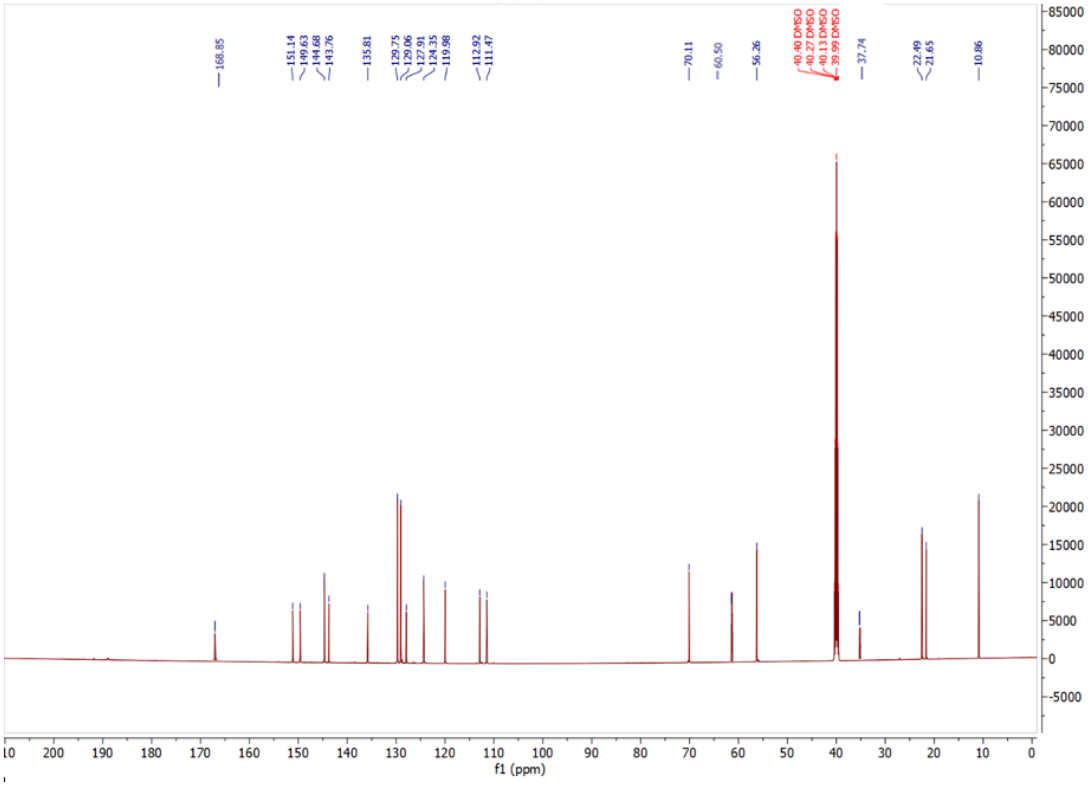

Figure S25. ^{13}C-NMR Spectrum of Compound (5B)

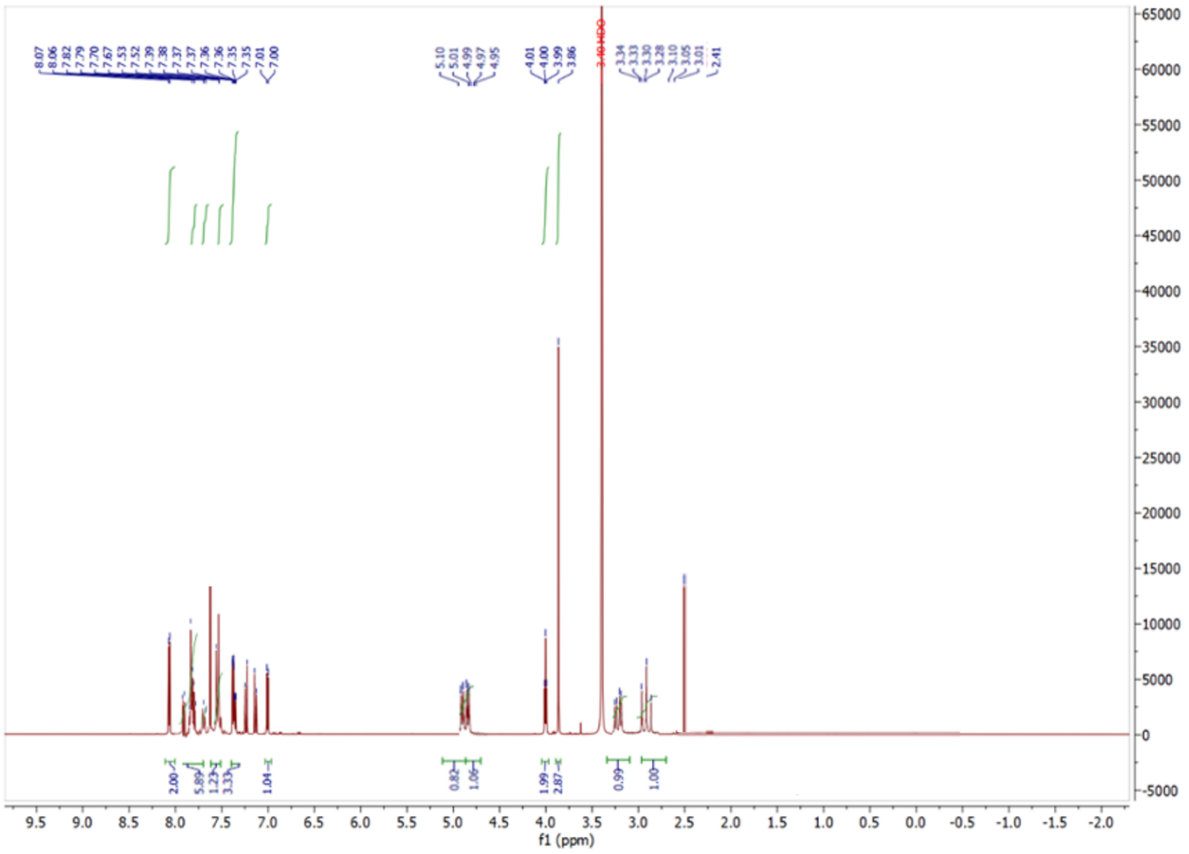

Figure S26. ^{1}H-NMR Spectrum of Compound (6B)

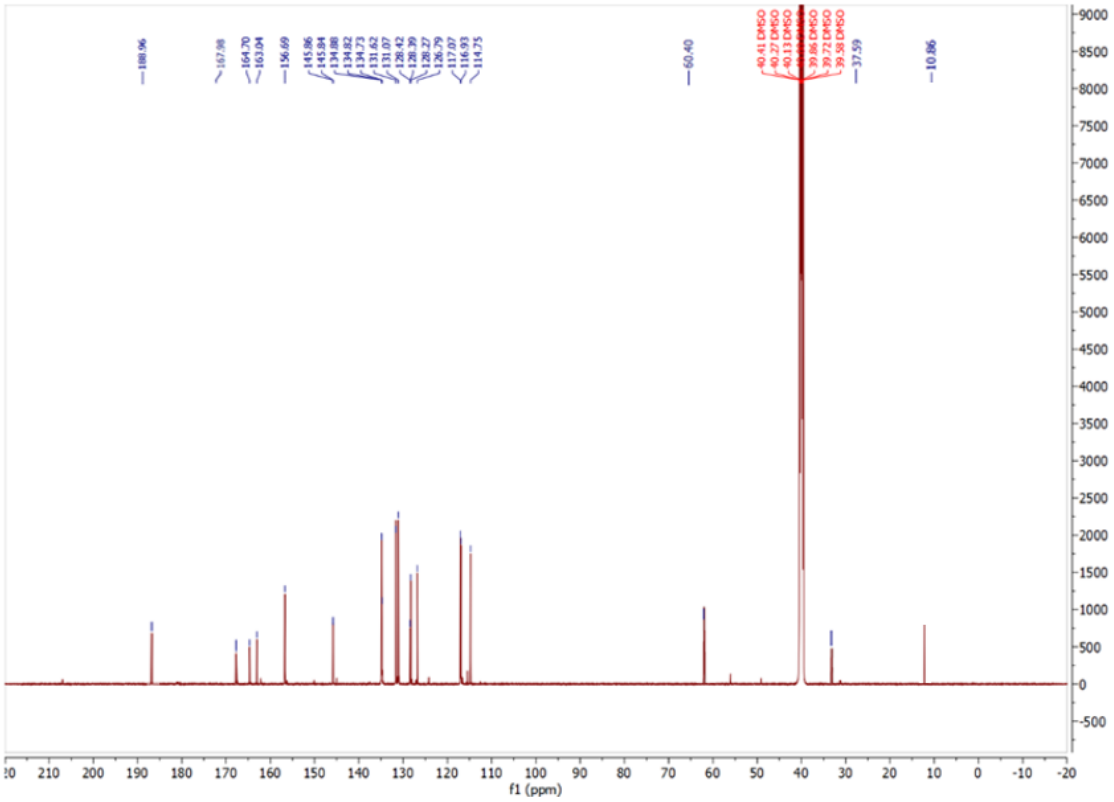

Figure S27. ^{13}C-NMR Spectrum of Compound (6B)

