

Supporting Information for

Original article

Analysis on herbal medicines utilized for treatment of COVID-19

Lu Luo^a, Jingwen Jiang^b, Cheng Wang^c, Martin Fitzgerald^d, Weifeng Hu^e, Yumei Zhou^f, Hui Zhang^g, Shilin Chen^{a,*}

^a*Institute of Chinese Materia Medica, China Academy of Chinese Medical Sciences, Beijing 100700, China*

^b*West China Biomedical Big Data Center, West China Hospital, Sichuan University, Chengdu 610041, China*

^c*Institute of Basic Medical Sciences, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing 100006, China*

^d*Ashdale Clinic, Cork T12 T2VK, Ireland*

^e*The Third Clinical Medical College, Zhejiang Chinese Medical University, Hangzhou 310000, China*

^f*The Fourth Clinical Medical College of Guangzhou University of Chinese Medicine, Guangzhou 518033, China*

^g*Akupunktur Akademiet, Aabyhoej 8230, Denmark*

Received 30 March 2020; received in revised form 29 April 2020; accepted 9 May 2020

*Corresponding author. Tel: +86 10 64032658, fax: +86 10 64013996.

E-mail address: slchen@icmm.ac.cn (Shilin Chen).

Table of contents

Table S1 List of 99 classic formulas utilized for COVID-19 with ingredients, and frequency	3
Table S2 Top ten most frequently used herbal formulas in COVID-19 treatment	6
Table S3.1 List of 179 herbs and corresponding properties.....	7
Table S3.2 Frequency of therapeutic effects of 179 herbs ($n=179$).....	10
Table S3.3 Frequency of medicinal properties of 179 herbs ($n=179$).....	11
Table S4 Frequency of therapeutic effects in five medicinal properties.....	11
Table S5.1 Top ten most frequently utilized individual herbs in COVID-19 treatment.....	12
Table S5.2 Information of the representative chemical components of top ten most frequently utilized herbs.....	12
Table S6.1 Eight groups of core combinations of herbs by hierarchical clustering.....	13
Table S6.2 Twelve groups of core combinations of chemical components by hierarchical clustering .	14
Table S7 Ten new formulas developed by unsupervised hierarchical clustering	15
Table S8 List of eight clusters and corresponding active pharmacophores	16
Table S9 Number of 22 chemical structures	16
Figure S1 Heat map of the frequency of top 10 frequently appeared chemical components in top 20 frequently utilized herbs	18

Table S1 List of 99 classic formulas utilized for COVID-19 with ingredients, and frequency.

Classic herbal formula	Ingredient	Frequency
Newly developed formula		55
An Gong Niu Huang Pill	Curcumae radix, Coptidis rhizoma, Gardeniae fructus, Scutellariae radix	21
Ma Xing Shi Gan Decoction	Forsythiae fructus, Armeniacae semen amarum, Glycyrrhizae radix et rhizoma	18
Xuan Bai Cheng Qi Decoction	Armeniacae semen amarum, Trichosanthis fructus, Rhei radix et rhizoma	13
Xie Bi Jing Injection	Carthamus tinctorius, Paeoniae radix rubra, Chuanxiong rhizoma, Salviae miltiorrhizae radix et rhizoma, Angelicae sinensis radix	13
Yin Qiao Powder	Forsythiae fructus, Lonicerae japonicae Flos, Platycodonis radix, Menthae haplocalycis herba, Lophatheri herba, Glycyrrhizae radix et rhizoma, Schizonepetae herba, Sojae semen praeparatum, Arctii fructus	13
Huo Po Xia Ling Decoction	Pogostemon cablin, Pinelliae rhizoma, Poria, Armeniacae semen amarum, Coicis semen, Amomi fructus rotundus, Tetrapanacis medulia, Polyporus, Sojae semen praeparatum, Alismatis rhizoma, Magnoliae officinalis cortex	12
Lian Hua Qing Wen Granule	Forsythiae fructus, Lonicerae japonicae Flos, Forsythiae fructus, Armeniacae semen amarum, Isatidis radix, Cyrtomium fortunei, Houத்துyniae herba, Pogostemon cablin, Rhei radix et rhizoma, Rhodiola crenulatae radix et rhizoma, Menthae haplocalycis herba, Glycyrrhizae radix et rhizoma	12
Huo Xiang Zheng Qi Powder	Areca catechu, Angelicae dahuricae radix, Perillae fructus, Poria, Pinelliae rhizoma, Atractylodis macrocephalae rhizoma, Citri reticulatae pericarpium, Magnoliae officinalis cortex, Zingiberis rhizoma recens, Platycodonis radix, Pogostemon cablin, Glycyrrhizae radix et rhizoma	11
Sheng Jiang Powder	Curcumae longae rhizoma, Rhei radix et rhizoma	11
Shu he Xiang Pill	Liquidambar, Benzoinum, Aucklandiae radix, Cyperi rhizoma, Santalum album, Caryophylli Flos, Aquilariae lignum resinatum, Piperis longi fructus, Olibanum, Atractylodis macrocephalae rhizoma, Chebulae fructus	11
Zi Xue Pill	Aucklandiae radix, Aquilariae lignum resinatum, Scrophulariae radix, Cimicifugae rhizoma, Glycyrrhizae radix et rhizoma, Caryophylli Flos	10
Cen Fu Injection	Ginseng radix et rhizoma rubra, Aconiti lateralis radix praeparata	9
Da Yuan Decoction	Arecae semen, Magnoliae officinalis cortex, Tsaoko fructus, Anemarrhenae rhizoma, Paeoniae radix alba, Scutellariae radix, Glycyrrhizae radix et rhizoma	9
Jie She Huo Xie Decoction	Forsythiae fructus, Puerariae lobatae radix, Bupleuri radix, Angelicae sinensis radix, Rehmanniae radix, Paeoniae radix rubra, Persicae semen, Carthamus tinctorius, Aurantii fructus, Glycyrrhizae radix et rhizoma	8
Ma Xing Yi Gan Decoction	Forsythiae fructus, Armeniacae semen amarum, Glycyrrhizae radix et rhizoma, Coicis semen	8
Huang Lian Jie Du Decoction	Coptidis rhizoma, Scutellariae radix, Phellodendri chinensis cortex, Gardeniae fructus	7
Jin Hua Qing Gan Granule	Lonicerae japonicae Flos, Fritillariae thunbergii bulbus, Scutellariae radix, Arctii fructus, Artemisiae annuae herba	7
Qing Wen Bai Du Decoction	Rehmanniae radix, Coptidis rhizoma, Gardeniae fructus, Platycodonis radix, Scutellariae radix, Anemarrhenae rhizoma, Paeoniae radix rubra, Scrophulariae radix, Forsythiae fructus, Glycyrrhizae radix et rhizoma, Moutan cortex, Lophatheri herba	7
Si Ni Jia Ren Cen Decoction	Glycyrrhizae radix et rhizoma, Aconiti lateralis radix praeparata, Zingiberis rhizoma recens, Ginseng radix et rhizoma	7
Fang Feng Tong Sheng Pill	Saposhnikoviae radix, Schizonepetae herba, Menthae haplocalycis herba, Forsythiae fructus, Rhei radix et rhizoma, Gardeniae fructus, Platycodonis radix, Chuanxiong rhizoma, Angelicae sinensis radix, Scutellariae radix, Forsythiae fructus, Glycyrrhizae radix et rhizoma, Atractylodis macrocephalae rhizoma, Paeoniae radix alba	6
Gan Lu Xiao Du Pill	Scutellariae radix, Artemisiae scopariae herba, Acori tatarinowii rhizoma, Fritillariae cirrhosae bulbus, Akebiae caulis, Pogostemon cablin, Forsythiae fructus, Amomi fructus rotundus, Menthae haplocalycis herba, Belamcandae rhizoma	6
Qing Kai Ling Syrup	Scutellariae radix, Gardeniae fructus, Isatidis radix, Lonicerae japonicae Flos	6
Sheng Mai Injection	Ginseng radix et rhizoma rubra, Ophiopogonis radix, Schisandrae chinensis fructus	6
Shu Feng Jie Du Granule	Polygoni cuspidati rhizoma et radix, Forsythiae fructus, Isatidis radix, Bupleuri radix, Patrinia scabiosifolia, Verbenae herba, Phragmitis rhizoma, Glycyrrhizae radix et rhizoma	5
Tan Re Qing Injection	Scutellariae radix, Lonicerae japonicae Flos, Forsythiae fructus	5
Xiao Chai Hu Decoction	Bupleuri radix, Scutellariae radix, Ginseng radix et rhizoma, Pinelliae rhizoma, Glycyrrhizae radix et rhizoma, Zingiberis rhizoma recens, Jujubae fructus	5
Cen Fu Decoction	Ginseng radix et rhizoma, Aconiti lateralis radix praeparata	4
Wang Ren Decoction	Armeniacae semen amarum, Tetrapanacis medulia, Amomi fructus rotundus, Lophatheri herba, Magnoliae officinalis cortex, Coicis semen, Pinelliae rhizoma	4
Xi Yan Ping Injection	Andrographis paniculata	4
Yu Ping Feng Powder	Saposhnikoviae radix, Astragali radix, Atractylodis macrocephalae rhizoma	4
Zhu Ye Shi Gao Decoction	Lophatheri herba, Pinelliae rhizoma, Ginseng radix et rhizoma, Ophiopogonis radix, Glycyrrhizae radix et rhizoma, Oryza sativa	4
Bai Hu Decoction	Anemarrhenae rhizoma, Oryza sativa, Glycyrrhizae radix et rhizoma	3

