Electronic Supplementary Material (ESI) for Molecular BioSystems.

Lipid Dynamics in Zebrafish Embryonic Development Observed by DESI-MS Imaging and nanoelectrospray-MS †

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†Electronic supplementary information (ESI) available: Supplementary Figures S1-S5.

SUPPLEMENTARY INFORMATION

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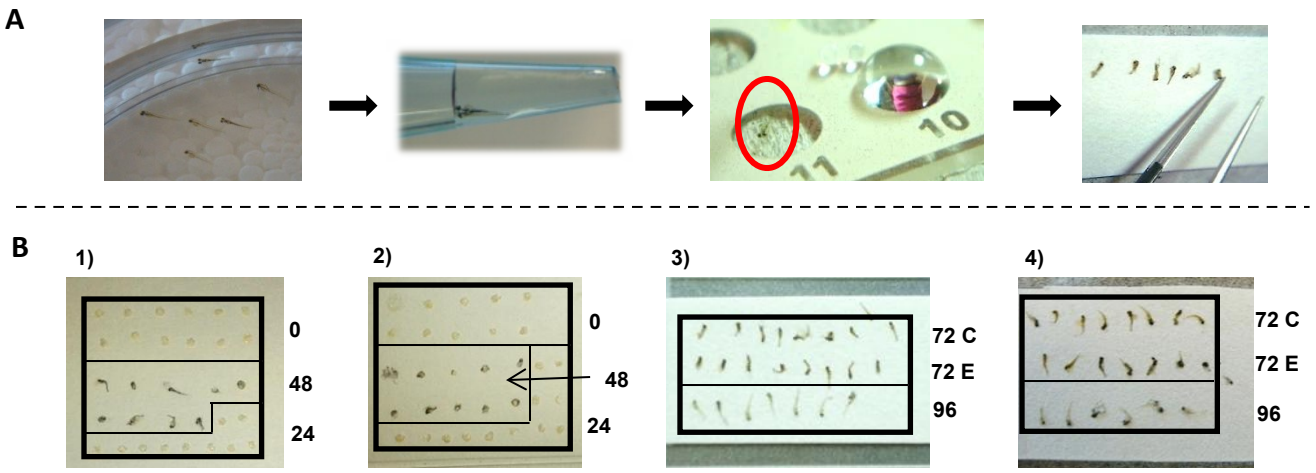

Figure S1. A. Workflow of zebrafish embryo handling: embryos were individually transferred alive from a Petri, excessive liquid was removed to minimize the movement of the hatched embryos; then with the aid of fine tweezers, each embryo was placed onto a rectangular-shaped piece of Whatman grade 1 cellulose filter paper, taped onto a glass microscope slide. **B.** Arrangement of the zebrafish embryos on filter paper taped to a glass microscope slide for DESI-MS analysis. Paper arrays are numbered from 1 to 4. Embryos are identified by their stage of development (0, 24, 48, 72, and 96 hpf); 72 C and 72 E represent controls and TCE exposed embryos.

