**Table S3. Chemical compositions and pharmacological activities of the single components of *Xiaoyao-san*.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Scientific name**  **(family)** | **Latin name** | **Chinese**  **name** | **Parts used** | **Chemical compositions** | **Pharmacological activities** |
| *Bupleurum chinese* DC.  (family *Apiaceae*) | *Bupleuri radix* | *Chai-Hu*  (柴胡) | Root | Saikosaponin a, Saikosaponin c, Saikosaponin d, Saikosaponin e, Prosaikogenin G, Prosaikogenin F, 2”-O-Acetylsaikosaponin a, 3”-O-Acetylsaikosaponin a, 6”-O-Acetylsaikosaponin a, 23-O-Acetylsaikosaponin a, 6”-O-Acetylsaikosaponin d, 23-Hydroxy-13𝛽, 28𝛽-epoxy-olean-11-ene-16-one 3-O-𝛽-D-glucopyranosyl-(1→3)-𝛽-D-fucopyranoside, 3𝛽,16𝛽-Dihydroxy-23-O-acetyl-13𝛽, 28𝛽-epoxy-olean-11-ene 3-O-𝛽-D-fucopyranoside, Bupleuroside I, Saikosaponin b1, Saikosaponin b2, 6”-O-Acetyl-saikosaponin b2, Saikosaponin h, Prosaikogenin D, Prosaikogenin A, 3𝛽,23,28-Trihydroxy-11, 13(18)-diene-16-one 3-O-𝛽-D-glucopyranosyl-(1→ 3)-𝛽-D-fucopyranoside, Bupleuroside V, Bupleuroside X, Bupleuroside XII, Saikosaponin v-1, Saikosaponin b3, Saikosaponin b4, Saikosaponin f, 3𝛽,16𝛽,23,28-Tetrahydroxy-11𝛼-methoxy-olean-12-ene 3-O-𝛽-D-fucopyranoside, 3𝛽,16𝛽,28-Trihydroxyl-11𝛼-methoxy-olean-12-ene-O-𝛽-D-fucopyranoside, Bupleuroside VII , Saikosaponin g, Saikosaponin i, Bupleuroside VIII, Bupleuroside XI, (2Z,8Z,10E)-pentadecatriene-4,6-diyne-1-ol, (2Z,8E,10E)-pentadecatriene-4,6-diyne-1-ol, (2Z,8Z,10E)-heptadecatriene-4,6-diyne-1-ol, Bupleurynol, Quercetin, Isorhamnetin, Isorhamnetin-3-O-glucoside, Puerarin, Rutin, Narcissin, Eugenin, Saikochrome A, Saikochromic acid, 7,4’-Dihydroxy-isoflavone-7-O-𝛽-D-glucoside, Saikochromoside A, Saikoisoflavonoside A, Nortrachelogenin, Nemerosin, Kaerophyllin, Isochaihulactone, Isokaerophyllin, (−)-yatein, Chinensinaphthol, Chaihunaphthone, Fumaric acid, Butanedioic acid, Pentadecanoic acid, Palmitoleic acid, Palmitic acid, Oleic acid, Stearic acid, 11-Hexadecenoic acid, 13-Octadecenoic acid, Linoleic acid, Tetracosanoic acid, 9S,12S,13S-Trihydroxy-10E-octadecenoic acid, 𝛼-Spinasterol, 24𝜉-Methylcholesta-7, 22E-diene-3𝛽,5𝛼,6𝛽-triol, 24𝜉-Ethylcholest-22E-end-3𝛽,5𝛼,6𝛽-Triol (Yang et al., 2017) | Antidepressant (Li et al., 2017; Wang et al., 2015), hepatoprotective (Li et al., 2015) |
| *Angelica sinensis* (Oliv.) Diels  (family *Apiaceae*) | *Angelicae sinensis radix* | *Dang-Gui*  (当归) | Root | ferulic acid, 3-butylphthalide, Z-butylidenephthalide, 3-butylidene-4-hydroxyphthalide, E-butylidenephthalide, senkyunolide A, Z-ligustilide, E-ligustilide, 6,7-epoxyligustilide, senkyunolide F, senkyunolide H, senkyunolide I, 6,7-dihydroxyligustilide (Lao et al., 2004) | Antidepressant (Gong et al., 2019), antispasmodic (Du et al., 2006), neuroprotective (Gong et al., 2016) |
