

Synthesis, Structural Characterization and Anticancer Activity of New 5-trifluoromethyl-2-thioxo-thiazolo[4,5-*d*]pyrimidine derivatives

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Table of contents

Figures S1-S15. ¹ H NMR spectra of compounds 1c , 1d , 2a-2e , 3a-e , 4a-c	S2-S9
Figures S16-S28. ¹³ C NMR spectra of compounds 2a-2e , 3a-e , 4a-c	S9-S15
Figures S29-S41. MS spectra of compounds 2a-2e , 3a-e , 4a-c	S16-S20
Figures S42-S54. IR spectra of compounds 2a-2e , 3a-e , 4a-c	S20-S26
Figure S55. The crystal packing of the 2e viewed along a axis. Disordered toluene molecules are marked with a purple wire/stick model. Dashed lines (in black) indicate intermolecular interactions, with N—H···O in black, C—H···S in orange and C—H···F in light green.....	S27
Table S1. Selected X-ray single-crystal data and structure refinement details of compounds 2e and 4b	S28

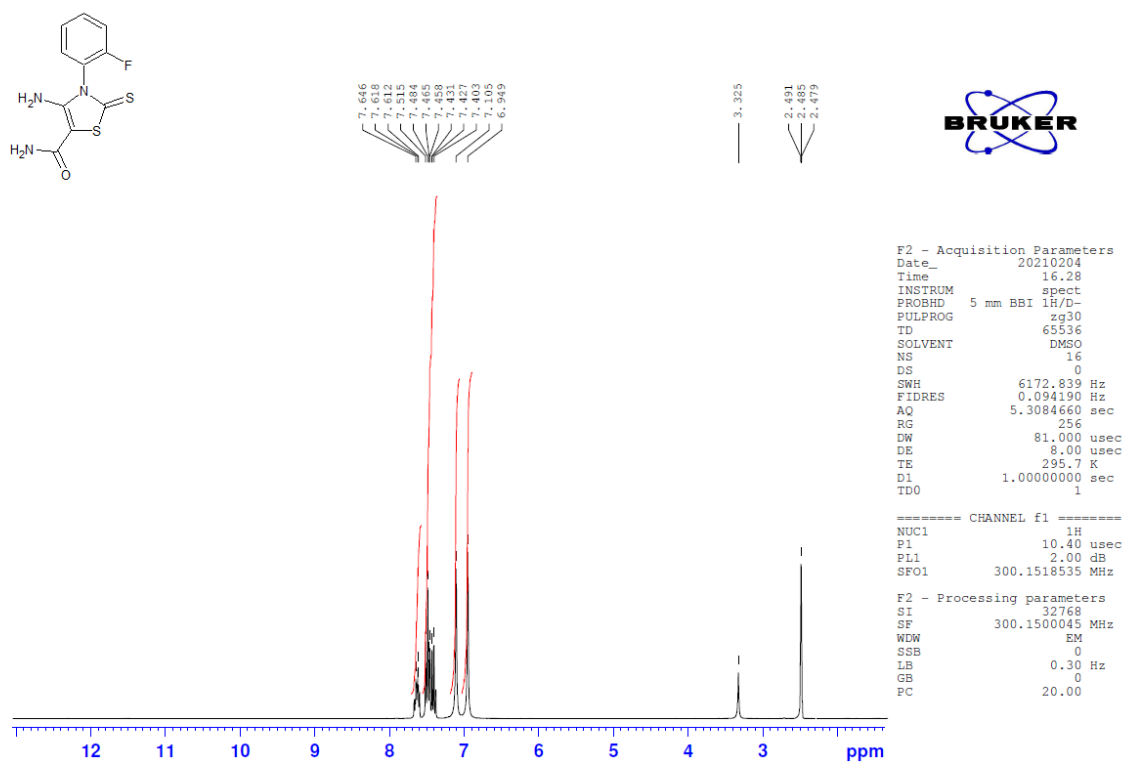


Figure S1. ¹HNMR spectrum of compound **1c** (300MHz, DMSO).

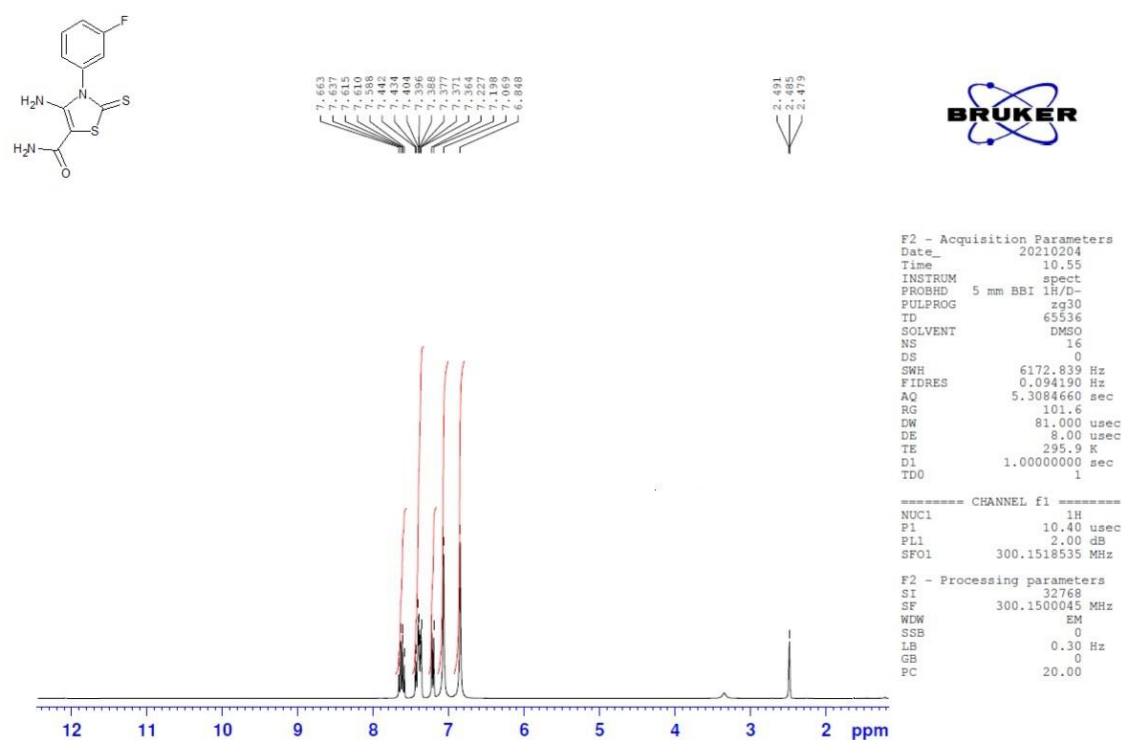


Figure S2. ¹HNMR spectrum of compound **1d** (300MHz, DMSO).

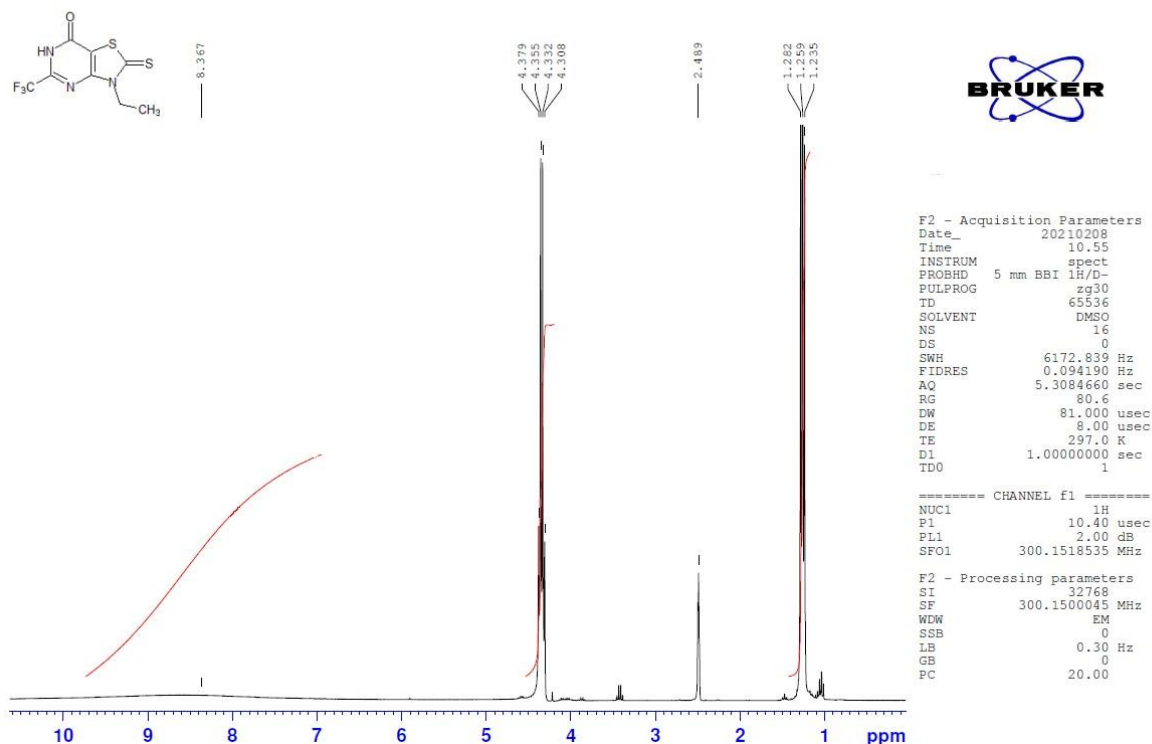


Figure S3. ^1H NMR spectrum of compound **2a** (300MHz, DMSO).

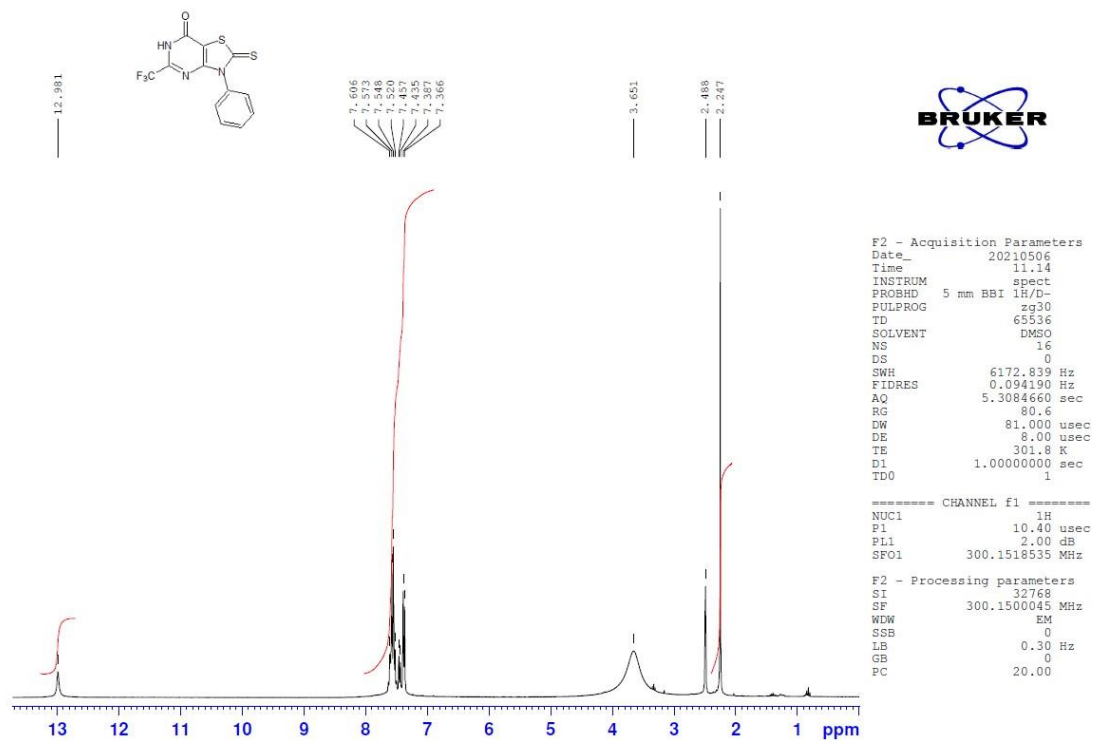


Figure S4. ^1H NMR spectrum of compound **2b** (300MHz, DMSO).

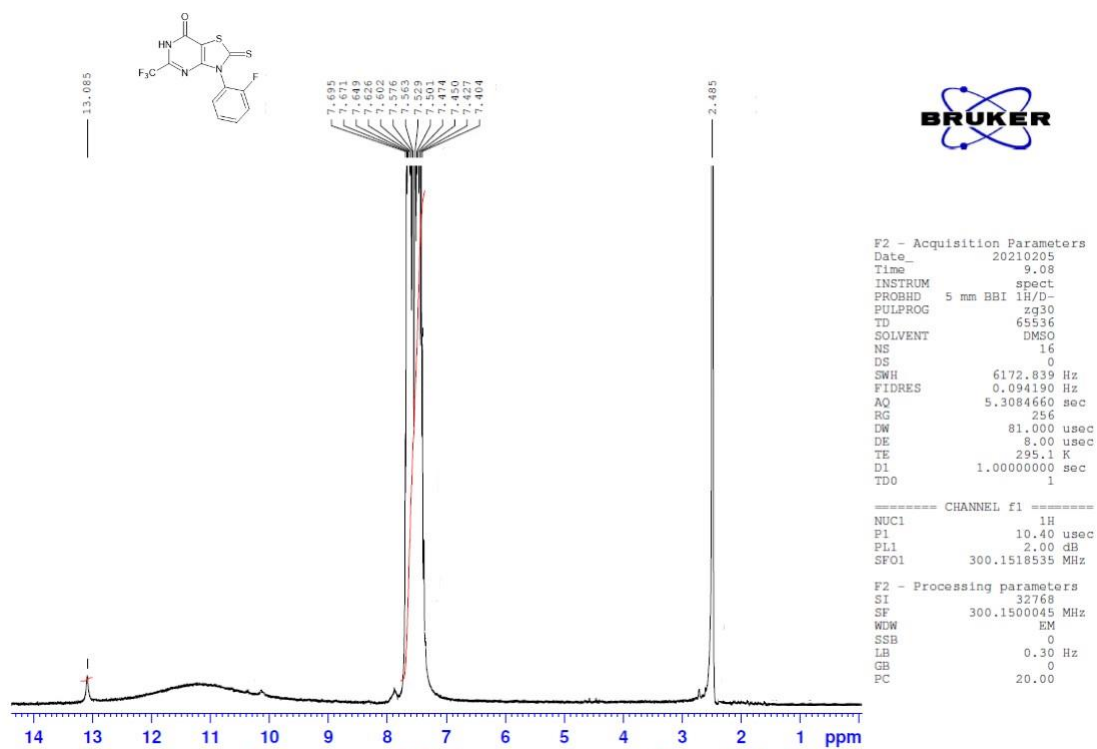


Figure S5. ¹H NMR spectrum of compound **2c** (300MHz, DMSO).

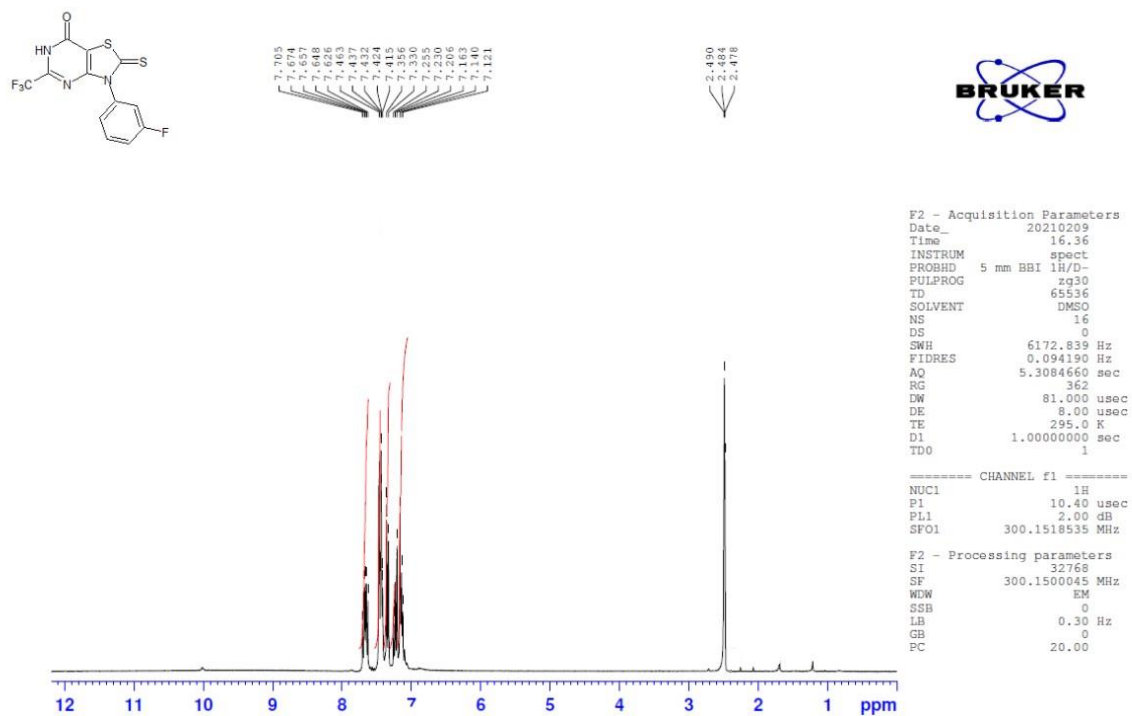


Figure S6. ¹H NMR spectrum of compound **2d** (300MHz, DMSO).

