

Supplementary Material

Targeting *Leishmania infantum* Mannosyl-oligosaccharide glucosidase with natural products: pH-dependent inhibition explored through computer-aided drug design.

Luis Daniel Goyzueta-Mamani, Haruna Luz Barazorda-Ccahuana, Mayron Antonio Candia-Puma, Alessandro Sobreira Galdino, Ricardo Andrez Machado-de-Avila, Rodolfo Cordeiro Giunchetti, José L. Medina-Franco, Mónica Florin-Christensen, Eduardo Antonio Ferraz Coelho, Miguel Angel Chávez-Fumagalli*

* **Correspondence:** Corresponding Author: mchavezf@ucsm.edu.pe

Table S1. Docking results for NPs ligands from BIOFACQUIM, PERUNPDB, and NuBBEDB with AutoDock 4.0.

Compound	Binding energy (kcal/mol)
perunpdb126	-12.2
fqnp233	-11.76
fqnp231	-11.3
nubbe1048	-11.1
nubbe463	-10.88
zinc000095551509	-10.85
fqnp326	-10.65
nubbe1826	-10.44
nubbe962	-10.44
nubbe1697	-10.4
zinc000100008319	-10.37
nubbe1728	-10.35
zinc000019632706	-10.34
nubbe946	-10.22
nubbe1061	-10.09
nubbe74	-10.09
nubbe71	-10.02
zinc000001319780	-10.02
fqnp48	-9.97
zinc000150338708	-9.95
nubbe1698	-9.86
zinc000003812988	-9.82
nubbe428	-9.8
fqnp271	-9.77
nubbe956	-9.74
nubbe429	-9.72
fqnp327	-9.66
fqnp49	-9.64
nubbe1051	-9.6
nubbe2281	-9.6
zinc000053683271	-9.6
fqnp269	-9.55
nubbe1062	-9.48
nubbe364uff	-9.48
nubbe1347	-9.42
nubbe1706	-9.42
zinc000100037890	-9.42
nubbe1348	-9.41
nubbe589uff	-9.4
perunpdb268	-9.39
nubbe2503	-9.38
nubbe366uff	-9.36

Supplementary Material

nubbe1523	-9.34
nubbe438	-9.34
nubbe133	-9.33
nubbe2301	-9.33
nubbe72	-9.29
nubbe72uff	-9.29
nubbe71uff	-9.28
fqnp281	-9.27
nubbe1033	-9.26
nubbe1063	-9.26
nubbe1430	-9.26
nubbe190uff	-9.25
zinc000004097383	-9.25
nubbe21	-9.23
nubbe1370	-9.2
nubbe364	-9.19
nubbe347	-9.17
nubbe415	-9.17
fqnp325	-9.15
zinc70673654	-9.15
nubbe1271	-9.14
zinc000001280665	-9.14
nubbe2161	-9.13
nubbe415uff	-9.13
nubbe78	-9.12
nubbe1365	-9.11
zinc000003861599	-9.11
nubbe585uff	-9.1
nubbe1064	-9.07
nubbe1130	-9.07
nubbe263uff	-9.07
fqnp153	-9.06
zinc000012503291	-9.05
nubbe2303	-9.01
zinc000410428674	-9.01
nubbe2491	-9
zinc68590493	-9
fqnp152	-8.99
nubbe1005	-8.97
nubbe87uff	-8.96
nubbe438uff	-8.94
nubbe1042	-8.93
nubbe1038	-8.92

nubbe1257	-8.91
nubbe589	-8.91
nubbe1144	-8.89
nubbe2378	-8.86
nubbe1928	-8.85
nubbe1204	-8.84
nubbe256uff	-8.84
nubbe1355	-8.83
nubbe1891	-8.83
nubbe228	-8.83
perunpdb147	-8.79
zinc000003927200	-8.79
nubbe607uff	-8.78
nubbe2264	-8.77
zinc000100037885	-8.77
nubbe1455	-8.74
nubbe621	-8.74
zinc000003813047	-8.74
zinc000013831141	-8.74
zinc000256433948	-8.74
nubbe191	-8.71
zinc000014768621	-8.7
nubbe1863	-8.69
nubbe1353	-8.68
nubbe439	-8.68
perunpdb22	-8.68
nubbe1416	-8.67
nubbe410	-8.67
perunpdb267	-8.67
nubbe1037	-8.66
nubbe1052	-8.66
nubbe928	-8.66
fqnp106	-8.66
zinc000003973334	-8.66
nubbe386	-8.65
nubbe2426	-8.64
nubbe87	-8.64
nubbe92	-8.64
zinc000052509463	-8.64
nubbe960	-8.63
zinc000002568036	-8.63
nubbe190	-8.61
nubbe959	-8.6

nubbe1146	-8.59
nubbe388	-8.59
fqnp207	-8.59
nubbe1176	-8.58
nubbe1110	-8.56
nubbe2484	-8.56
fqnp235	-8.56
zinc000003915154	-8.56
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nubbe416uff	-8.55
nubbe75uff	-8.55
fqnp143	-8.54
nubbe1131	-8.53
nubbe240uff	-8.53
nubbe1431	-8.52
fqnp265	-8.52
fqnp270	-8.52
nubbe458uff	-8.51
nubbe146	-8.5
nubbe21uff	-8.5
nubbe462uff	-8.5
nubbe2006	-8.48
fqnp303	-8.48
zinc000100371951	-8.48
nubbe1438	-8.47
nubbe479	-8.47
nubbe247uff	-8.45
perunpdb129	-8.45
fqnp133	-8.45
zinc000001493878	-8.45
fqnp446	-8.44
zinc000000020253	-8.43
zinc000100370145	-8.43
nubbe1039	-8.42
fqnp307	-8.4
nubbe1034	-8.39
zinc000003813003	-8.39
zinc000043206370	-8.39
fqnp282	-8.38
zinc000013648755	-8.38
nubbe268uff	-8.35
zinc000034089131	-8.35
zinc000043450324	-8.34
nubbe1025	-8.33

perunpdb28	-8.33
nubbe1035	-8.32
nubbe966	-8.31
zinc000256433955	-8.31
nubbe1046	-8.3
nubbe1727	-8.3
fqnp154	-8.3
nubbe1926	-8.29
nubbe2360	-8.29
nubbe2495	-8.29
fqnp268	-8.29
fqnp349	-8.29
nubbe1729	-8.28
nubbe1050	-8.27
nubbe2073	-8.27
nubbe1602	-8.25
nubbe407	-8.25
nubbe1168	-8.24
nubbe177uff	-8.24
nubbe2068	-8.24
nubbe608	-8.24
nubbe1096	-8.23
nubbe314	-8.23
nubbe365uff	-8.23
nubbe89uff	-8.23
perunpdb243	-8.23
fqnp201	-8.23
zinc000003818726	-8.23
zinc000003875483	-8.22
nubbe961	-8.21
nubbe266	-8.19
nubbe75	-8.19
fqnp169	-8.19
zinc000030691797	-8.19
nubbe2354	-8.18
nubbe574	-8.18
nubbe1827	-8.17
zinc000006094354	-8.17
nubbe1707	-8.16
nubbe240	-8.16
nubbe605	-8.16
fqnp287	-8.15
nubbe1356	-8.14
nubbe1360	-8.14

Supplementary Material

nubbe1318	-8.13
nubbe2171	-8.13
fqnp275	-8.13
fqnp386	-8.13
zinc000003927822	-8.12
zinc000004097305	-8.12
zinc000118912393	-8.12
nubbe1047	-8.11
nubbe1141	-8.11
nubbe1725	-8.11
nubbe1357	-8.1
nubbe1453	-8.09
nubbe416	-8.09
nubbe1095	-8.08
nubbe1317	-8.08
nubbe2077	-8.08
nubbe1232	-8.07
nubbe1652	-8.07
zinc000000402954	-8.07
nubbe191uff	-8.06
nubbe1949	-8.06
nubbe2244	-8.06
zinc000011677837	-8.06
nubbe1550	-8.05
nubbe395	-8.05
perunpdb207	-8.05
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nubbe2357	-8.04
nubbe479uff	-8.04
nubbe73	-8.04
nubbe216uff	-8.03
nubbe2326	-8.03
nubbe954	-8.03
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nubbe2033	-8.01
nubbe2280	-8.01
nubbe2432	-8.01
nubbe384	-8.01
nubbe2072	-8
nubbe2286	-8
nubbe455uff	-8
fqnp202	-8
zinc000002008310	-8

zinc000100378061	-8
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nubbe958	-7.99
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nubbe1632	-7.97
nubbe379	-7.97
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nubbe1653	-7.96
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perunpdb232	-7.95
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nubbe1231	-7.91
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fqnp142	-7.91
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fqnp285	-7.9
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nubbe2344	-7.89
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nubbe1661	-7.86
nubbe469	-7.86
nubbe590uff	-7.86
fqnp236	-7.86
nubbe1026	-7.85
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nubbe1553	-7.84
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nubbe268	-7.84
nubbe365	-7.84
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nubbe257uff	-7.83
nubbe381	-7.83
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nubbe1322	-7.81
nubbe1327	-7.81
nubbe329	-7.81
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zinc000000002299	-7.81

