

SPECIAL SEMINAR
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Marine Organic Geochemistry on a Computer

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We increasingly discover natural and anthropogenic organic chemicals in the ocean that can affect marine organisms or modulate their interactions. Examples include biotoxins from harmful algal blooms, petroleum compounds from oil seeps or oil spills, marine natural products, and industrial and commercial pollutants. But we often find that the more we sample, the less we seem to know: marine organic geochemists are increasingly overwhelmed by system complexity in the increasingly charted domains of space, time, and chemistry. To address this complexity, we are developing a flexible toolkit of advanced computational techniques, including quantum chemical computations, analysis of big data, and coupled simulations of transport, chemistry, and biology. In selected examples that I present, advanced computational methods are used: (i) to explain molecular mechanisms of the formation and degradation of bioactive chemicals in aquatic systems; (ii) to identify the environmental processes that control chemical impacts on aquatic organisms and/or human health; and (iii) to evaluate technical strategies for response and intervention during a major chemical event (e.g., an oil spill). These rapidly advancing computational tools are expected to revolutionize our understanding of marine organic geochemistry, including the roles of organic chemicals in ecological function, climate change, and socioeconomic security.