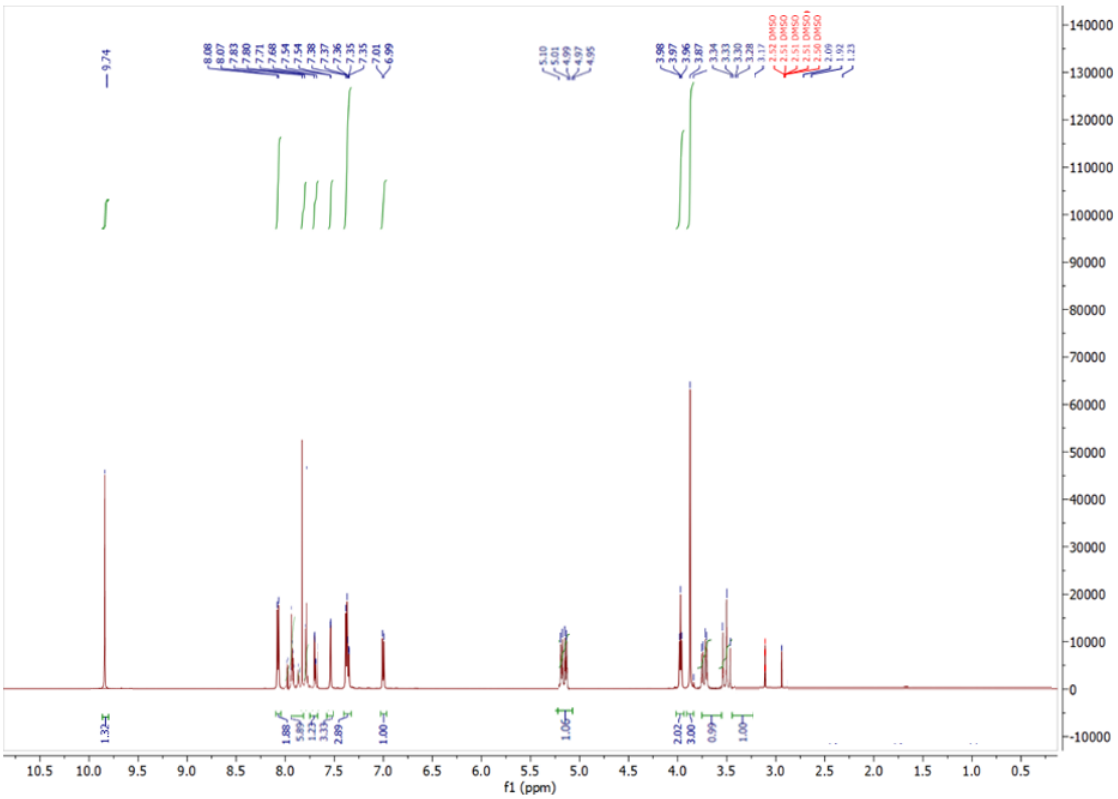

Figure S28. ^{1}H-NMR Spectrum of Compound (7B)

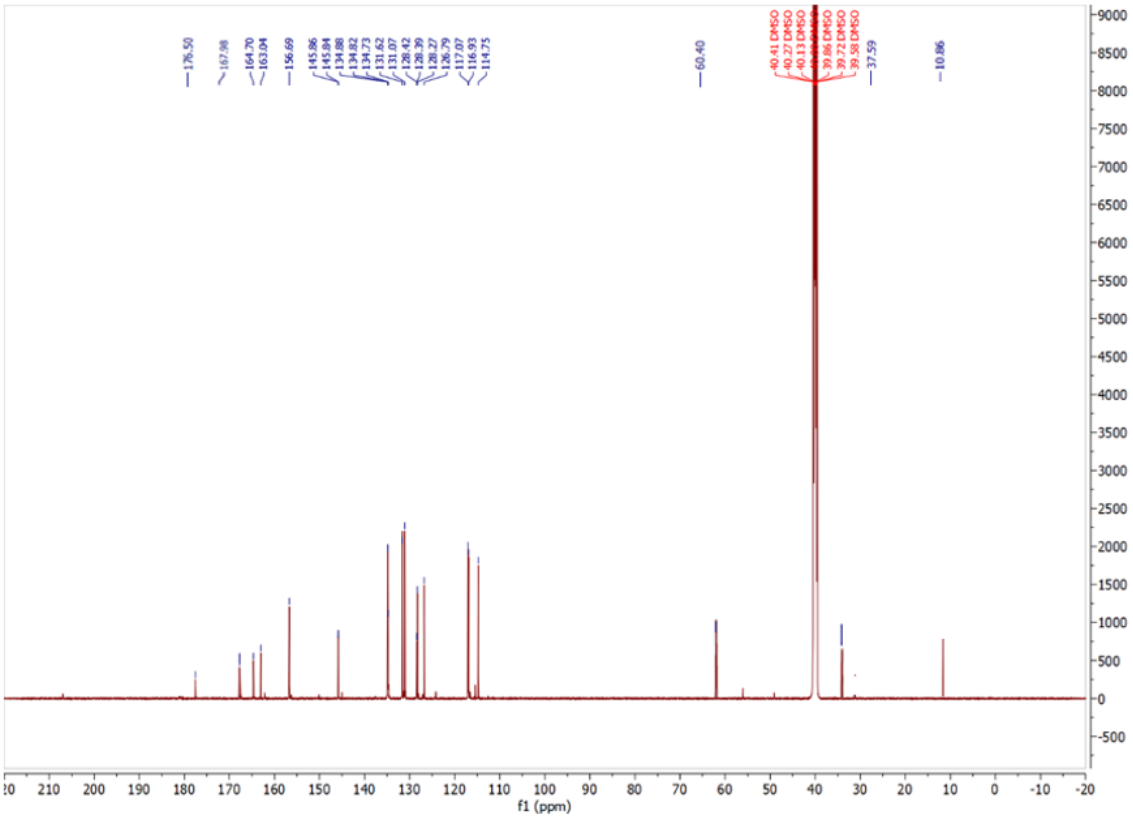

Figure S29. ^{13}C-NMR Spectrum of Compound (7B)

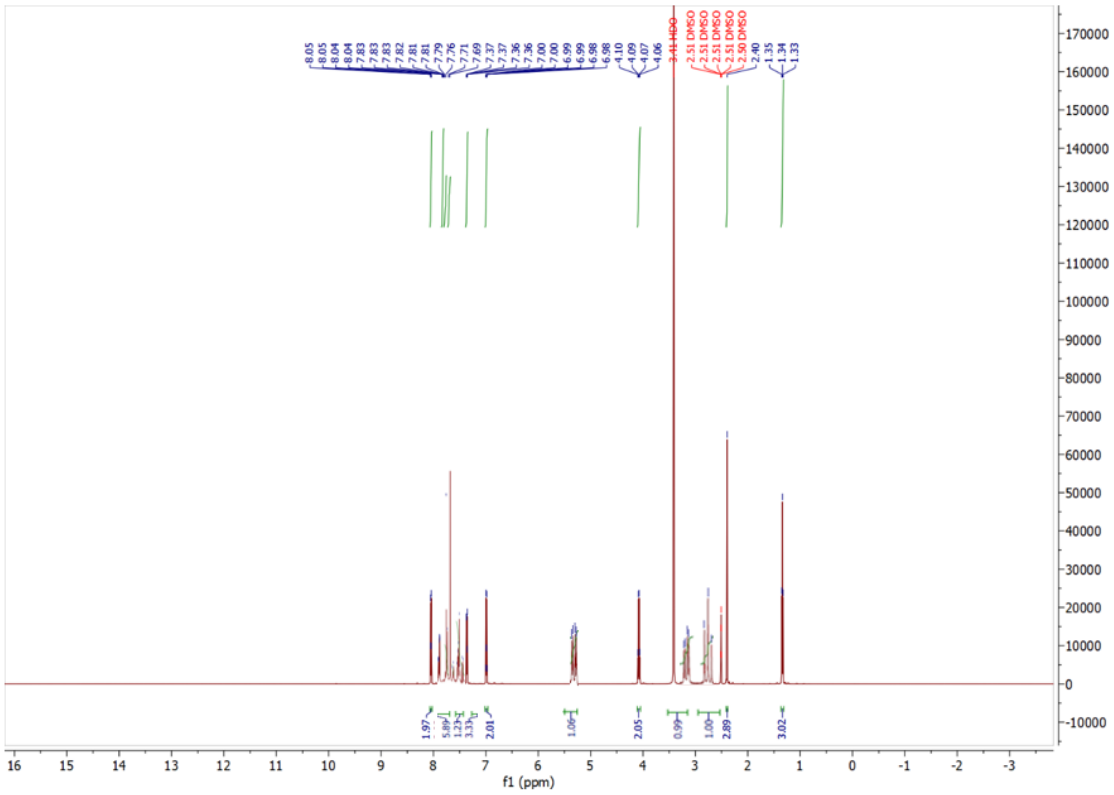

Figure S30. ^{1}H-NMR Spectrum of Compound (8B)

