

Table S3. Complete list of interacting herbal ingredients with important targets

Upstream targets		
S.No	Target	Related herbal Ingredients
1	HIPK2	NA
2	MAPK14	12-o-tetradecanoylphorbol-13-acetate taxol rottlerin mallotoxin aesculetin esculetin genistein curcumin curcumine piceatannol cinnamaldehyde cinna mic aldehyde trans-cinnamaldehyde hyperoxide resveratrol trans- resveratrol arachidonic acid quinazolinone 4- methoxyhonokiol epigallocatechin 3-gallate coleonol forskolin 12- tetradecanoylphorbol 13-acetate manganese taurodeoxycholic acid emetine 2-propenal rotenone adenosine diphosphate adenosine triphosphate sorbitol 17-beta-estradiol estradiol alpha-estradiol beta- estradiol 17beta-oestradiol 3,4-benzopyrenemagnesium lipoic acid alpha- lipoic acid glycerol formaldehyde ketone 3,4,5-trihydroxybenzoic acid gallic acid
3	CDK2	ginsenoside rh2 gnidimacrin isosilybin b silymarin ceramide isosilybin aaristololactam a iiiia indirubin isoindigo daidzein baicalein genistein vitamin d vitamin d3 luteolin quercetin eupatilin piceatannol apicidin (+)- arteannuinartemisinin resveratrol trans-resveratrol tetrandrine hanfangchin a epigallocatechin 3-gallate silybin camptothecin manganese perillyl alcohol perilla alcohol 4-(1-methylethenyl)-1-cyclohexene-1- methanol citrulline camp adenosine diphosphateandrogen adenosine triphosphate thymidine mimosine purine magnesiumglycerol formic acid fatty acids butanoic acid butyric acid ethyl aldehydeacetaldehyde arachidonic acid 18alpha-glycyrrhetic acid licochalcone a panaxydolursolic acid 15,16-dihydrotanshinone i fisetin (-)-epigallocatechin-3- gallate esculetinsilydianin heparin tangeretin catechin berberine aloe- emodin saponincaffeine geraniol apigenin progesterone aldosterone
4	ATM	silybin camptothecin iron adenosine diphosphate testosterone androgenadenosine triphosphate 17-beta- estradiol estradiol alpha-estradiol beta-estradiol17beta- oestradiol serotonin serotoninine caffeine genistein vitamin c
5	MAPK1	ceramide phosphatidylinositol 12-o-tetradecanoylphorbol-13- acetate bufalin seselenium arsenicum glycitein rottlerin mallotoxin daidzei n baicaleinamentoflavone aesculetin esculetin genistein kaempferol luteoli n quercetincapsaicin cinnamaldehyde cinnamic aldehyde trans-

		<p>cinnamaldehyde thapsigarginferulic acid resveratrol trans-resveratrol arachidonic acid hyperforin g-strophanthin vitamin u 7alpha-hydroxycholesterol picropodophyllin malvidinbetulic acid betulinic acid adenosine adenosin coleonol forskolin 12-tetradecanoylphorbol 13-acetate zinc manganese helenalin beta-phenylethyl isothiocyanate dihydrotestosterone (+)-catechin catechin d-catechin 2-propenalphenylalanine camp folic acid adenosine diphosphate progesterone adenosine triphosphate 3,5,3'-triiodothyronine aldosterone glucose 17-beta-estradiol estradiolalpha-estradiol beta-estradiol 17beta-oestradiol serotonin serotonin quinonefluoxetine chelerythrine 3,4-benzopyrene atrazine phytin phytic acidhydroquinone p-dihydroxybenzene ethanol alcohol dopamine calciumacetylcholine ethyl aldehyde acetaldehyde gossypin deoxypodophyllotoxinnicotine rosmarinic acid pectin naringenin berberine salvianolic acid b rotenoneandrographolide irisolidone rhapontigenin vitamin a curcumin morphinedelta(9)-tetrahydrocannabinol gallic acid paeonol beta-hydroxyisovalerylshikonin caffeine vitamin e (-)-epigallocatechin-3-gallate melanin alpha-amyrin evodiaminephosphatidic acid delphinidin licochalcone a costunolide vanillin cocaine</p>
6	ATR	silicon atropine copper chloride atractyloside copper cuprum 2-methylbutanoic acid styrene acrylic acid glycol
7	WEE1	flavokawain a resveratrol trans-resveratrol adenosine diphosphate adenosine triphosphate magnesium glycerol berberine
8	MAP3K1	12-o-tetradecanoylphorbol-13-acetate curcumin curcumine epigallocatechin 3-gallate7-epitaxol 12-tetradecanoylphorbol 13-acetate taxol (-)-epigallocatechin-3-gallate
9	ABL1	rottlerin mallotoxin myristic acid tetradecanoic acid adenosine diphosphateadenosine triphosphate sodium chloride magnesium glycerol
10	CSNK2A1	ellagic acid daidzein apigenin quercetin resveratrol trans-resveratrol zincheparin adenosine diphosphate emodin spermine spermidine glycerol 1-butanol
11	AKT1	ceramide phosphatidylinositol 12-o-tetradecanoylphorbol-13-acetate 120tauroursodeoxycholic acid gambogic acid se selenium parthenolide taxolgamma-tocotrienol rottlerin mallotoxin psoralidin orientin myricetin 3,3',4',5,5',7-hexahydroxyflavone isorhamnetin 3-methylquercetin chrysin baicalein genisteinvitamin d vitamin d3 linoleic acid (z,z)-9,12-octadecadienoic

