**Enzyme – ligand docking model list.**

**Table 1.** A list of *P. megaterium* tyrosinase GOLD docking PDB files. All .pdb files can be found at [www.github.com/J-Britton-IE/Tyrosinase\_docking](http://www.github.com/J-Britton-IE/Tyrosinase_docking)

|  |  |  |
| --- | --- | --- |
| **Substrate** | **Crystal structure with substrate** | **Docked substrate file** |
| Tyrosine | 4p6r.pdb | PmTyr\_Tyrosine.pdb |
| Tyrosol | 4p6t.pdb | PmTyr\_Tyrosol.pdb |

**Table 2. A list of *R. pseudosolanacearum* tyrosinase GOLD docking PDB files.** All .pdb files can be found at [www.github.com/J-Britton-IE/Tyrosinase\_docking](http://www.github.com/J-Britton-IE/Tyrosinase_docking)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Model type** | | | | |
| **Substrate** | **7xio full length** | **7xio catalytic** | **SWISS-MODEL** | **AlphaFold 3 full length** | **AlphaFold 3 catalytic** |
| **Tyrosine** | Tyrosine\_7xio-II.pdb | Tyrosine\_7xio\_catalytic.pdb | Tyrosine\_SM.pdb | Tyrosine\_AF3.pdb | Tyrosine\_AF3\_catalytic.pdb |
| **Octopamine** | N/A | N/A | Octopamine\_SM.pdb | N/A | Octopamine\_AF3\_catalytic.pdb |
| **Tyramine** | N/A | N/A | Tyramine\_SM.pdb | N/A | Tyramine\_AF3\_catalytic.pdb |
| **Tyrosol** | Tyrosol\_7xio-II.pdb | Tyrosol\_7xio\_catalytic.pdb | Tyrosol\_SM.pdb | Tyrosine\_AF3.pdb | Tyrosol\_AF3\_catalytic.pdb |
| **Resveratrol** | N/A | N/A | Resveratrol\_SM.pdb | N/A | Resveratrol\_AF3\_catalytic.pdb |
| **4-hydroxybenzoic acid** | N/A | N/A | 4HBA\_SM.pdb | N/A | 4HBA\_AF3\_catalytic.pdb |
| **4-hydroxymandelic acid** | N/A | N/A | 4HMA\_SM.pdb | N/A | 4HMA\_AF3\_catalytic.pdb |
| **4-hydroxyphenylacetic acid** | N/A | N/A | 4HPAA\_SM.pdb | N/A | 4HPAA\_AF3\_catalytic.pdb |
| **Phenol** | N/A | N/A | Phenol\_SM.pdb | N/A | Phenol\_AF3\_catalytic.pdb |
| **2-fluorophenol** | N/A | N/A | 2FP\_SM.pdb | N/A | 2FP\_AF3\_catalytic.pdb |
| **3-fluorophenol** | N/A | N/A | 3FP\_SM.pdb | N/A | 3FP\_AF3\_catalytic.pdb |
| **4-methoxyphenylacetic acid** | N/A | N/A | 4MPAA\_SM.pdb | N/A | 4MPAA\_AF3\_catalytic.pdb |