



SUPPLEMENTARY MATERIAL TO
***In silico* identification of novel allosteric inhibitors of Dengue
virus NS2B/NS3 serine protease**

RENATO A. DA COSTA¹, JOÃO A. P. DA ROCHA^{2*}, ALAN S. PINHEIRO³,
ANDRÉIA S. S. DA COSTA⁴, ELAINE C. M. DA ROCHA⁵, LUIZ P. C. JOSINO³,
ARLAN DA SILVA GONÇALVES⁶, ANDERSON H. L. LIMA³ and DAVI S. B. BRASIL⁴

¹Federal Institute of Education, Science and Technology of Pará - Campus Castanhal, 68740-970, Castanhal-PA, Brazil, ²Federal Institute of Education, Science and Technology of Pará - Campus Bragança, 68600-000, Bragança-PA, Brazil, ³Graduate Program in Chemistry, Institute of Exact and Natural Sciences, Federal University of Pará (UFPA), 66075-110 Belém-PA, Brazil, ⁴Graduate Program in Science and Environment, Institute of Exact and Natural Sciences, Federal University of Pará (UFPA), 66075-110 Belém-PA, Brazil, ⁵Federal Rural University of the Amazon Campus Capanema (UFRA), 68700-665 Capanema-PA, Brazil and ⁶Federal Institute of Education, Science and Technology of Espírito Santo Campus Vila Velha, 29106-010 Vila Velha-ES, Brazil

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TABLE S-I. Docking energy in final rank of all compounds

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_493-P10	55.0145	-40.4792	1.05
Compound_494-P10	48.3619	-40.6335	0.94
Compound_498-P10	47.2003	-33.1897	0.70
Compound_499-P10	42.4681	-32.8555	0.61
Compound_500-P10	49.1437	-35.1738	0.79
Compound_501-P10	45.8524	-35.1685	0.74
Compound_502-P10	42.9861	-34.5863	0.67
Compound_505-P10	43.5991	-35.0761	0.69
Compound_506-P10	35.3827	-34.7362	0.55
Compound_508-P10	49.0915	-37.4725	0.86
Compound_525-P10	43.4997	-34.5456	0.68
Compound_526-P10	39.5333	-34.9957	0.62
Compound_527-P10	53.3547	-36.2203	0.89
Compound_528-P10	46.6404	-37.0252	0.80
Compound_529-P10	43.2136	-37.0475	0.75
Compound_532-P10	51.9567	-41.3784	1.02
Compound_533-P10	66.5579	-45.3406	1.38

* Corresponding author. E-mail: joao.rocha@ifpa.edu.br

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_534-P10	66.3429	-44.8105	1.36
Compound_535-P10	54.8078	-46.4996	1.22
Compound_555-P10	47.1294	-42.0086	0.96
Compound_559-P10	72.8622	-43.7078	1.44
Compound_560-P10	53.2122	-43.6176	1.11
Compound_660-P10	43.7724	-42.6863	0.92
Compound_661-P10	51.1173	-43.8134	1.08
Compound_662-P10	37.5227	-43.0681	0.82
Compound_663-P10	48.0049	-41.0775	0.94
Compound_667-P10	60.6392	-44.2672	1.25
Compound_669-P10	59.9525	-44.3928	1.24
Compound_671-P10	43.0997	-44.2358	0.95
Compound_808-P10	47.4178	-44.9295	1.05
Compound_814-P10	43.6496	-38.7764	0.80
Compound_817-P10	48.6523	-40.2933	0.93
Compound_818-P10	53.1156	-44.8452	1.14
Compound_822-P10	52.9414	-40.9323	1.02
Compound_833-P10	63.2860	-41.3482	1.21
Compound_834-P10	53.6338	-37.4700	0.93
Compound_846-P10	40.7596	-36.3473	0.68
Compound_1267-P10	36.9559	-38.9872	0.70
Compound_1277-P10	64.6098	-42.0334	1.25
Compound_1301-P10	59.8522	-41.5171	1.16
Compound_1302-P10	54.2002	-42.6608	1.10
Compound_1314-P10	57.7154	-44.2496	1.20
Compound_1316-P10	41.4238	-43.2699	0.90
Compound_1320-P10	57.0063	-42.7086	1.14
Compound_1321-P10	46.9147	-42.1110	0.96
Compound_1323-P10	53.5591	-34.9115	0.86
Compound_1325-P10	60.4689	-41.5155	1.17
Compound_1326-P10	49.1343	-41.4219	0.97
Compound_1330-P10	53.6180	-44.0684	1.13
Compound_1632-P10	53.8111	-45.7540	1.18
Compound_1833-P10	42.6250	-31.3776	0.57
Compound_2036-P10	61.8467	-37.5276	1.08
Compound_2037-P10	50.6276	-31.6351	0.71
Compound_2038-P10	60.7469	-36.6313	1.03
Compound_2061-P10	69.9754	-43.6064	1.39
Compound_2092-P10	57.9794	-44.8444	1.22
Compound_2093-P10	40.4366	-46.7546	0.98
Compound_2094-P10	61.2447	-44.7289	1.27
Compound_2095-P10	60.2489	-45.1089	1.27
Compound_2096-P10	45.0966	-44.4462	0.99
Compound_2097-P10	59.4450	-43.3326	1.20
Compound_2100-P10	51.1354	-41.5047	1.01
Compound_2105-P10	48.4534	-33.6467	0.74

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2106-P10	48.1227	-35.4610	0.78
Compound_2109-P10	44.1434	-43.4043	0.95
Compound_2114-P10	50.9913	-43.1084	1.05
Compound_2115-P10	67.3150	-43.6992	1.35
Compound_2118-P10	34.3255	-42.4298	0.75
Compound_2119-P10	54.3968	-43.9169	1.13
Compound_2121-P10	53.7670	-39.4133	0.99
Compound_2122-P10	42.4321	-40.5701	0.83
Compound_2125-P10	38.0393	-33.2455	0.55
Compound_2131-P10	44.0794	-45.0650	0.99
Compound_2136-P10	48.9384	-46.9752	1.13
Compound_2137-P10	42.4597	-42.3731	0.89
Compound_2138-P10	40.7445	-35.0601	0.65
Compound_2139-P10	60.8563	-45.3153	1.29
Compound_2140-P10	34.9478	-46.1151	0.87
Compound_2144-P10	38.3626	-46.3833	0.93
Compound_2145-P10	53.1406	-46.4414	1.19
Compound_2146-P10	36.3688	-43.3671	0.81
Compound_2147-P10	38.3319	-46.8173	0.95
Compound_2155-P10	39.4951	-46.2351	0.95
Compound_2159-P10	48.3234	-47.2788	1.13
Compound_2160-P10	39.0845	-45.1868	0.91
Compound_2180-P10	32.8939	-30.8277	0.39
Compound_2219-P10	41.3088	-34.5854	0.64
Compound_2254-P10	55.0989	-35.7801	0.91
Compound_2278-P10	49.1206	-39.4010	0.91
Compound_2339-P10	53.8117	-43.1300	1.10
Compound_2359-P10	60.1688	-36.6478	1.02
Compound_2424-P10	56.7177	-42.6482	1.14
Compound_2565-P10	68.5571	-42.2957	1.33
Compound_2577-P10	66.5549	-47.4789	1.44
Compound_2579-P10	41.1970	-41.3316	0.84
Compound_2583-P10	54.2175	-46.0503	1.19
Compound_2616-P10	57.9462	-42.7637	1.16
Compound_2664-P10	67.7664	-40.7089	1.27
Compound_2727-P10	65.7697	-44.9486	1.36
Compound_2737-P10	59.7896	-43.1793	1.21
Compound_2766-P10	46.2643	-35.6101	0.76
Compound_2767-P10	51.5390	-36.7953	0.88
Compound_2776-P10	51.2687	-37.9631	0.91
Compound_2440-P11	39.7743	-32.3569	0.55
Compound_2441-P11	50.1818	-32.1041	0.72
Compound_2463-P11	48.3836	-36.9779	0.83
Compound_2539-P11	53.3664	-37.9739	0.94
Compound_2546-P11	45.2918	-38.4890	0.82
Compound_2547-P11	63.4939	-39.4801	1.16

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2548-P11	51.8828	-40.3744	0.99
Compound_2550-P11	41.3962	-43.2997	0.90
Compound_2551-P11	39.1605	-42.6747	0.84
Compound_2552-P11	55.3679	-41.9173	1.09
Compound_2554-P11	59.3719	-45.4047	1.26
Compound_2555-P11	45.2353	-45.6473	1.03
Compound_2569-P11	44.5374	-35.2276	0.72
Compound_2570-P11	42.4711	-37.3101	0.74
Compound_2571-P11	54.3922	-40.1765	1.03
Compound_2572-P11	49.8883	-40.0611	0.95
Compound_2573-P11	49.3663	-40.3050	0.94
Compound_2574-P11	67.9678	-44.0928	1.37
Compound_2584-P11	38.6052	-39.0160	0.72
Compound_2585-P11	49.7889	-43.4295	1.04
Compound_2586-P11	52.5446	-42.5088	1.06
Compound_2588-P11	57.9195	-44.7613	1.22
Compound_2589-P11	58.5917	-43.6817	1.20
Compound_2591-P11	53.3422	-46.7401	1.20
Compound_2592-P11	62.6974	-39.6109	1.15
Compound_2593-P11	52.2059	-40.6821	1.00
Compound_2594-P11	60.2085	-46.9019	1.32
Compound_2595-P11	45.6377	-45.2476	1.02
Compound_2596-P11	53.1575	-42.0078	1.06
Compound_2598-P11	54.1807	-42.3687	1.09
Compound_2599-P11	54.0687	-46.4592	1.20
Compound_2652-P11	31.5918	-38.9124	0.60
Compound_2657-P11	44.9156	-38.7006	0.82
Compound_2665-P11	43.7432	-40.3750	0.85
Compound_2667-P11	65.9916	-40.7361	1.24
Compound_2668-P11	52.5808	-39.2773	0.97
Compound_2669-P11	56.2488	-40.9469	1.08
Compound_2670-P11	44.6478	-43.0276	0.94
Compound_2689-P11	37.4111	-37.7554	0.67
Compound_2690-P11	41.7158	-40.8678	0.83
Compound_2691-P11	44.4737	-42.7648	0.93
Compound_2692-P11	46.0591	-41.3822	0.92
Compound_2693-P11	61.5882	-42.0828	1.20
Compound_2695-P11	41.9024	-41.6596	0.86
Compound_2696-P11	66.3707	-44.0720	1.34
Compound_2698-P11	43.7714	-39.8152	0.84
Compound_2699-P11	44.4826	-39.8318	0.85
Compound_2700-P11	45.5816	-45.3305	1.03
Compound_2701-P11	64.5427	-45.6295	1.36
Compound_2703-P11	62.0708	-48.1437	1.39
Compound_2714-P11	44.5524	-36.0907	0.74
Compound_2715-P11	61.4006	-40.9367	1.17

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2716-P11	48.4413	-42.1222	0.98
Compound_2717-P11	39.0429	-41.6999	0.81
Compound_2718-P11	50.2161	-42.3834	1.02
Compound_2720-P11	70.4130	-45.8771	1.46
Compound_2734-P11	63.5645	-44.2241	1.30
Compound_2735-P11	48.2251	-44.6284	1.05
Compound_2736-P11	64.2626	-46.7529	1.38
Compound_2743-P11	49.5718	-41.4932	0.98
Compound_2744-P11	41.9503	-44.4549	0.94
Compound_2745-P11	67.8441	-45.6421	1.41
Compound_2746-P11	60.8689	-42.2971	1.20
Compound_2747-P11	54.1800	-41.2640	1.05
Compound_2748-P11	51.7120	-47.0152	1.18
Compound_2750-P11	54.9374	-46.3364	1.21
Compound_2751-P11	43.5952	-45.1259	0.99
Compound_2818-P11	38.3860	-38.5915	0.71
Compound_2926-P11	63.1888	-42.1957	1.23
Compound_2939-P11	67.1451	-40.8512	1.26
Compound_2947-P11	79.2870	-43.8454	1.56
Compound_2948-P11	43.0468	-41.9508	0.88
Compound_2950-P11	66.7275	-41.3116	1.27
Compound_2951-P11	62.4857	-42.7354	1.24
Compound_2952-P11	59.7380	-42.4072	1.18
Compound_2960-P11	63.5794	-41.7107	1.23
Compound_2961-P11	60.0337	-41.6643	1.17
Compound_2963-P11	43.2168	-43.8173	0.94
Compound_2977-P11	38.9457	-39.8107	0.75
Compound_2978-P11	58.2777	-41.4194	1.13
Compound_2987-P11	54.3138	-42.0076	1.08
Compound_2988-P11	48.8261	-45.7669	1.09
Compound_2989-P11	63.9906	-45.9240	1.36
Compound_2990-P11	55.9811	-44.1223	1.17
Compound_2991-P11	54.2087	-44.0480	1.14
Compound_2992-P11	57.2201	-43.9059	1.18
Compound_2993-P11	49.6923	-45.3260	1.10
Compound_7-P12	58.1285	-41.2478	1.12
Compound_11-P12	39.2064	-43.7520	0.87
Compound_16-P12	64.3475	-46.0334	1.37
Compound_17-P12	62.3227	-43.6602	1.26
Compound_18-P12	50.2518	-43.8827	1.06
Compound_19-P12	47.6999	-44.1428	1.03
Compound_20-P12	45.6626	-45.8612	1.04
Compound_21-P12	53.6205	-45.2832	1.16
Compound_22-P12	45.4960	-46.5368	1.06
Compound_23-P12	49.0648	-45.1276	1.08
Compound_24-P12	44.6797	-44.9049	1.00

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_25-P12	47.3316	-44.8282	1.04
Compound_34-P12	44.8141	-45.1385	1.01
Compound_35-P12	57.1023	-48.3877	1.31
Compound_36-P12	48.1950	-42.3645	0.98
Compound_42-P12	43.9065	-44.7252	0.98
Compound_43-P12	46.8825	-45.9323	1.07
Compound_44-P12	43.6752	-46.7260	1.03
Compound_69-P12	44.6811	-43.9480	0.97
Compound_73-P12	50.2951	-43.2508	1.05
Compound_74-P12	64.9289	-47.9564	1.43
Compound_82-P12	60.9698	-44.9682	1.28
Compound_83-P12	65.7484	-47.5668	1.43
Compound_87-P12	34.7672	-45.9655	0.86
Compound_88-P12	51.4550	-46.9608	1.17
Compound_126-P12	45.2388	-43.5365	0.97
Compound_129-P12	45.4882	-44.4994	1.00
Compound_136-P12	42.7748	-44.3435	0.95
Compound_137-P12	58.1166	-43.9229	1.20
Compound_138-P12	51.4574	-45.2706	1.12
Compound_146-P12	53.2765	-42.2250	1.07
Compound_147-P12	53.6617	-44.1477	1.13
Compound_150-P12	41.2204	-42.0893	0.86
Compound_151-P12	52.7339	-46.6455	1.19
Compound_152-P12	79.9672	-42.3993	1.53
Compound_153-P12	52.5741	-43.9431	1.10
Compound_155-P12	70.1897	-45.3428	1.44
Compound_156-P12	53.7179	-47.0722	1.21
Compound_157-P12	48.5293	-43.7938	1.03
Compound_183-P12	66.5172	-42.4638	1.30
Compound_220-P12	48.2077	-37.4034	0.84
Compound_221-P12	47.5117	-39.0119	0.88
Compound_222-P12	38.0102	-38.4851	0.70
Compound_223-P12	62.4553	-41.2578	1.19
Compound_224-P12	62.2008	-46.5198	1.34
Compound_225-P12	56.9408	-44.6311	1.20
Compound_232-P12	42.5467	-35.8072	0.70
Compound_233-P12	47.0232	-40.1599	0.90
Compound_234-P12	50.5868	-40.4429	0.97
Compound_235-P12	33.7772	-41.1330	0.70
Compound_237-P12	29.4502	-43.2434	0.69
Compound_238-P12	66.1052	-44.4000	1.35
Compound_239-P12	46.4590	-43.8220	1.00
Compound_260-P12	47.1868	-41.9991	0.96
Compound_261-P12	61.1859	-42.7580	1.22
Compound_263-P12	43.6539	-42.3964	0.91
Compound_264-P12	55.7679	-43.5930	1.15

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_265-P12	55.9379	-46.3870	1.23
Compound_266-P12	46.9191	-43.5543	1.00
Compound_267-P12	59.0686	-43.6316	1.21
Compound_268-P12	60.4902	-39.6845	1.12
Compound_269-P12	50.9549	-39.7859	0.96
Compound_270-P12	52.8004	-39.8881	0.99
Compound_271-P12	43.1304	-42.5918	0.90
Compound_272-P12	50.7148	-44.0636	1.08
Compound_275-P12	64.5592	-45.7428	1.36
Compound_317-P12	45.2689	-39.4437	0.85
Compound_318-P12	38.1824	-38.0762	0.69
Compound_319-P12	47.3405	-41.1609	0.93
Compound_320-P12	33.5390	-41.5117	0.71
Compound_321-P12	39.7915	-38.5122	0.73
Compound_322-P12	50.0678	-39.9441	0.95
Compound_323-P12	49.0724	-40.4058	0.94
Compound_324-P12	52.7995	-43.0872	1.08
Compound_326-P12	37.1693	-39.4723	0.71
Compound_327-P12	53.4869	-44.0562	1.12
Compound_328-P12	46.0680	-39.2524	0.86
Compound_329-P12	61.8525	-40.9092	1.17
Compound_330-P12	42.1432	-45.6131	0.98
Compound_331-P12	43.7936	-45.4231	1.00
Compound_339-P12	52.7022	-41.6552	1.04
Compound_340-P12	38.5761	-43.5686	0.86
Compound_341-P12	47.4463	-39.0420	0.88
Compound_342-P12	51.1874	-41.4556	1.01
Compound_343-P12	61.6994	-42.6910	1.22
Compound_344-P12	47.6461	-44.4160	1.03
Compound_345-P12	68.7693	-45.5231	1.43
Compound_346-P12	39.0499	-43.5352	0.86
Compound_347-P12	47.8762	-44.4228	1.04
Compound_362-P12	45.5614	-42.9589	0.96
Compound_363-P12	56.5986	-42.3588	1.13
Compound_364-P12	70.3903	-42.7190	1.37
Compound_365-P12	47.8858	-41.5470	0.96
Compound_366-P12	49.6425	-42.9748	1.03
Compound_367-P12	52.1089	-40.0191	0.98
Compound_368-P12	50.7542	-40.3889	0.97
Compound_369-P12	58.6640	-38.7588	1.06
Compound_370-P12	71.6724	-40.1290	1.32
Compound_371-P12	50.0969	-40.0148	0.95
Compound_372-P12	57.3259	-42.9412	1.16
Compound_373-P12	60.5865	-40.4950	1.14
Compound_374-P12	45.9589	-41.1502	0.91
Compound_375-P12	55.4855	-45.8678	1.21

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_376-P12	46.9243	-43.8303	1.01
Compound_377-P12	50.6913	-42.9026	1.04
Compound_378-P12	55.7973	-40.1780	1.05
Compound_379-P12	59.6804	-42.4551	1.18
Compound_380-P12	51.6952	-45.1844	1.13
Compound_381-P12	55.4237	-40.6277	1.06
Compound_382-P12	39.4086	-43.1960	0.86
Compound_383-P12	46.4308	-42.8481	0.97
Compound_384-P12	51.9058	-47.4080	1.19
Compound_718-P12	51.8337	-40.0717	0.98
Compound_720-P12	59.4739	-46.5939	1.30
Compound_739-P12	49.0808	-34.7179	0.78
Compound_741-P12	43.0800	-38.9961	0.80
Compound_742-P12	61.0861	-44.0639	1.25
Compound_743-P12	68.0726	-43.5887	1.36
Compound_747-P12	47.2582	-38.2264	0.85
Compound_748-P12	45.7214	-34.9126	0.73
Compound_780-P12	41.1400	-26.5671	0.41
Compound_782-P12	50.2483	-35.4410	0.82
Compound_783-P12	44.0104	-37.0640	0.76
Compound_785-P12	46.5577	-41.6131	0.93
Compound_789-P12	51.0346	-35.9160	0.85
Compound_814-P12	56.5264	-39.7178	1.05
Compound_815-P12	53.2572	-37.0403	0.92
Compound_822-P12	56.2107	-41.0110	1.08
Compound_824-P12	55.4603	-36.9822	0.95
Compound_842-P12	43.5716	-33.9995	0.66
Compound_846-P12	41.9325	-34.3117	0.64
Compound_847-P12	49.1093	-38.8561	0.90
Compound_850-P12	43.0629	-37.8122	0.77
Compound_868-P12	49.2019	-36.5176	0.83
Compound_869-P12	46.6886	-38.1351	0.84
Compound_870-P12	68.1718	-41.4734	1.30
Compound_875-P12	43.3789	-40.2097	0.84
Compound_883-P12	52.9995	-39.8665	0.99
Compound_884-P12	64.3404	-43.4453	1.29
Compound_885-P12	45.2835	-41.7532	0.92
Compound_889-P12	42.8562	-39.7402	0.82
Compound_896-P12	48.0709	-38.5519	0.87
Compound_899-P12	54.2277	-42.7077	1.10
Compound_900-P12	40.5952	-39.5418	0.77
Compound_901-P12	33.6413	-41.1663	0.70
Compound_902-P12	48.1626	-42.2867	0.98
Compound_909-P12	66.0470	-47.6562	1.44
Compound_910-P12	58.5755	-40.8439	1.12
Compound_911-P12	61.2639	-42.1278	1.20

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_912-P12	46.5436	-44.3495	1.01
Compound_914-P12	65.3786	-42.8472	1.29
Compound_915-P12	40.1401	-45.8248	0.95
Compound_934-P12	55.1278	-46.6926	1.23
Compound_943-P12	57.9137	-44.7958	1.22
Compound_946-P12	35.3749	-36.9199	0.61
Compound_958-P12	69.5183	-42.6556	1.36
Compound_961-P12	63.2124	-43.4353	1.27
Compound_966-P12	54.2059	-39.6576	1.01
Compound_968-P12	45.4178	-39.6811	0.86
Compound_970-P12	52.6497	-41.9318	1.05
Compound_975-P12	36.8547	-39.0582	0.70
Compound_978-P12	65.2279	-40.5311	1.22
Compound_982-P12	55.5538	-41.3965	1.08
Compound_983-P12	63.1675	-44.9975	1.32
Compound_984-P12	46.9892	-41.5429	0.94
Compound_986-P12	66.2708	-43.7086	1.33
Compound_1004-P12	50.4445	-39.8501	0.95
Compound_1005-P12	60.6039	-41.1211	1.16
Compound_1007-P12	52.5963	-38.5765	0.95
Compound_1064-P12	53.5345	-42.3624	1.08
Compound_1070-P12	54.0613	-36.2323	0.91
Compound_1086-P12	57.7422	-35.7439	0.95
Compound_1088-P12	46.9075	-39.3295	0.87
Compound_1098-P12	57.1922	-35.1776	0.93
Compound_1109-P12	53.5266	-36.2018	0.90
Compound_1116-P12	51.2038	-43.1477	1.06
Compound_1119-P12	46.8142	-40.3522	0.90
Compound_1122-P12	58.1418	-44.0157	1.20
Compound_1229-P12	40.8363	-39.6448	0.78
Compound_1230-P12	41.1799	-32.6199	0.58
Compound_1238-P12	57.0396	-49.1078	1.33
Compound_1746-P12	38.8517	-46.3792	0.94
Compound_1748-P12	67.8588	-44.8080	1.39
Compound_1751-P12	57.7686	-48.8908	1.34
Compound_1757-P12	66.6318	-44.1677	1.35
Compound_1769-P12	42.4267	-44.5245	0.95
Compound_1770-P12	47.0593	-39.7181	0.89
Compound_2313-P12	36.2422	-44.2302	0.84
Compound_2321-P12	46.4107	-42.6761	0.96
Compound_2324-P12	44.8323	-42.7807	0.94
Compound_2327-P12	52.8229	-42.8714	1.08
Compound_2339-P12	59.3147	-43.9784	1.22
Compound_2428-P12	34.2659	-44.0945	0.80
Compound_2430-P12	35.8132	-43.9411	0.82
Compound_2444-P12	48.8790	-45.4703	1.09

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2477-P12	35.0684	-45.9967	0.87
Compound_2513-P12	57.7514	-40.8408	1.10
Compound_2516-P12	41.5891	-40.3276	0.81
Compound_2519-P12	58.0976	-43.4975	1.19
Compound_2576-P12	45.1658	-41.7509	0.92
Compound_2579-P12	58.8898	-43.0667	1.19
Compound_2582-P12	62.9167	-42.9882	1.25
Compound_2593-P12	33.4096	-42.8882	0.75
Compound_2614-P12	37.7373	-44.7578	0.88
Compound_2634-P12	42.8016	-45.6161	0.99
Compound_2686-P12	46.7598	-40.2014	0.90
Compound_2689-P12	58.0220	-42.0360	1.14
Compound_2692-P12	44.0234	-44.3581	0.97
Compound_2702-P12	41.1141	-43.9412	0.91
Compound_2797-P12	64.3679	-44.7752	1.33
Compound_2800-P12	52.6577	-44.8663	1.13
Compound_2803-P12	48.2608	-45.5384	1.08
Compound_2814-P12	38.7355	-45.1140	0.90
Compound_2882-P12	49.5151	-44.6195	1.07
Compound_2883-P12	36.2996	-43.4463	0.81
Compound_2886-P12	63.2164	-44.9135	1.31
Compound_2948-P12	24.8651	-43.4045	0.62
Compound_11-P13	50.8179	-42.7679	1.04
Compound_12-P13	44.0068	-41.3465	0.88
Compound_15-P13	60.5646	-39.1283	1.10
Compound_2452-P13	68.8033	-45.8146	1.43
Compound_2454-P13	54.0255	-43.0710	1.10
Compound_2455-P13	53.1834	-44.9230	1.14
Compound_2460-P13	54.5596	-41.1024	1.06
Compound_2463-P13	57.4093	-42.4225	1.14
Compound_2507-P13	57.8295	-35.9483	0.96
Compound_2511-P13	46.1377	-33.8329	0.70
Compound_2513-P13	45.3246	-40.4507	0.88
Compound_2518-P13	47.5901	-36.5015	0.80
Compound_2520-P13	44.3699	-38.5697	0.81
Compound_2524-P13	51.5027	-38.8883	0.94
Compound_2529-P13	60.6094	-39.3514	1.11
Compound_2530-P13	46.6495	-33.1950	0.69
Compound_2532-P13	56.5132	-39.8657	1.05
Compound_2540-P13	42.9762	-36.2652	0.72
Compound_2542-P13	54.2782	-38.7066	0.98
Compound_2549-P13	62.5866	-39.4564	1.14
Compound_2550-P13	48.7098	-37.6657	0.86
Compound_2558-P13	46.1899	-34.6363	0.73
Compound_2601-P13	79.3081	-44.3116	1.57
Compound_2602-P13	52.7671	-46.3412	1.18

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2667-P13	39.0287	-43.8395	0.87
Compound_2704-P13	47.9596	-33.7660	0.73
Compound_2706-P13	50.2584	-36.2616	0.84
Compound_2719-P13	52.3933	-40.2722	1.00
Compound_2721-P13	47.6982	-41.2643	0.94
Compound_2731-P13	43.4613	-34.8812	0.69
Compound_2771-P13	68.3343	-41.1504	1.29
Compound_2772-P13	69.7717	-42.3348	1.35
Compound_2789-P13	54.0643	-34.8607	0.87
Compound_2806-P13	49.1660	-33.3193	0.74
Compound_2807-P13	56.4184	-36.2483	0.95
Compound_2820-P13	37.0031	-44.6431	0.86
Compound_2821-P13	54.7284	-46.4566	1.21
Compound_2822-P13	57.7087	-45.0919	1.23
Compound_2829-P13	45.1063	-43.0206	0.95
Compound_2833-P13	29.7739	-45.7938	0.77
Compound_2834-P13	50.4251	-43.3978	1.05
Compound_2835-P13	48.9238	-44.6719	1.06
Compound_2836-P13	55.6036	-42.6940	1.12
Compound_2837-P13	32.8043	-43.3681	0.75
Compound_2844-P13	75.9887	-43.9979	1.50
Compound_2851-P13	39.8603	-48.3251	1.02
Compound_2854-P13	55.6174	-43.1775	1.13
Compound_2857-P13	52.0878	-46.0637	1.16
Compound_2858-P13	60.4387	-45.6487	1.29
Compound_2859-P13	55.8397	-46.8769	1.25
Compound_2861-P13	57.8992	-41.7518	1.13
Compound_2862-P13	55.8713	-46.1819	1.23
Compound_2863-P13	49.5151	-47.0837	1.14
Compound_2865-P13	43.6891	-44.6283	0.97
Compound_2868-P13	50.7243	-41.9483	1.02
Compound_2870-P13	57.0489	-41.3935	1.11
Compound_2871-P13	45.2534	-43.1990	0.96
Compound_2878-P13	34.7022	-39.0567	0.66
Compound_2879-P13	52.3703	-43.1414	1.08
Compound_2880-P13	62.1641	-42.0084	1.21
Compound_2881-P13	53.9229	-41.9310	1.07
Compound_2894-P13	62.5096	-44.3977	1.29
Compound_2909-P13	46.3798	-51.4962	1.22
Compound_2911-P13	42.1408	-49.1917	1.08
Compound_2916-P13	41.1081	-44.1473	0.92
Compound_2921-P13	55.0710	-50.5722	1.34
Compound_2928-P13	53.5942	-42.6343	1.08
Compound_2938-P13	55.8512	-47.3414	1.26
Compound_2970-P13	66.0422	-45.8864	1.39
Compound_42-P14	55.3744	-32.6016	0.82

