**Supplementary tables**

Table S1. The traditional and clinical use of the fruits of *Zanthoxylum bungeanum*

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| --- | --- | --- | --- | --- |
|  | **Preparation name** | **Main Compositions** | **Traditional Usages** | **Origin** |
| **1** | *Da-Jian-Zhong* Decoction *(Dai-kenchu-to*) (大建中汤) | Fruits of *Zanthoxylum bungeanum* (花椒); roots of *Zingiber officinale* Rosc. (干姜); roots of *Panax ginseng* C. A. Mey. (人参) | Warming energizer and tonifying deficiency (温中补虚); lowering the adverse flow of qi and relieving pain (降逆止痛) | *Synopsis of the Golden Chamber* (金匮要略) |
| **2** | *Da-Xiao-Si-Shen* Pill | Fruits of *Zanthoxylum bungeanum* (花椒); Roots of *Aconitum kusnezoffii* Reichb. (草乌); Atractylodes lancea (Thunb.) DC. (苍术); roots of *Zingiber officinale* Rosc. (干姜); | Strengthening mind and Qi (壮神益气), nourishing marrow and essence (添精髓); strengthening strength (倍气力); sharpening hearing and brightening the eyes (聪耳明目)  | *Prescriptions for Universal Relief* (普济方) |
| **3** | Jiao-Ai Pill (椒艾丸) | Fruits of *Zanthoxylum bungeanum* (花椒); leaves of *Artemisia argyi* Levl.et Vant. (艾叶); roots of *Zingiber officinale* Rosc. (干姜); fruits of *Prunus mume* (Sieb.) Sieb. et Zucc. (乌梅). | Stopping diarrhea and promoting digestion (止泻痢，促消化); tonifying Yang of the spleen and kidney (补益脾肾阳) | *Valuable prescriptions for emergency* (备急千金要方) |
| **4** | *Jiao-Mei* Decoction (椒梅汤) | Fruits of *Zanthoxylum bungeanum* (花椒); fruits of *Prunus mume* (Sieb.) Sieb. et Zucc. (乌梅); roots of *Paeonia lactiflora Pall*. (白芍); roots of *Coptis chinensis* Franch. (黄连); roots of *Zingiber officinale* Rosc. (干姜); roots of *Panax ginseng* C. A. Mey. (人参); young fruits of Citrus aurantium L. (枳实) | Relieving summer-heat and expelling roundworm (解暑驱蛔) | *Item differentiation of warm febrile diseases* (温病条辨) |
| **5** | Jiao-Hong Pill (椒红丸) | Fruits of *Zanthoxylum bungeanum* (花椒); roots of Zingiber officinale Rosc. (干姜); roots of *Aconitum carmichaelii* Debx. (附子) | Warming kidney and bowel, and relieving pain (补暖下元) | *Peaceful holy benevolent prescriptions* (太平圣惠方) |
| **6** | *Jiao-Pu-Jian-Pi Powder* (椒朴健脾散) | Fruits of *Zanthoxylum bungeanum* (花椒); barks of Mgnolia officinalis Rehd.et Wils. (厚朴); seeds of Myristica fragrans Houtt. (肉豆蔻); fruits of Terminalia chebula Retz. (诃子); barks of Citrus reticulata Blanco (广陈皮); roots of *Aconitum carmichaelii* Debx. (附子); roots of Aucklandia lappa Decne. (木香). | Strengthening spleen and warming stomach (健脾温胃); promoting appetite and digestion (消谷嗜食); cultivating Qi and nourishing mind (育气养神), strengthening visceral function (厚固脏腑). | *Yang's Familiy Heritage Formulas* (杨氏家藏方) |
| **7** | *Jiao-Shen* Pill (椒肾丸) | Fruits of *Zanthoxylum bungeanum* (花椒); roots of *Atractylodes macrocephala* Koidz. (白术); barks of *Cinnamomum cassia* Presl (肉桂); juvenile horn of *Cervus nippon* Temminck (鹿茸); fruits of *Psoralea corylifolia* L. (补骨脂); roots of *Zingiber officinale* Rosc. (干姜); | Warming kidney and tonifying deficiency (温肾补虚); securing essence and reducing urination (固精缩尿) | *Peaceful holy benevolent prescriptions* (太平圣惠方) |
| **8** | *Jiao-Zhu* Decoction (椒茱汤) | Fruits of *Zanthoxylum bungeanum* (花椒); fruits of Euodia rutaecarpa (Juss.) Benth. (吴茱萸); fruits of Cnidium monnieri (L.) Cuss. (蛇床子)  | Destroying parasites and relieving itching | *Medical Complete Book* (医统大全) |
| **9** | *Jie-Ji-Shu-Jiao* Decoction (解急蜀椒汤) | Fruits of *Zanthoxylum bungeanum* (花椒); roots of Zingiber officinale Rosc. (干姜); roots of *Pinellia ternate* (Thunb.) Breit.; roots of *Glycyrrhiza uralensis* Fisch. (甘草); roots of *Aconitum carmichaelii* Debx. (附子) | Warming energizer, eliminating cold and relieving pain (温中, 解结; 逐寒, 止痛) | *Medical secrets of an official* (外台秘要) |
