

An integrated antiarrhythmic target network of compound Chinese medicine Wenxin Keli revealed by a combined machine learning and molecular pathway analysis

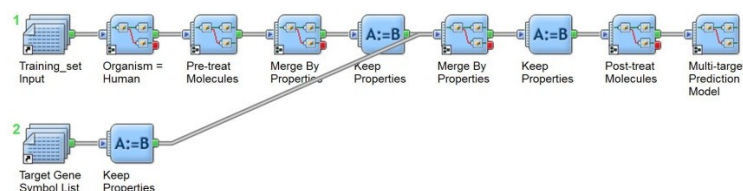


Figure S1 Protocol for establishing multi-target prediction model

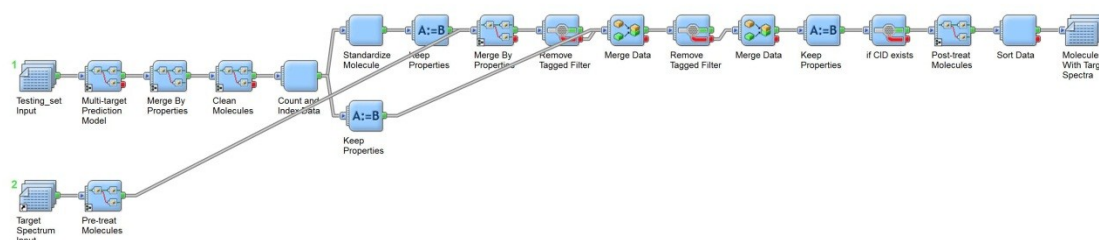


Figure S2 Protocol for outputting the target spectrum for testing molecules

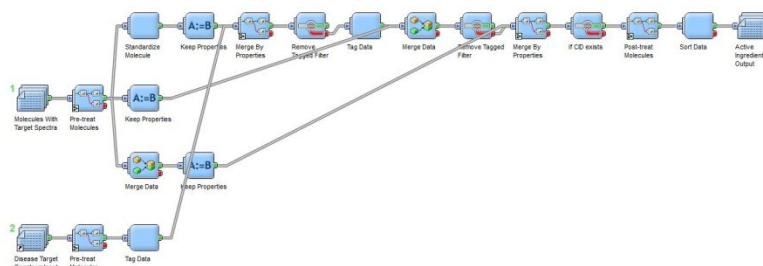


Figure S3 Protocol for overlapping the component and disease target spectra.

Table S1 Components of five herbs in Wenxin Keli

Library_Index	Component_Name	PubChem_CID	ChemSpider_ID	Chemdraw_ID
dangshen_004	taraxeryl acetate	94225		
dangshen_006	(-)-nicotine	942		
dangshen_007	friedelan-3-one	244297		
dangshen_017	daturic acid	67956		
dangshen_030	5-hydroxymethyl-2-furaldehyde	237332		
dangshen_044	pyro-glutamic acid-N-furctoside			
dangshen_047	alpha-pinene	6654		

dangshen_052	stigmatetyl-beta-D-glucoside	70699355
dangshen_055	stigmasterol	50930798
dangshen_057	7-stigmasterol-3-o-beta-d-glucoside	
dangshen_062	n-butyl allophanate	5315565
dangshen_063	taraxerol	11876269
dangshen_064	ethyl-alpha-d-fructoside	
dangshen_072	O-(O-methoxyphenoxy) phenol	
dangshen_074	syringaldehyde	8655
dangshen_079	perlolyrine	10706796
dangshen_089	1. N'-[N-(2a,3b-Dihydroxy-12-oleanen-28-oyl)-L-alanyl]-glycine	44570740
dangshen_093	tangshenoside I	6441191
dangshen_100	n-hexyl-beta-D-glucopyranoside	181215
dangshen_106	stigmasta-5,22-dien-3-one	5321507
dangshen_108	5alpha-stigmasta-7,22-dien-3-one	
dangshen_123	syringin	24847743
dangshen_132	ferulic acid	445858
dangshen_136	alpha-spinasteryl-beta-D-glucoside	
dangshen_140	5-metyoxymethy-2-furaldehyde	74711
dangshen_144	2,4-nonadienicacid	
dangshen_153	atractylenolide II	11736433
dangshen_154	atractylenolide III	11311230
dangshen_155	1,5-di-isobutyl-3,3-dimethyl[3,1,0]cyclohexa-dione	
dangshen_172	delta-guaiene	
huangjing_007	polyspirostanol po5	
huangjing_008	5,6-dihydroxy-7-o-glucoside-flavone	
huangjing_012	polyspirostanol po3	
huangjing_013	polyspirostanol poe	
huangjing_014	polyspirostanol po6	
huangjing_015	polyspirostanol po2	
huangjing_016	polyspirostanol po1	
huangjing_020	Apigenin	4444100
sanqi_001	ginsenoside rd	24721561

