Supplementary Information

NOVEL APPROACHES TO TOXICITY TESTING IN *DAPHNIA MAGNA*

by

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A thesis submitted to
The University of Birmingham
for the degree of
DOCTOR OF PHILOSOPHY

School of Biosciences
The University of Birmingham
March 2010

Table SI1. List of putative metabolite identities for polar extracts of *D. magna* neonates exposed to varying copper concentrations analysed in negative ion mode (chapter 3).

Empirical formula	Metabolite name [a]	Ion form	Observed mass (Da)	Theoretical mass (Da)	Absolute mass error (ppm)	Fold change [b]	*p*-value [c]	Significance [d]
HSO3	HSO3-	[M-H]-	79.95736	79.95737	0.070	0.03258	2.51167	
HSO3		[M+e]-	80.96519	80.96519	0.007	0.0173	2.00138	
HNO2	Nitrite	[M+^{35}Cl]-	81.97013	81.97013	0.007	0.02665	1.83226	
H2SO3	Sulfite	[M-H]-	80.96519	80.96519	0.007	0.0173	2.00138	
H2SO4	Sulfate	[M-H]-	96.96010	96.96011	0.058	0.03898	0.75177	
H2S4O6	Tetrathionate	[M+^{37}Cl]-	262.83974	262.83988	0.531	0.04647	0.99287	
PH3O3	Phosphonate	[M+Ac]-	140.99582	140.99584	0.118	0.02384	1.18875	
HO3Cl	Chlorate	[M+Ac]-	142.97521	142.97528	0.466	0.04298	0.93891	
CH2O2	Formate	[M+^{37}Cl]-	82.97193	82.97193	0.019	0.02677	1.49285	
CH3NO	Formamide	[M+^{39}K-2H]-	81.97013	81.97007	0.725	0.03348	1.35629	
CH3NO		[M+Ac]-	104.03532	104.03532	0.023	0.02804	0.83808	
C2H3ClO2	Chloroacetic acid	[M+Ac]-	152.99599	152.99601	0.141	0.02331	0.70344	
C2H4O	Acetaldehyde(2)	[M+Ac]-	103.04006	103.04007	0.083	0.01331	0.81693	
C2H4O2	Acetate(2)	[M+^{37}Cl]-	96.98758	96.98758	0.016	0.02477	0.7947	
C2H4O2	Acetate(2)	[M+Ac]-	119.03498	119.03498	0.030	0.02585	1.54541	

C3H4O3	Pyruvate(3)	[M-H]-	87.00877	87.00877	0.016	0.00917	1.34198	
C3H4O3		[M+Ac]-	147.02991	147.02990	0.078	0.00857	0.98878	
C3H5O5P	3-(Hydrohydroxyphosphoryl) pyruvate	[M+Ac]-	211.00133	211.00132	0.064	0.02744	0.78177	
C3H5NO2	2-Aminoacrylate(2)	[M+Ac]-	146.04588	146.04588	0.018	0.00597	0.6463	
C3H6O2S	S-Methylthioglycolate	[M+^{37}Cl]-	142.97521	142.97530	0.655	0.04298	0.93891	
C3H6O3	Glycerone(8)	[M+Ac]-	149.04553	149.04555	0.125	0.03262	1.01517	
C3H6O4	D-Glycerate	[M+^{39}K-2H]-	142.97521	142.97522	0.046	0.04298	0.93891	
C3H6ClNO2	3-Chloro-D-alanine(2)	[M+Ac]-	182.02257	182.02256	0.052	0.00218	0.5435	*
C3H7NO2	L-Alanine(8)	[M-H]-	88.04041	88.04040	0.084	0.01648	0.88921	
C3H7NO2		[M+Ac]-	148.06151	148.06153	0.153	0.01677	0.87141	
C3H7NO3	L-Serine(3)	[M-H]-	104.03532	104.03532	0.023	0.02804	0.83808	
C3H8O3	Glycerol	[M+Ac]-	151.06119	151.06120	0.057	0.04874	1.05764	
C3H8NO6P	O-Phospho-L-serine(2)	[M+Ac]-	244.02291	244.02278	0.530	0.00064	0.41877	*
C3H9O4P	2-Hydroxypropylphosphonate	[M+Ac]-	199.03772	199.03770	0.092	0.03801	1.17911	
C3H9O6P	sn-Glycerol 3-phosphate(4)	[M+Na-2H]-	192.98833	192.98835	0.086	0.03037	0.52374	
C3H10NO3P	N-Monomethyl-2-aminoethylphosphonate	[M+Ac]-	198.05381	198.05369	0.628	0.01405	1.45599	
C3H10NO4P	N-Methylethanolamine	[M+Ac]-	214.04862	214.04860	0.091	0.03865	0.83763	

	phosphate(3)							
C4H4O5	Oxaloacetate(3)	[M+Ac]-	191.01971	191.01973	0.097	0.03675	0.5615	
C4H4N2O2	Uracil	[M-H]-	111.01998	111.02000	0.195	0.02881	0.82837	
C4H6O4	Succinate(3)	[M+^{35}Cl]-	152.99599	152.99601	0.141	0.02331	0.70344	
C4H6O4		[M+Ac]-	177.04046	177.04046	0.020	0.02894	1.0569	
C4H7NO2	1-Aminocyclopropane-1-carboxylate(5)	[M+Ac]-	160.06154	160.06153	0.046	0.00625	0.65257	
C4H8O2S	3-(Methylthio)propionic acid	[M+^{37}Cl]-	156.99088	156.99095	0.469	0.0126	0.72668	
C4H8O3	4-Hydroxybutanoic acid(7)	[M-H]-	103.04006	103.04007	0.083	0.01331	0.81693	
C4H8O4	D-Erythrose(4)	[M-H]-	119.03498	119.03498	0.030	0.02585	1.54541	
C4H8O4		[M+^{39}K-2H]-	156.99088	156.99087	0.085	0.0126	0.72668	
C4H8O4		[M+Ac]-	179.05611	179.05611	0.020	0.04393	1.26391	
C4H8O5	Threonate	[M+Ac]-	195.05104	195.05103	0.058	0.03381	1.2199	
C4H8N2O4	O-Carbamoyl-L-serine(2)	[M-H]-	147.04113	147.04113	0.011	0.02128	1.34775	
C4H9O7P	D-Erythrose 4-phosphate(4)	[M+Ac]-	259.02250	259.02245	0.206	0.01292	0.56928	
C4H9NO4	2-Hydroxymethylserine(2)	[M+Na-2H]-	156.02784	156.02783	0.079	0.04444	1.62606	
C4H10O2	(R,R)-Butane-2,3-diol(3)	[M+Ac]-	149.08194	149.08193	0.043	0.04596	1.07859	
C4H10NO6P	O-Phospho-L-homoserine(4)	[M+Ac]-	258.03845	258.03843	0.075	0.0042	0.65941	*
C4H11O4P	Diethylphosphoric acid	[M+^{35}Cl]-	189.00904	189.00890	0.743	0.0277	0.55548	

C4H11O4P		[M+Ac]-	213.05351	213.05335	0.743	0.02435	0.72123	
C4H12NO4P	Phosphodimethylethanolamine	[M+Ac]-	228.06440	228.06425	0.655	0.02401	0.79408	
C5H6O5	2-Oxoglutarate(4)	[M+Ac]-	205.03538	205.03538	0.007	0.02558	0.69336	
C5H8O3	3-Methyl-2-oxobutanoic acid(4)	[M+^{39}K-2H]-	152.99599	152.99595	0.251	0.02331	0.70344	
C5H8O4	Glutarate(8)	[M+Ac]-	191.05610	191.05611	0.071	0.01587	1.25056	
C5H8O5	D-Arabinono-1,4-lactone(18)	[M-H]-	147.02991	147.02990	0.078	0.00857	0.98878	
C5H8O5		[M+Ac]-	207.05104	207.05103	0.055	0.02723	0.86356	
C5H9NO2	L-Proline(3)	[M-H]-	114.05605	114.05605	0.023	0.00118	0.68914	*
C5H9NO3	5-Aminolevulinate(12)	[M+Ac]-	190.07205	190.07210	0.250	0.01755	1.41381	
C5H9NO3S	Acetylcysteine	[M+^{39}K-2H]-	199.97892	199.97892	0.013	0.04633	1.15393	
C5H9NO4	L-Glutamate(10)	[M-H]-	146.04588	146.04588	0.018	0.00597	0.6463	
C5H9NO4		[M+^{35}Cl]-	182.02257	182.02256	0.052	0.00218	0.5435	*
C5H10O	Prenol(5)	[M+Ac]-	145.08700	145.08702	0.128	0.03256	1.21153	
C5H10O4	Deoxyribose(6)	[M+Ac]-	193.07175	193.07176	0.070	0.02433	1.49269	
C5H10O5	D-Ribose(25)	[M-H]-	149.04553	149.04555	0.125	0.03262	1.01517	
C5H10O5		[M+^{35}Cl]-	185.02221	185.02223	0.090	0.01688	0.68911	
C5H10O5		[M+^{39}K-2H]-	187.00143	187.00143	0.009	0.02734	0.65305	
C5H10O5		[M+^{37}Cl]-	187.01926	187.01928	0.089	0.02484	0.70783	

C5H10O5		[M+Ac]-	209.06669	209.06668	0.055	0.02241	0.95461	
C5H10O6	D-Xylonate(5)	[M+Na-2H]-	187.02237	187.02241	0.206	0.04961	0.93683	
C5H10N2O2	Casein K(2)	[M+Ac]-	189.08807	189.08808	0.061	0.00727	0.61233	
C5H10N2O3	L-Glutamine(4)	[M-H]-	145.06186	145.06187	0.045	0.0278	0.8475	
C5H10N2O3		[M+^{35}Cl]-	181.03854	181.03854	0.025	0.00774	0.59933	
C5H10N2O3		[M+^{37}Cl]-	183.03554	183.03559	0.298	0.02509	0.6721	
C5H10N2O3		[M+Ac]-	205.08302	205.08300	0.114	0.04097	0.96079	
C5H11O7P	2-Deoxy-D-ribose 1-phosphate(4)	[M+Ac]-	273.03828	273.03810	0.672	0.01706	0.50081	
C5H11NO2	L-Valine(10)	[M+^{35}Cl]-	152.04838	152.04838	0.004	0.0246	1.17958	
C5H11NO2		[M+Ac]-	176.09284	176.09283	0.042	0.00916	1.68653	
C5H11NO2S	L-Methionine(4)	[M-H]-	148.04377	148.04377	0.031	0.00086	0.49729	*
C5H11NO2S		[M+^{37}Cl]-	186.01741	186.01750	0.498	0.00372	0.60663	*
C5H11NO3S	L-Methionine S-oxide(3)	[M+^{37}Cl]-	202.01234	202.01242	0.384	0.01962	0.78895	
C5H12O5	Ribitol(4)	[M-H]-	151.06119	151.06120	0.057	0.04874	1.05764	
C5H12O5		[M+^{35}Cl]-	187.03787	187.03788	0.035	0.04372	1.14292	
C5H12O5		[M+^{37}Cl]-	189.03489	189.03493	0.194	0.04521	1.26412	
C5H12O5		[M+Ac]-	211.08234	211.08233	0.054	9.7E-05	0.27984	*
C5H12O8P2	1-Hydroxy-2-methyl-2-butenyl 4-diphosphate	[M+^{39}K-2H]-	298.94947	298.94935	0.393	0.04385	0.80093	
C5H13O8P	D-Ribitol 5-phosphate(4)	[M+Na-2H]-	253.00953	253.00948	0.211	0.02416	0.82181	

C5H13O8P		[M+Ac]-	291.04866	291.04866	0.005	0.03054	1.45616	
C5H14NO6P	sn-glycero-3-Phosphoethanolamine	[M-H]-	214.04862	214.04860	0.091	0.03866	0.83763	
C5H15N4O3P	N4-Phosphoagmatine	[M+e]-	210.08870	210.08873	0.131	4.2E-05	0.31794	*
C6H6O2S	Thien-2-ylacetate	[M+Ac]-	201.02274	201.02271	0.171	0.00985	0.8016	
C6H6O5S	3-Sulfocatechol(2)	[M-H]-	188.98633	188.98632	0.050	0.03647	1.19332	
C6H6O6	cis-Aconitate(3)	[M-H]-	173.00911	173.00916	0.310	0.00429	0.66635	*
C6H6O6		[M+^{35}Cl]-	208.98584	208.98584	0.008	0.01582	0.40374	
C6H6O6		[M+^{37}Cl]-	210.98287	210.98289	0.102	0.01239	0.50478	
C6H6N2O	Nicotinamide(3)	[M+Ac]-	181.06187	181.06187	0.019	0.02581	0.917	
C6H8O7	Citrate(9)	[M-H]-	191.01971	191.01973	0.097	0.03676	0.5615	
C6H8N2O2	Methylimidazoleacetic acid(2)	[M+Ac]-	199.07243	199.07243	0.008	0.00713	0.74918	
C6H9N2O5P	3-(Imidazol-4-yl)-2-oxopropyl phosphate	[M+Ac]-	279.03896	279.03876	0.700	0.00747	0.40671	
C6H9N3O2	L-Histidine(4)	[M-H]-	154.06219	154.06220	0.069	0.00456	0.58364	*
C6H9N3O2		[M+^{35}Cl]-	190.03887	190.03888	0.045	0.00131	0.28766	*
C6H9N5	N3-Metyladenine	[M+^{39}K-2H]-	188.03449	188.03440	0.470	0.04336	0.96686	
C6H10O2S	THAT (2-tetrahydrothiopheneacetic acid)	[M+Ac]-	205.05394	205.05401	0.320	0.01931	0.60249	

C6H10O3	4-Methyl-2-oxopentanoate(15)	[M+Ac]-	189.07685	189.07685	0.007	0.04178	0.99687	
C6H10O4	2-Aceto-2-hydroxybutanoate(11)	[M+Ac]-	205.07178	205.07176	0.080	0.02295	1.27249	
C6H10O5	Lichenin(18)	[M+^{35}Cl]-	197.02211	197.02223	0.592	0.03582	1.46381	
C6H10O5		[M+Ac]-	221.06669	221.06668	0.052	0.03602	1.12812	
C6H10O6	D-Glucono-1,5-lactone(19)	[M-H]-	177.04046	177.04046	0.020	0.02894	1.0569	
C6H10O6	D-Glucono-1,5-lactone(19)	[M+Na-2H]-	199.02240	199.02241	0.043	0.04839	0.97753	
C6H10NO4PS	4-Methyl-5-(2-phosphoethyl)-thiazole	[M+Ac]-	282.02048	282.02067	0.683	0.00411	0.57093	*
C6H10N2O2	Ectoine	[M+Ac]-	201.08811	201.08808	0.141	0	1.10166	
C6H11O8P	D-myo-Inositol 1,2-cyclic phosphate	[M-H]-	241.01205	241.01188	0.699	0.01841	0.40385	
C6H11NO2	L-Pipecolate(5)	[M+Ac]-	188.09283	188.09283	0.014	0.02912	1.10156	
C6H11NO3	Allysine(6)	[M+^{39}K-2H]-	182.02257	182.02250	0.381	0.00218	0.5435	*
C6H11NO3		[M+Ac]-	204.08774	204.08775	0.037	0.02117	1.20122	
C6H11NO4	L-2-Aminoadipate(7)	[M-H]-	160.06154	160.06153	0.046	0.00625	0.65257	
C6H11NO5	4-Hydroxy-4-methylglutamate	[M+^{35}Cl]-	212.03307	212.03313	0.262	0.00229	0.73973	*
C6H11NO5		[M+Ac]-	236.07756	236.07758	0.075	0.0055	0.46467	
C6H12O2	Hexanoic acid(6)	[M+Ac]-	175.09759	175.09758	0.037	0.04985	1.05448	

C6H12O4	(R)-Mevalonate(7)	[M+^{35}Cl]-	183.04297	183.04296	0.046	0.04587	1.26244	
C6H12O4		[M+^{39}K-2H]-	185.02221	185.02217	0.235	0.01688	0.68911	
C6H12O4S	5-Methylthio-D-ribose	[M+Ac]-	239.05965	239.05949	0.688	0.0455	0.98929	
C6H12O5	L-Rhamnose(19)	[M+Na-2H]-	185.04315	185.04314	0.035	0.01102	0.87036	
C6H12O5		[M+^{37}Cl]-	201.03495	201.03493	0.116	0.04747	1.10166	
C6H12O6	D-Glucose(41)	[M-H]-	179.05611	179.05611	0.020	0.04393	1.26391	
C6H12O6		[M+^{35}Cl]-	215.03282	215.03279	0.132	0.04383	1.42394	
C6H12O6		[M+^{37}Cl]-	217.02988	217.02984	0.177	0.04911	0.92243	
C6H12O6		[M+Ac]-	239.07724	239.07724	0.015	0.0405	1.16384	
C6H12O7	D-Gluconic acid(8)	[M-H]-	195.05104	195.05103	0.058	0.03383	1.2199	
C6H12N2O	L-Lysine 1,6-lactam(2)	[M+Ac]-	187.10881	187.10882	0.035	0.01224	0.52665	
C6H13O9P	D-Fructose 6-phosphate(38)	[M-H]-	259.02250	259.02245	0.206	0.01293	0.56928	
C6H13NO3	Fagomine	[M+Ac]-	206.10340	206.10340	0.012	0.02049	1.30893	
C6H13NO4	Deoxymannojirimycin(4)	[M+Na-2H]-	184.05912	184.05913	0.041	0.01009	0.85526	
C6H13NO4		[M+^{35}Cl]-	198.05381	198.05386	0.255	0	1.45599	
C6H13NO5	D-Glucosamine(8)	[M+Na-2H]-	200.05405	200.05404	0.037	0.00447	0.70645	*
C6H13NO5		[M+^{35}Cl]-	214.04862	214.04878	0.727	0.03868	0.83763	
C6H14O6	D-Iditol(2)	[M+^{35}Cl]-	217.04843	217.04844	0.053	0.03429	2.3633	
C6H14O6		[M+Ac]-	241.09288	241.09289	0.056	0.03544	2.12141	
C6H14NO8P	D-Glucosamine 6-phosphate(7)	[M-H]-	258.03845	258.03843	0.075	0.00421	1.65941	*

C6H14NO8P		[M+Na-2H]-	280.02044	280.02038	0.230	0.0299	0.95034	
C6H14N2O2	L-Lysine(6)	[M-H]-	145.09825	145.09825	0.011	0.00467	0.58636	
C6H14N2O2		[M+^{35}Cl]-	181.07491	181.07493	0.108	0.00313	0.33646	*
C6H14N2O2		[M+Ac]-	205.11940	205.11938	0.090	0.00595	0.71719	
C6H14N2O3	N6-Hydroxy-L-lysine(3)	[M+^{35}Cl]-	197.06987	197.06984	0.129	0.04467	1.23478	
C6H14N4O2	L-Arginine(3)	[M-H]-	173.10440	173.10440	0.002	0.00088	0.57805	*
C6H14N4O2		[M+^{35}Cl]-	209.08110	209.08108	0.107	0.00181	0.38495	*
C6H14N4O2		[M+^{37}Cl]-	211.07814	211.07813	0.059	0.00176	0.36748	*
C6H14N4O3	N-(omega)-Hydroxyarginine(2)	[M+Na-2H]-	211.08115	211.08126	0.519	2.8E-05	0.35053	*
C6H15O8P	Glycerophosphoglycerol	[M-H]-	245.04326	245.04318	0.320	0.00742	0.62345	
C6H15O8P		[M+Na-2H]-	267.02522	267.02513	0.350	0.00764	0.62411	
C7H6O2	Benzoate(6)	[M+Ac]-	181.05064	181.05063	0.035	0.03444	3.45205	
C7H6O3	4-Hydroxybenzoate(5)	[M-H]-	137.02442	137.02442	0.010	0.03965	1.18972	
C7H6O4S	4-Sulfobenzaldehyde	[M+^{35}Cl]-	220.96811	220.96808	0.119	0.00546	0.61355	
C7H7NO	Benzamide	[M+Ac]-	180.06662	180.06662	0.013	0.00089	0.34832	*
C7H7NO2	Anthranilate(4)	[M+Ac]-	196.06152	196.06153	0.064	0.01735	1.12231	
C7H8O2	Orcinol(7)	[M+Ac]-	183.06628	183.06628	0.020	0.00696	0.68005	
C7H8O3S	Toluene-4-sulfonate	[M+^{37}Cl]-	208.98584	208.98587	0.137	0.01584	0.40374	
C7H8O3S		[M+Ac]-	231.03321	231.03327	0.262	0.03812	1.91098	
C7H8O5	3-Dehydroshikimate(6)	[M+^{39}K-2H]-	208.98584	208.98578	0.279	0.01585	0.40374	

C7H8O7	Oxaloglutarate	[M+Ac]-	263.04090	263.04086	0.157	0.04287	1.39195	
C7H10O2	Toluene-cis-dihydrodiol(2)	[M+Ac]-	185.08192	185.08193	0.073	0.02553	1.21442	
C7H10O5	Shikimate(3)	[M+^{39}K-2H]-	211.00133	211.00143	0.482	0.02745	0.78177	
C7H10O7	2-Hydroxybutane-1,2,4-tricarboxylate(4)	[M-H]-	205.03538	205.03538	0.007	0	0.69336	
C7H10O7		[M+^{35}Cl]-	241.01205	241.01206	0.027	0.01842	0.40385	
C7H10O7		[M+^{37}Cl]-	243.00910	243.00911	0.027	0.00779	0.27946	
C7H10O7		[M+Ac]-	265.05651	265.05651	0.005	0.02528	0.63594	
C7H11NO5	N-Acetyl-L-glutamate(3)	[M+Na-2H]-	210.03841	210.03839	0.083	0.04023	1.53737	
C7H11N3O	4-(beta-Acetylaminoethyl)imidazole (2)	[M+^{39}K-2H]-	190.03887	190.03882	0.270	0.00132	1.28766	*
C7H12O2	Ethyl 2-methylbut-2-enoate(7)	[M+Ac]-	187.09758	187.09758	0.019	0.04817	1.13042	
C7H12O4	6-Carboxyhexanoate(3)	[M+^{39}K-2H]-	197.02211	197.02217	0.287	0	1.46381	
C7H12O6	Quinate(3)	[M-H]-	191.05610	191.05611	0.071	0.01588	1.25056	
C7H12O6		[M+Na-2H]-	213.03805	213.03806	0.040	0.02644	1.30202	
C7H13NO	N-Cyclohexylformamide	[M+Ac]-	186.11356	186.11357	0.041	0.02663	1.13393	
C7H13NO2	Stachydrine	[M+Ac]-	202.10849	202.10848	0.037	0.01999	1.26504	
C7H13NO3	5-Acetamidopentanoate(4)	[M+Ac]-	218.10342	218.10340	0.103	0.01785	0.87707	
C7H13NO4	Calystegin B2	[M+Na-2H]-	196.05913	196.05913	0.012	0.00649	0.86127	

