Table SI. Sequences of primers used for reverse transcription-quantitative PCR.

Gene	Sequence of primers (5'-3')	(Refs.)
Slc5a8	F: CTCCATGCAAAACTGTCCCTCT	*
	R: CCAACACCAAATAAGGCATAAGC	
Arhgap9	F: GCGCGCTGCGGACTGTCAT	*
	R: CTGCACACCGACTGGAAGTTCT	
Cybb	F: CCTAAGATAGCAGTTGATGGAC	*
	R: CCTGCACAGCCAGTAGAAGTA	
Actb	F: CCTTCTTGGGTATGGAATCCTGT	(40)
	R: CACTGTGTTGGCATAGAGGTCTTTAC	
Bcl2	F: GGAGAAATCAAACAGAGGTCGC	(41)
	R: CGTCAACAGGGAGATGTCACC	
Bax	F: CAAGGCCCTGTGCACTAAAGT	(41)
	R: AAGTAGGAGAGGAGGCCTTCC	
Casp8	F: CTCCGAAAAATGAAGGACAGA	(42)
	R: CGTGGGATAGGATACAGCAGA	
Casp9	F: AGTTCCCGGGTGCTGTCTAT	(43)
	R: GCCATGGTCTTTCTGCTCA	

*Designed in the present study. F, forward; R, reverse.

Table SII. Identification of metabolite compound in TTFM extracts in the negative ion mode.

Metabolite name	RT (min)	Average m/z	Formula	Ontology	InChIKey	Average peak intensity
6-chloro-4,5,7-trihydroxy-9,10-dioxoanthracene-2-carboxylic acid	0.061	332.9794	$C_{15}H_7ClO_7$	Anthracenecarboxylic acids	JGHTWRZCNLXYPF-UHFFFAOYSA-N	25214.40
L-HISTIDINE	3.430	154.06197	$C_6H_9N_3O_2$	Histidine and derivatives	HNDVDQJCIGZPNO-UHFFFAOYSA-N	29131.46
PC(17:0/9-HODE)	5.164	846.58325	$C4_3H_{82}NO_9P$	Phosphatidylcholines	AFBYJAHNLYKEPA-CRWFHCLENA-N	20534.87
Chloroxynil	5.166	185.94843	$C_7H_3Cl_2NO$	Dichlorobenzenes	YRSSHOVRSMQULE-UHFFFAOYSA-N	217632.48
DL-4-Hydroxy-3-methoxymandelic acid	5.167	196.97162	$C_9H_{10}O_5$	Methoxyphenols	CGQCWMIAEPEHNQ-UHFFFAOYSA-N	68812.04
Urocanic acid	5.168	137.03453	$C_6H_6N_2O_2$	Imidazolyl carboxylic acids and derivatives	LOIYMIARKYCTBW-OWOJBTEDSA-N	77836.50
Cyclamate	5.168	178.06061	$C_6H_{13}NO_3S$	Cyclamates	HCAJEUSONLESMK-UHFFFAOYSA-N	29690.54
Catechol	5.169	109.03942	$C_6H_6O_2$	Catechols	YCIMNLLNPGFGHC-UHFFFAOYSA-N	780681.23

Benzotriazole	5.169	118.03995	$C_6H_5N_3$	Benzotriazoles	QRUDEWIWKLJBPS-UHFFFAOYSA-N	94210.57
5-METHYLCYTOSINE HYDROCLORIDE	5.169	124.0501	$C_5H_7N_3O$	Hydroxypyrimidines	LRSASMSXMSNRBT-UHFFFAOYSA-N	124364.42
1-Hydroxybenzotriazole	5.169	134.03467	$C_6H_5N_3O$	Benzotriazoles	ASOKPJOREAFHNY-UHFFFAOYSA-N	216696.62
TYRAMINE	5.169	136.0504	$C_8H_{11}NO$	Phenethylamines	DZGWFCGJZKJUFP-UHFFFAOYSA-N	152637.79
4-Nitrophenol	5.169	138.06567	$C_6H_5NO_3$	Nitrophenols	BTJIUGUIPKRLHP-UHFFFAOYSA-N	38629.78
(-)-Citramalic acid	5.169	147.06619	$C_5H_8O_5$	Hydroxy fatty acids	XFTRTWQBIOMVPK-RXMQYKEDSA-N	64211.00
METHIONINE	5.169	148.0506	$C_5H_{11}NO_2S$	Methionine and derivatives	FFEARJCKVFRZRR-BYPYZUCNSA-N	212062.18
1,4-naphthalene-dione	5.169	158.03476	$C_{10}H_6O_2$	Naphthoquinones	FRASJONUBLZVQX-UHFFFAOYSA-N	17545.55
3-Methyladipic acid	5.169	159.06648	$C_7H_{12}O_4$	Medium-chain fatty acids	SYEOWUNSTUDKGM-UHFFFAOYSA-N	74349.11
L-Rhamnose	5.169	163.06114	$C_6H_{12}O_5$	Hexoses	PNNNRSAQSRJVSB-BXKVDMCESA-N	121535.68

5-acetyl-2,6-dimethyl-2,3-dihydro-1H-pyridin-4-one	5.169	166.06157	$C_9H_{13}NO_2$	Tetrahydropyridines	ZVVZLQBYQRVNQJ-UHFFFAOYSA-N	42111.48
FA 9:0+1O	5.169	173.11662	$C_9H_{18}O_3$	Medium-chain hydroxy acids and derivatives	XBUXARJOYUQNTC-UHFFFAOYSA-N	56709.08
2-Isopropylmalic acid	5.169	175.06154	$C_7H_{12}O_5$	Hydroxy fatty acids	BITYXLXUCSKTJS-UHFFFAOYSA-N	77890.13
6-Aminoindazole	5.170	132.05527	$C_7H_7N_3$	Indazoles	KEJFADGISRFLFO-UHFFFAOYSA-N	157461.48
2-Methylglutaric acid	5.170	145.05075	$C_6H_{10}O_4$	Methyl-branched fatty acids	AQYCMVICBNBXNA-UHFFFAOYSA-N	166003.28
2,4-Dihydroxyacetophenone	5.170	151.05029	$C_8H_8O_3$	Alkyl-phenylketones	SULYEHHGGXARJS-UHFFFAOYSA-N	42758.26
SHIKIMATE	5.170	155.03534	$C_7H_{10}O_5$	Shikimic acids and derivatves	JXOHGGNKMLTUBP-HSUXUTPPSA-N	22829.51
Hydroxysuberic acid	5.170	189.07756	$C_8H_{14}O_5$	Medium-chain hydroxy acids and derivatives	ARJZZFJXSNJKGR-UHFFFAOYSA-N	48047.33
Ketoisovaleric acid	5.171	115.03866	$C_5H_8O_3$	Short-chain keto acids and derivatives	QHKABHOOEWYVLI-UHFFFAOYSA-N	102642.81

5,6-dihydropenicillic acid	5.171	171.06697	$C_8H_{12}O_4$	Butenolides	XMLBVCBGTUQJHY-UHFFFAOYSA-N	73688.27
CP-457920	5.171	322.12616	$C_{18}H_{17}N_3O_3$	Naphthyridines	DGFVZQGXKQCQGK-UHFFFAOYSA-N	31242.13
3-Hydroxybenzaldehyde	5.172	121.02834	$C_7H_6O_2$	Hydroxybenzaldehydes	IAVREABSGIHHMO-UHFFFAOYSA-N	159449.33
3-Methyl-2-oxovaleric acid	5.173	129.05473	$C_6H_{10}O_3$	Short-chain keto acids and derivatives	JVQYSWDUAOAHFM-UHFFFAOYSA-N	60286.28
cis-Aconitate	5.178	173.01363	$C_6H_6O_6$	Tricarboxylic acids and derivatives	GTZCVFVGUGFEME-IWQZZHSRSA-N	102164.84
2-Oxobutyrate	5.179	101.02344	$C_4H_6O_3$	Short-chain keto acids and derivatives	TYEYBOSBBBHJIV-UHFFFAOYSA-N	96049.99
Thiophanic acid	5.188	392.89423	$C_{14}H_6Cl_4O_5$	Xanthones	MYBIAUJNAXMGTF-UHFFFAOYSA-N	138930.31
p-Coumarate	5.210	163.00409	$C_9H_8O_3$	Hydroxycinnamic acids	NGSWKAQJJWESNS-ZZXKWVIFSA-N	31087.77
N-Formylmethionine	5.372	176.00496	$C_6H_{11}NO_3S$	Methionine and derivatives	PYUSHNKNPOHWEZ-YFKPBYRVSA-N	20633.78
Methanesulfonate	5.583	94.99426	CH_4O_3S	Organosulfonic acids	AFVFQIVMOAPDHO-UHFFFAOYSA-N	57853.65