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_65-P14	41.2803	-34.6891	0.64
Compound_90-P14	62.7892	-35.2004	1.02
Compound_116-P14	75.0843	-40.9241	1.40
Compound_140-P14	51.2651	-34.8180	0.82
Compound_143-P14	49.2783	-35.1801	0.79
Compound_177-P14	44.8657	-37.1976	0.78
Compound_244-P14	45.3575	-39.0454	0.84
Compound_258-P14	40.2202	-35.6684	0.65
Compound_271-P14	50.5715	-38.4632	0.91
Compound_272-P14	50.1430	-40.8325	0.97
Compound_330-P14	57.0592	-36.0526	0.95
Compound_341-P14	61.0548	-36.2365	1.03
Compound_342-P14	31.0110	-33.2370	0.43
Compound_343-P14	46.1652	-36.7920	0.79
Compound_1577-P14	61.4422	-42.4758	1.21
Compound_2140-P14	52.7434	-44.2709	1.12
Compound_2141-P14	54.8068	-45.3000	1.18
Compound_2143-P14	47.1215	-50.1559	1.19
Compound_2144-P14	46.7221	-45.9093	1.06
Compound_2146-P14	44.1755	-45.6099	1.01
Compound_2147-P14	56.7071	-46.2304	1.24
Compound_2148-P14	40.3410	-47.3501	1.00
Compound_2149-P14	53.0775	-43.2231	1.09
Compound_2150-P14	60.6179	-48.4633	1.37
Compound_2152-P14	36.3999	-44.3614	0.84
Compound_2155-P14	52.9803	-47.3252	1.21
Compound_2156-P14	32.8452	-50.1278	0.95
Compound_2160-P14	41.0716	-44.0075	0.91
Compound_2161-P14	51.8595	-44.8165	1.12
Compound_2172-P14	31.8272	-50.2355	0.93
Compound_2175-P14	41.5615	-45.0386	0.95
Compound_2176-P14	66.8294	-48.7733	1.49
Compound_2181-P14	58.5780	-43.9837	1.21
Compound_2182-P14	54.1331	-45.7173	1.18
Compound_2187-P14	38.0742	-46.3311	0.93
Compound_2189-P14	46.7889	-47.5741	1.11
Compound_2190-P14	54.3031	-48.4801	1.27
Compound_2199-P14	35.9274	-44.9020	0.85
Compound_2203-P14	57.8520	-47.8872	1.31
Compound_2208-P14	64.8630	-42.1623	1.26
Compound_2209-P14	32.6154	-44.4828	0.78
Compound_2210-P14	48.1178	-43.6813	1.02
Compound_2211-P14	60.8221	-51.5269	1.46
Compound_2213-P14	51.9480	-47.6416	1.20
Compound_2217-P14	63.1143	-47.6602	1.39
Compound_2315-P14	49.3407	-45.2599	1.09

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_60-P15	32.3295	-44.9280	0.79
Compound_67-P15	30.6566	-42.7533	0.70
Compound_68-P15	39.0790	-45.1744	0.91
Compound_71-P15	33.5893	-49.7783	0.95
Compound_78-P15	46.0844	-46.9450	1.08
Compound_79-P15	42.7280	-47.2661	1.03
Compound_85-P15	32.2533	-47.6859	0.87
Compound_93-P15	37.4089	-48.1520	0.97
Compound_94-P15	47.3043	-45.1388	1.05
Compound_97-P15	48.3480	-49.3361	1.19
Compound_100-P15	51.3545	-48.0847	1.20
Compound_109-P15	49.9687	-46.1713	1.12
Compound_135-P15	37.4457	-46.7330	0.93
Compound_169-P15	32.9391	-48.6293	0.91
Compound_175-P15	31.4659	-44.5367	0.76
Compound_186-P15	34.5471	-49.2542	0.95
Compound_193-P15	42.9731	-48.1355	1.06
Compound_252-P15	37.2600	-45.2948	0.88
Compound_256-P15	34.9926	-43.9475	0.81
Compound_257-P15	45.6171	-43.1089	0.96
Compound_258-P15	49.9877	-45.7923	1.11
Compound_264-P15	33.1361	-44.8677	0.80
Compound_265-P15	45.6921	-43.9153	0.99
Compound_268-P15	54.2503	-46.1010	1.20
Compound_274-P15	45.9556	-47.0223	1.08
Compound_275-P15	47.8914	-46.2281	1.09
Compound_277-P15	52.9905	-50.5947	1.30
Compound_279-P15	28.0927	-44.4183	0.70
Compound_306-P15	45.9079	-47.4787	1.09
Compound_331-P15	46.8655	-47.3582	1.11
Compound_337-P15	26.8009	-44.6027	0.69
Compound_338-P15	22.9179	-43.7928	0.60
Compound_342-P15	32.3415	-46.1482	0.82
Compound_346-P15	46.4526	-43.4514	0.99
Compound_347-P15	52.5922	-46.4871	1.18
Compound_350-P15	38.0346	-46.4183	0.93
Compound_358-P15	30.4845	-47.3617	0.83
Compound_359-P15	63.7881	-45.4389	1.34
Compound_360-P15	45.9847	-50.9792	1.20
Compound_362-P15	60.0864	-48.4227	1.36
Compound_370-P15	61.5580	-46.6328	1.34
Compound_392-P15	46.6412	-46.9900	1.09
Compound_422-P15	26.4722	-46.8790	0.75
Compound_428-P15	42.5447	-43.8131	0.93
Compound_430-P15	31.7284	-46.5914	0.83
Compound_439-P15	30.8850	-45.6602	0.79

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_442-P15	49.6041	-45.4664	1.10
Compound_487-P15	38.2995	-45.9030	0.92
Compound_516-P15	32.3646	-47.3933	0.86
Compound_523-P15	34.0456	-47.3401	0.89
Compound_524-P15	25.0075	-47.3510	0.73
Compound_526-P15	54.9836	-48.1793	1.27
Compound_535-P15	53.9476	-48.6813	1.27
Compound_538-P15	38.2954	-48.7358	1.00
Compound_546-P15	28.8341	-47.2486	0.80
Compound_579-P15	59.1526	-49.7576	1.39
Compound_605-P15	51.5081	-46.9275	1.17
Compound_610-P15	32.5445	-46.8332	0.85
Compound_613-P15	29.4016	-47.9031	0.83
Compound_632-P15	53.9406	-48.2980	1.25
Compound_670-P15	41.7274	-50.3554	1.11
Compound_692-P15	39.3112	-41.1517	0.80
Compound_693-P15	44.0866	-45.0908	0.99
Compound_695-P15	57.6035	-45.1391	1.22
Compound_702-P15	47.7467	-44.4198	1.04
Compound_706-P15	61.8490	-44.6390	1.28
Compound_773-P15	27.2407	-46.5854	0.75
Compound_780-P15	26.3601	-44.6025	0.68
Compound_781-P15	43.6357	-44.2313	0.96
Compound_782-P15	54.5992	-48.1450	1.26
Compound_784-P15	28.8929	-47.3242	0.80
Compound_792-P15	48.8650	-47.1912	1.14
Compound_799-P15	55.9166	-45.1213	1.20
Compound_1181-P15	51.0767	-41.7666	1.02
Compound_1182-P15	35.3816	-45.0646	0.84
Compound_1183-P15	36.4037	-44.0670	0.83
Compound_1208-P15	44.2462	-44.1954	0.97
Compound_1209-P15	43.4463	-44.3126	0.96
Compound_1235-P15	64.1974	-44.2686	1.31
Compound_1241-P15	49.1386	-45.2867	1.09
Compound_1243-P15	62.5753	-45.4635	1.32
Compound_1256-P15	58.8681	-45.4229	1.25
Compound_1301-P15	51.3504	-46.2105	1.15
Compound_1303-P15	47.0571	-40.3263	0.91
Compound_1306-P15	45.7446	-41.9908	0.93
Compound_1307-P15	41.9399	-40.4053	0.82
Compound_1309-P15	60.1089	-43.9201	1.23
Compound_1311-P15	55.9244	-44.2489	1.17
Compound_1313-P15	58.8805	-38.0490	1.04
Compound_1320-P15	59.3806	-41.7253	1.16
Compound_1321-P15	65.6545	-43.6465	1.32
Compound_1323-P15	58.3101	-37.4927	1.02

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1644-P15	60.8990	-43.6940	1.24
Compound_1645-P15	47.6756	-41.9188	0.96
Compound_1648-P15	50.7563	-38.6211	0.92
Compound_1649-P15	56.5494	-31.4920	0.81
Compound_1685-P15	48.8819	-43.7566	1.04
Compound_1712-P15	38.5345	-42.3829	0.82
Compound_1728-P15	57.5719	-38.7876	1.04
Compound_1729-P15	49.5271	-36.7886	0.85
Compound_1732-P15	65.0854	-35.2740	1.07
Compound_1733-P15	35.6220	-30.3358	0.42
Compound_1750-P15	57.5548	-40.1350	1.08
Compound_1762-P15	57.2331	-40.6421	1.09
Compound_1785-P15	67.5036	-41.1095	1.28
Compound_1857-P15	41.7836	-29.7616	0.51
Compound_1859-P15	47.8030	-32.4814	0.69
Compound_1860-P15	39.0058	-30.6567	0.49
Compound_1932-P15	49.5756	-41.6036	0.99
Compound_1934-P15	50.6396	-40.5538	0.97
Compound_1957-P15	52.9920	-42.7341	1.08
Compound_1977-P15	70.0229	-44.2620	1.41
Compound_1993-P15	58.3564	-39.3281	1.07
Compound_2005-P15	48.9091	-34.1063	0.76
Compound_2057-P15	53.9821	-42.7896	1.10
Compound_2065-P15	63.7709	-43.7793	1.29
Compound_2076-P15	41.1918	-46.0370	0.97
Compound_2077-P15	63.4482	-41.7132	1.22
Compound_2078-P15	54.2703	-43.4468	1.12
Compound_2079-P15	54.6507	-41.7211	1.08
Compound_2095-P15	53.3392	-42.1439	1.07
Compound_2103-P15	49.1762	-40.1984	0.94
Compound_2110-P15	54.1972	-41.4947	1.06
Compound_2111-P15	56.1692	-43.0690	1.14
Compound_2112-P15	57.0978	-38.7341	1.03
Compound_2113-P15	54.7997	-39.1574	1.00
Compound_2114-P15	60.0865	-43.8622	1.23
Compound_2118-P15	52.2012	-38.4421	0.94
Compound_2121-P15	59.1667	-43.7910	1.21
Compound_2125-P15	51.8480	-39.1995	0.95
Compound_2163-P15	38.3008	-32.3324	0.53
Compound_2164-P15	33.9065	-31.3917	0.42
Compound_2177-P15	48.1718	-37.0025	0.83
Compound_2178-P15	39.5657	-36.8605	0.68
Compound_2206-P15	42.6848	-38.9908	0.79
Compound_2214-P15	42.8826	-40.0391	0.83
Compound_2215-P15	48.3048	-37.3888	0.84
Compound_2218-P15	38.9508	-37.9610	0.70

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2221-P15	64.1949	-37.6293	1.12
Compound_2225-P15	41.6237	-32.3240	0.58
Compound_2227-P15	40.8592	-39.8476	0.79
Compound_2427-P15	37.3116	-31.4091	0.48
Compound_2554-P15	44.0038	-42.2172	0.91
Compound_2555-P15	46.0343	-41.7871	0.93
Compound_2556-P15	48.2442	-40.6091	0.93
Compound_2557-P15	49.5253	-35.3491	0.80
Compound_2558-P15	52.1322	-37.1202	0.90
Compound_2560-P15	60.5354	-47.9124	1.36
Compound_2561-P15	58.7299	-47.4359	1.31
Compound_2562-P15	46.0176	-44.6051	1.01
Compound_2565-P15	59.1507	-47.6397	1.32
Compound_2566-P15	63.7380	-43.7822	1.29
Compound_2568-P15	52.8986	-41.4391	1.04
Compound_2571-P15	61.0430	-44.6434	1.27
Compound_2572-P15	59.1238	-42.7411	1.18
Compound_2574-P15	57.3728	-45.4308	1.23
Compound_2575-P15	43.1054	-44.5721	0.96
Compound_2576-P15	58.8568	-45.9396	1.27
Compound_2577-P15	58.7662	-45.3395	1.25
Compound_2578-P15	52.4911	-44.9423	1.13
Compound_2581-P15	50.2484	-46.0829	1.13
Compound_2584-P15	51.8196	-42.4146	1.05
Compound_2592-P15	71.7780	-45.0486	1.46
Compound_2593-P15	53.4809	-47.4443	1.22
Compound_2595-P15	55.5752	-45.2087	1.19
Compound_2596-P15	54.1647	-42.6255	1.09
Compound_2601-P15	42.6830	-35.2035	0.68
Compound_2604-P15	50.1052	-39.8099	0.94
Compound_2607-P15	70.0806	-43.2477	1.38
Compound_2608-P15	51.5240	-39.3056	0.95
Compound_2617-P15	51.6089	-40.7447	1.00
Compound_2619-P15	42.8593	-40.0761	0.83
Compound_2627-P15	50.5989	-37.6181	0.89
Compound_2631-P15	49.3238	-39.5076	0.92
Compound_2642-P15	56.3187	-38.3923	1.01
Compound_2643-P15	45.7776	-33.2832	0.68
Compound_2644-P15	50.4238	-44.3790	1.08
Compound_2645-P15	81.3018	-45.3161	1.63
Compound_2646-P15	53.9802	-43.0922	1.10
Compound_2648-P15	70.3747	-46.1624	1.47
Compound_2652-P15	75.4642	-43.2966	1.48
Compound_2654-P15	61.3965	-42.6950	1.22
Compound_2657-P15	48.8215	-44.6131	1.06
Compound_2658-P15	43.9239	-43.4404	0.94

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2661-P15	50.2732	-43.7017	1.06
Compound_2664-P15	72.6534	-43.6379	1.44
Compound_2669-P15	52.4027	-40.3921	1.00
Compound_2677-P15	48.1132	-43.8065	1.02
Compound_2678-P15	45.7188	-45.8239	1.04
Compound_2680-P15	57.1952	-44.0820	1.19
Compound_2682-P15	47.0028	-40.4378	0.91
Compound_2837-P15	47.6584	-42.0570	0.97
Compound_2892-P15	48.6865	-42.5318	1.00
Compound_2977-P15	55.1704	-43.2227	1.13
Compound_2979-P15	67.2393	-43.0887	1.33
Compound_2981-P15	49.7755	-43.9746	1.06
Compound_124-P16	52.4495	-44.9170	1.13
Compound_131-P16	60.1977	-44.4027	1.25
Compound_140-P16	52.0827	-42.2185	1.05
Compound_142-P16	57.7677	-41.0080	1.11
Compound_144-P16	48.9522	-41.4201	0.97
Compound_159-P16	47.6440	-44.2410	1.03
Compound_171-P16	58.5275	-43.3978	1.19
Compound_177-P16	57.6102	-43.8220	1.19
Compound_317-P16	45.7847	-40.8902	0.90
Compound_321-P16	37.8708	-45.2762	0.89
Compound_334-P16	53.9178	-39.7262	1.01
Compound_337-P16	62.9704	-40.4457	1.18
Compound_348-P16	38.0308	-42.8054	0.82
Compound_351-P16	44.1183	-45.1353	1.00
Compound_454-P16	52.4464	-40.5505	1.00
Compound_455-P16	41.3746	-39.2035	0.78
Compound_463-P16	61.3136	-42.7951	1.22
Compound_489-P16	50.7249	-43.2933	1.05
Compound_558-P16	31.8131	-42.3571	0.71
Compound_570-P16	59.5072	-46.8233	1.31
Compound_663-P16	55.5288	-44.8932	1.18
Compound_667-P16	37.4258	-43.0287	0.82
Compound_683-P16	51.7006	-44.9901	1.12
Compound_769-P16	49.9098	-42.3585	1.01
Compound_1357-P16	66.1906	-41.2510	1.26
Compound_1377-P16	57.3907	-43.8614	1.18
Compound_1391-P16	52.0908	-45.7779	1.15
Compound_1437-P16	45.4896	-45.3549	1.03
Compound_1479-P16	31.9536	-45.5066	0.80
Compound_1492-P16	60.6088	-47.7705	1.35
Compound_2123-P16	51.9581	-34.6681	0.83
Compound_2124-P16	42.2631	-31.3513	0.56
Compound_2125-P16	42.8302	-32.3024	0.60
Compound_2126-P16	41.1547	-32.7854	0.59

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2127-P16	39.3869	-31.6594	0.52
Compound_2128-P16	41.5567	-31.8395	0.57
Compound_2129-P16	50.2926	-32.1875	0.72
Compound_2130-P16	40.4039	-32.4652	0.56
Compound_2131-P16	47.9443	-32.4849	0.69
Compound_2132-P16	44.6951	-33.7888	0.68
Compound_2133-P16	35.4693	-28.6157	0.37
Compound_2352-P16	64.6752	-38.3925	1.15
Compound_2357-P16	53.7315	-37.3640	0.93
Compound_2358-P16	53.7148	-36.2203	0.90
Compound_2360-P16	44.6103	-36.2844	0.75
Compound_2455-P16	50.0787	-42.2774	1.01
Compound_2457-P16	47.7185	-43.3636	1.01
Compound_2458-P16	56.9074	-42.2748	1.13
Compound_2459-P16	48.6665	-44.2148	1.05
Compound_2460-P16	53.9491	-45.1302	1.16
Compound_2461-P16	43.7045	-43.2457	0.93
Compound_2462-P16	54.1436	-45.4115	1.17
Compound_2472-P16	48.2059	-41.0919	0.95
Compound_2475-P16	52.6139	-43.2361	1.08
Compound_2627-P16	66.8982	-36.4001	1.13
Compound_2630-P16	46.6629	-37.6086	0.82
Compound_2631-P16	51.7221	-39.3665	0.96
Compound_2651-P16	49.9435	-37.6244	0.88
Compound_2652-P16	46.2248	-37.5736	0.81
Compound_2654-P16	49.7225	-37.9376	0.88
Compound_2659-P16	36.5227	-30.5166	0.44
Compound_2660-P16	51.1211	-37.5821	0.90
Compound_2661-P16	54.5194	-36.1991	0.91
Compound_2662-P16	47.7907	-36.5050	0.81
Compound_2707-P16	49.4028	-41.0740	0.97
Compound_2708-P16	39.4753	-40.7519	0.79
Compound_2717-P16	51.2964	-42.6839	1.05
Compound_2719-P16	47.1152	-44.7233	1.03
Compound_2722-P16	55.6537	-44.8379	1.18
Compound_2784-P16	49.4411	-42.0685	1.00
Compound_2787-P16	49.1795	-42.4673	1.00
Compound_533-P17	51.2692	-42.3004	1.03
Compound_534-P17	64.9323	-39.1565	1.18
Compound_535-P17	53.6961	-39.9897	1.01
Compound_605-P17	53.5001	-38.5964	0.97
Compound_608-P17	43.9293	-35.5325	0.71
Compound_623-P17	49.4270	-39.5870	0.92
Compound_634-P17	60.7085	-40.7726	1.15
Compound_721-P17	49.0744	-42.0801	0.99
Compound_772-P17	42.3118	-43.9820	0.93

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_773-P17	47.6912	-42.8445	0.99
Compound_774-P17	41.8753	-37.5698	0.74
Compound_775-P17	67.9827	-45.1521	1.40
Compound_776-P17	71.4452	-47.1162	1.52
Compound_777-P17	47.5593	-46.2752	1.09
Compound_779-P17	55.2081	-48.9935	1.30
Compound_780-P17	47.6416	-45.3834	1.06
Compound_781-P17	73.0370	-46.0913	1.52
Compound_787-P17	37.6163	-45.2412	0.89
Compound_789-P17	50.4900	-49.3306	1.23
Compound_790-P17	61.7092	-47.3133	1.36
Compound_791-P17	70.7876	-47.9107	1.53
Compound_792-P17	45.1031	-46.7589	1.06
Compound_795-P17	51.2514	-47.8907	1.20
Compound_797-P17	53.1722	-48.7654	1.25
Compound_808-P17	43.8569	-46.0572	1.02
Compound_810-P17	44.2197	-45.7135	1.01
Compound_811-P17	49.9819	-47.7311	1.17
Compound_816-P17	64.9593	-47.6965	1.42
Compound_968-P17	47.8106	-40.9960	0.94
Compound_987-P17	65.3041	-42.1414	1.27
Compound_1009-P17	40.8505	-42.2598	0.86
Compound_1010-P17	56.3070	-41.2587	1.09
Compound_1015-P17	51.8829	-44.1294	1.10
Compound_1021-P17	53.7931	-41.7998	1.06
Compound_1022-P17	59.7375	-40.4266	1.12
Compound_1023-P17	50.8909	-42.5343	1.04
Compound_1024-P17	52.5244	-44.1059	1.11
Compound_1025-P17	39.4157	-41.4701	0.81
Compound_1031-P17	65.4147	-38.9928	1.18
Compound_1101-P17	57.9656	-41.4027	1.12
Compound_1420-P17	53.6367	-41.8422	1.06
Compound_1434-P17	51.3604	-38.2585	0.92
Compound_1461-P17	62.7630	-36.7154	1.07
Compound_1499-P17	47.4332	-38.8108	0.87
Compound_1500-P17	56.5873	-41.4155	1.10
Compound_1922-P17	39.4114	-35.3593	0.63
Compound_1939-P17	32.0445	-36.4906	0.54
Compound_1956-P17	34.0169	-36.6275	0.58
Compound_2023-P17	39.6930	-37.5380	0.70
Compound_2035-P17	44.5120	-35.2791	0.72
Compound_2043-P17	36.5173	-36.7516	0.62
Compound_2074-P17	59.7928	-35.9209	0.99
Compound_2688-P17	62.6735	-40.5096	1.18
Compound_2754-P17	59.4220	-43.0009	1.19
Compound_2982-P17	50.2026	-45.2009	1.10

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2983-P17	38.1697	-42.4606	0.82
Compound_2984-P17	38.9068	-43.5795	0.86
Compound_2985-P17	48.7949	-42.8186	1.01
Compound_2990-P17	57.9452	-44.8733	1.22
Compound_7-P18	48.1272	-45.1446	1.06
Compound_12-P18	65.7802	-43.0451	1.30
Compound_703-P18	53.9190	-38.3648	0.97
Compound_705-P18	41.7242	-42.6024	0.88
Compound_709-P18	54.8831	-42.2655	1.10
Compound_713-P18	50.7650	-37.8667	0.90
Compound_714-P18	53.4571	-39.7973	1.00
Compound_715-P18	25.8035	-38.8792	0.50
Compound_716-P18	40.6429	-37.9756	0.73
Compound_717-P18	37.3795	-39.5573	0.72
Compound_718-P18	58.4892	-39.8162	1.09
Compound_719-P18	39.4414	-38.6070	0.73
Compound_720-P18	48.6751	-39.7485	0.92
Compound_721-P18	46.8555	-41.1915	0.93
Compound_723-P18	59.6604	-40.9862	1.14
Compound_724-P18	55.2125	-41.3037	1.07
Compound_735-P18	50.7487	-42.5265	1.03
Compound_736-P18	61.3985	-42.2070	1.20
Compound_742-P18	61.6744	-42.3897	1.21
Compound_743-P18	29.6019	-43.4504	0.70
Compound_744-P18	55.9017	-42.8997	1.13
Compound_745-P18	49.9978	-40.8856	0.97
Compound_746-P18	60.4094	-42.8778	1.21
Compound_782-P18	52.5304	-46.3234	1.17
Compound_818-P18	58.2595	-39.9032	1.08
Compound_819-P18	52.6216	-38.6911	0.95
Compound_820-P18	43.1711	-38.1142	0.78
Compound_840-P18	43.8606	-38.5295	0.80
Compound_841-P18	47.8748	-39.1663	0.89
Compound_848-P18	47.6013	-39.8695	0.90
Compound_849-P18	38.8294	-40.0181	0.76
Compound_865-P18	31.2535	-44.0680	0.75
Compound_867-P18	44.1860	-37.6432	0.78
Compound_868-P18	38.4658	-37.3854	0.67
Compound_871-P18	48.7854	-37.9044	0.87
Compound_873-P18	25.1743	-37.4437	0.45
Compound_879-P18	47.8473	-36.6262	0.81
Compound_885-P18	47.7792	-38.1566	0.86
Compound_888-P18	53.9354	-37.8858	0.95
Compound_945-P18	43.6949	-43.5656	0.94
Compound_947-P18	25.4351	-44.6409	0.66
Compound_952-P18	36.4785	-47.2050	0.93

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_957-P18	42.6647	-44.8725	0.96
Compound_959-P18	42.3601	-45.5220	0.98
Compound_961-P18	23.3454	-41.8400	0.55
Compound_962-P18	39.9807	-41.3895	0.82
Compound_963-P18	58.8655	-40.5795	1.11
Compound_971-P18	43.6614	-43.2640	0.93
Compound_972-P18	49.3106	-49.8042	1.22
Compound_977-P18	48.8926	-45.0998	1.08
Compound_987-P18	35.1285	-48.7679	0.95
Compound_996-P18	55.3720	-44.0286	1.15
Compound_997-P18	40.6848	-47.8666	1.02
Compound_1042-P18	41.1127	-39.4130	0.78
Compound_1047-P18	50.8675	-40.2877	0.97
Compound_1048-P18	54.1436	-41.8955	1.07
Compound_1057-P18	69.3621	-42.4581	1.35
Compound_1059-P18	33.3993	-42.7991	0.75
Compound_1082-P18	51.5548	-41.8388	1.03
Compound_1085-P18	51.9438	-36.9464	0.89
Compound_1086-P18	36.4177	-40.4483	0.73
Compound_1087-P18	51.9892	-43.2757	1.08
Compound_1088-P18	29.5077	-43.6467	0.70
Compound_1091-P18	37.7620	-45.3097	0.89
Compound_1093-P18	59.4624	-44.2239	1.23
Compound_1108-P18	56.1209	-31.6580	0.81
Compound_1110-P18	41.4434	-31.1492	0.54
Compound_1111-P18	44.9902	-30.2159	0.58
Compound_1114-P18	48.0206	-36.8853	0.82
Compound_1118-P18	44.4421	-29.8637	0.56
Compound_1120-P18	45.8803	-29.0904	0.56
Compound_1123-P18	43.1116	-37.0432	0.74
Compound_1125-P18	49.9017	-35.7130	0.82
Compound_1126-P18	42.6408	-29.3065	0.51
Compound_2373-P18	52.8613	-34.3359	0.83
Compound_2661-P18	44.3483	-41.5203	0.89
Compound_2664-P18	46.9535	-32.9651	0.69
Compound_2665-P18	50.3171	-30.7221	0.68
Compound_2667-P18	46.4664	-35.3501	0.75
Compound_2668-P18	53.1194	-34.8296	0.85
Compound_2669-P18	46.2173	-32.3664	0.66
Compound_2670-P18	37.5517	-29.2327	0.42
Compound_2671-P18	33.8878	-32.1066	0.44
Compound_2672-P18	31.6705	-26.8557	0.25
Compound_2673-P18	43.9961	-33.4592	0.65
Compound_2678-P18	54.0282	-34.1937	0.85
Compound_2680-P18	49.0198	-39.5344	0.92
Compound_2681-P18	48.6102	-34.4593	0.76

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2683-P18	44.7049	-33.1393	0.66
Compound_2684-P18	41.3823	-43.7072	0.91
Compound_2685-P18	41.3245	-37.6868	0.73
Compound_2686-P18	47.8214	-38.1406	0.86
Compound_2687-P18	33.1189	-35.9685	0.54
Compound_2688-P18	47.9522	-40.0911	0.91
Compound_2691-P18	58.5036	-41.5314	1.14
Compound_2693-P18	39.4441	-41.5193	0.81
Compound_2694-P18	41.3051	-37.7864	0.73
Compound_2695-P18	40.9183	-33.9117	0.62
Compound_2696-P18	56.8132	-39.4019	1.05
Compound_2697-P18	52.8807	-33.7136	0.81
Compound_2698-P18	47.5149	-33.5569	0.72
Compound_2700-P18	53.3278	-38.7362	0.97
Compound_2701-P18	49.0645	-41.9010	0.99
Compound_2726-P18	57.3266	-34.8446	0.92
Compound_2734-P18	42.7746	-37.3884	0.75
Compound_2737-P18	48.2100	-39.9646	0.92
Compound_2740-P18	43.5814	-37.4258	0.76
Compound_2741-P18	38.5688	-29.7682	0.46
Compound_2742-P18	63.9009	-37.1037	1.10
Compound_2743-P18	42.4683	-35.1000	0.68
Compound_2744-P18	54.2458	-40.6883	1.04
Compound_2747-P18	57.5007	-37.9556	1.01
Compound_2748-P18	38.9087	-41.6218	0.80
Compound_2757-P18	38.7761	-34.0572	0.58
Compound_2765-P18	38.9456	-39.9749	0.76
Compound_2767-P18	37.1455	-34.6151	0.57
Compound_2772-P18	39.0484	-31.7681	0.52
Compound_2773-P18	43.4703	-28.4667	0.50
Compound_2774-P18	26.5100	-28.0408	0.20
Compound_2775-P18	36.8545	-23.2490	0.24
Compound_2776-P18	31.2249	-31.8513	0.39
Compound_2777-P18	34.8815	-27.9856	0.34
Compound_2778-P18	46.2998	-31.6880	0.64
Compound_2779-P18	43.7258	-30.9712	0.58
Compound_2780-P18	38.8679	-28.3339	0.42
Compound_2791-P18	37.8782	-33.2534	0.54
Compound_2792-P18	51.3478	-30.8954	0.71
Compound_2793-P18	41.4913	-35.6056	0.67
Compound_2800-P18	48.0613	-35.1340	0.77
Compound_2801-P18	38.8983	-39.7673	0.75
Compound_2805-P18	42.5077	-33.0831	0.62
Compound_2808-P18	50.0865	-34.5618	0.79
Compound_2813-P18	44.9705	-33.0059	0.66
Compound_2814-P18	37.2571	-34.8121	0.58

