

Supplementary Table 1: Chemical compounds characterized by LC/FIA-LTQ-Orbitrap

Compounds	Raw Formulae	Monoisotopic mass	theoretical [M+H] ⁺	theoretical [M-H] ⁻
acetic acid	C ₂ H ₄ O ₂	60.02113	61.02841	59.01385
glyoxylic acid	C ₂ H ₂ O ₃	74.00094	ND	72.99366
glycine	C ₂ H ₅ NO ₂	75.03203	76.03930	74.02475
cysteamine	C ₂ H ₇ NS	77.02992	78.03720	ND
2-pyrrolidinone	C ₄ H ₇ NO	85.05276	86.06004	ND
R-3-pyrrolidinol	C ₄ H ₉ NO	87.06841	88.07569	86.06113
pyruvic acid	C ₃ H ₄ O ₃	88.01604	ND	87.00876
isobutyric acid	C ₄ H ₈ O ₂	88.05243	89.05971	ND
putrescine	C ₄ H ₁₁ N ₂	88.10005	89.10733	ND
beta-alanine	C ₃ H ₇ NO ₂	89.04768	90.05496	88.04040
sarcosine	C ₃ H ₇ NO ₂	89.04768	90.05496	88.04040
L-lactic acid	C ₃ H ₆ O ₃	90.03169	91.03897	89.02441
isovaleric acid (3-methyl-butyric acid)	C ₅ H ₁₀ O ₂	102.06753	ND	101.06025
valeric acid (pentanoic acid)	C ₅ H ₁₀ O ₂	102.06808	103.07536	101.06080
2-methyl-butanic acid	C ₅ H ₁₀ O ₂	102.06808	103.07536	101.06080
cadaverine	C ₅ H ₁₄ N ₂	102.11570	103.12298	ND
2-aminoisobutyric acid	C ₄ H ₉ NO ₂	103.06333	104.07061	102.05605
gamma-amino butyric acid	C ₄ H ₉ NO ₂	103.06333	104.07061	102.05605
N,N'dimethylglycine	C ₄ H ₉ O ₂ N	103.06333	104.07061	102.05605
malonic acid	C ₃ H ₄ O ₄	104.01096	ND	103.00368
3-hydroxybutyric acid	C ₄ H ₈ O ₃	104.04734	ND	103.04006
2-hydroxyethyltrimethylammonium acetate (choline acetate)	C ₅ H ₁₄ NO	104.10699	105.11427	103.09971

L-serine	$C_3H_7NO_3$	105.04259	106.04987	104.03531
L-glyceric acid	$C_3H_6O_4$	106.02716	107.03444	105.01988
cytosine	$C_4H_5N_3O$	111.04326	112.05054	110.03598
histamine	$C_5H_9N_3$	111.07965	112.08693	ND
uracil	$C_4H_4N_2O_2$	112.02728	113.03456	111.02000
creatinine	$C_4H_7N_3O$	113.05892	114.06620	112.05164
Proline	$C_5H_9NO_2$	115.06334	116.07062	114.05606
fumaric acid	$C_4H_4O_4$	116.01096	117.01824	115.00368
maleic acid	$C_4H_4O_4$	116.01096	117.01824	115.00368
caproic acid	$C_6H_{12}O_2$	116.08373	ND	115.07645
betaïne	$C_5H_{11}NO_2$	117.07898	118.08626	116.07170
L-valine	$C_5H_{11}NO_2S$	117.07898	118.08626	116.07170
succinic acid	$C_4H_6O_4$	118.02661	ND	117.01933
methylmalonic acid	$C_4H_6O_4$	118.02661	ND	117.01933
homoserine	$C_4H_9NO_3$	119.05824	120.06552	118.05096
L-threonine	$C_4H_9NO_3$	119.05824	120.06551	118.05096
L-Cysteine	$C_3H_7NO_2S$	121.01975	122.02702	ND
nicotinamide	$C_6H_6N_2O$	122.04801	123.05528	ND
nicotinic acid	$C_6H_5NO_2$	123.03258	124.03985	122.02530
taurine	$C_2H_7NO_3S$	125.01466	126.02193	124.00738
5-methyl-cytosine	$C_5H_7N_3O$	125.05891	126.06618	124.05163
thymine	$C_5H_6N_2O_2$	126.04348	127.05075	125.03620
L-pyroglutamic acid	$C_5H_7NO_3$	129.04259	130.04986	128.03531
D,L-pipecolic acid	$C_6H_{11}NO_2$	129.07898	130.08625	128.07170
4-methyl-2-oxovaleric acid	$C_6H_{10}O_3$	130.06299	ND	129.05571

