

Let $g \in \mathbf{G}$ be the coordinates of grid points representing the volume of the pocket.

1. Start with two neurons x and y at random positions w_x and w_y in $\mathbf{R}^3$.
2. Generate an input signal g according to $\mathbf{G}$.
3. Find the nearest and second-nearest neurons s_1 and s_2 .
4. Increment the age of all edges emanating from s_1 .
5. Add the squared distance between the input signal and the nearest neuron in input space to a local counter variable:

$$\Delta error(s_1) = \|w_{s_1} - g\|^2.$$

6. Move s_1 and its topological neighbors towards g by fractions ϵ_w and ϵ_n , respectively, of the total distance:

$$\Delta w_{s_1} = \epsilon_w (g - w_{s_1})$$

$$\Delta w_n = \epsilon_n (g - w_n).$$

7. If s_1 and s_2 are connected by an edge, set the age of this edge to zero. If such an edge does not exist, create it.
8. Remove edges with an age larger than $a_{\max}$. If this results in neurons having no emanating edges, remove them as well.
9. If the number of input signals generated so far is an integer multiple of parameter λ , insert a new neuron as follows:
 - Determine the neuron q with the maximum accumulated error.
 - Insert a new neuron r halfway between q and its neighbor p with the largest error variable:

$$w_r = 0.5 * (w_q + w_p).$$

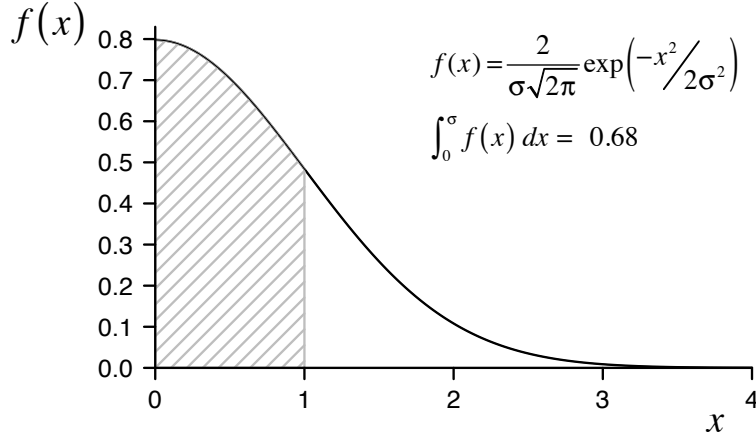
- Insert edges connecting the new neuron r with neurons q and p , and remove the original edge between q and p .
 - Decrease the error variables of q and p by multiplying them with a constant α .
 - Initialize the error variable of r with the new value of the error variable of q .
10. Decrease all error variables by multiplying them with a constant δ .
 11. If the average distance from the input vectors to the nearest neurons is greater than MQE go to step 1.

Figure S1. Pseudo-code of the growing neural gas algorithm. The algorithm is shown according to Fritzke 1994.

Table S1. Parameterization of the growing neural gas algorithm.

Parameter	Value
Number of inputs (update cycles) before next neuron is added (λ)	600
Jump size of winner neuron as fraction of distance towards input signal (ϵ_w)	0.05
Jump size of winner neuron's topological neighbors as fraction of distance towards input signal (ϵ_n)	0.0006
Scaling factor of the error variable for a pair of vertices in between which a new neuron was inserted (α)	0.5
Scaling factor of the error variables of all neurons (δ)	0.0005
Maximum age of an edge between neurons ($a_{\max}$)	16
Stopping Criterion: Mean Quantization Error (MQE)	1.8 Å

A



B

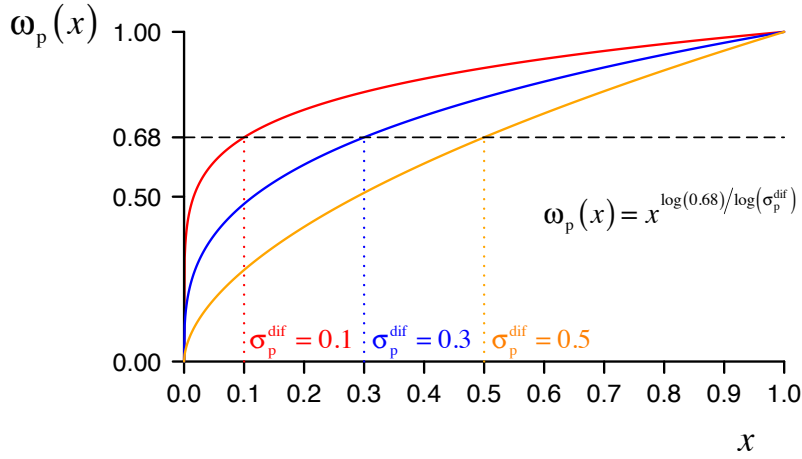


Figure S2. Amplification of minor differences between vertices of the pocket graphs. A) Half-normal probability function with $\sigma = 1$. The dashed area under the curve in the interval from 0 to 1σ is equal to 0.68. The differences $x = |\lambda_p^1(u) - \lambda_p^2(v)|$ between vertices of the graphs in a property p follow a half-normal distribution. With a mean of approximately 0.13 the parameters σ_p^{dif} of these half-normal distributions tend to be small in comparison to a maximum possible difference value of 1. B) Three different runs of the weighting function $\omega_p(x)$ with varied values of σ_p^{dif} . To enhance the discrimination between vertices, difference values are transformed so that the range $[0, \sigma_p^{\text{dif}}]$ is mapped to the range $[0, 0.68]$. This ensures that 68% of the difference values are transformed in 68% of the possible distance range $[0, 1]$.

Example

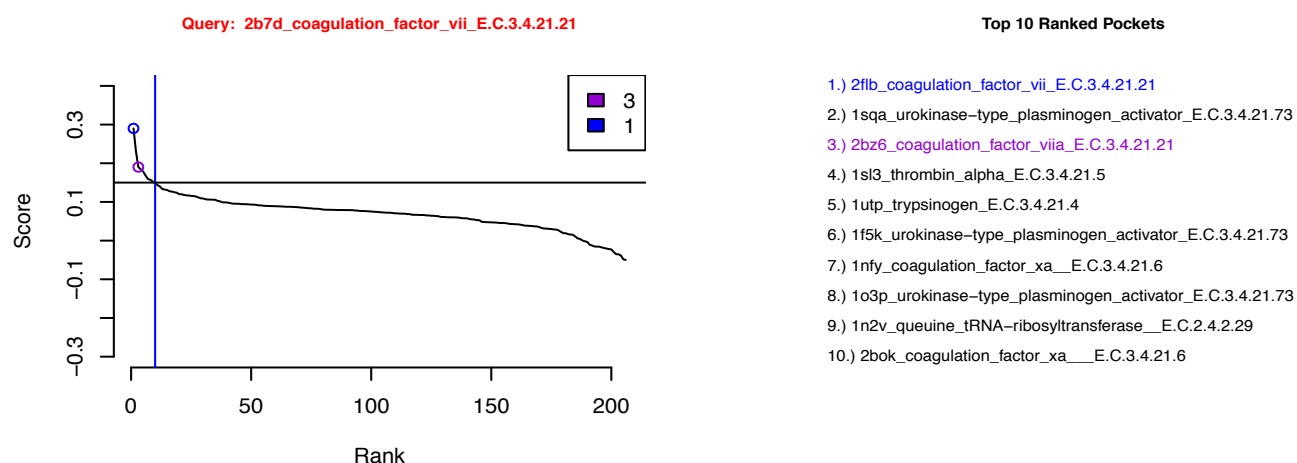
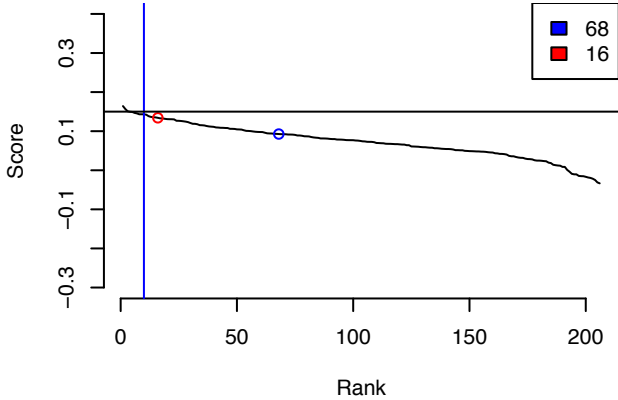


Figure S3. Score distributions within the PDBbind core set. For each protein the score distribution and the 10 top ranked proteins are shown. Each of the following pages contains plots derived from three queries coming from one predefined cluster. Information about the first protein of a cluster is shown in violet, about the second protein in blue, and about the third protein in red. In the shown example, PDB-structure 2b7d was taken as query. 2b7d is the third protein of its cluster (colored in red). The second protein of the cluster 2flb (colored in blue) was ranked first, the first protein of the cluster 2bz6 (colored in purple) was ranked third. Ranks of both proteins are indicated in the plot in the upper right corner. The blue vertical line in the plot marks the tenth rank. The black horizontal line indicates the reliability threshold τ .

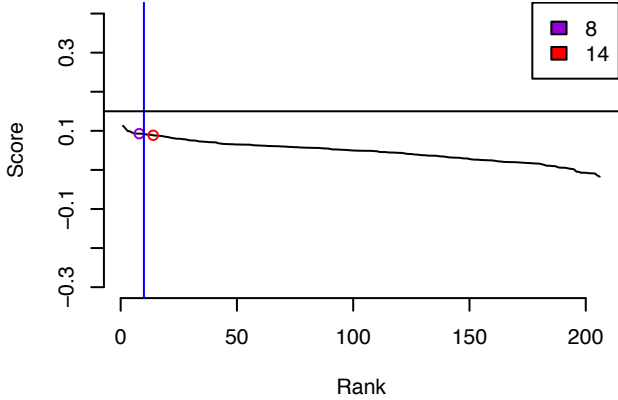
Query: 1hk4_serum_albumin_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 2.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 3.) 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 4.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 5.) 1flr_antibody_fab_E.C.-.-.-.-
- 6.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 7.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 8.) 2d3u_polyprotein_E.C.2.7.7.48
- 9.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 10.) 1l2s_beta-lactamase_E.C.3.5.2.6

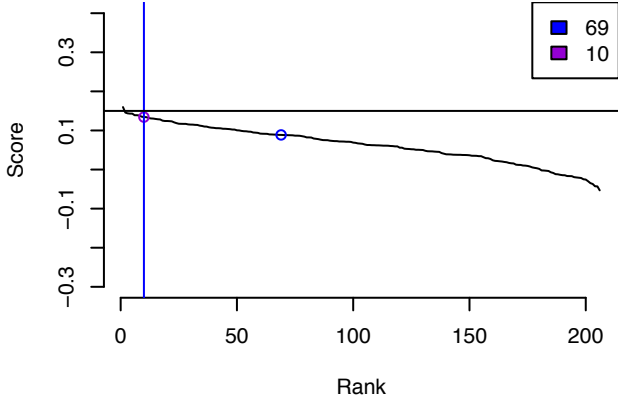
Query: 1ha2_serum_albumin_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 2.) 1kv1_mitogen-activated_protein_kinase_p38_E.C.2.7.1.37
- 3.) 1jqe_histamine_n-methyltransferase_E.C.2.1.1.8
- 4.) 10gs_glutathione_s-transferase_E.C.2.5.1.18
- 5.) 1nja_thymidylate_synthase_E.C.2.1.1.45
- 6.) 1lol_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 7.) 2ayr_estrogen_receptor_E.C.-.-.-.-
- 8.) 1hk4_serum_albumin_E.C.-.-.-.-
- 9.) 1fkn_secretase_beta_E.C.3.4.23.-
- 10.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37

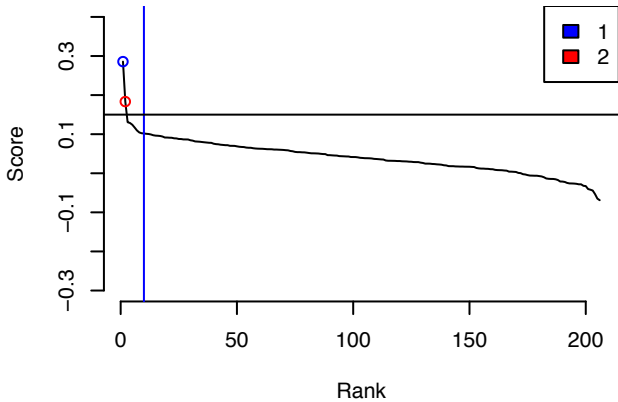
Query: 1gni_serum_albumin_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 2.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 3.) 2d3u_polyprotein_E.C.2.7.7.48
- 4.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 5.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 6.) 2d3z_polyprotein_E.C.2.7.7.48
- 7.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 8.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 9.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3
- 10.) 1hk4_serum_albumin_E.C.-.-.-.-

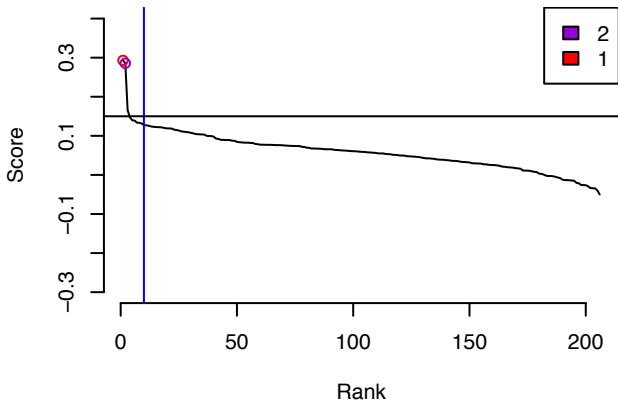
Query: 1nhu_hepatitis_c_virus_ns5b_RNA_polymerase_E.C.2.7.7.48



Top 10 Ranked Pockets

- 1.) 2d3z_polyprotein_E.C.2.7.7.48
- 2.) 2d3u_polyprotein_E.C.2.7.7.48
- 3.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 4.) 1if7_carbonic_anhydrase_ii_E.C.4.2.1.1
- 5.) 1gni_serum_albumin_E.C.-.-.-.-
- 6.) 1nny_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 7.) 1hk4_serum_albumin_E.C.-.-.-.-
- 8.) 2fai_estrogen_receptor_E.C.-.-.-.-
- 9.) 1b11_FIV_protease_E.C.3.4.23.16
- 10.) 6fiv_FIV_protease_E.C.3.4.23.16

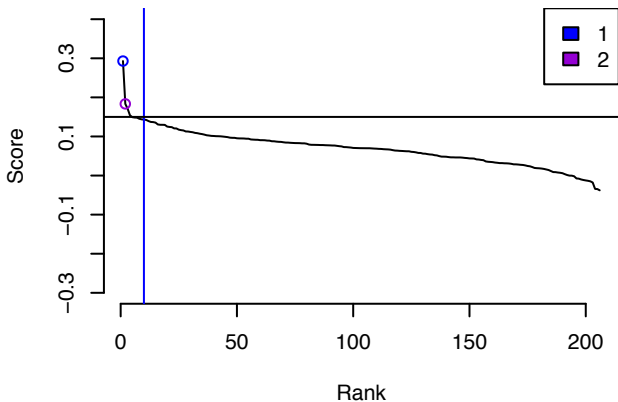
Query: 2d3z_polyprotein_E.C.2.7.7.48



Top 10 Ranked Pockets

- 1.) 2d3u_polyprotein_E.C.2.7.7.48
- 2.) 1nhu_hepatitis_c_virus_ns5b_RNA_polymerase_E.C.2.7.7.48
- 3.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 4.) 1d7j_FK506_binding_protein_E.C.5.2.1.8
- 5.) 1if7_carbonic_anhydrase_ii_E.C.4.2.1.1
- 6.) 1gni_serum_albumin_E.C.-.-.-.-
- 7.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 8.) 1c84_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 9.) 1hk4_serum_albumin_E.C.-.-.-.-
- 10.) 1sv3_phospholipase_a2_E.C.3.1.1.4

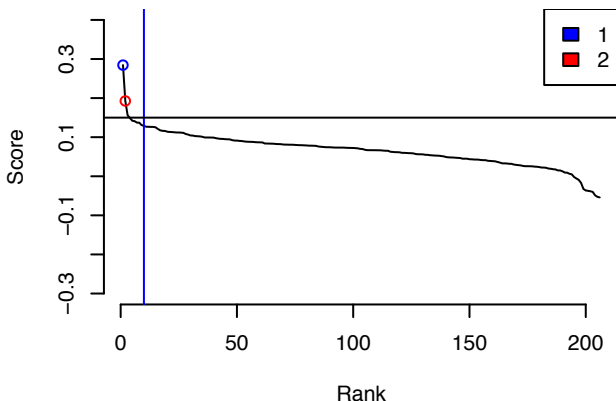
Query: 2d3u_polyprotein_E.C.2.7.7.48



Top 10 Ranked Pockets

- 1.) 2d3z_polyprotein_E.C.2.7.7.48
- 2.) 1nhu_hepatitis_c_virus_ns5b_RNA_polymerase_E.C.2.7.7.48
- 3.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 4.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 5.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 6.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 7.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 8.) 1flr_antibody_fab_E.C.-.-.-.-
- 9.) 1gni_serum_albumin_E.C.-.-.-.-
- 10.) 1hk4_serum_albumin_E.C.-.-.-.-

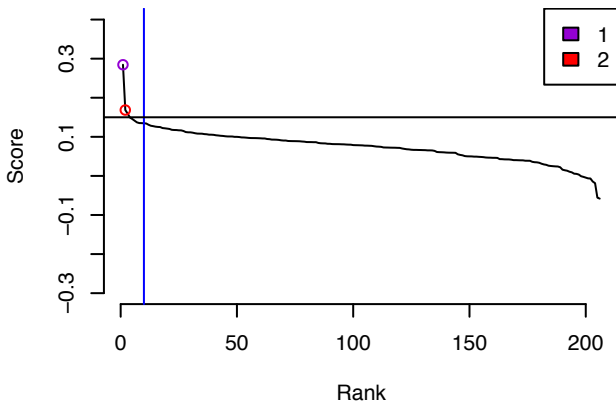
Query: 1ajp_penicillin_amidohydrolase_E.C.3.5.1.11



Top 10 Ranked Pockets

- 1.) 1ai5_penicillin_amidohydrolase_E.C.3.5.1.11
- 2.) 1ajq_penicillin_amidohydrolase_E.C.3.5.1.11
- 3.) 1df8_streptavidin_E.C.-.-.-.-
- 4.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 5.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 6.) 1jq9_phospholipase_a2_E.C.3.1.1.4
- 7.) 1m2q_casein_kinase_ii_E.C.2.7.1.37
- 8.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 9.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 10.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37

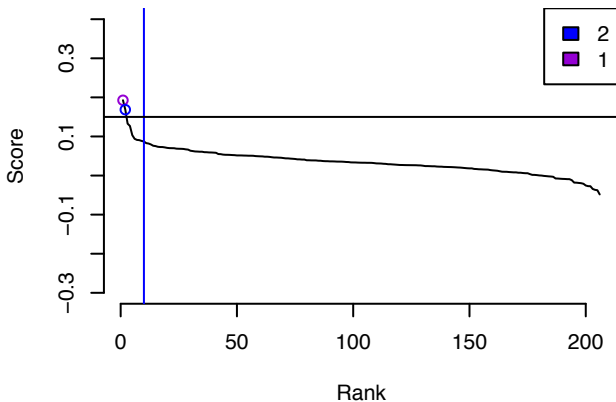
Query: 1ai5_penicillin_amidohydrolase_E.C.3.5.1.11



Top 10 Ranked Pockets

- 1.) 1ajp_penicillin_amidohydrolase_E.C.3.5.1.11
- 2.) 1ajq_penicillin_amidohydrolase_E.C.3.5.1.11
- 3.) 2f01_streptavidin_E.C.-.-.-.-
- 4.) 1df8_streptavidin_E.C.-.-.-.-
- 5.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 6.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 7.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 8.) 1m2q_casein_kinase_ii_E.C.2.7.1.37
- 9.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 10.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3

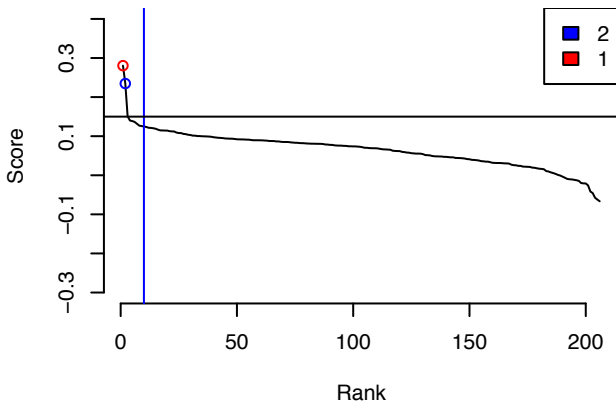
Query: 1ajq_penicillin_amidohydrolase_E.C.3.5.1.11



Top 10 Ranked Pockets

- 1.) 1ajp_penicillin_amidohydrolase_E.C.3.5.1.11
- 2.) 1ai5_penicillin_amidohydrolase_E.C.3.5.1.11
- 3.) 1df8_streptavidin_E.C.-.-.-.-
- 4.) 2f01_streptavidin_E.C.-.-.-.-
- 5.) 3pcj_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 6.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 7.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 8.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 9.) 8cpa_carboxypeptidase_a_E.C.3.4.17.1
- 10.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6

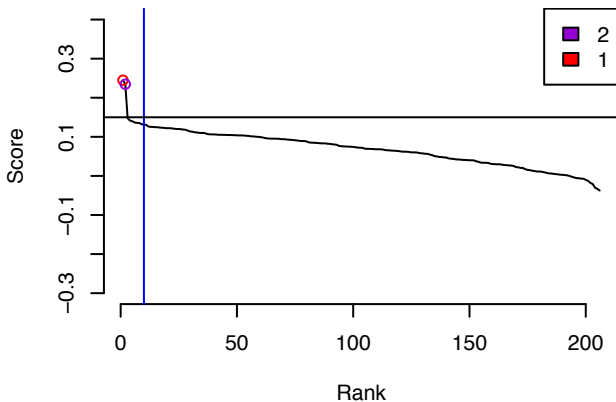
Query: 1gpk_acetylcholinesterase_E.C.3.1.1.7



Top 10 Ranked Pockets

- 1.) 1e66_acetylcholinesterase_E.C.3.1.1.7
- 2.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 3.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 4.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 5.) 1ndz_adenosine_deaminase_E.C.3.5.4.4
- 6.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 7.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 8.) 1jqe_histamine_n-methyltransferase_E.C.2.1.1.8
- 9.) 1toj_aspartate_aminotransferase_E.C.2.6.1.1
- 10.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37

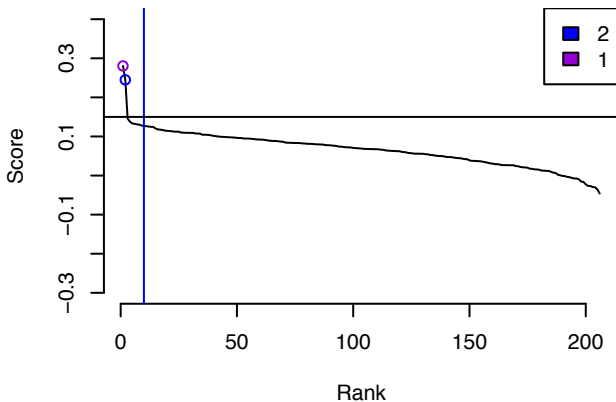
Query: 1h23_acetylcholinesterase_E.C.3.1.1.7



Top 10 Ranked Pockets

- 1.) 1e66_acetylcholinesterase_E.C.3.1.1.7
- 2.) 1gpk_acetylcholinesterase_E.C.3.1.1.7
- 3.) 1ndw_adenosine_deaminase_E.C.3.5.4.4
- 4.) 1jqe_histamine_n-methyltransferase_E.C.2.1.1.8
- 5.) 1slg_streptavidin_E.C.-.-.-.-
- 6.) 1ndy_adenosine_deaminase_E.C.3.5.4.4
- 7.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 8.) 2bak_mitogen-activated_protein_kinase_14_E.C.2.7.1.37
- 9.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 10.) 1f4g_thymidylate_synthase_E.C.2.1.1.45

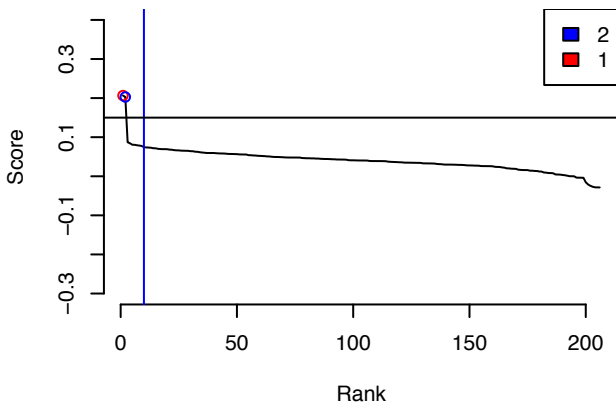
Query: 1e66_acetylcholinesterase_E.C.3.1.1.7



Top 10 Ranked Pockets

- 1.) 1gpk_acetylcholinesterase_E.C.3.1.1.7
- 2.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 3.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1jqe_histamine_n-methyltransferase_E.C.2.1.1.8
- 5.) 1ndz_adenosine_deaminase_E.C.3.5.4.4
- 6.) 1ndy_adenosine_deaminase_E.C.3.5.4.4
- 7.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 8.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 9.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 10.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29

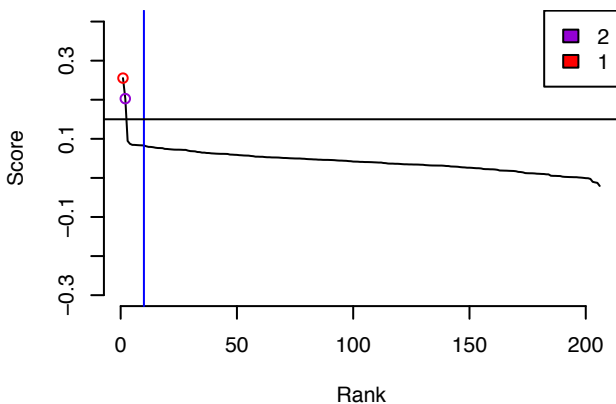
Query: 2rkm_oligo-peptide_binding_protein_E.C.-.-.-



Top 10 Ranked Pockets

- 1.) 1b7h_oligo-peptide_binding_protein_E.C.-.-.-
- 2.) 1b9j_oligo-peptide_binding_protein_E.C.-.-.-
- 3.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 4.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 5.) 1toi_aspartate_aminotransferase_E.C.2.6.1.1
- 6.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 7.) 3gss_glutathione_s-transferase_E.C.2.5.1.18
- 8.) 1g7q_h-2_class_i_histocompatibility_antigen_E.C.-.-.-
- 9.) 1olu_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4
- 10.) 1toj_aspartate_aminotransferase_E.C.2.6.1.1

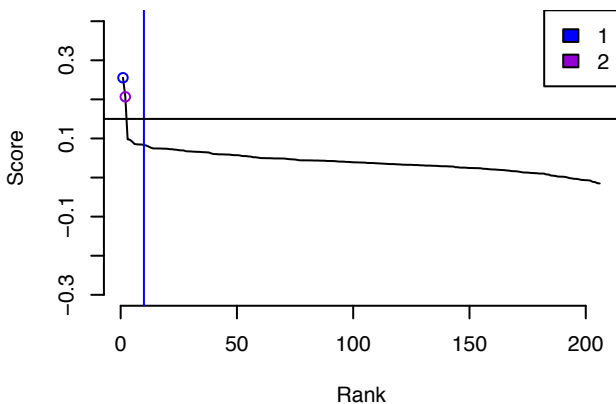
Query: 1b9j_oligo-peptide_binding_protein_E.C.-.-.-



Top 10 Ranked Pockets

- 1.) 1b7h_oligo-peptide_binding_protein_E.C.-.-.-
- 2.) 2rkm_oligo-peptide_binding_protein_E.C.-.-.-
- 3.) 4fiv_FIV_protease_E.C.3.4.23.16
- 4.) 3gss_glutathione_s-transferase_E.C.2.5.1.18
- 5.) 1g7q_h-2_class_i_histocompatibility_antigen_E.C.-.-.-
- 6.) 1olu_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4
- 7.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 8.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 9.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 10.) 1e66_acetylcholinesterase_E.C.3.1.1.7

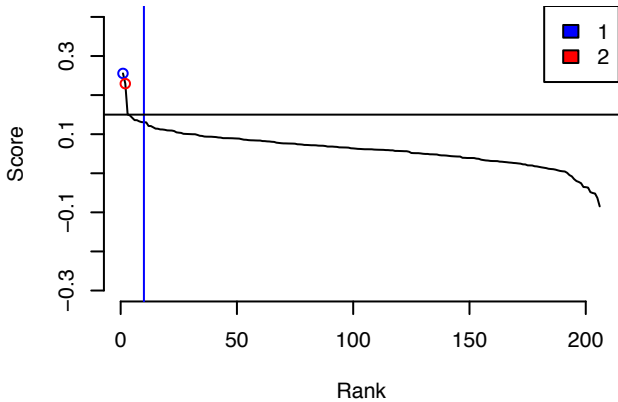
Query: 1b7h_oligo-peptide_binding_protein_E.C.-.-.-



Top 10 Ranked Pockets

- 1.) 1b9j_oligo-peptide_binding_protein_E.C.-.-.-
- 2.) 2rkm_oligo-peptide_binding_protein_E.C.-.-.-
- 3.) 1olu_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4
- 4.) 1toi_aspartate_aminotransferase_E.C.2.6.1.1
- 5.) 4fiv_FIV_protease_E.C.3.4.23.16
- 6.) 2hdq_beta-lactamase_E.C.3.5.2.6
- 7.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 8.) 1tok_aspartate_aminotransferase_E.C.2.6.1.1
- 9.) 1v16_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4
- 10.) 1toj_aspartate_aminotransferase_E.C.2.6.1.1

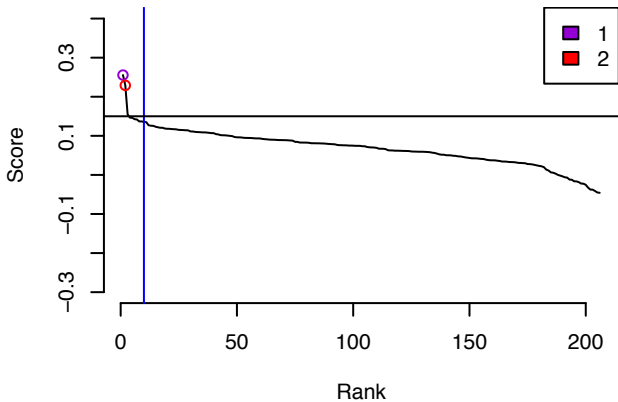
Query: 1u2y_alpha-amylase_E.C.3.2.1.1



Top 10 Ranked Pockets

- 1.) 1u33_alpha-amylase_E.C.3.2.1.1
- 2.) 1xd1_alpha-amylase_E.C.3.2.1.1
- 3.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 4.) 2usn_stromelysin-1_E.C.3.4.24.17
- 5.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 6.) 1ndw_adenosine_deaminase_E.C.3.5.4.4
- 7.) 1ndy_adenosine_deaminase_E.C.3.5.4.4
- 8.) 1fkn_secretase_beta_E.C.3.4.23.-
- 9.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 10.) 2g94_beta-secretase_1_E.C.3.4.23.46

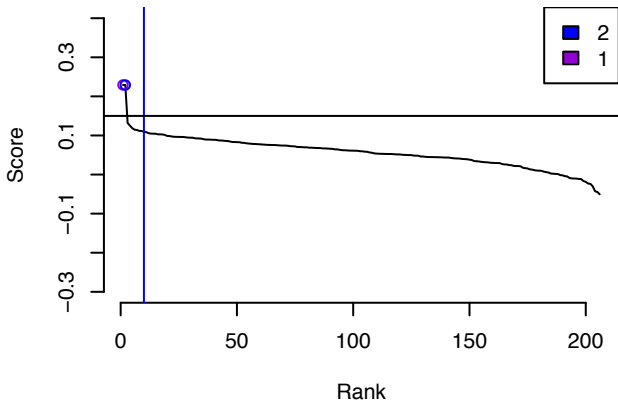
Query: 1u33_alpha-amylase_E.C.3.2.1.1



Top 10 Ranked Pockets

- 1.) 1u2y_alpha-amylase_E.C.3.2.1.1
- 2.) 1xd1_alpha-amylase_E.C.3.2.1.1
- 3.) 1ndz_adenosine_deaminase_E.C.3.5.4.4
- 4.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 5.) 1jq9_phospholipase_a2_E.C.3.1.1.4
- 6.) 2ceq_beta-galactosidase_E.C.3.2.1.23
- 7.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 8.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 9.) 1ndw_adenosine_deaminase_E.C.3.5.4.4
- 10.) 2j78_beta-glucosidase_a_E.C.3.2.1.21

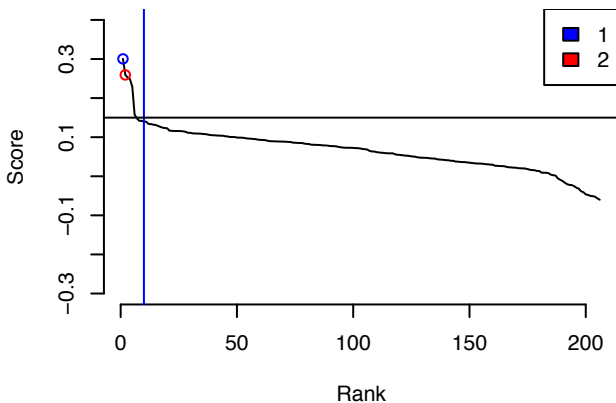
Query: 1xd1_alpha-amylase_E.C.3.2.1.1



Top 10 Ranked Pockets

- 1.) 1u2y_alpha-amylase_E.C.3.2.1.1
- 2.) 1u33_alpha-amylase_E.C.3.2.1.1
- 3.) 1ppm_penicillopepsin_E.C.3.4.23.20
- 4.) 5er1_endothiaepsin_bw624_E.C.3.4.23.22
- 5.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 6.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 7.) 1fkn_secretase_beta_E.C.3.4.23.-
- 8.) 4er2_endothiaepsin_E.C.3.4.23.22
- 9.) 1apw_penicillopepsin_E.C.3.4.23.20
- 10.) 1uwt_beta-galactosidase_E.C.3.2.1.23

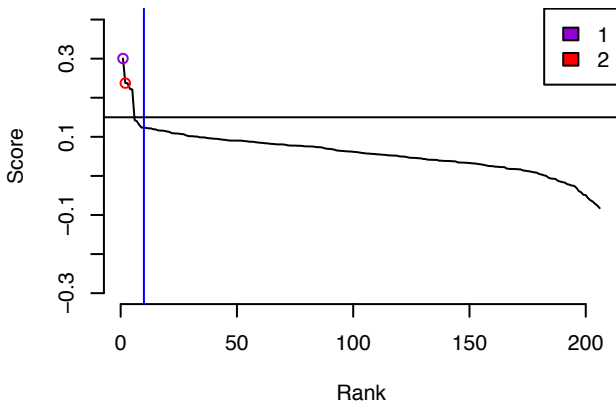
Query: 1uwt_beta-galactosidase_E.C.3.2.1.23



Top 10 Ranked Pockets

- 1.) 2ceq_beta-galactosidase_E.C.3.2.1.23
- 2.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 3.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 4.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 5.) 2j77_beta-glucosidase_a_E.C.3.2.1.21
- 6.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 7.) 1ndz_adenosine_deaminase_E.C.3.5.4.4
- 8.) 1u33_alpha-amylase_E.C.3.2.1.1
- 9.) 1u2y_alpha-amylase_E.C.3.2.1.1
- 10.) 1f4e_thymidylate_synthase_E.C.2.1.1.45

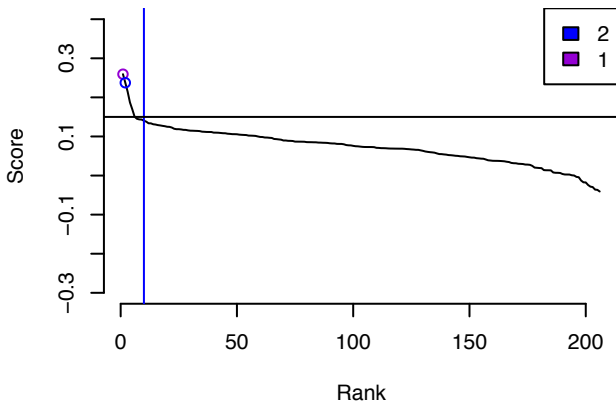
Query: 2ceq_beta-galactosidase_E.C.3.2.1.23



Top 10 Ranked Pockets

- 1.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 2.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 3.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 4.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 5.) 2j77_beta-glucosidase_a_E.C.3.2.1.21
- 6.) 1u33_alpha-amylase_E.C.3.2.1.1
- 7.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 8.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 9.) 1gpk_acetylcholinesterase_E.C.3.1.1.7
- 10.) 1fh9_xylanase_beta-1,4_E.C.3.2.1.91

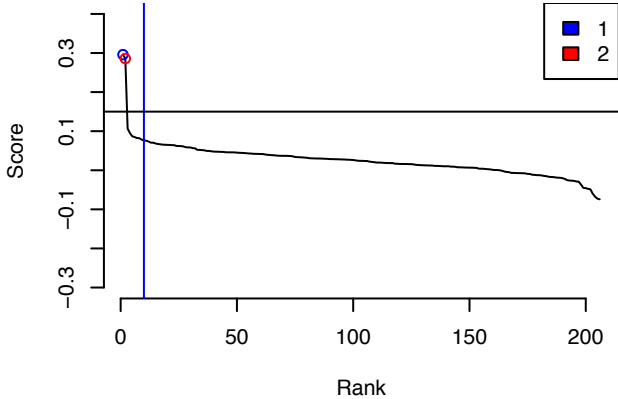
Query: 2cer_beta-glucosidase_a_E.C.3.2.1.21



Top 10 Ranked Pockets

- 1.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 2.) 2ceq_beta-galactosidase_E.C.3.2.1.23
- 3.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 4.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 5.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 6.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 7.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 8.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 9.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3
- 10.) 2bok_coagulation_factor_xa__E.C.3.4.21.6

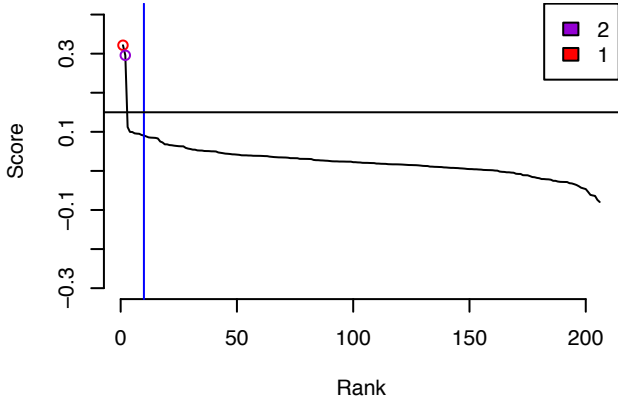
Query: 2qwb_neuraminidase_E.C.3.2.1.18



Top 10 Ranked Pockets

- 1.) 2qwd_neuraminidase_E.C.3.2.1.18
- 2.) 2qwe_neuraminidase_E.C.3.2.1.18
- 3.) 1q8t_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 4.) 7cpa_carboxypeptidase_a_E.C.3.4.17.1
- 5.) 2baj_mitogen-activated_protein_kinase_14_E.C.2.7.1.37
- 6.) 10gs_glutathione_s-transferase_E.C.2.5.1.18
- 7.) 2fzc_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 8.) 3gss_glutathione_s-transferase_E.C.2.5.1.18
- 9.) 1pr5_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 10.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73

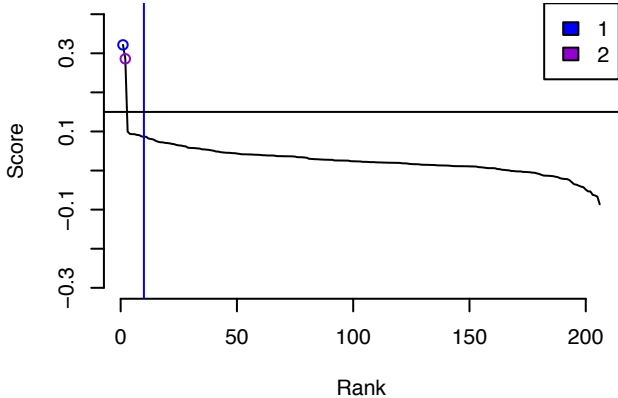
Query: 2qwd_neuraminidase_E.C.3.2.1.18



Top 10 Ranked Pockets

- 1.) 2qwe_neuraminidase_E.C.3.2.1.18
- 2.) 2qwb_neuraminidase_E.C.3.2.1.18
- 3.) 2fzc_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 4.) 1q8t_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 5.) 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4
- 6.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 7.) 1utp_trypsinogen_E.C.3.4.21.4
- 8.) 8cpa_carboxypeptidase_a_E.C.3.4.17.1
- 9.) 10gs_glutathione_s-transferase_E.C.2.5.1.18
- 10.) 2flb_coagulation_factor_vii_E.C.3.4.21.21

