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

Design, Synthesis, Anticancer Activity, Molecular Docking and ADME Studies of Novel Methylsulfonyl Indole-benzimidazoles in Comparison with Ethylsulfonyl Counterparts

Supplementary Data

Suppl.Table 1. % Viability scores of triplicates and statistical significance obtained by one-way ANOVA/Dunnett statistics with respect to the DMSO control samples for each experimental group (*).

	Compound	Rep1 (%)	Rep2 (%)	Rep3 (%)	Mean (%)	Adj. P-val	Experimental group
1	23	71.28	85.7	77.5	78.16	0.0013	A
2	24	54.25	51.26	51.76	52.42	< 0.0001	A
3	25	74.64	78.99	78.24	77.29	0.0008	A
4	26	31.87	29.76	31.37	31	< 0.0001	A
5	27	50.89	49.68	45.04	48.54	< 0.0001	B
6	28	98.02	97.59	102.06	99.23	> 0.9999	B
7	29	56.39	50.11	50.97	52.49	< 0.0001	B
8	30	52.61	54.67	51.58	52.95	< 0.0001	B
9	31	42.44	43.93	45.42	43.93	< 0.0001	A
10	32	93.12	88.39	92.6	91.37	0.9621	B
11	33	84.26	77.72	71.62	77.87	0.0702	B
12	34	52.52	51.15	50.29	51.32	< 0.0001	B
13	35	106.71	103.36	98.76	102.94	0.9991	A
14	36	49.77	40.32	45.92	45.34	< 0.0001	A
15	37	90.37	88.82	87.61	88.93	0.8268	B
16	38	89.25	90.8	86.93	88.99	0.8307	B
17	39	46.17	43.31	40.82	43.43	< 0.0001	A
18	40	73.25	75.66	70.76	73.22	0.0139	B
19	41	63.57	58.85	56.73	59.72	< 0.0001	A
20	42	89.56	99.25	79.36	89.39	0.3467	A
21	43	45.79	41.19	43.93	43.64	< 0.0001	A
22	44	70.33	66.46	56.91	64.56	0.0003	B
23	45	98.41	102.04	99.29	99.91	> 0.9999	C

24	46	83.62	90.09	89.82	87.84	0.0148	C
25	47	81.59	88.32	83.18	84.36	0.0014	C
26	48	42.64	42.2	42.55	42.46	< 0.0001	C
27	49	74.24	76.19	72.2	74.21	< 0.0001	C
28	50	41.57	44.92	38.96	41.82	< 0.0001	A
29	51	56.61	54	49.52	53.38	< 0.0001	A
30	52	72.99	58.37	49.43	60.26	< 0.0001	B
31	53	70.24	64.65	50.63	61.84	< 0.0001	B
32	54	54.5	45.99	35.06	45.18	< 0.0001	B
33	55	49.43	49.77	36.01	45.07	< 0.0001	B
34	56	80.61	78.93	70.61	76.72	< 0.0001	C
35	57	79.64	76.54	75.66	77.28	< 0.0001	C
36	58	79.11	88.49	90.09	85.9	0.0038	C
--	DMSO (%0.1)	99.75	110.32	89.93	100	--	A
--	DMSO (%0.1)	99.48	94.50	106.02	100	--	B
--	DMSO (%0.1)	102.57	93.98	103.45	100	--	C

*: Significance scores are derived from log2 scaled viability percentiles and one-way ANOVA/Dunnett statistics. The analyses were seperately performed for each experimental group/batch, by taking their respective DMSO control values into account.

Suppl.Table 2. Docking scores and SwissADME results of methylsulfonyl indole-benzimidazole derivatives, CPT and BZ.

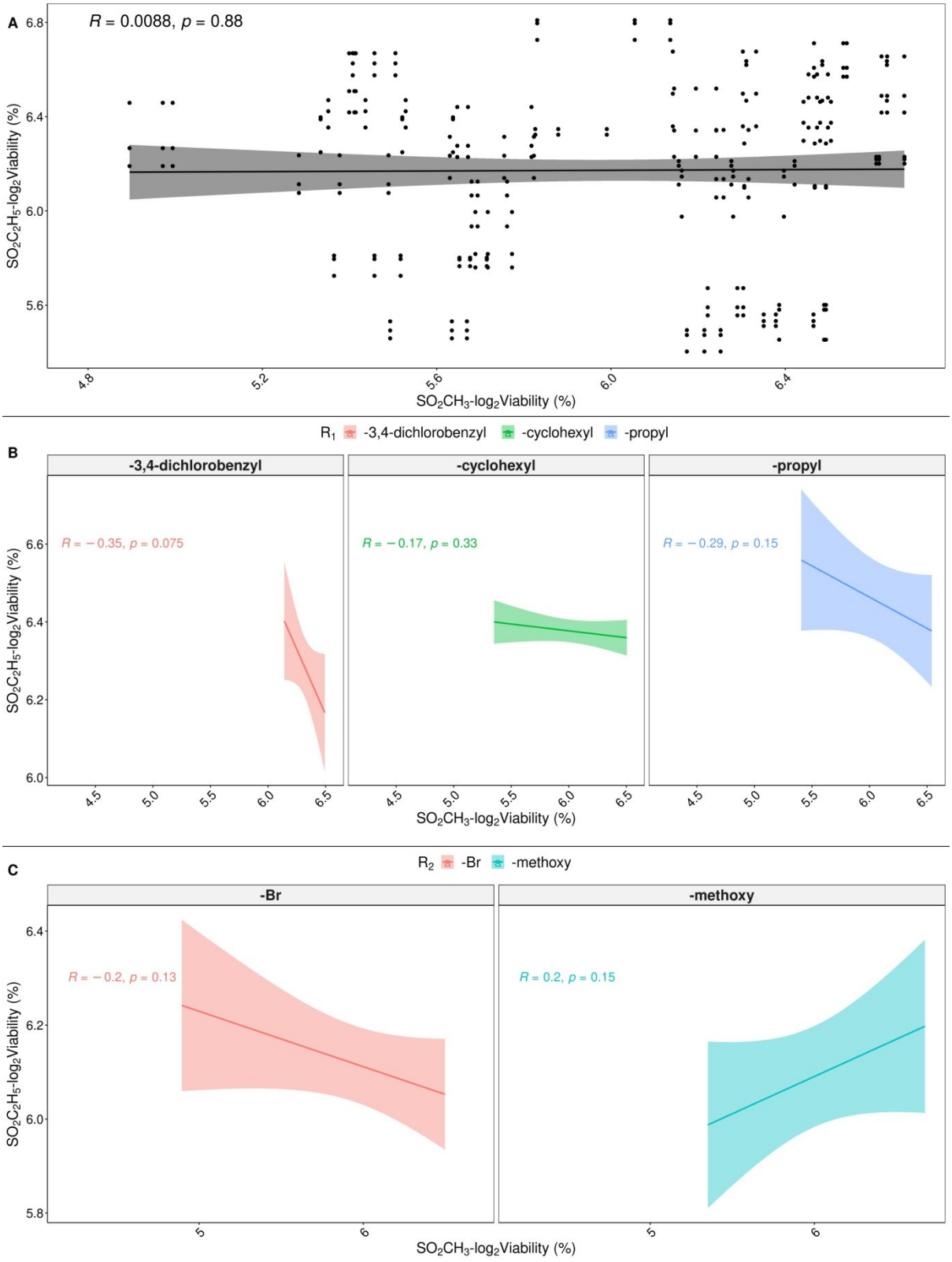
NO	Docking score (kcal/mol)	Count of H-bond acceptors/donors	Number of rotatable bonds	Consensus Computational LogP	Lipinski Violations	Muegge Filter Violations	Leadlikeness
23	-8.2	3/1	2	0.92	0	0	Yes
24	-7.6	4/1	3	1.81	0	0	No, MW>350
25	-7.7	3/1	2	2.35	0	0	No, MW>350
26	-7.8	3/1	2	2.42	0	0	No, MW>350
27	-8.2	3/1	3	2.14	0	0	Yes
28	-7.5	4/1	4	2.09	0	0	No; MW>350
29	-7.5	3/1	3	2.63	0	0	No; MW>350
30	-7.7	3/1	3	2.63	0	0	No; MW>350
31	-7.5	3/1	4	2.45	0	0	No; MW>350
32	-7.5	4/1	5	2.39	0	0	No; MW>350
33	-7.6	3/1	4	2.93	0	0	No; MW>350 XLOGP3>3.5
34	-7.4	3/1	4	3.00	0	0	No; MW>350, XLOGP3>3.5
35	-7.4	4/1	6	2.67	0	0	No; MW>350
36	-7.6	3/1	5	3.21	0	0	No; MW>350, XLOGP3>3.5
37	-7.6	3/1	5	3.27	0	0	No; MW>350, XLOGP3>3.5
38	-8.6	3/1	5	3.27	0	0	No; MW>350, XLOGP3>3.5
39	-8.6	3/1	5	3.27	0	0	No; MW>350, XLOGP3>3.5
40	-8.8	3/1	3	3.53	0	0	No; MW>350, XLOGP3>3.5
41	-8.0	3/1	3	3.60	0	0	No; MW>350, XLOGP3>3.5
42	-8.9	3/1	4	3.00	0	0	No; MW>350, XLOGP3>3.5
43	-8.1	4/1	5	2.94	0	0	No; MW>350, XLOGP3>3.5
44	-8.3	3/1	4	3.48	0	0	No; MW>350, XLOGP3>3.5
45	-8.4	4/1	4	3.29	0	0	No; MW>350, XLOGP3>3.5
46	-8.5	4/1	4	3.77	1 violation: MLOGP>4.15	0	No; MW>350, XLOGP3>3.5
47	-8.4	4/1	4	3.83	1 violation: MLOGP>4.15	0	No; MW>350, XLOGP3>3.5
48	-9.1	5/1	4	3.58	0	0	No; MW>350,

							XLOGP3>3.5
49	-8.5	6/1	5	3.52	0	0	No; MW>350, XLOGP3>3.5
50	-8.9	5/1	4	4.06	0	0	No; MW>350, XLOGP3>3.5
51	-8.6	5/1	4	4.12	2 violations: MW>500, MLOGP>4.15	0	No; MW>350, XLOGP3>3.5
52	-8.3	3/1	4	3.48	0	0	No; MW>350, XLOGP3>3.5
53	-8.4	4/1	5	3.42	0	0	No; MW>350, XLOGP3>3.5
54	-8.4	3/1	4	3.96	1 violation: MLOGP>4.15	1 violation: XLOGP3>5	No; MW>350, XLOGP3>3.5
55	-8.5	3/1	4	4.02	2 violations: MW>500, MLOGP>4.15	1 violation: XLOGP3>5	No; MW>350, XLOGP3>3.5
56	-8.5	3/1	4	3.96	1 violation: MLOGP>4.15	1 violation: XLOGP3>5	No; MW>350, XLOGP3>3.5
57	-8.5	3/1	4	4.43	2 violations: MW>500, MLOGP>4.15	1 violation: XLOGP3>5	No; MW>350, XLOGP3>3.5
58	-8.1	3/1	4	4.50	2 violations: MW>500, MLOGP>4.15	1 violation: XLOGP3>5	No; MW>350, XLOGP3>3.5
CPT	-8.5	5/1	1	2.20	0	0	Yes
BZ	-10.7	4/2	7	5.07	0	1 violation: XLOGP3>5	No; MW>350, XLOGP3>3.5

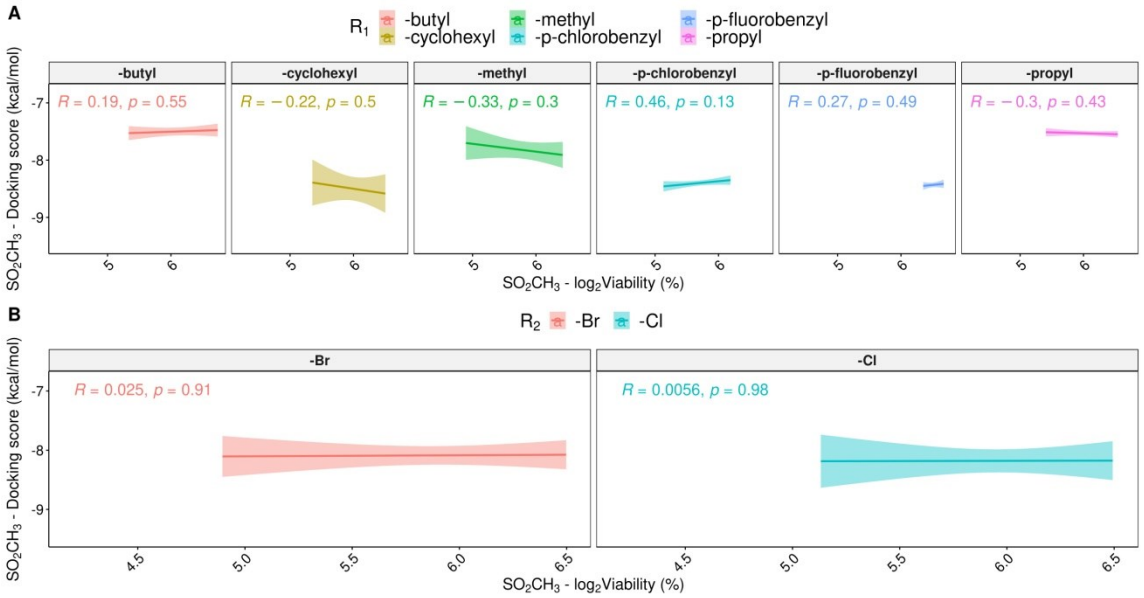
Suppl. Table 3. Physical and spectral data for compounds **23-58.**

