Table S1. The six physicochemical descriptors used to filter potential bioactive ingredients.

|  |  |  |
| --- | --- | --- |
| Property | Index name | Range for active compounds |
| lipophilicity | XLOGP3 | [-0.7, 5] |
| size | MW | [150, 500] |
| polarity | TPSA | [20, 130] |
| solubility | log S | ≤6 |
| saturation | fraction of Csp3 | ≥0.25 |
| flexibility | rotatable bonds | ≤9 |

The useful active compounds were filtrated by SwissADME web tool, according lipophilicity, size, polarity, solubility, flexibility and saturation.

Table S2. 12 key targets of TMGTY acting on AD.

|  |  |  |  |
| --- | --- | --- | --- |
| **NODE** | **Degree** | **Betweenness** | **Closeness** |
| EGFR | 114 | 22332.19 | 0.172029 |
| ESR1 | 98 | 17755.73 | 0.169604 |
| PTGS2 | 86 | 8567.221 | 0.167829 |
| NOS3 | 77 | 5376.635 | 0.166522 |
| GSK3β | 71 | 3818.449 | 0.165591 |
| BACE1 | 53 | 1550.05 | 0.163413 |
| MPO | 53 | 2428.807 | 0.162037 |
| IGF1R | 47 | 1272.595 | 0.163274 |
| NOS2 | 44 | 1974.361 | 0.161697 |
| F2 | 42 | 2388.462 | 0.161155 |
| ABCB1 | 37 | 3696.756 | 0.162928 |
| PLAU | 33 | 1328.186 | 0.161833 |

A total of 12 genes had a DC > 26 (twice median value) in network.

Table S3. KEGG enrichment analysis for 12 key targets.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ID | Description | pvalue | symbol name | Count |
| hsa05215 | Prostate cancer | 8.82E-06 | EGFR/GSK3B/PLAU/IGF1R | 4 |
| hsa04066 | HIF-1 signaling pathway | 1.40E-05 | EGFR/NOS3/IGF1R/NOS2 | 4 |
| hsa05224 | Breast cancer | 4.57E-05 | ESR1/EGFR/GSK3B/IGF1R | 4 |
| hsa05205 | Proteoglycans in cancer | 0.000167 | ESR1/EGFR/PLAU/IGF1R | 4 |
| hsa05206 | MicroRNAs in cancer | 0.000811 | PTGS2/EGFR/PLAU/ABCB1 | 4 |
| hsa04151 | PI3K-Akt signaling pathway | 0.001333 | EGFR/NOS3/GSK3B/IGF1R | 4 |
| hsa05010 | Alzheimer disease | 0.001804 | PTGS2/BACE1/GSK3B/NOS2 | 4 |
| hsa01521 | EGFR tyrosine kinase inhibitor resistance | 0.000183 | EGFR/GSK3B/IGF1R | 3 |
| hsa01522 | Endocrine resistance | 0.000347 | ESR1/EGFR/IGF1R | 3 |
| hsa04926 | Relaxin signaling pathway | 0.000777 | EGFR/NOS3/NOS2 | 3 |
| hsa04915 | Estrogen signaling pathway | 0.000946 | ESR1/EGFR/NOS3 | 3 |
| hsa05226 | Gastric cancer | 0.001182 | EGFR/GSK3B/ABCB1 | 3 |
| hsa04921 | Oxytocin signaling pathway | 0.0013 | PTGS2/EGFR/NOS3 | 3 |
| hsa05225 | Hepatocellular carcinoma | 0.001671 | EGFR/GSK3B/IGF1R | 3 |
| hsa05202 | Transcriptional misregulation in cancer | 0.002487 | MPO/PLAU/IGF1R | 3 |
| hsa04510 | Focal adhesion | 0.002792 | EGFR/GSK3B/IGF1R | 3 |
| hsa05163 | Human cytomegalovirus infection | 0.003844 | PTGS2/EGFR/GSK3B | 3 |
