**Tables**

**Table 1.** The selected 10 compounds from *Folium sennae*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Molecule ID** | **Molecule Name** | **Molecular Structure** | OB% 1 | DL 2 |
| MOL002259 | Physciondiglucoside |  | 41.65 | 0.63 |
| MOL002268 | rhein |  | 47.07 | 0.28 |
| MOL002276 | Sennoside E\_qt |  | 50.69 | 0.61 |
| MOL002288 | Emodin-1-O-beta-D-glucopyranoside |  | 44.81 | 0.80 |
| MOL002293 | Sennoside D\_qt |  | 61.06 | 0.61 |
| MOL002369 | Dihydroxydianthrone |  | 74.55 | 0.57 |
| MOL002372 | (6Z,10E,14E,18E)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene |  | 33.55 | 0.42 |
| MOL000359 | sitosterol |  | 36.91 | 0.75 |
| MOL000422 | kaempferol |  | 41.88 | 0.24 |
| MOL000449 | Stigmasterol |  | 43.83 | 0.76 |

1 oral bioavailability; 2 drug-likeness.

**Table 2.** VMH simulation of tryptophan metabolism in intestinal flora.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Bacteria** | **Reactions** | | **Score** | **Metabolites** | |
|  | Abbreviation | Description |  | Abbreviation | Description |
| *Streptococcus* | 5HLTDL | 5-Hydroxy-L-Tryptophan Decarboxy-Lyase | 4 | Trp-L  5htrp | L-Tryptophan  5-Hydroxy-L-tryptophan |
|  | LTDCL | L-Tryptophan Decarboxy-Lyase | 4 |
|  | 5HXKYNDCL | 5-Hydroxykynurenamine Decarboxy-Lyase | 1 |
|  | EX\_5htrp(e) | Exchange of 5-Hydroxy-L-Tryptophan | 1 |
|  | EX\_trp\_L(e) | Exchange of L-Tryptophan | 1 |
|  | ACACT1r | Acetyl Coenzyme A C-Acetyltransferase | 0 |
|  | TRPt2r | L-tryptophan reversible transport via proton symport | 0 |
| *Sutterella* | FKYNH | N-Formyl-L-Kynurenine Amidohydrolase | 4 | Trp-L | L-Tryptophan |
|  | EX\_trp\_L(e) | Exchange of L-Tryptophan | 1 |
|  | TRPS1 | Tryptophan synthase (indoleglycerol phosphate) | 0 |
|  | TRPS2 | tryptophan synthase (indole) | 0 |
|  | TRPS3 | tryptophan synthase (indoleglycerol phosphate) | 0 |
|  | TRPt2r | L-tryptophan reversible transport via proton symport | 0 |
| *Dorea* | EX\_trp\_L(e) | Exchange of L-Tryptophan | 1 | Trp-L | L-Tryptophan |
|  | ANPRT | Anthranilate phosphoribosyltransferase | 0 |
|  | ANS | Anthranilate synthase | 0 |
|  | ANS2 | Anthranilate synthase 2 | 0 |
|  | IGPS | Indole-3-glycerol-phosphate synthase | 0 |
|  | PRAI | Phosphoribosylanthranilate isomerase | 0 |
|  | TRPS1 | Tryptophan synthase (indoleglycerol phosphate) | 0 |
|  | TRPS2 | tryptophan synthase (indole) | 0 |
|  | TRPS3 | tryptophan synthase (indoleglycerol phosphate) | 0 |
|  | TRPt2r | L-tryptophan reversible transport via proton symport | 0 |  |  |
|  | TRPTA | tryptophan transaminase | 0 |
| *Lactobacillus* | EX\_trp\_L(e) | Exchange of L-Tryptophan | 1 | Trp-L | L-Tryptophan |
|  | ACACT1r | Acetyl Coenzyme A C-Acetyltransferase | 0 |
|  | TRPt2r | L-tryptophan reversible transport via proton symport | 0 |
| *Mycoplasma* | EX\_trp\_L(e) | Exchange of L-Tryptophan | 1 | Trp-L | L-Tryptophan |
|  | TRPt2r | L-tryptophan reversible transport via proton symport | 0 |
| *Adlercreutzia* | EX\_trp\_L(e) | Exchange of L-Tryptophan | 1 | Trp-L | L-Tryptophan |
|  | TRPt2r | L-tryptophan reversible transport via proton symport | 0 |
| *Paraprevotella* | ANPRT | Anthranilate phosphoribosyltransferase | 0 | Trp-L | L-Tryptophan |
|  | ANS | Anthranilate synthase | 0 |
|  | ANS2 | Anthranilate synthase 2 | 0 |
|  | IGPS | Indole-3-glycerol-phosphate synthase | 0 |
|  | PRAI | Phosphoribosylanthranilate isomerase | 0 |
|  | TRPS1 | Tryptophan synthase (indoleglycerol phosphate) | 0 |
|  | TRPS2 | tryptophan synthase (indole) | 0 |
|  | TRPS3 | tryptophan synthase (indoleglycerol phosphate) | 0 |
|  | TRPTA | tryptophan transaminase | 0 |