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**Figure S1.** Photo of *A. Kastambulense*

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**Figure S2.** Docking conformation and interactions of **Atorvastatin** with HMG\_CoA R.

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**Figure S3**. Docking conformation and interactions of **Acarbose (ACR)** with Amylase.

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**Figure S4.** Docking conformation and interactions of **Acarbose (ACR)** with Glycosidase.



**Figure S5.** Docking conformation and interactions of **Orlistat** with Lipase.

**Table S1.** Interactions types and distances of top pose compound **1, 2** and **3** against ACE, AChE, BChE, HMG\_CoA R, Amylase, Collagenase, Glycosidase, Lipase, Tyrosinase and Urease, respectively. \*Captopril (for ACE), Tacrine (TAC) (for AChE and BChE), Atorvastatin (for HMG-CoAR), Acarbose (ACR) (for Amylase and Glycoside), EGCG (for Collagenase), Orlistat (for Lipase), Kojic acid (for Tyrosinase) and Thiourea (for Urease) as positive compounds of the related targets.

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| --- | --- | --- | --- | --- | --- |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (ACE )** | **Binding site of ligand (Captopril )** |
| :Captopril:H28 - A:ASP393:OD1 | 2.6861 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP393:OD1 | :Captopril:H28 |
| A:HIS361:HE1 - :Captopril:O4 | 3.0635 | Hydrogen Bond | Carbon Hydrogen Bond | A:HIS361:HE1 | :Captopril:O4 |
| :Captopril:H28 - A:HIS361 | 2.6725 | Hydrogen Bond | Pi-Donor Hydrogen Bond | A:HIS361 | :Captopril:H28 |
| A:HIS331 - :Captopril:C14 | 5.0672 | Hydrophobic | Pi-Alkyl | A:HIS331 | :Captopril:C14 |
| A:HIS361 - :Captopril:C14 | 4.1989 | Hydrophobic | Pi-Alkyl | A:HIS361 | :Captopril:C14 |
| A:PHE435 - :Captopril | 4.6340 | Hydrophobic | Pi-Alkyl | A:PHE435 | :Captopril |
| A:TYR501 - :Captopril | 4.4576 | Hydrophobic | Pi-Alkyl | A:TYR501 | :Captopril |
| A:TYR501 - :Captopril:C14 | 5.2844 | Hydrophobic | Pi-Alkyl | A:TYR501 | :Captopril:C14 |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (ACE )** | **Binding site of ligand (1 )** |
| A:GLN259:HE21 - :Gentisic Acid:O4 | 2.3926 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLN259:HE21 | :Gentisic Acid:O4 |
| :Gentisic Acid:H17 - A:GLU431:O | 2.7535 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU431:O | :Gentisic Acid:H17 |
| A:LYS432:NZ - :Gentisic Acid | 4.9859 | Electrostatic | Pi-Cation | A:LYS432:NZ | :Gentisic Acid |
| A:GLU431:OE2 - :Gentisic Acid | 4.2827 | Electrostatic | Pi-Anion | A:GLU431:OE2 | :Gentisic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (ACE )** | **Binding site of ligand (2 )** |
| A:ALA332:HN - :Catechin:O6 | 1.9218 | Hydrogen Bond | Conventional Hydrogen Bond | A:ALA332:HN | :Catechin:O6 |
| A:THR358:HG1 - :Catechin:O1 | 2.2095 | Hydrogen Bond | Conventional Hydrogen Bond | A:THR358:HG1 | :Catechin:O1 |
| :Catechin:H34 - A:ALA332:O | 2.1158 | Hydrogen Bond | Conventional Hydrogen Bond | A:ALA332:O | :Catechin:H34 |
| :Catechin:H32 - A:GLU431:OE2 | 2.2259 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU431:OE2 | :Catechin:H32 |
| :Catechin:H33 - A:SER357:O | 2.2582 | Hydrogen Bond | Conventional Hydrogen Bond | A:SER357:O | :Catechin:H33 |
| A:ASP393:OD1 - :Catechin | 3.7757 | Electrostatic | Pi-Anion | A:ASP393:OD1 | :Catechin |
| A:HIS331 - :Catechin | 4.9420 | Hydrophobic | Pi-Pi Stacked | A:HIS331 | :Catechin |
| :Catechin - A:ALA332 | 4.5766 | Hydrophobic | Pi-Alkyl | A:ALA332 | :Catechin |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (ACE )** | **Binding site of ligand (3 )** |
| A:TYR501:HH - :Rosmarinic Acid:O5 | 2.2343 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR501:HH | :Rosmarinic Acid:O5 |
| :Rosmarinic Acid:H41 - A:GLU431:OE2 | 2.4928 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU431:OE2 | :Rosmarinic Acid:H41 |
| :Rosmarinic Acid:H42 - A:SER260:OG | 2.4257 | Hydrogen Bond | Conventional Hydrogen Bond | A:SER260:OG | :Rosmarinic Acid:H42 |
| :Rosmarinic Acid:H42 - A:GLU431:O | 2.2985 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU431:O | :Rosmarinic Acid:H42 |
| :Rosmarinic Acid:H40 - A:ASP393:OD2 | 1.8006 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP393:OD2 | :Rosmarinic Acid:H40 |
| :Rosmarinic Acid:H38 - A:ALA332:O | 2.6592 | Hydrogen Bond | Conventional Hydrogen Bond | A:ALA332:O | :Rosmarinic Acid:H38 |
| :Rosmarinic Acid:H38 - A:GLU362:OE2 | 2.7344 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU362:OE2 | :Rosmarinic Acid:H38 |
| A:HIS331:HE1 - :Rosmarinic Acid:O6 | 2.5655 | Hydrogen Bond | Carbon Hydrogen Bond | A:HIS331:HE1 | :Rosmarinic Acid:O6 |
| A:ASP393:OD1 - :Rosmarinic Acid | 4.1686 | Electrostatic | Pi-Anion | A:ASP393:OD1 | :Rosmarinic Acid |
