

Synthesis, Anticancer, Antioxidant, Anti-inflammatory, Antimicrobial Activities, Molecular Docking, and DFT Studies of Sultams Derived from Saccharin

Nourah Al-Fayez ¹, Hany Elsayy ^{1,2}, Mohammed A. Mansour ^{2,3}, Mohamad Akbar Ali ^{1,4} and Ibrahim Elghamry ^{1,*}

¹ Department of Chemistry, College of Science Al Hufuf, King Faisal University, P.O. Box 380, Saudi Arabia

² Biochemistry Division, Department of Chemistry, Faculty of Science, Tanta University, Tanta 31527, Egypt

³ Cancer Biology and Therapy Lab, Division of Human Sciences, School of Applied Sciences, London South Bank University, London SE1 0AA, UK

⁴ Department of Chemistry, College of Art and Science, Khalifa University, 127788, Abu Dhabi, United Arab Emirates

* Correspondence: ielghamry@kfu.edu.sa or elghamry@hotmail.com; Tel.: +966-135-899-557

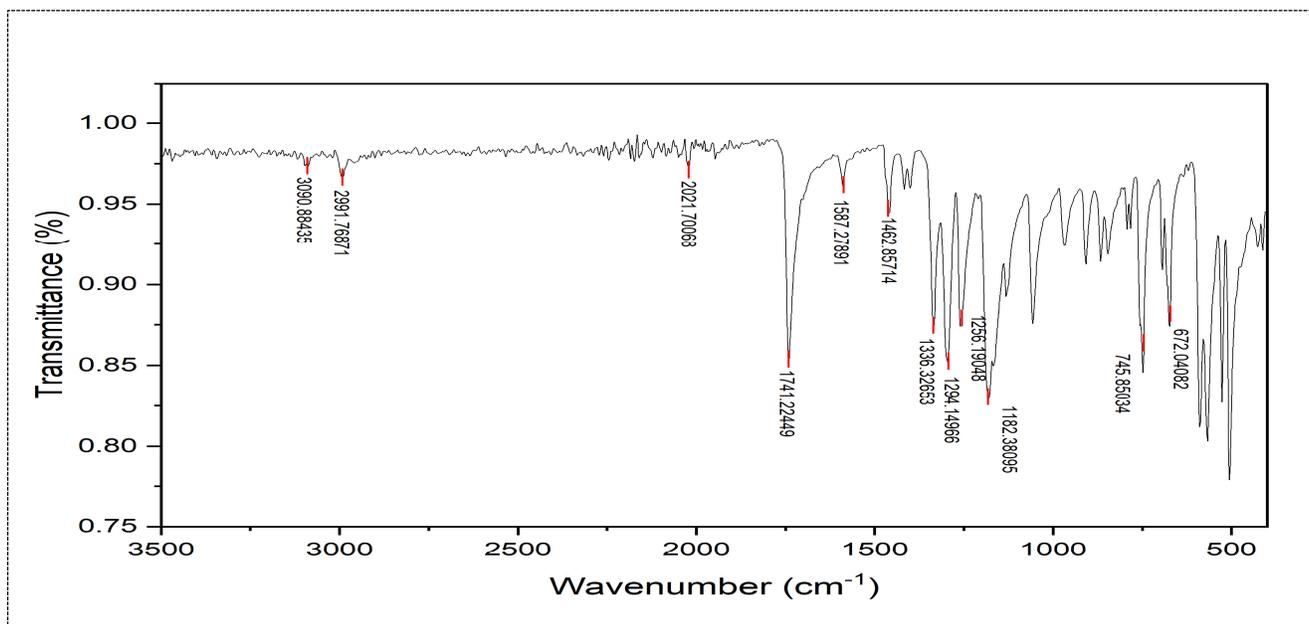


Figure S1. IR spectra of compound 2.

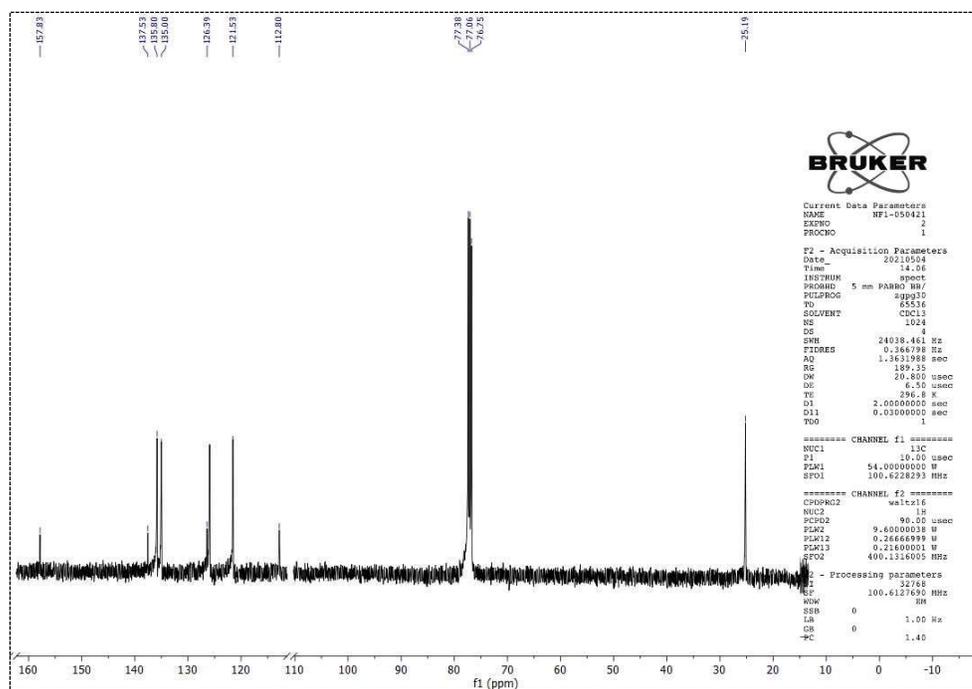


Figure S3. ¹³C NMR spectra of compound 2.

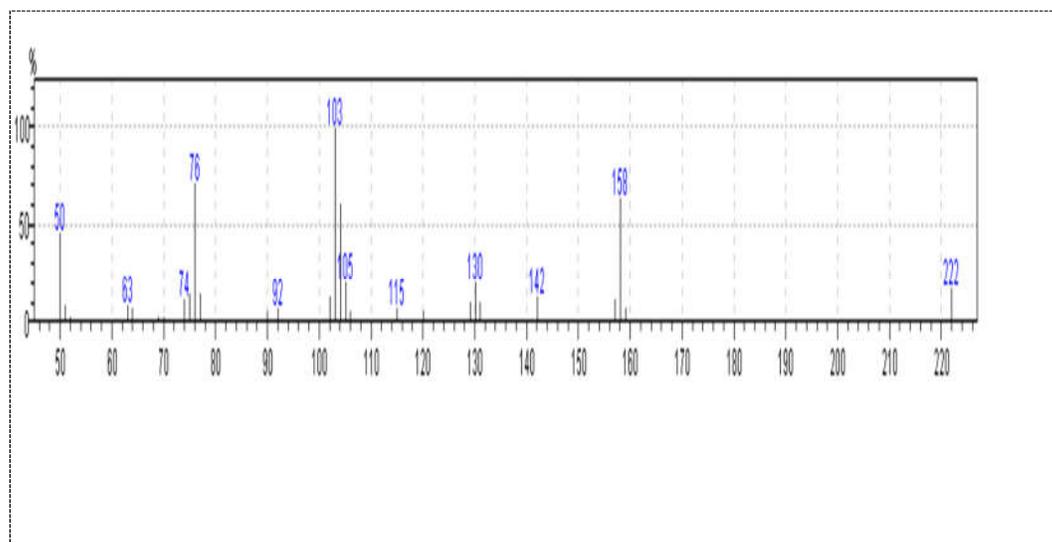


Figure S4. MS spectra of compound 2.

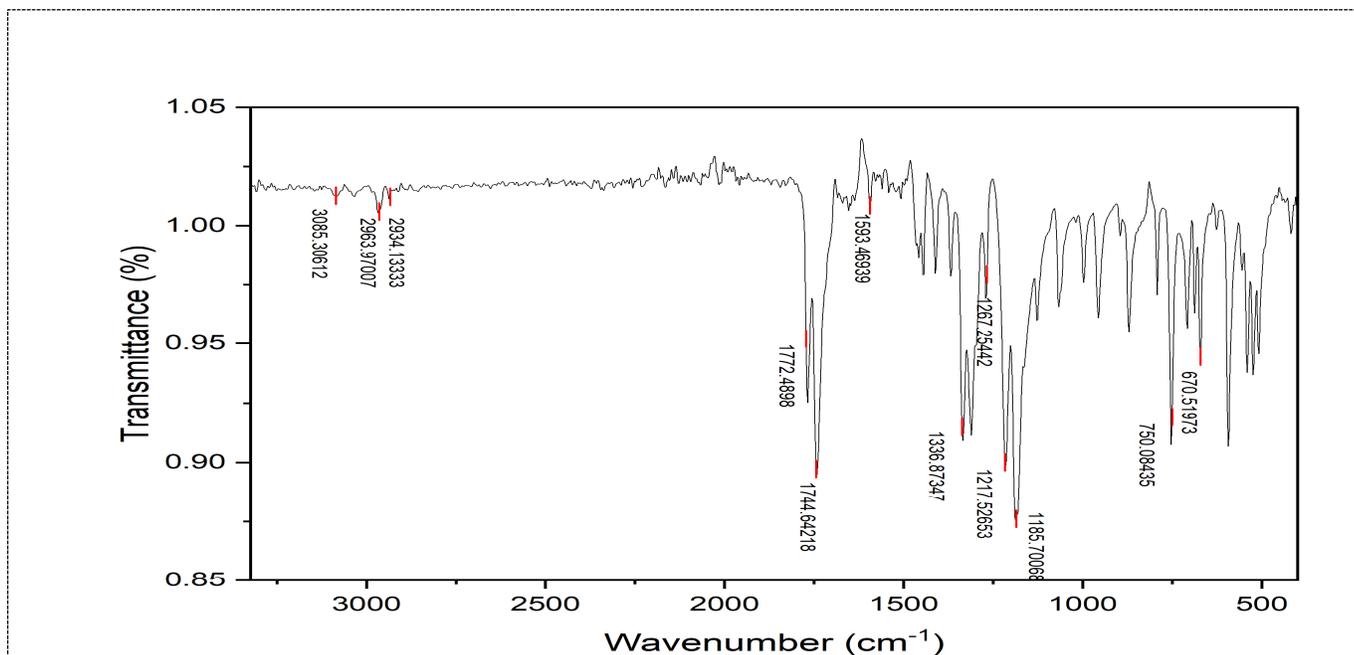


Figure S5. IR spectra of compound 3a.

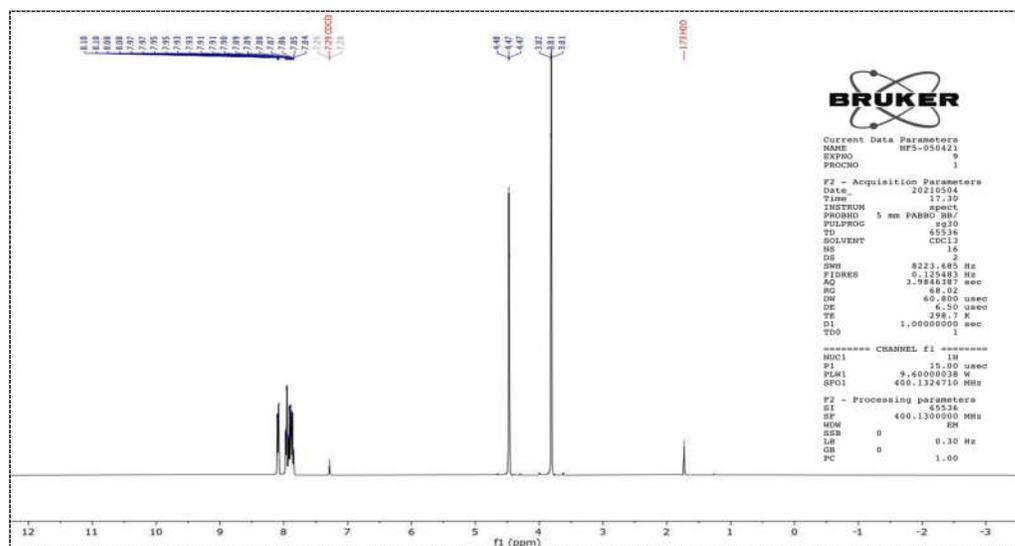


Figure S6. ¹H NMR spectra of compound 3a.

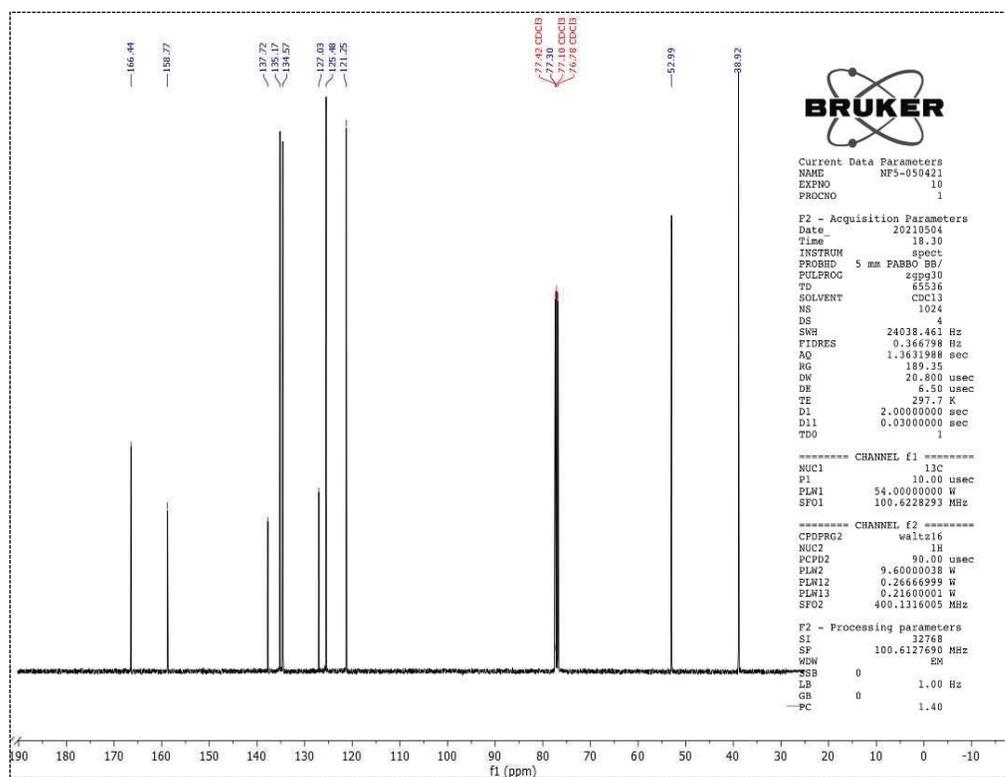


Figure S7. ¹³C NMR spectra of compound 3a.

Chemical Formula: C₁₀H₉NO₅S
 Molecular Weight: 255.25 g/mol

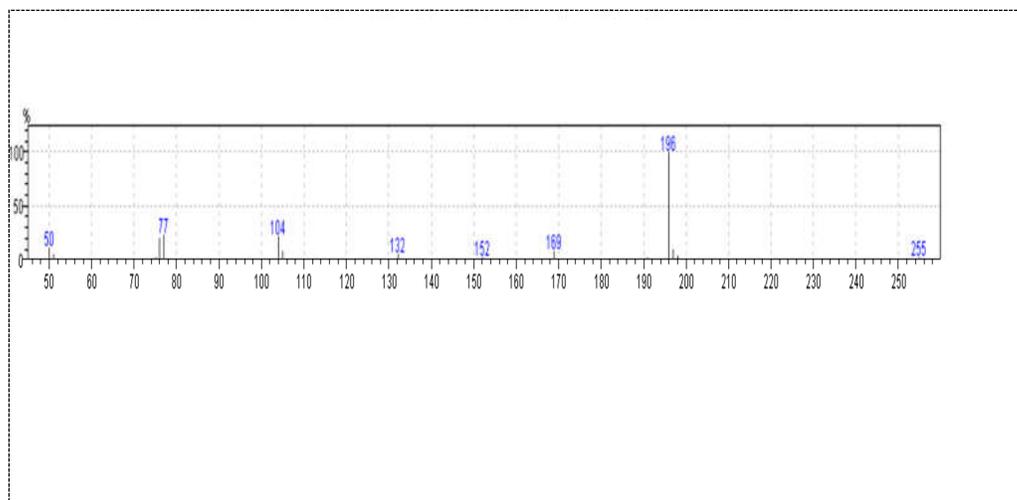


Figure S8. MS spectra of compound 3a.

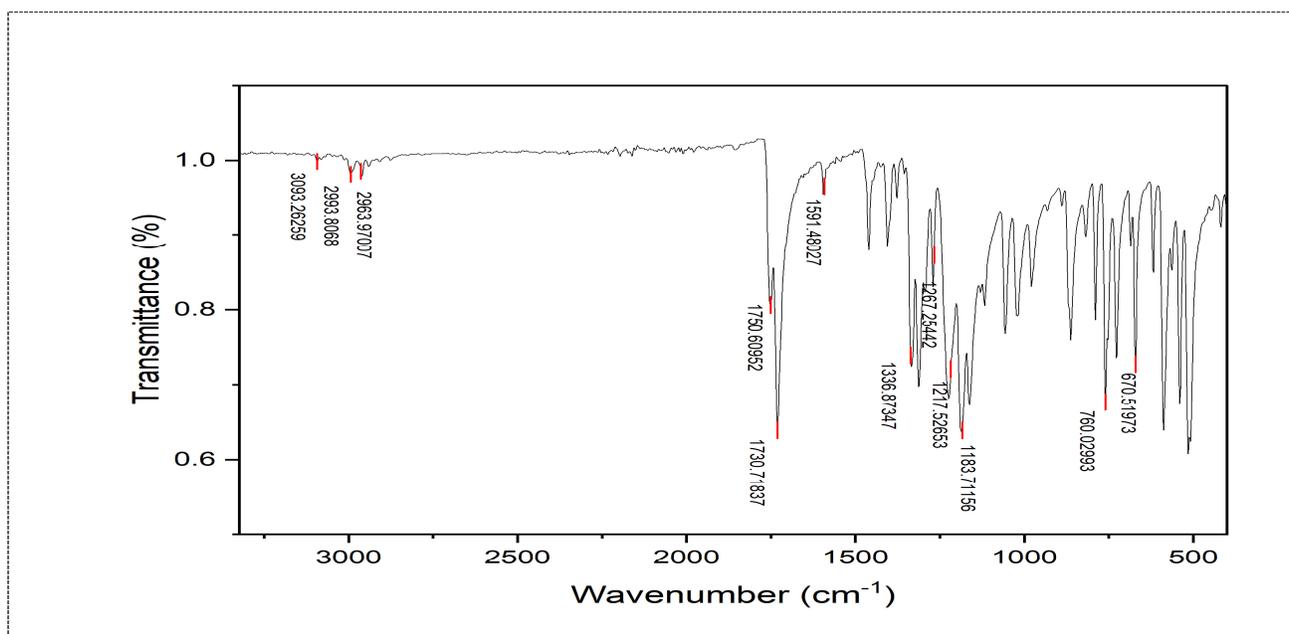


Figure S9. IR spectra of compound 3b.

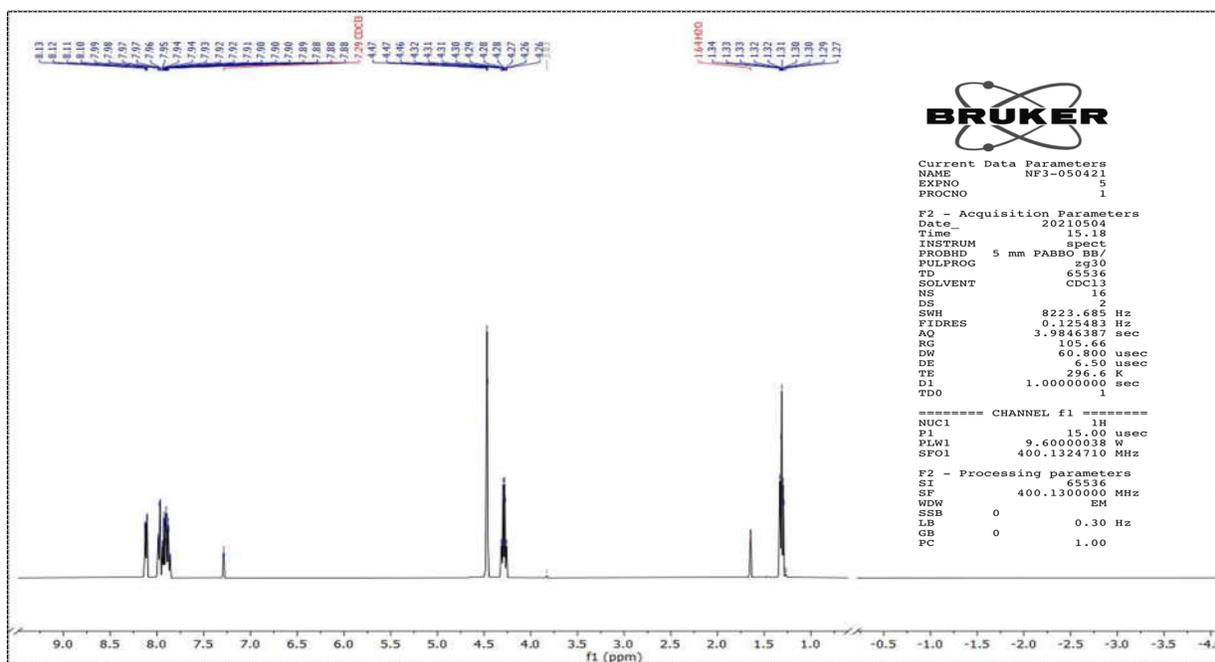


Figure S10. ¹H NMR spectra of compound 3b.

