

Supplementary Table 1 - Metabolomics Report Extended

[illegible]

377	en Zaan	015545	Other	5.13E-05	5.39E-05	5.33E-05	5.42E-05	5.39E-05	5.21E-05	1.24E-05	1.27E-05	1.0	2.4	1.5
378	2-Pyridylmethanol	015546	Other	5.13E-05	5.39E-05	5.33E-05	5.42E-05	5.39E-05	5.21E-05	1.24E-05	1.27E-05	1.0	2.4	1.5
379	2-Pyridylmethanol	015547	Other	5.13E-05	5.39E-05	5.33E-05	5.42E-05	5.39E-05	5.21E-05	1.24E-05	1.27E-05	1.0	2.4	1.5
380	6-Undecyloxy-2,3-bis(methylthio)hexan-3-ol	015548	Other	5.13E-05	5.39E-05	5.33E-05	5.42E-05	5.39E-05	5.21E-05	1.24E-05	1.27E-05	1.0	2.4	1.5
381	6-Undecyloxy-2,3-bis(methylthio)hexan-3-ol	015549	Other	5.13E-05	5.39E-05	5.33E-05	5.42E-05	5.39E-05	5.21E-05	1.24E-05	1.27E-05	1.0	2.4	1.5
382	Propane-1,2-diol	015550	Other	7.88E-04	8.15E-04	8.15E-04	7.88E-04	7.81E-04	6.92E-04	7.64E-04	6.92E-04	1.0	1.5	1.0
383	Methylvinylcarbazole	015551	Other	2.44E-04	2.58E-04	2.62E-04	2.44E-04	2.43E-04	6.98E-05	4.71E-05	1.78E-04	1.0	1.5	1.0
384	2-Methylpentane	015552	Other	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.0	1.5	1.0
385	2-Deoxy-alpha-D-glucopyranose	015553	Other	4.92E-04	1.05E-04	1.05E-04	1.27E-05	8.13E-05	2.13E-05	4.87E-05	4.87E-05	1.0	1.5	1.0
386	2-Deoxy-beta-D-glucopyranose	015554	Other	4.92E-04	1.11E-04	7.51E-04	4.92E-04	4.92E-04	4.21E-04	4.73E-04	6.81E-04	1.0	1.5	1.0
387	N-oxyl-2,2,6,6-tetramethylpiperidine	015555	Other	2.07E-03	1.33E-03	0.95E-03	2.07E-03	3.11E-03	5.92E-03	5.92E-03	5.92E-03	1.0	1.5	1.0
388	NH-Methyl-L-lysine	015556	Other	4.98E-05	4.98E-05	4.88E-05	4.98E-05	4.98E-05	3.97E-05	4.88E-05	4.28E-05	1.0	1.5	1.0
389	Mucic acid	015557	Other	3.38E-04	3.31E-04	2.11E-04	2.18E-04	2.18E-04	2.18E-04	2.20E-04	2.21E-04	1.0	1.5	1.0
390	Octan-2-ol	015558	Other	3.03E-05	1.97E-05	3.51E-05	2.28E-05	3.11E-05	3.52E-05	3.42E-05	3.42E-05	1.0	1.5	1.0
391	1,7-Annulene	015559	Other	4.07E-05	4.33E-05	5.61E-05	5.55E-05	5.57E-05	6.53E-05	1.18E-05	1.32E-05	1.0	1.5	1.0
392	1,7-Annulene	015560	Other	4.07E-05	4.33E-05	5.61E-05	5.55E-05	5.57E-05	6.53E-05	1.18E-05	1.32E-05	1.0	1.5	1.0
393	1-Phenyl-2-methylpropan-1-ol	015561	Other	3.38E-04	3.31E-04	2.11E-04	2.18E-04	2.18E-04	2.18E-04	2.20E-04	2.21E-04	1.0	1.5	1.0
394	Thiophene	015562	Other	1.38E-05	1.43E-05	1.48E-05	1.37E-05	1.59E-05	7.51E-05	6.41E-04	6.41E-04	1.0	1.5	1.0
395	Methanol	015563	Other	1.01E-05	1.11E-05	1.11E-05	1.11E-05	1.11E-05	1.11E-05	1.00E-05	1.00E-05	1.0	1.5	1.0
396	8-Hydroxy-2-hexadecanoic acid	015564	Other	6.77E-04	5.98E-04	4.43E-04	6.98E-04	1.67E-05	1.68E-05	9.48E-04	9.48E-04	1.0	1.5	1.0
397	Galactol	015565	Other	6.32E-05	7.48E-05	4.28E-05	2.23E-04	6.24E-05	4.21E-05	1.08E-04	1.08E-04	1.0	1.5	1.0
