#Ligand	TotalEnergy	VDW	AverConPair
1xak-1-HexacosanolStructure2D_-0.pdb	-515.259	-515.259	141.481
1xak-2-Benzoxazolinone 2737-0.pdb	-485.327	-485.327	25.8
1xak-3-Carboxy-pentaric acid-0.pdb	220.642	220.642	178.462
1xak-5ursane 33-0.pdb	-573.146	-573.146	14.2
1xak-9-cis-Antheraxanthin 2742-0.pdb	914.142	914.142	113.256
1xak-4584RA-XIII-0.pdb	201.061	201.061	123.429
1xak-6948crotonate-0.pdb	-367.977	-367.977	391.667
1xak-abyssinica_CID_3083701-0.pdb	539.462	539.462	237.879
1xak-Acacia_CID_5320844-0.pdb	-693.664	-693.664	137.879
1xak-acetovanilloneStructure2D_CID_2214-0.pdb	-494.316	-494.316	250.833
1xak-acteosideStructure2D_CID_5281800_-0.pdb	318.918	318.918	196.591
1xak-AdenosineStructure2D_CID_60961-0.pdb	-592.854	-592.854	184.737
1xak-Africanal_CID_342943-0.pdb	243.629	243.629	253.704
1xak-Agarin_CID_4266-0.pdb	-425.086	-425.086	28
1xak-Aloe-emodinStructure2D_CID_10207-0.pdb	189.113	189.113	24.2
1xak-alpha-L-Rhamnose_CID_439710-0.pdb	-446.613	-446.613	24
1xak-alpha-TocopherolStructure2D_CID_14985-0.pdb	275.423	275.423	14.129
1xak-alpha-TurmeroneStructure2D_CID_14632996-0.pdb	-458.915	-458.915	20.125
1xak-Ammonium glycyrrhizate_CID_62074-0.pdb	1038.94	1038.94	262.542
1xak-Anemone blue anthocyanin 1_CID_11979368-0.pdb	766.296	766.296	155.934
1xak-anilineStructure2D_CID_6115-0.pdb	-382.959	-382.959	33
1xak-AnnonaStructure2D_CID_5459105-0.pdb	496.246	496.246	194.545
1xak-AntitrypsinStructure2D_CID_165580(1)-0.pdb	-568.106	-568.106	129.048
1xak-Arachidonic AcidStructure2D_CID_444899-0.pdb	-607.407	-607.407	162.273
1xak-Aristolochiac acid C_CID_165274-0.pdb	119.629	119.629	15.25
1xak-Aristolochic acid_CID_2236-0.pdb	-445.479	-445.479	13.64
1xak-Asparagusate_CID_16070001-0.pdb	-397.462	-397.462	28.125
1xak-aspartic acid 101-0.pdb	649.365	649.365	212.222
1xak-AstragalinStructure2D_CID_5282102-0.pdb	100.05	100.05	162.813
1xak-atraric acid 102-0.pdb	-534.367	-534.367	214.286
1xak-AtrazineStructure2D_CID_2256-0.pdb	-538.712	-538.712	21.5
1xak-avicine103-0.pdb	173.506	173.506	17.28
1xak-azadirachtinStructure2D_CID_5281303-0.pdb	314.876	314.876	193.725
1xak-Baicalein-7-methyl ether 3673-0.pdb	-647.723	-647.723	181.429
1xak-balanitin 3 106-0.pdb	696.002	696.002	720.968
1xak-balanitin 4 107-0.pdb	764.265	764.265	672.603
1xak-balanitin 5 108-0.pdb	-724.282	-724.282	834.722
1xak-balanitin 7 110-0.pdb	-762.913	-762.913	835.211
1xak-baueronol 111-0.pdb	-573.615	-573.615	15.129
1xak-b-Chlorogenin 7651-0.pdb	-603.049	-603.049	136.129
1xak-behenic acid 112-0.pdb	-549.741	-549.741	152.083
1xak-benzo[c]phenanthridine113-0.pdb	-537.074	-537.074	229.286
1xak-Benzyl alcohol 2614-0.pdb	-433.616	-433.616	28.875
1xak-benzyl isothiocyanate (BITC) 114-0.pdb	210.926	210.926	16.8
1xak-benzylic amines 115-0.pdb	280.504	280.504	242.917
1xak-Berberine alkaloids 116-0.pdb	570.879	570.879	17.56
1xak-Bergapten 2716-0.pdb	-559.986	-559.986	22.25
1xak-beta,beta-Caroten-2-ol 2832-0.pdb	138.504	138.504	156.098
1xak-beta-Bisabolol 3343-0.pdb	-594.561	-594.561	25.625
1xak-beta-Cubebene 3151-0.pdb	-473.974	-473.974	21.2
1xak-beta-D-Galactopyranose 3590-0.pdb	-462.436	-462.436	22.5
1xak-beta-D-Glucopyranuronic acid 2555-0.pdb	221.972	221.972	204.615
1xak-Betaine 117-0.pdb	-395.206	-395.206	31.125
1xak-beta-iononeStructure2D_CID_638014-0.pdb	-198.402	-198.402	143.571
1xak-beta-L-Fructofuranosyl beta-L-glucopyranoside 2543-0.pdb	143.955	143.955	198.261
1xak-beta-L-Fructofuranosyl beta-L-glucopyranoside-0.pdb	-544.572	-544.572	143.913
1xak-betulin 118-0.pdb	156.212	156.212	154.375
1xak-Betulinic acidStructure2D_CID_64971-0.pdb	-593.081	-593.081	135.152
1xak-b-Eudesmol 3142-0.pdb	-500.951	-500.951	21.75
1xak-biochanin A 120-0.pdb	973.772	973.772	203.333
1xak-Biotin 2443-0.pdb	-527.776	-527.776	20.25
1xak-bis-(5-formylfurfuryl) ether 121-0.pdb	-607.503	-607.503	229.412
1xak-Bisabola-3,10-diene-2-one 3403-0.pdb	-496.823	-496.823	19.25
1xak-Bisacumol 3283-0.pdb	-522.462	-522.462	195.625
1xak-bisindole alkaloids 122-0.pdb	333.578	333.578	163.913
1xak-bisjatrorrhizine 123-0.pdb	117.166	117.166	10.18
1xak-Blumenol A 3174-0.pdb	-523.396	-523.396	191.875
1xak-b-Ocimene 3386-0.pdb	-474.659	-474.659	24.9
1xak-Brassicasterol 3178-0.pdb	242.816	242.816	197.586

1xak-brassinolides 124-0.pdb	205.409	205.409		118.235
1xak-Butanoic acidConformer3D_CID_549297-0.pdb	-467.194	-467.194		235.833
1xak-ButenylamineConformer3D_CID_12415240-0.pdb	-335.784	-335.784	35.8	
1xak-Butyric AcidStructure2D_CID_264-0.pdb	-124.721	-124.721		206.667
