University of Glasgow

STEM Research Opportunities for SMU students Summer 2017

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SMU in Glasgow UK
Summer STEM Research 2017

SMU-in- Glasgow UK is a 6-week intensive summer research program for students in STEM fields hosted at the University of Glasgow, Scotland. The University of Glasgow (UG) is a large (17,000+ students) top-tier international research institution in a city that is trendy, vibrant and energetic. The second oldest university in Scotland (founded in 1451), the UG has a long history of achievement; former faculty include engineer James Watt, economist Adam Smith, and physicist Lord Kelvin.

The University: Study abroad at University of Glasgow offers you a green campus setting in the up-scale West End of Glasgow in an institution that is consistently ranked among the UK's top universities. The University of Glasgow has more than 6,000 staff which includes 2000+ active researchers with an annual research income of more than £200m.

The Opportunities: The STEM departments are some of the largest in the UK, and they are equipped with cutting-edge research equipment. Students work in an intimate setting with faculty and other students on their selected research topic. Cultural excursions with STEM students (all disciplines) provide a chance to tour the UK and meet other international students.

The Organization: In the STEM fields, the University of Glasgow partners with Arcadia University to offer summer intensive research courses. Arcadia organizes program related activities (orientations, presentation of student projects) as well as extra-curricular cultural activities (historical tours, museum visits, and field trips). At the end of the program, the students present their research to the group.

The Benefits: The program provides intensive research experience, and this is highly desirable for scholarship applications and graduate school applications. Research during the semester is typically limited to a few hours/week; summer research allows for concentrated and collaborative work, and the resulting research output is significantly increased.

The Research: As part of the program, students may have the opportunity to work with UG faculty with specialized equipment, depending on the specific project. For example, the UG Psychology department has an MRI facility on-site allowing students to perform projects integrating real-time brain scans into their research. The Chemistry department can perform in-house x-ray crystallography, and the Physics department has a gravity wave interferometer. This environment provides a wide range of facilities and research topics to choose from. Students would be working with a diverse mix of faculty and students from different countries and universities.

The Experience: Glasgow is the largest city in Scotland with a variety of museums and historical sites. There is also easy access to Edinburgh (1 hour), Stirling Castel (1 hour), Loch Ness and the highlands (day trip), as well as London (5 hours).

Frequently Asked Questions

SMU Credits:

The students receive 6 SMU credits (equivalent of 2 courses) for this program. This may count for general elective credits, and may also satisfy University Curriculum "Proficiencies & Experiences" such as Global Engagement, Information Literacy, Oral Communication, Quantitative Reasoning, Writing. The specific equivalences depend on the details of the research program; these should be approved in advance. These courses may also satisfy the student's degree requirements. Again, the specific equivalences depend on the details of the research program; these should be approved in advance with the departmental advisor.

Format Of The Program:

The program is an intensive 6-week course for which the students receive 6 credits. The 2016 course ran from 18 June to 29 July (including the orientation). There are typically 20 students in the program across all STEM fields. Cultural activities involve all STEM disciplines so students can meet other international students.

Many of the students have completed 2 or 3 years of course work; for some fields this is the recommended preparation, but there are other fields (such as life sciences) where first-year students (rising freshmen) are welcome. See the example projects to determine the appropriate prerequisites.

A literature review is assigned (and due) before the start of the program so the students can do some preparation in advance to make the most of the 6 weeks. At Glasgow, the students then work on their projects under the direction of the faculty. At the end of term they submit a written report of their project and give an oral presentation (which is video taped).

The specific format of the course varies by field; sample projects are described in the attached material.

Logistical Support:

Arcadia provides support for the program in several forms; assisting with pairing the students to the advising faculty, providing local logistics (housing arrangements, orientations), student assistance (24/7 support), and local cultural activities.

Life Sciences

Sample Projects

From Previous Years

20th June – 29th July 2016.
6 weeks.

ARCADIA SUMMER PROJECT 2016

Viruses in Freshwater: A Historical Record of Past Pollution?

Faculty from the School of Life Sciences

Many species of bacteria present in natural environments act as hosts for viruses ("bacteriophage") that enter, replicate and destroy the microbial host. Vast numbers of these viruses are found in aquatic and marine environments – typically each milliliter of seawater contains 10 million of these agents – and they play important roles in regulating bacterial populations, driving bacterial evolution and in consequence, impacting upon multiple ecosystems.

Although viral infectivity can decline with time depending upon the virus, ambient temperature, pH and other parameters, they remain an important indicator of water quality. But can they persist in the absence of the bacteria in which they grow? Can they provide a historical record of past pollution?

The aim of this project will be to characterize the bacteria of faecal origin in a local watercourse, to establish which indicator organisms are present and which are absent, and then to attempt detection of bacteriophage for both groups of microbes. Students on the project will develop skills in environmental monitoring, virology and molecular biology.

Desirable background: Some basic knowledge of ecology and microbiology would be useful but training can be provided.

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ARCADIA SUMMER PROJECT 2016

Extremophiles in the Urban Environment

Faculty from the School of Life Sciences

Microbes are able to colonize natural environments in which extremes of temperature, pH or osmolarity are found. Members of the Archaea are particularly notes for these attributes. Modern domestic and urban environments can present equally challenging conditions yet the ability of microbes to exist in these niches and the substrates that they utilize for growth are much less well understood.

The project will use conventional microbiological techniques to sample from a range of urban environments that present thermal challenge and seek out thermophilic organisms able to survive and grow in these conditions. The properties of these bacteria will be analyzed and identification will be attempted by sequencing of genes that encode ribosomal RNA. Students on the project will develop skills in microbiology and molecular biology and the project will offer substantial opportunity for independent investigation.

Desirable background: Some basic knowledge of microbiology and aseptic technique would be useful but training can be provided.

ARCADIA SUMMER PROJECT 2016

Using Caenorhabditis elegans as a Model Organism for Genetic Screens

Faculty from the School of Life Sciences

The nematode Caenorhabditis elegans has achieved great utility as a model organism for the biology of multicellular organisms. Despite its simplicity – typically, the animal comprises just over 1000 cells – it has a sophisticated nervous system and all the neuronal pathways have been mapped. Today, *C. elegans* is used to study a much larger variety of biological processes including apoptosis, cell signalling, cell cycle, cell polarity, gene regulation, metabolism, ageing and sex determination. Many key discoveries, both in basic biology and medically relevant areas, were first made in the worm

As an experimental system, *Caenorhabditis elegans*, offers a unique opportunity to interrogate *in vivo* the genetic and molecular functions of human disease-related genes. For example, *C. elegans* has provided crucial insights into fundamental biological processes such as cell death and cell fate determinations, as well as pathological processes such as neurodegeneration and microbial susceptibility. The *C. elegans* model has several distinct advantages including a completely sequenced genome that shares extensive homology with that of mammals, ease of cultivation and storage, a relatively short lifespan and techniques for generating null and transgenic animals.

