Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Hybrid Dihydropyrimidinones as Dual-Functional Bioactive Molecules: Fluorescent Probes and Cytotoxic Agents to Cancer Cells

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Supplementary Information

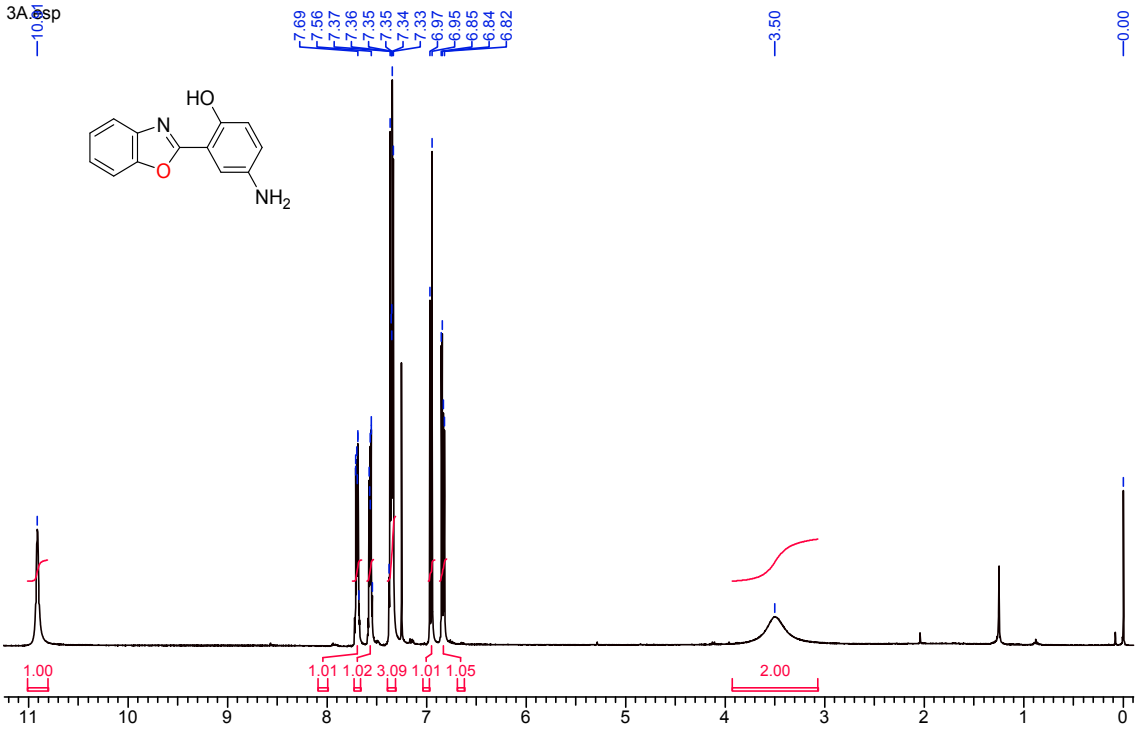


Figure S1. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3a**.

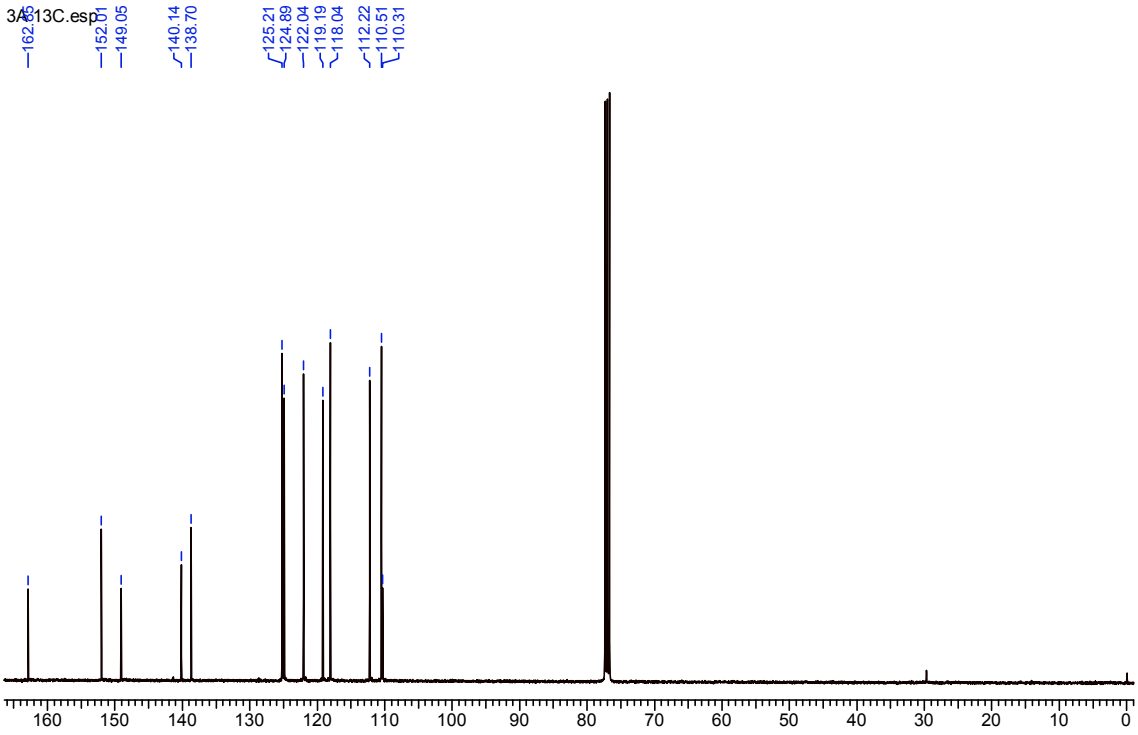


Figure S2. ^{13}C NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3a**.

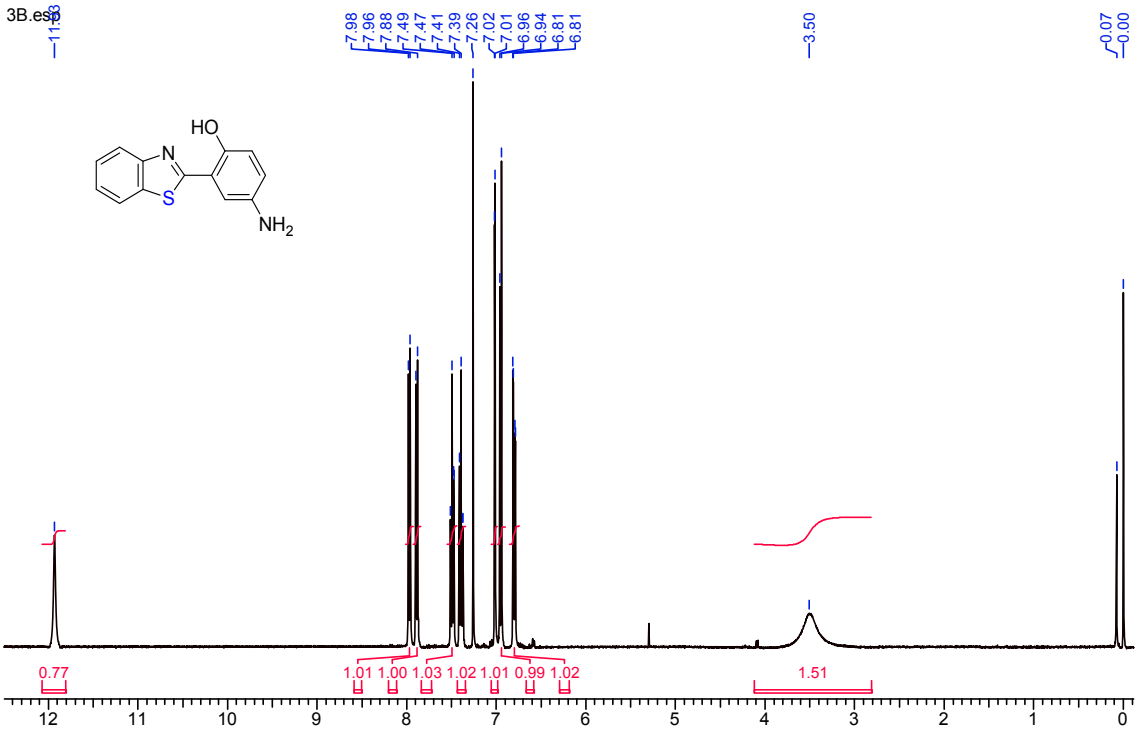


Figure S3. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3b**.

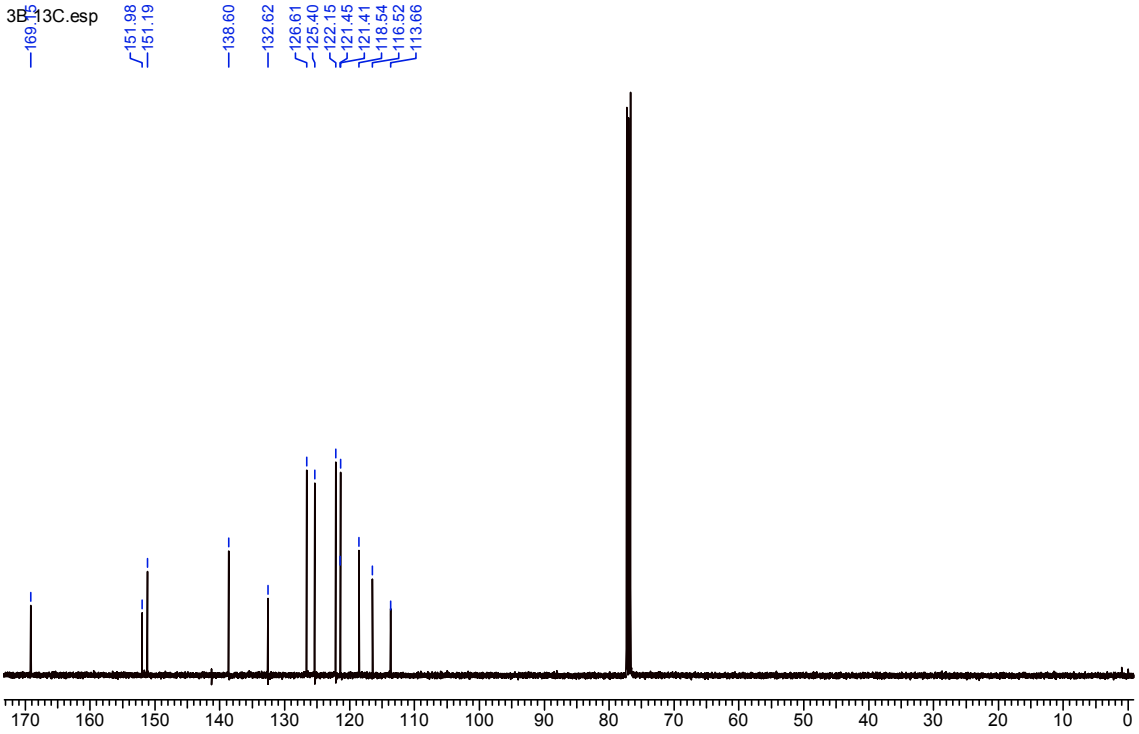


Figure S4. ^{13}C NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3b**.

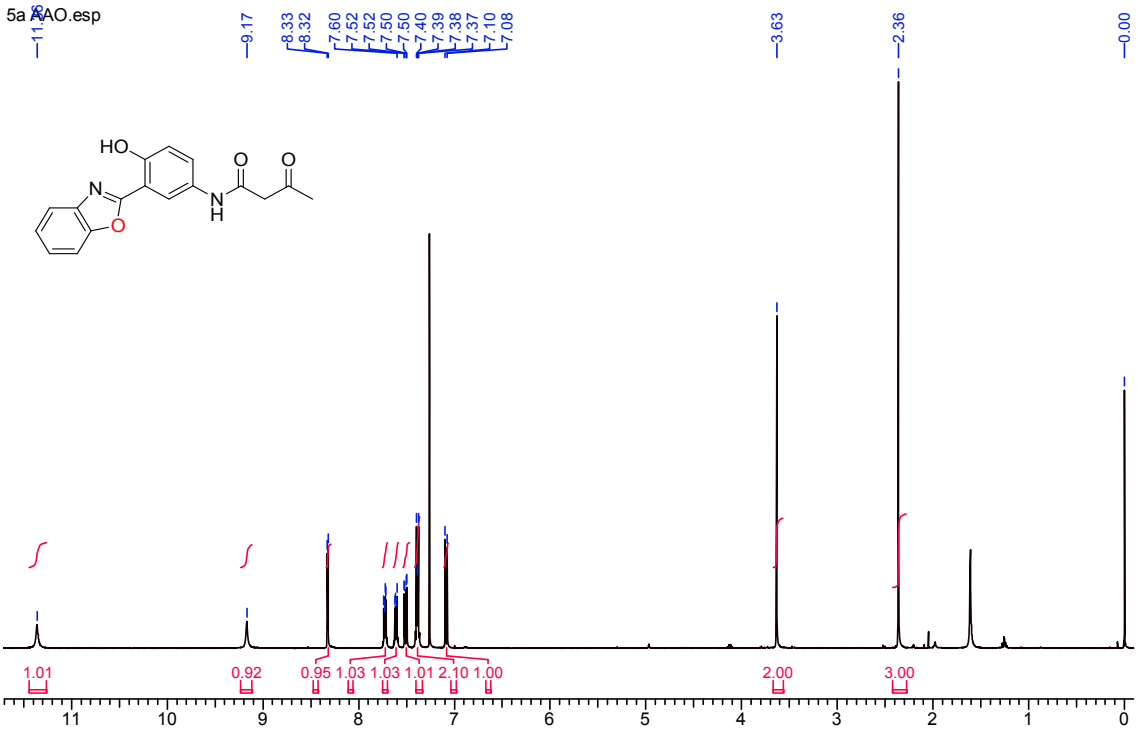


Figure S5. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **5a**.

