

## Supplementary Materials

# Tracing the thermal history of seafood products through *lyso*-phospholipid analysis by hydrophilic interaction liquid chromatography-electrospray ionization Fourier-transform mass spectrometry

Ilario Losito<sup>1,2,\*</sup>, Laura Facchini<sup>1</sup>, Rosa Catucci<sup>1</sup>, Cosima Damiana Calvano<sup>1,2</sup>, Tommaso R.I. Cataldi<sup>1,2</sup>, Francesco Palmisano<sup>1,2</sup>

<sup>1</sup> Dipartimento di Chimica, Università degli Studi di Bari "Aldo Moro", Via E. Orabona 4, 70126 Bari, Italy; ilario.losito@uniba.it

<sup>2</sup> Centro Interdipartimentale SMART, Università degli Studi di Bari "Aldo Moro", Via E. Orabona 4, 70126 Bari, Italy

\* Correspondence: ilario.losito@uniba.it; Tel.: +39-080-544-2506

### Titles of supplementary figures, as reported at the end of the main manuscript:

**Figure S1.** Comparison of typical ESI(+)-FTMS spectra obtained for PC in fresh seafood products

**Figure S2.** Comparison of typical ESI(+)-FTMS spectra obtained for LPC in fresh seafood products

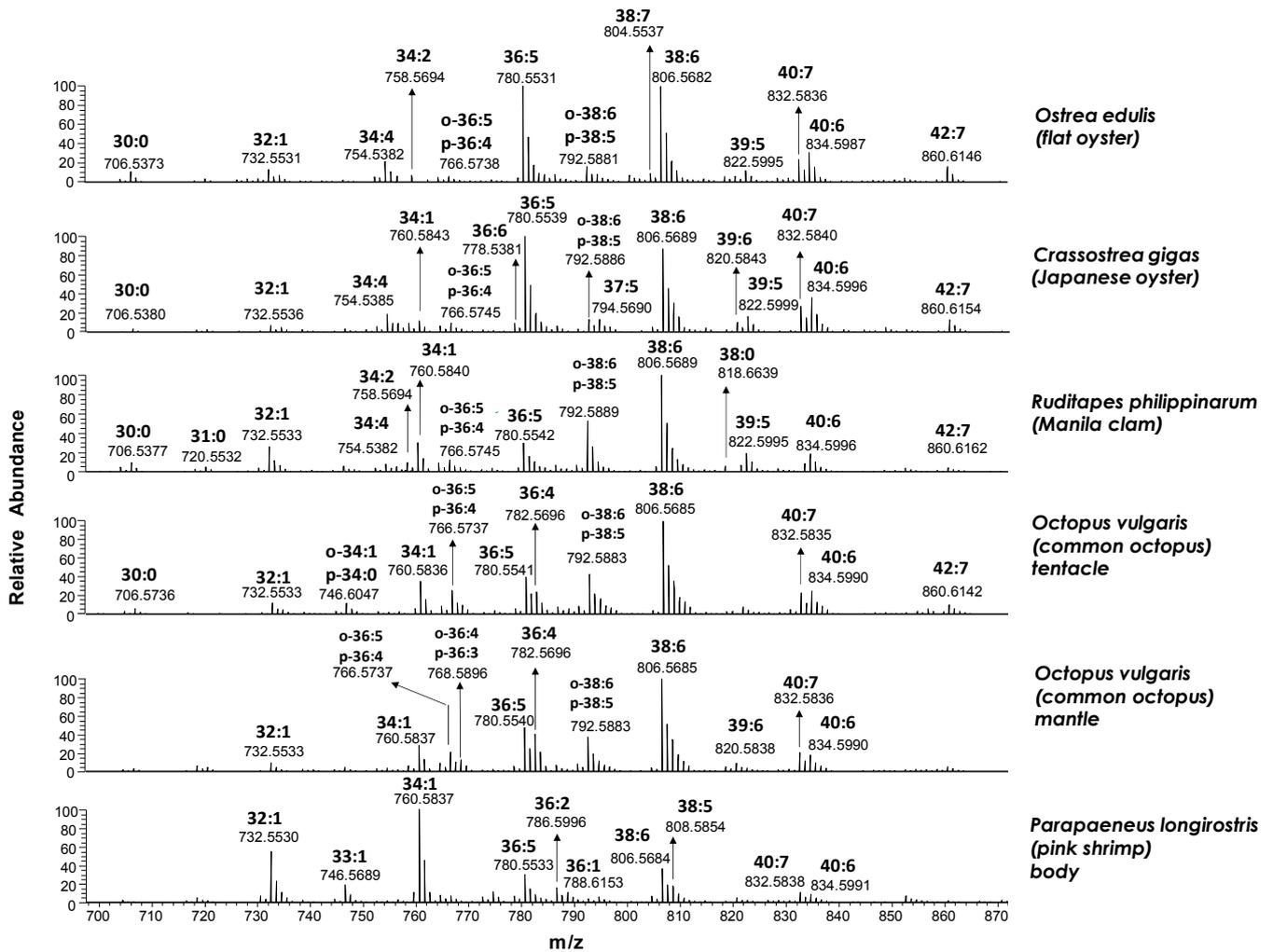
**Figure S3.** Comparison of typical ESI(+)-FTMS spectra obtained for PE in fresh seafood products