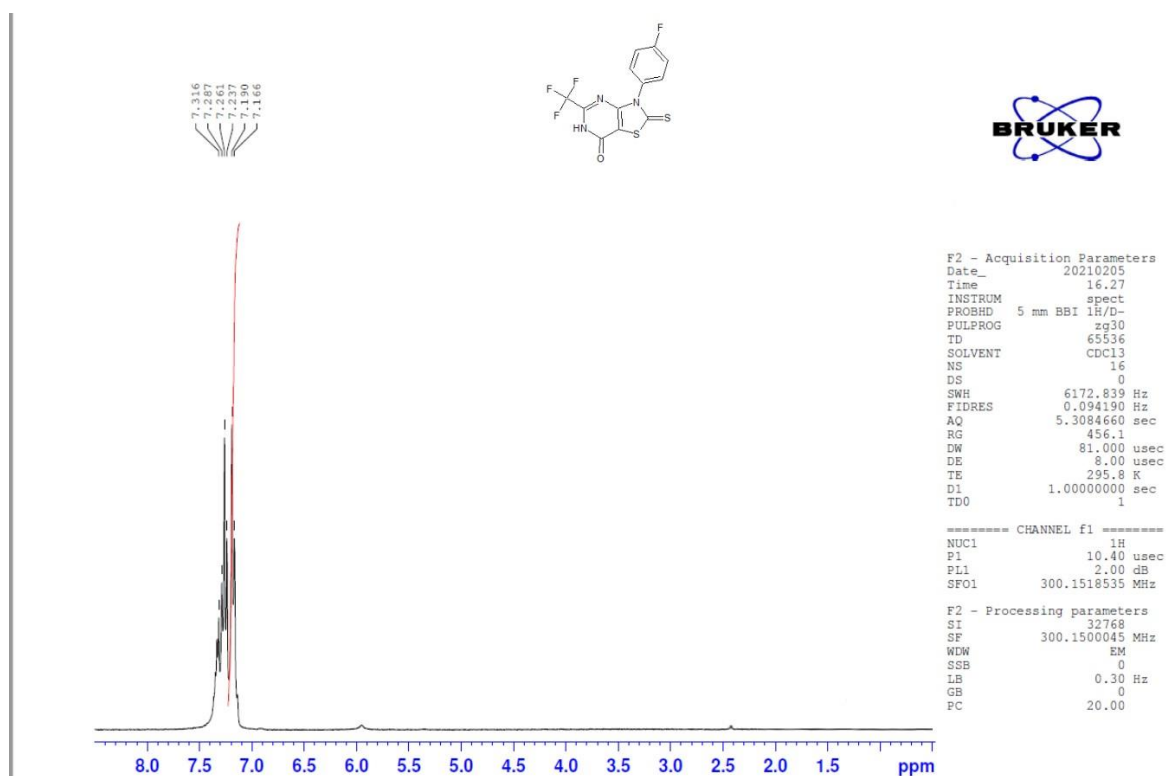


Figure S7. ¹H NMR spectrum of compound **2e** (300 MHz, CDCl₃).

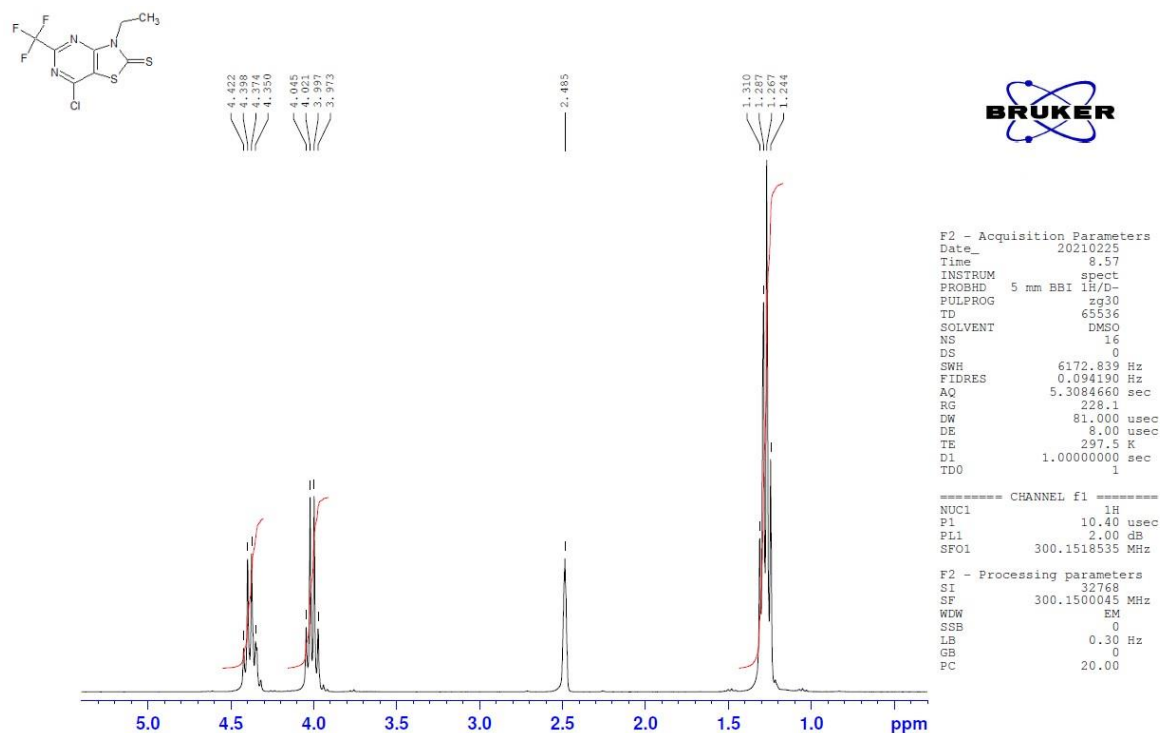


Figure S8. ¹H NMR spectrum of compound **3a** (300 MHz, DMSO).

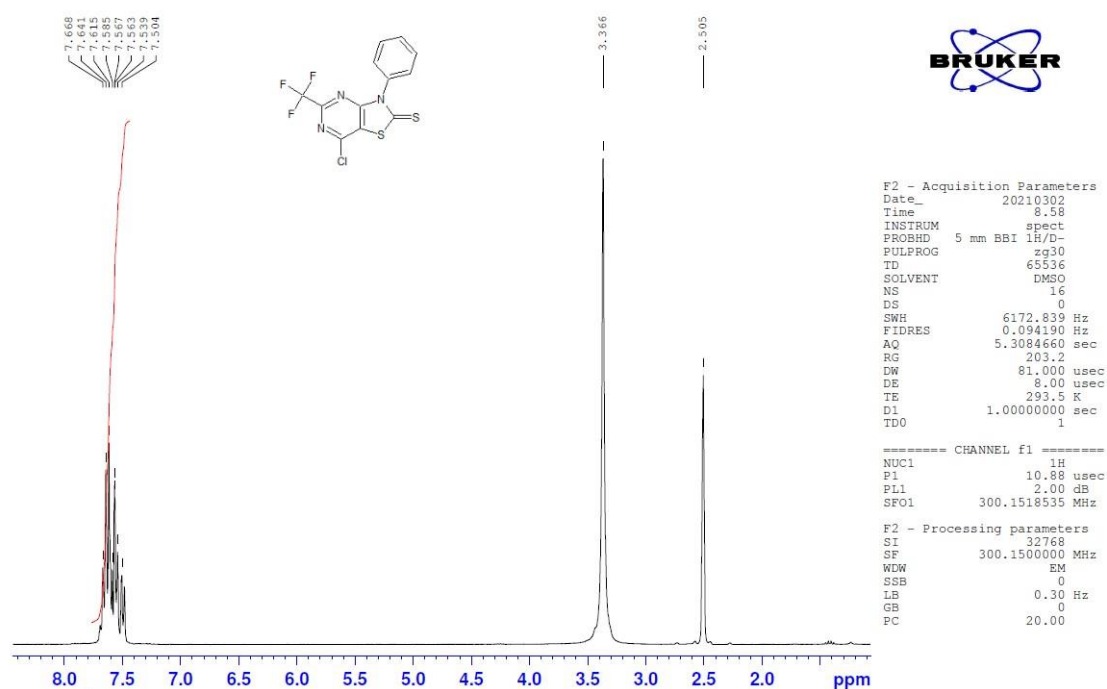


Figure S9. ^1H NMR spectrum of compound **3b** (300MHz, DMSO).

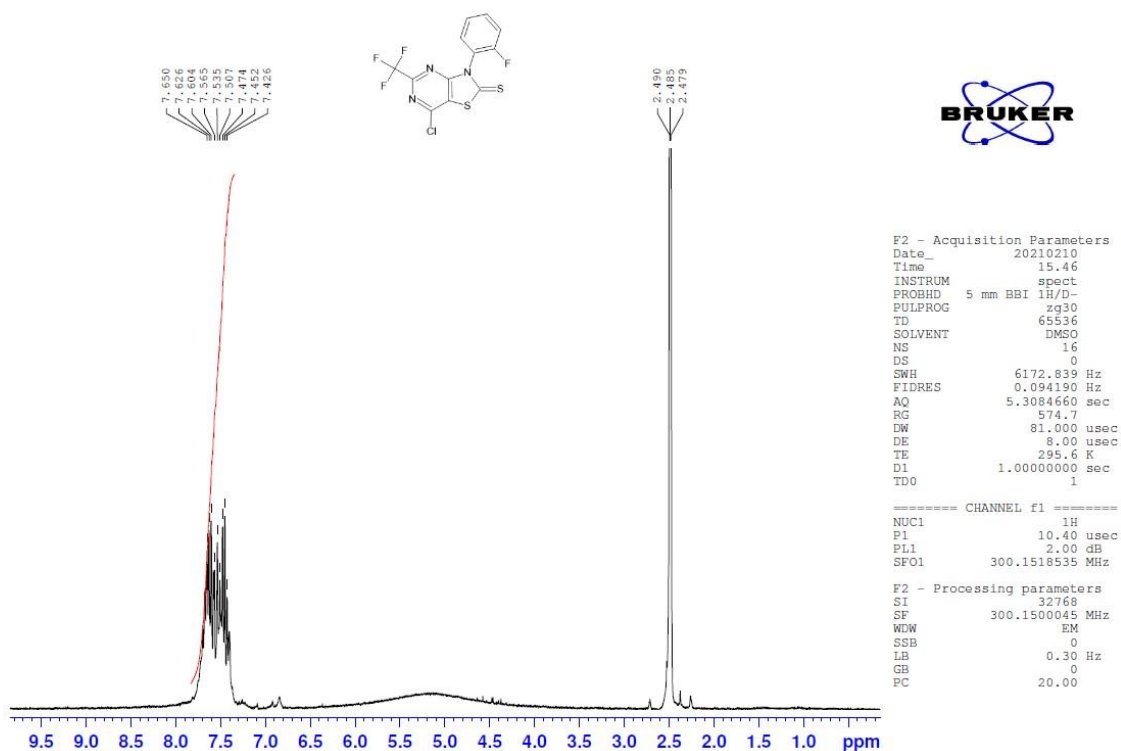


Figure S10. ^1H NMR spectrum of compound **3c** (300MHz, DMSO).

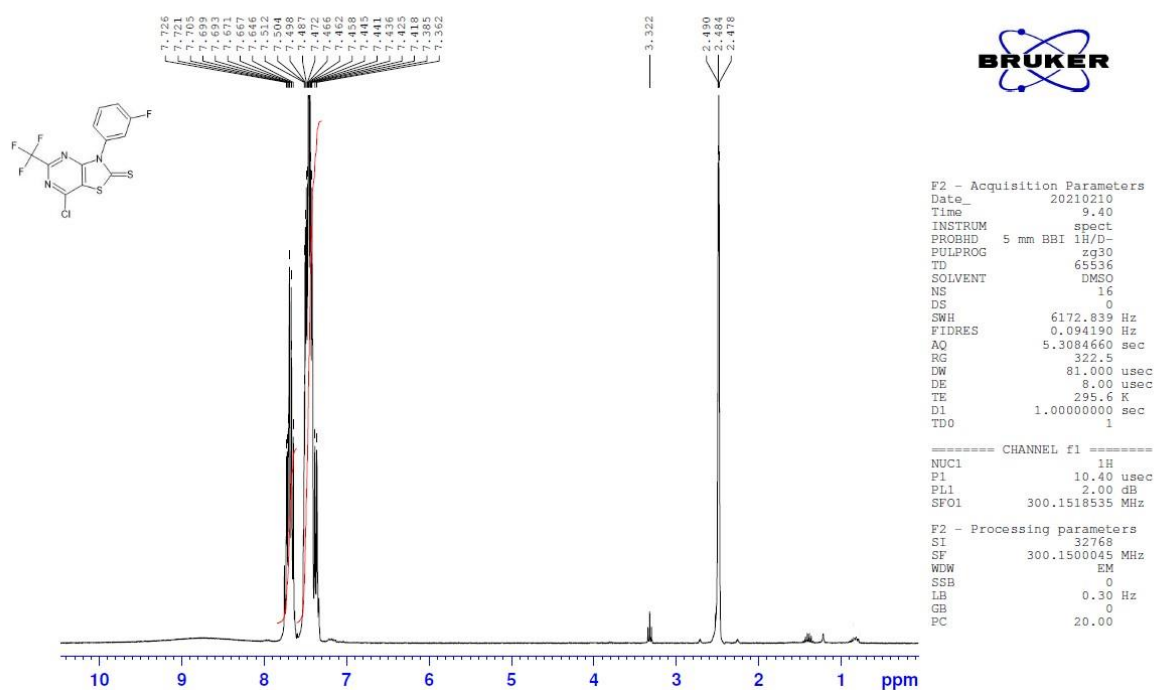


Figure S11. ¹HNMR spectrum of compound **3d** (300MHz, DMSO).

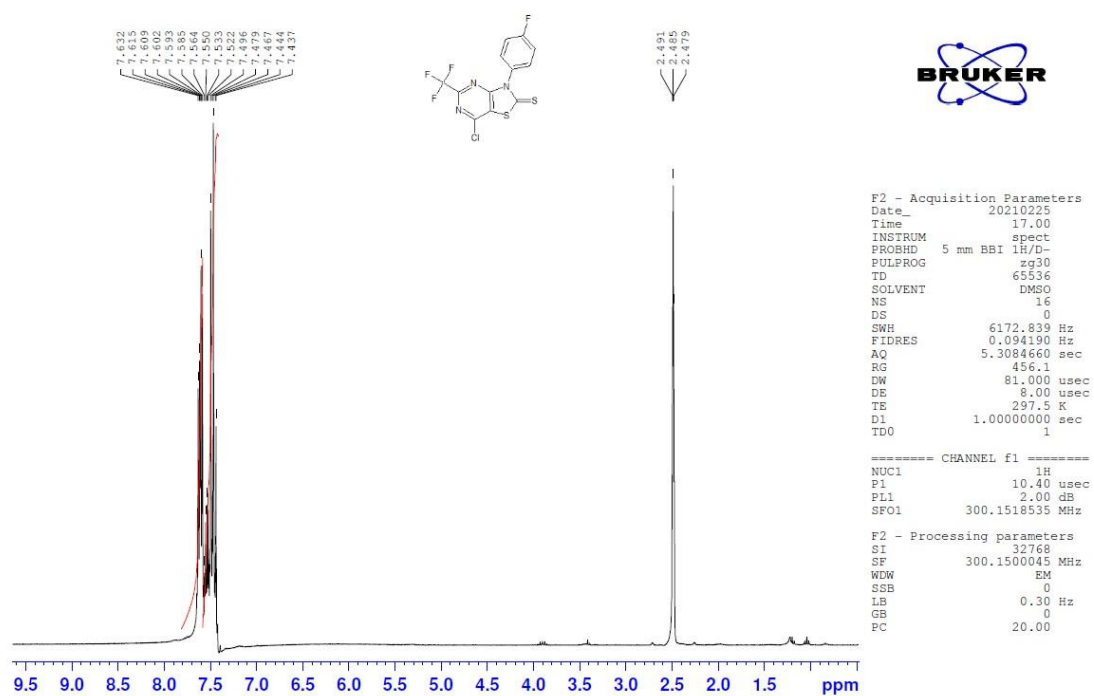


Figure S12. ¹HNMR spectrum of compound **3e** (300MHz, DMSO).