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2816-P18	51.7890	-35.2531	0.84
Compound_2817-P18	37.6119	-33.6597	0.55
Compound_2819-P18	33.9733	-38.7617	0.64
Compound_2821-P18	45.1838	-36.4662	0.76
Compound_2823-P18	48.5255	-33.1486	0.72
Compound_2824-P18	48.8884	-37.1275	0.84
Compound_2825-P18	45.5927	-41.0466	0.90
Compound_2836-P18	44.1235	-39.8603	0.84
Compound_2837-P18	44.5509	-35.9233	0.74
Compound_2943-P18	40.0764	-45.7037	0.94
Compound_2946-P18	48.2217	-40.6703	0.94
Compound_2947-P18	37.0229	-40.6138	0.74
Compound_2948-P18	44.4439	-39.5095	0.84
Compound_2972-P18	63.3247	-50.5631	1.48
Compound_2999-P18	59.5477	-40.9061	1.14
Compound_3000-P18	65.1723	-43.8721	1.32
Compound_6-P19	44.3074	-44.5106	0.98
Compound_7-P19	35.2933	-45.3531	0.85
Compound_9-P19	65.0941	-46.5354	1.39
Compound_138-P19	45.8869	-35.2536	0.74
Compound_139-P19	49.4719	-36.6764	0.84
Compound_150-P19	47.2633	-37.3139	0.82
Compound_156-P19	52.9781	-38.4495	0.95
Compound_163-P19	47.0599	-38.2792	0.85
Compound_180-P19	38.1420	-37.5590	0.67
Compound_187-P19	40.1973	-38.0297	0.72
Compound_191-P19	51.1396	-35.9205	0.85
Compound_348-P19	49.8115	-39.5414	0.93
Compound_349-P19	33.2567	-39.2863	0.64
Compound_350-P19	36.7458	-38.2978	0.67
Compound_351-P19	53.3319	-36.7740	0.91
Compound_353-P19	34.8623	-33.6476	0.50
Compound_357-P19	55.4755	-42.1813	1.10
Compound_359-P19	47.8868	-44.3044	1.04
Compound_360-P19	38.6299	-41.8870	0.81
Compound_363-P19	40.2338	-46.4591	0.97
Compound_364-P19	54.3007	-41.8593	1.07
Compound_366-P19	45.5168	-42.1410	0.93
Compound_368-P19	52.6406	-45.5691	1.15
Compound_377-P19	49.8562	-41.3665	0.98
Compound_378-P19	53.5929	-43.7447	1.12
Compound_379-P19	54.7375	-43.5894	1.13
Compound_380-P19	65.0321	-42.2134	1.27
Compound_381-P19	42.9079	-42.1550	0.89
Compound_382-P19	49.5514	-42.0562	1.00
Compound_384-P19	66.3114	-44.2590	1.35

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_388-P19	62.9252	-47.0196	1.37
Compound_392-P19	49.7143	-39.0531	0.91
Compound_396-P19	46.4255	-41.9484	0.94
Compound_397-P19	54.5856	-41.5966	1.07
Compound_402-P19	45.7707	-43.1309	0.97
Compound_403-P19	48.7414	-42.9119	1.01
Compound_404-P19	61.4852	-44.2437	1.26
Compound_406-P19	58.0569	-42.7491	1.16
Compound_408-P19	51.2843	-39.5322	0.95
Compound_413-P19	52.2200	-45.7202	1.15
Compound_414-P19	47.1290	-43.1244	0.99
Compound_654-P19	61.9789	-45.9705	1.32
Compound_655-P19	57.8314	-40.8139	1.10
Compound_692-P19	53.1820	-37.9619	0.94
Compound_693-P19	55.8534	-40.1468	1.05
Compound_694-P19	47.0840	-40.4775	0.91
Compound_711-P19	52.7027	-40.7125	1.01
Compound_712-P19	41.2678	-39.3768	0.78
Compound_727-P19	44.9386	-43.2542	0.95
Compound_742-P19	58.7186	-40.7332	1.12
Compound_749-P19	55.3089	-35.2595	0.90
Compound_751-P19	41.1812	-36.1155	0.68
Compound_756-P19	50.0977	-35.8771	0.83
Compound_767-P19	48.0756	-34.2355	0.75
Compound_768-P19	50.8859	-33.2033	0.76
Compound_771-P19	59.0929	-38.1013	1.05
Compound_772-P19	47.5089	-37.5411	0.83
Compound_784-P19	54.4735	-35.3938	0.89
Compound_788-P19	59.0346	-35.1613	0.96
Compound_790-P19	42.1735	-34.6326	0.66
Compound_799-P19	53.6600	-36.2690	0.90
Compound_804-P19	53.2965	-33.1012	0.80
Compound_811-P19	53.5804	-43.7337	1.12
Compound_823-P19	45.5421	-34.7739	0.72
Compound_835-P19	48.4364	-38.5315	0.88
Compound_836-P19	45.8590	-38.1765	0.82
Compound_837-P19	48.6907	-37.5119	0.85
Compound_840-P19	39.5688	-31.5952	0.53
Compound_854-P19	34.1498	-32.6718	0.46
Compound_862-P19	49.9185	-37.0740	0.86
Compound_863-P19	55.7602	-40.1102	1.05
Compound_864-P19	48.9547	-36.8476	0.84
Compound_867-P19	47.0354	-39.7645	0.89
Compound_868-P19	40.3310	-40.9032	0.81
Compound_869-P19	46.1659	-39.4092	0.86
Compound_873-P19	44.8826	-33.2144	0.66

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_874-P19	44.3529	-34.8560	0.70
Compound_876-P19	37.4223	-30.8314	0.47
Compound_878-P19	46.5360	-29.0431	0.57
Compound_888-P19	45.0754	-38.1268	0.81
Compound_893-P19	49.9788	-32.5239	0.73
Compound_894-P19	47.9031	-30.9960	0.65
Compound_897-P19	55.9827	-28.0014	0.70
Compound_900-P19	48.8830	-34.3000	0.76
Compound_902-P19	50.3124	-32.0555	0.72
Compound_903-P19	40.3077	-27.7988	0.43
Compound_905-P19	44.8586	-34.5649	0.70
Compound_911-P19	53.7554	-35.7985	0.89
Compound_912-P19	40.7090	-33.5434	0.60
Compound_933-P19	45.3791	-38.9924	0.84
Compound_951-P19	63.5275	-40.0152	1.18
Compound_958-P19	54.9209	-34.8170	0.88
Compound_959-P19	46.8039	-34.0570	0.72
Compound_964-P19	45.4306	-36.6807	0.77
Compound_965-P19	42.2932	-35.3341	0.68
Compound_966-P19	47.6798	-33.8220	0.73
Compound_975-P19	55.7516	-37.8758	0.98
Compound_976-P19	49.5146	-35.4944	0.81
Compound_979-P19	51.9169	-35.9787	0.86
Compound_980-P19	43.3741	-34.0677	0.66
Compound_985-P19	44.6039	-36.5865	0.76
Compound_986-P19	51.0791	-34.8250	0.81
Compound_994-P19	52.2508	-33.9653	0.81
Compound_995-P19	53.8626	-34.0651	0.84
Compound_996-P19	49.8827	-33.6874	0.76
Compound_1000-P19	54.2383	-34.9787	0.87
Compound_1001-P19	43.8734	-33.7084	0.66
Compound_1011-P19	49.8949	-38.2766	0.89
Compound_1012-P19	46.0276	-38.4556	0.83
Compound_1017-P19	55.1627	-35.5567	0.91
Compound_1018-P19	43.5936	-33.4179	0.65
Compound_1019-P19	44.9945	-33.2032	0.66
Compound_1034-P19	48.9689	-31.5827	0.68
Compound_1052-P19	47.9186	-35.7912	0.79
Compound_1053-P19	55.6747	-35.3573	0.91
Compound_1056-P19	40.2838	-32.4244	0.56
Compound_1081-P19	51.2181	-41.9048	1.02
Compound_1082-P19	54.3931	-41.0739	1.05
Compound_1083-P19	44.2686	-40.5334	0.86
Compound_1087-P19	54.2213	-38.1415	0.96
Compound_1088-P19	46.2163	-36.6740	0.79
Compound_1093-P19	50.2417	-32.2778	0.73

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1094-P19	54.0245	-33.1573	0.82
Compound_1096-P19	41.2786	-33.5010	0.61
Compound_1105-P19	50.0705	-39.1624	0.92
Compound_1111-P19	61.3292	-32.7504	0.93
Compound_1112-P19	44.4731	-32.4586	0.63
Compound_1114-P19	37.7098	-30.7275	0.47
Compound_1117-P19	60.9053	-31.6603	0.89
Compound_1120-P19	42.1654	-29.3942	0.51
Compound_1122-P19	47.4651	-37.3467	0.83
Compound_1123-P19	48.7371	-37.4366	0.85
Compound_1124-P19	58.7640	-34.0345	0.92
Compound_1127-P19	49.5807	-33.5966	0.75
Compound_1128-P19	45.0447	-33.6904	0.68
Compound_1150-P19	40.1852	-36.2042	0.67
Compound_1175-P19	46.7146	-40.6346	0.91
Compound_1188-P19	43.3506	-34.2727	0.67
Compound_1190-P19	41.0564	-28.3900	0.46
Compound_1195-P19	50.3015	-38.8191	0.92
Compound_1196-P19	43.3101	-34.3217	0.67
Compound_1197-P19	45.7354	-25.7859	0.46
Compound_1208-P19	44.1975	-35.2433	0.71
Compound_1260-P19	55.1546	-46.6992	1.23
Compound_1263-P19	53.2898	-43.8229	1.11
Compound_1348-P19	62.0831	-40.6267	1.17
Compound_1349-P19	63.9169	-40.9800	1.21
Compound_1350-P19	32.7956	-43.6419	0.76
Compound_1351-P19	54.9087	-40.2681	1.04
Compound_1369-P19	48.5091	-37.3771	0.85
Compound_1411-P19	46.8608	-34.9670	0.75
Compound_1420-P19	37.9236	-37.2662	0.66
Compound_1443-P19	44.7146	-28.5593	0.52
Compound_1705-P19	59.3836	-44.4411	1.23
Compound_1709-P19	53.7171	-47.1859	1.22
Compound_1712-P19	53.2987	-40.4852	1.02
Compound_1716-P19	51.3835	-42.9556	1.06
Compound_1725-P19	36.9072	-46.0693	0.90
Compound_1842-P19	60.0227	-31.9646	0.88
Compound_2191-P19	48.9228	-31.0282	0.67
Compound_2989-P19	38.9140	-31.1741	0.50
Compound_188-P1	45.7733	-38.0209	0.82
Compound_189-P1	52.5142	-43.8409	1.10
Compound_370-P1	46.7556	-42.1784	0.95
Compound_530-P1	41.4861	-41.9434	0.86
Compound_672-P1	32.7816	-32.5210	0.44
Compound_751-P1	49.4778	-37.3502	0.86
Compound_771-P1	55.9456	-38.6238	1.01

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_851-P1	51.2702	-39.1796	0.94
Compound_853-P1	52.5064	-37.1493	0.91
Compound_865-P1	37.6504	-32.3977	0.52
Compound_890-P1	47.2072	-36.9125	0.81
Compound_891-P1	44.8696	-35.7664	0.74
Compound_892-P1	40.3265	-35.1897	0.64
Compound_894-P1	41.1637	-37.4576	0.72
Compound_985-P1	51.0694	-43.2225	1.06
Compound_986-P1	41.4665	-34.2860	0.64
Compound_1027-P1	50.2264	-39.3076	0.93
Compound_1066-P1	41.3851	-39.5438	0.79
Compound_1166-P1	45.2830	-37.5549	0.80
Compound_1192-P1	41.3554	-33.0645	0.60
Compound_1221-P1	49.4055	-34.9437	0.79
Compound_1336-P1	45.8612	-41.3780	0.92
Compound_1337-P1	54.0925	-43.8430	1.13
Compound_1385-P1	48.2290	-36.1998	0.81
Compound_1407-P1	51.3227	-37.9468	0.91
Compound_1469-P1	47.0385	-38.2233	0.84
Compound_1472-P1	42.3044	-31.9142	0.58
Compound_1474-P1	40.1100	-32.1383	0.55
Compound_1606-P1	47.7148	-42.5239	0.98
Compound_1607-P1	50.2809	-37.3254	0.87
Compound_1636-P1	49.2539	-35.4009	0.80
Compound_1651-P1	61.0846	-43.1661	1.23
Compound_1715-P1	49.3389	-37.6323	0.87
Compound_1725-P1	41.8657	-27.8953	0.46
Compound_1754-P1	43.6031	-37.4005	0.76
Compound_1784-P1	52.8471	-40.5714	1.01
Compound_1785-P1	42.1036	-39.6049	0.80
Compound_1786-P1	50.3460	-38.2159	0.90
Compound_1794-P1	38.1559	-33.975	0.57
Compound_1795-P1	46.8089	-36.4657	0.79
Compound_1796-P1	49.9783	-39.3874	0.93
Compound_1797-P1	38.8844	-36.7301	0.66
Compound_1804-P1	55.6323	-37.5051	0.97
Compound_1805-P1	56.8035	-37.4806	0.99
Compound_1873-P1	46.8691	-36.0224	0.78
Compound_1924-P1	29.8855	-44.2065	0.73
Compound_1938-P1	51.0436	-43.4280	1.06
Compound_1939-P1	49.8509	-46.8226	1.14
Compound_1940-P1	48.2612	-41.4959	0.96
Compound_1955-P1	43.1855	-42.5290	0.90
Compound_1962-P1	47.6298	-40.8750	0.93
Compound_1986-P1	41.7985	-46.4207	0.99
Compound_2090-P1	56.3740	-39.1430	1.03

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2147-P1	55.2153	-39.2223	1.01
Compound_2151-P1	48.4837	-37.9815	0.86
Compound_2155-P1	46.0551	-35.8144	0.76
Compound_2274-P1	47.3442	-38.5784	0.86
Compound_2275-P1	42.9640	-36.7927	0.73
Compound_2276-P1	38.7735	-37.1531	0.67
Compound_2279-P1	40.1856	-38.6084	0.74
Compound_2280-P1	47.6738	-39.7615	0.90
Compound_2287-P1	46.6132	-38.1428	0.84
Compound_2288-P1	45.8882	-36.1515	0.76
Compound_2295-P1	56.4527	-40.8720	1.08
Compound_2299-P1	50.3383	-34.7932	0.80
Compound_2300-P1	39.8669	-33.9974	0.60
Compound_2301-P1	55.1002	-38.0583	0.98
Compound_2317-P1	50.8961	-32.3080	0.74
Compound_2384-P1	48.5193	-37.4172	0.85
Compound_2389-P1	43.0082	-35.2004	0.69
Compound_2390-P1	51.8695	-37.0355	0.89
Compound_2391-P1	48.2416	-38.6694	0.88
Compound_2399-P1	51.4178	-39.6501	0.96
Compound_2400-P1	45.8709	-40.5779	0.89
Compound_2409-P1	45.1807	-35.5990	0.74
Compound_2414-P1	45.4891	-34.6046	0.71
Compound_2415-P1	49.7350	-36.3606	0.84
Compound_2421-P1	48.2003	-38.2169	0.86
Compound_2422-P1	49.9433	-39.1626	0.92
Compound_2453-P1	48.0252	-35.7347	0.79
Compound_2695-P1	43.1010	-34.9401	0.68
Compound_2810-P1	55.4221	-44.1011	1.16
Compound_2812-P1	50.1788	-37.5453	0.88
Compound_2813-P1	52.8589	-44.3778	1.12
Compound_2819-P1	56.1674	-39.8642	1.05
Compound_2820-P1	43.9184	-41.1261	0.88
Compound_2821-P1	55.2055	-42.0001	1.09
Compound_2822-P1	62.4376	-40.9447	1.19
Compound_2823-P1	52.9541	-38.0968	0.94
Compound_2824-P1	58.2865	-39.9983	1.09
Compound_2825-P1	54.0658	-38.2005	0.96
Compound_2827-P1	40.4912	-41.4373	0.83
Compound_2828-P1	48.6306	-39.8172	0.92
Compound_2835-P1	62.2363	-44.4676	1.28
Compound_2905-P1	57.6916	-40.3382	1.09
Compound_2985-P1	56.9140	-44.8783	1.21
Compound_4-P20	47.2373	-37.5831	0.83
Compound_8-P20	52.2456	-36.2770	0.88
Compound_18-P20	54.4898	-39.8425	1.02

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_19-P20	39.4755	-34.9926	0.62
Compound_21-P20	48.2209	-35.9581	0.80
Compound_40-P20	49.9410	-38.9077	0.91
Compound_41-P20	54.9698	-35.5985	0.90
Compound_43-P20	49.9768	-38.1576	0.89
Compound_44-P20	58.2847	-37.7453	1.02
Compound_45-P20	45.7981	-36.7932	0.78
Compound_48-P20	42.9312	-38.5150	0.78
Compound_50-P20	47.3909	-37.6691	0.83
Compound_64-P20	55.7161	-32.8364	0.84
Compound_75-P20	47.2395	-36.5848	0.80
Compound_76-P20	43.0483	-38.3223	0.78
Compound_88-P20	39.5176	-31.8613	0.53
Compound_100-P20	50.9323	-43.1232	1.05
Compound_118-P20	53.3136	-42.2320	1.07
Compound_120-P20	47.1924	-36.6702	0.80
Compound_128-P20	50.9761	-39.0669	0.94
Compound_129-P20	55.2128	-39.0490	1.01
Compound_130-P20	47.1924	-37.8846	0.84
Compound_134-P20	46.2483	-38.8362	0.85
Compound_135-P20	37.2670	-37.8499	0.67
Compound_139-P20	56.4995	-43.4741	1.16
Compound_141-P20	61.5949	-39.7043	1.14
Compound_736-P20	47.1548	-38.0939	0.84
Compound_742-P20	53.8893	-36.8363	0.92
Compound_743-P20	54.6919	-40.1230	1.03
Compound_744-P20	54.6562	-43.8956	1.14
Compound_748-P20	52.1262	-37.9993	0.92
Compound_787-P20	48.5125	-38.3731	0.87
Compound_788-P20	38.7202	-39.5314	0.74
Compound_789-P20	50.4095	-40.8466	0.98
Compound_790-P20	42.1697	-37.9980	0.76
Compound_800-P20	48.3315	-41.1332	0.95
Compound_802-P20	49.9569	-43.6114	1.05
Compound_804-P20	61.3303	-44.0072	1.26
Compound_864-P20	48.1587	-39.5842	0.90
Compound_866-P20	25.0719	-38.0390	0.47
Compound_868-P20	48.5298	-40.5310	0.94
Compound_898-P20	39.1607	-32.3247	0.54
Compound_900-P20	38.7676	-43.1134	0.85
Compound_901-P20	37.0507	-30.6419	0.45
Compound_902-P20	37.8428	-33.6363	0.56
Compound_903-P20	42.2485	-35.9948	0.70
Compound_904-P20	32.6209	-39.3472	0.63
Compound_905-P20	40.2484	-37.8880	0.72
Compound_906-P20	56.6482	-35.7666	0.94

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_907-P20	55.3290	-37.7977	0.97
Compound_908-P20	39.2947	-36.6559	0.67
Compound_909-P20	36.3065	-34.1416	0.54
Compound_910-P20	34.7343	-34.0624	0.51
Compound_911-P20	43.7893	-37.4319	0.77
Compound_913-P20	40.5744	-39.5917	0.77
Compound_915-P20	48.0120	-37.6511	0.84
Compound_916-P20	46.2088	-37.8146	0.82
Compound_933-P20	57.0508	-38.7602	1.03
Compound_934-P20	51.5258	-40.7731	0.99
Compound_935-P20	53.5548	-44.9848	1.15
Compound_936-P20	38.7576	-45.9705	0.93
Compound_938-P20	55.1472	-36.0139	0.92
Compound_939-P20	47.4134	-34.5338	0.74
Compound_940-P20	46.4727	-34.5534	0.73
Compound_941-P20	62.9269	-38.8224	1.13
Compound_943-P20	55.1663	-42.3451	1.10
Compound_953-P20	39.8264	-36.6816	0.68
Compound_955-P20	49.7221	-40.5529	0.96
Compound_956-P20	37.2109	-28.7686	0.40
Compound_957-P20	44.1767	-32.9350	0.64
Compound_960-P20	41.4051	-35.7321	0.68
Compound_968-P20	63.2407	-40.7471	1.19
Compound_972-P20	41.1019	-32.9714	0.59
Compound_981-P20	45.2392	-42.8393	0.95
Compound_982-P20	50.0335	-36.3658	0.84
Compound_988-P20	41.5113	-33.0425	0.60
Compound_989-P20	41.7070	-33.0803	0.60
Compound_990-P20	43.5727	-34.6274	0.68
Compound_991-P20	43.1329	-36.8295	0.74
Compound_992-P20	45.2134	-36.3690	0.76
Compound_1005-P20	34.2049	-33.7888	0.50
Compound_1006-P20	43.4794	-37.3573	0.76
Compound_1007-P20	32.7415	-33.6963	0.47
Compound_1008-P20	35.1082	-34.2604	0.53
Compound_1009-P20	51.1905	-35.6619	0.84
Compound_1010-P20	61.0697	-37.2607	1.06
Compound_1012-P20	52.8861	-42.5919	1.07
Compound_1014-P20	56.6650	-38.8221	1.03
Compound_1016-P20	48.0607	-36.4743	0.81
Compound_1039-P20	35.1842	-33.4781	0.51
Compound_1040-P20	42.3744	-36.3041	0.71
Compound_1041-P20	47.8614	-37.0537	0.82
Compound_1042-P20	25.6296	-29.3219	0.22
Compound_1043-P20	33.0862	-34.6831	0.50
Compound_1050-P20	63.7649	-44.0363	1.30

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1086-P20	40.4423	-46.7327	0.98
Compound_1093-P20	51.8696	-37.1846	0.90
Compound_1094-P20	53.7561	-42.8220	1.09
Compound_1095-P20	47.0708	-37.0197	0.81
Compound_1097-P20	51.1108	-42.2384	1.03
Compound_1101-P20	60.6178	-44.8460	1.27
Compound_1103-P20	35.5308	-37.3624	0.62
Compound_1104-P20	35.5043	-33.4754	0.51
Compound_1105-P20	38.5386	-34.7593	0.60
Compound_1106-P20	51.3025	-33.3902	0.78
Compound_1108-P20	49.6975	-37.6050	0.87
Compound_1110-P20	36.7866	-33.6733	0.54
Compound_1111-P20	38.2891	-34.6834	0.59
Compound_1113-P20	42.9141	-40.8382	0.85
Compound_1114-P20	46.0229	-33.8141	0.70
Compound_1123-P20	47.3492	-40.0615	0.90
Compound_1125-P20	42.2151	-40.1559	0.82
Compound_1185-P20	35.4616	-43.8363	0.81
Compound_1187-P20	47.6967	-44.0974	1.03
Compound_1193-P20	59.0395	-43.5560	1.20
Compound_1261-P20	41.6968	-45.9409	0.98
Compound_1262-P20	36.6163	-43.1475	0.81
Compound_1290-P20	47.8853	-40.7867	0.93
Compound_1291-P20	52.2645	-44.2484	1.11
Compound_1311-P20	30.0768	-39.7482	0.60
Compound_1322-P20	45.6856	-35.1867	0.73
Compound_1326-P20	54.4994	-36.8929	0.93
Compound_1327-P20	41.3433	-34.8881	0.65
Compound_1328-P20	47.5949	-34.3418	0.74
Compound_1329-P20	51.0505	-39.3329	0.95
Compound_1334-P20	46.2608	-37.7071	0.82
Compound_1337-P20	35.2979	-33.3913	0.50
Compound_1417-P20	57.6220	-40.8189	1.10
Compound_1418-P20	38.3346	-37.2462	0.67
Compound_1421-P20	44.1931	-39.0777	0.82
Compound_1439-P20	62.7599	-43.7083	1.27
Compound_1455-P20	65.1042	-42.4724	1.28
Compound_1459-P20	62.8124	-42.2647	1.23
Compound_1462-P20	62.0588	-43.1627	1.24
Compound_1464-P20	50.3724	-43.4750	1.05
Compound_1465-P20	64.1062	-43.0453	1.27
Compound_1495-P20	57.0610	-38.8148	1.03
Compound_1501-P20	58.4298	-41.3646	1.13
Compound_1503-P20	47.0229	-40.6064	0.91
Compound_1504-P20	52.6580	-41.0202	1.02
Compound_1506-P20	55.7860	-40.7974	1.07

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1508-P20	55.6971	-41.8094	1.10
Compound_1544-P20	60.2396	-41.4775	1.16
Compound_1662-P20	46.8395	-41.2498	0.93
Compound_1668-P20	36.6564	-47.2668	0.93
Compound_1669-P20	66.2982	-43.7038	1.33
Compound_1670-P20	59.2275	-44.4737	1.23
Compound_1671-P20	61.3081	-42.5833	1.21
Compound_1764-P20	53.3124	-33.6836	0.82
Compound_1766-P20	54.1464	-39.8037	1.01
Compound_1767-P20	61.1432	-38.1590	1.08
Compound_1770-P20	44.3317	-38.9390	0.82
Compound_1776-P20	46.6417	-40.1366	0.89
Compound_1777-P20	36.9439	-41.0954	0.76
Compound_1778-P20	52.1695	-41.5365	1.03
Compound_1782-P20	52.1088	-37.0285	0.90
Compound_1783-P20	40.1960	-41.4939	0.82
Compound_1784-P20	42.8503	-40.0084	0.83
Compound_1789-P20	59.5260	-39.9101	1.11
Compound_1791-P20	47.4126	-40.1249	0.91
Compound_1792-P20	37.2035	-41.8176	0.78
Compound_1795-P20	54.7666	-41.4768	1.07
Compound_1796-P20	51.9281	-44.5724	1.11
Compound_1798-P20	51.1196	-38.7129	0.93
Compound_1799-P20	50.0267	-37.6472	0.88
Compound_1833-P20	55.6795	-43.0723	1.13
Compound_1834-P20	33.1493	-43.8321	0.77
Compound_1835-P20	47.6039	-42.9787	0.99
Compound_1836-P20	40.4522	-38.9515	0.75
Compound_1837-P20	45.2165	-40.1505	0.87
Compound_1846-P20	40.9976	-37.7203	0.73
Compound_1847-P20	55.1244	-37.4314	0.96
Compound_1853-P20	39.1061	-38.9025	0.73
Compound_1854-P20	45.5418	-40.4389	0.88
Compound_1865-P20	52.6835	-39.9931	0.99
Compound_1866-P20	47.6847	-42.1448	0.97
Compound_1869-P20	52.8948	-40.5046	1.01
Compound_1889-P20	64.8486	-43.0385	1.29
Compound_1890-P20	59.4902	-42.2794	1.17
Compound_1899-P20	44.7253	-38.6712	0.82
Compound_1900-P20	47.1703	-40.6245	0.92
Compound_1911-P20	46.7001	-39.7667	0.88
Compound_1912-P20	49.4574	-40.8834	0.96
Compound_1917-P20	46.0342	-39.8914	0.88
Compound_1918-P20	52.0909	-38.6772	0.94
Compound_1919-P20	56.2928	-38.0288	1.00
Compound_1920-P20	53.0737	-38.7453	0.96

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1921-P20	52.4948	-40.6234	1.01
Compound_1925-P20	62.0506	-43.6445	1.26
Compound_1926-P20	53.7117	-40.6719	1.03
Compound_1930-P20	41.3891	-36.3827	0.70
Compound_1937-P20	44.4917	-38.6927	0.81
Compound_1939-P20	46.9295	-37.5647	0.82
Compound_1940-P20	41.4992	-36.6272	0.70
Compound_1941-P20	41.0335	-41.0912	0.83
Compound_1944-P20	61.2642	-39.8674	1.13
Compound_1945-P20	61.5886	-39.4240	1.13
Compound_1950-P20	46.8587	-37.3562	0.82
Compound_1974-P20	54.5598	-41.7479	1.07
Compound_1975-P20	43.2308	-43.0071	0.92
Compound_1976-P20	67.1734	-41.5208	1.28
Compound_1979-P20	38.8333	-39.2272	0.73
Compound_1980-P20	53.9995	-41.5778	1.06
Compound_1988-P20	41.0484	-38.5647	0.75
Compound_1989-P20	63.7526	-40.6108	1.20
Compound_1991-P20	58.8442	-41.9440	1.15
Compound_1995-P20	62.0584	-39.6983	1.14
Compound_1996-P20	52.8185	-40.3744	1.01
Compound_2008-P20	53.0026	-40.2162	1.00
Compound_2009-P20	55.1120	-41.5028	1.08
Compound_2013-P20	42.2243	-41.2654	0.85
Compound_2014-P20	49.0981	-40.5044	0.95
Compound_2024-P20	43.3753	-44.6582	0.97
Compound_2025-P20	48.4383	-41.9249	0.98
Compound_2030-P20	46.0566	-39.2977	0.86
Compound_2031-P20	57.9856	-42.3691	1.15
Compound_2037-P20	48.0534	-40.0889	0.92
Compound_2040-P20	37.3627	-39.6138	0.72
Compound_2041-P20	31.5315	-40.2709	0.64
Compound_2042-P20	38.5870	-37.4337	0.68
Compound_2047-P20	54.9237	-37.3698	0.95
Compound_2048-P20	48.9983	-36.5413	0.83
Compound_2049-P20	60.8614	-38.5957	1.09
Compound_2050-P20	44.7106	-38.4175	0.81
Compound_2051-P20	56.9392	-41.5393	1.11
Compound_2057-P20	47.7987	-38.8330	0.88
Compound_2058-P20	45.3166	-39.9968	0.87
Compound_2059-P20	49.2034	-41.5309	0.98
Compound_2060-P20	42.6464	-41.7792	0.87
Compound_2061-P20	54.2473	-41.4250	1.06
Compound_2063-P20	51.3565	-33.8150	0.79
Compound_2064-P20	59.6600	-36.0208	1.00
Compound_2065-P20	45.8178	-40.3901	0.89

