

Conferencia: Structural Analysis of Natural and Synthetic Small Organic Molecules Using NMR in Anisotropic Media

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The 2D structure of most small molecules can be in principle straightforwardly determined by manual or automatic analysis of a set of experimental data that includes the molecular formula, a series of 1D and 2D NMR experiments providing through-bond connectivity (COSY, TOCSY, HSQC, HMBC and ADEQUATE/INADEQUATE based experiments), and chemical shift predictions. This is the main concept embedded in automatic structure elucidation programs. Once the 2D structure is available, the determination of the relative spatial arrangement (configuration and preferred conformation) of all atoms in the molecule is a more challenging task that it is commonly addressed in NMR by using NOE and 3J coupling constants analysis, as well as recent developments on the application of DFT calculation of ^{13}C chemical shifts. However, it is difficult to assess how many samples are sitting on the laboratory's refrigerators waiting for an independent methodology that could lift some of the ambiguities generated by the use of conventional NMR methods. The development of the application of Residual Dipolar Couplings (RDCs) to the configurational and conformational analysis of small molecules has matured enough in the recent years to perform this task in an almost straightforward way, without even the need of using NOE and 3J coupling analysis, as it will be presented here for the analysis of rigid and semi-rigid small molecules. Except for cases of very high flexibility, the methodology has proven to be extremely powerful, particularly in situations where the use of conventional NMR experiments, such as J coupling constants analysis and NOE-derived distances cannot provide a unique solution to the structural problem. Recent results on the application of Residual Chemical Shift Anisotropy (RCSAs) to the discrimination of molecular configuration will also be presented. Most of the results presented here use poly(methylmethacrylate) (PMMA) and poly(2-hydroxyethylmethacrylate) (poly-HEMA) based flexible gels, whose degree of alignment can be easily tuned by variable and reversible compression.

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Roberto R. Gil was born in Catamarca, Argentina in 1961. He received the degrees of BS/MS in Organic Chemistry (1983) and Ph.D. in Natural Products Chemistry (1989) from the University of Córdoba, Córdoba, Argentina. In 1992 he received an external post-doctoral fellowship from the National Research Council of Argentina (CONICET) to work with Professors Geoffrey A. Cordell and A. Douglas Kinghorn at the University of Illinois at Chicago in the field of bioactive natural products from plants. In 1995, he returned to the University of Córdoba where he started his own research group as Assistant Professor. He was later inducted to the CONICET research track. In 1995 received the award "Top Ten Youngsters of the Year" given by the Chamber of Commerce of Córdoba City and also the award "CATAMARCA 96" sponsored by the Government of the Province of Catamarca. In 2000 he spent a year as Visiting Professor at Carnegie Mellon University working in Protein NMR with Professor Miguel Llinás. In 2001 he returned to UNC for a brief period of time where he continued his teaching and research activities as Associate Professor and he was also appointed Associate Dean for Science and Technology Affairs of the UNC College of Chemistry. In 2002, he moved to Pittsburgh, Pennsylvania, where he currently holds the position of Research Professor and Director of the NMR Laboratory of the Department of Chemistry at Carnegie Mellon University. His research interest is aimed at the development and application of NMR methodologies to the analysis of the structural and physical properties of small molecules in general, with particular interest on NMR oriented media.

The US National Science Foundation supports his research. In 2012 he was the Program Chair of SMASH-NMR, the NMR conference for small molecules and he is currently a permanent member of the SMASH organizing committee. In 2012 he also edited a special supplementary issue for the journal *Magnetic Resonance in Chemistry* on "NMR of Small Molecules in Anisotropic Media", and since 2014 he is the Features Editor of the same journal. At Carnegie Mellon he is strongly involved in programs oriented to increase the representation of underrepresented groups in Science. He has been serving in the CMU President Diversity Advisory Council since 2006. He has given NMR courses locally, as well as in Argentina, Peru, Colombia and Spain. He has over 100 presentations to meetings and is co-author of three book chapters and 104 articles in peer-reviewed journals.

