

New pyrazolyl thioureas active against the *Staphylococcus* genus

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Supporting Material:

Table S1. Elemental analysis of compounds **1** and **4d**.

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Figure S22: ¹³C NMR (101 MHz) of compound **1k**.

Figure S23: ¹H NMR (400 MHz) of compound **1l**.

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Figure S25: ¹H NMR (400 MHz) of compound **1m**.

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Figure S27: ¹H NMR (400 MHz) of compound **1n**.

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Figure S29: ¹H NMR (400 MHz) of compound **o**.

Figure S30: ¹³C NMR (101 MHz) of compound **1o**.

Figure S31: ¹H NMR (400 MHz) of compound **4d**

Figure S32: ¹³C NMR (101 MHz) of compound **4d**.

Figure S33: BOILED-Egg diagram for compounds **1a-o**

Figure S34: radar plot calculated for compounds **1a-o**

Table S1. Elemental analysis of compounds **1** and **4d**. Compounds have been considered pure when the difference between calculated and found values is ± 0.4 .

Comp.	Values	%C	%H	%N	%S
1a	Calcd.	54.24	5.36	14.88	8.52
	Found	54.00	5.21	15.69	8.22
1b	Calcd.	51.77	4.86	14.20	8.13
	Found	51.20	4.66	14.10	7.99
1c	Calcd.	51.77	4.86	14.20	8.13
	Found	51.52	5.00	14.32	8.00
1d	Calcd.	51.77	4.86	14.20	8.13
	Found	51.61	4.52	13.91	8.00
1e	Calcd.	55.37	5.68	14.35	8.21
	Found	55.63	5.69	14.46	8.31
1f	Calcd.	52.93	5.18	13.72	7.85
	Found	52.77	5.00	13.56	7.44
1g	Calcd.	52.93	5.18	13.72	7.85
	Found	52.87	5.10	13.56	7.56
1h	Calcd.	52.93	5.18	13.72	7.85
	Found	52.71	5.08	13.74	7.52
1i	Calcd.	56.42	5.98	13.85	7.93
	Found	56.60	5.95	13.98	8.10
1j	Calcd.	54.02	5.49	13.26	7.59
	Found	54.14	5.50	13.30	8.00
1k	Calcd.	54.02	5.49	13.26	7.59
	Found	54.00	5.40	13.10	7.80
1l	Calcd.	54.02	5.49	13.26	7.59
	Found	54.26	5.50	13.55	7.90
1m	Calcd.	57.40	6.26	13.39	7.66
	Found	57.69	6.83	13.56	7.13
1n	Calcd.	55.03	5.77	12.84	7.34
	Found	55.00	5.55	12.65	7.14
1o	Calcd.	55.03	5.77	12.84	7.34
	Found	55.02	5.65	12.84	6.33
4d	Calcd.	56.45	8.29	16.46	//
	Found	56.23	8.00	16.54	//

Chemical Structure: 1-(4-hydroxy-2-methyl-1H-imidazol-5-yl)-N-phenylacetamide

¹H NMR Spectrum (DMSO-d₆):

Chemical Shift (ppm)	Integration
7.95, 7.93, 7.89, 7.88, 7.87, 7.87, 7.71, 7.70, 7.69, 7.68, 7.67, 7.67, 7.58, 7.56, 7.55, 7.54, 7.52, 7.50, 7.46, 7.46, 7.45, 7.44, 7.43, 7.37, 6.11	1.06, 1.01
5.06, 5.05, 5.05, 4.15, 4.15, 4.11, 4.05, 4.03, 4.02, 4.01, 3.99, 3.97, 3.97, 3.96, 3.95, 3.93, 3.91, 3.36, 3.25, 3.24, 3.23, 3.23, 3.18, 3.16, 3.09, 3.09, 3.07, 3.06, 3.05, 3.03, 3.02, 3.01	6.90, 1.00, 5.59, 6.86

Chemical structure of compound 10 is shown. The ^{13}C NMR spectrum (CDCl₃) shows peaks at the following chemical shifts (ppm): 180.47, 168.88, 161.44, 140.22, 139.93, 134.94, 132.02, 128.50, 128.09, 103.44, 66.87, 60.12, 57.55, 20.94, and 14.28.

Figure S3: ^1H NMR (400 MHz) of compound **1b**.

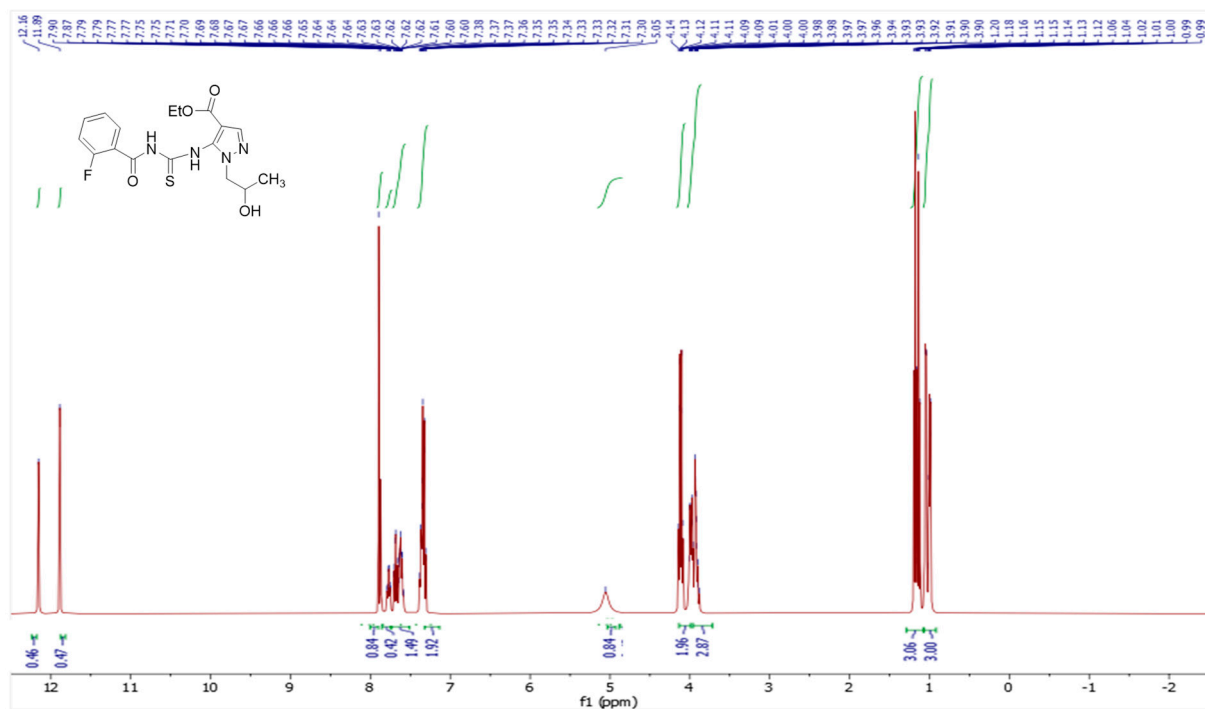


Figure S4: ^{13}C NMR (100 MHz) of compound **1b**.

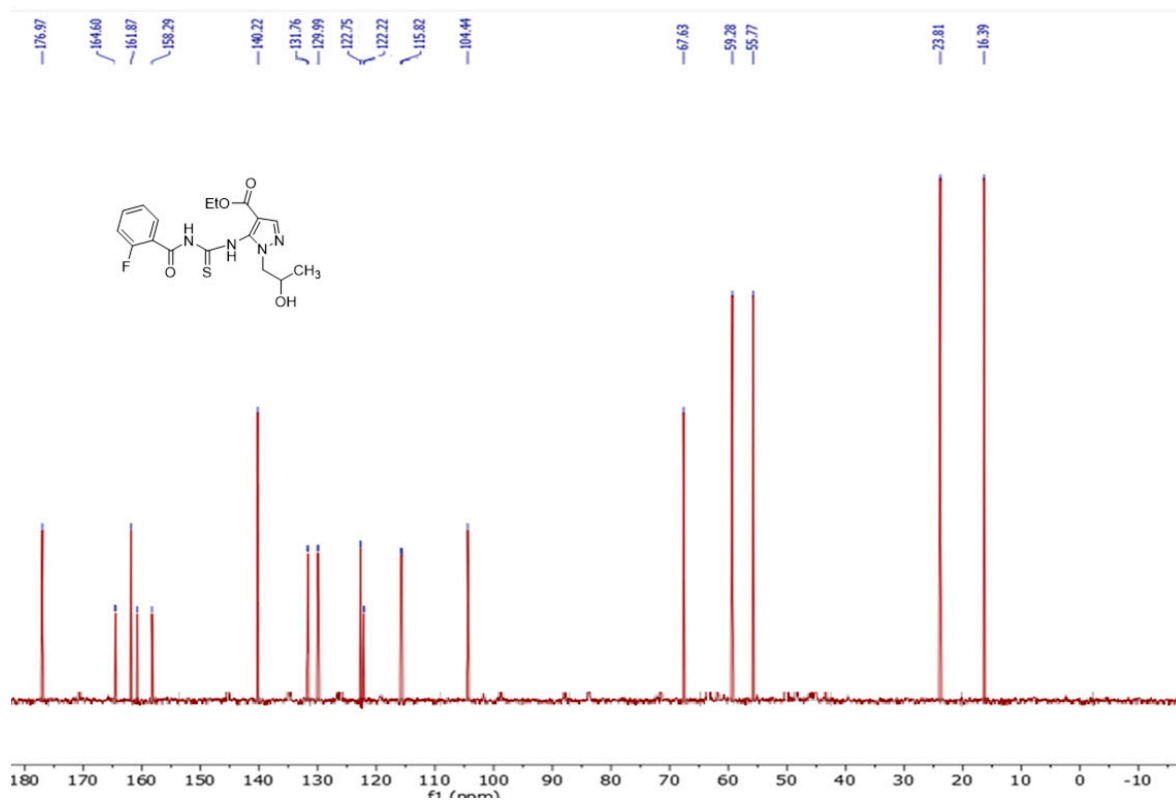


Figure S5: ^1H NMR (400 MHz) of compound 1c.

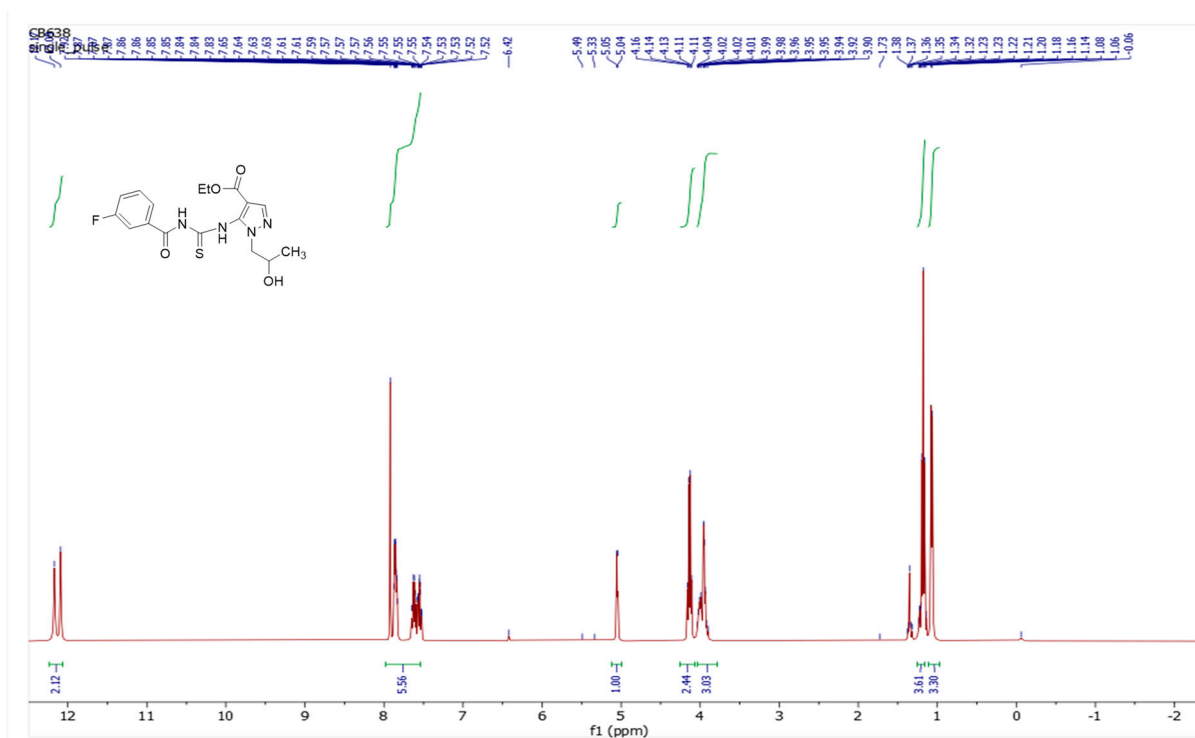


Figure S6: ^{13}C NMR (100 MHz) of compound 1c.

