

Supplementary information

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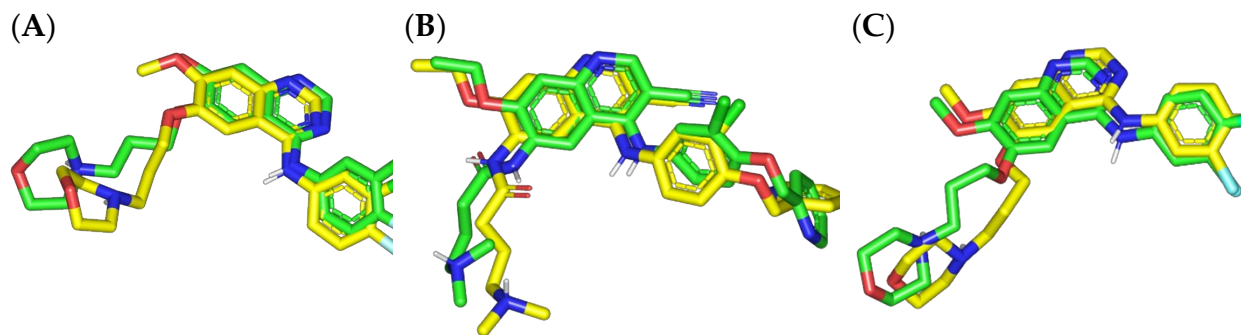


Figure S1. Superimposing the co-crystallized (green sticks) and redocked (yellow sticks) ligands at (A) EGFR^{WT}; (B) EGFR^{T790M}; (C) EGFR^{L858R} for validating the adopted docking protocol.