| **10** | *Shu-Jiao-Jiu-Zhong* Decoction (蜀椒救中汤) | Fruits of *Zanthoxylum bungeanum* (花椒); roots of *Zingiber officinale* Rosc. (干姜); barks of *Mgnolia officinalis* Rehd.et Wils. (厚朴); seeds of *Areca catechu* L. (槟榔); barks of Citrus reticulata Blanco (广陈皮). | Warming energizer and promoting Qi (温中行气); dispelling dampness and removing filth (化湿辟秽) | *Item differentiation of warm febrile diseases* (温病条辨) |
| **11** | *Wen-Zhong Decoction* (温中汤) | Fruits of *Zanthoxylum bungeanum* (花椒); roots of *Angelica sinensis* (Oliv.) Diels (当归); roots of *Atractylodes macrocephala* Koidz. (白术); roots of *Panax ginseng* C. A. Mey. (人参); roots of *Aconitum carmichaelii* Debx. (附子); roots of Zingiber officinale Rosc. (干姜); roots of *Glycyrrhiza uralensis* Fisch. (甘草); | Warming energizer (温中), dispelling cold and wind (祛风散寒), and stopping sweat (止汗) | *Wonderful well-tried recipes* (奇效良方) |
| **12** | *Wu-Jia-Pi* Decoction (五加皮汤) | Fruits of *Zanthoxylum bungeanum* (花椒); roots of *Angelica sinensis* (Oliv.) Diels (当归); Resins of Commiphora myrrha Engl. (没药); barks of the roots of *Acanthopanax gracilistylus* W. W. Smith. (五加皮); pericarps of *Citrus reticulata* Blanco (青皮); barks of the roots of *Paeonia suffruticosa* Andr. (牡丹皮); buds of *Eugenia caryophyllata* Thunb (丁香) | Promoting blood circulation and resolving blood stasis (活血化瘀); Reducing swelling and pain (消肿止痛) | *The Golden mirror of medicine* (医宗金鉴) |
| **13** | *Wu-Mei* Pills (乌梅丸) | Fruits of *Zanthoxylum bungeanum* (花椒); fruits of *Prunus mume* (Sieb.) Sieb. et Zucc. (乌梅); roots of *Asarum heterotropoides* Fr. Schmidt var. mandshuricum (Maxim.) Kitag. (细辛); roots of *Coptis chinensis* Franch. (黄连); roots of *Zingiber officinale* Rosc. (干姜); roots of *Panax ginseng* C. A. Mey. (人参); roots of *Aconitum carmichaelii* Debx. (附子) | Warm visceras and expelling roundworms (温脏安蛔) | *Treatise on Febrile Diseases* (伤寒论) |
| **14** | *Untitled Prescription* 1 | Fruits of *Zanthoxylum bungeanum* (花椒); feldspar (长石); Gypsum Rubrum (凝水石); twigs of *Cinnamomum cassia* Presl (桂枝); seeds of Cuscuta australis R.Br.(菟丝子); fresh roots of *Zingiber officinale* Rosc. (生姜). | Treating “*Thirst disorder syndrome*” which also known as Diabetes” | *Blending decoctions to treat sixty ailments* (治六十病方和齐汤法) |
| **15** | *Untitled Prescription* 2 | Fruits of *Zanthoxylum bungeanum* (花椒); roots of *Sophora flavescens* Ait. (苦参); twigs of *Cinnamomum cassia* Presl (桂枝); fresh roots of *Zingiber officinale* Rosc. (生姜); roots of *Anemarrhena asphodeloides* Bge. (知母); roots of *Gentiana manshurica* Kitag. (龙胆); roots of *Trichosanthes kirilowii* Maxim. (栝楼根); roots of *Aconitum carmichaelii* Debeaux (乌头). | Treating “*Thirst disorder syndrome*” which also known as Diabetes” | *Blending decoctions to treat sixty ailments* (治六十病方和齐汤法) |
| **16** | *Untitled Prescription* 3 | Fruits of *Zanthoxylum bungeanum* (花椒); feldspar (长石); seeds of Cuscuta australis R.Br.(菟丝子); fresh roots of *Zingiber officinale* Rosc. (生姜); Gypsum Rubrum (凝水石) | Treating “*Thirst disorder syndrome*” which also known as Diabetes” | *Blending decoctions to treat sixty ailments* (治六十病方和齐汤法) |
| **17** | *Untitled Prescription* 4 | Fruits of *Zanthoxylum bungeanum* (花椒); roots of *Trichosanthes kirilowii* Maxim. (栝楼根); feldspar (长石); Gypsum Rubrum (凝水石)  | Treating “*Thirst disorder syndrome*” which also known as Diabetes” | *Blending decoctions to treat sixty ailments* (治六十病方和齐汤法) |

