Multiproxy Characterization of Sedimentary Biomarker Archives using Ultrahigh Resolution Mass Spectrometry

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In order to better understand paleoenvironmental molecular proxies in marine sediments, and the changes in their compositions and distributions caused by complex processes (e.g. source organism dynamics, component degradation and diagenesis, etc.), more comprehensive, multiproxy approaches are needed. Herein, we demonstrate a novel ultrahigh resolution mass spectrometry approach that relies on in-house developed algorithms and analytical tools for rapid identification and visualization of thousands of species detected in marine sediments [1,2]. Such complex sets of biomarkers, ranging from 150 to 1500 Da, can be assessed from microgram quantities of whole sediment extract after a 12-minute analysis. Putatively identified classes of sedimentary biomarkers include chlorophyll and carotenoid pigments, ether lipids (branched and isoprenoid glycerol dialkyl glycerol tetraethers, GDGTs), their diagenetic products, and some novel and/or unexpected species. We also observed tentative compound groups of still unknown specific molecular structure, but with clear potential geochemical relevance (e.g. sphingolipids). Compositional variations along the sediment core profile are explored and applicability of ultrahigh resolution mass spectrometry data for calculation of common paleoenviromental indices, e.g. $TEX^{L}86$ or BIT is evaluated.

[1] Radovic et al. (2016) Anal. Chem., **88** (2), 1128–1137.

[2] Radović et al. (in press) Rapid Commun. Mass Spectrom., DOI: 10.1002/rcm.7556.