



PhD exit seminar: Interpreting resonance energy transfer experiments with Monte-Carlo and molecular dynamic simulations

Thursday 12 June 1 – 2pm

Speaker

Katarzyna Walczewska-Szewc, Corry Lab, BSB

Location

Slatyer Seminar Room
R.N. Robinson Building (Bldg 46),
Cunningham Close, ANU

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This lecture is free and open to the public

BSB event information:
biology.anu.edu.au/News/events-bsb.php



Förster resonance energy transfer (FRET) is a photochemical process in which an electronically excited chromophore spontaneously transfers energy to another molecule by a non-radiative dipole-dipole interaction.

While this occurs naturally in processes such as light harvesting in photosynthetic organisms, it is now commonly used as a tool in molecular biophysics to examine the proximity and structure of biological macromolecules and to report on biochemical events. One of features making FRET so widely used is the strong dependence of transfer on the distance between the participating molecules. Due to this, it has been termed a “spectroscopic ruler” enabling the measurement of

intermolecular distances and conformations of proteins and nucleic acids.

Although the utility of this method is now well appreciated, many difficulties arise in interpreting FRET experiments to gain detailed quantitative information. One complication is that the chance of transfer taking place is dependent on the orientation of the participating molecules, something that is difficult (if not impossible) to measure. Another difficulty comes from the fact that the commonly used fluorescent dyes are characterised by high conformational flexibility, which allows them to sample substantial space around the point of attachment introducing further uncertainty to the distance measurements. Moreover, the range of possible application of FRET to as the spectroscopic ruler is limited to 10 nm, whereas many of biological events that could potentially be signaled by FRET occur on larger distances.

In my work, I aim to use computational techniques to address these difficulties, by developing tools that can be used to better interpret the results of FRET experiments and to contribute to the design of new experiments employing FRET.

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