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Supplementary Information

New PPARα/γ/δ Optimal Activator Rationally Designed by Computational Methods

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Table S1. Molecules and physicochemical properties

Name	MW	MV	Polarizability	AlogP98	NHBD	NHBA	DM	SA	Ki
1RDT	550.66	413.70	23655.62	5.70	4.00	6.00	2.66	489.06	1.10
18944089	432.48	320.30	18027.82	5.20	1.00	6.00	0.84	358.64	0.40
446642	510.60	387.20	21846.00	5.22	2.00	6.00	5.78	461.11	1.00
9843045	384.44	289.40	15171.62	3.78	1.00	6.00	1.86	365.29	2.50
10578809	561.60	414.40	23793.06	6.00	2.00	7.00	2.38	477.37	5.10
77999	357.44	266.40	14855.22	3.46	1.00	5.00	3.57	318.34	10.00
10433070	434.61	351.90	16866.92	5.52	1.00	5.00	1.59	437.27	20.00
44383664	487.60	382.40	20160.84	7.63	1.00	6.00	5.47	465.15	26.00
10004390	459.55	353.10	19134.32	6.75	1.00	6.00	4.92	437.39	30.00
44385396	503.60	389.00	20505.64	7.35	1.00	7.00	7.98	476.19	41.00
10068664	385.47	294.50	17132.64	6.01	2.00	3.00	1.79	333.89	50.00
9827261	477.59	359.20	20328.46	6.60	1.00	7.00	13.85	394.74	60.00
44419783	396.45	298.30	15771.82	2.91	1.00	7.00	1.68	380.02	73.00
11464352	422.49	320.50	16657.58	3.84	1.00	7.00	2.03	379.79	81.00
447458	419.48	321.80	17507.60	5.04	1.00	5.00	2.42	387.21	90.00
44345164	404.21	265.00	17214.48	4.49	2.00	9.00	2.14	319.65	100.00

MW: molecular weight; MV: molecular volume; NHBD: number of hydrogen bond donors, NHBA: number of hydrogen bond acceptors; DM: dipole magnitude; SA: surface area; Ki: affinity constant.

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Table S2. GOLD Score of candidates, crystallographic molecule 1RDT and PPARγ ligands docked with PPARγ receptor

Fitness	S(hb_ext)	S(vdw_ext)	S(int)	File name
91.46	10.75	62.92	–5.81	candidate 1
70.00	0.38	55.12	–6.17	candidate 2
68.41	6.74	49.09	–5.83	candidate 3
62.91	6.00	50.43	–12.43	candidate 4
64.06	0.35	46.73	–0.54	candidate 5
67.01	0.00	56.04	–10.04	candidate 6
96.19	3.91	82.19	–20.73	candidate 7
68.00	5.66	49.69	–5.99	‘9843045’
85.61	3.05	73.34	–18.28	‘1RDT’
65.04	0.06	49.45	–3.02	‘77999’
84.47	3.97	72.86	–19.68	‘446642’
72.06	4.93	55.79	–9.57	‘447458’
81.73	1.04	66.29	–10.47	‘9827261’
79.15	0.47	64.02	–9.35	‘10004390’
68.28	5.98	49.24	–5.41	‘10068664’
72.14	2.02	59.36	–11.49	‘10433070’
81.13	3.46	65.11	–11.86	‘10578809’
71.91	3.55	52.63	–3.99	‘11464352’
80.90	3.64	58.46	–3.13	‘18944089’
57.78	2.59	47.71	–10.41	‘5289162’
72.09	1.53	62.25	–15.03	‘44383664’
75.14	1.37	66.57	–17.77	‘44385396’
71.97	4.24	52.19	–4.04	‘44419783’

Table S3. Binding affinity of candidates 1, 2 and 7 and specific PPAR ligands. The binding affinity of ligands was assessed with AutoDock/Vina software

entry	Alpha	Delta	Gamma
Candidate 1	−9.7	−10.8	−12.9
Candidate 2	−9.2	−9.0	−9.5
Candidate 7	−7.6	−8.1	−12.1
Rosiglitazone (gamma)	−8.7	−8.4	−8.4
Tesaglitazar (alpha/gamma)	−8.5	−7.9	−8.1