Alpha amylase

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **P/L** | **Estimated Free Energy of Binding (kcal/mol)** | **Ki (mikromolar)** | **Final Intermolecular Energy (kcal/mol)** | **vdW + Hbond + desolv Energy (kcal/mol)** | **Electrostatic Energy (kcal/mol)** | **Final Total Internal Energy (kcal/mol)** | **Torsional Free Energy (kcal/mol)** | **Unbound System's Energy [=(2)] (kcal/mol)** |
| **Anestezin** | -4.06 | 1.05 mM | -5.26 | -5.12 | -0.14 | -0.24 | 1.19 | -0.24 |
| **Cynaroside** | -6.85 | 9.57 | -10.13 | -9.81 | -0.32 | -4.49 | 3.28 | -4.49 |
| **Dihidroquercetin** | -6.06 | 36.37 | -7.85 | -7.14 | -0.7 | -2.15 | 1.79 | -2.15 |
| **Ecdysteron** | -6.72 | 11.96 | -10 | -9.69 | -0.31 | -1.77 | 3.28 | -1.77 |
| **Firul acid** | -4.64 | 395.3 | -6.13 | -5.5 | -0.63 | -0.97 | 1.49 | -0.97 |
| **Galic acid** | -6.88 | 9.04 | -10.76 | -9.9 | -0.86 | -3.4 | 3.88 | -3.4 |
| **Lutiolin** | -6.87 | 9.28 | -8.36 | -8.07 | -0.28 | -1.51 | 1.49 | -1.51 |
| **Plantaginin** | -11.12 | 7.06 nM | -14.4 | -14.4 | 0 | -5.4 | 3.28 | -5.4 |
| **Quercetin** | -6 | 39.72 | -7.79 | -7.43 | -0.36 | -2.59 | 1.79 | -2.59 |
| **Rosavin** | -5.1 | 183.78 | -8.97 | -8.43 | -0.54 | -5.83 | 3.88 | -5.83 |
| **Rutin** | -5.98 | 41.33 | -10.75 | -10.3 | -0.45 | -6.57 | 4.77 | -6.57 |
| **Salidrodside** | -5.24 | 143.07 | -8.23 | -7.61 | -0.62 | -2.47 | 2.98 | -2.47 |
| **Turkesterone** | -6.82 | 10.03 | -10.4 | -10.1 | -0.3 | -2.3 | 3.58 | -2.3 |

Beta glucosidase

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **P/L** | **Estimated Free Energy of Binding (kcal/mol)** | **Ki (mikromolar)** | **Final Intermolecular Energy (kcal/mol)** | **vdW + Hbond + desolv Energy (kcal/mol)** | **Electrostatic Energy (kcal/mol)** | **Final Total Internal Energy (kcal/mol)** | **Torsional Free Energy (kcal/mol)** | **Unbound System's Energy [=(2)] (kcal/mol)** |
| **Anestezin** | -4.25 | 766.34 | -5.44 | -5.42 | -0.02 | -0.19 | 1.19 | -0.19 |
| **Cynaroside** | -5.72 | 64.07 | -9 | -8.98 | -0.02 | -4.68 | 3.28 | -4.68 |
| **Dihidroquercetin** | -6.22 | 27.72 | -8.01 | -7.65 | -0.36 | -2.35 | 1.79 | -2.35 |
| **Ecdysteron** | -8.24 | 908.29 | -11.52 | -11.57 | 0.05 | -2.17 | 3.28 | -2.17 |
| **Firul acid** | -4.65 | 389.71 | -6.14 | -6.03 | -0.11 | 0.97 | 1.49 | -0.97 |
| **Galic acid** | -6.72 | 11.8 | -10.6 | -10.51 | -0.09 | -4.64 | 3.88 | -4.64 |
| **Lutiolin** | -6.76 | 11.01 | -8.26 | -7.88 | -0.37 | -2.01 | 1.49 | -2.01 |
| **Plantaginin** | -11.99 | 1.64 nM | -15.27 | -15.27 | 0 | -4.48 | 3.28 | -4.48 |
| **Quercetin** | -5.95 | 43.82 | -7.74 | -7.45 | -0.28 | -2.59 | 1.79 | -2.59 |
| **Rosavin** | -6.12 | 32.39 | -10 | -9.95 | -0.05 | -5.4 | 3.88 | -5.4 |
| **Rutin** | -7.45 | 3.47 | -12.22 | -12.08 | -0.14 | -7.18 | 4.77 | -7.18 |
| **Salidrodside** | -5.12 | 177.5 | -8.1 | -7.95 | -0.15 | -2.35 | 2.98 | -2.35 |
| **Turkesterone** | -7.16 | 5.63 | -10.74 | -10.71 | -0.03 | -3.03 | 3.58 | -3.03 |