sanqi_002	ginsenoside Re	73149
sanqi_003	ginsenoside rc	100018
sanqi_004	ginsenoside Rb1	432524
sanqi_005	ginsenoside Rb2	432450
sanqi_008	ginsenoside Rg1	441923
sanqi_009	cyperene	12308843
sanqi_012	alpha-copaene	636457
sanqi_014	daucosterol	52940117
sanqi_017	methylhexadecanate	
sanqi_021	6-o-beta-d-glucopyranosyl-20-o-beta-d-glucopyra-nosyl-3beta,6alpha,12beta,20(s),25-pentahydroxydam-mar-23-ene	
sanqi_023	20(s)-ginsenoside-rh1	
sanqi_024	delta-cadinene	441005
sanqi_033	3-ene-nonanone-2	
sanqi_036	L-alpha-amino-beta-oxalylaminopropionic acid	25201828
sanqi_037	alpha,alpha-dimethylbenzene methanol	
sanqi_038	cyclododecanone	13246
sanqi_040	3beta-o-beta-d-glucopyranosyl-20-o-[alpha-l-arabino-pyranosyl(1→2)-beta-d-glucopyranosyl]3beta,12beta,20(s)-trihydroxydammar-24-ene	
sanqi_041	acetophenone	7410
sanqi_044	stigmasterol	50930798
sanqi_045	dicapryl phthalate	8558
sanqi_046	1,1,5,5-tetramethyl-4-methano-2,3,4,6,7,10-hexahydronaphthalene	5321892
sanqi_047	notoginsenoside l	
sanqi_048	notoginsenoside k	
sanqi_049	notoginsenoside n	
sanqi_050	notoginsenoside m	
sanqi_051	notoginsenoside r1	53399243
sanqi_053	notoginsenoside r3	11968802
sanqi_055	isobutyl pyroglutamate	
sanqi_056	2,8-dimethyl-5-acetyl-bicyclo[5,3,0]deca-diene-1,8	
sanqi_058	sanchinoside b1	11968918
sanqi_059	alpha-guriunene	

sanqi_062	notoginsenoside c	
sanqi_064	alpha-murolene	12306047
sanqi_065	beta-sitosterol	222284
sanqi_070	1-methyl-4-isoallyl-cyclohexane	5319687
sanqi_073	notoginsenoside r4	5320225
sanqi_074	notoginsenoside r6	73351440
sanqi_083	n-butyl pyroglutamate	
sanqi_087	notoginsenoside a	6451129
sanqi_092	2,6-ditertbutyl-4-methyl phenol	
sanqi_094	ditertbutyl phthalate	121712
sanqi_095	methyl pyroglutamate	
sanqi_097	(s)-dencichine	
sanqi_104	notoginsenoside i	
sanqi_105	notoginsenoside j	
sanqi_107	notoginsenoside b	
sanqi_108	panaxatriol	12313936
sanqi_109	notoginsenoside d	
sanqi_110	notoginsenoside fe	
sanqi_111	notoginsenoside g	
sanqi_112	notoginsenoside h	
sanqi_113	cuparene	11084908
sanqi_116	panaxytriol	11108666
sanqi_117	panaxynol	5469789
sanqi_118	panaxydol	10825263
sanqi_119	gamma-elemene	6432312
sanqi_120	panaxadiol	10072981
sanqi_121	20-o-beta-d-xylopyranosyl(1→6)-beta-d-glucopyranosyl-20(s)-protopanaxadiol	
sanqi_129	quinquenoside ii	
sanqi_132	ethyl pyroglutamate	643508
sanqi_133	diisocapryl phthalate	
sanqi_134	nonanoic acid	
sanqi_136	quercetin	46906036

sanqi_145	beta-elemene	6918391	
sanqi_147	delta-guaiene	94275	
sanqi_148	alpha-guaiene	5317844	
sanqi_152	quinquenoside i		
sanqi_153	quinquenoside iii		
sanqi_154	ethylpalmitate		
sanqi_155	quinquenoside iv		
sanqi_156	quinquenoside v		
sanqi_157	3-o-[beta-d-glucopyranosyl(1→6)-beta-d-glucopyranosyl]-20-o-beta-d-glucopyranosyl-3beta,12beta,20(s)-trihydroxydammar-24-ene		
sanqi_192	20(S)-Notoginsenoside R2		
sanqi_193	20(R)-Notoginsenoside R2		
dangshen_001	2,4,4-trimethyl-1-pentene	7868	
dangshen_002	delta7-stigmastenone-3	5748344	
dangshen_005	nicotinic acid	938	
dangshen_008	alpha-stigmasterol-beta-d-glucoside		10142723
dangshen_009	furanodiene	5317424	
dangshen_011	2-furancarboxylic acid		10251740
dangshen_012	friedelin	11870449	
dangshen_013	alpha-curcumene	442360	
dangshen_014	5alpha-stigmastan-3,6-dione	10025616	
dangshen_015	1-peroxyferolide	442290	
dangshen_016	daturilin		4475392
dangshen_020	hexyl-beta-d-glucopyranosyl-(1-2)-beta-d-glucopyranoside		
dangshen_021	tangshenoside ii	5321613	
dangshen_022	5-hydroxy-2-pyridinemethanol		371355
dangshen_024	borneol	44630107	
dangshen_025	5-methoxy-3-(2-phenyl-e-e-ethenyl)-2,4-bis(4-hydroxybenzyl)phenol		4477772
dangshen_027	codonolactone	155948	
dangshen_029	alpha-curcumene	3083834	
dangshen_031	myristicin	4276	
dangshen_038	fritillaziebinol	24893863	