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nubbe678	-7.77
nubbe952	-7.77
zinc000000897251	-7.77
zinc000004097416	-7.77
nubbe132uff	-7.76
nubbe1359	-7.76
nubbe396uff	-7.76
nubbe836	-7.76
perunpdb155	-7.76
fqnp107	-7.76
fqnp118	-7.76
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nubbe548uff	-7.75
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Supplementary Material

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zinc000003814422	-7.68
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zinc68590487	-7.68
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nubbe12	-7.67
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nubbe461uff	-7.67
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perunpdb112	-7.58
nubbe1142	-7.57
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nubbe180	-7.57
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nubbe834	-7.57
nubbe1507	-7.56
nubbe22	-7.56
nubbe2288	-7.56
nubbe2402	-7.56
nubbe258	-7.56
nubbe93	-7.56
perunpdb217	-7.56
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nubbe1720	-7.54
nubbe202uff	-7.54
nubbe581uff	-7.54
fqnp141	-7.54
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nubbe1248	-7.53
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nubbe1626	-7.53
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nubbe2492	-7.5
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fqnp162	-7.45

Supplementary Material

fqnp329	-7.45
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zinc000004097467	-7.43
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nubbe2159	-7.42
nubbe2481	-7.42
nubbe1990	-7.41
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nubbe79uff	-7.41
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fqnp402	-7.41
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nubbe992	-7.4
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zinc000053229445	-7.4
zinc000256433946	-7.4
nubbe1210	-7.39
nubbe22uff	-7.39
nubbe591uff	-7.39
perunpdb206	-7.39
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fqnp426	-7.39
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fqnp380	-7.38

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perunpdb3	-7.37
nubbe179uff	-7.36
nubbe2009	-7.36
nubbe2189	-7.36
nubbe2351	-7.36
nubbe264	-7.36
nubbe384uff	-7.36
nubbe933	-7.36
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zinc000004097440	-7.36
zinc000049643479	-7.36
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nubbe228uff	-7.35
nubbe2290	-7.35
nubbe2353	-7.35
nubbe674	-7.35
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zinc000043207238	-7.35
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nubbe2261	-7.34
nubbe2289	-7.34
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nubbe2515	-7.31
nubbe567	-7.31
zinc000030726187	-7.31
nubbe1426	-7.3
nubbe1719	-7.3
nubbe606	-7.3
perunpdb216	-7.3
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Supplementary Material

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fqn123	-3.68
zinc000000057146	-3.68
zinc000000155905	-3.68
zinc000003791297	-3.68
zinc06385059	-3.68
zinc39060242	-3.68
nubbe1704	-3.67
nubbe2143	-3.67
nubbe56	-3.67
perunpdb173	-3.67
zinc000000403609	-3.67
zinc000001530652	-3.67
zinc000003830959	-3.67
zinc000004658562	-3.67
zinc000085534336	-3.67
zinc15442203	-3.67
zinc40186615	-3.67
zinc76599673	-3.67
nubbe1565	-3.66
nubbe2146	-3.66
nubbe270	-3.66

perunpdb172	-3.66
fqnp429	-3.66
zinc000000000494	-3.66
zinc000002539484	-3.66
nubbe1386	-3.65
nubbe378uff	-3.65
zinc000000057147	-3.65
zinc000001543916	-3.65
zinc000003981610	-3.65
zinc000013818943	-3.65
zinc000100006770	-3.65
nubbe46uff	-3.64
nubbe6uff	-3.64
fqnp273	-3.64
zinc000000896546	-3.64
zinc000001530762	-3.64
zinc000003830453	-3.64
zinc000004474405	-3.64
zinc000252286876	-3.64
nubbe117	-3.63
nubbe39	-3.63
nubbe635	-3.63
zinc000001843099	-3.63
zinc000003831050	-3.63
nubbe1987	-3.62
fqnp390	-3.62
zinc000000895099	-3.62
zinc000253529561	-3.62
zinc03794711	-3.62
nubbe975	-3.61
perunpdb194	-3.61
perunpdb197	-3.61
zinc000002169830	-3.61
zinc000100052681	-3.61
nubbe1295	-3.6
nubbe748uff	-3.6
perunpdb171	-3.6
fqnp53	-3.6
zinc000001530718	-3.6
zinc000003830713	-3.6
zinc000004658603	-3.6
zinc000100070233	-3.6
zinc02077807	-3.6

zinc48857970	-3.6
zinc77292284	-3.6
nubbe2120	-3.59
nubbe457uff	-3.59
zinc21798212	-3.59
zinc76599400	-3.59
nubbe2124	-3.58
zinc000001530639	-3.58
zinc000008034120	-3.58
zinc35649798	-3.58
nubbe452	-3.57
fqnp470	-3.57
zinc000001530654	-3.57
zinc22054075	-3.57
zinc36533584	-3.57
zinc000001529266	-3.56
zinc38864631	-3.56
nubbe1185	-3.55
nubbe1972	-3.55
nubbe443uff	-3.55
perunpdb59	-3.55
zinc000000394284	-3.55
zinc39088366	-3.55
nubbe1084	-3.54
nubbe176uff	-3.54
zinc000000114124	-3.54
zinc000006661227	-3.54
zinc38433749	-3.54
zinc39089965	-3.54
nubbe107	-3.53
nubbe185	-3.53
fqnp120	-3.53
zinc000028467879	-3.53
nubbe233	-3.52
perunpdb50	-3.52
fqnp458	-3.52
fqnp460	-3.52
zinc000001482049	-3.52
zinc000001540998	-3.52
zinc000001995484	-3.52
zinc000003812867	-3.52
nubbe213	-3.51
perunpdb80	-3.51

zinc000001530660	-3.51
zinc000072320327	-3.51
zinc000100019007	-3.51
nubbe116	-3.5
nubbe1884	-3.5
nubbe274uff	-3.5
nubbe304uff	-3.5
nubbe743uff	-3.5
zinc04098894	-3.5
zinc11681339	-3.5
nubbe1643	-3.49
nubbe913	-3.49
zinc000085432549	-3.49
zinc000085540223	-3.49
nubbe1190	-3.48
nubbe173	-3.48
nubbe173uff	-3.48
nubbe2110	-3.48
zinc000145401681	-3.48
nubbe1690	-3.47
nubbe339	-3.47
zinc000043194409	-3.47
zinc13545227	-3.47
nubbe104uff	-3.46
nubbe413	-3.46
perunpdb202	-3.46
zinc000001530575	-3.46
zinc000003978028	-3.46
zinc000004214955	-3.46
zinc000005224188	-3.46
zinc38234157	-3.46
zinc76599396	-3.46
nubbe107uff	-3.45
nubbe1645	-3.45
nubbe1684	-3.45
nubbe307uff	-3.45
perunpdb248	-3.45
zinc000001530717	-3.44
zinc000253529562	-3.44
nubbe303uff	-3.43
perunpdb12	-3.43
zinc000003995807	-3.43
zinc43419392	-3.43
zinc000000901552	-3.42

zinc000003803652	-3.42
zinc000012468792	-3.42
nubbe1503	-3.41
nubbe1683	-3.41
nubbe1802	-3.41
nubbe1998	-3.41
zinc000001530728	-3.41
zinc000003831051	-3.41
nubbe288uff	-3.4
nubbe875	-3.4
zinc000001530775	-3.4
zinc38433752	-3.4
nubbe389	-3.39
nubbe632	-3.39
fqn timer	-3.39
zinc000000895040	-3.39
nubbe114uff	-3.38
nubbe1703	-3.38
nubbe1876	-3.38
fqn timer	-3.38
zinc39088369	-3.38
nubbe123	-3.37
nubbe166uff	-3.37
nubbe1971	-3.37
zinc000008214402	-3.37
zinc11681341	-3.37
nubbe280uff	-3.36
nubbe282	-3.36
perunpdb275	-3.36
zinc000001532529	-3.36
zinc000008551180	-3.36
nubbe285	-3.35
nubbe311uff	-3.35
nubbe453	-3.35
perunpdb69	-3.35
perunpdb74	-3.35
fqn timer	-3.35
zinc000001532805	-3.35
nubbe1792	-3.34
nubbe2145	-3.34
zinc000000000353	-3.34
zinc000000538509	-3.34
zinc000003806063	-3.34
nubbe978	-3.33

perunpdb190	-3.33
zinc000001529425	-3.33
zinc000004658552	-3.33
zinc000008437287	-3.33
zinc000028957444	-3.33
zinc000253529560	-3.33
zinc38864628	-3.33
nubbe270uff	-3.32
nubbe560	-3.32
zinc000000901061	-3.32
zinc000001530569	-3.32
zinc000002016052	-3.32
zinc000005819214	-3.32
zinc000053022902	-3.32
nubbe1880	-3.31
nubbe303	-3.31
nubbe341uff	-3.31
zinc000000000257	-3.31
zinc000001487602	-3.31
zinc000001530635	-3.31
zinc000001530737	-3.31
zinc000001532728	-3.31
zinc000003830957	-3.31
zinc000029571072	-3.31
zinc39937087	-3.31
zinc62454731	-3.31
nubbe205	-3.29
zinc000000001505	-3.29
zinc000000002176	-3.29
zinc000100052691	-3.29
nubbe167uff	-3.28
perunpdb15	-3.28
zinc000001530580	-3.28
zinc000003785276	-3.28
zinc000252678020	-3.28
nubbe1505	-3.27
nubbe230	-3.27
zinc39088367	-3.27
nubbe1793	-3.26
zinc000004658557	-3.26
zinc38864637	-3.26
nubbe124	-3.25
zinc000000895103	-3.25