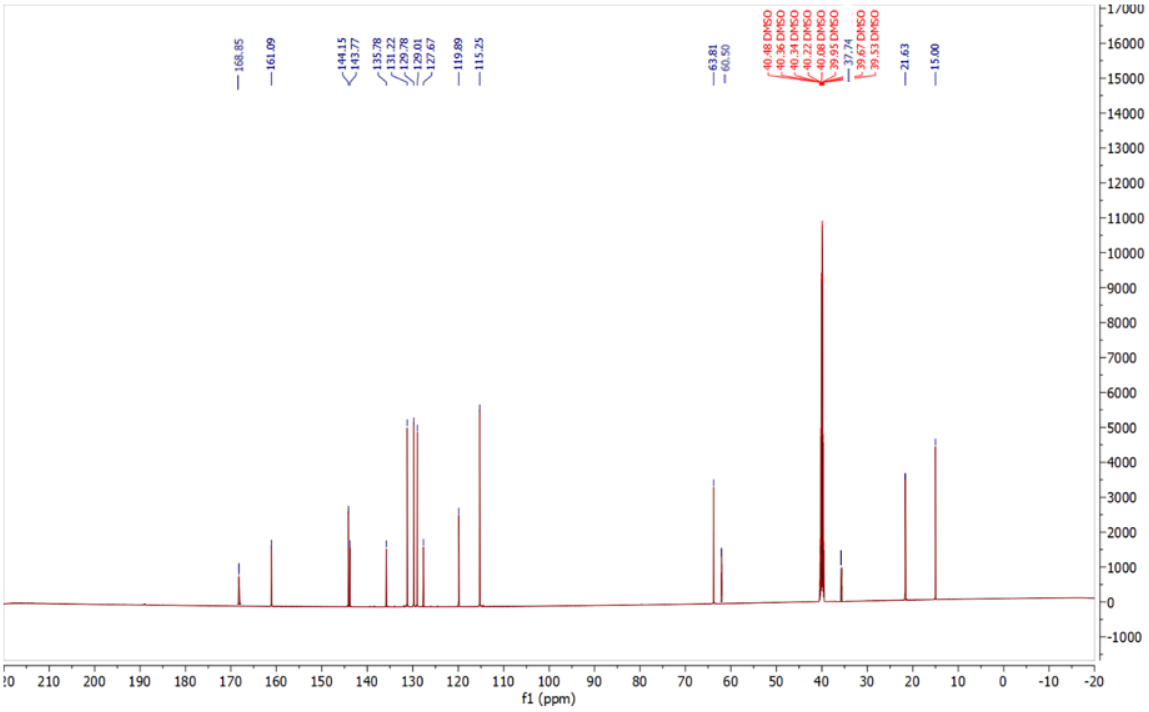

Figure S31. ^{13}C-NMR Spectrum of Compound (8B)

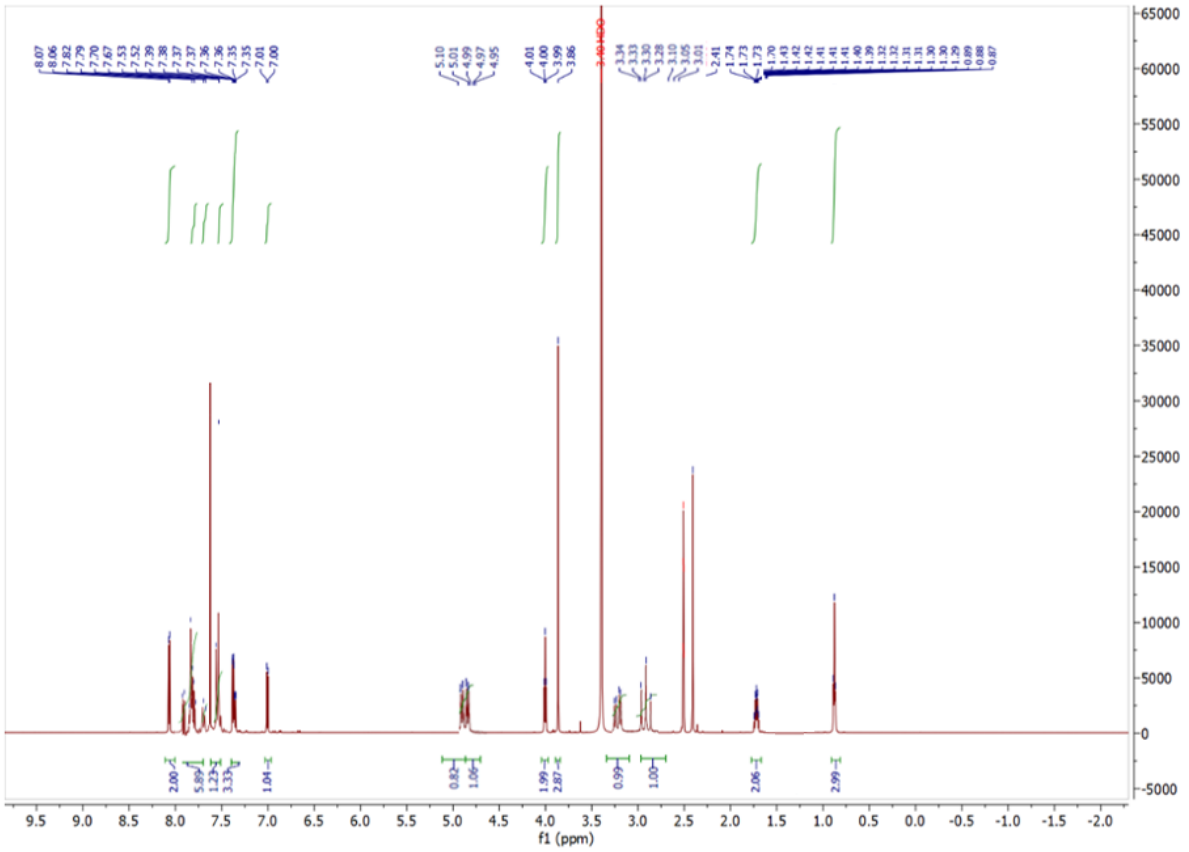

Figure S32. ^{1}H-NMR Spectrum of Compound (9B)