Pertusaric acid	8.093	753.45135	$C_{21}H_{34}O_5$	Gamma butyrolactones	SKQHRBRVCRUFSX-UHFFFAOYSA-N	24502.45
2'-Deoxycytidine	10.522	225.99612	$C_9H_{13}N_3O_4$	Pyrimidine 2'-deoxyribonucleosides	CKTSBUTUHBMZGZ-SHYZEUOFSA-N	25379.40
Ampicillin	12.162	348.10324	$C_{16}H_{19}N_3O_4S$	Penicillins	AVKUERGKIZMTKX-UHFFFAOYSA-N	21614.15
3-[6-[[(2R,3R,4R,5S,6S)-3,5-dihydroxy-6-methyl-4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxychromen-4-one	13.220	753.22919	$C_{34}H_{42}O_{19}$	Flavonoid-3-O-glycosides	MQMTVWHXCSRCER-OHWKTECQSA-N	17411.49
4,5-dihydroxy-3-propylcyclopent-2-en-1-one	14.450	155.07338	$C_8H_{12}O_3$	1,2-diols	LFRFNLMDZHTVHB-UHFFFAOYSA-N	26321.18

[(1R,3R,10S,13R,14S,17R)-3-[(2R)-5-(3,5-dihydroxy-4-methoxy-6-methyloxan-2-yl)oxy-3,4-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-14-hydroxy-10,13-dimethyl-17-(5-oxo-2H-furan-3-yl)-1,2,3,4,5,6,7,8,9,11,12,15,16,17-tetradecahydrocyclopenta[a]phenanthren-1-yl] acetate	14.676	753.3714	$C_{38}H_{58}O_{15}$	Cardenolide glycosides and derivatives	XWYDFNHNSVTJFP-CSVIMRPTSA-N	23676.48
Fluorescein	17.003	331.05615	$C_{20}H_{12}O_5$	Xanthenes	GNBHRKFJIUUOQI-UHFFFAOYSA-N	23031.06
COSTUNOLIDE	17.095	267.1452	$C_{15}H_{20}O_2$	Germacranolides and derivatives	HRYLQFBHBWLLLL-IKTIWSOHSA-N	22143.73
5-[[(2R,3S,4S,5R,6S)-3,4-dihydroxy-6-[[5-hydroxy-2-(4-hydroxy-3-	21.359	753.17719	$C_{34}H_{42}O_{19}$	Flavonoid-7-O-glycosides	VUXVICJLLYFORC-FQRWNCDPSA-N	28008.59

methoxyphenyl)-4-oxo-2,3-dihydrochromen-7-yl]oxy]-5-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]methoxy]-3-hydroxy-3-methyl-5-oxopentanoic acid						
VERATRIC ACID	23.438	180.98793	$C_9H_{10}O_4$	P-methoxybenzoic acids and derivatives	DAUAQNGYDSHRET-UHFFFAOYSA-N	25750.18
[(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[(2S,3S,4R,5R)-4-hydroxy-3-[(E)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoyl]oxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxyoxan-2-yl]methyl (E)-3-(4-hydroxy-3,5-	30.659	753.21704	$C_{34}H_{42}O_{19}$	Coumaric acids and derivatives	FHIJMQWMMZEFBL-OPSYHMPNSA-N	29498.82

dimethoxyphenyl)prop-2-enoate						
2,4-diacetylphloroglucinol	31.812	209.04607	$C_{10}H_{10}O_5$	Alkyl-phenylketones	PIFFQYJYNWXNGE-UHFFFAOYSA-N	207278.24
Gly	37.647	74.00267	$C_2H_5NO_2$	Alpha amino acids	DHMQDGOQFOQNFH-UHFFFAOYSA-N	29992.12
(2E,4E)-12-hydroxy-13-(hydroxymethyl)-3,5,7-trimethyltetradeca-2,4-dienedioic acid	39.631	341.25186	$C_{18}H_{30}O_6$	Long-chain fatty acids	QFZISQBFEIXWDM-UTLPMFLDSA-N	31005.85
(2R,3S,4S,5R,6R)-2-[[(2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]-6-oct-1-en-3-yloxyoxane-3,4,5-triol	40.050	467.2164	$C_{19}H_{34}O_{10}$	Fatty acyl glycosides of mono- and disaccharides	MUPQSGHACLOUTE-PARKKQJRSA-N	52648.85
Perfluorooctylsulfonic acid	41.043	498.91837	$C_8HF_{17}O_3S$	Perfluorooctane sulfonic acid and derivatives	YFSUTJLHUFNCNZ-UHFFFAOYSA-N	86403.93

AZELAIC ACID	41.194	187.0959	$C_9H_{16}O_4$	Medium-chain fatty acids	BDJRBEYXGGNYIS-UHFFFAOYSA-N	171121.15
5,7-dihydroxy-2-(3-hydroxy-4,5-dimethoxyphenyl)-3,6-dimethoxy-4H-chromen-4-one	41.725	389.08505	$C_{19}H_{18}O_9$	6-O-methylated flavonoids	WTTGIVJDHDPLCL-UHFFFAOYSA-N	36763.37
Ticlopidine	42.540	262.04779	$C_{14}H_{14}ClNS$	Thienopyridines	PHWBOXQYWZNQIN-UHFFFAOYSA-N	32703.08
(4S,5Z,6S)-4-(2-methoxy-2-oxoethyl)-5-[2-[(E)-3-phenylprop-2-enoyl]oxyethylidene]-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4H-pyran-3-carboxylic acid	43.436	201.11357	$C_{10}H_{18}O_4$	Oxolanes	IVOODSRSVJPWLY-UHFFFAOYSA-N	70005.35
Hexosyl LPE 18:2	44.265	638.3324	$C_{29}H_{54}NO_{12}P$	Monosaccharide phosphates	HQYLDWZNTJHJNQ-AVQMFFATSA-N	87048.79

4-O-Methylphloracetophenone	44.559	180.97049	$C_9H_{10}O_4$	Alkyl-phenylketones	GKSGTWUNURZTKD-UHFFFAOYSA-N	33935.80
SPARTEINE SULFATE	44.730	330.90067	$C_{15}H_{28}N_2O_4S$	Sparteine, lupanine, and related alkaloids	FCEHFCFHANDXMB-UMEYXWOPSA-N	54095.64
Succinate	44.966	248.96025	$C_4H_6O_4$	Dicarboxylic acids and derivatives	KDYFGRWQOYBRFD-UHFFFAOYSA-N	6462155.50
Hexosyl LPE 18:3	44.968	636.32196	$C_{29}H_{52}NO_{12}P$	Monosaccharide phosphates	QFDVZERXJLVROF-IUQGRGSQSA-N	1383950.69
2-Deoxyribose 1-phosphate	45.150	212.99863	$C_5H_{11}O_7P$	Pentoses	KBDKAJNTYKVSEK-VPENINKCSA-N	9379322.75
Carbamimidothioic acid	45.391	182.98775	$C_3H_8N_2O_3S_2$	Organosulfonic acids	LTHWZZOUNJCHES-UHFFFAOYSA-N	2182143.94

RT, retention time; InChIKey, international chemical identifier key.

Table SIII. Identification of metabolite compound in TTFM extracts in the positive ion mode.