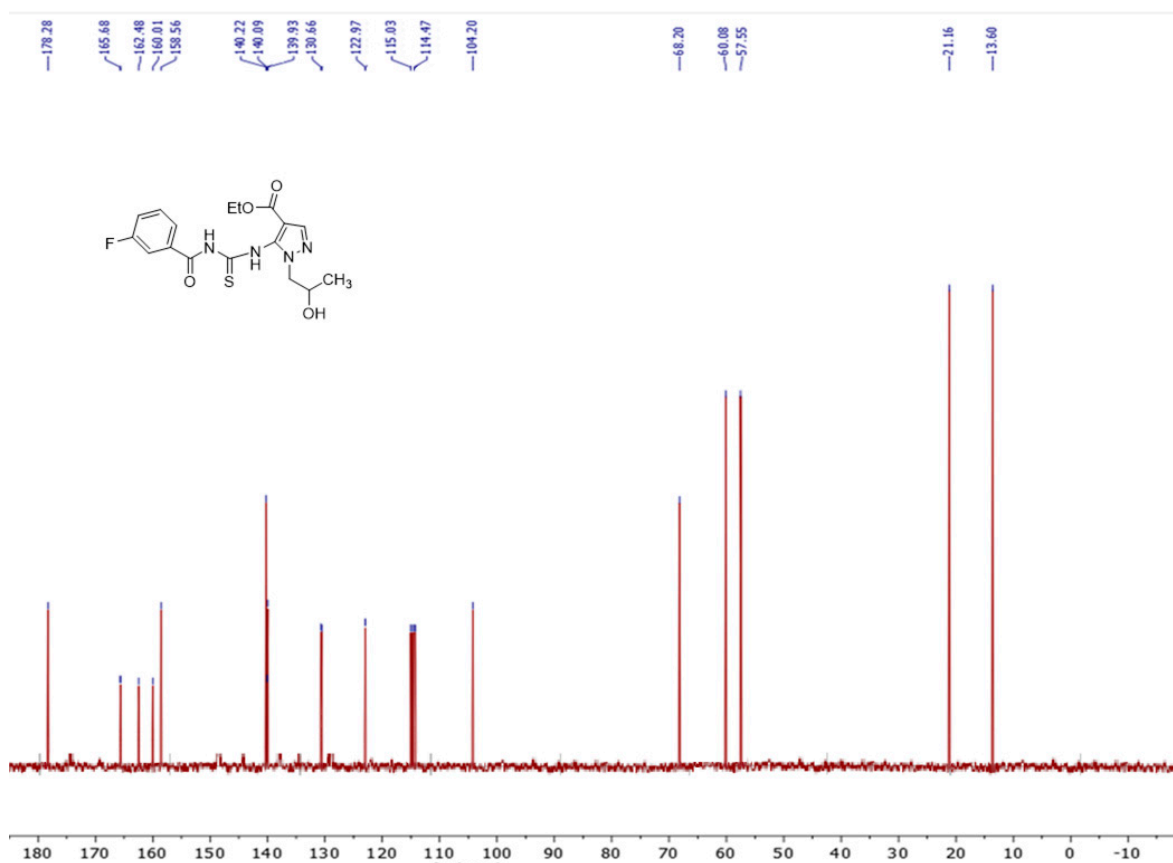


Figure S7: ^1H NMR (400 MHz) of compound **1d**.

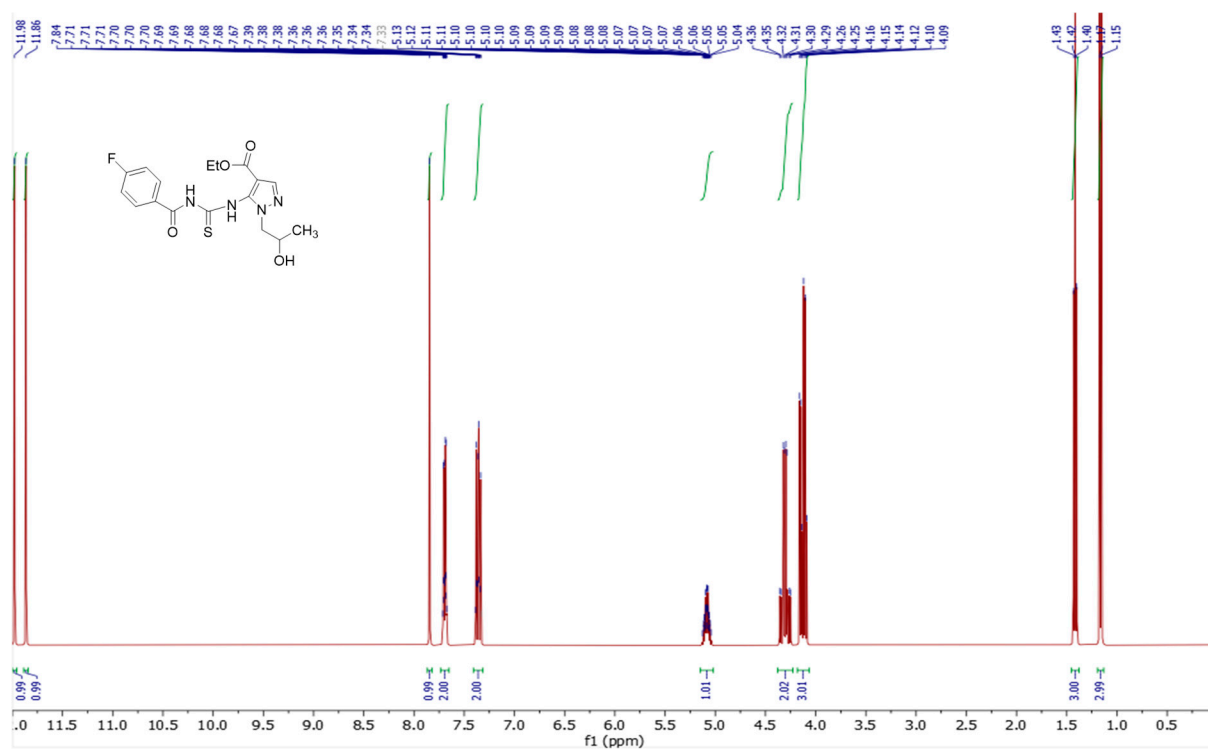


Figure S8: ^{13}C NMR (100 MHz) of compound **1d**.

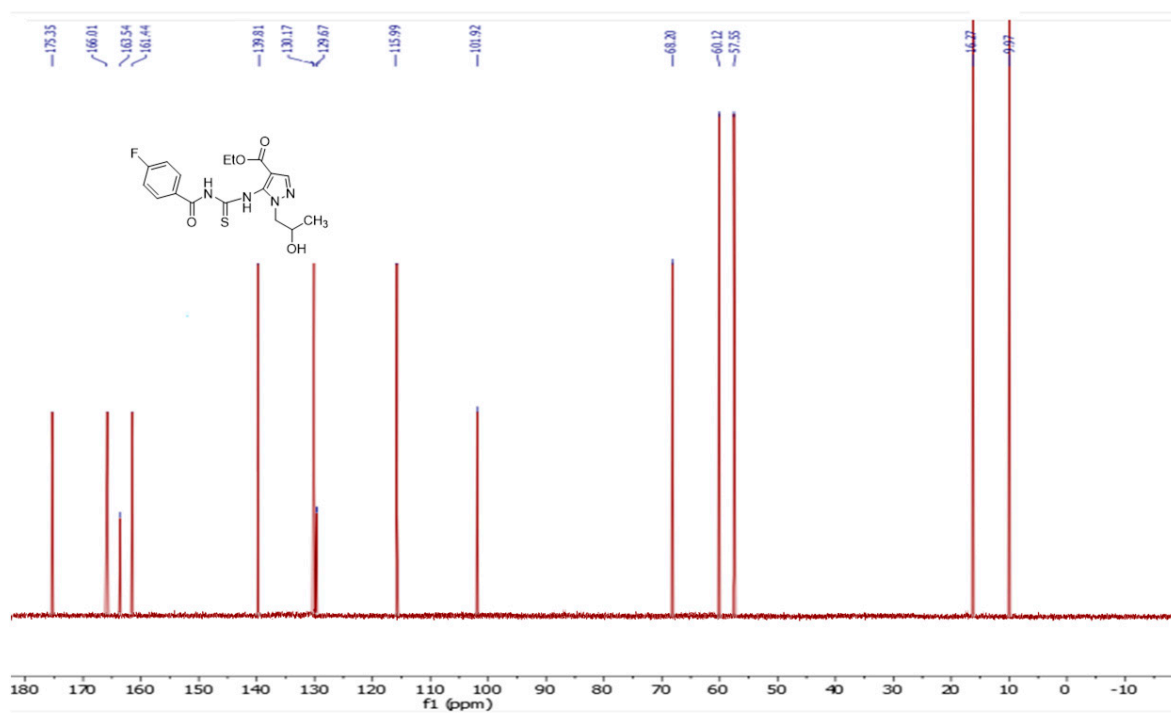


Figure S9: ^1H NMR (400 MHz) of compound **1e**.

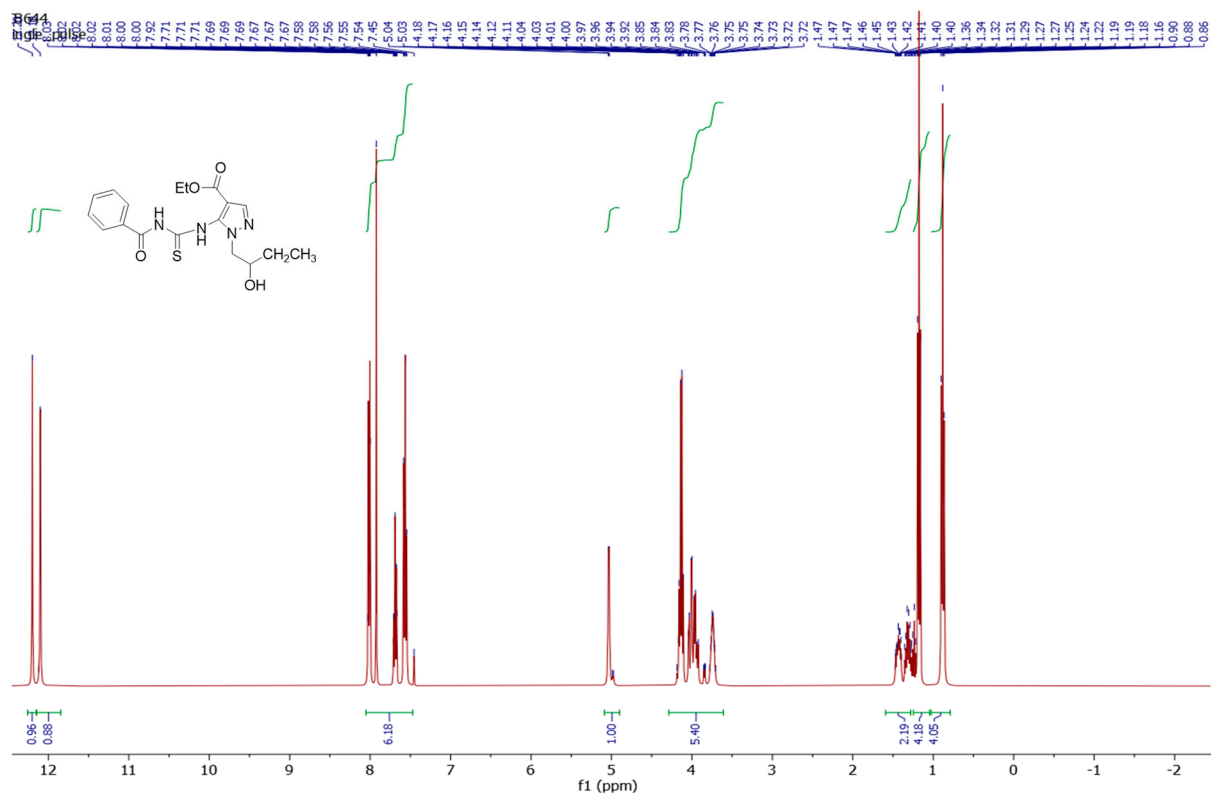


Figure S10: ^{13}C NMR (100 MHz) of compound **1e**.

