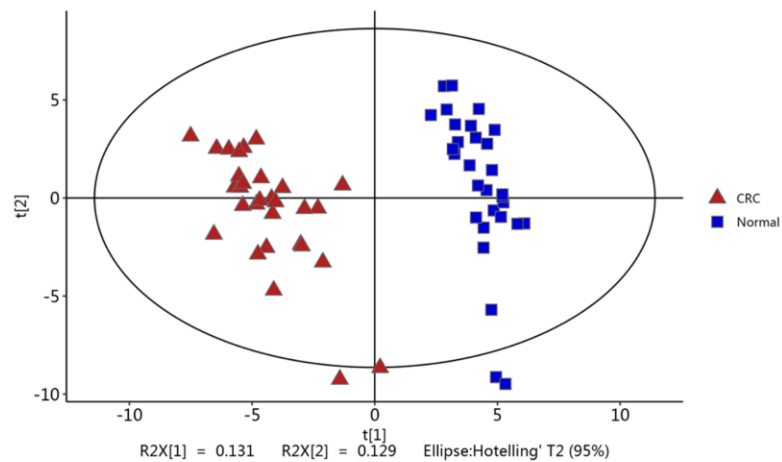
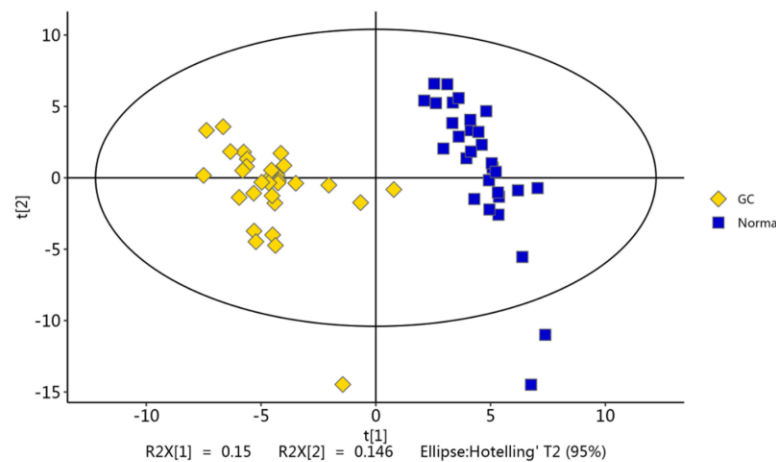


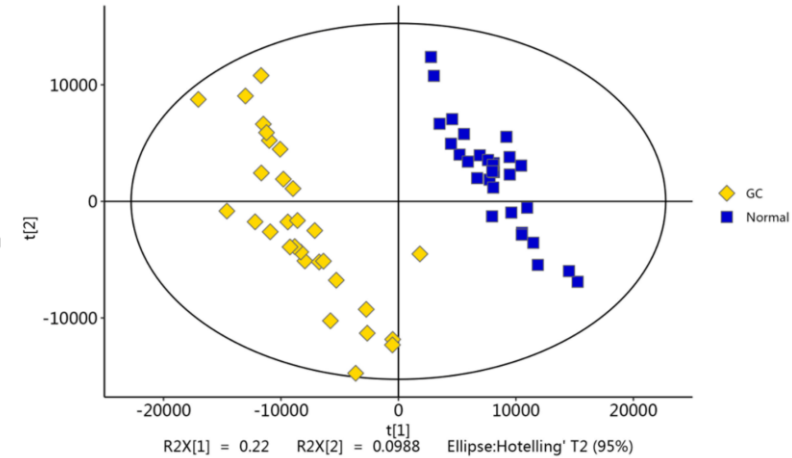
A



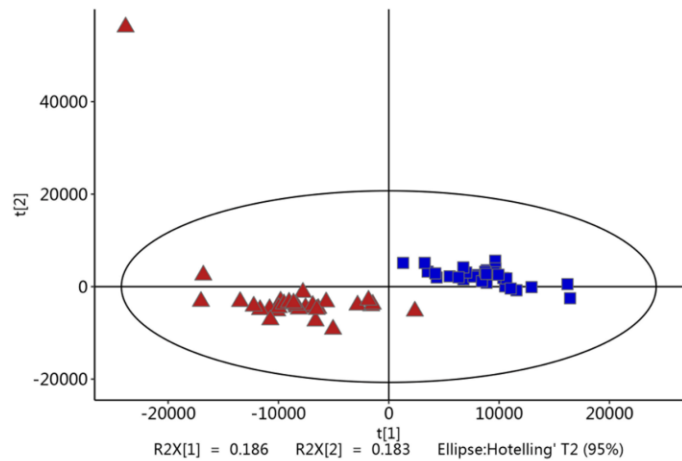
B



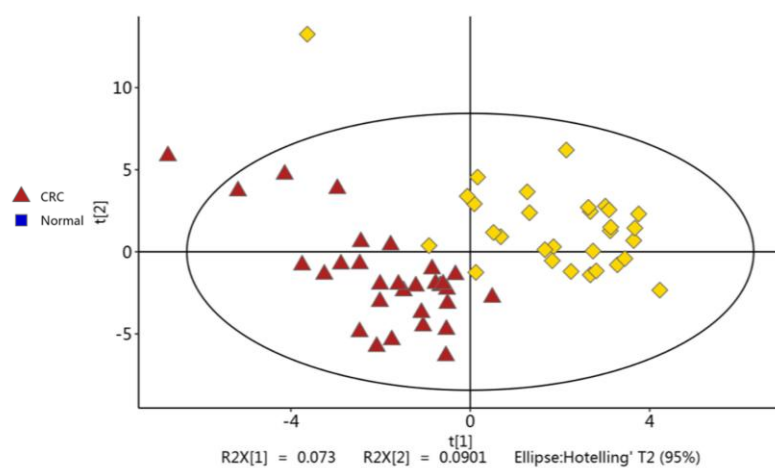
C



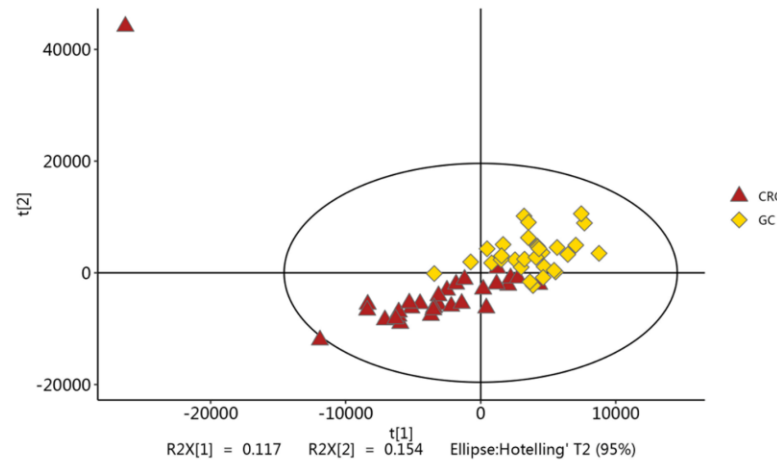
D



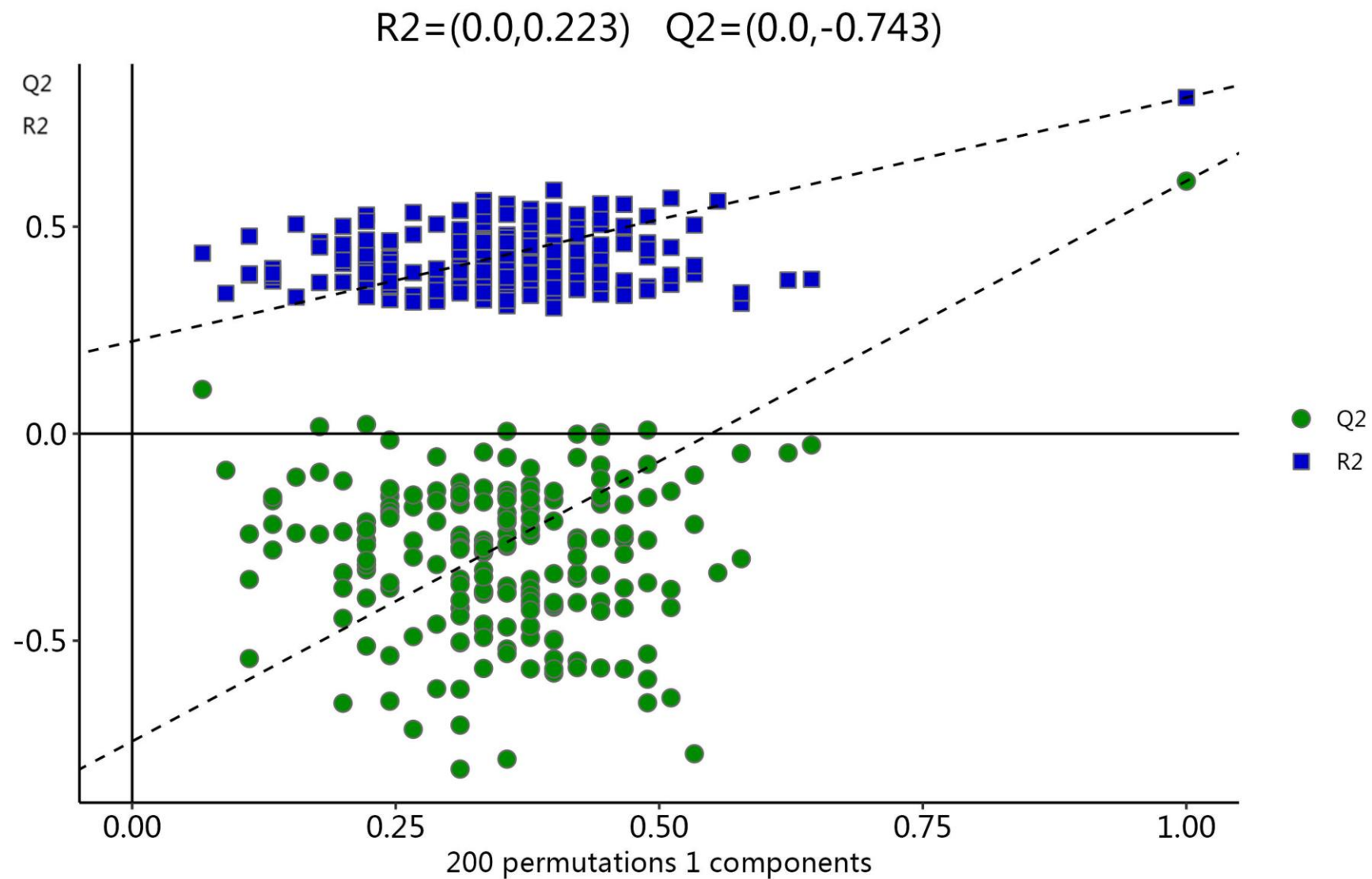
E



F



Supplementary Figure 1



Supplementary Figure 2

Supplementary Table 1

CRC_Normal

Dataclass	Metabolites	VIP	P-value
LC	Propofol glucuronide	42.49817221	8.55861E-10
LC	LysoPC(0:0/18:2(9Z,12Z))	39.47754279	4.36019E-11
LC	Edetic Acid	17.2619243	0.002920995
LC	Floridin	13.59326069	0.005470616
LC	PC(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/P-18:1(11Z))	12.48540157	0.000941439
LC	Carissanol	11.908102	2.5157E-17
LC	LysoPC(20:4(5Z,8Z,11Z,14Z)/0:0)	11.63081531	0.000659239
LC	Cefazolin	11.13027078	0.037648397
LC	Lidocaine	10.25208078	2.4692E-07
LC	L-Acetylcarnitine	9.568914567	1.35872E-06
LC	PC(P-18:1(11Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))	9.539132309	1.2835E-07
LC	Dehydroepiandrosterone sulfate	9.420918289	3.87093E-06
LC	N-(2-Hydroxyethyl)-2-(1-isoquinolinylmethylene)hydrazinecarbothioamide	9.034904108	1.32234E-14
LC	1-O-(2-methoxy-4Z-hexadecenyl)-sn-glycero-3-phosphocholine	8.387712311	8.27263E-11
LC	Isocitric acid	8.268257009	3.77399E-11
LC	1-(O-alpha-D-glucopyranosyl)-29-keto-(1,3R,31R)-dotriacontanetriol	8.137192793	7.66668E-08
LC	Myristyl linoleate	7.293027309	1.53382E-05
LC	2-C-methyl-D-erythritol-4-phosphate	6.608794507	2.82786E-06
LC	2-Methyl-4'-(methylthio)-2-morpholinopropiophenone	6.526906048	2.63902E-16
LC	LysoPC(0:0/18:0)	6.473041889	4.97807E-05
LC	SM(d19:1/17:1)	6.461664278	0.000474572
GC	P-Cresol Glucuronide	6.169756794	3.46361E-09
LC	UTILIN	5.865190773	1.18555E-14
LC	PC(0:0/14:0)	5.650490153	1.21615E-07
LC	19-Epischolaricine	5.489759575	7.3543E-13
LC	SM(d18:0/16:1(9Z))	5.427568515	0.048506935
LC	SM(d18:1/16:1(9Z))	5.424866725	0.00772874
LC	S-Japonin	5.305731909	2.72318E-08
LC	Benzoxazole	5.189941289	0.006969556
GC	Equilenin	5.019844924	5.65742E-12
LC	Chenodeoxycholic acid glycine conjugate	4.914568141	0.00250336
LC	N-Nitrosoanatabine	4.908067503	9.0431E-08
LC	13-Hydroxyoctadecanoylcarnitine	4.692914047	9.00106E-06
LC	4-(2-Aminoethylamino)-3-[bis(carboxymethyl)amino]-3-(carboxymethyl)hexanedioic acid	4.575558576	7.80926E-16
LC	GM4(d18:1/16:0)	4.547326604	0.002240535

LC	PE(20:3(8Z,11Z,14Z)/19:1(9Z))	4.257968073	0.004986593
LC	L-Carnitine	4.196477586	0.019107079
LC	TG(8:0/8:0/a-17:0)[rac]	4.192833218	0.001807578
LC	O-Linoleoylcarnitine	4.158315188	0.000124559
LC	Oxotremorine	4.10126294	3.47602E-10
GC	M-Toluamide	4.07408551	1.09868E-11
LC	Vignatic acid B	4.047582595	8.15219E-09
LC	Pulverulentoside I; (1aS,1bS,2S,5aR,6S,6aS)-6-({3-O-Acetyl-6-deoxy-2-O-[(2E)-3-(4-methoxyphenyl)-2-propenoyl]-?-L-mannopyranosyl}oxy)-1a-(hydroxymethyl)-1a 1b 2 5a 6 6a-hexahydrooxireno[4,5]cycloocta[1,2-c]nran-2-yl 2-D-	3.858844175	4.23574E-07
LC	Disodium ethylenediaminetetraacetate	3.816321676	0.001501447
LC	PE(17:0/22:4(7Z,10Z,13Z,16Z))	3.811016687	0.018020845
LC	Ecabet	3.756021836	1.65235E-08
LC	2,2'-Methylenebis(4-methyl-6-tert-butylphenol)	3.737504178	4.48394E-09
LC	LysoPE(18:1(9Z)/0:0)	3.690409776	0.003272017
LC	6-Butyryl-5-hydroxy-4-phenylseselin	3.628337528	3.44845E-06
LC	(Z)-1-(Methylthio)-5-phenyl-1-penten-3-yne	3.610219464	3.75868E-17
LC	Phyllocoumarin	3.586812347	1.44928E-14
LC	Armillaripin	3.567906255	3.75531E-13
GC	Lactulose	3.495048836	1.17209E-08
GC	3-(Pyrazol-1-yl)-L-Alanine	3.478503833	1.07455E-05
LC	GM4(d18:1/18:0)	3.427226609	0.00077003
LC	Enterodiol sulfate	3.42070736	2.46749E-05
LC	Decanoylcarnitine	3.411000528	0.040108029
LC	21H-Bilene-8,12-dipropanoicacid, 3,18-diethenyl-1,19,22,24-tetrahydro-2,7,13,17-tetramethyl-1,19-dioxo-	3.400435988	3.20379E-10
LC	LysoPC(20:4(8Z,11Z,14Z,17Z)/0:0)	3.39666242	0.014970982
LC	3-(4-Iodophenyl)-2-mercapto-(Z)-2-propenoic acid	3.26460273	0.000643291
LC	PI(O-18:0/18:0)	3.240315512	0.000414215
LC	LysoPC(18:0/0:0)	3.233124088	0.000246821
LC	Fluroxene	3.230422598	6.13729E-08
LC	Allopregnanolone sulfate	3.220783822	0.000694672
LC	Cichorioside K	3.188583861	1.87411E-07
LC	PS(P-20:0/22:2(13Z,16Z))	3.159384796	0.000497199
LC	Isoscoparin 2"-O-glucoside	3.158622876	0.011737836
LC	PC(14:1(9Z)/20:3(8Z,11Z,14Z))	3.158472497	0.000655833
LC	2-beta-d-Ribofuranosyl thiazole-4-carboxamide	3.142837949	0.033532879
GC	2,6-Pyridinedicarboxylic Acid	3.04429804	0.000467607
LC	EUPARIN	3.041424033	8.53003E-07

LC	2-Methoxy-4-(2-(methylamino)propyl)phenyl beta-D-glucopyranosiduronic acid	2.998019222	1.56684E-11
LC	Thiamine	2.986735683	9.89438E-16
GC	Maltotriose	2.967438411	3.93626E-08
LC	LysoPE(P-16:0/0:0)	2.943208684	2.00632E-15
LC	GM4(d18:1/20:0)	2.896561691	1.35716E-05
LC	Sphingosine 1-phosphate	2.872973969	4.17964E-06
LC	PS(P-20:0/0:0)	2.869241249	1.94025E-11
GC	Cis-Aconitic Acid	2.839031115	1.91216E-07
LC	Caffeine	2.836388459	2.98414E-05
LC	LysoPC(O-18:0/0:0)	2.813916526	6.88096E-11
LC	6-Thioxanthilic acid	2.802940246	5.21422E-05
LC	PE(22:4(7Z,10Z,13Z,16Z)/21:0)	2.792774107	0.002827525
LC	LysoPE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	2.739654725	0.002262948
LC	lysine phosphoester	2.738394426	1.10672E-16
LC	alpha-Hydroxyisobutyric acid	2.713289561	4.89805E-08
GC	Mannobiose	2.702951156	4.04999E-06
LC	Plantacyanin	2.692902203	6.32772E-07
LC	dIDP	2.680611052	3.6366E-05
LC	LysoPC(0:0/20:4(5Z,8Z,11Z,14Z))	2.665988563	0.001932634
LC	Vaccenic acid	2.657321417	5.07884E-18
LC	2-Oxoarginine	2.616648409	2.34915E-06
LC	PC(12:0/20:1(11Z))	2.615534205	0.024230165
GC	Lactitol	2.598859082	4.1221E-08
LC	3,7-Dihydroxycholan-24-oic acid	2.596328246	0.002277093
LC	PE-NMe2(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	2.572915343	0.000184811
LC	LysoPE(0:0/18:2(9Z,12Z))	2.55685943	0.041348246
LC	Gravolenic acid	2.535145661	1.25085E-15
LC	Ptilosaponoside B	2.534596132	1.39127E-15
LC	PC(17:2(9Z,12Z)/0:0)	2.530884685	2.01802E-12
LC	Pyridine N-oxide glucuronide	2.525441791	1.41685E-17
LC	APC	2.522022165	1.035E-16
LC	PC(18:0/P-16:0)	2.483996322	0.006576642
LC	Theophylline	2.473532016	3.40937E-05
LC	3-Hydroxy-1,10-bisaboladien-9-one	2.460036938	8.1062E-05
LC	Methyl 3-epi-4,5-didehydrojasmonate	2.459175956	0.000160245
GC	Quinic Acid	2.444090937	0.001652102
LC	Octenoyl-L-carnitine	2.428760739	0.002018958
LC	1-O-Hexadecyl-sn-glycero-3-phosphocholine	2.415245297	3.53666E-12
LC	Hydroxyzine	2.406651062	1.24797E-05

LC	9-tridecynoic acid	2.397123658	1.8413E-06
LC	3-Hydroxylidocaine	2.395202512	6.85042E-10
LC	(-)-1-(Methylthio)propyl 1-propenyl disulfide	2.392819976	0.004134558
LC	DG(18:3(9,11,15)-OH(13)/15:0/0:0)	2.350536602	4.77286E-07
GC	Melezitose	2.33823233	0.004851492
LC	PC(O-16:1(11Z)/0:0)	2.318896321	6.45531E-10
LC	TG(8:0/8:0/a-13:0)[rac]	2.314677188	2.86545E-07
LC	[(2S,4R,5R,6R,14S,16R)-14-Hydroxy-7,11-dimethyl-6-(2-oxopyran-4-yl)-3-oxapentacyclo[8.8.0.0.2.4.0.2.7.0]11,16]octadecan-5-yl acetate	2.298391961	2.36295E-13
LC	Salvianolic acid D	2.296432304	0.042377746
LC	PC(P-18:1(11Z)/18:2(9Z,12Z))	2.29304248	0.033194972
LC	LysoPE(0:0/18:1(11Z))	2.29203755	0.000965336
LC	SM(d16:2(4E,8Z)/TXB2)	2.256344468	0.006823403
LC	2-Hydroxycinnamic acid	2.239594123	0.000407668
GC	Oleic Acid	2.235259281	5.47719E-15
LC	3,4-Dimethylethcathinone	2.222408403	6.81941E-13
LC	5-Phosphoribosyl-4-carboxy-5-aminoimidazole	2.21742822	0.004402249
LC	(-)-Salvisyriacolide	2.207861118	2.15026E-07
GC	Ribonic Acid	2.206744123	5.17386E-08
LC	27-Hydroxycholesterol	2.201059461	5.37126E-12
LC	(5Z,9Z)-2-methoxy-hexacosadienoic acid	2.196545835	1.54517E-13
LC	LysoPC(22:5(7Z,10Z,13Z,16Z,19Z)/0:0)	2.19313766	0.032264472
LC	5,6-Carboxyfluorescein	2.187386078	0.023292318
LC	4-Allylphenol sulfate	2.185962233	1.54636E-10
LC	2-((2-Methoxy-2-(3-(trifluoromethyl)phenyl)ethyl)amino)ethyl 4-(2-(2-(9H-fluoren-9-yl)acetamido)ethyl)benzoate	2.178340441	1.07007E-16
LC	Galactotriose	2.159792907	0.000268063
LC	Spiropiperidine	2.143751302	4.59915E-13
LC	gamma-Glutamylserine	2.140807688	1.35977E-06
LC	3,4-Bis(carboxymethyl)-3,4-dihydroxyhexanedioic acid	2.137505791	7.15661E-17
LC	3-hexanoyl-NBD Cholesterol	2.133973148	4.87466E-15
GC	Levo-glucosan	2.104786048	0.001889958
GC	3-Hydroxybutyric Acid	2.102690259	2.82965E-07
LC	Trihydroxycoprostanic acid	2.102329678	1.38215E-10
GC	3-Methylbutane-1,2-Diol	2.096532824	0.000302983
LC	6"-Acetylliquiritin	2.090160826	5.71294E-08
LC	Glycocholic acid	2.080174705	0.011366738
LC	BAY-u9773	2.076332055	1.98401E-09
LC	indoprofen	2.071726504	9.51453E-07

LC	3-[(1R,4S,5S,6R)-6-[(1E,3S,5Z,8Z,11Z)-3-Hydroperoxytetradeca-1,5,8,11-tetraen-1-yl]-2,3-dioxabicyclo[2.2.1]heptan-5-yl]propanoic carnitine	2.067666959	0.002917231
LC	Octadec-5-enoic acid	2.05946082	6.94076E-09
LC	Demissidine	2.045613252	2.44702E-11
LC	PI-Cer(t18:0/18:0(2OH))	2.042118723	3.44384E-06
LC	Kuguacin E	2.034175757	1.63259E-08
LC	Dehydropachyrrhizone	2.032633963	1.76064E-14
LC	3-Methyl-2Z,4E-decadienoic acid	2.031471123	2.95136E-10
LC	SM(d18:1/14:0)	2.019353736	0.009694017
LC	Zearalenone	2.015782898	1.38073E-10
LC	Ansamitocin P3	2.003818393	1.0961E-15
LC	6-Hydroxy-3,4-dihydro-2(1H)-quinolinone	1.993867973	1.55654E-16
LC	LysoPC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	1.979809839	0.034813181
GC	Lathosterol	1.973611905	0.00047797
LC	Ambrettolic acid	1.953670578	1.2543E-06
LC	Artemoin A	1.952474323	0.000250384
LC	Desacetycefapirin	1.951657459	9.52697E-20
LC	N-Choloylglycine	1.94278213	0.004378367
LC	Ammonia aspartate	1.940393697	0.015065224
LC	Melibiose	1.939323645	2.26121E-07
LC	16-oxo-palmitate	1.927899179	7.85485E-11
LC	Mactraxanthin 3-linoleate 3'-dipalmitoleate	1.922054407	0.015831232
LC	3b-Hydroxy-5-cholenoic acid	1.916556959	0.001774865
LC	Isothankunic acid	1.915111552	4.9734E-10
LC	N-Palmitoyl Arginine	1.914045288	0.000998682
LC	SM(d18:1/12:0)	1.90773961	1.5654E-08
LC	5alpha-Cholestane-3alpha,7alpha,12alpha,24-tetrol	1.890016505	5.78885E-13
LC	Quercetin 3'-isobutyrate	1.886251033	0.043292328
LC	Cohibin A	1.872758156	2.6842E-09
LC	2-Deoxybrassinolide	1.872576165	3.55804E-09
LC	LysoPC(P-18:1(9Z)/0:0)	1.866329038	8.91119E-09
LC	UDP-D-galacturonic acid	1.847146006	0.000197803
LC	PE-Cer(d15:2(4E,6E)/20:0)	1.838616812	1.8686E-07
GC	10-Heptadecenoic Acid	1.836594218	0.00263448
LC	Bis(2-ethylhexyl) phthalate	1.829509305	0.004088095
LC	(1R)-5-[2-[(1R,7Ar)-7a-methyl-1-[(2R)-6-methylheptan-2-yl]-2,3,3a,5,6,7-hexahydro-1H-inden-4-ylidene]ethylidene]-4-methylidenecyclohexane-1,3-diol	1.825263451	1.6188E-10
LC	5alpha-Pregnan-3beta,20beta-diol 20-sulfate	1.820247968	0.004380918
GC	3,5-Dimethylphenol	1.818722124	0.002529207