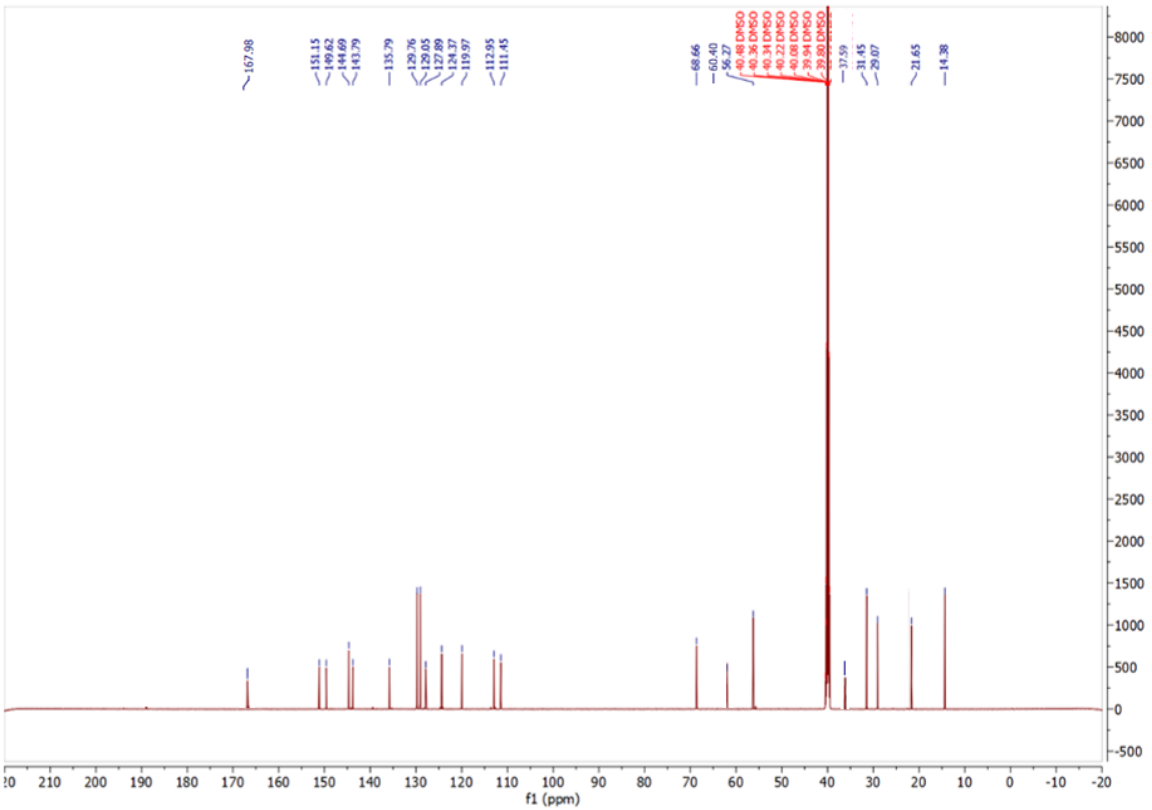

Figure S33. ^{13}C-NMR Spectrum of Compound (9B)

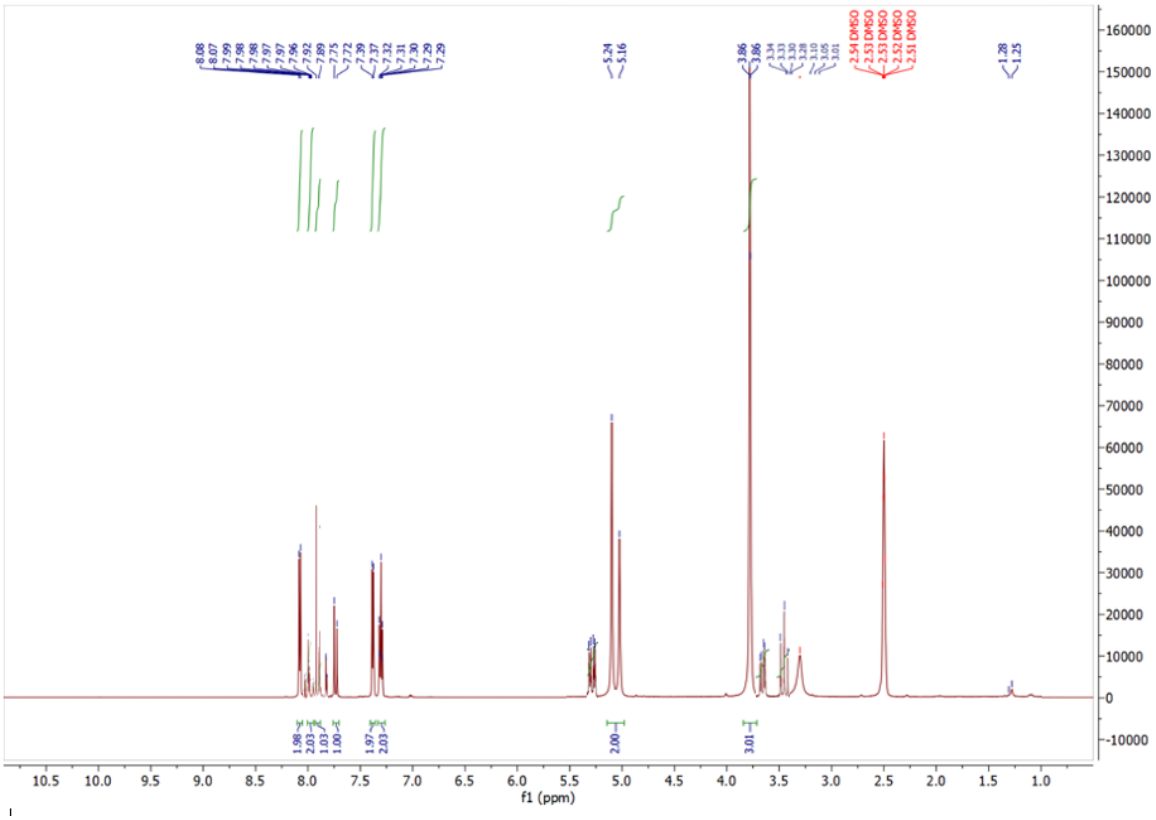

Figure S34. ^{1}H-NMR Spectrum of Compound (12B)

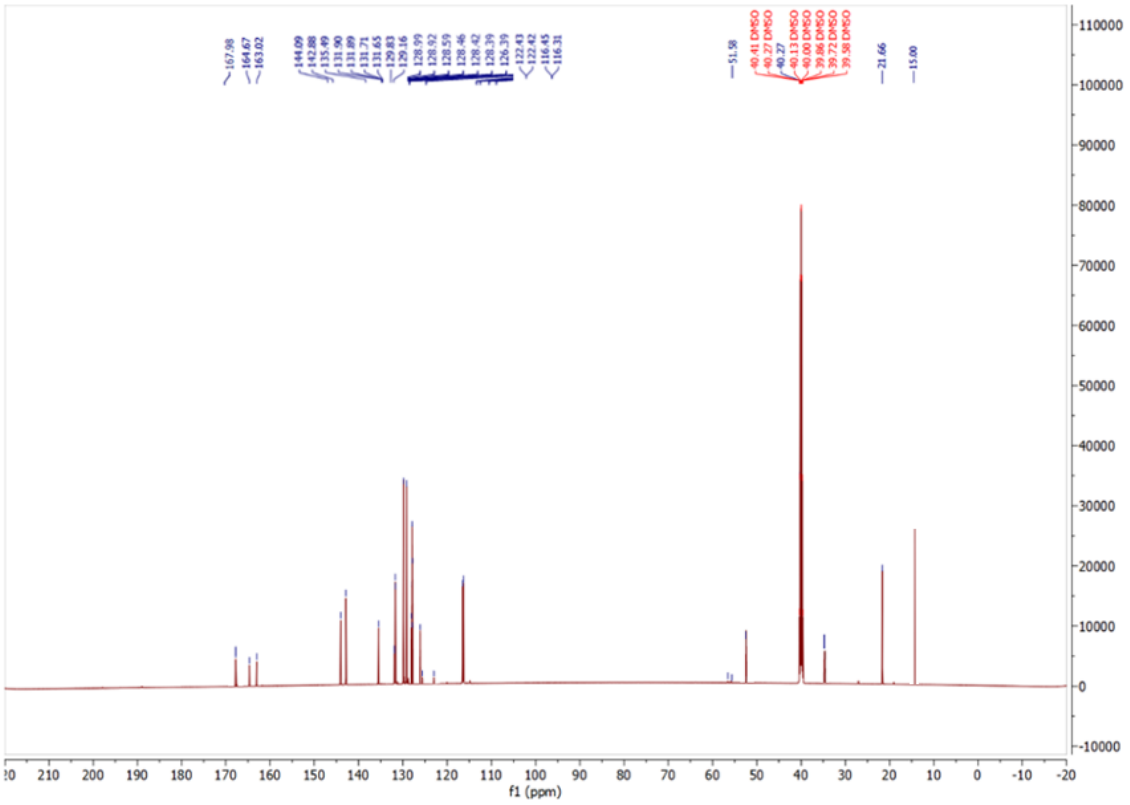

Figure S35. ^{13}C-NMR Spectrum of Compound (12B)