**Figure S4.** Comparison of typical ESI(+)-FTMS spectra obtained for LPE in fresh seafood products

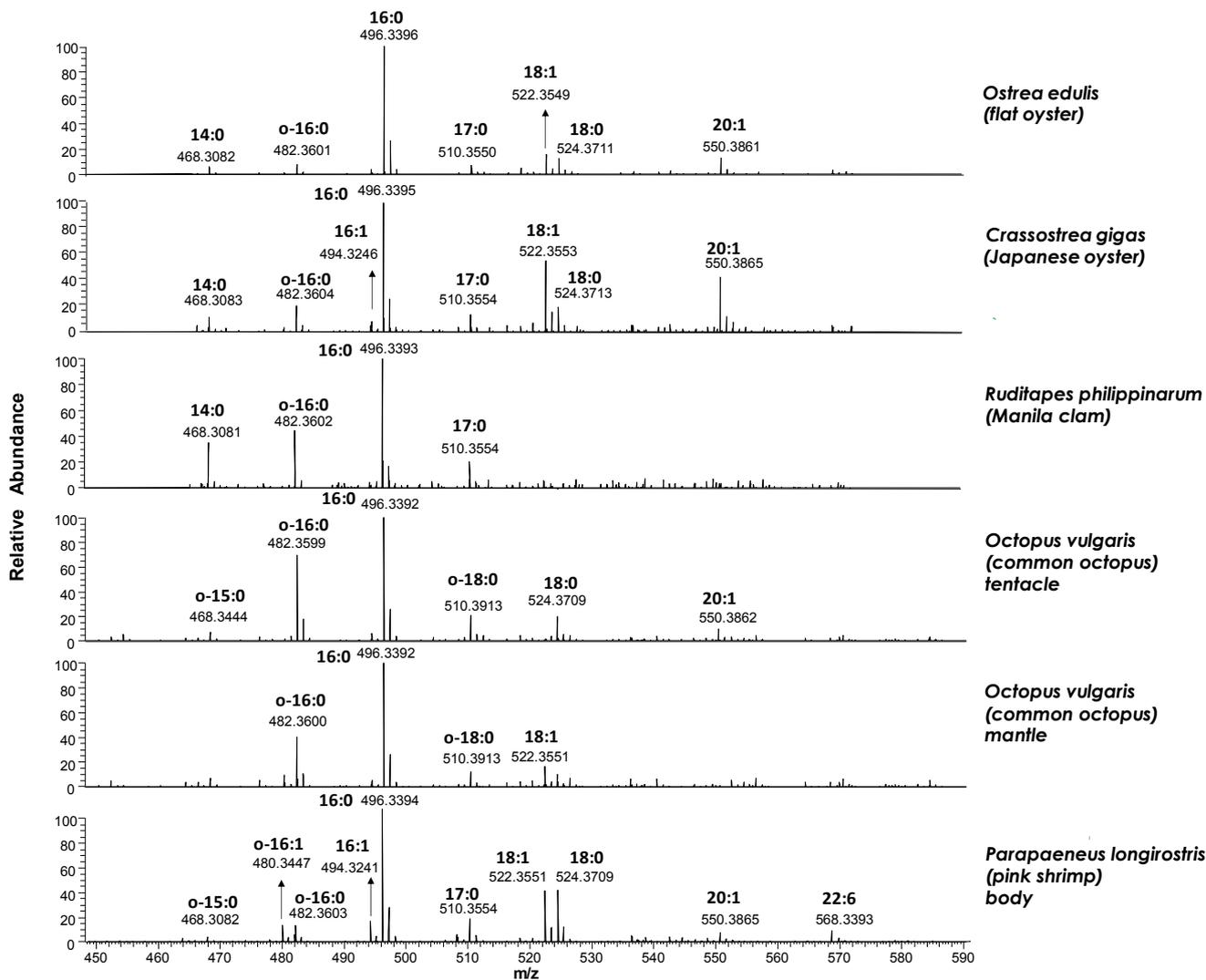
**Figure S5.** Comparison of LPE/PE and LPC/PC ESI(+)-FTMS response ratios obtained for fresh or refrigerated European flat oysters (*Ostrea Edulis*)

