Table A.1. Chemical ingredients isolated from BF and their targets predicted in SwissTargetPrediction.

No.	Category	Compound	Molecular formula	Exact Mass	Targets
YDZ1	quassinoids	yadanziolide S	$C_{20}H_{28}O_9$	412.17333	#N/A
YDZ2	quassinoids	bruceine E	$C_{20}H_{28}O_9$	412.17333	#N/A
YDZ3	quassinoids	bruceine F	$C_{20}H_{28}O_{10}$	428.16825	TERT, JUN, PRKCA, HSD11B1, PRKCG, PRKCD, PRKCB, VAV1, PRKCE, PRKCH, PRKCQ, TRPV4, HMGCR, FNTB, PGGT1B, FNTA, F2, PLA2G2A, PTGS2, F2RL1, AR, NR3C2, NR3C1, METAP2, KCNA3, CYP19A1, PDE4D, ABCB1, CXCR1, NOS2, ATP2A1, GSTM1, IARS, PTPN1, BCL2L1, SLC6A2, TACR2, SLC6A3, GLRA2, SLC2A1, ADCY1, PRSS1, CTRC, GLI1, TLR9, IL1B, CES2, ACHE
YDZ4	quassinoids	hydroisobrucein B	$C_{23}H_{30}O_{11}$	482.17881	#N/A
YDZ5	quassinoids	bruceine L	$C_{26}H_{34}O_{11}$	522.21011	#N/A
YDZ6	quassinoids	hydroisobrucein A	$C_{26}H_{36}O_{11}$	524.22576	JUN, PRKCD, TERT, PTGS2, KCNA3, PRKCA, PRKCG, PRKCB, VAV1, PRKCE, PRKCH, PRKCQ, PGGT1B, FNTA, FNTB, TRPV4, ATP2A1, ADCY1, MAPK14, ADORA3, TMIGD3, IRAK4, TK2, PDE4D, PLEC, ADORA2A, F2RL1, DNMT1, JAK2, SLC5A2, SLC5A1, ADORA2B, ELOC, ELOB, VHL, ABCB1, ADAM17, PYGL, MAP2K1, HSD11B1, SLC29A1, PIM1, CCNA2, MMP2, MAPK1, CHEK1, SYK, HK2, HK1, NTRK1, SLC28A2, ADK, LGALS3, LGALS1, IMPDH2, GBA, BDKRB1, PDE10A, TRPA1, SORD, SLC2A1, F10, PSMB8, MET, PTPN1, TOP1, PIK3CG, PSMB2, CASP8, PSMB1, PIM2, PSMB5, CASP1, PIM3, GAPDH, CDC7, CDK5R1, CDK5, PDGFRB, CCNA1, DYRK1A, LCK, MAPK10, MAPK11, EPHA5, MAPK9, GAK, CDK1, CCNB1, CCNE1, CDK2, CDK7, CCNH, CDK9, CCNT1, CSNK1A1, MAPK3, MAPK15, CAMKK2, INSRR, FLT3, CXCR2, MPI, SIGMAR1, PIK3CD, PIK3CA, CFD
YDZ7	quassinoids	javanicolide D	$C_{28}H_{38}O_{12}$	566.23633	JUN, PRKCA
YDZ8	quassinoids	bruceine M	$C_{21}H_{30}O_9$	426.18898	#N/A
YDZ9	quassinoids	yadanzigan	$C_{26}H_{38}O_{14}$	574.22616	#N/A
YDZ10	quassinoids	20-hydroxyyadanzigan	$C_{26}H_{38}O_{15}$	590.22107	PTPN1, PPM1B, PPP1CC, PPP2R5A, PPP2CA, BCL2L1, GLI1, JUN, PRKCA, GLRA1, GLRA2, PRKCD, PRKCE, PRKCH, PRKCQ, STAT3, TYR, EPHX2, PTAFR, PDE4D, TERT, F2, RORC, ATP1A1, KCNA3, NEU4, ATP2A1, HSD11B2, HSD11B1, ADORA2A, FUCA1
YDZ11	quassinoids	yadanzioside D	$C_{29}H_{40}O_{16}$	644.23164	GLI1, PPM1B, PPP1CC, PPP2R5A, PTPN1, KCNA3, PRKCA, JUN, PPP2CA, F2, PRKCD, PRKCE, PRKCH, PRKCQ, TERT, ATP2A1, FDFT1, PDE4D, HSD11B2, HSD11B1, TOP1, BCL2L1, SLC5A2, EPHX2, GLRA1, GLRA2, ADORA2A, ADORA2B, ADORA3
YDZ12	quassinoids	yadanzioside E	$C_{32}H_{44}O_{16}$	684.26294	GLI1, PPM1B, PPP2R5A, KCNA3, PTPN1, F2, PTGS2, FDFT1, PRKCA, PRKCD, PRKCE, PRKCH, PRKCQ, JUN, ATP2A1, SLC5A2, HSD11B2, HSD11B1, PPP2CA, GLRA1, GLRA2, TOP1, RORC, ATP1A1, EIF4A1, EPHX2
YDZ13	quassinoids	yadanzioside H	$C_{32}H_{46}O_{16}$	686.27859	PTPN1, GLI1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, HSD11B2, HSD11B1, DRD4, SLC5A2, SLC5A1, JUN, MMP13, MMP8, EPHX2
YDZ14	quassinoids	desmethyl-bruceolide	$C_{20}H_{24}O_{10}$	424.13695	#N/A
YDZ15	quassinoids	Desmethyl-bruceine B	$C_{22}H_{26}O_{11}$	466.14751	JUN, KCNA3, AR, NR3C2, NR3C1, GLI1, FNTB, TERT, F2, GLRA2, SERPINA6, PRKCA, PRKCG, PRKCD, PRKCB, VAV1, PRKCE, PRKCH, PRKCQ, TRPV4, PTGS2, F2RL1, HSD11B1, ATP2A1, NOS2, PGGT1B, FNTA, HSD11B2, ABCB1, HMGCR, PDE4D
YDZ16	quassinoids	desmethyl_brusatol	$C_{25}H_{30}O_{11}$	506.17881	KCNA3, JUN, PRKCA, TERT, ATP2A1, PRKCE, F2RL1, CASP1, TOP1, GLI1, MME, AR, NR3C2, PTGDR2, PRKCG, VAV1, PRKCH, PRKCQ, TRPV4, PTGS2, CASP3, LTA4H, CASP6, CASP7, CASP8, SLC2A1, ADCY1, TBXAS1, OPRD1, AGTR1, GLRA2
YDZ17	quassinoids	bruceine J	$C_{25}H_{32}O_{11}$	508.19446	KCNA3, AR, NR3C2, GLI1, FNTA, FNTB, CASP1, GLRA2, SERPINA6, JUN, NR3C1, PRKCG, VAV1, PRKCE, PRKCH, PRKCQ, TRPV4, MME, F2RL1, CASP3, ATP2A1, TOP1, PTGDR2, TBXAS1, BMP1, CASP7, HMGCR, ABCB1, ACE, MMP1, PIK3CA, MMP10, MMP8, CASP6, CASP8, AGTR1, PIM1, AMPD3, KDM4C, MET, ITGB1, ITGA4, ADK, LTA4H
YDZ18	quassinoids	Desmethyl-bruceine C	$C_{27}H_{34}O_{12}$	550.20503	KCNA3, PRKCA, JUN, PDE4D, PTGS2, ATP2A1, TERT, PRKCE, PRKCD, F2RL1, PTPN1, OPRD1, OPRK1, GSTM1, GLI1, FNTB, PGGT1B, FNTA, NOS2, PRKCB, PRKCH, PRKCQ, PRKCG, VAV1, TRPV4, AR, NR3C2, NR3C1
YDZ19	quassinoids	bruceantinol B	$C_{29}H_{36}O_{13}$	592.21559	KCNA3, PTGS2, ATP2A1, PDE4D, F2RL1, TERT, PRKCE, PRKCD, GSTM1, PPP1CA, PRKCB, PRKCH, PRKCQ, PRKCA, MMP10, MMP8, GLI1, ACE2, PCSK7, CAPN2, CTSB, CASP3, CASP7, CASP8, CASP1, OPRD1, OPRK1, HCAR2, DUSP3, JUN, PTPA, NOS2, FDFT1
YDZ20	quassinoids	bruceolide	$C_{21}H_{26}O_{10}$	438.15260	#N/A

YDZ21	quassinoids	bruceine B	$C_{23}H_{28}O_{11}$	480.16316	#N/A
YDZ22	quassinoids	bruceine A	$C_{26}H_{34}O_{11}$	522.21011	#N/A
YDZ23	quassinoids	brusatol	$C_{26}H_{32}O_{11}$	520.19446	#N/A
YDZ24	quassinoids	bruceantarin	$C_{28}H_{30}O_{11}$	542.17881	#N/A
YDZ25	quassinoids	aglycone of yadanzioside J	$C_{26}H_{34}O_{12}$	538.20503	JUN, KCNA3, AR, NR3C2, NR3C1, GLI1, FNTB, TERT, F2, GLRA2, SERPINA6, PRKCA, PRKCG, PRKCD, PRKCB, VAV1, PRKCE, PRKCH, PRKCQ, TRPV4, PTGS2, F2RL1, HSD11B1, ATP2A1, NOS2, PGGT1B, FNTA, HSD11B2, ABCB1, HMGCR, PDE4D
YDZ26	quassinoids	bruceantin	$C_{28}H_{36}O_{11}$	548.22576	KCNA3, PRKCD, ATP2A1, PRKCA, JUN, F2RL1, PRKCE, PTGS2, ADCY1, CDK2, CDK1, CTSV, RET, SLC2A1, GLI1, CXCR2, VAV1, SRC, MMP1, CHEK1, WEE1, PAK3, PAK2, PAK1, OPRK1, PDE4D, MMP14, TERT, HSP90AB1, PRKCG, NOS2, MMP3, MMP8, LNPEP, PARP1, BDKRB1, PCSK7, GSTM1, HDAC6, HDAC2, HDAC1, AR, TOP1, CCR1, FCER2, ADAM17, PIK3CA, PIK3R1
YDZ27	quassinoids	bruceine C	$C_{28}H_{36}O_{12}$	564.22068	PRKCA, KCNA3
YDZ28	quassinoids	bruceantinol A	$C_{30}H_{38}O_{13}$	606.23124	KCNA3, ATP2A1, PRKCA, PTGS2, F2RL1, TERT, PDE4D, OPRK1, PRKCE, JUN, PRKCD, GSTM1, PRKCB, PRKCH, PRKCQ, CDK2, CDK1, OPRD1, ADCY1, GLI1, MMP1, PCSK7, FLT1, SYK, SOAT1, FGFR1, SOAT2, PIK3CA, PIK3R1, ADORA3, RET, PARP1, ADAM17, MMP14, ADAM10, PRKCG, P2RX3, P2RY12, PPP2CA, ADRB3
