Table S4. Chemical compositions of single components in Tong Xie Yao Fang.

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| **Scientific name** | **Chemical compositions** |
| Rhizome of *Atractylodes macrocephala* Koidz (Zhu et al., 2021) | Atractylenolide III, atractylenolide IV, 3-acetyl-atractylon, β-eudesmol, biatractylenolide II |
| Root of *Saposhnikovia divaricata* (Turcz.) Schischk (Yokosuka et al., 2017) | 3’-O-angeloylhamaudol, ledebouriellol, divaricatol, sec-O-methylvisammioside, (9Z)-heptadeca-1,9-diene-4,6-diyn-3-ol, (9Z)-heptadeca-1,9-diene-4,6-diyne-3,8-diol, (9Z)-1-methoxy-9-heptadecene-4,6-diyn-3-ol, (8E)-heptadeca-1,8-diene-4,6-diyne-3,10-diol, (8E)-10-hydroperoxy-1,8-heptadecadiene-4,6-diyn-3-ol |
| Peel of *Citrus reticulatae* Blanco. (Boughendjioua and Boughendjioua, 2017) | α-Thuyene, α-Pinene, sabinene, myrcene, α-Terpinene, limonene, β -phellandrene, γ-Terpinene, p- Cymene, octanal, decanal, linalol, terpinene-4-ol, l-Caryophyllene, α- Terpinenol, N-N-butylpyrrole, l-Caryophyllene, dimethylAnthranilate, germacrene-d, thymol, δ-muurolen, β-Cubebene, copaen, 2-isopropyl-5metylphenol |
| Root of *Paeonia lactiflora* Pall. (Tan et al., 2020) | Desbenzoyl paeoniflorin, D-catechin, paeoniflorin, albiflorin, oxypaeoniflorin, benzoylpaeoniflorin, gallolpaeoniflorin, galloylalbiflorin, 1’-O-galloyl sucrose, 6’-O- galloyl sucrose, 6-O- galloyl sucrose, benzoyloxypaeniflorin, paeonol, methyl gallate, gallic acid, paeoniflorin sulfonate, tetragalloyl glucose, monoterpene, glycosides sulfite |

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