**Figure S6.** Comparison of typical ESI(+)-FTMS spectra obtained for LPC in seafood products after thermal treatments leading to the maximum accumulation of LPC

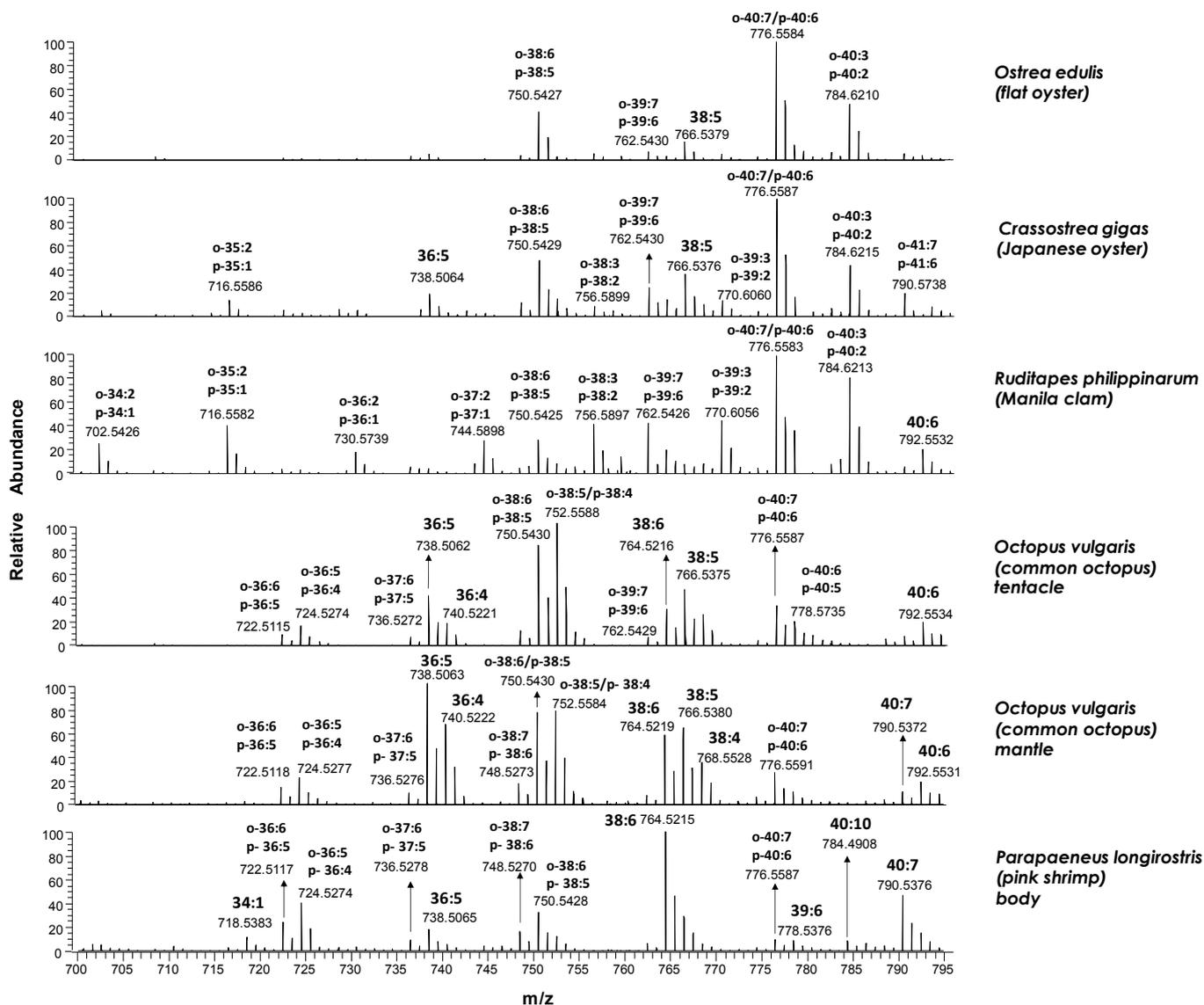
**Figure S7.** Comparison of typical ESI(+)-FTMS spectra obtained for LPE in seafood products after thermal treatments leading to the maximum accumulation of LPE



