

Supplementary Table 1: Summary of herbal components.

Mol ID	Molecule Name	OB (%)	DL	SMILE
MOL000273	(2R)-2-[(3S,5R,10S,13R,14R,16R,17R)-3,16-dihydroxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-methylhept-5-enoic acid	30.93	0.81	<chem>CC(=CCCC(C1C(CC2(C1(CC=C3C2=CCC4C3(CCC(C4(C)C)O)C)C)C)O)C(=O)O)C</chem>
MOL000275	trametenolic acid	38.71	0.8	<chem>CC(=CCCC(C1CCC2(C1(CCC3=C2CCC4C3(CCC(C4(C)C)O)C)C)C)C(=O)O)C</chem>
MOL000276	7,9(11)-dehydropachymic acid	35.11	0.81	<chem>CC(C)C(C)C=CC(C)C1CCC2C1(CCC3C2=CC(C4(C3(CCC(C4)O)C)O)O)C</chem>
MOL000279	Cerevisterol	37.96	0.77	<chem>CC(C)C(C)C=CC(C)C1CCC2C1(CCC3C2=CC(C4(C3(CCC(C4)O)C)O)O)C</chem>
MOL000280	(2R)-2-[(3S,5R,10S,13R,14R,16R,17R)-3,16-dihydroxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-5-isopropyl-hex-5-enoic acid	31.07	0.82	/
MOL000282	ergosta-7,22E-dien-3beta-ol (Stellasterol)	43.51	0.72	<chem>CC(C)C(C)C=CC(C)C1CCC2C1(CCC3C2=CCC4C3(CCC(C4)O)C)C</chem>
MOL000283	Ergosterol peroxide	40.36	0.81	<chem>CC(C)C(C)C=CC(C)C1CCC2C1(CCC3C24C=CC5(C3(CCC(C5)O)C)OO4)C</chem>
MOL000285	(2R)-2-[(5R,10S,13R,14R,16R,17R)-16-hydroxy-3-keto-4,4,10,13,14-pentamethyl-1,2,5,6,12,15,16,17-octahydrocyclopenta[a]phenanthren-17-yl]-5-isopropyl-hex-5-enoic acid	38.26	0.82	/
MOL000287	3beta-Hydroxy-24-methylene-8-lanostene-21-oic acid (Eburicoic acid)	38.7	0.81	<chem>CC(C)C(=C)CCC(C1CCC2(C1(CC3=C2CCC4C3(CCC(C4(C)C)O)C)C)C(=O)O</chem>
MOL000289	pachymic acid	33.63	0.81	<chem>CC(C)C(=C)CCC(C1C(CC2(C1(CCC3=C2CCC4C3(CCC(C4(C)C)O)C(=O)C)C)C)O)C(=O)O</chem>
MOL000290	Poricoic acid A	30.61	0.76	<chem>CC(C)C(=C)CCC(C1C(CC2(C1(C=C3C2=CCC(C3(C)CCC(=O)O)C(=C)C)C)O)C(=O)O</chem>
MOL000291	Poricoic acid B	30.52	0.75	<chem>CC(=CCCC(C1C(CC2(C1(CC=C3C2=CCC(C3(C)CCC(=O)O)C(=C)C)C)O)C(=O)O)C</chem>
MOL000292	poricoic acid C	38.15	0.75	<chem>CC(C)C(=C)CCC(C1CCC2(C1(CC=C3C2=CCC(C3(C)CCC(=O)O)C(=C)C)C)C)C(=O)O</chem>
MOL000296	hederagenin	36.91	0.75	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)CO)O)C)C)C2C1)C)C(=O)O)C</chem>
MOL000300	dehydroeburicoic acid	44.17	0.83	<chem>CC(C)C(=C)CCC(C1CCC2(C1(CC=C3C2=CCC4C3(CCC(C4(C)C)O)C)C)C(=O)O</chem>

Supplementary Table 2: Gene Ontology Biological Process (GO_BP) analysis results of potential targets of the formula for disease Intervention.

Category	Term
GOTERM_BP_DIRECT	GO:0043066~negative regulation of apoptotic process
GOTERM_BP_DIRECT	GO:0009410~response to xenobiotic stimulus
GOTERM_BP_DIRECT	GO:0045944~positive regulation of transcription from RNA polymerase II promoter
GOTERM_BP_DIRECT	GO:0010629~negative regulation of gene expression
GOTERM_BP_DIRECT	GO:0030522~intracellular receptor signaling pathway
GOTERM_BP_DIRECT	GO:0001666~response to hypoxia
GOTERM_BP_DIRECT	GO:0070374~positive regulation of ERK1 and ERK2 cascade
GOTERM_BP_DIRECT	GO:0043065~positive regulation of apoptotic process
GOTERM_BP_DIRECT	GO:0033138~positive regulation of peptidyl-serine phosphorylation
GOTERM_BP_DIRECT	GO:0008284~positive regulation of cell proliferation
GOTERM_BP_DIRECT	GO:0071456~cellular response to hypoxia
GOTERM_BP_DIRECT	GO:0045893~positive regulation of transcription, DNA-templated
GOTERM_BP_DIRECT	GO:1902895~positive regulation of pri-miRNA transcription from RNA polymerase II promoter
GOTERM_BP_DIRECT	GO:0048661~positive regulation of smooth muscle cell proliferation
GOTERM_BP_DIRECT	GO:0042593~glucose homeostasis
GOTERM_BP_DIRECT	GO:0006954~inflammatory response
GOTERM_BP_DIRECT	GO:0010628~positive regulation of gene expression
GOTERM_BP_DIRECT	GO:0009755~hormone-mediated signaling pathway
GOTERM_BP_DIRECT	GO:0050796~regulation of insulin secretion

Supplementary Table 3: Gene Ontology Cellular Component (GO_CC) analysis results of potential targets of the formula for disease Intervention.

