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Structural studies of the Eu(III) and U(VI) interactions with pentapeptides

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In the wake of the Fukushima accident, it is of great importance to assess the mechanisms governing radionuclide impact on the environment (particularly the biosphere) and to unravel the molecular processes underlying actinide transport and deposition in tissues. 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 structural data are essential to understand structure, function and affinity interdependence, which governs the organ deposition of such elements. In this poster, we will present first results on the complexation of Eu3+, which we used as a surrogate of trivalent actinides, and UO22+ with peptides containing various, biologically relevant, geometrical constraints. Three pentapeptides have been synthesized, DGDGD, ADPDA and DPDPD. The latter two contain proline (P) residues that induce an angular strain that is absent while the first peptide contains two flexible glycin (G) residues. The expected complexing residues are in all cases the carboxylate function of the aspartate aminoacids (D). The number of carboxylic side chains was also varied between 2 and 3. Furthermore, the influence of the intrinsic geometry of the cation is also investigated by comparing the complexation of the linear uranyl(VI) oxo-cation versus the "spherical"europium(III).
Among structural investigation techniques, X-ray Absorption Spectroscopy (XAS) was found adequate since it is an element specific local structural and electronic probe that is increasingly used to sense metal centres in biological systems. This technique coupled with other spectroscopic methods such as infra-red spectroscopy and SLRT enables us to draw a full understanding of the metal environment. To screen the affinity of peptides with both Eu(III) and U(VI), Isothermal Tiration Calorimetry (ITC) was also used. Additionally, theoretical tools such as molecular mechanics and dynamics were used to model the actinide complex stability.

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