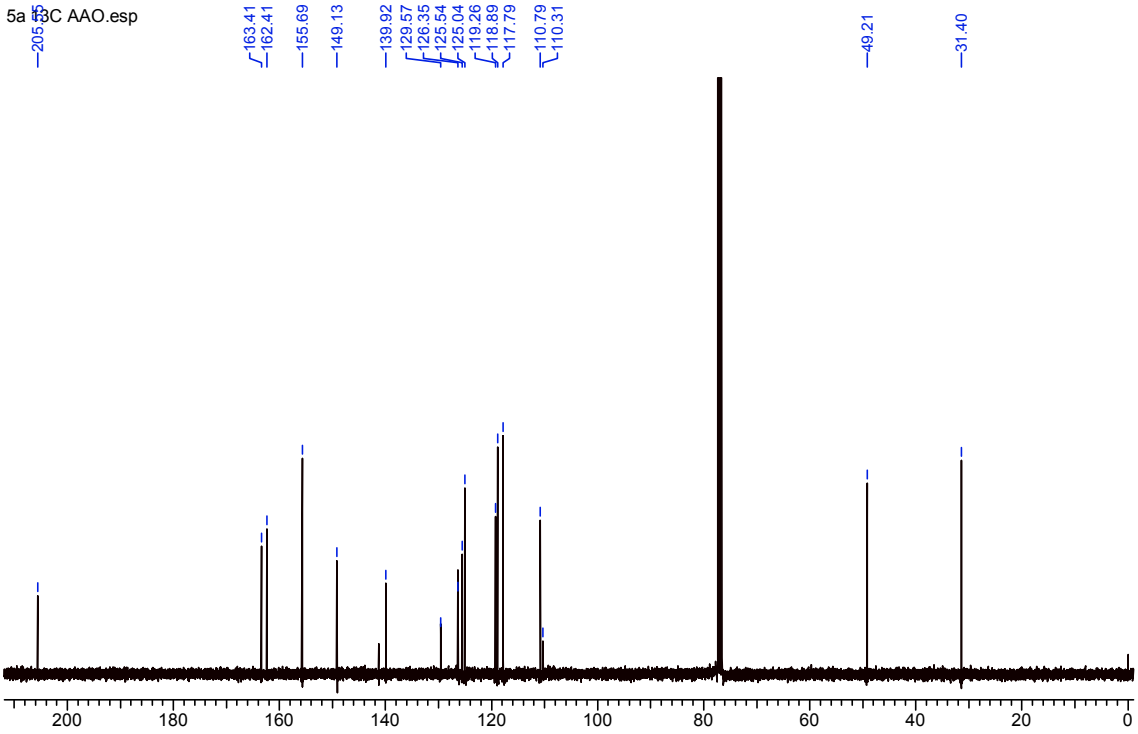


Figure S6. ^{13}C NMR Spectrum (400 MHz, $CDCl_3$) of Compound **5a**.

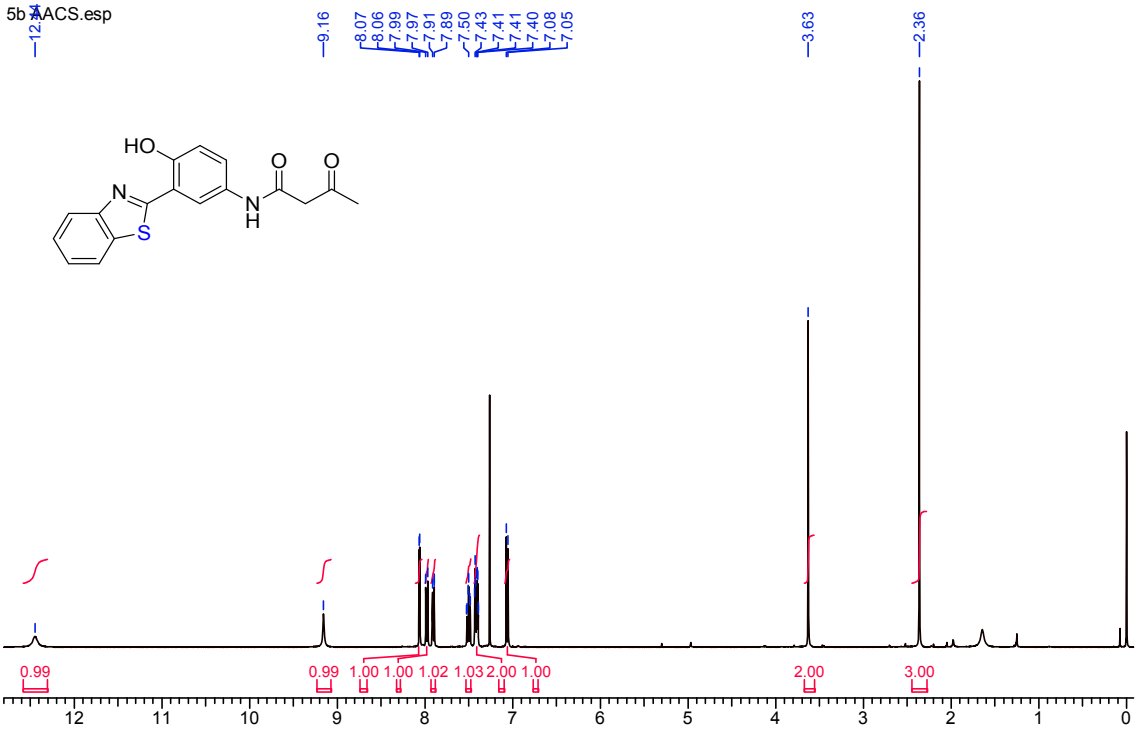


Figure S7. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **5b**.

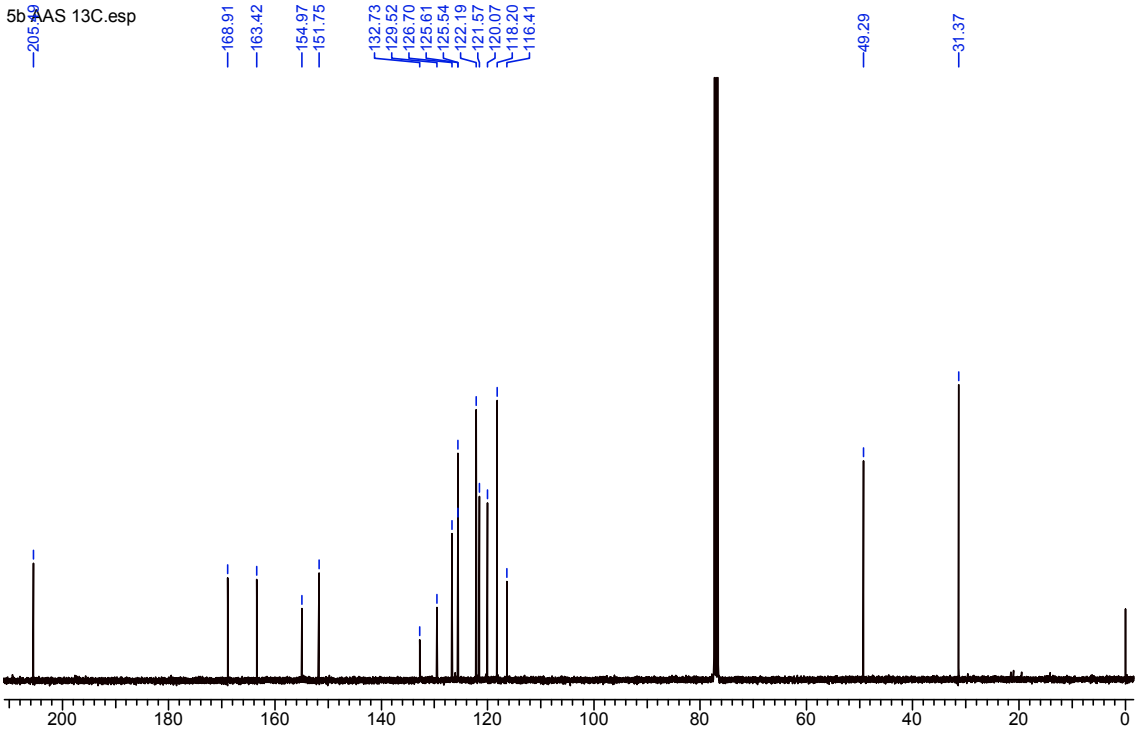


Figure S8. ^{13}C NMR Spectrum (400 MHz, $CDCl_3$) of Compound **5b**.

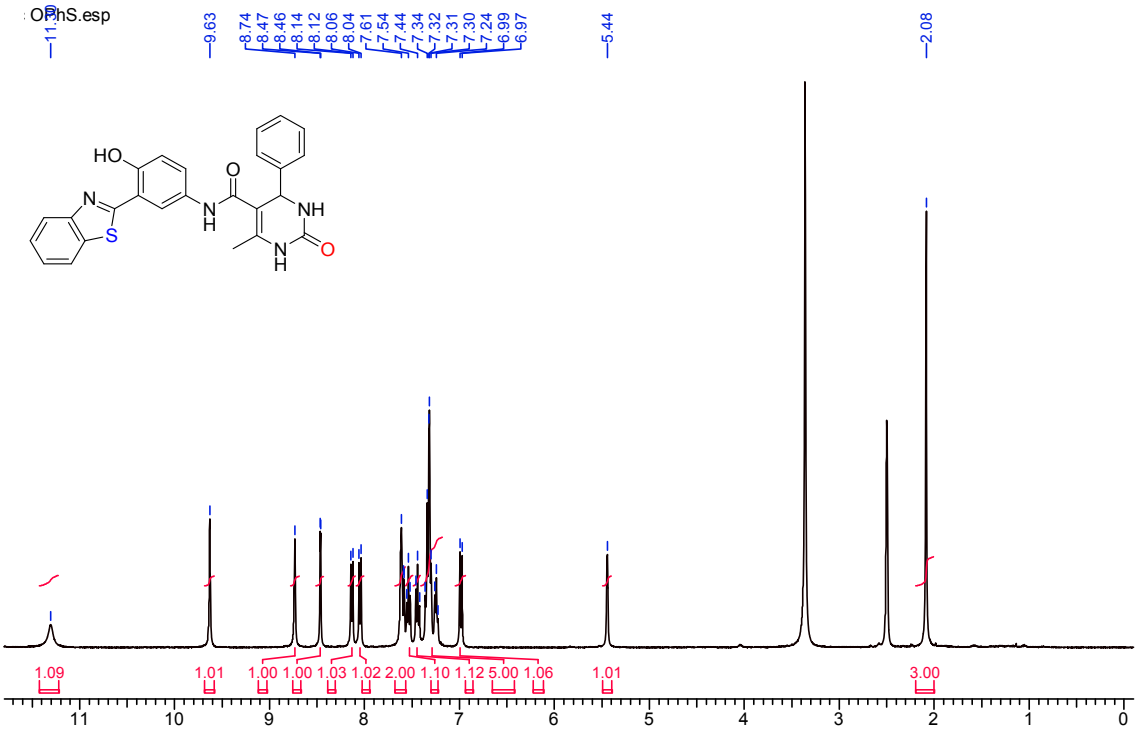


Figure S9. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8a**.