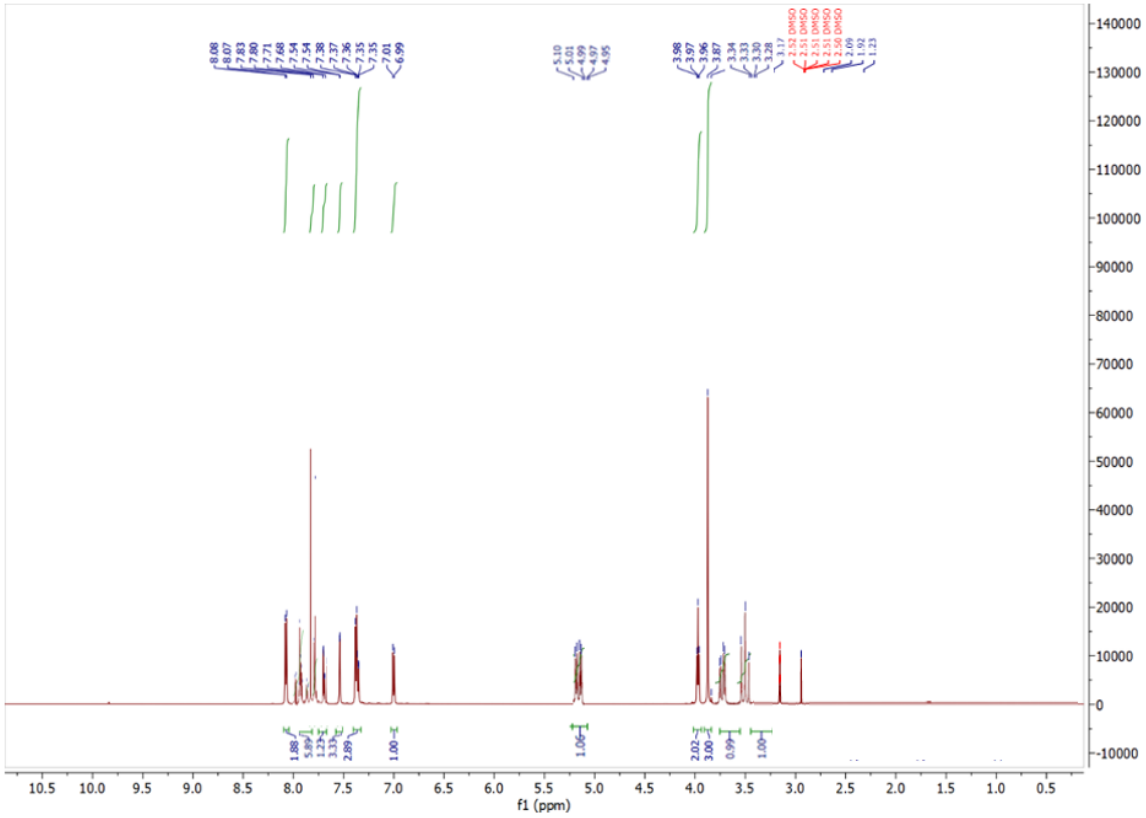

Figure S36. ^{1}H-NMR Spectrum of Compound (13B)

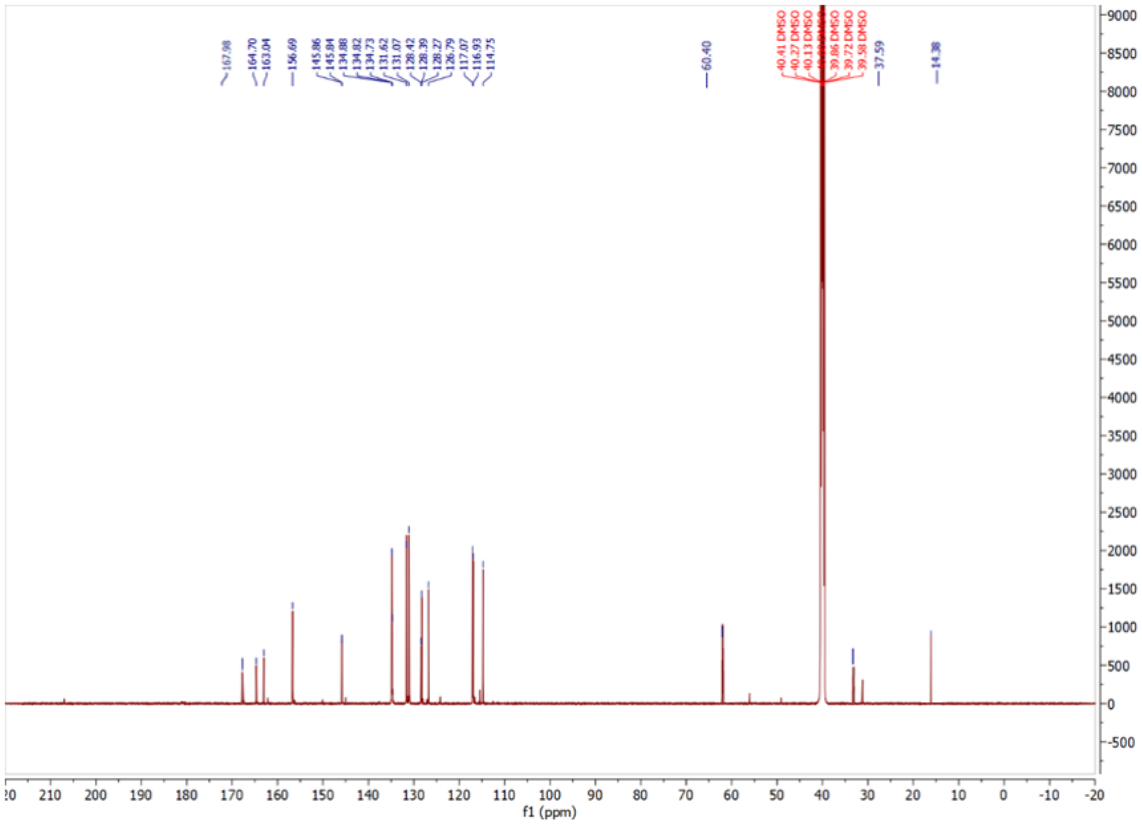

Figure S37. ^{13}C-NMR Spectrum of Compound (13B)

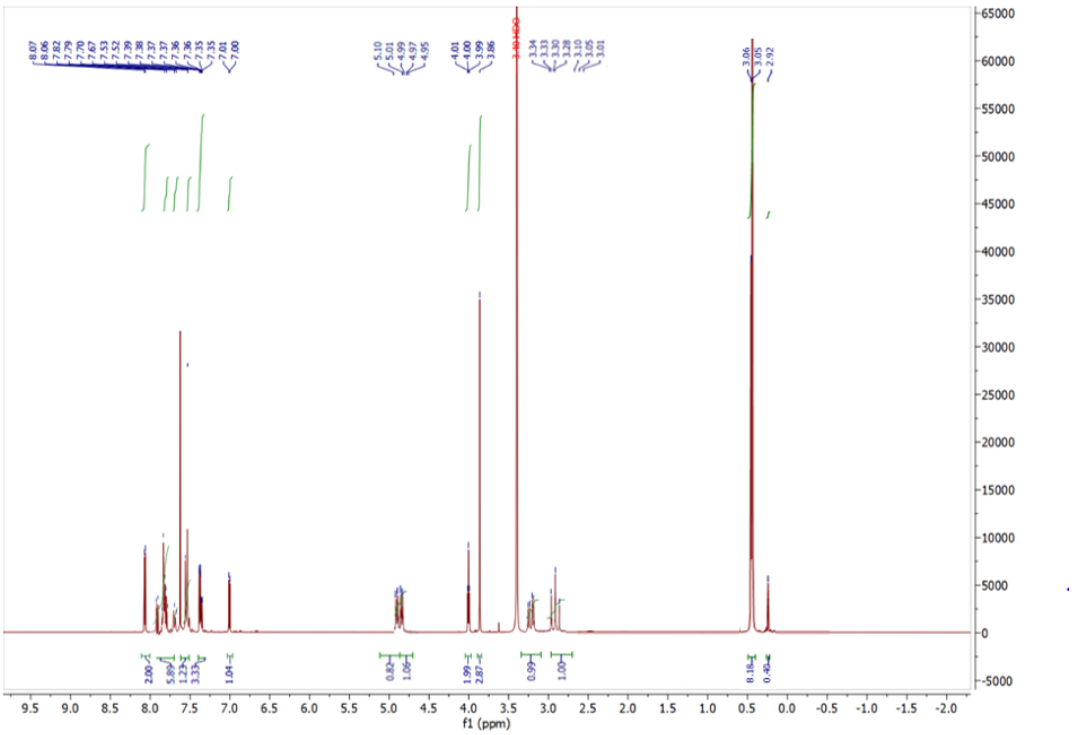

Figure S38. ^{1}H-NMR Spectrum of Compound (14B)