Table S2. Amides isolated from the fruits of *Zanthoxylum bungeanum.*

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Name** | **Molecular formula** | **Chemical structure** |
| 1 | Hydroxy-α-Sanshool | C16H25NO2 |  |
| 2 | α-Sanshool | C16H25NO |  |
| 3 | Hydroxy-β-Sanshool | C16H25NO2 |  |
| 4 | β-Sanshool | C16H25NO |  |
| 5 | Hydroxy-γ-Sanshool | C18H27NO2 |  |
| 6 | γ-Sanshool | C18H27NO |  |
| 7 | Tetrahydrobungeanool | C18H33NO2 |  |
| 8 | dihydrobungeanool | C18H31NO |  |
| 9 | dehydro-7-sanshool | C18H25NO |  |
| 10 | isobungeanool | C18H29NO2 |  |
| 11 | Qinbunamide A | C18H31NO4 |  |
| 12 | Qinbunamide B | C18H31NO4 |  |
| 13 | Qinbunamide C | C15H23NO4 |  |
| 14 | hydroxy-γ-isosanshool | C18H27NO2 |  |
| 15 | (2E,4E,8E,10E,12E)-N-Isobutyl-2,4,8,10,12-tetradecapentaenamide | C18H27NO |  |
| 16 | Bungeanool | C18H29NO2 |  |
| 17 | (2E,6E,8E)-N-(2-Hydroxy-2-methylpropyl) -10-oxo-2,6,8-decatrienamide | C14H21NO3 |  |
| 18 | 2’-Hydroxy-N-isobytyl-[trans-2,6,8,10] dodecatetraenamide | C16H25NO2 |  |
| 19 | (6RS)-(2E,7E,9E)-6-Hydroxy-N-(2-hydroxy- 2-methylpropyl)-11-oxo-2,7,9-dodecatrienamide | C16H25NO4 |  |
| 20 | N- [2-(3,4- Dimethoxyphenyl) ethyl]-3-phenyl-acrylamide | C19H21NO3 |  |
| 21 | Bugeanumamide A | C16H23NO4 |  |
| 22 | (11RS)-(2E,7E,9E)-11-Hydroxy-N-(2-hydroxy-2-methylpropyl)-6-oxo-2,7,9-dodecatrienamide | C16H25NO4 |  |
| 23 | (10RS,11RS)-(2E,6Z,8E)-10,11-Dihydroxy-N-(2-hydroxy-2-methylpropyl)-2,6,8-dodecatrienamide | C18H29NO4 |  |
| 24 | (6RS,11RS)-(2E,7E,9E)-N-(2-Hydroxy-2-methylpropyl)-6,11-dioxo-2,7,9-dodecatrienamide | C16H27NO4 |  |
| 25 | (2E,4E,9E,11E)-N-(2-Hydroxy-2-methypropyl)-8-hydroxy-13-oxo-2,4,9,11-tetradecatetraenamide | C18H27NO4 |  |
| 26 | (2E,4E,9E,11E)-N-(Hydroxy-2-methypropyl)-8,13-dihydroxy-2,4,9,11-tetradecatetraenamide | C14H23NO4 |  |
| 27 | (2E)-6,6-Dimethoxy-N-(2-hydroxy-2-methylpropyl)-2-hexenamide | C12H23NO4 |  |
| 28 | hydroxy-ε-sanshool | C16H25NO2 |  |