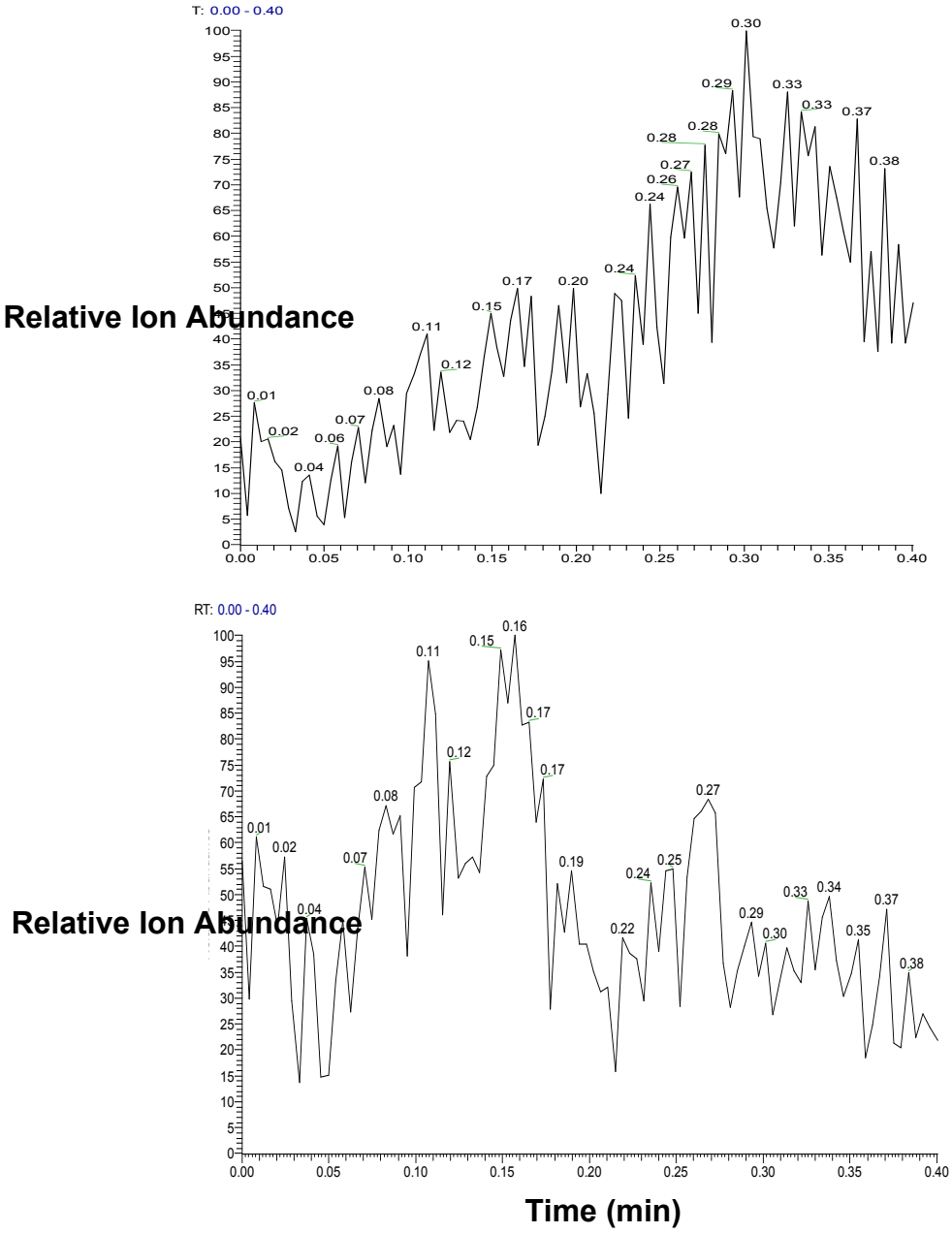

Figure S2. Chronogram of the ion of *m/z* 511 acquired over 24 s by nESI-MS, illustrating the increase of relative signal intensity for the FA dimers compared to the ion of *m/z* 794.

