

Supplementary material

Natural compounds as DPP-4 inhibitors: 3D similarity search, ADME toxicity, and molecular docking approaches

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Table S1. The selected NPs by best 3D-similarity coefficients vs linagliptin (Tanimoto Combo, TC >1, ShapeTanimoto, ShT >0.75, and Combo Score, CS >1.2)

Name	TC	ShT	CS	Name	TC	ShT	CS	Name	TC	ShT	CS
ZINC1094329	1.328	0.807	1.345	ZINC5387327	1.196	0.761	1.259	ZINC8926323	1.169	0.760	1.258
ZINC8916385	1.323	0.800	1.340	ZINC8926342	1.196	0.761	1.259	ZINC4116049	1.168	0.758	1.236
ZINC789645	1.303	0.781	1.320	ZINC8589983	1.195	0.760	1.258	ZINC13116156	1.167	0.781	1.258
ZINC838142	1.302	0.781	1.319	ZINC2488345	1.194	0.759	1.257	ZINC1108640	1.167	0.757	1.235
ZINC832612	1.279	0.790	1.330	ZINC9601609	1.194	0.758	1.257	ZINC640985	1.167	0.752	1.234
ZINC2334127	1.267	0.780	1.318	ZINC9601608	1.192	0.783	1.281	ZINC9601615	1.162	0.776	1.254
ZINC1094334	1.266	0.780	1.318	ZINC8606274	1.187	0.770	1.254	ZINC13142224	1.161	0.774	1.252
ZINC6565526	1.250	0.763	1.301	ZINC838204	1.184	0.751	1.269	ZINC12296449	1.097	0.757	1.228
ZINC13512682	1.215	0.805	1.283	ZINC2488384	1.178	0.791	1.269	ZINC33833997	1.048	0.785	1.291
ZINC6732655	1.206	0.796	1.274	ZINC838200	1.171	0.769	1.260	ZINC33833796	1.016	0.762	1.268
ZINC9601596	1.203	0.767	1.266	ZINC2488377	1.170	0.760	1.238	ZINC84153787	1.004	0.768	1.273
ZINC2488364	1.202	0.792	1.270	ZINC4147162	1.169	0.783	1.261				

Table S2. The selected NPs by best 3D-similarity coefficients vs sitagliptin (Tanimoto Combo, TC >1, ShapeTanimoto, ShT >0.75, and Combo Score, CS >1.2)

Name	TC	ShT	CS	Name	TC	ShT	CS	Name	TC	ShT	CS
ZINC253398618	1.294	0.788	1.376	ZINC85879230	1.078	0.785	1.238	ZINC85876049	1.043	0.771	1.226
ZINC89363727	1.284	0.777	1.366	ZINC72324985	1.076	0.794	1.261	ZINC217722740	1.043	0.831	1.224
ZINC59572517	1.248	0.786	1.379	ZINC90130383	1.076	0.752	1.242	ZINC2151699	1.042	0.781	1.221
ZINC136757666	1.211	0.784	1.383	ZINC12389255	1.076	0.760	1.240	ZINC96114431	1.041	0.755	1.339
ZINC85876175	1.200	0.818	1.405	ZINC20762885	1.075	0.759	1.239	ZINC72324714	1.040	0.756	1.254
ZINC604405970	1.200	0.766	1.333	ZINC604403934	1.073	0.789	1.231	ZINC96296242	1.040	0.758	1.225
ZINC12296782	1.195	0.781	1.367	ZINC36370102	1.073	0.753	1.207	ZINC524732317	1.039	0.782	1.243
ZINC2508009	1.187	0.752	1.321	ZINC8614482	1.072	0.769	1.293	ZINC10146685	1.038	0.762	1.222
ZINC89914549	1.171	0.773	1.378	ZINC96112842	1.072	0.784	1.259	ZINC6767083	1.038	0.770	1.220
ZINC96114503	1.167	0.768	1.374	ZINC2123570	1.072	0.801	1.228	ZINC2121295	1.037	0.751	1.278
ZINC218315564	1.158	0.775	1.363	ZINC40313093	1.070	0.806	1.250	ZINC226848468	1.037	0.792	1.210
ZINC12296887	1.153	0.778	1.358	ZINC2707927	1.070	0.775	1.230	ZINC96115667	1.035	0.786	1.259
ZINC85879571	1.149	0.789	1.352	ZINC381318	1.070	0.758	1.204	ZINC72324924	1.035	0.764	1.217
ZINC20676820	1.146	0.782	1.382	ZINC20761191	1.067	0.788	1.252	ZINC8611816	1.034	0.751	1.275
ZINC217928409	1.139	0.755	1.344	ZINC2120824	1.066	0.787	1.277	ZINC6766260	1.033	0.777	1.236
ZINC89915303	1.138	0.768	1.308	ZINC79193641	1.066	0.751	1.200	ZINC30952814	1.033	0.757	1.216
ZINC217927992	1.137	0.754	1.342	ZINC6075837	1.064	0.786	1.221	ZINC4046819	1.032	0.760	1.214
ZINC12296682	1.137	0.753	1.342	ZINC96115407	1.063	0.762	1.224	ZINC79194115	1.031	0.759	1.239
ZINC20715640	1.133	0.794	1.395	ZINC4074101	1.063	0.791	1.218	ZINC8764612	1.031	0.754	1.214
ZINC12322314	1.132	0.766	1.336	ZINC96116537	1.062	0.787	1.300	ZINC96112029	1.030	0.762	1.238
ZINC96116458	1.128	0.752	1.299	ZINC6766255	1.061	0.786	1.245	ZINC253389136	1.028	0.795	1.267
ZINC11692316	1.126	0.773	1.361	ZINC12895627	1.061	0.762	1.222	ZINC85878975	1.028	0.753	1.212
ZINC12296795	1.125	0.786	1.356	ZINC72325880	1.058	0.765	1.246	ZINC8765456	1.028	0.755	1.210
ZINC10384610	1.117	0.796	1.252	ZINC943432	1.058	0.758	1.220	ZINC170625251	1.027	0.750	1.238

ZINC2096678	1.114	0.760	1.316	ZINC72325031	1.058	0.773	1.216	ZINC6075833	1.027	0.770	1.205
ZINC72324690	1.112	0.786	1.247	ZINC5956697	1.057	0.779	1.214	ZINC96116557	1.026	0.759	1.207
ZINC6912954	1.108	0.755	1.212	ZINC6075832	1.056	0.777	1.213	ZINC8490844	1.025	0.782	1.246
ZINC96114432	1.107	0.767	1.307	ZINC9900130	1.054	0.761	1.242	ZINC8587150	1.025	0.769	1.228
ZINC253395761	1.107	0.755	1.210	ZINC945277	1.054	0.756	1.215	ZINC96116527	1.022	0.774	1.246
ZINC10384551	1.102	0.781	1.237	ZINC2707925	1.054	0.764	1.213	ZINC2126493	1.022	0.762	1.226
ZINC2998244	1.101	0.780	1.236	ZINC96269279	1.053	0.772	1.238	ZINC20427677	1.022	0.764	1.225
ZINC90000481	1.099	0.783	1.323	ZINC265220	1.053	0.754	1.215	ZINC20616123	1.022	0.751	1.204
ZINC2113602	1.099	0.819	1.256	ZINC35045981	1.052	0.827	1.287	ZINC13583976	1.020	0.752	1.202
ZINC2707930	1.099	0.779	1.234	ZINC8587149	1.052	0.776	1.235	ZINC85878476	1.019	0.775	1.216
ZINC9902281	1.099	0.773	1.234	ZINC40312847	1.052	0.788	1.232	ZINC96296243	1.017	0.755	1.222
ZINC21646922	1.097	0.782	1.321	ZINC72324571	1.052	0.751	1.214	ZINC4046623	1.014	0.765	1.213
ZINC72324535	1.096	0.770	1.231	ZINC72324692	1.052	0.751	1.213	ZINC35361886	1.013	0.787	1.248
ZINC85878147	1.095	0.796	1.256	ZINC85875372	1.051	0.755	1.212	ZINC6767084	1.013	0.763	1.213
ZINC89916271	1.094	0.763	1.260	ZINC20760451	1.050	0.751	1.326	ZINC12899028	1.013	0.769	1.210
ZINC85876531	1.094	0.796	1.255	ZINC4043624	1.050	0.773	1.207	ZINC12663453	1.012	0.754	1.216
ZINC6912833	1.091	0.768	1.226	ZINC170625248	1.049	0.790	1.253	ZINC12893479	1.011	0.754	1.214
ZINC8762389	1.086	0.771	1.250	ZINC12296927	1.048	0.764	1.206	ZINC85875832	1.009	0.780	1.222
ZINC2707928	1.086	0.765	1.220	ZINC2115413	1.047	0.788	1.225	ZINC4046622	1.008	0.766	1.205
ZINC72324473	1.084	0.768	1.218	ZINC72324751	1.046	0.780	1.279	ZINC35442480	1.007	0.766	1.227
ZINC96116515	1.083	0.750	1.344	ZINC2120822	1.046	0.802	1.243	ZINC79192051	1.006	0.750	1.234
ZINC20762547	1.082	0.763	1.246	ZINC12296399	1.046	0.755	1.234	ZINC4040633	1.006	0.766	1.201
ZINC20761936	1.082	0.805	1.239	ZINC72326026	1.046	0.753	1.234	ZINC4046932	1.005	0.760	1.203
ZINC6912811	1.082	0.760	1.217	ZINC41428634	1.044	0.752	1.232	ZINC96112189	1.001	0.751	1.226
ZINC30615924	1.079	0.777	1.270	ZINC6075836	1.044	0.765	1.201	ZINC35361885	1.000	0.759	1.220

Table S3. The selected NPs by best 3D-similarity coefficients vs alogliptin (Tanimoto Combo, TC >1, ShapeTanimoto, ShT >0.75, and Combo Score, CS >1.2)

Name	TC	ShT	CS	Name	TC	ShT	CS	Name	TC	ShT	CS
ZINC1000110	1.317	0.834	1.449	ZINC487437	1.094	0.775	1.259	ZINC677506	1.052	0.751	1.239
ZINC14961096	1.276	0.883	1.416	ZINC36025434	1.094	0.914	1.218	ZINC8926363	1.052	0.766	1.235
ZINC1789891	1.274	0.813	1.374	ZINC525915112	1.093	0.842	1.556	ZINC568533	1.052	0.772	1.209
ZINC1789905	1.270	0.822	1.372	ZINC95913545	1.093	0.828	1.480	ZINC59586736	1.051	0.816	1.493
ZINC1791330	1.258	0.810	1.360	ZINC4098455	1.093	0.757	1.399	ZINC85644634	1.051	0.847	1.431
ZINC6720720	1.247	0.828	1.386	ZINC604404518	1.093	0.761	1.343	ZINC1101493	1.051	0.750	1.239
ZINC19703085	1.241	0.853	1.505	ZINC9781377	1.093	0.757	1.259	ZINC13738998	1.051	0.789	1.228
ZINC330295	1.237	0.762	1.334	ZINC6569127	1.091	0.831	1.542	ZINC5126030	1.050	0.756	1.236
ZINC100632953	1.234	0.819	1.406	ZINC14806402	1.091	0.763	1.312	ZINC225438310	1.050	0.787	1.203
ZINC5444758	1.229	0.824	1.400	ZINC1446419	1.091	0.754	1.258	ZINC4044108	1.049	0.779	1.252
ZINC217991216	1.229	0.796	1.366	ZINC1127268	1.091	0.772	1.256	ZINC4026036	1.049	0.880	1.233
ZINC6499528	1.224	0.860	1.394	ZINC5441698	1.091	0.757	1.202	ZINC976542	1.049	0.789	1.224
ZINC1245404	1.223	0.808	1.394	ZINC119512	1.091	0.775	1.201	ZINC49542475	1.048	0.770	1.254
ZINC872110	1.222	0.846	1.363	ZINC95099212	1.090	0.829	1.588	ZINC4083211	1.048	0.763	1.207
ZINC189799	1.222	0.793	1.327	ZINC85531793	1.090	0.821	1.551	ZINC13515283	1.047	0.808	1.516
ZINC942551	1.217	0.788	1.322	ZINC28540146	1.090	0.829	1.543	ZINC95912387	1.047	0.790	1.494
ZINC706774	1.214	0.784	1.319	ZINC192293	1.090	0.823	1.245	ZINC95914670	1.047	0.772	1.492
ZINC2091112	1.206	0.875	1.400	ZINC5728766	1.089	0.772	1.280	ZINC4097731	1.047	0.819	1.480
ZINC872109	1.206	0.839	1.347	ZINC622396	1.089	0.766	1.200	ZINC253398313	1.047	0.772	1.204
ZINC1458727	1.206	0.820	1.346	ZINC2867973	1.089	0.758	1.200	ZINC4102354	1.046	0.832	1.498
ZINC151198	1.205	0.760	1.410	ZINC33833729	1.088	0.825	1.518	ZINC25763686	1.046	0.791	1.491
ZINC217940798	1.204	0.796	1.344	ZINC38396388	1.088	0.866	1.452	ZINC33831146	1.046	0.794	1.487
ZINC5730717	1.204	0.810	1.343	ZINC263585279	1.088	0.782	1.277	ZINC33832524	1.046	0.829	1.464
ZINC490166	1.202	0.752	1.338	ZINC1133310	1.088	0.751	1.255	ZINC13056335	1.046	0.796	1.241
ZINC941313	1.200	0.771	1.305	ZINC14952519	1.087	0.828	1.537	ZINC838160	1.046	0.786	1.221
ZINC36646378	1.195	0.753	1.332	ZINC1094337	1.087	0.768	1.252	ZINC225434522	1.046	0.783	1.200
ZINC525500	1.195	0.777	1.301	ZINC59872849	1.086	0.852	1.548	ZINC33833455	1.045	0.788	1.492