agmatine	C ₅ H ₁₄ N ₄	130.12185	131.12912	ND
cis-hydroxyproline	C ₅ H ₉ NO ₃	131.05824	132.06551	130.05096
creatine	C ₄ H ₉ N ₃ O ₂	131.06948	132.07675	130.06220
Isoleucine	C ₆ H ₁₃ NO ₂	131.09463	132.10190	130.08735
L-leucine	C ₆ H ₁₃ NO ₂	131.09463	132.10190	130.08735
oxaloacetic acid	C ₄ H ₄ O ₅	132.00587	ND	ND
glutaric acid	C ₅ H ₈ O ₄	132.04226	133.04953	131.03498
L-asparagine	C ₄ H ₈ N ₂ O ₃	132.05349	133.06076	131.04621
L-ornithine	C ₅ H ₁₂ N ₂ O ₂	132.08988	133.09715	131.08260
aspartic acid	C ₄ H ₇ NO ₄	133.03751	134.04478	132.03023
D-malic acid	C ₄ H ₆ O ₅	134.02207	ND	133.01479
adenine	C ₅ H ₅ N ₅	135.05450	136.06178	134.04722
hypoxanthine	C ₅ H ₄ N ₄ O	136.03906	137.04634	135.03178
trigonelline	C ₇ H ₇ NO ₂	137.04768	138.05496	136.04040
p-aminobenzoic acid	C ₇ H ₇ NO ₂	137.04768	138.05496	136.04040
tyramine	C ₈ H ₁₁ NO	137.08406	138.09134	ND
caprylic acid	C ₈ H ₁₆ O ₂	144.11503	ND	143.10775
spermidine	C ₇ H ₁₉ N ₃	145.15790	146.16518	ND
alpha-ketoglutaric acid	C ₅ H ₆ O ₅	146.02152	ND	145.01424
adipic acid	C ₆ H ₁₀ O ₄	146.05791	147.06519	145.05063
L-glutamine	C ₅ H ₁₀ N ₂ O ₃	146.06914	147.07642	145.06186
L-lysine	C ₆ H ₁₄ N ₂ O ₂	146.10553	147.11281	145.09825
L-glutamic acid	C ₅ H ₉ NO ₄	147.05316	148.06044	146.04588
L-methionine	C ₅ H ₁₁ NO ₂ S	149.05105	150.05833	148.04377
4-hydroxyphenylacetic acid	C ₈ H ₈ O ₃	152.04734	ND	151.04006
3 hydroxytyramine (dopamine)	C ₈ H ₁₁ NO ₂	153.17844	154.18572	152.17116