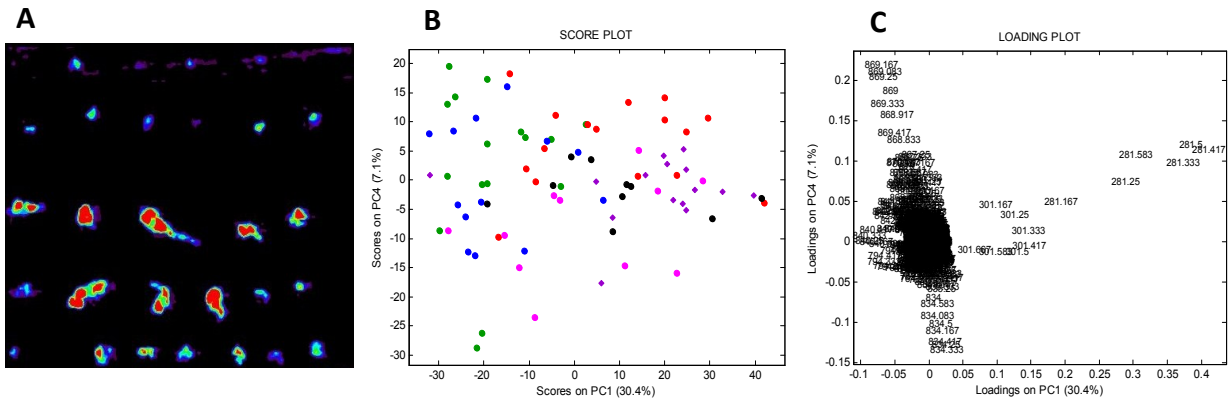

Figure S3. A. DESI image of slide # 1 (embryos at 0, 24, and 48 hpf) for the ion of *m/z* 281. **B.** Score plot of PC1 and PC2. Samples have been color-coded as follows: 0 hpf, green; 24 hpf, blue; 48 hpf, red; 72 hpf controls, black; 72 hpf exposed to TCE, purple; 96 hpf, magenta. **C.** Loading plot of PC1 and PC2. Variables are labeled in terms of their *m/z* ratio.