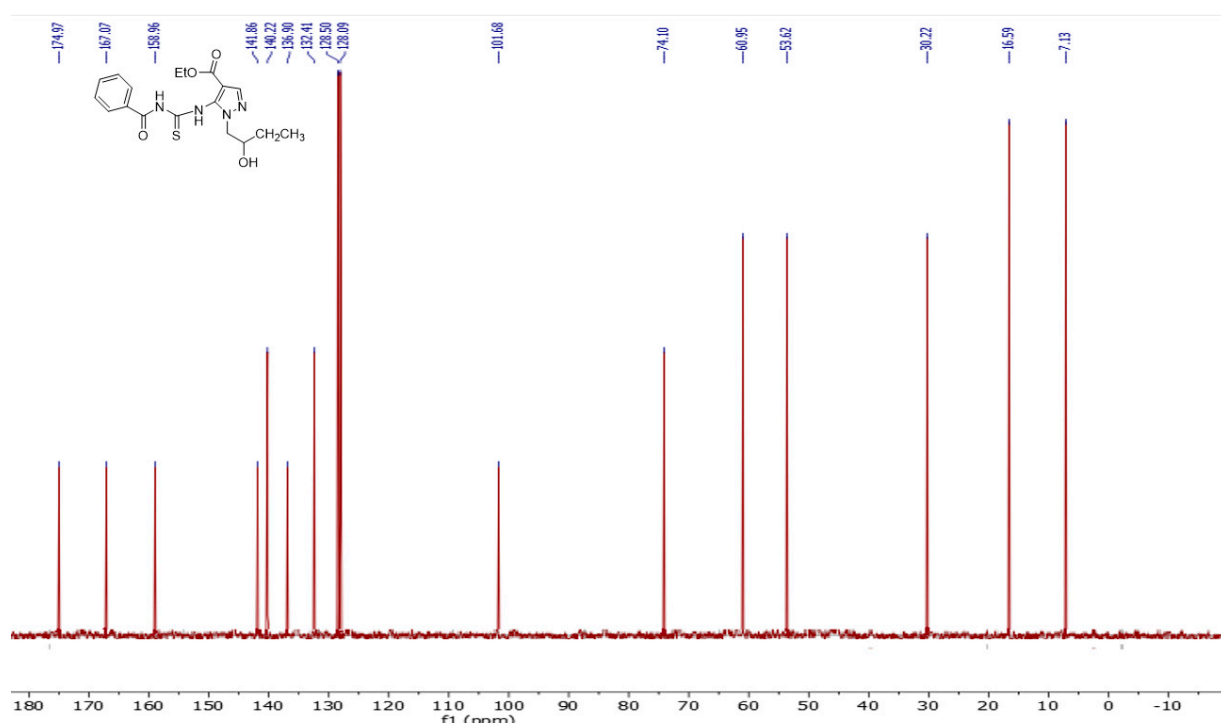


Figure S11: ^1H NMR (400 MHz) of compound **1f**.

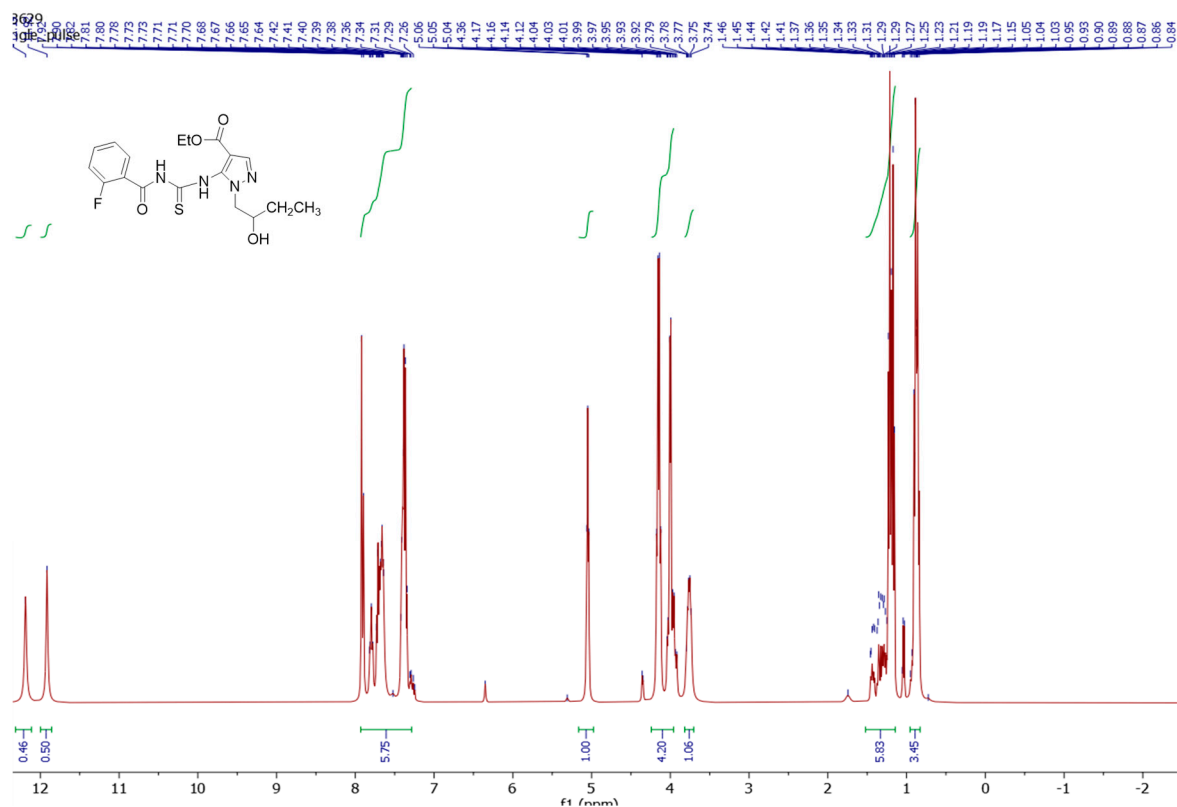


Figure S12: ^{13}C NMR (100 MHz) of compound **1f**.

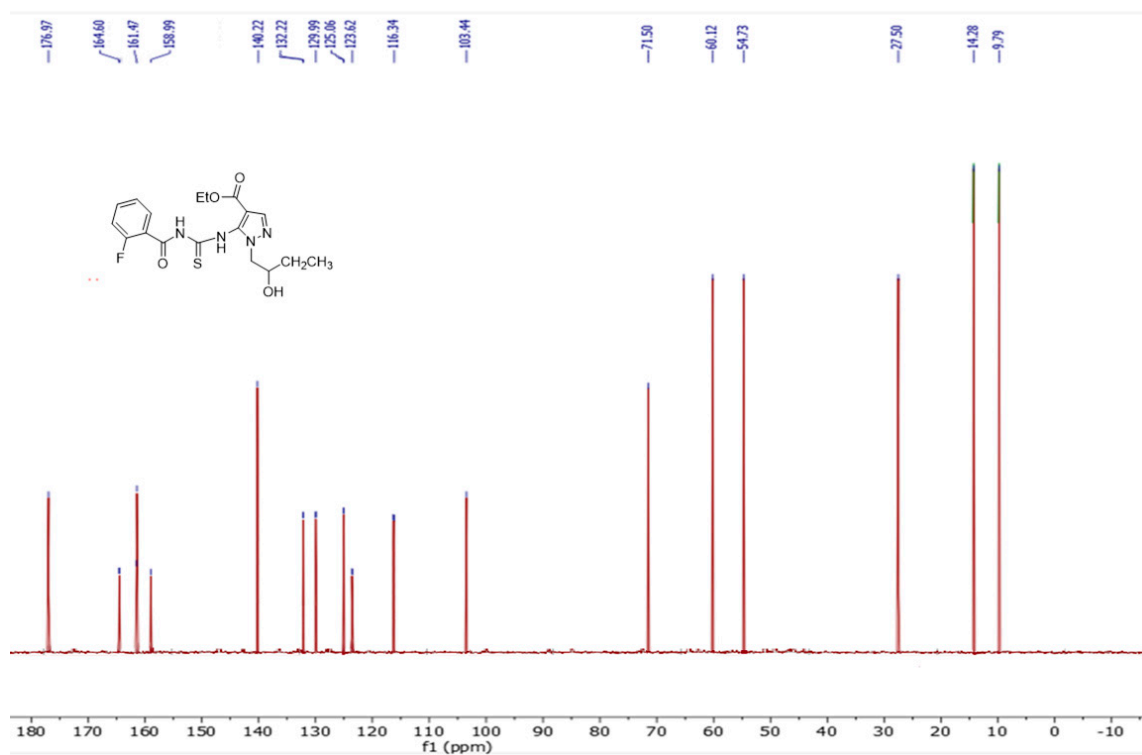


Figure S13: ^1H NMR (400 MHz) of compound **1g**.

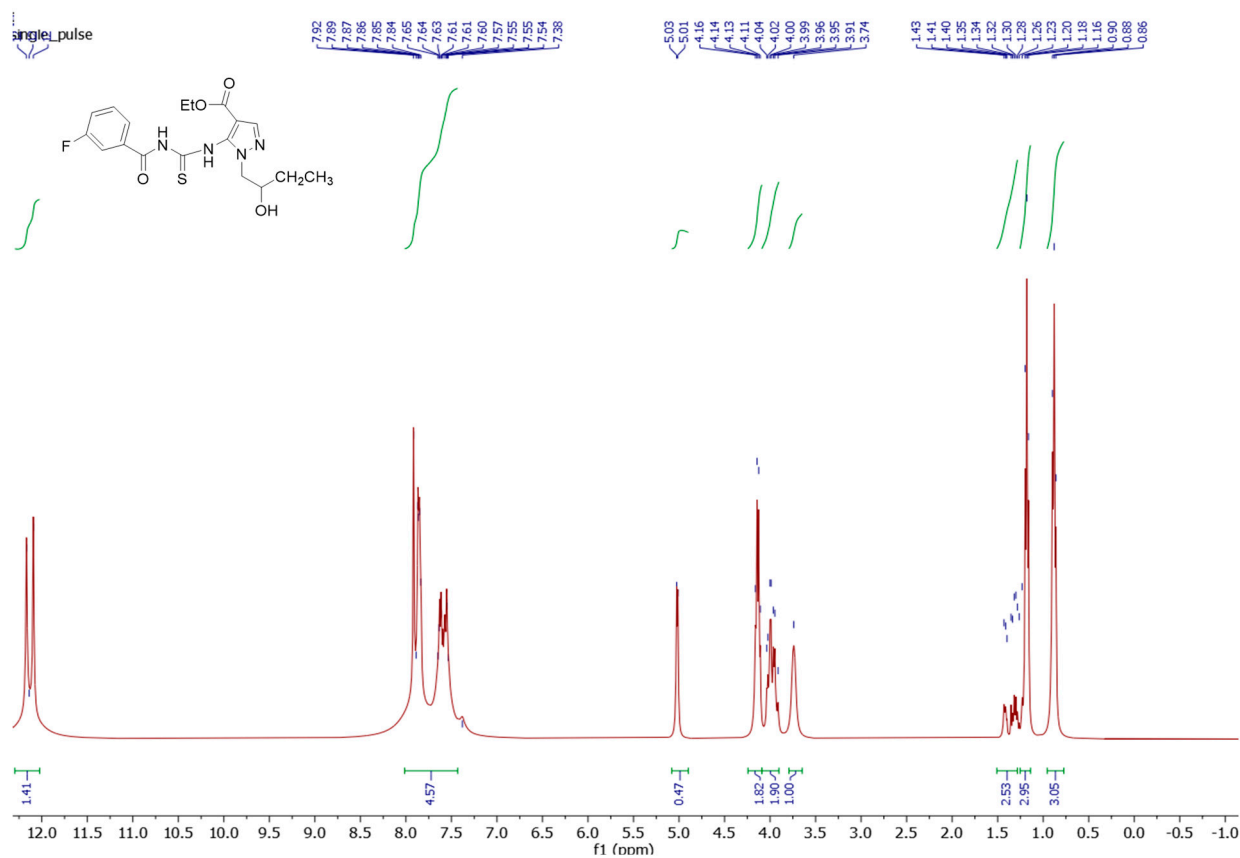


Figure S14: ^{13}C NMR (100 MHz) of compound **1g**.