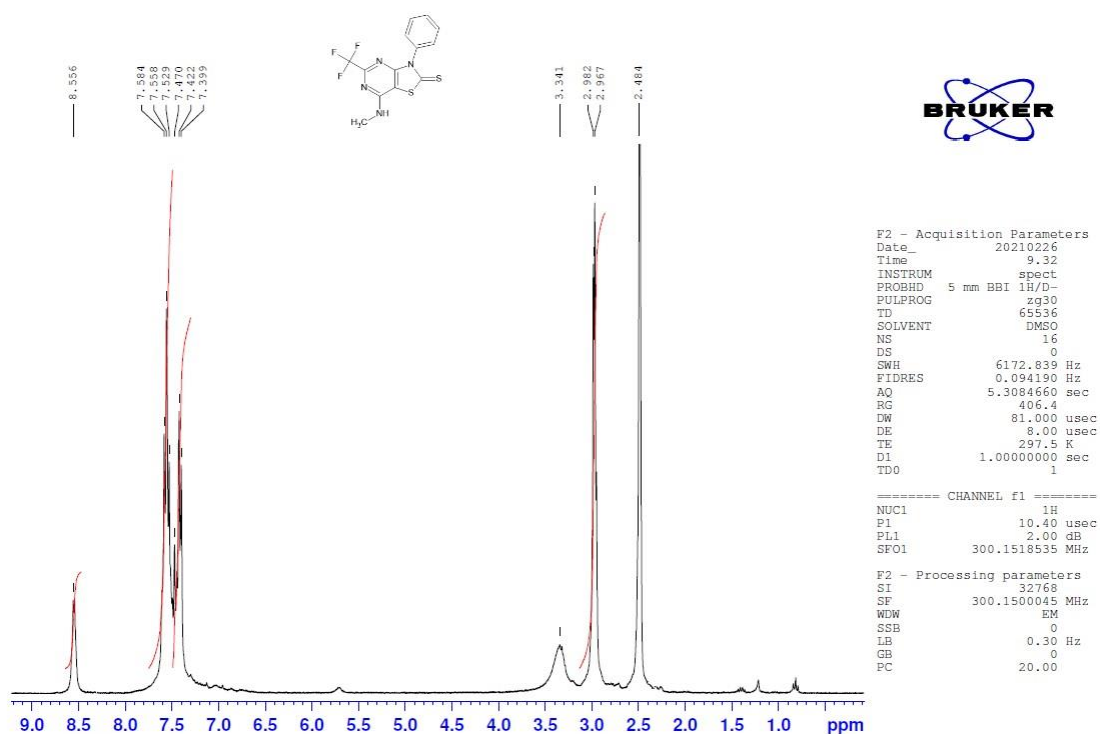


Figure S13. ^1H NMR spectrum of compound **4a** (300MHz, DMSO).

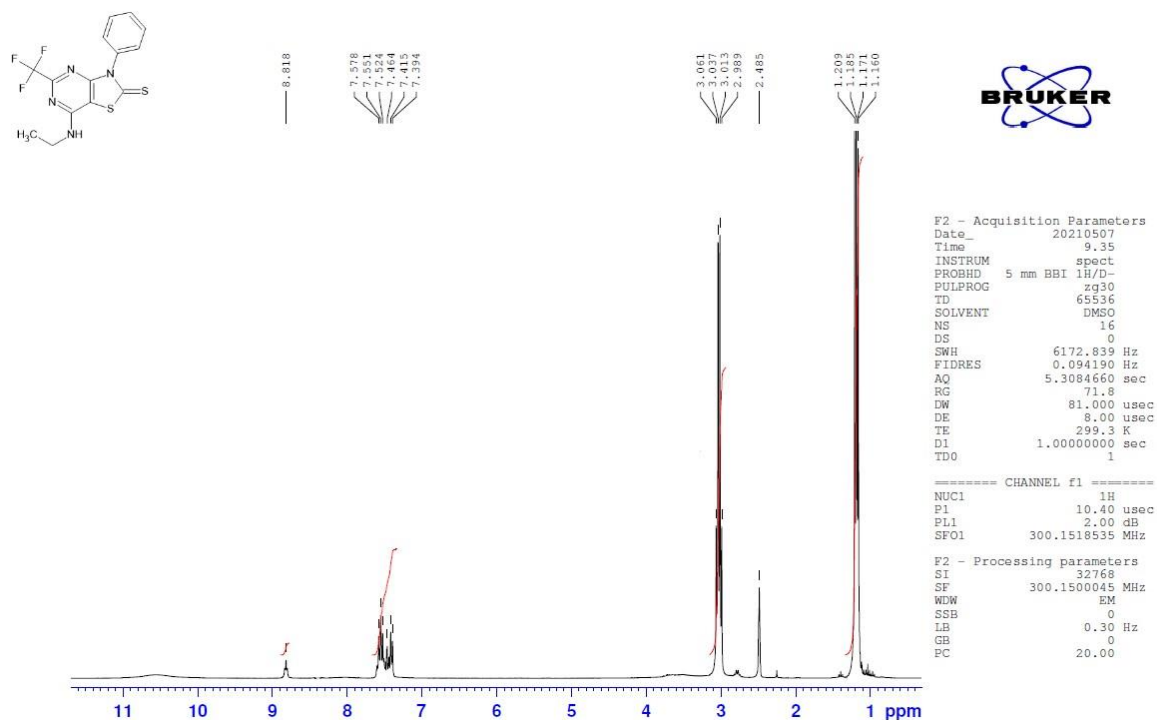


Figure S14. ^1H NMR spectrum of compound **4b** (300MHz, DMSO).

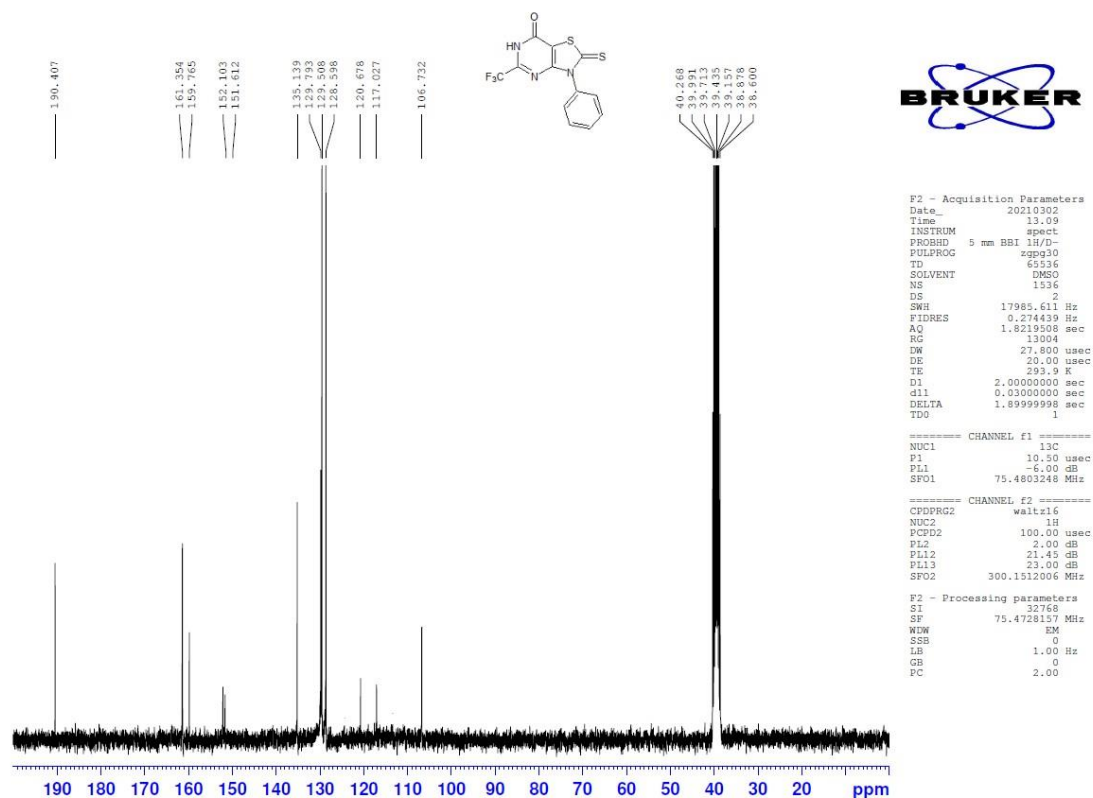


Figure S17. ¹³CNMR spectrum of compound **2b** (75MHz, DMSO).

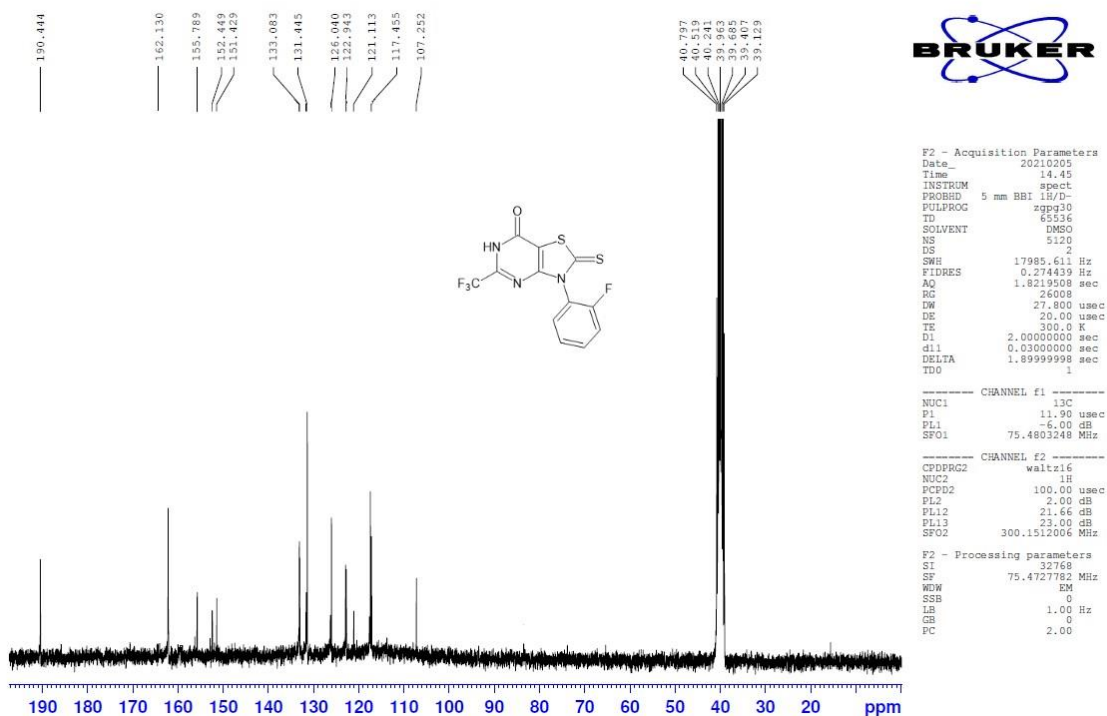


Figure S18. ¹³CNMR spectrum of compound **2c** (75MHz, DMSO).

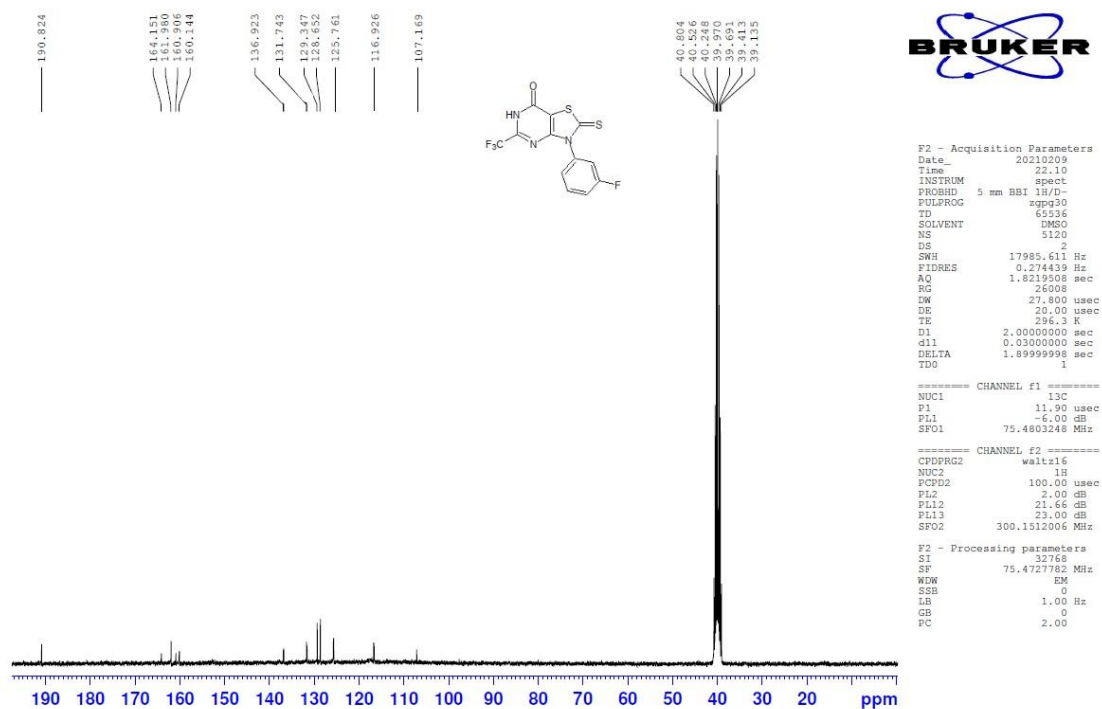


Figure S19. ^{13}C NMR spectrum of compound **2d** (75MHz, DMSO).

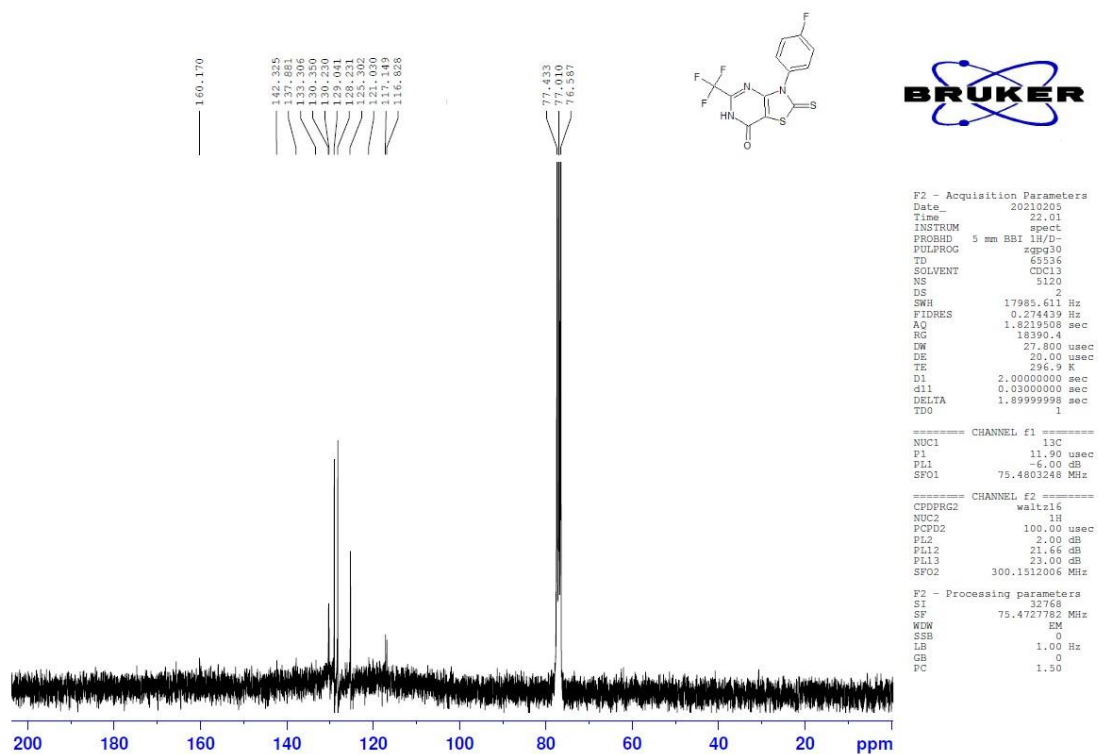


Figure S20. ^{13}C NMR spectrum of compound **2e** (75MHz, CDCl_3).