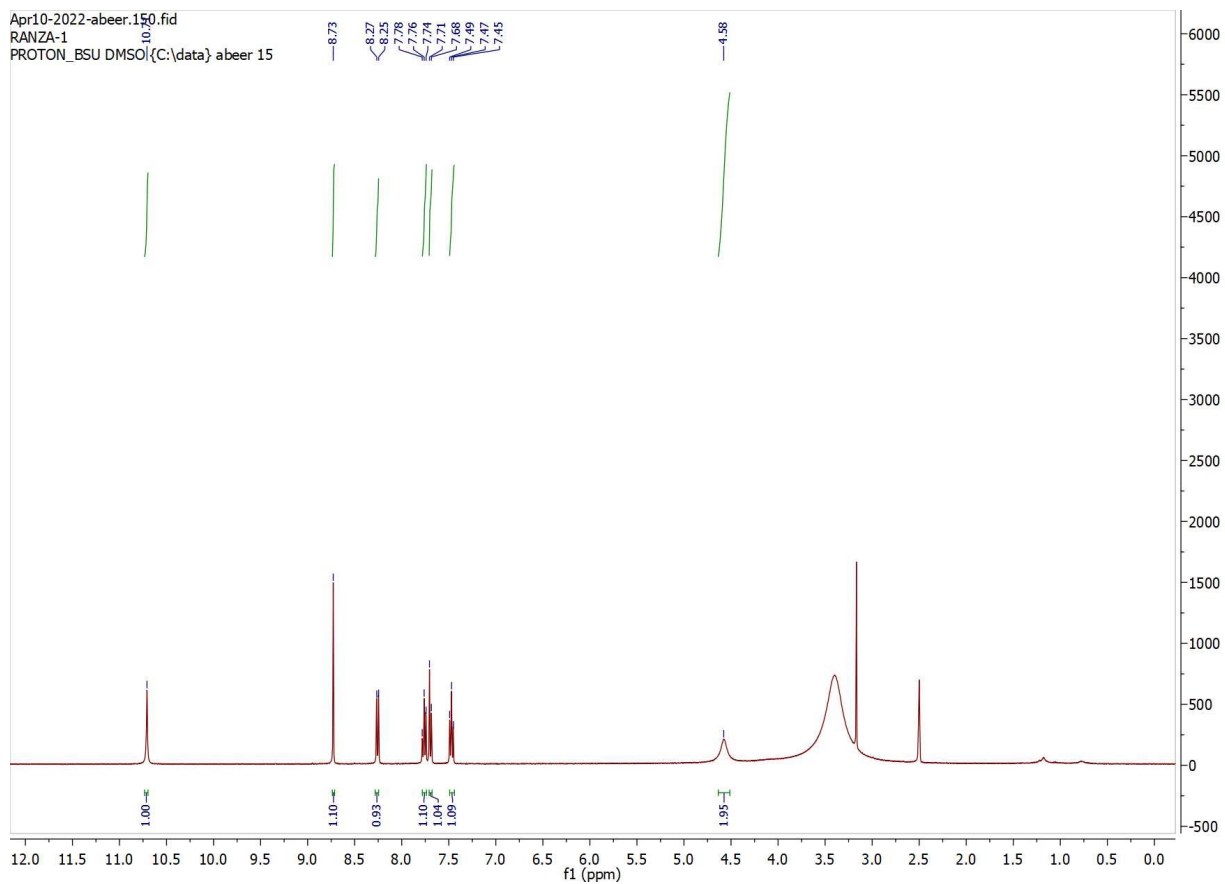


Figure 2. ^1H NMR of Compound 3

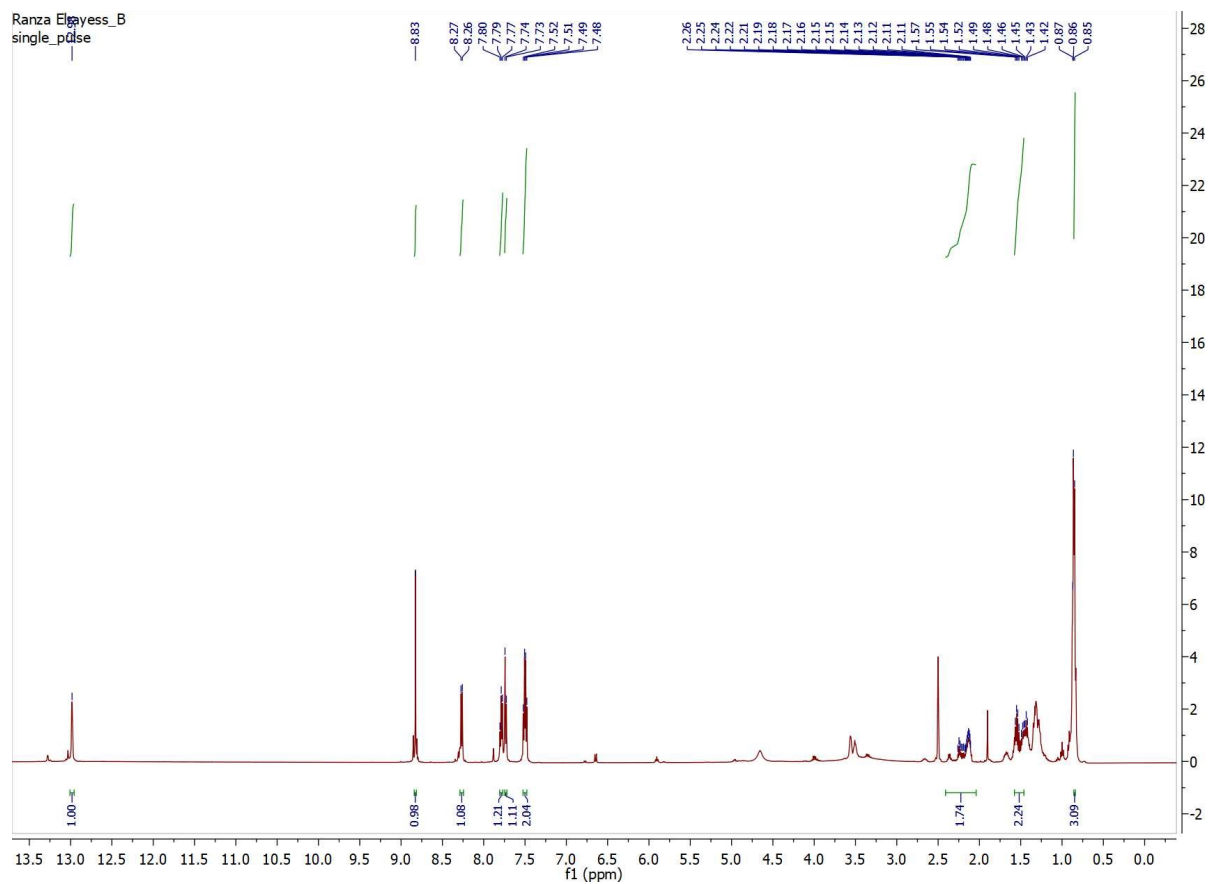


Figure 3. ^1H NMR of Compound 4

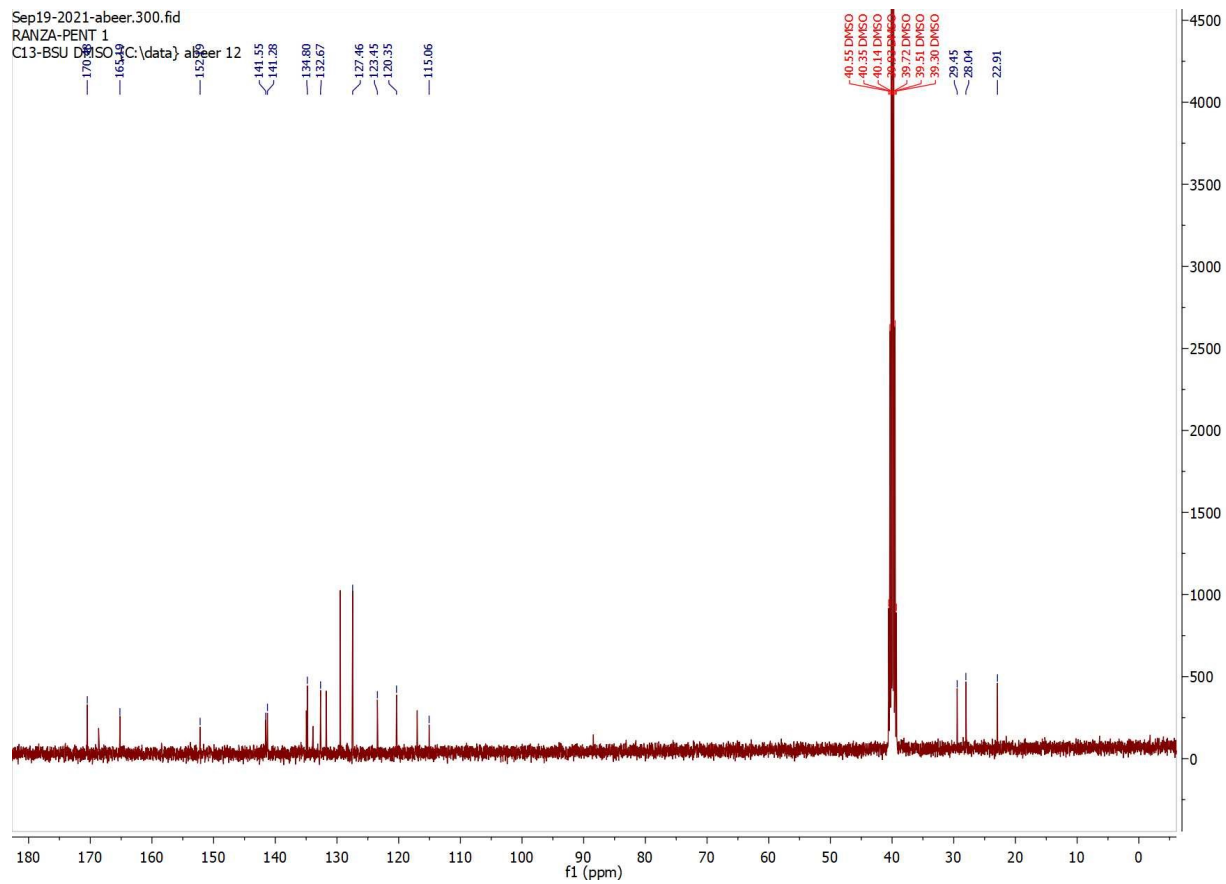


Figure 4. ^{13}C NMR of Compound 4

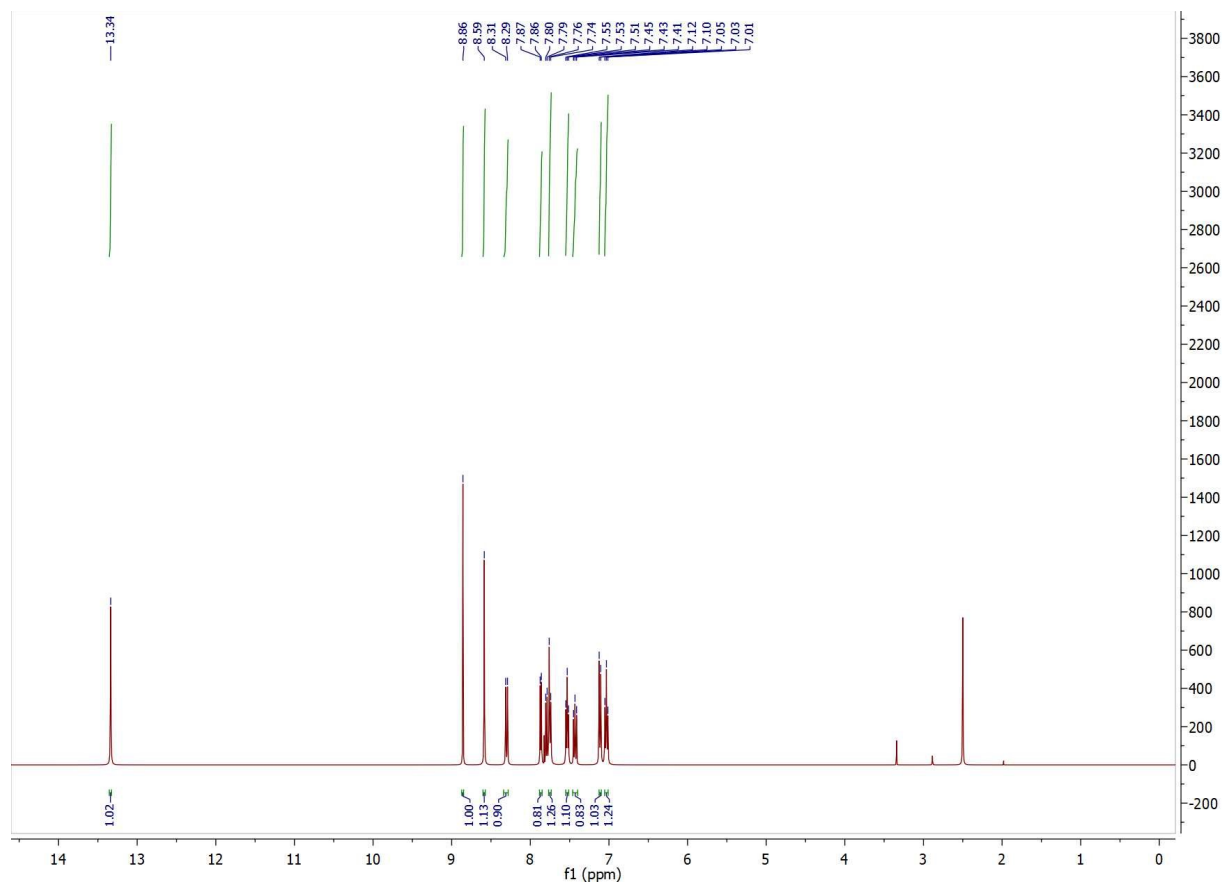


Figure 5. ^1H NMR of Compound 5

