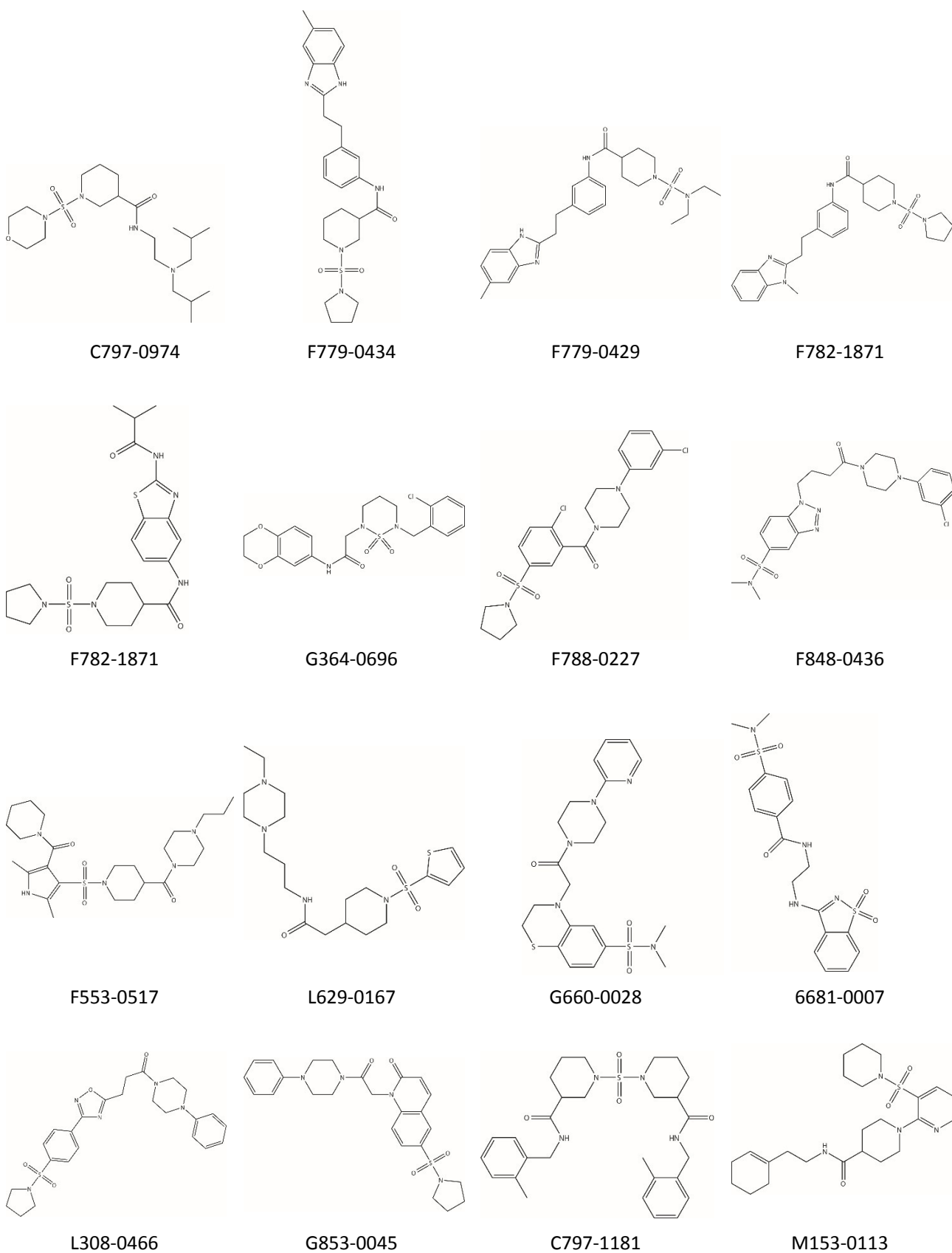
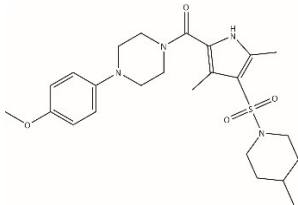
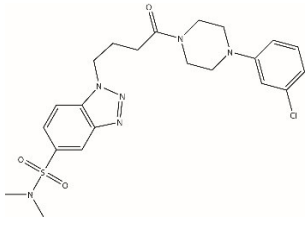


Table S1. Structures of top 30 chemicals in docking analysis.

