

CHEMICAL AND RADIOPHARMACEUTICAL SCIENCES

Mission and Objectives | Achievements

Mission and Objectives

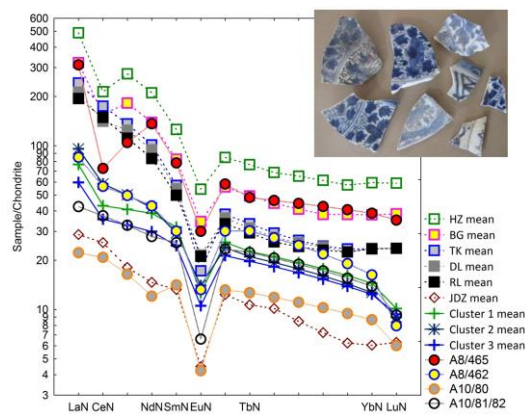
- Promote and provide a focus for networks aiming at the development of research and expertise in the synthesis and characterization of inactive and radioactive compounds, and characterization of cultural, geological and biogenic materials, and hydrological resources.
- Development and application of nuclear methods and luminescence to geoenvironmental and cultural heritage issues; geochemical, mineralogical and absolute dating tools.
- Elemental and Isotopic Analysis and Radiocarbon Dating- applications in the fields of Environmental Geochemistry, Isotope Hydrology, Oceanography and Archaeometry.
- f-Element chemistry studies at fundamental and applied levels in the areas of nuclear science, catalysis and new materials.
- Basic/oriented research and technology transfer on specific halogen- and metal-based nuclear tools for SPECT and PET Molecular Imaging and Targeted Radiotherapy.
- Exploration of ternary intermetallic phase diagrams based on f- and d- elements and studies of exotic ground state properties such as strongly correlated electron behaviour, superconductivity and magnetism.
- Development of multifunctional molecular materials by combination of magnetic and electroactive centres.

Main Achievements

Nuclear methods applied to Cultural Heritage

The chemical characterization of porcelain fragments from archaeological sites from Lisbon and Coimbra obtained by INAA showed a general provenance from southern China kilns. A few porcelains were attributed to Jingdezhen and Zhangzhou kilns. An increasing improvement of the production procedure from late 15th till the 17th centuries of the Chinese porcelains sent to Portugal was found.

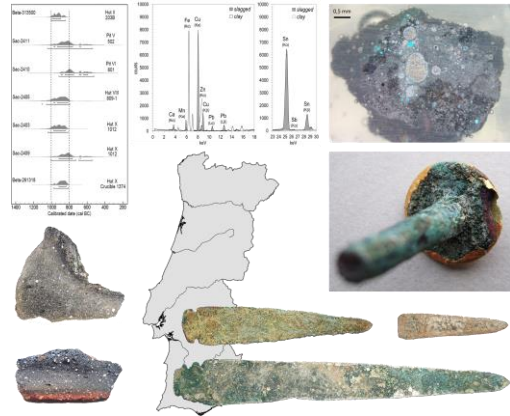
REE patterns of porcelains found in Portugal, and Chinese kilns (Zhangzhou and Jingdezhen).



Archaeometallurgy

Although the production of bronze alloys in the Southwestern Iberia was established to have been initiated during the third quarter of the II Millennium BC, the introduction of these alloys could be pushed backward to the second quarter of the II Millennium BC, probably as imports.

SW Bronze Age metallurgical remains and metallic artefacts (chemical and microstructural characterization and dating).



Environmental Geochemistry

Diverse trends of sea level, climatic fluctuations, Bond events, humid episodes and/or Human intervention in the landscape, have been recognized to be recorded in the filling up of alluvial plain estuaries in the Iberian Peninsula over the last 5000 years.

Alluvial plain at southern Portuguese coast.



Groundwater sampling at Santiago Island, Cape Verde (sustainable groundwater management).

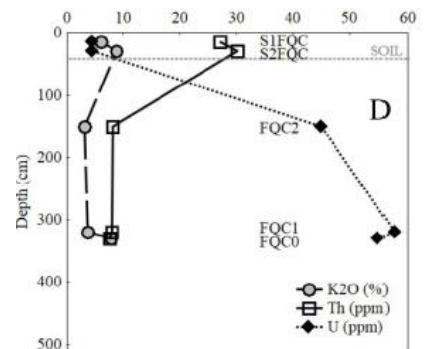
Isotope Hydrology

Salinity sources and renewability of groundwater on coastal aquifers of Algarve, Sado (Portugal), Cap Bon (Tunisia) and Cape Verde were recognised. The conceptual hydrogeological circulation models of Cabeço de Vide mineral waters and in Melgaço-Messagães (N of Portugal) could be established.

Dose rate evaluation from natural radioisotopes

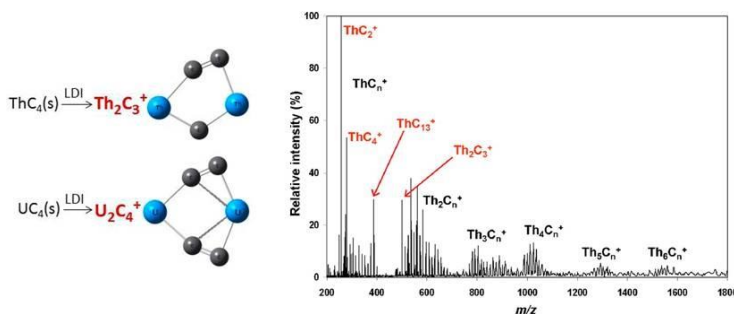
The concentrations of natural radionuclides obtained using two methods for comparison - the field gamma spectrometry (FGS) and instrumental neutron activation analysis (INAA) - as their combination may help detect spatial variations and disequilibrium in the U series.