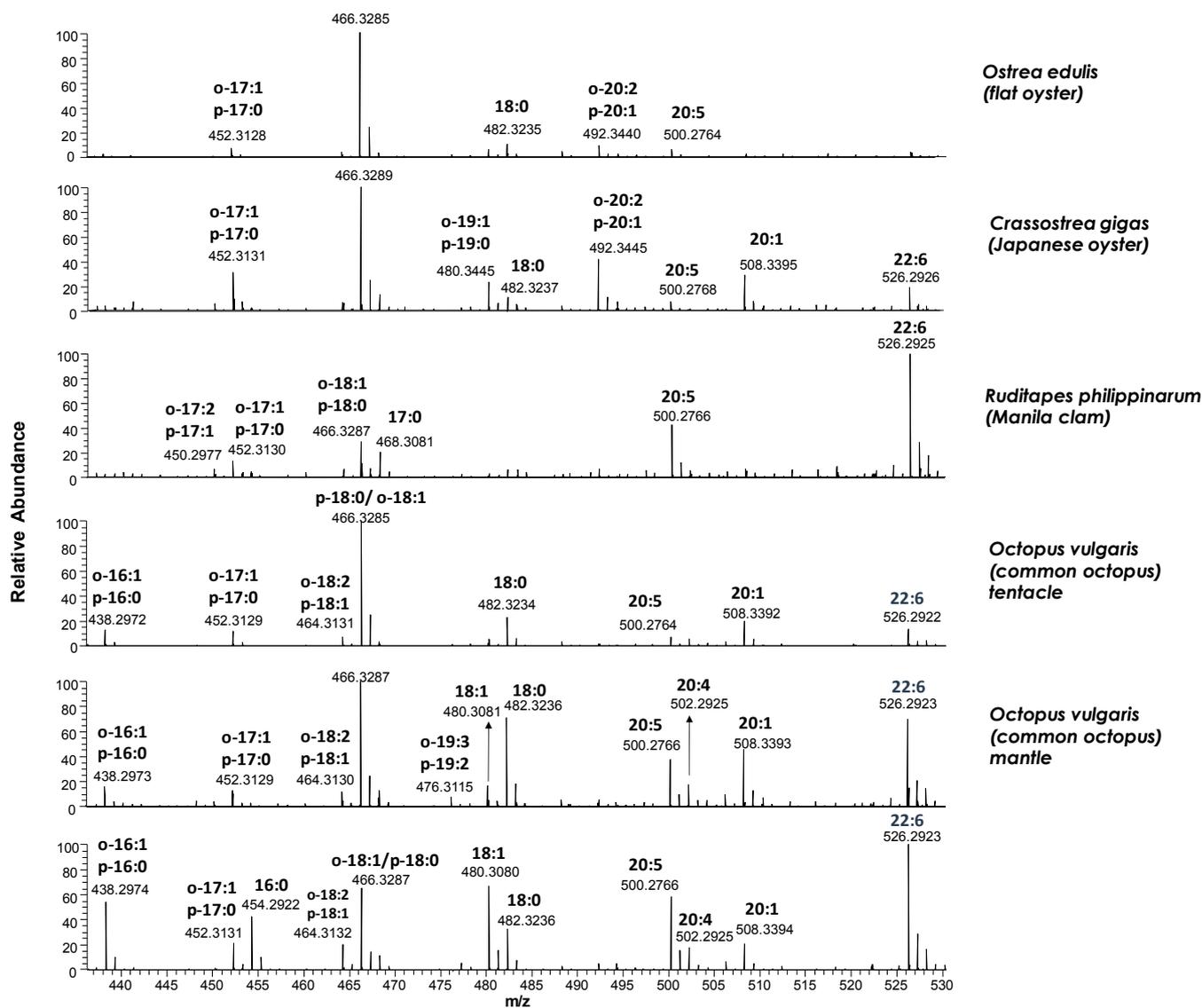
**Figure S1.** Comparison between typical ESI(+)-FTMS spectra obtained for the PC class during the HILIC-ESI(+)-FTMS analysis of lipid extracts obtained from different fresh seafood products. Spectra were averaged in the retention time interval 7.3 - 11.6 min (see Figure 1 in the paper).