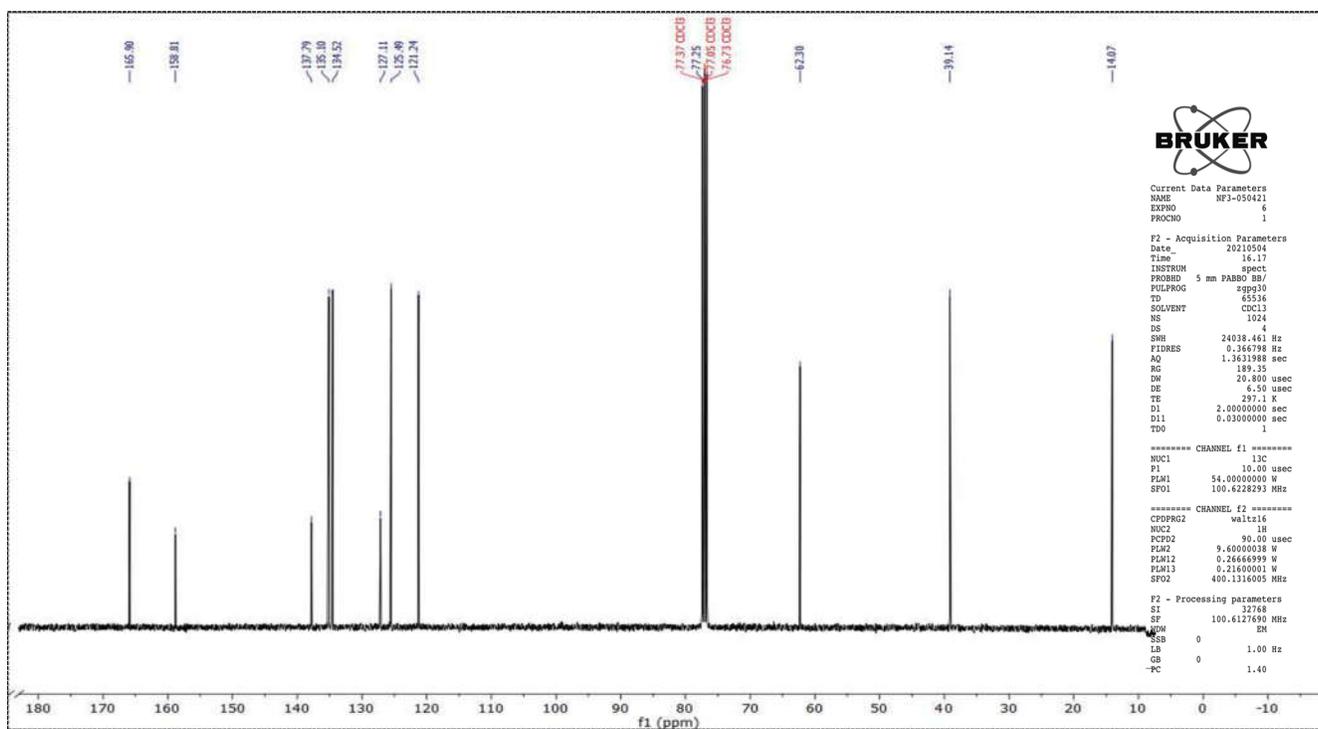


Figure S11. ¹³C NMR spectra of compound 3b.

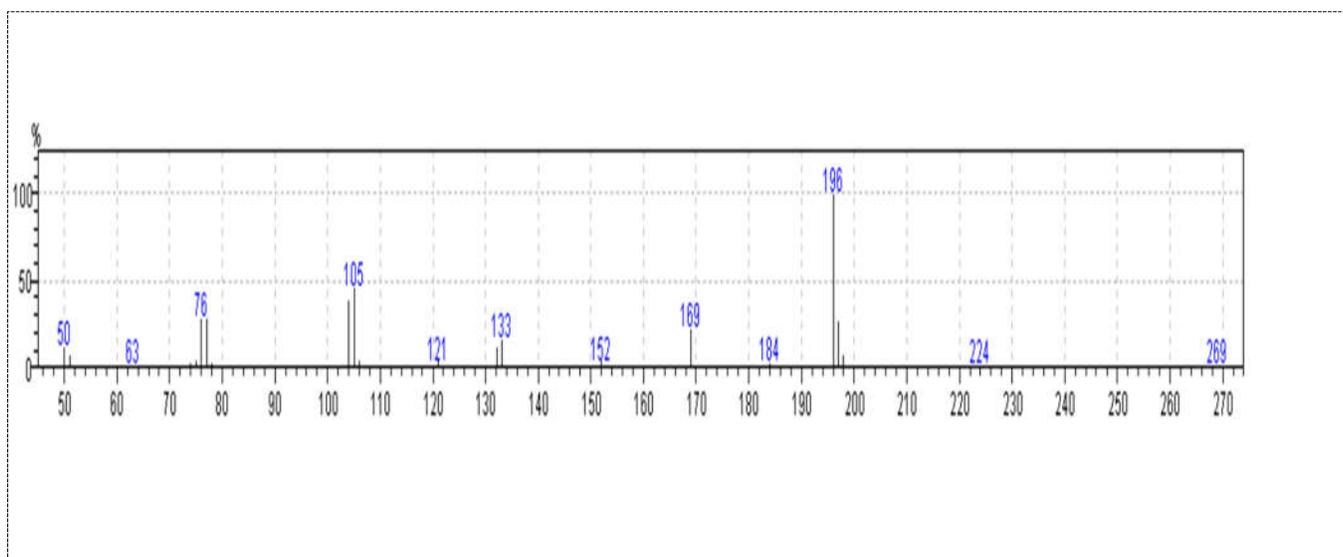


Figure S12. MS spectra of compound 3b.

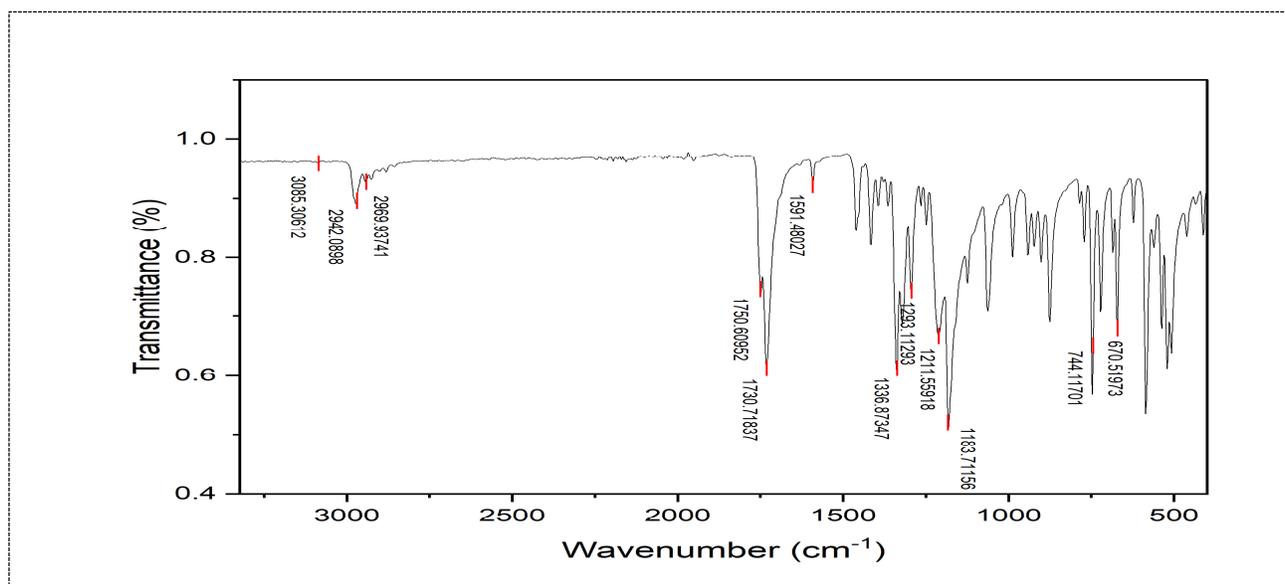


Figure S13. IR spectra of compound 3c.

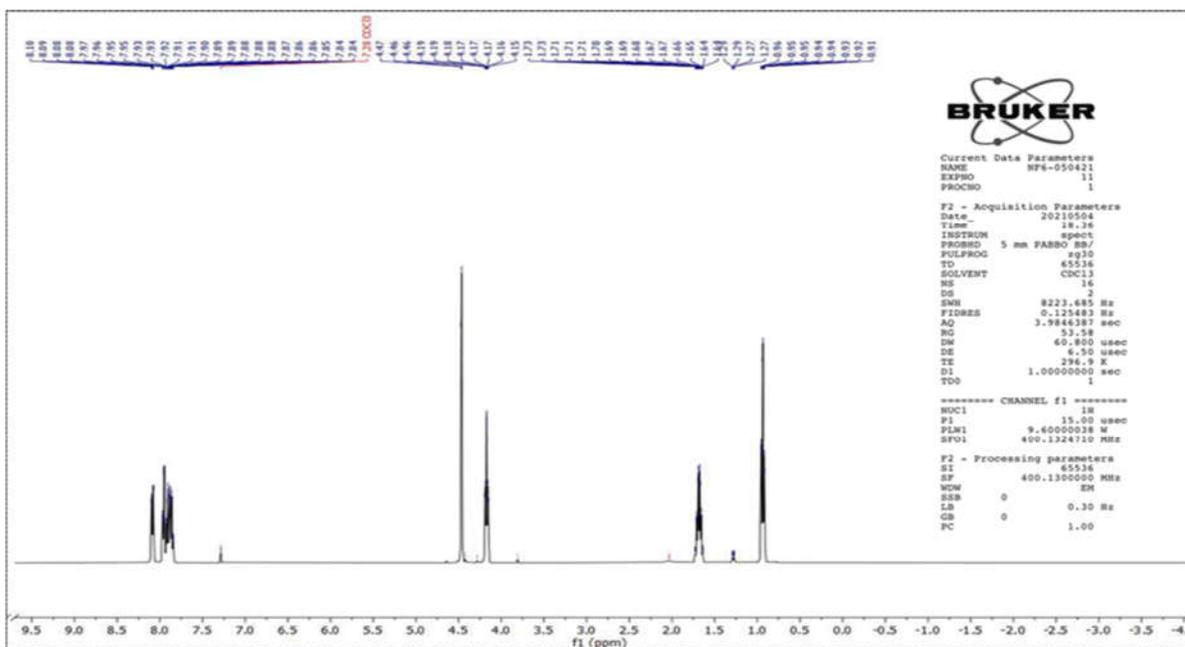


Figure S14. ¹H NMR spectra of compound 3c.

