

SUPPLEMENTARY INFORMATION

for

Metabolomics study of the Giant Clam *Tridacna maxima* reveals presence of marine microplastics

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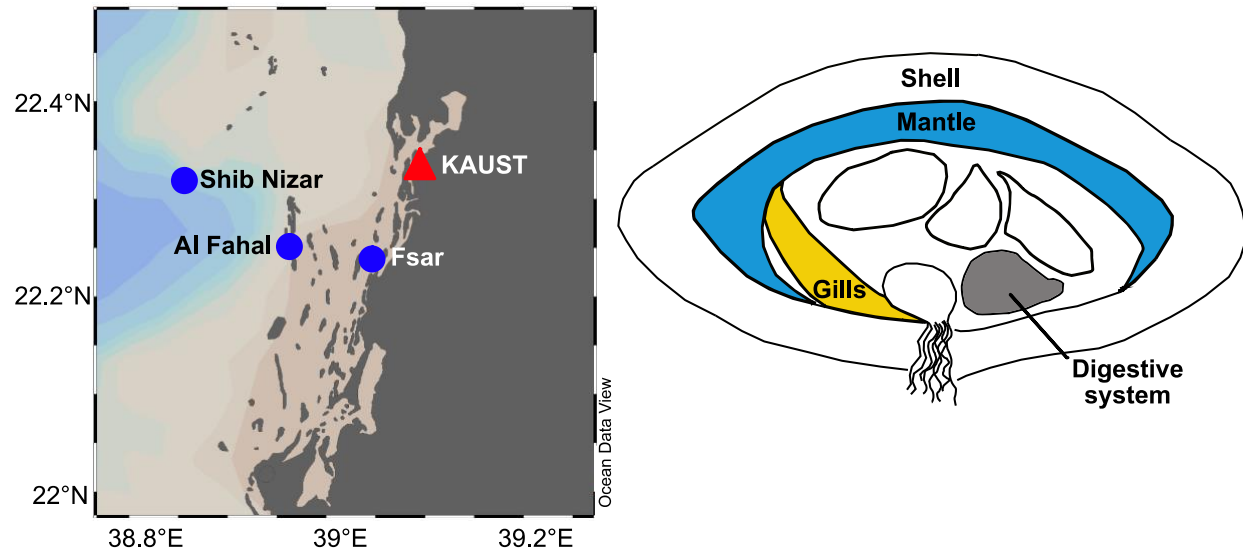


Figure 1. Sampling sites in the central Red Sea and schematic of *Tridacna maxima*, highlighting the sampled tissues (Left panel) Map showing sampled reef sites (inshore – Fsar reef, midshore – Al Fahal reef, off-shore – Shib Nizar reef). (Right panel) Schematic cross section of *T. maxima* indicating the tissue compartments sampled: outer mantle (blue), gills (yellow), and digestive system (grey).

Table 1. Summary of metabolites identified by the tissue type. (✓) indicates the metabolites detection in each tissue.

Metabolite	GC-MS	LC-MS	NMR
1-Hexadecanol	✓		
1-Kestose	✓		
1,10-Phenanthroline	✓		
1,3-Dihydroxyacetone dimer	✓		
1,5-Anhydrosorbitol	✓		
1,6-Anhydroglucose	✓		
16-hydroxypalmitic acid	✓		
2-Aminopimelic acid	✓		
2-Hydroxybutyric acid	✓		
2-Hydroxyethanesulfonate		✓	
2-Hydroxyisobutyric acid	✓		
2-Hydroxyphenylacetic acid	✓		
2-Hydroxypyridine	✓		
2-Isopropylmalic acid	✓		
2-Methylbutyrylcarnitine		✓	
2-Methylbutyrylglycine		✓	
2-Phenylglycine	✓		
2-Thiouracil	✓		
2-Toluic acid	✓		
2,3-Diaminopropionic acid	✓		
2,3-dihydroxypropyl hexadecanoate		✓	
2,3-Diphosphoglyceric acid	✓		
2,6-Diaminopurine	✓		
2,6-Pyridinedicarboxylic acid	✓		
2'-Deoxyadenosine	✓		
3-Aminopropionitrile	✓		
3-Dehydroquinate		✓	
3-Hydroxyaspartic acid	✓		
3-Hydroxybenzoic acid	✓		
3-hydroxybenzoic acid-3-O-sulphate		✓	
3-Hydroxybutyric acid	✓		
3-Hydroxypyruvate	✓		
3-Indoleacetonitrile	✓		
3-Methyl-2-oxovaleric acid	✓		
3-Methyladenine	✓		
3-Oxoadipic acid	✓		

3-Pyridylacetic acid	✓		
3,4-Dihydroxymandelic acid	✓		
3,4-Methyleneazelaic acid		✓	
3,4-Methylenesebacic acid		✓	
4-Aminohippuric acid	✓		
4-Hydroxybenzaldehyde	✓		
4-Hydroxybenzoic acid	✓		
4-Hydroxyphenylacetic acid	✓		
4-Hydroxyproline	✓		
4-Hydroxypyridine	✓		
4-Methylumbelliferone	✓		
4-O-methylolivetolcarboxylic acid		✓	
5-Aminovaleric acid	✓		
5-Dehydroquinic acid	✓		
5-Hydroxy-L-tryptophan	✓		
5-Hydroxymethyluracil	✓		
5-Keto-D-Gluconate	✓		
5,6-Dihydrouracil			✓
6-(gamma,gamma-Dimethylallylamino)purine	✓		
6-Amino-1-Methyluracil	✓		
6-Hydroxynicotinic acid	✓		
Acetaminophen		✓	
Adenine	✓		
Adenosine	✓	✓	
Adenosine monophosphate		✓	
Adipic acid	✓		
Alanylalanine	✓		
Allantoin	✓		
alpha-Ketoglutaric acid	✓		
alpha-Ketoisovaleric acid	✓		
Alpha-Lactose	✓		
alpha-Tocopherol	✓		
Amantadine	✓		
Aminoadipic acid	✓		
Aniline		✓	
Anthracene	✓		
Anthranilic acid	✓		
Apigenin	✓		
Arachidic acid	✓		
Behenic acid	✓		

Benzoic acid	✓		
beta-Alanine	✓	✓	
Beta-D-Fructose 6-phosphate	✓	✓	
Betaine			✓
Bicine	✓		
Biopterin	✓		
Cadaverine	✓		
Caffeic acid	✓		
Chlorogenic acid	✓		
Ciliatine	✓		
cis-Aconitic acid	✓		
cis-p-Coumaric acid	✓		
Citramalic acid	✓		
Citric acid	✓	✓	
Coniferaldehyde	✓		
Coniferyl alcohol	✓		
Coumarinic acid	✓		
Creatinine	✓		
Cyanine	✓		
Cystamine	✓		
Cysteamine	✓		
Cysteinyglycine	✓		
Cytosine	✓		
D-Allose	✓		
D-Allulose	✓		
D-Arabinose-5-phosphate	✓		
D-Fucose	✓		
D-Galactosamine	✓		
D-Galactose	✓		
D-Glucose	✓	✓	✓
D-Glucose-6-phosphate	✓		
D-Glutamine	✓		
D-Maltose	✓		
D-Phenyllactic acid	✓		
D-Raffinose	✓		
D-Ribulose	✓		
D-Ribulose-1,5-Bisphosphate	✓		
D-Ribulose-5-phosphate	✓		
D-Sorbitol	✓		
D-Sorbitol-6-phosphate	✓		

D-Threitol	✓		
D-Trehalose	✓		
D-Turanose	✓		
D-Xylitol	✓		
D-Xylulose	✓		
Daidzein	✓		
Deoxyadenosine monophosphate	✓		
Deoxyinosine	✓	✓	
Deoxyuridine	✓		
Dethiobiotin	✓		
Diaminopimelic acid	✓		
Dihydroxyacetone	✓		
Dimethylbenzimidazole	✓		
Dimethylglycine		✓	
DL-2-Aminooctanoic acid		✓	
DMSP			✓
Dopamine	✓		
Epigallocatechin	✓		
Epinephrine	✓		
Erucamide		✓	
Erythronic acid		✓	
Eserine	✓		
Ethionine	✓		
Ethyl glucuronide		✓	
Ethylmalonic acid	✓		
Ferulic acid	✓		
Formate			✓
Fumarate			✓
Fumaric acid	✓		
Galactitol	✓		
Galactonic acid		✓	
Gallic acid	✓		
Genistein	✓		
Gentisic acid	✓		
Glucaric acid	✓		
Gluconic acid	✓		
Glucose 6-phosphate		✓	
Glutaconic acid		✓	
Glutamylphenylalanine		✓	
Glutaric acid	✓		

Glyceraldehyde	✓			
Glyceric acid	✓			
Glycerol	✓			
Glycerol 1-phosphate	✓			
Glycine	✓			✓
Glycolic acid	✓			
Guanine	✓	✓		
Guanosine	✓			
Guanosine monophosphate		✓		
Harmaline	✓			
Heptadecanoic acid	✓			
Hippurate	✓			
Homogentisic acid	✓			
Homoserine lactone	✓			
Hydrocinnamic acid	✓			
Hydroxylamine	✓			
Hypotaurine		✓		
Hypoxanthine	✓			
Indole-3-carboxyaldehyde	✓			
Indoleacetic acid	✓			
Inosine	✓	✓		✓
Isocitric acid	✓			
Isophthalic acid	✓			
Isovalerylcarnitine		✓		
Isovalerylglycine		✓		
Kaempferol	✓			
Ketoleucine	✓			
Kojic acid	✓			
Kynurenate	✓			
L-3-Cyanoalanine	✓			
L-Alanine	✓			✓
L-Arginine	✓	✓		
L-Ascorbic acid	✓			
L-Asparagine	✓			
L-Aspartic acid		✓		
L-Carnitine		✓		
L-Citrulline	✓			
L-Cysteic acid	✓			
L-Cysteine	✓			
L-Dopa	✓			

L-Glutamic acid	✓	✓	✓
L-Glutamine	✓		✓
L-Histidine	✓		✓
L-Homocarnosine	✓		
L-Isoleucine		✓	✓
L-Leucine			✓
L-Lysine	✓		
L-Mandelic acid	✓		
L-Methionine	✓		✓
L-Norleucine	✓		
L-Ornithine	✓		
L-Phenylalanine	✓	✓	✓
L-Prolinamide	✓		
L-Proline	✓	✓	
L-Rhamnose	✓		
L-Tryptophan	✓	✓	✓
L-Tyrosine		✓	✓
L-Valine			✓
Lactate			✓
Lactic acid	✓	✓	
Lactitol	✓		
Lauric acid	✓		
Lignoceric acid	✓		
Linoleic acid	✓		
Maleamic acid	✓		
Malic acid	✓	✓	
Malonic acid	✓		
Maltotriose	✓		
Mesaconic acid	✓		
Methyldopa	✓		
Methylmalonic acid	✓	✓	
Methylsuccinic acid	✓		
Methyluracil	✓		
Minoxidil	✓		
Monoethylhexyl phthalic acid		✓	
Myo-Inositol	✓		
Myricetin	✓		
N-Acetyl-L-aspartic acid	✓		
N-Acetylleucine	✓		
N-Acetylmannosamine	✓		