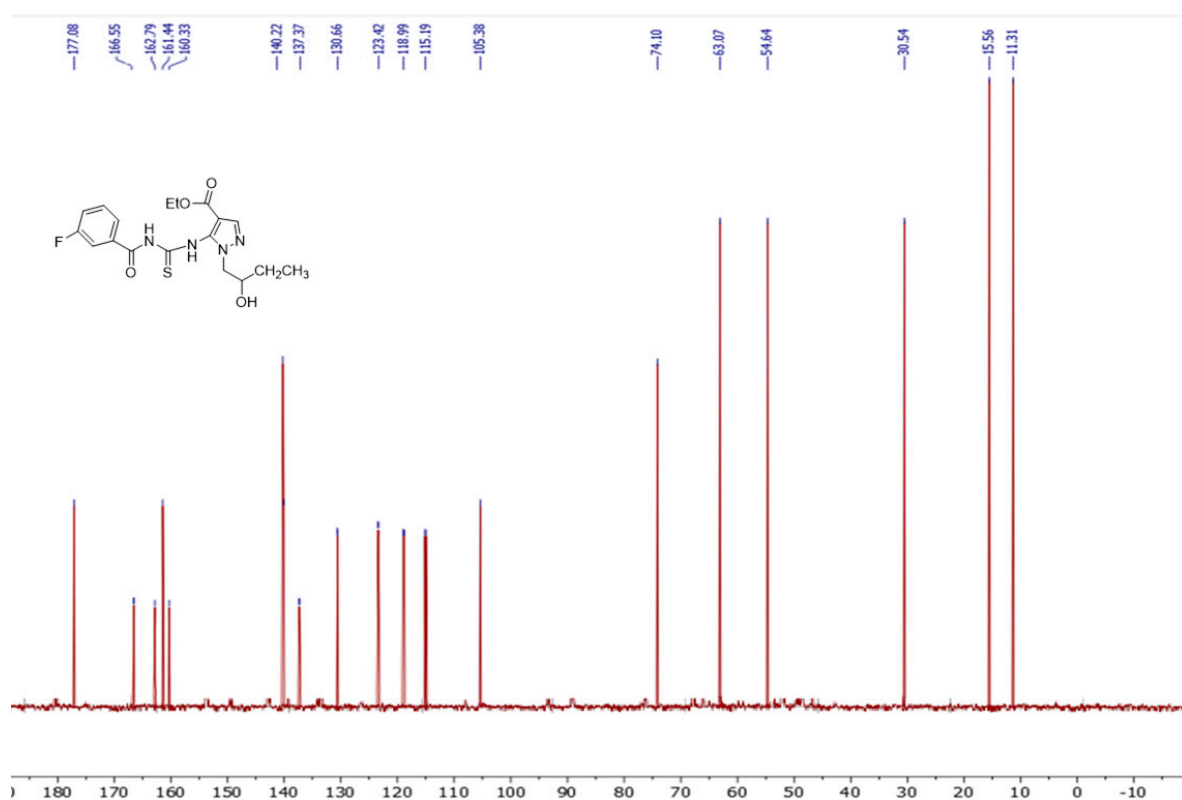


Figure S15: ^1H NMR (400 MHz) of compound 1h.

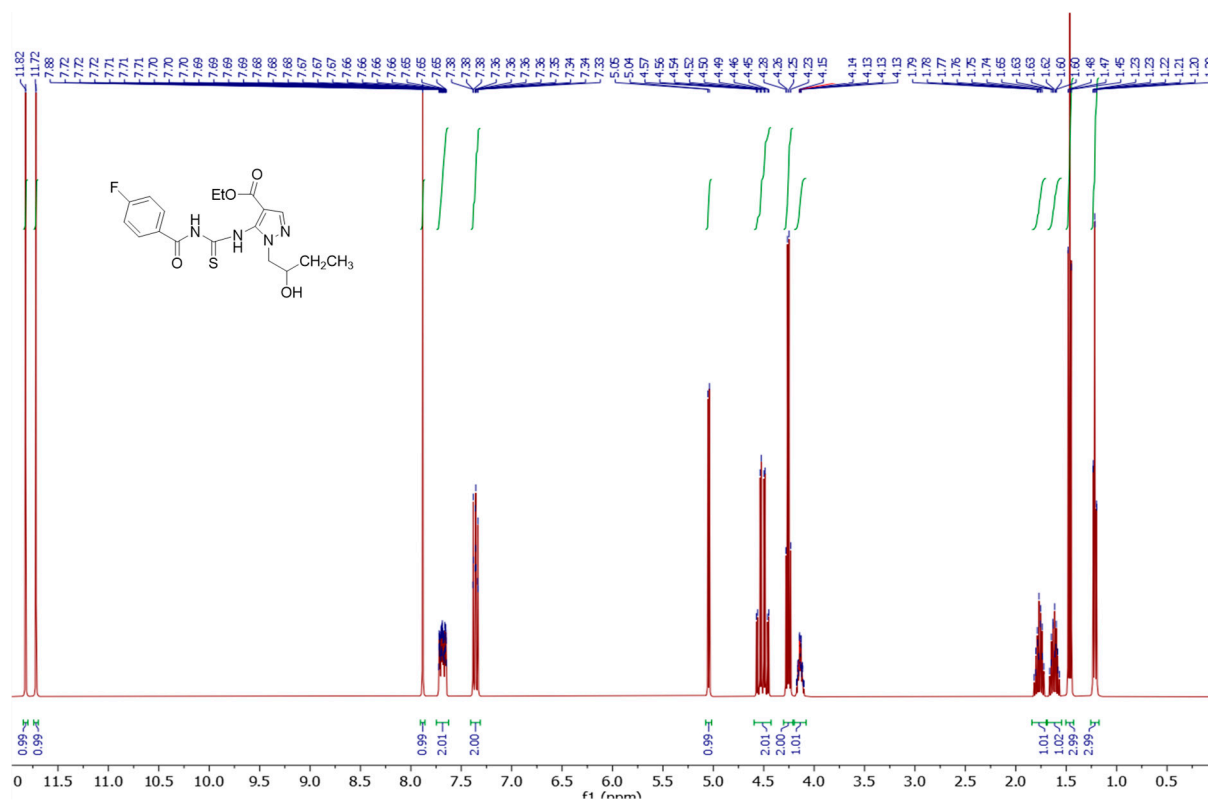


Figure S16: ^{13}C NMR (100 MHz) of compound 1h.

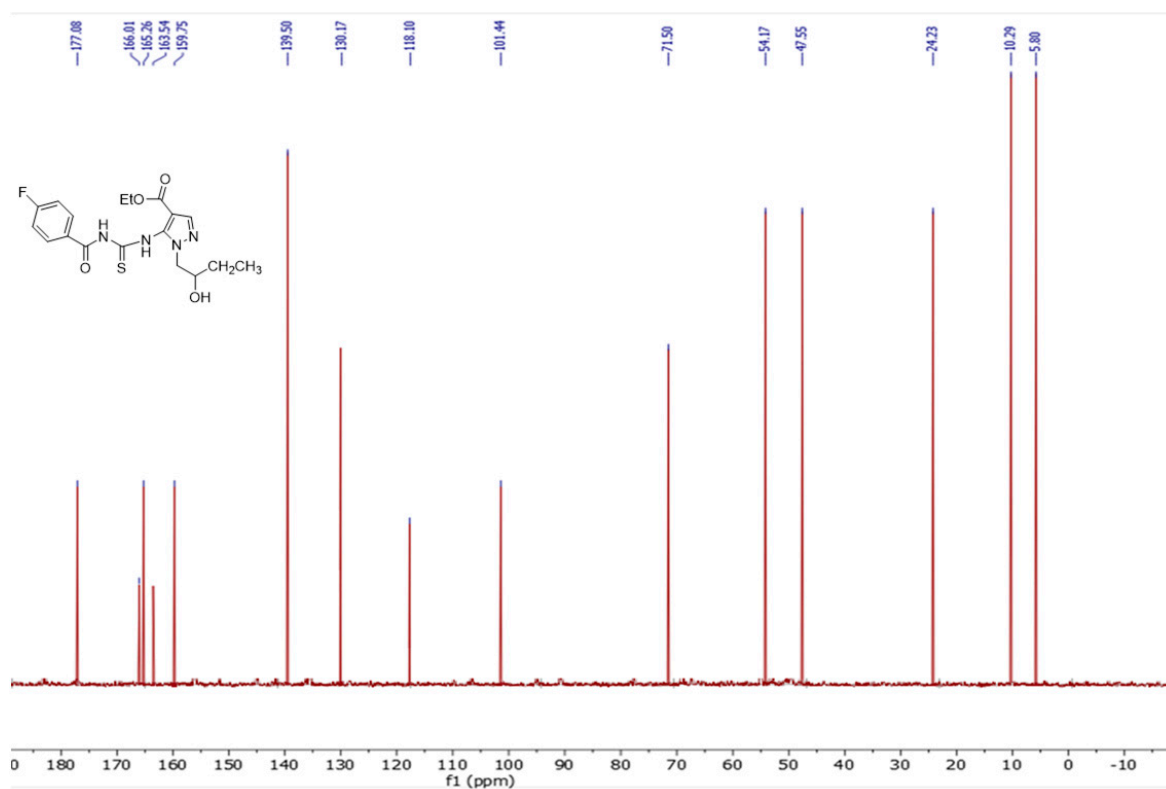


Figure S17: ^1H NMR (400 MHz) of compound **1i**.