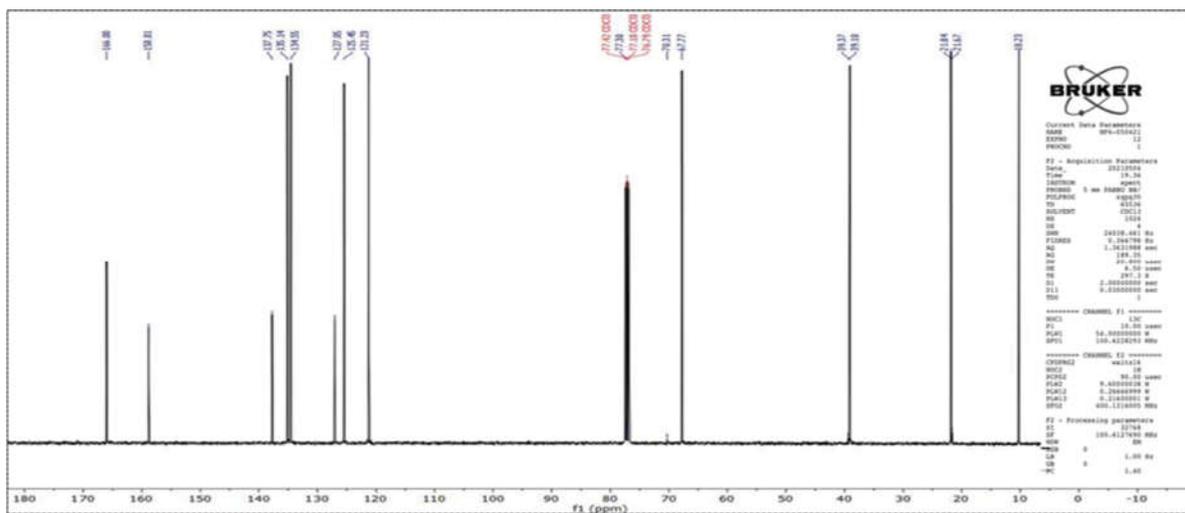


Figure S15. ¹³C NMR spectra of compound 3c.

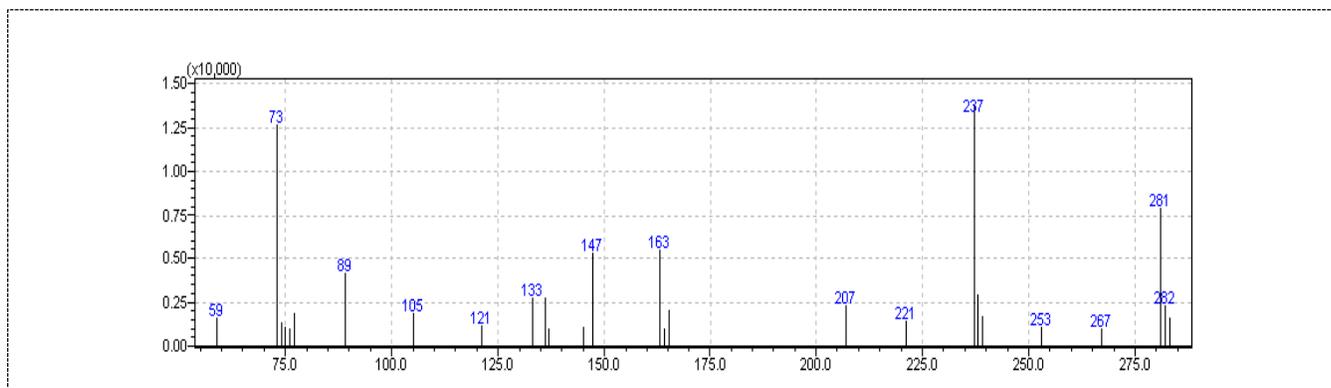


Figure S16. MS spectra of compound 3c.

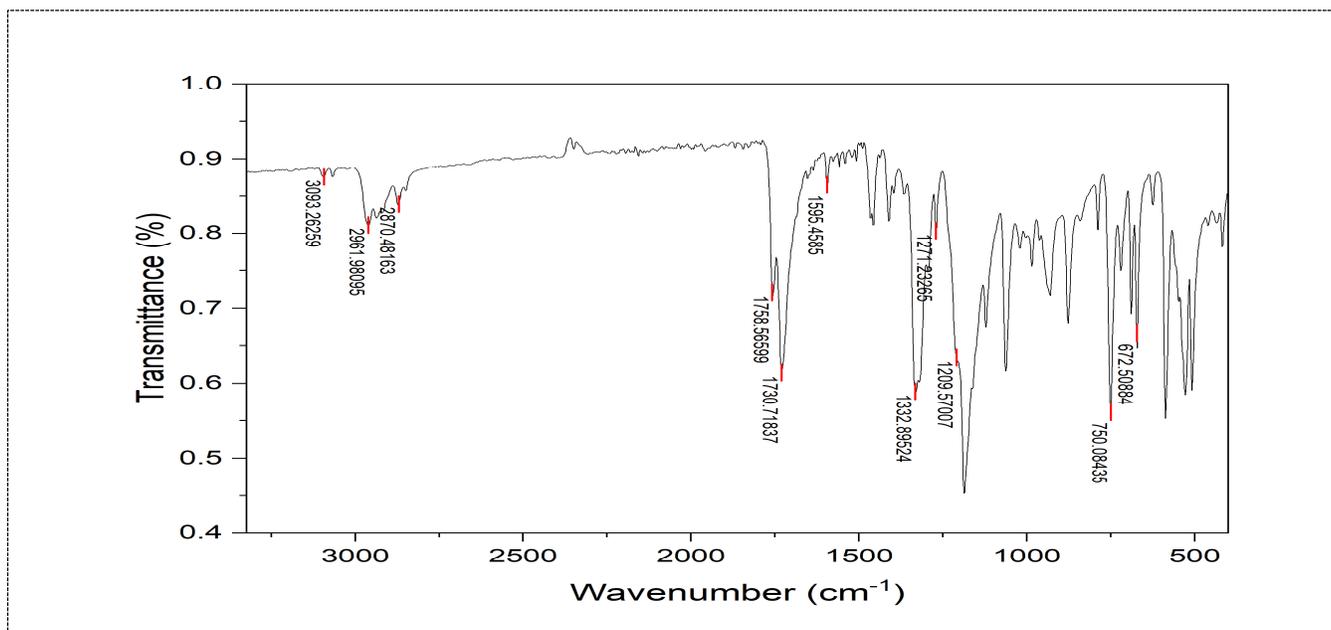


Figure S17. IR spectra of compound 3d.

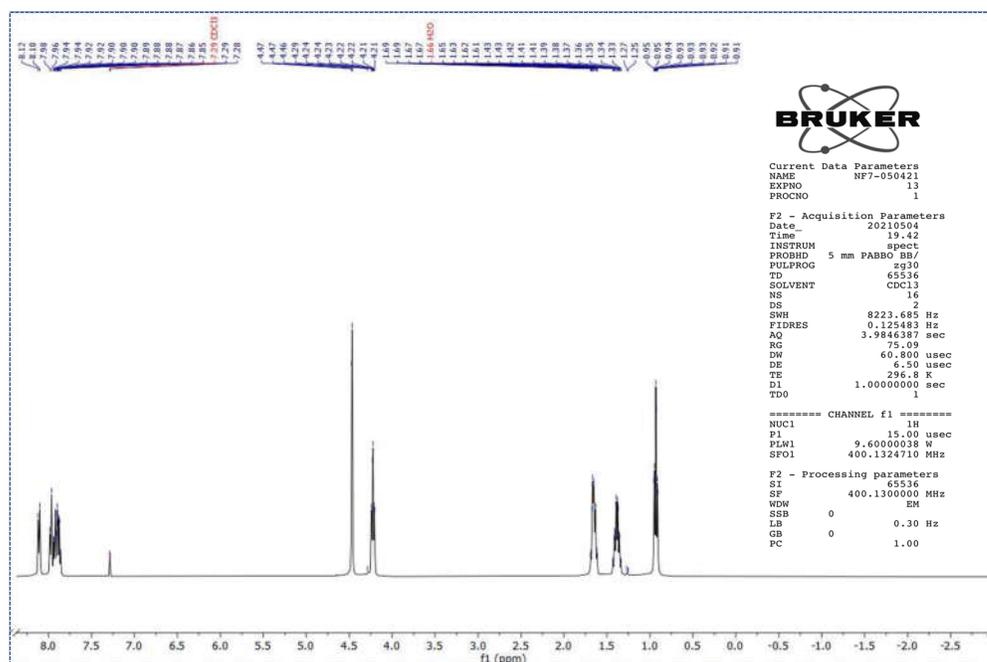


Figure S18. ¹H NMR spectra of compound 3d.

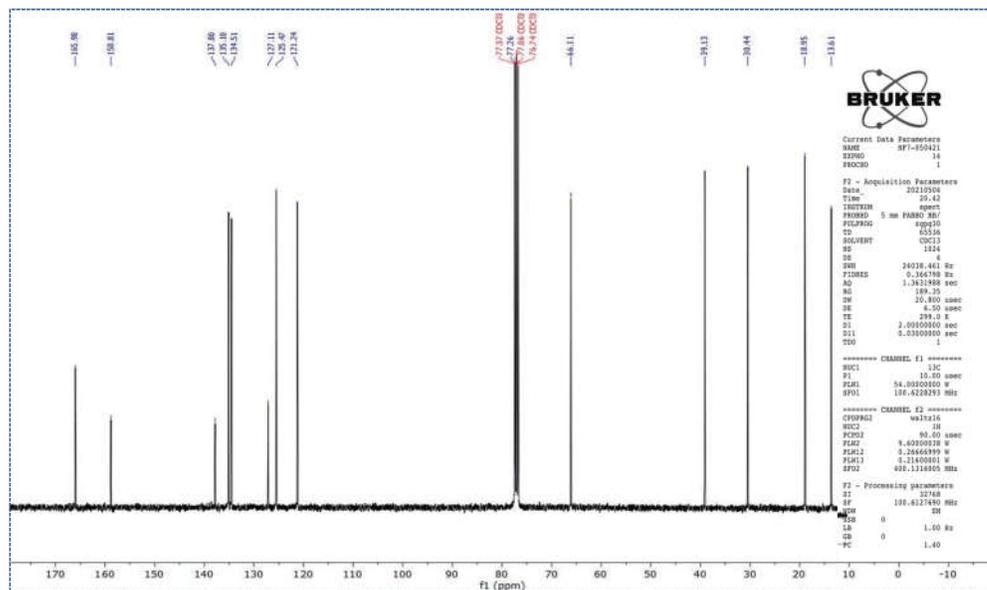


Figure S19. ¹³C NMR spectra of compound 3d.