GC	Methyl L-Alaninate	1.802826861	0.012661837
LC	Melatonin glucuronide	1.792198449	1.42574E-14
LC	2-[(2-Fluorophenyl)sulfanylmethyl]-5-[6-[(2-hydroxycyclopentyl)amino]purin-9-ylloxolane-3,4-diol	1.782733747	5.28971E-08
LC	Ethyl n-allyl-n-[(e)-2-methyl-3-[4-(4-amidinophenoxy carbonyl)-phenyl]propenoyl]amino acetate	1.767588186	1.37606E-17
LC	SALSOLIDINE	1.767323834	0.002745276
LC	Sesamol	1.7477448	0.003461947
LC	2,4-Diamino-6-nitrotoluene	1.729521819	4.28708E-11
GC	2,4-Dihydroxypentanedioic Acid	1.729366659	0.005339578
LC	D-Lactic acid	1.727906981	0.001370748
LC	1,1,1,2,3,3,3-Heptafluoropropane	1.72709705	1.23953E-15
GC	Galactonic Acid	1.723181484	0.002930658
LC	OOB-PE	1.71806048	0.000625607
LC	Piperine	1.717747084	0.045463612
LC	bhos#40	1.701051713	5.85616E-14
LC	Cefodizime,(S)	1.70104054	3.69182E-06
LC	Chenodeoxycholic acid	1.69184219	0.003761494
LC	Mayolene-17	1.682907933	6.74861E-11
LC	Bryacarpene 2	1.681136132	0.036196184
LC	DG(18:3(9Z,12Z,15Z)/15:0/0:0)	1.680670717	0.000398678
GC	D-Xylose	1.678417919	4.47381E-06
LC	3-Amino-6-{4-[(4-Methylpiperazin-1-Yl)sulfonyl]phenyl}-N-Pyridin-3-Ylpyrazine-2-Carboxamide	1.677061072	2.71856E-06
LC	PC(O-16:0/3:0)	1.675656576	4.82045E-08
LC	1,5-Naphthalenediamine	1.669077005	5.41393E-17
LC	Stercobilinogen	1.656342892	0.028153421
GC	Cis-Erucic Acid	1.65616121	1.90766E-08
LC	3alpha-Hydroxy-5beta-chola-7,9(11)-dien-24-oic Acid	1.648741771	0.013952712
LC	Uridine 2',3'-cyclic phosphate	1.644484835	0.001941689
LC	(11E)-Octadec-11-enedioylcarnitine	1.644262612	0.000522049
LC	Androstenediol 3-sulfate	1.633455669	0.000701675
GC	1,3-Benzenedicarboxylic Acid	1.614876192	0.014436224
LC	Gorgostane-3beta,5alpha,6beta,11alpha,12beta-pentol 12-acetate	1.610606835	2.57361E-11
LC	Marmesin rhamnoside	1.603789166	4.52583E-09
LC	Heptafluorobutyric acid	1.60117464	4.58913E-14
LC	beta-D-fructose 2,6-bisphosphate	1.599411315	0.01680882
LC	5-Hydroxy-2-imino-1-methylimidazolidin-4-one	1.599012897	3.31356E-18
LC	Propylparaben	1.598017866	0.03477292

LC	(20R)-24-Hydroxygeminivitamin D3	1.596799428	2.452E-10
LC	PE(10:0/10:0)	1.58684232	9.93136E-12
LC	Mesobilirubinogen	1.58270969	0.04744512
GC	Dodecanol	1.578848163	0.001955347
LC	3-Hydroxymethyl-picumast	1.576352661	0.003291373
LC	1-Hydroxy-2,2,5,5-tetramethylpyrrolidine-3-carboxamide	1.575555982	0.029295932
LC	Symmetric dimethylarginine	1.567192762	1.38255E-05
GC	Maltitol	1.562290949	0.007377188
LC	PE-Cer(d14:2(4E,6E)/23:0)	1.561452325	0.000912827
LC	3beta,4beta-dihydroxycholest-23-one	1.558053457	2.32937E-11
LC	(2S)-1,1,1-Trifluoro-2-(4-pyrazol-1-ylphenyl)-3-[5-[[1-(trifluoromethyl)cyclopropyl]methyl]-1H-imidazol-2-yl]propan-2-ol	1.557118943	2.72246E-23
LC	Ganoderiol C	1.5523282	1.92293E-11
LC	Demethyltorosaflavone C	1.551043667	0.0332785
LC	4-(2-Aminoethyl)benzenesulfonyl fluoride	1.545317659	1.12302E-06
LC	Dodecylbenzene	1.527097902	5.25338E-05
LC	Uridine diphosphate glucose	1.526628066	4.79333E-06
LC	Blumealactone C	1.521426184	5.96746E-10
GC	Cellobiose	1.51852037	2.91857E-07
LC	7beta,25-dihydroxycholesterol	1.51118216	1.04413E-10
LC	Zierin	1.505109076	8.64151E-12
LC	LysoPE(P-18:0/0:0)	1.499681041	5.33839E-13
LC	Ikarisoside D	1.493017706	1.21604E-07
LC	Cabozantinib	1.491279376	7.61124E-07
LC	Oxdralazine	1.490592189	6.27694E-09
LC	16-Deoxymyxinol	1.482235131	6.07781E-10
LC	Darexaban glucuronide	1.479381022	5.15096E-05
LC	(4S,6R)-6-[(1E)-4,4-Bis(4-fluorophenyl)-3-(1-methyltetrazol-5-yl)buta-1,3-dienyl]-4-hydroxvoxan-2-one	1.457682746	2.12112E-06
GC	1,2-Propanediol	1.456349934	3.94499E-06
LC	Pregnenolone sulfate	1.447412635	0.000877283
LC	Cholestane-3,5,6-triol	1.446615871	3.78705E-12
LC	Daucic acid	1.44185227	5.58056E-16
GC	L-Tryptophan	1.439971595	1.67086E-08
LC	Sulfaethidole	1.431763613	0.00868341
LC	2,2':6',2''-Terpyridine	1.431065901	9.25407E-07
LC	8-Azaguanine	1.42830507	4.10414E-06
LC	N-(2-(Mercaptomethyl)-3-phenylbutanoyl)-L-alanine	1.422836682	1.19975E-10
LC	Gcdcs	1.420296646	0.002699526

LC	Hydroquinone sulfate	1.418006261	5.97496E-05
LC	Dodecanoylcarnitine	1.412810369	0.005912259
LC	15S-HTPE	1.404250593	2.74552E-10
LC	7-Amino-4-hydroxy-2-naphthalenesulfonic acid	1.404216962	9.0741E-05
GC	Cytidine Monophosphate	1.399725205	0.010015967
LC	6alpha-Hydroxycastasterone	1.395935429	1.46313E-13
LC	2,4-Thiazolidinedicarboxylic acid, 2-methyl-	1.395544257	0.000361617
LC	27-Norcholestanehexol	1.392746479	2.72704E-10
GC	Delta-Tocopherol	1.389674181	0.004810235
LC	3-Hydroxy-4-aminopyridine sulfate	1.389455693	0.03521443
GC	(S)-3,4-Dihydroxybutyric Acid	1.384606819	2.79936E-06
LC	makisterone B	1.382937153	2.07571E-11
LC	Campesterol glucoside	1.381441258	0.000185431
LC	Armatinol B	1.377061535	2.48033E-08
LC	DG(i-15:0/0:0/i-12:0)	1.372289758	3.59805E-09
LC	5b-Cholestane-3a,7a,12a,23-Tetrol	1.362759764	2.96439E-08
LC	LysoPC(20:0/0:0)	1.356829162	3.49368E-07
GC	Linoelaidic Acid	1.353034593	2.53053E-11
LC	5beta-Cholestane-3alpha,7alpha,27-triol	1.351151855	2.76785E-13
LC	3a,7a-Dihydroxycholanoic acid	1.350516778	1.03822E-08
GC	Beta-Lactose	1.349787046	1.22367E-06
LC	Callyspongenol A	1.348393927	2.57369E-09
GC	Uric Acid	1.345972703	1.28136E-06
LC	N-(1-Deoxy-1-fructosyl)glycine	1.343728118	3.44768E-17
LC	7alpha,26-dihydroxy-5beta-cholestan-3-one	1.342471151	2.61432E-11
LC	Serylmethionine	1.336601876	3.56649E-05
LC	virginiamycin m1	1.335630052	1.99958E-07
LC	oscr#36	1.335110552	3.16455E-10
GC	5-Hydroxyindoleacetic Acid	1.334281623	5.85205E-09
LC	2-Ethoxy-3-[4-[2-(4-methylsulfonyloxyphenyl)ethoxy]phenyl]propanoic acid	1.331426993	4.59265E-08
LC	Pyrogallol-1-O-sulphate	1.327814193	0.000393374
GC	4-Hydroxyproline	1.325624423	1.21322E-05
LC	19-oxodesacetylcinobufagin	1.321657751	9.35251E-07
LC	Tribufos	1.318951795	2.33202E-06
LC	Methylenediphosphonic acid	1.317842217	0.001058028
LC	Polysorbate 80	1.314193555	4.25862E-12
LC	20a,22b-Dihydroxycholesterol	1.313033184	1.0543E-10
LC	(25R)-4beta,26-dihydroxycholesterol	1.311645931	8.89506E-12
LC	Helianthin	1.31141562	0.000312475

GC	O-Phosphoethanolamine	1.309591481	0.008407344
LC	13'-Hydroxy-alpha-tocopherol	1.306369995	0.001323398
LC	19-Oic-deoxycorticosterone	1.30446905	2.72747E-17
LC	Cholesterol sulfate	1.303754069	4.32418E-07
LC	SM(d18:1/16:0(2OH))	1.302108362	0.008388629
LC	Callyspongendiol	1.301850646	8.28469E-15
LC	Dexamethasone	1.300429431	0.000149214
LC	chrysoeriol 7-O-neohesperidoside	1.299711384	2.21659E-06
LC	Sitostanol-beta	1.299676074	2.0544E-10
LC	Melanettin	1.294633946	4.91123E-14
GC	Ketoleucine	1.292038711	1.96617E-07
LC	Benzyloxycarbonyl-Val-Ala-Asp(OMe)-fluoromethylketone	1.286389889	1.10289E-07
LC	Propionylcarnitine	1.285707694	0.001922986
LC	3-(3,4-Difluorophenyl)-4-(4-(methylsulfonyl)phenyl)-2(5H)-furanone	1.284798019	3.66351E-07
LC	3 alpha,7 alpha,26-Trihydroxy-5beta-cholestane	1.282845729	9.87938E-13
LC	Citrusinine I	1.280523477	8.9544E-11
GC	Butane-1,2,4-Triol	1.279754132	0.029697615
LC	4,6,2',4'-Tetramethoxychalcone 2'-beta-glucoside	1.278496938	8.46346E-07
LC	Naematolone	1.273946744	2.8444E-09
LC	(2S,4R)-4-(9H-Pyrido[3,4-b]indol-1-yl)-1,2,4-butanetriol	1.271660543	2.01546E-14
LC	C16 Sphinganine	1.271276738	2.45049E-14
LC	Sphinganine 1-phosphate	1.26979324	1.08666E-05
LC	IODODIFLUNISAL	1.265024342	0.002573601
LC	1alpha-Hydroxycorticosterone	1.260150798	0.010989918
GC	3,4-Dihydroxyphenylglycol	1.254746809	0.000238717
LC	Bilirubin	1.250083168	1.00946E-07
LC	typhasterol	1.246317652	5.31502E-09
LC	PC(19:0/0:0)	1.246096088	1.51154E-10
LC	Fusaroskyrin	1.243441946	0.016964902
LC	LysoPE(P-18:1(9Z)/0:0)	1.241220213	2.784E-13
GC	Gluconolactone	1.240246029	0.000255877
LC	25-Acetylvulgaroside	1.236974491	0.000513819
LC	isoleucyl-thiazolidine	1.236358137	0.000546623
LC	Longilactone, delta-4(18)-Isomer, 2alpha-alchoh;	1.235857192	1.02386E-07
	(1R,2R,3R,3aS,5aS,6R,6aS,9S,10S,10aS,10bR,10cR)-1,2,6,9,10-Pentahydroxy-		
	3 10a 10c-trimethyl-7-methylenetetradecahydro-4H-phenanthro[10 1-b]furan-4-one		
LC	PA(17:0/12:0)	1.235006671	7.75427E-06
LC	Pregnanediol-3-glucuronide	1.233043587	0.006201122
LC	Methiuron	1.231771366	0.036659617

GC	Pectin	1.230538708	0.02249332
GC	Udp-N-Acetylglucosamine	1.22933857	0.000250452
GC	Sorbitol-6-Phosphate	1.228255933	0.035595175
LC	Bentazone	1.227224272	9.37737E-19
LC	POB-PS	1.226652287	3.62922E-06
LC	(3alpha,5alpha,22R,23R)-Cholestane-3,22,23-triol	1.224368162	2.77123E-10
LC	Penicisteroid H	1.223169484	4.35585E-08
LC	Bergaptol	1.217677104	0.001399244
GC	L-(-)-Sorbose	1.21655086	4.33363E-05
LC	PE(DiMe(11,5)/20:4(5Z,8Z,11Z,13E)-OH(15S))	1.214397699	0.026419723
LC	LysoPC(18:3(9Z,12Z,15Z)/0:0)	1.213288176	0.012002897
GC	Leucrose	1.212746219	0.000461067
LC	2-Hydroxy-3-methylbutyric acid	1.210678862	0.011042545
LC	Teasterone	1.210226285	6.12047E-11
GC	Hypoxanthine	1.204971604	0.036703896
GC	L-Erythrulose	1.20475443	0.00644521
LC	Avideoxycholic acid	1.204206817	3.24537E-07
LC	[1,1'-Biphenyl]-4-ol, 3-amino-	1.202625535	3.09893E-06
GC	D-Galactose	1.193413669	5.63244E-05
GC	N-Acetyl-Tryptophan	1.193371694	1.19932E-07
LC	PE(20:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	1.193029564	0.005136758
GC	Mq(0:0/16:0/0:0)	1.193029203	0.017707552
LC	Deoxycytidine	1.192780342	1.11849E-08
GC	2-Hydroxybutyric Acid	1.192265965	4.27599E-06
LC	Sarothrin	1.188657266	0.034792195
LC	5-Amino-1-[carboxy(methyl)amino]pentane-1,1,2,2,3,3,4,4,5-nonacarboxylic acid	1.186002074	0.006816995
LC	PS(24:0/20:3(5Z,8Z,11Z)-O(14R,15S))	1.183478475	7.30648E-06
LC	Schisanhenol	1.181114152	3.48468E-06
LC	Ephedrine	1.180348068	0.003913201
LC	1-Octen-3-yl acetate	1.180217394	3.25388E-10
LC	Sorafenib beta-D-Glucuronide	1.178826579	4.78587E-06
LC	Benzylpenicilloyl	1.176030668	8.8688E-10
GC	3-Methyl-2-Oxovaleric Acid	1.175406016	0.000265624
LC	LysoPC(15:0/0:0)	1.17511826	7.89638E-06
LC	2-Hydroxy-4-[(1R)-1-hydroxy-8-methyl-6-oxononyl]-3-methyl-2H-furan-5-one	1.169781465	0.042924805
LC	GDP-mannuronate	1.166629508	8.42862E-06
LC	PE(14:1(9Z)/12:0)	1.166448449	1.00365E-08
LC	PC(P-18:0/20:4(5Z,8Z,11Z,14Z)-OH(16R))	1.158664652	0.005779348
LC	Axillarin 7-sulfate	1.156452978	3.06896E-05

LC	5-Methoxysalicylic acid	1.156210528	0.009399317
LC	PA(a-25:0/20:4(5Z,8Z,10E,14Z)-OH(12S))	1.15548637	0.012286157
LC	Phosphoric acid, mono(4-cyanophenyl) monomethyl ester	1.14996127	1.1305E-05
LC	Undecanoylcarnitine	1.145632031	8.51401E-06
LC	Methacrifos	1.141927844	1.14759E-07
LC	Momordol	1.138092343	8.19004E-12
LC	N-3-hydroxy-13-methyl-hexadecanoyl glycy-L-serine	1.134444097	1.37727E-07
LC	2-Hexadecyloctadec-9-enal	1.131273104	0.000150582
LC	5-((8Z,11Z)-nonadeca-8,11-dien-1-yl)resorcinol	1.127771991	7.54806E-10
LC	(11E,13Z)-10-Hydroxyoctadeca-11,13-dienoylcarnitine	1.118321026	6.98624E-05
GC	Alpha-D-Lactose	1.114578621	0.012936834
LC	Phenylalanyltryptophan	1.114363258	0.000786901
LC	Alisol A	1.113997306	2.213E-08
LC	Isoquinolinesulfonamide	1.113185717	0.033123431
GC	1h-Indole-2-Acetic Acid	1.106535927	0.004289838
LC	15-hydroxycembra-1,3,7,11-tetraene	1.106360009	1.5044E-07
LC	PIM1(19:0/16:0)	1.106272763	0.000186753
LC	Edetate trisodium	1.105598041	0.002528702
LC	5-Nonadecyl-1,3-benzenediol	1.105246109	8.91573E-09
LC	Bisantrene	1.102782867	8.22966E-08
LC	Etodolac acyl glucuronide	1.100811961	0.006397494
GC	Phthalic Acid	1.098809128	0.000592117
LC	Stercobilin	1.09701035	0.026576372
LC	Berkeleylactone G	1.094370571	0.026450811
LC	Dihydroxyacetone phosphate	1.093204547	0.002647595
LC	Manbeta1-4Glc-beta-Cer(d18:1/16:0)	1.093093559	2.19053E-06
LC	2-(Trifluoromethyl)isonicotinic acid	1.091777906	0.002612161
LC	Piridronic acid	1.091020748	0.000107916
LC	Nitroglycerin	1.09023557	3.11375E-08
LC	Lumirubin	1.088202444	3.73598E-07
LC	Ambrisentan	1.085436211	1.59647E-14
LC	3-Amino-5-(3-thiophenyl)-2-thiophenecarboxamide	1.085349842	6.3644E-06
LC	Taurodeoxycholic acid 3-glucuronide	1.08530765	0.011973246
LC	Isoflupredone acetate	1.084720317	0.00091987
GC	Glutaconic Acid	1.079652709	0.007363395
LC	6-Nitrotryptophan	1.077416891	9.7226E-15
GC	Phenol	1.075743007	0.04215171
LC	(3Z,5E,7E)-Decatrienoylcarnitine	1.074612588	0.017119473
LC	Thiazolidine-4-carboxylic acid	1.074482326	3.06448E-07

LC	(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone	1.073906842	0.023693826
LC	7-Chloroemodin	1.072981428	1.61205E-17
LC	2-[(1r,3s)-3-Hydroxycyclohexyl]-5-(2-methyloctan-2-yl)phenol	1.072497043	7.07017E-12
LC	N6,N6,N6-Trimethyl-L-lysine	1.070947656	0.014584338
LC	(2S)-3-[3-[(4-Carbamimidoylbenzoyl)amino]propanoylamino]-2-[(4-ethylphenyl)sulfonylamino]propanoic acid	1.068161136	0.000147419
LC	gamma-Glutamylacetamide	1.06608525	0.000293257
LC	farnesyl triphosphate	1.063720574	1.66623E-13
LC	7alpha,12alpha-Dihydroxy-5beta-chol-3-en-24-oic Acid	1.06144848	5.97344E-09
LC	Eszopiclone	1.055627597	8.16875E-14
LC	NNAL-N-glucuronide	1.054646494	7.71277E-05
GC	D-Fructose	1.054643771	5.89727E-07
LC	D-Mannose	1.052024395	0.001951394
LC	LysoPI(18:1(9Z)/0:0)	1.04753716	4.58379E-08
LC	N-Stearoyl Lysine	1.044744203	9.76573E-05
LC	24-Nor-5beta-chol-22-ene-3alpha,12alpha-diol	1.043975788	6.1191E-09
GC	L-Glutamic Acid	1.042986929	0.002390984
LC	Carbimazole	1.04230476	0.033589365
LC	Indole-3-propionic acid	1.039522069	0.008463226
LC	Tropisetron	1.039362858	0.001320556
LC	Gelsenicine	1.038741342	4.32525E-07
LC	Succinylsulfathiazole	1.03858209	0.014530326
LC	Phosphovanillin	1.038564305	7.14284E-14
LC	Spinoflavanone A	1.035733755	2.15839E-08
LC	Kinetin	1.035117724	3.80474E-15
LC	2,2-Difluoro-n-(2-hydroxyethyl)-3-(2-nitro-1h-imidazol-1-yl)propanamide	1.034474162	0.008034367
GC	Glucuronic Acid	1.031929507	0.000928279
LC	PC(O-17:0/0:0)	1.028848524	4.08683E-11
LC	plaunotol	1.027944612	2.01481E-09
LC	reparixin	1.027229951	4.37947E-17
LC	DG(18:0/20:4(8Z,11Z,14Z,17Z)/0:0)	1.026748997	0.024320454
LC	7 alpha,24-Dihydroxy-4-cholesten-3-one	1.020770275	8.78812E-12
LC	U-75302	1.019661338	6.84454E-13
LC	Thyroxine	1.017362606	7.64838E-06
LC	3,5,9-Trihydroxyergost-7-en-6-one	1.016717812	1.17301E-07
LC	4-Vinylphenol sulfate	1.016351425	0.004227491
LC	PHODA-PI	1.014968976	1.17941E-10
LC	Leucyl-leucine	1.014123166	1.18257E-06
LC	MEK1-2-inhibitor	1.01056178	0.004804795

LC	5beta-Pregnane-3alpha,20alpha-diol	1.009112388	1.39851E-09
LC	(1(10)E,4a,5E)-1(10),5-Germacradiene-12-acetoxy-4,11-diol	1.005521022	0.022071093
LC	Ribosylhopane	1.003760993	6.16628E-12
LC	4-Deoxybryaquinone	1.002770403	1.01653E-08
LC	19Z-pentacosenoic acid	1.00182327	1.30003E-10
LC	Confusoside	1.00151958	3.52174E-06

GC Normal

Dataclass	Metabolites	VIP	P-value
LC	Propofol glucuronide	53.94652497	4.45672E-15
LC	LysoPC(0:0/18:2(9Z,12Z))	38.31488806	6.16049E-10
LC	Edetic Acid	26.86598179	3.83159E-05
LC	Carissanol	14.37844613	1.39673E-26
LC	LysoPC(20:4(5Z,8Z,11Z,14Z)/0:0)	12.08499396	0.000493465
LC	Dehydroepiandrosterone sulfate	11.19017239	8.46707E-08
LC	Isocitric acid	10.16648213	6.1962E-12
LC	SM(d18:1/16:1(9Z))	9.715301146	2.74592E-05
LC	Lidocaine	8.939153154	5.31002E-05
LC	N-(2-Hydroxyethyl)-2-(1-isoquinolinylmethylene)hydrazinecarbothioamide	8.816521427	2.02231E-15
LC	PC(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/P-18:1(11Z))	8.4669964	0.02855219
LC	1-(O-alpha-D-glucopyranosyl)-29-keto-(1,3R,31R)-dotriacontanetriol	8.215099913	3.13532E-07
LC	PC(P-18:1(11Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))	8.191727526	1.18243E-06
LC	UTILIN	7.350631376	2.15176E-23
LC	SM(d19:1/17:1)	7.342634715	0.000642955
LC	19-Epischolaricine	6.848364743	1.48997E-19
LC	2-C-methyl-D-erythritol-4-phosphate	6.38754549	0.000101689
LC	1-O-(2-methoxy-4Z-hexadecenyl)-sn-glycero-3-phosphocholine	6.281443908	5.92016E-05
GC	P-Cresol Glucuronide	6.057556488	4.01438E-15
LC	Myristyl linoleate	5.991049997	0.031623979
LC	N-Nitrosoanatabine	5.90988211	1.60368E-09
LC	2-Methyl-4'-(methylthio)-2-morpholinopropiophenone	5.89166591	9.90643E-13
LC	Chenodeoxycholic acid glycine conjugate	5.884162488	0.000620503
LC	4-(2-Aminoethylamino)-3-[bis(carboxymethyl)amino]-3-(carboxymethyl)hexanedioic acid	5.600909303	3.80096E-25
LC	L-Acetylcarnitine	5.589893334	0.001881515
LC	S-Japonin	5.567984988	6.97297E-09
LC	LysoPE(18:1(9Z)/0:0)	5.433082918	4.14667E-06
LC	(±)-(Z)-2-(5-Tetradecenyl)cyclobutanone	5.364835164	0.019070874
LC	Isoscoparin 2"-O-glucoside	5.17440409	0.000552038
LC	Pulverulentoside I; (1aS,1bS,2S,5aR,6S,6aS)-6-({3-O-Acetyl-6-deoxy-2-O-[(2E)-3-(4-me	5.037663029	1.05476E-10

LC	13-Hydroxyoctadecanoylcarnitine	4.933345605	1.68573E-05
GC	Equilenin	4.932257964	1.9879E-16
LC	LysoPC(20:4(8Z,11Z,14Z,17Z)/0:0)	4.751566938	0.000651503
LC	Enterodiol sulfate	4.556738685	3.78655E-09
LC	PC(0:0/14:0)	4.503660424	0.000185342
LC	TG(8:0/8:0/a-17:0)[rac]	4.456641938	0.001664105
LC	6-Butyryl-5-hydroxy-4-phenylseselin	4.31490091	6.24884E-08
LC	Oxotremorine	4.293933171	2.58891E-12
LC	Benzoxazole	4.284956005	0.01913489
LC	p-Cresol sulfate	4.205993242	0.017654745
LC	PC(12:0/20:1(11Z))	4.190891176	0.001363777
LC	dIDP	4.178355858	9.1202E-15
LC	2,2'-Methylenebis(4-methyl-6-tert-butylphenol)	4.15865175	3.59592E-14
LC	Ecabet	4.150657042	2.74776E-09
LC	LysoPC(0:0/18:1(9Z))	4.131967354	0.023274943
LC	O-Linoleoylcarnitine	4.108912325	0.000562633
GC	Lactulose	4.103276426	4.46051E-12
LC	LysoPC(0:0/18:0)	4.041917952	0.039107379
LC	Indoxyl sulfate	4.007344508	9.16702E-10
GC	M-Toluamide	3.978343556	1.85085E-11
LC	Cichorioside K	3.805460545	3.1816E-12
LC	L-Alloisoleucine	3.794286905	0.008302739
LC	PC(18:0/P-16:0)	3.789733332	9.00938E-05
GC	3-(Pyrazol-1-Yl)-L-Alanine	3.770363952	0.000130677
LC	2-Methoxy-4-(2-(methylamino)propyl)phenyl beta-D-glucopyranosiduronic acid	3.741584163	4.11721E-17
LC	Armillaripin	3.658880068	3.8297E-13
LC	21H-Bilane-8,12-dipropanoicacid, 3,18-diethenyl-1,19,22,24-tetrahydro-2,7,13,17-tetramethyl-	3.658494082	4.8298E-11
LC	Decanoylcarnitine	3.642436159	0.03128563
LC	(Z)-1-(Methylthio)-5-phenyl-1-penten-3-yne	3.618887447	1.79317E-14
GC	Lactitol	3.611330271	3.20936E-12
LC	Phyllocoumarin	3.528669441	1.64083E-15
LC	Vignatic acid B	3.463578533	1.0499E-06
GC	Maltotriose	3.442438543	3.32747E-11
LC	LysoPE(0:0/18:1(11Z))	3.395511207	2.61986E-07
LC	Plantacyanin	3.391050708	5.16825E-10
LC	Allopregnanolone sulfate	3.382748995	0.001129506
LC	Octenoyl-L-carnitine	3.369514045	1.40229E-06
LC	Disodium ethylenediaminetetraacetate	3.347200615	0.003664457
LC	PS(P-20:0/22:2(13Z,16Z))	3.261628398	0.000431688