| A:HIS361 - :Rosmarinic Acid | 3.8503 | Hydrophobic | Pi-Pi Stacked | A:HIS361 | :Rosmarinic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (AChE )** | **Binding site of ligand (TAC )** |
| :TAC:H27 - A:GLU202:OE1 | 1.9707 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU202:OE1 | :TAC:H27 |
| A:TRP86 - :TAC | 4.0979 | Hydrophobic | Pi-Pi Stacked | A:TRP86 | :TAC |
| A:TRP86 - :TAC | 4.9290 | Hydrophobic | Pi-Pi Stacked | A:TRP86 | :TAC |
| A:TRP86 - :TAC | 3.7454 | Hydrophobic | Pi-Pi Stacked | A:TRP86 | :TAC |
| A:TRP86 - :TAC | 4.6814 | Hydrophobic | Pi-Pi Stacked | A:TRP86 | :TAC |
| A:TRP86 - :TAC | 4.9323 | Hydrophobic | Pi-Alkyl | A:TRP86 | :TAC |
| A:TRP86 - :TAC | 4.6616 | Hydrophobic | Pi-Alkyl | A:TRP86 | :TAC |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (AChE )** | **Binding site of ligand (1 )** |
| A:GLY121:HN - :Gentisic Acid:O3 | 2.8755 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLY121:HN | :Gentisic Acid:O3 |
| :Gentisic Acid:H17 - A:GLU202:OE1 | 2.2471 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU202:OE1 | :Gentisic Acid:H17 |
| :Gentisic Acid:H15 - A:GLU202:OE2 | 2.5639 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU202:OE2 | :Gentisic Acid:H15 |
| A:GLY448:HA1 - :Gentisic Acid:O1 | 2.5742 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLY448:HA1 | :Gentisic Acid:O1 |
| A:TRP86 - :Gentisic Acid | 3.8345 | Hydrophobic | Pi-Pi Stacked | A:TRP86 | :Gentisic Acid |
| A:TRP86 - :Gentisic Acid | 3.7605 | Hydrophobic | Pi-Pi Stacked | A:TRP86 | :Gentisic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (hAChE )** | **Binding site of ligand (2 )** |
| :Catechin:H35 - A:TYR72:O | 1.7625 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR72:O | :Catechin:H35 |
| :Catechin:H34 - A:TYR72:O | 2.4369 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR72:O | :Catechin:H34 |
| :Catechin:H32 - A:GLU202:OE1 | 2.3493 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU202:OE1 | :Catechin:H32 |
| :Catechin:H33 - A:HIS447:O | 2.3868 | Hydrogen Bond | Conventional Hydrogen Bond | A:HIS447:O | :Catechin:H33 |
| A:GLY121:HA1 - :Catechin:O2 | 2.9141 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLY121:HA1 | :Catechin:O2 |
| :Catechin:H6 - A:SER125:OG | 3.0859 | Hydrogen Bond | Carbon Hydrogen Bond | A:SER125:OG | :Catechin:H6 |
| A:TRP86 - :Catechin | 3.8391 | Hydrophobic | Pi-Pi Stacked | A:TRP86 | :Catechin |
| A:TRP86 - :Catechin | 3.7959 | Hydrophobic | Pi-Pi Stacked | A:TRP86 | :Catechin |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (hAChE )** | **Binding site of ligand (3)** |
| A:TYR124:HH - :Rosmarinic Acid:O2 | 2.4799 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR124:HH | :Rosmarinic Acid:O2 |
| A:PHE295:HN - :Rosmarinic Acid:O7 | 2.2589 | Hydrogen Bond | Conventional Hydrogen Bond | A:PHE295:HN | :Rosmarinic Acid:O7 |
| :Rosmarinic Acid:H41 - A:PHE338:O | 2.3412 | Hydrogen Bond | Conventional Hydrogen Bond | A:PHE338:O | :Rosmarinic Acid:H41 |
| :Rosmarinic Acid:H42 - A:SER293:O | 2.9314 | Hydrogen Bond | Conventional Hydrogen Bond | A:SER293:O | :Rosmarinic Acid:H42 |
| :Rosmarinic Acid:H40 - A:GLU202:OE1 | 2.1911 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU202:OE1 | :Rosmarinic Acid:H40 |
| A:VAL294:HA - :Rosmarinic Acid:O7 | 3.0052 | Hydrogen Bond | Carbon Hydrogen Bond | A:VAL294:HA | :Rosmarinic Acid:O7 |
| A:GLY448:HA1 - :Rosmarinic Acid:O4 | 2.9524 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLY448:HA1 | :Rosmarinic Acid:O4 |
| A:TRP86 - :Rosmarinic Acid | 3.9091 | Hydrophobic | Pi-Pi Stacked | A:TRP86 | :Rosmarinic Acid |
| A:TRP86 - :Rosmarinic Acid | 3.7961 | Hydrophobic | Pi-Pi Stacked | A:TRP86 | :Rosmarinic Acid |
| A:TYR341 - :Rosmarinic Acid | 4.7102 | Hydrophobic | Pi-Pi Stacked | A:TYR341 | :Rosmarinic Acid |
| A:PHE297 - :Rosmarinic Acid | 5.8705 | Hydrophobic | Pi-Pi T-shaped | A:PHE297 | :Rosmarinic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (BChE )** | **Binding site of ligand (TAC)** |
| :TAC:H26 - A:TRP82:O | 2.0179 | Hydrogen Bond | Conventional Hydrogen Bond | A:TRP82:O | :TAC:H26 |
| :TAC:H27 - A:GLN67:OE1 | 1.9669 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLN67:OE1 | :TAC:H27 |
| A:THR120:OG1 - :TAC | 2.8443 | Other | Pi-Lone Pair | A:THR120:OG1 | :TAC |
| A:TRP82 - :TAC | 5.3361 | Hydrophobic | Pi-Alkyl | A:TRP82 | :TAC |
| A:TRP82 - :TAC | 5.0819 | Hydrophobic | Pi-Alkyl | A:TRP82 | :TAC |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (BChE )** | **Binding site of ligand (1)** |
| A:GLY115:HN - :Gentisic Acid:O4 | 3.0051 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLY115:HN | :Gentisic Acid:O4 |
| A:TYR128:HH - :Gentisic Acid:O4 | 2.7309 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR128:HH | :Gentisic Acid:O4 |