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2066-P20	54.6862	-39.5302	1.01
Compound_2069-P20	34.2227	-39.3566	0.66
Compound_2070-P20	51.8876	-40.0315	0.98
Compound_2071-P20	45.7058	-41.0240	0.90
Compound_2072-P20	36.8466	-40.7402	0.74
Compound_2077-P20	56.7363	-41.2678	1.10
Compound_2078-P20	61.6675	-42.3239	1.21
Compound_2079-P20	50.6615	-44.1706	1.08
Compound_2080-P20	45.7835	-35.5593	0.75
Compound_2081-P20	60.1745	-39.9495	1.12
Compound_2084-P20	44.9425	-39.5686	0.85
Compound_2087-P20	43.0768	-38.5208	0.79
Compound_2092-P20	39.6129	-42.1005	0.83
Compound_2093-P20	38.4286	-41.7239	0.80
Compound_2094-P20	41.7703	-42.3771	0.88
Compound_2095-P20	50.8339	-35.5530	0.83
Compound_2096-P20	51.9070	-37.3471	0.90
Compound_2097-P20	34.2944	-41.7104	0.73
Compound_2099-P20	63.1917	-41.7047	1.22
Compound_2100-P20	51.3382	-41.4486	1.01
Compound_2101-P20	52.6780	-38.9220	0.96
Compound_2105-P20	46.4973	-39.5948	0.88
Compound_2106-P20	54.8318	-40.8760	1.05
Compound_2108-P20	40.9246	-42.4679	0.86
Compound_2112-P20	44.8146	-37.6125	0.79
Compound_2113-P20	47.7471	-41.9587	0.96
Compound_2128-P20	41.5196	-42.4736	0.87
Compound_2130-P20	45.7366	-43.5349	0.98
Compound_2134-P20	49.6503	-42.9900	1.03
Compound_2135-P20	43.4970	-42.9508	0.92
Compound_2138-P20	48.4097	-39.1152	0.89
Compound_2139-P20	49.9014	-40.0395	0.95
Compound_2140-P20	34.3418	-41.4644	0.72
Compound_2141-P20	55.4306	-41.8926	1.09
Compound_2142-P20	47.1080	-40.1773	0.90
Compound_2143-P20	46.0869	-42.0539	0.94
Compound_2149-P20	57.7322	-39.6219	1.07
Compound_2150-P20	44.4876	-42.9204	0.94
Compound_2151-P20	51.7468	-41.3269	1.01
Compound_2154-P20	51.7576	-39.2785	0.96
Compound_2155-P20	46.2823	-40.9488	0.91
Compound_2166-P20	34.8253	-44.1919	0.81
Compound_2168-P20	44.8483	-40.2969	0.87
Compound_2169-P20	42.5350	-41.8737	0.87
Compound_2171-P20	41.5520	-38.7447	0.77
Compound_2172-P20	41.7339	-41.0473	0.84

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2183-P20	56.2545	-41.6955	1.10
Compound_2184-P20	58.0324	-42.8440	1.17
Compound_2185-P20	67.8677	-42.3419	1.32
Compound_2192-P20	61.2011	-38.7465	1.10
Compound_2193-P20	50.5935	-40.8976	0.98
Compound_2200-P20	53.8695	-40.4379	1.03
Compound_2204-P20	52.0480	-39.7767	0.97
Compound_2207-P20	43.7845	-39.7073	0.83
Compound_2208-P20	56.1962	-39.6687	1.04
Compound_2209-P20	42.9411	-40.4515	0.84
Compound_2210-P20	62.7111	-39.8886	1.16
Compound_2214-P20	51.4698	-35.7576	0.85
Compound_2215-P20	47.8897	-38.0605	0.85
Compound_2218-P20	43.1822	-42.1067	0.89
Compound_2219-P20	51.7244	-42.4641	1.05
Compound_2222-P20	42.7810	-42.0953	0.88
Compound_2223-P20	45.8189	-39.6974	0.87
Compound_2230-P20	51.6863	-39.8597	0.97
Compound_2233-P20	51.8606	-36.8298	0.89
Compound_2234-P20	46.2380	-40.4727	0.90
Compound_2235-P20	47.8241	-43.4129	1.01
Compound_2238-P20	42.0623	-40.4964	0.83
Compound_2239-P20	75.3779	-43.4974	1.48
Compound_2255-P20	68.5071	-45.1179	1.41
Compound_2256-P20	41.6689	-44.2828	0.93
Compound_2257-P20	52.6019	-44.2303	1.11
Compound_2264-P20	44.4206	-39.7962	0.85
Compound_2265-P20	50.5031	-42.0209	1.01
Compound_2269-P20	45.6076	-41.3622	0.91
Compound_2270-P20	60.0763	-38.8687	1.09
Compound_2280-P20	28.0228	-45.9083	0.74
Compound_2283-P20	52.6815	-42.0062	1.05
Compound_2284-P20	51.6036	-43.5254	1.08
Compound_2287-P20	50.6985	-40.6441	0.98
Compound_2288-P20	53.0094	-42.9799	1.08
Compound_2302-P20	54.9517	-40.9521	1.06
Compound_2303-P20	56.1798	-43.0132	1.14
Compound_2307-P20	59.0296	-41.2494	1.14
Compound_2308-P20	52.7870	-37.5051	0.92
Compound_2309-P20	51.8253	-38.5068	0.93
Compound_2311-P20	44.4172	-37.5936	0.78
Compound_2312-P20	30.8006	-38.7066	0.58
Compound_2313-P20	45.0748	-38.7811	0.83
Compound_2318-P20	53.5334	-34.4157	0.84
Compound_2319-P20	55.6671	-35.3954	0.91
Compound_2323-P20	37.0303	-40.6920	0.75

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2328-P20	38.2381	-36.5919	0.65
Compound_2330-P20	48.4147	-40.9305	0.95
Compound_2331-P20	43.1801	-40.2455	0.84
Compound_2336-P20	32.2742	-35.4194	0.51
Compound_2337-P20	46.1068	-36.4985	0.78
Compound_2339-P20	54.8363	-41.9866	1.09
Compound_2340-P20	58.0980	-39.6967	1.08
Compound_2343-P20	58.5008	-40.9924	1.12
Compound_2345-P20	49.0782	-36.5190	0.83
Compound_2346-P20	38.7279	-37.6272	0.69
Compound_2363-P20	42.4406	-40.8809	0.84
Compound_2365-P20	48.5773	-41.2990	0.96
Compound_2368-P20	52.3573	-44.6349	1.12
Compound_2370-P20	37.7360	-38.4379	0.69
Compound_2371-P20	60.3305	-42.3751	1.19
Compound_2376-P20	41.9904	-39.4740	0.79
Compound_2378-P20	37.4372	-41.0037	0.76
Compound_2388-P20	52.5724	-40.4651	1.00
Compound_2391-P20	49.9655	-44.2550	1.07
Compound_2396-P20	46.3500	-40.7132	0.91
Compound_2405-P20	46.5935	-38.2597	0.84
Compound_2406-P20	49.8264	-37.6098	0.87
Compound_2409-P20	37.3003	-44.1776	0.85
Compound_2415-P20	46.1044	-38.9846	0.85
Compound_2416-P20	33.4095	-41.6022	0.71
Compound_2417-P20	44.4062	-35.7987	0.73
Compound_2418-P20	50.4811	-38.6211	0.91
Compound_2420-P20	47.1613	-41.4818	0.94
Compound_2421-P20	46.8811	-41.8984	0.95
Compound_2422-P20	46.6664	-41.9250	0.95
Compound_2425-P20	46.8667	-41.2638	0.93
Compound_2426-P20	42.1588	-43.3449	0.91
Compound_2427-P20	36.3856	-42.9205	0.80
Compound_2428-P20	37.2468	-42.0404	0.79
Compound_2434-P20	56.8162	-44.1448	1.18
Compound_2435-P20	56.0653	-43.7206	1.16
Compound_2436-P20	42.5377	-38.7110	0.78
Compound_2437-P20	53.1946	-39.4543	0.98
Compound_2438-P20	55.1826	-42.4213	1.10
Compound_2439-P20	50.3089	-43.2028	1.04
Compound_2441-P20	49.7795	-37.2383	0.86
Compound_2442-P20	32.2811	-39.5798	0.63
Compound_2444-P20	42.8857	-42.0334	0.88
Compound_2446-P20	45.6453	-37.8555	0.81
Compound_2447-P20	45.6206	-38.7284	0.84
Compound_2449-P20	42.3145	-42.3208	0.88

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2450-P20	50.5618	-44.4376	1.08
Compound_2451-P20	46.8829	-42.5238	0.97
Compound_2453-P20	60.3772	-42.3802	1.19
Compound_2454-P20	52.1756	-43.6856	1.09
Compound_2458-P20	48.5926	-39.5652	0.91
Compound_2459-P20	48.9583	-41.1455	0.96
Compound_2483-P20	32.3273	-46.7898	0.84
Compound_2484-P20	39.1000	-46.9158	0.96
Compound_2486-P20	38.6578	-42.4338	0.82
Compound_2487-P20	46.9934	-44.0738	1.01
Compound_2489-P20	41.4154	-44.3254	0.93
Compound_2490-P20	48.3376	-44.6652	1.05
Compound_2493-P20	62.6533	-40.6192	1.18
Compound_2494-P20	55.7760	-41.9151	1.10
Compound_2498-P20	50.8971	-41.7902	1.01
Compound_2499-P20	53.8329	-43.1124	1.10
Compound_2510-P20	32.7193	-40.7777	0.68
Compound_2526-P20	60.6222	-40.8084	1.15
Compound_2527-P20	45.0699	-42.8887	0.95
Compound_2529-P20	50.0703	-41.2802	0.98
Compound_2530-P20	61.9276	-42.1644	1.21
Compound_2531-P20	47.8621	-40.6083	0.93
Compound_2533-P20	42.0606	-40.5928	0.83
Compound_2534-P20	55.5328	-41.2223	1.08
Compound_2535-P20	54.3247	-42.1969	1.08
Compound_2542-P20	60.2846	-42.0712	1.18
Compound_2543-P20	51.5187	-37.2278	0.89
Compound_2544-P20	60.9812	-38.3942	1.09
Compound_2546-P20	36.7415	-40.3610	0.73
Compound_2550-P20	51.1993	-39.9930	0.97
Compound_2551-P20	39.5081	-39.2563	0.75
Compound_2557-P20	37.7314	-35.8314	0.62
Compound_2558-P20	47.7286	-37.1571	0.83
Compound_2564-P20	34.8365	-35.2032	0.55
Compound_2565-P20	30.8959	-36.4412	0.52
Compound_2566-P20	41.6868	-39.2353	0.78
Compound_2569-P20	49.4959	-38.5332	0.90
Compound_2571-P20	34.3131	-44.4463	0.81
Compound_2572-P20	63.7537	-38.2888	1.13
Compound_2573-P20	56.0141	-40.1590	1.05
Compound_2590-P20	35.4080	-41.5822	0.74
Compound_2591-P20	53.2701	-40.6822	1.02
Compound_2599-P20	54.2608	-38.4120	0.97
Compound_2600-P20	49.2665	-40.3457	0.94
Compound_2602-P20	57.0597	-42.4615	1.14
Compound_2603-P20	48.0228	-41.8076	0.97

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2613-P20	60.1746	-43.5899	1.22
Compound_2616-P20	47.9872	-44.9737	1.06
Compound_2631-P20	49.5947	-45.0039	1.08
Compound_2636-P20	53.9330	-40.5066	1.03
Compound_2640-P20	51.2475	-40.3634	0.98
Compound_2643-P20	52.9772	-40.6465	1.02
Compound_2644-P20	39.2803	-41.8984	0.82
Compound_2649-P20	48.1839	-35.0458	0.77
Compound_2654-P20	24.9414	-36.9540	0.43
Compound_2655-P20	51.7612	-39.0107	0.95
Compound_2657-P20	47.5894	-40.6997	0.93
Compound_2658-P20	47.8391	-39.9446	0.91
Compound_2659-P20	58.7360	-45.4741	1.25
Compound_2660-P20	62.0732	-45.7128	1.32
Compound_2661-P20	41.3586	-42.2060	0.86
Compound_2672-P20	29.3482	-45.6107	0.76
Compound_2675-P20	57.2938	-39.9112	1.07
Compound_2676-P20	51.1162	-41.1858	1.00
Compound_2678-P20	48.2153	-43.8341	1.03
Compound_2683-P20	46.7592	-40.2224	0.90
Compound_2684-P20	30.5087	-43.1504	0.71
Compound_2697-P20	47.0001	-43.1345	0.99
Compound_2701-P20	53.3451	-41.6223	1.05
Compound_2702-P20	37.9133	-42.0519	0.80
Compound_2717-P20	57.0880	-41.1643	1.10
Compound_2725-P20	59.0604	-45.7349	1.27
Compound_2730-P20	54.8740	-36.9105	0.94
Compound_2731-P20	53.2472	-38.0170	0.94
Compound_2732-P20	33.0719	-39.8222	0.65
Compound_2740-P20	38.6503	-35.4302	0.62
Compound_2741-P20	39.8412	-39.5159	0.76
Compound_2744-P20	49.7199	-34.7759	0.79
Compound_2745-P20	50.4153	-34.6399	0.80
Compound_2746-P20	41.0427	-41.5217	0.84
Compound_2749-P20	55.8703	-38.8723	1.01
Compound_2750-P20	48.0936	-35.4785	0.78
Compound_2751-P20	49.3530	-38.5381	0.89
Compound_2763-P20	40.0523	-42.3867	0.85
Compound_2764-P20	49.2972	-36.0784	0.82
Compound_2771-P20	55.8050	-35.2836	0.91
Compound_2772-P20	43.1117	-37.0858	0.74
Compound_2773-P20	47.9112	-40.0828	0.91
Compound_2782-P20	39.3098	-41.1261	0.80
Compound_2784-P20	44.3741	-42.0452	0.91
Compound_2795-P20	45.3835	-37.0950	0.78
Compound_2796-P20	68.1320	-40.8568	1.28

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2798-P20	60.5011	-39.4322	1.11
Compound_2800-P20	54.1514	-42.9674	1.10
Compound_2803-P20	44.5115	-38.1391	0.80
Compound_2804-P20	44.1127	-41.4173	0.89
Compound_2811-P20	40.5254	-43.5847	0.89
Compound_2812-P20	38.6924	-40.4369	0.77
Compound_2816-P20	56.7695	-43.7863	1.17
Compound_2818-P20	46.1659	-37.9595	0.82
Compound_2822-P20	60.8497	-38.7500	1.09
Compound_2824-P20	54.4909	-39.9321	1.02
Compound_2832-P20	38.3162	-39.6510	0.74
Compound_2838-P20	48.8312	-37.5309	0.85
Compound_2841-P20	51.6045	-37.6873	0.91
Compound_2845-P20	47.7608	-41.2271	0.94
Compound_2863-P20	56.9436	-42.1684	1.13
Compound_2866-P20	33.8354	-45.1391	0.82
Compound_2867-P20	47.9376	-40.6511	0.93
Compound_2869-P20	54.2137	-39.4403	1.00
Compound_2871-P20	55.1501	-44.7662	1.17
Compound_2873-P20	66.3993	-36.5893	1.13
Compound_2874-P20	55.3653	-38.9314	1.01
Compound_2894-P20	59.5290	-39.8102	1.10
Compound_2895-P20	37.2975	-44.3245	0.86
Compound_2906-P20	50.8415	-46.1295	1.14
Compound_2913-P20	44.7081	-43.4897	0.96
Compound_2914-P20	52.2120	-43.9610	1.10
Compound_2917-P20	60.5291	-39.0770	1.10
Compound_2926-P20	56.8378	-42.0827	1.12
Compound_2930-P20	45.9377	-43.0360	0.97
Compound_2931-P20	59.8000	-41.5908	1.16
Compound_2934-P20	42.0213	-42.5522	0.88
Compound_2935-P20	43.2191	-41.8190	0.88
Compound_2936-P20	59.6786	-44.9079	1.25
Compound_2937-P20	56.9473	-37.6587	1.00
Compound_2938-P20	60.6126	-40.0444	1.13
Compound_2943-P20	43.6097	-38.6411	0.80
Compound_2946-P20	48.7175	-42.7870	1.01
Compound_2947-P20	44.4019	-43.0146	0.94
Compound_2949-P20	44.9274	-41.2155	0.90
Compound_2963-P20	51.5463	-42.7902	1.05
Compound_2965-P20	42.4670	-41.4828	0.86
Compound_2970-P20	38.8775	-45.5296	0.92
Compound_2974-P20	63.0047	-39.3148	1.15
Compound_2975-P20	48.4616	-42.1787	0.98
Compound_2979-P20	51.7337	-40.0263	0.98
Compound_2980-P20	45.0788	-42.6923	0.94

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2995-P20	53.4670	-42.1637	1.07
Compound_2996-P20	45.9670	-43.9964	0.99
Compound_2998-P20	37.1226	-43.0113	0.81
Compound_9-P2	55.2653	-44.7582	1.17
Compound_22-P2	41.2397	-43.5645	0.90
Compound_24-P2	46.1508	-45.4218	1.04
Compound_110-P2	53.1964	-34.7250	0.85
Compound_112-P2	47.4644	-42.2660	0.97
Compound_113-P2	46.2341	-41.0134	0.91
Compound_118-P2	46.8434	-42.8512	0.98
Compound_120-P2	38.5798	-35.1944	0.61
Compound_122-P2	49.3046	-39.0021	0.91
Compound_123-P2	41.4380	-37.9708	0.74
Compound_129-P2	41.7378	-36.7641	0.71
Compound_131-P2	37.3168	-41.9137	0.79
Compound_142-P2	53.9650	-32.3761	0.79
Compound_143-P2	51.6997	-33.4637	0.79
Compound_147-P2	38.5198	-27.9737	0.40
Compound_150-P2	58.9588	-37.6252	1.03
Compound_156-P2	45.3552	-39.1067	0.84
Compound_160-P2	48.2470	-33.8176	0.74
Compound_166-P2	56.4127	-34.5775	0.90
Compound_209-P2	50.1403	-39.1654	0.92
Compound_210-P2	50.0800	-38.3564	0.90
Compound_230-P2	45.2953	-37.5568	0.80
Compound_234-P2	60.1448	-41.7892	1.17
Compound_328-P2	60.4353	-40.9585	1.15
Compound_333-P2	47.1658	-34.5049	0.74
Compound_341-P2	55.3774	-38.0279	0.98
Compound_430-P2	44.2333	-29.6579	0.55
Compound_463-P2	47.2158	-39.6697	0.89
Compound_466-P2	30.5912	-39.0835	0.59
Compound_470-P2	51.0755	-43.9973	1.08
Compound_473-P2	51.8213	-44.3024	1.10
Compound_475-P2	59.5938	-41.9150	1.17
Compound_476-P2	49.9768	-40.3047	0.95
Compound_478-P2	56.1760	-44.1138	1.17
Compound_497-P2	42.2531	-43.6377	0.92
Compound_498-P2	55.2655	-40.2258	1.04
Compound_503-P2	60.7608	-42.9657	1.22
Compound_511-P2	65.3407	-42.5305	1.28
Compound_514-P2	52.1467	-40.7620	1.01
Compound_515-P2	46.2021	-35.7633	0.76
Compound_548-P2	63.5626	-42.0082	1.24
Compound_589-P2	53.9779	-40.7805	1.04
Compound_612-P2	36.5516	-50.9958	1.04

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_619-P2	66.4298	-46.1925	1.41
Compound_622-P2	63.1300	-37.2779	1.09
Compound_723-P2	63.2842	-42.5811	1.25
Compound_745-P2	37.1222	-42.7961	0.81
Compound_747-P2	47.4629	-42.7842	0.98
Compound_764-P2	45.6719	-44.0303	0.99
Compound_776-P2	64.6085	-43.2070	1.29
Compound_846-P2	45.3191	-44.6434	1.00
Compound_947-P2	59.4647	-44.0085	1.22
Compound_948-P2	51.7558	-42.3395	1.04
Compound_949-P2	44.4432	-40.3243	0.86
Compound_952-P2	38.5339	-46.3370	0.94
Compound_1020-P2	56.5300	-45.1857	1.21
Compound_1023-P2	54.3292	-44.9802	1.16
Compound_1072-P2	41.8648	-39.5667	0.80
Compound_1073-P2	49.8048	-39.5665	0.93
Compound_1089-P2	37.7552	-40.7328	0.76
Compound_1091-P2	36.3674	-35.0488	0.57
Compound_1092-P2	54.8765	-40.1982	1.04
Compound_1093-P2	44.5843	-43.4346	0.95
Compound_1103-P2	45.8569	-39.9308	0.87
Compound_1104-P2	36.1701	-40.4850	0.73
Compound_1117-P2	53.5569	-41.5691	1.05
Compound_1119-P2	53.1302	-45.0865	1.15
Compound_1125-P2	41.9972	-34.3285	0.65
Compound_1126-P2	36.5210	-32.4523	0.50
Compound_1129-P2	32.5827	-44.0136	0.77
Compound_1130-P2	55.2567	-39.8426	1.03
Compound_1131-P2	35.0896	-41.4862	0.74
Compound_1151-P2	55.4872	-42.3484	1.11
Compound_1153-P2	38.6614	-37.3289	0.68
Compound_1164-P2	48.7131	-36.7129	0.83
Compound_1165-P2	42.6935	-34.0675	0.65
Compound_1166-P2	42.3792	-35.6382	0.69
Compound_1173-P2	43.9900	-38.8769	0.81
Compound_1182-P2	38.1026	-34.6323	0.59
Compound_1244-P2	55.4161	-43.6182	1.14
Compound_1246-P2	58.3536	-49.1160	1.35
Compound_1394-P2	44.4020	-40.7070	0.87
Compound_1396-P2	51.5752	-38.9659	0.94
Compound_1397-P2	40.8691	-40.7717	0.81
Compound_1398-P2	37.8556	-30.9075	0.48
Compound_1399-P2	39.5882	-37.9256	0.71
Compound_1400-P2	54.7730	-40.9177	1.05
Compound_1409-P2	48.8841	-35.5741	0.80
Compound_1435-P2	43.0699	-40.4570	0.84

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1447-P2	48.8540	-31.4717	0.68
Compound_1455-P2	44.6498	-31.2212	0.60
Compound_1546-P2	47.9023	-41.6371	0.96
Compound_1547-P2	69.8251	-45.5243	1.44
Compound_1606-P2	44.3452	-44.3909	0.98
Compound_1809-P2	62.9775	-46.6216	1.36
Compound_1828-P2	47.4243	-44.3539	1.03
Compound_1832-P2	46.0262	-39.9295	0.88
Compound_1842-P2	51.2745	-42.8205	1.05
Compound_1851-P2	46.7041	-34.3643	0.73
Compound_1855-P2	52.2443	-39.3671	0.97
Compound_1857-P2	46.5851	-39.0246	0.86
Compound_1863-P2	49.5324	-41.1981	0.97
Compound_1978-P2	40.8616	-38.5986	0.75
Compound_2028-P2	39.6926	-39.1667	0.75
Compound_2174-P2	41.2540	-40.9200	0.82
Compound_2175-P2	49.9404	-39.4581	0.93
Compound_2177-P2	45.3667	-45.0981	1.02
Compound_2182-P2	52.4605	-44.0678	1.11
Compound_2193-P2	48.8114	-42.9310	1.01
Compound_2194-P2	56.5924	-39.7800	1.05
Compound_2244-P2	64.1343	-44.3433	1.31
Compound_2263-P2	52.0155	-39.2207	0.96
Compound_2264-P2	52.7445	-43.7705	1.10
Compound_2353-P2	51.5283	-38.1098	0.92
Compound_2368-P2	65.7495	-46.0764	1.39
Compound_2371-P2	67.2480	-46.9933	1.44
Compound_2372-P2	48.5103	-43.0831	1.01
Compound_2374-P2	43.0768	-44.3294	0.95
Compound_2375-P2	47.4112	-48.1953	1.14
Compound_2391-P2	41.7257	-47.4531	1.02
Compound_2392-P2	50.5350	-47.3056	1.17
Compound_2394-P2	37.9301	-47.1841	0.95
Compound_2411-P2	52.9866	-41.2910	1.03
Compound_2412-P2	52.5620	-46.1588	1.17
Compound_2414-P2	37.0041	-52.2249	1.08
Compound_2448-P2	38.3916	-42.3894	0.82
Compound_2517-P2	50.7271	-41.5953	1.01
Compound_2522-P2	48.8318	-44.9158	1.07
Compound_2531-P2	52.2662	-35.6993	0.86
Compound_2532-P2	58.8413	-44.4437	1.23
Compound_2533-P2	58.0308	-44.3953	1.21
Compound_2616-P2	45.7688	-39.3945	0.86
Compound_2721-P2	55.1269	-43.0005	1.12
Compound_2723-P2	43.5502	-42.5240	0.91
Compound_2786-P2	42.8761	-39.8269	0.82

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2787-P2	46.3103	-40.8670	0.91
Compound_2788-P2	46.7562	-36.1581	0.78
Compound_2789-P2	57.3871	-41.5185	1.12
Compound_2791-P2	50.2076	-36.5387	0.85
Compound_2792-P2	61.4160	-49.5119	1.42
Compound_2820-P2	48.1275	-41.5088	0.96
Compound_2821-P2	51.3970	-43.8518	1.08
Compound_2822-P2	44.5361	-32.4341	0.63
Compound_2823-P2	62.4160	-41.2394	1.19
Compound_2852-P2	45.4143	-31.8115	0.63
Compound_2854-P2	47.4291	-34.7189	0.75
Compound_2856-P2	39.6198	-32.4772	0.55
Compound_2861-P2	50.1237	-43.2838	1.04
Compound_2867-P2	43.5306	-35.5902	0.71
Compound_2868-P2	52.0374	-36.6872	0.89
Compound_2869-P2	51.0459	-39.4449	0.95
Compound_2870-P2	47.2751	-38.6886	0.86
Compound_2907-P2	44.7120	-43.5481	0.96
Compound_2925-P2	30.3815	-27.0788	0.24
Compound_2926-P2	43.0538	-37.5758	0.76
Compound_2941-P2	41.9792	-31.9010	0.58
Compound_2942-P2	52.3818	-32.6381	0.77
Compound_2949-P2	25.7030	-25.1083	0.10
Compound_2950-P2	46.2701	-25.3758	0.46
Compound_2951-P2	30.7584	-27.8851	0.27
Compound_2952-P2	34.7939	-27.6349	0.33
Compound_2953-P2	38.7039	-27.4849	0.39
Compound_2954-P2	35.3172	-26.5562	0.31
Compound_2955-P2	35.5159	-29.1544	0.39
Compound_2956-P2	31.4698	-28.3726	0.29
Compound_2957-P2	36.2478	-30.8706	0.45
Compound_3-P4	64.8396	-41.8643	1.25
Compound_34-P4	35.1408	-38.5929	0.65
Compound_43-P4	44.8774	-35.3229	0.72
Compound_44-P4	42.8558	-34.4959	0.67
Compound_45-P4	52.5763	-36.5612	0.89
Compound_46-P4	47.8773	-36.7727	0.82
Compound_84-P4	43.3467	-37.6203	0.76
Compound_86-P4	49.4063	-39.2242	0.91
Compound_90-P4	47.3623	-39.7788	0.90
Compound_391-P4	55.9498	-44.1598	1.17
Compound_392-P4	35.7724	-43.2654	0.80
Compound_393-P4	51.7638	-47.8267	1.20
Compound_396-P4	52.2459	-44.7974	1.12
Compound_397-P4	38.2379	-44.3156	0.87
Compound_398-P4	59.8581	-46.1690	1.29

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_405-P4	48.7911	-40.9687	0.95
Compound_424-P4	43.2388	-38.7308	0.79
Compound_427-P4	52.1795	-45.2714	1.14
Compound_455-P4	42.3026	-41.4418	0.86
Compound_457-P4	42.1628	-38.8949	0.78
Compound_514-P4	50.7049	-35.6579	0.83
Compound_529-P4	39.6904	-32.3732	0.55
Compound_621-P4	42.5315	-47.7133	1.04
Compound_623-P4	36.1954	-42.3638	0.78
Compound_628-P4	54.0081	-47.5665	1.23
Compound_676-P4	50.5759	-42.7368	1.04
Compound_677-P4	50.2263	-43.7986	1.06
Compound_698-P4	56.9422	-45.4387	1.22
Compound_699-P4	35.2207	-40.5453	0.71
Compound_708-P4	37.9417	-34.3708	0.58
Compound_721-P4	49.9226	-40.9443	0.97
Compound_725-P4	42.7958	-43.1067	0.91
Compound_726-P4	48.1453	-42.9922	1.00
Compound_728-P4	56.5104	-44.1085	1.18
Compound_957-P4	44.9744	-40.2148	0.87
Compound_962-P4	57.3223	-45.4819	1.23
Compound_991-P4	51.5424	-44.4777	1.10
Compound_992-P4	49.8424	-42.8239	1.03
Compound_993-P4	40.4780	-45.2554	0.94
Compound_994-P4	55.9599	-37.3483	0.97
Compound_995-P4	46.4700	-43.1942	0.98
Compound_999-P4	61.1665	-40.6328	1.15
Compound_1160-P4	44.5154	-42.0208	0.91
Compound_1161-P4	49.3359	-43.9000	1.05
Compound_1162-P4	40.9367	-43.3998	0.89
Compound_1163-P4	39.7497	-50.0681	1.06
Compound_1166-P4	48.7200	-42.8007	1.01
Compound_1167-P4	52.4006	-38.2477	0.94
Compound_1169-P4	48.6625	-46.8934	1.12
Compound_1176-P4	55.8167	-42.7526	1.13
Compound_1177-P4	38.1200	-38.0263	0.69
Compound_1181-P4	53.5731	-42.7639	1.09
Compound_1183-P4	46.7899	-41.5695	0.94
Compound_1184-P4	57.9176	-43.4204	1.18
Compound_1222-P4	47.0546	-34.5120	0.74
Compound_1223-P4	45.7119	-39.7514	0.87
Compound_1229-P4	58.0825	-40.0292	1.08
Compound_1230-P4	38.4174	-35.8689	0.63
Compound_1242-P4	54.6107	-41.2791	1.06
Compound_1243-P4	49.7547	-39.9635	0.94
Compound_1245-P4	53.7566	-38.3779	0.96

