

Resubmission Molecules (MS# molecules - 1866652)

Structure Activity Relationship Development Efforts Towards Peripherally Selective Analogs of the Cannabinoid Receptor Partial Agonist BAY 59-3074

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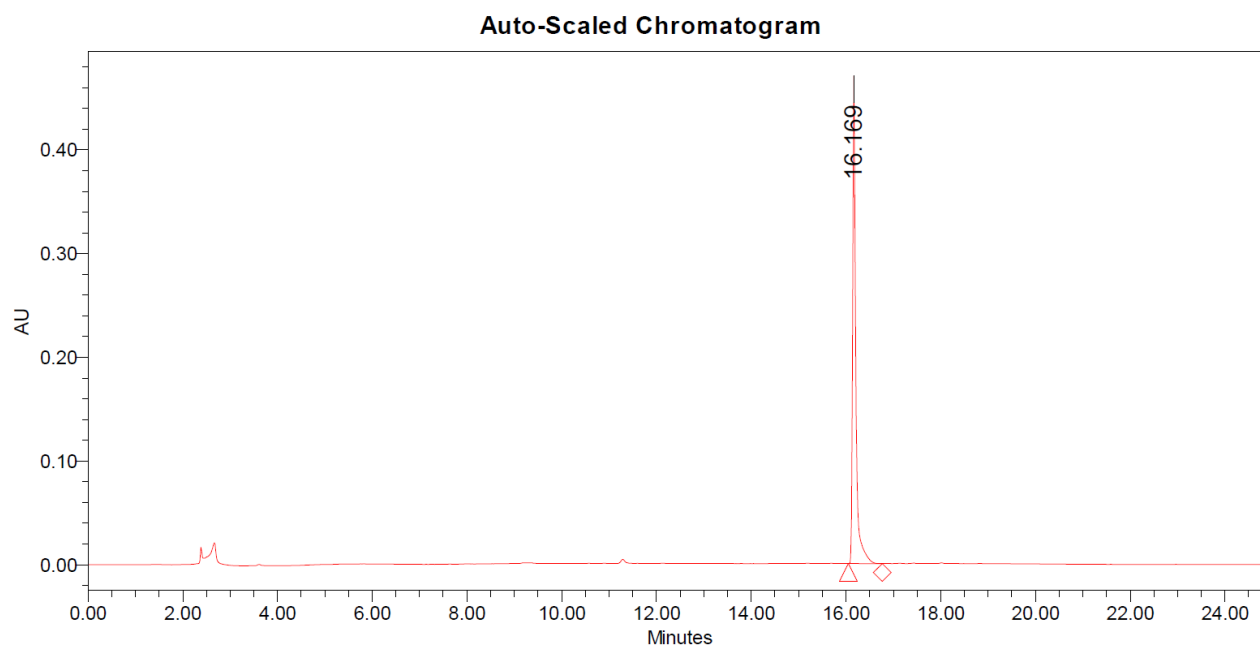
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Table S1. Calculated Properties of Compounds					
#	MW^a	cLogP^b	TPSA^b	HBD	HBA
1	453	5.1	76	0	5
4	452	4.2	79	1	5
5	462	5.0	55	1	5
6	384	3.4	79	1	5
7	412	4.5	79	1	5
8	432	4.5	79	1	5
9	442	5.2	55	1	5
10	364	3.6	79	1	5
11	467	5.1	79	1	5
12	467	5.1	79	1	5
13	467	5.1	79	1	5
14	502	6.1	88	1	6
15	502	6.1	88	1	6
16	376	5.5	62	1	4
17	378	5.4	71	1	5
18	377	4.7	74	2	6
19	391	4.9	65	1	6

20	396	5.3	62	1	4
21	439	4.2	91	2	6
22	412	4.5	79	1	5
23	432	4.5	79	1	5
24	396	5.3	62	1	4
a. Calculated with ChemDraw suite. b. Calculated with ChemAxon suite.					