| :Gentisic Acid:H15 - A:GLU197:OE2 | 2.1096 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU197:OE2 | :Gentisic Acid:H15 |
| A:GLY115:HA1 - :Gentisic Acid:O4 | 3.0912 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLY115:HA1 | :Gentisic Acid:O4 |
| A:GLY439:HA1 - :Gentisic Acid:O1 | 2.7609 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLY439:HA1 | :Gentisic Acid:O1 |
| A:GLY439:HA2 - :Gentisic Acid:O1 | 3.0814 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLY439:HA2 | :Gentisic Acid:O1 |
| A:TRP82 - :Gentisic Acid | 3.8310 | Hydrophobic | Pi-Pi Stacked | A:TRP82 | :Gentisic Acid |
| A:TRP82 - :Gentisic Acid | 3.8285 | Hydrophobic | Pi-Pi Stacked | A:TRP82 | :Gentisic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (BChE )** | **Binding site of ligand (2)** |
| A:ASP70:HN - :Catechin:O6 | 2.7961 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP70:HN | :Catechin:O6 |
| :Catechin:H35 - A:ASN68:O | 2.8623 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASN68:O | :Catechin:H35 |
| A:ILE69:HA - :Catechin:O6 | 2.5365 | Hydrogen Bond | Carbon Hydrogen Bond | A:ILE69:HA | :Catechin:O6 |
| A:HIS438:NE2 - :Catechin | 4.9261 | Electrostatic | Pi-Cation | A:HIS438:NE2 | :Catechin |
| A:ASP70:OD2 - :Catechin | 4.5891 | Electrostatic | Pi-Anion | A:ASP70:OD2 | :Catechin |
| A:TRP82 - :Catechin | 3.7200 | Hydrophobic | Pi-Pi Stacked | A:TRP82 | :Catechin |
| A:TRP82 - :Catechin | 3.8774 | Hydrophobic | Pi-Pi Stacked | A:TRP82 | :Catechin |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (BChE )** | **Binding site of ligand (3)** |
| A:TRP82:HE1 - :Rosmarinic Acid:O3 | 2.7739 | Hydrogen Bond | Conventional Hydrogen Bond | A:TRP82:HE1 | :Rosmarinic Acid:O3 |
| :Rosmarinic Acid:H41 - A:TYR128:OH | 2.4586 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR128:OH | :Rosmarinic Acid:H41 |
| :Rosmarinic Acid:H42 - A:GLU197:OE2 | 2.4222 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU197:OE2 | :Rosmarinic Acid:H42 |
| A:TRP82 - :Rosmarinic Acid | 4.4522 | Hydrophobic | Pi-Pi Stacked | A:TRP82 | :Rosmarinic Acid |
| A:TRP82 - :Rosmarinic Acid | 4.0754 | Hydrophobic | Pi-Pi Stacked | A:TRP82 | :Rosmarinic Acid |
| A:TRP82 - :Rosmarinic Acid | 5.3330 | Hydrophobic | Pi-Pi T-shaped | A:TRP82 | :Rosmarinic Acid |
| A:PHE329 - :Rosmarinic Acid | 5.3953 | Hydrophobic | Pi-Pi T-shaped | A:PHE329 | :Rosmarinic Acid |
| :Rosmarinic Acid - A:ALA328 | 3.7207 | Hydrophobic | Pi-Alkyl | A:ALA328 | :Rosmarinic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (HMG\_CoA R )** | **Binding site of ligand (Atorvastatin)** |
| :Atorvastatin:H67 - A:ILE746:O | 2.4515 | Hydrogen Bond | Conventional Hydrogen Bond | A:ILE746:O | :Atorvastatin:H67 |
| :Atorvastatin:H61 - A:SER745:OG | 2.7988 | Hydrogen Bond | Conventional Hydrogen Bond | A:SER745:OG | :Atorvastatin:H61 |
| :Atorvastatin:H64 - A:ALA751:O | 1.7578 | Hydrogen Bond | Conventional Hydrogen Bond | A:ALA751:O | :Atorvastatin:H64 |
| A:SER775:HB1 - :Atorvastatin:F1 | 2.5107 | Hydrogen Bond | Carbon Hydrogen Bond | A:SER775:HB1 | :Atorvastatin:F1 |
| :Atorvastatin:H9 - A:SER745:OG | 2.7805 | Hydrogen Bond | Carbon Hydrogen Bond | A:SER745:OG | :Atorvastatin:H9 |
| A:VAL772:O - :Atorvastatin:F1 | 3.3953 | Halogen | Halogen (Fluorine) | A:VAL772:O | :Atorvastatin:F1 |
| :Atorvastatin - A:ALA754 | 4.2001 | Hydrophobic | Pi-Alkyl | A:ALA754 | :Atorvastatin |
| :Atorvastatin - A:LEU853 | 4.8288 | Hydrophobic | Pi-Alkyl | A:LEU853 | :Atorvastatin |
| :Atorvastatin - A:ALA754 | 4.2077 | Hydrophobic | Pi-Alkyl | A:ALA754 | :Atorvastatin |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (HMG\_CoA R )** | **Binding site of ligand (1)** |
| Gentisic Acid:H16 - A:LEU862:O | 2.4633 | Hydrogen Bond | Conventional Hydrogen Bond | A:LEU862:O | Gentisic Acid:H16 |
| Gentisic Acid:- A:ALA856 | 4.1262 | Hydrophobic | Pi-Alkyl | A:ALA856 | Gentisic Acid: |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (HMG\_CoA R )** | **Binding site of ligand (2)** |
| A:ARG568:HH11 - :Catechin:O2 | 3.0060 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG568:HH11 | :Catechin:O2 |
| A:HIS861:HD1 - :Catechin:O5 | 2.3767 | Hydrogen Bond | Conventional Hydrogen Bond | A:HIS861:HD1 | :Catechin:O5 |
| A:ARG568:NH1 - :Catechin | 3.6727 | Electrostatic | Pi-Cation | A:ARG568:NH1 | :Catechin |
| :Catechin - A:CYS561 | 4.3174 | Hydrophobic | Pi-Alkyl | A:CYS561 | :Catechin |
| :Catechin - A:LEU862 | 5.1012 | Hydrophobic | Pi-Alkyl | A:LEU862 | :Catechin |
| :Catechin - A:ALA856 | 4.7913 | Hydrophobic | Pi-Alkyl | A:ALA856 | :Catechin |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (HMG\_CoA R )** | **Binding site of ligand (3)** |
| A:ARG568:HH11 - :Rosmarinic Acid:O2 | 2.8202 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG568:HH11 | :Rosmarinic Acid:O2 |
