Predicting Nano-bio Interactions by Integrating Nanoparticle Libraries and Quantitative Nanostructure Activity Relationship Modeling

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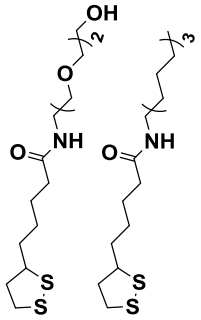
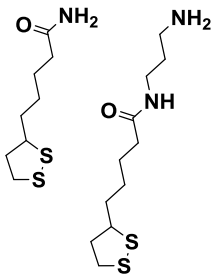
Supplementary Table SI. Experimental characterization of the GNP library members including seven series

Series 1

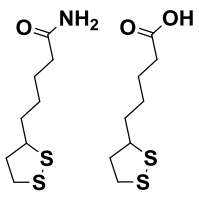
GNP index	# Ligand / GNP 		Size (TEM) (nm)	Zeta potential in water (mV)	Zeta potential in 10% FBS (mV)	Hydrodynamic diameters in water (nm)	PDI in water	Hydrodynamic diameters in 10% FBS (nm)	PDI in 10% FBS	LogP	HO-1 level in A549	Cell uptake in A549 (10^7 GNP/cell)	Cell uptake in HEK293 (10^7 GNP/cell)
1	459 (100%)	0 (0%)	7.3	-13.1±1.6	-19.4±0.4	221.0±10.0	0.367	133.2±0.7	0.224	-2.67±0.06	0.44±0.11	0.2±0.02	0.43±0.03
2	346 (90%)	40 (10%)	6.8	-10.0±1.3	-18.5±0.9	149.9±7.21	0.145	151.1±1.1	0.124	-2.47±0.08	0.47±0.08	0.41±0.33	0.5±0.18
3	311 (74%)	107 (26%)	8.5	-10.3±0.2	-18.3±0.8	156.5±8.06	0.2	157.7±0.7	0.222	-1.61±0.15	1.33±0.13	1.32±0.23	1.71±0.21
4	240 (49%)	251 (51%)	8	-14.1±0.3	-18.5±1.0	301.2±4.8	0.211	216.6±2.9	0.176	-0.88±0.17	1.93±0.12	1.73±0.08	1.93±0.08
5	147 (27%)	390 (73%)	7.5	-17.5±1.2	-18.5±0.8	247.8±8.8	0.139	252.8±4.8	0.205	-0.66±0.05	3.4±0.28	2.41±0.18	3.18±0.19
6	86 (15%)	477 (85%)	8	-20.7±0.1	-17.3±0.7	261.0±2.1	0.207	329.8±3.0	0.322	-0.02±0.26	3.23±0.18	2.51±0.27	3.33±0.08
7	0 (0%)	727 (100%)	6.7	-21.1±0.2	-19.4±1.0	269±0.8	0.232	303.8±1.1	0.343	2.4±0.1	4.1±0.41	6.13±1.24	5.39±0.55

Series 2

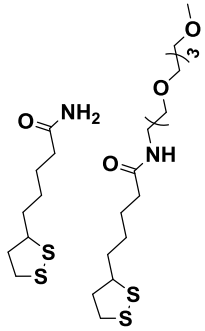
GNP index	# Ligand / GNP 		Size (TEM) (nm)	Zeta potential in water (mV)	Zeta potential in 10% FBS (mV)	Hydrodynamic diameters in water (nm)	PDI in water	Hydrodynamic diameters in 10% FBS (nm)	PDI in 10% FBS	LogP	HO-1 level in A549	Cell uptake in A549 (10^7 GNP/cell)	Cell uptake in HEK293 (10^7 GNP/cell)
8*	232 (100%)	0 (0%)	5.8	-7.2±0.3	-21.4±0.3	106.1±1.4	0.154	133.5±2.5	0.238	-2.56±0.02	1.42±0.44	0.49±0.02	0.49±0.02
9	116 (85%)	21 (15%)	5.8	39.4±0.5	-23.1±0.2	105.5±2.3	0.208	127.4±5.4	0.176	-2.52±0.11	1.95±0.54	0.75±0.02	0.65±0.03
10	101 (77%)	31 (23%)	5.8	42.9±0.6	-26.1±0.7	105.4±1.6	0.183	102.2±3.4	0.149	-2.68±0.11	2.98±0.4	1.64±0.03	1.81±0.27
11	75 (48%)	82 (52%)	5.8	47.6±1.2	-29.3±0.9	70.8±7.4	0.423	99.2±5.8	0.338	-2.35±0.11	3.75±0.44	2.39±0.11	2.64±0.32
12	0 (0%)	144 (100%)	5.8	65.3±1.7	-22.4±0.2	70.7±7.8	0.332	102.4±6.9	0.294	-1.74±0.19	3.93±0.60	4.86±0.41	4.12±0.69

***This one (GNP #8) is same as the first ones in the following three series (series 3,4,5), thus they are all marked as GNP #8.**

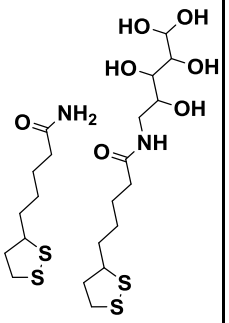
Series 3

GNP index	# Ligand / GNP 		Size (TEM) (nm)	Zeta potential in water (mV)	Zeta potential in 10% FBS (mV)	Hydrodynamic diameters in water (nm)	PDI in water	Hydrodynamic diameters in 10% FBS (nm)	PDI in 10% FBS	LogP	HO-1 level in A549	Cell uptake in A549 (10^7 GNP/cell)	Cell uptake in HEK293 (10^7 GNP/cell)
8	232 (100%)	0 (0%)	5.8	-7.2±0.3	-21.4±0.3	106.1±1.4	0.154	133.5±2.5	0.238	-2.56±0.02	1.42±0.44	0.49±0.02	0.49±0.02
13	201 (87%)	31 (13%)	5.8	-30.7±0.2	-26.3±0.8	121.6±1.1	0.122	102.5±3.7	0.283	-2.59±0.07	0.94±0.17	0.41±0.03	0.45±0.05
14	108 (47%)	124 (53%)	5.8	-33.9±1.2	-30.6±0.9	130.8±1.8	0.188	124.6±2.6	0.183	-2.4±0.07	1.26±0.1	0.48±0.04	0.46±0.02
15	62 (27%)	170 (73%)	5.8	-38.8±0.5	-29.3±0.5	137.7±2.9	0.167	145.3±2.9	0.174	-2.3±0.16	0.88±0.32	0.42±0.02	0.44±0.04
16	0 (0%)	287 (100%)	5.8	-41.5±1.1	-25.9±0.7	147.7±0.9	0.191	112.4±4.6	0.116	-2.21±0.12	0.89±0.32	0.44±0.04	0.42±0.04

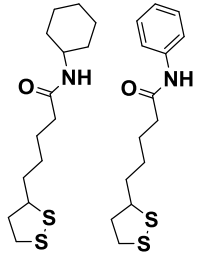
Series 4

GNP index	# Ligand / GNP 		Size (TEM) (nm)	Zeta potential in water (mV)	Zeta potential in 10% FBS (mV)	Hydrodynamic diameters in water (nm)	PDI in water	Hydrodynamic diameters in 10% FBS (nm)	PDI in 10% FBS	LogP	HO-1 level in A549	Cell uptake in A549 (10^7 GNP/cell)	Cell uptake in HEK293 (10^7 GNP/cell)
8	232 (100%)	0 (0%)	5.8	-7.2±0.3	-21.4±0.3	106.1±1.4	0.154	133.5±2.5	0.238	-2.56±0.02	1.42±0.44	0.49±0.02	0.49±0.02
17	676 (91%)	67 (9%)	6.9	-25.1±0.8	-9.19±0.4	160.1±3.3	0.193	167.9±3.0	0.191	-1.72±0.35	2.86±0.32	0.69±0.02	0.69±0.03
18	472 (75%)	158 (25%)	6.6	-25.3±1.1	-10.2±0.3	207.9±4.6	0.366	175.9±3.2	0.288	-2.08±0.06	2.38±0.29	0.61±0.03	0.59±0.02
19	327 (55%)	268 (45%)	6.4	-17.8±0.4	-12.9±0.2	162.5±8.7	0.261	184.9±3.9	0.295	-2.19±0.16	2.07±0.27	0.58±0.07	0.57±0.04
20	0 (0%)	720 (100%)	6.5	-11.3±0.2	-21.4±0.7	154.7±2.7	0.003	143.3±4.7	0.392	-1.92±0.06	2.46±0.25	0.62±0.05	0.6±0.02