Cen Fu Long Mu Li Decoction	Ginseng radix et rhizoma, Aconiti lateralis radix praeparata, Zingiberis rhizoma recens, Jujubae fructus	3
Da Qing Long Decoction	Forsythiae fructus, Cinnamomi ramulus, Glycyrrhizae radix et rhizoma, Armeniacae semen amarum, Zingiberis rhizoma recens, Jujubae fructus	3
Jing Fang Bai Du Powder	Notopterygii rhizoma et radix, Radix angelicae biseratae, Bupleuri radix, Peucedani radix, Aurantii fructus, Poria, Schizonepetae herba, Saposhnikoviae radix, Platycodonis radix, Chuanxiong rhizoma, Glycyrrhizae radix et rhizoma	3
Qian Jin Wei Jing Decoction	Phragmitis rhizoma, Benincasae semen, Coicis semen, Persicae semen	3
Sang Bei Powder	Mori cortex, Fritillariae cirrhosae bulbus	3
Sheng Mai Decoction	Ginseng radix et rhizoma, Ophiopogonis radix, Schisandrae chinensis fructus	3
Xiang Sha Liu Jun Zi Decoction	Ginseng radix et rhizoma, Atractylodis macrocephalae rhizoma, Poria, Glycyrrhizae radix et rhizoma, Citri reticulatae pericarpium, Pinelliae rhizoma, Amomi fructus, Aucklandiae radix, Zingiberis rhizoma recens	3
Cen Qin Bai Shu Powder	Nelumbinis semen, Coicis semen, Amomi fructus, Platycodonis radix, Lablab semen album, Poria, Ginseng radix et rhizoma, Glycyrrhizae radix et rhizoma, Atractylodis macrocephalae rhizoma, Dioscoreae rhizoma	2
Cen Mai Decoction	Panacis quinquefolii radix, Schisandrae chinensis fructus, Ophiopogonis radix	2
Er Chen Decoction	Pinelliae rhizoma, Citri exocarpium rubrum, Poria, Glycyrrhizae radix et rhizoma	2
Gui Zhi Decoction	Cinnamomi ramulus, Paeoniae radix alba, Zingiberis rhizoma recens, Jujubae fructus, Glycyrrhizae radix et rhizoma	2
Anti-virus Syrup	Isatidis radix, Phragmitis rhizoma, Rehmanniae radix, Curcumae radix, Anemarrhenae rhizoma, Acori tatarinowii rhizoma, Pogostemon cablin, Forsythiae fructus	2
Long Dan Xie Gan Decoction	Gentianae radix et rhizoma, Gardeniae fructus, Scutellariae radix, Alismatis rhizoma, Plantaginis semen, Akebiae caulis, Rehmanniae radix, Angelicae sinensis radix, Bupleuri radix, Glycyrrhizae radix et rhizoma	2
Qing Fei Pai Du Decoction	Forsythiae fructus, Glycyrrhizae radix et rhizoma, Armeniacae semen amarum, Cinnamomi ramulus, Alismatis rhizoma, Polyporus, Atractylodis macrocephalae rhizoma, Poria, Bupleuri radix, Scutellariae radix, Pinelliae rhizoma, Zingiberis rhizoma recens, Asteris radix et rhizoma, Farfarae Flos, Belamcandae rhizoma, Asari radix et rhizoma, Dioscoreae rhizoma, Aurantii fructus immaturus, Citri reticulatae pericarpium, Pogostemon cablin	2
Qing Qi Hua Tan Decoction	Citri reticulatae pericarpium, Armeniacae semen amarum, Aurantii fructus immaturus, Scutellariae radix, Trichosanthis fructus, Poria, Pinelliae rhizoma	2
Qing Ying Decoction	Rehmanniae radix, Scrophulariae radix, Lophatheri herba, Ophiopogonis radix, Salviae miltiorrhizae radix et rhizoma, Coptidis rhizoma, Lonicerae japonicae Flos, Forsythiae fructus	2
Re Du Ning Injection	Artemisiae annuae herba, Lonicerae japonicae Flos, Gardeniae fructus	2
Ren Cen Bai Du Powder	Ginseng radix et rhizoma, Bupleuri radix, Platycodonis radix, Glycyrrhizae radix et rhizoma, Poria, Aurantii fructus, Notopterygii rhizoma et radix, Radix angelicae biseratae, Peucedani radix, Chuanxiong rhizoma	2
Sang Ju Decoction	Mori folium, Chrysanthemi Flos, Armeniacae semen amarum, Forsythiae fructus, Menthae haplocalycis herba, Platycodonis radix, Glycyrrhizae radix et rhizoma, Phragmitis rhizoma	2
Sha Cen Mai Dong Decoction	Glehniae radix, Polygonati odorati rhizoma, Glycyrrhizae radix et rhizoma, Mori folium, Ophiopogonis radix, Lablab semen album, Trichosanthis radix	2
Sheng Mai Decoction	Codonopsis radix, Ophiopogonis radix, Schisandrae chinensis fructus	2
Si Jun Zi Decoction	Ginseng radix et rhizoma, Atractylodis macrocephalae rhizoma, Poria, Glycyrrhizae radix et rhizoma	2
Wang Shi Qing Shu Yi Qi Decoction	Panacis quinquefolii radix, Dendrobii caulis, Ophiopogonis radix, Coptidis rhizoma, Lophatheri herba, Nymphaea tetragona, Anemarrhenae rhizoma, Glycyrrhizae radix et rhizoma, Oryza sativa, Trichosanthis fructus	2
Xiao Xian Xiong Decoction	Coptidis rhizoma, Pinelliae rhizoma, Trichosanthis fructus	2
Zhi Bao Pill	Benzoinum	2
Bu Zhong Yi Qi Pill	Astragali radix, Codonopsis radix, Atractylodis macrocephalae rhizoma, Angelicae sinensis radix, Cimicifugae rhizoma, Bupleuri radix, Citri reticulatae pericarpium, Glycyrrhizae radix et rhizoma	1
Cen Mai Injection	Ginseng radix et rhizoma rubra, Ophiopogonis radix	1
Chai Ge Jie Ji Decoction	Bupleuri radix, Puerariae lobatae radix, Glycyrrhizae radix et rhizoma, Scutellariae radix, Notopterygii rhizoma et radix, Angelicae dahuricae radix, Paeoniae radix alba, Platycodonis radix, Jujubae fructus, Zingiberis rhizoma recens	1
Chai Hu Xian Xiong Decoction	Bupleuri radix, Pinelliae rhizoma, Coptidis rhizoma, Platycodonis radix, Scutellariae radix, Trichosanthis fructus, Aurantii fructus immaturus, Zingiberis rhizoma recens	1
Fu Fang Jin Yin Hua Granule	Lonicerae japonicae Flos, Forsythiae fructus, Scutellariae radix	1
Fu Fang Qin Syrup	Lonicerae japonicae Flos, Scutellariae radix, Forsythiae fructus, Isatidis radix	1
Gui Zhi Fu Ling Pill	Cinnamomi ramulus, Poria, Moutan cortex, Paeoniae radix rubra, Persicae semen	1
Hao Ling Qing Dan Decoction	Artemisiae annuae herba, Bambusae caulis in taenias, Pinelliae rhizoma, Poria, Scutellariae radix, Aurantii fructus, Citri reticulatae pericarpium, Glycyrrhizae radix et rhizoma, Indigo naturalis	1
Huang Shi Liu Jun Zi Decoction	Ginseng radix et rhizoma, Atractylodis macrocephalae rhizoma, Poria, Glycyrrhizae radix et rhizoma, Pinelliae rhizoma, Citri reticulatae pericarpium, Astragali radix, Dioscoreae rhizoma	1
Jin Shi Qing Wen Jie Du Syrup	Anemarrhenae rhizoma, Lonicerae japonicae Flos, Forsythiae fructus, Paridis rhizoma, Platycodonis radix, Aurantii fructus, Fritillariae thunbergii bulbus, Bupleuri radix, Scutellariae radix, Schizonepetae herba, Arctii fructus, Coicis semen, Trichosanthis radix, Ophiopogonis radix, Paeoniae radix rubra, Glycyrrhizae radix et rhizoma	1
Li Zhong Pill	Ginseng radix et rhizoma, Zingiberis rhizoma recens, Glycyrrhizae radix et rhizoma, Atractylodis macrocephalae rhizoma	1

