**Table S3.** Molecular docking data and affinity values (binding free energies) of ligands binding with *Xoo* 5CY8

and *M. oryzae* 4LXZ enzymes.

|  |  |  |  |
| --- | --- | --- | --- |
| **CID** | **Compound name** | **Xoo**  **5CY8**  **Docking score [kcal/mol]** | **M. oryzae**  **4LXZ Docking score [kcal/mol]** |
| [5365037](https://pubchem.ncbi.nlm.nih.gov/compound/5365037) | **9-eicosene** | **-7.773** | **-7.612** |
| [6329112](https://pubchem.ncbi.nlm.nih.gov/compound/6329112) | 3-(Dimethylsiloxy)-3,3-dimethyl-1-propene | -6.518 | -6.463 |
| 6421864 | l-Alanine, N-methoxycarbonyl-, methyl ester | -6.302 | -6.068 |
| 5375190 | 4-(1,3-Butadienyl)-3,5,5-trimethylcyclohex-2-en-1one | -7.237 | -7.054 |
| 5366244 | Phytol | -7.450 | -7.323 |
| 5354176 | Flexricin P-4 | -6.869 | **-7.575** |
| 145561 | **Methyl 10,12-pentacosadiynoate** | **-7.919** | **-7.915** |
| 91181716 | Cyclohexene-d1 | **-7.543** | -6.172 |
| 12932773 | 2-Chlorocycloheptanol | -6.769 | -6.346 |
| 5366075 | 3-Hydroxy-beta-damascone | -6.428 | -7.005 |
| 1549095 | (E)-4-(3-Hydroxyprop-1-en-1-yl)-2-methoxyphenol | -6.895 | -6.370 |
| 605654 | 1-(3,6,6-Trimethyl-1,6,7,7a-tetrahydrocyclopenta[c]pyran-1-yl) ethanone | -7.175 | -7.081 |
| 5363097 | **E-15-Heptadecenal** | **-7.573** | **-7.535** |
| 5352711 | 4-(2,6,6-Trimethylcyclohexa-1,3-dienyl) but-3-en-2-one | -7.156 | -7.053 |
| 601977 | 6-Methoxycoumaran-7-ol-3-one | -7.489 | -6.791 |
| 575987 | **5H-Cyclopenta[b]pyridine** | **-7.817** | -6.481 |
| 561778 | 1-Oxaspiro [3.5] nona-5,8-dien-7-one, 3-methylene- | -6.985 | -6.412 |
| 560888 | 2-Vinylbicyclo [2.1.1] hexan-2-ol | -6.127 | -6.643 |
| 558931 | alpha-[5-Methyl-2,3,4,5-tetrahydro-2-furyl] glucine | -6.466 | -6.544 |
| 557922 | 1,3-Oxathiane, 5-isopropyl-2-methyl- | -6.544 | -6.799 |
| 554455 | Ethylene glycol, TMS derivative | -6.449 | -6.316 |
| 553025 | 3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane | **-7.697** | **-8.012** |
| 543693 | 7-Methyl-2-oxepanone | -6.734 | -6.399 |
| 538757 | 2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one | -6.217 | -6.263 |
| 533712 | Pentanedioic acid, ethyl methyl ester | -6.050 | -6.620 |
| 521348 | 3-Mercaptohexanol | -6.623 | -6.237 |
| 347424 | Benzeneacetic acid, alpha-hydroxy-, pentyl ester | -6.659 | -7.064 |
| 329061 | Pentanamide, 5-hydroxy- | -6.101 | -5.987 |
| 246673 | N-Carbobenzoxy-DL-leucine | -6.187 | -7.123 |
| 181561 | 5-Methoxypyrrolidin-2-one | -6.228 | -6.054 |
| 141615 | 2-Methoxy-5-methylthiophene | -8.358 | -6.579 |
| 137941 | 2,2-Dimethoxybutane | -6.559 | -6.344 |
| 102642 | 2-Methylbutanoic anhydride | -6.274 | -6.274 |
| 119838 | 3,5-dihydroxy-6-methyl-2,3-dihydropyran-4-one | -6.619 | -6.341 |
| 98431 | 5-Hydroxymethyl-dihydro-furan-2-one | -6.199 | -6.198 |
| 78475 | 1,3-Dioxan-5-ol | -6.045 | -5.942 |
| 70945 | 2-Methylcyclohexane-1,3-dione | -6.336 | -6.316 |
| 70227 | Diazene, bis(1,1-dimethylethyl)- | -6.615 | -6.536 |
| 69340 | Octanoic anhydride | -6.610 | -7.058 |
| 66948 | Protoanemonin | -7.283 | -6.447 |
| 62719 | Silane, ethoxydimethyl[3-(oxiranylmethoxy)propyl]- | -6.701 | -7.213 |
| 61278 | Formic acid, allyl ester | -6.411 | -6.008 |
| 61209 | 3-Methyl-1,2-cyclopentanedione | -6.233 | -6.385 |
| 25209 | **Tetradec-7-ene** | **-7.555** | -7.089 |
| 19309 | 2,5-Anhydro-1,6-dideoxyhexo-3,4-diulose | -7.490 | -6.377 |
| 18829 | 4-Hydroxy-3-methylbutan-2-one | -6.220 | -6.200 |
| 13006 | Cyclohexane-1,2-dione | -6.254 | -6.348 |
| 12206 | Methyl pentanoate | -6.203 | -6.558 |
| 11559 | 5-Methyl-2(3H)-furanone | -7.040 | -6.459 |
| 12266 | Furan, 2,5-dimethyl- | -7.534 | -6.634 |
| 11254 | 2,2'-Bioxirane | -6.983 | -6.243 |
| 8452 | Ketocyclopentane | -6.135 | -6.306 |
| 7136 | Eugenol acetate | -6.633 | -6.557 |
| 7041 | Syringol | -7.316 | -6.874 |
| 6175 | Cytosine riboside | -6.243 | -6.452 |
| 6818 | Butyl 2-ethylhexyl phthalate | -6.943 | **-7.890** |
| 4765 | 4-Hydroxybenzenesulfonic acid | -6.974 | -6.801 |
| 785 | hydroquinone | -6.482 | -6.542 |
| 1064 | Kinic acid | -6.756 | -6.400 |
| 460 | Guaiacol | -6.884 | -6.545 |
| 332 | 2-Methoxy-4-vinylphenol | -7.132 | -7.203 |

**Table7.** Molecular docking data and affinity values (binding free energies)