

Biomolecular NMR - USC

Name of the entity:	Biomolecular NMR Group – University of Santiago de Compostela
Country	Spain
Thematic Areas of interest (key words)	NMR; structure; protein; nucleic acid; drug discovery; SAR; library screening; fragment-based screening; interaction; binding
Topics of interest	<ul style="list-style-type: none"> – HEALTH.2010.1.2-1: Tools for the identification and the detection of biomarkers in clinical samples and patients. – HEALTH.2010.2.3.2-1: Target characterisation and hit-to-lead progression in tuberculosis (TB) Drug development. – HEALTH.2010.2.3.2-2: Lead optimisation and late preclinical development in TB drugs. – HEALTH.2010.2.3.3-2: Drug lead discovery against RNA viruses.
Description of Research activity	<p>NMR is a powerful tool to investigate the structure, dynamics and interactions of biomolecules (proteins and nucleic acids) in solution. More precisely, we are interested in the investigation of intermolecular interactions, focusing especially on drug/target recognition. The experimental approach depends on the particular conditions of the system and the specific biological question to be addressed: (i) determination of the 3D structure of the biomolecules; (ii) investigation of weak ligand/target interactions by tr-NOE, STD and other methods; (iii) screening, fragment-based drug discovery, structure-based drug design.</p> <p>We have some papers on the structure determination of some drug/target complexes such as (i) the antitumour drug Etoposide in complex with Tubulin, and (ii) ligand/RNA complex with an RNA hairpin from the HIV virus.</p>
Expertise offered	<ul style="list-style-type: none"> – Protein and nucleic acid (DNA, RNA) structure determination by Nuclear Magnetic Resonance (NMR). – Study of ligand / target interaction by NMR. – Screening of chemical combinatorial libraries against their biological targets. – Fragment-based screening and drug discovery. – Contribution to derivation of Structure-Activity Relationships (SAR) and Structure-Based Drug Design. – High-field NMR spectrometers available. – Software development for NMR.
Expected results for your organisation	We wish to collaborate with partners from academia and industry in projects related to biomolecule structure and drug discovery. In particular, we would like to find partners with expertise in target identification or in protein characterization and over-expression.

Former Participation in European Projects	"Development of late transition metalloenzymes for highly efficient catalytic processes (ARTIZYMES)": an interdisciplinary approach for a 'de novo' design of artificial metalloenzymes. The design process is to be aided by molecular modelling and by structure determination using NMR and X-ray crystallography.
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