| hsa04020 | Calcium signaling pathway | 0.004611 | EGFR/NOS3/NOS2 | 3 |
| hsa05165 | Human papillomavirus infection | 0.011243 | PTGS2/EGFR/GSK3B | 3 |

Table S4. GO enrichment analysis for 33 key targets.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ONTOLOGY | ID | Description | pvalue | geneID | Count |
| BP | GO:0048511 | rhythmic process | 6.88E-07 | ESR1/NOS3/GSK3B/IGF1R/NOS2 | 5 |
| BP | GO:0032355 | response to estradiol | 8.29E-07 | EGFR/ESR1/PTGS2/IGF1R | 4 |
| BP | GO:0098754 | detoxification | 1.83E-06 | PTGS2/NOS3/MPO/ABCB1 | 4 |
| BP | GO:1903034 | regulation of response to wounding | 2.75E-06 | NOS3/IGF1R/F2/PLAU | 4 |
| BP | GO:0009612 | response to mechanical stimulus | 5.87E-06 | PTGS2/BACE1/MPO/IGF1R | 4 |
| BP | GO:0072593 | reactive oxygen species metabolic process | 1.02E-05 | NOS3/MPO/NOS2/F2 | 4 |
| BP | GO:0009636 | response to toxic substance | 1.33E-05 | PTGS2/NOS3/MPO/ABCB1 | 4 |
| BP | GO:0019932 | second-messenger-mediated signaling | 2.96E-05 | EGFR/NOS3/GSK3B/NOS2 | 4 |
| BP | GO:0062197 | cellular response to chemical stress | 4.23E-05 | EGFR/PTGS2/NOS3/MPO | 4 |
| BP | GO:0032496 | response to lipopolysaccharide | 4.28E-05 | PTGS2/NOS3/MPO/NOS2 | 4 |
| BP | GO:0062012 | regulation of small molecule metabolic process | 4.75E-05 | PTGS2/NOS3/GSK3B/NOS2 | 4 |
| BP | GO:0002237 | response to molecule of bacterial origin | 5.43E-05 | PTGS2/NOS3/MPO/NOS2 | 4 |
| BP | GO:0032102 | negative regulation of response to external stimulus | 0.000114 | NOS3/BACE1/F2/PLAU | 4 |
| BP | GO:0006979 | response to oxidative stress | 0.000119 | EGFR/PTGS2/NOS3/MPO | 4 |
| BP | GO:0048608 | reproductive structure development | 0.000119 | EGFR/ESR1/PTGS2/NOS3 | 4 |
| BP | GO:0061458 | reproductive system development | 0.000122 | EGFR/ESR1/PTGS2/NOS3 | 4 |
| BP | GO:1903829 | positive regulation of protein localization | 0.000133 | EGFR/PTGS2/GSK3B/F2 | 4 |
| BP | GO:1901652 | response to peptide | 0.000193 | PTGS2/GSK3B/BACE1/IGF1R | 4 |
| BP | GO:0007263 | nitric oxide mediated signal transduction | 5.76E-07 | EGFR/NOS3/NOS2 | 3 |
| BP | GO:0071392 | cellular response to estradiol stimulus | 1.94E-06 | EGFR/ESR1/IGF1R | 3 |
| BP | GO:1904646 | cellular response to amyloid-beta | 2.78E-06 | GSK3B/BACE1/IGF1R | 3 |
| BP | GO:0030195 | negative regulation of blood coagulation | 3.38E-06 | NOS3/F2/PLAU | 3 |
| BP | GO:1900047 | negative regulation of hemostasis | 3.60E-06 | NOS3/F2/PLAU | 3 |
| BP | GO:0050819 | negative regulation of coagulation | 4.31E-06 | NOS3/F2/PLAU | 3 |
| BP | GO:1904645 | response to amyloid-beta | 5.12E-06 | GSK3B/BACE1/IGF1R | 3 |
| BP | GO:0030193 | regulation of blood coagulation | 8.89E-06 | NOS3/F2/PLAU | 3 |