Figure S1. Compound 21 HPLC



Peak Results

	RT	Area	% Area	Height
1	16.169	2196004	100.00	453142

Figure S2. Compound 21 ^1H NMR spectra

^1H NMR (300 MHz, $\text{CHLOROFORM-}d$) δ ppm 7.53 - 7.70 (m, 1 H), 7.47 (d, $J=7.54$ Hz, 1 H), 7.36 (t, $J=8.19$ Hz, 1 H), 7.08 (d, $J=8.48$ Hz, 1 H), 7.00 (br. s., 3 H), 6.81 (d, $J=7.54$ Hz, 1 H), 4.66 (d, $J=6.78$ Hz, 1 H), 3.13 - 3.38 (m, 1 H), 1.77 - 1.96 (m, 2 H), 1.65 (br. s., 3 H), 1.47 - 1.59 (m, 1 H), 1.06 - 1.37 (m, 6 H)

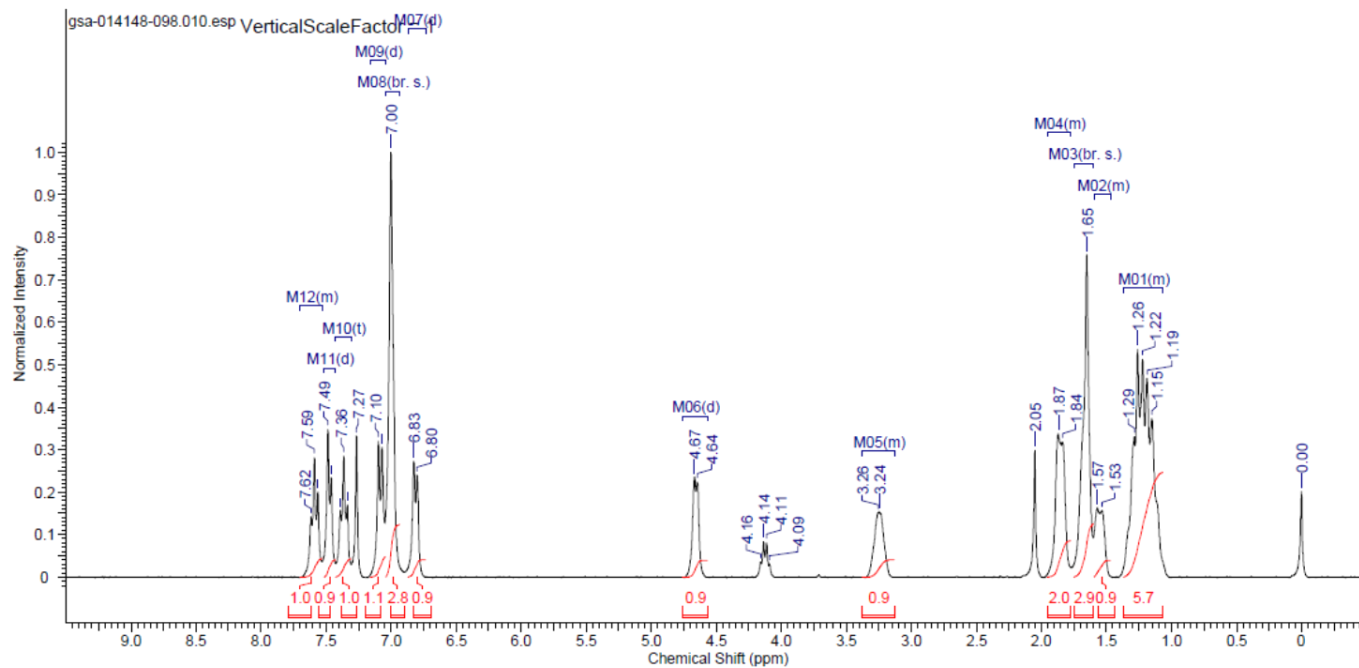
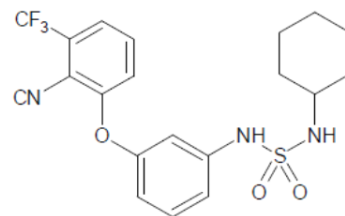