C7H13NO4		[M+^{39}K-2H]-	212.03307	212.03307	0.021	0.00231	1.73973	*
C7H13NO4S	S-(2-Hydroxyethyl)-N-acetyl-L-cysteine	[M+^{37}Cl]-	244.02291	244.02298	0.298	0.00065	1.41877	*
C7H14O	Heptan-2-one(2)	[M+Ac]-	173.11832	173.11832	0.008	0.00427	1.60379	*
C7H14O2S	7-Mercaptoheptanoic acid	[M+Ac]-	221.08531	221.08531	0.020	8.3E-05	0.25721	*
C7H14O4	beta-Cymaropyranose(2)	[M+Na-2H]-	183.06386	183.06388	0.102	0.03911	1.25653	
C7H14O4		[M+^{35}Cl]-	197.05856	197.05861	0.262	0.03101	1.22969	
C7H14O4		[M+^{39}K-2H]-	199.03772	199.03782	0.485	0	1.17911	
C7H14O5	beta-D-Digitalopyranose(2)	[M+^{35}Cl]-	213.05351	213.05353	0.078	0.02437	0.72123	
C7H14O5		[M+^{39}K-2H]-	215.03282	215.03273	0.411	0.04385	1.42394	
C7H14O6	5-O-Methyl-myo-inositol(9)	[M-H]-	193.07175	193.07176	0.070	0.02434	1.49269	
C7H14O6		[M+^{35}Cl]-	229.04843	229.04844	0.051	0.02655	0.75765	
C7H14O6		[M+^{37}Cl]-	231.04552	231.04549	0.123	0.01382	0.77425	
C7H14O6		[M+Ac]-	253.09290	253.09289	0.025	0.03094	0.9529	
C7H14O7	Sedoheptulose(3)	[M-H]-	209.06669	209.06668	0.055	0.02242	0.95461	
C7H14O7		[M+^{35}Cl]-	245.04326	245.04336	0.394	0.00743	0.62345	
C7H14O7		[M+Ac]-	269.08783	269.08781	0.080	0.0481	1.29844	
C7H14N2O3	N-Acetylornithine(2)	[M+^{39}K-2H]-	211.04913	211.04905	0.381	0.04657	0.93322	
C7H14N2O4	LL-2,6-Diaminoheptanedioate(2)	[M-H]-	189.08807	189.08808	0.061	0.00728	0.61233	
C7H14N2O4Se	Selenocystathionine(2)	[M-H]-	269.00450	269.00460	0.381	0.04937	0.94484	

C7H15O9P	1-Deoxy-D-altro-heptulose 7-phosphate	[M-H]-	273.03828	273.03810	0.672	0.01707	0.50081	
C7H15NO3	L-Carnitine(2)	[M+^{35}Cl]-	196.07462	196.07460	0.124	0.04059	1.17983	
C7H15NO3		[M+^{39}K-2H]-	198.05381	198.05380	0.047	0	1.45599	
C7H15NO3		[M+Ac]-	220.11913	220.11905	0.374	0.03295	0.84987	
C7H15Cl2N2O3P	4-Hydroxycyclophosphamide(4)	[M+^{35}Cl]-	310.98916	310.98914	0.069	0.04248	1.15317	
C7H15Cl2N2O4P	Carboxyphosphamide(2)	[M-H]-	291.00745	291.00738	0.256	0.02563	1.74511	
C7H15Cl2N2O4P		[M+^{35}Cl]-	326.98410	326.98405	0.142	0.02738	1.60202	
C7H16O7	Perseitol(2)	[M-H]-	211.08234	211.08233	0.054	0.00011	1.27984	*
C7H16N2O2	N6-Methyl-L-lysine	[M+^{39}K-2H]-	197.06987	197.06978	0.433	0	1.23478	
C7H16N4O	Acetylagmatine	[M+^{39}K-2H]-	209.08110	209.08102	0.394	0.00182	1.38495	*
C7H16N4O3	(+)-gamma-Hydroxy-L-homoarginine	[M+Ac]-	263.13600	263.13609	0.360	0.02926	0.55869	
C7H18N4O7P	N1-Amidinostreptamine 6-phosphate	[M+^{35}Cl]-	336.06057	336.06072	0.433	0.0065	0.48327	
C8H5NO2	Indole-5,6-quinone(2)	[M+Ac]-	206.04589	206.04588	0.036	0.0015	0.35256	*
C8H6O3	alpha-Oxo-benzeneacetic acid(3)	[M+Ac]-	209.04556	209.04555	0.055	0.03968	1.30802	
C8H8O	Phenylacetaldehyde(7)	[M+Ac]-	179.07136	179.07137	0.048	0.04308	1.1429	

C8H8O2	Phenyl acetate(14)	[M+Ac]-	195.06630	195.06628	0.084	0.04906	0.99066	
C8H8O3	4-Hydroxyphenylacetate(21)	[M-H]-	151.04006	151.04007	0.057	0.04321	1.1601	
C8H8O3		[M+^{35}Cl]-	187.01673	187.01675	0.089	0.04094	0.64067	
C8H8O3		[M+^{37}Cl]-	189.01380	189.01380	0.018	0.04818	0.89539	
C8H8O3		[M+Ac]-	211.06121	211.06120	0.054	0.04161	1.08837	
C8H8N2O2	Ricinine	[M+^{35}Cl]-	199.02796	199.02798	0.098	0.04715	0.95665	
C8H8N2O2		[M+Ac]-	223.07246	223.07243	0.127	0.00811	0.53154	
C8H9NO	2-Phenylacetamide(5)	[M+Ac]-	194.08225	194.08227	0.091	0.04558	1.09226	
C8H9NO2	N-Acetoxyarylamine(9)	[M+Ac]-	210.07718	210.07718	0.012	0.01078	0.6984	
C8H12O2	cis-1,2-Dihydro-3-ethylcatechol(3)	[M+Ac]-	199.09760	199.09758	0.082	0.01749	1.29122	
C8H12N2O4	3-(3,4-Dihydroxypyridin-1-yl)-L-alanine(2)	[M-H]-	199.07243	199.07243	0.008	0	0.74918	
C8H13NO	Supinidine	[M+Ac]-	198.11357	198.11357	0.012	0.02548	1.38877	
C8H13NO2	Retronecine(4)	[M+Ac]-	214.10849	214.10848	0.035	0.01256	0.95421	
C8H13NO5	N2-Acetyl-L-aminoadipate	[M-H]-	202.07210	202.07210	0.012	0.03902	0.95738	
C8H13NO5		[M+Ac]-	262.09324	262.09323	0.047	0.03008	0.88767	
C8H14O	Sulcatone	[M+Ac]-	185.11831	185.11832	0.046	0.03851	1.24818	
C8H14O4	Suberic acid(3)	[M+^{35}Cl]-	209.05859	209.05861	0.103	0.01423	1.07888	
C8H14O5	(R)-3-((R)-3-	[M-H]-	189.07685	189.07685	0.007	0.04179	0.99687	

	Hydroxybutanoyloxy)butanoate							
C8H14O5		[M+Na-2H]-	211.05881	211.05879	0.078	0.0365	1.41863	
C8H14O7	6-Acetyl-D-glucose	[M-H]-	221.06669	221.06668	0.052	0.03604	1.12812	
C8H14O7		[M+^{39}K-2H]-	259.02250	259.02256	0.238	0.01295	0.56928	
C8H14O8	3-Deoxy-D-manno-octulosonate	[M+^{35}Cl]-	273.03828	273.03827	0.031	0.01709	0.50081	
C8H14NO8P	N2-Acetyl-L-aminoadipyl-delta-phosphate	[M-H]-	282.03833	282.03843	0.357	0.02345	0.71126	
C8H14N2O4	Proclavaminic acid(2)	[M-H]-	201.08811	201.08808	0.141	0	1.10166	
C8H14N4S2	Thiaburimamide	[M+Ac]-	289.07990	289.07984	0.195	0.02902	1.40867	
C8H15NO	Tropine(7)	[M+Ac]-	200.12923	200.12922	0.062	0.02872	1.186	
C8H15NO2	Homostachydrine(2)	[M+Ac]-	216.12415	216.12413	0.081	0.003	1.6191	*
C8H15NO2S	Prenyl-L-cysteine	[M+^{37}Cl]-	226.04880	226.04880	0.012	0.01924	0.57007	
C8H15NO3	N-Acetyl-L-leucine(2)	[M-H]-	172.09791	172.09792	0.044	0.01952	1.10343	
C8H15NO3		[M+^{35}Cl]-	208.07454	208.07460	0.267	0.03081	1.2217	
C8H15NO4	Castanospermine(5)	[M-H]-	188.09283	188.09283	0.014	0.02913	1.10156	
C8H15NO4		[M+^{39}K-2H]-	226.04880	226.04872	0.373	0.01926	0.57007	
C8H15NO5	N-Acetyl-D-fucosamine(2)	[M-H]-	204.08774	204.08775	0.037	0	1.20122	
C8H15NO6	N-Acetyl-D-glucosamine(7)	[M+^{35}Cl]-	256.05935	256.05934	0.037	0.03319	1.17749	
C8H15NO6		[M+^{39}K-2H]-	258.03845	258.03855	0.370	0.00422	2.65941	*

C8H15NO6		[M+^{37}Cl]-	258.05642	258.05639	0.114	0.03131	1.21588	
C8H15NO6		[M+Ac]-	280.10381	280.10379	0.062	0.03001	1.23978	
C8H15NO7		[M-H]-	236.07756	236.07758	0.075	0.00552	0.46467	
C8H16O	1-Octanal(3)	[M+Ac]-	187.13396	187.13397	0.046	0.04455	0.97918	
C8H16O3	Ethyl (R)-3-hydroxyhexanoate(5)	[M+^{39}K-2H]-	197.05856	197.05855	0.043	0.03102	1.22969	
C8H16O4	L-Cladinose	[M-H]-	175.09759	175.09758	0.037	0.04985	1.05448	
C8H16O4		[M+^{39}K-2H]-	213.05351	213.05347	0.204	0.02438	0.72123	
C8H16O5	D-Mycinose	[M+^{39}K-2H]-	229.04843	229.04838	0.211	0.02656	0.75765	
C8H16NO9P	N-Acetyl-D-glucosamine 6-phosphate(5)	[M-H]-	300.04900	300.04900	0.015	0.02945	0.69132	
C8H16N2O3	Glycyl-leucine(4)	[M-H]-	187.10881	187.10882	0.035	0.01225	0.52665	
C8H16N2O4	N6-Acetyl-N6-hydroxy-L-lysine(2)	[M-H]-	203.10375	203.10373	0.091	0.00032	0.41029	*
C8H16N2O5	N-Acetyl-beta-D-glucosaminylamine	[M+Ac]-	279.11982	279.11978	0.155	0.00952	1.1668	
C8H17NO5	N-Ethylglycocyamine(3)	[M-H]-	206.10340	206.10340	0.012	0.02051	1.30893	
C8H17NO5		[M+^{39}K-2H]-	244.05917	244.05928	0.453	0.04954	0.95282	
C8H18O2	Octane-1,8-diol(3)	[M+Ac]-	205.14454	205.14453	0.031	0.03858	1.18828	
C8H21N6O7P	Streptidine 6-phosphate	[M+Ac]-	403.13455	403.13479	0.597	0.01778	1.4938	
C9H7NO2	4,8-Dihydroxyquinoline(5)	[M-H]-	160.04041	160.04040	0.046	0.00632	0.68124	

C9H7NO2		[M+^{35}Cl]-	196.01708	196.01708	0.003	0.00149	0.56174	*
C9H8O2	trans-Cinnamate(6)	[M-H]-	147.04515	147.04515	0.024	0.00547	0.64238	
C9H8O2		[M+Ac]-	207.06628	207.06628	0.017	0.0256	1.40273	
C9H8O4	3-(4-Hydroxyphenyl)pyruvate(7)	[M-H]-	179.03497	179.03498	0.076	0.03144	1.2386	
C9H10O	Indan-1-ol(3)	[M+Ac]-	193.08700	193.08702	0.096	0.01827	0.80394	
C9H10O2	Tolylacetate(5)	[M+^{39}K-2H]-	187.01673	187.01669	0.232	0.04096	0.64067	
C9H10O3	3-(2-Hydroxyphenyl)propanoate(12)	[M+^{35}Cl]-	201.03238	201.03240	0.083	0.04914	1.02336	
C9H10O4	3-(4-Hydroxyphenyl)lactate(9)	[M-H]-	181.05064	181.05063	0.035	0.03444	3.45205	
C9H10O4		[M+Na-2H]-	203.03259	203.03258	0.056	0	1.26504	
C9H10N2	Dimethylbenzimidazole(2)	[M+^{39}K-2H]-	183.03304	183.03300	0.193	0.01998	1.14627	
C9H10N2O	1-Ethyl-2-benzimidazolinone	[M+^{39}K-2H]-	199.02796	199.02792	0.203	0	0.95665	
C9H11NO2	L-Phenylalanine(4)	[M-H]-	164.07171	164.07170	0.045	0.00135	0.44545	*
C9H11NO2		[M+^{35}Cl]-	200.04838	200.04838	0.003	0.00785	0.43126	
C9H11NO3	L-Tyrosine(5)	[M-H]-	180.06662	180.06662	0.013	0.00089	0.34832	*
C9H11NO3		[M+Ac]-	240.08775	240.08775	0.010	0.00128	0.35003	*
C9H11NO4	3,4-Dihydroxy-L-	[M-H]-	196.06152	196.06153	0.064	0	2.12231	

	phenylalanine(2)							
C9H11N2O8P	2',3'-Cyclic UMP(2)	[M-H]-	305.01810	305.01803	0.231	0.00281	0.50571	*
C9H11N5O4	Neopterin	[M+Ac]-	312.09510	312.09496	0.453	0.02008	0.55653	
C9H12O2	3-Isopropylcatechol	[M+Ac]-	211.09759	211.09758	0.030	0.02267	1.45606	
C9H12O4	7-Methyl-2-hydroxy-6-oxoocta-2,4-dienoate(6)	[M-H]-	183.06628	183.06628	0.020	0.00696	0.68005	
C9H12N2O5	Deoxyuridine	[M+Ac]-	287.08863	287.08848	0.534	0.00189	0.46326	*
C9H12N2O6	Uridine(2)	[M-H]-	243.06228	243.06226	0.076	0.00222	0.48409	*
C9H12N2O6		[M+^{35}Cl]-	279.03896	279.03894	0.073	0.00749	0.40671	
C9H12N2O6		[M+^{37}Cl]-	281.03598	281.03599	0.034	0.00718	0.39977	
C9H12N2O6		[M+Ac]-	303.08340	303.08339	0.028	0.00942	0.64405	
C9H13NO	N-Methyltyramine(6)	[M+Ac]-	210.11361	210.11357	0.202	0.00867	1.35389	
C9H13N2O9P	UMP(4)	[M-H]-	323.02867	323.02859	0.233	0.00013	0.35298	*
C9H13N3O5	Cytidine(3)	[M+^{35}Cl]-	278.05501	278.05492	0.311	0.0171	0.61562	
C9H13N3O5		[M+Ac]-	302.09936	302.09938	0.052	0.01956	0.73192	
C9H14O2	Boschnialactone	[M-H]-	153.09208	153.09210	0.154	0.02301	1.45665	
C9H14O4	cis-2-Carboxycyclohexyl-acetic acid	[M-H]-	185.08192	185.08193	0.073	0.02555	1.21442	
C9H14O4		[M+Ac]-	245.10308	245.10306	0.067	0.0044	0.73263	*
C9H14N3O8P	CMP(3)	[M-H]-	322.04468	322.04458	0.315	0.00203	0.42418	*
C9H14N3O9P	1-(5-Phospho-D-ribosyl)-5-	[M+^{39}K-2H]-	375.99563	375.99538	0.674	0.02253	2.53361	

	amino-4-imidazolecarboxylate(2)							
C9H14N4O3	Carnosine	[M+^{35}Cl]-	261.07601	261.07599	0.067	0.00788	0.55934	
C9H15NO	Pseudopelletierine	[M+Ac]-	212.12923	212.12922	0.058	0.00961	1.24171	
C9H15NO3	Otonecine(3)	[M-H]-	184.09793	184.09792	0.067	0.04629	1.21276	
C9H15NO3		[M+Ac]-	244.11905	244.11905	0.010	0.04173	0.8275	
C9H15N2O6P	Pyrimidine 5'-deoxynucleotide	[M-H]-	277.05969	277.05950	0.687	0.0026	0.30332	*
C9H15N2O15P3	UTP	[M+e]-	483.96875	483.96909	0.693	0.04868	1.13577	
C9H16O3	9-Oxononanoic acid	[M+^{35}Cl]-	207.07936	207.07935	0.065	0.0307	0.78958	
C9H16O3		[M+^{39}K-2H]-	209.05859	209.05855	0.184	0.01424	1.07888	
C9H16O3		[M+Ac]-	231.12383	231.12380	0.136	0.03969	1.17616	
C9H16O4	Azelaic acid	[M-H]-	187.09758	187.09758	0.019	0.04818	1.13042	
C9H16O4		[M+Ac]-	247.11870	247.11871	0.055	0.02624	0.86921	
C9H16N2O4	gamma-Glutamyl-gamma-aminobutyraldehyde	[M+Ac]-	275.12493	275.12486	0.249	0.02201	1.18075	
C9H16N2O5	N2-Succinyl-L-ornithine(3)	[M+Ac]-	291.11981	291.11978	0.115	0.0395	1.11848	
C9H17N	Pinidine	[M+Ac]-	198.14997	198.14995	0.088	0.02706	1.19094	
C9H17NO	N-Methylpelletierine	[M+Ac]-	214.14488	214.14487	0.058	0.03915	1.03647	
C9H17NO3	8-Amino-7-oxononanoate(2)	[M-H]-	186.11356	186.11357	0.041	0.02665	1.13393	

C9H17NO3		[M+^{35}Cl]-	222.09028	222.09025	0.155	0.03955	1.00283	
C9H17NO3		[M+Ac]-	246.13470	246.13470	0.010	0.01853	1.10545	
C9H17NO5	Pantothenate	[M-H]-	218.10342	218.10340	0.103	0.01787	0.87707	
C9H17NO5		[M+^{39}K-2H]-	256.05935	256.05928	0.271	0.0332	1.17749	
C9H17NO5		[M+Ac]-	278.12462	278.12453	0.332	0.03065	1.18487	
C9H17NO7	Muramic acid	[M-H]-	250.09324	250.09323	0.050	0.01619	0.74775	
C9H17NO7		[M+Ac]-	310.11437	310.11436	0.040	0.03966	1.30409	
C9H18O8	3-beta-D-Galactosyl-sn-glycerol(2)	[M-H]-	253.09290	253.09289	0.025	0.03095	0.9529	
C9H18O8		[M+^{39}K-2H]-	291.04866	291.04878	0.401	0.03055	1.45616	
C9H18NO4	O-Acetylcarnitine	[M+e]-	204.12415	204.12413	0.085	0.0372	1.28788	
C9H18N2O4	N2-(D-1-Carboxyethyl)-L-lysine	[M-H]-	217.11939	217.11938	0.039	0.02233	1.39961	
C9H18N2O4		[M+Ac]-	277.14058	277.14051	0.247	0.0322	1.12423	
C9H19NO4	Pantothenol	[M-H]-	204.12415	204.12413	0.085	0	1.28788	
C9H19NO4		[M+^{35}Cl]-	240.10082	240.10081	0.039	0.04876	0.75444	
C9H19NO4		[M+^{39}K-2H]-	242.07989	242.08002	0.519	0.0181	1.37641	
C9H19NO4		[M+Ac]-	264.14527	264.14526	0.028	0.04851	1.08055	
C9H22O13P2	Bis(glycerophospho)-glycerol	[M-H]-	399.04638	399.04629	0.214	0.00025	3.23648	*
C9H22O13P2		[M+Na-2H]-	421.02822	421.02824	0.047	0.00346	3.58933	*

C10H8O3	1,3,8-Naphthalenertriol(3)	[M+Na-2H]-	197.02211	197.02201	0.489	0	1.46381	
C10H9NO	Indole-3-acetaldehyde(4)	[M+^{39}K-2H]-	196.01708	196.01702	0.303	0.0015	1.56174	*
C10H9NO3	5-Hydroxyindoleacetate(3)	[M+Na-2H]-	212.03307	212.03291	0.742	0.00232	2.73973	*
C10H9NO4	4-(2-Aminophenyl)-2,4-dioxobutanoate(4)	[M-H]-	206.04589	206.04588	0.036	0.00151	1.35256	*
C10H9NO5	7,8-Dihydro-7,8-dihydroxykynurenate(4)	[M+Na-2H]-	244.02291	244.02274	0.686	0.00067	2.41877	*
C10H10O2	cis-1,2-Dihydronaphthalene-1,2-diol(9)	[M+Ac]-	221.08197	221.08193	0.165	0.01744	1.73735	
C10H10O3	Coniferyl aldehyde(3)	[M+Na-2H]-	199.03772	199.03766	0.283	0	1.17911	
C10H10O4	6-Hydroxymellein(6)	[M-H]-	193.05065	193.05063	0.085	0.04294	1.25106	
C10H10O5	5-Hydroxyferulate	[M-H]-	209.04556	209.04555	0.055	0.03969	1.30802	
C10H11NO3	(3-Arylcarbonyl)-alanine(7)	[M+Na-2H]-	214.04862	214.04856	0.268	0.03869	0.83763	
C10H12O	p-Cumic aldehyde(4)	[M+^{39}K-2H]-	185.03731	185.03742	0.603	0.03231	1.33574	
C10H12O2	p-Cumate(7)	[M+^{39}K-2H]-	201.03238	201.03234	0.216	0	1.02336	
C10H12O3	Coniferyl alcohol(2)	[M-H]-	179.07136	179.07137	0.048	0.04308	1.1429	
C10H12O4	2,3-Dihydroxy-p-cumate(5)	[M-H]-	195.06630	195.06628	0.084	0.04907	0.99066	
C10H12O5	Danielone(2)	[M-H]-	211.06121	211.06120	0.054	0.04162	1.08837	
C10H12N2O4	3-Hydroxykynurenine(4)	[M-H]-	223.07246	223.07243	0.127	0.00813	0.53154	
C10H12N4O5	Inosine	[M-H]-	267.07350	267.07349	0.020	0.03472	1.19435	