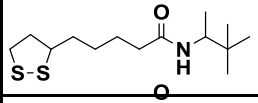
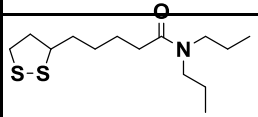
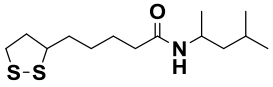
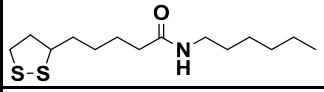
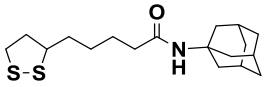
Series 5

GNP index	# Ligand / GNP 		Size (TEM) (nm)	Zeta potential in water (mV)	Zeta potential in 10% FBS (mV)	Hydrodynamic diameters in water (nm)	PDI in water	Hydrodynamic diameters in 10% FBS (nm)	PDI in 10% FBS	LogP	HO-1 level in A549	Cell uptake in A549 (10^7 GNP/cell)	Cell uptake in HEK293 (10^7 GNP/cell)
8	232 (100%)	0 (0%)	5.8	-7.2±0.3	-21.4±0.3	106.1±1.4	0.154	133.5±2.5	0.238	-2.56±0.02	1.42±0.44	0.49±0.02	0.49±0.02
21	673 (88%)	92 (12%)	4.9	-13.0±0.2	-24.6±1.3	459.8±10.2	0.314	260.2±3.6	0.145	-1.8±0.2	2.89±0.24	0.85±0.04	0.81±0.01
22	502 (69%)	226 (31%)	5	-4.0±0.1	-20.9±0.9	450.0± 9.8	0.395	252.3±3.3	0.235	-0.96±0.05	1.41±0.24	0.68±0.04	0.7±0.04
23	221 (29%)	542 (71%)	5.7	-11.6±0.4	-12.2±0.3	546.3±10.4	0.391	218.0±2.2	0.066	-2.42±0.04	1.73±0.1	0.49±0.06	0.47±0.02
24	0 (0%)	810 (100%)	8	-15.8±0.3	-18.5±0.5	149.6±1.8	0.431	192.4±1.9	0.18	-2.28±0.13	1.06±0.11	0.48±0.02	0.45±0.06

Series 6

GNP index	# Ligand / GNP		Size (TEM) (nm)	Zeta potential in water (mV)	Zeta potential in 10% FBS (mV)	Hydrodynamic diameters in water (nm)	PDI in water	Hydrodynamic diameters in 10% FBS (nm)	PDI in 10% FBS	LogP	HO-1 level in A549	Cell uptake in A549 (10^7 GNP/cell)	Cell uptake in HEK293 (10^7 GNP/cell)
													
25	869 (100%)	0 (0%)	7.3	-24.4±0.6	-29.3±0.5	273.2±2.1	0.138	224.5±4.3	0.248	2.06±0.28	2.58±0.3	4.87±0.47	5.04±0.55
26	695 (80%)	174 (20%)	7.3	-27.9±1.1	-32.4±0.9	281.2±3.4	0.283	224.3±2.9	0.195	2.38±0.19	2.28±0.23	5.03±0.59	5.31±0.66
27	348 (40%)	521 (60%)	7.3	-22.0±1.1	-28.6±0.7	236.3±5.7	0.199	233.2±1.8	0.374	2.72±0.2	2.21±0.14	5.39±0.60	5.58±0.26
28	174 (20%)	695 (80%)	7.3	-22.5±0.5	-23.4±0.2	249.5±4.6	0.273	244.9±4.3	0.294	2.67±0.07	1.89±0.15	5.59±0.73	5.26±0.33
29	0 (0%)	869 (100%)	7.3	-23.0±0.5	-28.3±0.7	238.2±7.5	0.263	213.8±5.3	0.327	2.7±0.14	2.21±0.28	5.8±0.65	5.26±0.49

Series 7

GNP index	# Ligand / GNP	Size (TEM) (nm)	Zeta potential in water (mV)	Zeta potential in 10% FBS (mV)	Hydrodynamic diameters in water (nm)	PDI in water	Hydrodynamic diameters in 10% FBS (nm)	PDI in 10% FBS	LogP	HO-1 level in A549	Cell uptake in A549 (10^7 GNP/cell)	Cell uptake in HEK293 (10^7 GNP/cell)
30	 795 (100%)	5.9	-8.0±0.8	-13.8±0.3	236.0±6.1	0.178	212.0±5.0	0.299	2.52±0.13	2.28±0.14	5.33±0.75	5.16±0.65
31	 682 (100%)	5.9	-8.5±0.2	-21.1±0.4	252.5±5.5	0.259	154.0±2.7	0.444	2.28±0.25	2.06±0.16	5.84±0.4	5.27±0.76
32	 830 (100%)	5.9	-7.4±0.3	-21.8±0.5	225.8±8.5	0.185	189.9±3.0	0.342	2.57±0.07	1.92±0.19	5.4±0.49	5.09±0.43
33	 698(100%)	5.9	-12.4±0.6	-11.7±0.4	232.4±1.6	0.219	189.1±3.3	0.389	1.76±0.06	2.11±0.28	5.39±0.58	5.2±0.58
34	 703 (100%)	5.9	-5.7±0.4	-17.0±0.2	284.5±8.3	0.213	210.7±5.8	0.407	1.98±0.07	2.21±0.23	5.55±0.48	5.19±0.67

Supplementary Table SII. The calculated nanodescriptors with their nano-composition and structure

Index	Series	Radius(Ang)	#lig1	#lig2	total#Ligand	TotalSurface Area	AverageSurfaceAreaPerLigand
1	HY 1	36.5	459	0	459	76,869	167
2	HY 2	34	346	40	386	69,746	181
3	HY 3	42.5	311	107	418	100,385	240
4	HY 4	40	240	251	491	98,719	201
5	HY 5	37.5	147	390	537	89,277	166
6	HY 6	40	86	477	563	99,999	178
7	HY 7	33.5	0	727	727	83,923	115
8	PO 1	29	0	232	232	39,980	172
9	PO 2	29	21	116	137	38,158	279
10	PO 3	29	31	101	132	37,158	281
11	PO 4	29	82	75	157	39,017	249
12	PO 5	29	144	0	144	40,072	278
13	NE 2	29	31	201	232	40,324	174
14	NE 3	29	124	108	232	40,960	177
15	NE 4	29	170	62	232	42,036	181
16	NE 5	29	287	0	287	44,688	156
17	HA 2	34.5	67	676	743	59,553	80
18	HA 3	33	158	472	630	55,987	89
19	HA 4	32	268	327	595	62,725	105
20	HA 5	32.5	720	0	720	65,224	91
21	HD 2	24.5	92	673	765	39,259	51
22	HD 3	25	226	502	728	42,573	58
23	HD 4	28.5	542	221	763	52,685	69
24	HD 5	40	810	0	810	99,863	123
25	PI 1	36.5	0	869	869	78,732	91
26	PI 2	36.5	174	695	869	76,487	88
27	PI 3	36.5	521	348	869	76,351	88
28	PI 4	36.5	695	174	869	75,533	87
29	PI 5	36.5	869	0	869	74,966	86
30	MG 1	29.5	795	0	795	45,299	57
31	MG 2	29.5	682	0	682	43,279	63
32	MG 3	29.5	830	0	830	48,982	59
33	MG 4	29.5	698	0	698	54,508	78
34	MG 5	29.5	703	0	703	47,638	68
35	HY_e	32.5	0	536	536	79,934	149
36	Po_e	29	42	102	144	38,379	267
37	Ne_e	29	47	185	232	40,446	174
38	HA_e	26	380	126	506	47,689	94
39	HD_e	25	235	275	510	43,634	86
40	PI_e	36.5	348	521	869	78,833	91
41	MG_e	29.5	869	0	869	48,407	56