| A:ASN755:HD22 - :Rosmarinic Acid:O4 | 3.0369 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASN755:HD22 | :Rosmarinic Acid:O4 |
| A:ASN755:HD22 - :Rosmarinic Acid:O3 | 3.0718 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASN755:HD22 | :Rosmarinic Acid:O3 |
| A:SER852:HG - :Rosmarinic Acid:O2 | 1.8669 | Hydrogen Bond | Conventional Hydrogen Bond | A:SER852:HG | :Rosmarinic Acid:O2 |
| :Rosmarinic Acid:H42 - A:GLU559:OE2 | 2.2139 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU559:OE2 | :Rosmarinic Acid:H42 |
| :Rosmarinic Acid:H38 - A:SER852:O | 2.6986 | Hydrogen Bond | Conventional Hydrogen Bond | A:SER852:O | :Rosmarinic Acid:H38 |
| :Rosmarinic Acid - A:CYS561 | 4.7875 | Hydrophobic | Pi-Alkyl | A:CYS561 | :Rosmarinic Acid |
| :Rosmarinic Acid - A:LEU853 | 4.8352 | Hydrophobic | Pi-Alkyl | A:LEU853 | :Rosmarinic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Amylase)** | **Binding site of ligand (ACR )** |
| A:GLN63:HE22 - :ACR:O18 | 1.6702 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLN63:HE22 | :ACR:O18 |
| A:ASN298:HD21 - :ACR:O7 | 2.0254 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASN298:HD21 | :ACR:O7 |
| A:ASN301:HN - :ACR:O9 | 2.6100 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASN301:HN | :ACR:O9 |
| :ACR:H77 - A:ASP300:OD2 | 2.9104 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP300:OD2 | :ACR:H77 |
| :ACR:H87 - A:TRP59:O | 1.7371 | Hydrogen Bond | Conventional Hydrogen Bond | A:TRP59:O | :ACR:H87 |
| :ACR:H70 - A:ASP197:OD1 | 2.2595 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP197:OD1 | :ACR:H70 |
| :ACR:H72 - A:GLU233:OE2 | 1.9303 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU233:OE2 | :ACR:H72 |
| :ACR:H73 - A:GLU233:OE2 | 1.7352 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU233:OE2 | :ACR:H73 |
| :ACR:H74 - A:ASP300:OD1 | 2.2284 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP300:OD1 | :ACR:H74 |
| :ACR:H81 - A:ASP300:OD1 | 1.6743 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP300:OD1 | :ACR:H81 |
| :ACR:H86 - A:ASP300:OD1 | 2.5189 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP300:OD1 | :ACR:H86 |
| A:ASN301:HA - :ACR:O17 | 1.9122 | Hydrogen Bond | Carbon Hydrogen Bond | A:ASN301:HA | :ACR:O17 |
| :ACR:H15 - A:GLU233:OE2 | 2.8086 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLU233:OE2 | :ACR:H15 |
| :ACR:H20 - A:GLU233:OE2 | 2.3565 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLU233:OE2 | :ACR:H20 |
| :ACR:H27 - A:ASP197:OD1 | 2.7183 | Hydrogen Bond | Carbon Hydrogen Bond | A:ASP197:OD1 | :ACR:H27 |
| :ACR:H27 - A:GLU233:OE1 | 2.5169 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLU233:OE1 | :ACR:H27 |
| :ACR:H37 - A:ASP300:OD1 | 2.8195 | Hydrogen Bond | Carbon Hydrogen Bond | A:ASP300:OD1 | :ACR:H37 |
| A:ALA198 - :ACR:C35 | 4.4052 | Hydrophobic | Alkyl | A:ALA198 | :ACR:C35 |
| :ACR:C35 - A:LEU162 | 4.5427 | Hydrophobic | Alkyl | A:LEU162 | :ACR:C35 |
| A:HIS201 - :ACR:C35 | 5.1708 | Hydrophobic | Pi-Alkyl | A:HIS201 | :ACR:C35 |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Amylase)** | **Binding site of ligand (1)** |
| A:THR314:HG1 - :Gentisic Acid:O4 | 2.6979 | Hydrogen Bond | Conventional Hydrogen Bond | A:THR314:HG1 | :Gentisic Acid:O4 |
| A:ARG346:HH12 - :Gentisic Acid:O1 | 2.1996 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG346:HH12 | :Gentisic Acid:O1 |
| A:ARG346:HH22 - :Gentisic Acid:O4 | 2.3628 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG346:HH22 | :Gentisic Acid:O4 |
| A:ARG346:HH22 - :Gentisic Acid:O1 | 2.2531 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG346:HH22 | :Gentisic Acid:O1 |
| :Gentisic Acid:H17 - A:ASP317:OD2 | 2.0385 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP317:OD2 | :Gentisic Acid:H17 |
| :Gentisic Acid:H16 - A:ALA310:O | 1.8533 | Hydrogen Bond | Conventional Hydrogen Bond | A:ALA310:O | :Gentisic Acid:H16 |
| A:HIS305:HD2 - :Gentisic Acid:O4 | 2.8977 | Hydrogen Bond | Carbon Hydrogen Bond | A:HIS305:HD2 | :Gentisic Acid:O4 |
| A:ASP317:OD2 - :Gentisic Acid | 3.8054 | Electrostatic | Pi-Anion | A:ASP317:OD2 | :Gentisic Acid |
| :Gentisic Acid - A:ALA310 | 5.4112 | Hydrophobic | Pi-Alkyl | A:ALA310 | :Gentisic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Amylase)** | **Binding site of ligand (2)** |
| A:GLN63:HE22 - :Catechin:O3 | 2.6581 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLN63:HE22 | :Catechin:O3 |
| A:HIS299:HE2 - :Catechin:O6 | 2.7107 | Hydrogen Bond | Conventional Hydrogen Bond | A:HIS299:HE2 | :Catechin:O6 |
| :Catechin:H35 - A:GLU233:OE2 | 2.2179 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU233:OE2 | :Catechin:H35 |
| :Catechin:H34 - A:ASP197:OD1 | 2.3060 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP197:OD1 | :Catechin:H34 |
| :Catechin:H34 - A:GLU233:OE1 | 2.4579 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU233:OE1 | :Catechin:H34 |
