

Supplementary Table 4: Normal VS Model_metabolites

#ID	name	Normal_vs_Model_log2FC	Normal_vs_Model_Pvalue	Normal_vs_Model_VIP	Normal_vs_Model_(FC_2_Pvalue_0.05_VIP_1)_regulated
pos_7178	Dodecylbenzene	0.668230753	4.57E-07	2.131076348	unchanged
neg_1268	Taurocholate	0.738730849	1.26E-06	2.124237895	unchanged
neg_2037	S-Methyl hexadecanethioate	0.658053461	6.04E-06	2.122646176	unchanged
neg_2057	Mevastatin	-0.633302061	1.20E-05	2.096138302	unchanged
neg_14	Fructose-lysine	0.682499067	2.04E-05	2.122458661	unchanged
neg_1817	5(S)-HPETE	1.02262616	2.60E-05	2.130515829	up
pos_1376	alpha-D-Sedoheptulopyranose 7-phosphate	0.884054788	3.88E-05	2.063835155	unchanged
neg_2053	Taxa-4(20),11(12)-dien-5alpha,13alpha-diol	-0.678911874	5.47E-05	2.057753135	unchanged
neg_2055	(±)13-HDoHE	0.872244402	6.32E-05	2.04708922	unchanged
neg_2060	Erinacine C	-0.875843994	7.17E-05	2.082213994	unchanged
neg_2231	11-Dehydro-thromboxane B2	3.310184751	7.25E-05	2.051435947	up
neg_1680	Methyl octynecarboxylate	0.941298824	7.73E-05	2.048540384	unchanged
neg_1497	Cyanoketone	1.820228254	9.54E-05	2.041236393	up
pos_7184	Sphingosine-1-phosphate	-0.597790074	0.000112317	2.008892653	unchanged
neg_1506	Tetradecanedioic acid	1.973724385	0.000181223	2.011496144	up
neg_2108	PC(P-16:0/PGE1)	1.137828946	0.000216699	2.028914164	up
neg_1514	Caprylic acid	1.83058955	0.000231052	2.020830071	up
neg_2019	PE(20:1(11Z)/16:0)	2.390171638	0.000326519	2.00345998	up
neg_2258	CP 47,497-C8-homolog C-8-hydroxy metabolite	1.397685296	0.000330292	2.013886729	up
neg_1545	Pikromycin	2.221016653	0.00039127	2.000526259	up
neg_1571	Pentolame	-0.459514833	0.000463592	1.962952211	unchanged
neg_1574	Piriprost	2.826583748	0.0004672	1.974431221	up
neg_1576	Pravastatin	-0.747641862	0.00047159	1.972976217	unchanged
neg_1581	Pregnenolone-3,21-disulfate	-1.671144101	0.000558305	2.002701975	down
neg_2141	(R)-3,4-Dihydro-8-hydroxy-3-tridecyl-1H-2-benzopyran-1-one	0.475785432	0.000626352	1.910843901	unchanged
neg_1612	3-[(3aS,4S,7aS)-7a-Methyl-1,5-dioxo-octahydro-1H-inden-4-yl]propanoate	1.061857201	0.000638906	2.041040021	up
neg_1613	5-((6-((Aminomethyl)amino)-1-oxohexyl)amino)pentanoic acid	1.706070237	0.000699712	1.94561333	up
neg_522	6-Thioxanthine 5'-monophosphate	1.152520902	0.000723266	1.956367226	up
neg_1618	Propofol glucuronide	2.927510994	0.000737336	1.995123027	up
pos_1375	2-epi-5-epi-Valiolone 7-phosphate	2.300352639	0.000738623	2.023421239	up
neg_521	dTDP	0.72928325	0.000799229	1.962574748	unchanged
neg_1650	LysoPE(0:0/18:3(6Z,9Z,12Z))	1.467920913	0.000829587	1.931113864	up
neg_1662	LysoPC(18:3(6Z,9Z,12Z)/0:0)	1.225953801	0.000839474	1.945228756	up
neg_1665	N-Palmitoyl Arginine	1.545177998	0.000861153	1.953682552	up
neg_1668	Trypanothione disulfide	2.205949323	0.00100399	1.98836014	up
neg_1670	LysoPE(0:0/16:1(9Z))	0.909929375	0.001052055	1.92766431	unchanged
neg_1675	2'''-N-Acetyl-6'''-deamino-6'''-hydroxyneomycin	1.639099157	0.001059749	1.922254156	up
neg_1932	PE(20:3(6,8,11)-OH(5)/P-18:1(11Z))	-0.714635123	0.001079421	1.916268062	unchanged
neg_1682	C12272	3.517099984	0.001107732	1.977574127	up
neg_1683	Bardoxolone methyl	2.38514621	0.001121349	1.926786608	up
neg_1684	5b-Cyprinol sulfate	2.526097337	0.001216661	1.957291394	up
neg_1693	24,25-Diacetylvulgaroside	1.796266582	0.001248812	1.971716223	up
neg_1765	20-Hydroxyecdysone	1.598203277	0.001263565	1.984596555	up
neg_2096	(±)16-HETE	1.135611362	0.001269776	1.914697968	up
neg_1799	Phytolaccatoxin	1.888256744	0.001326897	1.905653678	up
neg_1810	Decanoylcholine	1.597746773	0.001415308	1.890936639	up
pos_9740	Icosadienoic acid	-0.711789714	0.001417756	1.864668242	unchanged

neg	1818	C11134	-0.641911726	0.001487916	1.949194818	unchanged
neg	1848	Lucidenic acid M	1.418524105	0.001489044	1.910458464	up
neg	1852	LysoPE(0:0/18:2(9Z,12Z))	2.091431527	0.001503351	1.908267378	up
neg	1855	PKG Inhibitor	0.855014179	0.001543955	1.944622066	unchanged
neg	1857	Pubescenol	0.654519535	0.001580302	1.872760613	unchanged
neg	2229	PC(P-18:0/PGF1alpha)	2.247079838	0.001642734	1.893774578	up
neg	1874	(E)-3,7-Dimethyl-1,5,7-octatrien-3-ol	2.028932219	0.001689865	1.995184767	up
neg	1875	LysoPE(0:0/18:1(11Z))	-0.511512458	0.001696166	1.827491696	unchanged
neg	2118	PE-NMe2(18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))	2.12366813	0.00170959	1.912063088	up
neg	2230	Siderol	1.593143617	0.001717856	1.893027432	up
neg	1927	(6Z,9Z,12Z)-Octadecatrienoic acid	3.110486369	0.001718526	1.945265003	up
neg	1498	(3beta,5alpha,6beta,7alpha,22E,24R)-Ergosta-8,22-diene-3,5,6,7-tetrol	2.651603471	0.001724226	1.921722392	up
neg	2088	Eicosapentaenoic acid	2.426777643	0.001769061	1.898155937	up
neg	1972	C16143	0.991972491	0.001810993	1.861625878	unchanged
neg	2158	8(S)-HETrE	1.84541022	0.00181234	1.881363478	up
pos	9088	(5Z,8Z,11Z,14Z,17Z)-Icosapentaenoic acid	1.058099421	0.001814996	1.866479907	up
neg	1925	PC(20:2(11Z,14Z)/PGJ2)	-0.656496223	0.001882338	1.841238345	unchanged
pos	9302	DEHYDROCHOLIC ACID	2.507088518	0.001967735	1.896309084	up
neg	1923	PC(P-16:0/PGF2alpha)	-0.241026985	0.002051331	1.873620847	unchanged
neg	2115	PE(22:1(13Z)/6 keto-PGF1alpha)	-0.487117576	0.00205958	1.860094837	unchanged
pos	9335	19(S)-HETE	-0.630778284	0.002151982	1.821836435	unchanged
pos	8991	1,2-dihydroxyheptadec-16-en-4-yl acetate	-0.769698738	0.002185285	1.856543681	unchanged
pos	806	UDP-4-dehydro-6-deoxy-D-glucose	1.762550973	0.0023542	1.873396485	up
neg	1629	geranate	0.371491778	0.002388336	1.819733101	unchanged
neg	2114	PE(20:1(11Z)/20:3(5Z,8Z,11Z))	0.824380813	0.002395206	1.923292466	unchanged
neg	1993	5-Methoxytryptamine	0.845111827	0.002402584	1.869124971	unchanged
neg	1998	LysoPE(0:0/18:0)	-1.007020359	0.00249423	1.859412312	down
neg	1985	Hexadecanoic acid	-0.577390032	0.002519721	1.83483556	unchanged
neg	2015	Polyporusterone B	1.424998646	0.002573617	1.854816013	up
neg	1931	14-Fluoro-6-thiaheptadecanoic acid	2.235644657	0.002581103	1.897778166	up
neg	2101	Deoxyloganin	2.043485071	0.00259134	1.879902451	up
neg	2038	Tenofovir exalidex	0.942717067	0.002714319	1.894885521	unchanged
neg	875	Azamethiphos	-2.416910959	0.002724883	1.919470694	down
neg	1930	1-(3-Methylbutanoyl)-6-apiosylglucose	-0.349854715	0.002784611	1.84523007	unchanged
pos	9091	17-Hydroxymethylethisterone	-0.73789951	0.002838969	1.949818073	unchanged
neg	1988	13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid	1.45175175	0.002853659	1.868866069	up
neg	1609	Undecylprodigiosin	1.238282068	0.003056362	1.792775097	up
neg	2068	1-Stearoylglycerophosphoserine	2.550155409	0.003345603	1.852916857	up
neg	2086	Dihydroactinidiolide	-0.574150981	0.003376642	1.841911346	unchanged
neg	1986	13(S)-HODE	-0.358891383	0.003490217	1.806548141	unchanged
pos	781	Uric acid	-0.457449702	0.00353728	1.783270975	unchanged
pos	7049	(±)-Myristoylcarnitine	1.457988384	0.003623911	1.867958719	up
neg	1922	11,12,13-Trinor-1(10)-spirovetivene-2,7-dione	1.106574086	0.003805577	1.811178439	up
neg	2103	1alpha-Hydroxyarbusculin A	1.406320337	0.003904338	1.905056848	up
neg	2042	PC(15:0/P-16:0)	-0.435435014	0.004071465	1.821180955	unchanged
neg	1360	Bilirubin	1.842579052	0.004125249	1.814941249	up
pos	9082	L-2-Amino adipate 6-semialdehyde	0.957655644	0.004136909	1.797288283	unchanged
neg	576	5-Fluorodeoxyuridine	0.713028203	0.004238395	1.916912795	unchanged
neg	2116	Glycochenodeoxycholate	1.122862538	0.00428839	1.795118298	up
pos	9090	(+)-Camphor	-0.632205197	0.004327244	1.809544308	unchanged

neg_2131	Cholylcitrulline	0.944809638	0.004501519	1.836583	unchanged
neg_1881	PE(P-18:0/PGE2)	-0.540062912	0.004545152	1.754787911	unchanged
pos_9416	prostaglandin a1 ethyl ester	-0.472099462	0.004552808	1.802970636	unchanged
neg_2156	CDP-DG(a-17:0/i-24:0)	-0.722369291	0.004740062	1.762344835	unchanged
neg_881	5-Methoxytryptophan	-0.663292376	0.00487351	1.778509573	unchanged
neg_2177	Bifonazole	0.995534963	0.004957286	1.776077305	unchanged
neg_2185	3-Oxohehexadecanoic acid	-0.524003949	0.005044207	1.76231919	unchanged
neg_2188	PI(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	1.295090075	0.005084368	1.73061469	up
neg_2189	Bis(beta-D-glucosyl) crocetin	2.030396205	0.005172896	1.826122918	up
neg_2196	Prolylhydroxyproline	-0.634619202	0.005196423	1.712770494	unchanged
neg_2212	delta-Terpineol	1.161279912	0.005341652	1.854983197	up
pos_1920	Carmofur	2.437334435	0.005592653	1.835657726	up
neg_1869	PC(P-18:0/PGE2)	1.386872298	0.005634015	1.761092329	up
pos_4789	Coenzyme F420	-1.171963905	0.005681468	1.831915096	down
neg_2253	16-Oxopalmitate	2.342021938	0.005754155	1.888839584	up
neg_1508	Hymenoxon	1.924156826	0.005769766	1.835984158	up
neg_2255	3alpha,11beta,21-Trihydroxy-20-oxo-5beta-pregnan-18-al	0.782548004	0.005848261	1.757549569	unchanged
neg_2405	(7Z,10Z,13Z,16Z,19Z)-Docosapentaenoic acid	1.800336451	0.005860013	1.774603381	up
neg_2315	(9Z)-Hexadecenoic acid	2.021075497	0.005913241	1.870255022	up
neg_2353	(R)-3-Hydroxy-hexadecanoic acid	0.536659493	0.006229001	1.706720651	unchanged
neg_2356	C21481	-0.50696724	0.006506328	1.818664863	unchanged
neg_2386	LysoPA(0:0/18:0)	1.170282821	0.006652145	1.793314601	up
neg_2403	3b,12a-Dihydroxy-5a-cholanoic acid	1.082147064	0.006883947	1.758262266	up
pos_5642	Urocortisol	-0.801449899	0.00689562	1.772001242	unchanged
neg_2465	Hept-2-en-1-yl isovalerate	1.083101418	0.007146442	1.737942535	up
neg_2492	1-Lyso-2-arachidonoyl-phosphatidate	1.577689823	0.007186147	1.820764278	up
neg_2504	DG(22:0/6 keto-PGF1alpha/0:0)	0.9412831	0.007190117	1.74926781	unchanged
neg_2511	Calcidiol	3.306125059	0.007219784	1.814203309	up
neg_2546	15-Hydroxy-11alpha,9alpha-(epoxymethano)prosta-5,13-dienoic acid	0.664730754	0.007231403	1.725924351	unchanged
neg_2556	8,11-eicosadiynoic acid	-0.290733465	0.007286091	1.729403053	unchanged
neg_2562	Tetrahydrofolate	0.608658273	0.007575774	1.774274018	unchanged
neg_2568	6-Ethylchenodeoxycholic acid	-1.730374014	0.007714112	1.699168127	down
neg_2599	Vofopitant	-0.36382275	0.007715911	1.727279852	unchanged
neg_2607	Filipin II	0.838231716	0.00777278	1.718734328	unchanged
neg_2615	(-)-3-Cyanomethyl-3-hydroxy-1H-indol-2(3H)-	0.97916813	0.008173336	1.783657553	unchanged
neg_2621	Biotin sulfone	1.340067714	0.0082144	1.705036743	up
neg_2635	Teasterone	0.763915531	0.008317769	1.724113988	unchanged
neg_2660	trans-16-Octadecenoic acid	-0.255201107	0.008506191	1.704026793	unchanged
neg_2670	Tetrahydrocorticosterone	1.461085093	0.008576197	1.717092456	up
neg_2672	1,2,10-Trihydroxydihydro-trans-linalyl oxide 7-O-beta-D-glucopyranoside	2.297391489	0.008912505	1.819347864	up
neg_2678	(R)-Mevalonate	1.123587912	0.009014282	1.71700808	up
neg_2682	7-[(1R,2R,3R,5S)-3,5-Dihydroxy-2-[(3S)-3-hydroxyoctyl]cyclopentyl]heptanoylcarnitine	1.666942573	0.00906613	1.824490265	up
neg_2689	Farnesoic acid	-0.174268523	0.009176819	1.709330994	unchanged
neg_2713	Galaxolide	-0.976597566	0.0092969	1.726021905	unchanged
neg_2716	3-Hexaprenyl-4,5-dihydroxybenzoate	-0.355829227	0.009672502	1.81695731	unchanged
neg_2724	Octadecanoic acid	-1.675827914	0.009840062	1.776574735	down
neg_2748	20,26-Dihydroxyecdysone	-0.292981026	0.009857091	1.697047479	unchanged
neg_2763	2,6,10,10-Tetramethyl-1-oxaspiro[4.5]decan-6-ol	-1.027356587	0.01026635	1.702797648	down