1xak-cadinene 127-0.pdb	161.904	161.904		184.667
1xak-caffeic acidStructure2D_CID_689043-0.pdb	-566.001	-566.001		301.538
1xak-Caffeine_Conformer3D_CID_2519-0.pdb	-548.426	-548.426		223.571
1xak-CannabidiolStructure2D_CID_644019-0.pdb	189.867	189.867		195.217
1xak-CAPENSIN_CID_644959-0.pdb	-584.085	-584.085	19.35	
1xak-Catechin gallateConformer3D_CID_5276454-0.pdb	194.116	194.116		21.625
1xak-celecoxibStructure2D_CID_2662-0.pdb	-649.317	-649.317		157.692
1xak-chelerythrineStructure2D_CID_2703-0.pdb	-655.144	-655.144		165.385
1xak-Chlorogenic AcidStructure2D_CID_1794427-0.pdb	-689.379	-689.379	16.4	
1xak-chrysinStructure2D_CID_5281607-0.pdb	-658.065	-658.065		207.895
1xak-CiglitazoneStructure2D_CID_2750-0.pdb	651.517	651.517		137.391
1xak-Cinchonidine_CID_2757-0.pdb	-686.143	-686.143	20.5	
1xak-cinnamic acidStructure2D_CID_444539-0.pdb	-485.478	-485.478		236.364
1xak-CitrininStructure2D_CID_54680783-0.pdb	41.981	41.981		149.444
1xak-Clematin_CID_42608007-0.pdb	115.075	115.075		129.767
1xak-cresolStructure2D_CID_2879 (2)-0.pdb	-42.135	-42.135		27.875
1xak-CresolStructure2D_CID_2879-0.pdb	-41.542	-41.542		27.875
1xak-DaidzeinStructure2D_CID_5281708-0.pdb	-701.467	-701.467		185.789
1xak-Dalbergia_CID_5481240-0.pdb	-134.199	-134.199		146.667
1xak-Dalbergin_CID_442768-0.pdb	-67.719	-67.719	19.05	
1xak-demethoxycurcuminStructure2D_CID_5469424-0.pdb	668.607	668.607	14.96	
1xak-DiosgeninStructure2D_CID_99474-0.pdb	-313.904	-313.904	15.2	
1xak-ecdysterone-0.pdb	163.048	163.048		177.353
1xak-echinacin-0.pdb	618.283	618.283		721.429
1xak-echinacoside-0.pdb	355.874	355.874		165.818
1xak-ehtyl-12-oxododecanoate-0.pdb	-63.751	-63.751		24
1xak-Eicosapentanoic acid-0.pdb	183.783	183.783		167.273
1xak-Eicosen-1-ol-0.pdb	-571.997	-571.997		15.381
1xak-ekeberginine_CID_10379640-0.pdb	-246.614	-246.614		149.091
1xak-Elaidic Acid-0.pdb	-579.373	-579.373	19.8	
1xak-Eldecalcitol-0.pdb	305.259	305.259		220.571
1xak-Elemicin-0.pdb	-527.084	-527.084		210.667
1xak-elemol-0.pdb	531.673	531.673		228.125
1xak-Ellagic acid acetyl-arabinoside-0.pdb	838.424	838.424	13.5	
1xak-Ellagic acid acetyl-xyloside-0.pdb	-753.878	-753.878		15
1xak-Ellagic AcidStructure2D_CID_5281855-0.pdb	-653.774	-653.774		167.273
1xak-ellagicacid-0.pdb	-622.001	-622.001		173.636
1xak-embelin-0.pdb	-686.852	-686.852		22.381
1xak-E-Mix D-0.pdb	104.836	104.836		12.931
1xak-Emodin-0.pdb	-627.955	-627.955	19.1	
1xak-EmodinStructure2D_CID_3220-0.pdb	-639.791	-639.791	18.6	
1xak-energy-0.pdb	-441.375	-441.375		244.167
1xak-epi-Cubenol-0.pdb	-113.211	-113.211		171.875
1xak-epigallocatechin gallateStructure2D_CID_65064-0.pdb	189.787	189.787		156.061
1xak-epimaslinic acid-0.pdb	-594.067	-594.067		132.941
1xak-epitaxifolin-0.pdb	-630.919	-630.919		168.636
1xak-epitetraphyllin B-0.pdb	-535.015	-535.015	19.1	
1xak-Epoxyazadiradione-0.pdb	97.677	97.677		158.824
1xak-epsilon-phytol-0.pdb	-54.091	-54.091		160.952
1xak-epsilon-Viniferin-0.pdb	269.121	269.121		137.059
1xak-ergocalciferol-0.pdb	-616.061	-616.061		153.103
1xak-Ergosta-0.pdb	-651.931	-651.931		15.069
1xak-Eriodictyol-7-O-beta-D-glucopyranoside-0.pdb	551.697	551.697		934.375
1xak-EriodictyolStructure2D_CID_440735-0.pdb	-609.552	-609.552		184.286
1xak-Eruboside B-0.pdb	299.208	299.208		505.333
1xak-erucinStructure2D_CID_78160-0.pdb	-389.963	-389.963		254.444
1xak-erycristagallin-0.pdb	-158.929	-158.929		105.862
1xak-erysodine-0.pdb	-622.269	-622.269		169.545
1xak-erysotrine-0.pdb	-611.382	-611.382		167.826
1xak-erysovine-0.pdb	-624.957	-624.957		182.727
1xak-erythritol-0.pdb	-416.518	-416.518	26.5	
1xak-erythrono-1-4-lactone-0.pdb	-396.392	-396.392		28
1xak-erythro-pentaric acid 2510-0.pdb	-178.271	-178.271		123.846
1xak-esculeoside c-0.pdb	888.728	888.728		138.864
1xak-esculetinStructure2D_CID_5281416-0.pdb	-521.382	-521.382		261.538
1xak-esculin-0.pdb	624.437	624.437	15.88	

1xak-estragole-0.pdb	-487.548	-487.548	242.727
1xak-Estriol-0.pdb	235.194	235.194	252.857
1xak-Estrone-0.pdb	-610.718	-610.718	19.15
1xak-ethanal-0.pdb	-24.753	-24.753	483.333
1xak-Ethyl 2-propene sulfinate-0.pdb	192.565	192.565	263.333
1xak-ethyl methyl disulfide-0.pdb	-30.958	-30.958	34.2
1xak-ethylamine-0.pdb	-252.557	-252.557	456.667
1xak-ethylisopropyl sulfide-0.pdb	-368.023	-368.023	223.636
1xak-ethyllaurate-0.pdb	-201.352	-201.352	11.5
1xak-ethylparaben-0.pdb	-499.779	-499.779	231.667
1xak-ethylpropionate-0.pdb	-390.167	-390.167	288.571