| *Paeonia lactiflora* Pall. (family *Paeoniaceae*) | *Paeoniae radix alba* | *Bai-Shao*  (白芍) | Root | paeoniflorin sulfonate, tetragalloyl glucose, monoterpene, glycosides sulfite, paeoniflorin, albiflorin, oxypaeoniflorin, benzoylpaeoniflorin, gallolpaeoniflorin, galloylalbiflorin, 1’-O-galloyl sucrose, 6’-O-galloyl sucrose, 6-O-galloyl sucrose, benzoyloxypaeniflorin, paeonol, methyl gallate, gallic acid (Tan et al., 2020) | Anticonvulsant (Zhang et al., 1994), antidepressant (Jin et al., 2016; Wang et al., 2016), neuroprotective (Zhang et al., 2017) |
| *Atractylodes macrocephala* Koidz.  (family *Compositae*) | *Atractylodis macrocephalae*  *rhizoma* | *Bai-Zhu*  (白术) | Rhizome | atractylenolide III, atractylenolide IV, 3-acetyl-atractylon, β-eudesmol, biatractylenolide II (Zhu et al., 2021) | Improving disordered intestinal flora (Wang et al., 2014), inhibiting the gastrointestinal movement and spasm (Zhang et al., 1999), promoting the healing of intestinal mucosa injury (Song et al., 2014) |
| *Poria cocos* (Schw.) Wolf.  (family *Polyporaceae*) | *Poria cocos* | *Fu-Ling*  (茯苓) | Sclerotium | Pachymic acid, Tumulosic acid, Trametenolic acid, Eburicoic acid, 3-O-acetyl-16α-hydroxytrametenolic acid, 16α-Hydroxytrametenolic acid, O-acetylpachymic acid, O-acetylpachymic acid-25-ol, Methyl-O-acetylpachymate, Pachymic acid methyl ester, Ganoderic acid, 25-Hydroxypachymic acid, 25-Hydroxy-3-epitumulosic acid, 16α,25-Dihydroxyeburiconic acid, 16α-Hydroxyeburiconic acid, 3β,16α-Dihydroxy-7-oxo-24-methyllanosta-8,24(31)-dien-21-oic acid, 3α,16α-Dihydroxy-7-oxo-24-methyllanosta-8,24(31)-dien-21-oic acid, Oxotrametenolic acid, Acetyl eburicoic acid, Poricoic acid ZH, Poricoic acid ZU, Poricoic acid ZW, 3β,15α-Dihydroxy-24-oxolanosta-8-en- 21-oic acid, 3β-Acetyloxy-16α-hydroxy-24-oxolanost-8-en-21-oic acid, Daedaleanic acid B, 15α-Hydroxyeburiconic acid, 3α,16α,25-Trihydroxylanosta-8,24-dien- 21-oic acid, 16α,29-Dihydroxyeburiconic acid, 3β-Acetyloxy-16α,26-dihydroxylanosta-8,24-dien-21-oic acid, 15α-Hydroxy-3-oxolanosta-8,24-dien-21-oic acid, 16α-Hydroxy-3-oxolanosta-8,24-dien-21-oic acid, 3β,16α-Bis(acetyloxy)-29-hydroxylanosta-8,24-dien-21-oic acid, Hispindic acid B, 3β,15α-Bis(acetyloxy)-24- methylenelanost-8-en-21-oic acid, 16α-Acetyloxyeburiconic acid, 3-Epi-pachymic acid, Ceanphytamic acid A, Ceanphytamic acid B, Dehydrotrametenolic acid, Dehydropachymic acid, Dehydroeburicoic acid, 