Comp.	Mp (°C)	Formulas	Yield (%)	^{1}H- and ^{13}C-NMR (DMSO-d_6) δ ppm	MS (ESI+) m/z	Isolation
23	249	**$C_{17}H_{15}N_3O_2S_{\cdot 0.25H2O}$:** C, 61.89; H, 4.73; N, 12.74; S, 9.70; Found: C, 61.77; H, 4.96; N, 13.05; S, 9.69.	9	**^{1}H NMR:** δ 3.22 (s, 3H), 4.04 (s, 3H), 7.17-7.26 (m, 2H), 7.51 (d, *J*=7.2 Hz, 1H), 7.75 (dd, *J*=8.8 Hz, *J*=1.6 Hz, 1H), 7.81 (d, *J*=8.8 Hz, 1H), 8.17-8.18 (m, 2H), 8.41 (d, *J*=7.2 Hz, 1H), 11.90 (brd s, 1H). **^{13}C NMR:** 31.92, 44.22, 104.27, 110.28, 111.76, 117.33, 119.72, 120.43, 121.45, 122.46, 126.22, 127.66, 133.81, 136.01, 139.15, 142.40, 152.81.	326	$CHCl_3$: EtOAc: n-Hexane (2:2:1) cc
24	278	**$C_{18}H_{17}N_3O_2S_{\cdot 0.2H2O}$:** C, 60.21; H, 4.88; N, 11.71; S, 8.91; Found: C, 59.83; H, 4.86; N, 11.86; S, 8.91.	8	**^{1}H NMR:** 3.22 (s, 3H), 3.81 (s, 3H), 4.03 (s, 3H), 6.88 (dd, *J*=8.6 Hz, *J*=2.8 Hz, 1H), 7.41 (d, *J*=9.2 Hz, 1H), 7.74 (dd, *J*=8.6 Hz, *J*=2.8 Hz, 1H), 7.80 (d, *J*=8.0 Hz, 1H), 7.95 (d, *J*=2.8 Hz, 1H), 8.13 (*d*, *J*=2.8 Hz, 1H), 8.17 (d, *J*=1.6 Hz, 1H), 11.78 (brd d, 1H). **^{13}C NMR:** 32.00, 44.30, 55.36, 103.23, 104.10, 110.26, 112.53, 112.68, 117.40, 119.72, 126.94, 128.04, 131.10, 133.81, 139.19, 142.44, 153.05, 154.52.	356	$CHCl_3$: EtOAc: n-Hexane (2:2:1) cc
25	280	**$C_{17}H_{14}ClN_3O_2S_{\cdot 0.65H2O}$:** C, 55.02; H, 4.15; N, 11.71; S, 8.91; Found: C, 54.70; H, 3.89; N, 11.67; S, 8.63.	28	**^{1}H NMR:** 3.25 (s, 3H), 4.08 (s,3H), 7.28 (dd, *J*=8.4 Hz, *J*=2.0 Hz, 1H), 8.4 (d, *J*=8.4 Hz, 1H), 7.78 (dd, *J*=8.4 Hz, *J*=1.6 Hz, 1H), 7.85 (d, *J*=8.4 Hz, 1H), 8.25 (d, *J*=1.6 Hz, 1H), 8.31 (brd s, 1H), 8.52 (d, *J*=2.0 Hz, 1H), 12.13 (brd s, 1H). **^{13}C NMR:** 31.99, 44.23, 104.11, 110.33, 113.41, 117.52, 119.80, 120.69, 122.54, 125.19, 127.38, 129.10, 133.95, 134.53, 139.06, 142.28, 152.21	360	$CHCl_3$: EtOAc: n-Hexane (1:2:2) cc
26	265	**$C_{17}H_{14}BrN_3O_2S$:** C, 50.51; H, 3.49; N, 10.39; S, 7.93; Found: C, 50.13; H, 3.62; N, 10.77; S, 7.92.	22	**^{1}H NMR:** 3.25 (s, 3H), 4.08 (s, 3H), 7.39 (dd, *J*=8.4 Hz, *J*=2.0 Hz, 1H), 7.52 (d, *J*=8.4 Hz, 1H), 7.78 (dd, *J*=8.4 Hz, *J*=1.6 Hz, 1H), 7.85 (d, *J*=8.0 Hz, 1H), 8.29 (s, 1H), 8.67 (d, *J*=2.0 Hz, 1H), 12.13 (brd s, 1H). **^{13}C NMR:** 31.99, 44.21, 104.06, 110.40, 113.28, 113.92, 117.61, 119.87, 123.77, 125.15, 128.07, 129.00, 134.03, 134.83, 139.13, 142.33, 152.24.	404	$CHCl_3$: EtOAc: n-Hexane (2:2:1) cc
27	311	**$C_{18}H_{17}N_3O_2S_{\cdot 0.35\ H2O}$:** C, 62.37; H, 5.18; N, 12.13; S, 9.23; Found: C, 62.10; H, 4.75; N, 12.53; S, 9.29.	34	**^{1}H NMR:** 1.41 (t, 3H), 3.25 (s, 3H), 4.57 (q, 2H), 7.19-7.28 (m, 2H), 7.55 (d, *J*=8.0 Hz, 1H), 7.78 (dd, *J*=8.4 Hz, *J*=1.6 Hz, 1H), 7.86 (d, *J*=8.0 Hz, 1H), 8.09 (d, *J*=3.2 Hz, 1H), 8.21 (d, *J*=1.6 Hz, 1H), 8.40 (d, *J*=7.6 Hz, 1H), 11.89 (brd s, 1H). **^{13}C NMR:** 14.67, 44.29, 56.00, 104.13, 110.45, 111.86, 117.58, 119.97, 120.50, 121.49, 122.52, 126.43, 126.78, 134.04, 136.11, 138.28, 142.66, 151.95.	340	$CHCl_3$: EtOAc: n-Hexane (2:2:1) cc
28	251	**$C_{19}H_{19}N_3O_2S$:** C, 61.77; H, 5.18; N, 11.37; S, 8.68; Found: C, 61.76; H, 5.05; N, 11.70; S, 8.76.	32	**^{1}H NMR:** 1.41 (t, 3H), 3.24 (s, 3H), 3.82 (s, 3H), 4.55 (q, 2H), 6.91 (dd, *J*=8.8 Hz, *J*=2.4 Hz, 1H), 7.44 (d, *J*=8.8 Hz, 1H), 7.77 (dd, *J*=8.4 Hz, *J*=1.6 Hz, 1H), 7.85 (d, *J*=8 Hz, 1H), 7.95 (d, *J*=2.4 Hz, 1H), 8.04 (s, 1H), 8.21 (d, *J*=1.6 Hz, 1H), 11.77 (brd s, 1H). **^{13}C NMR:** 14.65, 39.21, 44.30, 55.35, 103.18, 103.89, 110.36, 112.57, 112.71, 117.58, 119.90, 127.07, 127.09, 131.14, 133.96, 138.27, 142.65, 152.13, 154.51	370	$CHCl_3$: EtOAc: n-Hexane (2:2:1) cc
29	298	**For $C_{18}H_{16}ClN_3O_2S_{\cdot 0.25\ H2O}$:** C, 57.20; H, 4.40; N, 11.12; S, 8.46; Found: C, 56.98; H, 4.56; N, 11.55; S, 8.66.	47	**^{1}H NMR:**1.42 (t, 3H), 3.25 (s. 3H), 4.58 (q, 2H), 7.28 (dd, *J*=8.4 Hz, *J*=2.4 Hz, 1H), 7.57 (d, *J*=8.4 Hz, 1H), 7.79 (dd, *J*=8.8 Hz, *J*=2.0 Hz, 1H), 7.87 (d, *J*=8.8 Hz, 1H), 8.21 (s, 1H), 8.27 (d, *J*=1.6 Hz, 1H), 8.50 (d, *J*=2.0 Hz, 1H), 12.10 (brd s, 1H). **^{13}C NMR:** 14.64, 39.22, 44.22, 103.93, 110.46, 113.51, 117.75, 120.05, 120.79, 122.63, 125.27, 127.59, 128.27, 134.19, 134.63, 138.21, 142.52, 151.31	374	$CHCl_3$: EtOAc: n-Hexane (2:2:1) cc
30	288	**$C_{18}H_{16}BrN_3O_2S_{\cdot 0.15\ H2O}$:** C, 51.46; H, 3.91; N, 10.00; S, 7.61; Found: C, 51.02; H, 4.12; N, 10.43; S, 7.71.	56	**^{1}H NMR:** 1.42 (t, 3H), 3.25 (s, 3H), 4.08 (s, 3H), 7.39 (dd, *J*=8.4 Hz, *J*=2.0 Hz, 1H), 7.52 (d, *J*=8.4 Hz, 1H), 7.78 (dd, *J*=8.4 Hz, *J*=1.6 Hz, 1H), 7.85 (d, *J*=8.0 Hz, 1H), 8.25 (d, *J*=1.6 Hz, 1H), 8.29 (s, 1H), 8.67 (d, *J*=2.0 Hz, 1H), 12.13 (brd s, 1H). **^{13}C NMR:** 31.99, 44.21, 104.06, 110.40, 113.28, 113.92, 117.61, 119.87, 123.77, 125.15, 128.07, 129.00, 134.03, 134.83, 139.13, 142.33, 152.24.	417	$CHCl_3$: EtOAc: n-Hexane (2:2:1) cc
31	256	**$C_{19}H_{19}N_3O_2S$:** C, 64.57; H, 5.42; N, 11.89; S, 9.07; Found: C, 64.32; H, 5.53; N, 12.02; S, 9.02.	54	**^{1}H NMR:** 0.85 (t, 3H), 1.79 (m, 2H), 3.23 (s, 3H), 4.47 (t, 2H), 7.15-7.25 (m, 2H), 7.52 (d, *J*=8.0 Hz, 1H), 7.75 (dd, *J*=8.4 Hz, *J*=1.6 Hz, 1H), 7.85 (d, *J*=8.4 Hz, 1H), 8.05 (d, *J*=2.4 Hz, 1H), 8.18 (d, *J*=1.6 Hz, 1H), 8.36 (d, *J*=8.0 Hz, 1H), 11.83 (brd s, 1H) **^{13}C NMR:** 10.85, 22.28, 44.19, 45.48, 104.20, 110.66, 111.79, 117.52, 119.86, 120.42, 121.39, 122.43, 126.40, 126.67, 133.92, 135.98, 138.73, 142.42, 152.15.	354	$CHCl_3$: EtOAc: n-Hexane (1:2:1) cc
32	244	**$C_{20}H_{21}N_3O_2S$:** C, 62.64; H, 5.52; N, 10.96; S, 8.36; Found: C, 62.32; H, 5.55; N, 10.98; S, 8.26.	37	**^{1}H NMR:** 0.87 (t, 3H), 1.79 (m, 2H), 3.22 (s, 3H), 3.79 (s, 3H), 4.46 (t, 2H), 6.88 (dd, *J*=8.8 Hz, *J*=2.4 Hz, 1H), 7.41 (d, *J*=9.2 Hz, 1H), 7.74 (dd, *J*=8.8 Hz, *J*=1.6 Hz, 1H), 7.84 (d, *J*=8.4 Hz, 1H), 7.92 (d, *J*=2.4 Hz, 1H), 8.00 (d, *J*=3.2 Hz, 1H), 8.18 (d, *J*=1.6 Hz, 1H), 11.70 (brd s, 1H). **^{13}C NMR:** 10.92, 22.34, 44.27, 45.54, 55.33, 103.18, 104.02, 110.62, 112.55, 112.67, 117.58, 119.85, 127.04, 127.11, 131.07, 133.90, 138.79, 142.48, 152.36, 154.50.	384	$CHCl_3$: EtOAc: n-Hexane (1:2:1) cc
33	249	**$C_{19}H_{18}ClN_3O_2S_{\cdot 0.15\ H2O}$:** C, 58.49; H, 4.73; N, 10.77; S, 8.20; Found: C, 58.21; H, 4.79; N, 11.07; S, 8.20.	22	**^{1}H NMR:** 0.87 (t, 3H), 1.79 (m, 2H), 3.23 (s, 3H), 4.48 (t, 2H), 7.24 (dd, *J*=8.8 Hz, *J*=2.4 Hz, 1H), 7.54 (d, *J*=8.8 Hz, 1H), 7.75 (dd, *J*=8.4 Hz, *J*=1.6 Hz, 1H), 7.77 (dd, *J*=8.4 Hz, *J*=8.4 Hz, 1H), 8.16 (s, 1H), 8.23 (d, *J*=1.6 Hz, 1H), 8.46 (d, *J*=1.6 Hz, 1H), 12.02 (brd s, 1H). **^{13}C NMR:** 10.91, 22.34, 44.19, 45.51, 104.06, 110.74, 113.51, 117.75, 120.00, 120.76, 122.59, 125.25, 127.63, 128.23, 134.13, 134.56, 138.76, 142.35, 151.55.	388	$CHCl_3$: EtOAc: n-Hexane (1:2:1) cc
34	195	**$C_{19}H_{18}ClN_3O_2S$-0.15 H_2O:** C, 64.89; H, 5.80; N, 11.35; S, 8.64; Found: C, 64.67; H, 5.86; N, 11.45; S, 8.61.	55	**^{1}H NMR:** 0.84 (t, 3H), 1.31 (m, 2H),1.75 (m, 2H), 3.25 (s, 3H), 4.53 (t, 2H), 7.18-7.28 (m, 2H), 7.54 (d, *J*=8.0 Hz, 1H), 7.77 (dd, *J*=8.4 Hz, *J*=1.6 Hz, 1H), 7.86 (d, *J*=8.4 Hz, 1H), 8.08 (d, *J*=2.8 Hz, 1H), 8.20 (d, *J*=1.6 Hz, 1H), 8.37 (d, *J*=8.0 Hz, 1H), 11.86 (brd s, 1H). **^{13}C NMR:** 13.49, 19.36, 31.08, 43.95, 44.26, 104.27, 110.69, 111.87, 117.61, 119.95, 120.49, 121.42, 122.50, 126.45, 126.76, 133.99, 136.05, 138.72, 142.52, 152.19.	368	$CHCl_3$: EtOAc: n-Hexane (1:2:1) cc
35	215	**$C_{21}H_{23}N_3O_2S_{\cdot 0.35\ H2O}$:** C, 62.46; H, 5.92; N, 10.41; S, 7.92; Found: C, 62.16; H, 5.87; N, 10.48; S, 8.29.	25	**^{1}H NMR**: 0.85 (t, 3H), 1.32 (m, 2H),1.76 (m, 2H), 3.25 (s, 3H), 3.82 (s, 3H), 4.52 (t, 2H), 6.91 (dd, *J*=8.8 Hz, *J*=2.4 Hz, 1H), 7.44 (d, *J*=8.8 Hz, 1H), 7.77 (dd, *J*=8.4 Hz, *J*=2.0 Hz, 1H), 7.86 (d, *J*=8.4 Hz, 1H), 7.91 (d, *J*=2.4 Hz, 1H), 8.04 (d, *J*=3.2 Hz, 1H), 8.20 (d, *J*=2.0 Hz, 1H), 11.74 (brd s, 1H). **^{13}C NMR:** 13.50, 19.38, 31.06, 44.00, 44.26, 55.35, 103.09, 103.79, 110.71, 112.61, 112.71, 117.48, 119.99, 127.04, 127.23, 131.07, 134.05, 138.61, 142.15, 152.27, 154.54.	398	$CHCl_3$: EtOAc: n-Hexane (1:2:1) cc
36	129	**$C_{20}H_{20}ClN_3O_2S_{\cdot H2O}$:** C, 57.26; H, 5.29; N, 10.02; S, 7.62; Found: C, 57.00; H, 5.37; N, 9.89; S, 7.26.	28	**^{1}H NMR:** 0.87 (t, 3H), 1.33 (m, 2H), 1.76 (m, 2H), 3.26 (s, 3H), 4.54 (t, 2H), 7.27 (d, *J*=7.2 Hz, 1H), 7.57 (d, *J*=8.4 Hz, 1H), 7.78 (d, *J*=8.0 Hz, 1H), 7.87 (d, *J*=8.8 Hz, 1H), 8.19 (s, 1H), 8.25 (s, 1H), 8.47 (s, 1H), 12.06 (brd s, 1H). **^{13}C NMR:** 13.46, 19.31, 31.02, 43.88, 44.12, 103.99, 110.64, 113.46, 117.70, 119.96, 120.67, 122.54, 125.20, 127.55, 128.18, 134.07, 134.49, 138.61, 142.30, 151.46.	402	$CHCl_3$: EtOAc: n-Hexane (1:2:1) cc
37	129	**$C_{20}H_{20}ClN_3O_2S_{\cdot H2O}$:** C, 57.26; H, 5.29; N, 10.02; S, 7.62; Found: C, 57.00; H, 5.37; N, 9.89; S, 7.26.	27	**^{1}H NMR:** 0.87 (t, 3H), 1.33 (m, 2H), 1.76 (m, 2H), 3.26 (s, 3H), 4.54 (t, 2H), 7.27 (d, *J*=7.2 Hz, 1H), 7.57 (d, *J*=8.4 Hz, 1H), 7.78 (d, *J*=8.0 Hz, 1H), 7.87 (d, *J*=8.8 Hz, 1H), 8.19 (s, 1H), 8.25 (s, 1H), 8.47 (s, 1H), 12.06 (brd s, 1H). **^{13}C NMR:**13.46, 19.31, 31.02, 43.88, 44.12, 103.99, 110.64, 113.46, 117.70, 119.96, 120.67, 122.54, 125.20, 127.55, 128.18, 134.07, 134.49, 138.61, 142.30, 151.46.	402	$CHCl_3$: EtOAc: n-Hexane (1.5:2:1) cc
38	240	**$C_{22}H_{23}N_3O_2S$-0.$_{\cdot 5H2O}$:** C, 65.64; H, 6.01; N, 10.43; S, 7.96; Found: C, 65.61; H, 6.45; N, 10.28; S, 7.74.	42	**^{1}H NMR:** 1.36 (m, 3H), 1.64 (d, 1H), 1.90 (m, 4H), 2.32 (m, 2H), 3.20 (s, 3H), 4.63 (m, 1H), 7.13-7.25 (m, 2H), 7.53 (d, *J*=8.0 Hz, 1H), 7.71 (dd, *J*=8.4 Hz, *J*=1.6 Hz, 1H), 7.83 (d, *J*=2.8 Hz, 1H), 7.95 (d, *J*=8.0 Hz, 1H), 8.08 (d, *J*=8.4 Hz, 1H), 8.18 (d, *J*=1.6 Hz, 1H), 11.80 (brd s, 1H, NH). **^{13}C NMR:** 18.46, 24.30, 25.48, 30.45, 44.19, 55.93, 56.55,104.14, 111.97, 113.17, 118.06, 119.51, 120.15, 120.32, 122.30, 126.45, 127.1.4,133.73, 136.04, 136.71, 143.34, 152.18.	394	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
39	210	**$C_{22}H_{23}N_3O_2S_{\cdot 0.5H2O}$:** C, 63.86; H, 6.05; N, 9.71; S, 7.41; Found: C, 63.47; H, 6.29; N, 9.34; S, 7.05.	37	**^{1}H NMR:** 1.340 (m, 3H), 1.68 (d, 1H), 1.93 (m, 4H), 2.34 (m, 2H), 3.24 (s, 3H), 3.78 (s, 3H), 4.64 (m, 1H), 6.90 (dd, *J*=8.8 Hz, *J*=2.8 Hz, 1H), 7.44 (m, 2H), 7.73 (dd, *J*=8.4 Hz, *J*=1.6 Hz, 1H), 7.80 (d, *J*=2.8 Hz, 1H), 8.10 (d, *J*=8.4 Hz, 1H), 8.20 (d, *J*=2.0 Hz, 1H), 11.70 (brd d, 1H). **^{13}C NMR:** 14.05, 24.38, 25.57, 30.55, 44.26, 55.25, 56.63, 59.72, 101.52, 104.02, 112.75, 112.82, 113.20, 118.11, 119.53, 126.98, 127.61, 131.11, 133.76, 136.80, 143.43, 152.44, 154.44.	424	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc

