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Selective ligands for uranyl via combinatorial peptoid libraries: A synthetic, structural, thermodynamic and computational study

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Collaborators: N/A

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ABSTRACT: Estimates of the total mass of uranium in seawater are on the order of 4.5 billion tons, one thousand times that present in terrestrial ores (the total ocean volume is approximately 1.4×10^9 km^3; uranium is present at ca. 3 ppb). Despite this abundance, there are several major impediments to using uranium from seawater as a viable economic source of uranium. First, the concentration of uranium is very low; second, there are relatively high concentrations of other ions that interfere with uranium separation; and third, the volumes involved are extremely high. Our research is aimed at developing our fundamental understanding of how donor ligands bind to the uranyl ion, UO_2^{2+}, with the longer-term goal of using this information to tackle selective recognition of uranyl in aqueous solution. The results of these studies will impact the science and technology underlying our approaches to controlling the behavior of uranium in these systems, and will lead to a fundamental change in how scientists formulate models of bonding for uranyl. Our goal is to explore a combinatorial library approach to uranyl selectivity. The rational design of selective ligands for U(VI) is challenging due to the limited number of ligands that are currently known. Combinatorial chemistry, which has previously been applied to identify new transition-metal complexes and catalysts, provides a particularly attractive approach for the identification of uranyl-selective ligand systems. We anticipate that this fundamental science will find use beyond actinide separation technologies in areas such as nuclear waste remediation and nuclear materials.

[For Sections A and B, provide a one-page maximum summary of the project, including background and objectives and replace text here. For Section C, two pages are allowed.]