CCPN Conference 2019
University of Leicester, UK
4th-6th September 2019

Session Abstracts

Session 1: Sensitivity Enhancement in Biomolecular NMR
Session Chair: Phil Williamson (University of Southampton)

Sensitivity represents a major limitation for the application of NMR in the biosciences. Recently however, a number of technological developments in the fields of liquid-state and solid-state NMR have revolutionised the limits of detection. This session will discuss how these developments are revolutionising how we utilize NMR for a range of methods from metabolomics, through to the study of large biomolecular assemblies and membrane proteins. We are delighted that **Tony Watts** (University of Oxford) will begin this session by describing some of the approaches he has used in his work with membranes and membrane proteins. **Józef Lewanowski** (University of Warwick) will then speak to us about the increased use of proton-detection in solid-state NMR. Our third speaker, **Matt Goodwin** from the University of Bristol, will describe how he has been using a cryo-microprobe within a metabolomics context. Finally, **Guido Pintaduda** will join us from Lyon to tell us about his work on magic-angle spinning DNP NMR of biomolecular assemblies.

Session 2 : NMR-guided Docking
Session Chair: Helen Mott (University of Cambridge)

In this session the speakers will explore how the power of NMR is being utilised in data-driven docking. The session will start with an introduction to HADDOCK, one of the oldest and most widely used docking servers run by the Bonvin lab in Utrecht. **Gary Thompson** (University of Kent) and **Helen Mott** (University of Cambridge) will describe the methodology of the approach and also give several examples from their work where HADDOCK has been used. In the next talk, **Luca Codutti** who works with Theresa Carlomagno at the University of Hannover, will describe their INPHARMA approach, which is used for docking small molecule ligands to a common target. **Tobias Madl** from the University of Graz will talk about how surface accessibility data from NMR and CS-Rosetta can be combined for structure determination and docking of complexes. Finally, **Andreas Lingel** from Norvartis will give us an industry perspective on the use of NMR for understanding how small molecules bind to protein targets.

Session 3 : Complementary Techniques
Session Chair: Rivka Isaakson (King's College, London)

At CCPN, no one needs convincing about the power of NMR and many of us also rely on alternative techniques to add value/validation to our data and answer remaining questions. In this session, we are pleased to welcome some exciting speakers who will expand on different ways to complement NMR data and tell us some stories from their own research. First up, **Katherine Stott**, Director of the Biophysics facility at Cambridge University, will give us an overview of methods that can be used to visualise disorder. She will explain how CD, ITC, AUC, SAXS, luminescence & cross-linking combined to tell her latest research story. **Janet Lovett**, a URF and lecturer at St Andrews, will give us recent insight into electron paramagnetic spectroscopy and ways in which it can work in concert with NMR. Next we will hear from **Helen Walden**, Professor of Structural Biology at Glasgow University, who will tell us a story of E3 ligases in Parkinson's Disease that was elucidated using X-ray crystallography, analytical ultracentrifugation and NMR. Last but not least we look forward to a talk by **Jeddidiah Bellamy-Carter** on his work improving software for carbene footprinting mass-spectrometry in the group of Neil Oldham at Nottingham University.