Lian Pu Decoction	Magnoliae officinalis cortex, Coptidis rhizoma, Acori tatarinowii rhizoma, Pinelliae rhizoma, Sojae semen praeparatum, Gardeniae fructus, Phragmitis rhizoma	1
Lian Qiao Bai Du Powder	Schizonepetae herba, Saposhnikoviae radix, Bupleuri radix, Peucedani radix, Scutellariae radix, Platycodonis radix, Arctii fructus, Lonicerae japonicae Flos, Fritillariae cirrhosae bulbus, Forsythiae fructus, Aurantii fructus, Poria, Chuanxiong rhizoma, Glycyrrhizae radix et rhizoma	1
Ma Huang Lian Qiao Chi Xiao Dou Decoction	Forsythiae fructus, Forsythiae fructus, Armeniacae semen amarum, Vignae semen, Jujubae fructus, Mori cortex, Zingiberis rhizoma recens, Glycyrrhizae radix et rhizoma	1
Ma Xing Yin Qiao Powder	Forsythiae fructus, Armeniacae semen amarum, Glycyrrhizae radix et rhizoma, Forsythiae fructus, Lonicerae japonicae Flos, Platycodonis radix, Menthae haplocalycis herba, Lophatheri herba, Glycyrrhizae radix et rhizoma, Schizonepetae herba, Sojae semen praeparatum, Arctii fructus	1
Mai Wei Bu Zhong Yi Qi Decoction	Pseudostellariae radix, Ophiopogonis radix, Schisandrae chinensis fructus, Astragali radix, Glycyrrhizae radix et rhizoma, Ginseng radix et rhizoma, Angelicae sinensis radix, Citri reticulatae pericarpium, Cimicifugae rhizoma, Bupleuri radix, Atractylodis macrocephalae rhizoma,	1
Pu Di Lan Qiao Du Pill	Taraxaci herba, Scutellariae radix, Corydalis Bungeanae Herba, Isatidis radix	1
Qi Wei Decoction	Bupleuri radix, Magnoliae officinalis cortex, Glycyrrhizae radix et rhizoma, Cinnamomi ramulus, Forsythiae fructus, Citri reticulatae pericarpium, Pinelliae rhizoma	1
Qiang Huo Sheng Shi Decoction	Notopterygii rhizoma et radix, Radix angelicae biseratae, Artemisia rupestris, Saposhnikoviae radix, Glycyrrhizae radix et rhizoma, Vitis fructus, Chuanxiong rhizoma	1
Qing Re Jie Du Granule	Lonicerae japonicae Flos, Forsythiae fructus, Isatidis folium, Coptidis rhizoma, Rehmanniae radix, Anemarrhenae rhizoma, Scrophulariae radix	1
Qing Zao Jiu Fei Decoction	Mori folium, Ginseng radix et rhizoma, Glycyrrhizae radix et rhizoma, Helicteres angustifolia, Ophiopogonis radix, Eriobotryae folium, Armeniacae semen amarum	1
Ren Cen Bai Hu Decoction	Anemarrhenae rhizoma, Glycyrrhizae radix et rhizoma, Oryza sativa, Ginseng radix et rhizoma	1
San Shi Decoction	Armeniacae semen amarum, Bambusae caulis in taenias, Tetrapanacis medulia, Lonicerae japonicae Flos	1
Sang Bei Zhi Ke Powder	Mori cortex, Fritillariae thunbergii bulbus, Platycodonis radix, Schizonepetae herba, Asteris radix et rhizoma, Stemonae radix, Cynanchum glaucescens, Glycyrrhizae radix et rhizoma, Citri reticulatae pericarpium	1
Shen Gan Ma Huang Decoction	Belamcandae rhizoma, Forsythiae fructus, Zingiberis rhizoma recens, Asari radix et rhizoma, Asteris radix et rhizoma, Farfarae Flos, Schisandrae chinensis fructus, Jujubae fructus, Pinelliae rhizoma	1
Shen Shu Powder	Atractylodis rhizoma, Citri reticulatae pericarpium, Magnoliae officinalis cortex, Glycyrrhizae radix et rhizoma, Pogostemon cablin, Amomi fructus	1
Sheng Yang Yi Wei Decoction	Astragali radix, Pinelliae rhizoma, Ginseng radix et rhizoma, Glycyrrhizae radix et rhizoma, Radix angelicae biseratae, Saposhnikoviae radix, Paeoniae radix alba, Notopterygii rhizoma et radix, Citri reticulatae pericarpium, Poria, Bupleuri radix, Alismatis rhizoma, Atractylodis macrocephalae rhizoma, Coptidis rhizoma	1
Shuang Huang Lian Syrup	Lonicerae japonicae Flos, Scutellariae radix, Forsythiae fructus	1
Ting Li Xie Fei Decoction	Descurainiae semen lepidii semen, Trichosanthis fructus, Fagopyri dibotryis rhizoma, Tripirospermum chinense, Scutellariae radix, Perillae fructus, Allium macrostemon, Pinelliae rhizoma, Cinnamomi ramulus, Paeoniae radix alba, Chuanxiong rhizoma, Sinapis semen	1
Tong Xuan Li Fei Pill	Perillae folium, Peucedani radix, Platycodonis radix, Armeniacae semen amarum, Forsythiae fructus, Glycyrrhizae radix et rhizoma, Citri reticulatae pericarpium, Pinelliae rhizoma, Poria, Aurantii fructus, Scutellariae radix	1
Wu Ling Powder	Polyporus, Poria, Atractylodis macrocephalae rhizoma, Alismatis rhizoma, Cinnamomi ramulus	1
Wu Ye Lu Gen Decoction	Pogostemon cablin, Menthae haplocalycis herba, Nelumbinis folium, Eriobotryae folium, Eupatorii herba, Phragmitis rhizoma, Benincasae semen	1
Xi Jiao Di Huang Decoction	Rehmanniae radix, Paeoniae radix alba, Moutan cortex	1
Xin Xue Granule	Andrographis paniculata, Polygonati odorati rhizoma, Cimicifugae rhizoma, Aquilariae lignum resinatum, Gardeniae fructus	1
Xing Nao Jing Injection	Curcumae radix, Gardeniae fructus	1
Yin Huang Qing Fei Capsule	Descurainiae semen lepidii semen, Forsythiae fructus, Armeniacae semen amarum, Fritillariae thunbergii bulbus, Eriobotryae folium, Isatidis folium, Acori tatarinowii rhizoma, Dioscorea nipponica, Artemisia rupestris, Ginkgo folium, Schisandrae chinensis fructus, Aurantii fructus immaturus, Glycyrrhizae radix et rhizoma	1
Yin Lian Qing Wen Jie Du Syrup	Not published	1
Yin Qiao Bai Du Powder	Lonicerae japonicae Flos, Lasiosphaera calvatia, Puerariae lobatae radix, Arctii fructus, Forsythiae fructus, Isatidis radix	1
Yin Qiao Ma Bo Powder	Forsythiae fructus, Arctii fructus, Lonicerae japonicae Flos, Belamcandae rhizoma, Lasiosphaera calvatia	1
Zhen Qi Fu Zheng Pill	Astragali radix, Ligustri lucidi fructus	1
Zhi Shu Powder	Platycodonis radix, Schizonepetae herba, Asteris radix et rhizoma, Stemonae radix, Cynanchum glaucescens, Glycyrrhizae radix et rhizoma, Citri reticulatae pericarpium	1
Tong Shi Wu Han Anti-epidemic Formula	Not published	1
Total		423

Table S2 Top ten most frequently used herbal formulas in COVID-19 treatment.

Frequency	Clinic stage	Syndrome differentiation	Symptom	Treatment principle	Formula	Herbal ingredient
25	Critical stage	Internal blockage and external detachment	Dizziness, irritability, hot chest and abdomen, cold hands and feet, shortness of breath or need of auxiliary ventilation. The tongue is red and crimson, with yellow or dry coating. The pulse is rapid, broad or rootless.	Open the orifices, dissolve the phlegm, and heat-toxin, tonify Qi and nourish Yin	An Gong Niu Huang Pill	Curcumae radix, Coptidis rhizoma, Gardeniae fructus, and Scutellariae radix
13				Clear away the heat, dissolve the phlegm, invigorate the Qi and Yang, and open the orifices	Zi Xue Powder	Aucklandiae radix, Aquilariae lignum resinatum, Scrophulariae radix, Cimicifugae rhizoma, Glycyrrhizae radix et rhizoma, and Caryophylli flos
11				Dissolve the dampness, open the orifices, invigorate the Qi and nourish Yin	Su He Xiang Pill	Liquidambar, Benzoinum, Aucklandiae radix, Cyperi rhizoma, Santalum album, Caryophylli flos, Aquilariae lignum resinatum, Piperis longi fructus, Olibanum, Atractylodis macrocephalae rhizoma, and Chebulae fructus
18	Mild, moderate, and critical stages	Heat-toxin obstructing the lung	High fever, cough, yellow or thick phlegm, fatigue, headache, aching, dry and bitter mouth, vexation, constipation, red urine, red tongue, yellow and greasy coating, slippery and rapid pulse	Clear away the heat, remove the toxin, disperse the lung Qi and expel the external pathogenic factors	Modification of Ephedra, Apricot Kernel, Gypsum and Licorice Decoction (Ma Huang Xing Ren Gan Cao Shi Gao Tang)	Ephedrae herba, Armeniacae semen amarum, and Glycyrrhizae radix et rhizoma
13	Moderate and critical stages	Heat-toxin congesting the lung	Fever, cough, yellow thick sputum, chest distention, asthma, thirst, foul breath, abdominal distention and constipation, dark red tongue, thick fur and yellow turbid fur, slippery or tight pulse	Clear away the heat, disperse lung Qi, promote bowel movement to remove the heat	Xuan Bai Cheng Qi Decoction	Armeniacae semen amarum, Trichosanthis fructus, and Rhei radix et rhizoma
13				Clear away the heat, dissolve the phlegm, remove heat-toxin, tonify Qi, and nourish Yin	Xue Bi Jing Decoction	Carthamus tinctorius, Paeoniae radix rubra, Chuanxiong rhizoma, and Salviae miltiorrhizae radix et rhizoma
13	Mild stage	Heat-damp accumulating in the lung	Fever, chills, sore throat, dry cough and less phlegm, aching limbs and muscles, fatigue, headache, red tongue edge, thin white or yellowish coating, floating pulse.	Expel the wind, relieve the exterior, and remove heat-toxin	Yin Qiao Powder	Forsythiae fructus, Lonicerae japonicae flos, Platycodonis radix, Menthae haplocalycis herba, Lophatheri herba, Glycyrrhizae radix et rhizoma, Schizonepetae herba, and Arctii fructus
12				Dissolve the phlegm, remove the heat-toxin, regulate Qi and spleen	Hou Po Xia Ling Decoction	Pogostemon cablin, Pogostemon cablin, Rubra Poria, Pinelliae rhizoma, Armeniacae semen amarum, Coicis semen, Amomi fructus rotundus, Tetrapanacis medulia, Polyporus, Schizonepetae herba, Alismatis rhizoma, and Magnoliae officinalis cortex
12				Clear the lung, relieve the exterior, invigorate Qi and dissolve the dampness	Lian Hua Qing Wen Decoction	Forsythiae fructus, Lonicerae japonicae flos, Ephedrae herba, Armeniacae semen amarum, Isatidis radix, Cyrtomium fortunei, Pogostemon cablin, Houttuyniae herba, Pogostemon cablin, Rhei radix et rhizoma, Rhodiolae crenulatae radix et rhizoma, Menthae haplocalycis herba, and Glycyrrhizae radix et rhizoma
11	Mild and moderate stage	Heat-toxin obstructing the lung	In the early stage of fever, dry cough, fatigue, stomach distention, aversion to cold, headache, nausea, sore throat, slightly dry mouth, light red tongue, thin, white and slightly greasy coating, tight or slow pulse.	Dissolve the dampness, relieve the exterior, disperse lung Qi and clear the heat	Upbearing and Downbearing Powder (Sheng Jiang San)	Liquidambar, Benzoinum, Aucklandiae radix, Cyperi rhizoma, Santalum album, Caryophylli flos, Aquilariae lignum resinatum, Piperis longi fructus, Olibanum, Atractylodis macrocephalae rhizoma, and Chebulae fructus