ZINC1142676	1.193	0.763	1.298	ZINC9147122	1.086	0.825	1.537	ZINC2306198	1.045	0.778	1.223
ZINC1152507	1.189	0.760	1.293	ZINC9781351	1.086	0.772	1.276	ZINC838181	1.045	0.781	1.222
ZINC6556411	1.188	0.774	1.360	ZINC238783892	1.085	0.823	1.537	ZINC13512151	1.045	0.785	1.221
ZINC100495199	1.187	0.794	1.264	ZINC789648	1.084	0.769	1.274	ZINC067657	1.045	0.826	1.206
ZINC524730033	1.185	0.755	1.323	ZINC13424725	1.083	0.846	1.548	ZINC70455510	1.044	0.784	1.518
ZINC5907073	1.183	0.779	1.355	ZINC59765889	1.083	0.839	1.536	ZINC59771847	1.044	0.834	1.469
ZINC20760691	1.182	0.817	1.322	ZINC5728767	1.083	0.766	1.274	ZINC59764680	1.044	0.811	1.462
ZINC4170026	1.181	0.834	1.321	ZINC9601619	1.083	0.769	1.273	ZINC31164103	1.044	0.800	1.453
ZINC832607	1.178	0.839	1.317	ZINC604406189	1.083	0.755	1.249	ZINC2344777	1.044	0.768	1.225
ZINC218066667	1.175	0.776	1.346	ZINC9781391	1.083	0.770	1.246	ZINC31164099	1.043	0.792	1.505
ZINC838145	1.175	0.837	1.314	ZINC4540569	1.082	0.798	1.290	ZINC70454560	1.043	0.822	1.467
ZINC9782470	1.174	0.827	1.314	ZINC2488348	1.082	0.769	1.272	ZINC59726158	1.043	0.822	1.467
ZINC851616	1.173	0.835	1.312	ZINC1446420	1.082	0.769	1.272	ZINC95486354	1.043	0.829	1.416
ZINC1127254	1.172	0.835	1.312	ZINC640993	1.082	0.790	1.267	ZINC12402877	1.043	0.797	1.235
ZINC2091110	1.171	0.854	1.362	ZINC31160874	1.082	0.811	1.261	ZINC3894228	1.043	0.752	1.228
ZINC12438112	1.171	0.835	1.310	ZINC838163	1.082	0.822	1.258	ZINC4349710	1.042	0.832	1.467
ZINC707150	1.170	0.838	1.336	ZINC34685248	1.082	0.879	1.235	ZINC12378086	1.042	0.775	1.220
ZINC263586879	1.170	0.802	1.310	ZINC180678	1.082	0.802	1.216	ZINC13358870	1.042	0.776	1.219
ZINC838148	1.169	0.830	1.308	ZINC4349549	1.081	0.820	1.579	ZINC2488382	1.042	0.780	1.218
ZINC1448012	1.168	0.775	1.308	ZINC4349372	1.081	0.847	1.542	ZINC1626068	1.042	0.780	1.218
ZINC263586880	1.167	0.843	1.306	ZINC4812655	1.081	0.751	1.275	ZINC079009	1.042	0.822	1.202
ZINC753717	1.166	0.769	1.338	ZINC20762493	1.081	0.767	1.272	ZINC067653	1.042	0.822	1.202
ZINC450480	1.166	0.791	1.306	ZINC789712	1.081	0.764	1.272	ZINC59765936	1.041	0.824	1.518
ZINC12342485	1.166	0.827	1.305	ZINC6815073	1.081	0.815	1.235	ZINC39433939	1.041	0.835	1.442
ZINC9782466	1.164	0.828	1.303	ZINC225439439	1.081	0.784	1.216	ZINC15830200	1.041	0.822	1.262
ZINC13282205	1.164	0.825	1.303	ZINC033179	1.080	0.884	1.267	ZINC1127270	1.041	0.764	1.245
ZINC863247	1.163	0.824	1.303	ZINC9781410	1.080	0.778	1.242	ZINC38472655	1.040	0.813	1.532
ZINC044493	1.162	0.849	1.325	ZINC067669	1.080	0.792	1.214	ZINC4102357	1.040	0.846	1.405

ZINC12342488	1.162	0.818	1.302	ZINC46153069	1.080	0.836	1.207	ZINC838156	1.040	0.782	1.214
ZINC13282203	1.160	0.816	1.300	ZINC1807495	1.079	0.771	1.216	ZINC8974182	1.040	0.790	1.212
ZINC789709	1.160	0.823	1.299	ZINC1095264	1.078	0.766	1.268	ZINC9782440	1.039	0.762	1.244
ZINC5095098	1.160	0.821	1.299	ZINC36289482	1.077	0.863	1.255	ZINC85510518	1.038	0.814	1.404
ZINC5607398	1.159	0.795	1.329	ZINC61997014	1.077	0.770	1.240	ZINC85592725	1.038	0.812	1.242
ZINC12393369	1.159	0.820	1.298	ZINC627172	1.077	0.781	1.238	ZINC754303	1.038	0.860	1.213
ZINC1143247	1.158	0.764	1.298	ZINC20762071	1.077	0.755	1.215	ZINC13739028	1.038	0.778	1.213
ZINC2334130	1.157	0.822	1.297	ZINC225435746	1.077	0.780	1.212	ZINC90711737	1.037	0.806	1.453
ZINC151199	1.155	0.768	1.357	ZINC21992895	1.076	0.822	1.566	ZINC70454743	1.037	0.842	1.422
ZINC706775	1.155	0.761	1.294	ZINC84154015	1.076	0.823	1.497	ZINC84154202	1.037	0.817	1.418
ZINC753718	1.153	0.756	1.324	ZINC4654800	1.076	0.863	1.468	ZINC70454681	1.037	0.826	1.407
ZINC832594	1.153	0.840	1.317	ZINC1106316	1.076	0.751	1.324	ZINC2502268	1.037	0.788	1.231
ZINC2595059	1.153	0.819	1.292	ZINC838158	1.076	0.818	1.251	ZINC812594	1.037	0.798	1.226
ZINC8926216	1.153	0.814	1.292	ZINC14684628	1.075	0.811	1.530	ZINC1756437	1.037	0.868	1.221
ZINC5575620	1.151	0.757	1.323	ZINC15830182	1.075	0.860	1.293	ZINC85509713	1.036	0.804	1.516
ZINC9782474	1.151	0.815	1.290	ZINC253403806	1.075	0.778	1.210	ZINC2008803	1.036	0.812	1.401
ZINC12342483	1.151	0.813	1.290	ZINC25763680	1.074	0.814	1.525	ZINC12661119	1.036	0.769	1.260
ZINC5484332	1.150	0.787	1.320	ZINC256004463	1.074	0.841	1.492	ZINC13282213	1.036	0.793	1.227
ZINC450481	1.149	0.768	1.289	ZINC8642820	1.074	0.812	1.251	ZINC32066887	1.035	0.779	1.482
ZINC6766372	1.149	0.755	1.289	ZINC13739027	1.074	0.814	1.249	ZINC4692014	1.035	0.817	1.475
ZINC13282204	1.149	0.811	1.288	ZINC281024	1.074	0.885	1.238	ZINC680572	1.035	0.754	1.242
ZINC625431	1.148	0.835	1.312	ZINC20763682	1.074	0.752	1.212	ZINC5483900	1.035	0.786	1.207
ZINC5441686	1.147	0.767	1.317	ZINC253500608	1.073	0.847	1.504	ZINC33832113	1.034	0.819	1.429
ZINC623390	1.147	0.832	1.312	ZINC256004465	1.073	0.840	1.491	ZINC40891808	1.034	0.768	1.421
ZINC9782468	1.147	0.813	1.286	ZINC33832091	1.073	0.851	1.435	ZINC3984976	1.034	0.761	1.262
ZINC604404074	1.146	0.753	1.348	ZINC9601618	1.073	0.761	1.263	ZINC524731654	1.034	0.752	1.240
ZINC985539	1.145	0.814	1.339	ZINC1425463	1.073	0.767	1.235	ZINC104891686	1.033	0.802	1.449
ZINC832608	1.144	0.832	1.307	ZINC34065053	1.072	0.829	1.546	ZINC137894960	1.032	0.819	1.405

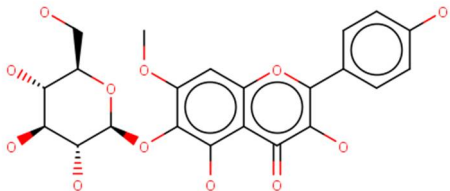
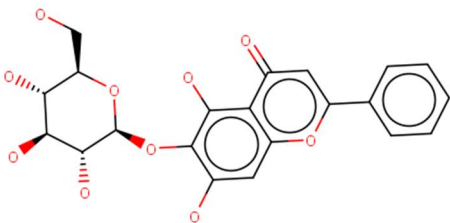
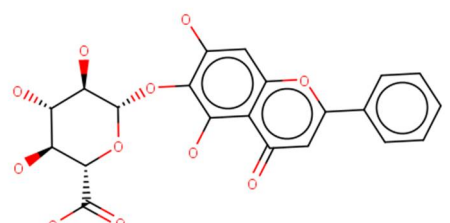
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ZINC044026	1.143	0.851	1.329	ZINC100790789	1.072	0.757	1.262	ZINC524730659	1.032	0.763	1.328
ZINC1578553	1.142	0.777	1.282	ZINC253529745	1.071	0.825	1.527	ZINC13508152	1.032	0.770	1.324
ZINC842264	1.140	0.825	1.304	ZINC85948413	1.071	0.859	1.443	ZINC38321668	1.031	0.759	1.471
ZINC1127183	1.139	0.825	1.303	ZINC13510653	1.071	0.757	1.262	ZINC33832038	1.031	0.806	1.418
ZINC789670	1.139	0.824	1.303	ZINC694159	1.071	0.764	1.233	ZINC824146928	1.031	0.754	1.212
ZINC28641045	1.139	0.782	1.279	ZINC217840572	1.071	0.750	1.209	ZINC5126035	1.031	0.774	1.206
ZINC1516664	1.138	0.846	1.323	ZINC5612099	1.071	0.763	1.208	ZINC39109040	1.030	0.765	1.418
ZINC604404011	1.136	0.770	1.365	ZINC5004613	1.070	0.835	1.534	ZINC15830055	1.030	0.814	1.248
ZINC20111175	1.136	0.820	1.353	ZINC838184	1.070	0.807	1.246	ZINC9781369	1.030	0.756	1.234
ZINC100790987	1.134	0.796	1.301	ZINC14952515	1.069	0.809	1.520	ZINC85592762	1.030	0.788	1.221
ZINC1463136	1.134	0.754	1.212	ZINC4097706	1.069	0.845	1.495	ZINC101192143	1.030	0.797	1.217
ZINC5564120	1.131	0.767	1.300	ZINC1004760	1.069	0.775	1.280	ZINC754342	1.030	0.852	1.205
ZINC9782397	1.131	0.820	1.295	ZINC9601602	1.069	0.754	1.260	ZINC70454402	1.029	0.803	1.520
ZINC4416338	1.130	0.879	1.570	ZINC13282210	1.069	0.771	1.256	ZINC71316154	1.029	0.794	1.429
ZINC12818365	1.129	0.775	1.269	ZINC4098556	1.068	0.834	1.528	ZINC3903396	1.029	0.785	1.221
ZINC19793157	1.127	0.752	1.328	ZINC14728216	1.068	0.760	1.310	ZINC838170	1.028	0.785	1.220
ZINC6350710	1.126	0.787	1.321	ZINC1823150	1.068	0.771	1.255	ZINC40312435	1.027	0.776	1.312
ZINC8934438	1.125	0.804	1.263	ZINC5126036	1.068	0.810	1.243	ZINC1831406	1.027	0.862	1.208
ZINC524729822	1.121	0.755	1.350	ZINC1814239	1.068	0.777	1.203	ZINC771868	1.027	0.849	1.202
ZINC95099184	1.120	0.875	1.509	ZINC4416340	1.067	0.831	1.490	ZINC641059	1.026	0.752	1.206
ZINC604403850	1.120	0.752	1.320	ZINC524731545	1.067	0.781	1.276	ZINC5126033	1.026	0.762	1.203
ZINC272757	1.119	0.788	1.230	ZINC789673	1.067	0.752	1.257	ZINC34582172	1.025	0.792	1.401
ZINC4416342	1.118	0.867	1.558	ZINC35183154	1.067	0.864	1.220	ZINC95909527	1.025	0.811	1.359
ZINC832596	1.118	0.824	1.304	ZINC4349347	1.066	0.835	1.523	ZINC95910756	1.024	0.762	1.478
ZINC79188978	1.118	0.816	1.228	ZINC256004464	1.066	0.831	1.486	ZINC4102355	1.024	0.809	1.459
ZINC4136393	1.117	0.796	1.309	ZINC9601620	1.066	0.754	1.256	ZINC85489357	1.024	0.818	1.386
ZINC985538	1.117	0.804	1.307	ZINC188472	1.066	0.888	1.241	ZINC59765534	1.023	0.817	1.442

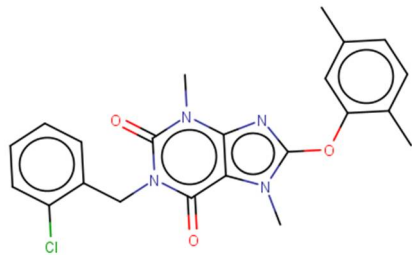
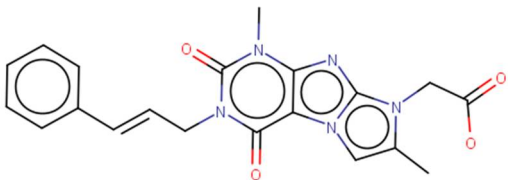
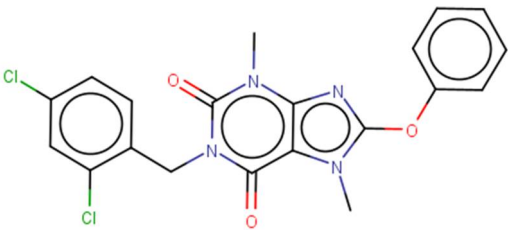
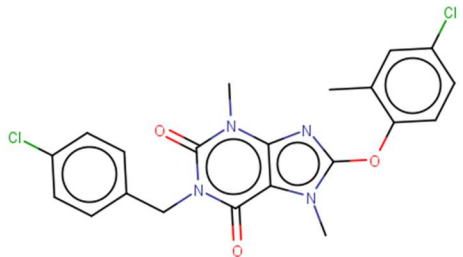
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ZINC5126026	1.116	0.823	1.302	ZINC59587489	1.065	0.832	1.546	ZINC85531479	1.023	0.832	1.384
ZINC4950181	1.116	0.825	1.301	ZINC838172	1.065	0.821	1.257	ZINC19624606	1.023	0.766	1.243
ZINC5126016	1.116	0.822	1.301	ZINC789678	1.065	0.751	1.255	ZINC59767459	1.022	0.771	1.485
ZINC263585280	1.116	0.840	1.296	ZINC85592752	1.065	0.810	1.240	ZINC59771840	1.022	0.814	1.447
ZINC784692	1.116	0.754	1.256	ZINC4349341	1.064	0.829	1.526	ZINC14684626	1.022	0.789	1.440
ZINC524732009	1.114	0.759	1.341	ZINC33832036	1.064	0.852	1.436	ZINC13756081	1.022	0.777	1.215
ZINC891969	1.114	0.777	1.281	ZINC8589992	1.064	0.767	1.275	ZINC9781363	1.022	0.781	1.213
ZINC35183146	1.114	0.898	1.253	ZINC4785836	1.064	0.750	1.254	ZINC12656812	1.022	0.755	1.200
ZINC9601600	1.114	0.794	1.252	ZINC976543	1.064	0.802	1.240	ZINC31494764	1.020	0.808	1.469
ZINC043090	1.113	0.763	1.224	ZINC408712	1.064	0.896	1.200	ZINC43465446	1.020	0.796	1.427
ZINC629087	1.111	0.774	1.279	ZINC59769582	1.063	0.830	1.543	ZINC33831890	1.019	0.778	1.489
ZINC637501	1.110	0.811	1.323	ZINC85509222	1.063	0.804	1.513	ZINC95914666	1.018	0.783	1.500
ZINC780279	1.110	0.817	1.295	ZINC145236354	1.063	0.829	1.482	ZINC59588314	1.018	0.811	1.421
ZINC12342456	1.110	0.773	1.277	ZINC524731655	1.063	0.801	1.263	ZINC15830180	1.018	0.759	1.261
ZINC524732095	1.110	0.810	1.272	ZINC4416344	1.062	0.801	1.513	ZINC12660384	1.018	0.751	1.242
ZINC84153777	1.109	0.845	1.610	ZINC14684624	1.062	0.829	1.480	ZINC107430606	1.018	0.751	1.219
ZINC59764672	1.109	0.857	1.550	ZINC31155769	1.062	0.840	1.426	ZINC8434862	1.018	0.784	1.206
ZINC14684625	1.109	0.858	1.549	ZINC95486355	1.062	0.842	1.423	ZINC95098946	1.017	0.794	1.502
ZINC641063	1.109	0.772	1.276	ZINC35623187	1.062	0.860	1.215	ZINC526567	1.017	0.769	1.255
ZINC85643658	1.108	0.846	1.561	ZINC15657732	1.061	0.839	1.425	ZINC22289134	1.016	0.760	1.235
ZINC524731546	1.108	0.849	1.306	ZINC678123	1.061	0.761	1.249	ZINC839517	1.016	0.766	1.233
ZINC824764557	1.106	0.763	1.387	ZINC12342533	1.061	0.764	1.247	ZINC59764696	1.015	0.808	1.456
ZINC36367814	1.106	0.914	1.218	ZINC85531795	1.060	0.800	1.511	ZINC59586922	1.015	0.792	1.441
ZINC35183249	1.106	0.914	1.218	ZINC1071126	1.060	0.772	1.244	ZINC20113041	1.015	0.773	1.249
ZINC12427889	1.105	0.775	1.299	ZINC12402879	1.060	0.798	1.236	ZINC95912862	1.014	0.801	1.446
ZINC192121	1.105	0.837	1.259	ZINC5126032	1.060	0.815	1.231	ZINC34356282	1.014	0.787	1.383
ZINC20761678	1.105	0.755	1.216	ZINC85540925	1.059	0.809	1.564	ZINC101269056	1.014	0.754	1.304