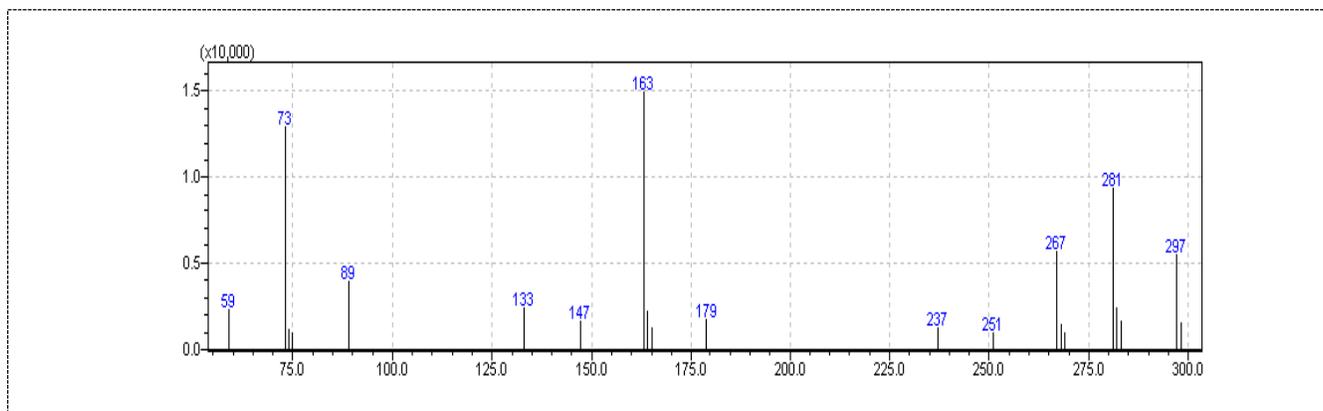


Figure S20. MS spectra of compound 3d.

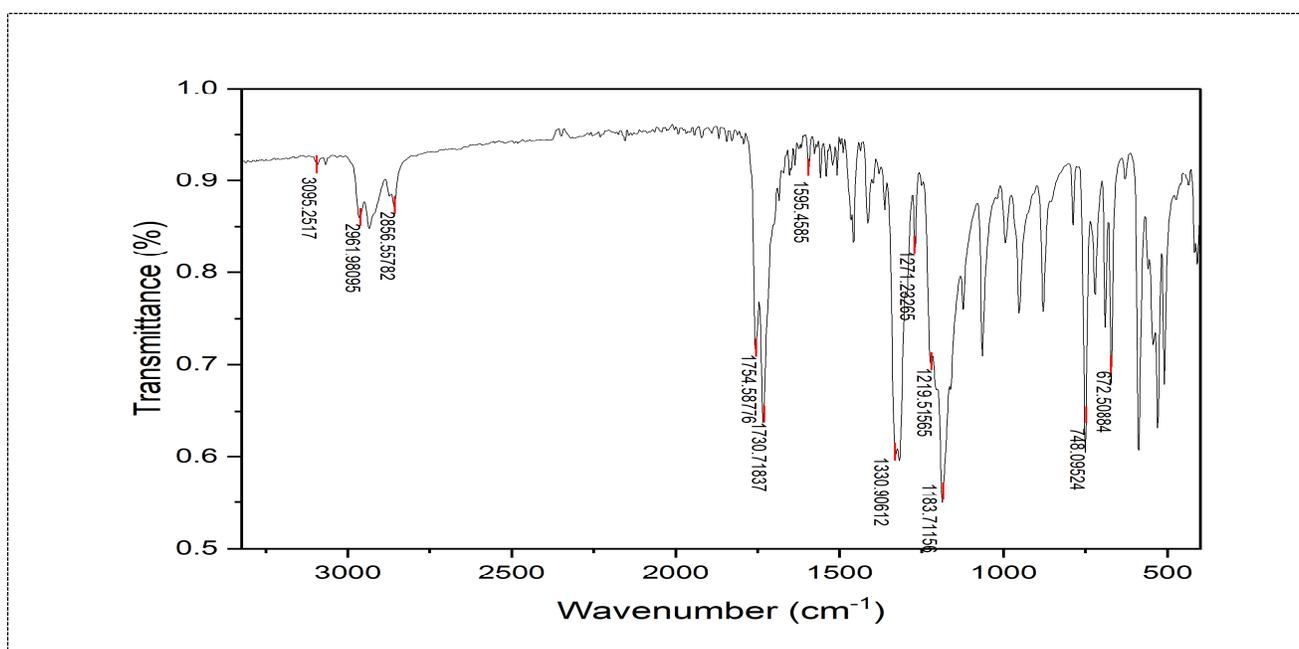


Figure S21. IR spectra of compound 3e.

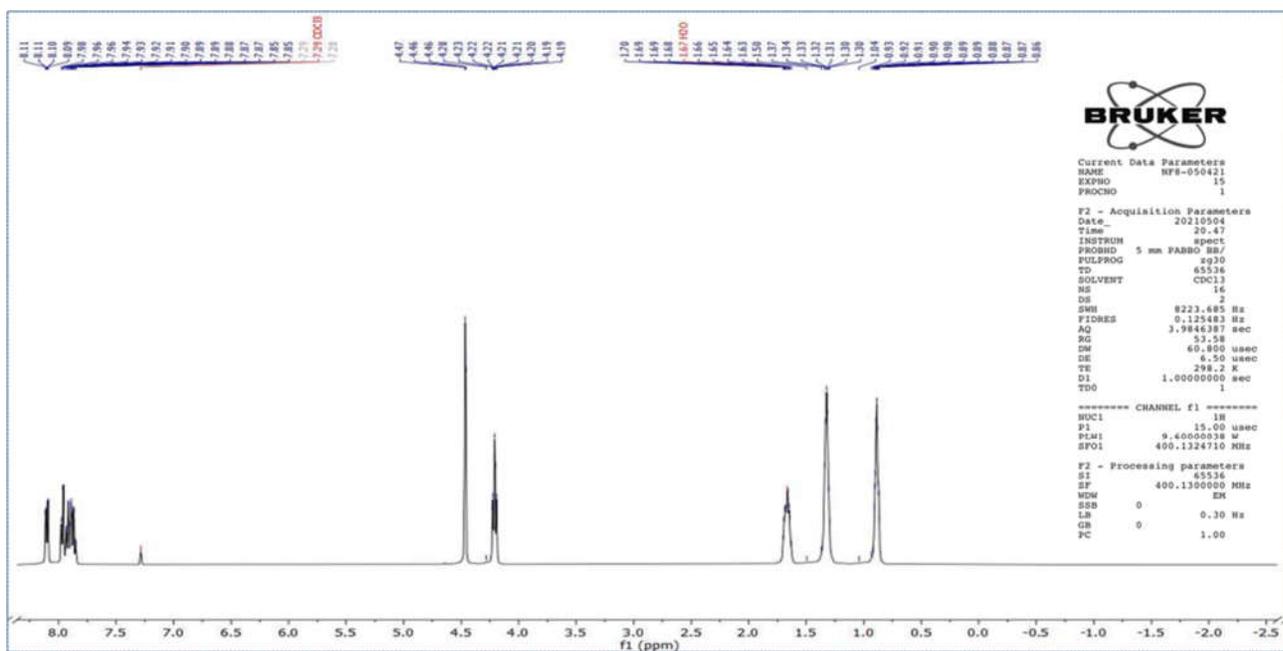


Figure S22. ^1H NMR spectra of compound 3e.

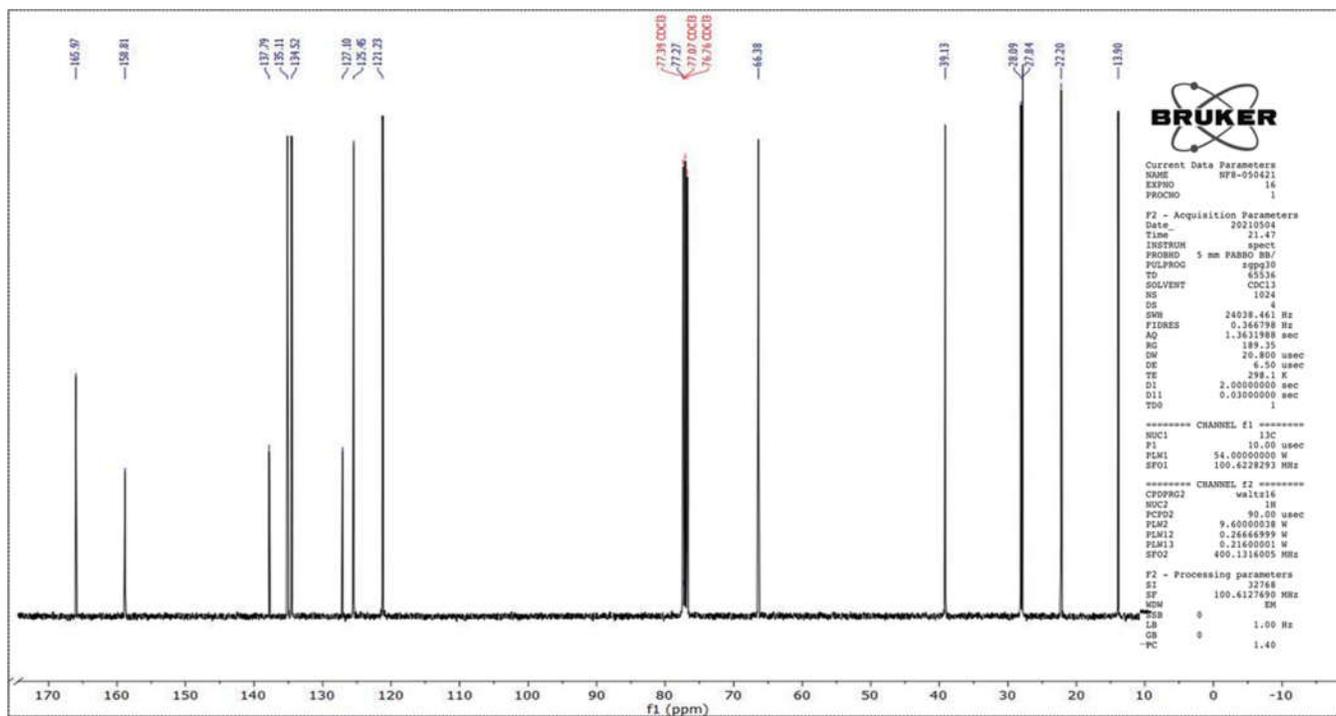


Figure S23. ^{13}C NMR spectra of compound 3e.

