

ANALYSIS OF SPECIFIC INTERACTIONS BETWEEN GLYCANS AND WATER BY NUCLEAR MAGNETIC RESONANCE

<u>Hana Ishikawa</u>^a, Tatsuya Moriguchi^a, Kohtaro Hirao^{a,b}, Yuta Maki^{a,b}, Ryo Okamoto^{a,b}, Yasuhiro Kajihara^{a,b}

^a Grad. Sch. Sci., Osaka Univ., 1-1, Machikaneyama, Toyonaka, 560-0043 Japan ishikawah23@chem.sci.osaka-u.ac.jp

^b FRC, Grad. Sch. Sci. Osaka Univ., 1-1, Machikaneyama, Toyonaka, 560-0043 Japan

Glycans of glycoproteins regulate stability and functions of proteins. However, the detailed mechanisms remain unclear. We have hypothesized that glycans regulate water behavior around glycoproteins. To analyze the interaction between glycan and water, we succeeded in the development of a unique sampling method for NMR measurement.

After dissolving the sugar in dried deuterium-d6-DMSO, we added a further drying agent to reduce the water amount that was less than 1 equivalent of the sugar. From this state, proton NMR and the T1 and T2 relaxation times of the water were measured while the amount of water was gradually increased to about 100 equivalents. The resultant spectra revealed that sialic acid at the end of the glycans lower the mobility of water molecules around glycans.

Then, we especially focused on sialic acid which is found at the end of the glycan. Sialic acid has a unique fonctional group, the carboxylic acid. Therefore, methyl α -sialoside and its methyl ester form were analyzed to investigate how the carboxylic acid influences the water behavior. The contributions of each hydroxy group were also analyzed through synthesizing each deoxyzed analog.

In this presentation, we will present the details of the our experiment and discuss the specific interactions between glycans and water.