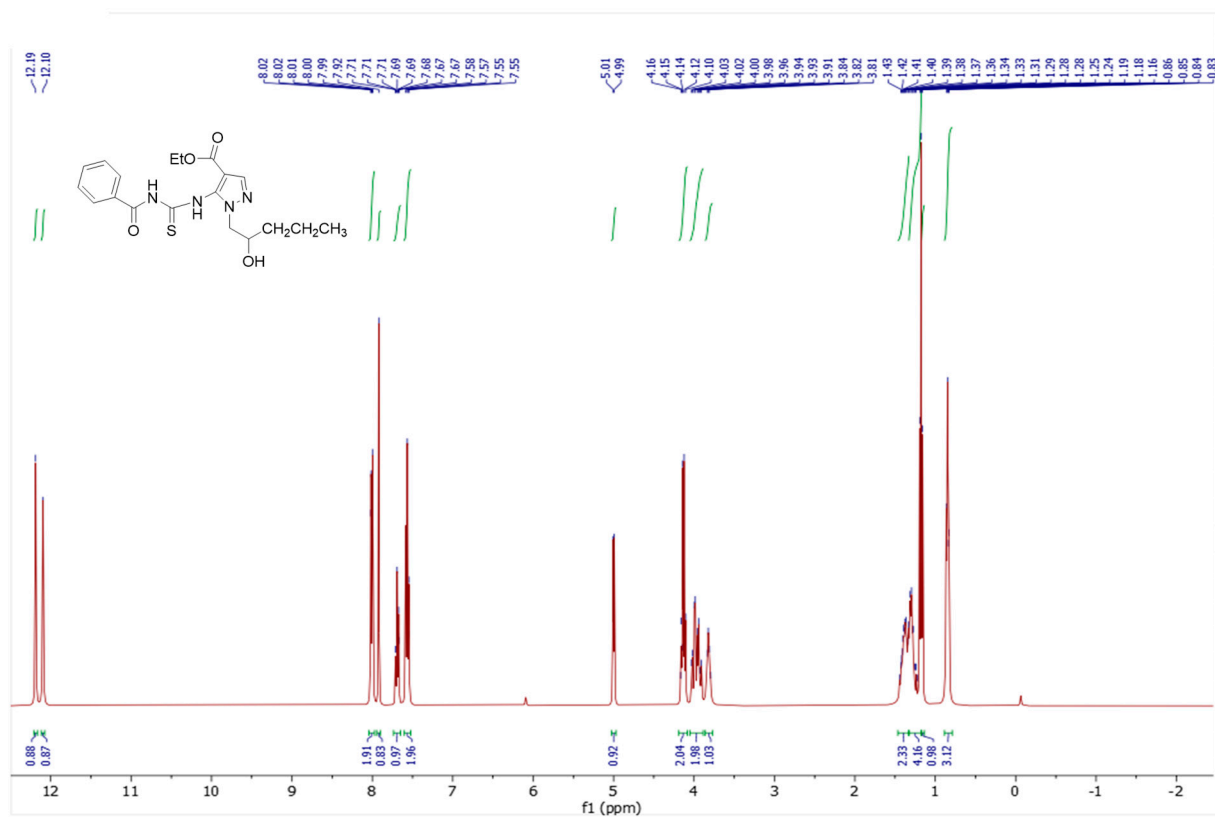


Figure S18: ^{13}C NMR (100 MHz) of compound **1i**.

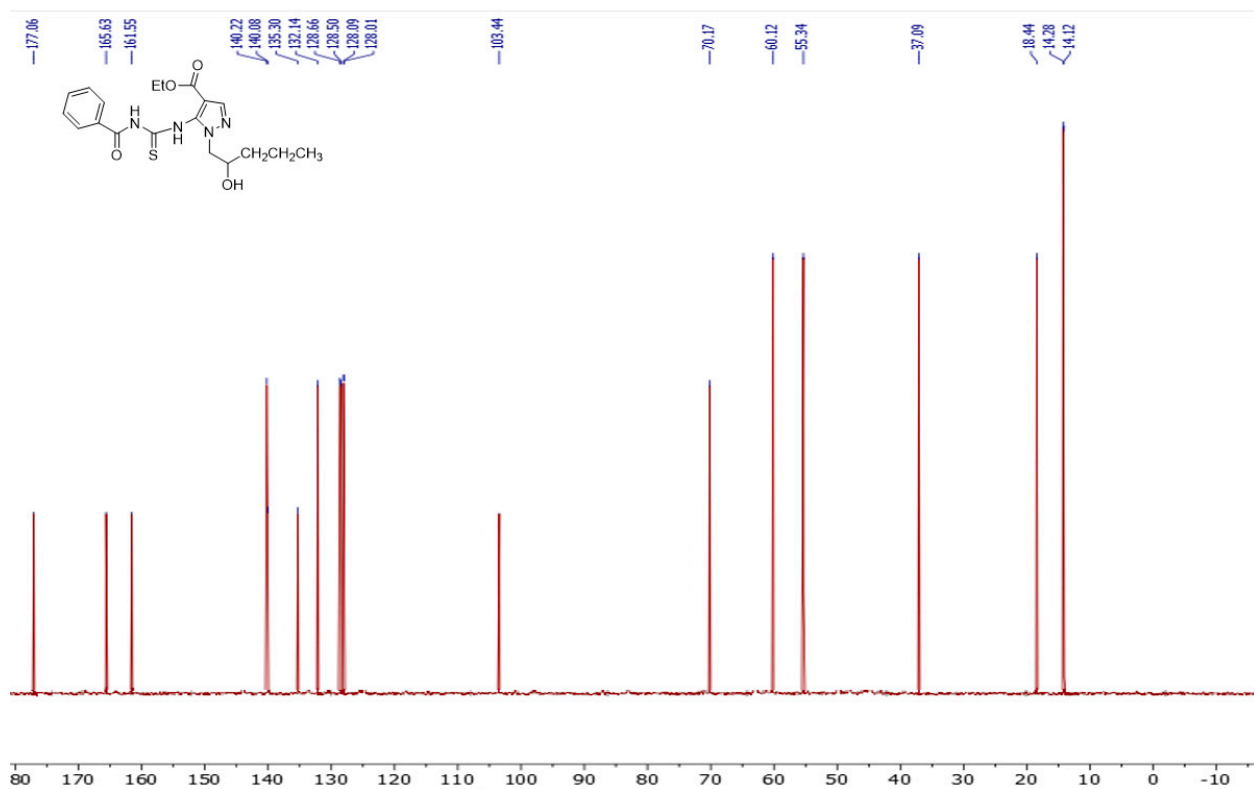


Figure S19: ^1H NMR (400 MHz) of compound 1j.

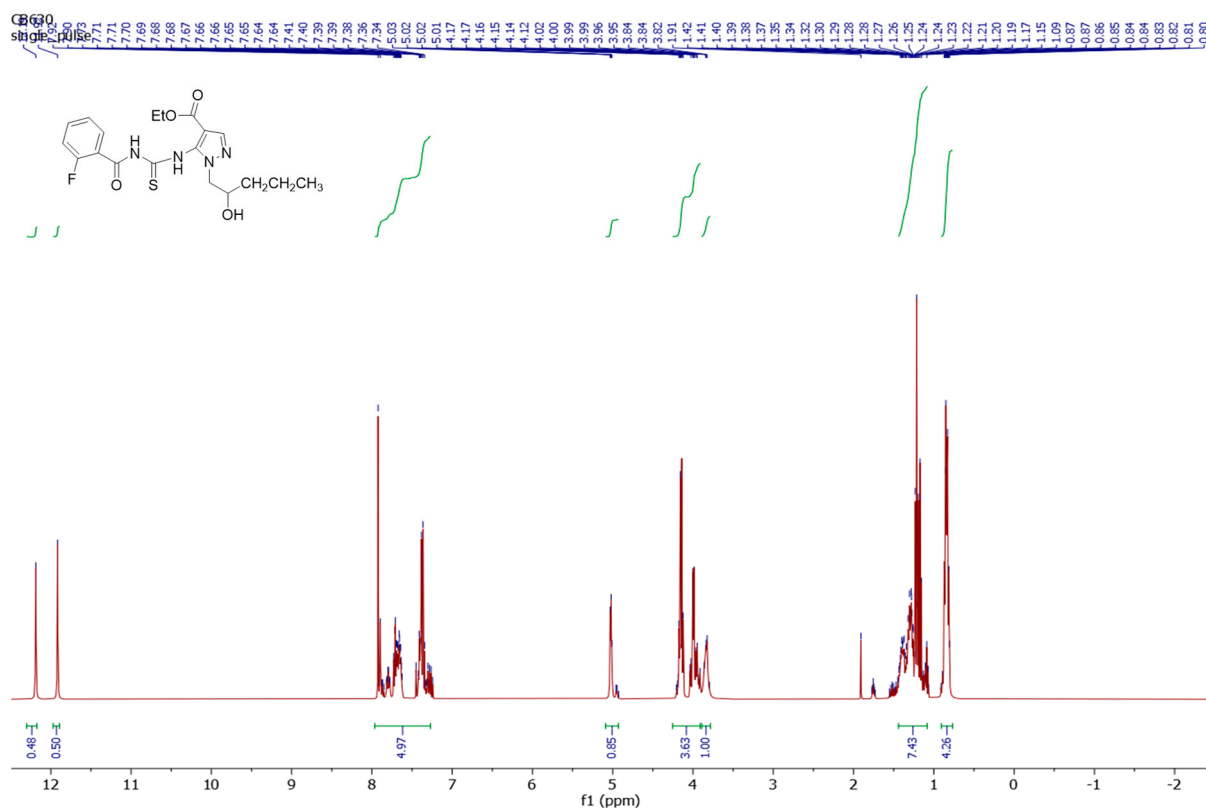


Figure S20: ^{13}C NMR (100 MHz) of compound 1j.

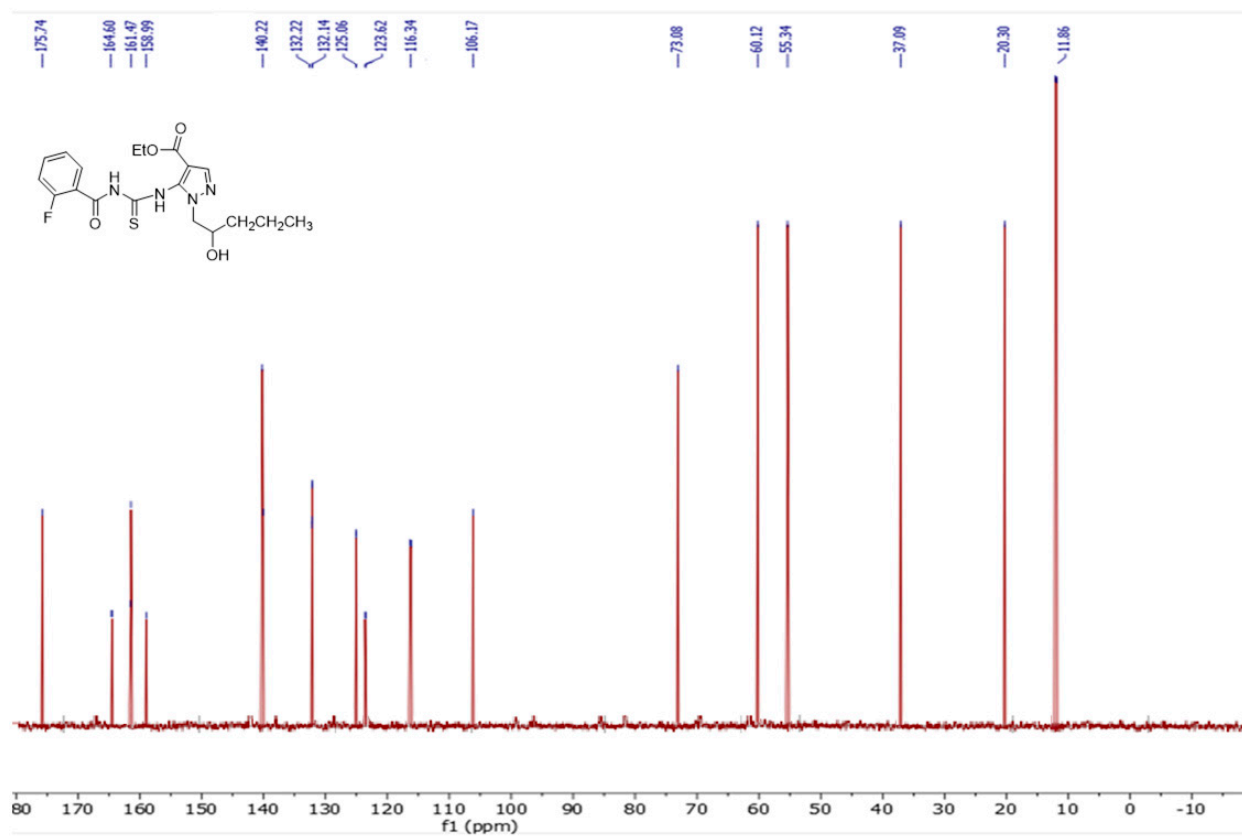


Figure S21: ^1H NMR (400 MHz) of compound 1k.