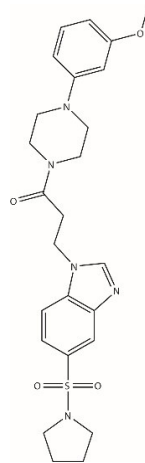




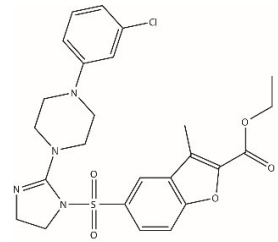
F379-0958



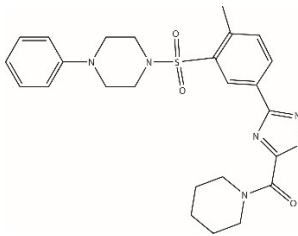
F848-0394



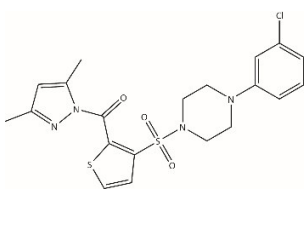
F513-0046



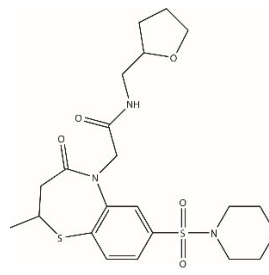
C066-5575



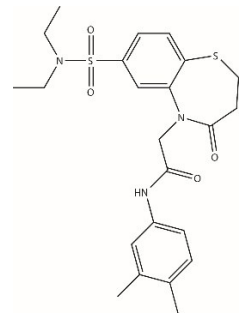
L286-0466



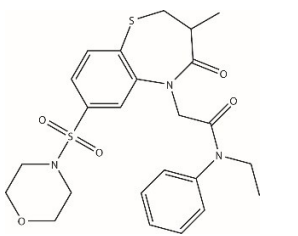
C200-9226



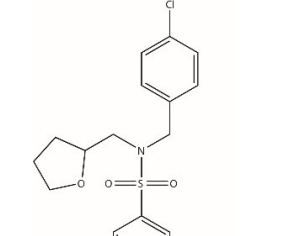
G640-1014



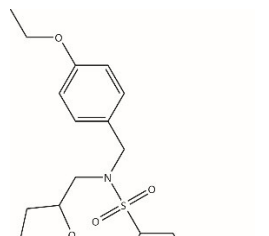
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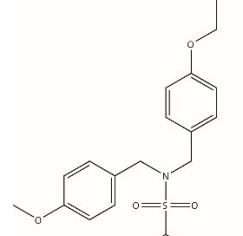
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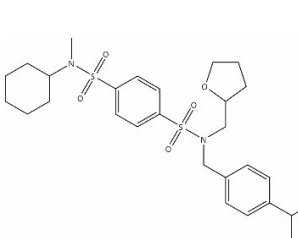
D207-0130



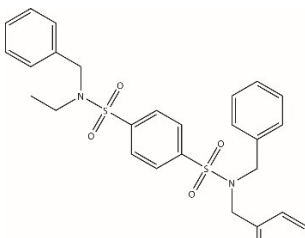
D207-0125



D207-0136



D207-0090



D207-0052

Table S2. ADMET properties of top 30 chemicals in docking analysis.