N-alpha-Acetyl-L-lysine	✓	
N-Methylalanine	✓	
N-Methylethanolamine	✓	
Nicotinic acid		✓
Norvaline	✓	
O-Acetylserine	✓	
O-Phosphoethanolamine	✓	
O-Succinyl-L-Homoserine	✓	
Octacosanoic acid	✓	
Oxoglutaric acid		✓
Palmitic acid	✓	
Pantothenic acid	✓	✓
Pelargonic acid	✓	
Penicillamine	✓	
Pentachlorophenol	✓	
Phenylephrine	✓	
Phenylhydrazine	✓	
Phosphoenolpyruvic acid	✓	
Phosphoric acid		✓
Picolinic acid	✓	
Pimelic acid	✓	
Pipecolic acid	✓	
Pirbuterol		✓
Podophyllotoxin	✓	
Prephenate	✓	
Proline betaine		✓
Propyleneglycol	✓	
Protocatechuic acid	✓	
Psoralen	✓	
Putrescine	✓	
Pyrogalllic acid	✓	
Pyroglutamic acid	✓	✓
Pyrophosphate	✓	
Pyruvic acid	✓	
Quinic acid	✓	
Quinolinic acid	✓	
S-Adenosylmethionine	✓	
S-Carboxymethyl-L-cysteine	✓	
Sakuranetin	✓	
Sarcosine	✓	

Serotonin	✓		
Shikimic acid	✓		
Sinapic acid	✓		
Sinapyl aldehyde	✓		
Sinigrin	✓		
Spermine	✓		
Stearic acid	✓		
Suberic acid	✓		
Succinic acid	✓		✓
Sucrose	✓		
Tartaric acid	✓		
Taurine	✓	✓	✓
Terephthalic acid	✓		
Tetrahydro-2,5-furan-diacetic acid		✓	
Thymine	✓		
Tranexamic Acid		✓	
Trifluoroacetic acid		✓	
Trigonelline		✓	✓
Uracil	✓		✓
Urea	✓		
Ureidosuccinic acid	✓		
Uric acid	✓		
Uridine	✓		
Uridine 5-diphosphate N-acetylgalactosamine		✓	
Uridine 5-diphospho-N-acetylglucosamine	✓	✓	
Uridine 5_monophosphate		✓	
Vanillylmandelic acid	✓		
Xanthine	✓		
Xanthosine	✓		
Xanthurenic acid	✓		

Table 2. List of the quantified signal and their relative assignment and multiplicity detected by NMR

Metabolite	Assignment
nicotinic acid derivate 1	9.26 (s)
nicotinic acid derivate 2	9.24 (s)
nicotinic acid derivate 3	9.22 (s)
trigonelline	<u>9.12 (s)</u>
nicotinic acid derivate 4	8.98 (s)
nicotinamide derivate 1	8.71 (d)
nicotinamide derivate 2	8.69 (s)
nicotinamide derivate 4	8.82 (s)
nicotinamide derivate 8	8.65 (s)
aminohippuric acid related	8.54 (t)
formate	<u>8.44 (s)</u>
pyridinecarboxylic acid derivate 1	8.41 (d)
pyridinecarboxylic acid derivate 2	8.39 (d)
6-oxopurine derivate 1	8.27 (s)
6-oxopurine derivate 2	8.26 (s)
	<u>8.23 (s);</u>
inosine	6.09 (d)
6-oxopurine derivate 3	8.19 (s)
6-oxopurine derivate 4	8.04 (s)
6-oxopurine derivate 5	8.03 (s)
6-oxopurine derivate 6	8.00 (s)
nicotinic acid derivate 5	7.97 (t)
6-oxopurine derivate 7	7.68 (s)
6-oxopurine derivate 8	7.59 (s)
tryptophan	<u>7.74 (d)</u>
phenylalanine	<u>7.42 (m)</u>
	7.19 (m);
tyrosine	<u>6.89 (m)</u>
histidine	<u>7.10 (s)</u>
fumarate	<u>6.54 (s)</u>
nucleotide related 1	6.14 (d)
nucleotide related 2	6.12 (d)
uracil	<u>5.80 (d)</u>
carbohydrate 1	5.41 (d)
carbohydrate 2	5.40 (d)
carbohydrate 3	5.34 (d)
carbohydrate 4	5.26 (d)
glucose	<u>5.23 (d)</u>
	<u>3.90 (s);</u>
betaine	3.27 (s)
glycine	<u>3.56 (s)</u>
5,6-dihydrouracil	<u>3.46 (t)</u>
taurine	<u>3.43 (t)</u>
	3.46(t);
	<u>2.91 (s);</u>
DMSP	<u>2.74(t)</u>
methionine related	2.74 (t)
methionine	<u>2.64 (t)</u>
glutamine	<u>2.45 (d)</u>
succinate	<u>2.41 (s)</u>
glutamate	<u>2.37 (s)</u>
4-aminobutyric acid related 1	2.30 (t)

4-aminobutyric acid related 2	2.26 (t)
alanine related	1.51 (d)
alanine	<u>1.48 (d)</u>
lactate	<u>1.35 (d)</u>
unidentified methyl signal 1	1.09 (s)
	<u>1.04 (d);</u>
valine	0.99 (d)
	<u>1.01 (d);</u>
isoleucine	0.94 (t)
	<u>0.96 (d);</u>
leucine	0.96 (d)
unidentified methyl signal 2	0.89 (s)

* underline indicated the signals used for the following analysis

s=singlet; d=doublet; t=triplet; m=multiplet

Table 3. Comparison analysis among different tissues.

metabolite	Tissue, median [95%CI]			p-value	FDR
	Gills	Outer mantle	Digestive system		
nicotinic acid derivates 1	0.572 [0.423 1.258]	1.353 [0.843 2.059]	0.772 [0.553 1.484]	6.13E-06	9.54E-06
nicotinic acid derivates 2	0.63 [0 4.269]	0.7 [0.084 1.675]	0.653 [0 3.735]	9.80E-01	9.80E-01
nicotinic acid derivates 3	0.373 [0 3.108]	0.762 [0.265 1.33]	0.919 [0 5.311]	5.52E-02	6.18E-02
nicotinic acid derivates 4	0.633 [0.298 1.514]	1.416 [0.522 2.147]	0.561 [0.429 2.229]	2.17E-02	2.54E-02
nicotinamides derivates 1	0.76 [0.502 1.265]	0.256 [0.157 0.491]	1.823 [1.197 3.285]	1.33E-10	3.13E-09
nicotinamides derivates 2	0.185 [0 0.463]	2.549 [0.98 4.062]	0.306 [0 0.806]	9.33E-09	3.48E-08
nicotinamides derivates 3	0.077 [0 0.437]	2.506 [1.352 4.173]	0.264 [0.05 0.704]	5.20E-09	2.08E-08
nicotinamides derivates 4	0.192 [0 0.521]	2.54 [0.831 3.89]	0.345 [0.103 1.01]	1.23E-08	4.31E-08
Aminohippuric acid related	0.759 [0.488 1.229]	0.275 [0.163 0.524]	1.789 [1.169 3.239]	1.78E-10	3.13E-09
pyridinecarboxylic acids derivates 1	0.252 [0.059 0.704]	2.284 [1.273 3.746]	0.227 [0 1.375]	3.86E-08	1.03E-07
pyridinecarboxylic acids derivates 2	0.104 [0.014 0.379]	2.589 [1.337 3.663]	0.33 [0.058 0.803]	2.28E-09	1.41E-08
6-Oxopurine derivate 1	0.348 [0.116 0.982]	2.51 [0.906 3.554]	0.042 [0 0.236]	3.74E-10	4.18E-09
6-Oxopurine derivate 2	0.439 [0.086 0.716]	1.155 [0 5.371]	0.613 [0.026 2.326]	6.41E-01	6.53E-01
6-Oxopurine derivate 3	0.268 [0.111 2.102]	0.238 [0.106 0.382]	1.903 [0.872 4.825]	1.38E-07	3.09E-07
6-Oxopurine derivate 4	0.784 [0.498 1.175]	0.19 [0.082 0.428]	1.928 [1.247 3.801]	9.86E-11	3.13E-09
6-Oxopurine derivate 5	1.072 [0.677 2.045]	0.217 [0.107 0.354]	1.48 [0.98 2.756]	4.26E-09	1.84E-08
6-Oxopurine derivate 6	0.995 [0.518 1.712]	0.644 [0.177 2.4]	1.03 [0.179 2.711]	2.58E-02	2.95E-02
nicotinic acid derivates 5	0.632 [0.44 0.972]	1.093 [0.454 1.509]	1.292 [0.829 2.419]	1.24E-05	1.86E-05
6-Oxopurine derivate 7	1.185 [0.445 3.349]	0.672 [0.271 1.195]	0.42 [0.076 3.331]	1.09E-03	1.39E-03
6-Oxopurine derivate 8	0.106 [0 4.358]	0.064 [0.006 0.283]	2.099 [0.019 6.551]	1.79E-02	2.13E-02
nucleotides related 1	0.51 [0.08 1.282]	1.749 [0.432 3.815]	0.502 [0 1.21]	2.53E-06	4.17E-06
nucleotides related 2	0.565 [0.205 1.562]	1.102 [0.587 3.389]	0.73 [0.121 1.998]	2.56E-04	3.42E-04
carbohydrated 1	0.09 [0 1.277]	0.61 [0.141 2.236]	1.937 [0 6.286]	5.49E-05	7.51E-05
carbohydrated 2	0.016 [0 2.336]	0.199 [0.02 1.501]	2.344 [0.314 5.845]	1.85E-06	3.23E-06
carbohydrated 3	0.141 [0 0.494]	1.149 [0.661 2.803]	1.596 [0.18 2.825]	1.56E-07	3.24E-07
carbohydrated 4	0 [0 0.493]	2.701 [1.122 4.444]	0 [0 1.861]	1.81E-09	1.27E-08
methionine related	1.287 [1.013 1.566]	1.377 [0.729 2.303]	0.217 [0 0.434]	2.96E-08	8.37E-08
4-Aminobutyric acid related 1	0 [0 0.625]	2.874 [0.913 5.133]	0 [0 0]	2.24E-10	3.13E-09
4-Aminobutyric acid related 2	0.172 [0 0.683]	2.537 [1.279 4.314]	0 [0 0]	4.67E-10	4.36E-09
L-Alanine related	0.053 [0 0.536]	2.237 [0.654 5.68]	0 [0 0.866]	3.99E-09	1.84E-08
unidentified methyl signal 1	0.311 [0.165 0.708]	1.031 [0.395 2.286]	1.419 [0.267 3.082]	4.93E-06	7.89E-06
unidentified methyl signal 2	0 [0 2.362]	1.597 [0.548 3.167]	0.82 [0.166 1.935]	1.80E-06	3.23E-06
Trigonelline	0.639 [0.401 1.133]	1.192 [0.872 1.699]	1.163 [0.632 1.942]	1.97E-06	3.34E-06
Formate	0.469 [0.301 0.859]	1.753 [1.079 3.062]	0.59 [0.253 1.141]	2.99E-08	8.37E-08
Inosine	0.804 [0.462 1.315]	1.116 [0.94 1.421]	1.037 [0.703 1.45]	5.32E-05	7.45E-05
L-Tryptophan	0.915 [0.439 1.732]	0.483 [0.349 0.634]	1.102 [0.366 3.452]	6.48E-04	8.44E-04
L-Phenylalanine	1.437 [0.708 2.031]	0.495 [0.406 0.595]	1.022 [0.613 2.429]	1.86E-08	6.11E-08
L-Histidine	1.155 [0.481 2.715]	0.783 [0.45 1.178]	NA [NA NA]	1.29E-02	1.57E-02
L-Tyrosine	1.258 [0.645 2.454]	0.721 [0.619 0.866]	0.802 [0.671 1.156]	2.48E-05	3.56E-05
Fumarate	1.425 [0.865 1.695]	0.381 [0.144 1.001]	1.172 [0.428 2.186]	5.43E-07	1.05E-06
Uracil	0.944 [0.638 2.509]	0.611 [0.517 0.959]	0.927 [0.126 3.239]	7.45E-03	9.27E-03
D-Glucose	0.338 [0.132 0.794]	0.943 [0.579 1.654]	1.676 [0.911 3.385]	3.25E-09	1.65E-08
Betaine	0.791 [0.596 1.164]	0.875 [0.615 1.121]	1.277 [0.891 1.715]	1.73E-06	3.23E-06
Glycine	0.188 [0.123 0.339]	0.722 [0.407 1.291]	2.224 [0.471 3.193]	1.47E-09	1.18E-08
5,6-Dihydrouracil	1.225 [0.831 1.44]	1.254 [0.767 2.168]	0.341 [0.17 0.634]	6.08E-08	1.55E-07
Taurine	1.008 [0.75 1.257]	0.883 [0.643 1.411]	1.002 [0.715 1.409]	4.11E-01	4.26E-01
DMSP	1.262 [0.998 1.521]	1.351 [0.843 2.12]	0.277 [0.077 0.559]	2.64E-08	8.20E-08
L-Methionine	0.457 [0.265 0.809]	1.572 [0.714 2.853]	0.813 [0.412 1.422]	8.60E-08	2.09E-07
L-Glutamine	1.083 [0.28 2.643]	0.863 [0.449 1.541]	0.786 [0.251 1.198]	1.37E-01	1.45E-01
Succinate	0.601 [0.297 0.797]	1.992 [1.2 3.002]	0.151 [0.033 1.151]	2.51E-09	1.41E-08
L-Glutamate	0.951 [0.571 1.543]	0.856 [0.411 1.483]	1.234 [0.308 1.858]	5.66E-02	6.21E-02
L-Alanine	0.895 [0.69 1.387]	0.952 [0.625 1.21]	1.019 [0.784 1.616]	1.27E-01	1.37E-01
Lactate	1.039 [0.818 1.618]	1.294 [0.851 1.645]	0.679 [0.082 1.059]	2.32E-07	4.64E-07
L-Valine	1.382 [0.56 3.107]	0.495 [0.368 0.626]	0.815 [0.387 1.254]	1.45E-07	3.11E-07
L-Isoleucine	1.291 [0.484 3.361]	0.575 [0.354 0.686]	0.756 [0.286 1.254]	1.26E-05	1.86E-05
L-Leucine	1.373 [0.562 3.784]	0.498 [0.307 0.593]	0.783 [0.369 1.259]	9.44E-08	2.20E-07