Index	TotalPartialCharge	AveragePartialChargePerLigand	Hydrophobic Potential	PotentialEnergy	contactpreference_hyd.grid_ave	contactpreference_hyd.grid_aboveThreshold	contactpreference_lpa.grid_ave
1	-78	-0.17	-0.37	7.95E+08	0.68	8,368	0.56
2	-71	-0.18	0.01	6.59E+08	0.69	7,542	0.55
3	-54	-0.13	0.47	7.11E+08	0.67	7,236	0.55
4	-61	-0.12	1.17	8.55E+08	0.70	8,345	0.53
5	-68	-0.13	1.83	9.21E+08	0.71	9,065	0.52
6	-96	-0.17	2.18	9.82E+08	0.71	9,574	0.52
7	-83	-0.11	3.62	1.26E+09	0.72	10,355	0.49
8	-55	-0.24	0.65	3.85E+08	0.64	14,221	0.58
9	-6	-0.04	0.52	2.31E+08	0.61	11,263	0.58
10	2	0.01	0.31	2.25E+08	0.61	9,947	0.58
11	43	0.27	0.22	2.63E+08	0.62	8,733	0.58
12	105	0.73	0.07	2.49E+08	0.63	7,757	0.58
13	-69	-0.30	0.65	3.91E+08	0.64	14,298	0.58
14	-165	-0.71	0.50	3.93E+08	0.63	13,913	0.58
15	-220	-0.95	0.45	3.92E+08	0.63	14,359	0.58
16	-346	-1.20	0.24	4.87E+08	0.63	12,972	0.59
17	-125	-0.17	-0.06	1.27E+09	0.67	10,857	0.59
18	-107	-0.17	-0.01	1.08E+09	0.69	9,651	0.56
19	-98	-0.16	0.15	1.01E+09	0.70	9,606	0.55
20	-87	-0.12	1.05	1.23E+09	0.72	8,307	0.52
21	-81	-0.11	-1.62	1.35E+09	0.62	9,698	0.63
22	-118	-0.16	-1.92	1.25E+09	0.62	7,928	0.62
23	-134	-0.18	-2.12	1.30E+09	0.62	6,603	0.63
24	-134	-0.17	-1.16	1.37E+09	0.64	8,292	0.62
25	-128	-0.15	2.92	1.49E+09	0.72	8,789	0.50
26	-149	-0.17	3.04	1.50E+09	0.72	9,562	0.51
27	-115	-0.13	3.34	1.49E+09	0.72	12,183	0.51
28	-90	-0.10	3.65	1.50E+09	0.71	13,700	0.51
29	-101	-0.12	4.22	1.50E+09	0.71	15,243	0.51
30	-138	-0.17	4.99	1.38E+09	0.72	16,759	0.45
31	-145	-0.21	6.38	1.18E+09	0.72	16,226	0.46
32	-130	-0.16	4.10	1.45E+09	0.72	17,354	0.47
33	-90	-0.13	2.68	1.21E+09	0.72	13,643	0.49
34	-101	-0.14	5.03	1.23E+09	0.73	6,783	0.50
35	-61	-0.11	3.04	9.38E+08	0.72	11,031	0.50
36	-11	-0.08	0.37	2.41E+08	0.62	10,930	0.58
37	-98	-0.42	0.60	3.90E+08	0.64	14,379	0.58
38	-67	-0.13	0.59	8.79E+08	0.71	11,098	0.53
39	-91	-0.18	-1.12	8.75E+08	0.64	9,344	0.61
40	-118	-0.14	3.06	1.48E+09	0.72	11,075	0.51
41	-109	-0.13	4.33	1.51E+09	0.72	4,788	0.49

Index	contactpreference_lpa.grid_aboveThreshold	electrondensity.grid_ave	electrondensity.grid_aboveThreshold	electrostaticmap_acc.grid_avelog	electrostaticmap_acc.grid_aboveThreshold	electrostaticmap_don.grid_avelog	electrostaticmap_don.grid_aboveThreshold
1	8,602	-3.46	113,728	0.55	82,444	0.66	82,403
2	7,121	-1.71	96,320	0.35	66,018	0.53	65,924
3	5,928	-3.47	147,206	0.24	60,422	0.49	60,444
4	5,152	-1.89	123,387	0.27	57,445	0.49	57,459
5	3,959	1.30	113,758	0.44	68,064	0.57	68,361
6	3,686	0.98	130,611	0.46	71,326	0.59	71,368
7	1,661	3.22	87,989	0.66	86,678	0.71	86,934
8	18,212	1.83	59,880	0.36	60,618	0.55	60,694
9	15,993	-1.35	63,071	0.32	62,267	0.50	62,144
10	16,091	-0.46	57,257	0.24	52,672	0.47	52,440
11	14,193	0.55	63,345	0.22	56,077	0.45	56,197
12	14,651	2.45	59,098	0.20	48,729	0.44	48,656
13	17,903	0.23	67,533	0.43	72,184	0.58	72,020
14	18,802	-0.27	66,248	0.43	71,752	0.58	71,638
15	19,784	-1.69	62,861	0.47	71,993	0.59	71,819
16	19,659	0.19	58,549	0.50	65,536	0.60	65,517
17	13,086	-0.12	89,320	0.57	77,223	0.66	77,094
18	9,944	1.27	89,900	0.52	70,359	0.62	70,405
19	7,089	-2.52	84,782	0.44	65,115	0.57	65,228
20	3,185	-6.14	83,007	0.87	92,134	1.42	196,239
21	21,345	0.37	55,887	0.86	105,525	0.87	105,339
22	21,829	3.02	60,001	0.88	107,789	0.87	107,584
23	22,829	-0.95	65,320	0.98	114,291	0.92	114,039
24	19,647	4.04	141,632	0.70	89,442	0.75	89,319
25	3,865	0.47	119,384	0.95	109,215	0.89	109,247
26	3,607	-3.10	113,058	0.90	107,931	0.89	107,914
27	3,464	-5.18	107,103	0.91	105,749	0.90	105,695
28	3,319	-3.35	108,897	0.90	104,350	0.89	104,287
29	3,127	-0.79	116,524	0.84	103,367	0.84	103,234
30	1,247	5.59	64,612	1.16	116,160	1.04	115,976
31	798	4.98	69,283	1.19	123,430	1.05	123,880
32	1,628	0.00	63,942	1.13	119,301	1.03	119,649
33	2,838	-3.40	58,519	0.87	90,823	0.83	91,161
34	1,548	-0.11	62,331	1.14	120,280	1.02	120,720
35	2,639	-2.41	90,678	0.57	73,854	0.63	74,236
36	16,499	1.15	59,137	0.26	54,062	0.48	53,639
37	18,770	0.35	57,760	0.42	60,192	0.56	60,148
38	5,482	-0.33	57,272	0.85	90,725	0.82	91,024
39	20,506	1.11	53,507	0.72	90,526	0.76	90,359
40	3,973	-3.15	111,636	0.91	106,720	0.89	106,656
41	1,373	-0.30	64,126	1.17	129,708	1.05	130,137