The aim of this project will be to establish an experimental system with C. elegans in which these topics can be explored using a forward genetic approach. Using ethylmathanesulforate (EMS), a mutagen that induces direct mutations in DNA, such as missense and nonsense mutations you will screen populations of C. elegans looking for any phenotypic changes that may be biologically interesting and attempt to further characterize the mutants. This is a very exciting project as the outcome is unknown and it may lead to the identification of a new mutant phenotype.

Students on the project will develop skills in molecular biology and the project will offer substantial opportunity for independent investigation.

Desirable background: Some basic knowledge of molecular biology or biochemistry would be useful but training can be provided.

Psychology

Sample Projects

From Previous Years

Psychology Arcadia projects – Summer 2016

Proposal 1:

Title: Using fMRI Intersubject Correlation to assess neural variability in the action observation network of individuals on the autism spectrum

Abstract: Intersubject Correlation (ISC) provides a means to understand how brain activity is correlated among a group of observers. It has provided insight into the processes involved in viewing naturalistic stimuli. Previous research has indicated that, compared to typically developed (TD) individuals, groups of individuals on the autism spectrum (AS) produce less ISC. With a set of data previously collected from AS and TD observers we will more closely examine this question in the context of claims that high functioning AS participants use compensatory networks in visual motion areas to process actions. Namely, we will address the question - Can we find evidence that variability in the ASD group arises from this compensatory network? The project will involve several components including: 1) using specialized software in Matlab for the calculation of ISC and the comparison of ISC maps across conditions, 2) using the fMRI analysis software Brain-voyager to visualize ISC maps, 3) using Brain-voyager to evaluate how quantitative measures of body motion predict brain activity. These results will contribute to understanding the social neuroscience of autism.

Proposal 2:

Title: Automatic Neuronal Processing To Threatening Voices

Abstract: The first impressions that we make about another's character, be it from their voice, face, or appearance, have been shown to heavily influence any future interactions we may have with that person. In regards to approach/avoidance behavior, one of the rapid judgments we must make is whether a person may or may not be a threat to us. Previous literature has shown that such information can be rapidly derived from hearing the person say a simple word or from a brief glance at their face. For faces, it has been shown via functional Magnetic Resonance Imaging (fMRI) that the amygdalae, and extended areas of the limbic region of the brain, are attuned to varying levels of threat and are proposed to process such judgments automatically, without the requirement of conscious decision-making. If such a process also occurs for voices, and the possibility of threat derived from speech, is an active question in the field and one that our group is currently researching. Thus the aim of this project would be to establish if amygdala activity is modulated in accordance with perceived threat or aggression from novel speakers via fMRI. Students on the project would obtain hands on experience in the running of auditory behavioral experiments; develop skills and understanding in experimental design and analysis for behavioral and fMRI protocols; learn about auditory morphing and synthesis techniques; and acquire a solid grounding in research relating to social cognitive neuroscience with scope for further independent analysis and study.

Desirable background: General experience of experimental design and statistical analysis in psychology is desirable, as is an understanding of fMRI and brain imaging, but training can be provided.

Mathematics

Sample Projects

From Previous Years

University of Glasgow

Arcadia project: Voronoi diagrams and optimal location problems

School of Mathematics and Statistics, University of Glasgow
Supervisor: Dr. Steve Roper

Description

Given a convex domain Ω (for example the unit square) and a function ρ defined on Ω (we imagine this to be population density for example). We ask the question, given N locations $\boldsymbol{x}_i$, $i = 1, \dots, N$ (these might represent post offices for example), where do we place these $\boldsymbol{x}_i$ in order to minimise

$$\int_\Omega \min_i |\boldsymbol{x} - \boldsymbol{x}_i|^2 \rho(x)\, dx$$

This problem is called an optimal location problem and its solution gives rise to an object called a *Voronoi diagram* in which Ω is partitioned into cells V_i. For every point in V_i, the distance to $\boldsymbol{x}_i$ is less than the distance to any other $\boldsymbol{x}_j$. This means if, ρ is population density, that everyone in cell V_i travels to post office $\boldsymbol{x}_i$. An example is shown below

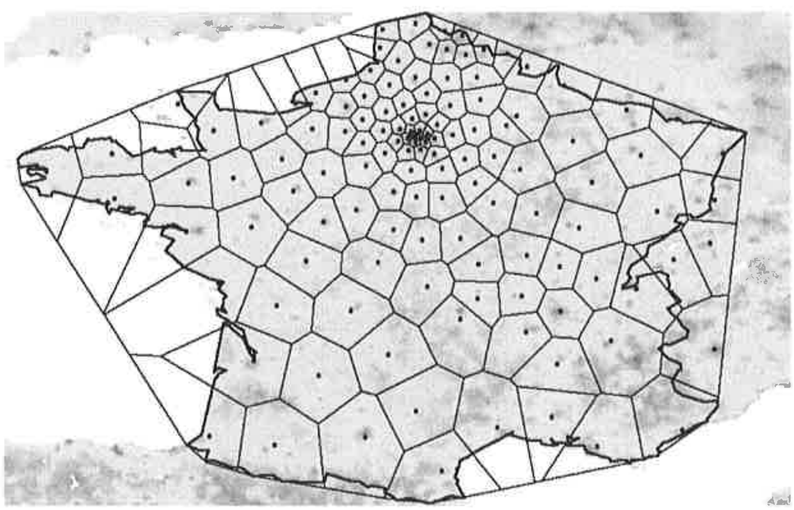


Figure 1: A generalised Voronoi diagram used to partition metropolitan France. The colour represents population density (data from EuroStat).

This project will study Voronoi diagrams, their properties and algorithms for their calculation, together with generalisations (Apollonius diagram, Power Diagram, Median Line). This work has applications to numerous fields, including logistics and even international law (where to draw maritime boundaries for example).