6α-Hydroxypolyporenic acid C, 3-Epi-dehydrotumulosic acid, 25-Hydroxy-3-epi-dehydrotumulosic acid, Dehydrotumulosic acid, Dehydroeburiconic acid, 3-O-Acetyl-16α-hydroxydehydrotrametenolic acid, 3-Epidehydropachymic acid, 3β,16α-Dihydroxylanosta-7,9(11),24-trien-21-oic acid, 6α-Hydroxydehydropachymic acid, 3β-p-Hydroxybenzoyldehydrotumulosic acid, 3β-Hydroxy-16α-acetoxy-lanosta-7,9(11),24-trien-21-oic acid, Polyporenic acid C, Dehydrotrametenonic acid, 15α-Hydroxydehydrotumulosic acid, 16α,25-Dihydroxydehydroeburicoic acid, 29-Hydroxypolyporenic acid C, Poriacosones A, Poriacosones B, 16α,27-Dihydroxydehydrotrametenoic acid, 3β,16α,30-Trihydroxy-24-methyllanosta-7,9(11),24(31)-trien-21-oic acid, 3β-Acetoxy-16α,24β-dihydroxylanosta-7,9(11),25-trien-21-oic acid, 29-Hydroxydehydrotumulosic acid, 29-Hydroxydehydropachymic acid, 3β,15α-Dihydroxylanosta-7,9(11),24-triene-21-oic acid, Dehydrosulphurenic acid, Dehydroeburicoic acid monoacetate, 3β-Acetoxylanosta-7,9(11),24-trien-21-oic acid, Poricoic acid ZE, Poricoic acid ZI, Poricoic acid ZL, Poricoic acid ZV, Coriacoic acid B, Coriacoic acid C, 6,16α-Dihydroxydehydrotrametenonic acid, 16α-Hydroxydehydrotrametenonic acid, 25,26-Dihydroxydehydropachymic acid, 3β,16α-Dihydroxy-24-hydroxymethyllanosta-7,9(11)-dien-21-oic acid, 15α-Hydroxydehydrotrametenolic acid, 16α-Hydroxydehydrotrametenoic acid, 16-Hydroxy-3,24-dioxolanosta-7,9(11)-dien-21-oic acid, 16α-Acetyloxy-24-methylene-3-oxolanosta-7,9(11)-dien-21-oic acid, Poricoic acid G, Poricoic acid H, 25-Hydroxyporicoic acid H, Poricoic acid GM, Poricoic acid HM, Poricoic acid GE, Poricoic acid ZA, Poricoic acid ZJ, Poricoic acid ZK, Poricoic acid ZR, 25-Methoxy-29-hydroxyporicoic acid HM, Poricoic acid A, Poricoic acid B, Poricoic acid C, Poricoic acid D, Poricoic acid DM, Poricoic acid AM, Poricoic acid E, Poricoic acid BM, Poricoic acid F, 16-Deoxyporicoic acid B, Poricoic acid CM, 25-Methoxyporicoic acid A, 26-Hydroxyporicoic acid DM, 25-Hydroxyporicoic acid C, Poricoic acid AE, Poricoic acid CE, 3,4-Secolanosta-4(28),7,9,24Z-tetraen-3,26-dioic acid, Poricoic acid BE, 16α-Hydroxy-3,4-secolanosta-4(28),7,9(11),24(31),25(27)-pentaene-3,21-dioic acid, Poricoic acid ZB, Poricoic acid ZC, Poricoic acid ZD, Poricoic acid ZG, Poricoic acid ZM, Poricoic acid ZO, Poricoic acid ZP, Poricoic acid ZN, Poricoic acid ZT, Poricoic acid ZQ, 5α,8α-Peroxydehydrotumulosic acid, 3-(2-Hydroxyacetoxy)-5α,8α-peroxydehydrotumulosic acid, Daedaleanic acid A, 11β-Ethoxydaedaleanic acid A, (3β,16α)-3-Acetyloxy-16-hydroxy-24-methylenelanosta-5,7(9),11-tetraene-21-oic acid, 16α-Hydroxy-3-oxo-24-methyllanosta-5,7,9(11),24(31)-tetraen-21-oic