zinc000003800475	-3.25
zinc39088365	-3.25
nubbe51uff	-3.24
nubbe226uff	-3.23
zinc000003079342	-3.23
zinc000004474564	-3.23
zinc39088364	-3.23
nubbe194uff	-3.22
nubbe312uff	-3.22
perunpdb191	-3.22
zinc000008214514	-3.22
zinc38433751	-3.22
nubbe456	-3.21
perunpdb94	-3.21
perunpdb212	-3.2
perunpdb9	-3.2
zinc000035454991	-3.2
nubbe324uff	-3.19
nubbe636	-3.19
nubbe759uff	-3.19
zinc42375786	-3.19
nubbe1377	-3.18
nubbe38	-3.18
zinc000000895042	-3.18
zinc000001542392	-3.18
zinc76599670	-3.18
nubbe1397	-3.17
nubbe62uff	-3.17
zinc000003079340	-3.17
zinc000003977737	-3.17
zinc05688736	-3.17
nubbe324	-3.16
perunpdb14	-3.16
zinc13511397	-3.16
zinc38864633	-3.16
nubbe106uff	-3.15
zinc000003941496	-3.15
zinc02508225	-3.15
nubbe603	-3.14
zinc000000113415	-3.13
zinc000003812913	-3.13
zinc000006845860	-3.13
zinc000008143864	-3.13

zinc000035454995	-3.13
nubbe302uff	-3.12
nubbe312	-3.12
nubbe1811	-3.11
nubbe981	-3.11
zinc000001532526	-3.11
nubbe2167	-3.1
zinc000000895316	-3.1
zinc000003813088	-3.1
zinc000008220878	-3.1
nubbe318uff	-3.09
zinc000003939013	-3.09
nubbe1820	-3.08
nubbe211uff	-3.08
zinc000001532522	-3.08
zinc39937088	-3.08
nubbe17	-3.07
nubbe37uff	-3.07
zinc000000000507	-3.07
zinc08627075	-3.07
zinc36378001	-3.07
nubbe1821	-3.06
nubbe334	-3.06
zinc000001530600	-3.06
zinc000003830958	-3.06
zinc22054059	-3.06
nubbe1803	-3.05
nubbe233uff	-3.05
nubbe310uff	-3.05
fqnp428	-3.05
zinc000004474603	-3.05
nubbe111uff	-3.04
zinc000003831138	-3.04
zinc000100001964	-3.04
nubbe642uff	-3.03
zinc000095617679	-3.03
nubbe172uff	-3.02
nubbe448uff	-3.02
zinc000003872952	-3.02
nubbe231	-3.01
nubbe50	-3.01
zinc22053713	-3.01
nubbe1795	-3
perunpdb73	-3

nubbe2113	-2.99
zinc000000901159	-2.99
nubbe2471	-2.98
zinc000001535101	-2.98
zinc000003801919	-2.98
zinc01593341	-2.98
nubbe17uff	-2.97
fqnp405	-2.97
fqnp94	-2.97
zinc000000901555	-2.97
zinc000000403079	-2.96
zinc000003079337	-2.96
zinc000008551178	-2.96
zinc000012503177	-2.96
zinc000253529563	-2.96
zinc000000895034	-2.95
zinc000004097426	-2.95
zinc000008034121	-2.95
nubbe1186	-2.94
nubbe1689	-2.94
nubbe660uff	-2.94
zinc000001532525	-2.94
zinc000003794794	-2.94
zinc000100001965	-2.94
nubbe65uff	-2.93
perunpdb195	-2.93
nubbe1567	-2.92
nubbe1679	-2.92
fqnp224	-2.92
zinc04523240	-2.92
nubbe636uff	-2.91
nubbe766uff	-2.91
nubbe309uff	-2.9
zinc000242437512	-2.9
nubbe231uff	-2.89
nubbe299	-2.89
fqnp226	-2.89
zinc39097926	-2.89
nubbe283	-2.88
nubbe339uff	-2.88
zinc05157115	-2.88
zinc22054067	-2.88
nubbe1032	-2.87
zinc000003872605	-2.87

nubbe116uff	-2.86
nubbe206uff	-2.86
nubbe560uff	-2.86
zinc000003830813	-2.86
zinc04523242	-2.86
perunpdb72	-2.85
zinc000011615926	-2.84
zinc000049637509	-2.84
zinc04533798	-2.84
zinc06562444	-2.84
zinc22054079	-2.84
nubbe1699	-2.83
nubbe1810	-2.83
nubbe186uff	-2.83
nubbe1796	-2.82
perunpdb18	-2.82
zinc000000896695	-2.82
zinc02562349	-2.82
nubbe212	-2.81
zinc000003875342	-2.81
zinc000003830945	-2.8
zinc000003871832	-2.8
nubbe206	-2.79
zinc000003812306	-2.78
zinc000003944422	-2.78
zinc04566616	-2.78
nubbe104	-2.77
nubbe1641	-2.77
perunpdb17	-2.77
zinc000001532179	-2.77
zinc000242437511	-2.77
nubbe282uff	-2.76
zinc000003785268	-2.76
zinc05063416	-2.76
nubbe169	-2.75
zinc000003830943	-2.75
zinc000085537053	-2.75
zinc36533537	-2.74
nubbe168uff	-2.73
nubbe301	-2.72
zinc000001554392	-2.71
zinc000008035377	-2.71
nubbe2472	-2.7

zinc98089939	-2.7
zinc000052971887	-2.69
zinc36387027	-2.69
perunpdb203	-2.68
zinc000003812960	-2.68
zinc000001530760	-2.66
zinc000514288136	-2.66
zinc04404234	-2.66
nubbe223uff	-2.65
zinc000000156792	-2.65
zinc000001846431	-2.65
nubbe193uff	-2.64
nubbe420	-2.63
zinc000000895318	-2.63
zinc000245224194	-2.63
nubbe172	-2.62
nubbe318	-2.62
fqnpl49	-2.62
zinc22054071	-2.62
zinc000100052685	-2.61
zinc000150338698	-2.61
nubbe2332	-2.6
nubbe760uff	-2.6
nubbe963	-2.6
zinc000008214703	-2.59
nubbe330uff	-2.58
zinc000085540219	-2.58
nubbe451uff	-2.57
zinc000001531008	-2.57
nubbe193	-2.56
nubbe176	-2.55
nubbe2423	-2.55
nubbe48	-2.55
zinc000008214681	-2.55
nubbe236	-2.54
zinc000003812888	-2.54
zinc24817559	-2.54
nubbe281uff	-2.53
nubbe452uff	-2.53
nubbe769uff	-2.53
nubbe1031	-2.52
nubbe187uff	-2.52
nubbe302	-2.51

nubbe448	-2.51
nubbe236uff	-2.5
zinc000028232746	-2.5
perunpdb93	-2.49
nubbe114	-2.48
nubbe1162	-2.48
nubbe332uff	-2.48
zinc000000895048	-2.48
zinc05167490	-2.46
nubbe1157	-2.44
nubbe210	-2.43
nubbe272uff	-2.43
nubbe301uff	-2.43
zinc000100009383	-2.43
nubbe313uff	-2.42
nubbe340uff	-2.42
zinc000514288134	-2.42
fqnp121	-2.41
zinc000003830635	-2.41
zinc04566615	-2.41
zinc000085540215	-2.4
zinc13532457	-2.4
nubbe208	-2.38
nubbe389uff	-2.38
nubbe636buff	-2.38
nubbe642	-2.36
fqnp116	-2.36
zinc000003951740	-2.36
zinc000004097392	-2.36
nubbe1187	-2.35
nubbe2454	-2.35
zinc000253500687	-2.34
zinc000019364219	-2.32
nubbe454	-2.31
nubbe142	-2.3
nubbe169uff	-2.3
nubbe337	-2.3
nubbe443	-2.3
nubbe445	-2.3
zinc000027641461	-2.3
nubbe603uff	-2.29
nubbe63	-2.29
zinc000035454987	-2.29
zinc000049841054	-2.29

nubbe204uff	-2.28
fqnp430	-2.28
zinc000003776875	-2.28
nubbe987	-2.27
zinc000242437513	-2.27
fqnp431	-2.26
zinc000003830891	-2.26
zinc000008035395	-2.26
zinc000216450933	-2.25
nubbe192uff	-2.24
fqnp151	-2.24
zinc000000643046	-2.24
nubbe110uff	-2.23
nubbe207uff	-2.23
nubbe337uff	-2.23
nubbe204	-2.22
fqnp463	-2.22
nubbe1088	-2.21
nubbe1801	-2.21
nubbe453uff	-2.2
zinc000008577218	-2.2
nubbe174uff	-2.19
nubbe194	-2.19
nubbe1800	-2.18
zinc000257355149	-2.18
nubbe223	-2.17
nubbe335	-2.16
nubbe185uff	-2.15
zinc000003955219	-2.15
nubbe110	-2.14
nubbe313	-2.14
zinc000003830946	-2.14
zinc02020190	-2.14
zinc000004102194	-2.13
zinc38644575	-2.13
zinc000008551179	-2.12
nubbe635uff	-2.1
zinc000038238855	-2.1
nubbe272	-2.07
zinc13532465	-2.07
nubbe103	-2.06
perunpdb89	-2.06
zinc000003941829	-2.06
zinc000008035268	-2.06