Prerequisites. This project would suit a student who has studied multivariable calculus and who may have an interest in scientific computation and/or computational geometry.

University of Glasgow

Arcadia project: Mechanics of Heavy Chains

School of Mathematics and Statistics, University of Glasgow
Supervisor: Dr. Steve Roper

Description

A heavy chain is a deformable one-dimensional object with mass. It can bend but not extend (it cannot change its length). This project will study the rational derivation of the equations of motion of a heavy chain and study some applications (the motion of a single chain, and multiple chains). A useful reference is [2]. More general models involving fibres, chains and elastic ropes can be constructed to model human hair [1]. The theory has applications in engineering but serves as a useful introduction to continuum mechanics.

Prerequisites. Students must have studied multivariable calculus, have some exposure to ordinary and partial differential equations and have studied Newton's laws of motion. The project could have some computational element for a student interested in scientific computation.

References

[1] Raymond E. and Warren Goldstein Patrick B. and Ball, *Shape of a Ponytail and the Statistical Physics of Hair Fiber Bundles*, Physical Review Latters **108** (2012), no. 7.

[2] Darryl Yong, *Strings, chains, and ropes*, SIAM Rev. **48** (2006), no. 4, 771–781 (electronic).

Arcadia — Langton's Ant

This project will investigate an example of a *cellular automaton* called Langton's Ant. A cellular automaton is composed of a grid of *cells*, each cell can have one of a finite number of states. The states of all the cells at a particular time is called a *generation* and a cellular automaton has a rule to create a new generation. This rule updates the state of every cell and is typically a function of a cell's state and that of its neighbours (a definition of the neighbours of a cell must be provided).

As an example we consider a one-dimensional array of cells. A cell can have one of two states 'black' or 'white' (represented by '1' or '0' respectively). A generation is represented by a row in the following figure which is an illustration of applying 'Rule 110' (an elementary celluar automaton). Langton's Ant is an example of a cellular automaton, it is most easily described as an 'ant' walking

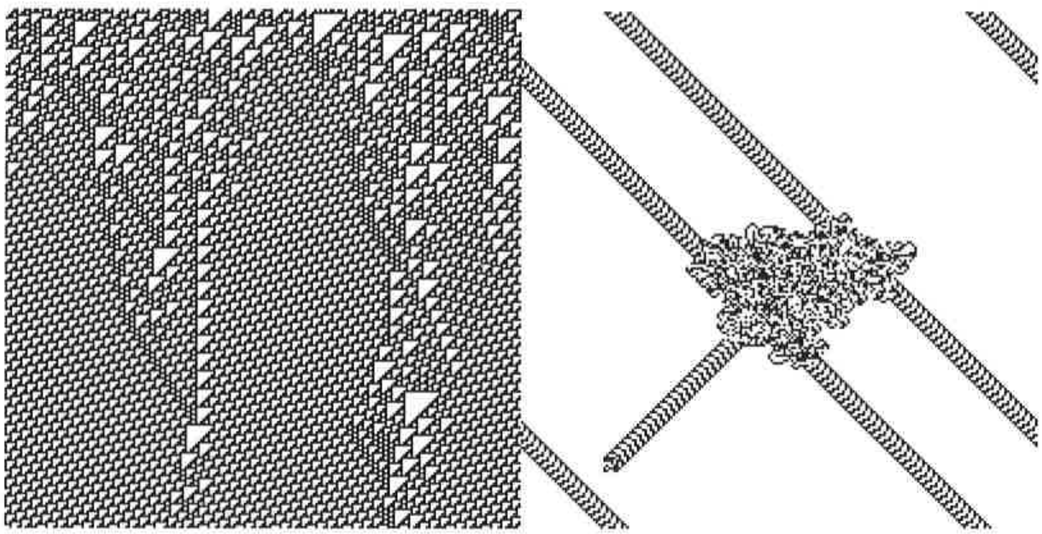


Figure 1: On the left, a simulation of Rule 110. On the right, simulation of Langton's Ant walking on a doubly periodic square array.

on a two-dimensional array of cells. The cells are coloured black and white, and are initially all white. The ant starts on any cell. If the cell is white, the ant turns 90 degrees right, changes the state of the cell to black and walks forward one cell. If the cell is black, the ant turns 90 degrees left, changes the state of the cell to white and walks forward one cell. The behaviour is complex.

The project will involve investigating cellular automata, in particular simulations of Langton's Ant, and variations on it. There are many variations to investigate such as

- More than two states for the cell, with different left and right turning rules.
- Multiple ants.
- Different geometry of cells (infinite array or periodic).
- Different initial conditions.
- Three-dimensional 'ants'.

This project might suit students with an interest in difference equations, chaos, computing. There is something here for mathematicians of all kinds.

<u>Physics & Astronomy</u>

Sample Projects

From Previous Years

Physics and Astronomy Arcadia projects – Summer 2016

1. The "Beta pen": a hand-held device for detecting beta radiation

Principal Supervisor: Dr Bjoern Seitz - Physics and Astronomy

Radioactive isotopes emitting beta radiation are frequently embedded in living organisms, either as the result of exposure to natural or man-made radioisotopes emitted into the environment or as radioactive tracers to monitor biological functions in a living organism. An example for man-made exposure to beta-radiation would be ingestion of Strontium-90 with seafood as encountered in the aftermath of the Fukushima Dai-ichi powerplant's accident. Beta-emitting radioactive tracers could e.g. be employed in radio-guided surgery of cancer lesions.

The broad energy spectrum and short penetration length make it in general difficult to detect and identify beta-emitting isotopes. We propose to study a hand-held device, currently dubbed the "beta-Pen", to identify beta-radiation at short range with applications ranging from food monitoring to novel ways of radio-guided surgery in mind. The project will comprise of identifying and testing a novel combination of scintillating material with small area photon detection systems to prove the feasibility of this approach and provide a pilot study of its uses.

2. Investigating the astronomical signatures of artificial structures in extra-solar planetary systems

Principal supervisor: Prof Martin Hendry – Physics and Astronomy

Recently there has been growing interest within the SETI (Search for Extra-Terrestrial Intelligence) community about the possibility of using future giant ground- and space-based optical and infra-red telescopes to search for evidence artificial structures associated with extra-solar planets in the solar neighbourhood. Indeed in autumn 2015 observations of an extra-solar planetary system with the NASA Kepler telescope displayed intriguing, strongly varying light curves which led to speculation that they might be the result of artificial structures. While there is no clear evidence to support this hypothesis, it has nonetheless placed the modelling of astronomical signatures from such structures firmly in the limelight.