YDZ29	quassinoids	aglycone of yadanzioside O	$C_{31}H_{40}O_{13}$	620.24689	KCNA3, PTGS2, ATP2A1, PRKCA, JUN, PDE4D, F2RL1, TERT, OPRD1, OPRK1, PRKCE, PRKCD, GSTM1, PTPN1, PRKCB, PRKCH, PRKCQ, GLI1, PCSK7, PTPA, PPP2CA, FNTB, PGGT1B, FNTA, NOS2
YDZ30	quassinoids	bruceine I	$C_{22}H_{28}O_{9}$	436.17333	#N/A
YDZ31	quassinoids	Deacetyl-Yadanzioside I	$C_{27}H_{36}O_{15}$	600.20542	GLI1, PTPN1, HSD11B2, HSD11B1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, SLC5A2, MMP13, MMP2, MMP8, MLNR, TOP1, TACR2
YDZ32	quassinoids	yadanzioside I	$C_{29}H_{38}O_{16}$	642.21599	PTPN1, GLI1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, HSD11B2, HSD11B1, DRD4, SLC5A2, SLC5A1, JUN, MMP13, MMP8, EPHX2
YDZ33	quassinoids	bruceoside B	$C_{32}H_{42}O_{16}$	682.24729	PTPN1, GLI1, SQLE, TACR2, SLC5A2, SLC5A1, CHRM4, CHRM5, EIF4A1, CHRM2, CHRM1, CHRM3, ADORA2A, ADORA3, DRD4, F7
YDZ34	quassinoids	javanicoside A	$C_{32}H_{42}O_{16}$	682.24729	PTPN1, EIF4A1, GLI1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, SLC5A2, ADORA2A, ADORA2B, ADORA3, F7, S1PR3, S1PR1, TACR2, TOP1, SLC5A1, DRD4, MAPK14, CSNK1D, TYMS, CHRM4, CHRM5, CHRM2, CHRM1, CHRM3
YDZ35	quassinoids	yadanzioside P	$C_{34}H_{46}O_{16}$	710.27859	PTPN1, KCNA3, GLI1, SQLE, EIF4A1, MMP13, GRM2, S1PR3, S1PR1, PPARG, PPARA
YDZ36	quassinoids	yadanzioside L	$C_{34}H_{46}O_{17}$	726.27350	PTPN1, KCNA3, GLI1, SQLE, EPHX2, PPARG, PPARA
YDZ37	quassinoids	yadanzioside K	$C_{36}H_{48}O_{18}$	768.28406	KCNA3, GLI1, TOP1, EIF4A1, ADORA2A, ADORA3, MMP13
YDZ38	quassinoids	bruceoside C	$C_{32}H_{42}O_{16}$	682.24729	GLI1, EIF4A1, SLC5A2, SLC5A1, MMP13, MMP8, LGALS3, LGALS1, LGALS7, LGALS9, SIRT2, ADORA3, TOP1, PDE10A, MAP2K1, TERT, ADK, BCL2A1, ADORA2A, ADORA2B, PTPN1
YDZ39	quassinoids	yadanziolide C	$C_{20}H_{26}O_{9}$	410.15768	#N/A
YDZ40	quassinoids	Yadanziolide E	$C_{20}H_{26}O_{9}$	410.15768	#N/A
YDZ41	quassinoids	bruceine D	$C_{20}H_{26}O_{9}$	410.15768	AR, NR3C2, NR3C1, JUN
YDZ42	quassinoids	yadanziolide A	$C_{20}H_{26}O_{10}$	426.15260	AR, NR3C2, JUN, F2, ABCB1, NR3C1, TERT, PRKCA, PRKCG, PRKCD, PRKCB, VAV1, PRKCE, PRKCH, PRKCQ, TRPV4, FNTB, PGGT1B, FNTA, PLA2G2A, SERPINA6, F2RL1, PRSS1, CTRC, GLI1, CDA, ADA, CES2, HSD11B2, KCNA3, TYR, ATP2A1, GSTM1, CYP19A1, PDE4D, PGR, OGA, NOS2, EPAS1, PNP, PREP, IARS, GBA, BCL2L1, PTGS2, SLC5A2, GAA, MANBA, SLC6A2, TACR2, ADK, PTGES, METAP2, ACHE, FUCA1, HSD11B1, PTPN1, HSPA8, HSD17B2, DAO, HMGCR, CDK2, CCNA1, CCNA2, GSK3B
YDZ43	quassinoids	deacetylated isobrucein B	$C_{21}H_{26}O_{10}$	438.15260	#N/A
YDZ44	quassinoids	yadanziolide B	$C_{20}H_{26}O_{11}$	442.14751	JUN, AR, NR3C2, NR3C1, TERT, PRKCG, PRKCD, PRKCA, PRKCB, VAV1, PRKCE, PRKCH, PRKCQ, TRPV4, ABCB1, GLI1, ATP2A1, F2, PDE4D, FNTB, PGGT1B, FNTA, MGAM, F2RL1, KCNA3, TLR9, ADA, PLA2G2A, SERPINA6, GSTM1, PRSS1, CTRC, CDA, PGR, NOS2, CES2, HSD11B2, ADORA2A, GLRA2, OGA, CYP19A1, IARS, PTPN1, PTGS2, GAA, MANBA, TYR, BCL2L1, PNP, CDK2, CCNA1, CCNA2, EPAS1, ACHE, ALOX5, PREP, ADK
YDZ45	quassinoids	yadanziolide W	$C_{22}H_{28}O_{12}$	484.15808	TERT, JUN, PDE4D, PGGT1B, GLI1, NR3C2, PTGS2, PTPN1, PRKCG, PRKCD, PRKCB, VAV1, PRKCE, PRKCH, PRKCQ, TRPV4,

					ATP2A1, F2, AR, NOS2, FNTA, FNTB, KCNA3, PRKCA, F2RL1, CYP19A1, ABCB1, TYR, OGA, SLC5A2, ADK, MMP1, MMP7, MMP8, ACHE, IARS, NR3C1, ADA, HK2, HK1, ADORA2A, ADORA3, GLRA2, SLC29A1, SLC5A1, GBA, TNF, CA2, CA1, CA12, CA9, PNP, TACR2, HRAS, MAPK10, MMP3, ADAM17, CDA, GSK3B, METAP2, CA14, GAA, MANBA, ADORA1
YDZ46	quassinoids	yadanzioside B	$C_{32}H_{44}O_{17}$	700.25785	GLI1, PTPN1, MLNR, HSD11B2, F2
YDZ47	quassinoids	bruceoside D	$C_{31}H_{40}O_{16}$	668.23164	GLI1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, KCNA3, PTPN1, SQLE, PRKCD, HSD11B2, HSD11B1
YDZ48	quassinoids	bruceoside E	$C_{31}H_{42}O_{16}$	670.24729	GLI1, PTPN1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, HSD11B2, HSD11B1
YDZ49	quassinoids	bruceantinoside A	$C_{34}H_{46}O_{16}$	710.27859	PTPN1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, GLI1, TACR2, S1PR3, S1PR1, PRKCD, SQLE, SLC5A2, MMP13, FDFT1, JUN, ADORA2A, ADORA3, TOP1, EIF4A1, SIRT2
YDZ50	quassinoids	bruceoside F	$C_{35}H_{46}O_{18}$	754.26841	KCNA3, GLI1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, FDFT1, CD22, TYMS
YDZ51	quassinoids	yadanzioside F	$C_{29}H_{38}O_{16}$	642.21599	GLI1, PTPN1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, TOP1, HSD11B2, HSD11B1, EPHX2, SLC29A1, ADORA1, SLC5A2, JUN, DRD4, ADORA2A, ADORA2B, ADORA3, MMP13, MMP8, EIF4A1, SLC5A1
YDZ52	quassinoids	bruceoside A	$C_{32}H_{42}O_{16}$	682.24729	PTPN1, SLC5A2, GLI1, KCNA3, EIF4A1, CHRM4, CHRM5, CHRM2, CHRM1, CHRM3, FDFT1, TOP1, SLC5A1, ADORA2A, ADORA3, MAPK14, CSNK1D, S1PR3, S1PR1, DRD4, TACR2, HSD11B2
YDZ53	quassinoids	javanicoside G	$C_{31}H_{40}O_{15}$	652.23672	PTPN1, GLI1, KCNA3, EIF4A1, GABRA5, TACR2, MAPK14, CSNK1D, MMP8, SLC5A2, CHRM4, CHRM5, CHRM2, CHRM1, CHRM3, DRD4, SLC5A1, ICAM1, BCL2A1, ADORA2A, TOP1, HSD11B2
YDZ54	quassinoids	yadanzioside A	$C_{32}H_{44}O_{16}$	684.26294	PTPN1, GLI1, HSD11B2, S1PR3, S1PR1, SLC5A2, ADORA1, SIRT2, TYMS, DRD4, CHRM4, CHRM5, CHRM2, CHRM1, CHRM3, TOP1, TACR2, EIF4A1, ADORA2A
YDZ55	quassinoids	javanicoside H	$C_{35}H_{46}O_{17}$	738.27350	PTPN1, TOP1, KCNA3, GLI1, SQLE, CHRM4, CHRM5, CHRM2, CHRM1, CHRM3, MAPK14, ADORA2A
YDZ56	quassinoids	yadanzioside J	$C_{32}H_{44}O_{17}$	700.25785	PTPN1, GLI1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, HSD11B2, HSD11B1, SLC5A2, SLC5A1, JUN, ADORA1, ADORA2A, ADORA3, TYMS, EPHX2, F2