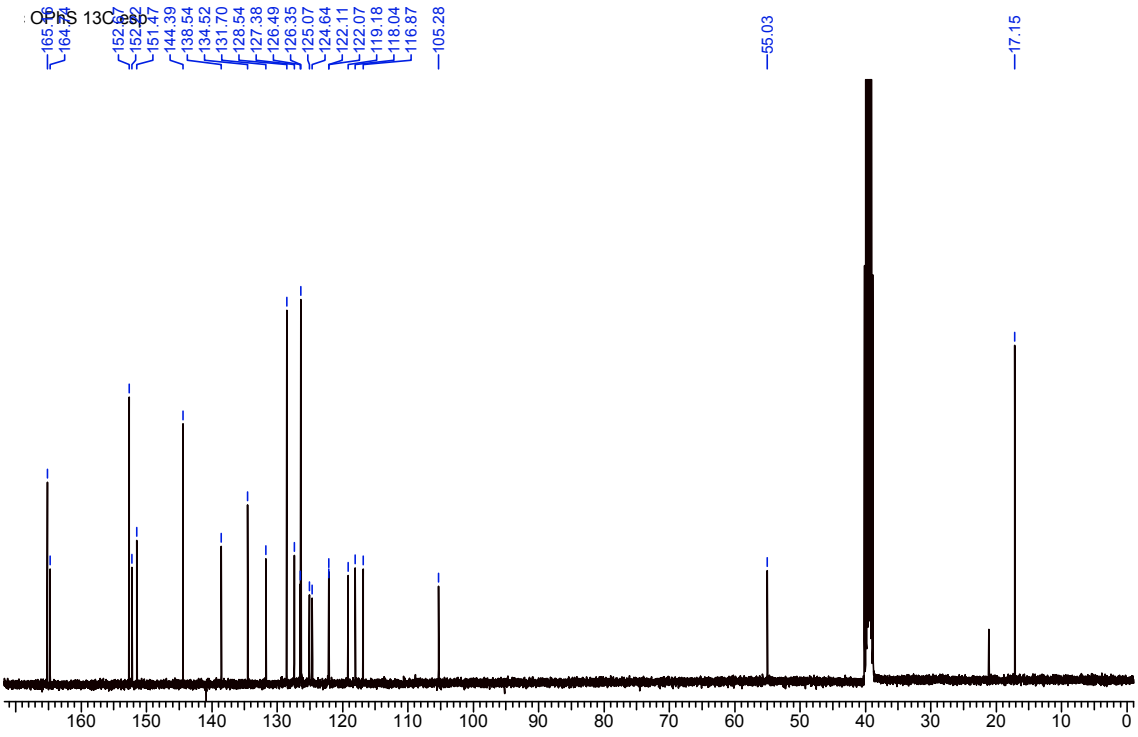


Figure S10. ^{13}C NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8a**.

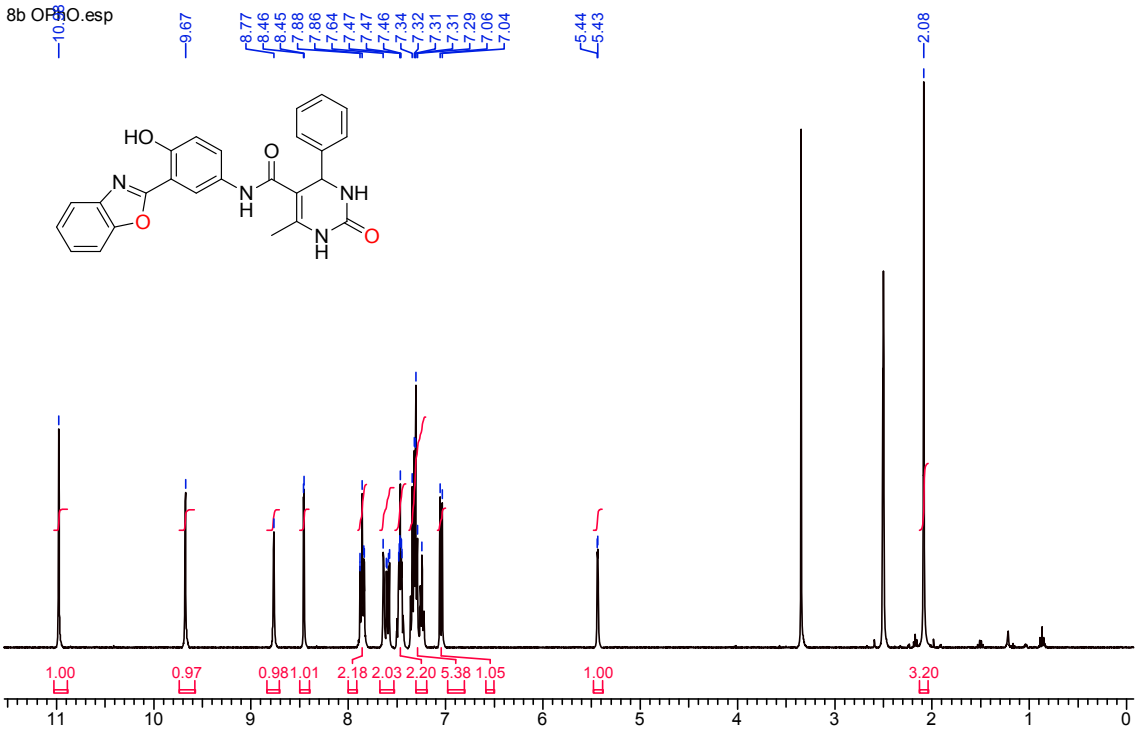


Figure S11. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8b**.

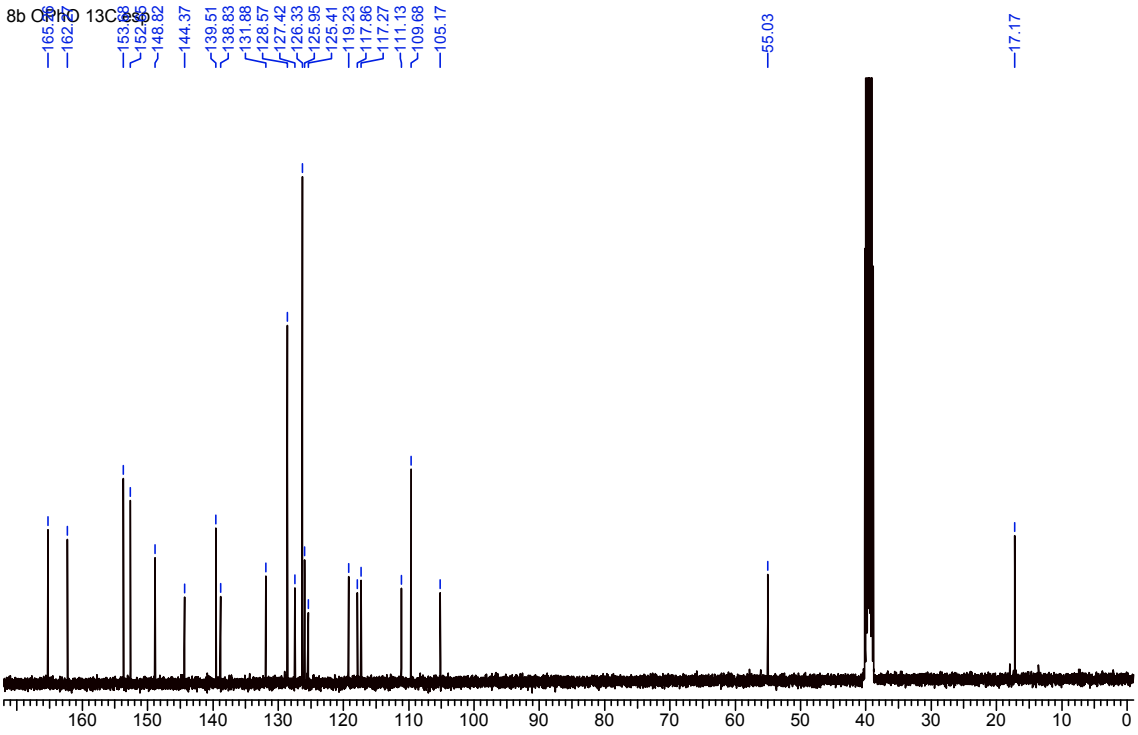


Figure S12. ^{13}C NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8b**.

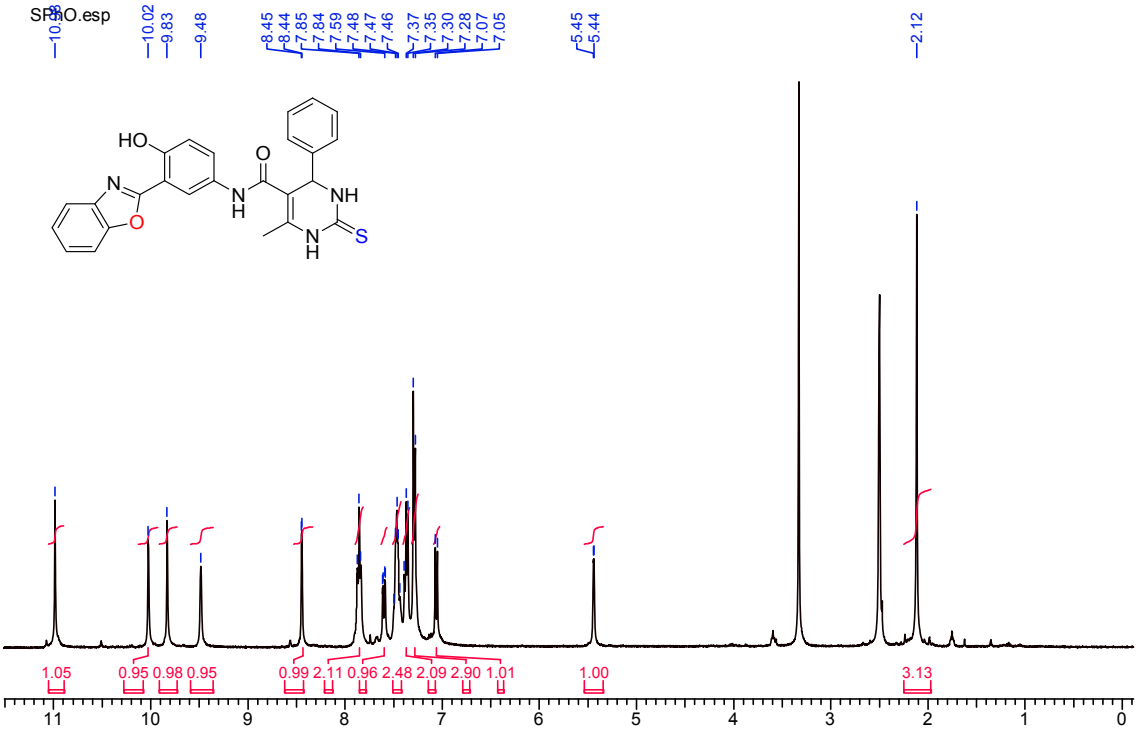


Figure S13. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8c**.

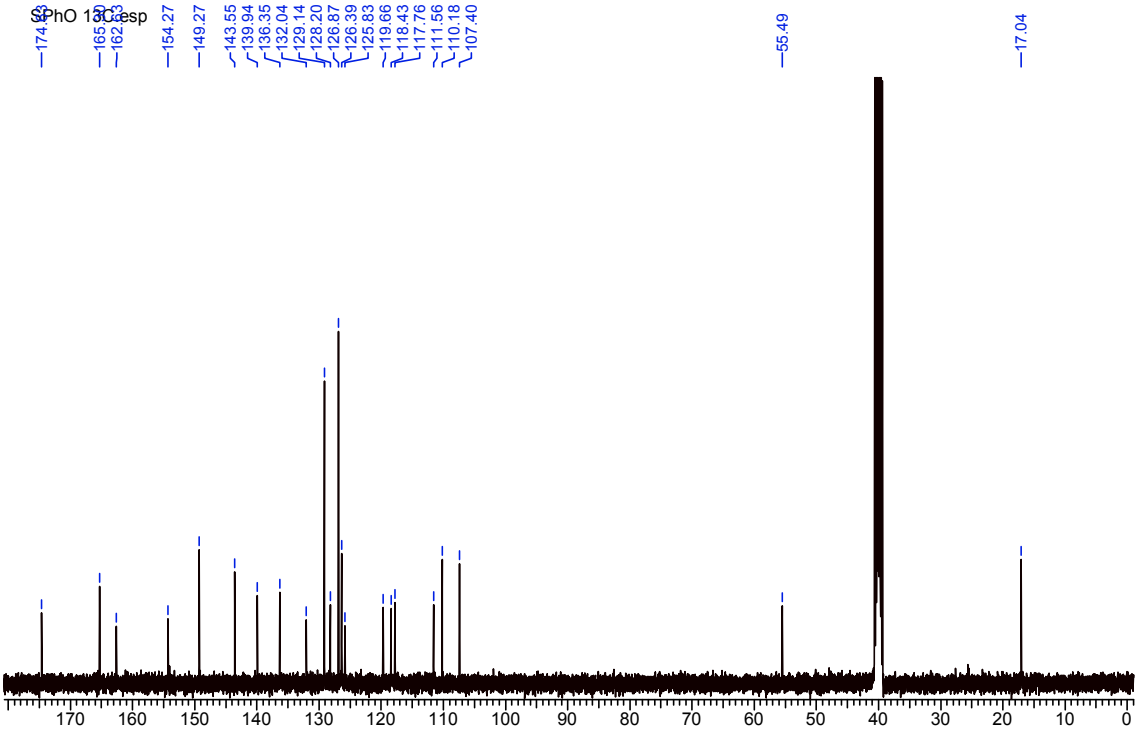


Figure S14. ^{13}C NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8c**.