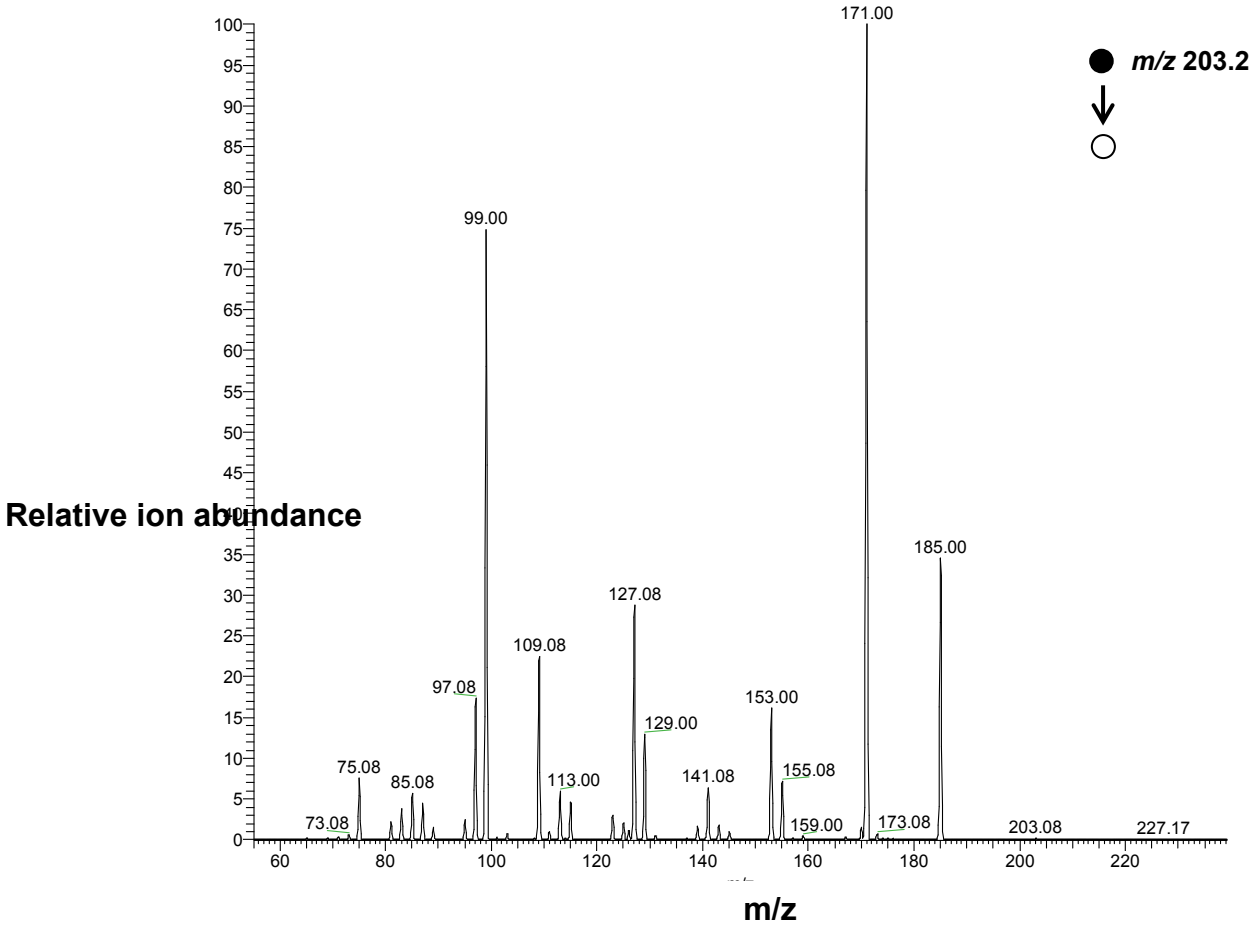

Figure S4. Product ion scan for the precursor ion of *m/z* 203.2 acquired by nESI-MS/MS. The average product ion spectrum was collected from a representative sample from an embryo at 48 hpf.