Table S3.1 List of 179 herbs and corresponding properties.

Herb CN	Herb EN	Frequency	Therapeutic effect	Medicinal property	Proportion (n=166)
Gan Cao	Glycyrrhizae radix et rhizoma	139	Qi-tonic	Rhizoma & radix	83.73%
Huang Qin	Scutellariae radix	101	Heat-clearing	Rhizoma & radix	60.84%
Ku Xing Ren	Armeniacaese semen amarum	87	Expectorant & cough-suppressing	Fructus & semen	52.41%
Jin Yin Hua	Lonicerae japonicae Flos	82	Heat-clearing	Flos	49.40%
Lian Qiao	Forsythiae fructus	81	Heat-clearing	Fructus & semen	48.80%
Ma Huang	Ephedrae herba	74	Exterior-relieving	Herba & others	44.58%
Fu Ling	Poria	65	Dampness-resolving	Herba & others	39.16%
Guang Huo					
Xiang	Pogostemon cablin	63	Dampness-resolving	Herba & others	37.95%
Chen Pi	Citri reticulatae pericarpium	57	Qi-regulating	folium & cortex	34.34%
Jie Geng	Platycodonis radix	55	Expectorant & cough-suppressing	Radix & rhizoma	33.13%
Ban Xia	Pinelliae rhizoma	54	Expectorant & cough-suppressing	Radix & rhizoma	32.53%
Bai Zhu	Atractylodis macrocephalae rhizoma	51	Qi-tonic	Radix & rhizoma	30.72%
Cang Zhu	Atractylodis rhizoma	50	Dampness-resolving	Radix & rhizoma	30.12%
Da Huang	Rhei radix et rhizoma	48	Heat-clearing	Radix & rhizoma	28.92%
Zhi Zi	Gardeniae fructus	46	Heat-clearing	Fructus & semen	27.71%
Hou Po	Magnoliae officinalis cortex	44	Dampness-resolving	folium & cortex	26.51%
Mai Dong	Ophiopogonis radix	42	Yin-nourishing	Radix & rhizoma	25.30%
Huang Lian	Coptidis rhizoma	42	Heat-clearing	Radix & rhizoma	25.30%
Lu Gen	Phragmitis rhizoma	39	Heat-clearing	Radix & rhizoma	23.49%
Huang Qi	Astragali radix	38	Qi-tonic	Radix & rhizoma	22.89%
Bo He	Menthae haplocalycis herba	36	Exterior-relieving	Herba & others	21.69%
Ren Shen	Ginseng radix et rhizoma	32	Qi-tonic	Radix & rhizoma	19.28%
Guan Zhong	Cyrtomium fortunei	31	Heat-clearing	Radix & rhizoma	18.67%
Yu Jin	Curcuma radix	30	Blood-activating	Radix & rhizoma	18.07%
Chai Hu	Bupleuri radix	30	Exterior-relieving	Radix & rhizoma	18.07%
Fu Zi	Aconiti lateralis radix praeparata	29	Interior-warming	Radix & rhizoma	17.47%
Chi Shao	Paeoniae radix rubra	29	Heat-clearing	Radix & rhizoma	17.47%
Zhi Mu	Anemarrhenae rhizoma	28	Heat-clearing	Radix & rhizoma	16.87%
Ban Lan Gen	Isatidis radix	28	Heat-clearing	Radix & rhizoma	16.87%
Yi Yi Ren	Coicis semen	28	Dampness-resolving	Fructus & semen	16.87%
Xuan Shen	Scrophulariae radix	27	Heat-clearing	Fructus & semen	16.27%
Gua Lou	Trichosanthis fructus	27	Expectorant & cough-suppressing	Fructus & semen	16.27%
Dan Zhu Ye	Lophatheri herba	28	Heat-clearing	Herba & others	16.87%
Ting Li Zi	Descurainiae semen lepidii semen	26	Expectorant & cough-suppressing	Fructus & semen	15.66%
Niu Bang Zi	Arctii fructus	26	Exterior-relieving	Fructus & semen	15.66%
Fang Feng	Saposhnikovia radix	25	Exterior-relieving	Radix & rhizoma	15.06%
Chuan Xiong	Chuanxiong rhizoma	24	Blood-activating	Radix & rhizoma	14.46%
Dang Gui	Angelicae sinensis radix	23	Blood-nourishing	Radix & rhizoma	13.86%
Chen Xiang	Aquilariae lignum resinatum	23	Qi-regulating	Herba & others	13.86%
Cao Guo	Tsaoko fructus	23	Dampness-resolving	Fructus & semen	13.86%
Ding Xiang	Caryophylli Flos	22	Interior-warming	Flos	13.25%
Bing Lang	Arecae semen	22	Insect repellent	Fructus & semen	13.25%
Zi Su Ye	Perillae folium	21	Exterior-relieving	folium & cortex	12.65%
Zhe Bei Mu	Fritillariae thunbergii bulbus	21	Expectorant & cough-suppressing	Radix & rhizoma	12.65%
Sheng Jiang	Zingiberis rhizoma recens	21	Exterior-relieving	Radix & rhizoma	12.65%
Tao Ren	Persicae semen	20	Blood-activating	Fructus & semen	12.05%
Dan Shen	Salviae miltiorrhizae radix et rhizoma	20	Blood-activating	Radix & rhizoma	12.05%
Shan Zhu Yu	Corni fructus	18	Astringent	Fructus & semen	10.84%
Hong Shen	Ginseng radix et rhizoma rubra	18	Qi-tonic	Radix & rhizoma	10.84%