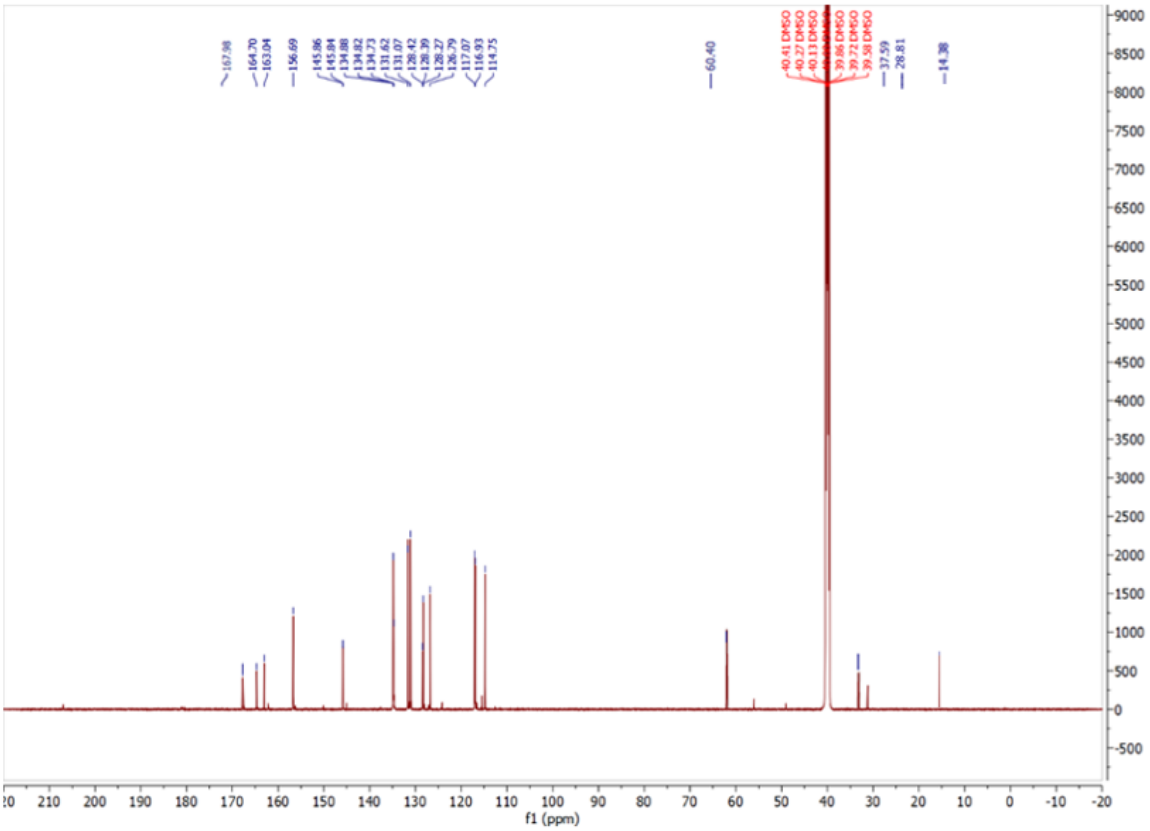

Figure S39. ^{13}C-NMR Spectrum of Compound (14B)

