2018 Winter Research Projects at CAI

Project title:	**Imaging chemical exchange processes by magnetic resonance techniques**
Project duration:	4 – 6 weeks
Description:	Exchange of labile protons from metabolites with bulk water can be detected by appropriate magnetic resonance methods. Current methods are limited because the spectral resolution acquired is very poor and subject to experimental time constraints. Emerging methods such as frequency labelled exchange (FLEX) (van Zijl, *Magn. Reson. Med.*, 65:927 – 948 (2011)), while also time consuming nonetheless offers the possibility of identifying individual metabolites involved in the exchange process without ambiguity. In this project, using an implementation of FLEX on a 9.4Tesla pre-clinical MRI instrument, the student will collect a dataset from a solution of metabolites with exchangeable protons and explore the potential of non-uniform-sampling (or sparse sampling) as a means to accelerate data acquisition times whilst still retaining quantitative results.
Expected outcomes and deliverables:	Scholars will gain skills in operating an MRI spectrometer and use of modern data analysis techniques for investigating chemical exchange processes.
Suitable for:	This project is open to students with a strong background in physical chemistry and a basic knowledge of nuclear magnetic resonance (NMR) spectroscopy. Some programming skills (C, C++) will be advantageous.
Primary Supervisor:	Yasvir (Yas) Tesiram
Further info:	yas.tesiram@cai.uq.edu.au

2018 Winter Research Projects at CAI

Project title:	Develop simultaneous fMRI and calcium recording system for the rodent brain
Project duration:	6 weeks
Description:	Functional MRI based on blood oxygen level-dependent (BOLD) contrast is widely used for observing brain activity and functional connectivity, but it's only an indirect measure of the actual neural activity. To understand its underlying neural mechanism, we are developing a system to combine optical recordings of fluorescent calcium signals inside MRI to measure neural circuit activity in the mouse brain. In order to achieve simultaneous acquisition of multi-modality data, optical excitation/stimulation/signal recording has to be synced to the MRI scanner. This project will focus on setting up the fibre-optic system, calibrate/optimise the system, designing the in vivo acquisition scheme, collecting and analysing the preliminary data.
Expected outcomes and deliverables:	The student will help to build up and test the optic system and its control program. S/he will gain skills and experience in fMRI and fluorescent imaging. At the end of the project the student is expected to be able to setup and operate the optical recording system, to collect data and do basic analysis. The student will give a written report and presentation at the conclusion of the project.
Suitable for:	This project is open to students with programming skills (eg, Matlab or C/C++). Familiarity with I/O control and experience with Matlab/Labview software will be ideal..
Primary Supervisor:	A/Prof. Kai-Hsiang Chuang
Further info:	k.chuang@uq.edu.au

2018 Winter Research Projects at CAI

Project title:	**Developing Mathematical Techniques for Structural Biology using DEER Spectroscopy**
Project duration:	4-6 weeks
Description:	The project will centre on using the Electron Paramagnetic Resonance technique of DEER (a magnetic resonant technique) to measure distances between paramagnetic spin labels introduced onto a protein. The main part of the project will investigate regularisation algorithms with the aim of using the DEER experimental constraints to determine protein structure. The project tasks and aims are: • Gain an understanding of the theory of distance measurements using paramagnetic spin labels. The Electron Paramagnetic Resonance technique is called DEER. • Learn how to measure on the spectrometer - carry out DEER measurements on a protein system with spin labels. This experiments involves understanding the operation of LHe cryostats and vacuum systems. • Simulate DEER data to determine the distance distribution between the spin labels, using Matlab. • Investigate regularisation algorithms to extract protein structure from the data and structural models of the protein– this will involve developing Matlab code to compute protein conformational distributions from the DEER data.
Expected outcomes and deliverables:	• Applicant will learn about the theory of magnetic resonance, particularly an understanding of DEER spectroscopy • A working knowledge of LHe cryostats will be gained • Develop analysis skills, simulated DEER data using Matlab • Understand and develop regularisation algorithms • Develop Matlab coding skills for data analysis • This project may provide data for a research paper.
Suitable for:	This project is open to 3rd and 4th year students with a background in chemistry, biochemistry, physics or mathematics. It will suit someone interested in coding with Matlab and developing algorithms for fitting experimental data to molecular models.
Primary Supervisor:	A/Prof Jeffrey Harmer
Further info:	For further information email jeffrey.harmer@cai.uq.edu.au

2018 Winter Research Projects at CAI

Project title:	**Cytochrome P450 – understanding drug, substrate and inhibitor interactions using Electron Paramagnetic Resonance**
Project duration:	4-6 weeks
Description:	The project will use Electron Paramagnetic Resonance spectroscopy (a magnetic resonant technique) to investigate the active site of a P450 enzyme, and in particular how drugs (substrates) and inhibitors interact with the P450 catalytic site. The activities and aims are: • Learn about the theory of continuous wave and pulse Electron Paramagnetic Resonance techniques • Background theory of reactions carried out by P450 enzymes in biology and in biotechnology reactions • Learn how to operate the EPR spectrometer • Carry out a variety of EPR measurements on selected P450 enzymes with a range of substrates and inhibitors • Simulate the EPR data using MatLab • Using the experimental data, characterise the coordination environment of the P450 active site when interaction with a range of substrates and inhibitors
Expected outcomes and deliverables:	• Develop an understanding of the theory of magnetic resonance, particularly an understanding of magnetic resonance techniques for paramagnetic materials • Gain an understanding of enzymatic reactions carried out by P450 enzymes • Learn how to simulate EPR data and use the data to build a model for the molecular structure around the P450 paramagnetic centre • Learn MatLab coding for data analysis and fitting • This project may provide data for a research paper.
Suitable for:	This project is open to 3rd and 4th year students with a background in chemistry, biochemistry, physics or Mathematics.
Primary Supervisor:	A/Prof Jeffrey Harmer
Further info:	For further information email jeffrey.harmer@cai.uq.edu.au