dangshen_040	encecalin	114703
dangshen_041	5-methoxylfuradehyde3	
dangshen_042	stigmasteryl ferulate	10769701
dangshen_048	delta7-stigmasterol	
dangshen_049	butyl-cyclohexane	15506
dangshen_054	7-(beta-xylosyl)cephalomannine	
dangshen_059	nicotine	6919000
dangshen_060	frutinone a	441965
dangshen_061	taraxerone	11877466
dangshen_067	2-furancarboxylate	5460151
dangshen_068	chrysanthemaxanthin	5376313
dangshen_070	12-o-nicotinoylisolineolone	5320138
dangshen_071	beta-curcumene	14014430
dangshen_076	dl-syringaresinol	
dangshen_078	20-hexadecanoylingenol	5318035
dangshen_083	4-methylsulfinyl butyl isothiocyanate	5350
dangshen_084	delta22-stigmasterol	
dangshen_085	2,6,10,14-tetramethyl hexadecane	
dangshen_088	2-[[[(2S)-2- [[[(4aS,6aR,6aS,6bR,8aR,10R,11R,12aR, 14bS)-10,11-dihydroxy- 2,2,6a,6b,9,9,12a-heptamethyl- 1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b- tetradecahydronicene-4a- carbonyl]amino]propanoyl]amino]acetic acid	11994876
dangshen_091	22-dine-3-one	
dangshen_095	3-beta-hydroxymethylenetanshiquinone	
dangshen_096	4-phenylbicyclo[2,2,2]octan-1-ol	
dangshen_097	codpiloic acid	178371
dangshen_098	8alpha-methoxyfuranodiene	6325622
dangshen_099	stigmasta-5	
dangshen_104	alpha-spinasterol	5281331
dangshen_105	inulin	44630352
dangshen_107	menthyl acetate	220674

dangshen_109	1-ethyl-beta-d-galactoside	
dangshen_112	tansehnoside	
dangshen_113	tert-butylbenzene	7366
dangshen_117	alpha-pinene	82227
dangshen_118	pyridine	11738823
dangshen_124	scutellarein glucoside	
dangshen_125	alpha-spinasterol-beta-d-glucoside	11968950
dangshen_127	atractylinolide ii	14448070
dangshen_128	3-methylcarbazole	20746
dangshen_130	coelogen	442697
dangshen_134	codonopsine	442631
dangshen_138	spinoside a	6326071
dangshen_139	7-methoxy-2-methyl isoflavone	
dangshen_141	11-hydroxyrankinidine	5318332
dangshen_145	alpha-stigmasta-7,22-dien-3-one	
dangshen_146	tangshenoside	
dangshen_152	7alpha-l-rhamnosyl-6-methoxylutcolin	
dangshen_156	stigmasta-7,22-dien-3-one	
dangshen_157	capsaicin (e)	1548943
dangshen_160	diisocapryl phthalate	
dangshen_162	vanillic acid	54675858
dangshen_163	2,6-nonadienol	
dangshen_168	beta-pinene	14896
dangshen_171	guajaverin	44259215
dangshen_174	methionine sulfoxide	56932118
dangshen_175	6,6'-dimethoxygossypol	5316861
dangshen_176	ethyl-p-digallate	5317260
dangshen_179	ricinine	2786702
dangshen_182	delta7-sitgmas-tenyl-beta-D-glucoside	
dangshen_183	methyl-11,14-eicosadenoate	
dangshen_184	stigmast-7-en-3beta-ol	
dangshen_185	Taraxasteryl acetate	

dangshen_186	Lobetyolin		24534044
gansong_001	orotic acid	23683036	
gansong_002	debneyol	5316408	
gansong_005	cineole	2758	
gansong_006	alpha-pinene	82227	
gansong_007	nardosinonediol		nardosinonediol
gansong_008	nardosinone	168136	
gansong_009	nardonoxide		
gansong_010	nardol	5320013	
gansong_011	nardoguaianone k		
gansong_012	nardoguaianone j	5320012	
gansong_013	nardofuran	170651	
gansong_014	paulownin	11068649	
gansong_015	patchouli alcohol	10955174	
gansong_016	calarenol	6324867	
gansong_017	calarene	6432176	
gansong_018	4-methyl-1,2-benzenediamine	10332	
gansong_019	nardostachone	5320015	
gansong_020	nardostachin	196699	
gansong_021	isovaleroxy-hydroxy dihydrovaltrate	5318683	
gansong_022	valeranone	171455	
gansong_024	eudesobovatol a	442837	
gansong_025	angelicin	457801	
gansong_026	beta-caryophyllen	5281522	
gansong_027	beta-eudesmol		
gansong_028	alpha-guriunene	5317859	
gansong_029	kanshone E		
gansong_030	kanshone C		
gansong_031	kanshone D		
gansong_032	oroselol	160600	
gansong_033	1,2,9,10-tetradehydroaristolane	5321842	
gansong_034	tetradymol	3512330	

gansong_035	(+)-car-3-ene-2,5-dione	
gansong_036	jatropham	5325835
gansong_037	beta-patchoulene	101731
gansong_038	valerenic acid	42608162
gansong_039	jatamansinol	
gansong_040	calaxin	5281431
gansong_041	jatamansin	668081
gansong_042	9-aristolen-1alpha-ol	5320089
gansong_043	isonardosinone	
gansong_046	elemene	9859094
gansong_047	beta-pinene	14896
gansong_049	aristolan-9beta-ol	
gansong_050	9-aristolene	
gansong_053	1(10)-aristolen-2-one	5320095
gansong_054	gansong_015	
gansong_055	debilone	5316407
gansong_056	narchinol A	
gansong_057	kanshone B	14021478
gansong_058	kanshone A	15694585
gansong_059	carene-3	
gansong_060	naringenin	667495
gansong_061	jatamansinlo	
gansong_062	1,5-naphthalene diol	
gansong_063	aristolene	530421
gansong_064	1(10)-aristolene	
gansong_065	eudesm-11-en-2,4alpha-diol	
gansong_066	9-aristolen-2-one	
gansong_067	beta-Maaliene	
gansong_068	beta-sitosterol	
gansong_069	1(10)-aristolen-9beta-ol	1(10)-aristolen-9beta-ol
gansong_070	gansongone	
gansong_071	nardosinonediol	

gansong_072	oleanolic acid	10062	
gansong_073	de-oxonarchinol A		de-oxonarchinol A
gansong_074	ursolic acid	58472	
gansong_075	ethyl-beta-D-glucopy-ranoside	121667	
gansong_A01	delta(1,10)-aristolene		gansong_A01
gansong_A02	delta9-aristolene		gansong_A02
gansong_A03	1,2,9,10-tetradehydroaristolan		gansong_A03
gansong_A04	1,2,9,10-tetradehydroaristolan-2-one		gansong_A04
gansong_A05	delta(1,10)-aristolene-2-one		gansong_A05
gansong_A06	Gansongone		gansong_A06
gansong_A07	Aristolone		gansong_A07
gansong_A08	Debilon		gansong_A08
gansong_A09	delta(1,10)-aristolene-9beta-ol		gansong_A09
gansong_A10	Calarenol		gansong_A10
gansong_A11	Kanshone G		gansong_A11
gansong_A12	Kanshone C		gansong_A12
gansong_A13	Kanshone F		gansong_A13
gansong_A14	Nardonoxide		gansong_A14
gansong_A15	Nardofuran		gansong_A15
gansong_A16	Kanshone A		gansong_A16
gansong_A17	Nardosinonediol		gansong_A17
gansong_A18	Kanshone D		gansong_A18
gansong_A19	Kanshone E		gansong_A19
gansong_A20	Isonardosinone		gansong_A20
gansong_A21	Nardosinone		gansong_A21
gansong_A22	Kanshone B		gansong_A22
gansong_A23	Narchinol A		gansong_A23
gansong_A24	Desoxo-narchinol-A		gansong_A24
gansong_A25	Nardoguaianone A		gansong_A25
gansong_A26	Nardoperoxide		gansong_A26
gansong_A27	Nardoguaianone C		gansong_A27
gansong_A28	Nardoguaianone B		gansong_A28

gansong_A29	Nardoguaianone D	gansong_A29
gansong_A30	Isonardoperoxide	gansong_A30
gansong_A31	Nardoguaianone E	gansong_A31
gansong_A32	Nardoguaianone F	gansong_A32
gansong_A33	Nardoguaianone G	gansong_A33
gansong_A34	Nardoguaianone H	gansong_A34
gansong_A35	Nardoguaianone I	gansong_A35
gansong_A36	Nardoguaianone J	gansong_A36
gansong_A37	Nardoguaianone K	gansong_A37
gansong_A38	Nardol	gansong_A38
gansong_A39	Jatamansic acid	gansong_A39
gansong_A40	Nardoxide	gansong_A40
gansong_A41	beta-Maaliene	gansong_A41
gansong_A42	beta-Maaliol	gansong_A42
gansong_A43	Valeranone	gansong_A43
gansong_A44	Nardostachone	gansong_A44
gansong_A45	Eudesm-11-2,4alpha-diol	gansong_A45
gansong_A46	beta-Eudesmol	gansong_A46
gansong_A47	Jatamol A	gansong_A47
gansong_A48	Jatamol B	gansong_A48
gansong_A49	Elemol	gansong_A49
gansong_A50	Patchouli alcohol	gansong_A50
gansong_A51	beta-Patchoulene	gansong_A51
gansong_A52	alpha-Patchoulene	gansong_A52
gansong_A53	Seychellane	gansong_A53
gansong_A54	Seychellene	gansong_A54
gansong_A55	Norseychellanone	gansong_A55
gansong_A56	Spirojatamol	gansong_A56
gansong_A57	alpha-Pinene	gansong_A57
gansong_A58	beta-Pinene	gansong_A58
gansong_A59	3-Carene	gansong_A59
gansong_A60	beta-Ionone	gansong_A60