zinc98089938	-2.05
fqp122	-2.03
zinc000003991624	-2.03
nubbe1167	-2.02
nubbe1985	-2.02
zinc000019364225	-2.02
nubbe111	-2.01
fqp432	-2.01
zinc000003830960	-2.01
zinc000100055899	-2.01
zinc000514288311	-2.01
fqp291	-2
zinc000008214635	-2
zinc000087496092	-2
nubbe109	-1.99
nubbe124uff	-1.99
zinc000103650667	-1.99
nubbe331	-1.97
zinc000008214651	-1.96
zinc000001530810	-1.9
zinc000004474682	-1.9
zinc000257355148	-1.89
nubbe109uff	-1.88
zinc000006920384	-1.88
nubbe125uff	-1.86
nubbe330	-1.86
zinc000035454983	-1.86
zinc000257355145	-1.83
zinc000150339323	-1.82
nubbe112uff	-1.81
zinc04566614	-1.8
fqp67	-1.79
zinc000003799072	-1.78
zinc98089940	-1.78
nubbe210uff	-1.77
zinc000018279893	-1.77
nubbe118	-1.76
nubbe174	-1.73
nubbe332	-1.73
zinc000004217475	-1.73
zinc98089944	-1.73
nubbe1649	-1.72
zinc000003977952	-1.72

zinc000085536932	-1.72
zinc000009164421	-1.7
nubbe604	-1.68
zinc000004393164	-1.67
nubbe112	-1.66
zinc000001533877	-1.62
zinc000008551177	-1.62
zinc98089943	-1.61
zinc02556386	-1.58
nubbe118uff	-1.56
zinc000002041302	-1.56
nubbe420uff	-1.55
nubbe635buff	-1.55
zinc000514288135	-1.55
zinc000001543475	-1.54
zinc000003943279	-1.54
zinc000019363537	-1.51
zinc000085537014	-1.47
perunpdb90	-1.42
zinc000038945666	-1.38
zinc000257355146	-1.38
nubbe187	-1.35
nubbe207	-1.35
nubbe444	-1.33
zinc000242437514	-1.33
zinc000008214614	-1.31
zinc000003830944	-1.29
zinc000238809664	-1.29
zinc000003930376	-1.26
perunpdb86	-1.22
nubbe602	-1.2
nubbe546	-1.19
perunpdb85	-1.18
zinc04566617	-1.18
nubbe331uff	-1.17
nubbe1806	-1.16
perunpdb88	-1.14
zinc000014881137	-1.09
zinc000238809662	-1.06
zinc000000896409	-1.05
perunpdb87	-1.02
fqp434	-1.01
zinc000008214692	-1.01

nubbe338	-0.94	zinc000095564694	0.21
zinc000238809665	-0.93	zinc000060392785	0.26
nubbe2274	-0.83	perunpdb83	0.3
nubbe1807	-0.82	zinc000060183170	0.33
nubbe280	-0.8	zinc000022448097	0.35
zinc000028108825	-0.78	zinc000085537017	0.46
zinc000003929022	-0.71	perunpdb84	0.48
zinc000008214483	-0.7	fqnp74	1.03
zinc000257355147	-0.62	zinc000033965961	1.25
nubbe390	-0.55	zinc000022851765	1.63
nubbe286	-0.54	zinc000003830276	1.72
zinc000257355150	-0.46	zinc000021982937	1.89
zinc000096006013	-0.35	nubbe361	2.21
perunpdb92	-0.3	zinc000019855121	2.32
perunpdb91	-0.11	fqnp73	2.36
zinc000238809663	-0.06	zinc000022447798	2.52
nubbe360	-0.03	zinc000096309558	2.89
nubbe271	0.1		

Table S2. PASSer predictions for allosteric site probabilities in MOGS protein pockets.

Pocket Number	Parameter	Amount
Pocket 1		
	Score	0.118
	Druggability Score	0.006
	Number of Alpha Spheres	50.000
	Total SASA	130.671
	Polar SASA	69.082
	Apolar SASA	61.589
	Volume	488.359
	Mean local hydrophobic density	5.250
	Mean alpha sphere radius	3.932
	Mean alp. sph. solvent access	0.707
	Apolar alpha sphere proportion	0.160
	Hydrophobicity score	-3.000
	Volume score	3.308
	Polarity score	10.000
	Charge score	-2.000
	Proportion of polar atoms	51.351
	Alpha sphere density	6.177
	Cent. of mass - Alpha Sphere max dist	14.690
	Flexibility	0.922

Pocket 2

Score	0.084
Druggability Score	0.002
Number of Alpha Spheres	20.000
Total SASA	18.505
Polar SASA	6.429
Apolar SASA	12.076
Volume	96.898
Mean local hydrophobic density	7.000
Mean alpha sphere radius	3.624
Mean alp. sph. solvent access	0.414
Apolar alpha sphere proportion	0.400
Hydrophobicity score	9.889
Volume score	4.556
Polarity score	5.000
Charge score	2.000
Proportion of polar atoms	40.000
Alpha sphere density	1.723
Cent. of mass - Alpha Sphere max dist	3.745
Flexibility	0.897

Pocket 3

Score	0.074
Druggability Score	0.001
Number of Alpha Spheres	19.000
Total SASA	11.554
Polar SASA	4.308
Apolar SASA	7.246
Volume	83.399
Mean local hydrophobic density	8.000
Mean alpha sphere radius	3.606
Mean alp. sph. solvent access	0.454
Apolar alpha sphere proportion	0.474
Hydrophobicity score	-5.000
Volume score	4.500
Polarity score	6.000
Charge score	1.000
Proportion of polar atoms	33.333
Alpha sphere density	1.325
Cent. of mass - Alpha Sphere max dist	2.830
Flexibility	0.941

Pocket 4

Score	0.066
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Druggability Score	0.541
Number of Alpha Spheres	53.000
Total SASA	151.351
Polar SASA	48.703
Apolar SASA	102.648
Volume	648.796
Mean local hydrophobic density	20.857
Mean alpha sphere radius	3.872
Mean alp. sph. solvent access	0.530
Apolar alpha sphere proportion	0.528
Hydrophobicity score	-4.857
Volume score	4.857
Polarity score	10.000
Charge score	7.000
Proportion of polar atoms	41.463
Alpha sphere density	6.007
Cent. of mass - Alpha Sphere max dist	16.279
Flexibility	0.982

Pocket 5

Score	0.047
Druggability Score	0.001
Number of Alpha Spheres	16.000
Total SASA	24.021
Polar SASA	10.737
Apolar SASA	13.284
Volume	89.878
Mean local hydrophobic density	6.000
Mean alpha sphere radius	3.567
Mean alp. sph. solvent access	0.402
Apolar alpha sphere proportion	0.438
Hydrophobicity score	22.143
Volume score	4.571
Polarity score	4.000
Charge score	0.000
Proportion of polar atoms	42.857
Alpha sphere density	1.646
Cent. of mass - Alpha Sphere max dist	3.684
Flexibility	0.663

Pocket 6

Score	0.045
Druggability Score	0.002
Number of Alpha Spheres	26.000
Total SASA	35.891
Polar SASA	12.946

	Apolar SASA	22.945
	Volume	131.564
	Mean local hydrophobic density	6.000
	Mean alpha sphere radius	3.700
	Mean alp. sph. solvent access	0.421
	Apolar alpha sphere proportion	0.269
	Hydrophobicity score	23.700
	Volume score	4.400
	Polarity score	5.000
	Charge score	0.000
	Proportion of polar atoms	38.889
	Alpha sphere density	1.915
	Cent. of mass - Alpha Sphere max dist	5.526
	Flexibility	0.970
Pocket 7		
	Score	0.023
	Druggability Score	0.001
	Number of Alpha Spheres	18.000
	Total SASA	40.583
	Polar SASA	26.091
	Apolar SASA	14.492
	Volume	117.018
	Mean local hydrophobic density	2.000
	Mean alpha sphere radius	3.545
	Mean alp. sph. solvent access	0.367
	Apolar alpha sphere proportion	0.167
	Hydrophobicity score	25.500
	Volume score	5.125
	Polarity score	5.000
	Charge score	3.000
	Proportion of polar atoms	52.941
	Alpha sphere density	2.061
	Cent. of mass - Alpha Sphere max dist	4.677
	Flexibility	0.910
Pocket 8		
	Score	0.010
	Druggability Score	0.023
	Number of Alpha Spheres	28.000
	Total SASA	57.172
	Polar SASA	17.320
	Apolar SASA	39.852
	Volume	182.406
	Mean local hydrophobic density	19.000

Mean alpha sphere radius	3.663
Mean alp. sph. solvent access	0.419
Apolar alpha sphere proportion	0.714
Hydrophobicity score	5.714
Volume score	4.429
Polarity score	6.000
Charge score	-1.000
Proportion of polar atoms	38.889
Alpha sphere density	2.417
Cent. of mass - Alpha Sphere max dist	5.293
Flexibility	0.721

