

Supporting Information

Supporting materials and methods

1. HPLC-DAD analysis of the preferred prescription

To facilitate the identification of the preferred prescription components, the preferred prescription aqueous extract was analyzed by the HPLC-DAD. The extracts of the preferred prescription were filtered with a 0.22 µm filter membrane, a Phenomenex Synergi 4µ Fusion-RP 80A (250 mm*4.6 mm, 5 µm) column was used for chromatographic separation. The mobile phase was composed of acetonitrile (A) and aqueous solution (B). The linear elution gradient was 0-40 min, 5-35% A; 40-50 min, 35-70% A; 50-55 min, 70-90% A; and 55-58 min, 90-5% A. The injection volume was 10 µL, and the flow rate was 1.0 mL/min. The reference compounds were precisely weighted and diluted in methanol with fixed volume. The detection wavelengths were as follows: 248 nm (calycosin 7-O-glucoside, calycosin, and formononetin), 356 nm (rutin), 282 nm (naringin, hesperidin, and neohesperidin), 288 nm (naringenin), 266 nm (kaempferol), 330 nm (nobiletin), and 220 nm (atractylenolide II). The linear range, average recovery, precision, exclusivity, and stability data were analyzed. HPLC-DAD, high-performance liquid chromatography diode array detection

2. MTT assay

AGS, HGC-27, MKN28, SGC-7901 cells (5×10^3 cells/well) were seeded into 96-well plates separately for 24 h to allow adherence to the walls. To determine the decoction dose, GC cells were treated with different concentrations (0, 1, 2, 8, 16 mg/mL) of the preferred prescription for 48 h. MTT (120 µL, 5 mg/mL) (Sigma, USA) was added after the medium was removed, and the cells were incubated for 4 h in the incubator. The supernatant was removed, and 150 µL of dimethyl sulfoxide (DMSO) was added for 10 min. Absorbance at 490 nm was detected on an ELX800 Automatic microplate reader (Bio-Tek, USA) to calculate the absorbance (OD₄₉₀). The IC₅₀ was calculated by Graphpad software. MTT, 3-(4,5-Dimethyl-2-thiazolyl)-2,5-diphenylterazolium bromide; IC₅₀, half-maximal inhibitory concentration

Table S1 Top 24 principal function-categorized herbs

No.	Herb	Functional category	Occurrence frequency (%)	Number of occurrences	Frequency of use (%)	Classification category
1	<i>Atractylodis Macrocephalae Rhizoma</i>	a1	26.37	145	74.74	Tonifying and replenishing medicinal
2	<i>Poria</i>	i	10.07	126	64.95	Dampness-draining diuretic medicinal
3	<i>Astragali Radix</i>	a1	26.37	107	55.15	Tonifying and replenishing medicinal
4	<i>Codonopsis Radix</i>	a1	26.37	105	54.12	Tonifying and replenishing medicinal
5	<i>Glycyrrhizae Radix</i>	a1	26.37	96	49.48	Tonifying and replenishing medicinal
6	<i>Pinelliae Rhizoma</i>	e	6.51	85	43.81	Cough-suppressing and panting-calming medicinal
7	<i>Citri Reticulatae Pericarpium</i>	d	8.74	77	39.69	Qi-regulating medicinal
8	<i>Coicis Semen</i>	i	10.07	63	32.47	Dampness-draining diuretic medicinal
9	<i>Herba Hedyotidis Diffusae</i>	b1	8.08	54	27.84	Heat-clearing medicinal
10	<i>Angelicae Sinensis Radix</i>	a3	5.04	48	24.74	Tonifying and replenishing medicinal
11	<i>Galli Gigeriae Endothelium Corneum</i>	h	5.51	38	19.59	Digestant medicinal
12	<i>Curcumae Rhizoma</i>	c	6.89	34	17.53	Blood-activating and stasis-dispelling medicinal
13	<i>Aucklandiae Radix</i>	d	8.74	30	15.46	Qi-regulating medicinal
14	<i>Pseudostellariae Radix</i>	a1	26.37	29	14.95	Tonifying and replenishing medicinal
15	<i>Paeoniae Radix Alba</i>	a3	5.04	29	14.95	Tonifying and replenishing medicinal
16	<i>Scutellariae Barbatae Herba</i>	b1	8.08	29	14.95	Heat-clearing medicinal
17	<i>Amomi Fructus</i>	k	2.57	28	14.43	Dampness-resolving medicinal
18	<i>Dioscoreae Rhizoma</i>	a1	26.37	26	13.40	Tonifying and replenishing medicinal
19	<i>Hordei Fructus Germinatus</i>	h	5.51	25	12.89	Digestant medicinal
20	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>	c	6.89	24	12.37	Blood-activating and stasis-dispelling medicinal
21	<i>Ligustri Lucidi Fructus</i>	a2	4.18	24	12.37	Tonifying and replenishing medicinal
22	<i>Aurantii Fructus</i>	d	8.74	23	11.86	Qi-regulating medicinal
23	<i>Radix Actinidiae Chinensis</i>	m	2.38	23	11.86	Wind-dampness dispelling medicinal
24	<i>Crataegi Fructus</i>	h	5.51	21	10.82	Digestant medicinal

