Article

**Exploring the mechanism of XieBai San in treating liver injury based on network pharmacology and experimental verification**

**Supplementary materials**

**Table S1.** Thirty two compounds in Cortex Mori screened by “oral bioavailability” (OB) ≥ 30% and “drug likeness” (DL).

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Mol ID** | **Molecule Name** | **MW** | **AlogP** | **Hdon** | **Hacc** | **OB (%)** | **Caco-2** | **BBB** | **DL** | **FASA-** | **HL** |
| MOL012681 | Dimethyl(methylenedi-4,1-phenylene) biscarbamate | 314.37 | 3.33 | 2 | 6 | 50.84 | 0.62 | 0.08 | 0.26 | 0.3 | 0.78 |
| MOL012686 | 7-methoxy-5,4′-dihydroxyflavanonol | 302.3 | 2.16 | 3 | 6 | 51.72 | 0.11 | −0.57 | 0.26 | 0.34 | 16.16 |
| MOL012689 | cyclomulberrochromene | 418.47 | 4.58 | 2 | 6 | 36.79 | 0.86 | −0.19 | 0.87 | 0.32 | 15.19 |
| MOL012692 | kuwanon D | 422.51 | 4 | 3 | 6 | 31.09 | 0.43 | −0.2 | 0.8 | 0.33 | 24.51 |
| MOL012714 | Moracin A | 286.3 | 3.38 | 2 | 5 | 64.39 | 0.84 | −0.04 | 0.23 | 0.22 | 6.52 |
| MOL012717 | moracin M-6,3′-di-O-β-D-glucopyranoside | 566.56 | −0.67 | 9 | 14 | 37.81 | −2.26 | −3.85 | 0.74 | 0 | 12.26 |
| MOL012719 | moracin O | 326.37 | 3.54 | 3 | 5 | 62.33 | 0.52 | −0.34 | 0.44 | 0.3 | 6.8 |
| MOL012726 | mulberrofuran G | 562.6 | 6.95 | 5 | 8 | 92.19 | 0.35 | −0.75 | 0.24 | 0.34 | 9.34 |
| MOL012735 | mulberroside C\_qt | 326.37 | 3.54 | 3 | 5 | 71.39 | 0.41 | −0.75 | 0.46 | 0.29 | 3.69 |
| MOL012743 | resveratrol-3,4′-di-O-β-D-glucopyranoside | 552.58 | −0.79 | 9 | 13 | 35.08 | −2.28 | −3.86 | 0.76 | 0.34 | 3.38 |
| MOL012749 | sanggenone B | 570.63 | 5.75 | 5 | 9 | 115.44 | −0.07 | −1.07 | 0.3 | 0.35 | 28.97 |
| MOL012753 | sanggenone F | 354.38 | 3.09 | 3 | 6 | 62.42 | 0.48 | −0.18 | 0.54 | 0.35 | 16.79 |
| MOL012755 | sanggenone H | 354.38 | 3.09 | 3 | 6 | 37.5 | 0.42 | −0.28 | 0.53 | 0.35 | 18.92 |
| MOL012760 | sanggenone M | 436.49 | 4.4 | 3 | 7 | 68.29 | −0.05 | −0.65 | 0.85 | 0.36 | 23.83 |
| MOL001474 | sanguinarine | 332.35 | 3.47 | 0 | 4 | 37.81 | 1.26 | 0.15 | 0.86 | 0.3 | 7.84 |
| MOL000211 | Mairin | 456.78 | 6.52 | 2 | 3 | 55.38 | 0.73 | 0.22 | 0.78 | 0.26 | 8.87 |
| MOL000358 | beta-sitosterol | 414.79 | 8.08 | 1 | 1 | 36.91 | 1.32 | 0.99 | 0.75 | 0.23 | 5.36 |
| MOL003758 | Iristectorigenin (9CI) | 330.31 | 2.03 | 3 | 7 | 71.55 | 0.55 | −0.16 | 0.34 | 0.23 | 16.32 |
| MOL003856 | Moracin B | 286.3 | 3.38 | 2 | 5 | 55.85 | 0.83 | −0.09 | 0.23 | 0.24 | 5.3 |
| MOL003857 | Moracin C | 310.37 | 5 | 3 | 4 | 82.13 | 0.87 | −0.07 | 0.29 | 0.31 | 9.13 |
| MOL003858 | Moracin D | 308.35 | 4.2 | 2 | 4 | 60.93 | 1.03 | 0.12 | 0.38 | 0.32 | 6.44 |
| MOL003860 | Moracin F | 286.3 | 3.38 | 2 | 5 | 53.81 | 0.81 | −0.02 | 0.23 | 0.26 | 4.84 |
| MOL004912 | Glabrone | 336.36 | 3.12 | 2 | 5 | 52.51 | 0.59 | −0.11 | 0.5 | 0 | 16.09 |
| MOL000098 | quercetin | 302.25 | 1.5 | 5 | 7 | 46.43 | 0.05 | −0.77 | 0.28 | 0.38 | 14.4 |
| MOL001004 | pelargonidin | 271.26 | 1.93 | 4 | 5 | 37.99 | 0.31 | −0.33 | 0.21 | 0.38 | 0.48 |
| MOL012800 | 3,5,7-trihydroxy-2-(3-hydroxyphenyl)chromone | 286.25 | 1.77 | 4 | 6 | 59.71 | 0.25 | −0.37 | 0.24 | 0.4 | 15.5 |
| MOL002514 | Sexangularetin | 316.28 | 1.76 | 4 | 7 | 62.86 | 0.31 | −0.5 | 0.3 | 0.32 | 15.19 |
| MOL000422 | kaempferol | 286.25 | 1.77 | 4 | 6 | 41.88 | 0.26 | −0.55 | 0.24 | 0 | 14.74 |
| MOL005043 | campest-5-en-3beta-ol | 400.76 | 7.63 | 1 | 1 | 37.58 | 1.32 | 0.94 | 0.71 | 0.23 | 4.43 |
| MOL000554 | gallic acid-3-O-(6′-O-galloyl)-glucoside | 484.4 | −0.03 | 9 | 14 | 30.25 | −1.96 | −2.76 | 0.67 | 0.36 |  |
| MOL009653 | Cycloeucalenol | 426.8 | 7.59 | 1 | 1 | 39.73 | 1.42 | 1.04 | 0.79 | 0.23 | 5.01 |
| MOL000098 | quercetin | 302.25 | 1.5 | 5 | 7 | 46.43 | 0.05 | −0.77 | 0.28 | 0.38 | 14.4 |