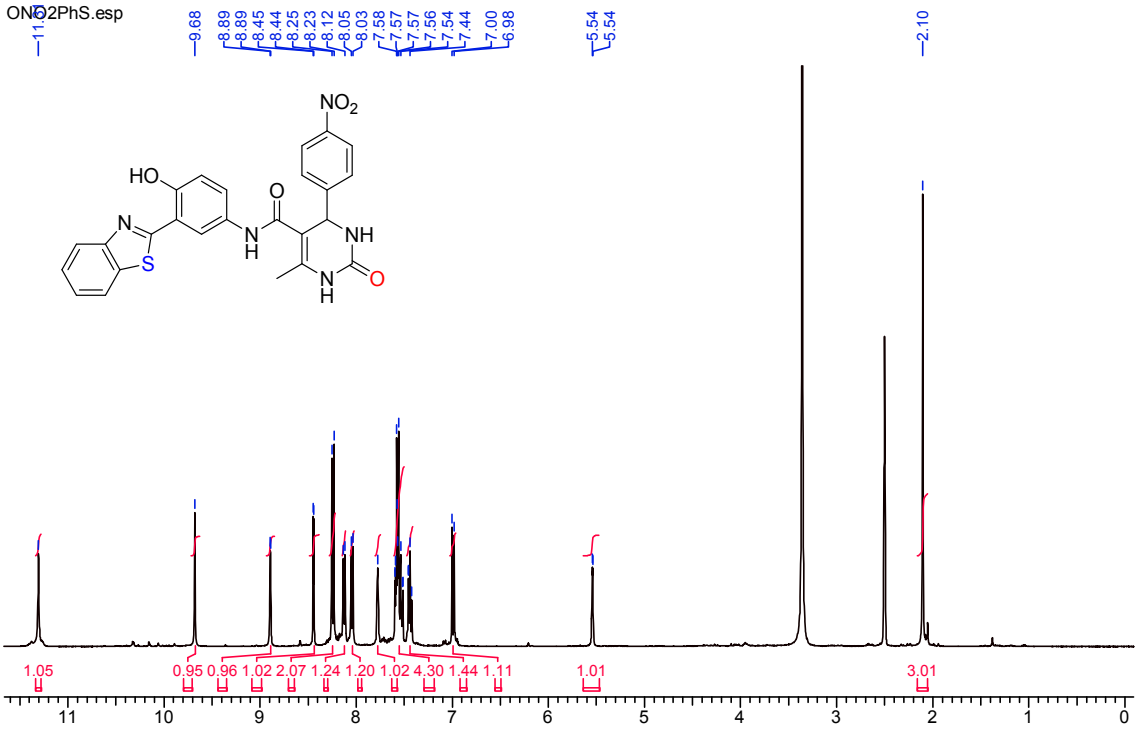


Figure S15. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8d**.

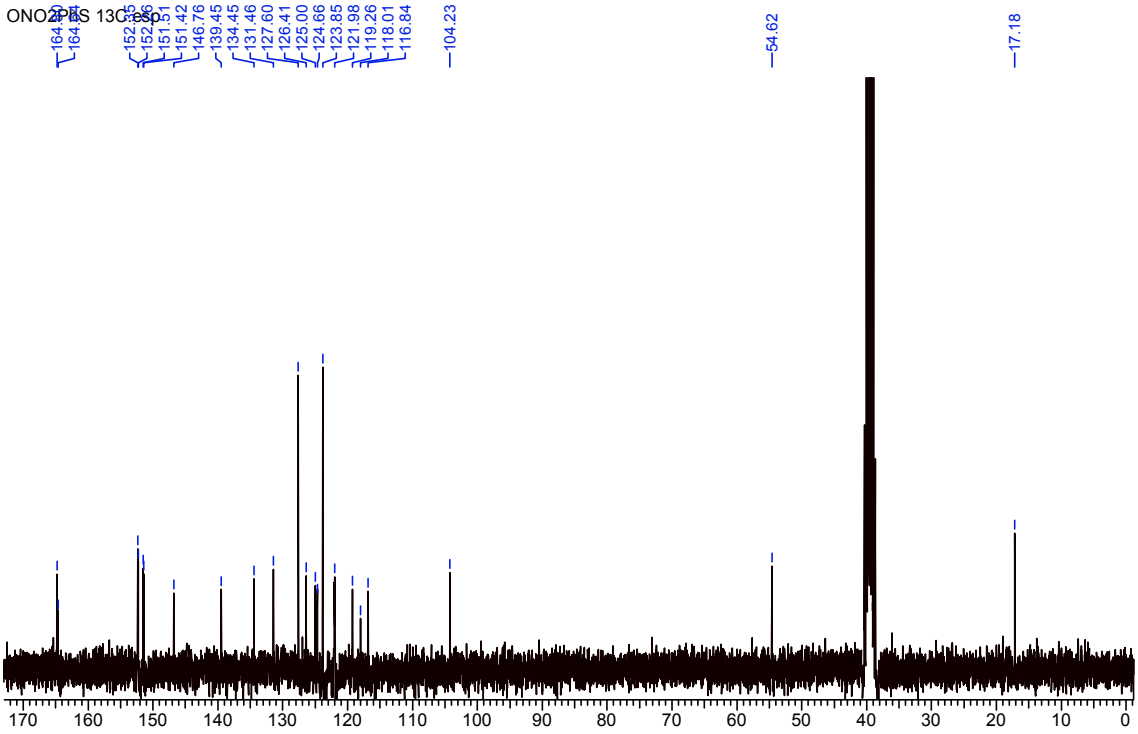


Figure S16. ^{13}C NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8d**.

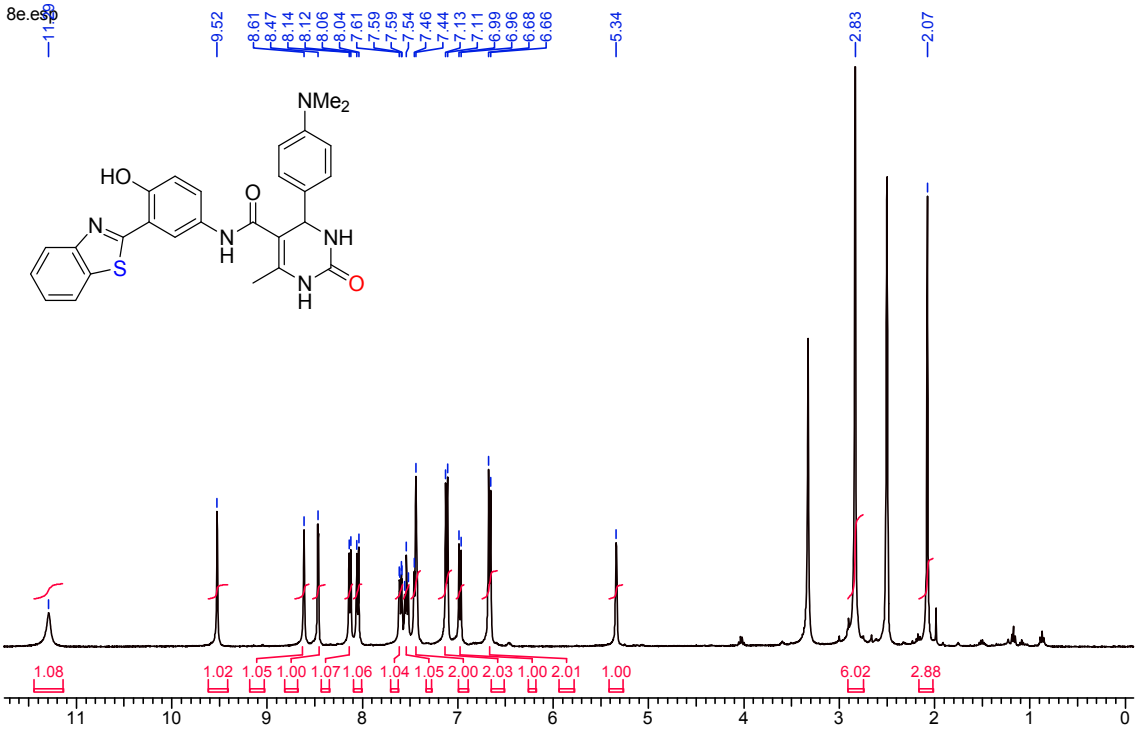


Figure S17. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8e**.

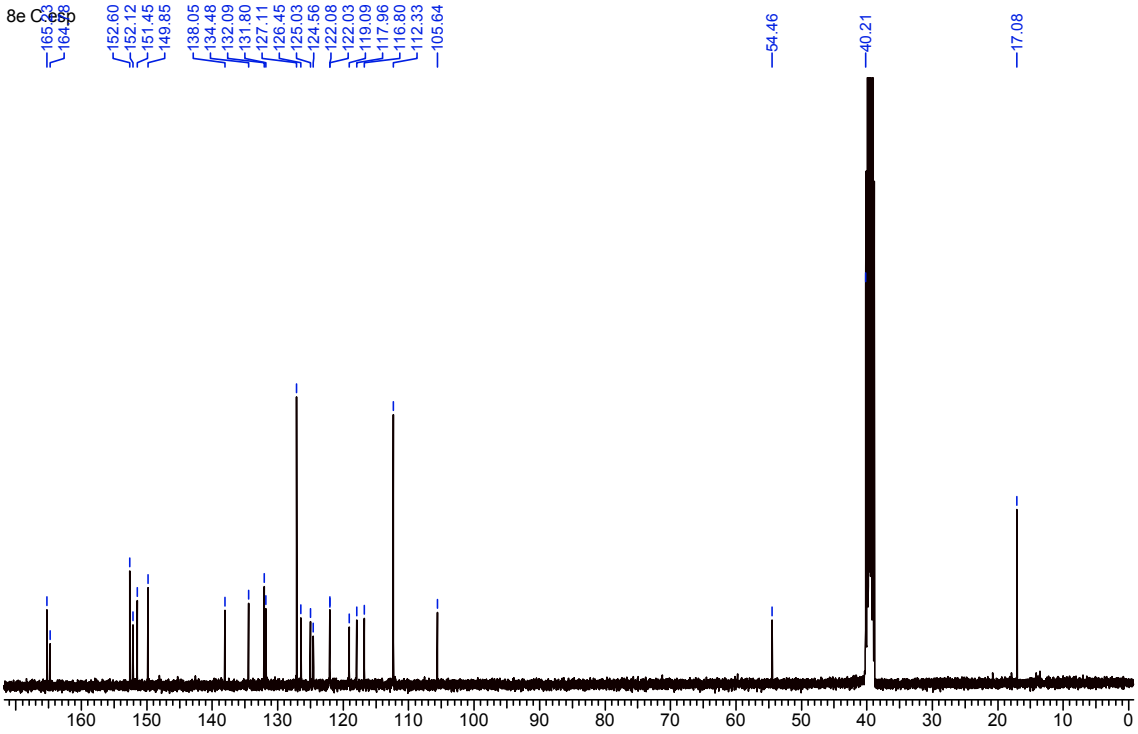


Figure S18. ^{13}C NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8e**.

