

PyDockSAXS Top100 results

Conf	Ele	Desolv	VDW	PyDock	Crysol	pyDockSAXS	RANK
6367	-7.268	-8.294	57.23	-9.839	3.8	58.389	1
3057	-10.327	0.673	22.29	-7.425	3.604	59.02	2
16	-7.341	-9.325	76.99	-8.967	4.806	67.762	3
3536	5.175	-5.623	56.351	5.187	3.669	72.228	4
5503	-8.398	11.501	43.408	7.444	3.614	73.981	5
4722	-5.241	-10.226	53.554	-10.112	5.845	74.506	6
2636	-6.273	14.214	1.569	8.097	3.655	75.01	7
2253	-7.281	11.796	50.262	9.541	3.669	76.582	8
8008	-8.994	6.053	19.842	-0.957	5.026	77.509	9
2637	-8.721	-0.215	16.322	-7.304	5.999	78.421	10
2634	-6.511	0.344	104.84	4.317	4.632	79.644	11
9144	1.303	7.433	12.219	9.959	4.337	82.848	12
5913	-8.111	11.122	60.6	9.071	4.566	83.86	13
995	-6.631	-9.649	98.605	-6.419	6.668	83.96	14
7332	-4.623	-1.674	27.115	-3.585	6.333	84.494	15
6908	-5.063	10.098	26.201	7.655	4.92	85.289	16
9725	-1.402	12.315	22.138	13.127	4.496	87.34	17
2618	-14.482	-6.41	47.451	-16.146	8.827	87.84	18
1952	-4.201	0.713	48.687	1.38	6.406	89.965	19
1245	-6.787	-9.588	47.038	-11.67	8.565	90.761	20
782	-13.767	-8.985	17.653	-20.987	10.201	90.8	21
184	-9.113	-9.458	48.245	-13.747	9.017	91.352	22
5498	-4.581	8.917	68.954	11.231	5.259	91.495	23
6861	-7.97	3.172	24.083	-2.389	7.424	92.976	24
7362	1.495	8.935	7.52	11.182	5.647	94.354	25
4125	-4.252	0.47	35.026	-0.279	7.355	94.641	26
5120	-13.792	-0.131	67.671	-7.156	8.476	94.741	27
1681	-8.853	-7.224	75.021	-8.575	8.917	95.94	28
6427	-3.273	10.159	42.6	11.146	5.908	96.218	29
380	-9.959	11.686	21.215	3.849	7.159	97.496	30
5474	-5.368	9.835	27.573	7.224	6.989	99.753	31
1694	-8.846	11.266	-10.124	1.407	8.241	101.882	32
3063	-10.463	13.695	32.292	6.461	7.68	103.456	33