GC	Cis-Aconitic Acid	3.154253894	3.89001E-10
LC	PE-NMe2(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	3.040954905	1.67904E-05
LC	Vaccenic acid	3.031525829	1.50499E-20
LC	PI(O-18:0/18:0)	3.028972281	0.002887081
LC	[3-Methoxy-2-phosphonooxy-6-[(E)-2-(3,4,5-trimethoxyphenyl)ethenyl]phenyl] dihydroge	3.010458194	0.017237678
LC	LysoPC(0:0/20:4(5Z,8Z,11Z,14Z))	2.950013103	0.00121253
LC	3-(4-Iodophenyl)-2-mercapto-(Z)-2-propenoic acid	2.948505766	0.001760034
LC	gamma-Glutamylserine	2.946838817	7.49733E-09
LC	alpha-Hydroxyisobutyric acid	2.882413071	2.08052E-12
LC	Galactotriose	2.882409673	5.59696E-08
LC	Caffeine	2.866566449	2.80265E-05
LC	Fluorene	2.842166756	4.52853E-07
LC	Sphingosine 1-phosphate	2.838054454	7.75174E-06
LC	Hydroxyzine	2.836639859	4.42442E-07
LC	3,4-Dimethylethcathinone	2.836429107	2.09715E-21
LC	2-Oxoarginine	2.814642957	5.92824E-07
GC	2,6-Pyridinedicarboxylic Acid	2.813096475	0.002839778
LC	PS(P-20:0/0:0)	2.80210582	3.98979E-10
LC	Glycocholic acid	2.762208825	0.001078465
LC	PE(22:4(7Z,10Z,13Z,16Z)/21:0)	2.753488411	0.005457149
LC	9-tridecynoic acid	2.749320526	7.30832E-07
LC	LysoPE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	2.722823168	0.001383361
LC	lysine phosphoester	2.71285795	6.39359E-14
LC	PC(17:2(9Z,12Z)/0:0)	2.678348283	2.22589E-13
LC	Ptilosaponoside B	2.677181483	7.77624E-16
GC	Octaethylene Glycol	2.66154083	7.31284E-07
LC	Methyl 3-epi-4,5-didehydrojasmonate	2.651237028	7.99368E-06
LC	APC	2.649821373	2.78165E-17
LC	Melibiose	2.644487256	1.16746E-11
LC	EUPARIN	2.622642915	1.97339E-06
LC	Thiamine	2.606164504	3.56529E-11
LC	Zearalenone	2.592859771	1.47316E-16
LC	LysoPE(P-16:0/0:0)	2.589484635	3.0235E-10
LC	Gravolenic acid	2.560480712	1.89272E-17
LC	Theophylline	2.547771811	3.06009E-05
LC	3-[(1R,4S,5S,6R)-6-[(1E,3S,5Z,8Z,11Z)-3-Hydroperoxytetradeca-1,5,8,11-tetraen-1-yl]-2	2.534435874	0.000541287
LC	Matraxanthin 3-linoleate 3'-dipalmitoleate	2.533171882	0.011558246
GC	Melezitose	2.506016185	0.005991462
LC	5-{2-Fluoro-5-[3-(3-hydroxy-2-methoxycarbonyl-phenoxy)-propenyl]-phenyl}-isoxazole-3-	2.480937881	0.0487224

LC	6"-Acetylliquiritin	2.472937151	2.34793E-12
LC	3-Methyl-2Z,4E-decadienoic acid	2.467781535	6.58734E-14
LC	GM4(d18:1/18:0)	2.465713887	0.042240365
GC	Ribonic Acid	2.453976277	0.005684684
GC	3-Methylbutane-1,2-Diol	2.444183466	3.26707E-07
LC	DG(18:3(9,11,15)-OH(13)/15:0/0:0)	2.429438144	1.85007E-06
LC	PI-Cer(t18:0/18:0(2OH))	2.424038317	9.07158E-06
LC	Pyridine N-oxide glucuronide	2.419406205	2.8962E-13
LC	[(2S,4R,5R,6R,14S,16R)-14-Hydroxy-7,11-dimethyl-6-(2-oxopyran-4-yl)-3-oxapentacycl	2.367365409	2.35006E-13
LC	N-Choloylglycine	2.35980136	0.0011058
LC	PC(O-16:1(11Z)/0:0)	2.352273921	1.93406E-10
LC	2-[(2-Fluorophenyl)sulfanylmethyl]-5-[6-[(2-hydroxycyclopentyl)amino]purin-9-yl]oxolane	2.344109746	1.56976E-11
LC	2,4-Thiazolidinedicarboxylic acid, 2-methyl-	2.301708405	4.45013E-07
LC	3b-Hydroxy-5-cholenoic acid	2.300600053	0.00026945
LC	PC(14:1(9Z)/20:3(8Z,11Z,14Z))	2.299527329	0.022306549
LC	2-(5,8-Tetradecadienyl)cyclobutanone	2.299305213	0.021249907
LC	2-((2-Methoxy-2-(3-(trifluoromethyl)phenyl)ethyl)amino)ethyl 4-(2-(2-(9H-fluoren-9-yl)ace	2.288621689	7.86744E-17
LC	3,7-Dihydroxycholan-24-oic acid	2.286392283	0.011569648
LC	Octadec-5-enoic acid	2.279438	6.39647E-09
LC	Propylparaben	2.278729795	0.007900314
GC	P-Cresol	2.273388205	0.017876409
LC	SM(d18:1/14:0)	2.222411694	0.00667243
LC	LysoPC(O-18:0/0:0)	2.218996093	1.28915E-05
LC	LysoPE(0:0/16:0)	2.214984416	0.023646247
LC	(-)-Salvisyriacolide	2.2108962	3.74573E-07
LC	Desacetycefapirin	2.209933168	4.30069E-25
LC	Melatonin glucuronide	2.181274399	1.29343E-22
LC	3-Hydroxylidocaine	2.176948804	3.8166E-09
GC	Cellobiose	2.176237082	2.55371E-11
LC	Ansamitocin P3	2.1664012	1.07531E-16
LC	Cabozantinib	2.161336002	1.36062E-09
LC	1-O-Hexadecyl-sn-glycero-3-phosphocholine	2.155677345	6.40337E-09
LC	PE-Cer(d14:2(4E,6E)/23:0)	2.145256236	4.57363E-05
LC	(5Z,9Z)-2-methoxy-hexacosadienoic acid	2.144522665	3.25487E-12
LC	27-Hydroxycholesterol	2.141978776	1.08849E-11
LC	Artemoin A	2.139000219	9.3166E-05
GC	Quinic Acid	2.135311955	0.002375503
LC	16-oxo-palmitate	2.128104247	8.7475E-13
LC	Ikariside D	2.115382588	5.24926E-11

LC	4-(2-Aminoethyl)benzenesulfonyl fluoride	2.113026735	3.21214E-12
LC	Chenodeoxycholic acid	2.105068385	0.000439192
LC	Bis(2-ethylhexyl) phthalate	2.097021044	0.00174431
LC	Cohibin A	2.088519059	1.22597E-10
LC	6-Thioxanthylic acid	2.087715016	0.001821187
LC	Spiropiperidine	2.066201663	4.30362E-11
LC	Trihydroxycoprostanic acid	2.063272269	9.69794E-10
GC	Oleic Acid	2.057633839	3.1445E-14
LC	3,4-Bis(carboxymethyl)-3,4-dihydroxyhexanedioic acid	2.052894979	8.38911E-13
GC	Beta-Lactose	2.042600146	1.56114E-09
LC	DG(18:3(9Z,12Z,15Z)/15:0/0:0)	2.032596067	5.35984E-05
LC	UDP-D-galacturonic acid	2.018912892	0.000273723
LC	Dehydropachyrrhizone	2.014906972	5.00503E-16
LC	5alpha-Pregnan-3beta,20beta-diol 20-sulfate	2.014892652	0.002721915
LC	3-Amino-6-{4-[(4-Methylpiperazin-1-yl)sulfonyl]phenyl}-N-Pyridin-3-ylpyrazine-2-Carbox	2.011397905	5.26767E-08
LC	2-Deoxybrassinolide	2.006936039	2.76346E-10
LC	Glycerol 5-hydroxydecanoate	2.005981312	6.30227E-13
LC	6-Hydroxy-3,4-dihydro-2(1H)-quinolinone	1.984964911	6.1025E-14
LC	4-Allylphenol sulfate	1.984378099	4.47979E-08
LC	(4E,7E,10Z,13E,16E,19E)-docosa-4,7,10,13,16,19-hexaenoic acid	1.979862868	0.003727707
LC	Demissidine	1.957965106	1.95426E-10
LC	SM(d18:1/12:0)	1.952154348	5.64912E-08
LC	Glycoursodeoxycholic acid	1.950015511	0.017673265
LC	2-Hydroxycinnamic acid	1.930980092	0.003988207
LC	PE-Cer(d15:2(4E,6E)/20:0)	1.923098256	3.88038E-07
LC	Marmesin rhamnoside	1.917955165	1.18024E-12
GC	10-Heptadecenoic Acid	1.909167384	0.000359808
LC	(4E,15E)-Bilirubin	1.897076068	8.03285E-08
LC	(3Z,5E,7E)-Decatrienoylcarnitine	1.89679357	6.01807E-08
LC	Sesamol	1.892132742	0.001044249
LC	3-hexanoyl-NBD Cholesterol	1.881761628	3.34977E-11
LC	3-Hydroxymethyl-picumast	1.873705086	0.000437715
LC	Isothankunic acid	1.871586314	6.69361E-09
LC	5alpha-Cholestane-3alpha,7alpha,12alpha,24-tetrol	1.870393826	6.74343E-12
LC	Piperine	1.867684191	0.043012498
LC	Porson	1.866593245	0.000546435
GC	Galacturonic Acid	1.856685583	7.8056E-05
GC	Levogluconan	1.854603568	3.51654E-06
GC	3-Hydroxybutyric Acid	1.854059215	1.10462E-05

LC	Ethyl n-allyl-n-[(e)-2-methyl-3-[4-(4-amidinophenoxy carbonyl)-phenyl]propenoyl]amino a	1.847265413	1.20864E-17
LC	Fusaroskyrin	1.843849422	0.00191085
LC	Androstenediol 3-sulfate	1.837543969	0.000285111
LC	2,4-Diamino-6-nitrotoluene	1.813782868	2.1726E-12
LC	Methiuron	1.804156623	0.003221871
LC	Hippuric acid	1.803684657	2.45259E-05
LC	TG(8:0/8:0/a-13:0)[rac]	1.802239019	0.000203891
GC	Delta-Tocopherol	1.802200522	0.00040632
LC	Zierin	1.797289473	1.32646E-15
LC	3-(3,4-Difluorophenyl)-4-(4-(methylsulfonyl)phenyl)-2(5H)-furanone	1.792263897	9.49353E-15
LC	Sulfaethidole	1.786998554	0.00279293
LC	PC(18:1(9Z)-O(12,13)/16:0)	1.777252797	0.005137805
LC	LysoPC(P-18:1(9Z)/0:0)	1.775479339	2.36195E-07
LC	(1R)-5-[2-[(1R,7Ar)-7a-methyl-1-[(2R)-6-methylheptan-2-yl]-2,3,3a,5,6,7-hexahydro-1H-i	1.772930178	2.84645E-10
LC	Hexazinone	1.759318895	0.003982387
LC	(4S,6R)-6-[(1E)-4,4-Bis(4-fluorophenyl)-3-(1-methyltetrazol-5-yl)buta-1,3-dienyl]-4-hydro	1.758349855	2.53494E-13
LC	Uridine 2',3'-cyclic phosphate	1.756411896	0.001611442
LC	(2S)-1,1,1-Trifluoro-2-(4-pyrazol-1-ylphenyl)-3-[5-[[1-(trifluoromethyl)cyclopropyl]methyl]-	1.755297126	3.44173E-29
LC	Ephedrine	1.755138777	0.037941192
LC	SALSOLIDINE	1.75436815	0.044209272
LC	Tribufos	1.752575299	2.82091E-10
LC	Cefodizime,(S)	1.73968369	2.54541E-05
LC	5-Hydroxy-2-imino-1-methylimidazolidin-4-one	1.733205725	9.94897E-22
LC	Dodecanoylcarnitine	1.730478547	0.000804712
LC	Mayolene-17	1.725599502	5.86416E-10
LC	Heliangin	1.723957331	6.23056E-06
LC	Uridine diphosphate glucose	1.718394768	5.03324E-07
LC	PGP(a-13:0/i-24:0)	1.710503078	0.048877201
LC	2-(Trifluoromethyl)isonicotinic acid	1.705726042	2.8419E-06
LC	2-Ethoxy-3-[4-[2-(4-methylsulfonyloxyphenyl)ethoxy]phenyl]propanoic acid	1.701428547	4.52184E-13
LC	(11E)-Octadec-11-enedioylcarnitine	1.689703326	4.98632E-05
LC	chrysoeriol 7-O-neohesperidoside	1.685669224	2.25755E-09
LC	virginiamycin m1	1.684168361	2.72755E-10
LC	Nitroflurbiprofen	1.679466869	0.004636533
LC	(1(10)E,4a,5E)-1(10),5-Germacradiene-12-acetoxy-4,11-diol	1.678126272	1.54075E-06
GC	Cis-Erucic Acid	1.674884692	5.24756E-15
LC	Callyspongenol A	1.674200425	5.43577E-14
GC	Mg(0:0/16:0/0:0)	1.665463275	0.000293167
GC	Sorbitol-6-Phosphate	1.663949206	0.005671253

LC	Kuguacin E	1.657918258	7.61822E-05
LC	LysoPE(0:0/18:0)	1.654915013	0.003270896
LC	1,5-Naphthalenediamine	1.654703348	4.73111E-14
LC	indoprofen	1.622851906	2.47715E-06
LC	N-(1-Deoxy-1-fructosyl)glycine	1.62230885	6.7269E-25
LC	Longilactone, delta-4(18)-Isomer, 2alpha-alcohol; (1R,2R,3R,3aS,5aS,6R,6aS,9S,10S,11R,12R,12aR,12bS,13R,13aS,14S,14aR,15S,15aR,16S,16aR,17R,17aR,18R,18aR)-18,18-dimethyl-1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18-octadecahydro-4H-benzofuro[3,2-b]pyridine-4-one	1.604978458	1.40755E-10
LC	gamma-Glutamylacetamide	1.60471643	8.53726E-07
LC	Symmetric dimethylarginine	1.603999405	4.19675E-07
LC	Creatine	1.593905884	0.01464511
LC	Sitostanol-beta	1.591968643	2.71244E-14
LC	Blumealactone C	1.589542394	2.56249E-12
LC	4,6,2',4'-Tetramethoxychalcone 2'-beta-glucoside	1.582224572	3.0114E-09
GC	Sitosterol	1.581459281	0.011367669
LC	Ganoderiol C	1.577912643	5.15331E-11
LC	Oxdralazine	1.573165585	2.60479E-12
LC	PE(20:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	1.571052151	0.000268259
LC	Pregnanediol-3-glucuronide	1.569011146	0.000935353
LC	DG(i-15:0/0:0/i-12:0)	1.564774242	1.20268E-11
LC	PC(2:0/PGE1)	1.560547429	0.001644284
LC	Schisanhenol	1.558844509	1.81423E-09
GC	D-Xylofuranose	1.557412914	3.22198E-13
LC	Naematolone	1.546891339	2.27814E-11
LC	Confusoside	1.534774964	1.86749E-10
LC	PE(10:0/10:0)	1.532944261	2.25749E-09
LC	27-Norcholestanehexol	1.529780646	3.60434E-11
LC	1-Hydroxy-2,2,5,5-tetramethylpyrrolidine-3-carboxamide	1.526350416	0.026131412
LC	Armatinol B	1.523137964	7.88902E-10
LC	N-Palmitoyl Arginine	1.509384497	0.036985273
LC	Pentaethylene glycol	1.507723353	6.7933E-05
LC	2-Hexadecyloctadec-9-enal	1.505430918	1.74759E-07
LC	Glycerol 1-propanoate diacetate	1.504739382	1.00346E-09
LC	bhos#40	1.498592116	4.73597E-10
LC	Perfluoroundecanoic acid	1.49584195	5.70822E-05
LC	Hydroquinone sulfate	1.490832585	5.38712E-05
LC	2-[(1r,3s)-3-Hydroxycyclohexyl]-5-(2-methyloctan-2-yl)phenol	1.486159369	1.27985E-16
LC	Clausarinol	1.483893959	0.000407528
LC	Gorgostane-3beta,5alpha,6beta,11alpha,12beta-pentol 12-acetate	1.478907343	3.05601E-08
LC	Dodecylbenzene	1.477164371	0.000110538
LC	5b-Cholestane-3a,7a,12a,23-Tetrol	1.472891383	1.15106E-09

LC	BAY-u9773	1.468296896	0.00013998
GC	Glucuronic Acid	1.46481744	8.04168E-06
LC	2-Hydroxy-3-methylbutyric acid	1.458146757	0.000634845
GC	(2r,3r)-2-Amino-3-Hydroxybutanedioic Acid	1.453899838	2.42443E-09
LC	Myricanene B 5-[arabinosyl-(1->6)-glucoside]	1.450317109	1.27471E-07
LC	(2S)-3-[3-[(4-Carbamimidoylbenzoyl)amino]propanoylamino]-2-[(4-ethylphenyl)sulfonyl]amino-1-propanol	1.448708574	7.21837E-08
LC	Bilirubin diglucuronide	1.448590242	3.93493E-08
LC	(2R,4S)-Pyrrolidine-2,4-dicarboxylic acid	1.43910938	0.000270192
GC	Mannobiose	1.434713195	0.014811044
LC	[1,1'-Biphenyl]-4-ol, 3-amino-	1.431367306	6.00949E-08
LC	2,12alpha-Dihydroxy-3-oxo-5beta-chol-1-en-24-oic Acid	1.431040894	0.010274667
GC	2,4-Dihydroxypentanedioic Acid	1.418385824	0.02357389
GC	L-(-)-Sorbose	1.418018011	4.01186E-07
LC	Pyrogallol-1-O-sulphate	1.41688468	0.00036034
GC	2-Hydroxybutyric Acid	1.415181276	9.56613E-11
LC	Sorafenib beta-D-Glucuronide	1.41482535	5.64284E-08
LC	Polyglycerol esters of fatty acids	1.409600437	0.001772705
LC	6alpha-Hydroxycastasterone	1.409372819	7.91987E-13
LC	Citrusinine I	1.407464648	4.932E-12
GC	Galactonic Acid	1.403051197	0.008091077
LC	Bentazone	1.40281291	3.88983E-25
LC	SM(d18:1/16:0(2OH))	1.401822443	0.025057923
LC	PI(18:3(6Z,9Z,12Z)/20:1(11Z))	1.398100284	0.004675007
LC	Cholestane-3,5,6-triol	1.386584578	1.16517E-10
LC	Tiazotic acid	1.383825135	2.50538E-09
LC	Melanettin	1.377371632	1.94571E-14
LC	(Z)-7-Dodecenyl butyrate	1.373676492	2.03243E-10
LC	N-(2-(Mercaptomethyl)-3-phenylbutanoyl)-L-alanine	1.37038432	7.69199E-12
LC	(2S,4R)-4-(9H-Pyrido[3,4-b]indol-1-yl)-1,2,4-butanetriol	1.367882721	2.98472E-15
LC	(11E,13Z)-10-Hydroxyoctadeca-11,13-dienoylcarnitine	1.367125321	9.15086E-07
GC	Leucrose	1.363766502	3.59385E-05
LC	Daucic acid	1.36327816	1.16083E-11
LC	Methacrifos	1.359796055	4.03021E-13
LC	(20R)-24-Hydroxygeminivitamin D3	1.357641186	3.85118E-07
LC	15S-HTPE	1.356677686	3.31388E-09
LC	Isoferulic acid 3-sulfate	1.348738588	0.007312743
LC	Methylenediphosphonic acid	1.34567188	0.001055644
GC	L-Tryptophan	1.344537361	5.89222E-08
LC	3beta,4beta-dihydroxycholest-23-one	1.341571151	1.82387E-08

GC	Glutaconic Acid	1.335572767	0.002869039
LC	2,2-Difluoro-n-(2-hydroxyethyl)-3-(2-nitro-1h-imidazol-1-yl)propanamide	1.334721464	0.000358464
LC	Ambrettolic acid	1.333773865	0.001347852
LC	Ambrisentan	1.330924408	6.93096E-22
LC	16-Deoxymyxinol	1.327185441	2.54802E-08
LC	Etodolac acyl glucuronide	1.321159427	0.001050768
LC	13'-Hydroxy-alpha-tocopherol	1.320662404	0.000550501
LC	Benzyloxycarbonyl-Val-Ala-Asp(OMe)-fluoromethylketone	1.31564306	9.51472E-08
LC	TETRAHYDROURIDINE	1.315640201	9.88862E-06
LC	Laninamivir	1.315078295	4.72882E-11
GC	Galactinol	1.314662258	0.026922345
LC	Phosphoric acid, mono(4-cyanophenyl) monomethyl ester	1.314512855	1.63562E-06
LC	3-Methyl-2-oxovaleric acid	1.31435357	0.001572127
LC	7beta,25-dihydroxycholesterol	1.313284326	1.62478E-08
LC	5beta-Cholestane-3alpha,7alpha,27-triol	1.309030157	1.23141E-11
LC	Eszopiclone	1.308072301	1.94372E-21
LC	Darexaban glucuronide	1.297878588	9.3707E-06
GC	Glucaric Acid	1.29347667	0.007820373
LC	7alpha,26-dihydroxy-5beta-cholestan-3-one	1.292758055	2.29368E-10
LC	(S)-3-(6-Methoxypyridin-3-yl)-3-(2-oxo-3-(3-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)pro	1.290923367	3.50156E-06
LC	Polysorbate 80	1.290314954	1.13316E-10
LC	(all-E)-3,5,7-Tridecatriene-9,11-diyn-1-ol	1.287141303	5.90686E-14
GC	3-Cyclohexene-1-Methanol	1.284516484	0.049951838
LC	(11E)-Tridec-11-enoylcarnitine	1.284000902	3.82809E-08
LC	1-Octen-3-yl acetate	1.281472594	8.28176E-11
LC	PS(24:0/20:3(5Z,8Z,11Z)-O(14R,15S))	1.281317653	2.97647E-06
LC	beta-D-fructose 2,6-bisphosphate	1.276343754	0.046504248
LC	19-oxodesacetylcinobufagin	1.275461979	4.11745E-06
LC	Tiaprost	1.273791552	1.43271E-07
LC	Lithocholic acid glucuronide	1.273546523	0.002439931
GC	Fructose 1-Phosphate	1.27175649	0.01133481
LC	LysoPI(18:2(9Z,12Z)/0:0)	1.266056939	0.000504996
LC	Lactobionic acid	1.258384781	3.79206E-11
LC	16beta-OH-Dhea sulfate	1.257892209	0.046511497
LC	Scutellarein 4'-methyl ether 7-glucuronide	1.254363732	3.87717E-05
LC	Glutarate semialdehyde	1.251914886	3.29138E-09
LC	(25R)-4beta,26-dihydroxycholesterol	1.24748465	3.06453E-10
GC	3,4-Dihydroxyphenylglycol	1.242660091	2.77563E-05
LC	LysoPE(P-18:0/0:0)	1.240490755	2.68332E-07

LC	Gelsenicine	1.238704491	4.54946E-12
GC	D-Xylose	1.237233244	0.000232236
LC	2,2':6',2"-Terpyridine	1.237051707	1.92734E-06
GC	Udp-N-Acetylglucosamine	1.236231064	5.38843E-05
GC	Gluconolactone	1.233841205	2.84597E-05
LC	Deoxycytidine	1.232408908	3.43009E-08
LC	Desflurane	1.231162652	1.61316E-13
GC	3-Aminopropane-1,2-Diol	1.229821745	0.016804042
LC	20a,22b-Dihydroxycholesterol	1.229431942	1.41191E-09
LC	Sphinganine 1-phosphate	1.22819153	7.18708E-05
LC	19-Oic-deoxycorticosterone	1.224931346	3.64464E-13
LC	Pregnenolone sulfate	1.223923983	0.020210567
LC	C16 Sphinganine	1.223794593	6.05841E-13
GC	D-Galactose	1.221376193	3.27561E-05
LC	Dexamethasone	1.219943867	1.21459E-06
LC	PE(O-18:0/0:0)	1.218139912	2.06224E-12
LC	Phosphovanillin	1.218037437	5.42545E-19
GC	D-Threo-Isocitric Acid	1.217746415	4.28734E-08
GC	Uric Acid	1.21620351	3.86109E-07
LC	Benzylpenicilloyl	1.216151883	5.07065E-11
LC	Serylvalylglycylglutamic acid	1.211251221	5.76314E-12
LC	3a,7a-Dihydroxycholanoic acid	1.210925986	7.36321E-07
LC	Undecanoylcarnitine	1.209550184	7.35925E-06
LC	L-Glutamic acid	1.205394744	0.00027443
GC	Linoelaidic Acid	1.202108658	3.03119E-09
LC	makisterone B	1.201886078	1.02461E-06
LC	GDP-mannuronate	1.197507335	9.71077E-05
GC	Dodecanol	1.19660098	0.018447715
LC	Succinylsulfathiazole	1.195668093	0.008454725
LC	LysoPE(0:0/20:4(8Z,11Z,14Z,17Z))	1.192939815	2.8019E-08
LC	Valylserine	1.183143626	3.56503E-05
LC	D-Lactic acid	1.182897022	0.001931519
LC	N6,N6,N6-Trimethyl-L-lysine	1.181879605	0.007052275
LC	PGP(PGF1alpha/18:0)	1.180323101	0.001613153
LC	8-Carboxymethyldihydrochelerythrine	1.179327724	4.23409E-08
LC	Bursin	1.178633568	1.45748E-08
GC	Ketoleucine	1.175660419	6.68119E-08
LC	IODODIFLUNISAL	1.174970878	0.004948984
LC	Dextrothyroxine	1.174004762	1.36097E-07

LC	Safingol (L-threo-sphinganine)	1.170975064	0.018387348
LC	m-Trifluoromethylhippuric acid	1.170540167	1.46622E-05
LC	Edetate trisodium	1.169722684	0.001185079
LC	(S)-Nerolidol 3-O-[a-L-rhamnopyranosyl-(1->2)-b-D-glucopyranoside]	1.169566391	0.000611494
LC	1,1,1,2,3,3,3-Heptafluoropropane	1.169402501	1.79597E-07
LC	Bergaptol	1.169017972	0.001743079
LC	Bisantrene	1.163179334	1.71798E-08
LC	LysoPI(18:1(9Z)/0:0)	1.162667162	1.01072E-08
LC	4,6-O-Ethylidene-D-glucose	1.160518728	1.06436E-10
LC	Phenylalanyltryptophan	1.159325965	0.000509969
LC	Triphenylphosphine oxide	1.156975715	9.58183E-07
LC	Apremilast	1.156293509	2.92863E-13
LC	Diguanosine diphosphate	1.153739413	7.17078E-08
LC	PHODA-PI	1.151062287	5.53769E-15
LC	6-(1,2,3,4-Tetrahydroxybutyl)oxane-2,3,4,5-tetrol	1.149845018	3.31884E-06
GC	N-Acetyl-Tryptophan	1.141870085	1.88594E-07
LC	5-Nonadecyl-1,3-benzenediol	1.139761748	1.92617E-09
GC	1,2-Propanediol	1.136035086	8.93271E-08
LC	N-3-hydroxy-13-methyl-hexadecanoyl glycyL-L-serine	1.133261547	7.96892E-07
LC	Isoflupredone acetate	1.130907838	0.001683722
GC	N-Alpha-Acetyl-L-Lysine	1.129653169	5.81088E-05
LC	Icotinib	1.12655806	6.91081E-19
LC	ChenodeoxycholyLtaurine	1.125916628	0.001474018
LC	(8Z,11Z,13E,15S)-15-Hydroxyicosa-8,11,13-trienoylcarnitine	1.12137012	0.00149066
LC	Campesteryl glucoside	1.119815162	0.005620214
LC	5-Hydroxyoctanoylcarnitine	1.114416716	5.72702E-05
LC	Glucosyl 6-hydroxy-2,6-dimethyl-2E,7-octadienoate	1.112204063	5.28866E-09
LC	15-hydroxycembra-1,3,7,11-tetraene	1.110551009	2.57608E-07
LC	PIM1(19:0/16:0)	1.110355082	0.000410268
LC	Glycinexylidide	1.108467857	4.14218E-09
LC	7-Amino-4-hydroxy-2-naphthalenesulfonic acid	1.105374419	0.000433706
LC	typhasterol	1.105348837	1.77229E-07
LC	Gyrophoric acid	1.102093794	0.012441174
LC	4-(4-Methoxyphenyl)-2-butanone	1.099769732	2.40176E-08
LC	3 alpha,7 alpha,26-Trihydroxy-5beta-cholestane	1.097658435	9.36945E-09
LC	5-Methoxysalicylic acid	1.09583463	0.01276689
LC	3-beta-Hydroxy-4-beta-methyl-5-alpha-cholest-7-ene-4-alpha-carboxylate	1.095648704	4.84528E-07
LC	Hirsutin	1.092191363	2.75445E-18
LC	Gluconic acid	1.08961736	3.5624E-05

