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Structural studies of actinide-peptide complexes

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In the wake of the Fukushima accident assessing the mechanisms governing radionucleide impact on the environment (particularly the biosphere) is of great importance.
Most data available on the interaction of actinides with biological systems are based on physiological or biokinetic measurements, with scarce information on the microscopic factors such as structure of the actinide coordination site within biological molecules (proteins, peptides...). These biomolecules are essentially responsible for specific migration pathways towards various organs in vivo. This structural data is essential for developing the understanding structure, function and affinity interdependence. Here-in we describe an approach for structural elucidation of several uranyle and europium (used as a trivalent actinide surrogate) biological complexes combining both experimental and theoretical techniques.
the discribed approach overcomes the intricacy of actinide chemistry combined with the complexicity of protein tertiary structure by using biomimetic peptides. The chosen peptides cover a wide spectrum of structural as well as functional (amide, carboxylate et phosphonate$\cdots$) properties. Isothermal calorimetric titration provided primordial thermodynamic information (affinity constant, stoechiometry), additional functional and structural analysis techniques (IR,TRLFS, EXAFS) led to elucidate the complexe's structure. In parallel DFT calculations have been used to optimize the proposed structures and fit the experimental data.

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