acid, 6,7-Dehydroporicoic acid H, Coriacoic acid A, Coriacoic acid D, β-Amyrin acetate, Oleanolic acid, 3-O-acetyloleanolic acid, 7-oxo-15-Hydroxydehydroabietic acid, Dehydroabietic acid methyl ester, Poricoic acid ZF, Dehydroabietic acid, 7-Oxocallitrisic acid, Pimaric acid, Ergosterol, (22E)-ergosta-5,7,9(11),22-tetraen-3β-ol, Ergosta-5,7-dien-3β-ol, (22E)-Ergosta-8(14),22-dien-3β-ol, (22E)-Ergosta-6,8(14),22-trien-3β-ol, (22E)-Ergosta-7,22-dien-3β-ol, Ergost-7-en-3β-ol, Ergosterol peroxide, Daucosterol, Cerevisterol, Biemnasterol, Β-Sitosterol, 3β,5α-Dihydroxy-ergosta-7,22-diene-6-one, 3β,5α,9α-Trihydroxy-ergosta-7,-dien-6-one, Ergosta-7,22-diene-3-one, 6,9-Epoxy-ergosta-7,22-diene-3-ol, Ergosta-4,22-diene-3-one, Ergosta-5,6-epoxy-7,22-dien-3-ol, Pregn-7-ene-2β,3α,15α,20-tetrol, Peroxy-ergosterol, Ergot sterone, 9,11-Dehydroergosterol peroxide, Pachyman, PolysaccharideH11, PC1, PC2, PC2-A, PC3, PC4, PCSC22, PCM1, PCM2, PCM3, PCM4, ac-PCM0, ac-PCM1, ac-PCM2, PCPWP, PCPWPS, ac-PCM3-I, ac-PCM3-II, ac-PCM4-I, ac-PCM4-II, wb-PCM1, wb-PCM2, wc-PCM1, wc-PCM2, wb-PCM3-I, wc-PCM3-I, wb-PCM3-II, wb-PCM4-I, wb, PCM4-II, wc-PCM3-II, wc-PCM4I, wc-PCM4-II, WIP, wb-PCM0, wc-PCM0, ab-PCM0, ab-PCM1, ab-PCM2-I, ab-PCM2-I, ab-PCM3-I, ab-PCM3-II, ab-PCM4-I, abPCM4-II, PCS1, PCS2, PCS3-I, PCS3-II, PCS4-I, PCS4-II, PC-PS, PCSG, Pi-PCM0, Pi-PCM1, Pi-PCM2, Pi-PCM3-I, Pi-PCM4-I, Pi-PCM3-II, Pi-PCM4-II, Polysaccharides from *Poria*, WSP, WSP-1, WSP-2, PCII, PCP, ATPCP, PCP-II, CMP33, PAC, FMGP, CMP3, PPS, CMP, PPSW-1, Sul-W-1, S-CMP, Polysaccharides (WRP), PPC, PCP-M, Sulfated pachymaran, PCWPW and PCWPS (Lu et al., 2021) | Antidepressant (Zhang et al., 2019), antispasmodic (Xiao et al., 2020), enteroprotective (Zou, 2019) |
| *Zingiber officinale* Roscoe  (family *Zingiberaceae*) | *Zingiberis rhizoma recens* | *Sheng-Jiao*  (生姜) | Rhizome | [6]-Paradol, [7]-Paradol, [8]-Paradol, [9]-Paradol, [10]-Paradol, [11]-Paradol, [13]-Paradol, Methyl [6]-paradol, [4]-Gingerol, [6]-Gingerol, [7]-Gingerol, [8]-Gingerol, [10]-Gingerol, Methyl [4]-gingerol, Methyl [6]-gingerol, [4]-Shogaol, [6]-Shogaol, [8]-Shogaol, [10]-Shogaol, [12]-Shogaol, Methyl [6]-shogaol, Methyl [8]-shogaol, Acetoxy-[4]-gingerol, Acetoxy-[6]-gingerol, Acetoxy-[8]-gingerol, Acetoxy-[10]-gingerol, Methyl acetoxy-[6]-gingerol, 1-Dehydro-[3]-gingerdione, 1-Dehydro-[6]-gingerdione, 1-Dehydro-[8]-gingerdione, 1-Dehydro-[10]-gingerdione, [4]-Gingerdiol, [6]-Gingerdiol, [8]-Gingerdiol, [10]-Gingerdiol, 5-Acetoxy-[4]-gingerdiol, 5-Acetoxy-[6]-gingerdiol, 5-Acetoxy-[7]-gingerdiol, Methyl 5-acetoxy-[4]-gingerdiol, Methyl 