398	Calcitriol	015566	Other	1.17E-04	2.37E-04	2.65E-04	1.53E-04	3.05E-04	4.05E-04	6.11E-04	5.45E-04	1.0	1.5	1.0
399	Peris decanoate	015567	Other	6.98E-04	6.98E-04	7.98E-04	6.98E-04	6.98E-04	5.94E-05	1.43E-05	1.43E-05	1.0	1.5	1.0
400	Euphorbia	015568	Other	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.07E-04	2.01E-05	1.00E-05	1.00E-05	1.0	1.5	1.0
401	Sodium decanoate	015569	Other	2.03E-05	2.52E-05	2.37E-05	2.03E-05	1.65E-04	5.95E-04	4.97E-04	1.98E-04	1.0	1.5	1.0
402	Galactol	015570	Other	1.48E-05	1.55E-05	1.88E-05	1.78E-05	1.67E-05	6.95E-04	1.92E-05	1.92E-05	1.0	1.5	1.0
403	6-Tetradecenoic acid	015571	Other	1.48E-05	1.55E-05	1.88E-05	1.78E-05	1.67E-05	6.95E-04	1.92E-05	1.92E-05	1.0	1.5	1.0
404	Decanoic acid	015572	Other	2.33E-04	2.25E-04	2.25E-04	2.33E-04	2.33E-04	2.33E-04	2.33E-04	2.33E-04	1.0	1.5	1.0
405	D-Ribose-5-phosphate	015573	Other	1.68E-05	1.43E-05	1.43E-05	1.43E-05	1.68E-05	1.68E-05	1.68E-05	5.95E-04	1.0	1.5	1.0
406	Galactol	015574	Other	1.95E-05	1.84E-05	1.84E-05	1.95E-05	1.95E-05	1.95E-05	1.95E-05	1.95E-05	1.0	1.5	1.0
407	Galactol	015575	Other	6.77E-04	3.11E-04	6.97E-04	2.14E-03	6.10E-04	1.17E-04	1.18E-04	1.18E-04	1.0	1.5	1.0
408	Glucosamine	015576	Other	1.44E-05	0.98E-05	8.18E-05	2.23E-03	4.08E-03	2.23E-03	3.08E-03	3.08E-03	1.0	1.5	1.0
409	Decanoic acid	015577	Other	1.68E-05	1.43E-05	1.43E-05	1.43E-05	1.68E-05	1.68E-05	1.68E-05	1.68E-05	1.0	1.5	1.0
410	D-Ribose-5-phosphate	015578	Other	1.33E-05	1.33E-05	1.33E-05	1.33E-05	1.33E-05	1.33E-05	1.33E-05	1.33E-05	1.0	1.5	1.0
411	Thiophene diethyl	015579	Other	4.92E-04	7.18E-04	7.18E-04	3.13E-04	2.59E-04	1.24E-04	1.23E-04	1.41E-04	1.0	1.5	1.0
412	alpha-Hydroxy-L-glutamic acid	015580	Other	4.92E-04	5.95E-04	1.51E-05	7.63E-04	5.95E-04	5.92E-04	5.92E-04	5.92E-04	1.0	1.5	1.0
413	D-Alanyl-alanine	015581	Other	5.32E-04	5.32E-04	5.32E-04	5.32E-04	5.32E-04	7.67E-04	7.13E-04	6.45E-04	1.0	1.5	1.0
414	alpha-Hydroxy-L-glutamic acid	015582	Other	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E-04	2.20E-05	1.00E-05	1.0	1.5	1.0
415	Galactol	015583	Other	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E-04	2.20E-05	1.00E-05	1.0	1.5	1.0
416	2-Acetylthiophene	015584	Other	1.03E-05	6.32E-05	7.54E-05	3.20E-05	7.43E-04	2.34E-04	5.14E-05	7.14E-05	1.0	1.5	1.0
417	2-Acetylthiophene	015585	Other	1.03E-05	6.32E-05	7.54E-05	3.20E-05	7.43E-04	2.34E-04	5.14E-05	7.14E-05	1.0	1.5	1.0
418	Galactol	015586	Other	6.98E-04	6.98E-04	7.98E-04	6.98E-04	6.98E-04	5.94E-05	1.43E-05	1.43E-05	1.0	1.5	1.0
419	Prothionamide	015587	Other	1.08E-04	1.07E-04	1.08E-04	1.44E-04	1.08E-04	5.95E-04	3.27E-04	3.27E-04	1.0	1.5	1.0