C10H12N4O6	Xanthosine	[M-H]-	283.06851	283.06841	0.355	0.00475	0.37733	
C10H12N5O5P	3',5'-Cyclic dAMP	[M+^{37}Cl]-	350.02403	350.02406	0.085	0.0182	0.70518	
C10H12N5O6P	3',5'-Cyclic AMP(3)	[M-H]-	328.04538	328.04525	0.407	0.00496	0.53412	
C10H13N	Actinidine	[M+Ac]-	206.11868	206.11865	0.133	0.03126	1.67518	
C10H13NO	(R)-2-Methylimino-1-phenylpropan-1-ol(3)	[M+^{39}K-2H]-	200.04838	200.04832	0.297	0	0.43126	
C10H13NO3	L-Tyrosine methyl ester(5)	[M-H]-	194.08225	194.08227	0.091	0.0456	1.09226	
C10H13NO4	Enicoflavine	[M-H]-	210.07718	210.07718	0.012	0.01079	0.6984	
C10H13NO5	L-Arogenate	[M+^{35}Cl]-	262.04873	262.04878	0.174	0.00132	0.39764	*
C10H13NO6S	L-Tyrosine methyl ester 4-sulfate	[M-H]-	274.03913	274.03908	0.166	0.02612	1.12227	
C10H13N4O9P	Xanthosine 5'-phosphate	[M+Ac]-	423.05558	423.05587	0.692	0.02642	1.18307	
C10H13N5O4	Adenosine(3)	[M-H]-	266.08948	266.08948	0.005	0.01493	0.56859	
C10H13N5O4		[M+^{35}Cl]-	302.06616	302.06616	0.011	0.01336	0.39109	
C10H13N5O4		[M+^{37}Cl]-	304.06325	304.06321	0.143	0.01171	0.40342	
C10H13N5O4		[M+Ac]-	326.11072	326.11061	0.342	0.01828	0.53493	
C10H13N5O5	Guanosine(2)	[M-H]-	282.08443	282.08439	0.129	0.01563	0.73871	
C10H14O	(-)-Carvone(24)	[M+Ac]-	209.11835	209.11832	0.150	0.02722	1.2147	
C10H14N2O5	Thymidine	[M+^{35}Cl]-	277.05969	277.05967	0.056	0.00261	1.30332	*
C10H14N2O5		[M+^{39}K-2H]-	279.03896	279.03888	0.288	0.0075	0.40671	
C10H14N2O5		[M+Ac]-	301.10413	301.10413	0.011	0.00164	0.55938	*

C10H14N4O10P2	dIDP	[M+^{37}Cl]-	448.98476	448.98497	0.476	0.04921	0.85318	
C10H14N4O12P2	XDP	[M-H]-	443.00132	443.00108	0.552	0.03455	2.08074	
C10H14N5O6PS2	Molybdopterin	[M-H]-	394.00477	394.00504	0.687	0.03177	1.364	
C10H14N5O7PS	6-Thioguanosine monophosphate	[M+^{37}Cl]-	416.00186	416.00161	0.597	0.03693	1.16005	
C10H14N5O8P	GMP(2)	[M-H]-	362.05076	362.05073	0.092	0.00185	0.44656	*
C10H15O3	(3R)-3-Isopropenyl-6-oxoheptanoate(2)	[M+e]-	183.10267	183.10267	0.008	0.03947	1.18455	
C10H15NO	Ephedrine(4)	[M+Ac]-	224.12923	224.12922	0.055	0.02574	1.08578	
C10H15NO3	L-Metanephrine(2)	[M+Ac]-	256.11907	256.11905	0.087	0.00563	1.15116	
C10H15N2O9P	1-(5-Phosphoribosyl)imidazole-4-acetate	[M-H]-	337.04439	337.04424	0.431	0.00279	0.52191	*
C10H15N3O4	5-Methyl-2'-deoxycytidine	[M+^{39}K-2H]-	278.05501	278.05486	0.527	0.01712	0.61562	
C10H15N4O9P	1-(5'-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide	[M+^{39}K-2H]-	403.00656	403.00628	0.706	0.0441	1.10924	
C10H15N5O9P2	dADP	[M+^{37}Cl]-	448.00098	448.00096	0.050	0.0131	0.66412	
C10H15N5O10P2	ADP(4)	[M-H]-	426.02233	426.02214	0.435	0.02813	0.6333	
C10H16	(-)-Limonene(21)	[M+Ac]-	195.13909	195.13905	0.187	0.01485	1.38757	
C10H16O	(+)-Camphor(27)	[M+Ac]-	211.13399	211.13397	0.101	0.00647	1.3418	

C10H16O3	5-exo-Hydroxy-1,2-campholide(2)	[M-H]-	183.10267	183.10267	0.008	0.03947	1.18455	
C10H16O3		[M+Ac]-	243.12381	243.12380	0.047	0.00545	0.68816	
C10H16N2O4	(S)-ATPA	[M+Ac]-	287.12489	287.12486	0.099	0.01007	1.6909	
C10H16N4O3	Homocarnosine(3)	[M+Na-2H]-	261.09676	261.09691	0.573	0.00172	0.49317	*
C10H17O3	(3R)-6-Hydroxy-3-isopropenyl-heptanoate(4)	[M+e]-	185.11831	185.11832	0.046	0.03852	1.24818	
C10H17NO2	Acetyltropine(2)	[M-H]-	182.11866	182.11865	0.041	0.04755	1.23514	
C10H17NO2		[M+Ac]-	242.13980	242.13978	0.072	0.04578	0.89107	
C10H17NO3	Tussilagine(2)	[M-H]-	198.11357	198.11357	0.012	0	1.38877	
C10H17NO3		[M+Ac]-	258.13470	258.13470	0.009	0.00879	1.56802	
C10H17NO4	2-Amino-9,10-epoxy-8-oxodecanoic acid	[M-H]-	214.10849	214.10848	0.035	0.01257	0.95421	
C10H17NO4		[M+Ac]-	274.12970	274.12961	0.319	0.01532	1.05	
C10H17N3O6S	Glutathione	[M-H]-	306.07654	306.07653	0.024	0.01851	0.07874	
C10H17N3O6S		[M+Na-2H]-	328.05862	328.05848	0.434	0.02023	0.1526	
C10H18O	(-)-Menthone(28)	[M+Ac]-	213.14963	213.14962	0.053	0.03362	1.45988	
C10H18O2	6-endo-Hydroxycineole(5)	[M+^{39}K-2H]-	207.07936	207.07929	0.354	0.03072	0.78958	
C10H18O2		[M+Ac]-	229.14456	229.14453	0.115	0.04129	1.21574	
C10H18O3	10-Oxodecanoate(2)	[M-H]-	185.11831	185.11832	0.046	0.03854	1.24818	
C10H18O3		[M+Ac]-	245.13945	245.13945	0.006	0.04172	1.06543	

C10H18O4	Sebacic acid(2)	[M+Ac]-	261.13437	261.13436	0.025	0.04448	1.1323	
C10H18O9	Xylobiose	[M+Na-2H]-	303.06954	303.06975	0.705	0.01314	0.45661	
C10H19NO	Lupinine	[M+^{39}K-2H]-	206.09534	206.09527	0.337	0.02164	1.06454	
C10H19NO4	O-Propanoylcarnitine	[M-H]-	216.12415	216.12413	0.081	0.00301	2.6191	*
C10H19NO4		[M+^{35}Cl]-	252.10080	252.10081	0.042	0.03199	0.82955	
C10H19NO4		[M+Ac]-	276.14530	276.14526	0.135	0.02141	1.50293	
C10H20O2	Decanoic acid(4)	[M-H]-	171.13905	171.13905	0.021	0.02758	1.19347	
C10H20O2		[M+^{35}Cl]-	207.11575	207.11573	0.089	0.01652	0.92658	
C10H20O2		[M+Ac]-	231.16020	231.16018	0.071	0.01967	0.89525	
C10H20O3	10-Hydroxydecanoic acid	[M-H]-	187.13396	187.13397	0.046	0.04457	0.97918	
C10H20O3		[M+^{37}Cl]-	225.10771	225.10770	0.060	0.00039	0.419	*
C11H12O4	6-Methoxymellein(3)	[M-H]-	207.06628	207.06628	0.017	0.02562	1.40273	
C11H12O5	Sinapate	[M+Na-2H]-	245.04326	245.04314	0.475	0.00745	0.62345	
C11H12N2O2	L-Tryptophan(7)	[M-H]-	203.08261	203.08260	0.041	0.0342	8.93663	
C11H12N2O2		[M+Ac]-	263.10374	263.10373	0.032	0.0019	0.59048	*
C11H12N2O6	Portulacaxanthin III	[M+^{39}K-2H]-	305.01810	305.01814	0.146	0.00282	1.50571	*
C11H13ClN2	Epibatidine	[M+^{37}Cl]-	245.04326	245.04318	0.336	0.00746	0.62345	
C11H14O2	Eugenol methyl ether(4)	[M-H]-	177.09212	177.09210	0.093	0.02226	1.21124	
C11H14O2		[M+Ac]-	237.11340	237.11323	0.702	0.00014	0.64268	*
C11H14O4	Sinapyl alcohol(3)	[M+Ac]-	269.10306	269.10306	0.013	0.04926	0.93838	
C11H14N2	N-Methyltryptamine(2)	[M+Na-2H]-	195.09032	195.09037	0.239	0.01731	1.67566	

C11H15N5O3	N6-Methyl-2'-deoxyadenosine	[M+^{39}K-2H]-	302.06616	302.06610	0.210	0.01338	0.39109	
C11H15N5O3S	5'-Methylthioadenosine	[M+Ac]-	356.10345	356.10342	0.097	0.02752	0.84768	
C11H16O2	3-tert-Butyl-5-methylcatechol	[M+Ac]-	239.12889	239.12888	0.027	0.01942	1.17198	
C11H16N2O8	N-Acetyl-aspartyl-glutamate	[M-H]-	303.08340	303.08339	0.028	0.00943	0.64405	
C11H16N2O8		[M+Na-2H]-	325.06541	325.06534	0.226	0.01728	0.61404	
C11H17NO3	Mescaline(5)	[M-H]-	210.11361	210.11357	0.202	0.00868	1.35389	
C11H17NO3		[M+Ac]-	270.13473	270.13470	0.120	0.01368	1.31474	
C11H17NO6	Proacacipetalin	[M-H]-	258.09830	258.09831	0.049	0.00463	0.63625	
C11H19NO3	N-Heptanoylhomoserine lactone	[M-H]-	212.12923	212.12922	0.058	0.00963	1.24171	
C11H19NO3		[M+Ac]-	272.15039	272.15035	0.156	0.01416	1.62833	
C11H20N2O6	N6-(L-1,3-Dicarboxypropyl)-L-lysine	[M-H]-	275.12493	275.12486	0.249	0.02202	1.18075	
C11H21NO4	O-Butanoylcarnitine(2)	[M-H]-	230.13981	230.13978	0.119	0.00539	1.4542	
C11H21NO4		[M+^{35}Cl]-	266.11647	266.11646	0.035	0.03794	1.20408	
C11H21NO4		[M+^{37}Cl]-	268.11352	268.11351	0.035	0.03973	1.11942	
C11H21NO4		[M+Ac]-	290.16094	290.16091	0.094	0.00703	1.39339	
C11H22O	2-Undecanone	[M+^{39}K-2H]-	207.11575	207.11567	0.379	0.01653	0.92658	
C11H22NO7PS	N-(7-	[M+Na-2H]-	364.06022	364.06013	0.240	0.01588	0.86237	

	Mercaptoheptanoyl)threonine 3-O-phosphate							
C11H22NO7PS		[M+^{35}Cl]-	378.05486	378.05487	0.015	0.04525	1.04178	
C11H22NO7PS		[M+^{39}K-2H]-	380.03418	380.03407	0.288	0.00675	0.69786	
C11H22N2O4S	Pantetheine	[M-H]-	277.12275	277.12275	0.013	0.00963	0.37148	
C11H22N2O4S		[M+^{35}Cl]-	313.09963	313.09943	0.634	0.01264	0.40175	
C11H22N2O4S		[M+^{37}Cl]-	315.09651	315.09648	0.090	0.00428	0.40829	*
C12H10O2S	cis-1,2-Dihydroxy-1,2-dihydrodibenzothiophene	[M+Na-2H]-	239.01492	239.01482	0.416	0.03055	0.96331	
C12H10O2S		[M+^{35}Cl]-	253.00953	253.00955	0.093	0.02417	0.82181	
C12H10O2S		[M+^{39}K-2H]-	254.98880	254.98876	0.162	0.03691	0.86192	
C12H13NO2	Shihunine(2)	[M+Ac]-	262.10860	262.10848	0.448	0.00425	0.5859	*
C12H14O4	Apiole(3)	[M-H]-	221.08197	221.08193	0.165	0.01745	1.73735	
C12H16O2	Thymyl acetate	[M-H]-	191.10772	191.10775	0.176	0.03394	0.993	
C12H16O4	Aspidinol	[M+Ac]-	283.11879	283.11871	0.270	0.03789	1.22411	
C12H16O7	Arbutin(2)	[M+Na-2H]-	293.06441	293.06427	0.465	0.04533	1.01164	
C12H16O12	4-(4-Deoxy-beta-D-gluc-4-enuronosyl)-D-galacturonate(2)	[M+^{37}Cl]-	389.03045	389.03063	0.467	0.01109	1.9671	
C12H16N2O	Bufotenine(3)	[M+^{37}Cl]-	241.09288	241.09271	0.686	0.03545	2.12141	
C12H16N2O		[M+Ac]-	263.14012	263.14012	0.013	0.02308	0.64037	

C12H16N2O2	Phenylacetylglycine dimethylamide	[M+Ac]-	279.13511	279.13503	0.281	0.01989	0.96405	
C12H16N5O8P	Acetyl adenylate	[M+Na-2H]-	410.04834	410.04832	0.045	0.00096	0.64227	*
C12H16N5O8P		[M+^{39}K-2H]-	426.02233	426.02226	0.165	0.02815	0.6333	
C12H17NO2	3-(Dimethylamino)propyl benzoate(2)	[M-H]-	206.11868	206.11865	0.133	0.03127	1.67518	
C12H18O3	(-)-Jasmonic acid(2)	[M-H]-	209.11835	209.11832	0.150	0.02723	1.2147	
C12H18O3		[M+Ac]-	269.13946	269.13945	0.042	0.01578	1.47857	
C12H19NO4	N-(3-Oxooctanoyl)homoserine lactone	[M-H]-	240.12417	240.12413	0.156	0.03877	0.79791	
C12H19NO4		[M+Ac]-	300.14525	300.14526	0.042	0.02344	0.72906	
C12H20O2	Ethyl(E,Z)-decadienoate(9)	[M-H]-	195.13909	195.13905	0.187	0.01487	1.38757	
C12H20O3	Cucurbic acid(4)	[M-H]-	211.13399	211.13397	0.101	0.00649	1.3418	
C12H20O3		[M+Ac]-	271.15510	271.15510	0.005	0.02702	1.34781	
C12H20N3O6S	Glutathione episulfonium ion	[M+^{35}Cl]-	369.07665	369.07669	0.096	0.04286	1.12492	
C12H20N4O3	His-Leu	[M+Ac]-	327.16754	327.16739	0.444	0.00104	0.37719	*
C12H21NO2	Elaeokanine C	[M-H]-	210.14997	210.14995	0.083	0.03027	1.32744	
C12H21NO2		[M+Ac]-	270.17106	270.17108	0.084	0.02342	1.1323	
C12H21N3O6	Nicotianamine	[M-H]-	302.13578	302.13576	0.064	0.01306	0.64119	

C12H22O3	3-Oxododecanoic acid	[M-H]-	213.14963	213.14962	0.053	0.03363	1.45988	
C12H22O3		[M+^{37}Cl]-	251.12337	251.12335	0.093	0.02309	0.67058	
C12H22O3		[M+Ac]-	273.17080	273.17075	0.188	0.0324	1.20783	
C12H22O4	Dodecanedioic acid(2)	[M-H]-	229.14456	229.14453	0.115	0.0413	1.21574	
C12H22O11	Sucrose(30)	[M+^{35}Cl]-	377.08566	377.08562	0.115	0.03356	0.77167	
C12H22O11		[M+^{37}Cl]-	379.08271	379.08267	0.114	0.03194	0.76964	
C12H22O11		[M+Ac]-	401.13016	401.13007	0.228	0.04686	0.99592	
C12H22FeO14	Fe(III)dicitrate	[M+^{37}Cl]-	483.00259	483.00235	0.496	0.01128	2.46377	
C12H23NO10	6-(alpha-D-Glucosaminyl)-1D-myo-inositol	[M+Na-2H]-	362.10695	362.10687	0.228	0.04407	0.97796	
C12H24O2	Dodecanoic acid	[M-H]-	199.17036	199.17035	0.032	0.03695	1.7552	
C12H24O2		[M+Ac]-	259.19149	259.19148	0.025	0.03056	1.65626	
C12H24O3	12-Hydroxydodecanoic acid	[M+^{39}K-2H]-	253.12122	253.12115	0.270	0.02977	0.91667	
C12H24N2O3	N-(6-Aminohexanoyl)-6-aminohexanoate(2)	[M-H]-	243.17144	243.17142	0.096	0.00966	0.42523	
C12H24N2O3		[M+Ac]-	303.19260	303.19255	0.176	0.02227	1.31944	
C12H24N2O7	Fructoselysine	[M-H]-	307.15111	307.15108	0.109	0.01074	1.60287	
C13H8	1-Phenylhepta-1,3,5-triyne	[M+Na-2H]-	185.03731	185.03727	0.224	0.03231	1.33574	
C13H8S2	Thiarubrine A(2)	[M+Ac]-	287.02066	287.02060	0.217	0.01182	1.50631	
C13H8O5	1,3,5-Trihydroxyxanthone	[M+Ac]-	303.05120	303.05103	0.566	0.04212	1.02564	
C13H12O4S	(1R,2R)-3-[(1,2-Dihydro-2-	[M-H]-	263.03855	263.03836	0.739	0.03815	0.73086	

	hydroxy-1-naphthalenyl)thio]-2-							
C13H16N2O	Tetrahydroharmine(2)	[M+^{35}Cl]-	251.09582	251.09566	0.619	0.00068	0.42479	*
C13H16N2O		[M+^{37}Cl]-	253.09290	253.09271	0.733	0.03097	0.9529	
C13H16N2O2	Melatonin(2)	[M+^{37}Cl]-	269.08783	269.08763	0.745	0.04811	1.29844	
C13H16N2O4	alpha-N-Phenylacetyl-L-glutamine(3)	[M-H]-	263.10374	263.10373	0.032	0.00192	1.59048	*
C13H16N2O4		[M+Na-2H]-	285.08572	285.08568	0.152	0.00208	0.49927	*
C13H18O3	Dehydrovomifoliol(2)	[M+Ac]-	281.13948	281.13945	0.112	0.01887	1.42278	
C13H18N2O	5-Methoxy-N,N-dimethyltryptamine	[M+^{35}Cl]-	253.11149	253.11131	0.693	0.00075	0.41257	*
C13H18N2O		[M+Ac]-	277.15584	277.15577	0.265	0.03191	0.62334	
C13H18N2O3	N-Caffeoylputrescine	[M+Na-2H]-	271.10653	271.10641	0.437	0.00957	0.83811	
C13H20O3	Vomifoliol(4)	[M+^{37}Cl]-	261.10770	261.10770	0.013	0.00201	0.53518	*
C13H20O3		[M+Ac]-	283.15514	283.15510	0.146	0.00974	1.61683	
C13H21NO2	Tigloidine	[M+Ac]-	282.17112	282.17108	0.133	0.02016	1.27545	
C13H21NO4	Meteloidine	[M-H]-	254.13982	254.13978	0.147	0.04785	1.08939	
C13H21NO4		[M+Ac]-	314.16103	314.16091	0.374	0.04435	1.14194	
C13H23NO3	Valeroidine	[M+^{39}K-2H]-	278.11637	278.11640	0.110	0.01505	1.22775	
C13H23N3O4	Leu-Gly-Pro	[M-H]-	284.16162	284.16158	0.139	0.01844	0.55315	
C13H24O10	Methyl-2-alpha-L-	[M+^{39}K-2H]-	377.08566	377.08556	0.274	0.03358	0.77167	

	fucopyranosyl-beta-D-galactoside							
C13H25N2O8PS	S-Acetylphosphopantetheine	[M+Na-2H]-	421.08164	421.08160	0.103	0.04573	1.28564	
C14H10O8	2-Protocatechoylphloroglucinolcarboxylate	[M+Ac]-	365.05139	365.05142	0.092	0.03884	0.83218	
C14H11NO3	N-Benzoylanthranilate(4)	[M+Na-2H]-	262.04873	262.04856	0.639	0.00133	1.39764	*
C14H11NO4	N-Benzoyl-4-hydroxyanthranilate	[M+Na-2H]-	278.04362	278.04348	0.512	0.0021	0.31816	*
C14H15NO6	(+)-2,7-Dideoxypancratistatin	[M+Na-2H]-	314.06457	314.06461	0.120	0.01424	0.35143	
C14H15N3	4-(Dimethylamino)azobenzene(2)	[M+^{37}Cl]-	262.09324	262.09305	0.730	0.03009	0.88767	
C14H15N3O	4-(Dimethylamino)phenylazoxybenzene(2)	[M+e]-	241.12201	241.12206	0.210	0.04592	0.84549	
C14H17NO10	Triglochinin	[M+^{35}Cl]-	394.05478	394.05465	0.328	0.03105	1.40314	
C14H18O4	Methylripariochromene A(3)	[M+Na-2H]-	271.09536	271.09518	0.669	0.03475	0.96736	