Occurrence frequency = number of occurrences for the herbs appearing in 194 prescriptions / total cumulative occurrences for 148 herbs appearing in 194 prescriptions (i.e. 2,103); Frequency of use = number of prescriptions recording the herbs in use/ total number of the eligible prescriptions (i.e. 194). Abbreviations: a1: Qi-tonifying medicinal; a2: Yin-tonifying medicinal; a3: Blood-tonifying medicinal; a4: Yang-tonifying medicinal; b: heat-clearing medicinal; c: blood-activating and stasis-dispelling medicinal; d: Qi-regulating medicinal; e: cough-suppressing and panting-calming medicinal; f: interior-warming medicinal; g: Liver-pacifying medicinal; h: digestant medicinal; i: dampness-draining diuretic medicinal; j: exterior-releasing medicinal; k: dampness-resolving medicinal; l: hemostatic medicinal; m: wind-dampness dispelling medicinal; n: astringent medicinal; o: purgative medicinal; p: orifice-opening medicinal; q: repellent medicinal; r: attacking poison, insects and itch-relieving medicinal.

Table S2 Principal functional categorizations and clinical application of the most recorded herbs

Herbal nature	Principal functional categorizations	Number of decoctions using the herbs	Frequency of use (%)	Syndromes	Key signs & symptoms	Treatment principles	Representative herbs
Sweet, warm	Qi-tonifying	182	93.81	<i>Middle-Jiao</i> Deficiency	Poor appetite, dislike to talk, lassitude, weak limbs, borborygmus, loose stools, heavy descending sensation in abdominal cavity, prolapse of rectum.	Tonify Middle-Jiao Qi	<i>Atractylodis Macrocephalae Rhizoma, Astragali Radix, Codonopsis Radix, Glycyrrhizae Radix, Pseudostellariae Radix, Dioscoreae Rhizoma</i>
Bitter, warm/ pungent, warm	Dampness-draining	149	76.80	Cold damp obstructs Spleen	Fullness sensation in upper abdomen, poor appetite, sticky sensation in mouth, heavy sensation on head, loose stools or diarrhea.	Tonify Spleen to transform damp	<i>Poria, Coicis Semen, Amomi Fructus</i>
				Damp-heat stagnates interiorly	Full abdomen & hypochondrium distension, no desire for food, bitter taste in mouth, thirsty, heavy sensation on body, yellow urine, loose stools, jaundice, itchy skin.	Remove damp and heat	
				Damp from Spleen affecting Lung	Cough/vomiting of phlegm, saliva, congestion in chest, shortness of breath (SOB), poor appetite.	Dry damp, remove phlegm	
Pungent, warm/ bitter, warm	Qi-regulating	119	61.34	Stagnation of Liver Qi	Mental depression, restlessness, sighing, distension, wandering pain in the costal and hypochondriac region, distress in epigastrium, poor appetite or vomiting, irregular bowel movements, thin greasy tongue coating, wiry pulse.	Disperse Liver Qi	<i>Citri Reticulatae Pericarpium, Aucklandiae Radix, Aurantii Fructus, Fructus Evodiae</i>
				Qi stagnation transforming into Fire	Irritability, stuffiness in the chest, hypochondriac distension, acid regurgitation, dry & bitter mouth, constipation or headache, tinnitus, red tongue & yellow coating, wiry-rapid pulse.	Purge Fire from Liver	
Pungent, warm/ bitter, warm	Blood-activating and stasis-dispelling	84	42.27	Qi stagnation, Blood stasis	Moving/fixed pain, distending pain on hypochondrium, masses in abdominal cavity, stabbing pain aggravated by pressure, purplish tongue body, purple spots; thready, string-taut pulse.	Invigorate blood circulation, eliminate blood stasis	<i>Curcumae Rhizoma, Salviae Miltiorrhizae Radix et Rhizoma</i>