L-histidine	C ₆ H ₉ N ₃ O ₂	155.06948	156.07676	154.06220
orotic acid	C ₅ H ₄ N ₂ O ₄	156.01711	157.02439	155.00983
allantoin	C ₄ H ₆ N ₄ O ₃	158.04399	159.05127	157.03671
2-amino-octanoic acid	C ₈ H ₁₇ NO ₂	159.12593	160.13321	158.11865
pimelic acid	C ₇ H ₁₂ O ₄	160.07356	161.08084	159.06628
tryptamine	C ₁₀ H ₁₂ N ₂	160.10005	161.10733	ND
terbutyl-hydroxybutyrate	C ₈ H ₁₆ O ₃	160.10994	161.11722	ND
L-carnitine	C ₇ H ₁₅ NO ₃	161.10519	162.11247	ND
D,L-5-hydroxylysine	C ₆ H ₁₄ N ₂ O ₃	162.10044	163.10772	161.09316
phenylpyruvic acid	C ₉ H ₈ O ₃	164.04789	ND	163.04061
L-phenylalanine	C ₉ H ₁₁ NO ₂	165.07898	166.08626	164.07170
phthalic acid	C ₈ H ₆ O ₄	166.02661	167.03389	165.01933
3-(4-hydroxyphenyl) propionic acid	C ₉ H ₁₀ O ₃	166.06354	ND	165.05626
L-3-phenyllactic acid	C ₉ H ₁₀ O ₃	166.06354	ND	165.05626
pyridoxal	C ₈ H ₉ NO ₃	167.05824	168.06552	166.05096
3-hydroxy-4-methoxyphenethylamine	C ₉ H ₁₃ NO ₂	167.09463	168.10191	ND
3-methoxytyramine	C ₉ H ₁₃ NO ₂	167.09463	168.10191	ND
synephrine	C ₉ H ₁₃ NO ₂	167.09463	168.10191	166.08735
uric acid	C ₅ H ₄ N ₄ O ₃	168.02834	169.03562	167.02106
pyridoxamine	C ₈ H ₁₂ N ₂ O ₂	168.08988	169.09716	167.08260
pyridoxine	C ₈ H ₁₁ NO ₃	169.07389	170.08117	168.06661
N-methyl-histidine	C ₇ H ₁₁ N ₃ O ₂	169.08513	170.09241	168.07785
beta-glycerophosphate	C ₃ H ₉ O ₆ P	172.01422	173.02150	171.00694
glycylproline	C ₇ H ₁₂ N ₂ O ₃	172.08479	173.09207	171.07751
cis-aconitic acid	C ₆ H ₆ O ₆	174.01644	175.02372	173.00916
L-arginine	C ₆ H ₁₄ N ₄ O ₂	174.11113	175.11841	173.10385

3-indoleacetic acid	C ₁₀ H ₉ NO ₂	175.06388	176.07116	174.05660
citrulline	C ₆ H ₁₃ N ₃ O ₃	175.09569	176.10297	174.08841
serotonin	C ₁₀ H ₁₂ N ₂ O	176.09496	177.10224	ND
hippuric acid	C ₉ H ₉ NO ₃	179.05824	180.06552	178.05096
caffeic acid	C ₉ H ₈ O ₄	180.04226	181.04954	179.03498
L-tyrosine	C ₉ H ₁₁ NO ₃	181.07389	182.08117	180.06661
mannitol	C ₆ H ₁₄ O ₆	182.07904	183.08632	181.07176
3-phosphoglyceric acid	C ₃ H ₇ O ₇ P	185.99349	ND	184.98621
L-2-phosphoglyceric acid	C ₃ H ₇ O ₇ P	185.99349	ND	184.98621
azelaic acid	C ₉ H ₁₆ O ₄	188.10486	189.11214	187.09758
L-homoarginine	C ₇ H ₁₆ N ₄ O ₂	188.12733	189.13461	187.12005
N-acetyl-L-glutamic acid	C ₇ H ₁₁ NO ₅	189.06427	190.07155	188.05699
5-hydroxyindole-3-acetic acid	C ₁₀ H ₉ NO ₃	191.05824	192.06552	190.05096
citric acid	C ₆ H ₈ O ₇	192.02700	193.03428	191.01972
glucuronic acid	C ₆ H ₁₀ O ₇	194.04265	ND	193.03537
caffeine	C ₈ H ₁₀ N ₄ O ₂	194.08038	195.08766	ND
2-hydroxyhippuric acid	C ₉ H ₉ NO ₄	195.05371	196.06099	194.04643
methyl-L-tyrosine	C ₁₀ H ₁₃ NO ₃	195.08954	ND	ND
dimethyl-suberate	C ₁₀ H ₁₈ O ₄	202.12051	203.12779	201.11323
N,N-dimethyl-arginine	C ₈ H ₁₈ N ₄ O ₂	202.14298	203.15026	201.13570
spermine	C ₁₀ H ₂₆ N ₄	202.21575	203.22303	ND
o-acetyl-carnitine	C ₉ H ₁₇ NO ₄	203.11576	204.12304	202.10848
L-tryptophane	C ₁₁ H ₁₂ N ₂ O ₂	204.08988	205.09716	203.08260
L- kynurenine	C ₁₀ H ₁₂ N ₂ O ₃	208.08534	209.09262	207.07806
D,L-panthothenic acid	C ₉ H ₁₇ NO ₅	219.11120	220.11848	218.10392
carnosine	C ₉ H ₁₄ N ₄ O ₃	226.10659	227.11387	225.09931