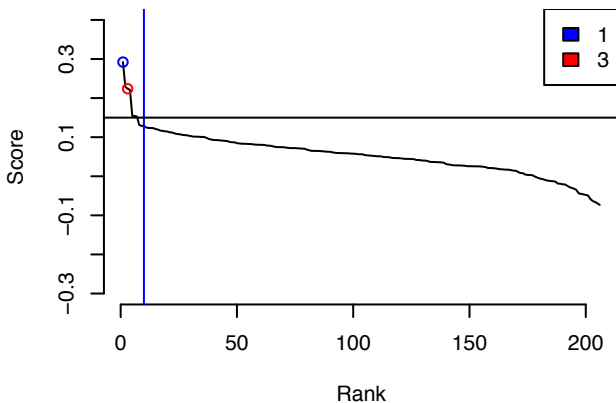
Query: 2qwe_neuraminidase_E.C.3.2.1.18



Top 10 Ranked Pockets

- 1.) 2qwd_neuraminidase_E.C.3.2.1.18
- 2.) 2qwb_neuraminidase_E.C.3.2.1.18
- 3.) 1utp_trypsinogen_E.C.3.4.21.4
- 4.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 5.) 1o3f_trypsin_beta_E.C.3.4.21.4
- 6.) 1q8t_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 7.) 10gs_glutathione_s-transferase_E.C.2.5.1.18
- 8.) 2fzc_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 9.) 3gss_glutathione_s-transferase_E.C.2.5.1.18
- 10.) 7cpa_carboxypeptidase_a_E.C.3.4.17.1

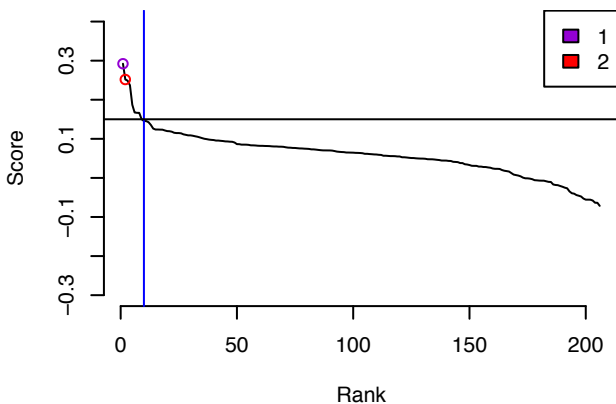
Query: 2j77_beta-glucosidase_a_E.C.3.2.1.21



Top 10 Ranked Pockets

- 1.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 2.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 3.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 4.) 2ceq_beta-galactosidase_E.C.3.2.1.23
- 5.) 1fh9_xylanase_beta-1,4_E.C.3.2.1.91
- 6.) 1fh7_xylanase_beta-1,4_E.C.3.2.1.91
- 7.) 1fh8_xylanase_beta-1,4_E.C.3.2.1.91
- 8.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 9.) 2cgr_antibody_fab_E.C.-.-.-.-
- 10.) 2cer_beta-glucosidase_a_E.C.3.2.1.21

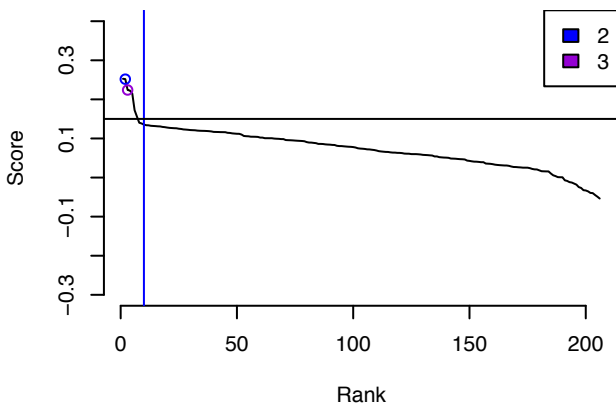
Query: 2j78_beta-glucosidase_a_E.C.3.2.1.21



Top 10 Ranked Pockets

- 1.) 2j77_beta-glucosidase_a_E.C.3.2.1.21
- 2.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 3.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 4.) 2ceq_beta-galactosidase_E.C.3.2.1.23
- 5.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 6.) 1fh9_xylanase_beta-1,4_E.C.3.2.1.91
- 7.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 8.) 2usn_stromelysin-1_E.C.3.4.24.17
- 9.) 1u2y_alpha-amylase_E.C.3.2.1.1
- 10.) 1fh8_xylanase_beta-1,4_E.C.3.2.1.91

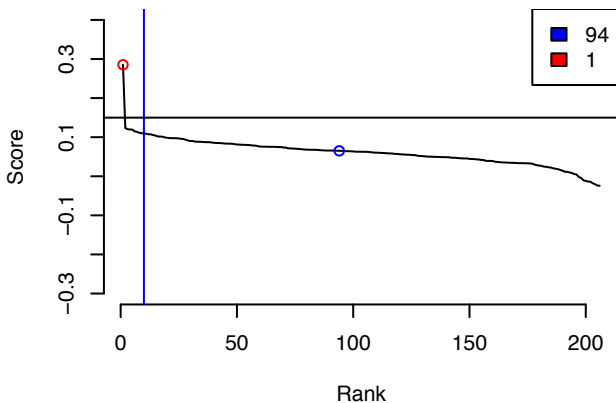
Query: 2cet_beta-glucosidase_a_E.C.3.2.1.21



Top 10 Ranked Pockets

- 1.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 2.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 3.) 2j77_beta-glucosidase_a_E.C.3.2.1.21
- 4.) 2ceq_beta-galactosidase_E.C.3.2.1.23
- 5.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 6.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 7.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 8.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 9.) 4tmn_thermolysin_E.C.3.4.24.27
- 10.) 1ndy_adenosine_deaminase_E.C.3.5.4.4

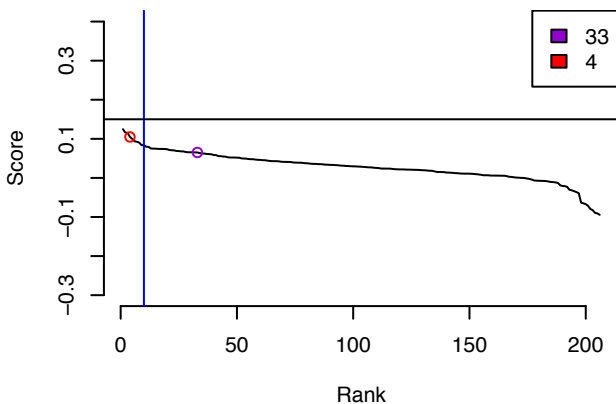
Query: 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64



Top 10 Ranked Pockets

- 1.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 2.) 2hdq_beta-lactamase_E.C.3.5.2.6
- 3.) 1tok_aspartate_aminotransferase_E.C.2.6.1.1
- 4.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 5.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 6.) 2f01_streptavidin_E.C.-.-.-.-
- 7.) 2g5u_transthyretin_E.C.-.-.-.-
- 8.) 1syh_glutamate_receptor_2_E.C.-.-.-.-
- 9.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 10.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37

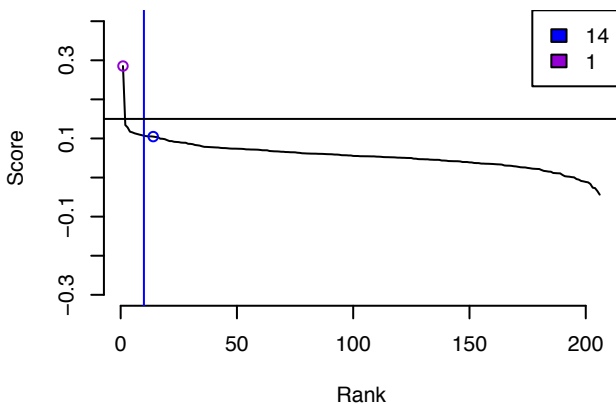
Query: 1zc9_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64



Top 10 Ranked Pockets

- 1.) 1kv5_triosephosphate_isomerase_E.C.5.3.1.1
- 2.) 1trd_triosephosphate_isomerase_E.C.5.3.1.1
- 3.) 4tim_triosephosphate_isomerase_E.C.5.3.1.1
- 4.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 5.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 6.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6
- 7.) 2hdq_beta-lactamase_E.C.3.5.2.6
- 8.) 1nny_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 9.) 1nwl_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 10.) 1bcu_thrombin_alpha_E.C.3.4.21.5

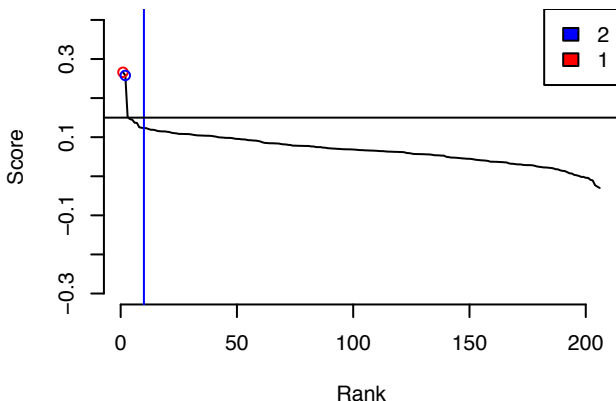
Query: 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64



Top 10 Ranked Pockets

- 1.) 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 2.) 2g5u_transthyretin_E.C.-.-.-.-
- 3.) 1y1m_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 4.) 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 5.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 6.) 2f01_streptavidin_E.C.-.-.-.-
- 7.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 8.) 1syh_glutamate_receptor_2_E.C.-.-.-.-
- 9.) 2hdq_beta-lactamase_E.C.3.5.2.6
- 10.) 1ols_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4

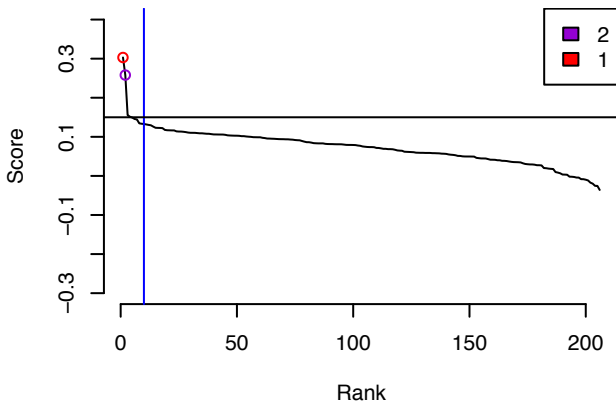
Query: 2fdp_beta-secretase_1_E.C.3.4.23.46



Top 10 Ranked Pockets

- 1.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 2.) 1fkn_secretase_beta_E.C.3.4.23.-
- 3.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 4.) 2i0d_HIV-1_protease_E.C.3.4.23.16
- 5.) 4fiv_FIV_protease_E.C.3.4.23.16
- 6.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 7.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 8.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 9.) 1kv1_mitogen-activated_protein_kinase_p38_E.C.2.7.1.37
- 10.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37

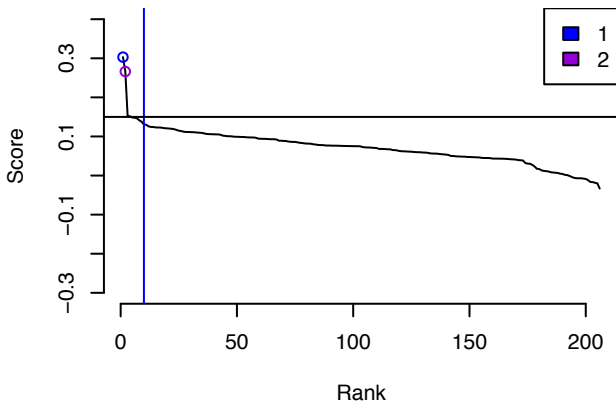
Query: 1fkn_secretase_beta_E.C.3.4.23.-



Top 10 Ranked Pockets

- 1.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 2.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 3.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 4.) 2i0d_HIV-1_protease_E.C.3.4.23.16
- 5.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 6.) 4fiv_FIV_protease_E.C.3.4.23.16
- 7.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 8.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 9.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 10.) 1u2y_alpha-amylase_E.C.3.2.1.1

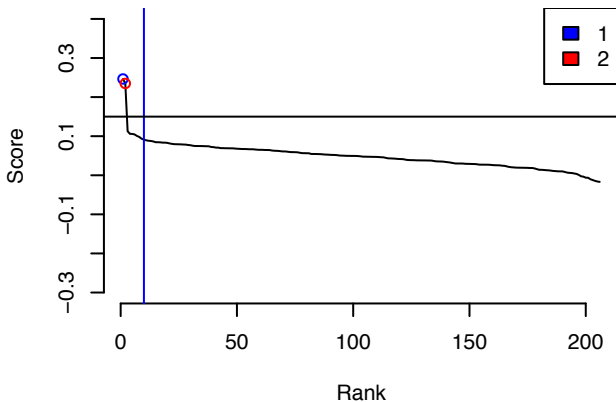
Query: 2g94_beta-secretase_1_E.C.3.4.23.46



Top 10 Ranked Pockets

- 1.) 1fkn_secretase_beta_E.C.3.4.23.-
- 2.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 3.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 4.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 5.) 2i0d_HIV-1_protease_E.C.3.4.23.16
- 6.) 4fiv_FIV_protease_E.C.3.4.23.16
- 7.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 8.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 9.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 10.) 1u2y_alpha-amylase_E.C.3.2.1.1

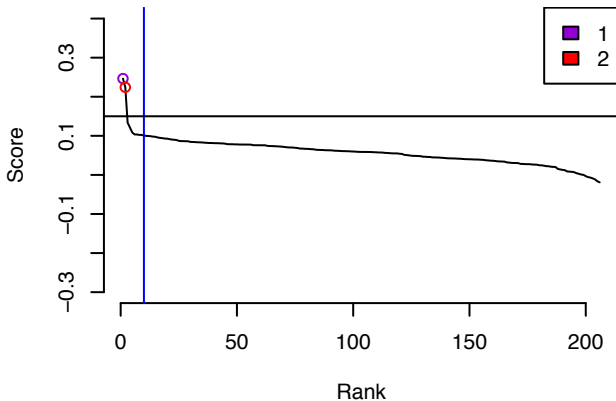
Query: 1v16_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4



Top 10 Ranked Pockets

- 1.) 1olu_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4
- 2.) 1ols_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4
- 3.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 4.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 5.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 6.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 7.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3
- 8.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 9.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 10.) 2ceq_beta-galactosidase_E.C.3.2.1.23

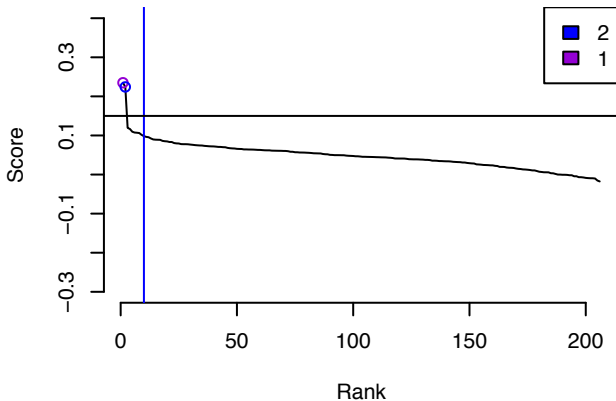
Query: 1olu_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4



Top 10 Ranked Pockets

- 1.) 1v16_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4
- 2.) 1ols_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4
- 3.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 4.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 5.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 6.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 7.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 8.) 1jq9_phospholipase_a2_E.C.3.1.1.4
- 9.) 1gni_serum_albumin_E.C.-.-.-
- 10.) 1ndz_adenosine_deaminase_E.C.3.5.4.4

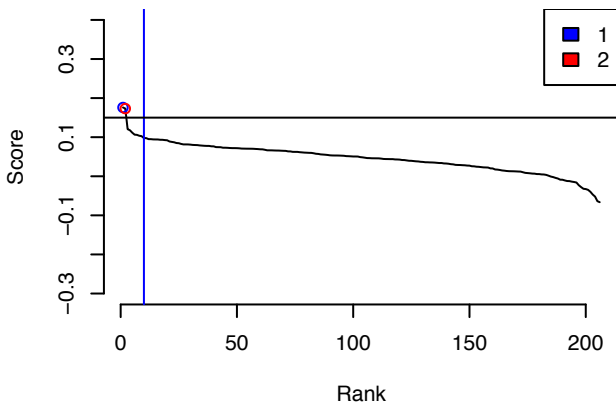
Query: 1ols_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4



Top 10 Ranked Pockets

- 1.) 1v16_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4
- 2.) 1olu_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4
- 3.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 4.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 5.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 6.) 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 7.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 8.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 9.) 2j77_beta-glucosidase_a_E.C.3.2.1.21
- 10.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3

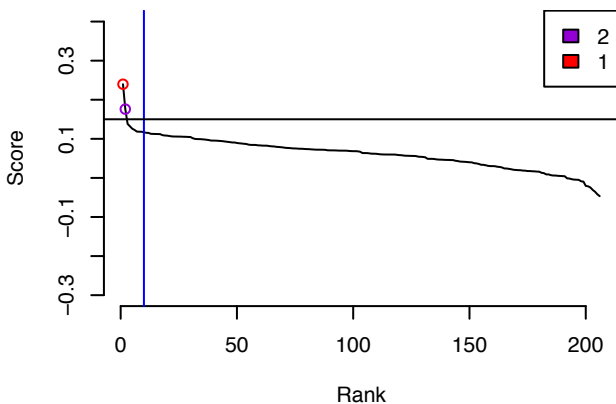
Query: 1tok_aspartate_aminotransferase_E.C.2.6.1.1



Top 10 Ranked Pockets

- 1.) 1toj_aspartate_aminotransferase_E.C.2.6.1.1
- 2.) 1toi_aspartate_aminotransferase_E.C.2.6.1.1
- 3.) 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 4.) 1lol_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 5.) 1nwl_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 6.) 2hdq_beta-lactamase_E.C.3.5.2.6
- 7.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 8.) 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 9.) 4fiv_FIV_protease_E.C.3.4.23.16
- 10.) 2f80_pol_polyprotein_E.C.3.4.23.16

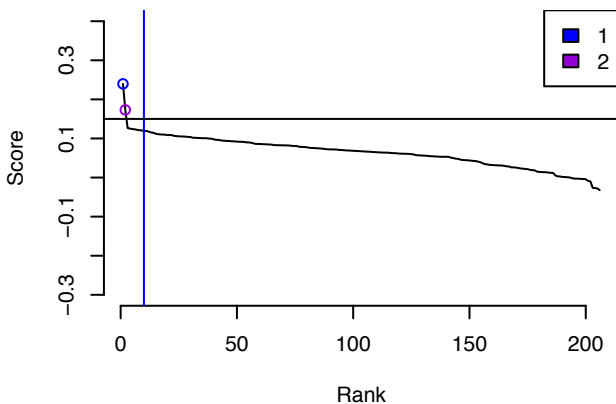
Query: 1toj_aspartate_aminotransferase_E.C.2.6.1.1



Top 10 Ranked Pockets

- 1.) 1toi_aspartate_aminotransferase_E.C.2.6.1.1
- 2.) 1tok_aspartate_aminotransferase_E.C.2.6.1.1
- 3.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 4.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 5.) 1gpk_acetylcholinesterase_E.C.3.1.1.7
- 6.) 1syh_glutamate_receptor_2_E.C.-.-.-.-
- 7.) 1q8t_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 8.) 1vfn_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 9.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 10.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37

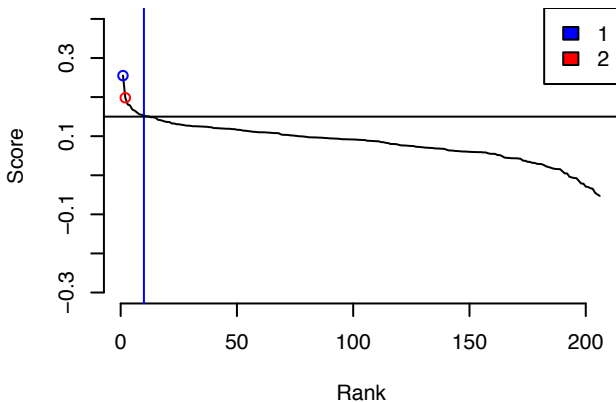
Query: 1toi_aspartate_aminotransferase_E.C.2.6.1.1



Top 10 Ranked Pockets

- 1.) 1toj_aspartate_aminotransferase_E.C.2.6.1.1
- 2.) 1tok_aspartate_aminotransferase_E.C.2.6.1.1
- 3.) 2bak_mitogen-activated_protein_kinase_14_E.C.2.7.1.37
- 4.) 4fiv_FIV_protease_E.C.3.4.23.16
- 5.) 1re8_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 6.) 1ydt_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 7.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 8.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 9.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 10.) 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-.-

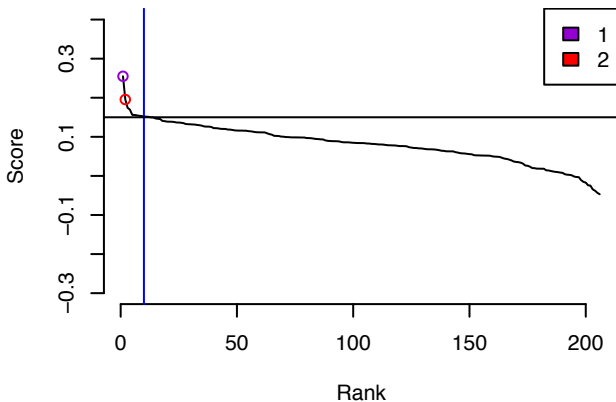
Query: 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29



Top 10 Ranked Pockets

- 1.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 2.) 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 3.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 4.) 1pz5_antibody_fab_E.C.-.-.-.-
- 5.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 6.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 7.) 1zs0_neutrophil_collagenase_E.C.3.4.24.34
- 8.) 1syh_glutamate_receptor_2_E.C.-.-.-.-
- 9.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 10.) 2b7d_coagulation_factor_vii_E.C.3.4.21.21

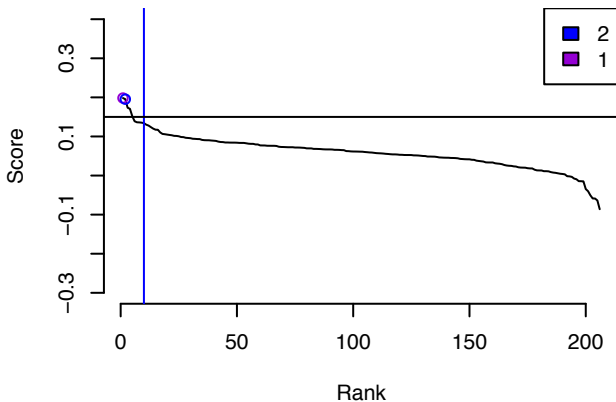
Query: 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29



Top 10 Ranked Pockets

- 1.) 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 2.) 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 3.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 4.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 5.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 6.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 7.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 8.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 9.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 10.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37

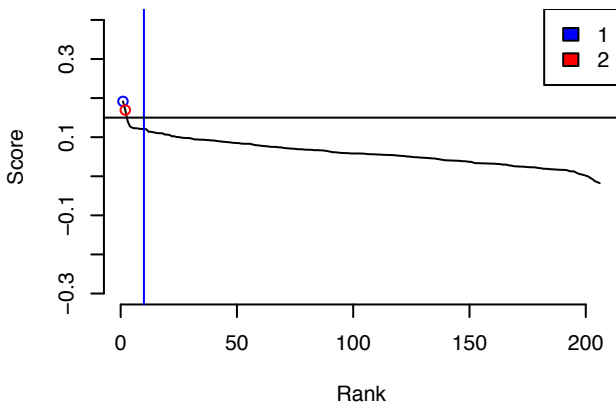
Query: 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29



Top 10 Ranked Pockets

- 1.) 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 2.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 3.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 4.) 1syh_glutamate_receptor_2_E.C.-.-.-.-
- 5.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34
- 6.) 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 7.) 1vfn_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 8.) 1pz5_antibody_fab_E.C.-.-.-.-
- 9.) 1zs0_neutrophil_collagenase_E.C.3.4.24.34
- 10.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34

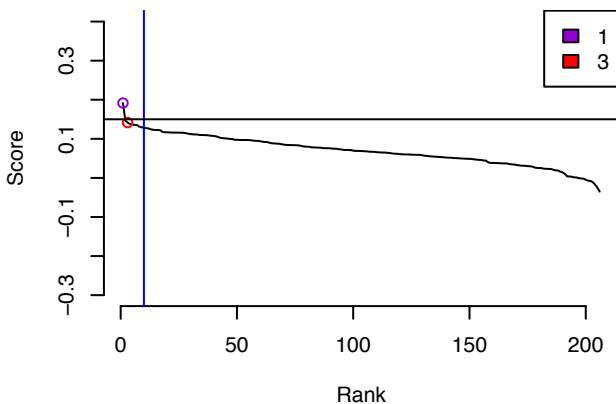
Query: 1kv1_mitogen-activated_protein_kinase_p38_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 2bak_mitogen-activated_protein_kinase_14_E.C.2.7.1.37
- 2.) 2baj_mitogen-activated_protein_kinase_14_E.C.2.7.1.37
- 3.) 4fiv_FIV_protease_E.C.3.4.23.16
- 4.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 5.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 6.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 7.) 1fkn_secretase_beta_E.C.3.4.23.-
- 8.) 2i0d_HIV-1_protease_E.C.3.4.23.16
- 9.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 10.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8

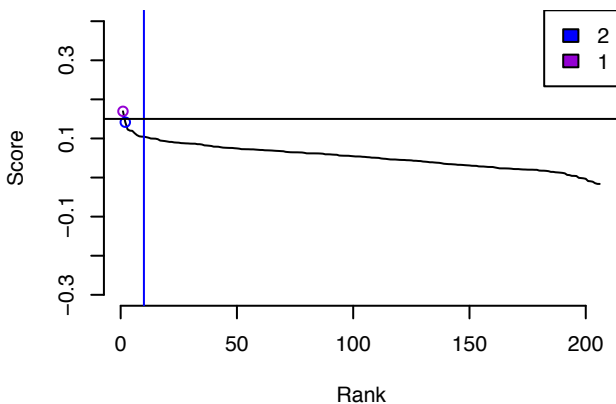
Query: 2bak_mitogen-activated_protein_kinase_14_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 1kv1_mitogen-activated_protein_kinase_p38_E.C.2.7.1.37
- 2.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 3.) 2baj_mitogen-activated_protein_kinase_14_E.C.2.7.1.37
- 4.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 5.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 6.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 7.) 4fiv_FIV_protease_E.C.3.4.23.16
- 8.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 9.) 1fkn_secretase_beta_E.C.3.4.23.-
- 10.) 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37

Query: 2baj_mitogen-activated_protein_kinase_14_E.C.2.7.1.37

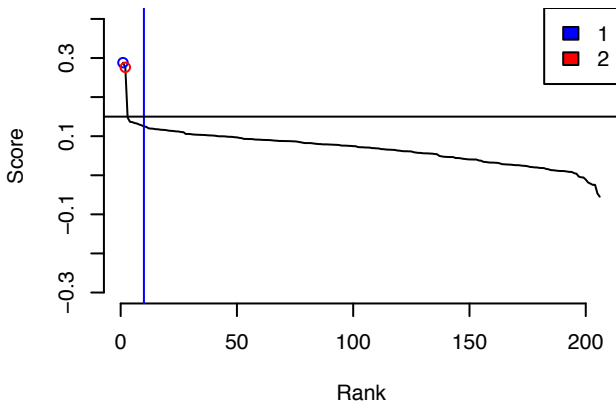


Top 10 Ranked Pockets

- 1.) 1kv1_mitogen-activated_protein_kinase_p38_E.C.2.7.1.37
- 2.) 2bak_mitogen-activated_protein_kinase_14_E.C.2.7.1.37
- 3.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 4.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 5.) 2b1v_estrogen_receptor_E.C.-.-.-.-
- 6.) 2fai_estrogen_receptor_E.C.-.-.-.-
- 7.) 1q8t_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 8.) 1fzk_h-2_class_i_histocompatibility_antigen_E.C.-.-.-.-
- 9.) 1ydt_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 10.) 1h23_acetylcholinesterase_E.C.3.1.1.7

Query: 1ndw_adenosine_deaminase_E.C.3.5.4.4

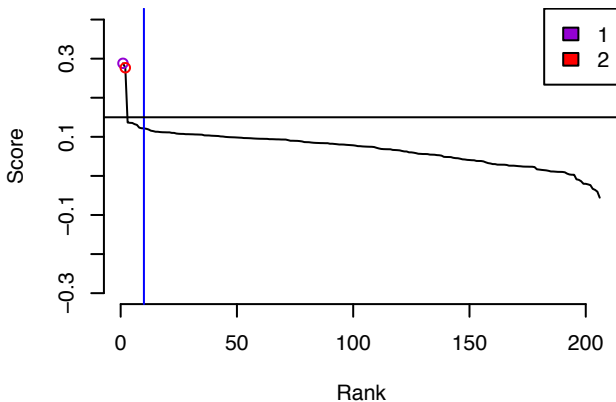
Top 10 Ranked Pockets



- 1.) 1ndy_adenosine_deaminase_E.C.3.5.4.4
- 2.) 1ndz_adenosine_deaminase_E.C.3.5.4.4
- 3.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 4.) 1u33_alpha-amylase_E.C.3.2.1.1
- 5.) 1u2y_alpha-amylase_E.C.3.2.1.1
- 6.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 7.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 8.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 9.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 10.) 2cer_beta-glucosidase_a_E.C.3.2.1.21

Query: 1ndy_adenosine_deaminase_E.C.3.5.4.4

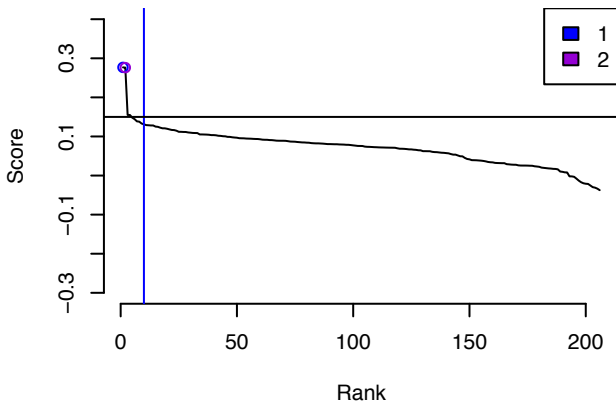
Top 10 Ranked Pockets



- 1.) 1ndw_adenosine_deaminase_E.C.3.5.4.4
- 2.) 1ndz_adenosine_deaminase_E.C.3.5.4.4
- 3.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 4.) 1u2y_alpha-amylase_E.C.3.2.1.1
- 5.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 6.) 1e66_acetylcholinesterase_E.C.3.1.1.7
- 7.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 8.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 9.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 10.) 1gpk_acetylcholinesterase_E.C.3.1.1.7

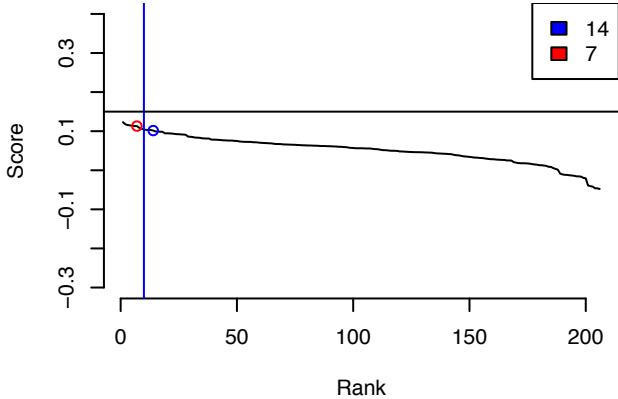
Query: 1ndz_adenosine_deaminase_E.C.3.5.4.4

Top 10 Ranked Pockets



- 1.) 1ndy_adenosine_deaminase_E.C.3.5.4.4
- 2.) 1ndw_adenosine_deaminase_E.C.3.5.4.4
- 3.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1u33_alpha-amylase_E.C.3.2.1.1
- 5.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 6.) 2i0d_HIV-1_protease_E.C.3.4.23.16
- 7.) 1gpk_acetylcholinesterase_E.C.3.1.1.7
- 8.) 4fiv_FIV_protease_E.C.3.4.23.16
- 9.) 1e66_acetylcholinesterase_E.C.3.1.1.7
- 10.) 2cet_beta-glucosidase_a_E.C.3.2.1.21

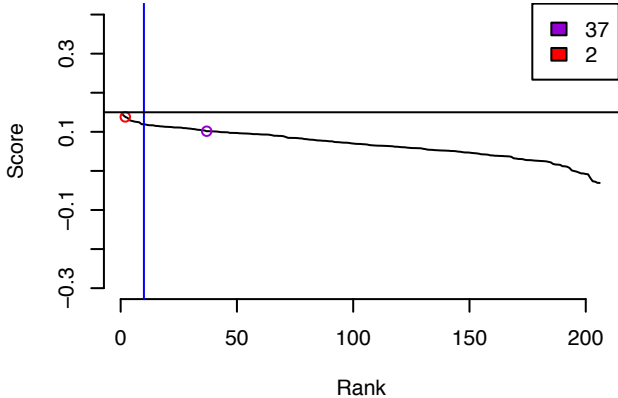
Query: 2hdq_beta-lactamase_E.C.3.5.2.6



Top 10 Ranked Pockets

- 1.) 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 2.) 1hk4_serum_albumin_E.C.-.-.-.-
- 3.) 1loI_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 4.) 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 5.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 6.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 7.) 1xgj_beta-lactamase_E.C.3.5.2.6
- 8.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 9.) 1tok_aspartate_aminotransferase_E.C.2.6.1.1
- 10.) 2i0d_HIV-1_protease_E.C.3.4.23.16

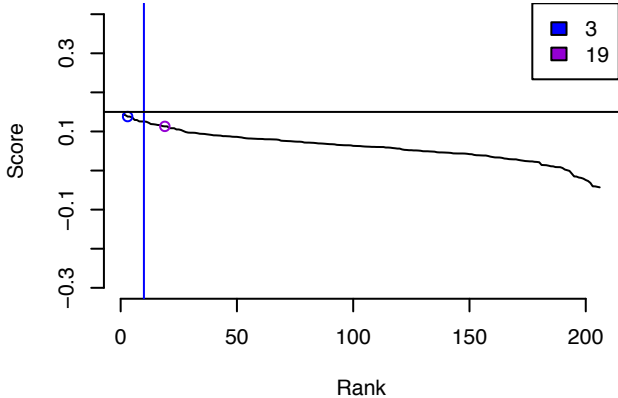
Query: 1l2s_beta-lactamase_E.C.3.5.2.6



Top 10 Ranked Pockets

- 1.) 1hk4_serum_albumin_E.C.-.-.-.-
- 2.) 1xgj_beta-lactamase_E.C.3.5.2.6
- 3.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 4.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 5.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 6.) 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 7.) 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 8.) 2d3u_polyprotein_E.C.2.7.7.48
- 9.) 1loI_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 10.) 1slg_streptavidin_E.C.-.-.-.-

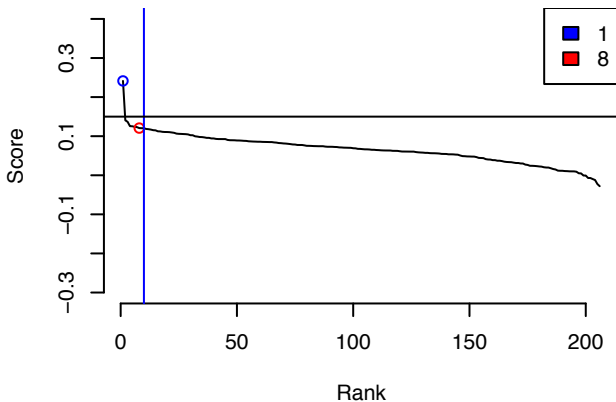
Query: 1xgj_beta-lactamase_E.C.3.5.2.6



Top 10 Ranked Pockets

- 1.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 2.) 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 3.) 1l2s_beta-lactamase_E.C.3.5.2.6
- 4.) 1nny_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 5.) 1hk4_serum_albumin_E.C.-.-.-.-
- 6.) 1ax0_lectin_E.C.-.-.-.-
- 7.) 1axz_lectin_E.C.-.-.-.-
- 8.) 6fiv_FIV_protease_E.C.3.4.23.16
- 9.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 10.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5

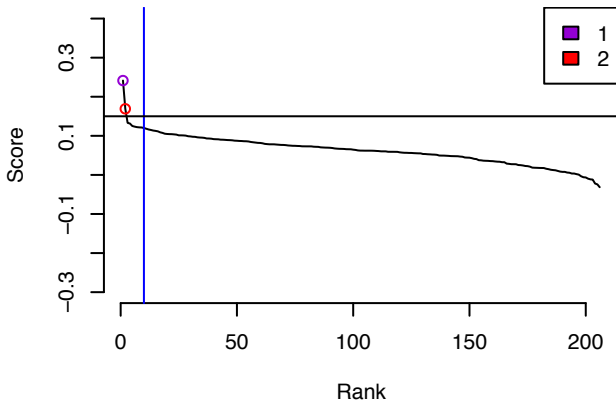
Query: 1q8t_cyclin_dependent_kinase_2_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 1ydt_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 2.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 3.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 4.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 5.) 4fiv_FIV_protease_E.C.3.4.23.16
- 6.) 2i0d_HIV-1_protease_E.C.3.4.23.16
- 7.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 8.) 1re8_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 9.) 1kv1_mitogen-activated_protein_kinase_p38_E.C.2.7.1.37
- 10.) 1om1_casein_kinase_ii_E.C.2.7.1.37

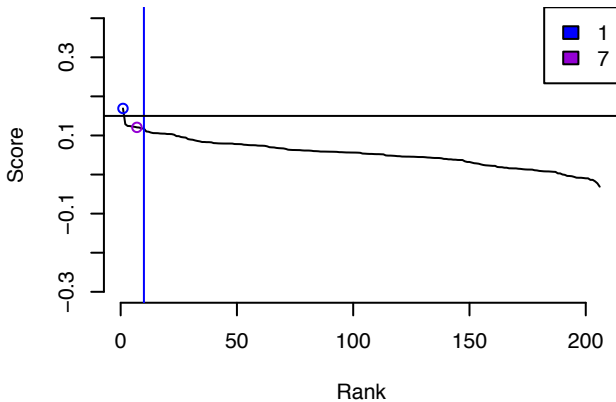
Query: 1ydt_cyclin_dependent_kinase_2_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 1q8t_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 2.) 1re8_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 3.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 4.) 4fiv_FIV_protease_E.C.3.4.23.16
- 5.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 6.) 1toi_aspartate_aminotransferase_E.C.2.6.1.1
- 7.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 8.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 9.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 10.) 2i0d_HIV-1_protease_E.C.3.4.23.16

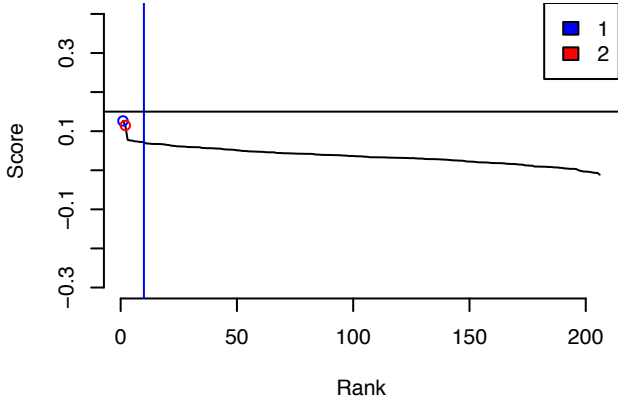
Query: 1re8_cyclin_dependent_kinase_2_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 1ydt_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 2.) 4er2_endothiaepsin_E.C.3.4.23.22
- 3.) 1ppm_penicillopepsin_E.C.3.4.23.20
- 4.) 1toi_aspartate_aminotransferase_E.C.2.6.1.1
- 5.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 6.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 7.) 1q8t_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 8.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 9.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 10.) 1apw_penicillopepsin_E.C.3.4.23.20

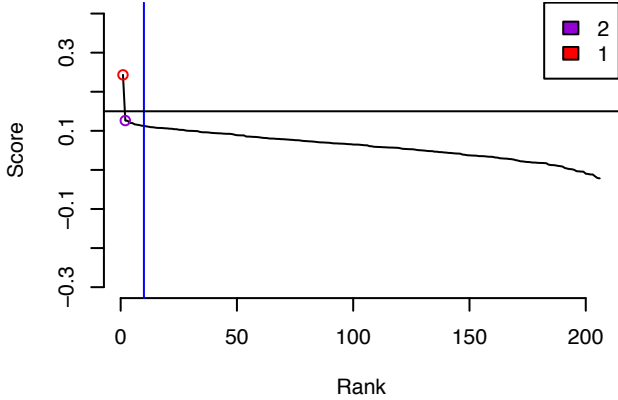
Query: 1fo0_h-2_class_i_histocompatibility_antigen_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1g7q_h-2_class_i_histocompatibility_antigen_E.C.-.-.-.-
- 2.) 1fzk_h-2_class_i_histocompatibility_antigen_E.C.-.-.-.-
- 3.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 4.) 2baj_mitogen-activated_protein_kinase_14_E.C.2.7.1.37
- 5.) 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 6.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 7.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 8.) 1nja_thymidylate_synthase_E.C.2.1.1.45
- 9.) 1b9j_oligo-peptide_binding_protein_E.C.-.-.-.-
- 10.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37

