**Supplementary Material S3.** Characteristics of single components in the included studies.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Category of traditional usage** | **Frequency of herbs** | **Scientific name** | **Toxicity** **(daily dose)** | **Bioactive compounds** | **References** |
| Tranquilizing | 9 | *Ziziphus jujuba* Mill. | Non-toxic | Sanjoinine A, jujubosides | Shergis et al. (2017) |
| 7 | Fossilia Ossis Mastodi | Non-toxic | Calcium carbonate, calcium phosphate | Zhang et al. (2011) |
| 6 | *Ostrea gigas* Thunberg | N/A | Calcium carbonate | Zhang et al. (2011) |
| 6 | *Poria cocos* (Schw.) Wolf | Non-toxic | Pachymic acid, poricoic acid B | Ríos. (2011) |
| 5 | *Polygala tenuifolia* Willd. | Non-toxic | Tenuifoliside B | Ikeya et al. (2004) |
| 3 | *Dimocarpus longan* Lour. | Non-toxic | Corilagin, ellagic acid | Yang et al. (2011) |
| 3 | *Lilium lancifolium* Thunb. | Non-toxic | Kaempferol, *p*-coumaric acid | Jin et al. (2012) |
| 2 | *Nelumbo nucifera* Gaertn | Non-toxic | Isoliensinine, neferine | Mukherjee et al. (2009) |
| 1 | *Acorus calamus* var. *angustatus* Besser | Mild toxic (3–10 g) | α-Asarone, β-asarone | Han et al. (2013) |
| 1 | Magnetite | Non-toxic | Iron oxide mineral magnetite | Wang et al. (1997) |
| 1 | *Platycladus orientalis* (L.) Franco | Non-toxic | d-Limonene, cedrol | Zhu et al. (2020) |
| 1 | *Valeriana officinalis* L. | Non-toxic | Valepotriates, linarin | Fernández et al. (2004) |
| Qi tonifying | 5 | *Glycyrrhiza uralensis* Fisch. ex DC. | Non-toxic | Glycyrrhetinic acid, liquiritin | Chen et al. (2014) |
| 3 | *Panax ginseng* C.A.Mey. | Non-toxic | Ginsenosides, ployacetylene | Choi. (2008) |
| 3 | *Astragalus mongholicus* Bunge | Non-toxic | APS, *Astragalus* saponins VII | Fu et al. (2014) |
| 3 | *Codonopsis pilosula* (Franch.) Nannf. | Non-toxic | Lobetyolin, lobetyolinin | Bailly et al. (2021) |
| 3 | *Schisandra chinensis* (Turcz.) Baill. | Non-toxic | Schisandrin, deoxyschisandrin | Sowndhararajan et al. (2018) |
| 2 | *Dioscorea oppositifolia* L. | Non-toxic | YP-1 | Zao et al. (2005) |
| 1 | *Pseudostellaria heterophylla* (Miq.) Pax | Non-toxic | Heterophyllin B, rhamnogalacturonan I | Hu et al. (2019) |
| Heat clearing | 4 | *Scutellaria baicalensis* Gerogi | Non-toxic | Baicalein, baicalin | Liao et al. (2021) |
| 2 | *Anemarrhena asphodeloides* Bunge | Non-toxic | Timosaponin BIII, trans-hinokiresinol | Wang et al. (2018) |
| 2 | *Coptis chinensis* Franch. | Mild toxic (2–5 g) | Berberine, coptisine | Wang J. et al. (2018) |
| 2 | *Lophatherum gracile* Brongn. | Non-toxic | Isoorientin, swertiajaponin | Tang et al. (2015) |
| 2 | *Rheum officinale* Baill. | Non-toxic | Emodin, aloe-emodin | Huang et al. (2007) |
| 1 | *Fritillaria thunbergii* Miq. | Non-toxic | Peimine, peiminine | Nile et al. (2021) |
| 1 | *Fritillaria cirrhosa* D.Don | Non-toxic | Imperialine, peiminine | Chen T. et al. (2020) |
| 1 | *Gardenia jasminoides* J.Ellis | Non-toxic | Geniposide, genipin | Chen L. et al. (2020) |
| 1 | *Prunella vulgaris* L. | Non-toxic | Ursolic acid, 2α-hydroxyursolic acid | Ryu et al. (2000) |
| 1 | *Scrophularia buergeriana* Miq. | Non-toxic | Buergeriside C1, buergeriside A1 | Shin et al. (2018) |
| 1 | *Scrophularia ningpoensis* Hemsl. | Non-toxic | Scrophuside, ningposides | Hua et al. (2014) |