The aim of this project will therefore be to review some of the recent literature on this novel topic, and use simple numerical codes to simulate telescopic observations of realistic artificial structures that might conceivably be built by advanced extra-terrestrial civilisations, in order to investigate the feasibility of detecting such structures - or at least placing constraints on the telescope technology required to do so - in the future. The project will benefit from some prior knowledge of astronomy, but this is not essential. Some prior experience in scientific computing, using e.g. MATLAB, would be very beneficial, however. The research will involve some collaboration with colleagues in the School of Engineering.

3. Electrical testing of Silicon Strip Detectors for the ATLAS experiment at the Large Hadron Collider

Principal Supervisor: Dr Andrew Blue – Physics and Astronomy

In 2021, installation will begin on the upgrade of the ATLAS experiment at the high luminosity (HL) LHC at CERN. The new silicon based particle tracker will require over 20,000 strip detectors, and these will all be assembled and tested over a range of 20 institutes over a 3 year periosd. At present the UK will build 50% of the strip barrel tracker, with the remainder built by the US. For the next 2 years, an R&D stage continues to study the design and performance of the detectors that will be used in the upgrade of ATLAS. This involves characterization of both the semiconductor silicon sensors and the electrical performance of the readout CMOS chips. We would be looking for students who are keen to study hardware used for particle physics experiments. Work could include the use of FPGA systems for DAQ readout, semiconductor characterization of silicon detectors (for charge collection & noise levels) or analysis of detector performance from preliminary particle test beams. Knowledge of computer programming and semiconductor physics is preferred but not essential.

4. Multi-instrument solar prominence diagnostics: Prominence contribution to solar irradiance

Principal Supervisor: Dr Nicolas Labrosse – Physics and Astronomy

Being able to detect the presence of above-the-limb solar prominences in solar irradiance measurements would be extremely useful to characterize their properties over a wide range of temperatures. In this exploratory project, the student will analyse data from the three instruments embarked on the Solar Dynamics Observatory (SDO) satellite:

- the EVE spectrometer which monitors the solar irradiance in the extreme ultraviolet
- the AIA imager which observes the full Sun at high spatial and temporal resolution over a large range of temperatures
- the HMI imager and magnetograph, observing the Sun in the visible range.

After identifying the largest prominences observed since the start of operations of SDO on AIA images, a detailed analysis of the EVE spectra and HMI observations will be carried out to look for signatures of the presence of these prominences above the limb of the Sun. This measurement has not been fully explored so far, so this could be a very exciting project... or a very deceptive one!

The data analysis will be done preferably using IDL (Interactive Data Language). During the project the student will learn:

1. basic physics of solar prominences,
2. how to program using Interactive Data Language (IDL),
3. how to analyse data from space-based observatories using SolarSoft IDL routines (SSW).

<u>Geosciences</u>

Sample Projects

From Previous Years

For possible projects, please see:

http://www.gla.ac.uk/schools/ges/

Chemistry

Sample Projects

From Previous Years

Undergraduate Research Project 2015–2016

- **3d Printing and Chemical Robotics:** One of the great challenges in synthetic chemistry is to effectively discover, synthesise and apply new molecular entities to a range of problems e.g. drug discovery. However it is clear that exploring this parameter space can be limited. We have been exploring the idea of combining the concept of merging the **reaction** with the **reactor** by fabricating the reactor with incorporated reagents using a 3d-printer. *In this project we will design new reactionware for drug-discovery and to see if we can take complex multi-step organic synthetic reactions and deploy them into a 3d printed reactionware matrix.*

- **Protein-Engineering:** Proteins are the ultimate catalysts, evolved by nature, and highly effective, but the post synthetic modification of proteins has been limited to the incorporation of 'new' amino acids or post translational modification of the amino acids. *In this project we will examine the idea of incorporating cluster-hybrids with pendent amino-acids to link into a protein e.g. take AA-AA-AA-AA → AA-AA-POM-Cluster-AA-AA and look at protein folding, function to make the first truly bio-ionic protein.*

- **Using Self Assembly to Build Molecular Architectures:** The problem with chemical synthesis is that the concept of designing a complete blue-print for a complex functional molecule. However, by using 'self-assembly' it is possible to build very complex architectures very quickly if the ligand building block is designed correctly. *In this project we will be examining the influence of **ligand design** (using simple organic chemistry) to grow and build complex architectures that involved many tens of thousands of atoms in a single growth process.*

- **The Origin of Life:** Understanding the origin of life is a vast challenge. In biology the ribosomal machinery is responsible for producing almost all the complex molecules of biology but where did it come from?? In this project we will be using complex-network flow systems to produce complex molecular systems and structures. *The aim is to produce a range of new organic, inorganic and hybrid molecular systems of vast complexity that simply cannot be achieved on a reasonable timescale in the laboratory using conventional synthetic techniques.*

Metal-Organic Frameworks for Catalysis, Drug Delivery and CO_2 Capture

Background. A current area of focus is **Metal-Organic Frameworks (MOFs)** – porous, stable, crystalline materials (**Fig. 1**) comprised of organic ligand molecules (struts) linked by transition metal ions or clusters. MOFs have infinite ordered arrays of nanocavities and exhibit prodigious capacities for the uptake of gases and small organic molecules, and, as such, are implicated in green technologies such as carbon capture and storage and hydrogen fuel cells. Catalysis *within* the pores of MOFs is a small but nascent research area, with the added advantage of the reagents and products being able to diffuse in and out of the material.

We seek to prepare MOFs with highly functionalised pores – analogous to enzyme binding sites – for the selective binding of targeted guest molecules and their subsequent catalytic transformation to compounds of interest.

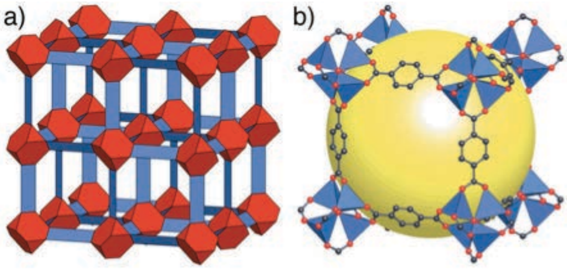


Fig 1. a) Schematic MOF diagram showing organic struts connected by clusters. **b)** One of the many spherical nanopores in MOF-5.

