**Supplementary data**

**Network pharmacology-based study on the mechanism of Yiwei Decoction in chronic atrophic gastritis and experimental assessment**

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Supplementary 1. Screening of potential active chemicals of YWD

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NO. | Name | GI absorption | Lipinski | Ghose | Veber | Egan | Muegge |
| 1 | xanthotoxol triglucoside | Low | × | × | × | × | × |
| 2 | verbascotetrose | Low | × | × | × | × | × |
| 3 | dunnisinoside | Low | × | × | × | × | × |
| 4 | iactose | Low | × | × | × | × | × |
| 5 | trehalose | Low | × | × | × | × | × |
| 6 | nystose | Low | × | × | × | × | × |
| 7 | melittoside | Low | × | × | × | × | × |
| 8 | 6,7-dimethoxy-2-oxo-2*H*-chromen-8-yl *β*-*D*-glucopyranoside | Low | √ | × | × | × | √ |
| 9\* | catalpol | High | √ | × | × | × | √ |
| 10 | aucubin | Low | √ | × | × | × | × |
| 11 | leonuride | Low | √ | × | × | × | × |
| 12\* | diffractic acid | High | √ | √ | √ | √ | √ |
| 13 | geniposidic acid | Low | √ | × | × | × | × |
| 14 | mussaenosidic acid | Low | √ | × | × | × | × |
| 15 | 8-epiloganic acid | Low | √ | × | × | × | × |
| 16 | decaffeoylverbascoside | Low | √ | × | × | × | × |
| 17\* | 4-hydroxybenzoic acid | High | √ | × | √ | √ | × |
| 18 | glucosyl 6-hydroxy-2,6-dimethyl-2*E*,7-octadienoate | Low | √ | × | √ | × | √ |
| 19 | purpureaside | Low | × | × | × | × | × |
| 20 | echinacoside | Low | × | × | × | × | × |
| 21 | jionoside A1 | Low | × | × | × | × | × |
| 22 | isomaltulose | Low | × | × | × | × | × |
| 23\* | *N*-cis-*p*-coumaroyloctopamine | High | √ | √ | √ | √ | √ |
| 24 | acteoside | Low | × | × | × | × | × |
| 25\* | *N*-trans-*p*-coumaroyloctopamine | High | √ | √ | √ | √ | √ |
| 26 | isoacteoside | Low | × | × | × | × | × |
| 27 | 6-*O*-*E*-feruloylajugol | Low | × | × | × | × | × |
| 28 | martynoside | Low | × | × | × | × | × |
| 29 | isomartynoside | Low | × | × | × | × | × |
| 30\* | violanone | High | √ | √ | √ | √ | √ |
| 31\* | rehmapicroside | High | √ | × | √ | × | √ |
| 32\* | 5,7-dihydroxy-3',4',5'-trimethoxyflavanone | High | √ | √ | √ | √ | √ |
| 33 | gardoside | Low | √ | × | × | × | × |
| 34\* | 5,7,4'-trihydroxy-6-methyl homoisoflavanone | High | √ | √ | √ | √ | √ |
| 35\* | 8-formyl ophiopogonone B | High | √ | √ | √ | √ | √ |
| 36\* | 5-hydroxy-3',4'-dimethoxy-6,8-dimethyl homoisoflavanone | High | √ | √ | √ | √ | √ |
| 37\* | 5,7,2'-trihydroxy-4'-methoxy-6,8-dimethyl homoisoflavanone | High | √ | √ | √ | √ | √ |
| 38\* | ophiopogonanone E | High | √ | √ | √ | √ | √ |
| 39\* | diosbulbin D | High | √ | √ | √ | √ | √ |
| 40\* | ophiopogonanone C | High | √ | √ | √ | √ | √ |
| 41 | bis(4-ethylbenzylidene)sorbitol | Low | × | × | × | × | × |
| 42\* | bergaptol | High | √ | √ | √ | √ | √ |
| 43 | rehmannioside D | Low | × | × | × | × | × |
| 44 | ophiopogonin D | Low | × | × | × | × | × |
| 45\* | methylophiopogonanone A | High | √ | √ | √ | √ | √ |
| 46\* | 14-hydroxycholesta-4,7-diene-3,6-dione | High | √ | × | √ | √ | × |
| 47\* | imperatorin | High | √ | √ | √ | √ | √ |
| 48 | (6a*R*,11a*R*)-10-(3-hydroxy-3-methylbutyl)-6a,11a-dihydro-6*H*-[1]benzofuro[3,2-c]chromene-3,9-diol | Low | × | × | × | × | × |
| 49\* | xanthotoxol | High | √ | √ | √ | √ | √ |

\*Potential active chemicals.

Supplementary 2. Degree value of the potential active chemicals in YWD

|  |  |  |
| --- | --- | --- |
| NO. | Name | Degree |
| YWD17 | methylophiopogonanone A | 39 |
| YWD19 | imperatorin | 30 |
| YWD2 | diffractic acid | 28 |
| YWD14 | diosbulbin D | 24 |
| YWD6 | violanone | 20 |
| YWD15 | ophiopogonanone C | 19 |
| YWD13 | ophiopogonanone E | 17 |
| YWD16 | bergaptol | 16 |
| YWD4 | *N-cis-p-coumaroyloctopamine* | 15 |
| YWD11 | 5-hydroxy-3',4'-dimethoxy-6,8-dimethyl homoisoflavanone | 10 |
| YWD20 | xanthotoxol | 10 |
| YWD8 | 5,7-dihydroxy-3',4',5'-trimethoxyflavanone | 9 |
| YWD12 | 5,7,2'-trihydroxy-4'-methoxy-6,8-dimethyl homoisoflavanone | 8 |
| YWD7 | rehmapicroside | 5 |
| YWD9 | 5,7,4'-trihydroxy-6-methyl homoisoflavanone | 5 |
| YWD1 | catalpol | 4 |
| YWD18 | 14-hydroxycholesta-4,7-diene-3,6-dione | 4 |
| YWD5 | *N-trans-p-coumaroyloctopamine* | 3 |
| YWD10 | 8-formyl ophiopogonone B | 3 |
| YWD3 | 4-hydroxybenzoic acid | 2 |

Supplementary3. 10 genes identified according to four algorithms

|  |  |  |  |
| --- | --- | --- | --- |
| MCC | Degree | MNC | EPC |
| EGFR | EGFR | EGFR | EGFR |
| NFKB1 | AKT1 | AKT1 | AKT1 |
| AKT1 | NFKB1 | NFKB1 | NFKB1 |
| MTOR | HIF1A | HIF1A | HIF1A |
| TNF | TNF | TNF | TNF |
| HIF1A | SRC | SRC | SRC |
| SRC | MAPK3 | MAPK3 | MAPK3 |
| STAT3 | MMP9 | MMP9 | MMP9 |
| MMP9 | STAT3 | STAT3 | HSP90AB1 |
| PTGS2 | PTGS2 | PTGS2 | STAT3 |