

NMR in drug discovery: From an analytical to a biophysical technique

Juan F. Espinosa

Eli Lilly – Discovery Chemistry Research and Technologies

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NMR in drug discovery: From an analytical to a biophysical technique

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This presentation highlights some examples of application of NMR spectroscopy in drug discovery, from structural elucidation to ligand binding, including methodological developments.



Dr. **Juan F. Espinosa** is Group Leader in the Spanish Site of Lilly Research Laboratories in Alcobendas (Madrid). He studied Chemistry at the University of Alcala where he obtained a Master degree in Organic Chemistry in 1994 under the supervision of Dr. Antonio Lorente. He received a doctorate in Chemistry in 1998 for work on conformational analysis of carbohydrate analogues and the study of their interactions with proteins, under the supervision of Jesús Jiménez Barbero in the Spanish Research Council in Madrid. During his Ph.D. he spent research stays in the University of Lübeck (Germany) with Prof. Thomas Peters, in the German Cancer Research Center in Heidelberg (Germany) with Dr. Claus-Wilhelm von der Lieth and in INRA and CERMAV (Nantes and Grenoble, France) with Prof. Anne Imberty and Prof. Serge Perez. He moved to USA to complete a postdoctoral fellowship in the laboratory of Prof. Samuel Gellman at the University of Madison-Wisconsin from 1998 to 1999, working on the design and conformational analysis of beta-hairpin forming peptides. He returned to Spain in

2000 to join the Spanish Lilly site as Senior NMR Spectroscopy where he has managed the NMR group since its creation. He was promoted to Senior Research Scientist in 2003, to Principal Research Scientist in 2007 and to Research Advisor in 2012 and became group leader of the Alcobendas biophysics group in 2013.

His expertise includes application of NMR to the structural elucidation and conformational analysis of organic molecules, development of new NMR methodologies and detection and study of ligand binding by ligand-based NMR approaches and other biophysical methods. He is coauthor of 70 publications in peer-reviewed international journals and has supervised 1 Ph. D. Thesis.

Awards and Honors:

- 1994 Extraordinary graduate award from University of Alcala
 - 1998 Extraordinary doctorate award from University of Alcala
 - 1998 Fulbright Scholarship to conduct research in USA
 - 2011 Lilly's President Award for scientific achievements
- Former Treasurer of the NMR group of the Spanish Royal Society of Chemistry
Former Member of the SMASH NMR organizing committee