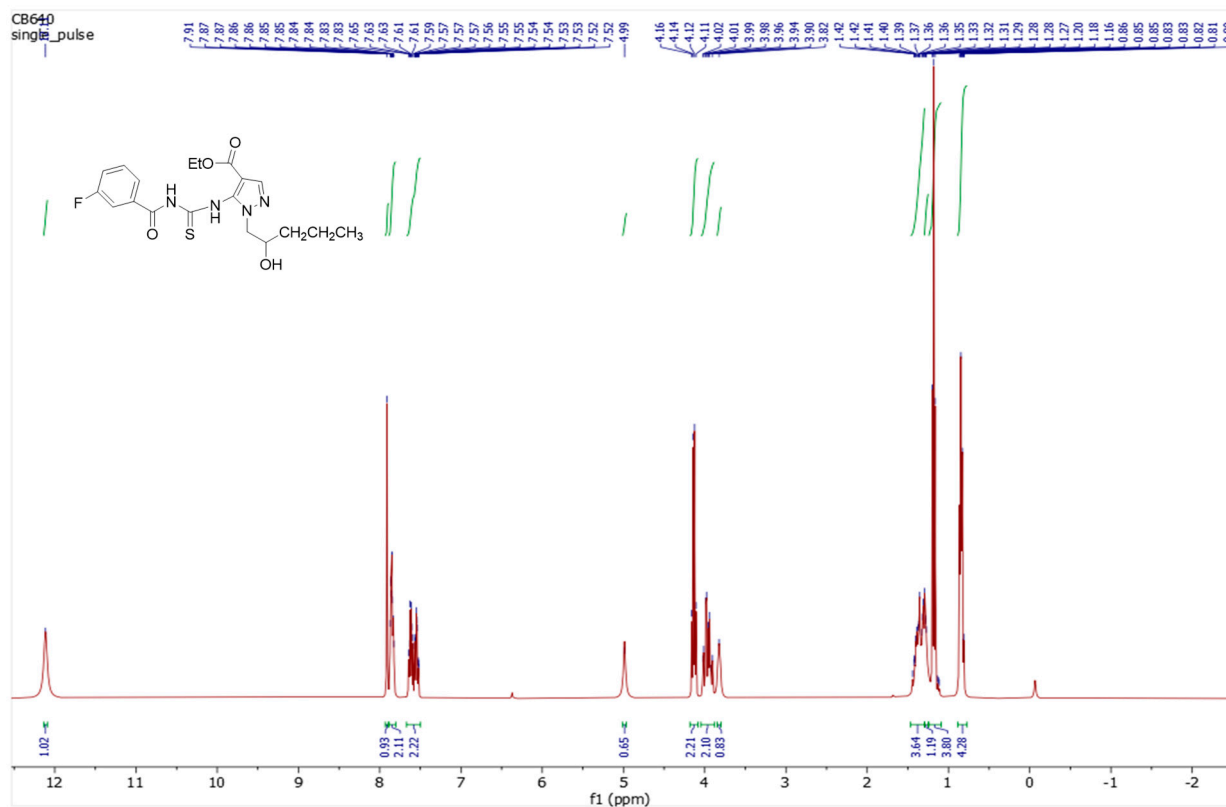


Figure S22: ^{13}C NMR (100 MHz) of compound 1k.

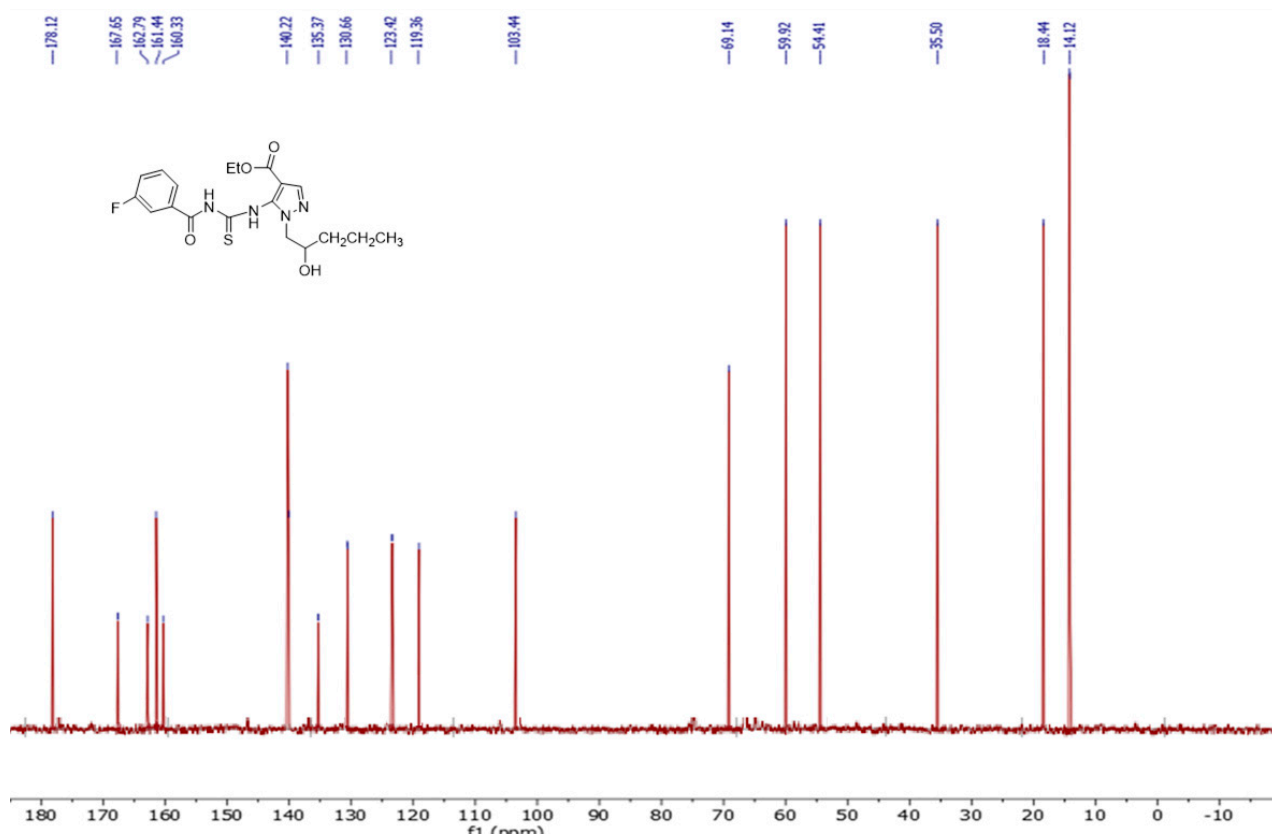


Figure S23: ^1H NMR (400 MHz) of compound 11.

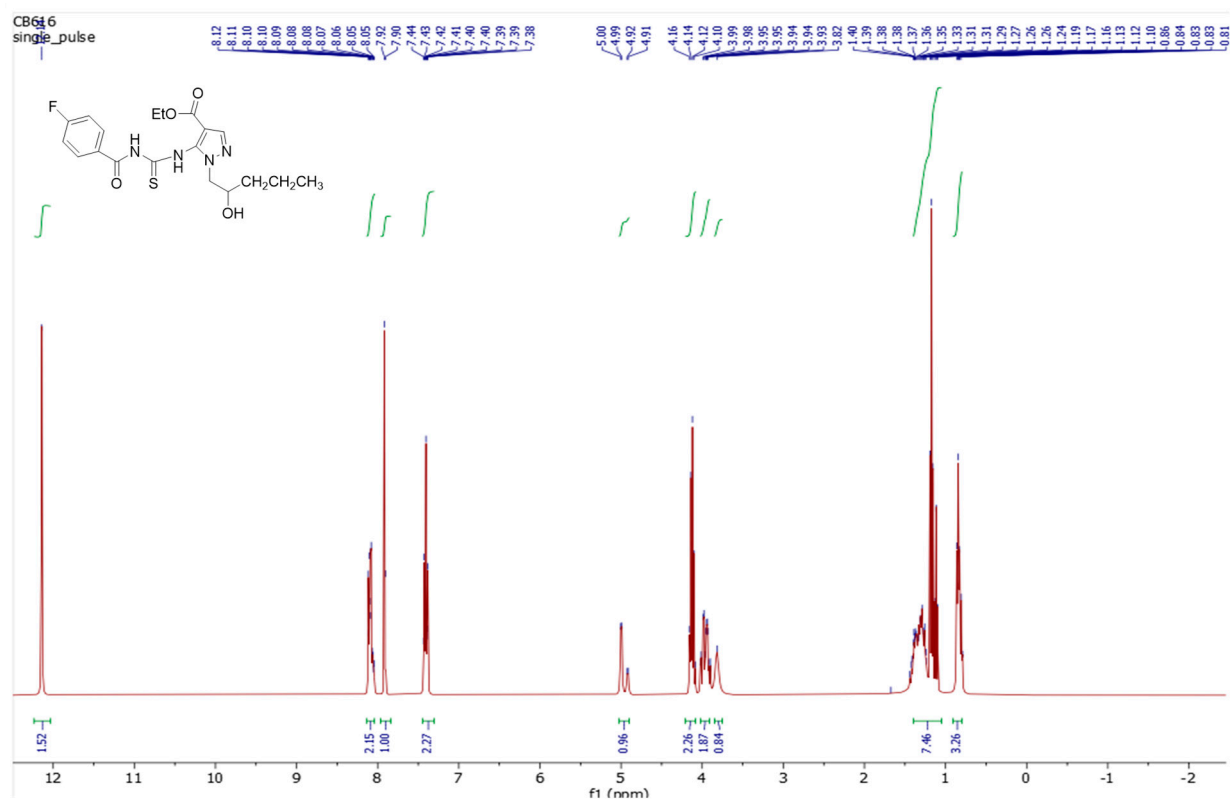
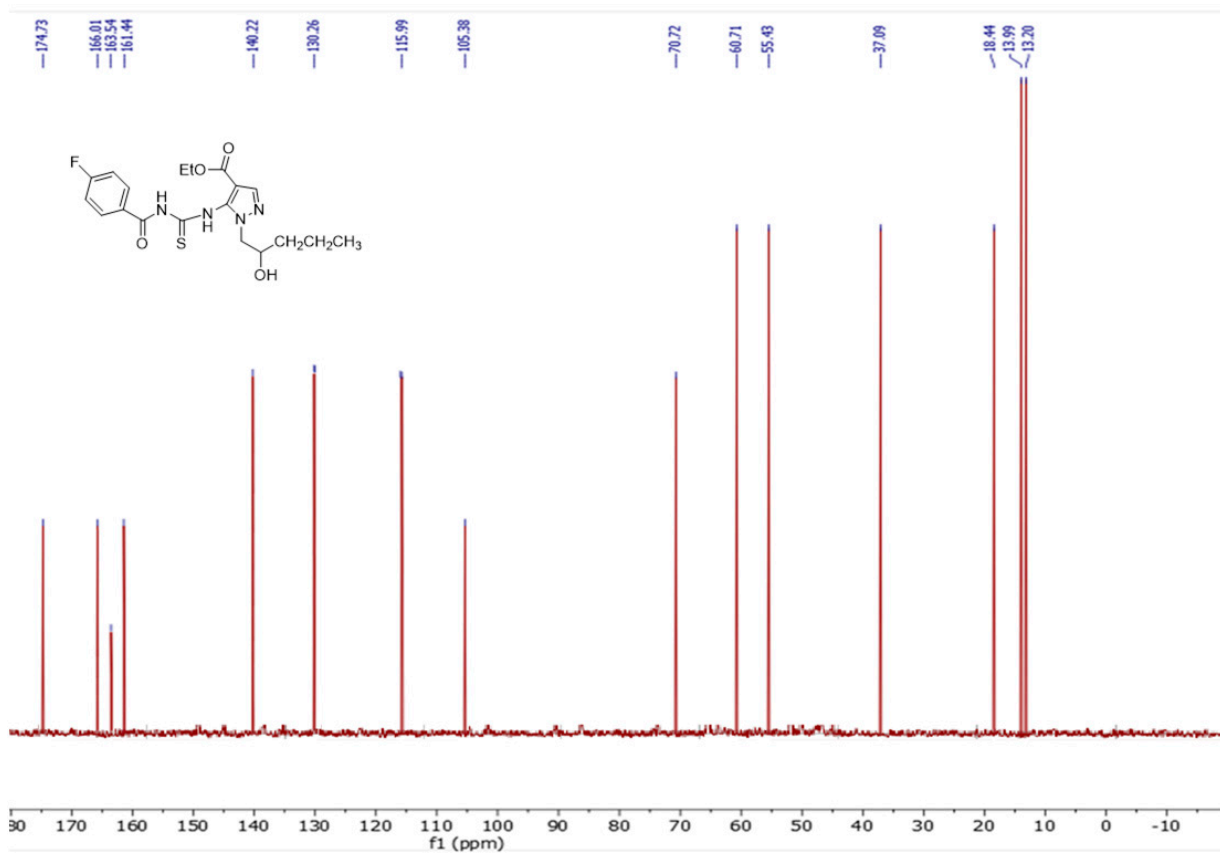


Figure S24: ^{13}C NMR (100 MHz) of compound 11.