Pocket 9

Score	-0.003
Druggability Score	0.001
Number of Alpha Spheres	39.000
Total SASA	120.430
Polar SASA	92.654
Apolar SASA	27.775
Volume	430.069
Mean local hydrophobic density	3.667
Mean alpha sphere radius	3.811
Mean alp. sph. solvent access	0.493
Apolar alpha sphere proportion	0.154
Hydrophobicity score	17.429
Volume score	4.357
Polarity score	8.000
Charge score	1.000
Proportion of polar atoms	53.571
Alpha sphere density	4.628
Cent. of mass - Alpha Sphere max dist	11.598
Flexibility	0.975

Pocket 10

Score	-0.004
Druggability Score	0.002
Number of Alpha Spheres	32.000
Total SASA	99.213
Polar SASA	66.607
Apolar SASA	32.606
Volume	310.538
Mean local hydrophobic density	1.000
Mean alpha sphere radius	3.711
Mean alp. sph. solvent access	0.395
Apolar alpha sphere proportion	0.062
Hydrophobicity score	16.429

	Volume score	4.071
	Polarity score	9.000
	Charge score	0.000
	Proportion of polar atoms	60.000
	Alpha sphere density	3.904
	Cent. of mass - Alpha Sphere max dist	10.958
	Flexibility	0.935
Pocket 11		
	Score	-0.011
	Druggability Score	0.003
	Number of Alpha Spheres	35.000
	Total SASA	64.448
	Polar SASA	25.804
	Apolar SASA	38.644
	Volume	177.237
	Mean local hydrophobic density	4.667
	Mean alpha sphere radius	3.704
	Mean alp. sph. solvent access	0.460
	Apolar alpha sphere proportion	0.171
	Hydrophobicity score	45.462
	Volume score	4.231
	Polarity score	5.000
	Charge score	1.000
	Proportion of polar atoms	47.619
	Alpha sphere density	2.336
	Cent. of mass - Alpha Sphere max dist	7.087
	Flexibility	0.951
Pocket 12		
	Score	-0.012
	Druggability Score	0.004
	Number of Alpha Spheres	39.000
	Total SASA	127.083
	Polar SASA	72.739
	Apolar SASA	54.343
	Volume	336.074
	Mean local hydrophobic density	7.778
	Mean alpha sphere radius	3.932
	Mean alp. sph. solvent access	0.432
	Apolar alpha sphere proportion	0.231
	Hydrophobicity score	23.769
	Volume score	4.385
	Polarity score	8.000
	Charge score	4.000

	Proportion of polar atoms	46.154
	Alpha sphere density	4.882
	Cent. of mass - Alpha Sphere max dist	10.925
	Flexibility	0.980
Pocket 13		
	Score	-0.014
	Druggability Score	0.009
	Number of Alpha Spheres	25.000
	Total SASA	47.080
	Polar SASA	9.643
	Apolar SASA	37.436
	Volume	132.102
	Mean local hydrophobic density	15.000
	Mean alpha sphere radius	3.775
	Mean alp. sph. solvent access	0.442
	Apolar alpha sphere proportion	0.640
	Hydrophobicity score	11.667
	Volume score	4.444
	Polarity score	6.000
	Charge score	1.000
	Proportion of polar atoms	41.176
	Alpha sphere density	1.799
	Cent. of mass - Alpha Sphere max dist	3.916
	Flexibility	0.847
Pocket 14		
	Score	-0.016
	Druggability Score	0.000
	Number of Alpha Spheres	22.000
	Total SASA	44.894
	Polar SASA	29.195
	Apolar SASA	15.699
	Volume	131.939
	Mean local hydrophobic density	1.000
	Mean alpha sphere radius	3.725
	Mean alp. sph. solvent access	0.487
	Apolar alpha sphere proportion	0.091
	Hydrophobicity score	6.222
	Volume score	3.778
	Polarity score	7.000
	Charge score	-2.000
	Proportion of polar atoms	47.059
	Alpha sphere density	1.726
	Cent. of mass - Alpha Sphere max dist	3.307
	Flexibility	0.662

Pocket 15

Score	-0.019
Druggability Score	0.005
Number of Alpha Spheres	33.000
Total SASA	95.612
Polar SASA	55.760
Apolar SASA	39.852
Volume	341.750
Mean local hydrophobic density	15.000
Mean alpha sphere radius	3.953
Mean alp. sph. solvent access	0.546
Apolar alpha sphere proportion	0.485
Hydrophobicity score	20.273
Volume score	3.909
Polarity score	6.000
Charge score	1.000
Proportion of polar atoms	37.500
Alpha sphere density	3.561
Cent. of mass - Alpha Sphere max dist	8.618
Flexibility	0.955

Pocket 16

Score	-0.019
Druggability Score	0.001
Number of Alpha Spheres	61.000
Total SASA	128.326
Polar SASA	68.994
Apolar SASA	59.332
Volume	425.414
Mean local hydrophobic density	3.000
Mean alpha sphere radius	3.987
Mean alp. sph. solvent access	0.561
Apolar alpha sphere proportion	0.066
Hydrophobicity score	11.417
Volume score	3.500
Polarity score	7.000
Charge score	-1.000
Proportion of polar atoms	45.946
Alpha sphere density	4.254
Cent. of mass - Alpha Sphere max dist	9.492
Flexibility	0.860

Pocket 17

Score	-0.020
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Druggability Score	0.000
Number of Alpha Spheres	16.000
Total SASA	23.590
Polar SASA	13.929
Apolar SASA	9.661
Volume	67.593
Mean local hydrophobic density	3.000
Mean alpha sphere radius	3.601
Mean alp. sph. solvent access	0.406
Apolar alpha sphere proportion	0.250
Hydrophobicity score	21.375
Volume score	4.625
Polarity score	6.000
Charge score	-1.000
Proportion of polar atoms	50.000
Alpha sphere density	0.899
Cent. of mass - Alpha Sphere max dist	2.064
Flexibility	0.952

Pocket 18

Score	-0.023
Druggability Score	0.003
Number of Alpha Spheres	41.000
Total SASA	160.190
Polar SASA	93.770
Apolar SASA	66.420
Volume	544.982
Mean local hydrophobic density	5.333
Mean alpha sphere radius	3.970
Mean alp. sph. solvent access	0.566
Apolar alpha sphere proportion	0.220
Hydrophobicity score	8.688
Volume score	3.438
Polarity score	9.000
Charge score	-1.000
Proportion of polar atoms	52.941
Alpha sphere density	6.182
Cent. of mass - Alpha Sphere max dist	16.326
Flexibility	0.683

Pocket 19

Score	-0.025
Druggability Score	0.017
Number of Alpha Spheres	33.000
Total SASA	127.982
Polar SASA	49.486

	Apolar SASA	78.496
	Volume	489.355
	Mean local hydrophobic density	13.000
	Mean alpha sphere radius	3.987
	Mean alp. sph. solvent access	0.524
	Apolar alpha sphere proportion	0.424
	Hydrophobicity score	20.778
	Volume score	2.778
	Polarity score	2.000
	Charge score	2.000
	Proportion of polar atoms	45.833
	Alpha sphere density	4.765
	Cent. of mass - Alpha Sphere max dist	10.461
	Flexibility	0.425
Pocket 20		
	Score	-0.030
	Druggability Score	0.022
	Number of Alpha Spheres	37.000
	Total SASA	90.221
	Polar SASA	43.124
	Apolar SASA	47.097
	Volume	252.489
	Mean local hydrophobic density	11.000
	Mean alpha sphere radius	3.864
	Mean alp. sph. solvent access	0.429
	Apolar alpha sphere proportion	0.324
	Hydrophobicity score	-1.231
	Volume score	3.154
	Polarity score	9.000
	Charge score	-2.000
	Proportion of polar atoms	54.167
	Alpha sphere density	3.172
	Cent. of mass - Alpha Sphere max dist	8.628
	Flexibility	0.921
Pocket 21		
	Score	-0.031
	Druggability Score	0.002
	Number of Alpha Spheres	22.000
	Total SASA	54.209
	Polar SASA	22.810
	Apolar SASA	31.398
	Volume	174.297
	Mean local hydrophobic density	7.000

	Mean alpha sphere radius	3.758
	Mean alp. sph. solvent access	0.463
	Apolar alpha sphere proportion	0.364
	Hydrophobicity score	12.500
	Volume score	4.375
	Polarity score	5.000
	Charge score	3.000
	Proportion of polar atoms	47.059
	Alpha sphere density	1.982
	Cent. of mass - Alpha Sphere max dist	5.074
	Flexibility	0.959
Pocket 22		
	Score	-0.031
	Druggability Score	0.011
	Number of Alpha Spheres	25.000
	Total SASA	130.159
	Polar SASA	55.286
	Apolar SASA	74.873
	Volume	428.973
	Mean local hydrophobic density	8.000
	Mean alpha sphere radius	4.123
	Mean alp. sph. solvent access	0.613
	Apolar alpha sphere proportion	0.400
	Hydrophobicity score	9.556
	Volume score	3.444
	Polarity score	4.000
	Charge score	3.000
	Proportion of polar atoms	41.667
	Alpha sphere density	5.111
	Cent. of mass - Alpha Sphere max dist	12.705
	Flexibility	0.831
Pocket 23		
	Score	-0.035
	Druggability Score	0.000
	Number of Alpha Spheres	27.000
	Total SASA	121.655
	Polar SASA	72.142
	Apolar SASA	49.513
	Volume	507.733
	Mean local hydrophobic density	0.000
	Mean alpha sphere radius	4.125
	Mean alp. sph. solvent access	0.597
	Apolar alpha sphere proportion	0.037
	Hydrophobicity score	10.111

