

Supplementary Information

Acridone Derivatives as Photosystem II Inhibitors: Synthesis, Herbicidal Activity, and Structure-Activity

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Molecular docking poses of compounds **10a-10e** with D1 protein of photosystem II

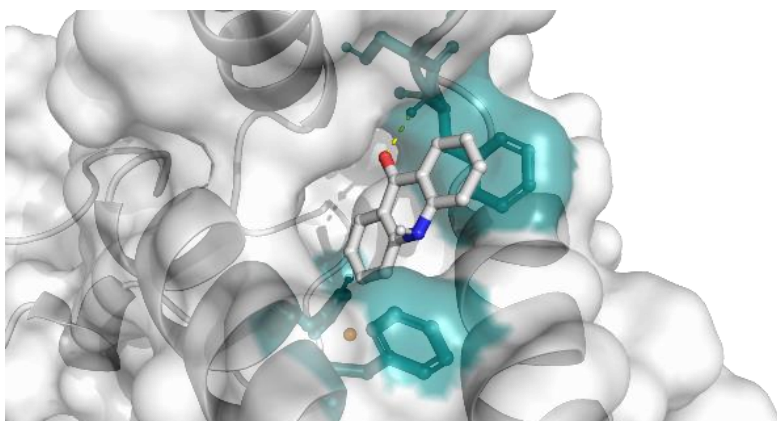


Figure S1. Binding mode of compound **10a** with the pocket site of D1 protein of PSII (PDB ID: 4V82).

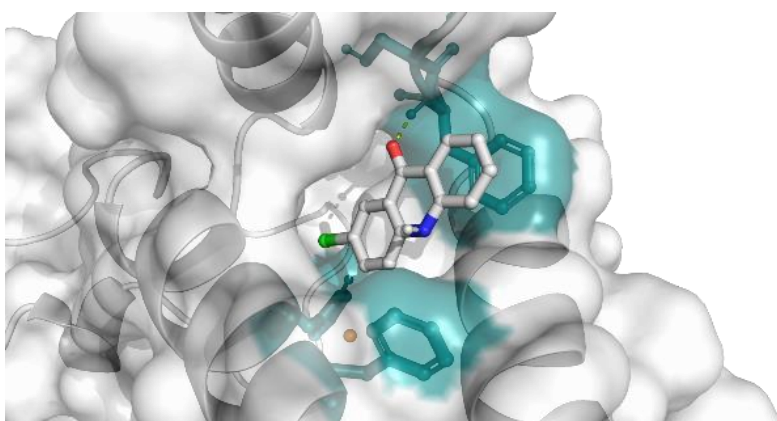


Figure S2. Binding mode of compound **10b** with the pocket site of D1 protein of PSII (PDB ID: 4V82).

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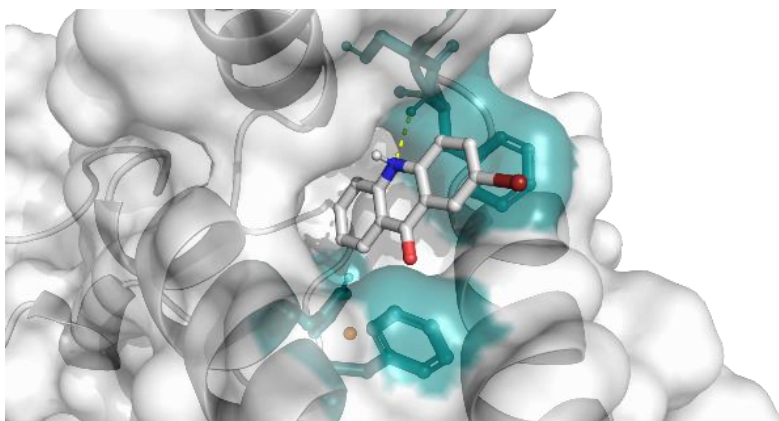


Figure S3. Binding mode of compound **10c** with the pocket site of D1 protein of PSII (PDB ID: 4V82).

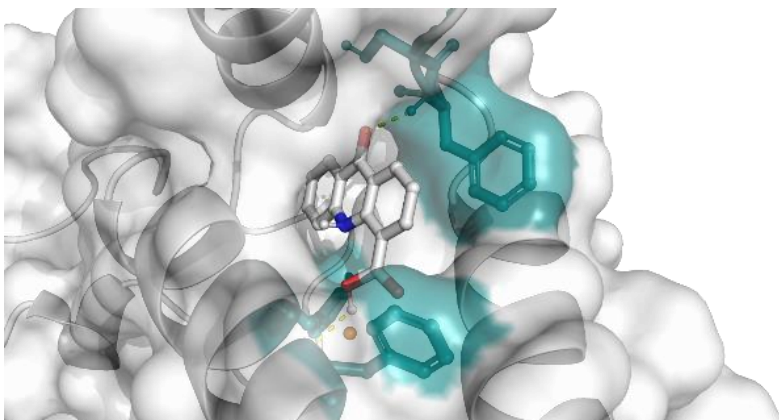


Figure S4. Binding mode of compound **10d** with the pocket site of D1 protein of PSII (PDB ID: 4V82).

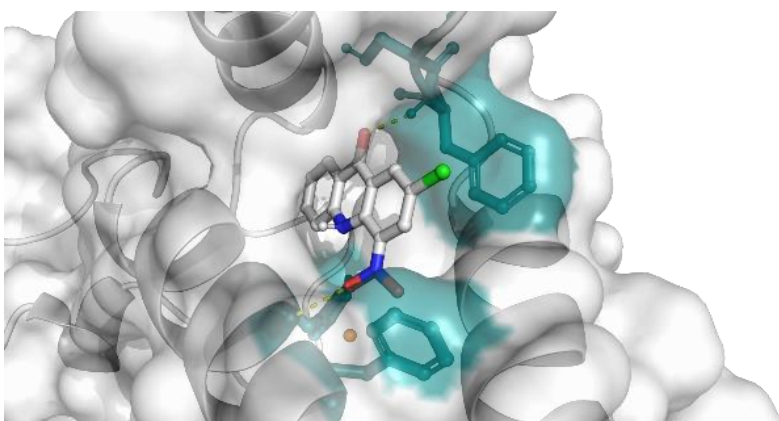


Figure S5. Binding mode of compound **10e** with the pocket site of D1 protein of PSII (PDB ID: 4V82).

Molecular docking poses of compounds **10a-10e** with HPPD enzyme

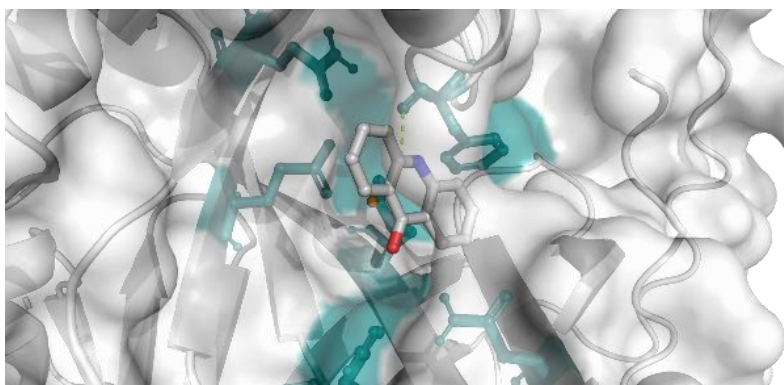


Figure S6. Binding mode of compound **10a** with the pocket site of HPPD enzyme (PDB ID: 6J63).

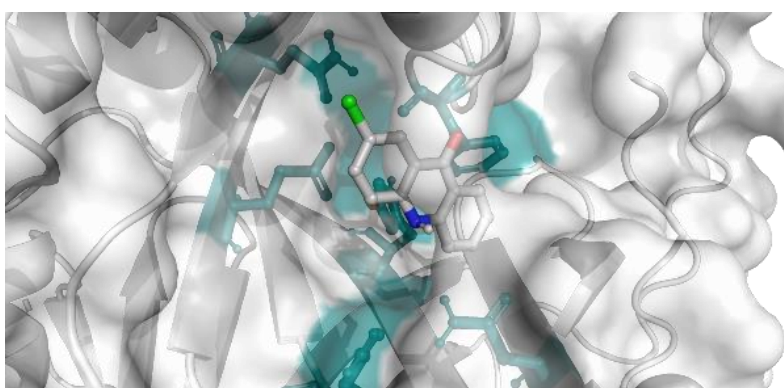


Figure S7. Binding mode of compound **10b** with the pocket site of HPPD enzyme (PDB ID: 6J63).