1xak-eucalyptol-0.pdb	-425.539	-425.539	232.727
1xak-Eudesobovatol A-0.pdb	632.713	632.713	293.514
1xak-EugenolStructure2D_CID_3314-0.pdb	-488.687	-488.687	240.833
1xak-euglobal ia1-0.pdb	892.296	892.296	13.25
1xak-Euglobal Ib-0.pdb	-612.392	-612.392	144.643
1xak-Euglobal Ic-0.pdb	-671.833	-671.833	151.786
1xak-euglobal iii-0.pdb	-591.196	-591.196	132.727
1xak-euglobal Iia-0.pdb	-667.041	-667.041	156.786
1xak-euglobal v-0.pdb	156.684	156.684	176.061
1xak-Euglobal VII-0.pdb	-698.738	-698.738	143.333
1xak-euglobal-iii-0.pdb	-689.861	-689.861	158.788
1xak-eupafolin-7-glucoside-0.pdb	-70.467	-70.467	135.294
1xak-euphol-0.pdb	-599.983	-599.983	133.226
1xak-exo-2-Bornanol-0.pdb	-428.573	-428.573	218.182
1xak-exo-borneol-0.pdb	-42.862	-42.862	223.636
1xak-ferulic acidStructure2D_CID_445858-0.pdb	188.289	188.289	173.571
1xak-formononetinStructure2D_CID_5280378-0.pdb	42.222	42.222	19.15
1xak-FructoseStructure2D_CID_2723872-0.pdb	-403.541	-403.541	199.167
1xak-Fumaric acidStructure2D_CID_444972-0.pdb	-433.168	-433.168	35.25
1xak-galactinol 4177-0.pdb	-836.178	-836.178	13
1xak-galacturonic acid 236-0.pdb	-48.612	-48.612	223.077
1xak-galanginStructure2D_CID_5281511-0.pdb	265.833	265.833	21
1xak-Gallic acid_Conformer3D_CID_370-0.pdb	-487.358	-487.358	250.833
1xak-geduninStructure2D_CID_12004512-0.pdb	983.332	983.332	140.857
1xak-Genistein_Conformer3D_CID_5280961-0.pdb	-623.726	-623.726	19.85
1xak-geraniolStructure2D_CID_637566-0.pdb	-509.282	-509.282	298.182
1xak-g-Glutamylcysteine 7654-0.pdb	207.653	207.653	156.875
1xak-Grandifloric acid_CID_433554-0.pdb	174.762	174.762	183.913
1xak-Grandiflorone_CID_3014646-0.pdb	-600.256	-600.256	175.652
1xak-gum arabic-0.pdb	919.101	919.101	20.561
1xak-H14 saponins-0.pdb	-436.274	-436.274	263.333
1xak-hayatidine-0.pdb	241.462	241.462	205.111
1xak-heliotrine-0.pdb	-649.734	-649.734	194.545
1xak-Helioxanthin-0.pdb	422.397	422.397	139.231
1xak-Heptacosane-0.pdb	-460.452	-460.452	142.222
1xak-heptanol-0.pdb	-385.706	-385.706	31
1xak-Heptanonitril-0.pdb	-401.999	-401.999	27.625
1xak-Hesperetin-0.pdb	358.416	358.416	254.091
1xak-hesperetin-5-glucoside-0.pdb	171.297	171.297	13.303
1xak-hesperetinStructure2D_CID_72281-0.pdb	-62.784	-62.784	171.818
1xak-Hesperidin-0.pdb	449.139	449.139	164.186
1xak-HesperidinStructure2D_CID_10621-0.pdb	-685.723	-685.723	13
1xak-hespertitinic acid-0.pdb	-578.118	-578.118	228.571
1xak-HexacosanolStructure2D_CID_68171 (2)-0.pdb	-453.643	-453.643	142.593
1xak-HexacosanolStructure2D_CID_68171-0.pdb	-448.077	-448.077	142.222
1xak-HexahydroxyflavyliumStructure2D_CID_128853-0.pdb	-708.105	-708.105	190.909
1xak-Hexitol-0.pdb	-460.883	-460.883	211.667
1xak-Hexopyranuronate-0.pdb	659.903	659.903	236.923
1xak-Hibiscetin-0.pdb	250.532	250.532	229.143
1xak-hibiscic-0.pdb	-496.654	-496.654	209.231
1xak-hibiscin-0.pdb	326.955	326.955	214.286
1xak-Hirsutanonol_CID_9928190-0.pdb	-584.897	-584.897	14.6
1xak-Hirsutatin A_CID_11707361-0.pdb	120.322	120.322	10.625
1xak-hirsutidine-0.pdb	-721.742	-721.742	17.44
1xak-Hopenone I-0.pdb	113.944	113.944	243.548
1xak-hopeyhopin-0.pdb	-60.564	-60.564	21.05
1xak-hordenine-0.pdb	-515.827	-515.827	230.833
1xak-Huangqiyenin A-0.pdb	269.089	269.089	161.778
1xak-Humulene-0.pdb	-462.883	-462.883	204.667

1xak-hydrolyzable tannins-0.pdb	999.426	999.426		274.667
1xak-hydroxycinnamic derivatives-0.pdb	-544.547	-544.547		236.667
1xak-hydroxyflavone-0.pdb	210.546	210.546		306.667
1xak-Hymenolin-0.pdb	-538.821	-538.821		185.263
1xak-hypaconitine-0.pdb	778.699	778.699		284.091
1xak-hyperin-0.pdb	-729.166	-729.166		14
1xak-juglone 2677-0.pdb	-538.393	-538.393		243.077
1xak-Kaempferide-0.pdb	299.549	299.549		290.909
1xak-Kaempferol-3-O-alpha-L-arabinoside-0.pdb	362.008	362.008		177.667
1xak-kaempferol-7-O-glucoside-0.pdb	-955.888	-955.888		147.188
1xak-kaempferolStructure2D_CID_5280863-0.pdb	-689.035	-689.035		19.619
1xak-Keracyanin 5089-0.pdb	605.888	605.888		194.524
1xak-khatamines (-)-cathinone-0.pdb	-457.468	-457.468		252.727
1xak-kigelinol-0.pdb	124.627	124.627		176.957
1xak-kolanin-0.pdb	-275.951	-275.951		36
1xak-kryptogenin-0.pdb	1020.45	1020.45		343.871
1xak-Kumatakenin-0.pdb	-685.391	-685.391		182.174
1xak-L-(+)-Cysteine-0.pdb	-378.011	-378.011		291.429
1xak-lanciaquinone-0.pdb	204.683	204.683		852.941
1xak-leucopelargonidin-0.pdb	-632.214	-632.214		182.857
1xak-leucosceptoside a-0.pdb	375.189	375.189		161.778
1xak-L-gamma-Glutamyl-S-allylthio-L-cysteine-0.pdb	-560.612	-560.612	18.85	