Figure S3. Compound 21 ^{13}C NMR spectra

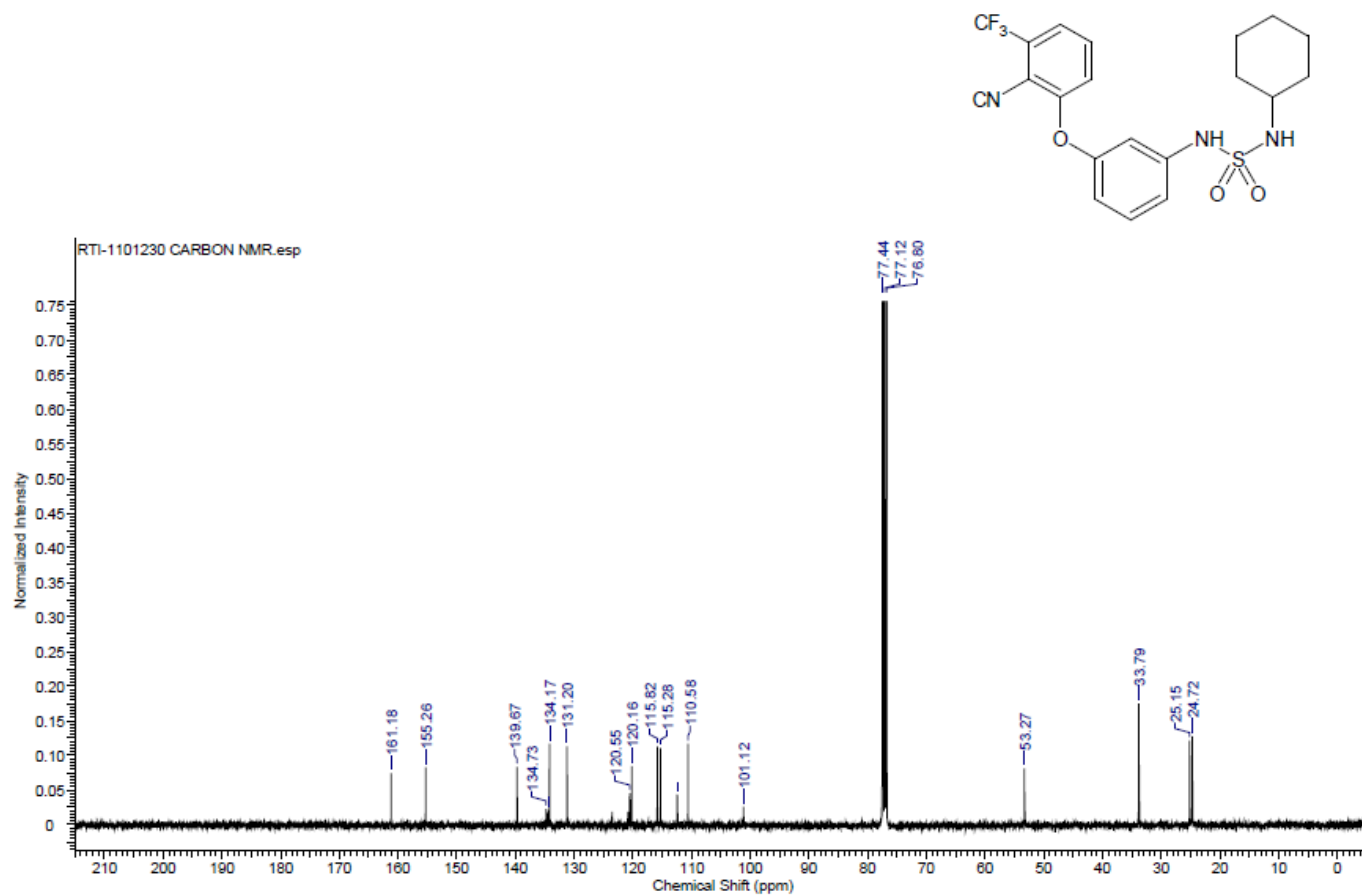
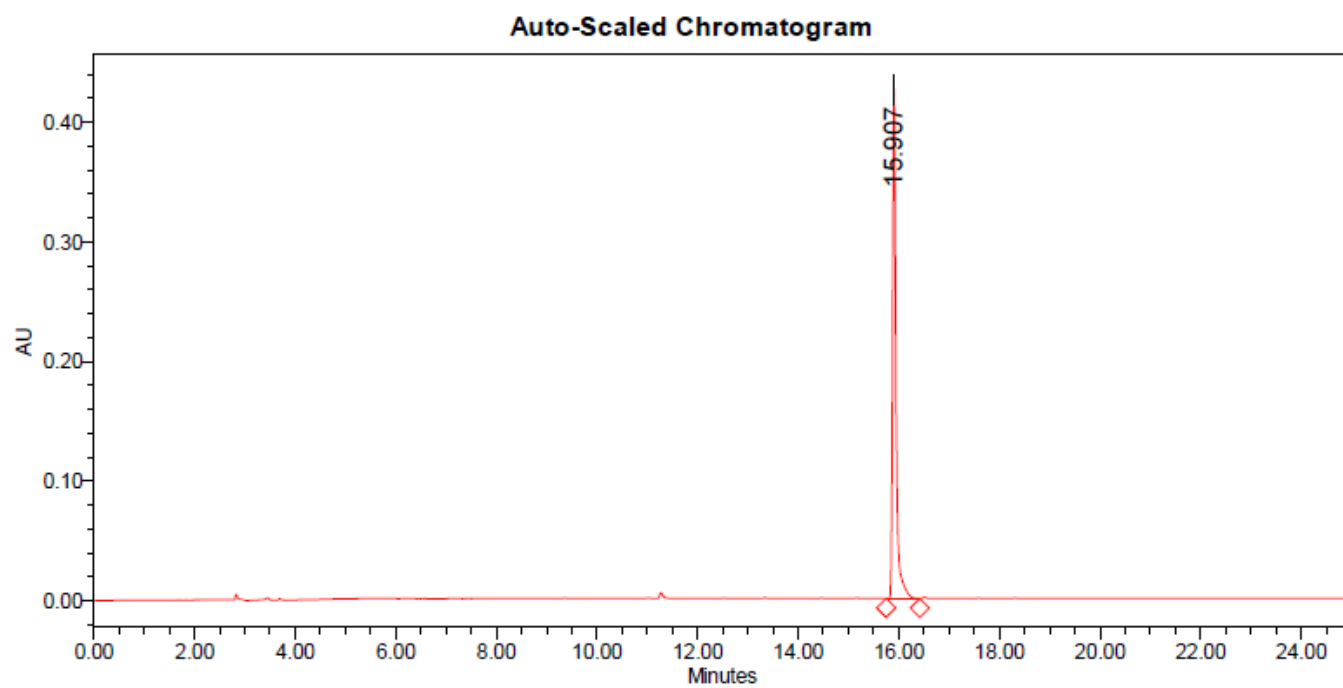


Figure S4. Compound 24 HPLC



Peak Results

	RT	Area	% Area	Height
1	15.907	2037104	100.00	425766

Figure S5. Compound 24 ^1H NMR spectra

^1H NMR (300 MHz, CHCl_3) δ ppm 7.46 - 7.60 (m, 3 H), 7.37 (s, 3 H), 7.41 (s, 3 H), 7.19 (br. s., 1 H), 6.93 - 7.11 (m, 3 H), 3.77 (br. s., 2 H)