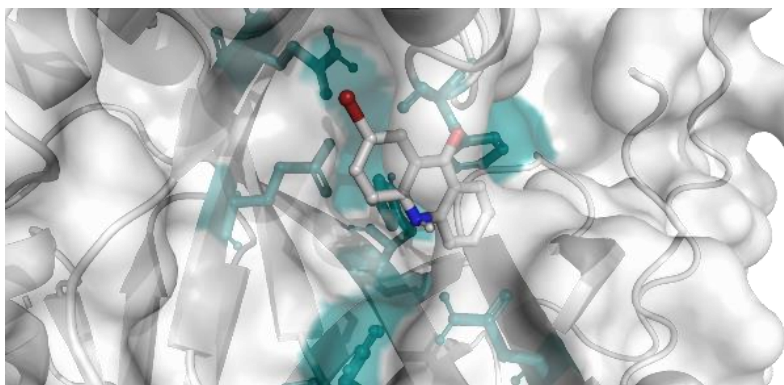


Figure S8. Binding mode of compound **10c** with the pocket site of HPPD enzyme (PDB ID: 6J63).

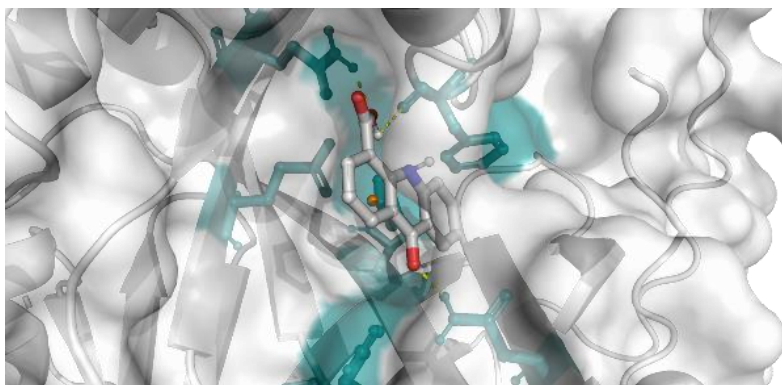


Figure S9. Binding mode of compound **10d** with the pocket site of HPPD enzyme (PDB ID: 6J63).

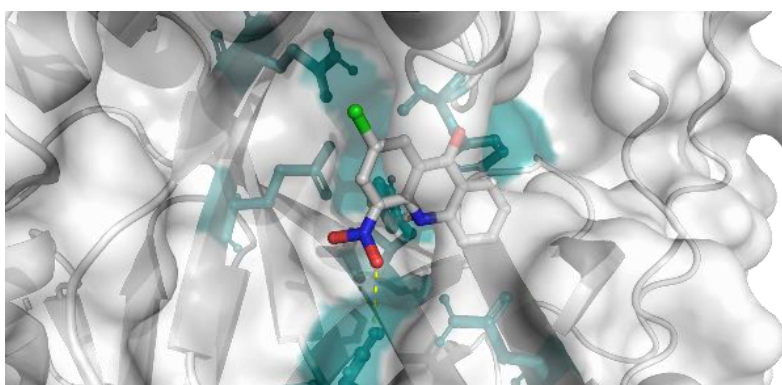


Figure S10. Binding mode of compound **10e** with the pocket site of HPPD enzyme (PDB ID: 6J63).

NMR spectra of compounds **10a-10e**

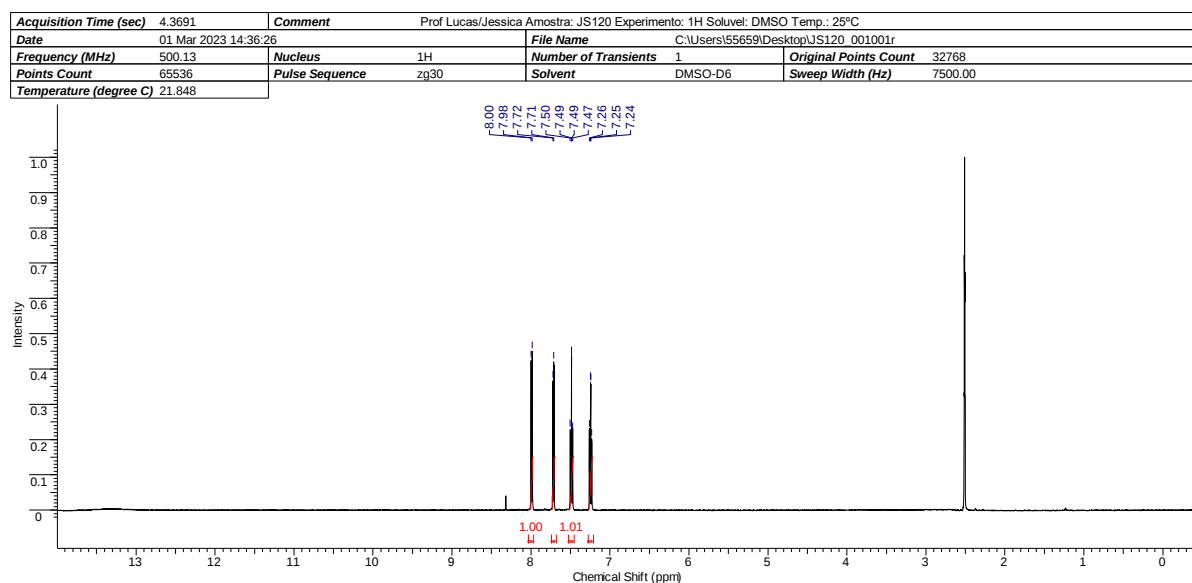


Figure S11. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of compound **7**.

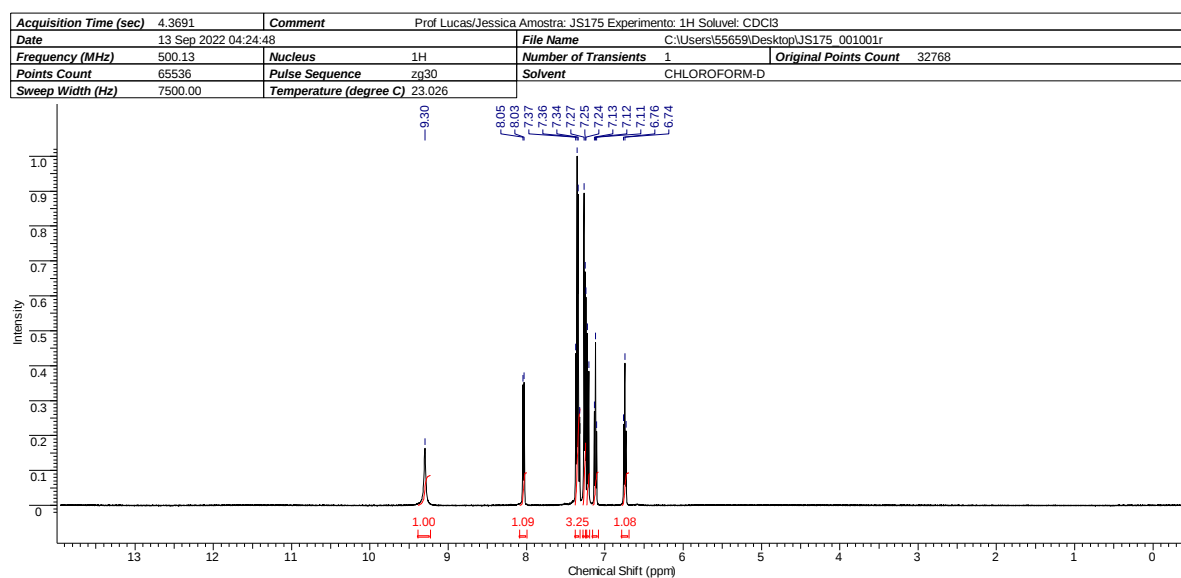


Figure S12. ^1H NMR spectrum (500 MHz, CDCl_3) of compound **9a**.

