Dial-a-Molecule

An EPSRC Grand Challenge network

Directed Assembly of Extended Structures with Targeted Properties

D E T A S P

An EPSRC Grand Challenge Network

Launch Meeting

Your chance to take a leading role in shaping the future for chemical & material synthesis in the UK

20th October 2010

The ICC, Birmingham

EPSRC

Engineering and Physical Sciences Research Council

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Vision: In 20-40 years, scientists will be able to deliver any desired molecule within a timeframe useful to the end-user, using safe, economically viable and sustainable processes.

Synthesis of molecules is both a central driver for, and a serious constraint in a myriad of research disciplines, associated industries and other grand challenges. Recently a pan-industry report on synthetic chemistry in the healthcare environment stated that "when synthetic enablement is lacking, we see projects stall, even those with the best biological or clinical rationale". Emerging challenges in fields such as (nano)materials, chemical biology and next-generation healthcare pose synthetic problems that are beyond the scope of existing technologies.

The UK has a strong, internationally leading chemical industry generating huge revenue for the exchequer but is experiencing significant and growing pressures from competitors in the emerging economies. It is vital that UK retains a vibrant presence in this sector, and this can only be achieved by leading in the area of generation of new intellectual property. A critical bottleneck to progress is the availability and time taken to synthesise target molecules which **Dial-a-Molecule** aims to address, helping secure the future economic health of the sector.

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Vision: To control the assembly of matter with sufficient certainty and precision to yield materials and molecular assemblies with far more sophisticated and tuneable properties and functions than currently accessible.

Focus: Develop the ability to "design" a condensed phase material with a desired function and then to "engineer" that material, using molecular and materials building blocks in a fully controllable manner.

Value: In the current socio-economic environment it is apparent that the chemical sciences will be central in the drive for cleaner, more efficient energy sources and in solutions to issues of environmental pollution and global warming, while also underpinning advances in healthcare and global security. Fundamental to all these issues is a deeper understanding of how processes occur at the molecular and nanometre level, how this knowledge may be applied to generate materials with particular properties across all the size scales from molecules to bulk materials, and how these materials may find applications in modern society that will be of benefit to all. The **DAESTP Grand Challenge** tackles just these ambitious targets.

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Dial-a-Molecule & DAESTP Joint Launch Meeting

Time	Event	Hall
9.30 - 10.30	*Coffee and Registration*	Foyer Lower Level, Foyer Upper Level
10.30 - 11.40	*Welcome and Introduction to the Grand Challenges* Andrew Bourne **EPSRC**, Richard Whitby **Dial-a-Molecule**, David Hollinshead **AstraZeneca**, Paul Raithby **DAESTP**, Bob Docherty **Pfizer**.	Hall 5
11.40 - 12.30	*Plenary Lecture* **Dial-a-Molecule: Can Flow Chemistry Help?** Prof. S. V. Ley, FRS	Hall 5
12.30 - 13.30	*Lunch break*	All Foyers
13.30 – 14.00	*Question&answer session about Dial-a-Molecule and DAESTP Grand Challenges*	Hall 5 (Dial-a-Molecule) Hall 7 (DAESTP)
14.00 – 14.30	*Group discussion about the themes of Dial-a-Molecule and DAESTP*	Hall 7(DAESTP) Hall 8 (Dial-a-Molecule)
14.30 – 15.00	*Group discussion about the themes of Dial-a-Molecule and DAESTP*	
15.00 - 15.30	*Coffee break*	All Foyers
15.30 – 16.00	*Group discussion about the themes of Dial-a-Molecule and DAESTP*	Hall 7 (DAESTP) Hall 8(Dial-a-Molecule)
16.00 – 16.20	*Discussion break*	
16.20 - 17.10	*Plenary Lecture* **Chemical Control of Extended Structures – Grand Challenges and Opportunities** Prof. M. J. Rosseinsky, FRS	Hall 5
17.10 - 17.30	*Concluding remarks and next steps*	Hall 5

The organizing committee would like to thank the following companies for their sponsorship of the event:

- ✓ ACD Labs
- ✓ Sigma Aldrich
- ✓ Vapourtec

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Flow Chemistry - the next big discovery

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SIGMA-ALDRICH

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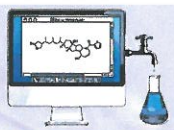
www.dial-a-molecule.org



How can we make molecules in DAYS not YEARS?

Network Themes

Synthetic route selection

- **T**he capability to predict how well a particular transformation will work is crucial.
- **H**ow can we best to use data on reaction outcomes to predict success and optimum conditions for proposed transformations?
- **H**ow can we collect and make available high quality data on reaction outcomes in the future?
- **C**an theoretical methods usefully predict reaction outcomes under real conditions?
- **W**ith reliable predictions on individual steps AI systems could be used to determine optimum synthetic routes to compounds under variable constraints.

Lab of the future

- **T**he equipment we use to carry out synthesis must develop if the aims of **Dial-a-Molecule** are to be achieved.
- **R**eactors which allow easy capture of full information on reaction conditions, and good repeatability.
- **F**lexible modular reactors capable of adapting to the problems posed.
- **R**eactors (flow or batch) and work-up/purification systems designed to be used in sequence.
- **R**eal time monitoring of reaction compositions enabling smart "self-optimisation".

Catalytic paradigms for 100% efficient synthesis

- **C**atalysis is key to achievement of **Dial-a-Molecule**. The fundamental conflicts between scope, activity and selectivity have to be tackled.
- **N**ew approaches to selectivity in catalysis (e.g. shape or electronic-surface recognition elements for regiocontrol).
- **C**ross-compatibility in catalysts for multi-catalyst processing (including chemo/biocatalytic cascades).
- **M**ultifunctional catalysts for sequential reactions;
- **F**orced chemocatalyst evolution;
- **P**hase-separation of catalysts for sequential processing.