Sweet, warm/sweet, cold	Blood-tonifying	69	35.57	Blood deficiency	Pale or yellowish complexion, pale lustreless lips & nails, dizziness, vertigo, palpitations, insomnia, numbness of limbs, pale tongue body, thready-weak pulse.	Replenish Blood	<i>Angelicae Sinensis Radix, Paeoniae Radix Alba</i>
Sweet, neutral	Food abating	55	28.35	Stomach excessive	Epigastric and abdominal distension and fullness or pain, which are aggravated by food intake, belching with foul smell, anorexia, constipation, acidic regurgitation, nausea, vomiting, diarrhea with foul smell or fermented contents or constipation.	Dissolve the stagnation	<i>Galli Gigeriae Endothelium Corneum, Hordei Fructus Germinatus, Crataegi Fructus</i>
Sweet, cold	Yin-tonifying	55	28.35	Stomach Yin deficiency	Dry mouth & lips, thirsty, hunger but no desire for food, retching, hiccups, constipation/dry stools, red dry tongue with little coating or mirror red tongue, thready-rapid pulse.	Tonify Stomach Yin fluids	<i>Herba Dendrobii, Rhizoma Polygonati Odorati</i>
Sweet, warm/ pungent, warm	Yang-tonifying	27	13.92	Spleen Yang deficiency	Lustreless withered yellow complexion, cold sensation at epigastric region, vomiting clear water, poor appetite, distension, preference for hot drinks, etc.	Warm Middle-Jiao Yang	<i>Semen Cuscutae, Fructus Psoraleae, Semen Myristicae, Rhizoma Zingiberis</i>
				Yang deficiency of Spleen & Kidney	SOB, dislike to talk, cold & sore loins & knees, pre-dawn diarrhea.	Warm Spleen & Kidney Yang	
				Cold in Stomach	Cold pain in Stomach, aggravated by cold, relieved by warmth, no thirst, vomiting clear water, hiccup.	Warm Stomach to dispel cold	

Frequency of use = number of prescriptions recording the herbs in use/ total number of the eligible prescriptions (i.e. 194). SOB, shortness of breath.

Table S3 Top 10 triplet herbal combinations

Herb (LHS)	Number of decoctions	Herbs (RHS)	Number of occurrences	Support (LHS) (%)	Confidence (LHS=>RHS) (%)	LIFT
<i>Poria</i>	126	<i>Aucklandiae Radix, Glycyrrhizae Radix</i> →	21	10.82	100.00	1.54
<i>Atractylodis Macrocephalae Rhizoma</i>	145	<i>Aucklandiae Radix, Codonopsis Radix</i> →	20	10.31	100.00	1.34
<i>Atractylodis Macrocephalae Rhizoma</i>	145	<i>Galli Gigeriae Endothelium Corneum, Codonopsis Radix</i> →	20	10.31	100.00	1.34
<i>Atractylodis Macrocephalae Rhizoma</i>	145	<i>Coicis Semen, Glycyrrhizae Radix</i> →	29	14.95	96.55	1.29
<i>Atractylodis Macrocephalae Rhizoma</i>	145	<i>Aucklandiae Radix, Poria</i> →	25	12.89	96.00	1.28
<i>Poria</i>	126	<i>Pseudostellariae Radix, Atractylodis Macrocephalae Rhizoma</i> →	24	12.37	95.83	1.48
<i>Atractylodis Macrocephalae Rhizoma</i>	145	<i>Hordei Fructus Germinatus, Codonopsis Radix</i> →	21	10.82	95.24	1.27
<i>Codonopsis Radix</i>	105	<i>Hordei Fructus Germinatus, Atractylodis Macrocephalae Rhizoma</i> →	21	10.82	95.24	1.76
<i>Atractylodis Macrocephalae Rhizoma</i>	145	<i>Aucklandiae Radix, Glycyrrhizae Radix</i> →	21	10.82	95.24	1.27
<i>Atractylodis Macrocephalae Rhizoma</i>	145	<i>Paeoniae Radix Alba, Poria</i> →	20	10.31	95.00	1.27