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1247-P4	46.6590	-41.6424	0.94
Compound_1251-P4	52.9296	-43.5040	1.10
Compound_1253-P4	55.0565	-40.2190	1.04
Compound_1255-P4	70.9198	-43.0144	1.39
Compound_1260-P4	50.7472	-40.4363	0.97
Compound_1261-P4	46.1446	-41.6075	0.93
Compound_1263-P4	60.8911	-46.5662	1.32
Compound_1278-P4	54.7742	-40.5639	1.04
Compound_1279-P4	49.5799	-39.2958	0.92
Compound_1280-P4	55.6884	-41.0141	1.07
Compound_1281-P4	58.5202	-38.2166	1.04
Compound_1282-P4	52.5101	-41.5027	1.03
Compound_1283-P4	50.0610	-30.8856	0.68
Compound_1288-P4	40.1303	-42.3511	0.85
Compound_1290-P4	46.3151	-39.7881	0.88
Compound_1291-P4	56.7440	-43.5972	1.17
Compound_1292-P4	54.7256	-44.7010	1.16
Compound_1293-P4	57.1668	-47.2251	1.28
Compound_1296-P4	42.9606	-33.6094	0.64
Compound_1299-P4	53.6746	-37.4307	0.93
Compound_1300-P4	52.4333	-41.6470	1.04
Compound_1303-P4	68.1046	-40.2834	1.26
Compound_1304-P4	41.9075	-40.2285	0.82
Compound_1305-P4	54.2735	-37.0532	0.93
Compound_1306-P4	51.3084	-40.4878	0.98
Compound_1307-P4	47.5185	-31.9356	0.67
Compound_1308-P4	49.4747	-30.3534	0.66
Compound_1312-P4	47.0433	-42.2575	0.96
Compound_1313-P4	38.7049	-43.9013	0.87
Compound_1315-P4	58.7582	-41.1243	1.13
Compound_1318-P4	56.0773	-42.6518	1.13
Compound_1320-P4	72.5038	-46.3616	1.51
Compound_1321-P4	66.3441	-46.1531	1.40
Compound_1322-P4	45.0911	-41.1785	0.90
Compound_1324-P4	49.3214	-32.2603	0.71
Compound_1326-P4	48.6279	-36.6961	0.83
Compound_1327-P4	51.0655	-41.7116	1.01
Compound_1328-P4	55.7923	-37.7429	0.98
Compound_1329-P4	59.9370	-40.4538	1.13
Compound_1332-P4	64.4020	-41.1249	1.22
Compound_1333-P4	43.2280	-40.1171	0.83
Compound_1334-P4	46.3811	-43.0096	0.97
Compound_1335-P4	44.1123	-38.3881	0.80
Compound_1336-P4	48.2341	-33.7950	0.74
Compound_1337-P4	46.8008	-30.8633	0.63
Compound_1342-P4	50.7846	-41.6918	1.01

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1343-P4	53.1073	-42.8981	1.08
Compound_1345-P4	49.9691	-47.7974	1.17
Compound_1347-P4	37.4611	-38.5327	0.69
Compound_1348-P4	45.9722	-37.6753	0.81
Compound_1349-P4	45.2244	-39.1792	0.84
Compound_1353-P4	44.7903	-39.9238	0.86
Compound_1354-P4	37.1166	-41.4137	0.77
Compound_1355-P4	55.1301	-35.7098	0.91
Compound_1356-P4	45.7881	-41.7557	0.93
Compound_1357-P4	43.5694	-38.1443	0.78
Compound_1359-P4	39.0405	-33.8627	0.58
Compound_1360-P4	44.6897	-32.4048	0.64
Compound_1368-P4	42.3879	-41.9675	0.87
Compound_1370-P4	43.5283	-38.9883	0.81
Compound_1372-P4	53.5965	-41.8191	1.06
Compound_1373-P4	42.1747	-43.2747	0.91
Compound_1375-P4	53.1847	-33.4957	0.81
Compound_1378-P4	46.8351	-37.7155	0.83
Compound_1379-P4	38.7476	-39.1844	0.73
Compound_1450-P4	49.1950	-41.4019	0.97
Compound_1451-P4	33.9352	-40.1768	0.68
Compound_1452-P4	61.3817	-40.5301	1.16
Compound_1453-P4	35.9869	-42.6054	0.78
Compound_1454-P4	50.5686	-35.4567	0.82
Compound_1457-P4	53.2844	-43.9944	1.12
Compound_1461-P4	48.3152	-43.4954	1.02
Compound_1462-P4	55.1740	-48.1113	1.27
Compound_1464-P4	47.5909	-42.4415	0.98
Compound_1465-P4	38.6454	-40.7794	0.78
Compound_1468-P4	52.5291	-42.0476	1.05
Compound_1469-P4	45.1014	-43.3616	0.96
Compound_1470-P4	48.3787	-40.7274	0.94
Compound_1471-P4	53.6530	-44.1429	1.13
Compound_1472-P4	51.3192	-38.3767	0.92
Compound_1473-P4	46.4168	-37.4980	0.81
Compound_1477-P4	40.4579	-44.2904	0.91
Compound_1479-P4	59.0527	-44.3485	1.23
Compound_1481-P4	42.7480	-37.2267	0.74
Compound_1483-P4	60.3982	-42.2795	1.19
Compound_1484-P4	39.2777	-43.4469	0.86
Compound_1553-P4	46.8519	-40.2420	0.90
Compound_1555-P4	52.1259	-44.6131	1.12
Compound_1556-P4	49.9801	-42.2106	1.01
Compound_1558-P4	43.5489	-44.1419	0.96
Compound_1559-P4	54.8696	-43.6420	1.13
Compound_1560-P4	53.1644	-45.9706	1.17

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1562-P4	57.5095	-43.5080	1.18
Compound_1563-P4	50.1186	-44.7398	1.09
Compound_1565-P4	54.0870	-40.4273	1.03
Compound_1566-P4	42.5727	-40.9659	0.85
Compound_1567-P4	60.8653	-43.1023	1.22
Compound_1568-P4	57.9583	-43.8787	1.19
Compound_1570-P4	61.1500	-44.0336	1.25
Compound_1571-P4	62.0724	-45.4361	1.31
Compound_1572-P4	48.1641	-45.2930	1.07
Compound_1573-P4	39.2575	-40.3922	0.78
Compound_1574-P4	49.7983	-40.4956	0.96
Compound_1575-P4	55.6365	-44.6076	1.18
Compound_1576-P4	74.0539	-47.0347	1.56
Compound_1577-P4	53.8425	-45.5121	1.17
Compound_1579-P4	38.5607	-42.6510	0.83
Compound_1580-P4	52.9020	-46.2713	1.18
Compound_1583-P4	50.1295	-42.5809	1.02
Compound_1586-P4	51.0613	-39.1192	0.94
Compound_1587-P4	68.4840	-42.3231	1.33
Compound_1590-P4	56.6619	-44.7564	1.20
Compound_1594-P4	47.4786	-44.4655	1.03
Compound_1595-P4	52.8482	-45.2243	1.15
Compound_1597-P4	59.2344	-46.6137	1.30
Compound_1598-P4	51.9690	-46.3821	1.17
Compound_1600-P4	54.8253	-45.8941	1.20
Compound_1603-P4	43.3834	-44.1781	0.96
Compound_1607-P4	39.6197	-39.0822	0.74
Compound_1608-P4	47.4663	-40.0037	0.90
Compound_1613-P4	54.2144	-38.5349	0.98
Compound_1614-P4	47.4265	-38.6852	0.86
Compound_1621-P4	50.3469	-43.0010	1.04
Compound_1622-P4	50.9257	-42.0635	1.02
Compound_1682-P4	50.8647	-39.8069	0.96
Compound_1683-P4	40.6868	-38.6724	0.75
Compound_1684-P4	63.6591	-39.0154	1.15
Compound_1685-P4	46.6192	-38.9345	0.86
Compound_1686-P4	54.4201	-41.0134	1.05
Compound_1687-P4	47.0157	-38.6472	0.86
Compound_1691-P4	50.1081	-39.6955	0.94
Compound_1717-P4	55.7154	-39.6172	1.03
Compound_1722-P4	49.4059	-37.7106	0.87
Compound_1723-P4	48.6438	-37.7271	0.86
Compound_1724-P4	33.6288	-34.8455	0.52
Compound_1725-P4	44.6506	-32.2867	0.63
Compound_1796-P4	40.2086	-42.5825	0.85
Compound_1797-P4	45.8542	-40.1611	0.88

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1798-P4	48.7802	-38.8192	0.89
Compound_1799-P4	44.3908	-40.0405	0.85
Compound_1800-P4	43.1898	-38.2718	0.78
Compound_1801-P4	37.8841	-38.0866	0.68
Compound_1802-P4	44.2290	-39.4203	0.83
Compound_1803-P4	33.3616	-37.9477	0.60
Compound_1806-P4	50.5455	-42.8202	1.04
Compound_1826-P4	48.7858	-42.7723	1.01
Compound_1831-P4	45.2964	-39.2994	0.85
Compound_1832-P4	42.9362	-35.7109	0.70
Compound_1833-P4	44.0457	-37.2159	0.76
Compound_1834-P4	33.7373	-38.9214	0.64
Compound_1835-P4	40.6549	-38.7868	0.75
Compound_1836-P4	39.1013	-34.3265	0.60
Compound_1837-P4	46.2963	-35.8333	0.76
Compound_1838-P4	40.9736	-38.0857	0.74
Compound_1841-P4	40.1099	-36.3618	0.67
Compound_1844-P4	33.5500	-35.0059	0.52
Compound_1845-P4	41.3507	-37.3205	0.72
Compound_1846-P4	50.1780	-42.9483	1.04
Compound_1883-P4	53.7150	-38.7923	0.97
Compound_1886-P4	61.3802	-40.2562	1.15
Compound_1898-P4	61.8682	-38.1925	1.10
Compound_1899-P4	53.5348	-38.8137	0.97
Compound_1900-P4	53.1504	-42.0040	1.06
Compound_2003-P4	42.7755	-40.1476	0.83
Compound_2004-P4	35.2888	-38.7606	0.66
Compound_2009-P4	45.5491	-43.4474	0.97
Compound_2011-P4	45.4722	-48.1904	1.11
Compound_2014-P4	43.3663	-49.7047	1.12
Compound_2016-P4	39.5825	-45.0216	0.91
Compound_2022-P4	42.6503	-40.8646	0.85
Compound_2023-P4	42.0405	-44.2359	0.93
Compound_2024-P4	40.9123	-45.1518	0.94
Compound_2025-P4	46.3980	-47.6410	1.11
Compound_2028-P4	50.7817	-46.2146	1.14
Compound_2030-P4	47.9754	-49.0606	1.17
Compound_2033-P4	35.8685	-50.6124	1.01
Compound_2080-P4	54.6273	-39.3000	1.00
Compound_2081-P4	52.0896	-42.1022	1.04
Compound_2089-P4	43.3842	-44.4139	0.96
Compound_2091-P4	66.3032	-47.3571	1.44
Compound_2117-P4	54.0288	-43.4021	1.11
Compound_2118-P4	48.3983	-42.4276	0.99
Compound_2123-P4	64.1809	-46.8474	1.39
Compound_2125-P4	45.4061	-47.1303	1.08

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2128-P4	50.1467	-48.1581	1.19
Compound_2131-P4	33.4585	-41.6958	0.71
Compound_2132-P4	56.8461	-46.8574	1.26
Compound_2133-P4	57.7937	-48.6395	1.33
Compound_2134-P4	33.0025	-37.9317	0.60
Compound_2135-P4	42.5853	-39.6755	0.81
Compound_2136-P4	42.8285	-44.1783	0.95
Compound_2137-P4	55.1004	-46.4951	1.22
Compound_2138-P4	67.1081	-46.8034	1.43
Compound_2139-P4	64.0940	-44.9093	1.33
Compound_2140-P4	57.3536	-46.1236	1.25
Compound_2151-P4	38.4933	-37.4440	0.68
Compound_2152-P4	52.5681	-38.8963	0.96
Compound_2155-P4	43.7776	-43.3893	0.94
Compound_2157-P4	48.0119	-44.4854	1.04
Compound_2160-P4	46.8027	-45.2795	1.05
Compound_2166-P4	42.1285	-42.7328	0.89
Compound_2167-P4	36.5834	-43.2411	0.81
Compound_2168-P4	56.6917	-47.1238	1.27
Compound_2173-P4	51.4238	-46.2763	1.15
Compound_2180-P4	40.8223	-46.3117	0.97
Compound_2314-P4	34.2845	-33.0871	0.48
Compound_2315-P4	37.2828	-28.4651	0.40
Compound_2371-P4	53.4385	-47.0057	1.21
Compound_2372-P4	37.5626	-45.6671	0.90
Compound_2377-P4	43.1331	-42.5496	0.90
Compound_2378-P4	44.6380	-42.9963	0.94
Compound_2379-P4	46.0620	-42.4138	0.95
Compound_2380-P4	38.6706	-43.6165	0.86
Compound_2381-P4	37.8001	-45.6111	0.90
Compound_2382-P4	56.1160	-45.3342	1.21
Compound_2653-P4	65.9770	-39.4781	1.20
Compound_2657-P4	45.3024	-41.4858	0.91
Compound_2659-P4	42.9155	-36.2111	0.72
Compound_2663-P4	46.7489	-36.9540	0.80
Compound_2669-P4	56.8967	-38.3031	1.01
Compound_2679-P4	55.8411	-39.7994	1.04
Compound_2696-P4	50.2721	-36.6761	0.85
Compound_2697-P4	51.3207	-36.4222	0.87
Compound_2698-P4	45.6292	-38.0340	0.82
Compound_2700-P4	49.3852	-38.0764	0.88
Compound_2741-P4	39.3740	-54.7273	1.19
Compound_2743-P4	40.5606	-34.5158	0.63
Compound_2745-P4	48.2048	-37.6243	0.85
Compound_2751-P4	48.3303	-36.9094	0.83
Compound_2754-P4	42.2264	-35.1774	0.67

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2756-P4	56.2616	-39.5942	1.04
Compound_2758-P4	47.6676	-39.8452	0.90
Compound_2779-P4	56.0812	-43.5328	1.15
Compound_2794-P4	60.4013	-38.6582	1.08
Compound_2800-P4	46.6625	-40.1538	0.89
Compound_2876-P4	35.3833	-45.1179	0.85
Compound_2877-P4	47.8093	-46.3575	1.09
Compound_2889-P4	45.6986	-43.2878	0.97
Compound_2891-P4	55.1729	-42.5653	1.11
Compound_2893-P4	50.2159	-46.5270	1.14
Compound_2894-P4	48.2016	-47.2498	1.13
Compound_2896-P4	54.5995	-41.4752	1.07
Compound_2897-P4	53.7311	-43.5776	1.11
Compound_2898-P4	55.7255	-42.8226	1.13
Compound_2899-P4	61.2710	-46.1960	1.32
Compound_2900-P4	64.5871	-46.1375	1.37
Compound_2901-P4	55.4712	-48.7930	1.29
Compound_2903-P4	60.3972	-46.8923	1.32
Compound_2905-P4	52.3028	-45.9515	1.16
Compound_2908-P4	51.4424	-47.1259	1.18
Compound_2909-P4	41.1266	-44.3335	0.92
Compound_2910-P4	53.9262	-45.6568	1.18
Compound_2917-P4	51.7524	-37.7412	0.91
Compound_2918-P4	56.8506	-40.7251	1.08
Compound_2924-P4	65.2797	-42.5369	1.28
Compound_2926-P4	41.7955	-43.4656	0.91
Compound_2927-P4	47.0122	-47.3023	1.11
Compound_2929-P4	47.2537	-45.7527	1.07
Compound_2931-P4	50.0217	-42.1048	1.01
Compound_2932-P4	43.7152	-42.0594	0.90
Compound_2933-P4	51.1196	-44.3410	1.09
Compound_2935-P4	31.1730	-39.7081	0.62
Compound_2936-P4	64.3870	-40.6084	1.21
Compound_2937-P4	62.7215	-44.5098	1.29
Compound_2938-P4	47.6632	-47.1987	1.12
Compound_2939-P4	69.2399	-48.6792	1.53
Compound_2940-P4	55.1414	-46.7122	1.23
Compound_2942-P4	51.8905	-45.2026	1.13
Compound_2944-P4	56.7918	-45.6392	1.23
Compound_2946-P4	50.9874	-45.9844	1.14
Compound_2947-P4	48.7430	-44.8538	1.07
Compound_2948-P4	35.8922	-47.0134	0.91
Compound_2949-P4	39.2538	-40.9193	0.79
Compound_2951-P4	51.9817	-44.7726	1.12
Compound_2952-P4	42.8958	-43.2260	0.92
Compound_2953-P4	55.4342	-46.7473	1.23

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2954-P4	56.6655	-39.7670	1.05
Compound_2955-P4	45.6682	-40.5815	0.89
Compound_2956-P4	56.5035	-43.1577	1.15
Compound_2957-P4	81.0314	-42.5339	1.55
Compound_2958-P4	50.0491	-44.6677	1.08
Compound_2960-P4	54.9285	-44.1309	1.15
Compound_2962-P4	54.6272	-44.6485	1.16
Compound_2963-P4	57.2218	-48.5572	1.32
Compound_2965-P4	39.2056	-45.4320	0.92
Compound_2966-P4	53.6360	-43.0639	1.10
Compound_2967-P4	49.5127	-42.9369	1.02
Compound_2972-P4	41.1540	-41.7526	0.85
Compound_2978-P4	44.3810	-44.9418	0.99
Compound_2980-P4	51.0935	-45.2592	1.12
Compound_2983-P4	46.1072	-45.7275	1.05
Compound_2984-P4	54.4354	-41.4305	1.06
Compound_2985-P4	50.3303	-44.7293	1.09
Compound_2991-P4	56.1446	-43.4777	1.15
Compound_2992-P4	48.1392	-44.3723	1.04
Compound_2993-P4	53.6253	-47.4065	1.22
Compound_2998-P4	51.7928	-47.3983	1.19
Compound_2-P5	40.4799	-45.0664	0.93
Compound_3-P5	73.3080	-50.0978	1.64
Compound_10-P5	42.8506	-43.2061	0.92
Compound_11-P5	38.4490	-45.6078	0.91
Compound_12-P5	57.9826	-47.3254	1.29
Compound_24-P5	60.3688	-44.3826	1.25
Compound_25-P5	55.9169	-46.6615	1.24
Compound_27-P5	61.9207	-48.5159	1.40
Compound_28-P5	47.0937	-47.9874	1.13
Compound_30-P5	50.0907	-39.2070	0.93
Compound_31-P5	67.8346	-40.2421	1.26
Compound_32-P5	54.5447	-45.0408	1.17
Compound_33-P5	76.9626	-48.4025	1.65
Compound_34-P5	53.3445	-48.4883	1.25
Compound_35-P5	61.1948	-47.6792	1.36
Compound_37-P5	55.5826	-46.9374	1.24
Compound_39-P5	53.9618	-48.7174	1.27
Compound_42-P5	62.5841	-47.2883	1.37
Compound_43-P5	46.5313	-42.1676	0.95
Compound_44-P5	59.4122	-45.5692	1.27
Compound_51-P5	52.8071	-38.6758	0.96
Compound_52-P5	32.7595	-40.4604	0.67
Compound_58-P5	58.1447	-43.3433	1.18
Compound_60-P5	53.2720	-44.2074	1.12
Compound_61-P5	60.1981	-49.9015	1.41

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_63-P5	42.5509	-43.5243	0.92
Compound_65-P5	43.5981	-44.3731	0.96
Compound_69-P5	51.1257	-40.4852	0.98
Compound_70-P5	54.7070	-40.7664	1.05
Compound_74-P5	67.0215	-46.7196	1.43
Compound_76-P5	45.1461	-45.0017	1.01
Compound_79-P5	43.4350	-46.9259	1.04
Compound_81-P5	45.1087	-44.3023	0.99
Compound_103-P5	49.2023	-42.0978	0.99
Compound_104-P5	34.7205	-42.1047	0.75
Compound_106-P5	59.5949	-46.0615	1.29
Compound_107-P5	43.6168	-44.8696	0.98
Compound_109-P5	56.4977	-41.9924	1.11
Compound_110-P5	38.6820	-42.1488	0.82
Compound_111-P5	36.5764	-46.2549	0.90
Compound_112-P5	46.2182	-45.6770	1.05
Compound_113-P5	53.9656	-47.4672	1.23
Compound_114-P5	40.6887	-48.0226	1.02
Compound_116-P5	63.1109	-47.3176	1.38
Compound_118-P5	51.2778	-45.7736	1.14
Compound_121-P5	47.5834	-46.7166	1.10
Compound_122-P5	52.6081	-43.9007	1.10
Compound_123-P5	34.4510	-45.6823	0.85
Compound_124-P5	50.3888	-40.7382	0.97
Compound_125-P5	55.8954	-43.8938	1.16
Compound_126-P5	41.5311	-39.5551	0.79
Compound_128-P5	40.8590	-43.1917	0.88
Compound_129-P5	45.8889	-42.9615	0.96
Compound_130-P5	41.7789	-44.6405	0.94
Compound_131-P5	34.5220	-36.7159	0.59
Compound_132-P5	47.1587	-38.0250	0.84
Compound_133-P5	41.9327	-40.2123	0.82
Compound_134-P5	46.3439	-41.8564	0.94
Compound_135-P5	52.4827	-42.0476	1.05
Compound_136-P5	58.1602	-44.3281	1.21
Compound_139-P5	26.2221	-43.0346	0.63
Compound_140-P5	51.1534	-45.5507	1.13
Compound_142-P5	51.9802	-43.3501	1.08
Compound_143-P5	55.9774	-41.8720	1.10
Compound_144-P5	43.5300	-41.7710	0.89
Compound_145-P5	44.1167	-41.7100	0.90
Compound_146-P5	37.2128	-41.8575	0.78
Compound_148-P5	50.9771	-45.0876	1.11
Compound_149-P5	42.8780	-43.8695	0.94
Compound_150-P5	56.0432	-45.9184	1.22
Compound_151-P5	45.9821	-39.8223	0.87

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_152-P5	46.6931	-41.0108	0.92
Compound_153-P5	50.2256	-41.8796	1.00
Compound_154-P5	43.0917	-44.9124	0.97
Compound_155-P5	40.3501	-45.0136	0.93
Compound_156-P5	40.2018	-46.4097	0.97
Compound_158-P5	40.8406	-44.9715	0.93
Compound_164-P5	64.9247	-41.9668	1.26
Compound_167-P5	51.0975	-41.5322	1.01
Compound_168-P5	46.0196	-38.6617	0.84
Compound_174-P5	58.4288	-44.1452	1.21
Compound_176-P5	48.3839	-45.6130	1.08
Compound_178-P5	47.0532	-44.3760	1.02
Compound_179-P5	40.7799	-42.4218	0.86
Compound_180-P5	44.9260	-45.2271	1.01
Compound_186-P5	41.1485	-41.2279	0.83
Compound_187-P5	49.4445	-43.8545	1.05
Compound_188-P5	50.7279	-46.3907	1.14
Compound_193-P5	54.1547	-47.9984	1.25
Compound_199-P5	58.5493	-48.4961	1.34
Compound_200-P5	58.9677	-46.8934	1.30
Compound_207-P5	60.9423	-44.9913	1.28
Compound_208-P5	43.3978	-45.2777	0.99
Compound_209-P5	50.3704	-47.8472	1.18
Compound_222-P5	48.0295	-43.3256	1.01
Compound_223-P5	56.3713	-45.1164	1.20
Compound_225-P5	51.5265	-47.0803	1.18
Compound_226-P5	47.7416	-46.2624	1.09
Compound_228-P5	42.8128	-38.6811	0.79
Compound_229-P5	39.5821	-43.5299	0.87
Compound_230-P5	68.4123	-43.9286	1.37
Compound_231-P5	51.0410	-46.0128	1.14
Compound_232-P5	68.4364	-45.1292	1.41
Compound_233-P5	73.5798	-47.5240	1.57
Compound_235-P5	69.8391	-45.9459	1.46
Compound_239-P5	57.5506	-45.2669	1.23
Compound_240-P5	41.1676	-42.7695	0.88
Compound_241-P5	49.7668	-44.0768	1.06
Compound_247-P5	34.7152	-38.1543	0.63
Compound_248-P5	39.0731	-41.4817	0.80
Compound_254-P5	51.5685	-45.8028	1.14
Compound_256-P5	42.2385	-43.9623	0.93
Compound_257-P5	45.0243	-46.2938	1.04
Compound_259-P5	55.5468	-45.0744	1.19
Compound_261-P5	55.2298	-44.2667	1.16
Compound_265-P5	47.4001	-40.8107	0.93
Compound_266-P5	45.3443	-42.7965	0.95

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_271-P5	56.1760	-46.4395	1.24
Compound_273-P5	55.3269	-46.9777	1.24
Compound_276-P5	51.9491	-47.9317	1.21
Compound_278-P5	53.8563	-46.2525	1.19
Compound_300-P5	33.9699	-45.1431	0.82
Compound_301-P5	47.1354	-44.5879	1.03
Compound_303-P5	44.3079	-45.2061	1.00
Compound_304-P5	35.2433	-46.9295	0.90
Compound_305-P5	59.0213	-47.3939	1.31
Compound_306-P5	48.1068	-39.9674	0.91
Compound_307-P5	34.9992	-40.0354	0.69
Compound_308-P5	53.7818	-43.1904	1.10
Compound_309-P5	46.9950	-47.2307	1.11
Compound_310-P5	59.7847	-46.1881	1.29
Compound_311-P5	55.2883	-48.1222	1.27
Compound_312-P5	40.9707	-44.3149	0.92
Compound_314-P5	47.0531	-50.6705	1.21
Compound_315-P5	46.7144	-47.3676	1.10
Compound_316-P5	53.6081	-45.4622	1.17
Compound_317-P5	55.0648	-44.9473	1.18
Compound_320-P5	56.1079	-40.0275	1.05
Compound_326-P5	55.0941	-35.6331	0.91
Compound_327-P5	51.0107	-35.3571	0.83
Compound_331-P5	49.1322	-36.2684	0.82
Compound_360-P5	38.8158	-31.0422	0.50
Compound_363-P5	50.5423	-37.3681	0.88
Compound_365-P5	56.2222	-39.7196	1.04
Compound_366-P5	53.6292	-39.0633	0.98
Compound_578-P5	49.2361	-36.4673	0.83
Compound_581-P5	45.3371	-33.7885	0.69
Compound_685-P5	46.3201	-39.1703	0.86
Compound_686-P5	42.5681	-42.6200	0.90
Compound_734-P5	55.7011	-42.8275	1.13
Compound_738-P5	46.9505	-40.5126	0.91
Compound_743-P5	56.7710	-44.6501	1.20
Compound_750-P5	46.6732	-42.3114	0.96
Compound_752-P5	64.2460	-46.0005	1.36
Compound_753-P5	46.4858	-40.3088	0.90
Compound_760-P5	46.6440	-45.0071	1.03
Compound_761-P5	51.6921	-41.2305	1.01
Compound_763-P5	70.6863	-43.2598	1.39
Compound_768-P5	55.6140	-46.6724	1.24
Compound_769-P5	47.1584	-39.5244	0.88
Compound_770-P5	41.9009	-41.6524	0.86
Compound_771-P5	37.7792	-31.2564	0.49
Compound_772-P5	47.2692	-32.5921	0.69

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_778-P5	60.9020	-40.0407	1.13
Compound_786-P5	49.4677	-42.5369	1.01
Compound_793-P5	33.3068	-31.0297	0.40
Compound_794-P5	39.1815	-34.5651	0.60
Compound_882-P5	53.3321	-46.3812	1.19
Compound_883-P5	52.5986	-46.4243	1.18
Compound_884-P5	47.4617	-44.5343	1.03
Compound_896-P5	46.3656	-48.3423	1.13
Compound_898-P5	54.9235	-50.3225	1.33
Compound_903-P5	50.9155	-48.5939	1.21
Compound_909-P5	42.5553	-48.3538	1.06
Compound_922-P5	72.2317	-48.9625	1.58
Compound_929-P5	54.2439	-47.7438	1.24
Compound_954-P5	46.5957	-35.4873	0.76
Compound_968-P5	48.0017	-31.5160	0.67
Compound_969-P5	50.3639	-34.0084	0.78
Compound_1007-P5	44.0113	-42.9447	0.93
Compound_1008-P5	43.5492	-43.5727	0.94
Compound_1039-P5	47.1754	-41.6341	0.95
Compound_1041-P5	55.7439	-42.3185	1.11
Compound_1042-P5	47.7070	-38.7574	0.87
Compound_1044-P5	43.9553	-41.0389	0.87
Compound_1058-P5	49.0337	-45.6764	1.09
Compound_1059-P5	52.9447	-40.4071	1.01
Compound_1064-P5	45.2330	-46.6665	1.06
Compound_1065-P5	43.4695	-44.6442	0.97
Compound_1078-P5	45.0487	-44.7492	1.00
Compound_1111-P5	71.5005	-40.5855	1.33
Compound_1112-P5	45.4010	-41.0664	0.90
Compound_1113-P5	54.4409	-42.2894	1.09
Compound_1114-P5	42.9298	-43.9216	0.94
Compound_1115-P5	50.3552	-39.4523	0.94
Compound_1116-P5	55.9959	-34.6850	0.89
Compound_1117-P5	39.9356	-32.5834	0.56
Compound_1121-P5	53.7296	-44.3871	1.14
Compound_1123-P5	62.5683	-43.9180	1.27
Compound_1126-P5	45.9825	-45.0286	1.02
Compound_1127-P5	42.4210	-48.1396	1.05
Compound_1130-P5	42.7218	-38.7525	0.79
Compound_1132-P5	56.2104	-41.4647	1.09
Compound_1133-P5	50.7714	-41.4585	1.00
Compound_1136-P5	51.7903	-37.8502	0.91
Compound_1137-P5	55.0474	-42.4779	1.10
Compound_1138-P5	45.2039	-37.0256	0.78
Compound_1139-P5	41.2826	-32.2927	0.57
Compound_1146-P5	40.6848	-43.9863	0.90