neg_2783	QUINALPHOS	-0.592449931	0.010293481	1.690791152	unchanged
neg_2803	(2R,3R)-3-Methylornithinyl-N6-lysine	1.993040835	0.010678018	1.796008888	up
neg_2805	Ginsenoside C-K	-0.754122304	0.010699571	1.761511833	unchanged
neg_2814	PG(20:1(11Z)/PGE2)	1.349318995	0.010700764	1.745197247	up
neg_2815	alpha-Tocopherol	3.273020874	0.010737105	1.795704278	up
neg_2825	(Z,Z)-3,6-Dodecadien-1-ol	-1.061121579	0.010771214	1.630734586	down
neg_2829	(3alphaOH,20S,24S)-3,19:20,24-Diepoxydammarane-3,25-diol	0.531770153	0.011122954	1.631444153	unchanged
neg_2844	alpha-Valerenol	1.082807747	0.011496077	1.8074758	up
neg_2846	6-((3-Cyclobutyl-2,3,4,5-tetrahydro-1H-3-benzazepin-7-yl)oxy)-N-methyl-3-oxvridinecarboxamide	0.668759117	0.01154162	1.678563639	unchanged
neg_2932	Germacrenone	-0.892826778	0.011983475	1.681067766	unchanged
neg_3051	LysoPI(0:0/18:0)	1.457173041	0.011992423	1.700676322	up
pos_9085	D-Lysopine	-1.142749535	0.012027081	1.7042684	down
neg_515	Nicotinate D-ribonucleotide	-0.715555018	0.012060358	1.678312052	unchanged
neg_518	2-Methylpropyl glucosinolate	-1.737238169	0.012323366	1.673692793	down
pos_8155	9-OxoODE	-0.291046607	0.012568983	1.653787835	unchanged
neg_2008	3alpha,7alpha,12beta-Trihydroxy-5beta-cholanoic acid	-0.687830061	0.012596375	1.653806854	unchanged
neg_575	Uridine	-0.71511394	0.012779874	1.735421555	unchanged
pos_1916	Timolol	1.259822166	0.0128285	1.711742743	up
neg_1774	PE(15:0/20:3(8Z,11Z,14Z)-2OH(5,6))	-0.604272997	0.012998992	1.688698084	unchanged
neg_643	(R)-Mevalonate 3-phosphate	0.996892606	0.013109966	1.704758292	unchanged
neg_651	Azvadine	1.891036847	0.013169383	1.669047358	up
neg_670	(+)-2-Amino-7-phosphonoheptanoic acid	-1.39131738	0.013170567	1.640109141	down
neg_723	L-Tryptophan	-0.468687033	0.013422797	1.61253887	unchanged
neg_728	Dihydrokalafungin	-0.819467293	0.013610866	1.664187415	unchanged
neg_732	S-Nitrosocaptopril	0.830700576	0.013660796	1.659049843	unchanged
neg_733	5-L-Glutamyl-taurine	-0.598204589	0.013714775	1.707285369	unchanged
neg_736	Apigenin 7-di-O-xyloside	-1.082357687	0.013870969	1.698317698	down
neg_737	3-Maleimidobenzoic acid N-hydroxysuccinimide ester	-0.914307396	0.013959235	1.669076704	unchanged
neg_738	Aldotetrauronic acid	-0.571242349	0.014057787	1.621782271	unchanged
neg_745	5'-Phosphoribosylglycinamide	1.321848493	0.014092449	1.786025644	up
neg_746	C06397	-0.41853961	0.014137844	1.639674784	unchanged
neg_749	UDP-3-O-(3-hydroxytetradecanoyl)-D-Zeanoside B	-0.378718385	0.014215367	1.607737521	unchanged
neg_802	Zeanoside B	1.033033735	0.014351872	1.696016621	up
neg_807	2'-Deoxy-5'-O-thiophosphonouridine	-1.240597946	0.014426306	1.654688698	down
neg_873	4-Hydroxybenzenesulfonic acid	2.913418565	0.014543486	1.766275371	up
neg_1885	PS(18:0/18:2(9Z,12Z))	1.445060173	0.014567264	1.731468989	up
pos_9279	(-)-Amijiol	0.966073241	0.014636342	1.640531585	unchanged
neg_970	2-Isopropylmalic acid	0.663292144	0.014704633	1.68008937	unchanged
neg_971	Niridazole	-0.655547934	0.01492884	1.632472432	unchanged
neg_977	5-Phosphooxy-L-lysine	-0.454712911	0.015254964	1.605266276	unchanged
neg_978	Shikimate 3-phosphate	1.355584755	0.015489172	1.77877656	up
pos_1000	dUMP	-0.526560885	0.015498633	1.562402678	unchanged
pos_1007	1,3-Dichloro-2-propanol	-0.50879745	0.015536541	1.613123263	unchanged
pos_10073	2-Aminoethane-1,1,1-triol	-0.459843592	0.015596681	1.590604326	unchanged
pos_10074	6-thio-dg	-0.479744056	0.015599104	1.643072047	unchanged
pos_1021	Cyanuric acid	4.412030746	0.015638372	1.783958726	up
pos_6792	3-Hydroxy-9-hexadecenoylcarnitine	0.727634624	0.016050055	1.547807933	unchanged

pos_1046	4-Hydroxy-6-methyl-3-(1H-pyrazol-3-yl)-2H-pyran-2-one	-0.77128289	0.016217651	1.603012548	unchanged
pos_10477	cis-3-Hexenyl b-primeveroside	-1.077760805	0.016232855	1.679102676	down
pos_10834	Ascorbyl stearate	-0.481210281	0.016235078	1.642411042	unchanged
pos_11106	Lactyltrimethylammonium betaine	1.139288049	0.01644815	1.680790794	up
pos_11107	Pyrano(2,3-c)pyrazol-6(2H)-one, 3,4-dimethyl-2-(2-thienylmethyl)-	-0.931178088	0.016599234	1.611716511	unchanged
pos_11108	(1R,6R)-6-Hydroxy-2-succinylcyclohexa-2,4-diene-1-carboxylate	-0.452641935	0.01663836	1.673901147	unchanged
pos_11109	2-Amino-2-deoxyisochorismate	-0.495844545	0.016817724	1.668910386	unchanged
pos_11111	Thymidine	-2.817719553	0.016949685	1.678584768	down
pos_11113	Moparin	-0.45590225	0.017070278	1.621289571	unchanged
pos_11114	CMP	1.069052655	0.017120653	1.626035382	up
pos_11116	Desidustat	-0.739383311	0.01717548	1.63649151	unchanged
pos_11392	Alacepril	-0.578965056	0.017223424	1.597024111	unchanged
pos_11441	Quercetin 3-O-glucoside	-1.108943377	0.017303954	1.577182286	down
neg_1882	PS(20:4(6E,8Z,11Z,14Z))+O(5)/22:0)	-1.405049288	0.018042982	1.582363217	down
pos_1172	Norsalsolinol	-0.476516125	0.018371264	1.656685067	unchanged
pos_11722	Sibenadet	-0.419909463	0.018403998	1.653237905	unchanged
pos_1173	2-Ethyl-4-hydroxy-5-methyl-3(2H)-furanone	2.348480106	0.018465067	1.737413837	up
pos_1174	Isoquinoline N-oxide	1.502955071	0.018686928	1.693870111	up
pos_1175	3h-Serotonin	-1.306676768	0.019257907	1.540943868	down
pos_1176	Indoleacrylic acid	1.779275334	0.01946433	1.634181151	up
pos_1179	N-Acetyl-L-glutamate	-1.805216078	0.019691548	1.545824989	down
pos_1181	Carbamazepine-o-quinone	1.387301407	0.01996116	1.703776706	up
pos_1182	5-(4-Carboxybutylperoxy)pentanoic acid	-0.687644295	0.020049237	1.567194494	unchanged
pos_1188	CMP-2-aminoethylphosphonate	-0.2872578	0.020162261	1.613316804	unchanged
pos_1190	[(2R,3S,4S,5R,6S)-3,4,5-trihydroxy-6-[(E)-3-phenylprop-2-enoyl]oxyoxan-2-yl]methyl 3,4-dihydroxy-2-methylidenebutanoate	0.98715024	0.020466222	1.601832231	unchanged
pos_12215	floctafenine	0.505927668	0.02051977	1.52372168	unchanged
pos_12225	2,2,4,4,6,6-Hexamethyl-1,3,5-trithiane	1.14881684	0.020658252	1.600709722	up
pos_12226	N3-Fumaroyl-L-2,3-diaminopropanoate	-0.581826237	0.020736052	1.588724673	unchanged
pos_12227	Deoxythioguanosine	0.833844893	0.020852585	1.628580884	unchanged
pos_12228	(2R,3R,4S,5R)-5-Fluoro-2,3,4-trihydroxy-6-oxohexyl dihydrogen phosphate	-1.666998453	0.02104349	1.583724208	down
pos_12234	Grixazone B	-0.474775306	0.021055921	1.513570102	unchanged
pos_12236	Lipoyl-AMP	1.015660551	0.021078814	1.679041993	up
pos_12395	Cytidine monophosphate	-0.670959472	0.021572217	1.683377007	unchanged
pos_1263	UDP-glucuronate	1.771578197	0.021759179	1.689436784	up
neg_2102	DG(2:0/18:2(10E,12Z))+O(9)/0:0)	-0.899980949	0.021953884	1.656619954	unchanged
pos_1033	S-(3-Oxo-3-carboxy-n-propyl)cysteine	1.02183313	0.021989724	1.627336139	up
neg_1891	2-[(L-Alanin-3-ylcarbamoyl)methyl]-3-(2-aminoethylcarbamoyl)-2-hydroxypropanoate	-1.66879374	0.022556384	1.644037704	down
pos_1460	Eremopetasitenin C1	5.777807053	0.022654649	1.701553004	up
pos_6988	Morinidazole	-0.738289203	0.022872567	1.690322021	unchanged
pos_8341	MG(0:0/20:1(11Z)/0:0)	0.899488772	0.022931506	1.592910856	unchanged
neg_640	D-Glucose	1.632504477	0.023022694	1.61425367	up
pos_1702	Hydrocortisone succinate	-0.509138341	0.023875752	1.549535922	unchanged
pos_5000	Traumatic acid	4.385945748	0.025185518	1.687711809	up
neg_508	Pseudouridine 5'-phosphate	-0.268513443	0.02553223	1.555985278	unchanged
neg_1915	16-hydroxy hexadecanoic acid	-0.884292299	0.025641306	1.506173087	unchanged

pos_2181	Aeruginosin 98-B	-0.645946758	0.025890279	1.543732769	unchanged
pos_6255	1,2-dihydroxyheptadec-16-yn-4-yl acetate	-0.843957011	0.025991318	1.511465231	unchanged
pos_2070	Sphinganine 1-phosphate	-0.348595748	0.026212766	1.493251496	unchanged
pos_6433	N6-(L-1,3-Dicarboxypropyl)-L-lysine	0.874198478	0.026300818	1.541796602	unchanged
neg_1884	PE(16:0/20:3(8Z,11Z,14Z)-2OH(5,6))	-0.628148902	0.027096736	1.52983697	unchanged
pos_867	7-Cyano-7-carbaguanine	-0.32313638	0.027272617	1.527204587	unchanged
pos_2203	Retinoyl-AZT	-1.148601193	0.027442022	1.581513289	down
pos_1356	N-acetyl zonisamide	2.441496041	0.027698608	1.585067655	up
pos_6730	Cholic Acid, Methyl Ester	-0.156584974	0.027743124	1.500640512	unchanged
neg_1616	2,3-Dimethoxy-5-methyl-6-(9'-carboxynonyl)-1,4-benzoquinone	-0.561088769	0.027836643	1.484171094	unchanged
pos_5473	Deoxyguanidinoproclavaminic acid	0.206874564	0.027846622	1.498606026	unchanged
pos_5555	3-Amino-4-(3-hexylphenylamino)-4-oxobutylphosphonic acid	-1.314607312	0.028008649	1.50257188	down
pos_5617	Versicotide C	-0.997776777	0.028218095	1.52780071	unchanged
pos_778	2-Pyrone-4,6-dicarboxylate	4.000825736	0.028513681	1.635773099	up
pos_6477	delta-Tocotrienol	1.102829789	0.028912214	1.582317804	up
pos_6262	Chenodeoxycholate	1.210852838	0.029319042	1.580163308	up
pos_6303	6-Keto-prostaglandin E1	1.515548536	0.029325959	1.539997423	up
pos_6394	N-Oleoylglycine	-0.503531776	0.029412752	1.520805341	unchanged
pos_6395	N-Arachidonyl dopamine	-0.967484286	0.02958504	1.506311915	unchanged
pos_7307	delta-Dodecalactone	0.589306537	0.029793085	1.551115471	unchanged
neg_2143	N-Lauroyl Asparagine	4.912531926	0.031214231	1.636002377	up
pos_6588	7-Sulfocholic acid	0.197387346	0.031293145	1.533933634	unchanged
pos_668	PS(20:5(5Z,8Z,11Z,14Z,17Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))	-0.33874854	0.031843211	1.476057436	unchanged
pos_669	PA(16:1(9Z)/LTE4)	-0.699119438	0.032132194	1.517947454	unchanged
pos_1755	Melibiotol	-0.237939166	0.032187031	1.50221698	unchanged
neg_2106	all-trans-4-Hydroxyretinoic acid	-1.364885308	0.032227147	1.442534128	down
pos_685	N-Acetylhistidine	-1.486070913	0.032258164	1.544470067	down
pos_2158	20-Hydroxyleukotriene E4	-1.008153847	0.032313449	1.582356548	down
pos_2173	6,7-Didehydrofevicordin F 3-[glucosyl-(1->6)-glucoside]	1.224875667	0.032722083	1.538734449	up
pos_7088	Citrinin	2.52913648	0.032902251	1.630454027	up
pos_7134	Casokefamide	1.263908749	0.033094547	1.510616926	up
pos_7168	Avizafone	-0.985667605	0.033203325	1.552447671	unchanged
pos_7169	Precorin 6Y	-0.326879821	0.033610374	1.488499022	unchanged
pos_7173	Sialyllacto-N-tetraose a	0.985147545	0.033655408	1.493575041	unchanged
pos_7177	3-Dehydroshikimate	0.432626501	0.03385306	1.53428978	unchanged
neg_2254	(Z)-9-Cycloheptadecen-1-one	-0.338023976	0.034920487	1.447857128	unchanged
pos_7179	9-Oxononanoic acid	1.571843857	0.034976195	1.508518723	up
pos_7183	cis-2,3-Dihydro-2,3-dihydroxybiphenyl	1.822500199	0.035478907	1.5729442	up
pos_1602	Apramycin	-0.597292308	0.035489277	1.483869632	unchanged
neg_1118	3"-Oxoribostamycin	0.94312956	0.035565471	1.517189752	unchanged
pos_7311	(2S)-2-Hydroxyhexadecanoylcarnitine	2.391765055	0.035712724	1.613183017	up
neg_1286	C01056	1.012320009	0.036284569	1.563264626	up
pos_7441	7alpha,27-Dihydroxycholesterol	-1.120834136	0.036525022	1.552597893	down
pos_7442	(9Z,12Z,15Z)-3-	-0.274222373	0.036628486	1.495602141	unchanged
pos_7462	6"-Deamino-6"-oxoparomomycin II	2.98219033	0.036962216	1.598263681	up
pos_7511	1-(3-Carboxypropylcarbamoyl)-5-fluorouracil	-0.152594984	0.037035078	1.466152977	unchanged
pos_7513	trp-gly	-0.260361672	0.037147892	1.506618668	unchanged
pos_7517	3-Hydroxy-11Z-octadecenoylcarnitine	-2.305315612	0.037326208	1.536079729	down

pos 7538	Ruboxistaurin	-0.515059442	0.037345587	1.518025425	unchanged
pos 7539	PC(18:3(6Z,9Z,12Z)/0:0)[U]	-0.159250766	0.037945822	1.536339131	unchanged
pos 7542	(3Z)-Phytochromobilin	-0.332806892	0.038227513	1.489431964	unchanged
pos 7559	Guanidinoacetate	-0.904262277	0.038929843	1.49084355	unchanged
pos 7582	Glu Gly Met Phe	-0.895964809	0.039012148	1.416702923	unchanged
pos 759	METHACHOLINE	-0.683784612	0.03946126	1.406410121	unchanged
pos 7605	phe-ile-gly	-2.352636886	0.039696287	1.561203825	down
pos 7615	Pedin B	-0.378949748	0.039852547	1.477894033	unchanged
pos 7672	Lucidenic acid D1	0.505175558	0.039863621	1.381772201	unchanged
pos 1693	Verruculogen	2.075606138	0.0400069	1.532137839	up
neg 1463	10-Deacetyl-2-debenzoylbaccatin III	2.106048958	0.040383639	1.46958315	up
pos 787	(S)-Chiral alcohol	-0.545787481	0.040784502	1.440848863	unchanged
pos 7970	7alpha-Hydroxycholesterol	-0.216562373	0.041334155	1.447395325	unchanged
pos 799	5-Fluorouridine diphosphate	-0.228849316	0.041387474	1.494387639	unchanged
pos 8005	Lepidiumterpenyl ester	0.253888813	0.041399545	1.489525521	unchanged
pos 8014	Cyclo(glycylleucylvalylleucylprolylseryl)	-0.387435433	0.041574733	1.480624943	unchanged
neg 1525	3-Oxotetradecanoic acid	-0.462149841	0.041627133	1.453533936	unchanged
pos 8118	Methyl jasmonate	2.994235021	0.041681741	1.576559865	up
pos 812	2-(Dimethylamino)ethyl methacrylate	-0.465568692	0.041712207	1.51785735	unchanged
pos 8130	Cucurbitacin IIa	1.028625435	0.041719417	1.489693977	up
neg 1495	milbemycin alpha10	-0.447440701	0.041983402	1.439323943	unchanged
pos 1725	Prunasin	-0.91213481	0.041999642	1.394710072	unchanged
neg 1462	(Z)-5-[(2R,3S,4S)-4-Hydroxy-2-[(E)-3-hydroxyoct-1-enyl]oxan-3-yl]pent-3-enoic acid	0.517971531	0.04231982	1.480871356	unchanged
pos 8546	HYDROCHLORIDE SALT	-1.946006858	0.042692793	1.471823847	down
pos 8620	Phosphocholine	-0.531073936	0.04316533	1.43655076	unchanged
pos 863	5-Hydroxyectoine	-0.647377968	0.043623509	1.403340362	unchanged
pos 8712	Cucurbitacin C	-0.779369974	0.043779018	1.533036425	unchanged
pos 869	L-Methionine sulfoximine	-0.179663472	0.043912105	1.479533573	unchanged
pos 733	5-Hydroxymethyluridine	-0.401595983	0.043944416	1.403406914	unchanged
pos 8719	LysoPC(22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	1.190056799	0.04399767	1.487453398	up
pos 1714	Gly-Trp-Gly	-0.578485325	0.044223058	1.469076082	unchanged
pos 904	Methyl beta-D-galactoside	1.014680953	0.044390361	1.440244662	up
neg 1486	Dhesn	-2.890182718	0.044674142	1.495472605	down
neg 1464	Decitabine	6.320147581	0.044802506	1.557563056	up
pos 829	Xanthine	0.255994323	0.045406885	1.440828727	unchanged
neg 1460	Acoric acid	-0.149752978	0.045528642	1.42517597	unchanged
neg 1649	PE(14:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))	0.564190157	0.045940657	1.376738876	unchanged
pos 9098	Volicitin	-0.255872557	0.046245159	1.388636617	unchanged
pos 9100	trans,trans-Farnesyl phosphate	-1.032704334	0.04660378	1.403769521	down
neg 1515	LysoPC(P-16:0/0:0)	0.56400081	0.046901626	1.355473683	unchanged
pos 9291	LysoPI(18:2(9Z,12Z)/0:0)	-0.256793292	0.046964261	1.473214741	unchanged
pos 9301	O-Arachidonoyl Glycidol (2R,3R,4S,5S,6R)-2-[1,7-bis(4-hydroxyphenyl)heptan-3-yloxy]-6-[[[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]oxane-3,4,5-triol	-0.438104578	0.04712963	1.483516927	unchanged
pos 1633	LysoPA(20:4(8Z,11Z,14Z,17Z)/0:0)	-0.401305998	0.047209271	1.406692672	unchanged
pos 9303	Tilisolol	1.317335976	0.047567878	1.424451048	up
pos 1166	n,n-bis(2-hydroxyethyl)dodecanamide	-0.483749638	0.047747587	1.455556797	unchanged
pos 9386	Sarecycline	2.735404926	0.04806125	1.522658579	up
pos 940	5-Oxoavermectin "1a" aglycone	-0.319953323	0.048097357	1.422487533	unchanged
pos 9402		-0.396103863	0.048292362	1.333811299	unchanged

neg_1488	Penitrem B	-0.197380789	0.048321912	1.3984425	unchanged
pos_952	Cystine-glutamate	0.113308607	0.048405492	1.384230371	unchanged
pos_9602	Imiquimod	-0.718008572	0.048703749	1.406424912	unchanged
pos_9604	cmpentylf	-0.512952645	0.048975881	1.352747757	unchanged
pos_9636	9,10-Epoxy-13-hydroxy-11-octadecenoate	-2.036637981	0.048989845	1.503691488	down
pos_9685	1-Octadecanoyl-sn-glycero-3-	-0.917969261	0.049229745	1.4096171	unchanged
pos_2215	Levanbiose	-0.586250054	0.049255677	1.409235761	unchanged
pos_990	7-Methyluric acid	-0.757386211	0.049272303	1.336939173	unchanged
pos_991	12-Tridecene-4,6,8,10-tetraynal	2.057596278	0.049392029	1.513415551	up
pos_995	[Acetyl-[2-(5-methoxy-1H-indol-3-yl)ethyl]amino]oxy hydrogen sulfate	2.023112537	0.049777012	1.509005071	up