Dang Shen	Codonopsis radix	18	Qi-tonic	Radix & rhizoma	10.84%
Yu Xing Cao	Houttuyniae herba	17	Heat-clearing	Herba & others	10.24%
Qing Hao	Artemisiae annuae herba	17	Heat-clearing	Herba & others	10.24%
Jing Jie	Schizonepetae herba	17	Exterior-relieving	Herba & others	10.24%
Dou Kou	Amomi fructus rotundus	18	Dampness-resolving	Fructus & semen	10.84%
Di Huang	Rehmanniae radix	17	Blood-nourishing	Radix & rhizoma	10.24%
Sang Bai Pi	Mori cortex	16	Expectorant & cough-suppressing	folium & cortex	9.64%
Mu Xiang	Aucklandiae radix	16	Qi-regulating	Radix & rhizoma	9.64%
Bai Shao	Paeoniae radix alba	16	Blood-nourishing	Radix & rhizoma	9.64%
Wu Wei Zi	Schisandrae chinensis fructus	14	Astringent	Fructus & semen	8.43%
Mu Dan Pi	Moutan cortex	14	Heat-clearing	folium & cortex	8.43%
Bai Zhi	Angelicae dahuricae radix	14	Exterior-relieving	Radix & rhizoma	8.43%
An Xi Xiang	Benzoinum	14	Resuscitation-inducing	Herba & others	8.43%
Sheng Ma	Cimicifugae rhizoma	13	Exterior-relieving	Radix & rhizoma	7.83%
Sang Ye	Mori folium	13	Exterior-relieving	folium & cortex	7.83%
Qiang Huo	Notopterygii rhizoma et radix	13	Exterior-relieving	Radix & rhizoma	7.83%
Hong Hua	Carthamus tinctorius	13	Blood-activating	Flos	7.83%
Xiang Fu	Cyperii rhizoma	12	Qi-regulating	Radix & rhizoma	7.23%
Tan Xiang	Santalum album	12	Qi-regulating	Herba & others	7.23%
Su He Xiang	Liquidambar	12	Resuscitation-inducing	Herba & others	7.23%
Ru Xiang	Olibanum	12	Blood-activating	Herba & others	7.23%
Pei Lan	Eupatorii herba	12	Dampness-resolving	Herba & others	7.23%
Ke Zi	Chebulae fructus	12	Astringent	Fructus & semen	7.23%
Bi Ba	Piperis longi fructus	12	Interior-warming	Fructus & semen	7.23%
Tai Zi Shen	Pseudostellariae radix	11	Qi-tonic	Radix & rhizoma	6.63%
Shi Chang Pu	Acori tatarinowii rhizoma	11	Resuscitation-inducing	Radix & rhizoma	6.63%
Sha Ren	Amomi fructus	11	Dampness-resolving	Fructus & semen	6.63%
Hong Jing	Rhodiolae crenulatae radix et rhizoma	11	Qi-tonic	Radix & rhizoma	6.63%
Tian	Belamcandae rhizoma	10	Heat-clearing	Radix & rhizoma	6.02%
Sheg An	Cinnamomi ramulus	10	Exterior-relieving	Radix & rhizoma	6.02%
Gui Zhi	Jujubae fructus	10	Qi-tonic	Radix & rhizoma	6.02%
Da Zao	Glehniae radix	10	Yin-nourishing	Radix & rhizoma	6.02%
Bei Sha Shen	Polyporus	10	Dampness-resolving	Herba & others	6.02%
Zhu Ling	Aurantii fructus	9	Qi-regulating	Fructus & semen	5.42%
Zhi Ke	Alismatis rhizoma	10	Dampness-resolving	Radix & rhizoma	6.02%
Ze Xie	Panax quinquefolii radix	9	Qi-tonic	Radix & rhizoma	5.42%
Xi Yang	Tetrapanax medulia	10	Dampness-resolving	Radix & rhizoma	6.02%
Shen	Peucedani radix	9	Expectorant & cough-suppressing	Radix & rhizoma	5.42%
Tong Cao	Curcuma longae rhizoma	10	Blood-activating	Radix & rhizoma	6.02%
Qian Hu	Areca catechu	9	Qi-regulating	folium & cortex	5.42%
Jiang Huang	Sabia schumanniana	8	Qi-regulating	Radix & rhizoma	4.82%
Da Fu Pi	Verbenae herba	8	Heat-clearing	Herba & others	4.82%
Qing Mu	Chrysanthemi Flos	8	Exterior-relieving	Flos	4.82%
Xiang	Sojae semen praeparatum	12	Exterior-relieving	Fructus & semen	7.23%
Ma Bian Cao	Lablab semen album	8	Qi-tonic	Fructus & semen	4.82%
Ju Hua	Aurantii fructus immaturus	7	Qi-regulating	Fructus & semen	4.22%
Dan Dou Chi	Polygoni cuspidati rhizoma et radix	7	Dampness-resolving	Radix & rhizoma	4.22%
Bai Bian Dou	Isatidis folium	7	Heat-clearing	folium & cortex	4.22%
Zhi Shi	Expectorant & cough-suppressing	6	Radix & rhizoma	3.61%	
Hu Zhang	Asteris radix et rhizoma	6	Radix & rhizoma	3.61%	
Da Qing Ye	Dioscoreae rhizoma	6	Qi-tonic	Radix & rhizoma	3.61%
Zi Wan	Puerariae lobatae radix	6	Exterior-relieving	Radix & rhizoma	3.61%
Shan Yao	Expectorant & cough-suppressing	6	Radix & rhizoma	3.61%	
Ge Gen	Fritillariae cirrhosae bulbos	6	Radix & rhizoma	3.61%	
Chuan Bei	Dendrobii caulis	5	Yin-nourishing	Radix & rhizoma	3.01%
Mu	Taraxaci herba	5	Heat-clearing	Herba & others	3.01%
Shi Hu	Eriobotryae folium	5	Expectorant &	folium & cortex	3.01%
Pu Gong					
Ying					
Pi Pa Ye					

		cough-suppressing			
Chuan Xin					
Lian	Andrographis paniculata	5	Heat-clearing	Herba & others	3.01%
Bai Jiang	Patrinia scabiosifolia	5	Heat-clearing	Herba & others	3.01%
Zhu Ru	Bambusae caulis in taenias	4	Expectorant & cough-suppressing	Radix & rhizoma	2.41%
Yu Zhu	Polygonati odorati rhizoma	4	Yin-nourishing	Radix & rhizoma	2.41%
Yin Chen	Artemisiae scopariae herba	4	Dampness-resolving	Herba & others	2.41%
Tian Hua Fen	Trichosanthis radix	4	Heat-clearing	Radix & rhizoma	2.41%
Tian Dong	Asparagi radix	4	Yin-nourishing	Radix & rhizoma	2.41%
Shan Zha	Crataegi fructus	4	Digestant	Fructus & semen	2.41%
Mu Tong	Akebiae caulis	4	Dampness-resolving	Radix & rhizoma	2.41%
Mai Ya	Hordei fructus germinatus	4	Digestant	Fructus & semen	2.41%
Jing Mi	Oryza sativa	4	Yin-nourishing	Fructus & semen	2.41%
Jin Qiao Mai	Fagopyri dibotryis rhizoma	4	Heat-clearing	Radix & rhizoma	2.41%
Di Gu Pi	Lycii cortex	4	Heat-clearing	folium & cortex	2.41%
Bai Mao Gen	Imperatae rhizoma	4	Hemostatics	Radix & rhizoma	2.41%
Ai Di Cha	Ardisiae japonicae herba	4	Expectorant & cough-suppressing	Herba & others	2.41%
Xi Xin	Asari radix et rhizoma	3	Exterior-relieving	Radix & rhizoma	1.81%
Nan Sha					
Shen	Adenophorae radix	3	Yin-nourishing	Radix & rhizoma	1.81%
Kuan Dong			Expectorant & cough-suppressing		
Hua	Farfarae Flos	3		Flos	1.81%
Dong Gua Zi	Benincasae semen	3	Dampness-resolving	Fructus & semen	1.81%
Bai He	Lilii bulbus	3	Yin-nourishing	folium & cortex	1.81%
Bai Bu	Stemonae radix	3	Expectorant & cough-suppressing	Radix & rhizoma	1.81%
Bai Qian	Cynanchum glaucescens	3	Expectorant & cough-suppressing	Radix & rhizoma	1.81%
Zi Su Zi	Perillae fructus	2	Expectorant & cough-suppressing	Fructus & semen	1.20%
Zi Su Geng	Perillae caulis	2	Exterior-relieving	Radix & rhizoma	1.20%
Zi Cao	Abnebiae radix	2	Heat-clearing	Radix & rhizoma	1.20%
Chong Lou	Paridis rhizoma	2	Heat-clearing	Radix & rhizoma	1.20%
Yin Chai Hu	Stellaria dichotoma	1	Heat-clearing	Radix & rhizoma	0.60%
Tu Fu Ling	Smilar glabra	2	Heat-clearing	Radix & rhizoma	1.20%
San Qi	Notoginseng radix et rhizoma	2	Hemostatics	Radix & rhizoma	1.20%
Qing Guo	Citri reticulatae pericarpium viride	2	Heat-clearing	Fructus & semen	1.20%
Nv Zhen Zi	Ligustri lucidi fructus	2	Yin-nourishing	Fructus & semen	1.20%
Ma Bo	Lasiosphaera calvatia	2	Heat-clearing	Herba & others	1.20%
Lv Dou	Vigna radiata	2	Heat-clearing	Fructus & semen	1.20%
Long Dan	Gentianae radix et rhizoma	2	Heat-clearing	Radix & rhizoma	1.20%
Lian Zi	Nelumbinis semen	2	Astringent	Fructus & semen	1.20%
Ju Hong	Citri exocarpium rubrum	2	Expectorant & cough-suppressing	folium & cortex	1.20%
Jin Lian Hua	Trollius chinensis	2	Heat-clearing	Flos	1.20%
He Ye	Nelumbinis folium	2	Heat-clearing	folium & cortex	1.20%
Gu Ya	Setariae fructus germinatus	2	Digestant	Fructus & semen	1.20%
Gou Qi Zi	Lycii fructus	2	Yin-nourishing	Fructus & semen	1.20%
Gan Jiang	Zingiberis rhizoma	2	Interior-warming	Radix & rhizoma	1.20%
Fu Xiao Mai	Triticum aestivum	2	Astringent	Fructus & semen	1.20%
Du Huo	Radix angelicae biseratae	2	Dampness-resolving	Radix & rhizoma	1.20%
Chi Xiao Dou	Vignae semen	2	Dampness-resolving	Fructus & semen	1.20%
Che Qian Zi	Plantaginis semen	2	Dampness-resolving	Fructus & semen	1.20%
Zi Hua Di					
Ding	Viola philippica	1	Heat-clearing	Herba & others	0.60%
Yuan Zhi	Polygalae radix	1	Sedative	Radix & rhizoma	0.60%
Yu Mi Xu	Maydis seigma	1	Dampness-resolving	Flos	0.60%
Yin Xing Ye	Ginkgo folium	1	Expectorant & cough-suppressing	folium & cortex	0.60%
Yi Zhi Hao	Artemisia rupestris	1	Exterior-relieving	Herba & others	0.60%