* p-value calculated using Kruskal-Wallis rank sum test

NA= metabolites present but couldn't quantify it

Table 4. Correlation between metabolites identified by NMR and distance of sample collection.

metabolite	Gill			Outer mantle			Digestive system		
	rho	p-value	FDR	rho	p-value	FDR	rho	p-value	FDR
nicotinic acid derivates 1	0.1	6.79E-01	8.92E-01	0.37	1.34E-01	3.35E-01	0.02	9.33E-01	9.89E-01
nicotinic acid derivates 2	-0.05	8.35E-01	9.37E-01	-0.24	3.46E-01	5.53E-01	0.18	4.84E-01	7.77E-01
nicotinic acid derivates 3	-0.22	3.89E-01	7.06E-01	-0.16	5.33E-01	7.65E-01	0.72	1.16E-03	1.53E-02
nicotinic acid derivates 4	-0.25	3.19E-01	6.61E-01	0.26	2.93E-01	5.13E-01	0.41	1.05E-01	2.79E-01
nicotinamides derivates 1	0.05	8.36E-01	9.37E-01	-0.08	7.56E-01	9.41E-01	-0.04	8.90E-01	9.89E-01
nicotinamides derivates 2	-0.33	1.75E-01	5.06E-01	-0.34	1.66E-01	3.45E-01	0.28	2.73E-01	5.16E-01
nicotinamides derivates 3	-0.43	7.76E-02	2.72E-01	-0.3	2.24E-01	4.32E-01	0.54	2.64E-02	1.27E-01
nicotinamides derivates 4	0.09	7.17E-01	8.92E-01	-0.37	1.34E-01	3.35E-01	0.54	2.47E-02	1.27E-01
Aminohippuric acid related	0.04	8.77E-01	9.37E-01	-0.33	1.84E-01	3.68E-01	0.02	9.25E-01	9.89E-01
pyridinecarboxylic acids derivates 1	-0.16	5.33E-01	8.29E-01	0	1.00E+00	1.00E+00	0.58	1.50E-02	1.25E-01
pyridinecarboxylic acids derivates 2	-0.29	2.46E-01	5.73E-01	-0.39	1.06E-01	3.31E-01	0.52	3.35E-02	1.48E-01
6-Oxopurine derivate 1	-0.13	6.04E-01	8.67E-01	-0.16	5.33E-01	7.65E-01	-0.06	8.11E-01	9.89E-01
6-Oxopurine derivate 2	-0.18	4.66E-01	7.45E-01	0.11	6.69E-01	9.05E-01	0.39	1.18E-01	2.98E-01
6-Oxopurine derivate 3	0.09	7.17E-01	8.92E-01	0.01	9.59E-01	9.94E-01	0.49	4.60E-02	1.74E-01
6-Oxopurine derivate 4	0.09	7.17E-01	8.92E-01	-0.17	4.99E-01	7.55E-01	0.2	4.35E-01	7.21E-01
6-Oxopurine derivate 5	-0.12	6.41E-01	8.75E-01	-0.35	1.49E-01	3.35E-01	0.32	2.07E-01	4.57E-01
6-Oxopurine derivate 6	-0.31	2.03E-01	5.18E-01	-0.52	2.54E-02	1.29E-01	-0.63	6.85E-03	7.26E-02
nicotinic acid derivates 5	-0.08	7.56E-01	9.01E-01	-0.47	4.79E-02	1.92E-01	0.05	8.35E-01	9.89E-01
6-Oxopurine derivate 7	0.46	5.53E-02	2.21E-01	-0.51	3.00E-02	1.40E-01	-0.81	8.68E-05	2.30E-03
6-Oxopurine derivate 8	0.05	8.36E-01	9.37E-01	-0.03	9.18E-01	9.88E-01	0.57	1.81E-02	1.25E-01
nucleotides related 1	-0.28	2.69E-01	6.02E-01	-0.37	1.34E-01	3.35E-01	0.03	9.01E-01	9.89E-01
nucleotides related 2	-0.12	6.41E-01	8.75E-01	-0.5	3.53E-02	1.52E-01	0.11	6.73E-01	9.39E-01
unidentified carbohydrated 1	0.65	3.53E-03	3.22E-02	-0.01	9.59E-01	9.94E-01	-0.27	2.94E-01	5.28E-01
unidentified carbohydrated 2	0.74	4.21E-04	2.36E-02	0.07	7.96E-01	9.48E-01	-0.05	8.39E-01	9.89E-01
unidentified carbohydrated 3	0.24	3.40E-01	6.81E-01	-0.68	1.82E-03	4.49E-02	-0.82	5.08E-05	2.30E-03
unidentified carbohydrated 4	-0.02	9.25E-01	9.59E-01	-0.35	1.49E-01	3.35E-01	-0.01	9.79E-01	9.96E-01
methione related	-0.01	9.59E-01	9.76E-01	-0.62	6.44E-03	7.22E-02	-0.29	2.61E-01	5.16E-01
4-Aminobutyric acid related 1	-0.04	8.87E-01	9.37E-01	-0.07	7.96E-01	9.48E-01	-	-	-
4-Aminobutyric acid related 2	0.21	3.97E-01	7.06E-01	-0.29	2.46E-01	4.58E-01	-	-	-
L-Alanine related	0.51	2.93E-02	1.26E-01	0.56	1.48E-02	1.20E-01	0.04	8.81E-01	9.89E-01
unidentified methyl signal 1	-0.13	6.04E-01	8.67E-01	-0.34	1.66E-01	3.45E-01	0.55	2.12E-02	1.25E-01
unidentified methyl signal 2	0.34	1.63E-01	5.06E-01	0.05	8.36E-01	9.56E-01	0.13	6.12E-01	9.06E-01
Trigonelline	0.41	9.41E-02	3.10E-01	0.04	8.77E-01	9.82E-01	0.73	8.20E-04	1.45E-02
Formate	0	1.00E+00	1.00E+00	-0.14	5.68E-01	7.95E-01	0.48	5.30E-02	1.83E-01
Inosine	0.31	2.03E-01	5.18E-01	0.55	1.78E-02	1.20E-01	0.38	1.35E-01	3.24E-01
L-Tryptophan	-0.74	1.11E-03	2.55E-02	0.1	7.21E-01	9.18E-01	0.47	7.53E-02	2.35E-01
L-Phenylalanine	-0.66	3.13E-03	3.22E-02	-0.17	4.99E-01	7.55E-01	0.47	5.52E-02	1.83E-01
L-Histidine	-0.35	1.81E-01	5.06E-01	0.56	2.01E-02	1.20E-01	-	-	-
L-Tyrosine	-0.6	8.04E-03	5.00E-02	0	1.00E+00	1.00E+00	0.12	6.59E-01	9.39E-01
Fumarate	0.64	4.02E-03	3.22E-02	0.35	1.49E-01	3.35E-01	0	9.96E-01	9.96E-01
Uracil	0.2	4.34E-01	7.36E-01	-0.54	2.14E-02	1.20E-01	-0.46	9.84E-02	2.74E-01
D-Glucose	0.6	8.04E-03	5.00E-02	-0.45	6.36E-02	2.38E-01	-0.13	6.16E-01	9.06E-01
Betaine	0.21	4.03E-01	7.06E-01	0.25	3.19E-01	5.41E-01	-0.08	7.66E-01	9.89E-01
Glycine	0.14	5.68E-01	8.60E-01	0.64	4.02E-03	5.63E-02	-0.25	3.29E-01	5.63E-01
5,6-Dihydrouracil	-0.18	4.66E-01	7.45E-01	-0.67	2.40E-03	4.49E-02	0.18	5.01E-01	7.81E-01
Taurine	-0.04	8.77E-01	9.37E-01	-0.37	1.34E-01	3.35E-01	0.01	9.55E-01	9.92E-01
DMSP	-0.3	2.24E-01	5.45E-01	-0.72	7.29E-04	4.08E-02	0.1	7.06E-01	9.60E-01
L-Methionine	0.56	1.48E-02	6.90E-02	0.41	9.41E-02	3.29E-01	0.27	2.99E-01	5.28E-01
L-Glutamine	-0.58	1.22E-02	6.81E-02	0.03	9.18E-01	9.88E-01	-0.46	9.46E-02	2.74E-01
Succinate	0.08	7.56E-01	9.01E-01	0.24	3.46E-01	5.53E-01	-0.03	9.13E-01	9.89E-01
L-Glutamate	0.7	1.36E-03	2.55E-02	0.39	1.06E-01	3.31E-01	-0.53	4.40E-02	1.74E-01
L-Alanine	-0.26	2.93E-01	6.31E-01	0.55	1.78E-02	1.20E-01	0.55	2.08E-02	1.25E-01
Lactate	0.21	4.03E-01	7.06E-01	0.05	8.36E-01	9.56E-01	-0.09	7.36E-01	9.75E-01
L-Valine	-0.64	4.02E-03	3.22E-02	-0.28	2.69E-01	4.85E-01	-0.29	2.66E-01	5.16E-01
L-Isoleucine	-0.45	6.36E-02	2.38E-01	-0.1	6.79E-01	9.05E-01	-0.33	2.16E-01	4.57E-01
L-Leucine	-0.56	1.48E-02	6.90E-02	0.09	7.17E-01	9.18E-01	-0.35	1.74E-01	4.02E-01

* p-value calculated using Spearman's correlation test; Positive rho = the concentration increases with the distance from the coast; Negative rho = the concentration decreases with the distance from the coast; Zero= No change in the concentrations among the shores; Dash= metabolites not found

