QBiC SEMINAR

Speaker

Piotr Fajer, Ph.D.

Institute of Molecular Biophysics, Florida State University

Date & Location

Friday, June 23, 2017
16:00 - 17:00
Osaka, QBiC Bldg. A 1F lounge
(6-2-3 Furuedai, Suita, Osaka 565-0874, Japan)
There will be a TV broadcast at CDB bldg.D E-206

Title

The GOOD and the BAD about spin labeling EPR

Abstract

Electron Paramagnetic Resonance (EPR/ESR) is a technique capable of characterizing molecular dynamics, intra- and inter-domain distances and secondary structure. It is a low resolution structural technique particularly usefull in large molecules/complexes that are not amenable to NMR, or too disordered for X-ray crystallography. Verification of putative models by distance measurements between statretgically placed vantage points (spin labels attached to single cysteine mutants) is a common application of the method. We will discuss some of those examples: acto-myosin complex, troponin complex.

More recently the EPR has been employed to determine structural models ab initio. Measurement of 10 distance restraints allowed us to develop a model of unphosphorylated myosin heads.

A considerable weakness of EPR and fluorescent methods in structural biology is the use of extrinsic labels. EPR and fluorescent signals originate from the groups that are 8-20 Angstroms away from the protein backbone, separated by 5-7 single bonds. The interpretation of those signals in terms of protein demands knowledge of rotameric state of the label. We have developed computational methods based on simulated scaling to exhaustively sample possible configurations of the label and determine its free energy.

Host

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