Chemical structure of the compound is shown above the spectrum. The structure is a thiazole derivative with a phenyl group, an ethyl ester, and a butyl chain. The spectrum displays peaks corresponding to the protons in the molecule, with chemical shifts ranging from approximately 0.7 to 12.0 ppm. Key peaks are labeled with their chemical shifts: 12.0, 11.8, 11.6, 11.4, 11.2, 11.0, 10.8, 10.6, 10.4, 10.2, 10.0, 9.8, 9.6, 9.4, 9.2, 9.0, 8.8, 8.6, 8.4, 8.2, 8.0, 7.8, 7.6, 7.4, 7.2, 7.0, 6.8, 6.6, 6.4, 6.2, 6.0, 5.8, 5.6, 5.4, 5.2, 5.0, 4.8, 4.6, 4.4, 4.2, 4.0, 3.8, 3.6, 3.4, 3.2, 3.0, 2.8, 2.6, 2.4, 2.2, 2.0, 1.8, 1.6, 1.4, 1.2, 1.0, 0.8, 0.6, 0.4, 0.2, 0.0.

Chemical structure of compound 10 is shown. The ^{13}C NMR spectrum (CDCl₃) shows peaks at the following chemical shifts (ppm): 174.73, 166.52, 159.98, 140.22, 140.08, 137.13, 133.20, 128.09, 127.68, 102.23, 71.74, 63.63, 57.32, 36.52, 25.26, 21.32, 14.46, and 13.20.

Figure S27: ^1H NMR (400 MHz) of compound **1n**.

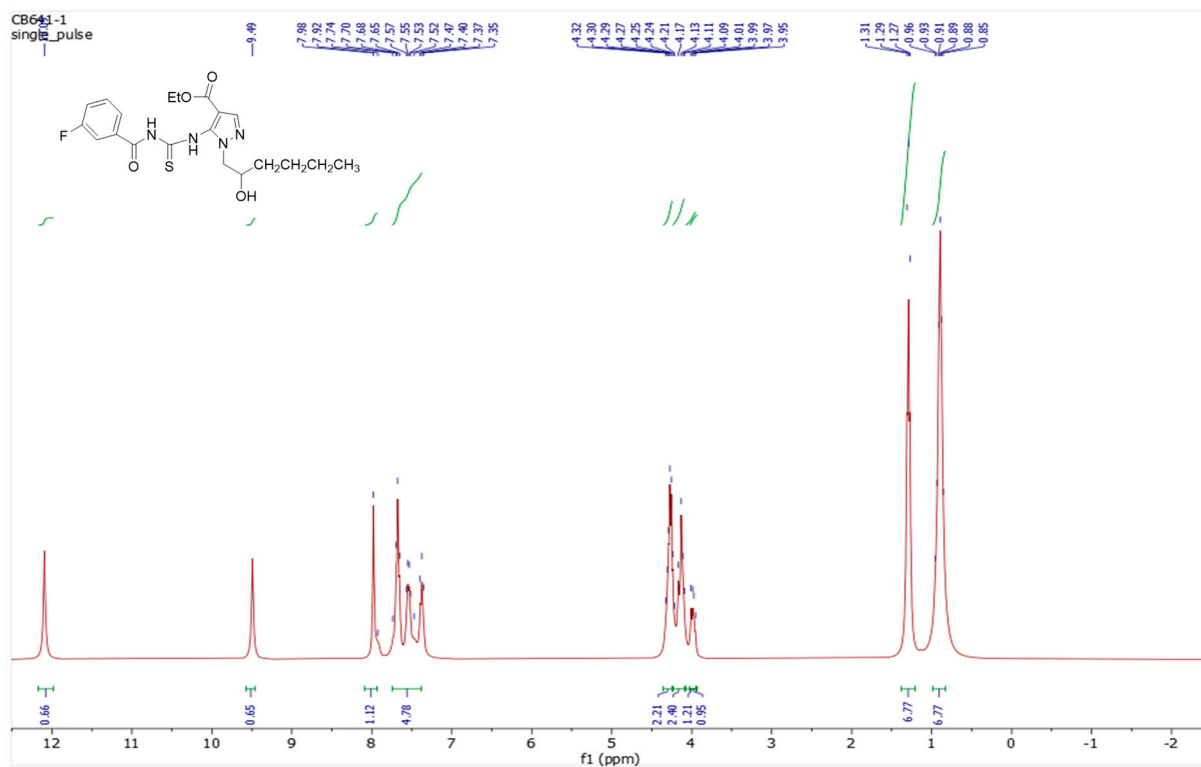


Figure S28: ^{13}C NMR (100 MHz) of compound **1n**.

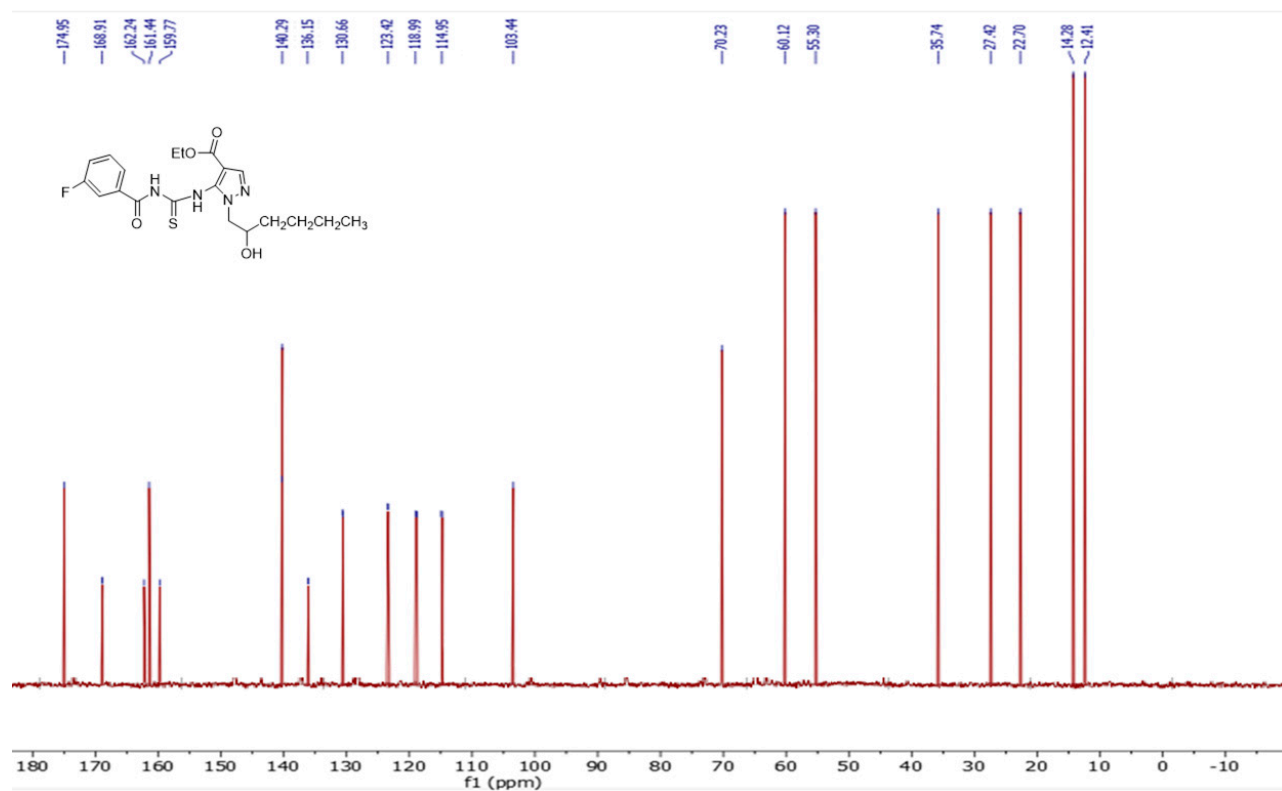


Figure S29: ^1H NMR (400 MHz) of compound **1o**.

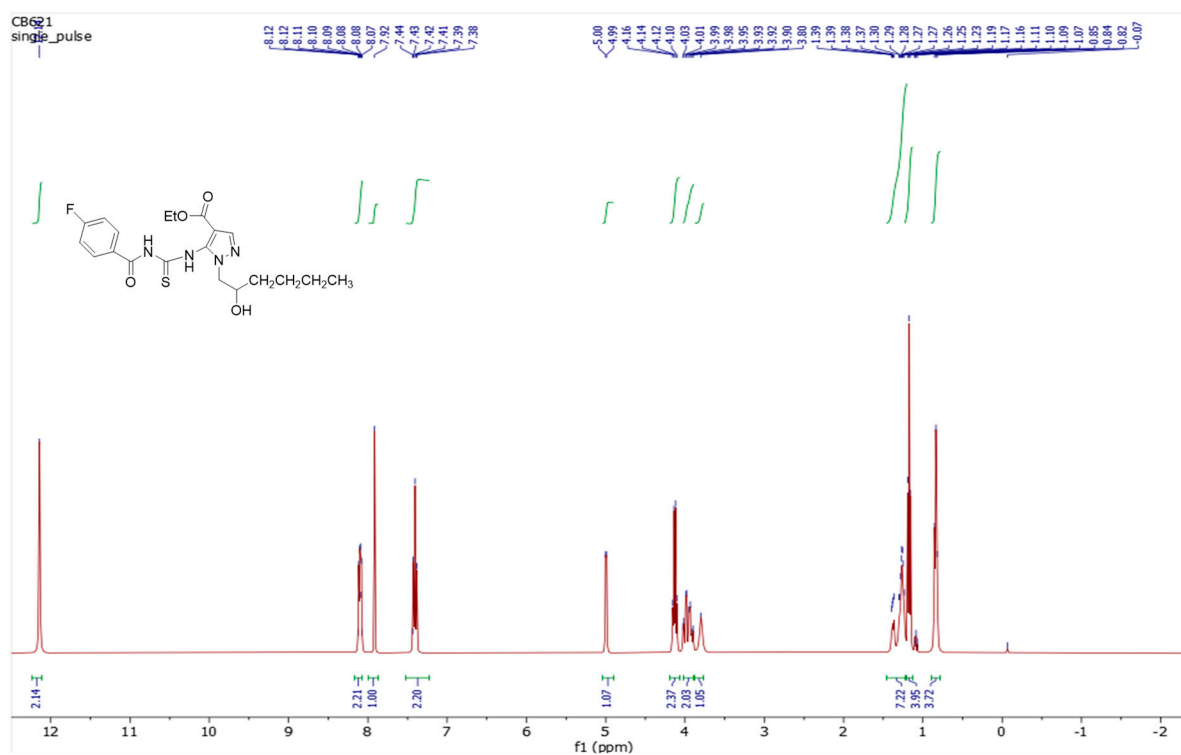


Figure S30: ^{13}C NMR (100 MHz) of compound **1o**.