LC	D-Mannose	1.087547276	0.000905525
LC	Callyspongendiol	1.087395071	3.46008E-10
LC	Momordol	1.082154252	2.15574E-10
GC	Quebrachitol	1.081787968	2.16818E-06
LC	2-Quinolinylmethanol	1.077081886	6.96285E-07
LC	Melanthugenin	1.074188386	7.00923E-07
LC	omega-linoleoyloxy-Cer(d20:1/32:0)	1.072884949	8.65716E-06
LC	3-Amino-5-(3-thiophenyl)-2-thiophenecarboxamide	1.072449973	8.95864E-05
LC	3-hydroxydecanoyl carnitine	1.07014953	1.59785E-05
LC	N-Acetylserotonin glucuronide	1.064802095	2.72532E-18
LC	LysoPE(P-18:1(9Z)/0:0)	1.055516617	5.19698E-08
GC	Phthalic Acid	1.055235543	0.007076062
LC	NNAL-N-glucuronide	1.05506139	1.82075E-08
LC	25-Acetylvulgaroside	1.054460118	0.006206929
LC	4-Hydroxybenzoic acid	1.054414052	2.33657E-09
GC	1h-Indole-2-Acetic Acid	1.054373789	0.000459681
LC	PE(14:1(9Z)/12:0)	1.052910636	3.19574E-07
GC	Shikimic Acid	1.050427422	5.0944E-05
LC	Serylmethionine	1.05021726	0.000192059
LC	7-Chloroemodin	1.049950067	6.12867E-14
LC	Leucyl-leucine	1.04923988	5.68426E-07
LC	2-hydroxy-9Z,12Z-Octadecadienoic acid	1.047346217	1.34841E-07
LC	farnesyl triphosphate	1.04205051	3.94004E-11
LC	plaunotol	1.041525176	9.62516E-09
LC	Indole	1.040677766	8.36688E-17
LC	Teleocidin B 2	1.040098076	0.000547234
LC	3-Hydroxy-1,10-bisaboladien-9-one	1.03818934	0.004548154
LC	12-tridecynoic acid	1.034793857	3.63108E-20
LC	Mulberrofuran Q	1.033107969	3.52486E-11
LC	SNAG-delta5-CT	1.028376595	1.98698E-05
LC	6-Nitrotryptophan	1.027077565	3.82194E-11
LC	Ribosylhopane	1.02643103	2.82385E-11
LC	Penicisteroid H	1.018244517	1.08954E-05
LC	7 alpha,24-Dihydroxy-4-cholesten-3-one	1.014163859	4.4465E-11
LC	1-Methyladenosine	1.012217471	7.60465E-10
LC	Tropisetron	1.012113342	0.016069794
LC	Dihydroxyacetone phosphate	1.010750013	0.004264067
LC	Dodecenoylcarnitine	1.009241096	2.54326E-05
LC	(7'S,8'S)-4,7'-Epoxy-3,8'-bilign-7-ene-3',5-dimethoxy-4',9,9'-triol 4'-glucoside	1.001694241	0.028532372

CRC_GC		VIP	P-value	log2(FC)
Dataclass	Metabolites			
LC	Edetic Acid	29.77516675	0.022670974	-0.25967
LC	GM4(d18:1/16:0)	7.184613967	0.048162072	-0.17694
LC	[3-Methoxy-2-phosphonooxy-6-[(E)-2-(3,4,5-trimethoxyphenyl)ethenyl]phenyl] dihydroge	6.552317172	0.017655846	-7.96095
LC	3,5-Dihydroxytetradecanoylcarnitine	5.943436346	0.006308104	-0.28801
LC	5-{2-Fluoro-5-[3-(3-hydroxy-2-methoxycarbonyl-phenoxy)-propenyl]-phenyl}-isoxazole-3-	5.353048266	0.048760356	-10.4705
GC	Maltitol	2.626025751	0.03783258	2.35471
GC	L-Erythrulose	2.620536925	0.028482614	1.9649
GC	3,5-Dimethylphenol	2.578842677	0.01772745	2.28505
GC	Lathosterol	4.768870042	0.000508801	-2.12474
GC	2-Mercaptoethanol	2.367790154	0.024028827	2.05919
LC	LysoPC(16:1(9Z)/0:0)	4.525791969	0.04651496	-0.29079
GC	Xanthine	4.439662586	0.025835897	-1.93149
GC	Dimethylethanolamine	2.201838452	0.005466176	0.54232
GC	Caprylic Acid	2.014069712	0.018419962	1.75179
LC	Porson	4.246862757	0.000912709	-4.55394
LC	D-Proline	3.886934209	0.008972325	-0.26759
LC	PC(18:0/P-16:0)	3.814656164	0.015266796	-0.15921
LC	Perfluorooctanoic acid	3.476109662	0.008211101	-1.35326
GC	3-Aminopropane-1,2-Diol	3.403750621	0.013318306	-5.84518
LC	Clausarinol	3.357039457	0.000700403	-4.76074
GC	Mannobiose	2.88155096	0.014160457	-1.84871
LC	Vignatic acid B	2.856005484	0.010424846	-0.21669
GC	3r-Hydroxy-Butanoic Acid	1.329260436	7.34299E-06	0.26004
GC	Butane-1,2,4-Triol	2.834360691	0.048089921	-1.17745
GC	N,N-Dimethylglycine	1.311597281	0.007004374	0.30644
LC	17-phenyl trinor Prostaglandin D2	2.829094507	0.022889968	-0.09852
LC	gamma-Glutamylserine	2.821546841	0.007138767	-0.27067
GC	Carbonate	1.151224436	0.012540237	0.25774
GC	4-Hydroxybutyric Acid	1.147027581	0.026514211	0.24627
LC	trans-Allo-ocimene	2.606566072	2.31574E-12	-0.69229
GC	Lactitol	2.448048327	0.002530042	-0.83861
LC	3-Methyl-2-oxovaleric acid	2.413185742	0.027742674	-0.21588
LC	Cefazolin	26.87268368	0.047223285	4.53798
LC	Floridin	23.69982568	0.031313835	2.30073
LC	L-Acetylcarnitine	12.43515769	0.006328427	0.32006
LC	2-beta-d-Ribofuranosyl thiazole-4-carboxamide	7.526381597	0.044079037	4.31218

GC	Galacturonic Acid	2.349145131	0.009708227	-0.39255
GC	M-Toluic Acid	2.293530163	0.030712237	-4.08416
LC	2,4-Thiazolidinedicarboxylic acid, 2-methyl-	2.270979323	0.027267598	-0.41446
LC	PC(O-16:0/3:0)	2.258363371	0.002950626	-0.46026
LC	Glycochenodeoxycholate-3-sulfate	5.219354802	0.030183959	1.84359
LC	5,6-Carboxyfluorescein	5.182990808	0.033576893	3.7299
LC	3-Hydroxy-1,10-bisaboladien-9-one	4.735234255	0.003239068	1.44526
LC	GlcCer(d16:1/18:0)	2.195754371	2.252E-07	-0.58391
LC	3,4-Dimethylethcathinone	2.146733367	0.00187812	-0.07746
LC	(-)-1-(Methylthio)propyl 1-propenyl disulfide	4.182592541	0.025664373	2.32976
LC	Bryacarpene 2	4.012370436	0.048971484	4.16378
LC	5-Phosphoribosyl-4-carboxy-5-aminoimidazole	3.909689964	0.025172517	2.37596
LC	TG(8:0/8:0/a-13:0)[rac]	2.074885094	0.007541406	-0.72771
LC	Demethyltorosaflavone C	3.817654526	0.037761495	4.22719
LC	LysoPC(O-18:0/0:0)	2.056633565	0.030030356	-0.22712
LC	Malyngamide H	3.721994212	0.031233529	1.55589
LC	Glyceryl 5-hydroxydecanoate	3.559163206	7.31512E-08	0.25425
LC	4-Oxo-2-nonenal	2.049888373	2.823E-11	-0.40525
GC	(2r,3r)-2-Amino-3-Hydroxybutanedioic Acid	1.982907116	0.002793685	-0.5333
LC	Sarothrin	2.861222763	0.044346613	4.48052
GC	3-Methylbutane-1,2-Diol	1.95298856	0.032235974	-0.45724
GC	Cellobiose	1.911133547	0.006070391	-0.60835
LC	Perfluoroundecanoic acid	1.909131699	0.027396209	-0.91331
LC	(4E,15E)-Bilirubin	2.676110561	0.000203163	0.96022
LC	Isoquinolinesulfonamide	2.659137825	0.044430335	4.22057
LC	5-Methyl-6-hydroxyluteolinidin	1.908173546	0.045511329	-7.32687
LC	Ammonia aspartate	2.593631785	0.030986133	0.09162
LC	2-Hydroxy-4-[(1R)-1-hydroxy-8-methyl-6-oxononyl]-3-methyl-2H-furan-5-one	2.586642917	0.044371367	3.62261
LC	lithocholic acid sulfate	2.582439584	0.023410221	2.11533
LC	Carbimazole	2.486578963	0.045123897	4.15221
LC	Hexazinone	2.422523608	0.023529577	0.56596
LC	(Z)-7-Dodecenyl butyrate	1.884306361	5.20106E-06	-0.13312
LC	Taurodeoxycholic acid 3-glucuronide	2.350948639	0.015884461	3.45959
LC	3,5,6-Trihydroxy-3',4',7-trimethoxyflavone	2.321275773	0.04906031	4.19963
LC	Polyglycerol esters of fatty acids	1.878380792	0.0351343	-1.29306
GC	Maltotriose	1.873118024	0.007957779	-0.76856
LC	Heptafluorobutyric acid	2.195780226	1.55365E-06	0.09094
LC	TETRAHYDROURIDINE	1.849918965	0.003863083	-0.55368
LC	1,1,1,2,3,3,3-Heptafluoropropane	2.151258512	3.45751E-06	0.08728

LC	8-Azaguanine	1.831626601	0.015093467	-0.25531
LC	LysoPE(P-16:0/0:0)	1.819436392	0.019624532	-0.2903
GC	Lactulose	1.813766191	0.002940747	-0.82536
LC	Ambrettolic acid	1.808463015	0.030272548	-0.54778
LC	(3a,5b,7a,12a)-24-[(carboxymethyl)amino]-1,12-dihydroxy-24-oxocholan-3-yl-b-D-Glucoside	1.980598216	0.0075181	2.86866
LC	Methiuron	1.942811121	0.005774556	0.93603
LC	OOB-PS	1.772428714	0.045272241	-0.30246
LC	gamma-Glutamylacetamide	1.723825124	0.005782317	-0.23477
GC	Beta-Lactose	1.672854373	0.006405899	-0.67661
LC	LysoPC(20:0/0:0)	1.615624101	0.020372364	-0.29978
LC	Cholesterol sulfate	1.604265337	0.000214304	-0.50714
LC	(2R,4S)-Pyrrolidine-2,4-dicarboxylic acid	1.574833899	0.046485761	-0.22905
LC	N,N-Dimethylformamide dimethyl acetal	1.823916213	2.54701E-06	0.25436
LC	Monocyclic botryococcane	1.81967258	0.010969127	0.06601
LC	Glutarate semialdehyde	1.481142595	0.004097102	-1.05415
GC	Beta-Mannosylglycerate	1.466603784	0.029746324	-0.43299
GC	Deoxyuridine	1.463188423	0.040305326	-6.0944
LC	Valylserine	1.451603516	0.038767102	-0.75568
LC	Tuberoside B (<i>Ullucus tuberosus</i>)	1.70597436	0.009508105	0.07965
LC	13-Heptadecyn-1-ol	1.666197563	2.43263E-05	0.16674
LC	2-Benzoyloxycinnamaldehyde	1.638354863	0.039426282	3.89545
LC	Glycerol 1-propanoate diacetate	1.446750041	0.01736237	-0.7105
LC	oscr#36	1.362422484	0.003092806	-0.89601
LC	13-methoxy-heneicosanoic acid	1.357647113	0.014643881	-0.49213
LC	Ponasteroside A	1.57086904	0.009271459	0.64045
LC	Rifamycin	1.552461516	0.020723001	3.7297
LC	Saxitoxin	1.517499776	0.013142771	0.89133
LC	Lithocholyltaurine	1.517230388	0.013556489	3.98357
LC	p-Hydroxylevamisole	1.50021901	0.014861087	1.95751
LC	Dihydropyridazine	1.50011764	0.002116766	0.0728
LC	Tamarixetin 3-O-sulfate	1.482665059	0.026482362	2.48241
LC	PS(P-16:0/19:0)	1.351866944	0.028876487	-0.1927
LC	Fostriecin	1.464631211	0.019206057	3.41658
LC	2-Nonenoic acid	1.330272899	0.002033766	-0.88084
LC	2-[(1r,3s)-3-Hydroxycyclohexyl]-5-(2-methyloctan-2-yl)phenol	1.329491557	0.002469223	-0.64868
LC	3-Methoxy-4-hydroxyphenylethyleneglycol sulfate	1.423705742	0.037115937	2.19083
LC	(Z)-6-Tetradecene-1,3-diyne-5,8-diol	1.421721402	1.54539E-05	0.15704
LC	ZOPOLRESTAT	1.414905564	0.029435701	2.25422
LC	Taurodeoxycholic acid	1.379342345	0.013754289	3.07354

LC	21H-Biline-8,12-dipropanoicacid, 3,18-diethenyl-1,19,22,24-tetrahydro-2,7,13,17-tetram	1.370880365	0.002355786	0.63337
GC	11alpha-Hydroxyprogesterone	1.315516821	0.043706312	-0.34546
LC	bhos#40	1.305421279	0.0015141	-0.75067
LC	Lumirubin	1.355086486	0.005764541	0.64079
LC	3beta,4beta-dihydroxycholest-23-one	1.26982742	0.004217943	-0.5981
LC	Spisulosine	1.340966539	0.005089286	0.06979
LC	(20R)-24-Hydroxygeminivitamin D3	1.257186406	0.014754447	-0.54405
LC	Riluzole	1.329808699	0.027400548	2.14942
LC	Avideoxycholic acid	1.255004282	0.006917716	-0.63218
GC	DI-Glyceric Acid	1.251478171	0.043820331	-0.48855
LC	17-hydroxy-heptadecanoic acid	1.291905642	0.000153753	1.38562
LC	(2E,4E,6E,8E)-3,7-Dimethyl-9-(2-nonoxyphenyl)nona-2,4,6,8-tetraenoic acid	1.270761216	0.028040061	2.17595
GC	D-Threo-Isocitric Acid	1.249851433	0.001022715	-0.42115
LC	Pseudouridine	1.268085652	0.012157611	0.48756
LC	(E)-2-Amino-5-phosphonopent-3-enoic acid	1.26233334	0.025920273	2.17567
LC	ecdysone 25-O-D-glucopyranoside	1.260502789	0.006236336	0.67945
LC	Glutaconic acid	1.247914231	0.009193061	-0.18971
LC	(3alpha,5alpha,22R,23R)-Cholestane-3,22,23-triol	1.246486825	0.003188049	-0.59827
LC	gailiapenta	1.25401377	0.012588399	3.11332
LC	PC(18:0(11cp)/0:0)	1.244611253	0.037237118	-0.27052
LC	LysoPC(P-16:0/0:0)	1.238345382	0.006273982	-1.04145
LC	9Z,12Z-Octadecadienyl acetate	1.245201228	0.038801338	1.48336
LC	Teasterone	1.225733939	0.000785992	-0.8026
LC	Phaeophorbide b	1.238654881	0.00013429	1.10202
LC	PC(19:0/0:0)	1.194045957	0.00367676	-0.45495
LC	3alpha,7alpha-Dihydroxy-5beta-cholest-23-en-26-oic acid	1.230582972	0.005647096	1.20929
LC	4-Allylphenol sulfate	1.193015311	0.035845463	-0.82601
LC	3-Ketosphingosine	1.223682017	0.033171307	0.28988
LC	4-Amino-4-deoxyarabinose	1.182288463	0.006595695	-0.24498
LC	LysoPE(P-18:0/0:0)	1.164045545	0.008061839	-0.37904
LC	Manbeta1-4Glcbeta-Cer(d18:1/16:0)	1.154426661	0.000327995	-0.4417
LC	Foliandrin	1.179990855	0.047079257	4.32235
LC	Bilirubin	1.17843603	0.024596628	0.56067
LC	5-Sulfo-1,3-benzenedicarboxylic acid	1.17420845	0.003973469	0.10632
LC	(all-E)-3,5,7-Tridecatriene-9,11-diyn-1-ol	1.148817812	0.000960469	-0.08935
LC	6alpha-Glucuronosylhyodeoxycholate	1.161798811	0.040305612	3.49025
LC	Cholestane-3,7,12,25-tetrol-3-glucuronide	1.158626103	0.009941161	0.78577
LC	Dihydroxyphenyl-valerolactone	1.144199193	0.003137417	-1.06209
LC	Myricanene B 5-[arabinosyl-(1->6)-glucoside]	1.153929742	0.033337232	0.52454

LC	(E)-4-(trimethylammonio)but-2-enoyl-CoA	1.153265086	0.018291021	4.18088
LC	1-(Methylthio)propyl propyl disulfide	1.151357372	0.02676249	2.08437
LC	7beta,25-dihydroxycholesterol	1.139582966	0.015660126	-0.44355
LC	CDP-DG(i-22:0/PGD1)	1.146894701	0.001699511	0.30382
LC	Pyrogallol Red	1.14484573	0.025552229	2.11805
LC	S-3-oxodecanoyl cysteamine	1.136962639	0.005065822	-0.22184
LC	Tiaprost	1.135368839	0.029600304	-0.5408
LC	Methyl (Z)-5-(5-methyl-2-thienyl)-2-penten-4-ynoate	1.110722479	0.014435592	-5.70255
LC	24-Nor-5beta-chol-22-ene-3alpha,12alpha-diol	1.103922851	0.002170175	-0.769
LC	N-Carboxyacetyl-D-phenylalanine	1.114894	0.009467115	0.57818
LC	N-docosahexaenoyl GABA	1.112112251	0.023555155	2.17533
LC	PE(O-16:0/0:0)	1.089043893	0.002725111	-0.39278
LC	Petroselinic acid	1.081810946	0.000162406	-0.34975
LC	O-(17-Carboxyheptadecanoyl)carnitine	1.097507213	0.041499541	0.52778
GC	Sedoheptulose	1.077896138	0.041317571	-0.42735
LC	Gorgostane-3beta,5alpha,6beta,11alpha,12beta-pentol 12-acetate	1.075552343	0.007886535	-0.83258
LC	16-Deoxymyxinol	1.070480113	0.026083594	-0.44939
LC	3-Phenyl-4-pentenal	1.063313394	0.023846647	-1.88341
LC	serofendic acid	1.068732163	0.022626909	1.20411
LC	LysoPC(20:1(11Z)/0:0)	1.060316811	0.028691702	-0.26485
LC	3 alpha,7 alpha,26-Trihydroxy-5beta-cholestane	1.056981192	0.001750616	-0.65
LC	Penicisteroid H	1.045368822	0.028769014	-0.5516
LC	Kresoxim-Methyl	1.05068649	0.000313871	0.85248
GC	Cis-Aconitic Acid	1.044812137	0.027003586	-0.51825
LC	1,2-Dioctanoyl PC	1.044831489	0.029187496	4.16999
LC	11beta,12beta-Dihydroxy-5beta-cholan-24-oic Acid	1.044345481	0.000513227	-1.04593
LC	5-Nitro-2-(3-phenylpropylamino)benzoic acid	1.043969003	0.020831934	0.612
LC	DG(8:0/PGE2/0:0)	1.032918845	0.048925666	2.02484
LC	Heptaethylene glycol monododecyl ether	1.030444418	0.037899143	0.28302
LC	Phenyl vinyl sulfide	1.025510498	0.014137733	0.10453
LC	Bis(2-propoxyethyl) 2,6-dimethyl-4-(3-nitrophenyl)-3,4-dihydropyridine-3,5-dicarboxylate	1.023274891	1.03907E-05	0.24781
LC	Pregnanediol-3-glucuronide	1.013366218	0.033694708	0.88129
LC	5-(3',5'-Dihydroxyphenyl)-gamma-valerolactone-O-sulphate-O-methyl	1.011818038	0.042436923	3.95919
LC	Glucosyl 6-hydroxy-2,6-dimethyl-2E,7-octadienoate	1.010425731	0.038990323	-0.68619

Supplementary Table 2

CRC					
Dataclass	Metabolites	Score	VIP	P-value	log2(FC)
LC	Propofol glucuronide	51.7	42.49817221	8.55861E-10	19.07257438
LC	LysoPC(0:0/18:2(9Z,12Z))	75.2	39.47754279	4.36019E-11	-0.727652673
LC	Edetic Acid	64.2	17.2619243	0.002920995	0.509698064
LC	Floridin	37.2	13.59326069	0.005470616	12.54389347
LC	PC(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/P-18:1(11Z))	44.7	12.48540157	0.000941439	0.369119974
LC	Carissanol	49.2	11.908102	2.5157E-17	46.71698349
LC	LysoPC(20:4(5Z,8Z,11Z,14Z)/0:0)	71.5	11.63081531	0.000659239	-0.380526211
LC	Cefazolin	50.8	11.13027078	0.037648397	16.60945755
LC	Lidocaine	67.4	10.25208078	2.4692E-07	10.4153208
LC	L-Acetylcarnitine	65	9.568914567	1.35872E-06	0.632826879
LC	PC(P-18:1(11Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))	46.7	9.539132309	1.2835E-07	0.635860039
LC	Dehydroepiandrosterone sulfate	55	9.420918289	3.87093E-06	-1.044090391
LC	N-(2-Hydroxyethyl)-2-(1-isoquinolinylmethylene)hydrazinecarbothioamide	38	9.034904108	1.32234E-14	8.843472801
LC	1-O-(2-methoxy-4Z-hexadecenyl)-sn-glycero-3-phosphocholine	56.2	8.387712311	8.27263E-11	-0.669886089
LC	Isocitric acid	63.8	8.268257009	3.77399E-11	0.904076446
LC	1-(O-alpha-D-glucopyranosyl)-29-keto-(1,3R,31R)-dotriacontanetriol	54.1	8.137192793	7.66668E-08	-0.54734215
LC	Myristyl linoleate	39.3	7.293027309	1.53382E-05	14.76594422
LC	2-C-methyl-D-erythritol-4-phosphate	39.3	6.608794507	2.82786E-06	0.292099645
LC	2-Methyl-4'-(methylthio)-2-morpholinopropiophenone	50	6.526906048	2.63902E-16	44.97719463
LC	LysoPC(0:0/18:0)	74.6	6.473041889	4.97807E-05	-0.290628331
LC	SM(d19:1/17:1)	47.5	6.461664278	0.000474572	-0.348223403
GC	P-Cresol Glucuronide	82.2	6.169756794	3.46361E-09	15.35038527
LC	UTILIN	37.1	5.865190773	1.18555E-14	14.95453522
LC	PC(0:0/14:0)	73.2	5.650490153	1.21615E-07	-1.023676176
LC	19-Epischolaricine	49.6	5.489759575	7.3543E-13	13.68437485
LC	SM(d18:0/16:1(9Z))	55.9	5.427568515	0.048506935	-0.226502234
LC	SM(d18:1/16:1(9Z))	55	5.424866725	0.00772874	-0.174288833
LC	S-Japonin	42	5.305731909	2.72318E-08	1.588389631

LC	Benzoxazole	38.6	5.189941289	0.006969556	0.307546864
GC	Equilenin	77.7	5.019844924	5.65742E-12	10.17264487
LC	Chenodeoxycholic acid glycine conjugate	60.5	4.914568141	0.00250336	-1.704015561
LC	N-Nitrosoanatabine	42	4.908067503	9.0431E-08	0.137617405
LC	13-Hydroxyoctadecanoylcarnitine	68.9	4.692914047	9.00106E-06	0.753871157
LC	4-(2-Aminoethylamino)-3-[bis(carboxymethyl)amino]-3-(carboxymethyl)hexanedioic acid	38.6	4.575558576	7.80926E-16	12.52684064
LC	GM4(d18:1/16:0)	44.4	4.547326604	0.002240535	-0.226897789
LC	PE(20:3(8Z,11Z,14Z)/19:1(9Z))	55	4.257968073	0.004986593	0.350544693
LC	L-Carnitine	71.8	4.196477586	0.019107079	0.205124901
LC	TG(8:0/8:0/a-17:0)[rac]	46.1	4.192833218	0.001807578	-0.88258484
LC	O-Linoleoylcarnitine	70.2	4.158315188	0.000124559	0.762378005
LC	Oxotremorine	43.5	4.10126294	3.47602E-10	10.08617735
GC	M-Toluamide	71.5	4.07408551	1.09868E-11	7.168033275
LC	Vignatic acid B	38	4.047582595	8.15219E-09	-0.80393699
LC	Pulverulentoside I; (1aS,1bS,2S,5aR,6S,6aS)-6-({3-O-Acetyl-6-deoxy-2-O-[(2E)-3-(4-methoxyphenyl)-2-propenoyl]-?-L-mannopyranosyl}oxy)-1a-(hydroxymethyl)-1a,1b,2,5a,6,6a-hexahydrooxireno[4,5]cyclopenta[1,2-c]pyran-2-y I ?-D-glucopyranoside	36	3.858844175	4.23574E-07	44.00579231
LC	Disodium ethylenediaminetetraacetate	39.4	3.816321676	0.001501447	0.448632265
LC	PE(17:0/22:4(7Z,10Z,13Z,16Z))	54.7	3.811016687	0.018020845	0.249631195
LC	Ecabet	45.3	3.756021836	1.65235E-08	1.080698266
LC	2,2'-Methylenebis(4-methyl-6-tert-butylphenol)	58.3	3.737504178	4.48394E-09	11.7457015
LC	LysoPE(18:1(9Z)/0:0)	72.8	3.690409776	0.003272017	0.493191335
LC	6-Butyryl-5-hydroxy-4-phenylseselin	39	3.628337528	3.44845E-06	-1.021114355
LC	(Z)-1-(Methylthio)-5-phenyl-1-penten-3-yne	45.2	3.610219464	3.75868E-17	-0.887478814
LC	Phyllocoumarin	52.4	3.586812347	1.44928E-14	9.450965066
LC	Armilaripin	56.8	3.567906255	3.75531E-13	-4.232566273
GC	Lactulose	89.8	3.495048836	1.17209E-08	5.208099944
GC	3-(Pyrazol-1-Yl)-L-Alanine	91	3.478503833	1.07455E-05	-3.187666237
LC	GM4(d18:1/18:0)	42.3	3.427226609	0.00077003	-0.614313666
LC	Enterodiol sulfate	37.4	3.42070736	2.46749E-05	1.579700736
LC	Decanoylcarnitine	62.7	3.411000528	0.040108029	-1.602939568

