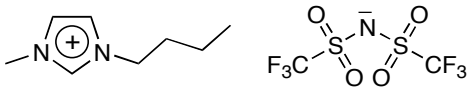
Faculty of Science Vacation Research Scholarships (Summer Scholarships 2009/2010)

(Closing Date 9th October 2009)

Projects	Supervisors	Comments
"Novel Organometallic Complexes – New Catalysts for multistep processes" We are interested in all aspects of organometallic chemistry and catalysis, as well as inorganic chemistry, with a particular emphasis upon designing transition metal catalysts for key organic transformations (synthetic/industrial catalysis and green chemistry). Much of our work relies on the chemistry of multidentate ligand systems, bearing mixed (P, N, O and S) donor atoms. Our research projects involve the investigation of catalytic mechanisms, as well as molecular structure determination In particular, we are interested in making catalysts to promote multiple step reactions in one pot. These are in some cases bimetallic catalysts, with two or more catalysts attached to a molecular scaffold. This project will involve making new scaffolds and attaching metal complexes to these"	Prof. Barbara A Messerle School of Chemistry Phone: 9385 4653 e-mail b.messerle@unsw.edu.au	2nd or 3rd year student
"Understanding organic processes in ionic liquids" The use of traditional organic solvents is becoming more limited as the community becomes aware of their environmental impacts. As such there is a great trend towards more environmentally benign, 'green' chemistry. One alternative is to use a solvent that simply doesn't evaporate such that it can be readily reused and not lost to the environment. Ionic liquids, such as that shown in Figure 1, fit this criteria.  **Figure 1.** An example of an ionic liquid.	Dr Jason Harper School of Chemistry Tel: 9385 4692 e-mail j.harper@unsw.edu.au	2nd or 3rd year student

Many organic reactions have been found to proceed well in ionic liquids, and the rates and selectivities are often improved. However, this not currently predicatable and work in this group aims to rectify this by taking representative organic processes and *understanding* any changes on going to an ionic liquid as a solvent. This project would suit a student with a strong background in physical and analytical chemistry (particularly rate analysis) and organic chemistry (particularly an understanding of organic reaction mechanisms).	*(this project is only offered from mid January, for more details please contact the supervisor directly)*	

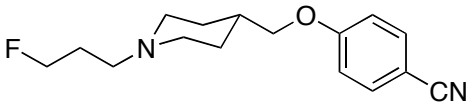
Three Projects are being offered **1. Synthesis of new azaflavonoids** The role of dietary phytoestrogens especially the flavonoids and isoflavonoids in human health is well documented in the literature. These compounds resemble in structure to the endogenous estradiol and have been shown to display weak estrogenic activity. The aim of this project is to synthesize novel azaflavonoids for evaluation of their anti-tumour and anti-atherosclerosis activities. **2. Novel anti-microbial biomaterials** The use of medical devices has increased immensely over the last decade. Although, this increase in device use has resulted in a better quality of life and longer patient survival, device-related bacterial infections have emerged as a serious problem with the increased use of medical implants. The aim of this project is to develop methodologies for the covalent attachment of novel anti-microbial compounds including specially designed peptides and nitric oxide donors onto biomaterial surfaces**.**	Dr Naresh Kumar Ph: 9385 4698 Email: n.kumar@unsw.edu.au	2nd or 3rd year student – Who is interested in organic synthetic chemistry
Dr Graham Ball Dalton 129 ***In silico* coordination chemistry** How much we *really* know as chemists can be related to how accurately we can predict observations using theory *before* we do the experiment. This project aims to use emerging computational chemical methods, in particular density functional theory (DFT) to predict the stability, structure and spectroscopic properties of new compounds with unusual bonding topologies such as alkane or xenon complexes. Scores of interesting molecules and not a reaction vessel in sight!	Dr Graham Ball Ph: 9385 4720 g.ball@unsw.edu.au	2nd or 3rd year student

RESEARCH PROJECTS: MOLECULES FOR PROBING σ RECEPTOR BINDING AFFINITIES

Supervisor:
A/Prof. Roger Read,
Room 227 Dalton Bld.
e-mail
Ph 9385 54712

2nd or 3rd year student

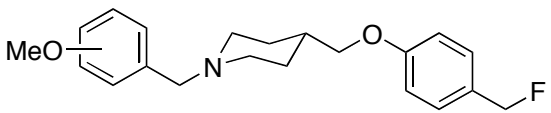
Sigma receptors are found in high densities in various tumours and have been implicated in sections of the human chromosome associated with psychiatric disorders. Since their discovery in 1976, two major sub-types have been recognised and named sigma-1 and sigma-2. Little is known of either receptor protein although the sigma-1 receptor has been most studied. A number of classes of drugs will bind to sigma receptors, but to be useful in radiolabelled diagnostics the molecules must bind with high selectively to sigma-1 or sigma-2 sub-type receptors.[1]



1

FPS

Ki (sigma-1) = 0.5 nM
Ki (sigma-2) = 144 nM



2

2-, 3-, 4-OMe

A number of piperidine derivatives, including FPS **1**, have shown excellent high affinity binding and selectivity towards the sigma-1 sub-type.[2,3] Meanwhile, in parallel studies, it has been found that in certain trishomocubane and piperazine derivatives, the sub-type selectivity can be switched by subtly changing substituents at the nitrogen.
As part of our ongoing interest in receptor ligand interactions,[4] in this project, piperidine molecules will be synthesised that will probe the structure activity relationship within the piperidines in an attempt to control selectivity towards the alternative sigma-2 sub-type. As a start, target molecules will have structure **2** and they will include 2-, 3- and 4-methoxylated aryl derivatives.

Objectives

Tasks within this project will be:

1. Planning and design of the syntheses based on literature precedents.
2. Purification and full characterisation of the compounds.
3. Testing of a method for the introduction of the critical fluorine atom in each of the molecules.
4. Conformational studies of the products by NMR spectroscopy.

References
1. Collier, T. L.; Waterhouse, R. N.; Kassiou, M., *Curr. Pharm. Design*, **2007**, *13*, 51-72.
2. Waterhouse, R.N.; Slifstein, M.; Talbot, P.; Sultana, A.; Sudo, Y.; *et al*., *NeuroImage*, **2002**, *16*, S6.
3. Collier, T. L.; O'Brien, J. C.; Waterhouse, R. N., *J. Labelled Cmpd. And Radiopharm*., **1996**, *37*, 785-794.
4. Kassiou, M.; Read, R.W.; Shi, X.-Q., *Bioorg. Med. Chem. Lett*., **1997**, *7*, 799-

For Applications please go to the Chemistry School website or see

Ken McGuffin
School of Chemistry
Dalton Building, Room 106
University of New South Wales 2052
PH: 9385 4611
k.mcguffin@unsw.edu.au

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