Index	electrostatic map_hyd.grid_avelog	electrostatic map_hyd.grid_aboveThreshold	interactionpotential_br.grid_avelog	interactionpotential_br.grid_aboveThreshold	interactionpotential_br-.grid_avelog	interactionpotential_br-.grid_aboveThreshold	interactionpotential_c1=.grid_avelog
1	1.11	82,774	2.88	32,358	2.89	32,512	2.70
2	0.91	66,297	2.69	26,278	2.70	26,402	2.52
3	0.82	60,545	2.66	20,910	2.67	20,995	2.49
4	0.84	57,651	2.70	22,712	2.72	22,800	2.54
5	0.99	68,053	2.82	29,300	2.84	29,434	2.66
6	1.01	71,480	2.86	29,437	2.88	29,585	2.70
7	1.20	86,921	3.20	38,889	3.23	39,106	3.01
8	0.95	61,014	2.21	22,278	2.05	17,892	2.05
9	0.87	62,551	1.99	20,487	1.99	20,563	1.85
10	0.81	52,512	2.02	17,331	2.02	17,383	1.89
11	0.78	56,391	2.10	19,331	2.10	19,391	1.97
12	0.76	48,936	2.09	17,154	2.09	17,218	1.97
13	1.00	72,527	2.22	26,066	2.23	26,185	2.06
14	1.00	72,021	2.19	25,880	2.20	26,005	2.02
15	1.02	72,257	2.17	25,714	2.18	25,835	2.00
16	1.05	65,664	2.25	24,501	2.28	24,615	2.07
17	1.10	77,540	3.04	33,200	3.06	33,399	2.84
18	1.07	70,443	2.88	33,245	2.90	33,437	2.70
19	0.98	65,279	2.91	29,219	2.93	29,390	2.74
20	1.42	92,136	3.41	45,302	3.43	45,598	3.21
21	1.40	105,927	3.33	48,688	3.36	48,983	3.11
22	1.42	108,243	3.29	50,938	3.33	51,222	3.07
23	1.52	115,086	3.38	57,271	3.42	57,584	3.15
24	1.27	89,708	3.09	38,928	3.12	39,114	2.86
25	1.46	109,531	3.33	47,126	3.36	47,365	3.14
26	1.46	108,246	3.35	46,682	3.37	46,937	3.15
27	1.47	106,171	3.33	45,560	3.36	45,822	3.14
28	1.45	104,751	3.34	45,278	3.36	45,545	3.14
29	1.37	103,737	3.34	44,542	3.36	44,801	3.13
30	1.69	116,286	3.58	57,161	3.61	57,489	3.39
31	1.73	123,513	3.50	59,249	3.53	59,591	3.30
32	1.68	119,326	3.53	60,346	3.56	60,685	3.34
33	1.41	90,897	3.22	44,224	3.24	44,480	3.03
34	1.66	120,133	3.56	60,373	3.58	60,716	3.39
35	1.11	73,883	2.80	35,063	2.82	35,244	2.63
36	0.83	54,271	2.04	18,178	2.04	18,222	1.91
37	0.96	60,291	2.21	21,660	2.22	21,747	2.05
38	1.38	90,727	3.15	43,632	3.17	43,861	2.97
39	1.28	90,916	2.98	41,108	3.02	41,304	2.77
40	1.46	107,103	3.31	46,097	3.34	46,335	3.12
41	1.70	129,772	3.65	64,360	3.68	64,739	3.47

Index	interactionpotential_c1=.grid_aboveThreshold	interactionpotential_c2.grid_avelog	interactionpotential_c2.grid_aboveThreshold	interactionpotential_c3.grid_avelog	interactionpotential_c3.grid_aboveThreshold	interactionpotential_cl.grid_avelog	interactionpotential_cl.grid_aboveThreshold
1	31,789	2.69	31,818	2.76	31,912	2.22	20,047
2	25,871	2.50	25,881	2.57	25,939	2.55	27,736
3	20,537	2.48	20,632	2.55	20,670	2.52	22,046
4	22,304	2.53	22,333	2.60	22,390	2.57	23,933
5	28,979	2.64	29,081	2.71	29,102	2.68	31,092
6	29,004	2.68	29,002	2.70	27,702	2.72	31,142
7	38,365	3.00	38,517	3.07	38,539	3.05	41,309
8	22,001	2.04	21,973	2.10	21,987	2.07	23,272
9	20,037	1.84	20,088	1.89	20,163	1.86	21,547
10	16,913	1.88	16,898	1.93	16,912	1.89	18,031
11	19,073	1.96	19,041	2.02	19,055	1.98	20,225
12	16,837	1.96	16,856	2.01	16,897	1.98	18,077
13	25,600	2.05	25,650	2.11	25,712	1.67	16,166
14	25,394	2.01	25,432	2.07	25,534	2.05	27,283
15	25,303	1.99	25,325	2.05	25,391	2.02	27,084
16	24,220	2.06	24,186	2.12	24,203	2.10	25,986
17	32,831	2.82	32,817	2.90	32,860	2.88	35,193
18	32,815	2.68	32,792	2.76	32,835	2.74	35,320
19	28,868	2.72	28,853	2.79	28,893	2.77	31,037
20	44,837	3.20	44,778	3.28	44,823	3.26	48,071
21	48,171	3.09	48,128	3.17	48,197	3.16	51,604
22	50,407	3.05	50,370	3.13	50,439	3.12	54,160
23	56,945	3.13	56,869	3.21	56,907	3.21	60,407
24	38,323	2.85	38,356	2.92	38,486	2.91	41,385
25	46,493	3.12	46,501	3.20	46,577	3.18	49,944
26	46,156	3.14	46,138	3.22	46,218	3.19	49,540
27	45,025	3.12	44,992	3.20	45,071	3.18	48,352
28	44,712	3.12	44,674	3.20	44,757	3.18	47,915
29	43,978	3.11	43,970	3.19	44,034	3.18	47,152
30	56,717	3.38	56,656	3.45	56,699	3.43	61,196
31	58,648	3.28	58,605	3.36	58,671	3.34	62,865
32	58,549	3.33	59,217	3.40	59,879	3.38	63,704
33	43,793	3.01	43,746	3.09	43,796	3.07	46,870
34	59,295	3.37	59,235	3.44	59,335	3.41	63,890
35	34,673	2.61	34,645	2.68	34,683	2.66	37,178
36	17,920	1.90	17,907	1.95	17,910	1.92	18,751
37	21,570	2.04	21,542	2.10	21,552	2.07	22,881
38	43,328	2.95	43,284	3.03	43,307	3.01	46,965
39	40,641	2.76	40,620	2.83	40,689	2.82	43,543
40	45,524	3.10	45,506	3.18	45,580	3.16	48,868
41	63,917	3.45	63,801	3.53	63,834	3.51	68,271

Index	interactionpotential_cl-.grid_avelog	interactionpotential_cl-.grid_aboveThreshold	interactionpotential_dry.grid_avelog	interactionpotential_dry.grid_aboveThreshold	interactionpotential_f.grid_avelog	interactionpotential_f.grid_aboveThreshold	interactionpotential_f-.grid_avelog
1	2.74	32,059	0	791,925	2.22	30,817	2.22
2	2.55	26,089	0	800,191	2.07	25,126	2.07
3	2.52	20,760	0	784,821	2.04	19,790	2.03
4	2.57	22,483	0	744,465	2.09	21,629	2.09
5	2.69	29,300	0	781,004	2.19	28,167	2.19
6	2.73	29,234	0	773,937	2.22	28,125	2.22
7	3.06	38,854	0	811,750	2.50	37,326	2.52
8	2.07	22,117	0	656,566	1.66	21,304	1.64
9	1.85	20,198	0	710,979	1.49	19,359	1.45
10	1.88	16,975	0	645,912	1.52	16,345	1.48
11	1.97	19,170	0	755,050	1.59	18,475	1.56
12	1.97	16,968	0	664,449	1.59	16,199	1.55
13	2.08	25,838	0	736,749	1.67	24,763	1.65
14	2.05	25,615	0	739,343	1.64	24,536	1.62
15	2.03	25,500	0	728,877	1.61	24,428	1.59
16	2.11	24,359	0	665,605	1.67	23,129	1.65
17	2.90	33,084	0	753,607	2.35	31,868	2.36
18	2.75	33,121	0	783,571	2.23	31,886	2.24
19	2.78	29,123	0	773,368	2.27	28,054	2.28
20	3.27	45,211	0	777,623	2.68	43,675	2.71
21	3.18	48,569	0	802,977	2.65	46,832	2.66
22	3.14	50,844	0	825,749	2.61	49,054	2.63
23	3.22	57,367	0	879,447	2.66	55,783	2.69
24	2.93	38,659	0	806,684	2.39	37,357	2.40
25	3.19	46,865	0	769,463	2.61	45,130	2.63
26	3.21	46,534	0	752,886	2.62	44,832	2.64
27	3.19	45,381	0	721,663	2.61	43,695	2.63
28	3.19	45,074	0	721,763	2.61	43,375	2.63
29	3.19	44,332	0	762,127	2.60	42,716	2.62
30	3.45	57,150	0	720,884	2.88	55,377	2.89
31	3.36	59,142	0	780,155	2.78	57,041	2.79
32	3.40	59,811	0	752,179	2.83	56,748	2.85
33	3.08	44,144	0	722,520	2.53	42,597	2.55
34	3.43	59,808	0	790,540	2.85	56,892	2.88
35	2.67	34,951	0	794,424	2.16	33,757	2.17
36	1.91	18,004	0	653,996	1.54	17,509	1.50
37	2.07	21,669	0	647,665	1.66	20,736	1.64
38	3.02	43,647	0	762,599	2.47	42,409	2.49
39	2.84	40,952	0	801,699	2.33	39,463	2.34
40	3.17	45,883	0	739,142	2.59	44,158	2.61
41	3.52	64,404	0	799,286	2.92	62,417	2.96