Supplementary Table 4: Model VS L-YP metabolites

#ID	name	Model_vs_L-YP_1	Model_vs_L-YP_1	Model_vs_L-YP_VIP	Model_vs_L-YP (FC_2_Pvalue_0.05_VIP_1)_regulated
neg_1100	Perfluoroheptanoic acid	0.399645063	0.000270888	2.243058608	unchanged
neg_2878	DG(i-14:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/0:0)	1.003999063	0.001057048	2.10451688	up
neg_746	C06397 (5E)-4-[(E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy-2-methyl-5-[2-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyethoxy]hexanoic acid	-0.555230502	0.001660134	2.059622374	unchanged
pos_5214	Gabapentin	-2.318691844	0.001852569	2.097967279	down
pos_2332	6-[[3-Fluoro-5-(4-methoxyoxan-4-yl)phenoxy]methyl]-1-methylquinolin-2-one	0.828790013	0.001878742	2.058902943	unchanged
neg_2788	Ramifenazone	0.66977427	0.002016296	2.101837295	unchanged
pos_10279	Sophoraflavanone B	2.121295474	0.002297416	2.087605595	up
pos_2342	4-Carboxy-4-hydroxy-2-oxoadipate	-3.709482155	0.00247579	2.189825904	down
neg_1098	(-)-Huperzine A (HupA)	0.37862314	0.002910943	2.042599632	unchanged
pos_9286	LysoPC(20:1(11Z)/0:0)	2.22139543	0.003612404	2.067903267	up
pos_10286	Lucidenic acid D1	1.18634359	0.003651511	2.024599527	up
pos_7672	Valnemulin	1.149573478	0.004122618	1.956984421	up
neg_1788	Diflorasone	-0.400247115	0.004486471	2.077357216	unchanged
neg_2725	4-Methylene-L-glutamate	0.638041997	0.004731104	2.067674385	unchanged
pos_839	Methyl sterculate	0.4512012	0.005163722	2.07080891	unchanged
neg_2588	Sulfate	0.749544538	0.005344158	2.005894373	unchanged
neg_264	Carboxyethylphosphoramidate	0.180643826	0.005346135	1.965595012	unchanged
pos_5303	Sclareol	-1.434862183	0.005399719	1.984205564	down
neg_2685	PG(20:1(11Z)/PGE2)	0.65967479	0.005761395	1.99526765	unchanged
neg_2814	C16506	0.905415851	0.006117227	1.981946665	unchanged
neg_2271	Cyanuric acid	-1.394716081	0.006477484	1.885392886	down
pos_1021	(4E,7E,10Z,13E,16E,19E)-docosa-4,7,10,13,16,19-hexaenoic acid	-0.483522697	0.006723097	1.948756163	unchanged
neg_2478	Acarbose 7IV-phosphate	0.644014737	0.007148761	1.936388485	unchanged
pos_11550	Rumenic acid	0.908788705	0.007178406	1.975393301	unchanged
neg_2618	Gentamicin X2	0.395133992	0.007360453	1.963003249	unchanged
neg_2414	Glu Gly Met Phe	0.81152994	0.008054574	2.076823781	unchanged
pos_7582	Edoxudine	0.769927319	0.008290444	1.994322067	unchanged
pos_6989	trichostatin A	0.82896298	0.008291875	1.930220571	unchanged
pos_5728	(S)-9-Hydroxy-10-undecenoic acid	-0.628145307	0.009225687	1.92791718	unchanged
pos_9661	2-hydroxyhexadecanoic acid	1.043181134	0.009688784	1.938376742	up
neg_2425	Guanidinoacetate	0.554239226	0.010669982	1.906660782	unchanged
pos_7559	Cilengitide	0.601790942	0.010905423	1.995730818	unchanged
pos_7061	Methyl jasmonate	1.763594778	0.010959056	1.956235044	up
pos_8118	Capecitabine	-1.165545302	0.010989566	1.872211397	down
pos_5314	1'-Hydroxybufuralol	-1.459115447	0.011050167	1.807589248	down
pos_11728		1.100451998	0.011310179	1.854505167	up

neg_2748	20,26-Dihydroxyecdysone	0.291317961	0.011502072	1.838417527	unchanged
pos_1362	Isochorismate	-1.634262946	0.011750812	1.892605123	down
pos_9504	beta-Alanyl-L-lysine	1.267019483	0.011794944	1.816424526	up
neg_2720	Quinceoxepine	0.85995735	0.011908565	1.83582023	unchanged
pos_10282	PAF (Platelet Activating Factor)	1.068626929	0.012712665	1.939975628	up
neg_2689	Farnesoic acid	0.434389149	0.012720726	1.806836659	unchanged
neg_2322	(6E)-8-Hydroxygeraniol	1.374896422	0.01294468	1.865818806	up
pos_5473	Deoxyguanidinoproclavaminic acid	0.993152805	0.013144873	1.936549718	unchanged
pos_1172	Norsalsolinol	-0.601521755	0.013211618	1.939585816	unchanged
pos_7557	Phenylpropanoate	0.452961527	0.013376818	1.803225895	unchanged
neg_2413	N-Oleoyl Histidine	1.137866007	0.013433425	2.002222844	up
neg_2320	Cyclohexaneundecanoic acid	1.199320805	0.0134748	1.849221383	up
neg_1665	N-Palmitoyl Arginine	0.590550478	0.013683057	1.802469806	unchanged
pos_7615	Pedein B	2.060328495	0.013866673	1.824578217	up
neg_857	UDP-L-Ara4FN	-1.37124038	0.01412798	1.759021752	down
neg_2759	Limonene aldehyde	0.684790322	0.014632573	1.898541385	unchanged
pos_863	5-Hydroxyectoine	0.336743395	0.0146815	1.698573014	unchanged
neg_2658	C06633	0.540652712	0.014845691	1.798437826	unchanged
pos_10275	5(Z),8(Z),11(Z)-Eicosatrienoic acid	0.990701398	0.016221142	1.817902158	unchanged
pos_1147	Epigallocatechin 3-caffeate	-1.305793145	0.016341934	1.745939934	down
pos_669	PA(16:1(9Z)/LTE4)	-0.682992131	0.01649068	1.923041647	unchanged
neg_744	C18034	-1.144785522	0.016628039	1.728986414	down
neg_2323	Palmitoyl glucuronide	1.015997008	0.016714349	1.818350078	up
pos_10990	1-(8Z,11Z,14Z-eicosatrienoyl)-sn-glycero-3-phosphocholine	0.616900135	0.016996454	1.797564806	unchanged
pos_5457	Gln Ser His Thr	-3.176775411	0.017076799	1.825160781	down
neg_2687	9'-Carboxy-gamma-chromanol	0.471802852	0.017268648	1.784494378	unchanged
pos_7213	Solasodienone (not validated)	1.38431252	0.017453321	1.826247737	up
neg_2859	Oleandolide	0.412149993	0.017783059	1.814932476	unchanged
pos_6588	7-Sulfocholic acid	1.419333429	0.017992951	1.800969665	up
neg_2287	xi-5-Hexyldihydro-2(3H)-furanone	1.412414106	0.018331787	1.800705679	up
pos_7511	1-(3-Carboxypropylcarbamoyl)-5-fluorouracil	0.427021358	0.019292846	1.850040488	unchanged
pos_5776	3-Hydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione	-0.632050069	0.019301529	1.737848351	unchanged
pos_2177	trans-Crocetin (beta-D-glucosyl) (beta-D-gentibiosyl) ester	-2.451292305	0.019374809	1.858014608	down
pos_9397	1尾,3伪,7伪,12伪-Tetrahydroxy-5尾-cholan-24-oic Acid	1.220883818	0.019973809	1.773765125	up
pos_10168	PC(18_3(9Z,12Z,15Z)_20_0)	0.628672976	0.020172046	1.704804425	unchanged
pos_910	(R)-3-hydroxybutyrylcarnitine	-0.638232071	0.02032862	1.716570863	unchanged
neg_881	5-Methoxytryptophan	-1.255791732	0.020644362	1.702908868	down
neg_2783	QUINALPHOS	0.204325476	0.020897028	1.771669614	unchanged
pos_9288	Alanylarginine	1.515617521	0.021145726	1.783434774	up
neg_2724	Octadecanoic acid	1.104170075	0.021366469	1.84590123	up

neg_2813	Dicrocin	0.635756503	0.021674034	1.716930875	unchanged
pos_1128	Phenylacetylglutamine	-1.057862805	0.021718802	1.709521665	down
neg_1581	Pregnenolone-3,21-disulfate	1.152459136	0.022165599	1.759052892	up
neg_2842	C17582	0.404425786	0.022218807	1.810089116	unchanged
pos_8076	Ubiquinone-10	2.062042473	0.022334419	1.812987428	up
pos_1009	7,8-Dihydro-7,8-dihydroxykynurenate	-0.47008991	0.022455963	1.675886563	unchanged
pos_5450	(E)-4,5-Dihydro-6-(2-(4-pyridinyl)ethenyl)-3(2H)-pyridazinone	-2.522226689	0.022803031	1.77580409	down
pos_9395	3a,7b,21-Trihydroxy-5b-cholanoic acid	0.980407228	0.023393529	1.747962925	unchanged
neg_2131	Cholylcitrulline	-0.213267665	0.023442344	1.717736607	unchanged
pos_6635	5,6,7,8-Tetrahydromonapterin	0.873778644	0.023780617	1.719730118	unchanged
neg_2473	Pregnenolone	0.559394761	0.024256443	1.81562312	unchanged
neg_3051	LysoPI(0:0/18:0)	1.291749271	0.025356176	1.90840097	up
pos_10770	3-Ethyl-4-(9-hydroxy-4,6,8,10-tetramethyl-7-oxododec-4-en-2-yl)oxetan-2-one	0.786584962	0.025709516	1.794410822	unchanged
neg_1682	C12272	0.554485989	0.025731087	1.72900001	unchanged
pos_3113	ENOXACIN	0.933403148	0.025902775	1.741165298	unchanged
pos_1149	Ser Asn Phe	-1.179242641	0.026034718	1.67680598	down
neg_753	N-Acetyl-N6,O-didemethylpuromycin-5'-	-0.933385122	0.026253737	1.636164995	unchanged
pos_7501	5.9-tetracosadienoic acid	2.854665351	0.026359024	1.897108849	up
pos_6990	Tryptophyl-Glycine	2.179718535	0.026415228	1.839119758	up
pos_1657	Butanoylphosphate	-1.532684438	0.026874767	1.749925072	down
pos_10669	Laprafylline	0.863070916	0.027135931	1.813497771	unchanged
neg_2633	Topotecan	0.468078157	0.027286918	1.777136139	unchanged
pos_12299	Rhizocticin C	-1.80855272	0.027529574	1.700155801	down
pos_11508	PC(18:0/TXB2)	1.672025455	0.02848327	1.694510424	up
pos_5000	Traumatic acid	-1.780015123	0.028580849	1.784237973	down
neg_2784	n-octyl-beta-D-thioglucopyranoside	0.632914562	0.028652899	1.78492549	unchanged
pos_1127	Tryptophan 2-C-mannoside	-1.064170817	0.028750999	1.630340635	down
neg_2458	Oleamide	0.616869246	0.029112606	1.66261941	unchanged
pos_11768	PC(P-18:1(11Z)/PGE2)	1.587228653	0.029132092	1.67289147	up
neg_2500	DG(15:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z))-	0.46278306	0.02914488	1.714788144	unchanged
neg_2660	trans-16-Octadecenoic acid	0.664941969	0.029174959	1.852546221	unchanged
neg_2492	1-Lyso-2-arachidonoyl-phosphatidate	1.03461155	0.029235583	1.885370385	up
pos_1146	5-(L-Alanin-3-yl)-2-hydroxy-cis,cis-muconate 6-semialdehyde	-0.99116066	0.029796246	1.638556796	unchanged
pos_10784	Procaine	0.719943167	0.030172049	1.775386417	unchanged
pos_1447	N-Carbamoylsarcosine	-0.687976547	0.030296628	1.654241251	unchanged
neg_1576	Pravastatin	0.757164173	0.030575273	1.689553664	unchanged
pos_7968	Oleoylcarnitine	2.555286581	0.031045567	1.858986188	up
pos_6255	1,2-dihydroxyheptadec-16-yn-4-yl acetate	-0.898686971	0.031308978	1.700520424	unchanged
neg_2285	Deacetylnomilin	0.778542883	0.031520719	1.693565117	unchanged
pos_6743	Nvp dpp 728 dihydrochloride	1.074734449	0.03164285	1.76491996	up
neg_2635	Teasterone	0.407217704	0.031671201	1.779215033	unchanged

neg_2426	Petasitenine	0.599256377	0.031690525	1.684779786	unchanged
pos_7915	Diaminobutyric acid	1.515678197	0.031979645	1.834667015	up
neg_2256	Emindole SB	0.882192752	0.032007319	1.640630569	unchanged
neg_2815	alpha-Tocopherol	0.624322504	0.032281721	1.765262499	unchanged
neg_2493	Methyl salicylate O-[rhamnosyl-(1->6)-	0.859382768	0.032341486	1.679291543	unchanged
neg_1364	Brevianamide F	-0.843572519	0.03249595	1.664654688	unchanged
neg_2211	3b,17b-Dihydroxyetiocholine	1.203834364	0.032824385	1.650489098	up
neg_2137	C07909	-1.744016803	0.033426884	1.696253151	down
pos_8341	MG(0:0/20:1(11Z)/0:0)	-0.903218788	0.033601254	1.786282523	unchanged
pos_752	L-Carnitine	1.039673238	0.03373096	1.569708286	up
pos_2087	Trp Ser Gly	-1.696405974	0.033985503	1.747258563	down
neg_737	3-Maleimidobenzoic acid N-hydroxysuccinimide ester	-1.086983879	0.034081901	1.781624455	down
pos_6975	Olitoriusin	1.077952031	0.034499822	1.681576803	up
pos_1179	N-Acetyl-L-glutamate	-0.605876186	0.034578852	1.634501089	unchanged
neg_718	Eterobarb	-1.019322748	0.034608398	1.587684129	down
neg_715	Aranidipine	-0.972315262	0.034634138	1.57369628	unchanged
pos_7856	Solasodine	2.295325192	0.034668444	1.819051998	up
neg_2757	DL-2-hydroxy stearic acid	0.779652521	0.034701274	1.694147844	unchanged
neg_2709	L-Nicotianine	0.502441835	0.034858733	1.652447796	unchanged
pos_10001	Stearoylcarnitine	2.47987947	0.03516626	1.847635782	up
neg_2325	Leukotriene D4	1.144692945	0.035289331	1.718539247	up
pos_9324	dehydroabietadienol	0.781809883	0.035392466	1.838038663	unchanged
pos_8804	1-Palmitoyl Lysophosphatidic Acid	-0.326978432	0.03562599	1.594878443	unchanged
pos_8577	Trihexosylceramide (d18_1_16_0)	-0.273455966	0.035957074	1.672909914	unchanged
neg_2485	Rostafuroxin	0.374125485	0.036463058	1.667817116	unchanged
neg_855	N-Acetylneuraminic acid	-1.226654507	0.036472358	1.616871786	down
pos_9461	Calcitriol	0.4558085	0.03658735	1.782881006	unchanged
neg_2628	Ecabet	0.308286098	0.036755463	1.676413586	unchanged
pos_6192	6-Deoxocastasterone	0.458677397	0.037327217	1.71768935	unchanged
neg_1122	Brexiprazole	-2.949394599	0.037580929	1.744046053	down
pos_10451	2'''-N-Acetyl-6'''-deamino-6'''-hydroxyparomomycin II	1.202940643	0.037725558	1.633845894	up
pos_11549	Mitomycin A	1.277454699	0.038345575	1.591582208	up
pos_668	PS(20:5(5Z,8Z,11Z,14Z,17Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))	-0.412834323	0.038458178	1.725102642	unchanged
pos_7561	Levamisole	0.386537265	0.03863063	1.651308711	unchanged
pos_6792	3-Hydroxy-9-hexadecenoylcarnitine	-0.860521442	0.038896074	1.603060545	unchanged
neg_2899	Pyridinolone	0.68736012	0.039022562	1.662194696	unchanged
neg_2898	2'-N-Acetylparomamine	1.066391008	0.039146992	1.692556053	up
pos_769	Deoxyinosine	-0.259941981	0.039218311	1.669238635	unchanged
pos_724	2R-Hydroxymethyl-3S-hydroxypyrolidine	-1.063454319	0.039877984	1.705810245	down
pos_1176	Indoleacrylic acid	-0.436818192	0.040011714	1.601926504	unchanged
pos_990	7-Methyluric acid	-0.646451527	0.04021109	1.679087589	unchanged

