

Monday, March 4 10:30 am – 12:00 pm Room 301 Bruker Corporation

## USING NMR (NUCLEAR MAGNETIC RESONANCE) AND EPR (ELECTRON PARAMAGNETIC RESONANCE) IN BIOPHYISCS

Magnetic resonance offers many insights into how biological systems function. The two techniques shed light on the identity of species, dynamics, and structures of proteins, peptides, nucleotides, and lipids. The speakers will present an overview of these techniques and applications for people who may be new to the field and wish to incorporate them in their studies.

NMR is a valuable tool for the study of structures and dynamic processes of proteins, peptides and nucleotides. NMR is also well suited to study the interaction of such molecules. Various NMR methods exist to study the interaction of proteins with small molecules in drug discovery, interactions of proteins with each other or with peptides and nucleotides.

In drug discovery fragment based screening by NMR is a well-established technique. A brief presentation of these methods will be included.

The investigation of interaction between larger molecules is facilitated by several NMR methods and by the use of isotopic labeling. Interactions such as protein oligomerization, protein-protein and protein-nucleotide interaction in solutions can be investigated. An overview of these techniques and applications will be included.

In contrast to NMR, EPR detects unpaired electrons in free radicals and transition metal ions. One electron transfer reactions result in unpaired electrons. Examples of paramagnetic species encountered in biology are:

- ROS (Reactive Oxygen Species), RNS (Reactive Nitrogen Species)
- Amino acid radicals such as tyrosine and tryptophan radicals
- Paramagnetic intermediates in photosynthesis
- Metalloenzymes

In addition to these naturally occurring paramagnetic species, spin labels can be incorporated into a number of biomolecules via SDSL (Site Directed Spin Labeling). Applications and techniques are:

- Motional dynamics of proteins, peptides, and nucleotides via linsehape analysis
- Accessibility studies in membrane proteins or peptides via saturation measurements
- Distance measurements (2-8 nm) via DEER (Double Electron-Electron Resonance) to complement other structural methods such as X-ray, NMR, CryoEM and FRET

An introduction to the techniques and applications will be presented.

## Speakers

Ralph Weber, Senior Application Scientist, Bruker Corporation Clemens Anklin, Vice President Applications, Bruker Corporation