gansong_A61	Nardosatchin		gansong_A61
gansong_A62	Oleanolic acid		gansong_A62
gansong_A63	Nardostachysin		gansong_A63
gansong_A64	Jatamansin		gansong_A64
gansong_A65	Jatamansinol		gansong_A65
gansong_A66	Oroselol		gansong_A66
gansong_A67	Angelicin		gansong_A67
gansong_A68	Erythro-(3,4-dimethoxyphenyl)-2-(2-methoxy-4-(E)-(propenylphenoxy)-propan-1-ol		gansong_A68
gansong_A69	Virolin		gansong_A69
gansong_A70	Erythro-1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxy-4(E)-(propenylphenoxy)-propan-1-ol		gansong_A70
gansong_A71	(+)-Pinoresinol		gansong_A71
gansong_A72	(+)-1-Hydroxyinoresinol		gansong_A72
gansong_A73	Dinardokanshones A		gansong_A73
gansong_A74	Dinardokanshones B		gansong_A74
huangjing_002	vitexin xyloside	5364006	
huangjing_004	azetidine-2-carboxylic acid	5248351	
huangjing_005	neoprazerigenin A3-O-beta-lycotetraoside		
huangjing_006	digitalis glycoside	53477737	
huangjing_009	5,4'-dihydroxyflavone-6-c-beta-d-glycosyl-rhamnoside-7-o-glycoside		
huangjing_017	14alpha-hydroxysibiricoside A		
huangjing_018	sibiricoside A	46173928	
huangjing_019	sibiricoside B	46173929	
huangjing_A13	Liquiritigenin		huangjing_A13
huangjing_A14	Vitexinxyloside I		huangjing_A14
huangjing_A15	Vitexinxyloside II		huangjing_A15
huangjing_A18	8-C-galactosylapigenin		huangjing_A18
huangjing_A19	6-C-galactosyl-8-C-galactosylapigenin		huangjing_A19
huangjing_A22	Isoliquiritigenin		huangjing_A22
huangjing_A23	7-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-4H-chromen-4-one		huangjing_A23
huangjing_A24	vitexin		huangjing_A24
huangjing_A28	Tectoridin isoflavone		huangjing_A28
huangjing_A39	syringaresinol		huangjing_A39

huangjing_A40	Syringaresinol-O-beta-D-glucopyranoside		huangjing_A40
huangjing_A41	Liriodendron glycosides		huangjing_A41
hupo_001	succinosilvic acid		
hupo_002	succinic acid	53338995	
hupo_003	succinoabietol		
hupo_004	succinoresinol		
hupo_005	diabietinolic acid		
hupo_006	succinoa bietinolic acid		
hupo_007	succoxyabietic acid		
hupo_008	borneol	64685	
sanqi_006	bata-caryophyllene	5281515	
sanqi_010	cyperol	14076601	
sanqi_011	alpha-cuparenol	5318539	
sanqi_015	delta-elemene	12004383	
sanqi_016	alpha-guttiferin		
sanqi_018	20(s)-ginsenoside-rh2		
sanqi_019	20(r)-ginsenoside-rh1		
sanqi_020	gamma-sitosterol	636741	
sanqi_026	(-)-dicentrine	317843	
sanqi_029	engeletin	44584103	
sanqi_031	encecalin	114703	
sanqi_035	diterbutyl phthalate		
sanqi_039	mycosinol	5281153	
sanqi_042	ginsenoside	3086007	
sanqi_043	isoaloesin	11972379	
sanqi_052	cycloeucaenol	50986194	
sanqi_060	xi-cadinene	5315590	
sanqi_061	20-hexadecanoylingenol	5318035	
sanqi_063	quercetin-3-l-arabinon-7-d-glucoside		
sanqi_066	delta-guaiene	11958028	
sanqi_069	methyl isobutyl ketone	7909	
sanqi_071	(-)-trifara-9,14-diene	6326198	

sanqi_075	flavonoid glycoside	
sanqi_076	notopterol	5320227
sanqi_080	guaijaverin	44259215
sanqi_081	1-tridecene-3,5,7,9,11-pentyne	
sanqi_090	gypenoside XVII	45479307
sanqi_091	stigmasterol-beta-d-glucoside	
sanqi_093	dithiocyclopentene	5316944
sanqi_096	4,4'-diketo-3-hydroxy-beta-carotene	10303691
sanqi_098	dauricine	45358120
sanqi_099	elemicin	10248
sanqi_103	sanqi_087	
sanqi_106	sandaracopimarinol	10446844
sanqi_123	pancratistatin	6713165
sanqi_124	3,4-dimethylbenzoic acid	12073
sanqi_125	beta,beta-dimethylacrylalkannin	442720
sanqi_127	ethyl-p-digallate	5317260
sanqi_131	14-methyl hexadecanoic acid	
sanqi_151	coprine	4479242
sanqi_158	1,10-dimethoxy-3-one-7-acetylenedecahydronaphthalene	
sanqi_159	1,9,9-Trimethyl-4,7-dimethano-2,3,5,6,7,8-hexahydroazulene	
sanqi_160	1-methoxyethylbenzene	19913
sanqi_161	1-methyl-4-dioximethylthino-bicycol(2,2,2) octane	
sanqi_162	20-O-glucoginsenoside Rf	
sanqi_166	cyclodecanone	73918
sanqi_167	dammar-20(22)-ene-3beta,12beta,25-TCMLIBio1-6-O-beta-D-glucopyranoside	
sanqi_168	dencichine	2360
sanqi_169	dicaplate	
sanqi_170	ethyloctadecadienoate	
sanqi_172	ginsenoside Rg2	6441009
sanqi_173	ginsenoside Rh1	12855920
sanqi_175	methylheptadecadieneoate	
sanqi_180	notoginsenoside R7	

sanqi_185	alpha-cedrene	6431015
sanqi_186	alpha-elemene	
sanqi_187	beta-cubebene	93081
sanqi_188	beta-guaiene	6949
sanqi_189	gamma-cadinene	92313
sanqi_190	gamma-murolene	12313020
sanqi_191	xi-guaiene	

