

NEW NMR STRATEGIES TO INVESTIGATE GLYCAN-LECTIN INTERACTIONS OF COMPLEX GLYCOCONJUGATES

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The molecular recognition of glycans is at the heart of numerous biological processes within living organisms and plays crucial roles in health and disease. Understanding these interactions at the molecular/atomic level is of paramount importance for developing novel therapeutic approaches, improving disease diagnostics and/or advancing in biotechnological applications [1].

Given the dynamic nature of glycans, NMR has been extensively used to study glycan-lectin interactions and remains at the forefront of existing approaches [2]. In this context, ¹⁹F-labelled glycan probes have been exploited in diverse applications [3] and fluorine NMR has emerged as a powerful strategy to interrogate biological systems in complex environments closely resembling native conditions [4].

Herein, we describe the NMR analysis of the molecular recognition of complex glycoconjugates, even in complex environments such as the cell, by the exploitation of ¹⁹F-NMR spectroscopy. This novel approach allowed easily detecting complex glycans, monitoring binding events and/or profiling the glycosylation of intact cells.

References:

- 1. Essentials of Glycobiology, 4th edition. Varki A, Cummings RD, Esko JD, et al., editors. Cold Spring Harbor (NY): Cold Spring Harbor Laboratory Press; **2022**.
- 2. J. Angulo, A. Ardá, S. Bertuzzi, A. Canales, J. Ereño-Orbea, A. Gimeno, M. Gomez-Redondo, J. C. Muñoz-García, P. Oquist, S. Monaco, A. Poveda, L. Unione, J. Jimenez-Barbero, *Prog. Nucl. Magn. Reson. Spectrosc.* **2024**, *144-145*, 97-152.
- 3. B. Linclau, A. ardá, N-C. Reichardt, M. sollogoub, L. unione, S. P. Vincent, J. Jiménez-Barbero, *Chem. Soc. Rev.*, **2020**, *49*, 3863-3888.
- 4. A. M. Gronenborn, Structure, 2022, 30, 6-14.