**Table S2.** Thirteen compounds in Radix Paeoniae Alba screened by “oral bioavailability” (OB) ≥ 30% and “drug likeness” (DL).

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Mol ID** | **Molecule Name** | **MW** | **AlogP** | **Hdon** | **Hacc** | **OB (%)** | **Caco-2** | **BBB** | **DL** | **FASA-** | **HL** |
| MOL001689 | acacetin | 284.28 | 2.59 | 2 | 5 | 34.97 | 0.67 | −0.05 | 0.24 | 0.35 | 17.25 |
| MOL002219 | Atropine | 289.41 | 2 | 2 | 4 | 34.53 | 0.15 | −0.3 | 0.21 | 0.31 | 3.12 |
| MOL002224 | aurantiamide acetate | 444.57 | 4.53 | 2 | 6 | 58.38 | 0.41 | −0.22 | 0.59 | 0.37 | 7.04 |
| MOL000358 | beta-sitosterol | 414.79 | 8.08 | 1 | 1 | 36.91 | 1.32 | 0.99 | 0.75 | 0.23 | 5.36 |
| MOL000953 | CLR | 386.73 | 7.38 | 1 | 1 | 37.87 | 1.43 | 1.13 | 0.68 | 0.2 | 4.52 |
| MOL000296 | hederagenin | 414.79 | 8.08 | 1 | 1 | 36.91 | 1.32 | 0.96 | 0.75 | 0 | 5.35 |
| MOL002228 | Kulactone | 452.74 | 6.23 | 0 | 3 | 45.44 | 0.86 | 0.16 | 0.82 | 0.31 | 5.52 |
| MOL001790 | Linarin | 592.6 | −0.18 | 7 | 14 | 39.84 | −1.68 | −2.77 | 0.71 | 0.27 | 16.07 |
| MOL001645 | Linoleyl acetate | 308.56 | 6.85 | 0 | 2 | 42.1 | 1.36 | 1.08 | 0.2 | 0.21 | 7.48 |
| MOL001552 | OIN | 289.41 | 1.72 | 1 | 4 | 45.97 | 0.43 | 0.09 | 0.19 | 0.31 | 4.47 |
| MOL002218 | scopolin | 354.34 | −0.29 | 4 | 9 | 56.45 | −1.05 | −1.75 | 0.39 | 0.27 | 3.01 |
| MOL000449 | Stigmasterol | 412.77 | 7.64 | 1 | 1 | 43.83 | 1.44 | 1 | 0.76 | 0.22 | 5.57 |
| MOL002222 | sugiol | 300.48 | 4.99 | 1 | 2 | 36.11 | 1.14 | 0.7 | 0.28 | 0.27 | 14.62 |