Index	interactionpotential_f-.grid_aboveThreshold	interactionpotential_i.grid_avelog	interactionpotential_i.grid_aboveThreshold	interactionpotential_k+.grid_avelog	interactionpotential_k+.grid_aboveThreshold	interactionpotential_n..grid_avelog	interactionpotential_n..grid_aboveThreshold
1	29,435	3.05	32,990	2.44	31,854	2.45	31,601
2	23,996	2.85	26,771	2.26	25,940	2.28	25,733
3	20,398	2.82	21,409	2.25	20,367	2.26	20,376
4	20,492	2.86	23,148	2.28	22,359	2.31	22,195
5	29,040	2.98	29,926	2.38	29,146	2.41	28,968
6	29,103	3.03	30,017	2.42	29,171	2.45	28,881
7	38,678	3.38	39,700	2.70	38,750	2.75	38,248
8	21,855	2.38	22,630	1.87	21,914	1.86	21,821
9	19,832	2.14	21,027	1.71	19,821	1.67	19,824
10	16,673	2.17	17,439	1.75	16,711	1.70	16,740
11	18,919	2.25	19,477	1.81	18,965	1.77	19,078
12	16,698	2.22	17,551	1.81	16,680	1.77	16,649
13	25,501	2.39	26,679	1.88	25,528	1.86	25,417
14	25,318	2.37	26,441	1.84	25,303	1.83	25,210
15	25,154	2.35	26,325	1.81	25,156	1.80	25,101
16	23,833	2.44	25,081	1.86	23,914	1.86	23,895
17	33,049	3.22	33,821	2.56	33,085	2.59	32,673
18	33,056	3.04	33,889	2.43	33,177	2.46	32,712
19	29,156	3.07	29,764	2.46	29,212	2.49	28,793
20	45,370	3.59	46,058	2.91	45,537	2.94	44,787
21	48,582	3.53	49,586	2.82	48,726	2.86	48,050
22	50,890	3.50	51,842	2.79	51,069	2.82	50,292
23	57,743	3.60	57,970	2.86	57,976	2.89	56,972
24	38,602	3.31	39,840	2.58	38,747	2.61	38,112
25	46,776	3.52	47,998	2.83	46,851	2.87	46,304
26	46,408	3.53	47,603	2.85	46,467	2.88	45,965
27	45,239	3.52	46,397	2.83	45,329	2.86	44,821
28	44,991	3.52	46,112	2.84	45,097	2.86	44,523
29	44,257	3.53	45,337	2.83	44,397	2.86	43,792
30	57,522	3.76	58,620	3.08	57,733	3.12	56,696
31	59,268	3.69	60,179	2.99	59,502	3.02	58,521
32	59,049	3.71	61,110	3.03	59,270	3.07	58,316
33	44,241	3.39	44,857	2.73	44,400	2.76	43,686
34	59,239	3.74	61,182	3.07	59,364	3.11	59,251
35	34,976	2.96	35,638	2.34	35,087	2.38	34,573
36	17,884	2.20	18,279	1.76	17,933	1.72	17,923
37	21,427	2.38	22,194	1.87	21,328	1.85	21,401
38	43,919	3.32	44,980	2.68	44,100	2.71	43,334
39	40,920	3.19	41,816	2.50	41,034	2.54	40,485
40	45,762	3.50	46,977	2.82	45,873	2.85	45,329
41	64,832	3.83	65,221	3.15	65,108	3.19	63,898

Index	interactionpotential_n1.grid_avelog	interactionpotential_n1.grid_aboveThreshold	interactionpotential_n1..grid_avelog	interactionpotential_n1..grid_aboveThreshold	interactionpotential_n1+.grid_avelog	interactionpotential_n1+.grid_aboveThreshold	interactionpotential_n1=.grid_avelog
1	2.50	31,651	2.50	31,650	2.52	31,649	2.56
2	2.33	25,764	2.33	25,764	2.35	25,764	2.39
3	2.30	20,407	2.31	20,407	2.34	20,407	2.37
4	2.35	22,224	2.35	22,224	2.37	22,223	2.41
5	2.46	29,023	2.46	29,023	2.48	29,021	2.52
6	2.50	28,931	2.50	28,929	2.51	28,929	2.55
7	2.80	38,324	2.80	38,324	2.81	38,323	2.85
8	1.88	21,856	1.89	21,855	1.94	21,855	1.97
9	1.69	19,842	1.70	19,842	1.78	19,842	1.80
10	1.72	16,750	1.73	16,750	1.82	16,750	1.84
11	1.80	19,094	1.81	19,094	1.88	19,094	1.90
12	1.80	16,671	1.81	16,671	1.87	16,671	1.90
13	1.89	25,453	1.86	24,256	1.95	25,453	1.97
14	1.86	25,262	1.86	25,262	1.91	25,261	1.94
15	1.83	25,137	1.83	25,137	1.88	25,137	1.91
16	1.90	23,939	1.90	23,938	1.93	23,937	1.96
17	2.64	32,733	2.64	32,730	2.65	32,729	2.69
18	2.50	32,785	2.50	32,785	2.51	32,784	2.55
19	2.54	28,863	2.54	28,862	2.55	28,861	2.59
20	3.00	44,866	3.00	44,865	3.00	44,863	3.05
21	2.90	48,131	2.90	48,131	2.91	48,130	2.95
22	2.86	50,386	2.87	50,386	2.87	50,386	2.91
23	2.94	57,088	2.93	57,088	2.94	57,083	2.99
24	2.65	38,177	2.66	38,176	2.67	38,174	2.71
25	2.92	46,379	2.92	46,379	2.93	46,379	2.98
26	2.94	46,065	2.94	46,065	2.94	46,062	2.99
27	2.92	44,919	2.92	44,919	2.93	44,918	2.98
28	2.92	44,601	2.92	44,601	2.93	44,601	2.98
29	2.92	43,875	2.92	43,875	2.92	43,873	2.97
30	3.18	56,813	3.18	56,813	3.18	56,813	3.23
31	3.08	58,650	3.08	58,650	3.09	58,647	3.14
32	3.13	58,438	3.13	58,437	3.13	58,437	3.18
33	2.82	43,787	2.82	43,786	2.82	43,785	2.87
34	3.17	59,407	3.17	59,407	3.17	59,406	3.22
35	2.43	34,632	2.43	34,632	2.44	34,632	2.48
36	1.74	17,940	1.75	17,940	1.83	17,939	1.85
37	1.88	21,426	1.88	21,426	1.94	21,426	1.96
38	2.76	43,421	2.76	43,421	2.77	43,421	2.81
39	2.57	40,555	2.57	40,555	2.58	40,554	2.62
40	2.91	45,413	2.91	45,413	2.91	45,412	2.96
41	3.25	64,036	3.25	64,036	3.25	64,032	3.30