C14H18O4		[M+Ac]-	309.13455	309.13436	0.603	0.00777	1.21536	
C14H18NO9S2	Glucotropeolin	[M+^{35}Cl]-	443.01157	443.01170	0.304	0.04104	1.09773	
C14H20O2	Glutinosone	[M+Ac]-	279.16028	279.16018	0.345	0.03504	1.64438	
C14H20N2O3	Subaphyllin	[M-H]-	263.14012	263.14012	0.013	0.02309	0.64037	
C14H21N	N-(Cyclohexylmethyl)-N-methylbenzenamine	[M+^{39}K-2H]-	240.11597	240.11601	0.148	0.02562	0.47285	
C14H21N		[M+Ac]-	262.18127	262.18125	0.066	0.00824	1.98213	
C14H21NO	Fabianine(2)	[M+^{39}K-2H]-	256.11082	256.11092	0.393	0.00292	-0.3869	*
C14H22O2	Rishitin	[M+Ac]-	281.17584	281.17583	0.023	0.00517	1.52594	
C14H24O12	Acetyl-maltose	[M+Ac]-	443.14095	443.14063	0.714	0.0475	0.98181	
C14H26O4Si	2,3,4-Trioxycyclopentanone	[M+^{35}Cl]-	321.12963	321.12944	0.593	0.01324	1.57374	
C14H27N4O10P2	CMP-N-trimethyl-2-aminoethylphosphonate	[M-H]-	472.11264	472.11297	0.700	0.01838	1.52475	
C14H28O2	Tetradecanoic acid	[M+^{35}Cl]-	263.17826	263.17833	0.272	0.02206	0.65676	
C15H11O7	Delphinidin(2)	[M+e]-	303.05120	303.05103	0.566	0.01184	1.50631	
C15H11NO3	2-(4-Hydroxybenzyl)isoindole-1,3-dione(3)	[M+Na-2H]-	274.04838	274.04856	0.666	0.04712	1.20149	
C15H12O7	Taxifolin(3)	[M-H]-	303.05120	303.05103	0.566	0.01185	1.50631	
C15H12O7		[M+^{35}Cl]-	339.02755	339.02771	0.462	0.03669	0.94231	
C15H16O5	Lactucin(4)	[M+^{37}Cl]-	313.06611	313.06623	0.372	0.01106	0.39294	

C15H18N2	6-Methylergoline	[M+^{35}Cl]-	261.11658	261.11640	0.691	0.00253	0.48542	*
C15H20O2	Alantolactone(10)	[M+Ac]-	291.16021	291.16018	0.091	0.0264	1.5237	
C15H20O3	1,2-Dihydrosantonin(18)	[M+Na-2H]-	269.11582	269.11591	0.348	0.03351	0.93363	
C15H20O4	Abscisate(23)	[M+Na-2H]-	285.11104	285.11083	0.741	0.01866	0.94269	
C15H20N2O	Anagyrine(6)	[M+Na-2H]-	265.13238	265.13223	0.560	0.02948	1.05925	
C15H20N5O6S	S-Adenosyl-4-methylthio-2-oxobutanoate	[M+^{37}Cl]-	435.08014	435.07988	0.589	0.02131	2.43573	
C15H22	alpha-Curcumene	[M+^{39}K-2H]-	239.12086	239.12076	0.432	0.0009	0.49957	*
C15H22O	alpha-Sinensal(6)	[M+Ac]-	277.18096	277.18092	0.149	0.04875	0.85443	
C15H22O2	Bakkenolide A(10)	[M-H]-	233.15472	233.15470	0.070	0.044	0.83712	
C15H22O2		[M+Ac]-	293.17593	293.17583	0.329	0.01213	1.72816	
C15H22O3	Xanthoxin(3)	[M-H]-	249.14963	249.14962	0.046	0.02998	0.88782	
C15H22O5	Hymenoxon(3)	[M-H]-	281.13948	281.13945	0.112	0.01888	1.42278	
C15H22N2O	5,6-Dehydrolupanine(2)	[M+^{35}Cl]-	281.14270	281.14261	0.304	0.02992	1.17046	
C15H22N2O2	Argyrolobine	[M+e]-	262.16871	262.16868	0.127	0.03401	6.99424	
C15H24	Pentalenene(28)	[M+^{39}K-2H]-	241.13647	241.13641	0.263	0.02058	0.61018	
C15H24O	2-trans,6-trans-Farnesal(6)	[M+Ac]-	279.19660	279.19657	0.112	0.03201	1.39949	
C15H24O2	Latia luciferin(7)	[M+Ac]-	295.19150	295.19148	0.056	0.03896	1.16493	
C15H24O3	Cuauhtemone(2)	[M+Ac]-	311.18638	311.18640	0.060	0.02856	2.86393	
C15H25NO4	Amabiline(2)	[M-H]-	282.17112	282.17108	0.133	0.02017	1.27545	
C15H25NO5	Intermedine(4)	[M-H]-	298.16606	298.16600	0.209	0.03555	1.23547	

C15H26O4	(10S)-Juvenile hormone III acid diol	[M-H]-	269.17586	269.17583	0.098	0.03743	1.12967	
C15H30O	Pentadecanal	[M+^{39}K-2H]-	263.17826	263.17827	0.044	0.02208	0.65676	
C15H30O		[M+Ac]-	285.24353	285.24352	0.040	0.03934	0.91319	
C16H14O5	(-)-Vestitone(15)	[M-H]-	285.07690	285.07685	0.180	0.03373	1.2193	
C16H14O6	Hesperetin(7)	[M+^{39}K-2H]-	339.02755	339.02765	0.285	0.0367	0.94231	
C16H16N2S	2-p-Tolyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazole	[M+e]-	268.10382	268.10397	0.554	0.00866	0.78108	
C16H19NO2	(+)-Elaeocarpine(2)	[M+Na-2H]-	278.11637	278.11625	0.440	0.01506	1.22775	
C16H19NO3	alpha-Erythroidine(7)	[M+Na-2H]-	294.11137	294.11116	0.705	0.04018	1.10005	
C16H19NO3		[M+^{35}Cl]-	308.10576	308.10590	0.440	0.04537	1.00528	
C16H20N2O6S	Indolylmethyl-desulfoglucosinolate	[M+^{37}Cl]-	405.07056	405.07066	0.251	0.00804	1.57889	
C16H23NO2	Acrifoline(5)	[M+Na-2H]-	282.14771	282.14755	0.576	0.02883	0.85293	
C16H24O3	Dehydrojuvabione	[M-H]-	263.16533	263.16527	0.233	0.01874	1.40326	
C16H24O5	Graphinone	[M-H]-	295.15512	295.15510	0.073	0.0135	0.56124	
C16H24N5O8P	O-Hexanoyl-adnosine monophosphate	[M+^{37}Cl]-	482.10268	482.10270	0.051	0.00885	0.53779	
C16H25NO	Lycopodine	[M+Ac]-	306.20744	306.20747	0.090	0.01167	1.55126	
C16H25NO4	Serratanidine	[M+Ac]-	354.19220	354.19221	0.036	0.03038	1.34065	

C16H25N5O6	Dihydrozeatin-O-glucoside	[M-H]-	382.17337	382.17321	0.422	0.04779	0.93195	
C16H26O2	Methyl farnesoate	[M-H]-	249.18602	249.18600	0.066	0.02852	0.51436	
C16H26O3	(2E,6E)-(10R,11S)-10,11-Epoxy-3,7,11-trimethyltrideca-2,6-dienoic(3)	[M-H]-	265.18092	265.18092	0.005	0.02888	1.54667	
C16H26O3		[M+Ac]-	325.20210	325.20205	0.158	0.03651	1.25525	
C16H26O4	12-trans-Hydroxy juvenile hormone III	[M-H]-	281.17584	281.17583	0.023	0.00518	1.52594	
C16H26O7	8-Epiiridodial glucoside(2)	[M+^{35}Cl]-	365.13744	365.13726	0.502	0.02296	0.89304	
C16H27NO4	N-(3-Oxododecanoyl)homoserine lactone	[M-H]-	296.18674	296.18673	0.025	0.02203	1.09835	
C16H27NO4		[M+Ac]-	356.20792	356.20786	0.161	0.01002	1.32728	
C16H27NO5	Heliotrine	[M+Ac]-	372.20286	372.20278	0.221	0.04258	0.95229	
C16H28O4	(10S)-Juvenile hormone III diol	[M-H]-	283.19146	283.19148	0.083	0.03395	1.31235	
C16H28N4O6	(Ac)2-L-Lys-D-Ala-D-Ala	[M+Ac]-	431.21496	431.21474	0.511	0.00125	0.47109	*
C16H29N3O6S	S-Hexyl-glutathione	[M+Na-2H]-	412.15253	412.15238	0.370	0.00458	0.38921	
C16H30O	2-trans-Hexadecenal(2)	[M+Ac]-	297.24353	297.24352	0.038	0.03905	0.71871	
C16H30O2	(9Z)-Hexadecenoic acid	[M+^{35}Cl]-	289.19400	289.19398	0.064	0.03068	0.41984	

C16H30O4	2,3-Dihydroxycyclopentaneundecanoic acid	[M+^{35}Cl]-	321.18391	321.18381	0.306	0.03127	1.20663	
C16H30O4		[M+^{37}Cl]-	323.18079	323.18086	0.222	0.02398	1.12496	
C16H32O	Hexadecanal(2)	[M+Ac]-	299.25917	299.25917	0.005	0.04751	0.9676	
C16H32O2		[M-H]-	255.23295	255.23295	0.014	0.04693	0.97245	
C16H32O2		[M+^{35}Cl]-	291.20962	291.20963	0.040	0.01889	0.74679	
C16H32O2		[M+^{37}Cl]-	293.20673	293.20668	0.165	0.0157	0.62721	
C16H32O2		[M+Ac]-	315.25415	315.25408	0.211	0.04869	1.07881	
C17H12O7	(-)-Acanthocarpan	[M+e]-	328.05862	328.05885	0.712	0.02024	0.1526	
C17H12O8	3,4,3'-Tri-O-methylellagic acid	[M+^{39}K-2H]-	381.00160	381.00183	0.595	0.01127	1.68171	
C17H17N	(S)-7,8,13,14-Tetrahydroprotoberberine	[M+Na-2H]-	256.11082	256.11077	0.205	0.00293	0.61311	*
C17H24O4	Trichodermin(2)	[M-H]-	291.16021	291.16018	0.091	0.02641	1.5237	
C17H24N2O	beta-Obscurine	[M+^{37}Cl]-	309.15540	309.15531	0.276	0.03407	1.31628	
C17H26O3	[6]-Paradol	[M-H]-	277.18096	277.18092	0.149	0.04876	0.85443	
C17H26O4	Phytuberin(3)	[M-H]-	293.17593	293.17583	0.329	0.01214	1.72816	
C17H27NO	Cryptophorine	[M+Ac]-	320.22323	320.22312	0.351	0.04776	1.03096	
C17H28O4	10-Deoxymethynolide	[M-H]-	295.19150	295.19148	0.056	0.03897	1.16493	
C17H28O4S	Steryl sulfate	[M+^{37}Cl]-	365.13744	365.13728	0.428	0.02298	0.89304	

C17H29NO11	Neolinustatin	[M+Na-2H]-	444.14891	444.14873	0.399	0.0333	1.62105	
C17H30O	(+)-12-(2-Cyclopenten-1-yl)-2-dodecanone	[M+Ac]-	309.24350	309.24352	0.060	0.04822	0.83698	
C17H32O3	2-Methoxy-5Z-hexadecenoic acid(3)	[M+^{39}K-2H]-	321.18391	321.18375	0.493	0.03129	1.20663	
C17H33NO4	O-Decanoyl-L-carnitine	[M-H]-	314.23367	314.23368	0.040	0.02492	1.41289	
C17H33NO4		[M+^{39}K-2H]-	352.18968	352.18957	0.325	0.00245	1.21055	*
C17H33NO4		[M+Ac]-	374.25484	374.25481	0.073	0.0105	1.5909	
C17H34O3	3-Hydroxy-palmitic acid methyl ester(2)	[M-H]-	285.24353	285.24352	0.040	0.03936	0.91319	
C18H14O7	Dihydromethylsterigmatocystin	[M+Ac]-	401.08796	401.08781	0.377	0.02491	1.48377	
C18H16O6	Betagarin(5)	[M+^{37}Cl]-	365.06121	365.06114	0.187	0.04919	0.97341	
C18H20N2	(-)-Apparicine	[M+^{35}Cl]-	299.13226	299.13205	0.703	0.02445	0.88046	
C18H23NO2	Isococculidine	[M+Na-2H]-	306.14777	306.14755	0.726	0.03043	1.00743	
C18H25NO2	Isolobinine(3)	[M+Na-2H]-	308.16340	308.16320	0.657	0.01623	1.16044	
C18H28O3	12-OPDA(9)	[M-H]-	291.19665	291.19657	0.280	0.02691	1.15355	
C18H28O4	5-O-Methylembelin	[M+Ac]-	367.21266	367.21261	0.126	0.03561	1.3433	
C18H30O2	(6Z,9Z,12Z)-Octadecatrienoic acid(6)	[M-H]-	277.21734	277.21730	0.131	0.04285	0.75264	
C18H30O3	(9Z)-(13S)-12,13-	[M-H]-	293.21217	293.21222	0.166	0.02709	1.25246	

	Epoxyoctadeca-9,11-dienoic acid(9)							
C18H30O5	2,3-Dinor-8-iso prostaglandin F2alpha	[M-H]-	325.20210	325.20205	0.158	0.03652	1.25525	
C18H30O5		[M+^{35}Cl]-	361.17889	361.17873	0.452	0.00525	0.43594	
C18H31NO4	10-Nitro-9Z,12Z-octadecadienoic acid(2)	[M-H]-	324.21813	324.21803	0.300	0.01543	1.38936	
C18H31NO4		[M+^{35}Cl]-	360.19473	360.19471	0.054	0.02041	1.23709	
C18H31NO4		[M+^{39}K-2H]-	362.17390	362.17392	0.043	0.01361	0.70013	
C18H31NO4		[M+^{37}Cl]-	362.19165	362.19176	0.305	0.01974	1.11829	
C18H31NO4		[M+Ac]-	384.23923	384.23916	0.175	0.00803	1.4794	
C18H32O2	9-cis,11-trans-Octadecadienoate4	[M-H]-	279.23298	279.23295	0.095	0.04897	0.87077	
C18H32O3	(9Z,12Z)-(8S)-Hydroxyoctadeca-9,12-dienoic acid(6)	[M-H]-	295.22789	295.22787	0.072	0.0449	0.85276	
C18H32O4	(9Z,11E)-(13S)-13-Hydroperoxyoctadeca-9,11-dienoic acid(8)	[M-H]-	311.22279	311.22278	0.021	0.04572	0.8701	
C18H34O2	(9Z)-Octadecenoic acid(5)	[M-H]-	281.24863	281.24860	0.094	0.04861	0.80545	
C18H34O3	2-Oxooctadecanoic acid(3)	[M-H]-	297.24353	297.24352	0.038	0.03907	0.71871	

C18H34O4	(9Z)-(7S,8S)-Dihydroxyoctadecenoic acid(3)	[M+Ac]-	373.25955	373.25956	0.036	0.03876	0.55475	
C18H35NO2	3-Ketosphingosine(3)	[M-H]-	296.25952	296.25950	0.059	0.02062	1.37223	
C18H35NO2		[M+Ac]-	356.28058	356.28063	0.148	0.00745	1.40263	
C18H35NO3	(+)-Prosopinine	[M-H]-	312.25453	312.25442	0.360	0.01077	1.56464	
C18H35NO3		[M+Ac]-	372.27553	372.27555	0.047	0.00363	1.74695	*
C18H36O2	Octadecanoic acid	[M-H]-	283.26424	283.26425	0.048	0.04853	0.9887	
C18H36O2		[M+^{37}Cl]-	321.23804	321.23798	0.182	0.01371	0.65415	
C18H36O3	(R)-2-Hydroxystearate(3)	[M-H]-	299.25917	299.25917	0.005	0.04753	0.9676	
C18H36O4	(9R,10R)-Dihydroxyoctadecanoic acid(2)	[M-H]-	315.25415	315.25408	0.211	0.04871	1.07881	
C18H36O4		[M+^{39}K-2H]-	353.21017	353.20997	0.576	0.04557	0.81286	
C18H37NO	Octadecanamide	[M+^{35}Cl]-	318.25700	318.25692	0.265	0.0289	0.90356	
C18H37NO		[M+^{37}Cl]-	320.25408	320.25397	0.357	0.03266	0.94607	
C18H37NO2	Sphingosine(3)	[M+Ac]-	358.29628	358.29628	0.007	0.00771	1.25246	
C18H38NO5P	Sphingosine 1-phosphate	[M-H]-	378.24168	378.24149	0.514	0.01323	1.26284	
C18H38NO5P		[M+^{37}Cl]-	416.21523	416.21521	0.039	0.00122	0.53132	*
C18H39NO3	Phytosphingosine	[M+^{37}Cl]-	354.25949	354.25945	0.125	0.01278	1.38631	
C19H26O3S2	1alpha,5alpha-Epidithio-	[M-H]-	365.12521	365.12506	0.404	0.01163	0.44064	

	17a-oxa-D-homoandrostan-3,17-dione							
C19H26O3S2		[M+Na-2H]-	387.10714	387.10701	0.342	0.0082	0.37029	
C19H26O6S	2-Methoxyestradiol-17beta 3-sulfate	[M+Na-2H]-	403.11983	403.11968	0.371	0.03281	0.52784	
C19H26O7	Orizabin(2)	[M+^{37}Cl]-	403.13455	403.13431	0.604	0.0178	1.4938	
C19H26N2	(-)-Quebrachamine	[M+Ac]-	341.22329	341.22345	0.474	0.04799	0.86693	
C19H33NO	17beta-Amino-5alpha-androstan-11beta-ol	[M+^{39}K-2H]-	328.20500	328.20482	0.547	0.02374	1.06623	
C19H37O7P	Palmitoylglycerone phosphate	[M+^{39}K-2H]-	445.17623	445.17630	0.156	0.02795	1.32518	
C19H40O3	1-O-Hexadecyl-sn-glycerol	[M+Ac]-	375.31139	375.31160	0.556	0.0478	1.15509	
C20H11Cl2NO2	3-[(2,6-Dichlorobenzylidene)amino]-6H-dibenzo[b,d]pyran-6-one(2)	[M+^{35}Cl]-	401.98618	401.98609	0.232	0.03186	1.08109	
C20H11Cl2NO2		[M+Ac]-	426.03072	426.03054	0.426	0.0309	1.66448	
C20H15NO5	10-Hydroxydihydrosanguinarine	[M+Na-2H]-	370.06946	370.06969	0.629	0.04071	1.09693	
C20H18O9	1-Hydroxy-2-(beta-D-	[M-H]-	401.08796	401.08781	0.377	0.02492	1.48377	

	glucosyloxy)-9,10-anthraquinone(2)							
C20H22O4	8-(3,3-Dimethylallyl)spatheliachromene(5)	[M+Ac]-	385.16577	385.16566	0.276	0.03479	1.12834	
C20H22O9	Astringin(2)	[M+^{39}K-2H]-	443.07479	443.07499	0.455	0.02258	0.8522	
C20H24O4	Crocetin(4)	[M+^{35}Cl]-	363.13690	363.13686	0.106	0.04554	1.05651	
C20H24O4		[M+Ac]-	387.18143	387.18131	0.301	0.01682	1.11464	
C20H28O2	Retinoate(11)	[M-H]-	299.20166	299.20165	0.021	0.02833	0.72064	
C20H32O2	(5Z,8Z,11Z,14Z)-Icosatetraenoic acid(10)	[M-H]-	303.23302	303.23295	0.219	0.04328	1.33774	
C20H32O4	Prostaglandin B1(19)	[M+^{39}K-2H]-	373.17885	373.17867	0.491	0.00307	0.2087	*
C20H32O6	Prostaglandin G2(4)	[M-H]-	367.21266	367.21261	0.126	0.03562	1.3433	
C20H34O5	Prostaglandin F2alpha(11)	[M+Ac]-	413.25476	413.25448	0.681	0.04215	0.45416	
C20H34O6	6-Keto-prostaglandin F1alpha(2)	[M+Ac]-	429.24968	429.24939	0.667	0.0254	1.99075	
C20H38O3	2-Oxophytanate	[M+^{39}K-2H]-	363.23086	363.23070	0.436	0.0349	0.13583	
C20H38O3		[M+^{37}Cl]-	363.24844	363.24855	0.293	0.02637	1.05404	
C20H38O3		[M+Ac]-	385.29595	385.29595	0.004	0.04981	1.02405	
C20H40O	Phytol	[M+Ac]-	355.32175	355.32177	0.052	0.04639	1.17076	
C20H40O3	L-2-Hydroxyphytanate	[M+^{39}K-2H]-	365.24651	365.24635	0.434	0.03925	0.28072	

C20H41NO2	N,N-Dimethylsphing-4-enine	[M+^{35}Cl]-	362.28333	362.28313	0.550	0.03909	0.63737	
C20H41NO2		[M+^{39}K-2H]-	364.26239	364.26234	0.149	0.01463	1.11255	
C20H41NO2		[M+Ac]-	386.32759	386.32758	0.019	0.0499	0.95852	
C21H18O7	12-Deoxyaklanonic acid	[M+Na-2H]-	403.07975	403.07992	0.431	0.04496	1.07136	
C21H20O9	Daidzin(5)	[M+^{35}Cl]-	451.08018	451.08014	0.096	0.04968	0.95466	
C21H21O12	Delphinidin 3-O-glucoside	[M+e]-	465.10370	465.10385	0.330	0.02077	1.95471	
C21H22O12	Quercetin 7-O-glucoside	[M-H]-	465.10370	465.10385	0.330	0.02078	1.95471	
C21H24O5	Rutamarin(4)	[M+Ac]-	415.17642	415.17623	0.461	0.02769	1.23602	
C21H34O2	3alpha-Hydroxy-5beta-pregnane-20-one(7)	[M-H]-	317.24865	317.24860	0.146	0.03648	0.9636	
C21H39O7P	Oleoylglycerone phosphate	[M+^{37}Cl]-	471.21002	471.20979	0.478	0.01066	0.04856	
C21H42O3	1-O-Octadec-9-enyl glycerol	[M+^{39}K-2H]-	379.26223	379.26200	0.602	0.04132	0.41739	
C22H20NO5	Chelilutine(2)	[M+^{35}Cl]-	413.10383	413.10355	0.676	0.0424	0.79668	
C22H26O4	3,6-Dimethoxyestra-1,3,5(10)	[M+Ac]-	413.19706	413.19696	0.233	0.02829	1.17898	
C22H26O6	Burseran(2)	[M-H]-	385.16577	385.16566	0.276	0.0348	1.12834	
C22H26O6		[M+^{35}Cl]-	421.14230	421.14234	0.099	0.04935	1.02722	
C22H26O6		[M+^{37}Cl]-	423.13943	423.13939	0.091	0.04922	1.04158	
C22H26O6		[M+Ac]-	445.18679	445.18679	0.008	0.02327	1.4146	
C22H26O10	Auriculoside	[M+^{39}K-2H]-	487.10094	487.10121	0.547	0.01913	1.40208	