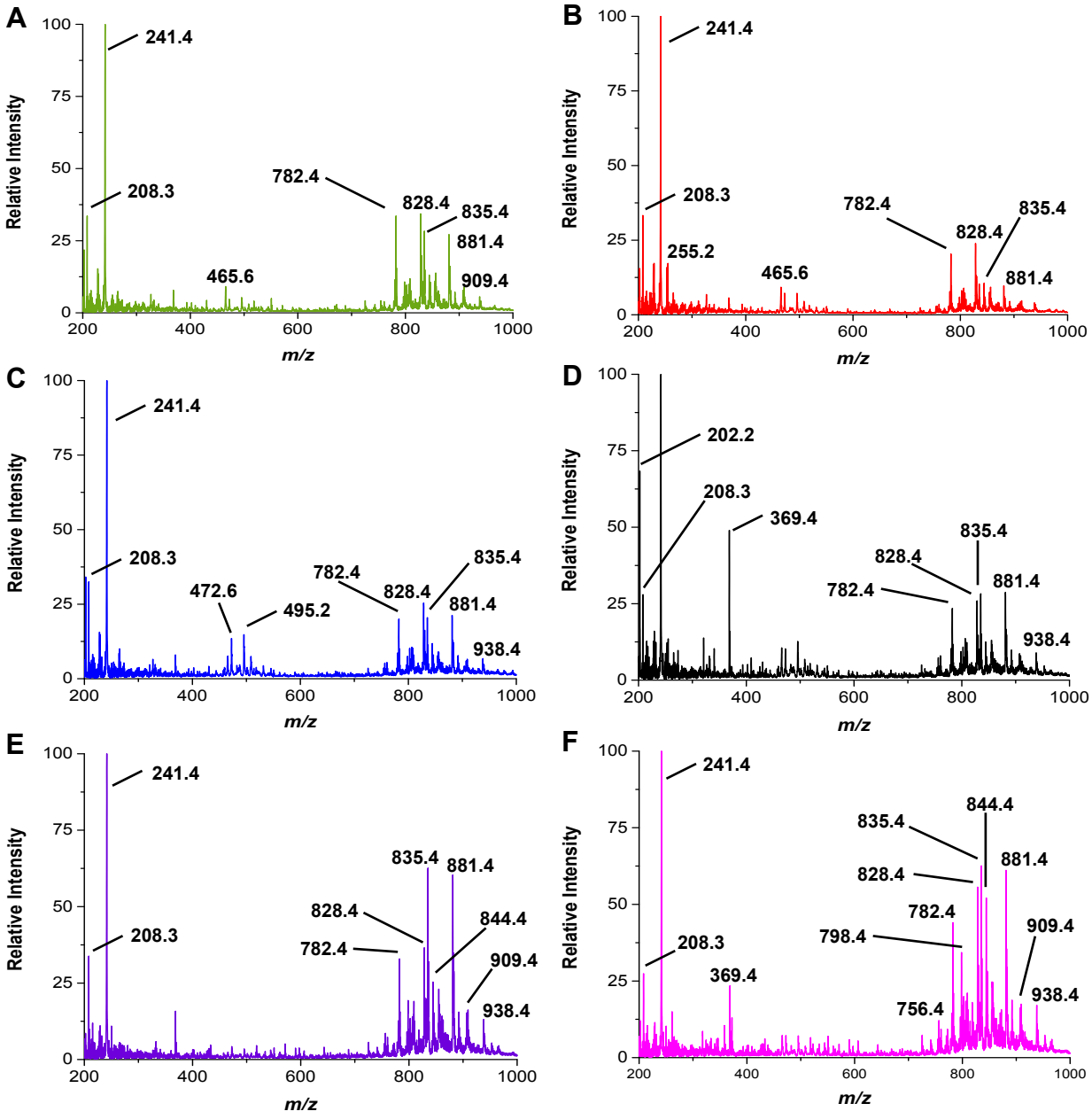

Figure S5. Averaged nESI-MS spectra in positive ion mode. **A.** 0 hpf (N=12 samples). **B.** 24 hpf (N=17 samples). **C.** 48 hpf (N=16 samples). **D.** 72 hpf, controls (N=11 samples). **E.** 72 hpf, exposed to TCE (N=13 samples). **F.** 96 hpf (N=12 samples).

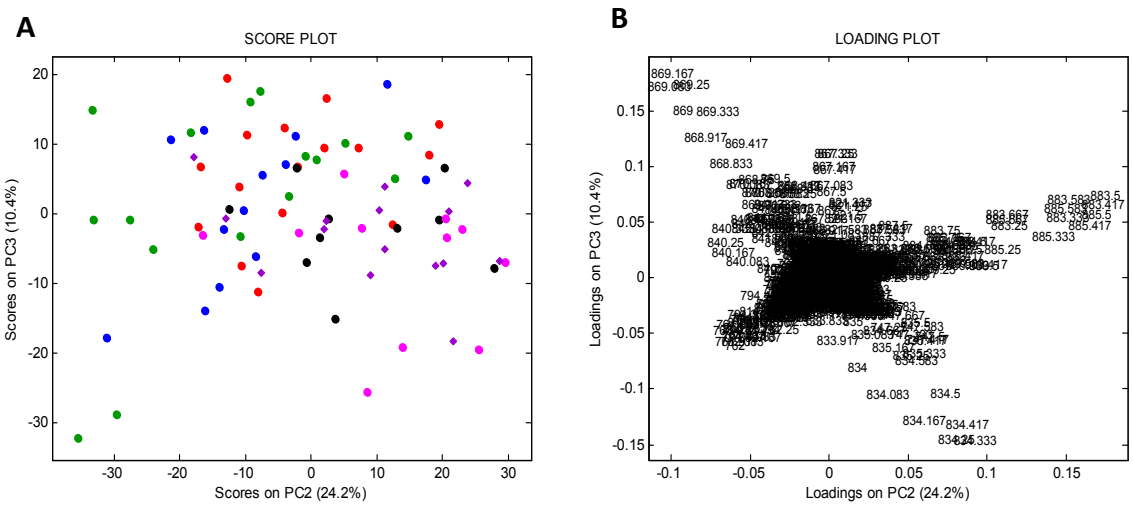

Figure S6. Negative ion mode data acquired by nESI-MS. **A.** Score plot of PC2 and PC3 for the truncated data between *m/z* 700-1000. Samples have been color-coded as follows: 0 hpf, green; 24 hpf, blue; 48 hpf, red; 72 hpf controls, black; 72 hpf exposed to TCE, purple; 96 hpf, magenta. **B.** Loading plot of PC2 and PC3. Variables are labeled in terms of their *m/z* ratio.