pos_6730	Cholic Acid, Methyl Ester	-0.9993508	0.040330938	1.6171242	unchanged
neg_706	C12368	-1.253663766	0.040954357	1.574680949	down
pos_8059	Alpha-Linoleoylcholine	2.438101098	0.041039187	1.78359083	up
pos_7118	Clausarinol	0.504495801	0.041167116	1.652176152	unchanged
neg_2741	Levomethadyl acetate	0.741387877	0.041185818	1.589317906	unchanged
pos_7076	alpha-Methylstyrene	0.682372685	0.04150911	1.627553775	unchanged
pos_9303	LysoPA(20:4(8Z,11Z,14Z,17Z)/0:0)	0.964491293	0.041597722	1.81325699	unchanged
neg_2354	2-Phytyl-1,4-naphthoquinone	1.344901552	0.041875421	1.64282554	up
pos_5194	M1dG	1.168527196	0.042014503	1.587711854	up
neg_1578	24,24-Difluoro-1 alpha,25-dihydroxyvitamin D3	0.56718037	0.042509592	1.659529892	unchanged
pos_5425	Asp Lys Ile Ser	-1.193498937	0.042625144	1.646690532	down
neg_600	(S)-DNPA	-0.519335377	0.044167508	1.602120859	unchanged
pos_991	12-Tridecene-4,6,8,10-tetraynal	-0.543256853	0.044321361	1.639287074	unchanged
pos_952	Cystine-glutamate	-0.423574445	0.044380595	1.4656835	unchanged
pos_2134	5-Fluorodeoxyuridine monophosphate	0.391422624	0.044553378	1.582877353	unchanged
neg_2167	Norbicycloekasantalal	0.956783173	0.045069331	1.570462383	unchanged
neg_2491	5,10-Methenyltetrahydrofolate	0.473242182	0.045253474	1.612719945	unchanged
pos_8485	linoleyl-L-carnitine	3.495386806	0.046352696	1.777725195	up
pos_2772	L-Histidine	0.440494358	0.04669665	1.662666763	unchanged
pos_4310	dCDP	0.798842689	0.046722149	1.547888257	unchanged
neg_1148	Indolelactic acid	-0.654543634	0.046991124	1.516308156	unchanged
pos_779	Daunosamine	0.29061763	0.047294876	1.55086853	unchanged
pos_7100	alpha-1,5-L-Arabinobiose	0.750748775	0.047314991	1.587353435	unchanged
pos_10785	Diethyl decanedioate	0.329626969	0.047408504	1.583032354	unchanged
neg_2576	Bruceine D	0.547541583	0.047447836	1.559632446	unchanged
neg_1913	PC(DiMe(11,3)/18:1(12Z)-2OH(9,10))	1.174593825	0.048092264	1.639646241	up
neg_2494	C17960	0.558279653	0.048431037	1.562665159	unchanged
neg_1612	3-[(3aS,4S,7aS)-7a-Methyl-1,5-dioxo-octahydro-1H-inden-4-yl]propanoate	0.233742377	0.048906723	1.528936863	unchanged
pos_8077	PC(22:3(10Z,13Z,16Z)/20:3(6,8,11)-OH(5))	1.520662101	0.048999005	1.544056822	up
neg_2556	8,11-eicosadiynoic acid	0.520231663	0.049151982	1.611016788	unchanged
neg_2627	N-[Diaminophosphoryloxy-[di(propan-2-yl)amino]phosphoryl]-N-propan-2-ylpropan-2-	0.35851238	0.049375646	1.642165298	unchanged
pos_10671	Platelet-activating factor	0.684649738	0.049624795	1.63306903	unchanged
pos_6587	Hexadecanedioic acid mono-L-carnitine ester	-0.773168983	0.04977077	1.544786311	unchanged
pos_6262	Chenodeoxycholate	-0.844560069	0.049986861	1.549155056	unchanged
pos_2215	Levanbiose	-2.015984849	0.049994696	1.691030735	down

Supplementary Table 4: Model_VS H-YP_metabolites

#ID	name	Model_vs_H-YP_log2FC	Model_vs_H-YP Pvalue	Model_vs_H-YP_VIP	Model_vs_H-YP (FC 2 Pvalue 0.05 VIP 1) regulated
neg_1612	3-[(3aS,4S,7aS)-7a-Methyl-1,5-dioxo-octahydro-1H-inden-4-yl]propanoate	0.640259223	2.08E-05	2.102480847	unchanged
neg_2607	Filipin II	1.129689769	2.83E-05	2.061436357	up
pos_6588	7-Sulfocholic acid	3.245359234	3.77E-05	2.109408334	up
neg_1521	C01844	0.901824119	8.82E-05	2.002778272	unchanged
neg_1581	Pregnenolone-3,21-disulfate	2.179284034	9.32E-05	2.029509104	up
neg_1576	Pravastatin	1.562992581	0.000119736	1.995870984	up
pos_7173	Sialyllacto-N-tetraose a	2.866815763	0.000175745	2.018407111	up
pos_6635	5,6,7,8-Tetrahydromonapterin	1.592465741	0.000197926	1.943317086	up
neg_1498	(3beta,5alpha,6beta,7alpha,22E,24R)-Ergosta-8,22-diene-3,5,6,7-tetrol	0.919234282	0.000211359	1.991591369	unchanged
pos_6615	3-Phenyl-2-propenyl	0.940773006	0.000363682	1.941605503	unchanged
neg_1568	1-Nonen-3-ol	1.232541547	0.000406526	1.987877618	up
pos_7100	alpha-1,5-L-Arabinobiose	1.504476983	0.00041975	1.952777889	up
pos_7099	L-4-Hydroxyglutamate semialdehyde	1.431028643	0.000461672	1.93672009	up
pos_7067	1-(2-Furyl)butan-3-one	2.302162047	0.000468546	1.94341165	up
pos_7104	Cicaprost	1.520802585	0.000487481	1.933100885	up
pos_863	5-Hydroxyectoine	0.507968394	0.000506187	2.004440831	unchanged
pos_6395	N-Arachidonyl dopamine	1.179721002	0.000578	1.985855933	up
pos_7076	alpha-Methylstyrene	1.239398921	0.000635608	1.915458223	up
neg_807	2'-Deoxy-5'-O-thiophosphonouridine	0.800391658	0.00065247	1.966156631	unchanged
pos_799	5-Fluorouridine diphosphate	-0.86341193	0.00072425	1.933784207	unchanged
pos_10639	Avermectin B1b monosaccharide	1.881243364	0.00088439	1.942591066	up
pos_6633	3-Dimethylallyl-4-hydroxymandelic acid	0.743360186	0.000960552	1.869449607	unchanged
pos_897	PHENACYLAMINE	0.561864094	0.001332583	1.937657506	unchanged
pos_866	L-Tyrosine	0.604678298	0.001448713	1.954519345	unchanged
pos_7168	Avizafone	2.936228236	0.001449482	1.974122729	up
pos_7088	Citrinin	2.48236234	0.001457725	1.948539045	up
pos_7078	(4-Methylphenyl)acetaldehyde	1.195092673	0.001515848	1.90364296	up
neg_515	Nicotinate D-ribonucleotide	-0.680139365	0.001523594	1.834724784	unchanged
pos_898	Ectoine	0.588737593	0.00157051	1.931457099	unchanged
neg_2798	8,8a-Deoxyoleandolide	0.778370085	0.001707776	1.924556886	unchanged
pos_7077	L-Fucono-1,5-lactone	1.053693664	0.001821739	1.899554375	up
pos_7098	2'-O-methyladenosine	1.137937695	0.002151268	1.88204656	up
pos_10770	3-Ethyl-4-(9-hydroxy-4,6,8,10-tetramethyl-7-oxododec-4-en-2-yl)oxetan-2-one	1.152628543	0.002285174	1.837537375	up
pos_7074	Hydrocinnamic acid	1.612658317	0.002431411	1.870790926	up
pos_7134	Casokefamide	2.353773398	0.00252588	1.918059663	up
neg_522	6-Thioxanthine 5'-monophosphate	-0.985698259	0.002845414	1.835414833	unchanged
pos_7177	3-Dehydroshikimate	1.990700499	0.00295495	1.888326161	up
pos_7136	Diacetazotol	2.412131528	0.002958049	1.913768773	up
neg_521	dTDP	-0.923389405	0.003084944	1.773545749	unchanged
pos_1045	Methylcysteine	-1.710885443	0.003096877	1.816783284	down
pos_806	UDP-4-dehydro-6-deoxy-D-glucose	-1.979402411	0.00310118	1.846523464	down
pos_7169	Precorrin 6Y	2.95612591	0.00322339	1.923789616	up
pos_7165	Tunicamycin VI	2.348090224	0.003243138	1.8495421	up
pos_7511	1-(3-Carboxypropylcarbamoyl)-5-fluorouracil	0.59137524	0.003288969	1.8485709	unchanged

neg_1613	5-((6-((Aminomethyl)amino)-1-oxohexyl)amino)pentanoic acid	-1.393511677	0.003395689	1.847531555	down
pos_1046	4-Hydroxy-6-methyl-3-(1H-pyrazol-3-yl)-2H-pyran-2-one	0.831793818	0.003425295	1.972503365	unchanged
neg_1818	C11134	1.523287279	0.003722608	1.860255106	up
pos_5728	trichostatin A	-0.985838187	0.003867612	1.899840584	unchanged
neg_1618	Propofol glucuronide	-1.357822242	0.004011039	1.83521142	down
neg_1774	PE(15:0/20:3(8Z,11Z,14Z)-2OH(5,6))	-1.726298127	0.004137923	1.823550466	down
pos_1021	Cyanuric acid	-0.574677295	0.004188214	1.757823532	unchanged
neg_2152	8-[(1R,2R)-3-Oxo-2-{(Z)-pent-2-enyl}cyclopentyl]octanoate	-0.647871489	0.004526865	1.826205822	unchanged
pos_7049	(±)-Myristoylcarnitine	-1.26590345	0.004647669	1.827023411	down
neg_841	(S)-3-Sulfolactate	0.471996956	0.004759263	1.892343173	unchanged
pos_7118	Clausarinol	0.760518824	0.004777745	1.821113043	unchanged
pos_6636	16-Methylheptadecanoic acid	0.52475952	0.005107333	1.941336611	unchanged
pos_6988	Morinidazole	-2.348554141	0.005111244	1.766017302	down
pos_8005	Lepidiumterpenyl ester	-0.620705686	0.005436879	1.792806376	unchanged
pos_7559	Guanidinoacetate	0.722168403	0.005493037	1.719077415	unchanged
pos_7311	(2S)-2-Hydroxyhexadecanoylcarnitine	-1.073255602	0.006250498	1.727038954	down
neg_2609	SM(d16:1/20:3(8Z,11Z,14Z)-2OH(5,6))	0.285434292	0.006652636	1.688759233	unchanged
neg_1637	PS(14:0/18:0)	-2.066789031	0.006718586	1.779002488	down
neg_2270	6-Phenylhexyl isothiocyanate	1.871636456	0.00681499	1.764343299	up
pos_6792	3-Hydroxy-9-hexadecenoylcarnitine	-1.65792207	0.006902501	1.817059809	down
neg_1665	N-Palmitoyl Arginine	0.692049152	0.007030123	1.712259741	unchanged
pos_7121	O-(1->4)-alpha-L-Dihydrostreptosyl-streptidine 6-phosphate	0.985350163	0.00751675	1.827839314	unchanged
pos_7497	N,N-dimethyl-Safingol	0.804829432	0.00755133	1.716781479	unchanged
pos_5642	Urocortisol	-1.512431377	0.007595574	1.752153612	down
neg_737	3-Maleimidobenzoic acid N-hydroxysuccinimide ester	0.971415835	0.00789415	1.744014131	unchanged
neg_1809	PS(22:5(4Z,7Z,10Z,13Z,16Z)/22:2(13Z,16Z))	1.227908778	0.008083988	1.762810314	up
neg_1891	2-[(L-Alanine-3-ylcarbamoyl)methyl]-3-(2-aminoethylcarbamoyl)-2-hydroxypropanoate	-1.649897363	0.008103182	1.713398309	down
pos_7126	Desisobutyrylciclesonide	1.286925956	0.00813785	1.81230475	up
pos_7582	Glu Gly Met Phe	0.932464121	0.008523496	1.674988484	unchanged
pos_1009	7,8-Dihydro-7,8-dihydroxykynurenate	-0.430630207	0.008616033	1.744407379	unchanged
pos_6718	LysoPC 16-2	-1.292194066	0.008831871	1.697780272	down
pos_960	Formyl-5-hydroxykynurenamine	-1.093338261	0.008945292	1.67494097	down
pos_7517	3-Hydroxy-11Z-octadecenoylcarnitine	1.618997686	0.009275367	1.639196923	up
pos_2772	L-Histidine	0.62592386	0.00935074	1.716518475	unchanged
pos_7557	Phenylpropanoate	0.474500454	0.009487452	1.637535514	unchanged
pos_7354	Digitoxigenin 3-[glucosyl-(1->6)-glucosyl-(1->4)-2,6-dideoxyribohexoside]	1.154119702	0.009872477	1.8429518	up
pos_6255	1,2-dihydroxyheptadec-16-yn-4-yl acetate	-1.39040922	0.009923053	1.761976518	down
neg_1885	PS(18:0/18:2(9Z,12Z))	-1.512434775	0.009986646	1.718465945	down
pos_7184	Sphingosine-1-phosphate	-0.556472202	0.01009188	1.64378866	unchanged
pos_7615	Pedin B	2.226825257	0.010108197	1.70256651	up
pos_7442	(9Z,12Z,15Z)-3-Hydroxyoctadecatrienoylcarnitine	-0.870070316	0.010191467	1.694395016	unchanged
pos_7179	9-Oxononanoic acid	-0.409780313	0.010273177	1.64699057	unchanged
neg_2339	Thromboxane B2	1.212535186	0.010515945	1.672634383	up
neg_1506	Tetradecanedioic acid	-0.784111055	0.010864152	1.72459489	unchanged
pos_8804	1-Palmitoyl Lysophosphatidic Acid	0.734195224	0.010943336	1.771173832	unchanged

pos_7915	Diaminobutyric acid	1.089376748	0.011275457	1.619015267	up
pos_7307	delta-Dodecalactone	-1.5126103	0.011445173	1.70047071	down
neg_2805	Ginsenoside C-K	0.241159817	0.011499983	1.615910037	unchanged
pos_7095	Linamarin	0.781859787	0.01155801	1.712382253	unchanged
pos_12083	1-Monostearin	0.787165293	0.011942749	1.670082783	unchanged
pos_5000	Traumatic acid	-3.465145192	0.011987153	1.746077684	down
neg_2786	(S)-6-Hydroxynicotine	1.344055813	0.012016124	1.656546679	up
pos_931	(E)-Casimiroedine	-0.911843528	0.01263029	1.695045173	unchanged
pos_6730	Cholic Acid, Methyl Ester	-1.72533818	0.01273097	1.759917217	down
pos_814	5,6-Dihydrouridine	-0.516459305	0.013151016	1.665634483	unchanged
pos_7061	Cilengitide	1.460722923	0.013297445	1.635020711	up
neg_1993	5-Methoxytryptamine	1.288070142	0.0133041	1.655001535	up
neg_1460	Acoric acid	-2.446093774	0.013556971	1.743475985	down
neg_2678	(R)-Mevalonate	0.672748282	0.013573201	1.639512935	unchanged
pos_6746	Miltefosine	1.674240256	0.013621481	1.694824329	up
pos_7375	Viloxazine	-0.520851901	0.01382541	1.668971021	unchanged
pos_1044	Difluorodeoxyuridine	-1.674097185	0.01398707	1.688379676	down
pos_8118	Methyl jasmonate	-1.069282454	0.014291211	1.62455429	down
pos_8341	MG(0:0/20:1(11Z)/0:0)	-1.29747611	0.014505051	1.759909995	down
neg_1654	2,3-Dinor-8-iso prostaglandin F2alpha	1.017978393	0.014530348	1.628396291	up
pos_7180	Arg Ala Trp	0.917455008	0.015294258	1.719933461	unchanged
neg_1616	2,3-Dimethoxy-5-methyl-6-(9'-carboxynonyl)-1,4-benzoquinone	-1.427319706	0.015507496	1.651336811	down
pos_7216	3-O-Acetylepisamarcandin	1.223422667	0.015883944	1.707709049	up
neg_2789	Panaquinquecol 5	0.306215207	0.015902108	1.635804141	unchanged
neg_2467	20-Hydroxy-6Z,15Z-eicosadienoic acid	-0.572400125	0.01603771	1.819635817	unchanged
pos_6587	Hexadecanedioic acid mono-L-carnitine ester	-1.095186988	0.016509875	1.67879487	down
pos_1035	3,4-Dihydro-7-methoxy-2-methylene-3-oxo-2H-1,4-benzoxazine-5-carboxylic acid	-2.651899873	0.016595976	1.732240634	down
neg_702	CDP	0.209255777	0.01687684	1.664464758	unchanged
pos_8577	Trihexosylceramide (d18 1 16 0)	-0.345678592	0.017044871	1.602259195	unchanged
pos_769	Deoxyinosine	-0.339448207	0.017051907	1.667012511	unchanged
pos_11498	PC(P-18:1(11Z)/18:3(10,12,15)-OH(9))	0.958541805	0.017143528	1.736780349	unchanged
pos_5630	1-Deoxy-11beta-hydroxypentalenate	2.02427771	0.017602769	1.66261333	up
pos_781	Uric acid	-0.682518225	0.018270028	1.636530225	unchanged
neg_1873	L-Oleandrosyl-oleandolide	0.580432327	0.018460338	1.602430192	unchanged
neg_1508	Hymenoxon	-1.171329154	0.018512786	1.687882067	down
pos_6477	delta-Tocotrienol	-1.950543103	0.018590454	1.702494535	down
neg_1692	Contignasterol	-0.883341513	0.01867766	1.643561661	unchanged
pos_7097	Richter	0.679111243	0.018816277	1.633672281	unchanged
pos_7488	L-Leucine	1.041335141	0.01922667	1.583318324	up
neg_2216	C11999	-1.164193643	0.019353413	1.588587208	down
pos_4174	1-Guanidino-1-deoxy-scylo-inositol 4-phosphate	1.244335828	0.019370161	1.627353091	up
pos_7513	trp-gly	-0.50925178	0.01967799	1.642410702	unchanged
neg_1649	PE(14:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))	-1.443400904	0.019756946	1.615024192	down
pos_910	(R)-3-hydroxybutyrylcarnitine	-0.779948689	0.019817537	1.553920741	unchanged
neg_868	5-(3-Hydroxybenzoyl)-2-thiophenesulfonamide	0.201829895	0.020247308	1.597832054	unchanged
neg_1525	3-Oxotetradecanoic acid	-1.507732267	0.020357047	1.610165184	down
pos_10399	Dextran-70	0.947898531	0.020490257	1.674232259	unchanged
neg_1972	C16143	-1.253637006	0.020633374	1.666436002	down