Occurrence= number of occurrences of the herbal pairs appearing in the eligible prescriptions (i.e. 194). LHS, left hand side; RHS, right hand side

Table S4 Bioactive compounds of the 24 core herbs

Molecule ID	Compound	Abbr. of Compounds	MW	OB (%)	DL	Herb
MOL000028	alpha-Amyrin	01BZ	426.8	39.51	0.76	<i>Attractylodes Macrocephalae Rhizoma</i>
MOL000049	3β-acetoxyatractylone	02BZ	274.39	54.07	0.22	<i>Attractylodes Macrocephalae Rhizoma</i>
MOL000072	8β-ethoxy atractylonolide III	03BZ	276.41	35.95	0.21	<i>Attractylodes Macrocephalae Rhizoma</i>
MOL000211	Betulinic acid	01HQ	456.78	55.38	0.78	<i>Astragal Radix</i>
MOL000239	Kumatakenin	02HQ	314.31	50.83	0.29	<i>Astragal Radix</i>
MOL000296	Hederagenin	03HQ	414.79	36.91	0.75	<i>Astragal Radix</i>
MOL000354	Isorhamnetin	04HQ	316.28	49.6	0.31	<i>Astragal Radix</i>
MOL000387	Bifendate	05HQ	418.38	31.1	0.67	<i>Astragal Radix</i>
MOL000392	Formononetin	06HQ	268.28	69.67	0.21	<i>Astragal Radix</i>
MOL000398	Isoflavanone	07HQ	224.25	109.99	0.3	<i>Astragal Radix</i>
MOL000417	Calycosin	08HQ	284.28	47.75	0.24	<i>Astragal Radix</i>
MOL000422	Kaempferol	09HQ	286.25	41.88	0.24	<i>Astragal Radix</i>
MOL000098	Quercetin	10HQ	302.25	46.43	0.28	<i>Astragal Radix</i>
MOL002670	Cavidine	01BX	353.45	35.64	0.81	<i>Pinelliae Rhizoma</i>
MOL002714	Baicalin	02BX	270.25	33.52	0.21	<i>Pinelliae Rhizoma</i>
MOL002776	Baicalin	03BX	446.39	40.12	0.75	<i>Pinelliae Rhizoma</i>
MOL000358	beta-Sitosterol	04BX	414.79	36.91	0.75	<i>Pinelliae Rhizoma</i>
MOL000449	Stigmasterol	05BX	412.77	43.83	0.76	<i>Pinelliae Rhizoma</i>
MOL005030	11-Eicosenoic acid	06BX	310.58	30.7	0.2	<i>Pinelliae Rhizoma</i>
MOL000519	(-)-Neocryptotanshinone	07BX	314.41	31.11	0.32	<i>Pinelliae Rhizoma</i>
MOL000378	Cyclo(L-tyrosyl-L-phenylalanyl)	08BX	310.3	38.69	0.78	<i>Pinelliae Rhizoma</i>
MOL000359	beta-Sitosterol	01CP	414.79	36.91	0.75	<i>Citri Reticulatae Pericarpium</i>
MOL004328	Naringenin	02CP	272.27	59.29	0.21	<i>Citri Reticulatae Pericarpium</i>
MOL005828	Nobiletin	03CP	402.43	61.67	0.52	<i>Citri Reticulatae Pericarpium</i>
MOL001659	Poriferasterol	01BHSSC	412.77	43.83	0.76	<i>Herba Hedycotis</i>
MOL000449	Stigmasterol	02BHSSC	412.77	43.83	0.76	<i>Herba Hedycotis</i>
MOL000358	beta-Sitosterol	03BHSSC	414.79	36.91	0.75	<i>Herba Hedycotis</i>
MOL000098	Quercetin	04BHSSC	302.25	46.43	0.28	<i>Herba Hedycotis</i>
MOL010828	Cynaropicrin	01MX	346.41	67.5	0.38	<i>Aucklandiae Radix</i>
MOL010839	Lappadilactone	02MX	494.68	38.56	0.73	<i>Aucklandiae Radix</i>
MOL000211	Betulinic acid	03MX	456.78	55.38	0.78	<i>Aucklandiae Radix</i>
MOL000359	beta-Sitosterol	04MX	414.79	36.91	0.75	<i>Aucklandiae Radix</i>
MOL000449	Stigmasterol	05MX	412.77	43.83	0.76	<i>Aucklandiae Radix</i>
MOL0001973	beta-Sitosterol acetate	01SR	456.83	40.39	0.85	<i>Amomi Fructus</i>
MOL000358	beta-Sitosterol	02SR	414.79	36.91	0.75	<i>Amomi Fructus</i>
MOL000449	Stigmasterol	03SR	412.77	43.83	0.76	<i>Amomi Fructus</i>
MOL007180	Glimperide	04SR	490.69	32.29	0.7	<i>Amomi Fructus</i>
MOL007514	11,14-Eicosadienoic acid, methyl ester	05SR	322.59	39.67	0.23	<i>Amomi Fructus</i>