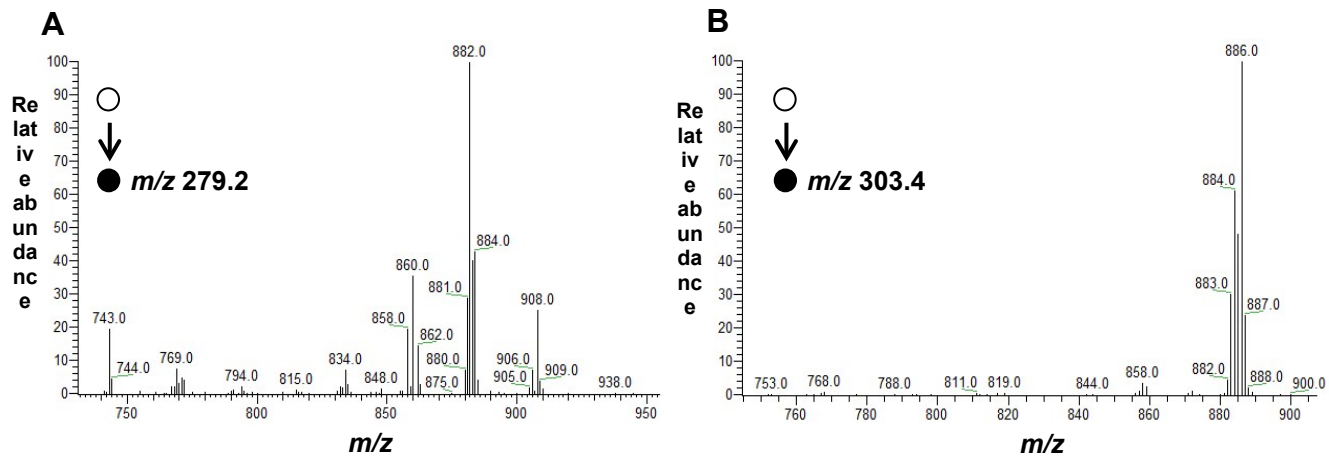

Figure S7. A. Precursor ion scan for the product ion of *m/z* 279.2. **B.** Precursor ion scan for the product ion of *m/z* 303.4. Average precursor scan spectra were collected from a representative zebrafish embryo at 72 hdf by nESI-MS/MS in negative ion mode.

