

**Table S1.** 117 potential active chemicals in Wuweizi.

| Molecule Name   | MW     | OB (%) | Caco-2 |
|---|--------|--------|--------|
| (L)-alpha-Terpineol   | 154.28 | 48.8   | 1.39   |
| ZINC02040970  | 222.41 | 40.43  | 1.44   |
| schisantherin A   | 270.24 | 9.73   | 1.57   |
| schisandrin b   | 400.46 | 6.25   | 1.85   |
| (-)nopinene   | 136.26 | 44.84  | 1.8    |
| calarene  | 204.39 | 52.16  | 1.82   |
| Linalool  | 170.28 | 49.37  | 0.86   |
| beta-Chamigrene   | 204.39 | 31.99  | 1.82   |
| Nootkatin   | 232.35 | 31.82  | 1.1    |
| L-Bornyl acetate  | 196.32 | 65.52  | 1.29   |
| schisandrol B   | 514.57 | 31.8   | 1.33   |
| Moslene   | 136.26 | 33.02  | 1.88   |
| (+)-beta-Phellandrene   | 136.26 | 40.3   | 1.83   |
| (-)Cuparene   | 202.37 | 38.26  | 1.88   |
| 1H-Cycloprop(e)azulen-7-ol,<br>decahydro-1,1,7-trimethyl-4-methylene-,<br>(1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))- | 220.39 | 82.33  | 1.37   |
| Hemo-sol  | 136.26 | 39.84  | 1.83   |
| delta-Terpineol   | 154.28 | 55.11  | 1.28   |
| beta-Gurjunene  | 204.39 | 51.36  | 1.81   |
| (-)Comphene   | 136.26 | 34.98  | 1.81   |
| beta-Citronellol  | 156.3  | 38.89  | 1.2    |
| [(1S)-endo]-(-)-Borneol   | 154.28 | 83.54  | 1.22   |
| (E)-oct-2-en-4-one  | 126.22 | 64.62  | 1.36   |
| T-Muurolol  | 222.41 | 30.41  | 1.36   |
| (-)alpha-Longipinene  | 204.39 | 57.47  | 1.81   |
| Aristolone  | 218.37 | 45.31  | 1.29   |
| 3-Furaldehyde   | 96.09  | 50.96  | 1.04   |
| (5S)-5-butyloxolan-2-one  | 142.22 | 65.08  | 1.16   |
| Limetin   | 206.21 | 36.63  | 0.88   |
| beta-Terpinene  | 136.26 | 42.29  | 1.85   |
| (Z)-2-methyl-5-[(1S,2R,4R)-2-methyl-3-methylene-2-norbornan<br>yl]pent-2-en-1-ol  | 220.39 | 35.28  | 1.28   |
| (-)Terpinen-4-ol  | 154.28 | 81.41  | 1.36   |
| DBP   | 278.38 | 64.54  | 0.8    |
| β-terpineol   | 154.28 | 47.89  | 1.29   |
| Arnebin 7   | 272.32 | 73.85  | 0.74   |
| beta-Sesquiphellandrene   | 218.42 | 30.58  | 1.82   |
| Thymoquinol   | 166.24 | 44.44  | 1.19   |
| (9aS)-2,5,9,9-tetramethyl-3,4,6,7,8,9a-hexahydrobenzo[7]annul<br>ene  | 204.39 | 45.36  | 1.86   |
| (E)-9-Isopropyl-6-methyl-5,9-decadiene-2-one  | 208.38 | 60.25  | 1.45   |
| 1,1alpha,4,5,6,7,7alpha,7beta-Octahydro-1,1,7,7alpha-tetramet<br>hyl-2H-cyclopropan(alpha)-naphthalen-2-one             | 218.37 | 43.91  | 1.3    |
| 1-(1,5-Dimethyl-4-hexenyl)-4-methyl benzene   | 208.43 | 30.94  | 1.83   |
| 3alpha-Tigloyloxytropane  | 223.35 | 90.82  | 1      |
| 4-Ethenyl-2,2,4-trimethyl-3-(1-methylethethyl)-cyclo-hexane-m<br>ethanol  | 222.41 | 39.67  | 1.31   |
| Angeloylgomisin O   | 498.62 | 31.97  | 0.83   |
| Schizandrider B   | 514.62 | 30.71  | 0.66   |
| Clupanodonic acid   | 276.46 | 44.01  | 1.22   |
| Epiguaiipyridine  | 215.37 | 36.98  | 1.66   |