2-deoxycytidine	$C_9H_{13}N_3O_4$	227.09061	228.09789	226.08333
thymidine	$C_{10}H_{14}N_2O_5$	242.09027	243.09755	241.08299
uridine	$C_9H_{12}N_2O_6$	244.06954	245.07682	243.06226
gamma-glutamylcysteine	$C_8H_{14}N_2O_5S$	250.06234	251.06962	249.05506
5-methylcytidine	$C_{10}H_{15}N_3O_5$	257.10845	258.11573	256.10117
tetradecanedioic acid	$C_{14}H_{26}O_4$	258.18311	259.19039	257.17583
hexanoyl-carnitine	$C_{13}H_{25}NO_4$	259.17836	260.18564	258.17108
alpha-D-glucose-1-phosphate	$C_6H_{13}O_9P$	260.02972	261.03700	259.02244
adenosine	$C_{10}H_{13}N_5O_4$	267.09675	268.10403	266.08947
Inosine	$C_{10}H_{12}N_4O_5$	268.08077	269.08805	267.07349
5-deoxy-5-methylthioadenosine	$C_{11}H_{15}N_5O_3S$	297.08956	298.09684	296.08228
glutathione	$C_{10}H_{17}N_3O_6S$	307.08381	308.09109	306.07653
uridine-5'-monophosphate	$C_9H_{13}N_2O_9P$	324.03587	325.04315	323.02859
inosine-5'-monophosphate	$C_{10}H_{13}N_4O_8P$	348.04710	349.05438	347.03982
cortisone	$C_{21}H_{28}O_5$	360.19367	361.20095	359.18639
guanosine-5'-monophosphate	$C_{10}H_{14}N_5O_8P$	363.05800	364.06528	362.05072
riboflavine	$C_{17}H_{20}N_4O_6$	376.13828	377.14556	375.13100
cholesterol	$C_{27}H_{46}O$	386.35487	387.36215	ND
chenodeoxycholic acid	$C_{24}H_{40}O_4$	392.29266	393.29994	391.28538
deoxycholic acid	$C_{24}H_{40}O_4$	392.29266	393.29994	391.28538
L-palmitoyl carnitine	$C_{23}H_{45}NO_4$	399.33486	400.34214	398.32758
S-5-adenosyl-L-methionine	$C_{15}H_{23}N_6O_5S$	400.15179	401.15907	ND
cholic acid	$C_{24}H_{40}O_5$	408.28757	409.29485	407.28029
folic acid	$C_{19}H_{19}N_7O_6$	441.13968	442.14696	440.13240
glycoursodeoxycholic acid	$C_{26}H_{43}NO_5$	449.31412	450.32140	448.30684
LPE 16:0/0:0	$C_{21}H_{44}NO_7P$	453.28499	454.29227	452.27771

glycocholic acid	$C_{26}H_{43}NO_6$	465.30904	466.31632	464.30176
LPC 16:0/0:0	$C_{24}H_{50}NO_7P$	495.33304	496.34032	ND
taurocholic acid	$C_{26}H_{45}NO_7S$	515.29167	516.29895	514.28439