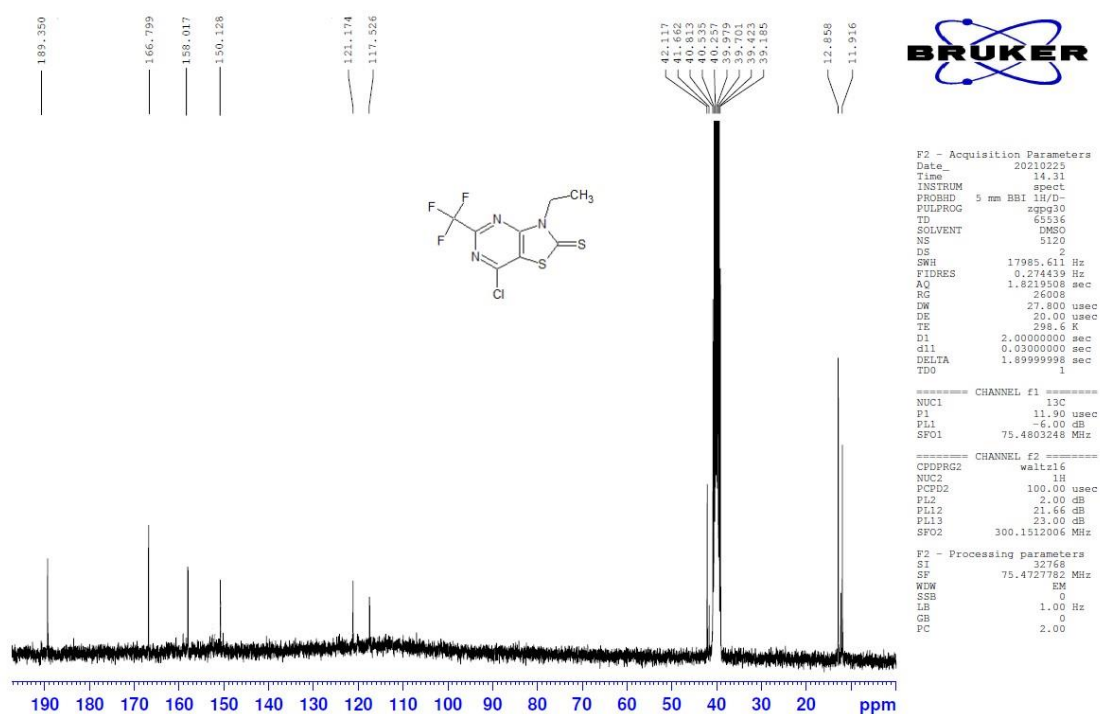


Figure S21. ¹³CNMR spectrum of compound 3a (75MHz, DMSO).

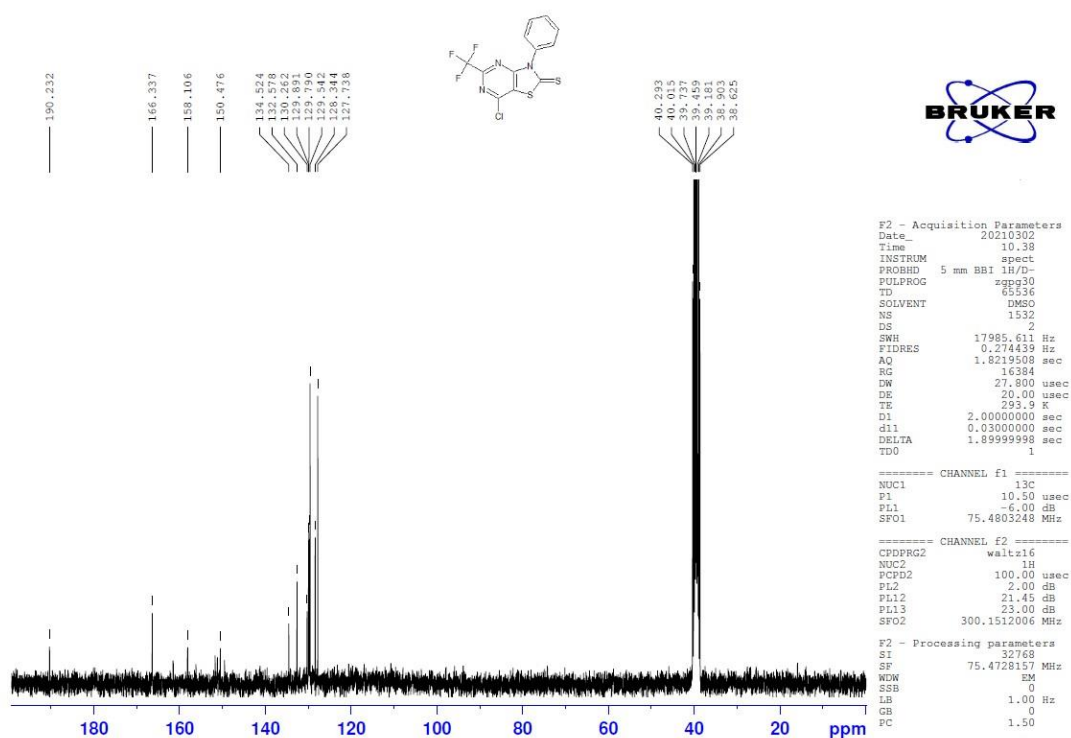


Figure S22. ¹³CNMR spectrum of compound 3b (75MHz, DMSO).

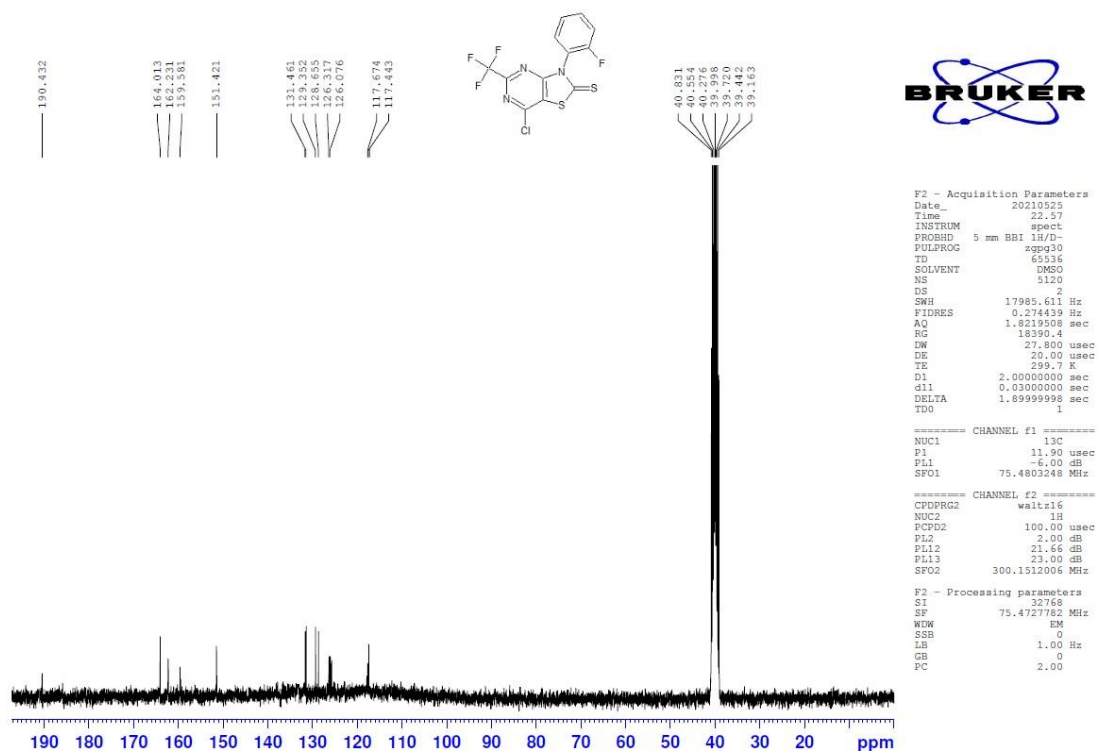


Figure S23. ^{13}C NMR spectrum of compound **3c** (75MHz, DMSO).

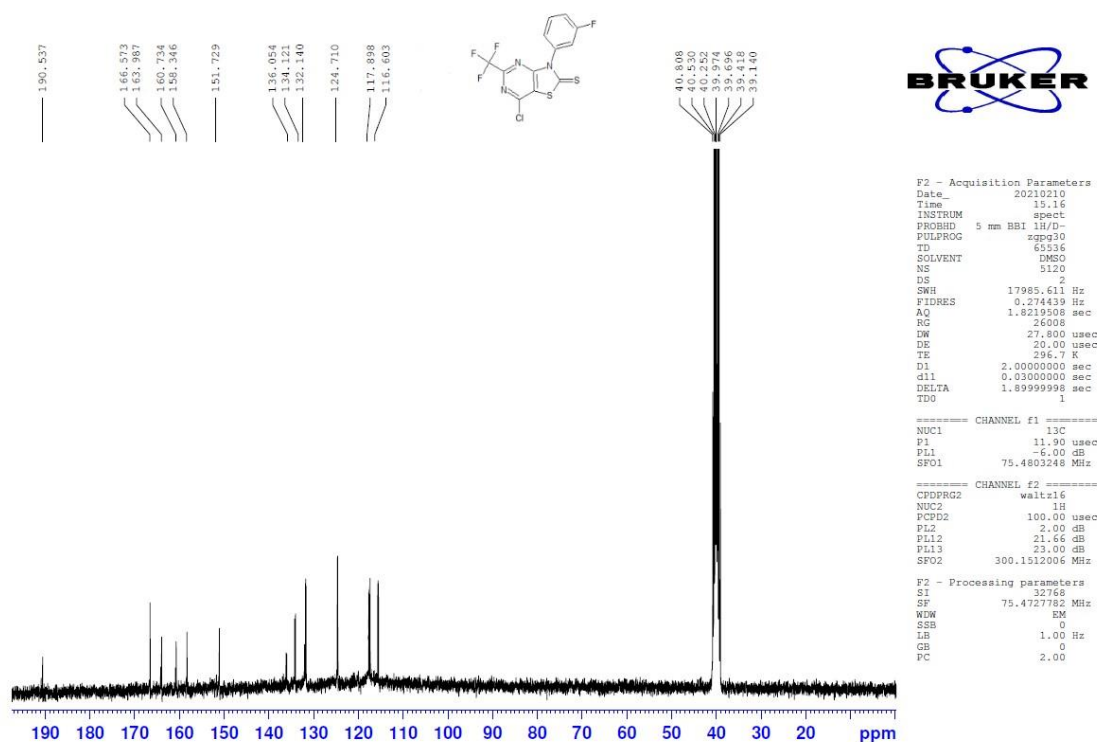


Figure S24. ^{13}C NMR spectrum of compound **3d** (75MHz, DMSO).

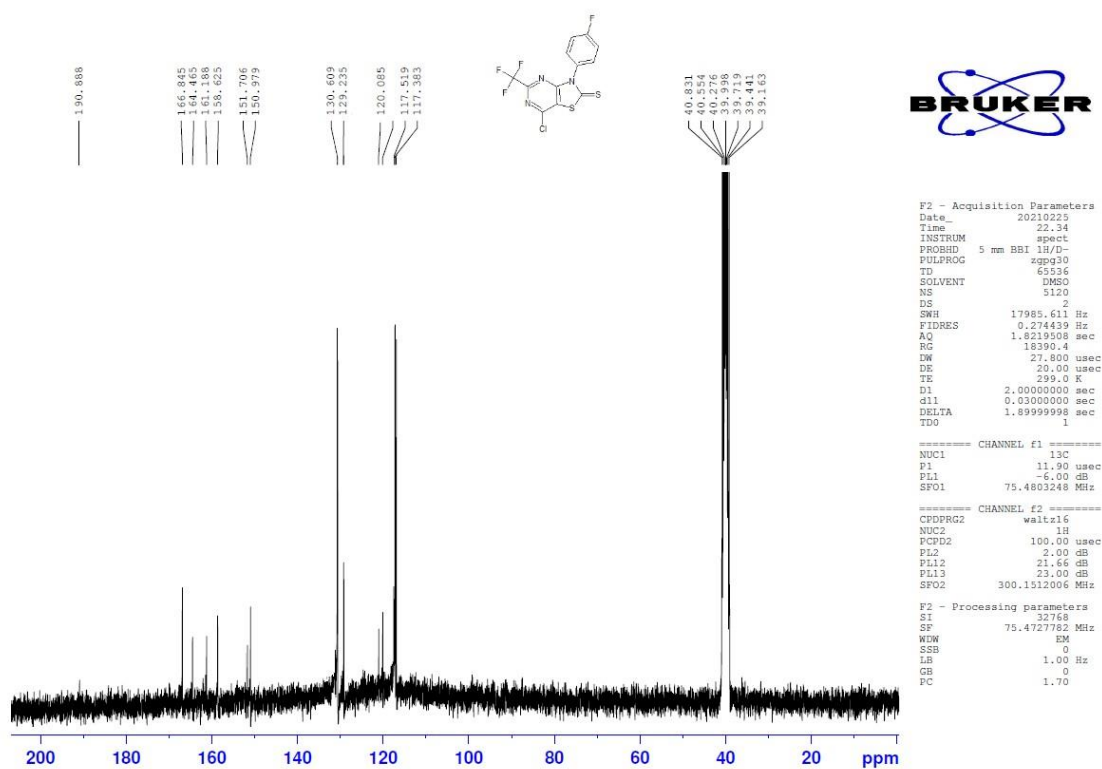


Figure S25. ^{13}C NMR spectrum of compound **3e** (75MHz, DMSO).

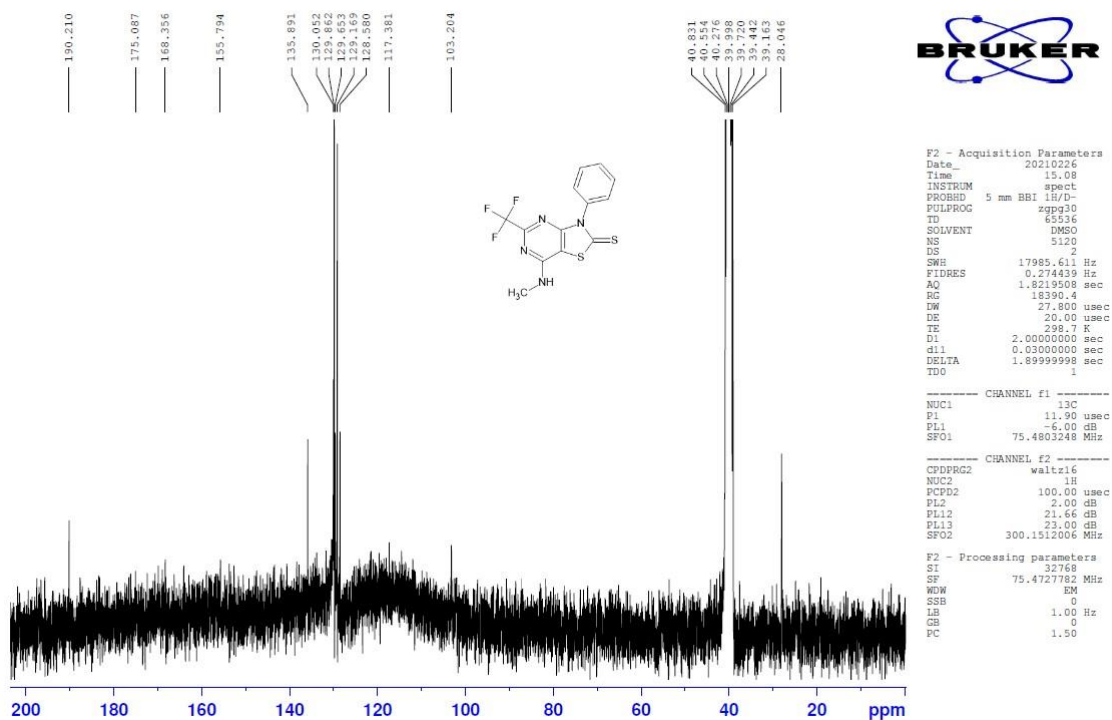


Figure S26. ^{13}C NMR spectrum of compound **4a** (75MHz, DMSO).

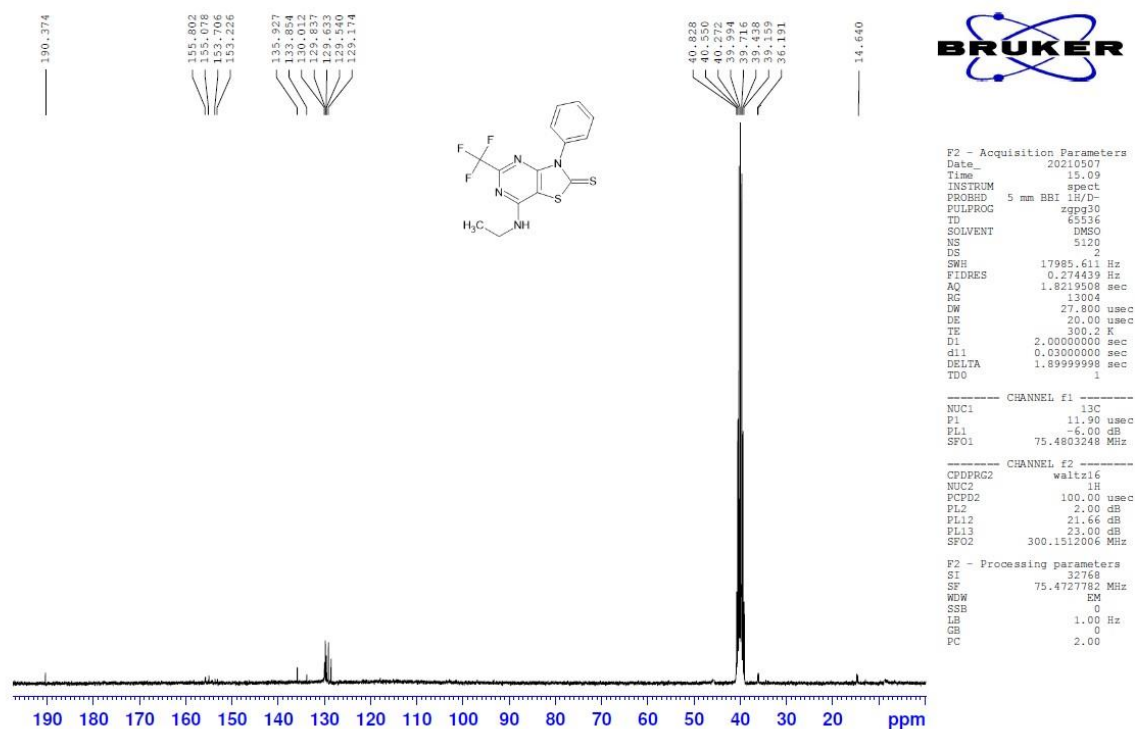


Figure S27. ^{13}C NMR spectrum of compound **4b** (75MHz, DMSO).