MOL010846	Decoxynivalenol	01MY	296.35	31.16	0.25	<i>Hordei Fructus Germinatus</i>
MOL005088	Nivalenol	02MY	312.35	35.68	0.28	<i>Hordei Fructus Germinatus</i>
MOL002322	Isovitexin	03MY	432.41	31.29	0.72	<i>Hordei Fructus Germinatus</i>
MOL000358	beta-Sitosterol	04MY	414.79	36.91	0.75	<i>Hordei Fructus Germinatus</i>
MOL004798	Delphinidin	05MY	338.69	40.63	0.28	<i>Hordei Fructus Germinatus</i>
MOL000492	Ciandanol	06MY	290.29	54.83	0.24	<i>Hordei Fructus Germinatus</i>
MOL000569	Digallic acid	07MY	322.24	61.85	0.26	<i>Hordei Fructus Germinatus</i>
MOL000006	Luteolin	08MY	286.25	36.16	0.25	<i>Hordei Fructus Germinatus</i>
MOL007180	Glimperide	09MY	490.69	32.29	0.7	<i>Hordei Fructus Germinatus</i>
MOL000073	(+)-Epicatechin	10MY	290.29	48.96	0.24	<i>Hordei Fructus Germinatus</i>
MOL013381	Marmarin	01ZQ	332.43	38.23	0.31	<i>Aurantii Fructus</i>
MOL002341	Hesperetin	02ZQ	302.3	70.31	0.27	<i>Aurantii Fructus</i>
MOL000358	beta-Sitosterol	03ZQ	414.79	36.91	0.75	<i>Aurantii Fructus</i>
MOL004328	Naringenin	04ZQ	272.27	59.29	0.21	<i>Aurantii Fructus</i>
MOL005828	Nobiletin	05ZQ	402.43	61.67	0.52	<i>Aurantii Fructus</i>
MOL000358	beta-Sitosterol	01TLG	414.79	36.91	0.75	<i>Radix Actinidiae Chinesis</i>
MOL000359	beta-Sitosterol	02TLG	414.79	36.91	0.75	<i>Radix Actinidiae Chinesis</i>
MOL000471	Aloe-emodin	03TLG	270.25	83.38	0.24	<i>Radix Actinidiae Chinesis</i>
MOL000492	Ciandanol	04TLG	290.29	54.83	0.24	<i>Radix Actinidiae Chinesis</i>
MOL000073	(+)-Epicatechin	05TLG	290.29	48.96	0.24	<i>Radix Actinidiae Chinesis</i>
MOL000098	Quercetin	06TLG	302.25	46.43	0.28	<i>Radix Actinidiae Chinesis</i>
MOL0001919	paeoniflorgenone	01BS	318.35	87.59	0.57	<i>Paeoniae Radix Alba</i>
MOL001918	Palbinone	02BS	358.52	43.56	0.33	<i>Paeoniae Radix Alba</i>
MOL001921	(+)-Lactiflorin	03BS	462.49	49.12	0.8	<i>Paeoniae Radix Alba</i>
MOL001924	Paeoniflorin	04BS	480.51	53.87	0.79	<i>Paeoniae Radix Alba</i>
MOL001928	Albiflorin	05BS	480.5	66.64	0.33	<i>Paeoniae Radix Alba</i>
MOL001930	Benzoyloxy-paeoniflorin	06BS	600.6	31.27	0.75	<i>Paeoniae Radix Alba</i>
MOL000211	Betulinic acid	07BS	456.78	55.38	0.78	<i>Paeoniae Radix Alba</i>
MOL000359	beta-Sitosterol	08BS	414.79	36.91	0.75	<i>Paeoniae Radix Alba</i>
MOL000422	Kaempferol	09BS	286.25	41.88	0.24	<i>Paeoniae Radix Alba</i>
MOL000492	Ciandanol	10BS	290.29	54.83	0.24	<i>Paeoniae Radix Alba</i>
MOL002776	Baicalin	01BZL	446.39	40.12	0.75	<i>Scutellariae Barbatae Herba</i>
MOL005043	Campesterol	02BZL	400.76	37.58	0.71	<i>Scutellariae Barbatae Herba</i>
MOL000953	Cholesterol	03BZL	386.73	37.87	0.68	<i>Scutellariae Barbatae Herba</i>
MOL000358	beta-Sitosterol	04BZL	414.79	36.91	0.75	<i>Scutellariae Barbatae Herba</i>
MOL012266	Rivularin (flavone)	05BZL	344.34	37.94	0.37	<i>Scutellariae Barbatae Herba</i>
MOL0001973	beta-Sitosterol acetate	06BZL	456.83	40.39	0.85	<i>Scutellariae Barbatae Herba</i>
MOL000449	Stigmasterol	07BZL	412.77	43.83	0.76	<i>Scutellariae Barbatae Herba</i>
MOL000173	Wogonin	08BZL	284.28	30.68	0.23	<i>Scutellariae Barbatae Herba</i>
MOL001735	Hispidulin	09BZL	300.28	30.97	0.27	<i>Scutellariae Barbatae Herba</i>
