

## SUPPLEMENTARY TABLES

**Supplementary Table 1. A total of 124 different active ingredients from TCMSP and literature in YBD.**

<b>Ingredients</b>	<b>Herb</b>	<b>Symbol</b>
(+)-Catechin	MH	A1
(+)-Leucocyanidin	MH	MH1
24-Ethylcholest-4-en-3-one	MH	MH2
Beta-sitosterol	MH	B1
Campest-5-en-3beta-ol	MH	MH3
Delphinidin	MH	MH4
Diosmetin	MH	MH5
Eriodictyol	MH	MH6
Genkwanin	MH	MH7
Herbacetin	MH	MH8
Kaempferol	MH	E1
Leucopelargonidin	MH	MH9
Luteolin	MH	MH10
Mandenol	MH	MH11
Naringenin	MH	E2
Pectolarigenin	MH	MH12
Poriferast-5-en-3beta-ol	MH	D1
Quercetin	MH	C1
Resivit	MH	MH13
Stigmasterol	MH	B2
Taxifolin	MH	MH14
Truflex OBP	MH	MH15
stepharine	DZ	DZ1
zizyphus saponin I Qt	DZ	DZ2
coumestrol	DZ	DZ3
Daechuine S7	DZ	DZ4
Jujubasaponin V Qt	DZ	DZ5
Mauritine D	DZ	DZ6
berberine	DZ	DZ7
(S)-Coclaurine	DZ	DZ8
Mairin	DZ	F1
Stigmasterol	DZ	B2
beta-sitosterol	DZ	B1
Ruvoside Qt	DZ	DZ9
(+)-catechin	DZ	A1
Stepholidine	DZ	DZ10
Nuciferin	DZ	DZ11
Fumarine	DZ	DZ12
beta-carotene	DZ	DZ13
(-)-catechin	DZ	DZ14
quercetin	DZ	C1
beta-sitosterol	SJ	B1
6-methylgingediacetate2	SJ	SJ1
Stigmasterol	SJ	B2

poriferast-5-en-3beta-ol	SJ	D1
Dihydrocapsaicin	SJ	SJ2
CaSO4	SG	SG
quercetin	GC	C1
Mairin	GC	F1
Jaranol	GC	GC1
isorhamnetin	GC	GC2
sitosterol	GC	GC3
formononetin	GC	GC4
Calycosin	GC	GC5
kaempferol	GC	GC6
licochalcone a	GC	E1
Vestitol	GC	GC7
Inermine	GC	GC8
DFV	GC	GC9
Glycyrol	GC	GC10
Medicarpin	GC	GC11
Lupiwighteone	GC	GC12
7-Methoxy-2-methyl isoflavone	GC	GC13
naringenin	GC	GC14
(2S)-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]-8,8-dimethyl-2,3-dihydropyrano[2,3-f]chromen-4-one	GC	E2
euchrenone	GC	GC15
glyasperin B	GC	GC16
glyasperin F	GC	GC17
Glyasperin C	GC	GC18
Isotrifoliol	GC	GC19
(E)-1-(2,4-dihydroxyphenyl)-3-(2,2-dimethylchromen-6-yl)prop-2-en-1-one	GC	GC20
kanzonols W	GC	GC21
(2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one	GC	GC22
Semilicoisoflavone B	GC	GC23
Glepidotin A	GC	GC24
Glepidotin B	GC	GC25
Phaseolinisoflavan	GC	GC26
Glypallichalcone	GC	GC27
8-(6-hydroxy-2-benzofuranyl)-2,2-dimethyl-5-chromenol	GC	GC28
Licochalcone B	GC	GC29
licochalcone G	GC	GC30
3-(2,4-dihydroxyphenyl)-8-(1,1-dimethylprop-2-enyl)-7-hydroxy-5-methoxy-coumarin	GC	GC31
Licoricone	GC	GC32
Gancaonin A	GC	GC33
Gancaonin B	GC	GC34
3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-8-(3-methylbut-2-enyl)chromone	GC	GC35
5,7-dihydroxy-3-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)chromone	GC	GC36
2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-(3-methylbut-2-enyl)chromone	GC	GC37
Glycyrin	GC	GC38
Licocoumarone	GC	GC39
Licoisoflavone	GC	GC40
Licoisoflavone B	GC	GC41