Radionuclide concentrations through an aplite dyke, which locally exceeded minimum reference levels for gamma radiation despite release of up to 590 Bq. kg⁻¹ of ²²⁰Rn.



Molecular thorium and uranium carbide clusters

Laser ionization of solid thorium and uranium carbide targets resulted in molecular actinide carbide clusters. Intriguing high abundances for both ThC₁₃⁺ and UC₁₃⁺ and for Th₁₃C_n⁺ were observed. A disparity between An = Th and U in the relative abundances of the bimetallic ions An₂C₃⁺ and An₂C₄⁺ was apparent and elucidated by computations based on density functional theory.

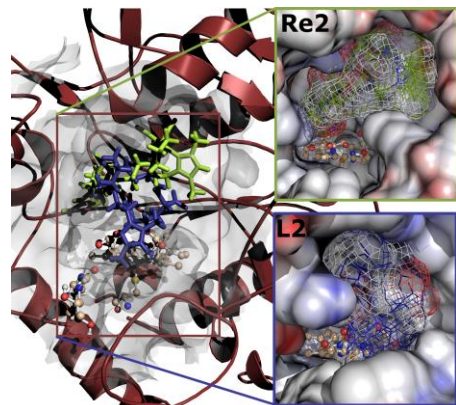


Molecular actinide carbide clusters.

Targeting of Inducible Nitric Oxide Synthase with M(CO)₃-Complexes (M = ^{99m}Tc/Re)

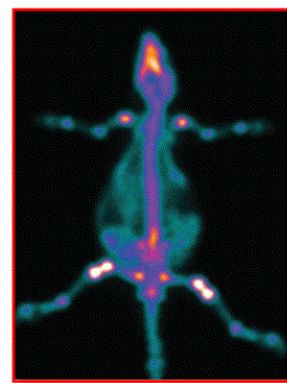
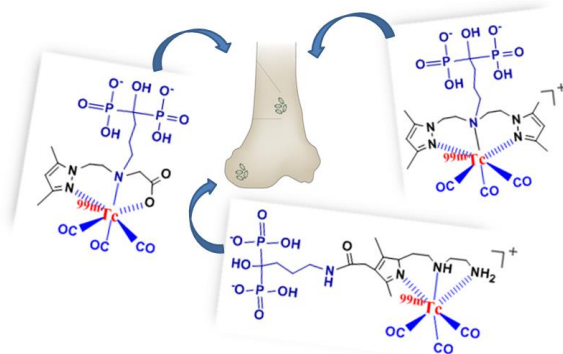
Computational studies, molecular docking, MD simulations and FEP calculations, allowed the identification of the interactions responsible for the iNOS-recognizing ability of the complexes, showing that electrostatic interactions between the Re(CO)₃ core and R260/R382 are a key issue. These findings will allow a more rational design of M(CO)₃-complexes (M = ^{99m}Tc/Re) for in vivo NOS targeting, offering better opportunities to obtain best performing compounds.

Molecular surfaces of the active site of the complexes L2:iNOS and Re2:iNOS colored according to electrostatic potential.



Bisphosphonate-containing $^{99m}\text{Tc(I)}/\text{Re(I)}$ -complexes for theranostic of MBD

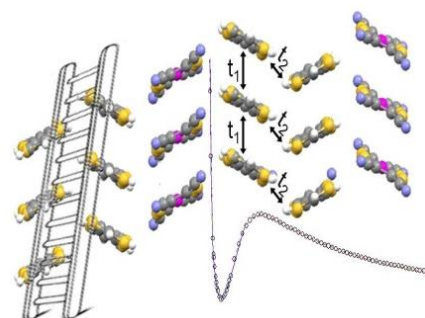
Complexes of the type $\text{fac}[\text{M}(\text{CO})_3(\text{k}^3\text{-L})]^+$ ($\text{M} = ^{99m}\text{Tc}, \text{Re}$) stabilized by azolyl-containing bifunctional chelators with different molecular weight, overall charge, (lipo)hydrophilic nature and different positions of BP attachment were synthesized. Biodistribution studies in mice have shown that complexes bearing the BP unit at position 4 of the azolyl ring ($^{99m}\text{Tc1}/^{188}\text{Re}$) present the most favourable pharmacokinetics, and the highest accumulation in the cytosol.



Schematic drawing of selected examples of BP-containing $\text{fac}[\text{M}(\text{CO})_3(\text{k}^3\text{-L})]^+$ complexes and planar whole-body gamma camera image of a rat injected with a radioactive complex.

A Weakly Disordered Molecular Spin-Ladder System

$(\alpha\text{-DT-TTF})_2[\text{Au}(\text{mnt})_2]$ not only enlarges reduced the number of organic spin-ladder systems in a unique series of closely related molecular compounds, but also provides an interesting example of a weakly disordered spin-ladder system.



Schematic ladder arrangement of donor molecules in the crystal structure of $(\alpha\text{-DT-TTF})_2[\text{Au}(\text{mnt})_2]$ and magnetic susceptibility behaviour.

Magnetic properties of f-element materials

$\text{Dy}_8(\text{OH})_{20}\text{Cl}_4 \cdot 6\text{H}_2\text{O}$ is the first example of a layered lanthanide compound displaying slow magnetic relaxation below 5 K, even in the absence of an external field, with a blocking temperature of 3 K and an energy barrier of 36.1 K, a behaviour characteristic of single-molecule magnets. The work was highlighted in the cover of issue 29 (October 2013) of the European Journal of Inorganic Chemistry.

Slow magnetic relaxation in a layered lanthanide hydroxide.