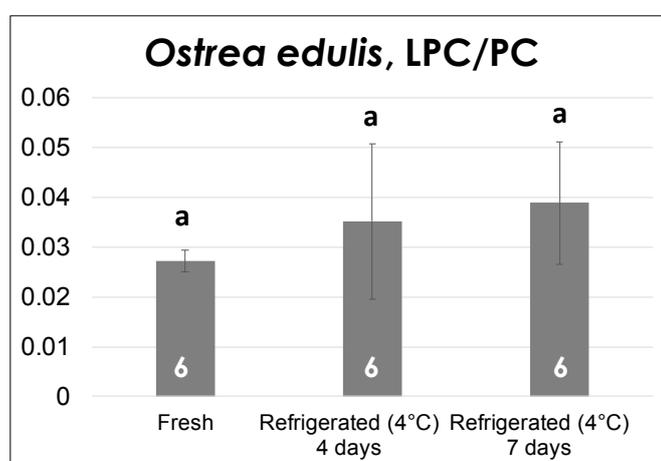
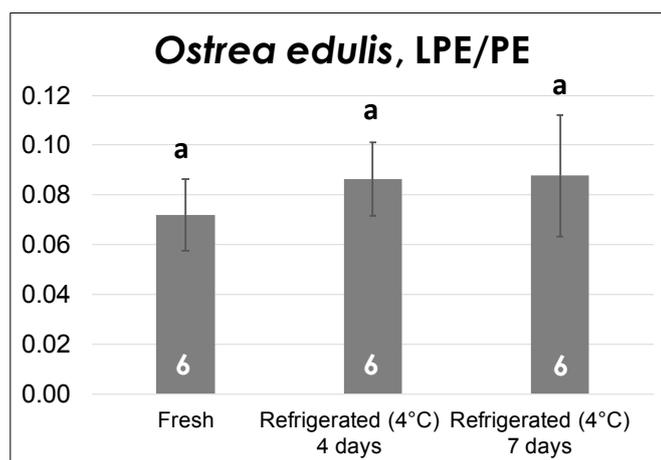
**Figure S2.** Comparison between typical ESI(+)-FTMS spectra obtained for the LPC class during the HILIC-ESI(+)-FTMS analysis of lipid extracts obtained from different fresh seafood products. Spectra were averaged in the retention time interval 14.6 - 16.7 min (see Figure 1 in the paper).