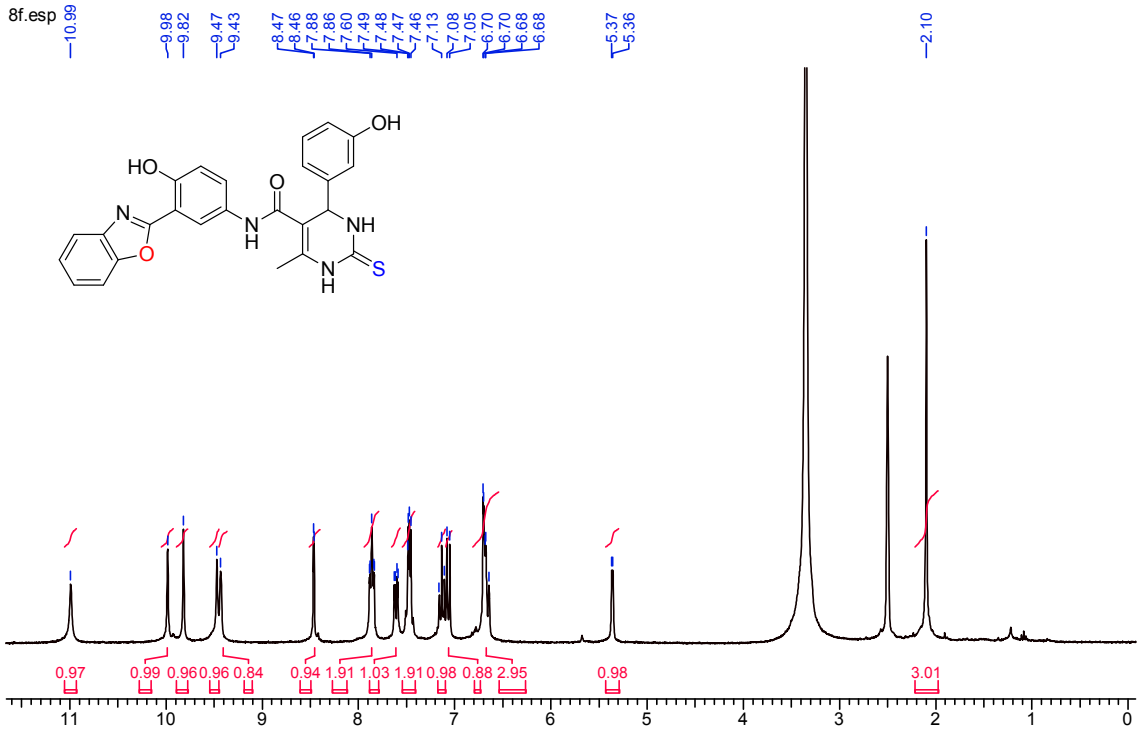


Figure S19. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8f**.

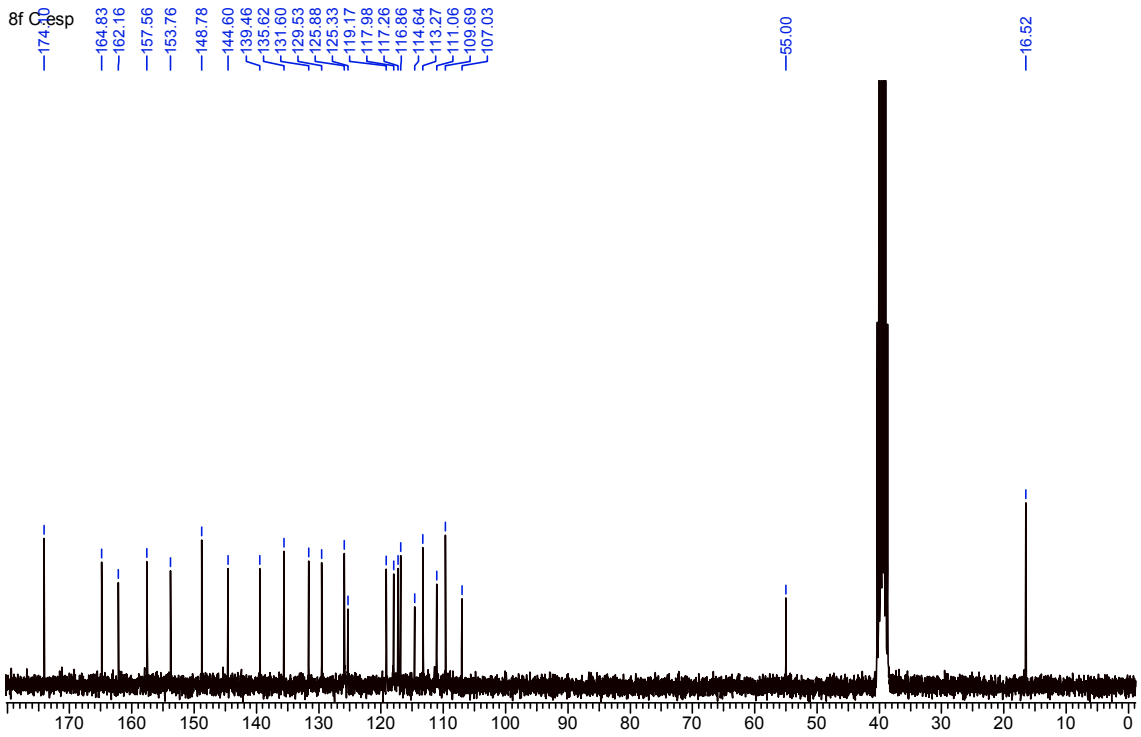


Figure S20. ^{13}C NMR Spectrum (400 MHz, DMSO-d_6) of Compound **8f**.

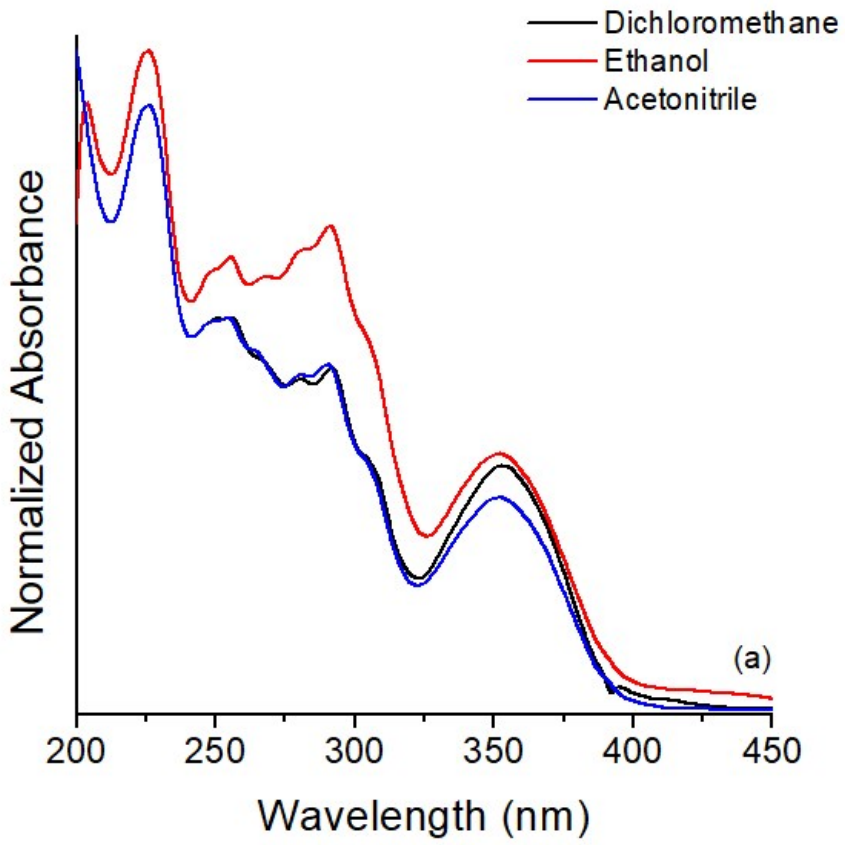


Figure S21. Normalized UV-Vis absorption spectra of compound **5b** (a) **i**n different organic solvents [10^{-5}M].

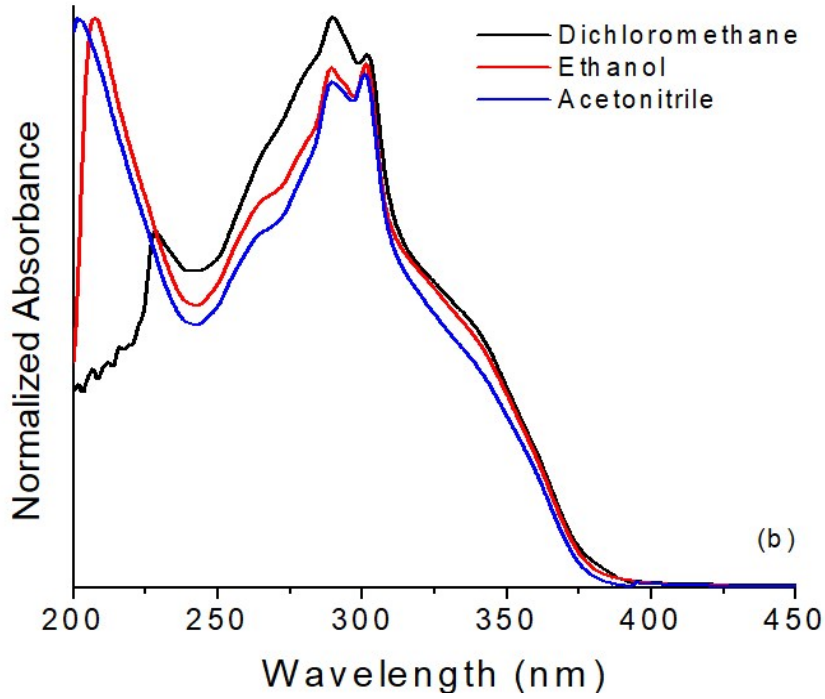


Figure S22. Normalized UV-Vis absorption spectra of compound **8c** (b) **i**n different organic solvents [10^{-5}M].

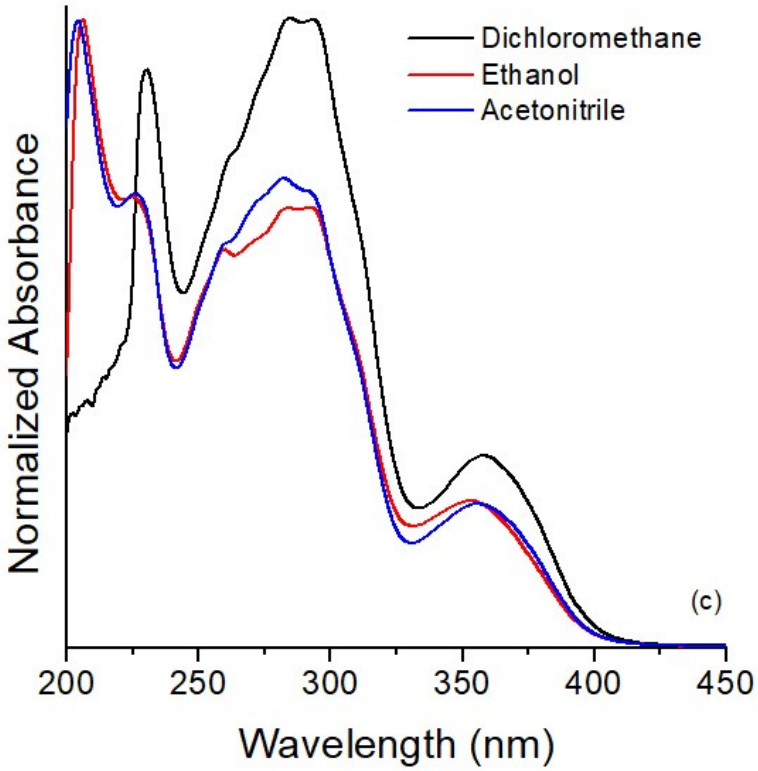


Figure S23. Normalized UV-Vis absorption spectra of compound **8d** (c) **i**n different organic solvents [10^{-5}M].

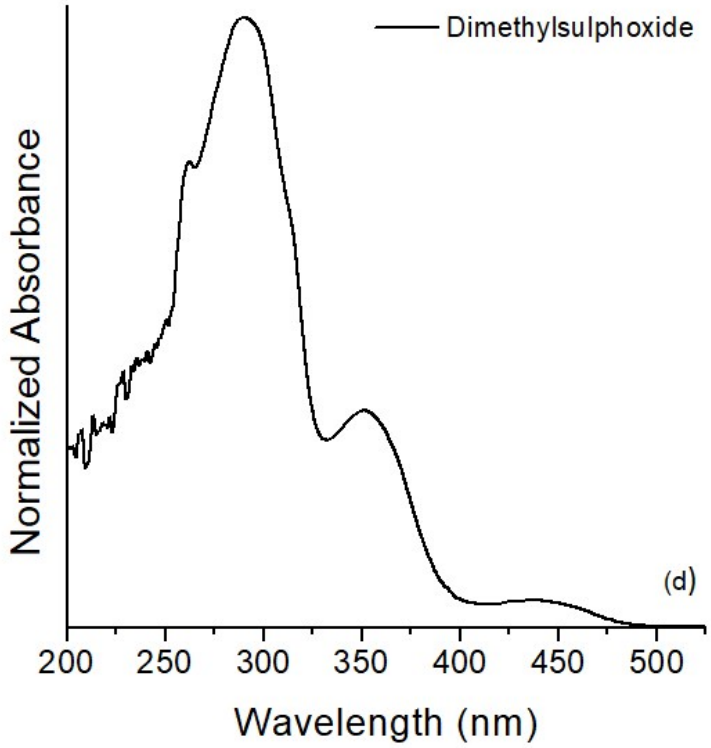


Figure S24. Normalized UV-Vis absorption spectra of compound **8e** (d) **i**n DMSO [10^{-5}M].