| BP | GO:1900046 | regulation of hemostasis | 9.73E-06 | NOS3/F2/PLAU | 3 |
| BP | GO:0042698 | ovulation cycle | 1.06E-05 | ESR1/NOS3/IGF1R | 3 |
| BP | GO:0050818 | regulation of coagulation | 1.11E-05 | NOS3/F2/PLAU | 3 |
| BP | GO:0006801 | superoxide metabolic process | 1.16E-05 | NOS3/MPO/NOS2 | 3 |
| BP | GO:0006809 | nitric oxide biosynthetic process | 1.31E-05 | PTGS2/NOS3/NOS2 | 3 |
| BP | GO:0061045 | negative regulation of wound healing | 1.36E-05 | NOS3/F2/PLAU | 3 |
| BP | GO:0046209 | nitric oxide metabolic process | 1.65E-05 | PTGS2/NOS3/NOS2 | 3 |
| BP | GO:2001057 | reactive nitrogen species metabolic process | 1.71E-05 | PTGS2/NOS3/NOS2 | 3 |
| BP | GO:1903035 | negative regulation of response to wounding | 2.42E-05 | NOS3/F2/PLAU | 3 |
| BP | GO:0098869 | cellular oxidant detoxification | 3.10E-05 | PTGS2/NOS3/MPO | 3 |
| BP | GO:0009408 | response to heat | 4.02E-05 | PTGS2/NOS3/GSK3B | 3 |
| BP | GO:0014066 | regulation of phosphatidylinositol 3-kinase signaling | 4.24E-05 | EGFR/IGF1R/F2 | 3 |
| BP | GO:1990748 | cellular detoxification | 4.71E-05 | PTGS2/NOS3/MPO | 3 |
| BP | GO:0097237 | cellular response to toxic substance | 5.76E-05 | PTGS2/NOS3/MPO | 3 |
| BP | GO:1900180 | regulation of protein localization to nucleus | 7.11E-05 | PTGS2/GSK3B/F2 | 3 |
| BP | GO:0061041 | regulation of wound healing | 7.27E-05 | NOS3/F2/PLAU | 3 |
| BP | GO:0014065 | phosphatidylinositol 3-kinase signaling | 9.20E-05 | EGFR/IGF1R/F2 | 3 |
| BP | GO:0062013 | positive regulation of small molecule metabolic process | 9.59E-05 | PTGS2/NOS3/NOS2 | 3 |
| BP | GO:0034614 | cellular response to reactive oxygen species | 9.79E-05 | EGFR/NOS3/MPO | 3 |
| BP | GO:0045834 | positive regulation of lipid metabolic process | 0.00011 | PTGS2/IGF1R/F2 | 3 |
| BP | GO:0021543 | pallium development | 0.000148 | EGFR/GSK3B/IGF1R | 3 |
| BP | GO:0048660 | regulation of smooth muscle cell proliferation | 0.000151 | PTGS2/NOS3/IGF1R | 3 |
| BP | GO:0048659 | smooth muscle cell proliferation | 0.000159 | PTGS2/NOS3/IGF1R | 3 |
| BP | GO:0048015 | phosphatidylinositol-mediated signaling | 0.00017 | EGFR/IGF1R/F2 | 3 |
| BP | GO:0009266 | response to temperature stimulus | 0.000178 | PTGS2/NOS3/GSK3B | 3 |
| BP | GO:0048017 | inositol lipid-mediated signaling | 0.000181 | EGFR/IGF1R/F2 | 3 |
| BP | GO:0008217 | regulation of blood pressure | 0.000187 | PTGS2/NOS3/NOS2 | 3 |
| BP | GO:0071248 | cellular response to metal ion | 0.000212 | EGFR/PTGS2/BACE1 | 3 |
| BP | GO:0000302 | response to reactive oxygen species | 0.000254 | EGFR/NOS3/MPO | 3 |
