

S2 Table Results of analog screen

Compound number	Rank	Compound	Inhibition of Gli-Luciferase	IC ₅₀ μM (range, n)	Inhibition - mGli1 qPCR	IC ₅₀ μM (range, n)	Binding	IC ₅₀ μM (range, n)
1b	61	C72129543	<i>aggregator*</i>					
2b	43	C72146912	no					
3b	48	C72158134	yes				yes	
4b	28	C72167017	yes				yes	
5b	53	C72168261	yes				yes	
6b	41	C72172828	no					
7b	52	C72419993	yes				yes	
8b	4	C72426960	yes					
9b	178	C72481543	yes					
10b	33	C72431634	no					
11b	11	C72473625	yes					
12b	68	C72429353	yes				yes	
13b	N/A	C55271488	yes	10.9 (8.2-14.5, 3)				
14b	2	C72129787	yes					
15b	18	C72149026	no				yes	
16b	12	C72149186	yes					
17b	20	C72149758	yes					
18b	229	C72150023	no				no	
19b	5	C72150480	yes	22.4 (5.7-87.2, 3)				
20b	9	C72153124	<i>aggregator*</i>					
21b	6	C72158119	yes	bell-shape (3)				
22b	13	C72163209	yes					
23b	36	C72163710	no				yes	
24b	15	C72168023	yes	bell-shape (3)				
25b	34	C72168579	yes	2.3 (1.5-3.6, 3)	yes	7.8 (4.0-15.1, 3)		
26b	3	C72408285	yes					
27b	1	C72420973	<i>aggregator*</i>					
28b	228	C72435718	no				yes	
29b	107	C72447326	yes					
30b	10	C72448241	yes					
31b	227	C72457741	yes				no	
32b	224	C72477710	yes	9.4 (5.8-15.0, 3)	yes	12.7 (3.8-42.3, 3)	yes	
33b	19	C72476169	yes					
34b	35	C72480679	yes					
35b	159	C72428267	no					
36b	96	C72433192	no					
37b	54	C72146027	yes	5.4 (3.8-7.6, 3)	yes	8.8 (5.2-14.9, 3)		
38b	231	C72170378	no					
39b	204	C72152697	no					
40b	114	C72167102	<i>aggregator*</i>					
41b	126	C72479818	no					
42b	186	C72162059	no					
43b	31	C72447879	yes	13.3 (5.7-31.2, 3)	yes			
44b	185	C72163442	yes					
45b	76	C72475536	yes	3.1 (1.9-5.1, 3)	yes	5.3 (3.8-7.5, 3)	yes	12.7 (9.4-17.3, 3)
46b	230	C72447458	yes	15.8 (9.0-27.8, 3)	yes			
		vismodegib (nM)	yes	30.6 (12.3-76.3, 3)	yes	1.8 (1.4-2.2, 3)	yes	21.0 (13.3-33.3)

**aggregator*: see S3 Table