	Volume score	4.111
	Polarity score	7.000
	Charge score	-2.000
	Proportion of polar atoms	56.522
	Alpha sphere density	4.643
	Cent. of mass - Alpha Sphere max dist	12.729
	Flexibility	0.904
Pocket 24		
	Score	-0.041
	Druggability Score	0.010
	Number of Alpha Spheres	20.000
	Total SASA	83.737
	Polar SASA	29.394
	Apolar SASA	54.343
	Volume	323.576
	Mean local hydrophobic density	13.733
	Mean alpha sphere radius	4.132
	Mean alp. sph. solvent access	0.691
	Apolar alpha sphere proportion	0.750
	Hydrophobicity score	54.000
	Volume score	6.000
	Polarity score	3.000
	Charge score	1.000
	Proportion of polar atoms	33.333
	Alpha sphere density	3.203
	Cent. of mass - Alpha Sphere max dist	8.473
	Flexibility	0.579
Pocket 25		
	Score	-0.042
	Druggability Score	0.000
	Number of Alpha Spheres	15.000
	Total SASA	71.437
	Polar SASA	55.738
	Apolar SASA	15.699
	Volume	173.548
	Mean local hydrophobic density	0.000
	Mean alpha sphere radius	3.690
	Mean alp. sph. solvent access	0.641
	Apolar alpha sphere proportion	0.000
	Hydrophobicity score	-4.000
	Volume score	3.400
	Polarity score	3.000
	Charge score	1.000

	Proportion of polar atoms	53.333
	Alpha sphere density	2.763
	Cent. of mass - Alpha Sphere max dist	5.657
	Flexibility	0.045
Pocket 26		
	Score	-0.045
	Druggability Score	0.000
	Number of Alpha Spheres	15.000
	Total SASA	87.649
	Polar SASA	55.043
	Apolar SASA	32.606
	Volume	307.814
	Mean local hydrophobic density	0.000
	Mean alpha sphere radius	3.923
	Mean alp. sph. solvent access	0.480
	Apolar alpha sphere proportion	0.067
	Hydrophobicity score	-16.500
	Volume score	4.100
	Polarity score	8.000
	Charge score	0.000
	Proportion of polar atoms	68.750
	Alpha sphere density	3.426
	Cent. of mass - Alpha Sphere max dist	7.776
	Flexibility	0.805
Pocket 27		
	Score	-0.046
	Druggability Score	0.001
	Number of Alpha Spheres	15.000
	Total SASA	65.284
	Polar SASA	31.471
	Apolar SASA	33.814
	Volume	186.697
	Mean local hydrophobic density	6.000
	Mean alpha sphere radius	3.805
	Mean alp. sph. solvent access	0.609
	Apolar alpha sphere proportion	0.467
	Hydrophobicity score	13.333
	Volume score	5.000
	Polarity score	3.000
	Charge score	1.000
	Proportion of polar atoms	35.294
	Alpha sphere density	2.477
	Cent. of mass - Alpha Sphere max dist	6.343
	Flexibility	0.997

Pocket 28

Score	-0.048
Druggability Score	0.417
Number of Alpha Spheres	69.000
Total SASA	155.534
Polar SASA	61.339
Apolar SASA	94.195
Volume	467.668
Mean local hydrophobic density	31.029
Mean alpha sphere radius	3.908
Mean alp. sph. solvent access	0.496
Apolar alpha sphere proportion	0.507
Hydrophobicity score	10.000
Volume score	3.867
Polarity score	8.000
Charge score	1.000
Proportion of polar atoms	34.146
Alpha sphere density	4.860
Cent. of mass - Alpha Sphere max dist	10.044
Flexibility	0.938

Pocket 29

Score	-0.048
Druggability Score	0.018
Number of Alpha Spheres	53.000
Total SASA	127.865
Polar SASA	51.784
Apolar SASA	76.081
Volume	424.183
Mean local hydrophobic density	12.714
Mean alpha sphere radius	3.896
Mean alp. sph. solvent access	0.467
Apolar alpha sphere proportion	0.264
Hydrophobicity score	-7.750
Volume score	3.917
Polarity score	9.000
Charge score	1.000
Proportion of polar atoms	43.750
Alpha sphere density	4.109
Cent. of mass - Alpha Sphere max dist	12.084
Flexibility	0.800

Pocket 30

Score	-0.053
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Druggability Score	0.000
Number of Alpha Spheres	17.000
Total SASA	48.653
Polar SASA	28.123
Apolar SASA	20.530
Volume	185.780
Mean local hydrophobic density	6.000
Mean alpha sphere radius	3.997
Mean alp. sph. solvent access	0.631
Apolar alpha sphere proportion	0.412
Hydrophobicity score	13.500
Volume score	5.167
Polarity score	5.000
Charge score	1.000
Proportion of polar atoms	46.154
Alpha sphere density	1.611
Cent. of mass - Alpha Sphere max dist	3.107
Flexibility	0.887

Pocket 31

Score	-0.065
Druggability Score	0.000
Number of Alpha Spheres	37.000
Total SASA	118.953
Polar SASA	68.232
Apolar SASA	50.720
Volume	407.559
Mean local hydrophobic density	3.000
Mean alpha sphere radius	3.961
Mean alp. sph. solvent access	0.574
Apolar alpha sphere proportion	0.108
Hydrophobicity score	-5.385
Volume score	4.615
Polarity score	12.000
Charge score	4.000
Proportion of polar atoms	62.069
Alpha sphere density	3.982
Cent. of mass - Alpha Sphere max dist	11.189
Flexibility	0.868

Pocket 32

Score	-0.069
Druggability Score	0.007
Number of Alpha Spheres	30.000
Total SASA	103.317
Polar SASA	35.690

	Apolar SASA	67.627
	Volume	311.939
	Mean local hydrophobic density	10.667
	Mean alpha sphere radius	3.863
	Mean alp. sph. solvent access	0.514
	Apolar alpha sphere proportion	0.400
	Hydrophobicity score	13.455
	Volume score	3.545
	Polarity score	3.000
	Charge score	0.000
	Proportion of polar atoms	37.500
	Alpha sphere density	3.418
	Cent. of mass - Alpha Sphere max dist	8.972
	Flexibility	0.532
Pocket 33		
	Score	-0.069
	Druggability Score	0.001
	Number of Alpha Spheres	19.000
	Total SASA	69.871
	Polar SASA	31.227
	Apolar SASA	38.644
	Volume	228.409
	Mean local hydrophobic density	6.000
	Mean alpha sphere radius	3.936
	Mean alp. sph. solvent access	0.537
	Apolar alpha sphere proportion	0.368
	Hydrophobicity score	23.167
	Volume score	3.500
	Polarity score	3.000
	Charge score	0.000
	Proportion of polar atoms	43.750
	Alpha sphere density	2.306
	Cent. of mass - Alpha Sphere max dist	5.844
	Flexibility	0.697
Pocket 34		
	Score	-0.083
	Druggability Score	0.002
	Number of Alpha Spheres	19.000
	Total SASA	62.900
	Polar SASA	22.810
	Apolar SASA	40.089
	Volume	216.789
	Mean local hydrophobic density	11.000

	Mean alpha sphere radius	3.956
	Mean alp. sph. solvent access	0.533
	Apolar alpha sphere proportion	0.632
	Hydrophobicity score	38.333
	Volume score	4.000
	Polarity score	2.000
	Charge score	1.000
	Proportion of polar atoms	35.714
	Alpha sphere density	1.881
	Cent. of mass - Alpha Sphere max dist	5.156
	Flexibility	0.584
Pocket 35		
	Score	-0.084
	Druggability Score	0.005
	Number of Alpha Spheres	58.000
	Total SASA	160.254
	Polar SASA	116.780
	Apolar SASA	43.475
	Volume	456.786
	Mean local hydrophobic density	5.750
	Mean alpha sphere radius	3.785
	Mean alp. sph. solvent access	0.475
	Apolar alpha sphere proportion	0.138
	Hydrophobicity score	6.059
	Volume score	4.059
	Polarity score	11.000
	Charge score	2.000
	Proportion of polar atoms	56.098
	Alpha sphere density	4.854
	Cent. of mass - Alpha Sphere max dist	14.097
	Flexibility	0.833
Pocket 36		
	Score	-0.094
	Druggability Score	0.000
	Number of Alpha Spheres	15.000
	Total SASA	76.028
	Polar SASA	39.799
	Apolar SASA	36.229
	Volume	219.278
	Mean local hydrophobic density	0.000
	Mean alpha sphere radius	4.016
	Mean alp. sph. solvent access	0.546
	Apolar alpha sphere proportion	0.067
	Hydrophobicity score	11.714

