**PROTEIN LIGAND INTERACTION**

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| --- | --- | --- | --- |
| Compound | Hydrogen Bonding | Hydrogen bond length | Hydrophobic Interactions |
| 4,5-di-p-trans-coumaroylquinic\_acid | Trp20, His110, Ile260, Asn160, Thr113 | 2.81, 3.11, 3.05, 3.28, 2.70 | Val47, Trp111, Trp219, Ala299, Trp309, Leu300, Trp 309, Cys298, Phe115, Cys303, Phe122, Tyr209, Trp79, Ser210, Gln183, Ser210, Tyr48, Asp43 |
| (+)-pipoxide | His 110, Trp111 | 3,01, 3.03 | Trp309, Lue300, Thr114, Cys303, Phe122, Phe115, Trp79, Val47, Gln183, Tyr209, Asp43, Tyr48, Ile3260, Ser210, Trp20, Cys298 |
| Thymelol | His110, Ile 260 | 2.83, 2.67 | Trp219, Trp111, Lys77, Tyr48, Cys298, Gln183, Asp43, Ser210, Gly18, Lys21, Ser214, Tyr209, Trp20, Phe122, Leu300, Gln183 |
| Zinc000095485961 | Trp20, Ile260, His110, Thr113 | 2.81, 2.78, 3.03, 2.87 | Cys303, Phe122, Tyr309, Trp111, Trp79, Leu300, Tyr48, Asp43, Lys262, Ser210, Tyr209, Cys298, Trp219, Phe115 |
| Rutamontine | Trp111, Asn160 | 3.14, 2.81 | His110, Phe122, Tyr48, Gln183, Trp20, Ile260,Asp43,Lys262,Ser210,Ser214,Tyr209 |
| (-)-tingtanoxide | His110 | 2.97 | Thr113,Trp219,Leu300,Phe115,Trp111,Tyr209,Cys298,Gln183,Lys77,Trp20,Val47,Trp79,Tyr48,Phe122, Tyr309,Cys303,Trp219 |
| Tricoccin\_s13\_acetate | - | - | Trp111,Tyr48,Trp20,Val47, Pro218,Phe122,Leu300,Cys298,Trp219,His110,Trp79,Tyr209 |
| Lactupicrin | Thr113, Trp20 | 2.90,2.94 | Trp219,Phe122,Leu300,Tyr309,Cys303,Trp11,Phe115,Trp79,Ala299,Tyr48 |
| Naamidine\_a | Trp20, Thr113 | 3.01,2.93 | Ala299,Phe115,Tyr209,Tyr48,Cys298,His110,Trp111,Val47,Trp219,Trp79,Leu300,Cys303,Tyr309 |
| Zinc000000134782 | Trp20, Thr113 | 3.01,2.93 | Ala299,Phe115,Tyr209,Tye48,Cys298,His110,Trp111,Val47,Trp219,Trp79,Leu300,Phe122,Cys303,Tyr309 |
| Sigmoidin\_b\_4'-methylether\_diacetate | Gln183, Asn160, Ser210, Trp20 | 2.42, 2.83,2.99,3.14 | Lys262,Tyr209,Lys77,His110,Trp111,Phe115,Leu300,Cys298,Phe122AAla299,Phe122,Trp219,Tyr48,Lys21 |
| (-)-pipoxide | His110  Cys298 | 2.87, 3.27 3.33 | Trp111,Trp79, Phe115, Tyr309, Val 47, Tyr48, Tyr209, Ser210,Asp43, Trp20, Gln183, Phe122,Leu300, Thr113, Cys303 |
| Abyssinone\_ii | Gln183, Asn160 | 2.48,2.85 | Tyr209,His110,Tyr48,Trp20,Trp219,Cys303,Phe122,Phe115,Leu300,Trp111 |
| (+)-strigol | Trp111, Asn160 | 3.16,3.05 | Cys298,Tyr48,Phe122,Trp219,Val47,Trp20,Lys262,Gly18,Tyr209,Ser210,His110 |
| Norisojamicin | Asn160 | 2.63 | Leu300, Phe122,Cys298,Trp111,His110, Tyr209,Gln183, Tyr48, Trp20,Trp219 |
| Calopogonium\_isoflavone\_b |  |  | Leu300,Trp219,His110,Asn160,Trp111,Try48,Gln183,Tyr209,Trp20,Cys298,Phe122,Try70,Trp20,Val47 |
| Isosamarcandin | - | - | Arg69, Tyr103, Asp105,Arg69, Tyr103, Asp105,Ile58, Leu62, Arg69, Leu72, Lys100, Leu101, Asp102, Tyr103, Lys154 |
| (+)-pipoxide-2-methyl\_ether | His110  Trp111 | 3.09  3.03,3.12 | Tryp20,Tyr209,Ile260,Gln183,Tyr48,Ser210,Asp43,Trp79,Val47,Leu300,Ala299,Phe122,Tyr309,Cys303,Phe155,Cys298 |
| 1,6-di-O-p-hydroxybenzoyl-beta-D-glucopyranoside | Thr113, His110, Trp111, Ile260 | 2.96,3.29,2.78,3.31 | Phe122,Phe115,Tyr209,Gln183,Ser210,Trp20,Trp48,Asp43,Leu300,Trp79,Tyr309,Ala299,Cys3030 |
| Zinc000095485890 |  |  | Cys80,Leu300,Ala299,Phe115,Trp111,Trp79,Cys298,His110,Tyr48,Trp20,Val47,Trp219,Trp219,Thr113,Phe122,Cys303 |