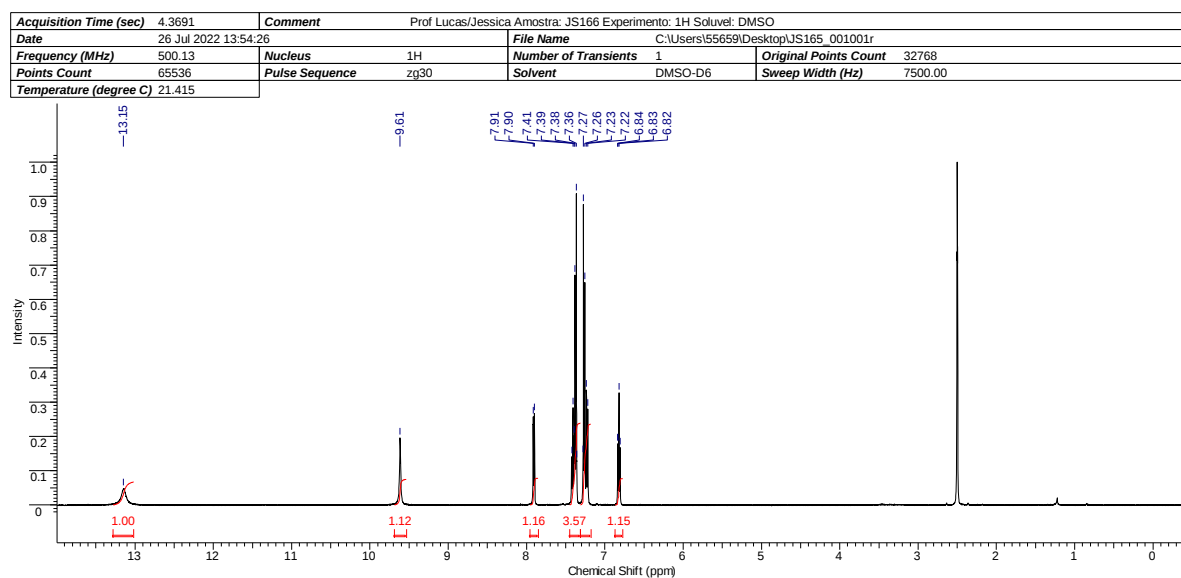


Figure S13. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of compound **9b**.

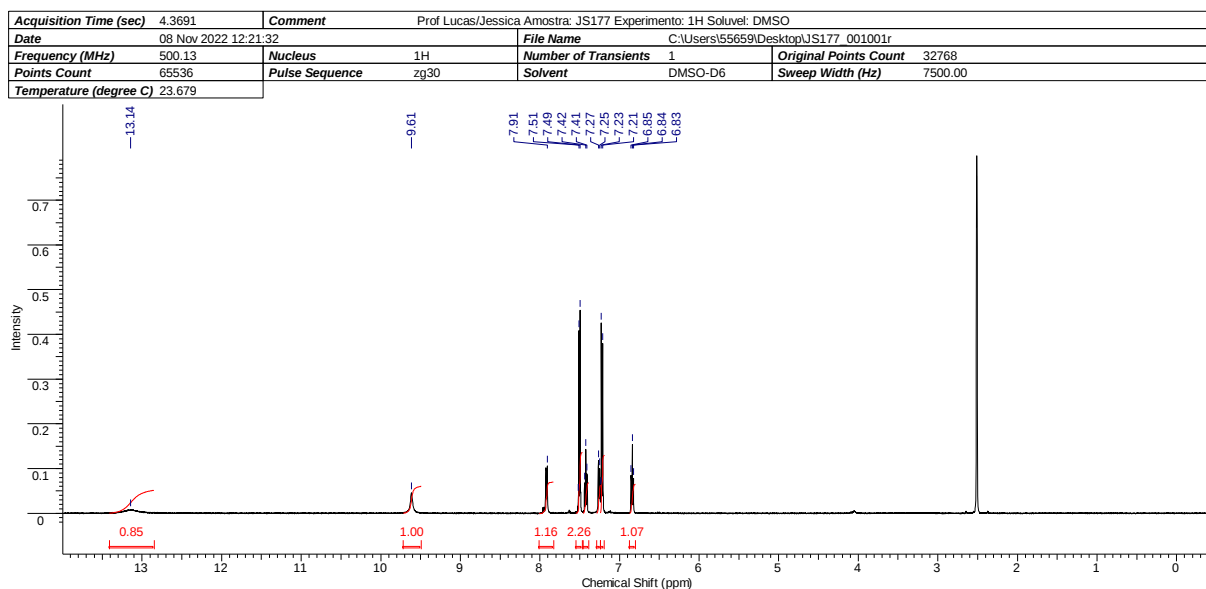


Figure S14. ^1H NMR spectrum (500 MHz, DMSO-d_6) of compound **9c**.

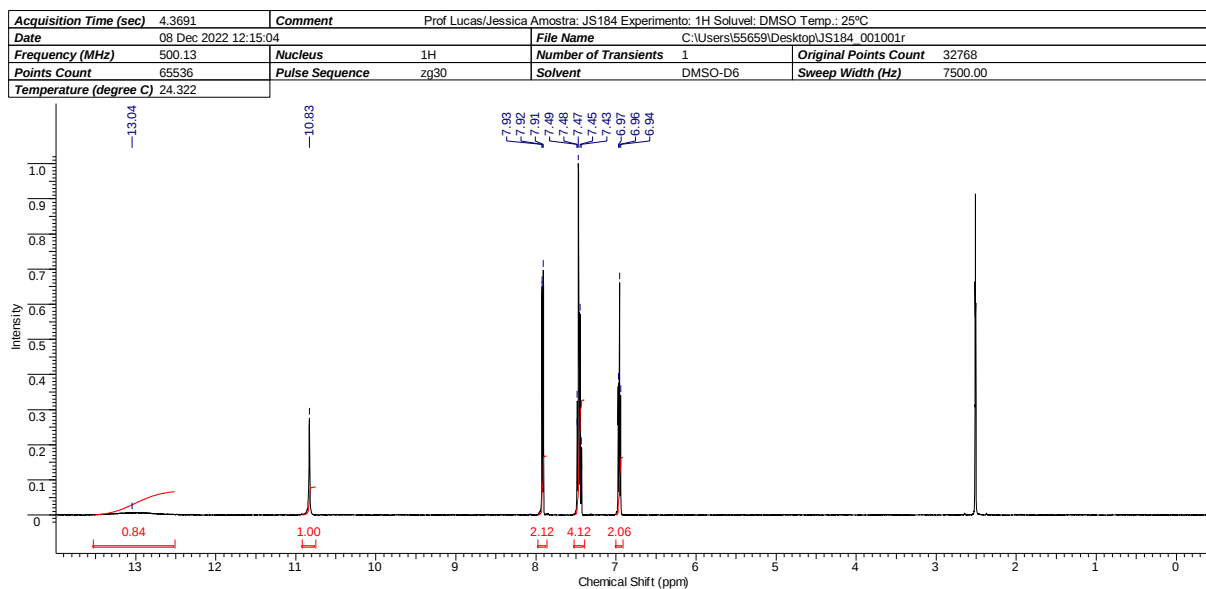


Figure S15. ^1H NMR spectrum (500 MHz, DMSO-d_6) of compound **9d**.