**Table S3.** Ninety-two compounds in Glycyrrhiza uralens is screened by “oral bioavailability” (OB) ≥ 30% and “drug likeness” (DL).

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Mol ID** | **Molecule Name** | **MW** | **AlogP** | **Hdon** | **Hacc** | **OB (%)** | **Caco-2** | **BBB** | **DL** | **FASA-** | **HL** |
| MOL001484 | Inermine | 284.28 | 2.44 | 1 | 5 | 75.18 | 0.89 | 0.4 | 0.54 | 0.3 | 11.72 |
| MOL001792 | DFV | 256.27 | 2.57 | 2 | 4 | 32.76 | 0.51 | −0.29 | 0.18 | 0.42 | 17.89 |
| MOL000211 | Mairin | 456.78 | 6.52 | 2 | 3 | 55.38 | 0.73 | 0.22 | 0.78 | 0.26 | 8.87 |
| MOL002311 | Glycyrol | 366.39 | 4.85 | 2 | 6 | 90.78 | 0.71 | −0.2 | 0.67 | 0.28 | 9.85 |
| MOL000239 | Jaranol | 314.31 | 2.09 | 2 | 6 | 50.83 | 0.61 | −0.22 | 0.29 | 0.29 | 15.5 |
| MOL002565 | Medicarpin | 270.3 | 2.66 | 1 | 4 | 49.22 | 1 | 0.53 | 0.34 | 0.31 | 8.46 |
| MOL000354 | isorhamnetin | 316.28 | 1.76 | 4 | 7 | 49.6 | 0.31 | −0.54 | 0.31 | 0.32 | 14.34 |
| MOL000359 | sitosterol | 414.79 | 8.08 | 1 | 1 | 36.91 | 1.32 | 0.87 | 0.75 | 0.22 | 5.37 |
| MOL003656 | Lupiwighteone | 338.38 | 3.92 | 3 | 5 | 51.64 | 0.68 | −0.23 | 0.37 | 0.36 | 15.63 |
| MOL003896 | 7-Methoxy-2-methyl isoflavone | 266.31 | 3.36 | 0 | 3 | 42.56 | 1.16 | 0.56 | 0.2 | 0.33 | 16.89 |
| MOL000392 | formononetin | 268.28 | 2.58 | 1 | 4 | 69.67 | 0.78 | 0.02 | 0.21 | 0 | 17.04 |
| MOL000417 | Calycosin | 284.28 | 2.32 | 2 | 5 | 47.75 | 0.52 | −0.43 | 0.24 | 0 | 17.1 |
| MOL000422 | kaempferol | 286.25 | 1.77 | 4 | 6 | 41.88 | 0.26 | −0.55 | 0.24 | 0 | 14.74 |
| MOL004328 | naringenin | 272.27 | 2.3 | 3 | 5 | 59.29 | 0.28 | −0.37 | 0.21 | 0.4 | 16.98 |
| MOL004805 | (2S)-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]-8,8-dimethyl-2,3-dihydropyrano[2,3-f]chromen-4-one | 390.51 | 5.48 | 1 | 4 | 31.79 | 1 | 0.25 | 0.72 | 0.35 | 14.82 |
| MOL004806 | euchrenone | 406.56 | 6.35 | 1 | 4 | 30.29 | 1.09 | 0.39 | 0.57 | 0 | 15.89 |
| MOL004808 | glyasperin B | 370.43 | 4.02 | 3 | 6 | 65.22 | 0.47 | −0.09 | 0.44 | 0 | 16.1 |
| MOL004810 | glyasperin F | 354.38 | 2.97 | 3 | 6 | 75.84 | 0.43 | −0.15 | 0.54 | 0 | 15.64 |
| MOL004811 | Glyasperin C | 356.45 | 4.73 | 3 | 5 | 45.56 | 0.71 | 0.07 | 0.4 | 0 | 3.13 |
| MOL004814 | Isotrifoliol | 298.26 | 2.99 | 2 | 6 | 31.94 | 0.53 | −0.25 | 0.42 | 0 | 7.91 |
| MOL004815 | (E)-1-(2,4-dihydroxyphenyl)-3-(2,2-dimethylchromen-6-yl)prop-2-en-1-one | 322.38 | 3.96 | 2 | 4 | 39.62 | 0.66 | −0.12 | 0.35 | 0 | 16.16 |