Table S2 Acting target spectrum of the active components in Wenxin Keli

Library Index	Name	Target Name	Target Score
dangshen_005	nicotinic acid	TBXA2R	16.225
dangshen_005	nicotinic acid	ADRB1	11.038
dangshen_009	furanodiene	RAPGEF4	9.3555
dangshen_011	2-furancarboxylic acid	RAPGEF4	6.7818
dangshen_013	alpha-curcumene	RAPGEF4	12.452
dangshen_013	alpha-curcumene	PLA2G6	6.3923
dangshen_016	daturilin	PTGFR	6.9179
dangshen_025	5-methoxy-3-(2-phenyl-e-e-ethenyl)-2,4-bis(4-hydroxybenzyl)phenol	TTR	12.684
dangshen_027	codonolactone	FKBP1A	7.0532
dangshen_029	alpha-curcumene	RAPGEF4	12.452
dangshen_029	alpha-curcumene	PLA2G6	6.3923
dangshen_031	myristicin	FKBP1A	7.1848
dangshen_031	myristicin	ADRA2C	8.4596
dangshen_031	myristicin	CHRM2	8.5561
dangshen_031	myristicin	ADRA2B	9.3420
dangshen_040	encecalin	KCNA1	6.3261
dangshen_040	encecalin	ADRA2A	6.2615
dangshen_040	encecalin	ADRA2C	6.0779
dangshen_049	butyl-cyclohexane	CHRM2	9.1093
dangshen_049	butyl-cyclohexane	RAPGEF4	7.4867
dangshen_049	butyl-cyclohexane	TBXA2R	6.8168
dangshen_059	nicotine	TGM2	12.256
dangshen_059	nicotine	TBXA2R	6.6544
dangshen_059	nicotine	RAPGEF4	6.4446
dangshen_060	frutinone a	ADRA2B	8.0783
dangshen_060	frutinone a	ADRA2A	9.5874
dangshen_060	frutinone a	ADRA2C	9.9038
dangshen_060	frutinone a	HCN4	10.035
dangshen_060	frutinone a	TTR	10.952
dangshen_067	2-furancarboxylate	RAPGEF4	10.295
dangshen_068	chrysanthemaxanthin	FKBP1A	14.349
dangshen_068	chrysanthemaxanthin	PTGFR	9.5650
dangshen_074	syringaldehyde	TTR	17.991
dangshen_074	syringaldehyde	KCNA1	7.1404
dangshen_078	20-hexadecanoylinganol	PTGFR	16.300
dangshen_078	20-hexadecanoylinganol	FKBP1A	14.503
dangshen_079	perlolyrine	CAMK2D	6.2019
dangshen_088	2-[(2S)-2-[(4aS,6aR,6aS,6bR,8aR,10R,11R,12aR,14bS)-10,11-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydricene-4a-carbonyl]amino]propanoyl]amino]acetic acid	KCNA1	7.6843
dangshen_088	2-[(2S)-2-[(4aS,6aR,6aS,6bR,8aR,10R,11R,12aR,14bS)-10,11-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydricene-4a-carbonyl]amino]propanoyl]amino]acetic acid	TTR	13.286
dangshen_089	1. N'-[N-(2a,3b-Dihydroxy-12-oleanen-28-oyl)-L-alanyl]-glycine	PROC	8.6201
dangshen_089	1. N'-[N-(2a,3b-Dihydroxy-12-oleanen-28-oyl)-L-alanyl]-glycine	FKBP1B	8.0267
dangshen_089	1. N'-[N-(2a,3b-Dihydroxy-12-oleanen-28-oyl)-L-alanyl]-glycine	NPPA	7.8441
dangshen_098	8alpha-methoxyfuranodiene	RAPGEF4	8.7152
dangshen_104	alpha-spinasterol	PTGFR	13.2200
dangshen_105	inulin	HSPA1A	9.5556
dangshen_107	menthyl acetate	FKBP1A	13.375
dangshen_107	menthyl acetate	ACE	10.657
dangshen_127	atractylinolide ii	FKBP1A	11.531
dangshen_128	3-methylcarbazole	PLA2G6	6.5614
dangshen_128	3-methylcarbazole	ADRA2C	8.4190
dangshen_128	3-methylcarbazole	CAMK2D	8.8653
dangshen_128	3-methylcarbazole	ADRA2A	9.7986
dangshen_128	3-methylcarbazole	ADRA2B	9.8543

