**Supplementary Table 1 Predicted interactions between Myricetin and ERp5 (4GWR) interaction**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Pose** | **Myricetin** | **Distance (Å)** | **Intermolecular Interaction** | **Protein** | **Affinity (kcal/mol)** |
| 1 | O1 | 2.5 |  = O – HN | H192 | -5.3 |
| O1 | 2.6 |  = O – HN | R256 |
| H3 | 2.2 | OH – O = | H192 |
| 2 | O1 | 2.3 |  = O – HN | W189 | -4.8 |
| O18 | 2 |  = O – HN | Y186 |
| O21 | 2 | HO – HN | G191 |
| 7 | O17 | 2.1 | HO – HN | W189 | -4.6 |
| O18 | 2.2 |  = O – HN | F237 |
| O19 | 2.2 | OH – O = | F237 |
| H6 | 2.2 | OH – O = | W189 |
| O21 | 1.9 | HO – HN | G191 |
| H1 | 2.3 | HO – HN | F237 |
| 8 | H9 | 2.4 | OH – O = | F237 | -4.4 |
| O19 | 2.7 | HO – HN | G191 |
| O19 | 2.3 | HO – HN | H192 |
| 14 | O17 | 2.1 | HO – HN | G191 | -4.2 |
| H9 | 2.3 | OH – O = | W189 |
| O21 | 2.1 | HO – HN | W189 |
| O22 | 2.2 | HO – HN | F237 |
| H7 | 2.4 | OH – O = | F237 |
| 16 | O22 | 2.4 | HO – HN | F237 | -4.2 |
| H7 | 2.1 | OH – O = | F237 |
| O21 | 2 | HO – HN | W189 |
| O1 | 2.2 |  = O – HN | G191 |
| O20 | 2.2 | HO – HN | K194 |

**Supplementary Table 2 Predicted interactions between Myricetin and PDI (4EL1) interaction**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Pose** | **Myricetin** | **Distance (Å)** | **Intermolecular Interaction** | **Protein** | **Affinity (kcal/mol)** |
| 1 | O17 | 1.9 | HO – HN | Y99 | -5.5 |
| H9 | 2.3 | OH – O = | Y99 |
| O21 | 2.4 | HO – HN | H55 |
| O22 | 2 | HO – HN | H55 |
| O22 | 2.7 | HO – HN | H55 |
| O22 | 2.5 | HO – HN | G54 |
| O23 | 2 | HO – HN | G54 |
| 3 | O21 | 2.2 | HO – HN | K81 | -5.2 |
| O17 | 2.2 | HO – HO | Y49 |
| H9 | 2 | OH – OH | D83 |
| 5 | O19 | 2.4 | HO – HN | K81 | -5.2 |
| O18 | 2.4 |  = O – HN | K81 |
| 7 | O17 | 2.9 | HO – HN | K81 | -5.1 |
| H9 | 2.2 | OH – O = | E23 |
| H9 | 2.9 | OH – OH | E23 |
| O22 | 2 | HO – HN | K57 |
| 11 | O21 | 2 | HO – HN | G54 | -4.9 |
| O22 | 2.4 | HO – HN | G54 |
| O22 | 2.4 | HO – HN | H55 |
| O22 | 1.9 | HO – HN | H55 |
| O23 | 2.8 | HO – HN | H55 |
| O1 – C10 | 4 – 4,2 | π – π  | W52 |
| 14 | O17 | 2 | HO – HN | G54 | -4.9 |
| H7 | 2.4 | OH – O = | Y99 |
| O22 | 2.4 | HO – HN | Y99 |
| O21 | 2.3 | HO – HN | Y99 |
| 15 | O19 | 2.3 | HO – HN | Q92 | -4.8 |
| H3 | 1.9 | OH – O = | A84 |
| C11 – C16 | 3.7 | π – π  | W52 |
| O21 | 2.4 | HO – HN | Y99 |