Kreatine kinase

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **P/L** | **Estimated Free Energy of Binding (kcal/mol)** | **Ki (mikromolar)** | **Final Intermolecular Energy (kcal/mol)** | **vdW + Hbond + desolv Energy (kcal/mol)** | **Electrostatic Energy (kcal/mol)** | **Final Total Internal Energy (kcal/mol)** | **Torsional Free Energy (kcal/mol)** | **Unbound System's Energy [=(2)] (kcal/mol)** |
| **Anestezin** | -3.39 | 3.27 | -4.58 | -4.42 | -0.16 | -0.21 | 1.19 | -0.21 |
| **Cynaroside** | -4.3 | 707.07 | -7.58 | -7.01 | -0.57 | -3.76 | 3.28 | -3.76 |
| **Dihidroquercetin** | -5.23 | 146.49 | -7.02 | -6.44 | -0.58 | -2.35 | 1.79 | -2.35 |
| **Ecdysteron** | -4.79 | 309.19 | -8.07 | -7.69 | -0.38 | -3.24 | 3.28 | -3.24 |
| **Firul acid** | -4.3 | 706.77 | -5.79 | -5.03 | -0.76 | -0.97 | 1.49 | -0.97 |
| **Galic acid** | -5.85 | 51.77 | -9.72 | -8.97 | -0.76 | -3.86 | 3.88 | -3.86 |
| **Lutiolin** | -4.9 | 256.67 | -6.39 | -5.89 | -0.5 | -2 | 1.49 | -2 |
| **Plantaginin** | -8.53 | 558.94 | -11.81 | -11.81 | 0 | -4.15 | 3.28 | -4.15 |
| **Quercetin** | -5.42 | 106.81 | -7.21 | -6.96 | -0.25 | -2.44 | 1.79 | -2.44 |
| **Rosavin** | -4.42 | 572.29 | -8.3 | -8 | -0.3 | -5.43 | 3.88 | -5.43 |
| **Rutin** | -4.57 | 448.81 | -9.34 | -8.65 | -0.69 | -8.05 | 4.77 | -8.05 |
| **Salidrodside** | -4.94 | 240.36 | -7.92 | -7.45 | -0.47 | -2.18 | 2.98 | -2.18 |
| **Turkesterone** | -4.82 | 294.82 | -8.4 | -7.84 | -0.56 | -1.19 | 3.58 | -1.19 |

Cav1.1 PDB-ID: 6JPA

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Estimated Free Energy of Binding (kcal/mol)** | **Estimated Inhibition Constant, Ki (mikromolar)** | **Final Intermolecular Energy (kcal/mol)** | **vdW + Hbond + desolv Energy (kcal/mol)** | **Electrostatic Energy (kcal/mol)** | **Final Total Internal Energy (kcal/mol)** | **Torsional Free Energy (kcal/mol)** | **Unbound System's Energy [=(2)] (kcal/mol)** |
| **Anestezin** | -4.18 | 868.15 | -5.37 | -5.2 | -0.17 | -0.19 | 1.19 | -0.19 |
| Cynaroside | -6.54 | 16.13 | -9.82 | -9.66 | -0.16 | -4.57 | 3.28 | -4.57 |
| **Dihidroquercetin** | -5.57 | 83.19 | -7.36 | -6.91 | -0.45 | -2.72 | 1.79 | -2.72 |
| **Ecdysteron** | -6.67 | 12.87 | -9.95 | -9.74 | -0.22 | -4.73 | 3.28 | -4.73 |
| **Firul acid** | -3.75 | 1.78 mM | -5.24 | -4.68 | -0.56 | -0.97 | 1.49 | -0.97 |
| Galic acid | -4.66 | 383.34 | -8.54 | -8.42 | -0.12 | -4.83 | 3.88 | -4.83 |
| Lutiolin | -5.87 | 50 | -7.36 | -7.18 | -0.18 | -1.96 | 1.49 | -1.96 |
| **Plantaginin** | -10.89 | 10.39 | -14.17 | -14.17 | 0 | -5.51 | 3.28 | -5.51 |
| Quercetin | -5.36 | 118.28 | -7.15 | -6.65 | -0.49 | -2.34 | 1.79 | -2.34 |
| Rosavin | -4.13 | 944.82 | -8 | -7.64 | -0.36 | -3.99 | 3.88 | -3.99 |
| **Rutin** | -4.18 | 865.54 | -8.95 | -8.72 | -0.23 | -8.18 | 4.77 | -8.18 |
| **Salidrodside** | -4.2 | 832.08 | -7.18 | -6.73 | -0.45 | -2.3 | 2.98 | -2.3 |
| Turkesterone | -7.9 | 1.63 | -11.48 | -11.07 | -0.41 | -1.32 | 3.58 | -1.32 |