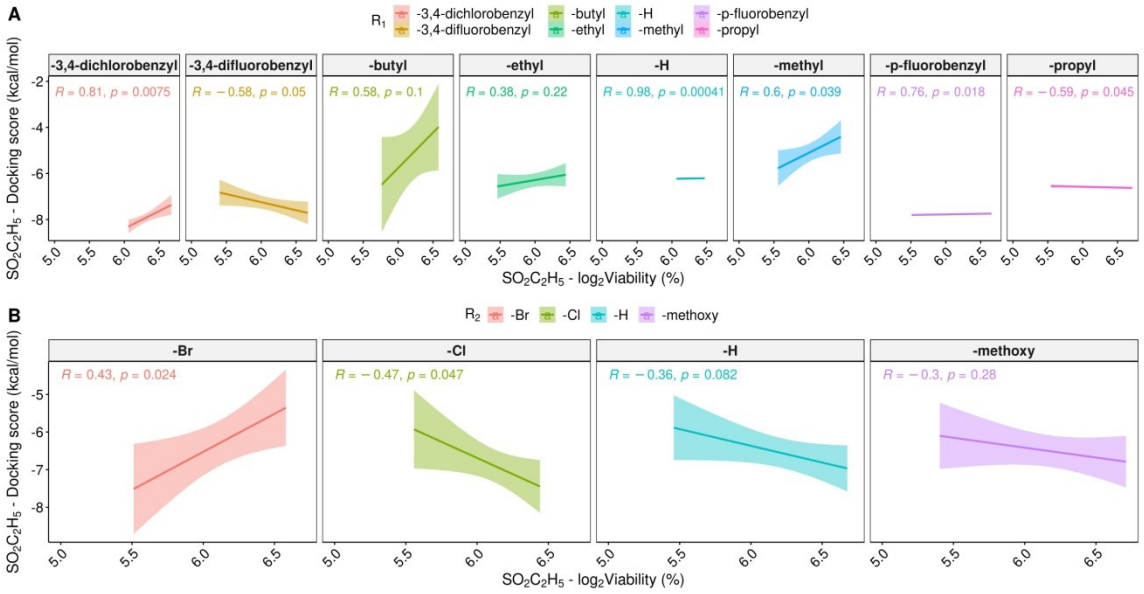
40	178	**$C_{22}H_{22}ClN_3O_2S$-$_{0.9\ H2O}$:** C, 59.55; H, 5.41; N, 9.47; S, 7.21; Found: C, 59.36; H, 5.55; N, 9.68; S, 7.10.	43	**^{1}H NMR:** 1.43 (m, 3H), 1.68 (s, 1H), 1.87-1.98 (m, 4H), 2.33 (m, 2H), 3.35 (s, 3H), 4.67 (m, 1H), 7.27 (dd, *J*= 8.4 Hz, *J*=2.0 Hz, 1H), 7.58 (d, *J*=9.2 Hz, 1H), 7.74 (dd, *J*=8.4 Hz, *J*=1.6 Hz, 1H), 7.96 (d, *J*=2.8 Hz, 1H), 8.07 (d, *J*=1.6 Hz, 1H), 8.11 (d, *J*=8.4 Hz, 1H), 8.25 (d, *J*=1.6 Hz, 1H), 12.02 (brd s, 1H, NH). **^{13}C NMR:** 24.38, 25.49, 30.48, 44.20, 48.57, 56.66, 103.98, 113.30, 113.65, 118.24, 119.64, 119.76, 122.48, 125.15, 127.75, 128.61, 133.94, 134.65, 136.72, 143.31, 151.53.	428	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
41	230	**$C_{22}H_{22}BrN_3O_2S$:** C, 55.94; H, 4.69; N, 8.90; S, 6.79; Found: C, 55.40; H, 4.65; N, 9.30; S, 6.67.	69	**^{1}H NMR:** 1.40 (m, 3H), 1.65 (s, 1H), 1.84-1.95 (m, 4H), 2.31 (m, 2H), 3.22 (s, 3H), 4.64 (m, 1H), 7.35 (dd, *J*=8.4 Hz, *J*=2 Hz, 1H), 7.51 (d, *J*=8.8 Hz, 1H), 7.71 (dd, *J*= 8.4 Hz, *J*=2.0 Hz, 1H), 7.92 (s, 1H), 8.08 (d, *J*=8.4 Hz, 1H), 8.21 (dd, *J*=11 Hz, *J*=2 Hz, 2H), 12.0 (brd s, 1H). **^{13}C NMR:** 24.31, 25.42, 30.42, 44.13, 56.59, 103.80, 113.04, 113.23, 114.01, 118.19, 119.56, 122.73, 124.93, 128.32, 128.37, 133.87, 134.82, 136.66, 143.26, 151.44.	474.	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
42	252	**$C_{23}H_{19}N_3O_2S$-$_{0.3\ H2O}$:** C, 67.89; H, 4.85; N, 10.33; S, 7.86; Found: C, 67.49; H, 4.83; N, 10.50; S, 7.84.	13	**^{1}H NMR:** 3.26 (s, 3H), 5.86 (s, 2H), 7.08 (d, *J*=7.2 Hz, 2H), 7.19-7.34 (m, 5H), 7.50 (dd, *J*=7.0 Hz, *J*=1.6 Hz, 1H), 7.75-7.79 (m, 3H), 8.26 (s, 1H), 8.45 (dd, *J*=7.2 Hz, *J*=1.6 Hz, 1H), 11.79 (brd s, 1H). **^{13}C NMR:** 44.21, 47.37, 103.95, 110.75, 111.90, 117.73, 120.33, 120.66, 121.53, 122.66, 125.97, 126.36, 126.85, 127.50, 128.96,134.42, 136.00, 136.61, 139.01, 142.66, 152.63.	402.	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
43	309	**$C_{23}H_{19}N_3O_2S$-$_{H2O}$:** C, 63.43; H, 4.86; N, 9.64; S, 7.36; Found: C, 63.69; H, 4.70; N, 9.44; S, 7.57.	44	**^{1}H NMR:** 3.23 (s, 3H), 3.79 (s, 3H), 5.81 (s, 2H), 6.87 (dd, *J*=8.8 Hz, *J*=2.4 Hz, 1H), 7.07 (d, *J*=7.6 Hz, 2H), 7.23-7.39 (m, 4H), 7.68-7.73 (m, 3H), 7.94 (d, *J*=2.4 Hz, 1H), 8.25 (s, 1H), 11.61 (brd s, 1H). **^{13}C NMR:** 44.22, 47.37, 55.31, 103.13, 103.71, 110.64, 112.60, 112.79, 117.72, 120.23, 125.96, 126.97, 127.20, 127.46, 128.93, 131.00, 134.34, 136.59, 138.98, 142.65, 152.81, 154.58	432	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
44	301	**$C_{23}H_{18}ClN_3O_2S$:** C, 63.36; H, 4.16; N, 9.63; S, 7.35; Found: C, 62.78; H, 4.16; N, 9.48; S, 7.02.	19	**^{1}H NMR:** 3.26 (s, 3H), 5.88 (s, 2H), 7.08 (d, *J*=7.6 Hz, 2H), 7.25-7.34 (m, 4H), 7.53 (d, *J*=8.4 Hz, 1H), 7.76 (s, 2H), 7.89 (s, 1H), 8.32 (s, 1H), 8.53 (d, *J*=2.0 Hz, 1H), 11.97 (brd s, 1H, NH). **^{13}C NMR:** 44.07, 47.25, 103.68, 110.67, 113.47, 117.83, 120.33, 120.69, 122.65, 125.32, 125.87, 127.43, 128.21, 128.88, 134.42, 134.50, 136.39, 138.89, 142.44, 151.91.	436	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
45	179	**$C_{23}H_{18}FN_3O_2S$-$_{1.6\ H2O}$:** C, 61.61; H, 4.76; N, 9.37; S, 7.13; Found: C, 61.31; H, 4.24; N, 9.45; S, 7.10.	47	**^{1}H NMR:** 3.25 (s, 3H), 5.84 (s, 2H), 7.10-7.27 (m, 6H), 7.51 (dd, *J*=7.2 Hz, *J*=1.2 Hz, 1H), 7.75 (d, *J*=1.2, 2H), 7.82 (d, *J*=2.8 Hz, 1H), 8.25 (t, 1H), 8.42 (d, *J*=8.4 Hz, 1H), 11.79 (brd s, 1H). **^{13}C NMR:** 44.19, 46.73, 103.88, 110.72, 111.89, 115.76 (d, J=21.3 Hz), 117.74, 120.35, 120.64, 121.49, 122.65, 126.33, 126.85, 128.08 (d, J=8.4 Hz), 132.73 (d, J=3.1 Hz), 134.48, 136.00, 138.86, 142.66, 152.53, 161.38 (d, J=241.6 Hz).	420	$CHCl_3$: EtOAc: n-Hexane (1:1:1) cc
46	273	**$C_{23}H_{17}ClFN_3O_2S$:** C, 60.86; H, 3.78; N, 9.26; S, 7.06; Found: C, 60.46; H, 3.75; N, 9.30; S, 6.96.	59	**^{1}H NMR:** 3.25 (s, 3H), 5.85 (s, 2H), 7.09-7.17 (m, 4H), 7.25 (dd, *J*=8.8 Hz, *J*=2.0 Hz, 1H), 7.52 (d, *J*=8.4 Hz, 1H), 7.76 (s, 2H), 7.91 (s, 1H), 8.30 (s, 1H), 8.50 (d, *J*=2.4 Hz, 1H). **^{13}C NMR:** 44.14, 46.70, 103.70, 110.74, 113.56, 115.78 (d, J=21.3 Hz), 117.93, 120.45, 120.75, 122.74, 125.41, 127.49, 128.77 (d, J=7.6 Hz), 128.32, 132.59 (d, J=3.1 Hz), 134.52, 134.63, 138.84, 142.54, 151.90, 161.40 (d, J=242.3 Hz)	454	$CHCl_3$: EtOAc: n-Hexane (1:1:1) cc
47	183	**$C_{23}H_{17}BrFN_3O_2S$-$_{1.0\ H2O}$:** C, 53.49; H, 3.70; N, 8.13; S, 6.21; Found: C, 53.11; H, 3.54; N, 8.13; S, 6.84.	54	**^{1}H NMR:** 3.24 (s, 3H), 5.84 (s, 2H), 7.08-7.16 (m, 4H), 7.36 (dd, *J*=8.8 Hz, *J*=1.6 Hz, 1H), 7.47 (d, *J*=8.4 Hz, 1H), 7.76 (s, 2H), 7.91 (d, *J*=2.8 Hz, 1H), 8.29 (s, 1H), 8.60 (d, *J*=1.6 Hz, 1H), 12.01 (brd s, 1H). **^{13}C NMR:** 44.10, 46.79, 103.12, 110.96, 113.50, 114.07, 115.79 (d, J=21.4 Hz), 117.69, 120.68, 123.65, 125.34, 128.05 (d, J=7.6 Hz),128.16, 128.48, 132.45 (d, J=3.1 Hz), 134.78, 134.88, 138.62, 141.79, 151.70, 161.42 (d, J=242.3 Hz).	500	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
48	193	**$C_{24}H_{18}F_2N_3O_3S$:** C, 63.15; H, 3.92; N, 9.61; S, 7.33; Found: C, 62.89; H, 3.72; N, 9.82; S, 7.30.	68	**^{1}H NMR:** δ ppm 3.23 (s, 3H), 5.82 (s, 2H), 6.76 (m, 1H), 7.17-7.37 (m, 4H), 7.48 (m, 1H), 7.49-7.81 (m, 3H), 8.23 (t, 1H), 8.41 (dd, *J*=7.2 Hz, *J*=1.6 Hz, 1H), 11.78 (s, 1H).	438	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
49	281	**$C_{24}H_{19}F_2N_3O_3S$:** C, 61.66; H, 4.10; N, 8.99; S, 6.86; Found: C, 61.34; H, 3.97; N, 9.08; S, 6.86.	49	**^{1}H NMR:** 3.23 (s, 3H), 3.79. (s, 3H), 5.80 (s, 2H), 6.75 (m, 1H), 6.87 (dd, *J*=9.2 Hz, *J*=2.4 Hz, 1H), 7.23-7.39 (m, 3H), 7.73-7.76 (m, 3H), 7.93 (d, *J*=2.4 Hz, 1H), 8.24 (d, *J*=1.2 Hz, 1H), 11.65 (brd d, 1H).	468	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
50	292	**$C_{23}H_{16}ClF_2N_3O_2S$:** C, 58.54; H, 3.42; N, 8.90; S, 6.79; Found: C, 58.26; H, 3.21; N, 9.06; S, 6.80.	50	**^{1}H NMR:** 3.26 (s, 3H), 5.86 (s, 2H), 6.76 (m, 1H), 7.25-7.39 (m, 3H), 7.53 (d, *J*=8.8 Hz, 1H), 7.78 (s, 2H), 7.93 (s, 1H), 8.31 (s, 1H), 8.50 (d, *J*=2.0 Hz, 1H), 12.00 (brd s, 1H).	472	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
51	285	**$C_{23}H_{16}BrF_2N_3O_2S$:** C, 53.50; H, 3.12; N, 8.14; S, 6.21; Found: C, 53.11; H, 2.78; N, 8.42; S, 6.19.	65	**^{1}H NMR:** 3.26 (s, 3H), 5.86 (s, 2H), 6.76 (m, 1H), 7.27-7.39 (m, 3H), 7.49 (d, *J*=8.4 Hz, 1H), 7.78 (s, 2H), 7.91 (s, 1H), 8.32 (d, *J*=1.2 Hz, 1H), 8.64 (d, *J*=1.6 Hz, 1H), 12.00 (brd s, 1H).	518	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
52	148	**$C_{23}H_{18}ClN_3O_2S$-$_{0.2\ H2O}$:** C, 62.85; H, 4.21; N, 9.56; S, 7.29; Found: C, 62.62; H, 4.51; N, 9.27; S, 6.95.	15	**^{1}H NMR:** 3.23 (s, 3H), 5.83 (s, 2H), 7.07 (d, J=8.8, 2H), 7.17-7.25 (m, 2H), 7.36 (m, 2H), 7.48 (dd, *J*=7.2 Hz, *J*=1.2 Hz, 1H), 7.73 (d, *J*=1.2, 2H), 7.77 (s, 1H), 8.23 (d, 1H), 8.42 (m, 1H), 11.76 (brd s, 1H). **^{13}C NMR:** 44.18, 46.78, 103.83, 110.67, 111.89, 117.74, 120.37, 120.64, 121.51, 122.65, 126.32, 126.84, 127.90, 128.90, 132.07, 134.51, 135.62, 135.99, 138.86, 142.66, 152.52.	436.	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
53	236	**$C_{24}H_{20}ClN_3O_3S$-$_{0,1H2O}$:** C, 61.62; H, 4.35; N, 8.98; S, 6.85; Found: C, 61.34; H, 4.64; N, 8.89; S, 6.62.	19	**^{1}H NMR:** 3.23 (s, 3H), 3.79 (s, 3H), 5.82 (s, 2H), 6.87 (dd, *J*=9.0 Hz, *J*=2.4 Hz, 1H), 7.89 (d, *J*=8.4, 2H), 7.37 (d, *J*=8.8 Hz, 3H), 7.71-7.72 (m, 3H), 7.94 (d, *J*=2.4 Hz, 1H), 8.23 (s, 1H), 11.64 (brd s, 1H). **^{13}C NMR:** 44.20, 46.79, 55.31, 103.15, 103.59, 110.59, 112.61, 112.81, 117.75, 120.31, 126.96, 127.20, 127.91, 128.90, 131.00, 132.07, 134.45, 135.63, 138.86, 142.66, 152.72, 154.60.	466	$CHCl_3$: isopropanol (10:0.5) cc
54	233	**$C_{23}H_{17}Cl_2N_3O_2S$-$_{1.2\ H2O}$:** C, 56.14; H, 3.97; N, 8.54; S, 6.51; Found: C, 55.82; H, 3.30; N, 8.89; S, 6.54.	24	**^{1}H NMR:** 3.24 (s, 3H), 5.85 (s, 2H), 7.07 (d, J=8.8 Hz, 2H), 7.24 (dd, *J*=9.0 Hz, *J*=2.0 Hz, 1H), 7.37 (dd, *J*=6.8 Hz, *J*=2.0, 2H), 7.51 (d, *J*=8.4 Hz, 1H), 7.75 (d, *J*=0.8 Hz, 2H), 7.88 (s, 1H), 8.29 (s, 1H), 8.50 (d, *J*=2.0 Hz, 1H), 11.95 (brd s, 1H). **^{13}C NMR:** 44.04, 46.65, 103.56, 110.62, 113.49, 117.86, 120.39, 120.70, 122.67, 125.33, 127.40, 127.82, 128.24, 128.84, 132.01, 134.42, 134.59, 135.42, 138.77, 142.44, 151.82	470	$CHCl_3$: isopropanol (10:0.5) cc
55	239	**$C_{23}H_{17}BrClN_3O_2S$-1.3 H_2O:** C, 51.32; H, 3.67; N, 7.80; S, 5.95; Found: C, 50.98; H, 3.19; N, 7.90; S, 5.85.	14	**^{1}H NMR:** 3.26 (s, 3H), 5.87 (s, 2H), 7.09 (d, *J*=8.4, 2H), 7.38 (m, 3H), 7.49 (d, J=8.4, 1H), 7.72 (d, *J*=0.8, 2H), 7.89 (s, 1H), 8.32 (s, 1H), 8.66 (d, *J*=2.0, 1H), 11.98 (brd s, 1H). **^{13}C NMR:** 44.04, 46.65, 103.45, 110.62, 113.34, 113.92, 117.87, 120.39, 123.71, 125.20, 127.81, 128.02, 128.07, 128.84, 132.02, 134.60, 134.66, 135.41, 138.76, 142.43, 151.78	516	$CHCl_3$: EtOAc: n-Hexane (1:1.5:0.5) cc
56	260	**$C_{23}H_{17}Cl_2N_3O_2S$-$_{1.1\ H2O}$:** C, 56.35; H, 3.94; N, 8.57; S, 6.54; Found: C, 56.01; H, 3.69; N, 8.58; S, 6.43.	27	**^{1}H NMR:** 3.26 (s, 3H), 5.88 (s, 2H), 6.90 (dd, *J*=8.4 Hz, *J*=2.4 Hz, 1H), 7.20-7.28 (m, 2H), 7.48-7.56 (m, 3H), 7.77 (d, *J*=1.2 Hz, 2H), 7.83 (d, *J*=3.2 Hz, 1H), 8.27 (d, *J*=0.8 Hz, 1H), 8.45 (d, *J*=7.2 Hz, 1H), 11.80 (brd s, 1H). **^{13}C NMR:** 44.10, 46.26, 103.62, 110.56, 111.84, 117.72, 120.42, 120.62, 121.42, 122.62, 126.01, 126.24, 126.82, 128.34, 130.06, 131.08, 131.39, 134.58, 135.93, 137.74, 138.70, 142.58, 152.40.	470	$CHCl_3$: isopropanol (10:0.5) cc
57	296	**$C_{23}H_{16}Cl_3N_3O_2S$-0.6-$_{1.0\ \ H2O}$:** C, 53.57; H, 3.36; N, 8.14; S, 6.21; Found: C, 53.26; H, 3.16; N, 8.20; S, 6.13.	17	**^{1}H NMR:** 3.27 (s, 3H), 5.89 (s, 2H), 6.88 (dd, *J*=8.8 Hz, *J*=2.0 Hz, 1H), 7.27 (dd, *J*=8.4 Hz, *J*=2.4 Hz, 1H), 7.50-7.56 (m, 3H), 7.79 (d, *J*=0.8 Hz, 2H), 7.93 (s, 1H), 8.30 (s, 1H), 8.51 (d, *J*=2.0 Hz, 1H), 11.99 (brd s, 1H). **^{13}C NMR:** 44.09, 46.29, 103.50, 110.64, 113.57, 117.97, 120.57, 120.72, 122.76, 125.43, 126.02, 127.45, 128.34, 128.41, 130.14, 131.15, 131.46, 134.50, 134.78, 137.66, 138.74, 142.50, 151.84.	504	$CHCl_3$: isopropanol (10:0.5) cc
58	309	**$C_{23}H_{16}BrCl_2N_3O_2S$-$_{1.0H2O}$:** C, 48.69; H, 3.19; N, 7.40; S, 5.65; Found: C, 48.35; H, 2.97; N, 7.48; S, 5.59.	29	**^{1}H NMR:** 3.24 (s, 3H), 5.86 (s, 2H), 6.85 (dd, *J*=8.2 Hz, *J*=1.6 Hz, 1H), 7.35 (dd, *J*=8.8 Hz, *J*=1.6 Hz, 1H), 7.46 (s, 1H), 7.47 (d, *J*=2.0 Hz, 1H), 7.53 (d, *J*=8.8 Hz, 1H), 7.76 (d, *J*=1.2 Hz, 2H), 7.88 (s, 1H), 8.31 (s, 1H), 8.63 (d, *J*=2.0 Hz, 1H), 11.97 (brd s, 1H). **^{13}C NMR:** 44.02, 46.23, 103.32, 110.58, 113.38, 113.95, 117.93, 120.52, 123.68, 125.23, 125.96, 128.01, 128.13, 128.35, 130.08, 131.10, 131.41, 134.69, 134.74, 137.60, 138.68, 142.43, 151.75.	550	$CHCl_3$: isopropanol (10:0.5) cc