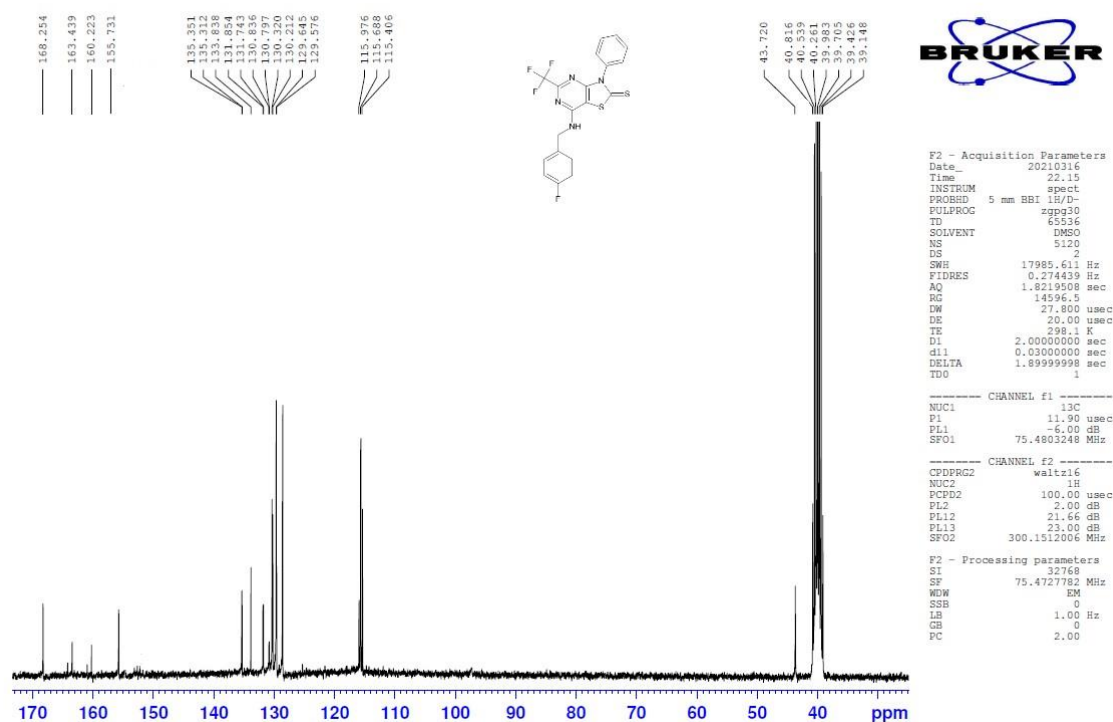


Figure S28. ^{13}C NMR spectrum of compound **4c** (75MHz, DMSO).

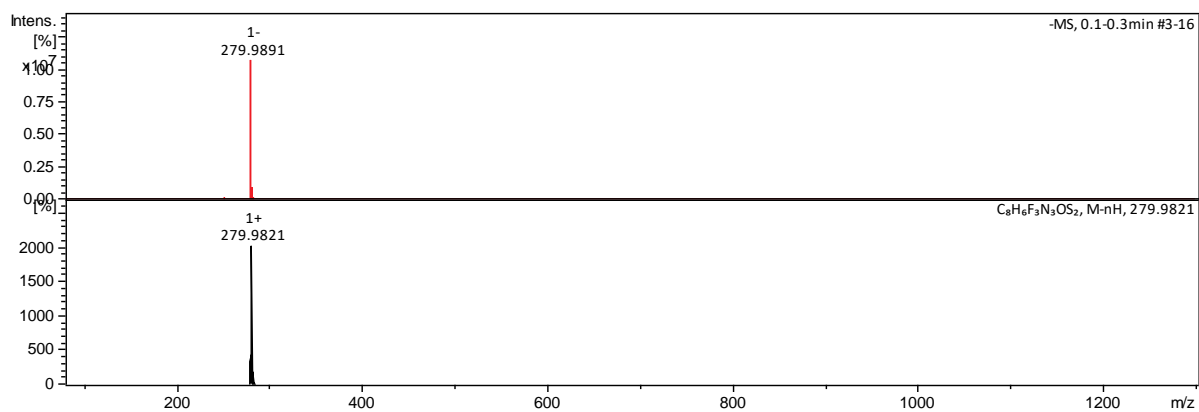


Figure S29. MS spectrum of compound 2a.

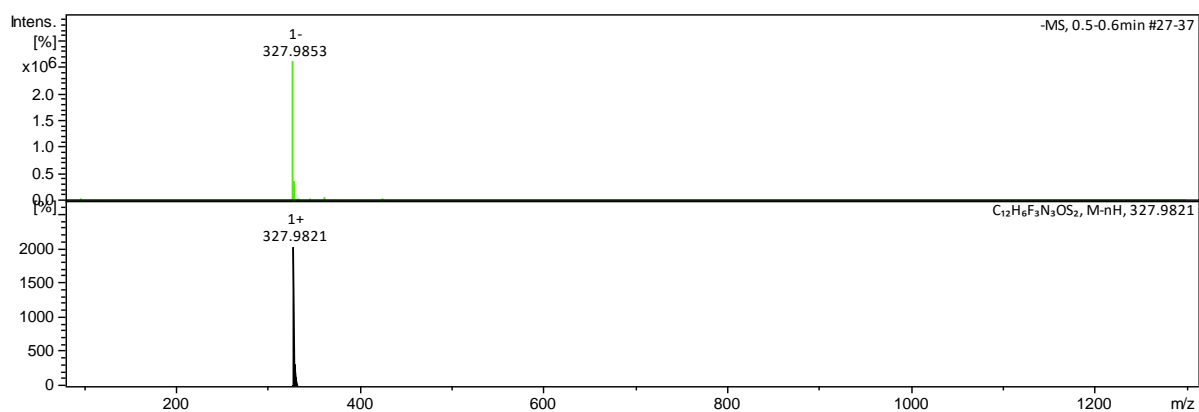


Figure S30. MS spectrum of compound 2b.

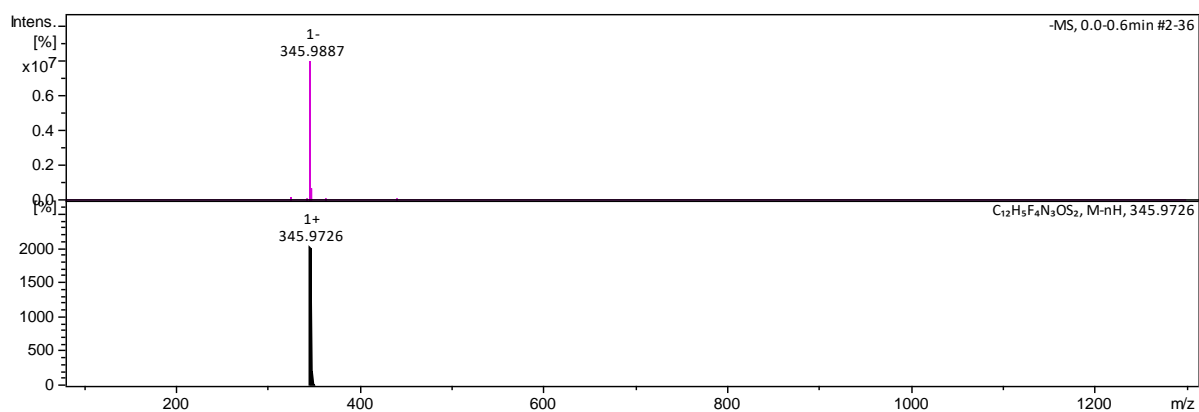


Figure S31. MS spectrum of compound 2c.

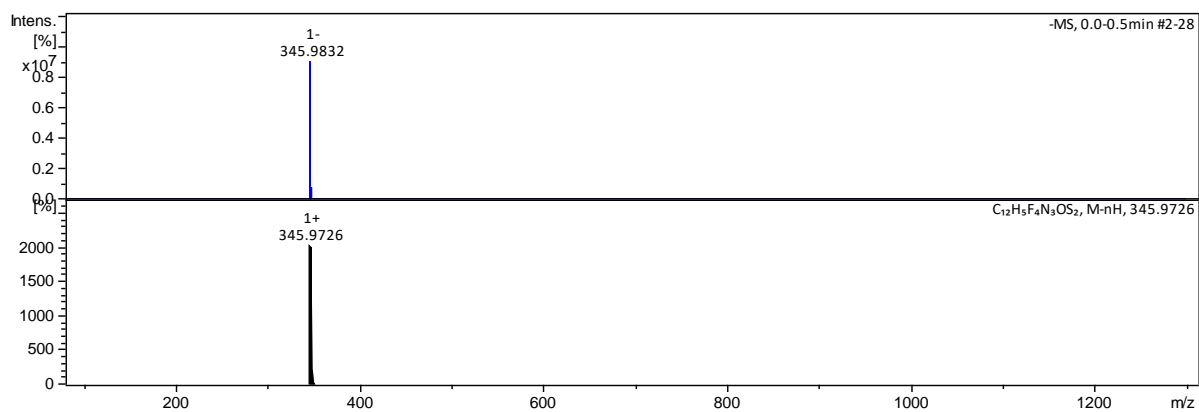


Figure S32. MS spectrum of compound 2d.

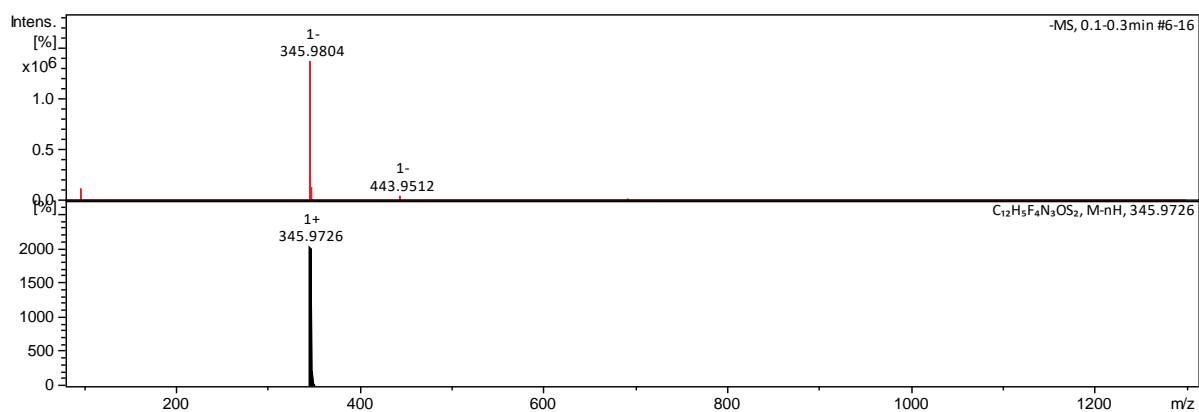


Figure S33. MS spectrum of compound 2e.

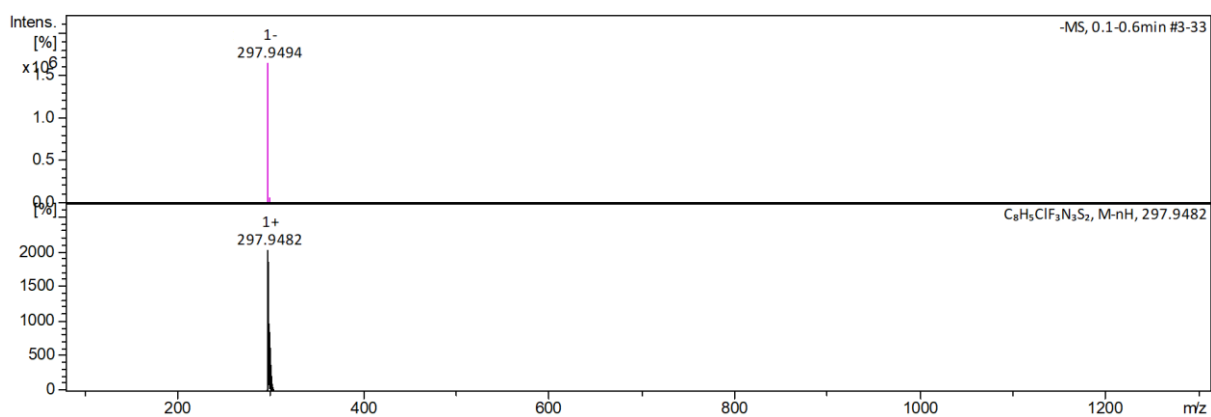


Figure S34. MS spectrum of compound 3a.

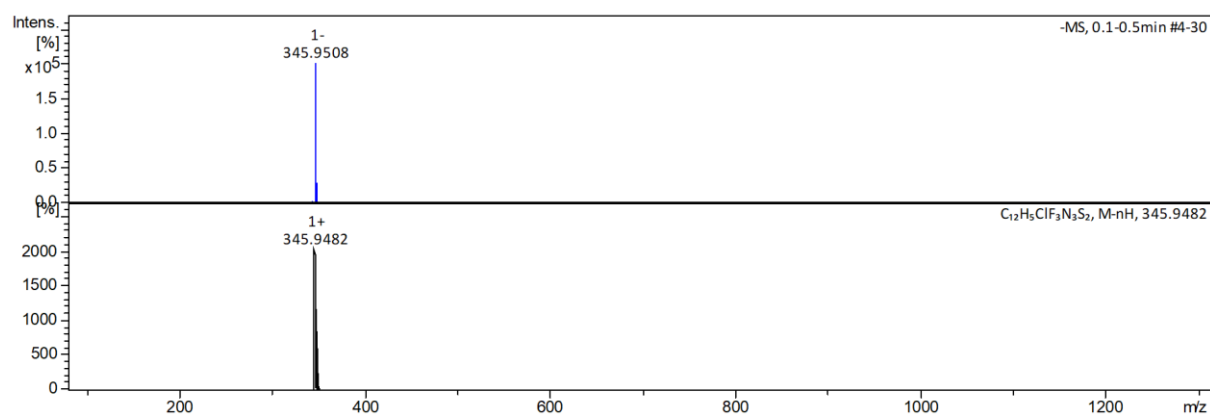


Figure S35. MS spectrum of compound 3b.

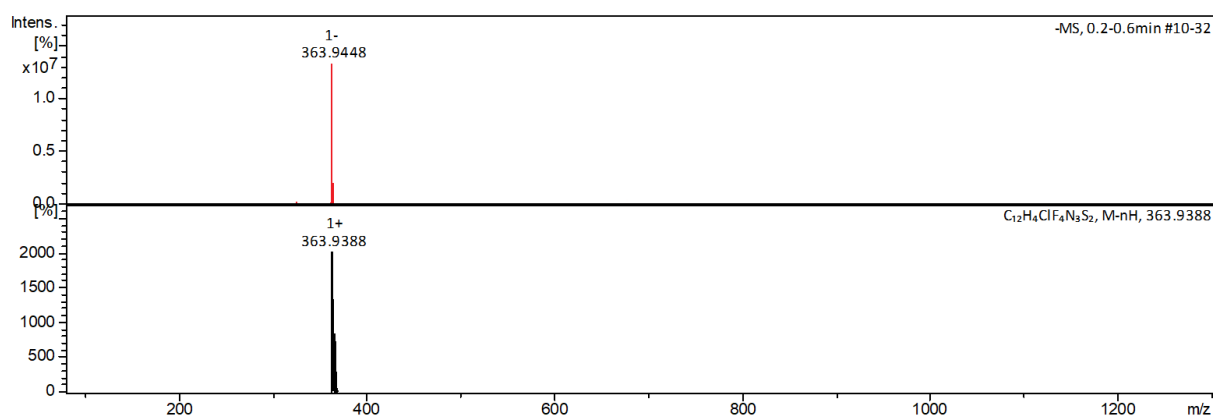


Figure S36. MS spectrum of compound 3c.