**Table S3.** (*Continued*).

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Mol ID** | **Molecule Name** | **MW** | **AlogP** | **Hdon** | **Hacc** | **OB (%)** | **Caco-2** | **BBB** | **DL** | **FASA-** | **HL** |
| MOL004820 | kanzonols W | 336.36 | 3.63 | 2 | 5 | 50.48 | 0.63 | 0.04 | 0.52 | 0 | 0.15 |
| MOL004824 | (2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one | 384.41 | 2.96 | 3 | 7 | 60.25 | 0 | −0.76 | 0.63 | 0 | 4.31 |
| MOL004827 | Semilicoisoflavone B | 352.36 | 2.85 | 3 | 6 | 48.78 | 0.45 | −0.33 | 0.55 | 0 | 17.02 |
| MOL004828 | Glepidotin A | 338.38 | 3.9 | 3 | 5 | 44.72 | 0.79 | 0.06 | 0.35 | 0 | 16.09 |
| MOL004829 | Glepidotin B | 340.4 | 3.88 | 3 | 5 | 64.46 | 0.46 | −0.09 | 0.34 | 0 | 15.98 |
| MOL004833 | Phaseolinisoflavan | 324.4 | 3.95 | 2 | 4 | 32.01 | 1.01 | 0.46 | 0.45 | 0 | 2.66 |
| MOL004835 | Glypallichalcone | 284.33 | 3.4 | 1 | 4 | 61.6 | 0.76 | 0.23 | 0.19 | 0 | 17.01 |
| MOL004838 | 8-(6-hydroxy-2-benzofuranyl)-2,2-dimethyl-5-chromenol | 308.35 | 4.2 | 2 | 4 | 58.44 | 1 | 0.34 | 0.38 | 0.34 | 8.71 |
| MOL004841 | Licochalcone B | 286.3 | 2.88 | 3 | 5 | 76.76 | 0.47 | −0.46 | 0.19 | 0 | 17.02 |
| MOL004848 | licochalcone G | 354.43 | 4.35 | 3 | 5 | 49.25 | 0.64 | −0.04 | 0.32 | 0.35 | 15.75 |
| MOL004849 | 3-(2,4-dihydroxyphenyl)-8-(1,1-dimethylprop-2-enyl)-7-hydroxy-5-methoxy-coumarin | 368.41 | 4.03 | 3 | 6 | 59.62 | 0.4 | −0.23 | 0.43 | 0 | 0.69 |
| MOL004855 | Licoricone | 382.44 | 4.16 | 2 | 6 | 63.58 | 0.53 | −0.14 | 0.47 | 0 | 16.37 |
| MOL004856 | Gancaonin A | 352.41 | 4.17 | 2 | 5 | 51.08 | 0.8 | 0.13 | 0.4 | 0 | 16.82 |
| MOL004857 | Gancaonin B | 368.41 | 3.91 | 3 | 6 | 48.79 | 0.58 | −0.1 | 0.45 | 0 | 16.49 |
| MOL004860 | licorice glycoside E | 693.71 | 1.59 | 7 | 14 | 32.89 | −2.06 | −2.8 | 0.27 | 0.31 | 25.39 |
| MOL004863 | 3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-8-(3-methylbut-2-enyl)chromone | 354.38 | 3.65 | 4 | 6 | 66.37 | 0.52 | −0.13 | 0.41 | 0 | 15.81 |