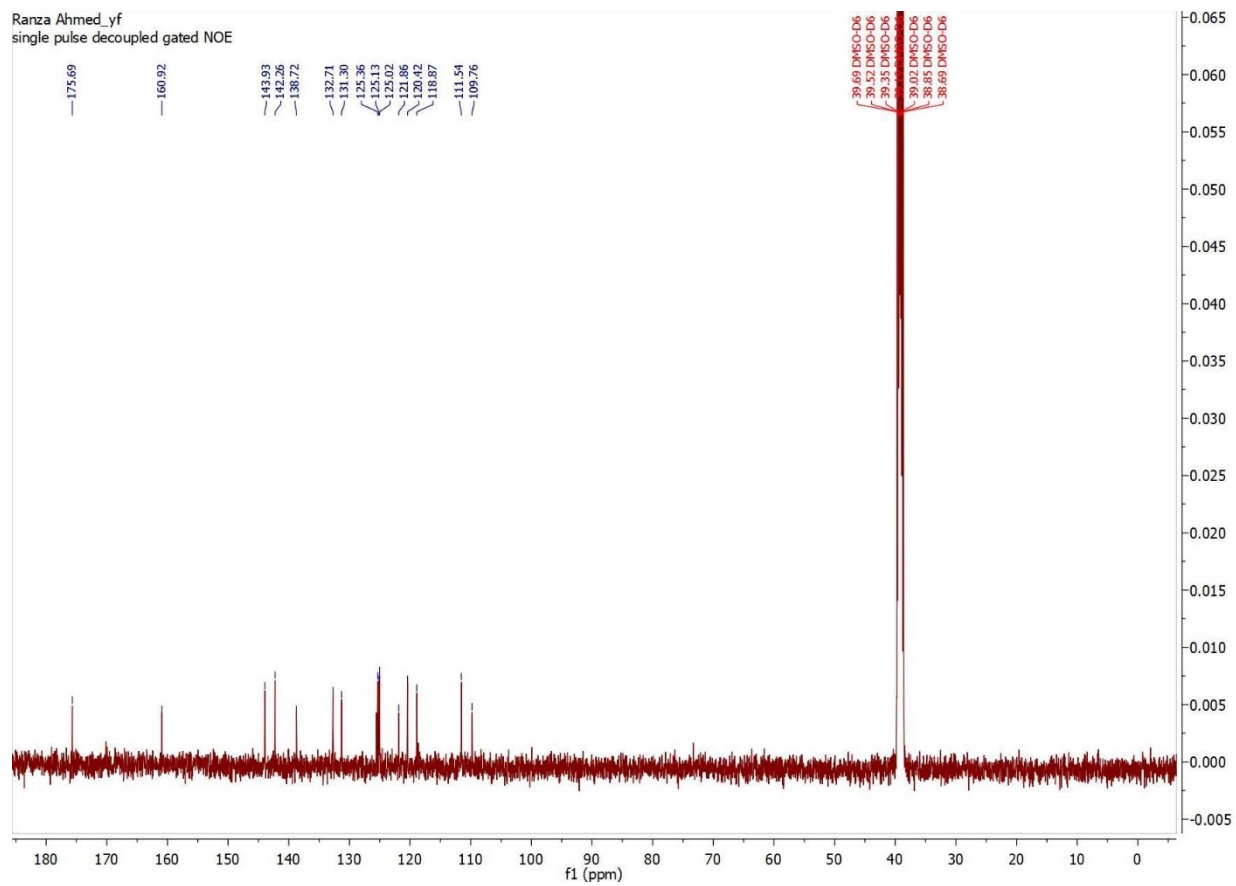


Figure 6. ^{13}C NMR of Compound 5

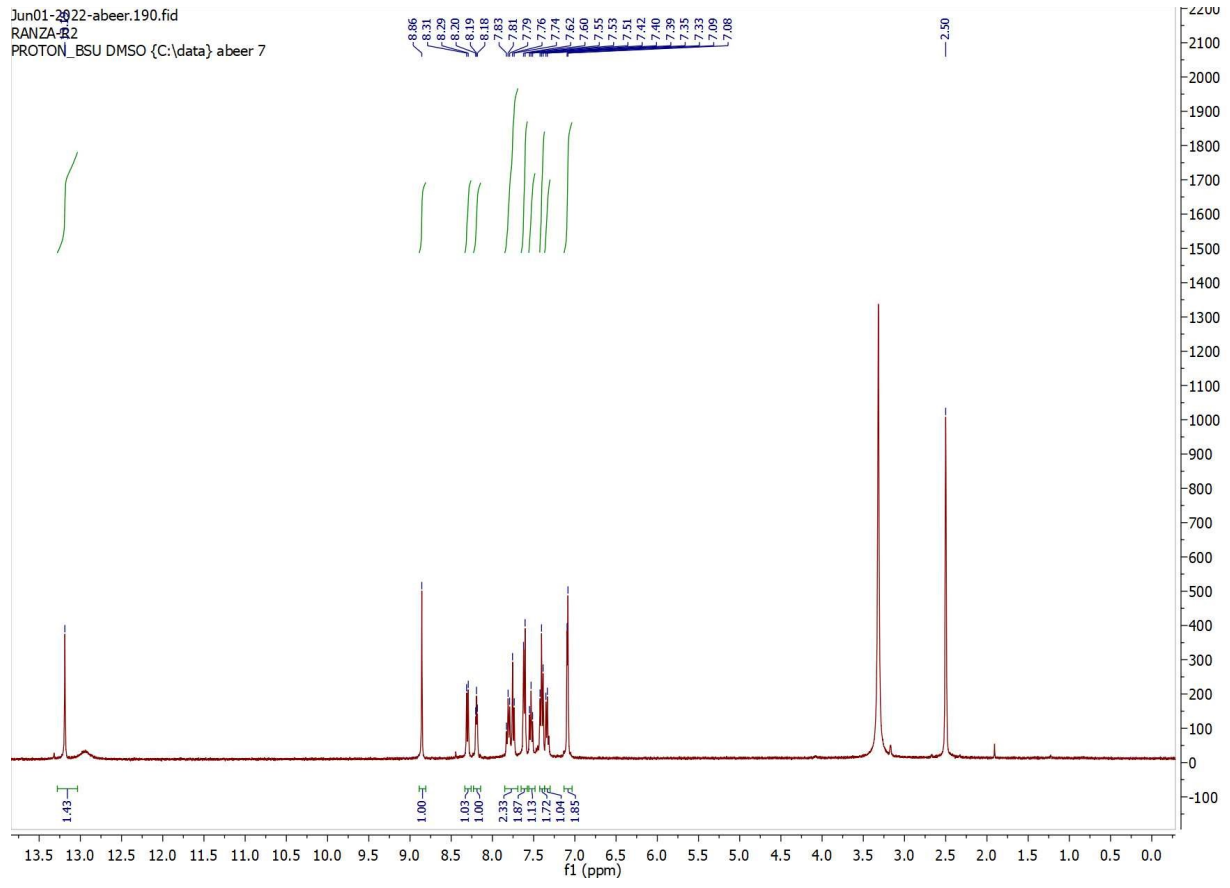


Figure 7. ^1H NMR of Compound 6

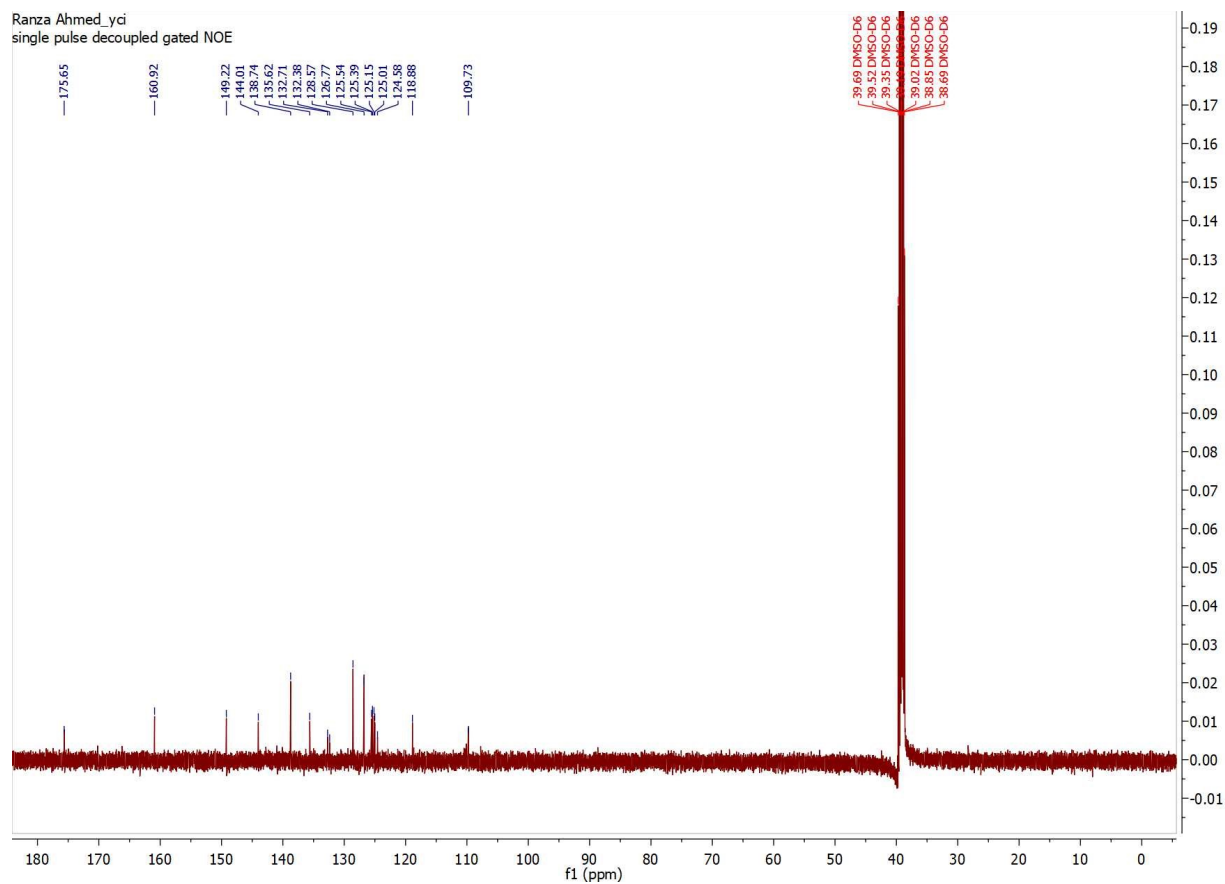


Figure 8. ¹³C NMR of Compound 6

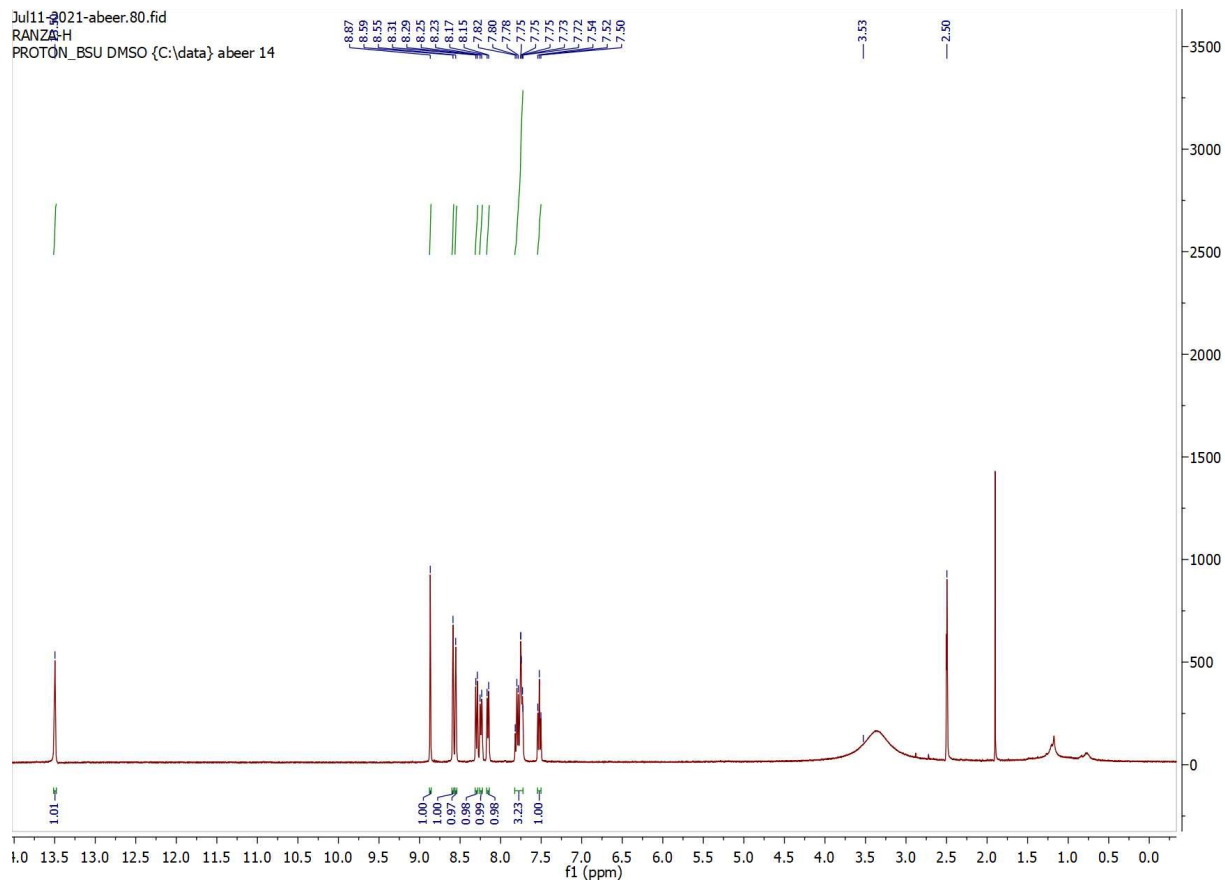


Figure 9. ^1H NMR of Compound 7

