**Table S1:** Interaction of selected phytomolecules with bacterial efflux pump of *Bacillus subtilis*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Test Compound** | **Amino acid Residue** | **Type of bond Interactions** | **ATOM** | **Bond Length** | **Ligand Pose** | **Dock Score** |
| **Berberine** | PRO144A | Hydrophobic | 19C | 4.334 | LP1 | -62.04 |
| ASN149A | Hydrophobic | 1C | 4.344 |
| TYR170A | Hydrophobic | 25C | 3.401 |
| GLY171A | Hydrophobic | 25C | 4.961 |
| PRO226A | Hydrophobic | 19C | 3.388 |
| TYR229A | Hydrophobic | 19C | 4.342 |
| ILE255A | Hydrophobic | 15C | 3.440 |
| PHE224A | Aromatic | 13C | 4.459 |
|  |  |  |  |  |  |  |
| **Gallic acid** | PHE224A | Aromatic | 1C | 3.931 | LP5 | -33.85 |
|  |  |  |  |  |  |  |
| **Piperine** | VAL147A | Hydrophobic | 20C | 7.948 | LP2 | -43.66 |
| TYR170A | Hydrophobic | 20C | 4.772 |
| GLY171A | Hydrophobic | 20C | 3.905 |
| ALA172A | Hydrophobic | 20C | 3.104 |
| ILE190A | Hydrophobic | 20C | 3.903 |
| PRO226A | Hydrophobic | 2C | 3.096 |
| GLU253A | Hydrophobic | 20C | 4.864 |
| ILE255A | Hydrophobic | 20C | 4.592 |
|  |  |  |  |  |  |  |
| **Rutin** | GLU145A | Hydrophobic | 1C | 4.395 | LP1 | -59.76 |
| TYR120A | Aromatic | 30C | 4.986 |
| TYR268A | Aromatic | 30C | 4.220 |
| TYR268A | Hydrogen bond | 38O | 1.686 |
|  |  |  |  |  |  |  |
| **Tetracycline** | VAL147A | Hydrophobic | 3C | 4.135 | LP1 | -77.78 |
| PRO226A | Hydrophobic | 31C | 3.918 |
| ILE255A | Hydrophobic | 1C | 4.763 |
| TYR152A | Aromatic | 16C | 5.214 |
| TYR170A | Aromatic | 16C | 5.245 |
| TYR152A | Hydrogen Bond | 44H | 2.178 |

**Table S2:** Interaction of selected phytomolecules with bacterial efflux pump of *Escherichia coli*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule Name** | **Amino acid Residue** | **Type of bond Interactions** | **Ligand Atom** | **Bond Length** | **Ligand Pose** | **Dock Score** |
| **Berberine** | MET380A | Hydrophobic | 19C | 3.618 | LP5 | -64.34 |
| ASP393A | Hydrophobic | 20C | 3.692 |
| ASP396A | Hydrophobic | 19C | 3.234 |
| ALA397A | Hydrophobic | 19C | 4.691 |
| THR400A | Hydrophobic | 22C | 3.127 |
| ASN178B | Hydrophobic | 22C | 4.551 |
| ALA181B | Hydrophobic | 22C | 2.717 |
| GLN182B | Hydrophobic | 22C | 4.383 |
| VAL392B | Hydrophobic | 25C | 4.665 |
| ASP393B | Hydrophobic | 1C | 3.880 |
| ASP396B | Hydrophobic | 1C | 3.586 |
| ASP393A | Charge | 7N | 3.724 |
|  |  |  |  |  |  |  |
| **Gallic acid** | ASP396A | Hydrogen Bond | 18H | 2.273 | LP4 | -32.10 |
| GLN182B | Hydrogen Bond | 16H | 2.221 |
|  |  |  |  |  |  |  |
| **Piperine** | ALA373A | Hydrophobic | 20C | 4.407 | LP2 | -57.52 |
| SER376A | Hydrophobic | 20C | 3.178 |
| ALA397A | Hydrophobic | 20C | 4.373 |
| THR400A | Hydrophobic | 20C | 3.628 |
| ALA181B | Hydrophobic | 20C | 3.278 |
| VAL392B | Hydrophobic | 5C | 3.540 |
| ASP393B | Hydrophobic | 1C | 3.526 |
| ASP396B | Hydrophobic | 6C | 2.802 |
|  |  |  |  |  |  |  |
| **Rutin** | TH4399A | Hydrophobic | 9C | 4.298 | LP4 | -59.82 |
| THR400A | Hydrophobic | 3C | 4.050 |
| ASN403A | Hydrophobic | 5C | 4.271 |
| GLN182B | Hydrophobic | 1C | 3.466 |
| THR185B | Hydrophobic | 3C | 4.118 |
| GLN182B | Hydrogen Bond | 28O | 2.330 |
|  |  |  |  |  |  |  |
| **Tetracycline** | ASP396A | Hydrophobic | 5C | 4.306 | LP1 | -57.16 |
| THR400A | Hydrophobic | 30C | 3.673 |
| ASN178B | Hydrophobic | 31C | 3.621 |
| ALA181B | Hydrophobic | 31C | 3.947 |
| GLN182B | Hydrophobic | 30C | 3.278 |
| THR185B | Hydrophobic | 1C | 4.882 |
| ASP396A | Hydrogen Bond | 47H | 2.519 |
| THR400A | Hydrogen Bond | 29N | 2.201 |
| ASN178B | Hydrogen Bond | 48H | 1.744 |

