**Table S1. Total docking ranking**

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| --- | --- |
| **Ligand** | **Docking score (kcal/mol)** |
| **6LU7** | **1R4L** | **SUM** |
| Hesperidin | -8.5 | -11.4 | -19.9 |
| Saikosaponin A | -8.8 | -11 | -19.8 |
| Rutin | -8.9 | -10.7 | -19.6 |
| Corosolic acid | -8.8 | -10.2 | -19 |
| Verbascoside | -8.4 | -10.6 | -19 |
| Baicalin | -8.4 | -10.5 | -18.9 |
| Glycyrrhizin | -8.9 | -9.9 | -18.8 |
| Mulberroside A | -7.7 | -11 | -18.7 |
| Cynaroside | -8.4 | -10.2 | -18.6 |
| Bilirubin | -7.8 | -10.7 | -18.5 |
| Vincetoxicoside B | -7.9 | -10.6 | -18.5 |
| Morusin | -8.6 | -9.8 | -18.4 |
| Puerarin | -8.6 | -9.8 | -18.4 |
| Orientin | -8.1 | -10.2 | -18.3 |
| Cynancersicoside A | -8.3 | -9.9 | -18.2 |
| Protostemonine | -8.1 | -10.1 | -18.2 |
| Amygdalin | -8.1 | -10 | -18.1 |
| Ilexgenin A | -7.9 | -10.1 | -18 |
| Prim-*O*-glucosylcimifugin | -7.6 | -10.4 | -18 |
| Corynoline | -7.7 | -10.2 | -17.9 |
| Astragaloside A | -7.6 | -10.2 | -17.8 |
| Paeoniflorin | -7.7 | -10 | -17.7 |
| Polyphyllin I | -8.5 | -9.1 | -17.6 |
| Nodakenin | -7.9 | -9.6 | -17.5 |
| Tectoridin | -7.9 | -9.5 | -17.4 |
| Ursolic acid | -7.4 | -10 | -17.4 |
| Swertiajaponin | -8 | -9.4 | -17.4 |
| Berberine | -7.5 | -9.7 | -17.2 |
| Timosaponin BII | -7.7 | -9.4 | -17.1 |
| Dryocrassin | -7.4 | -9.5 | -16.9 |
| Columbianadin | -7.2 | -9.6 | -16.8 |
| Arctiin | -7.3 | -9.5 | -16.8 |
| Oleanic acid | -7.4 | -9.3 | -16.7 |
| Luteolin | -7.6 | -9.1 | -16.7 |
| Quercetin | -7.7 | -9 | -16.7 |
| Forsythiaside A | -7.6 | -9.1 | -16.7 |
| Radix isatidis A | -7.6 | -9.1 | -16.7 |
| Genistein | -7.5 | -9.1 | -16.6 |
| Indirubin | -7.3 | -9.3 | -16.6 |
| Curcumin | -7 | -9.5 | -16.5 |
| Trisalbaspidin ABA | -7.2 | -9.3 | -16.5 |
| Artemisinin | -7.3 | -9.1 | -16.4 |
| Emodin | -7.2 | -9.2 | -16.4 |
| Cholic acid | -7 | -9.3 | -16.3 |
| Hyodeoxycholic acid | -7 | -9.3 | -16.3 |
| Daidzein | -7.4 | -8.8 | -16.2 |
| Xanthiside | -7.3 | -8.9 | -16.2 |
| Chlorogenic acid | -7.3 | -8.8 | -16.1 |
| Verbenalin | -7.4 | -8.7 | -16.1 |
| Poricoic acid A | -6.9 | -9.2 | -16.1 |
| Andrographolide | -6.9 | -8.8 | -15.7 |
| Dipsacoside B | -8.9 | -6.7 | -15.6 |
| Codeine | -7 | -8.5 | -15.5 |
| Rosmarinic acid | -7 | -8.4 | -15.4 |
| Notopterol | -7 | -8.4 | -15.4 |
| Harpagide | -7 | -8.3 | -15.3 |
| Imperatorin | -7.1 | -8.2 | -15.3 |
| Papaverine | -6.9 | -8.3 | -15.2 |
| Geniposide | -6.7 | -8.5 | -15.2 |
| Catalpol | -7.1 | -7.9 | -15 |
| Salidroside | -6.9 | -7.9 | -14.8 |
| Morphine | -6.6 | -8.1 | -14.7 |
| Atractylenolide I | -6.3 | -8.2 | -14.5 |
| Magnolol | -6.4 | -7.9 | -14.3 |
| Lobetyolin | -6.4 | -7.7 | -14.1 |
| Matrine | -6.1 | -7.9 | -14 |
| Pterodontic acid | -6 | -7.7 | -13.7 |
| Isoevodionol | -6.2 | -7.1 | -13.3 |
| Esculetin | -6.2 | -6.9 | -13.1 |
| Platycodin D | -7.5 | -5.5 | -13 |
| Scopoletin | -5.8 | -6.8 | -12.6 |
| [Dhelwangin](https://www.so.com/link?m=aTIJ%2Fdd1QsjrXW3oaXW3D6jeP3M2PCkfB1GUykGLqFxidCSgxIQ1orzM%2BGzZkrQqsFwhfyyQUVXA%2FrcVII6fYR%2BMrNMKa2soqAk8ujOaxJpo2Ysdfdf5f0hkPBfKb2ZQjbz0DeI1lOTzh5W3ozV5B2A%3D%3D) | -5.2 | -7.1 | -12.3 |
| Caffeic acid | -5.7 | -6.5 | -12.2 |
| Ferulic acid | -5.4 | -6.5 | -11.9 |
| 6-Gingerol | -4.8 | -6.6 | -11.4 |
| L(+)–Ascorbic acid | -5.1 | -6.1 | -11.2 |
| Atractylodin | -4.9 | -6.3 | -11.2 |
| Ephedrine | -5.1 | -6.1 | -11.2 |
| Pulegone | -4.9 | -6.2 | -11.1 |
| α–Asarone | -5.1 | -5.9 | -11 |
| Coumalic acid | -4.9 | -5.9 | -10.8 |
| Citrulline | -4.9 | -5.8 | -10.7 |
| Linolenic acid | -4.6 | -6.1 | -10.7 |
| Amantadine Hydrochloride | -4.4 | -6.2 | -10.6 |
| L-Menthol | -4.7 | -5.7 | -10.4 |
| trans–Cinnamaldehyde | -4.4 | -5.7 | -10.1 |
| β–Pinene | -4.3 | -5.7 | -10 |
| Arecoline | -4.6 | -5.4 | -10 |
| Glutamic acid | -4.5 | -5.3 | -9.8 |
| α–Pinene | -4.1 | -5.6 | -9.7 |
| Tetramethyl pyrazine | -4.5 | -5.1 | -9.6 |
| Succinic acid | -4.4 | -4.9 | -9.3 |
| Decanoy acetaldehyde | -3.9 | -4.9 | -8.8 |
| Taurine | -3.7 | -4.2 | -7.9 |
| Betaine | -3.5 | -4.1 | -7.6 |