Table 5.A. Metabolites found in the *mantle* detected by GC-MS

metabolite	rho	p-value	FDR
Caffeic acid	0.70	1.36E-03	2.02E-01
L-Histidine	0.67	2.40E-03	2.02E-01
Eserine	0.64	4.02E-03	2.02E-01
L-Alanine	0.63	5.12E-03	2.02E-01
Deoxyuridine	-0.63	5.12E-03	2.02E-01
beta-Alanine	0.59	9.93E-03	2.44E-01
D-Galactosamine	-0.59	9.93E-03	2.44E-01
Quinic acid	-0.59	9.93E-03	2.44E-01
Glycine	0.56	1.48E-02	2.91E-01
Succinic acid	0.56	1.48E-02	2.91E-01
L-Glutamic acid	0.55	1.78E-02	3.19E-01
Ethionine	-0.54	2.14E-02	3.24E-01
5-Dehydroquinic acid	-0.54	2.14E-02	3.24E-01
Pyroglutamic acid	0.52	2.54E-02	3.34E-01
Sarcosine	-0.52	2.54E-02	3.34E-01
Maleamic acid	-0.50	3.53E-02	3.66E-01
Lauric acid	-0.50	3.53E-02	3.66E-01
Vanillylmandelic acid	0.50	3.53E-02	3.66E-01
Ferulic acid	0.50	3.53E-02	3.66E-01
Coniferyl alcohol	-0.49	4.12E-02	4.06E-01
Dopamine	0.46	5.53E-02	4.96E-01
Sakuranetin	0.46	5.53E-02	4.96E-01
Glycolic acid	0.45	6.36E-02	4.98E-01
Cysteinylglycine	0.45	6.36E-02	4.98E-01
Xanthine	-0.45	6.36E-02	4.98E-01
Heptadecanoic acid	-0.43	7.28E-02	4.98E-01
Sinapic acid	-0.43	7.28E-02	4.98E-01
Epinephrine	0.42	8.30E-02	4.98E-01
L-Ascorbic acid	-0.42	8.30E-02	4.98E-01
Ferulic acid	-0.42	8.30E-02	4.98E-01
6-Amino-1-Methyluracil	-0.42	8.30E-02	4.98E-01
Ketoleucine	-0.41	9.41E-02	4.98E-01
Citric acid	-0.41	9.41E-02	4.98E-01
Malic acid	0.41	9.41E-02	4.98E-01
Uridine	0.41	9.41E-02	4.98E-01
Amantadine	0.41	9.41E-02	4.98E-01
Inosine	0.41	9.41E-02	4.98E-01

D-Maltose	0.39	1.06E-01	4.98E-01
2,3-Diaminopropionic acid	0.39	1.06E-01	4.98E-01
Cytosine	0.39	1.06E-01	4.98E-01
L-Ornithine	0.39	1.06E-01	4.98E-01
D-Turanose	-0.39	1.06E-01	4.98E-01
Aminoadipic acid	-0.38	1.19E-01	5.23E-01
Serotonin	-0.38	1.19E-01	5.23E-01
Uridine diphosphate-N-acetylglucosamine	0.38	1.19E-01	5.23E-01
2,3-Diphosphoglyceric acid	-0.37	1.34E-01	5.45E-01
O-Acetylserine	0.37	1.34E-01	5.45E-01
L-Citrulline	-0.37	1.34E-01	5.45E-01
Alanylanine	0.35	1.49E-01	5.45E-01
Hydrocinnamic acid	-0.35	1.49E-01	5.45E-01
Indole-3-carboxyaldehyde	0.35	1.49E-01	5.45E-01
Harmaline	0.35	1.49E-01	5.45E-01
N-alpha-Acetyl-L-lysine	0.35	1.49E-01	5.45E-01
Dimethylbenzimidazole	-0.35	1.49E-01	5.45E-01
3-Pyridylacetic acid	-0.34	1.66E-01	5.55E-01
1-Kestose	-0.34	1.66E-01	5.55E-01
cis-p-Coumaric acid	-0.34	1.66E-01	5.55E-01
Creatinine	0.34	1.66E-01	5.55E-01
6-Hydroxynicotinic acid	0.34	1.66E-01	5.55E-01
3-Oxoadipic acid	0.33	1.84E-01	5.67E-01
D-Fucose	-0.33	1.84E-01	5.67E-01
S-Adenosylmethionine	-0.33	1.84E-01	5.67E-01
Coumarinic acid	-0.33	1.84E-01	5.67E-01
Putrescine	-0.33	1.84E-01	5.67E-01
Spermine	0.31	2.03E-01	5.80E-01
L-Asparagine	0.31	2.03E-01	5.80E-01
Dethiobiotin	0.31	2.03E-01	5.80E-01
D-Ribulose-5-phosphate	0.31	2.03E-01	5.80E-01
3-Methyl-2-oxovaleric acid	-0.31	2.03E-01	5.80E-01
Linoleic acid	-0.30	2.24E-01	5.88E-01
Protocatechuic acid	-0.30	2.24E-01	5.88E-01
Pimelic acid	0.30	2.24E-01	5.88E-01
Methyluracil	-0.30	2.24E-01	5.88E-01
Anthracene	-0.30	2.24E-01	5.88E-01
D-Arabinose-5-phosphate	0.30	2.24E-01	5.88E-01
2-Hydroxypyridine	-0.29	2.46E-01	6.20E-01
4-Hydroxybenzoic acid	-0.29	2.46E-01	6.20E-01

4-Hydroxyproline	0.29	2.46E-01	6.20E-01
alpha-Tocopherol	0.28	2.69E-01	6.34E-01
L-3-Cyanoalanine	-0.28	2.69E-01	6.34E-01
Glutaric acid	-0.28	2.69E-01	6.34E-01
3-Hydroxypyruvate	0.28	2.69E-01	6.34E-01
2'-Deoxyadenosine	-0.26	2.93E-01	6.34E-01
N-Methylalanine	-0.26	2.93E-01	6.34E-01
Phosphoenolpyruvic acid	-0.26	2.93E-01	6.34E-01
Benzoic acid	-0.26	2.93E-01	6.34E-01
Picolinic acid	0.26	2.93E-01	6.34E-01
1,5-Anhydrosorbitol	-0.26	2.93E-01	6.34E-01
Xanthosine	-0.26	2.93E-01	6.34E-01
5-Hydroxymethyluracil	-0.26	2.93E-01	6.34E-01
Adenosine	0.26	2.93E-01	6.34E-01
D-Ribulose	-0.25	3.19E-01	6.34E-01
Gallic acid	-0.25	3.19E-01	6.34E-01
L-Glutamine	-0.25	3.19E-01	6.34E-01
Adipic acid	-0.25	3.19E-01	6.34E-01
Stearic acid	-0.25	3.19E-01	6.34E-01
Biopterin	-0.25	3.19E-01	6.34E-01
2,6-Diaminopurine	0.25	3.19E-01	6.34E-01
Isophthalic acid	0.25	3.19E-01	6.34E-01
Homogentisic acid	-0.24	3.46E-01	6.74E-01
Pantothenic acid	0.24	3.46E-01	6.74E-01
4-Hydroxypyridine	0.22	3.74E-01	6.88E-01
Phenylhydrazine	-0.22	3.74E-01	6.88E-01
L-Norleucine	0.22	3.74E-01	6.88E-01
Tartaric acid	0.22	3.74E-01	6.88E-01
3-Hydroxyaspartic acid	0.22	3.74E-01	6.88E-01
Beta-D-Fructose 6-phosphate	0.22	3.74E-01	6.88E-01
Lactic acid	0.21	4.03E-01	6.97E-01
L-Mandelic acid	0.21	4.03E-01	6.97E-01
L-Homocarnosine	0.21	4.03E-01	6.97E-01
L-Norvaline	0.21	4.03E-01	6.97E-01
L-Methionine	0.21	4.03E-01	6.97E-01
D-Allose	0.21	4.03E-01	6.97E-01
Myricetin	-0.21	4.03E-01	6.97E-01
L-Lysine	0.20	4.34E-01	7.01E-01
Homoserine lactone	0.20	4.34E-01	7.01E-01
Adenine	0.20	4.34E-01	7.01E-01

4-Hydroxybenzaldehyde	0.20	4.34E-01	7.01E-01
D-Allulose	0.20	4.34E-01	7.01E-01
D-Glucose-6-phosphate	0.20	4.34E-01	7.01E-01
Kynurenate	-0.20	4.34E-01	7.01E-01
Epigallocatechin	-0.20	4.34E-01	7.01E-01
Hydroxylamine	-0.18	4.66E-01	7.40E-01
Daidzein	-0.18	4.66E-01	7.40E-01
Pyroglutamic acid	-0.18	4.82E-01	7.60E-01
Ureidosuccinic acid	-0.17	4.99E-01	7.74E-01
Propyleneglycol	0.17	4.99E-01	7.74E-01
N-Acetylucine	-0.16	5.33E-01	8.20E-01
Malonic acid	0.14	5.68E-01	8.41E-01
Uracil	-0.14	5.68E-01	8.41E-01
Penicillamine	-0.14	5.68E-01	8.41E-01
Galactitol	-0.14	5.68E-01	8.41E-01
Palmitic acid	-0.14	5.68E-01	8.41E-01
Myo-Inositol	0.13	6.04E-01	8.50E-01
Fumaric acid	0.13	6.04E-01	8.50E-01
Glycerol	0.13	6.04E-01	8.50E-01
D-Phenyllactic acid	0.13	6.04E-01	8.50E-01
L-Tryptophan	0.13	6.04E-01	8.50E-01
Isocitric acid	-0.13	6.04E-01	8.50E-01
Apigenin	-0.13	6.04E-01	8.50E-01
L-Dopa	0.12	6.41E-01	8.71E-01
3-Indoleacetonitrile	0.12	6.41E-01	8.71E-01
Pyrogalllic acid	0.12	6.41E-01	8.71E-01
Pyrophosphate	-0.12	6.41E-01	8.71E-01
D-Trehalose	-0.12	6.41E-01	8.71E-01
2-Hydroxybutyric acid	-0.10	6.79E-01	8.85E-01
Norvaline	-0.10	6.79E-01	8.85E-01
1,6-Anhydroglucose	-0.10	6.79E-01	8.85E-01
16-hydroxypalmitic acid	-0.10	6.79E-01	8.85E-01
L-Proline	0.10	6.79E-01	8.85E-01
2-Phenylglycine	0.10	6.79E-01	8.85E-01
3-Methyladenine	-0.09	7.17E-01	9.11E-01
Hippurate	-0.09	7.17E-01	9.11E-01
Methyldopa	0.09	7.17E-01	9.11E-01
cis-Aconitic acid	-0.09	7.17E-01	9.11E-01
5-Aminovaleric acid	0.08	7.56E-01	9.14E-01
Octacosanoic acid	0.08	7.56E-01	9.14E-01

Bicine	0.08	7.56E-01	9.14E-01
Glucaric acid	0.08	7.56E-01	9.14E-01
Genistein	0.08	7.56E-01	9.14E-01
Citramalic acid	-0.08	7.56E-01	9.14E-01
Allantoin	-0.08	7.56E-01	9.14E-01
N-Acetylmannosamine	-0.08	7.56E-01	9.14E-01
L-Cysteic acid	-0.07	7.96E-01	9.15E-01
alpha-Ketoglutaric acid	0.07	7.96E-01	9.15E-01
Ciliatine	0.07	7.96E-01	9.15E-01
Quinolinic acid	0.07	7.96E-01	9.15E-01
Guanine	0.07	7.96E-01	9.15E-01
Behenic acid	0.07	7.96E-01	9.15E-01
D-Threitol	0.05	8.36E-01	9.15E-01
4-Aminohippuric acid	0.05	8.36E-01	9.15E-01
5-Keto-D-Gluconate	0.05	8.36E-01	9.15E-01
Cystamine	0.05	8.36E-01	9.15E-01
2-Hydroxyphenylacetic acid	0.05	8.36E-01	9.15E-01
D-Ribulose-1,5-Bisphosphate	0.05	8.36E-01	9.15E-01
Pipecolic acid	-0.05	8.36E-01	9.15E-01
2-Toluic acid	-0.05	8.36E-01	9.15E-01
Shikimic acid	-0.05	8.36E-01	9.15E-01
S-Carboxymethyl-L-cysteine	-0.05	8.36E-01	9.15E-01
Gentisic acid	-0.05	8.36E-01	9.15E-01
Minoxidil	-0.04	8.77E-01	9.34E-01
Taurine	-0.04	8.77E-01	9.34E-01
Arachidic acid	-0.04	8.77E-01	9.34E-01
D-Sorbitol-6-phosphate	0.04	8.77E-01	9.34E-01
Alpha-Lactose	-0.04	8.77E-01	9.34E-01
L-Prolinamide	-0.03	9.18E-01	9.52E-01
2-Hydroxybutyric acid	-0.03	9.18E-01	9.52E-01
D-Glucose	-0.03	9.18E-01	9.52E-01
Cyanine	-0.03	9.18E-01	9.52E-01
Maltotriose	0.03	9.18E-01	9.52E-01
1,3-Dihydroxyacetone dimer	0.01	9.59E-01	9.79E-01
Thymine	0.01	9.59E-01	9.79E-01
D-Galactose	0.01	9.59E-01	9.79E-01
Suberic acid	0.00	1.00E+00	1.00E+00
Glycerol 1-phosphate	0.00	1.00E+00	1.00E+00
Uric acid	0.00	1.00E+00	1.00E+00
5-Hydroxy-L-tryptophan	0.00	1.00E+00	1.00E+00

