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| --- | --- | --- | --- | --- | --- |
|  | **Affinity (kcal/mol)** | **RMSD l.b. \*** | **RMSD u.b.\*** | **H-bond a.a.** | **Picture** |
| **Chlorogenic acid** | -7 | 6.361 | 9.87 | GLU-363, GLY-705, ASN-741, THR-1113 |  |
| **Cynarine** | -7.1 | 12.247 | 14.785 | SER-1112, THR-1113, PHE-1114, TYR-1460 |  |
| **Hyperoside** | -7.4 | 2.778 | 4.252 | THR-361, GLU-363, SER-393, PHE-1114, GLU-1115 |  |
| **Malic acid** | -4.2 | 7.155 | 8.06 | GLU-1115, THR-1414 |  |
| **Quinic acid** | -5.9 | 1.705 | 4.672 | GLY-705, GLU-1115, THR-1414 |  |
| **Rutin** | -8.1 | 6.456 | 10.965 | ASN-741, GLU-1115, GLY-1415, TYR-1460 |  |
| **Tricin** | -6.6 | 0.94 | 2.703 | TYR-742 |  |

1. **RMSD values** are calculated relative to the best mode and use only movable heavy atoms. Two variants of RMSD metrics are provided, rmsd/lb (RMSD lower bound) and rmsd/ub (RMSD upper bound), differing in how the atoms are matched in the distance calculation:
   1. - **rmsd/ub** matches each atom in one conformation with itself in the other conformation, ignoring any symmetry
   2. - **rmsd'** matches each atom in one conformation with the closest atom of the same element type in the other conformation (rmsd' can not be used directly, because it is not symmetric)
   3. - **rmsd/lb** is defined as follows: rmsd/lb(c1, c2) = max(rmsd'(c1, c2), rmsd'(c2, c1))

So: if your ligand has no internal symmetry, rmsd/ub is the value to use. However, if you are docking e.g. benzene, this would give you different values depending on your ligand is rotates and which of the six equivalent CH point into your binding pocket, therefore rmsd/lb gives you a better ranking of docking solutions also see: <http://mgldev.scripps.edu/pipermail/autodock/2009-March/005265.html>

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