Table S3. Volatile substances isolated from the fruits of *Zanthoxylum bungeanum.*

|  |  |  |  |
| --- | --- | --- | --- |
| **No.** | **Name** | **Molecular formula** | **Chemical structure** |
| 29 | α-Thujene | C10H16 |  |
| 30 | α-Pinene | C10H16 |  |
| 31 | Sabinene | C10H16 |  |
| 32 | β-Pinene | C10H16 |  |
| 33 | Myrcene | C10H16 |  |
| 34 | α-Phellandrene | C10H16 |  |
| 35 | α-Terpinene  | C10H16 |  |
| 36 | p-Cymene | C10H16 |  |
| 37 | β-Phellandrene | C10H16 |  |
| 38 | Cineol | C10H18O |  |
| 39 | γ-Terpinene | C10H16 |  |
| 40 | 2-Carene | C10H16 |  |
| 41 | Linalool | C10H18O |  |
| 42 | α-Terpineol | C10H18O |  |
| 43 | 1-Methyl-4- (1-methylethyl) | C10H18O |  |
| 44 | 3-Cyclohexene-1-methanol | C10H18O |  |
| 45 | Terpinolene | C10H16 |  |
| 46 | Limonene | C10H16 |  |
| 47 | Geranyl acetate | C12H20O2 |  |
| 48 | Acetosyringone | C10H12O4 |  |
| 49 | (-)-Terpinen-4-ol | C10H18O |  |
| 50 | Cuminaldehyde | C10H12O |  |
| 51 | Dibutyl phthalate | C16H22O4 |  |
| 52 | 1- Methoxy- 4- (1- propenyl)- Benzene | C10H12O |  |
| 53 | Myrtenyl acetate | C12H18O2 |  |

Table S4. Flavonoids isolated from the fruits of *Zanthoxylum bungeanum*.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Name** | **Molecular formula** | **Chemical structure** |
| 54 | Quercetin-3-O-α-L-Rhamnopyranosyl-(1-6)-β-D-glucopy ranoside | C27H30O16 |  |
| 55 | Quercetin-3-O-α-L-Rhamnopyranosyl | C21H20H11 |  |
| 56 | Quercetin 3-O-β-glucopyranoside | C21H20O12 |  |
| 57 | Quercetin | C15H10O7 |  |
| 58 | Rutin | C27H30O16 |  |
| 59 | Isorhamnetin | C16H12O7 |  |
| 60 | Hyperoside | C21H20O12 |  |
| 61 | Vitexin | C21H20O10 |  |

Table S5. Lignans isolated from the fruits of *Zanthoxylum bungeanum.*

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Name** | **Molecular formula** | **Chemical structure** |
| 62 | 7-methoxycoumarin | C10H8O3 |  |
| 63 | Herniarin | C10H8O3 |  |
| 64 | Neochlorogenic acid | C16H18O9 |  |
| 65 | Sesamin | C20H18O6 |  |
| 66 | Eudesmin | C22H26O6 |  |
| 67 | Chlorogenic acid | C16H18O9 |  |

Table S6. Other components in fruits of *Zanthoxylum bungeanum.*

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Name** | **Molecular formula** | **Chemical structure** |
| 68 | 2-Phenylethyl-6-O-β-D-glucopyranoside | C14H20O6 |  |
| 69 | Isobutyl-O-β-D-Glucopyranoside | C10H20O6 |  |
| 70 | 3-methoxyphenethyl alcohol-4-O-β-D-glucopyranoside | C15H22O8 |  |
| 71 | (1′R, 3′R, 5′R, 8′S)-epidihydrophaseic acid-O-β-D-glucoside | C21H32O10 |  |
| 72 | Benzyl -1-O- β-D-glucopyranoside | C13H18O6 |  |
| 73 | Benzenepropanoic acid-O-β-D-glucopyranosyloxy | C15H20O8 |  |
| 74 | Orcinol glucoside | C13H18O7 |  |
| 75 | 3-Methoxy-5-hydroxyphe nol-1-O-β-D-glucopyranoside | C13H18O8 |  |
| 76 | 4-Hydroxyl-3, 5-dimethoxyl-6-O-β-D-glucosebenzene | C14H20O9 |  |
| 77 | 2-(4-Hydroxy-3-methoxyphenyl) ethyl-O-β-D-glucopyranoside | C15H22O8 |  |
| 78 | Coumaric Acid-4-O-β-D-Glucopyranoside | C15H18O8 |  |
| 79 | Hloroglucinol 1-O-β-D-glucopyranoside | C12H16O8 |  |
| 80 | 3,5-dihydroxy phenethyl alcohol 3-O-β-glucopyranoside | C14H20O8 |  |
| 81 | Betulalbuside A | C16H28O7 |  |
| 82 | 1-hydroxylinaloyl-6-O-β-D-glucopyranoside | C16H28O7 |  |
| 83 | Guanosine | C10H12N4O5 |  |
| 84 | Arbutin | C12H16O7 |  |
| 85 | Syringin | C17H24O9 |  |
| 86 | skimmiamine | C14H13NO4 |  |