YDZ57	quassinoids	javanicoside E	$C_{36}H_{50}O_{18}$	770.29971	PTPN1, GLI1, JUN, ADORA1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, S1PR3, S1PR1, HSD11B2, TACR2, CHRM4, CHRM5, CHRM2, CHRM1, CHRM3, MMP13, ADORA2A, CDK2, CDK1, MAPK14, PIK3CD, PIK3CG, PIK3CA, GABRA5, BTK
YDZ58	quassinoids	javanicoside F	$C_{33}H_{44}O_{16}$	696.26294	EIF4A1, FDFT1, SLC5A2, PTPN1, ADORA3, GLI1, ADORA2A, TACR2, SLC5A1, SLC29A1, TOP1, TNF, CHRM4, P2RY12, CHRM5, CHRM2, CHRM1, CHRM3, ADORA2B, MAPK14, CDK2, CDK1, GPR55, PTPRA
YDZ59	quassinoids	yadanzioside C	$C_{34}H_{46}O_{17}$	726.27350	PTPN1, KCNA3, SLC5A2, SLC5A1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, GLI1, TYMS, SQLE, ADORA3
YDZ60	quassinoids	yadanzioside G	$C_{36}H_{48}O_{18}$	768.28406	PTPN1, KCNA3, GLI1, SQLE, CHRM4, CHRM5, CHRM2, CHRM1, CHRM3, TOP1, TYMS, ADORA2A, GRM2, TK2, MAPK14, S1PR3, S1PR1
YDZ61	quassinoids	desmethyl_bruceantinoside A	$C_{33}H_{44}O_{16}$	696.26294	FDFT1, KCNA3, PTPN1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, GLI1, PRKCD, SQLE, JUN, PRKCA
YDZ62	quassinoids	javanicoside D	$C_{35}H_{48}O_{17}$	740.28915	PTPN1, KCNA3, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, GLI1, F7, PDE5A, PTPRA
YDZ63	quassinoids	yadanzioside O	$C_{37}H_{50}O_{18}$	782.29971	P2RY12, LGALS3, LGALS1, LGALS7, LGALS9, ADORA2A, ADORA3, GLI1, SLC5A2, MMP13, CDK1, CCNE2, CDK2, CCNE1, ACE, MME, EIF4A1, ECE1, TOP1, S1PR3, S1PR1, PARP1, ADORA2B, PTPN1, PDE5A, PTPN22
YDZ64	quassinoids	yadanzioside M	$C_{34}H_{40}O_{16}$	704.23164	HSP90AA1, SLC5A2, TOP1, SLC5A1, EIF4A1, F7, ADORA1, DRD4, PPARG, PPARA, ADORA2A, MAPK14, CSNK1D, GLI1, CHRM4, CHRM5, CHRM2, CHRM1, CHRM3, MMP13, MMP8, PTPN1
YDZ65	quassinoids	butyl ester of bruceoside D	$C_{35}H_{48}O_{16}$	724.29424	PTPN1, GLI1, TACR2, ADORA2A, JUN, MAPK14, CSNK1D, ADORA3, SLC5A2, S1PR3, S1PR1, SLC5A1, TYMS, TK2, TOP1, CHRM4, CHRM5, CHRM2, CHRM1, CHRM3, HSD11B2
YDZ66	quassinoids	dehydrobruceine B	$C_{23}H_{26}O_{11}$	478.14751	#N/A
YDZ67	quassinoids	dehydrobrusatol	$C_{26}H_{30}O_{11}$	518.17881	#N/A
YDZ68	quassinoids	Demethyl-dehydrobrusatol	$C_{25}H_{28}O_{11}$	504.16316	TERT, ATP2A1, PRKCE, PTPN1, KCNA3, JUN, AR, PTGDR2, TOP1, MAG, MME, MMP10, MMP8, NEU4, SLC5A1, GLI1, ABL1, EPHA2, LCK, SRC, KDR, MAP3K9, FGFR1, AURKA, BTK, PTGS2, ITGB1, ITGA4, ACE2, SLC5A2, HK2, HK1
YDZ69	quassinoids	dehydrobruceine A	$C_{26}H_{32}O_{11}$	520.19446	#N/A
YDZ70	quassinoids	dehydrobruceine C	$C_{28}H_{34}O_{12}$	562.20503	#N/A
YDZ71	quassinoids	dehydrobruceantinol	$C_{30}H_{36}O_{13}$	604.21559	#N/A

YDZ72	quassinoids	javanicoside C	$C_{32}H_{40}O_{16}$	680.23164	ADORA2A, ADORA3, ECE1, GLI1, ADORA2B, LGALS3, LGALS1, LGALS7, LGALS9, SLC5A2, P2RY12, PTPN1, TOP1, MMP13, MMP8, EIF4A1
YDZ73	quassinoids	bruceanic acid F	$C_{24}H_{30}O_{12}$	510.17373	CASP3, CASP6, CASP7, CASP8, CASP1, KCNA3, PSMB5, SLC2A1, ADCY1, ACE, MME, PRKCA, GLRA2, PTGER1, PTGER4, PTGER2, PTGFR, PTGIR, PTGER3, SELP, TOP1, SLC5A1, TYMS, CASP2, PIK3CA, AKT1, HK2, HK1, NEU2, PRKCE, TYR, LGALS3, OPRK1, ABCB1
YDZ74	quassinoids	bruceaketolic acid	$C_{22}H_{28}O_{12}$	484.15808	ABCB1, PRKCA, OPRK1, OPRM1, TRPV4, GLRA2, GLRA1, PTAFR, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, PPM1A, SLC2A1, ADCY1, FDFT1, PRKCG, PRKCE, PRKCH, PRKCQ, CASP3, CASP1, HMGCR, PSMB5, PPP5C, PPM1B, ITGB1, ITGA4, SLC5A1, PRKCD, CASP6, CASP7, CASP8, VDR, TBXAS1, MMP10, MMP8
YDZ75	quassinoids	bruceanic acid E	$C_{25}H_{32}O_{12}$	524.18938	ABCB1, KCNA3, SLC2A1, ADCY1, CASP3, PRKCA, GLRA2, ITGB1, TBXAS1, PTGIS, CASP1, CASP7, MME, ECE1, PIK3CA, OPRK1, MAPK14, MAPK10, CASP8, CTSA, SLC5A1, CDK5R1, CDK5, SLC5A2, DGAT1, PRKCE, PTGS2, PTGDR2, PDE5A, PTGIR, ITGB7, ITGA4
YDZ76	quassinoids	javanic acid A	$C_{26}H_{34}O_{13}$	554.19994	ABCB1, KCNA3, SLC2A1, ADCY1, MME, CASP3, CASP6, CASP7, CASP8, CASP1, HK2, HK1, PRKCA, TYMS, GLRA2, PTGER1, PTGER4, PTGER2, PTGFR, PTGIR, PTGER3, SELP, PIK3CA, LGALS3, PSMB5, ACE, ITGB1, ITGA4, TYR, SLC5A1, PTGDR2, DHFR, BACE1, HAO2, ITGB3, IMPDH2, ITGB5, ITGAV, PRKCE, OPRM1, TOP1, PDE5A, FPGS, ACLY, GART, MAP3K14, AMPD3, LRP6, DKK1, ANPEP, ENPEP, CSNK2A1, LAP3, DLG4, GSTP1, AMPD2, CASP2
YDZ77	quassinoids	javanic acid B	$C_{27}H_{36}O_{13}$	568.21559	#N/A
YDZ78	quassinoids	bruceanic acid E methyl ester	$C_{26}H_{34}O_{12}$	538.20503	#N/A
YDZ79	quassinoids	bruceene	$C_{20}H_{26}O_{8}$	394.16277	#N/A
YDZ80	quassinoids	bruceene A	$C_{20}H_{26}O_{9}$	410.15768	#N/A
YDZ81	quassinoids	javanicolide C	$C_{26}H_{36}O_{11}$	524.22576	ABCB1, SLC2A1, ADCY1, MMP9, PRKCA, ADORA2A, KCNA3, SLC5A2, SLC5A1, OPRK1, IRAK4, MAP2K1, GLRA2, SLC29A1, SYK, PDE10A, PLEC, ADORA3, AKT1, ELOC, ELOB, VHL, MAPK8, RPS6KA3, MAPK14, MAPK10, JAK2, RPS6KA4, MAPK11, MAPK9, CSNK1E, NLK, MAP2, PRKCE, UPP1, ADAM17, PIM1, ADK, CDC7, P2RY12, DNMT1, IMPDH2, CDK1, TMIGD3, SLC28A2, TOP1, HSP90AA1, CCKBR, MET, CXCR2, CCNE2, CDK2, CCNE1, CHEK1, MTOR, TK2, CASP1, ABL1, ADORA2B, SRC, PIK3CD, PRKDC, PIK3CB, HCK, PIK3CG, PI4KB, CASP8, PIK3CA, CTSK, CTSS, MAP3K5, JAK3, JAK1, PARP1, TYK2, PIM2, AGTR1, SOAT1, SLC16A1, DGAT1, MMP2, PYGL, CFD, DPP4, MCHR1, GAPDH, F10, CTSL, MMP14, OGA, NTRK1, BCL2A1, CHRM1, CASP3, LRRK2, GRK7, STK38, HIPK4, ERN1, OXSR1, STK39, MAP3K13
YDZ82	quassinoids	javanicolide H	$C_{26}H_{34}O_{11}$	522.21011	ABCB1, ADCY1, SLC2A1, PRKCA, OPRK1, KCNA3, ADORA2A, MMP9, IRAK4, SLC5A2, SLC5A1, PLEC, MAPK8, RPS6KA3, MAPK14, MAPK10, RPS6KA4, MAPK11, MAPK9, CSNK1E, NLK, GLRA2, PRKCE, PDE10A, ADAM17, SYK, MAP2K1, TOP1, NTRK1, CYP51A1, ELOC, ELOB, VHL, CFD, AKT1, LRRK2, GRK7, STK38, HIPK4, ERN1, OXSR1, STK39, MAP3K13, ICK, MAP3K15, MAST1, SBK1, HUNK, FYN, CSF1R, ABL1, FLT1, PRPF4B, SNRK, DSTYK, MAP3K12, PDGFRB, KIT, FLT4, FLT3, INSR, PDGFRA, RET, YES1, MAP2K3, PRKAA2, JAK3, MAP2K6, AURKB, BLK, DYRK1A, PHKG2, CSNK1G1, MYLK, DAPK3, CAMK1, CAMK4, CHEK2, PDPK1, CSNK1G2, RPS6KA1, DAPK1, LCK, PRKD3, SRC, PTK2, MAP3K11, FGFR3, MYLK2, CSNK1A1, KDR, CAMK2D, CSNK1D, JAK1, MAP3K9, MAP2K4, ITK, MAP2K2, JAK2, ROCK2, PAK3