ZINC70454948	1.104	0.843	1.602	ZINC31156122	1.059	0.854	1.459	ZINC15830202	1.014	0.757	1.257
ZINC5166457	1.104	0.752	1.301	ZINC59733192	1.059	0.839	1.439	ZINC1322114	1.014	0.772	1.248
ZINC1127263	1.104	0.767	1.271	ZINC851296	1.059	0.763	1.271	ZINC31156160	1.013	0.800	1.386
ZINC637757	1.104	0.767	1.271	ZINC9781365	1.059	0.816	1.250	ZINC40395299	1.013	0.781	1.367
ZINC524732094	1.104	0.763	1.271	ZINC13403091	1.059	0.763	1.245	ZINC839520	1.013	0.752	1.235
ZINC32124293	1.104	0.771	1.215	ZINC9782507	1.059	0.761	1.245	ZINC5126043	1.013	0.752	1.213
ZINC8846457	1.103	0.814	1.312	ZINC4084083	1.059	0.774	1.218	ZINC38139689	1.012	0.760	1.453
ZINC13282202	1.102	0.766	1.269	ZINC31158282	1.058	0.815	1.509	ZINC604404017	1.012	0.756	1.322
ZINC9601585	1.102	0.764	1.269	ZINC85540917	1.057	0.814	1.531	ZINC8964561	1.012	0.753	1.256
ZINC189499	1.101	0.789	1.238	ZINC136163915	1.057	0.822	1.478	ZINC96115985	1.012	0.793	1.212
ZINC69482277	1.100	0.826	1.377	ZINC40412761	1.057	0.813	1.466	ZINC95911739	1.011	0.778	1.408
ZINC13739123	1.100	0.763	1.267	ZINC12342497	1.057	0.796	1.232	ZINC85877411	1.011	0.757	1.230
ZINC1068770	1.100	0.763	1.267	ZINC35880132	1.056	0.816	1.419	ZINC59766885	1.010	0.777	1.407
ZINC631628	1.100	0.783	1.264	ZINC524729083	1.056	0.755	1.320	ZINC15988049	1.010	0.766	1.223
ZINC19851363	1.100	0.839	1.253	ZINC882630	1.056	0.755	1.243	ZINC59767653	1.009	0.785	1.415
ZINC4692013	1.099	0.867	1.558	ZINC9782503	1.056	0.761	1.242	ZINC59767342	1.008	0.785	1.433
ZINC14648312	1.099	0.759	1.407	ZINC13282211	1.056	0.790	1.233	ZINC59588414	1.008	0.783	1.374
ZINC851295	1.099	0.762	1.266	ZINC525915108	1.055	0.802	1.520	ZINC31162312	1.008	0.773	1.345
ZINC9601606	1.098	0.762	1.265	ZINC85877634	1.055	0.770	1.213	ZINC15674091	1.006	0.762	1.220
ZINC789659	1.098	0.782	1.262	ZINC101192117	1.055	0.789	1.209	ZINC15830196	1.005	0.797	1.236
ZINC14648310	1.097	0.758	1.405	ZINC4012524	1.055	0.897	1.201	ZINC95910262	1.004	0.790	1.416
ZINC5642047	1.097	0.760	1.264	ZINC33833250	1.054	0.830	1.523	ZINC85511982	1.003	0.805	1.357
ZINC9782399	1.096	0.824	1.299	ZINC34013285	1.054	0.819	1.474	ZINC95918982	1.003	0.756	1.307
ZINC13510361	1.096	0.758	1.263	ZINC2316884	1.054	0.794	1.230	ZINC15120654	1.003	0.756	1.307
ZINC086265	1.096	0.851	1.245	ZINC59585959	1.053	0.792	1.528	ZINC59765346	1.002	0.807	1.442
ZINC272761	1.096	0.790	1.233	ZINC1532699	1.053	0.766	1.411	ZINC59181830	1.002	0.779	1.428
ZINC9782477	1.095	0.767	1.288	ZINC15657718	1.052	0.818	1.471	ZINC824654903	1.002	0.765	1.212
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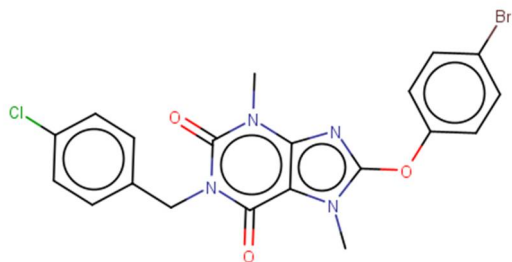
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ZINC6732641	1.094	0.756	1.261								

Table S4. 2D structures of selected NPs and docking score values

ID	Structure	CG4	CG3: Steric	CG3: Clash	CG3: ProDesov	CG3: LigDesov	CG3: LigDesovHB	CG4: HB
ZINC84153787		-8.931	-10.724	0.575	5.283	4.773	-1.097	-7.742
ZINC33833997		-8.354	-9.435	0.439	4.085	3.750	-0.956	-6.237
ZINC33833796		-8.209	-8.885	0.442	4.839	4.652	-2.049	-7.328

ZINC8926342		-6.555	-13.748	0.402	6.696	1.213	-0.385	-0.733
ZINC12296449		-6.354	-12.324	0.630	7.377	4.811	-2.615	-4.234
ZINC8606274		-6.350	-13.193	0.384	6.329	1.225	-0.390	-0.706
ZINC9601609		-6.208	-13.566	0.459	6.864	1.239	-0.430	-0.776

ZINC8926323



-6.177

-13.200

0.444

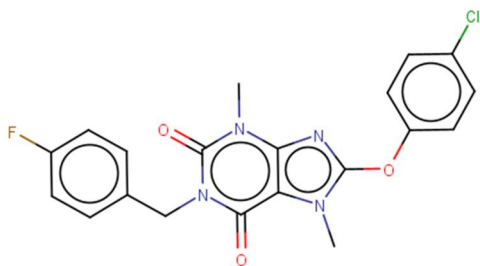
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1.263

-0.487

-0.887

ZINC2488345



-6.005

-13.278

0.436

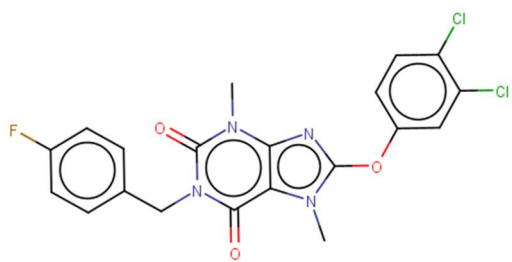
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1.285

-0.485

-0.907

ZINC9601596



-5.765

-11.394

0.546

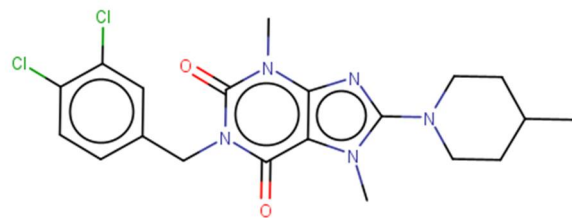
4.857

1.055

-0.245

-0.585

ZINC1094329



-5.719

-11.853

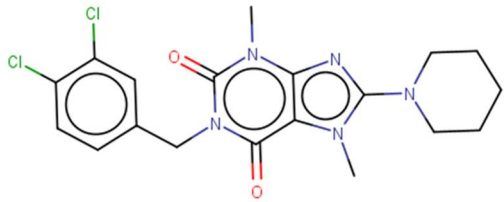
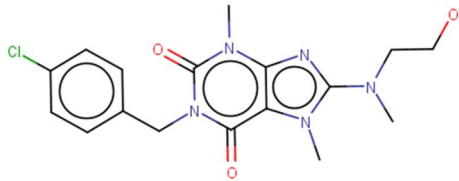
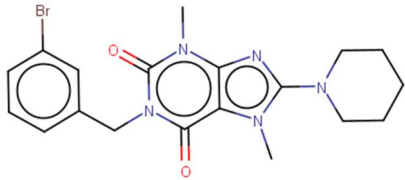
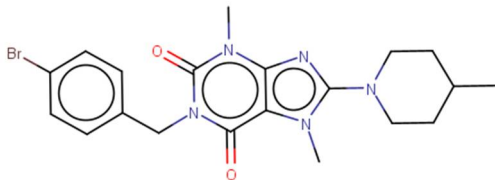
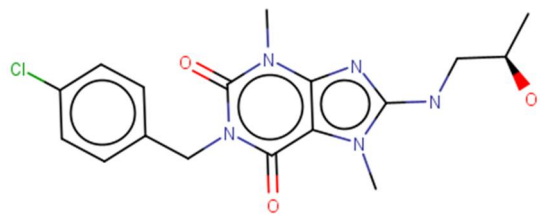
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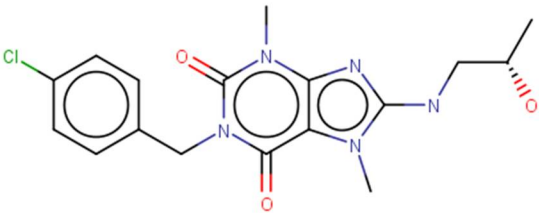
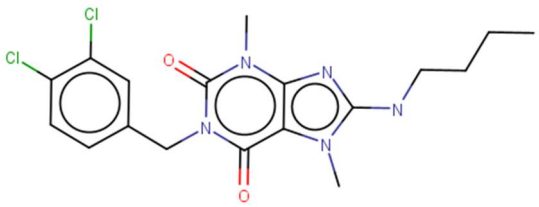
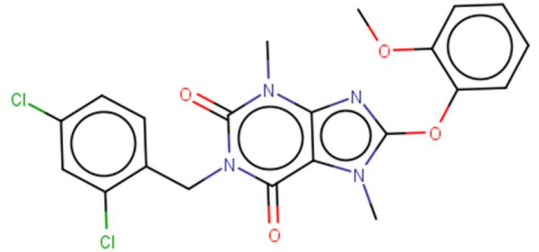
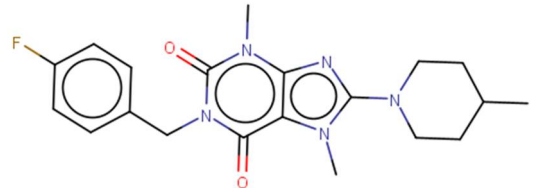
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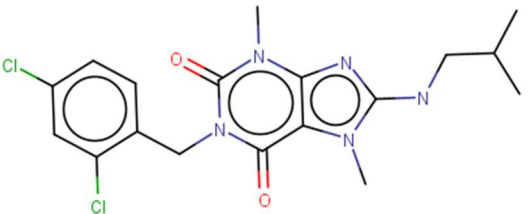
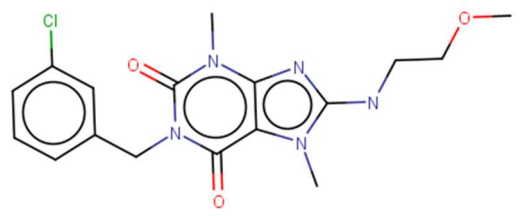
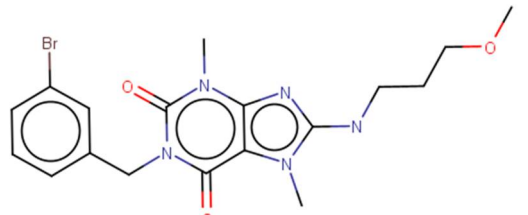
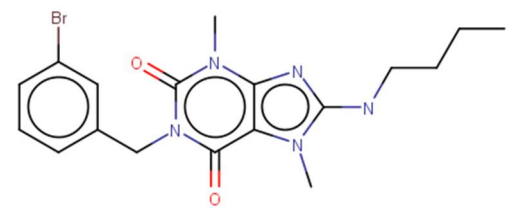
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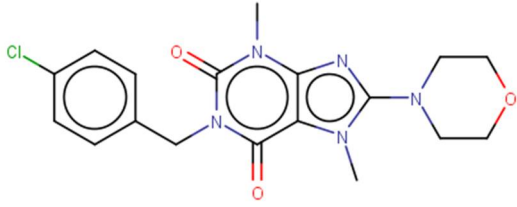
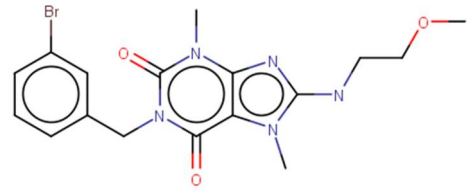
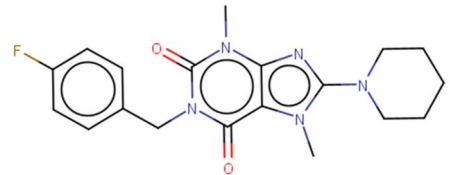
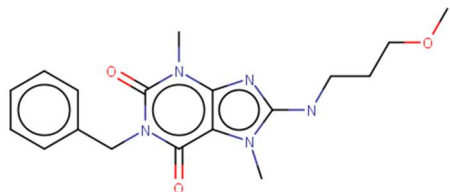
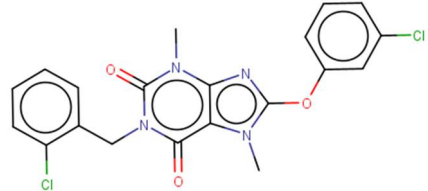
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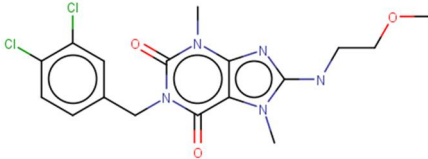
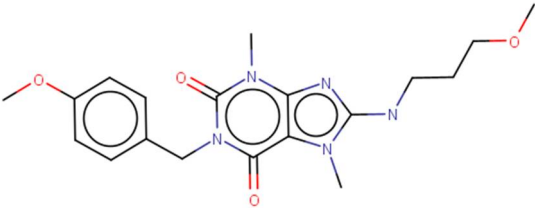
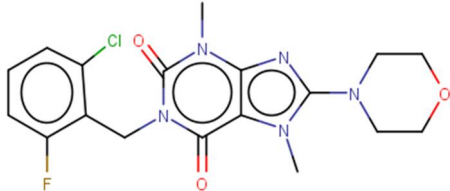
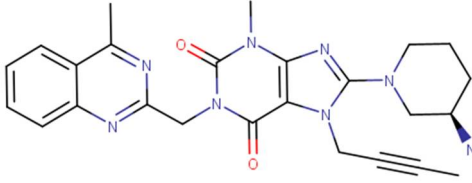
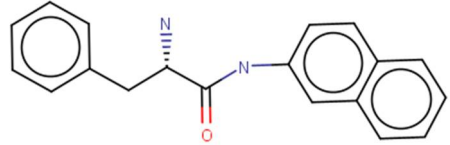
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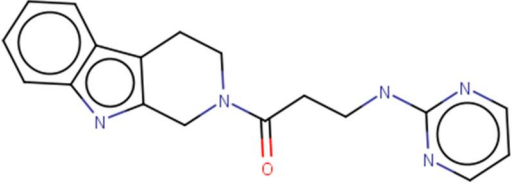
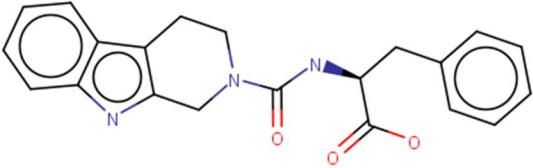
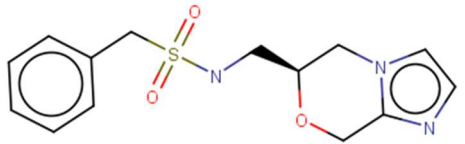
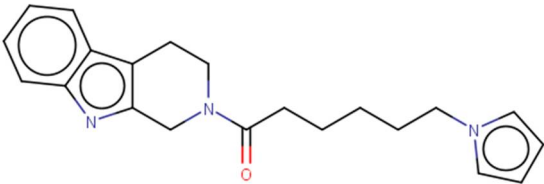
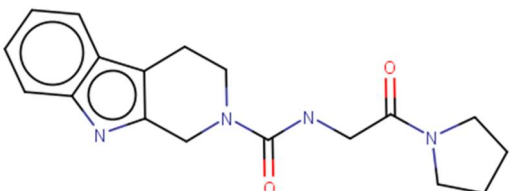
ZINC8916385		-5.618	-11.121	0.352	5.615	1.152	-0.677	-0.938
ZINC640985		-5.496	-9.718	0.292	4.591	1.737	-0.486	-1.911
ZINC832612		-5.467	-11.065	0.361	5.453	1.293	-0.667	-0.842
ZINC2334127		-5.462	-11.049	0.383	5.695	0.976	-0.589	-0.878
ZINC838204		-5.433	-9.915	0.692	3.922	3.320	-1.734	-1.718