MOL001755	Stigmast-4-en-3-one	10BZL	412.77	36.08	0.76	<i>Scutellariae Barbatae Herba</i>
MOL002714	Baicalin	11BZL	270.25	33.52	0.21	<i>Scutellariae Barbatae Herba</i>
MOL002719	Carthamin	12BZL	288.27	33.23	0.24	<i>Scutellariae Barbatae Herba</i>
MOL002915	Salvigenin	13BZL	328.34	49.07	0.33	<i>Scutellariae Barbatae Herba</i>
MOL000351	Rhamnazin	14BZL	330.31	47.14	0.34	<i>Scutellariae Barbatae Herba</i>
MOL000359	beta-Sitosterol	15BZL	414.79	36.91	0.75	<i>Scutellariae Barbatae Herba</i>
MOL005190	Eriodictyol	16BZL	288.27	71.79	0.24	<i>Scutellariae Barbatae Herba</i>
MOL000006	Luteolin	17BZL	286.25	36.16	0.25	<i>Scutellariae Barbatae Herba</i>
MOL008206	5-Hydroxy-7,8-dimethoxyflavone	18BZL	298.31	44.09	0.25	<i>Scutellariae Barbatae Herba</i>
MOL000098	Quercetin	19BZL	302.25	46.43	0.28	<i>Scutellariae Barbatae Herba</i>
MOL001601	Trijuganone B	01DANS	280.34	38.75	0.36	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL001659	Poriferasterol	02DANS	412.77	43.83	0.76	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL001771	Clicosterol	03DANS	414.79	36.91	0.75	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL001942	Isoimperatorin	04DANS	370.3	45.46	0.23	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL002222	Sugiol	05DANS	200.48	36.11	0.28	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL002651	Dehydrotanshinone II A	06DANS	292.35	43.76	0.4	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL002776	Baicalin	07DANS	446.39	40.12	0.75	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL000569	Digallic acid	08DANS	322.24	61.85	0.26	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL000006	Luteolin	09DANS	286.25	36.16	0.25	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL006824	o-aramylin	10DANS	426.8	39.51	0.76	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007036	Arucadiol	11DANS	298.41	33.77	0.29	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007048	Touranetholic acid A	12DANS	312.29	48.24	0.31	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007061	Methylenanthraquinone	13DANS	178.32	37.07	0.36	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007064	Przewalskin B	14DANS	330.46	110.32	0.44	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007068	Przewalskinone B	15DANS	292.3	62.24	0.41	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007069	Tanshinol B	16DANS	296.34	55.74	0.4	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007079	Tanshinolaldehyde	17DANS	310.3	52.47	0.45	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007081	Danshenol B	18DANS	354.48	57.95	0.56	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007082	Danshenol A	19DANS	336.41	56.97	0.52	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007085	Salvilenone	20DANS	292.4	30.38	0.38	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007088	Cryptotanshinone	21DANS	296.39	52.34	0.4	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007098	Deoxyneocryptotanshinone	22DANS	298.41	49.4	0.29	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007101	1,2-Dihydrotanshinquinone	23DANS	278.32	45.04	0.36	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007105	