C22H27NO3	Spiredine	[M+Na-2H]-	374.17388	374.17376	0.314	0.00406	0.55418	*
C22H27NO4	Thalicsessine(2)	[M+Ac]-	428.20809	428.20786	0.531	0.04555	1.20652	
C22H28F2O4S	Archangelicin(2)	[M+e]-	426.16832	426.16819	0.313	0.04856	0.9234	
C22H28O6	Quassin(2)	[M-H]-	387.18143	387.18131	0.301	0.01684	1.11464	
C22H28N2O3	17-O-Acetylajmaline	[M+Na-2H]-	389.18486	389.18466	0.510	0.016	1.98332	
C22H29NO2	Lobelanidine(2)	[M+Na-2H]-	360.19473	360.19450	0.645	0.02042	1.23709	
C22H29NO3	Spirasine I	[M+Na-2H]-	376.18967	376.18941	0.684	0.01029	1.56468	
C22H30F2O3	4,4-Difluoro-17beta-hydroxyandrost-5-en-3-one propionate	[M-H]-	379.20876	379.20902	0.698	0.00561	1.42699	
C22H30N2O2	Aspidospermine	[M+Na-2H]-	375.20559	375.20540	0.515	0.01644	1.54045	
C22H33NO2	Veatchine(6)	[M+Na-2H]-	364.22605	364.22580	0.693	0.00836	1.10482	
C22H33N3O5S	Formylmethionyl-leucyl-phenylalanine methyl ester	[M+^{39}K-2H]-	488.16295	488.16270	0.511	0.0243	0.66903	
C22H34O7	Coleonol	[M+^{35}Cl]-	445.19957	445.19986	0.644	0.02349	1.17008	
C22H44O2	Docosanoic acid	[M+Ac]-	399.34797	399.34798	0.034	0.03979	1.45585	
C22H44O3	13-Hydroxydocosanoic acid	[M-H]-	355.32175	355.32177	0.052	0.0464	1.17076	
C22H44O3		[M+^{39}K-2H]-	393.27785	393.27765	0.504	0.04087	0.64184	
C23H28N4	Calycanthidine	[M+Na-2H]-	381.20591	381.20606	0.406	0.02756	1.42666	
C23H31NO3	3-Hydroxy-2-(4-morpholinylmethyl)estra-	[M+Na-2H]-	390.20533	390.20506	0.685	0.01056	1.91834	

	1,3,5(10)-trien-17-one							
C23H38O4	2-Arachidonoylglycerol(2)	[M+Ac]-	437.29115	437.29086	0.655	0.04535	0.70063	
C23H38O6	Sterol 3-beta-D-glucoside	[M+^{35}Cl]-	445.23621	445.23624	0.071	0.04658	1.06135	
C23H39NO	Irehine	[M+Na-2H]-	366.27807	366.27783	0.648	0.00834	0.98242	
C23H41NO2	Terminaline	[M+^{39}K-2H]-	400.26247	400.26234	0.336	0.03654	1.29396	
C23H41NO2		[M+Ac]-	422.32777	422.32758	0.444	0.00688	1.48624	
C23H45NO4	L-Palmitoylcarnitine	[M-H]-	398.32769	398.32758	0.270	0.04398	1.17632	
C24H30O8	Yangambin(2)	[M-H]-	445.18679	445.18679	0.008	0.02328	1.4146	
C24H33NO4	Spiramine A	[M+Na-2H]-	420.21592	420.21563	0.696	0.02766	1.25697	
C24H36O2	(4Z,7Z,10Z,13Z,16Z,19Z)-Docosahexaenoic acid ethyl ester	[M+e]-	356.27189	356.27208	0.529	0.0096	1.62912	
C24H38O4	3alpha,12alpha-Dihydroxy-5beta-chol-6-enoate4	[M+e]-	390.27749	390.27756	0.176	0.0037	1.76099	*
C24H40O	3beta-Cyclopentyl-5alpha-androstan-17beta-ol	[M+e]-	344.30835	344.30846	0.330	0.02994	1.14905	
C24H40O3	3alpha-Hydroxy-5beta-cholanate	[M+e]-	376.29805	376.29829	0.647	0.01274	1.32303	
C24H40O5	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholanate(3)	[M+^{39}K-2H]-	445.23621	445.23618	0.064	0.0466	1.06135	

C24H48O2	Tetracosanoic acid	[M+Ac]-	427.37937	427.37928	0.202	0.03662	1.8001	
C25H24O6	Pomiferin	[M+Ac]-	479.17125	479.17114	0.222	0.00183	0.08851	*
C25H32O5	3beta,21-Dihydroxy-pregna-5,7,9(11)-trien-20-one diacetate	[M+^{35}Cl]-	447.19448	447.19438	0.231	0.02221	1.38707	
C25H36O5	16alpha,17beta-Dihydroxyandrost-4-en-3-one dipropionate(2)	[M+^{37}Cl]-	453.22265	453.22273	0.169	0.02515	1.94506	
C25H36O6	Glycinoeclepin A	[M+^{37}Cl]-	469.21751	469.21764	0.280	0.03069	1.85675	
C25H39NO2	3beta-(1-Pyrrolidinyl)-5alpha-pregnane-11,20-dione	[M+Na-2H]-	406.27273	406.27275	0.043	0.00454	1.34597	*
C25H39NO3	Myxalamid B	[M-H]-	400.28562	400.28572	0.244	0.03188	6.13633	
C25H41NO4	Myxalamid S	[M-H]-	418.29645	418.29628	0.400	0.03448	6.0193	
C25H41NO7	Browniine(3)	[M+e]-	467.28854	467.28885	0.669	0.00192	0.37366	*
C25H42N2O	Cyclobuxine D	[M+Ac]-	445.34388	445.34357	0.704	0.00997	0.48941	
C26H21N3O3	Oplophorus luciferin	[M+e]-	423.15882	423.15884	0.049	0.02173	1.80867	
C26H43NO3	N-Oleoyl dopamine	[M-H]-	416.31711	416.31702	0.222	0.02306	1.67185	
C27H44O	Cholest-4-en-3-one(8)	[M+e]-	384.33951	384.33976	0.660	0.0253	1.35915	
C28H42O2	beta-Tocotrienol(2)	[M-H]-	409.31128	409.31120	0.187	0.03922	1.45537	
C28H46O	4alpha-Methyl-5alpha-	[M+e]-	398.35525	398.35541	0.411	0.01692	1.29616	

	cholest-7-en-3-one(8)							
C30H42N4O2	Homaline	[M+e]-	490.33139	490.33132	0.133	0.02148	1.12921	
C30H50O	(S)-2,3-Epoxysqualene(13)	[M+e]-	426.38659	426.38671	0.290	0.02378	1.33271	
C31H52O	24-Methylenecycloartanol(2)	[M+e]-	440.40243	440.40236	0.151	0.01049	1.33799	

[a] Following removal of assignments in which the match was a non-endogenous metabolite such as a drug, plasticiser or pesticide. However, compounds such as secondary alkaloid metabolites and bacterial metabolites have not been removed and the presence of these reflects the fact that empirical formulae are insufficient for unambiguous metabolite identification. The number in parentheses represents the total number of possible metabolites that match the stated empirical formula.

[b] Fold change between the control and high dose group.

[c] Determined from t-test of peak intensities between control and high dose group.

[d] * indicates significant fold change following FDR (<5%), $p = \leq 0.05$

Table SI2. List of putative metabolite identities for polar extracts of *D. magna* neonates exposed to varying copper concentrations analysed in positive ion mode (chapter 3).

Empirical formula	Metabolite name [a]	Ion form	Observed mass (Da)	Theoretical mass (Da)	Absolute mass error (ppm)	Fold change [b]	*p*-value [c]	Significance [d]
HO3Cl	Chlorate	[M+Na]+	106.95059	106.95064	0.509	0.00666	0.80166	
C2H5NO2	Glycine (3)	[M+H]+	76.03931	76.03931	0.060	0.03401	0.93623	
C2H7NO3S	Taurine	[M+Na]+	148.00389	148.00389	0.018	0.04502	1.36281	
C2H7NO3S		[M+^{39}K]+	163.97785	163.97783	0.150	0.04805	1.14463	
C2H7NO3S		[M+2Na-H]+	169.98583	169.98583	0.014	0.04859	1.00163	
C3H5NO2	2-Aminoacrylate (2)	[M+H]+	88.03931	88.03931	0.052	0.04686	0.98053	
C3H6O3	Glycerone (3)	[M+Na]+	113.02093	113.02092	0.120	0.03926	0.86177	
C3H7O6P	Glycerone phosphate (10)	[M+H]+	171.00543	171.00530	0.734	0.00525	0.78188	
C3H7NO2	L-Alanine (8)	[M+H]+	90.05495	90.05496	0.060	0.03179	0.8486	
C3H7NO2		[M+Na]+	112.03691	112.03690	0.086	0.03617	0.86724	
C3H7NO3	L-Serine (3)	[M+H]+	106.04987	106.04987	0.004	0.04499	0.95872	
C3H8NO6P	O-Phospho-L-serine (11)	[M+H]+	186.01630	186.01620	0.519	0.00492	0.6113	
C3H8NO6P		[M+Na]+	207.99819	207.99815	0.200	0.01166	0.67259	
C3H10N2	1,3-Diaminopropane	[M+H]+	75.09168	75.09167	0.075	0.0447	0.88266	

C4H6O2	Diacetyl (5)	[M+H]+	87.04406	87.04406	0.041	0.02835	0.86196	
C4H7NO4	L-Aspartate (3)	[M+H]+	134.04477	134.04479	0.115	0.04862	1.06609	
C4H8O2S	3-(Methylthio)propionic acid (2)	[M+2Na-H]+	164.99565	164.99567	0.112	0.02982	1.09359	*
C4H9O5P	Butanoylphosphate (2)	[M+H]+	169.02615	169.02604	0.654	0.00409	0.34178	
C4H9O6P	3,4-Dihydroxy-2-butanone 4-phosphate	[M+H]+	185.02106	185.02095	0.571	0.00035	0.46747	
C4H9NO	4-Aminobutanal (3)	[M+H]+	88.07569	88.07569	0.005	0.00089	0.62907	
C4H9NO2	4-Aminobutanoate (6)	[M+H]+	104.07061	104.07061	0.044	0.03682	0.83057	
C4H9NO3	L-Threonine (2)	[M+H]+	120.06552	120.06552	0.003	0.00216	0.66749	
C4H10O2	(R,R)-Butane-2,3-diol (3)	[M+Na]+	113.05731	113.05730	0.076	0.04792	0.8704	*
C4H10O2		[M+2^{39}K-H]+	166.98720	166.98712	0.465	0.03125	1.10124	
C4H12NO4P	Phosphodimethylethanolamine	[M+H]+	170.05779	170.05767	0.686	0.0342	0.84042	
C4H12N2	Putrescine (4)	[M+H]+	89.10732	89.10732	0.049	0.00371	0.63442	
C5H7NO3	4-Oxoproline	[M+H]+	130.04987	130.04987	0.003	0.02081	0.86987	
C5H7NO3		[M+^{39}K]+	168.00577	168.00575	0.099	0.03869	0.85168	
C5H8O	Cyclopentanone	[M+H]+	85.06479	85.06479	0.016	0.04167	0.84011	
C5H8N2O2	5,6-Dihydrothymine (3)	[M+H]+	129.06585	129.06585	0.034	0.05	1.00291	
C5H8N2O2		[M+Na]+	151.04781	151.04780	0.070	0.01085	0.82743	*
C5H9NO2	L-Proline (2)	[M+H]+	116.07061	116.07061	0.040	0.02165	1.15135	

C5H9NO2		[M+^{39}K]+	154.02647	154.02649	0.119	0.00076	0.75917	
C5H9NO4	L-Glutamate (3)	[M+H]+	148.06044	148.06044	0.031	0.00982	0.62421	
C5H9NO4		[M+Na]+	170.04237	170.04238	0.061	0.00928	0.78676	
C5H9NO4		[M+2Na-H]+	192.02428	192.02433	0.236	0.01502	0.77471	
C5H9N3	1H-Imidazole-4-ethanamine (3)	[M+H]+	112.08693	112.08692	0.059	0.01991	0.89381	
C5H10O	Prenol (2)	[M+H]+	87.08044	87.08044	0.016	0.027	0.99234	*
C5H10N2O3	L-Glutamine (2)	[M+H]+	147.07643	147.07642	0.072	0.0085	0.97853	
C5H10N2O3		[M+Na]+	169.05836	169.05836	0.026	0.00473	0.72202	
C5H10N2O3		[M+^{39}K]+	185.03229	185.03230	0.067	0.03263	1.00942	
C5H11N	Piperidine (3)	[M+H]+	86.09642	86.09643	0.063	0.00214	0.63322	
C5H11NO2	L-Valine (2)	[M+H]+	118.08626	118.08626	0.039	0.02944	1.52306	*
C5H11NO2		[M+Na]+	140.06822	140.06820	0.140	0.01236	1.55116	
C5H11NO2		[M+^{39}K]+	156.04217	156.04214	0.203	0.04159	1.16036	
C5H11NO2		[M+^{41}K]+	158.04029	158.04026	0.219	0.04459	1.04896	
C5H11NO2S	L-Methionine (3)	[M+H]+	150.05832	150.05833	0.049	0.00111	0.57014	
C5H11NO2S		[M+Na]+	172.04027	172.04027	0.014	0.01258	0.69353	
C5H11NO3S	L-Methionine S-oxide	[M+H]+	166.05325	166.05324	0.046	0.0155	0.78516	
C5H14NO	Choline (2)	[M-e]+	104.10700	104.10699	0.092	0.01218	1.18248	
C6H7N	Aniline (4)	[M+H]+	94.06513	94.06513	0.049	0.01948	0.80907	*
C6H8O2	cis-1,2-Dihydrobenzene-	[M+^{39}K]+	151.01559	151.01559	0.004	0.01943	0.57661	

	1,2-diol (4)							
C6H9N3O2	L-Histidine (2)	[M+H]+	156.07679	156.07675	0.235	0.0131	0.8005	
C6H9N3O2		[M+Na]+	178.05873	178.05870	0.177	0.00917	0.80724	
C6H9N3O2		[M+^{39}K]+	194.03261	194.03264	0.136	0.01126	0.63591	
C6H10O2	2-Hydroxycyclohexan-1-one	[M+^{39}K]+	153.03123	153.03124	0.061	0.03699	0.98423	
C6H10N2O2	Ectoine (2)	[M+H]+	143.08152	143.08150	0.109	0.0224	0.83523	
C6H11O6PS	2,3-Diketo-5-methylthiopentyl-1-phosphate (2)	[M-e]+	242.00068	242.00085	0.708	0.00663	0.67786	*
C6H11NO2	L-Pipecolate (4)	[M+H]+	130.08625	130.08626	0.042	0.00503	0.89194	
C6H11NO4	L-2-Aminoadipate (5)	[M+H]+	162.07612	162.07609	0.213	0.02784	0.93536	
C6H11NO4		[M+Na]+	184.05802	184.05803	0.057	0.01182	1.72967	
C6H12O3	D-2-Hydroxyisocaproate	[M+Na]+	155.06791	155.06787	0.281	0.00092	0.46578	
C6H12O3		[M+^{39}K]+	171.04179	171.04180	0.084	0.04429	1.05531	
C6H12O6	D-Glucose (3)	[M+^{39}K]+	219.02661	219.02655	0.277	0.04175	0.75235	
C6H12N2O3	D-Alanyl-D-alanine (2)	[M+H]+	161.09211	161.09207	0.252	0.01172	1.21671	*
C6H13NO2	L-Leucine (4)	[M+H]+	132.10190	132.10191	0.041	0.00262	0.67281	
C6H13NO2		[M+Na]+	154.08384	154.08385	0.067	0.01364	0.80595	
C6H13NO3	Fagomine	[M+H]+	148.09682	148.09682	0.003	0.04911	0.95574	*
C6H13NO4	Deoxymannojirimycin (2)	[M+2Na-H]+	208.05558	208.05563	0.218	0.00969	1.82682	

C6H14N2O2	L-Lysine (3)	[M+H]+	147.11282	147.11280	0.106	0.00179	0.58758	
C6H14N2O2		[M+Na]+	169.09475	169.09475	0.004	0.01613	0.67085	
C6H14N2O2		[M+^{39}K]+	185.06870	185.06869	0.068	0.00836	0.64544	
C6H14N4O2	L-Arginine (2)	[M+H]+	175.11897	175.11895	0.101	0.00038	0.5913	
C6H14N4O2		[M+Na]+	197.10095	197.10090	0.267	0.00419	0.69732	
C6H14N4O2		[M+^{39}K]+	213.07475	213.07484	0.401	0.00211	0.47838	
C6H15O4P	Diisopropyl phosphate	[M+H]+	183.07819	183.07807	0.631	0.01935	0.82022	
C6H15N4O5P	L-Arginine phosphate (9)	[M+H]+	255.08527	255.08529	0.060	0.01034	0.81589	
C7H7NO2	Anthranilate (5)	[M+H]+	138.05497	138.05496	0.106	0.02316	1.28021	
C7H7NO2		[M+Na]+	160.03694	160.03690	0.247	0.03355	1.32573	
C7H7NO2		[M+^{39}K]+	176.01088	176.01084	0.236	0.03964	0.93669	
C7H7NO2		[M+^{41}K]+	178.00901	178.00896	0.307	0.04345	0.86097	
C7H11N3O2	N(pi)-Methyl-L-histidine (2)	[M+H]+	170.09240	170.09240	0.020	0.04015	1.16156	
C7H12O2	Ethyl 2-methylbut-2-enoate (3)	[M+^{39}K]+	167.04690	167.04689	0.063	0.01775	1.6699	
C7H12O3	trans-4-Hydroxycyclohexanecarboxylate	[M+^{39}K]+	183.04179	183.04180	0.079	0.04765	0.92249	
C7H12N2O4S	AMCC (2)	[M+2Na-H]+	265.02301	265.02295	0.240	0.00703	0.86713	
C7H13NO2	Stachydrine	[M+Na]+	166.08385	166.08385	0.002	0.01864	1.53225	*

C7H13NO2		[M+^{39}K]+	182.05781	182.05779	0.119	0.04708	1.04542	*
C7H14O6	5-O-Methyl-myo-inositol (3)	[M+Na]+	217.06832	217.06826	0.270	0.02957	1.18961	
C7H14O6		[M+^{39}K]+	233.04226	233.04220	0.260	0.02146	1.11505	*
C7H14NO2	4-(Trimethylammonio)but-2-enoate	[M-e]+	144.10192	144.10191	0.101	0.0289	1.32233	
C7H14NO3	3-Dehydrocarnitine (2)	[M-e]+	160.09687	160.09682	0.310	0.03948	1.2538	
C7H14N2O3	N-Acetylornithine (2)	[M+H]+	175.10774	175.10772	0.118	0.00828	0.7205	
C7H14N2O4	LL-2,6-Diaminoheptanedioate (3)	[M+H]+	191.10267	191.10263	0.186	0.00106	0.50124	
C7H15NO3	L-Carnitine (7)	[M+H]+	162.11251	162.11247	0.244	0.02825	1.24871	
C7H15NO3		[M+Na]+	184.09442	184.09442	0.025	0.01843	1.11045	
C7H16NO2	4-Trimethylammoniobutanoate	[M-e]+	146.11757	146.11756	0.100	0.04491	1.17981	
C7H16N4O2	Homoarginine	[M+H]+	189.13458	189.13460	0.118	0.00384	1.38291	
C7H16N4O3	(+)-gamma-Hydroxy-L-homoarginine	[M+Na]+	227.11134	227.11146	0.539	0.03839	1.01804	
C7H17N2O2	L-Carnitinamide	[M-e]+	161.12848	161.12845	0.159	0.00441	0.63299	
C7H19N3	Spermidine (2)	[M+H]+	146.16519	146.16517	0.114	0.04751	0.70195	
C8H9NO4	4-Pyridoxate (2)	[M+2Na-H]+	228.02425	228.02433	0.331	0.02903	1.39774	

C8H10O2	Tyrosol (3)	[M+^{39}K]+	177.03127	177.03124	0.173	0.02714	0.71194	
C8H11N3O3	N-Acetyl-L-histidine	[M+H]+	198.08738	198.08732	0.311	0.024	1.1549	*
C8H12N2O2	Pyridoxamine (2)	[M+H]+	169.09717	169.09715	0.092	0.02478	0.83641	
C8H12N2O4	3-(3,4-Dihydroxypyridin-1-yl)-L-alanine	[M+H]+	201.08707	201.08698	0.426	0.00265	0.48388	
C8H14O2	Cycloheptanecarboxylic acid (2)	[M+^{39}K]+	181.06256	181.06254	0.114	0.0066	0.6908	
C8H14N2O4	Proclavaminic acid (2)	[M+H]+	203.10264	203.10263	0.028	0.00484	0.59323	
C8H14N2O5	gamma-L-Glutamyl-D-alanine	[M+H]+	219.09762	219.09755	0.322	0.00306	0.57293	
C8H15NO2	Homostachydrine	[M+H]+	158.11758	158.11756	0.156	0.01591	1.31336	
C8H15NO2		[M+Na]+	180.09952	180.09950	0.109	0.01567	1.00989	
C8H15NO3	N-Acetyl-L-leucine	[M+H]+	174.11246	174.11247	0.060	0.04107	1.1989	
C8H15NO3		[M+Na]+	196.09447	196.09442	0.278	0.03285	1.03239	
C8H15NO4	Castanospermine	[M+Na]+	212.08922	212.08933	0.521	0.02332	1.06533	
C8H15N3O4	N-Acetyl-L-citrulline	[M+H]+	218.11357	218.11353	0.168	0.00403	0.40248	*
C8H16NO	Crotono-betaine	[M+41K]+	183.08454	183.08447	0.407	8.1E-05	0.41152	
C8H16N2O3	Glycyl-leucine (2)	[M-e]+	188.11554	188.11554	0.023	0.0375	0.86839	
C8H16N2O3		[M+H]+	189.12335	189.12337	0.103	0.00206	0.44608	
C8H16N2O4	N6-Acetyl-N6-hydroxy-L-lysine (2)	[M+H]+	205.11828	205.11828	0.021	0.00373	0.58367	