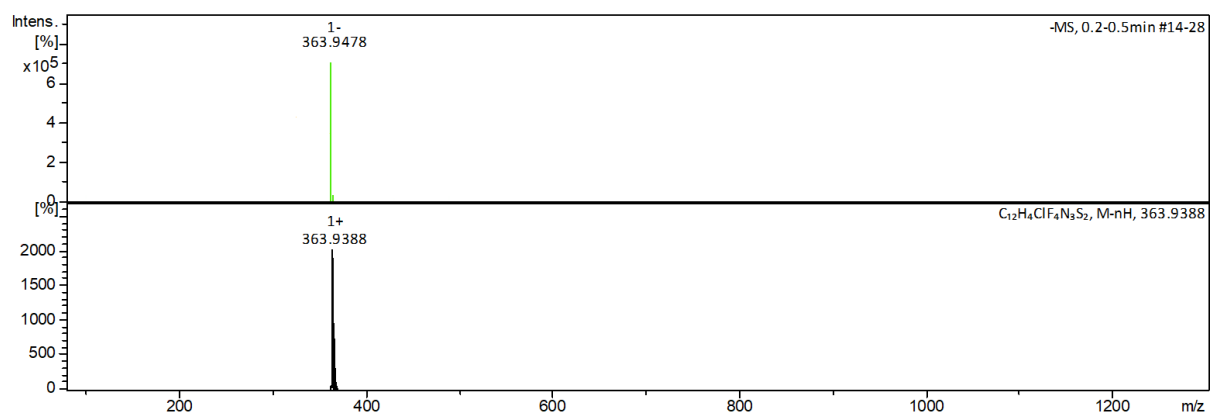


Figure S37. MS spectrum of compound 3d.

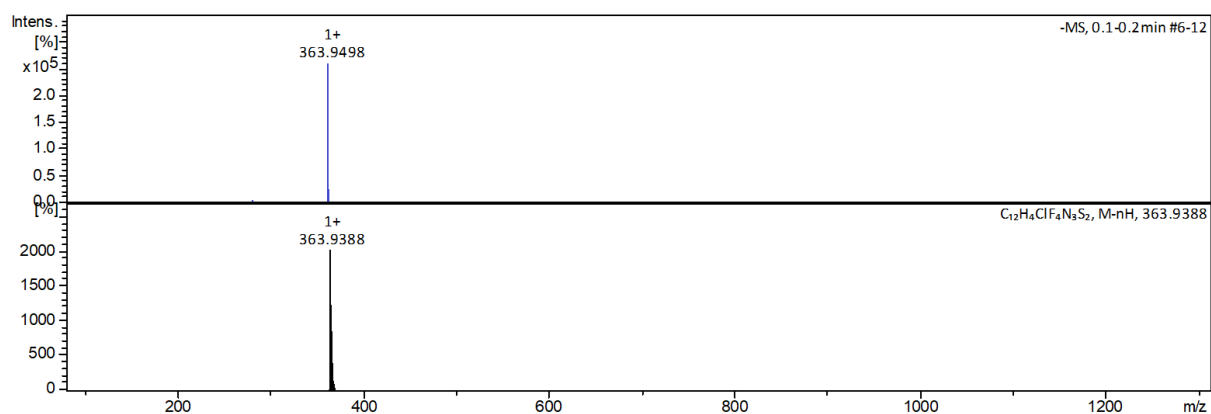


Figure S38. MS spectrum of compound 3e.

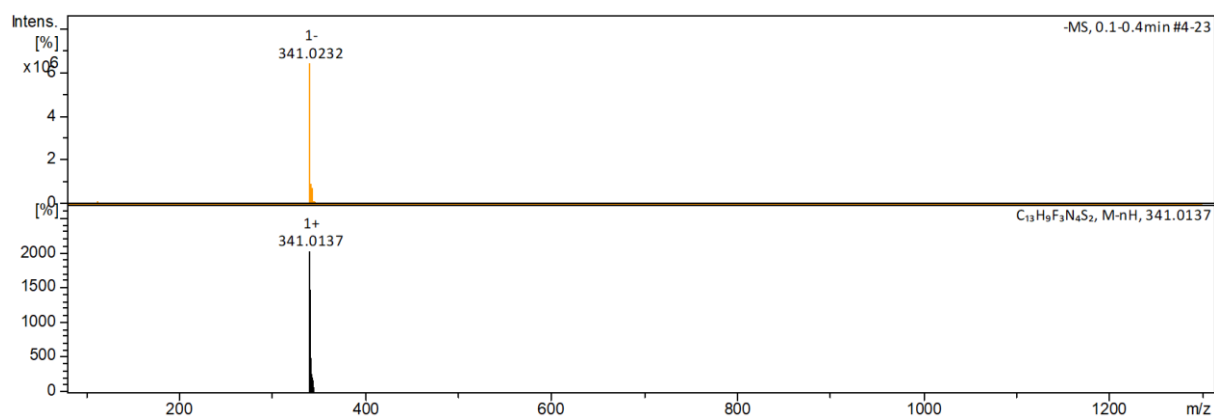


Figure S39. MS spectrum of compound 4a.

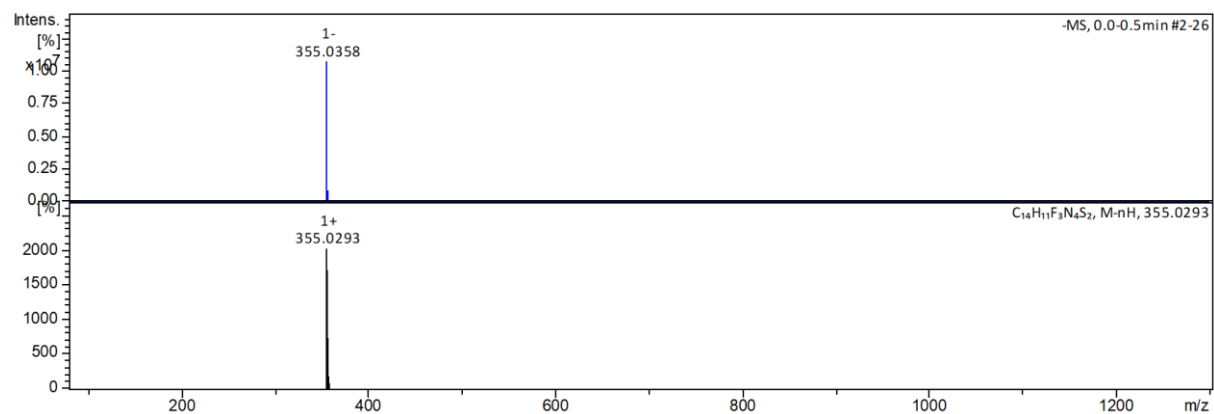


Figure S40. MS spectrum of compound 4b.

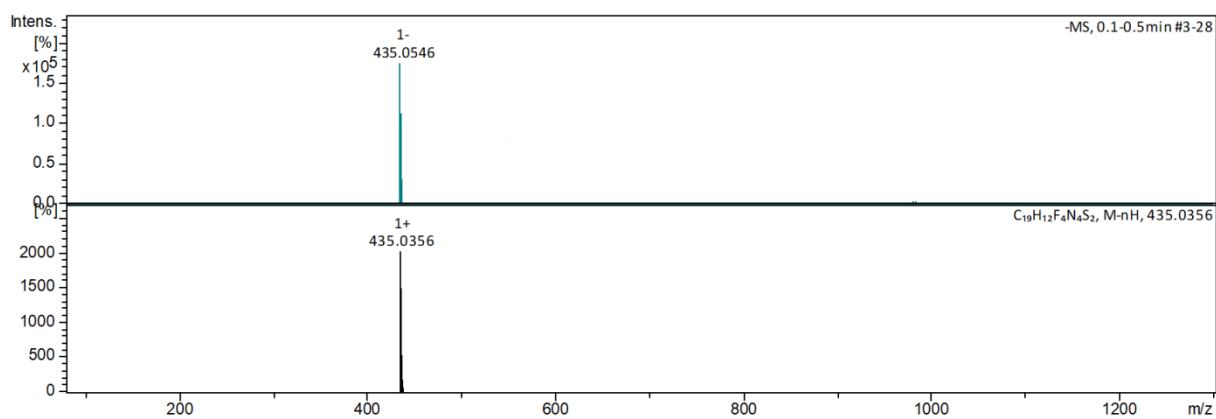


Figure S41. MS spectrum of compound 4c.

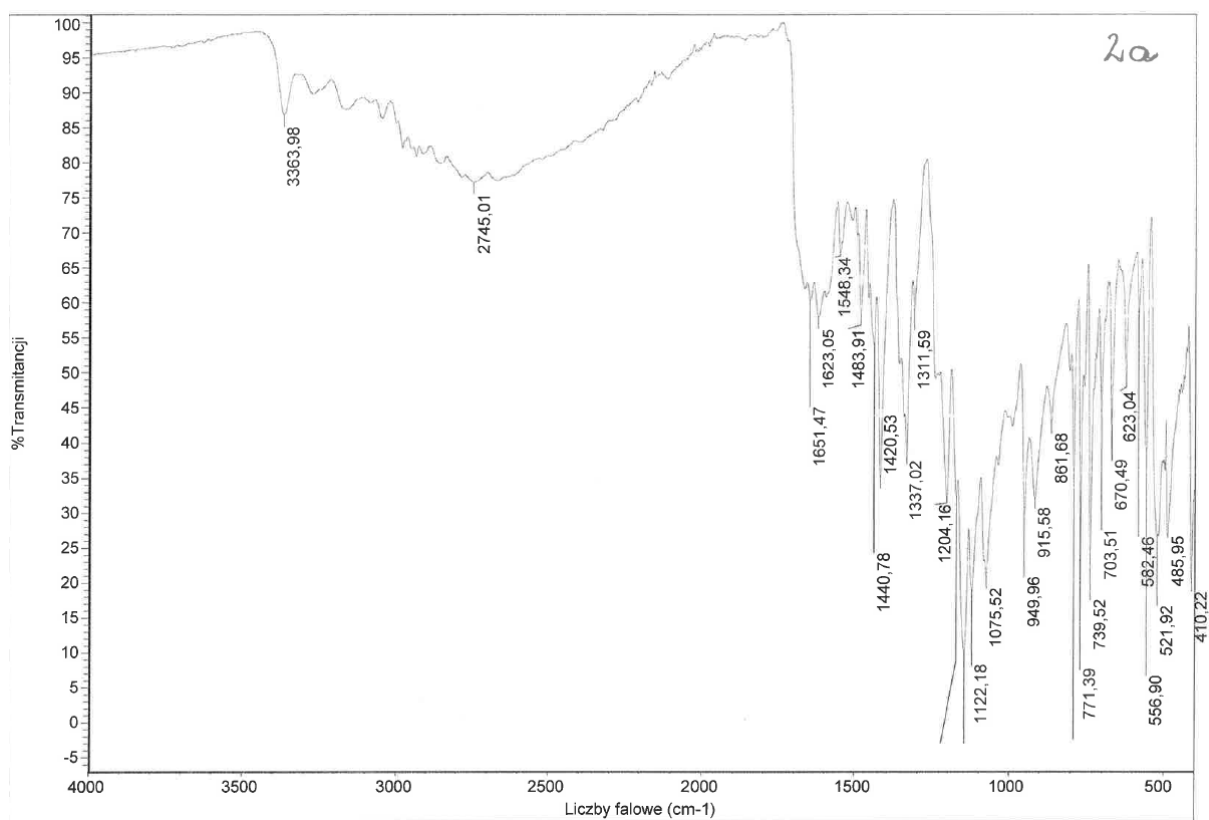


Figure S42. IR spectrum of compound 2a.

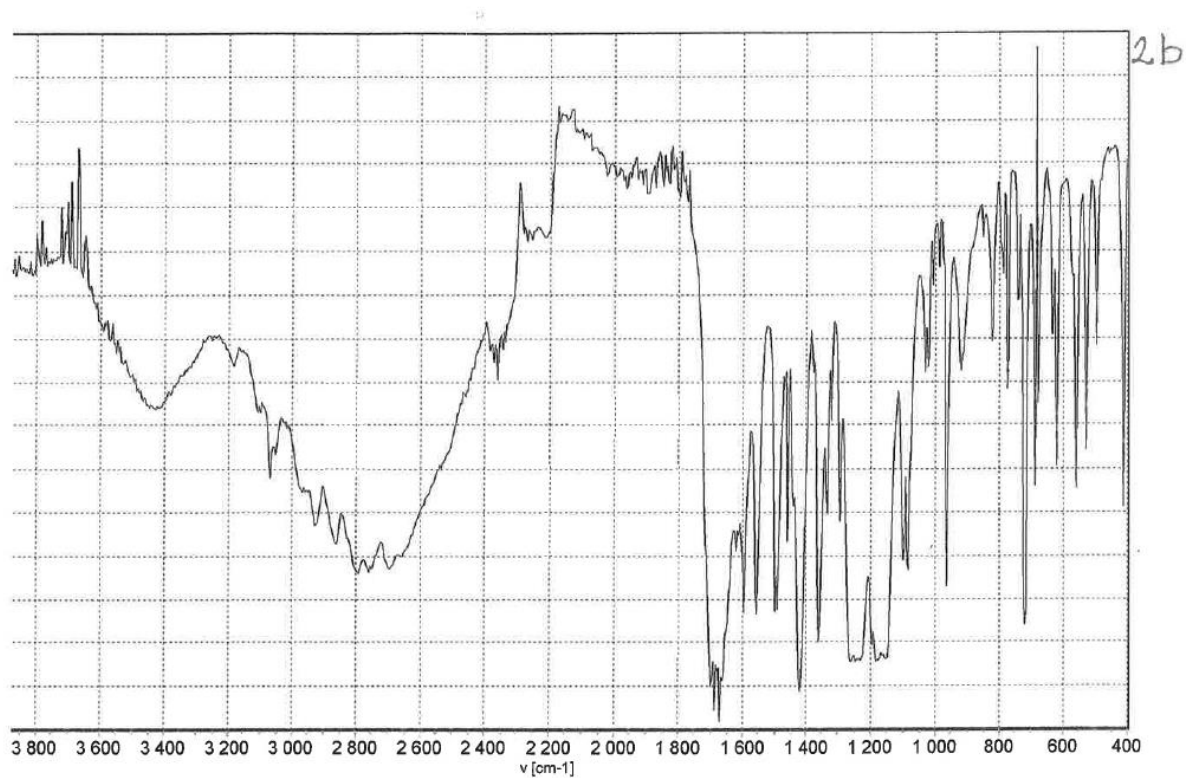


Figure S43. IR spectrum of compound 2b.

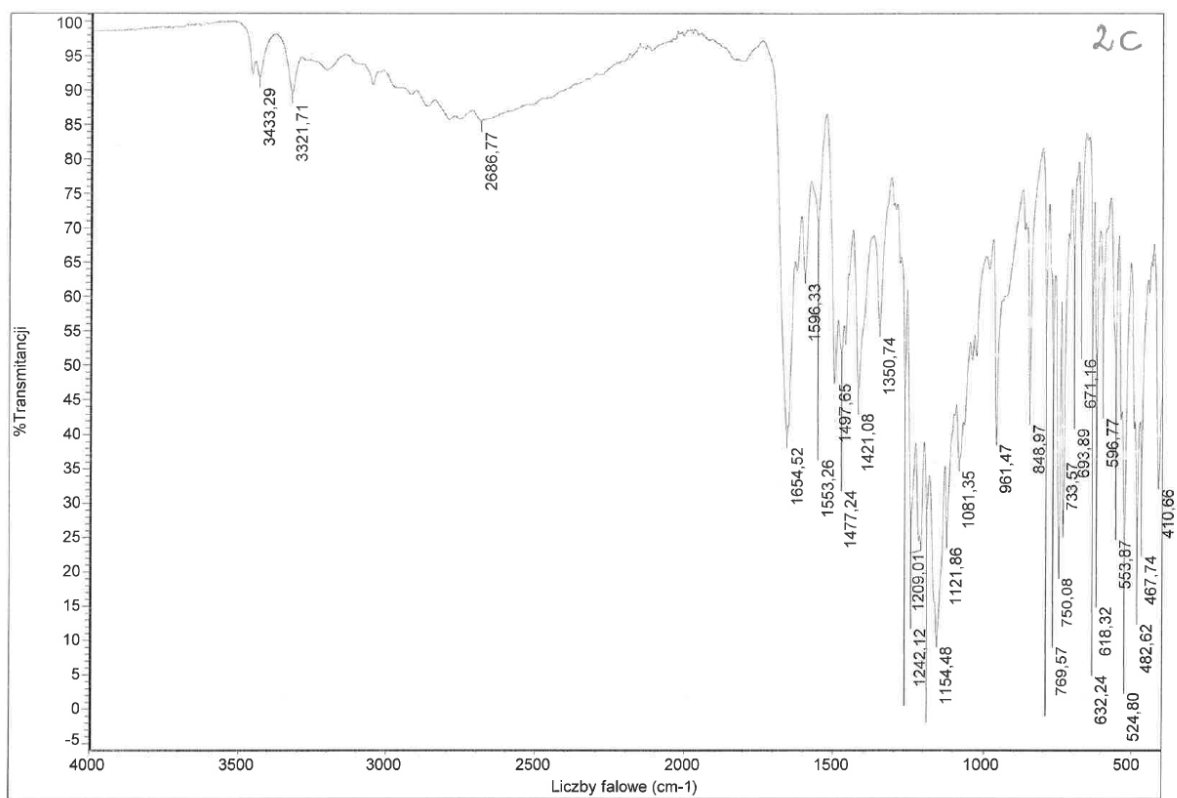


Figure S44. IR spectrum of compound 2c.