Project 1: Surface Modulation of MOF Nanoparticles. New synthetic protocols will be developed to prepare and functionalise *nanoparticulate* MOFs while exercising strict control over crystal morphology. Post-synthetic modification will be used to generate bioactive drug-delivery vectors – **artificial viruses** – as well as solution-based nanocatalysts. Interactions with biomolecules will be examined in the context of developing new self-assembly protocols. The effect of surface modification on a number of properties will be examined, including molecular storage and release and stability. Collaborations will be developed with biological sciences to test the drug delivery properties of these materials in cells and develop MOF protein/DNA hybrids.

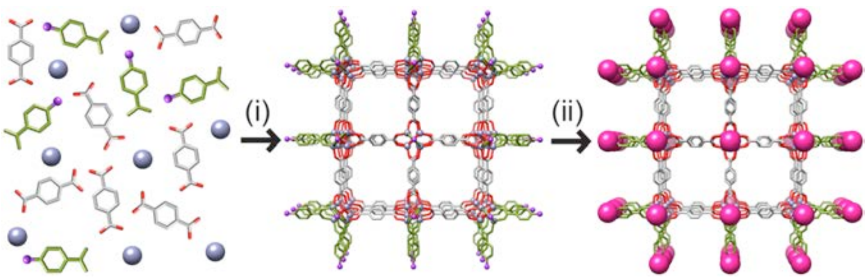


Fig 2. Surface modification of MOFs through a two step-procedure.

Project 2: Functionalising MOFs to act as Receptors. Incorporation of functional groups into MOFs will be achieved using novel struts such as those shown in **Fig. 2**. The target struts contain many H-bond donors and acceptors and are of the same length, allowing multivariate MOFs with mixed struts to be prepared. Differing metal coordination units can be incorporated in a modular fashion to prepare MOFs with different topologies. This diversity of both strut functionality and accessible MOF topologies dictates that many different MOFs can be synthesised to generate a wide variety of binding sites. Upon preparation of a series of new MOFs, the binding of small molecules, after their diffusion into the nanopores in organic solvents, will be examined. Nucleophilic groups are also known to promote selective capture of CO_2, and so gas uptake will be investigated in detail.

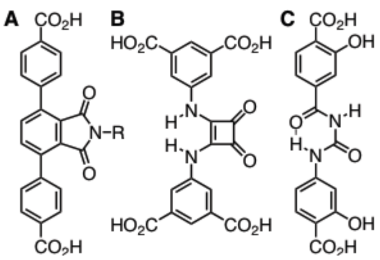


Fig 2. Three examples of functionalised MOF struts.

Project 3: Catalytic and Organocatalytic MOFs. The introduction of catalytically active sites into MOFs allows for size-selective heterogeneous catalysis. We use several strategies to incorporate functionality into MOFs both before and after their synthesis. Model catalytic reactions are used to assess efficacy and develop methodology, with comparison to analogous homogenous catalysts also utilised. Successful catalytic species may also be used in natural product synthesis.

Overview: Students can expect to learn a broad range of **organic and inorganic synthetic skills**, as well as gain experience in state-of-the-art solution and solid-state characterisation techniques.

Redox-Active Dithione Ligands

All molybdenum- and tungsten-containing enzymes with the exception of nitrogenase possess at least one ene-1,2-dithiolate.[1] This entity can exist in three different oxidation levels: a dianionic dithiolate, monoanionic radical, or a neutral dithione.[2] The latter has been sparingly used in coordination chemistry on account of the difficulty of preparing the organic moiety, which can then be attached to a metal ion. The use of non-aromatic heterocycles is the only accessible means to a genuine dithione ligand – the archetypal *N*,*N′*-dialkylpiperazine-2,3-dithiones (pipdt; Figure 1).

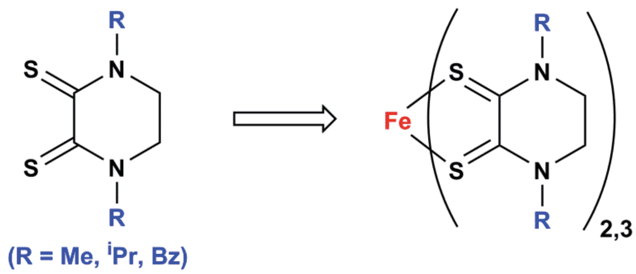
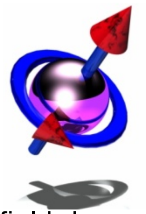


Figure 1. Structures of pipdt ligand and iron complexes

The aim of the project is to synthesise novel Fe(II) and Fe(III) complexes with pipdt ligands using air-sensitive laboratory techniques (Schlenk line, glovebox). Specifically, the hitherto unknown $[Fe(pipdt)_3]^z$ (z = 3+, 2+, 1+, 0) series (Figure 1), where examination of the electrochemistry will enable each member to be isolated and characterised. We will employ a battery of physical methods – electronic absorption, IR, MS, NMR, electron paramagnetic resonance, Mössbauer and X-ray absorption spectroscopy, SQUID magnetometry, X-ray crystallography – to fully elucidate their electronic and molecular structure. We will also target mixed-ligand $[Fe^{II}(pipdt)_2X_2]$ (X = Cl, Br, SCN) complexes, namely their magnetic properties and potential spin cross-over behaviour. The applicability of the synthetic process will be applied to Co and contrasted with the Fe chemistry.

1. R. Hille, J. Hall and P. Basu, *Chem. Rev.*, 2014, **114**, 3963 – 4038.
2. S. Sproules, *Prog. Inorg. Chem.*, 2014, **58**, 1 – 144.



Spin Entanglement in Molecular Farfalle

Quantum information science promises to revolutionise information and communications technologies via secure communication, precision measurement, and ultra-powerful simulation and computation.[1] Some concepts of quantum computing (QC) have been demonstrated on a variety of physical systems, yet the field has not advanced to the state where a quantum computer exists that is capable of implementing advanced algorithms. Single electron spins represent a natural choice for the implementation of a quantum bit (qubit). They are two-level systems that are relatively decoupled from the environment, and thus have sufficiently long coherence times. The implementation of QC in quantum dots and superconducting devices are among the most developed activities in solid state systems but the consensus is that the optimal (reliable, scalable and cheap) hardware to encode qubits still needs to be defined. Molecules with an $S = {}^{1}/_{2}$ ground state have been deployed as qubits, and these have manifested as either polymetallic clusters or organic radicals.[2] In order to attain the desired performance characteristics, the electron spin-spin coupling between qubits must be carefully stage managed. This is achieved by using ligand design to position spin centres (metal ions) and manipulate their interaction.