licoisoflavanone	GC	GC42
shinpterocarpin	GC	GC43
(E)-3-[3,4-dihydroxy-5-(3-methylbut-2-enyl)phenyl]-1-(2,4-dihydroxyphenyl)prop-2-en-1-one	GC	GC44
liquiritin	GC	GC45
licopyranocoumarin	GC	GC46
Glyzaglabrin	GC	GC47
Glabridin	GC	GC48
Glabranin	GC	GC49
Glabrene	GC	GC50
Glabrone	GC	GC51
1,3-dihydroxy-9-methoxy-6-benzofurano[3,2-c]chromenone	GC	GC52
1,3-dihydroxy-8,9-dimethoxy-6-benzofurano[3,2-c]chromenone	GC	GC53
Eurycarpin A	GC	GC54
(-)-Medicocarpin	GC	GC55
Sigmoidin-B	GC	GC56
(2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one	GC	GC57
(2S)-7-hydroxy-2-(4-hydroxyphenyl)-8-(3-methylbut-2-enyl)chroman-4-one	GC	GC58
Isoglycyrol	GC	GC59
Isolicoflavonol	GC	GC60
HMO	GC	GC61
1-Methoxyphaseollidin	GC	GC62
Quercetin der.	GC	GC63
3'-Hydroxy-4'-O-Methylglabridin	GC	GC64
3'-Methoxyglabridin	GC	GC65
2-[(3R)-8,8-dimethyl-3,4-dihydro-2H-pyrano[6,5-f]chromen-3-yl]-5-methoxyphenol	GC	GC66
Inflacoumarin A	GC	GC67
icos-5-enoic acid	GC	GC68
Kanzonol F	GC	GC69
6-prenylated eriodictyol	GC	GC70
7,2',4'-trihydroxy-5-methoxy-3-arylcoumarin	GC	GC71
7-Acetoxy-2-methylisoflavone	GC	GC72
8-prenylated eriodictyol	GC	GC73
gadelaidic acid	GC	GC74
Gancaonin G	GC	GC75
Gancaonin H	GC	GC76
Licoagrocarpin	GC	GC77
Glyasperins M	GC	GC78
Glycyrrhiza flavonol A	GC	GC79
Licoagroisoflavone	GC	GC80
Odoratin	GC	GC81
Phaseol	GC	GC82
Xambioona	GC	GC83
dehydroglyasperins C	GC	GC84

**Supplementary Table 2. Targets information of different ingredients in YBD through SwissTargetPrediction and TCMSP.**

PSMD3	target	HSPB1	target	RAF1	target	GABRA2	target	CHRNA7	target
MMP2	target	HMOX1	target	RASSF1	target	IKBKB	target	CHRNA2	target
HSPA5	target	HK2	target	RASA1	target	MAPK8	target	JUN	target
ACHE	target	NKX3-1	target	ERBB2	target	CHRM2	target	TGFB1	target
ACACA	target	HAS2	target	ERBB3	target	SLC6A2	target	F10	target
AHSA1	target	HIF1A	target	RB1	target	CA2	target	ADH1C	target
AKR1B1	target	CHUK	target	RXRA	target	CDK4	target	ADRA2A	target
MAOB	target	INSR	target	RUNX2	target	FOSL2	target	MAOA	target
AR	target	IGF2	target	CHEK2	target	STAT3	target	CTRB1	target
BAX	target	IGFBP3	target	PON1	target	HTR2A	target	DRD5	target
BCL2	target	ICAM1	target	STAT1	target	CHRM4	target	ADRA2B	target
ALOX5	target	IFNG	target	SCN5A	target	HTR3A	target	DRD2	target
AHR	target	IRF1	target	SLC2A4	target	ADRA1D	target	CYP2B6	target
BIRC5	target	IL1A	target	MMP3	target	IGHG1	target	CDC37	target
BCL2L1	target	IL1B	target	SOD1	target	CHRM3	target	PDE10A	target
ADRB2	target	IL10	target	THBD	target	OPRM1	target	ADRA2C	target
CASP3	target	IL2	target	F3	target	KDR	target	LACTB	target
CASP8	target	IL6	target	PLAT	target	OPRD1	target	DRD4	target
CASP9	target	CXCL8	target	E2F1	target	DRD1	target	HTR2C	target
CTSD	target	MMP1	target	E2F2	target	MAPK10	target	TOP2	target
CAV1	target	MMP9	target	RELA	target	CHRM5	target	PDE4	target
CCL2	target	MAPK1	target	PRSS1	target	ADRB1	target	CACNA1S	target
CD40LG	target	MYC	target	NFATC3	target	LTA4H	target	CYP2B1	target
TP53	target	MPO	target	DIO1	target	HMGCR	target	ALB	target
CLDN4	target	NQO1	target	PLAU	target	ABAT	target	CTNNB1	target
F7	target	POR	target	VCAM1	target	ADIPOQ	target	CASP7	target
COL1A1	target	NCF1	target	VEGFA	target	AKR1C1	target	MMP10	target
COL3A1	target	NFKBIA	target	PPP3CA	target	APOB	target	KLF7	target
CRP	target	NOS3	target	PGR	target	GOT1	target	GRP78	target
CXCL10	target	NFE2L2	target	CDK2	target	BAD	target	ABCG2	target
CXCL11	target	NCOA2	target	ESR2	target	CAT	target	CDC2	target
CXCL2	target	NR1I2	target	NOS2	target	CYP19A1	target	CDKN2A	target
CDKN1A	target	NR1I3	target	CHEK1	target	FASN	target	IL8	target
CYP1A1	target	ODC1	target	CCNA2	target	GSR	target	MGAM	target
CYP1A2	target	SPP1	target	ESR1	target	CES1	target	HERC5	target
CYP1B1	target	PPARG	target	GRIA2	target	LDLR	target	F2	target
CYP3A4	target	PPARA	target	PYGM	target	MTTP	target	PPP3CB	target
DCAF5	target	PPARD	target	GSK3B	target	MAPK3	target	ADCY2	target
DPP4	target	PTEN	target	MAPK14	target	ABCC1	target	APP	target
TOP1	target	PIK3CG	target	NCOA1	target	PLB1	target	XIAP	target
TOP2A	target	SERPINE1	target	OLR1	target	SOAT1	target	MDM2	target
DUOX2	target	PARP1	target	NR3C2	target	SOAT2	target	MET	target
EGFR	target	KCNH2	target	HSD3B1	target	SREBF1	target	MCL1	target
SELE	target	PCOLCE	target	HSD3B2	target	UGT1A1	target	NUF2	target
SULT1E1	target	EGF	target	ADRA1A	target	RXRB	target	PCNA	target
ELK1	target	PTGER3	target	ATP5F1B	target	KCNMA1	target	PTGES	target
EIF6	target	PTGS1	target	PKIA	target	TFRC	target	TYR	target
CCND1	target	PTGS2	target	IL4	target	FN1	target	XDH	target
CCNB1	target	ACP3	target	CHRM1	target	TRPC6	target	DGAT2	target
GABRA1	target	RUNX1T1	target	MT-ND6	target	PDE3A	target		
GJA1	target	PRKCA	target	SLC6A3	target	GABRA3	target		
GSTM1	target	PRKCB	target	SLC6A4	target	GABRA5	target		