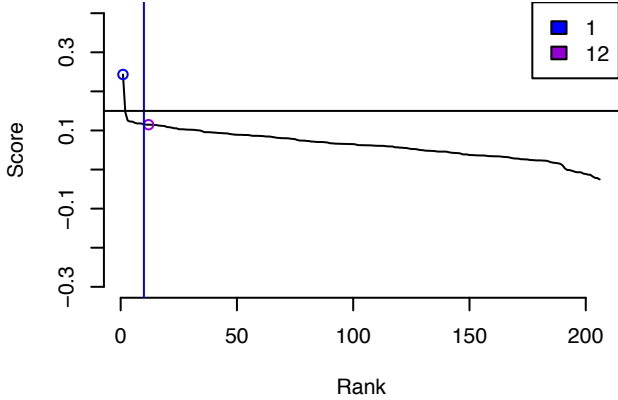
Query: 1g7q_h-2_class_i_histocompatibility_antigen_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1fzk_h-2_class_i_histocompatibility_antigen_E.C.-.-.-.-
- 2.) 1fo0_h-2_class_i_histocompatibility_antigen_E.C.-.-.-.-
- 3.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 4.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 5.) 2i0d_HIV-1_protease_E.C.3.4.23.16
- 6.) 1l2s_beta-lactamase_E.C.3.5.2.6
- 7.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 8.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 9.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 10.) 4tmn_thermolysin_E.C.3.4.24.27

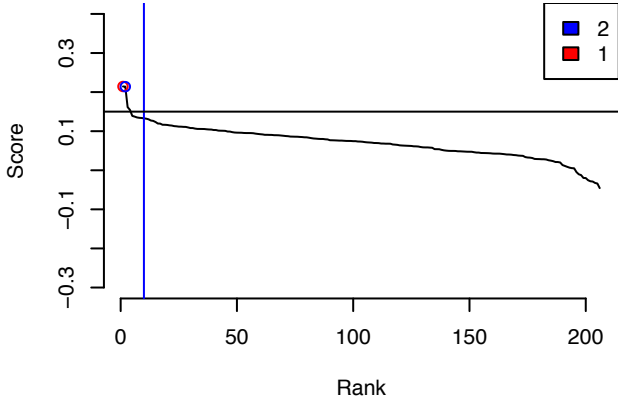
Query: 1fzk_h-2_class_i_histocompatibility_antigen_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1g7q_h-2_class_i_histocompatibility_antigen_E.C.-.-.-.-
- 2.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 3.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 4.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 5.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 6.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 7.) 1ndz_adenosine_deaminase_E.C.3.5.4.4
- 8.) 4tmn_thermolysin_E.C.3.4.24.27
- 9.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 10.) 2bak_mitogen-activated_protein_kinase_14_E.C.2.7.1.37

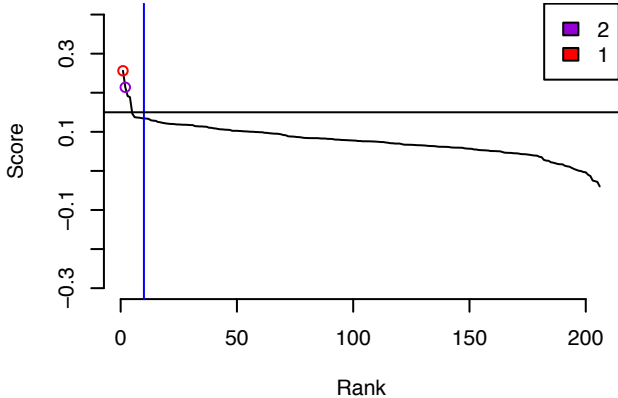
Query: 1m2q_casein_kinase_ii_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 2.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 3.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 4.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 5.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 6.) 1ajp_penicillin_amidohydrolase_E.C.3.5.1.11
- 7.) 1ai5_penicillin_amidohydrolase_E.C.3.5.1.11
- 8.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 9.) 1flr_antibody_fab_E.C.-.-.-.-
- 10.) 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37

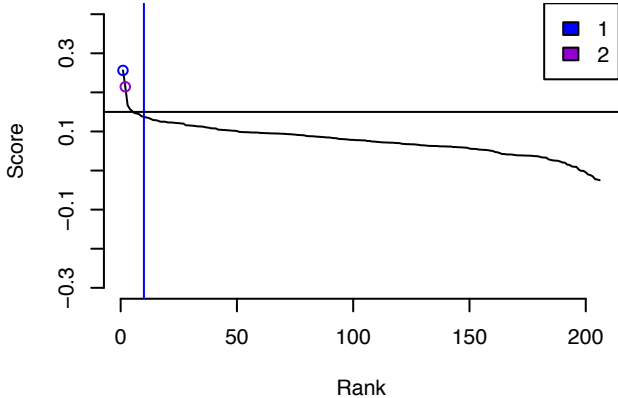
Query: 1om1_casein_kinase_ii_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 2.) 1m2q_casein_kinase_ii_E.C.2.7.1.37
- 3.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 4.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 5.) 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 6.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 7.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 8.) 1slg_streptavidin_E.C.-.-.-.-
- 9.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 10.) 1ai5_penicillin_amidohydrolase_E.C.3.5.1.11

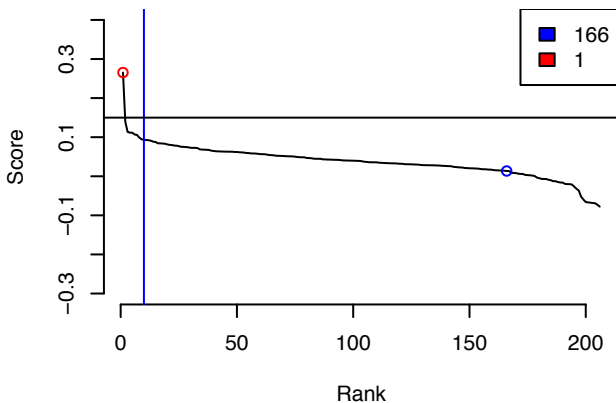
Query: 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 2.) 1m2q_casein_kinase_ii_E.C.2.7.1.37
- 3.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 4.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 5.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 6.) 2bak_mitogen-activated_protein_kinase_14_E.C.2.7.1.37
- 7.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 8.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 9.) 1gni_serum_albumin_E.C.-.-.-.-
- 10.) 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37

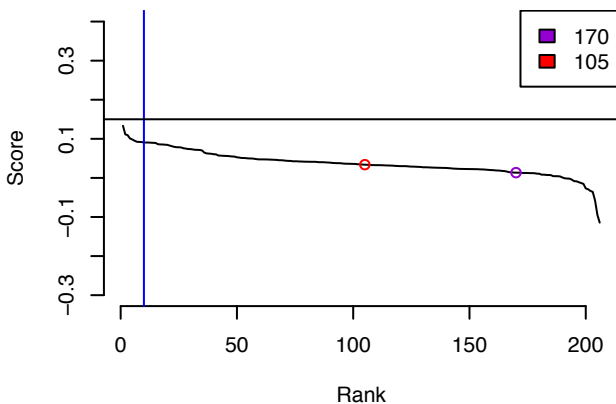
Query: 1nwl_tyrosine_phosphatase_1b_E.C.3.1.3.48



Top 10 Ranked Pockets

- 1.) 1nny_tyrosine_phosphatase_1b__E.C.3.1.3.48
- 2.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 3.) 4tim_triosephosphate_isomerase_E.C.5.3.1.1
- 4.) 1hk4_serum_albumin_E.C.-.-.-.-
- 5.) 1tok_aspartate_aminotransferase_E.C.2.6.1.1
- 6.) 2fzc_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 7.) 2ctc_carboxypeptidase_a_E.C.3.4.17.1
- 8.) 1l2s_beta-lactamase_E.C.3.5.2.6
- 9.) 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 10.) 1a08_tyrosine_kinase_src_E.C.2.7.1.112

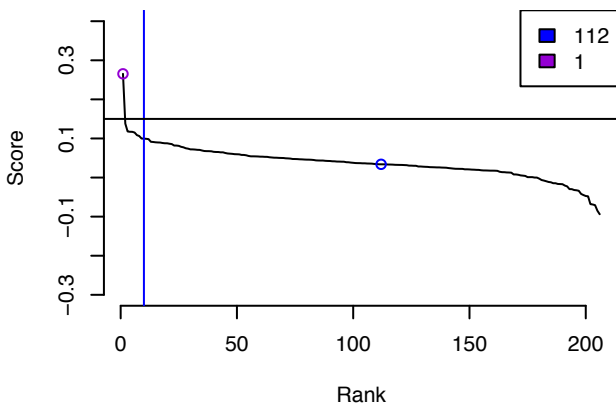
Query: 1c84_tyrosine_phosphatase_1b_E.C.3.1.3.48



Top 10 Ranked Pockets

- 1.) 2d3z_polyprotein_E.C.2.7.7.48
- 2.) 1ela_elastase_E.C.3.4.21.36
- 3.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 4.) 1nhu_hepatitis_c_virus_ns5b_rna_polymerase_E.C.2.7.7.48
- 5.) 1flr_antibody_fab_E.C.-.-.-.-
- 6.) 6fiv_FIV_protease_E.C.3.4.23.16
- 7.) 1d7l_FK506_binding_protein_E.C.5.2.1.8
- 8.) 1gz9_lectin_E.C.-.-.-.-
- 9.) 1df8_streptavidin_E.C.-.-.-.-
- 10.) 1y1m_glutamate_[nmda]_receptor_E.C.-.-.-.-

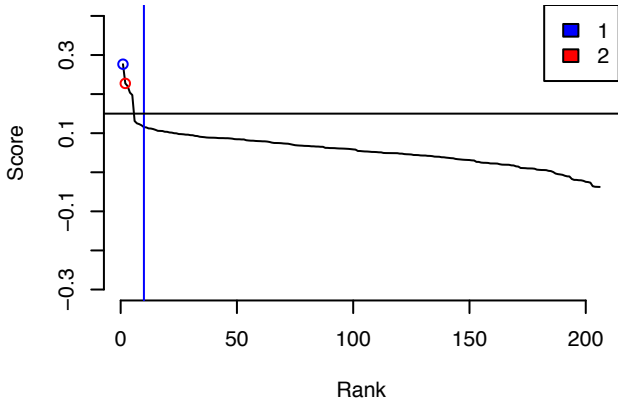
Query: 1nny_tyrosine_phosphatase_1b_E.C.3.1.3.48



Top 10 Ranked Pockets

- 1.) 1nwl_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 2.) 1xgj_beta-lactamase_E.C.3.5.2.6
- 3.) 1kv5_triosephosphate_isomerase_E.C.5.3.1.1
- 4.) 1nhu_hepatitis_c_virus_ns5b_rna_polymerase_E.C.2.7.7.48
- 5.) 4tim_triosephosphate_isomerase_E.C.5.3.1.1
- 6.) 1l2s_beta-lactamase_E.C.3.5.2.6
- 7.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 8.) 1o0h_ribonuclease_a_E.C.3.1.27.5
- 9.) 2flb_coagulation_factor_vii_E.C.3.4.21.21
- 10.) 2fzc_aspartate_carbamoyltransferase_E.C.2.1.3.2

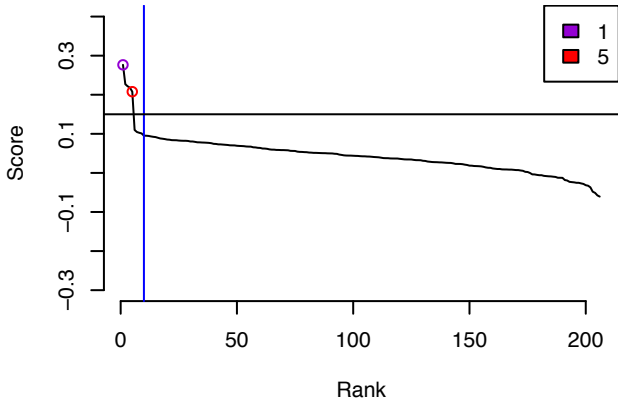
Query: 5er1_endothiapepsin_bw624_E.C.3.4.23.22



Top 10 Ranked Pockets

- 1.) 2er9_endothiapepsin_E.C.3.4.23.22
- 2.) 4er2_endothiapepsin_E.C.3.4.23.22
- 3.) 1apw_penicillopepsin_E.C.3.4.23.20
- 4.) 1ppm_penicillopepsin_E.C.3.4.23.20
- 5.) 1bxo_penicillopepsin_E.C.3.4.23.20
- 6.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 7.) 1xd1_alpha-amylase_E.C.3.2.1.1
- 8.) 1fkn_secretase_beta_E.C.3.4.23.-
- 9.) 4tmn_thermolysin_E.C.3.4.24.27
- 10.) 1vzq_thrombin_alpha_E.C.3.4.21.5

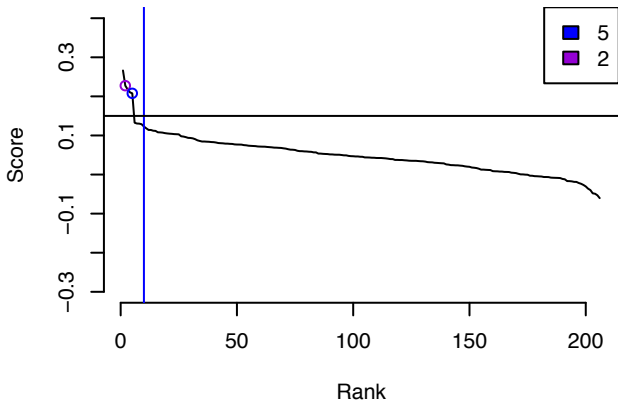
Query: 2er9_endothiapepsin_E.C.3.4.23.22



Top 10 Ranked Pockets

- 1.) 5er1_endothiapepsin_bw624_E.C.3.4.23.22
- 2.) 1ppm_penicillopepsin_E.C.3.4.23.20
- 3.) 1bxo_penicillopepsin_E.C.3.4.23.20
- 4.) 1apw_penicillopepsin_E.C.3.4.23.20
- 5.) 4er2_endothiapepsin_E.C.3.4.23.22
- 6.) 3gss_glutathione_s-transferase_E.C.2.5.1.18
- 7.) 1re8_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 8.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 9.) 10gs_glutathione_s-transferase_E.C.2.5.1.18
- 10.) 2i0d_HIV-1_protease_E.C.3.4.23.16

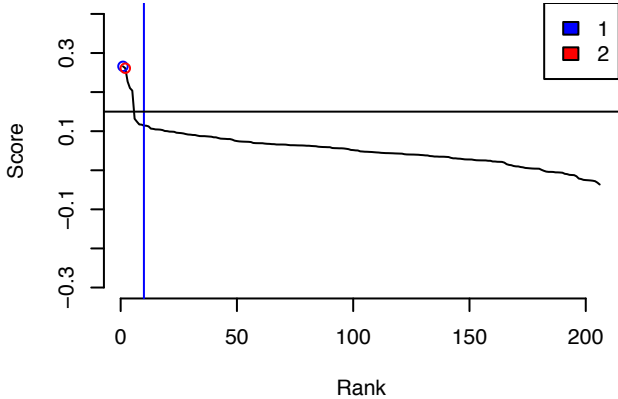
Query: 4er2_endothiapepsin_E.C.3.4.23.22



Top 10 Ranked Pockets

- 1.) 1apw_penicillopepsin_E.C.3.4.23.20
- 2.) 5er1_endothiapepsin_bw624_E.C.3.4.23.22
- 3.) 1bxo_penicillopepsin_E.C.3.4.23.20
- 4.) 1ppm_penicillopepsin_E.C.3.4.23.20
- 5.) 2er9_endothiapepsin_E.C.3.4.23.22
- 6.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 7.) 1vzq_thrombin_alpha_E.C.3.4.21.5
- 8.) 1u2y_alpha-amylase_E.C.3.2.1.1
- 9.) 1re8_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 10.) 1fkn_secretase_beta_E.C.3.4.23.-

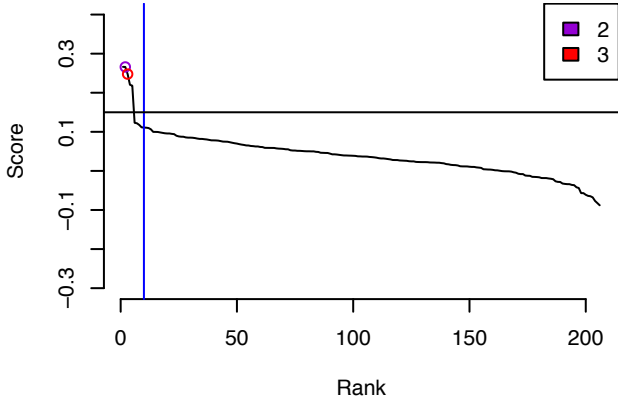
Query: 1ppm_penicillopepsin_E.C.3.4.23.20



Top 10 Ranked Pockets

- 1.) 1apw_penicillopepsin_E.C.3.4.23.20
- 2.) 1bxo_penicillopepsin_E.C.3.4.23.20
- 3.) 2er9_endothiaepsin_E.C.3.4.23.22
- 4.) 4er2_endothiaepsin_E.C.3.4.23.22
- 5.) 5er1_endothiaepsin_bw624_E.C.3.4.23.22
- 6.) 1xd1_alpha-amylase_E.C.3.2.1.1
- 7.) 1re8_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 8.) 1u33_alpha-amylase_E.C.3.2.1.1
- 9.) 1ndw_adenosine_deaminase_E.C.3.5.4.4
- 10.) 1u2y_alpha-amylase_E.C.3.2.1.1

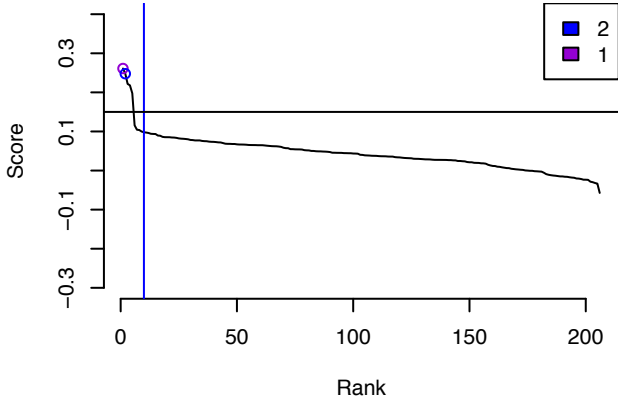
Query: 1apw_penicillopepsin_E.C.3.4.23.20



Top 10 Ranked Pockets

- 1.) 4er2_endothiaepsin_E.C.3.4.23.22
- 2.) 1ppm_penicillopepsin_E.C.3.4.23.20
- 3.) 1bxo_penicillopepsin_E.C.3.4.23.20
- 4.) 5er1_endothiaepsin_bw624_E.C.3.4.23.22
- 5.) 2er9_endothiaepsin_E.C.3.4.23.22
- 6.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 7.) 1u33_alpha-amylase_E.C.3.2.1.1
- 8.) 1re8_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 9.) 1xd1_alpha-amylase_E.C.3.2.1.1
- 10.) 1fkn_secretase_beta_E.C.3.4.23.-

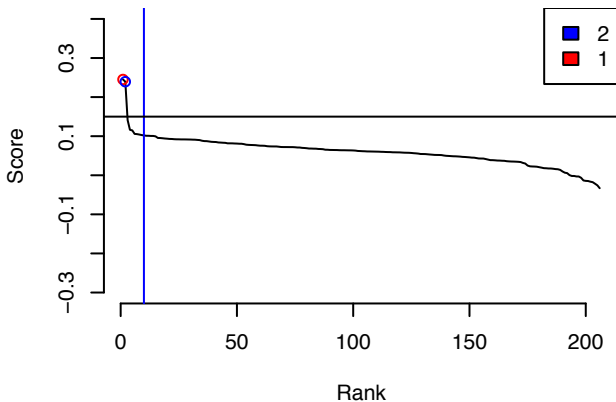
Query: 1bxo_penicillopepsin_E.C.3.4.23.20



Top 10 Ranked Pockets

- 1.) 1ppm_penicillopepsin_E.C.3.4.23.20
- 2.) 1apw_penicillopepsin_E.C.3.4.23.20
- 3.) 2er9_endothiaepsin_E.C.3.4.23.22
- 4.) 4er2_endothiaepsin_E.C.3.4.23.22
- 5.) 5er1_endothiaepsin_bw624_E.C.3.4.23.22
- 6.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 7.) 1vzq_thrombin_alpha_E.C.3.4.21.5
- 8.) 1re8_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 9.) 1u2y_alpha-amylase_E.C.3.2.1.1
- 10.) 1ndy_adenosine_deaminase_E.C.3.5.4.4

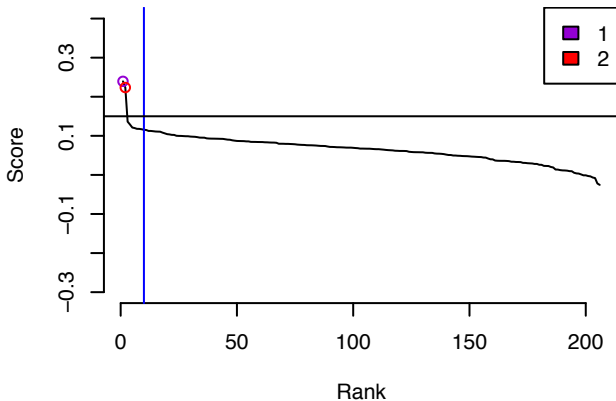
Query: 1nje_thymidylate_synthase_E.C.2.1.1.45



Top 10 Ranked Pockets

- 1.) 1nja_thymidylate_synthase_E.C.2.1.1.45
- 2.) 1tsy_thymidylate_synthase_E.C.2.1.1.45
- 3.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 5.) 1pr5_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 6.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 7.) 1hfs_stromelysin-1_E.C.3.4.24.17
- 8.) 3gss_glutathione_s-transferase_E.C.2.5.1.18
- 9.) 2fzc_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 10.) 2gss_glutathione_s-transferase_E.C.2.5.1.18

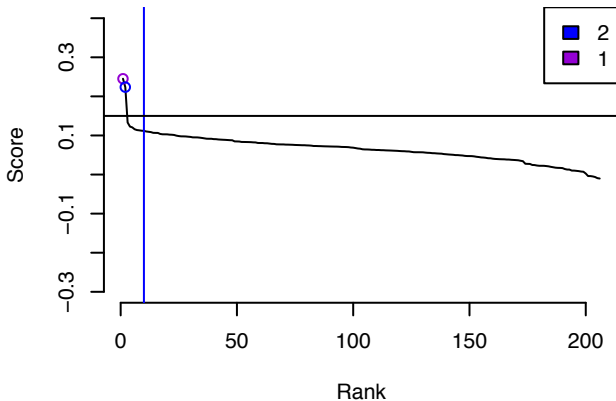
Query: 1tsy_thymidylate_synthase_E.C.2.1.1.45



Top 10 Ranked Pockets

- 1.) 1nje_thymidylate_synthase_E.C.2.1.1.45
- 2.) 1nja_thymidylate_synthase_E.C.2.1.1.45
- 3.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 5.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 6.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 7.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 8.) 1pz5_antibody_fab_E.C.-.-.-.-
- 9.) 1hfs_stromelysin-1_E.C.3.4.24.17
- 10.) 1slg_streptavidin_E.C.-.-.-.-

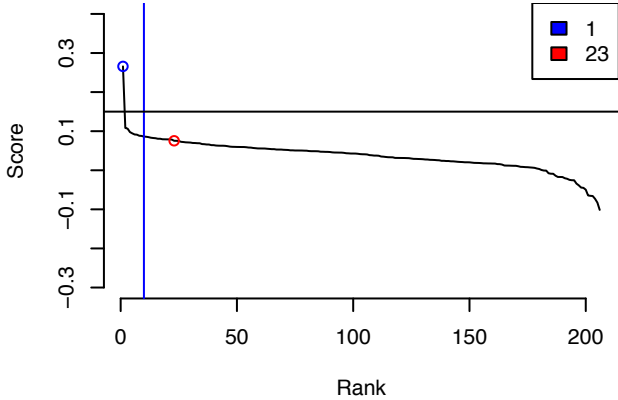
Query: 1nja_thymidylate_synthase_E.C.2.1.1.45



Top 10 Ranked Pockets

- 1.) 1nje_thymidylate_synthase_E.C.2.1.1.45
- 2.) 1tsy_thymidylate_synthase_E.C.2.1.1.45
- 3.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 5.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 6.) 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 7.) 1slg_streptavidin_E.C.-.-.-.-
- 8.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 9.) 1jqe_histamine_n-methyltransferase_E.C.2.1.1.8
- 10.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3

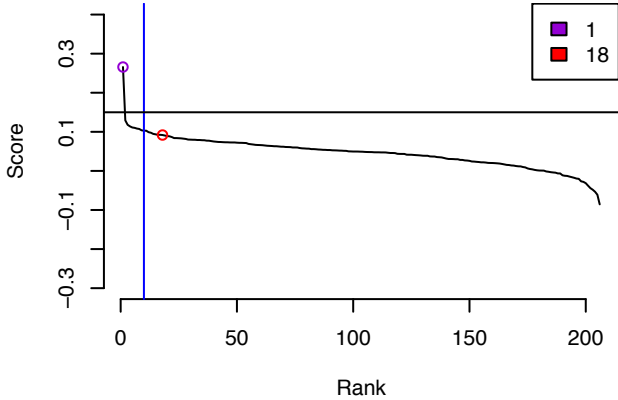
Query: 4tl_n_thermolysin_E.C.3.4.24.27



Top 10 Ranked Pockets

- 1.) 1tmn_thermolysin_E.C.3.4.24.27
- 2.) 2usn_stromelysin-1_E.C.3.4.24.17
- 3.) 1fh8_xylanase_beta-1,4_E.C.3.2.1.91
- 4.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34
- 5.) 1u33_alpha-amylase_E.C.3.2.1.1
- 6.) 2j77_beta-glucosidase_a_E.C.3.2.1.21
- 7.) 1fkn_secretase_beta_E.C.3.4.23.-
- 8.) 2ctc_carboxypeptidase_a_E.C.3.4.17.1
- 9.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 10.) 1ndy_adenosine_deaminase_E.C.3.5.4.4

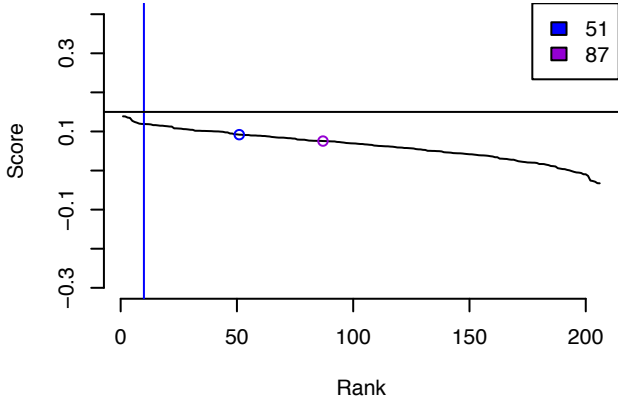
Query: 1tmn_thermolysin_E.C.3.4.24.27



Top 10 Ranked Pockets

- 1.) 4tl_n_thermolysin_E.C.3.4.24.27
- 2.) 2usn_stromelysin-1_E.C.3.4.24.17
- 3.) 1rvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 4.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 5.) 1u33_alpha-amylase_E.C.3.2.1.1
- 6.) 1fkn_secretase_beta_E.C.3.4.23.-
- 7.) 1fh8_xylanase_beta-1,4_E.C.3.2.1.91
- 8.) 1pz5_antibody_fab_E.C.-.-.-.-
- 9.) 1u2y_alpha-amylase_E.C.3.2.1.1
- 10.) 1a30_HIV-1_protease_E.C.3.4.23.16

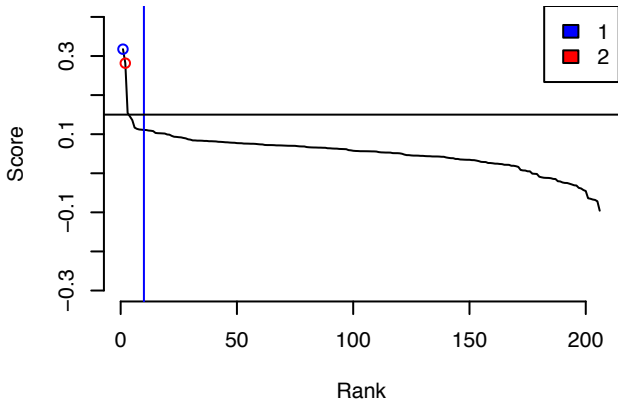
Query: 4tmn_thermolysin_E.C.3.4.24.27



Top 10 Ranked Pockets

- 1.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 2.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 3.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 5.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 6.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 7.) 2usn_stromelysin-1_E.C.3.4.24.17
- 8.) 5er1_endothiaepsin_bw624_E.C.3.4.23.22
- 9.) 1flr_antibody_fab_E.C.-.-.-.-
- 10.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29

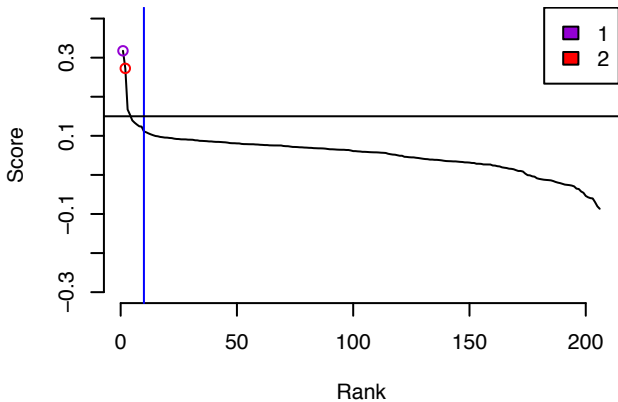
Query: 1fh7_xylanase_beta-1,4_E.C.3.2.1.91



Top 10 Ranked Pockets

- 1.) 1fh9_xylanase_beta-1,4_E.C.3.2.1.91
- 2.) 1fh8_xylanase_beta-1,4_E.C.3.2.1.91
- 3.) 2j77_beta-glucosidase_a_E.C.3.2.1.21
- 4.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 5.) 1pz5_antibody_fab_E.C.-.-.-.-
- 6.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 7.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 8.) 1u2y_alpha-amylase_E.C.3.2.1.1
- 9.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 10.) 1a30_HIV-1_protease_E.C.3.4.23.16

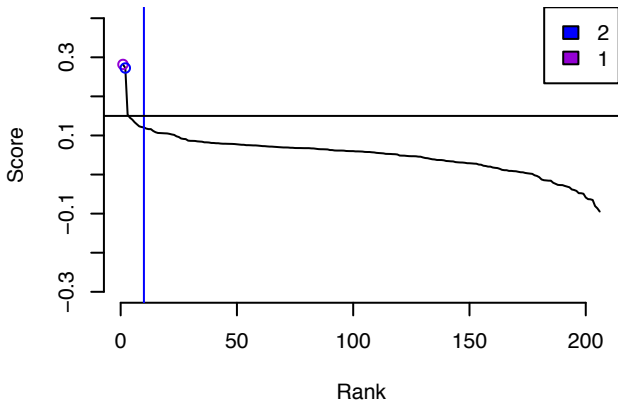
Query: 1fh9_xylanase_beta-1,4_E.C.3.2.1.91



Top 10 Ranked Pockets

- 1.) 1fh7_xylanase_beta-1,4_E.C.3.2.1.91
- 2.) 1fh8_xylanase_beta-1,4_E.C.3.2.1.91
- 3.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 4.) 2j77_beta-glucosidase_a_E.C.3.2.1.21
- 5.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 6.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 7.) 1flr_antibody_fab_E.C.-.-.-.-
- 8.) 2usn_stromelysin-1_E.C.3.4.24.17
- 9.) 2ceq_beta-galactosidase_E.C.3.2.1.23
- 10.) 1u33_alpha-amylase_E.C.3.2.1.1

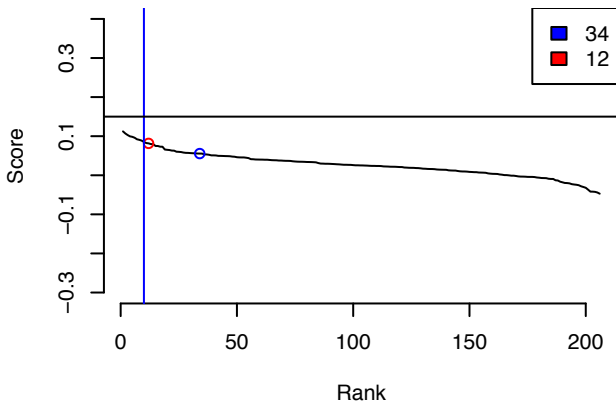
Query: 1fh8_xylanase_beta-1,4_E.C.3.2.1.91



Top 10 Ranked Pockets

- 1.) 1fh7_xylanase_beta-1,4_E.C.3.2.1.91
- 2.) 1fh9_xylanase_beta-1,4_E.C.3.2.1.91
- 3.) 2j77_beta-glucosidase_a_E.C.3.2.1.21
- 4.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 5.) 2usn_stromelysin-1_E.C.3.4.24.17
- 6.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 7.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 8.) 1u33_alpha-amylase_E.C.3.2.1.1
- 9.) 1flr_antibody_fab_E.C.-.-.-.-
- 10.) 2gss_glutathione_s-transferase_E.C.2.5.1.18

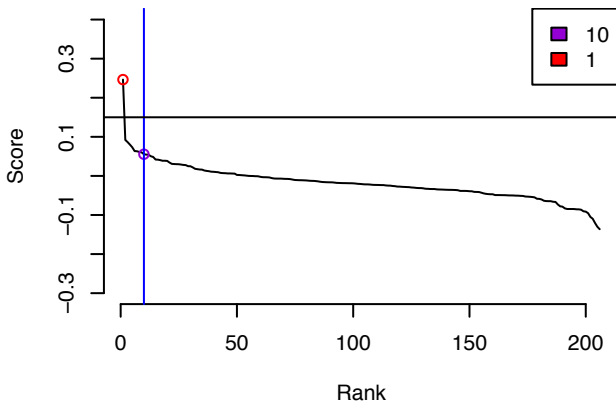
Query: 2fzc_aspartate_carbamoyltransferase_E.C.2.1.3.2



Top 10 Ranked Pockets

- 1.) 2qwd_neuraminidase_E.C.3.2.1.18
- 2.) 1nwl_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 3.) 1nje_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1nny_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 5.) 2hdq_beta-lactamase_E.C.3.5.2.6
- 6.) 1pr5_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 7.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 8.) 2qwe_neuraminidase_E.C.3.2.1.18
- 9.) 1l2s_beta-lactamase_E.C.3.5.2.6
- 10.) 1lol_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23

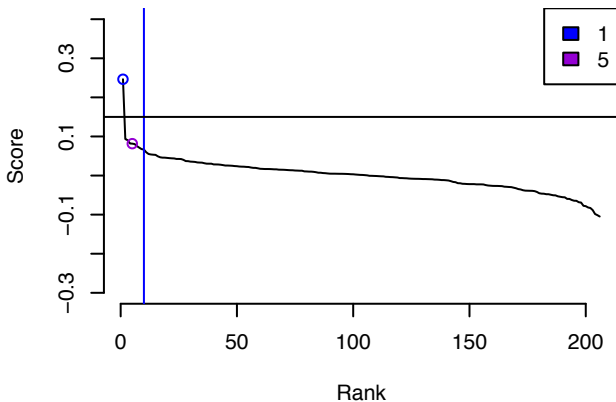
Query: 2h3e_aspartate_carbamoyltransferase_E.C.2.1.3.2



Top 10 Ranked Pockets

- 1.) 1d09_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 2.) 1a1b_tyrosine_kinase_C-src_E.C.2.7.1.112
- 3.) 1is0_tyrosine_kinase_C-src_E.C.2.7.1.112
- 4.) 1x1z_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 5.) 1a08_tyrosine_kinase_C-src_E.C.2.7.1.112
- 6.) 4tim_triosephosphate_isomerase_E.C.5.3.1.1
- 7.) 1nje_thymidylate_synthase_E.C.2.1.1.45
- 8.) 1kv5_triosephosphate_isomerase_E.C.5.3.1.1
- 9.) 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 10.) 2fzc_aspartate_carbamoyltransferase_E.C.2.1.3.2

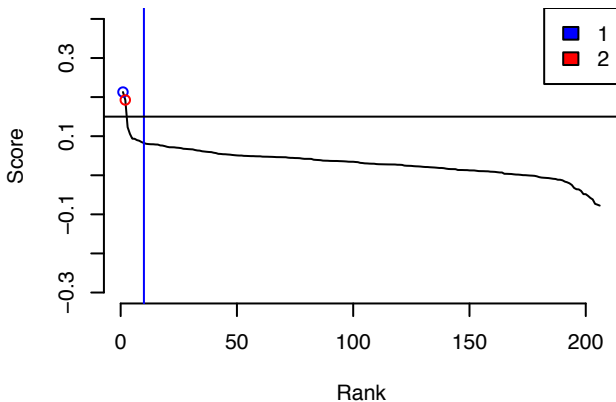
Query: 1d09_aspartate_carbamoyltransferase_E.C.2.1.3.2



Top 10 Ranked Pockets

- 1.) 2h3e_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 2.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 3.) 1a08_tyrosine_kinase_C-src_E.C.2.7.1.112
- 4.) 1a1b_tyrosine_kinase_C-src_E.C.2.7.1.112
- 5.) 2fzc_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 6.) 1x1z_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 7.) 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 8.) 1kv5_triosephosphate_isomerase_E.C.5.3.1.1
- 9.) 2hdq_beta-lactamase_E.C.3.5.2.6
- 10.) 1v16_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4

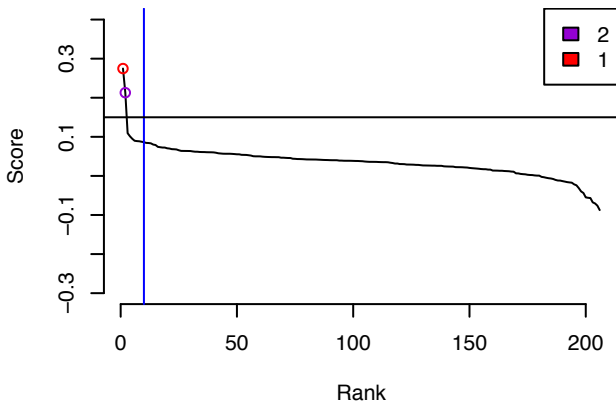
Query: 2ctc_carboxypeptidase_a_E.C.3.4.17.1



Top 10 Ranked Pockets

- 1.) 8cpa_carboxypeptidase_a_E.C.3.4.17.1
- 2.) 7cpa_carboxypeptidase_a_E.C.3.4.17.1
- 3.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 4.) 1nwl_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 5.) 2f01_streptavidin_E.C.-.-.-.-
- 6.) 1tok_aspartate_aminotransferase_E.C.2.6.1.1
- 7.) 1loI_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 8.) 4tlN_thermolysin_E.C.3.4.24.27
- 9.) 1q8t_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 10.) 1e5a_tranthyretin_E.C.-.-.-.-

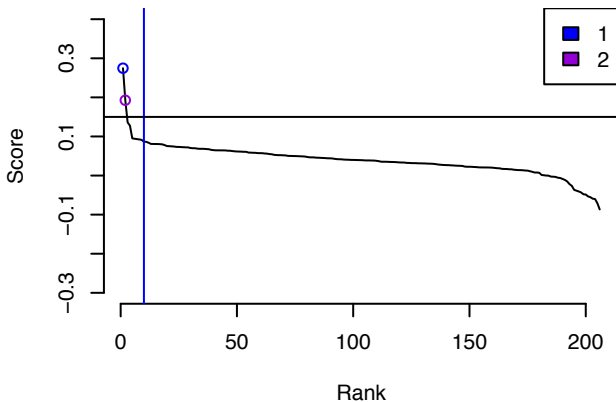
Query: 8cpa_carboxypeptidase_a_E.C.3.4.17.1



Top 10 Ranked Pockets

- 1.) 7cpa_carboxypeptidase_a_E.C.3.4.17.1
- 2.) 2ctc_carboxypeptidase_a_E.C.3.4.17.1
- 3.) 1loI_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 4.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 5.) 2qwd_neuraminidase_E.C.3.2.1.18
- 6.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 7.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 8.) 1ajq_penicillin_amidohydrolase_E.C.3.5.1.11
- 9.) 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 10.) 2qwe_neuraminidase_E.C.3.2.1.18

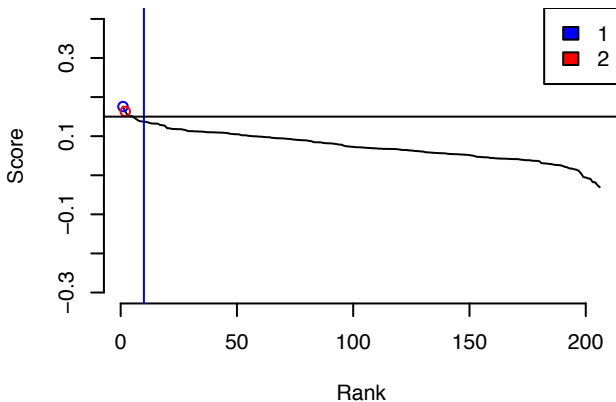
Query: 7cpa_carboxypeptidase_a_E.C.3.4.17.1



Top 10 Ranked Pockets

- 1.) 8cpa_carboxypeptidase_a_E.C.3.4.17.1
- 2.) 2ctc_carboxypeptidase_a_E.C.3.4.17.1
- 3.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 4.) 1loI_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 5.) 2qwb_neuraminidase_E.C.3.2.1.18
- 6.) 1tok_aspartate_aminotransferase_E.C.2.6.1.1
- 7.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 8.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34
- 9.) 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 10.) 2qwe_neuraminidase_E.C.3.2.1.18