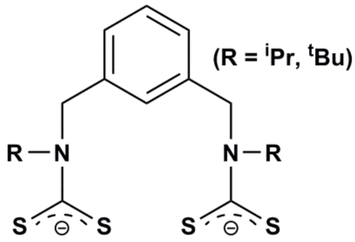


Figure 1. Structure of bisdithiocarbamate ligand

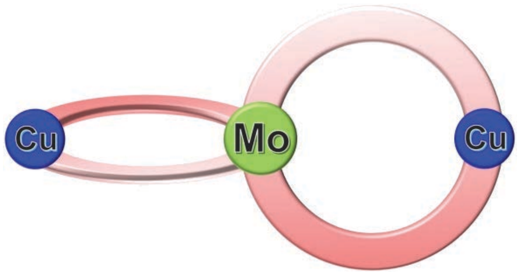


Figure 2. Cartoon representation of a trimetallic molecular farfalle where metal ions are linked by bis(dithiocarbamate) ligands.

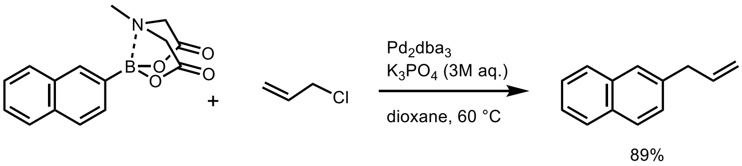
This project explores chemical entities that can switch the interaction between two weakly coupled electron spins in a quantum device we will use to take over the world. The synthetic target is a self-assembled dicopper(II) complex using two bis(dithiocarbamate) ligands (Figure 1).[3] The spin-spin interaction is modulated by the spatial separation of the two Cu^{II} ions, generating a bipartite system with accessible levels. The programme combines the synthesis of mono- and multinuclear complexes and characterisation by spectroscopy (NMR, electronic absorption, EPR), SQUID magnetometry and X-ray crystallography. This will be followed by testing electrochemical control over the spin ground state by selective oxidation of one of the Cu^{II} ions. By constructing smaller building units, more elaborate trimetallic systems are envisaged (Figure 2), where the spin-spin interaction is tuned by the ligand size and switched electrochemically.

3. M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press: Cambridge, UK, 2010.
4. G. Aromí, D. Aguilà, P. Gamex, F Luis and O. Roubeau, *Chem. Soc. Rev.*, 2012, **41**, 537–546.
5. W. W. H. Wong, J. Cookson, E. A. L. Evans, E. J. L. McInnes, J. Wolowska, J. P. Maher, P. Bishop and P. Beer, *Chem. Commun.*, 2005, 2214–2216.

New C–C bond forming strategies.

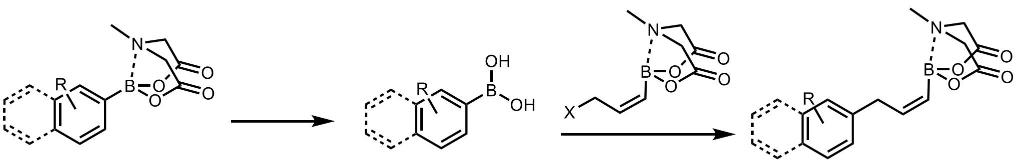
One of the main goals of organic synthesis is the ability to build up complex, biologically active molecules quickly from simple starting materials. Recent research into MIDA boronates has shown their potential to be powerful tools for synthesis, allowing several complex molecules to be quickly constructed from simple building blocks.[1] The commercial availability of ~200 of these MIDA boronates provides easy access to the necessary starting materials.[2]

Recent results in the group have shown that a MIDA boronate can be coupled with an allyl halide in good yield (Scheme 1). The reactivity is unique because it makes a new bond to an sp^3-hybridised carbon, a challenging feat in Pd-catalysed couplings.

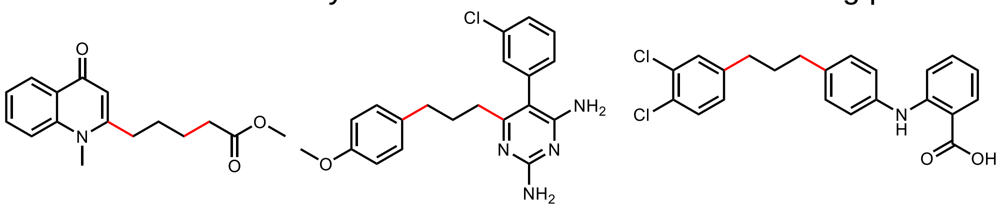


Scheme 1: Coupling of MIDA boronate with allyl halide

The project will extend this chemistry in new directions. For example, by using a MIDA boronate containing allyl halide we can make use of an iterative sequence (Scheme 2). By deprotecting the original MIDA boronate before coupling, we can obtain a product that also contains a MIDA boronate. This product can then be used in further coupling reactions, giving the ability to rapidly prepare bioactive targets such as those shown in Figure 1.



Scheme 2: Iterative synthesis of MIDA boronate containing product



Evollionine C | anti-malarial | Alzheimer's disease

Figure 1: Potential targets for iterative synthesis

(1) Li, J.; Ballmer, S. G.; Gillis, E. P.; Fujii, S.; Schmidt, M. J.; Palazzolo, A. M. E.; Lehmann, J. W.; Morehouse, G. F.; Burke, M. D. *Science* **2015**, *347*, 1221.