YDZ83	quassinoids	javanicolide E	$C_{26}H_{34}O_{11}$	522.21011	ABCB1, ADCY1, PRKCA, OPRK1, SLC2A1, KCNA3, ADORA2A, MAPK14, SOAT1, DGAT1, MTOR, PIK3CA, GLRA2, SORD, IRAK4, PRKCE, KLK3, MMP9, ADORA3, ADK, MKNK2, SLC29A1, TK2, MAP2, SYK, PDE10A, CCNA2, CDK2, MAPK1, MAPK8, RPS6KA3, MAPK10, RPS6KA4, SLC5A2, MAPK11, MAPK9, CSNK1E, SLC5A1, NLK, LRRK2, GRK7, STK38, HIPK4, ERN1, OXSR1, STK39, MAP3K13, ICK, MAP3K15, MAST1, SBK1, HUNK, FYN, CSF1R, ABL1, FLT1, PRPF4B, SNRK, DSTYK, MAP3K12, PDGFRB, KIT, FLT4, FLT3, INSR, PDGFRA, RET, YES1, MAP2K3, PRKAA2, JAK3, MAP2K6, AURKB, BLK, DYRK1A, PHKG2, CSNK1G1, MYLK, DAPK3, CAMK1, CAMK4, CHEK2, PDPK1, CSNK1G2, RPS6KA1, DAPK1, LCK, PRKD3, SRC, PTK2, MAP3K11, FGFR3, MYLK2, CSNK1A1, KDR, CAMK2D, NTRK1, CSNK1D, JAK1, MAP3K9, MAP2K4
YDZ84	quassinoids	dihydrobruceine A	$C_{26}H_{36}O_{11}$	524.22576	ABCB1, PRKCA, OPRK1, OPRM1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, TRPV4, GLRA2, PRKCD, ADCY1, PRKCG, PRKCE, PRKCH, PRKCQ, FDFT1, GLRA1, PPM1A, MAPK14, SLC2A1, KLK3, ADORA2A, EGFR, MAPK8, MAPK10, MAPK3, MAPK9, PDE10A, ADORA1, ADK, MKNK2, ADORA3, MAPK1, MAP2, SYK, MMP9, PTAFR, TK2, HSP90AA1, SLC29A1, SORD, CXCR2, CDK1, MAP2K1, IRAK4, CXCR1, CCNA1, CCNA2, SOAT1, PIK3CA, DGAT1, SRC, MTOR, PIK3CB, RPS6KA3, RPS6KA4,

					MAPK11, CSNK1E, NLK, GHRHR, TACR2, NTRK1, P2RX3, CYP3A4, CCR1, CDK4, MET, ELOC, ELOB, VHL, SLC5A2, PTPN1, SLC16A1, CALM1, PPP1CA, PPM1B, HMGCR, CFD, REN, MMP1, ADAM17, AKT1, SLC5A1, BCL2A1, CCNE2, CDK2, CCNE1, EDNRA, MCHR1, LRRK2, JAK3, PRKACA, CHEK1, GRK7, STK38, HIPK4, ERN1, OXSR1, STK39, MAP3K13, BRD4, ICK, MAP3K15, MAST1
YDZ85	quassinoids	javanicolide F	$C_{30}H_{40}O_{13}$	608.24689	KCNA3, PRKCA, PRKCE, PTGS2, PRKCD, ABCB1, HSP90AA1, TACR2, REN, TOP1, PDE10A, TNF, ATP2A1, GAPDH, PRKCB, PRKCH, PRKCQ, ADORA2A, ADORA3, PDE5A, MAPK8, MAPK14, MAP3K14, KLK3, PIK3CD, PIK3CA, MAPK10, MAPK3, MAPK9, AURKA, PIK3CB, PIK3CG, JAK3, CNR1, JAK2, EIF4A1, F10, SCARB1, SYK, CXCR2, MAP2K1, CFD, PRKDC, HSP90AB1, MMP8, AURKB, P2RY12, CCNA2, CDK2, CDK4, MAPK1, PIM1
YDZ86	quassinoids	javanicoside B	$C_{32}H_{44}O_{16}$	684.26294	PTPN1, GLI1, HSD11B2, TK2, SLC5A2, ADORA1, ADORA2A, ADORA3, EIF4A1, TACR2, SLC5A1, BCL2A1, DRD4, TYMS, P2RY12
YDZ87	quassinoids	yadanzioside N	$C_{34}H_{46}O_{16}$	710.27859	PTPN1, FDFT1, PRKCD, TACR2, ADORA2A, ADORA3, TYMS, GLI1, SLC5A2, TK2, MMP8, HSD11B2, JUN, MAPK14, S1PR3, S1PR1, PTGFR, GBA, SIRT2
YDZ88	quassinoids	quassilactone A	$C_{26}H_{34}O_{12}$	538.20503	GLRA1, PTAFR, GLRA2, VDR, PPM1A, FDFT1, PRKCA, OPRK1, KCNA3, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, JUN, PPP1CC, ABCB1, PTPA
YDZ89	quassinoids	quassilactone B	$C_{26}H_{36}O_{12}$	540.22068	GLRA1, PTAFR, GLRA2, VDR, PPM1A, FDFT1, OPRK1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, ABCB1, OPRM1, RORC, HTR2B, ADRA2A, ADRA2C, ADRA2B, DRD1, DRD2, ADRA1D, HTR2A, HTR2C, DRD3, CYP2D6, HTR6, ADRA1A, HTR1B, PRKCA
YDZ90	quassinoids	Sergeolide A	$C_{28}H_{32}O_{11}$	544.19446	KCNA3
YDZ91	quassinoids	javanicin	$C_{24}H_{28}O_{12}$	508.15808	ABCB1, PRKCA, OPRK1, OPRM1, PRKCD, FDFT1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, PPM1A, GLRA2, SLC2A1, ADCY1, TRPV4, GLRA1, PTAFR, PPP5C, PPP1CA, PPM1B, PTPN1, PPP1CC, PRKCG, PRKCE, PRKCH, PRKCQ
YDZ92	quassinoids	yadanziolide D	$C_{19}H_{24}O_{9}$	396.14203	KCNA3, PRKCA, PTGS2, F2RL1, IARS, JUN, PTPN1, GSTM1, GLRA1, GLRA2, RPS6KA5, ABCB1, ATP2A1, SLC2A1, ADCY1, PDE4D, HSD11B1, CYP19A1, TERT, AR, NR3C2, NR3C1, PLA2G1B, STAT3, PRKCE, HMGCR, PRKCD, OPRD1, OPRK1, PGR, PDCD4, ATP12A, TTL, RORC, ATP1A1, PRKCB, PRKCH, PRKCQ, PRKCG, VAV1, TRPV4, PPP2CA, F2
YDZ93	quassinoids	javanicolide A	$C_{19}H_{24}O_{9}$	396.14203	KCNA3, PRKCA, JUN, PTGS2, F2RL1, SLC2A1, ADCY1, PDE4D, TERT, PRKCD, IARS, PRKCE, PRKCG, PRKCB, VAV1, PRKCH, PRKCQ, TRPV4, PTPN1, ATP2A1, GSTM1, HSD11B1, RORC, ATP1A1, STAT3, ABCB1, NOS2, PTPA, PPP2CA, GLRA1, GLRA2, AR, PDCD4, TTL, PPP1CC, RPS6KA5, CYP19A1, FNTB, PGGT1B, FNTA
YDZ94	quassinoids	2-dihydroailanthone	$C_{20}H_{26}O_{7}$	378.16785	JUN, BCL2L1, F2, PRKCA, TERT, PRKCG, PRKCD, PRKCB, PRKCE, PRKCH, PRKCQ, FNTB, PGGT1B, FNTA, GLI1, VAV1, TRPV4, PTGS2, F2RL1, CYP19A1, HSD11B1, AR, NR3C2, NR3C1, HMGCR, PDE4D, IARS, TLR9, NOS2, IL2, PPM1B, PTPN1, PPP1CC, PPP2CA, PPP2R5A, SLC6A2, TACR2, SLC6A3, PLA2G2A, PTAFR
YDZ95	quassinoids	shinjulactone M	$C_{20}H_{26}O_{9}$	410.15768	JUN
YDZ96	quassinoids	javanicolide B	$C_{20}H_{26}O_{10}$	426.15260	JUN, F2, GLI1, AR, NR3C2, BCL2L1, ADA, CDA, TLR9, GBA, GAA, HSD11B2, ABCB1, PRKCA, AHCY, ADORA2A, TERT, TYR, TK1, PNP, ADORA3, ADK, FUCA1, PRKCG, PRKCD, PRKCB, VAV1, PRKCE, PRKCH, PRKCQ, TRPV4, GAPDH, NR3C1, HSPA5, OGA, MAPK1, FNTB, PGGT1B, FNTA, HMGCR, CDK9, CCNT1, CSNK2A1, CDK2, CCNA1, CCNA2, HSPA8, PLA2G2A, F2RL1, SERPINA6, EPHX2, MMP3, MMP1, ADAM17, KCNA3, PRSS1, CTRC, SLC5A2, TYMP, PTPA, ATP2A1, PIM1, PDE4D, CES2, GSTM1
YDZ97	quassinoids	bruceine K	$C_{20}H_{28}O_{9}$	412.17333	#N/A
YDZ98	terpenoids	Pregnenolone	$C_{21}H_{32}O_{2}$	316.24023	SERPINA6, SHBG, G6PD, CYP19A1, CYP17A1, ESR2, NR3C1, SIGMAR1, NR1H3, HSD11B1, AR, PTGES, ESR1, CES2, RORA, HMGCR, PTPN6, PTPN2, SREBF2, PTPN1, PTGER1, PTGER2, FDFT1, PPARA, PPARD, PGR, PREP, SRD5A2, FABP4, PPARG, TERT, FABP3, FABP5, FABP1, FNTA, FNTB, PTGER4, IDO1, CDC25A, PTGIR, CDC25B, SCD, ADORA3, MAPK3, PTPN11, AKR1B10, POLB, PDE4D, PTPRF, PLA2G1B, ACP1, NPC1L1, RORC, CD81, SLC6A3, CYP51A1, PTGFR, PTGER3, FFAR1, SLC22A6, TNF, ALOX5, TOP1, FAAH, CNR1, PTGDR, SAE1, UBA2, NOS2, BCHE, BACE1, PRKCH, JAK2, LTB4R, STS, F2R, HSD11B2, CTSD, PTGS2, SLC6A4, CES1, NR1H4