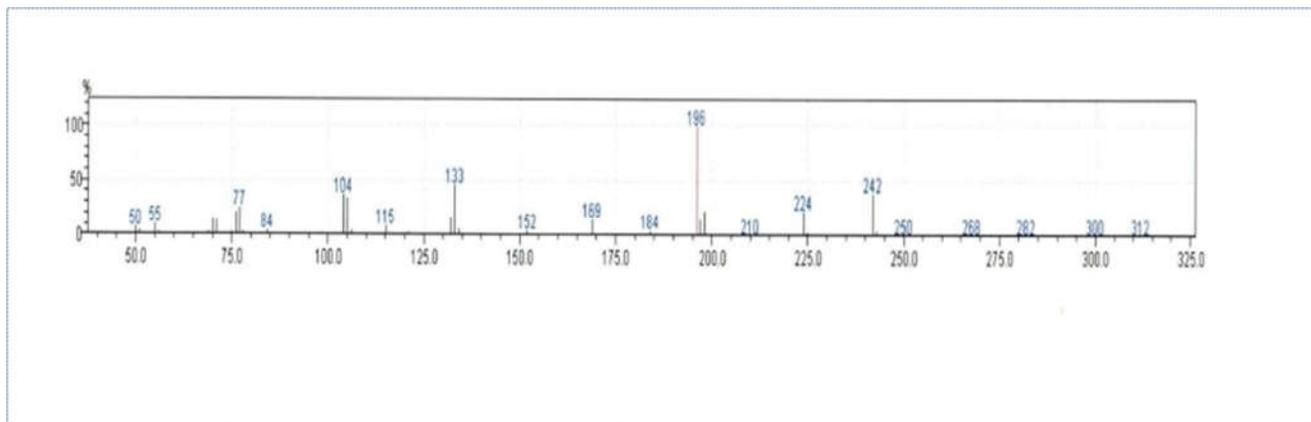


Figure S24. MS spectra of compound 3e.

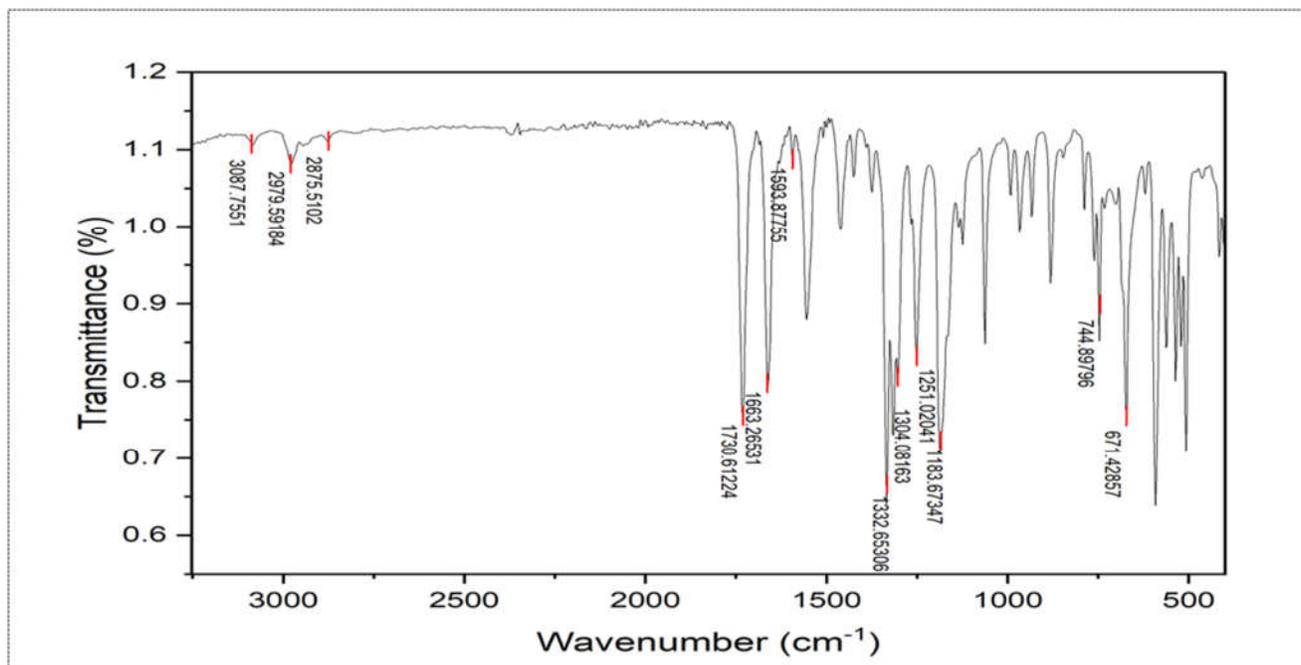
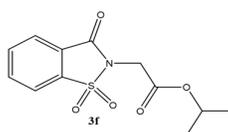


Figure S25. IR spectra of compound 3f.

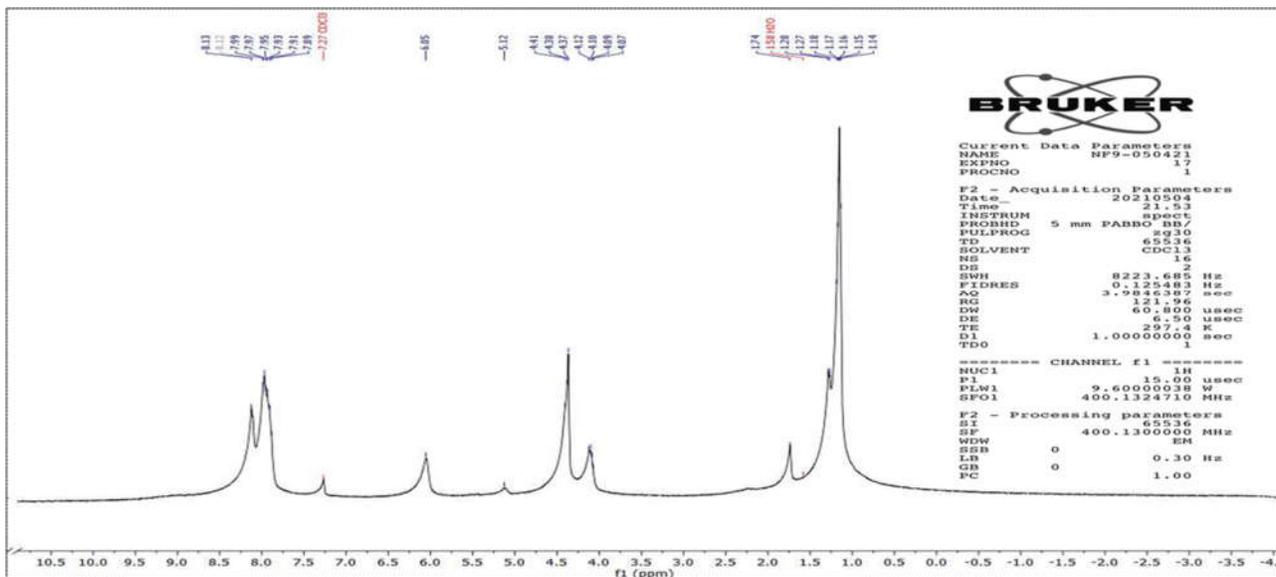


Figure S26. ¹H NMR spectra of compound 3f.

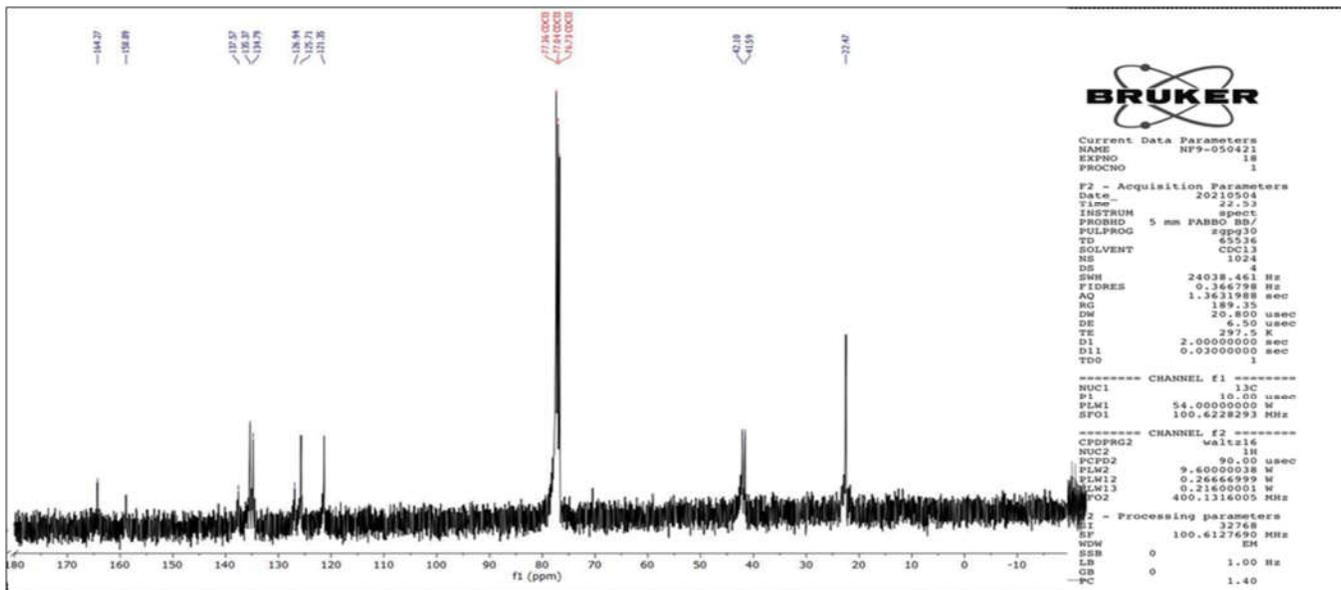


Figure S27. ¹³C NMR spectra of compound 3f.