Index	interactionpotential_n1=.grid_aboveThreshold	interactionpotential_n2.grid_avelog	interactionpotential_n2.grid_aboveThreshold	interactionpotential_n2+.grid_avelog	interactionpotential_n2+.grid_aboveThreshold	interactionpotential_n2=.grid_avelog	interactionpotential_n2=.grid_aboveThreshold
1	31,756	2.57	31,738	2.59	31,738	2.63	31,750
2	25,859	2.40	25,834	2.41	25,834	2.45	25,840
3	20,472	2.37	20,453	2.40	20,451	2.43	20,463
4	22,301	2.42	22,294	2.44	22,293	2.47	22,303
5	29,136	2.53	29,040	2.54	29,040	2.58	29,079
6	29,063	2.57	28,990	2.58	28,990	2.62	29,018
7	38,514	2.88	38,350	2.88	38,349	2.92	38,430
8	21,932	1.94	22,042	1.99	22,040	2.02	21,903
9	19,898	1.75	19,932	1.82	19,932	1.84	19,912
10	16,799	1.78	16,761	1.86	16,761	1.88	16,774
11	19,160	1.87	19,104	1.93	19,104	1.95	19,127
12	16,714	1.86	16,731	1.92	16,731	1.94	16,725
13	25,544	1.95	25,520	2.00	25,519	2.02	25,529
14	25,343	1.92	25,336	1.96	25,335	1.99	25,334
15	25,217	1.89	25,217	1.93	25,216	1.96	25,221
16	24,037	1.96	24,097	1.99	24,095	2.01	24,140
17	32,882	2.71	32,791	2.72	32,787	2.76	32,833
18	32,956	2.58	32,820	2.58	32,819	2.62	32,887
19	28,981	2.61	28,910	2.62	28,908	2.65	28,949
20	45,081	3.08	44,938	3.08	44,936	3.12	45,000
21	48,349	2.98	48,204	2.98	48,204	3.02	48,272
22	50,638	2.94	50,457	2.94	50,455	2.98	50,541
23	57,360	3.01	57,111	3.02	57,108	3.06	57,217
24	38,348	2.73	38,388	2.74	38,387	2.78	38,455
25	46,594	3.00	46,476	3.01	46,474	3.05	46,523
26	46,250	3.02	46,153	3.02	46,152	3.06	46,207
27	45,113	3.00	45,016	3.01	45,016	3.05	45,058
28	44,819	3.00	44,695	3.01	44,694	3.04	44,760
29	44,090	3.00	43,955	3.00	43,954	3.04	44,025
30	57,117	3.26	56,863	3.26	56,860	3.30	56,956
31	58,942	3.16	58,720	3.17	58,719	3.21	58,825
32	58,739	3.21	58,586	3.21	58,583	3.25	58,630
33	43,991	2.90	43,834	2.90	43,832	2.94	43,910
34	59,149	3.25	59,446	3.25	59,444	3.29	59,559
35	34,801	2.50	34,687	2.51	34,685	2.54	34,732
36	17,983	1.80	17,951	1.87	17,951	1.89	17,967
37	21,505	1.94	21,431	1.99	21,431	2.01	21,460
38	43,604	2.84	43,448	2.84	43,445	2.88	43,518
39	40,726	2.65	40,612	2.65	40,611	2.69	40,658
40	45,604	2.98	45,488	2.99	45,488	3.03	45,533
41	64,359	3.33	64,075	3.33	64,073	3.37	64,191

Index	interactionpotential_n3+.grid_avelog	interactionpotential_n3+.grid_aboveThreshold	interactionpotential_na+.grid_avelog	interactionpotential_na+.grid_aboveThreshold	interactionpotential_o.grid_avelog	interactionpotential_o.grid_aboveThreshold	interactionpotential_o-.grid_avelog
1	2.66	31,791	1.94	29,840	2.39	31,572	2.52
2	2.48	25,872	2.85	75,214	2.22	25,710	2.34
3	2.47	20,518	1.81	19,083	2.19	20,341	2.31
4	2.51	22,322	1.82	20,812	2.24	22,167	2.37
5	2.61	29,052	1.88	27,083	2.32	27,578	2.48
6	2.65	29,050	1.91	27,298	2.37	28,850	2.51
7	2.96	38,378	2.12	36,510	2.67	38,233	2.83
8	2.05	22,048	1.54	20,208	1.79	21,811	1.88
9	1.87	19,996	1.44	18,354	1.60	19,807	1.68
10	1.91	16,939	1.48	15,419	1.63	16,727	1.71
11	1.98	19,110	1.51	17,942	1.70	19,068	1.80
12	1.97	16,782	1.51	15,410	1.70	16,635	1.80
13	2.05	25,569	1.54	23,734	1.79	25,393	1.89
14	2.02	25,392	1.50	23,568	1.76	25,189	1.86
15	1.99	25,294	1.48	23,471	1.73	25,070	1.83
16	2.05	24,106	1.49	22,718	1.78	23,719	1.91
17	2.80	32,857	2.03	31,082	2.52	32,643	2.66
18	2.66	32,872	1.91	31,406	2.39	32,693	2.53
19	2.69	28,937	1.95	27,503	2.42	28,780	2.56
20	3.16	44,982	2.28	43,152	2.86	44,762	3.03
21	3.06	48,250	2.28	46,003	2.80	48,012	2.94
22	3.02	50,512	2.24	48,308	2.77	50,254	2.90
23	3.10	57,131	2.27	52,948	2.84	56,949	2.97
24	2.82	38,404	2.05	36,536	2.56	38,094	2.68
25	3.09	46,545	2.23	44,083	2.79	46,271	2.95
26	3.10	46,202	2.24	43,760	2.80	45,927	2.97
27	3.09	45,078	2.23	42,669	2.79	44,783	2.95
28	3.09	44,764	2.23	42,401	2.78	44,491	2.95
29	3.08	44,023	2.22	41,764	2.78	43,766	2.95
30	3.34	56,882	2.47	54,101	3.04	56,673	3.21
31	3.25	58,785	2.38	56,246	2.95	58,481	3.12
32	3.29	58,682	2.42	56,378	2.99	58,263	3.17
33	2.98	43,871	2.15	41,972	2.70	43,661	2.85
34	3.33	59,476	2.43	56,652	3.03	58,437	3.20
35	2.58	34,716	1.83	33,117	2.31	34,558	2.46
36	1.92	17,957	1.48	16,235	1.65	17,921	1.74
37	2.04	21,435	1.53	20,152	1.78	21,395	1.88
38	2.92	43,474	2.10	41,217	2.64	43,329	2.80
39	2.73	40,673	2.00	38,673	2.49	40,461	2.60
40	3.07	45,557	2.22	43,181	2.77	45,294	2.94
41	3.41	64,105	2.50	62,206	3.11	63,858	3.29

Index	interactionpotential_o-.grid_aboveThreshold	interactionpotential_o...grid_avelog	interactionpotential_o...grid_aboveThreshold	interactionpotential_o=.grid_avelog	interactionpotential_o=.grid_aboveThreshold	interactionpotential_o1.grid_avelog	interactionpotential_o1.grid_aboveThreshold
1	31,799	2.52	31,799	2.52	31,799	2.52	33,245
2	25,895	2.34	25,895	2.34	25,895	2.30	25,634
3	20,417	2.31	20,417	2.31	20,417	2.28	20,264
4	22,330	2.37	22,330	2.37	22,330	2.37	23,363
5	29,127	2.48	29,127	2.48	29,127	2.43	28,893
6	29,119	2.52	29,119	2.52	29,119	2.47	28,748
7	38,626	2.83	38,626	2.83	38,626	2.77	38,127
8	21,847	1.88	21,847	1.89	21,847	1.87	21,761
9	19,870	1.68	19,870	1.68	19,870	1.67	19,781
10	16,661	1.72	16,661	1.72	16,661	1.71	16,703
11	19,050	1.80	19,050	1.80	19,050	1.78	19,036
12	16,712	1.80	16,712	1.80	16,712	1.78	16,602
13	25,554	1.89	25,554	1.89	25,554	1.87	25,334
14	25,351	1.86	25,351	1.86	25,351	1.84	25,127
15	25,192	1.84	25,192	1.84	25,192	1.81	25,006
16	23,976	1.91	23,976	1.91	23,976	1.87	23,652
17	33,026	2.66	33,026	2.66	33,026	2.61	32,558
18	33,044	2.53	33,044	2.53	33,044	2.48	32,592
19	29,099	2.57	29,099	2.57	29,099	2.51	28,675
20	45,273	3.03	45,273	3.03	45,273	2.97	44,607
21	48,550	2.94	48,550	2.94	48,550	2.88	47,857
22	50,854	2.90	50,854	2.90	50,854	2.84	50,092
23	57,654	2.97	57,654	2.97	57,654	2.91	56,770
24	38,526	2.68	38,526	2.68	38,526	2.63	38,001
25	46,757	2.95	46,757	2.95	46,757	2.89	46,138
26	46,395	2.97	46,395	2.97	46,395	2.91	45,789
27	45,230	2.95	45,230	2.95	45,230	2.89	44,646
28	44,979	2.95	44,979	2.95	44,979	2.89	44,352
29	44,249	2.95	44,249	2.95	44,249	2.88	43,626
30	57,423	3.21	57,423	3.21	57,423	3.15	56,524
31	59,198	3.12	59,198	3.12	59,198	3.05	58,317
32	58,998	3.17	58,998	3.17	58,998	3.10	58,059
33	44,203	2.85	44,203	2.85	44,203	2.79	43,515
34	59,125	3.20	59,126	3.20	59,125	3.14	58,228
35	34,927	2.46	34,928	2.46	34,927	2.40	34,469
36	17,872	1.74	17,872	1.74	17,872	1.73	17,885
37	21,403	1.88	21,403	1.88	21,403	1.86	21,357
38	43,820	2.80	43,820	2.80	43,819	2.73	43,202
39	40,878	2.60	40,878	2.61	40,878	2.55	40,363
40	45,748	2.94	45,748	2.94	45,747	2.88	45,182
41	64,713	3.29	64,713	3.29	64,713	3.22	63,681