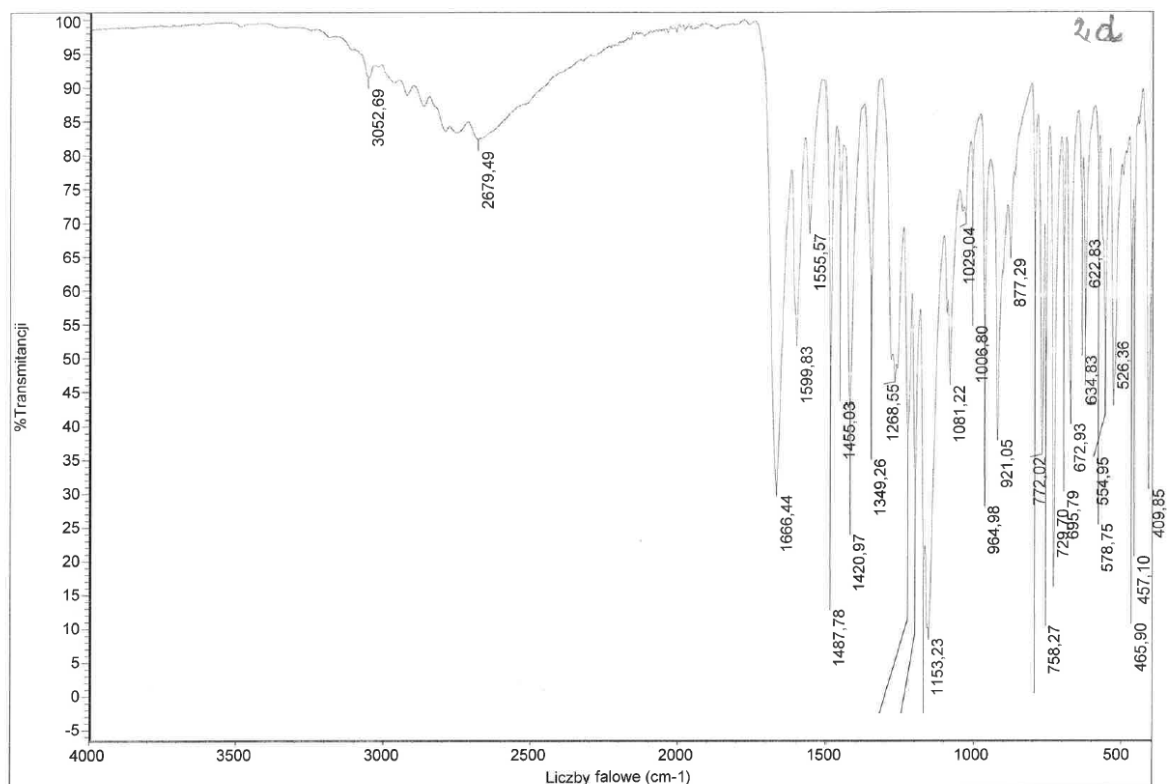


Figure S45. IR spectrum of compound **2d**.

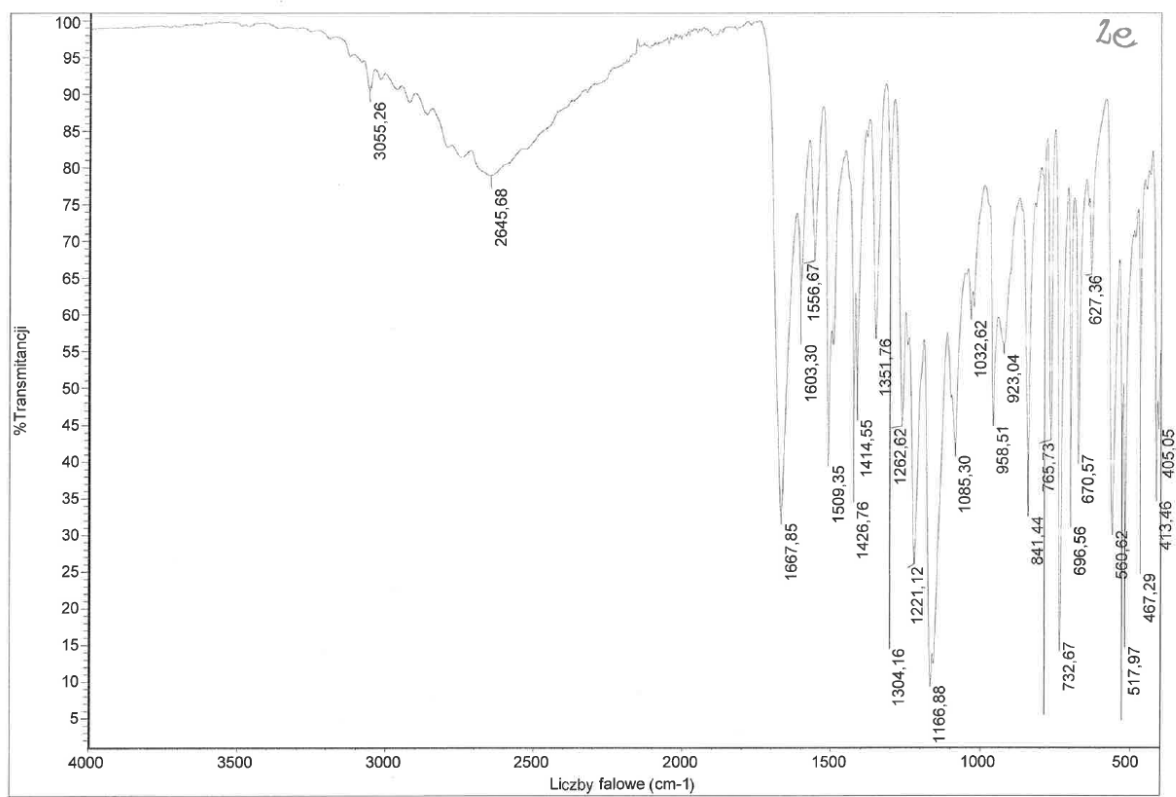


Figure S46. IR spectrum of compound **2e**.

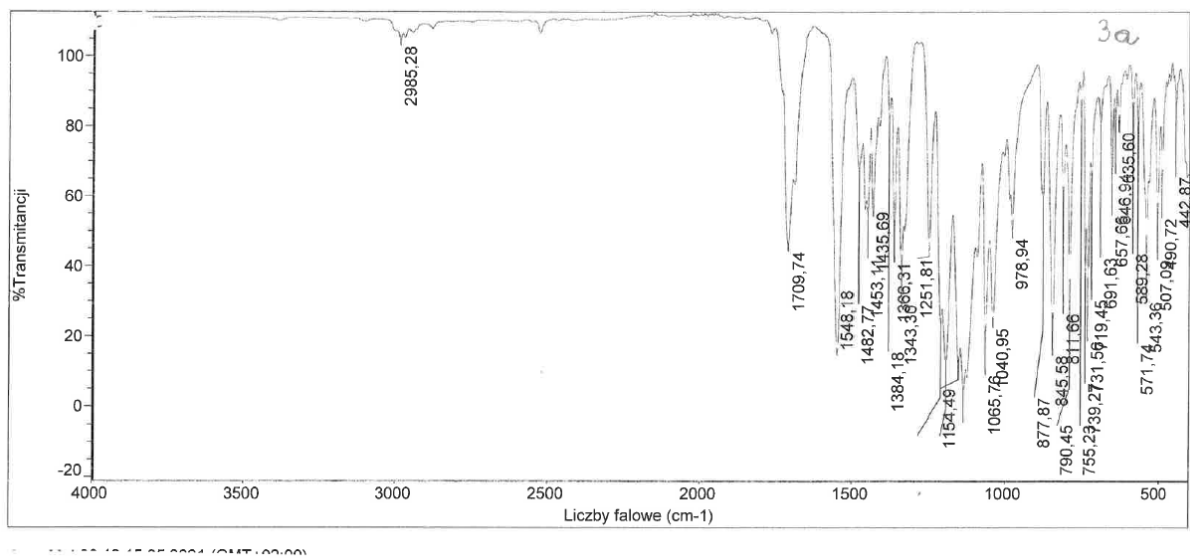


Figure S47. IR spectrum of compound 3a.

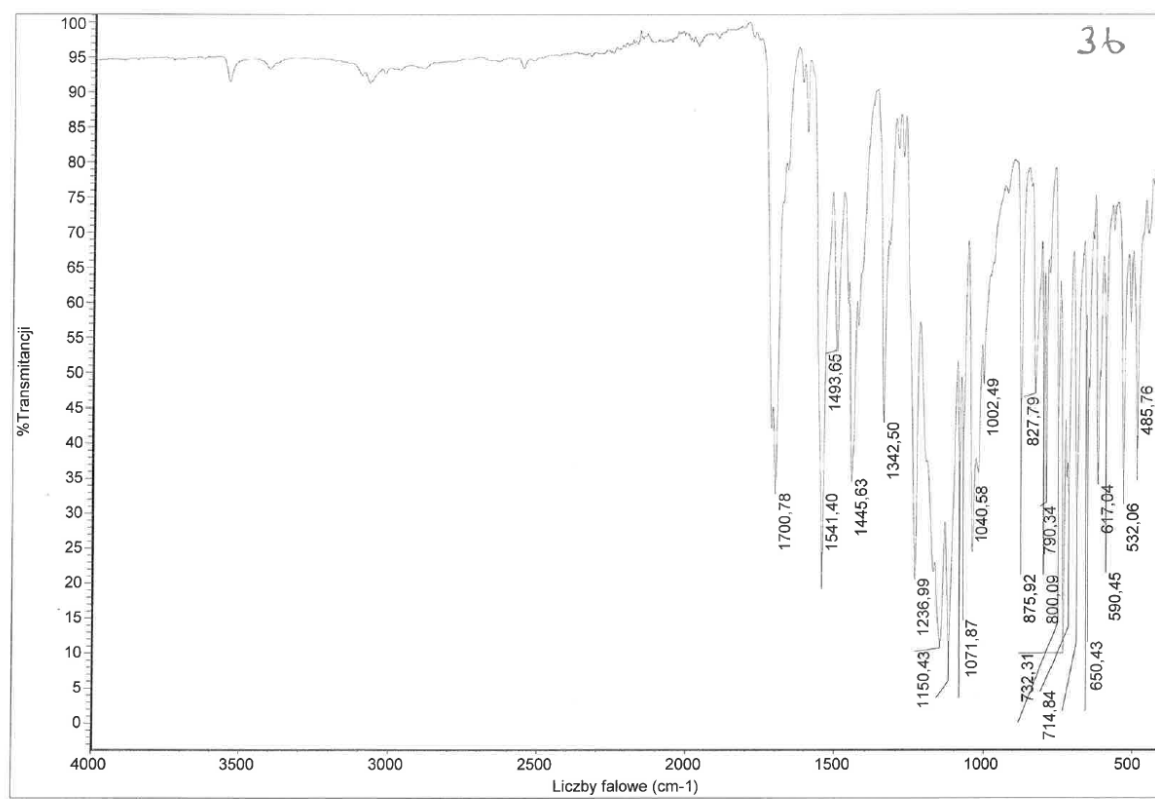


Figure S48. IR spectrum of compound 3b.

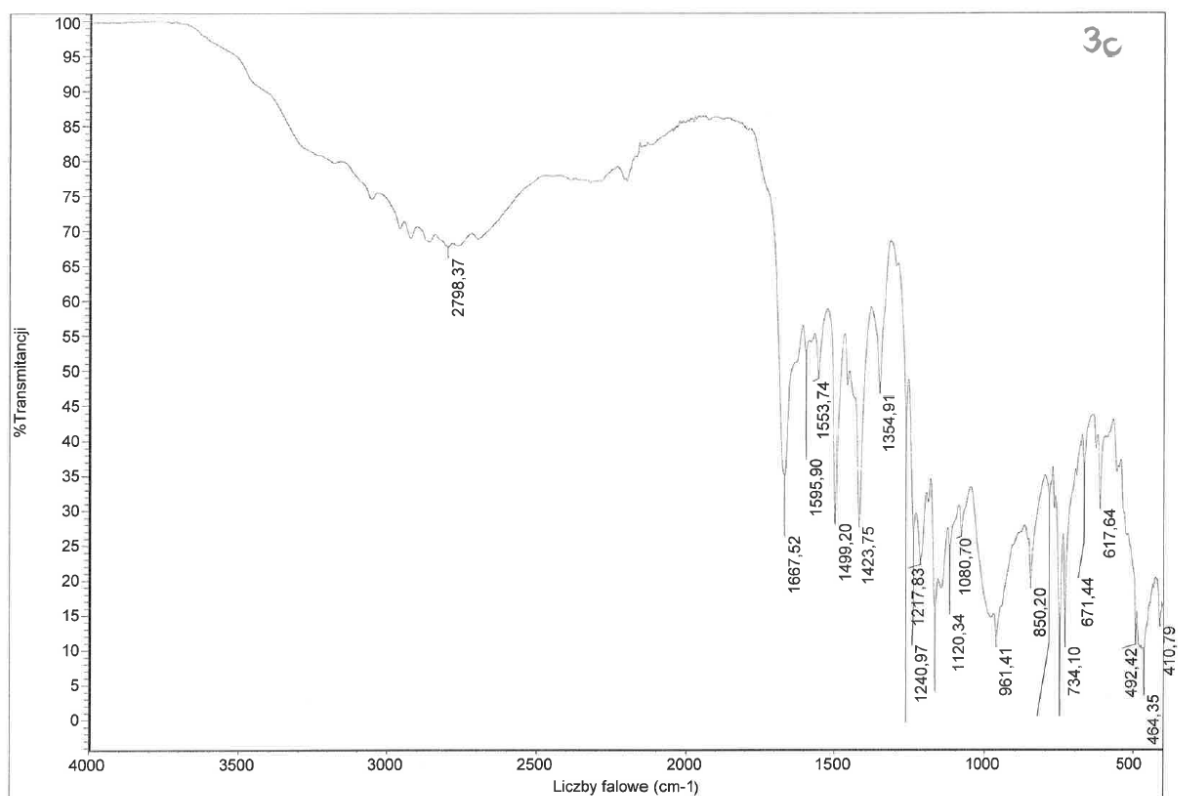


Figure S49. IR spectrum of compound 3c.

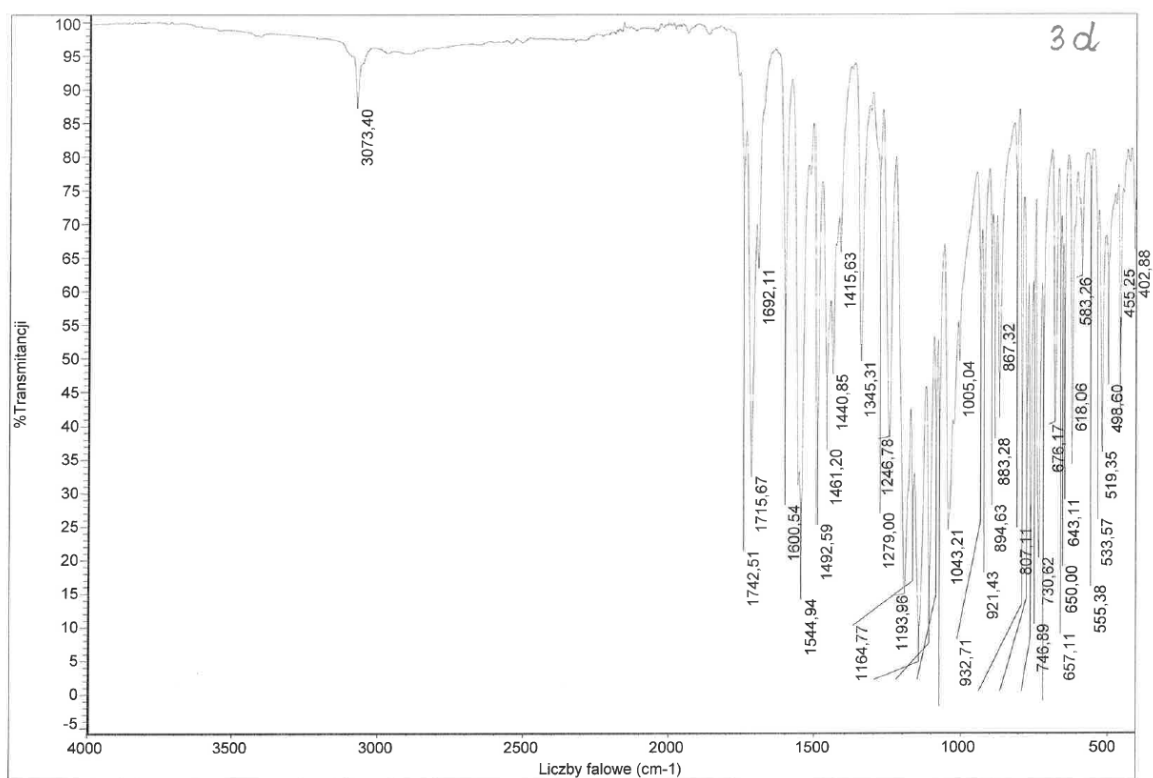


Figure S50. IR spectrum of compound 3d.

