

... THE NEW DEAL
FOR THE NANO WORLD

Seminar

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Studying protein electrostatics by NMR experiments

Nuclear Magnetic Resonance (NMR) spectroscopy has the unrivalled potential to quantify electrostatic interactions in proteins experimentally. We have made significant progress over the years in developing new NMR methodology that allows unambiguous access to all amino acids in proteins, using ^{13}C and ^{15}N chemical shifts as strategic reporters. This improved methodology has allowed accurate insights into the microscopic charge states and nature of electrostatic coupling in small proteins. We have extended this now also to the study of intrinsically disordered proteins (IDPs). In addition, the electrostatic potential present at the polypeptide backbone amide groups can be approximated by computation. We demonstrate that this potential significantly alters the concentration of ions in the immediate vicinity of proteins. This in turn influences paramagnetic relaxation effects from co-solute molecules as well as hydrogen exchange (HX) kinetics, providing novel ways to study protein electrostatics.

DATE: 28/11/2022
VENUE: Room C12
TIME: 9.30-11.00