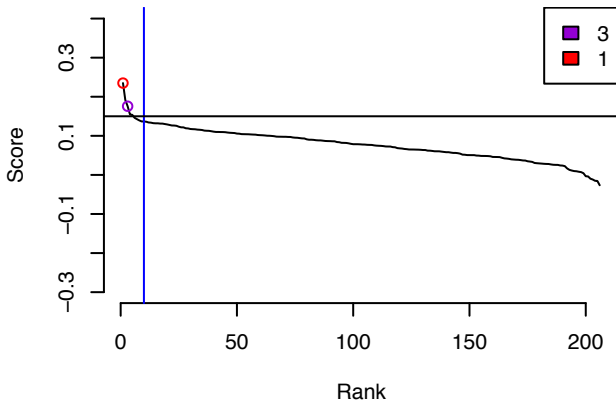
Query: 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 2.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 3.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 4.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 5.) 1hk4_serum_albumin_E.C.-.-.-.-
- 6.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 7.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 8.) 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 9.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 10.) 2f80_pol_polyprotein_E.C.3.4.23.16

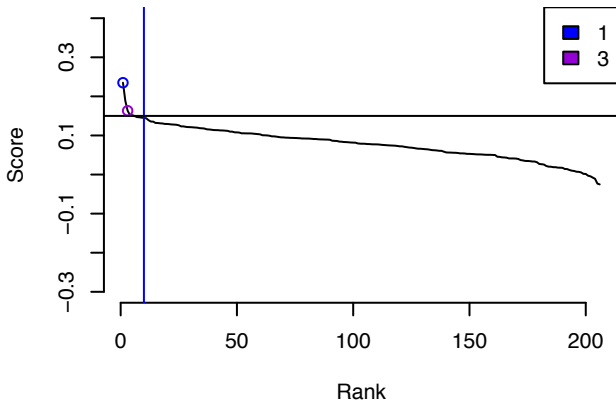
Query: 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 2.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 3.) 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 4.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 5.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 6.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 7.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 8.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 9.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 10.) 1q8t_cyclin_dependent_kinase_2_E.C.2.7.1.37

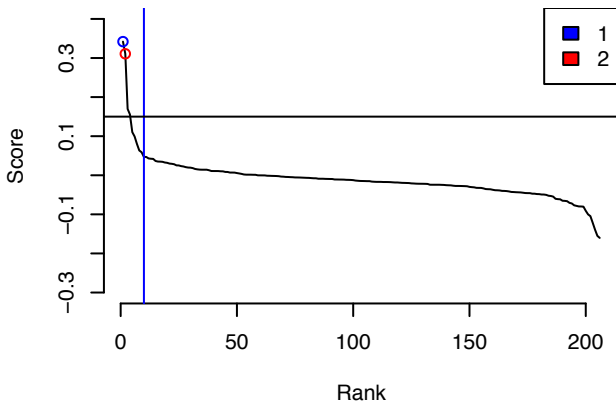
Query: 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 2.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 3.) 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 4.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 5.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 6.) 1hk4_serum_albumin_E.C.-.-.-.-
- 7.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 8.) 1jq9_phospholipase_a2_E.C.3.1.1.4
- 9.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 10.) 1q7a_phospholipase_a2_E.C.3.1.1.4

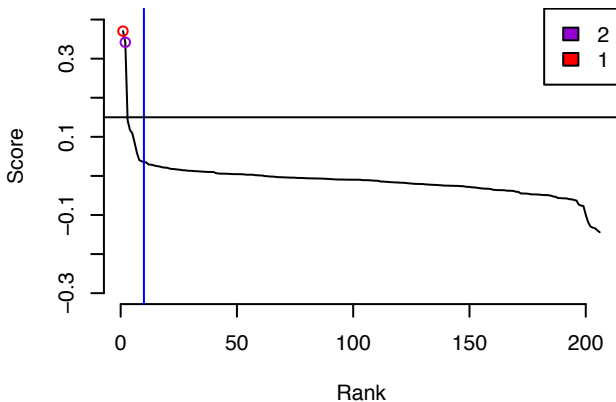
Query: 1abf_apolipoprotein_E.C.-.-.-



Top 10 Ranked Pockets

- 1.) 5abp_apolipoprotein_E.C.-.-.-
- 2.) 8abp_apolipoprotein_E.C.-.-.-
- 3.) 1ftm_glutamate_receptor_2_E.C.-.-.-
- 4.) 1p1q_glutamate_receptor_2_E.C.-.-.-
- 5.) 1x1z_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 6.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 7.) 1trd_triosephosphate_isomerase_E.C.5.3.1.1
- 8.) 7cpa_carboxypeptidase_a_E.C.3.4.17.1
- 9.) 1pb9_glutamate_[nmda]_receptor_E.C.-.-.-
- 10.) 1zc9_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64

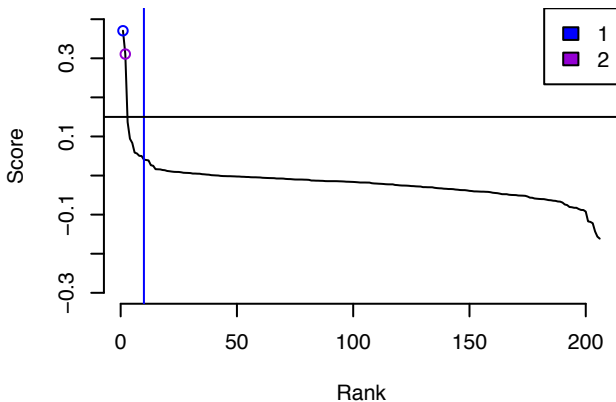
Query: 5abp_apolipoprotein_E.C.-.-.-



Top 10 Ranked Pockets

- 1.) 8abp_apolipoprotein_E.C.-.-.-
- 2.) 1abf_apolipoprotein_E.C.-.-.-
- 3.) 1ftm_glutamate_receptor_2_E.C.-.-.-
- 4.) 1pb9_glutamate_[nmda]_receptor_E.C.-.-.-
- 5.) 1p1q_glutamate_receptor_2_E.C.-.-.-
- 6.) 1x1z_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 7.) 1trd_triosephosphate_isomerase_E.C.5.3.1.1
- 8.) 7cpa_carboxypeptidase_a_E.C.3.4.17.1
- 9.) 2d3z_polyprotein_E.C.2.7.7.48
- 10.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64

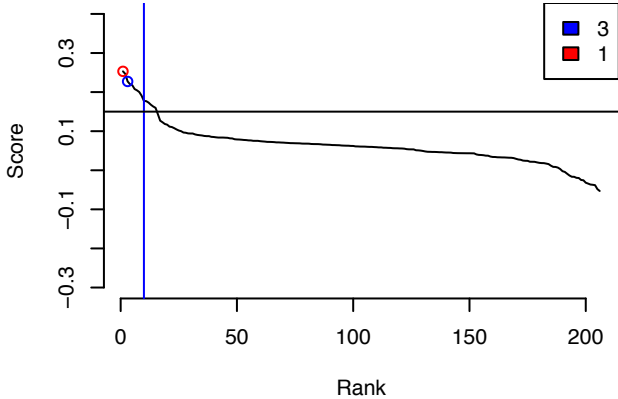
Query: 8abp_apolipoprotein_E.C.-.-.-



Top 10 Ranked Pockets

- 1.) 5abp_apolipoprotein_E.C.-.-.-
- 2.) 1abf_apolipoprotein_E.C.-.-.-
- 3.) 1ftm_glutamate_receptor_2_E.C.-.-.-
- 4.) 1p1q_glutamate_receptor_2_E.C.-.-.-
- 5.) 1x1z_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 6.) 7cpa_carboxypeptidase_a_E.C.3.4.17.1
- 7.) 1pb9_glutamate_[nmda]_receptor_E.C.-.-.-
- 8.) 2ctc_carboxypeptidase_a_E.C.3.4.17.1
- 9.) 1trd_triosephosphate_isomerase_E.C.5.3.1.1
- 10.) 1zc9_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64

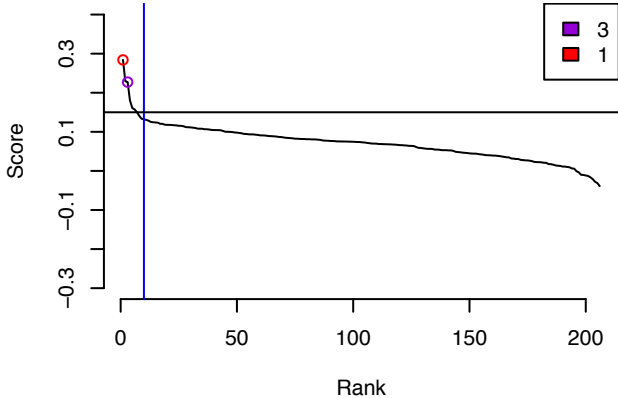
Query: 1bcu_thrombin_alpha_E.C.3.4.21.5



Top 10 Ranked Pockets

- 1.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 2.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6
- 3.) 1vzq_thrombin_alpha_E.C.3.4.21.5
- 4.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 5.) 2bok_coagulation_factor_xa_E.C.3.4.21.6
- 6.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 7.) 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4
- 8.) 1j17_trypsin_beta_E.C.3.4.21.4
- 9.) 1utp_trypsinogen_E.C.3.4.21.4
- 10.) 2bz6_coagulation_factor_viiia_E.C.3.4.21.21

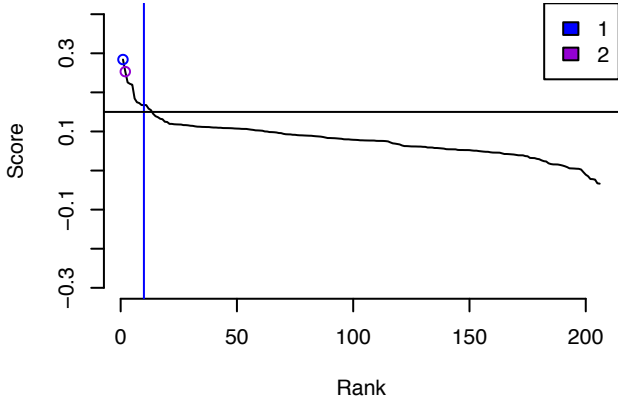
Query: 1vzq_thrombin_alpha_E.C.3.4.21.5



Top 10 Ranked Pockets

- 1.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 2.) 2bok_coagulation_factor_xa_E.C.3.4.21.6
- 3.) 1bcu_thrombin_alpha_E.C.3.4.21.5
- 4.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6
- 5.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 6.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 7.) 2bz6_coagulation_factor_viiia_E.C.3.4.21.21
- 8.) 2flb_coagulation_factor_vii_E.C.3.4.21.21
- 9.) 2b7d_coagulation_factor_vii_E.C.3.4.21.21
- 10.) 1utp_trypsinogen_E.C.3.4.21.4

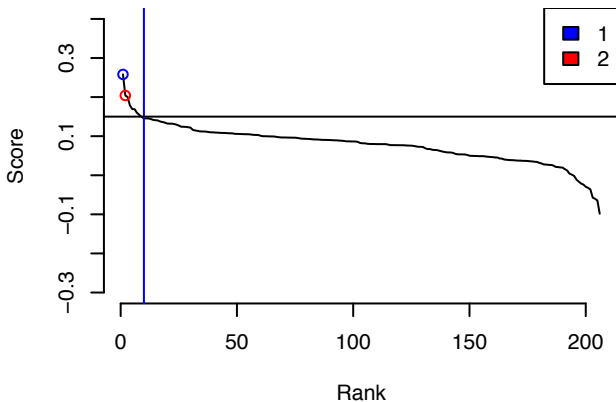
Query: 1sl3_thrombin_alpha_E.C.3.4.21.5



Top 10 Ranked Pockets

- 1.) 1vzq_thrombin_alpha_E.C.3.4.21.5
- 2.) 1bcu_thrombin_alpha_E.C.3.4.21.5
- 3.) 2bok_coagulation_factor_xa_E.C.3.4.21.6
- 4.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 5.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6
- 6.) 2b7d_coagulation_factor_vii_E.C.3.4.21.21
- 7.) 2flb_coagulation_factor_vii_E.C.3.4.21.21
- 8.) 1j17_trypsin_beta_E.C.3.4.21.4
- 9.) 2bz6_coagulation_factor_viiia_E.C.3.4.21.21
- 10.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73

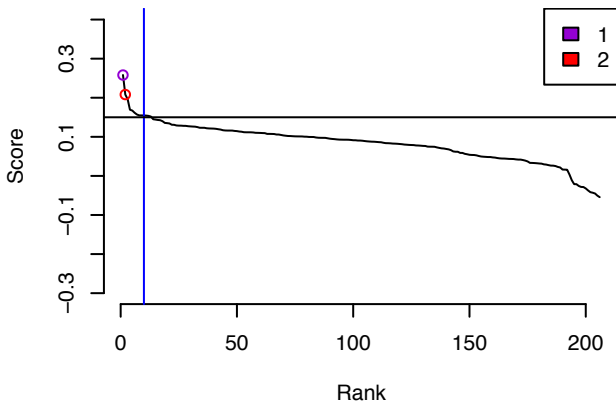
Query: 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 2.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 3.) 1jq9_phospholipase_a2_E.C.3.1.1.4
- 4.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 5.) 1flr_antibody_fab_E.C.-.-.-.-
- 6.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 7.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 8.) 1m2q_casein_kinase_ii_E.C.2.7.1.37
- 9.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 10.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37

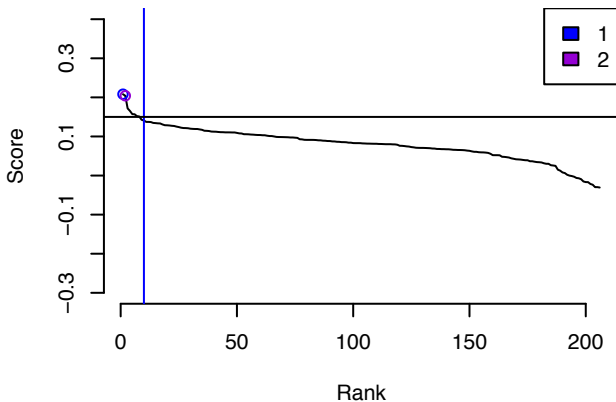
Query: 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 2.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 3.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 4.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 5.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 6.) 1m2q_casein_kinase_ii_E.C.2.7.1.37
- 7.) 1jq9_phospholipase_a2_E.C.3.1.1.4
- 8.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 9.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 10.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29

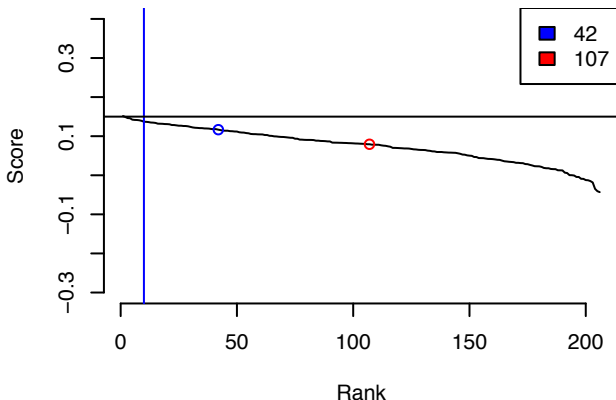
Query: 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37



Top 10 Ranked Pockets

- 1.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 2.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 3.) 1jq9_phospholipase_a2_E.C.3.1.1.4
- 4.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 5.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 6.) 1hk4_serum_albumin_E.C.-.-.-.-
- 7.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 8.) 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 9.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 10.) 1flr_antibody_fab_E.C.-.-.-.-

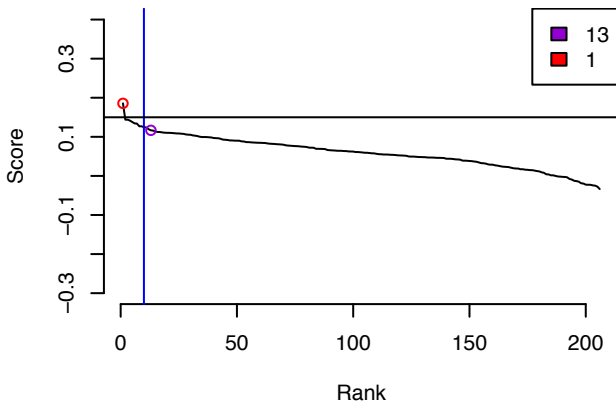
Query: 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8



Top 10 Ranked Pockets

- 1.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 2.) 1fkn_secretase_beta_E.C.3.4.23.-
- 3.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 4.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 5.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 6.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 7.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 8.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 9.) 4fiv_FIV_protease_E.C.3.4.23.16
- 10.) 2fdp_beta-secretase_1_E.C.3.4.23.46

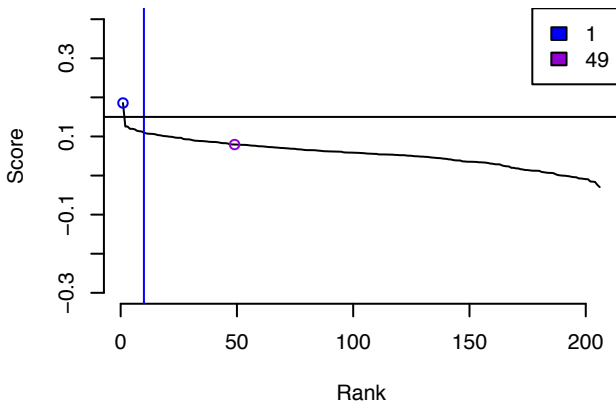
Query: 1jqe_histamine_n-methyltransferase_E.C.2.1.1.8



Top 10 Ranked Pockets

- 1.) 2aou_histamine_n-methyltransferase_E.C.2.1.1.8
- 2.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 3.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 5.) 1e66_acetylcholinesterase_E.C.3.1.1.7
- 6.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3
- 7.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 8.) 1gpk_acetylcholinesterase_E.C.3.1.1.7
- 9.) 1hfs_stromelysin-1_E.C.3.4.24.17
- 10.) 2cer_beta-glucosidase_a_E.C.3.2.1.21

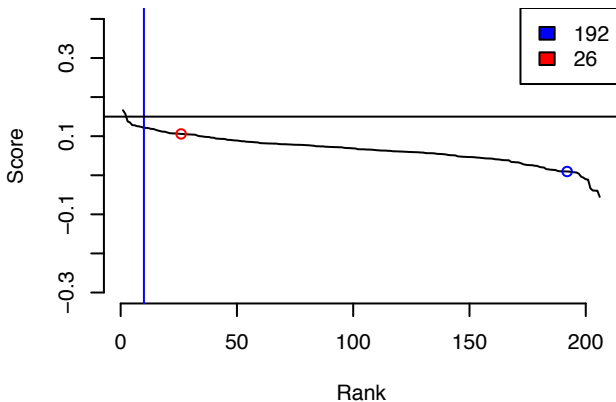
Query: 2aou_histamine_n-methyltransferase_E.C.2.1.1.8



Top 10 Ranked Pockets

- 1.) 1jqe_histamine_n-methyltransferase_E.C.2.1.1.8
- 2.) 1e66_acetylcholinesterase_E.C.3.1.1.7
- 3.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 4.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 5.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 6.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3
- 7.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 8.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 9.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 10.) 1gni_serum_albumin_E.C.-.-.-.-

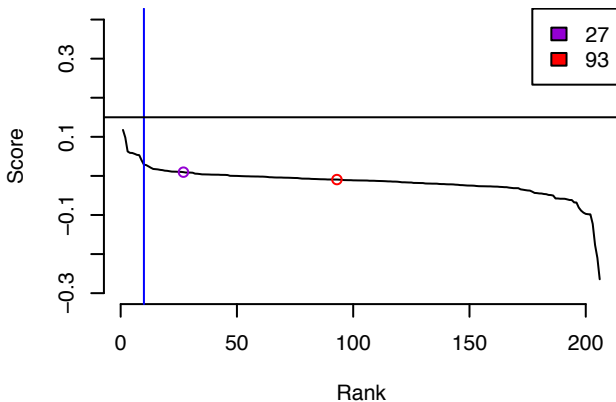
Query: 1y1m_glutamate_[nmda]_receptor_E.C.-.-.-



Top 10 Ranked Pockets

- 1.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 2.) 1flr_antibody_fab_E.C.-.-.-
- 3.) 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 4.) 3pcj_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 5.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 6.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 7.) 2f01_streptavidin_E.C.-.-.-
- 8.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 9.) 2j77_beta-glucosidase_a_E.C.3.2.1.21
- 10.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37

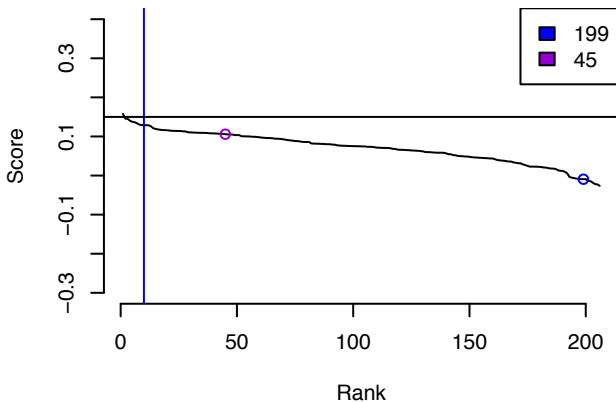
Query: 1pb9_glutamate_[nmda]_receptor_E.C.-.-.-



Top 10 Ranked Pockets

- 1.) 5abp_apolipoprotein_E.C.-.-.-
- 2.) 1ftm_glutamate_receptor_2_E.C.-.-.-
- 3.) 1p1q_glutamate_receptor_2_E.C.-.-.-
- 4.) 1abf_apolipoprotein_E.C.-.-.-
- 5.) 1trd_triosephosphate_isomerase_E.C.5.3.1.1
- 6.) 8abp_apolipoprotein_E.C.-.-.-
- 7.) 2cgr_antibody_fab_E.C.-.-.-
- 8.) 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 9.) 1syh_glutamate_receptor_2_E.C.-.-.-
- 10.) 2j78_beta-glucosidase_a_E.C.3.2.1.21

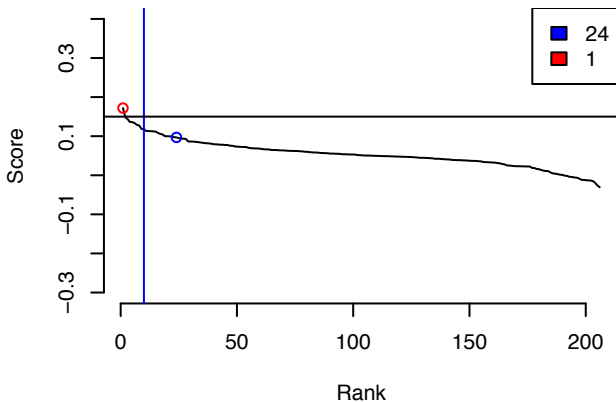
Query: 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-



Top 10 Ranked Pockets

- 1.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 2.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3
- 3.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 5.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 6.) 10gs_glutathione_s-transferase_E.C.2.5.1.18
- 7.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 8.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 9.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 10.) 1tsy_thymidylate_synthase_E.C.2.1.1.45

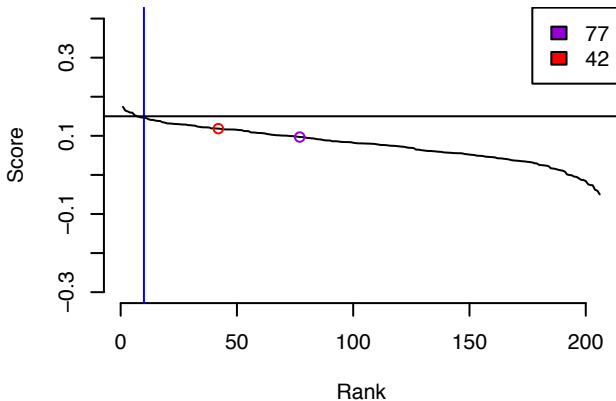
Query: 1vfn_purine_nucleoside_phosphorylase_E.C.2.4.2.1



Top 10 Ranked Pockets

- 1.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 2.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 3.) 1zs0_neutrophil_collagenase_E.C.3.4.24.34
- 4.) 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 5.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 6.) 1syh_glutamate_receptor_2_E.C.-.-.-.-
- 7.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 8.) 2f01_streptavidin_E.C.-.-.-.-
- 9.) 1toj_aspartate_aminotransferase_E.C.2.6.1.1
- 10.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34

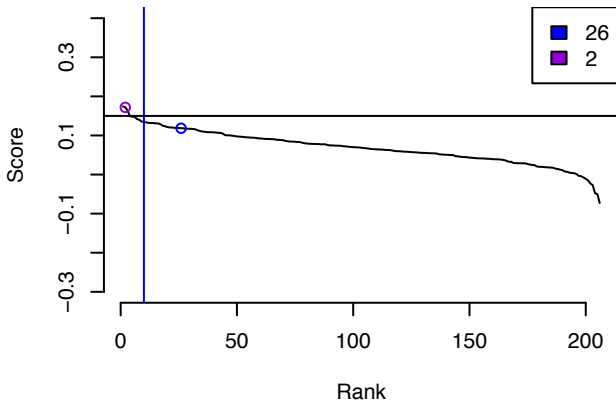
Query: 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1



Top 10 Ranked Pockets

- 1.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 2.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 3.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 4.) 1slg_streptavidin_E.C.-.-.-.-
- 5.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 6.) 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 7.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 8.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 9.) 1jq9_phospholipase_a2_E.C.3.1.1.4
- 10.) 2i0d_HIV-1_protease_E.C.3.4.23.16

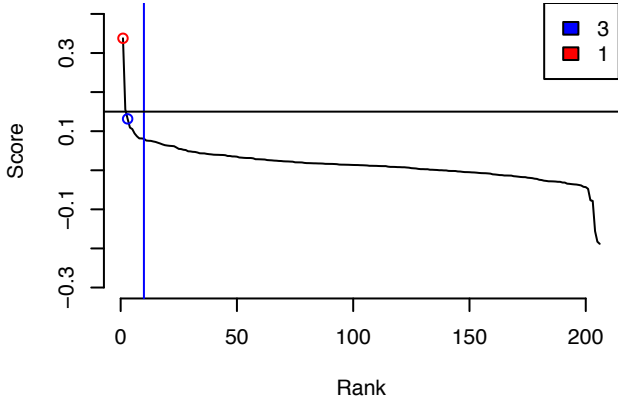
Query: 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1



Top 10 Ranked Pockets

- 1.) 1if7_carbonic_anhydrase_ii_E.C.4.2.1.1
- 2.) 1vfn_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 3.) 1flr_antibody_fab_E.C.-.-.-.-
- 4.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 5.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 6.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 7.) 1hk4_serum_albumin_E.C.-.-.-.-
- 8.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 9.) 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1
- 10.) 2f01_streptavidin_E.C.-.-.-.-

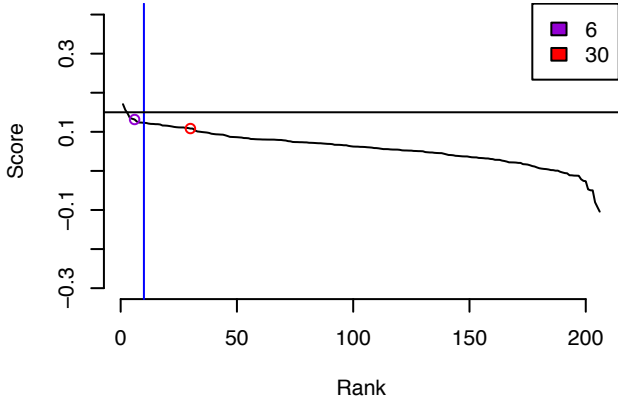
Query: 1p1q_glutamate_receptor_2_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1ftm_glutamate_receptor_2_E.C.-.-.-.-
- 2.) 1abf_apolipoprotein_E.C.-.-.-.-
- 3.) 1syh_glutamate_receptor_2_E.C.-.-.-.-
- 4.) 5abp_apolipoprotein_E.C.-.-.-.-
- 5.) 1ela_elastase_E.C.3.4.21.36
- 6.) 8abp_apolipoprotein_E.C.-.-.-.-
- 7.) 2f01_streptavidin_E.C.-.-.-.-
- 8.) 1axz_lectin_E.C.-.-.-.-
- 9.) 1bma_elastase_E.C.3.4.21.36
- 10.) 1det_ribonuclease_T1_E.C.3.1.27.3

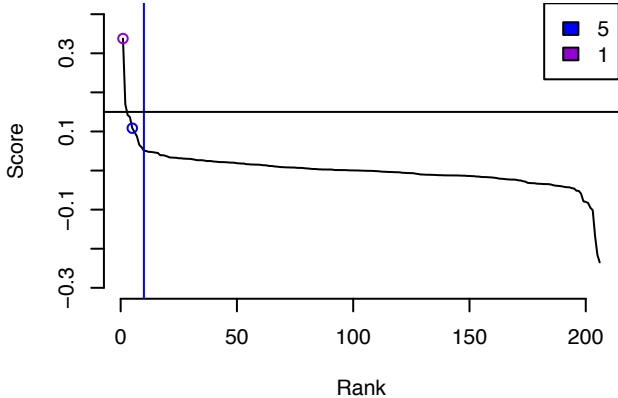
Query: 1syh_glutamate_receptor_2_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 2.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 3.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 4.) 2usn_stromelysin-1_E.C.3.4.24.17
- 5.) 1vfn_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 6.) 1p1q_glutamate_receptor_2_E.C.-.-.-.-
- 7.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34
- 8.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 9.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 10.) 1a30_HIV-1_protease_E.C.3.4.23.16

Query: 1ftm_glutamate_receptor_2_E.C.-.-.-.-

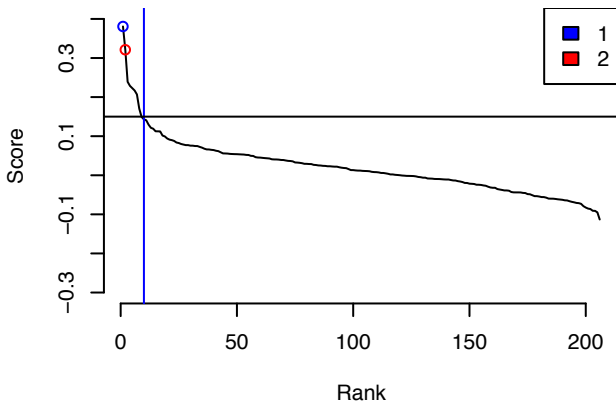


Top 10 Ranked Pockets

- 1.) 1p1q_glutamate_receptor_2_E.C.-.-.-.-
- 2.) 1abf_apolipoprotein_E.C.-.-.-.-
- 3.) 5abp_apolipoprotein_E.C.-.-.-.-
- 4.) 8abp_apolipoprotein_E.C.-.-.-.-
- 5.) 1syh_glutamate_receptor_2_E.C.-.-.-.-
- 6.) 1pb9_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 7.) 1det_ribonuclease_T1_E.C.3.1.27.3
- 8.) 1vfn_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 9.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 10.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34

Query: 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-

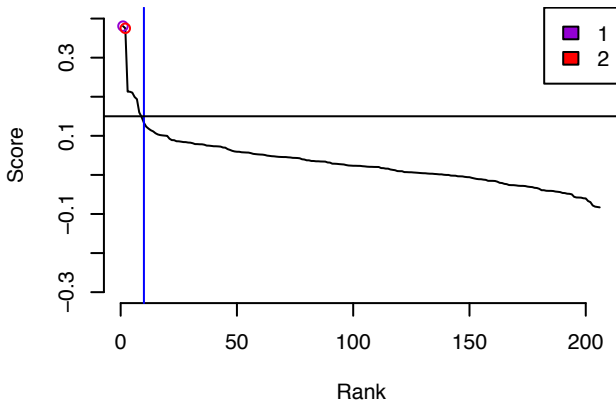
Top 10 Ranked Pockets



- 1.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-
- 2.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-
- 3.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 4.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 5.) 2std_scytalone_dehydratase_E.C.4.2.1.94
- 6.) 2b1v_estrogen_receptor_E.C.-.-.-
- 7.) 2fai_estrogen_receptor_E.C.-.-.-
- 8.) 1nc1_mta/sah_nucleosidase_E.C.3.2.2.9
- 9.) 2d3u_polyprotein_E.C.2.7.7.48
- 10.) 1gni_serum_albumin_E.C.-.-.-

Query: 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-

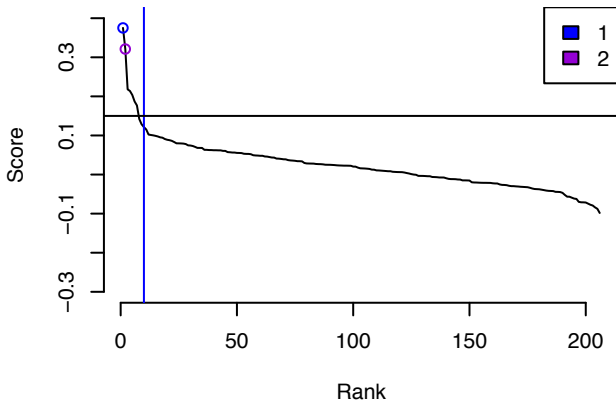
Top 10 Ranked Pockets



- 1.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-
- 2.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-
- 3.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 4.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 5.) 2std_scytalone_dehydratase_E.C.4.2.1.94
- 6.) 2fai_estrogen_receptor_E.C.-.-.-
- 7.) 2b1v_estrogen_receptor_E.C.-.-.-
- 8.) 1gni_serum_albumin_E.C.-.-.-
- 9.) 2d3u_polyprotein_E.C.2.7.7.48
- 10.) 2ayr_estrogen_receptor_E.C.-.-.-

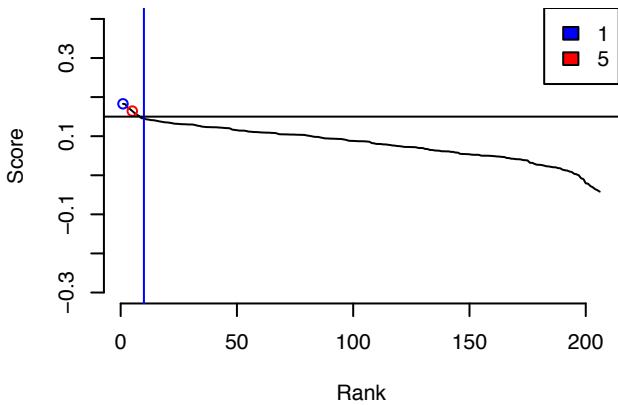
Query: 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-

Top 10 Ranked Pockets



- 1.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-
- 2.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-
- 3.) 2fai_estrogen_receptor_E.C.-.-.-
- 4.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 5.) 2b1v_estrogen_receptor_E.C.-.-.-
- 6.) 2std_scytalone_dehydratase_E.C.4.2.1.94
- 7.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 8.) 2d3u_polyprotein_E.C.2.7.7.48
- 9.) 1gni_serum_albumin_E.C.-.-.-
- 10.) 1nc1_mta/sah_nucleosidase_E.C.3.2.2.9

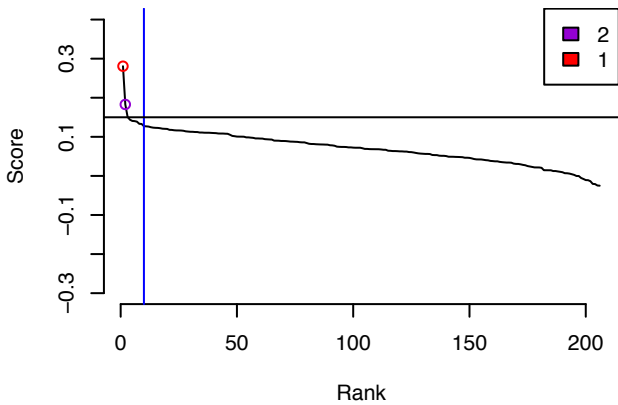
Query: 1f4e_thymidylate_synthase_E.C.2.1.1.45



Top 10 Ranked Pockets

- 1.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 2.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 3.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 4.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 5.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 6.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 7.) 1ndz_adenosine_deaminase_E.C.3.5.4.4
- 8.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 9.) 1e66_acetylcholinesterase_E.C.3.1.1.7
- 10.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3

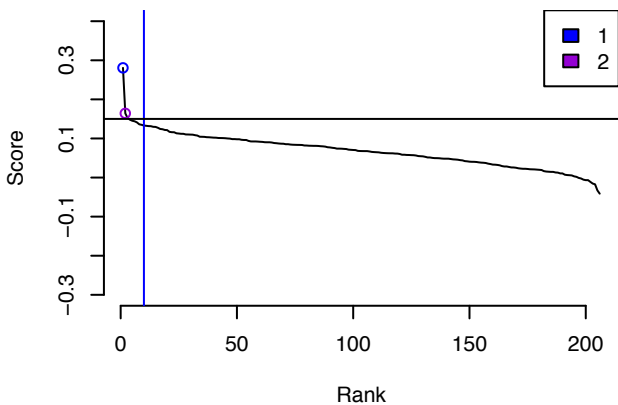
Query: 1f4f_thymidylate_synthase_E.C.2.1.1.45



Top 10 Ranked Pockets

- 1.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 2.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 3.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 4.) 1jqe_histamine_n-methyltransferase_E.C.2.1.1.8
- 5.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3
- 6.) 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 7.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 8.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 9.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 10.) 4tmn_thermolysin_E.C.3.4.24.27

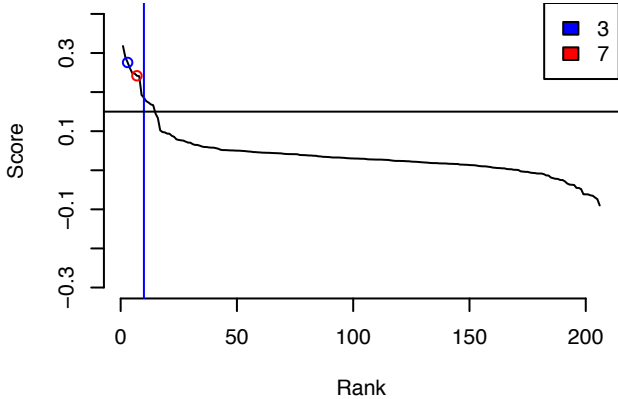
Query: 1f4g_thymidylate_synthase_E.C.2.1.1.45



Top 10 Ranked Pockets

- 1.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 2.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 3.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 4.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 5.) 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 6.) 1jqe_histamine_n-methyltransferase_E.C.2.1.1.8
- 7.) 1nje_thymidylate_synthase_E.C.2.1.1.45
- 8.) 1tsy_thymidylate_synthase_E.C.2.1.1.45
- 9.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 10.) 1nja_thymidylate_synthase_E.C.2.1.1.45

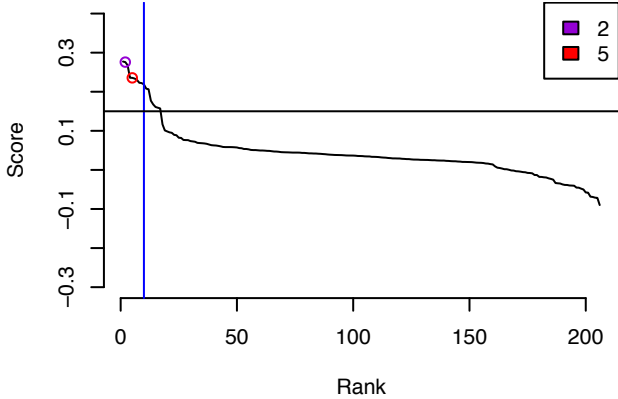
Query: 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73



Top 10 Ranked Pockets

- 1.) 1v2o_trypsin_beta_E.C.3.4.21.4
- 2.) 1o3f_trypsin_beta_E.C.3.4.21.4
- 3.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 4.) 1utp_trypsinogen_E.C.3.4.21.4
- 5.) 1j17_trypsin_beta_E.C.3.4.21.4
- 6.) 1j16_trypsin_beta_E.C.3.4.21.4
- 7.) 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 8.) 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4
- 9.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 10.) 2bz6_coagulation_factor_viia_E.C.3.4.21.21

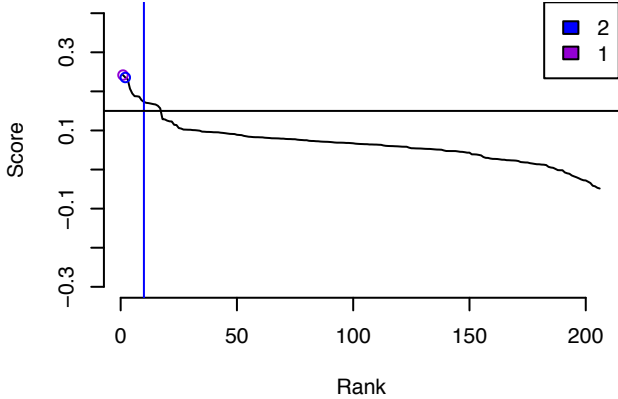
Query: 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73



Top 10 Ranked Pockets

- 1.) 1o3f_trypsin_beta_E.C.3.4.21.4
- 2.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 3.) 1utp_trypsinogen_E.C.3.4.21.4
- 4.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6
- 5.) 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 6.) 1j17_trypsin_beta_E.C.3.4.21.4
- 7.) 2bz6_coagulation_factor_viia_E.C.3.4.21.21
- 8.) 1j16_trypsin_beta_E.C.3.4.21.4
- 9.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 10.) 1v2o_trypsin_beta_E.C.3.4.21.4

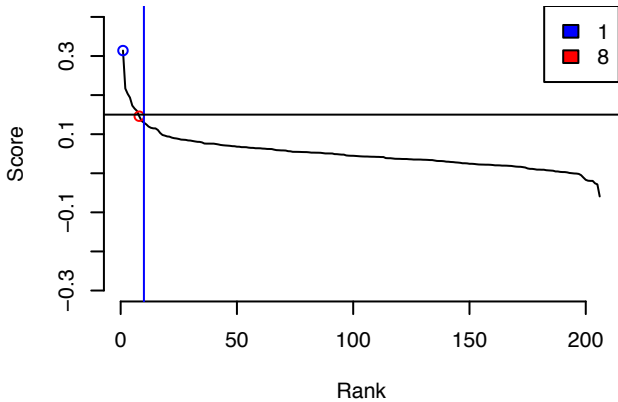
Query: 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73