| MOL004864 | 5,7-dihydroxy-3-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)chromone | 352.41 | 4.17 | 2 | 5 | 30.49 | 0.9 | 0.21 | 0.41 | 0 | 14.99 |
| MOL004866 | 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-(3-methylbut-2-enyl)chromone | 354.38 | 3.92 | 4 | 6 | 44.15 | 0.48 | −0.28 | 0.41 | 0 | 16.77 |
| MOL004879 | Glycyrin | 382.44 | 4.67 | 2 | 6 | 52.61 | 0.59 | −0.13 | 0.47 | 0 | 1.31 |
| MOL004882 | Licocoumarone | 340.4 | 4.98 | 3 | 5 | 33.21 | 0.84 | 0.06 | 0.36 | 0 | 9.66 |
| MOL004883 | Licoisoflavone | 354.38 | 3.65 | 4 | 6 | 41.61 | 0.37 | −0.27 | 0.42 | 0 | 16.09 |
| MOL004884 | Licoisoflavone B | 352.36 | 2.85 | 3 | 6 | 38.93 | 0.46 | −0.18 | 0.55 | 0 | 15.73 |
| MOL004885 | licoisoflavanone | 354.38 | 2.97 | 3 | 6 | 52.47 | 0.39 | −0.22 | 0.54 | 0 | 15.67 |
| MOL004891 | shinpterocarpin | 322.38 | 3.46 | 1 | 4 | 80.3 | 1.1 | 0.68 | 0.73 | 0.32 | 6.5 |
| MOL004898 | (E)-3-[3,4-dihydroxy-5-(3-methylbut-2-enyl)phenyl]-1-(2,4-dihydroxyphenyl)prop-2-en-1-one | 340.4 | 4.49 | 4 | 5 | 46.27 | 0.41 | −0.4 | 0.31 | 0.43 | 15.24 |
| MOL004903 | liquiritin | 418.43 | 0.66 | 5 | 9 | 65.69 | −1.06 | −1.93 | 0.74 | 0 | 17.96 |
| MOL004904 | licopyranocoumarin | 384.41 | 3.04 | 3 | 7 | 80.36 | 0.13 | −0.62 | 0.65 | 0 | 0.08 |
| MOL004905 | 3,22-Dihydroxy-11-oxo-delta(12)-oleanene-27-alpha-methoxycarbonyl-29-oic acid | 512.75 | 4.37 | 1 | 6 | 34.32 | −0.06 | −0.75 | 0.55 | 0 | 3.56 |
| MOL004907 | Glyzaglabrin | 298.26 | 2.1 | 2 | 6 | 61.07 | 0.34 | −0.2 | 0.35 | 0 | 21.2 |
| MOL004908 | Glabridin | 324.4 | 3.95 | 2 | 4 | 53.25 | 0.97 | 0.36 | 0.47 | 0 | 0.03 |
| MOL004910 | Glabranin | 324.4 | 4.42 | 2 | 4 | 52.9 | 0.97 | 0.31 | 0.31 | 0 | 16.24 |
| MOL004911 | Glabrene | 322.38 | 3.77 | 2 | 4 | 46.27 | 0.99 | 0.04 | 0.44 | 0 | 3.63 |
| MOL004912 | Glabrone | 336.36 | 3.12 | 2 | 5 | 52.51 | 0.59 | −0.11 | 0.5 | 0 | 16.09 |