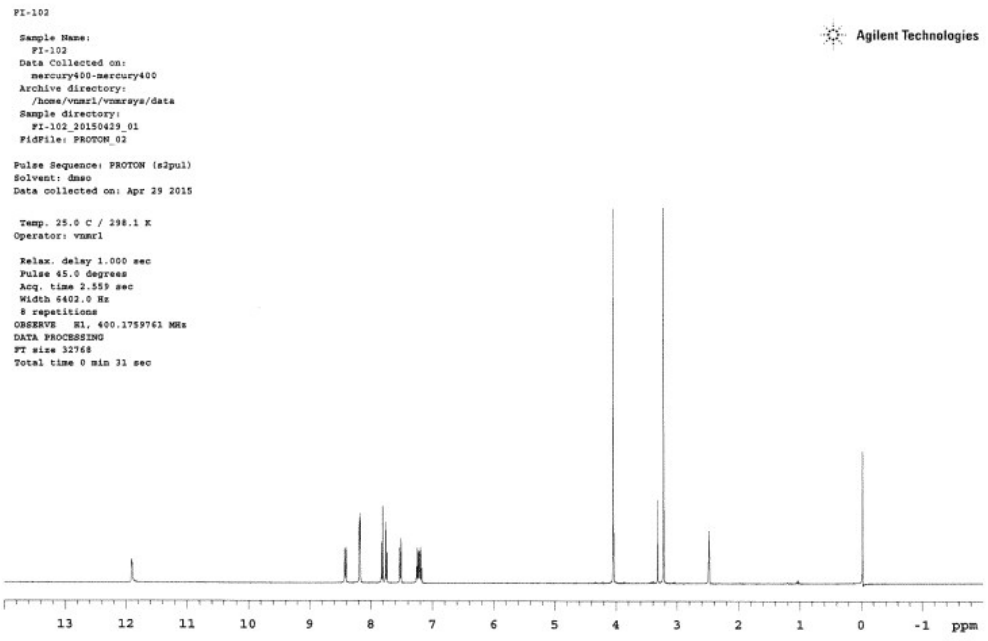
Suppl.Figure 1. Viability correlations between methylsulfonyl (20 µM) (x-axes) and ethylsulfonyl (16 µM) (y-axes) indole-benzimidazole exposures on MCF-7 for 24 hours. (A) Overall comparisons, (B) nonsignificant R_1 and (C) nonsignificant R_2 correlation assessments. Pearson's correlations were performed on the viability scores from the biological triplicates where the lines and shadow regions represent the linear correlations and confidence intervals, respectively.



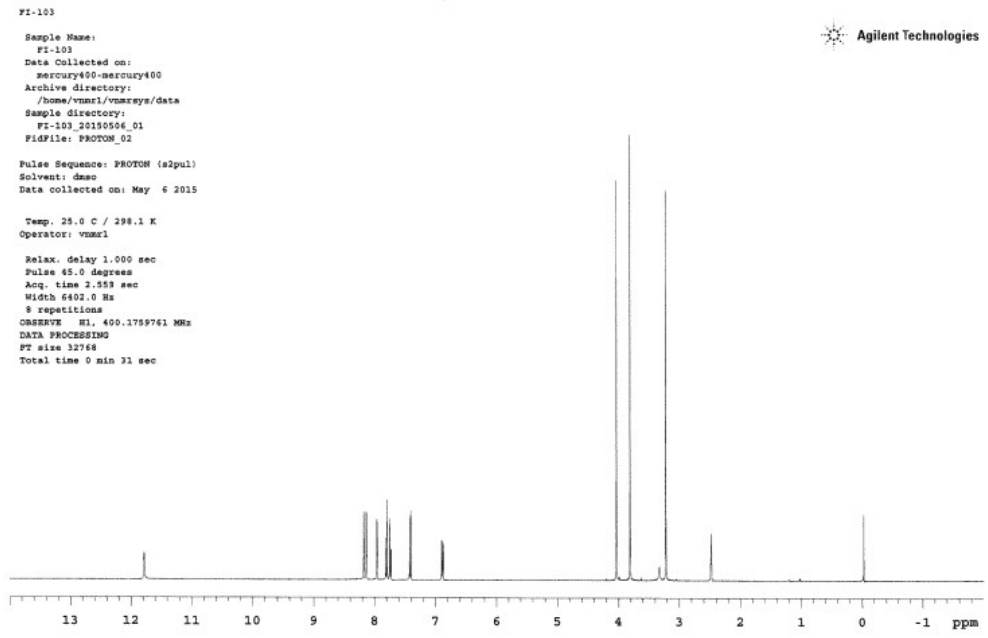
Suppl.Figure 2. Nonsignificant correlation maps between *in silico* docking scores (kcal/mol) (y-axes) and *in vitro* log2 transformed viability percentiles (x-axes) obtained from methylsulfonyl derivative exposures on MCF-7 cell line in triplicates: (A) R_1 and (B) R_2. Each R_1 and R_2 groups are color coded along with the confidence intervals, as Pearson's correlation and significancy scores are depicted inside the plots with the respective color codes for each group.



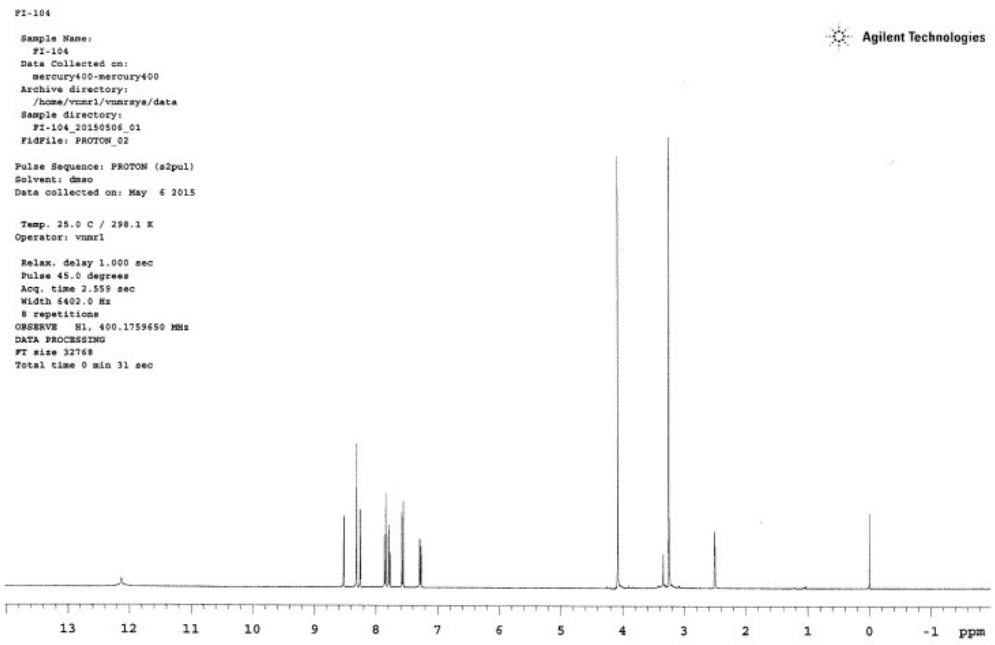
Suppl.Figure 3. Correlation maps between *in silico* docking scores (kcal/mol) (y-axes) and *in vitro* log2 transformed viability percentiles (x-axes) obtained from ethylsulfonyl derivative exposures on MCF-7 cell line in triplicates: (A) R_1 and (B) R_2. Each R_1 and R_2 groups are color coded along with the confidence intervals, as Pearson's correlation and significancy scores are depicted inside the plots with the respective color codes for each group.



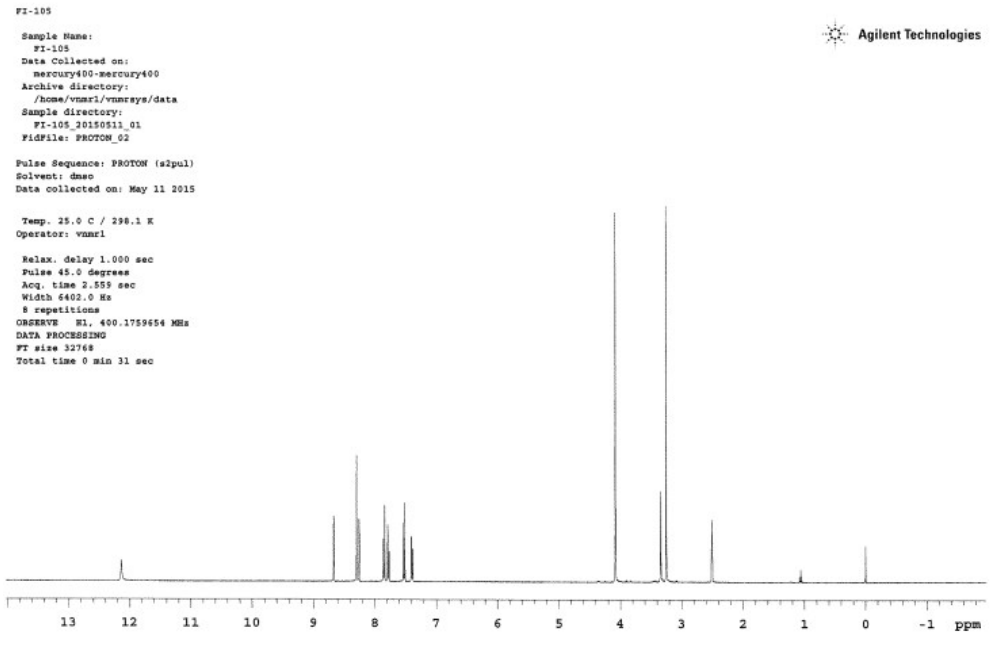
Suppl. Figure 4. ^{1}H NMR spectrum of compound **23.**



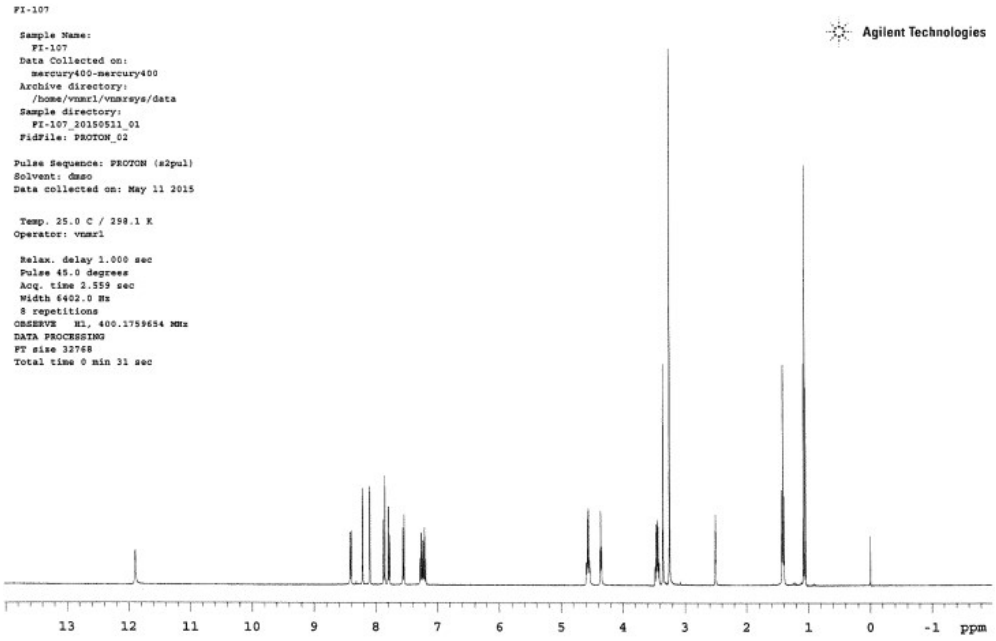
Suppl. Figure 5. ^{1}H NMR spectrum of compound **24.**