LC	21H-Bilane-8,12-dipropanoicacid, 3,18-diethenyl-1,19,22,24-tetrahydro-2,7,13,17-tetramethyl-1,19-dioxo-	62.3	3.400435988	3.20379E-10	-2.811250528
LC	LysoPC(20:4(8Z,11Z,14Z,17Z)/0:0)	73.5	3.39666242	0.014970982	-0.253895079
LC	3-(4-Iodophenyl)-2-mercapto-(Z)-2-propenoic acid	38.4	3.26460273	0.000643291	0.418225743
LC	PI(O-18:0/18:0)	36.3	3.240315512	0.000414215	0.468715233
LC	LysoPC(18:0/0:0)	59.6	3.233124088	0.000246821	-0.35944229
LC	Fluroxene	46.1	3.230422598	6.13729E-08	2.293039304
LC	Allopregnanolone sulfate	41.8	3.220783822	0.000694672	-0.862715685
LC	Cichorioside K	52.1	3.188583861	1.87411E-07	9.753205695
LC	PS(P-20:0/22:2(13Z,16Z))	53	3.159384796	0.000497199	0.418856311
LC	Isoscoparin 2"-O-glucoside	36.5	3.158622876	0.011737836	0.522152731
LC	PC(14:1(9Z)/20:3(8Z,11Z,14Z))	39	3.158472497	0.000655833	-0.633461507
LC	2-beta-d-Ribofuranosyl thiazole-4-carboxamide	40.2	3.142837949	0.033532879	9.860432416
GC	2,6-Pyridinedicarboxylic Acid	73.2	3.04429804	0.000467607	-2.894086621
LC	EUPARIN	37.4	3.041424033	8.53003E-07	2.963091245
LC	2-Methoxy-4-(2-(methylamino)propyl)phenyl beta-D-glucopyranosiduronic acid	40	2.998019222	1.56684E-11	15.04521702
LC	Thiamine	43.2	2.986735683	9.89438E-16	15.10938615
GC	Maltotriose	94.5	2.967438411	3.93626E-08	5.019357256
LC	LysoPE(P-16:0/0:0)	59.2	2.943208684	2.00632E-15	-1.021100062
LC	GM4(d18:1/20:0)	43.3	2.896561691	1.35716E-05	-0.582422757
LC	Sphingosine 1-phosphate	72.9	2.872973969	4.17964E-06	0.719163797
LC	PS(P-20:0/0:0)	54.8	2.869241249	1.94025E-11	-0.869696826
GC	Cis-Aconitic Acid	91.3	2.839031115	1.91216E-07	2.571242221
LC	Caffeine	60.3	2.836388459	2.98414E-05	-7.352759987
LC	LysoPC(O-18:0/0:0)	56.4	2.813916526	6.88096E-11	-0.674477043
LC	6-Thioxanthylic acid	41	2.802940246	5.21422E-05	0.539086555
LC	PE(22:4(7Z,10Z,13Z,16Z)/21:0)	46.1	2.792774107	0.002827525	0.305318458
LC	LysoPE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	73	2.739654725	0.002262948	0.479695908
LC	lysine phosphoester	42.7	2.738394426	1.10672E-16	-0.926138618
LC	alpha-Hydroxyisobutyric acid	62.9	2.713289561	4.89805E-08	1.413276248
GC	Mannobiose	81.8	2.702951156	4.04999E-06	-2.821771229
LC	Plantacyanin	37.3	2.692902203	6.32772E-07	11.74308534

LC	dIDP	38.6	2.680611052	3.6366E-05	6.70806104
LC	LysoPC(0:0/20:4(5Z,8Z,11Z,14Z))	73.6	2.665988563	0.001932634	-0.333905535
LC	Vaccenic acid	52.5	2.657321417	5.07884E-18	0.535180914
LC	2-Oxoarginine	41.7	2.616648409	2.34915E-06	-2.152693903
LC	PC(12:0/20:1(11Z))	40.8	2.615534205	0.024230165	0.3557155
GC	Lactitol	95.8	2.598859082	4.1221E-08	4.47494889
LC	3,7-Dihydroxycholan-24-oic acid	58.2	2.596328246	0.002277093	-3.95099439
LC	PE-NMe2(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	39	2.572915343	0.000184811	0.190814951
LC	LysoPE(0:0/18:2(9Z,12Z))	76.1	2.55685943	0.041348246	-0.326553943
LC	Gravolenic acid	38.2	2.535145661	1.25085E-15	9.112039998
LC	Ptilosaponoside B	43.3	2.534596132	1.39127E-15	-4.6583077
LC	PC(17:2(9Z,12Z)/0:0)	68.8	2.530884685	2.01802E-12	-0.651265755
LC	Pyridine N-oxide glucuronide	45.1	2.525441791	1.41685E-17	-0.689359056
LC	APC	60.4	2.522022165	1.035E-16	-3.916759138
LC	PC(18:0/P-16:0)	38.3	2.483996322	0.006576642	0.307080036
LC	Theophylline	57	2.473532016	3.40937E-05	-6.190365882
LC	3-Hydroxy-1,10-bisaboladien-9-one	60.1	2.460036938	8.1062E-05	2.540579182
LC	Methyl 3-epi-4,5-didehydrojasmonate	55.4	2.459175956	0.000160245	-0.739698332
GC	Quinic Acid	87.5	2.444090937	0.001652102	-7.577062134
LC	Octenoyl-L-carnitine	77.4	2.428760739	0.002018958	-0.646576895
LC	1-O-Hexadecyl-sn-glycero-3-phosphocholine	59.6	2.415245297	3.53666E-12	-0.793006309
LC	Hydroxyzine	41.3	2.406651062	1.24797E-05	1.080385732
LC	9-tridecynoic acid	47.9	2.397123658	1.8413E-06	0.137193724
LC	3-Hydroxylidocaine	42.3	2.395202512	6.85042E-10	9.629763433
LC	(-)-1-(Methylthio)propyl 1-propenyl disulfide	39.1	2.392819976	0.004134558	16.35224975
LC	DG(18:3(9,11,15)-OH(13)/15:0/0:0)	50	2.350536602	4.77286E-07	-3.098868289
GC	Melezitose	82.7	2.33823233	0.004851492	1.912543881
LC	PC(O-16:1(11Z)/0:0)	58.5	2.318896321	6.45531E-10	-0.762657036
LC	TG(8:0/8:0/a-13:0)[rac]	41.9	2.314677188	2.86545E-07	-1.695088807
LC	[(2S,4R,5R,6R,14S,16R)-14-Hydroxy-7,11-dimethyl-6-(2-oxopyran-4-yl)-3-oxapentacyclo[8.8.0.02,4.02,7.011,16]octadecan-5-yl] acetate	53.8	2.298391961	2.36295E-13	-4.847549212
LC	Salvianolic acid D	45	2.296432304	0.042377746	15.72436875

LC	PC(P-18:1(11Z)/18:2(9Z,12Z))	47.1	2.29304248	0.033194972	-0.297761551
LC	LysoPE(0:0/18:1(11Z))	74	2.29203755	0.000965336	0.57448127
LC	SM(d16:2(4E,8Z)/TXB2)	40.1	2.256344468	0.006823403	-0.400896323
LC	2-Hydroxycinnamic acid	51.2	2.239594123	0.000407668	-0.281846321
GC	Oleic Acid	97	2.235259281	5.47719E-15	1.757303873
LC	3,4-Dimethylethcathinone	39.7	2.222408403	6.81941E-13	0.275666558
LC	5-Phosphoribosyl-4-carboxy-5-aminoimidazole	41.2	2.21742822	0.004402249	13.60453314
LC	(-)-Salvisyriacolide	48.4	2.207861118	2.15026E-07	-3.619466846
GC	Ribonic Acid	87.7	2.206744123	5.17386E-08	-1.199087785
LC	27-Hydroxycholesterol	68.7	2.201059461	5.37126E-12	-1.398358181
LC	(5Z,9Z)-2-methoxy-hexacosadienoic acid	55.6	2.196545835	1.54517E-13	-1.873803557
LC	LysoPC(22:5(7Z,10Z,13Z,16Z,19Z)/0:0)	69.6	2.19313766	0.032264472	-0.317606977
LC	5,6-Carboxyfluorescein	42.9	2.187386078	0.023292318	5.655920492
LC	4-Allylphenol sulfate	47.8	2.185962233	1.54636E-10	-2.769470207
LC	2-((2-Methoxy-2-(3-(trifluoromethyl)phenyl)ethyl)amino)ethyl 4-(2-(2-(9H-fluoren-9-yl)acetamido)ethyl)benzoate	46.2	2.178340441	1.07007E-16	-6.469499445
LC	Galactotriose	51.6	2.159792907	0.000268063	10.33512266
LC	Spiropiperidine	38.1	2.143751302	4.59915E-13	-0.934288114
LC	gamma-Glutamylserine	69.9	2.140807688	1.35977E-06	0.777438447
LC	3,4-Bis(carboxymethyl)-3,4-dihydroxyhexanedioic acid	42.4	2.137505791	7.15661E-17	-0.624690652
LC	3-hexanoyl-NBD Cholesterol	39	2.133973148	4.87466E-15	0.475067214
GC	Levogluconan	92.4	2.104786048	0.001889958	1.884892529
GC	3-Hydroxybutyric Acid	97.8	2.102690259	2.82965E-07	2.700566654
LC	Trihydroxycoprostanic acid	62.7	2.102329678	1.38215E-10	-1.447375613
GC	3-Methylbutane-1,2-Diol	82.2	2.096532824	0.000302983	1.346167904
LC	6"-Acetylliquiritin	37.5	2.090160826	5.71294E-08	7.329463621
LC	Glycocholic acid	63.6	2.080174705	0.011366738	-1.354030874
LC	BAY-u9773	45.8	2.076332055	1.98401E-09	41.9625605
LC	indoprofen	48.6	2.071726504	9.51453E-07	1.552228677
LC	3-[(1R,4S,5S,6R)-6-[(1E,3S,5Z,8Z,11Z)-3-Hydroperoxytetradeca-1,5,8,11-tetraen-1-yl]-2,3-dioxabicyclo[2.2.1]heptan-5-yl]propanoylcarnitine	38.2	2.067666959	0.002917231	-1.586522506
LC	Octadec-5-enoic acid	58.2	2.05946082	6.94076E-09	0.918075284
LC	Demissidine	66.5	2.045613252	2.44702E-11	-1.420633139

LC	PI-Cer(t18:0/18:0(2OH))	36.2	2.042118723	3.44384E-06	0.39688878
LC	Kuguacin E	64	2.034175757	1.63259E-08	-0.880482257
LC	Dehydropachyrrhizone	37.7	2.032633963	1.76064E-14	6.807383024
LC	3-Methyl-2Z,4E-decadienoic acid	41.3	2.031471123	2.95136E-10	41.88999038
LC	SM(d18:1/14:0)	55.9	2.019353736	0.009694017	-0.384824166
LC	Zearalenone	52.3	2.015782898	1.38073E-10	9.601335307
LC	Ansamitocin P3	44.2	2.003818393	1.0961E-15	-3.261857205
LC	6-Hydroxy-3,4-dihydro-2(1H)-quinolinone	56.3	1.993867973	1.55654E-16	-0.833218963
LC	LysoPC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	72.5	1.979809839	0.034813181	0.315373898
GC	Lathosterol	95.8	1.973611905	0.00047797	-2.312623188
LC	Ambrettolic acid	54.2	1.953670578	1.2543E-06	-1.188437843
LC	Artemoin A	52.1	1.952474323	0.000250384	-0.905715209
LC	Desacetycefapirin	37.4	1.951657459	9.52697E-20	41.44828786
LC	N-Choloylglycine	65.8	1.94278213	0.004378367	-1.46358351
LC	Ammonia aspartate	39.6	1.940393697	0.015065224	0.267699292
LC	Melibiose	57.4	1.939323645	2.26121E-07	12.10636651
LC	16-oxo-palmitate	42.3	1.927899179	7.85485E-11	-1.555943324
LC	Mactraxanthin 3-linoleate 3'-dipalmitoleate	37.1	1.922054407	0.015831232	0.197523174
LC	3b-Hydroxy-5-cholenoic acid	62.9	1.916556959	0.001774865	-2.141789281
LC	Isothankunic acid	36.6	1.915111552	4.9734E-10	-1.450415863
LC	N-Palmitoyl Arginine	44.8	1.914045288	0.000998682	-0.673158619
LC	SM(d18:1/12:0)	43.3	1.90773961	1.5654E-08	-1.672821426
LC	5alpha-Cholestane-3alpha,7alpha,12alpha,24-tetrol	38.8	1.890016505	5.78885E-13	-1.84347603
LC	Quercetin 3'-isobutyrate	41.4	1.886251033	0.043292328	12.70449811
LC	Cohibin A	50.7	1.872758156	2.6842E-09	-1.422733737
LC	2-Deoxybrassinolide	67	1.872576165	3.55804E-09	-1.504216643
LC	LysoPC(P-18:1(9Z)/0:0)	56.4	1.866329038	8.91119E-09	-0.60806642
LC	UDP-D-galacturonic acid	41.1	1.847146006	0.000197803	0.095169929
LC	PE-Cer(d15:2(4E,6E)/20:0)	38.9	1.838616812	1.8686E-07	-0.957108623
GC	10-Heptadecenoic Acid	85.9	1.836594218	0.00263448	1.836018508
LC	Bis(2-ethylhexyl) phthalate	59.1	1.829509305	0.004088095	2.016224841

LC	(1R)-5-[2-[(1R,7Ar)-7a-methyl-1-[(2R)-6-methylheptan-2-yl]-2,3,3a,5,6,7-hexahydro-1H-inden-4-ylidene]ethylidene]-4-methylidenecyclohexane-1,3-diol	65.6	1.825263451	1.6188E-10	-1.352564586
LC	5alpha-Pregnan-3beta,20beta-diol 20-sulfate	41.6	1.820247968	0.004380918	-2.660953117
GC	3,5-Dimethylphenol	85.2	1.818722124	0.002529207	6.221310855
GC	Methyl L-Alaninate	73	1.802826861	0.012661837	-1.069537125
LC	Melatonin glucuronide	36.9	1.792198449	1.42574E-14	14.45199518
LC	2-[(2-Fluorophenyl)sulfanylmethyl]-5-[6-[(2-hydroxycyclopentyl)amino]purin-9-yl]oxolane-3,4-diol	37.1	1.782733747	5.28971E-08	41.7120456
LC	Ethyl n-allyl-n-[(e)-2-methyl-3-[4-(4-amidinophenoxy)carbonyl]-phenyl]propenoyl]amino acetate	45.4	1.767588186	1.37606E-17	-5.666991119
LC	SALSOLIDINE	42.4	1.767323834	0.002745276	-2.01397683
LC	Sesamol	49.1	1.7477448	0.003461947	-1.85550569
LC	2,4-Diamino-6-nitrotoluene	39.3	1.729521819	4.28708E-11	0.261560617
GC	2,4-Dihydroxypentanedioic Acid	77.1	1.729366659	0.005339578	0.875400907
LC	D-Lactic acid	71.1	1.727906981	0.001370748	0.470349851
LC	1,1,1,2,3,3,3-Heptafluoropropane	40.9	1.72709705	1.23953E-15	0.211655581
GC	Galactonic Acid	81.9	1.723181484	0.002930658	-1.658612334
LC	OOB-PE	44.5	1.71806048	0.000625607	-0.19805063
LC	Piperine	74.8	1.717747084	0.045463612	-4.354265638
LC	bhos#40	53.5	1.701051713	5.85616E-14	-1.884077234
LC	Cefodizime,(S)	44.1	1.70104054	3.69182E-06	0.124587545
LC	Chenodeoxycholic acid	57.7	1.69184219	0.003761494	-2.026284303
LC	Mayolene-17	56.4	1.682907933	6.74861E-11	-2.855823215
LC	Bryacarpene 2	44.5	1.681136132	0.036196184	11.75327241
LC	DG(18:3(9Z,12Z,15Z)/15:0/0:0)	49.2	1.680670717	0.000398678	-0.648332957
GC	D-Xylose	88.2	1.678417919	4.47381E-06	0.948883928
LC	3-Amino-6-{4-[(4-Methylpiperazin-1-Yl)sulfonyl]phenyl}-N-Pyridin-3-Ylpyrazine-2-Carboxamide	50.2	1.677061072	2.71856E-06	-1.026960415
LC	PC(O-16:0/3:0)	45.6	1.675656576	4.82045E-08	-0.720124752
LC	1,5-Naphthalenediamine	44	1.669077005	5.41393E-17	-0.886254474
LC	Stercobilinogen	50.5	1.656342892	0.028153421	4.731643316
GC	Cis-Erucic Acid	92.4	1.65616121	1.90766E-08	1.377869366
LC	3alpha-Hydroxy-5beta-chola-7,9(11)-dien-24-oic Acid	54.3	1.648741771	0.013952712	-2.764290301

LC	Uridine 2',3'-cyclic phosphate	45.6	1.644484835	0.001941689	0.569436791
LC	(11E)-Octadec-11-enedioly carnitine	48.1	1.644262612	0.000522049	1.955096252
LC	Androstenediol 3-sulfate	43.1	1.633455669	0.000701675	-0.819162473
GC	1,3-Benzenedicarboxylic Acid	85.7	1.614876192	0.014436224	1.580355248
LC	Gorgostane-3beta,5alpha,6beta,11alpha,12beta-pentol 12-acetate	41.3	1.610606835	2.57361E-11	-2.282503635
LC	Marmesin rhamnoside	37.8	1.603789166	4.52583E-09	13.53489803
LC	Heptafluorobutyric acid	50.8	1.60117464	4.58913E-14	0.192910174
LC	beta-D-fructose 2,6-bisphosphate	38.8	1.599411315	0.01680882	-0.520181997
LC	5-Hydroxy-2-imino-1-methylimidazolidin-4-one	41	1.599012897	3.31356E-18	0.477526774
LC	Propylparaben	45.5	1.598017866	0.03477292	0.754434844
LC	(20R)-24-Hydroxygeminivitamin D3	47.1	1.596799428	2.452E-10	-1.345330723
LC	PE(10:0/10:0)	39.2	1.58684232	9.93136E-12	-0.922517835
LC	Mesobilirubinogen	49.8	1.58270969	0.04744512	1.77003862
GC	Dodecanol	81.4	1.578848163	0.001955347	-1.778273366
LC	3-Hydroxymethyl-picumast	50.5	1.576352661	0.003291373	-0.75390454
LC	1-Hydroxy-2,2,5,5-tetramethylpyrrolidine-3-carboxamide	50.5	1.575555982	0.029295932	3.076914156
LC	Symmetric dimethylarginine	58.6	1.567192762	1.38255E-05	0.573107336
GC	Maltitol	82.6	1.562290949	0.007377188	6.470752849
LC	PE-Cer(d14:2(4E,6E)/23:0)	56.7	1.561452325	0.000912827	-0.22617225
LC	3beta,4beta-dihydroxycholest-23-one	48.2	1.558053457	2.32937E-11	-1.533531601
LC	(2S)-1,1,1-Trifluoro-2-(4-pyrazol-1-ylphenyl)-3-[5-[[1-(trifluoromethyl)cyclopropyl]methyl]-1H-imidazol-2-yl]propan-2-ol	52	1.557118943	2.72246E-23	16.14219439
LC	Ganoderiol C	45.5	1.5523282	1.92293E-11	-1.729436293
LC	Demethyltorosaflavone C	45.1	1.551043667	0.0332785	4.988859923
LC	4-(2-Aminoethyl)benzenesulfonyl fluoride	37.3	1.545317659	1.12302E-06	2.249331937
LC	Dodecylbenzene	37.7	1.527097902	5.25338E-05	-0.550848332
LC	Uridine diphosphate glucose	52.1	1.526628066	4.79333E-06	-2.247777858
LC	Blumealactone C	41.5	1.521426184	5.96746E-10	9.171915163
GC	Cellobiose	99.5	1.51852037	2.91857E-07	1.664617881
LC	7beta,25-dihydroxycholesterol	38.7	1.51118216	1.04413E-10	-1.218481834
LC	Zierin	37.4	1.505109076	8.64151E-12	11.88020816
LC	LysoPE(P-18:0/0:0)	53.1	1.499681041	5.33839E-13	-1.067831034
LC	Ikarisoside D	36.7	1.493017706	1.21604E-07	41.24749127

LC	Cabozantinib	39.1	1.491279376	7.61124E-07	41.28624367
LC	Oxdralazine	37.3	1.490592189	6.27694E-09	5.553402149
LC	16-Deoxymyxinol	55.4	1.482235131	6.07781E-10	-1.250056864
LC	Darexaban glucuronide	40	1.479381022	5.15096E-05	1.509001985
LC	(4S,6R)-6-[(1E)-4,4-Bis(4-fluorophenyl)-3-(1-methyltetrazol-5-yl)buta-1,3-dienyl]-4-hydroxyoxan-2-one	39.3	1.457682746	2.12112E-06	9.2470834
GC	1,2-Propanediol	95.2	1.456349934	3.94499E-06	2.510698016
LC	Pregnenolone sulfate	53.2	1.447412635	0.000877283	-0.733588232
LC	Cholestane-3,5,6-triol	72.8	1.446615871	3.78705E-12	-1.758012878
LC	Daucic acid	45.5	1.44185227	5.58056E-16	-0.606770814
GC	L-Tryptophan	88.5	1.439971595	1.67086E-08	-0.973861622
LC	Sulfaethidole	37.5	1.431763613	0.00868341	0.518310694
LC	2,2':6',2"-Terpyridine	36.4	1.431065901	9.25407E-07	3.016849598
LC	8-Azaguanine	39.5	1.42830507	4.10414E-06	-0.47833826
LC	N-(2-(Mercaptomethyl)-3-phenylbutanoyl)-L-alanine	43.8	1.422836682	1.19975E-10	10.43344325
LC	Gcdcs	68.8	1.420296646	0.002699526	0.911581526
LC	Hydroquinone sulfate	42.4	1.418006261	5.97496E-05	-5.082394612
LC	Dodecanoylcarnitine	59.3	1.412810369	0.005912259	-0.909132607
LC	15S-HTPE	51.9	1.404250593	2.74552E-10	-2.814750637
LC	7-Amino-4-hydroxy-2-naphthalenesulfonic acid	38.7	1.404216962	9.0741E-05	3.839991208
GC	Cytidine Monophosphate	83.7	1.399725205	0.010015967	2.987902867
LC	6alpha-Hydroxycastasterone	48.3	1.395935429	1.46313E-13	-2.000545072
LC	2,4-Thiazolidinedicarboxylic acid, 2-methyl-	63.8	1.395544257	0.000361617	0.780629771
LC	27-Norcholestanehexol	44.7	1.392746479	2.72704E-10	-1.513703836
GC	Delta-Tocopherol	84.3	1.389674181	0.004810235	2.745777645
LC	3-Hydroxy-4-aminopyridine sulfate	43.3	1.389455693	0.03521443	0.246254109
GC	(S)-3,4-Dihydroxybutyric Acid	93.6	1.384606819	2.79936E-06	0.815702189
LC	makisterone B	48.7	1.382937153	2.07571E-11	-0.904051784
LC	Campesteryl glucoside	37.7	1.381441258	0.000185431	-1.215649001
LC	Armatinol B	51.5	1.377061535	2.48033E-08	-1.368984289
LC	DG(i-15:0/0:0/i-12:0)	44.4	1.372289758	3.59805E-09	-1.401142819
LC	5b-Cholestane-3a,7a,12a,23-Tetrol	61.2	1.362759764	2.96439E-08	-1.248209565
LC	LysoPC(20:0/0:0)	59.4	1.356829162	3.49368E-07	-0.537571825

GC	Linoelaidic Acid	96.5	1.353034593	2.53053E-11	0.980867202
LC	5beta-Cholestane-3alpha,7alpha,27-triol	75.4	1.351151855	2.76785E-13	-1.803098512
LC	3a,7a-Dihydroxycholanoic acid	69	1.350516778	1.03822E-08	-3.211079086
GC	Beta-Lactose	95	1.349787046	1.22367E-06	1.603701093
LC	Callyspongenol A	43.3	1.348393927	2.57369E-09	40.78996746
GC	Uric Acid	94.5	1.345972703	1.28136E-06	-0.811614381
LC	N-(1-Deoxy-1-fructosyl)glycine	39	1.343728118	3.44768E-17	3.347465371
LC	7alpha,26-dihydroxy-5beta-cholestan-3-one	46.9	1.342471151	2.61432E-11	-1.365043048
LC	Serylmethionine	55.9	1.336601876	3.56649E-05	4.522043965
LC	virginiamycin m1	38.8	1.335630052	1.99958E-07	8.262323087
LC	oscr#36	42.9	1.335110552	3.16455E-10	-1.672643654
GC	5-Hydroxyindoleacetic Acid	74.1	1.334281623	5.85205E-09	-0.88097067
LC	2-Ethoxy-3-[4-[2-(4-methylsulfonyloxyphenyl)ethoxy]phenyl]propanoic acid	36.4	1.331426993	4.59265E-08	40.84418899
LC	Pyrogallol-1-O-sulphate	49.7	1.327814193	0.000393374	-5.850026126
GC	4-Hydroxyproline	90.4	1.325624423	1.21322E-05	-1.098236295
LC	19-oxodesacetylcinobufagin	40.1	1.321657751	9.35251E-07	-0.748289201
LC	Tribufos	36.1	1.318951795	2.33202E-06	40.99655021
LC	Methylenediphosphonic acid	40.4	1.317842217	0.001058028	-0.188909471
LC	Polysorbate 80	40.9	1.314193555	4.25862E-12	-0.897909853
LC	20a,22b-Dihydroxycholesterol	58.9	1.313033184	1.0543E-10	-1.215864384
LC	(25R)-4beta,26-dihydroxycholesterol	71	1.311645931	8.89506E-12	-1.288361277
LC	Heliangin	46.8	1.31141562	0.000312475	7.621662891
GC	O-Phosphoethanolamine	87	1.309591481	0.008407344	-0.716287605
LC	13'-Hydroxy-alpha-tocopherol	55.5	1.306369995	0.001323398	0.187723651
LC	19-Oic-deoxycorticosterone	67.9	1.30446905	2.72747E-17	-1.275579023
LC	Cholesterol sulfate	38.4	1.303754069	4.32418E-07	-1.028054725
LC	SM(d18:1/16:0(2OH))	38.6	1.302108362	0.008388629	-0.209438497
LC	Callyspongendiol	38.9	1.301850646	8.28469E-15	0.363360629
LC	Dexamethasone	70.7	1.300429431	0.000149214	10.15614893
LC	chrysoeriol 7-O-neohesperidoside	49.3	1.299711384	2.21659E-06	-0.96461299
LC	Sitostanol-beta	41.3	1.299676074	2.0544E-10	9.81375311
LC	Melanettin	45.9	1.294633946	4.91123E-14	-3.019368335