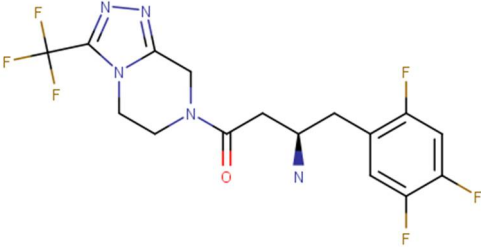
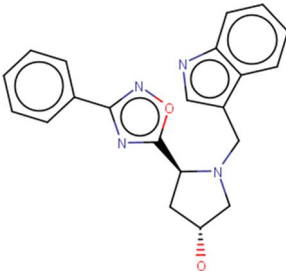
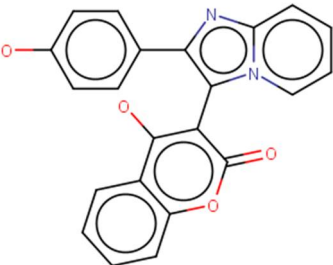
ZINC838200		-5.433	-9.915	0.692	3.922	3.320	-1.734	-1.718
ZINC9601608		-5.428	-10.591	0.379	5.135	1.091	-0.678	-0.764
ZINC6732655		-5.385	-11.569	0.407	6.060	1.077	-0.528	-0.832
ZINC838142		-5.353	-10.193	0.295	4.872	1.008	-0.589	-0.747

ZINC1108640		-5.265	-10.287	0.254	5.188	0.959	-0.671	-0.708
ZINC2488364		-5.058	-9.481	0.648	3.946	3.487	-1.764	-1.894
ZINC9601615		-5.012	-11.365	0.316	5.355	1.681	-0.355	-0.645
ZINC4147162		-4.938	-10.745	0.357	5.175	1.453	-0.427	-0.752

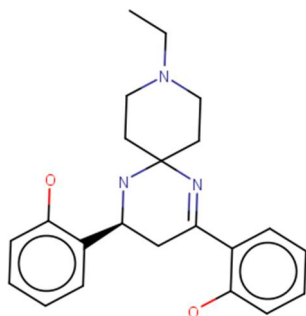
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ZINC2488384		-4.883	-11.425	0.611	4.753	3.251	-1.085	-0.988
ZINC789645		-4.880	-10.261	0.360	5.359	1.236	-0.713	-0.860
ZINC2488377		-4.865	-9.962	0.685	5.021	3.044	-1.446	-2.207
ZINC8589983		-4.776	-11.736	0.487	5.829	2.207	-1.103	-0.460

ZINC13512682		-4.767	-10.221	0.393	5.056	1.444	-0.629	-0.810
ZINC13142224		-4.745	-10.847	0.375	4.950	1.948	-0.600	-0.571
ZINC6565526		-4.550	-11.020	0.549	6.459	2.273	-1.333	-1.479
Linagliptin		-4.46	-11.595	0.451	6.384	3.254	-1.946	-1.008
ZINC2508009		-10.551	-13.226	0.282	4.557	2.848	-1.197	-3.815

ZINC85879571		-9.829	-14.484	0.471	6.275	5.084	-3.593	-3.582
ZINC11692316		-9.682	-13.000	0.703	7.300	4.382	-3.422	-5.645
ZINC96112842		-9.297	-10.873	0.283	2.794	2.910	-2.182	-2.229
ZINC604405970		-9.149	-15.395	0.497	7.919	1.802	-1.899	-2.073
ZINC12296782		-9.138	-15.055	0.466	6.659	3.408	-2.042	-2.574

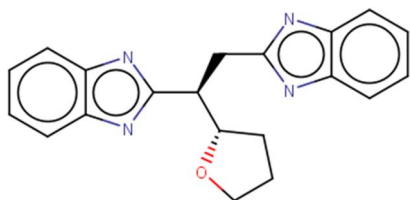
Sitagliptin		-8.859	-15.328	1.057	8.670	2.924	-2.423	-3.760
ZINC15674091		-11.613	-15.359	0.639	4.5601	3.369	-2.475	-2.347
ZINC524732009		-11.498	-16.260	0.385	6.205	2.612	-0.5131	-3.928

ZINC15830055



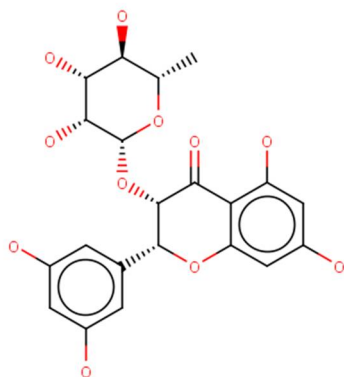
-11.158 -13.655 0.465 5.597 2.691 -3.077 -3.179

ZINC3984976



-11.003 -13.108 0.552 4.932 2.584 -3.215 -2.748

ZINC85509222



-10.850 -16.481 0.542 6.656 4.889 -1.320 -5.137



Table S5. Absorption parameters for selected NPs and drugs (pkCSM online tool was engaged)

Molecule	Water solubility (log mol/L)	Caco2 permeability (log cm/s) high Caco2 permeability >0.9	Human intestinal absorption (% Absorbed) poorly absorbed <30%	Skin Permeability low skin permeability, log Kp>-2.5	P-glycoprotein substrate	P-glycoprotein I inhibitor	P-glycoprotein II inhibitor
ZINC84153787	-2.953	-0.829	43.287	-2.735	Yes	No	No
ZINC33833997	-2.907	-0.425	26.427	-2.735	Yes	No	No
ZINC33833796	-2.906	-0.453	26.115	-2.735	Yes	No	No
ZINC8926342	-2.979	1.504	94.892	-2.735	No	Yes	Yes
ZINC12296449	-2.890	0.964	67.835	-2.735	Yes	No	No
ZINC8606274	-3.044	1.393	92.916	-2.737	No	Yes	Yes
ZINC9601609	-2.943	1.473	92.500	-2.735	Yes	Yes	Yes
ZINC8926323	-3.063	1.443	93.155	-2.737	No	Yes	Yes
ZINC2488345	-3.016	1.333	94.403	-2.736	No	Yes	Yes
ZINC9601596	-3.024	1.302	94.011	-2.736	No	Yes	Yes
ZINC1094329	-2.996	1.502	99.222	-2.777	Yes	Yes	No

ZINC8916385	-2.874	1.056	100.000	-2.787	Yes	No	No
ZINC640985	-2.770	1.492	75.968	-2.735	No	No	No
ZINC832612	-2.733	1.023	100.000	-2.788	Yes	No	No
ZINC2334127	-2.976	1.525	99.564	-2.780	No	No	No
ZINC838204	-2.659	0.679	72.249	-2.735	Yes	No	No
ZINC838200	-2.912	0.049	72.588	-2.735	Yes	No	No
ZINC6732655	-2.977	1.414	94.163	-2.735	Yes	Yes	No
ZINC9601608	-2.937	1.437	91.389	-2.735	No	Yes	Yes
ZINC838142	-2.923	1.502	100.000	-2.755	No	No	No
ZINC1108640	-3.074	1.475	92.427	-2.735	Yes	Yes	No
ZINC2488364	-2.875	1.403	77.058	-2.735	No	No	No
ZINC9601615	-2.981	1.357	96.997	-2.735	No	No	No
ZINC4147162	-2.981	1.413	95.045	-2.735	Yes	No	No
ZINC1094334	-2.758	0.530	89.257	-2.769	No	No	No
ZINC2488384	-2.887	1.399	77.004	-2.735	No	No	No
ZINC789645	-2.692	1.452	100.000	-2.778	No	No	No
ZINC2488377	-2.949	1.378	71.507	-2.735	No	No	No
ZINC8589983	-3.054	1.370	93.475	-2.737	No	Yes	Yes
ZINC13512682	-2.872	1.401	97.236	-2.735	No	No	No
ZINC13142224	-2.887	0.278	83.907	-2.735	No	No	No
ZINC6565526	-2.924	1.544	93.399	-2.747	No	No	No
Linagliptin	-2.976	1.295	83.771	-2.737	Yes	Yes	No
ZINC2508009	-4.219	1.338	92.203	-2.723	Yes	Yes	Yes
ZINC85879571	-4.046	0.952	93.871	-3.069	Yes	No	No
ZINC11692316	-3.755	0.741	93.771	-2.707	Yes	No	No
ZINC96112842	-2.567	0.485	87.431	-2.774	Yes	No	No
ZINC604405970	-4.551	1.108	91.284	-2.792	Yes	Yes	Yes
ZINC12296782	-3.905	0.746	97.117	-3.000	Yes	No	No

Sitagliptin	-4.159	1.331	90.851	-2.950	No	No	No
ZINC15674091	-3.458	0.814	89.606	-2.738	Yes	Yes	Yes
ZINC524732009	-2.892	0.861	86.834	-2.735	Yes	No	Yes
ZINC15830055	-3.310	0.914	86.807	-2.736	Yes	Yes	Yes
ZINC3984976	-2.892	0.858	78.915	-2.735	Yes	No	No
ZINC85509222	-3.129	-0.314	56.114	-2.735	Yes	No	No
Alogliptin	-2.531	0.293	79.038	-3.081	No	No	No

Table S6. Distribution parameters parameters for selected NPs and drugs (pkCSM online tool was engaged)

Molecule	Human volume of distribution (VDss) (log L/kg) VDss low, logVDss<-0.15 VDss high, logVDss>0.45	Human fraction unbound (Fu)	BBB permeability (log BB) readily cross the BBB, logBB>0.3 poorly distributed, logBB<-1	CNS permeability (log PS) to Penetrate the CNS, logPS>-2 unable to penetrate the CNS, logPS<-3
ZINC84153787	0.817	0.137	-1.912	-4.447
ZINC33833997	0.134	0.152	-1.464	-4.429
ZINC33833796	0.116	0.145	-1.571	-4.455
ZINC8926342	0.277	0.230	-1.128	-2.238
ZINC12296449	0.326	0.372	-1.628	-2.908
ZINC8606274	-0.035	0.188	-1.085	-2.216
ZINC9601609	0.092	0.240	-1.152	-2.184
ZINC8926323	0.045	0.208	-1.105	-2.192
ZINC2488345	-0.102	0.247	-1.129	-2.403
ZINC9601596	-0.066	0.257	-1.302	-2.290
ZINC1094329	0.488	0.321	0.297	-2.865
ZINC8916385	0.731	0.311	-0.008	-2.873

ZINC640985	0.329	0.401	-1.414	-3.099
ZINC832612	0.747	0.303	0.021	-2.858
ZINC2334127	0.507	0.317	0.344	-2.857
ZINC838204	-0.410	0.409	-1.449	-3.488
ZINC838200	-0.285	0.276	-1.360	-3.034
ZINC6732655	0.222	0.270	-1.364	-2.935
ZINC9601608	-0.042	0.263	-1.375	-2.498
ZINC838142	0.353	0.387	0.100	-2.921
ZINC1108640	0.173	0.252	-1.251	-2.482
ZINC2488364	-0.023	0.324	-1.386	-3.071
ZINC9601615	0.058	0.285	-1.415	-3.053
ZINC4147162	0.239	0.253	-1.197	-2.922
ZINC1094334	0.552	0.350	-1.354	-2.988
ZINC2488384	-0.015	0.322	-1.395	-3.069
ZINC789645	0.580	0.370	-0.207	-2.918
ZINC2488377	0.055	0.257	-1.222	-3.189
ZINC8589983	-0.009	0.181	-1.092	-2.211
ZINC13512682	-0.023	0.339	-1.562	-3.082
ZINC13142224	-0.074	0.337	-1.454	-3.151
ZINC6565526	0.415	0.400	-1.568	-3.025
Linagliptin	0.376	0.245	-1.436	-2.939
ZINC2508009	0.752	0.000	0.043	-1.942
ZINC85879571	0.454	0.257	-0.828	-2.448
ZINC11692316	-0.167	0.110	-0.538	-2.295
ZINC96112842	-0.091	0.378	-0.923	-2.956
ZINC604405970	0.875	0.161	0.273	-1.758
ZINC12296782	0.258	0.389	-0.793	-2.469
Sitagliptin	-0.314	0.294	-1.523	-3.115

ZINC15674091	0.458	0.141	-0.769	-2.153
ZINC524732009	-0.018	0.308	0.145	-1.947
ZINC15830055	2.089	0.370	-0.451	-2.106
ZINC3984976	0.657	0.224	0.388	-2.077
ZINC85509222	0.048	0.263	-1.487	-4.557
Alogliptin	0.359	0.369	-0.575	-2.685

Table S7. Metabolism and excretion parameters for selected NPs and drugs (pkCSM online tool was engaged)

Molecule	CYP2D6 substrate	CYP3A4 substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Total Clearance (log ml/min/kg)	Renal OCT2 sub- strate
ZINC84153787	No	No	No	No	No	No	No	0.526	No
ZINC33833997	No	No	No	No	No	No	No	0.162	No
ZINC33833796	No	No	No	No	No	No	No	0.129	No
ZINC8926342	No	No	Yes	Yes	Yes	No	Yes	0.255	Yes
ZINC12296449	No	No	No	No	No	No	No	0.315	No
ZINC8606274	No	Yes	Yes	Yes	Yes	No	Yes	0.136	Yes
ZINC9601609	No	No	Yes	Yes	Yes	No	Yes	0.201	Yes
ZINC8926323	No	Yes	Yes	Yes	Yes	No	Yes	0.243	Yes
ZINC2488345	No	Yes	Yes	Yes	Yes	No	Yes	0.226	Yes
ZINC9601596	No	Yes	Yes	Yes	Yes	No	Yes	0.262	Yes
ZINC1094329	No	Yes	No	Yes	No	No	No	0.370	Yes
ZINC8916385	No	Yes	Yes	Yes	No	No	No	0.484	No
ZINC640985	No	No	Yes	No	No	No	No	0.342	No
ZINC832612	No	Yes	Yes	Yes	No	No	No	0.334	No
ZINC2334127	No	Yes	Yes	Yes	No	No	No	0.318	Yes