Top 10 Ranked Pockets

- 1.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 2.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 3.) 2b7d_coagulation_factor_vii_E.C.3.4.21.21
- 4.) 2flb_coagulation_factor_vii_E.C.3.4.21.21
- 5.) 1v2o_trypsin_beta_E.C.3.4.21.4
- 6.) 1o3f_trypsin_beta_E.C.3.4.21.4
- 7.) 1j17_trypsin_beta_E.C.3.4.21.4
- 8.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 9.) 1utp_trypsinogen_E.C.3.4.21.4
- 10.) 1pz5_antibody_fab_E.C.-.-.-.-

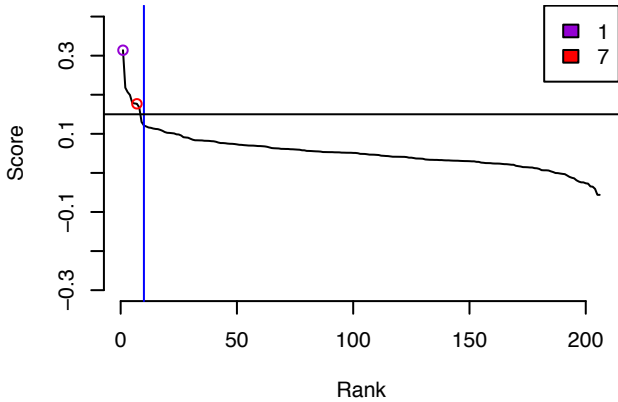
Query: 2b1v_estrogen_receptor_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 2fai_estrogen_receptor_E.C.-.-.-.-
- 2.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 3.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 4.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 5.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 6.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 7.) 2std_scytalone_dehydratase_E.C.4.2.1.94
- 8.) 2ayr_estrogen_receptor_E.C.-.-.-.-
- 9.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 10.) 2d3u_polyprotein_E.C.2.7.7.48

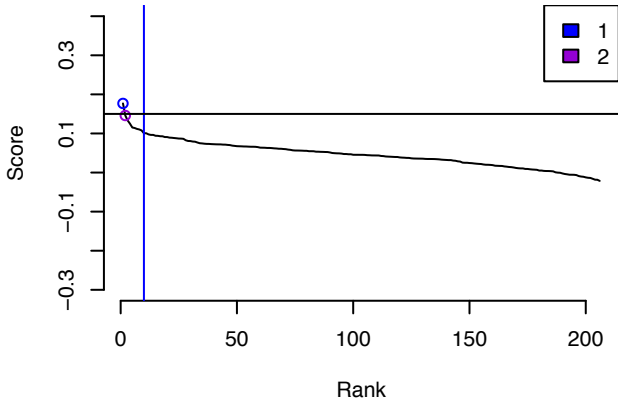
Query: 2fai_estrogen_receptor_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 2b1v_estrogen_receptor_E.C.-.-.-.-
- 2.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 3.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 4.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 5.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 6.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 7.) 2ayr_estrogen_receptor_E.C.-.-.-.-
- 8.) 2std_scytalone_dehydratase_E.C.4.2.1.94
- 9.) 1m2q_casein_kinase_ii_E.C.2.7.1.37
- 10.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37

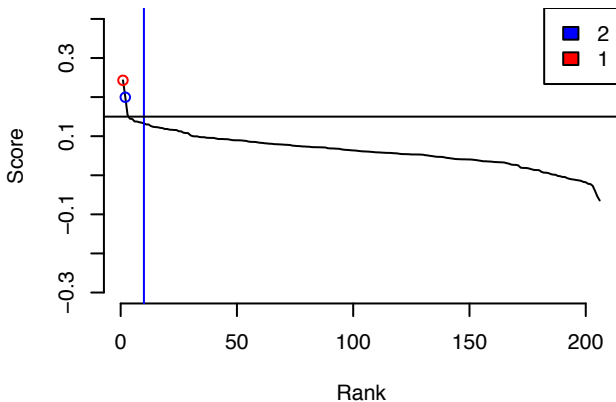
Query: 2ayr_estrogen_receptor_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 2fai_estrogen_receptor_E.C.-.-.-.-
- 2.) 2b1v_estrogen_receptor_E.C.-.-.-.-
- 3.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 4.) 1gni_serum_albumin_E.C.-.-.-.-
- 5.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 6.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 7.) 1m2q_casein_kinase_ii_E.C.2.7.1.37
- 8.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 9.) 2aou_histamine_n-methyltransferase_E.C.2.1.1.8
- 10.) 2bak_mitogen-activated_protein_kinase_14_E.C.2.7.1.37

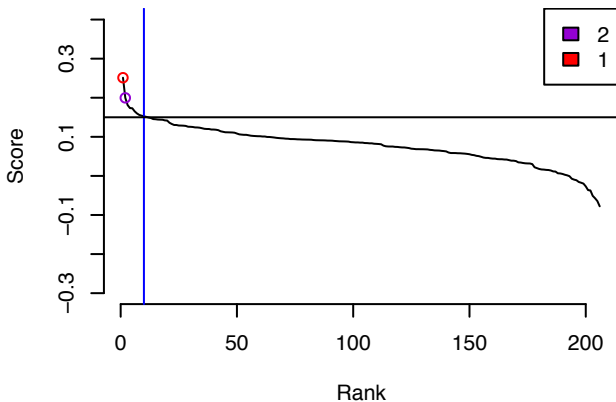
Query: 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1



Top 10 Ranked Pockets

- 1.) 1if7_carbonic_anhydrase_ii_E.C.4.2.1.1
- 2.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 3.) 1axz_lectin_E.C.-.-.-.-
- 4.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 5.) 1u1b_ribonuclease_a_E.C.3.1.27.5
- 6.) 6fiv_FIV_protease_E.C.3.4.23.16
- 7.) 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 8.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 9.) 1b11_FIV_protease_E.C.3.4.23.16
- 10.) 1hk4_serum_albumin_E.C.-.-.-.-

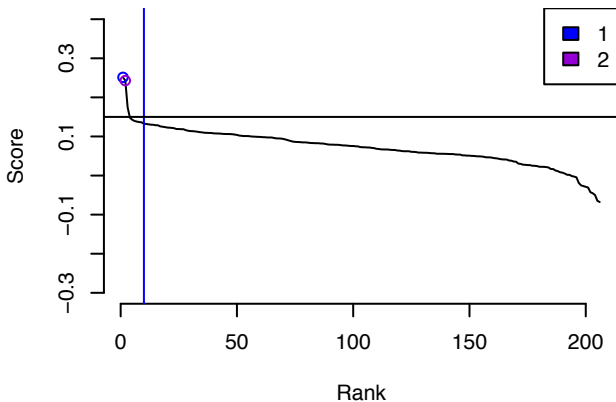
Query: 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1



Top 10 Ranked Pockets

- 1.) 1if7_carbonic_anhydrase_ii_E.C.4.2.1.1
- 2.) 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1
- 3.) 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 4.) 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 5.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 6.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3
- 7.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 8.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 9.) 2d3u_polyprotein_E.C.2.7.7.48
- 10.) 1flr_antibody_fab_E.C.-.-.-.-

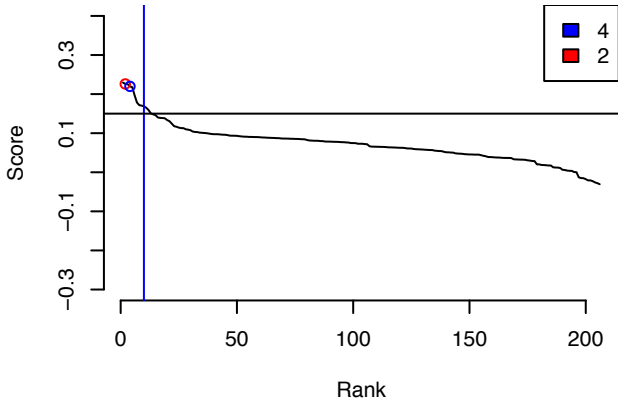
Query: 1if7_carbonic_anhydrase_ii_E.C.4.2.1.1



Top 10 Ranked Pockets

- 1.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 2.) 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1
- 3.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 4.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 5.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 6.) 2d3z_polyprotein_E.C.2.7.7.48
- 7.) 1b11_FIV_protease_E.C.3.4.23.16
- 8.) 2d3u_polyprotein_E.C.2.7.7.48
- 9.) 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 10.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3

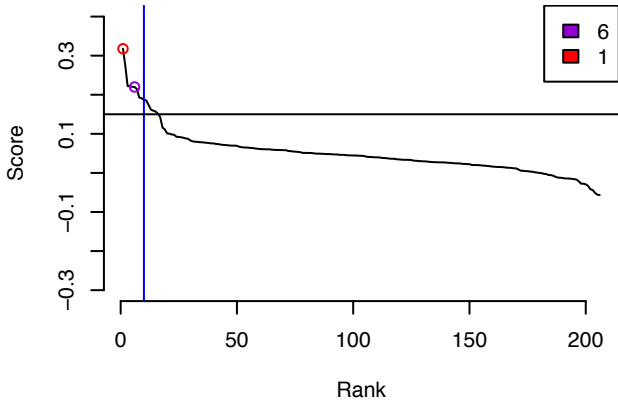
Query: 2bok_coagulation_factor_xa_E.C.3.4.21.6



Top 10 Ranked Pockets

- 1.) 1vzq_thrombin_alpha_E.C.3.4.21.5
- 2.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6
- 3.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 4.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 5.) 1bcu_thrombin_alpha_E.C.3.4.21.5
- 6.) 2bz6_coagulation_factor_viaa_E.C.3.4.21.21
- 7.) 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4
- 8.) 1j17_trypsin_beta_E.C.3.4.21.4
- 9.) 2flb_coagulation_factor_vii_E.C.3.4.21.21
- 10.) 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73

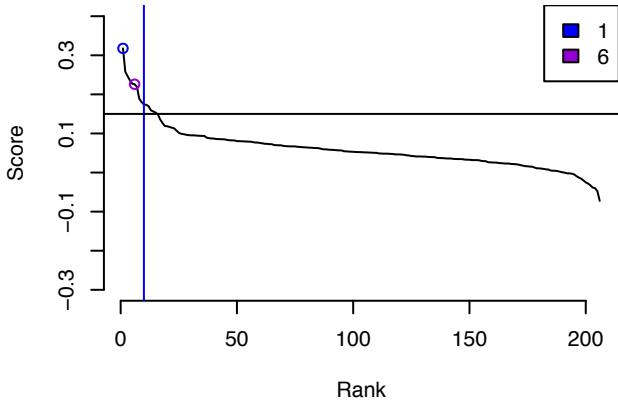
Query: 1nfy_coagulation_factor_xa_E.C.3.4.21.6



Top 10 Ranked Pockets

- 1.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6
- 2.) 1j17_trypsin_beta_E.C.3.4.21.4
- 3.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 4.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 5.) 1bcu_thrombin_alpha_E.C.3.4.21.5
- 6.) 2bok_coagulation_factor_xa_E.C.3.4.21.6
- 7.) 1j16_trypsin_beta_E.C.3.4.21.4
- 8.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 9.) 2bz6_coagulation_factor_viaa_E.C.3.4.21.21
- 10.) 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73

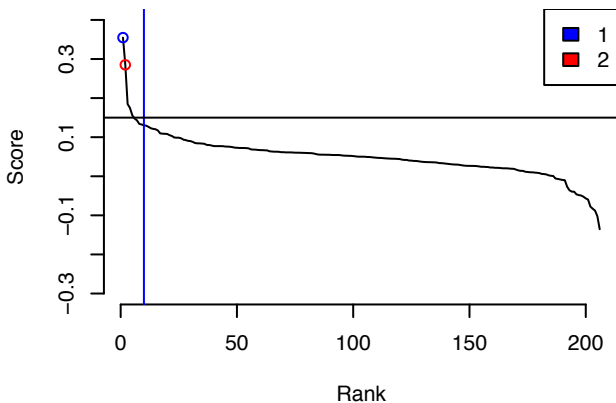
Query: 1mq6_coagulation_factor_xa_E.C.3.4.21.6



Top 10 Ranked Pockets

- 1.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 2.) 1j17_trypsin_beta_E.C.3.4.21.4
- 3.) 1bcu_thrombin_alpha_E.C.3.4.21.5
- 4.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 5.) 1j16_trypsin_beta_E.C.3.4.21.4
- 6.) 2bok_coagulation_factor_xa_E.C.3.4.21.6
- 7.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 8.) 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4
- 9.) 1vzq_thrombin_alpha_E.C.3.4.21.5
- 10.) 2bz6_coagulation_factor_viaa_E.C.3.4.21.21

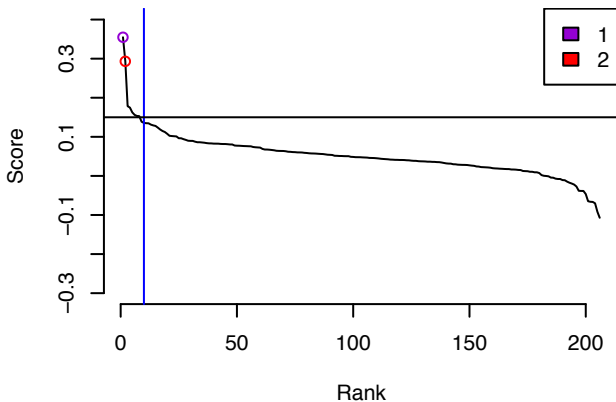
Query: 1ax0_lectin_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1axz_lectin_E.C.-.-.-.-
- 2.) 1gz9_lectin_E.C.-.-.-.-
- 3.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 4.) 1rnt_ribonuclease_T1_E.C.3.1.27.3
- 5.) 1bma_elastase_E.C.3.4.21.36
- 6.) 2g8r_ribonuclease_pancreatic_E.C.3.1.27.5
- 7.) 1ela_elastase_E.C.3.4.21.36
- 8.) 6fiv_FIV_protease_E.C.3.4.23.16
- 9.) 6rnt_ribonuclease_T1_E.C.3.1.27.3
- 10.) 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1

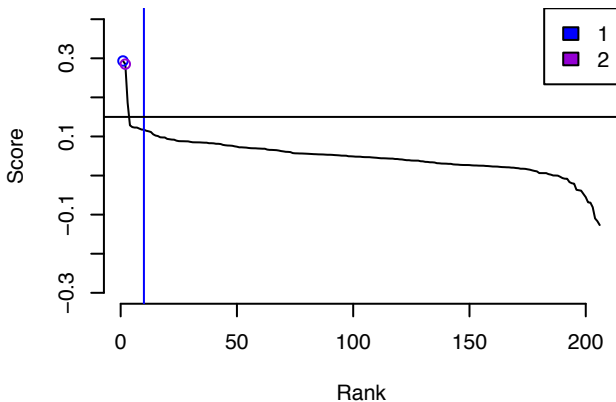
Query: 1axz_lectin_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1ax0_lectin_E.C.-.-.-.-
- 2.) 1gz9_lectin_E.C.-.-.-.-
- 3.) 1rnt_ribonuclease_T1_E.C.3.1.27.3
- 4.) 1bma_elastase_E.C.3.4.21.36
- 5.) 1ela_elastase_E.C.3.4.21.36
- 6.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 7.) 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1
- 8.) 6rnt_ribonuclease_T1_E.C.3.1.27.3
- 9.) 2g8r_ribonuclease_pancreatic_E.C.3.1.27.5
- 10.) 1o0h_ribonuclease_a_E.C.3.1.27.5

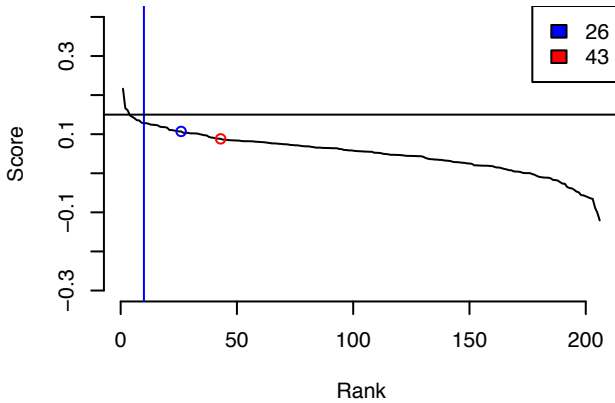
Query: 1gz9_lectin_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1axz_lectin_E.C.-.-.-.-
- 2.) 1ax0_lectin_E.C.-.-.-.-
- 3.) 1rnt_ribonuclease_T1_E.C.3.1.27.3
- 4.) 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 5.) 2ush_stromelysin-1_E.C.3.4.24.17
- 6.) 2g8r_ribonuclease_pancreatic_E.C.3.1.27.5
- 7.) 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1
- 8.) 1ela_elastase_E.C.3.4.21.36
- 9.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 10.) 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29

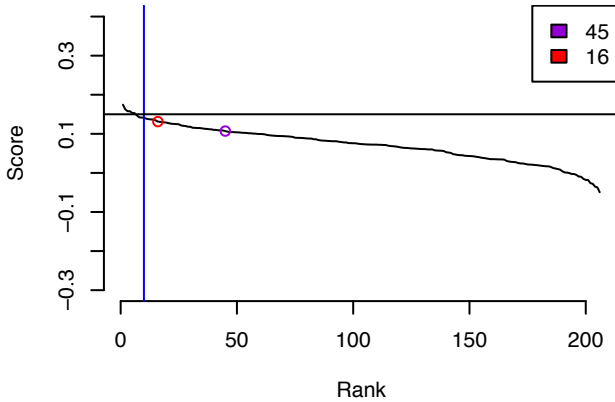
Query: 2usn_stromelysin-1_E.C.3.4.24.17



Top 10 Ranked Pockets

- 1.) 1pz5_antibody_fab_E.C.-.-.-.-
- 2.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 3.) 2cgr_antibody_fab_E.C.-.-.-.-
- 4.) 1u2y_alpha-amylase_E.C.3.2.1.1
- 5.) 1zs0_neutrophil_collagenase_E.C.3.4.24.34
- 6.) 1fh8_xylanase_beta-1,4_E.C.3.2.1.91
- 7.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 8.) 1syh_glutamate_receptor_2_E.C.-.-.-.-
- 9.) 1tmn_thermolysin_E.C.3.4.24.27
- 10.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5

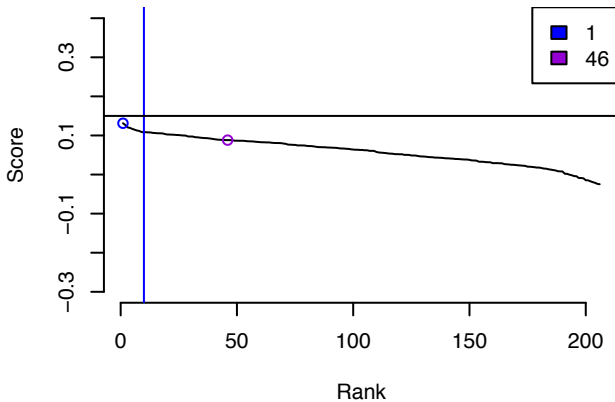
Query: 2d1o_stromelysin-1_E.C.3.4.24.17



Top 10 Ranked Pockets

- 1.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 2.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 3.) 2l0d_HIV-1_protease_E.C.3.4.23.16
- 4.) 4fiv_FIV_protease_E.C.3.4.23.16
- 5.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 6.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 7.) 1fzk_h-2_class_i_histocompatibility_antigen_E.C.-.-.-.-
- 8.) 1zs0_neutrophil_collagenase_E.C.3.4.24.34
- 9.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 10.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8

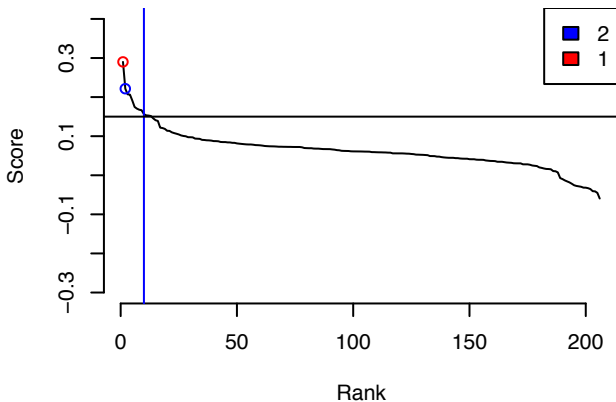
Query: 1hfs_stromelysin-1_E.C.3.4.24.17



Top 10 Ranked Pockets

- 1.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 2.) 1jqe_histamine_n-methyltransferase_E.C.2.1.1.8
- 3.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 5.) 1tsy_thymidylate_synthase_E.C.2.1.1.45
- 6.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 7.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 8.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 9.) 1ndz_adenosine_deaminase_E.C.3.5.4.4
- 10.) 2fdp_beta-secretase_1_E.C.3.4.23.46

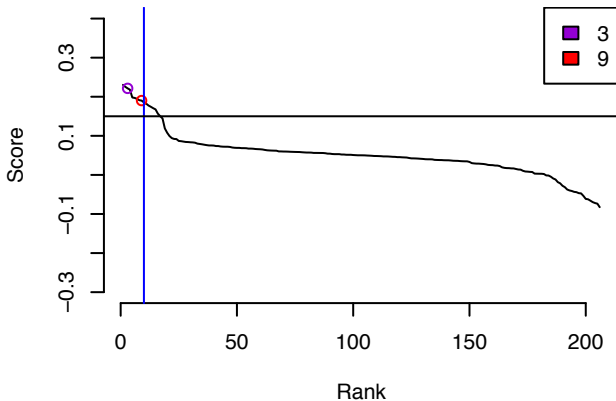
Query: 2flb_coagulation_factor_vii_E.C.3.4.21.21



Top 10 Ranked Pockets

- 1.) 2b7d_coagulation_factor_vii_E.C.3.4.21.21
- 2.) 2bz6_coagulation_factor_viaa_E.C.3.4.21.21
- 3.) 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 4.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 5.) 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4
- 6.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 7.) 2bok_coagulation_factor_xa__E.C.3.4.21.6
- 8.) 1bcu_thrombin_alpha_E.C.3.4.21.5
- 9.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 10.) 1mq6_coagulation_factor_xa__E.C.3.4.21.6

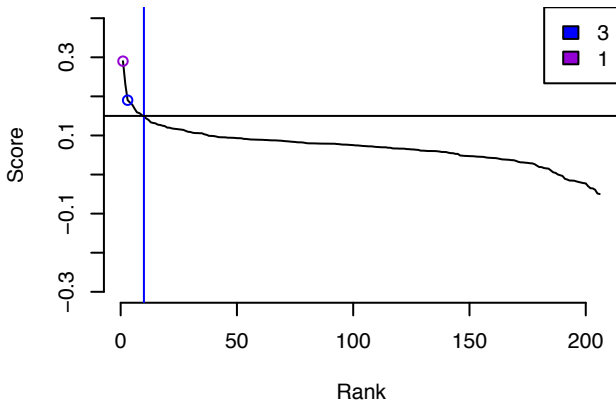
Query: 2bz6_coagulation_factor_viaa_E.C.3.4.21.21



Top 10 Ranked Pockets

- 1.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 2.) 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4
- 3.) 2flb_coagulation_factor_vii_E.C.3.4.21.21
- 4.) 1utp_trypsinogen_E.C.3.4.21.4
- 5.) 1v2o_trypsin_beta_E.C.3.4.21.4
- 6.) 2bok_coagulation_factor_xa__E.C.3.4.21.6
- 7.) 1o3f_trypsin_beta_E.C.3.4.21.4
- 8.) 1nfy_coagulation_factor_xa__E.C.3.4.21.6
- 9.) 2b7d_coagulation_factor_vii_E.C.3.4.21.21
- 10.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73

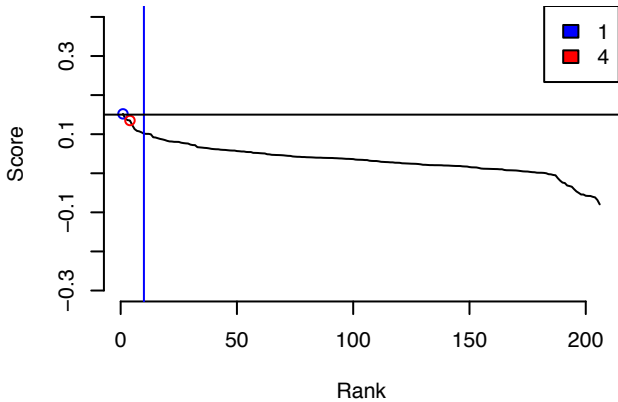
Query: 2b7d_coagulation_factor_vii_E.C.3.4.21.21



Top 10 Ranked Pockets

- 1.) 2flb_coagulation_factor_vii_E.C.3.4.21.21
- 2.) 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 3.) 2bz6_coagulation_factor_viaa_E.C.3.4.21.21
- 4.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 5.) 1utp_trypsinogen_E.C.3.4.21.4
- 6.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 7.) 1nfy_coagulation_factor_xa__E.C.3.4.21.6
- 8.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 9.) 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 10.) 2bok_coagulation_factor_xa__E.C.3.4.21.6

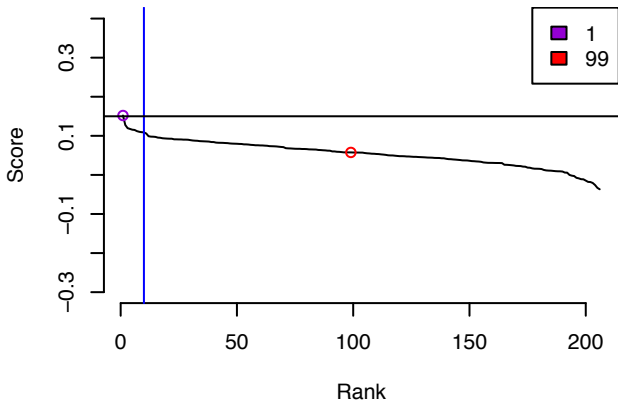
Query: 1loq_ortidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23



Top 10 Ranked Pockets

- 1.) 1lol_ortidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 2.) 1nwl_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 3.) 7cpa_carboxypeptidase_a_E.C.3.4.17.1
- 4.) 1x1z_ortidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 5.) 2ctc_carboxypeptidase_a_E.C.3.4.17.1
- 6.) 2hdq_beta-lactamase_E.C.3.5.2.6
- 7.) 1nny_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 8.) 4tim_triosephosphate_isomerase_E.C.5.3.1.1
- 9.) 1kv5_triosephosphate_isomerase_E.C.5.3.1.1
- 10.) 8cpa_carboxypeptidase_a_E.C.3.4.17.1

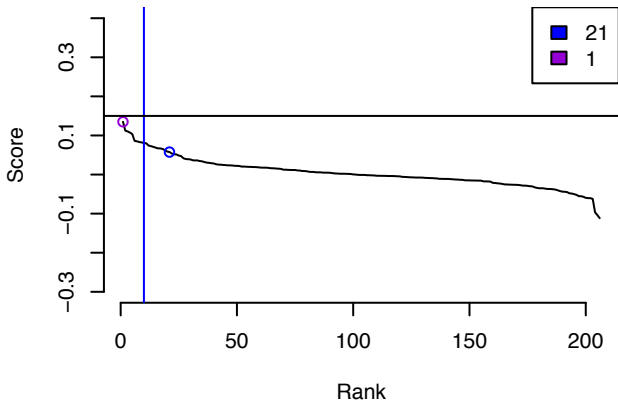
Query: 1lol_ortidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23



Top 10 Ranked Pockets

- 1.) 1loq_ortidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 2.) 7cpa_carboxypeptidase_a_E.C.3.4.17.1
- 3.) 1l2s_beta-lactamase_E.C.3.5.2.6
- 4.) 1tok_aspartate_aminotransferase_E.C.2.6.1.1
- 5.) 2hdq_beta-lactamase_E.C.3.5.2.6
- 6.) 1ydt_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 7.) 1toj_aspartate_aminotransferase_E.C.2.6.1.1
- 8.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 9.) 8cpa_carboxypeptidase_a_E.C.3.4.17.1
- 10.) 1e1v_cyclin_dependent_kinase_2_E.C.2.7.1.37

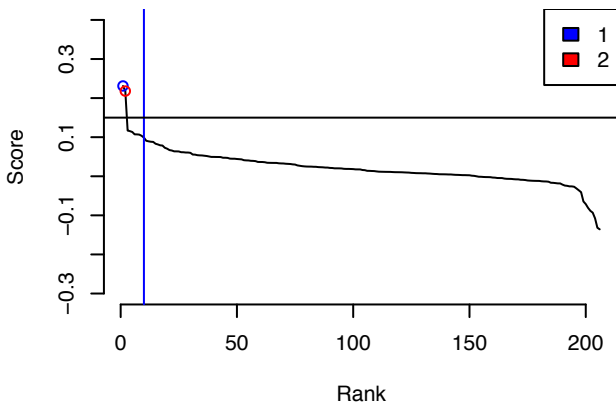
Query: 1x1z_ortidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23



Top 10 Ranked Pockets

- 1.) 1loq_ortidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 2.) 2g5u_transthyretin_E.C.-.-.-.-
- 3.) 1abf_apolipoprotein_E.C.-.-.-.-
- 4.) 4tim_triosephosphate_isomerase_E.C.5.3.1.1
- 5.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 6.) 2hdq_beta-lactamase_E.C.3.5.2.6
- 7.) 5abp_apolipoprotein_E.C.-.-.-.-
- 8.) 8abp_apolipoprotein_E.C.-.-.-.-
- 9.) 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 10.) 1d09_aspartate_carbamoyltransferase_E.C.2.1.3.2

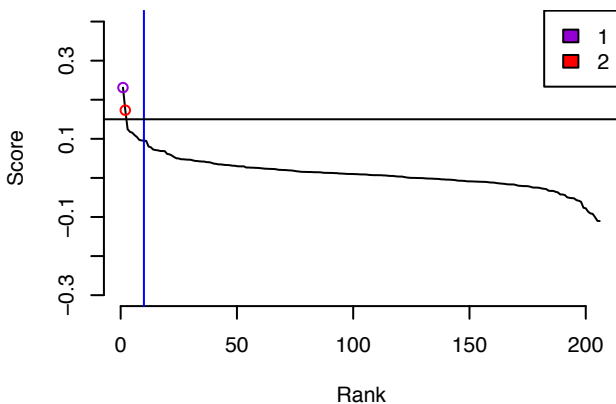
Query: 4tim_triosephosphate_isomerase_E.C.5.3.1.1



Top 10 Ranked Pockets

- 1.) 1kv5_triosephosphate_isomerase_E.C.5.3.1.1
- 2.) 1trd_triosephosphate_isomerase_E.C.5.3.1.1
- 3.) 1nny_tyrosine_phosphatase_1b__E.C.3.1.3.48
- 4.) 1zc9_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 5.) 1nwl_tyrosine_phosphatase_1b__E.C.3.1.3.48
- 6.) 1x1z_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 7.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 8.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 9.) 3pcj_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 10.) 1o0h_ribonuclease_a_E.C.3.1.27.5

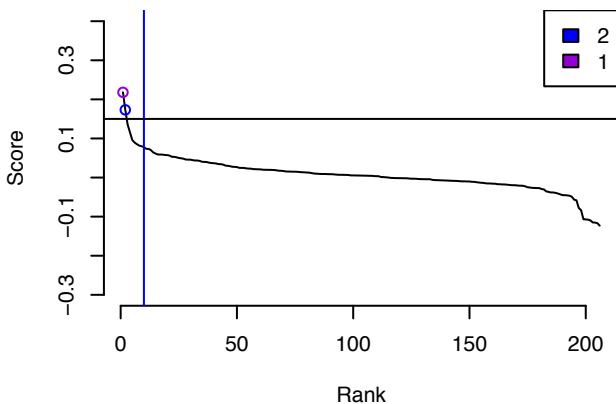
Query: 1kv5_triosephosphate_isomerase_E.C.5.3.1.1



Top 10 Ranked Pockets

- 1.) 4tim_triosephosphate_isomerase_E.C.5.3.1.1
- 2.) 1trd_triosephosphate_isomerase_E.C.5.3.1.1
- 3.) 1zc9_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 4.) 1nny_tyrosine_phosphatase_1b__E.C.3.1.3.48
- 5.) 1o0h_ribonuclease_a_E.C.3.1.27.5
- 6.) 1a08_tyrosine_kinase_C-src_E.C.2.7.1.112
- 7.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 8.) 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 9.) 1a1b_tyrosine_kinase_C-src_E.C.2.7.1.112
- 10.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64

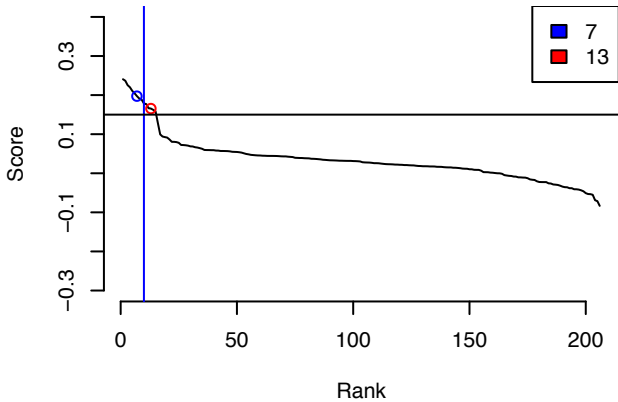
Query: 1trd_triosephosphate_isomerase_E.C.5.3.1.1



Top 10 Ranked Pockets

- 1.) 4tim_triosephosphate_isomerase_E.C.5.3.1.1
- 2.) 1kv5_triosephosphate_isomerase_E.C.5.3.1.1
- 3.) 1a08_tyrosine_kinase_C-src_E.C.2.7.1.112
- 4.) 1zc9_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 5.) 1a1b_tyrosine_kinase_C-src_E.C.2.7.1.112
- 6.) 1nny_tyrosine_phosphatase_1b__E.C.3.1.3.48
- 7.) 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 8.) 1nwl_tyrosine_phosphatase_1b__E.C.3.1.3.48
- 9.) 1abf_apolipoprotein_E.C.-.-.-
- 10.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6

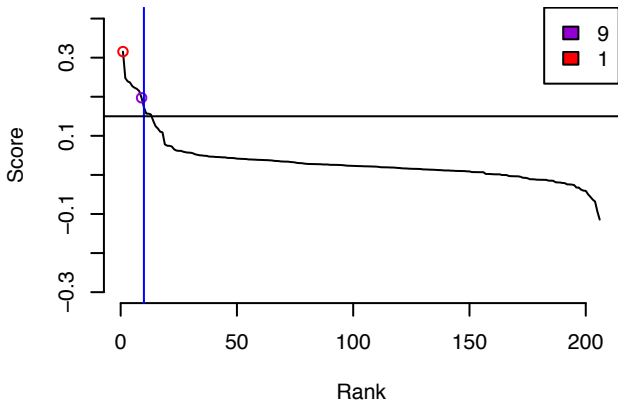
Query: 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4



Top 10 Ranked Pockets

- 1.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 2.) 1o3f_trypsin_beta_E.C.3.4.21.4
- 3.) 2bz6_coagulation_factor_viiia_E.C.3.4.21.21
- 4.) 1utp_trypsinogen_E.C.3.4.21.4
- 5.) 1v2o_trypsin_beta_E.C.3.4.21.4
- 6.) 1bcu_thrombin_alpha_E.C.3.4.21.5
- 7.) 1j16_trypsin_beta_E.C.3.4.21.4
- 8.) 2flb_coagulation_factor_vii_E.C.3.4.21.21
- 9.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6
- 10.) 2bok_coagulation_factor_xa_E.C.3.4.21.6

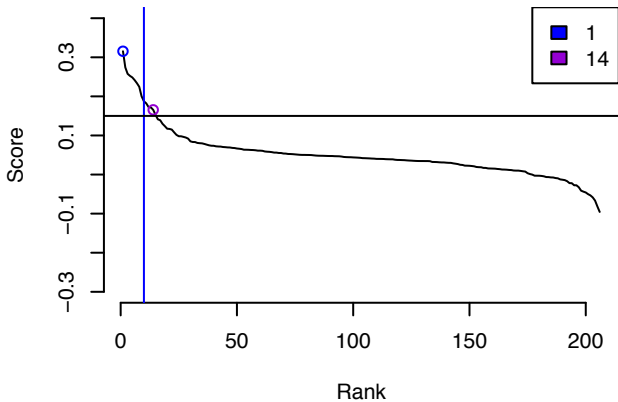
Query: 1j16_trypsin_beta_E.C.3.4.21.4



Top 10 Ranked Pockets

- 1.) 1j17_trypsin_beta_E.C.3.4.21.4
- 2.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 3.) 1v2o_trypsin_beta_E.C.3.4.21.4
- 4.) 1o3f_trypsin_beta_E.C.3.4.21.4
- 5.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6
- 6.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 7.) 1utp_trypsinogen_E.C.3.4.21.4
- 8.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 9.) 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4
- 10.) 1bcu_thrombin_alpha_E.C.3.4.21.5

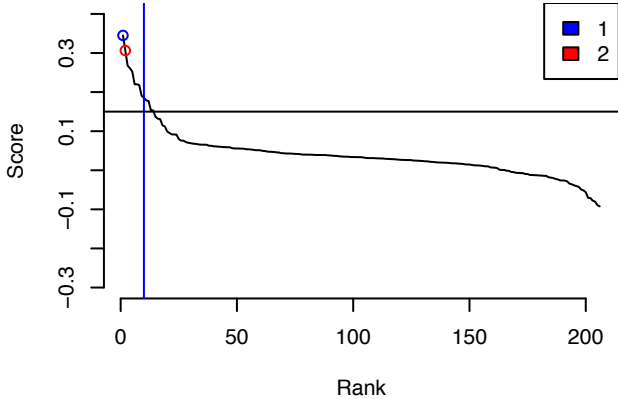
Query: 1j17_trypsin_beta_E.C.3.4.21.4



Top 10 Ranked Pockets

- 1.) 1j16_trypsin_beta_E.C.3.4.21.4
- 2.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 3.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6
- 4.) 1utp_trypsinogen_E.C.3.4.21.4
- 5.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 6.) 1o3f_trypsin_beta_E.C.3.4.21.4
- 7.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 8.) 1v2o_trypsin_beta_E.C.3.4.21.4
- 9.) 1bcu_thrombin_alpha_E.C.3.4.21.5
- 10.) 1sq_a_urokinase-type_plasminogen_activator_E.C.3.4.21.73

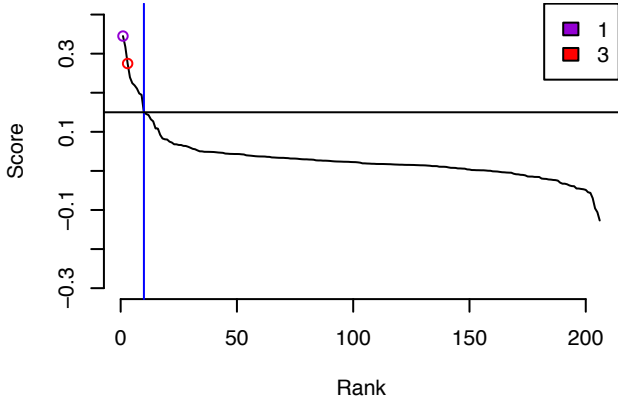
Query: 1utp_trypsinogen_E.C.3.4.21.4



Top 10 Ranked Pockets

- 1.) 1v2o_trypsin_beta_E.C.3.4.21.4
- 2.) 1o3f_trypsin_beta_E.C.3.4.21.4
- 3.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 4.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 5.) 1j17_trypsin_beta_E.C.3.4.21.4
- 6.) 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4
- 7.) 1j16_trypsin_beta_E.C.3.4.21.4
- 8.) 2bz6_coagulation_factor_viiia_E.C.3.4.21.21
- 9.) 1bcu_thrombin_alpha_E.C.3.4.21.5
- 10.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6

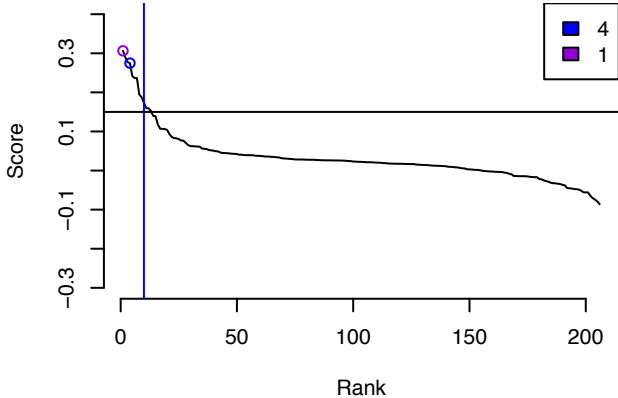
Query: 1v2o_trypsin_beta_E.C.3.4.21.4



Top 10 Ranked Pockets

- 1.) 1utp_trypsinogen_E.C.3.4.21.4
- 2.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 3.) 1o3f_trypsin_beta_E.C.3.4.21.4
- 4.) 1j16_trypsin_beta_E.C.3.4.21.4
- 5.) 1j17_trypsin_beta_E.C.3.4.21.4
- 6.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 7.) 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4
- 8.) 2bz6_coagulation_factor_viiia_E.C.3.4.21.21
- 9.) 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 10.) 1mq6_coagulation_factor_xa_E.C.3.4.21.6