| BP | GO:0007596 | blood coagulation | 0.000326 | NOS3/F2/PLAU | 3 |
| BP | GO:0071241 | cellular response to inorganic substance | 0.000326 | EGFR/PTGS2/BACE1 | 3 |
| BP | GO:0046777 | protein autophosphorylation | 0.000339 | EGFR/GSK3B/IGF1R | 3 |
| BP | GO:0050817 | coagulation | 0.000348 | NOS3/F2/PLAU | 3 |
| BP | GO:0007599 | hemostasis | 0.000353 | NOS3/F2/PLAU | 3 |
| BP | GO:2001234 | negative regulation of apoptotic signaling pathway | 0.000366 | PTGS2/NOS3/GSK3B | 3 |
| BP | GO:0033002 | muscle cell proliferation | 0.000381 | PTGS2/NOS3/IGF1R | 3 |
| BP | GO:0021537 | telencephalon development | 0.000452 | EGFR/GSK3B/IGF1R | 3 |
| BP | GO:0051924 | regulation of calcium ion transport | 0.000473 | PTGS2/NOS3/F2 | 3 |
| BP | GO:0071216 | cellular response to biotic stimulus | 0.000501 | NOS3/GSK3B/NOS2 | 3 |
| BP | GO:0003018 | vascular process in circulatory system | 0.000542 | PTGS2/NOS3/ABCB1 | 3 |
| BP | GO:0034599 | cellular response to oxidative stress | 0.000678 | EGFR/NOS3/MPO | 3 |
| BP | GO:0001666 | response to hypoxia | 0.000692 | PTGS2/NOS2/PLAU | 3 |
| BP | GO:0034504 | protein localization to nucleus | 0.00075 | PTGS2/GSK3B/F2 | 3 |
| BP | GO:0036293 | response to decreased oxygen levels | 0.000788 | PTGS2/NOS2/PLAU | 3 |
| BP | GO:0018105 | peptidyl-serine phosphorylation | 0.000916 | EGFR/PTGS2/GSK3B | 3 |
| BP | GO:0070482 | response to oxygen levels | 0.000994 | PTGS2/NOS2/PLAU | 3 |
| BP | GO:0048545 | response to steroid hormone | 0.001048 | ESR1/PTGS2/IGF1R | 3 |
| BP | GO:0018209 | peptidyl-serine modification | 0.001123 | EGFR/PTGS2/GSK3B | 3 |
| BP | GO:0019216 | regulation of lipid metabolic process | 0.001133 | PTGS2/IGF1R/F2 | 3 |
| BP | GO:0010038 | response to metal ion | 0.001252 | EGFR/PTGS2/BACE1 | 3 |
| BP | GO:1901653 | cellular response to peptide | 0.001358 | GSK3B/BACE1/IGF1R | 3 |
| BP | GO:0042742 | defense response to bacterium | 0.001391 | MPO/NOS2/F2 | 3 |
| BP | GO:2001233 | regulation of apoptotic signaling pathway | 0.001458 | PTGS2/NOS3/GSK3B | 3 |
| BP | GO:0051346 | negative regulation of hydrolase activity | 0.001469 | PTGS2/NOS3/GSK3B | 3 |
| BP | GO:0030900 | forebrain development | 0.001527 | EGFR/GSK3B/IGF1R | 3 |
| BP | GO:0050878 | regulation of body fluid levels | 0.001598 | NOS3/F2/PLAU | 3 |
| BP | GO:0042176 | regulation of protein catabolic process | 0.001758 | EGFR/GSK3B/NOS2 | 3 |
| BP | GO:0010959 | regulation of metal ion transport | 0.001862 | PTGS2/NOS3/F2 | 3 |
| BP | GO:0043434 | response to peptide hormone | 0.001876 | PTGS2/GSK3B/IGF1R | 3 |
| BP | GO:0009410 | response to xenobiotic stimulus | 0.00197 | PTGS2/NOS2/ABCB1 | 3 |