Metabolite name	RT (min)	Average m/z	Formula	Ontology	InChIKey	Average peak intensity
Sinapic acid	5.153	225.22137	$C_{11}H_{12}O_5$	Hydroxycinnamic acids	PCMORTLOPMLEFB-ONEGZZNKSA-N	9965.84
(1R,2R,4aS,8aS)-1-((S)-3-hydroxy-3-methylpentyl)-2,5,5,8a-tetramethyldecahydronaphthalen-2-ol	5.153	311.29132	$C_{20}H_{38}O_2$	Diterpenoids	VWPNQCLIQCRCCG-HHUCQEJWSA-N	8640.11
(Z)-5-[(1S,2R,4aR,8aR)-5-(hydroxymethyl)-1,2,4a-trimethyl-2,3,4,7,8,8a-hexahydronaphthalen-1-yl]-3-(hydroxymethyl)pent-2-enoic acid	5.153	319.22525	$C_{20}H_{32}O_4$	Colensane and clerodane diterpenoids	LRLROPFPFABQRF-CBYQQGIISA-N	8974.22
N-Methylanthranilic Acid	5.154	151.98055	$C_8H_9NO_2$	Aminobenzoic acids	WVMBPWMAQDVZCM-UHFFFAOYSA-N	21229.58

7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-2,3,4,5,6,7,8,8a-octahydronaphthalen-1-ol	5.154	241.21538	$C_{15}H_{28}O_2$	Eudesmane, isoeudesmane or cycloeudesmane sesquiterpenoids	LKKDASYGWYYFIK-UHFFFAOYSA-N	15477.82
Oleic acid	5.154	283.26205	$C_{18}H_{34}O_2$	Long-chain fatty acids	ZQPPMHVWECSIRJ-MDZDMXLPSA-N	120390.47
3-dihydro-7,8-dehydrodiscorhabdin C (+2)	5.154	463.89383	$C_{18}H_{14}Br_2N_3O_2$	Phenanthrolines	RZRKLCBSFPOTIQ-UHFFFAOYSA-O	178439.49
Cearoin	5.163	266.99109	$C_{14}H_{12}O_4$	Benzophenones	NFJVELXCUBWAFL-UHFFFAOYSA-N	26546.74
2,4-dihydroxyheptadecyl acetate	5.163	313.27356	$C_{19}H_{38}O_4$	Long-chain fatty alcohols	ZBVKFVTUHVIICH-UHFFFAOYSA-N	7413.27
Oxolinic acid	5.165	262.07501	$C_{13}H_{11}NO_5$	Quinoline carboxylic acids	KYGZCKSPAKDVKC-UHFFFAOYSA-N	14592.08
2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6,8-dimethoxychromen-4-one	5.167	369.0538	$C_{17}H_{14}O_8$	8-O-methylated flavonoids	GLMWHQIFJIURES-UHFFFAOYSA-N	12633.32
Etodolac	5.168	287.99814	$C_{17}H_{21}NO_3$	Indolyl carboxylic acids and derivatives	NNYBQONXHNTVIJ-UHFFFAOYSA-N	23177.23

Cyanidin	5.170	288.07693	$C_{15}H_{11}O_6$	7-hydroxyflavonoids	VEVZSMAEJFVWIL-UHFFFAOYSA-O	22024.79
Nicosulfuron-TP UCSN	5.170	316.07031	$C_{10}H_{13}N_5O_5S$	Pyridinesulfonamides	DGJDFJVBNQLVJW-UHFFFAOYSA-N	34841.48
Methoxamine	7.389	212.12869	$C_{11}H_{17}NO_3$	Dimethoxybenzenes	WJAJPNHVVFWKKL-UHFFFAOYSA-N	6624.51
ascr#17	19.356	331.2103	$C_{17}H_{30}O_6$	Sugar acids and derivatives	NEVPBIQTDNVVMK-CSKARUKUSA-N	5749.11
11b-hydroxypristimerin	28.153	463.2702	$C_{30}H_{40}O_5$	Triterpenoids	MRLNWXSZJIGUHQ-XEFXFLPWSA-N	7476.89
2-Butenoic acid, 2-methyl-, (2Z)-2-[[1-(3,4-dimethoxyphenyl)propoxy]carbonyl]-2-buten-1-yl ester, (2E)-	30.655	394.21545	$C_{21}H_{28}O_6$	Benzyloxycarbonyls	LKOARHYUMOKAPJ-GOBHWCIESA-N	9693.54
2-[2-[2-[[2-[2-(2-hydroxypropanoylamino)-3-methylbutanoyl]oxy-3-methylbutanoyl]amino]-3-methylbutanoyl]oxypropan	32.300	560.32196	$C_{26}H_{45}N_3O_{10}$	Depsipeptides	YBUWNKPGCLTWJO-UHFFFAOYSA-N	6766.97

oylamino]-3-methylbutanoic acid						
beta-D-Xylopyranoside, 1,3,4,6,7,7a,7b,8,9,10,11,13,13a,15,15a-pentadecahydro-13-hydroxy-11-(1-hydroxy-1-methylethyl)-1,1,7a,8,13a-pentamethyl-10,12a-epoxy-2H,5H-cyclopropa[1',8'a]naphth[2',1':4,5]indeno[2,1-b]oxepin-2-yl	33.288	636.41327	$C_{35}H_{54}O_9$	Cycloartanols and derivatives	LTVCFOSNIVVOBK-RSGHPYSYSA-N	6295.82
Esmolol	33.289	296.18292	$C_{16}H_{25}NO_4$	Phenol ethers	AQNDDEOPVVGCPG-UHFFFAOYSA-N	7318.11
9-hydroxy-5b,8,11a-trimethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7a,9,10,11,11b,12,13,13a,13b-hexadecahydrocyclopenta[	34.122	534.34717	$C_{30}H_{44}O_7$	Triterpenoids	FTGKHGAVFGGOMW-UHFFFAOYSA-N	6164.38

a]chrysene-3a,5a,8-tricarboxylic acid						
MMV676182	34.353	373.21228	$C_{22}H_{24}N_6$	Naphthalenes	MMRLNUFECMEMSQ-UHFFFAOYSA-N	7275.53
[5-Hydroxy-2-(3-hydroxybutyl)-3,3-dimethylcyclohexyl]methyl beta-D-glucopyranoside	34.648	393.24966	$C_{19}H_{36}O_8$	Terpene glycosides	GQUCOZSVXCLPKQ-SQNVVSGMSA-N	6113.67
[(3aS,4S,5S,6E,10E,11aR)-6-formyl-5-methoxy-10-methyl-3-methylidene-2-oxo-3a,4,5,8,9,11a-hexahydrocyclodeca[b]furan-4-yl] 2-methylpropanoate	34.694	401.76373	$C_{20}H_{26}O_6$	Germacranolides and derivatives	SKCDPGIEMVQDCR-VBMXKYFYSA-N	7086.55
4-[3-methyl-5-(5,6,7-trihydroxy-1,2,4a,5-tetramethyl-3,4,6,7,8,8a-hexahydro-2H-naphthalen-	35.122	465.28247	$C_{24}H_{42}O_7$	Colensane and clerodane diterpenoids	DQOOFQPFNNGTHL-UHFFFAOYSA-N	6069.77

1-yl)pentoxy]-4-oxobutanoic acid						
Spiro[naphthalene-1(2H),2'-oxirane]-2,3-diol, octahydro-5,6,8a-trimethyl-5-[2-(tetrahydro-3,4-dihydroxy-2,5-dimethoxy-3-furanyl)ethyl]	35.697	472.2847	$C_{22}H_{38}O_8$	O-glycosyl compounds	RLYPFWBODVDUHT-UHFFFAOYSA-N	5788.33
2,3,14-trihydroxy-10,13-dimethyl-17-(2,3,6,7-tetrahydroxy-5,6-dimethylheptan-2-yl)-2,3,4,5,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-6-one	35.905	511.32574	$C_{28}H_{46}O_8$	Hydroxy bile acids, alcohols and derivatives	GGLFMIALTLLMEJ-UHFFFAOYSA-N	8273.33
FUSIDIC ACID	36.240	555.35004	$C_{31}H_{48}O_6$	Steroid esters	IECPWNUMDGFDKC-MZJAQBGESA-N	5023.66
Threonine	37.722	120.10156	$C_4H_9NO_3$	L-alpha-amino acids	AYFVYJQAPQTCCC-GBXIJSLDSA-N	9716.30