**Table S3.** (*Continued*).

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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Mol ID** | **Molecule Name** | **MW** | **AlogP** | **Hdon** | **Hacc** | **OB (%)** | **Caco-2** | **BBB** | **DL** | **FASA-** | **HL** |
| MOL004913 | 1,3-dihydroxy-9-methoxy-6-benzofurano[3,2-c]chromenone | 298.26 | 2.99 | 2 | 6 | 48.14 | 0.48 | −0.19 | 0.43 | 0 | 8.87 |
| MOL004914 | 1,3-dihydroxy-8,9-dimethoxy-6-benzofurano[3,2-c]chromenone | 328.29 | 2.98 | 2 | 7 | 62.9 | 0.4 | −0.34 | 0.53 | 0 | 9.32 |
| MOL004915 | Eurycarpin A | 338.38 | 3.92 | 3 | 5 | 43.28 | 0.43 | −0.06 | 0.37 | 0 | 17.1 |
| MOL004917 | glycyroside | 562.57 | −0.73 | 6 | 13 | 37.25 | −1.58 | −2.56 | 0.79 | 0 | 14.62 |
| MOL004924 | (-)-Medicocarpin | 432.46 | 0.75 | 4 | 9 | 40.99 | −0.6 | −1.34 | 0.95 | 0 | 13.2 |
| MOL004935 | Sigmoidin-B | 356.4 | 3.89 | 4 | 6 | 34.88 | 0.42 | −0.41 | 0.41 | 0 | 14.49 |
| MOL004941 | (2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one | 256.27 | 2.57 | 2 | 4 | 71.12 | 0.41 | −0.25 | 0.18 | 0 | 18.09 |
| MOL004945 | (2S)-7-hydroxy-2-(4-hydroxyphenyl)-8-(3-methylbut-2-enyl)chroman-4-one | 324.4 | 4.42 | 2 | 4 | 36.57 | 0.72 | −0.04 | 0.32 | 0 | 17.95 |
| MOL004948 | Isoglycyrol | 366.39 | 4.36 | 1 | 6 | 44.7 | 0.91 | 0.05 | 0.84 | 0 | 6.69 |
| MOL004949 | Isolicoflavonol | 354.38 | 3.63 | 4 | 6 | 45.17 | 0.54 | −0.42 | 0.42 | 0 | 15.55 |
| MOL004957 | HMO | 268.28 | 2.58 | 1 | 4 | 38.37 | 0.79 | 0.25 | 0.21 | 0 | 16.56 |
| MOL004959 | 1-Methoxyphaseollidin | 354.43 | 4.25 | 2 | 5 | 69.98 | 1.01 | 0.48 | 0.64 | 0 | 9.53 |
| MOL004961 | Quercetin der. | 330.31 | 1.82 | 3 | 7 | 46.45 | 0.39 | −0.44 | 0.33 | 0 | 16.61 |
| MOL004966 | 3′-Hydroxy-4′-O-Methylglabridin | 354.43 | 3.93 | 2 | 5 | 43.71 | 1 | 0.73 | 0.57 | 0 | −0.61 |
| MOL000497 | licochalcone a | 338.43 | 4.62 | 2 | 4 | 40.79 | 0.82 | −0.21 | 0.29 | 0 | 16.2 |
| MOL004974 | 3′-Methoxyglabridin | 354.43 | 3.93 | 2 | 5 | 46.16 | 0.94 | 0.47 | 0.57 | 0 | 0.52 |
| MOL004978 | 2-[(3R)-8,8-dimethyl-3,4-dihydro-2H-pyrano[6,5-f]chromen-3-yl]-5-methoxyphenol | 338.43 | 4.2 | 1 | 4 | 36.21 | 1.12 | 0.61 | 0.52 | 0 | −0.13 |
| MOL004980 | Inflacoumarin A | 322.38 | 4.7 | 2 | 4 | 39.71 | 0.73 | −0.24 | 0.33 | 0 | 2.31 |