C8H18O2	Octane-1,8-diol (2)	[M+Na]+	169.11990	169.11990	0.008	0.01199	0.93409	
C8H18O2		[M+^{39}K]+	185.09381	185.09384	0.159	0.01356	0.71147	
C8H21N3	Homospermidine (2)	[M+H]+	160.18087	160.18082	0.291	0.00579	0.19734	*
C9H8O3	Phenylpyruvate (5)	[M+H]+	165.05464	165.05462	0.113	0.00032	0.55819	
C9H9NO3	Hippurate (4)	[M+2Na-H]+	224.02956	224.02941	0.668	0.01115	1.47879	*
C9H10O2	Tolylacetate (3)	[M+Na]+	173.05743	173.05730	0.743	0.03052	0.65241	
C9H11NO2	L-Phenylalanine (2)	[M+H]+	166.08627	166.08626	0.088	0.00146	0.50188	
C9H11NO2		[M+Na]+	188.06818	188.06820	0.108	0.00195	0.49689	
C9H11NO2		[M+^{39}K]+	204.04215	204.04214	0.057	0.00073	0.44479	
C9H11NO3	L-Tyrosine (3)	[M+H]+	182.08119	182.08117	0.108	5.4E-05	0.39336	
C9H11NO3		[M+Na]+	204.06317	204.06312	0.268	0.00709	0.57026	
C9H11NO3		[M+^{39}K]+	220.03712	220.03705	0.303	0.00438	0.55821	
C9H11N3O3	4-Acetamido-2-amino-6-nitrotoluene	[M+H]+	210.08727	210.08732	0.230	0.04808	0.93826	
C9H12O2	3-Isopropylcatechol	[M+H]+	153.09101	153.09101	0.024	0.01144	1.2109	
C9H12O4	7-Methyl-2-hydroxy-6-oxoocta-2,4-dienoate	[M+Na]+	207.06274	207.06278	0.200	0.01669	0.77132	
C9H12N2O6	Uridine	[M+Na]+	267.05870	267.05876	0.222	0.00344	0.68752	
C9H13N3O5	Cytidine	[M+H]+	244.09285	244.09280	0.211	0.00768	0.61063	
C9H14N4O3	Carnosine (2)	[M+H]+	227.11381	227.11387	0.253	0.03923	0.99404	
C9H14N4O3		[M+Na]+	249.09579	249.09581	0.090	0.023	0.96799	

C9H15N5O4	4a-Hydroxytetrahydrobiopterin (4)	[M+H]+	258.11974	258.11968	0.227	0.00446	1.24177	
C9H16N2O5	N2-Succinyl-L-ornithine (2)	[M+H]+	233.11333	233.11320	0.560	0.0003	0.47231	
C9H17NO3	8-Amino-7-oxononanoate (2)	[M+H]+	188.12811	188.12812	0.055	0.0279	1.18948	*
C9H17NO3		[M+Na]+	210.11001	210.11007	0.264	0.02746	1.10496	
C9H17NO5	Pantothenate (3)	[M+H]+	220.11799	220.11795	0.180	0.01783	0.83099	
C9H17NO5		[M+Na]+	242.09998	242.09990	0.349	0.00942	0.67344	
C9H17NO5		[M+^{39}K]+	258.07396	258.07383	0.491	0.0372	0.80169	
C9H18NO4	O-Acetylcarnitine (2)	[M-e]+	204.12304	204.12304	0.023	0.04269	0.87975	
C9H18N2O4	N2-(D-1-Carboxyethyl)-L-lysine (3)	[M+H]+	219.13400	219.13393	0.299	0.00376	0.43744	
C9H19NO4	Pantothenol (28)	[M+H]+	206.13866	206.13869	0.123	0.04045	0.88425	
C9H19N3O3	beta-Alanyl-L-lysine	[M+H]+	218.14998	218.14992	0.282	0.01082	0.5087	
C9H19N5O3	beta-Alanyl-L-arginine	[M+H]+	246.15608	246.15607	0.055	0.00985	0.53396	
C9H20N2O2	7,8-Diaminononanoate	[M+H]+	189.15973	189.15975	0.129	0.0421	1.07104	
C9H21N2O3	3-Hydroxy-N6,N6,N6-trimethyl-L-lysine	[M-e]+	205.15468	205.15467	0.052	0.02449	0.87601	
C9H21N3O	N1-Acetylspermidine	[M+H]+	188.17572	188.17574	0.098	0.00051	2.94837	*
C10H8O3	1,3,8-Naphthalenertriol (2)	[M+H]+	177.05465	177.05462	0.162	0.03834	0.82356	

C10H9NO4	4-(2-Aminophenyl)-2,4-dioxobutanoate	[M+H]+	208.06039	208.06044	0.218	0.02008	1.07011	
C10H11NO	Indole-3-ethanol (2)	[M+Na]+	184.07333	184.07329	0.242	0.00395	1.90844	
C10H11NO		[M+2Na-H]+	206.05527	206.05523	0.192	0.00422	1.82137	
C10H12O	p-Cumic aldehyde (2)	[M+Na]+	171.07816	171.07804	0.722	0.03374	0.78038	
C10H12O2	p-Cumate	[M+H]+	165.09102	165.09101	0.082	0.00668	1.22434	
C10H12O2		[M+Na]+	187.07308	187.07295	0.687	0.03252	0.60001	
C10H12N2O4	3-Hydroxykynurenine (2)	[M+H]+	225.08699	225.08698	0.025	0.00081	0.47466	
C10H12N4O5	Inosine	[M+H]+	269.08800	269.08805	0.176	0.03517	1.41782	
C10H12N4O5		[M+Na]+	291.06994	291.06999	0.180	0.04464	1.04424	
C10H13N5O4	Adenosine	[M+H]+	268.10392	268.10403	0.416	0.0063	0.42414	
C10H13N5O5	Guanosine	[M+H]+	284.09899	284.09895	0.153	0.0086	0.78916	
C10H14N2	Nicotine (2)	[M+H]+	163.12302	163.12297	0.280	0.02273	1.34564	
C10H14N2O4	Porphobilinogen	[M+H]+	227.10256	227.10263	0.328	0.02259	0.86805	
C10H14N5O7P	AMP (8)	[M+H]+	348.07020	348.07036	0.472	0.04489	1.04395	
C10H14N5O7P		[M+Na]+	370.05228	370.05231	0.079	0.03745	1.00842	
C10H16O	(+)-Camphor (2)	[M+H]+	153.12739	153.12739	0.009	0.04318	0.94521	
C10H16O		[M+Na]+	175.10938	175.10934	0.249	0.03874	0.87017	*
C10H16O		[M+^{39}K]+	191.08325	191.08327	0.128	0.02362	0.54641	*
C10H16O2	6-Oxocineole (2)	[M+^{39}K]+	207.07817	207.07819	0.094	0.01713	0.6855	
C10H16O3	5-exo-Hydroxy-1,2-	[M+^{39}K]+	223.07312	223.07310	0.070	0.01147	0.69304	

	campholide							
C10H17NO2	Acetyltropine (2)	[M+H]+	184.13321	184.13321	0.025	0.03628	1.11637	*
C10H17NO2		[M+Na]+	206.11513	206.11515	0.099	0.01036	0.91674	
C10H18O	(-)-Menthone (3)	[M+Na]+	177.12502	177.12499	0.190	0.03593	0.70372	
C10H18O2	6-endo-Hydroxycineole	[M+^{39}K]+	209.09376	209.09384	0.380	0.00787	0.75997	
C10H18O3	10-Oxodecanoate	[M+H]+	187.13284	187.13287	0.168	0.04881	0.96508	*
C10H18N2O3	Dethiobiotin (2)	[M+H]+	215.13907	215.13902	0.235	0.01526	0.73933	
C10H19NO4	O-Propanoylcarnitine (2)	[M+H]+	218.13873	218.13869	0.204	0.00181	0.66928	
C10H19NO4		[M+Na]+	240.12071	240.12063	0.332	0.02741	1.00986	
C11H8O3	1-Hydroxy-2-naphthoate (3)	[M+Na]+	211.03665	211.03657	0.396	0.04675	1.11188	*
C11H8O4	1,4-Dihydroxy-2-naphthoate	[M+H]+	205.04958	205.04954	0.213	0.04085	1.48906	
C11H12N2O2	L-Tryptophan (3)	[M+H]+	205.09715	205.09715	0.021	0.00043	0.52118	
C11H12N2O2		[M+Na]+	227.07913	227.07910	0.135	0.00244	0.58427	
C11H14O2	Eugenol methyl ether (2)	[M+H]+	179.10669	179.10666	0.188	0.03631	0.99012	
C11H15NO2	Heliamine	[M+H]+	194.11752	194.11756	0.182	0.02021	0.63816	
C11H15N2O5	N-Ribosylnicotinamide (2)	[M-e]+	255.09767	255.09755	0.473	0.02984	0.36298	
C11H16O2	3-tert-Butyl-5-methylcatechol	[M+Na]+	203.10425	203.10425	0.007	0.04275	1.01639	*
C11H21NO4	O-Butanoylcarnitine	[M+H]+	232.15446	232.15434	0.537	0.00444	0.75062	

C11H21NO4		[M+Na]+	254.13628	254.13628	0.002	0.0319	1.03769	
C12H10O	2-Hydroxybiphenyl (3)	[M+Na]+	193.06251	193.06239	0.640	0.00993	0.6823	
C12H10O2	Biphenyl-2,3-diol (3)	[M+Na]+	209.05738	209.05730	0.376	0.03055	0.86912	
C12H10O3	2,2',3-Trihydroxybiphenyl	[M+^{41}K]+	243.02421	243.02427	0.253	0.03785	0.98569	
C12H10O5	2-Hydroxy-6-oxo-6-(2-hydroxyphenyl)-hexa-2,4-dienoate	[M+Na]+	257.04219	257.04205	0.559	0.02898	1.20863	
C12H10N4O2	Carnosine	[M+Na]+	265.06971	265.06960	0.425	0.01899	0.88701	*
C12H12O2	cis-2,3-Dihydro-2,3-dihydroxybiphenyl (3)	[M+Na]+	211.07302	211.07295	0.325	0.00303	0.75869	
C12H12O3	3-Butylidene-7-hydroxyphthalide	[M+H]+	205.08593	205.08592	0.042	0.01918	1.04941	*
C12H12O3		[M+Na]+	227.06797	227.06787	0.456	0.01445	0.86996	*
C12H13NO2	Shihunine	[M+Na]+	226.08399	226.08385	0.617	0.02246	0.80384	
C12H14O3	Benzyl 2-methyl-3-oxobutanoate	[M+Na]+	229.08344	229.08352	0.334	0.01177	0.95219	
C12H15NO2	Bellendine	[M+Na]+	228.09960	228.09950	0.437	0.01723	0.69081	
C12H16O2	Thymyl acetate	[M+H]+	193.12227	193.12231	0.188	0.0023	0.5642	
C12H16O3	Benzyl (2R,3S)-2-methyl-3-hydroxybutanoate	[M+H]+	209.11718	209.11722	0.198	0.03777	0.96689	
C12H16O3		[M+Na]+	231.09908	231.09917	0.374	0.03493	1.15379	

C12H16O12	4-(4-Deoxy-beta-D-gluc-4-enuronosyl)-D-galacturonate	[M-e]+	352.06348	352.06363	0.430	0.01631	0.9485	
C12H16N2O4	3-Hydroxyhexobarbital	[M+H]+	253.11835	253.11828	0.259	0.03796	0.73911	
C12H17N4OS	Thiamin (5)	[M-e]+	265.11169	265.11176	0.262	0.00141	0.4759	
C12H20O	(Z,Z,Z)-3,6,9-Dodecatrien-1-ol	[M+H]+	181.15870	181.15869	0.047	0.00154	0.468	
C12H20O2	Ethyl(E,Z)-decadienoate (3)	[M+Na]+	219.13557	219.13555	0.085	0.03506	0.89375	
C12H20O10	Bis-D-fructose 2',1:2,1'-dianhydride	[M+H]+	325.11309	325.11293	0.503	0.0214	0.92342	
C12H20N4O3	His-Leu	[M+H]+	269.16072	269.16082	0.362	0.04267	0.1959	
C12H21NO2	Elaeokanine C	[M+H]+	212.16444	212.16451	0.308	0.03057	1.32514	*
C12H22O	Geosmin (3)	[M+H]+	183.17435	183.17434	0.047	0.01531	1.16781	
C12H22O11	Sucrose (4)	[M+Na]+	365.10541	365.10544	0.072	0.04494	1.21837	
C12H22O11		[M+^{39}K]+	381.07955	381.07937	0.461	0.02197	0.83232	
C12H22N2O2	1,8-Diazacyclotetradecane-2,9-dione	[M+H]+	227.17532	227.17540	0.372	0.00785	0.71131	
C12H24O2	Dodecanoic acid (4)	[M+H]+	201.18495	201.18491	0.217	0.00417	0.71828	
C12H24O2		[M+^{39}K]+	239.14076	239.14079	0.123	0.02083	0.91638	

C12H24N2O3	N-(6-Aminohexanoyl)-6-aminohexanoate	[M+H]+	245.18602	245.18597	0.206	0.0039	0.49417	
C13H8O	Fluoren-9-one (2)	[M+H]+	181.06481	181.06479	0.103	0.04134	1.08318	
C13H8O		[M+Na]+	203.04678	203.04674	0.215	0.01878	0.86024	
C13H10O4	2,4,6-Trihydroxybenzophenone	[M+H]+	231.06520	231.06519	0.059	0.02224	0.71657	
C13H14O2	Tremetone	[M+Na]+	225.08863	225.08860	0.127	0.02692	0.8246	
C13H16O2	4'-Hydroxy-3'-prenylacetophenone	[M+H]+	205.12228	205.12231	0.129	0.00411	1.75763	
C13H16O2		[M+Na]+	227.10423	227.10425	0.094	0.00966	1.04995	
C13H16N2O2	Melatonin (2)	[M+Na]+	255.11047	255.11040	0.277	0.02979	0.8923	
C13H23N3O4	Leu-Gly-Pro	[M+H]+	286.17609	286.17613	0.152	0.0062	0.49373	
C14H18N2O2	Hypaphorine (2)	[M+Na]+	269.12596	269.12605	0.332	0.01123	1.4024	*
C14H20N2O3	Subaphyllin (2)	[M+H]+	265.15468	265.15467	0.040	0.00547	0.53559	
C14H28O2	Tetradecanoic acid (3)	[M+H]+	229.21612	229.21621	0.377	0.01575	1.1602	
C15H10O3	Flavonol	[M+Na]+	261.05236	261.05222	0.550	0.01788	0.79446	
C15H20O2	Alantolactone	[M+Na]+	255.13569	255.13555	0.543	0.00774	0.72739	
C15H22O	alpha-Sinensal	[M+Na]+	241.15643	241.15629	0.595	0.04142	0.26548	
C15H23N6O5S	S-Adenosyl-L-methionine (3)	[M-e]+	399.14463	399.14452	0.282	0.03718	1.11916	
C15H24	Pentalenene	[M+H]+	205.19506	205.19508	0.080	0.0142	1.01292	

C15H24O	2-trans,6-trans-Farnesal	[M+H]+	221.18998	221.18999	0.052	0.00915	1.14115	
C15H26O2	Centarol	[M+H]+	239.20061	239.20056	0.224	0.04575	0.52121	
C16H16	cis-1,2-Diphenylcyclobutane	[M+Na]+	231.11450	231.11442	0.340	0.03442	0.78679	
C16H26O2	Methyl farnesoate	[M+H]+	251.20049	251.20056	0.264	0.02073	1.26183	
C16H30O4	2,3-Dihydroxycyclopentane undecanoic acid	[M+H]+	287.22161	287.22169	0.266	0.02027	1.1416	
C16H30O4		[M+^{39}K]+	325.17772	325.17757	0.463	0.00517	0.72973	
C16H32O2	Hexadecanoic acid (6)	[M+H]+	257.24755	257.24751	0.169	0.02524	1.31708	
C17H30O	(+)-12-(2-Cyclopenten-1-yl)-2-dodecanone	[M+H]+	251.23688	251.23694	0.244	0.04232	1.20366	*
C18H18O2	(S)-Indenestrol A (4)	[M+2^{39}K-H]+	343.04971	343.04972	0.036	0.00095	0.31902	
C18H32O2	9-cis,11-trans-Octadecadienoate (4)	[M+H]+	281.24754	281.24751	0.119	0.04361	1.07686	
C18H35NO2	3-Ketosphingosine	[M+Na]+	320.25603	320.25600	0.092	0.04061	1.08622	
C18H35NO2		[M+^{39}K]+	336.22994	336.22994	0.005	0.0243	0.86828	
C18H35NO2		[M+^{41}K]+	338.22797	338.22806	0.252	0.03011	0.8966	
C18H35NO3	(+)-Prosopinine	[M+Na]+	336.25091	336.25092	0.016	0.03017	1.48741	
C18H35NO3		[M+^{39}K]+	352.22511	352.22485	0.729	0.03634	1.06662	
C18H35NO3		[M+^{41}K]+	354.22315	354.22297	0.507	0.02454	1.09529	

C18H37NO	Octadecanamide (3)	[M+H]+	284.29479	284.29479	0.001	0.02048	1.37133	
C18H37NO		[M+^{39}K]+	322.25076	322.25067	0.269	0.03214	0.80431	
C18H37NO2	Sphingosine (4)	[M+H]+	300.28986	300.28971	0.515	0.01924	0.80319	
C18H37NO2		[M+Na]+	322.27177	322.27165	0.371	0.02381	0.86238	
C18H37NO2		[M+^{39}K]+	338.24558	338.24559	0.025	0.02392	0.90452	
C20H30O	Retinol (4)	[M+H]+	287.23687	287.23694	0.249	0.0089	1.51567	
C20H30O5	(5Z,13E)-11alpha-Hydroxy-9,15-dioxoprost-13-enoate (2)	[M-e]+	350.20900	350.20878	0.638	0.02078	0.94448	
C20H31NO6	Symlandine (2)	[M-e]+	381.21440	381.21459	0.499	0.01312	1.23104	
C20H32O	Kaur-16-en-18-ol (4)	[M-e]+	288.24468	288.24477	0.300	0.01529	1.3031	
C20H36O7P2	Geranylgeranyl diphosphate (4)	[M-e]+	450.19310	450.19308	0.039	0.02243	1.23443	
C20H41NO2	N,N-Dimethylsphing-4-enine	[M+H]+	328.32108	328.32101	0.227	0.01393	0.85724	
C20H41NO2		[M+Na]+	350.30275	350.30295	0.572	0.02037	1.04027	
C20H41NO2		[M+^{39}K]+	366.27687	366.27689	0.050	0.01161	0.6321	
C21H32O4	11beta,21-Dihydroxy-5beta-pregnane-3,20-dione (2)	[M-e]+	348.22975	348.22951	0.685	0.03479	1.05829	
C21H39N3O3	Cannabisativine	[M+H]+	382.30655	382.30642	0.344	0.04435	1.07866	

C22H20O	1,1-Diphenyl-2-(4-methoxyphenyl)propene	[M+^{39}K]+	339.11474	339.11457	0.488	0.00349	0.37577	*
C22H32O3	Medroxyprogesterone	[M-e]+	344.23482	344.23460	0.650	0.03577	1.02936	
C22H32O3		[M+Na]+	367.22410	367.22437	0.725	0.01902	1.45911	
C22H33NO2	Veatchine	[M+Na]+	366.24043	366.24035	0.217	0.04754	1.08386	
C22H33NO2		[M+2Na-H]+	388.22235	388.22230	0.141	0.02608	1.04999	
C23H36N4O5	N-Acetyl-leu-leu-tyr-amide (2)	[M+^{41}K]+	489.23004	489.22985	0.394	0.01015	1.02989	
C23H37O5P	3beta-Hydroxy-16-phosphonopregn-5-en-20-one monoethyl ester (3)	[M-e]+	424.23704	424.23731	0.647	0.00801	1.51723	
C23H41O6P	sn-3-O-(Geranylgeranyl) glycerol 1-phosphate	[M-e]+	444.26344	444.26353	0.201	0.00722	1.27886	
C23H45NO4	L-Palmitoylcarnitine	[M+H]+	400.34226	400.34214	0.311	0.01469	0.64321	
C23H45NO4		[M+Na]+	422.32400	422.32408	0.190	0.04997	1.06764	
C23H50N2O5P	Sphingosyl-phosphocholine	[M-e]+	465.34496	465.34519	0.489	0.0115	1.42536	
C26H42O	B-Norcholest-4-en-3-one	[M+H]+	371.33107	371.33084	0.616	0.03433	1.18576	
C26H43NO4	Glycolithocholate (2)	[M+Na]+	456.30861	456.30843	0.394	0.04694	1.11852	
C28H41NO3	Arachidonoyl dopamine	[M+H]+	440.31617	440.31592	0.567	0.01964	1.64545	
C28H45O	5,7,24(28)-Ergostatrienol	[M+^{39}K]+	436.31032	436.31020	0.276	0.02175	1.46872	

C30H44O2	2-Phytyl-1,4-naphthoquinone (2)	[M+H]+	437.34132	437.34141	0.198	0.02154	1.17798	

[a] Following removal of assignments in which the match was a non-endogenous metabolite such as a drug, plasticiser or pesticide. However, compounds such as secondary alkaloid metabolites and bacterial metabolites have not been removed and the presence of these reflects the fact that empirical formulae are insufficient for unambiguous metabolite identification. The number in parentheses represents the total number of possible metabolites that match the stated empirical formula.
[b] Fold change between the control and high dose group.
[c] Determined from t-test of peak intensities between control and high dose group.
[d] * indicates significant fold change following FDR (<5%), $p = \leq 0.05$

Table SI3 List of peaks from the 21 day chronic exposure of individual *D. magna* to cadmium (Chapter 6). These peaks are the top 107 absolute regression vectors determined from the PLS-R model for predicting reproductive output; corresponding to the fewest number of peaks that could be incorporated into the model whilst maintaining a mean cross-validated R^2 value of within 1% of the maximum cross-validated R^2. From the 107 peaks 6 can be putatively matched to one or more empirical formula in the KEGG database, and 3 unknown metabolites have both ^{12}C and ^{13}C forms (indicated as M1-M3).