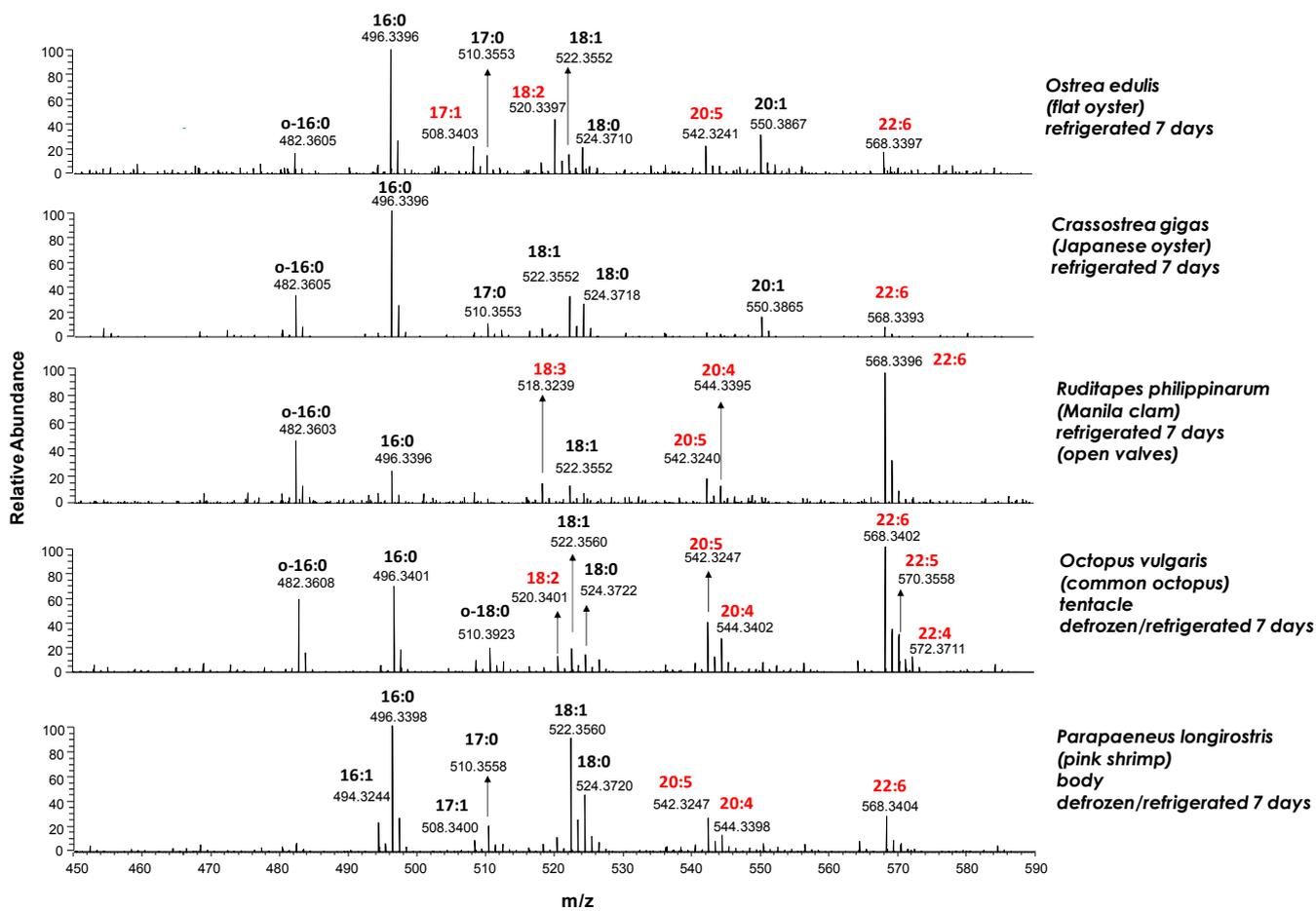
**Figure S3.** Comparison between typical ESI(+)-FTMS spectra obtained for the PE class during the HILIC-ESI(+)-FTMS analysis of lipid extracts obtained from different fresh seafood products. Spectra were averaged in the retention time interval 2.3 – 3.4 min (see Figure 1 in the paper).