pos_6622	Armillarin	0.833463199	0.020863939	1.709620893	unchanged
pos_12085	MG(0:0/20:2(11Z,14Z)/0:0)	0.464984778	0.021482149	1.718120806	unchanged
pos_1024	4-Thialysine	-2.225897484	0.021565369	1.678873174	down
pos_10299	PG 17 0-18 1-d5	0.652946753	0.021769237	1.53142887	unchanged
pos_940	Sarecycline	-0.897392834	0.021970356	1.556225512	unchanged
pos_10400	Estrone glucuronide	0.933526791	0.02248804	1.699451102	unchanged
pos_11492	PC(14:0/20:2(11Z,14Z))	1.189335842	0.022875373	1.671442795	up
pos_5473	Deoxyguanidinoproclavaminic acid	1.281468049	0.023313979	1.617516426	up
pos_1755	Melibiotol	-1.615173821	0.023912076	1.584720876	down
pos_9544	PC(P-18:1(11Z)/20:3(6,8,11)-OH(5))	0.529066241	0.023933792	1.484668308	unchanged
neg_1386	C07493	1.887694864	0.024164043	1.598098227	up
pos_5346	3-hydroxy-C10-homoserine lactone	1.011895685	0.024314038	1.564330969	up
neg_2426	Petasitenine	0.827463981	0.025036318	1.564185925	unchanged
pos_11501	PG(18 0 22 4(7Z,10Z,13Z,16Z))	0.774871832	0.025785519	1.585007075	unchanged
pos_7620	Linoelaidylcarnitine	-1.303596256	0.026252441	1.521691145	down
pos_6745	N-Docosahexaenoyl Lysine	1.570354959	0.026423613	1.587823614	up
pos_12237	Rutin	0.323509545	0.026533926	1.546277238	unchanged
neg_2255	3alpha,11beta,21-Trihydroxy-20-oxo-5beta-pregnan-18-al	-0.880900762	0.026613374	1.608923165	unchanged
pos_7439	Octadecyl fumarate	-0.761892093	0.026754776	1.608242661	unchanged
pos_5776	3-Hydroxy-9,10-secoandrost-1,3,5(10)-triene-9,17-dione	-0.530150709	0.026785774	1.522440198	unchanged
neg_1731	C16500	-1.065870227	0.026789339	1.491764381	down
pos_1725	Prunasin	-2.151451255	0.026957497	1.636375792	down
pos_8621	Docosanoic acid	1.463200743	0.027078682	1.607956511	up
pos_11550	Acarbose 7IV-phosphate	0.78677177	0.02713745	1.54901492	unchanged
pos_958	Lanthionine ketimine	-0.612822023	0.027184228	1.517850318	unchanged
neg_1452	Pinometostat	1.155816141	0.027214915	1.73272284	up
pos_1038	alpha-D-Ribose 1-methylphosphonate 5-phosphate	-0.873493429	0.027231646	1.603527052	unchanged
neg_1410	C75	-2.424725811	0.027391479	1.637973802	down
neg_470	(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone	-0.918090334	0.027481642	1.573025722	unchanged
pos_7161	Pristinamycin IA	1.844808256	0.02755565	1.593432362	up
pos_9308	N-Nervonoyl Tyrosine	0.364942392	0.028015792	1.574407706	unchanged
neg_2254	(Z)-9-Cycloheptadecen-1-one	-1.127621013	0.028997182	1.580276478	down
pos_6433	N6-(L-1,3-Dicarboxypropyl)-L-lysine	-1.137388939	0.029320641	1.561835446	down
neg_826	GDP-L-fucose	0.601506094	0.029495393	1.543600465	unchanged
neg_2236	C11961	1.248583825	0.029656234	1.624549134	up
pos_53	FA 13 3+10	0.352839455	0.030302953	1.530520804	unchanged
neg_2231	11-Dehydro-thromboxane B2 (2R,3R,4S,5S,6R)-2-[1,7-bis(4-hydroxyphenyl)heptan-3-yl-oxo]-6-[[[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]oxane-3,4,5-triol	-0.968331011	0.030309236	1.538789204	unchanged
pos_1633	ylxy]-6-[[[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]oxane-3,4,5-triol	-1.725287599	0.030585217	1.468350079	down
neg_618	Alanyltyrosine	-0.928495067	0.030605082	1.476960719	unchanged
neg_1948	N-Glycoloylganglioside GM2	0.254980548	0.031900767	1.510473408	unchanged
pos_867	7-Cyano-7-carbaguanine	-1.161815599	0.032226699	1.50197161	down
pos_11020	Daidzin	0.445003318	0.032270974	1.513781085	unchanged
neg_1578	24,24-Difluoro-1alpha,25-dihydroxyvitamin D3	0.80015776	0.032443466	1.512086331	unchanged
neg_1884	PE(16:0/20:3(8Z,11Z,14Z)-2OH(5,6))	-1.648377013	0.032656882	1.545310234	down
pos_5606	Cervonoyl ethanolamide	1.492814919	0.03315694	1.499500947	up
pos_2131	Clavulanate-9-aldehyde	0.215300618	0.03317796	1.44584995	unchanged
pos_7130	ophiocordin	0.868319712	0.033627619	1.566330146	unchanged
pos_1167	GDP-4-dehydro-6-deoxy-D-mannose	2.816530259	0.033951754	1.675470755	up

pos_10694	PC(16:0/20:5(5E,8E,11E,14E,17E))[U]	1.037453528	0.034091495	1.520834629	up
neg_1864	Penitrem D	0.220003307	0.035747555	1.463023989	unchanged
neg_736	Apigenin 7-di-O-xyloside	1.507732011	0.035781107	1.641638215	up
neg_1682	C12272	0.485848064	0.036028073	1.406347898	unchanged
neg_656	Ethyl beta-D-glucopyranoside	-1.128952687	0.036216043	1.463673941	down
pos_6310	L-2,4-Diaminobutanoate	-0.623090528	0.036254356	1.545998743	unchanged
neg_797	Hippurate	0.163255534	0.037177467	1.488607626	unchanged
neg_791	Tetracenomycin D3	0.332558562	0.037262469	1.483098085	unchanged
neg_2038	Tenofovir exalidex	0.399072614	0.037285735	1.468730971	unchanged
neg_727	1-Methylinosine	0.366629827	0.037457678	1.588096102	unchanged
neg_2806	(15S)-15-Hydroxy-5,8,11-cis-13-trans-eicosatetraenoate	0.237058456	0.037519595	1.459209131	unchanged
pos_986	2-Phenylacetamide	0.635514417	0.037536588	1.613235425	unchanged
neg_2572	Glycohyocholate	0.506713866	0.038036988	1.465315095	unchanged
pos_8229	G-418	-1.282838062	0.038284587	1.381948318	down
pos_969	1-(5'-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide	-1.265421824	0.039049801	1.372729118	down
pos_776	(1R)-Hydroxy-(2R)-N-acetyl-L-cysteinyl-1,2-dihydronaphthalene	-1.307143316	0.039197811	1.457110311	down
pos_5602	Decarbamoylsaxitoxin	1.268674193	0.03929767	1.459687711	up
neg_2787	Reduced riboflavin	0.616022787	0.039317854	1.539880806	unchanged
pos_5597	gamma-Aminobutyryllysine	1.666305927	0.039423011	1.458752211	up
neg_53	dTDP-4-oxo-alpha-D-xylose	0.29844919	0.039579113	1.478996979	unchanged
neg_1734	CPA(16:0/0:0)	0.962455639	0.039656439	1.458374153	unchanged
pos_10785	Diethyl decanedioate	0.324305398	0.039733512	1.486229925	unchanged
neg_2886	Lanabecestat	0.356579379	0.039811117	1.394064307	unchanged
neg_648	L-3,4-Dihydroxybutan-2-one 4-phosphate	0.478632626	0.039906661	1.433885005	unchanged
pos_9710	C16 Sphingosine	0.621876374	0.040081891	1.490884927	unchanged
neg_1495	milbemycin alpha10	-1.358688578	0.040206245	1.478742132	down
pos_10168	PC(18 3(9Z,12Z,15Z) 20 0)	0.553164175	0.040415823	1.467712153	unchanged
pos_9927	O-(13-Carboxytridecanoyl)carntine	0.476326162	0.04044212	1.455736302	unchanged
pos_11753	PC(18:4(2E,4E,6E,11Z)/18:1(11Z))[U]	0.943525289	0.040818208	1.4887185	unchanged
pos_8220	Taxa-4(20),11(12)-dien-5alpha-ol	-0.58923536	0.040824619	1.465265476	unchanged
neg_1650	LysoPE(0:0/18:3(6Z,9Z,12Z))	-0.652087478	0.04094614	1.50265031	unchanged
neg_1100	Perfluoroheptanoic acid	0.553856868	0.040986477	1.508119497	unchanged
neg_2386	LysoPA(0:0/18:0)	0.184787262	0.041444584	1.470763519	unchanged
pos_7561	Levamisole	0.418821458	0.04145219	1.392257336	unchanged
pos_9994	Cer(d17:1/PGE2)	0.42453554	0.041618677	1.440511537	unchanged
pos_6245	7-Methylxanthine	-4.609679008	0.041889926	1.538840159	down
neg_2185	3-Oxohexadecanoic acid	-0.721332874	0.042300506	1.541485717	unchanged
pos_12299	Rhizocticin C	-1.439936996	0.04248856	1.509943289	down
neg_2494	C17960	0.562242153	0.042705575	1.403297443	unchanged
pos_9638	trans-Dec-2-enoic acid	0.307337443	0.042866875	1.564903131	unchanged
neg_680	Aflatoxin B1 diol	-2.10450184	0.043102422	1.500419783	down
neg_2628	Ecabet	0.293416765	0.043126353	1.401999291	unchanged
neg_2188	PI(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	0.974146565	0.043132678	1.465969582	unchanged
neg_2541	7alpha-Hydroxydehydroepiandrosterone	-0.482162718	0.043598652	1.484546311	unchanged
neg_819	Hexanitrohexaazaisowurtzitane	0.311346805	0.043608637	1.433102368	unchanged
neg_2658	C06633	0.776491136	0.043713475	1.361487318	unchanged
neg_847	UDP-2,3-diacetamido-2,3-dideoxy-alpha-D-glucuronate	0.483406293	0.043741882	1.420426925	unchanged
pos_10373	C16 Sphinganine	0.675107283	0.044077195	1.447372035	unchanged

pos_5303	Carboxyethylphosphoramidate	-0.741417199	0.044392172	1.373762983	unchanged
neg_1632	Ciliatocholate	-0.27260403	0.04450539	1.453431648	unchanged
pos_11317	Icosanoic acid	0.751631309	0.044588982	1.535071156	unchanged
pos_7539	PC(18:3(6Z,9Z,12Z)/0:0)[U]	-0.353670265	0.044933951	1.51020017	unchanged
neg_2565	C02033	0.440726367	0.044999497	1.485799031	unchanged
neg_1685	(S)-10,16-Dihydroxyhexadecanoic acid	-0.625541062	0.045170183	1.502899429	unchanged
neg_2784	n-octyl-beta-D-thioglucopyranoside	0.567442512	0.04548172	1.488412943	unchanged
neg_2859	Oleandolide	0.304350988	0.045792285	1.413774052	unchanged
neg_2418	Icosanoic acid	-0.494510491	0.04580426	1.468112014	unchanged
neg_809	Glucoiberverin	0.849783058	0.046106964	1.455529911	unchanged
neg_856	2-Hydroxy-1,4-benzoxazin-3-one sulfate	0.274307096	0.047228494	1.45407024	unchanged
pos_1356	N-acetyl zonisamide	-1.200493341	0.047230751	1.422439579	down
neg_1870	Sirolimus	0.780161078	0.047568764	1.410084868	unchanged
pos_3113	ENOXACIN	0.811719295	0.048736389	1.432320511	unchanged
neg_1313	2-Octynoic acid	-2.097960016	0.0489796	1.466790042	down
pos_7605	phe-ile-gly	0.946090559	0.049031439	1.342250286	unchanged
neg_1925	PC(20:2(11Z,14Z)/PGJ2)	0.382652987	0.049376709	1.421032297	unchanged
neg_2713	Galaxolide	0.176130342	0.049542131	1.329344852	unchanged
neg_2042	PC(15:0/P-16:0)	-0.648884543	0.049558105	1.493514808	unchanged
pos_7701	Cholytyrosine	-1.084042431	0.049976164	1.435997695	down

Supplementary Table 4: Model VS WP metabolites

#ID	name	Model_vs_WP_log2FC	Model_vs_WP_Pvalue	Model_vs_WP_VIP	Model_vs_WP_(FC_2_Pvalue_0.05_VIP_1)_regulated
neg_1923	PC(P-16:0/PGF2alpha)	-1.792861556	7.53E-06	2.079665229	down
pos_1046	4-Hydroxy-6-methyl-3-(1H-pyrazol-3-yl)-2H-pyran-2-one	1.020122462	5.04E-05	2.054448842	up
neg_1932	PE(20:3(6,8,11)-OH(5)/P-18:1(11Z))	-1.665209228	6.04E-05	2.018205014	down
neg_2037	S-Methyl hexadecanethioate	-2.369391854	0.000110674	2.032356596	down
pos_10069	Cyclopassifloic acid A	-0.469093661	0.000121783	1.990708767	unchanged
neg_2060	Erinacine C	-1.159916978	0.00013411	2.000417843	down
neg_1927	(6Z,9Z,12Z)-Octadecatrienoic acid	-1.14637653	0.000145246	1.982292179	down
neg_1930	1-(3-Methylbutanoyl)-6-apiosylglucose	-2.134506353	0.000150067	2.006095759	down
pos_6394	N-Oleoylglycine	-0.374891478	0.000223741	2.00519419	unchanged
pos_903	Indoleacetaldehyde	0.5952067	0.000349197	2.022989531	unchanged
pos_839	4-Methylene-L-glutamate	0.437411587	0.000391022	2.000831201	unchanged
neg_2057	Mevastatin	-1.59186079	0.000466846	2.073997484	down
neg_2053	Taxa-4(20),11(12)-dien-5alpha,13alpha-diol	-1.65630602	0.000910125	2.055841332	down
neg_971	Niridazole	0.888504581	0.001080176	1.915788107	unchanged
neg_1985	Hexadecanoic acid	-1.261147135	0.001111711	1.90831281	down
neg_2055	(±)13-HDoHE	-2.084122334	0.001132186	2.03404879	down
neg_1497	Cyanoketone	-0.31936725	0.001284657	1.861386146	unchanged
neg_2141	(R)-3,4-Dihydro-8-hydroxy-3-tridecyl-1H-2-benzopyran-1-one	-2.110849026	0.00131629	2.028489919	down
neg_2229	PC(P-18:0/PGF1alpha)	-2.182247504	0.001532275	1.944043072	down
neg_970	2-Isopropylmalic acid	0.807987106	0.001537718	1.891158731	unchanged
neg_2467	20-Hydroxy-6Z,15Z-eicosadienoic acid	-0.504139668	0.001545124	1.994384854	unchanged
neg_2205	35S-Methylokadaic acid 7-hexadecanoate	-0.529070714	0.001617974	1.80175035	unchanged
neg_2115	PE(22:1(13Z)/6 keto-PGF1alpha)	-1.148346461	0.001712721	1.891449616	down
neg_2231	11-Dehydro-thromboxane B2	-1.917128494	0.001738324	2.027634173	down
pos_896	4-Hydroxy-3-methyl-2-(2-propynyl)-2-cyclopentene-1-one	0.488051631	0.00181382	1.875087277	unchanged
neg_2230	Siderol	-1.820468629	0.00183504	2.008011577	down
neg_2258	CP 47,497-C8-homolog C-8-hydroxy metabolite	-2.565760898	0.001865868	2.012067717	down
neg_1650	LysoPE(0:0/18:3(6Z,9Z,12Z))	-0.4966428	0.00189439	1.89052765	unchanged
neg_2158	8(S)-HETrE	-1.416431179	0.001921837	1.962429187	down
pos_9740	Icosadienoic acid	-4.359441048	0.002024583	2.019014956	down
pos_5214	(5E)-4-[(E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy-2-methyl-5-[2-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxvethylidene]cyclopentene-1-carboxylic acid	-2.167710603	0.00208683	1.850057104	down
pos_769	Deoxyinosine	-0.565303138	0.002177859	1.914840975	unchanged
neg_1613	5-((6-((Aminomethyl)amino)-1-oxohexyl)amino)pentanoic acid	-1.123886921	0.002452666	1.820861962	down
neg_2118	PE-NMe2(18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))	-2.540869883	0.00250755	2.000021806	down
neg_2114	PE(20:1(11Z)/20:3(5Z,8Z,11Z))	-1.246379204	0.002565908	1.897699197	down
neg_977	5-Phospho-L-lysine	1.096942102	0.002709455	1.88090862	up
pos_9454	Ser-Leu-Ile-Gly-Lys-Val	-0.276973077	0.002777759	1.846071139	unchanged
neg_2101	Deoxyloganin	-1.032323003	0.002903422	1.854757094	down
pos_5728	trichostatin A	-0.754355689	0.002908535	1.85010348	unchanged
neg_1972	C16143	-1.151088115	0.003022832	1.767714802	down
neg_2096	(±)16-HETE	-0.932789546	0.003050323	1.87501865	unchanged
neg_2108	PC(P-16:0/PGE1)	-0.922224312	0.003123762	1.869845216	unchanged
pos_8220	Taxa-4(20),11(12)-dien-5alpha-ol	-0.531849082	0.003166445	1.849737289	unchanged
pos_7178	Dodecylbenzene	-0.462609078	0.003299339	1.837375489	unchanged
neg_2672	1,2,10-Trihydroxydihydro-trans-linalyl oxide 7-O-beta-D-glucopyranoside	0.596782329	0.003422261	1.840358728	unchanged
neg_1931	14-Fluoro-6-thiaheptadecanoic acid	-2.392285106	0.003434542	1.934310422	down
neg_978	Shikimate 3-phosphate	0.814208216	0.003491076	1.869397466	unchanged
neg_1637	PS(14:0/18:0)	-2.120107835	0.003511747	1.857214804	down
pos_5314	Capecitabine	-2.170188522	0.003511897	1.758641726	down