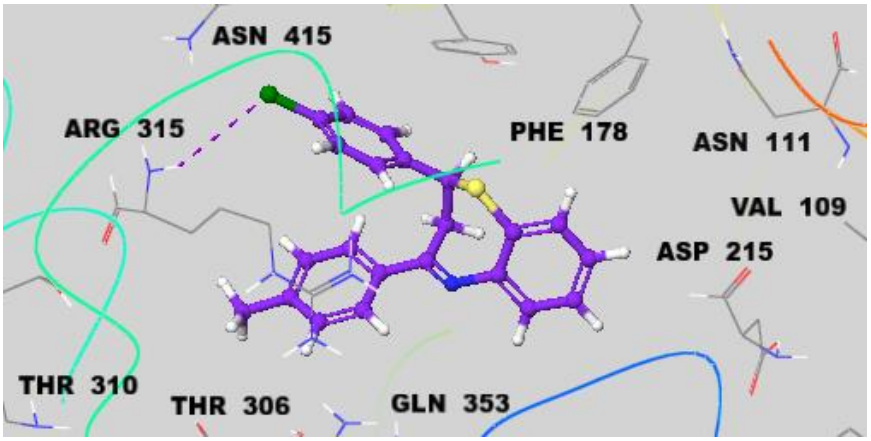

Figure S40. Docking Image of Compound 1B

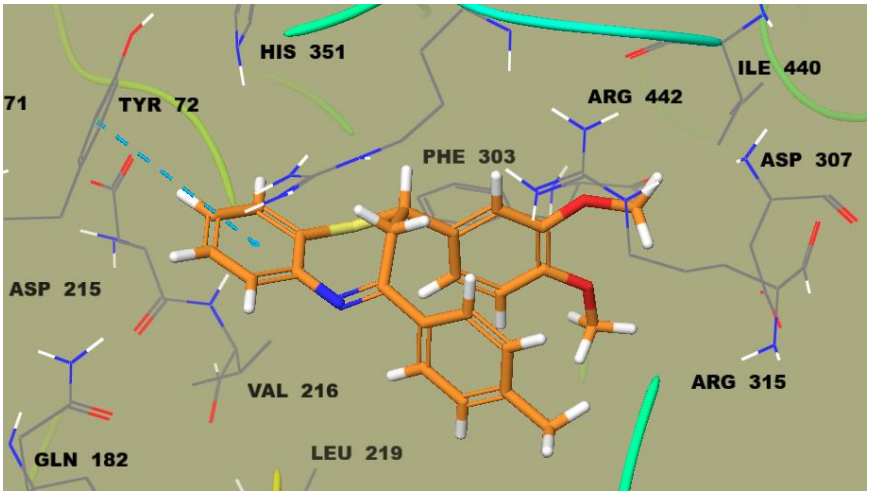

Figure S41. Docking Image of Compound 2B

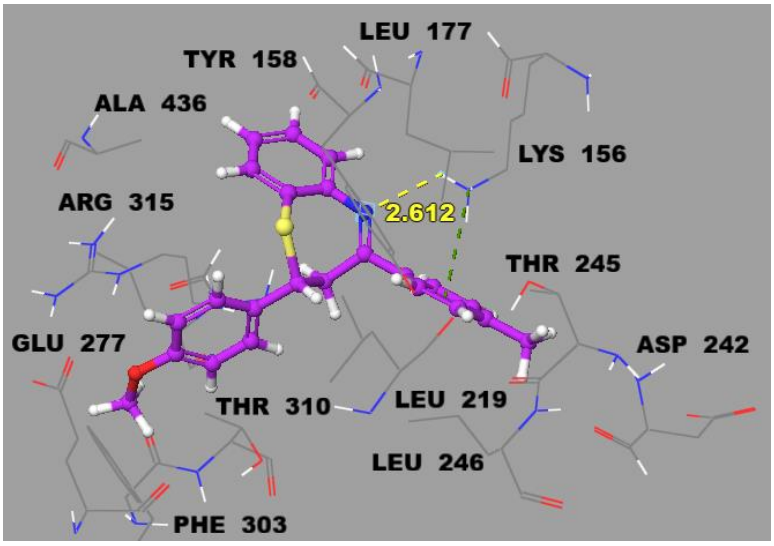

Figure S42. Docking Image of Compound 3B

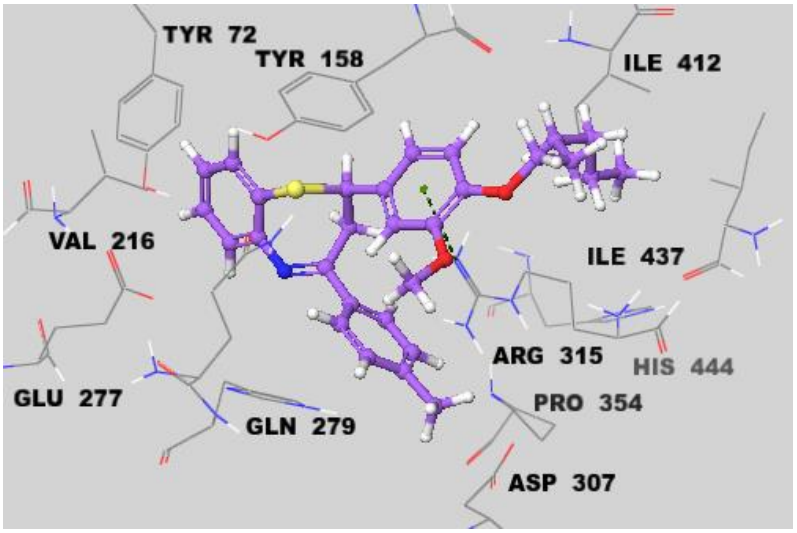

Figure S43. Docking Image of Compound 4B

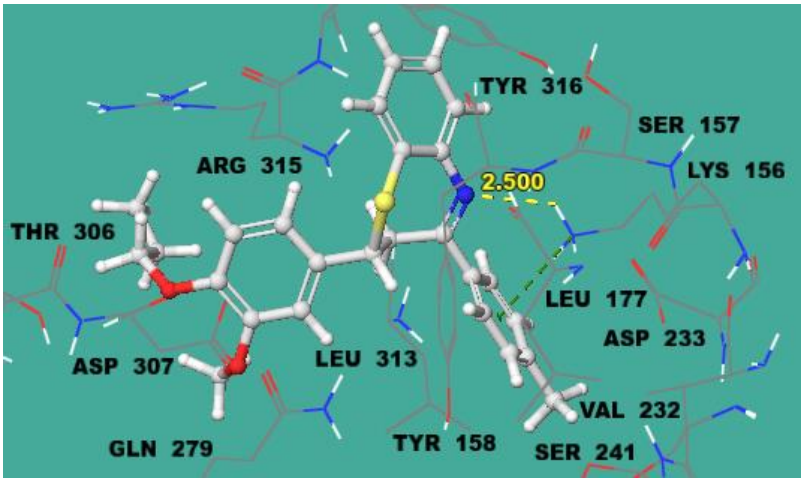

Figure S44. Docking Image of Compound 5B

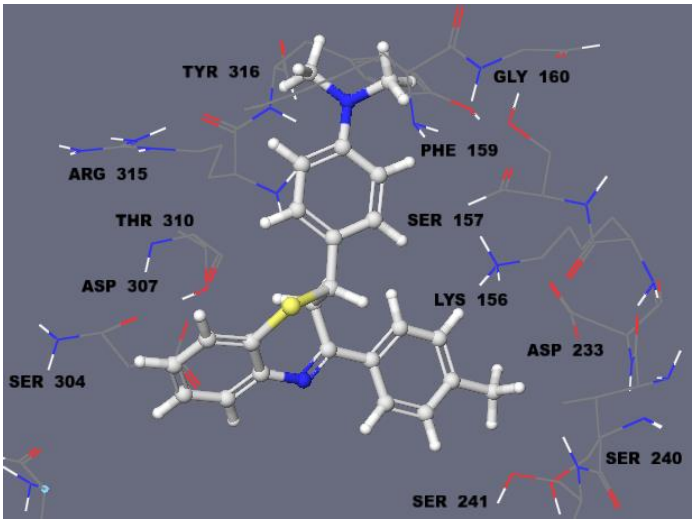

Figure S45. Docking Image of Compound 6B

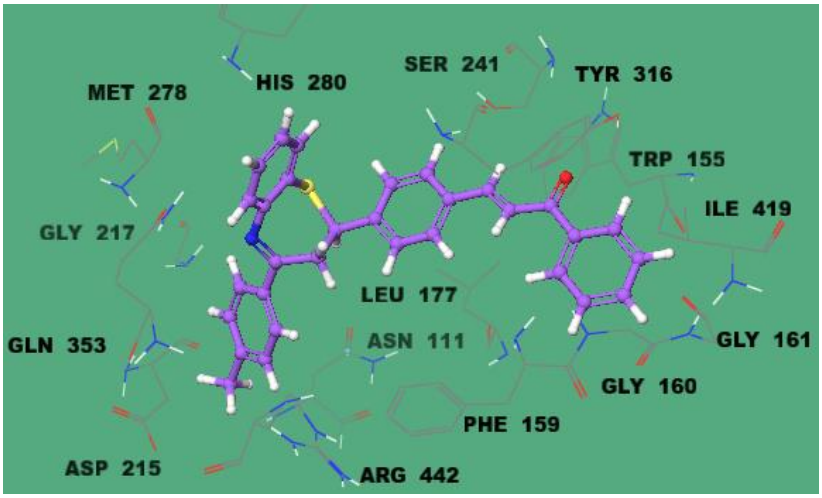

Figure S46. Docking Image of Compound 7B

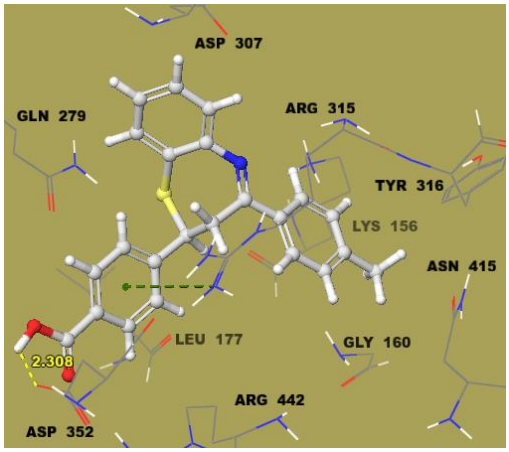

Figure S47. Docking Image of Compound 8

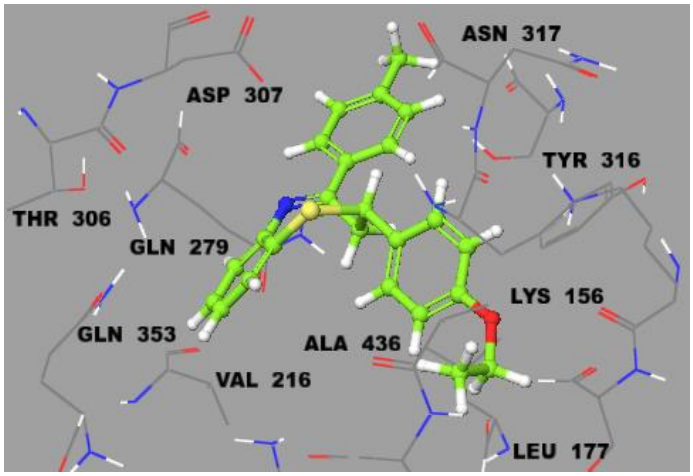

Figure S48. Docking Image of Compound 9B

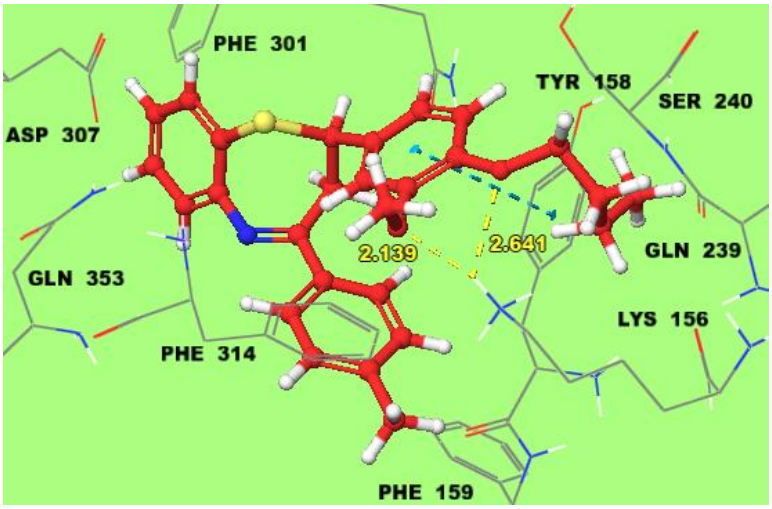

Figure S49. Docking Image of Compound 10B

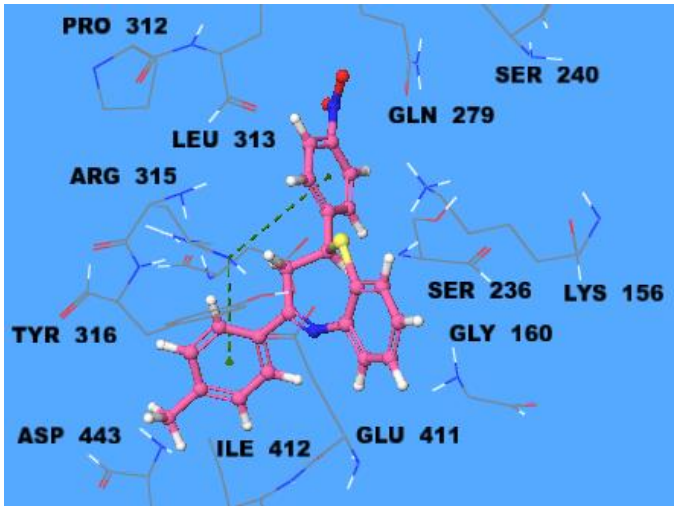

Figure S50. Docking Image of Compound 11B