Index	interactionpotential_oc2.grid_avelog	interactionpotential_oc2.grid_aboveThreshold	interactionpotential_oes.grid_avelog	interactionpotential_oes.grid_aboveThreshold	interactionpotential_oh.grid_avelog	interactionpotential_oh.grid_aboveThreshold	interactionpotential_oh2.grid_avelog
1	2.37	31,264	2.37	31,264	2.51	31,679	2.51
2	2.20	25,465	2.20	25,465	2.34	26,324	2.33
3	2.18	20,110	2.18	20,110	2.31	20,418	2.31
4	2.22	21,942	2.22	21,942	2.36	22,239	2.36
5	2.32	28,581	2.32	28,581	2.47	29,053	3.06
6	2.35	28,565	2.35	28,565	2.51	28,957	2.50
7	2.64	37,816	2.64	37,816	2.81	38,371	2.80
8	1.77	21,496	1.76	21,496	1.89	21,876	1.90
9	1.58	19,667	1.58	19,667	1.69	19,850	1.71
10	1.62	16,591	1.61	16,590	1.73	16,765	1.74
11	1.69	18,777	1.69	18,777	1.81	19,110	1.82
12	1.69	16,485	1.69	16,485	1.80	16,685	1.81
13	1.77	25,174	1.77	25,174	1.89	25,472	1.90
14	1.74	24,949	1.74	24,949	1.86	25,270	1.87
15	1.71	24,820	1.71	24,820	1.83	25,151	1.84
16	1.76	23,514	1.76	23,514	1.90	23,962	1.90
17	2.48	32,337	2.48	32,337	2.65	32,761	2.64
18	2.36	32,323	2.36	32,323	2.51	32,823	2.51
19	2.40	28,469	2.40	28,469	2.55	28,891	2.54
20	2.83	44,251	2.83	44,251	3.01	44,916	3.00
21	2.78	47,480	2.78	47,480	2.92	48,185	2.91
22	2.75	49,706	2.75	49,706	2.88	50,443	2.87
23	2.81	56,380	2.81	56,380	2.95	57,149	2.94
24	2.53	37,755	2.53	37,755	2.67	38,211	2.66
25	2.76	45,809	2.76	45,809	2.94	46,421	2.93
26	2.78	45,478	2.78	45,478	2.95	46,116	2.94
27	2.76	44,346	2.76	44,346	2.93	44,976	2.92
28	2.76	44,026	2.76	44,026	2.93	44,654	2.92
29	2.75	43,314	2.75	43,314	2.93	43,930	2.92
30	3.01	56,111	3.01	56,111	3.19	56,875	3.18
31	2.92	57,858	2.92	57,858	3.10	58,716	3.08
32	2.97	57,586	2.97	57,586	3.14	58,504	3.13
33	2.67	43,175	2.67	43,175	2.83	43,831	2.82
34	3.00	57,778	3.00	57,778	3.18	59,341	3.17
35	2.29	34,230	2.29	34,230	2.44	34,672	2.43
36	1.64	17,806	1.64	17,806	1.75	17,954	1.76
37	1.76	21,084	1.76	21,084	1.88	21,443	1.89
38	2.61	42,890	2.61	42,890	2.78	43,464	2.76
39	2.47	40,059	2.47	40,059	2.59	40,600	2.58
40	2.74	44,835	2.74	44,835	2.92	45,460	2.91
41	3.07	63,171	3.07	63,171	3.26	64,103	3.25

Index	interactionpotential_oh2.grid_aboveThreshold	interactionpotential_on.grid_avelog	interactionpotential_on.grid_aboveThreshold	interactionpotential_po4.grid_avelog	interactionpotential_po4.grid_aboveThreshold	interactionpotential_po4h.grid_avelog	interactionpotential_po4h.grid_aboveThreshold
1	31,685	2.53	31,799	3.13	32,985	3.13	32,985
2	25,800	2.35	25,895	2.92	26,745	2.92	26,745
3	20,460	2.32	20,417	2.89	21,401	2.89	21,402
4	22,271	2.38	22,330	2.93	23,154	2.94	23,154
5	49,860	2.49	29,127	3.06	29,880	3.06	29,880
6	28,918	2.52	29,119	3.11	29,989	3.11	29,989
7	38,250	2.83	38,626	3.47	39,622	3.47	39,622
8	21,996	1.90	21,847	2.43	22,782	2.44	22,782
9	19,936	1.70	19,870	2.18	21,036	2.19	21,039
10	16,737	1.73	16,661	2.21	17,791	2.22	17,791
11	19,069	1.82	19,050	2.29	19,629	2.30	19,629
12	16,727	1.81	16,712	2.27	17,575	2.28	17,575
13	25,485	1.90	25,554	2.44	26,688	2.45	26,689
14	25,300	1.87	25,351	2.43	26,458	2.43	26,458
15	25,188	1.85	25,192	2.41	26,325	2.42	26,325
16	24,032	1.92	23,977	2.52	25,040	2.52	25,040
17	32,721	2.67	33,026	3.31	33,788	3.31	33,788
18	32,746	2.53	33,044	3.12	33,845	3.12	33,845
19	28,816	2.57	29,098	3.15	29,734	3.15	29,734
20	44,805	3.03	45,273	3.68	45,989	3.68	45,989
21	48,077	2.94	48,550	3.62	49,555	3.62	49,557
22	50,315	2.90	50,854	3.59	51,789	3.58	51,790
23	56,953	2.97	57,654	3.69	57,859	3.69	57,861
24	38,291	2.69	38,526	3.39	39,754	3.39	39,755
25	46,382	2.96	46,757	3.60	47,968	3.61	47,968
26	46,039	2.97	46,396	3.62	47,586	3.62	47,588
27	44,917	2.96	45,230	3.61	46,355	3.61	46,358
28	44,592	2.96	44,979	3.61	46,057	3.61	46,059
29	43,853	2.95	44,249	3.61	45,297	3.62	45,298
30	56,699	3.22	57,423	3.85	58,497	3.85	58,499
31	58,561	3.12	59,197	3.78	60,111	3.78	60,112
32	58,434	3.17	58,998	3.80	60,995	3.80	60,995
33	43,727	2.86	44,203	3.48	44,794	3.48	44,794
34	59,271	3.21	59,125	3.83	61,095	3.83	61,096
35	34,617	2.46	34,927	3.04	35,582	3.05	35,582
36	17,922	1.76	17,872	2.24	18,270	2.25	18,270
37	21,398	1.90	21,403	2.44	22,163	2.45	22,163
38	43,339	2.80	43,819	3.40	44,894	3.40	44,895
39	40,529	2.61	40,878	3.27	41,783	3.27	41,783
40	45,403	2.94	45,746	3.58	46,923	3.58	46,924
41	63,894	3.29	64,712	3.92	65,099	3.92	65,100

Supplementary Table SIII. Nanodescriptors list

Descriptions		Nanodescriptors
Estimation of the exposed water-accessible surface area of the vGNP		TotalSurfaceArea
Average surface area per ligand to estimate the exposure level of the surface ligands calculated by the surface area devided by number of ligands		AverageSurfaceAreaPerLigand
Total atomic partial charges		TotalPartialCharge
Average atomic partial charges per ligand		AveragePartialChargePerLigand
Van der Waals accessible surfaces (Interaction surfaces) that contour the regions of space accessible to the center of ligand atoms, hydrophobic potential accessed from hydrophobicity of the surface		HydrophobicPotential
The Potential Energy Functions are used to evaluate the potential energy function on the current system. The potential energy of the system can be affected by atom properties, crystal cell properties, geometric restraints and the currently loaded forcefield parameters.		PotentialEnergy
Probabilistic receptor preference maps that predict non-bonded contact preferences -- the preferred locations of hydrophobic and hydrophilic ligand atoms		contactpreference_hyd.grid_ave
		contactpreference_hyd.grid_aboveThreshold
		contactpreference_lpa.grid_ave
		contactpreference_lpa.grid_aboveThreshold
An electron density surface is a representation of the electron-density distribution in a unit cell, sampled over a grid and visualized as an isosurface.		electrondensity.grid_ave
		electrondensity.grid_aboveThreshold
Electrostatic Feature Maps that predict the electrostatically preferred locations of hydrophobic, H-bond acceptor and H-bond donor sites from the solutions of the Poisson-Boltzmann Equation		electrostaticmap_acc.grid_avelog
		electrostaticmap_acc.grid_aboveThreshold
		electrostaticmap_don.grid_avelog
		electrostaticmap_don.grid_aboveThreshold
		electrostaticmap_hyd.grid_avelog
		electrostaticmap_hyd.grid_aboveThreshold
An Interaction Potential map provides a graphical representation of where a chemical probe has favorable interactions with a molecular surface. To calculate these descriptors, a probe is an atom representation of a particular chemical functionality. These descriptors cover basic physico-chemical properties of surface ligands such as sizes, charges, and hydrogen bond	Bromine atom	interactionpotential_br.grid_avelog
		interactionpotential_br.grid_aboveThreshold
	Bromide ion	interactionpotential_br-.grid_avelog
		interactionpotential_br-.grid_aboveThreshold
	Aromatic CH group	interactionpotential_c1=.grid_avelog
		interactionpotential_c1=.grid_aboveThreshold
	Methylene CH group	interactionpotential_c2.grid_avelog