Ginkgolide A	38.305	409.14572	$C_{20}H_{24}O_9$	Ginkgolides and bilobalides	FPUXKXIZEIDQKW-VTPWKYHPSA-N	5492.24
Vinpocetine	38.397	351.20541	$C_{22}H_{26}N_2O_2$	Eburnan-type alkaloids	DDNCQMVWWZOMLN-UHFFFAOYSA-N	8012.91
Anemarsaponin C	39.259	925.4765	$C_{45}H_{74}O_{18}$	Steroidal saponins	ROHLIYKWVMBBFX-AMMIEGAUSA-N	4822.70
N-Methyldodecylamine	39.389	200.23688	$C_{13}H_{29}N$	Dialkylamines	OMEMQVZNTDHENJ-UHFFFAOYSA-N	7406.95
2-(2-hydroxybut-3-en-2-yl)-3a,6,6,9a-tetramethyl-2,4,5,5a,7,8,9,9b-octahydro-1H-benzo[e][1]benzofuran-4,5-diol	39.443	356.27731	$C_{20}H_{34}O_4$	Naphthofurans	UNORIIWPFZFSEC-UHFFFAOYSA-N	10039.84
[1-(6-hydroxy-1-methoxy-8-methyl-12-oxo-10H-benzo[b][1,5]benzodioxocin-2-yl)-3-methylbutyl] acetate	41.246	846.36755	$C_{23}H_{26}O_7$	Diarylethers	NUYFKDBCHFKOBT-UHFFFAOYSA-N	5106.42

Atalaphylline	41.263	380.19119	$C_{23}H_{25}NO_4$	Acridones	GLXYKTASIIUSRC-UHFFFAOYSA-N	6555.90
5-chloro-3-[(E)-3,4-dihydroxy-3,5-dimethylhept-1-enyl]-7,8-dihydroxy-7-methyl-8H-isochromen-6-one	41.432	385.14441	$C_{19}H_{25}ClO_6$	Azaphilones	BRELKNNWUMEGDN-VOTSOKGWSA-N	10234.69
3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy-6-[[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-6-methoxy-7-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxychromen-4-one	41.852	917.2923	$C_{40}H_{52}O_{24}$	Flavonoid-7-O-glycosides	TXZUPPVCNIMVHW-AJMZACEDSA-N	7056.08

4-hydroxy-7-methyl-2-[2-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropan-2-yl]-2,3-dihydrofuro[3,2-g]chromen-5-one	42.039	439.1582	$C_{21}H_{26}O_{10}$	Furanochromones	KHWKLNXMSVVKCH-UHFFFAOYSA-N	11626.99
Leu-Gly-Gly	42.260	246.1496	$C_{10}H_{19}N_3O_4$	Peptides	VWHGTYCRDRBSFI-ZETCQYMHSA-N	13188.03
Loggerpeptin A	42.414	1015.51874	$C_{50}H_{72}N_8O_{13}$	Cyclic depsipeptides	UAVAEWGJORGZNS-RRDHTEHZSA-N	6929.67
Maedamide	42.696	963.04486	$C_{51}H_{74}N_6O_{12}$	Depsipeptides	YOPVXOUHYSYHKL-IJRNZAOCSA-N	5476.55
(Z)-N-hexadec-9-enoyl-L-phenylalanine	43.141	402.3024	$C_{25}H_{39}NO_3$	Phenylalanine and derivatives	OIDVFUQQVKYQTG-YLNCNTMDSA-N	5285.25
(4R)-4-((3R,5R,7R,9S,10S,13R,14S,17R)-7-hydroxy-10,13-dimethyl-3-(sulfooxy)hexadecahydro-1H-	43.338	945.5061	$C_{24}H_{40}O_7S$	Monohydroxy bile acids, alcohols and derivatives	WHMOBEGYTDWMIG-BSWAIDMHSA-N	4670.78

cyclopenta[a]phenanthren-17-yl)pentanoic acid						
Amphotericin X/B2	43.438	938.51404	$C_{48}H_{75}NO_{17}$	Aminoglycosides	IJLVDQCUUOUTLI-GSEDQWGASA-N	6545.79
Moroidin	43.495	494.25781	$C_{47}H_{66}N_{14}O_{10}$	Cyclic peptides	UCSHFBQCLZMAJY-QFMFBHDYSA-N	14127.74
2-(4-Methyl-3-cyclohexen-1-yl)-2-propanyl 6-O-(6-deoxy-alpha-L-mannopyranosyl)-beta-D-glucopyranoside	43.584	485.23413	$C_{22}H_{38}O_{10}$	O-glycosyl compounds	JIDXOGPQCVBGSC-BXUICYMCSA-N	6434.50
(E)-3-(4-methoxyphenyl)-1-[2,4,6-trimethoxy-3-(3-methylbut-2-enyl)phenyl]prop-2-en-1-one	44.033	419.22745	$C_{24}H_{28}O_5$	3-prenylated chalcones	GGNVSANPVOEGII-GXDHUFHOSA-N	17174.55
(9Z,12E)-15,16-dihydroxyoctadeca-9,12-dienoic acid	44.140	313.23572	$C_{18}H_{32}O_4$	Lineolic acids and derivatives	LKLLJYJTYPVCID-JVVXYUKTSA-N	6672.07
[8,8-dimethyl-9-(3-methylbut-2-enoyloxy)-2-	44.233	870.36847	$C_{24}H_{26}O_7$	Angular pyranocoumarins	UHWIZIJICYWABA-UHFFFAOYSA-N	7613.79

oxo-9,10-dihydropyrano[2,3-f]chromen-10-yl] 3-methylbut-2-enoate						
2-[1-hydroxy-1-(4-methoxyphenyl)propan-2-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol	44.262	345.15396	$C_{16}H_{24}O_8$	O-glycosyl compounds	JYWSARFDLXXOHT-UHFFFAOYSA-N	13501.34
(3R,5R,7R,8R,9S,10S,12S,13R,14S,17R)-17-((2R)-6,7-dihydroxy-6-methylheptan-2-yl)-10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthrene-3,7,12-triol	44.654	927.68823	$C_{27}H_{48}O_5$	Pentahydroxy bile acids, alcohols and derivatives	XZDHXPDYLPEFQI-HANXKNDOSA-N	5629.40
(4aS)-6,7-dihydroxy-1,1,4a-trimethyl-3,4,10,10a-tetrahydro-2H-phenanthren-9-one	44.839	292.18991	$C_{17}H_{22}O_3$	Diterpenoids	JMBKXUYCBVKSSY-OMOCHNIRSA-N	11843.90

3-[(2S,3R,4S,5R,6R)-3-[(2S,3R,4R,5S,6S)-3,5-dihydroxy-6-methyl-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-4,5-dihydroxy-6-[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-2-(3,4-dihydroxyphenyl)-5,7-dihydroxychromen-4-one	44.959	957.11743	$C_{39}H_{50}O_{25}$	Flavonoid-3-O-glycosides	CBSLALAKOKYDBZ-SFGFBRIDSA-N	8129.93
Betaine	44.967	118.08655	$C_5H_{11}NO_2$	Alpha amino acids	KWIUHFFTVRNATP-UHFFFAOYSA-N	2215418.88
3-hydroxy-C4-homoserine lactone	45.599	188.09177	$C_8H_{13}NO_4$	N-acyl-alpha amino acids and derivatives	FIXDIFPJOFIIEC-UHFFFAOYSA-N	113605.18
7-Hydroxy-4-methylcoumarin	45.719	177.16403	$C_{10}H_8O_3$	7-hydroxycoumarins	HSHNITRMYYLLCV-UHFFFAOYSA-N	11219.89