	Volume score	3.429
	Polarity score	4.000
	Charge score	0.000
	Proportion of polar atoms	57.143
	Alpha sphere density	2.401
	Cent. of mass - Alpha Sphere max dist	5.719
	Flexibility	0.544
Pocket 37		
	Score	-0.098
	Druggability Score	0.000
	Number of Alpha Spheres	16.000
	Total SASA	87.516
	Polar SASA	54.910
	Apolar SASA	32.606
	Volume	254.181
	Mean local hydrophobic density	1.000
	Mean alpha sphere radius	3.871
	Mean alp. sph. solvent access	0.588
	Apolar alpha sphere proportion	0.125
	Hydrophobicity score	-4.714
	Volume score	4.000
	Polarity score	6.000
	Charge score	1.000
	Proportion of polar atoms	53.333
	Alpha sphere density	2.837
	Cent. of mass - Alpha Sphere max dist	7.218
	Flexibility	0.814
Pocket 38		
	Score	-0.098
	Druggability Score	0.222
	Number of Alpha Spheres	60.000
	Total SASA	162.716
	Polar SASA	81.488
	Apolar SASA	81.228
	Volume	633.485
	Mean local hydrophobic density	29.355
	Mean alpha sphere radius	3.915
	Mean alp. sph. solvent access	0.521
	Apolar alpha sphere proportion	0.517
	Hydrophobicity score	22.812
	Volume score	4.625
	Polarity score	9.000
	Charge score	3.000

	Proportion of polar atoms	37.209
	Alpha sphere density	4.558
	Cent. of mass - Alpha Sphere max dist	10.708
	Flexibility	0.733
Pocket 39		
	Score	-0.099
	Druggability Score	0.000
	Number of Alpha Spheres	23.000
	Total SASA	78.389
	Polar SASA	54.237
	Apolar SASA	24.153
	Volume	209.590
	Mean local hydrophobic density	1.000
	Mean alpha sphere radius	3.890
	Mean alp. sph. solvent access	0.492
	Apolar alpha sphere proportion	0.087
	Hydrophobicity score	26.714
	Volume score	4.286
	Polarity score	5.000
	Charge score	1.000
	Proportion of polar atoms	58.824
	Alpha sphere density	2.264
	Cent. of mass - Alpha Sphere max dist	5.355
	Flexibility	0.970
Pocket 40		
	Score	-0.101
	Druggability Score	0.000
	Number of Alpha Spheres	16.000
	Total SASA	79.534
	Polar SASA	52.966
	Apolar SASA	26.568
	Volume	190.175
	Mean local hydrophobic density	2.000
	Mean alpha sphere radius	3.898
	Mean alp. sph. solvent access	0.512
	Apolar alpha sphere proportion	0.188
	Hydrophobicity score	15.833
	Volume score	5.000
	Polarity score	5.000
	Charge score	2.000
	Proportion of polar atoms	60.000
	Alpha sphere density	2.471
	Cent. of mass - Alpha Sphere max dist	5.287
	Flexibility	0.462

Pocket 41

Score	-0.106
Druggability Score	0.014
Number of Alpha Spheres	25.000
Total SASA	87.337
Polar SASA	18.502
Apolar SASA	68.835
Volume	282.314
Mean local hydrophobic density	18.000
Mean alpha sphere radius	4.009
Mean alp. sph. solvent access	0.608
Apolar alpha sphere proportion	0.760
Hydrophobicity score	36.200
Volume score	5.000
Polarity score	3.000
Charge score	0.000
Proportion of polar atoms	23.810
Alpha sphere density	2.544
Cent. of mass - Alpha Sphere max dist	6.396
Flexibility	0.903

Pocket 42

Score	-0.112
Druggability Score	0.017
Number of Alpha Spheres	43.000
Total SASA	121.716
Polar SASA	51.673
Apolar SASA	70.042
Volume	411.515
Mean local hydrophobic density	14.000
Mean alpha sphere radius	4.059
Mean alp. sph. solvent access	0.509
Apolar alpha sphere proportion	0.349
Hydrophobicity score	20.500
Volume score	4.000
Polarity score	8.000
Charge score	1.000
Proportion of polar atoms	44.828
Alpha sphere density	3.466
Cent. of mass - Alpha Sphere max dist	9.818
Flexibility	0.942

Pocket 43

Score	-0.113
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Druggability Score	0.001
Number of Alpha Spheres	44.000
Total SASA	136.831
Polar SASA	76.450
Apolar SASA	60.381
Volume	464.167
Mean local hydrophobic density	9.000
Mean alpha sphere radius	3.956
Mean alp. sph. solvent access	0.535
Apolar alpha sphere proportion	0.227
Hydrophobicity score	-4.200
Volume score	4.500
Polarity score	8.000
Charge score	0.000
Proportion of polar atoms	48.485
Alpha sphere density	4.064
Cent. of mass - Alpha Sphere max dist	12.052
Flexibility	0.928

Pocket 44

Score	-0.118
Druggability Score	0.187
Number of Alpha Spheres	41.000
Total SASA	155.589
Polar SASA	54.148
Apolar SASA	101.441
Volume	530.394
Mean local hydrophobic density	22.160
Mean alpha sphere radius	3.940
Mean alp. sph. solvent access	0.509
Apolar alpha sphere proportion	0.610
Hydrophobicity score	7.100
Volume score	4.300
Polarity score	8.000
Charge score	2.000
Proportion of polar atoms	35.484
Alpha sphere density	4.749
Cent. of mass - Alpha Sphere max dist	12.554
Flexibility	0.967

Pocket 45

Score	-0.121
Druggability Score	0.002
Number of Alpha Spheres	15.000
Total SASA	115.627
Polar SASA	54.038

	Apolar SASA	61.589
	Volume	349.232
	Mean local hydrophobic density	8.000
	Mean alpha sphere radius	4.095
	Mean alp. sph. solvent access	0.698
	Apolar alpha sphere proportion	0.600
	Hydrophobicity score	5.750
	Volume score	4.500
	Polarity score	5.000
	Charge score	1.000
	Proportion of polar atoms	43.478
	Alpha sphere density	3.838
	Cent. of mass - Alpha Sphere max dist	8.174
	Flexibility	0.959
Pocket 46		
	Score	-0.121
	Druggability Score	0.000
	Number of Alpha Spheres	21.000
	Total SASA	92.135
	Polar SASA	36.585
	Apolar SASA	55.551
	Volume	259.709
	Mean local hydrophobic density	1.000
	Mean alpha sphere radius	3.924
	Mean alp. sph. solvent access	0.573
	Apolar alpha sphere proportion	0.095
	Hydrophobicity score	3.625
	Volume score	3.125
	Polarity score	4.000
	Charge score	-2.000
	Proportion of polar atoms	47.368
	Alpha sphere density	2.617
	Cent. of mass - Alpha Sphere max dist	5.316
	Flexibility	0.577
Pocket 47		
	Score	-0.129
	Druggability Score	0.003
	Number of Alpha Spheres	20.000
	Total SASA	81.657
	Polar SASA	32.144
	Apolar SASA	49.513
	Volume	192.281
	Mean local hydrophobic density	12.000

	Mean alpha sphere radius	3.802
	Mean alp. sph. solvent access	0.507
	Apolar alpha sphere proportion	0.650
	Hydrophobicity score	20.400
	Volume score	3.200
	Polarity score	1.000
	Charge score	-1.000
	Proportion of polar atoms	33.333
	Alpha sphere density	2.173
	Cent. of mass - Alpha Sphere max dist	4.736
	Flexibility	0.882
Pocket 48		
	Score	-0.132
	Druggability Score	0.008
	Number of Alpha Spheres	28.000
	Total SASA	117.142
	Polar SASA	59.196
	Apolar SASA	57.946
	Volume	305.573
	Mean local hydrophobic density	11.000
	Mean alpha sphere radius	3.982
	Mean alp. sph. solvent access	0.650
	Apolar alpha sphere proportion	0.429
	Hydrophobicity score	19.200
	Volume score	3.800
	Polarity score	5.000
	Charge score	2.000
	Proportion of polar atoms	44.000
	Alpha sphere density	3.415
	Cent. of mass - Alpha Sphere max dist	10.477
	Flexibility	0.926
Pocket 49		
	Score	-0.132
	Druggability Score	0.006
	Number of Alpha Spheres	23.000
	Total SASA	81.444
	Polar SASA	36.762
	Apolar SASA	44.682
	Volume	185.406
	Mean local hydrophobic density	15.000
	Mean alpha sphere radius	3.930
	Mean alp. sph. solvent access	0.476
	Apolar alpha sphere proportion	0.696
	Hydrophobicity score	38.333

	Volume score	4.444
	Polarity score	3.000
	Charge score	1.000
	Proportion of polar atoms	35.294
	Alpha sphere density	2.043
	Cent. of mass - Alpha Sphere max dist	5.135
	Flexibility	0.930
Pocket 50		
	Score	-0.140
	Druggability Score	0.013
	Number of Alpha Spheres	49.000
	Total SASA	193.174
	Polar SASA	82.073
	Apolar SASA	111.102
	Volume	596.227
	Mean local hydrophobic density	17.895
	Mean alpha sphere radius	3.911
	Mean alp. sph. solvent access	0.577
	Apolar alpha sphere proportion	0.388
	Hydrophobicity score	18.867
	Volume score	3.867
	Polarity score	8.000
	Charge score	-1.000
	Proportion of polar atoms	44.737
	Alpha sphere density	5.646
	Cent. of mass - Alpha Sphere max dist	12.261
	Flexibility	0.862
Pocket 51		
	Score	-0.143
	Druggability Score	0.000
	Number of Alpha Spheres	22.000
	Total SASA	108.236
	Polar SASA	35.779
	Apolar SASA	72.458
	Volume	342.493
	Mean local hydrophobic density	4.000
	Mean alpha sphere radius	4.103
	Mean alp. sph. solvent access	0.511
	Apolar alpha sphere proportion	0.227
	Hydrophobicity score	12.571
	Volume score	4.571
	Polarity score	3.000
	Charge score	1.000