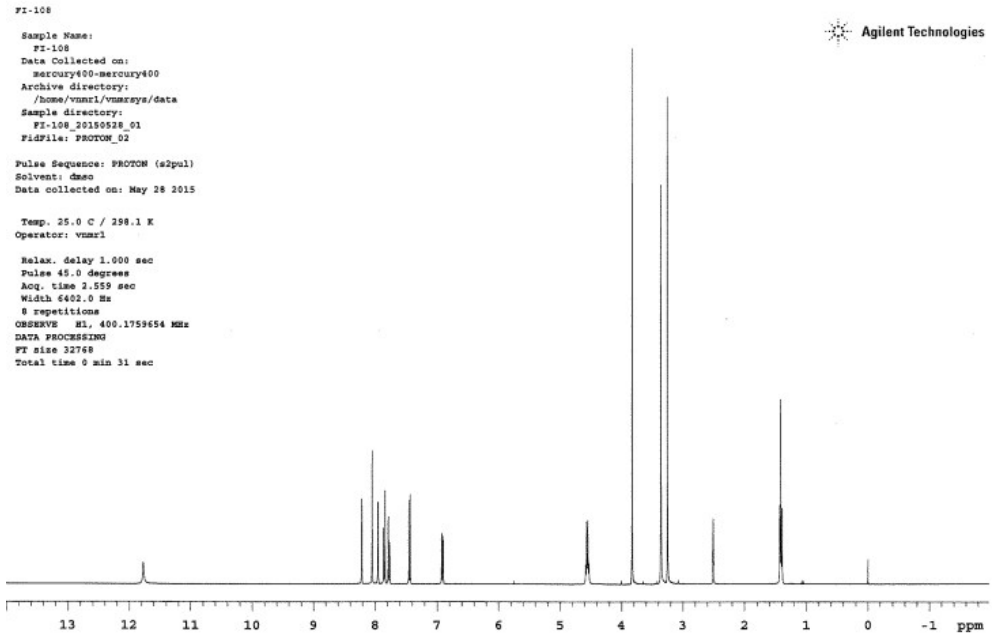
Suppl. Figure 6. ^{1}H NMR spectrum of compound **25.**



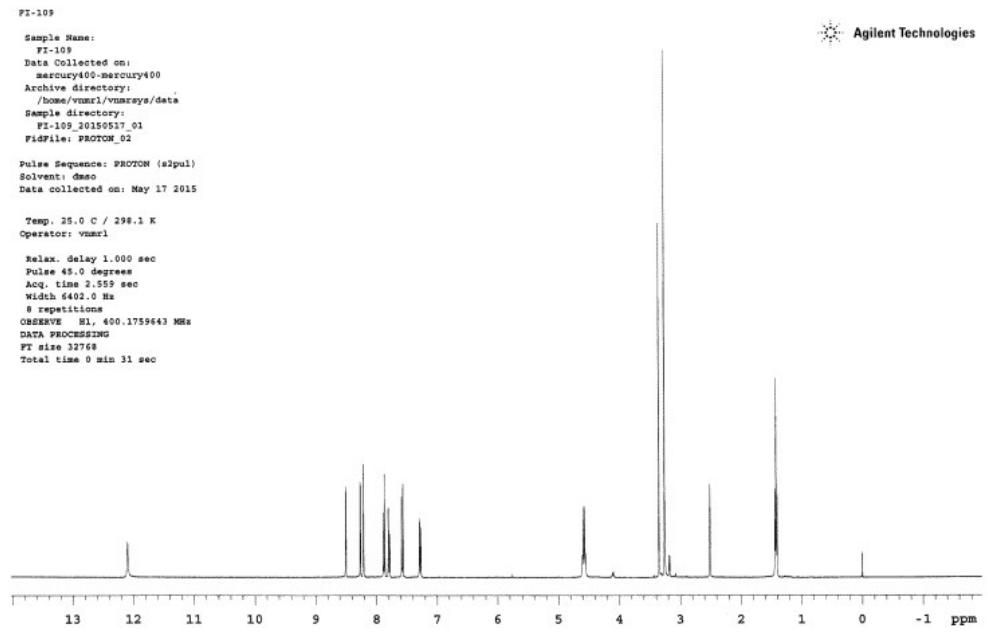
Suppl. Figure 7. ^{1}H NMR spectrum of compound **26.**



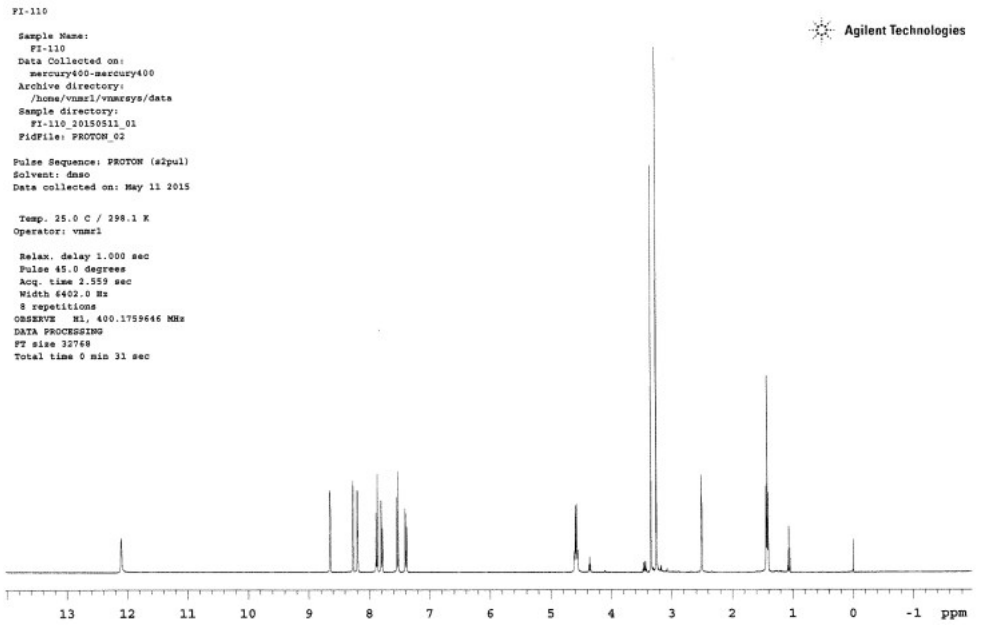
Suppl. Figure 8. ^{1}H NMR spectrum of compound **27.**



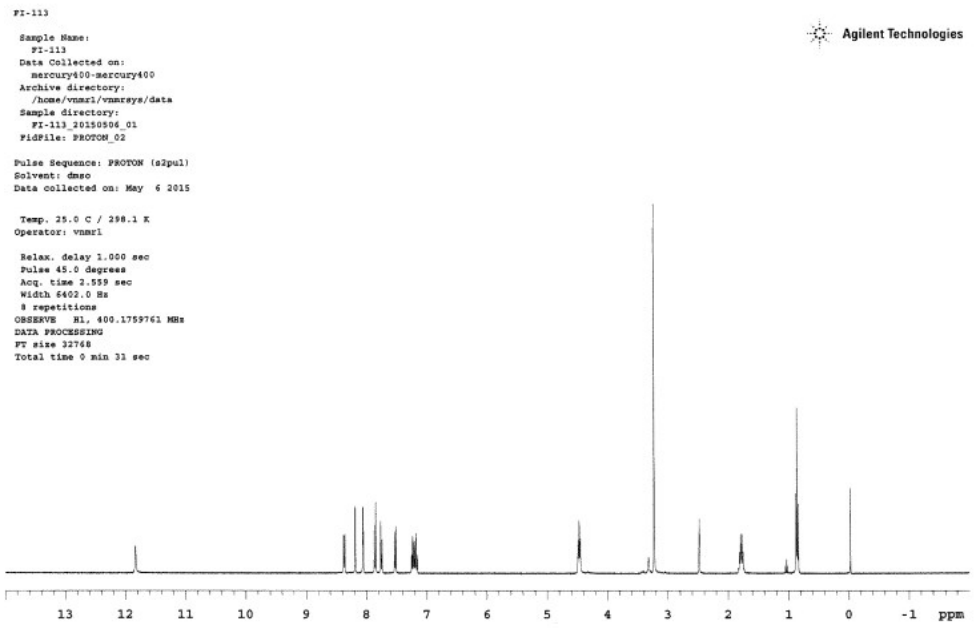
Suppl. Figure 9. ^{1}H NMR spectrum of compound **28.**



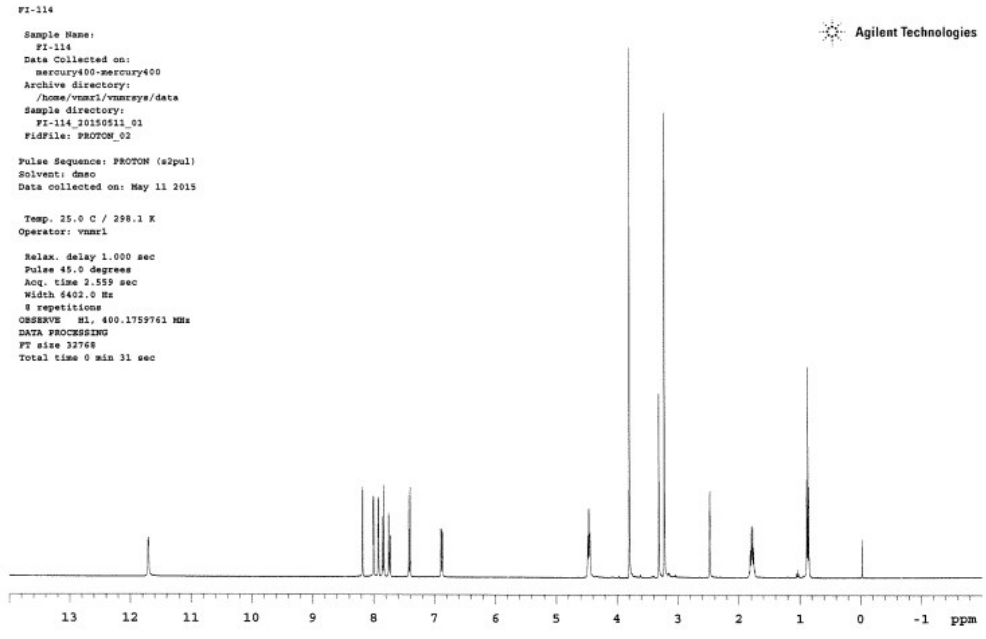
Suppl. Figure 10. ^{1}H NMR spectrum of compound **29.**



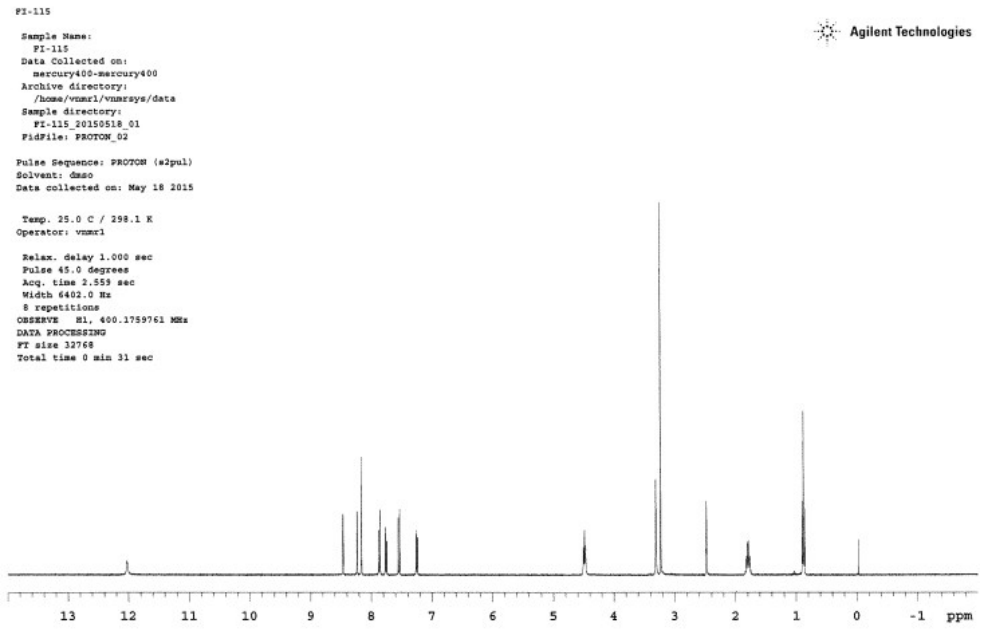
Suppl. Figure 11. ^{1}H NMR spectrum of compound **30.**



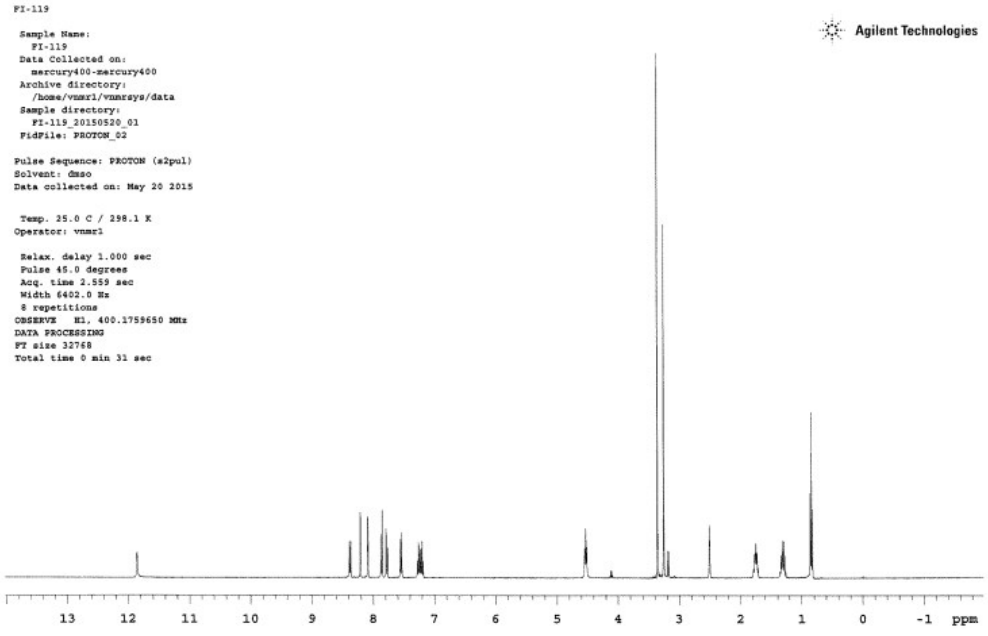
Suppl. Figure 12. ^{1}H NMR spectrum of compound **31.**