OMEGA-HYDROXYDODECANOATE	45.953	181.15886	$C_{12}H_{24}O_3$	Medium-chain hydroxy acids and derivatives	ZDHCZVWCTKTBRY-UHFFFAOYSA-N	12351.50
Geranic acid	46.389	169.12213	$C_{10}H_{16}O_2$	Acyclic monoterpenoids	ZHYZQXUYZJNEHD-VQHVLOKHSA-N	8940.16
2-Hydroxycinnamic acid, predominantly trans	46.531	165.16362	$C_9H_8O_3$	Hydroxycinnamic acids	PMOWTIHVNWZYFI-AATRIKPKSA-N	11248.31
TYRAMINE	46.583	138.08577	$C_8H_{11}NO$	Phenethylamines	DZGWFCGJZKJUFP-UHFFFAOYSA-N	8217.68
Quinoclamine	46.630	210.01254	$C_{10}H_6ClNO_2$	Naphthoquinones	OBLNWSCLAYSJJR-UHFFFAOYSA-N	8294.31
N-Butylbenzenesulfonamide	46.693	214.08813	$C_{10}H_{15}NO_2S$	Benzenesulfonamides	IPRJXAGUEGOFGG-UHFFFAOYSA-N	7591.48
Lupinine	46.738	170.153	$C_{10}H_{19}NO$	Lupinine-type alkaloids	HDVAWXXJVMJBAR-VHSXEESVSA-N	8488.00
TRYPTANTHRINE	47.016	249.05952	$C_{15}H_8N_2O_2$	Indoloquinazolines	VQQVWGVXDIPORV-UHFFFAOYSA-N	7964.69
L-beta-Homolysine	47.035	161.13213	$C_7H_{16}N_2O_2$	Beta amino acids and derivatives	PJDINCOFOROBQW-LURJTMIESA-N	15102.42
PYROCATECHUIC ACID	47.279	192.98097	$C_7H_6O_4$	Salicylic acids	GLDQAMYCGOIJDV-UHFFFAOYSA-N	9977.91

4-(1H-indol-3-yl)butan-2-one	47.329	188.10661	$C_{12}H_{13}NO$	3-alkylindoles	ZJCUUXGLZWBCIL-UHFFFAOYSA-N	6703.02
NEROL	47.348	177.12274	$C_{10}H_{18}O$	Acyclic monoterpenoids	GLZPCOQZEFWAFX-YFHOEESVSA-N	13807.92
Dimethenamid-ESA	47.637	322.07486	$C_{12}H_{19}NO_5S_2$	Heteroaromatic compounds	YMYKMSAZEZQEER-UHFFFAOYSA-N	7424.77
pentadecanoic acid	47.665	243.22794	$C_{15}H_{30}O_2$	Long-chain fatty acids	WQEPLUUGTLDZJY-UHFFFAOYSA-N	5061.78
Indole-3-acetaldehyde	47.676	160.07899	$C_{10}H_9NO$	3-alkylindoles	WHOOUMGHGSPMGR-UHFFFAOYSA-N	10616.96
4-oxododecanedioic acid	47.716	262.16617	$C_{12}H_{20}O_5$	Medium-chain keto acids and derivatives	HHXMOTDTSDYYEI-UHFFFAOYSA-N	5493.20
A alpha C	47.862	184.08415	$C_{11}H_9N_3$	Alpha carbolines	FJTNLJLPLJDTRM-UHFFFAOYSA-N	11338.45
Stearoyl-L-Carnitine	47.874	428.37347	$C_{25}H_{49}NO_4$	Acyl carnitines	FNPHNLNTJNMAEE-UHFFFAOYSA-N	7947.41
Dicyclohexylamine	47.885	182.1909	$C_{12}H_{23}N$	Cyclohexylamines	XBPCUCUWBYBCDP-UHFFFAOYSA-N	9303.55
ISO E Super	47.886	235.20526	$C_{16}H_{26}O$	Ketones	FVUGZKDGWGKCFE-UHFFFAOYSA-N	11635.49

L-Tyrosine	47.983	182.18971	$C_9H_{11}NO_3$	Tyrosine and derivatives	OUYCCCASQSFEME-QMMMGPOBSA-N	9770.23
hexadecyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate	48.093	419.30884	$C_{26}H_{42}O_4$	Coumaric acids and derivatives	ZISDTRGMDDVTKY-CZIZESTLSA-N	9344.03
3-Phenoxybenzylalcohol	48.156	201.09489	$C_{13}H_{12}O_2$	Diphenylethers	KGANAERDZBAECK-UHFFFAOYSA-N	15093.22
Phenolsulfonphthalein	48.239	355.06668	$C_{19}H_{14}O_5S$	Benzofuranones	BELBBZDIHDAJOR-UHFFFAOYSA-N	9954.42
6-Ethoxy-3(4'-hydroxyphenyl)-4-methylcoumarin	48.256	297.11429	$C_{18}H_{16}O_4$	Isoflav-3-enones	MOBDZHABRVPJCH-UHFFFAOYSA-N	10281.14
Myristoyl Ethanolamide	48.371	272.26486	$C_{16}H_{33}NO_2$	N-acylethanolamines	JHIXEZNTXMFXEK-UHFFFAOYSA-N	11268.34
ISOPALMITIC ACID	48.471	257.24677	$C_{16}H_{32}O_2$	Long-chain fatty acids	ZONJATNKKGGVSU-UHFFFAOYSA-N	10153.41
2-Aminoisobutyric acid	48.545	104.0793	$C_4H_9NO_2$	Alpha amino acids	FUOOLUPWFVMBKG-UHFFFAOYSA-N	12923.60

Pargyline	48.586	160.11159	$C_{11}H_{13}N$	Phenylmethylamines	DPWPWRLQFGFJFI-UHFFFAOYSA-N	12094.66
LUMICHROME	48.589	243.08884	$C_{12}H_{10}N_4O_2$	Flavins	ZJTJUVIJVLLGSP-UHFFFAOYSA-N	5776.42
Pirimicarb-desamido	49.111	168.11288	$C_8H_{13}N_3O$	Dialkylarylamines	MUEHLDAHWSCFAG-UHFFFAOYSA-N	16627.52
Methyprylon	49.161	184.13329	$C_{10}H_{17}NO_2$	Piperidinediones	SIDLZWOQUZRBRU-UHFFFAOYSA-N	22756.59
L-Citrulline	49.162	159.07632	$C_6H_{13}N_3O_3$	L-alpha-amino acids	RHGKLRLOHDJJDR-BYPYZUCNSA-N	457584.56
Glycyl-L-proline	49.162	173.09218	$C_7H_{12}N_2O_3$	Dipeptides	KZNQNBZMBZJQJO-YFKPBYRVSA-N	45456.52
L-Arginine	49.162	176.11871	$C_6H_{14}N_4O_2$	L-alpha-amino acids	ODKSFYDXXFIFQN-BYPYZUCNSA-N	30983.01
Isovaleric acid	49.163	103.07582	$C_5H_{10}O_2$	Methyl-branched fatty acids	GWYFCOCPABKNJV-UHFFFAOYSA-N	264643.91
HISTIDINOL	49.163	124.08705	$C_6H_{11}N_3O$	Aralkylamines	ZQISRDCJNBUVMM-YFKPBYRVSA-N	14641654.53
Thymine	49.163	127.08672	$C_5H_6N_2O_2$	Hydroxypyrimidines	RWQNBRDOKXIBIV-UHFFFAOYSA-N	365159.11