| 1 | *Scutellaria barbata* D.Don | Non-toxic | Pheophorbide a | Tang et al. (2006) |
| Yin-blood tonifying | 4 | *Rehmannia glutinosa* (Gaertn.) DC. | Non-toxic | Catalpol, RPS | Zhang et al. (2008) |
| 2 | *Angelica sinensis* (Oliv.) Diels | Mild toxic (6–12 g) | Ferulic acid, Z-ligustilide | Chao et al. (2011) |
| 2 | *Eclipta prostrata* (L.) L. | Non-toxic | Echinocystic acid, eclalbasaponin II | Lee et al. (2008) |
| 2 | *Paeonia lactiflora* Pall. | Mild toxic (6–15 g) | Paeoniflorin | He et al. (2011) |
| 1 | *Angelica acutiloba* (Siebold & Zucc.) Kitag. | Non-toxic | Butylidene phthalide, furfural | Sowndhararajan et al. (2017)Yun et al., 2017 |
| 1 | *Asparagus cochinchinensis* (Lour.) Merr. | Non-toxic | Quercetin,asparacoside | Son et al. (2013) |
| 1 | *Equus qsinus* | N/A | Collagen α1, collagen α2 | Wang et al. (2014) |
| 1 | *Ophiopogon japonicus* (Thunb.) Ker Gawl. | Non-toxic | Ophiopogonin D, saponins | Chen et al. (2016) |
| 1 | *Trionyx sinensis* Wiegmann | N/A | CTEP | Tang et al. (2013) |
| Exterior-releasing | 3 | *Bupleurum chinense* DC. | Mild toxic (3–10 g) | Saikosaponins A, saikosaponins D | Liu et al. (2017) |
| 3 | *Zingiber officinale* Roscoe | Non-toxic | 6-Gingerol | de Lima et al. (2108) |
| 1 | *Bupleurum falcatum* L. | Mild toxic (3–10 g) | Saikosaponin A | Park et al. (2002) |
| Dampness-phlegm resolving | 3 | *Pinellia ternata* (Thunb.) Makino, 10g | Average toxic (internal use, 3–9 g after processed) | Pinellic acid | Nagai et al. (2002) |
| 2 | *Platycodon grandiflorus* (Jacq.) A.DC. | Non-toxic | Platycodin D, PGS | Zhang et al. (2015) |
| 1 | *Atractylodes lancea* (Thunb.) DC. | Non-toxic | Atractylodin, atractylodinol | Nakai et al. (2003) |
| Blood activating | 2 | *Conioselinum anthriscoides* 'Chuanxiong' | Mild toxic (3–10 g) | Ligustilide, senkyunolide A | Ran et al. (2001) |
| 1 | *Curcuma phaeocaulis* Valeton | Non-toxic | Phaeocaulisin A, phaeocaulisin B | Liu et al. (2013) |
| 1 | *Salvia miltiorrhiza* Bunge | Non-toxic | Danshensu, salvianolic acid B | Wang et al. (2017) |
| Yang-tonifying | 2 | *Eucommia ulmoides* Oliv. | Non-toxic | Eucommiol, astragalin | Wang C.Y. et al. (2019) |
| 1 | *Aconitum carmichaelii* Debeaux | Average toxic (3–15 g after processed) | Aconitine, mesaconitine | Zhao et al. (2020) |
| 1 | *Epimedium brevicornu* Maxim. | Mild toxic (6–10 g) | Icariin, epimedin B | Meng et al. (2004) |
| Wind-dampness dispelling | 2 | *Nanhaia speciosa* (Champ. ex Benth.) J.Compton & Schrire | Non-toxic | Formononetin, maackiain | Zhao et al. (2017) |
| Qi-regulating | 1 | *Aucklandia costus* Falc. | Non-toxic | Costunolide, dehydrocostuslactone | Lin et al. (2015) |

APS, *Astragalus mongholicus* polysaccharides; CTEP, *Carapax Trionycis* extract peptide; N/A, not available; PGS, *Platycodon grandiflorus* saponins; RPS, *Rehmannia glutinosa* polysaccharides.

The toxicity of single components in the included trials was cited form Liu et al. (2020). The study provided non-toxic traditional Chinese medicines (TCMs) with potential toxicity and toxic-TCMs, documented in the Chinese Pharmacopeia, with the toxic grade (highly toxic, average toxic, and mild toxic) and daily dose for body weight 70 kg.

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