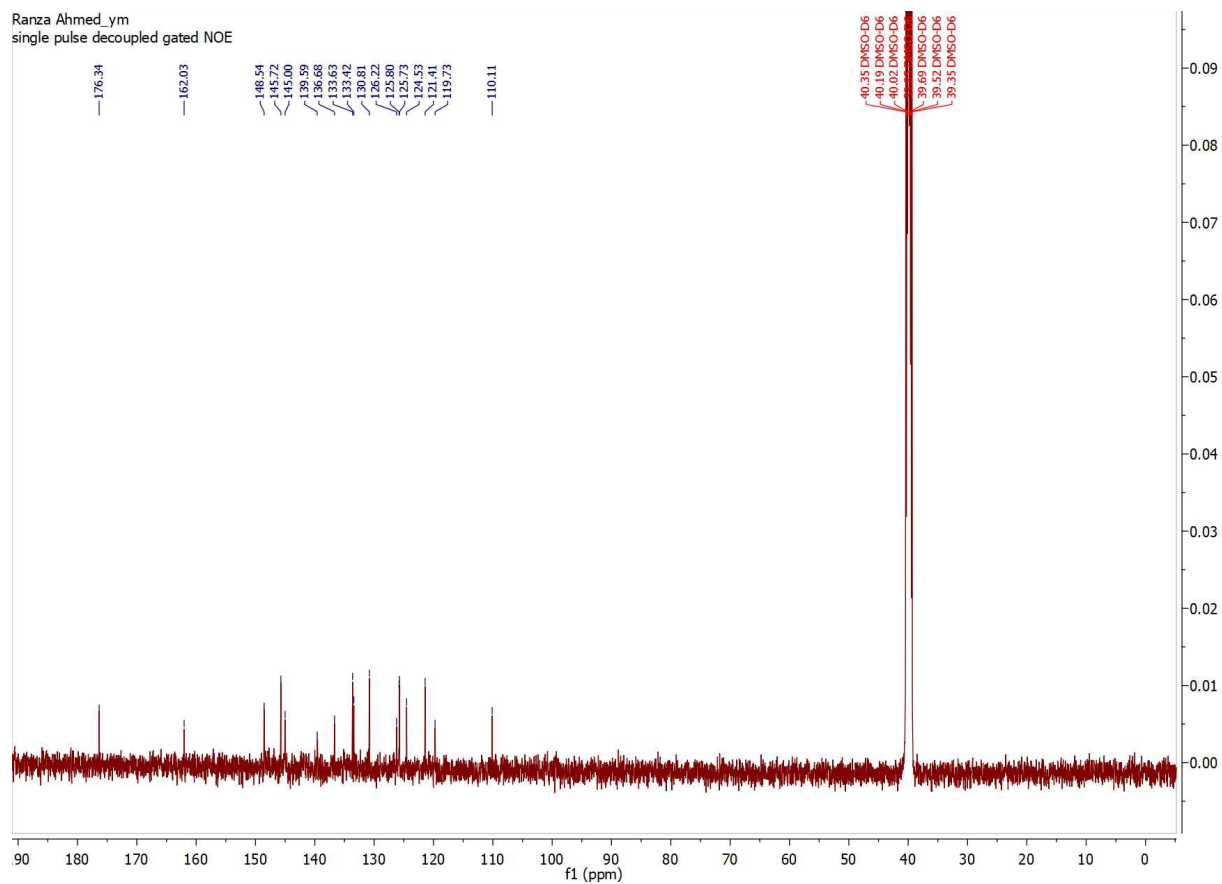


Figure 10. ^{13}C NMR of Compound 7

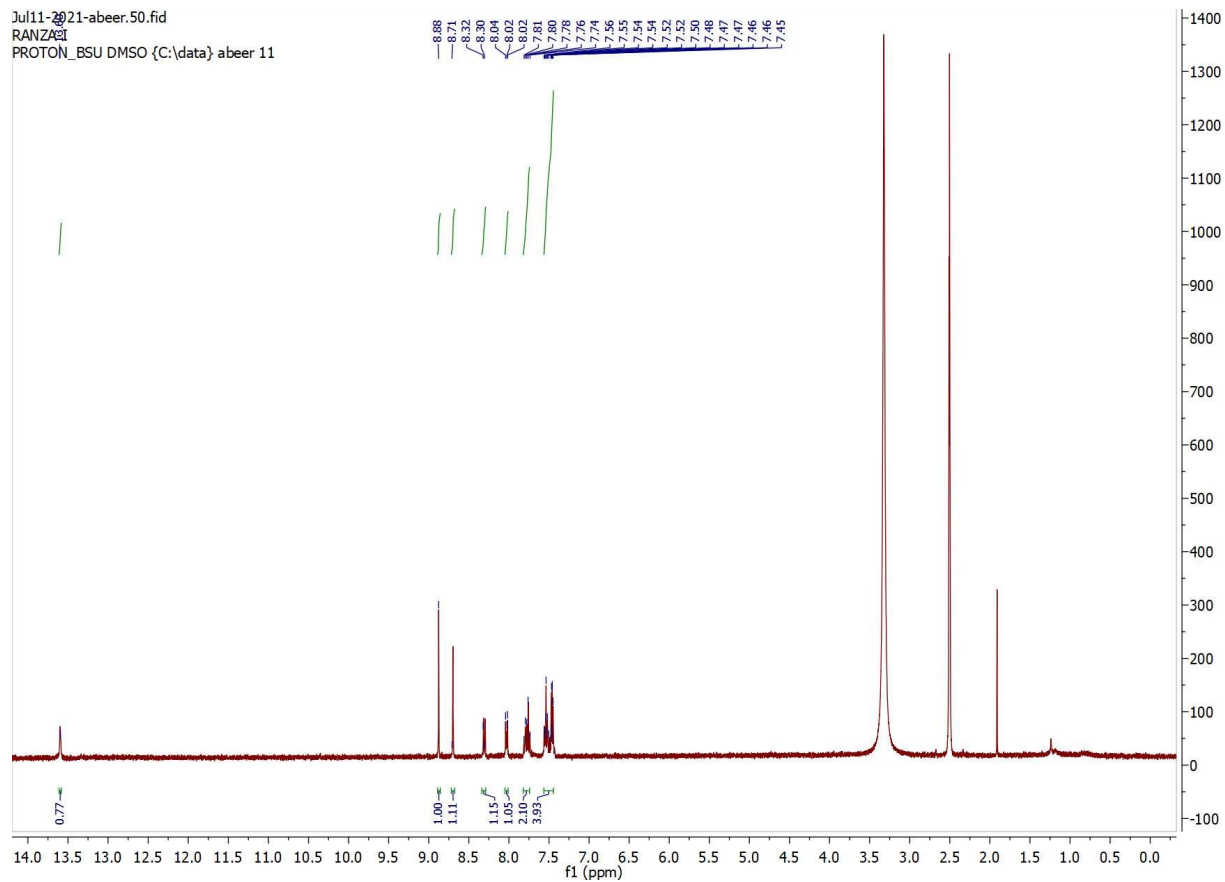


Figure 11. ^1H NMR of Compound 9

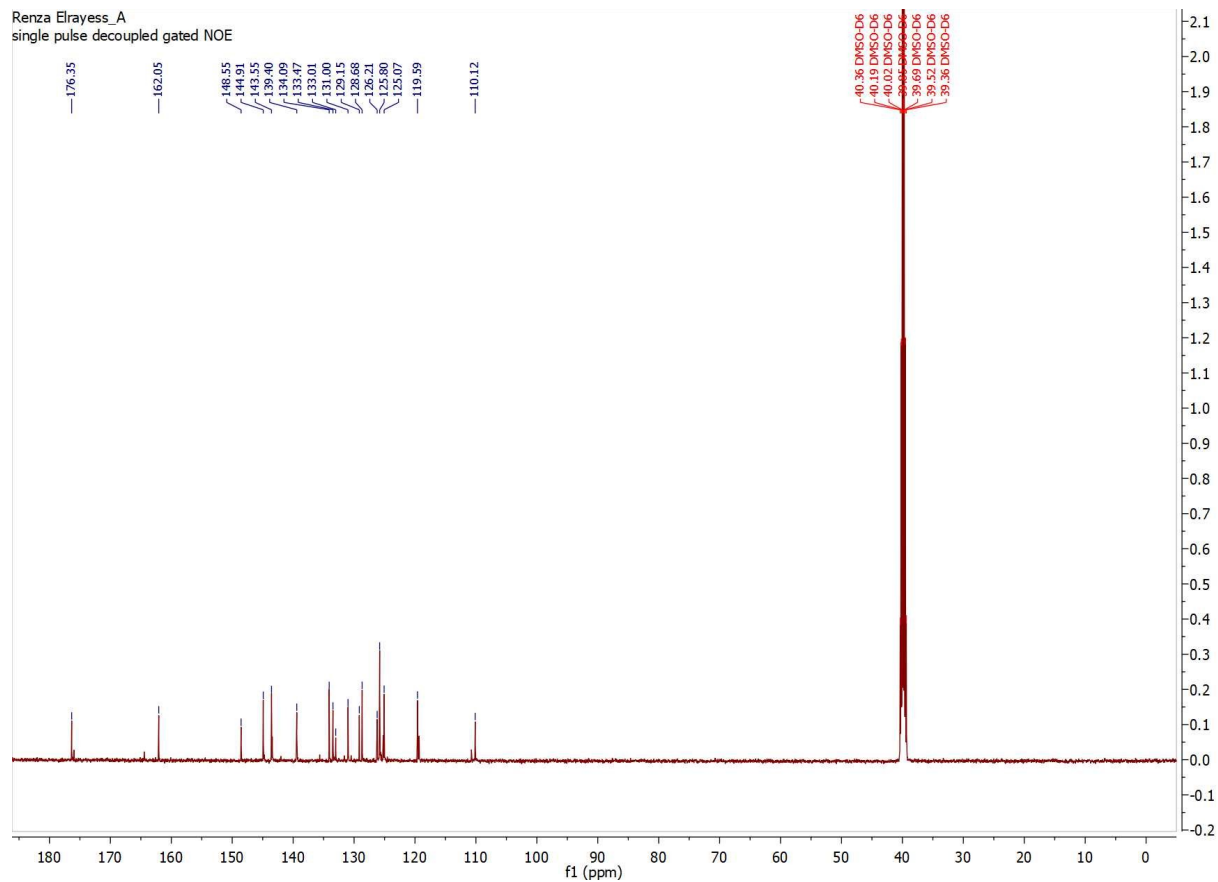


Figure 12. ^{13}C NMR of Compound 9

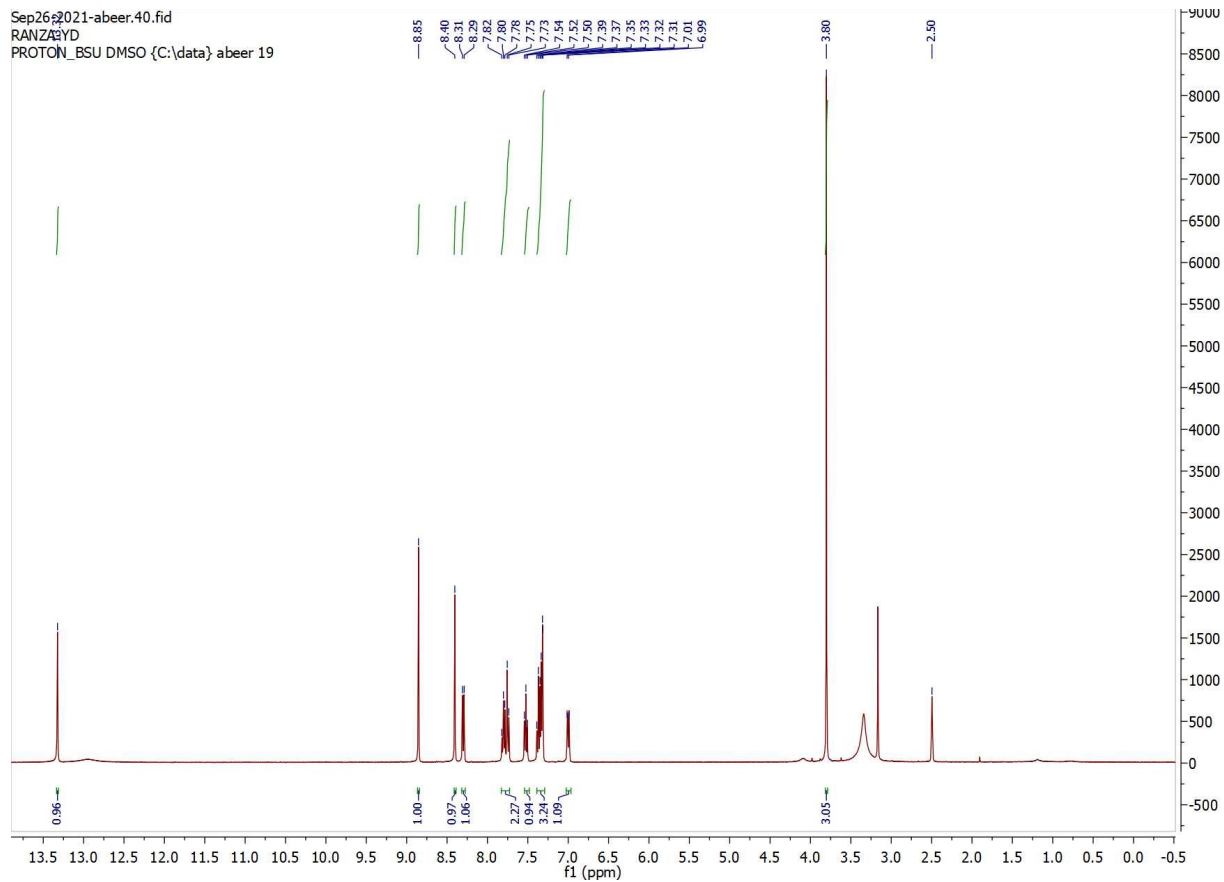


Figure 13. ^1H NMR of Compound 11