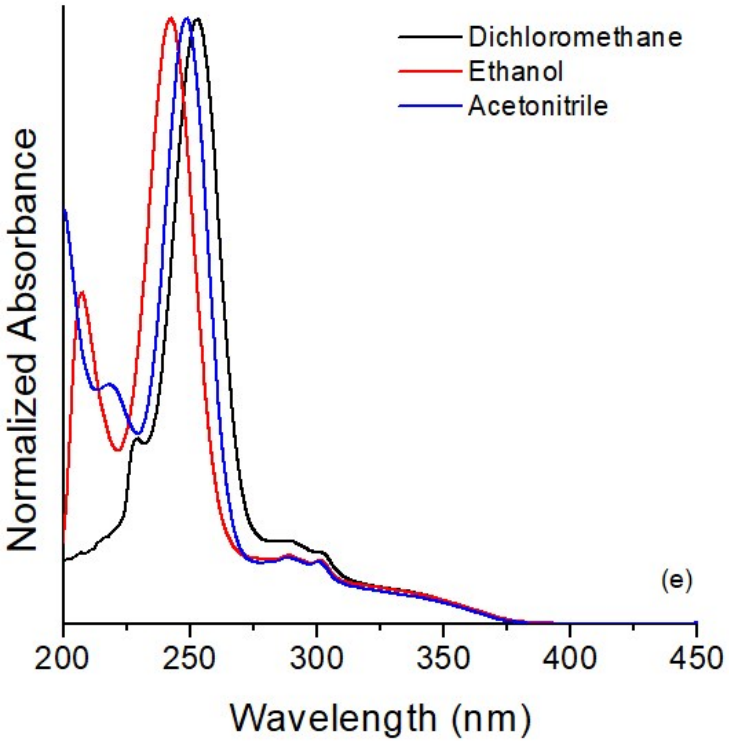


Figure S25. Normalized UV-Vis absorption spectra of compound **8f** (e) **i**n different organic solvents [10^{-5}M].

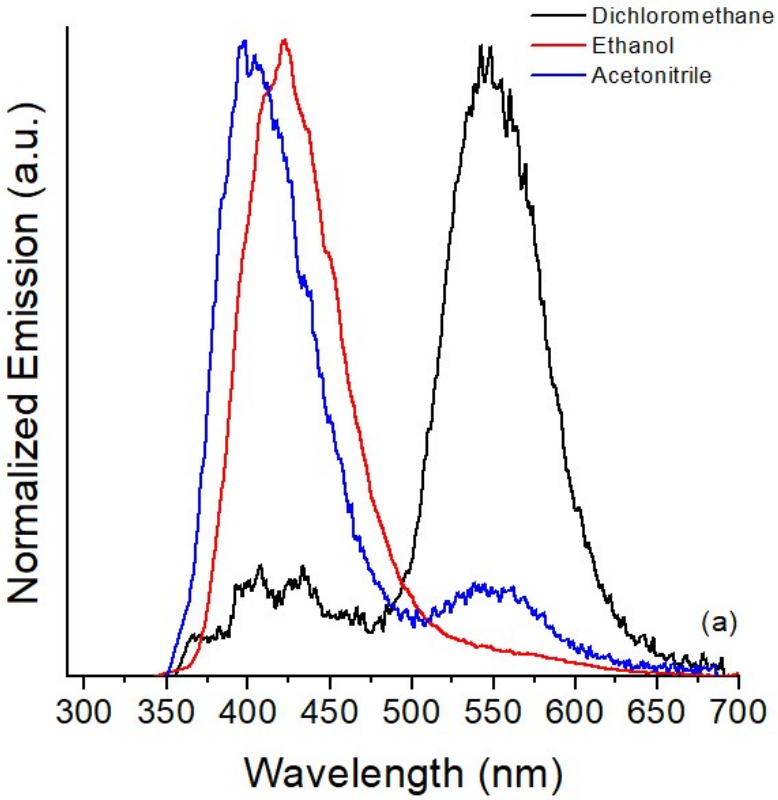


Figure S26. Normalized steady-state fluorescence emission spectra of **5b** (a) in different organic solvents [10^{-5} M].

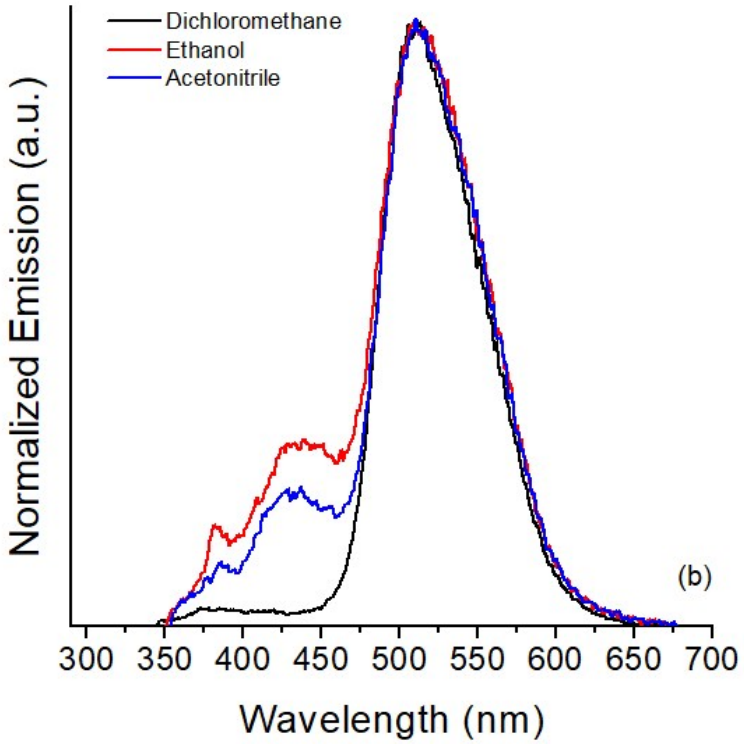


Figure S27. Normalized steady-state fluorescence emission spectra of **8c** (b) in different organic solvents [10^{-5} M].

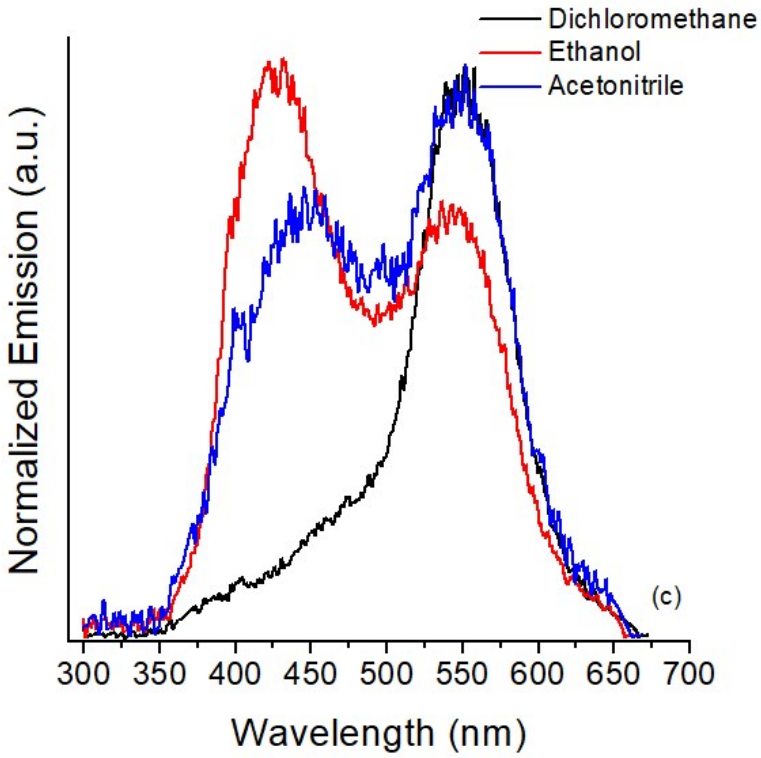


Figure S28. Normalized steady-state fluorescence emission spectra of **8d** (c) in different organic solvents [10^{-5} M].

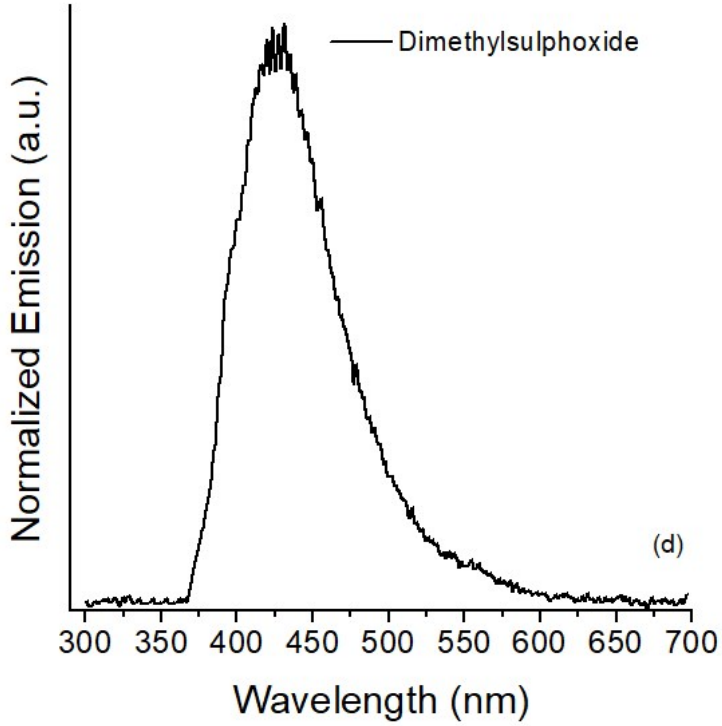


Figure S29. Normalized steady-state fluorescence emission spectra of **8e** (d) in DMSO [10^{-5} M].

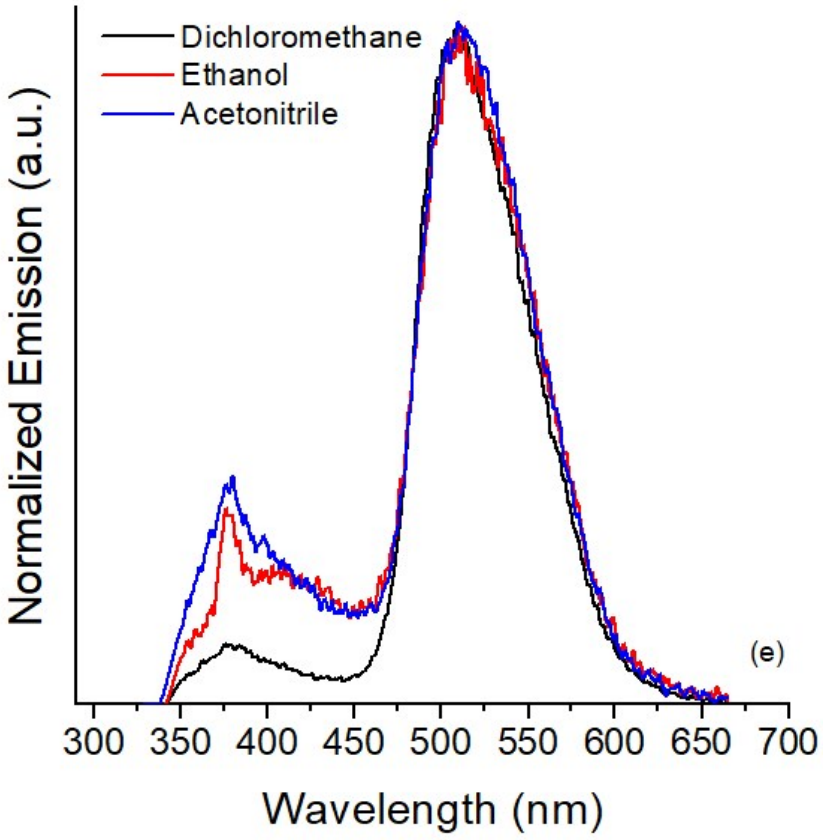
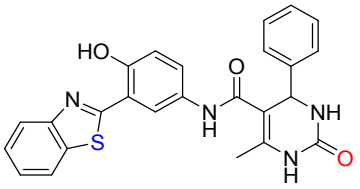
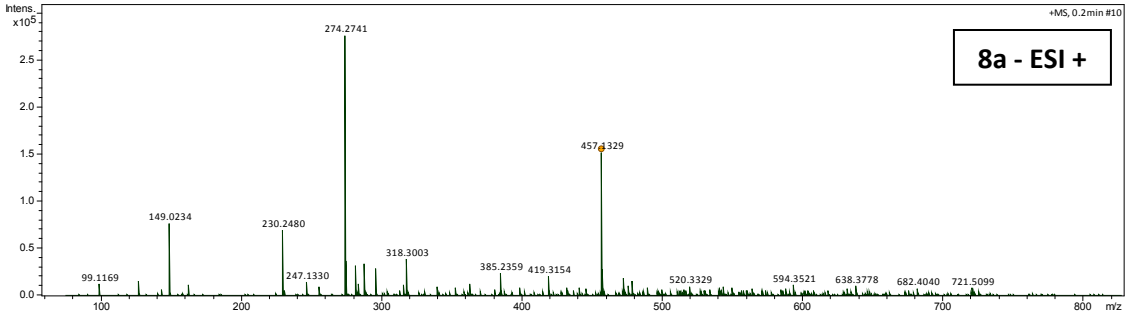
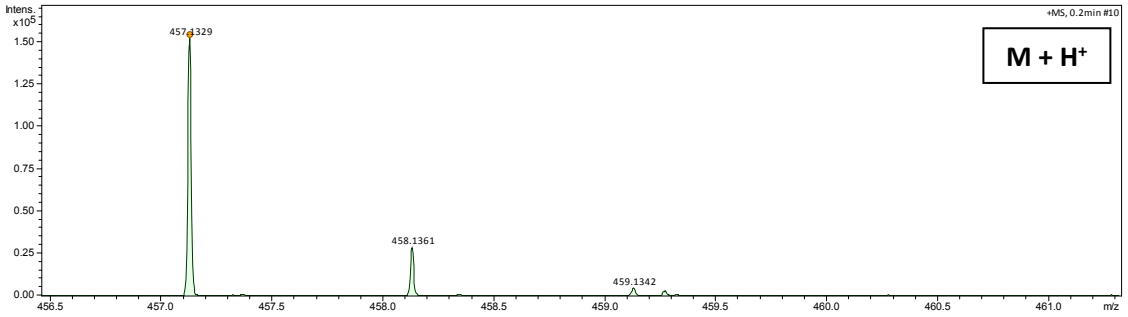


