Molecular characterization of dissolved organic matter (DOM) from the deep water of the South China Sea

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It has been estimated that dissolved organic carbon (DOC) is the largest pool of reduced carbon in the ocean with an estimated mass of 700 gigatons of carbon, equivalent to the carbon content of carbon dioxide in the atmosphere. However, we still do not know much about the chemical structure and composition of oceanic DOM and how the chemistry of DOM varies with depth in the oceans. In this study, water samples were collected at depths of 500, 800, and 1500 meters at three stations in the South China Sea (SCS) in 2012. A custom-built 9.4 Tesla (T) FT-ICR mass spectrometer, located at the National High Magnetic Field Laboratory in Tallahassee, Florida was used for molecular characterization of dissolved organic matter in the SCS water samples. The FT-ICRMS produces mass accuracy of approximately $\pm$0.2 ppm up to m/z ~800, with average resolving power ($m/\Delta m_{50\%}$) > 700,000 at 400 Da. Our results suggest that DOM in the SCS water samples is (1) very similar in composition, regardless of depth, as suggested by elemental ratios (H/C and O/C) of formulas identified in the DOM; and (2) composed primarily of molecules with high H/C and moderate O/C ratios. Similarities in the composition of marine DOM at these sites are also evident based on the relative abundance of double bond equivalents in each molecular formula and comparison of formulas elemental content, including heteroatoms N and S. Taken together, these data suggest that DOM in these South China Sea samples is largely refractory and composed primarily of refractory carboxyl-rich alicyclic molecules, which likely represent a molecular "island of stability", or bioreactivity, of marine DOM. Further, our data address the chemistry “wing” of the PDPMC model (POM-DOM-Piezophilic Microorganism Continuum) (Fang et al., 2015, Science China (Earth Sciences), doi: 10.1007/s11430-014-4985-2).