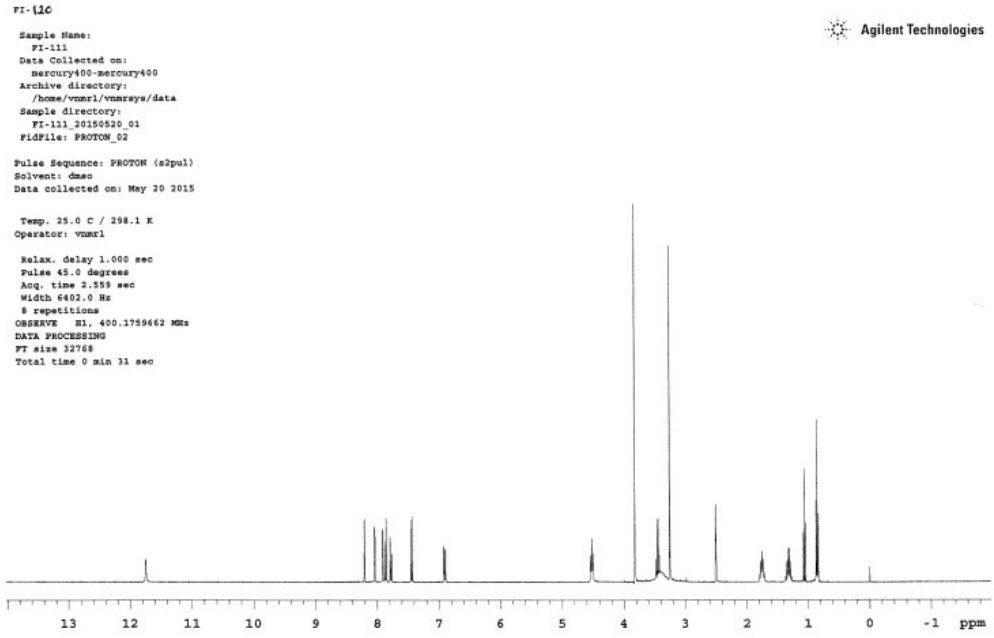
Suppl. Figure 13. ^{1}H NMR spectrum of compound **32.**



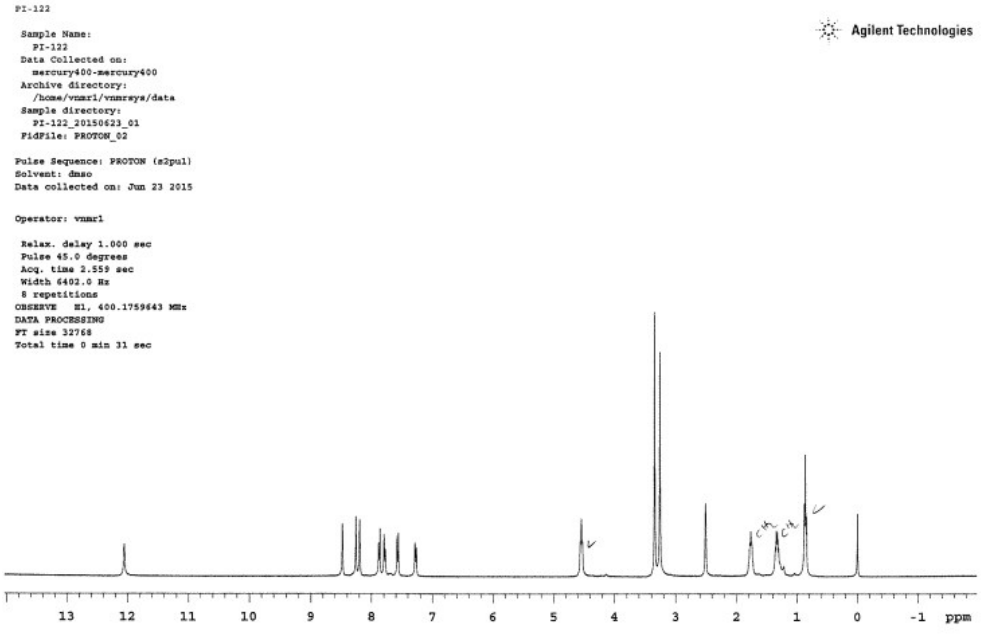
Suppl. Figure 14. ^{1}H NMR spectrum of compound **33.**



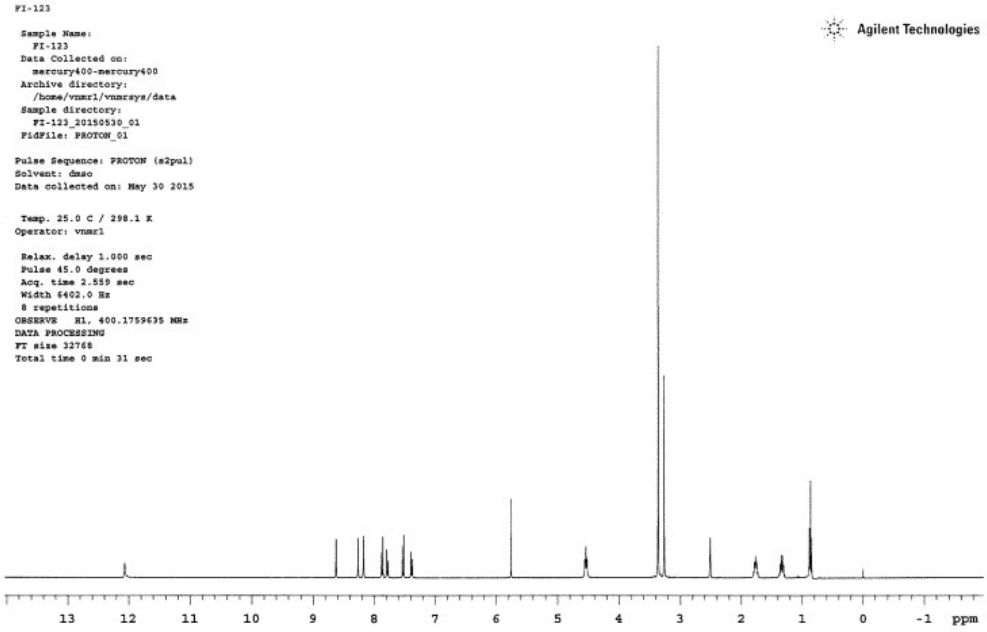
Suppl. Figure 15. ^{1}H NMR spectrum of compound **34.**



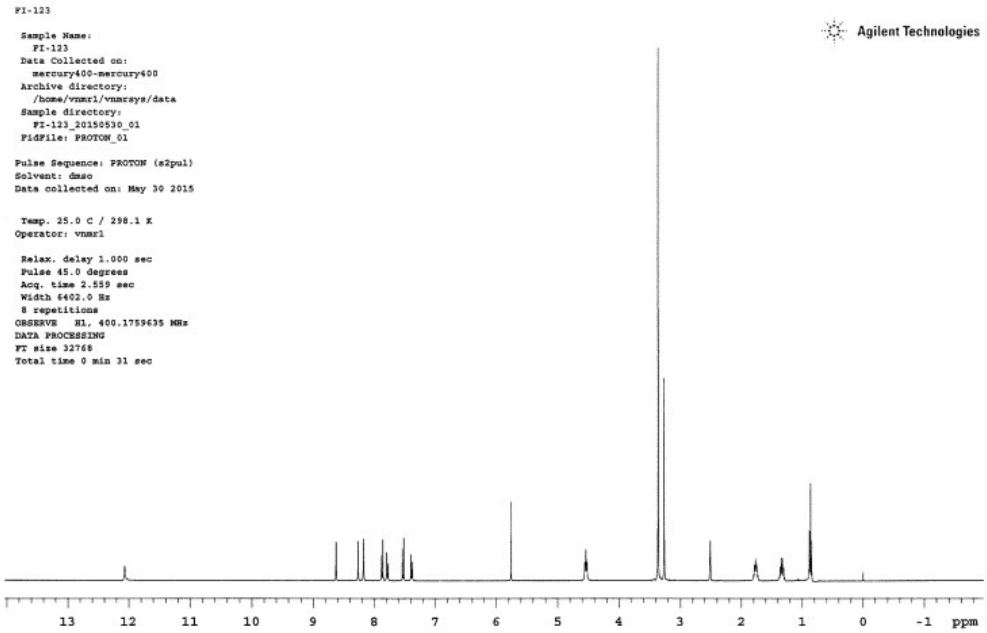
Suppl. Figure 16. ^{1}H NMR spectrum of compound **35.**



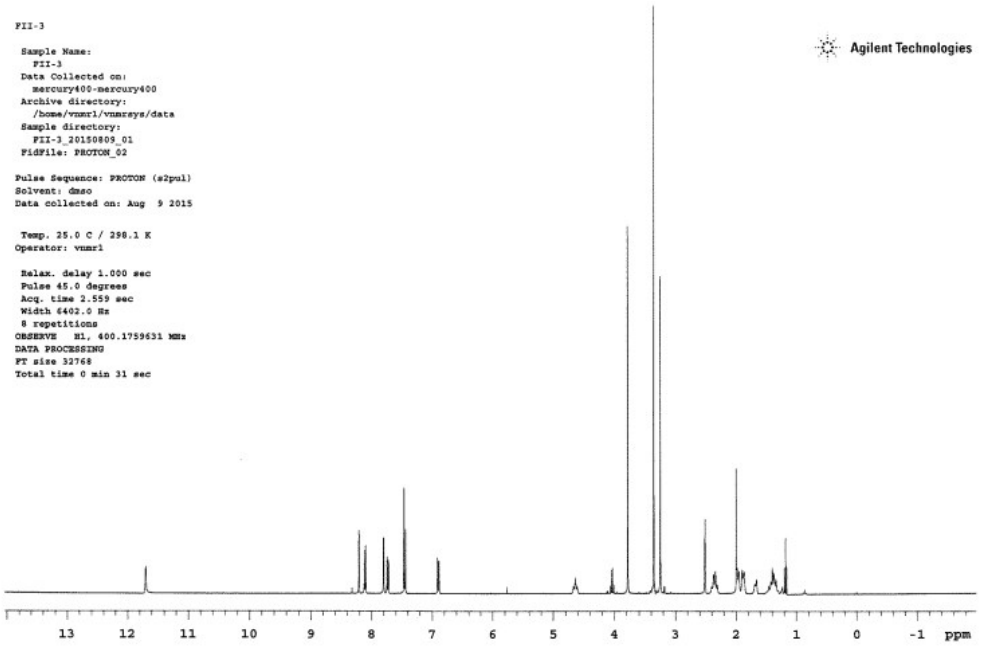
Suppl. Figure 17. ^{1}H NMR spectrum of compound **36.**



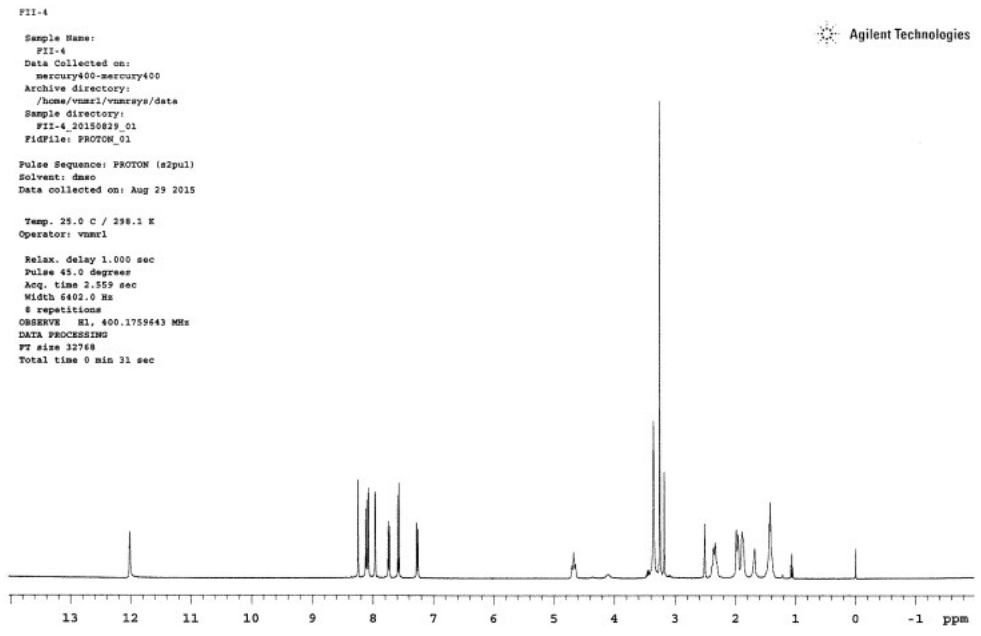
Suppl. Figure 18. ^{1}H NMR spectrum of compound **37.**



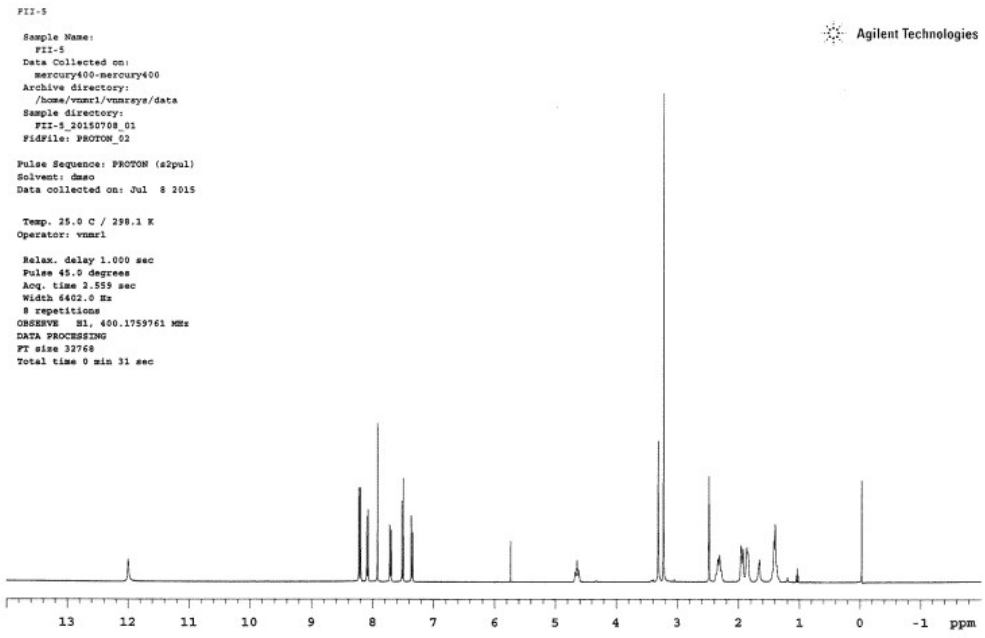
Suppl. Figure 19. ^{1}H NMR spectrum of compound **38.**



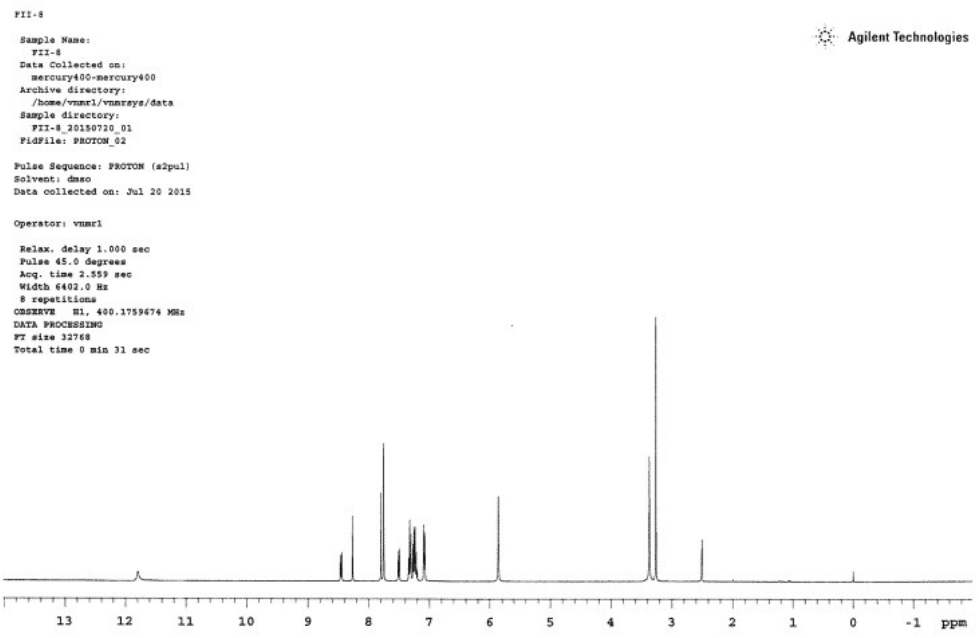
Suppl. Figure 20. ^{1}H NMR spectrum of compound **39.**