Class	Name	Docking Score	Molecular weight	Water Solubility	Consensus Log Po/w	TPSA	Log Kp (skin permeation)	Bioavailability Score	Synthetic accessibility
1	C797-0974	-73.04	432.62	Soluble	1.7	90.57 Å ²	-7.86 cm/s	0.55	4.51
	F779-0434	-65.4151	495.64	Moderately soluble	3.07	106.78 Å ²	-6.90 cm/s	0.55	4.13
	F779-0429	-63.9194	497.65	Moderately soluble	3.57	106.78 Å ²	-6.73 cm/s	0.55	3.69
	F779-1131	-59.0317	495.64	Moderately soluble	3.07	95.92 Å ²	-7.19 cm/s	0.55	3.63
	F782-1871	-54.7081	479.62	Soluble	2.31	148.33 Å ²	-7.63 cm/s	0.55	3.74
	G364-0696	-59.0589	451.92	Soluble	2.31	96.56 Å ²	-7.42 cm/s	0.55	3.39
2	F788-0227	-59.612	468.4	Moderately soluble	3.37	69.31 Å ²	-6.41 cm/s	0.55	3.03
	F848-0436	-59.2082	474.55	Soluble	2.08	100.02 Å ²	-8.00 cm/s	0.55	3.48
	F533-0517	-58.6479	507.69	Moderately soluble	2.06	105.41 Å ²	-8.25 cm/s	0.55	4.75
	L629-0167	-57.8019	442.64	Soluble	2.03	109.58 Å ²	-7.83 cm/s	0.55	4.25
	G660-0028	-57.7897	461.6	Soluble	1.59	110.74 Å ²	-7.80 cm/s	0.55	3.85
	6681-0007	-56.7435	436.51	Soluble	1.25	141.77 Å ²	-8.54 cm/s	0.55	3.72
	L308-0466	-56.3962	495.59	Moderately soluble	2.59	108.23 Å ²	-7.36 cm/s	0.55	3.88
	G853-0045	-55.8869	480.58	Moderately soluble	2.21	91.31 Å ²	-7.62 cm/s	0.55	3.49
	C797-1181	-55.8409	526.69	Moderately soluble	2.87	107.20 Å ²	-7.61 cm/s	0.55	4.45
	M153-0113	-55.7228	460.63	Moderately soluble	3.06	90.99 Å ²	-6.89 cm/s	0.55	4.65
	F379-0958	-54.4232	474.62	Moderately soluble	2.77	94.33 Å ²	-6.88 cm/s	0.55	4.17
3	F848-0394	-53.9121	491.01	Moderately soluble	2.29	100.02 Å ²	-7.73 cm/s	0.55	3.5
	F513-0046	-53.7898	497.61	Soluble	2.1	96.36 Å ²	-7.92 cm/s	0.55	3.58
	C066-5575	-57.764	531.02	Moderately soluble	3.48	104.04 Å ²	-6.64 cm/s	0.55	4.3
	L286-0466	-56.6176	495.59	Moderately soluble	2.95	108.23 Å ²	-6.80 cm/s	0.55	3.96
	C200-9226	-54.3811	464.99	Moderately soluble	3.42	112.13 Å ²	-6.32 cm/s	0.55	3.68
4	G640-1014	-58.6075	481.63	Soluble	2.15	129.70 Å ²	-8.05 cm/s	0.55	4.78
	G640-0011	-56.5278	475.62	Moderately soluble	3.12	120.47 Å ²	-7.06 cm/s	0.55	3.99
	G640-0825	-54.6971	503.63	Moderately soluble	2.55	120.91 Å ²	-7.74 cm/s	0.55	4.64
5	D207-0130	-62.968	513.07	Moderately soluble	3.45	100.75 Å ²	-6.88 cm/s	0.55	4.02
	D207-0125	-62.0309	522.68	Moderately soluble	3.24	109.98 Å ²	-7.15 cm/s	0.55	4.23
	D207-0052	-58.5663	535.68	Moderately soluble	3.82	104.41 Å ²	-6.71 cm/s	0.55	3.62
	D207-0090	-55.8444	548.76	Poorly soluble	4.5	100.75 Å ²	-6.05 cm/s	0.55	4.57
	D207-0136	-54.6747	558.71	Moderately soluble	4.11	109.98 Å ²	-6.61 cm/s	0.55	3.64