| :Catechin:H28 - A:TYR62:O | 2.6712 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR62:O | :Catechin:H28 |
| A:ASP197:OD2 - :Catechin | 4.9111 | Electrostatic | Pi-Anion | A:ASP197:OD2 | :Catechin |
| A:ASP300:OD2 - :Catechin | 4.5137 | Electrostatic | Pi-Anion | A:ASP300:OD2 | :Catechin |
| :Catechin:H33 - A:TRP59 | 3.2292 | Hydrogen Bond | Pi-Donor Hydrogen Bond | A:TRP59 | :Catechin:H33 |
| A:TRP59 - :Catechin | 4.2895 | Hydrophobic | Pi-Pi Stacked | A:TRP59 | :Catechin |
| A:TRP59 - :Catechin | 4.4697 | Hydrophobic | Pi-Pi Stacked | A:TRP59 | :Catechin |
| A:TYR62 - :Catechin | 4.4105 | Hydrophobic | Pi-Pi Stacked | A:TYR62 | :Catechin |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Amylase)** | **Binding site of ligand (3)** |
| :Rosmarinic Acid:H40 - A:GLU233:OE2 | 2.7439 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU233:OE2 | :Rosmarinic Acid:H40 |
| A:TYR62 - :Rosmarinic Acid | 4.3508 | Hydrophobic | Pi-Pi Stacked | A:TYR62 | :Rosmarinic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Collagenase)** | **Binding site of ligand (EGCG)** |
| A:TYR541:HH - EGCG:O7 | 3.0589 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR541:HH | EGCG:O7 |
| EGCG:H49 - A:HIS469:O | 2.0071 | Hydrogen Bond | Conventional Hydrogen Bond | A:HIS469:O | EGCG:H49 |
| EGCG:H42 - A:GLU466:OE2 | 2.3429 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU466:OE2 | EGCG:H42 |
| EGCG:H43 - A:TYR548:OH | 2.0578 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR548:OH | EGCG:H43 |
| A:ILE439:HA - EGCG:O5 | 2.5407 | Hydrogen Bond | Carbon Hydrogen Bond | A:ILE439:HA | EGCG:O5 |
| EGCG:H9 - A:TYR438:O | 2.7688 | Hydrogen Bond | Carbon Hydrogen Bond | A:TYR438:O | EGCG:H9 |
| A:GLU499:OE2 - EGCG | 4.0658 | Electrostatic | Pi-Anion | A:GLU499:OE2 | EGCG |
| A:PHE481 - EGCG | 4.1500 | Hydrophobic | Pi-Pi Stacked | A:PHE481 | EGCG |
| A:ILE437 - EGCG | 5.0859 | Hydrophobic | Alkyl | A:ILE437 | EGCG |
| A:HIS469 - EGCG | 5.3220 | Hydrophobic | Pi-Alkyl | A:HIS469 | EGCG |
| EGCG - A:ILE437 | 5.2568 | Hydrophobic | Pi-Alkyl | A:ILE437 | EGCG |
| EGCG - A:ILE439 | 5.3989 | Hydrophobic | Pi-Alkyl | A:ILE439 | EGCG |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Collagenase)** | **Binding site of ligand (1)** |
| :Gentisic Acid:H17 - A:GLU498:OE2 | 2.4557 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU498:OE2 | :Gentisic Acid:H17 |
| :Gentisic Acid:H16 - A:HIS469 | 2.7331 | Hydrogen Bond | Pi-Donor Hydrogen Bond | A:HIS469 | :Gentisic Acid:H16 |
| A:PHE481 - :Gentisic Acid | 3.7320 | Hydrophobic | Pi-Pi Stacked | A:PHE481 | :Gentisic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Collagenase)** | **Binding site of ligand (2)** |
| A:HIS469:HD1 - :Catechin:O5 | 2.7364 | Hydrogen Bond | Conventional Hydrogen Bond | A:HIS469:HD1 | :Catechin:O5 |
| :Catechin:H35 - A:GLU440:OE1 | 2.2822 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU440:OE1 | :Catechin:H35 |
| :Catechin:H34 - A:GLU498:OE2 | 1.8207 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU498:OE2 | :Catechin:H34 |
| :Catechin:H28 - A:TYR438:O | 2.3768 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR438:O | :Catechin:H28 |
| A:HIS469:HA - :Catechin:O5 | 3.0731 | Hydrogen Bond | Carbon Hydrogen Bond | A:HIS469:HA | :Catechin:O5 |
| A:HIS469:HD2 - :Catechin:O2 | 3.0087 | Hydrogen Bond | Carbon Hydrogen Bond | A:HIS469:HD2 | :Catechin:O2 |
| :Catechin:H7 - A:TYR438:O | 2.8008 | Hydrogen Bond | Carbon Hydrogen Bond | A:TYR438:O | :Catechin:H7 |
| A:GLU499:OE2 - :Catechin | 4.4306 | Electrostatic | Pi-Anion | A:GLU499:OE2 | :Catechin |
| A:PHE481 - :Catechin | 4.0748 | Hydrophobic | Pi-Pi Stacked | A:PHE481 | :Catechin |
| A:TYR541 - :Catechin | 5.1322 | Hydrophobic | Pi-Pi Stacked | A:TYR541 | :Catechin |
| A:TYR438 - :Catechin | 5.2840 | Hydrophobic | Pi-Pi T-shaped | A:TYR438 | :Catechin |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Collagenase)** | **Binding site of ligand (3)** |
| A:GLY441:HN - :Rosmarinic Acid:O8 | 2.2426 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLY441:HN | :Rosmarinic Acid:O8 |
| A:HIS469:HD1 - :Rosmarinic Acid:O3 | 2.9141 | Hydrogen Bond | Conventional Hydrogen Bond | A:HIS469:HD1 | :Rosmarinic Acid:O3 |
| :Rosmarinic Acid:H39 - A:HIS469:O | 2.1494 | Hydrogen Bond | Conventional Hydrogen Bond | A:HIS469:O | :Rosmarinic Acid:H39 |
| :Rosmarinic Acid:H38 - A:GLU466:OE1 | 2.8761 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU466:OE1 | :Rosmarinic Acid:H38 |
| A:GLY441:HA2 - :Rosmarinic Acid:O8 | 2.8884 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLY441:HA2 | :Rosmarinic Acid:O8 |
| :Rosmarinic Acid:H6 - A:TYR438:O | 2.6992 | Hydrogen Bond | Carbon Hydrogen Bond | A:TYR438:O | :Rosmarinic Acid:H6 |