YDZ99	terpenoids	Sitosterol	$C_{29}H_{50}O$	414.38617	NPC1L1, NR1H3, RORC, SHBG, HMGCR, CYP17A1, SREBF2, CYP19A1, AR, CYP51A1, RORA, ESR1, ESR2, PTPN1, CYP2C19, ACHE, SERPINA6, G6PD, SLC6A2, SLC6A4, BCHE, CHRM2, NR1I3, NR1H2, VDR, PTGER1, PTGER2, TBXAS1, PTGES, DHCR7, PPARD, SQLE, GLRA1, HSD11B1, PTPN6, PTPN2, FDFT1, CES2, NOS2, PPARG, UGT2B7, NR3C1, POLB
YDZ100	terpenoids	Stigmasterol	$C_{29}H_{48}O$	412.37052	NPC1L1, NR1H3, RORC, ESR1, ESR2, SHBG, SREBF2, HMGCR, CYP19A1, AR, CYP17A1, CYP51A1, RORA, CYP2C19, PTPN1, SERPINA6, G6PD, ACHE, SLC6A4, NR1I3, CHRM2, SLC6A2, BCHE, NR1H2, PTGER1, PTGER2, TBXAS1, PTGES, PPARA, PPARD,

					SQLE, VDR, DHCR7, PTPN6, PTPN2, FDFT1, HSD11B1, NOS2, PPARG, UGT2B7, GLRA1, POLB
YDZ101	terpenoids	*β*-daucosterol	$C_{35}H_{60}O_6$	576.43899	IL2, STAT3, BCL2L1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, PTAFR, PTPN1, S1PR3, S1PR1, PTPN2, CDC25B, ACP1, PPM1B, PPP1CC, PPP2CA, PPP2R5A, HSD11B2, DRD4, RBP4, PFKFB3
YDZ102	terpenoids	Stigmasterol-3-*O*-*β*-D-glucopyranoside	$C_{35}H_{58}O_6$	574.42334	IL2, STAT3, BCL2L1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, PTAFR, PTPN1, PFKFB3, PTPN2, S1PR3, S1PR1, CDC25B, ACP1, MET, F2, PPM1B, PPP1CC, PPP2CA, PPP2R5A, DRD4, HSD11B2, HSD11B1
YDZ103	terpenoids	(20R)-*O*-(3)-*β*-D-glucopyranosyl-(1→2)-*α*-L-arabinopyranosyl-pregn-5-en-3*β*,20-diol	$C_{32}H_{52}O_{11}$	612.35096	STAT3, IL2, PTAFR, SLC5A1, HSD11B2, PTPN1, SLC5A2, VEGFA, FGF1, FGF2, HPSE, MAPK14, ADORA1, ATP1A1
YDZ104	terpenoids	3*β*-hydroxy-5*α*-pregnan-20-one	$C_{21}H_{34}O_2$	318.25588	G6PD, SERPINA6, SHBG, CYP19A1, GABBR1, AR, CDC25A, VDR, NR1H4, POLB, GPBAR1, AKR1B10, HSD11B1, GABRA2, GABRB2, GABRG2, UGT2B7, HSD17B3, FNTA, FNTB, FABP4, PPARA, FABP3, FABP5, PPARD, FFAR1, FABP2, NPC1L1, SLC22A6, PTGER2, PTGFR, KDM2A, PHF8, KDM5C, CDC45, PTPRC, HSD11B2, PRKCA, ESR1, ESR2, CDC25B, PLG, HAO1, SAE1, UBA2, PTGES, PTPN1, STS, CYP17A1, NR1I3, SHH, CNR2, JAK2, F2R, CACNA2D1, TRPM8, CA4
YDZ105	terpenoids	(22E,24R)-5*α*,8*α*-epidioxy-ergosta-6,22-dien-3*β*-ol	$C_{28}H_{44}O$	396.33922	AR, CDC25A, VDR, GLRA1, NR1H3, PTPN1, CYP19A1
YDZ106	terpenoids	blumenol A	$C_{13}H_{20}O_3$	224.14124	#N/A
YDZ107	terpenoids	brucojavan 1	$C_{16}H_{28}O_8$	348.17842	VEGFA, FGF1, FGF2, STAT3, OGA, CDK2, CCNA1, CCNA2, GAPDH, ADK, ADORA1, HSPA8, ADA, GRK1, ADORA2A, ADORA3, SLC5A2, CDA, SLC5A1, MME, HK2, HK1, EGFR, LGALS3, HSPA5, PNP, AKR1C3, MANBA, AHCY, PTPN1, TK1, MAPK1, DAO, CCNB1, CDK1, GSK3B, DPP4, PTGES, ADRA2A, ADRA2C, ADRA2B, DRD1, DRD2, ADRA1D, HTR2C, ADRA1A, DRD3, CYP2D6, HTR6, HTR1B, IL2, SLC29A1, PSEN2, PSENEN, NCSTN, APH1A, PSEN1, APH1B, ADORA2B, MMP13, MMP1, MMP7, MMP8, PYGM, MCL1, ERN1, PIN1, PPP1CC, PPP2CA, PPP2R5A, MMP3, HDAC1, ADAM17, PYGL, AMD1
YDZ108	terpenoids	brucojavan 2	$C_{15}H_{26}O_3$	254.18819	NR1H4, SHH, CA4, TRPM8, NPC1L1, CA2, CA1, AR, CDC25B, NR1I3, ESR2, GPBAR1, NR1H3, UGT2B7, BRD4, BRD2, SHBG, POLA1, CDC25A, HSD11B1, PTGS1, CDC7, ESR1, FKBP1A, PTGS2, JAK1, APP, CA6, CA12, CA14, CA9, CA13, CA5B, CA5A, FAAH, MPO, PRKCA, HMGCR
YDZ109	terpenoids	brucojavan 3	$C_{15}H_{26}O_3$	254.18819	NR1H4, SHH, CA4, TRPM8, NPC1L1, CA1, AR, CA2, GPBAR1, NR1I3, NR1H3, ESR2, UGT2B7, POLA1, HSD11B1, SHBG, ESR1, PTGS1, BRD4, BRD2, CDC25A, JAK1, CDC7, FKBP1A, PARP1, PTGS2, PRKCA, NR3C1
YDZ110	terpenoids	(6S,7E)-6,9,10-trihydroxymegastigma-4,7-dien-3-one	$C_{13}H_{20}O_4$	240.13616	#N/A
YDZ111	terpenoids	(6S,7E)-6,9-dihydroxymegastigma-4,7-dien-3-one	$C_{13}H_{20}O_3$	224.14124	#N/A
YDZ112	flavone	angophorol	$C_{16}H_{14}O_5$	286.08412	CYP1B1, CA7, CA12, CA4, ABCC1, HSD17B1, ADORA3, MAOB, ESR1, ABCG2, CYP19A1, ESR2, ADORA1, TAS2R31, PTGS1, SHBG, CBR1, PLA2G1B, MMP13, SLC5A2, POLB, MMP12, PPARG, PLA2G2A, PLA2G5, CES1, BCHE, SERPINE1, CES2, CA2, GRM5, EDNRA, LCK, RXRA, GRM2, KLK1, KLK2, BACE1, AKR1C3, AKR1B1, ERN1, CA1, KIT, CA3, SRC, CHRNA7, HSD17B2, KDR, EZR, ACHE, CHEK1, WEE1, GRM4, PTGER4, PTGER3, NOX4, PTPN1, RET, MTOR, PIK3CA, CLK1, DYRK1B, PLA2G10, ALPL, ALPG, PDK1, PTGER1, GSK3B, PFKFB3, PTGS2, RPS6KA3, CHEK2, RPS6KA1, HNF4A, MET, ADCY5, PGF, VEGFA, CA9, ABCB1, CA6, CA13, CA5B, CA5A, VCP, PIK3R1, CDK2, EPHB2, CTSL, DYRK1A, MMP3, HSD17B3, MAOA, FFAR1, ALK, DNM1, KAT2B, GCGR, PDPK1, TAAR1
YDZ113	flavone	apigenin	$C_{15}H_{10}O_5$	270.05282	NOX4, AKR1B1, CDK5R1, CDK5, XDH, MAOA, FLT3, CYP19A1, ESR1, CCNB3, CCNB1, CCNB2, ACHE, ADORA1, PTGS2, ESR2, CDK6, ADORA2A, SYK, GSK3B, ABCC1, HSD17B1, TTR, CSNK2A1, CFTR, CYP1B1, ABCG2, AKR1B10, TNKS2, TNKS, ALOX5, PARP1, CA2, CA7, CA12, ABCB1, CA4, ALOX12, PTPRS, GLO1, APP, MMP9, MMP2, MMP12, CD38, TOP1, ARG1, ESRRA, PFKFB3, ALOX15, AMY1A, GRK6, TYR, HSD17B2, AHR, CA1, CA9, CBR1, AR, TERT, PIM1, EGFR, CDK1, KDM4E, LCK, AURKB, NAE1, TBXAS1, IGF1R, KDR, PLK1, MET, ALK, AXL, BCHE, ADORA3, CDK2, HTR2C, GPR35, DAPK1, MPG, SLC22A12, ST6GAL1, F2, PLG, AVPR2, DRD4, MPO, PIK3R1, PYGL, SRC, PTK2, MMP13, MMP3, CA3, CA6, PKN1, CA14, NEK2, CXCR1, CAMK2B, AKT1,

					NEK6
YDZ114	flavone	luteolin	$C_{15}H_{10}O_6$	286.04774	NOX4, AKR1B1, CDK5R1, CDK5, XDH, MAOA, FLT3, CA2, CCNB3, CCNB1, CCNB2, ALOX5, ADORA1, CA7, GLO1, APP, SYK, GSK3B, PARP1, TTR, MMP9, CA12, MMP2, CA4, MMP12, CD38, CYP1B1, ABCG2, AKR1B10, TNKS2, TNKS, TOP1, ARG1, PTPRS, ABCC1, HSD17B1, ACHE, CDK6, ABCB1, HSD17B2, CYP19A1, ESR2, ADORA2A, CSNK2A1, ALOX15, ALOX12, ESR1, PTGS2, CFTR, AMY1A, GRK6, CA1, CA9, CDK2, TERT, CDK1, TYR, AHR, ESRRA, GPR35, AVPR2, IGF1R, EGFR, F2, PIM1, AURKB, DRD4, MPO, PIK3R1, DAPK1, PYGL, SRC, PTK2, KDR, MMP13, MMP3, CA3, PLK1, CA6, PKN1, CA14, MET, NEK2, CXCR1, CAMK2B, ALK, AKT1, NEK6, PLA2G1B, CA5A, BACE1, AXL, NUAK1, AKR1C2, AKR1C1, AKR1C3, AKR1C4, CA13, AKR1A1, PFKFB3, PLG, KDM4E, AR