Xu Chang					
Qing	Cynanchum paniculatum	1	Dampness-resolving	Radix & rhizoma	0.60%
Xie Bai	Allium macrostemon	1	Qi-regulating	Radix & rhizoma	0.60%
Tian Zhu			Expectorant &		
Huang	Bambusae concretio silicea	1	cough-suppressing	Herba & others	0.60%
Suan Zao					
Ren	Ziziphi spinosae semen	1	Sedative	Fructus & semen	0.60%
Su Mu	Caesalpinia sappan	1	Blood-activating	Herba & others	0.60%
Shu Di					
Huang	Rehmanniae radix praeparata	1	Blood-nourishing	Radix & rhizoma	0.60%
Qing Pi	Citrus reticulata blanco	1	Qi-regulating	folium & cortex	0.60%
Qing Dai	Indigo naturalis	1	Heat-clearing	Radix & rhizoma	0.60%
			Expectorant &		
Pang Da Hai	Scaphium wallichii	1	cough-suppressing	Fructus & semen	0.60%
Ou Jie	Nelumbinis rhizomatis nodus	1	Hemostatics	Radix & rhizoma	0.60%
Mu Hu Die	Oroxylum indicum	1	Heat-clearing	Fructus & semen	0.60%
Man Jing Zi	Vitidis fructus	1	Exterior-relieving	Fructus & semen	0.60%
			Expectorant &		
Jie Zi	Sinapis semen	1	cough-suppressing	Fructus & semen	0.60%
Huang Bai	Phellodendri chinensis cortex	1	Heat-clearing	folium & cortex	0.60%
Shan Zhi Ma	Helicteres angustifolia	1	Heat-clearing	Fructus & semen	0.60%
He Geng	Nymphaea tetragona	1	Heat-clearing	folium & cortex	0.60%
Gou Teng	Uncaria rhynchophylla	1	Heat-clearing	Radix & rhizoma	0.60%
Gong Lao					
Mu	Mahoniae caulis	1	Heat-clearing	Radix & rhizoma	0.60%
Fo Shou	Citrus medica	1	Qi-regulating	Fructus & semen	0.60%
Fei Xing Cao	Tripierospermum chinense	1	Heat-clearing	Radix & rhizoma	0.60%
Chuan Shan					
Long	Dioscorea nipponica	1	Blood-activating	Radix & rhizoma	0.60%
Cha Shu Gen	Camellia sinensis	1	Heat-clearing	Herba & others	0.60%
Ce Bai Ye	Platycladi cacumen	1	Hemostatics	folium & cortex	0.60%
Bu Zha Ye	Microctis folium	1	Heat-clearing	folium & cortex	0.60%
Ku Di Ding	Corydalis Bungeanae Herba	1	Heat-clearing	Herba & others	0.60%
Total		2760			

Table S3.2 Frequency of therapeutic effects of 179 herbs ($n=179$).

Therapeutic effect	Number of herbs	Frequency
Heat-clearing (antipyretic)	47	26.26%
Expectorant and cough-suppressing	22	12.29%
Dampness-resolving	21	11.73%
Exterior-relieving	20	11.17%
Qi-tonic	12	6.70%
Qi-regulating	12	6.70%
Yin-tonic	10	5.59%
Blood-activating	9	5.03%
Astringent	5	2.79%
Interior-warming	4	2.23%
Hemostatics	4	2.23%
Blood-tonic	4	2.23%
Resuscitation-inducing	3	1.68%
Digestant	3	1.68%
Sedative	2	1.12%
Insect repellent	1	0.56%

Table S3.3 Frequency of medicinal properties of 179 herbs ($n=179$).

Medicinal property	Number of herbs	Frequency
Radix & Rhizoma	83	46.37%
Fructus & Semen	42	23.46%
Herba & others	28	15.64%
Folium & Cortex	19	10.61%
Flos	7	3.91%

Table S4 Frequency of therapeutic effects in five medicinal properties.

Therapeutic effect	Medicinal properties					Total
	Flos	Folium & Cortex	Fructus & Semen	Herba & others	Radix & Rhizoma	
Astringent			5			5
Blood-activating	1		1	2	5	9
Blood-nourishing					4	4
Dampness-resolving	1	1	7	5	7	21
Digestant			3			3
Expectorant & cough-suppressing	1	4	6	2	9	22
Exterior-relieving	1	2	3	4	10	20
Heat-clearing	2	7	7	11	20	47
Hemostatics		1			3	4
Insect repellent			1			1
Interior-warming	1		1		2	4
Qi-regulating		3	3	2	4	12
Qi-tonic			1		11	12
Resuscitation-inducing				2	1	3
Sedative			1		1	2
Yin-nourishing		1	3		6	10
Total	7	19	42	28	83	179

Table S5.1 Top ten most frequently utilized individual herbs in COVID-19 treatment.

Herb	Frequency	Medicinal property	Natural property	Therapeutic effect	Chief chemical component
Glycyrrhizae radix et rhizoma	139	Radix & Rhizoma	Sweet and bland	Qi-tonic	Glycyrrhetic acid, glycyrrhizin, licoricidin, glabridin, glycyrrhiza polysaccharides, glutathione, isoangustone A, dehydroglyasperin C, licochalcone A,B,C,D,E, and liquiritigenin, etc.
Scutellariae radix	101	Radix & Rhizoma	Bitter and cold	Heat-clearing	Baicalein, phenyletha-noid glycosides, iridoid glycosides, diterpenes, triter-penoids, alkaloids, phytosterols, and polysaccharides, etc.
Armeniacaе semen amarum	87	Fructus & Semen	Bitter and slightly warm	Expectorant & cough-suppressing	Amygdalin, etc.
Lonicerae japonicae flos	82	Flos	Pungent, slightly bitter and warm	Heat-clearing	Chlorogenic acid, flavonoids, iridoids, organic acids, saponins, chlorogenic acid, luteolin, loganin, loniceroside A, hexadecanoic acid, octadecadienoic acid, ethyl palmitate, and dihydrocarveol, etc.
Forsythiae fructus	81	Fructus & Semen	Sweet and bland	Heat-clearing	Forsythiaside, forsythin, and rutin, etc.
Ephedrae herba	74	Herba & others	Pungent and slightly warm	Exterior-relieving	Ephedrine, pseudophedrine, <i>N</i> -Methylephedrine, <i>N</i> -Methylpseudoephedrine, norephedrine, and norpseudophedrine. etc.
Poria	65	Herba & others	Bitter, pungent, and warm	Dampness-resolving	Pachymic acid, triterpenes, and polysaccharides, etc.
Pogostemon cablin	63	Herba & others	Pungent and slightly warm	Dampness-resolving	Patchouli alcohol
Citri reticulatae pericarpium	57	Folium & Cortex	Bitter, pungent, and warm	Qi-regulating	Hesperidin, alkaloids, flavonoids, and essential oils, etc.
Platycodonis radix	55	Radix & Rhizoma	Bitter, pungent, and bland	Expectorant & cough-suppressing	Platycodin D, platycodonate, polygalacic acid, flavonoids, polysaccharides, sterols, phenols, polyacetylenes, fatty acids, and essential oils, etc.

Table S5.2 Information of the representative chemical components of top ten most frequently utilized herbs.

No.	Herbal medicine	Representative component	chemical	Molecular weight (g/mol)	Molecular formula
1	Glycyrrhizae radix et rhizoma	Glycyrrhetic acid		470.7	C ₃₀ H ₄₆ O _{4∞}
2	Scutellariae radix	baicalein		270.24	C ₁₅ H ₁₀ O ₅
3	Armeniacaе semen amarum	Amygdalin		457.48	C ₂₀ H ₂₇ NO ₁₁
4	Lonicerae japonicae flos	Chlorogenic acid		354.31	C ₁₆ H ₁₈ O _{9∞}
5	Forsythiae fructus	Forsythiaside		624.65	C ₂₉ H ₃₆ O _{15∞}
6	Ephedrae herba	Ephedrine		165.23	C ₁₀ H ₁₅ NO _∞
7	Poria	pachymic acid		528.85	C ₃₃ H ₅₂ O ₅
8	Pogostemon cablin	Patchouli alcohol		222.37	C ₁₅ H ₂₆ O
9	Citri reticulatae pericarpium	Hesperidin		610.62	C ₂₈ H ₃₄ O ₁₅
10	Platycodonis radix	Platycodin D		1,225.49	C ₅₇ H ₉₂ O ₂₈

Table S6.1 Eight groups of core combinations of herbs by hierarchical clustering.

Herb EN	Herb CN	Herb EN	Herb CN
Group One		Tetrapanax medulia	Tong Cao
Aconiti lateralis radix praeparata	Fu Zi	Group Four	
Aquilariae lignum resinatum	Chen Xiang	Angelicae sinensis radix	Dang Gui
Caryophylli flos	Ding Xiang	Carthamus tinctorius	Hong Hua
Cimicifugae rhizoma	Sheng Ma	Chuanxiong rhizoma	Chuan Xiong
Coptidis rhizoma	Huang Lian	Ginseng radix et rhizoma rubra	Hong Shen
Corni fructus	Shan Zhu Yu	Paeoniae radix rubra	Chi Shao
Curcumae radix	Yu Jin	Salviae miltiorrhizae radix et rhizoma	Dan Shen
Fritillariae cirrhosae bulbus	Chuan Bei Mu	Group Five	
Gardeniae fructus	Zhi Zi	Arctii fructus	Niu Bang Zi
Ginseng radix et rhizoma	Ren Shen	Armeniacae semen amarum	Ku Xing Ren
Sabia schumanniana	Qing Mu Xiang	Artemisiae annuae herba	Qing Hao
Scrophulariae radix	Xuan Shen	Aurantii fructus	Zhi Ke
Scutellariae radix	Huang Qin	Aurantii fructus immaturus	Zhi Shi
Group Two		Bupleuri radix	Chai Hu
Acori tatarinowii rhizoma	Shi Chang Pu	Cyrtomium fortunei	Guan Zhong
Anemarrhenae rhizoma	Zhi Mu	Descurainiae semen lepidii semen	Ting Li Zi
Moutan cortex	Mu Dan Pi	Ephedrae herba	Ma Huang
Paeoniae radix alba	Bai Shao	Eupatorii herba	Pei Lan
Panacis quinquefolii radix	Xi Yang Shen	Forsythiae fructus	Lian Qiao
Rehmanniae radix	Di Huang	Fritillariae thunbergii bulbus	Zhe Bei Mu
Group Three		Glycyrrhizae radix et rhizoma	Gan Cao Yu Xing Cao
Alismatis rhizoma	Ze Xie	Houttuyniae herba	Cao
Amomi fructus	Sha Ren	Isatidis folium	Da Qing Ye
Amomi fructus rotundus	Dou Kou	Isatidis radix	Ban Lan Gen
Angelicae dahuricae radix	Bai Zhi	Lonicerae japonicae flos	Jin Yin Hua
Asteris radix et rhizoma	Zi Wan	Menthae haplocalycis herba	Bo He
Belamcandae rhizoma	Sheng An	Mori cortex	Sang Bai Pi
Citri reticulatae pericarpium	Chen Pi	Persicae semen	Tao Ren
Coicis semen	Yi Yi Ren	Peucedani radix	Qian Hu
Curcumae longae rhizoma	Jiang Huang	Phragmitis rhizoma	Lu Gen
Lablab semen album	Bai Bian Dou	Platycodonis radix	Jie Geng
Lophatheri herba	Dan Zhu Ye	Puerariae lobatae radix	Ge Gen
Magnoliae officinalis cortex	Hou Po	Rhei radix et rhizoma	Da Huang
Perillae folium	Zi Su Ye	Rhodiolae crenulatae radix et rhizoma	Hong Jing Tian
Pinelliae rhizoma	Ban Xia	Schizonepetae herba	Jing Jie
Pogostemon cablin	Guang Huo Xiang	Trichosanthis fructus	Gua Lou
Polyporus	Zhu Ling	Group Six	
Poria	Fu Ling	Arecae semen	Bing Lang
Sojae semen praeparatum	Dan Dou Chi	Atractylodis rhizoma	Cang Zhu