AST

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Estimated Free Energy of Binding (kcal/mol)** | **Estimated Inhibition Constant, Ki (mikromolar)** | **Final Intermolecular Energy (kcal/mol)** | **vdW + Hbond + desolv Energy (kcal/mol)** | **Electrostatic Energy (kcal/mol)** | **Final Total Internal Energy (kcal/mol)** | **Torsional Free Energy (kcal/mol)** | **Unbound System's Energy [=(2)] (kcal/mol)** |
| **Anestezin** | 3.33 |  | 2.14 | 2.17 | -0.03 | -0.17 | 1.19 | -0.17 |
| **Cynaroside** | -6.53 | 16.39 | -9.81 | -9.28 | -0.53 | -3.93 | 3.28 | -3.93 |
| **Dihidroquercetin** | -8.22 | 947.47 | -10.01 | -9.69 | -0.32 | -2.77 | 1.79 | -2.77 |
| **Ecdysteron** | 7.19 |  | 3.91 | 4.04 | -0.13 | -3.41 | 3.28 | -3.41 |
| **Firul acid** | -5.81 | 54.91 | -7.3 | -7 | -0.31 | -0.96 | 1.49 | -0.96 |
| **Galic acid** | -7.15 | 3.44 | -11.33 | -11.15 | -0.18 | -4.81 | 3.88 | -4.81 |
| **Lutiolin** | -8.17 | 1.03 | -9.66 | -9.22 | -0.43 | -1.99 | 1.49 | -1.99 |
| **Plantaginin** | -13.28 | 183 | -16.57 | -16.57 | 0 | -4.47 | 3.28 | -4.47 |
| **Quercetin** | -8.02 | 1.32 | -9.81 | -9.44 | -0.37 | -2.57 | 1.79 | -2.57 |
| **Rosavin** | -7.18 | 5.42 | -11.06 | -10.4 | -0.67 | -3.36 | 3.88 | -3.36 |
| **Rutin** | 7.41 |  | 2.63 | 3.65 | -1.02 | 3.7 | 4.77 | 3.7 |
| **Salidrodside** | -6.9 | 8.79 | -9.88 | -9.19 | -0.69 | -1.98 | 2.98 | -1.98 |
| **Turkesterone** | 8.85 |  | 5.27 | 5.61 | -0.34 | -1.29 | 3.58 | -1.29 |

Catalase

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Estimated Free Energy of Binding (kcal/mol)** | **Estimated Inhibition Constant, Ki (mikromolar)** | **Final Intermolecular Energy (kcal/mol)** | **vdW + Hbond + desolv Energy (kcal/mol)** | **Electrostatic Energy (kcal/mol)** | **Final Total Internal Energy (kcal/mol)** | **Torsional Free Energy (kcal/mol)** | **Unbound System's Energy [=(2)] (kcal/mol)** |
| **Anestezin** | -5.04 | 201.57 | -6.23 | -5.93 | -0.3 | -0.22 | 1.19 | -0.22 |
| **Cynaroside** | -5.56 | 83.83 | -8.84 | -8.57 | -0.27 | -3.82 | 3.28 | -3.82 |
| **Dihidroquercetin** | -5.94 | 44.38 | -7.73 | -7.48 | -0.25 | -2.63 | 1.79 | -2.63 |
| **Ecdysteron** | -5.18 | 158.7 | -8.46 | -8.23 | -0.23 | -3.43 | 3.28 | -3.43 |
| **Firul acid** | -3.9 | 1.37 | -5.4 | -4.89 | -0.51 | -0.33 | 1.49 | -0.33 |
| **Galic acid** | -3.76 | 1.74 | -7.64 | -7.23 | -0.41 | -5.37 | 3.88 | -5.37 |
| **Lutiolin** | -6.47 | 18.24 | -7.96 | -7.49 | -0.46 | -1.97 | 1.49 | -1.97 |
| **Plantaginin** | -8.74 | 395.47 | -12.02 | -12.02 | 0 | -4.85 | 3.28 | -4.85 |
| **Quercetin** | -6.29 | 24.52 | -8.08 | -7.72 | -0.36 | -2.17 | 1.79 | -2.17 |
| **Rosavin** | -3.96 | 1.25 mM | -7.84 | -7.67 | -0.17 | -4.66 | 3.88 | -4.66 |
| **Rutin** | -3.92 | 1.33 mM | -8.7 | -8.1 | -0.59 | -7.55 | 4.77 | -7.55 |
| **Salidrodside** | -3.97 | 1.23 mM | -6.95 | -6.59 | -0.36 | -2.76 | 2.98 | -2.76 |
| **Turkesterone** | -4.77 | 318.8 | -8.35 | -8.11 | -0.24 | -3.44 | 3.58 | -3.44 |