**Table S3:** Interaction of selected phytomolecules with efflux protein of *Pseudomonas aeruginosa*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule Name** | **Amino acid Residue** | **Type of bond Interactions** | **Ligand Atom** | **Bond Length** | **Ligand Pose** | **Dock Score** |
| **Berberine** | ALA271A | Hydrophobic | 22C | 3.103 | LP2 | -48.41 |
| ARG274A | Hydrophobic | 22C | 3.841 |
| ASP281A | Hydrophobic | 1C | 4.992 |
| ASP343A | Hydrophobic | 1C | 4.305 |
| SER350A | Hydrophobic | 22C | 3.903 |
| TYR351A | Hydrophobic | 22C | 4.671 |
|  |  |  |  |  |  |  |
| **Gallic acid** | ARG274A | Hydrogen Bond | 18H | 2.427 | LP1 | -27.22 |
|  |  |  |  |  |  |  |
| **Piperine** | ALA271A | Hydrophobic | 20C | 3.373 | LP2 | -52.96 |
| ARG274A | Hydrophobic | 20C | 4.383 |
| ASP343A | Hydrophobic | 3C | 4.725 |
| SER350A | Hydrophobic | 20C | 4.322 |
| GLN354A | Hydrophobic | 20C | 4.107 |
|  |  |  |  |  |  |  |
| **Rutin** | LEU134A | Hydrophobic | 1C | 3.376 | LP3 | -61.54 |
| ARG274A | Hydrophobic | 1C | 3.733 |
|  |  |  |  |  |  |  |
| **Tetracycline** | LEU134A | Hydrophobic | 1C | 3.491 | LP4 | -47.03 |
| ALA271A | Hydrophobic | 30C | 4.752 |
| ARG274A | Hydrophobic | 30C | 2.327 |
| ALA277A | Hydrophobic | 1C | 3.862 |
| SER278A | Hydrophobic | 1C | 4.469 |
| ALA347A | Hydrophobic | 6C | 3.974 |
| SER350A | Hydrophobic | 31C | 2.817 |
| SER350A | Hydrogen Bond | 48H | 1.921 |

**Table S4:** Interaction of selected phytomolecules with efflux protein of *Staphylococcus aureus*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule Name** | **Amino acid Residue** | **Type of bond Interactions** | **Ligand Atom** | **Bond Length** | **Ligand Pose** | **Dock Score** |
| **Berberine** | SER13A | Hydrophobic | 22C | 4.212 | LP1 | -55.77 |
| MET16A | Hydrophobic | 22C | 4.060 |
| ALA20A | Hydrophobic | 19C | 4.274 |
| GLY38A | Hydrophobic | 25C | 3.814 |
| TYR39A | Hydrophobic | 1C | 4.548 |
| PHE108A | Hydrophobic | 20C | 4.109 |
| SER6B | Hydrophobic | 22C | 4.353 |
| PHE9B | Hydrophobic | 22C | 4.085 |
| ARG10B | Hydrophobic | 22C | 3.636 |
| HIS35A | Aromatic | 3C | 4.657 |
|  |  |  |  |  |  |  |
| **Gallic acid** | HIS35A | Aromatic | 1C | 4.222 | LP4 | -22.59 |
| ARG10B | Charge | 11O | 4.305 |
| ARG10B | Hydrogen Bond | 11O | 2.425 |
|  |  |  |  |  |  |  |
| **Piperine** | SER13A | Hydrophobic | 2C | 3.155 | LP4 | -47.82 |
| MET16A | Hydrophobic | 6C | 3.292 |
| GLY38A | Hydrophobic | 20C | 3.666 |
| VAL101A | Hydrophobic | 20C | 4.486 |
| SER6B | Hydrophobic | 5C | 4.010 |
| PHE9B | Hydrophobic | 1C | 3.753 |
| ARG10B | Hydrophobic | 3C | 2.877 |
| PHE108A | Aromatic | 13C | 5.118 |
|  |  |  |  |  |  |  |
| **Rutin** | PHE108A | Hydrophobic | 5C | 3.552 | LP2 | -66.74 |
| SER6B | Hydrophobic | 5C | 4.606 |
| ARG10B | Hydrophobic | 13C | 4.207 |
| HIS35A | Aromatic | 30C | 4.422 |
| ARG10B | Hydrogen Bond | 27O | 2.102 |
|  |  |  |  |  |  |  |
| **Tetracycline** | PHE108A | Hydrophobic | 31C | 3.537 | LP5 | -56.22 |
| SER6B | Hydrophobic | 11C | 4.892 |
| HIS35A | Aromatic | 16C | 4.087 |
| ARG10B | Hydrogen Bond | 32O | 2.548 |