donor/acceptor properties. The descriptor calculation was based upon the work of GRID [Goodford 1985] [Boobbyer 1989], including calculating a three-term interaction energy for each point in a rectilinear grid. Interaction Potentials that predict the preferred location of user-specified probe atoms of varying parameters, based on a force field incorporating van der Waals, charge and hydrogen bonding terms		interactionpotential_c2.grid_aboveThreshold
	Methyl CH3 group	interactionpotential_c3.grid_avelog
		interactionpotential_c3.grid_aboveThreshold
	Chlorine atom	interactionpotential_cl.grid_avelog
		interactionpotential_cl.grid_aboveThreshold
	Chloride ion	interactionpotential_cl-.grid_avelog
		interactionpotential_cl-.grid_aboveThreshold
	Dry (hydrophobic) probe	interactionpotential_dry.grid_avelog
		interactionpotential_dry.grid_aboveThreshold
	Fluorine atom	interactionpotential_f.grid_avelog
		interactionpotential_f.grid_aboveThreshold
	Fluoride ion	interactionpotential_f-.grid_avelog
		interactionpotential_f-.grid_aboveThreshold
	Iodine atom	interactionpotential_i.grid_avelog
		interactionpotential_i.grid_aboveThreshold
	Potassium cation	interactionpotential_k+.grid_avelog
		interactionpotential_k+.grid_aboveThreshold
	Nitrogen atom with lone pair	interactionpotential_n..grid_avelog
		interactionpotential_n..grid_aboveThreshold
	Amide NH group	interactionpotential_n1.grid_avelog
		interactionpotential_n1.grid_aboveThreshold
	sp3 NH group with lone pair	interactionpotential_n1..grid_avelog
		interactionpotential_n1..grid_aboveThreshold
	sp3 NH cation	interactionpotential_n1+.grid_avelog
		interactionpotential_n1+.grid_aboveThreshold
	sp2 cationic NH group	interactionpotential_n1=.grid_avelog
		interactionpotential_n1=.grid_aboveThreshold
	Amide NH2 group	interactionpotential_n2.grid_avelog
		interactionpotential_n2.grid_aboveThreshold
	sp3 cationic NH2 group	interactionpotential_n2+.grid_avelog
		interactionpotential_n2+.grid_aboveThreshold
	sp2 cationic NH2 group	interactionpotential_n2=.grid_avelog
		interactionpotential_n2=.grid_aboveThreshold
	sp3 cationic NH3 group	interactionpotential_n3+.grid_avelog

		interactionpotential_n3+.grid_aboveThreshold
	Sodium cation	interactionpotential_na+.grid_avelog
		interactionpotential_na+.grid_aboveThreshold
	Carbonyl oxygen atom	interactionpotential_o.grid_avelog
		interactionpotential_o.grid_aboveThreshold
	Anionic phenolate oxygen atom	interactionpotential_o-.grid_avelog
		interactionpotential_o-.grid_aboveThreshold
	Carboxy oxygen atom	interactionpotential_o...grid_avelog
		interactionpotential_o...grid_aboveThreshold
	Phosphate oxygen atom	interactionpotential_o=.grid_avelog
		interactionpotential_o=.grid_aboveThreshold
	Aliphatic hydroxyl group	interactionpotential_o1.grid_avelog
		interactionpotential_o1.grid_aboveThreshold
	Ether oxygen atom	interactionpotential_oc2.grid_avelog
		interactionpotential_oc2.grid_aboveThreshold
	Ester oxygen atom	interactionpotential_oes.grid_avelog
		interactionpotential_oes.grid_aboveThreshold
	Phenolic hydroxyl group	interactionpotential_oh.grid_avelog
		interactionpotential_oh.grid_aboveThreshold
	Water	interactionpotential_oh2.grid_avelog
		interactionpotential_oh2.grid_aboveThreshold
	Nitro oxygen atom	interactionpotential_on.grid_avelog
		interactionpotential_on.grid_aboveThreshold
	PO4 dianion	interactionpotential_po4.grid_avelog
		interactionpotential_po4.grid_aboveThreshold
	PO4H phosphate anion	interactionpotential_po4h.grid_avelog
		interactionpotential_po4h.grid_aboveThreshold

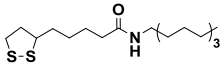
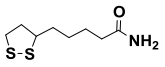
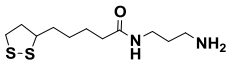
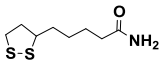
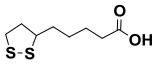
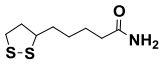
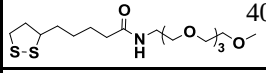
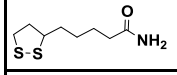
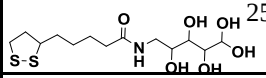
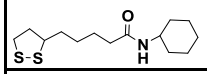
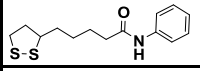
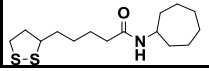
*All descriptors were calculated against the vGNPs

*_avelog: average of the log values of the interaction potential for each point in a rectilinear grid

*_aboveThreshold: number of points that possess interaction potential above the user-defined interaction threshold

*For more details describing the surface feature extraction, please refer to ChemicalComputingGroupInc. Molecular Operating Environment (MOE). (2016).

Supplementary table SIV. The seven new GNPs external set

GNP index	vGNPs		Predicted properties				Experimentally characterized properties					
	# Ligand / vGNP*	Size (nm)	LogP	HO-1 level in A549	Cell uptake in A549 (10^7 GNP/cell)	Cell uptake in HEK293 (10^7 GNP/cell)	# Ligand / GNP	Size (TEM) (nm)	LogP	HO-1 level in A549	Cell uptake in A549 (10^7 GNP/cell)	Cell uptake in HEK293 (10^7 GNP/cell)
35	 500 (100%)	6.5	0.81	2.76	4.61	4.61	536 (100%)	6.5	0.55±0.12	2.38±0.15	5.11±0.4	4.22±0.25
36	 100 (67%)  50 (33%)	5.8	-2.32	2.85	1.3	1.47	102 (71%) 42 (29%)	5.8	-2.54±0.07	2.7±0.66	2.34±0.14	2.31±0.42
37	 200 (80%)  50 (20%)	5.8	-2.46	1.19	0.55	0.55	185 (80%) 47 (20%)	5.8	-2.13±0.5	0.9±0.21	0.4±0.02	0.4±0.01
38	 100 (25%)  400 (75%)	5.2	-0.79	1.99	1.65	1.88	126 (25%) 380 (75%)	5.2	-2.29±0.06	2.41±0.37	0.63±0.02	0.61±0.04
39	 250 (50%)  250 (50%)	5	-1.84	1.91	0.63	0.66	275 (54%) 235 (46%)	5	-2.3±0.15	2.04±0.28	0.58±0.05	0.59±0.03
40	 540 (60%)  360 (40%)	7.3	2.32	2.28	5.04	5.26	521 (60%) 348 (40%)	7.3	2.39±0.2	2.16±0.15	5.3±0.57	5.58±0.35
41	 850 (100%)	5.9	2.12	2.17	5.47	5.16	869 (100%)	5.9	2.3±0.03	1.87±0.23	5.04±0.38	5.34±0.67

*The number of ligands per GNP is approximated according to our rational design