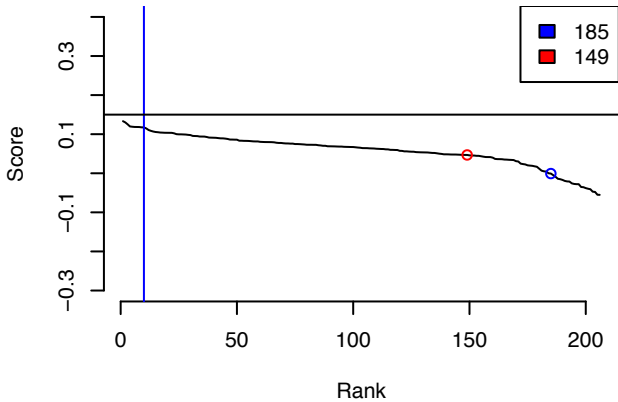
Query: 1o3f_trypsin_beta_E.C.3.4.21.4



Top 10 Ranked Pockets

- 1.) 1utp_trypsinogen_E.C.3.4.21.4
- 2.) 1f5k_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 3.) 1o3p_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 4.) 1v2o_trypsin_beta_E.C.3.4.21.4
- 5.) 1j17_trypsin_beta_E.C.3.4.21.4
- 6.) 1bra_trypsin_beta_D189G_G226D_E.C.3.4.21.4
- 7.) 1j16_trypsin_beta_E.C.3.4.21.4
- 8.) 2bz6_coagulation_factor_viiia_E.C.3.4.21.21
- 9.) 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 10.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6

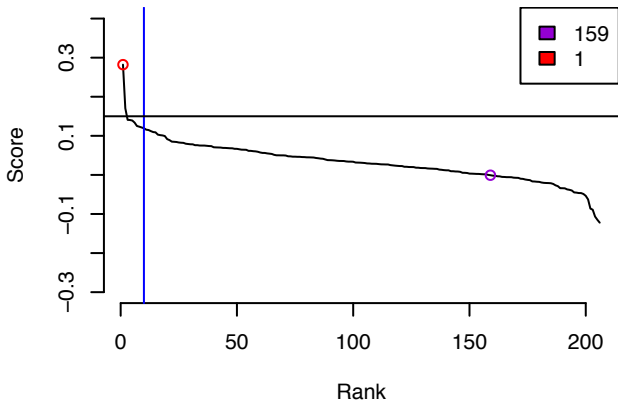
Query: 1jys_mta/sah_nucleosidase_E.C.3.2.2.9



Top 10 Ranked Pockets

- 1.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 2.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 3.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 4.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 5.) 2bz6_coagulation_factor_viiia_E.C.3.4.21.21
- 6.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 7.) 1bcu_thrombin_alpha_E.C.3.4.21.5
- 8.) 1pr5_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 9.) 1vzq_thrombin_alpha_E.C.3.4.21.5
- 10.) 1pz5_antibody_fab_E.C.-.-.-.-

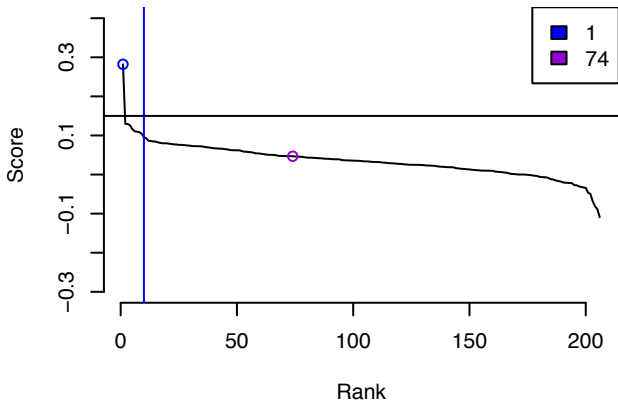
Query: 1nc1_mta/sah_nucleosidase_E.C.3.2.2.9



Top 10 Ranked Pockets

- 1.) 1y6q_mta/sah_nucleosidase_E.C.3.2.2.9
- 2.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 3.) 2std_scytalone_dehydratase_E.C.4.2.1.94
- 4.) 1fkb_FK506_binding_protein_E.C.5.2.1.8
- 5.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 6.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 7.) 2b1v_estrogen_receptor_E.C.-.-.-.-
- 8.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 9.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 10.) 1fki_FK506_binding_protein_E.C.5.2.1.8

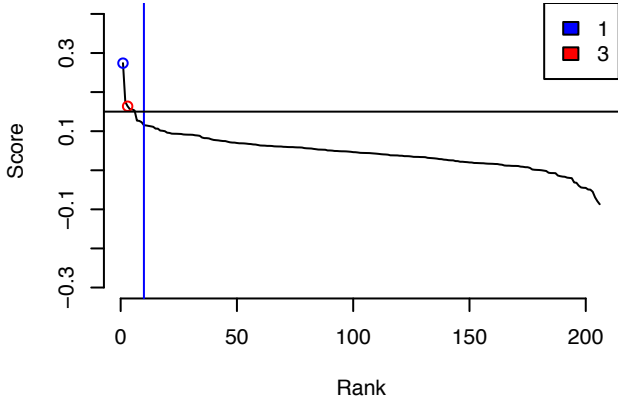
Query: 1y6q_mta/sah_nucleosidase_E.C.3.2.2.9



Top 10 Ranked Pockets

- 1.) 1nc1_mta/sah_nucleosidase_E.C.3.2.2.9
- 2.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 3.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 4.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 5.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 6.) 2b1v_estrogen_receptor_E.C.-.-.-.-
- 7.) 1fkb_FK506_binding_protein_E.C.5.2.1.8
- 8.) 2std_scytalone_dehydratase_E.C.4.2.1.94
- 9.) 1fki_FK506_binding_protein_E.C.5.2.1.8
- 10.) 2fai_estrogen_receptor_E.C.-.-.-.-

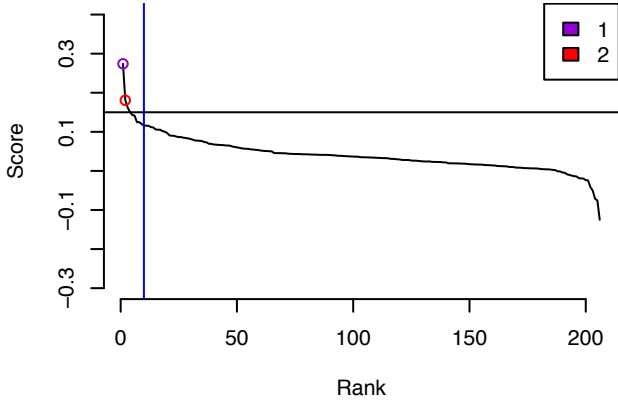
Query: 1bma_elastase_E.C.3.4.21.36



Top 10 Ranked Pockets

- 1.) 1ela_elastase_E.C.3.4.21.36
- 2.) 1axz_lectin_E.C.-.-.-.-
- 3.) 1elb_elastase_E.C.3.4.21.36
- 4.) 1ax0_lectin_E.C.-.-.-.-
- 5.) 1tyr_transthyretin_E.C.-.-.-.-
- 6.) 1j17_trypsin_beta_E.C.3.4.21.4
- 7.) 2g8r_ribonuclease_pancreatic_E.C.3.1.27.5
- 8.) 6rnt_ribonuclease_T1_E.C.3.1.27.3
- 9.) 1b11_FIV_protease_E.C.3.4.23.16
- 10.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29

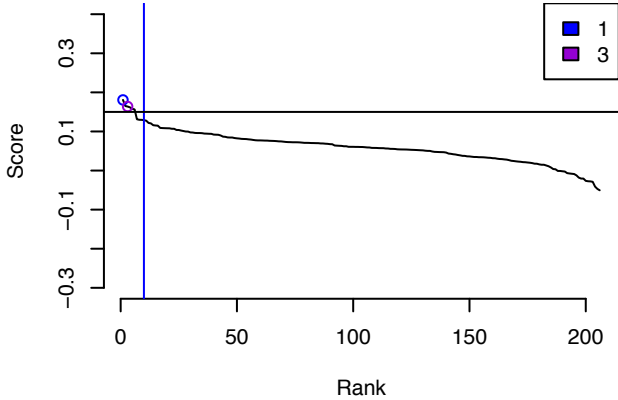
Query: 1ela_elastase_E.C.3.4.21.36



Top 10 Ranked Pockets

- 1.) 1bma_elastase_E.C.3.4.21.36
- 2.) 1elb_elastase_E.C.3.4.21.36
- 3.) 1axz_lectin_E.C.-.-.-.-
- 4.) 1tyr_transthyretin_E.C.-.-.-.-
- 5.) 1ax0_lectin_E.C.-.-.-.-
- 6.) 1j17_trypsin_beta_E.C.3.4.21.4
- 7.) 1j16_trypsin_beta_E.C.3.4.21.4
- 8.) 2bzz_nonsecretory_ribonuclease_E.C.3.1.27.5
- 9.) 1gz9_lectin_E.C.-.-.-.-
- 10.) 1nfy_coagulation_factor_xa_E.C.3.4.21.6

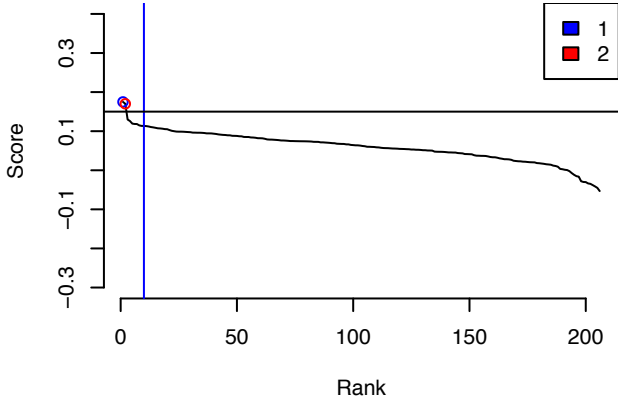
Query: 1elb_elastase_E.C.3.4.21.36



Top 10 Ranked Pockets

- 1.) 1ela_elastase_E.C.3.4.21.36
- 2.) 2bok_coagulation_factor_xa_E.C.3.4.21.6
- 3.) 1bma_elastase_E.C.3.4.21.36
- 4.) 2bzz_nonsecretory_ribonuclease_E.C.3.1.27.5
- 5.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 6.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 7.) 1axz_lectin_E.C.-.-.-.-
- 8.) 1j17_trypsin_beta_E.C.3.4.21.4
- 9.) 1slg_streptavidin_E.C.-.-.-.-
- 10.) 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73

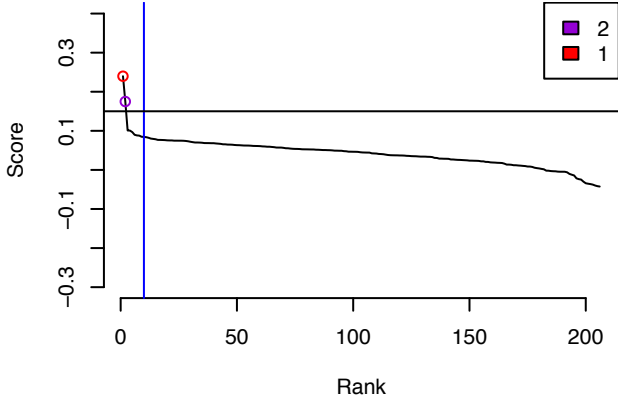
Query: 1pr5_purine_nucleoside_phosphorylase_E.C.2.4.2.1



Top 10 Ranked Pockets

- 1.) 1a69_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 2.) 1k9s_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 3.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 5.) 1m2q_casein_kinase_ii_E.C.2.7.1.37
- 6.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 7.) 1jys_mta/sah_nucleosidase_E.C.3.2.2.9
- 8.) 1nje_thymidylate_synthase_E.C.2.1.1.45
- 9.) 1flr_antibody_fab_E.C.-.-.-.-
- 10.) 1fkn_secretase_beta_E.C.3.4.23.-

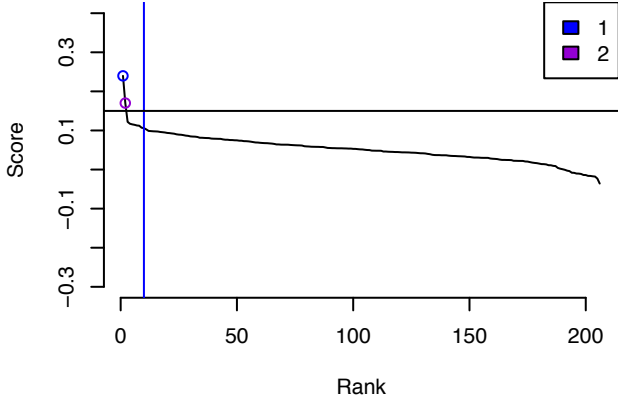
Query: 1a69_purine_nucleoside_phosphorylase_E.C.2.4.2.1



Top 10 Ranked Pockets

- 1.) 1k9s_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 2.) 1pr5_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 3.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 4.) 1nje_thymidylate_synthase_E.C.2.1.1.45
- 5.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 6.) 1ols_2-oxoisovalerate_dehydrogenase_E.C.1.2.4.4
- 7.) 1m2q_casein_kinase_ii_E.C.2.7.1.37
- 8.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 9.) 1nja_thymidylate_synthase_E.C.2.1.1.45
- 10.) 1om1_casein_kinase_ii_E.C.2.7.1.37

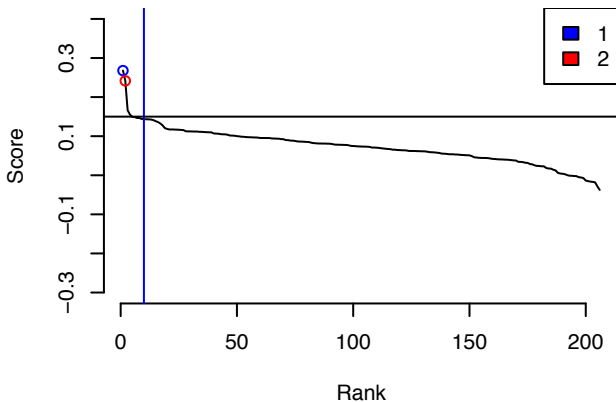
Query: 1k9s_purine_nucleoside_phosphorylase_E.C.2.4.2.1



Top 10 Ranked Pockets

- 1.) 1a69_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 2.) 1pr5_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 3.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 4.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 5.) 1b11_FIV_protease_E.C.3.4.23.16
- 6.) 1m2q_casein_kinase_ii_E.C.2.7.1.37
- 7.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 8.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 9.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 10.) 1h23_acetylcholinesterase_E.C.3.1.1.7

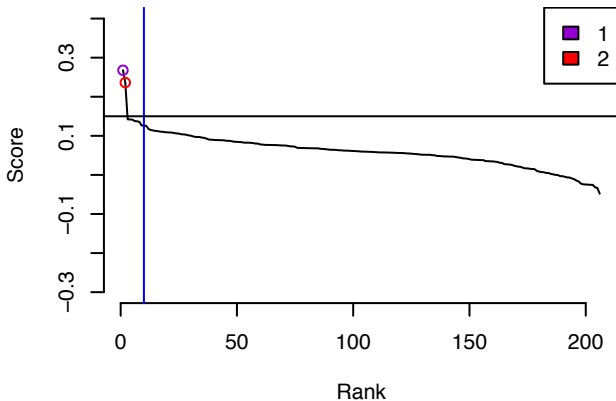
Query: 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3



Top 10 Ranked Pockets

- 1.) 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 2.) 3pcj_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 3.) 1y1m_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 4.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 5.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 6.) 1ajp_penicillin_amidohydrolase_E.C.3.5.1.11
- 7.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 8.) 1df8_streptavidin_E.C.-.-.-.-
- 9.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 10.) 1xgj_beta-lactamase_E.C.3.5.2.6

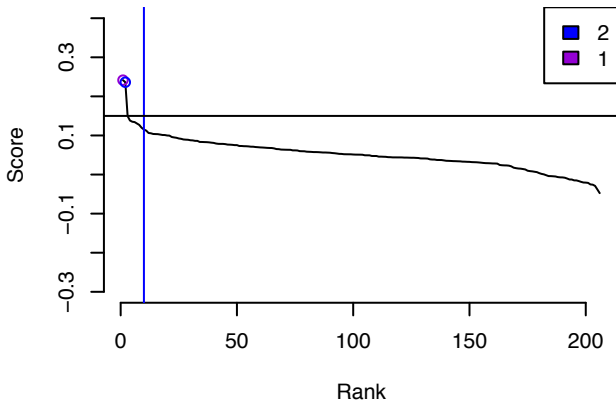
Query: 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3



Top 10 Ranked Pockets

- 1.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 2.) 3pcj_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 3.) 1df8_streptavidin_E.C.-.-.-.-
- 4.) 1xgj_beta-lactamase_E.C.3.5.2.6
- 5.) 1flr_antibody_fab_E.C.-.-.-.-
- 6.) 1y1m_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 7.) 2g5u_transthyretin_E.C.-.-.-.-
- 8.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 9.) 1hk4_serum_albumin_E.C.-.-.-.-
- 10.) 1l2s_beta-lactamase_E.C.3.5.2.6

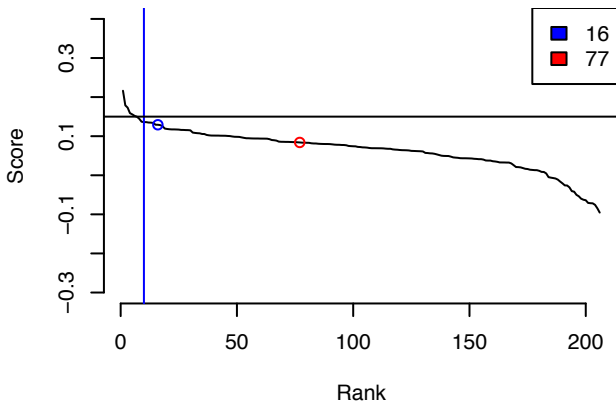
Query: 3pcj_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3



Top 10 Ranked Pockets

- 1.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 2.) 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 3.) 1df8_streptavidin_E.C.-.-.-.-
- 4.) 2g5u_transthyretin_E.C.-.-.-.-
- 5.) 1y1m_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 6.) 1flr_antibody_fab_E.C.-.-.-.-
- 7.) 1hk4_serum_albumin_E.C.-.-.-.-
- 8.) 2f01_streptavidin_E.C.-.-.-.-
- 9.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 10.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5

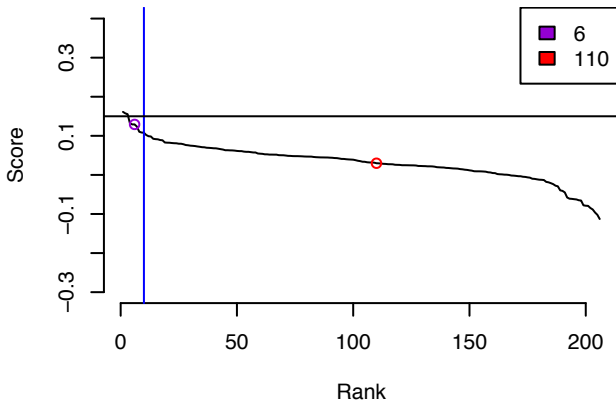
Query: 1pz5_antibody_fab_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 2usn_stromelysin-1_E.C.3.4.24.17
- 2.) 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 3.) 1sqa_urokinase-type_plasminogen_activator_E.C.3.4.21.73
- 4.) 1zs0_neutrophil_collagenase_E.C.3.4.24.34
- 5.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 6.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 7.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 8.) 2bz6_coagulation_factor_viiia_E.C.3.4.21.21
- 9.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34
- 10.) 1fh7_xylanase_beta-1,4_E.C.3.2.1.91

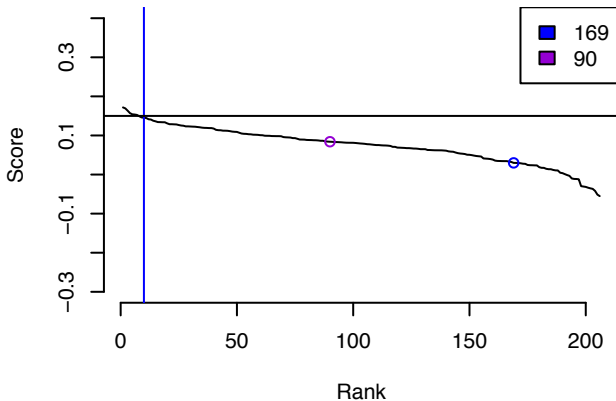
Query: 2cgr_antibody_fab_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 2usn_stromelysin-1_E.C.3.4.24.17
- 2.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34
- 3.) 1zs0_neutrophil_collagenase_E.C.3.4.24.34
- 4.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 5.) 2j77_beta-glucosidase_a_E.C.3.2.1.21
- 6.) 1pz5_antibody_fab_E.C.-.-.-.-
- 7.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 8.) 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 9.) 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 10.) 2bz6_coagulation_factor_viiia_E.C.3.4.21.21

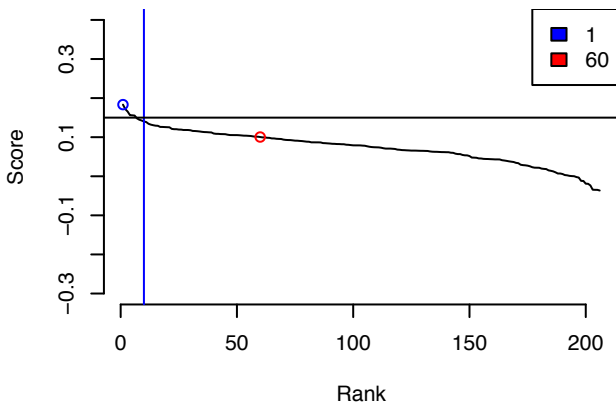
Query: 1flr_antibody_fab_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 2.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 3.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 4.) 1y1m_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 5.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 6.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 7.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 8.) 1hk4_serum_albumin_E.C.-.-.-.-
- 9.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3
- 10.) 2d3u_polyprotein_E.C.2.7.7.48

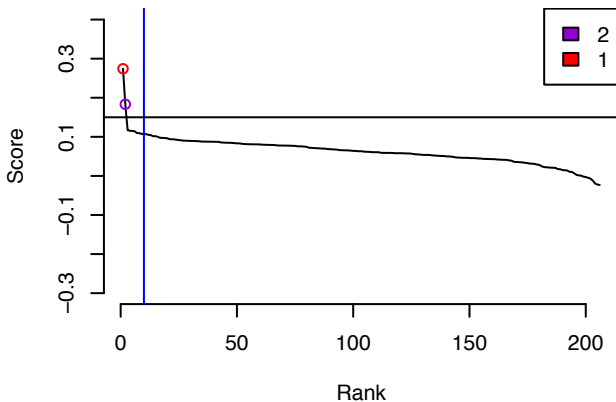
Query: 2gss_glutathione_s-transferase_E.C.2.5.1.18



Top 10 Ranked Pockets

- 1.) 3gss_glutathione_s-transferase_E.C.2.5.1.18
- 2.) 1flr_antibody_fab_E.C.-.-.-
- 3.) 2d3z_polyprotein_E.C.2.7.7.48
- 4.) 1elb_elastase_E.C.3.4.21.36
- 5.) 6fiv_FIV_protease_E.C.3.4.23.16
- 6.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 7.) 2d3u_polyprotein_E.C.2.7.7.48
- 8.) 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1
- 9.) 1if7_carbonic_anhydrase_ii_E.C.4.2.1.1
- 10.) 1b11_FIV_protease_E.C.3.4.23.16

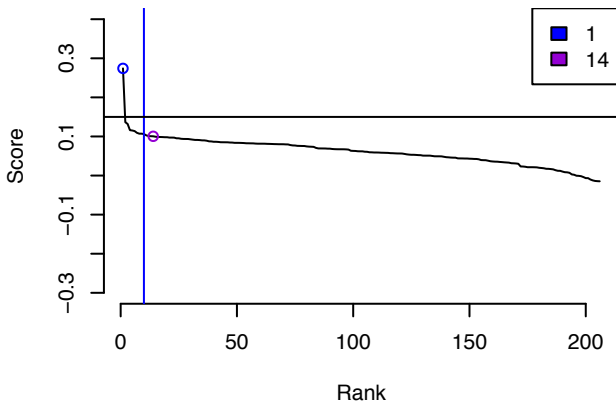
Query: 3gss_glutathione_s-transferase_E.C.2.5.1.18



Top 10 Ranked Pockets

- 1.) 10gs_glutathione_s-transferase_E.C.2.5.1.18
- 2.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 3.) 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-
- 4.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 5.) 2b7d_coagulation_factor_vii_E.C.3.4.21.21
- 6.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-
- 7.) 2er9_endothiaepsin_E.C.3.4.23.22
- 8.) 2bak_mitogen-activated_protein_kinase_14_E.C.2.7.1.37
- 9.) 4tmn_thermolysin_E.C.3.4.24.27
- 10.) 4er2_endothiaepsin_E.C.3.4.23.22

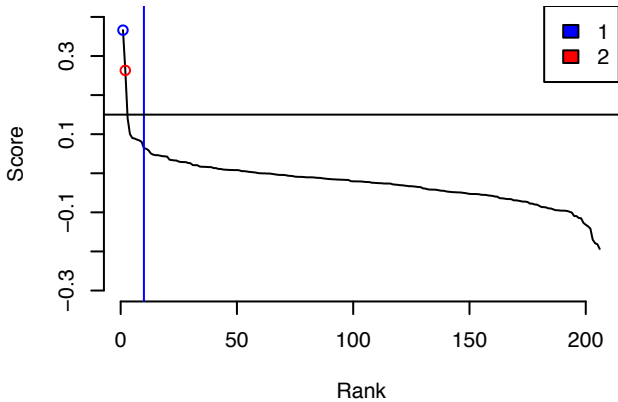
Query: 10gs_glutathione_s-transferase_E.C.2.5.1.18



Top 10 Ranked Pockets

- 1.) 3gss_glutathione_s-transferase_E.C.2.5.1.18
- 2.) 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-
- 3.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 4.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 5.) 1elb_elastase_E.C.3.4.21.36
- 6.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 7.) 2b7d_coagulation_factor_vii_E.C.3.4.21.21
- 8.) 1sl3_thrombin_alpha_E.C.3.4.21.5
- 9.) 1l2s_beta-lactamase_E.C.3.5.2.6
- 10.) 1jqe_histamine_n-methyltransferase_E.C.2.1.1.8

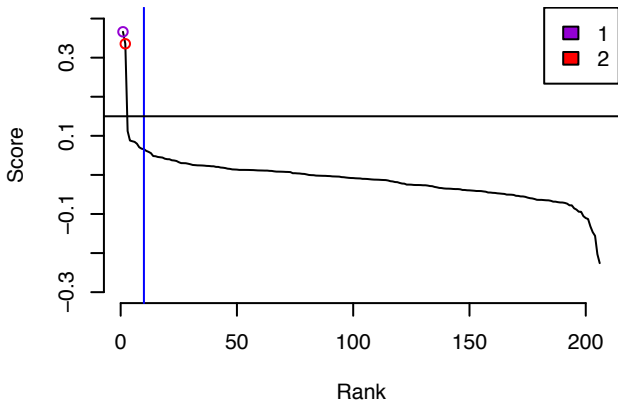
Query: 1l83_lysozyme_C54T_C97A_L99A_E.C.3.2.1.17



Top 10 Ranked Pockets

- 1.) 1li6_lysozyme_mutant_I99a/m102q_E.C.3.2.1.17
- 2.) 1li3_lysozyme_E.C.3.2.1.17
- 3.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 4.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 5.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 6.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 7.) 2b1v_estrogen_receptor_E.C.-.-.-.-
- 8.) 1fkb_FK506_binding_protein_E.C.5.2.1.8
- 9.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 10.) 1fki_FK506_binding_protein_E.C.5.2.1.8

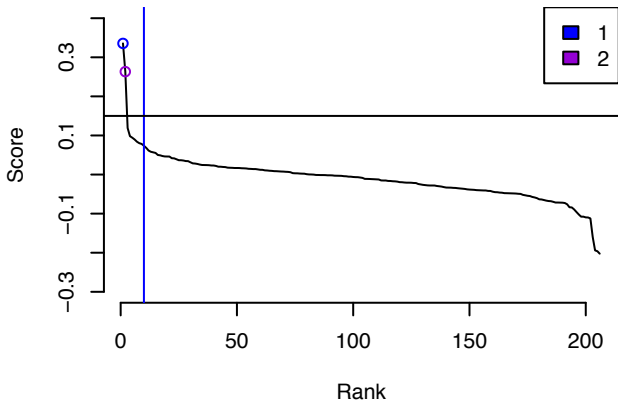
Query: 1li6_lysozyme_mutant_I99a/m102q_E.C.3.2.1.17



Top 10 Ranked Pockets

- 1.) 1l83_lysozyme_C54T_C97A_L99A_E.C.3.2.1.17
- 2.) 1li3_lysozyme_E.C.3.2.1.17
- 3.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 4.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 5.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 6.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 7.) 1d7l_FK506_binding_protein_E.C.5.2.1.8
- 8.) 2b1v_estrogen_receptor_E.C.-.-.-.-
- 9.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 10.) 1b11_FIV_protease_E.C.3.4.23.16

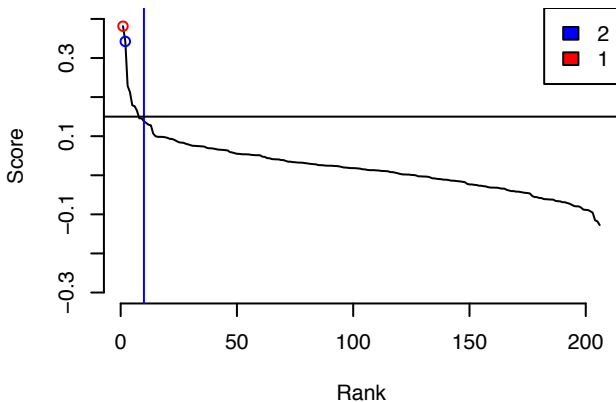
Query: 1li3_lysozyme_E.C.3.2.1.17



Top 10 Ranked Pockets

- 1.) 1li6_lysozyme_mutant_I99a/m102q_E.C.3.2.1.17
- 2.) 1l83_lysozyme_C54T_C97A_L99A_E.C.3.2.1.17
- 3.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 4.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 5.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 6.) 1c84_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 7.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 8.) 2b1v_estrogen_receptor_E.C.-.-.-.-
- 9.) 6fiv_FIV_protease_E.C.3.4.23.16
- 10.) 2std_scytalone_dehydratase_E.C.4.2.1.94

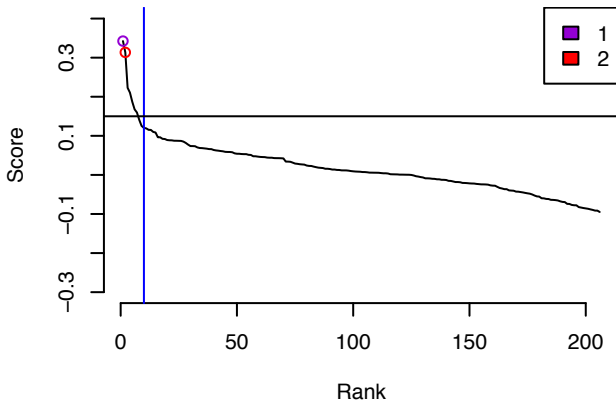
Query: 6std_scytalone_dehydratase_E.C.4.2.1.94



Top 10 Ranked Pockets

- 1.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 2.) 2std_scytalone_dehydratase_E.C.4.2.1.94
- 3.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 4.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 5.) 2fai_estrogen_receptor_E.C.-.-.-.-
- 6.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 7.) 2b1v_estrogen_receptor_E.C.-.-.-.-
- 8.) 1gni_serum_albumin_E.C.-.-.-.-
- 9.) 1fkb_FK506_binding_protein_E.C.5.2.1.8
- 10.) 1fki_FK506_binding_protein_E.C.5.2.1.8

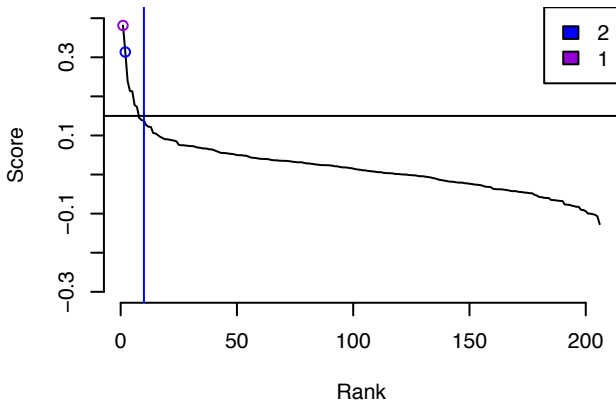
Query: 2std_scytalone_dehydratase_E.C.4.2.1.94



Top 10 Ranked Pockets

- 1.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 2.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 3.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 4.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 5.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 6.) 2fai_estrogen_receptor_E.C.-.-.-.-
- 7.) 2b1v_estrogen_receptor_E.C.-.-.-.-
- 8.) 1nc1_mta/sah_nucleosidase_E.C.3.2.2.9
- 9.) 1fki_FK506_binding_protein_E.C.5.2.1.8
- 10.) 1d7j_FK506_binding_protein_E.C.5.2.1.8

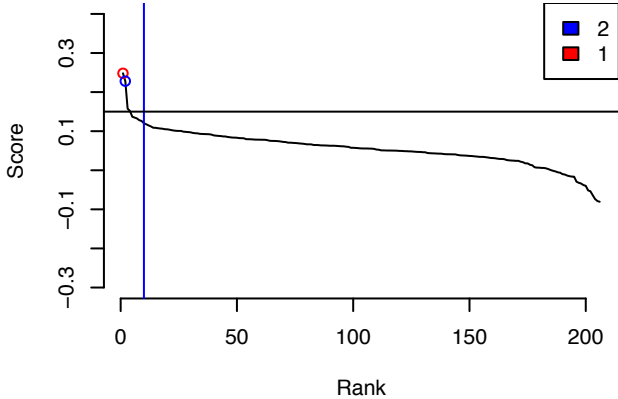
Query: 3std_scytalone_dehydratase_E.C.4.2.1.94



Top 10 Ranked Pockets

- 1.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 2.) 2std_scytalone_dehydratase_E.C.4.2.1.94
- 3.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 4.) 1fcz_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 5.) 1fd0_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 6.) 2fai_estrogen_receptor_E.C.-.-.-.-
- 7.) 2b1v_estrogen_receptor_E.C.-.-.-.-
- 8.) 1fki_FK506_binding_protein_E.C.5.2.1.8
- 9.) 1nc1_mta/sah_nucleosidase_E.C.3.2.2.9
- 10.) 1gni_serum_albumin_E.C.-.-.-.-

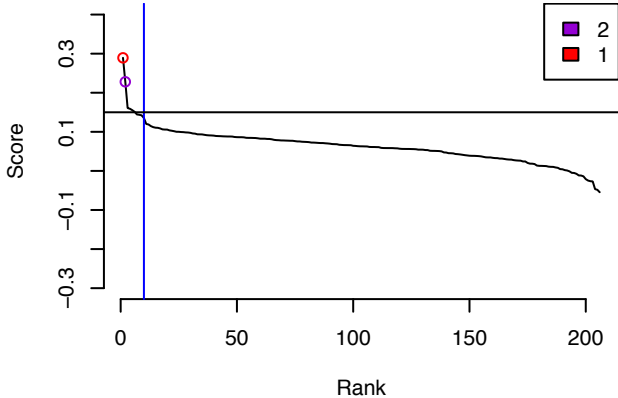
Query: 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34



Top 10 Ranked Pockets

- 1.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 2.) 1zs0_neutrophil_collagenase_E.C.3.4.24.34
- 3.) 2cgr_antibody_fab_E.C.-.-.-.-
- 4.) 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 5.) 1pz5_antibody_fab_E.C.-.-.-.-
- 6.) 1u1b_ribonuclease_a_E.C.3.1.27.5
- 7.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 8.) 2usn_stromelysin-1_E.C.3.4.24.17
- 9.) 1syh_glutamate_receptor_2_E.C.-.-.-.-
- 10.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29

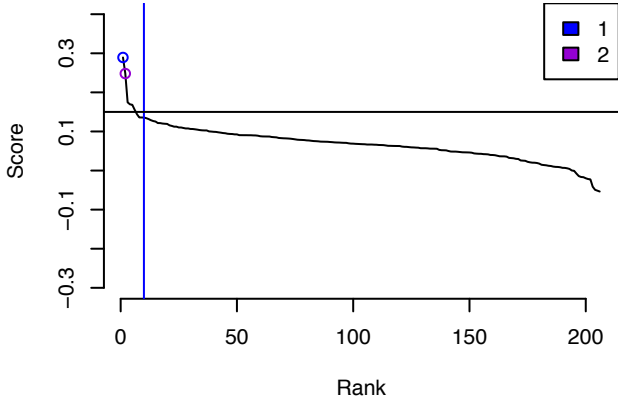
Query: 1zs0_neutrophil_collagenase_E.C.3.4.24.34



Top 10 Ranked Pockets

- 1.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 2.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34
- 3.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 4.) 1pz5_antibody_fab_E.C.-.-.-.-
- 5.) 2cgr_antibody_fab_E.C.-.-.-.-
- 6.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 7.) 2usn_stromelysin-1_E.C.3.4.24.17
- 8.) 1vfn_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 9.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 10.) 1s39_tRNA-guanine_transglycosylase_E.C.2.4.2.29

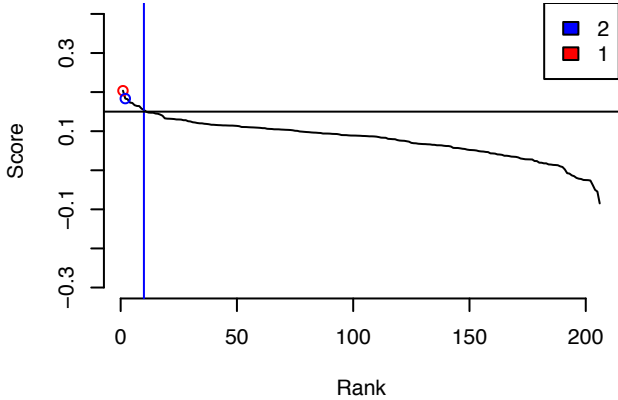
Query: 1zvx_neutrophil_collagenase_E.C.3.4.24.34



Top 10 Ranked Pockets

- 1.) 1zs0_neutrophil_collagenase_E.C.3.4.24.34
- 2.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34
- 3.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 4.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 5.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 6.) 1pz5_antibody_fab_E.C.-.-.-.-
- 7.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 8.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 9.) 2usn_stromelysin-1_E.C.3.4.24.17
- 10.) 2f01_streptavidin_E.C.-.-.-.-

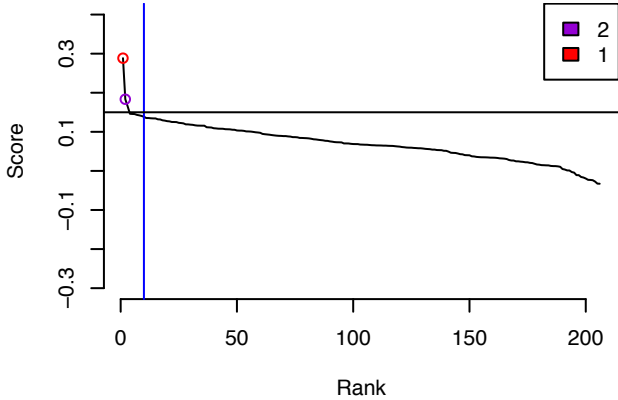
Query: 2d0k_dihydrofolate_reductase_E.C.1.5.1.3



Top 10 Ranked Pockets

- 1.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 2.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3
- 3.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 5.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 6.) 2j78_beta-glucosidase_a_E.C.3.2.1.21
- 7.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 8.) 1hk4_serum_albumin_E.C.-.-.-.-
- 9.) 1uwt_beta-galactosidase_E.C.3.2.1.23
- 10.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37

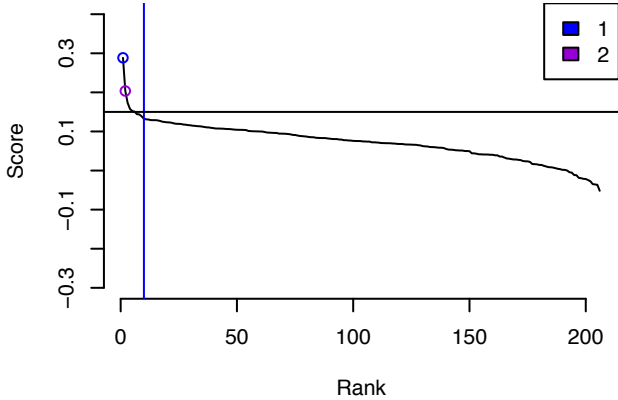
Query: 1dhi_dihydrofolate_reductase_E.C.1.5.1.3



Top 10 Ranked Pockets

- 1.) 2drc_dihydrofolate_reductase_E.C.1.5.1.3
- 2.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 3.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 4.) 1flr_antibody_fab_E.C.-.-.-.-
- 5.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 6.) 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 7.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 8.) 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 9.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 10.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29

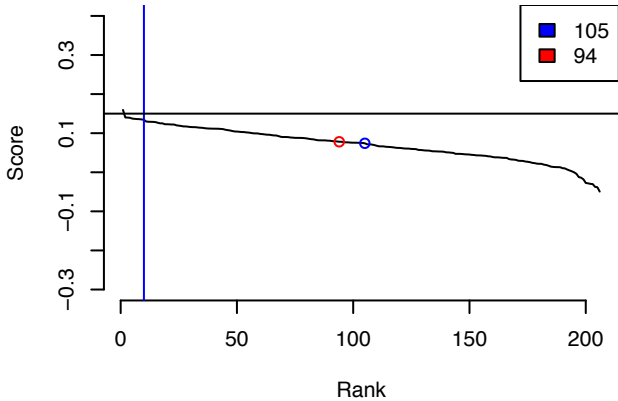
Query: 2drc_dihydrofolate_reductase_E.C.1.5.1.3