| BP | GO:0001558 | regulation of cell growth | 0.002025 | EGFR/GSK3B/F2 | 3 |
| BP | GO:0001503 | ossification | 0.002096 | EGFR/PTGS2/GSK3B | 3 |
| BP | GO:0006816 | calcium ion transport | 0.002153 | PTGS2/NOS3/F2 | 3 |
| BP | GO:0042060 | wound healing | 0.002227 | NOS3/F2/PLAU | 3 |
| BP | GO:0050804 | modulation of chemical synaptic transmission | 0.002227 | PTGS2/GSK3B/BACE1 | 3 |
| BP | GO:0099177 | regulation of trans-synaptic signaling | 0.002241 | PTGS2/GSK3B/BACE1 | 3 |
| BP | GO:0009314 | response to radiation | 0.002362 | EGFR/PTGS2/BACE1 | 3 |
| BP | GO:0032103 | positive regulation of response to external stimulus | 0.002424 | PTGS2/IGF1R/F2 | 3 |
| BP | GO:0031667 | response to nutrient levels | 0.002487 | PTGS2/MPO/IGF1R | 3 |
| BP | GO:0023061 | signal release | 0.002567 | GSK3B/BACE1/NOS2 | 3 |
| BP | GO:0033674 | positive regulation of kinase activity | 0.002992 | EGFR/IGF1R/F2 | 3 |
| BP | GO:0009991 | response to extracellular stimulus | 0.003046 | PTGS2/MPO/IGF1R | 3 |
| BP | GO:0016049 | cell growth | 0.003137 | EGFR/GSK3B/F2 | 3 |
| BP | GO:0090066 | regulation of anatomical structure size | 0.003192 | PTGS2/NOS3/GSK3B | 3 |
| BP | GO:0051223 | regulation of protein transport | 0.003343 | PTGS2/GSK3B/NOS2 | 3 |
| BP | GO:0010817 | regulation of hormone levels | 0.003362 | ESR1/IGF1R/NOS2 | 3 |
| CC | GO:0045121 | membrane raft | 8.90E-07 | EGFR/PTGS2/NOS3/BACE1/IGF1R | 5 |
| CC | GO:0098857 | membrane microdomain | 9.03E-07 | EGFR/PTGS2/NOS3/BACE1/IGF1R | 5 |
| CC | GO:0005901 | caveola | 1.51E-05 | PTGS2/NOS3/IGF1R | 3 |
| CC | GO:0044853 | plasma membrane raft | 3.96E-05 | PTGS2/NOS3/IGF1R | 3 |
| CC | GO:0005788 | endoplasmic reticulum lumen | 0.000783 | PTGS2/BACE1/F2 | 3 |
| CC | GO:0031983 | vesicle lumen | 0.000906 | EGFR/BACE1/MPO | 3 |
| CC | GO:0030139 | endocytic vesicle | 0.001032 | EGFR/NOS3/MPO | 3 |
| MF | GO:0020037 | heme binding | 1.47E-06 | PTGS2/NOS3/MPO/NOS2 | 4 |
| MF | GO:0046906 | tetrapyrrole binding | 1.94E-06 | PTGS2/NOS3/MPO/NOS2 | 4 |
| MF | GO:0016705 | oxidoreductase activity, acting on paired donors, with incorporation or reduction of molecular oxygen | 0.00018 | PTGS2/NOS3/NOS2 | 3 |
| MF | GO:0031625 | ubiquitin protein ligase binding | 0.000829 | EGFR/GSK3B/ABCB1 | 3 |
| MF | GO:0044389 | ubiquitin-like protein ligase binding | 0.000991 | EGFR/GSK3B/ABCB1 | 3 |
| MF | GO:0004175 | endopeptidase activity | 0.002411 | BACE1/F2/PLAU | 3 |
| MF | GO:0004712 | protein serine/threonine/tyrosine kinase activity | 0.00264 | EGFR/GSK3B/IGF1R | 3 |

Table S5. The docking results and binding sites of the 12 predicted targets and the active compounds at the optimal location (LibDock score >110)