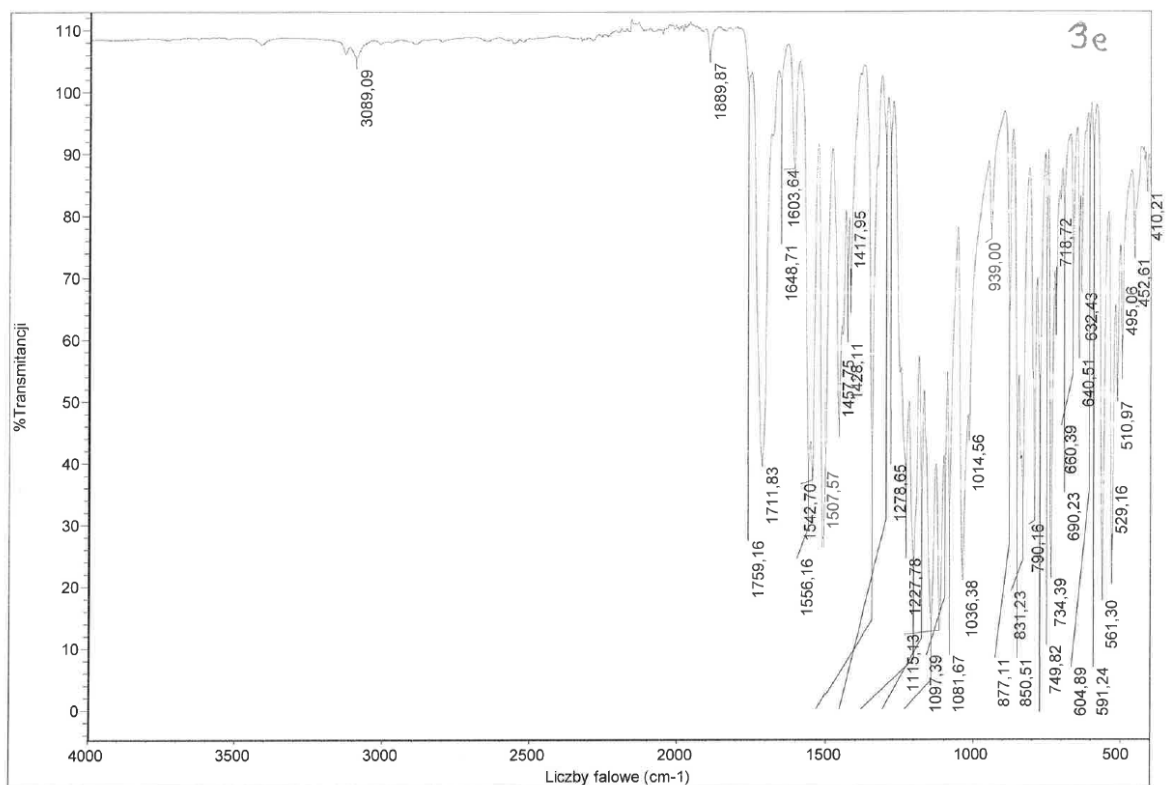


Figure S51. IR spectrum of compound **3e**.

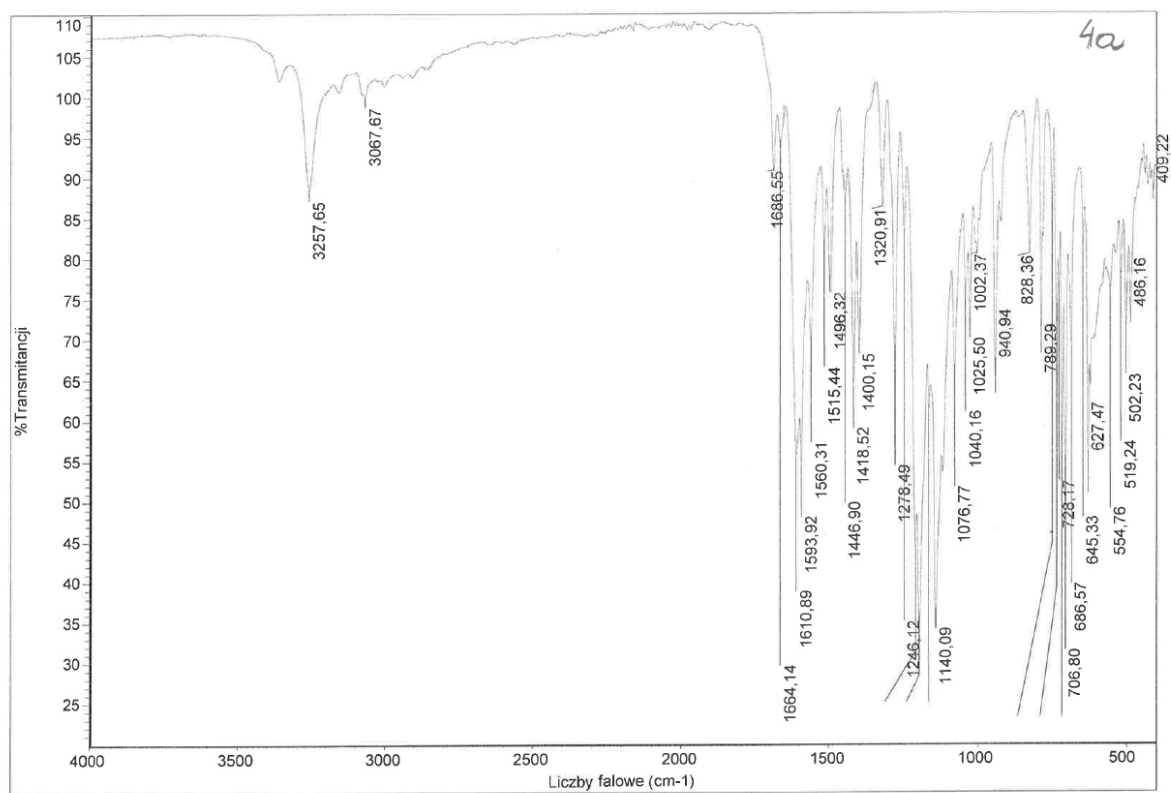


Figure S52. IR spectrum of compound **4a**.

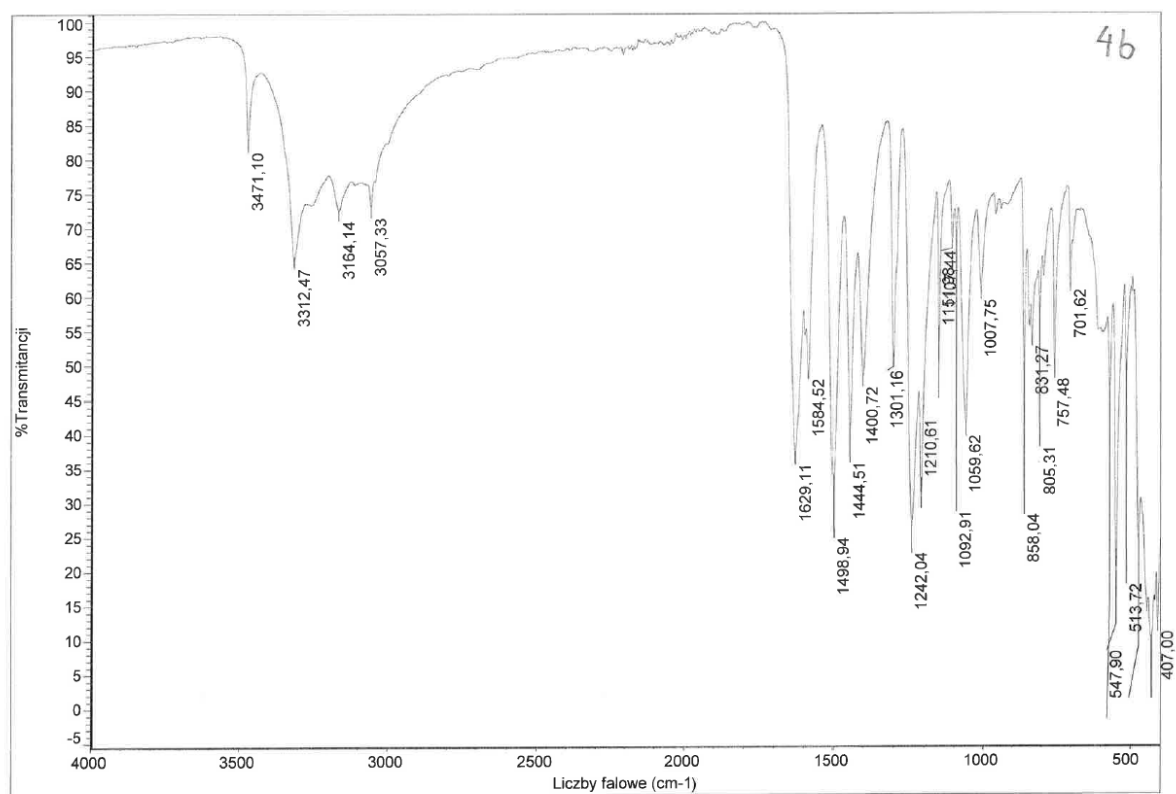


Figure S53. IR spectrum of compound 4b.

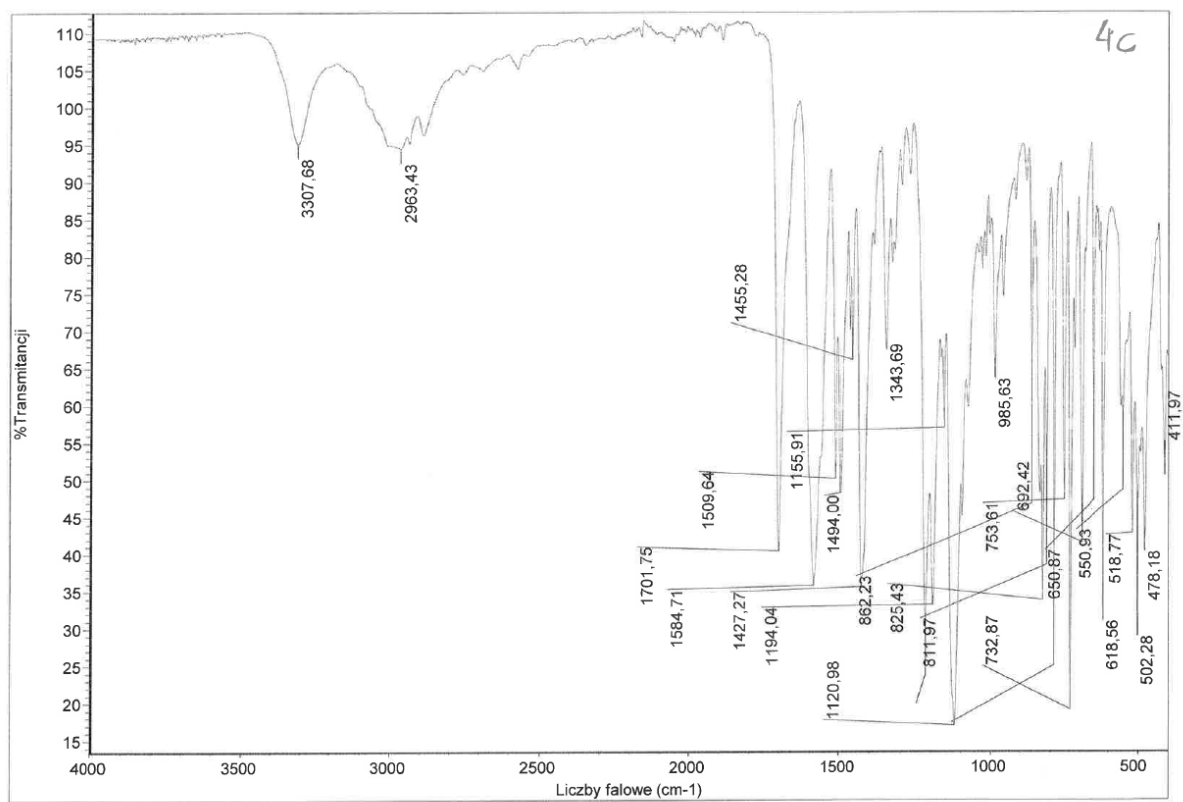


Figure S54. IR spectrum of compound 4c.

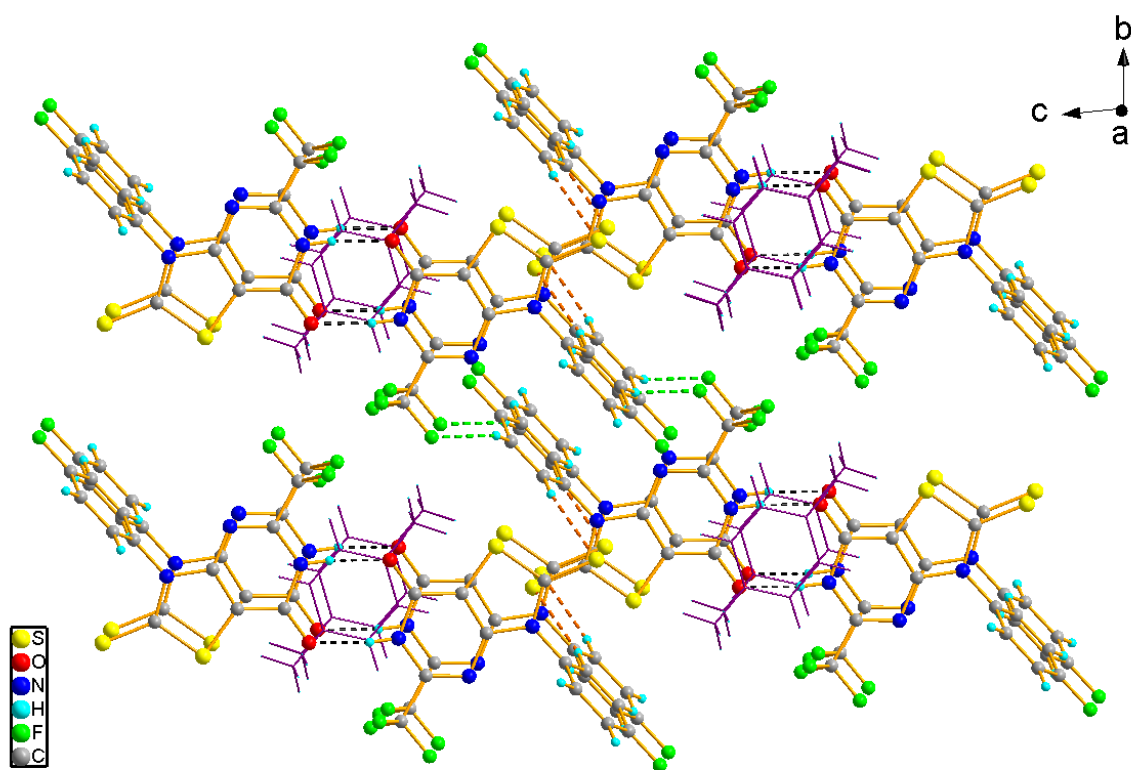


Figure S55. The crystal packing of the **2e** viewed along *a* axis. Disordered toluene molecules are marked with a purple wire/stick model. Dashed lines (in black) indicate intermolecular interactions, with N—H \cdots O in black, C—H \cdots S in orange and C—H \cdots F in light green.

Table S1. Selected X-ray single-crystal data and structure refinement details of compounds **2e** and **4b**.

	2e	4b
Chemical formula	2(C ₁₂ H ₅ F ₄ N ₃ OS ₂), C ₇ H ₈	C ₁₄ H ₁₁ F ₃ N ₄ S ₂
<i>M_r</i> (g/mol)	786.75	356.39
Crystal system, space group	triclinic, <i>P</i> -1	monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	100	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.217 (2), 9.362 (3), 12.381 (3)	16.228(4), 5.599(2), 17.631(4)
<i>α</i> , <i>β</i> , <i>γ</i> (°)	95.81 (2), 90.55 (2), 99.02 (2)	90, 111.050(5), 90
<i>V</i> (Å ³)	347.46 (17)	1495.1(7)
<i>Z</i>	1	4
<i>λ</i> (Å)	1.54184	1.54184
Crystal size (mm)	0.190 x 0.125 x 0.041	0.207 × 0.034 × 0.021
Crystal colour, shape	yellow, plate	light yellow, needle
<i>D_{calc}</i> (g/cm ³)	1.590	1.583
<i>μ</i> (mm ⁻¹)	3.45	3.58
<i>F</i> (000)	398	728
2 <i>θ</i> range (°)	3.6 - 75.7	3.2-75.5
No of measured, independent and observed [<i>I</i> > 2 <i>σ</i> (<i>I</i>)] reflections	16332, 3355, 3066	10153, 3044, 2463
<i>R_{int}</i>	0.030	0.085
Parameters, restraints	336, 0	209, 0
Goof on <i>F</i> ²	1.06	1.04
<i>R</i> ₁ [<i>I</i> > 2 <i>σ</i> (<i>I</i>)]	0.039	0.075
<i>wR</i> ₂ (all data)	0.111	0.215
<i>T_{min}</i> , <i>T_{max}</i>	0.69, 1.00	0.51, 1.00
<i>Δρ_{max}</i> , <i>Δρ_{min}</i> (e Å ⁻³)	0.52, -0.40	1.01, -0.66
CCDC No	2118584	2118585