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1149-P5	49.0489	-43.3667	1.03
Compound_1150-P5	45.2098	-41.0139	0.89
Compound_1152-P5	39.4279	-47.9891	1.00
Compound_1153-P5	39.3786	-41.7568	0.82
Compound_1158-P5	40.6239	-41.0484	0.82
Compound_1159-P5	46.5018	-43.3983	0.99
Compound_1162-P5	48.5072	-43.0819	1.01
Compound_1163-P5	50.5992	-40.8283	0.98
Compound_1164-P5	37.6430	-39.1259	0.71
Compound_1165-P5	40.7456	-35.7133	0.66
Compound_1169-P5	63.6556	-44.1151	1.30
Compound_1171-P5	53.4023	-45.1575	1.15
Compound_1173-P5	49.7500	-47.3569	1.16
Compound_1174-P5	58.6710	-48.2654	1.33
Compound_1177-P5	47.2297	-38.4063	0.85
Compound_1185-P5	53.3093	-41.4697	1.05
Compound_1186-P5	36.5509	-40.6167	0.74
Compound_1187-P5	46.9507	-41.7902	0.95
Compound_1188-P5	52.5556	-43.4057	1.09
Compound_1189-P5	49.7112	-39.2874	0.92
Compound_1190-P5	38.1808	-34.2151	0.58
Compound_1202-P5	37.6204	-44.6923	0.87
Compound_1205-P5	36.0750	-45.2756	0.86
Compound_1207-P5	59.4473	-46.5424	1.30
Compound_1208-P5	35.7806	-48.3565	0.95
Compound_1212-P5	55.3589	-38.0083	0.98
Compound_1213-P5	43.3510	-35.2204	0.69
Compound_1215-P5	52.4646	-38.9732	0.96
Compound_1217-P5	45.5987	-39.0415	0.84
Compound_1218-P5	37.5371	-40.8593	0.76
Compound_1292-P5	40.4061	-43.0651	0.87
Compound_1293-P5	65.4879	-40.1566	1.21
Compound_1294-P5	56.7240	-43.6090	1.17
Compound_1295-P5	38.6428	-42.0146	0.81
Compound_1296-P5	53.8152	-37.1327	0.93
Compound_1297-P5	55.5348	-34.5481	0.88
Compound_1300-P5	48.7405	-44.3501	1.05
Compound_1302-P5	62.5695	-42.2606	1.23
Compound_1305-P5	55.8117	-48.6641	1.30
Compound_1307-P5	57.6247	-35.9446	0.96
Compound_1310-P5	41.5466	-42.3989	0.87
Compound_1315-P5	41.5464	-42.9342	0.89
Compound_1316-P5	51.3826	-40.6815	0.99
Compound_1317-P5	46.7329	-41.7658	0.94
Compound_1318-P5	52.9514	-38.9757	0.97
Compound_1325-P5	60.1382	-46.3654	1.30

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1326-P5	41.5877	-42.6775	0.88
Compound_1328-P5	47.0467	-49.9331	1.18
Compound_1333-P5	46.7019	-43.3353	0.99
Compound_1348-P5	57.8882	-44.7270	1.22
Compound_1349-P5	57.7442	-40.6018	1.10
Compound_1351-P5	46.5659	-41.5295	0.93
Compound_1354-P5	51.4619	-36.7308	0.88
Compound_1384-P5	53.2378	-42.6699	1.08
Compound_1385-P5	53.3156	-43.5346	1.11
Compound_1398-P5	36.0160	-45.5073	0.87
Compound_1412-P5	43.5427	-44.9643	0.98
Compound_1416-P5	47.8538	-39.7105	0.90
Compound_1468-P5	42.4811	-49.3864	1.09
Compound_1470-P5	35.1816	-46.4673	0.88
Compound_1498-P5	46.9248	-46.8858	1.09
Compound_1499-P5	70.3351	-48.4254	1.54
Compound_1502-P5	49.7349	-47.4591	1.16
Compound_1503-P5	47.2068	-43.0559	0.99
Compound_1506-P5	57.8578	-39.6244	1.07
Compound_1522-P5	55.4131	-41.9227	1.09
Compound_1523-P5	57.5638	-41.8844	1.13
Compound_1525-P5	36.8099	-42.9154	0.81
Compound_1526-P5	67.3227	-43.4746	1.34
Compound_1530-P5	50.2977	-44.1743	1.07
Compound_1541-P5	61.2076	-44.3491	1.26
Compound_1545-P5	48.3143	-44.7506	1.06
Compound_1546-P5	52.7151	-44.8651	1.13
Compound_1553-P5	54.2046	-41.5940	1.06
Compound_1555-P5	52.5157	-40.2412	1.00
Compound_1557-P5	56.8176	-42.8188	1.14
Compound_1560-P5	43.1823	-45.6819	1.00
Compound_1561-P5	51.2729	-40.6325	0.99
Compound_1563-P5	40.4396	-43.9529	0.90
Compound_1569-P5	53.3739	-46.4255	1.19
Compound_1572-P5	51.4193	-43.7817	1.08
Compound_1581-P5	56.4135	-44.4856	1.19
Compound_1582-P5	54.0297	-41.9402	1.07
Compound_1588-P5	34.3010	-41.0870	0.71
Compound_1589-P5	53.6078	-44.9213	1.15
Compound_1594-P5	55.1991	-49.4713	1.31
Compound_1601-P5	52.6451	-47.3525	1.20
Compound_1622-P5	46.8891	-45.2300	1.05
Compound_1628-P5	39.8770	-42.2998	0.84
Compound_1629-P5	42.9470	-44.8493	0.97
Compound_1630-P5	46.6229	-46.5507	1.08
Compound_1633-P5	54.1216	-48.3686	1.26

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1640-P5	46.3231	-45.8279	1.05
Compound_1641-P5	66.0964	-41.2892	1.26
Compound_1642-P5	50.1123	-42.8098	1.03
Compound_1644-P5	67.7068	-44.4102	1.38
Compound_1645-P5	29.1007	-43.9583	0.71
Compound_1646-P5	49.9206	-45.7135	1.11
Compound_1647-P5	39.7208	-40.6115	0.79
Compound_1648-P5	54.9028	-41.6218	1.08
Compound_1649-P5	38.9492	-42.2105	0.82
Compound_1650-P5	37.1726	-44.4490	0.86
Compound_1651-P5	50.8008	-44.7957	1.10
Compound_1652-P5	61.9703	-45.9708	1.32
Compound_1654-P5	44.5271	-42.9852	0.94
Compound_1660-P5	38.2798	-43.8368	0.86
Compound_1661-P5	60.3380	-43.8913	1.24
Compound_1662-P5	53.1422	-45.0845	1.15
Compound_1663-P5	47.6691	-43.8727	1.02
Compound_1665-P5	43.2824	-46.6846	1.03
Compound_1666-P5	37.3402	-45.7824	0.90
Compound_1668-P5	52.5727	-39.7069	0.98
Compound_1669-P5	51.0932	-42.5778	1.04
Compound_1670-P5	54.9243	-44.1776	1.15
Compound_1671-P5	52.1183	-47.0454	1.19
Compound_1672-P5	69.2117	-46.9718	1.48
Compound_1675-P5	56.8145	-45.8560	1.23
Compound_1680-P5	51.9372	-45.2937	1.13
Compound_1685-P5	48.9439	-37.8676	0.87
Compound_1693-P5	38.9481	-44.5487	0.89
Compound_1697-P5	50.8341	-48.1195	1.20
Compound_1704-P5	42.3155	-43.2731	0.91
Compound_1705-P5	34.8485	-45.3127	0.84
Compound_1706-P5	36.4002	-47.5113	0.93
Compound_1723-P5	38.9467	-45.6172	0.92
Compound_1724-P5	42.3095	-46.3391	1.00
Compound_1735-P5	48.9862	-42.8787	1.01
Compound_1741-P5	47.9579	-43.6844	1.02
Compound_1742-P5	54.1197	-45.4857	1.18
Compound_1743-P5	54.0389	-43.9094	1.13
Compound_1744-P5	50.7757	-48.0453	1.19
Compound_1748-P5	50.8627	-46.8225	1.16
Compound_1755-P5	54.5270	-46.8520	1.22
Compound_1761-P5	36.7710	-38.6492	0.68
Compound_1762-P5	44.6850	-40.1291	0.86
Compound_1768-P5	45.3244	-44.8004	1.01
Compound_1770-P5	34.6063	-46.4898	0.87
Compound_1773-P5	39.3847	-46.9654	0.97

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1775-P5	42.4084	-44.2036	0.94
Compound_1801-P5	45.4592	-31.7044	0.63
Compound_1837-P5	49.3850	-39.0214	0.91
Compound_1848-P5	43.0344	-38.4109	0.78
Compound_1849-P5	41.4877	-37.1012	0.72
Compound_1850-P5	50.8645	-35.4917	0.83
Compound_1851-P5	66.8465	-38.3699	1.19
Compound_1852-P5	51.0373	-38.3689	0.92
Compound_1853-P5	42.9288	-37.4799	0.75
Compound_1861-P5	45.7499	-36.3736	0.77
Compound_1862-P5	52.2038	-38.3394	0.94
Compound_1863-P5	49.5927	-32.9516	0.74
Compound_1886-P5	45.0446	-36.5560	0.76
Compound_1975-P5	63.5885	-43.4039	1.28
Compound_1976-P5	54.5414	-42.5529	1.10
Compound_1977-P5	65.7635	-43.4240	1.31
Compound_1978-P5	68.6725	-43.7712	1.37
Compound_1979-P5	43.4721	-44.4866	0.97
Compound_1980-P5	48.2134	-43.0379	1.00
Compound_1985-P5	57.3361	-46.1887	1.25
Compound_1992-P5	44.6658	-38.4862	0.81
Compound_1993-P5	44.1682	-40.5949	0.86
Compound_1994-P5	61.0255	-41.4841	1.18
Compound_1995-P5	54.9185	-39.5243	1.02
Compound_1997-P5	55.2601	-39.6818	1.03
Compound_1998-P5	41.0012	-42.7832	0.87
Compound_2048-P5	51.0506	-33.1821	0.77
Compound_2109-P5	47.2566	-32.3932	0.68
Compound_2148-P5	33.6557	-33.4230	0.48
Compound_2250-P5	51.0774	-43.6636	1.07
Compound_2271-P5	54.1736	-43.0412	1.11
Compound_2272-P5	63.4586	-41.1395	1.21
Compound_2275-P5	47.2784	-45.0524	1.05
Compound_2287-P5	57.0384	-45.5006	1.23
Compound_2289-P5	63.6547	-43.5271	1.28
Compound_2292-P5	67.0451	-45.4917	1.40
Compound_2294-P5	46.2405	-34.2165	0.71
Compound_2295-P5	50.0192	-34.5654	0.79
Compound_2298-P5	54.0114	-44.8883	1.16
Compound_2305-P5	61.0604	-43.9419	1.25
Compound_2325-P5	52.1697	-35.1093	0.84
Compound_2326-P5	51.6397	-41.9718	1.03
Compound_2342-P5	51.7325	-41.5378	1.02
Compound_2343-P5	40.2525	-41.7727	0.83
Compound_2345-P5	44.9252	-40.1465	0.86
Compound_2355-P5	51.9398	-46.0995	1.16

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2356-P5	57.7635	-43.4514	1.18
Compound_2360-P5	44.9223	-32.6895	0.65
Compound_2361-P5	45.8766	-33.8631	0.70
Compound_2363-P5	48.3274	-48.7553	1.17
Compound_2364-P5	57.6031	-42.1575	1.14
Compound_2366-P5	40.8728	-40.6236	0.81
Compound_2372-P5	57.6945	-46.6770	1.27
Compound_2387-P5	64.6946	-43.4511	1.30
Compound_2400-P5	47.7145	-41.4251	0.95
Compound_2406-P5	68.5700	-47.3240	1.47
Compound_2409-P5	55.3495	-45.5356	1.20
Compound_2412-P5	60.7488	-45.9796	1.30
Compound_2413-P5	61.0984	-43.6082	1.24
Compound_2414-P5	56.7382	-33.9447	0.89
Compound_2415-P5	61.9121	-44.6612	1.28
Compound_2418-P5	49.1126	-47.0248	1.14
Compound_2419-P5	41.8056	-45.5415	0.97
Compound_2653-P5	48.7400	-43.8164	1.04
Compound_2655-P5	41.6806	-41.7970	0.86
Compound_2661-P5	47.2977	-34.7183	0.75
Compound_2673-P5	48.1002	-43.0344	1.00
Compound_2674-P5	55.1440	-41.7014	1.08
Compound_2675-P5	43.3029	-39.9987	0.83
Compound_2676-P5	46.7136	-40.3679	0.90
Compound_2679-P5	45.4279	-34.3726	0.71
Compound_2690-P5	44.3773	-47.5447	1.07
Compound_2692-P5	37.7797	-42.1780	0.80
Compound_2695-P5	63.9478	-46.3534	1.37
Compound_2696-P5	52.4796	-48.8669	1.25
Compound_2697-P5	70.7623	-45.9253	1.47
Compound_2699-P5	51.1130	-43.0946	1.06
Compound_2706-P5	50.6867	-41.8064	1.01
Compound_2707-P5	37.7840	-41.6297	0.79
Compound_2712-P5	58.4960	-46.3784	1.28
Compound_2719-P5	48.3060	-43.8949	1.03
Compound_2721-P5	49.3766	-36.1624	0.82
Compound_2728-P5	57.3348	-48.3502	1.31
Compound_2730-P5	47.8459	-45.2372	1.06
Compound_2733-P5	49.4623	-46.6155	1.13
Compound_2734-P5	54.3246	-41.6539	1.07
Compound_2738-P5	55.0175	-47.9282	1.26
Compound_2739-P5	52.2264	-50.3962	1.29
Compound_2740-P5	57.5978	-47.7960	1.30
Compound_2744-P5	50.7963	-40.4502	0.97
Compound_2745-P5	41.1266	-45.2430	0.95
Compound_2748-P5	53.1932	-45.4869	1.16

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2750-P5	52.3637	-46.1098	1.16
Compound_2755-P5	51.7107	-43.0837	1.07
Compound_2765-P5	58.8948	-49.3943	1.37
Compound_2769-P5	41.8108	-46.2488	0.99
Compound_51-P6	50.4464	-44.6464	1.09
Compound_60-P6	45.2243	-47.1530	1.07
Compound_97-P6	39.9459	-41.7794	0.83
Compound_99-P6	56.1093	-45.6552	1.21
Compound_112-P6	61.3602	-39.2664	1.12
Compound_116-P6	50.5681	-41.3995	1.00
Compound_120-P6	43.6167	-42.1042	0.90
Compound_151-P6	63.1773	-44.3950	1.30
Compound_165-P6	55.8268	-41.3409	1.08
Compound_171-P6	30.3903	-40.6505	0.63
Compound_293-P6	58.0073	-47.4506	1.30
Compound_299-P6	41.5593	-42.2017	0.87
Compound_300-P6	62.7522	-44.5477	1.30
Compound_301-P6	50.6694	-45.0428	1.10
Compound_302-P6	43.6003	-49.1364	1.10
Compound_306-P6	65.6874	-46.4082	1.40
Compound_308-P6	55.6688	-47.7453	1.27
Compound_311-P6	45.2769	-49.0770	1.13
Compound_313-P6	48.7929	-47.5400	1.14
Compound_314-P6	55.6742	-47.5767	1.26
Compound_321-P6	43.0572	-40.7953	0.85
Compound_322-P6	41.1691	-42.5978	0.87
Compound_328-P6	46.4051	-45.7544	1.05
Compound_330-P6	44.5651	-47.0357	1.06
Compound_333-P6	37.3959	-46.5899	0.92
Compound_335-P6	27.0547	-46.1973	0.74
Compound_479-P6	49.9384	-41.8468	1.00
Compound_480-P6	47.2195	-40.5943	0.92
Compound_481-P6	50.1435	-42.6716	1.03
Compound_482-P6	58.0918	-41.8754	1.14
Compound_483-P6	47.8874	-43.0377	1.00
Compound_484-P6	51.6902	-42.0171	1.03
Compound_491-P6	48.9227	-39.9429	0.93
Compound_503-P6	47.7601	-38.6887	0.87
Compound_504-P6	63.4299	-41.1098	1.21
Compound_726-P6	39.1830	-40.4303	0.77
Compound_727-P6	45.1490	-39.9779	0.86
Compound_732-P6	63.2549	-43.2229	1.27
Compound_734-P6	51.3500	-48.7099	1.22
Compound_736-P6	55.1071	-45.8663	1.20
Compound_738-P6	31.1933	-46.8285	0.82
Compound_760-P6	53.5832	-46.1667	1.19

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_765-P6	49.7470	-39.1204	0.92
Compound_766-P6	48.9969	-41.4774	0.97
Compound_767-P6	51.5408	-44.3499	1.10
Compound_768-P6	41.2397	-46.9122	1.00
Compound_772-P6	57.0199	-45.2082	1.22
Compound_774-P6	34.1856	-49.2218	0.94
Compound_777-P6	42.6035	-47.0123	1.02
Compound_779-P6	37.9115	-46.1888	0.92
Compound_780-P6	51.8116	-40.4524	0.99
Compound_781-P6	58.0704	-40.9717	1.11
Compound_782-P6	56.9545	-42.3176	1.13
Compound_783-P6	54.4938	-41.4184	1.06
Compound_784-P6	53.8753	-43.1890	1.10
Compound_785-P6	37.1390	-37.2342	0.65
Compound_786-P6	44.8764	-39.0528	0.83
Compound_787-P6	34.6463	-40.3040	0.69
Compound_788-P6	58.5163	-41.1290	1.12
Compound_789-P6	42.4238	-42.7858	0.90
Compound_790-P6	54.7003	-43.1056	1.12
Compound_792-P6	57.4329	-44.7208	1.21
Compound_794-P6	50.9387	-42.9447	1.05
Compound_795-P6	46.0883	-46.8414	1.08
Compound_797-P6	43.4548	-43.7644	0.94
Compound_798-P6	60.8150	-41.0164	1.16
Compound_799-P6	45.9311	-40.5796	0.89
Compound_800-P6	52.8726	-42.0156	1.05
Compound_801-P6	49.0784	-42.6064	1.01
Compound_802-P6	58.2600	-43.6497	1.19
Compound_803-P6	27.3434	-45.1232	0.71
Compound_804-P6	44.0660	-39.1426	0.82
Compound_805-P6	48.7103	-39.5080	0.91
Compound_806-P6	59.5982	-41.4564	1.15
Compound_807-P6	42.2788	-45.1411	0.96
Compound_808-P6	50.2744	-45.9844	1.12
Compound_810-P6	58.7128	-43.4333	1.19
Compound_815-P6	52.9987	-41.6413	1.05
Compound_816-P6	55.6012	-43.5764	1.15
Compound_822-P6	54.3674	-40.1554	1.03
Compound_823-P6	38.2708	-39.0644	0.72
Compound_831-P6	58.7400	-46.9013	1.30
Compound_834-P6	58.3037	-44.9807	1.23
Compound_836-P6	29.7462	-44.0335	0.72
Compound_843-P6	48.9998	-40.6747	0.95
Compound_844-P6	38.1141	-42.4139	0.81
Compound_845-P6	48.0342	-45.4214	1.07
Compound_856-P6	66.3551	-46.2762	1.41

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_862-P6	38.1656	-42.8514	0.83
Compound_863-P6	37.1613	-44.8710	0.87
Compound_864-P6	53.0795	-47.6399	1.22
Compound_876-P6	58.3312	-43.8906	1.20
Compound_881-P6	34.6680	-39.3945	0.67
Compound_882-P6	46.1036	-41.6318	0.93
Compound_883-P6	55.9002	-43.0013	1.13
Compound_884-P6	58.7698	-45.2571	1.25
Compound_888-P6	59.9289	-44.9800	1.26
Compound_890-P6	64.8469	-45.4194	1.36
Compound_893-P6	57.8888	-44.6294	1.21
Compound_895-P6	53.0834	-44.9984	1.14
Compound_901-P6	43.0008	-38.3846	0.78
Compound_902-P6	29.5707	-38.9036	0.57
Compound_908-P6	63.1825	-43.7910	1.28
Compound_910-P6	37.0118	-46.4463	0.91
Compound_913-P6	52.9514	-46.4463	1.18
Compound_915-P6	56.5836	-42.9668	1.14
Compound_969-P6	49.7072	-45.6896	1.11
Compound_970-P6	28.7941	-46.3626	0.77
Compound_971-P6	35.4003	-46.3508	0.88
Compound_972-P6	45.3993	-45.8403	1.04
Compound_973-P6	53.2140	-50.2033	1.30
Compound_974-P6	55.5982	-40.7305	1.06
Compound_975-P6	48.2208	-41.9725	0.97
Compound_976-P6	57.6311	-46.2159	1.26
Compound_977-P6	67.1099	-45.4562	1.40
Compound_978-P6	53.1439	-49.6677	1.28
Compound_979-P6	53.3794	-47.2209	1.21
Compound_981-P6	62.5783	-45.8531	1.33
Compound_985-P6	48.5479	-42.9542	1.01
Compound_986-P6	56.6337	-45.4417	1.22
Compound_992-P6	50.7492	-40.7630	0.98
Compound_993-P6	45.3965	-41.6186	0.92
Compound_1001-P6	50.9344	-46.4834	1.15
Compound_1003-P6	58.0818	-45.7922	1.25
Compound_1005-P6	39.5064	-41.9967	0.83
Compound_1012-P6	33.3123	-42.4892	0.73
Compound_1013-P6	47.2749	-45.5227	1.06
Compound_1032-P6	39.1264	-44.5913	0.89
Compound_1033-P6	41.1279	-47.4160	1.01
Compound_1034-P6	48.9822	-47.9953	1.16
Compound_1046-P6	69.5502	-48.0028	1.51
Compound_1051-P6	55.4010	-41.5582	1.08
Compound_1052-P6	45.5526	-44.0384	0.99
Compound_1053-P6	62.8403	-43.9457	1.28

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1054-P6	63.4844	-50.2235	1.47
Compound_1058-P6	54.9846	-46.2595	1.21
Compound_1060-P6	54.5985	-48.6323	1.28
Compound_1063-P6	57.2868	-48.1113	1.31
Compound_1065-P6	49.8374	-47.8103	1.17
Compound_1072-P6	51.8146	-38.9495	0.95
Compound_1073-P6	43.7179	-43.2362	0.93
Compound_1079-P6	61.4289	-47.8049	1.37
Compound_1081-P6	40.9999	-46.2771	0.98
Compound_1084-P6	50.7324	-47.6442	1.18
Compound_1331-P6	49.8654	-46.4896	1.13
Compound_1332-P6	31.5297	-45.2419	0.78
Compound_1333-P6	51.5287	-47.3719	1.19
Compound_1334-P6	56.3390	-44.3139	1.18
Compound_1335-P6	47.3041	-46.0053	1.07
Compound_1336-P6	44.5251	-42.0894	0.91
Compound_1337-P6	54.1005	-43.3568	1.11
Compound_1338-P6	72.5805	-42.7308	1.41
Compound_1339-P6	60.2624	-41.1936	1.16
Compound_1340-P6	38.1405	-42.0365	0.80
Compound_1341-P6	41.4365	-42.8746	0.88
Compound_1342-P6	46.3957	-43.9845	1.00
Compound_1344-P6	55.0333	-44.0411	1.15
Compound_1345-P6	53.3708	-44.2444	1.13
Compound_1346-P6	55.8194	-46.6348	1.24
Compound_1347-P6	47.0096	-41.3780	0.94
Compound_1351-P6	53.3699	-46.7229	1.20
Compound_1353-P6	37.8285	-47.2344	0.95
Compound_1354-P6	38.3075	-49.5809	1.03
Compound_1355-P6	38.1711	-50.0056	1.04
Compound_1362-P6	48.6578	-44.0038	1.04
Compound_1363-P6	46.8902	-47.2648	1.10
Compound_1364-P6	51.4221	-46.0964	1.15
Compound_1365-P6	44.9591	-44.2408	0.98
Compound_1366-P6	62.3652	-46.2181	1.34
Compound_1367-P6	58.0784	-44.9274	1.23
Compound_1369-P6	43.2536	-42.7881	0.91
Compound_1371-P6	50.5201	-44.3840	1.08
Compound_1372-P6	52.1946	-43.2979	1.08
Compound_1379-P6	54.8729	-45.7447	1.20
Compound_1385-P6	47.2221	-49.2449	1.17
Compound_1387-P6	53.7537	-48.6826	1.26
Compound_1390-P6	43.8729	-47.2841	1.05
Compound_1392-P6	49.8894	-46.4135	1.13
Compound_1417-P6	46.1290	-47.4769	1.10
Compound_1424-P6	34.4100	-43.3389	0.78

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1425-P6	44.2530	-46.8170	1.05
Compound_1426-P6	52.3842	-45.4414	1.14
Compound_1427-P6	54.7752	-47.7218	1.25
Compound_1431-P6	52.7185	-50.3784	1.29
Compound_1433-P6	43.5480	-47.2166	1.05
Compound_1436-P6	32.8650	-48.5968	0.90
Compound_1438-P6	36.3763	-47.4615	0.93
Compound_1439-P6	53.0719	-47.3038	1.21
Compound_1440-P6	49.6324	-41.3798	0.98
Compound_1441-P6	49.9649	-43.9460	1.06
Compound_1443-P6	49.1321	-45.6854	1.10
Compound_1444-P6	44.6460	-44.8394	1.00
Compound_1445-P6	49.1759	-46.9509	1.13
Compound_1446-P6	47.9443	-39.0591	0.88
Compound_1447-P6	41.7756	-40.3844	0.82
Compound_1448-P6	46.7770	-43.5878	1.00
Compound_1449-P6	47.8696	-44.2552	1.03
Compound_1450-P6	47.9834	-45.9072	1.08
Compound_1452-P6	45.1673	-44.3731	0.99
Compound_1454-P6	59.3630	-45.6760	1.27
Compound_1455-P6	43.5250	-48.3905	1.08
Compound_1457-P6	50.5180	-44.9264	1.10
Compound_1458-P6	50.0490	-43.5100	1.05
Compound_1459-P6	36.4804	-43.1963	0.81
Compound_1460-P6	60.1024	-42.8884	1.20
Compound_1461-P6	53.8543	-44.0098	1.13
Compound_1462-P6	56.4942	-45.6726	1.22
Compound_1464-P6	61.3845	-45.4174	1.30
Compound_1465-P6	41.8391	-46.0986	0.98
Compound_1466-P6	74.1660	-48.9269	1.62
Compound_1467-P6	49.9668	-41.2516	0.98
Compound_1468-P6	43.4099	-44.5804	0.97
Compound_1469-P6	57.8990	-46.8077	1.28
Compound_1470-P6	57.9500	-48.3207	1.32
Compound_1472-P6	45.7238	-45.7289	1.04
Compound_1476-P6	46.1221	-45.8825	1.05
Compound_1477-P6	39.8187	-43.6334	0.88
Compound_1478-P6	46.5908	-45.7837	1.06
Compound_1484-P6	46.2400	-41.1452	0.92
Compound_1485-P6	48.0662	-42.0548	0.97
Compound_1493-P6	45.0588	-48.6571	1.11
Compound_1496-P6	47.2350	-44.8485	1.04
Compound_1498-P6	36.1937	-43.3423	0.81
Compound_1506-P6	41.9781	-44.7919	0.95
Compound_1507-P6	37.7842	-44.7927	0.88
Compound_1508-P6	29.8843	-46.8959	0.80