1xak-lilagenin-0.pdb	114.173	114.173		154.839
1xak-linaloolStructure2D_CID_6549-0.pdb	-480.396	-480.396		29
1xak-Linifolin A_CID_442272-0.pdb	169.083	169.083		222.727
1xak-Linoleic AcidStructure2D_CID_5280450-0.pdb	-691.642	-691.642	20.55	
1xak-l-Menthol_CID_16666-0.pdb	-445.343	-445.343		239.091
1xak-L-METHIONINE SULFONE-0.pdb	-427.381	-427.381		259.091
1xak-lotoideside a-0.pdb	978.775	978.775		203.793
1xak-lotoideside e-0.pdb	-672.568	-672.568		129.038
1xak-L-Ribopyranose-0.pdb	-456.982	-456.982	25.9	
1xak-LuteolinStructure2D_CID_5280445-0.pdb	672.038	672.038		204.286
1xak-malvidinStructure2D_CID_159287-0.pdb	230.921	230.921		150.833
1xak-Mangiferin_Conformer3D_CID_5281647-0.pdb	102.381	102.381		973.333
1xak-MannitolStructure2D_CID_6251-0.pdb	-424.254	-424.254		224.167
1xak-MelatoninStructure2D_CID_896-0.pdb	444.957	444.957		214.118
1xak-MethoxsalenStructure2D_CID_4114-0.pdb	-600.347	-600.347		22.625
1xak-methylparabenStructure2D_CID_7456-0.pdb	-461.169	-461.169		228.182
1xak-Mevalonic AcidStructure2D_CID_439230-0.pdb	-42.172	-42.172	23.5	
1xak-MolluginStructure2D_CID_124219-0.pdb	112.479	112.479		196.667
1xak-MonocrotalineStructure2D_CID_9415-0.pdb	-580.142	-580.142		161.739
1xak-morinStructure2D_CID_5281670-0.pdb	-639.089	-639.089		187.273
1xak-myricetinStructure2D_CID_5281672-0.pdb	494.851	494.851		166.957
1xak-naringeninStructure2D_CID_932-0.pdb	-647.413	-647.413	20.5	
1xak-NiacinamideStructure2D_CID_936-0.pdb	-435.171	-435.171		291.111
1xak-NiacinStructure2D_CID_938-0.pdb	-448.059	-448.059		266.667
1xak-nicotinic_acid_Conformer3D_CID_938-0.pdb	-449.423	-449.423		273.333
1xak-Nomilin-0.pdb	936.156	936.156		307.027
1xak-octanoic acidStructure2D_CID_379-0.pdb	-425.444	-425.444	28.1	
1xak-Officinalic acid_CID_10577334-0.pdb	626.617	626.617		236.944
1xak-Oleic AcidStructure2D_CID_445639-0.pdb	-607.217	-607.217	21.25	
1xak-oleuropeinStructure2D_CID_5281544-0.pdb	305.561	305.561		192.105
1xak-ostholStructure2D_CID_10228-0.pdb	-619.146	-619.146		198.889
1xak-Oxalic AcidStructure2D_CID_971-0.pdb	-343.434	-343.434	32.5	
1xak-Palmitic AcidStructure2D_CID_985-0.pdb	197.833	197.833		190.556
1xak-PatulinStructure2D_CID_4696-0.pdb	-522.775	-522.775		254.545
1xak-pelargonic acidStructure2D_CID_8158-0.pdb	-48.592	-48.592		280.909
1xak-Periplocin_CID_14463159-0.pdb	351.842	351.842		160.816
1xak-phenethyl isothiocyanateStructure2D_CID_16741-0.pdb	-509.001	-509.001		260.909
1xak-Phenprobamate_CID_4770-0.pdb	-481.924	-481.924		182.308
1xak-PhlorhizinStructure2D_CID_3503(1)-0.pdb	315.094	315.094		203.158
1xak-Phytic AcidStructure2D_CID_890-0.pdb	-646.043	-646.043		132.778
1xak-picropodophyllinStructure2D_CID_72435-0.pdb	-616.296	-616.296		142.333
1xak-piperineStructure2D_CID_638024-0.pdb	-63.328	-63.328		183.333
1xak-Plantagoside_CID_174157-0.pdb	117.447	117.447		135.758
1xak-Platycodin D_CID_162859-0.pdb	581.942	581.942		153.882
1xak-plumbaginStructure2D_CID_10205-0.pdb	-551.709	-551.709		232.857
1xak-PolygalaConformer3D_CID_1689-0.pdb	299.273	299.273		18
1xak-Pregnenolone 2544-0.pdb	-613.658	-613.658		183.043
1xak-protocatechualdehydeStructure2D_CID_8768-0.pdb	-488.245	-488.245	30.3	

1xak-PrunusConformer3D_CID_353060-0.pdb	257.82	257.82	19.7	
1xak-Psammaplysene A_Structure2D_CID_11434210-0.pdb	-78.26	-78.26		137.838
1xak-pterostilbeneStructure2D_CID_5281727-0.pdb	-650.194	-650.194		228.421
1xak-Pyruvic AcidStructure2D_CID_1060-0.pdb	-342.375	-342.375		326.667
1xak-Raffinose-0.pdb	848.683	848.683		305.882
1xak-reserpiline-0.pdb	-721.062	-721.062		174.667
1xak-ResinConformer3D_CID_11290200-0.pdb	-759.523	-759.523		185.833
1xak-resveratrol e-dehydrodimer-0.pdb	176.808	176.808		141.176
1xak-Rhamnetin-0.pdb	-702.021	-702.021		186.522
1xak-Rhamnus Conformer3D_CID_437987-0.pdb	253.114	253.114	13.8	
1xak-Rhoifolin-0.pdb	-876.476	-876.476		148.049
1xak-RiboflavinStructure2D_CID_493570-0.pdb	-747.981	-747.981		162.963
1xak-riboprina-0.pdb	-683.167	-683.167		178.333
1xak-ricinoleic acidStructure2D_CID_643684-0.pdb	-615.813	-615.813		179.524
1xak-riddelliineStructure2D_CID_5281744-0.pdb	-268.996	-268.996	10.28	
1xak-rohituka 3-0.pdb	566.359	566.359		18
1xak-RosaStructure2D_CID_69438-0.pdb	-654.534	-654.534		169.714
1xak-Rosefuran-0.pdb	-481.883	-481.883		247.273
1xak-rottlerin-0.pdb	285.174	285.174		109.737
1xak-Rotundone-0.pdb	-517.185	-517.185		20
1xak-Rubian-0.pdb	664.691	664.691		101.316
1xak-Rubiarbonol B-0.pdb	-683.003	-683.003		13.303