YDZ115	flavone	quercetin	$C_{15}H_{10}O_7$	302.04265	NOX4, AVPR2, AKR1B1, XDH, MAOA, IGF1R, FLT3, CYP19A1, EGFR, F2, CA2, PIM1, ALOX5, AURKB, DRD4, ADORA1, CA7, GLO1, MPO, PIK3R1, ADORA2A, DAPK1, PYGL, CA1, GSK3B, SRC, PTK2, HSD17B2, KDR, MMP13, MMP3, CA3, ALOX15, ABCC1, PLK1, CA6, CDK1, MMP9, CA12, MMP2, PKN1, CA14, CA9, CSNK2A1, ALOX12, MET, CA4, NEK2, CXCR1, CAMK2B, ALK, AKT1, ABCB1, NEK6, PLA2G1B, CA5A, BACE1, CYP1B1, AXL, ABCG2, NUAK1, AKR1C2, AKR1C1, AKR1C3, AKR1C4, CA13, AKR1A1, GPR35, MAPT, KDM4E, TOP2A, INSR, ACHE, MYLK, SYK, PIK3CG, APEX1, PTPRS, ESR2, MPG, SLC22A12, CDK5R1, CDK5, CCNB3, CCNB1, CCNB2, ARG1, CDK6, CDK2, TYR, HSD17B1, AHR, ESRRA, APP, PARP1, TTR, MMP12, CD38, AKR1B10, TNKS2, TNKS, TOP1, TERT
YDZ116	flavone	3'-methoxy-luteolin	$C_{16}H_{12}O_6$	300.06339	ABCC1, CYP1B1, AKR1B1, XDH, CA2, CA7, CA12, CA4, CDK5R1, CDK5, CCNB3, CCNB1, CCNB2, ARG1, PTPRS, PLG, APP, ALOX5, PARP1, TNKS2, TNKS, ABCB1, NOX4, FLT3, ABCG2, MAOA, ADORA1, GLO1, SYK, GSK3B, TTR, MMP9, MMP2, MMP12, CD38, AKR1B10, TOP1, ESR2, ACHE, CDK6, ADORA2A, PLA2G2A, PIM1, TERT, HSD17B1, ALOX15, ALOX12, ESR1, CYP19A1, CSNK2A1, IGF1R, EGFR, OPRD1, CDK2, PTGS2, CFTR, MCL1, HSD17B2, CBR1, CA1, CA9, F2, CDK1, AVPR2, AURKB, DRD4, MPO, PIK3R1, DAPK1, PYGL, SRC, PTK2, KDR, MMP13, MMP3, CA3, PLK1, CA6, PKN1, CA14, MET, NEK2, CXCR1, CAMK2B, ALK, AKT1, NEK6, PLA2G1B, CA5A, BACE1, AXL, NUAK1, AKR1C2, AKR1C1, AKR1C3, AKR1C4, CA13, AKR1A1, GPR35, AMY1A, GRK6, TYR, ST6GAL1
YDZ117	flavone	luteolin-3'-*O*-*β*-D-glucoside	$C_{21}H_{20}O_{11}$	448.10056	AKR1B1, TNF, IL2, ADORA1, NOX4, ADRA2C, CA2, CA7, CA12, CA4, ACHE, XDH, NQO2, RPS6KA3, NMUR2, ADRA2A, CD38, ALDH2, SLC29A1, PTGS2
YDZ118	flavone	kaempferol-3-*O*-*α*-L-rhamoside	$C_{21}H_{20}O_{10}$	432.10565	NQO2, AKR1B1, CA2, CA7, CA12, CA4, RPS6KA3, ACHE, NOX4, ADRA2C, NMUR2, ADRA2A, CD38, PTGS2, PDE5A, ADORA1, XDH, TNF, IL2, SLC29A1, ALOX5
YDZ119	flavone	quercetin-3-*O*-*α*-L-rhamnoside	$C_{21}H_{20}O_{11}$	448.10056	AKR1B1, CA2, CA7, CA12, CA4, NQO2, NOX4, ADRA2C, ACHE, RPS6KA3, NMUR2, ADRA2A, CD38, PTGS2, XDH, TNF, IL2, ADORA1, PDE5A, ALOX5, SLC29A1
YDZ120	flavone	quercetin-3-*O*-*β*-D-galactoside	$C_{21}H_{20}O_{12}$	464.09548	AKR1B1, NOX4, ADRA2C, CA2, CA7, CA12, CA4, ACHE, NQO2, RPS6KA3, NMUR2, ADRA2A, PTGS2, CD38, PDE5A, TNF, IL2, XDH, ADORA1, ALOX5, SLC29A1, TERT
YDZ121	flavone	rutin	$C_{27}H_{30}O_{16}$	610.15338	NMUR2, ADRA2A, ADRA2C, ACHE, AKR1B1, NOX4, CA7, CA12, CA4, CA2, RPS6KA3, NQO2, XDH, CD38, PTGS2, PDE5A, TNF, IL2, ADORA1, ALOX5, TERT
YDZ122	flavone	apigenin-7-*O*-neohesperidoside	$C_{27}H_{30}O_{14}$	578.16356	TNF, IL2, AKR1B1, ADORA1, XDH, NMUR2, ADRA2A, ADRA2C, ACHE, CA7, CA12, CA4, EGFR, ALDH2, CA2, CA1, CA9, NQO2, NOX4, TP53, CD38, RPS6KA3, SQLE
YDZ123	flavone	thevetiaflavone	$C_{16}H_{12}O_5$	284.06847	ABCB1, CYP1B1, ABCG2, ESR2, ESR1, AKR1B1, ADORA1, ADORA2A, HSD17B1, ABCC1, TNKS2, TNKS, NOX4, CDK5R1, CDK5, XDH, MAOA, FLT3, CYP19A1, CCNB3, CCNB1, CCNB2, ACHE, PTGS2, CDK6, SYK, GSK3B, TTR, CSNK2A1, CFTR, AKR1B10, PIM1, PLG, CA2, CA7, CA12, TERT, MCL1, ALOX5, AR, CA4, ADORA3, PARP1, APP, PTPRS, AMY1A, GRK6, CA1, CA9, CBR1, ARG1, ALOX15, ALOX12, GLO1, MMP9, MMP2, MMP12, CD38, TOP1, HSD17B2, LCK, TYR, AHR, ESRRA, KIT, OPRD1, CDK1, NAE1, MAOB, PFKFB3, KDM4E, EGFR, IGF1R, PLA2G2A, SLC22A12, SIGMAR1, ODC1, NOS2, ST6GAL1, GPR35, DAPK1, MPG, F2, OPRM1, PTPN1, KDM5A, CALM1, PPARG, BACE1, CYP1A1, CYP1A2, CDK2, AVPR2, AURKB, DRD4, MPO, PIK3R1, PYGL, SRC, PTK2, KDR, MMP13, MMP3
YDZ124	flavone	isovitexin	$C_{21}H_{20}O_{10}$	432.10565	AKR1B1, CA7, CA12
YDZ125	flavone	7-methoxy-luteolin	$C_{16}H_{12}O_6$	300.06339	AKR1B1, ADORA1, ADORA2A, PIM1, NOX4, APP, PLG, CYP1B1, ABCC1, EGFR, CDK5R1, CDK5, TERT, PTPRS, XDH, CA2, CA7, CA12, CA4, ALOX5, FLT3, ABCG2, ESR2, MAOA, CCNB3, CCNB1, CCNB2, SYK, GSK3B, TTR, AKR1B10, TNKS2, TNKS, ABCB1, ESR1, OPRD1, GLO1, PARP1, MMP9, MMP2, MMP12, CD38, TOP1, ARG1, AMY1A, GRK6, HSD17B1, PLA2G2A, F2, IGF1R, KIT,

					CYP19A1, ACHE, PTGS2, CDK6, CSNK2A1, CFTR, BACE1, CBR1, HSD17B2, AR, ST6GAL1, NOS2, ADORA3, GPR35, DAPK1, CA1, CA9, KDM4E, ALOX15, CDK1, ALOX12, AVPR2, AURKB, DRD4, MPO, PIK3R1, PYGL, SRC, PTK2, KDR, MMP13, MMP3, CA3, PLK1, CA6, PKN1, CA14, MET, NEK2, CA13, CXCR1, CAMK2B, ALK, AKT1, NEK6, PLA2G1B, CA5A, AXL, NUAK1, AKR1C2, AKR1C1, AKR1C3
YDZ126	flavone	luteolin-7-*O*-*β*-D-glucoside	$C_{21}H_{20}O_{11}$	448.10056	TNF, IL2, AKR1B1, ADORA1, CA7, CA12, XDH, NMUR2, ADRA2A, ACHE, RPS6KA3, NQO2, ALDH2, EGFR, CD38, CA1, ALOX5, CA2, CA4, PDE5A, SLC29A1, NOX4, ADRA2C, PLG
YDZ127	flavone	apigenin-7-*O*-*β*-D-glucoside	$C_{21}H_{20}O_{10}$	432.10565	TNF, IL2, AKR1B1, ADORA1, CA7, CA12, XDH, RPS6KA3, ACHE, NQO2, ALDH2, NMUR2, ADRA2A, EGFR, CA1, CD38, PDE5A, SLC29A1, CA2, CA4, F10, ABCB1
YDZ128	nitrogen compound	thymine	$C_5H_6N_2O_2$	126.04293	DPYD
YDZ129	nitrogen compound	uracil	$C_4H_4N_2O_2$	112.02728	TYMS, AOC3, PARP1, SIGMAR1
YDZ130	nitrogen compound	3-pyridinecarboxylic acid	$C_6H_5NO_2$	123.03203	HCAR2, DDO, SIRT3, SIRT2, SLC22A6, FYN, LCK
YDZ131	nitrogen compound	5-methoxynicotinic acid	$C_7H_7NO_3$	153.04259	FEN1, MAOB, HCAR2, ERCC5, PIM1, PTGDR2, CAD, KDM5C, KDM4B, KDM5B, KDM4A, GPR35, CA2, CA1, RNPEP
YDZ132	nitrogen compound	3-formylindole	C_9H_7NO	145.05276	CYP2A6, IMPDH2, PARP1, PIM1, PIM2, NOS2, TPO, MALT1, CCR1