Epidianshenspiroketallactone	24DANS	268.31	68.27	0.31	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007107	Ferruginol	25DANS	286.5	36.07	0.25	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007108	Isocryptotanshinone	26DANS	296.39	54.98	0.39	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007111	Isotanshinone IIA	27DANS	294.37	49.92	0.4	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007115	Manool	28DANS	290.5	45.04	0.2	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007118	Microtopol	29DANS	298.46	39.61	0.28	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007121	Miltipolone	30DANS	300.43	36.56	0.37	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007122	Miltirone	31DANS	282.41	36.76	0.25	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007124	Deoxyneocryptotanshinone	32DANS	298.4	39.46	0.23	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007125	Neocryptotanshinone	33DANS	314.41	52.49	0.32	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007127	Nortanshinone	34DANS	280.29	34.72	0.37	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007141	Salvianolic acid G	35DANS	418.3	45.56	0.61	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007143	Salvilenone	36DANS	292.4	32.43	0.23	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007145	Salviolone	37DANS	268.38	31.72	0.24	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007149	Sugiol	38DANS	300.48	34.49	0.39	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007150	Tanshindiol A	39DANS	312.34	75.39	0.46	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007151	Tanshindiol B	40DANS	312.34	42.67	0.45	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007152	Tanshindiol C	41DANS	312.34	42.85	0.45	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007154	Tanshinone IIA	42DANS	294.37	49.89	0.4	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL007156	Danshenxinun A	43DANS	296.34	45.64	0.3	<i>Salviae Miltiorrhizae Radix et Rhizoma</i>
MOL000358	beta-Sitosterol	01NZZ	414.79	36.91	0.75	<i>Ligustri Lucidi Fructus</i>
MOL000422	Kaempferol	02NZZ	286.25	41.88	0.24	<i>Ligustri Lucidi Fructus</i>
MOL004576	Taxifolin	03NZZ	304.27	57.84	0.27	<i>Ligustri Lucidi Fructus</i>
MOL005190	Eriodictyol	04NZZ	288.27	71.79	0.24	<i>Ligustri Lucidi Fructus</i>
MOL005209	Lucidusculine	05NZZ	401.6	30.11	0.75	<i>Ligustri Lucidi Fructus</i>
MOL000006	Luteolin	06NZZ	286.25	36.16	0.25	<i>Ligustri Lucidi Fructus</i>
MOL000098	Quercetin	07NZZ	302.25	46.43	0.28	<i>Ligustri Lucidi Fructus</i>
MOL000275	Trametenolic acid	01FL	456.78	38.71	0.8	<i>Poria</i>
MOL000276	Dehydrochrysinic acid	02FL	526.83	35.11	0.81	<i>Poria</i>
MOL000279	Cerevisterol	03FL	430.74	37.96	0.77	<i>Poria</i>
MOL000280	Dehydrotumulolic acid	04FL	484.79	31.07	0.82	<i>Poria</i>
MOL000282	Stellasterol	05FL	398.74	43.51	0.72	<i>Poria</i>
MOL000283	Ergosterol peroxide	06FL	428.6	40.36	0.81	<i>Poria</i>
MOL000285	Polyprenic acid C	07FL	482.77	38.26	0.82	<i>Poria</i>
MOL000287	Eburicoic acid	08FL	470.81	38.7	0.81	<i>Poria</i>
MOL000289	Pachymic acid	09FL	528.85	33.63	0.81	<i>Poria</i>