**Table S5:** Interaction of selected phytomolecules with bacterial biofilm of *Bacillus subtilis*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule Name** | **Amino acid Residue** | **Type of bond Interactions** | **Ligand Atom** | **Bond Length** | **Ligand Pose** | **Dock Score** |
| **Berberine** | ARG118A | Hydrophobic | 1C | 4.476 | LP3 | -61.86 |
| PRO122A | Hydrophobic | 25C | 3.420 |
| PRO123A | Hydrophobic | 25C | 2.732 |
| PHE120C | Hydrophobic | 19C | 3.957 |
| PRO123D | Hydrophobic | 1C | 3.868 |
| PHE120C | Aromatic | 13C | 5.178 |
| **Gallic acid** | No Interaction | | | | LP1 | -33.61 |
|  |  |  |  |  |  |  |
| **Piperine** | THR119A | Hydrophobic | 3C | 2.615 | LP2 | -55.37 |
| PHE120A | Hydrophobic | 3C | 3.973 |
| THR119B | Hydrophobic | 20C | 4.876 |
| PRO122C | Hydrophobic | 20C | 4.259 |
| PRO123C | Hydrophobic | 20C | 3.213 |
| PRO123D | Hydrophobic | 2C | 4.029 |
| PHE120A | Hydrogen Bond | 4N | 1.878 |
|  |  |  |  |  |  |  |
| **Rutin** | PHE120B | Hydrophobic | 11C | 4.001 | LP5 | -77.14 |
| LEU121B | Hydrophobic | 5C | 3.955 |
| PRO122B | Hydrophobic | 5C | 3.418 |
| PRO123B | Hydrophobic | 4C | 4.499 |

**Table S6:** Interaction of selected phytomolecules with bacterial biofilm of *Escherichia coli*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule Name** | **Amino acid Residue** | **Type of bond Interactions** | **Ligand Atom** | **Bond Length** | **Ligand Pose** | **Dock Score** |
| **Berberine** | ARG36A | Hydrophobic | 20C | 4.710 | LP4 | -40.96 |
| GLN125A | Hydrophobic | 19C | 4.980 |
| ILE128A | Hydrophobic | 19C | 3.843 |
| PRO129A | Hydrophobic | 19C | 3.039 |
| ILE119B | Hydrophobic | 25C | 4.859 |
| MET121B | Hydrophobic | 25C | 4.242 |
| ILE128B | Hydrophobic | 19C | 4.365 |
| FLC201A | Hydrophobic | 25C | 3.763 |
| PHE84A | Aromatic | 13C | 4.728 |
| ARG36A | Hydrogen Bond | 7N | 1.729 |
| GLN125A | Hydrogen Bond | 7N | 2.429 |
|  |  |  |  |  |  |  |
| **Gallic acid** | PHE84A | Aromatic | 1C | 4.912 | LP3 | -23.93 |
| ARG36A | Hydrogen Bond | 9O | 2.138 |
|  |  |  |  |  |  |  |
| **Piperine** | TYR118A | Hydrophobic | 20C | 4.472 | LP2 | -40.52 |
| HIS120A | Hydrophobic | 20C | 4.443 |
| ILE119B | Hydrophobic | 6C | 4.287 |
| MET121B | Hydrophobic | 5C | 3.351 |
| FLC201A | Hydrophobic | 3C | 4.069 |
| PHE84A | Aromatic | 13C | 5.246 |
| TYR118A | Hydrogen Bond | 13C | 5.367 |
| GLN81A | Hydrogen Bond | 8O | 2.534 |
|  |  |  |  |  |  |  |
| **Rutin** | GLY79A | Hydrophobic | 11C | 4.151 | LP3 | 49.03 |
| ILE80A | Hydrophobic | 12C | 2.336 |
| GLN125A | Hydrophobic | 13C | 4.166 |
| ILE119B | Hydrophobic | 1C | 4.316 |
| MET121B | Hydrophobic | 14C | 3.911 |
| FLC201A | Hydrophobic | 6C | 3.368 |
| PHE84A | Aromatic | 30C | 5.402 |
| ARG36A | Hydrogen Bond | 19O | 1.807 |
| GLU116A | Hydrogen Bond | 62H | 2.103 |