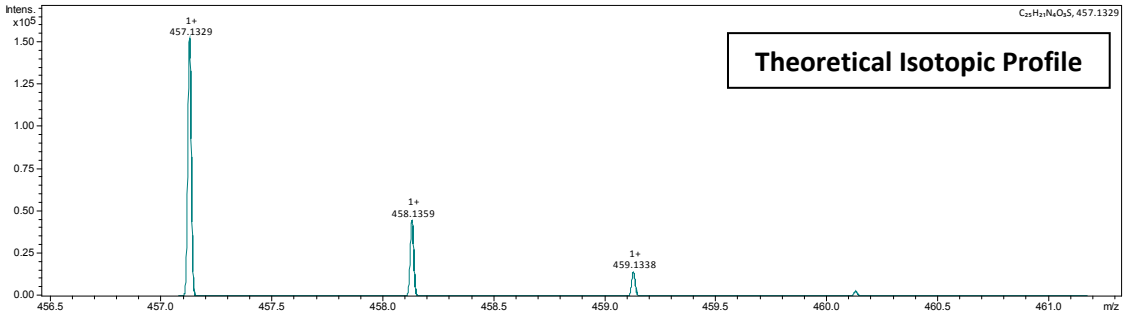
Figure S30. Normalized steady-state fluorescence emission spectra of **8f** (e) in different organic solvents [10-5 M].

Compound 8a





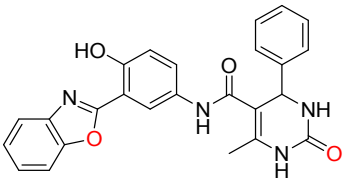


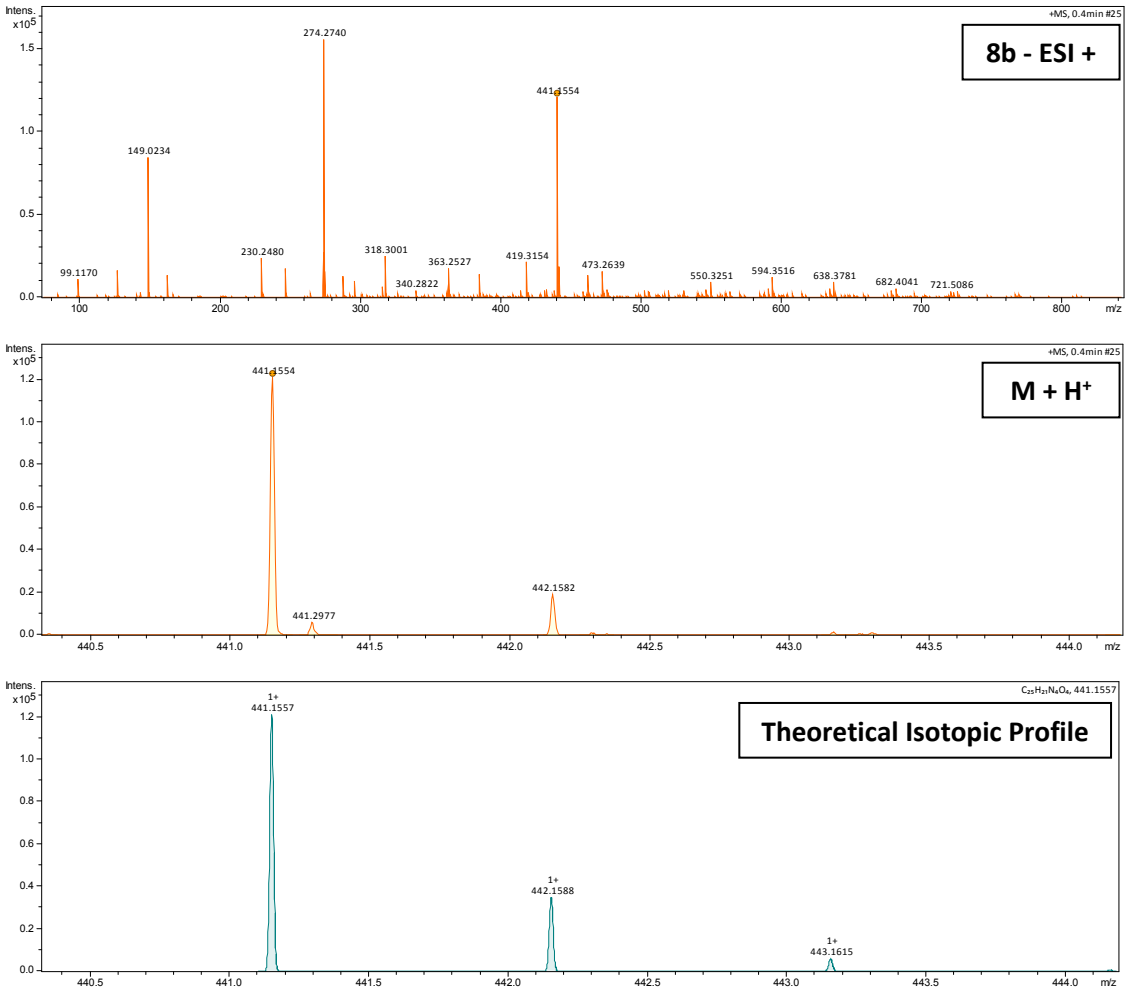


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
457,1329	$C_{25}H_{21}N_4O_3S$	457,1329	-0.1	63.1	17.5	even	ok

Figure S31. High Resolution Mass Spectrum (QTOF-MS) of Compound **8a**.

Compound 8b

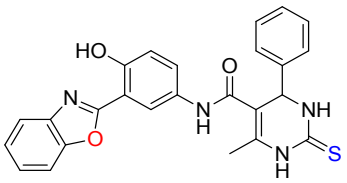


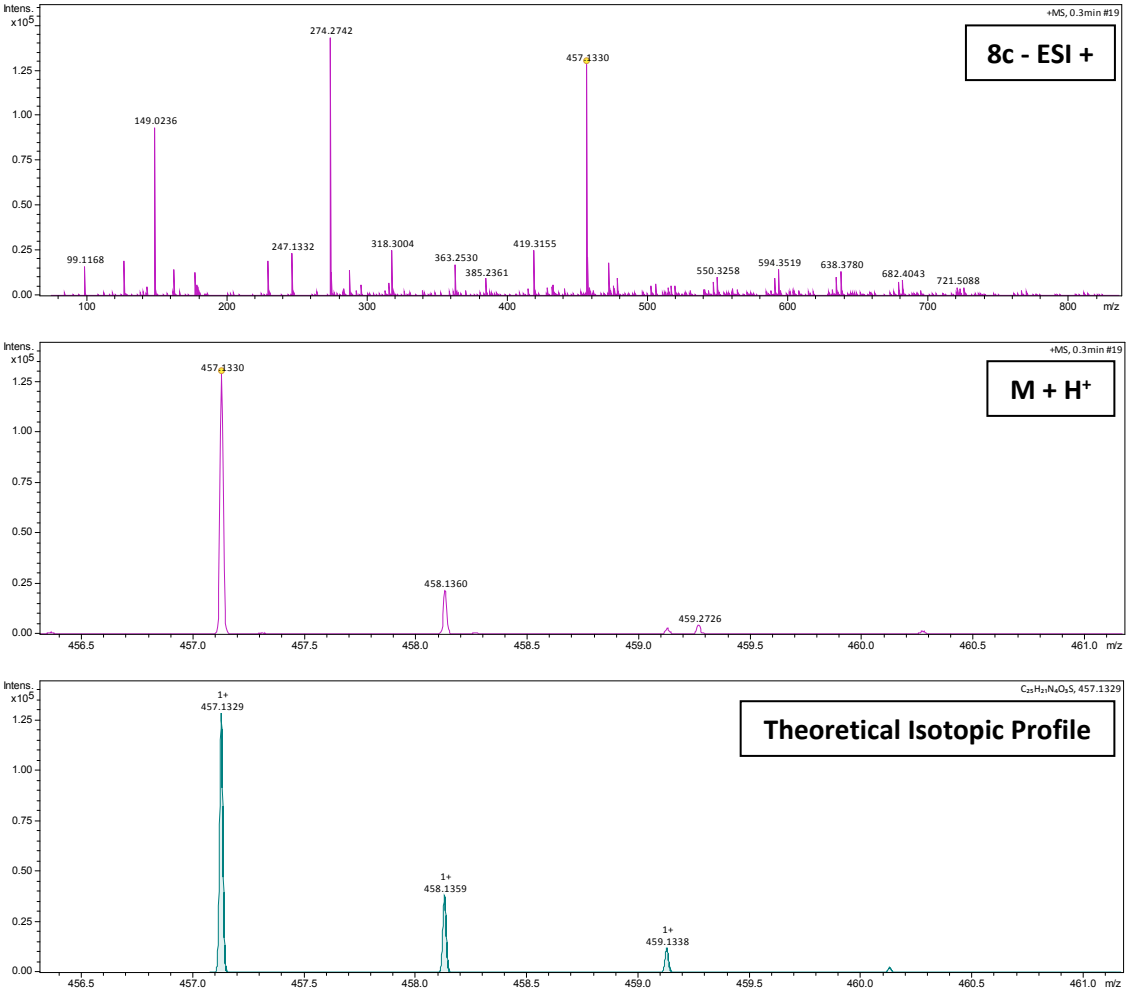


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
441,1554	$C_{25}H_{21}N_4O_4$	441,1557	0.9	79.0	17.5	even	ok

Figure S32. High Resolution Mass Spectrum (QTOF-MS) of Compound **8b**.