GSTM2	target	FOS	target	AKR1C3	target	HSP90	target
GSTP1	target	NPEPPS	target	ADRA1B	target	MAP2	target
HSF1	target	AKT1	target	SLPI	target	PRKACA	target

**Supplementary Table 3. Overlapping targets information of drug targets and disease targets.**

MMP2  
XDH  
HSPB1  
NOS2  
COL1A1  
PPP3CA  
BCL2  
CRP  
GSTP1  
FN1  
EGF  
IL1A  
LDLR  
SPP1  
F2  
XIAP  
PTGS2  
OLR1  
CTNNB1  
CCND1  
CDK4  
NFATC3  
VEGFA  
TGFB1  
MYC  
CCNA2  
MT-ND6  
MMP1  
STAT1  
HMGCR  
NR3C2  
GSR  
HMOX1  
MMP3  
PPP3CB  
GSTM1  
IL10  
MAPK1  
PLAT  
MDM2  
EGFR  
SOD1  
ERBB2  
IL4  
AKR1B1  
TRPC6  
IGHG1  
RUNX2  
CXCL10  
TP53  
CASP9  
CDKN1A  
CAT  
RASA1

IL1B  
NFKBIA  
IGFBP3  
ALB  
SLC6A3  
LTA4H  
PLAU  
PTEN  
ALOX5  
RXRA  
CLDN4  
PON1  
E2F1  
APOB  
CASP8  
PPARG  
CXCL8  
SELE  
THBD  
MAPK14  
MPO  
PCNA  
CHUK  
STAT3  
SLPI  
ADRB2  
CTSD  
TFRC  
MCL1  
CCL2  
IL6  
CASP3  
PARP1  
MGAM  
KDR  
IGF2  
PIK3CG  
IL2  
IFNG  
FOS  
HSPA5  
ICAM1  
BCL2L1  
MAPK3  
HIF1A  
RELA  
NOS3  
SERPINE1  
VCAM1  
INSR  
AKT1  
PTGS1  
F3  
PYGM  
CDKN2A  
JUN  
BAX  
PRKCA  
CD40LG  
CYP3A4  
SCN5A

APP  
MMP9  
TOP1  
ADIPOQ

**Supplementary Table 5. Detail information on the known ligands of the top five targets.**

Target	Known ligand	Full name of ligand	Molecular weight	Molecular formula	Affinity energy (kcal/mol)
AKT1	UC8	~{N}-methyl-6-[4-[[4-[2-oxidanylidene-6- (propanoylamino)-3~{H}-benzimidazol-1- yl]piperidin-1-yl]methyl]phenyl]-5-phenyl- pyridine-3-carboxamide	588.7	C35H36N6O3	-6.2
TRPC6	POV	(2S)-3-(hexadecanoyloxy)-2- [(9Z)-octadec-9- enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate	760.08	C42H82NO8P	-8.0
STAT3	KQV	[(2-{{[(5S,8S,10aR)-3-acetyl-8-((2S)-5-amino-1-[(diphenylmethyl)amino]- 1,5-dioxopentan-2- yl} carbamoyl)-6-oxodecahydropyrrolo[1,2-a][1,5]diazocin-5- yl} carbamoyl)-1H-indol-5- yl)(difluoro)methyl]phosphonic acid (non-preferred name)	835.79	40H44F2N7O9	-7.1
PPP3CA	PGE	TRIETHYLENE GLYCOL	150.17	C6H14O4	-7.8
NFATC	3ANP	PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER	506.2	10H17N6O12P	-8.2