pos_9302	DEHYDROCHOLIC ACID	-1.922493371	0.003607098	1.946784382	down
pos_1920	Carmofur	-1.940679536	0.003812403	1.848439776	down
pos_8991	1,2-dihydroxyheptadec-16-en-4-yl acetate	-2.762439387	0.003900784	1.9806062	down
neg_2008	3alpha,7alpha,12beta-Trihydroxy-5beta-cholanoic acid	-1.974956293	0.004006326	1.881316013	down
neg_1988	13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid	-1.407682325	0.004008054	1.912298961	down
pos_669	PA(16:1(9Z)/LTE4)	-0.483914893	0.004200182	1.812025494	unchanged
neg_2152	8-[(1R,2R)-3-Oxo-2-{(Z)-pent-2-enyl}cyclopentyl]octanoate	-0.460178962	0.004313313	1.766558243	unchanged
pos_8221	PGF2β Alcohol methyl ether	-0.506778116	0.004474626	1.821513138	unchanged
pos_668	PS(20:5(5Z,8Z,11Z,14Z,17Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))	-0.292681958	0.004542369	1.876984721	unchanged
neg_2271	C16506	-1.446230742	0.004564527	1.710934397	down
pos_904	Methyl beta-D-galactoside	0.450275125	0.004692005	1.731308834	unchanged
pos_7696	N-[(2S)-1-[[[(2S)-1-Amino-1-oxopropan-2-yl]amino]-3-naphthalen-2-yl]-1-oxopropan-2-yl]-N'-hydroxy-2-(2-methylpropyl)butanediamide	1.869702946	0.004770901	1.678308183	up
pos_7375	Viloxazine	-0.543899189	0.004775802	1.691896607	unchanged
pos_7517	3-Hydroxy-11Z-octadecenoylcarnitine	1.710928336	0.004796304	1.751989445	up
neg_1922	11,12,13-Trinor-1(10)-spirovetivene-2,7-dione	-1.139454341	0.004799445	1.69317158	down
neg_2088	Eicosapentaenoic acid	-1.171389931	0.004935771	1.852765716	down
pos_8155	9-OxoODE	-1.540651374	0.005178829	1.829375852	down
pos_1009	7,8-Dihydro-7,8-dihydroxykynurenate	-0.695132737	0.005211805	1.760658371	unchanged
neg_1508	Hymenoxon	-0.899840516	0.005338849	1.704405348	unchanged
neg_1821	Leukotriene C4	0.468971102	0.0054974	1.759869469	unchanged
pos_7442	(9Z,12Z,15Z)-3-Hydroxyoctadecatrienoylcarnitine	-0.710159814	0.005529538	1.788766477	unchanged
pos_5776	3-Hydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione	-0.853084533	0.005697275	1.813320063	unchanged
pos_910	(R)-3-hydroxybutyrylcarnitine	-0.876526422	0.005835485	1.740121865	unchanged
neg_1618	Propofol glucuronide	-0.921399717	0.005968177	1.719627261	unchanged
pos_1078	Phensuximide	1.195692069	0.006083162	1.760477577	up
pos_9082	L-2-Aminoadipate 6-semialdehyde	-1.901798372	0.006104259	1.84550711	down
pos_1038	alpha-D-Ribose 1-methylphosphonate 5-phosphate	-0.434649857	0.006433245	1.748229355	unchanged
pos_799	5-Fluorouridine diphosphate	-0.395241981	0.006474662	1.743013191	unchanged
neg_1774	PE(15:0/20:3(8Z,11Z,14Z)-2OH(5,6))	-1.301869059	0.006529358	1.711664712	down
neg_1986	13(S)-HODE	-1.258492493	0.006606749	1.862724532	down
pos_7049	(±)-Myristoylcarnitine	-1.104481126	0.00684126	1.792218065	down
pos_7511	1-(3-Carboxypropylcarbamoyl)-5-fluorouracil	0.525783778	0.006884939	1.785181491	unchanged
neg_2066	Ganodermic acid TQ	0.389070166	0.006968598	1.713907613	unchanged
neg_1680	Methyl octynecarboxylate	-1.084609987	0.007037157	1.755382759	down
pos_9088	(5Z,8Z,11Z,14Z,17Z)-Icosapentaenoic acid	-1.272993878	0.007188627	1.868440721	down
neg_1860	Ouabain	1.107922228	0.007539867	1.651055944	up
pos_1077	2-Methyl-2-[(1-oxo-2-propenyl)amino]-1-propanesulfonic acid	1.187873104	0.007628925	1.734064442	up
pos_871	Leu Pro	0.519120487	0.00772284	1.847309777	unchanged
pos_9416	prostaglandin a1 ethyl ester	-2.1595609	0.007841623	1.902417262	down
neg_2748	20,26-Dihydroxyecdysone	0.285483652	0.008069254	1.698171296	unchanged
pos_9335	19(S)-HETE	-1.063331221	0.008101217	1.865739107	down
pos_7672	Lucidenic acid D1	1.29620563	0.00812734	1.765875558	up
neg_2255	3alpha,11beta,21-Trihydroxy-20-oxo-5beta-pregnan-18-al	-0.808280925	0.008164999	1.642893483	unchanged
neg_2185	3-Oxoheptadecanoic acid	-0.607758534	0.008683005	1.650766827	unchanged
neg_2190	Aypgkf	0.382761347	0.008705482	1.666043296	unchanged
neg_2070	Deoxycholyphenylalanine	0.309243005	0.008906924	1.693809773	unchanged
pos_1743	trans-o-Hydroxybenzylidenepyruvate	0.788011696	0.008977203	1.607414957	unchanged
pos_8523	MG(0:0/16:0/0:0)	0.482753004	0.009293148	1.697990468	unchanged
pos_7179	9-Oxononanoic acid	-0.493259508	0.009348807	1.698601048	unchanged
neg_2102	DG(2:0/18:2(10E,12Z)+=O(9)/0:0)	-0.329910931	0.009680408	1.635028995	unchanged
neg_1891	2-[(L-Alanin-3-ylcarbamoyl)methyl]-3-(2-aminoethylcarbamoyl)-2-	-1.393059814	0.009803481	1.757760722	down
pos_1021	Cyanuric acid	-0.46677183	0.010135394	1.623560732	unchanged

neg_1810	Decanoylcholine	-0.636324994	0.010860084	1.646075267	unchanged
neg_610	Estradiol-17beta 3-sulfate	0.641757209	0.011030905	1.675373555	unchanged
neg_2086	Dihydroactinidiolide	-1.470614732	0.011558516	1.740665365	down
neg_1548	(-)-alpha-Bisabolol	-1.042539484	0.011705331	1.712264232	down
pos_6792	3-Hydroxy-9-hexadecenoylcarnitine	-1.300838146	0.011763235	1.743512362	down
pos_7439	Octadecyl fumarate	-0.98504964	0.012258068	1.684022784	unchanged
pos_5000	Traumatic acid	-3.536971595	0.012323721	1.805597166	down
neg_1655	Rhizoxin	0.48653478	0.012372015	1.580013584	unchanged
neg_1814	25-Hydroxyvitamin D3 3-sulfate ester	-0.252299078	0.012397168	1.726893865	unchanged
pos_9091	17-Hydroxymethylethisterone	-1.243151762	0.012582933	1.826692776	down
pos_931	(E)-Casimiroedine	-0.565548973	0.012631442	1.595955487	unchanged
pos_12299	Rhizocticin C	-2.958899114	0.012872274	1.682890039	down
neg_1665	N-Palmitoyl Arginine	0.667085998	0.0133858	1.699476416	unchanged
pos_7307	delta-Dodecalactone	-1.231096883	0.01342948	1.657826388	down
pos_1075	2-Propylsuccinic acid	0.581788192	0.013812556	1.588989919	unchanged
neg_2146	C21484	0.458624445	0.013865264	1.660179479	unchanged
neg_2019	PE(20:1(11Z)/16:0)	-0.554419175	0.013865429	1.80003949	unchanged
pos_1045	Methylcysteine	-1.017867954	0.013921276	1.688093112	down
pos_6730	Cholic Acid, Methyl Ester	-1.654390584	0.013979877	1.783167841	down
pos_9279	(-)-Amijiol	-1.821808107	0.014112957	1.796025739	down
neg_1460	Acoric acid	-2.26116594	0.014313122	1.771457254	down
neg_2587	(13R,14R)-7-Labdene-13,14,15-triol	-0.271614557	0.014414376	1.624885455	unchanged
neg_2006	PE(P-18:1(11Z)/18:1(12Z)-2OH(9,10))	0.90606317	0.014928292	1.62687752	unchanged
neg_1486	Dhesn	-6.719035436	0.015538447	1.831033819	down
pos_5642	Urocortisol	-1.183010186	0.015799336	1.76236246	down
neg_1616	2,3-Dimethoxy-5-methyl-6-(9'-carboxynonyl)-1,4-benzoquinone	-1.241449543	0.016170996	1.638852861	down
pos_6433	N6-(L-1,3-Dicarboxypropyl)-L-lysine	-0.945710763	0.016234649	1.597158034	unchanged
pos_9090	(+)-Camphor	-1.562225827	0.016322728	1.756683214	down
pos_2131	Clavulanate-9-aldehyde	0.192065447	0.016725564	1.61982939	unchanged
pos_8392	Phosphatidylcholine lyso alkyl 16_0	-0.520348423	0.016963252	1.548378728	unchanged
neg_611	beta-D-glucosaminyl-(1->4)-beta-D-glucosamine	0.575611863	0.017083682	1.591028999	unchanged
pos_9085	D-Lysopine	-2.057384507	0.017130005	1.788412118	down
pos_8202	beta-Acetyldigoxin	-0.258115417	0.018015562	1.695654994	unchanged
neg_904	2,2,2-Trifluoroethyl	0.2722695	0.018222981	1.524015662	unchanged
pos_1018	Pindolol	-1.787971181	0.018256685	1.644369201	down
pos_9625	PE(15:0/18:0)	0.238095849	0.018267371	1.565252821	unchanged
pos_1725	Prunasin	-2.809174797	0.018274217	1.666661182	down
neg_1884	PE(16:0/20:3(8Z,11Z,14Z)-2OH(5,6))	-2.385374721	0.018432281	1.767455713	down
pos_8005	Lepidiumterpenyl ester	-0.519588308	0.01853132	1.628832978	unchanged
neg_2068	1-Stearoylglycerophosphoserine	0.523577689	0.018552006	1.616795006	unchanged
pos_8677	Dapdiamide B	0.304187384	0.01873331	1.602166242	unchanged
pos_8577	Trihexosylceramide (d18_1_16_0)	-0.286617876	0.019252401	1.618536812	unchanged
pos_2158	20-Hydroxyleukotriene E4	-3.968863318	0.019484399	1.62718912	down
neg_1885	PS(18:0/18:2(9Z,12Z))	-1.149968004	0.019485525	1.6665228	down
pos_8341	MG(0:0/20:1(11Z)/0:0)	-1.083284137	0.019868374	1.718105255	down
pos_11498	PC(P-18:1(11Z)/18:3(10,12,15)-OH(9))	0.930423064	0.020243421	1.568171101	unchanged
neg_2885	6-beta-hydroxydexamethasone	-0.632854598	0.02058406	1.588484425	unchanged
pos_5346	3-hydroxy-C10-homoserine lactone	1.15538279	0.02100035	1.519657834	up
neg_1817	5(S)-HPETE	-0.719896361	0.021061319	1.571492383	unchanged
neg_429	Urea-1-carboxylate	0.561156626	0.021157683	1.604539799	unchanged
neg_1495	milbemycin alpha10	-2.087804155	0.02129633	1.780574432	down
neg_1649	PE(14:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))	-1.216467539	0.021336914	1.574544837	down
neg_2143	N-Lauroyl Asparagine	-30.54830853	0.021480484	1.75190699	down

pos_12498	CDP-ethanolamine	0.150909377	0.021848999	1.497062728	unchanged
neg_980	1-(5'-Phosphoribosyl)-5-amino-4-imidazolecarboxamide	1.638099391	0.022006261	1.603456527	up
pos_6367	2-[5-[(3,5-Dimethyl-1H-pyrrol-2-yl)methylidene]-4-methoxy-2-	-2.197479534	0.022013709	1.770017318	down
pos_2772	L-Histidine	0.528351612	0.022034277	1.637343131	unchanged
pos_958	Lanthionine ketimine	-0.377690643	0.022214361	1.583836964	unchanged
pos_7615	Pedin B	2.032191345	0.022262256	1.606240133	up
pos_6477	delta-Tocotrienol	-1.7386938	0.022364997	1.710054905	down
pos_8646	Hepoxilin A3	0.190227187	0.022658736	1.547300055	unchanged
pos_863	5-Hydroxyectoine	0.260221117	0.022783675	1.604734687	unchanged
neg_2609	SM(d16:1/20:3(8Z,11Z,14Z)-2OH(5,6))	0.191018646	0.022840797	1.543168561	unchanged
pos_7121	O-(1->4)-alpha-L-Dihydrostreptosyl-streptidine 6-phosphate	0.788549114	0.022853508	1.585199716	unchanged
pos_7126	Desisobutyrylciclesonide	1.076920131	0.023240026	1.63062768	up
pos_7118	Clausarinol	0.583305507	0.023337448	1.550147977	unchanged
neg_2196	Prolylhydroxyproline	-0.454449164	0.023366094	1.645560343	unchanged
neg_1950	Lithocholate 3-O-glucuronide	0.461493229	0.023408642	1.560802594	unchanged
pos_7077	L-Fucono-1,5-lactone	0.758962072	0.023489752	1.513893151	unchanged
pos_6255	1,2-dihydroxyheptadec-16-yn-4-yl acetate	-0.992225281	0.023833885	1.63459354	unchanged
pos_1033	S-(3-Oxo-3-carboxy-n-propyl)cysteine	-1.152101022	0.023840532	1.540648654	down
pos_8170	CL(8:0/10:0/10:0/14:0)	-0.314145541	0.02392414	1.676805372	unchanged
neg_2038	Tenofovir exalidex	0.442305335	0.024068887	1.681243732	unchanged
neg_2805	Ginsenoside C-K	0.193246561	0.024182112	1.515218519	unchanged
pos_8715	Ecgonine methyl ester	0.678379184	0.024292415	1.601695006	unchanged
pos_2332	Gabapentin	0.655960462	0.024307442	1.500253745	unchanged
pos_7582	Glu Gly Met Phe	0.817299616	0.024322866	1.585702683	unchanged
neg_465	Arabinonic acid	0.64857767	0.024442815	1.608772029	unchanged
pos_5473	Deoxyguanidinoproclavaminic acid	0.659306024	0.024837809	1.493914316	unchanged
neg_1874	(E)-3,7-Dimethyl-1,5,7-octatrien-3-ol	0.226216133	0.025179534	1.568410345	unchanged
neg_1506	Tetradecanedioic acid	-0.511248099	0.025419691	1.509483514	unchanged
pos_874	o-1821	0.288079234	0.025423757	1.547772289	unchanged
neg_1364	Brevianamide F	0.50769108	0.025708054	1.400483983	unchanged
pos_7561	Levamisole	0.407346699	0.025799543	1.582129794	unchanged
neg_1449	C20760	-1.190262056	0.026041606	1.693879792	down
neg_2789	Panaquinquecol 5	0.280609584	0.026339114	1.504930804	unchanged
pos_9190	PA(18:1(11Z)/15:0)	0.274131643	0.026367552	1.540518263	unchanged
pos_9710	C16 Sphingosine	0.631544665	0.026399637	1.608424095	unchanged
pos_1004	D-Glucono-1,5-lactone 6-phosphate	-0.51619223	0.026692336	1.475205035	unchanged
neg_2106	all-trans-4-Hydroxyretinoic acid	-3.861413526	0.027222811	1.728177788	down
neg_2268	11beta,21-Dihydroxy-3,20-oxo-5beta-pregnan-18-al	0.229922271	0.02761755	1.471171705	unchanged
pos_9033	(9E,11E)-Octadecadienoic acid	0.532961897	0.027636948	1.524566373	unchanged
neg_1410	C75	-2.33088989	0.028115157	1.680283403	down
pos_2181	Aeruginosin 98-B	-2.217209018	0.028189022	1.556216484	down
pos_8118	Methyl jasmonate	-0.838459659	0.028578225	1.638313149	unchanged
pos_1755	Melibiotol	-1.450453577	0.029570051	1.571665352	down
neg_2426	Petasitenine	0.626906749	0.029648334	1.444452768	unchanged
pos_8302	PI(20:1(11Z)/TXB2)	-0.494727047	0.029793932	1.540225233	unchanged
neg_1654	2,3-Dinor-8-iso prostaglandin F2alpha	0.714140702	0.029923319	1.419417197	unchanged
pos_6718	LysoPC 16-2	-0.745318837	0.029987196	1.546756202	unchanged
neg_2737	Juvenile hormone III acid	0.714465234	0.030083487	1.444771442	unchanged
pos_2727	DG(a-25:0/LTE4/0:0)	2.661532343	0.030145743	1.641362505	up
neg_2900	Ecdysone	-0.773810179	0.030203756	1.520285931	unchanged
pos_8128	LysoPC(20:4(5Z,8Z,11Z,14Z)/0:0)	0.323413774	0.030259341	1.547056678	unchanged
pos_7311	(2S)-2-Hydroxyhexadecanoylcarnitine	-0.7134987	0.030271409	1.528643279	unchanged
neg_1463	10-Deacetyl-2-debenzoylbaccatin III	-2.755231292	0.030429525	1.67533153	down

