Table B.1. XP GScore and MM-GBSA results

|  |  |
| --- | --- |
| α-Amylase (3DHP) | DPP-4 (6B1E Chain A) |
| Compounds | XP GScore | MM-GBSA (kcal/mol) | Compounds | XP GScore | MM-GBSA (kcal/mol) |
| 11-Deoxyisomogroside V | -17.060 | -35.81 | 11-O-Mogroside V | -14.657 | -40.65 |
| 11-O-Mogroside V | -14.560 | -39.52 | CHEBI:140096 | -12.192 | -37.43 |
| Mogroside IV | -12.930 | -30.36 | Mogroside IVa | -11.658 | -50.77 |
| Mogroside III | -12.716 | -41.43 | Salvianolic acid B | -11.523 | -30.91 |
| 6,8-Di-C-glucopyranosylnaringenin | -11.818 | -35.3 | 6,8-Di-C-glucopyranosylnaringenin | -11.298 | -44.11 |
| Sagerinic Acid | -11.700 | -30.45 | Sagerinic acid | -10.569 | -39.58 |
| Grosvenorine | -10.802 | -39.16 | Rutin | -10.148 | -39.23 |
| Mogroside IIe | -10.728 | -36.73 | Methyl hesperidin | -9.311 | -33.42 |
| Isoliquiritigenin 4'-O-glucoside 4-O-apiofuranosyl-(1'''->2''')-glucoside | -10.279 | -40.73 | Rhoifolin | -9.127 | -41.33 |
| 5,3',4',5'-Tetrahydroxy-6,7-dimethoxyflavone | -9.311 | -33.62 | Procyanidin B2, (+)- | -8.758 | -37.43 |
| Quercetin | -8.844 | -30.33 | Hinokiflavone | -8.717 | -42.26 |
| Mogroside III-E | -8.834 | -38.14 | SCHEMBL13206587 | -8.714 | -35.11 |
| Versiconal | -8.071 | -38.89 | Salvianolic acid A | -8.423 | -39.58 |
| Lumichrome | -7.677 | -35.48 | Salvianolic acid C | -8.376 | -33.69 |
| 3-Amino-2,3-Dideoxy-Scyllo-Inosose | -7.358 | -30.18 | Ginsenoside Rf | -8.239 | -33.3 |
| Methyl Hesperidin | -7.247 | -41.07 | Kaempferol 7-O-glucoside | -8.083 | -44.56 |
| Feruloylagmatine | -7.236 | -34.56 | Astragalin | -7.939 | -37.96 |
| Apigenin | -7.025 | -31.83 | Flazin | -7.762 | -42.64 |
| Cirsimaritin | -6.874 | -34.93 | N-[4-[[6-Methoxy-7-[3-(4-morpholinyl) propoxy]-4-quinazolinyl] amino] phenyl] benzamide | -7.688 | -52.91 |
| Hinokiflavone | -6.723 | -47.95 | Hesperidin | -7.554 | -35.36 |
| Curcumin | -6.720 | -44.06 | Quercetin 3,4'-dimethyl ether | -7.09 | -34.12 |
| Oxyayanin B | -6.644 | -36.87 | Hypoxanthine E | -6.908 | -32.94 |
| 1-(2-Quinoxalinyl)-1,2,3,4-butanetetrol | -6.58 | -33.79 | 13-azaprostanoic acid | -6.767 | -30.43 |
| 2-O-Methyladenosine | -6.473 | -34.71 | Beta-CCM | -6.596 | -33.19 |
| 5,9-Epoxy-3,6-megastigmadien-8-ol | -6.416 | -31.31 | SCHEMBL2214591 | -6.573 | -52.39 |
| 9H-Pyrido[3,4-B] indole | -6.053 | -30.73 | SCHEMBL2214758 | -6.474 | -35.67 |
|  |  |  | N-trans-Feruloyltyramine | -6.459 | -35.55 |
|  |  |  | (S)-5'-Deoxy-5'-(methylsulfinyl)adenosine | -6.457 | -30.35 |
|  |  |  | Dicyclomine | -6.404 | -31.64 |
|  |  |  | 2-O-Methyladenosine | -6.244 | -30.58 |
|  |  |  | YBYJEAFJEFYNQU-UHFFFAOYSA-N | -6.199 | -34.49 |
|  |  |  | [9H-Pyrido[3,4-B] indole](https://pubchem.ncbi.nlm.nih.gov/compound/64961) | -6.059 | -36.79 |