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| --- | --- | --- | --- | --- | --- | --- | --- |
| **Protein (species)** | **PDB** | **Restrained functional**  **site** | **Δ (kcal/mol)** | **Allosteric Site** | **Δ(kcal/mol)** | **Proximity (%)** | **AUC** |
| Acetyltransferase Pat (Mycobacterium tuberculosis) | 4avb | 1 x ACO | -4.92 | 1 x CMP | 3.74 | 0 | 0.67 |
| Amino-acid  acetyltransferase (Neisseria  gonorrhoeae) | 3d2p | 6 x COA | -1.14 | 6 x ARG | 1.21 | 0 | 0.41 |
| Anaerobic ribonucleoside-  triphosphate reductase (Enterobacteria phage T4) | 1h78 | 2 x DCF | -1.81 | 2 x DCP | 1.31 | 0 | 0.76 |
| Androgen receptor  (Homo sapiens) | 2pio | 1 x DHT | -4.61 | 1 x YLO | 0.74 | 0 | 0.70 |
| Androgen receptor  (Mus musculus) | 2qpy | 1 x DHT | -4.42 | 1 x 4HY | 2.0 | 0 | 0.71 |
| Antithrombin III  (Homo sapiens) | 1t1f | 1 x RCL | -4.62 | 1 x NTP | 0.96 | 0 | 0.72 |
| ATP phosphoribosyltransfe rase (Mycobacteriu  m tuberculosis) | 1nh8 | 2 x AMP | -1.59 | 2 x HIS | 0.97 | 0 | 0.69 |
| cAMP receptor protein (Mycobacterium tuberculosis) | 3d0s | 2 x DNA | -1.8 | 2 x CMP | 1.11 | 0 | 0.56 |
| Chorismate mutase (Saccharomyces  cerevisiae) | 3csm | 2 x TSA | -1.81 | 2 x TRP | 0.16 | 0.83 | 0.16 |
| Farnesyl pyrophosphate synthase (Homo sapiens) | 2qis | 2 x RIS | -1.38 | 4 x 3N1 | 0.44 | 0.63 | 0.47 |
| Fatty acid metabolism regulator protein (Escherichia coli) | 1hw1 | 2 x DNA | -5.44 | 2 x COA | 2.39 | 0 | 0.72 |
| Fructose-1,6- bisphosphatase 1 (Escherichia coli) | 2q8m | 4 x FBP | -0.77 | 4 x AMP  4 x BG6 | 1.67  -1.62 | 0  10 | 0.79  0 |
| Fructose-1,6- bisphosphatase 1 (Sus scrofa) | 1fbp | 4 x FBP | -1.01 | 4 x AMP  4 x PFE | 1.36  1.45 | 0  1.86 | 0.63  0.63 |
| Glucose-1-phosphate thymidylyltransferase 1 (Escherichia coli) | 1mc3 | 4 x TTP | 0.19 | 4 x TMP | 1.26 | 1.69 | 0.63 |
| Glutamate dehydrogenase 1,  mitochondrial (Bos taurus) | 1nr7 | 6 x GLU | -1.15 | 6 x GWD | -1.25 | 0 | 0.59 |
| Glycogen phosphorylase, liver  form (Homo sapiens) | 2ati | 2 x GLC | -0.66 | 2 x AVE  1 x CP4 | 0.45  0.5 | 0  0 | 0.79  0.89 |
| Glycogen phosphorylase, muscle form (Homo sapiens) | 1z8d | 2 x GLC | -0.5 | 2 x AMP | 0.4 | 0 | 0.69 |
| Glycogen phosphorylase, muscle form (Oryctolagus  cuniculus) | 2skc | 2 x GLC | -0.65 | 2 x FRY  2 x QUE | 0.67  0.02 | 0  0 | 0.88  0.24 |
| HTH-type transcriptional repressor PurR (Escherichia coli) | 1qp0 | 2 x DNA | -7.37 | 2 x HPA | 4.04 | 0 | 0.69 |
| Isocitrate dehydrogenase [NADP], mitochondrial (Homo sapiens) | 4ja8 | 2 x NDP | -1.6 | 1 x 1K9 | 0.95 | 0.32 | 0.5 |