pos_7859	Ser Gly Tyr Phe	-0.564868829	0.03055071	1.519455501	unchanged
pos_7184	Sphingosine-1-phosphate	-0.587819554	0.030622062	1.501384311	unchanged
pos_1413	L-Methionine	-0.72510047	0.031058421	1.514526443	unchanged
neg_2678	(R)-Mevalonate	0.566540235	0.031071787	1.589098481	unchanged
neg_2254	(Z)-9-Cycloheptadecen-1-one	-1.062868248	0.031731163	1.531577904	down
neg_1462	(Z)-5-[(2R,3S,4S)-4-Hydroxy-2-[(E)-3-hydroxyoct-1-enyl]oxan-3-yl]pent-3-enoic	-2.688607864	0.031781458	1.671046533	down
neg_1818	C11134	0.876457402	0.03179672	1.448927625	unchanged
neg_1852	LysoPE(0:0/18:2(9Z,12Z))	-0.255223011	0.031904485	1.503856201	unchanged
pos_1044	Difluorodeoxyuridine	-1.16525713	0.032132785	1.595090424	down
pos_7559	Guanidinoacetate	0.530206194	0.032223721	1.493963404	unchanged
neg_979	Cytosine	1.271282536	0.032426292	1.484127919	up
neg_1971	5-Oxoavermectin "1b" aglycone	0.356673124	0.032464508	1.465991721	unchanged
pos_7354	Digitoxigenin 3-[glucosyl-(1->6)-glucosyl-(1->4)-2,6-dideoxyribohexoside]	0.947773479	0.033362662	1.474416944	unchanged
neg_1947	[(2-Hexylcyclopentylidene)amino]thiourea	0.163733182	0.033778982	1.516548659	unchanged
pos_1417	5-amino-1-(5-phosphonato-D-ribosyl)imidazol-3-ium	-0.676204761	0.033901612	1.503311336	unchanged
pos_9638	trans-Dec-2-enoic acid	0.32752207	0.03396643	1.492069817	unchanged
pos_1056	lys-met	-1.931327601	0.034306899	1.485724276	down
pos_1187	NTP	0.68776086	0.034660566	1.426106546	unchanged
pos_6881	Hydroxyhomodestruxin B	-1.180289122	0.03469173	1.613044741	down
neg_1578	24,24-Difluoro-1alpha,25-dihydroxyvitamin D3	0.570356733	0.034787927	1.438627987	unchanged
neg_595	(R)-2-(4-(Tert-butoxycarbonyl)morpholin-3-yl)acetic acid	-1.06874814	0.035249161	1.498203425	down
neg_2831	Versalide	0.700325059	0.035276504	1.415988423	unchanged
pos_2173	6,7-Didehydrofevicordin F 3-[glucosyl-(1->6)-glucoside]	-3.038285415	0.035348113	1.52041973	down
pos_1356	N-acetyl zonisamide	-1.310555632	0.035481873	1.536472899	down
neg_2012	di-trans,poly-cis-Undecaprenyl diphosphate	0.321108806	0.035850515	1.440748835	unchanged
pos_9754	(S)-Hemiketal	0.834817849	0.035936999	1.583077879	unchanged
pos_9994	Cer(d17:1/PGE2)	0.424627015	0.036137446	1.581025279	unchanged
pos_1353	Indoxyl	-0.283876737	0.036594065	1.504709727	unchanged
pos_6564	D-Urobilinogen	-0.609034423	0.036764906	1.436404359	unchanged
neg_1685	(S)-10,16-Dihydroxyhexadecanoic acid	-0.678399491	0.036909829	1.577218534	unchanged
neg_2131	Cholylcitrulline	0.181220992	0.037025363	1.472258473	unchanged
neg_2386	LysoPA(0:0/18:0)	0.198394054	0.037250844	1.495876225	unchanged
pos_6245	7-Methylxanthine	-24.52607058	0.037569481	1.547249478	down
pos_1035	3,4-Dihydro-7-methoxy-2-methylene-3-oxo-2H-1,4-benzoxazine-5-carboxylic	-1.543487259	0.037582838	1.556916463	down
pos_8335	3-(2,4-Dimethyl-5-(2-oxo-1,2-dihydroindol-3-ylidenemethyl)-1H-pyrrol-3-yl)propionic acid	0.478550429	0.037910576	1.387461193	unchanged
pos_8810	PE(16:0/0:0)	0.327273735	0.038766641	1.442357284	unchanged
pos_6587	Hexadecanedioic acid mono-L-carnitine ester	-0.788480362	0.03885233	1.559708353	unchanged
neg_1612	3-[(3aS,4S,7aS)-7a-Methyl-1,5-dioxo-octahydro-1H-inden-4-yl]propanoate	0.43414626	0.039295291	1.533915344	unchanged
pos_7067	1-(2-Furyl)butan-3-one	1.650546216	0.03956776	1.455491677	up
neg_1881	PE(P-18:0/PGE2)	-0.904760336	0.039619037	1.489600165	unchanged
neg_1979	C05497	0.239751776	0.039700101	1.421650995	unchanged
pos_1020	N-Formyl-L-aspartate	-1.031544231	0.039705658	1.488204039	down
neg_1568	1-Nonen-3-ol	0.830478486	0.039915745	1.522696877	unchanged
pos_8846	(2-{{2-[hexadec-9-enamido]-3-hydroxyoctadec-4-en-1-yl}phosphono}oxy}ethyl)trimethylazanium	0.564730433	0.040130003	1.489096209	unchanged
neg_1581	Pregnenolone-3,21-disulfate	1.793183986	0.040346904	1.51744634	up
pos_7076	alpha-Methylstyrene	0.889597609	0.040677694	1.446005015	unchanged
pos_8643	2-Methylbutyroylcarnitine	0.217726166	0.040699115	1.439770242	unchanged
pos_7078	(4-Methylphenyl)acetaldehyde	0.86872888	0.041285957	1.423102717	unchanged
neg_1313	2-Octynoic acid	-2.407211376	0.041351586	1.53645785	down
neg_2944	C06054	0.199949615	0.041580304	1.423017975	unchanged
pos_1066	3-Amino-2,3-dideoxy-scylo-inosose	0.891392181	0.041706387	1.432729443	unchanged

pos_6622	Armillarin	0.71171792	0.04195804	1.45767368	unchanged
neg_1864	Penitrem D	0.18664563	0.042737031	1.433541322	unchanged
neg_1358	C05964	-2.733407199	0.042920103	1.523718435	down
neg_1267	2-(7'-Methylthio)heptylmalic acid	31.62419661	0.043003028	1.513696546	up
pos_4789	Coenzyme F420	-0.615408772	0.043038791	1.546925724	unchanged
neg_467	5,6-Dihydro-5-fluorouracil	-0.845536904	0.043598962	1.459929679	unchanged
neg_2405	(7Z,10Z,13Z,16Z,19Z)-Docosapentaenoic acid	-0.608223626	0.043635059	1.370256192	unchanged
neg_1525	3-Oxotetradecanoic acid	-1.065531757	0.043701458	1.500025767	down
pos_7165	Tunicamycin VI	1.936211634	0.044187348	1.373232272	up
neg_1629	geranate	-0.985834441	0.044373518	1.450396815	unchanged
neg_2356	C21481	-0.432791817	0.044459367	1.333011748	unchanged
neg_1464	Decitabine	-2.78942964	0.044621242	1.573123337	down
pos_8644	(6S)-Hydroxyhyoscyamine	0.202492424	0.045135323	1.411445139	unchanged
neg_2912	18-Hydroxycorticosterone	-0.814036211	0.045584225	1.391475267	unchanged
neg_1638	Microcystin LR	0.632645926	0.046348762	1.401324743	unchanged
pos_9435	4a-Hydroxytetrahydrobiopterin	2.799778342	0.04639452	1.467890446	up
pos_7098	2'-O-methyladenosine	0.825153594	0.046940669	1.390144818	unchanged
pos_7971	3beta,7alpha-Dihydroxy-5-cholestenoate	-0.342470991	0.048059834	1.413969734	unchanged
pos_7216	3-O-Acetylepisamarcandin	0.983987373	0.048160356	1.468578914	unchanged
pos_6312	APC	1.08164151	0.04817586	1.410819048	up
pos_7100	alpha-1,5-L-Arabinobiose	1.112227946	0.048280777	1.452205382	up
neg_2040	5beta-Cyprinolsulfate	0.214499632	0.048411284	1.505981151	unchanged
pos_6588	7-Sulfocholic acid	2.729161309	0.048504852	1.522359861	up
neg_2342	1-Octadecanoyl-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphoethanolamine	0.380924261	0.048670287	1.44370865	unchanged
neg_1857	Pubescenol	0.42854648	0.048795529	1.381838052	unchanged
pos_8800	Ricinoleic acid methyl ester	0.19575104	0.048797355	1.346672444	unchanged
pos_6310	L-2,4-Diaminobutanoate	-0.554504901	0.049049649	1.435426713	unchanged
pos_1051	2-Phenylethanol glucuronide	-1.314385578	0.049271291	1.41314723	down
pos_9972	Cholesterol-d7	0.556109969	0.049275664	1.463164805	unchanged
pos_6635	5,6,7,8-Tetrahydromonapterin	1.272228912	0.049372692	1.474893579	up
neg_1645	PC(2:0/PGE2)	0.367757998	0.04937824	1.529562027	unchanged
pos_6988	Morinidazole	-1.155615237	0.0499041	1.368291775	down

Supplementary Table 4: The intersection of DAMs

	The intersection of the comparisons among (Normal VS Model), (Model VS H-YP), and (Model VS WP)
	The intersection of (Model VS H-YP) and (Model VS WP)
	The intersection of (Model VS H-YP) and (Normal VS Model)
	The intersection of (Model VS WP) and (Normal VS Model)
	The absence of color represents their respective uniqueness

	#ID	name	(FC_2_Pvalue_0.05_VI P 1) regulated		#ID	name	(FC_2_Pvalue_0.05_VIP VIP 1) regulated		#ID	name	(FC_2_Pvalue_0.05_VIP_1)_r regulated
Normal VS Model	pos_7049	(±)-Myristoylcarnitine	up	Model VS H-YP	neg_1460	Acoric acid	down	Model VS WP	neg_1460	Acoric acid	down
	neg_1972	C16143	up		neg_1495	milbemycin alpha10	down		neg_1495	milbemycin alpha10	down
	neg_1885	PS(18:0/18:2(9Z,12Z))	up		neg_1525	3-Oxotetradecanoic acid	down		neg_1525	3-Oxotetradecanoic acid	down
	pos_5642	Urocortisol	up		neg_1581	Pregnenolone-3,21-disulfate	up		neg_1581	Pregnenolone-3,21-disulfate	up
						2,3-Dimethoxy-5-methyl-6-(9'-carboxynonyl)-1,4-				2,3-Dimethoxy-5-methyl-6-(9'-	
	pos_8341	MG(0:0/20:1(11Z)/0:0)	up		neg_1616	benzoquinone	down		neg_1616	carboxynonyl)-1,4-benzoquinone	down
	pos_5000	Traumatic acid	up		neg_1649	PE(14:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))	down		neg_1649	PE(14:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))	down
	pos_6792	3-Hydroxy-9-hexadecenoylcarnitine	up		neg_1774	PE(15:0/20:3(8Z,11Z,14Z)-2OH(5,6))	down		neg_1774	PE(15:0/20:3(8Z,11Z,14Z)-2OH(5,6))	down
	neg_1884	PE(16:0/20:3(8Z,11Z,14Z)-2OH(5,6))	up		neg_1884	PE(16:0/20:3(8Z,11Z,14Z)-2OH(5,6))	down		neg_1884	PE(16:0/20:3(8Z,11Z,14Z)-2OH(5,6))	down
	neg_1774	PE(15:0/20:3(8Z,11Z,14Z)-2OH(5,6))	up		neg_1885	PS(18:0/18:2(9Z,12Z))	down		neg_1885	PS(18:0/18:2(9Z,12Z))	down
										2-[(L-Alanin-3-ylcarbamoyl)methyl]-3-(2-	
	neg_1891	2-[(L-Alanin-3-ylcarbamoyl)methyl]-3-(2-aminoethylcarbamoyl)-2-hydroxypropanoate	up		neg_1891	2-[(L-Alanin-3-ylcarbamoyl)methyl]-3-(2-aminoethylcarbamoyl)-2-hydroxypropanoate	down		neg_1891	(2-aminoethylcarbamoyl)-2-	
	pos_6730	Cholic Acid, Methyl Ester	up		neg_1972	C16143	down		neg_1972	hydroxypropanoate	down
	pos_7615	Pedin B	down		neg_2254	(Z)-9-Cycloheptadecen-1-one	down		neg_1972	C16143	down
	pos_6477	delta-Tocotrienol	up		pos_1356	N-acetyl zonisamide	down		neg_2254	(Z)-9-Cycloheptadecen-1-one	down
	neg_1581	Pregnenolone-3,21-disulfate	down		pos_1725	Prunasin	down		pos_1356	N-acetyl zonisamide	down
	pos_6988	Morinidazole	up		pos_1755	Melibiitol	down		pos_1725	Prunasin	down
	pos_6588	7-Sulfocholic acid	down		pos_5000	Traumatic acid	down		pos_1755	Melibiitol	down
	pos_1356	N-acetyl zonisamide	up		pos_5642	Urocortisol	down		pos_5000	Traumatic acid	down
	pos_7307	delta-Dodecalactone	up		pos_6477	delta-Tocotrienol	down		pos_5642	Urocortisol	down
	pos_1755	Melibiitol	up		pos_6588	7-Sulfocholic acid	up		pos_6477	delta-Tocotrienol	down
		2,3-Dimethoxy-5-methyl-6-(9'-carboxynonyl)-1,4-							pos_6588	7-Sulfocholic acid	up
	neg_1616	benzoquinone	up		pos_6730	Cholic Acid, Methyl Ester	down		pos_6730	Cholic Acid, Methyl Ester	down
	neg_2254	(Z)-9-Cycloheptadecen-1-one	up		pos_6792	3-Hydroxy-9-hexadecenoylcarnitine	down		pos_6792	3-Hydroxy-9-hexadecenoylcarnitine	down
	pos_1725	Prunasin	up		pos_6988	Morinidazole	down		pos_6988	Morinidazole	down
	neg_1525	3-Oxotetradecanoic acid	up		pos_7049	(±)-Myristoylcarnitine	down		pos_7049	(±)-Myristoylcarnitine	down
	neg_1495	milbemycin alpha10	up		pos_7307	delta-Dodecalactone	down		pos_7307	delta-Dodecalactone	down
	pos_7517	3-Hydroxy-11Z-octadecenoylcarnitine	down		pos_7517	3-Hydroxy-11Z-octadecenoylcarnitine	up		pos_7517	3-Hydroxy-11Z-octadecenoylcarnitine	up
	neg_1460	Acoric acid	up		pos_7615	Pedin B	up		pos_7615	Pedin B	up
	neg_1649	PE(14:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))	up		pos_8341	MG(0:0/20:1(11Z)/0:0)	down		pos_8341	MG(0:0/20:1(11Z)/0:0)	down
	pos_806	UDP-4-dehydro-6-deoxy-D-glucose	up		neg_1508	Hymenoxon	down		neg_1313	2-Octynoic acid	down
	neg_736	Apigenin 7-di-O-xyloside	down		neg_1993	5-Methoxytryptamine	up		neg_1410	C75	down
										5-((6-((Aminomethyl)amino)-1-	
	neg_1508	Hymenoxon	up		neg_736	Apigenin 7-di-O-xyloside (2R,3R,4S,5S,6R)-2-[[1,1,1-tris(4-hydroxyphenyl)heptan-3-yloxy]-6-[[[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]oxane-3,4,5-triol	up		neg_1613	oxohexyl)amino]pentanoic acid	down
	pos_867	7-Cyano-7-carbaguanine	up		pos_1633	yl]oxymethyl]oxane-3,4,5-triol	down		neg_1637	PS(14:0/18:0) 3,4-Dihydro-1-methoxy-2-methylene-3-oxo-2H-1,4-benzoxazine-5-carboxylic acid	down
	pos_6255	1,2-dihydroxyheptadec-16-yn-4-yl acetate	up		pos_5473	Deoxyguanidinoproclavaminic acid	up		pos_1035	acid	down
	pos_6433	N6-(L-1,3-Dicarboxypropyl)-L-lysine	up		pos_6255	1,2-dihydroxyheptadec-16-yn-4-yl acetate	down		pos_1044	Difluorodeoxyuridine	down
	pos_7177	3-Dehydroshikimate	down		pos_6433	N6-(L-1,3-Dicarboxypropyl)-L-lysine	down		pos_1045	Methylcysteine	down
										2-Methyl-2-[(1-oxo-2-propenyl)amino]-	
	pos_7169	Precorin 6Y	down		pos_7088	Citrinin	up		pos_1077	1-propanesulfonic acid	up
	pos_5473	Deoxyguanidinoproclavaminic acid	down		pos_7168	Avizafone	up		pos_1229	Rhizoctin C	down
	neg_1993	5-Methoxytryptamine	down		pos_7169	Precorin 6Y	up		pos_5346	3-hydroxy-C10-homoserine lactone	up
	pos_7173	Sialyllacto-N-tetraose a	down		pos_7173	Sialyllacto-N-tetraose a	up		pos_6245	7-Methylxanthine	down
	pos_7168	Avizafone	down		pos_7177	3-Dehydroshikimate	up		pos_6635	5,6,7,8-Tetrahydromonapterin	up
	pos_7088	Citrinin (2R,3R,4S,5S,6R)-2-[[1,1,1-tris(4-hydroxyphenyl)heptan-3-yloxy]-6-[[[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]oxane-3,4,5-triol	down		pos_806	UDP-4-dehydro-6-deoxy-D-glucose	down		pos_7067	1-(2-Furyl)butan-3-one	up
	pos_1633	yl]oxymethyl]oxane-3,4,5-triol	up		pos_867	7-Cyano-7-carbaguanine	down		pos_7100	alpha-1,5-L-Arabinobiose	up
	neg_2037	S-Methyl hexadecanethioate	up		neg_1313	2-Octynoic acid	down		pos_7126	Desisobutyrylciclesonide	up
	neg_2057	Mevastatin	up		neg_1410	C75	down		pos_7165	Tunicamycin VI (Z)-2-[(2R,3S,4S)-4-Hydroxy-2-[(1E)-3-hydroxyoct-1-enyl]oxan-3-yl]pent-3-enoic acid	down
									neg_1462	enoic acid	down
	neg_2141	(R)-3,4-Dihydro-8-hydroxy-3-tridecyl-1H-2-benzopyran-1-one	up		neg_1613	oxohexyl)amino]pentanoic acid	down		neg_1463	10-Deacetyl-2-debenzoylbaccatin III	down
	neg_2053	Taxa-4(20),11(12)-dien-5alpha,13alpha-diol	up		neg_1637	PS(14:0/18:0)	down				