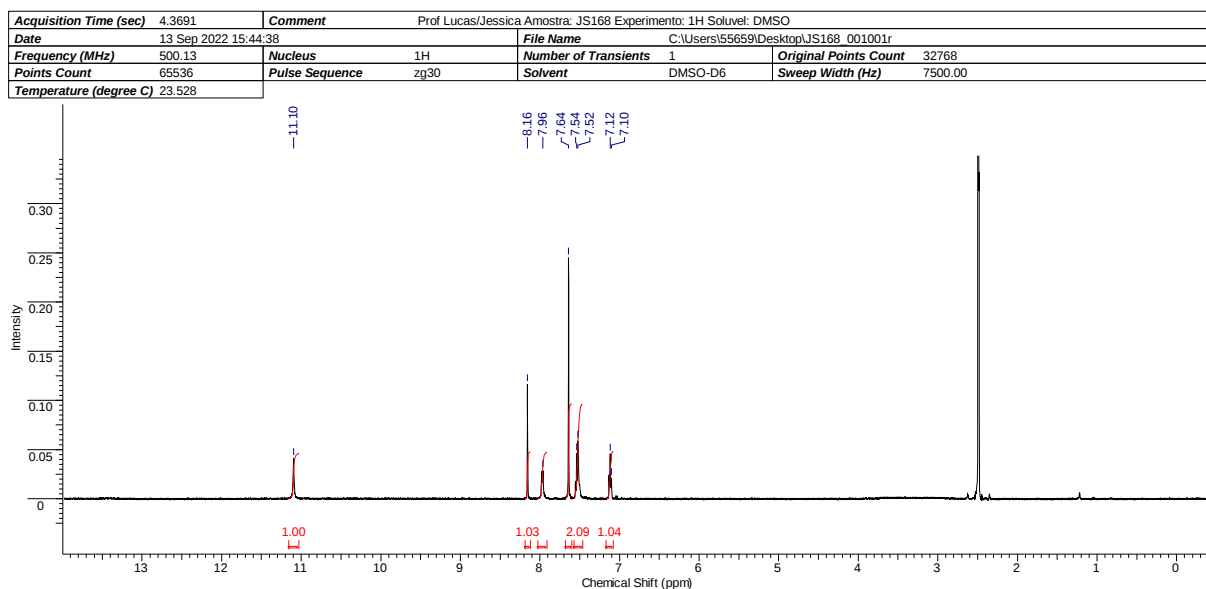


Figure S16. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of compound **9e**.

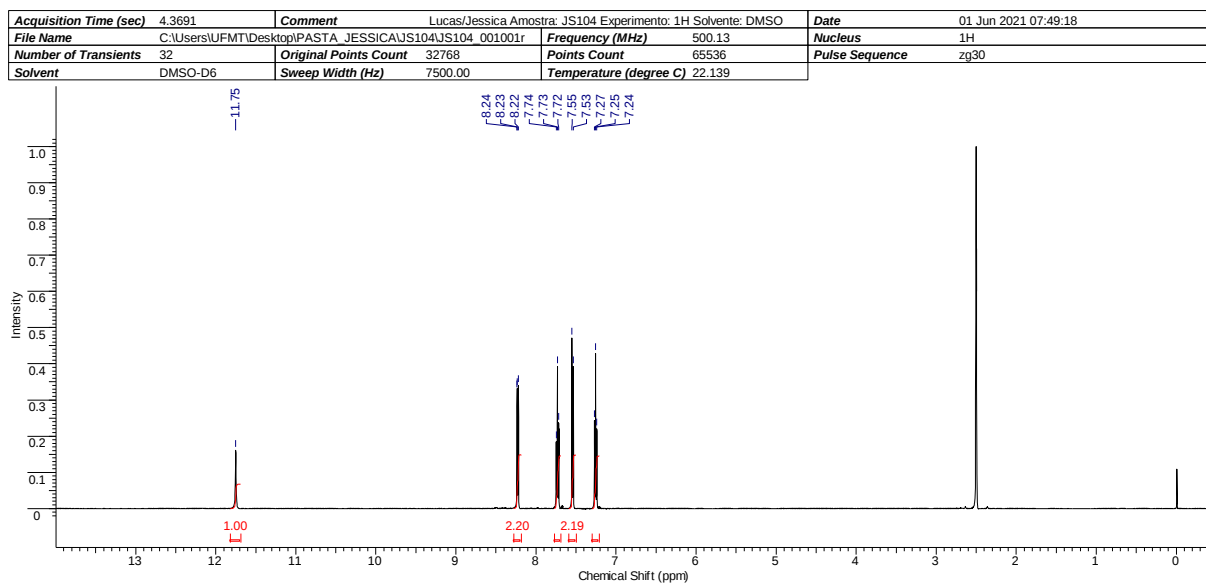


Figure S17. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of compound **10a**.

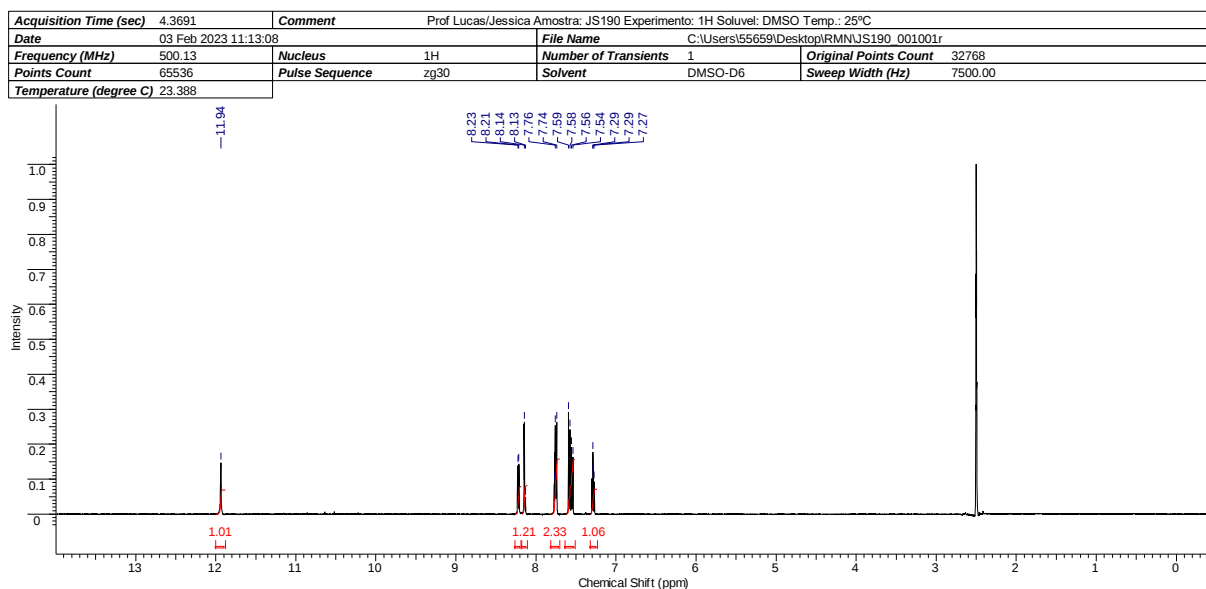


Figure S18. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of compound **10b**.

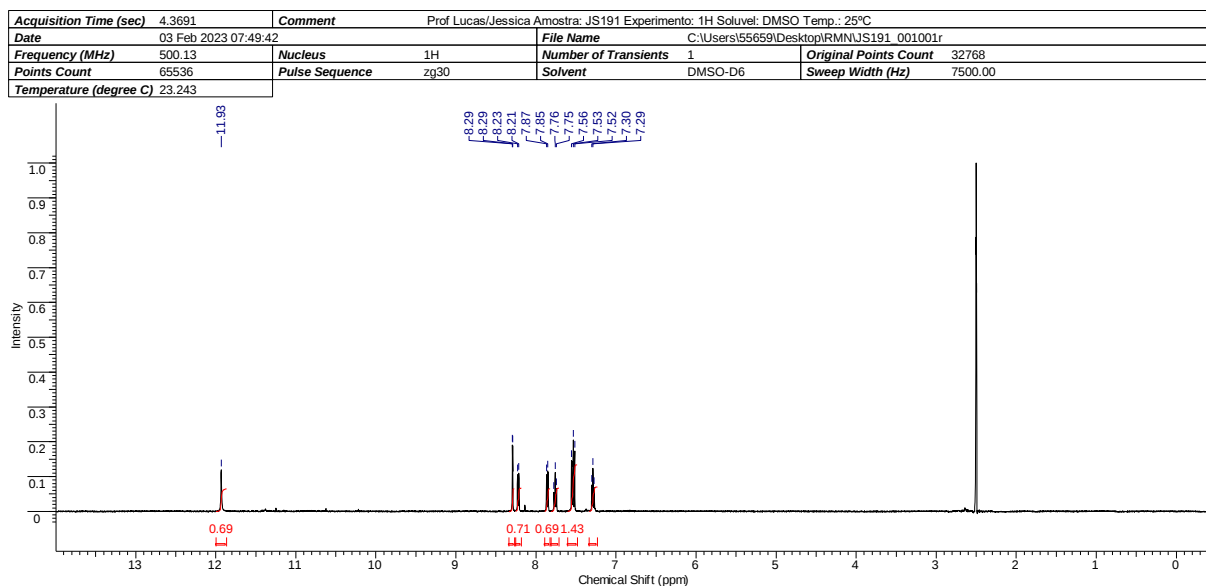


Figure S19. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of compound **10c**.

