## **SUPPLEMENTARY FIGURES**



Fig. S1. Raw Raman spectra of crustaceans. Black: *Thysanoessa raschii* (higher crustaceans, or *Euphausiacea*), red: *Calanus* spp. (copepod crustaceans of the *Calanoida* order), blue: liquid fat squeezed from *Calanus* spp.



Scheme S1. The schematic representation of ComDim.



**Fig. S2a.** PCA decomposition of LIB spectra (full dataset of 29 samples, full spectra), loadings. Black, red, and blue lines correspond to dark, medium-coloured, and light spots, respectively.





Fig. S2b. PCA decomposition of LIB spectra (full dataset of 29 samples, full spectra), cf. Fig. S2a. Shown are integrals of selected peaks on graphs of loadings, normalized to respective greatest absolute magnitudes among all the principal components. Wavelength positions of the peaks see in the main text. Black, red, and blue lines correspond to dark, medium-coloured, and light spots, respectively. The width of grey and white rings is 0.2.



**Fig. S3.** PCA decomposition of LIB spectra (full dataset of 29 samples, full spectra): scree plot of eigenvalues.



Shown are integrals of selected peaks on graphs of loadings, normalized to respective greatest absolute magnitudes among all the principal components. Wavelength positions of the peaks see in the main text. Black, red, and blue lines correspond to dark, medium-coloured, and light spots, respectively. The width of grey and white rings is 0.2.



**Fig. S5.** PCA decomposition of Raman spectra before (*a*) and after (*b*) masking of hydrocarbon chain signals. Dashed lines margin crustacean samples, cf. Fig. 4 in the main text.



Fig. S6. PCA decomposition of Raman spectra: a: loadings obtained for the full-length spectra (449 – 3151 cm<sup>-1</sup>); b: loadings obtained from spectra spanning the range of 449 – 1921 cm<sup>-1</sup>. Black, red, and blue lines correspond to dark, medium-coloured, and light spots, respectively.











## Fig. S9. CPCA decomposition of fused LIBS and Raman spectra (full dataset of 29 samples).



Fig. S10. CPCA decomposition of fused LIBS and Raman spectra (Calanoida dataset of 14 samples).



Fig. S11. NMF decomposition of fused LIBS and Raman spectra (*Calanoida* dataset of 14 samples).



Fig. S12. ComDim – PCA decomposition of fused LIBS and Raman spectra (full dataset of 29 samples).



Fig. S13. ComDim – PCA decomposition of fused LIBS and Raman spectra (*Calanoida* dataset of 14 samples). *Right*: loadings in the Raman domain. Left: integrals of selected peaks of LIBS loadings, normalized to respective greatest absolute magnitudes among all the principal components. Wavelength positions of the peaks see in the main text. Black, red, and blue lines correspond to dark, medium-coloured, and light spots, respectively. The width of grey and white rings is 0.2.



Fig. S14. ComDim – ICA decomposition of fused LIBS and Raman spectra (*Calanoida* dataset of 14 samples).



**Fig. S15.** PCA decomposition of fused LIBS and Raman spectra (*Calanoida* dataset of 14 samples, masked Li signals), cf. Fig. 3d in the main text. *a*: integrals of selected peaks of LIBS loadings, normalized to respective greatest absolute magnitudes among all the principal components; *b*: loadings in the Raman domain. Wavelength positions of the peaks see in the main text. Black, red, and blue lines correspond to dark, medium-coloured, and light spots, respectively. The width of grey and white rings is 0.2.