Observed mass (Da)	**Theoretical mass (Da)**	**Metabolite name** [a]	**Empirical formula of putatively identified metabolite**	**Ion form**	**Absolute mass error (ppm)**	**Fold change** [b]	***p*-value** [c]	**Significance** [d]
145.06265						0.93785	0.954	
146.04667						0.15051	0.200	
175.02481	175.0248136	Ascorbate (11)	$C_6H_8O_6$	[M-H]-	0.021	0.4982	0.200	
181.07302	181.0730996	Lathyrine	$C_7H_{10}N_4O_2$	[M-H]-	0.440	6.72194	1.10×10^{-7}	***
189.03395						3.36663	0.031	*
195.05276						2.62193	0.143	
196.04518						2.199	0.158	
215.03873						2.45648	0.058	
221.08435						1.21114	0.571	

223.07285						0.51409	0.202	
225.01738						2.93751	0.004	**
226.04919						2.24145	0.043	*
226.10457						0.46084	0.517	
231.07006						0.24627	1.10×10^{-5}	***
237.99488						1.35426	0.577	
239.16571						0.35288	1.40×10^{-4}	***
241.18136						0.25911	1.86×10^{-4}	***
242.00758						5.14699	0.002	**
243.19703						0.20662	1.70×10^{-4}	***
246.0891						0.15282	4.81×10^{-8}	***
251.09631						0.50339	0.017	*
255.16069						0.53202	0.001	**
257.17634						1.03663	0.782	
265.07559						0.51533	0.005	**
267.1971						0.84556	0.451	
271.15564						0.94511	0.573	
271.22841						0.72946	0.133	
275.00834						0.70417	0.131	
277.18142						1.75767	0.016	*
277.2178		M1 (^{12}C)				0.22881	0.076	

278.22116		M1 (^{13}C)				0.2599	0.085	
281.9728						0.22339	0.002	**
283.192						0.66865	0.117	
284.19538						0.80119	0.319	
293.14414						11.0755	0.002	**
295.12263						0.42829	1.81×10^{-4}	***
295.99316						0.43751	0.048	*
297.15354		M2 (^{12}C)				7.21596	0.004	**
298.15692		M2 (^{13}C)				7.33661	0.004	**
302.95482						0.61632	0.202	
309.15608						5.05566	2.22×10^{-4}	***
318.24263						2.04412	0.104	
321.13851						0.93575	0.896	
330.13876						0.21227	8.88×10^{-5}	***
331.06003						0.14082	0.018	*
339.24852						1.16626	0.808	
340.12549						11.9927	0.107	
349.08143						0.95069	0.921	
351.0628						1.52717	0.095	
355.15541	355.1550986	Rutamarin (4)	$C_{21}H_{24}O_5$	[M-H]-	0.877	1.13825	0.875	
358.17008						0.24322	2.57×10^{-4}	***

359.22133						0.33709	0.106	
362.09486						3.09977	1.10×10^{-5}	***
366.9908						25.2065	0.127	
372.11626						0.45412	0.003	**
374.16527						0.23424	0.000	***
374.16858						0.22644	8.97×10^{-5}	***
376.10272						2.44053	0.071	
376.1808						0.14804	3.09×10^{-5}	***
379.19814						12.0314	0.176	
381.15973						0.30744	2.09×10^{-5}	***
392.17592						0.246	6.19×10^{-6}	***
392.97009						0.12792	5.07×10^{-5}	***
393.17267						9.63537	0.001	***
395.24203						0.62357	0.707	
396.11651						0.16758	1.09×10^{-5}	***
396.14684						0.21266	1.93×10^{-5}	***
399.20654						3.84952	0.001	***
400.14692						20.7368	0.119	
404.08784						4.67643	2.31×10^{-4}	***
404.21238						0.07542	1.26×10^{-5}	***
407.18841						9.41069	0.002	**

408.19173						8.21735	0.001	**
411.27628						0.16445	0.059	
416.24889						0.19034	0.001	**
417.13637						1.48886	0.281	
417.22944						8.35696	0.013	*
418.23272						6.74578	0.014	*
418.26435						0.28728	0.002	**
419.12654	419.1266916	Wuweizisu C	$C_{22}H_{24}O_6$	$[M+^{35}Cl]-$	0.362	0.3841	8.17×10^{-5}	***
420.20722						0.17117	1.27×10^{-5}	***
424.17856						0.15707	4.88×10^{-5}	***
428.21611						0.21668	1.93×10^{-5}	***
429.13624						1.39585	0.473	
431.22168						0.50391	0.351	
431.2314						0.63365	0.065	
432.24378						0.10427	1.96×10^{-5}	***
433.01987						15.6532	0.001	**
436.20219						0.2985	3.09×10^{-5}	***
441.17365						0.53448	0.167	
446.22306		M3 (^{12}C)				0.05743	3.15×10^{-6}	***
447.22649		M3 (^{13}C)				0.5738	0.125	
448.23874						0.08015	7.57×10^{-6}	***

452.21014	452.2098296	Dihydrogeranylgeranyl diphosphate	$C_{20}H_{38}O_7P_2$	[M-H]-	0.686	0.18131	1.96×10^{-5}	***
455.01478						10.1727	0.006	**
459.27644						7.54462	0.024	*
461.10856	461.1089386	Isoscoparine (3)	$C_{22}H_{22}O_{11}$	[M-H]-	0.821	14.9972	0.246	
461.25911						11.3117	0.006	**
462.21789						0.07351	4.02×10^{-6}	***
463.22135						0.95954	0.938	
468.20505						0.12274	7.17×10^{-6}	***
472.29297						0.28676	0.001	***
474.30852						0.39828	0.003	**
474.97352						0.18151	3.92×10^{-4}	***
475.17612						10.7049	0.003	**
489.19171						11.0408	0.003	**
492.18481						0.79134	0.473	

[a] Following removal of assignments in which the match was a non-endogenous metabolite such as a drug, plasticiser or pesticide. However, compounds such as secondary alkaloid metabolites and bacterial metabolites have not been removed and the presence of these reflects the fact that empirical formulae are insufficient for unambiguous metabolite identification. The number in parentheses represents the total number of possible metabolites that match the stated empirical formula.

[b] Fold change between the control and high dose group.

[c] Determined from t-test of peak intensities between control and high dose group.

[d] Significance value following FDR (<5%): *** $p = 0.005$, ** $p = 0.01$, * $p = 0.05$

Table SI4 List of peaks from the 21 day chronic exposure of individual *D. magna* to DNP (Chapter 6). These peaks are the top 502 absolute regression vectors determined from the PLS-R model for predicting reproductive output; corresponding to the fewest number of peaks that could be incorporated into the model whilst maintaining a mean cross-validated R^2 value of within 1% of the maximum cross-validated R^2. From the 502 peaks 63 can be putatively matched to one or more empirical formula in the KEGG database, and 5 unknown metabolites have both ^{12}C and ^{13}C forms (indicated as M1-M5).

Observed mass (Da)	Theoretical mass (Da)	Metabolite name [a]	Empirical formula of putatively identified metabolite	Ion form	Absolute mass error (ppm)	Fold change [b]	*p*-value [c]	Significance [d]
145.06094						0.27658	0.49422	
145.06267						0.80248	0.92011	
147.04703						0.89174	0.79687	
154.91874						0.66821	0.2994	
156.99032						1.11588	0.39776	
161.06203						0.92203	0.87478	
164.07107						0.71063	0.62566	
166.0503						0.51052	0.55893	
171.04171						0.92469	0.9697	
173.00915	173.0091636	cis-Aconitate (3)	$C_6H_6O_6$	[M-H]-	0.079	3.00393	0.00157	**
173.03877						1.39969	0.62103	

175.0248	175.0248136	Ascorbate (11)	$C_6H_8O_6$	[M-H]-	0.078	0.63557	0.54329	
181.06186						1.002	0.99375	
181.07308	181.0730996	Lathyrine	$C_7H_{10}N_4O_2$	[M-H]-	0.108	0.5738	0.54002	
182.02256	182.0225606	Glutamate (10)	$C_5H_9NO_4$	$[M+^{35}Cl]-$	0.003	1.293	0.58832	
187.037						1.5525	0.47331	
191.01881						1.39156	0.73481	
193.07176	193.0717636	5-O-Methyl-myo-inositol (9)	$C_7H_{14}O_6$	[M-H]-	0.019	1.11695	0.62103	
194.04926						0.61264	0.62103	
195.0863						4.16276	0.36289	
196.04505						0.47843	0.46411	
197.02215	197.0222266	Lichenin (19)	$C_6H_{10}O_5$	$[M+^{35}Cl]-$	0.389	1.11807	0.73662	
199.02692						1.35202	0.6539	
200.94512						0.67225	0.11997	
201.12445						1.51953	0.06743	
202.90031						1.5077	0.53676	
203.03258						0.57887	0.57282	
203.0826	203.0826016	Tryptophan (7)	$C_{11}H_{12}N_2O_2$	[M-H]-	0.008	1.61486	0.33098	
203.10373	203.1037316	N6-Acetyl-N6-hydroxylysine (2)	$C_8H_{16}N_2O_4$	[M-H]-	0.008	1.43608	0.21354	
204.08595						1.51178	0.41452	

205.0343						2.68203	0.00156	**
207.05103						0.96971	0.94736	
208.89891						1.88465	0.42264	
208.98584	208.9858416	cis-Aconitate (3)	$C_6H_6O_6$	$[M+^{35}Cl]-$	0.008	2.40845	0.01525	*
209.0655						0.90641	0.87367	
209.08273						1.24759	0.27308	
210.98289	210.9828916	cis-Aconitate (3)	$C_6H_6O_6$	$[M+^{37}Cl]-$	0.008	2.18837	0.02143	*
211.05882						0.94035	0.73481	
216.91905						0.74952	0.33979	
219.01464	219.0146436	4-Carboxy-4-hydroxy-2-oxoadipate	$C_7H_8O_8$	[M-H]-	0.016	2.37944	0.00472	**
220.08268	220.0826626	N-Acetyl-D-glucosamine (7)	$C_8H_{15}NO_6$	[M-H]-	0.008	0.42503	0.30558	
220.11905						0.88452	0.74538	
220.93639						0.66572	0.32715	
221.06667	221.0666786	6-Acetyl-D-glucose	$C_8H_{14}O_7$	[M-H]-	0.039	1.61687	0.36024	
221.08399						1.41158	0.6181	
224.97686						0.62222	0.74961	
225.01554						0.85268	0.48807	
225.09659						0.72963	0.29933	
226.09993						1.25192	0.92011	

227.06912	227.0691766	D-Mycinose	$C_8H_{16}O_5$	[M+^{35}Cl]-	0.249	0.84703	0.65228	
227.2003						0.30989	0.31863	
228.04763						1.55448	0.66458	
229.04842	229.0484416	5-O-Methyl-myo-inositol (9)	$C_7H_{14}O_6$	[M+^{35}Cl]-	0.094	1.16991	0.56322	
230.13978	230.1397826	O-Butanoylcarnitine (2)	$C_{11}H_{21}NO_4$	[M-H]-	0.011	0.89176	0.80153	
232.05912						1.05657	0.80745	
233.08384						0.50548	0.67437	
234.11542						1.38774	0.679	
235.12992						1.13545	0.72161	
237.11505						33.1148	2.3E-07	***
237.99446						0.38556	0.36081	
238.1296						1.71436	0.22454	
240.02229						0.65907	0.22454	
241.01205	241.0120566	Homocitrate (4)	$C_7H_{10}O_7$	[M+^{35}Cl]-	0.027	2.48855	0.0056	**
243.00911	243.0091066	Homocitrate (4)	$C_7H_{10}O_7$	[M+^{37}Cl]-	0.014	2.26635	0.02143	*
243.0164						0.98478	0.93982	
246.07311						0.48684	0.57128	
249.04929						0.54327	0.12622	
249.0576						0.28818	0.12168	
249.08022	249.0800146	Harmaline	$C_{13}H_{14}N_2O$	[M+^{35}Cl]-	0.825	0.85061	0.47494	

	249.0802206	2-(5-Methylthio)pentylmalic acid (2)	$C_{10}H_{18}O_5S$	[M-H]-	0.002			
249.098						0.91585	0.72161	
250.11821						0.73354	0.8196	
251.04087						2.58966	0.00157	**
251.10375	251.1037316	3-Hydroxyhexobarbital	$C_{12}H_{16}N_2O_4$	[M-H]-	0.073	1.43006	0.0695	
252.13174						0.6493	0.02143	*
252.1435						2.97041	0.54149	
253.04609						0.88266	0.62837	
253.09292	253.0928936	2-(beta-D-Glucosyl)-sn-glycerol (2)	$C_9H_{18}O_8$	[M-H]-	0.104	1.27695	0.4156	
254.09628	254.0962936	2-(beta-D-Glucosyl)-sn-glycerol (2)	$C_9H_{18}O_8$	[M-(^{13}C)H]-	0.054	1.26899	0.38351	
256.05935	256.0593406	N-Acetyl-D-glucosamine (7)	$C_8H_{15}NO_6$	[M+^{35}Cl]-	0.037	0.35173	0.28678	
256.93418						0.67347	0.3969	
257.02782						0.62667	0.4222	
257.10306		M1 (^{12}C)				0.53704	0.57019	
258.04418						0.50945	0.57538	
258.05642	258.0563906	N-Acetyl-D-glucosamine	$C_8H_{15}NO_6$	[M+^{37}Cl]-	0.114	0.30731	0.26779	

		(7)						
258.10642		M1 (^{13}C)				0.51776	0.55269	
258.90378						0.71735	0.36512	
258.93123						0.67742	0.43688	
259.02066						0.88449	0.61644	
259.10696						0.83545	0.7574	
260.13076						1.2218	0.77673	
261.12777						1.19211	0.53093	
261.13743						0.63442	0.64554	
262.11826						0.28921	0.44942	
262.14088						0.87178	0.77757	
263.04087						2.42019	0.01004	*
263.07101						0.83388	0.23236	
263.10374	263.1037316	Phenylacetylglutamine (3)	$C_{13}H_{16}N_2O_4$	[M-H]-	0.032	1.3547	0.56663	
263.14012	263.1401166	Feruloylputrescine	$C_{14}H_{20}N_2O_3$	[M-H]-	0.013	1.41991	0.27088	
264.04664						1.026	0.89844	
264.06022						1.21621	0.62566	
265.05457		M2 (^{12}C)				2.72192	0.00157	**
265.05653						2.90391	0.00318	**
265.11006						0.98904	0.9794	

266.0599		M2 (^{13}C)				2.50396	0.00171	**
267.02752						1.09677	0.68009	
267.03975						0.7948	0.30451	
267.0608						2.24838	0.00514	**
271.10662						0.81937	0.56533	
273.00814						0.78528	0.82934	
273.01019						1.01471	0.96723	
273.03815	273.0380966	1-Deoxy-D-altro-heptulose 7-phosphate	$C_7H_{15}O_9P$	[M-H]-	0.196	2.45977	0.00025	***
	273.0382716	3-Deoxyoctulosonic acid	$C_8H_{14}O_8$	$[M+^{35}Cl]-$	0.445			
	273.0382986	2-(4-Methylthio)butylmalic acid (2)	$C_9H_{16}O_5S$	$[M+^{37}Cl]-$	0.544			
273.0979						0.74489	0.56663	
273.10362						0.9111	0.73662	
273.10913						1.05478	0.93192	
273.1277						1.03899	0.90055	
274.03899	274.0390846	L-Tyrosine methyl ester 4-sulfate	$C_{10}H_{13}NO_6S$	[M-H]-	0.345	0.37035	0.53744	
274.87761						0.67881	0.27762	
275.05254						1.21517	0.74761	

277.01512						1.1692	0.67262	
277.02337						0.6338	0.35636	
277.15569						1.66901	0.12086	
278.0993						1.43041	0.35836	
278.11482						1.53132	7.3E-05	***
279.06549						0.44223	0.3959	
280.10154						0.47076	0.37581	
280.10372						0.46703	0.36289	
280.98161						8.12012	0.00024	***
281.05135						1.73808	0.15027	
282.06519						0.85607	0.47429	
282.94811	282.9482176	Terthiophene	$C_{12}H_8S_3$	$[M+^{35}Cl]-$	0.380	0.66753	0.20979	
283.06698	283.0668946	N-Acetyl-D-tryptophan (2)	$C_{13}H_{14}N_2O_3$	$[M+^{37}Cl]-$	0.302	1.48662	0.23239	
283.10334						0.96468	0.93392	
283.12272						0.80065	0.65586	
283.97891						0.74928	0.20728	
285.02355						0.6901	0.45728	
285.03551						0.58541	0.4873	
285.06461						1.04534	0.88363	
285.0856	285.0854026	N-Glucosylnicotinate (2)	$C_{12}H_{16}NO_7$	[M-H]-	0.692	1.66836	0.28572	

285.18192	285.1819816	N-Acetyl-leucyl-leucine	$C_{14}H_{26}N_2O_4$	[M-H]-	0.216	0.76732	0.79687	
293.15056						1.13185	0.75985	
294.08321						3.35427	0.0056	**
294.99208						0.95557	0.89732	
295.06694						2.4098	0.0056	**
295.11199						1.71002	0.1876	
295.12191	295.1218796	Baptifoline	$C_{15}H_{20}N_2O_2$	$[M+^{35}Cl]-$	0.103	0.60576	0.00029	***
296.11387						1.41628	0.49422	
296.13973						1.10113	0.79283	
296.98965						1.00299	0.99375	
297.98082						0.72447	0.35138	
298.95167						1.54352	0.66458	
299.09173						0.94318	0.8377	
300.01584						0.57901	0.15343	
300.04886	300.0489956	N-Acetyl-D-glucosamine 6-phosphate (5)	$C_8H_{16}NO_9P$	[M-H]-	0.452	0.73008	0.57237	
300.18153						1.10461	0.44682	
301.00944						0.65022	0.56663	
301.05949						1.65515	0.29794	
301.18498						1.13575	0.52429	
302.06616	302.0661566	Adenosine (3)	$C_{10}H_{13}N_5O_4$	$[M+^{35}Cl]-$	0.011	0.99514	0.99307	

302.0967						0.96281	0.97148	
302.1608						1.63911	0.12307	
303.0655						0.73766	0.3718	
303.06979						1.80639	0.39276	
304.22258						0.62061	0.43942	
305.02648						1.1139	0.60343	
305.02762						1.22465	0.61357	
305.07307						1.91574	0.38351	
306.97876						0.82613	0.32807	
307.04648						1.2099	0.54679	
307.08557						0.90889	0.60973	
307.09989						0.25645	0.57205	
308.11718						0.73278	0.36089	
309.04407						2.21802	0.15689	
309.08264						3.83477	0.00042	***
309.09084						0.66758	0.03996	*
309.13016						0.60271	0.2432	
309.14537						1.05819	0.91266	
310.11427						0.30866	0.23406	
310.11735						0.2363	0.43635	
314.89291						0.65333	0.36442	

315.19262						0.44111	0.51253	
316.23848						4.86984	0.33438	
317.05478						0.73844	0.37459	
317.22602						0.62337	0.54962	
318.05795						0.75633	0.42716	
319.02829						2.66609	0.1507	
319.05065						0.7271	0.19849	
320.97113						1.11731	0.75128	
321.11931						1.93231	0.08314	
321.13498						0.74698	0.8365	
321.22005	321.2201966	2-Methoxyhexadecanoate (2)	$C_{17}H_{34}O_3$	$[M+^{35}Cl]-$	0.456	0.38216	0.61797	
322.04457	323.0285946	CMP (3)	$C_9H_{14}N_3O_8P$	[M-H]-	0.0267	1.02405	0.95937	
323.02858	323.0285946	UMP (4)	$C_9H_{13}N_2O_9P$	[M-H]-	0.0452	1.24013	0.52497	
323.12635						0.65272	0.15124	
324.03193	324.0319946	UMP (4)	$C_9H_{13}N_2O_9P$	$[M(^{13}C)-H]-$	0.199	1.20708	0.56991	
324.16833						0.71049	0.36685	
324.92148						0.7517	0.55453	
326.11079						1.47351	0.67262	

327.09319						1.42433	0.25784	
328.07479						0.76404	0.08565	
329.04689						1.70557	0.17343	
331.05934						0.31265	0.57505	
331.0834						1.06008	0.82389	
332.17144						1.11757	0.57614	
333.25642		M3 (^{12}C)				0.71229	0.43808	
334.25977		M3 (^{13}C)				0.78538	0.52663	
335.06135						0.6907	0.17097	
335.09371						1.20295	0.5541	
336.06014	336.0602286	2-Deoxy-5-hydroxymethylcytidine 5-phosphate	$C_{10}H_{16}N_3O_8P$	[M-H]-	0.264	1.30561	0.56663	
336.13018						2.22012	0.00536	**
336.94509						1.4857	0.21721	
337.16166						0.68939	0.38404	
337.19801						1.89974	0.00393	**
337.23291	337.2328966	(R)-2-Hydroxystearate (3)	$C_{18}H_{36}O_3$	[M+^{37}Cl]-	0.040	2.31828	0.57289	
338.26699						0.49253	0.71996	

338.93725						0.73947	0.56845	
339.03097						0.87712	0.86043	
340.09925						1.54912	0.20292	
340.12479	340.1247436	N6-[(Indol-3-yl)acetyl]-L-lysine	$C_{16}H_{21}N_3O_3$	[M+^{37}Cl]-	0.136	2.24803	0.04825	*
	340.1249226	6-(alpha-D-Glucosaminyl)-1D-myo-inositol	$C_{12}H_{23}NO_{10}$	[M-H]-	0.390			
340.19997						0.1631	0.4551	
340.90682						0.69384	0.33693	
340.93434						0.69114	0.50055	
341.10893	341.1089386	Sucrose (29)	$C_{12}H_{22}O_{11}$	[M-H]-	0.025	2.11035	0.03961	*
341.11511						1.19683	0.51855	
341.12773						0.8734	0.62103	
342.10768						0.72475	0.627	
342.11231						2.11994	0.03532	*
343.11335	343.1131766	Arnicolide A (14)	$C_{17}H_{22}O_5$	[M+^{37}Cl]-	0.505	2.3432	0.03068	*
343.11646						1.20812	0.3909	
345.01588						1.89244	0.1327	
345.14952						0.62694	0.28577	
345.15556	345.1553146	Affinisine (3)	$C_{20}H_{24}N_2O$	[M+^{37}Cl]-	0.710	1.47486	0.80745	

346.15883						0.56643	0.62776	
348.09097						0.60662	0.16608	
348.96258						0.83794	0.62889	
349.09644						0.93116	0.78529	
349.20202	349.2020486	Prostaglandin E3 (5)	$C_{20}H_{30}O_5$	[M-H]-	0.082	0.2956	0.26888	
350.04861						1.6666	0.03996	*
351.1774						0.54663	0.29811	
351.21352						1.5214	0.10529	
352.94483						1.26201	0.19583	
352.98922						2.15556	0.01004	*
353.07302						1.24539	0.38151	
354.17616						0.57114	0.56859	
354.94312						1.19329	0.31413	
355.12469						3.25011	0.16043	
355.19865						1.45809	0.32226	
356.20205						1.38734	0.29794	
357.14755						0.83898	0.50585	
358.00761						0.68858	0.48815	
359.17109						0.09152	0.27557	
360.04297	360.0428516	1-Methylethyl glucosinolate	$C_{10}H_{19}NO_9S_2$	[M-H]-	0.329	1.85181	0.70319	