YDZ133	nitrogen compound	2-hydroxycinchoninic acid	$C_{10}H_7NO_3$	189.04259	PARP1, KDM4E, KDM4A, KDM3A, KDM6B, FTO, KDM4C, CTBP2, ERN1, CPA1, KMO, AKR1B1, TPMT
YDZ134	nitrogen compound	4-ethoxycarbonyl-2-quinolone	$C_{12}H_{11}NO_3$	217.07389	PARP1, CSNK2A1, MAPK8, CHEK1, PDE7A, GRM4, NOTUM, GCK, ADORA1, NAAA, TDP2, ADORA2A, BRD2, BRDT, BRD3, CDK5R1, CCNA1, CCNA2, CDK9, CCNT1, CCNB3, CDK1, CCNB1, CCNB2, CTSS, ADORA2B, MAPK10, CTSK, MAPK9, MAOA, TGM2, PDE2A, RPS6KA2, FAAH, ELANE, PDE4B, CASP3, CASP7, MALT1, IDO1, ADORA3, JAK1, TYK2, MGLL, TMIGD3, MET, GSTP1, MTNR1A, MTNR1B, EGFR, HMOX1, GUSB, TBXAS1, CCNE1, CDK2, F2, CDK5, XPO1, HTR6, XDH, FLT3, GSR, HSD11B1, NR1H3, CCR3, ALDH3A1, NR1H2, PARP3, TAAR1, MAP3K20, ABL2, TGFBR2, TGFBR1, ACE, PDE5A, TERT, NOS2, GALR3, GRM2, CYP26A1, HTR2B, CDC7, KAT2B, CRHR1, MPO, PDE4D, DYRK1B, APP, HRH4, SHH, SLC6A2, MCL1, QPCT, P2RX7, PABPC1, TDO2, CHRM1, CCND3, CCND1, CDK4, CCND2, CHRM2, PLAU, CYP11B1, TRPA1, LRRK2, NOS1, BCAT2
YDZ135	nitrogen compound	2,3-dihydro-3-hydroxy-2-oxo-1*H*-indole-3-acetic acid	$C_{10}H_9NO_4$	207.05316	AKR1B1, KMO, AKR1A1, NQO2, FBP1, SLC13A5, FUCA1, PTGDR2
YDZ136	nitrogen compound	2'-deoxyadenosine	$C_{10}H_{13}N_5O_3$	251.10184	#N/A
YDZ137	nitrogen compound	thymidine	$C_{10}H_{14}N_2O_5$	242.09027	#N/A
YDZ138	nitrogen compound	adenosine	$C_{10}H_{13}N_5O_4$	267.09675	ADORA1, ADORA2A, ADORA3, DPP4, ADK, HSPA8, HSPA5, ADA, AHCY, GAPDH, EHMT1, EHMT2, MCL1, SETD7, AMD1, EGFR, SRM, PDCD4, SRC, ADORA2B, MAPK1, SLC29A1, PNP, SETD2, CARM1, PRMT1, DOT1L, GRK1, P2RY1, P2RY11, MTAP, ROCK2, PRKACA, SMS, FBP1, FHIT, CDA, KMT2A, SUV39H1, DNMT1, INMT, SMYD2, EZH2, EZH1, SETDB1, PNMT, DNMT3B, MAPKAPK2, HSPA1A, RARS, CA2, CA1, CA12, CA9, OGA, CCND1, CDK4, CA14, FUCA1, HSD17B1, PIM1, GBA, GAA, MARS, GSK3B, PRMT7, PARG, IDO1, SLC28A2, IARS, DAO, F2
YDZ139	nitrogen compound	flazine	$C_{17}H_{12}N_2O_4$	308.07971	PTGDR2, AKR1C3, VCP, IGFBP3, AKR1B1, P2RX3, IGFBP5, MMP9, MMP1, MMP2, MMP14, MMP8, MME, CA2, PYGL, PYGM, CA1, ACE, AMPD3, ANPEP, LTA4H, ECE1, HMGCR, REN, CSNK2A1, MKNK2, ITGAL, ICAM1, ITGB2, SLC22A12, METAP2, KDM4A, PNP, CREBBP, NOX4, EGFR, HCAR2, CDC25B, CAMKK2, FOLH1, MMP16, KDM3A, KDM5B, KDM4D, KDM4C, MMP3, SELE, SELP, BCL2A1, ERN1, CPT1A, PPARA, HSP90AA1, HSP90AB1, MET, MAPK8, PTGS2, ITGB1, ITGA4, SLC5A2, FDFT1, WEE1, PFKFB4, FBP1, PARP1
YDZ140	nitrogen compound	*N*-benzoyl-L-phenylalaninol	$C_{16}H_{17}NO_2$	255.12593	PIN1, CAPN1, ITGAL, ICAM1, ITGB2, CCR3, TGFBR1, CA2, BACE1, NQO2, PDE2A, PDE10A, CCNE1, CDK2, MMP2, BRD4, PARP1, PRKCQ, PIM1, PIM2, AKR1C3, CYP2C9, CYP2C19, CCR5, NQO1, JAK2, P2RX3, ABCC9, GABRA1, GABRB3, GABRG2, GABRA5,

					AMPD3, CA1, HDAC6, CDK5R1, CDK5, DYRK1A, MPO, KDR, IDO1, AURKA, ADORA1, ADORA2A, MKNK1, AXL, TYRO3, MERTK, CYP11B1, CYP11B2, MLYCD, CRHR1, P2RX7, LRRK2, KCNE1, KCNQ1, IL6ST, PARP3, PGR, JAK3, JAK1, BRPF1, MAP2K1, PDE7A, TYK2, OPRK1, ALOX15, EGFR, CCNB3, CDK1, CCNB1, CCNB2, TERT, PER2, EPHX2, CHRM1, ATP4B, ATP4A, MAPK8, PRKDC, MTOR, PIK3CA, TTK, PTGES, RASGRP1, SIGMAR1, NTRK1, CSNK1D, PAK1, CSNK1E, ADA, MYLK, KCNMA1, TRPM8, CFD, LIPE, HSD11B1, MAPK14, MET, HTR2A, DRD3, HMOX1, MCHR1, TK1, DRD2, CX3CR1, MAP3K14, NAMPT, NR3C1, AMPD2
YDZ141	others	cleomiscosin A	$C_{20}H_{18}O_8$	386.10017	#N/A
YDZ142	others	cleomiscosin C	$C_{21}H_{20}O_9$	416.11073	#N/A
YDZ143	others	cleomiscosin E	$C_{20}H_{18}O_8$	386.10017	#N/A
YDZ144	others	pinoresinol	$C_{20}H_{22}O_6$	358.14164	SHBG, ALOX5, MCL1, MAPK9, PTAFR, SLC5A2, SOAT1, HIF1A, SOAT2, OPRM1, PIK3CG, PIK3CA
YDZ145	others	guaiacylglycerol-*β*-*O*-6'-(2-methoxy) cinnamyl alcohol ether	$C_{20}H_{24}O_7$	376.15220	#N/A
YDZ146	others	secoisolariciresinol	$C_{20}H_{26}O_6$	362.17294	HTR1A, SHBG, NR3C1, ALOX15, TTR, SRC, IGF1R, ALOX12, CYP24A1, CHEK1, WEE1, POLA1, MKNK2, ALOX5, CA2, CA4, CA1, LYPLA1, LYPLA2, GSK3B, MAP2K1, ESR1, AR, PIK3R1, SLC6A4, FLT3, PLK4, CDK5, AXL, NTRK1, KDR, MAP3K14, ESR2, SLC6A3, ADORA1, ADCY10, XDH, LRRK2, MTOR, TTL, LTB4R, HSP90AA1, TYRO3, MERTK, ALK, CAPN1, CNR2, IRAK4, RCOR1, KDM1A, ITK, CDK1, CCNB1, CCNE1, CDK2, CDK7, CCNH, CDK9, CCNT1, DYRK1A, CSNK1A1, MAPK3, MAPK15, CAMKK2, INSRR, MMP2, HMGCR, ESRRA, ESRRB, GPER1, CNR1, ADORA2A, ERN1, SLC6A2, CYP19A1, CA6, LNPEP, ACVRL1, MAP3K7, AKR1B1, PIK3CD, PIK3CB, PIK3CG, PIK3CA, AKR1B10, PTGFR, SORD, CSF1R, ADCY1, ROCK2, HSP90AB1, RELA, GPR55, GPR18, HSD17B1
YDZ147	others	dihydrodehydrodiconiferyl alcohol	$C_{20}H_{22}O_7$	374.13655	CA2, CA1, CA12, GSK3B, MKNK2, CNR1, CNR2, NTRK1, CHEK1, WEE1, MTOR, ABCB1, SORD, PIK3CA, PIK3R1, CCNE2, CCNE1, MAPK1, SYK, SLC28A2, ACVRL1, ADORA2A, CDC25B, TOP1, HRAS, SLC5A1, IRAK4, ADAM17, MAP3K14, KLK1, KLK2, SLC29A1, ADK, AGTR1, MMP9, OPRM1, OPRD1, FLT3, LCK, MAP2K2, P2RX3, MAPKAPK5, TYK2, TYMS, CDC25C, NUDT1, CDC25A, CFTR, TLR9, MMP2, MMP14, MAP2K1, AMPD3, MAPK8, RPS6KA3, MAPK10, RPS6KA4, MAPK11, MAPK9, CSNK1E, NLK, MMP7, MMP8, CDK1, SERPINA6, HSD11B1, S1PR1, ALPL, HCAR2, CSF1R, TYRO3, MERTK, MAP3K7, MMP13, GABRA1, GABRB2, GABRG2, CA4, CDK5R1, CDK5, CDK2, CCNA1, CCNA2, KCNJ1, FLT4, UPP1, AKR1B10
YDZ148	others	7,8-epoxylignans	$C_{20}H_{24}O_7$	376.15220	SLC5A2, SOAT1, HIF1A, SOAT2, ALOX5, MCL1, LCK, MAP2K2, MAPKAPK5, TYK2, MAPK1, ALK, PTAFR, TOP1, CHEK1, WEE1, SLC5A1, MMP7, MMP8, ADORA2A, MAPK9, ADK, SLC5A4, CDC25B, ADORA1, PIK3CA, PIK3R1, MAP2K7, RELA, CDK5R1, CDK5, CCNA1, CCNA2, HRAS, NUDT1, IRAK4, GSK3B, CDK2, CDC25C, CDC25A, TLR9, NTRK1, ADORA3, CDK1, UPP1, ACVRL1, PTGS2, PYGL, CFTR
YDZ149	others	7'-hydroxylariciresinol	$C_{20}H_{24}O_7$	376.15220	SLC5A2, SOAT1, HIF1A, SOAT2, ALOX5, PTAFR, TOP1, MCL1, SLC5A1, CHEK1, WEE1, SLC5A4, MAPK9, ADK, ADORA1, MMP7, MMP8