|  |  |  |  |
| --- | --- | --- | --- |
| Target | Drug Information | Main Interaction Residues | Interactions |
| NOS3 | Squalene | VAL418,ILE188,ALA423,GLY186,TRP178,SER354,LEU193,PHE473,ALA181,ALA177,ALA472,PRO182,PHE468 | van der Waals, Alkyl, Pi-Sigma, Pi-Alkyl |
| NOS3 | Baicalein | SER354,ALA227,LEU193,PHE353,TRP178,CYS184,ALA181 | van der Waals, Pi-Pi Stacked, Conventional Hydrogen Bond, Pi-Alkyl |
| NOS3 | Quercetin | LEU193,PHE353,TRP178,CYS184,ALA181,ARG183 | van der Waals, Pi-Pi Stacked, Unfavorable Donor-Donor, Pi-Alkyl |
| NOS3 | Kaempferol | ALA181,CYS184,TRP178,PHE353,ILE228,LEU193 | van der Waals, Pi-Pi Stacked, Pi-Alkyl |
| EGFR | Squalene | LYS822,PRO717,LEU768,LYS704,LEU694,MET769,ALA719,LEU820, LEU764,LYS721,MET742 | van der Waals, Alkyl |
| IGF1R | Squalene | LEU1005,LEU1081,VAL1013,MET1079,VAL1053,LEU1065,MET1054,ALA1051,PHE1047,PHE1010,LYS1033 | van der Waals, Pi-Alkyl, Alkyl |
| GSK3β | Squalene | LEU329,HIS337,ALA336,PRO346,HIS381,PRO380 | van der Waals, Pi-Alkyl, Alkyl |
| GSK3β | Baicalein | SER368,GLU366,SER174,PRO331,HIS173,ALA170 | van der Waals, Pi-Alkyl, Unfavorable Acceptor-Acceptor, Conventional Hydrogen Bond, Pi-Pi T-shaped, Carbon Hydrogen Bond |
| BACE1 | Squalene | ILE118,LEU30,VAL69,ARG128,ILE126 | van der Walls, Alkyl |
| PTGS2 | Squalene | HIS214,VAL291,LEU390,HIS388,VAL295,LEU391,HIS386,PHE210,HIS207 | van der Waals, Alkyl, Pi-Sigma, Pi-Alkyl |
| PTGS2 | Quercetin | TRP387,HIS388,LEU390,ALA202,HIS386,HIS207,THR206 | van der Waals, Pi-Pi Stacked, Conventional Hydrogen Bond, Pi-Pi T-shaped, Pi-Sigma, Pi-Alkyl |
| PTGS2 | Kaempferol | HIS207,HIS386,HIS388,LEU390,TRP387,ALA199,THR206 | van der Waals, Pi-Pi T-shaped, Conventional Hydrogen Bond, Pi-Alkyl, Pi-Pi Stacked |
| PTGS2 | Baicalein | ASN382,THR206,HIS386,HIS207,LEU390,LEU391,HIS388,ALA199 | van der Waals, Pi-Pi Stacked, Conventional Hydrogen Bond, Pi-Pi T-shaped, Pi-Alkyl |
| PTGS2 | Wogonin | HIS388,ALA202,TRP387,HIS207,HIS386,LEU390 | van der Waals, Pi-Pi Stacked, Pi-Donor Hydrogen Bond, Pi-Pi T-shaped, Pi-Alkyl |
| NOS2 | Squalene | ILE201,MET374,CYS200,TYR489,PHE369,TRP194,ALA197,PHE488,PRO198,ARG199,LEU125 | van der Waals, Alkyl, Pi-Alkyl |
| NOS2 | Quercetin | THR190,TRP194,PHE369,TYR489,CYS200,ALA197,ARG199 | van der Waals, Pi-Pi Stacked, Conventional Hydrogen Bond, Pi-Pi T-shaped, Pi-Alkyl |
| NOS2 | Kaempferol | LEU209,ALA197,TRP194,CYS200 | van der Waals, Amide-Pi Stacked, Pi-Sulfur, Pi-Alkyl, Pi-Pi Stacked |
| NOS2 | Baicalein | PHE369,TRP194,CYS200,ALA197,MET355,ARG199,TYP489 | van der Waals, Pi-Pi Stacked, Carbon Hydrogen Bond, Pi-Pi T-shaped, Pi-Signa, Pi-Alkyl, Pi-Sulfur |