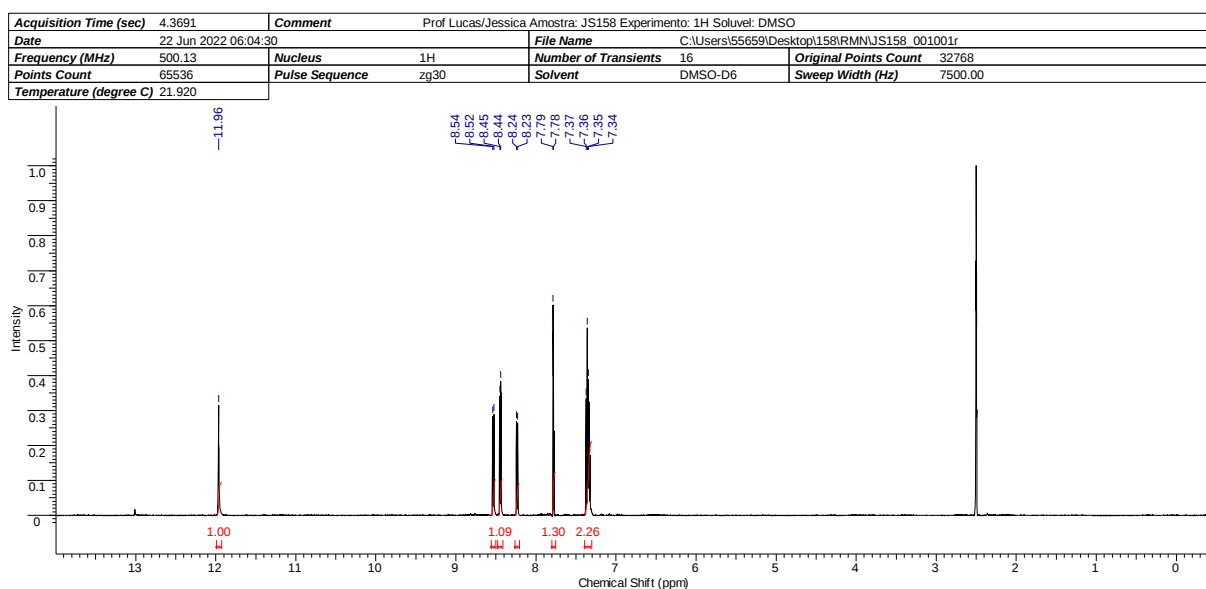


Figure S20. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of compound **10d**.

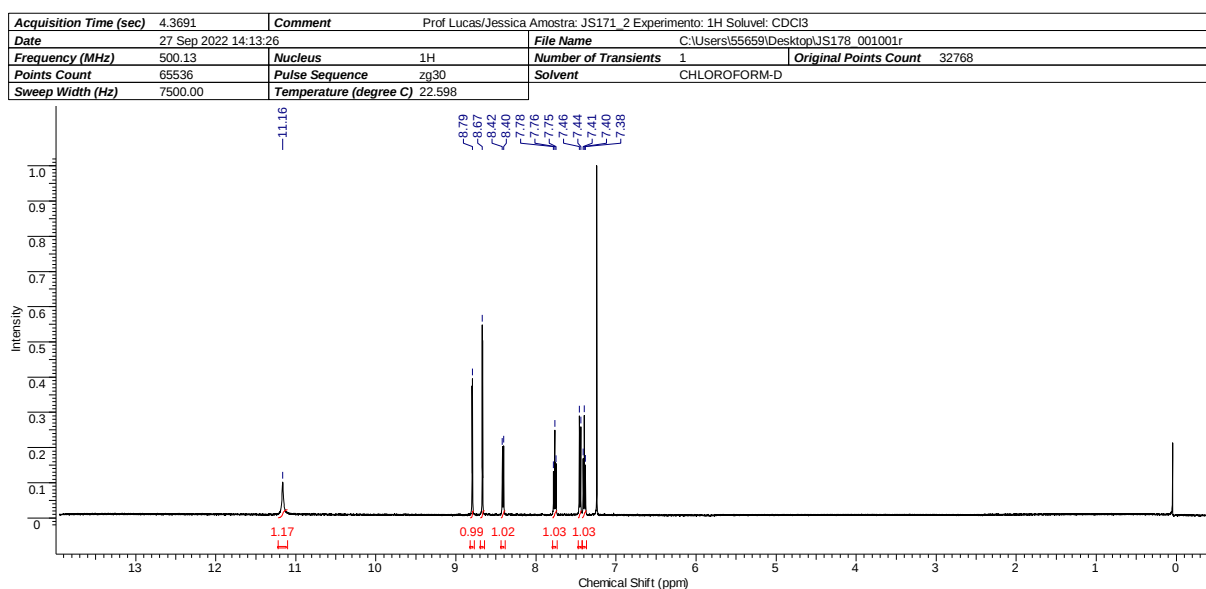


Figure S21. ^1H NMR spectrum (500 MHz, CDCl_3) of compound **10e**.

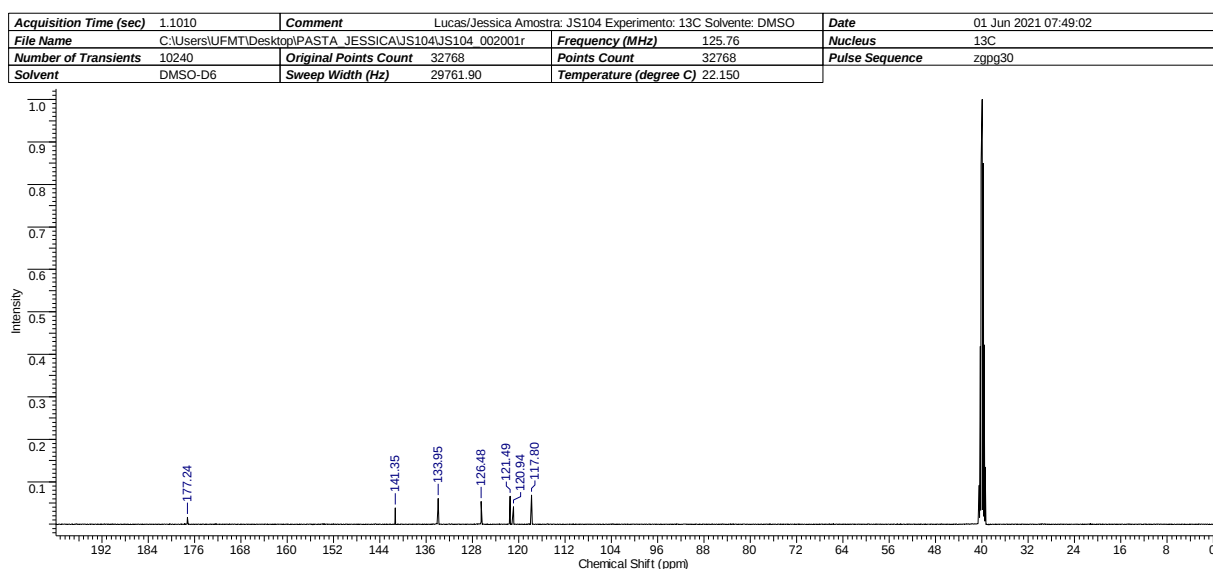


Figure S22. ^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of compound **10a**.