1xak-rubiatrol-0.pdb	-64.762	-64.762		149.697
1xak-Rubicoumaric acid-0.pdb	310.925	310.925		124.444
1xak-rubimaillin-0.pdb	-63.233	-63.233		189.524
1xak-rubiprasin b-0.pdb	-57.483	-57.483		140.833
1xak-Rubixanthin-0.pdb	-761.523	-761.523		13.122
1xak-Rubrobrassicin-0.pdb	-639.699	-639.699		445.283
1xak-Rubrofusarin-6-O-beta-gentiobioside-0.pdb	-833.763	-833.763		129.048
1xak-S-allylcysteineStructure2D_CID_9793905-0.pdb	-444.353	-444.353	27.9	
1xak-salsolinolStructure2D_CID_91588-0.pdb	400.201	400.201		184.615
1xak-sanguinarineStructure2D_CID_5154-0.pdb	-646.288	-646.288	12.72	
1xak-scoparoneStructure2D_CID_8417-0.pdb	-54.678	-54.678		225.333
1xak-Scutellarin_CID_185617-0.pdb	305.748	305.748		150.303
1xak-secoisolariciresinol diglucosideStructure2D_-0.pdb	352.988	352.988		145.417
1xak-SelenomethionineStructure2D_CID_15103-0.pdb	-419.318	-419.318		251.111
1xak-shogaolStructure2D_CID_5281794-0.pdb	128.485	128.485	23.9	
1xak-sinapinic acidStructure2D_CID_637775-0.pdb	-580.111	-580.111		21.125
1xak-SlaframineStructure2D_CID_88363-0.pdb	-544.438	-544.438		230.714
1xak-stearic acidStructure2D_CID_5281-0.pdb	194.284	194.284	21.75	
1xak-Succinic AcidStructure2D_CID_1110-0.pdb	-407.726	-407.726		29
1xak-sulforafanStructure2D_CID_5350-0.pdb	-0.285696	-0.285696	24.4	
1xak-TaurineStructure2D_CID_1123-0.pdb	-366.206	-366.206		282.857
1xak-terpinoleneStructure2D_CID_11463-0.pdb	-424.815	-424.815	23.3	
1xak-Tetrandrine-0.pdb	19.083	19.083		895.652
1xak-Thiamine 2459-0.pdb	-561.488	-561.488		195.556
1xak-UbiquinoneStructure2D_CID_5281915-0.pdb	635.728	635.728		157.143
1xak-ursolic acidStructure2D_CID_64945-0.pdb	-586.416	-586.416		132.727
1xak-vanillinStructure2D_CID_1183-0.pdb	-50.642	-50.642		28
1xak-Vitamin AStructure2D_CID_445354-0.pdb	158.806	158.806		132.381
1xak-Vitamin DStructure2D_CID_5280795-0.pdb	114.779	114.779	19.25	
1xak-volkenin-0.pdb	-54.88	-54.88	18.55	
1xak-wighteone 6599-0.pdb	204.034	204.034	11.04	
1xak-wighteone-0.pdb	-714.656	-714.656	18.96	
1xak-withanoside ii 6606-0.pdb	158.629	158.629		969.643
1xak-Wyerone-0.pdb	-588.092	-588.092		203.158
1xak-xanthorhamnin 556-0.pdb	982.722	982.722		197.593
1xak-xanthydrol 3319-0.pdb	-574.374	-574.374	22.6	
1xak-xapentacyclo (2)-0.pdb	414.032	414.032		152.687
1xak-xapentacyclo-0.pdb	-874.098	-874.098		991.045
1xak-yamogenin 558-0.pdb	-744.906	-744.906		175.667
1xak-yamogenin palmitate 6623-0.pdb	138.194	138.194		122.766
1xak-yrosine 560-0.pdb	-720.253	-720.253	17.7	
1xak-Zeatin 2985-0.pdb	-660.714	-660.714		238.125
1xak-Zeaxanthin 2759-0.pdb	-26.193	-26.193	6.5	
1xak-Zedoarondiol 3209-0.pdb	-501.301	-501.301		186.667
1xak-zerumboneStructure2D_CID_5470187-0.pdb	-516.596	-516.596	21.25	
1xak-zeta-carotene 2968-0.pdb	132.639	132.639	14.15	
1xak-Zidovudine 561-0.pdb	-615.566	-615.566		185.263
1xak-zingerone 3821-0.pdb	-588.174	-588.174		288.571

1xak-Zingiberene_CID_92776-0.pdb	-594.678	-594.678		282.667
1xak-Roccustyrna-0.pdb	-842.556	-628.451		153.714
1xak-1xak-Roccustyrna_fr1-0-0.pdb	473.938	473.938		143.623
1xak-1xak-Roccustyrna_fr1-1-0.pdb	-673.178	-673.178		837.681
1xak-1xak-Roccustyrna_fr2-0-0.pdb	-628.841	-628.841		141.212
1xak-1xak-Roccustyrna_fr2-1-0.pdb	-752.781	-752.781		148.485
1xak-1xak-Roccustyrna_fr3-0-0.pdb	49.582	49.582		145.897
1xak-1xak-Roccustyrna_fr3-1-0.pdb	-690.406	-690.406		133.846
1xak-1xak-Roccustyrna_fr4-0-0.pdb	-716.283	-716.283		145.833
1xak-1xak-Roccustyrna_fr4-1-0.pdb	-706.647	-706.647		142.778
1xak-1xak-Roccustyrna_fr5-0-0.pdb	248.088	248.088		130.392
1xak-1xak-Roccustyrna_fr5-1-0.pdb	-541.644	-541.644		128.824
1xak-1xak-Roccustyrna_fr6-0-0.pdb	-762.121	-762.121		148.684
1xak-1xak-Roccustyrna_fr6-1-0.pdb	-721.924	-721.924		135.263
1xak-1xak-Roccustyrna_fr7-0-0.pdb	-671.428	-671.428		139.429
1xak-1xak-Roccustyrna_fr7-1-0.pdb	-717.514	-717.514		156.571
1xak-1xak-Roccustyrna_gs1-0-0.pdb	128.984	128.984		144.348
1xak-1xak-Roccustyrna_gs1-1-0.pdb	-76.201	-76.201		12.913
1xak-1xak-Roccustyrna_gs2-0-0.pdb	-655.845	-655.845		206.316
1xak-1xak-Roccustyrna_gs2-1-0.pdb	-603.972	-603.972		197.368
1xak-1xak-Roccustyrna_gs3-0-0.pdb	394.05	394.05		186.383
1xak-1xak-Roccustyrna_gs3-1-0.pdb	-777.214	-777.214		129.149
1xak-1xak-Roccustyrna_gs4-0-0.pdb	-235.976	-235.976		686.275
1xak-1xak-Roccustyrna_gs4-1-0.pdb	-775.205	-775.205		152.157
1xak-1xak-Roccustyrna_gs5-0-0.pdb	183.447	183.447		740.625
1xak-1xak-Roccustyrna_gs5-1-0.pdb	-831.464	-831.464		105.313
1xak-1xak-Roccustyrna_gs6-0-0.pdb	-587.294	-587.294	18.65	