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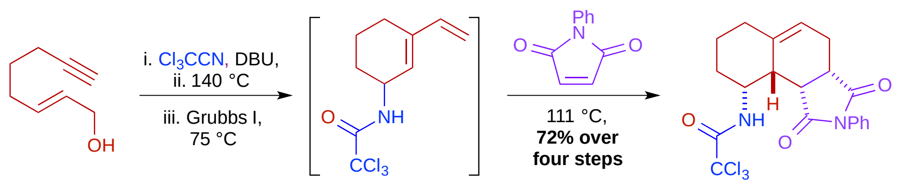
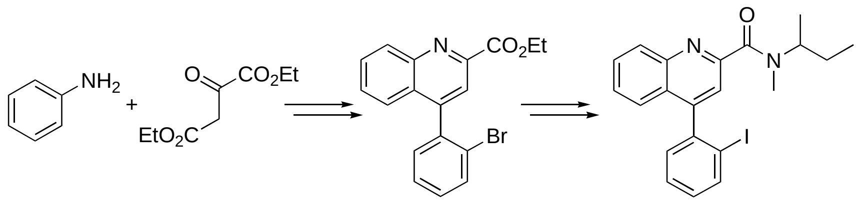
Multi-Bond Forming Tandem Reactions for the Rapid Synthesis of Biologically and Medicinally Important Compounds

We have developed new one-pot, multi-bond forming tandem processes involving Overman rearrangements, ring closing enyne metathesis reactions and hydrogen bonding directed Diels-Alder cyclisations for the rapid synthesis of drug-like polycyclic scaffolds.[1] Additional steps can also be added to this one-pot process resulting in the preparation of aromatic analogues. Work is currently underway to develop asymmetric versions of these processes for the total synthesis of natural products. A typical project in this area would involve the synthesis and application of new substrates for a tandem process followed by the use of the highly functionalised products as a key synthetic intermediate in a total synthesis.



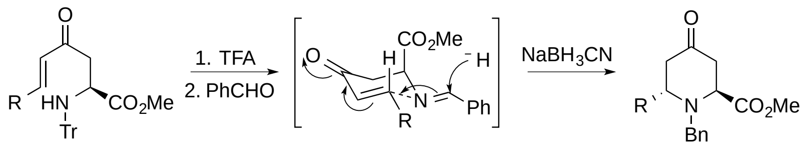
New Molecular Imaging Agents for Neurological Receptors

To gain a better understanding of many neurodegenerative diseases and various types of cancer, we are currently involved in a major collaboration with scientists from the departments of clinical physics/medicine and the Beatson Institute of Cancer Research to image various neurological receptors.[2] Our part in this project is to synthesise new compounds based on known affinity agents incorporating an iodine atom for SPECT imaging or fluorine atom for PET imaging. A typical project in this area would involve the multi-step synthesis of compounds such as new quinoline-2-carboxamides for the imaging of the translocator protein (TSPO) in stroke patients. Key steps during such a synthesis would involve quinoline ring synthesis, Suzuki reactions and metal catalysed halogen exchange reactions.[3]

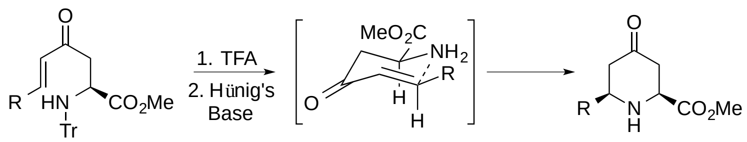


6-Endo-Trig Cyclisations For The Synthesis of Pipecolic Acid Derivatives

A recent project has led to the development of a rapid and highly efficient synthesis of enone derived α-amino acids. These compounds have been shown to be good substrates for a one-pot reductive amination/6-*endo-trig* cyclisation to give 2,6-*trans*-6-substituted-4-oxo-L-pipecolic acids.[4] The stereochemical outcome of the cyclisation step was rationalised by a Zimmerman-Traxler chair-like intermediate, which placed the R-group and the *N*-substituent in a pseudoequatorial position.



Based on this, it was proposed that a more direct 6-*endo-trig* cyclisation without a substituent on the nitrogen atom would result in an alternative chair-like reacting conformer where the R-group and ester moieties would be pseudoequatorial resulting in 2,6-*cis*-substituted compounds. As predicted, a one-pot process involving *N*-trityl deprotection followed by Hünig's based mediated cyclisation gave the desired *cis*-diastereomers very cleanly and in good overall yields.[5] Current projects in this programme of research seek to demonstrate the use of these compounds as general building blocks for the preparation of more complex targets.



Students working in the group will receive excellent training in all aspects of practical synthetic chemistry and will become familiar with a wide range of analytical and spectroscopic techniques for characterising all products.

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Femtosecond spectroscopy in the liquid phase

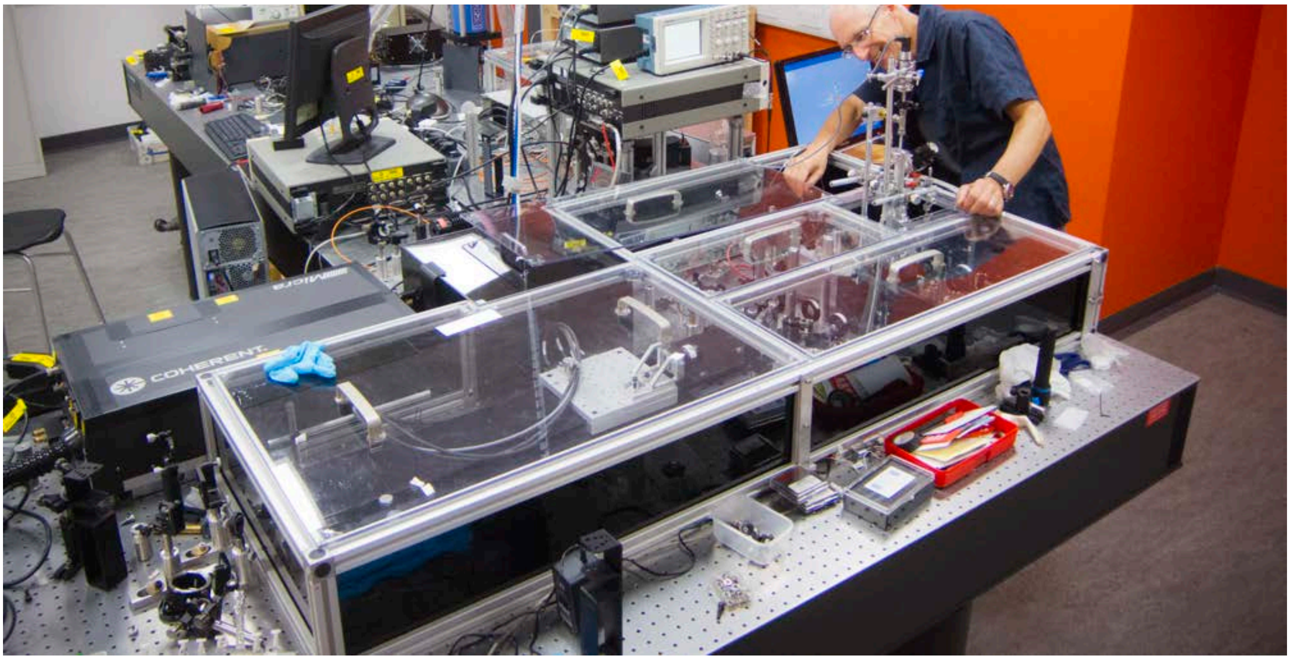
In the Ultra{fast/slow} Chemical Physics (UCP) group, we are interested in the dynamics and structure of liquids, solutions, proteins (treated as amorphous blobs), and phase transitions. These dynamics range from femtoseconds to kiloseconds. One of the techniques we use to study the femtosecond dynamics is called optical Kerr-effect (OKE) spectroscopy. To make a long story short, OKE measures a signal in the time domain using a pair of femtosecond laser pulses and the Fourier transform of this signal is proportional to the anisotropic Raman spectrum of the sample. With our set-up, we can carry out measurements from 20 fs to ~1 ns corresponding to frequencies from 1 GHz to ~10 THz. The UCP lab has two OKE set-ups, which are currently used by one PhD student and two postdocs.