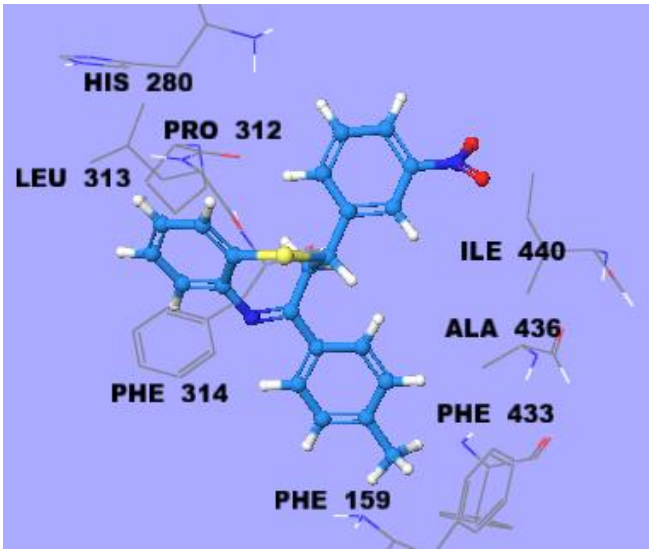

Figure S51. Docking Image of Compound 12

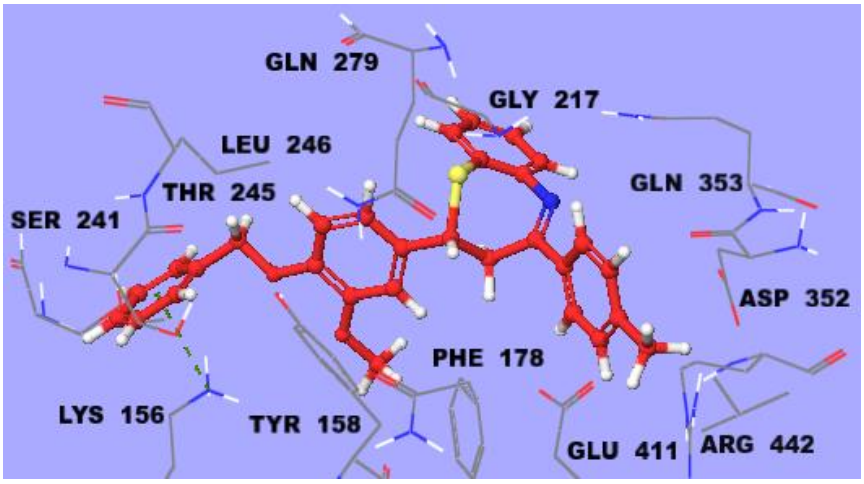

Figure S52. Docking Image of Compound 13

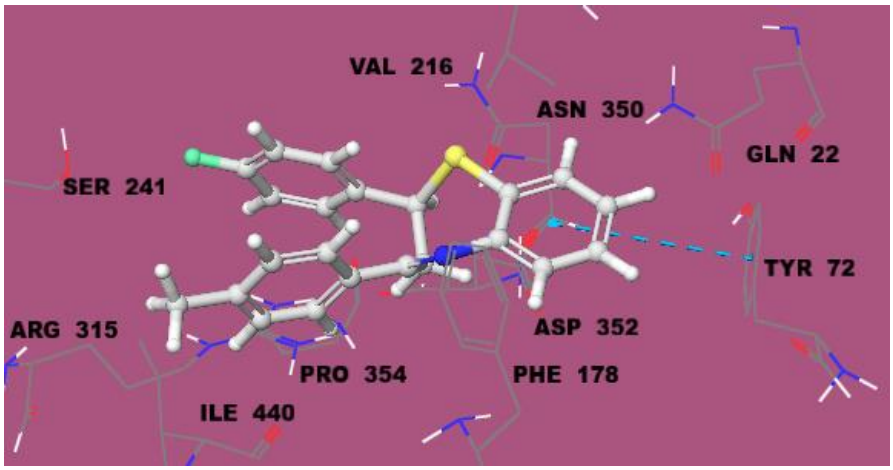

Figure S53. Docking Image of Compound 14B

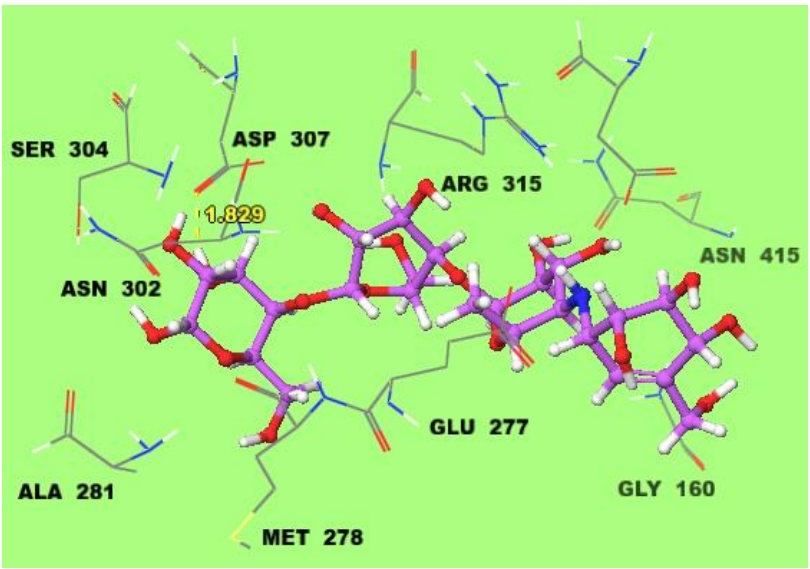

Figure S54. Docking Image of Acarbose

Table S1: Binding energies of the compounds **1B-14B** against various modes of glucosidase enzyme

Compound No.	**Docking score PDB ID 3AJ7 (kcal/mol)**	**Compound No.**	**Docking score PDB ID 3AJ7 (kcal/mol)**
1B	-6.5589	**8B**	-6.8165
2B	-9.5322	**9B**	-6.8547
3B	-8.8329	**10B**	-7.7301
4B	-6.2681	**11B**	-6.8232
5B	-7.5788	**12B**	-6.6822
6B	-7.7090	**13B**	-7.7702
7B	-7.9781	**14B**	-6.4343
Acarbose (Standard)	-5.5322		

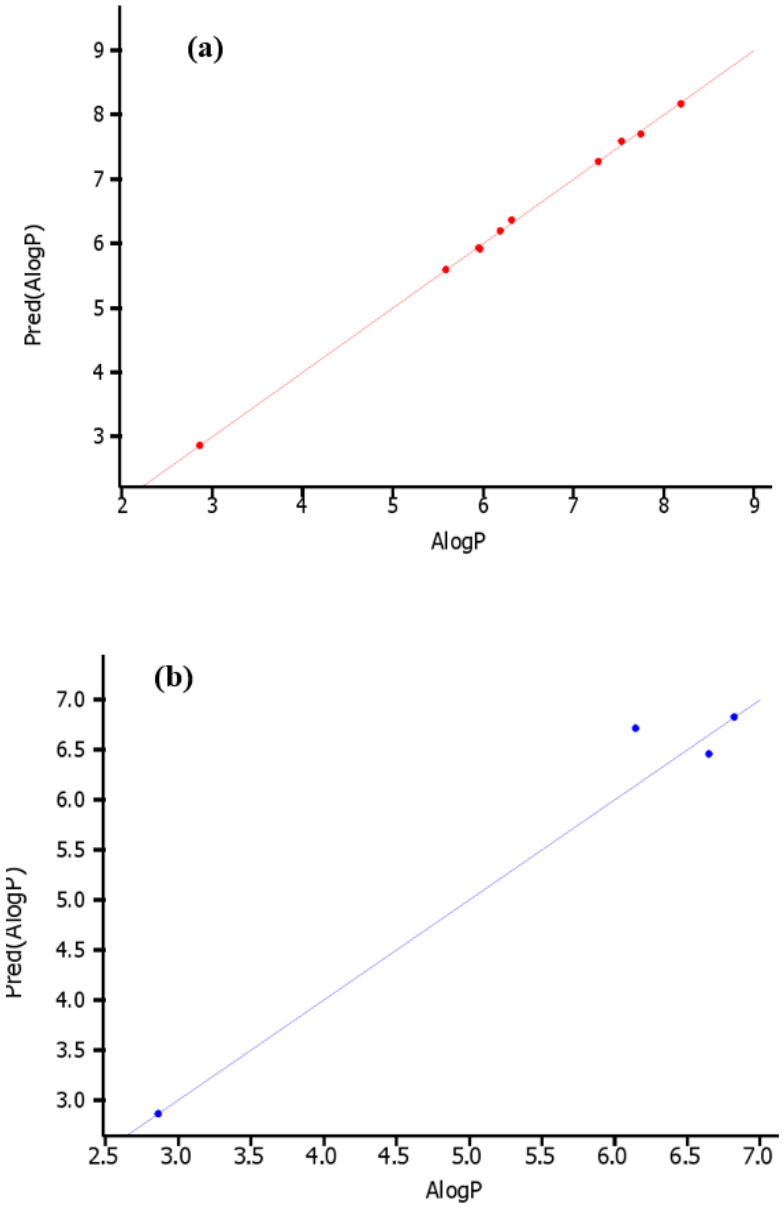

Figure S55: Plot of experimental versus predicted telomerase inhibitory activities of test set (a) and training set (b).