Table 5.B. Metabolites found in the *gills* detected by GC-MS

metabolite	rho	p-value	FDR
Myo-Inositol	-0.73	5.19E-04	4.35E-02
Pimelic acid	-0.72	7.29E-04	4.35E-02
Cyanine	0.72	7.29E-04	4.35E-02
Psoralen	0.71	1.01E-03	4.50E-02
Dopamine	-0.67	2.40E-03	8.61E-02
L-Norleucine	-0.64	4.02E-03	1.20E-01
Epinephrine	0.62	6.44E-03	1.28E-01
L-Lysine	0.62	6.44E-03	1.28E-01
L-Phenylalanine	-0.62	6.44E-03	1.28E-01
Glycerol	-0.60	8.04E-03	1.31E-01
L-Methionine	-0.60	8.04E-03	1.31E-01
L-3-Cyanoalanine	-0.58	1.22E-02	1.56E-01
2-Aminopimelic acid	-0.58	1.22E-02	1.56E-01
Maltotriose	0.58	1.22E-02	1.56E-01
Harmaline	-0.55	1.78E-02	1.88E-01
L-Ornithine	-0.55	1.78E-02	1.88E-01
Coniferyl alcohol	0.55	1.78E-02	1.88E-01
N-Acetylleucine	-0.54	2.14E-02	2.01E-01
L-Norvaline	-0.54	2.14E-02	2.01E-01
D-Maltose	0.52	2.54E-02	2.17E-01
L-Dopa	-0.52	2.54E-02	2.17E-01
Propyleneglycol	0.51	3.00E-02	2.44E-01
L-Proline	-0.50	3.53E-02	2.53E-01
D-Ribulose-5-phosphate	0.50	3.53E-02	2.53E-01
Gentisic acid	-0.50	3.53E-02	2.53E-01
Uric acid	0.49	4.12E-02	2.64E-01
Lignoceric acid	0.49	4.12E-02	2.64E-01
L-Alanine	-0.49	4.12E-02	2.64E-01
D-Trehalose	0.47	4.79E-02	2.86E-01
Myricetin	0.47	4.79E-02	2.86E-01
4-Hydroxybenzaldehyde	0.46	5.53E-02	3.00E-01
1-Hexadecanol	0.46	5.53E-02	3.00E-01
L-Mandelic acid	-0.46	5.53E-02	3.00E-01
Linoleic acid	0.45	6.36E-02	3.16E-01
L-Glutamic acid	-0.45	6.36E-02	3.16E-01
Adenine	-0.45	6.36E-02	3.16E-01
Serotonin	-0.43	7.28E-02	3.52E-01
2,3-Diphosphoglyceric acid	0.42	8.30E-02	3.71E-01

6-Amino-1-Methyluracil	0.42	8.30E-02	3.71E-01
Lauric acid	-0.42	8.30E-02	3.71E-01
N-Methylalanine	0.41	9.41E-02	4.05E-01
Glycolic acid	0.39	1.06E-01	4.05E-01
Hippurate	0.39	1.06E-01	4.05E-01
1,3-Dihydroxyacetone dimer	0.39	1.06E-01	4.05E-01
Malic acid	0.39	1.06E-01	4.05E-01
Fumaric acid	-0.39	1.06E-01	4.05E-01
4-Hydroxyproline	-0.39	1.06E-01	4.05E-01
Methyldopa	-0.38	1.19E-01	4.28E-01
D-Sorbitol	-0.38	1.19E-01	4.28E-01
Glyceraldehyde	0.38	1.19E-01	4.28E-01
D-Raffinose	0.37	1.33E-01	4.36E-01
D-Threitol	0.37	1.34E-01	4.36E-01
Hydroxylamine	0.37	1.34E-01	4.36E-01
3-Oxoadipic acid	0.37	1.34E-01	4.36E-01
Protocatechuic acid	0.37	1.34E-01	4.36E-01
Gallic acid	0.35	1.49E-01	4.46E-01
Alanylalanine	0.35	1.49E-01	4.46E-01
2-Toluic acid	0.35	1.49E-01	4.46E-01
Ureidosuccinic acid	0.35	1.49E-01	4.46E-01
Cysteinylglycine	-0.35	1.49E-01	4.46E-01
3-Pyridylacetic acid	0.34	1.66E-01	4.72E-01
Picolinic acid	0.34	1.66E-01	4.72E-01
Glutaric acid	0.34	1.66E-01	4.72E-01
L-Cysteic acid	-0.33	1.84E-01	5.07E-01
Norvaline	-0.33	1.84E-01	5.07E-01
Sarcosine	0.31	2.03E-01	5.13E-01
Caffeic acid	-0.31	2.03E-01	5.13E-01
Putrescine	0.31	2.03E-01	5.13E-01
Ciliatine	-0.31	2.03E-01	5.13E-01
D-Glucose	0.31	2.03E-01	5.13E-01
L-Tryptophan	-0.31	2.03E-01	5.13E-01
Spermine	0.30	2.24E-01	5.49E-01
1-Kestose	0.30	2.24E-01	5.49E-01
Octacosanoic acid	-0.29	2.46E-01	5.50E-01
D-Fucose	0.29	2.46E-01	5.50E-01
Minoxidil	0.29	2.46E-01	5.50E-01
Ketoleucine	0.29	2.46E-01	5.50E-01
N-Methylethanolamine	0.29	2.46E-01	5.50E-01

Anthracene	0.29	2.46E-01	5.50E-01
D-Galactose	0.29	2.46E-01	5.50E-01
Phenylephrine	0.28	2.69E-01	5.94E-01
L-Histidine	-0.26	2.93E-01	6.10E-01
L-Arginine	0.26	2.93E-01	6.10E-01
alpha-Tocopherol	0.26	2.93E-01	6.10E-01
2-Hydroxybutyric acid	0.26	2.93E-01	6.10E-01
D-Ribulose	-0.26	2.93E-01	6.10E-01
Stearic acid	-0.25	3.19E-01	6.41E-01
Ethionine	0.25	3.19E-01	6.41E-01
2-Hydroxybutyric acid	0.25	3.19E-01	6.41E-01
Galactitol	-0.24	3.46E-01	6.65E-01
Uridine	-0.24	3.46E-01	6.65E-01
1,5-Anhydrosorbitol	0.24	3.46E-01	6.65E-01
5-Hydroxymethyluracil	0.24	3.46E-01	6.65E-01
Pyroglutamic acid	-0.22	3.74E-01	6.97E-01
3,4-Dihydroxymandelic acid	0.22	3.74E-01	6.97E-01
Vanillylmandelic acid	0.22	3.74E-01	6.97E-01
Xanthine	0.21	4.03E-01	7.44E-01
4-Aminohippuric acid	0.20	4.34E-01	7.77E-01
Isophthalic acid	0.20	4.34E-01	7.77E-01
Malonic acid	-0.20	4.34E-01	7.77E-01
Thymine	-0.18	4.66E-01	8.10E-01
D-Arabinose-5-phosphate	-0.18	4.66E-01	8.10E-01
5-Hydroxy-L-tryptophan	0.18	4.66E-01	8.10E-01
Homoserine lactone	-0.17	4.99E-01	8.42E-01
Phenylhydrazine	0.17	4.99E-01	8.42E-01
Sakuranetin	0.17	4.99E-01	8.42E-01
2'-Deoxyadenosine	-0.16	5.33E-01	8.44E-01
3-Hydroxybenzoic acid	0.16	5.33E-01	8.44E-01
Benzoic acid	0.16	5.33E-01	8.44E-01
Coniferaldehyde	-0.16	5.33E-01	8.44E-01
Methyluracil	0.16	5.33E-01	8.44E-01
Quinic acid	0.16	5.33E-01	8.44E-01
Lactitol	-0.16	5.33E-01	8.44E-01
Lactic acid	0.14	5.68E-01	8.45E-01
Urea	0.14	5.68E-01	8.45E-01
Pelargonic acid	0.14	5.68E-01	8.45E-01
beta-Alanine	0.14	5.68E-01	8.45E-01
D-Allose	0.14	5.68E-01	8.45E-01

L-Asparagine	0.13	6.04E-01	8.45E-01
Glycerol 1-phosphate	0.13	6.04E-01	8.45E-01
Apigenin	0.13	6.04E-01	8.45E-01
N-Acetylmannosamine	0.13	6.04E-01	8.45E-01
Kynurenate	-0.13	6.04E-01	8.45E-01
Pyrophosphate	-0.13	6.04E-01	8.45E-01
Adipic acid	-0.13	6.04E-01	8.45E-01
Hydrocinnamic acid	-0.13	6.04E-01	8.45E-01
D-Allulose	-0.13	6.04E-01	8.45E-01
Alpha-Lactose	-0.13	6.04E-01	8.45E-01
Suberic acid	0.12	6.41E-01	8.63E-01
3-Indoleacetoneitrile	-0.12	6.41E-01	8.63E-01
1,6-Anhydroglucose	-0.12	6.41E-01	8.63E-01
Ethylmalonic acid	-0.12	6.41E-01	8.63E-01
Inosine	-0.12	6.41E-01	8.63E-01
Arachidic acid	-0.10	6.79E-01	8.85E-01
Indoleacetic acid	-0.10	6.79E-01	8.85E-01
3-Methyladenine	0.10	6.79E-01	8.85E-01
5-Keto-D-Gluconate	0.10	6.79E-01	8.85E-01
4-Hydroxypyridine	-0.09	7.17E-01	8.85E-01
Homogentisic acid	0.09	7.17E-01	8.85E-01
2,6-Diaminopurine	0.09	7.17E-01	8.85E-01
Bicine	-0.09	7.17E-01	8.85E-01
Heptadecanoic acid	0.09	7.17E-01	8.85E-01
Xanthosine	-0.09	7.17E-01	8.85E-01
D-Sorbitol-6-phosphate	-0.09	7.17E-01	8.85E-01
Daidzein	-0.09	7.17E-01	8.85E-01
Uracil	0.08	7.56E-01	9.15E-01
Sinapic acid	0.08	7.56E-01	9.15E-01
Cytosine	-0.08	7.56E-01	9.15E-01
2,3-Diaminopropionic acid	-0.07	7.96E-01	9.37E-01
Dihydroxyacetone	-0.07	7.96E-01	9.37E-01
Tartaric acid	0.07	7.96E-01	9.37E-01
D-Xylulose	0.07	7.96E-01	9.37E-01
Dethiobiotin	0.05	8.36E-01	9.60E-01
Diaminopimelic acid	0.05	8.36E-01	9.60E-01
Ferulic acid	0.05	8.36E-01	9.60E-01
Palmitic acid	-0.05	8.36E-01	9.60E-01
5-Aminovaleric acid	0.04	8.77E-01	9.63E-01
Shikimic acid	0.04	8.77E-01	9.63E-01