GC	Ketoleucine	89.3	1.292038711	1.96617E-07	-0.823428414
LC	Benzoyloxycarbonyl-Val-Ala-Asp(OMe)-fluoromethylketone	39.3	1.286389889	1.10289E-07	12.66651011
LC	Propionylcarnitine	64.7	1.285707694	0.001922986	-0.581867293
LC	3-(3,4-Difluorophenyl)-4-(4-(methylsulfonyl)phenyl)-2(5H)-furanone	37.7	1.284798019	3.66351E-07	40.91368901
LC	3 alpha,7 alpha,26-Trihydroxy-5beta-cholestane	71.8	1.282845729	9.87938E-13	-1.613287738
LC	Citrusinine I	49.3	1.280523477	8.9544E-11	-2.114667051
GC	Butane-1,2,4-Triol	89.1	1.279754132	0.029697615	-1.124191533
LC	4,6,2',4'-Tetramethoxychalcone 2'-beta-glucoside	38.9	1.278496938	8.46346E-07	40.90663332
LC	Naematolone	41.8	1.273946744	2.8444E-09	40.62262973
LC	(2S,4R)-4-(9H-Pyrido[3,4-b]indol-1-yl)-1,2,4-butanetriol	50	1.271660543	2.01546E-14	-2.752313019
LC	C16 Sphinganine	49.6	1.271276738	2.45049E-14	-0.875340694
LC	Sphinganine 1-phosphate	68.8	1.26979324	1.08666E-05	0.850801403
LC	IODODIFLUNISAL	37.2	1.265024342	0.002573601	0.334896358
LC	1alpha-Hydroxycorticosterone	64	1.260150798	0.010989918	-0.523231998
GC	3,4-Dihydroxyphenylglycol	72.3	1.254746809	0.000238717	1.187444513
LC	Bilirubin	58	1.250083168	1.00946E-07	2.181767855
LC	typhasterol	46.2	1.246317652	5.31502E-09	-1.335430214
LC	PC(19:0/0:0)	44.2	1.246096088	1.51154E-10	-1.027951581
LC	Fusaroskyrin	36.7	1.243441946	0.016964902	0.553013787
LC	LysoPE(P-18:1(9Z)/0:0)	51.9	1.241220213	2.784E-13	-1.185982164
GC	Gluconolactone	83.4	1.240246029	0.000255877	1.177241436
LC	25-Acetylvulgaroside	52.8	1.236974491	0.000513819	-3.895991278
LC	isoleucyl-thiazolidine	48.1	1.236358137	0.000546623	3.841199781
LC	Longilactone, delta-4(18)-Isomer, 2alpha-alchoh; (1R,2R,3R,3aS,5aS,6R,6aS,9S,10S,10aS,10bR,10cR)-1,2,6,9,10-Pentahydroxy-3,10a,10c-trimethyl-7-methylenetetradecahydro-4H-phenanthro[10,1-bc]furan-4-one	39.3	1.235857192	1.02386E-07	14.14533658
LC	PA(17:0/12:0)	39.2	1.235006671	7.75427E-06	40.7531877
LC	Pregnanediol-3-glucuronide	44	1.233043587	0.006201122	-1.748799894
LC	Methiuron	37.5	1.231771366	0.036659617	-1.149781843
GC	Pectin	77.2	1.230538708	0.02249332	1.782425039
GC	Udp-N-Acetylglucosamine	87.8	1.22933857	0.000250452	1.146457486
GC	Sorbitol-6-Phosphate	74.7	1.228255933	0.035595175	1.204818303

LC	Bentazone	38.4	1.227224272	9.37737E-19	40.1153453
LC	POB-PS	38	1.226652287	3.62922E-06	-0.878267787
LC	(3alpha,5alpha,22R,23R)-Cholestane-3,22,23-triol	69.7	1.224368162	2.77123E-10	-1.195963809
LC	Penicisteroid H	51.1	1.223169484	4.35585E-08	-1.265240646
LC	Bergaptol	38.8	1.217677104	0.001399244	0.360617489
GC	L-(-)-Sorbose	78.2	1.21655086	4.33363E-05	0.99523718
LC	PE(DiMe(11,5)/20:4(5Z,8Z,11Z,13E)-OH(15S))	36.1	1.214397699	0.026419723	0.290265274
LC	LysoPC(18:3(9Z,12Z,15Z)/0:0)	77.7	1.213288176	0.012002897	-0.539614602
GC	Leucrose	78.2	1.212746219	0.000461067	0.889487806
LC	2-Hydroxy-3-methylbutyric acid	63.1	1.210678862	0.011042545	0.475169506
LC	Teasterone	52.3	1.210226285	6.12047E-11	-1.59978806
GC	Hypoxanthine	87.4	1.204971604	0.036703896	0.604012647
GC	L-Erythrulose	82.3	1.20475443	0.00644521	3.35695436
LC	Avideoxycholic acid	53.9	1.204206817	3.24537E-07	-1.300295133
LC	[1,1'-Biphenyl]-4-ol, 3-amino-	36	1.202625535	3.09893E-06	-1.073576999
GC	D-Galactose	96.1	1.193413669	5.63244E-05	1.154238456
GC	N-Acetyl-Tryptophan	83.7	1.193371694	1.19932E-07	-1.087117184
LC	PE(20:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	37.9	1.193029564	0.005136758	0.250115308
GC	Mg(0:0/16:0/0:0)	79	1.193029203	0.017707552	0.989445385
LC	Deoxycytidine	52.9	1.192780342	1.11849E-08	0.171858909
GC	2-Hydroxybutyric Acid	94.7	1.192265965	4.27599E-06	1.023911673
LC	Sarothrin	40.6	1.188657266	0.034792195	41.71509368
LC	5-Amino-1-[carboxy(methyl)amino]pentane-1,1,2,2,3,3,4,4,5-nonacarboxylic acid	38.1	1.186002074	0.006816995	1.129929423
LC	PS(24:0/20:3(5Z,8Z,11Z)-O(14R,15S))	37.2	1.183478475	7.30648E-06	-2.841418692
LC	Schisanhenol	37.7	1.181114152	3.48468E-06	1.789489738
LC	Ephedrine	44.9	1.180348068	0.003913201	7.633618571
LC	1-Octen-3-yl acetate	53.8	1.180217394	3.25388E-10	-1.077597255
LC	Sorafenib beta-D-Glucuronide	37.5	1.178826579	4.78587E-06	-0.948443017
LC	Benzylpenicilloyl	44.6	1.176030668	8.8688E-10	40.31870753
GC	3-Methyl-2-Oxovaleric Acid	90.5	1.175406016	0.000265624	-0.664453881
LC	LysoPC(15:0/0:0)	69.5	1.17511826	7.89638E-06	-0.340836999

LC	2-Hydroxy-4-[(1R)-1-hydroxy-8-methyl-6-oxononyl]-3-methyl-2H-furan-5-one	47.7	1.169781465	0.042924805	3.753184152
LC	GDP-mannuronate	41.3	1.166629508	8.42862E-06	0.121800734
LC	PE(14:1(9Z)/12:0)	37.5	1.166448449	1.00365E-08	-0.617572897
LC	PC(P-18:0/20:4(5Z,8Z,11Z,14Z)-OH(16R))	46	1.158664652	0.005779348	0.264442168
LC	Axillarin 7-sulfate	36.2	1.156452978	3.06896E-05	0.677327584
LC	5-Methoxysalicylic acid	48.1	1.156210528	0.009399317	-2.51098847
LC	PA(a-25:0/20:4(5Z,8Z,10E,14Z)-OH(12S))	38.8	1.15548637	0.012286157	-3.625662068
LC	Phosphoric acid, mono(4-cyanophenyl) monomethyl ester	37.7	1.14996127	1.1305E-05	-0.676040503
LC	Undecanoylcarnitine	59.4	1.145632031	8.51401E-06	-2.740200184
LC	Methacrifos	38.5	1.141927844	1.14759E-07	0.952823056
LC	Momordol	59.8	1.138092343	8.19004E-12	-1.447244193
LC	N-3-hydroxy-13-methyl-hexadecanoyl glycy-L-serine	38.5	1.134444097	1.37727E-07	0.970513093
LC	2-Hexadecyloctadec-9-enal	40.5	1.131273104	0.000150582	0.208838894
LC	5-((8Z,11Z)-nonadeca-8,11-dien-1-yl)resorcinol	50.6	1.127771991	7.54806E-10	-1.17237788
LC	(11E,13Z)-10-Hydroxyoctadeca-11,13-dienoylcarnitine	56.2	1.118321026	6.98624E-05	0.796736353
GC	Alpha-D-Lactose	94.2	1.114578621	0.012936834	1.045866014
LC	Phenylalanyltryptophan	68.5	1.114363258	0.000786901	-1.484265301
LC	Alisol A	49.7	1.113997306	2.213E-08	-1.178671574
LC	Isoquinolinesulfonamide	40.2	1.113185717	0.033123431	9.698636979
GC	1h-Indole-2-Acetic Acid	86.9	1.106535927	0.004289838	-0.539360167
LC	15-hydroxycembra-1,3,7,11-tetraene	54.1	1.106360009	1.5044E-07	-3.339065921
LC	PIM1(19:0/16:0)	37.3	1.106272763	0.000186753	-0.965745109
LC	Edetate trisodium	38.9	1.105598041	0.002528702	0.401616075
LC	5-Nonadecyl-1,3-benzenediol	52.6	1.105246109	8.91573E-09	-1.057952702
LC	Bisantrene	37.8	1.102782867	8.22966E-08	1.598674205
LC	Etodolac acyl glucuronide	62.3	1.100811961	0.006397494	-2.207457798
GC	Phthalic Acid	77.5	1.098809128	0.000592117	0.896219219
LC	Stercobilin	53.7	1.09701035	0.026576372	4.983835506
LC	Berkeleylactone G	42.7	1.094370571	0.026450811	3.021326101
LC	Dihydroxyacetone phosphate	47.4	1.093204547	0.002647595	0.351907823
LC	Manbeta1-4Glcbeta-Cer(d18:1/16:0)	39	1.093093559	2.19053E-06	-1.21695946
LC	2-(Trifluoromethyl)isonicotinic acid	38.5	1.091777906	0.002612161	-0.585353358

LC	Piridronic acid	38.4	1.091020748	0.000107916	0.092492091
LC	Nitroglycerin	38.9	1.09023557	3.11375E-08	0.139294553
LC	Lumirubin	54.6	1.088202444	3.73598E-07	1.514202778
LC	Ambrisentan	36	1.085436211	1.59647E-14	13.14980442
LC	3-Amino-5-(3-thiophenyl)-2-thiophenecarboxamide	36.7	1.085349842	6.3644E-06	0.103268094
LC	Taurodeoxycholic acid 3-glucuronide	51.7	1.08530765	0.011973246	4.075794922
LC	Isoflupredone acetate	39.6	1.084720317	0.00091987	-0.870554404
GC	Glutaconic Acid	74.2	1.079652709	0.007363395	0.838171904
LC	6-Nitrotryptophan	45.1	1.077416891	9.7226E-15	-1.436652925
GC	Phenol	83.5	1.075743007	0.04215171	-1.04952031
LC	(3Z,5E,7E)-Decatrienoylcarnitine	63.7	1.074612588	0.017119473	-0.567103751
LC	Thiazolidine-4-carboxylic acid	37.2	1.074482326	3.06448E-07	-0.529643737
LC	(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone	39.4	1.073906842	0.023693826	-1.408937352
LC	7-Chloroemodin	48.5	1.072981428	1.61205E-17	-0.625869141
LC	2-[(1r,3s)-3-Hydroxycyclohexyl]-5-(2-methyloctan-2-yl)phenol	51	1.072497043	7.07017E-12	40.06607802
LC	N6,N6,N6-Trimethyl-L-lysine	64.1	1.070947656	0.014584338	-0.985784699
LC	(2S)-3-[3-[(4-Carbamimidoylbenzoyl)amino]propanoylamino]-2-[(4-ethylphenyl)sulfonylamino]propanoic acid	37.6	1.068161136	0.000147419	10.17773271
LC	gamma-Glutamylacetamide	65.9	1.06608525	0.000293257	0.564542451
LC	farnesyl triphosphate	38.4	1.063720574	1.66623E-13	-1.414171777
LC	7alpha,12alpha-Dihydroxy-5beta-chol-3-en-24-oic Acid	53.7	1.06144848	5.97344E-09	-1.119656192
LC	Eszopiclone	37.3	1.055627597	8.16875E-14	9.760947699
LC	NNAL-N-glucuronide	50.6	1.054646494	7.71277E-05	10.2067946
GC	D-Fructose	97.7	1.054643771	5.89727E-07	0.614272904
LC	D-Mannose	60.9	1.052024395	0.001951394	0.313657067
LC	LysoPI(18:1(9Z)/0:0)	53.4	1.04753716	4.58379E-08	-0.830867594
LC	N-Stearoyl Lysine	51.8	1.044744203	9.76573E-05	0.16260263
LC	24-Nor-5beta-chol-22-ene-3alpha,12alpha-diol	51.5	1.043975788	6.1191E-09	-1.515757001
GC	L-Glutamic Acid	92.9	1.042986929	0.002390984	0.673199405
LC	Carbimazole	39.7	1.04230476	0.033589365	8.210966104
LC	Indole-3-propionic acid	65.8	1.039522069	0.008463226	-2.472980946
LC	Tropisetron	42.5	1.039362858	0.001320556	11.11932231
LC	Gelsenicine	37.9	1.038741342	4.32525E-07	11.61306718

LC	Succinylsulfathiazole	36.9	1.03858209	0.014530326	0.513624537
LC	Phosphovanillin	38.4	1.038564305	7.14284E-14	0.433110326
LC	Spinoflavanone A	38.5	1.035733755	2.15839E-08	5.760187152
LC	Kinetin	41.1	1.035117724	3.80474E-15	-1.507144952
LC	2,2-Difluoro-n-(2-hydroxyethyl)-3-(2-nitro-1h-imidazol-1-yl)propanamide	39.3	1.034474162	0.008034367	-1.773443078
GC	Glucuronic Acid	83.6	1.031929507	0.000928279	1.109528919
LC	PC(O-17:0/0:0)	45	1.028848524	4.08683E-11	-1.690229651
LC	plaunotol	53.8	1.027944612	2.01481E-09	-1.171945365
LC	reparixin	40.4	1.027229951	4.37947E-17	8.979609018
LC	DG(18:0/20:4(8Z,11Z,14Z,17Z)/0:0)	44.2	1.026748997	0.024320454	0.370689066
LC	7 alpha,24-Dihydroxy-4-cholesten-3-one	54.5	1.020770275	8.78812E-12	-1.633359417
LC	U-75302	36.2	1.019661338	6.84454E-13	-0.903626488
LC	Thyroxine	58.2	1.017362606	7.64838E-06	0.364804046
LC	3,5,9-Trihydroxyergost-7-en-6-one	65.1	1.016717812	1.17301E-07	-1.223318493
LC	4-Vinylphenol sulfate	62.3	1.016351425	0.004227491	-3.974535492
LC	PHODA-PI	38.9	1.014968976	1.17941E-10	-3.259160956
LC	Leucyl-leucine	60	1.014123166	1.18257E-06	-2.813447767
LC	MEK1-2-inhibitor	41.3	1.01056178	0.004804795	10.3005391
LC	5beta-Pregnane-3alpha,20alpha-diol	72.7	1.009112388	1.39851E-09	-0.990606021
LC	(1(10)E,4a,5E)-1(10),5-Germacradiene-12-acetoxy-4,11-diol	69	1.005521022	0.022071093	-0.609840442
LC	Ribosylhopane	37.8	1.003760993	6.16628E-12	-3.040767604
LC	4-Deoxybryaquinone	51.7	1.002770403	1.01653E-08	10.02682053
LC	19Z-pentacosenoic acid	54.9	1.00182327	1.30003E-10	-1.558306974
LC	Confusoside	38.4	1.00151958	3.52174E-06	40.22868175

GC

Dataclass	Metabolites	Score	VIP	P-value	log2(FC)
LC	Propofol glucuronide	51.7	53.94652497	4.45672E-15	19.32397265
LC	LysoPC(0:0/18:2(9Z,12Z))	75.2	38.31488806	6.16049E-10	-0.642330056
LC	Edetic Acid	64.2	26.86598179	3.83159E-05	0.769365307
LC	Carissanol	49.2	14.37844613	1.39673E-26	46.96537401
LC	LysoPC(20:4(5Z,8Z,11Z,14Z)/0:0)	71.5	12.08499396	0.000493465	-0.371821984
LC	Dehydroepiandrosterone sulfate	55	11.19017239	8.46707E-08	-1.293133135

LC	Isocitric acid	63.8	10.16648213	6.1962E-12	1.097727866
LC	SM(d18:1/16:1(9Z))	55	9.715301146	2.74592E-05	-0.344062841
LC	Lidocaine	67.4	8.939153154	5.31002E-05	10.33492516
LC	N-(2-Hydroxyethyl)-2-(1-isoquinolinylmethylene)hydrazinecarbothioamide	38	8.816521427	2.02231E-15	8.566865141
LC	PC(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/P-18:1(11Z))	44.7	8.4669964	0.02855219	0.284839363
LC	1-(O-alpha-D-glucopyranosyl)-29-keto-(1,3R,31R)-dotriacontanetriol	54.1	8.215099913	3.13532E-07	-0.572102216
LC	PC(P-18:1(11Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))	46.7	8.191727526	1.18243E-06	0.523467932
LC	UTILIN	37.1	7.350631376	2.15176E-23	15.26443876
LC	SM(d19:1/17:1)	47.5	7.342634715	0.000642955	-0.390018794
LC	19-Epischolaricine	49.6	6.848364743	1.48997E-19	13.95110501
LC	2-C-methyl-D-erythritol-4-phosphate	39.3	6.38754549	0.000101689	0.269872277
LC	1-O-(2-methoxy-4Z-hexadecenyl)-sn-glycero-3-phosphocholine	56.2	6.281443908	5.92016E-05	-0.443793695
GC	P-Cresol Glucuronide	82.2	6.057556488	4.01438E-15	15.62833252
LC	Myristyl linoleate	39.3	5.991049997	0.031623979	14.96812108
LC	N-Nitrosoanatabine	42	5.90988211	1.60368E-09	0.174561009
LC	2-Methyl-4'-(methylthio)-2-morpholinopropiophenone	50	5.89166591	9.90643E-13	44.68122803
LC	Chenodeoxycholic acid glycine conjugate	60.5	5.884162488	0.000620503	-2.153627048
LC	4-(2-Aminoethylamino)-3-[bis(carboxymethyl)amino]-3-(carboxymethyl)hexanedioic acid	38.6	5.600909303	3.80096E-25	12.7992879
LC	L-Acetylcarnitine	65	5.589893334	0.001881515	0.312767034
LC	S-Japonin	42	5.567984988	6.97297E-09	1.5767264
LC	LysoPE(18:1(9Z)/0:0)	72.8	5.433082918	4.14667E-06	0.61441495
LC	(±)-(Z)-2-(5-Tetradecenyl)cyclobutanone	61.3	5.364835164	0.019070874	-0.310990762
LC	Isoscoparin 2"-O-glucoside	36.5	5.17440409	0.000552038	0.869988453
LC	Pulverulentoside I; (1aS,1bS,2S,5aR,6S,6aS)-6-({3-O-Acetyl-6-deoxy-2-O-[(2E)-3-(4-methoxyphenyl)-2-propenoyl]-?-L-mannopyranosyl}oxy)-1a-(hydroxymethyl)-1a,1b,2,5a,6,6a-hexahydrooxireno[4,5]cyclopenta[1,2-c]pyran-2-y I ?-D-glucopyranoside	36	5.037663029	1.05476E-10	44.24277203
LC	13-Hydroxyoctadecanoylcarnitine	68.9	4.933345605	1.68573E-05	0.735993044
GC	Equilenin	77.7	4.932257964	1.9879E-16	10.43989948
LC	LysoPC(20:4(8Z,11Z,14Z,17Z)/0:0)	73.5	4.751566938	0.000651503	-0.35893985

LC	Enterodiol sulfate	37.4	4.556738685	3.78655E-09	1.719136138
LC	PC(0:0/14:0)	73.2	4.503660424	0.000185342	-0.684771493
LC	TG(8:0/8:0/a-17:0)[rac]	46.1	4.456641938	0.001664105	-0.920074588
LC	6-Butyryl-5-hydroxy-4-phenylseselin	39	4.31490091	6.24884E-08	-1.26252097
LC	Oxotremorine	43.5	4.293933171	2.58891E-12	9.940634302
LC	Benzoxazole	38.6	4.284956005	0.01913489	0.266212151
LC	p-Cresol sulfate	54.8	4.205993242	0.017654745	-1.068851968
LC	PC(12:0/20:1(11Z))	40.8	4.190891176	0.001363777	0.569908711
LC	dIDP	38.6	4.178355858	9.1202E-15	6.991863788
LC	2,2'-Methylenebis(4-methyl-6-tert-butylphenol)	58.3	4.15865175	3.59592E-14	11.722534
LC	Ecabet	45.3	4.150657042	2.74776E-09	1.136402137
LC	LysoPC(0:0/18:1(9Z))	73.5	4.131967354	0.023274943	0.178266073
LC	O-Linoleoylcarnitine	70.2	4.108912325	0.000562633	0.714464023
GC	Lactulose	89.8	4.103276426	4.46051E-12	6.03345607
LC	LysoPC(0:0/18:0)	74.6	4.041917952	0.039107379	-0.165546837
LC	Indoxyl sulfate	57.3	4.007344508	9.16702E-10	-1.511932567
GC	M-Toluamide	71.5	3.978343556	1.85085E-11	7.106765825
LC	Cichorioside K	52.1	3.805460545	3.1816E-12	9.748547741
LC	L-Alloisoleucine	72.7	3.794286905	0.008302739	0.213750582
LC	PC(18:0/P-16:0)	38.3	3.789733332	9.00938E-05	0.466295029
GC	3-(Pyrazol-1-Yl)-L-Alanine	91	3.770363952	0.000130677	-2.88057344
LC	2-Methoxy-4-(2-(methylamino)propyl)phenyl beta-D-glucopyranosiduronic acid	40	3.741584163	4.11721E-17	15.2910691
LC	Armillaripin	56.8	3.658880068	3.8297E-13	-4.226104953
LC	21H-Bilane-8,12-dipropanoicacid, 3,18-diethenyl-1,19,22,24-tetrahydro-2,7,13,17-tetramethyl-1,19-dioxo-	62.3	3.658494082	4.8298E-11	-3.444619996
LC	Decanoylcarnitine	62.7	3.642436159	0.03128563	-1.748587976
LC	(Z)-1-(Methylthio)-5-phenyl-1-penten-3-yne	45.2	3.618887447	1.79317E-14	-0.812269404
GC	Lactitol	95.8	3.611330271	3.20936E-12	5.313556753
LC	Phyllocoumarin	52.4	3.528669441	1.64083E-15	9.195618265
LC	Vignatic acid B	38	3.463578533	1.0499E-06	-0.587246487
GC	Maltotriose	94.5	3.442438543	3.32747E-11	5.787915047
LC	LysoPE(0:0/18:1(11Z))	74	3.395511207	2.61986E-07	0.731373914

LC	Plantacyanin	37.3	3.391050708	5.16825E-10	11.88986752
LC	Allopregnanolone sulfate	41.8	3.382748995	0.001129506	-0.819885432
LC	Octenoyl-L-carnitine	77.4	3.369514045	1.40229E-06	-0.931860442
LC	Disodium ethylenediaminetetraacetate	39.4	3.347200615	0.003664457	0.424390458
LC	PS(P-20:0/22:2(13Z,16Z))	53	3.261628398	0.000431688	0.428436453
GC	Cis-Aconitic Acid	91.3	3.154253894	3.89001E-10	3.089494537
LC	PE-NMe2(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	39	3.040954905	1.67904E-05	0.203818073
LC	Vaccenic acid	52.5	3.031525829	1.50499E-20	0.613287691
LC	PI(O-18:0/18:0)	36.3	3.028972281	0.002887081	0.416880785
LC	[3-Methoxy-2-phosphonooxy-6-[(E)-2-(3,4,5-trimethoxyphenyl)ethenyl]phenyl] dihydrogen phosphate	38.8	3.010458194	0.017237678	13.04817123
LC	LysoPC(0:0/20:4(5Z,8Z,11Z,14Z))	73.6	2.950013103	0.00121253	-0.3567034
LC	3-(4-Iodophenyl)-2-mercapto-(Z)-2-propenoic acid	38.4	2.948505766	0.001760034	0.383270169
LC	gamma-Glutamylserine	69.9	2.946838817	7.49733E-09	1.048104931
LC	alpha-Hydroxyisobutyric acid	62.9	2.882413071	2.08052E-12	1.274201548
LC	Galactotriose	51.6	2.882409673	5.59696E-08	10.43028552
LC	Caffeine	60.3	2.866566449	2.80265E-05	-8.754283613
LC	Fluorene	46.1	2.842166756	4.52853E-07	1.972649203
LC	Sphingosine 1-phosphate	72.9	2.838054454	7.75174E-06	0.726247359
LC	Hydroxyzine	41.3	2.836639859	4.42442E-07	1.192601567
LC	3,4-Dimethylethcathinone	39.7	2.836429107	2.09715E-21	0.35312522
LC	2-Oxoarginine	41.7	2.814642957	5.92824E-07	-2.47374176
GC	2,6-Pyridinedicarboxylic Acid	73.2	2.813096475	0.002839778	-2.188464301
LC	PS(P-20:0/0:0)	54.8	2.80210582	3.98979E-10	-0.772322407
LC	Glycocholic acid	63.6	2.762208825	0.001078465	-1.671180862
LC	PE(22:4(7Z,10Z,13Z,16Z)/21:0)	46.1	2.753488411	0.005457149	0.285232471
LC	9-tridecynoic acid	47.9	2.749320526	7.30832E-07	0.17035804
LC	LysoPE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	73	2.722823168	0.001383361	0.43609798
LC	lysine phosphoester	42.7	2.71285795	6.39359E-14	-0.824551637
LC	PC(17:2(9Z,12Z)/0:0)	68.8	2.678348283	2.22589E-13	-0.683453722
LC	Ptilosaponoside B	43.3	2.677181483	7.77624E-16	-5.219475083
GC	Octaethylene Glycol	95.9	2.66154083	7.31284E-07	7.166165825
LC	Methyl 3-epi-4,5-didehydrojasmonate	55.4	2.651237028	7.99368E-06	-0.792357375