dangshen_130	coelogin	KCNA1	9.7035
dangshen_130	coelogin	TTR	7.6176
dangshen_132	ferulic acid	TTR	17.3280
dangshen_132	ferulic acid	RHOA	15.0950
dangshen_132	ferulic acid	CAMK2A	10.6990
dangshen_134	codonopsine	CHRM2	6.9209
dangshen_134	codonopsine	ADRA2A	7.4492
dangshen_134	codonopsine	ADRA2B	8.5885
dangshen_134	codonopsine	HCN4	9.2265
dangshen_134	codonopsine	ADRA2C	9.6791
dangshen_134	codonopsine	KCNQ1	13.4290
dangshen_138	spinoside a	PTGFR	10.9970
dangshen_140	5-metyoxymethy-2-furaldehyde	RAPGEF4	8.4385
dangshen_153	atractylenolide II	FKBP1A	11.5310
dangshen_154	atractylenolide III	FKBP1A	7.0532
dangshen_162	vanillic acid	TTR	16.5930
dangshen_162	vanillic acid	KCNA1	6.0052
dangshen_171	guaijaverin	ADRA2C	22.5770
dangshen_171	guaijaverin	ADRA2A	12.3510
dangshen_171	guaijaverin	CAMK2B	7.5441
dangshen_174	methionine sulfoxide	ACE	8.8460
dangshen_175	6,6'-dimethoxygossypol	KCNA1	6.0521
dangshen_176	ethyl-p-digallate	TTR	6.6936
dangshen_176	ethyl-p-digallate	RGS4	17.3070
dangshen_179	ricinine	RAPGEF4	10.0860
gansong_005	cineole	CHRM2	7.1038
gansong_005	cineole	ACE	6.4121
gansong_007	nardosinonediol	PTGFR	8.0948
gansong_007	nardosinonediol	FKBP1A	8.0337
gansong_014	paulownin	CHRM2	10.193
gansong_018	4-methyl-1,2-benzenediamine	RAPGEF4	6.1927
gansong_021	isovaleroxy-hydroxy dihydrovaltrate	FKBP1A	7.7265
gansong_022	valeranone	RAPGEF4	6.2753
gansong_025	angelicin	PTGFR	12.4520
gansong_028	alpha-guriunene	RAPGEF4	6.6487
gansong_037	beta-patchoulene	RAPGEF4	6.5374
gansong_040	calaxin	CACNA1C	6.1933
gansong_042	9-aristolen-1alpha-ol	PTGFR	7.2970
gansong_060	naringenin	KCNA1	7.3193
gansong_072	oleanolic acid	PTGFR	11.8430
gansong_073	de-oxonarchinol A	PTGFR	10.5240
gansong_074	ursolic acid	PTGFR	12.4320
gansong_A04	1,2,9,10-tetrahydroaristolane-2-one	FKBP1A	6.3946
gansong_A07	Aristolone	FKBP1A	7.5482
gansong_A12	Kanshone C	FKBP1A	6.9987
gansong_A13	Kanshone F	FKBP1A	15.2860
gansong_A16	Kanshone A	PTGFR	8.5507
gansong_A17	Nardosinonediol	PTGFR	8.0948
gansong_A17	Nardosinonediol	FKBP1A	8.0337
gansong_A18	Kanshone D	FKBP1A	6.8097
gansong_A19	Kanshone E	FKBP1A	8.2698
gansong_A38	Nardol	FKBP1A	6.4564
gansong_A39	Jatamansic acid	FKBP1A	6.1086
gansong_A40	Nardoxide	ACE	8.6075
gansong_A40	Nardoxide	FKBP1A	7.4223
gansong_A41	beta-Maaliene	RAPGEF4	6.6962
gansong_A44	Nardostachone	RGS4	6.7633
gansong_A48	Jatamol B	FKBP1A	7.3885
gansong_A51	beta-Patchoulene	RAPGEF4	6.5374
gansong_A55	Norseychellanone	RAPGEF4	6.1829
gansong_A65	Jatamansinol	ABCC9	16.925
gansong_A67	Angelicin	RHOA	6.9951
gansong_A67	Angelicin	KCNA1	12.1350
gansong_A68	Erythro-(3,4-dimethoxyphenyl)-2-(2-methoxy-4-(E)-(propenylphenoxy)-propan-1-ol	HCN4	6.2630
gansong_A70	Erythro-1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxy-4(E)-(propenylphenoxy)-propan-1-ol	TTR	6.0450
gansong_A73	Dinardokanshones A	PTGFR	7.6329
huangjing_002	vitexin xyloside	CAMK2A	6.8807
huangjing_002	vitexin xyloside	CAMK4	6.5751
huangjing_006	digitalis glycoside	FKBP1B	6.0442
huangjing_018	sibiricoside A	FKBP1B	9.6062
huangjing_020	Apigenin	CAMK2B	9.7539
huangjing_020	Apigenin	KCNA1	6.2698
huangjing_A13	Liquiritigenin	TTR	10.0890
huangjing_A14	Vitexinxyloside I	CAMK2B	6.6191
huangjing_A14	Vitexinxyloside I	CAMK4	8.8462
huangjing_A14	Vitexinxyloside I	CAMK2A	10.827
huangjing_A18	8-C-galactosylapigenin	CAMK4	8.0655
huangjing_A18	8-C-galactosylapigenin	CAMK2A	8.0427

