University of Reading

Chemical Analysis Facility

Autumn Newsletter

Cutting Edge Science in the Chemical Analysis Facility

Welcome to the first Chemical Analysis Facility Newsletter. We hope in these short newsletters to provide a flavour of the many research projects that are going on in CAF and offer you a glimpse of its cutting edge capabilities.

The Chemical Analysis Facility laboratories are the result of a £4.5 million investment by the University, recognising the need for state of the art analytical instrumentation to support and invigorate research in the chemical sciences.

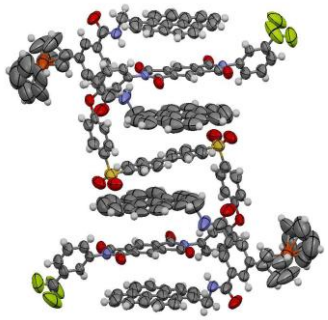
This issue has a strong Chemistry flavour, but we will be showcasing what CAF can do across the campus in future issues of the Newsletter.

Professor David Garner, President of the Royal Society of Chemistry opens CAF with the Vice-Chancellor earlier this year

Pathogenic Mildew Explored

Professor Rainer Cramer and Dr Laurence Bindschedler and collaborators from Imperial College have been awarded funding from BBSRC to improve analytical strategies towards identifying effectors of the economically important barley powdery mildew pathogen, *Blumeriagraminis*f. sp. *hordei*. The study aims to identify effectors at the site of interaction between the mildew and host (the haustoria). There is growing evidence that haustoria are are involved in the uptake of nutrients and in the delivering of the effectors into the host epidermal cells. To date 199 proteins of the haustori and 1076 proteins in sporulating hyphae have been identified via the detection of at least two significant peptides. A total of 36 these proteins were exclusively haustorial proteins. Out of the these 36 haustorial proteins, 24 are predicted to be secreted proteins, 17 (19 if considering secretion signal peptides) are smaller than 20kDa. These small secreted proteins (SSPs) are being investigated as they may play a role as effectors for the establishment of the disease. Some 18 proteins of the haustrial proteome have yet to be identified.

This work was presented as a poster at the recent ASMS meeting in Salt Lake City.



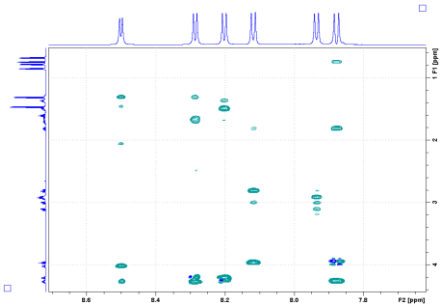
Molecular Tweezers Bind Selectively

A recent X-Ray crystal structure has shed light on the exquisite binding selectivity of a molecular tweezer molecule designed by Professor Howard Colquhoun and Dr Zhixue Zhu. The crystal grown by Dr Zhu was analysed on the CAF single crystal X-ray instrument and the structure was solved by Professor Christine Cardin. The solution revealed the binding of two tweezer molecules binding to an extended acceptor molecule that contained two different recognition sites.

'Sequence-specific assembly of tweezer molecules on oligomer chains: Evidence for frameshift-reading of sequence information.', Zhu, Cardin, Gan and Colquhoun, *Nature Chemistry*, **2**, 653, (2010).

Short Peptide - Defined Structure?

Professor Ian Hamley, Dr David Nutt and Dr Geoff Brown have collaborated together on a project that uses the Bruker 700 MHz NMR spectrometer to examine the self-assembly of peptides into amyloid fibrils. These fibrils are thought to play a role in a number of disease states, including Alzheimer's. A model peptide with the sequence AAKLVFF (based on a fragment of the amyloid β peptide Aβ16-20) has been shown to adopt a β-sheet structure in aqueous solution. Solving the solution structure of this heptapeptide required assignment of all protons by a variety of 2D-NMR techniques. Correlations observed between protons were then used to



generate distance constraints which were in turn used in molecular dynamics simulations leading to the solution structure.

'Influence of the Solvent on the Self-Assembly of a Modified Amyloid Beta Peptide Fragment. II. NMR and Computer Simulation Investigation', Hamley *et al.*, *J. Phys. Chem. B*, 114, 940 (2010)

The Chemical Analysis Facility is housed in two recently refurbished laboratories within the Chemistry/Pharmacy building. The main laboratory houses the NMR, Mass spectrometry, Thermal Analysis and Optical spectroscopy equipment. A second laboratory separately houses the X-ray equipment. The highlights of the instrumentation include a 700 MHz NMR spectrometer with a cryogenically cooled triple nucleus detection probe, an Orbitrap high resolution mass spectrometer, a Small Angle X-ray Scattering (SAXS) instrument, a Raman microscope and a small volume Isothermal Titration Calorimeter.

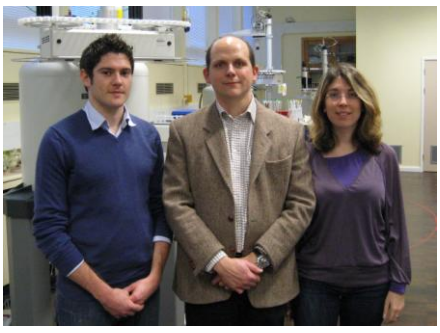
Acoustic Levitation

A NERC award to Dr Christian Pfrang aims to improve the understanding of the impact on climate change of the chemical interactions of organic atmospheric aerosols. To achieve this goal, Dr Pfrang will apply the technique of acoustic levitation to atmospheric sciences. The acoustic levitator will be directly coupled to the CAF laboratories Raman microscope using a fibre optic probe in order to be able to follow changes in the chemical composition of acoustically levitated particles. Acoustic levitation uses sound waves to sustain airborne particles and thus allows container-less reaction monitoring. Three important classes of aerosol will be studied: aqueous droplets, ice and mineral dust particles. Atmospherically important reactions of ozone and nitrogen oxides with organic species within acoustically levitated sea water droplets are to be examined.

New Appointments

Food and Nutritional Sciences have recently appointed three new lecturers who will take advantage of CAF in order to strengthen and develop areas of current internationally recognised research excellence. Dr Gunter Kuhnle (centre) was appointed as a lecturer in nutritional biochemistry. Dr Kunhle's current research activities include the use of mass spectrometry to identify and quantify phytoestrogens and their metabolites in serum and urine and in the characterisation of the polyphenolic content of dates with a view to finding polyphenols which may prove to be protective against colorectal cancer.

Dr Sandrine Claus (right) and Dr Jonathan Swann (left) have been appointed as lecturers in metabonomics. Appointments in this area were possible because of the instrumentation in the CAF laboratories which allows links to be established between nutritional studies and metabolite



profiles in blood and urine. The ultimate goals are to develop insights into how diet impacts heath at the molecular level.

Further Information about the Chemical Analysis Facility can be found at the CAF website:

www.reading.ac.uk/caf