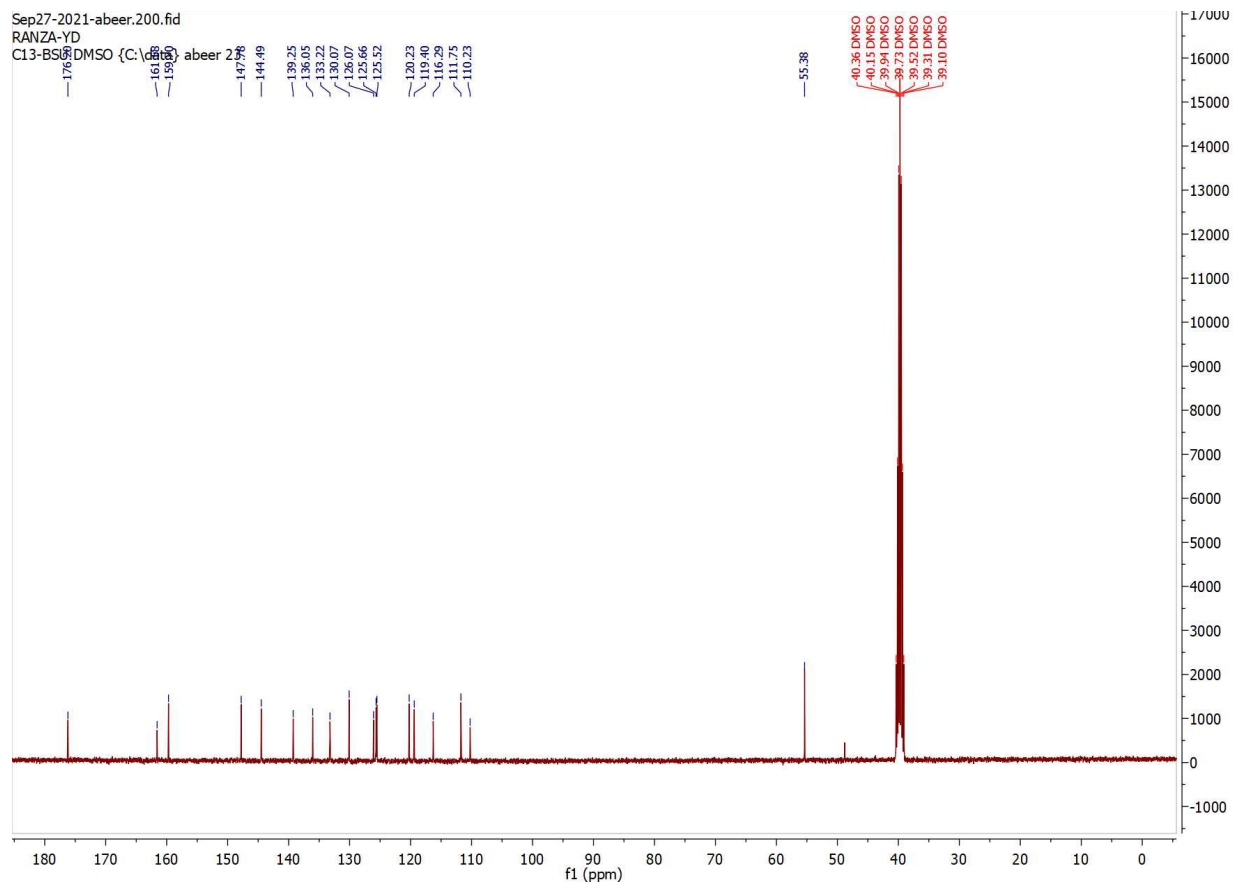


Figure 14. ^{13}C NMR of Compound 11

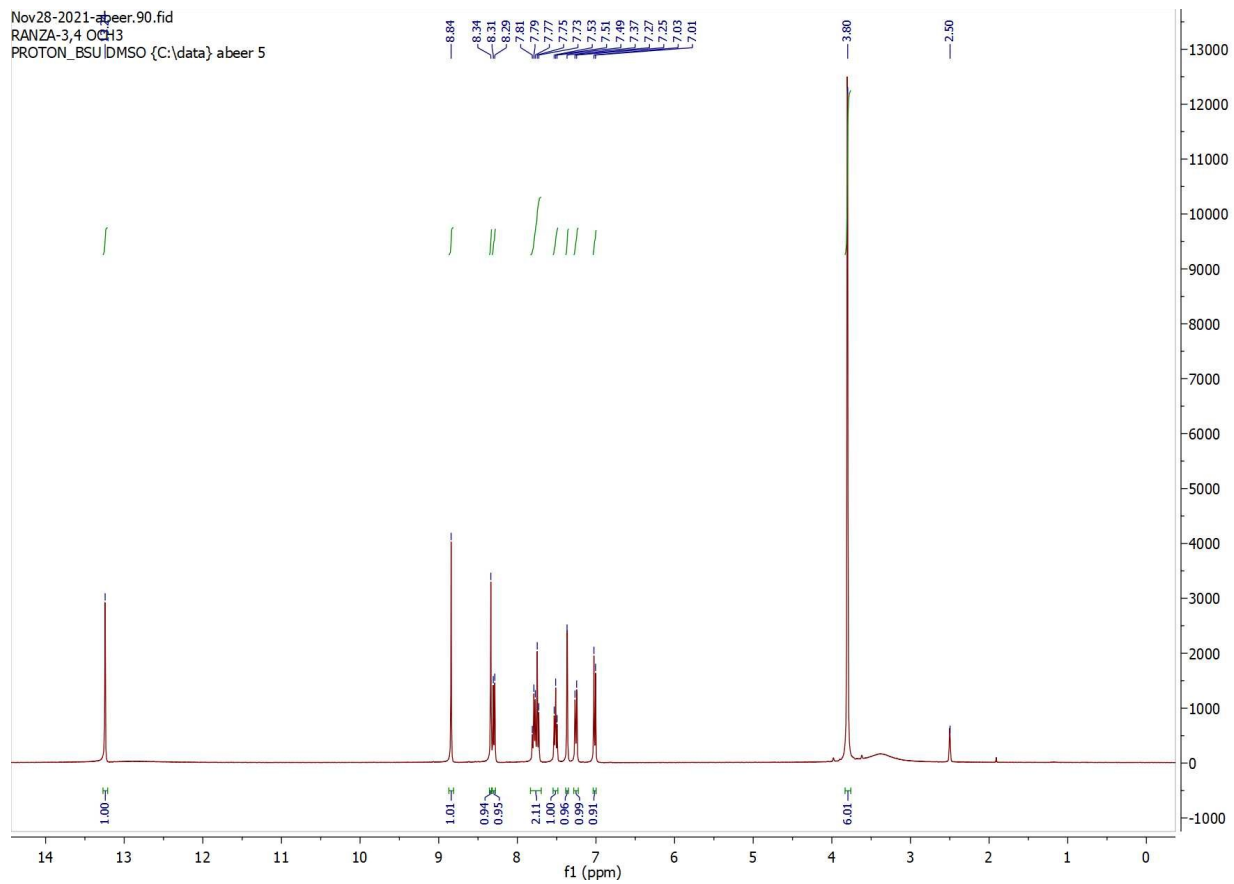


Figure 15. ¹H NMR of Compound 13

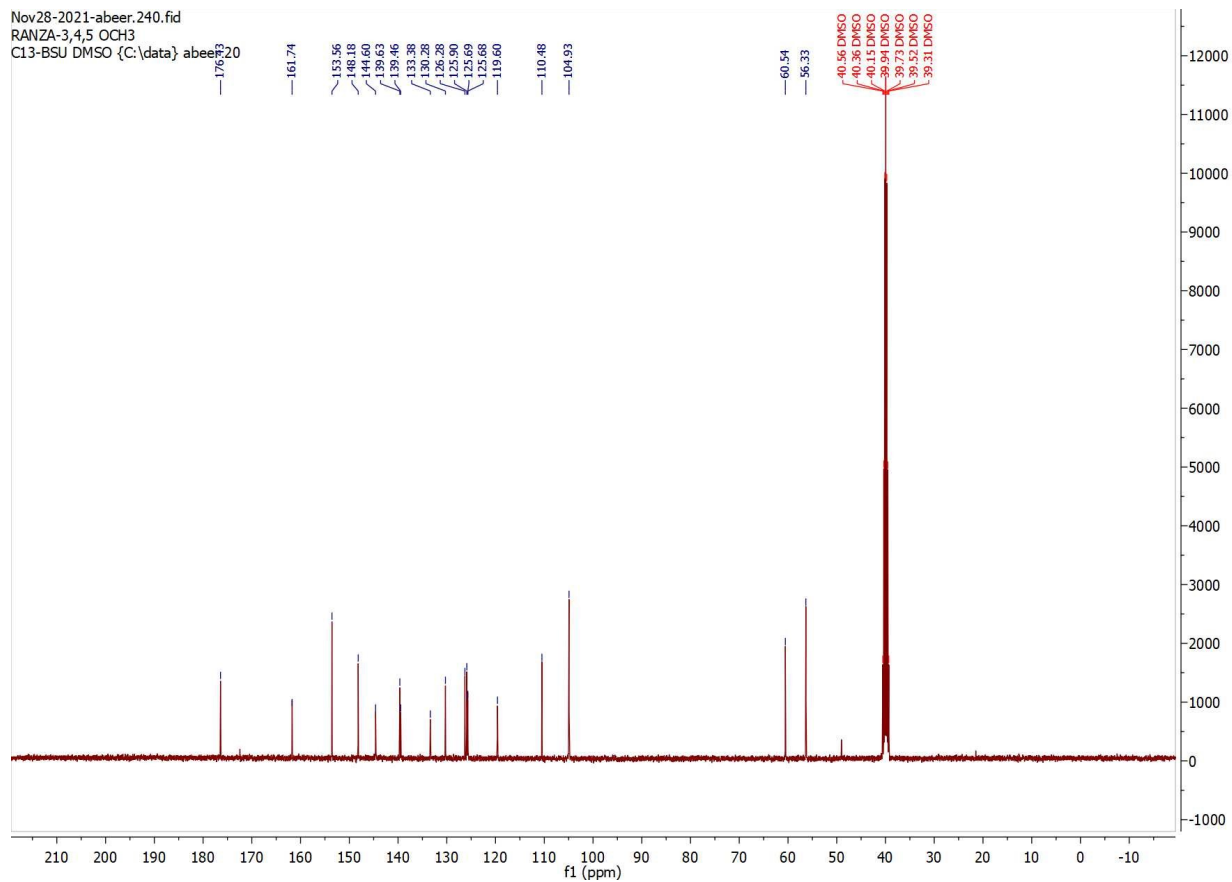


Figure 16. ^{13}C NMR of Compound 13

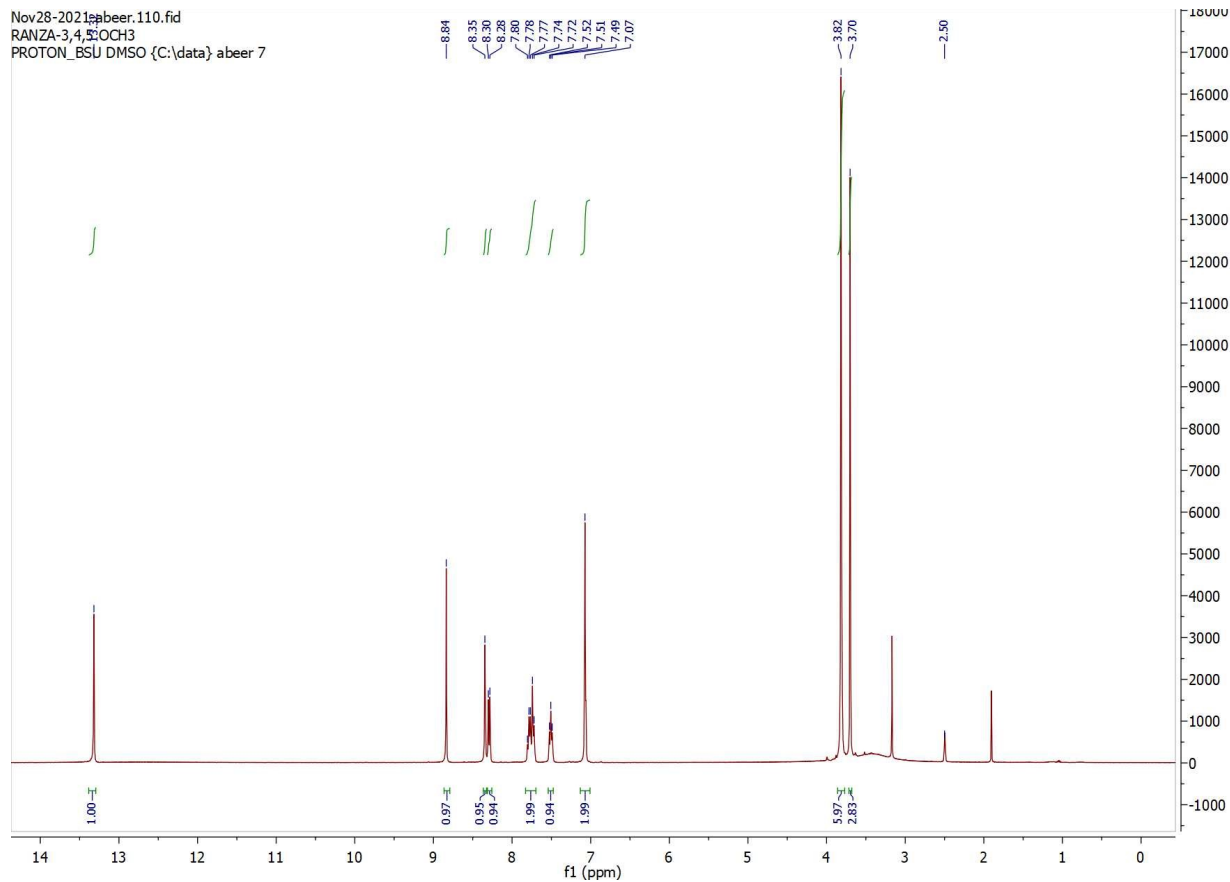