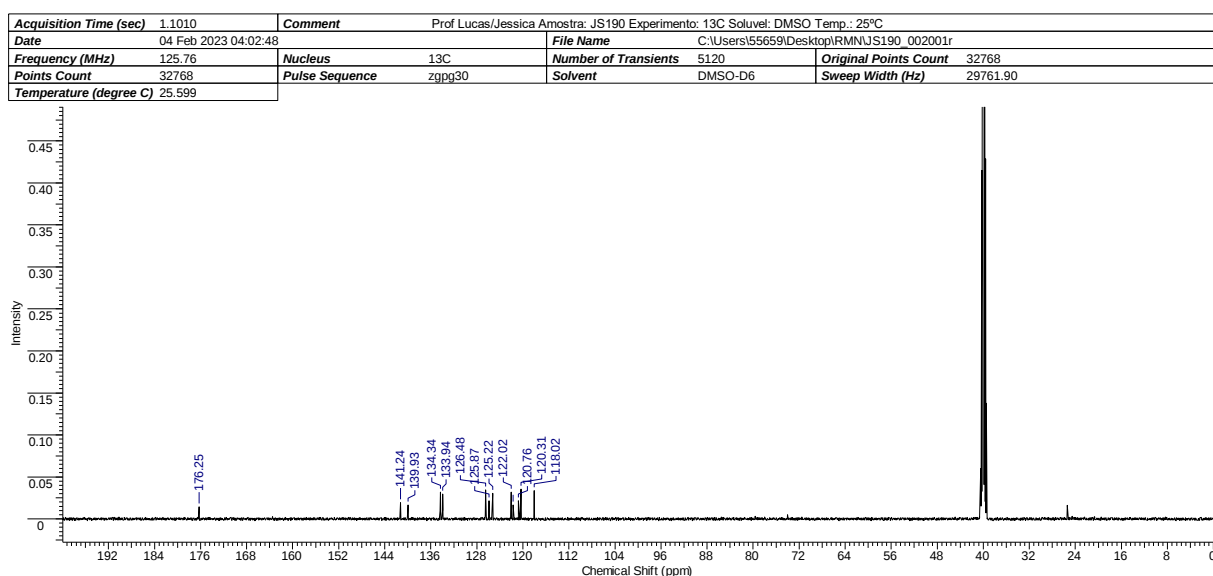


Figure S23. ^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of compound **10b**.

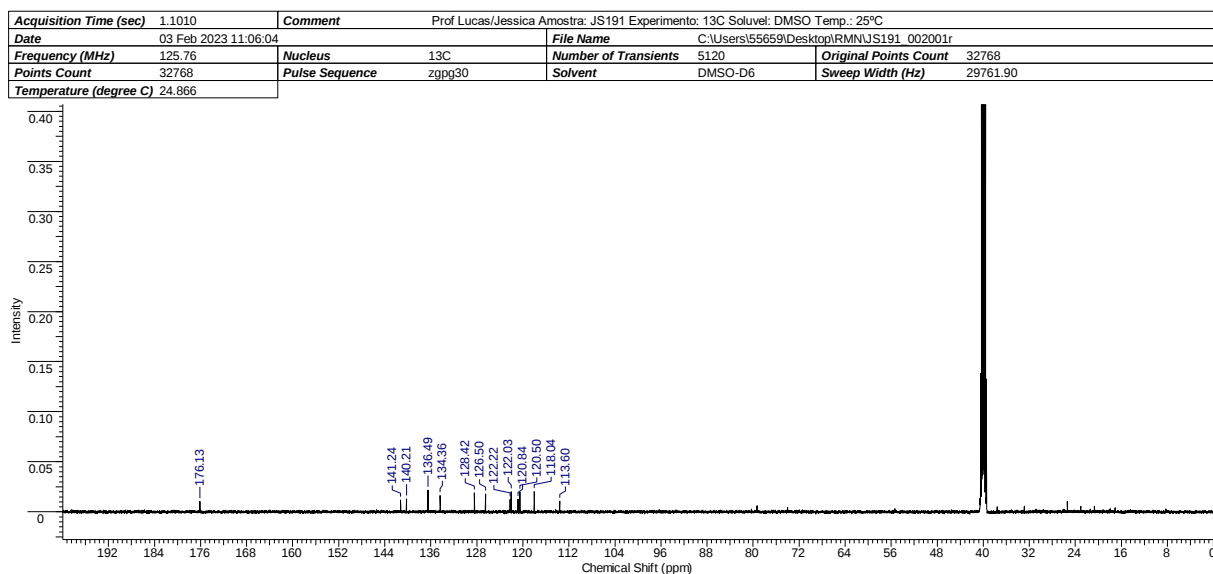


Figure S24. ^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of compound **10c**.

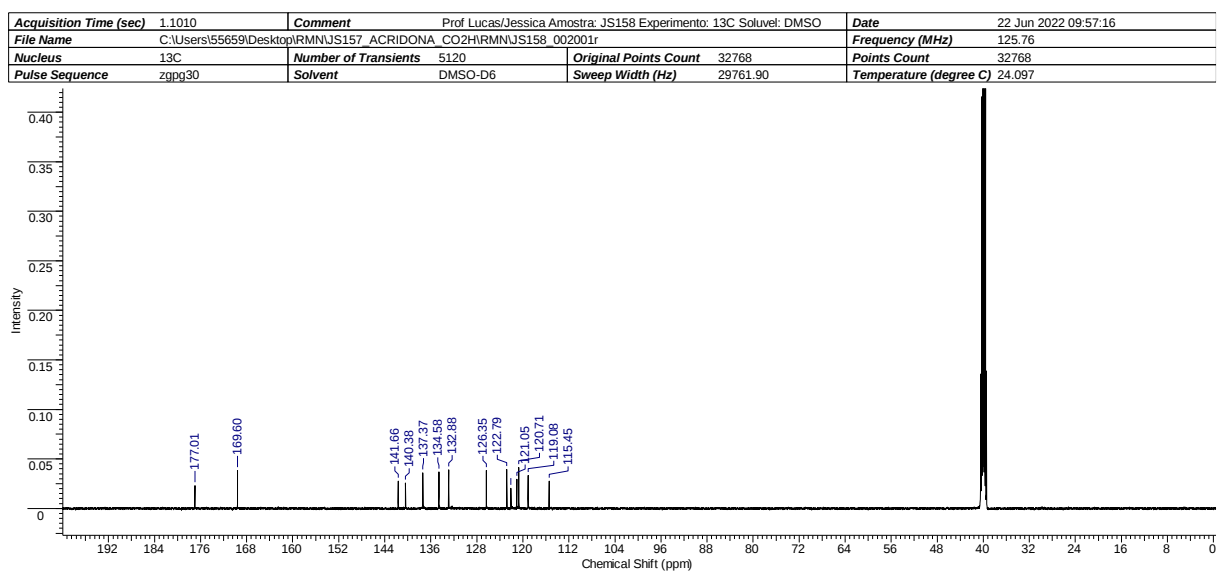


Figure S25. ^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of compound **10d**.

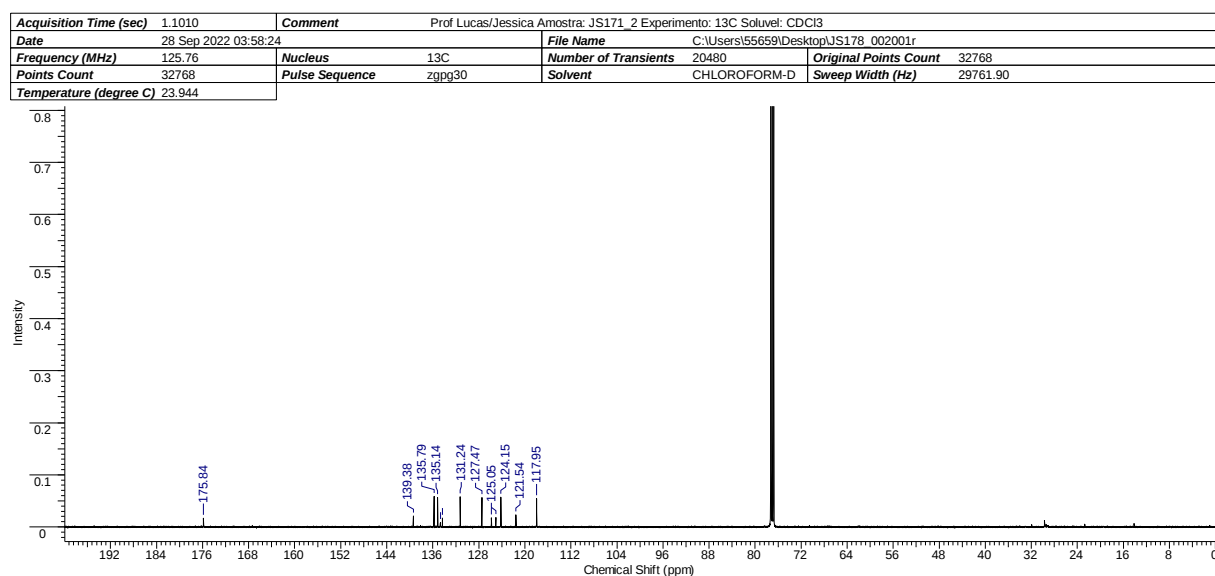


Figure S26. ^{13}C NMR spectrum (125 MHz, CDCl_3) of compound **10e**.