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1520-P6	43.9628	-49.8216	1.13
Compound_1521-P6	46.3800	-48.7942	1.14
Compound_1529-P6	26.9003	-47.7499	0.78
Compound_1530-P6	53.2425	-48.9772	1.26
Compound_1531-P6	34.7370	-49.5228	0.96
Compound_1551-P6	36.6521	-29.7434	0.42
Compound_1610-P6	43.9454	-37.8876	0.78
Compound_1621-P6	57.8002	-39.0244	1.05
Compound_1624-P6	48.0808	-37.1505	0.83
Compound_1639-P6	40.6384	-39.1761	0.76
Compound_1642-P6	49.2691	-44.9198	1.08
Compound_1643-P6	48.9159	-45.8339	1.10
Compound_1644-P6	66.1156	-38.0017	1.16
Compound_1657-P6	57.9108	-47.0329	1.29
Compound_1663-P6	46.0716	-43.6766	0.99
Compound_1665-P6	60.7189	-44.5762	1.26
Compound_1668-P6	67.4993	-47.1055	1.45
Compound_1670-P6	42.2411	-42.3437	0.88
Compound_1671-P6	51.1958	-43.8944	1.08
Compound_1675-P6	57.3188	-47.1114	1.28
Compound_1676-P6	48.6605	-46.5834	1.11
Compound_1678-P6	53.6614	-41.8420	1.06
Compound_1679-P6	43.2555	-44.2824	0.96
Compound_1684-P6	57.2643	-47.0006	1.27
Compound_1686-P6	48.7111	-43.4511	1.02
Compound_1689-P6	57.3012	-42.4334	1.14
Compound_1690-P6	47.6794	-45.7948	1.08
Compound_1691-P6	41.9843	-45.1843	0.96
Compound_1693-P6	50.4283	-45.1780	1.10
Compound_1708-P6	46.7089	-38.7095	0.85
Compound_1709-P6	57.7860	-44.2559	1.20
Compound_1748-P6	46.8392	-41.1496	0.93
Compound_1749-P6	43.8941	-43.2657	0.94
Compound_1750-P6	46.9460	-36.9812	0.81
Compound_1751-P6	42.5913	-34.7594	0.67
Compound_1752-P6	39.6692	-33.0841	0.57
Compound_1755-P6	56.3480	-39.0074	1.03
Compound_1756-P6	51.7021	-43.9399	1.09
Compound_1757-P6	58.6636	-44.0936	1.21
Compound_1764-P6	62.4800	-48.7616	1.41
Compound_1765-P6	41.6347	-40.7907	0.83
Compound_1766-P6	60.3491	-42.5657	1.20
Compound_1767-P6	39.1611	-35.5713	0.63
Compound_1768-P6	44.1998	-34.5234	0.69
Compound_1771-P6	52.6640	-44.0506	1.11
Compound_1772-P6	45.5447	-45.0455	1.02

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1773-P6	49.7359	-44.3025	1.07
Compound_1788-P6	49.0654	-46.1072	1.11
Compound_1799-P6	46.6521	-42.2928	0.96
Compound_1800-P6	48.7384	-41.8816	0.98
Compound_1801-P6	45.6810	-34.2342	0.71
Compound_1807-P6	48.0715	-43.2544	1.01
Compound_1809-P6	54.6670	-44.8931	1.17
Compound_1817-P6	44.6714	-48.4664	1.10
Compound_1823-P6	50.3549	-42.1575	1.02
Compound_1824-P6	49.5354	-39.1649	0.91
Compound_1825-P6	49.3856	-39.3309	0.92
Compound_1826-P6	50.1794	-33.7706	0.77
Compound_1830-P6	47.1595	-40.9590	0.93
Compound_1831-P6	53.8438	-44.4161	1.14
Compound_1832-P6	53.3143	-45.0179	1.15
Compound_1833-P6	70.2428	-46.9745	1.49
Compound_1834-P6	52.2382	-43.2175	1.08
Compound_1837-P6	65.2615	-47.3054	1.42
Compound_1840-P6	52.3870	-45.9167	1.16
Compound_1842-P6	57.5841	-48.7327	1.33
Compound_1845-P6	54.9612	-48.4048	1.27
Compound_1847-P6	56.5359	-50.0444	1.35
Compound_2134-P6	45.0349	-44.1511	0.98
Compound_2135-P6	50.4100	-43.0569	1.04
Compound_2136-P6	53.3177	-45.4808	1.16
Compound_2138-P6	58.1119	-42.5580	1.16
Compound_2172-P6	63.5886	-42.7498	1.26
Compound_2173-P6	65.1871	-41.1293	1.24
Compound_2174-P6	44.3719	-42.7091	0.93
Compound_2175-P6	51.1823	-42.3139	1.03
Compound_2176-P6	66.1535	-43.9635	1.34
Compound_2177-P6	63.2243	-46.2888	1.35
Compound_2187-P6	59.4059	-41.7919	1.16
Compound_2216-P6	59.7434	-40.3137	1.12
Compound_2217-P6	39.1817	-41.3381	0.80
Compound_2218-P6	54.5459	-39.4260	1.01
Compound_2221-P6	54.8399	-43.4413	1.13
Compound_2230-P6	41.3499	-37.5091	0.73
Compound_2231-P6	51.0841	-38.7195	0.93
Compound_2232-P6	39.1164	-41.5813	0.81
Compound_2234-P6	74.4927	-42.9391	1.45
Compound_2336-P6	62.7301	-42.8023	1.24
Compound_2359-P6	42.5867	-45.5805	0.98
Compound_2366-P6	49.7240	-42.4237	1.01
Compound_2367-P6	43.1073	-43.4179	0.93
Compound_2368-P6	51.5847	-45.8044	1.14

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2369-P6	38.1999	-48.5113	0.99
Compound_2372-P6	51.2030	-47.5318	1.19
Compound_2374-P6	36.2429	-47.7442	0.94
Compound_2376-P6	45.3437	-49.7471	1.15
Compound_2378-P6	52.5137	-48.2705	1.23
Compound_2379-P6	36.0774	-41.3555	0.75
Compound_2380-P6	54.5962	-42.8072	1.11
Compound_2383-P6	47.0036	-45.3011	1.05
Compound_2384-P6	38.9226	-43.7292	0.87
Compound_2385-P6	63.2745	-45.8639	1.34
Compound_2386-P6	48.4059	-38.6258	0.88
Compound_2387-P6	55.6064	-40.1175	1.05
Compound_2388-P6	57.3318	-41.7120	1.12
Compound_2389-P6	65.4981	-44.6551	1.35
Compound_2390-P6	58.0433	-45.6537	1.25
Compound_2392-P6	45.0123	-43.7127	0.97
Compound_2394-P6	42.0215	-43.3685	0.91
Compound_2395-P6	53.4870	-46.3779	1.19
Compound_2397-P6	51.9905	-43.9930	1.10
Compound_2398-P6	47.6521	-42.1769	0.97
Compound_2399-P6	42.1351	-44.2736	0.94
Compound_2400-P6	28.5443	-42.6247	0.66
Compound_2401-P6	52.7936	-43.3405	1.09
Compound_2402-P6	41.2170	-43.5690	0.90
Compound_2405-P6	59.0628	-44.6009	1.23
Compound_2406-P6	51.2349	-45.4141	1.12
Compound_2407-P6	54.3701	-47.0442	1.23
Compound_2408-P6	31.9370	-39.7971	0.63
Compound_2409-P6	44.8943	-41.5158	0.90
Compound_2410-P6	44.0949	-42.8349	0.93
Compound_2411-P6	66.6133	-45.6356	1.39
Compound_2412-P6	56.2100	-45.5691	1.21
Compound_2413-P6	58.2214	-47.4112	1.30
Compound_2415-P6	70.2745	-45.8801	1.46
Compound_2420-P6	51.7483	-43.7959	1.09
Compound_2421-P6	53.0547	-45.9756	1.17
Compound_2422-P6	39.1994	-44.2900	0.89
Compound_2427-P6	44.0012	-39.0373	0.82
Compound_2428-P6	38.0348	-39.6664	0.73
Compound_2435-P6	47.8549	-44.2968	1.03
Compound_2438-P6	32.5637	-45.3202	0.80
Compound_2439-P6	47.8679	-42.8591	0.99
Compound_2446-P6	58.6531	-45.3953	1.25
Compound_2447-P6	53.8319	-46.7593	1.21
Compound_2448-P6	43.3977	-47.1213	1.04
Compound_2458-P6	58.2577	-47.8182	1.31

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2466-P6	35.4375	-44.7302	0.84
Compound_2467-P6	50.6360	-49.1373	1.22
Compound_2468-P6	63.4655	-46.3407	1.36
Compound_2480-P6	52.7151	-46.8799	1.19
Compound_2487-P6	44.4375	-42.1343	0.91
Compound_2488-P6	47.1434	-45.6255	1.06
Compound_2489-P6	55.4144	-48.2990	1.28
Compound_2493-P6	41.6094	-46.3752	0.99
Compound_2495-P6	64.8917	-48.0992	1.43
Compound_2498-P6	58.3738	-48.9769	1.35
Compound_2500-P6	43.0768	-46.9613	1.03
Compound_2501-P6	51.9080	-46.4530	1.17
Compound_2507-P6	65.5177	-39.8242	1.21
Compound_2508-P6	52.4057	-43.0718	1.08
Compound_2513-P6	71.3994	-46.3243	1.49
Compound_2515-P6	67.6183	-45.6979	1.41
Compound_2518-P6	42.9403	-44.2777	0.95
Compound_2520-P6	44.1034	-44.0369	0.96
Compound_2563-P6	45.5901	-39.8988	0.87
Compound_2564-P6	53.5802	-40.6951	1.03
Compound_2569-P6	39.4710	-46.2030	0.95
Compound_2571-P6	52.2288	-43.8670	1.10
Compound_2574-P6	50.9330	-46.0304	1.14
Compound_2576-P6	50.4824	-44.2869	1.08
Compound_2601-P6	46.7664	-42.7037	0.97
Compound_2608-P6	55.7355	-39.4863	1.03
Compound_2609-P6	45.4806	-41.2287	0.91
Compound_2610-P6	43.2468	-43.4362	0.93
Compound_2611-P6	56.5976	-43.7154	1.17
Compound_2615-P6	56.8246	-45.6827	1.23
Compound_2617-P6	47.0505	-44.5543	1.03
Compound_2620-P6	40.5700	-44.2004	0.91
Compound_2622-P6	52.8200	-43.4582	1.09
Compound_2623-P6	52.3945	-43.1142	1.08
Compound_2624-P6	56.2089	-36.9598	0.96
Compound_2625-P6	55.8578	-38.1197	0.99
Compound_2628-P6	52.2332	-41.6073	1.03
Compound_2629-P6	57.3466	-40.9553	1.10
Compound_2630-P6	48.3184	-45.7091	1.08
Compound_2631-P6	44.1220	-35.8216	0.73
Compound_2632-P6	52.8900	-38.1505	0.94
Compound_2633-P6	42.7019	-39.5847	0.81
Compound_2634-P6	51.6706	-40.9101	1.00
Compound_2635-P6	50.9261	-43.0196	1.05
Compound_2636-P6	47.4943	-43.7167	1.01
Compound_2638-P6	46.0721	-43.5301	0.98

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2640-P6	49.5560	-43.0921	1.03
Compound_2641-P6	50.3298	-45.8005	1.12
Compound_2643-P6	44.1002	-42.2936	0.91
Compound_2644-P6	53.0905	-40.4392	1.01
Compound_2645-P6	44.3586	-42.3762	0.92
Compound_2646-P6	51.2614	-39.5683	0.96
Compound_2647-P6	55.7309	-40.1056	1.05
Compound_2650-P6	63.6777	-41.4938	1.22
Compound_2651-P6	50.2163	-42.1954	1.01
Compound_2652-P6	53.1214	-44.8713	1.14
Compound_2653-P6	45.7528	-39.2285	0.85
Compound_2654-P6	50.0775	-37.8074	0.88
Compound_2655-P6	50.3290	-42.3059	1.02
Compound_2656-P6	49.0027	-41.3366	0.97
Compound_2657-P6	54.0290	-42.6606	1.09
Compound_2658-P6	43.9424	-45.4759	1.00
Compound_2660-P6	56.4411	-43.0310	1.14
Compound_2665-P6	48.3460	-44.3903	1.05
Compound_2666-P6	44.4377	-43.1657	0.94
Compound_2667-P6	46.5363	-42.7073	0.97
Compound_2670-P6	47.9782	-37.6449	0.84
Compound_2671-P6	47.6430	-38.3888	0.86
Compound_2679-P6	44.6964	-41.3723	0.90
Compound_2682-P6	40.8739	-46.6378	0.98
Compound_2683-P6	29.3743	-41.0746	0.63
Compound_2689-P6	48.6946	-43.5111	1.03
Compound_2690-P6	64.5142	-41.7891	1.25
Compound_2691-P6	49.7811	-43.8721	1.06
Compound_2703-P6	53.4279	-42.2012	1.07
Compound_2704-P6	49.9536	-44.9878	1.09
Compound_2712-P6	48.6538	-47.1522	1.13
Compound_2713-P6	60.0110	-41.8142	1.17
Compound_2714-P6	42.7129	-45.5786	0.98
Compound_2727-P6	70.9962	-40.0377	1.30
Compound_2734-P6	50.0731	-38.0892	0.89
Compound_2735-P6	54.5046	-40.0956	1.03
Compound_2736-P6	53.9942	-40.8059	1.04
Compound_2737-P6	62.8412	-42.9370	1.25
Compound_2741-P6	61.0317	-44.0760	1.25
Compound_2743-P6	51.6358	-49.2391	1.24
Compound_2746-P6	46.2018	-43.9120	1.00
Compound_2748-P6	50.7618	-42.2378	1.02
Compound_2749-P6	55.0388	-42.8368	1.11
Compound_2755-P6	46.4314	-37.0166	0.80
Compound_2756-P6	49.1439	-38.5343	0.89
Compound_2762-P6	42.1179	-44.0763	0.93

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2764-P6	34.7611	-42.6164	0.76
Compound_2767-P6	42.0166	-41.7195	0.86
Compound_2769-P6	51.5455	-41.7859	1.02
Compound_2817-P6	50.7404	-43.3889	1.06
Compound_2818-P6	65.7862	-44.2814	1.34
Compound_2819-P6	65.4044	-45.8220	1.38
Compound_2820-P6	51.3518	-43.3648	1.07
Compound_2821-P6	60.4955	-43.3729	1.22
Compound_2842-P6	40.2198	-29.7428	0.48
Compound_2843-P6	36.2021	-31.3494	0.46
Compound_2887-P6	53.7702	-37.6527	0.94
Compound_47-P7	61.8755	-42.9410	1.23
Compound_48-P7	43.6514	-45.8497	1.01
Compound_63-P7	57.9493	-48.8234	1.34
Compound_70-P7	51.8349	-46.8244	1.18
Compound_71-P7	50.8437	-45.5807	1.12
Compound_72-P7	42.6438	-48.4208	1.07
Compound_84-P7	38.5424	-43.1026	0.84
Compound_85-P7	43.5337	-43.6958	0.94
Compound_88-P7	60.8070	-46.8732	1.33
Compound_89-P7	54.6031	-45.7743	1.19
Compound_91-P7	50.9865	-41.2154	1.00
Compound_92-P7	63.0303	-42.6940	1.25
Compound_93-P7	30.9479	-45.0055	0.77
Compound_94-P7	47.4531	-47.0964	1.11
Compound_97-P7	73.4931	-45.7643	1.51
Compound_103-P7	55.0877	-46.0915	1.21
Compound_106-P7	60.7930	-43.9610	1.24
Compound_107-P7	51.0736	-43.5744	1.07
Compound_112-P7	49.9584	-44.6845	1.08
Compound_113-P7	53.7700	-43.1781	1.10
Compound_124-P7	51.0181	-46.1299	1.14
Compound_131-P7	37.2220	-41.9500	0.79
Compound_132-P7	41.3889	-45.2200	0.95
Compound_138-P7	59.0413	-47.6961	1.32
Compound_151-P7	44.6865	-45.0706	1.00
Compound_152-P7	53.5934	-46.0789	1.18
Compound_173-P7	55.7339	-47.1185	1.25
Compound_188-P7	52.5551	-45.8819	1.16
Compound_195-P7	54.3727	-42.6789	1.10
Compound_196-P7	48.0436	-45.8900	1.08
Compound_197-P7	69.4811	-47.0461	1.48
Compound_202-P7	67.1843	-48.8797	1.50
Compound_208-P7	59.3863	-47.7759	1.33
Compound_216-P7	54.4183	-43.5846	1.13
Compound_217-P7	56.7802	-43.7733	1.17

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_218-P7	58.6574	-45.3853	1.25
Compound_223-P7	64.4202	-46.6939	1.39
Compound_229-P7	52.5132	-44.8437	1.13
Compound_230-P7	50.1921	-47.4301	1.17
Compound_282-P7	48.9524	-42.8780	1.01
Compound_283-P7	43.5952	-41.4295	0.88
Compound_284-P7	54.1433	-45.5645	1.18
Compound_289-P7	54.8432	-44.4055	1.16
Compound_296-P7	41.0421	-46.5911	0.99
Compound_297-P7	44.4024	-46.2205	1.03
Compound_298-P7	60.6413	-43.7811	1.24
Compound_299-P7	51.7654	-46.7936	1.17
Compound_305-P7	42.7782	-44.8143	0.96
Compound_306-P7	46.3618	-49.2895	1.15
Compound_310-P7	57.1940	-46.2092	1.25
Compound_313-P7	40.1338	-44.7752	0.92
Compound_314-P7	49.0286	-42.3826	1.00
Compound_315-P7	54.1867	-41.9478	1.07
Compound_318-P7	42.5344	-47.4822	1.04
Compound_319-P7	59.7270	-45.4947	1.27
Compound_320-P7	50.9504	-46.5025	1.15
Compound_321-P7	48.5441	-40.4111	0.93
Compound_322-P7	37.9116	-39.3828	0.72
Compound_323-P7	51.8383	-43.6303	1.08
Compound_324-P7	55.6086	-48.9604	1.30
Compound_325-P7	48.5144	-44.6440	1.06
Compound_327-P7	46.9796	-46.4611	1.08
Compound_333-P7	71.0834	-42.5380	1.38
Compound_334-P7	55.0384	-43.6896	1.14
Compound_335-P7	56.3812	-42.1630	1.12
Compound_336-P7	42.2563	-46.1024	0.99
Compound_339-P7	39.7453	-49.5577	1.05
Compound_340-P7	58.5732	-48.5191	1.34
Compound_342-P7	40.9529	-42.0708	0.85
Compound_343-P7	54.1325	-43.4812	1.12
Compound_344-P7	57.1287	-43.3495	1.16
Compound_345-P7	71.0577	-48.8984	1.56
Compound_348-P7	57.2438	-47.4928	1.29
Compound_353-P7	52.5812	-43.6599	1.10
Compound_362-P7	43.2056	-44.2119	0.95
Compound_363-P7	53.7203	-46.3518	1.19
Compound_364-P7	38.8999	-45.7555	0.92
Compound_383-P7	55.4987	-45.7105	1.21
Compound_384-P7	50.9824	-48.1120	1.20
Compound_396-P7	51.2548	-46.1300	1.15
Compound_397-P7	51.2244	-42.3470	1.04

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_403-P7	47.1635	-42.4813	0.97
Compound_404-P7	56.7815	-42.0000	1.12
Compound_405-P7	55.4553	-43.4231	1.14
Compound_406-P7	51.0742	-43.1046	1.05
Compound_410-P7	63.2271	-49.2774	1.44
Compound_416-P7	53.8381	-44.8445	1.15
Compound_417-P7	55.3687	-48.0488	1.27
Compound_418-P7	44.1689	-47.7923	1.07
Compound_419-P7	41.1193	-42.9188	0.88
Compound_423-P7	49.7050	-41.9523	1.00
Compound_424-P7	46.0735	-45.5293	1.04
Compound_426-P7	34.2426	-38.0964	0.62
Compound_427-P7	51.0134	-42.5845	1.04
Compound_428-P7	47.0479	-45.9601	1.07
Compound_429-P7	49.9917	-43.9303	1.06
Compound_433-P7	50.0393	-45.3116	1.10
Compound_435-P7	34.9448	-48.3269	0.93
Compound_438-P7	67.2594	-48.7786	1.49
Compound_440-P7	41.7704	-42.8927	0.89
Compound_441-P7	50.7287	-46.6395	1.15
Compound_491-P7	60.0033	-43.3995	1.22
Compound_492-P7	53.6260	-46.0269	1.18
Compound_497-P7	42.0318	-50.1116	1.10
Compound_503-P7	45.0105	-46.4631	1.05
Compound_504-P7	54.4168	-47.1932	1.23
Compound_505-P7	27.8368	-44.1594	0.69
Compound_506-P7	59.5712	-46.1338	1.29
Compound_512-P7	63.3786	-41.6824	1.22
Compound_513-P7	44.7969	-45.4168	1.02
Compound_514-P7	63.0252	-49.2109	1.44
Compound_515-P7	42.5631	-48.9451	1.08
Compound_519-P7	58.8225	-47.5591	1.32
Compound_525-P7	36.6566	-47.2137	0.93
Compound_526-P7	38.8735	-48.9553	1.02
Compound_527-P7	63.6320	-48.0952	1.41
Compound_528-P7	55.7065	-42.5877	1.12
Compound_529-P7	55.0275	-43.7948	1.14
Compound_532-P7	48.0804	-44.5346	1.05
Compound_533-P7	36.8649	-43.3708	0.82
Compound_534-P7	57.5201	-46.5198	1.26
Compound_535-P7	28.4751	-39.1946	0.56
Compound_536-P7	47.8897	-40.7104	0.93
Compound_537-P7	40.3546	-42.8663	0.87
Compound_538-P7	51.8337	-44.6102	1.11
Compound_539-P7	59.2676	-45.2622	1.26
Compound_540-P7	62.6605	-46.9015	1.36

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_542-P7	53.2690	-44.4052	1.13
Compound_547-P7	39.1288	-42.8016	0.84
Compound_548-P7	55.6706	-44.2329	1.17
Compound_549-P7	40.8567	-42.6019	0.87
Compound_550-P7	57.5311	-44.1264	1.19
Compound_551-P7	48.5801	-43.6281	1.03
Compound_554-P7	55.1745	-46.4190	1.22
Compound_555-P7	55.8267	-45.9231	1.22
Compound_557-P7	51.8231	-46.1747	1.16
Compound_558-P7	52.4433	-46.1038	1.17
Compound_559-P7	58.8429	-48.1063	1.33
Compound_562-P7	44.2092	-45.8203	1.02
Compound_567-P7	45.1722	-45.7881	1.03
Compound_575-P7	36.3140	-40.1496	0.72
Compound_576-P7	54.1816	-41.4414	1.06
Compound_582-P7	50.6838	-46.2138	1.14
Compound_587-P7	52.2550	-45.3085	1.14
Compound_596-P7	34.7073	-44.4974	0.82
Compound_597-P7	42.3632	-48.3040	1.06
Compound_598-P7	65.0987	-48.2946	1.44
Compound_616-P7	44.9856	-46.7043	1.06
Compound_617-P7	35.4250	-48.5027	0.95
Compound_631-P7	60.5947	-46.4641	1.31
Compound_632-P7	51.8732	-43.2625	1.07
Compound_638-P7	58.0488	-41.7640	1.13
Compound_639-P7	48.0521	-46.5003	1.10
Compound_640-P7	44.9445	-46.7717	1.06
Compound_641-P7	60.3131	-49.3209	1.39
Compound_645-P7	54.7256	-48.8541	1.28
Compound_651-P7	55.9006	-45.7770	1.21
Compound_652-P7	53.7272	-48.5893	1.26
Compound_653-P7	64.6774	-46.9398	1.40
Compound_654-P7	49.4077	-41.7048	0.99
Compound_658-P7	61.6856	-43.6430	1.25
Compound_659-P7	33.9288	-46.7147	0.87
Compound_661-P7	57.4340	-38.7755	1.04
Compound_662-P7	58.0144	-42.6120	1.16
Compound_663-P7	60.5544	-43.5015	1.23
Compound_664-P7	51.6558	-45.7524	1.14
Compound_668-P7	48.5560	-44.4393	1.05
Compound_670-P7	35.5997	-46.3179	0.88
Compound_672-P7	52.0472	-46.8103	1.18
Compound_674-P7	47.4989	-45.0857	1.05
Compound_675-P7	45.4854	-44.4555	1.00
Compound_988-P7	63.1445	-44.8086	1.31
Compound_989-P7	46.0425	-43.2745	0.97

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_990-P7	68.7976	-44.8573	1.41
Compound_991-P7	43.0879	-39.0598	0.80
Compound_992-P7	43.4406	-41.2573	0.87
Compound_993-P7	47.8244	-43.7736	1.02
Compound_994-P7	48.2157	-45.5070	1.08
Compound_995-P7	54.1487	-44.7404	1.15
Compound_996-P7	61.7700	-46.4941	1.34
Compound_998-P7	51.0344	-44.7981	1.10
Compound_1003-P7	56.0963	-45.0925	1.20
Compound_1004-P7	49.8601	-46.4468	1.13
Compound_1005-P7	41.4557	-44.4094	0.93
Compound_1006-P7	51.4131	-43.4204	1.07
Compound_1007-P7	44.6485	-46.6340	1.05
Compound_1010-P7	24.2092	-45.6451	0.67
Compound_1011-P7	50.0060	-47.4394	1.16
Compound_1013-P7	49.0411	-40.3595	0.94
Compound_1014-P7	31.3983	-44.0779	0.75
Compound_1015-P7	53.4778	-44.6068	1.14
Compound_1016-P7	43.0958	-45.9149	1.00
Compound_1017-P7	76.9825	-46.3706	1.59
Compound_1020-P7	56.4577	-46.0486	1.23
Compound_1025-P7	49.2571	-44.8950	1.08
Compound_1027-P7	41.0732	-45.5809	0.96
Compound_1030-P7	35.1609	-48.2846	0.93
Compound_1031-P7	61.5070	-45.1770	1.29
Compound_1032-P7	34.2633	-44.4699	0.81
Compound_1033-P7	38.7333	-40.1340	0.76
Compound_1034-P7	48.1150	-40.3839	0.93
Compound_1035-P7	50.0398	-44.9141	1.09
Compound_1036-P7	49.0007	-48.0321	1.16
Compound_1037-P7	57.8175	-49.3548	1.35
Compound_1039-P7	56.5373	-48.1990	1.30
Compound_1040-P7	43.4134	-43.3160	0.93
Compound_1046-P7	27.3222	-46.8431	0.76
Compound_1047-P7	62.2649	-43.4808	1.26
Compound_1048-P7	60.9192	-44.4013	1.26
Compound_1049-P7	48.5697	-41.0781	0.95
Compound_1050-P7	48.2960	-43.8128	1.03
Compound_1053-P7	56.7662	-46.2670	1.24
Compound_1054-P7	47.6393	-45.9481	1.08
Compound_1055-P7	34.5225	-46.3250	0.87
Compound_1056-P7	28.0052	-39.5815	0.56
Compound_1057-P7	45.7558	-41.9460	0.93
Compound_1058-P7	49.4618	-42.5955	1.01
Compound_1059-P7	48.8295	-43.9761	1.04
Compound_1060-P7	54.4170	-45.9272	1.19

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1061-P7	58.0496	-47.1278	1.29
Compound_1063-P7	55.4802	-45.0427	1.19
Compound_1069-P7	58.7877	-43.3827	1.19
Compound_1070-P7	53.2698	-44.9882	1.15
Compound_1071-P7	42.0649	-43.5490	0.91
Compound_1072-P7	55.1345	-43.1295	1.12
Compound_1073-P7	40.6190	-41.9544	0.84
Compound_1076-P7	52.0019	-44.3496	1.11
Compound_1077-P7	47.8801	-44.5240	1.04
Compound_1079-P7	46.1192	-40.0443	0.88
Compound_1080-P7	45.1577	-40.5355	0.88
Compound_1081-P7	49.9214	-43.0975	1.03
Compound_1082-P7	53.1543	-46.2784	1.18
Compound_1083-P7	55.2366	-45.6333	1.20
Compound_1084-P7	55.2415	-45.2812	1.19
Compound_1086-P7	53.5856	-44.3207	1.13
Compound_1092-P7	45.6870	-43.5625	0.98
Compound_1093-P7	48.7179	-44.8023	1.06
Compound_1094-P7	37.5584	-43.8543	0.85
Compound_1095-P7	56.5508	-46.3014	1.24
Compound_1100-P7	63.6211	-44.7881	1.32
Compound_1101-P7	42.1680	-47.1739	1.02
Compound_1102-P7	43.5070	-45.8370	1.01
Compound_1103-P7	42.3697	-44.3443	0.94
Compound_1106-P7	54.7315	-45.8848	1.20
Compound_1107-P7	48.7362	-47.0811	1.13
Compound_1109-P7	41.8113	-41.2703	0.84
Compound_1110-P7	43.0842	-43.0079	0.92
Compound_1111-P7	56.1495	-47.5263	1.27
Compound_1112-P7	57.4736	-46.6771	1.27
Compound_1113-P7	59.8331	-49.9864	1.40
Compound_1114-P7	26.0823	-50.2973	0.84
Compound_1116-P7	50.4961	-43.8373	1.07
Compound_1119-P7	55.5477	-47.5485	1.26
Compound_1120-P7	42.8729	-46.7575	1.02
Compound_1122-P7	35.4879	-41.3346	0.74
Compound_1123-P7	45.1618	-41.9521	0.92
Compound_1124-P7	53.8451	-43.8525	1.12
Compound_1125-P7	47.2094	-45.4283	1.06
Compound_1126-P7	50.0000	-48.2437	1.19
Compound_1127-P7	57.8107	-48.3901	1.32
Compound_1129-P7	53.8421	-45.9842	1.19
Compound_1134-P7	54.8289	-44.6972	1.16
Compound_1135-P7	47.2085	-44.2273	1.02
Compound_1136-P7	49.3701	-45.3852	1.09
Compound_1137-P7	49.3998	-49.0433	1.20