|   |        |       |      |
|---|--------|-------|------|
| Gomisin-A   | 416.51 | 30.69 | 0.63 |
| Gomisin G   | 508.61 | 32.68 | 0.73 |
| Gomisin R   | 400.46 | 34.84 | 0.6  |
| (1R)-1-phenylpropan-1-ol  | 136.21 | 70.32 | 1.26 |
| schizonepetoside A_qt   | 168.26 | 60.29 | 0.87 |
| 2-[(1R)-4-methyl-1-cyclohex-3-enyl]propan-2-yl acetate  | 196.32 | 33.05 | 1.37 |
| Thujyalcohol  | 154.28 | 73.08 | 1.2  |
| Wuweizisu C   | 384.46 | 46.27 | 1.08 |
| Wyerone   | 258.29 | 79.24 | 0.77 |
| alpha-Cuparenol   | 218.37 | 55.7  | 1.41 |
| (-)beta-Pinene  | 136.26 | 44.77 | 1.85 |
| Terpilene   | 136.26 | 33.95 | 1.84 |
| ACETIC ACID,BORNYL ESTER  | 196.32 | 67.15 | 1.26 |
| (L)-alpha-Terpineol   | 154.28 | 48.8  | 1.39 |
| ZINC02040970  | 222.41 | 40.43 | 1.44 |
| 1,8-cineole   | 154.28 | 39.73 | 1.57 |
| (-)alpha-Pinene   | 136.26 | 46.25 | 1.85 |
| (-)nopinene   | 136.26 | 44.84 | 1.8  |
| calarene  | 204.39 | 52.16 | 1.82 |
| Linalool  | 170.28 | 49.37 | 0.86 |
| beta-Chamigrene   | 204.39 | 31.99 | 1.82 |
| Nootkatin   | 232.35 | 31.82 | 1.1  |
| L-Bornyl acetate  | 196.32 | 65.52 | 1.29 |
| (R)-linalool  | 154.28 | 39.8  | 1.33 |
| Moslene   | 136.26 | 33.02 | 1.88 |
| (+)-beta-Phellandrene   | 136.26 | 40.3  | 1.83 |
| (-)Cuparene   | 202.37 | 38.26 | 1.88 |
| 1H-Cycloprop(e)azulen-7-ol,<br>decahydro-1,1,7-trimethyl-4-methylene-,<br>(1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))- | 220.39 | 82.33 | 1.37 |
| Hemo-sol  | 136.26 | 39.84 | 1.83 |
| delta-Terpineol   | 154.28 | 55.11 | 1.28 |
| beta-Gurjunene  | 204.39 | 51.36 | 1.81 |
| (-)Comphene   | 136.26 | 34.98 | 1.81 |
| beta-Citronellol  | 156.3  | 38.89 | 1.2  |
| [(1S)-endo]-(-)-Borneol   | 154.28 | 83.54 | 1.22 |
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| T-Muurolol  | 222.41 | 30.41 | 1.36 |
| (-)alpha-Longipinene  | 204.39 | 57.47 | 1.81 |
| Aristolone  | 218.37 | 45.31 | 1.29 |
| 3-Furaldehyde   | 96.09  | 50.96 | 1.04 |
| (5S)-5-butyloxolan-2-one  | 142.22 | 65.08 | 1.16 |
| Limetin   | 206.21 | 36.63 | 0.88 |
| beta-Terpinene  | 136.26 | 42.29 | 1.85 |
| (Z)-2-methyl-5-[(1S,2R,4R)-2-methyl-3-methylene-2-norbornan-<br>yl]pent-2-en-1-ol                                       | 220.39 | 35.28 | 1.28 |
| (-)Terpinen-4-ol  | 154.28 | 81.41 | 1.36 |
| DBP   | 278.38 | 64.54 | 0.8  |
| β-terpineol   | 154.28 | 47.89 | 1.29 |
| Arnebin 7   | 272.32 | 73.85 | 0.74 |
| beta-Sesquiphellandrene   | 218.42 | 30.58 | 1.82 |
| Thymoquinol   | 166.24 | 44.44 | 1.19 |
| (9aS)-2,5,9,9-tetramethyl-3,4,6,7,8,9a-hexahydrobenzo[7]annul-<br>ene   | 204.39 | 45.36 | 1.86 |
| (E)-9-Isopropyl-6-methyl-5,9-decadiene-2-one  | 208.38 | 60.25 | 1.45 |

|   |        |       |      |
|---|--------|-------|------|
| 1,1alpha,4,5,6,7,7alpha,7beta-Octahydro-1,1,7,7alpha-tetramethyl-2H-cyclopropano (alpha)-naphthalen-2-one | 218.37 | 43.91 | 1.3  |
| 1-(1,5-Dimethyl-4-hexenyl)-4-methyl benzene   | 208.43 | 30.94 | 1.83 |
| 3alpha-Tigloyloxytropane  | 223.35 | 90.82 | 1    |
| 4-Ethenyl-2,2,4-trimethyl-3-(1-methylethyl)-cyclohexane-methanol  | 222.41 | 39.67 | 1.31 |
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| Clupanodonic acid   | 276.46 | 44.01 | 1.22 |
| Epiguaiipyridine  | 215.37 | 36.98 | 1.66 |
| Gomisin-A   | 416.51 | 30.69 | 0.63 |
| Gomisin G   | 508.61 | 32.68 | 0.73 |
| Gomisin R   | 400.46 | 34.84 | 0.6  |
| (1R)-1-phenylpropan-1-ol  | 136.21 | 70.32 | 1.26 |
| schizonepetoside A_qt   | 168.26 | 60.29 | 0.87 |
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| Thujyalcohol  | 154.28 | 73.08 | 1.2  |
| Wyerone   | 258.29 | 79.24 | 0.77 |
| alpha-Cuparenol   | 218.37 | 55.7  | 1.41 |
| (-)beta-Pinene  | 136.26 | 44.77 | 1.85 |
| Terpilene   | 136.26 | 33.95 | 1.84 |
| ACETIC ACID,BORNYL ESTER  | 196.32 | 67.15 | 1.26 |