LOCATION

WORKSHOP

Coordenadas GPS : 42.167841,-8.682858

Integrated Techniques in Structural Elucidation

InTechSE

Marie Curie Action FP7

June, 4th - 5th 2015

Universidade de Vigo

Vigo (Spain)

Master in Chemical Research and Industrial Chemistry

http://webqo3.webs.uvigo.es/intechse/intechse.html

Summary

The International Network on Integrated Techniques in Structural Elucidation (INTECHSE) is a Marie Curie Action within Seventh Framework Programme.

INTECHSE aims at establishing collaborations among synthetic chemists, spectroscopists and theoreticians to improve the applicability of spectroscopy to molecular elucidation and to design new systems with specific chiroptical properties.

The INTECHSE research program resides in three major topics: i) preparation and study of anisotropic media to be used as aligned media in NMR; ii) synthesis and structural elucidation of π-conjugated systems; iii) analysis of chiroptical properties.

INTECHSE will celebrate a meeting at CITEXVI (Campus Lagoas-Marcosende) in Vigo on June 4th-5th, 2015 to share the outcome of this collaborative research towards gaining understanding on the mechanisms responsible of chiroptical responses and appropriate methodologies for structural elucidation.

June 4th

9:00 Opening Presentation

9:10 Richard Weiss (Georgetown University, USA)
Thixotropic gels

10:00 Milan Kivala (FAU, Germany)
Heteroatom - doped organic scaffolds by chemical synthesis

10:50 Sandra Míguez-Lago (UVigo, Spain)
Design and synthesis of covalent organic helical cages

11:10 Coffee Break

11:40 Antonio Rizzo (CNR-Pisa, Italy)
Nonlinear Optical Chiral Spectrosopy: a computational chemist viewpoint

12:30 Victor Sánchez Pedregal
NMR - based structural analysis of flexible molecules in aligned media

13:00 Félix Freire (USC, Spain)
The role of cation-pi interactions in polymer chemistry: helical sense and aggregation control

13:45 Lunch Break

15:30 Eduardo Troche Pesqueira (UVigo, Spain)
RDC studies on small organic molecules and characterization of the water-soluble alignment media cromolyn

16:00 Eurico Cabrita (FCT-UNL, Portugal)
NMR diffusion studies in alignment media

16:50 Teresa Sierra (CSIC, Spain)
Control of self - assembly of polycatenar mesogens; towards functional soft materials

June 5th

9:00 Fabrizio Santoro (CNR-Pisa, Italy)
Quantum - classical dynamical approaches for the calculation of vibronic chiral spectra

9:50 Luis Muñoz (UVigo, Spain)
Conformational analysis from 13C NMR chemical shifts

10:20 Teresa Duncan (GU, USA)
Poly(vinyl acetate)-Borate Networks with Glycol Ethers for Cleaning Objects of Cultural Heritage

10:50 Marta Castiñeira (UVigo, Spain)
Computational study of transition metal catalyzed process

11:10 Coffee Break

11:40 José Lorenzo Alonso (UVigo, Spain)
Chiroptics through chiral axes

12:10 Emilia Tojo
Ionic Liquids; structure activity relationships

12:40 Dolores Pérez (USC, Spain)
Aryne cycloaddition reactions in the synthesis of large PAHs and nanographenes.

13:30 Lunch