Superoxide-dismutase

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Estimated Free Energy of Binding (kcal/mol)** | **Estimated Inhibition Constant, Ki (mikromolar)** | **Final Intermolecular Energy (kcal/mol)** | **vdW + Hbond + desolv Energy (kcal/mol)** | **Electrostatic Energy (kcal/mol)** | **Final Total Internal Energy (kcal/mol)** | **Torsional Free Energy (kcal/mol)** | **Unbound System's Energy [=(2)] (kcal/mol)** |
| **Anestezin** | -3.38 | 3.33 | -4.57 | -4.56 | -0.02 | -0.21 | 1.19 | -0.21 |
| **Cynaroside** | -4.38 | 620.16 | -7.66 | -6.96 | -0.7 | -4.31 | 3.28 | -4.31 |
| **Dihidroquercetin** | -5.01 | 211.41 | -6.8 | -6.32 | -0.48 | -2.83 | 1.79 | -2.83 |
| **Ecdysteron** | -4.99 | 219.64 | -8.27 | -8.15 | -0.12 | -4.25 | 3.28 | -4.25 |
| **Firul acid** | -3.57 | 2.42 | -5.06 | -4.39 | -0.66 | -0.87 | 1.49 | -0.87 |
| **Galic acid** | -3.05 | 5.81 | -6.93 | -6.53 | -0.4 | -5.19 | 3.88 | -5.19 |
| **Lutiolin** | -4.77 | 320.24 | -6.26 | -5.9 | -0.36 | -2.01 | 1.49 | -2.01 |
| **Plantaginin** | -9.01 | 250.48 nM | -12.29 | -12.29 | 0 | -4.48 | 3.28 | -4.48 |
| **Quercetin** | -5.26 | 138.84 | -7.05 | -6.48 | -0.57 | -1.85 | 1.79 | -1.85 |
| **Rosavin** | -3.22 | 4.36 mM | -7.1 | -6.71 | -0.39 | -4.03 | 3.88 | -4.03 |
| **Rutin** | -3.11 | 5.23 mM | -7.89 | -7.55 | -0.34 | -8.72 | 4.77 | -8.72 |
| **Salidrodside** | -3.4 | 3.23 mM | -6.38 | -5.83 | -0.55 | -2.77 | 2.98 | -2.77 |
| **Turkesterone** | -4.72 | 348.19 | -8.3 | -7.92 | -0.38 | -3.94 | 3.58 | -3.94 |

Voltage dependent anion channel

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Estimated Free Energy of Binding (kcal/mol)** | **Estimated Inhibition Constant, Ki (mikromolar)** | **Final Intermolecular Energy (kcal/mol)** | **vdW + Hbond + desolv Energy (kcal/mol)** | **Electrostatic Energy (kcal/mol)** | **Final Total Internal Energy (kcal/mol)** | **Torsional Free Energy (kcal/mol)** | **Unbound System's Energy [=(2)] (kcal/mol)** |
| **Anestezin** | -5.15 | 166.69 | -6.35 | -6.33 | -0.02 | -0.23 | 1.19 | -0.23 |
| **Cynaroside** | -4.24 | 780.18 | -7.52 | -7.01 | -0.51 | -4.5 | 3.28 | -4.5 |
| **Dihidroquercetin** | -6.76 | 11.16 | -8.55 | -8.42 | -0.13 | -2.85 | 1.79 | -2.85 |
| **Ecdysteron** | -1.93 | 38.43 | -5.21 | -5.1 | -0.12 | -3.31 | 3.28 | -3.31 |
| **Firul acid** | -5.4 | 110.1 | -6.89 | -6.42 | -0.47 | -0.96 | 1.49 | -0.96 |
| **Galic acid** | -6.79 | 10.49 | -10.67 | -10.54 | -0.13 | -3.33 | 3.88 | -3.33 |
| **Lutiolin** | -7.56 | 2.87 | -9.05 | -8.99 | -0.06 | -2 | 1.49 | -2 |
| **Plantaginin** | -10.55 | 18.47 | -13.83 | -13.83 | 0 | -5.96 | 3.28 | -5.96 |
| **Quercetin** | -6.31 | 23.79 | -8.1 | -7.93 | -0.16 | -2.64 | 1.79 | -2.64 |
| **Rosavin** | -5.92 | 45.41 | -9.8 | -9.63 | -0.17 | -3.57 | 3.88 | -3.57 |
| **Rutin** | 22.92 |  | 18.15 | 18.13 | 0.02 | 3.75 | 4.77 | 3.75 |
| **Salidrodside** | -6.85 | 9.51 | -9.83 | -9.63 | -0.2 | -2.38 | 2.98 | -2.38 |
| **Turkesterone** | -1.08 | 161.02 | -4.66 | -4.38 | -0.29 | 1.92 | 3.58 | 1.92 |