ZINC838204	No	No	No	No	No	No	No	0.390	No
ZINC838200	No	No	Yes	No	No	No	No	0.450	Yes
ZINC6732655	No	No	Yes	Yes	Yes	No	No	0.572	Yes
ZINC9601608	No	No	Yes	Yes	Yes	No	Yes	0.182	Yes
ZINC838142	No	Yes	Yes	Yes	No	No	No	0.301	Yes
ZINC1108640	No	No	Yes	Yes	Yes	No	No	0.169	Yes
ZINC2488364	No	No	Yes	No	No	No	No	0.444	No
ZINC9601615	No	No	No	No	No	No	No	0.414	No
ZINC4147162	No	Yes	Yes	No	Yes	No	No	0.423	Yes
ZINC1094334	No	Yes	Yes	Yes	No	No	No	0.433	No
ZINC2488384	No	No	Yes	No	No	No	No	0.382	No
ZINC789645	No	Yes	Yes	Yes	No	No	No	0.415	No
ZINC2488377	No	No	Yes	No	No	No	No	0.538	Yes
ZINC8589983	No	Yes	Yes	Yes	Yes	No	Yes	0.172	Yes
ZINC13512682	No	No	No	No	No	No	No	0.531	No
ZINC13142224	No	No	No	No	No	No	No	0.566	No
ZINC6565526	No	Yes	Yes	No	No	No	No	0.318	No
Linagliptin	No	Yes	No	No	Yes	No	Yes	0.443	Yes
ZINC2508009	No	Yes	Yes	Yes	No	Yes	No	0.974	No
ZINC85879571	No	Yes	Yes	No	No	No	No	0.730	No
ZINC11692316	No	Yes	Yes	No	No	No	No	0.813	No
ZINC96112842	No	No	No	No	No	No	No	0.799	Yes
ZINC604405970	Yes	Yes	Yes	Yes	Yes	Yes	No	0.981	Yes
ZINC12296782	Yes	Yes	Yes	No	No	No	No	0.619	No
Sitagliptin	No	Yes	No	No	No	No	No	0.472	No
ZINC15674091	No	Yes	Yes	Yes	No	Yes	Yes	0.783	Yes
ZINC524732009	No	No	Yes	Yes	Yes	Yes	Yes	0.486	Yes
ZINC15830055	Yes	Yes	No	No	No	Yes	No	0.505	No

ZINC3984976	No	No	Yes	Yes	No	Yes	Yes	1.450	Yes
ZINC85509222	No	No	No	No	No	No	No	-0.074	No
Alogliptin	No	Yes	No	No	No	No	No	0.365	No

Table S8. Toxicity parameters for selected NPs and drugs (pkCSM online tool was engaged)

Molecule	AMES toxicity ^a	Max. Human tolerated Dose ^b (log mg/kg/day) Toxic effect > 0.477 log mg/kg/day	hERG I inhibitor ^c	hERG II inhibitor ^d	Oral Rat Acute Toxicity ^e (LD50) (mol/kg)	Oral Rat Chronic Toxicity ^f (LOAEL) (log mg/kg_bw/day)	Hepatotoxicity ^g	Skin Sensitization ^h	T.Pyiformis toxicity ⁱ (log ug/L)	Minnow toxicity ^j (log mM)
ZINC84153787	No	0.639	No	Yes	2.618	5.028	No	No	0.285	4.394
ZINC33833997	No	0.635	No	No	2.694	5.224	No	No	0.285	1.501
ZINC33833796	No	0.646	No	No	2.701	5.173	No	No	0.285	1.532
ZINC8926342	Yes	0.685	No	Yes	2.720	1.249	No	No	0.285	0.273
ZINC12296449	No	0.526	No	No	2.483	1.240	No	No	0.285	0.209
ZINC8606274	No	0.241	No	Yes	2.647	0.855	No	No	0.285	-0.041
ZINC9601609	Yes	0.456	No	Yes	2.678	1.008	No	No	0.285	-0.488
ZINC8926323	No	0.277	No	Yes	2.652	0.847	No	No	0.285	-0.164
ZINC2488345	No	0.151	No	Yes	2.632	1.013	No	No	0.285	0.661
ZINC9601596	No	0.239	No	Yes	2.771	0.838	No	No	0.285	-0.235
ZINC1094329	No	0.832	No	Yes	2.505	1.073	Yes	No	0.285	0.174
ZINC8916385	Yes	-0.091	No	Yes	2.820	1.028	Yes	No	0.286	-0.173
ZINC640985	Yes	1.249	No	No	2.236	1.132	Yes	No	0.285	2.361
ZINC832612	Yes	-0.121	No	Yes	2.764	1.074	Yes	No	0.286	0.152
ZINC2334127	No	0.830	No	Yes	2.435	1.105	Yes	No	0.285	0.937

ZINC838204	Yes	0.766	No	No	2.285	1.773	Yes	No	0.285	3.741
ZINC838200	Yes	0.770	No	Yes	1.986	1.047	Yes	No	0.285	2.940
ZINC6732655	Yes	0.801	No	Yes	2.695	1.012	Yes	No	0.285	1.492
ZINC9601608	Yes	0.393	No	Yes	2.571	1.023	No	No	0.285	-0.547
ZINC838142	Yes	0.627	No	Yes	2.402	1.207	Yes	No	0.285	1.612
ZINC1108640	Yes	0.781	No	Yes	2.719	1.038	Yes	No	0.285	1.918
ZINC2488364	Yes	0.773	No	No	2.321	0.975	Yes	No	0.285	2.122
ZINC9601615	Yes	0.809	No	Yes	2.420	0.988	Yes	No	0.285	1.895
ZINC4147162	Yes	0.783	No	Yes	2.625	1.047	Yes	No	0.285	1.817
ZINC1094334	Yes	0.110	No	Yes	2.566	1.083	Yes	No	0.285	0.499
ZINC2488384	Yes	0.774	No	No	2.325	0.975	Yes	No	0.285	1.976
ZINC789645	Yes	-0.139	No	Yes	2.745	1.167	Yes	No	0.286	1.317
ZINC2488377	Yes	0.790	No	Yes	2.354	1.016	Yes	No	0.285	2.853
ZINC8589983	Yes	0.312	No	Yes	2.782	0.856	No	No	0.285	-0.581
ZINC13512682	Yes	0.785	No	No	2.374	0.940	Yes	No	0.285	1.651
ZINC13142224	Yes	0.727	No	No	2.368	1.119	Yes	No	0.285	2.701
ZINC6565526	No	0.107	No	Yes	2.661	1.116	Yes	No	0.285	0.336
Linagliptin	Yes	0.722	No	Yes	2.677	1.264	Yes	No	0.285	0.670
ZINC2508009	Yes	0.323	No	Yes	2.105	0.835	Yes	No	0.753	-0.049
ZINC85879571	No	-0.410	No	Yes	2.285	1.618	Yes	No	0.521	0.325
ZINC11692316	No	-0.355	No	Yes	2.300	1.998	Yes	No	0.321	2.118
ZINC96112842	Yes	0.248	No	Yes	2.611	1.424	Yes	No	0.285	1.864
ZINC604405970	No	-0.688	No	Yes	2.568	1.026	Yes	No	1.100	-0.491
ZINC12296782	No	-0.409	No	Yes	2.223	1.157	Yes	No	0.324	2.605
Sitagliptin	No	0.570	No	No	2.496	1.145	Yes	No	0.350	0.672
ZINC15674091	Yes	0.024	No	Yes	3.205	1.350	Yes	No	0.285	-0.404
ZINC524732009	Yes	0.316	No	Yes	2.484	0.601	No	No	0.285	2.451
ZINC15830055	No	-0.434	No	Yes	3.313	1.330	Yes	No	0.291	3.747

ZINC3984976	Yes	0.434	Yes	Yes	2.396	1.859	No	No	0.285	1.344
ZINC85509222	Yes	0.827	No	No	2.781	3.865	No	No	0.285	2.605
Alogliptin	Yes	-0.685	No	Yes	2.385	1.428	Yes	No	0.789	2.671

^aA compound with a positive values of AMES mutagenicity test is mutagenic and therefore may act as a carcinogen; ^bA Maximum recommended tolerated dose (MRTD) is $\leq 0.477 \log \text{mg/kg/day}$ is considered to be low, while $> 0.477 \log \text{mg/kg/day}$ is considered to be high; A hERG ^cI/^dII inhibitors could cause the development of the acquired long QT syndrome, which leads to fatal ventricular arrhythmia; ^eA lethal dosage value LD50 (mol/kg) is consider a standard measurement of acute toxicity; ^fThe lowest dose of a compound that results in an observed adverse effect (LOAEL) is in $\log (\text{mg/kg}_{\text{bw}}/\text{day})$; ^gA compound with positive tests could be associated with disrupted normal function of the liver; ^hA compound with positive tests could have a high potential adverse effect for products applied to the skin, e.g. cosmetics and antifungals; ⁱA value $> -0.5 \log \mu\text{g/L}$ is considered to be toxic; ^jA $\log \text{LC50}$ values < -0.3 indicate high acute toxicity.

Table S9. Docked interaction analysis of selected NPs compounds with target proteins 2RGU and 2ONC

Molecule	Bonds length (Å)	Type	Category	Active site residues	NP:Atoms
ZINC12296449	3.173	Salt Bridge	Hydrogen Bond;Electrostatic	A:ARG669:NH2	ZINC12296449:O26
	4.145	Attractive Charge	Electrostatic	A:ARG358:NH1	ZINC12296449:O26
	2.604	Conventional Hydrogen Bond	Hydrogen Bond	A:ARG358:NH1	ZINC12296449:O29
	2.686	Conventional Hydrogen Bond	Hydrogen Bond	A:SER630:OG	ZINC12296449:O28
	3.711	Carbon Hydrogen Bond	Hydrogen Bond	A:GLU205:OE2	ZINC12296449:C18
	3.655	Carbon Hydrogen Bond	Hydrogen Bond	A:GLU206:OE2	ZINC12296449:C18
	3.594	Carbon Hydrogen Bond	Hydrogen Bond	A:ASN710:OD1	ZINC12296449:C18
	3.179	Carbon Hydrogen Bond	Hydrogen Bond	A:GLU205:O	ZINC12296449:C20
	3.924	Pi-Sigma	Hydrophobic	A:PHE357	ZINC12296449:C17
	5.020	Pi-Pi Stacked	Hydrophobic	A:TYR666	ZINC12296449
	5.261	Pi-Pi Stacked	Hydrophobic	A:TYR666	ZINC12296449
	4.725	Pi-Pi Stacked	Hydrophobic	A:PHE357	ZINC12296449
	4.603	Pi-Pi T-shaped	Hydrophobic	A:TYR547	ZINC12296449

	3.922	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC12296449
	4.268	Pi-Alkyl	Hydrophobic	A:TYR662	ZINC12296449:C18
ZINC8926342	3.383	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	ZINC8926342
	3.204	Conventional Hydrogen Bond	Hydrogen Bond	A:TYR631:N	ZINC8926342:O27
	3.606	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:OG	ZINC8926342:C20
	3.639	Pi-Anion	Electrostatic	A:GLU206:OE1	ZINC8926342
	2.895	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC8926342
	3.460	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC8926342
	3.878	Pi-Sigma	Hydrophobic	A:PHE357	ZINC8926342:C18
	3.614	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC8926342
	4.617	Pi-Pi Stacked	Hydrophobic	A:TRP629	ZINC8926342
	5.625	Pi-Pi Stacked	Hydrophobic	A:TRP629	ZINC8926342
	4.431	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC8926342
	5.211	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC8926342:C20
	5.089	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC8926342:C21
	5.481	Pi-Alkyl	Hydrophobic	A:TYR631	ZINC8926342:C20
ZINC8606274	3.893	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1020:O	ZINC08606274
	3.200	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	ZINC08606274
	3.224	Conventional Hydrogen Bond	Hydrogen Bond	A:TYR631:N	ZINC08606274:O25
	3.266	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:OG	ZINC08606274:C18
	3.469	Pi-Anion	Electrostatic	A:GLU206:OE1	ZINC08606274
	3.540	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC08606274
	3.407	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC08606274
	3.969	Pi-Sigma	Hydrophobic	A:TRP629:CB	ZINC08606274

	3.802	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC08606274
	4.870	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC08606274
	3.715	Pi-Alkyl	Hydrophobic	A:TRP629	ZINC08606274:CI28
	3.544	Pi-Alkyl	Hydrophobic	A:TRP629	ZINC08606274:CI28
ZINC9601609	4.020	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1020:O	ZINC9601609
	3.262	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	ZINC9601609
	3.133	Conventional Hydrogen Bond	Hydrogen Bond	A:TYR631:N	ZINC9601609:O26
	3.328	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:OG	ZINC9601609:C19
	3.624	Pi-Anion	Electrostatic	A:GLU206:OE1	ZINC9601609
	3.433	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC9601609
	3.292	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC9601609
	3.728	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC9601609
	4.828	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC9601609
	3.656	Pi-Alkyl	Hydrophobic	A:PHE357	ZINC9601609:C18
	5.239	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC9601609:C20
	3.866	Pi-Alkyl	Hydrophobic	A:TRP629	ZINC9601609:CI29
	3.701	Pi-Alkyl	Hydrophobic	A:TRP629	ZINC9601609:CI29
	4.261	Pi-Alkyl	Hydrophobic	A:TYR666	ZINC9601609:C18
ZINC8926323		Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	ZINC8926323
	3.094	Pi-Donor Hydrogen Bond			
	3.053	Conventional Hydrogen Bond	Hydrogen Bond	A:TYR631:N	ZINC8926323:O25
	2.894	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:CB	ZINC8926323:O25
	3.072	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:OG	ZINC8926323:C18
	3.713	Pi-Anion	Electrostatic	A:GLU206:OE1	ZINC8926323
	3.662	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC8926323

	3.311	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC8926323
	3.816	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC8926323
	4.707	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC8926323
	4.961	Pi-Alkyl	Hydrophobic	A:PHE357	ZINC8926323:Br29
	5.138	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC8926323:C19
	3.911	Pi-Alkyl	Hydrophobic	A:TRP629	ZINC8926323:Cl28
	3.605	Pi-Alkyl	Hydrophobic	A:TRP629	ZINC8926323:Cl28
	4.002	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1020:O	ZINC2488345
	3.056	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	ZINC2488345
	2.969	Conventional Hydrogen Bond	Hydrogen Bond	A:TYR631:N	ZINC2488345:O25
	3.171	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:OG	ZINC2488345:C18
	3.372	Pi-Anion	Electrostatic	A:GLU206:OE1	ZINC2488345
ZINC2488345	3.543	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC2488345
	3.526	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC2488345
	3.868	Pi-Sigma	Hydrophobic	A:TRP629:CB	ZINC2488345
	3.877	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC2488345
	5.026	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC2488345
	5.150	Alkyl	Hydrophobic	A:356901	ZINC2488345:C18
	3.794	Alkyl	Hydrophobic	A:356901	ZINC2488345:Cl29
	5.314	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC2488345:C19
	3.746	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	ZINC9601596
ZINC9601596	3.708	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	ZINC9601596
	3.220	Water Hydrogen Bond;	Hydrogen Bond	A:HOH1020:O	ZINC9601596:C20