Coumarinic acid	0.04	8.77E-01	9.63E-01
Pyroglutamic acid	0.04	8.77E-01	9.63E-01
Taurine	0.04	8.77E-01	9.63E-01
Pantothenic acid	-0.04	8.77E-01	9.63E-01
2-Thiouracil	-0.04	8.77E-01	9.63E-01
Cysteamine	0.03	9.18E-01	9.72E-01
Citramalic acid	0.03	9.18E-01	9.72E-01
Succinic acid	-0.03	9.18E-01	9.72E-01
4-Hydroxybenzoic acid	0.03	9.18E-01	9.72E-01
D-Glucose-6-phosphate	-0.03	9.18E-01	9.72E-01
Epigallocatechin	0.03	9.18E-01	9.72E-01
Glyceric acid	0.01	9.59E-01	9.92E-01
D-Galactosamine	-0.01	9.59E-01	9.92E-01
L-Ascorbic acid	-0.01	9.59E-01	9.92E-01
Glucaric acid	-0.01	9.59E-01	9.92E-01
2-Hydroxypyridine	0.00	1.00E+00	1.00E+00
3-Hydroxyaspartic acid	0.00	1.00E+00	1.00E+00
Phosphoenolpyruvic acid	0.00	1.00E+00	1.00E+00
Isocitric acid	0.00	1.00E+00	1.00E+00
L-Citrulline	0.00	1.00E+00	1.00E+00
Beta-D-Fructose 6-phosphate	0.00	1.00E+00	1.00E+00

Table 5.C. Metabolites found in the *digestive* system detected by GC-MS

metabolite	rho	p-value	FDR
Alpha-Lactose	-0.81	8.28E-05	1.72E-02
Quinic acid	0.77	3.07E-04	2.48E-02
L-Histidine	-0.76	3.57E-04	2.48E-02
Coumarinic acid	0.75	5.69E-04	2.96E-02
Serotonin	-0.73	9.03E-04	3.76E-02
Ciliatine	-0.71	1.27E-03	4.39E-02
Shikimic acid	0.70	1.75E-03	5.19E-02
Harmaline	0.69	2.18E-03	5.61E-02
2-Phenylglycine	0.68	2.43E-03	5.61E-02
D-Raffinose	0.67	3.07E-03	6.38E-02
Pentachlorophenol	-0.66	3.84E-03	7.10E-02
Mesaconic acid	-0.66	4.23E-03	7.10E-02
3-Indoleacetonitrile	0.65	4.44E-03	7.10E-02
Phosphoenolpyruvic acid	-0.64	5.73E-03	8.52E-02
L-Norvaline	-0.61	9.81E-03	1.12E-01
Cytosine	0.60	1.02E-02	1.12E-01
Hydroxylamine	0.59	1.22E-02	1.12E-01
Dihydroxyacetone	-0.59	1.24E-02	1.12E-01
L-Methionine	-0.59	1.24E-02	1.12E-01
4-Methylumbelliferone	0.59	1.29E-02	1.12E-01
Caffeic acid	-0.59	1.29E-02	1.12E-01
5-Aminovaleric acid	-0.59	1.34E-02	1.12E-01
alpha-Tocopherol	0.58	1.37E-02	1.12E-01
L-Cysteine	0.58	1.40E-02	1.12E-01
Psoralen	-0.58	1.42E-02	1.12E-01
Deoxyadenosine monophosphate	-0.58	1.45E-02	1.12E-01
Kynurenate	-0.58	1.51E-02	1.12E-01
Glycolic acid	-0.58	1.53E-02	1.12E-01
2-Isopropylmalic acid	0.57	1.65E-02	1.12E-01
Arachidic acid	0.57	1.81E-02	1.12E-01
Methyldopa	-0.57	1.81E-02	1.12E-01
Succinic acid	0.56	1.84E-02	1.12E-01
D-Ribulose	-0.56	1.87E-02	1.12E-01
Chlorogenic acid	-0.56	1.91E-02	1.12E-01
Citramalic acid	0.56	1.94E-02	1.12E-01
Vanillylmandelic acid	0.56	1.97E-02	1.12E-01
D-Ribulose-1,5-Bisphosphate	-0.56	2.05E-02	1.12E-01

L-Phenylalanine	-0.56	2.05E-02	1.12E-01
Citric acid	0.55	2.23E-02	1.15E-01
N-Acetylleucine	0.55	2.31E-02	1.15E-01
Methylsuccinic acid	0.55	2.35E-02	1.15E-01
L-3-Cyanoalanine	0.54	2.43E-02	1.15E-01
Podophyllotoxin	0.54	2.47E-02	1.15E-01
Ferulic acid	0.54	2.51E-02	1.15E-01
Glutaric acid	0.54	2.68E-02	1.15E-01
L-Ornithine	-0.54	2.68E-02	1.15E-01
Inosine	-0.53	2.73E-02	1.15E-01
Xanthurenic acid	0.53	2.77E-02	1.15E-01
Uric acid	-0.53	2.77E-02	1.15E-01
Amantadine	0.53	2.82E-02	1.15E-01
Biopterin	0.53	2.82E-02	1.15E-01
L-Prolinamide	0.53	2.96E-02	1.16E-01
L-Lysine	0.53	2.96E-02	1.16E-01
L-Glutamic acid	-0.52	3.10E-02	1.19E-01
5-Hydroxymethyluracil	-0.52	3.15E-02	1.19E-01
Gluconic acid	0.51	3.46E-02	1.28E-01
2-Thiouracil	-0.51	3.57E-02	1.30E-01
D-Arabinose-5-phosphate	-0.50	3.97E-02	1.42E-01
Tartaric acid	0.50	4.03E-02	1.42E-01
Diaminopimelic acid	0.50	4.15E-02	1.44E-01
3-Hydroxyaspartic acid	-0.49	4.46E-02	1.51E-01
2,3-Diaminopropionic acid	-0.49	4.60E-02	1.51E-01
Malic acid	-0.49	4.60E-02	1.51E-01
cis-Aconitic acid	0.49	4.73E-02	1.51E-01
Cysteinylglycine	-0.49	4.73E-02	1.51E-01
Glyceraldehyde	0.48	5.08E-02	1.57E-01
Pyrogalllic acid	-0.48	5.08E-02	1.57E-01
L-Dopa	-0.48	5.15E-02	1.57E-01
Kojic acid	0.48	5.22E-02	1.57E-01
Methylmalonic acid	0.48	5.37E-02	1.57E-01
Prephenate	0.48	5.37E-02	1.57E-01
Pyrophosphate	-0.47	5.52E-02	1.60E-01
O-Phosphoethanolamine	-0.47	5.83E-02	1.66E-01
3-Methyladenine	0.46	6.16E-02	1.73E-01
Pyruvic acid	0.45	6.75E-02	1.87E-01
Xanthosine	0.45	7.02E-02	1.90E-01
Spermine	-0.45	7.12E-02	1.90E-01

Homoserine lactone	-0.45	7.12E-02	1.90E-01
2,6-Diaminopurine	0.44	7.40E-02	1.95E-01
D-Ribulose-5-phosphate	-0.44	7.59E-02	1.97E-01
Uracil	-0.44	7.68E-02	1.97E-01
Sinapic acid	0.43	8.59E-02	2.18E-01
Xanthine	0.42	8.91E-02	2.21E-01
5-Keto-D-Gluconate	-0.42	8.91E-02	2.21E-01
2-Hydroxyisobutyric acid	0.42	9.13E-02	2.23E-01
Dethiobiotin	-0.42	9.24E-02	2.24E-01
Ethionine	0.41	1.00E-01	2.40E-01
Picolinic acid	0.41	1.04E-01	2.43E-01
Hypoxanthine	-0.41	1.04E-01	2.43E-01
Bicine	0.40	1.08E-01	2.46E-01
Adenine	-0.40	1.08E-01	2.46E-01
Glycerol	-0.40	1.09E-01	2.46E-01
Thymine	0.40	1.10E-01	2.46E-01
L-Ascorbic acid	0.39	1.25E-01	2.76E-01
Pimelic acid	-0.39	1.26E-01	2.76E-01
Isophthalic acid	-0.38	1.37E-01	2.95E-01
Quinolinic acid	0.37	1.39E-01	2.95E-01
cis-p-Coumaric acid	0.37	1.39E-01	2.95E-01
Taurine	0.37	1.45E-01	3.05E-01
Linoleic acid	0.37	1.50E-01	3.11E-01
Anthranilic acid	0.36	1.54E-01	3.18E-01
1-Kestose	-0.36	1.56E-01	3.18E-01
Isocitric acid	-0.35	1.69E-01	3.42E-01
Coniferaldehyde	-0.34	1.78E-01	3.55E-01
D-Trehalose	-0.34	1.83E-01	3.63E-01
L-Norleucine	-0.33	1.90E-01	3.73E-01
Ketoleucine	0.33	1.98E-01	3.84E-01
Pantothenic acid	-0.33	2.00E-01	3.84E-01
D-Galactosamine	0.33	2.01E-01	3.84E-01
Sucrose	0.32	2.17E-01	4.10E-01
2-Hydroxypyridine	0.30	2.38E-01	4.45E-01
3-Pyridylacetic acid	0.30	2.42E-01	4.45E-01
Terephthalic acid	0.30	2.42E-01	4.45E-01
3-Aminopropionitrile	0.29	2.53E-01	4.61E-01
O-Succinyl-L-Homoserine	-0.29	2.57E-01	4.65E-01
4-Hydroxyphenylacetic acid	-0.29	2.64E-01	4.73E-01
D-Sorbitol	-0.28	2.80E-01	4.93E-01

L-Cysteic acid	-0.28	2.82E-01	4.93E-01
Protocatechuic acid	0.28	2.82E-01	4.93E-01
Glycine	-0.28	2.85E-01	4.93E-01
2-Hydroxybutyric acid	0.27	3.01E-01	5.18E-01
L-Alanine	-0.26	3.14E-01	5.31E-01
L-Asparagine	0.26	3.14E-01	5.31E-01
2-Aminopimelic acid	-0.26	3.19E-01	5.35E-01
Fumaric acid	-0.25	3.24E-01	5.39E-01
Uridine	-0.25	3.29E-01	5.43E-01
3,4-Dihydroxymandelic acid	0.25	3.34E-01	5.47E-01
D-Galactose	-0.25	3.37E-01	5.47E-01
Phenylhydrazine	-0.24	3.45E-01	5.56E-01
6-Hydroxynicotinic acid	-0.24	3.53E-01	5.64E-01
2'-Deoxyadenosine	0.24	3.58E-01	5.64E-01
L-Glutamine	-0.24	3.58E-01	5.64E-01
Cadaverine	-0.23	3.72E-01	5.81E-01
L-Mandelic acid	-0.23	3.75E-01	5.81E-01
Glycerol 1-phosphate	0.23	3.77E-01	5.81E-01
4-Hydroxybenzaldehyde	0.22	3.86E-01	5.90E-01
Malonic acid	-0.22	3.89E-01	5.90E-01
Aminoadipic acid	-0.22	3.94E-01	5.94E-01
beta-Alanine	-0.21	4.15E-01	6.20E-01
6-(gamma,gamma-Dimethylallylamino)purine	0.21	4.17E-01	6.20E-01
Myo-Inositol	-0.21	4.26E-01	6.24E-01
alpha-Ketoisovaleric acid	0.21	4.29E-01	6.24E-01
Methyluracil	0.21	4.29E-01	6.24E-01
Heptadecanoic acid	0.20	4.35E-01	6.29E-01
Homogentisic acid	0.20	4.38E-01	6.29E-01
Uridine diphosphate-N-acetylglucosamine	0.19	4.54E-01	6.38E-01
N-Methylalanine	-0.19	4.54E-01	6.38E-01
Gallic acid	0.19	4.57E-01	6.38E-01
Octacosanoic acid	0.19	4.63E-01	6.38E-01
Propyleneglycol	0.19	4.66E-01	6.38E-01
1,6-Anhydroglucose	-0.19	4.69E-01	6.38E-01
Lactic acid	0.19	4.69E-01	6.38E-01
L-Citrulline	0.19	4.69E-01	6.38E-01
L-Rhamnose	0.18	4.82E-01	6.50E-01
4-Hydroxybenzoic acid	0.18	4.91E-01	6.59E-01
L-Tryptophan	-0.18	4.94E-01	6.59E-01
Guanine	-0.17	5.07E-01	6.72E-01