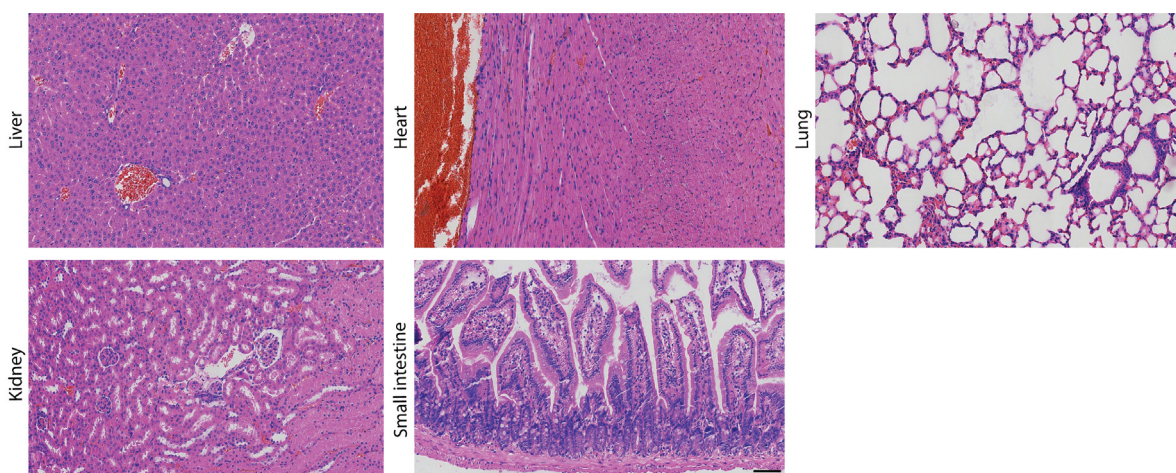


Figure S1 The preferred prescription had no toxic and side effect *in vivo*. Hematoxylin and eosin (H&E) staining of liver, heart, lung, kidney, and small intestine tissues of sacrificed nude mice (n = 5). The scale bar indicates 100 μ m. H&E, hematoxylin and eosin.

Treatment principles	Herbs	Indications of GC
Tonify <i>Middle-Jiao Qi</i> & invigorate Spleen	<i>Atractylodis Macrocephalae Rhizoma</i> , <i>Astragali Radix</i>	Fatigue, poor appetite, loose stools or diarrhea, SOB, spontaneous sweating, prolapse of rectum, etc.
Disperse <i>Qi</i> stagnation & dry dampness	<i>Citri Reticulatae Pericarpium</i> , <i>Pinelliae Rhizoma</i> , <i>Aucklandiae Radix</i> , <i>Amomi Fructus</i> , <i>Aurantii Fructus</i>	Fullness and painful in the abdomen, belching, sour regurgitation, nausea, vomiting, constipation or diarrhoea, etc.
Abate food & promote digestion	<i>Galli Gigeriae Endothelium Corneum</i> , <i>Hordei Fructus Germinatus</i> , <i>Crataegi Fructus</i>	Epigastric and abdominal distension and fullness or pain, which are aggravated by food intake, belching with foul smell, anorexia, constipation, acidic regurgitation, nausea, vomiting, diarrhea with foul smell or fermented contents or constipation, etc.
Clear heat & remove toxin	<i>Radix Actinidiae Chinensis</i> , <i>Herba Hedyotidis</i>	Internal abscesses, jaundice, indigestion, vomiting, diarrhea, etc.

Figure S2 Working mode of the preferred prescription. Treatment principles of the preferred prescription include tonifying *Middle-jiao* and invigorating the Spleen, dispersing *Qi* stagnation and drying dampness, abating food and promoting digestion, clearing heat, and removing toxins. SOB, short of breath.