420	8-Hydroxyoctanoic acid	015588	Other	6.92E-04	1.01E-04	7.92E-04	1.54E-05	1.07E-05	1.07E-05	1.04E-05	1.04E-05	1.0	1.5	1.0
421	N-Amino-L-lysine	015589	Other	1.18E-05	1.18E-05	1.18E-05	1.18E-05	6.67E-04	1.05E-05	2.64E-05	2.64E-05	1.0	1.5	1.0
422	Diethyl-2-hydroxy-L-glutamate	015590	Other	6.92E-04	7.92E-04	7.92E-04	7.92E-04	6.61E-05	6.61E-05	7.91E-05	6.89E-05	1.0	1.5	1.0
423	N-oxyl-2,2,6,6-tetramethylpiperidine	015591	Other	1.75E-05	1.85E-05	1.85E-05	2.15E-04	3.15E-04	3.15E-04	3.15E-04	3.15E-04	1.0	1.5	1.0
424	N-Methyl-L-lysine	015592	Other	6.95E-04	6.95E-04	7.95E-04	6.95E-04	6.95E-04	5.94E-05	1.43E-05	1.43E-05	1.0	1.5	1.0
425	Decanoic acid	015593	Other	2.14E-05	0.00E+00	0.00E+00	0.00E+00	3.68E-03	2.02E-03	2.02E-03	2.48E-03	1.0	1.5	1.0
426	Propanoic acid	015594	Other	2.05E-05	2.15E-05	2.15E-05	2.05E-05	2.05E-05	2.05E-05	2.05E-05	2.05E-05	1.0	1.5	1.0
427	Hydroxyacetone phosphate	015595	Other	2.14E-05	2.14E-05	2.14E-05	2.14E-05	2.14E-05	1.79E-05	1.51E-05	1.51E-05	1.0	1.5	1.0
428	N-Methyl-L-lysine	015596	Other	6.95E-04	6.95E-04	7.95E-04	6.95E-04	6.95E-04	5.94E-05	1.43E-05	1.43E-05	1.0	1.5	1.0
429	Galactol	015597	Other	6.98E-04	6.98E-04	7.98E-04	6.98E-04	6.98E-04	5.94E-05	1.43E-05	1.43E-05	1.0	1.5	1.0
430	N-Acetylthiophene	015598	Other	4.53E-05	3.32E-05	6.18E-05	1.50E-04	1.50E-04	6.98E-04	2.68E-04	2.68E-04	1.0	1.5	1.0
431	Diethyl-2-hydroxy-L-glutamate	015599	Other	6.92E-04	7.92E-04	7.92E-04	7.92E-04	6.61E-05	6.61E-05	7.91E-05	6.89E-05	1.0	1.5	1.0
432	7-Bis(methylthio)hexan-3-ol	015600	Other	6.41E-03	3.88E-03	3.11E-03	3.03E-03	1.11E-04	1.08E-04	0.00E+00	1.13E-04	1.0	1.5	1.0
433	10-Hydroxydecanoic acid	015601	Other	2.87E-04	3.61E-04	5.49E-04	1.49E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.0	1.5	1.0
434	Diethyl-2-hydroxy-L-glutamate	015602	Other	1.75E-05	1.85E-05	1.85E-05	1.75E-05	1.85E-05	1.85E-05	1.85E-05	1.85E-05	1.0	1.5	1.0
435	trans-Hydroxyoctanoic acid	015603	Other	2.38E-05	2.38E-05	2.47E-05	2.38E-05	4.73E-05	4.44E-05	2.13E-05	2.62E-05	1.0	1.5	1.0
436	Decanoic acid	015604	Other	6.82E-05	4.31E-04	3.68E-04	1.49E-04	4.60E-04	4.14E-04	1.97E-04	2.44E-04	1.0	1.5	1.0
437	N-Octanoic-L-glutamic acid	015605	Other	1.68E-05	1.74E-05	1.65E-05	1.68E-05	1.11E-05	1.16E-05	1.17E-05	1.17E-05	1.0	1.5	1.0
438	2-Oxo-7-methylthiohexanoic acid	015606	Other	1.48E-05	1.55E-05	1.55E-05	1.48E-05	6.86E-05	7.88E-05	2.23E-05	1.95E-05	1.0	1.5	1.0
439	L-Hydroxyoctanoic acid	015607	Other	1.48E-05	1.55E-05	1.55E-05	1.48E-05	6.86E-05	7.88E-05	2.23E-05	1.95E-05	1.0	1.5	1.0
440	N-Octanoic-L-glutamic acid	015608	Other	1.68E-05	1.74E-05	1.65E-05	1.68E-05	1.11E-05	1.16E-05	1.17E-05	1.17E-05	1.0	1.5	1.0