LC	APC	60.4	2.649821373	2.78165E-17	-4.596067807
LC	Melibiose	57.4	2.644487256	1.16746E-11	12.44996866
LC	EUPARIN	37.4	2.622642915	1.97339E-06	2.527372489
LC	Thiamine	43.2	2.606164504	3.56529E-11	14.77593025
LC	Zearalenone	52.3	2.592859771	1.47316E-16	9.907855111
LC	LysoPE(P-16:0/0:0)	59.2	2.589484635	3.0235E-10	-0.730796633
LC	Gravolenic acid	38.2	2.560480712	1.89272E-17	8.912222705
LC	Theophylline	57	2.547771811	3.06009E-05	-7.076581272
LC	3-[(1R,4S,5S,6R)-6-[(1E,3S,5Z,8Z,11Z)-3-Hydroperoxytetradeca-1,5,8,11-tetraen-1-yl]-2,3-dioxabicyclo[2.2.1]heptan-5-yl]propanoylcarnitine	38.2	2.534435874	0.000541287	-2.020774272
LC	Mastraxanthin 3-linoleate 3'-dipalmitoleate	37.1	2.533171882	0.011558246	0.229977306
GC	Melezitose	82.7	2.506016185	0.005991462	2.425334023
LC	5-{2-Fluoro-5-[3-(3-hydroxy-2-methoxycarbonyl-phenoxy)-propenyl]-phenyl}-isoxazole-3-carboxylic acid	50.9	2.480937881	0.0487224	10.87873151
LC	6"-Acetylliquiritin	37.5	2.472937151	2.34793E-12	7.339484367
LC	3-Methyl-2Z,4E-decadienoic acid	41.3	2.467781535	6.58734E-14	42.10504774
LC	GM4(d18:1/18:0)	42.3	2.465713887	0.042240365	-0.372005352
GC	Ribonic Acid	87.7	2.453976277	0.005684684	-0.814790759
GC	3-Methylbutane-1,2-Diol	82.2	2.444183466	3.26707E-07	1.803406484
LC	DG(18:3(9,11,15)-OH(13)/15:0/0:0)	50	2.429438144	1.85007E-06	-2.721899195
LC	PI-Cer(t18:0/18:0(2OH))	36.2	2.424038317	9.07158E-06	0.518874733
LC	Pyridine N-oxide glucuronide	45.1	2.419406205	2.8962E-13	-0.582787135
LC	[(2S,4R,5R,6R,14S,16R)-14-Hydroxy-7,11-dimethyl-6-(2-oxopyran-4-yl)-3-oxapentacyclo[8.8.0.02,4.02,7.011,16]octadecan-5-yl] acetate	53.8	2.367365409	2.35006E-13	-4.850046799
LC	N-Choloylglycine	65.8	2.35980136	0.0011058	-1.559056251
LC	PC(O-16:1(11Z)/0:0)	58.5	2.352273921	1.93406E-10	-0.713443735
LC	2-[(2-Fluorophenyl)sulfanylmethyl]-5-[6-[(2-hydroxycyclopentyl)amino]purin-9-yl]oxolane-3,4-diol	37.1	2.344109746	1.56976E-11	41.99695853
LC	2,4-Thiazolidinedicarboxylic acid, 2-methyl-	63.8	2.301708405	4.45013E-07	1.195094538
LC	3b-Hydroxy-5-cholenoic acid	62.9	2.300600053	0.00026945	-2.755913386
LC	PC(14:1(9Z)/20:3(8Z,11Z,14Z))	39	2.299527329	0.022306549	-0.446629272
LC	2-(5,8-Tetradecadienyl)cyclobutanone	52.7	2.299305213	0.021249907	-0.355364316

LC	2-((2-Methoxy-2-(3-(trifluoromethyl)phenyl)ethyl)amino)ethyl 4-(2-(2-(9H-fluoren-9-yl)acetamido)ethyl)benzoate	46.2	2.288621689	7.86744E-17	-7.838158462
LC	3,7-Dihydroxycholan-24-oic acid	58.2	2.286392283	0.011569648	-2.248293124
LC	Octadec-5-enoic acid	58.2	2.279438	6.39647E-09	0.994532364
LC	Propylparaben	45.5	2.278729795	0.007900314	0.931691163
GC	P-Cresol	95.2	2.273388205	0.017876409	-0.8403432
LC	SM(d18:1/14:0)	55.9	2.222411694	0.00667243	-0.426343438
LC	LysoPC(O-18:0/0:0)	56.4	2.218996093	1.28915E-05	-0.44735444
LC	LysoPE(0:0/16:0)	75.8	2.214984416	0.023646247	0.245271894
LC	(-)-Salvisyriacolide	48.4	2.2108962	3.74573E-07	-3.305087106
LC	Desacetycefapirin	37.4	2.209933168	4.30069E-25	41.6092499
LC	Melatonin glucuronide	36.9	2.181274399	1.29343E-22	14.67022399
LC	3-Hydroxylidocaine	42.3	2.176948804	3.8166E-09	9.243683703
GC	Cellobiose	99.5	2.176237082	2.55371E-11	2.272963723
LC	Ansamitocin P3	44.2	2.1664012	1.07531E-16	-4.03177861
LC	Cabozantinib	39.1	2.161336002	1.36062E-09	41.89804256
LC	1-O-Hexadecyl-sn-glycero-3-phosphocholine	59.6	2.155677345	6.40337E-09	-0.609512102
LC	PE-Cer(d14:2(4E,6E)/23:0)	56.7	2.145256236	4.57363E-05	-0.36042635
LC	(5Z,9Z)-2-methoxy-hexacosadienoic acid	55.6	2.144522665	3.25487E-12	-1.456913797
LC	27-Hydroxycholesterol	68.7	2.141978776	1.08849E-11	-1.084197256
LC	Artemoin A	52.1	2.139000219	9.3166E-05	-0.994449909
GC	Quinic Acid	87.5	2.135311955	0.002375503	-4.760463222
LC	16-oxo-palmitate	42.3	2.128104247	8.7475E-13	-1.602806553
LC	Ikariside D	36.7	2.115382588	5.24926E-11	41.72942822
LC	4-(2-Aminoethyl)benzenesulfonyl fluoride	37.3	2.113026735	3.21214E-12	2.478221168
LC	Chenodeoxycholic acid	57.7	2.105068385	0.000439192	-2.747293675
LC	Bis(2-ethylhexyl) phthalate	59.1	2.097021044	0.00174431	2.212837849
LC	Cohibin A	50.7	2.088519059	1.22597E-10	-1.628519805
LC	6-Thioxanthylic acid	41	2.087715016	0.001821187	0.431248782
LC	Spiropiperidine	38.1	2.066201663	4.30362E-11	-0.810713148
LC	Trihydroxycoprostanic acid	62.7	2.063272269	9.69794E-10	-1.118968077
GC	Oleic Acid	97	2.057633839	3.1445E-14	1.698645289
LC	3,4-Bis(carboxymethyl)-3,4-dihydroxyhexanedioic acid	42.4	2.052894979	8.38911E-13	-0.530688566

GC	Beta-Lactose	95	2.042600146	1.56114E-09	2.280310983
LC	DG(18:3(9Z,12Z,15Z)/15:0/0:0)	49.2	2.032596067	5.35984E-05	-0.808689056
LC	UDP-D-galacturonic acid	41.1	2.018912892	0.000273723	0.098413022
LC	Dehydropachyrrhizone	37.7	2.014906972	5.00503E-16	6.564337144
LC	5alpha-Pregnan-3beta,20beta-diol 20-sulfate	41.6	2.014892652	0.002721915	-3.140297231
LC	3-Amino-6-{4-[(4-Methylpiperazin-1-Yl)sulfonyl]phenyl}-N-Pyridin-3-Ylpyrazine-2-Carboxamide	50.2	2.011397905	5.26767E-08	-1.292492708
LC	2-Deoxybrassinolide	67	2.006936039	2.76346E-10	-1.491785435
LC	Glyceryl 5-hydroxydecanoate	42.8	2.005981312	6.30227E-13	-0.349226745
LC	6-Hydroxy-3,4-dihydro-2(1H)-quinolinone	56.3	1.984964911	6.1025E-14	-0.752365565
LC	4-Allylphenol sulfate	47.8	1.984378099	4.47979E-08	-1.943458324
LC	(4E,7E,10Z,13E,16E,19E)-docosa-4,7,10,13,16,19-hexaenoic acid	54.7	1.979862868	0.003727707	0.533008548
LC	Demissidine	66.5	1.957965106	1.95426E-10	-1.034297987
LC	SM(d18:1/12:0)	43.3	1.952154348	5.64912E-08	-1.582927148
LC	Glycoursodeoxycholic acid	58.1	1.950015511	0.017673265	-2.138435888
LC	2-Hydroxycinnamic acid	51.2	1.930980092	0.003988207	-0.226011502
LC	PE-Cer(d15:2(4E,6E)/20:0)	38.9	1.923098256	3.88038E-07	-0.954474993
LC	Marmesin rhamnoside	37.8	1.917955165	1.18024E-12	13.64481746
GC	10-Heptadecenoic Acid	85.9	1.909167384	0.000359808	2.087200932
LC	(4E,15E)-Bilirubin	53.7	1.897076068	8.03285E-08	-1.392719491
LC	(3Z,5E,7E)-Decatrienoylcarnitine	63.7	1.89679357	6.01807E-08	-1.041459047
LC	Sesamol	49.1	1.892132742	0.001044249	-2.102798648
LC	3-hexanoyl-NBD Cholesterol	39	1.881761628	3.34977E-11	0.396837152
LC	3-Hydroxymethyl-picumast	50.5	1.873705086	0.000437715	-0.95169791
LC	Isothankunic acid	36.6	1.871586314	6.69361E-09	-1.113059937
LC	5alpha-Cholestane-3alpha,7alpha,12alpha,24-tetrol	38.8	1.870393826	6.74343E-12	-1.438488445
LC	Piperine	74.8	1.867684191	0.043012498	-4.718978816
LC	Porson	54.9	1.866593245	0.000546435	6.902509666
GC	Galacturonic Acid	76.4	1.856685583	7.8056E-05	0.779065555
GC	Levogluconan	92.4	1.854603568	3.51654E-06	1.582384542
GC	3-Hydroxybutyric Acid	97.8	1.854059215	1.10462E-05	2.294931388
LC	Ethyl n-allyl-n-[(e)-2-methyl-3-[4-(4-amidinophenoxy carbonyl)-phenyl]propenoyl]amino acetate	45.4	1.847265413	1.20864E-17	-5.895514154

LC	Fusaroskyrin	36.7	1.843849422	0.00191085	0.788432637
LC	Androstenediol 3-sulfate	43.1	1.837543969	0.000285111	-0.944432953
LC	2,4-Diamino-6-nitrotoluene	39.3	1.813782868	2.1726E-12	0.276502393
LC	Methiuron	37.5	1.804156623	0.003221871	-2.085809771
LC	Hippuric acid	62	1.803684657	2.45259E-05	-2.562881823
LC	TG(8:0/8:0/a-13:0)[rac]	41.9	1.802239019	0.000203891	-0.967383729
GC	Delta-Tocopherol	84.3	1.802200522	0.00040632	2.977216719
LC	Zierin	37.4	1.797289473	1.32646E-15	12.06660044
LC	3-(3,4-Difluorophenyl)-4-(4-(methylsulfonyl)phenyl)-2(5H)-furanone	37.7	1.792263897	9.49353E-15	41.15496686
LC	Sulfaethidole	37.5	1.786998554	0.00279293	0.630348565
LC	PC(18:1(9Z)-O(12,13)/16:0)	38.7	1.777252797	0.005137805	-0.327055153
LC	LysoPC(P-18:1(9Z)/0:0)	56.4	1.775479339	2.36195E-07	-0.534905064
LC	(1R)-5-[2-[(1R,7Ar)-7a-methyl-1-[(2R)-6-methylheptan-2-yl]-2,3,3a,5,6,7-hexahydro-1H-inden-4-ylidene]ethylidene]-4-methylidenecyclohexane-1,3-diol	65.6	1.772930178	2.84645E-10	-1.078386904
LC	Hexazinone	39.5	1.759318895	0.003982387	-0.912085806
LC	(4S,6R)-6-[(1E)-4,4-Bis(4-fluorophenyl)-3-(1-methyltetrazol-5-yl)buta-1,3-dienyl]-4-hydroxyoxan-2-one	39.3	1.758349855	2.53494E-13	9.12340636
LC	Uridine 2',3'-cyclic phosphate	45.6	1.756411896	0.001611442	0.601525208
LC	(2S)-1,1,1-Trifluoro-2-(4-pyrazol-1-ylphenyl)-3-[5-[[1-(trifluoromethyl)cyclopropyl]methyl]-1H-imidazol-2-yl]propan-2-ol	52	1.755297126	3.44173E-29	16.28688995
LC	Ephedrine	44.9	1.755138777	0.037941192	9.059999145
LC	SALSOLIDINE	42.4	1.75436815	0.044209272	-1.678272879
LC	Tribufos	36.1	1.752575299	2.82091E-10	41.22711353
LC	Cefodizime,(S)	44.1	1.73968369	2.54541E-05	0.12152742
LC	5-Hydroxy-2-imino-1-methylimidazolidin-4-one	41	1.733205725	9.94897E-22	0.516597532
LC	Dodecanoylcarnitine	59.3	1.730478547	0.000804712	-1.155880107
LC	Mayolene-17	56.4	1.725599502	5.86416E-10	-2.597953131
LC	Heliangin	46.8	1.723957331	6.23056E-06	7.768929096
LC	Uridine diphosphate glucose	52.1	1.718394768	5.03324E-07	-2.881218763
LC	PGP(a-13:0/i-24:0)	36.3	1.710503078	0.048877201	0.171012909
LC	2-(Trifluoromethyl)isonicotinic acid	38.5	1.705726042	2.8419E-06	-0.868821663
LC	2-Ethoxy-3-[4-[2-(4-methylsulfonyloxyphenyl)ethoxy]phenyl]propanoic acid	36.4	1.701428547	4.52184E-13	41.02767595

LC	(11E)-Octadec-11-enedioylcarnitine	48.1	1.689703326	4.98632E-05	1.660971842
LC	chrysoeriol 7-O-neohesperidoside	49.3	1.685669224	2.25755E-09	-1.248093886
LC	virginiamycin m1	38.8	1.684168361	2.72755E-10	8.429222878
LC	Nitroflurbiprofen	39.3	1.679466869	0.004636533	7.366169284
LC	(1(10)E,4a,5E)-1(10),5-Germacradiene-12-acetoxy-4,11-diol	69	1.678126272	1.54075E-06	-0.957398207
GC	Cis-Erucic Acid	92.4	1.674884692	5.24756E-15	1.504736315
LC	Callyspongenol A	43.3	1.674200425	5.43577E-14	41.11941695
GC	Mg(0:0/16:0/0:0)	79	1.665463275	0.000293167	1.330630348
GC	Sorbitol-6-Phosphate	74.7	1.663949206	0.005671253	1.192244412
LC	Kuguacin E	64	1.657918258	7.61822E-05	-0.624110131
LC	LysoPE(0:0/18:0)	74.3	1.654915013	0.003270896	0.336510652
LC	1,5-Naphthalenediamine	44	1.654703348	4.73111E-14	-0.791882917
LC	indoprofen	48.6	1.622851906	2.47715E-06	1.15793968
LC	N-(1-Deoxy-1-fructosyl)glycine	39	1.62230885	6.7269E-25	3.57666039
LC	Longilactone, delta-4(18)-Isomer, 2alpha-alcohol; (1R,2R,3R,3aS,5aS,6R,6aS,9S,10S,10aS,10bR,10cR)-1,2,6,9,10-Pentahydroxy-3,10a,10c-trimethyl-7-methylenetetradecahydro-4H-phenanthro[10,1-bc]furan-4-one	39.3	1.604978458	1.40755E-10	14.40718799
LC	gamma-Glutamylacetamide	65.9	1.60471643	8.53726E-07	0.799316912
LC	Symmetric dimethylarginine	58.6	1.603999405	4.19675E-07	0.504143538
LC	Creatine	61.5	1.593905884	0.01464511	0.250174087
LC	Sitostanol-beta	41.3	1.591968643	2.71244E-14	10.04939922
LC	Blumealactone C	41.5	1.589542394	2.56249E-12	8.999255936
LC	4,6,2',4'-Tetramethoxychalcone 2'-beta-glucoside	38.9	1.582224572	3.0114E-09	41.03453652
GC	Sitosterol	91.5	1.581459281	0.011367669	1.315827379
LC	Ganoderiol C	45.5	1.577912643	5.15331E-11	-1.467813926
LC	Oxdralazine	37.3	1.573165585	2.60479E-12	5.349263974
LC	PE(20:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	37.9	1.571052151	0.000268259	0.321394856
LC	Pregnanediol-3-glucuronide	44	1.569011146	0.000935353	-2.630087788
LC	DG(i-15:0/0:0/i-12:0)	44.4	1.564774242	1.20268E-11	-1.50900226
LC	PC(2:0/PGE1)	43.1	1.560547429	0.001644284	0.193459969
LC	Schisanhenol	37.7	1.558844509	1.81423E-09	2.058870283
GC	D-Xylofuranose	84.1	1.557412914	3.22198E-13	1.589730272

LC	Naematolone	41.8	1.546891339	2.27814E-11	40.81635194
LC	Confusoside	38.4	1.534774964	1.86749E-10	40.85416906
LC	PE(10:0/10:0)	39.2	1.532944261	2.25749E-09	-0.823618561
LC	27-Norcholestanehexol	44.7	1.529780646	3.60434E-11	-1.623505584
LC	1-Hydroxy-2,2,5,5-tetramethylpyrrolidine-3-carboxamide	50.5	1.526350416	0.026131412	2.992688353
LC	Armatinol B	51.5	1.523137964	7.88902E-10	-1.339416539
LC	N-Palmitoyl Arginine	44.8	1.509384497	0.036985273	-0.441154127
LC	Pentaethylene glycol	69.4	1.507723353	6.7933E-05	-0.750413135
LC	2-Hexadecyloctadec-9-enal	40.5	1.505430918	1.74759E-07	0.282197718
LC	Glycerol 1-propanoate diacetate	38.4	1.504739382	1.00346E-09	3.089277713
LC	bhos#40	53.5	1.498592116	4.73597E-10	-1.133410586
LC	Perfluoroundecanoic acid	58.4	1.49584195	5.70822E-05	1.943429472
LC	Hydroquinone sulfate	42.4	1.490832585	5.38712E-05	-5.361109572
LC	2-[(1r,3s)-3-Hydroxycyclohexyl]-5-(2-methyloctan-2-yl)phenol	51	1.486159369	1.27985E-16	40.71476029
LC	Clausarinol	44	1.483893959	0.000407528	12.7273922
LC	Gorgostane-3beta,5alpha,6beta,11alpha,12beta-pentol 12-acetate	41.3	1.478907343	3.05601E-08	-1.449925546
LC	Dodecylbenzene	37.7	1.477164371	0.000110538	-0.527393281
LC	5b-Cholestane-3a,7a,12a,23-Tetrol	61.2	1.472891383	1.15106E-09	-1.253686045
LC	BAY-u9773	45.8	1.468296896	0.00013998	41.41473759
GC	Glucuronic Acid	83.6	1.46481744	8.04168E-06	1.323684439
LC	2-Hydroxy-3-methylbutyric acid	63.1	1.458146757	0.000634845	0.447082762
GC	(2r,3r)-2-Amino-3-Hydroxybutanedioic Acid	78	1.453899838	2.42443E-09	1.263424028
LC	Myricanene B 5-[arabinosyl-(1->6)-glucoside]	54.2	1.450317109	1.27471E-07	-1.323944733
LC	(2S)-3-[3-[(4-Carbamimidoylbenzoyl)amino]propanoylamino]-2-[(4-ethylphenyl)sulfonylamino]propanoic acid	37.6	1.448708574	7.21837E-08	10.35046035
LC	Bilirubin diglucuronide	56.4	1.448590242	3.93493E-08	4.894548341
LC	(2R,4S)-Pyrrolidine-2,4-dicarboxylic acid	59.2	1.43910938	0.000270192	0.688474374
GC	Mannobiose	81.8	1.434713195	0.014811044	-0.973065321
LC	[1,1'-Biphenyl]-4-ol, 3-amino-	36	1.431367306	6.00949E-08	-1.324417884
LC	2,12alpha-Dihydroxy-3-oxo-5beta-chol-1-en-24-oic Acid	41.1	1.431040894	0.010274667	-0.718439511
GC	2,4-Dihydroxypentanedioic Acid	77.1	1.418385824	0.02357389	0.670624347
GC	L-(-)-Sorbose	78.2	1.418018011	4.01186E-07	1.055322813
LC	Pyrogallol-1-O-sulphate	49.7	1.41688468	0.00036034	-6.585693362

GC	2-Hydroxybutyric Acid	94.7	1.415181276	9.56613E-11	1.077397714
LC	Sorafenib beta-D-Glucuronide	37.5	1.41482535	5.64284E-08	-1.18145105
LC	Polyglycerol esters of fatty acids	39.6	1.409600437	0.001772705	3.099179928
LC	6alpha-Hydroxycastasterone	48.3	1.409372819	7.91987E-13	-1.648359008
LC	Citrusinine I	49.3	1.407464648	4.932E-12	-2.509994588
GC	Galactonic Acid	81.9	1.403051197	0.008091077	-1.403085359
LC	Bentazone	38.4	1.40281291	3.88983E-25	40.29503191
LC	SM(d18:1/16:0(2OH))	38.6	1.401822443	0.025057923	-0.232932243
LC	PI(18:3(6Z,9Z,12Z)/20:1(11Z))	38.5	1.398100284	0.004675007	0.49250754
LC	Cholestane-3,5,6-triol	72.8	1.386584578	1.16517E-10	-1.309768773
LC	Tiazotic acid	39.5	1.383825135	2.50538E-09	-1.726210559
LC	Melanettin	45.9	1.377371632	1.94571E-14	-3.284301342
LC	(Z)-7-Dodecenyl butyrate	39	1.373676492	2.03243E-10	0.26313547
LC	N-(2-(Mercaptomethyl)-3-phenylbutanoyl)-L-alanine	43.8	1.37038432	7.69199E-12	10.10101417
LC	(2S,4R)-4-(9H-Pyrido[3,4-b]indol-1-yl)-1,2,4-butanetriol	50	1.367882721	2.98472E-15	-3.142406717
LC	(11E,13Z)-10-Hydroxyoctadeca-11,13-dienoylcarnitine	56.2	1.367125321	9.15086E-07	0.82769333
GC	Leucrose	78.2	1.363766502	3.59385E-05	1.074180275
LC	Daucic acid	45.5	1.36327816	1.16083E-11	-0.505608227
LC	Methacrifos	38.5	1.359796055	4.03021E-13	0.961238014
LC	(20R)-24-Hydroxygeminivitamin D3	47.1	1.357641186	3.85118E-07	-0.801281327
LC	15S-HTPE	51.9	1.356677686	3.31388E-09	-2.369491055
LC	Isoferulic acid 3-sulfate	40	1.348738588	0.007312743	-1.024892413
LC	Methylenediphosphonic acid	40.4	1.34567188	0.001055644	-0.188568392
GC	L-Tryptophan	88.5	1.344537361	5.89222E-08	-0.914546115
LC	3beta,4beta-dihydroxycholest-23-one	48.2	1.341571151	1.82387E-08	-0.935428182
GC	Glutaconic Acid	74.2	1.335572767	0.002869039	1.591296868
LC	2,2-Difluoro-n-(2-hydroxyethyl)-3-(2-nitro-1h-imidazol-1-yl)propanamide	39.3	1.334721464	0.000358464	-2.910804702
LC	Ambrettolic acid	54.2	1.333773865	0.001347852	-0.640662362
LC	Ambrisentan	36	1.330924408	6.93096E-22	13.40719786
LC	16-Deoxymyxinol	55.4	1.327185441	2.54802E-08	-0.800666617
LC	Etodolac acyl glucuronide	62.3	1.321159427	0.001050768	-3.261017575
LC	13'-Hydroxy-alpha-tocopherol	55.5	1.320662404	0.000550501	0.235100517

LC	Benzyloxycarbonyl-Val-Ala-Asp(OMe)-fluoromethylketone	39.3	1.31564306	9.51472E-08	12.58459523
LC	TETRAHYDROURIDINE	62.8	1.315640201	9.88862E-06	1.197547966
LC	Laninamivir	37.6	1.315078295	4.72882E-11	40.36701457
GC	Galactinol	82.8	1.314662258	0.026922345	2.298290345
LC	Phosphoric acid, mono(4-cyanophenyl) monomethyl ester	37.7	1.314512855	1.63562E-06	-0.776356559
LC	3-Methyl-2-oxovaleric acid	60.1	1.31435357	0.001572127	-0.222588034
LC	7beta,25-dihydroxycholesterol	38.7	1.313284326	1.62478E-08	-0.774929904
LC	5beta-Cholestane-3alpha,7alpha,27-triol	75.4	1.309030157	1.23141E-11	-1.392892746
LC	Eszopiclone	37.3	1.308072301	1.94372E-21	10.02060913
LC	Darexaban glucuronide	40	1.297878588	9.3707E-06	1.201798953
GC	Glucaric Acid	81.8	1.29347667	0.007820373	0.667343008
LC	7alpha,26-dihydroxy-5beta-cholestan-3-one	46.9	1.292758055	2.29368E-10	-1.043102429
LC	(S)-3-(6-Methoxypyridin-3-yl)-3-(2-oxo-3-(3-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)propyl)imidazolidin-1-yl)propanoic acid	46.7	1.290923367	3.50156E-06	10.11200681
LC	Polysorbate 80	40.9	1.290314954	1.13316E-10	-0.794285234
LC	(all-E)-3,5,7-Tridecatriene-9,11-diyn-1-ol	43.3	1.287141303	5.90686E-14	0.28752825
GC	3-Cyclohexene-1-Methanol	71.1	1.284516484	0.049951838	0.978242396
LC	(11E)-Tridec-11-enoylcarnitine	57.2	1.284000902	3.82809E-08	-1.087903702
LC	1-Octen-3-yl acetate	53.8	1.281472594	8.28176E-11	-1.074687074
LC	PS(24:0/20:3(5Z,8Z,11Z)-O(14R,15S))	37.2	1.281317653	2.97647E-06	-3.12192766
LC	beta-D-fructose 2,6-bisphosphate	38.8	1.276343754	0.046504248	-0.420784578
LC	19-oxodesacetylcinobufagin	40.1	1.275461979	4.11745E-06	-0.701854537
LC	Tiaprost	41.1	1.273791552	1.43271E-07	1.844380898
LC	Lithocholic acid glucuronide	40	1.273546523	0.002439931	0.151443928
GC	Fructose 1-Phosphate	84.2	1.27175649	0.01133481	2.815028352
LC	LysoPI(18:2(9Z,12Z)/0:0)	56.3	1.266056939	0.000504996	-0.527191022
LC	Lactobionic acid	47.3	1.258384781	3.79206E-11	40.2269431
LC	16beta-OH-Dhea sulfate	42.5	1.257892209	0.046511497	-0.491697064
LC	Scutellarein 4'-methyl ether 7-glucuronide	37.2	1.254363732	3.87717E-05	0.669947277
LC	Glutarate semialdehyde	52.2	1.251914886	3.29138E-09	9.974512386
LC	(25R)-4beta,26-dihydroxycholesterol	71	1.24748465	3.06453E-10	-0.942312061
GC	3,4-Dihydroxyphenylglycol	72.3	1.242660091	2.77563E-05	1.297538991
LC	LysoPE(P-18:0/0:0)	53.1	1.240490755	2.68332E-07	-0.688795769