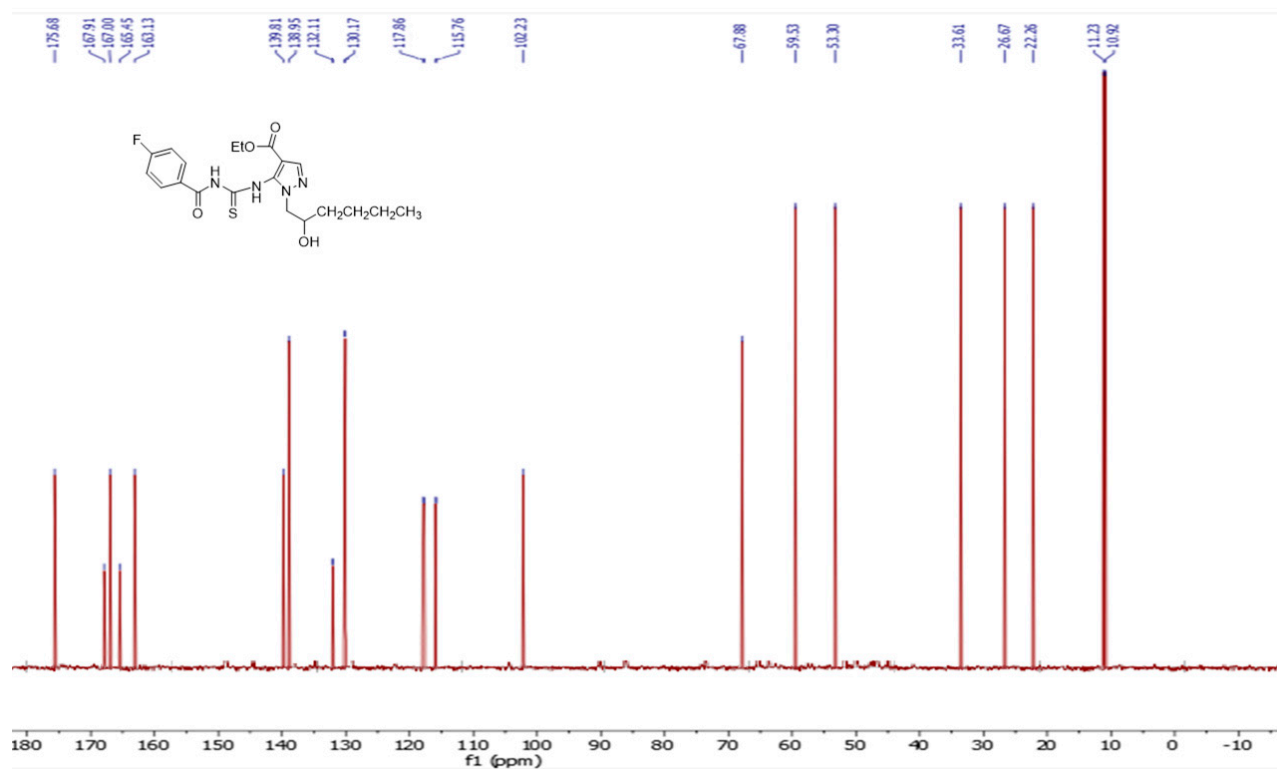


Figure S31: ^1H NMR (400 MHz) of compound **4d**.

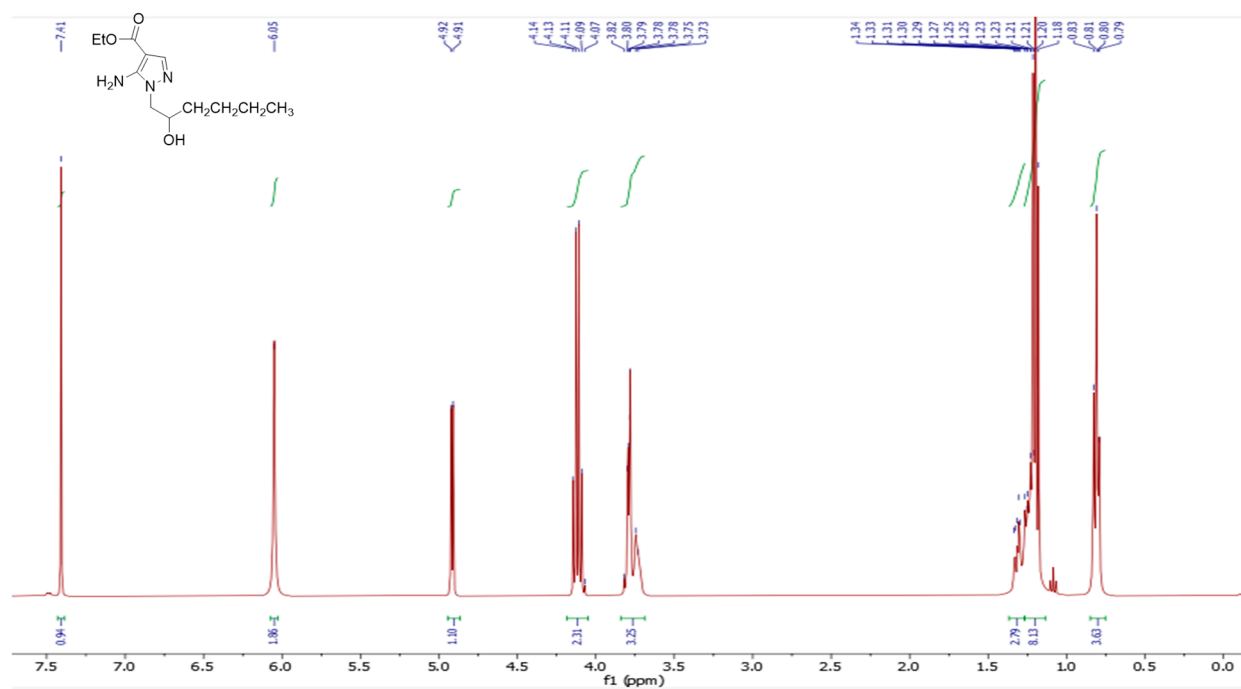


Figure S32: ^{13}C NMR (100 MHz) of compound **4d**.

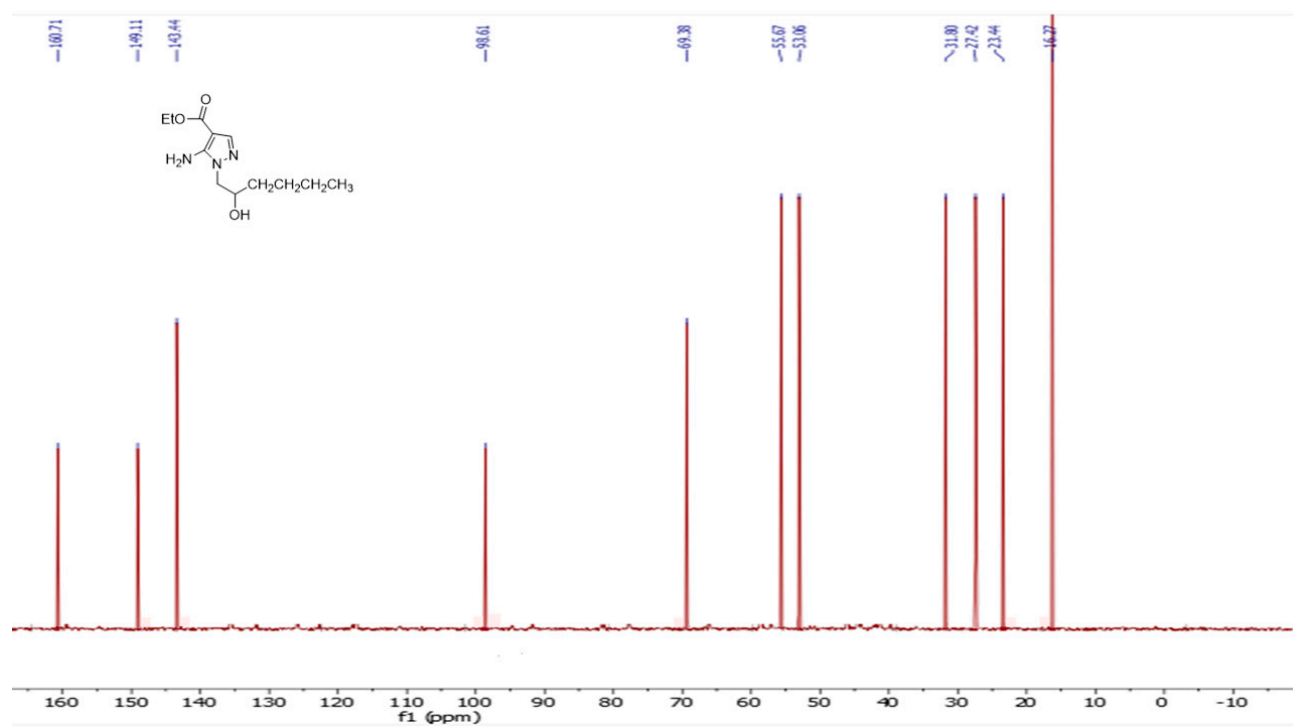


Figure S33: *BOILED-Egg* diagram for compounds **1a-o**

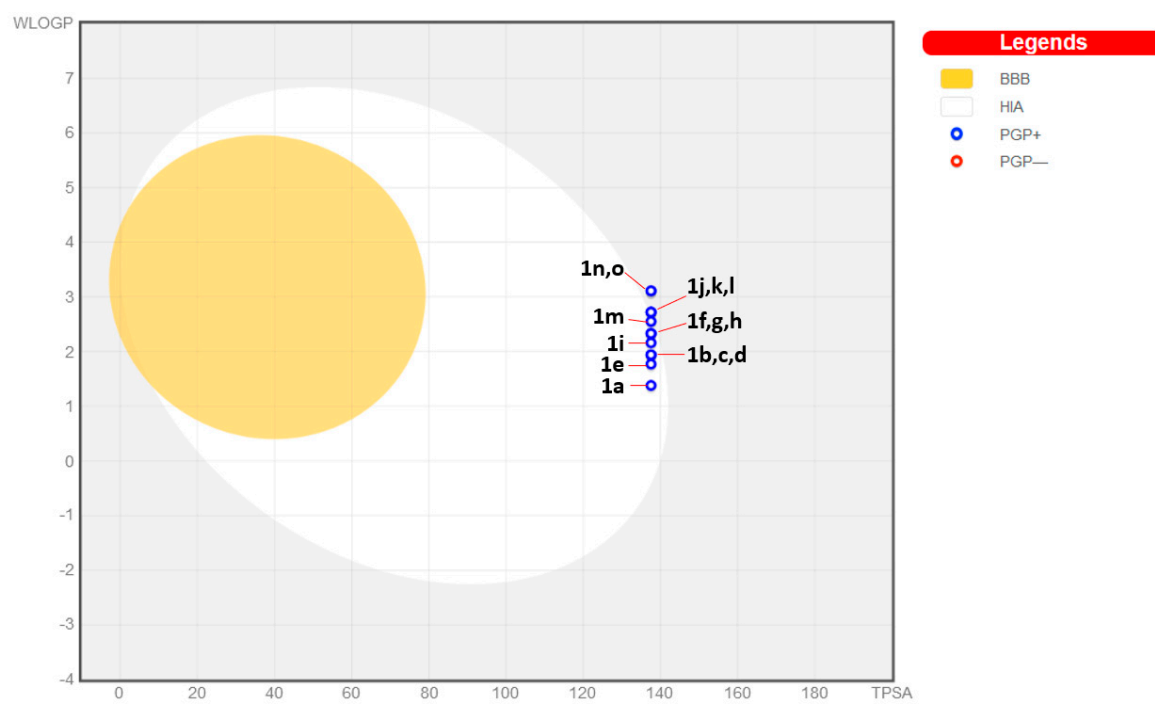


Figure S34: radar plot calculated for compounds **1a-o**

