|  |  |  |  |
| --- | --- | --- | --- |
|  | Affinity(kcal/mol) | H-bond | Picture |
| 1\_3\_4\_6\_Tetragalloylglucose | -10.67 | GLU-39, SER-41, GLY-147, TYR-275, LYS-1117, ALA-2, ARG-1144 |  |
| 4-methoxy-kaempferol-3-O-hexoside | -9.322 | GLU-39, TYR-275, ARG-38, ILE-148 |  |
| Chelidonic-acid | -6.681 | PHE-80, LEU-79, GLY-921, HIS-1064, ARG-386 |  |
| Digallic-acid | -9.073 | ASN-63, LYS-1075, SER-1242, ILE-4, GLY-1250, TYR-1252, TYR-1254, ASN-1119 |  |
| Gallic acid | -6.629 | GLY-921, ARG-386, LEU-79, PHE-80 |  |
| Gecsagalloylglucoside | -11.22 | ARG-38, LEU-1115, GLU-39, ARG-1144 |  |
| Geptagalloylglucoside | -11.5 | GLU-18, THR-13, ALA-2, ARG-1144, THR-34, LYS-1117, GLU-39, SER-41 |  |
| Kaempferol-3-O-arabinoside | -8.757 | GLY-1250, THY-1252, ASN-1068 |  |
| Keampherol-3-O-ramnoside | -9.167 | LYS-1243 |  |
| Myricetin | -9.015 | ILE-61, ASN-63, LYS-1075, ILE-4, ASP-1119, SER-1242, VAL-1244 |  |
| Pentagalloylglucoside | -10.6 | LEU-1115, GLN-146, GLY-147, GLU-39, SER-41, SER-11, THR-13, LYS-1117 |  |
| Protocatechuic-acid | -6.228 | GLU-88, LYS-430, ASN-1068, TYR-1252 |  |
| Quercetin-3-O-galactose | -9.224 | GLU-39, SER-41, TYR-275 |  |
| Shikimic-acid | -6.211 | LYS-175, TYR-102, PRO-101, ASN-107, LEU-108, LYS-109 |  |