| A:PHE481 - :Rosmarinic Acid | 5.4648 | Hydrophobic | Pi-Pi Stacked | A:PHE481 | :Rosmarinic Acid |
| A:PHE481 - :Rosmarinic Acid | 4.1594 | Hydrophobic | Pi-Pi Stacked | A:PHE481 | :Rosmarinic Acid |
| :Rosmarinic Acid - A:ILE439 | 4.0717 | Hydrophobic | Pi-Alkyl | A:ILE439 | :Rosmarinic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Glycosidase)** | **Binding site of ligand (ACR)** |
| A:ARG212:HH12 - :ACR:O16 | 2.7103 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG212:HH12 | :ACR:O16 |
| A:ARG212:HH22 - :ACR:O16 | 2.1753 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG212:HH22 | :ACR:O16 |
| A:ASN241:HD22 - :ACR:O10 | 2.1833 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASN241:HD22 | :ACR:O10 |
| A:ARG439:HH11 - :ACR:O3 | 1.8509 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG439:HH11 | :ACR:O3 |
| A:ARG439:HH11 - :ACR:O15 | 2.2442 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG439:HH11 | :ACR:O15 |
| A:ARG439:HH12 - :ACR:O4 | 2.3330 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG439:HH12 | :ACR:O4 |
| :ACR:H77 - A:ASN241:OD1 | 2.0611 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASN241:OD1 | :ACR:H77 |
| :ACR:H80 - A:ASN241:OD1 | 2.2174 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASN241:OD1 | :ACR:H80 |
| :ACR:H82 - A:SER156:O | 2.2023 | Hydrogen Bond | Conventional Hydrogen Bond | A:SER156:O | :ACR:H82 |
| :ACR:H87 - A:SER156:O | 1.9009 | Hydrogen Bond | Conventional Hydrogen Bond | A:SER156:O | :ACR:H87 |
| :ACR:H70 - A:GLU304:OE2 | 1.9899 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU304:OE2 | :ACR:H70 |
| :ACR:H72 - A:GLU304:OE2 | 1.7773 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU304:OE2 | :ACR:H72 |
| :ACR:H73 - A:GLU276:OE2 | 2.1563 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU276:OE2 | :ACR:H73 |
| :ACR:H81 - A:ASP68:OD2 | 2.4232 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP68:OD2 | :ACR:H81 |
| :ACR:H85 - A:HIS348:NE2 | 2.3192 | Hydrogen Bond | Conventional Hydrogen Bond | A:HIS348:NE2 | :ACR:H85 |
| :ACR:H85 - A:ASP349:OD2 | 1.9445 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP349:OD2 | :ACR:H85 |
| :ACR:H86 - A:ASP214:OD2 | 2.0583 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP214:OD2 | :ACR:H86 |
| :ACR:H38 - A:ASP68:OD2 | 2.3359 | Hydrogen Bond | Carbon Hydrogen Bond | A:ASP68:OD2 | :ACR:H38 |
| :ACR:H40 - A:ASP214:OD1 | 1.8479 | Hydrogen Bond | Carbon Hydrogen Bond | A:ASP214:OD1 | :ACR:H40 |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Glycosidase)** | **Binding site of ligand (1)** |
| A:LYS155:HZ1 - :Gentisic Acid:O3 | 2.1530 | Hydrogen Bond | Conventional Hydrogen Bond | A:LYS155:HZ1 | :Gentisic Acid:O3 |
| A:LYS155:HZ2 - :Gentisic Acid:O3 | 2.5642 | Hydrogen Bond | Conventional Hydrogen Bond | A:LYS155:HZ2 | :Gentisic Acid:O3 |
| :Gentisic Acid:H15 - A:ASP232:OD2 | 2.7899 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP232:OD2 | :Gentisic Acid:H15 |
| :Gentisic Acid:H15 - A:THR234:OG1 | 1.8628 | Hydrogen Bond | Conventional Hydrogen Bond | A:THR234:OG1 | :Gentisic Acid:H15 |
| A:SER235:HB1 - :Gentisic Acid:O1 | 2.6077 | Hydrogen Bond | Carbon Hydrogen Bond | A:SER235:HB1 | :Gentisic Acid:O1 |
| A:PHE420 - :Gentisic Acid | 4.7573 | Hydrophobic | Pi-Pi T-shaped | A:PHE420 | :Gentisic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Glycosidase)** | **Binding site of ligand (2)** |
| A:TYR313:HH - :Catechin:O5 | 2.3872 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR313:HH | :Catechin:O5 |
| :Catechin:H34 - A:ASP408:OD1 | 2.1379 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP408:OD1 | :Catechin:H34 |
| :Catechin:H32 - A:GLU276:OE2 | 1.8596 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU276:OE2 | :Catechin:H32 |
| A:ASP349:OD1 - :Catechin | 4.4981 | Electrostatic | Pi-Anion | A:ASP349:OD1 | :Catechin |
| A:ASP408:OD2 - :Catechin | 4.2540 | Electrostatic | Pi-Anion | A:ASP408:OD2 | :Catechin |
| A:TYR71 - :Catechin | 5.4021 | Hydrophobic | Pi-Pi T-shaped | A:TYR71 | :Catechin |
| :Catechin - A:ARG312 | 5.4861 | Hydrophobic | Pi-Alkyl | A:ARG312 | :Catechin |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Glycosidase)** | **Binding site of ligand (3)** |
| A:ARG312:HE - :Rosmarinic Acid:O3 | 3.0329 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG312:HE | :Rosmarinic Acid:O3 |
| A:ARG439:HH12 - :Rosmarinic Acid:O5 | 2.4087 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG439:HH12 | :Rosmarinic Acid:O5 |
| :Rosmarinic Acid:H39 - A:ASP349:O | 2.6714 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP349:O | :Rosmarinic Acid:H39 |
| :Rosmarinic Acid:H38 - A:GLU276:OE2 | 2.4335 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLU276:OE2 | :Rosmarinic Acid:H38 |
| :Rosmarinic Acid:H38 - A:ASP349:OD2 | 2.6335 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP349:OD2 | :Rosmarinic Acid:H38 |