**Table S7:** Interaction of selected phytomolecules with bacterial biofilm of *Pseudomonas aeruginosa*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule Name** | **Amino acid Residue** | **Type of bond Interactions** | **Ligand Atom** | **Bond Length** | **Ligand Pose** | **Dock Score** |
| **Berberine** | SERB | Hydrophobic | 22C | 4.441 | LP3 | -80.04 |
| ARGB | Hydrophobic | 19C | 4.938 |
| PHEB | Hydrophobic | 19C | 3.922 |
| GLY91B | Hydrophobic | 25C | 3.389 |
| GLN92B | Hydrophobic | 1C | 4.147 |
| ALA93B | Hydrophobic | 1C | 4.466 |
|  |  |  |  |  |  |  |
| **Gallic acid** | ARGB | Hydrogen Bond | 8O | 2.576 | LP3 | -40.17 |
|  |  |  |  |  |  |  |
| **Piperine** | ARGB | Hydrophobic | 5C | 4.849 | LP1 | -67.52 |
| PHEB | Hydrophobic | 20C | 4.271 |
| VAL67B | Hydrophobic | 2C | 4.172 |
| GLY91B | Hydrophobic | 3C | 4.071 |
| GLN92B | Hydrophobic | 5C | 3.738 |
| ALA93B | Hydrophobic | 1C | 4.745 |
| ARGB | Hydrogen Bond | 4N | 2.458 |
|  |  |  |  |  |  |  |
| **Rutin** | ARGB | Hydrophobic | 14C | 4.138 | LP4 | -81.50 |
| ALA64B | Hydrophobic | 11C | 4.824 |
| ALA88B | Hydrophobic | 5C | 4.813 |
| TRP89B | Hydrophobic | 11C | 4.569 |
| GLY91B | Hydrophobic | 12C | 3.324 |
| GLN92B | Hydrogen Bond | 19O | 2.293 |

**Table S8:** Interaction of selected phytomolecules with bacterial biofilm of *Staphylococcus aureus*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule Name** | **Amino acid Residue** | **Type of bond Interactions** | **Ligand Atom** | **Bond Length** | **Ligand Pose** | **Dock Score** |
| **Berberine** | LYS568A | Hydrophobic | 25C | 3.484 | LP4 | -61.86 |
| PRO571A | Hydrophobic | 19C | 4.553 |
| ASN658A | Hydrophobic | 22C | 3.450 |
| ASP663A | Hydrophobic | 22C | 3.077 |
| VAL665A | Hydrophobic | 22C | 4.261 |
| LYS653B | Hydrophobic | 20C | 4.367 |
| VAL669B | Hydrophobic | 19C | 4.817 |
| PHE569A | Aromatic | 13C | 4.528 |
|  |  |  |  |  |  |  |
| **Gallic acid** | ARG567A | Hydrogen Bond | 16H | 2.037 | LP3 | -33.61 |
|  | ASN658A | Hydrogen Bond | 11O | 1.733 |
|  |  |  |  |  |  |  |
| **Piperine** | LYS568A | Hydrophobic | 20C | 4.760 | LP2 | -55.37 |
| ASN658A | Hydrophobic | 2C | 3.494 |
| ASP663A | Hydrophobic | 2C | 3.047 |
| VAL665A | Hydrophobic | 1C | 3.109 |
| ARG666B | Hydrophobic | 6C | 3.928 |
| VAL669B | Hydrophobic | 5C | 3.939 |
|  |  |  |  |  |  |  |
| **Rutin** | LYS568A | Hydrophobic | 14C | 4.476 | LP3 | -77.14 |
| VAL650B | Hydrophobic | 9C | 3.931 |
| PRO651B | Hydrophobic | 5C | 3.709 |
| GLY652B | Hydrophobic | 3C | 4.589 |
| LYS653B | Hydrophobic | 1C | 3.054 |
| VAL669B | Hydrophobic | 2C | 4.909 |
| PHE569A | Aromatic | 20C | 5.414 |
| GLY652B | Hydrogen Bond | 73H | 1.340 |