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1142-P7	46.4063	-47.3593	1.10
Compound_1143-P7	55.4273	-44.9920	1.18
Compound_1144-P7	40.3648	-47.2221	0.99
Compound_1145-P7	39.7674	-44.4527	0.90
Compound_1148-P7	44.6979	-47.2099	1.07
Compound_1149-P7	46.4771	-50.3345	1.19
Compound_1151-P7	55.3563	-42.5174	1.11
Compound_1152-P7	53.0437	-43.5705	1.10
Compound_1153-P7	47.2235	-44.1946	1.02
Compound_1154-P7	47.7456	-49.8509	1.19
Compound_1155-P7	46.5206	-47.7123	1.11
Compound_1156-P7	43.4202	-47.4515	1.05
Compound_1158-P7	40.7167	-39.6695	0.78
Compound_1159-P7	44.5861	-40.5479	0.87
Compound_1162-P7	44.0260	-42.8209	0.93
Compound_1163-P7	35.3629	-42.5079	0.77
Compound_1165-P7	57.5551	-38.2776	1.03
Compound_1166-P7	40.0313	-38.9921	0.75
Compound_1167-P7	67.2561	-42.3947	1.31
Compound_1168-P7	54.0735	-42.4415	1.09
Compound_1169-P7	58.7526	-44.2039	1.22
Compound_1170-P7	57.2003	-44.0451	1.19
Compound_1172-P7	53.6726	-41.2468	1.05
Compound_1178-P7	54.7105	-41.5541	1.07
Compound_1179-P7	43.6681	-41.4372	0.88
Compound_1180-P7	39.8248	-41.4595	0.82
Compound_1181-P7	37.5349	-43.6808	0.84
Compound_1182-P7	46.5579	-45.6844	1.05
Compound_1185-P7	37.6943	-47.5357	0.96
Compound_1186-P7	48.7876	-45.8498	1.10
Compound_1188-P7	41.8693	-41.1316	0.84
Compound_1189-P7	55.4273	-42.3838	1.11
Compound_1190-P7	49.2750	-44.9783	1.08
Compound_1191-P7	60.1238	-47.2304	1.33
Compound_1192-P7	47.6756	-49.4890	1.18
Compound_1195-P7	60.7008	-47.9932	1.36
Compound_1201-P7	54.1487	-46.2430	1.20
Compound_1210-P7	56.7450	-47.3211	1.27
Compound_1213-P7	63.0518	-45.8191	1.34
Compound_1214-P7	39.5158	-48.2963	1.01
Compound_1220-P7	37.5482	-42.6021	0.81
Compound_1221-P7	42.5073	-43.5469	0.92
Compound_1227-P7	46.6020	-47.5940	1.11
Compound_1228-P7	38.6451	-48.3347	1.00
Compound_1231-P7	48.9072	-51.0712	1.25
Compound_1232-P7	44.2712	-44.6155	0.98

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1234-P7	48.7559	-42.2682	0.99
Compound_1235-P7	48.7508	-43.7393	1.03
Compound_1236-P7	44.4323	-42.2195	0.92
Compound_1237-P7	36.2023	-47.5739	0.93
Compound_1238-P7	47.1771	-47.5981	1.12
Compound_1241-P7	52.3447	-49.4171	1.26
Compound_1246-P7	51.7953	-44.3638	1.10
Compound_1248-P7	34.7258	-45.0281	0.83
Compound_1255-P7	52.0308	-41.9064	1.04
Compound_1256-P7	53.8280	-45.0526	1.16
Compound_1283-P7	52.7780	-43.2154	1.09
Compound_1289-P7	39.7204	-48.3789	1.01
Compound_1296-P7	52.2646	-42.2400	1.05
Compound_1297-P7	50.8190	-43.8688	1.07
Compound_1317-P7	57.0612	-45.6242	1.23
Compound_1324-P7	47.9153	-42.5070	0.98
Compound_1325-P7	42.2873	-44.2302	0.94
Compound_1347-P7	47.1938	-41.1026	0.93
Compound_1348-P7	33.1047	-42.6453	0.74
Compound_1361-P7	32.7711	-45.1943	0.80
Compound_1362-P7	46.6821	-45.9872	1.06
Compound_1393-P7	34.2026	-44.1673	0.80
Compound_1394-P7	41.1329	-46.2514	0.98
Compound_1407-P7	42.5194	-44.0975	0.94
Compound_1408-P7	52.5174	-45.4862	1.15
Compound_1438-P7	41.4382	-40.9327	0.83
Compound_1439-P7	40.6237	-42.5290	0.86
Compound_1452-P7	38.8575	-43.0128	0.84
Compound_1468-P7	50.8079	-35.1998	0.82
Compound_1469-P7	52.9611	-33.9433	0.82
Compound_1470-P7	41.0046	-36.7307	0.70
Compound_1482-P7	44.3074	-35.9517	0.73
Compound_1487-P7	52.3339	-40.9762	1.01
Compound_1498-P7	46.3969	-39.5598	0.87
Compound_1516-P7	55.9473	-39.6403	1.04
Compound_1517-P7	58.8236	-44.2129	1.22
Compound_1603-P7	56.2907	-43.0720	1.14
Compound_1605-P7	64.7256	-44.4147	1.33
Compound_1673-P7	63.4099	-42.5593	1.25
Compound_1676-P7	47.5411	-41.4944	0.95
Compound_1677-P7	70.2605	-41.6239	1.34
Compound_1683-P7	52.3164	-41.7790	1.04
Compound_1689-P7	44.8381	-41.7303	0.91
Compound_1690-P7	47.1889	-42.1786	0.96
Compound_1691-P7	57.9028	-35.3415	0.95
Compound_1932-P7	39.2067	-35.3415	0.63

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1939-P7	40.0871	-34.7056	0.62
Compound_1940-P7	36.9839	-33.3327	0.53
Compound_1948-P7	52.1477	-37.0139	0.90
Compound_1960-P7	27.8331	-32.9491	0.36
Compound_1969-P7	49.7203	-38.8223	0.91
Compound_2061-P7	40.6638	-42.3440	0.86
Compound_2062-P7	41.2426	-40.3393	0.81
Compound_2072-P7	50.0487	-37.6967	0.88
Compound_2075-P7	46.3665	-35.9147	0.77
Compound_2076-P7	41.1939	-36.2081	0.69
Compound_2077-P7	46.9229	-36.1600	0.78
Compound_2078-P7	50.2389	-37.1335	0.87
Compound_2219-P7	59.5093	-40.6528	1.13
Compound_2220-P7	48.5288	-41.5994	0.97
Compound_2222-P7	47.6792	-41.7915	0.96
Compound_2227-P7	43.7923	-39.2945	0.82
Compound_2233-P7	40.4422	-44.3447	0.91
Compound_2242-P7	57.1746	-41.1733	1.10
Compound_2261-P7	56.7244	-38.9581	1.03
Compound_2265-P7	32.7492	-39.9376	0.65
Compound_2266-P7	59.9447	-41.9562	1.17
Compound_2278-P7	42.3927	-44.2449	0.94
Compound_2284-P7	60.5630	-42.0874	1.19
Compound_2285-P7	54.1704	-42.0606	1.08
Compound_2286-P7	36.1607	-31.9691	0.48
Compound_2287-P7	51.5041	-32.4825	0.75
Compound_2289-P7	49.9213	-41.5895	0.99
Compound_2290-P7	49.5830	-40.2178	0.95
Compound_2295-P7	54.0634	-43.3870	1.11
Compound_2305-P7	58.6462	-40.3183	1.10
Compound_2306-P7	46.9475	-39.2798	0.87
Compound_2307-P7	49.7782	-45.4078	1.10
Compound_2338-P7	53.2778	-42.0251	1.06
Compound_2339-P7	38.3655	-48.1124	0.98
Compound_2345-P7	53.5066	-44.9871	1.15
Compound_2355-P7	55.6342	-42.4232	1.11
Compound_2357-P7	46.1940	-49.5161	1.16
Compound_2368-P7	52.2255	-52.0756	1.33
Compound_2374-P7	39.0901	-45.9000	0.93
Compound_2381-P7	45.3531	-43.1673	0.96
Compound_2382-P7	62.1530	-48.4448	1.40
Compound_2383-P7	59.9251	-50.5526	1.42
Compound_2391-P7	49.7859	-49.0996	1.21
Compound_2607-P7	29.1869	-35.6849	0.47
Compound_234-P8	66.7581	-43.3612	1.33
Compound_237-P8	51.2558	-35.2606	0.83

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_240-P8	48.3391	-39.1128	0.89
Compound_243-P8	43.7400	-34.1086	0.67
Compound_244-P8	52.2728	-43.5814	1.09
Compound_246-P8	49.5481	-39.0218	0.91
Compound_249-P8	63.1840	-39.4945	1.16
Compound_250-P8	41.1584	-38.2479	0.75
Compound_259-P8	47.3578	-35.5044	0.77
Compound_262-P8	64.8024	-39.8954	1.20
Compound_263-P8	40.0950	-38.9988	0.75
Compound_264-P8	48.7694	-41.4295	0.97
Compound_272-P8	48.6872	-35.5710	0.80
Compound_275-P8	39.6869	-34.3407	0.61
Compound_278-P8	47.2153	-44.0243	1.02
Compound_282-P8	50.9901	-41.3969	1.00
Compound_283-P8	52.8280	-38.0479	0.94
Compound_291-P8	43.7792	-37.7157	0.77
Compound_293-P8	49.1161	-34.8500	0.78
Compound_294-P8	49.8831	-36.8479	0.85
Compound_295-P8	46.8560	-34.8590	0.74
Compound_297-P8	50.9596	-37.8196	0.90
Compound_300-P8	62.0727	-41.9628	1.21
Compound_301-P8	56.6347	-38.9740	1.03
Compound_302-P8	58.9669	-38.4138	1.05
Compound_309-P8	50.1680	-36.3394	0.84
Compound_310-P8	49.7774	-34.9892	0.80
Compound_311-P8	47.3688	-36.9788	0.81
Compound_356-P8	53.4808	-42.9691	1.09
Compound_360-P8	48.4684	-37.7017	0.85
Compound_364-P8	43.3320	-37.8874	0.77
Compound_365-P8	51.8931	-36.8620	0.89
Compound_366-P8	41.6550	-36.7185	0.71
Compound_367-P8	39.8893	-38.4484	0.73
Compound_368-P8	46.6480	-35.2284	0.75
Compound_369-P8	52.1840	-41.5860	1.03
Compound_370-P8	53.9022	-42.9437	1.10
Compound_373-P8	54.3560	-36.4802	0.92
Compound_374-P8	63.3215	-44.7287	1.31
Compound_377-P8	47.8563	-44.6944	1.05
Compound_379-P8	47.1400	-40.0088	0.90
Compound_380-P8	42.5206	-40.0128	0.82
Compound_381-P8	41.8349	-40.3424	0.82
Compound_383-P8	45.9202	-42.4180	0.95
Compound_499-P8	45.1889	-38.5822	0.82
Compound_502-P8	37.6133	-36.8247	0.64
Compound_506-P8	53.5357	-40.8220	1.03
Compound_507-P8	54.9782	-44.7738	1.17

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_580-P8	50.9781	-39.5543	0.95
Compound_595-P8	48.0214	-31.7714	0.67
Compound_596-P8	48.5997	-42.0152	0.98
Compound_597-P8	60.5640	-40.7418	1.15
Compound_611-P8	35.0713	-39.7403	0.69
Compound_616-P8	50.2853	-36.8033	0.86
Compound_636-P8	51.8386	-41.9582	1.03
Compound_637-P8	56.7927	-42.2312	1.13
Compound_638-P8	44.2565	-43.2905	0.94
Compound_641-P8	47.8816	-44.8940	1.05
Compound_741-P8	59.5267	-34.5549	0.95
Compound_799-P8	44.6625	-40.7156	0.88
Compound_810-P8	48.3540	-30.3269	0.64
Compound_820-P8	49.9588	-35.6467	0.82
Compound_821-P8	41.5550	-38.7559	0.77
Compound_906-P8	62.6327	-40.6224	1.18
Compound_927-P8	42.1238	-37.9173	0.75
Compound_928-P8	44.1423	-38.4696	0.80
Compound_929-P8	32.6839	-37.8176	0.59
Compound_930-P8	30.5247	-35.4441	0.48
Compound_931-P8	38.0321	-35.7559	0.62
Compound_932-P8	35.3340	-30.2779	0.42
Compound_933-P8	48.3145	-38.2636	0.87
Compound_934-P8	35.9008	-35.6987	0.58
Compound_935-P8	44.8941	-32.1905	0.63
Compound_936-P8	38.7300	-35.8318	0.63
Compound_937-P8	56.0910	-40.1107	1.05
Compound_938-P8	48.6016	-37.1475	0.84
Compound_939-P8	45.4500	-36.2572	0.76
Compound_940-P8	47.9712	-34.3684	0.75
Compound_945-P8	47.3202	-35.6250	0.77
Compound_946-P8	38.9769	-34.1023	0.59
Compound_947-P8	47.8052	-38.6357	0.87
Compound_952-P8	47.2836	-37.9630	0.84
Compound_954-P8	58.2165	-37.4743	1.01
Compound_955-P8	53.6321	-38.4914	0.96
Compound_956-P8	45.8146	-40.0473	0.88
Compound_960-P8	44.5847	-36.1536	0.74
Compound_961-P8	40.9954	-35.5142	0.66
Compound_962-P8	42.2871	-35.4578	0.68
Compound_963-P8	39.6413	-39.5175	0.76
Compound_965-P8	45.8753	-36.0580	0.76
Compound_967-P8	39.2451	-34.5654	0.61
Compound_968-P8	34.1728	-34.1753	0.51
Compound_969-P8	36.5298	-34.7004	0.56
Compound_971-P8	53.2566	-38.5804	0.96

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_972-P8	45.6230	-36.7384	0.78
Compound_1008-P8	60.8023	-43.0194	1.22
Compound_1009-P8	47.4767	-43.1303	0.99
Compound_1022-P8	69.6801	-45.7845	1.45
Compound_1029-P8	47.4867	-45.5367	1.06
Compound_1030-P8	43.7360	-45.3438	0.99
Compound_1052-P8	51.8200	-42.6611	1.05
Compound_1053-P8	48.4235	-42.8833	1.00
Compound_1062-P8	61.2329	-46.9038	1.34
Compound_1075-P8	64.2151	-42.6068	1.26
Compound_1076-P8	54.8990	-44.2344	1.15
Compound_1085-P8	38.9881	-47.6185	0.98
Compound_1098-P8	43.2054	-42.0926	0.89
Compound_1099-P8	56.0493	-42.9997	1.14
Compound_1108-P8	56.4600	-46.2937	1.24
Compound_1119-P8	48.9683	-44.4081	1.06
Compound_1120-P8	52.0397	-47.8346	1.21
Compound_1128-P8	29.8796	-49.1313	0.87
Compound_1137-P8	49.9720	-45.2743	1.10
Compound_1138-P8	47.1697	-45.2544	1.05
Compound_1147-P8	56.3803	-50.7134	1.37
Compound_1159-P8	33.1459	-44.1839	0.78
Compound_1160-P8	48.7034	-44.2964	1.05
Compound_1169-P8	50.0077	-46.8630	1.15
Compound_1183-P8	44.9881	-42.9751	0.95
Compound_1184-P8	37.8612	-42.1564	0.80
Compound_1193-P8	46.5732	-45.6206	1.05
Compound_1207-P8	38.3617	-45.0213	0.89
Compound_1208-P8	30.6709	-45.3912	0.77
Compound_1209-P8	59.8290	-47.2808	1.32
Compound_1231-P8	30.6124	-49.1296	0.88
Compound_1232-P8	51.3203	-47.0736	1.17
Compound_1255-P8	45.0792	-43.6716	0.97
Compound_1256-P8	56.2279	-46.0730	1.23
Compound_1257-P8	31.1806	-46.2615	0.81
Compound_1582-P8	39.0920	-44.0604	0.88
Compound_1604-P8	29.9325	-45.3797	0.76
Compound_1605-P8	76.8056	-43.8847	1.52
Compound_1606-P8	48.7200	-44.6315	1.06
Compound_1612-P8	30.4653	-47.2524	0.82
Compound_1614-P8	63.0598	-43.2741	1.26
Compound_1615-P8	46.3273	-43.5493	0.99
Compound_1616-P8	45.7255	-43.5357	0.98
Compound_1617-P8	55.4224	-43.8335	1.15
Compound_1618-P8	52.2124	-42.9689	1.07
Compound_1619-P8	40.2125	-44.7658	0.92

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1620-P8	48.0125	-36.9973	0.83
Compound_1621-P8	39.7003	-44.3787	0.90
Compound_1622-P8	38.5066	-44.4851	0.88
Compound_1623-P8	50.2636	-42.9684	1.04
Compound_1624-P8	37.1187	-43.9392	0.84
Compound_1625-P8	52.3956	-43.9544	1.10
Compound_1626-P8	46.7194	-46.0731	1.07
Compound_1627-P8	46.4625	-44.7853	1.03
Compound_1628-P8	53.1812	-45.1513	1.15
Compound_1629-P8	61.8198	-41.9734	1.20
Compound_1630-P8	42.4086	-44.1176	0.94
Compound_1631-P8	41.1979	-45.1861	0.95
Compound_1651-P8	50.4131	-42.3743	1.02
Compound_1653-P8	56.3467	-43.8525	1.17
Compound_1654-P8	55.9789	-44.9659	1.19
Compound_1660-P8	53.7903	-45.7219	1.18
Compound_1677-P8	55.1174	-43.0060	1.12
Compound_1678-P8	49.6692	-45.3543	1.10
Compound_1679-P8	35.8870	-42.1969	0.77
Compound_1680-P8	54.5600	-43.1169	1.11
Compound_1681-P8	39.7469	-45.0686	0.92
Compound_1682-P8	53.6332	-43.7158	1.12
Compound_1683-P8	50.2368	-42.5862	1.03
Compound_1684-P8	34.3412	-46.4047	0.87
Compound_1713-P8	38.5986	-41.4477	0.79
Compound_1714-P8	56.2865	-44.8722	1.19
Compound_1715-P8	41.0827	-42.3735	0.86
Compound_1716-P8	35.5314	-41.7717	0.75
Compound_1717-P8	43.6846	-43.0485	0.93
Compound_1718-P8	35.9507	-42.9935	0.79
Compound_1719-P8	57.3505	-37.7274	1.01
Compound_1720-P8	44.8007	-43.1045	0.95
Compound_1721-P8	42.7316	-44.5330	0.95
Compound_1722-P8	40.3361	-44.2291	0.90
Compound_1723-P8	51.9612	-46.0525	1.16
Compound_1724-P8	39.6201	-41.5765	0.82
Compound_1725-P8	46.3607	-46.3702	1.07
Compound_1726-P8	45.1584	-45.2790	1.02
Compound_1727-P8	55.0489	-46.9348	1.23
Compound_1728-P8	58.3488	-42.7117	1.17
Compound_1729-P8	48.2737	-46.4172	1.10
Compound_1730-P8	51.3169	-48.2427	1.21
Compound_1731-P8	57.6523	-45.8649	1.25
Compound_1782-P8	53.2232	-42.4581	1.07
Compound_1783-P8	53.6952	-46.5468	1.20
Compound_1784-P8	52.7307	-42.4129	1.06

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1787-P8	44.7249	-45.7317	1.02
Compound_1821-P8	41.5617	-46.8208	1.00
Compound_1822-P8	37.8108	-43.9275	0.85
Compound_1823-P8	38.7755	-46.0004	0.93
Compound_1824-P8	49.6990	-44.5159	1.07
Compound_1825-P8	39.9135	-41.9044	0.83
Compound_1828-P8	55.1100	-46.8770	1.23
Compound_2154-P8	41.8642	-36.4461	0.71
Compound_2159-P8	51.6423	-39.5086	0.96
Compound_2162-P8	33.6694	-31.5508	0.42
Compound_2163-P8	37.1513	-33.3939	0.54
Compound_2165-P8	34.6978	-32.6078	0.47
Compound_2167-P8	44.3774	-33.2440	0.65
Compound_2173-P8	44.0840	-35.2711	0.71
Compound_6-P9	56.6723	-35.4705	0.93
Compound_35-P9	51.8540	-37.8461	0.92
Compound_59-P9	58.5436	-43.0203	1.18
Compound_60-P9	50.1989	-31.2840	0.70
Compound_85-P9	53.5339	-44.3993	1.13
Compound_86-P9	49.3914	-41.8339	0.99
Compound_87-P9	44.8840	-45.2601	1.01
Compound_92-P9	53.5161	-44.5448	1.14
Compound_93-P9	61.7821	-44.3497	1.27
Compound_102-P9	40.8128	-44.5186	0.92
Compound_105-P9	59.3451	-44.4403	1.23
Compound_108-P9	43.4862	-42.9345	0.92
Compound_109-P9	46.7786	-42.0374	0.95
Compound_110-P9	46.4726	-43.0904	0.98
Compound_111-P9	32.0345	-44.8822	0.78
Compound_117-P9	66.2463	-43.9321	1.34
Compound_132-P9	38.4395	-45.3696	0.91
Compound_133-P9	40.7431	-45.6136	0.95
Compound_134-P9	66.0641	-43.2382	1.31
Compound_139-P9	54.9778	-46.2290	1.21
Compound_169-P9	56.0238	-42.4957	1.12
Compound_170-P9	51.2486	-42.5217	1.04
Compound_171-P9	53.8857	-46.8513	1.21
Compound_184-P9	53.3823	-45.1516	1.15
Compound_187-P9	56.2059	-46.7496	1.25
Compound_190-P9	60.1112	-41.6768	1.17
Compound_191-P9	39.9297	-44.2897	0.90
Compound_192-P9	44.5439	-45.5641	1.02
Compound_197-P9	48.2938	-43.6699	1.02
Compound_211-P9	44.2379	-42.3409	0.92
Compound_212-P9	66.3741	-46.1872	1.40
Compound_213-P9	53.9485	-47.1849	1.22

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_219-P9	60.1285	-46.4408	1.31
Compound_249-P9	44.1133	-43.1929	0.94
Compound_250-P9	48.1389	-40.5958	0.93
Compound_251-P9	55.7430	-42.3900	1.11
Compound_255-P9	47.4842	-44.2210	1.03
Compound_267-P9	54.6465	-42.1503	1.09
Compound_285-P9	45.8549	-44.5520	1.01
Compound_286-P9	51.8638	-42.4697	1.05
Compound_287-P9	53.1295	-44.8534	1.14
Compound_326-P9	31.6662	-44.2477	0.76
Compound_327-P9	51.4042	-46.6229	1.16
Compound_328-P9	39.0728	-46.7401	0.96
Compound_347-P9	55.7397	-46.0147	1.22
Compound_348-P9	58.5378	-43.3956	1.19
Compound_349-P9	45.8451	-47.9201	1.11
Compound_367-P9	62.4658	-44.9364	1.30
Compound_368-P9	45.6230	-48.2249	1.11
Compound_1637-P9	47.0912	-42.0385	0.96
Compound_1638-P9	48.7201	-41.4095	0.97
Compound_1639-P9	52.7153	-37.6972	0.93
Compound_1641-P9	46.9770	-37.6918	0.83
Compound_1643-P9	58.6849	-37.1289	1.01
Compound_1644-P9	50.6211	-35.6836	0.83
Compound_1645-P9	41.4088	-35.2710	0.66
Compound_1646-P9	38.7933	-36.0257	0.64
Compound_1647-P9	51.4704	-38.5231	0.93
Compound_1655-P9	54.2538	-37.7755	0.95
Compound_1657-P9	51.7163	-36.1179	0.86
Compound_1659-P9	58.1652	-37.3293	1.01
Compound_1660-P9	59.7533	-38.7719	1.08
Compound_1739-P9	48.7904	-43.3774	1.02
Compound_1763-P9	61.3436	-38.7019	1.10
Compound_1764-P9	56.2121	-39.6824	1.04
Compound_1765-P9	58.6354	-41.1602	1.13
Compound_1766-P9	60.1777	-40.0006	1.12
Compound_1767-P9	68.6311	-39.4588	1.25
Compound_1769-P9	44.9763	-40.8157	0.88
Compound_1777-P9	44.1812	-33.6788	0.66
Compound_1778-P9	42.9588	-35.5958	0.70
Compound_1779-P9	50.7943	-42.0577	1.02
Compound_1781-P9	45.5567	-39.1373	0.85
Compound_1782-P9	50.7745	-40.4750	0.97
Compound_1789-P9	65.0951	-42.1232	1.26
Compound_1790-P9	60.4844	-42.6247	1.20
Compound_1791-P9	66.2567	-39.9695	1.22
Compound_1805-P9	46.3417	-47.5761	1.10

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_1806-P9	46.7299	-43.2352	0.98
Compound_1808-P9	68.8611	-46.9763	1.47
Compound_1809-P9	48.1966	-41.4197	0.96
Compound_1810-P9	54.6069	-45.2270	1.18
Compound_1814-P9	65.1453	-44.1495	1.32
Compound_1827-P9	57.8427	-44.4921	1.21
Compound_1828-P9	61.1266	-44.0879	1.25
Compound_1829-P9	53.5435	-44.9733	1.15
Compound_1963-P9	75.2702	-44.8408	1.52
Compound_1964-P9	64.6144	-44.9779	1.34
Compound_1965-P9	36.7678	-43.5817	0.83
Compound_1966-P9	60.1827	-43.9701	1.23
Compound_1980-P9	57.6712	-45.2954	1.23
Compound_1987-P9	57.4954	-42.8834	1.16
Compound_1988-P9	53.4074	-43.5373	1.11
Compound_2012-P9	57.0437	-46.0182	1.24
Compound_2013-P9	53.8472	-45.6514	1.18
Compound_2014-P9	58.3722	-47.6886	1.31
Compound_2062-P9	44.0666	-40.5500	0.86
Compound_2063-P9	58.6174	-40.7501	1.11
Compound_2064-P9	53.0274	-42.3817	1.07
Compound_2077-P9	46.4774	-44.0407	1.00
Compound_2084-P9	38.7815	-45.1497	0.91
Compound_2107-P9	57.3940	-42.9564	1.16
Compound_2108-P9	41.8756	-41.5723	0.85
Compound_2151-P9	45.6113	-42.8464	0.95
Compound_2152-P9	56.4150	-44.8409	1.20
Compound_2153-P9	64.8657	-44.1578	1.32
Compound_2166-P9	51.4718	-42.7985	1.05
Compound_2172-P9	46.9481	-47.1272	1.10
Compound_2195-P9	63.1438	-47.3715	1.38
Compound_2233-P9	45.7319	-41.2276	0.91
Compound_2234-P9	59.3901	-41.8725	1.16
Compound_2235-P9	39.6725	-44.4722	0.90
Compound_2236-P9	64.2093	-42.4152	1.26
Compound_2250-P9	60.1441	-42.7639	1.20
Compound_2256-P9	55.0731	-46.3385	1.22
Compound_2258-P9	57.1712	-44.3751	1.20
Compound_2259-P9	67.4395	-43.9396	1.36
Compound_2260-P9	51.6293	-46.5666	1.16
Compound_2283-P9	40.4029	-44.2979	0.91
Compound_2284-P9	55.8945	-44.6155	1.18
Compound_2285-P9	49.6169	-44.5675	1.07
Compound_2332-P9	50.4441	-46.0259	1.13
Compound_2354-P9	53.4648	-45.4808	1.16
Compound_2364-P9	42.9190	-46.2681	1.01

Compound	Docking energy, kJ mol ⁻¹		
	GOLD	DOCK6	RANK
Compound_2368-P9	51.1516	-45.6172	1.13
Compound_2379-P9	51.8825	-45.4440	1.14
Compound_2380-P9	39.2950	-47.9497	0.99
Compound_2401-P9	49.7271	-41.8335	1.00
Compound_2402-P9	47.3024	-44.9053	1.04
Compound_2415-P9	48.4849	-47.3998	1.14
Compound_2428-P9	34.6541	-45.4594	0.84
Compound_2436-P9	60.6219	-45.0694	1.27
Compound_2450-P9	41.8648	-45.0780	0.96
Compound_2457-P9	37.3772	-44.6400	0.87
Compound_2477-P9	42.6218	-46.7665	1.02
Compound_2487-P9	54.2181	-46.5911	1.21
Compound_2517-P9	63.1955	-45.9437	1.34

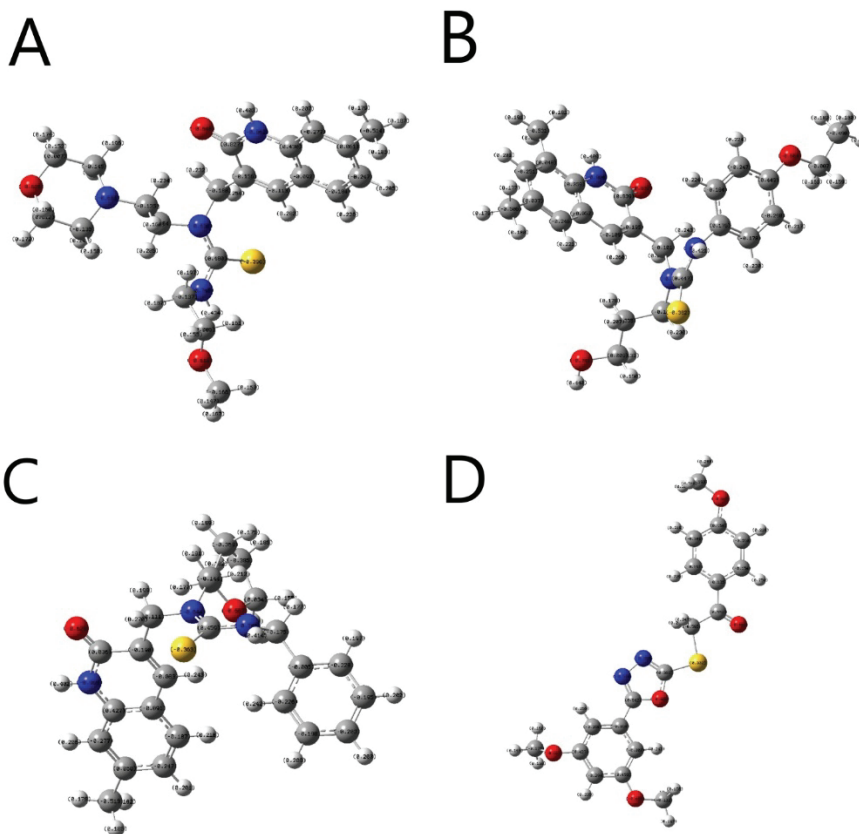


Fig. S-1. Atomic charges of the ligands were calculated using the restrained electrostatic potential (RESP) protocol at the HF/6-31G* level of theory using the Gaussian 09 software. A-3-P5; B-33-P5; C-1466-P6; D-2645-P15.