

International Conference on

Stereochemistry

August 18-19, 2016 São Paulo, Brazil

Residual chemical shift anisotropy (RCSA) and residual dipolar coupling (RDC): Tools for structural analyses of small molecules

Fernando Hallwass

Federal University of Pernambuco, Brazil

Recently, there have been developed a complementary methodology to the traditional NMR experiments applied to determine tridimensional structure or to solve assignment questions of small molecules, namely: RDC (Residual Dipolar Coupling) and RCSA (Residual Chemical Shift Anisotropy). This methodology is based on measuring anisotropic parameters produced by partial molecular alignment. Consequently, the geometrical dependent parameters of the NMR Hamiltonian are partially recovered, providing useful additional structural information, when the experiments in isotropic media are not sufficient. In this presentation will be shown our studies carried out with compounds with more than one stereocenter, for instance estrone and α -santonin, where RDC and RCSA measurement were applied to solve conformational and configurational problems.

Biography

Fernando Hallwass has completed his PhD in 2004 from University Federal of Pernambuco (Recife, Brazil) and Post-doctoral studies from Max Planck Institute for Biophysical Chemistry (Göttingen, Germany). He has published 25 papers in reputed journals. His research field is focused on Structural Determination using nuclear magnetic resonance (NMR) spectroscopy. During his Post-doctoral program, he studied new methodologies for determining relative configuration of natural compounds through residual dipolar coupling (RDC) and residual chemical shift anisotropy (RCSA) measurements.

hallwass@ufpe.br

Notes: