

Closing Lecture:

Breaking the limits in understanding glycan recognition by NMR



CIC bioGUNE
MEMBER OF BASQUE RESEARCH
& TECHNOLOGY ALLIANCE

Prof. Jesús Jiménez-Barbero

Ikerbasque Research Professor
Scientific Director | CIC bioGUNE
Bilbao, Spain



jjbarbero@cicbiogune.es
<https://www.cicbiogune.es/people/jjbarb>

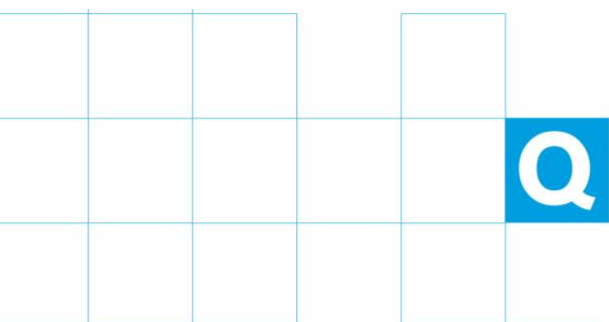
Abstract: Molecular recognition by specific targets is at the heart of the life processes. The interactions between proteins (lectins, enzymes, antibodies) and carbohydrates mediate a broad range of biological activities, from fertilization and tissue maturation to pathological processes. The elucidation of the mechanisms that govern how sugars are accommodated in the binding sites of these receptors is currently a topic of interest. Thus, unravelling the structural and conformational factors and the physicochemical features that rule the interactions of these molecules is of paramount interest.

Solution NMR is unique in providing stereochemical and conformational information. Given the inherent flexibility and dynamic properties of sugars, we use NMR as key tool for deducing at atomic resolution molecular recognition processes in which glycans are involved, also assisted by a variety of synthetic, molecular biology, computational and biophysical techniques.

This presentation is focused on the application of state-of-the-art NMR methods both from the ligand and receptor's perspective to study molecular recognition processes between receptors of biomedical interest and glycans. As recent examples, key details of glycan recognition by these receptors will be shown, with special emphasis in the application of novel ¹³C-based and paramagnetic-NMR methods, including the interactions of the spike protein of SARS CoV-2 with human immune lectins and cell glycans.¹⁻⁸

References

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6. Unione et al., *Curr. Opin. Struct. Biol.* **2021**, 68, 9-17.
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8. Unione et al., *submitted*



[ONLINE] - Zoom
February 8, 2022
12:00 p.m.

This event is part of the “Tutored Training Activities” at the

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CHEMISTRY
at the Interface with
BIOLOGY and
MATERIALS Science

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Biosketch: Jesús Jiménez-Barbero is Ikerbasque Research Professor and Scientific Director of CIC bioGUNE since November 2014.

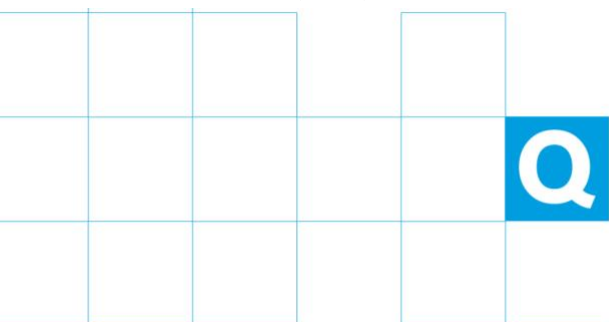
He received his PhD in Chemistry in 1987, working at the Institute for Organic Chemistry of CSIC. Earlier in his career, he worked at CERMAV-CNRS, Grenoble, 1986 (Predoc); Univ. Zurich (Switzerland), 1987 (Postdoc); National Institute for Medical Research (UK) 1988 (Postdoc; and Carnegie Mellon Univ., USA; 1990-92 (Postdoc and visiting).

Before moving to CIC bioGUNE where he has led the Centre towards its accreditation as Severo Ochoa Center of Excellence in 2017, he held a CSIC Research Professor position at CIB-CSIC since 2002. Previously, he was senior research scientist at Institute Organic Chemistry-CSIC (1996-2002). He has been Visiting Professor at École Normale Supérieure, Paris (2004), Univ. Pierre et Marie Curie (2009), Univ. Milano Bicocca (2009-12) and now at the University of the Basque Country since 2016.

From the management perspective, he has served as President of RSEQ (the Royal Society of Chemistry of Spain) since Jan 2012-Jan 2018, and was Secretary General of the same Institution (2004-11). He has also served as Head of the Chemistry Panel of the National Plan for Research of the Ministry of Economy and Competitiveness (2009-2018), and as the representative of Spain in the CMST committee of EU-COST (2012-14).

His scientific interests are centered in the field of Chemical Biology, especially in discovering the mechanisms of molecular recognition of carbohydrates, especially those related to processes of biomedical interest. In particular, he is focused in exploring molecular recognition studies from the atomic perspective. He has achieved major developments of general methodological aspects of NMR and, particularly, in their applications to the study of key features of molecular recognition processes involving sugars and proteins. His major contributions to the molecular recognition field include the unravelling of the molecular basis of the recognition of different ligands (glycans & other small molecules) by biological receptors in solution, using a multidisciplinary approach, which employs organic synthesis, protein biochemistry and molecular biology, biophysics, molecular modeling, and NMR, using a wide network of collaborations worldwide. Major contributions include his systematic studies on the interactions of glycans with lectins. Such detailed investigations are contributing to our general understanding of glycan-mediated interactions in health and disease and have been disseminated through more than 600 scientific publications and more than 300 invited and plenary lectures. These studies conducted to the International Whistler Award in Carbohydrate Chemistry in 2010 and the Gold Medal of RSEQ in 2018, among others. He has already supervised 33 PhD students as well as more than 40 postdocs.

Recent advances employ paramagnetic metals (lanthanides) and NMR-active molecular probes (^{19}F NMR) to scrutinize molecular recognition both in vitro and in-cell. The proposal focused on these last avenues has received the ERC Advanced Grant (2018).



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