Alanylalanine	0.17	5.20E-01	6.85E-01
Minoxidil	0.17	5.27E-01	6.89E-01
D-Glucose	-0.16	5.30E-01	6.89E-01
3-Hydroxybutyric acid	-0.16	5.37E-01	6.89E-01
Benzoic acid	-0.16	5.37E-01	6.89E-01
D-Maltose	-0.16	5.40E-01	6.89E-01
Stearic acid	-0.15	5.57E-01	7.06E-01
D-Turanose	-0.15	5.77E-01	7.28E-01
Guanosine	-0.14	5.81E-01	7.28E-01
Apigenin	-0.14	5.84E-01	7.28E-01
Adipic acid	0.14	6.05E-01	7.45E-01
Galactitol	0.14	6.05E-01	7.45E-01
Daidzein	0.13	6.12E-01	7.49E-01
Coniferyl alcohol	0.13	6.19E-01	7.53E-01
L-Arginine	0.13	6.30E-01	7.61E-01
D-Xylitol	-0.12	6.37E-01	7.61E-01
3-Oxoadipic acid	0.12	6.37E-01	7.61E-01
Sarcosine	-0.11	6.62E-01	7.87E-01
2,6-Pyridinedicarboxylic acid	-0.11	6.69E-01	7.91E-01
D-Glucose-6-phosphate	-0.11	6.77E-01	7.95E-01
L-Proline	-0.11	6.80E-01	7.95E-01
D-Fucose	-0.11	6.88E-01	7.99E-01
D-Allose	0.10	7.10E-01	8.16E-01
Glucaric acid	0.10	7.14E-01	8.16E-01
1,10-Phenanthroline	-0.10	7.14E-01	8.16E-01
Dopamine	-0.09	7.28E-01	8.27E-01
4-Aminohippuric acid	-0.09	7.40E-01	8.27E-01
D-Allulose	0.09	7.40E-01	8.27E-01
Beta-D-Fructose 6-phosphate	0.09	7.40E-01	8.27E-01
D-Glutamine	0.08	7.51E-01	8.35E-01
Deoxyinosine	-0.08	7.70E-01	8.52E-01
Ureidosuccinic acid	-0.07	7.81E-01	8.55E-01
Myricetin	0.07	7.81E-01	8.55E-01
N-Acetylmannosamine	0.07	7.89E-01	8.59E-01
Kaempferol	0.06	8.12E-01	8.80E-01
Palmitic acid	-0.05	8.59E-01	9.25E-01
Epinephrine	0.04	8.70E-01	9.33E-01
2,3-Diphosphoglyceric acid	-0.04	8.90E-01	9.48E-01
4-Hydroxybenzoic acid	-0.04	8.94E-01	9.48E-01
Lignoceric acid	0.03	8.98E-01	9.48E-01

Pyroglutamic acid	0.03	9.17E-01	9.62E-01
4-Hydroxypyridine	0.02	9.25E-01	9.62E-01
N-Acetyl-L-aspartic acid	0.02	9.25E-01	9.62E-01
Sinigrin	0.01	9.61E-01	9.89E-01
5-Hydroxy-L-tryptophan	0.01	9.61E-01	9.89E-01
Hippurate	-0.01	9.72E-01	9.90E-01
O-Acetylserine	0.01	9.72E-01	9.90E-01
Epigallocatechin	-0.01	9.76E-01	9.90E-01
Ferulic acid	-0.01	9.80E-01	9.90E-01
6-Amino-1-Methyluracil	0.00	9.96E-01	9.96E-01
Sinapyl aldehyde	0.00	9.96E-01	9.96E-01

Table 6. Metabolites detected by HPLC-MS

Tissue	m/z	Name	Formula
Mantle	190.10726	1-hydroxyhexanoylglycine	C8H15NO4
	124.99121	2-Hydroxyethanesulfonate	C2H6O4S
	246.17025	2-Methylbutyroylcarnitine	C12H23NO4
	160.09678	2-Methylbutyrylglycine	C7H13NO3
	211.09778	3,4-Methyleneazelaic acid	C11H16O4
	225.1133	3,4-Methylenesebacic acid	C12H18O4
	189.04058	3-Dehydroquinone	C7H10O6
	193.12365	4-Hydroxypropofol	C12H18O2
	237.11335	4-O-methylolivetolcarboxylic acid	C13H18O4
	152.07028	Acetaminophen	C8H9NO2
	268.10408	Adenosine	C10H13N5O4
	348.07028	Adenosine monophosphate	C10H14N5O7P
	117.05457	Alpha-ketoisovaleric acid	C5H8O3
	162.07607	Aminoadipic acid	C6H11NO4
	94.06518	Aniline	C6H7N
	191.01953	Citric acid	C6H8O7
	179.05591	D-Glucose	C6H12O6
	160.13315	DL-2-Aminooctanoic acid	C8H17NO2
	102.0562	Dimethylglycine	C4H9NO2
	221.06653	Ethyl glucuronide	C8H14O7
	259.02237	Glucose 6-phosphate	C6H13O9P
	129.01911	Glutaconic acid	C5H6O4
	295.12924	Glutamylphenylalanine	C14H18N2O5
	105.01944	Glyceric acid	C3H6O4
	362.051	Guanosine monophosphate	C10H14N5O8P
	108.01257	Hypotaurine	C2H7NO2S
	269.08846	Inosine	C10H12N4O5
	132.03006	L-Aspartic acid	C4H7NO4
	162.11231	L-Carnitine	C7H15NO3
	146.0458	L-Glutamic acid	C5H9NO4
	132.10192	L-Isoleucine	C6H13NO2
	89.02459	L-Lactic acid	C3H6O3
	133.01399	L-Malic acid	C4H6O5
	166.08641	L-Phenylalanine	C9H11NO2
	203.08285	L-Tryptophan	C11H12N2O2
	182.08086	L-Tyrosine	C9H11NO3

166.08626	L-phenylalanine	C9H11NO2
117.01914	Methylmalonic acid	C4H6O4
277.14475	Monoethylhexyl phthalic acid	C16H22O4
353.26589	2,3-dihydroxypropyl hexadecanoate	C19H38O4
124.03953	Nicotinic acid	C6H5NO2
145.01379	Oxoglutaric acid	C5H6O5
220.1183	Pantothenic acid	C9H17NO5
98.98438	Phosphoric acid	H3O4P
241.15463	Pirbuterol	C12H20N2O3
144.10195	Proline betaine	C7H13NO2
128.03504	Pyroglutamic acid	C5H7NO3
124.00728	Taurine	C2H7NO3S
187.06095	Tetrahydro-2,5-furan-diacetic acid	C8H12O5
351.25339	Tetrahydrocorticosterone	C21H34O4
158.11758	Tranexamic Acid	C8H15NO2
112.98555	Trifluoroacetic acid	C2HF3O2
606.07433	Uridine 5-diphospho-N-acetylglucosamine	C17H27N3O17P2
323.02877	Uridine 5_monophosphate	C9H13N2O9P
173.00912	cis-Aconitic acid	C6H6O6

Gills

124.99126	2-Hydroxyethanesulfonate	C2H6O4S
211.09783	3,4-Methyleneazelaic acid	C11H16O4
348.07064	Adenosine monophosphate	C10H14N5O7P
94.06533	Aniline	C6H7N
88.04057	Beta-Alanine	C3H7NO2
179.05608	D-Glucose	C6H12O6
102.05613	Dimethylglycine	C4H9NO2
338.3416	Erucamide	C22H43NO
135.0298	Erythronic acid	C4H8O5
259.0222	Fructose 6-phosphate	C6H13O9P
152.05706	Guanine	C5H5N5O
154.01777	Hypotaurine	C2H7NO2S
267.07351	Inosine	C10H12N4O5
246.1701	Isovalerylcarnitine	C12H23NO4
160.09643	Isovalerylglycine	C7H13NO3
132.03022	L-Aspartic acid	C4H7NO4
162.11242	L-Carnitine	C7H15NO3
146.04563	L-Glutamic acid	C5H9NO4
132.10203	L-Isoleucine	C6H13NO2
89.02461	L-Lactic acid	C3H6O3

133.01415	L-Malic acid	C4H6O5
166.08622	L-Phenylalanine	C9H11NO2
166.08636	L-Phenylalanine	C9H11NO2
116.07049	L-Proline	C5H9NO2
203.08264	L-Tryptophan	C11H12N2O2
117.01924	Methylmalonic acid	C4H6O4
353.26601	2,3-dihydroxypropyl hexadecanoate	C19H38O4
124.03946	Nicotinic acid	C6H5NO2
98.98435	Phosphoric acid	H3O4P
144.102	Proline betaine	C7H13NO2
124.00723	Taurine	C2H7NO3S
158.11757	Tranexamic Acid	C8H15NO2
112.98559	Trifluoroacetic acid	C2HF3O2
138.05506	Trigonelline	C7H7NO2
608.08838	Uridine 5-diphosphate N-acetylgalactosamine	C17H27N3O17P2

Digestive system	124.99144	2-Hydroxyethanesulfonate	C2H6O4S
	216.98118	3-hydroxybenzoic acid-3-O-sulphate	C7H6O6S
	94.06528	Aniline	C6H7N
	160.13325	DL-2-Aminooctanoic acid	C8H17NO2
	338.34169	Erucamide	C22H43NO
	195.05105	Galactonic acid	C6H12O7
	152.05699	Guanine	C5H5N5O
	267.07331	Inosine	C10H12N4O5
	246.16996	Isovalerylcarnitine	C12H23NO4
	160.0969	Isovalerylglycine	C7H13NO3
	175.11865	L-Arginine	C6H14N4O2
	162.11251	L-Carnitine	C7H15NO3
	132.10208	L-Isoleucine	C6H13NO2
	89.02464	L-Lactic acid	C3H6O3
	166.08627	L-Phenylalanine	C9H11NO2
	205.09718	L-Tryptophan	C11H12N2O2
	124.03958	Nicotinic acid	C6H5NO2
	220.11818	Pantothenic acid	C9H17NO5
	144.10189	Proline betaine	C7H13NO2
	128.03504	Pyroglutamic acid	C5H7NO3
	124.00741	Taurine	C2H7NO3S
	112.98559	Trifluoroacetic acid	C2HF3O2
	267.07371	inosine	C10H12N4O5

Table 7. Summary of metabolites identified by the tissue type. (✓) indicates the metabolites detection in each tissue.