FTIR spectra of compounds **10a-10e**

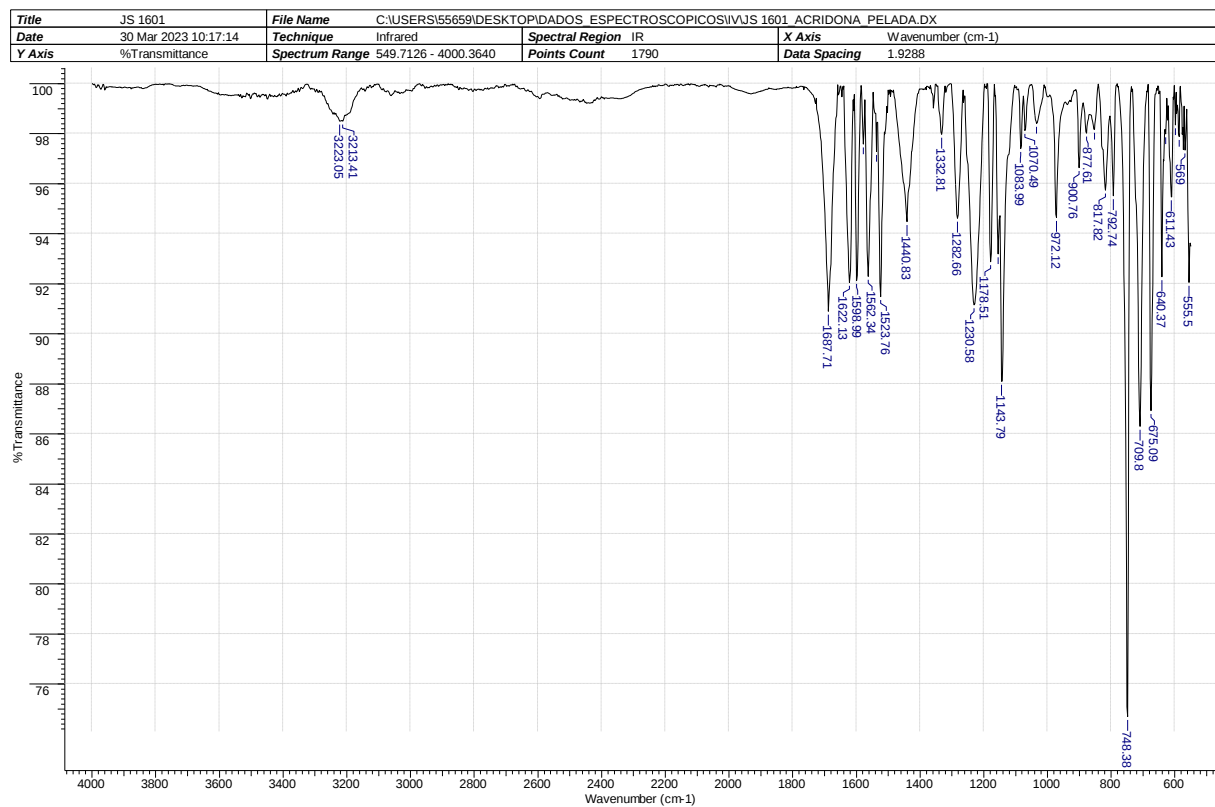


Figure S27. FTIR (KBr) spectrum of compound **10a**.

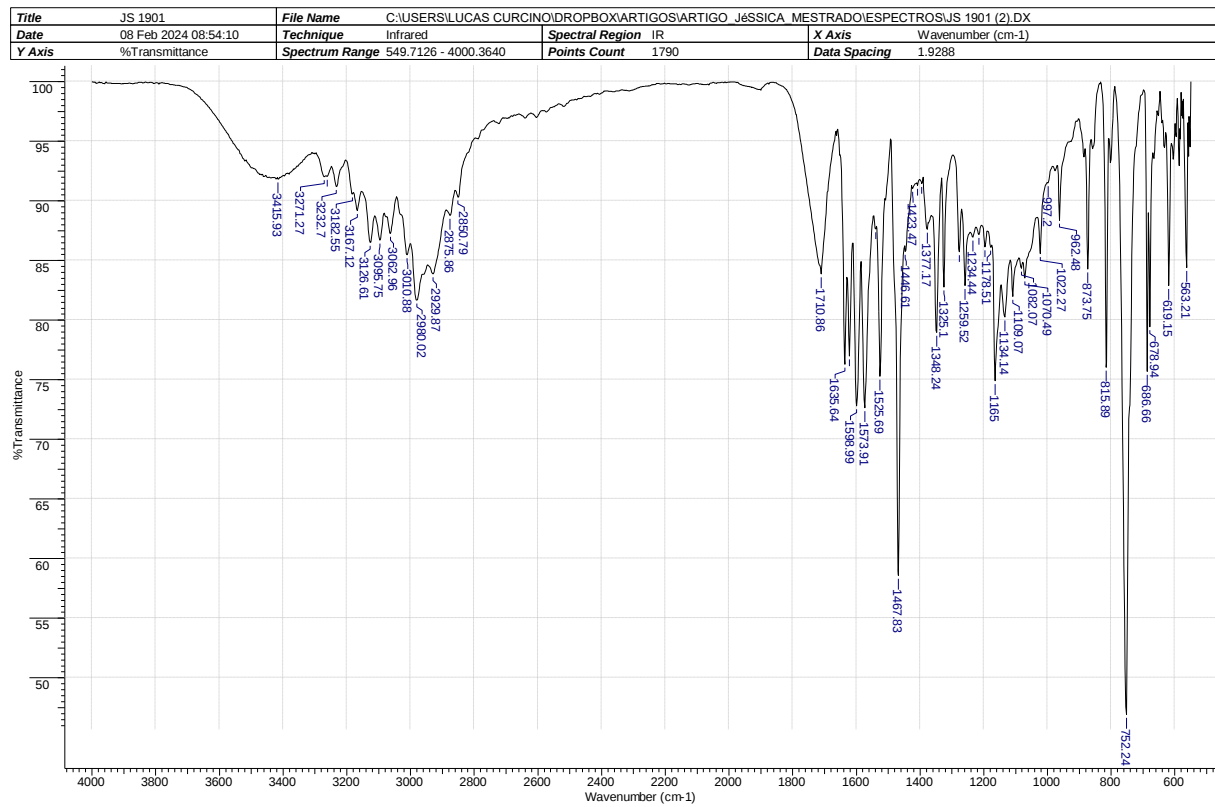


Figure S28. FTIR (KBr) spectrum of compound **10b**.

