2023 Winter Research Project Description

Project title:	**Protein structure and function using paramagnetic tags and Electron Paramagnetic Resonance**
Project duration, hours of engagement & delivery mode	Duration of the project, 4 weeks during Winter Vacation. Hours of engagement must be between 20-36hrs per week
Description:	Paramagnetic 'tags' are small molecules used in Electron Paramagnetic Resonance (EPR) spectroscopy to obtain distance measurements on the length scale 15-100 A. The tags are usually attached to a target protein system in pairs. Our group is developing a range of new tags based on nitroxides and Gd^{3+} centres. The project will look a range of tags and use molecular modelling techniques such as density function theory and molecular dynamics to predict how the tags behave when attached to the surface of a protein; i.e. how many conformations are populated, how well can we determine the position of the Gd^{3+} or nitroxide relative to the protein backbone at the attachment site.
Expected outcomes and deliverables:	*Understanding of nuclear magnetic resonance techniques* *Programming skills in Matlab* *Quantum Chemistry Calculations – density functional theory* *Molecular modelling*
Suitable for:	The project would suit a second or third year student interested in applying molecular modelling techniques to systems in biology, in particular, to determine the structure and function of protein systems.
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