5-acetoxy-[6]-gingerdiol, Diacetoxy-[4]-gingerdiol, Diacetoxy-[6]-gingerdiol, Methyl diacetoxy-[4]-gingerdiol, Methyl diacetoxy-[6]-gingerdiol, Methyl diacetoxy-[10]-gingerdiol, 3-Dihydro-[6]-demethoxyshogaol, 5-Methoxy-[6]-gingerol, 1,7-bis-(4’-Hydroxy-3’-methoxyphenyl)-4-heptene-3-one, 1,7-bis-(4’-Hydroxy-3’-methoxyphenyl)-3,5-heptadione, 1-Dehydro-3-dihydro-[10]-gingerdione, 6-Dihydroparadol, Acetoxy-6-dihydroparadol, 1-(4’-Hydroxy-3’-methoxyphenyl)-7-octen-3-one, 1-(4’-Hydroxy-3’-methoxyphenyl)-7-decen-3-one, 1-(4’-Hydroxy-3’-methoxyphenyl)-7-dodecen-3-one, [4]-Isogingerol, 4-(4-Hydroxyphenyl)-2-butanone, 4-Hydroxy-3-methoxybenzenepropanal, 3,4-Dimethoxybenzenepropanal, Zingerone, Zingerone methyl ether, Gingerol, Zingerol 2-methyl ether (Jolad et al., 2004) | Antiserotonergic (Yamahara et al., 1989), chemopreventative (Mahady et al. 2003), enhancing gastric emptying (Yamahara et al., 1990) |
| *Mentha canadensis* L.  (family *Lamiaceae*) | *Menthae herba* | *Bo-He*  (薄荷) | Aerial parts | (4S)-7-hydroxy-carvone 7-O-β-D-glucopyranoside, (3β,11α)-3-hydroxy-11α-methoxy-olean-12-en-3-yl palmitate, (4R,6R)-carveol β-d-glucoside, (4R,6S)-carveol β-d-glucoside, (+)-neodihydrocarvy β-D-glucoside, (−)-dihydrocarvy β-D-glucoside, uroterpenol β-D-glucoside, spicatoside A, spicatoside B, (3S,6S)-cislinalool-3,7-oxide, (3R,9S)-megastigman-5-en-3,9-diol 3-O-β-d-glucopyranoside, linarionoside A, 1,1,5-trimethyl- 6-(3-hydroxyl) cyclohexene5-yl-1-β-D-pyranoglucoside, linarionoside B, (9S)-linarionoside B, (+)-jasmololone glycoside, (‒)-5′-(β-d-glucopyranosyloxy) jasmonic acid, maniladiol, 3β,28- dihydroxy-olean-12-enyl palmitate, olean-12-ene-28-arboxy-3-palmitate, ursolic acid, 1-(β-D-ribofuranosyl)-1H-1,2,4-triazone, naphthisoxazol A, menthalactone, 6-amino9-[1-(3,4-dihydroxy phenyl)ethyl]-9H-purine (He et al., 2019) | Regulating intestinal flora (Fang et al., 2022) |
| *Glycyrrhiza uralensis* Fisch.  (family *Leguminosae*) | *Glycyrrhizae radix et rhizoma* | *Gan-Cao*  (甘草) | Root and rhizome | glycyrrhizic acid, 22β-acetoxyl-glycyrrhizin, licorice-saponin E2, licorice-saponin G2, licorice-saponin A3, liquiritigenin, liquiritin, liquiritin apioside, isoliquiritigenin, isoliquiritin, isoliquiritin apioside, glabrone, licoisoflavone B, glycyrrhisoflavone, isoangustone A, licoflavone B, isolicoflavonol, licochalcone A, echinatin, licoagrochalcone C, glycyrol, glyasperin D, licoricidin, glycycoumarin, glabridin, licoisoflavanone (Shang et al., 2022; Song et al., 2017) | Antispasmodic (Sato et al., 2007), antiulcer (Dehpour et al., 1995) |

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