Figure 17. ^1H NMR of Compound 14

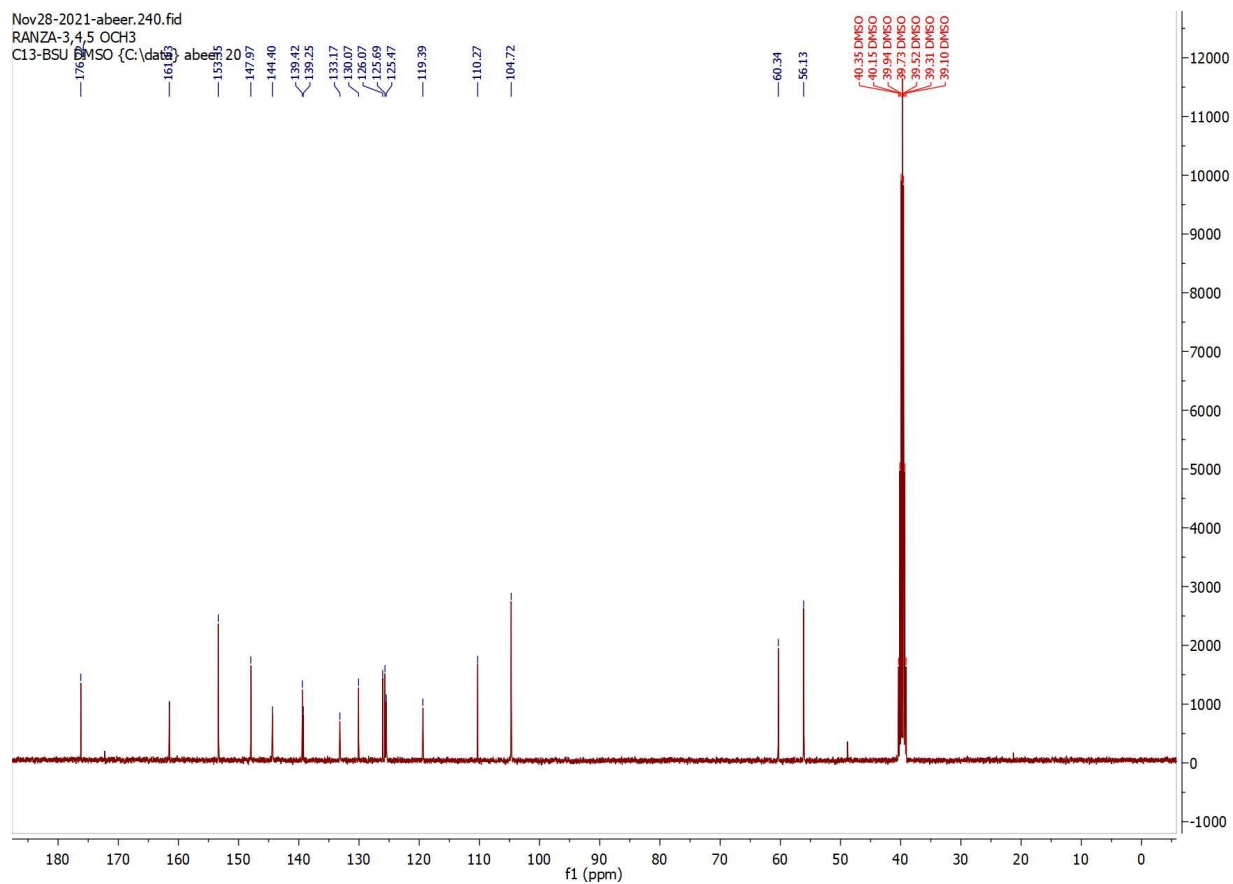


Figure 18. ^{13}C NMR of Compound 14

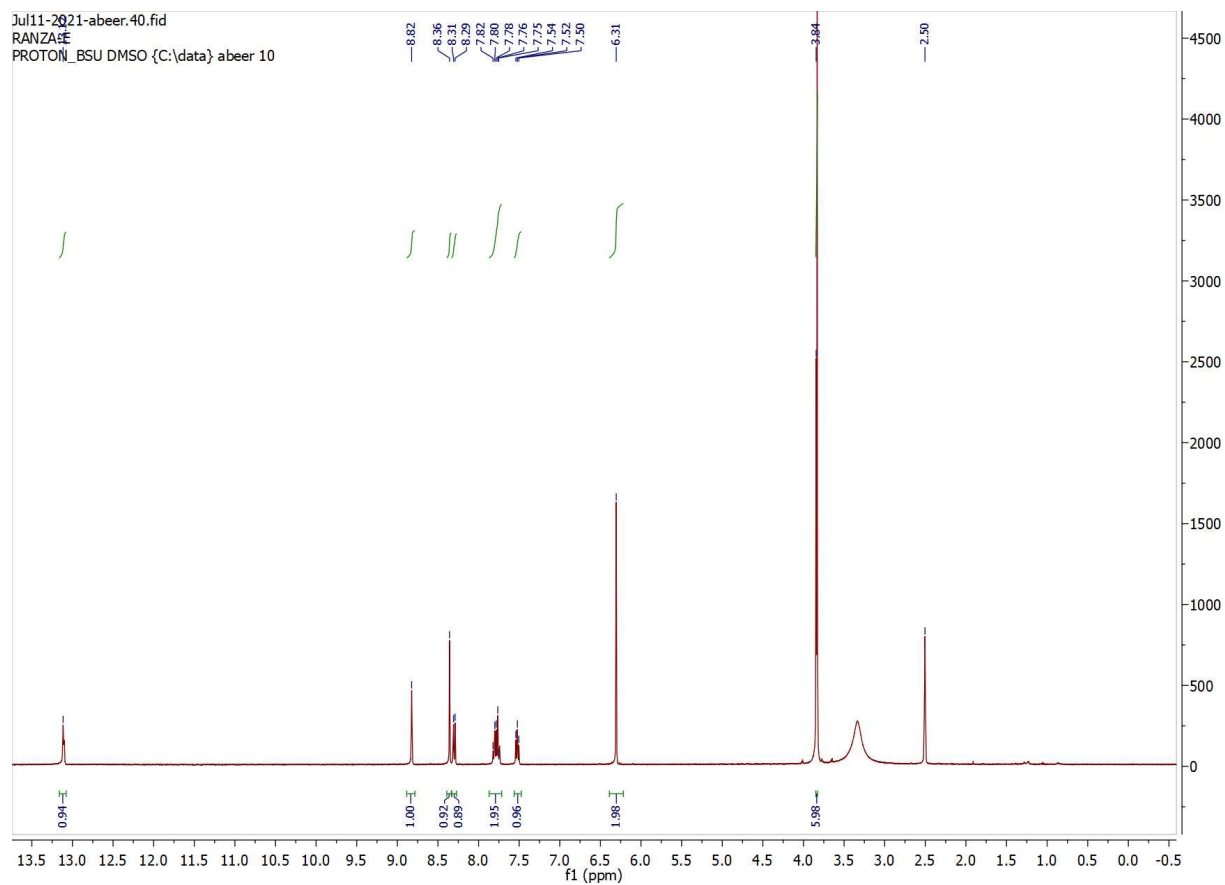


Figure 19. ^1H NMR of Compound 15

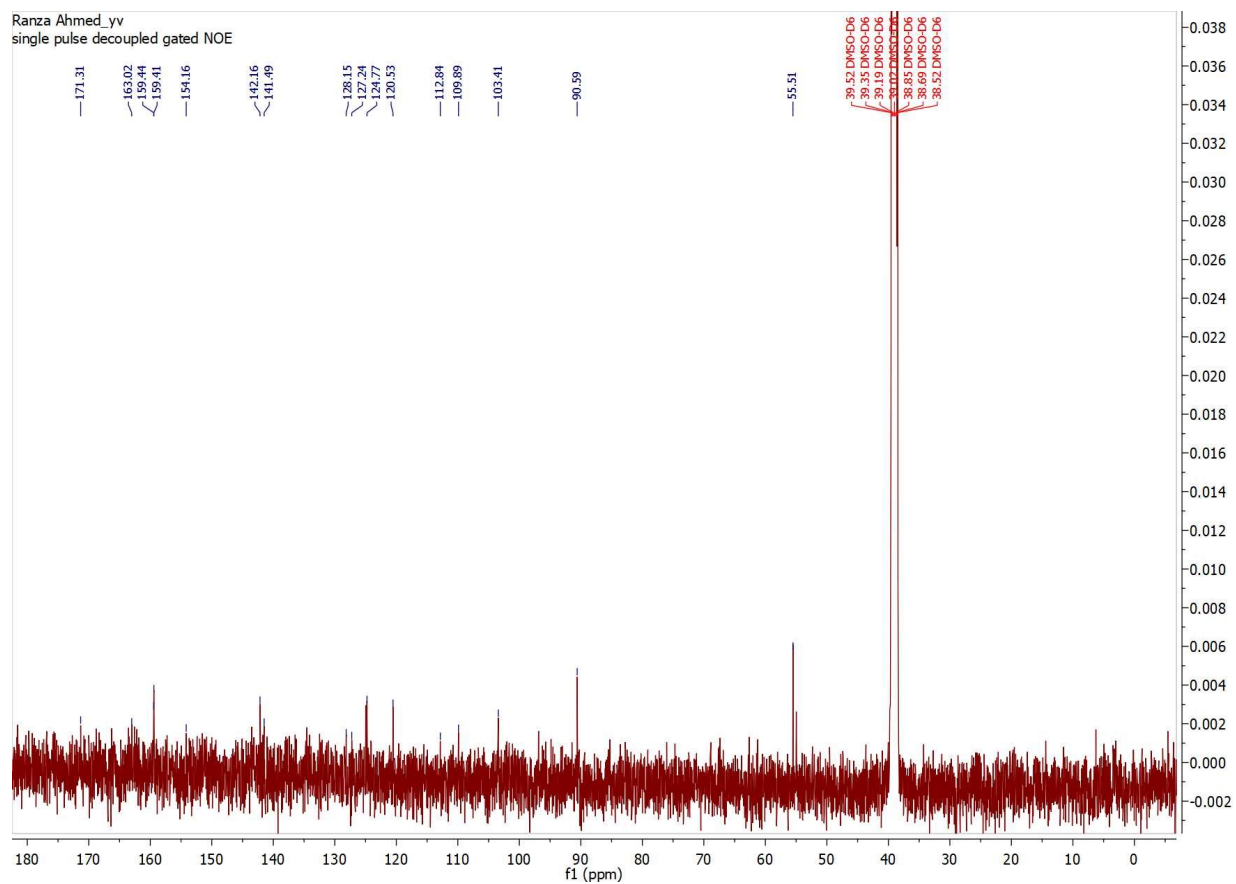


Figure 20. ^{13}C NMR of Compound 15

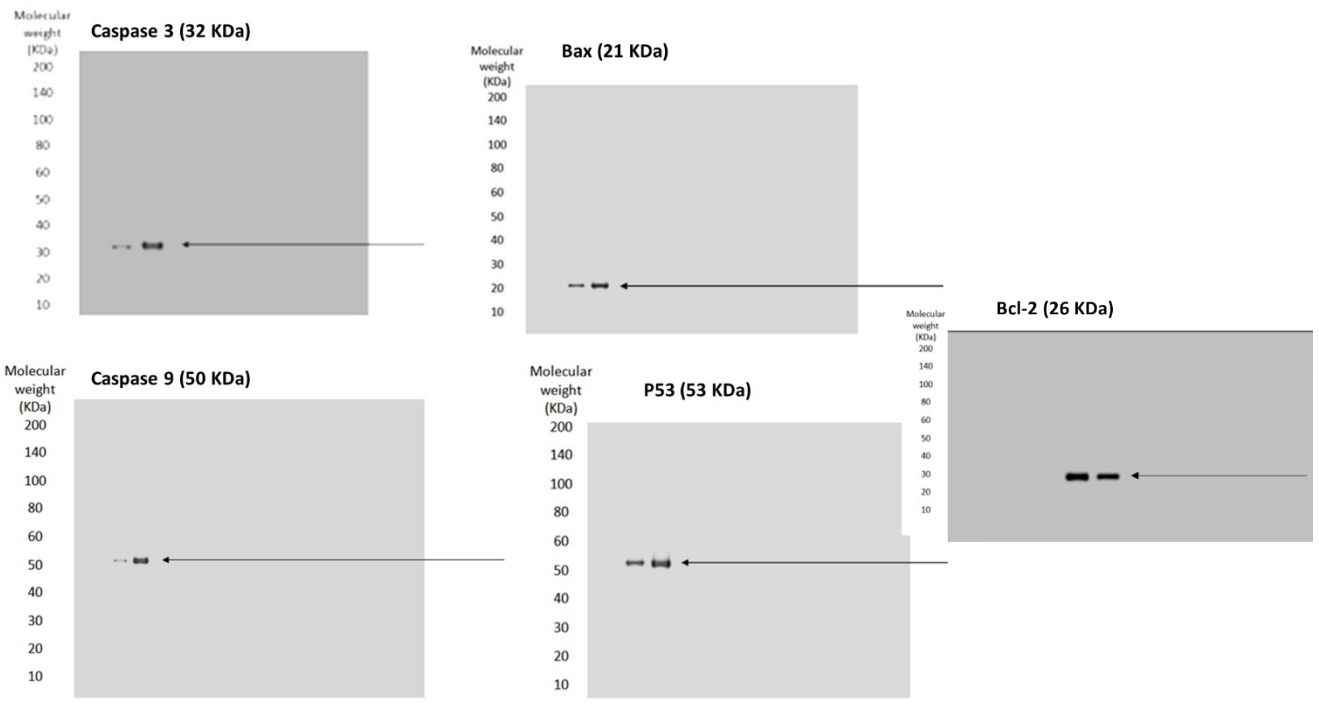