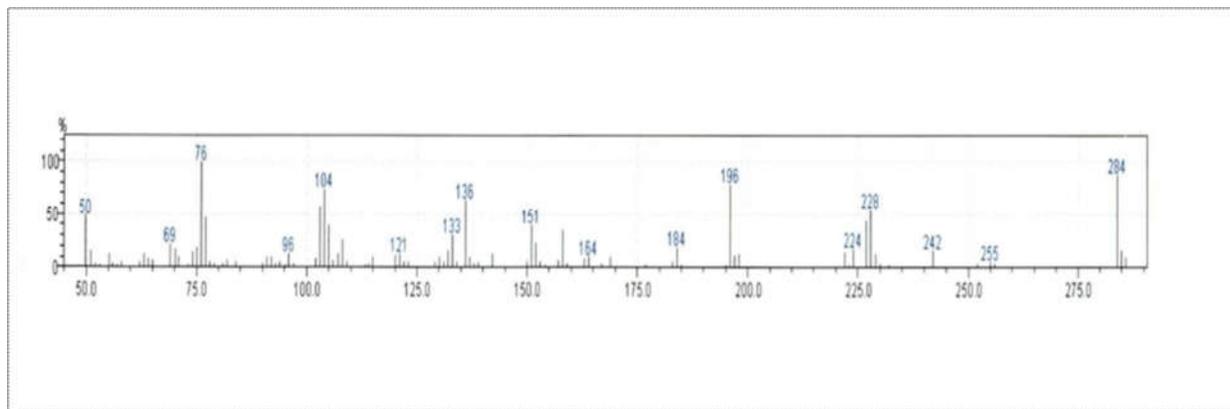


Figure S28. MS spectra of compound 3f.

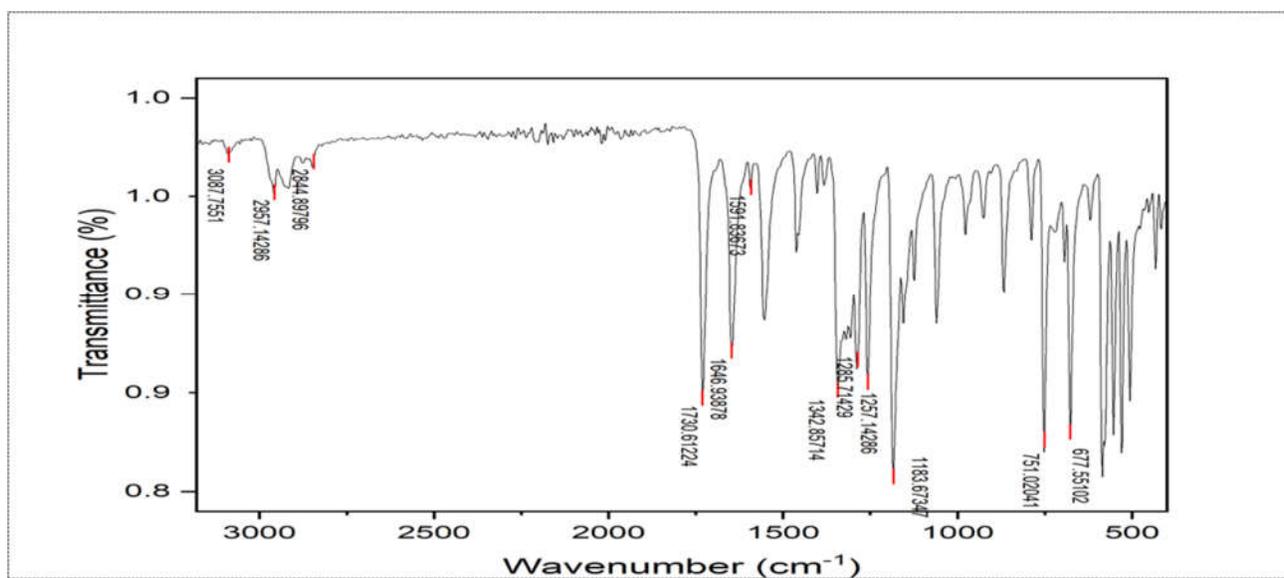
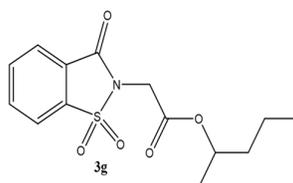


Figure S29: .IR spectra of compound 3g.

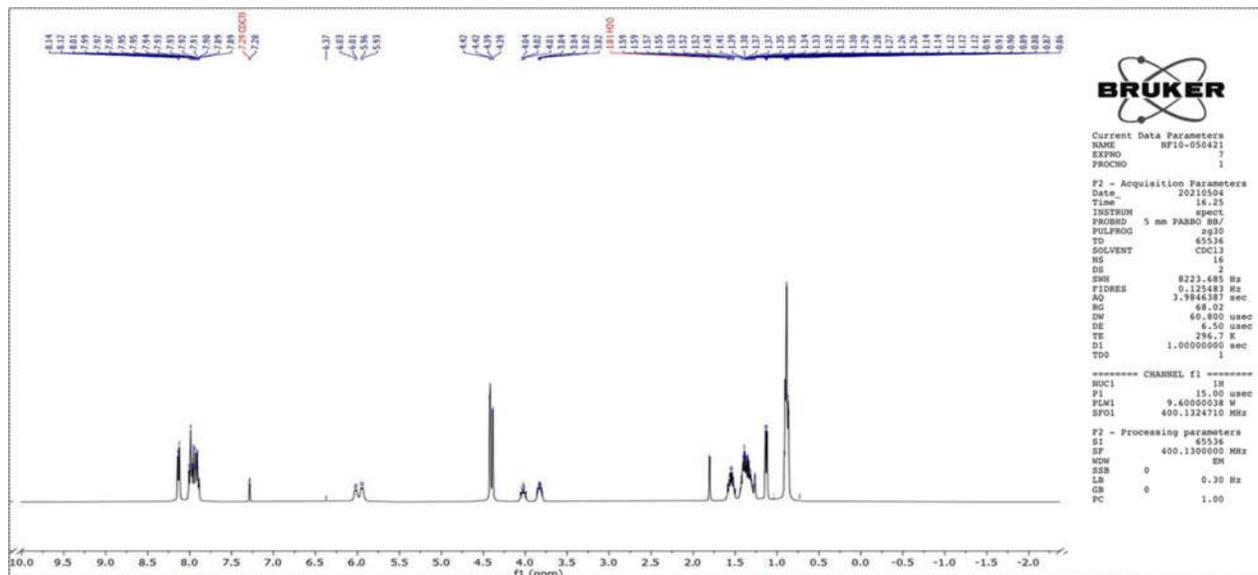


Figure S30. ¹H NMR spectra of compound 3g.

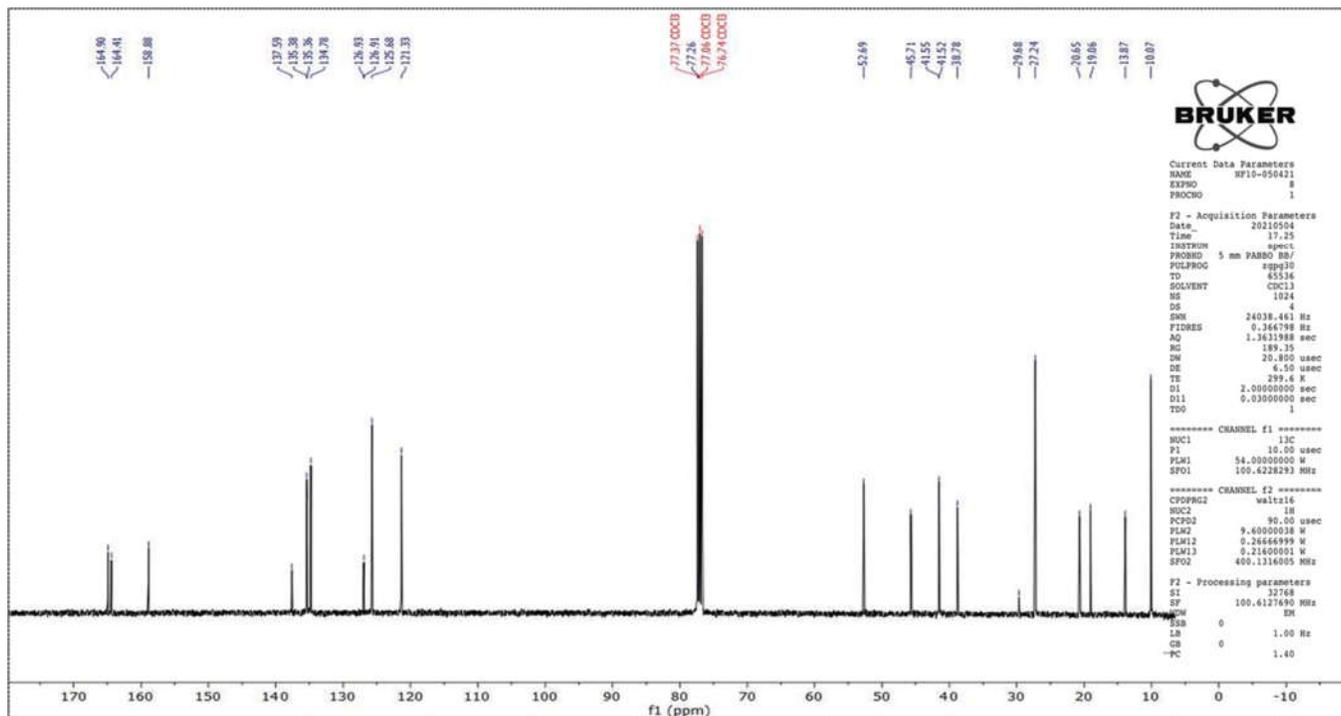


Figure S31. ¹³C NMR spectra of compound 3g.

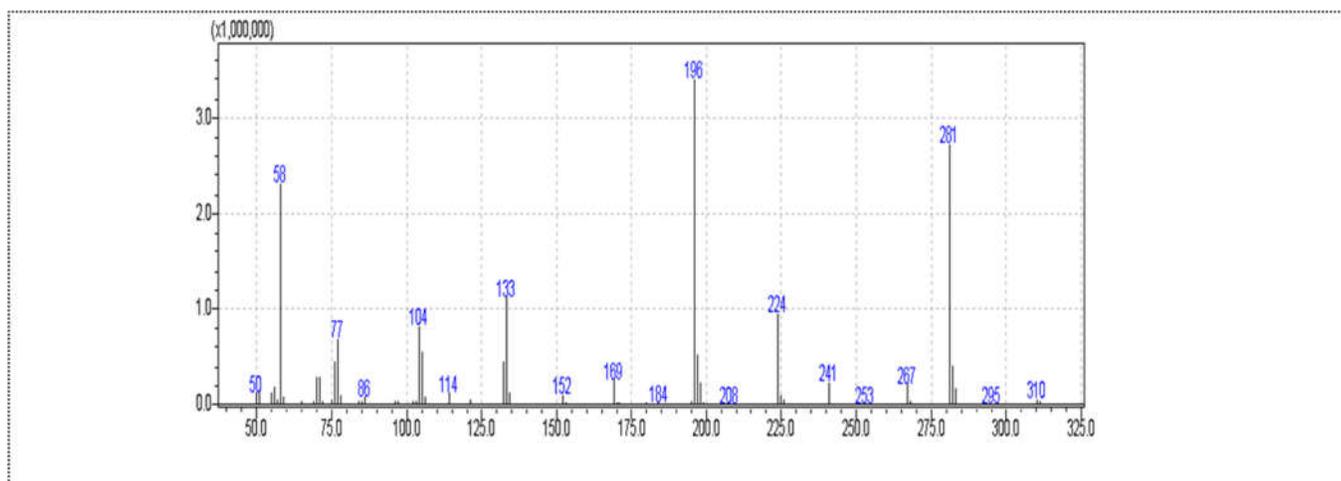


Figure S32. MS spectra of compound 3g.