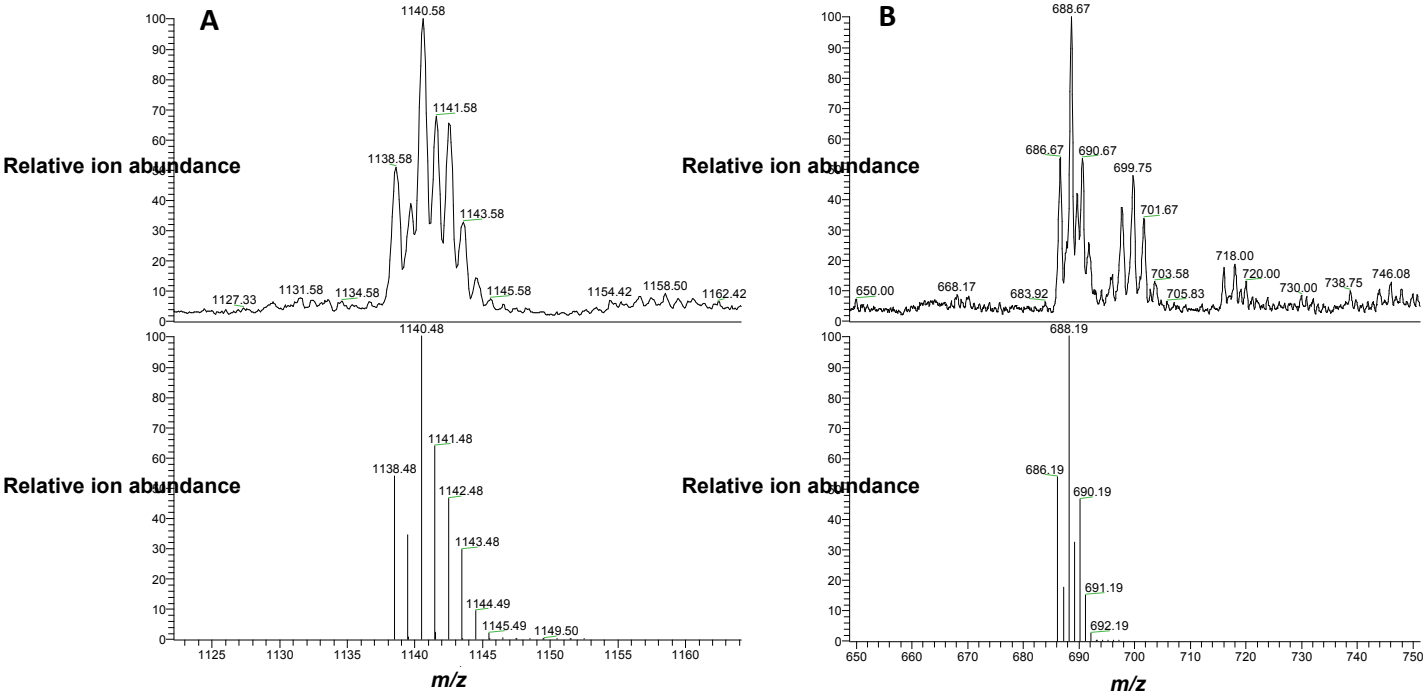

Figure S8. A. DESI-MS spectrum acquired in low mass resolution (zoomed over the range of *m/z* 1120-1165) from a representative zebrafish embryo at 96 hpf (top) compared with the theoretical isotopic distribution of ubiquinone detected as silver adduct $[M+Ag_2NO_3]^+$ (bottom). **B.** DESI-MS spectrum acquired in low mass resolution (zoomed over the range of *m/z* 650-750) from a representative zebrafish embryo at 96 hpf (top) compared with the theoretical isotopic distribution of squalene detected as silver adduct $[M+Ag_2NO_3]^+$ (bottom).

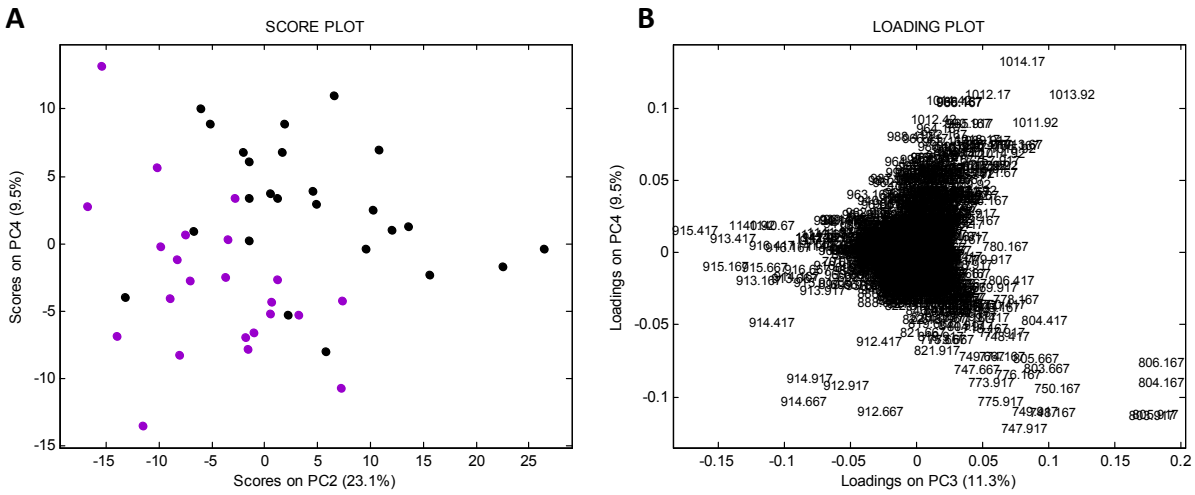

Figure S9. A. Score plot of PC2 and PC4. Samples have been color-coded as follows: 72 hpf controls, black; 72 hpf exposed to TCE, purple. **B.** Loading plot of PC2 and PC4. Variables are labeled in terms of their *m/z* ratio.