| A:ARG312:HD2 - :Rosmarinic Acid:O4 | 2.7021 | Hydrogen Bond | Carbon Hydrogen Bond | A:ARG312:HD2 | :Rosmarinic Acid:O4 |
| A:ARG439:NE - :Rosmarinic Acid | 4.1978 | Electrostatic | Pi-Cation | A:ARG439:NE | :Rosmarinic Acid |
| A:ARG439:HD2 - :Rosmarinic Acid | 2.3625 | Hydrophobic | Pi-Sigma | A:ARG439:HD2 | :Rosmarinic Acid |
| :Rosmarinic Acid - A:ARG312 | 4.9812 | Hydrophobic | Pi-Alkyl | A:ARG312 | :Rosmarinic Acid |
| :Rosmarinic Acid - A:ARG439 | 4.9918 | Hydrophobic | Pi-Alkyl | A:ARG439 | :Rosmarinic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Lipase)** | **Binding site of ligand (Orlistat)** |
| :Orlistat:N6 - A:ASP80:OD2 | 3.85309 | Electrostatic | Attractive Charge | A:ASP80:OD2 | :Orlistat:N6 |
| A:GLY77:HN - :Orlistat:O5 | 2.94844 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLY77:HN | :Orlistat:O5 |
| A:LEU154:HN - :Orlistat:O3 | 2.83933 | Hydrogen Bond | Conventional Hydrogen Bond | A:LEU154:HN | :Orlistat:O3 |
| :Orlistat:H54 - A:PHE78:O | 2.74148 | Hydrogen Bond | Conventional Hydrogen Bond | A:PHE78:O | :Orlistat:H54 |
| A:SER153:HB2 - :Orlistat:O3 | 2.69259 | Hydrogen Bond | Carbon Hydrogen Bond | A:SER153:HB2 | :Orlistat:O3 |
| A:ALA261 - :Orlistat:C32 | 4.06684 | Hydrophobic | Alkyl | A:ALA261 | :Orlistat:C32 |
| :Orlistat:C32 - A:ARG257 | 3.98395 | Hydrophobic | Alkyl | A:ARG257 | :Orlistat:C32 |
| :Orlistat:C32 - A:LEU265 | 3.58645 | Hydrophobic | Alkyl | A:LEU265 | :Orlistat:C32 |
| A:TYR115 - :Orlistat:C29 | 5.09789 | Hydrophobic | Pi-Alkyl | A:TYR115 | :Orlistat:C29 |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Lipase)** | **Binding site of ligand (1)** |
| A:GLY77:HN - :Gentisic Acid:O4 | 2.7376 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLY77:HN | :Gentisic Acid:O4 |
| A:HIS152:HD1 - :Gentisic Acid:O4 | 2.44546 | Hydrogen Bond | Conventional Hydrogen Bond | A:HIS152:HD1 | :Gentisic Acid:O4 |
| A:ARG257:HH12 - :Gentisic Acid:O2 | 2.86751 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG257:HH12 | :Gentisic Acid:O2 |
| A:ARG257:HH22 - :Gentisic Acid:O2 | 3.08009 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG257:HH22 | :Gentisic Acid:O2 |
| A:GLY77:HA2 - :Gentisic Acid:O3 | 2.89881 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLY77:HA2 | :Gentisic Acid:O3 |
| :Gentisic Acid - A:ALA261 | 4.53022 | Hydrophobic | Pi-Alkyl | A:ALA261 | :Gentisic Acid |
| :Gentisic Acid - A:LEU265 | 4.64892 | Hydrophobic | Pi-Alkyl | A:LEU265 | :Gentisic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Lipase)** | **Binding site of ligand (2)** |
| :Catechin:H32 - A:ASP80:OD1 | 3.06314 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP80:OD1 | :Catechin:H32 |
| :Catechin:H33 - A:ASP80:OD2 | 2.73389 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP80:OD2 | :Catechin:H33 |
| A:PRO181:HD1 - :Catechin:O5 | 2.3976 | Hydrogen Bond | Carbon Hydrogen Bond | A:PRO181:HD1 | :Catechin:O5 |
| A:HIS264:NE2 - :Catechin | 4.69536 | Electrostatic | Pi-Cation | A:HIS264:NE2 | :Catechin |
| A:TYR115 - :Catechin | 4.71204 | Hydrophobic | Pi-Pi Stacked | A:TYR115 | :Catechin |
| A:PHE216 - :Catechin | 4.11746 | Hydrophobic | Pi-Pi Stacked | A:PHE216 | :Catechin |
| A:HIS264 - :Catechin | 5.20624 | Hydrophobic | Pi-Pi Stacked | A:HIS264 | :Catechin |
| A:PHE78 - :Catechin | 5.45095 | Hydrophobic | Pi-Pi T-shaped | A:PHE78 | :Catechin |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Lipase)** | **Binding site of ligand (3)** |
| :Rosmarinic Acid:H38 - A:ASP80:OD1 | 1.97423 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP80:OD1 | :Rosmarinic Acid:H38 |
| A:HIS152:HE1 - :Rosmarinic Acid:O6 | 2.9702 | Hydrogen Bond | Carbon Hydrogen Bond | A:HIS152:HE1 | :Rosmarinic Acid:O6 |
| A:TYR115 - :Rosmarinic Acid | 4.16195 | Hydrophobic | Pi-Pi Stacked | A:TYR115 | :Rosmarinic Acid |
| A:PHE216 - :Rosmarinic Acid | 4.34645 | Hydrophobic | Pi-Pi Stacked | A:PHE216 | :Rosmarinic Acid |
| A:PHE216 - :Rosmarinic Acid | 5.31419 | Hydrophobic | Pi-Pi T-shaped | A:PHE216 | :Rosmarinic Acid |
| :Rosmarinic Acid - A:PRO181 | 5.32627 | Hydrophobic | Pi-Alkyl | A:PRO181 | :Rosmarinic Acid |
| :Rosmarinic Acid - A:ILE79 | 5.26216 | Hydrophobic | Pi-Alkyl | A:ILE79 | :Rosmarinic Acid |
| :Rosmarinic Acid - A:VAL260 | 4.98114 | Hydrophobic | Pi-Alkyl | A:VAL260 | :Rosmarinic Acid |
| :Rosmarinic Acid - A:ALA261 | 4.92185 | Hydrophobic | Pi-Alkyl | A:ALA261 | :Rosmarinic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Tyrosinase)** | **Binding site of ligand (Kojic acid)** |
| A:THR345:HG1 - :Kojic acid:O3 | 2.70184 | Hydrogen Bond | Conventional Hydrogen Bond | A:THR345:HG1 | :Kojic acid:O3 |
| A:PHE355 - :Kojic acid | 4.06124 | Hydrophobic | Pi-Pi Stacked | A:PHE355 | :Kojic acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Tyrosinase)** | **Binding site of ligand (1)** |