The project

You will learn about femtosecond lasers, optics, and time-resolved experiments. You will assist with the collection of data and can analyse data independently for a project report. For the data analysis, it would be very advantageous if you have appropriate computer skills.

Option 1: Liquids and solutions. One of the on-going experimental programmes involves the study of liquids and solutions [1] and in particular the effects of (pre)nucleation. Depending on how the research develops over the summer, you would be likely to study metastable supersaturated solutions with the aim to find evidence of pre-nuclei or possibly some room-temperature ionic liquid [2] with the aim to find optical phonon in a liquid.

Option 2: Dynamics of biomolecules. One of the other on-going programmes involves the study of biomolecules such as proteins and DNA. [3] We have discovered that both of these molecules can support acoustic and optical-phonon like modes that are likely to play a role in biochemical function. Again, by the time of the project you would be likely to be involved with a study of some protein.



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Sample Excursions

Summer 2016

(SUM16) LUSS HIGHLAND GAMES & THE HILL HOUSE

THEME: ACTIVE SCOTLAND, CREATING & IMAGINING SCOTLAND

The Hill House, high on a hill in Helensburgh overlooking the River Clyde, will be our first stop on the excursion. The Hill House is universally regarded as Charles Rennie Mackintosh's finest domestic creation with a visually arresting mix of Arts and Crafts, Art Nouveau, Scottish Baronial and Japonisme architecture and design. Mackintosh designed nearly everything inside the Hill House, along with his wife, Margaret Macdonald, who designed and made many of the textiles as well as a beautiful fireplace panel. Much of the house has been restored so it looks almost exactly as it did in 1904 when its first residents, Glasgow publisher Walter Blackie and his family, moved in.

In the afternoon the coach will drive to Luss, a village situated on the western shore of Loch Lomond, to watch the Luss Highland Games. The games began in 1967 to promote tourism by a group of local businessmen in the Balloch area. Today the games are known to be one of the top three Highland Games in all of Scotland and even includes over £15,000 in prize money. The traditional events include Running, Cycling, Wrestling, Tug o War, Tossing the Caber, Weight over the Bar, Throwing the Hammer, Ball and Weight and the Highland Dancing.

(SUM16) CEILIDH DANCE

THEME: CREATING & IMAGINING SCOTLAND

Ceilidh is the Gaelic word for a visit or gathering, a ceilidh (pronounced kay-lee) once involved a gathering of friends who sang, told stories, played music, recited poetry or debated the topics of the day, creating their own evening's entertainment. A modern-day ceilidh usually involves Scottish country dancing to traditional Scottish folk music. The ceilidh will be taking place at Summerhall, the former Royal School of Veterinary Studies in Edinburgh and now a creative hub for the arts, with a band and a caller who will teach the dances.

(SUM16) THE GOLF OPEN CHAMPIONSHIP

THEME: ACTIVE SCOTLAND

The Open was founded by pioneering golfers who had one guiding principle - to crown the Champion Golfer of the Year. Since 1860, The Open has been played over some of the world's most cherished links courses and has produced a remarkable legacy of great champions. It is the oldest and most international championship in professional golf and the Claret Jug - first presented in 1873 - is one of the most iconic trophies in all of sport.

From earlier greats such as Harry Vardon, Bobby Jones, Henry Cotton and Walter Hagen through modern legends such as Jack Nicklaus, Arnold Palmer, Tom Watson, Gary Player and Seve Ballesteros to exceptional talents of today, Tiger Woods, Phil Mickelson and Rory McIlroy, the greatest players in the world have faced the unrelenting challenge of The Open for more than 150 years.

This year, the open will be taking place at Royal Troon, founded in 1878 and is renowned as one of the greatest links courses. This year hosts some fantastic players including; Rory McIlroy, Zach Johnston, Ben Curtis, Phil Mickelson and many more. We will be heading to Royal Troon on the very last day of the Open Championship, therefore witnessing the finale and hand over of the trophy.

(SUM16) MUSIC BY MAIRI CAMPBELL

THEME: CREATING & IMAGINING SCOTLAND

Viola player and singer/songwriter, Mairi Campbell is an influential and pioneering figure in Scottish music. Her music has a rooted and powerful quality and her musical interests are wide ranging from playing Scottish dance music, to pushing the boundaries of the traditional music scene, and even singing the 'Auld Lang Syne' in the film Sex in the City.

(SUM16) CRAIGMILLAR CASTLE

THEME: ORIGINS

Craigmillar Castle is a 15th Century medieval stronghold located on the edge of Edinburgh. Originally built around an L'plan tower, the castle expanded over the 16th century to include private rooms and a great hall. The castle, gardens and pastureland was used as a home for over 250 years. It played an important part in the life of Mary Queen of Scots. It was here at Craigmillar Castle the plot to kill her husband, Lord Darnley, developed after she fled to the castle following Rizzio's murder. In the beautiful grounds you will also find two historic Yew trees situated at the entrance that are believed to have been used to make bow and arrows. Spectacular views of East Lothian from the high ramparts of Edinburgh's other castle.