

Supporting Information

Ligand-Based pharmacophore modeling, Virtual screening and Biological Evaluation to identify novel TGR5 agonists

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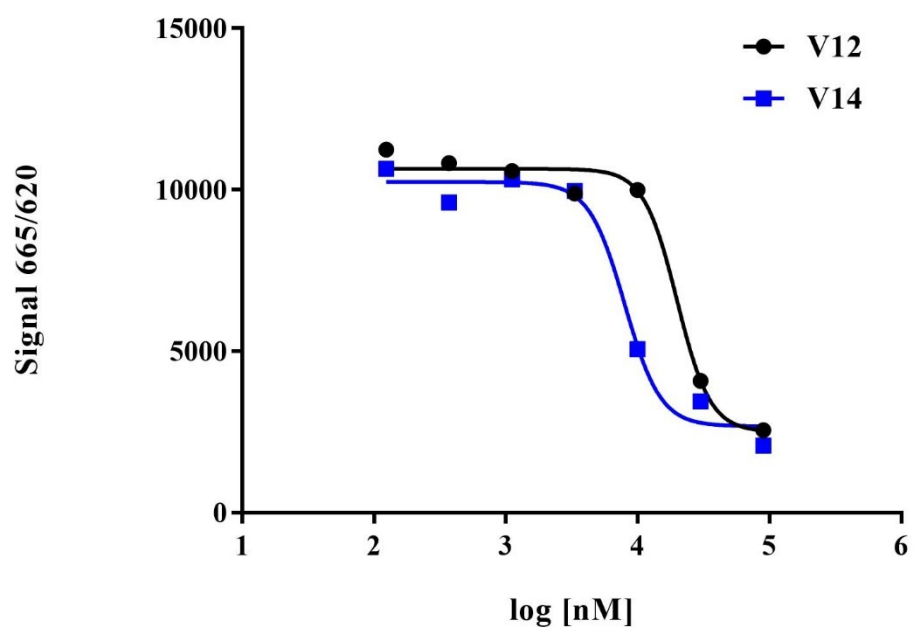


Figure S1 The dose–response curves of the compounds V12 and V14.

Table S1 The glide score and commercial source of hit compounds V1-20.

Comp.	Glide XP Gscore	Glide emodel (kcal·mol⁻¹)	commercial source
V1	-8.626	-80.012	Target Molecule Corp.
V2	-8.858	-71.579	Target Molecule Corp.
V3	-7.074	-80.520	Target Molecule Corp.
V4	-8.496	-56.935	Target Molecule Corp.
V5	-7.173	-63.129	Target Molecule Corp.
V6	-9.653	-56.652	Target Molecule Corp.
V7	-9.956	-67.126	Target Molecule Corp.
V8	-8.521	-84.647	Target Molecule Corp.
V9	-7.062	-63.258	Target Molecule Corp.
V10	-6.972	-47.228	Target Molecule Corp.
V11	-9.750	-50.516	Target Molecule Corp.
V12	7.002	-64.057	Target Molecule Corp.
V13	-6.967	-64.923	Target Molecule Corp.
V14	-8.160	-63.320	Target Molecule Corp.
V15	-7.805	-68.399	Target Molecule Corp.
V16	-7.021	-60.181	Target Molecule Corp.
V17	-8.164	-64.060	In our library
V18	-7.627	-54.656	Target Molecule Corp.
V19	-7.407	-56.082	Target Molecule Corp.
V20	-7.481	-56.435	Target Molecule Corp.

Table S2 The glide score of other top 65 compounds.

Ligand No.	CAS	Glide XP Gscore	Glide emodel (kcal·mol⁻¹)
1	1135242-13-5	-7.403	-63.866
2	117-81-7	-7.392	-61.343
3	298690-60-5	-7.383	-53.146
4	1445605-23-1	-7.337	-49.036
5	1226056-71-8	-7.286	-63.562
6	164650-44-6	-7.300	-51.468
7	956905-27-4	-7.259	-81.585
8	168626-94-6	-8.034	-61.678
9	162011-90-7	-7.256	-69.577
10	1346528-50-4	-7.409	-60.317
11	957485-64-2	-7.241	-65.118
12	985-13-7	-8.424	-75.227
13	1402836-58-1	-7.400	-55.780
14	52-86-8	-9.472	-64.050
15	5633-20-5	-8.449	-54.601
16	1246529-32-7	-7.236	-44.139
17	873652-48-3	-8.488	-77.078
18	122320-73-4	-8.551	-65.187
19	1173-88-2	-7.155	-59.045
20	133824-30-5	-7.131	-63.188
21	1108743-60-7	-7.126	-40.817
22	888216-25-9	-7.132	-71.594
23	1208315-24-5	-7.132	-56.807
24	1445251-22-8	-7.146	-67.307
25	694433-59-5	-7.503	-56.929
26	355025-24-0	-7.092	-84.005
27	68786-66-3	-7.270	-38.212
28	32672-69-7	-7.087	-59.870
29	1622921-15-6	-7.381	-60.607
30	1042224-63-4	-7.111	-62.009
31	64872-77-1	-7.445	-62.658
32	943962-47-8	-8.696	-75.134
33	14976-57-9	-7.054	-48.838
34	1110813-31-4	-8.318	-52.937
35	1135280-28-2	-8.331	-76.796
36	99592-39-9	-7.272	-69.721
37	89796-99-6	-6.969	-50.055
38	817194-38-0	-6.977	-67.735
39	298197-04-3	-6.944	-47.685
40	6138-79-0	-6.935	-47.373
41	896466-04-9	-8.320	-71.779

42	947914-18-3	-6.919	63.372
43	18010-40-7	-6.971	-41.379
44	792173-99-0	-6.903	-63.511
45	1439399-58-2	-8.476	-85.681
