Impact of biogeochemical zonation and depositional setting on molecular composition of dissolved organic matter in sediment pore waters

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Dissolved organic matter (DOM) in sediment pore waters is a complex mixture of individual molecules, which are important reactants in biogeochemical cycles and serve as substrates for benthic organisms. The molecular composition of DOM reflects the organic matter sources and quality, geochemical conditions in the sediment and microbial impact.

Aiming at a better understanding of the interactions between DOM and sediment biogeochemistry we analyzed 48 pore water samples from 8 sampling sites in the Eastern and Western Mediterranean, Black and Marmara Seas with ultrahigh-resolution Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FTICRMS) for the molecular composition in the context of comprehensive geochemical data and microbial cell abundances. The samples cover a broad range of geochemical conditions (oxic vs. sulfate-reducing vs. methanogenic conditions), organic matter sources (marine-dominated vs. terrestrial-influenced) and sedimentary systems. We detected more than 10,000 molecular species in the mass range of 300-600 Da including more than 3100 N-bearing and 2200 S-bearing molecules. Individual samples contained between 1170 and 5901 molecular species and showed considerable compositional variations. S-bearing molecules were elevated in the Black Sea, whereas N-bearing molecules were more abundant in the sediments from the Eastern Mediterranean Sea.

To elucidate the mechanisms controlling these molecular variations we performed multivariate statistical analyses to unravel the complex biogeochemical information encoded in the molecular composition of DOM and shed new light on the microbe-DOM-interactions in marine sediments.