

Electronic Supplementary Information (ESI) for Comparative Local Analysis of Metabolites, Lipids and Proteins in Intact Fish Tissues by LAESI Mass Spectrometry

Bindesh Shrestha,^a Robert Javonillo,^{b,c} John R. Burns,^b Zsolt Pirger,^d and Akos Vertes*^a

^aDepartment of Chemistry, W. M. Keck Institute for Proteomics Technology and Applications, The George Washington University, Washington, DC, 20052, USA

^bDepartment of Biological Sciences, The George Washington University, Washington, DC, 20052, USA

^cCurrent address: Department of Natural Sciences, Coppin State University, Baltimore, MD, 21216, USA

^dDepartment of Chemical-Ecology and Zoology, Centre for Ecological Research, Hungarian Academy of Sciences, Balaton Limnological Institute, Tihany, Hungary

*Corresponding author. E-mail: vertes@gwu.edu. Phone: +1 (202) 994-2717. Fax: +1 (202) 994-5873.

Table S1. Tentative assignments of metabolite and lipid ions observed in the gill glands of mature *A. anisitsi*. Lipid assignments included phosphatidylcholine (PC), phosphatidylserine (PS), phosphatidylinositol (PI), phosphatidylethanolamine (PE) sphingomyelin (SM) and phosphatidylglycerol (PG) species.

Metabolite and Lipid Ions ^a	m/z calc. ^b	m/z meas.	$\Delta m/z$
choline + NH ₄ ⁺	104.118	104.122	0.004
creatine + Na ⁺	131.081	131.058	0.023
acetylcholine + H ⁺	146.165	146.167	0.002
histidine + NH ₄ ⁺	155.092	155.068	0.024
-	-	131.058	-
lysine + H ⁺	146.165	146.167	0.002
-	-	149.060	-
-	-	165.052	-
-	-	118.994	-
tryptophan + Na ⁺	204.172	204.147	0.025
-	-	117.026	-
-	-	163.987	-
hexose + Na ⁺	180.097	180.050	0.047
acetylgalactosamine + H ⁺	221.128	221.135	0.007
thiamine (B1) + Na ⁺	300.998	300.961	0.037
-	-	219.079	-
coenzyme-A (CoA) + H ⁺	767.594	767.603	0.009
cholesterol + Na ⁺	369.349	369.356	0.007
dehydroepiandrosterone + H ⁺	288.424	288.379	0.045
-	-	286.124	-
dehydrotestosterone + H ⁺	290.442	290.522	0.080
-	-	289.665	-
-	-	300.115	-
11-ketotestosterone + H ⁺	302.407	302.397	0.010
5-androstenetriol + H ⁺	307.226	307.254	0.028
-	-	353.141	-
-	-	362.195	-

PC[32:0] + K ⁺	758.546	758.550	0.004
PC[34:4] + Na ⁺	760.525	760.575	0.050
PC[36:5] + H ⁺	780.553	780.556	0.003
PC[34:1] + K ⁺	782.546	782.560	0.014
PC[38:8] + H ⁺	802.538	802.534	0.004
PC[36:3] + Na ⁺	806.546	806.578	0.032
PC[40:10] + H ⁺	826.538	826.548	0.010
PC[40:9] + H ⁺	828.553	828.546	0.007
PC[40:5] + H ⁺	836.616	836.614	0.002
PC[38:6] + K ⁺	844.525	844.529	0.004
PC[42:11] + H ⁺	852.553	852.567	0.014
PS[38:2] + K ⁺	854.530	854.564	0.037
PS[38:1] + K ⁺	856.546	856.585	0.039
PI[35:2] + H ⁺	833.553	833.577	0.024
PI[33:1] + Na ⁺	845.517	845.522	0.005
PI[35:1] + Na ⁺	857.551	857.596	0.045
PI[40:1] + Na ⁺	929.645	929.622	0.023
PE[32:1] + H ⁺	732.553	732.546	0.007
PE[40:6] + H ⁺	808.548	808.582	0.034
PE[41:4] + H ⁺	810.600	810.611	0.011
PE[41:5] + Na ⁺	830.530	830.567	0.037
PE[42:11] + Na ⁺	832.525	832.570	0.045
PE[40:4] + K ⁺	834.541	834.496	0.047
PE[41:2] + Na ⁺	836.614	836.593	0.021
PE[40:6] + K ⁺	846.504	846.506	0.002
SM[34:1] + Na ⁺	725.556	725.561	0.005
SM[38:1] + H ⁺	835.589	835.605	0.016
SM[41:2] + K ⁺	837.624	837.645	0.021
PG[37:1] + K ⁺	829.535	829.561	0.026
PG[40:6] + Na ⁺	831.551	831.584	0.033
PG[40:4] + Na ⁺	835.584	835.605	0.021

^aPC, PS, PI, PE, SM, and PG species are identified by the total length of the acyl chain(s) and the number of double bonds in parentheses.

^bThe monoisotopic masses were calculated using the NIST Isotope Calculator package (ISOFORM, Version 1.02), and the measured *m/z* values were obtained from typical mass spectra.