1xak-1xak-Roccustyrna_gs6-1-0.pdb	-586.819	-586.819	18.8	
1xak-1xak-Roccustyrna_gs8-0-0.pdb	312.399	312.399	12.02	
1xak-1xak-Roccustyrna_gs8-1-0.pdb	-105.38	-105.38	15.66	
1xak-2g9t-Roccustyrna_fr1-0-0.pdb	334.614	334.614		119.855
1xak-2g9t-Roccustyrna-0-0.pdb	-717.828	-717.828		148.286
1xak-2ghv-Roccustyrna_fr1-0-0.pdb	61.313	61.313		695.652
1xak-2ghv-Roccustyrna_fr1-1-0.pdb	-893.183	-893.183		947.826
1xak-2ghv-Roccustyrna_fr2-0-0.pdb	-73.589	-73.589		160.303
1xak-2ghv-Roccustyrna_fr2-1-0.pdb	-756.836	-756.836		148.182
1xak-2ghv-Roccustyrna_fr3-0-0.pdb	68.636	68.636		121.795
1xak-2ghv-Roccustyrna_fr3-1-0.pdb	-728.905	-728.905		132.821
1xak-2ghv-Roccustyrna_fr4-0-0.pdb	-716.698	-716.698		145.278
1xak-2ghv-Roccustyrna_fr4-1-0.pdb	-726.485	-726.485		156.667
1xak-2ghv-Roccustyrna_fr5-0-0.pdb	304.145	304.145		149.804
1xak-2ghv-Roccustyrna_fr5-1-0.pdb	-842.276	-842.276		141.765
1xak-2ghv-Roccustyrna_fr6-0-0.pdb	-736.164	-736.164		138.421
1xak-2ghv-Roccustyrna_fr6-1-0.pdb	-776.917	-776.917		132.632
1xak-2ghv-Roccustyrna_fr7-0-0.pdb	-67.081	-67.081		134.571
1xak-2ghv-Roccustyrna_fr7-1-0.pdb	-598.901	-598.901		132.571
1xak-2ghv-Roccustyrna-0-0.pdb	-847.452	-729.162		144.286
1xak-6m2q-Roccustyrna_fr1-0-0.pdb	824.646	824.646		102.464
1xak-6m2q-Roccustyrna_fr2-0-0.pdb	-63.757	-63.757		132.424
1xak-6m2q-Roccustyrna_fr3-0-0.pdb	830.495	830.495		784.615
1xak-6m2q-Roccustyrna_fr4-0-0.pdb	-692.211	-692.211		135.278
1xak-6m2q-Roccustyrna_fr5-0-0.pdb	332.266	332.266		74.902
1xak-6m2q-Roccustyrna_fr6-0-0.pdb	-762.025	-762.025		148.947
1xak-6m2q-Roccustyrna_fr7-0-0.pdb	-717.556	-717.556		156.571
1xak-6m2q-Roccustyrna_gs1-0-0.pdb	319.542	319.542		182.391
1xak-6m2q-Roccustyrna_gs2-0-0.pdb	-655.824	-655.824		206.316
1xak-6m2q-Roccustyrna_gs3-0-0.pdb	582.636	582.636		23.234
1xak-6m2q-Roccustyrna_gs4-0-0.pdb	465.923	465.923		668.627
1xak-6m2q-Roccustyrna_gs5-0-0.pdb	725.764	725.764		570.313
1xak-6m2q-Roccustyrna_gs6-0-0.pdb	-587.777	-587.777	18.55	
1xak-6m2q-Roccustyrna_gs8-0-0.pdb	549.826	549.826	15.84	
1xak-6w9c-Roccustyrna-0-0.pdb	-758.537	-758.537		140.571
1xak-6xs6 (1)-Roccustyrna_fr1-0-0.pdb	239.687	239.687		572.464
1xak-6xs6-Roccustyrna-0-0.pdb	-733.162	-733.162		132.857
1xak-6zgg-Roccustyrna_fr1-0-0.pdb	742.847	742.847		54.058
1xak-7bv2-Roccustyrna_fr1-0-0.pdb	-69.915	-69.915		950.725
1xak-7bv2-Roccustyrna_fr1-1-0.pdb	-918.719	-918.719		969.565
1xak-7bv2-Roccustyrna_fr2-0-0.pdb	-680.734	-680.734		157.576
1xak-7bv2-Roccustyrna_fr2-1-0.pdb	-646.248	-646.248		132.727
1xak-7bv2-Roccustyrna_fr3-0-0.pdb	904.226	904.226		122.821

1xak-7bv2-Roccustyrna_fr3-1-0.pdb	-727.975	-727.975		132.821
1xak-7bv2-Roccustyrna_fr4-0-0.pdb	-744.451	-744.451		138.611
1xak-7bv2-Roccustyrna_fr4-1-0.pdb	-74.374	-74.374	13.75	
1xak-7bv2-Roccustyrna_fr5-0-0.pdb	346.969	346.969		145.098
1xak-7bv2-Roccustyrna_fr5-1-0.pdb	-777.695	-777.695		147.059
1xak-7bv2-Roccustyrna_fr6-0-0.pdb	-689.679	-689.679		132.895
1xak-7bv2-Roccustyrna_fr6-1-0.pdb	-721.703	-721.703		137.105
1xak-7bv2-Roccustyrna_fr7-0-0.pdb	-680.056	-680.056		144.286
1xak-7bv2-Roccustyrna_fr7-1-0.pdb	-71.762	-71.762		156.286
1xak-7bv2-Roccustyrna_gs1-0-0.pdb	-135.238	-135.238		958.696
1xak-7bv2-Roccustyrna_gs1-1-0.pdb	-761.809	-761.809		12.913
1xak-7bv2-Roccustyrna_gs2-0-0.pdb	-609.796	-609.796		187.895
1xak-7bv2-Roccustyrna_gs2-1-0.pdb	-549.452	-549.452		187.368
1xak-7bv2-Roccustyrna_gs3-0-0.pdb	502.167	502.167		18.383
1xak-7bv2-Roccustyrna_gs3-1-0.pdb	-741.929	-741.929		131.277
1xak-7bv2-Roccustyrna_gs4-0-0.pdb	353.952	353.952		923.529
1xak-7bv2-Roccustyrna_gs4-1-0.pdb	-800.072	-800.072		12.902
1xak-7bv2-Roccustyrna_gs5-0-0.pdb	-89.824	-89.824		55.625
1xak-7bv2-Roccustyrna_gs5-1-0.pdb	-851.849	-851.849		96.875
1xak-7bv2-Roccustyrna_gs6-0-0.pdb	-568.494	-568.494	18.5	
1xak-7bv2-Roccustyrna_gs6-1-0.pdb	-500.961	-500.961	18.5	
1xak-7bv2-Roccustyrna_gs8-0-0.pdb	494.848	494.848		16
1xak-7bv2-Roccustyrna_gs8-1-0.pdb	-105.501	-105.501	15.66	
1xak-7khp-Roccustyrna_fr1-0-0.pdb	210.995	210.995		113.768
1xak-7khp-Roccustyrna_fr2-0-0.pdb	-679.585	-679.585		14.303
1xak-7khp-Roccustyrna_fr3-0-0.pdb	349.214	349.214		106.154
1xak-7khp-Roccustyrna_fr4-0-0.pdb	-743.888	-743.888		139.167
1xak-7khp-Roccustyrna_fr5-0-0.pdb	164.215	164.215		132.353
1xak-7khp-Roccustyrna_fr6-0-0.pdb	-760.993	-760.993		148.684
1xak-7khp-Roccustyrna_fr7-0-0.pdb	-670.098	-670.098		139.714
1xak-7khp-Roccustyrna_gs1-0-0.pdb	269.415	269.415		133.696