LC	Gelsenicine	37.9	1.238704491	4.54946E-12	11.57452188
GC	D-Xylose	88.2	1.237233244	0.000232236	0.767781898
LC	2,2':6',2"-Terpyridine	36.4	1.237051707	1.92734E-06	2.579665828
GC	Udp-N-Acetylglucosamine	87.8	1.236231064	5.38843E-05	1.259139445
GC	Gluconolactone	83.4	1.233841205	2.84597E-05	1.286758602
LC	Deoxycytidine	52.9	1.232408908	3.43009E-08	0.16625119
LC	Desflurane	41.1	1.231162652	1.61316E-13	4.217595303
GC	3-Aminopropane-1,2-Diol	74.6	1.229821745	0.016804042	4.342858651
LC	20a,22b-Dihydroxycholesterol	58.9	1.229431942	1.41191E-09	-0.869569986
LC	Sphinganine 1-phosphate	68.8	1.22819153	7.18708E-05	0.833530046
LC	19-Oic-deoxycorticosterone	67.9	1.224931346	3.64464E-13	-1.017750249
LC	Pregnenolone sulfate	53.2	1.223923983	0.020210567	-0.52833252
LC	C16 Sphinganine	49.6	1.223794593	6.05841E-13	-0.780677052
GC	D-Galactose	96.1	1.221376193	3.27561E-05	1.075605716
LC	Dexamethasone	70.7	1.219943867	1.21459E-06	9.679703857
LC	PE(O-18:0/0:0)	49.2	1.218139912	2.06224E-12	1.550204696
LC	Phosphovanillin	38.4	1.218037437	5.42545E-19	0.472841303
GC	D-Threo-Isocitric Acid	91.4	1.217746415	4.28734E-08	0.885520275
GC	Uric Acid	94.5	1.21620351	3.86109E-07	-0.751637452
LC	Benzylpenicilloyl	44.6	1.216151883	5.07065E-11	40.2459073
LC	Serylvalylglycylglutamic acid	37.6	1.211251221	5.76314E-12	40.10637823
LC	3a,7a-Dihydroxycholanoic acid	69	1.210925986	7.36321E-07	-2.314184631
LC	Undecanoylcarnitine	59.4	1.209550184	7.35925E-06	-2.807619253
LC	L-Glutamic acid	64.9	1.205394744	0.00027443	0.273310866
GC	Linoelaidic Acid	96.5	1.202108658	3.03119E-09	0.897241912
LC	makisterone B	48.7	1.201886078	1.02461E-06	-0.686169382
LC	GDP-mannuronate	41.3	1.197507335	9.71077E-05	0.118552176
GC	Dodecanol	81.4	1.19660098	0.018447715	-1.222205621
LC	Succinylsulfathiazole	36.9	1.195668093	0.008454725	0.600593552
LC	LysoPE(0:0/20:4(8Z,11Z,14Z,17Z))	38.5	1.192939815	2.8019E-08	0.800394711
LC	Valylserine	50.8	1.183143626	3.56503E-05	2.073436849
LC	D-Lactic acid	71.1	1.182897022	0.001931519	0.221513843
LC	N6,N6,N6-Trimethyl-L-lysine	64.1	1.181879605	0.007052275	-1.067563438

LC	PGP(PGF1alpha/18:0)	36.7	1.180323101	0.001613153	0.591655076
LC	8-Carboxymethyldihydrochelerythrine	38.2	1.179327724	4.23409E-08	-1.314320959
LC	Bursin	40.1	1.178633568	1.45748E-08	2.140696885
GC	Ketoleucine	89.3	1.175660419	6.68119E-08	-0.781159082
LC	IODODIFLUNISAL	37.2	1.174970878	0.004948984	0.3142743
LC	Dextrothyroxine	48.8	1.174004762	1.36097E-07	-0.657876091
LC	Safingol (L-threo-sphinganine)	44.5	1.170975064	0.018387348	-0.234921176
LC	m-Trifluoromethylhippuric acid	40.2	1.170540167	1.46622E-05	-2.641315046
LC	Edetate trisodium	38.9	1.169722684	0.001185079	0.458215772
LC	(S)-Nerolidol 3-O-[a-L-rhamnopyranosyl-(1->2)-b-D-glucopyranoside]	40.1	1.169566391	0.000611494	-0.801239164
LC	1,1,1,2,3,3,3-Heptafluoropropane	40.9	1.169402501	1.79597E-07	0.124376432
LC	Bergaptol	38.8	1.169017972	0.001743079	0.351937392
LC	Bisantrene	37.8	1.163179334	1.71798E-08	1.592117747
LC	LysoPI(18:1(9Z)/0:0)	53.4	1.162667162	1.01072E-08	-0.835771306
LC	4,6-O-Ethylidene-D-glucose	40	1.160518728	1.06436E-10	3.313615091
LC	Phenylalanyltryptophan	68.5	1.159325965	0.000509969	-1.589599356
LC	Triphenylphosphine oxide	48.1	1.156975715	9.58183E-07	0.486960574
LC	Apremilast	36.9	1.156293509	2.92863E-13	12.61499288
LC	Diguanosine diphosphate	38.3	1.153739413	7.17078E-08	-1.208790112
LC	PHODA-PI	38.9	1.151062287	5.53769E-15	-4.621206282
LC	6-(1,2,3,4-Tetrahydroxybutyl)oxane-2,3,4,5-tetrol	42.1	1.149845018	3.31884E-06	0.461469759
GC	N-Acetyl-Tryptophan	83.7	1.141870085	1.88594E-07	-1.093699554
LC	5-Nonadecyl-1,3-benzenediol	52.6	1.139761748	1.92617E-09	-0.896064039
GC	1,2-Propanediol	95.2	1.136035086	8.93271E-08	2.565144123
LC	N-3-hydroxy-13-methyl-hexadecanoyl glycyL-L-serine	38.5	1.133261547	7.96892E-07	0.931168573
LC	Isoflupredone acetate	39.6	1.130907838	0.001683722	-0.8140645
GC	N-Alpha-Acetyl-L-Lysine	84.7	1.129653169	5.81088E-05	0.918986987
LC	Icotinib	38.7	1.12655806	6.91081E-19	39.70597332
LC	ChenodeoxycholyLtaurine	68.7	1.125916628	0.001474018	-1.437171611
LC	(8Z,11Z,13E,15S)-15-Hydroxyicosa-8,11,13-trienoylcarnitine	62.6	1.12137012	0.00149066	0.889053731
LC	Campesteryl glucoside	37.7	1.119815162	0.005620214	-0.797147378
LC	5-Hydroxyoctanoylcarnitine	63.6	1.114416716	5.72702E-05	-0.851615702

LC	Glucosyl 6-hydroxy-2,6-dimethyl-2E,7-octadienoate	39.1	1.112204063	5.28866E-09	3.267554974
LC	15-hydroxycembra-1,3,7,11-tetraene	54.1	1.110551009	2.57608E-07	-3.105080867
LC	PIM1(19:0/16:0)	37.3	1.110355082	0.000410268	-0.877398922
LC	Glycinexylidide	42.6	1.108467857	4.14218E-09	5.56626388
LC	7-Amino-4-hydroxy-2-naphthalenesulfonic acid	38.7	1.105374419	0.000433706	3.199223825
LC	typhasterol	46.2	1.105348837	1.77229E-07	-0.840338551
LC	Gyrophoric acid	39	1.102093794	0.012441174	1.027285565
LC	4-(4-Methoxyphenyl)-2-butanone	49.7	1.099769732	2.40176E-08	4.49849946
LC	3 alpha,7 alpha,26-Trihydroxy-5beta-cholestane	71.8	1.097658435	9.36945E-09	-0.963287826
LC	5-Methoxysalicylic acid	48.1	1.09583463	0.01276689	-2.23535692
LC	3-beta-Hydroxy-4-beta-methyl-5-alpha-cholest-7-ene-4-alpha-carboxylate	46.4	1.095648704	4.84528E-07	0.329611149
LC	Hirsutin	37.7	1.092191363	2.75445E-18	16.55159915
LC	Gluconic acid	70.9	1.08961736	3.5624E-05	0.78633826
LC	D-Mannose	60.9	1.087547276	0.000905525	0.282864932
LC	Callyspongendiol	38.9	1.087395071	3.46008E-10	0.302250787
LC	Momordol	59.8	1.082154252	2.15574E-10	-1.079477727
GC	Quebrachitol	85.5	1.081787968	2.16818E-06	0.760332767
LC	2-Quinolinylmethanol	59.4	1.077081886	6.96285E-07	-0.694387247
LC	Melanthugenin	42.4	1.074188386	7.00923E-07	40.13050409
LC	omega-linoleoyloxy-Cer(d20:1/32:0)	36.6	1.072884949	8.65716E-06	0.149054113
LC	3-Amino-5-(3-thiophenyl)-2-thiophenecarboxamide	36.7	1.072449973	8.95864E-05	0.09819849
LC	3-hydroxydecanoyl carnitine	57.2	1.07014953	1.59785E-05	-0.983544035
LC	N-Acetylserotonin glucuronide	39.1	1.064802095	2.72532E-18	39.61685605
LC	LysoPE(P-18:1(9Z)/0:0)	51.9	1.055516617	5.19698E-08	-0.807873634
GC	Phthalic Acid	77.5	1.055235543	0.007076062	1.287913683
LC	NNAL-N-glucuronide	50.6	1.05506139	1.82075E-08	9.599778114
LC	25-Acetylvulgaroside	52.8	1.054460118	0.006206929	-2.068018874
LC	4-Hydroxybenzoic acid	55.1	1.054414052	2.33657E-09	-1.839944175
GC	1h-Indole-2-Acetic Acid	86.9	1.054373789	0.000459681	-0.621492547
LC	PE(14:1(9Z)/12:0)	37.5	1.052910636	3.19574E-07	-0.504740578
GC	Shikimic Acid	86.6	1.050427422	5.0944E-05	0.785281379
LC	Serylmethionine	55.9	1.05021726	0.000192059	3.875084469

LC	7-Chloroemodin	48.5	1.049950067	6.12867E-14	-0.54394084
LC	Leucyl-leucine	60	1.04923988	5.68426E-07	-3.180942814
LC	2-hydroxy-9Z,12Z-Octadecadienoic acid	40.3	1.047346217	1.34841E-07	-1.975596055
LC	farnesyl triphosphate	38.4	1.04205051	3.94004E-11	-1.212171299
LC	plaunotol	53.8	1.041525176	9.62516E-09	-1.038554986
LC	Indole	50	1.040677766	8.36688E-17	-0.351241445
LC	Teleocidin B 2	36	1.040098076	0.000547234	-2.20998629
LC	3-Hydroxy-1,10-bisaboladien-9-one	60.1	1.03818934	0.004548154	1.095314722
LC	12-tridecynoic acid	51.3	1.034793857	3.63108E-20	0.484924232
LC	Mulberrofuran Q	42.6	1.033107969	3.52486E-11	39.71929984
LC	SNAG-delta5-CT	37.4	1.028376595	1.98698E-05	7.625205132
LC	6-Nitrotryptophan	45.1	1.027077565	3.82194E-11	-1.16579239
LC	Ribosylhopane	37.8	1.02643103	2.82385E-11	-2.705621997
LC	Penicisteroid H	51.1	1.018244517	1.08954E-05	-0.713641282
LC	7 alpha,24-Dihydroxy-4-cholesten-3-one	54.5	1.014163859	4.4465E-11	-1.311082054
LC	1-Methyladenosine	55.3	1.012217471	7.60465E-10	0.539969864
LC	Tropisetron	42.5	1.012113342	0.016069794	11.17734416
LC	Dihydroxyacetone phosphate	47.4	1.010750013	0.004264067	0.332881603
LC	Dodecenoylcarnitine	52.2	1.009241096	2.54326E-05	-0.821619191
LC	(7'S,8'S)-4,7'-Epoxy-3,8'-bilig-7-ene-3',5-dimethoxy-4',9,9'-triol 4'-glucoside	45.6	1.001694241	0.028532372	1.602952429

Supplementary Table 3
the Same Expressed Metabolites

P-Cresol Glucuronide
Equilenin
M-Toluamide
Lactulose
3-(Pyrazol-1-Yl)-L-Alanine
2,6-Pyridinedicarboxylic Acid
Maltotriose
Cis-Aconitic Acid
Mannobiose
Lactitol
Quinic Acid
Melezitose
Oleic Acid
Ribonic Acid
Levoglucozan
3-Hydroxybutyric Acid
3-Methylbutane-1,2-Diol
10-Heptadecenoic Acid
2,4-Dihydroxypentanedioic Acid
Galactonic Acid
D-Xylose
Cis-Erucic Acid
Dodecanol
Cellobiose
1,2-Propanediol
L-Tryptophan
Delta-Tocopherol
Linoelaidic Acid
Beta-Lactose
Uric Acid
Ketoleucine
3,4-Dihydroxyphenylglycol
Gluconolactone
Udp-N-Acetylglucosamine
Sorbitol-6-Phosphate
L-(-)-Sorbose
Leucrose
D-Galactose
N-Acetyl-Tryptophan
Mg(0:0/16:0/0:0)
2-Hydroxybutyric Acid
1h-Indole-2-Acetic Acid
Phthalic Acid
Glutaconic Acid
Glucuronic Acid
Propofol glucuronide
LysoPC(0:0/18:2(9Z,12Z))
Edetic Acid
PC(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/P-18:1(11Z))
Carissanol
LysoPC(20:4(5Z,8Z,11Z,14Z)/0:0)
Lidocaine
L-Acetylcarnitine
PC(P-18:1(11Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))
Dehydroepiandrosterone sulfate
N-(2-Hydroxyethyl)-2-(1-isoquinolinylmethylene)hydrazinecarbothioamide
1-O-(2-methoxy-4Z-hexadecenyl)-sn-glycero-3-phosphocholine

Isocitric acid
1-(O-alpha-D-glucopyranosyl)-29-keto-(1,3R,31R)-dotriacontanetriol
Myristyl linoleate
2-C-methyl-D-erythritol-4-phosphate
2-Methyl-4'-(methylthio)-2-morpholinopropiophenone
LysoPC(0:0/18:0)
SM(d19:1/17:1)
UTILIN
PC(0:0/14:0)
19-Epischolaricine
SM(d18:1/16:1(9Z))
S-Japonin
Benzoxazole
Chenodeoxycholic acid glycine conjugate
N-Nitrosoanatabine
13-Hydroxyoctadecanoylcarnitine
4-(2-Aminoethylamino)-3-[bis(carboxymethyl)amino]-3-(carboxymethyl)hexanedioic acid
TG(8:0/8:0/a-17:0)[rac]
O-Linoleoylcarnitine
Oxotremorine
Vignatic acid B
Pulverulentoside I; (1aS,1bS,2S,5aR,6S,6aS)-6-({3-O-Acetyl-6-deoxy-2-O-[(2E)-3-(4-methoxyphenyl)-2-propenoyl]-?-L-mannopyranosyl}oxy)-1a-(hydroxymethyl)-1a,1b,2,5a,6,6a-hexahydrooxireno[4,5]cyclopenta[1,2-c]pyran-2-y I ?-D-glucopyranoside
Disodium ethylenediaminetetraacetate
Ecabet
2,2'-Methylenebis(4-methyl-6-tert-butylphenol)
LysoPE(18:1(9Z)/0:0)
6-Butyryl-5-hydroxy-4-phenylseselin
(Z)-1-(Methylthio)-5-phenyl-1-penten-3-yne
Phyllocoumarin
Armillaripin
GM4(d18:1/18:0)
Enterodiol sulfate
Decanoylcarnitine
21H-Bilane-8,12-dipropanoic acid, 3,18-diethenyl-1,19,22,24-tetrahydro-2,7,13,17-tetramethyl-1,19-LysoPC(20:4(8Z,11Z,14Z,17Z)/0:0)
3-(4-Iodophenyl)-2-mercapto-(Z)-2-propenoic acid
PI(O-18:0/18:0)
Fluoxetine
Allopregnanolone sulfate
Cichorioside K
PS(P-20:0/22:2(13Z,16Z))
Isoscaparin 2''-O-glucoside
PC(14:1(9Z)/20:3(8Z,11Z,14Z))
EUPARIN
2-Methoxy-4-(2-(methylamino)propyl)phenyl beta-D-glucopyranosiduronic acid
Thiamine
LysoPE(P-16:0/0:0)
Sphingosine 1-phosphate
PS(P-20:0/0:0)
Caffeine
LysoPC(O-18:0/0:0)
6-Thioxanthyllic acid
PE(22:4(7Z,10Z,13Z,16Z)/21:0)
LysoPE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
lysine phosphoester
alpha-Hydroxyisobutyric acid
Plantacyanin

dIDP
LysoPC(0:0/20:4(5Z,8Z,11Z,14Z))
Vaccenic acid
2-Oxoarginine
PC(12:0/20:1(11Z))
3,7-Dihydroxycholan-24-oic acid
PE-NMe2(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))
Gravolenic acid
Ptilosaponoside B
PC(17:2(9Z,12Z)/0:0)
Pyridine N-oxide glucuronide
APC
PC(18:0/P-16:0)
Theophylline
3-Hydroxy-1,10-bisaboladien-9-one
Methyl 3-epi-4,5-didehydrojasmonate
Octenoyl-L-carnitine
1-O-Hexadecyl-sn-glycero-3-phosphocholine
Hydroxyzine
9-tridecynoic acid
3-Hydroxylidocaine
DG(18:3(9,11,15)-OH(13)/15:0/0:0)
PC(O-16:1(11Z)/0:0)
TG(8:0/8:0/a-13:0)[rac]
[(2S,4R,5R,6R,14S,16R)-14-Hydroxy-7,11-dimethyl-6-(2-oxopyran-4-yl)-3-oxapentacyclo[8.8.0.02,4.02,7.011,16]octadecan-5-yl] acetate
LysoPE(0:0/18:1(11Z))
2-Hydroxycinnamic acid
3,4-Dimethylethcathinone
(-)-Salvisyriacolide
27-Hydroxycholesterol
(5Z,9Z)-2-methoxy-hexacosadienoic acid
4-Allylphenol sulfate
2-((2-Methoxy-2-(3-(trifluoromethyl)phenyl)ethyl)amino)ethyl 4-(2-(2-(9H-fluoren-9-Galactotriose
Spiropiperidine
gamma-Glutamylserine
3,4-Bis(carboxymethyl)-3,4-dihydroxyhexanedioic acid
3-hexanoyl-NBD Cholesterol
Trihydroxycoprostanic acid
6''-Acetylliquiritin
Glycocholic acid
BAY-u9773
indoprofen
3-[(1R,4S,5S,6R)-6-[(1E,3S,5Z,8Z,11Z)-3-Hydroperoxytetradeca-1,5,8,11-tetraen-1-yl]-2,3-dioxabicyclo[2.2.1]heptan-5-yl]propanoylcarnitine
Octadec-5-enoic acid
Demissidine
PI-Cer(t18:0/18:0(2OH))
Kuguacin E
Dehydropachyrrhizone
3-Methyl-2Z,4E-decadienoic acid
SM(d18:1/14:0)
Zearalenone
Ansamitocin P3
6-Hydroxy-3,4-dihydro-2(1H)-quinolinone
Ambrettolic acid
Artemoin A
Desacetycefapirin

N-Choloylglycine
Melibiose
16-oxo-palmitate
Mactraxanthin 3-linoleate 3'-dipalmitoleate
3b-Hydroxy-5-cholenoic acid
Isothankunic acid
N-Palmitoyl Arginine
SM(d18:1/12:0)
5alpha-Cholestane-3alpha,7alpha,12alpha,24-tetrol
Cohibin A
2-Deoxybrassinolide
LysoPC(P-18:1(9Z)/0:0)
UDP-D-galacturonic acid
PE-Cer(d15:2(4E,6E)/20:0)
Bis(2-ethylhexyl) phthalate
(1R)-5-[2-[(1R,7Ar)-7a-methyl-1-[(2R)-6-methylheptan-2-yl]-2,3,3a,5,6,7-hexahydro-1H-inden-4-ylidene]ethylidene]-4-methylidenecyclohexane-1,3-diol
5alpha-Pregnan-3beta,20beta-diol 20-sulfate
Melatonin glucuronide
2-[(2-Fluorophenyl)sulfanylmethyl]-5-[6-[(2-hydroxycyclopentyl)amino]purin-9-yl]oxolane-3,4-diol
Ethyl n-allyl-n-[(e)-2-methyl-3-[4-(4-amidinophenoxy carbonyl)-phenyl]propenoyl]amino acetate
SALSOLIDINE
Sesamol
2,4-Diamino-6-nitrotoluene
D-Lactic acid
1,1,1,2,3,3,3-Heptafluoropropane
Piperine
bhos#40
Cefodizime,(S)
Chenodeoxycholic acid
Mayolene-17
DG(18:3(9Z,12Z,15Z)/15:0/0:0)
3-Amino-6-{4-[(4-Methylpiperazin-1-yl)sulfonyl]phenyl}-N-Pyridin-3-ylpyrazine-2-Carboxamide
1,5-Naphthalenediamine
Uridine 2',3'-cyclic phosphate
(11E)-Octadec-11-enedioylcarnitine
Androstenediol 3-sulfate
Gorgostane-3beta,5alpha,6beta,11alpha,12beta-pentol 12-acetate
Marmesin rhamnoside
beta-D-fructose 2,6-bisphosphate
5-Hydroxy-2-imino-1-methylimidazolidin-4-one
Propylparaben
(20R)-24-Hydroxygeminivitamin D3
PE(10:0/10:0)
3-Hydroxymethyl-picumast
1-Hydroxy-2,2,5,5-tetramethylpyrrolidine-3-carboxamide
Symmetric dimethylarginine
PE-Cer(d14:2(4E,6E)/23:0)
3beta,4beta-dihydroxycholest-23-one
(2S)-1,1,1-Trifluoro-2-(4-pyrazol-1-ylphenyl)-3-[5-[[1-(trifluoromethyl)cyclopropyl]methyl]-1H-Ganoderiol C
4-(2-Aminoethyl)benzenesulfonyl fluoride
Dodecylbenzene
Uridine diphosphate glucose
Blumealactone C
7beta,25-dihydroxycholesterol
Zierin
LysoPE(P-18:0/0:0)
Ikarisoside D

Cabozantinib
Oxdralazine
16-Deoxymyxinol
Darexaban glucuronide
(4S,6R)-6-[(1E)-4,4-Bis(4-fluorophenyl)-3-(1-methyltetrazol-5-yl)buta-1,3-dienyl]-4-hydroxyoxan-2-
Pregnenolone sulfate
Cholestane-3,5,6-triol
Daucic acid
Sulfaethidole
2,2':6',2''-Terpyridine
N-(2-(Mercaptomethyl)-3-phenylbutanoyl)-L-alanine
Hydroquinone sulfate
Dodecanoylcarnitine
15S-HTPE
7-Amino-4-hydroxy-2-naphthalenesulfonic acid
6alpha-Hydroxycastasterone
2,4-Thiazolidinedicarboxylic acid, 2-methyl-
27-Norcholestanehexol
makisterone B
Campesterol glucoside
Armatinol B
DG(i-15:0/0:0/i-12:0)
5b-Cholestane-3a,7a,12a,23-Tetrol
5beta-Cholestane-3alpha,7alpha,27-triol
3a,7a-Dihydroxycholanoic acid
Callyspongenol A
N-(1-Deoxy-1-fructosyl)glycine
7alpha,26-dihydroxy-5beta-cholestan-3-one
Serylmethionine
virginiamycin m1
2-Ethoxy-3-[4-[2-(4-methylsulfonyloxyphenyl)ethoxy]phenyl]propanoic acid
Pyrogallol-1-O-sulphate
19-oxodesacetylcinobufagin
Tribufos
Methylenediphosphonic acid
Polysorbate 80
20a,22b-Dihydroxycholesterol
(25R)-4beta,26-dihydroxycholesterol
Heliangin
13'-Hydroxy-alpha-tocopherol
19-Oic-deoxycorticosterone
SM(d18:1/16:0(2OH))
Callyspongendiol
Dexamethasone
chrysoeriol 7-O-neohesperidoside
Sitostanol-beta
Melanettin
Benzyloxycarbonyl-Val-Ala-Asp(OMe)-fluoromethylketone
3-(3,4-Difluorophenyl)-4-(4-(methylsulfonyl)phenyl)-2(5H)-furanone
3 alpha,7 alpha,26-Trihydroxy-5beta-cholestane
Citrusinine I
4,6,2',4'-Tetramethoxychalcone 2'-beta-glucoside
Naematolone
(2S,4R)-4-(9H-Pyrido[3,4-b]indol-1-yl)-1,2,4-butanetriol
C16 Sphinganine
Sphinganine 1-phosphate
IODODIFLUNISAL
typhasterol
Fusaroskyrin

LysoPE(P-18:1(9Z)/0:0)
25-Acetylvulgaroside
Longilactone, delta-4(18)-Isomer, 2alpha-alcohol; (1R,2R,3R,3aS,5aS,6R,6aS,9S,10S,10aS,10bR,10cR)-
1,2,6,9,10-Pentahydroxy-3,10a,10c-trimethyl-7-methylenetetradecahydro-4H-phenanthro[10,1-
Pregnanediol-3-glucuronide
Methiuron
Bentazone
Penicisteroid H
Bergaptol
2-Hydroxy-3-methylbutyric acid
[1,1'-Biphenyl]-4-ol, 3-amino-
PE(20:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))
Deoxycytidine
PS(24:0/20:3(5Z,8Z,11Z)-O(14R,15S))
Schisanhenol
Ephedrine
1-Octen-3-yl acetate
Sorafenib beta-D-Glucuronide
Benzylpenicilloyl
GDP-mannuronate
PE(14:1(9Z)/12:0)
5-Methoxysalicylic acid
Phosphoric acid, mono(4-cyanophenyl) monomethyl ester
Undecanoylcarnitine
Methacrifos
Momordol
N-3-hydroxy-13-methyl-hexadecanoyl glyceryl-L-serine
2-Hexadecyloctadec-9-enal
(11E,13Z)-10-Hydroxyoctadeca-11,13-dienoylcarnitine
Phenylalanyltryptophan
15-hydroxycembra-1,3,7,11-tetraene
PIM1(19:0/16:0)
Edetate trisodium
5-Nonadecyl-1,3-benzenediol
Bisantrene
Etodolac acyl glucuronide
Dihydroxyacetone phosphate
2-(Trifluoromethyl)isonicotinic acid
Ambrisentan
3-Amino-5-(3-thiophenyl)-2-thiophenecarboxamide
Isoflupredone acetate
6-Nitrotryptophan
(3Z,5E,7E)-Decatrienoylcarnitine
7-Chloroemodin
2-[(1R,3S)-3-Hydroxycyclohexyl]-5-(2-methyloctan-2-yl)phenol
N6,N6,N6-Trimethyl-L-lysine
(2S)-3-[3-[(4-Carbamimidoylbenzoyl)amino]propanoylamino]-2-[(4-
gamma-Glutamylacetamide
farnesyl triphosphate
Eszopiclone
NNAL-N-glucuronide
D-Mannose
LysoPI(18:1(9Z)/0:0)
Tropisetron
Gelsenicine
Succinylsulfathiazole
Phosphovanillin
2,2-Difluoro-n-(2-hydroxyethyl)-3-(2-nitro-1H-imidazol-1-yl)propanamide
plaunotol

7 α ,24-Dihydroxy-4-cholesten-3-one

PHODA-PI

Leucyl-leucine

(1(10)E,4a,5E)-1(10),5-Germacradiene-12-acetoxy-4,11-diol

Ribosylhopane

Confusoside