360.98454						1.3315	0.36664	
361.01288						0.73791	0.45321	
361.15351						1.01042	0.98678	
362.10687						0.39269	0.34331	
362.18203						0.9036	0.70288	
363.20229						0.54301	0.31165	
363.27526						0.9541	0.94114	
364.09137						0.95618	0.92166	
364.1724	364.1725406	2-N-Acetylparomamine	$C_{14}H_{27}N_3O_8$	[M-H]-	0.386	1.27361	0.28639	
364.95126						0.65312	0.26087	
366.14592						1.85084	0.1507	
366.18814						0.72399	0.36664	
367.03895						0.70985	0.72338	
367.08876						1.53063	0.26087	
368.09186						1.62115	0.21266	
370.07963						1.12028	0.80187	
371.20743						0.53954	0.2853	
372.03052						1.55607	0.02578	*
372.11494						0.68902	0.29383	
373.04725						0.78058	0.37533	
374.16194						0.92674	0.74548	

374.22145						0.37983	0.40265	
375.10255						1.34738	0.73481	
375.20239						0.70162	0.37533	
376.99516						0.99608	0.99359	
377.08558	377.0856166	Sucrose (29)	$C_{12}H_{22}O_{11}$	$[M+^{35}Cl]-$	0.097	1.42106	0.26888	
377.15413						0.97852	0.94677	
377.2908						0.99795	0.99737	
378.08092						0.52431	0.31328	
378.0849						0.1762	0.31282	
378.08906						1.30203	0.33318	
379.07798						1.35714	0.08585	
379.08262	379.0823286	Diphyllin	$C_{21}H_{16}O_7$	[M-H]-	0.769	1.42266	0.27557	
	379.0826666	Sucrose (29)	$C_{12}H_{22}O_{11}$	$[M+^{37}Cl]-$	0.123			
380.01544	380.0153286	N-Acetyl-D-glucosamine 1,6-bisphosphate	$C_8H_{17}NO_{12}P_2$	[M-H]-	0.293	1.4717	0.50002	
380.08623						1.42219	0.37693	
381.09497						0.90776	0.75227	
382.05206		M4 (^{12}C)				0.75571	0.62155	
382.1848						1.1776	0.55327	
383.01292						0.6371	0.62079	
383.05543		M4 (^{13}C)				0.73447	0.56793	

383.06265						1.7397	0.19023	
383.07587						0.83034	0.48836	
384.12534						0.78871	0.46411	
384.15645						1.33864	0.43106	
385.00275						0.86629	0.89678	
385.05406						1.79476	0.11219	
386.09464						0.799	0.27543	
386.10947	386.1090936	Anisessine (2)	$C_{20}H_{19}N_3O_3$	$[M+^{37}Cl]-$	0.975	1.84245	0.0466	*
387.11437						1.45679	0.20455	
388.00439						1.80702	0.03104	*
388.02508						1.67497	0.60919	
388.10978						1.0188	0.9361	
388.11771						1.41914	0.23655	
389.20994	389.2100266	Prostaglandin F2alpha (11)	$C_{20}H_{34}O_5$	$[M+^{35}Cl]-$	0.223	0.86611	0.56355	
389.21805	389.2180936	Rehmaionoside A (2)	$C_{19}H_{34}O_8$	[M-H]-	0.112	0.93618	0.75904	
390.20354						1.38393	0.20642	
391.01514						1.56646	0.16909	
391.01877						0.63768	0.29289	
391.06661						1.792	0.17597	
391.10288						1.69516	0.2732	

391.20777						0.78984	0.55783	
392.96904						1.04492	0.88645	
395.1705						0.25792	0.02287	*
395.20457						0.82533	0.64966	
396.17167						1.2943	0.27845	
397.14648						0.71485	0.25784	
397.15372						1.41761	0.39941	
398.89293						0.63095	0.49723	
399.05792						0.78518	0.41765	
399.06755						1.70077	0.18719	
399.13301						2.21339	0.23603	
401.12592						1.41821	0.26924	
401.13						1.44927	0.16909	
401.13602						1.55213	0.22389	
401.13824						1.3417	0.11796	
401.9975						1.43276	0.53676	
402.13344						1.45644	0.15978	
402.30141						0.22761	0.45935	
403.0662						1.73563	0.15689	
403.11522						1.52413	0.75624	
403.1342	403.1343066	Orizabin (2)	$C_{19}H_{26}O_7$	$[M+^{37}Cl]-$	0.140	1.53716	0.11287	

404.02856						0.67393	0.35673	
404.03395						0.72513	0.53921	
404.04758						1.12149	0.72732	
405.03172						1.34565	0.30307	
405.10443						0.55505	0.2949	
406.92461						0.66603	0.5098	
408.92166						0.5938	0.4248	
408.97423						0.82829	0.68204	
409.04951						1.16986	0.56663	
409.09637						1.53065	0.19849	
409.20745						0.57096	0.5846	
409.21999						0.59781	0.49654	
412.27854						2.18046	0.29383	
412.99786						1.30711	0.06814	
413.08678						0.8836	0.71996	
413.27687						0.88076	0.54466	
414.03189						1.10829	0.56859	
414.86676						0.6936	0.52783	
415.0416						1.91098	0.08268	
415.13837						0.68359	0.14321	
415.14588						1.73733	0.16182	

416.14882						1.46301	0.36664	
416.21506	416.2152136	Sphingosine 1-phosphate	$C_{18}H_{38}NO_5P$	$[M+^{35}Cl]-$	0.369	1.4401	0.2432	
417.03658						0.67362	0.26779	
417.21796						1.56859	0.25374	
418.13863						1.8526	0.02084	*
420.02148	420.0218536	S-(2-Chloroacetyl)glutathione (2)	$C_{12}H_{18}ClN_3O_7S$	$[M+^{37}Cl]-$	0.889	1.22702	0.60983	
420.06107						0.49192	0.21266	
420.18435						0.60785	0.23995	
420.94041						0.71083	0.56322	
421.00562						1.36177	0.30832	
421.20932						0.61512	0.64618	
422.90977						0.66782	0.38151	
422.93745						0.66278	0.52832	
423.09095						1.30541	0.23236	
423.11196		M5 (^{12}C)				1.64775	0.11219	
424.09416						1.071	0.77997	
424.11072						1.68349	0.35138	
424.11536		M5 (^{13}C)				1.62021	0.11287	

425.073						0.88578	0.90551	
425.13033						3.16352	0.21266	
426.02973	426.0300946	Glucoconringiin	$C_{11}H_{21}NO_{10}S_2$	[M+^{35}Cl]-	0.856	1.12522	0.67262	
426.06329						0.72994	0.67262	
426.13292						1.66585	0.27557	
426.23586						1.46309	0.28577	
429.05663						0.81247	0.79774	
429.07353						0.80893	0.43106	
430.00585						1.00483	0.98574	
430.15657						1.32956	0.22454	
430.17542						0.4449	0.32814	
431.13549						1.95781	0.52853	
431.14068						1.2961	0.44682	
431.2204						0.84574	0.49909	
432.14433						1.48351	0.35673	
432.22391						0.90695	0.70651	
433.0487						0.87853	0.64871	
433.07369						0.91289	0.78706	
433.15948						2.04779	0.20167	
433.22705						0.55494	0.43884	
433.23622	433.2360666	Oleoylglycerone	$C_{21}H_{39}O_7P$	[M-H]-	0.354	0.74704	0.36089	

		phosphate						
433.25483						0.63238	0.15978	
434.11907	434.1189906	Aureothin	$C_{22}H_{23}NO_6$	$[M+^{37}Cl]-$	0.183	0.66523	0.24195	
434.99271						2.28788	0.0056	**
435.04443						1.12779	0.72538	
436.25537						1.14817	0.43106	
438.88391						0.74152	0.40121	
438.91131						0.78883	0.61711	
439.08574						1.73116	0.06388	
439.19088						1.45097	0.37581	
440.99836						0.7242	0.28577	
441.14357						2.70793	0.00719	**
441.1727						0.72242	0.42256	
442.13362						0.72791	0.23995	
442.17597						0.71637	0.28805	
443.14059						2.44516	0.17815	
443.17742						1.28875	0.10618	
444.11102						0.36681	0.33294	
444.19108						0.45775	0.31848	
445.07321						1.25795	0.3969	
445.20906						0.73307	0.28577	

445.21968						1.13717	0.76932	
445.24432						0.79455	0.31581	
445.31719						0.92805	0.89922	
446.15139						1.58387	0.16909	
446.24682						0.77908	0.46463	
446.95438						0.67322	0.28572	
447.26157	447.2612946	N-Acetyl-leu-leu-tyr-amide	$C_{23}H_{36}N_4O_5$	[M-H]-	0.616	0.52639	0.31848	
449.02921						0.64175	0.54002	
450.17709						0.86386	0.77997	
451.01817						1.11488	0.63985	
451.17086						0.89817	0.82934	
451.18003						0.92982	0.88467	
452.17385						0.82482	0.77586	
454.17503						0.47769	0.32289	
455.10138						1.29186	0.29788	
456.01686						0.78154	0.41825	
456.19108						0.4399	0.34774	
456.21828						1.33961	0.43342	
456.97213						0.75665	0.55713	
457.08532						0.7357	0.49723	

457.15718						1.34231	0.24641	
457.2038						3.8578	0.0695	
458.0416						0.9281	0.72035	
458.18803						1.11569	0.66786	
458.99847						0.93841	0.88942	
459.08276						4.9376	0.47092	
459.08882						1.16485	0.55669	
459.13934						0.91944	0.73038	
459.15748						0.95331	0.9156	
459.20259	459.2024436	Aspidin (3)	$C_{25}H_{32}O_8$	[M-H]-	0.319	1.04772	0.92128	
460.16695						1.58813	0.23655	
460.19799						0.79078	0.58096	
460.20561						0.98324	0.9629	
461.08587						1.17885	0.54844	
461.10727						1.84968	0.11287	
461.18196						0.47953	0.42604	
461.20111						0.88012	0.75108	
461.26933						0.63957	0.67759	
462.27253						0.85739	0.85167	
462.96266						0.88437	0.91816	
463.19881						1.36114	0.57961	

464.05537						0.7342	0.6089	
464.25075						1.80364	0.10537	
464.98275						0.61599	0.19849	
465.06586						1.72177	0.1101	
465.12257						1.3088	0.69051	
465.30422						1.13389	0.92982	
466.24799						1.58935	0.06691	
468.24664						1.62139	0.33438	
469.11759						1.33179	0.2732	
469.15534						0.75763	0.4156	
469.20344						1.69159	0.32013	
470.00772						1.75891	0.07822	
470.1131						0.93531	0.77997	
470.12066						1.419	0.36677	
471.0328						0.69201	0.07883	
472.20359						1.34537	0.30103	
472.98616						0.76287	0.25439	
473.59174						1.31052	0.26849	
474.14668						1.47557	0.06814	
474.2859						0.89948	0.7797	
474.99544						0.68879	0.29788	

475.05587						1.53435	0.59367	
475.0627						1.29551	0.29879	
477.05985						1.27532	0.34479	
477.15477						0.64125	0.17597	
478.24776						1.34501	0.32462	
478.98157						1.61125	0.32458	
481.0612						0.87297	0.63341	
481.07037						1.29898	0.38151	
482.2067						0.61301	0.29972	
482.21624						1.27208	0.42852	
483.12635						1.27435	0.25682	
483.13321						1.36479	0.21266	
484.13653						1.36683	0.21266	
484.58268						1.34332	0.15392	
485.13654						1.52636	0.15919	
485.19199						1.21739	0.35673	
485.22448						1.15549	0.3653	
485.23665						1.22965	0.65897	
486.03695						0.65481	0.43342	
486.05095						1.02624	0.94915	
486.15457						1.33353	0.22973	

487.17793						1.18813	0.50034	
487.21507						1.39953	0.29365	
487.23418						1.19729	0.57538	
487.26003						0.74299	0.21626	
488.16224						1.51038	0.15689	
490.16048						1.57184	0.18323	
490.2161						1.56354	0.41961	

[a] Following removal of assignments in which the match was a non-endogenous metabolite such as a drug, plasticiser or pesticide. However, compounds such as secondary alkaloid metabolites and bacterial metabolites have not been removed and the presence of these reflects the fact that empirical formulae are insufficient for unambiguous metabolite identification. The number in parentheses represents the total number of possible metabolites that match the stated empirical formula.

[b] Fold change between the control and high dose group.

[c] Determined from t-test of peak intensities between control and high dose group.

[d] Significance value following FDR (<5%): *** $p = 0.005$, ** $p = 0.01$, * $p = 0.05$

Table SI5 List of peaks from the 21 day chronic exposure of individual *D. magna* to propranolol (Chapter 6). These peaks are the top 170 absolute regression vectors determined from the PLS-R model for predicting reproductive output; corresponding to the fewest number of peaks that could be incorporated into the model whilst maintaining a mean cross-validated R^2 value of within 1% of the maximum cross-validated R^2. From the 170 peaks 12 can be putatively matched to one or more empirical formula in the KEGG database, and 4 unknown metabolites have both ^{12}C and ^{13}C forms (indicated as M1-M4).

Observed mass (Da)	**Theoretical mass (Da)**	**Metabolite name** [a]	**Empirical formula of putatively identified metabolite**	**Ion form**	**Absolute mass error (ppm)**	**Fold change** [b]	***p*-value** [c]	**Significance** [d]
115.0761						0.42818	0.00698	**
116.97245						0.83571	0.5914	
156.99187						0.20532	0.39192	
175.02482	175.0248136	Ascorbate (11)	$C_6H_8O_6$	[M-H]-	0.037	0.57101	0.0507	
182.07436	182.0742006	Actinidine	$C_{10}H_{13}N$	[M+^{35}Cl]-	0.875	0.89189	0.86611	
197.07874						0.10059	0.00483	**
208.10137						0.07443	0.00027	***
209.10471						0.54013	0.11982	
221.06711						3.85882	4.26×10^{-5}	***
223.09999						1.27431	0.79598	
225.09572						1.42415	0.53489	

225.09698						0.22032	0.22271	
228.04803						0.07442	0.0005	***
232.10168						0.10031	0.00016	***
234.11734						0.0924	0.0003	***
235.09839						0.12457	0.00282	**
235.09978						0.42714	0.00834	**
236.09922						0.35346	0.14548	
237.9949						7.22542	0.27468	
238.13004						0.73208	0.27411	
239.0759						2.14605	0.4911	
241.01089						0.69969	0.51212	
242.17663						8.76496	0.05132	
249.08068						0.26201	6.10×10^{-6}	***
249.18649						0.85794	0.69933	
251.09627						0.18796	0.00077	***
253.07121						0.4974	0.00629	**
253.12867						0.65583	0.03402	*
259.09963						0.10183	0.00245	**
259.13761		M1 (^{12}C)				0.98503	0.96319	
260.14097		M1 (^{13}C)				1.1487	0.60335	
260.97627						0.38228	0.13467	

261.1133						1.74419	0.00075	***
263.11102						0.65258	0.61692	
263.13276						2.89818	0.00024	***
273.01076						0.39181	0.00447	**
274.03957						0.51928	0.3512	
275.00834						0.29806	0.00256	**
275.09446						0.06688	0.00766	**
276.95019						0.25888	0.12877	
277.2178		M2 (^{12}C)				0.73556	0.61936	
278.22116		M2 (^{13}C)				0.75308	0.63024	
279.12543						12.3816	1.13×10^{-5}	***
279.16407						1.13608	0.79051	
279.23348						1.14684	0.78468	
280.97691						0.40023	0.001	**
282.15636						1.12905	0.63192	
282.94652						0.47833	0.28005	
283.26757						0.0186	0.28351	
289.06607						1.86253	0.36869	
290.10485						0.12488	8.33×10^{-5}	***
293.0049						1.56224	0.0302	*
295.08476						1.97471	0.09612	

295.99326						0.38281	0.00736	**
296.14045						2.35782	0.08439	
296.99025						0.32987	0.00496	**
297.13679						2.52512	0.06509	
298.14028	298.1401726	Axisothiocyanate 3	$C_{16}H_{25}NS$	$[M+^{35}Cl]-$	0.360	3.60076	0.07258	
298.93225						0.59309	0.23372	
299.13285						0.69606	0.09997	
300.99552						1.33517	0.11912	
302.06417						0.88498	0.82374	
303.05067						0.36026	0.00013	***
305.01944						0.85982	0.51789	
305.06922						0.55234	0.31987	
306.07716	306.0771826	Stealthin C	$C_{18}H_{13}NO_4$	[M-H]-	0.0738	0.86455	0.65948	
307.10058	307.1007496	Sempervirine	$C_{19}H_{16}N_2$	$[M+^{35}Cl]-$	0.552	0.30932	0.4307	
309.09902						1.27737	0.45155	
310.1122						3.25818	0.25487	
310.11806						0.23676	0.29381	
313.56823						0.26134	0.00366	**
314.56673						0.3283	0.00459	**
315.12653						0.25304	0.0867	
317.24273						0.06529	0.01323	*

318.05127						0.80075	0.04979	*
318.05555						0.55775	0.01668	*
318.05873						0.28518	0.00039	***
318.23626						0.48711	0.23133	
321.00164						2.01783	0.00597	**
322.99305						0.23848	0.27198	
323.09931						4.41642	5.66×10^{-5}	***
328.0592	328.0593406	(+)-2,7-Dideoxypancratistatin	$C_{14}H_{15}NO_6$	$[M+^{35}Cl]^-$	0.429	1.0731	0.79629	
330.13317						0.19904	6.22×10^{-5}	***
331.07104						0.18658	9.76×10^{-5}	***
340.12564						5.28391	6.17×10^{-6}	***
341.02368						0.12381	0.01785	*
341.0998						1.76839	0.00039	***
342.95537						10.2996	0.00797	**
342.97964						0.45297	0.12502	
343.03803						4.51016	2.98×10^{-5}	***
343.11712						2.47688	0.00668	**
344.03324	344.0331256	N-(6-Oxo-6H-dibenzo[b,d]pyran-3-yl)maleamic acid	$C_{17}H_{11}NO_5$	$[M+^{35}Cl]^-$	0.333	0.64843	0.17408	

346.05134	346.0513056	7-Deoxypancratistatin (2)	$C_{14}H_{15}NO_7$	$[M+^{37}Cl]-$	0.099	1.56859	0.04833	*
348.1784						1.14728	0.44892	
348.96337						5.11099	0.08283	
354.17634						0.37509	0.36007	
355.1254						9.00662	1.37×10^{-5}	***
357.07507						1.69873	0.49604	
359.17181						0.28423	0.32759	
359.20245						1.03453	0.86935	
359.22124						0.93111	0.90912	
361.23688						1.45824	0.44371	
363.25248						1.92038	0.12407	
364.03564						1.21369	0.41998	
365.24721						1.33222	0.49874	
366.90146						0.84672	0.32337	
368.03863						0.57519	0.01577	*
372.10817						0.21124	0.00056	***
373.09995						1.134	0.45905	
375.01409						0.31293	0.00047	***
376.996	376.9958506	5-Fluorouridine	$C_9H_{12}FN_2O9P$	$[M+^{35}Cl]-$	0.396	0.37518	0.02111	*

		monophosphate						
379.07894						10.7353	0.05844	
380.94955						0.96903	0.87272	
382.04897	382.0487756	Hydroxysanguinarine	$C_{20}H_{13}NO_5$	$[M+^{35}Cl]-$	0.509	0.21889	0.11067	
383.24485						1.37037	0.46028	
385.26041						0.92714	0.78844	
387.23168		M3 (^{12}C)				1.16645	0.82166	
387.2761						1.52561	0.16358	
388.23506		M3 (^{13}C)				1.04104	0.92217	
389.0737						0.37384	0.5476	
390.09205						1.38393	0.05808	
390.98808						0.3687	0.00045	***
391.113	391.1131766	Cristacarpin (4)	$C_{21}H_{22}O_5$	$[M+^{37}Cl]-$	0.452	1.13714	0.6307	
392.19446						1.3899	0.22791	
392.96982						0.20406	0.00396	**
395.11796						0.1274	0.00319	**
395.1713						0.11725	0.00176	**
395.18139						4.11633	3.56×10^{-6}	***
397.14738						1.47974	0.1679	
397.18401						6.58333	0.00011	***
399.05429						0.37074	0.18785	

400.06204						0.43655	0.00411	**
400.14709						7.55816	1.13×10^{-5}	***
401.13696	401.1372566	Orizabin (2)	$C_{19}H_{26}O_7$	$[M+^{35}Cl]^-$	0.739	69.327	0.224	
404.04855						0.86311	0.579	
407.09685						0.1843	0.00061	***
409.13426						0.79052	0.42374	
411.27618						1.43253	0.55197	
413.29181		M4 (^{12}C)				0.83122	0.74325	
414.03293						6.85981	0.00104	**
414.29521		M4 (^{13}C)				0.86933	0.77587	
415.03284						0.33853	0.0002	***
415.30752						1.25509	0.58988	
419.30244						1.00314	0.99359	
425.01506						1.74457	0.24316	
425.13121						8.74011	1.26×10^{-5}	***
426.08445						0.59256	0.14996	
429.34543						1.76176	0.08283	
431.13646						0.42783	0.21567	
435.25078						0.5418	0.51463	
439.12921						0.48214	0.01668	*
441.17369						1.01089	0.97681	

441.28693						0.70301	0.21567	
442.04561						2.29842	0.06406	
443.14173						6.25407	1.19×10^{-5}	***
445.25581						1.51602	0.16132	
446.21744						0.26308	0.17408	
446.96487						1.58318	0.05009	
449.16951						1.58704	0.10502	
455.10279						1.65728	0.00672	**
457.20492						9.64834	7.83×10^{-6}	***
462.9389						0.98718	0.95373	
473.15238						4.02667	0.01582	*
474.97312						0.20876	0.0058	**
475.17586						0.62455	0.47525	
479.10855						0.31155	0.00088	***
479.18705						6.81362	3.36×10^{-5}	***
482.06567						0.42683	0.0025	**
484.99731						30.5226	0.03098	*
485.23758						0.84895	0.64104	

[a] Following removal of assignments in which the match was a non-endogenous metabolite such as a drug, plasticiser or pesticide. However, compounds such as secondary alkaloid metabolites and bacterial metabolites have not been removed and the presence of these reflects the fact that empirical formulae are insufficient for unambiguous metabolite identification. The number in parentheses represents the total number of possible metabolites that match the stated empirical formula.

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[c] Determined from t-test of peak intensities between control and high dose group.
[d] Significance value following FDR (<5%): *** $p = 0.005$, ** $p = 0.01$, * $p = 0.05$