Compoud 8c

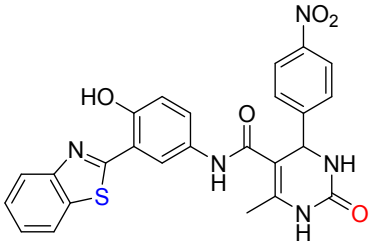


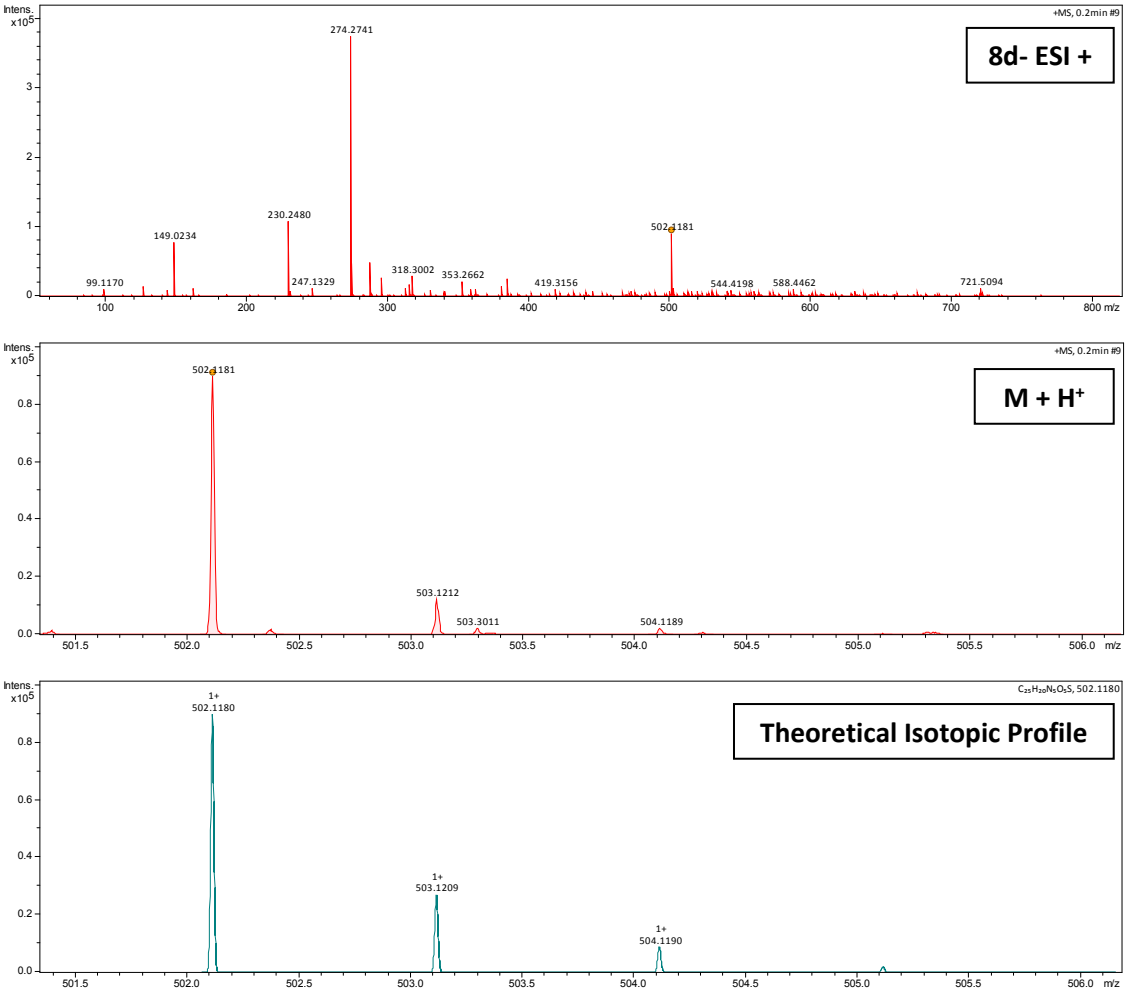


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
457,1330	$C_{25}H_{21}N_4O_3S$	457,1329	-0.3	72.9	17.5	even	ok

Figure S33. High Resolution Mass Spectrum (QTOF-MS) of Compound **8c**.

Compound 8d

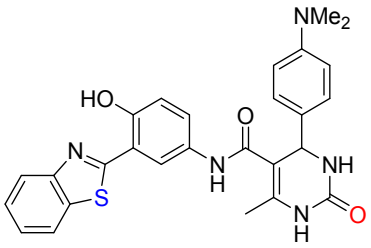


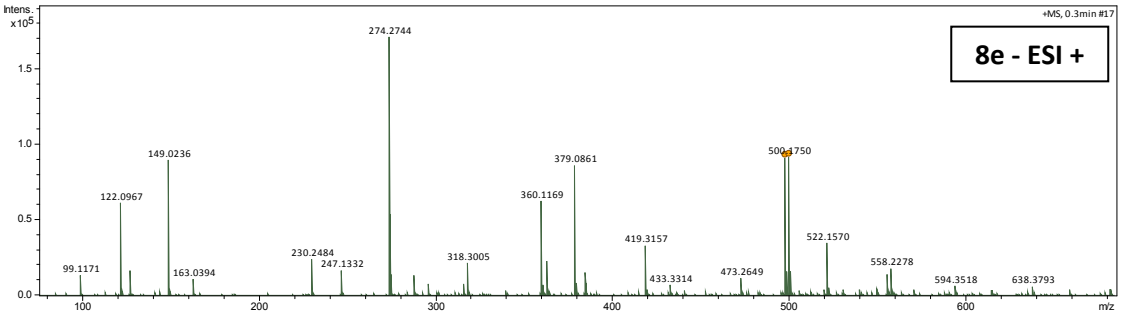


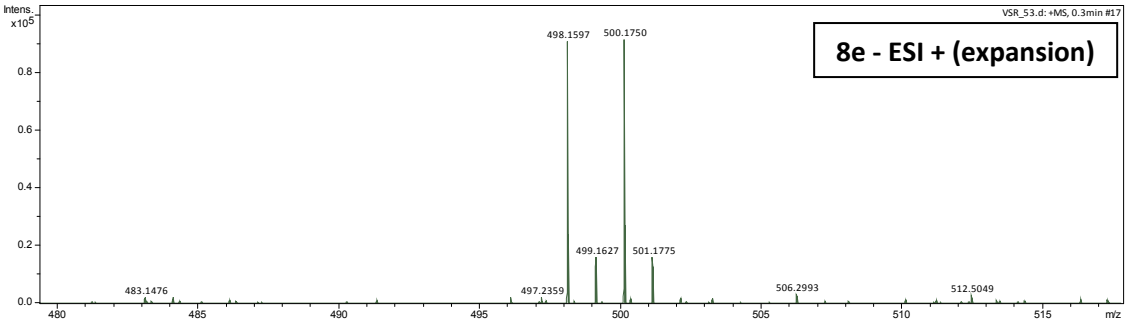
Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
502,1181	$C_{25}H_{20}N_5O_5S$	502,1180	-0.3	88.7	18.5	even	ok

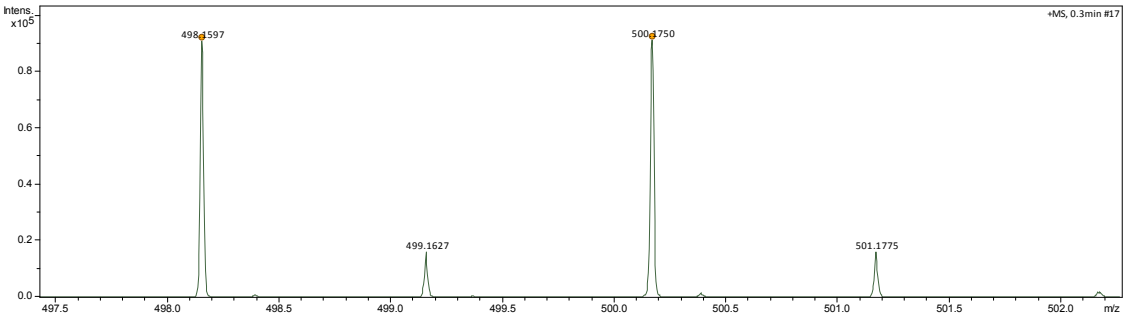
Figure S34. High Resolution Mass Spectrum (QTOF-MS) of Compound **8d**.

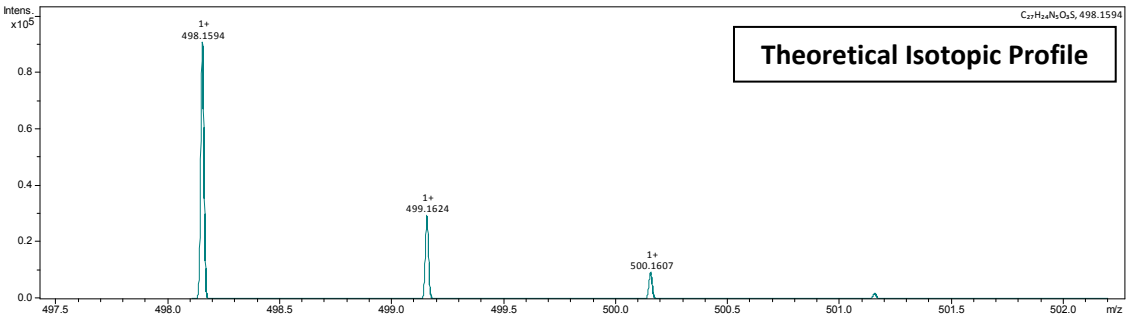
Compound 8e







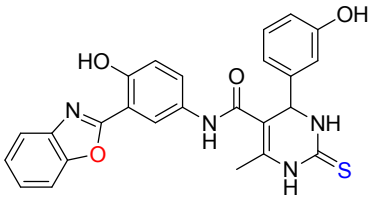


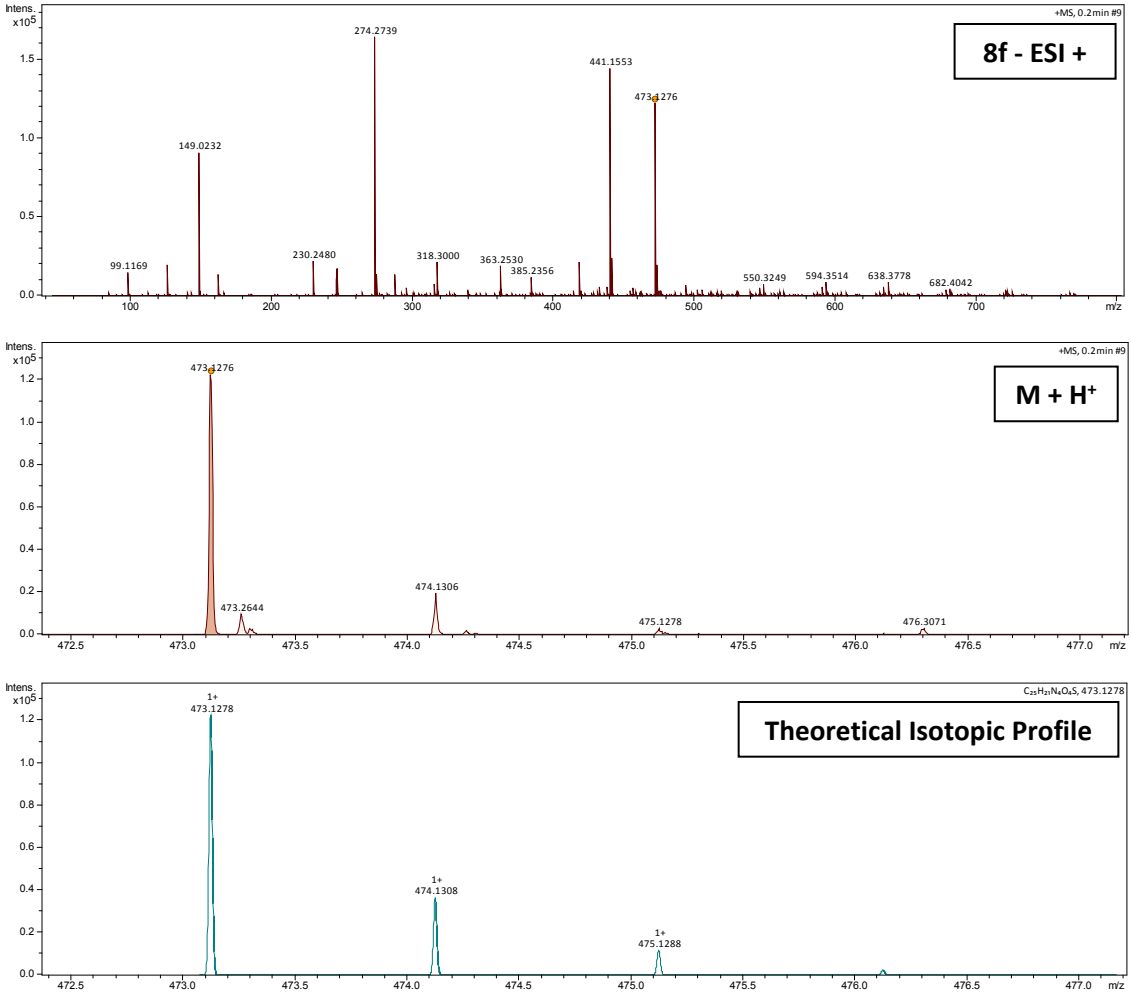


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e^- Conf	N-Rule
498,1597	$C_{27}H_{24}N_5O_3S$	498,1594	-0.6	88.2	18.5	even	ok

Figure S35. High Resolution Mass Spectrum (QTOF-MS) of Compound **8e**.

Compound 8f





Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
473,1276	$C_{25}H_{21}N_4O_4S$	473,1278	0.5	77.1	17.5	even	ok

Figure S35. High Resolution Mass Spectrum (QTOF-MS) of Compound **8e**