Category	Term
GOTERM_CC_DIRECT	GO:0043235~receptor complex
GOTERM_CC_DIRECT	GO:0045121~membrane raft
GOTERM_CC_DIRECT	GO:0005615~extracellular space
GOTERM_CC_DIRECT	GO:0005576~extracellular region
GOTERM_CC_DIRECT	GO:0005901~caveola
GOTERM_CC_DIRECT	GO:0005788~endoplasmic reticulum lumen
GOTERM_CC_DIRECT	GO:0099056~integral component of presynaptic membrane
GOTERM_CC_DIRECT	GO:0005886~plasma membrane
GOTERM_CC_DIRECT	GO:0030424~axon
GOTERM_CC_DIRECT	GO:0099055~integral component of postsynaptic membrane
GOTERM_CC_DIRECT	GO:0005737~cytoplasm
GOTERM_CC_DIRECT	GO:0005741~mitochondrial outer membrane
GOTERM_CC_DIRECT	GO:0005887~integral component of plasma membrane
GOTERM_CC_DIRECT	GO:0000785~chromatin
GOTERM_CC_DIRECT	GO:0005789~endoplasmic reticulum membrane
GOTERM_CC_DIRECT	GO:0031093~platelet alpha granule lumen
GOTERM_CC_DIRECT	GO:0090575~RNA polymerase II transcription factor complex
GOTERM_CC_DIRECT	GO:0005829~cytosol
GOTERM_CC_DIRECT	GO:0005634~nucleus

Supplementary Table 4: Gene Ontology Molecular Function (GO_MF) analysis results of potential targets of the formula for disease Intervention.

Category	Term
GOTERM_MF_DIRECT	GO:0004879~RNA polymerase II transcription factor activity, ligand-activated sequence-specific DNA binding
GOTERM_MF_DIRECT	GO:0042802~identical protein binding
GOTERM_MF_DIRECT	GO:0019899~enzyme binding
GOTERM_MF_DIRECT	GO:0005515~protein binding
GOTERM_MF_DIRECT	GO:0001223~transcription coactivator binding
GOTERM_MF_DIRECT	GO:0043565~sequence-specific DNA binding
GOTERM_MF_DIRECT	GO:0043560~insulin receptor substrate binding
GOTERM_MF_DIRECT	GO:0031994~insulin-like growth factor I binding
GOTERM_MF_DIRECT	GO:0042803~protein homodimerization activity
GOTERM_MF_DIRECT	GO:0008270~zinc ion binding
GOTERM_MF_DIRECT	GO:0031995~insulin-like growth factor II binding
GOTERM_MF_DIRECT	GO:1901363~heterocyclic compound binding
GOTERM_MF_DIRECT	GO:0004712~protein serine/threonine/tyrosine kinase activity
GOTERM_MF_DIRECT	GO:0002020~protease binding
GOTERM_MF_DIRECT	GO:0051378~serotonin binding
GOTERM_MF_DIRECT	GO:0005504~fatty acid binding
GOTERM_MF_DIRECT	GO:0016491~oxidoreductase activity
GOTERM_MF_DIRECT	GO:0001221~transcription cofactor binding
GOTERM_MF_DIRECT	GO:0000976~transcription regulatory region sequence-specific DNA binding

Supplementary Table 5: KEGG pathway analysis results of potential targets of the formula for disease intervention.

Category	Term
KEGG_PATHWAY	hsa04931:Insulin resistance
KEGG_PATHWAY	hsa04066:HIF-1 signaling pathway
KEGG_PATHWAY	hsa05200:Pathways in cancer
KEGG_PATHWAY	hsa04933:AGE-RAGE signaling pathway in diabetic complications
KEGG_PATHWAY	hsa05207:Chemical carcinogenesis - receptor activation
KEGG_PATHWAY	hsa04152:AMPK signaling pathway
KEGG_PATHWAY	hsa05415:Diabetic cardiomyopathy
KEGG_PATHWAY	hsa04920:Adipocytokine signaling pathway
KEGG_PATHWAY	hsa04936:Alcoholic liver disease
KEGG_PATHWAY	hsa04068:FoxO signaling pathway
KEGG_PATHWAY	hsa05418:Fluid shear stress and atherosclerosis
KEGG_PATHWAY	hsa05212:Pancreatic cancer
KEGG_PATHWAY	hsa05215:Prostate cancer
KEGG_PATHWAY	hsa04932:Non-alcoholic fatty liver disease
KEGG_PATHWAY	hsa04910:Insulin signaling pathway
KEGG_PATHWAY	hsa04917:Prolactin signaling pathway
KEGG_PATHWAY	hsa05205:Proteoglycans in cancer
KEGG_PATHWAY	hsa03320:PPAR signaling pathway
KEGG_PATHWAY	hsa01522:Endocrine resistance