Modeling Hydrogen-Deuterium Exchange Mass Spectrometry data via convolutions of exchange probabilities

Hydrogen-Deuterium Exchange Mass Spectrometry (HDX-MS) enables studying protein structure and dynamics by monitoring changes in masses of molecules due to exchange between hydrogens and their heavier isotope - hydrogen. A common approach to the analysis of data acquired in HDX-MS studies focuses on studying shifts in average masses molecules. However, this is insufficient to capture all types of exchange patterns. In this talk, I will present an alternative approach that uses isotopic distributions of peptides observed in mass spectra to describe complete exchange dynamics of both peptides observed directly, and their overlapping sub-sequences. Based on joint work with Jürgen Claesen (Amsterdam UMC) and Tomasz Burzykowski (UHAsselt).