| :Gentisic Acid:H17 - A:SER351:OG | 2.77465 | Hydrogen Bond | Conventional Hydrogen Bond | A:SER351:OG | :Gentisic Acid:H17 |
| A:PHE355 - :Gentisic Acid | 5.05423 | Hydrophobic | Pi-Pi T-shaped | A:PHE355 | :Gentisic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Tyrosinase)** | **Binding site of ligand (2)** |
| :Catechin:H28 - A:SER291:O | 3.0209 | Hydrogen Bond | Conventional Hydrogen Bond | A:SER291:O | :Catechin:H28 |
| :Catechin:H33 - A:THR343:OG1 | 2.11777 | Hydrogen Bond | Conventional Hydrogen Bond | A:THR343:OG1 | :Catechin:H33 |
| A:ASP344:OD1 - :Catechin | 4.99098 | Electrostatic | Pi-Anion | A:ASP344:OD1 | :Catechin |
| A:PHE355 - :Catechin | 4.29653 | Hydrophobic | Pi-Pi Stacked | A:PHE355 | :Catechin |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Tyrosinase)** | **Binding site of ligand (3)** |
| :Rosmarinic Acid:H41 - A:TYR297:O | 2.80301 | Hydrogen Bond | Conventional Hydrogen Bond | A:TYR297:O | :Rosmarinic Acid:H41 |
| :Rosmarinic Acid:H41 - A:VAL300:O | 2.38911 | Hydrogen Bond | Conventional Hydrogen Bond | A:VAL300:O | :Rosmarinic Acid:H41 |
| A:GLN294:HE21 - :Rosmarinic Acid | 3.20365 | Hydrogen Bond | Pi-Donor Hydrogen Bond | A:GLN294:HE21 | :Rosmarinic Acid |
| A:GLY299:HN - :Rosmarinic Acid | 2.89054 | Hydrogen Bond | Pi-Donor Hydrogen Bond | A:GLY299:HN | :Rosmarinic Acid |
| A:PHE355 - :Rosmarinic Acid | 4.05524 | Hydrophobic | Pi-Pi Stacked | A:PHE355 | :Rosmarinic Acid |
| A:TRP301 - :Rosmarinic Acid | 5.54003 | Hydrophobic | Pi-Pi T-shaped | A:TRP301 | :Rosmarinic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Urease)** | **Binding site of ligand (Thiourea)** |
| :Thiourea:H5 - A:ALA636:O | 2.72447 | Hydrogen Bond | Conventional Hydrogen Bond | A:ALA636:O | :Thiourea:H5 |
| :Thiourea:H6 - A:ASP633:OD1 | 2.43859 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP633:OD1 | :Thiourea:H6 |
| :Thiourea:H8 - A:HIS545:NE2 | 2.31351 | Hydrogen Bond | Conventional Hydrogen Bond | A:HIS545:NE2 | :Thiourea:H8 |
| :Thiourea:S1 - A:HIS492 | 4.91302 | Other | Pi-Sulfur | A:HIS492 | :Thiourea:S1 |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Urease)** | **Binding site of ligand (1)** |
| :Gentisic Acid:H17 - A:ALA440:O | 2.59569 | Hydrogen Bond | Conventional Hydrogen Bond | A:ALA440:O | :Gentisic Acid:H17 |
| :Gentisic Acid:H16 - A:ARG439:O | 2.61271 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG439:O | :Gentisic Acid:H16 |
| A:HIS492:HE1 - :Gentisic Acid:O1 | 2.45012 | Hydrogen Bond | Carbon Hydrogen Bond | A:HIS492:HE1 | :Gentisic Acid:O1 |
| A:ALA636:HA - :Gentisic Acid:O2 | 2.86271 | Hydrogen Bond | Carbon Hydrogen Bond | A:ALA636:HA | :Gentisic Acid:O2 |
| :Gentisic Acid - A:ALA440 | 4.2505 | Hydrophobic | Pi-Alkyl | A:ALA440 | :Gentisic Acid |
| :Gentisic Acid - A:ALA636 | 4.88588 | Hydrophobic | Pi-Alkyl | A:ALA636 | :Gentisic Acid |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Urease)** | **Binding site of ligand (2)** |
| A:ARG439:NE - :Catechin:O6 | 3.11145 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG439:NE | :Catechin:O6 |
| A:CYS592:SG - :Catechin:O2 | 3.44462 | Hydrogen Bond | Conventional Hydrogen Bond | A:CYS592:SG | :Catechin:O2 |
| :Catechin:H28 - A:ARG439:O | 2.81744 | Hydrogen Bond | Conventional Hydrogen Bond | A:ARG439:O | :Catechin:H28 |
| :Catechin:H32 - A:GLY550:O | 2.27725 | Hydrogen Bond | Conventional Hydrogen Bond | A:GLY550:O | :Catechin:H32 |
| :Catechin:H33 - A:ASP494:OD1 | 2.91358 | Hydrogen Bond | Conventional Hydrogen Bond | A:ASP494:OD1 | :Catechin:H33 |
| :Catechin:H6 - A:ARG439:O | 2.31951 | Hydrogen Bond | Carbon Hydrogen Bond | A:ARG439:O | :Catechin:H6 |
| A:ARG609:NH1 - :Catechin | 4.82368 | Electrostatic | Pi-Cation | A:ARG609:NH1 | :Catechin |
| A:CYS592:SG - :Catechin | 5.32607 | Other | Pi-Sulfur | A:CYS592:SG | :Catechin |
| :Catechin - A:ALA440 | 4.7488 | Hydrophobic | Pi-Alkyl | A:ALA440 | :Catechin |
| :Catechin - A:ARG439 | 4.67321 | Hydrophobic | Pi-Alkyl | A:ARG439 | :Catechin |
| :Catechin - A:ALA440 | 4.85292 | Hydrophobic | Pi-Alkyl | A:ALA440 | :Catechin |
| **Interactions** | **Distance Å** | **Bonding** | **Bonding Types** | **Binding site of target (Urease)** | **Binding site of ligand (3)** |
| :Rosmarinic Acid:H41 - A:PHE840:O | 1.99329 | Hydrogen Bond | Conventional Hydrogen Bond | A:PHE840:O | :Rosmarinic Acid:H41 |
| A:SER834:HB1 - :Rosmarinic Acid:O1 | 2.69934 | Hydrogen Bond | Carbon Hydrogen Bond | A:SER834:HB1 | :Rosmarinic Acid:O1 |
| A:SER834:HB2 - :Rosmarinic Acid:O1 | 2.92902 | Hydrogen Bond | Carbon Hydrogen Bond | A:SER834:HB2 | :Rosmarinic Acid:O1 |
| :Rosmarinic Acid:H6 - A:GLU642:OE1 | 2.36331 | Hydrogen Bond | Carbon Hydrogen Bond | A:GLU642:OE1 | :Rosmarinic Acid:H6 |
| A:PHE838 - :Rosmarinic Acid | 3.9611 | Hydrophobic | Pi-Pi Stacked | A:PHE838 | :Rosmarinic Acid |