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FACULDADE DE CIÊNCIAS E TECNOLOGIA
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HRMAS NMR applied to bio-materials

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MSI NMR group

Molecular Structure & Interactions NMR group

requimte

CQE Química Estrutural

Objectives

The new properties and multifunctional nature of advanced hybrid, bioactive materials are being exploited in many and diverse applications. However the complexity of these biosystems makes it difficult to understand the chemical and biochemical processes taking place in them at an atomic level. Nuclear Magnetic Resonance spectroscopy can provide information on structural and dynamic aspects of phenomena, allowing for process rationalization and optimization. My work plan focuses on applying HRMAS NMR to hybrid, bioactive materials, namely enzymes and living cells entrapped in porous sol-gel matrices (Fig. 1), in order to obtain structural and functional information on these biological-inorganic hybrid.

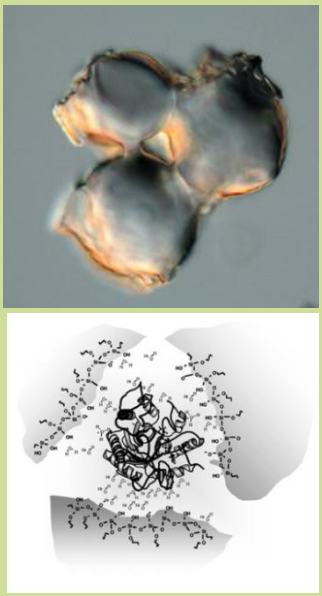

Fig. 1 – Sol-gel encapsulated enzyme.

Methodology

I use Liquid, Solid State and High Resolution Magic Angle Spinning (HRMAS) NMR (Fig. 2). Structural and dynamic studies will be performed using ^{13}C and ^{29}Si solid state MAS and CP MAS NMR techniques in the presence of the biomolecule to rationalize enzyme/matrix interactions. By using two-dimensional wide-line separation (WISE) NMR techniques we can correlate information on local mobility and chemical structure.
To study the accessibility of the entrapped biosystem to solvents and small molecules, we perform diffusion studies using Pulsed Field Gradient Spin Echo NMR (PFG NMR) adapted to HRMAS NMR spectroscopy.

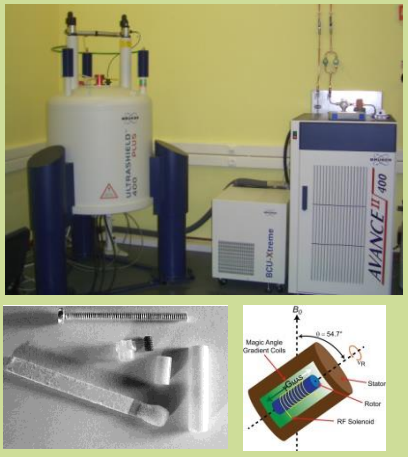

Fig. 2 – HR-MAS rotors.

Expected Results

By combining HRMAS with solid and liquid state NMR, we expect to study increasingly more complex sol-gel entrapped biosystems, to understand how the bioactive component and the matrix interact, as well as the mechanics of the processes taking place at atomic scale, thereby allowing the design of more efficient processes.

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