2102	-6.466	-0.024	67.03	0.213	8.858	104.381	34
6868	-8.587	-0.519	45.38	-4.568	9.748	104.708	35
3060	-3.872	-1.167	35.894	-1.449	9.691	107.507	36
3067	-1.756	13.527	36.471	15.418	6.925	107.522	37
7911	-12.461	-4.449	31.255	-13.785	12.247	108.7	38
2106	-1.452	12.402	9.81	11.931	7.697	109.033	39
5094	-6.873	3.879	11.173	-1.877	10.554	111.827	40
3077	-5.314	-3.076	57.39	-2.652	10.705	111.863	41
2858	-0.944	-2.565	33.17	-0.191	10.506	113.254	42
3051	-8.986	-1.058	26.581	-7.386	12.124	114.482	43
9183	-9.033	7.07	29.154	0.953	10.716	115.527	44
7402	-9.835	-1.928	9.978	-10.765	13.105	115.938	45
5940	-5.354	8.717	39.392	7.302	9.784	116.78	46
8489	-1.164	-10.373	61.633	-5.373	12.575	118.741	47
554	-0.052	-0.525	52.267	4.65	10.703	119.154	48
5518	-2.222	10.891	22.155	10.884	9.647	119.593	49
7363	0.483	-5.643	56.749	0.515	11.593	119.685	50
797	5.923	2.843	42.362	13.002	9.689	121.947	51
7970	-1.528	9.802	29.602	11.234	10.048	122.179	52
3561	-10.595	7.835	28.546	0.095	12.428	123.482	53
9184	-12.447	8.897	15.123	-2.038	13.007	124.19	54
866	-5.972	7.134	48.247	5.987	11.515	124.755	55
1452	0.15	15.769	17.744	17.694	9.58	126.025	56
7431	-7.702	3.735	33.387	-0.629	13.194	126.503	57
4759	-9.123	-0.263	60.691	-3.317	13.822	126.806	58
1464	-2.793	2.561	55.218	5.289	12.103	127.052	59
6905	-6.02	6.832	39.647	4.776	12.212	127.086	60
9650	-9.188	-6.62	32.391	-12.568	16.1	127.869	61
738	-10.452	8.654	82.516	6.453	12.097	128.186	62
2818	-8.024	-7.088	21.212	-12.991	16.295	128.294	63
2645	-6.217	2.255	25.068	-1.456	13.851	128.803	64
4099	-3.482	-7.878	42.517	-7.107	15.243	129.541	65
3294	-10.002	12.343	18.406	4.182	12.913	129.953	66
5519	-3.934	8.622	43.622	9.051	11.977	130.178	67
1555	-5.523	3.449	46.219	2.549	13.343	130.397	68
6867	-8.115	11.971	-0.745	3.782	13.329	131.563	69
6437	-1.312	9.944	19.101	10.541	12.092	132.248	70
441	-4.699	-3.561	51.654	-3.095	15.017	132.536	71

4116	-5.904	-3.025	22.842	-6.645	15.932	133.057	72
3075	-2.919	-1.653	82.899	3.717	13.728	133.397	73
3040	1.931	-4.628	44.243	1.728	14.21	133.665	74
476	-12.678	-6.957	34.513	-16.184	18.529	134.475	75
8559	-3.396	7.24	42.433	8.088	13.051	134.53	76
9794	-10.652	13.369	29.667	5.684	13.569	134.61	77
3570	-15.106	13.098	45.863	2.578	14.246	134.682	78
2408	-8.327	-0.23	58.016	-2.755	15.443	134.787	79
4439	-7.218	10.41	69.383	10.13	12.733	135.022	80
859	-7.715	-6.764	20.643	-12.414	17.889	135.62	81
795	-5.69	8.574	56.352	8.519	13.427	136.769	82
929	-8.818	10.336	34.593	4.977	14.207	136.9	83
9772	-4.596	2.043	4.72	-2.081	15.932	137.621	84
1571	3.644	7.502	52.195	16.366	12.145	138.34	85
2247	-7.984	14.415	5.833	7.013	14.083	138.359	86
3851	-10.32	13.273	1.202	3.073	15.027	138.749	87
4740	-8.208	-2.311	50.339	-5.485	17.08	139.163	88
4438	-4.06	4.695	20.715	2.706	15.542	140.688	89
1249	-3.744	2.764	49.912	4.011	15.439	141.535	90
6907	1.081	2.554	49.317	8.567	14.565	142.141	91
3502	-7.78	-4.326	34.175	-8.688	18.576	142.162	92
9143	-1.453	13.824	41.188	16.49	13.114	143.236	93
1804	-6.804	-6.287	57.001	-7.391	18.84	144.527	94
6874	-5.87	-5.327	26.511	-8.546	19.131	144.54	95
8507	-0.003	0.019	23.718	2.388	16.528	144.679	96
9156	-11.704	-2.06	101.453	-3.619	17.983	144.803	97
1352	-6.823	-3.433	19.836	-8.272	19.246	145.274	98
4418	-11.744	9.751	13.895	-0.603	17.468	145.679	99
7347	-6.269	0.138	18.725	-4.258	18.417	145.945	100