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ZINC9601596	3.639	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:CB	ZINC9601596:O25
	2.887	Halogen (Cl, Br, I)	Halogen	A:GLU206:OE1	ZINC9601596:Cl30
	2.716	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC9601596
	4.006	Pi-Pi Stacked	Hydrophobic	A:PHE357	ZINC9601596
	3.641	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC9601596
	4.394	Pi-Pi Stacked	Hydrophobic	A:TRP629	ZINC9601596
	5.166	Pi-Pi Stacked	Hydrophobic	A:TRP629	ZINC9601596
	3.748	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC9601596
	3.853	Pi-Alkyl	Hydrophobic	A:PHE357	ZINC9601596:Cl29
	4.132	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC9601596:C18
	5.310	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC9601596:C19
	5.390	Pi-Alkyl	Hydrophobic	A:TYR631	ZINC9601596:C18
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ZINC9601608	3.925	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1020:O	ZINC9601608
	3.246	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	ZINC9601608
	3.950	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	ZINC9601608
	2.919	Conventional Hydrogen Bond	Hydrogen Bond	A:TYR631:N	ZINC9601608:O27
	2.958	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:CB	ZINC9601608:O27
	3.337	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:OG	ZINC9601608:C19
	3.154	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC9601608
	3.570	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC9601608
	4.566	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC9601608
	4.954	Pi-Pi T-shaped	Hydrophobic	A:PHE357	ZINC9601608
	5.402	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC9601608:C18
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	5.051	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC9601608:C19
	4.237	Pi-Alkyl	Hydrophobic	A:TRP629	ZINC9601608:CI30
	3.985	Pi-Alkyl	Hydrophobic	A:TRP629	ZINC9601608:CI30
ZINC8589983	3.074	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	ZINC8589983
	3.589	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:OG	ZINC8589983:C19
	4.908	Pi-Anion	Electrostatic	A:GLU206:OE1	ZINC8589983
	2.790	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	ZINC8589983
	4.306	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC8589983
	4.665	Pi-Pi Stacked	Hydrophobic	A:TRP629	ZINC8589983
	5.733	Pi-Pi Stacked	Hydrophobic	A:TRP629	ZINC8589983
	3.646	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC8589983
	3.596	Pi-Alkyl	Hydrophobic	A:PHE357	ZINC8589983:CI29
	3.979	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC8589983:C18
	5.445	Pi-Alkyl	Hydrophobic	A:TYR631	ZINC8589983:C19
Linagliptin	2.969	Water Hydrogen Bond; Conventional Hydrogen Bond	Hydrogen Bond	A:HOH1020:O	A:356901:N25
	3.227	Water Hydrogen Bond; Pi-Donor Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	A:356901
	2.911	Water Hydrogen Bond; Conventional Hydrogen Bond	Hydrogen Bond	A:HOH1041:O	A:356901:N24
	3.053	Conventional Hydrogen Bond	Hydrogen Bond	A:TYR631:N	A:356901:O10
	3.141	Conventional Hydrogen Bond	Hydrogen Bond	A:TYR662:OH	A:356901:N27
	2.972	Conventional Hydrogen Bond	Hydrogen Bond	A:GLU205:OE2	A:356901:N27
	2.712	Conventional Hydrogen Bond	Hydrogen Bond	A:GLU206:OE1	A:356901:N27
	3.779	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:CB	A:356901:N24
	3.672	Carbon Hydrogen Bond	Hydrogen Bond	A:TYR666:OH	A:356901:C6

	2.973	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	A:356901
	3.501	Pi-Donor Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	A:356901
	3.660	Pi-Pi Stacked	Hydrophobic	A:TYR547	A:356901
	4.560	Pi-Pi Stacked	Hydrophobic	A:TRP629	A:356901
	3.653	Pi-Pi Stacked	Hydrophobic	A:TRP629	A:356901
	5.673	Pi-Pi Stacked	Hydrophobic	A:TRP629	A:356901
	4.390	Pi-Pi Stacked	Hydrophobic	A:TRP629	A:356901
	4.585	Pi-Pi Stacked	Hydrophobic	A:TYR547	A:356901
	4.964	Alkyl	Hydrophobic	A:VAL656	A:356901:C23
	4.537	Alkyl	Hydrophobic	A:VAL711	A:356901:C23
	5.146	Pi-Alkyl	Hydrophobic	A:PHE357	A:356901
	5.181	Pi-Alkyl	Hydrophobic	A:TYR547	A:356901:C14
	5.346	Pi-Alkyl	Hydrophobic	A:TRP627	A:356901:C32
	5.275	Pi-Alkyl	Hydrophobic	A:TRP629	A:356901:C32
	4.049	Pi-Alkyl	Hydrophobic	A:TYR662	A:356901:C23
	5.221	Pi-Alkyl	Hydrophobic	A:TYR666	A:356901
	2.687	Conventional Hydrogen Bond	Hydrogen Bond	A:ARG125:HH22	ZINC524732009:O26
	2.393	Conventional Hydrogen Bond	Hydrogen Bond	A:GLU205:O	ZINC524732009:O28
	2.154	Conventional Hydrogen Bond	Hydrogen Bond	A:GLU206:OE1	ZINC524732009:O28
	2.526	Carbon Hydrogen Bond	Hydrogen Bond	A:GLU206:HA	ZINC524732009:O28
	3.860	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC524732009
ZINC524732009	4.228	Pi-Pi Stacked	Hydrophobic	A:TYR662	ZINC524732009
	4.716	Pi-Pi Stacked	Hydrophobic	A:TYR547	ZINC524732009
	4.735	Pi-Pi T-shaped	Hydrophobic	A:TYR666	ZINC524732009
	5.713	Pi-Pi T-shaped	Hydrophobic	A:TYR666	ZINC524732009
	5.431	Pi-Pi T-shaped	Hydrophobic	A:TYR666	ZINC524732009
	5.466	Pi-Alkyl	Hydrophobic	A:VAL656	ZINC524732009

ZINC3984976	3.131	Conventional Hydrogen Bond	Hydrogen Bond	A:GLU206:OE1	ZINC3984976:N23
	3.895	Pi-Pi Stacked	Hydrophobic	A:PHE357	ZINC3984976
	4.617	Pi-Pi Stacked	Hydrophobic	A:TYR662	ZINC3984976
	4.612	Pi-Pi Stacked	Hydrophobic	A:PHE357	ZINC3984976
	5.484	Pi-Pi Stacked	Hydrophobic	A:TYR662	ZINC3984976
	4.413	Pi-Pi T-shaped	Hydrophobic	A:TYR666	ZINC3984976
	4.008	Amide-Pi Stacked	Hydrophobic	A:SER630:C,O;TYR631:N	ZINC3984976
	4.616	Pi-Alkyl	Hydrophobic	A:TYR547	ZINC3984976
	5.269	Pi-Alkyl	Hydrophobic	A:VAL656	ZINC3984976
Alogliptin	3.771	Water Hydrogen Bond; Carbon Hydrogen Bond	Hydrogen Bond	A:HOH939:O	A:SY1800:C2
	2.950	Conventional Hydrogen Bond	Hydrogen Bond	A:ARG125:HH22	A:SY1800:N27
	2.074	Conventional Hydrogen Bond	Hydrogen Bond	A:TYR631:HN	A:SY1800:O17
	3.108	Conventional Hydrogen Bond	Hydrogen Bond	A:GLU205:O	A:SY1800:N1
	2.555	Conventional Hydrogen Bond	Hydrogen Bond	A:GLU205:OE1	A:SY1800:N1
	3.385	Conventional Hydrogen Bond	Hydrogen Bond	A:GLU206:OE1	A:SY1800:N1
	2.362	Carbon Hydrogen Bond	Hydrogen Bond	A:SER630:HB1	A:SY1800:O17
	3.715	Carbon Hydrogen Bond	Hydrogen Bond	A:TYR547:OH	A:SY1800:C5
	4.395	Pi-Pi Stacked	Hydrophobic	A:TYR547	A:SY1800
	4.115	Pi-Pi Stacked	Hydrophobic	A:TYR547	A:SY1800
	4.503	Pi-Pi Stacked	Hydrophobic	A:TYR662	A:SY1800
	4.864	Pi-Pi T-shaped	Hydrophobic	A:TYR666	A:SY1800
	5.415	Pi-Alkyl	Hydrophobic	A:PHE357	A:SY1800

Table S10. The CSM values for the docked pose of each NPs

NPs ID	Type symmetry	Values	Direction vector [x,y,z]	Dipole Moments (Debye)
ZINC8926342	C2 SYM	21.11271189	[-0.9621419316919941, 0.2028967417687959, -0.1819775136097998]	X= -5.2740 Y= 3.0649 Z= 0.7447 Tot= 6.1452
	C3 SYM	21.4116737	[-0.9623080524897467, 0.2030447363354845, -0.18093105637188037]	
	C4 SYM	21.66063869	[-0.9621970639867214, 0.20510821059158382, -0.1791854681698597]	
	C5 SYM	21.66063869	[-0.9621970639867214, 0.20510821059158366, -0.17918546816985975]	
	C6 SYM	21.66063869	[-0.9621970639867212, 0.2051082105915841, -0.17918546816986]	
	C7 SYM	21.66063869	[-0.9621970639867214, 0.20510821059158355, -0.1791854681698596]	
	C8 SYM	21.66063869	[-0.9621970639867214, 0.20510821059158343, -0.17918546816985942]	
	C9 SYM	21.66063869	[-0.9621970639867214, 0.20510821059158366, -0.1791854681698598]	
	C10 SYM	21.66063869	[-0.9621970639867214, 0.20510821059158377, -0.17918546816985956]	
	C11 SYM	21.66063869	[-0.9621970639867214, 0.2051082105915837, -0.17918546816985959]	
	C12 SYM	21.66063869	[-0.9621970639867214, 0.2051082105915835, -0.17918546816985972]	
	C13 SYM	21.66063869	[-0.9621970639867212, 0.20510821059158413, -0.17918546816986028]	
	C14 SYM	21.66063869	[-0.9621970639867212, 0.2051082105915843, -0.17918546816986014]	
	C15 SYM	21.66063869	[-0.9621970639867214, 0.20510821059158404, -0.17918546816985972]	
	C16 SYM	21.66063869	[-0.9621970639867212, 0.20510821059158396, -0.1791854681698597]	
	C17 SYM	21.66063869	[-0.9621970639867214, 0.20510821059158382, -0.17918546816985953]	
	C18 SYM	21.66063869	[-0.9621970639867214, 0.20510821059158388, -0.17918546816985956]	
	C19 SYM	21.66063869	[-0.9621970639867214, 0.20510821059158355, -0.17918546816985953]	
	C20 SYM	21.66063869	[-0.9621970639867214, 0.20510821059158418, -0.17918546816985964]	
	S4 SYM	99.46065105	[0.37945566860260754, -0.8204492363656322, -0.4276405571416246]	
	S6 SYM	99.46065105	[0.37945566860260677, -0.8204492363656322, -0.4276405571416255]	
	S8 SYM	99.46065105	[0.37945566860260677, -0.8204492363656323, -0.42764055714162524]	
	S10 SYM	99.46065105	[0.3794556686026063, -0.8204492363656325, -0.4276405571416252]	
	S12 SYM	99.46065105	[0.3794556686026072, -0.820449236365632, -0.42764055714162535]	

ZINC12296449	S14 SYM	99.46065105	[0.3794556686026084, -0.8204492363656319, -0.4276405571416247]	
	S16 SYM	99.46065105	[0.37945566860260677, -0.8204492363656324, -0.42764055714162497]	
	S18 SYM	99.46065105	[0.37945566860261015, -0.8204492363656313, -0.42764055714162436]	
	S20 SYM	99.46065105	[0.3794556686026077, -0.8204492363656318, -0.4276405571416255]	
	INVERSION (S2)	99.34013556	[1.0, 0.0, 0.0]	
	MIRROR SYM	9.639780275	[0.214151606138893, 0.9749743963583917, -0.05969938051372397]	
	C2 SYM	24.04982074	[-0.891813636670858, 0.3630308795631635, -0.26995743725908866]	
	C3 SYM	26.89315539	[0.890827664172849, -0.35944343086564795, 0.27789655044976386]	
	C4 SYM	26.91219867	[0.8910768739290744, -0.36007857396721515, 0.2762705654218802]	
	C5 SYM	26.91219867	[0.8910768739290746, -0.3600785739672146, 0.2762705654218802]	
	C6 SYM	26.91219867	[0.8910768739290746, -0.3600785739672145, 0.27627056542188017]	
	C7 SYM	26.91219867	[0.8910768739290744, -0.3600785739672148, 0.2762705654218801]	
	C8 SYM	26.91219867	[0.8910768739290746, -0.36007857396721443, 0.27627056542188]	
	C9 SYM	26.91219867	[0.8910768739290746, -0.36007857396721454, 0.27627056542188005]	
	C10 SYM	26.91219867	[0.8910768739290743, -0.360078573967215, 0.2762705654218804]	
	C11 SYM	26.91219867	[0.8910768739290746, -0.3600785739672146, 0.27627056542188033]	X= 17.9660
	C12 SYM	26.91219867	[0.8910768739290748, -0.36007857396721443, 0.27627056542187994]	Y= -5.9141
	C13 SYM	26.91219867	[0.8910768739290746, -0.36007857396721443, 0.2762705654218802]	Z= 4.1409
	C14 SYM	26.91219867	[0.8910768739290742, -0.3600785739672153, 0.2762705654218802]	Tot= 19.3624
	C15 SYM	26.91219867	[0.8910768739290744, -0.36007857396721493, 0.27627056542188055]	
	C16 SYM	26.91219867	[0.8910768739290746, -0.3600785739672143, 0.27627056542187994]	
	C17 SYM	26.91219867	[0.8910768739290749, -0.3600785739672142, 0.27627056542187944]	
	C18 SYM	26.91219867	[0.8910768739290749, -0.36007857396721415, 0.27627056542188005]	
	C19 SYM	26.91219867	[0.8910768739290746, -0.3600785739672145, 0.2762705654218801]	
	C20 SYM	26.91219867	[0.8910768739290746, -0.36007857396721443, 0.27627056542188033]	
	S4 SYM	97.55050953	[-0.21189487460407433, -0.748928206261235, -0.6278591434253805]	
	S6 SYM	97.55050953	[-0.21189487460407427, -0.7489282062612354, -0.6278591434253801]	
	S8 SYM	97.55050953	[-0.21189487460407436, -0.7489282062612352, -0.6278591434253803]	