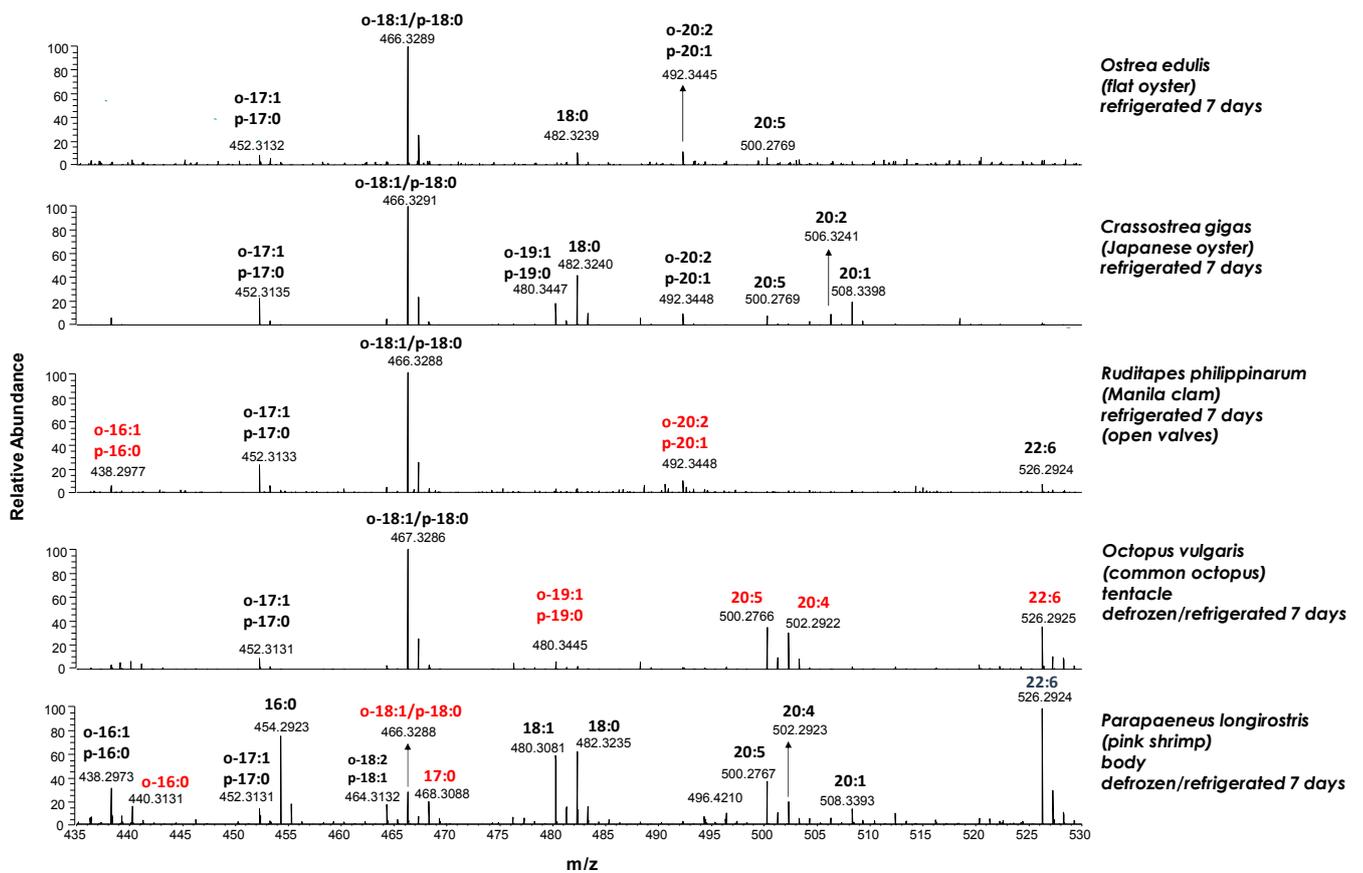
**Figure S4.** Comparison between typical ESI(+)-FTMS spectra obtained for the LPE class during the HILIC-ESI(+)-FTMS analysis of lipid extracts obtained from different fresh seafood products. Spectra were averaged in the retention time interval 3.4 – 4.3 min (see Figure 1 in the paper).



**Figure S5.** Comparison between LPE/PE and LPC/PC ratios of ESI(+)-FTMS responses obtained from the HILIC-ESI(+)-FTMS analysis of lipid extracts of European flat oysters (*O. edulis*) subjected to lipid extraction soon after purchase (as fresh product) or after refrigeration at 4°C for 4 or 7 days in a laboratory refrigerator. Mean values and standard deviations (indicated as error bars) are reported, referred to the number of replicates indicated for each type of sample. The results of a Tukey-Kramer test are reported in the form of sample type grouping, emphasized by letters. See the main text for details on the calculation of the LPE/PE and LPC/PC ratios from XIC chromatograms.



**Figure S6.** Comparison between ESI(+)-FTMS spectra obtained for the LPC class during the HILIC-ESI(+)-FTMS analysis of lipid extracts obtained from seafood products after thermal treatments leading to the maximum accumulation of LPC species. Red labels indicate LPC species that exhibited a significant variation (increase or decrease) in treated products with respect to fresh ones. Spectra were averaged in the retention time interval 14.6 - 16.7 min (see Figure 1 in the paper).



**Figure S7.** Comparison between ESI(+)-FTMS spectra obtained for the LPE class during the HILIC-ESI(+)-FTMS analysis of lipid extracts obtained from seafood products after thermal treatments leading to the maximum accumulation of LPE species. Red compositional labels indicate LPE species that exhibited a significant variation (increase or decrease) in treated products with respect to fresh ones. Spectra were averaged in the retention time interval 3.4 – 4.3 min (see Figure 1 in the paper).