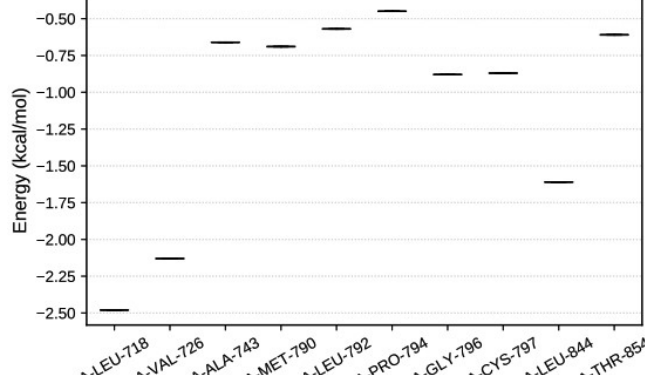
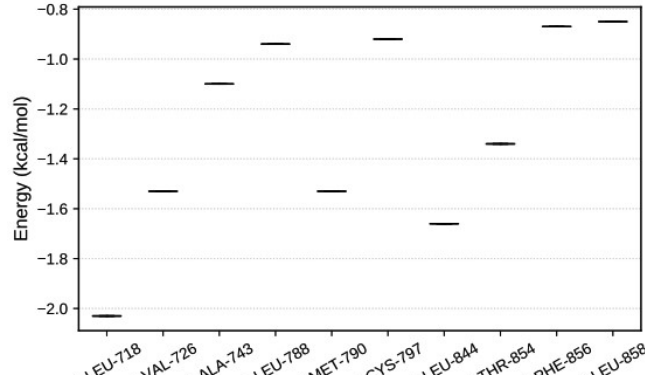
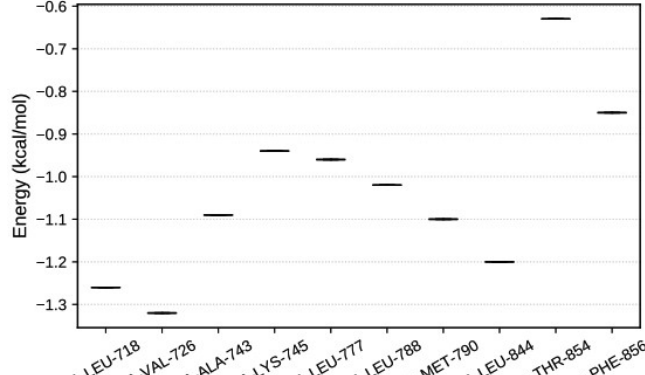
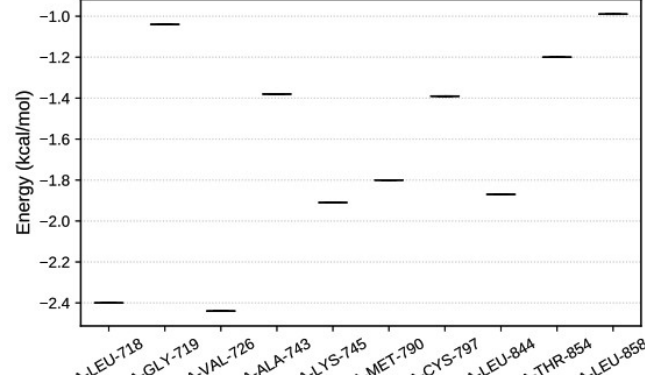
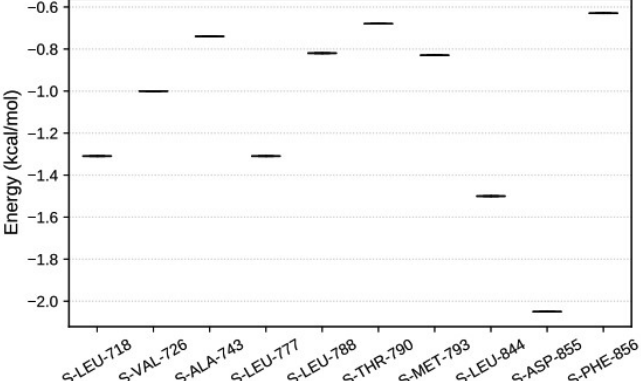
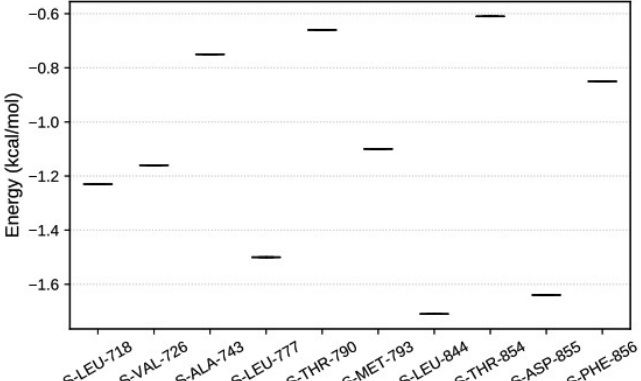
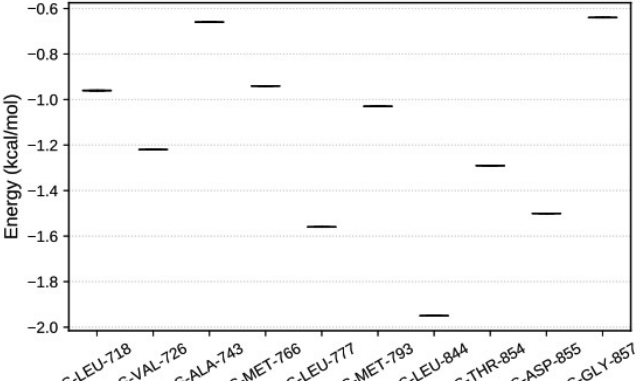


Figure 21. Western blotting images for the tested proteins

Target	Ligand	MM/GBSA	Per-residue MM/GBSA energy contributions
EGFR ^{WT}	13	-35.94	
	14	-42.59	
	15	-42.74	
	Gefitinib	-42.88	

EGFR ^{T790M}	13	-36.72	
	14	-59.23	
	15	-45.89	
Neratinib		-74.46	

EGFR ^{L858R}	13	-40.21	
	14	-49.23	
	15	-45.04	
Gefitinib		-40.33	