ZINC8606274	S10 SYM	97.55050953	[-0.21189487460407444, -0.7489282062612346, -0.6278591434253813]	
	S12 SYM	97.55050953	[-0.21189487460407433, -0.7489282062612355, -0.6278591434253803]	
	S14 SYM	97.55050953	[-0.21189487460407433, -0.7489282062612348, -0.6278591434253809]	
	S16 SYM	97.55050953	[-0.21189487460407444, -0.7489282062612347, -0.627859143425381]	
	S18 SYM	97.55050953	[-0.21189487460407436, -0.7489282062612355, -0.6278591434253801]	
	S20 SYM	97.55050953	[-0.211894874604074, -0.7489282062612357, -0.6278591434253799]	
	INVERSION (S2)	97.05581945	[1.0, 0.0, 0.0]	
	MIRROR SYM	5.215307877	[-0.43042319165417453, -0.8627491251147063, 0.2653296500582674]	
	C2 SYM	19.39617505	[-0.9503036781036427, 0.27956330355388814, -0.1369937176980213]	
	C3 SYM	22.02279929	[-0.9534629741308476, 0.26796563736266765, -0.13821278578473958]	
	C4 SYM	22.02279929	[-0.9534629741308476, 0.2679656373626675, -0.13821278578473958]	
	C5 SYM	22.02279929	[-0.9534629741308476, 0.26796563736266754, -0.13821278578473964]	
	C6 SYM	22.02279929	[-0.9534629741308476, 0.26796563736266726, -0.13821278578473967]	
	C7 SYM	22.02279929	[-0.9534629741308476, 0.26796563736266743, -0.13821278578473967]	
	C8 SYM	22.02279929	[-0.9534629741308474, 0.2679656373626681, -0.13821278578473972]	
	C9 SYM	22.02279929	[-0.9534629741308474, 0.26796563736266815, -0.1382127857847399]	
	C10 SYM	22.02279929	[-0.9534629741308474, 0.2679656373626679, -0.13821278578473986]	X= -6.4873
	C11 SYM	22.02279929	[-0.9534629741308476, 0.2679656373626672, -0.13821278578473936]	Y= 2.2160
	C12 SYM	22.02279929	[-0.9534629741308474, 0.26796563736266793, -0.1382127857847398]	Z= 0.5607
	C13 SYM	22.02279929	[-0.9534629741308474, 0.2679656373626679, -0.13821278578473972]	Tot= 6.8783
	C14 SYM	22.02279929	[-0.9534629741308474, 0.2679656373626677, -0.13821278578473975]	
	C15 SYM	22.02279929	[-0.9534629741308474, 0.26796563736266804, -0.13821278578473975]	
	C16 SYM	22.02279929	[-0.9534629741308476, 0.26796563736266743, -0.13821278578473964]	
	C17 SYM	22.02279929	[-0.9534629741308474, 0.2679656373626679, -0.1382127857847398]	
	C18 SYM	22.02279929	[-0.9534629741308474, 0.2679656373626679, -0.13821278578473997]	
	C19 SYM	22.02279929	[-0.9534629741308476, 0.26796563736266765, -0.1382127857847393]	
	C20 SYM	22.02279929	[-0.9534629741308474, 0.26796563736266815, -0.13821278578474]	
	S4 SYM	97.30740442	[0.40383698403762247, 0.8926133509272338, 0.20039235531789157]	

ZINC9601609	S6 SYM	97.30740442	[0.4038369840376223, 0.892613350927234, 0.20039235531789143]	
	S8 SYM	97.30740442	[0.4038369840376225, 0.8926133509272342, 0.20039235531789135]	
	S10 SYM	97.30740442	[0.4038369840376226, 0.8926133509272338, 0.2003923553178915]	
	S12 SYM	97.30740442	[0.4038369840376227, 0.8926133509272339, 0.20039235531789112]	
	S14 SYM	97.30740442	[0.40383698403762236, 0.8926133509272338, 0.2003923553178915]	
	S16 SYM	97.30740442	[0.40383698403762286, 0.8926133509272335, 0.20039235531789182]	
	S18 SYM	97.30740442	[0.4038369840376226, 0.8926133509272336, 0.2003923553178919]	
	S20 SYM	97.30740442	[0.4038369840376223, 0.8926133509272338, 0.20039235531789126]	
	INVERSION (S2)	97.08902452	[1.0, 0.0, 0.0]	
	MIRROR SYM	5.984689927	[-0.2565112496026603, -0.9523797561467064, -0.16484774462886068]	
	C2 SYM	19.91691427	[-0.9694718791805164, 0.16614609674205455, -0.18033233214146102]	
	C3 SYM	21.78860077	[-0.9707484935460979, 0.1814910707749704, -0.15718891025430567]	
	C4 SYM	21.78860077	[-0.9707484935460979, 0.18149107077497037, -0.1571889102543056]	
	C5 SYM	21.78860077	[-0.9707484935460979, 0.18149107077497045, -0.15718891025430554]	
	C6 SYM	21.78860077	[-0.9707484935460979, 0.18149107077497073, -0.15718891025430576]	
	C7 SYM	21.78860077	[-0.9707484935460979, 0.18149107077497037, -0.15718891025430573]	
	C8 SYM	21.78860077	[-0.9707484935460979, 0.18149107077497048, -0.1571889102543056]	
	C9 SYM	21.78860077	[-0.9707484935460979, 0.18149107077497081, -0.15718891025430584]	X= -4.7122
	C10 SYM	21.78860077	[-0.9707484935460982, 0.1814910707749703, -0.15718891025430545]	Y= -0.3364
	C11 SYM	21.78860077	[-0.9707484935460982, 0.1814910707749704, -0.15718891025430556]	Z= 0.8994
	C12 SYM	21.78860077	[-0.9707484935460979, 0.18149107077497073, -0.1571889102543057]	Tot= 4.8090
	C13 SYM	21.78860077	[-0.9707484935460979, 0.1814910707749707, -0.15718891025430556]	
	C14 SYM	21.78860077	[-0.9707484935460979, 0.1814910707749704, -0.15718891025430573]	
	C15 SYM	21.78860077	[-0.9707484935460979, 0.1814910707749706, -0.1571889102543058]	
	C16 SYM	21.78860077	[-0.9707484935460979, 0.18149107077497056, -0.15718891025430567]	
	C17 SYM	21.78860077	[-0.9707484935460979, 0.1814910707749705, -0.15718891025430534]	
	C18 SYM	21.78860077	[-0.9707484935460979, 0.1814910707749706, -0.1571889102543053]	
	C19 SYM	21.78860077	[-0.9707484935460979, 0.18149107077497045, -0.15718891025430587]	

ZINC8926323	C20 SYM	21.78860077	[-0.9707484935460979, 0.18149107077497068, -0.15718891025430584]	
	S4 SYM	97.40199476	[-0.47410089626313306, 0.5588695819241383, 0.6803624993798768]	
	S6 SYM	97.40199476	[-0.4741008962631332, 0.5588695819241379, 0.6803624993798769]	
	S8 SYM	97.40199476	[-0.47410089626313306, 0.558869581924138, 0.6803624993798769]	
	S10 SYM	97.40199476	[-0.47410089626313295, 0.5588695819241382, 0.6803624993798769]	
	S12 SYM	97.40199476	[-0.4741008962631335, 0.5588695819241383, 0.6803624993798766]	
	S14 SYM	97.40199476	[-0.47410089626313306, 0.5588695819241384, 0.6803624993798768]	
	S16 SYM	97.40199476	[-0.4741008962631334, 0.5588695819241382, 0.6803624993798768]	
	S18 SYM	97.40199476	[-0.4741008962631334, 0.5588695819241379, 0.6803624993798768]	
	S20 SYM	97.40199476	[-0.47410089626313295, 0.5588695819241379, 0.6803624993798771]	
	INVERSION (S2)	97.19949866	[1.0, 0.0, 0.0]	
	MIRROR SYM	8.505728756	[-0.03218284228812027, -0.8152987047035999, -0.5781455584633427]	
	C2 SYM	17.7775725	[-0.975794584243115, 0.14289788980486193, -0.16554492577884672]	
	C3 SYM	21.75997913	[-0.979551005929775, 0.14437960491038287, -0.1401226479477456]	
	C4 SYM	21.75997913	[-0.979551005929775, 0.1443796049103828, -0.14012264794774548]	
	C5 SYM	21.75997913	[-0.979551005929775, 0.14437960491038274, -0.1401226479477456]	
	C6 SYM	21.75997913	[-0.979551005929775, 0.14437960491038287, -0.14012264794774548]	
	C7 SYM	21.75997913	[-0.979551005929775, 0.14437960491038282, -0.14012264794774554]	
	C8 SYM	21.75997913	[-0.979551005929775, 0.14437960491038285, -0.14012264794774554]	X= -4.3286
	C9 SYM	21.75997913	[-0.979551005929775, 0.14437960491038304, -0.14012264794774565]	Y= -0.7382
	C10 SYM	21.75997913	[-0.979551005929775, 0.1443796049103828, -0.14012264794774557]	Z= 0.9113
	C11 SYM	21.75997913	[-0.979551005929775, 0.14437960491038254, -0.14012264794774526]	Tot= 4.4846
	C12 SYM	21.75997913	[-0.979551005929775, 0.14437960491038276, -0.14012264794774523]	
	C13 SYM	21.75997913	[-0.979551005929775, 0.14437960491038285, -0.14012264794774554]	
	C14 SYM	21.75997913	[-0.979551005929775, 0.14437960491038265, -0.14012264794774537]	
	C15 SYM	21.75997913	[-0.979551005929775, 0.1443796049103829, -0.14012264794774543]	
	C16 SYM	21.75997913	[-0.979551005929775, 0.14437960491038293, -0.14012264794774568]	
	C17 SYM	21.75997913	[-0.979551005929775, 0.14437960491038285, -0.14012264794774548]	

ZINC2488345	C18 SYM	21.75997913	[-0.979551005929775, 0.14437960491038268, -0.1401226479477456]	
	C19 SYM	21.75997913	[-0.9795510059297752, 0.14437960491038257, -0.14012264794774518]	
	C20 SYM	21.75997913	[-0.979551005929775, 0.1443796049103828, -0.14012264794774518]	
	S4 SYM	96.3216667	[-0.09850848487743787, 0.8824641644900733, 0.4599489936916794]	
	S6 SYM	96.3216667	[-0.09850848487743807, 0.8824641644900731, 0.45994899369168013]	
	S8 SYM	96.3216667	[-0.09850848487743792, 0.882464164490073, 0.45994899369167985]	
	S10 SYM	96.3216667	[-0.0985084848774378, 0.8824641644900734, 0.45994899369167935]	
	S12 SYM	96.3216667	[-0.09850848487743774, 0.8824641644900734, 0.45994899369167935]	
	S14 SYM	96.3216667	[-0.09850848487743762, 0.8824641644900733, 0.4599489936916796]	
	S16 SYM	96.3216667	[-0.09850848487743778, 0.882464164490073, 0.45994899369167963]	
	S18 SYM	96.3216667	[-0.09850848487743813, 0.8824641644900729, 0.45994899369167996]	
	S20 SYM	96.3216667	[-0.09850848487743692, 0.8824641644900743, 0.4599489936916782]	
	INVERSION (S2)	94.68763708	[1.0, 0.0, 0.0]	
	MIRROR SYM	5.751807312	[0.1436511089128776, 0.9849214832273672, 0.09640555370570508]	
	C2 SYM	17.67139639	[-0.9488041886846206, 0.25328513065018915, -0.18872534044487915]	
	C3 SYM	21.6724115	[-0.9531352744911457, 0.25478300333794546, -0.16315259645738062]	
	C4 SYM	21.6724115	[-0.9531352744911457, 0.25478300333794573, -0.16315259645738073]	
	C5 SYM	21.6724115	[-0.9531352744911457, 0.25478300333794557, -0.16315259645738073]	
	C6 SYM	21.6724115	[-0.9531352744911457, 0.2547830033379454, -0.16315259645738062]	
	C7 SYM	21.6724115	[-0.9531352744911459, 0.25478300333794535, -0.16315259645738062]	X= -3.7486
	C8 SYM	21.6724115	[-0.9531352744911457, 0.2547830033379455, -0.16315259645738067]	Y= 0.2076
	C9 SYM	21.6724115	[-0.9531352744911459, 0.25478300333794524, -0.16315259645738062]	Z= 0.7553
	C10 SYM	21.6724115	[-0.9531352744911457, 0.2547830033379455, -0.1631525964573806]	Tot= 3.8295
	C11 SYM	21.6724115	[-0.9531352744911457, 0.25478300333794535, -0.16315259645738056]	
	C12 SYM	21.6724115	[-0.9531352744911459, 0.2547830033379453, -0.16315259645738056]	
	C13 SYM	21.6724115	[-0.9531352744911459, 0.25478300333794507, -0.1631525964573806]	
	C14 SYM	21.6724115	[-0.9531352744911457, 0.25478300333794557, -0.16315259645738053]	
	C15 SYM	21.6724115	[-0.9531352744911459, 0.25478300333794496, -0.1631525964573806]	

ZINC9601596	C16 SYM	21.6724115	[-0.9531352744911457, 0.25478300333794573, -0.16315259645738064]	
	C17 SYM	21.6724115	[-0.9531352744911457, 0.2547830033379453, -0.16315259645738073]	
	C18 SYM	21.6724115	[-0.9531352744911459, 0.25478300333794507, -0.16315259645738037]	
	C19 SYM	21.6724115	[-0.9531352744911457, 0.2547830033379457, -0.1631525964573806]	
	C20 SYM	21.6724115	[-0.9531352744911459, 0.25478300333794524, -0.16315259645738048]	
	S4 SYM	96.29976254	[-0.017458570550689126, 0.8775582418738583, 0.47915209530334874]	
	S6 SYM	96.29976254	[-0.017458570550688966, 0.8775582418738584, 0.4791520953033483]	
	S8 SYM	96.29976254	[-0.017458570550689327, 0.8775582418738581, 0.4791520953033494]	
	S10 SYM	96.29976254	[-0.01745857055068906, 0.8775582418738583, 0.47915209530334907]	
	S12 SYM	96.29976254	[-0.017458570550688755, 0.8775582418738587, 0.47915209530334835]	
	S14 SYM	96.29976254	[-0.017458570550689254, 0.8775582418738586, 0.47915209530334874]	
	S16 SYM	96.29976254	[-0.017458570550689213, 0.8775582418738584, 0.4791520953033486]	
	S18 SYM	96.29976254	[-0.017458570550689598, 0.8775582418738581, 0.47915209530334946]	
	S20 SYM	96.29976254	[-0.017458570550689227, 0.8775582418738582, 0.4791520953033489]	
	INVERSION (S2)	94.65597897	[1.0, 0.0, 0.0]	
	MIRROR SYM	5.606379643	[0.24847141843767956, 0.960951473469428, 0.12179581214681834]	
	C2 SYM	20.26444167	[0.967227445019236, -0.044182121918766304, 0.2500380165181215]	
	C3 SYM	20.67769685	[-0.9673748663411472, 0.04659686165409366, -0.24902730865396516]	
	C4 SYM	20.67769685	[-0.9673748663411472, 0.04659686165409363, -0.249027308653965]	
	C5 SYM	20.67769685	[-0.967374866341147, 0.04659686165409367, -0.24902730865396516]	
	C6 SYM	20.67769685	[-0.9673748663411472, 0.04659686165409355, -0.24902730865396489]	X= -2.0730
	C7 SYM	20.67769685	[-0.9673748663411472, 0.046596861654093755, -0.2490273086539651]	Y= -0.6196
	C8 SYM	20.67769685	[-0.9673748663411472, 0.04659686165409366, -0.24902730865396527]	Z= -0.0767
	C9 SYM	20.67769685	[-0.967374866341147, 0.046596861654093685, -0.24902730865396494]	Tot= 2.1650
	C10 SYM	20.67769685	[-0.9673748663411472, 0.04659686165409357, -0.24902730865396477]	
	C11 SYM	20.67769685	[-0.967374866341147, 0.0465968616540937, -0.2490273086539655]	
	C12 SYM	20.67769685	[-0.9673748663411472, 0.046596861654093685, -0.24902730865396505]	
	C13 SYM	20.67769685	[-0.9673748663411472, 0.0465968616540935, -0.24902730865396444]	