	Proportion of polar atoms	41.176
	Alpha sphere density	3.105
	Cent. of mass - Alpha Sphere max dist	6.645
	Flexibility	0.799
Pocket 52		
	Score	-0.146
	Druggability Score	0.000
	Number of Alpha Spheres	39.000
	Total SASA	139.074
	Polar SASA	71.447
	Apolar SASA	67.627
	Volume	411.859
	Mean local hydrophobic density	5.000
	Mean alpha sphere radius	3.842
	Mean alp. sph. solvent access	0.438
	Apolar alpha sphere proportion	0.154
	Hydrophobicity score	12.929
	Volume score	3.714
	Polarity score	8.000
	Charge score	0.000
	Proportion of polar atoms	51.852
	Alpha sphere density	3.832
	Cent. of mass - Alpha Sphere max dist	7.323
	Flexibility	0.923
Pocket 53		
	Score	-0.147
	Druggability Score	0.000
	Number of Alpha Spheres	32.000
	Total SASA	125.518
	Polar SASA	84.459
	Apolar SASA	41.059
	Volume	345.878
	Mean local hydrophobic density	2.000
	Mean alpha sphere radius	3.802
	Mean alp. sph. solvent access	0.469
	Apolar alpha sphere proportion	0.094
	Hydrophobicity score	1.182
	Volume score	4.364
	Polarity score	8.000
	Charge score	3.000
	Proportion of polar atoms	54.167
	Alpha sphere density	3.489
	Cent. of mass - Alpha Sphere max dist	7.513
	Flexibility	0.814

Pocket 54

Score	-0.153
Druggability Score	0.000
Number of Alpha Spheres	20.000
Total SASA	96.633
Polar SASA	59.771
Apolar SASA	36.862
Volume	238.236
Mean local hydrophobic density	1.000
Mean alpha sphere radius	3.906
Mean alp. sph. solvent access	0.597
Apolar alpha sphere proportion	0.100
Hydrophobicity score	3.833
Volume score	3.833
Polarity score	5.000
Charge score	1.000
Proportion of polar atoms	58.824
Alpha sphere density	2.530
Cent. of mass - Alpha Sphere max dist	4.823
Flexibility	0.718

Pocket 55

Score	-0.154
Druggability Score	0.006
Number of Alpha Spheres	40.000
Total SASA	138.765
Polar SASA	82.006
Apolar SASA	56.759
Volume	505.517
Mean local hydrophobic density	15.000
Mean alpha sphere radius	4.094
Mean alp. sph. solvent access	0.447
Apolar alpha sphere proportion	0.400
Hydrophobicity score	4.556
Volume score	4.111
Polarity score	7.000
Charge score	-1.000
Proportion of polar atoms	43.333
Alpha sphere density	3.685
Cent. of mass - Alpha Sphere max dist	8.359
Flexibility	0.968

Pocket 56

Score	-0.159
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Druggability Score	0.007
Number of Alpha Spheres	40.000
Total SASA	167.935
Polar SASA	64.079
Apolar SASA	103.856
Volume	496.651
Mean local hydrophobic density	15.143
Mean alpha sphere radius	3.871
Mean alp. sph. solvent access	0.546
Apolar alpha sphere proportion	0.525
Hydrophobicity score	26.900
Volume score	5.200
Polarity score	7.000
Charge score	2.000
Proportion of polar atoms	32.258
Alpha sphere density	4.927
Cent. of mass - Alpha Sphere max dist	9.689
Flexibility	0.860

Pocket 57

Score	-0.173
Druggability Score	0.003
Number of Alpha Spheres	38.000
Total SASA	126.095
Polar SASA	76.583
Apolar SASA	49.513
Volume	348.897
Mean local hydrophobic density	12.000
Mean alpha sphere radius	4.140
Mean alp. sph. solvent access	0.409
Apolar alpha sphere proportion	0.342
Hydrophobicity score	10.556
Volume score	4.222
Polarity score	8.000
Charge score	0.000
Proportion of polar atoms	52.381
Alpha sphere density	3.188
Cent. of mass - Alpha Sphere max dist	9.370
Flexibility	0.843

Pocket 58

Score	-0.179
Druggability Score	0.009
Number of Alpha Spheres	75.000
Total SASA	193.565
Polar SASA	107.269

	Apolar SASA	86.296
	Volume	630.895
	Mean local hydrophobic density	18.000
	Mean alpha sphere radius	4.004
	Mean alp. sph. solvent access	0.491
	Apolar alpha sphere proportion	0.253
	Hydrophobicity score	-0.571
	Volume score	4.143
	Polarity score	10.000
	Charge score	4.000
	Proportion of polar atoms	53.191
	Alpha sphere density	4.782
	Cent. of mass - Alpha Sphere max dist	12.088
	Flexibility	0.895
Pocket 59		
	Score	-0.194
	Druggability Score	0.003
	Number of Alpha Spheres	24.000
	Total SASA	125.629
	Polar SASA	39.887
	Apolar SASA	85.742
	Volume	347.772
	Mean local hydrophobic density	10.000
	Mean alpha sphere radius	4.064
	Mean alp. sph. solvent access	0.586
	Apolar alpha sphere proportion	0.458
	Hydrophobicity score	21.000
	Volume score	4.250
	Polarity score	5.000
	Charge score	1.000
	Proportion of polar atoms	45.000
	Alpha sphere density	3.278
	Cent. of mass - Alpha Sphere max dist	8.997
	Flexibility	0.899
Pocket 60		
	Score	-0.209
	Druggability Score	0.666t
	Number of Alpha Spheres	157.000
	Total SASA	436.409
	Polar SASA	147.786
	Apolar SASA	288.623
	Volume	1667.223
	Mean local hydrophobic density	20.340

	Mean alpha sphere radius	4.062
	Mean alp. sph. solvent access	0.507
	Apolar alpha sphere proportion	0.299
	Hydrophobicity score	27.125
	Volume score	4.229
	Polarity score	29.000
	Charge score	0.000
	Proportion of polar atoms	39.796
	Alpha sphere density	9.556
	Cent. of mass - Alpha Sphere max dist	25.332
	Flexibility	0.844
Pocket 61		
	Score	-0.221
	Druggability Score	0.001
	Number of Alpha Spheres	19.000
	Total SASA	98.818
	Polar SASA	25.153
	Apolar SASA	73.665
	Volume	195.952
	Mean local hydrophobic density	10.000
	Mean alpha sphere radius	3.903
	Mean alp. sph. solvent access	0.542
	Apolar alpha sphere proportion	0.579
	Hydrophobicity score	43.250
	Volume score	5.500
	Polarity score	2.000
	Charge score	1.000
	Proportion of polar atoms	33.333
	Alpha sphere density	1.951
	Cent. of mass - Alpha Sphere max dist	5.180
	Flexibility	0.636
Pocket 62		
	Score	-0.233
	Druggability Score	0.004
	Number of Alpha Spheres	46.000
	Total SASA	181.659
	Polar SASA	91.087
	Apolar SASA	90.572
	Volume	598.479
	Mean local hydrophobic density	14.000
	Mean alpha sphere radius	4.154
	Mean alp. sph. solvent access	0.523
	Apolar alpha sphere proportion	0.326
	Hydrophobicity score	8.643

	Volume score	4.643
	Polarity score	10.000
	Charge score	5.000
	Proportion of polar atoms	52.941
	Alpha sphere density	4.318
	Cent. of mass - Alpha Sphere max dist	12.678
	Flexibility	0.414
Pocket 63		
	Score	-0.297
	Druggability Score	0.001
	Number of Alpha Spheres	233.000
	Total SASA	643.190
	Polar SASA	320.436
	Apolar SASA	322.753
	Volume	2208.325
	Mean local hydrophobic density	27.644
	Mean alpha sphere radius	3.985
	Mean alp. sph. solvent access	0.459
	Apolar alpha sphere proportion	0.386
	Hydrophobicity score	3.833
	Volume score	4.119
	Polarity score	25.000
	Charge score	2.000
	Proportion of polar atoms	41.406
	Alpha sphere density	10.983
	Cent. of mass - Alpha Sphere max dist	26.566
	Flexibility	0.588
Pocket 64		
	Score	-0.328
	Druggability Score	0.018
	Number of Alpha Spheres	197.000
	Total SASA	495.749
	Polar SASA	230.070
	Apolar SASA	265.678
	Volume	1990.677
	Mean local hydrophobic density	28.841
	Mean alpha sphere radius	3.927
	Mean alp. sph. solvent access	0.465
	Apolar alpha sphere proportion	0.350
	Hydrophobicity score	12.600
	Volume score	4.800
	Polarity score	23.000
	Charge score	5.000

Proportion of polar atoms	39.806
Alpha sphere density	8.845
Cent. of mass - Alpha Sphere max dist	20.290
Flexibility	0.879