Isophorone	49.163	139.11166	$C_9H_{14}O$	Cyclohexenones	HJOVHMDZYOCNQW-UHFFFAOYSA-N	53011.75
Nordeprenyl	49.163	174.1283	$C_{12}H_{15}N$	Amphetamines and derivatives	UUFAJPMQSFXDFR-UHFFFAOYSA-N	18730.09
Glycocyamine	49.165	118.07798	$C_3H_7N_3O_2$	Alpha amino acids and derivatives	BPMFZUMJYQTVII-UHFFFAOYSA-N	194932.14
N-(n-octyl)-2-pyrrolidinone	49.165	198.18542	$C_{12}H_{23}NO$	N-alkylpyrrolidines	WPPOGHDFAVQKLN-UHFFFAOYSA-N	16082.37
N-(3,4-dimethoxyphenethyl)-1H-indole-3-carboxamide	49.165	325.16013	$C_{19}H_{20}N_2O_3$	Dimethoxybenzenes	ODKYLYWWBHXMRV-UHFFFAOYSA-N	11969.00
(1S,3R,4S,5R)-1,3,4,5-tetrahydroxycyclohexane-1-carboxylic acid	49.166	193.07057	$C_7H_{12}O_6$	Quinic acids and derivatives	AAWZDTNXLSGCEK-WYWMIBKRSA-N	7333.44
CP-457920	49.167	324.13766	$C_{18}H_{17}N_3O_3$	Naphthyridines	DGFVZQGXKQCQGK-UHFFFAOYSA-N	11693.78
BUTANAL	49.168	73.06557	C_4H_8O	Alpha-hydrogen aldehydes	ZTQSAGDEMFDKMZ-UHFFFAOYSA-N	3443483.80
Piperazine	49.168	87.08109	$C_4H_{10}N_2$	Piperazines	GLUUGHFHXGJENI-UHFFFAOYSA-N	710179.88

Isobutyric acid	49.168	89.06031	$C_4H_8O_2$	Carboxylic acids	KQNPFQTWMSNSAP-UHFFFAOYSA-N	530537.78
trans-2-Hexenal	49.168	99.08096	$C_6H_{10}O$	Medium-chain aldehydes	MBDOYVRWFFCFHM-SNAWJCMRSA-N	4987298.88
L-2,3-DIAMINOPROPIONIC ACID	49.168	105.07031	$C_3H_8N_2O_2$	L-alpha-amino acids	PECYZEOJVXMISF-UHFFFAOYSA-N	2711496.00
Phenylhydrazine	49.168	109.10168	$C_6H_8N_2$	Phenylhydrazines	HKOOXMFOFWEVGF-UHFFFAOYSA-N	274645.20
Pyrocatechol	49.168	111.04439	$C_6H_6O_2$	Catechols	YCIMNLLNPGFGHC-UHFFFAOYSA-N	338701.01
Histamine	49.168	112.11243	$C_5H_9N_3$	2-arylethylamines	NTYJJOPFIAHURM-UHFFFAOYSA-N	215323.33
CREATININE	49.168	114.07365	$C_4H_7N_3O$	Alpha amino acids and derivatives	DDRJAANPRJIHGJ-UHFFFAOYSA-N	931742.20
4-Methylvaleric acid	49.168	117.09129	$C_6H_{12}O_2$	Methyl-branched fatty acids	FGKJLKRYENPLQH-UHFFFAOYSA-N	360699.16
beta-N-Methylaminoalanine	49.168	119.08576	$C_4H_{10}N_2O_2$	Alpha amino acids	UJVHVMNGOZXSOZ-VKHMYHEASA-N	1118196.94

alpha-Methyl-DL-serine	49.168	120.09359	$C_4H_9NO_3$	Alpha amino acids	CDUUKBXTEOFITR-SCSAIBSYSA-N	5843672.20
Benzamidine hydrochloride hydrate	49.168	121.10162	$C_7H_8N_2$	Benzene and substituted derivatives	PXXJHWLDUBFPOL-UHFFFAOYSA-N	4388108.78
2-Aminoethylphosphonic acid	49.168	126.05511	$C_2H_8NO_3P$	Organic phosphonic acids	QQVDJLLNRSOCEL-UHFFFAOYSA-N	68930.26
Agmatine sulfate salt	49.168	131.0881	$C_5H_{14}N_4$	Guanidines	QYPPJABKJHAVHS-UHFFFAOYSA-N	109526.24
Carveol	49.168	135.11694	$C_{10}H_{16}O$	Menthane monoterpenoids	BAVONGHXFVOKBV-UHFFFAOYSA-N	194496.80
Benzothiazole	49.168	136.02155	C_7H_5NS	Benzothiazoles	IOJUPLGTWVMSFF-UHFFFAOYSA-N	149011.92
d-LIMONENE	49.168	137.13254	$C_{10}H_{16}$	Menthane monoterpenoids	XMGQYMWWDOXHJM-JTQLQIEISA-N	728178.80
S-Citramalic acid	49.168	149.04482	$C_5H_8O_5$	Hydroxy fatty acids	XFTRTWQBIOMVPK-YFKPBYRVSA-N	568791.20
10-HYDROXYDECANOATE	49.168	153.12733	$C_{10}H_{20}O_3$	Medium-chain hydroxy acids and derivatives	YJCJVMMDTBEITC-UHFFFAOYSA-N	1296844.29
Uridine	49.168	171.14928	$C_9H_{12}N_2O_6$	Pyrimidine nucleosides	DRTQHJPVMGBUCF-XVFCMESISA-N	113667.03

Coniferylaldehyde	49.168	179.07002	$C_{10}H_{10}O_3$	Methoxyphenols	DKZBBWMURDFHNE-NSCUHMNNSA-N	161936.62
Xanthoxylin	49.168	197.08015	$C_{10}H_{12}O_4$	Alkyl-phenylketones	FBUBVLUPUDBFME-UHFFFAOYSA-N	65378.69
Norharman	49.168	207.03165	$C_{11}H_8N_2$	Beta carbolines	AIFRHYZBTHREPW-UHFFFAOYSA-N	180237.82
Eugenitin	49.168	221.08423	$C_{12}H_{12}O_4$	Chromones	RGTSAUBIQAKKLC-UHFFFAOYSA-N	867002.26
(2R)-8-ethyl-7-hydroxy-5-methoxy-2-methyl-2,3-dihydrochromen-4-one	49.168	237.11542	$C_{13}H_{16}O_4$	Chromones	BPIMOIWHAHUBPJ-SSDOTTSWSA-N	57276.92
5,6-Dihydrouracil	49.169	115.112	$C_4H_6N_2O_2$	Pyrimidones	OIVLITBTBDPEFK-UHFFFAOYSA-N	149085.37
1-Methylhistamine dihydrochloride	49.169	126.12764	$C_6H_{11}N_3$	2-arylethylamines	FHQDWPCFSJMNCT-UHFFFAOYSA-N	100391.59
Cuminyl alcohol	49.169	133.10127	$C_{10}H_{14}O$	Aromatic monoterpenoids	OIGWAXDAPKFNCQ-UHFFFAOYSA-N	67392.43
Tartaric acid	49.169	151.02412	$C_4H_6O_6$	Sugar acids and derivatives	FEWJPZIEWOKRBE-UHFFFAOYSA-N	73419.62

3-Methyladipic acid	49.169	161.08215	$C_7H_{12}O_4$	Medium-chain fatty acids	SYEOWUNSTUDKGM-UHFFFAOYSA-N	416905.57
Valerophenone	49.169	163.11177	$C_{11}H_{14}O$	Alkyl-phenylketones	XKGLSKVNOSHTAD-UHFFFAOYSA-N	103681.64
Hinokitiol	49.169	165.09164	$C_{10}H_{12}O_2$	Tropolones	FUWUEFKEXZQKKA-UHFFFAOYSA-N	37809.60
1-methylxanthine	49.169	167.05547	$C_6H_6N_4O_2$	Xanthines	MVOYJPOZRLFTCP-UHFFFAOYSA-N	321734.07
D-GLUCURONOLACTONE	49.169	177.03984	$C_6H_{10}O_7$	Glucuronic acid derivatives	AEMOLEFTQBMNLQ-UHFFFAOYSA-N	356403.19
Benzophenone	49.169	183.08121	$C_{13}H_{10}O$	Benzophenones	RWCCWEUUXYIKHB-UHFFFAOYSA-N	85513.79
5-Methoxytryptamine	49.169	190.99973	$C_{11}H_{14}N_2O$	Tryptamines and derivatives	JTEJPPKMYBDEMY-UHFFFAOYSA-N	24076.47
2(1H)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-6-hydroxy-3,8-dimethyl-5-(1-methylethyl)-, (4aR,5S,6S,8R,8aS)	49.169	219.17412	$C_{15}H_{24}O_2$	Sesquiterpenoids	KLDSZMWMGCWFKH-GIEZYDSUSA-N	1049940.44