ZINC9601608	C14 SYM	20.67769685	[-0.9673748663411472, 0.04659686165409362, -0.2490273086539651]	
	C15 SYM	20.67769685	[-0.967374866341147, 0.04659686165409359, -0.24902730865396516]	
	C16 SYM	20.67769685	[-0.967374866341147, 0.046596861654093706, -0.24902730865396533]	
	C17 SYM	20.67769685	[-0.9673748663411472, 0.0465968616540935, -0.2490273086539646]	
	C18 SYM	20.67769685	[-0.9673748663411472, 0.046596861654093456, -0.24902730865396505]	
	C19 SYM	20.67769685	[-0.9673748663411472, 0.04659686165409351, -0.24902730865396489]	
	C20 SYM	20.67769685	[-0.9673748663411472, 0.04659686165409365, -0.249027308653965]	
	S4 SYM	97.32722361	[-0.8231996804146058, 0.5657306349198479, -0.04786580071905857]	
	S6 SYM	97.32722361	[-0.8231996804146058, 0.565730634919848, -0.04786580071905857]	
	S8 SYM	97.32722361	[-0.823199680414606, 0.5657306349198477, -0.04786580071905846]	
	S10 SYM	97.32722361	[-0.8231996804146057, 0.5657306349198481, -0.04786580071905848]	
	S12 SYM	97.32722361	[-0.823199680414606, 0.5657306349198477, -0.04786580071905859]	
	S14 SYM	97.32722361	[-0.8231996804146061, 0.5657306349198474, -0.047865800719058604]	
	S16 SYM	97.32722361	[-0.8231996804146056, 0.5657306349198482, -0.04786580071905852]	
	S18 SYM	97.32722361	[-0.8231996804146064, 0.5657306349198471, -0.047865800719058785]	
	S20 SYM	97.32722361	[-0.8231996804146062, 0.5657306349198475, -0.04786580071905847]	
	INVERSION (S2)	97.11559126	[1.0, 0.0, 0.0]	
	MIRROR SYM	7.460768214	[0.004068109383117842, 0.9872603713238124, 0.15906102508036132]	
	C2 SYM	24.08007003	[-0.9100531613843446, 0.2805129580512492, -0.30514869132883143]	
	C3 SYM	24.55985674	[-0.9094413619271351, 0.28283947651302016, -0.3048249329401359]	
	C4 SYM	24.56447249	[-0.909049229559914, 0.2826817867332844, -0.3061380500457353]	
	C5 SYM	24.56447249	[-0.9090492295599137, 0.2826817867332846, -0.30613805004573547]	X= -6.2285
	C6 SYM	24.56447249	[-0.909049229559914, 0.28268178673328426, -0.30613805004573524]	Y= 1.0135
	C7 SYM	24.56447249	[-0.9090492295599137, 0.2826817867332847, -0.3061380500457356]	Z= -2.0799
	C8 SYM	24.56447249	[-0.9090492295599137, 0.28268178673328465, -0.30613805004573547]	Tot= 6.6443
	C9 SYM	24.56447249	[-0.909049229559914, 0.2826817867332839, -0.30613805004573563]	
	C10 SYM	24.56447249	[-0.9090492295599135, 0.28268178673328487, -0.30613805004573597]	
	C11 SYM	24.56447249	[-0.9090492295599135, 0.28268178673328465, -0.3061380500457357]	

ZINC8589983	C12 SYM	24.56447249	[-0.9090492295599137, 0.28268178673328426, -0.30613805004573524]	
	C13 SYM	24.56447249	[-0.9090492295599137, 0.2826817867332843, -0.3061380500457353]	
	C14 SYM	24.56447249	[-0.9090492295599137, 0.28268178673328426, -0.3061380500457354]	
	C15 SYM	24.56447249	[-0.9090492295599142, 0.2826817867332836, -0.3061380500457349]	
	C16 SYM	24.56447249	[-0.9090492295599137, 0.2826817867332845, -0.3061380500457352]	
	C17 SYM	24.56447249	[-0.9090492295599135, 0.282681786733285, -0.30613805004573585]	
	C18 SYM	24.56447249	[-0.909049229559914, 0.28268178673328437, -0.3061380500457351]	
	C19 SYM	24.56447249	[-0.9090492295599137, 0.28268178673328453, -0.30613805004573563]	
	C20 SYM	24.56447249	[-0.9090492295599137, 0.28268178673328487, -0.30613805004573524]	
	S4 SYM	99.60007075	[0.11887578488768842, 0.9829770032963924, -0.14008839622816946]	
	S6 SYM	99.60007075	[0.11887578488768867, 0.9829770032963923, -0.14008839622816874]	
	S8 SYM	99.60007075	[0.1188757848876891, 0.9829770032963924, -0.1400883962281688]	
	S10 SYM	99.60007075	[0.11887578488768927, 0.9829770032963924, -0.14008839622816874]	
	S12 SYM	99.60007075	[0.11887578488768864, 0.9829770032963923, -0.1400883962281696]	
	S14 SYM	99.60007075	[0.11887578488768837, 0.9829770032963923, -0.1400883962281692]	
	S16 SYM	99.60007075	[0.11887578488768911, 0.9829770032963921, -0.14008839622816954]	
	S18 SYM	99.60007075	[0.11887578488768749, 0.9829770032963921, -0.14008839622817104]	
	S20 SYM	99.60007075	[0.118875784887689, 0.9829770032963924, -0.14008839622816846]	
	INVERSION (S2)	99.44961417	[1.0, 0.0, 0.0]	
	MIRROR SYM	7.477888747	[-0.1783005176546555, -0.927292310437435, -0.3291472260367474]	
	C2 SYM	25.94479747	[-0.9312501985373083, 0.2623489492180896, -0.2528756543607714]	
	C3 SYM	26.22662571	[0.9331698090739374, -0.2573050276259713, 0.2509745608449379]	
	C4 SYM	26.22662571	[0.9331698090739374, -0.25730502762597096, 0.2509745608449378]	X= 3.3957
	C5 SYM	26.22662571	[0.9331698090739374, -0.2573050276259715, 0.2509745608449379]	Y= 1.6433
	C6 SYM	26.22662571	[0.9331698090739374, -0.25730502762597135, 0.25097456084493786]	Z= 0.6083
	C7 SYM	26.22662571	[0.9331698090739374, -0.2573050276259713, 0.25097456084493763]	Tot= 3.8211
	C8 SYM	26.22662571	[0.9331698090739377, -0.257305027625971, 0.2509745608449377]	
	C9 SYM	26.22662571	[0.9331698090739374, -0.257305027625971, 0.25097456084493797]	

	C10 SYM	26.22662571	[0.9331698090739372, -0.25730502762597135, 0.2509745608449382]	
	C11 SYM	26.22662571	[0.9331698090739372, -0.2573050276259716, 0.2509745608449381]	
	C12 SYM	26.22662571	[0.9331698090739377, -0.2573050276259708, 0.2509745608449377]	
	C13 SYM	26.22662571	[0.9331698090739374, -0.2573050276259715, 0.25097456084493786]	
	C14 SYM	26.22662571	[0.9331698090739372, -0.2573050276259718, 0.2509745608449383]	
	C15 SYM	26.22662571	[0.9331698090739374, -0.2573050276259713, 0.2509745608449382]	
	C16 SYM	26.22662571	[0.9331698090739374, -0.2573050276259715, 0.25097456084493813]	
	C17 SYM	26.22662571	[0.9331698090739377, -0.25730502762597124, 0.2509745608449374]	
	C18 SYM	26.22662571	[0.9331698090739372, -0.2573050276259716, 0.25097456084493824]	
	C19 SYM	26.22662571	[0.9331698090739372, -0.2573050276259718, 0.2509745608449383]	
	C20 SYM	26.22662571	[0.9331698090739377, -0.2573050276259711, 0.2509745608449374]	
	S4 SYM	99.62334649	[0.7482544567352265, 0.6623752861598822, 0.037070854596102265]	
	S6 SYM	99.62334649	[0.7482544567352251, 0.662375286159884, 0.03707085459610304]	
	S8 SYM	99.62334649	[0.7482544567352248, 0.662375286159884, 0.03707085459610221]	
	S10 SYM	99.62334649	[0.7482544567352246, 0.6623752861598843, 0.03707085459610249]	
	S12 SYM	99.62334649	[0.7482544567352264, 0.6623752861598823, 0.03707085459610188]	
	S14 SYM	99.62334649	[0.7482544567352227, 0.6623752861598816, 0.037070854596102334]	
	S16 SYM	99.62334649	[0.7482544567352257, 0.6623752861598833, 0.03707085459610152]	
	S18 SYM	99.62334649	[0.7482544567352282, 0.6623752861598802, 0.03707085459610227]	
	S20 SYM	99.62334649	[0.748254456735226, 0.6623752861598831, 0.037070854596102425]	
ZINC524732009	INVERSION (S2)	99.48607822	[1.0, 0.0, 0.0]	X= 1.3041 Y= -1.0397 Z= -0.3033 Tot= 1.6952
	MIRROR SYM	10.03930765	[-0.01464793373856027, -0.7213541529858972, -0.6924114557163172]	
	C2 SYM	48.2534009	[-0.8127497462420433, 0.5821164893280554, 0.024046680350396966]	
	C3 SYM	50.72262313	[0.8449971706563201, -0.5347225785453804, -0.0071795248166856285]	
	C4 SYM	50.72262313	[0.844997170656319, -0.5347225785453825, -0.007179524816683465]	
	C5 SYM	50.72262313	[0.8449971706563207, -0.5347225785453793, -0.00717952481668635]	
	C6 SYM	50.72262313	[0.8449971706563196, -0.5347225785453812, -0.007179524816684492]	
	C7 SYM	50.72262313	[0.8449971706563201, -0.5347225785453804, -0.007179524816685243]	

ZINC3984976	C8 SYM	50.72262313	[0.8449971706563207, -0.5347225785453794, -0.007179524816685849]	
	C9 SYM	50.72262313	[0.8449971706563194, -0.5347225785453815, -0.0071795248166845235]	
	C10 SYM	50.72262313	[0.8449971706563197, -0.534722578545381, -0.007179524816684829]	
	C11 SYM	50.72262313	[0.84499717065632, -0.5347225785453807, -0.0071795248166847975]	
	C12 SYM	50.72262313	[0.8449971706563199, -0.5347225785453807, -0.007179524816684988]	
	C13 SYM	50.72262313	[0.8449971706563197, -0.5347225785453811, -0.007179524816684683]	
	C15 SYM	50.72262313	[0.8449971706563207, -0.5347225785453795, -0.007179524816686714]	
	C14 SYM	50.72262313	[0.8449971706563199, -0.5347225785453811, -0.007179524816684437]	
	C16 SYM	50.72262313	[0.8449971706563204, -0.5347225785453802, -0.007179524816686134]	
	C17 SYM	50.72262313	[0.8449971706563197, -0.5347225785453811, -0.007179524816684352]	
	C18 SYM	50.72262313	[0.8449971706563224, -0.5347225785453766, -0.0071795248166894345]	
	C19 SYM	50.72262313	[0.8449971706563223, -0.5347225785453767, -0.007179524816688569]	
	C20 SYM	50.72262313	[0.8449971706563196, -0.5347225785453813, -0.007179524816685656]	
	S4 SYM	96.63320722	[0.7115242496624653, 0.38486788611024847, 0.5878860028809111]	
	S6 SYM	96.63320722	[0.7115242496624653, 0.38486788611024836, 0.587886002880911]	
	S8 SYM	96.63320722	[0.7115242496624653, 0.3848678861102485, 0.5878860028809111]	
	S10 SYM	96.63320722	[0.711524249662465, 0.38486788611024875, 0.5878860028809113]	
	S12 SYM	96.63320722	[0.7115242496624651, 0.38486788611024864, 0.5878860028809113]	
	S14 SYM	96.63320722	[0.7115242496624651, 0.3848678861102486, 0.5878860028809112]	
	S16 SYM	96.63320722	[0.7115242496624653, 0.3848678861102484, 0.587886002880911]	
	S18 SYM	96.63320722	[0.7115242496624655, 0.3848678861102483, 0.5878860028809109]	
	S20 SYM	96.63320722	[0.7115242496624652, 0.3848678861102486, 0.5878860028809112]	
	INVERSION (S2)	96.63320715	[1.0, 0.0, 0.0]	
	MIRROR SYM	6.034559767	[0.4334352953551223, 0.5765498701150279, 0.6926211749656246]	
	C2 SYM	21.83979639	[-0.8737354074943344, -0.17932894552088316, 0.4521366684854013]	X= 1.6984
	C3 SYM	22.3858577	[-0.875408693316454, -0.17494469952877736, 0.4506151038000887]	Y= 3.3236
	C4 SYM	22.3858577	[-0.8754086933164538, -0.17494469952877753, 0.4506151038000889]	Z= -3.7647
	C5 SYM	22.3858577	[-0.8754086933164542, -0.17494469952877728, 0.45061510380008823]	Tot= 5.3013

C6 SYM	22.3858577	[-0.875408693316454, -0.1749446995287773, 0.4506151038000885]
C7 SYM	22.3858577	[-0.875408693316454, -0.17494469952877767, 0.4506151038000886]
C8 SYM	22.3858577	[-0.8754086933164538, -0.1749446995287775, 0.4506151038000891]
C9 SYM	22.3858577	[-0.8754086933164535, -0.17494469952877728, 0.4506151038000891]
C10 SYM	22.3858577	[-0.8754086933164538, -0.1749446995287773, 0.4506151038000888]
C11 SYM	22.3858577	[-0.8754086933164542, -0.17494469952877734, 0.4506151038000885]
C12 SYM	22.3858577	[-0.875408693316454, -0.1749446995287774, 0.45061510380008846]
C13 SYM	22.3858577	[-0.8754086933164535, -0.1749446995287776, 0.45061510380008946]
C15 SYM	22.3858577	[-0.8754086933164538, -0.17494469952877736, 0.4506151038000888]
C14 SYM	22.3858577	[-0.8754086933164542, -0.1749446995287771, 0.450615103800088]
C16 SYM	22.3858577	[-0.8754086933164544, -0.17494469952877706, 0.45061510380008796]
C17 SYM	22.3858577	[-0.8754086933164541, -0.1749446995287776, 0.45061510380008807]
C18 SYM	22.3858577	[-0.8754086933164544, -0.1749446995287775, 0.45061510380008796]
C19 SYM	22.3858577	[-0.875408693316454, -0.17494469952877736, 0.4506151038000886]
C20 SYM	22.3858577	[-0.8754086933164538, -0.17494469952877745, 0.45061510380008907]
S4 SYM	99.41270981	[0.5245413088954336, -0.8492356548194772, 0.06045839764333173]
S6 SYM	99.41270981	[0.5245413088954332, -0.8492356548194775, 0.06045839764333212]
S8 SYM	99.41270981	[0.5245413088954333, -0.8492356548194774, 0.06045839764333197]
S10 SYM	99.41270981	[0.5245413088954327, -0.8492356548194777, 0.06045839764333223]
S12 SYM	99.41270981	[0.5245413088954328, -0.8492356548194776, 0.0604583976433318]
S14 SYM	99.41270981	[0.5245413088954343, -0.8492356548194768, 0.06045839764333169]
S16 SYM	99.41270981	[0.5245413088954319, -0.8492356548194783, 0.060458397643331954]
S18 SYM	99.41270981	[0.5245413088954344, -0.8492356548194767, 0.060458397643331246]
S20 SYM	99.41270981	[0.524541308895433, -0.8492356548194776, 0.06045839764333172]
INVERSION (S2)	99.31060232	[1.0, 0.0, 0.0]
MIRROR SYM	6.068432112	[-0.35003500325789333, -0.41348205543433597, -0.840540353777285]