1xak-7khp-Roccustyrna_gs2-0-0.pdb	-573.849	-573.849		184.737
1xak-7khp-Roccustyrna_gs3-0-0.pdb	708.216	708.216		262.553
1xak-7khp-Roccustyrna_gs4-0-0.pdb	107.261	107.261		698.039
1xak-7khp-Roccustyrna_gs5-0-0.pdb	-212.934	-212.934		901.563
1xak-7khp-Roccustyrna_gs6-0-0.pdb	-494.399	-494.399	18.5	
1xak-7khp-Roccustyrna_gs8-0-0.pdb	366.309	366.309	16.8	
1xak-cav2zu5_ZU5-Roccustyrna-0-0.pdb	-793.146	-488.916		162.286
1xak-cav3fqq_GOL-Roccustyrna-0-0.pdb	-731.629	-731.629		132.571
1xak-cav6lu7_02J-Roccustyrna_fr1-0-0.pdb	-302.048	-302.048		372.464
1xak-cav6lu7_02J-Roccustyrna_fr2-0-0.pdb	-736.318	-736.318		160.606
1xak-cav6lu7_02J-Roccustyrna_fr3-0-0.pdb	117.982	117.982		167.436
1xak-cav6lu7_02J-Roccustyrna_fr4-0-0.pdb	-685.705	-685.705		136.667
1xak-cav6lu7_02J-Roccustyrna_fr5-0-0.pdb	285.782	285.782		114.314
1xak-cav6lu7_02J-Roccustyrna_fr6-0-0.pdb	-671.069	-671.069		139.737
1xak-cav6lu7_02J-Roccustyrna_fr7-0-0.pdb	-671.155	-671.155		139.143
1xak-cav6lu7_02J-Roccustyrna_gs1-0-0.pdb	282.347	282.347		11.913
1xak-cav6lu7_02J-Roccustyrna_gs2-0-0.pdb	-65.547	-65.547		206.316
1xak-cav6lu7_02J-Roccustyrna_gs3-0-0.pdb	107.811	107.811		106.809
1xak-cav6lu7_02J-Roccustyrna_gs4-0-0.pdb	696.029	696.029		109.412
1xak-cav6lu7_02J-Roccustyrna_gs5-0-0.pdb	702.896	702.896		571.875
1xak-cav6lu7_02J-Roccustyrna_gs6-0-0.pdb	-587.538	-587.538	18.6	
1xak-cav6lu7_02J-Roccustyrna_gs8-0-0.pdb	-281.536	-281.536	10.8	
1xak-cav6w63_X77-Roccustyrna_fr1-0-0.pdb	543.913	543.913		731.884
1xak-cav6w63_X77-Roccustyrna_fr2-0-0.pdb	-736.384	-736.384		160.606
1xak-cav6w63_X77-Roccustyrna_fr3-0-0.pdb	-421.028	-421.028		100.769
1xak-cav6w63_X77-Roccustyrna_fr4-0-0.pdb	-706.366	-706.366	14.25	
1xak-cav6w63_X77-Roccustyrna_fr5-0-0.pdb	205.716	205.716		135.882
1xak-cav6w63_X77-Roccustyrna_fr6-0-0.pdb	-776.268	-776.268		132.632
1xak-cav6w63_X77-Roccustyrna_fr7-0-0.pdb	-67.114	-67.114		138.571
1xak-cav6w63_X77-Roccustyrna_gs1-0-0.pdb	127.002	127.002		109.348
1xak-cav6w63_X77-Roccustyrna_gs2-0-0.pdb	-608.733	-608.733		187.895
1xak-cav6w63_X77-Roccustyrna_gs3-0-0.pdb	404.872	404.872		250.851
1xak-cav6w63_X77-Roccustyrna_gs4-0-0.pdb	148.111	148.111		128.039
1xak-cav6w63_X77-Roccustyrna_gs5-0-0.pdb	416.317	416.317		49.375
1xak-cav6w63_X77-Roccustyrna_gs6-0-0.pdb	-587.241	-587.241	18.7	
1xak-cav6w63_X77-Roccustyrna_gs8-0-0.pdb	661.079	661.079	23.1	
1xak-cav6woj_APR-Roccustyrna_fr1-0-0.pdb	441.63	441.63		138.696
1xak-cav6woj_APR-Roccustyrna_fr2-0-0.pdb	-736.583	-736.583		160.909
1xak-cav6woj_APR-Roccustyrna_fr3-0-0.pdb	896.132	896.132		177.949

1xak-cav6woj_APR-Roccustyrna_fr4-0-0.pdb	-716.425	-716.425	145.833	
1xak-cav6woj_APR-Roccustyrna_fr5-0-0.pdb	673.204	673.204	200.784	
1xak-cav6woj_APR-Roccustyrna_fr6-0-0.pdb	-696.804	-696.804	136.053	
1xak-cav6woj_APR-Roccustyrna_fr7-0-0.pdb	-717.451	-717.451	15.6	
1xak-cav6woj_APR-Roccustyrna_gs1-0-0.pdb	108.826	108.826	126.739	
1xak-cav6woj_APR-Roccustyrna_gs2-0-0.pdb	-608.979	-608.979	187.895	
1xak-cav6woj_APR-Roccustyrna_gs3-0-0.pdb	424.213	424.213	710.638	
1xak-cav6woj_APR-Roccustyrna_gs4-0-0.pdb	318.469	318.469	22.549	
1xak-cav6woj_APR-Roccustyrna_gs5-0-0.pdb	-124.958	-124.958	378.125	
1xak-cav6woj_APR-Roccustyrna_gs6-0-0.pdb	-58.743	-58.743	18.7	
1xak-cav6woj_APR-Roccustyrna_gs8-0-0.pdb	288.087	288.087	16.96	
1xak-cav6wzu_GOL-Roccustyrna_fr1-0-0.pdb	688.159	688.159	164.783	
1xak-cav6wzu_GOL-Roccustyrna_fr2-0-0.pdb	-736.371	-736.371	160.303	
1xak-cav6wzu_GOL-Roccustyrna_fr3-0-0.pdb	741.214	741.214	105.385	
1xak-cav6wzu_GOL-Roccustyrna_fr4-0-0.pdb	-716.939	-716.939	145.833	
1xak-cav6wzu_GOL-Roccustyrna_fr5-0-0.pdb	-173.803	-173.803	631.373	
1xak-cav6wzu_GOL-Roccustyrna_fr6-0-0.pdb	-736.656	-736.656	137.895	
1xak-cav6wzu_GOL-Roccustyrna_fr7-0-0.pdb	-717.379	-717.379	157.143	
1xak-cav6wzu_GOL-Roccustyrna_gs1-0-0.pdb	167.576	167.576	141.522	
1xak-cav6wzu_GOL-Roccustyrna_gs2-0-0.pdb	-604.251	-604.251	198.421	
1xak-cav6wzu_GOL-Roccustyrna_gs3-0-0.pdb	83.545	83.545	885.106	
1xak-cav6wzu_GOL-Roccustyrna_gs4-0-0.pdb	207.453	207.453	122.941	
1xak-cav6wzu_GOL-Roccustyrna_gs5-0-0.pdb	686.627	686.627	127.031	
1xak-cav6wzu_GOL-Roccustyrna_gs6-0-0.pdb	-587.838	-587.838	18.65	
1xak-cav6wzu_GOL-Roccustyrna_gs8-0-0.pdb	356.161	356.161	14.58	
1xak-cav6wzu_GOL-Roccustyrna_less_admet_-0-0.pdb	-81.266	-81.266	15.4	
1xak-cav6wzu_GOL-Roccustyrna_less_admet_-1-0.pdb	-776.313	-776.313	151.143	
1xak-cav6wzu_GOL-Roccustyrna-0-0.pdb	0	0	0	
