^{15}N SPY IN CONFORMATIONAL ANALYSIS OF DISACCHARIDES

Radek Pohl, Nina Habanová

Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic
pohl@uochb.cas.cz

The interaction of carbohydrate-based molecules with proteins is essential for life and controls e.g. fertilization, immune response, or defense against pathogens and cancer. This interaction is driven by the recognition of specific carbohydrate conformation with a protein. Therefore, the development of analytical tools for their conformation prediction both in a free and bound state is of great importance. However, the determination of their conformational properties in solution remains a difficult task due to the structural complexity and inherent flexibility of saccharides.

NMR represents the most used and versatile method in conformational analysis of saccharides and their non-natural derivatives – glycomimetics. *J*-Coupling as a representative of NMR parameters is especially suitable in the conformational analysis since it is sensitive to the local geometric arrangement of interacting nuclei upon structural change. In this contribution, we introduce ^{15}N labeling directly in the glycosidic linkage, which offers redundant *J*-couplings useful in the conformational analysis (Figure 1). The ^{15}N labeling is used for the first time, however, ^{13}C ring labeling has been used for example in conformational analysis of methyl β-lactoside.[1]

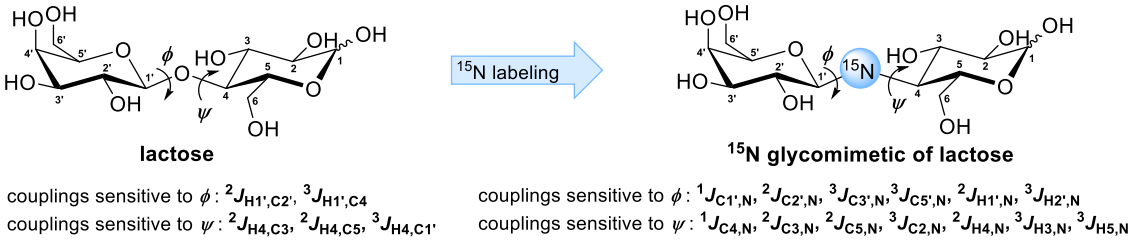

Figure 1. Redundant *J*-couplings across glycosidic linkage useful for conformational analysis.

The concept will be explained on bis(D-glucosyl)amine and bis(D-mannosyl)amine as examples of (1→1)-disaccharides. We will present in situ preparation of the disaccharides directly in an NMR tube, and their conformational analysis based on a combination of experimental NMR, molecular dynamics simulations, and DFT calculation of NMR parameters.

Acknowledgements. This work has been supported by the Czech Science Foundation – project 22-17586S.

REFERENCES

[1] W.Zhang, T. Turney, R. Meredith, Q. Pan, L. Sernau, X. Wang, X. Hu, R. J. Woods, I. Carmichael, A. S. Serianni, *J. Phys. Chem. B* **2017**, *121*, 3042–3058.