



Biotransformation monitoring, protein-ligand interactions and In-cell NMR spectroscopy in natural products research

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Abstract

A critical overview of the following developments of NMR spectroscopy will be summarized:

(a) rapid 'in situ' monitoring of enzymatic reaction products [1], and enriching the biological space of natural products, through real time biotransformation monitoring in the NMR tube. Investigation of interactions with the intrinsically disordered protein α -synuclein which is abundant in the human brain and a relevant target for neurodegenerative diseases [2].

(b) The combined use of saturation transfer difference (STD), Tr-NOESY and INPHARMA (Interligand Noes for PHarmacophore MApping) NMR techniques for mapping interactions, specific binding sites and structure elucidation of lipids with non-labelled serum albumin and the anti-apoptotic protein Bcl-2 [3,4].

(c) Application of in-cell NMR analytical methodology in the monitoring of the interaction of ligands with Bcl-2 inside living human cancer cells without requiring prior isotopic labeling of the target protein. STD and Tr-NOESY NMR were employed to evaluate the direct binding of the ligand to the nonlabelled Bcl-2 protein intracellularly [5], which was further validated in vitro. This approach has proved a very promising strategy for the real-time screening of the interaction profiling of drugs with their therapeutic targets in their native cellular environment in living eukaryotic cells, paving the way to the new field of intracellular rational drug design.

Biography

His academic career started as a "Premier Assistant" at the University of Lausanne, Institute of Organic Chemistry, 1981-1984. In 1984 he joined as a Lecturer to University of Ioannina, Section of Physical Chemistry, Department of Chemistry. He is Professor of Chemistry since 1997 in the University of Ioannina and an Adjunct faculty at the International Center for Chemical and Biological Sciences (ICCBS), University of Karachi. His research interests are focused on NMR applications in Bioorganic Chemistry, Structural Biology, Food Chemistry and Natural Products. He received numerous fellowships and awards in various Universities and Research Institutes (Honorary Research Fellow, QMW College, Medal of the Ministry of Education of Ukraine and D.Sc. University of EastAnglia). He has over 166 publications in international journals with total impact factor ~ 527, number of citations 5371 and h-index 40 (Google scholar). He is the Reviewer of more than 30 International journals.

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