2,6-Di-tert-butyl-1,4-benzoquinone	49.169	221.15515	$C_{14}H_{20}O_2$	Monocyclic monoterpenoids	RDQSIADLBQFVMY-UHFFFAOYSA-N	116024.07
2-[[(Guanidino)(imino)methyl]sulfanyl]ethanesulfonic Acid	49.169	227.022	$C_4H_{10}N_4O_3S_2$	Organosulfonic acids	MFFQNMFIVBUMBX-UHFFFAOYSA-N	434420.44
Aspergillusenes A	49.169	235.1705	$C_{15}H_{22}O_2$	Sesquiterpenoids	NWPUHDAIOGMKFI-WUXMJOGZSA-N	95283.34
heptadecanoic acid	49.169	271.26288	$C_{17}H_{34}O_2$	Long-chain fatty acids	KEMQGTRYUADPNZ-UHFFFAOYSA-N	95551.06
Crystamidine	49.169	278.09659	$C_{18}H_{15}NO_4$	Erythrinanes	NZMLLYZLUYBOGO-UHFFFAOYSA-N	80592.60
3-[(E)-2-(3-hydroxyphenyl)ethenyl]-5-methoxyphenol	49.169	281.05121	$C_{15}H_{14}O_3$	Stilbenes	VANIIUGEHGLNHB-AATRIKPKSA-N	297094.41
2',4',6'-Trihydroxydihydrochalcone	49.169	297.08218	$C_{15}H_{14}O_4$	2'-Hydroxy-dihydrochalcones	QWQGMMRHTWIOGH-UHFFFAOYSA-N	1458372.24
Uric acid	49.171	169.03487	$C_5H_4N_4O_3$	Xanthines	LEHOTFFKMJEONL-UHFFFAOYSA-N	43569.15

SyringicAcid	49.171	199.18147	$C_9H_{10}O_5$	Gallic acid and derivatives	JMSVCTWVEWCHDZ-UHFFFAOYSA-N	42748.88
Alanylleucine (isomer of 675)	49.171	203.14325	$C_9H_{18}N_2O_3$	Peptides	RDIKFPRVLJLMER-UHFFFAOYSA-N	25503.02
(-)-alpha-Copaene	49.171	205.15904	$C_{15}H_{24}$	Sesquiterpenoids	VLXDPFLIRFYIME-ZPWMNFGTSA-N	110528.60
(4S,5Z,6S)-4-(2-methoxy-2-oxoethyl)-5-[2-[(E)-3-phenylprop-2-enoyl]oxyethylidene]-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4H-pyran-3-carboxylic acid	49.171	225.0424	$C_{10}H_{18}O_4$	Oxolanes	IVOODSRSVJPWLY-UHFFFAOYSA-N	1496225.76
Parecoxib	49.171	371.10315	$C_{19}H_{18}N_2O_4S$	Benzenesulfonamides	TZRHLKRLEZJVIJ-UHFFFAOYSA-N	17338.80
Ephedrine	49.172	166.12242	$C_{10}H_{15}NO$	Phenylpropanes	KWGRBVOPPLSCSI-WPRPVWTQSA-N	45758.42

Phenyltetrazole	49.173	147.06606	$C_7H_6N_4$	Phenyltetrazoles and derivatives	MARUHZGHZWCEQU-UHFFFAOYSA-N	39219.30
PYRIDOXINE	49.191	187.10808	$C_8H_{11}NO_3$	Pyridoxines	LXNHXLLTXMVWPM-UHFFFAOYSA-N	12794.62
8-hydroxy-6,7-dimethoxy-2H-chromen-2-one	49.392	223.06326	$C_{11}H_{10}O_5$	Hydroxycoumarins	QNFBKOHHLAWWTC-UHFFFAOYSA-N	1904153.43
OCP_239.0946_17.0	49.392	239.09462	$C_{12}H_{15}ClN_2O$	Phenylpiperazines	LBSHKCUTMCYUOW-UHFFFAOYSA-N	399589.44
Phenethylacetate	49.440	165.09097	$C_{10}H_{12}O_2$	Benzene and substituted derivatives	MDHYEMXUFSJLGV-UHFFFAOYSA-N	15008.76
(4S,5Z,6S)-4-(2-methoxy-2-oxoethyl)-5-[2-[(E)-3-phenylprop-2-enoyl]oxyethylidene]-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-	49.452	235.16945	$C_{15}H_{22}O_2$	Eremophilane, 8,9-secoeremophilane and furoeremophilane sesquiterpenoids	FMWJHXDPCQWVEJ-JVLSTEMRSA-N	34965.87

yl]oxy-4H-pyran-3-carboxylic acid						
Tanshinone I	49.521	299.0596	$C_{18}H_{12}O_3$	Tanshinones, isotanshinones, and derivatives	AIGAZQPHXLWMOJ-UHFFFAOYSA-N	422626.60

RT, retention time; InChIKey, international chemical identifier key.

Table SIV. Representative protein-coding genes significantly affected by Thai traditional formulary medicine in 4T1 cells.

Genes	2-Fold change	*P*-value
Acta1	2.99	1.21×10^{-10}
Tnnc2	2.63	1.48×10^{-5}
0610039K10Rik	2.46	2.89×10^{-5}
Flacc1	2.41	7.80×10^{-5}
Arl5c	2.41	8.12×10^{-5}
Slc5a8	2.05	2.31×10^{-6}
Krt20	2.01	4.55×10^{-6}
BC147527	1.91	5.60×10^{-5}
Raet1e	1.43	3.07×10^{-6}
Snord72	1.36	2.97×10^{-5}
Acat3	1.22	1.51×10^{-4}
Otop1	1.08	8.58×10^{-9}
Arhgap9	1.08	9.44×10^{-6}
Eef1a2	1.01	1.10×10^{-4}
Hmgb1-ps7	0.98	1.76×10^{-4}
Ndufb4c	0.97	1.63×10^{-6}
Ccl20	0.09	1.88×10^{-7}
Ccdc39	-0.05	1.04×10^{-4}
Rbm6-ps1	-1.24	3.60×10^{-5}
Grin3b	-1.41	8.19×10^{-5}
SNORA21B	-1.57	3.78×10^{-5}
Cybb	-2.15	6.67×10^{-5}
B430219N15Rik	-2.40	1.48×10^{-4}
C1ql4	-2.43	7.71×10^{-5}
Bach2os	-2.43	1.55×10^{-4}

Table SV. Pathway categorization based on KEGG pathway enrichment analysis.

Pathway ID	Pathway	Level1	Level2	DEGs with pathway annotation	P-value	Gene list
ko04810	Regulation of actin cytoskeleton	Cellular Processes	Cell motility	1(7.69%)	$4.37x10^{-2}$	*Myh4*
ko00071	Fatty acid degradation	Metabolism	Lipid metabolism	1(7.69%)	$2.74x10^{-3}$	*Acat3*
ko00330	Arginine and proline metabolism	Metabolism	Amino acid metabolism	1(7.69%)	$2.56x10^{-3}$	*Ckm*
ko05134	Legionellosis	Human Diseases	Infectious disease: bacterial	1(7.69%)	$3.03x10^{-3}$	*Eef1a2*
ko04650	Natural killer cell mediated cytotoxicity	Organismal Systems	Immune system	1(7.69%)	$1.08x10^{-2}$	*Raet1e*
ko04270	Vascular smooth muscle contraction	Organismal Systems	Circulatory system	1(7.69%)	$1.78x10^{-2}$	*Myh4*
ko05010	Alzheimer disease	Human Diseases	Neurodegenerative disease	1(7.69%)	$1.00x10^{-1}$	*Cybb*
ko05030	Cocaine addiction	Human Diseases	Substance dependence	1(7.69%)	$2.12x10^{-3}$	*Grin3b*

Pathway ID	Pathway	Level1	Level2	DEGs with pathway annotation	P-value	Gene list
ko01200	Carbon metabolism	Metabolism	Global and overview maps	1(7.69%)	$1.28x10^{-2}$	*Acat3*
ko04668	TNF signaling pathway	Environmental Information Processing	Signal transduction	1(7.69%)	$1.24x10^{-2}$	*Ccl20*
ko01100	Metabolic pathways	Metabolism	Global and overview maps	2(15.38%)	$4.11x10^{-1}$	*Ckm, Acat3*
ko00900	Terpenoid backbone biosynthesis	Metabolism	Metabolism of terpenoids and polyketides	1(7.69%)	$6.17x10^{-4}$	*Acat3*
ko05034	Alcoholism	Human Diseases	Substance dependence	1(7.69%)	$3.26x10^{-4}$	*Grin3b*
ko05130	Pathogenic Escherichia coli infection	Human Diseases	Infectious disease: bacterial	1(7.69%)	$3.52x10^{-2}$	*Myh4*
ko00650	Butanoate metabolism	Metabolism	Carbohydrate metabolism	1(7.69%)	$6.64x10^{-4}$	*Acat3*
ko00280	Valine, leucine and isoleucine degradation	Metabolism	Amino acid metabolism	1(7.69%)	$2.84x10^{-3}$	*Acat3*

Pathway ID	Pathway	Level1	Level2	DEGs with pathway annotation	P-value	Gene list
ko00310	Lysine degradation	Metabolism	Amino acid metabolism	1(7.69%)	$3.44x10^{-3}$	*Acat3*
ko00720	Carbon fixation pathways in prokaryotes	Metabolism	Energy metabolism	1(7.69%)	$1.86x10^{-4}$	*Acat3*
ko00362	Benzoate degradation	Metabolism	Xenobiotics biodegradation and metabolism	1(7.69%)	$1.07x10^{-5}$	*Acat3*
ko05150	Staphylococcus aureus infection	Human Diseases	Infectious disease: bacterial	1(7.69%)	$1.15x10^{-2}$	*Krt20*
ko04933	AGE-RAGE signaling pathway in diabetic complications	Human Diseases	Endocrine and metabolic disease	1(7.69%)	$9.37x10^{-3}$	*Cybb*
ko04024	cAMP signaling pathway	Environmental Information Processing	Signal transduction	1(7.69%)	$3.67x10^{-3}$	*Grin3b*
ko03013	RNA transport	Genetic Information Processing	Translation	1(7.69%)	$3.61x10^{-2}$	*Eef1a2*

Pathway ID	Pathway	Level1	Level2	DEGs with pathway annotation	P-value	Gene list
ko05418	Fluid shear stress and atherosclerosis	Human Diseases	Cardiovascular disease	1(7.69%)	2.21×10^{-2}	*Cybb*
ko00380	Tryptophan metabolism	Metabolism	Amino acid metabolism	1(7.69%)	2.37×10^{-3}	*Acat3*
ko05168	Herpes simplex virus 1 infection	Human Diseases	Infectious disease: viral	2(15.38%)	7.72×10^{-2}	*Gm4631, Gm6710*
ko05031	Amphetamine addiction	Human Diseases	Substance dependence	1(7.69%)	3.88×10^{-3}	*Grin3b*
ko04657	IL-17 signaling pathway	Organismal Systems	Immune system	1(7.69%)	6.70×10^{-3}	*Ccl20*
ko05140	Leishmaniasis	Human Diseases	Infectious disease: parasitic	1(7.69%)	4.11×10^{-3}	*Eef1a2*
ko04975	Fat digestion and absorption	Organismal Systems	Digestive system	1(7.69%)	2.03×10^{-3}	*Acat3*
ko05131	Shigellosis	Human Diseases	Infectious disease: bacterial	1(7.69%)	5.21×10^{-2}	*Flacc1*
ko05033	Nicotine addiction	Human Diseases	Substance dependence	1(7.69%)	1.43×10^{-3}	*Grin3b*

Pathway ID	Pathway	Level1	Level2	DEGs with pathway annotation	P-value	Gene list
ko01120	Microbial metabolism in diverse environments	Metabolism	Global and overview maps	1(7.69%)	$2.51x10^{-2}$	*Acat3*
ko04060	Cytokine-cytokine receptor interaction	Environmental Information Processing	Signaling molecules and interaction	1(7.69%)	$6.48x10^{-2}$	*Ccl20*
ko04530	Tight junction	Cellular Processes	Cellular community - eukaryotes	1(7.69%)	$2.51x10^{-2}$	*Myh4*
ko04062	Chemokine signaling pathway	Organismal Systems	Immune system	1(7.69%)	$2.97x10^{-2}$	*Ccl20*
ko05323	Rheumatoid arthritis	Human Diseases	Immune disease	1(7.69%)	$8.54x10^{-3}$	*Ccl20*
ko02020	Two-component system	Environmental Information Processing	Signal transduction	1(7.69%)	$2.71x10^{-4}$	*Acat3*
ko00620	Pyruvate metabolism	Metabolism	Carbohydrate metabolism	1(7.69%)	$1.95x10^{-3}$	*Acat3*
ko04380	Osteoclast differentiation	Organismal Systems	Development and regeneration	1(7.69%)	$1.54x10^{-2}$	*Cybb*

Pathway ID	Pathway	Level1	Level2	DEGs with pathway annotation	P-value	Gene list
ko04020	Calcium signaling pathway	Environmental Information Processing	Signal transduction	1(7.69%)	4.33×10^{-2}	*Tnnc2*
ko04061	Viral protein interaction with cytokine and cytokine receptor	Environmental Information Processing	Signaling molecules and interaction	1(7.69%)	7.91×10^{-3}	*Ccl20*
ko04080	Neuroactive ligand-receptor interaction	Environmental Information Processing	Signaling molecules and interaction	1(7.69%)	8.76×10^{-2}	*Grin3b*
ko00072	Synthesis and degradation of ketone bodies	Metabolism	Lipid metabolism	1(7.69%)	1.17×10^{-4}	*Acat3*
ko05022	Pathways of neurodegeneration - multiple diseases	Human Diseases	Neurodegenerative disease	1(7.69%)	1.43×10^{-1}	*Cybb*
ko04724	Glutamatergic synapse	Organismal Systems	Nervous system	1(7.69%)	1.17×10^{-2}	*Grin3b*
ko05020	Prion disease	Human Diseases	Neurodegenerative disease	1(7.69%)	5.96×10^{-2}	*Grin3b*

Pathway ID	Pathway	Level1	Level2	DEGs with pathway annotation	P-value	Gene list
ko01212	Fatty acid metabolism	Metabolism	Global and overview maps	1(7.69%)	$3.24x10^{-3}$	*Acat3*
ko04915	Estrogen signaling pathway	Organismal Systems	Endocrine system	1(7.69%)	$1.57x10^{-2}$	*Krt20*
ko05017	Spinocerebellar ataxia	Human Diseases	Neurodegenerative disease	1(7.69%)	$1.46x10^{-2}$	*Grin3b*
ko00630	Glyoxylate and dicarboxylate metabolism	Metabolism	Carbohydrate metabolism	1(7.69%)	$9.24x10^{-4}$	*Acat3*
ko00640	Propanoate metabolism	Metabolism	Carbohydrate metabolism	1(7.69%)	$1.04x10^{-3}$	*Acat3*
ko01110	Biosynthesis of secondary metabolites	Metabolism	Global and overview maps	1(7.69%)	$1.43x10^{-1}$	*Acat3*

DEGs, differently expressed genes.