1xak-cav6wzu_GOL-roccustyrnareywarrior-0-0.pdb	256.67	256.67	842.424	
1xak-cav6wzu_GOL-roccustyrnareywarrior-1-0.pdb	-763.431	-763.431	836.364	
1xak-cav7b3o_NAG-Roccustyrna_fr1-0-0.pdb	-697.365	-697.365	96.087	
1xak-cav7b3o_NAG-Roccustyrna_fr2-0-0.pdb	-758.912	-758.912	161.818	
1xak-cav7b3o_NAG-Roccustyrna_fr3-0-0.pdb	60.608	60.608	109.487	
1xak-cav7b3o_NAG-Roccustyrna_fr4-0-0.pdb	-743.961	-743.961	139.167	
1xak-cav7b3o_NAG-Roccustyrna_fr5-0-0.pdb	345.033	345.033	117.647	
1xak-cav7b3o_NAG-Roccustyrna_fr6-0-0.pdb	-757.086	-757.086	149.737	
1xak-cav7b3o_NAG-Roccustyrna_fr7-0-0.pdb	-71.785	-71.785	156.286	
1xak-cav7b3o_NAG-Roccustyrna_gs1-0-0.pdb	116.253	116.253	149.348	
1xak-cav7b3o_NAG-Roccustyrna_gs2-0-0.pdb	-655.504	-655.504	206.842	
1xak-cav7b3o_NAG-Roccustyrna_gs3-0-0.pdb	539.08	539.08	189.574	
1xak-cav7b3o_NAG-Roccustyrna_gs4-0-0.pdb	-806.715	-806.715	288.235	
1xak-cav7b3o_NAG-Roccustyrna_gs5-0-0.pdb	-287.802	-287.802	278.125	
1xak-cav7b3o_NAG-Roccustyrna_gs6-0-0.pdb	-501.339	-501.339	18.5	
1xak-cav7b3o_NAG-Roccustyrna_gs8-0-0.pdb	870.413	870.413	20.58	
1xak-cav7bv2_POP-Roccustyrna-0-0.pdb	-758.535	-758.535	140.857	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr1-0-0.pdb	484.694	484.694	882.609	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr1-1-0.pdb	-670.768	-670.768	924.638	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr2-0-0.pdb	-708.248	-708.248	163.636	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr2-1-0.pdb	-671.047	-671.047	150.303	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr3-0-0.pdb	-0.787532	-0.787532	774.359	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr3-1-0.pdb	-692.613	-692.613	140.513	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr4-0-0.pdb	-702.345	-702.345	169.167	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr4-1-0.pdb	-743.901	-743.901	138.889	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr5-0-0.pdb	277.228	277.228	122.157	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr5-1-0.pdb	-820.294	-820.294	129.804	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr6-0-0.pdb	-762.082	-762.082	148.421	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr6-1-0.pdb	-776.662	-776.662	132.632	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr7-0-0.pdb	-689.043	-689.043	141.714	
1xak-cav7kdl (2)_NAG-Roccustyrna_fr7-1-0.pdb	-662.126	-662.126	133.143	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs1-0-0.pdb	-120.231	-120.231	663.043	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs1-1-0.pdb	-767.269	-767.269	129.348	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs2-0-0.pdb	-65.554	-65.554	206.316	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs2-1-0.pdb	-604.204	-604.204	198.421	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs3-0-0.pdb	794.282	794.282	115.745	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs3-1-0.pdb	-782.984	-782.984	129.149	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs4-0-0.pdb	-315.567	-315.567	539.216	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs4-1-0.pdb	-77.632	-77.632	150.196	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs5-0-0.pdb	511.832	511.832	123.281	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs5-1-0.pdb	-755.892	-755.892	834.375	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs6-0-0.pdb	-587.014	-587.014	18.6	

1xak-cav7kdl (2)_NAG-Roccustyrna_gs6-1-0.pdb	-501.581	-501.581	18.5	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs8-0-0.pdb	256.762	256.762	14.16	
1xak-cav7kdl (2)_NAG-Roccustyrna_gs8-1-0.pdb	-77.953	-77.953	12.9	
1xak-model1_6yi3-Roccustyrna_fr1-0-0.pdb	197.059	197.059		12.087
1xak-model1_6yi3-Roccustyrna_fr1-1-0.pdb	-862.917	-862.917		102.319
1xak-model1_6yi3-Roccustyrna_fr2-0-0.pdb	-690.622	-690.622		147.273
1xak-model1_6yi3-Roccustyrna_fr2-1-0.pdb	-736.384	-736.384		160.909
1xak-model1_6yi3-Roccustyrna_fr3-0-0.pdb	0.201151	0.201151		971.795
1xak-model1_6yi3-Roccustyrna_fr3-1-0.pdb	-722.328	-722.328		132.821
1xak-model1_6yi3-Roccustyrna_fr4-0-0.pdb	-671.058	-671.058		151.667
1xak-model1_6yi3-Roccustyrna_fr4-1-0.pdb	-700.879	-700.879		141.667
1xak-model1_6yi3-Roccustyrna_fr5-0-0.pdb	581.566	581.566		152.353
1xak-model1_6yi3-Roccustyrna_fr5-1-0.pdb	-56	-56		128.627
1xak-model1_6yi3-Roccustyrna_fr6-0-0.pdb	-761.833	-761.833		148.684
1xak-model1_6yi3-Roccustyrna_fr6-1-0.pdb	-721.795	-721.795	13.5	
1xak-model1_6yi3-Roccustyrna_fr7-0-0.pdb	-717.416	-717.416	15.6	