YDZ150	others	cleomiscosin B	$C_{20}H_{18}O_8$	386.10017	SYK, ADORA3, FLT1, ABCG2, MMP1, PIK3CA, PIK3R1, ADAM17, ERBB2, TYMS, EGFR, CFD, ABCB1, MMP13, ADCY1, MMP7, MMP8, ADAM10, MMP12, RET, EIF4A1, PIK3C2A, PIK3C2G, PIP4K2C, RAF1, FLT3, FKBP1A, MTOR, ADORA1, MYLK, DAPK3, ADORA2A, DAPK1, JAK1, CDK7, DAPK2, PIK3CD, PRKDC, PIK3CB, PIK3CG, PI4KB, CHUK, TYK2, MAP2K1, CSNK2A1, CSNK2A2, CLK1, CLK2, CLK3, DYRK2, CDC42BPA, HIPK2, HIPK3, BRAF, HIPK1, DYRK1B, PIK3C2B, LIMK2, RIOK2, MAP3K19, SLC2A1, GBA, ALPL, PLAA, ABCC1, PDE10A, AKR1B10, TYMP, CHEK1, WEE1, LNPEP, CRHR1, EIF2AK3, AKT1, CHRM1, HSP90AA1, NTRK1, MMP3, FCER2, HSP90AB1, CDK1, CCNB1, CCNE1, CDK2, IMPDH2, CDK3, GRK2, PIM1, PIM2, PIM3, HTR2B, F9, ADAMTS4, PAK4, MKNK2, SCN9A, TNK2, MAP3K14
YDZ151	others	2*β*,6*β*,9*β*-trihydroxyclovane	$C_{15}H_{26}O_3$	254.18819	NR1H4, SHH, NPC1L1, GPBAR1, AR, CDC25B, NR1I3, ESR1, ESR2, NR1H3, SHBG, CA4, CA1, CDC25A, CA2, TRPM8, UGT2B7, POLA1, HSD11B1, BRD4, BRD2, PTGS1, JAK1, PTGS2, CDC7, CYP19A1, MIF, NR3C1, CA6, CA12, CA14, CA9, CA13, CA5B, CA5A
YDZ152	others	glycerol 1,3-bisoleate	$C_{39}H_{72}O_5$	620.53798	PRKCD, PRKCA, PRKCQ, HSD11B1, FAAH, PTGES, PTGS2, CNR1, CNR2, HMGCR, PTPN1, LPAR6, LPAR3, ENPP2, LPAR2, LPAR1, TRPV1, LPAR5, LPAR4, CES2, PRKCG, PRKCE, PRKCH, ALOX5, PREP, PTPN2, AR, CYP19A1, CYP17A1, NOS2, BCL2L1, HSD17B2, HSD11B2, FNTA, FNTB, PGR, NR3C1, SERPINA6, METAP2, NR3C2

YDZ153	others	azelaic acid	$C_9H_{16}O_4$	188.10486	FABP4, FABP3, FABP5, PPARD, FFAR1, FABP2, PPARA, HSD11B1, AR, VDR, NR1H4, POLB, CDC25A, GPBAR1, SLC22A6, UGT2B7, CYP19A1, SERPINA6, SHBG, HSD17B3, G6PD, GABBR1, KDM2A, KDM5C, PTGFR, NPC1L1, GABRA2, GABRB2, GABRG2, AKR1B10, HSD11B2, PHF8, CA2, CA1, FNTA, FNTB, PLG, FOLH1, PTGER2, CDC45, LTA4H, CPA3, REN, HAO1, CACNA2D1, ACE, CHRNA7, KMO, GSTK1, PTPN1, FDPS, AKR1B1, EGLN3, GRM5, PTGES, FDFT1, AHR, PTGDR2, EDNRB, EDNRA, PTPRC
YDZ154	others	(±)-8-hydroxyhexadecanoic acid	$C_{16}H_{32}O_3$	272.23514	PPARA, PPARD, FFAR1, FABP4, FABP3, FABP5, HSD11B1, SLC22A6, FABP2, VDR, GPBAR1, NR1H4, PTGER2, KDM2A, PHF8, CDC25A, AR, UGT2B7, SERPINA6, SHBG, HSD17B3, G6PD, GABBR1, PTGFR, AKR1B10, CYP19A1, POLB, FNTA, FNTB, NPC1L1, GABRA2, GABRB2, GABRG2, KDM5C, HSD11B2, PTGER4, LTA4H, HAO1, CA2, CA1, PTGER3, GSTK1, PTPN1, TBXA2R, CDC45, HSD17B2, IMPDH2, PGR, THRA, THRB, AGTR1, PPARG, PTGDR, IMPDH1, PLA2G4A, HMGCR, PTPRC, BCL2, HDAC1, PTGDR2, CCR1, KDM7A, GCGR, PDE5A, CYP26B1, CYP26A1, CTSA, FDFT1, GSK3B, GSK3A, GIPR, AURKA, RARG, RARA, ADORA1, ADORA2A, ADORA2B, CHRNA7, DHCR7, CCKBR, PDE6D, AKR1C3, NR0B2, PLG, MMP12, MME, OPRK1, DUSP3, INSR, CCNE2, CCNE1, CCNB3, CCNB1, CCNB2, CCNA1, CCNA2, EPHX2, NTRK1, PTPN22, CDK2, CDK1, MAPK3, CDK5, NTRK2, ITGAV, ITGB3, RXRA, CHEK1
YDZ155	others	stearic acid	$C_{18}H_{36}O_2$	284.27153	PPARA, PPARD, FABP4, FABP5, FABP3, FABP2, FFAR1, SLC22A6, CDC25A, AKR1B10, HSD11B1, NR1H4, UGT2B7, PTGER2, POLB, CYP19A1, SERPINA6, SHBG, HSD17B3, G6PD, GABBR1, GPBAR1, NPC1L1, GABRA2, GABRB2, GABRG2, KDM2A, KDM5C, VDR, AR, FNTA, FNTB, PHF8, PLG, GSTK1, PTPN1, FAAH, PPARG, TERT, FABP1, RARG, RARB, RARA, GLRA1, HSD11B2, PTGFR, CDC45, PTPRC, HAO1, NR0B2, CYP26B1, CYP26A1, SCD, RXRB, RXRG, RXRA, CACNA2D1, HMGCR, PTGER4, CHRNA7, CA2, CA1, GCG, SAE1, UBA2, GRM5, PDE4A, PDE4B
YDZ156	others	4-hydroxy-3-methoxy-benzoic acid	$C_8H_8O_4$	168.04226	CA2, CA7, CA1, CA12, CA14, CA9, CA3, CA6, CA5A, CA4, TPMT, TTR, CA5B, CA13, FUT7, KDM4E, KDM4A, KDM3A, KDM6B, FTO, KDM4C, FYN, LCK, FBP1, AKR1C3, KDM2A, MMP9, MMP1, MMP2, MMP8, SQLE, POLA1, POLB, SERPINE1, TUBB1
YDZ157	others	3,4-dihydroxy benzoic acid	$C_7H_6O_4$	154.02661	#N/A
YDZ158	others	para-hydroxybenzaldehyde	$C_7H_6O_2$	122.03678	CA2, CA7, CA1, CA3, CA6, CA12, CA14, CA9, CA4, CA5B, CA5A, CA13, ERN1, COMT, ACHE, ALDH5A1, TYR, ABAT, FUT7
YDZ159	others	p-Hydroxybenzoic acid	$C_7H_6O_3$	138.03169	CA2, CA7, CA1, CA3, CA6, CA12, CA14, CA9, CA4, CA5B, CA5A, CA13, FUT7, SRD5A2, DAO, AKR1C2, AKR1C1, SQLE, HDAC6, HDAC8, ERN1, ESR2, LDHA, LDHB
YDZ160	others	vanillic acid	$C_8H_8O_4$	168.04226	CA2, CA7, CA1, CA12, CA14, CA9, CA3, CA6, CA5A, CA4, TPMT, TTR, CA5B, CA13, FUT7, KDM4E, KDM4A, KDM3A, KDM6B, FTO, KDM4C, FYN, LCK, FBP1, AKR1C3, KDM2A, MMP9, MMP1, MMP2, MMP8, SQLE, POLA1, POLB, SERPINE1, TUBB1
YDZ161	others	dihydroferulic acid	$C_{10}H_{12}O_4$	196.07356	FYN, LCK, SHBG, EGFR, MAP2K1, ALOX15, KDM4E, ACHE, TTR, HTR1A, FBP1, PTGFR, ALOX5, HSD11B1, LYPLA1, LYPLA2, NR3C1, PPARG, TUBB1, CA2, CA6, PPARD, CALM1, AMPD3, CTNNB1, ITGAL, ICAM1, ITGB2, PTGS2, POLA1, SLC6A2, HSD17B1, CYP1A2, ECE1, MAPK8, ACLY, HMGCR, KDM4C, PARP1, CYP19A1, SLC6A3, CA1, COMT
YDZ162	others	4-methoxy-guaiacylglycerol	$C_{11}H_{16}O_5$	228.09977	#N/A
YDZ163	others	vanillin	$C_8H_8O_3$	152.04734	ERN1, CA2, CA7, CA1, CA12, CA14, CA9, CA4, CA3, CA6, CA5A, CDC25B, PTPRC, EP300, TTR, NAT1, ALPG, PLAA
YDZ164	others	methyl 3,4-dihydroxybenzoate	$C_8H_8O_4$	168.04226	CA2, CA7, CA1, CA12, CA14, CA9, SQLE, FUT7, CA13, CA6, CA5B, SERPINE1, CA3, CA4, IGF1R, ALK, BCL2L1, CA5A, COMT, ADAMTS5, LDHA, LDHB, ESR2, ESR1, AURKB, SRC, PTK2, KDR, MET, NEK2, AXL
YDZ165	others	gallic acid	$C_7H_6O_5$	170.02152	CA2, CA7, CA1, CA3, CA6, CA12, CA14, CA9, FUT7, CA4, CA5B, CA5A, CA13, SQLE, LDHA, LDHB, TTR, IGF1R, ALK, SERPINE1, ESR2, BCL2L1, GPR35, COMT, TPMT
YDZ166	others	syringic acid	$C_9H_{10}O_5$	198.05282	CA2, CA7, CA1, CA3, CA6, CA12, CA14, CA9, CA5A, CA4, CA13, CA5B, FUT7, TPMT, AKR1C3, TUBB1, POLA1, POLB, SQLE, OGA, FYN, LCK, FBP1, SERPINE1, TTR, KDM4E, KDM4A, KDM3A, KDM2A, KDM6B, FTO, KDM4C, ERN1, NGFR, PTGDR2
YDZ167	others	7-carbonyl-guaiacylglycerol	$C_{10}H_{12}O_5$	212.06847	#N/A