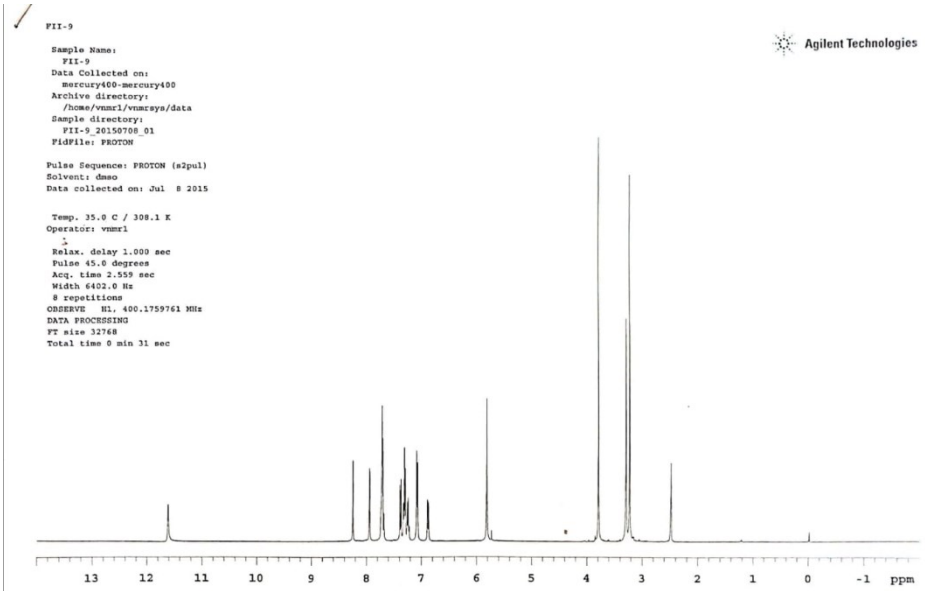
Suppl. Figure 21. ^{1}H NMR spectrum of compound **40.**



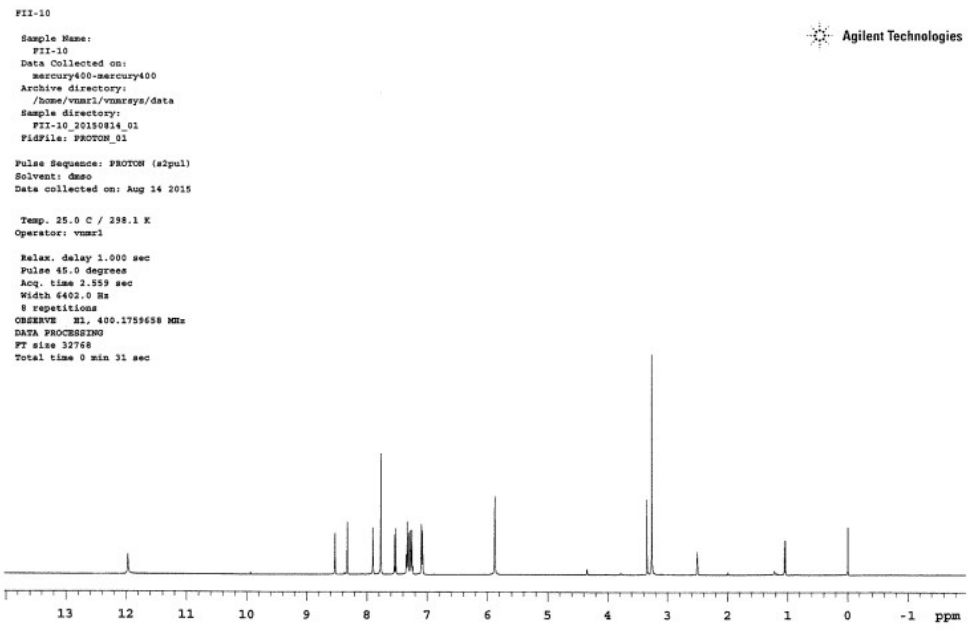
Suppl. Figure 22. ^{1}H NMR spectrum of compound **41.**



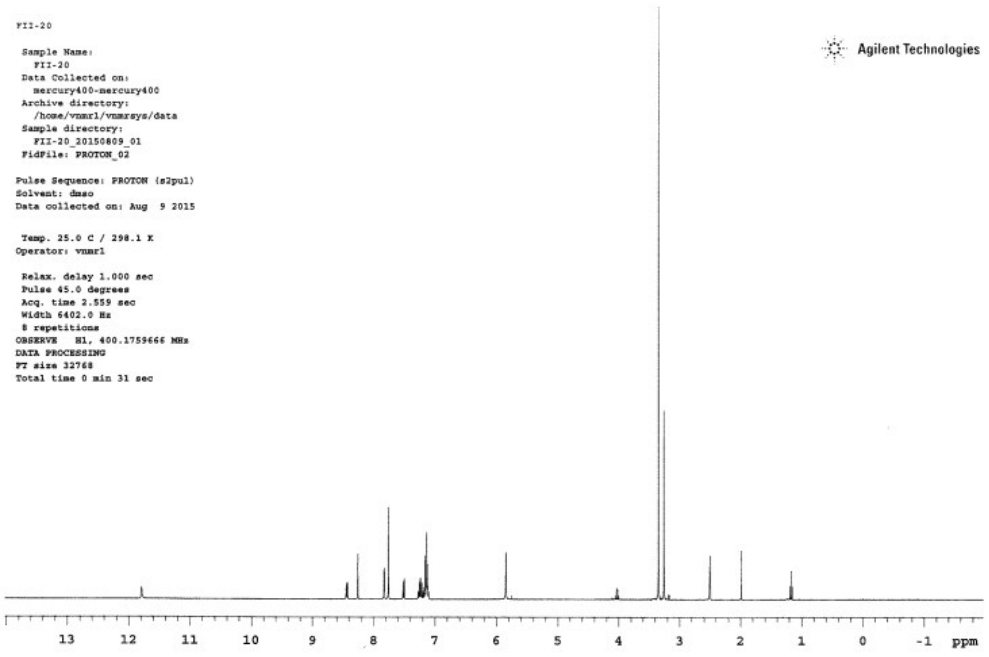
Suppl. Figure 23. ^{1}H NMR spectrum of compound **42.**



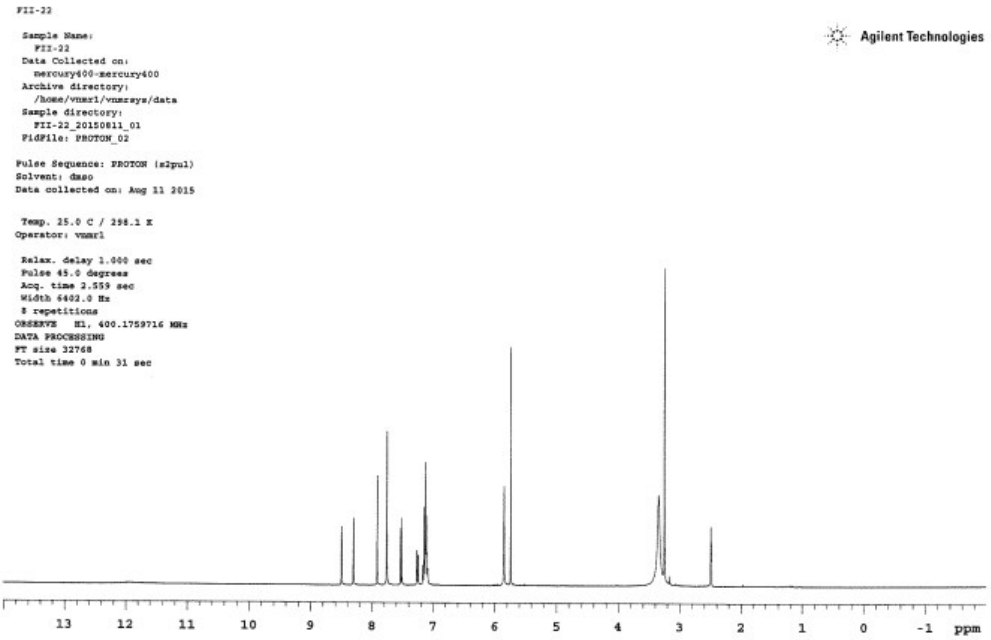
Suppl. Figure 24. ^{1}H NMR spectrum of compound **43.**



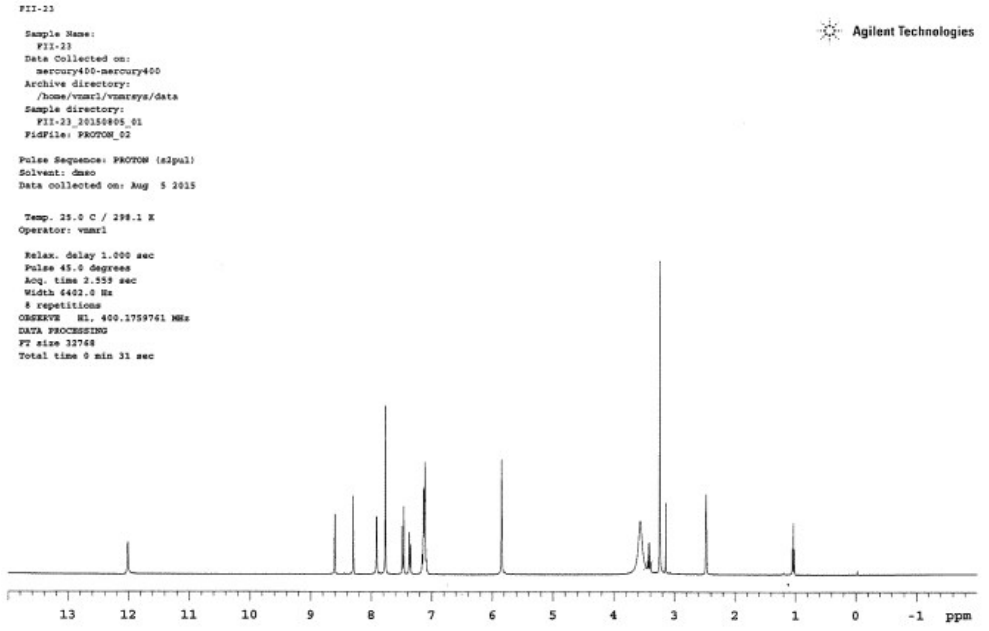
Suppl. Figure 25. ^{1}H NMR spectrum of compound **44.**



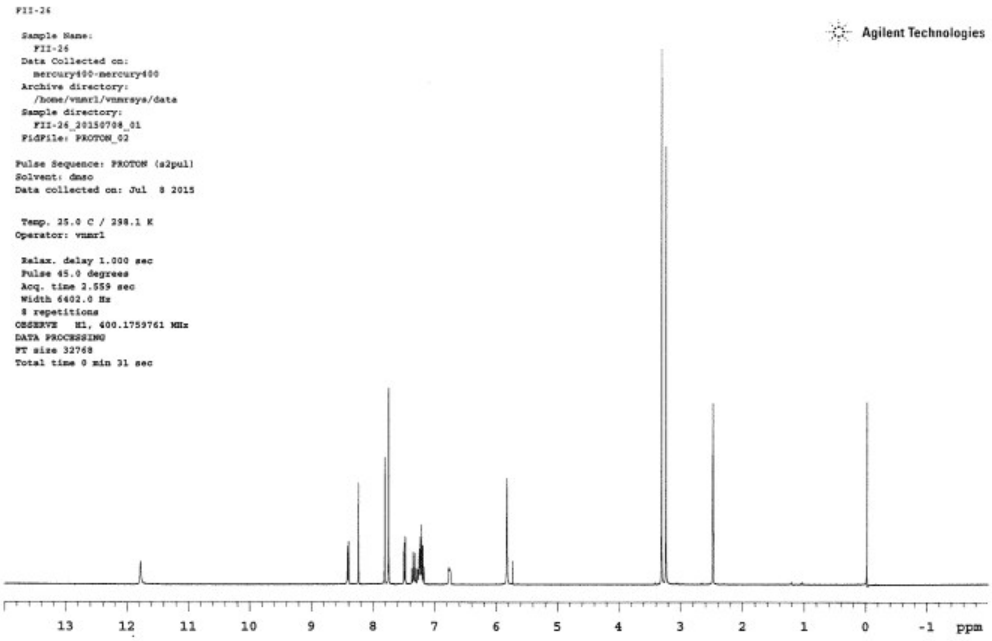
Suppl. Figure 26. ^{1}H NMR spectrum of compound **45.**



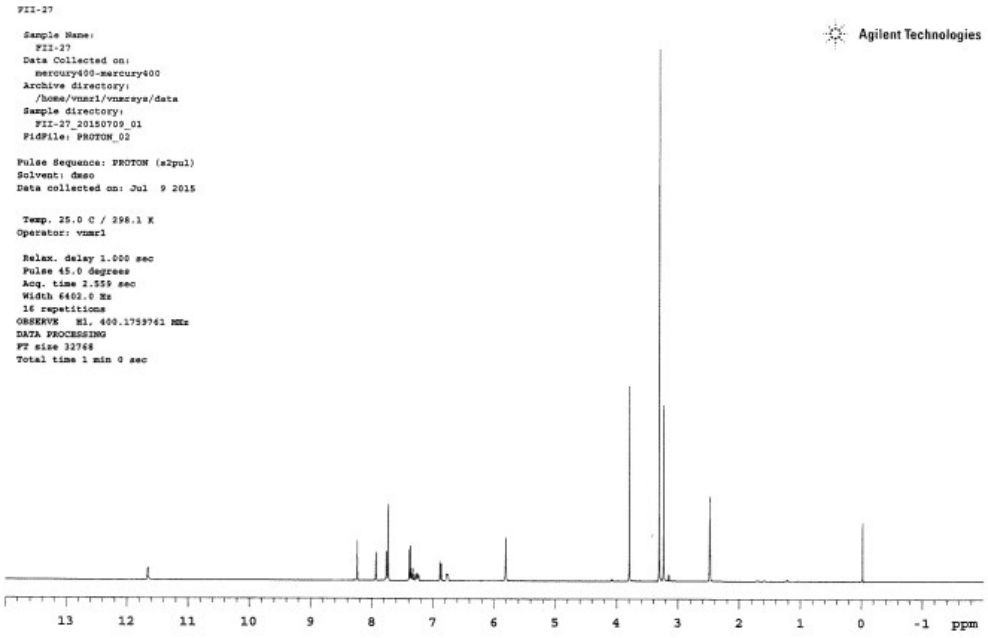
Suppl. Figure 27. ^{1}H NMR spectrum of compound **46.**



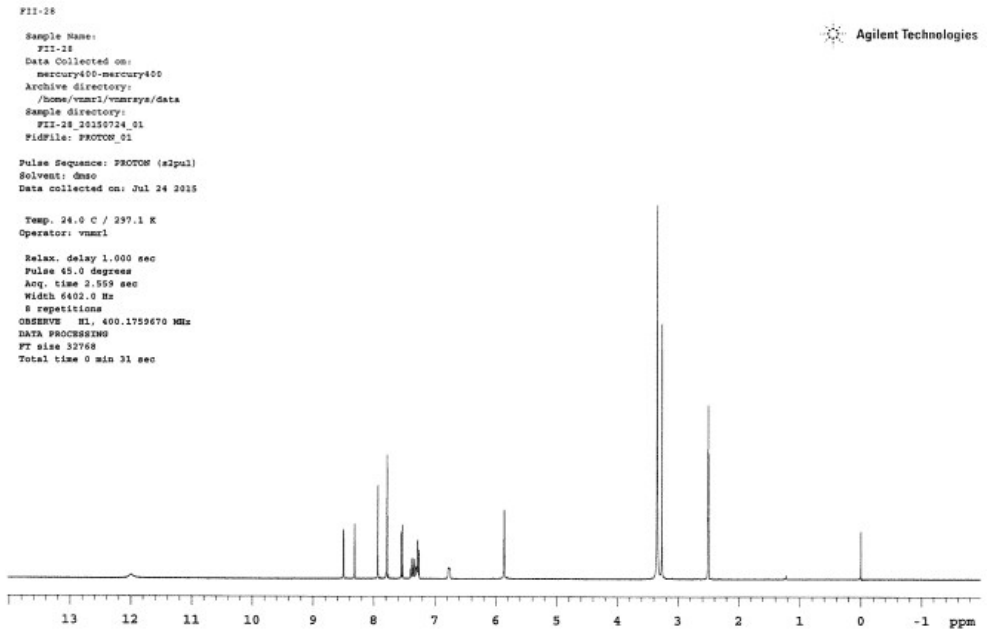
Suppl. Figure 28. ^{1}H NMR spectrum of compound **47.**