neg_2060	Erinacine C	up
neg_2055	(±)13-HDoHE	up
neg_2231	11-Dehydro-thromboxane B2	up
neg_1923	PC(P-16:0/PGF2alpha)	up
neg_2258	CP 47,497-C8-homolog C-8-hydroxy metabolite	up
neg_1932	PE(20:3(6,8,11)-OH(5)/P-18:1(11Z))	up
neg_1927	(6Z,9Z,12Z)-Octadecatrienoic acid	up
pos_9740	Icosadienoic acid	up
neg_1680	Methyl octynecarboxylate	up
neg_2230	Siderol	up
neg_2118	PE-NMe2(18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))	up
pos_8991	1,2-dihydroxyheptadec-16-en-4-yl acetate	up
neg_2229	PC(P-18:0/PGF1alpha)	up
neg_2115	PE(22:1(13Z)/6 keto-PGF1alpha)	up
neg_2158	8(S)-HETrE	up
pos_9088	(5Z,8Z,11Z,14Z,17Z)-Icosapentaenoic acid	up
neg_2088	Eicosapentaenoic acid	up
neg_1930	1-(3-Methylbutanoyl)-6-epiosylglucose	up
neg_1931	14-Fluoro-6-thiaheptadecanoic acid	up
pos_9302	DEHYDROCHOLIC ACID	up
pos_9335	19(S)-HETE	up
pos_9416	prostaglandin a1 ethyl ester	up
neg_2114	PE(20:1(11Z)/20:3(5Z,8Z,11Z))	up
pos_9091	17-Hydroxymethylthisterone	up
neg_2101	Deoxyloganin	up
neg_1988	13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid	up
neg_1986	13(S)-HODE	up
neg_1985	Hexadecanoic acid	up
neg_2086	Dihydroactinidiolide	up
pos_9090	(+)-Camphor	up
pos_9082	L-2-Aminoadipate 6-semialdehyde	up
neg_1922	11,12,13-Trinor-1(10)-spirovetivene-2,7-dione	up
pos_9085	D-Lysopine	up
pos_9279	(-)-Amijiol	up
pos_2181	Aeruginosin 98-B	up
pos_1920	Carmofur	up
neg_2008	3alpha,7alpha,12beta-Trihydroxy-5beta-cholanoic	up
pos_8155	9-OxoODE	up
pos_7672	Lucidenic acid D1	down
neg_2143	N-Lauroyl Asparagine	up
pos_1033	S-(3-Oxo-3-carboxy-n-propyl)cysteine	up
neg_2106	all-trans-4-Hydroxyretinoic acid	up
pos_2173	6,7-Didehydrofevicordin F 3-[glucosyl-(1->6)-glucoside]	up
neg_1463	10-Deacetyl-2-debenzoylbaccatin III	up
neg_1462	(Z)-5-[(2R,3S,4S)-4-Hydroxy-2-[(E)-3-hydroxyoct-1-enyl]oxan-3-yl]pent-3-enoic acid	up
pos_2158	20-Hydroxy leukotriene E4	up
neg_1464	Decitabine	up
neg_1486	Dhesn	up
pos_7178	Dodecylbenzene	up
pos_7184	Sphingosine-1-phosphate	up
pos_1376	alpha-D-Sedoheptulopyranose 7-phosphate	up
neg_1817	5(S)-HPETE	up
neg_1684	5b-Cyprinol sulfate	down
neg_2019	PE(20:1(11Z)/16:0)	up
neg_521	dTDP	up
neg_2108	PC(P-16:0/PGE1)	up

pos_1035	3,4-Dihydro-7-methoxy-2-methylene-3-oxo-2H-1,4-benzoxazine-5-carboxylic acid	down
pos_1044	Difluoro deoxyuridine	down
pos_1045	Methylcysteine	down
pos_1077	3-Ethyl-4-(9-hydroxy-4,6,8,10-tetramethyl-7-oxododec-4-en-2-yl)oxetan-2-one	up
pos_1229	Rhizoctacin C	down
pos_5346	3-hydroxy-C10-homoserine lactone	up
pos_6245	7-Methylxanthine	down
pos_6635	5,6,7,8-Tetrahydromonapterin	up
pos_7067	1-(2-Furyl)butan-3-one	up
pos_7100	alpha-1,5-L-Arabinobiose	up
pos_7126	Desisobutrylciclesonide	up
pos_7165	Tunicamycin VI	up
neg_1386	C07493	up
neg_1452	Pinometostat	up
neg_1568	1-Nonen-3-ol	up
neg_1576	Pravastatin	up
neg_1618	Propofol glucuronide	down
neg_1654	2,3-Dinor-8-iso prostaglandin F2alpha	up
neg_1731	C16500	down
neg_1809	PS(22:5(4Z,7Z,10Z,13Z,16Z)/22:2(13Z,16Z))	up
neg_1818	C11134	up
neg_2216	C11999	down
neg_2236	C11961	up
neg_2270	6-Phenylhexyl isothiocyanate	up
neg_2339	Thromboxane B2	up
neg_2607	Filipin II	up
neg_2786	(S)-6-Hydroxynicotine	up
neg_656	Ethyl beta-D-glucopyranoside	down
neg_680	Aflatoxin B1 diol	down
pos_1024	4-Thialysine	down
pos_10639	Avermectin B1b monosaccharide	up
pos_10694	PC(16:0/20:5(5E,8E,11E,14E,17E))[U]	up
pos_11492	PC(14:0/20:2(11Z,14Z))	up
pos_1167	GDP-4-dehydro-6-deoxy-D-mannose	up
pos_4174	1-Guanidino-1-deoxy-scylo-inositol 4-phosphate	up
pos_5597	gamma-Aminobutyryllysine	up
pos_5602	Decarbamoylsaxitoxin	up
pos_5606	Cervonoyl ethanolamide	up
pos_5630	1-Deoxy-11beta-hydroxypentalenate	up
pos_6395	N-Arachidonyl dopamine	up
pos_6587	Hexadecanedioic acid mono-L-carnitine ester	down
pos_6718	LysoPC 16-2	down
pos_6745	N-Docosahexaenoyl Lysine	up
pos_6746	Miltefosine	up
pos_7061	Cilengitide	up
pos_7074	Hydrocinnamic acid	up
pos_7076	alpha-Methylstyrene	up
pos_7077	L-Fucono-1,5-lactone	up
pos_7078	(4-Methylphenyl)acetaldehyde	up
pos_7098	2'-O-methyladenosine	up
pos_7099	L-4-Hydroxyglutamate semialdehyde	up
pos_7104	Cicaprost	up
pos_7134	Casokefamide	up
pos_7136	Diacetazotol	up
pos_7161	Pristinamycin IA	up
pos_7216	3-O-Acetylpisamarcandin	up

neg_1464	Decitabine	down
neg_1486	Dhesn	down
neg_1680	Methyl octynecarboxylate	down
neg_1922	11,12,13-Trinor-1(10)-spirovetivene-2,7-dione	down
neg_1923	PC(P-16:0/PGF2alpha)	down
neg_1927	(6Z,9Z,12Z)-Octadecatrienoic acid	down
neg_1930	1-(3-Methylbutanoyl)-6-epiosylglucose	down
neg_1931	14-Fluoro-6-thiaheptadecanoic acid	down
neg_1932	PE(20:3(6,8,11)-OH(5)/P-18:1(11Z))	down
neg_1985	Hexadecanoic acid	down
neg_1986	13(S)-HODE	down
neg_1988	13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid	down
neg_2008	3alpha,7alpha,12beta-Trihydroxy-5beta-cholanoic acid	down
neg_2037	S-Methyl hexadecanethioate	down
neg_2053	1axa-4(20),11(12)-dien-5alpha,13alpha-diol	down
neg_2055	(±)13-HDoHE	down
neg_2057	Mevastatin	down
neg_2060	Erinacine C	down
neg_2086	Dihydroactinidiolide	down
neg_2088	Eicosapentaenoic acid	down
neg_2101	Deoxyloganin	down
neg_2106	all-trans-4-Hydroxyretinoic acid	down
neg_2114	PE(20:1(11Z)/20:3(5Z,8Z,11Z))	down
neg_2115	PE(22:1(13Z)/6 keto-PGF1alpha)	down
neg_2118	NMe2(18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))	down
neg_2141	(R)-3,4-Dihydro-8-hydroxy-3-tridecyl-1H-2-benzopyran-1-one	down
neg_2143	N-Lauroyl Asparagine	down
neg_2158	8(S)-HETrE	down
neg_2229	PC(P-18:0/PGF1alpha)	down
neg_2230	Siderol	down
neg_2231	11-Dehydro-thromboxane B2	down
neg_2258	CP 47,497-C8-homolog C-8-hydroxy metabolite	down
pos_1033	S-(3-Oxo-3-carboxy-n-propyl)cysteine	down
pos_1920	Carmofur	down
pos_2158	20-Hydroxy leukotriene E4	down
pos_2173	6,7-Didehydrofevicordin F 3-[glucosyl-(1->6)-glucoside]	down
pos_2181	Aeruginosin 98-B	down
pos_7672	Lucidenic acid D1	up
pos_8155	9-OxoODE	down
pos_8991	1,2-dihydroxyheptadec-16-en-4-yl acetate	down
pos_9082	L-2-Aminoadipate 6-semialdehyde	down
pos_9085	D-Lysopine	down
pos_9088	(5Z,8Z,11Z,14Z,17Z)-Icosapentaenoic acid	down
pos_9090	(+)-Camphor	down
pos_9091	17-Hydroxymethylthisterone	down
pos_9279	(-)-Amijiol	down
pos_9302	DEHYDROCHOLIC ACID	down
pos_9335	19(S)-HETE	down
pos_9416	prostaglandin a1 ethyl ester	down
pos_9740	Icosadienoic acid	down
neg_1267	2-(7'-Methylthio)heptylmalic acid	up
neg_1358	C05964	down
neg_1449	C20760	down
neg_1548	(-)-alpha-Bisabolol	down
neg_1860	Ouabain	up
neg_2271	C16506	down

pos_1375	2-epi-5-epi-Valiolone 7-phosphate	up	pos_7311	(2S)-2-Hydroxyhexadecanoylcarnitine	down	neg_595	(R)-2-(4-(1-tert-butoxycarbonyl)morpholin-3-yl)acetic acid	down
neg_522	6-Thioxanthine 5'-monophosphate	up	pos_7354	Digitoxigenin 3-[glucosyl-(1->6)-glucosyl-(1->4)-	up	neg_977	5-Phosphooxy-L-lysine	up
neg_2096	(±)16-HETE	up	pos_7488	2,6-dideoxyribohexoside]	up	neg_979	Cytosine	up
neg_1268	Taurocholate	down	pos_7620	L-Leucine	down	neg_980	1-(5'-Phosphoribosyl)-5-amino-4-imidazolecarboxamide	up
neg_1498	(3beta,5alpha,6beta,7alpha,22E,24R)-Ergosta-8,22-diene-3,5,6,7-tetrol	up	pos_7701	Linoelaidylcarnitine	down	pos_1018	Pindolol	down
neg_1629	geranate	up	pos_776	Cholyltyrosine	down	pos_1020	N-Formyl-L-aspartate	down
neg_1869	PC(P-18:0/PGE2)	up	pos_7915	(1R)-Hydroxy-(2R)-N-acetyl-L-cysteinyl-1,2-dihydronaphthalene	down	pos_1046	4-Hydroxy-6-methyl-3-(1H-pyrazol-3-yl)-2H-pyran-2-one	up
neg_1668	Trypanothione disulfide	down	pos_8118	Diaminobutyric acid	up	pos_1051	2-Phenylethanol glucuronide	down
neg_576	5-Fluorodeoxyuridine	up	pos_8229	Methyl jasmonate	down	pos_1056	lys-met	down
neg_875	Azamethiphos	up	pos_8621	G-418	down	pos_1078	Phensuximide	up
neg_881	5-Methoxytryptophan	up	pos_960	Docosanoic acid	up	pos_2727	DG(a-25:0/LTE4(0:0))	up
				Formyl-5-hydroxykynurenamine	down		2-enoyl]oxy-2-methyl-5-[2-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyethylidene]cyclopentene-1-carboxylic acid	down
neg_1683	Bardoxolone methyl	down	pos_969	1-(5'-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide	down	pos_5214	carboxylic acid	down
pos_1916	Timolol	up				pos_5314	Capecitabine	down
pos_781	Uric acid	up				pos_6312	APC	up
neg_2102	DG(2:0/18:2(10E,12Z))+O(9)/0:0)	up					2-[2-[(3,5-Dimethyl-1H-pyrrrol-2-yl)methylidene]-4-methoxy-2-pyrrolylidene]indole	down
neg_1882	PS(20:4(6E,8Z,11Z,14Z))+O(5)/22:0)	up				pos_6367	pyrrolylidene]indole	down
						pos_6881	Hydroxyhomodestruxin B	down
neg_2042	PC(15:0/P-16:0)	up					1-[[[1-(2S)-1-[[[1-(2S)-1-[[[1-(2S)-1-oxopropan-2-yl]amino]-3-naphthalen-2-yl]-1-oxopropan-2-yl]-N'-hydroxy-2-(2-methylpropyl)butanediamide	up
pos_4789	Coenzyme F420	up				pos_7696	4a-Hydroxytetrahydrobiopterin	up
neg_1609	Undecylprodigiosin	up						
neg_1915	16-hydroxy hexadecanoic acid	up						
neg_1881	PE(P-18:0/PGE2)	up						
neg_2405	(7Z,10Z,13Z,16Z,19Z)-Docosapentaenoic acid	up						
neg_508	Pseudouridine 5'-phosphate	up						
neg_1360	Bilirubin	up						
neg_737	3-Maleimidobenzoic acid N-hydroxysuccinimide ester	down						
pos_10477	cis-3-Hexenyl b-primeveroside	down						
neg_640	D-Glucose	up						
pos_778	2-Pyrone-4,6-dicarboxylate	up						
pos_7441	7alpha,27-Dihydroxycholesterol	down						
pos_7605	phe-ile-gly	down						
pos_9402	5-Oxoavermectin "1a" aglycone	down						
neg_738	Aldotetrauronic acid	down						
neg_1286	C01056	up						
neg_518	2-Methylpropyl glucosinolate	down						
pos_733	5-Hydroxymethyluridine	up						
	[(2R,3S,4S,5R,6S)-3,4,5-trihydroxy-6-[(1E)-3-phenylprop-2-enoyl]oxyoxan-2-yl]methyl 3,4-dihydroxy-2-methylidenobutanoate	down						
pos_1190	dihydroxy-2-methylidenobutanoate	down						
pos_1602	Apramycin	up						
pos_8712	Cucurbitacin C	up						
pos_9100	trans,trans-Farnesyl phosphate	down						
neg_1515	LysoPC(P-16:0/0:0)	up						
neg_733	5-L-Glutamyl-taurine	down						
pos_2070	Sphinganine 1-phosphate	down						
neg_1118	3"-Oxoribostamycin	up						
pos_1693	Verruculogen	up						
pos_1188	CMP-2-aminoethylphosphonate	down						
pos_1714	Gly-Trp-Gly	up						
pos_1166	Tilisolol	up						
neg_1488	Penitrem B	up						
pos_2215	Levanbiose	up						
pos_5617	Versicotide C	down						
pos_5555	3-Amino-4-(3-hexylphenylamino)-4-oxobutylphosphonic acid	down						

pos_829	Xanthine	up
neg_749	UDP-3-O-(3-hydroxytetradecanoyl)-D-glucosamine	down
pos_7462	6"-Deamino-6"-oxoparomomycin II	down