| MOL004985 | icos-5-enoic acid | 310.58 | 7.75 | 1 | 2 | 30.7 | 1.22 | 1.09 | 0.2 | 0 | 5.28 |
| MOL004988 | Kanzonol F | 420.54 | 5.3 | 1 | 5 | 32.47 | 1.18 | 0.56 | 0.89 | 0.28 | 9.98 |
| MOL004989 | 6-prenylated eriodictyol | 356.4 | 3.89 | 4 | 6 | 39.22 | 0.4 | −0.29 | 0.41 | 0 | 16.52 |
| MOL004990 | 7,2′,4′-trihydroxy—20135-methoxy-3—arylcoumarin | 300.28 | 2.56 | 3 | 6 | 83.71 | 0.24 | −0.59 | 0.27 | 0 | 0.99 |
| MOL004991 | 7-Acetoxy-2-methylisoflavone | 294.32 | 3.15 | 0 | 4 | 38.92 | 0.74 | 0.16 | 0.26 | 0 | 17.49 |
| MOL004993 | 8-prenylated eriodictyol | 356.4 | 3.89 | 4 | 6 | 53.79 | 0.43 | −0.44 | 0.4 | 0 | 15.7 |
| MOL004996 | gadelaidic acid | 310.58 | 7.75 | 1 | 2 | 30.7 | 1.2 | 0.94 | 0.2 | 0 | 5.25 |
| MOL000500 | Vestitol | 272.32 | 3.15 | 2 | 4 | 74.66 | 0.86 | 0.3 | 0.21 | 0 | 3 |
| MOL005000 | Gancaonin G | 352.41 | 4.17 | 2 | 5 | 60.44 | 0.78 | 0.23 | 0.39 | 0 | 16.13 |
| MOL005001 | Gancaonin H | 420.49 | 4.71 | 3 | 6 | 50.1 | 0.6 | −0.14 | 0.78 | 0 | 16.64 |
| MOL005003 | Licoagrocarpin | 338.43 | 4.51 | 1 | 4 | 58.81 | 1.23 | 0.61 | 0.58 | 0.27 | 9.45 |
| MOL005007 | Glyasperins M | 368.41 | 3.22 | 2 | 6 | 72.67 | 0.49 | −0.04 | 0.59 | 0 | 15.57 |
| MOL005008 | Glycyrrhiza flavonol A | 370.38 | 2.17 | 4 | 7 | 41.28 | −0.09 | −0.81 | 0.6 | 0 | 13.71 |
| MOL005012 | Licoagroisoflavone | 336.36 | 3.48 | 2 | 5 | 57.28 | 0.71 | 0.09 | 0.49 | 0 | 19.64 |
| MOL005013 | 18α-hydroxyglycyrrhetic acid | 486.76 | 4.55 | 3 | 5 | 41.16 | −0.29 | −0.78 | 0.71 | 0 | 4.96 |
| MOL005016 | Odoratin | 314.31 | 2.3 | 2 | 6 | 49.95 | 0.42 | −0.24 | 0.3 | 0 | 16.35 |
| MOL005017 | Phaseol | 336.36 | 4.87 | 2 | 5 | 78.77 | 0.76 | −0.06 | 0.58 | 0 | 9.64 |
| MOL005018 | Xambioona | 388.49 | 4.68 | 0 | 4 | 54.85 | 1.09 | 0.52 | 0.87 | 0 | 14.5 |

**Table S3.** (*Continued*).

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Mol ID** | **Molecule Name** | **MW** | **AlogP** | **Hdon** | **Hacc** | **OB (%)** | **Caco-2** | **BBB** | **DL** | **FASA-** | **HL** |
| MOL005020 | dehydroglyasperins C | 340.4 | 4.3 | 4 | 5 | 53.82 | 0.68 | −0.12 | 0.37 | 0 | 2.75 |
| MOL000098 | quercetin | 302.25 | 1.5 | 5 | 7 | 46.43 | 0.05 | −0.77 | 0.28 | 0.38 | 14.4 |