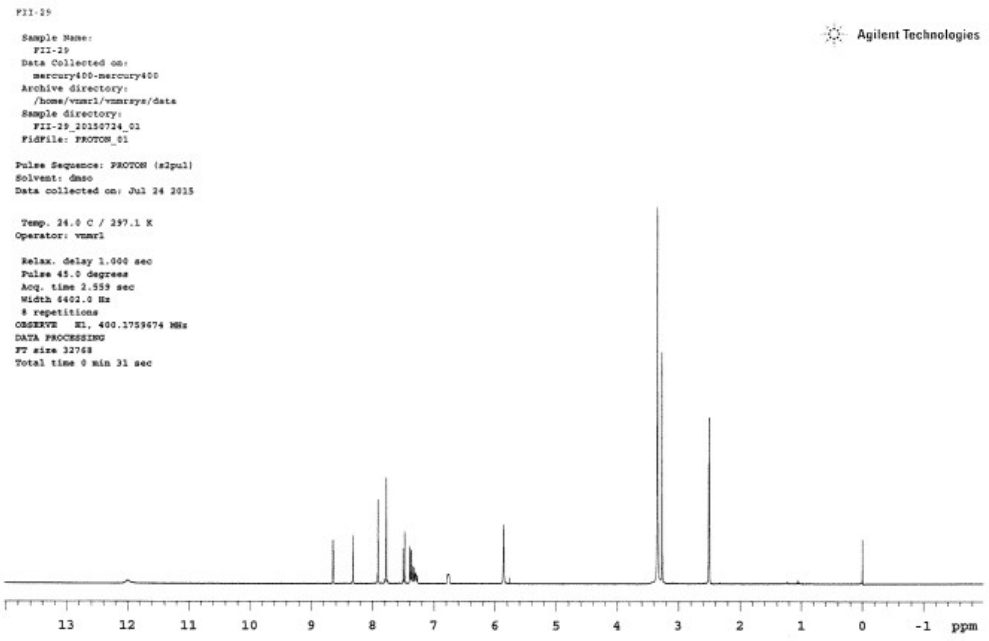
Suppl. Figure 29. ^{1}H NMR spectrum of compound **48.**



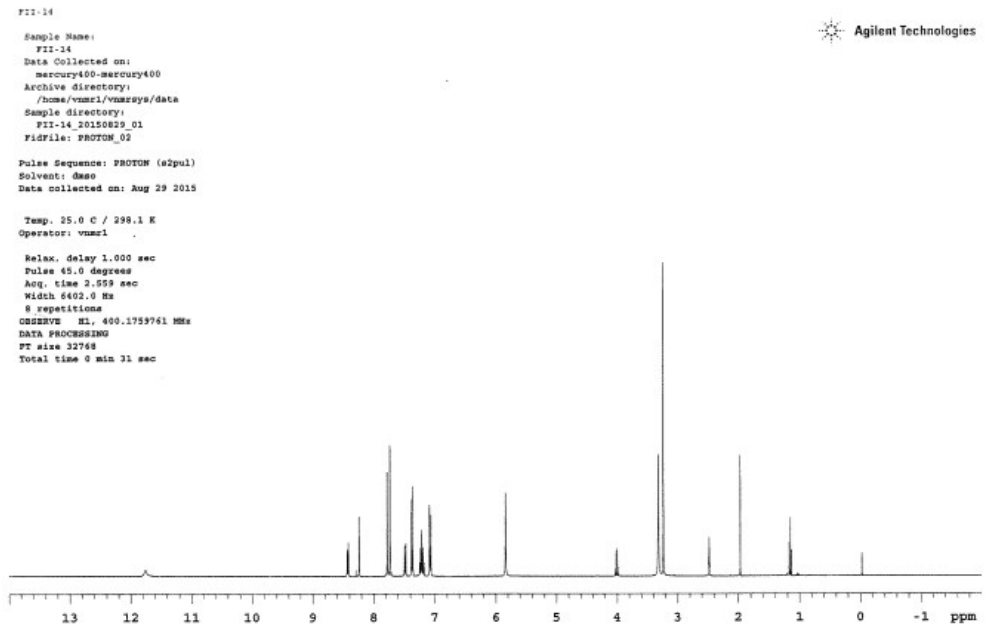
Suppl. Figure 30. ^{1}H NMR spectrum of compound **49.**



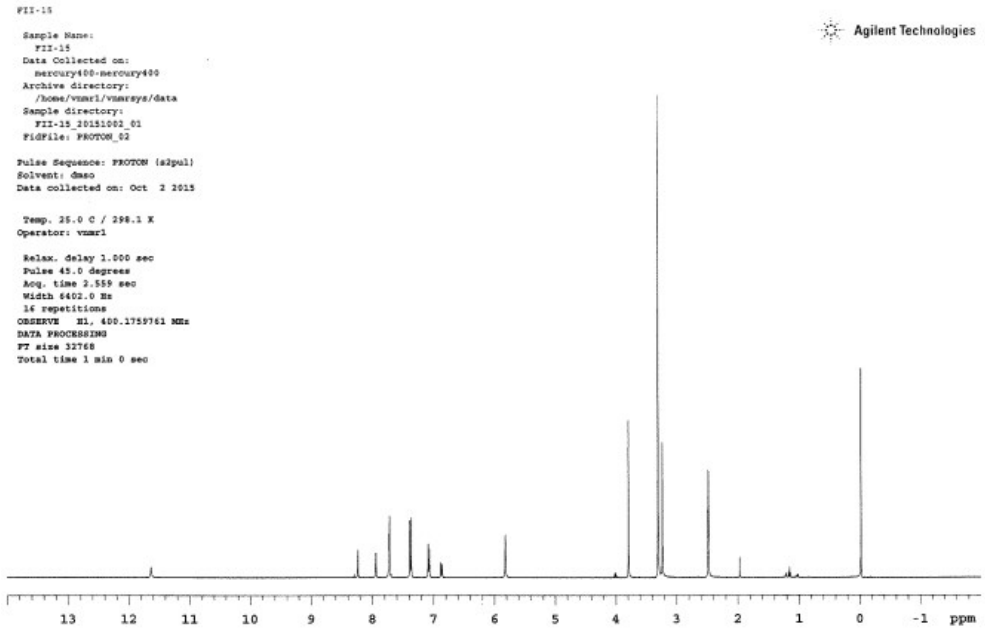
Suppl. Figure 31. ^{1}H NMR spectrum of compound **50.**



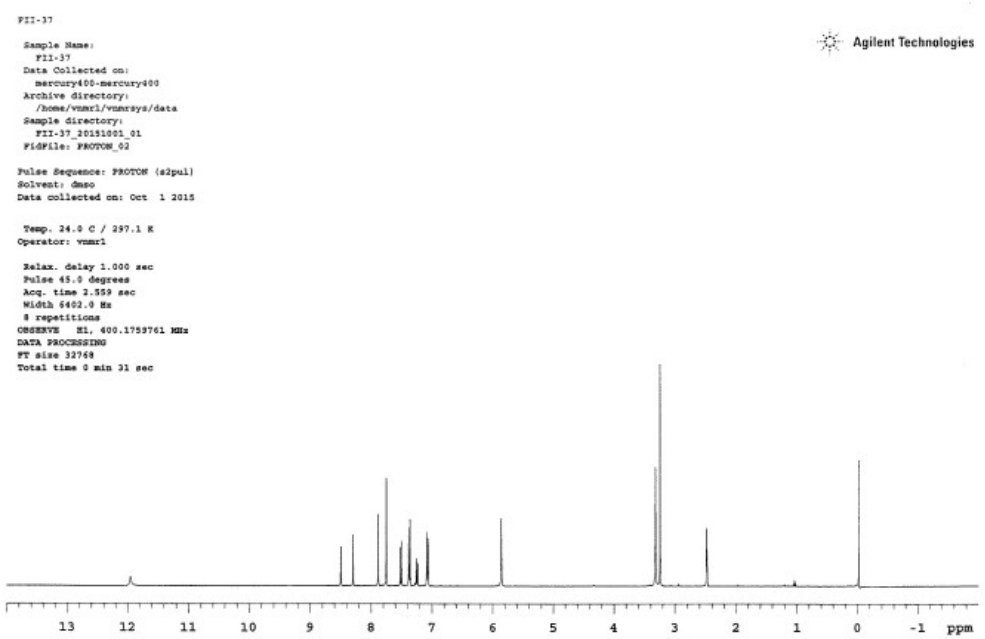
Suppl. Figure 32. ^{1}H NMR spectrum of compound **51.**



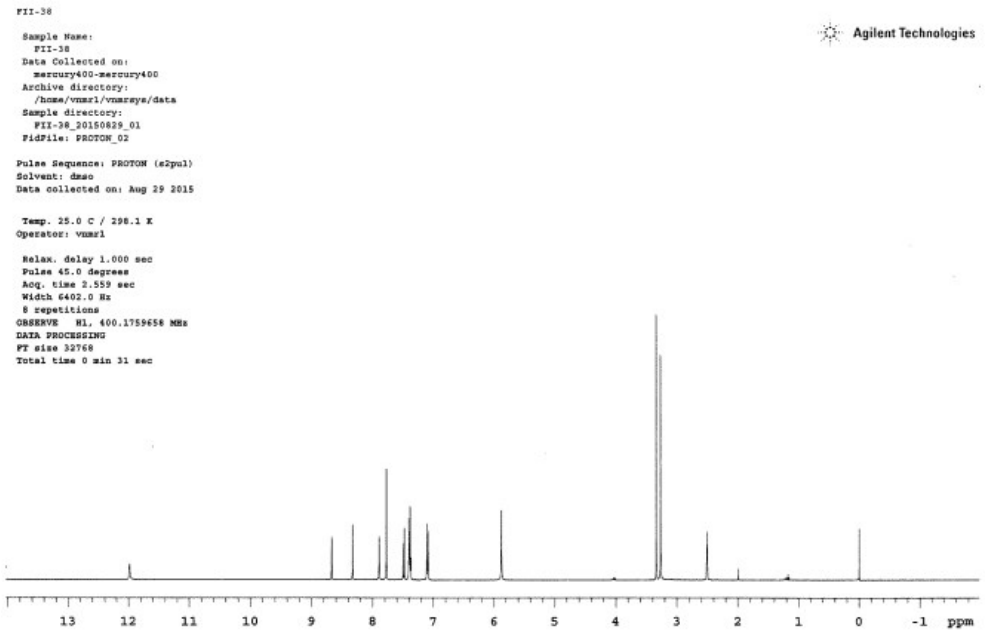
Suppl. Figure 33. ^{1}H NMR spectrum of compound **52.**



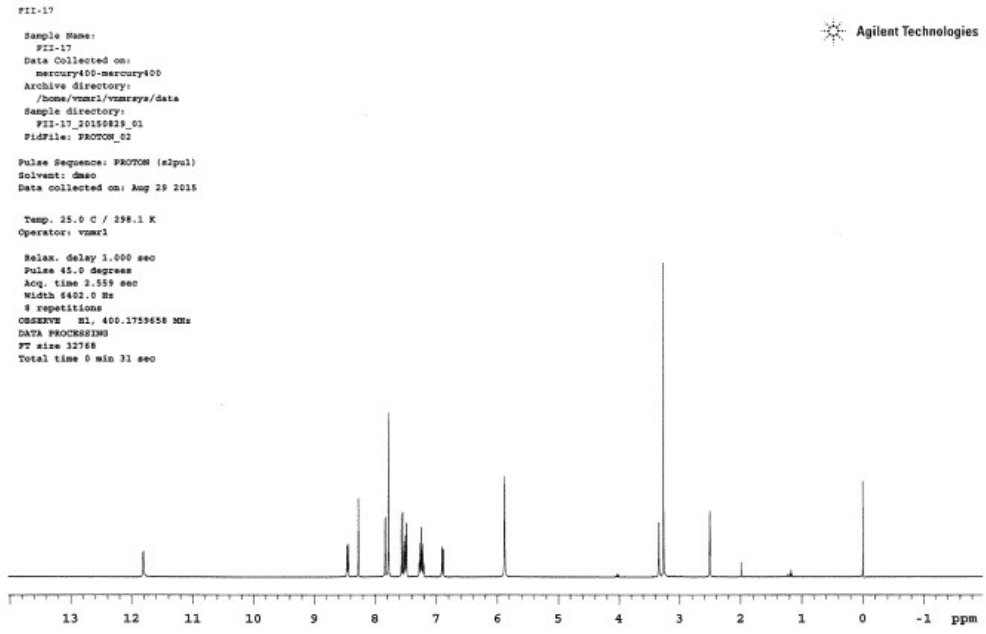
Suppl. Figure 34. ^{1}H NMR spectrum of compound **53.**



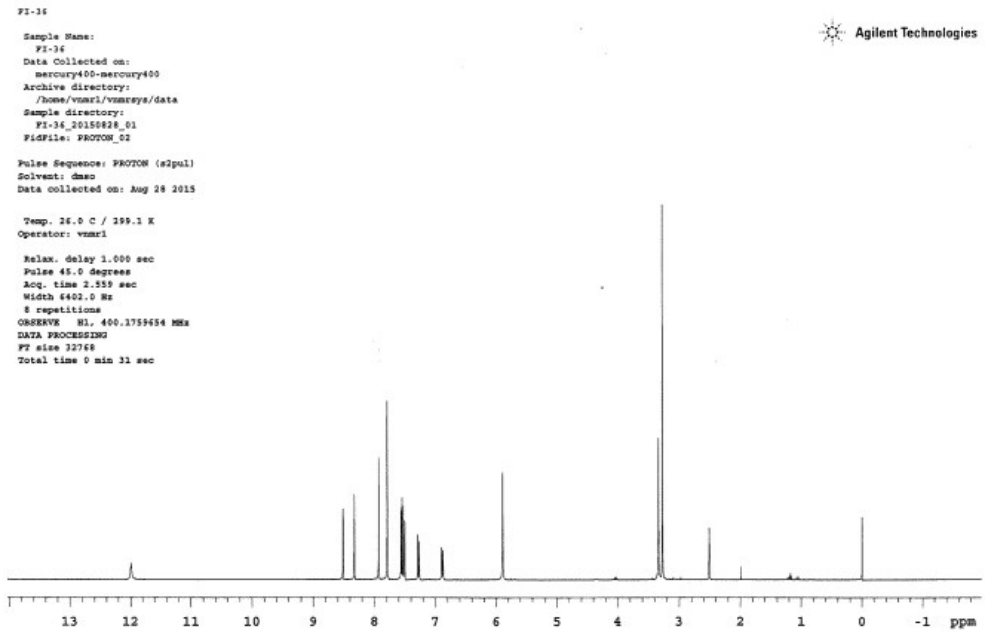
Suppl. Figure 35. ^{1}H NMR spectrum of compound **54.**



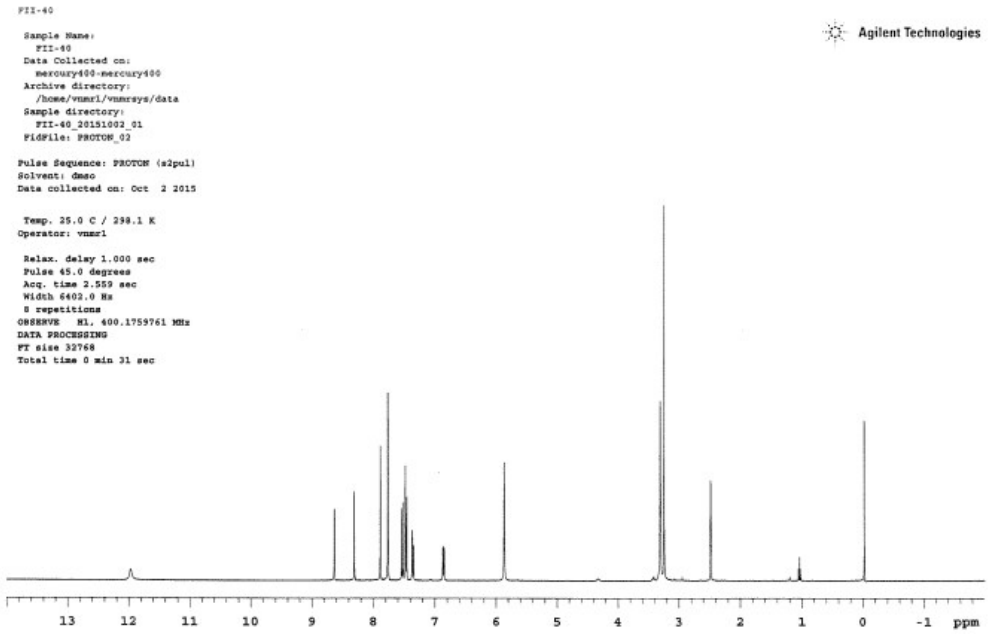
Suppl. Figure 36. ^{1}H NMR spectrum of compound **55.**



Suppl. Figure 37. ^{1}H NMR spectrum of compound **56.**



Suppl. Figure 38. ^{1}H NMR spectrum of compound **57.**



Suppl. Figure 39. ^{1}H NMR spectrum of compound **58.**