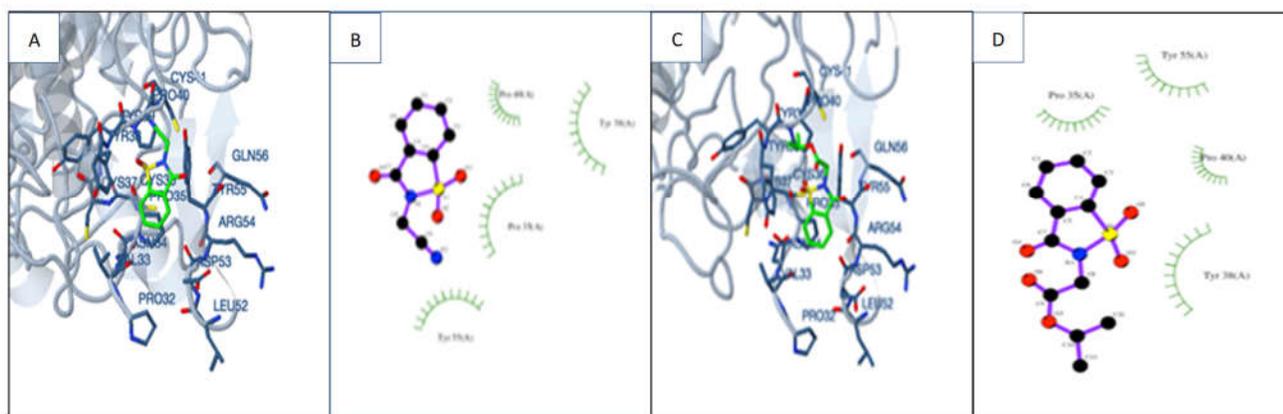


Figure S33. Molecular docking studies; A, B 3D, and 2D representations for compound 2, respectively; C, D 3D, and 2D representations for compound 3f, respectively; Hydrogen bonds highlighted in green with the respective distances between the atoms involved, whereas polar, hydrophobic, and other bonds are represented by an arc with spokes radiating towards the ligand atom.

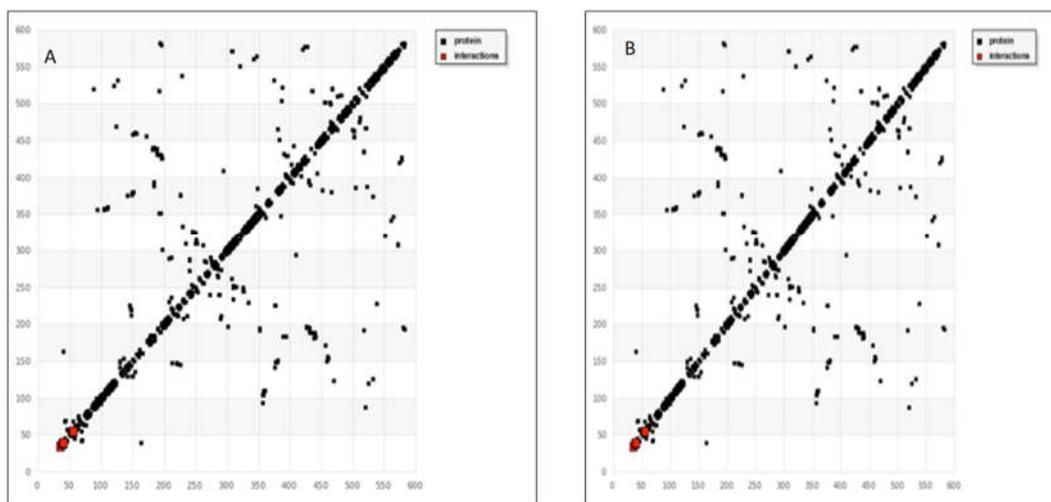


Figure S34. A, B, and C HB plot representations for compound **2**, and **3f**, respectively docking against COX-1 enzyme.

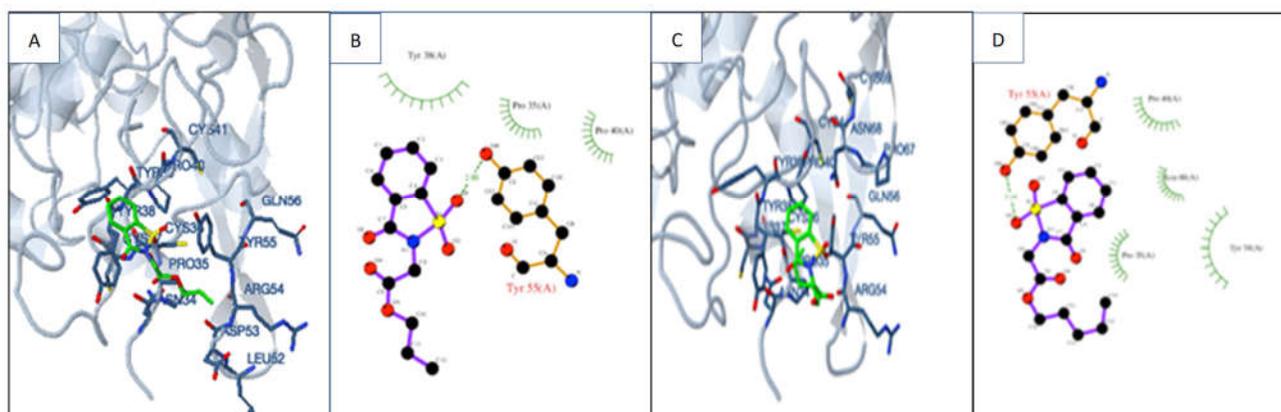


Figure S35. Molecular docking studies; A, B 3D, and 2D representations for compound **3c**, respectively; C, D 3D, and 2D representations for compound **3e**, respectively; Hydrogen bonds highlighted in green with the respective distances between the atoms involved, whereas polar, hydrophobic, and other bonds are represented by an arc with spokes radiating towards the ligand atom.

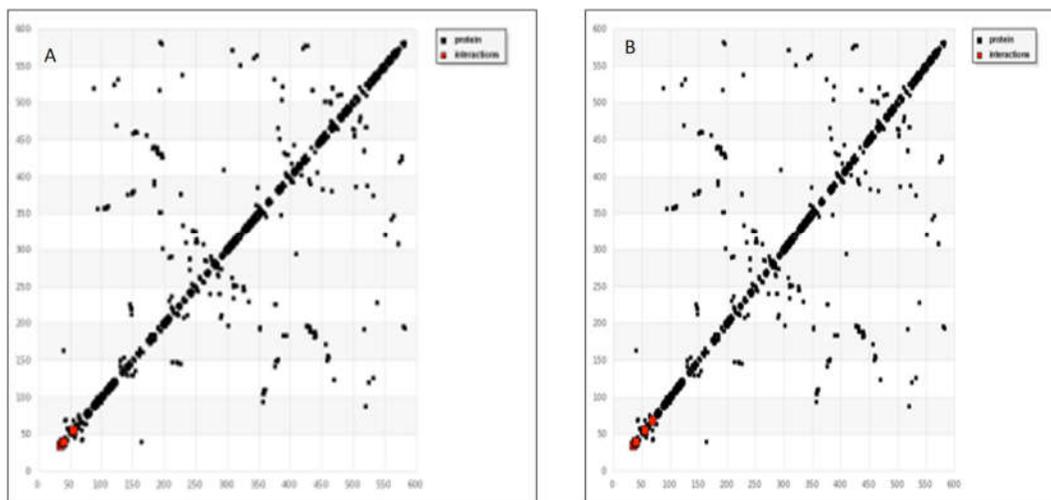


Figure S36. A, B, and C HB plot representations for compound **3c**, and **3e**, respectively docking against COX-1 enzyme.

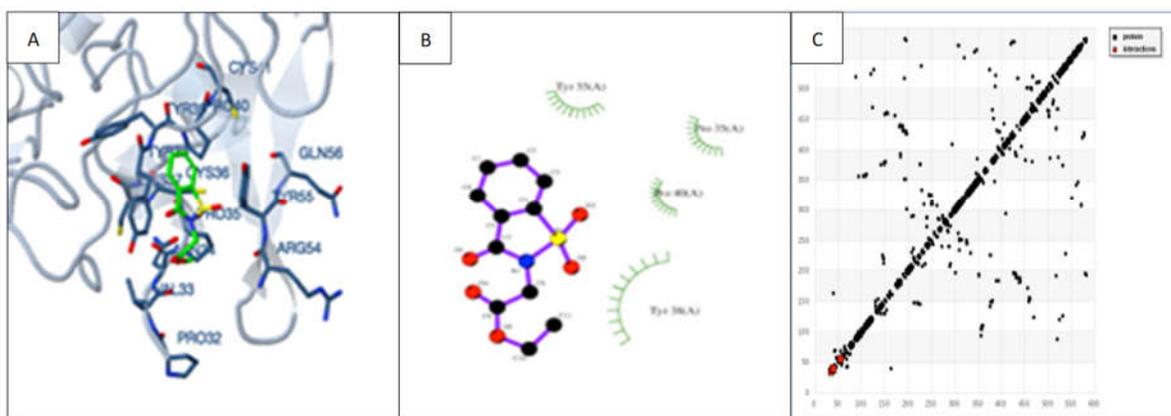


Figure S37. Molecular docking studies; A, B 3D, and 2D representations for compound **3b**, respectively; Hydrogen bonds highlighted in green with the respective distances between the atoms involved, whereas polar, hydrophobic, and other bonds are represented by an arc with spokes radiating towards the ligand atom. C HB plot representations for compound **3b** docking against COX-1 enzyme.

Table S1. MTT assay on normal cell lines (WI138).

Compounds (50μmol)	Number of dead cells(cells/ml)	Inhibition rate (%)
2	17	42.5
3a	4	10
3b	3	7.5
3c	11	27.5
3d	2	5
3e	15	37.5
3f	14	35
3g	16	40