huangjing_A22	Isoliquiritigenin	TTR	9.6680
huangjing_A23	7-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-4H-chromen-4-one	TTR	14.389
huangjing_A23	7-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-4H-chromen-4-one	CAMK2A	6.5134
huangjing_A24	vitexin	CAMK2A	8.9253
huangjing_A40	Syringaresinol-O-beta-D-glucopyranoside	KCNA1	6.1305
huangjing_A41	Liriodendron glycosides	CACNA1C	7.3095
sanqi_003	ginsenoside rc	HSPA1A	6.1163
sanqi_004	ginsenoside Rb1	HSPA1A	6.1447
sanqi_009	cyperene	RAPGEF4	6.5403
sanqi_011	alpha-cuparenol	RAPGEF4	8.413
sanqi_020	gamma-sitosterol	PTGFR	12.452
sanqi_024	delta-cadinene	FKBP1A	9.8775
sanqi_024	delta-cadinene	RAPGEF4	6.1903
sanqi_026	(-)-dicentrine	ADRA2B	30.631
sanqi_026	(-)-dicentrine	ADRA2A	29.272
sanqi_026	(-)-dicentrine	ADRA2C	27.8900
sanqi_026	(-)-dicentrine	HTR2A	17.421
sanqi_026	(-)-dicentrine	HCN4	14.283
sanqi_026	(-)-dicentrine	CHRM2	7.9162
sanqi_031	encecalin	KCNA1	6.3261
sanqi_031	encecalin	ADRA2A	6.2615
sanqi_031	encecalin	ADRA2C	6.0779
sanqi_038	cyclododecanone	RAPGEF4	6.6334
sanqi_052	cycloeucaleanol	PTGFR	7.2463
sanqi_060	xi-cadinene	RAPGEF4	7.1017
sanqi_061	20-hexadecanoylinganol	PTGFR	16.3000
sanqi_061	20-hexadecanoylinganol	FKBP1A	14.503
sanqi_064	alpha-murolene	FKBP1A	8.7718
sanqi_065	beta-sitosterol	PTGFR	12.452
sanqi_066	delta-guaiene	RAPGEF4	6.9636
sanqi_069	methyl isobutyl ketone	ACE	7.3420
sanqi_070	1-methyl-4-isoallyl-cyclohexane	FKBP1A	11.928
sanqi_073	notoginsenoside r4	HSPA1A	6.1447
sanqi_076	notopterol	KCNA1	8.9395
sanqi_080	guaijaverin	ADRA2C	22.577
sanqi_080	guaijaverin	ADRA2A	12.351
sanqi_080	guaijaverin	CAMK2B	7.5441
sanqi_087	notoginsenoside a	HSPA1A	8.0406
sanqi_087	notoginsenoside a	FKBP1B	7.1835
sanqi_090	gypenoside XVII	HSPA1A	6.3128
sanqi_093	dithiocyclopentene	CHRM2	6.7887
sanqi_094	diterbutyl phthalate	CHRM2	6.4315
sanqi_094	diterbutyl phthalate	UTS2	6.0559
sanqi_096	4,4'-diketo-3-hydroxy-beta-carotene	FKBP1A	6.1573
sanqi_098	dauricine	HCN4	11.336
sanqi_098	dauricine	TTR	9.7005
sanqi_098	dauricine	ADRA2B	7.3640
sanqi_099	elemicin	FKBP1A	15.3720
sanqi_099	elemicin	ADRA2C	8.3401
sanqi_099	elemicin	ADRA2B	8.1373
sanqi_108	panaxatriol	PTGFR	9.7340
sanqi_113	cuparene	RAPGEF4	13.6580
sanqi_116	panaxytriol	PTGFR	15.0540
sanqi_117	panaxynol	PTGFR	24.3920
sanqi_117	panaxynol	TBXA2R	15.2130
sanqi_118	panaxydol	TBXA2R	6.7792
sanqi_118	panaxydol	PTGFR	7.5974
sanqi_118	panaxydol	CHRM2	7.9951
sanqi_124	3,4-dimethylbenzoic acid	TTR	15.0160
sanqi_124	3,4-dimethylbenzoic acid	TBXA2R	10.4690
sanqi_124	3,4-dimethylbenzoic acid	RAPGEF4	10.3060
sanqi_127	ethyl-p-digallate	TTR	6.6936
sanqi_127	ethyl-p-digallate	RGS4	17.3070
sanqi_132	ethyl pyroglutamate	ACE	19.0520
sanqi_136	quercetin	ADRA2C	14.4540
sanqi_136	quercetin	CAMK2B	12.021
sanqi_136	quercetin	TTR	9.5662
sanqi_136	quercetin	ADRA2A	9.1196
sanqi_136	quercetin	KCNA1	7.4933
sanqi_147	delta-guaiene	RAPGEF4	6.9636
sanqi_148	alpha-guaiene	FKBP1A	6.7077
sanqi_148	alpha-guaiene	RAPGEF4	7.2353
sanqi_151	coprine	ACE	16.495
sanqi_151	coprine	NPPA	12.143
sanqi_160	1-methoxyethylbenzene	ADRA2B	11.058
sanqi_160	1-methoxyethylbenzene	ADRA2A	10.399
sanqi_160	1-methoxyethylbenzene	ADRA2C	9.7491
sanqi_160	1-methoxyethylbenzene	ACE	8.4289
sanqi_166	cyclodecanone	PLA2G6	6.1470
sanqi_168	dencichine	NPPA	11.3100

sanqi_168	dencichine	ACE	10.317
sanqi_187	beta-cubebene	RAPGEF4	6.3612
sanqi_188	beta-guaiene	RAPGEF4	7.2703
sanqi_189	gamma-cadinene	FKBP1A	9.8484
sanqi_190	gamma-murolene	FKBP1A	9.8484