		<p>acid luteolin apigeninquercetin cerebroside capsaicin curcumin curcumine piceatannol flavin mononucleotide flavin adenine dinucleotide hyperoxide phosphatidic acid lycopenethapsigargin resveratrol trans-resveratrol g-strophanthin naringenin withaferin atanshinone iia tanshinone ii tanshinone ii</p> <p>a leonurine evodiamine isoevodiaminecelastrol tripterine triptolide degueli n diosgenin butin nicotine diallyl tetrasulfide tetrandrine hanfangchin a picropodophyllin isoflavone honokioldelphinidin artesunate epigallocatechin 3-gallate betulic acid betulinic acid ursolic acid coleonol forskolin 7-epitaxol oridonin silybin tomatine 12-tetradecanoylphorbol 13-acetate camptothecin zinc copper cuprum manganesehelenalin allitridin di allyl trisulfide citrulline novobiocin guanosine rotenonel-arginine arginine camp adenosine diphosphate testosterone cholesterolandrogen progesterone adenosine triphosphate 3,5,3'-triiodothyronine coenzyme iiadrenaline 17-beta-estradiol estradiol alpha-estradiol beta-estradiol 17beta-oestradiol serotonin serotonine lauric acid dodecanoic acid chelerythrine caffeine3,4-benzopyrene atrazine acetovanillone apocynin palmitic acid fat hexadecanoic acid hexadecylic acid melatonin phytin phytic acid heteroauxin guaneglycerol ethanol alcohol 3,4,5-trihydroxybenzoic acid gallic acid calciumagmatine ethyl aldehyde acetaldehyde isobutyrylshikonin salvianolic acid ashikonin eupatilin brazilin (-)-epicatechin fisetin paeonol beta-carotenekaempferol selenocystine vitamin e wogonin icariin (-)-epigallocatechin-3-gallatepuerarin cardamomin sorbitol tylophorine andrographolide b-group soyasaponin</p>
12	TRIM28	zinc
13	PRKACA	l20 cgmp myristic acid tetradecanoic acid pentanal camp n-octane calcium
14	TAF1	NA
Downstream targets		
1	SELE	<p>anemoside b4 jatrorrhizine muscarine heparin colchicine berberine calciumnotoginsen oside r1 quercetin silymarin yakuchinone b curcumin genistein 17-beta-estradiol isoliquiritigenin kaempferol vitamin e vitamin k ursolic acidnicotine resveratrol</p>

2	ANGPT2	n-acetyl-d-glucosamine 2-acetamido-2-deoxy-d-glucose calcium
3	EPHA2	n-acetyl-d-glucosamine 2-acetamido-2-deoxy-d-glucose adenosine diphosphateadenosine triphosphate (-)-epigallocatechin-3-gallate
4	LUM	NA

TCMID prediction of interaction between natural ingredients and major targets through text mining and STITCH. NA-Not available