Table S6.2 Twelve groups of core combinations of chemical components by hierarchical clustering.

Label	Molecule name	Label	Molecule name
Group One		C7_1	7-Methoxy-2-methyl isoflavone
C1_1	(-)-Catechin	C7_2	Chrysanthemaxanthin
C1_2	(Z)-3-(4-Hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	C7_3	Diop
C1_3	Coumaroyltyramine	C7_4	11,14-Eicosadienoic acid
C1_4	(6Z,10E,14E,18E)-2,6,10,15,19,23-Hexamethyltetracos-2,6,10,14,18,22-hexaene	C7_5	Formononetin
C1_5	Digallate	C7_6	Glycyrol
C1_6	<i>ent</i> -Epicatechin	C7_7	Jaranol
C1_7	Eriodyctiol (flavanone)	C7_8	beta-Sitosterol
C1_8	DNOP	C7_9	Ginsenoside rh2
C1_9	Procyanidin B1	C7_10	Malkangunin
C1_10	Isopimaric acid	C7_11	Sesamin
C1_11	Resivit	C7_12	Sitosterol
C1_12	Sugiol	C7_13	Stigmasterol
C1_13	Vitamin-E	C7_14	Mairin
Group Two		C7_15	Suchilactone
C2_1	(-)-Taxifolin	Group Eight	
C2_2	Diosmetin	C8_1	Campesterol
C2_3	Eriodyctiol	C8_2	Campest-5- <i>en</i> -3beta-ol
C2_4	Chryseriol	C8_3	CLR
C2_5	Ergosta-7,22-dien-3-one	C8_4	Cycloartenol
C2_6	1-Monolinolein	C8_5	Cycloeucaleanol
C2_7	Linolenic acid ethyl ester	C8_6	Ethyl linolenate
C2_8	Peroxyergosterol	C8_7	Ethyl oleate (NF)
C2_9	Schottenol	C8_8	Glycitein
C2_10	Diosgenin	C8_9	Spinasterol
C2_11	Luteolin	C8_10	Mandenol
C2_12	Genkwanin	C8_11	Sitosterol alpha1
C2_13	Supraene	C8_12	ZINC03978781
C2_14	Taxifolin	Group Nine	
Group Three		C9_1	Ammidin
C3_1	5,7-Dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	C9_2	Cnidilin
C3_2	Naringenin	C9_3	Isoimperatorin
C3_3	Neohesperidin_qt	C9_4	Methyl icos-11,14-dienoate
C3_4	Nobiletin	C9_5	Nodakenin
C3_5	Sinensetin	C9_6	Phellopterin
Group Four		Group Ten	
C4_1	Areapillin	C10_1	Berberine
C4_2	Artemetin	C10_2	Coptisine
C4_3	Isorhamnetin	C10_3	Fumarine
C4_4	Kaempferol	C10_4	Obacunone
C4_5	Quercetin	C10_5	Palmatine
C4_6	Skrofulen	Group Eleven	
Group Five		C11_1	Aloe-emodin
C5_1	Baicalein	C11_2	Daucosterol_qt
C5_2	Baicalin	C11_3	Gallic acid-3- <i>O</i> -(6'- <i>O</i> -galloyl)-glucoside
C5_3	Oroxylin a	Group Twelve	
C5_4	Ellagic acid	C12_1	6-(3-Oxoindolin-2-ylidene)indolo[2,1- <i>b</i>]quinazolin-12-one
C5_5	Gondoic acid	C12_2	DFV
C5_6	Wogonin	C12_3	Acacetin
Group Six		C12_4	Dinatin
C6_1	(+)-Catechin	C12_5	Indigo
C6_2	Benzoyl paeoniflorin	C12_6	24-Ethylcholest-4-en-3-one
C6_3	Paeoniflorin	C12_7	Isovitexin
C6_4	Paeoniflorin_qt	C12_8	Linarin
Group Seven		C12_9	Poriferast-5- <i>en</i> -3beta-ol
		C12_10	Sinoacutine

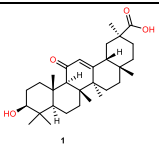
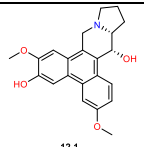
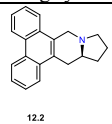
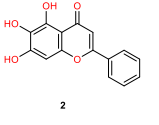
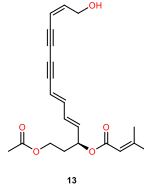
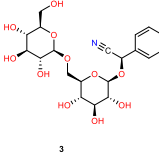
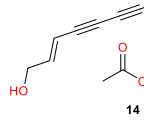
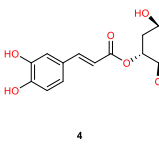
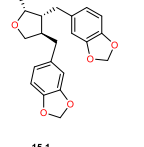
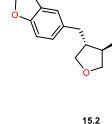
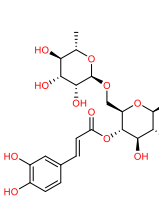
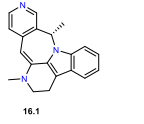
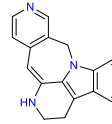
Table S7 Ten new formulas developed by unsupervised hierarchical clustering.

Herb EN	Herb CN	Herb EN	Herb CN
Formula One		Formula Five	
Aconiti lateralis radix praeparata	Fu Zi	Angelicae dahuricae radix	Bai Zhi
Acori tatarinowii rhizoma	Shi Chang Pu	Citri reticulatae pericarpium	Chen Pi
Armeniaca semen amarum	Ku Xing Ren	Magnoliae officinalis cortex	Hou Po
Asteris radix et rhizoma	Zi Wan	Perillae folium	Zi Su Ye
Aurantii fructus immaturus	Zhi Shi	Pinelliae rhizoma	Ban Xia
Belamcandae rhizoma	She Gan	Pogostemon cablin	Guang Huo Xiang
Chrysanthemi flos	Ju Hua	Poria	Fu Ling
Corni fructus	Shan Zhu Yu	Formula Six	
Dioscoreae rhizoma	Shan Yao	Angelicae sinensis radix	Dang Gui
Ephedrae herba	Ma Huang	Aurantii fructus	Zhi Ke
Eupatorii herba	Pei Lan	Bupleuri radix	Chai Hu
Fritillariae thunbergii bulbus	Zhe Bei Mu	Carthamus tinctorius	Hong Hua
Ginseng radix et rhizoma	Ren Shen	Chuanxiong rhizoma	Chuan Xiong
Isatidis folium	Da Qing Ye	Fritillariae cirrhosae bulbus	Chuan Bei Mu
Mori cortex	Sang Bai Pi	Ginseng radix et rhizoma rubra	Hong Shen
Mori folium	Sang Ye	Paeoniae radix rubra	Chi Shao
Formula Two		Peucedani radix	Qian Hu
Alismatis rhizoma	Ze Xie	Platycodonis radix	Jie Geng
Amomi fructus rotundus	Dou Kou	Puerariae lobatae radix	Ge Gen
Coicis semen	Yi Yi Ren	Salviae miltiorrhizae radix et rhizoma	Dan Shen
Curcumae longae rhizoma	Jiang Huang	Schizonepetae herba	Jing Jie
Polyporus	Zhu Ling	Formula Seven	
Sojae semen praeparatum	Dan Dou Chi	Arctii fructus	Niu Bang Zi
Tetrapanax medulia	Tong Cao	Codonopsis radix	Dang Shen
Formula Three		Forsythiae fructus	Lian Qiao
Amomi fructus	Sha Ren	Glycyrrhizae radix et rhizoma	Gan Cao
Descurainiae semen lepidii semen	Ting Li Zi	Lophatheri herba	Dan Zhu Ye
Lablab semen album	Bai Bian Dou	Menthae haplocalycis herba	Bo He
Persicae semen	Tao Ren	Phragmitis rhizoma	Lu Hui
Rhei radix et rhizoma	Da Huang	Formula Eight	
Trichosanthis fructus	Gua Lou	Arecae semen	Bing Lang
Formula Four		Atractylodis rhizoma	Cang Zhu
Anemarrhenae rhizoma	Zhi Mu	Lonicerae japonicae flos	Jin Yin Hua
Aquilariae lignum resinatum	Chen Xiang	Notopterygii rhizoma et radix	Qiang Huo
Aucklandiae radix	Mu Xiang	Tsaoko fructus	Cao Guo
Benzoinum	An Xi Xiang	Zingiberis rhizoma recens	Sheng Jiang
Caryophylli flos	Ding Xiang	Formula Nine	
Chebulae fructus	Ke Zi	Artemisiae annuae herba	Qing Hao
Cimicifugae rhizoma	Sheng Ma	Cinnamomi ramulus	Gui Zhi
Coptidis rhizoma	Huang Lian	Cyrtomium fortunei	Guan Zhong
Curcumae radix	Yu Jin	Glehniae radix	Bei Sha Shen
Cyperi rhizoma	Xiang Fu	Houttuyniae herba	Yu Xing Cao
Gardeniae fructus	Zhi Zi	Isatidis radix	Ban Lan Gen
Liquidambar	Su He Xiang	Jujubae fructus	Da Zao
Moutan cortex	Mu Dan Pi	Ophiopogonis radix	Mai Dong
Olibanum	Ru Xiang	Panacis quinquefolii radix	Xi Yang Shen
Paeoniae radix alba	Bai Shao	Rhodiola crenulatae radix et rhizoma	Hong Jing Tian
Piperis longi fructus	Bi Ba	Schisandrae chinensis fructus	Wu Wei Zi
Rehmanniae radix	Di Huang	Formula Ten	
Sabia schumanniana	Qing Mu Xiang	Astragali radix	Huang Qi
Santalum album	Chan Xiang	Atractylodis macrocephalae rhizoma	Bai Zhu
Scrophulariae radix	Xuan Shen	Pseudostellariae radix	Tai Zi Shen
Scutellariae radix	Huang Qin	Saposhnikovia radix	Fang Feng