Top 10 Ranked Pockets

- 1.) 1dhi_dihydrofolate_reductase_E.C.1.5.1.3
- 2.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 3.) 1f4e_thymidylate_synthase_E.C.2.1.1.45
- 4.) 1pbq_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 5.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 6.) 1f4f_thymidylate_synthase_E.C.2.1.1.45
- 7.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 8.) 2cer_beta-glucosidase_a_E.C.3.2.1.21
- 9.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 10.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37

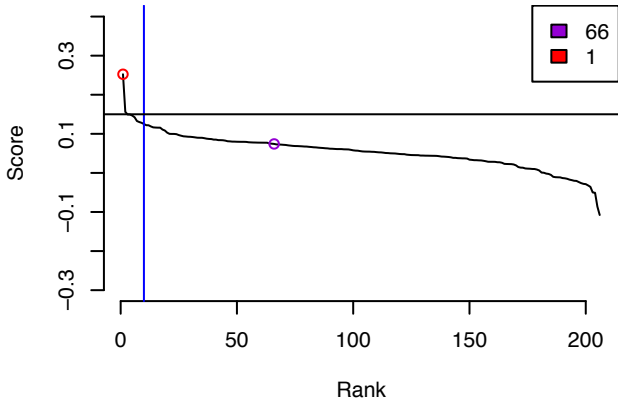
Query: 1slg_streptavidin_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 2.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 3.) 1h23_acetylcholinesterase_E.C.3.1.1.7
- 4.) 2d3u_polyprotein_E.C.2.7.7.48
- 5.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 6.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 7.) 1om1_casein_kinase_ii_E.C.2.7.1.37
- 8.) 1zoe_protein_kinase_ck2_alpha_subunit_E.C.2.7.1.37
- 9.) 1b11_FIV_protease_E.C.3.4.23.16
- 10.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37

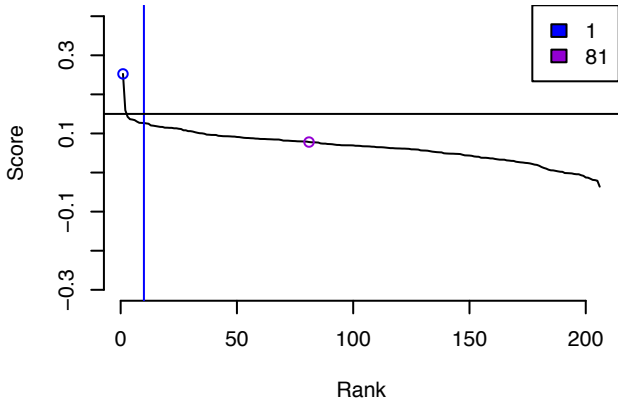
Query: 1df8_streptavidin_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 2f01_streptavidin_E.C.-.-.-.-
- 2.) 1ajp_penicillin_amidohydrolase_E.C.3.5.1.11
- 3.) 3pcj_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 4.) 1ai5_penicillin_amidohydrolase_E.C.3.5.1.11
- 5.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 6.) 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 7.) 1ajq_penicillin_amidohydrolase_E.C.3.5.1.11
- 8.) 1hk4_serum_albumin_E.C.-.-.-.-
- 9.) 1flr_antibody_fab_E.C.-.-.-.-
- 10.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1

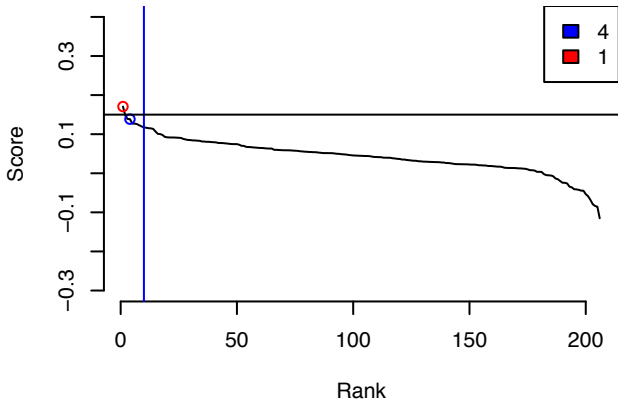
Query: 2f01_streptavidin_E.C.-.-.-.-



Top 10 Ranked Pockets

- 1.) 1df8_streptavidin_E.C.-.-.-.-
- 2.) 1ai5_penicillin_amidohydrolase_E.C.3.5.1.11
- 3.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 4.) 1hk4_serum_albumin_E.C.-.-.-.-
- 5.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 6.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 7.) 1n2v_queueine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 8.) 1vfn_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 9.) 3pcj_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 10.) 1ajq_penicillin_amidohydrolase_E.C.3.5.1.11

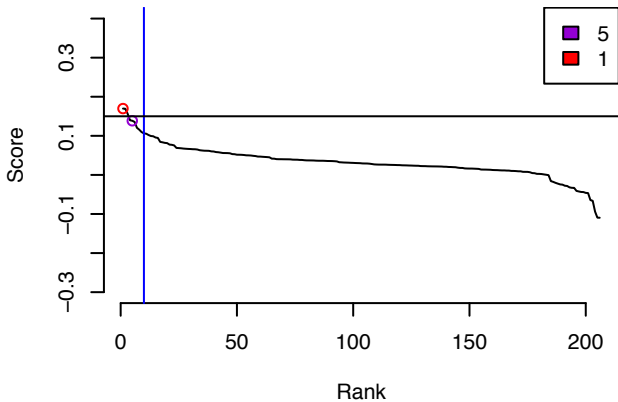
Query: 2g8r_ribonuclease_pancreatic_E.C.3.1.27.5



Top 10 Ranked Pockets

- 1.) 1u1b_ribonuclease_a_E.C.3.1.27.5
- 2.) 1ax0_lectin_E.C.-.-.-.-
- 3.) 1axz_lectin_E.C.-.-.-.-
- 4.) 1o0h_ribonuclease_a_E.C.3.1.27.5
- 5.) 1bma_elastase_E.C.3.4.21.36
- 6.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 7.) 1if7_carbonic_anhydrase_ii_E.C.4.2.1.1
- 8.) 1gz9_lectin_E.C.-.-.-.-
- 9.) 2b7d_coagulation_factor_vii_E.C.3.4.21.21
- 10.) 1j17_trypsin_beta_E.C.3.4.21.4

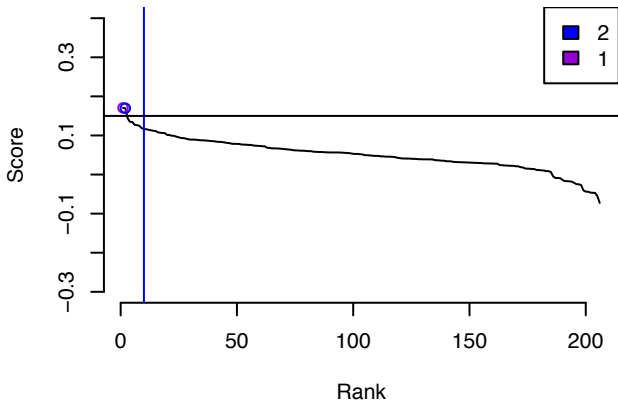
Query: 1o0h_ribonuclease_a_E.C.3.1.27.5



Top 10 Ranked Pockets

- 1.) 1u1b_ribonuclease_a_E.C.3.1.27.5
- 2.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 3.) 1hl4_ribonuclease_2_E.C.3.1.27.5
- 4.) 2bzz_nonsecretory_ribonuclease_E.C.3.1.27.5
- 5.) 2g8r_ribonuclease_pancreatic_E.C.3.1.27.5
- 6.) 1axz_lectin_E.C.-.-.-.-
- 7.) 1rnt_ribonuclease_T1_E.C.3.1.27.3
- 8.) 1kv5_triosephosphate_isomerase_E.C.5.3.1.1
- 9.) 1ax0_lectin_E.C.-.-.-.-
- 10.) 1nny_tyrosine_phosphatase_1b_E.C.3.1.3.48

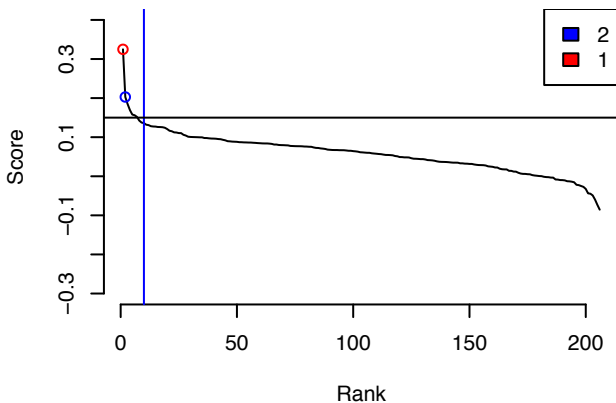
Query: 1u1b_ribonuclease_a_E.C.3.1.27.5



Top 10 Ranked Pockets

- 1.) 2g8r_ribonuclease_pancreatic_E.C.3.1.27.5
- 2.) 1o0h_ribonuclease_a_E.C.3.1.27.5
- 3.) 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1
- 4.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34
- 5.) 1axz_lectin_E.C.-.-.-.-
- 6.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 7.) 1ax0_lectin_E.C.-.-.-.-
- 8.) 1xgj_beta-lactamase_E.C.3.5.2.6
- 9.) 1flr_antibody_fab_E.C.-.-.-.-
- 10.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29

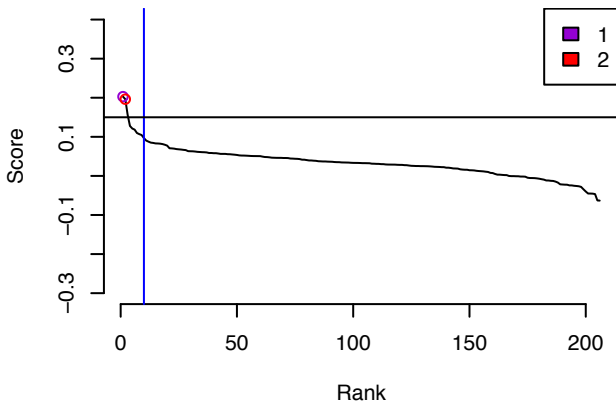
Query: 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5



Top 10 Ranked Pockets

- 1.) 2bzz_nonsecretory_ribonuclease_E.C.3.1.27.5
- 2.) 1hi4_ribonuclease_2_E.C.3.1.27.5
- 3.) 1ax0_lectin_E.C.-.-.-.-
- 4.) 1o0h_ribonuclease_a_E.C.3.1.27.5
- 5.) 1elb_elastase_E.C.3.4.21.36
- 6.) 1axz_lectin_E.C.-.-.-.-
- 7.) 1pz5_antibody_fab_E.C.-.-.-.-
- 8.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 9.) 1b11_FIV_protease_E.C.3.4.23.16
- 10.) 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3

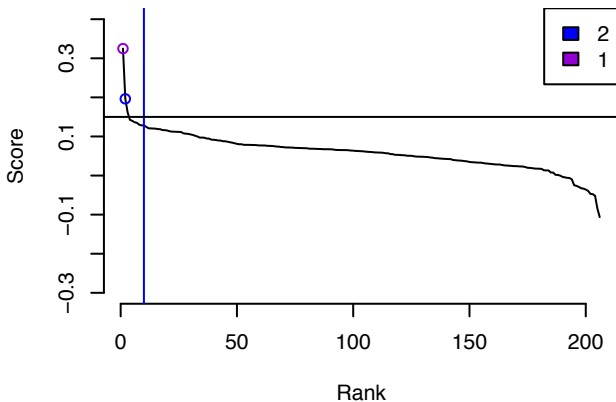
Query: 1hi4_ribonuclease_2_E.C.3.1.27.5



Top 10 Ranked Pockets

- 1.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 2.) 2bzz_nonsecretory_ribonuclease_E.C.3.1.27.5
- 3.) 1o0h_ribonuclease_a_E.C.3.1.27.5
- 4.) 1axz_lectin_E.C.-.-.-.-
- 5.) 1ax0_lectin_E.C.-.-.-.-
- 6.) 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1
- 7.) 1rnt_ribonuclease_T1_E.C.3.1.27.3
- 8.) 1elb_elastase_E.C.3.4.21.36
- 9.) 1y1m_glutamate_[nmda]_receptor_E.C.-.-.-.-
- 10.) 1xgj_beta-lactamase_E.C.3.5.2.6

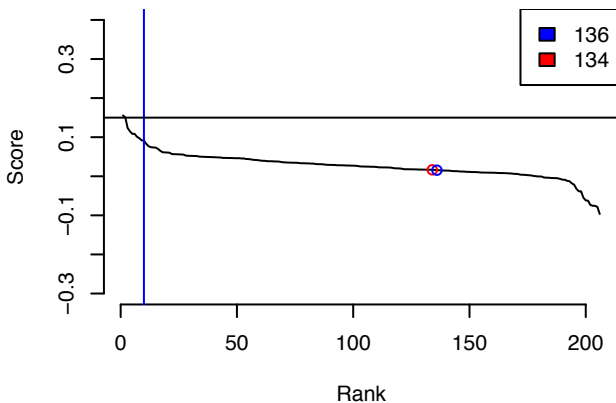
Query: 2bzz_nonsecretory_ribonuclease_E.C.3.1.27.5



Top 10 Ranked Pockets

- 1.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 2.) 1hi4_ribonuclease_2_E.C.3.1.27.5
- 3.) 1elb_elastase_E.C.3.4.21.36
- 4.) 1b11_FIV_protease_E.C.3.4.23.16
- 5.) 1o0h_ribonuclease_a_E.C.3.1.27.5
- 6.) 1n2v_queuine_tRNA-ribosyltransferase_E.C.2.4.2.29
- 7.) 1axz_lectin_E.C.-.-.-.-
- 8.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 9.) 1pz5_antibody_fab_E.C.-.-.-.-
- 10.) 6fiv_FIV_protease_E.C.3.4.23.16

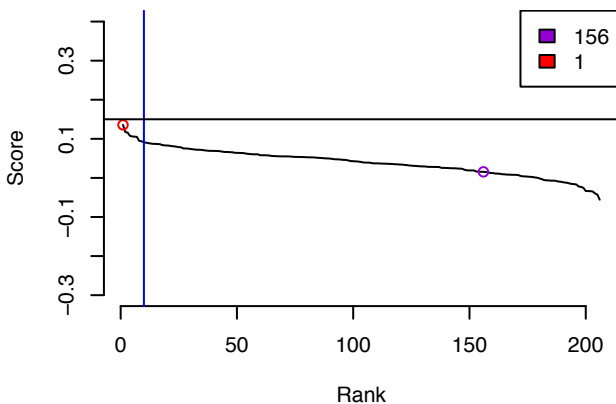
Query: 1tyr_tranthyretin_E.C.-.-.-



Top 10 Ranked Pockets

- 1bma_elastase_E.C.3.4.21.36
- 1ela_elastase_E.C.3.4.21.36
- 1axz_lectin_E.C.-.-.-
- 1j17_trypsin_beta_E.C.3.4.21.4
- 1ax0_lectin_E.C.-.-.-
- 1v20_trypsin_beta_E.C.3.4.21.4
- 6rnt_ribonuclease_T1_E.C.3.1.27.3
- 1gz9_lectin_E.C.-.-.-
- 1nfy_coagulation_factor_xa_E.C.3.4.21.6
- 1utp_trypsinogen_E.C.3.4.21.4

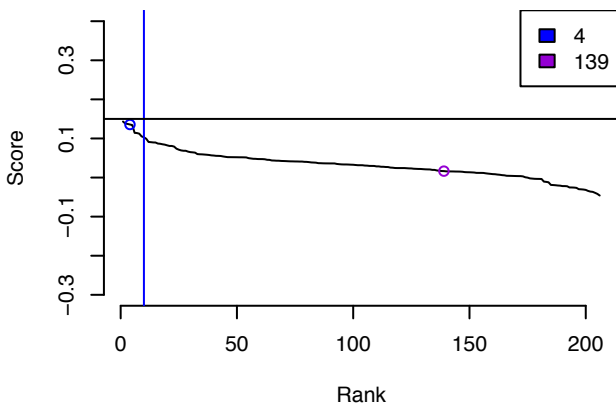
Query: 1e5a_tranthyretin_E.C.-.-.-



Top 10 Ranked Pockets

- 2g5u_tranthyretin_E.C.-.-.-
- 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 1df8_streptavidin_E.C.-.-.-
- 2fai_estrogen_receptor_E.C.-.-.-
- 1hk4_serum_albumin_E.C.-.-.-
- 3pcj_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 2f01_streptavidin_E.C.-.-.-
- 1ai5_penicillin_amidohydrolase_E.C.3.5.1.11
- 2hdq_beta-lactamase_E.C.3.5.2.6
- 1ha2_serum_albumin_E.C.-.-.-

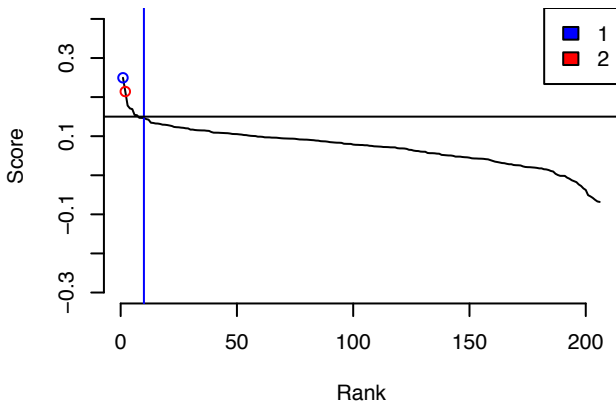
Query: 2g5u_tranthyretin_E.C.-.-.-



Top 10 Ranked Pockets

- 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 3pcj_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 3pch_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3
- 1e5a_tranthyretin_E.C.-.-.-
- 1m0q_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 2f01_streptavidin_E.C.-.-.-
- 1m0n_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 1x1z_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 2hdq_beta-lactamase_E.C.3.5.2.6

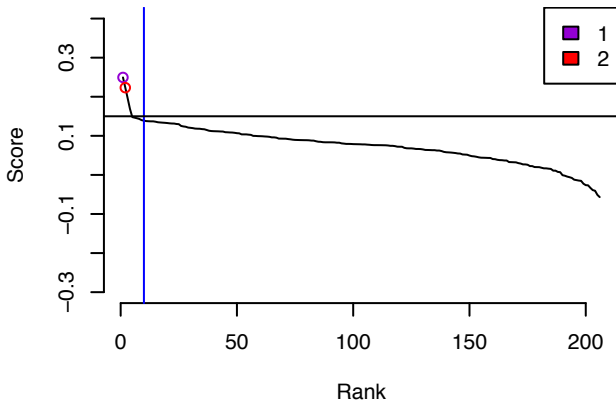
Query: 1sv3_phospholipase_a2_E.C.3.1.1.4



Top 10 Ranked Pockets

- 1.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 2.) 1jq9_phospholipase_a2_E.C.3.1.1.4
- 3.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 4.) 2d3u_polyprotein_E.C.2.7.7.48
- 5.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 6.) 1flr_antibody_fab_E.C.-.-.-.-
- 7.) 1k4g_tRNA-guanine_transglycosylase_E.C.2.4.2.29
- 8.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 9.) 1hk4_serum_albumin_E.C.-.-.-.-
- 10.) 3pce_protocatechuate_3,4-dioxygenase_E.C.1.13.11.3

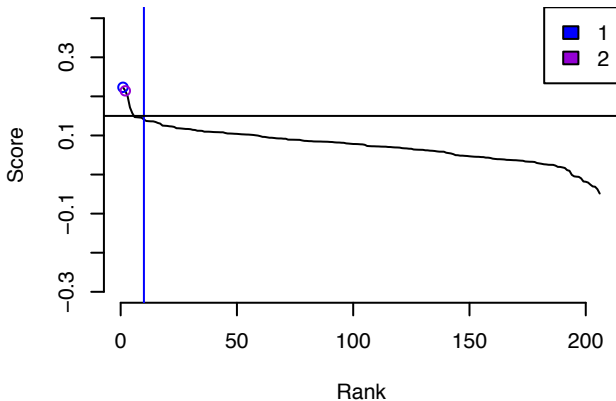
Query: 1q7a_phospholipase_a2_E.C.3.1.1.4



Top 10 Ranked Pockets

- 1.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 2.) 1jq9_phospholipase_a2_E.C.3.1.1.4
- 3.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 4.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 5.) 1f4g_thymidylate_synthase_E.C.2.1.1.45
- 6.) 1u33_alpha-amylase_E.C.3.2.1.1
- 7.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 8.) 1hk4_serum_albumin_E.C.-.-.-.-
- 9.) 2cet_beta-glucosidase_a_E.C.3.2.1.21
- 10.) 2d1o_stromelysin-1_E.C.3.4.24.17

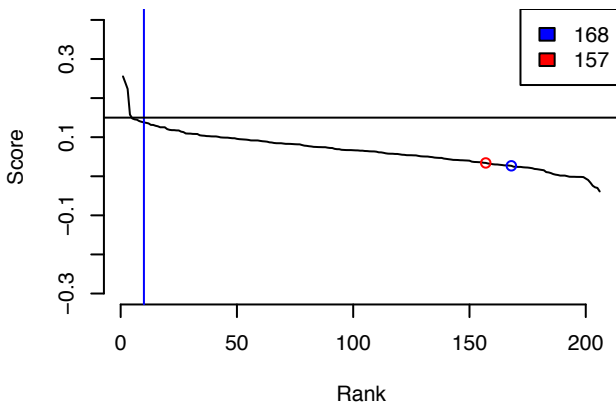
Query: 1jq9_phospholipase_a2_E.C.3.1.1.4



Top 10 Ranked Pockets

- 1.) 1q7a_phospholipase_a2_E.C.3.1.1.4
- 2.) 1sv3_phospholipase_a2_E.C.3.1.1.4
- 3.) 2brb_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 4.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 5.) 2brm_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37
- 6.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 7.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 8.) 1u33_alpha-amylase_E.C.3.2.1.1
- 9.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 10.) 1ajp_penicillin_amidohydrolase_E.C.3.5.1.11

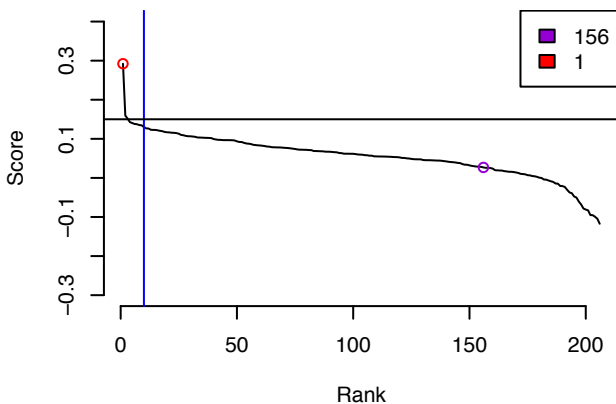
Query: 4fiv_FIV_protease_E.C.3.4.23.16



Top 10 Ranked Pockets

- 1.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 2.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 3.) 2i0d_HIV-1_protease_E.C.3.4.23.16
- 4.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 5.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 6.) 1fkn_secretase_beta_E.C.3.4.23.-
- 7.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 8.) 1kv1_mitogen-activated_protein_kinase_p38_E.C.2.7.1.37
- 9.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 10.) 1ndz_adenosine_deaminase_E.C.3.5.4.4

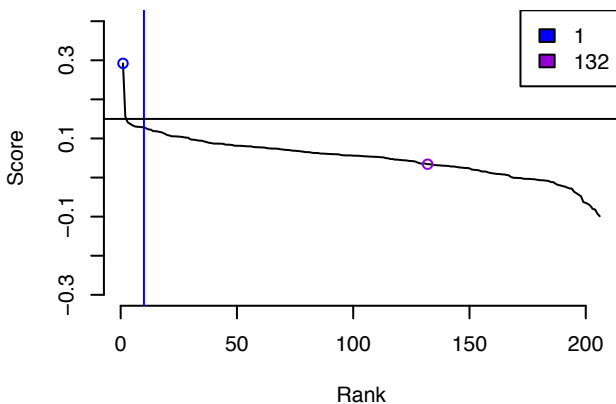
Query: 1b11_FIV_protease_E.C.3.4.23.16



Top 10 Ranked Pockets

- 1.) 6fiv_FIV_protease_E.C.3.4.23.16
- 2.) 1fki_FK506_binding_protein_E.C.5.2.1.8
- 3.) 1d7J_FK506_binding_protein_E.C.5.2.1.8
- 4.) 2bzz_nonsecretory_ribonuclease_E.C.3.1.27.5
- 5.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 6.) 1if7_carbonic_anhydrase_ii_E.C.4.2.1.1
- 7.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 8.) 1slg_streptavidin_E.C.-.-.-.-
- 9.) 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1
- 10.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1

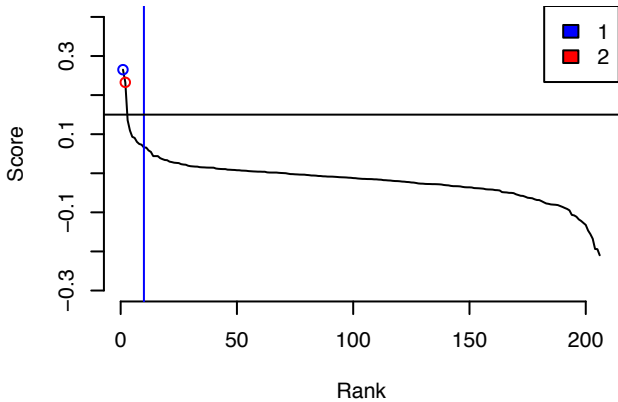
Query: 6fiv_FIV_protease_E.C.3.4.23.16



Top 10 Ranked Pockets

- 1.) 1b11_FIV_protease_E.C.3.4.23.16
- 2.) 2gss_glutathione_s-transferase_E.C.2.5.1.18
- 3.) 1ttm_carbonic_anhydrase_ii_E.C.4.2.1.1
- 4.) 1avn_carbonic_anhydrase_ii_E.C.4.2.1.1
- 5.) 1ax0_lectin_E.C.-.-.-.-
- 6.) 1if7_carbonic_anhydrase_ii_E.C.4.2.1.1
- 7.) 1fki_FK506_binding_protein_E.C.5.2.1.8
- 8.) 2d0k_dihydrofolate_reductase_E.C.1.5.1.3
- 9.) 1d7J_FK506_binding_protein_E.C.5.2.1.8
- 10.) 2bzz_nonsecretory_ribonuclease_E.C.3.1.27.5

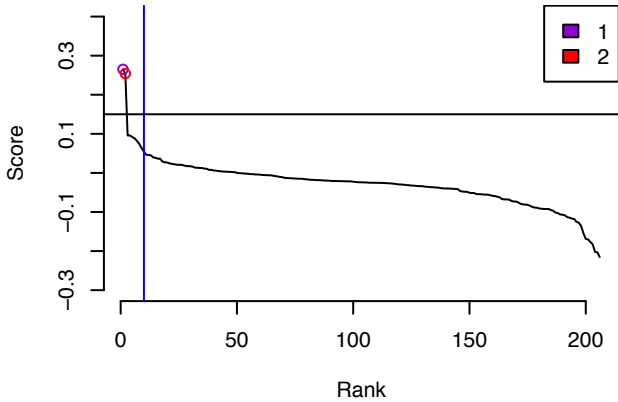
Query: 1a08_tyrosine_kinase_C-src_E.C.2.7.1.112



Top 10 Ranked Pockets

- 1.) 1a1b_tyrosine_kinase_C-src_E.C.2.7.1.112
- 2.) 1is0_tyrosine_kinase_C-src_E.C.2.7.1.112
- 3.) 1trd_triosephosphate_isomerase_E.C.5.3.1.1
- 4.) 1kv5_triosephosphate_isomerase_E.C.5.3.1.1
- 5.) 1nwl_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 6.) 1d09_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 7.) 1loq_orotidine_5'-monophosphate_decarboxylase_E.C.4.1.1.23
- 8.) 1nny_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 9.) 2h3e_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 10.) 4tim_triosephosphate_isomerase_E.C.5.3.1.1

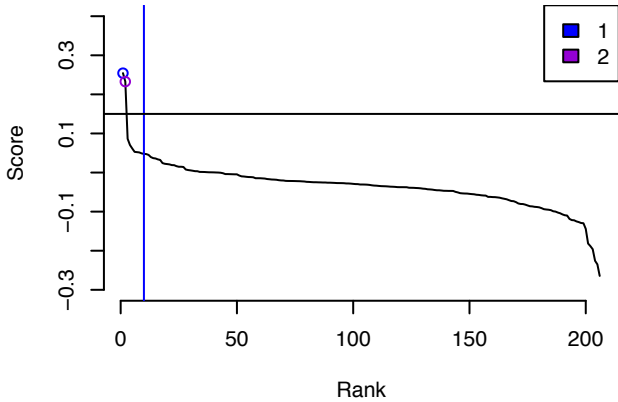
Query: 1a1b_tyrosine_kinase_C-src_E.C.2.7.1.112



Top 10 Ranked Pockets

- 1.) 1a08_tyrosine_kinase_C-src_E.C.2.7.1.112
- 2.) 1is0_tyrosine_kinase_C-src_E.C.2.7.1.112
- 3.) 1trd_triosephosphate_isomerase_E.C.5.3.1.1
- 4.) 1kv5_triosephosphate_isomerase_E.C.5.3.1.1
- 5.) 2h3e_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 6.) 4tim_triosephosphate_isomerase_E.C.5.3.1.1
- 7.) 1d09_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 8.) 1nwl_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 9.) 7cpa_carboxypeptidase_a_E.C.3.4.17.1
- 10.) 1nny_tyrosine_phosphatase_1b_E.C.3.1.3.48

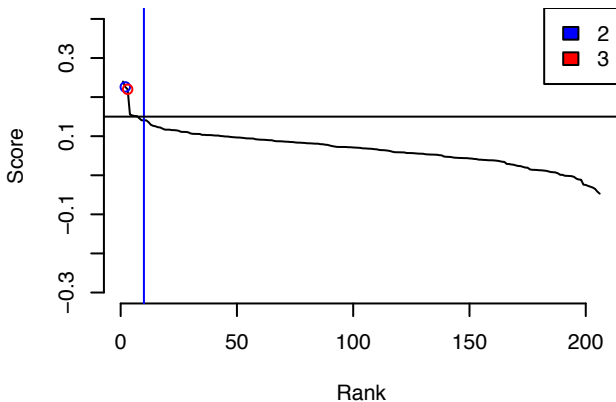
Query: 1is0_tyrosine_kinase_C-src_E.C.2.7.1.112



Top 10 Ranked Pockets

- 1.) 1a1b_tyrosine_kinase_C-src_E.C.2.7.1.112
- 2.) 1a08_tyrosine_kinase_C-src_E.C.2.7.1.112
- 3.) 2h3e_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 4.) 1kv5_triosephosphate_isomerase_E.C.5.3.1.1
- 5.) 1nje_thymidylate_synthase_E.C.2.1.1.45
- 6.) 1trd_triosephosphate_isomerase_E.C.5.3.1.1
- 7.) 1zc9_2,2-dialkylglycine_decarboxylase_E.C.4.1.1.64
- 8.) 1nwl_tyrosine_phosphatase_1b_E.C.3.1.3.48
- 9.) 2fzc_aspartate_carbamoyltransferase_E.C.2.1.3.2
- 10.) 1pr5_purine_nucleoside_phosphorylase_E.C.2.4.2.1

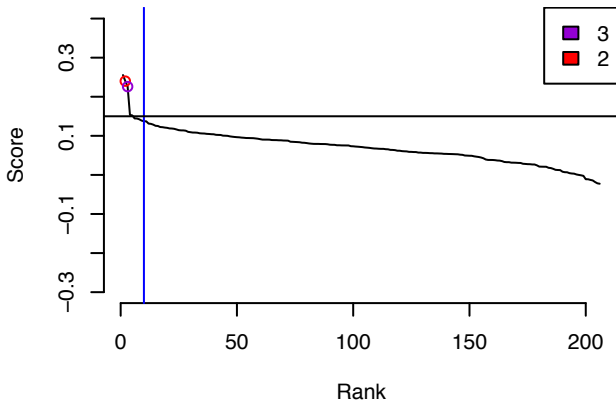
Query: 1a30_HIV-1_protease_E.C.3.4.23.16



Top 10 Ranked Pockets

- 1.) 4fiv_FIV_protease_E.C.3.4.23.16
- 2.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 3.) 2i0d_HIV-1_protease_E.C.3.4.23.16
- 4.) 1fkn_secretase_beta_E.C.3.4.23.-
- 5.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 6.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 7.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 8.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 9.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 10.) 1q8t_cyclin_dependent_kinase_2_E.C.2.7.1.37

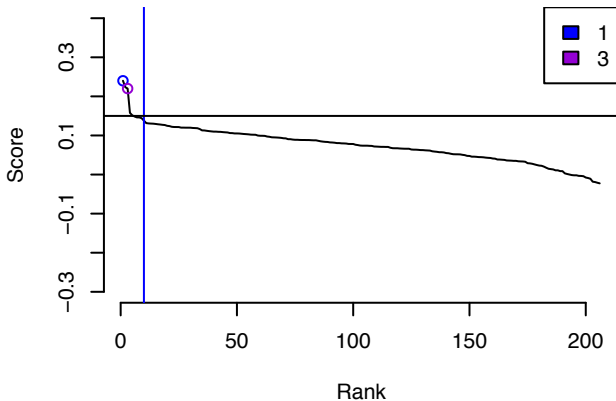
Query: 2f80_pol_polyprotein_E.C.3.4.23.16



Top 10 Ranked Pockets

- 1.) 4fiv_FIV_protease_E.C.3.4.23.16
- 2.) 2i0d_HIV-1_protease_E.C.3.4.23.16
- 3.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 4.) 1b39_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 5.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 6.) 1fkn_secretase_beta_E.C.3.4.23.-
- 7.) 1zvx_neutrophil_collagenase_E.C.3.4.24.34
- 8.) 1jqd_histamine_n-methyltransferase_E.C.2.1.1.8
- 9.) 1pxo_cyclin_dependent_kinase_2_E.C.2.7.1.37
- 10.) 1nvq_serine/threonine-protein_kinase_chk1_E.C.2.7.1.37

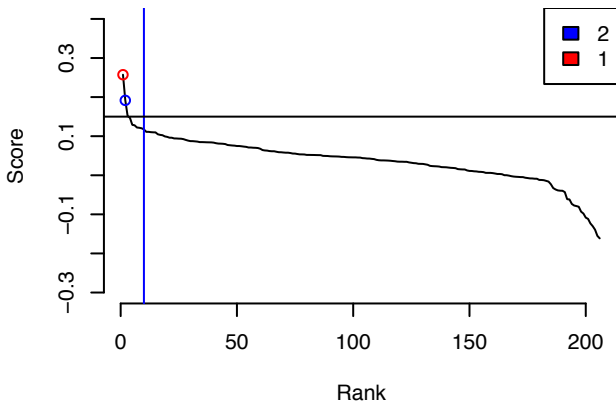
Query: 2i0d_HIV-1_protease_E.C.3.4.23.16



Top 10 Ranked Pockets

- 1.) 2f80_pol_polyprotein_E.C.3.4.23.16
- 2.) 4fiv_FIV_protease_E.C.3.4.23.16
- 3.) 1a30_HIV-1_protease_E.C.3.4.23.16
- 4.) 2d1o_stromelysin-1_E.C.3.4.24.17
- 5.) 1fkn_secretase_beta_E.C.3.4.23.-
- 6.) 2g94_beta-secretase_1_E.C.3.4.23.46
- 7.) 2fdp_beta-secretase_1_E.C.3.4.23.46
- 8.) 1v48_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 9.) 1ndz_adenosine_deaminase_E.C.3.5.4.4
- 10.) 2cer_beta-glucosidase_a_E.C.3.2.1.21

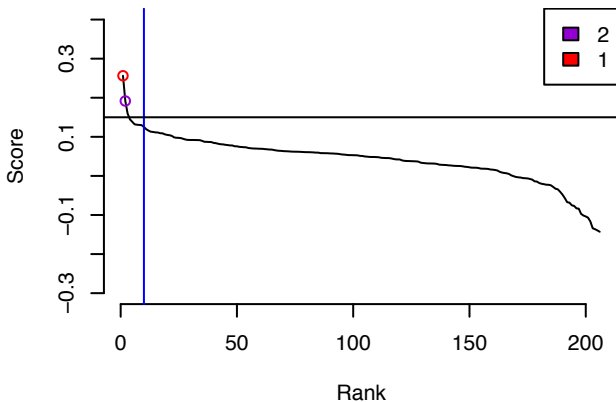
Query: 1d7j_FK506_binding_protein_E.C.5.2.1.8



Top 10 Ranked Pockets

- 1.) 1fkb_FK506_binding_protein_E.C.5.2.1.8
- 2.) 1fki_FK506_binding_protein_E.C.5.2.1.8
- 3.) 1b11_FIV_protease_E.C.3.4.23.16
- 4.) 2d3z_polyprotein_E.C.2.7.7.48
- 5.) 6fiv_FIV_protease_E.C.3.4.23.16
- 6.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 7.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 8.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 9.) 2std_scytalone_dehydratase_E.C.4.2.1.94
- 10.) 2d3u_polyprotein_E.C.2.7.7.48

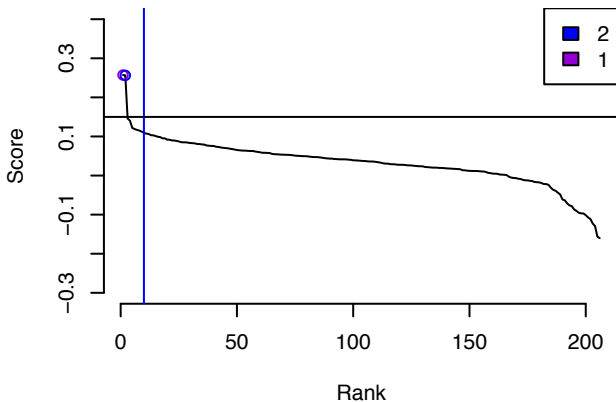
Query: 1fki_FK506_binding_protein_E.C.5.2.1.8



Top 10 Ranked Pockets

- 1.) 1fkb_FK506_binding_protein_E.C.5.2.1.8
- 2.) 1d7j_FK506_binding_protein_E.C.5.2.1.8
- 3.) 1b11_FIV_protease_E.C.3.4.23.16
- 4.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 5.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 6.) 1b8o_purine_nucleoside_phosphorylase_E.C.2.4.2.1
- 7.) 1flr_antibody_fab_E.C.-.-.-.-
- 8.) 1gni_serum_albumin_E.C.-.-.-.-
- 9.) 6fiv_FIV_protease_E.C.3.4.23.16
- 10.) 2std_scytalone_dehydratase_E.C.4.2.1.94

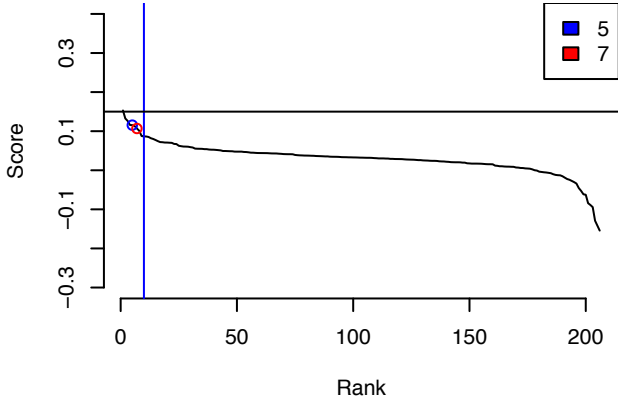
Query: 1fkb_FK506_binding_protein_E.C.5.2.1.8



Top 10 Ranked Pockets

- 1.) 1d7j_FK506_binding_protein_E.C.5.2.1.8
- 2.) 1fki_FK506_binding_protein_E.C.5.2.1.8
- 3.) 6std_scytalone_dehydratase_E.C.4.2.1.94
- 4.) 1nc1_mta/sah_nucleosidase_E.C.3.2.2.9
- 5.) 3std_scytalone_dehydratase_E.C.4.2.1.94
- 6.) 2ceq_beta-galactosidase_E.C.3.2.1.23
- 7.) 1gni_serum_albumin_E.C.-.-.-.-
- 8.) 2std_scytalone_dehydratase_E.C.4.2.1.94
- 9.) 1fcx_retinoic_acid_receptor_gamma-1_E.C.-.-.-.-
- 10.) 1y6q_mta/sah_nucleosidase_E.C.3.2.2.9

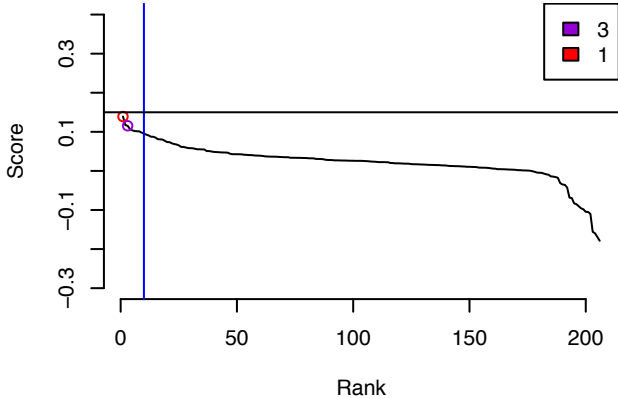
Query: 6rnt_ribonuclease_T1_E.C.3.1.27.3



Top 10 Ranked Pockets

- 1.) 1axz_lectin_E.C.-.-.-
- 2.) 1ax0_lectin_E.C.-.-.-
- 3.) 1bma_elastase_E.C.3.4.21.36
- 4.) 1ela_elastase_E.C.3.4.21.36
- 5.) 1det_ribonuclease_T1_E.C.3.1.27.3
- 6.) 1gz9_lectin_E.C.-.-.-
- 7.) 1rnt_ribonuclease_T1_E.C.3.1.27.3
- 8.) 1tyr_transthyretin_E.C.-.-.-
- 9.) 1b11_FIV_protease_E.C.3.4.23.16
- 10.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5

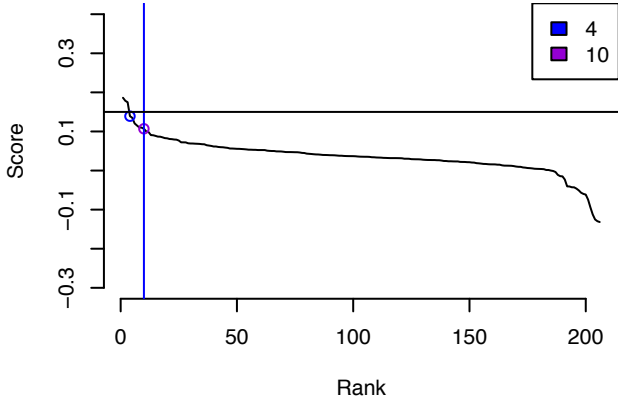
Query: 1det_ribonuclease_T1_E.C.3.1.27.3



Top 10 Ranked Pockets

- 1.) 1rnt_ribonuclease_T1_E.C.3.1.27.3
- 2.) 1ax0_lectin_E.C.-.-.-
- 3.) 6rnt_ribonuclease_T1_E.C.3.1.27.3
- 4.) 1o3f_trypsin_beta_E.C.3.4.21.4
- 5.) 1jaq_matrix_metalloproteinase-8_E.C.3.4.24.34
- 6.) 2cgr_antibody_fab_E.C.-.-.-
- 7.) 1axz_lectin_E.C.-.-.-
- 8.) 1pz5_antibody_fab_E.C.-.-.-
- 9.) 2g8r_ribonuclease_pancreatic_E.C.3.1.27.5
- 10.) 1bma_elastase_E.C.3.4.21.36

Query: 1rnt_ribonuclease_T1_E.C.3.1.27.3



Top 10 Ranked Pockets

- 1.) 1gz9_lectin_E.C.-.-.-
- 2.) 1axz_lectin_E.C.-.-.-
- 3.) 1ax0_lectin_E.C.-.-.-
- 4.) 1det_ribonuclease_T1_E.C.3.1.27.3
- 5.) 1pz5_antibody_fab_E.C.-.-.-
- 6.) 1o0h_ribonuclease_a_E.C.3.1.27.5
- 7.) 2bzz_nonsecretory_ribonuclease_E.C.3.1.27.5
- 8.) 2c02_nonsecretory_ribonuclease_E.C.3.1.27.5
- 9.) 1hi4_ribonuclease_2_E.C.3.1.27.5
- 10.) 6rnt_ribonuclease_T1_E.C.3.1.27.3

Table S2. Pocket pairs from different predefined clusters in the PDBbind core set that achieved a score > T.