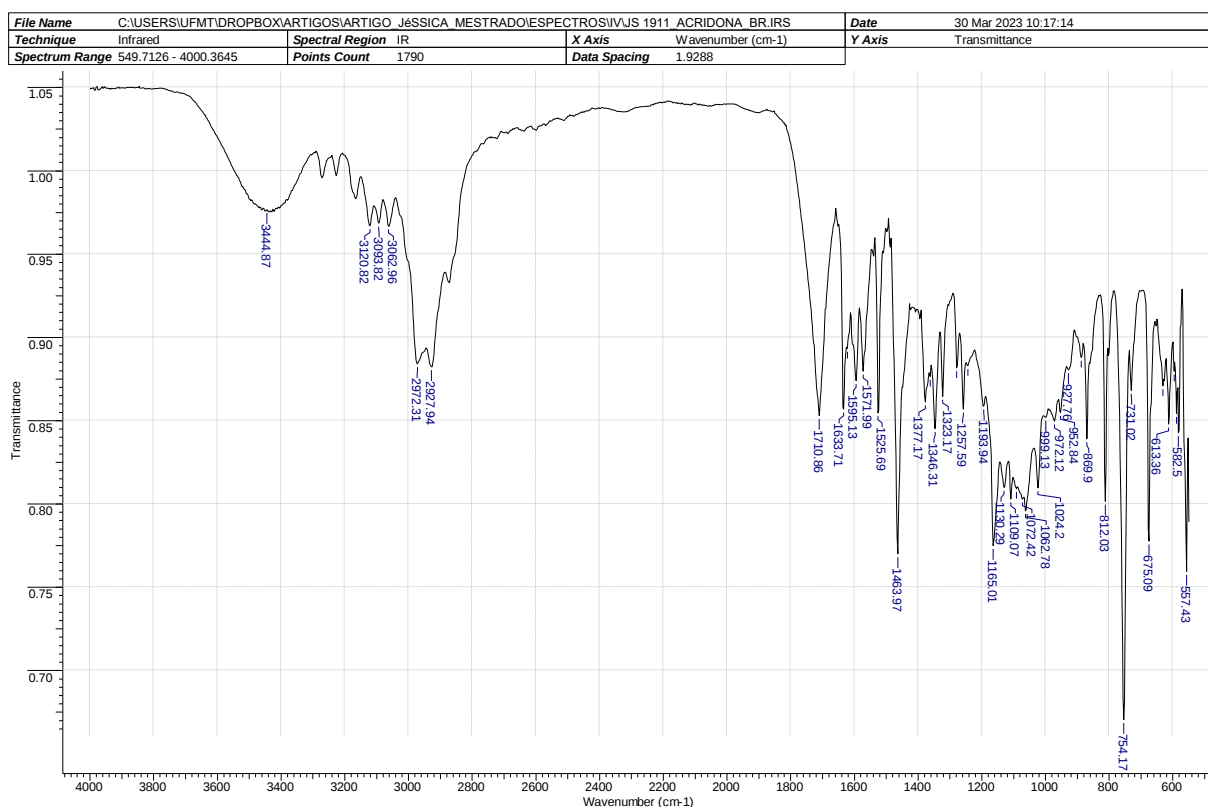


Figure S29. FTIR (KBr) spectrum of compound **10c**.

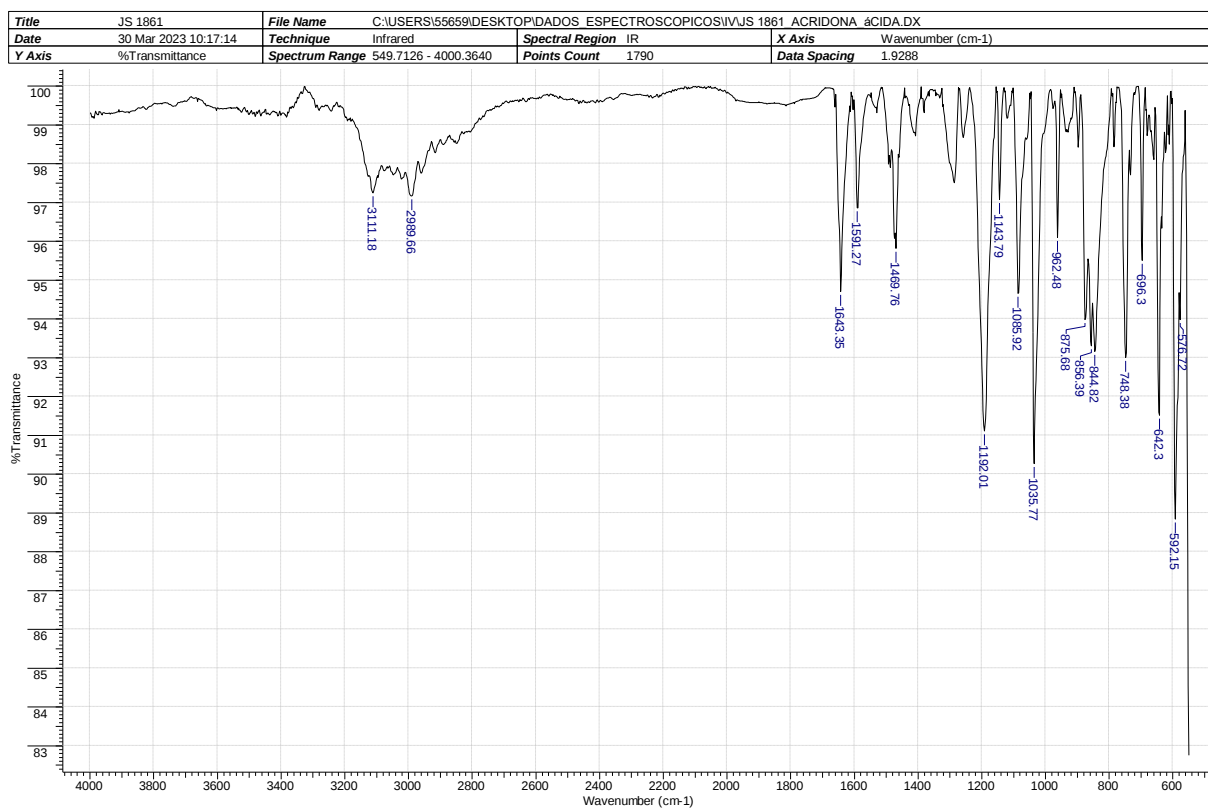


Figure S30. FTIR (KBr) spectrum of compound **10d**.

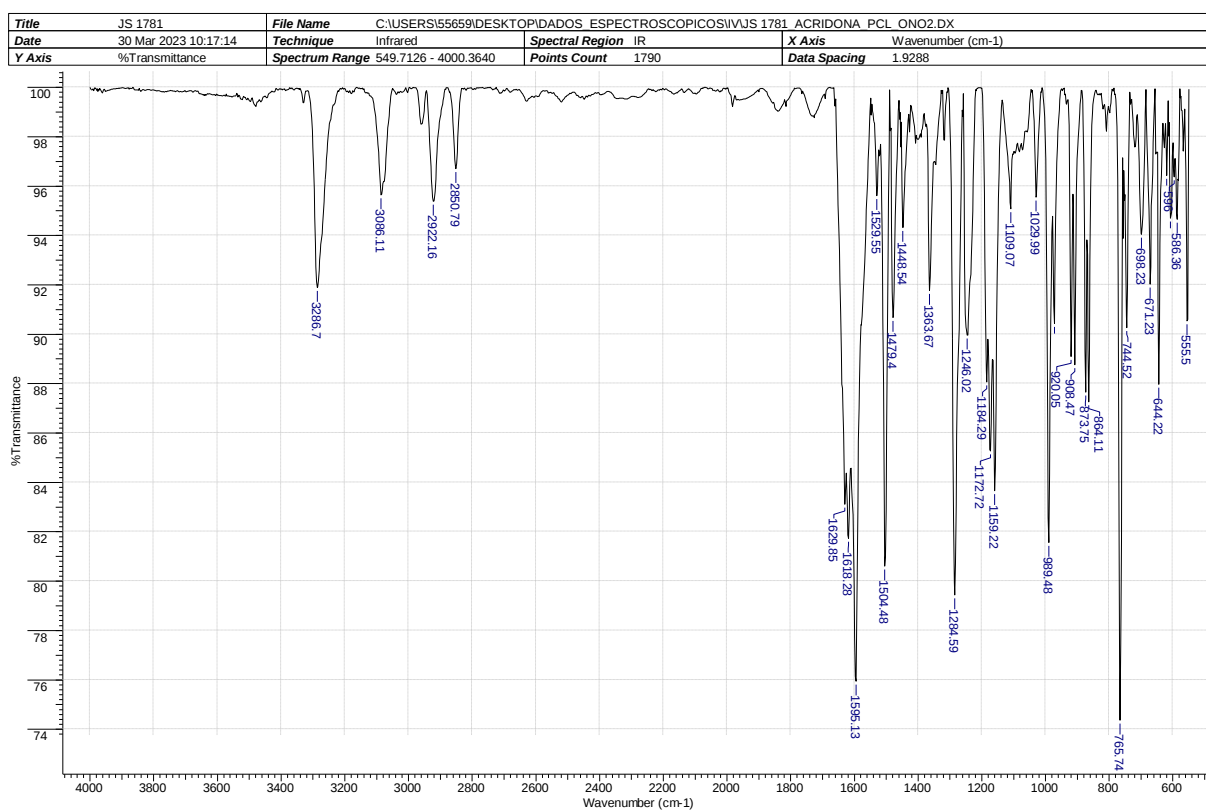


Figure S31. FTIR (KBr) spectrum of compound **10e**.