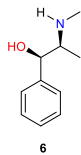
Table S8 List of eight clusters and corresponding active pharmacophores.

Mod ID	Cluster structure	Basic ring system
MOL0 13094	8-(2,3-Dihydroxy-3-methylbutyl)-5,7-dimethoxy-2 <i>H</i> -chromen-2-one	2 <i>H</i> -Chromen-2-one
MOL0 13287	(3 <i>aR</i> ,8 <i>aR</i>)-3 <i>a</i> ,8-Dimethyl-3,3 <i>a</i> ,8,8 <i>a</i> -tetrahydro-2 <i>H</i> -furo[2,3- <i>b</i>]indol-5-yl methylcarbamate	3,3 <i>a</i> ,8,8 <i>a</i> -Tetrahydro-2 <i>H</i> -furo[2,3- <i>b</i>]indole
MOL0 13117	(2 <i>S</i> ,4 <i>R</i>)-4,7-Dihydroxy-5-methoxy-6-methyl-2-phenyl-8-chromanecarbaldehyde	2-Phenylchromane
MOL0 12893	(<i>E</i>)-1-(4-Methylphenyl)- <i>N</i> -(4-phenyl-1 <i>H</i> -1,2,3-triazol-1-yl)methanimine	(<i>E</i>)-1-Phenyl- <i>N</i> -(4-phenyl-1 <i>H</i> -1,2,3-triazol-1-yl)methanimine
MOL0 12933	(13 <i>aR</i> ,14 <i>R</i>)-3,7-Dimethoxy-9,11,12,13,13 <i>a</i> ,14-hexahydrodibenzo[<i>f,h</i>]pyrrolo[1,2- <i>b</i>]isoquinolin-6,14-diol	9,11,12,13,13 <i>a</i> ,14-Hexahydrodibenzo[<i>f,h</i>]pyrrolo[1,2- <i>b</i>]isoquinoline
MOL0 13081	7,13-Dimethyl-5,6,7,13-tetrahydro-7,11,13 <i>a</i> -triazabenz[5,6]cyclohepta[1,2,3- <i>jk</i>]fluorene	1,2,3,8-Tetrahydro-1,7 <i>b</i> ,10-triazabenz[5,6]cyclohepta[1,2,3- <i>jk</i>]fluorene
MOL0 13187	(2 <i>S</i> ,3 <i>R</i> ,4 <i>R</i>)-3,4-Bis(1,3-benzodioxol-5-ylmethyl)tetrahydro-2-furanol	5,5'-[(3 <i>R</i> ,4 <i>R</i>)-Tetrahydrofuran-3,4-diylbis(methylene)]bis(1,3-benzodioxole)
MOL0 13037	2-(2-Phenylethyl)-6-[[[(6 <i>R</i> ,7 <i>R</i>)-5,6,7-trihydroxy-4-oxo-2-(2-phenylethyl)-5,6,7,8-tetrahydro-4 <i>H</i> -chromen-8-yl]oxy]-4 <i>H</i> -chromen-4-one	6-((4-Oxo-2-phenethyl-5,6,7,8-tetrahydro-4 <i>H</i> -chromen-8-yl)oxy)-2-phenethyl-4 <i>H</i> -chromen-4-one

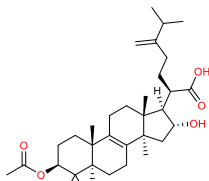
Table S9 Number of 22 chemical structures.

No.	Structure	Ring system	No.	Structure	Ring system
1			12		 12.2
2			13		
3			14		
4			15		 15.2
5			16		 16.2

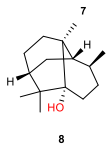
6



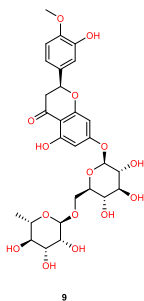
7



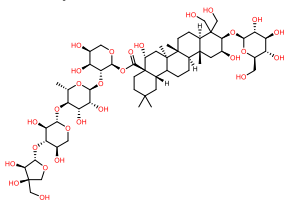
8



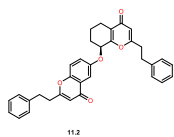
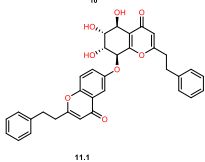
9



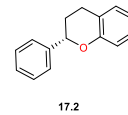
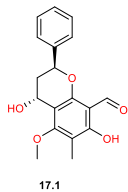
10



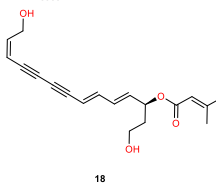
11



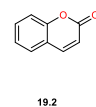
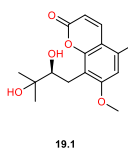
17



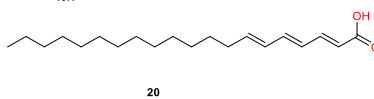
18



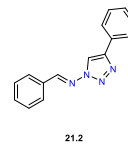
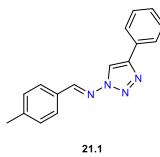
19



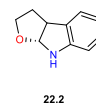
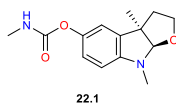
20



21



22



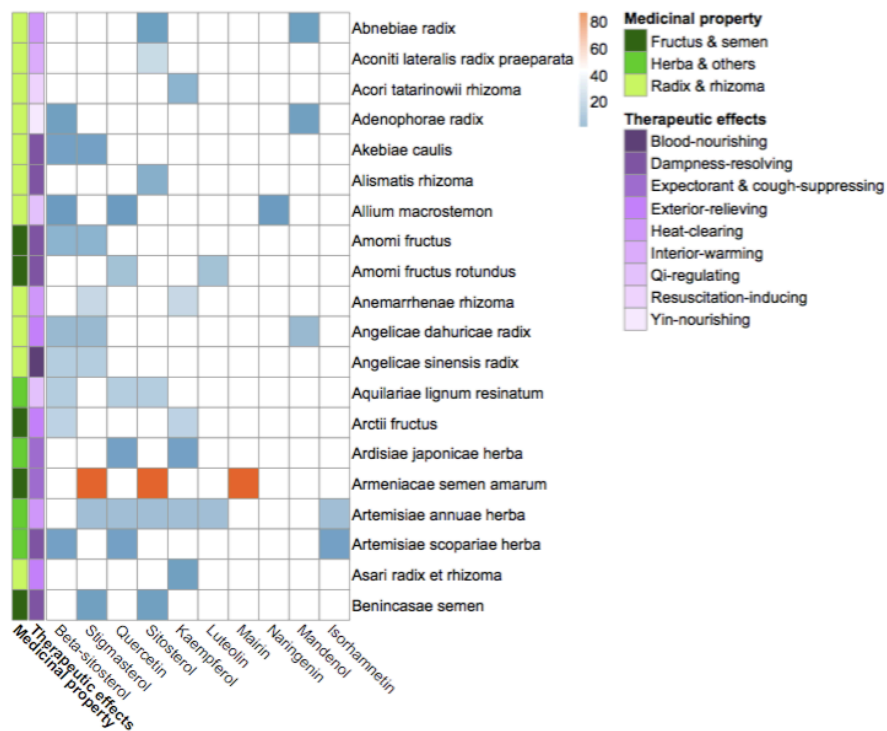


Figure S1 Heat map of the frequency of top 10 frequently appeared chemical components in top 20 frequently utilized herbs. Among the top 20 most frequently utilized herbal medicines containing top ten most frequently appeared components showing in the heat map, five of them belong to fructus & semen, 11 are applied by radix & rhizome, four are herba & others. While six of them belong to dampness-resolving class, three are antipyretic and another three are exterior-relieving, two are expectorant & cough-suppressing and another two Qi-regulating, one blood-nourishing, one interior-warming, one Yin-nourishing, and one resuscitation-inducing.