Query

Most Similar Pockets

PDB-ID	Protein Name	EC-Number	PDB-ID	Protein Name	EC-Number	Score
1abf	apolipoprotein	E.C.-.-.-.-	1ftm	glutamate_receptor_2	E.C.-.-.-.-	0.17
1abf	apolipoprotein	E.C.-.-.-.-	1p1q	glutamate_receptor_2	E.C.-.-.-.-	0.16
1ai5	penicillin_amidohydrolase	E.C.3.5.1.11	2f01	streptavidin	E.C.-.-.-.-	0.16
1ajp	penicillin_amidohydrolase	E.C.3.5.1.11	1df8	streptavidin	E.C.-.-.-.-	0.16
1avn	carbonic_anhydrase_ii	E.C.4.2.1.1	1axz	lectin	E.C.-.-.-.-	0.15
1ax0	lectin	E.C.-.-.-.-	2c02	nonsecretory_ribonuclease	E.C.3.1.27.5	0.18
1ax0	lectin	E.C.-.-.-.-	1mrt	ribonuclease_T1	E.C.3.1.27.3	0.17
1ax0	lectin	E.C.-.-.-.-	1bma	elastase	E.C.3.4.21.36	0.16
1axz	lectin	E.C.-.-.-.-	1mrt	ribonuclease_T1	E.C.3.1.27.3	0.18
1axz	lectin	E.C.-.-.-.-	1bma	elastase	E.C.3.4.21.36	0.17
1axz	lectin	E.C.-.-.-.-	1ela	elastase	E.C.3.4.21.36	0.16
1axz	lectin	E.C.-.-.-.-	2c02	nonsecretory_ribonuclease	E.C.3.1.27.5	0.16
1axz	lectin	E.C.-.-.-.-	6mrt	ribonuclease_T1	E.C.3.1.27.3	0.15
1b11	FIV_protease	E.C.3.4.23.16	1fki	FK506_binding_protein	E.C.5.2.1.8	0.16
1b11	FIV_protease	E.C.3.4.23.16	1d7j	FK506_binding_protein	E.C.5.2.1.8	0.15
1b39	cyclin_dependent_kinase_2	E.C.2.7.1.37	2brn	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.15
1b39	cyclin_dependent_kinase_2	E.C.2.7.1.37	2f80	pol_polyprotein	E.C.3.4.23.16	0.15
1b80	purine_nucleoside_phosphorylase	E.C.2.4.2.1	1if7	carbonic_anhydrase_ii	E.C.4.2.1.1	0.17
1b80	purine_nucleoside_phosphorylase	E.C.2.4.2.1	1flr	antibody_fab	E.C.-.-.-.-	0.16
1bcu	thrombin_alpha	E.C.3.4.21.5	1mq6	coagulation_factor_xa	E.C.3.4.21.6	0.25
1bcu	thrombin_alpha	E.C.3.4.21.5	1nfy	coagulation_factor_xa	E.C.3.4.21.6	0.22
1bcu	thrombin_alpha	E.C.3.4.21.5	2bok	coagulation_factor_xa	E.C.3.4.21.6	0.22
1bcu	thrombin_alpha	E.C.3.4.21.5	1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	0.21
1bcu	thrombin_alpha	E.C.3.4.21.5	1bra	trypsin_beta_D189G_G226D	E.C.3.4.21.4	0.20
1bcu	thrombin_alpha	E.C.3.4.21.5	1j17	trypsin_beta	E.C.3.4.21.4	0.20
1bcu	thrombin_alpha	E.C.3.4.21.5	1utp	trypsinogen	E.C.3.4.21.4	0.19
1bcu	thrombin_alpha	E.C.3.4.21.5	2bz6	coagulation_factor_viiia	E.C.3.4.21.21	0.18
1bcu	thrombin_alpha	E.C.3.4.21.5	1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	0.18
1bcu	thrombin_alpha	E.C.3.4.21.5	1j16	trypsin_beta	E.C.3.4.21.4	0.17
1bcu	thrombin_alpha	E.C.3.4.21.5	2ffb	coagulation_factor_vii	E.C.3.4.21.21	0.17
1bcu	thrombin_alpha	E.C.3.4.21.5	1sqa	urokinase-type_plasminogen_activator	E.C.3.4.21.73	0.16
1bcu	thrombin_alpha	E.C.3.4.21.5	1o3f	trypsin_beta	E.C.3.4.21.4	0.16
1bma	elastase	E.C.3.4.21.36	1tyr	transhyretin	E.C.-.-.-.-	0.16

Query

Most Similar Pockets

PDB-ID	Protein Name	EC-Number	PDB-ID	Protein Name	EC-Number	Score
1bra	trypsin_beta_D189G_G226D	E.C.3.4.21.4	1o3f	trypsin_beta	E.C.3.4.21.4	0.24
1bra	trypsin_beta_D189G_G226D	E.C.3.4.21.4	1utp	trypsinogen	E.C.3.4.21.4	0.22
1bra	trypsin_beta_D189G_G226D	E.C.3.4.21.4	1v2o	trypsin_beta	E.C.3.4.21.4	0.21
1e1v	cyclin_dependent_kinase_2	E.C.2.7.1.37	1v48	purine_nucleoside_phosphorylase	E.C.2.4.2.1	0.15
1e1v	cyclin_dependent_kinase_2	E.C.2.7.1.37	1nvq	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.15
1ela	elastase	E.C.3.4.21.36	1tyr	transhyretin	E.C.-.-.-.-	0.15
1elb	elastase	E.C.3.4.21.36	2bzz	nonsecretory_ribonuclease	E.C.3.1.27.5	0.16
1elb	elastase	E.C.3.4.21.36	2c02	nonsecretory_rbonuclease	E.C.3.1.27.5	0.16
1elb	elastase	E.C.3.4.21.36	2gss	glutathione_s-transferase	E.C.2.5.1.18	0.16
1f4e	thymidylate_synthase	E.C.2.1.1.45	2d0k	dihydrofolate_reductase	E.C.1.5.1.3	0.18
1f4e	thymidylate_synthase	E.C.2.1.1.45	2drc	dihydrofolate_reductase	E.C.1.5.1.3	0.17
1f4e	thymidylate_synthase	E.C.2.1.1.45	1ttm	carbonic_anhydrase_ii	E.C.4.2.1.1	0.15
1f4f	thymidylate_synthase	E.C.2.1.1.45	2drc	dihydrofolate_reductase	E.C.1.5.1.3	0.15
1f4g	thymidylate_synthase	E.C.2.1.1.45	2drc	dihydrofolate_reductase	E.C.1.5.1.3	0.15
1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1v2o	trypsin_beta	E.C.3.4.21.4	0.32
1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1o3f	trypsin_beta	E.C.3.4.21.4	0.29
1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1utp	trypsinogen	E.C.3.4.21.4	0.26
1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1j17	trypsin_beta	E.C.3.4.21.4	0.25
1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1j16	trypsin_beta	E.C.3.4.21.4	0.25
1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1bra	trypsin_beta	E.C.3.4.21.4	0.24
1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1nfy	coagulation_factor_xa	E.C.3.4.21.6	0.19
1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	2bz6	coagulation_factor_via	E.C.3.4.21.21	0.19
1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1mq6	coagulation_factor_xa	E.C.3.4.21.6	0.17
1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	2b7d	coagulation_factor_vii	E.C.3.4.21.21	0.17
1f5k	urokinase-type_plasminogen_activator	E.C.3.4.21.73	2flb	coagulation_factor_vii	E.C.3.4.21.21	0.17
1fcx	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	3std	scytalone_dehydratase	E.C.4.2.1.94	0.24
1fcx	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	6std	scytalone_dehydratase	E.C.4.2.1.94	0.23
1fcx	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	2std	scytalone_dehydratase	E.C.4.2.1.94	0.22
1fcx	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	2b1v	estrogen_receptor	E.C.-.-.-.-	0.22
1fcx	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	2fai	estrogen_receptor	E.C.-.-.-.-	0.21
1fcx	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	1nc1	mta/sah_nucleosidase	E.C.3.2.2.9	0.17
1fcz	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	2fai	estrogen_receptor	E.C.-.-.-.-	0.22
1fcz	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	3std	scytalone_dehydratase	E.C.4.2.1.94	0.21

Query

Most Similar Pockets

PDB-ID	Protein Name	EC-Number	PDB-ID	Protein Name	EC-Number	Score
1fcz	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	2b1v	estrogen_receptor	E.C.-.-.-.-	0.20
1fcz	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	2std	scytalone_dehydratase	E.C.4.2.1.94	0.19
1fcz	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	6std	scytalone_dehydratase	E.C.4.2.1.94	0.18
1fd0	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	3std	scytalone_dehydratase	E.C.4.2.1.94	0.21
1fd0	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	6std	scytalone_dehydratase	E.C.4.2.1.94	0.21
1fd0	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	2std	scytalone_dehydratase	E.C.4.2.1.94	0.21
1fd0	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	2fai	estrogen_receptor	E.C.-.-.-.-	0.20
1fd0	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	2b1v	estrogen_receptor	E.C.-.-.-.-	0.19
1fkn	secretase_beta	E.C.3.4.23.-	1a30	HIV-1_protease	E.C.3.4.23.16	0.16
1fkn	secretase_beta	E.C.3.4.23.-	2i0d	HIV-1_protease	E.C.3.4.23.16	0.15
1flr	secretase_beta	E.C.-.-.-.-	2gss	glutathione_s-transferase	E.C.2.5.1.18	0.17
1flr	antibody_fab	E.C.-.-.-.-	1sv3	phospholipase_a2	E.C.3.1.1.4	0.15
1flr	antibody_fab	E.C.-.-.-.-	1fd0	retinoic_acid_receptor_gamma-1	E.C.-.-.-.-	0.16
1gni	serum_albumin	E.C.-.-.-.-	1n2v	retinoic_acid_receptor_gamma-1	E.C.2.4.2.29	0.15
1gpk	acetylcholinesterase	E.C.3.1.1.7	1n2v	retinoic_acid_receptor_gamma-1	E.C.2.4.2.29	0.15
1gz9	lectin	E.C.-.-.-.-	1rnt	queuine_tRNA-ribosyltransferase	E.C.3.1.27.3	0.19
1hk4	serum_albumin	E.C.-.-.-.-	2d0k	ribonuclease_T1	E.C.1.5.1.3	0.16
1hk4	serum_albumin	E.C.-.-.-.-	1nvq	dihydrofolate_reductase	E.C.2.7.1.37	0.16
1hk4	serum_albumin	E.C.-.-.-.-	1nvq	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.15
1hk4	serum_albumin	E.C.-.-.-.-	1e1v	cyclin_dependent_kinase_2	E.C.2.7.1.37	0.15
1j16	trypsin_beta	E.C.3.4.21.4	1v20	trypsin_beta	E.C.3.4.21.4	0.24
1j16	trypsin_beta	E.C.3.4.21.4	1o3f	trypsin_beta	E.C.3.4.21.4	0.24
1j16	trypsin_beta	E.C.3.4.21.4	1utp	trypsinogen	E.C.3.4.21.4	0.22
1j16	trypsin_beta	E.C.3.4.21.4	1utp	trypsinogen	E.C.3.4.21.4	0.25
1j17	trypsin_beta	E.C.3.4.21.4	1o3f	trypsin_beta	E.C.3.4.21.4	0.24
1j17	trypsin_beta	E.C.3.4.21.4	1v20	trypsin_beta	E.C.3.4.21.4	0.22
1j17	trypsin_beta	E.C.3.4.21.4	1bma	elastase	E.C.3.4.21.36	0.15
1k4g	tRNA-guanine_transglycosylase	E.C.2.4.2.29	1v48	purine_nucleoside_phosphorylase	E.C.2.4.2.1	0.17
1k4g	tRNA-guanine_transglycosylase	E.C.2.4.2.29	1zvx	neutrophil_collagenase	E.C.3.4.24.34	0.17
1k4g	tRNA-guanine_transglycosylase	E.C.2.4.2.29	1ttm	carbonic_anhydrase_ii	E.C.4.2.1.1	0.16
1k4g	tRNA-guanine_transglycosylase	E.C.2.4.2.29	2brm	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.15
1k4g	tRNA-guanine_transglycosylase	E.C.2.4.2.29	1sv3	phospholipase_a2	E.C.3.1.1.4	0.15
1k4g	tRNA-guanine_transglycosylase	E.C.2.4.2.29	2d10	stromelysin-1	E.C.3.4.24.17	0.15
1k4g	tRNA-guanine_transglycosylase	E.C.2.4.2.29	1nvq	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.15
1k4g	tRNA-guanine_transglycosylase	E.C.2.4.2.29	1jqd	histamine_n-methyltransferase	E.C.2.1.1.8	0.15

Query

Most Similar Pockets

PDB-ID	Protein Name	EC-Number	PDB-ID	Protein Name	EC-Number	Score
1k4g	tRNA-guanine_transglycosylase	E.C.2.4.2.29	1zso	neutrophil_collagenase	E.C.3.4.24.34	0.15
1m2q	casein_kinase_ii	E.C.2.7.1.37	2brm	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.16
1m2q	casein_kinase_ii	E.C.2.7.1.37	2brb	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.15
1mq6	coagulation_factor_xa	E.C.3.4.21.6	1j17	trypsin_beta	E.C.3.4.21.4	0.26
1mq6	coagulation_factor_xa	E.C.3.4.21.6	1j16	trypsin_beta	E.C.3.4.21.4	0.23
1mq6	coagulation_factor_xa	E.C.3.4.21.6	1bra	trypsin_beta_D189G_G226D	E.C.3.4.21.4	0.19
1mq6	coagulation_factor_xa	E.C.3.4.21.6	2bz6	coagulation_factor_viaa	E.C.3.4.21.21	0.17
1mq6	coagulation_factor_xa	E.C.3.4.21.6	1o3f	trypsin_beta	E.C.3.4.21.4	0.16
1mq6	coagulation_factor_xa	E.C.3.4.21.6	2flb	coagulation_factor_vii	E.C.3.4.21.21	0.16
1mq6	coagulation_factor_xa	E.C.3.4.21.6	1utp	trypsinogen	E.C.3.4.21.4	0.15
1n2v	queuine_tRNA-ribosyltransferase	E.C.2.4.2.29	1ttm	carbonic_anhydrase_ii	E.C.4.2.1.1	0.18
1n2v	queuine_tRNA-ribosyltransferase	E.C.2.4.2.29	1pz5	antibody_fab	E.C.-.-.-.-	0.18
1n2v	queuine_tRNA-ribosyltransferase	E.C.2.4.2.29	1zvx	neutrophil_collagenase	E.C.3.4.24.34	0.17
1n2v	queuine_tRNA-ribosyltransferase	E.C.2.4.2.29	1nvq	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.17
1n2v	queuine_tRNA-ribosyltransferase	E.C.2.4.2.29	1zso	neutrophil_collagenase	E.C.3.4.24.34	0.16
1n2v	queuine_tRNA-ribosyltransferase	E.C.2.4.2.29	1syh	glutamate_receptor_2	E.C.-.-.-.-	0.16
1n2v	queuine_tRNA-ribosyltransferase	E.C.2.4.2.29	2brm	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.15
1n2v	queuine_tRNA-ribosyltransferase	E.C.2.4.2.29	2b7d	coagulation_factor_vii	E.C.3.4.21.21	0.15
1n2v	queuine_tRNA-ribosyltransferase	E.C.2.4.2.29	2bok	coagulation_factor_xa	E.C.3.4.21.6	0.15
1ndz	adenosine_deaminase	E.C.3.5.4.4	1f4e	thymidylate_synthase	E.C.2.1.1.45	0.16
1nfy	coagulation_factor_xa	E.C.3.4.21.6	1j17	trypsin_beta	E.C.3.4.21.4	0.27
1nfy	coagulation_factor_xa	E.C.3.4.21.6	1j16	trypsin_beta	E.C.3.4.21.4	0.21
1nfy	coagulation_factor_xa	E.C.3.4.21.6	2bz6	coagulation_factor_viaa	E.C.3.4.21.21	0.19
1nfy	coagulation_factor_xa	E.C.3.4.21.6	1utp	trypsinogen	E.C.3.4.21.4	0.19
1nfy	coagulation_factor_xa	E.C.3.4.21.6	1o3f	trypsin_beta	E.C.3.4.21.4	0.17
1nfy	coagulation_factor_xa	E.C.3.4.21.6	1bra	trypsin_beta_D189G_G226D	E.C.3.4.21.4	0.16
1nfy	coagulation_factor_xa	E.C.3.4.21.6	2b7d	coagulation_factor_vii	E.C.3.4.21.21	0.16
1nfy	coagulation_factor_xa	E.C.3.4.21.6	2flb	coagulation_factor_vii	E.C.3.4.21.21	0.15
1nvq	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	1jq9	phospholipase_a2	E.C.3.1.1.4	0.17
1o0h	ribonuclease_a	E.C.3.1.27.5	2c02	nonsecretory_ribonuclease	E.C.3.1.27.5	0.17
1o0h	ribonuclease_a	E.C.3.1.27.5	1h14	ribonuclease_2	E.C.3.1.27.5	0.16
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1o3f	trypsin_beta	E.C.3.4.21.4	0.28
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1utp	trypsinogen	E.C.3.4.21.4	0.27

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PDB-ID	Protein Name	EC-Number	PDB-ID	Protein Name	EC-Number	Score
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1mq6	coagulation_factor_xa	E.C.3.4.21.6	0.24
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1j17	trypsin_beta	E.C.3.4.21.4	0.23
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	2bz6	coagulation_factor_viiia	E.C.3.4.21.21	0.23
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1j16	trypsin_beta	E.C.3.4.21.4	0.22
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1nfy	coagulation_factor_xa	E.C.3.4.21.6	0.22
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1v2o	trypsin_beta	E.C.3.4.21.4	0.22
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	2flb	coagulation_factor_vii	E.C.3.4.21.21	0.21
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1bra	trypsin_beta_D189G_G226D	E.C.3.4.21.4	0.18
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	2bok	coagulation_factor_xa	E.C.3.4.21.6	0.16
1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	2b7d	coagulation_factor_vii	E.C.3.4.21.21	0.16
1om1	casein_kinase_ii	E.C.2.7.1.37	1b39	cyclin_dependent_kinase_2	E.C.2.7.1.37	0.19
1om1	casein_kinase_ii	E.C.2.7.1.37	1pxo	cyclin_dependent_kinase_2	E.C.2.7.1.37	0.19
1pbq	glutamate_[nmda]_receptor	E.C.2.7.1.37	2drc	dihydrofolate_reductase	E.C.1.5.1.3	0.16
1pxo	cyclin_dependent_kinase_2	E.C.2.7.1.37	2brm	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.15
1pz5	antibody_fab	E.C.-.-.-.-	1zso	neutrophil_collagenase	E.C.3.4.24.34	0.16
1pz5	antibody_fab	E.C.-.-.-.-	1zvx	neutrophil_collagenase	E.C.3.4.24.34	0.16
1pz5	antibody_fab	E.C.-.-.-.-	2c02	nonsecretory_ribonuclease	E.C.3.1.27.5	0.15
1s39	tRNA-guanine_transglycosylase	E.C.2.4.2.29	1ttm	carbonic_anhydrase_ii	E.C.4.2.1.1	0.17
1s39	tRNA-guanine_transglycosylase	E.C.2.4.2.29	1syh	glutamate_receptor_2	E.C.-.-.-.-	0.17
1s39	tRNA-guanine_transglycosylase	E.C.2.4.2.29	1jaq	matrix_metalloproteinase-8	E.C.3.4.24.34	0.15
1s13	thrombin_alpha	E.C.3.4.21.5	2bok	coagulation_factor_xa	E.C.3.4.21.6	0.23
1s13	thrombin_alpha	E.C.3.4.21.5	1nfy	coagulation_factor_xa	E.C.3.4.21.6	0.22
1s13	thrombin_alpha	E.C.3.4.21.5	1mq6	coagulation_factor_xa	E.C.3.4.21.6	0.22
1s13	thrombin_alpha	E.C.3.4.21.5	2b7d	coagulation_factor_vii	E.C.3.4.21.21	0.18
1s13	thrombin_alpha	E.C.3.4.21.5	2flb	coagulation_factor_vii	E.C.3.4.21.21	0.17
1s13	thrombin_alpha	E.C.3.4.21.5	1j17	trypsin_beta	E.C.3.4.21.4	0.17
1s13	thrombin_alpha	E.C.3.4.21.5	2bz6	coagulation_factor_viiia	E.C.3.4.21.21	0.17
1s13	thrombin_alpha	E.C.3.4.21.5	1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	0.17
1s13	thrombin_alpha	E.C.3.4.21.5	1sqa	urokinase-type_plasminogen_activator	E.C.3.4.21.73	0.17
1s13	thrombin_alpha	E.C.3.4.21.5	1bra	trypsin_beta_D189G_G226D	E.C.3.4.21.4	0.16
1s13	thrombin_alpha	E.C.3.4.21.5	1j16	trypsin_beta	E.C.3.4.21.4	0.15
1sqa	urokinase-type_plasminogen_activator	E.C.3.4.21.73	2b7d	coagulation_factor_vii	E.C.3.4.21.21	0.23
1sqa	urokinase-type_plasminogen_activator	E.C.3.4.21.73	2flb	coagulation_factor_vii	E.C.3.4.21.21	0.21

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PDB-ID	Protein Name	EC-Number	PDB-ID	Protein Name	EC-Number	Score
1sqg	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1v2o	trypsin_beta	E.C.3.4.21.4	0.19
1sqg	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1o3f	trypsin_beta	E.C.3.4.21.4	0.19
1sqg	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1j17	trypsin_beta	E.C.3.4.21.4	0.19
1sqg	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1nfy	coagulation_factor_xa	E.C.3.4.21.6	0.19
1sqg	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1utp	trypsinogen	E.C.3.4.21.4	0.18
1sqg	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1p25	antibody_fab	E.C.-.-.-.-	0.17
1sqg	urokinase-type_plasminogen_activator	E.C.3.4.21.73	2bz6	coagulation_factor_viiia	E.C.3.4.21.21	0.17
1sqg	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1mq6	coagulation_factor_xa	E.C.3.4.21.6	0.17
1sqg	urokinase-type_plasminogen_activator	E.C.3.4.21.73	2bok	coagulation_factor_xa	E.C.3.4.21.6	0.17
1sqg	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1bra	trypsin_beta_D189G_G226D	E.C.3.4.21.4	0.17
1sqg	urokinase-type_plasminogen_activator	E.C.3.4.21.73	1j16	trypsin_beta	E.C.3.4.21.4	0.16
1ttm	carbonic_anhydrase_ii	E.C.4.2.1.1	2d0k	dlhydrofolate_reductase	E.C.1.5.1.3	0.17
1ttm	carbonic_anhydrase_ii	E.C.4.2.1.1	1dhi	dlhydrofolate_reductase	E.C.1.5.1.3	0.17
1ttm	carbonic_anhydrase_ii	E.C.4.2.1.1	1flr	antibody_fab	E.C.-.-.-.-	0.15
1u2y	alpha-amylase	E.C.3.2.1.1	2j78	beta-glucosidase_a	E.C.3.2.1.21	0.15
1u33	alpha-amylase	E.C.3.2.1.1	1ndz	adenosine_deaminase	E.C.3.5.4.4	0.15
1uwt	beta-galactosidase	E.C.3.2.1.23	2cet	beta-glucosidase_a	E.C.3.2.1.21	0.25
1uwt	beta-galactosidase	E.C.3.2.1.23	2j78	beta-glucosidase_a	E.C.3.2.1.21	0.25
1uwt	beta-galactosidase	E.C.3.2.1.23	2j77	beta-glucosidase_a	E.C.3.2.1.21	0.23
1uwt	beta-galactosidase	E.C.3.2.1.23	2d0k	dlhydrofolate_reductase	E.C.1.5.1.3	0.16
1v48	purine_nucleoside_phosphorylase	E.C.2.4.2.1	2d0k	dlhydrofolate_reductase	E.C.1.5.1.3	0.16
1v48	purine_nucleoside_phosphorylase	E.C.2.4.2.1	2d1o	stromelysin-1	E.C.3.4.24.17	0.16
1v48	purine_nucleoside_phosphorylase	E.C.2.4.2.1	1slg	streptavidin	E.C.-.-.-.-	0.16
1v48	purine_nucleoside_phosphorylase	E.C.2.4.2.1	1f4e	thymidylate_synthase	E.C.2.1.1.45	0.16
1v48	purine_nucleoside_phosphorylase	E.C.2.4.2.1	2bok	coagulation_factor_xa	E.C.3.4.21.6	0.23
1vzq	thrombin_alpha	E.C.3.4.21.5	1mq6	coagulation_factor_xa	E.C.3.4.21.6	0.18
1vzq	thrombin_alpha	E.C.3.4.21.5	1o3p	urokinase-type_plasminogen_activator	E.C.3.4.21.73	0.16
1vzq	thrombin_alpha	E.C.3.4.21.5	1nfy	coagulation_factor_xa	E.C.3.4.21.6	0.16
1vzq	thrombin_alpha	E.C.3.4.21.5	2bz6	coagulation_factor_viiia	E.C.3.4.21.21	0.15
1vzm	glutamate_[nmda]_receptor	E.C.-.-.-.-	3pce	protocatechuate_3,4-dioxygenase	E.C.1.13.11.3	0.17
1ylm	glutamate_[nmda]_receptor	E.C.-.-.-.-	1flr	antibody_fab	E.C.-.-.-.-	0.16
1zoe	protein_kinase_ck2_alpha_subunit	E.C.2.7.1.37	2brm	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.17
1zoe	protein_kinase_ck2_alpha_subunit	E.C.2.7.1.37	1nvq	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	0.16

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PDB-ID	Protein Name	EC-Number	PDB-ID	Protein Name	EC-Number	Score
1zoe	protein_kinase_ck2_alpha_subunit	E.C.2.7.1.37	1pxo	cyclin_dependent_kinase_2	E.C.2.7.1.37	0.15
2b1v	estrogen_receptor	E.C.-.-.-.-	3std	scytalone_dehydratase	E.C.4.2.1.94	0.17
2b1v	estrogen_receptor	E.C.-.-.-.-	6std	scytalone_dehydratase	E.C.4.2.1.94	0.17
2b1v	estrogen_receptor	E.C.-.-.-.-	2std	scytalone_dehydratase	E.C.4.2.1.94	0.16
2b7d	coagulation_factor_vii	E.C.3.4.21.21	1utp	trypsinogen	E.C.3.4.21.4	0.18
2bok	coagulation_factor_xa	E.C.3.4.21.6	2bz6	coagulation_factor_via	E.C.3.4.21.21	0.20
2bok	coagulation_factor_xa	E.C.3.4.21.6	1bra	trypsin_beta_D189G_G226D	E.C.3.4.21.4	0.18
2bok	coagulation_factor_xa	E.C.3.4.21.6	1j17	trypsin_beta	E.C.3.4.21.4	0.17
2bok	coagulation_factor_xa	E.C.3.4.21.6	2flb	coagulation_factor_vii	E.C.3.4.21.21	0.17
2bok	coagulation_factor_xa	E.C.3.4.21.6	1elb	elastase	E.C.3.4.21.36	0.17
2brb	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	1jq9	phospholipase_a2	E.C.3.1.1.4	0.20
2brb	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	1sv3	phospholipase_a2	E.C.3.1.1.4	0.18
2brb	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	1flr	antibody_fab	E.C.-.-.-.-	0.17
2brb	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	1q7a	phospholipase_a2	E.C.3.1.1.4	0.17
2brb	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	1ttm	carbonic_anhydrase_ii	E.C.4.2.1.1	0.16
2brm	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	1q7a	phospholipase_a2	E.C.3.1.1.4	0.20
2brm	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	1sv3	phospholipase_a2	E.C.3.1.1.4	0.17
2brm	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	1jq9	phospholipase_a2	E.C.3.1.1.4	0.16
2brm	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	2d0k	dihydrofolate_reductase	E.C.1.5.1.3	0.15
2brm	serine/threonine-protein_kinase_chk1	E.C.2.7.1.37	1flr	antibody_fab	E.C.-.-.-.-	0.15
2bz6	coagulation_factor_via	E.C.3.4.21.21	1bra	trypsin_beta_D189G_G226D	E.C.3.4.21.4	0.23
2bz6	coagulation_factor_via	E.C.3.4.21.21	1utp	trypsinogen	E.C.3.4.21.4	0.22
2bz6	coagulation_factor_via	E.C.3.4.21.21	1v2o	trypsin_beta	E.C.3.4.21.4	0.20
2bz6	coagulation_factor_via	E.C.3.4.21.21	1o3f	trypsin_beta	E.C.3.4.21.4	0.19
2bz6	coagulation_factor_via	E.C.3.4.21.21	1j17	trypsin_beta	E.C.3.4.21.4	0.18
2bz6	coagulation_factor_via	E.C.3.4.21.21	1j16	trypsin_beta	E.C.3.4.21.4	0.16
2ceq	beta-galactosidase	E.C.3.2.1.23	2j78	beta-galactosidase_a	E.C.3.2.1.21	0.24
2ceq	beta-galactosidase	E.C.3.2.1.23	2cet	beta-galactosidase_a	E.C.3.2.1.21	0.22
2ceq	beta-galactosidase	E.C.3.2.1.23	2j77	beta-galactosidase_a	E.C.3.2.1.21	0.22
2cer	beta-glucosidase_a	E.C.3.2.1.21	2cet	beta-glucosidase_a	E.C.3.2.1.21	0.21
2cer	beta-glucosidase_a	E.C.3.2.1.21	2j78	beta-glucosidase_a	E.C.3.2.1.21	0.19
2cer	beta-glucosidase_a	E.C.3.2.1.21	1f4e	thymidylate_synthase	E.C.2.1.1.45	0.17
2cer	beta-glucosidase_a	E.C.3.2.1.21	1v48	purine_nucleoside_phosphorylase	E.C.2.4.2.1	0.15

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PDB-ID	Protein Name	EC-Number	PDB-ID	Protein Name	EC-Number	Score
2cet	beta-glucosidase_a	E.C.3.2.1.21	2d0k	dlhydrofolate_reductase	E.C.1.5.1.3	0.17
2cet	beta-glucosidase_a	E.C.3.2.1.21	1k4g	tRNA-guanine_transglycosylase	E.C.2.4.2.29	0.16
2cgr	antibody_fab	E.C.-.-.-.-	1jaq	matrix_metalloproteinase-8	E.C.3.4.24.34	0.16
2cgr	antibody_fab	E.C.-.-.-.-	1zs0	neutrophil_collagenase	E.C.3.4.24.34	0.16
2d1o	stromelysin-1	E.C.3.4.24.17	1zvx	neutrophil_collagenase	E.C.3.4.24.34	0.17
2d1o	stromelysin-1	E.C.3.4.24.17	2i0d	HIV-1_protease	E.C.3.4.23.16	0.16
2d1o	stromelysin-1	E.C.3.4.24.17	4fiv	FIV_protease	E.C.3.4.23.16	0.16
2d1o	stromelysin-1	E.C.3.4.24.17	1a30	HIV-1_protease	E.C.3.4.23.16	0.15
2d3u	polyprotein	E.C.2.7.7.48	1sv3	phospholipase_a2	E.C.3.1.1.4	0.17
2d3u	polyprotein	E.C.2.7.7.48	1ttm	carbonic_anhydrase_ii	E.C.4.2.1.1	0.15
2d3z	polyprotein	E.C.2.7.7.48	2gss	glutathione_s-transferase	E.C.2.5.1.18	0.17
2er9	endothiapsin	E.C.3.4.23.22	1ppm	penicillopepsin	E.C.3.4.23.20	0.23
2er9	endothiapsin	E.C.3.4.23.22	1bxo	penicillopepsin	E.C.3.4.23.20	0.22
2er9	endothiapsin	E.C.3.4.23.22	1apw	penicillopepsin	E.C.3.4.23.20	0.22
2fai	estrogen_receptor	E.C.-.-.-.-	6std	scytalone_dehydratase	E.C.4.2.1.94	0.18
2fai	estrogen_receptor	E.C.-.-.-.-	3std	scytalone_dehydratase	E.C.4.2.1.94	0.18
2fai	estrogen_receptor	E.C.-.-.-.-	2std	HIV-1_protease	E.C.4.2.1.94	0.17
2fdp	beta-secretase_1	E.C.3.4.23.46	1a30	trypsin_beta_D189G_G226D	E.C.3.4.23.16	0.15
2flb	coagulation_factor_vii	E.C.3.4.21.21	1bra	trypsinogen	E.C.3.4.21.4	0.19
2flb	coagulation_factor_vii	E.C.3.4.21.21	1utp	trypsin_beta	E.C.3.4.21.4	0.15
2flb	coagulation_factor_vii	E.C.3.4.21.21	1o3f	pol_polyprotein	E.C.3.4.23.16	0.15
2g94	beta-secretase_1	E.C.3.4.23.46	2f80	HIV-1_protease	E.C.3.4.23.16	0.15
2g94	beta-secretase_1	E.C.3.4.23.46	1a30	pol_polyprotein	E.C.3.4.23.16	0.15
2gss	glutathione_s-transferase	E.C.2.5.1.18	6fiv	FIV_protease	E.C.3.4.23.16	0.16
2j77	beta-glucosidase_a	E.C.3.2.1.21	1fh9	xylianase_beta-1,4	E.C.3.2.1.91	0.15
2j77	beta-glucosidase_a	E.C.3.2.1.21	1fh7	xylianase_beta-1,4	E.C.3.2.1.91	0.15
2j77	beta-glucosidase_a	E.C.3.2.1.21	1fh8	xylianase_beta-1,4	E.C.3.2.1.91	0.15
2j78	beta-glucosidase_a	E.C.3.2.1.21	1fh9	xylianase_beta-1,4	E.C.3.2.1.91	0.17
2j78	beta-glucosidase_a	E.C.3.2.1.21	2d0k	dlhydrofolate_reductase	E.C.1.5.1.3	0.17
2usn	stromelysin-1	E.C.3.4.24.17	2usn	stromelysin-1	E.C.3.4.24.17	0.17
2usn	stromelysin-1	E.C.3.4.24.17	1p25	antibody_fab	E.C.-.-.-.-	0.22
3pce	protocatechuate_3,4-dioxygenase	E.C.1.13.11.3	2cgr	antibody_fab	E.C.-.-.-.-	0.16
3pce	protocatechuate_3,4-dioxygenase	E.C.1.13.11.3	2gss	glutathione_s-transferase	E.C.2.5.1.18	0.16

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PDB-ID	Protein Name	EC-Number	PDB-ID	Protein Name	EC-Number	Score
4er2	endothiapsin	E.C.3.4.23.22	1apw	penicillopepsin	E.C.3.4.23.20	0.27
4er2	endothiapsin	E.C.3.4.23.22	1bxo	penicillopepsin	E.C.3.4.23.20	0.22
4er2	endothiapsin	E.C.3.4.23.22	1ppm	penicillopepsin	E.C.3.4.23.20	0.21
4fiv	FIV_protease	E.C.3.4.23.16	2f80	pol_polyprotein	E.C.3.4.23.16	0.26
4fiv	FIV_protease	E.C.3.4.23.16	1a30	HIV-1_protease	E.C.3.4.23.16	0.24
4fiv	FIV_protease	E.C.3.4.23.16	2i0d	HIV-1_protease	E.C.3.4.23.16	0.22
5er1	endothiapsin_bw624	E.C.3.4.23.22	1apw	penicillopepsin	E.C.3.4.23.20	0.22
5er1	endothiapsin_bw624	E.C.3.4.23.22	1ppm	penicillopepsin	E.C.3.4.23.20	0.20
5er1	endothiapsin_bw624	E.C.3.4.23.22	1bxo	penicillopepsin	E.C.3.4.23.20	0.20

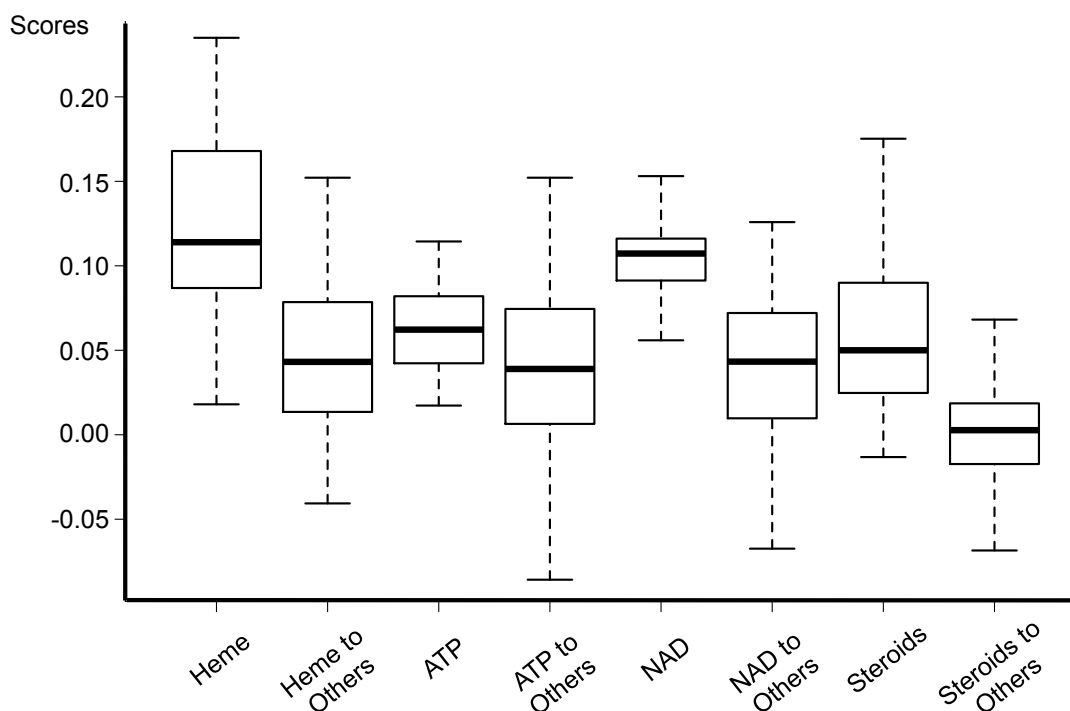


Figure S4. Score distributions from the pairwise comparisons in the benchmark example as proposed by Das et al. 2007. “Heme”, “ATP”, “NAD”, and “Steroids” depict score distributions within the respective binding site classes. “Heme to Others”, “ATP to Others”, “NAD to Others”, and “Steroids to Others” show inter class matching score distributions between pockets of e.g. Heme containing binding sites to pockets binding to the other 3 structure classes.