| NOS2 | Wogonin | ALA197,CYS200,TYR489,PHE369,TRP194,SER242 | van der Waals, Pi-Pi Stacked, Conventional Hydrogen Bond, Pi-Pi T-shaped, Pi-Alkyl, Pi-Sulfur |
| ESR1 | Squalene | ALA350,ILE424,LEU428,MET388,LEU346,PHE404,LEU391,LEU387,LEU525,LEU354,TRP383 | van der Waals, Alkyl, Pi-Alkyl |
| PLAU | Squalene | LEU73,TYR151,HIS57,VAL213,CYS220 | van der Waals, Alkyl, Pi-Alkyl |
| PLAU | Baicalein | GLN192,CYS191,TRP215CYS220,GLY219,SER190,GLY226 | van der Waals, Pi-Alkyl, Pi-Signa, Conventional Hydrogen Bond, Amide-Pi Stacked, Carbon Hydrogen Bond, Unfavorable Donor-Don |
| PLAU | Kaempferol | HIS57,GLN192,CYS191,TRP215,CYS220,GLY219 | van der Waals, Pi-Sigma, Attractive Charge, Amide-Pi Stacked, Conventional Hydrogen Bond, Pi-Alkyl, Carbon Hydrogen Bond |
| PLAU | Wogonin | CYS191,TRP215,CYS220,GLY219 | van der Waals, Pi-Sulfur, Conventional Hydrogen Bond, Amide-Pi Stacked, Carbon Hydrogen Bond, Pi-Alkyl, Unfavorable Acceptor-Acceptor |
| PLAU | Quercetin | HIS57,SER195,CYS191,SER190,ASP189,CYS220,TRP215 | van der Walls, Pi-Donor Hydrogen Bond, Conventional Hydrogen Bond, Carbon Hydrogen Bond, Pi-Pi T-shaped, Amide-Pi Stacked, Unfavorable Donor-Donor, Pi-Alkyl, Pi-Cation |
| ABCB1 | Squalene | PHE994,VAL991,TRP232,ALA302,PHE343,ALA229,LEU65,ILE340,ILE306,LEU225,MET876,LEU236 | van der Walls, Pi-Alkyl, Alkyl |
| F2 | Squalene | ILE174,TRP215,LEU99,CYS220,TYR228,VAL213,ALA190 | van der Walls, Pi-Alkyl, Alkyl |
| F2 | Quercetin | GLU192,TRP215,PHE227,GLY226,ALA190,ASP189,SER214,VAL213,CYS191,CYS220 | van der Walls, Unfavorable Acceptor-Acceptor, Conventional Hydrogen Bond, Pi-Sulfur, Carbon Hydrogen Bond, Amide-Pi Stacked, Unfavorable Negative-Negative, Pi-Alkyl |
| F2 | Baicalein | VAL213,GLU192,CYS220,CYS191,ALA190,TRP215,TYR228,GLY226 | van der Walls, Unfavorable Negative-Negative, Conventional Hydrogen Bond, Amide-Pi Stacked, Carbon Hydrogen Bond, Pi-Alkyl |
| MPO | Squalene | HIS336,MET87,MET243,ILE339,TYR334,PHE332,PHE99,LEU417,LEU420,ARG424,PHE146 | van der Walls, Pi-Alkyl, Alkyl |
| MPO | Quercetin | ILE339,MET243,MET87,LEU338,TYR296 | van der Walls, Pi-Sulfur, Conventional Hydrogen Bond, Pi-Alkyl, Carbon Hydrogen Bond |
| MPO | Kaempferol | MET243,ILE339,PHE332,TYR296,LEU338,MET87 | van der Walls, Pi-Sulfur, Conventional Hydrogen Bond, Pi-Alkyl |
| MPO | Baicalein | GLU242,MET243,ILE339,TYR334,GLY335,MET87 | van der Walls, Pi-Sulfur, Pi-Anion, Pi-Pi T-shaped, Pi-Sigma, Pi-Alkyl |
| MPO | Wogonin | ASP94,GLY90,GLY335,MET87,ILE339,MET243,GLU242 | van der Walls, Pi-Sulfur, Conventional Hydrogen Bond, Amide-Pi Stacked, Carbon Hydrogen Bond, Pi-Alkyl, Pi-Anion |