Metabolite	Mantle	Gills	Digestive system
1-Hexadecanol		✓	
1-Kestose	✓	✓	✓
1,10-Phenanthroline			✓
1,3-Dihydroxyacetone dimer	✓	✓	✓
1,5-Anhydrosorbitol	✓	✓	
1,6-Anhydroglucose	✓	✓	✓
16-hydroxypalmitic acid	✓		
2-Aminopimelic acid		✓	✓
2-Hydroxybutyric acid	✓	✓	✓
2-Hydroxyethanesulfonate	✓	✓	✓
2-Hydroxyisobutyric acid			✓
2-Hydroxyphenylacetic acid	✓		
2-Hydroxypyridine	✓	✓	✓
2-Isopropylmalic acid			✓
2-Methylbutyrylcarnitine	✓		
2-Methylbutrylglycine	✓		
2-Phenylglycine	✓		✓
2-Thiouracil		✓	✓
2-Toluic acid	✓	✓	
2,3-Diaminopropionic acid	✓	✓	✓
2,3-dihydroxypropyl hexadecanoate	✓	✓	
2,3-Diphosphoglyceric acid		✓	✓
2,6-Diaminopurine	✓	✓	✓
2,6-Pyridinedicarboxylic acid			✓
2'-Deoxyadenosine	✓	✓	✓
3-Aminopropionitrile			✓
3-Dehydroquinone	✓		
3-Hydroxyaspartic acid	✓	✓	✓
3-Hydroxybenzoic acid		✓	
3-hydroxybenzoic acid-3-O-sulphate			✓
3-Hydroxybutyric acid			✓
3-Hydroxypyruvate	✓		
3-Indoleacetonitrile	✓	✓	✓
3-Methyl-2-oxovaleric acid	✓		
3-Methyladenine	✓	✓	✓
3-Oxoadipic acid	✓	✓	✓

3-Pyridylacetic acid	✓	✓	✓
3,4-Dihydroxymandelic acid		✓	✓
3,4-Methyleneazelaic acid	✓	✓	
3,4-Methylenesebacic acid	✓		
4-Aminohippuric acid	✓	✓	✓
4-Hydroxybenzaldehyde	✓	✓	✓
4-Hydroxybenzoic acid	✓	✓	✓
4-Hydroxyphenylacetic acid			✓
4-Hydroxyproline	✓	✓	
4-Hydroxypyridine	✓	✓	✓
4-Methylumbelliferone			✓
4-O-methylolivetolcarboxylic acid	✓		
5-Aminovaleric acid	✓	✓	✓
5-Dehydroquinic acid	✓		
5-Hydroxy-L-tryptophan	✓	✓	✓
5-Hydroxymethyluracil	✓	✓	✓
5-Keto-D-Gluconate	✓	✓	✓
5,6-Dihydrouracil	✓	✓	✓
6-(gamma,gamma-Dimethylallylamino)purine			✓
6-Amino-1-Methyluracil	✓	✓	✓
6-Hydroxynicotinic acid	✓		✓
Acetaminophen	✓		
Adenine	✓	✓	✓
Adenosine	✓		
Adenosine monophosphate	✓	✓	
Adipic acid	✓	✓	✓
Alanylalanine	✓	✓	✓
Allantoin	✓		
alpha-Ketoglutaric acid	✓		
alpha-Ketoisovaleric acid			✓
Alpha-Lactose	✓	✓	✓
alpha-Tocopherol	✓	✓	✓
Amantadine	✓		✓
Aminoadipic acid	✓		✓
Aniline	✓	✓	✓
Anthracene	✓	✓	
Anthranilic acid			✓
Apigenin	✓	✓	✓
Arachidic acid	✓	✓	✓
Behenic acid	✓		

Benzoic acid	✓	✓	✓
beta-Alanine	✓	✓	✓
Beta-D-Fructose 6-phosphate	✓	✓	✓
Betaine	✓	✓	✓
Bicine	✓	✓	✓
Biopterin	✓		✓
Cadaverine			✓
Caffeic acid	✓	✓	✓
Chlorogenic acid			✓
Ciliatine	✓	✓	✓
cis-Aconitic acid	✓		✓
cis-p-Coumaric acid	✓		✓
Citramalic acid	✓	✓	✓
Citric acid	✓		✓
Coniferaldehyde		✓	✓
Coniferyl alcohol	✓	✓	✓
Coumarinic acid	✓	✓	✓
Creatinine	✓		
Cyanine	✓	✓	
Cystamine	✓		
Cysteamine		✓	
Cysteinyglycine	✓	✓	✓
Cytosine	✓	✓	✓
D-Allose	✓	✓	✓
D-Allulose	✓	✓	✓
D-Arabinose-5-phosphate	✓	✓	✓
D-Fucose	✓	✓	✓
D-Galactosamine	✓	✓	✓
D-Galactose	✓	✓	✓
D-Glucose	✓	✓	✓
D-Glucose-6-phosphate	✓	✓	✓
D-Glutamine			✓
D-Maltose	✓	✓	✓
D-Phenyllactic acid	✓		
D-Raffinose		✓	✓
D-Ribulose	✓	✓	✓
D-Ribulose-1,5-Bisphosphate	✓		✓
D-Ribulose-5-phosphate	✓	✓	✓
D-Sorbitol		✓	✓
D-Sorbitol-6-phosphate	✓	✓	

D-Threitol	✓	✓	
D-Trehalose	✓	✓	✓
D-Turanose	✓		✓
D-Xylitol			✓
D-Xylulose		✓	
Daidzein	✓	✓	✓
Deoxyadenosine monophosphate			✓
Deoxyinosine			✓
Deoxyuridine	✓		
Dethiobiotin	✓	✓	✓
Diaminopimelic acid		✓	✓
Dihydroxyacetone		✓	✓
Dimethylbenzimidazole	✓		
Dimethylglycine	✓	✓	
DL-2-Aminooctanoic acid	✓		✓
DMSP	✓	✓	✓
Dopamine	✓	✓	✓
Epigallocatechin	✓	✓	✓
Epinephrine	✓	✓	✓
Erucamide		✓	✓
Erythronic acid		✓	
Eserine	✓		
Ethionine	✓	✓	✓
Ethyl glucuronide	✓		
Ethylmalonic acid		✓	
Ferulic acid	✓	✓	✓
Formate	✓	✓	✓
Fumarate	✓	✓	✓
Fumaric acid	✓	✓	✓
Galactitol	✓	✓	✓
Galactonic acid			✓
Gallic acid	✓	✓	✓
Genistein	✓		
Gentisic acid	✓	✓	
Glucaric acid	✓	✓	✓
Gluconic acid			✓
Glucose 6-phosphate	✓		
Glutaconic acid	✓		
Glutamylphenylalanine	✓		
Glutaric acid	✓	✓	✓

Glyceraldehyde		✓	✓
Glyceric acid	✓	✓	
Glycerol	✓	✓	✓
Glycerol 1-phosphate	✓	✓	✓
Glycine	✓		✓
Glycolic acid	✓	✓	✓
Guanine	✓	✓	✓
Guanosine			✓
Guanosine monophosphate	✓		
Harmaline	✓	✓	✓
Heptadecanoic acid	✓	✓	✓
Hippurate	✓	✓	✓
Homogentisic acid	✓	✓	✓
Homoserine lactone	✓	✓	✓
Hydrocinnamic acid	✓	✓	
Hydroxylamine	✓	✓	✓
Hypotaurine	✓	✓	
Hypoxanthine			✓
Indole-3-carboxyaldehyde	✓		
Indoleacetic acid		✓	
Inosine	✓	✓	✓
Isocitric acid	✓	✓	✓
Isophthalic acid	✓	✓	✓
Isovalerylcarnitine		✓	✓
Isovalerylglycine		✓	✓
Kaempferol			✓
Ketoleucine	✓	✓	✓
Kojic acid			✓
Kynurenate	✓	✓	✓
L-3-Cyanoalanine	✓	✓	✓
L-Alanine	✓	✓	✓
L-Arginine		✓	✓
L-Ascorbic acid	✓	✓	✓
L-Asparagine	✓	✓	✓
L-Aspartic acid	✓	✓	
L-Carnitine	✓	✓	✓
L-Citrulline	✓	✓	✓
L-Cysteic acid	✓	✓	✓
L-Cysteine			✓
L-Dopa	✓	✓	✓

L-Glutamic acid	✓	✓	✓
L-Glutamine	✓		✓
L-Histidine	✓	✓	✓
L-Homocarnosine	✓		
L-Isoleucine	✓	✓	✓
L-Leucine	✓	✓	✓
L-Lysine	✓	✓	✓
L-Mandelic acid	✓	✓	✓
L-Methionine	✓	✓	✓
L-Norleucine	✓	✓	✓
L-Ornithine	✓	✓	✓
L-Phenylalanine	✓	✓	✓
L-Prolinamide	✓		✓
L-Proline	✓	✓	✓
L-Rhamnose			✓
L-Tryptophan	✓	✓	✓
L-Tyrosine	✓	✓	✓
L-Valine	✓	✓	✓
Lactate	✓	✓	✓
Lactic acid	✓	✓	✓
Lactitol		✓	
Lauric acid	✓	✓	
Lignoceric acid		✓	✓
Linoleic acid	✓	✓	✓
Maleamic acid	✓		
Malic acid	✓	✓	✓
Malonic acid	✓	✓	✓
Maltotriose	✓	✓	
Mesaconic acid			✓
Methyldopa	✓	✓	✓
Methylmalonic acid	✓	✓	✓
Methylsuccinic acid			✓
Methyluracil	✓	✓	✓
Minoxidil	✓	✓	✓
Monoethylhexyl phthalic acid	✓		
Myo-Inositol	✓	✓	✓
Myricetin	✓	✓	✓
N-Acetyl-L-aspartic acid			✓
N-Acetylleucine	✓	✓	✓
N-Acetylmannosamine	✓	✓	✓

N-alpha-Acetyl-L-lysine	✓		
N-Methylalanine	✓	✓	✓
N-Methylethanolamine		✓	
Nicotinic acid	✓	✓	✓
Norvaline	✓	✓	✓
O-Acetylserine	✓		✓
O-Phosphoethanolamine			✓
O-Succinyl-L-Homoserine			✓
Octacosanoic acid	✓	✓	✓
Oxoglutaric acid	✓		
Palmitic acid	✓	✓	✓
Pantothenic acid	✓	✓	✓
Pelargonic acid		✓	
Penicillamine	✓		
Pentachlorophenol			✓
Phenylephrine		✓	
Phenylhydrazine	✓	✓	✓
Phosphoenolpyruvic acid	✓	✓	✓
Phosphoric acid	✓	✓	
Picolinic acid	✓	✓	✓
Pimelic acid	✓	✓	✓
Pipecolic acid	✓		
Pirbuterol	✓		
Podophyllotoxin			✓
Prephenate			✓
Proline betaine	✓	✓	✓
Propyleneglycol	✓	✓	✓
Protocatechuic acid	✓	✓	✓
Psoralen		✓	✓
Putrescine	✓	✓	
Pyrogalllic acid	✓		✓
Pyroglutamic acid	✓	✓	✓
Pyrophosphate	✓	✓	✓
Pyruvic acid			✓
Quinic acid	✓	✓	✓
Quinolinic acid	✓		✓
S-Adenosylmethionine	✓		
S-Carboxymethyl-L-cysteine	✓		
Sakuranetin	✓	✓	
Sarcosine	✓	✓	✓

Serotonin	✓	✓	✓
Shikimic acid	✓	✓	✓
Sinapic acid	✓	✓	✓
Sinapyl aldehyde			✓
Sinigrin			✓
Spermine	✓	✓	✓
Stearic acid	✓	✓	✓
Suberic acid	✓	✓	
Succinic acid	✓	✓	✓
Sucrose			✓
Tartaric acid	✓	✓	✓
Taurine	✓	✓	✓
Terephthalic acid			✓
Tetrahydro-2,5-furan-diacetic acid	✓		
Thymine	✓	✓	✓
Tranexamic Acid	✓	✓	
Trifluoroacetic acid	✓	✓	✓
Trigonelline	✓	✓	✓
Uracil	✓	✓	✓
Urea		✓	
Ureidosuccinic acid	✓	✓	✓
Uric acid	✓	✓	✓
Uridine	✓	✓	✓
Uridine 5-diphosphate N-acetylgalactosamine		✓	
Uridine 5-diphospho-N-acetylglucosamine	✓		✓
Uridine 5_monophosphate	✓		
Vanillylmandelic acid	✓	✓	✓
Xanthine	✓	✓	✓
Xanthosine	✓	✓	✓
Xanthurenic acid			✓