| Isocitrate dehydrogenase kinase/phosphatase (Escherichia coli) | 3eps | 1 x ATP | -3.58 | 1 x AMP | 0.67 | 0.28 | 0.51 |
| L-lactate dehydrogenase (Geobacillus stearothermophilus) | 1ldn | 4 x NAD | -1.85 | 2 x FBP | 2.89 | 0.41 | 0.79 |
| L-lactate dehydrogenase 2 (Bifidobacterium longum subsp. Longum) | 1lld | 4 x NAD | -2.78 | 2 x FBP | 3.26 | 0.52 | 0.78 |
| Lactose operon repressor (Eschericia coli) | 1efa | 2 x DNA | -5.97 | 2 x NPF | 3.16 | 0 | 0.64 |
| Leukotriene A-4 hydrolase (Homo sapiens) | 5fwq | 1 x BES | -2.47 | 1 x 692 | 2.08 | 0 | 0.87 |
| Lysine-sensitive  aspartokinase 3 (Escherichia coli) | 2j0w | 2 x ADP | -0.56 | 2 x LYS | 0.74 | 0 | 0.53 |
| Mitogen-activated protein kinase 14 (Homo sapiens) | 1wfc | 1 x L9G | -3.48 | 1 x 0O8 | 1.88 | 0 | 0.8 |
| Mitogen-activated  protein kinase 8 (Homo sapiens) | 1ukh | 1 x 537 | -2.92 | 1 x 46A | 0.82 | 0 | 0.36 |
| Multifunctional 2- oxoglutarate  metabolism enzyme (Mycobacterium  smegmatis) | 2y0p | 2 x TD7 | -2.85 | 2 x ACO | 0.62 | 0 | 0.61 |
| Myosin-2 heavy chain (Dictyostelium  discoideum) | 1yv3 | 1 x ADP | -2.94 | 1 x PBQ | 0.58 | 0 | 0.58 |
| NAD(P)-dependent glyceraldehyde-3- phosphate  dehydrogenase (Thermoproteus  tenax) | 1uxu | 4 x NAP | -1.93 | 4 x AMP | 3.52 | 0 | 0.84 |
| Ornithine decarboxylase (Trypanosoma brucei gambiense) | 1njj | 2 x ORX | -2.87 | 2 x GET | 1.23 | 0.77 | 0.8 |
| Parathion hydrolase (Brevundimonas diminuta) | 1qw7 | 4 x CO | -1.42 | 2 x EBP | 0.22 | 0 | 0.33 |
| Plasminogen activator inhibitor 1 (Homo sapiens) | 1oc0 | 1 x Bchain | -2.19 | 1 x 96P | 1.09 | 0 | 0.47 |
| Pyruvate dehydrogenase kinase  isozyme 2 (Homo sapiens) | 2bu2 | 2 x ATP | -3.3 | 2 x TF2  2 x TF3  2 x TF4 | 2.67  0.85  1.14 | 0  0.94  0 | 0.85  0.22  0.34 |
| Pyruvate kinase PKLR (Homo sapiens) | 2vgb | 4 x PGA | -0.13 | 4 x FBP | 1.05 | 0 | 0.75 |
| Pyruvate kinase PKM (Homo sapiens) | 3gqy | 6 x TLA | -0.22 | 4 x FBP  2 x NZT  4 x SER | 1.25  1.8  1.22 | 0  0  1.58 | 0.59  0.83  0.58 |
| Ribonucleoside- diphosphate reductase 1 subunit alpha (Escherichia coli) | 4r1r | 1 x GDP | -4.39 | 1 x ATP  1 x TTP | 2.12  1.28 | 0  0 | 0.79  0.69 |
| Tyrosine-protein kinase ABL1 (Homo sapiens) | 3pyy | 1 x STI | -4.13 | 1 x 3YY | 2.93 | 0 | 0.58 |
| Tyrosine-protein  kinase ABL1 (Mus musculus) | 3k5v | 1 x STI | -4.56 | 1 x STJ | 2.38 | 0 | 0.54 |
| Uridylate kinase (Helicobacter pylori) | 4a7x | 1 x UDP | -4.24 | 2 x GTP | 0.05 | 1.82 | 0.54 |