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Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares

Conferencia:

Computer-Assisted 3D Structure Elucidation (CASE-3D) of Natural Products

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25/01/18

Aula de Seminarios do CIQUS

12:30 h

Más información:
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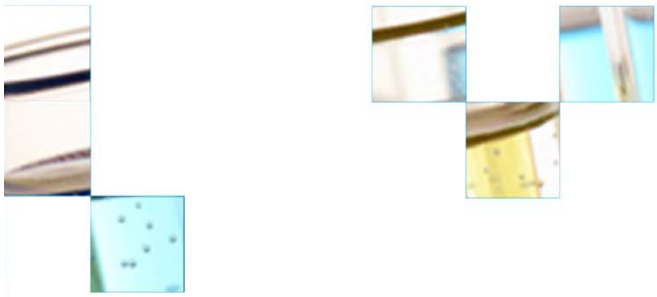

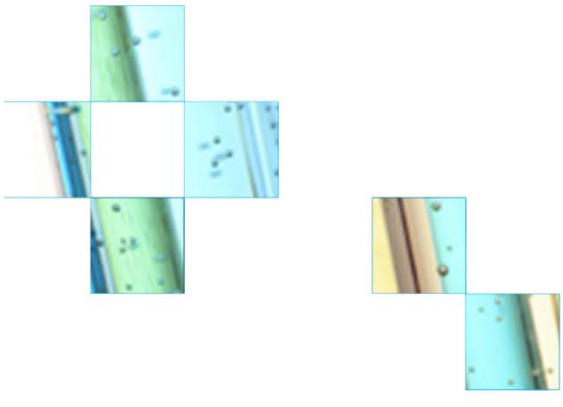

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Computer-Assisted 3D Structure Elucidation (CASE-3D) of Natural Products

Abstract: A multiparameter automated methodology which extends currently available computer-assisted structure elucidation (CASE) software for the relative configuration analysis of small molecules is presented. This CASE-3D methodology, implemented in the StereoFitter program, is based on the selection on a parsimonious selection of conformational models and can make a combined use of anisotropic and isotropic NMR parameters. Relative configuration was successfully predicted for a variety of natural products.

Photo:

Webpage: https://www.ufpe.br/dqf

Biographical sketch:
Armando Navarro got his PhD in Compostela under the mentoring of professors Domingo Domínguez and Carlos Sáa. After post-doc stays at the groups of prof. Javier Sardina in Compostela and Prof. Peter Schreiner in the Institut fur Organische Chemie (Giessen Germany) he holded IPP and RyC positions at the Universities of Vigo and Santiago de Compostela. In 2014 he moved for a short period to the Karlsruhe Institut of Technology and joined in this very year the Universidade Federal de Pernambuco as a visiting professor. From 2017 he is full professor at the Departamento de Química Fundamental of this university.
He has done research in different aspects of physical organic chemistry with more than sixty papers on the field and his current research interests involve the development of new NMR based methodologies for the structural analysis of organic compounds with an emphasis on computer and automation procedures. He has written several NMR related programs among them the MSpin program.