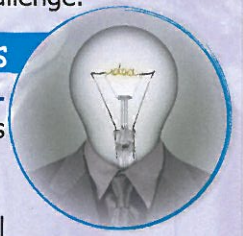
A step change in molecular synthesis

- **C**hallenges us to develop new strategies and methods in molecular synthesis.
- **T**oolbox of ultra-robust processes designed for sequencing.
- **H**olistic approaches to targets - cutting loose from the 'disconnection' approach.
- **R**eagentless synthesis
- **A**bolition of work-ups.
- **E**ngineered/evolved enzyme systems.
- **S**ynthetic Biology.
- **P**hase separation of substrates and reagents.

Aims of the network

- **F**orm new research communities directed at **Dial-a-Molecule** that extend beyond chemistry and chemical engineering and involve academia, industry and users.
- **I**dentify research priorities and the major barriers associated with them.
- **D**evelop community driven research agendas in the area of the Grand Challenge.
- **I**dentify the major societal and economic benefits associated with the Grand Challenge and widely disseminate the information in an accessible way.
- **D**rive a step change in the ambition of scientists involved in molecular synthesis encouraging highly innovative approaches with the potential to transform the subject.
- **E**ncourage and facilitate grant applications in the area of the Grand Challenge.
- **P**rovide routes to maximize UK commercial benefit from the Grand Challenge.

Tools



- **A** set of workshops and meetings to develop the ideas of **Dial-a-Molecule**, and to facilitate the formation of groups to tackle aspects of the Grand Challenge.
- **A** website describing the challenge and a forum for engagement.
- **E**ngagement of other disciplines with the chemistry/chemical engineering community.
- **C**lose co-operation with industry.

Outcomes

- **A** clear roadmap identifying priorities, bottlenecks and intermediate targets with justification for the Grand Challenge.
- **E**ngagement of policy makers (politicians, funding bodies, professional bodies) and scientific community in the Grand Challenge. **D**evelop a strategy to engage the wider public.
- **I**dentification of any areas which are crucial for the Grand Challenge but need targeted investment to develop.
- **F**ormation of groups actively applying for funding to tackle aspects of the Grand Challenge.

Structure

Overall management of the network and long term view of development is done by the **Grand Challenge Steering group** (GCSG). The network is structured around an advisory group and 4 themes. Each is lead by a steering group but with open membership.

The **Focusing our efforts** advisory group will have a predominantly industrial representation. It will guide priorities in developing the roadmap to maximise early stage (commercial) return. It also facilitates the crucial two-way flow of information between academia and industry. Users, manufacturers of molecules and companies involved in the supply of equipment and software to facilitate synthesis should be involved.

Directed Assembly of Extended Structures with Targeted Properties

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www.daestp.org.uk

Network Themes

Controlling the assembly of designed molecular frameworks and hybrid materials with targeted properties

Outline Target: To develop a better understanding of how the assembly process works in molecular framework and hybrid materials. Impact will be in energy and sustainability including gas storage, fuel cell and battery materials. The aim is to make complex materials architectures accessible and controllable.

Core Network Champions: Ward, Raithby, Rosseinsky

Controlling nucleation and crystallisation processes leading to the design of physical forms of pharmaceuticals with pre-targeted properties

Outline Target: Elucidation of the fundamental physics and chemistry that governs the structure of the nucleation transition state. Impact will be in pharmaceutical and other industries, including energy, food & drink, dyes & pigments and others. Improving processes for production of crystalline and microcrystalline solid-state materials.

Core Network Champions: Wilson, Price, Roberts

Controlling the molecular self-assembly in biological and biomimetic systems

Outline Target: To develop biomimetic methods to achieve some of the special selectivities that enzymes display. Impact will be in health and therapy, drug delivery, energy and sustainability through optimised membrane and other biologically-inspired systems. New approaches to making biologically-active materials, harnessing the power of biology in creating and optimising chemically-important processes will be developed.

Core Network Champions: Hunter, Wilson, Yaliraki

Controlling surface-based molecular self-assembly for applications in interface science

Outline Target: Building large volumes of nanostructured, self-assembled materials in three dimensions. Impact in creating novel materials with electrical, magnetic and switchable properties, with tailored nanoscale architectures to optimise desired physical characteristics. The aim is to move molecular self-assembly into longer length scales, retaining and enhancing control of growth processes.

Core Network Champions: Jackson, Makatsoris, Roberts, Ward

Developing self-optimised chemical systems through self-evolution

Outline Target: An intelligent integration approach in which pre-organised arrangements of chemical building blocks are brought together spontaneously to form nanostructures or larger arrays with a particular functionality. Impact will be in rational materials design, towards automated optimisation of materials for a given property - "Dial-a-Property". The aim is to harness the power of modern computational and algorithmic approaches together with ideas of self-assembly and evolutionary chemistry.

Core Network Champions: Yaliraki, Jackson, Makatsoris, Price

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Welcome to the launch meeting of the Directed Assembly Grand Challenge Network.

We are very pleased that you are able to join us at the beginning of an enterprise that we hope will shape the development of aspects of scientific research over the next several decades, and will strengthen the interactions between academics, industrialists, policy makers and the general public.

The network aims to form new research communities, drawing from Chemistry, Chemical Engineering and other disciplines, involving academia, industry and end users of research. Within these communities we will develop agendas for transformative research focussed on scientific impact, societal and economic issues, and together create a road map to identify priorities and tackle the barriers to achieving our goals.

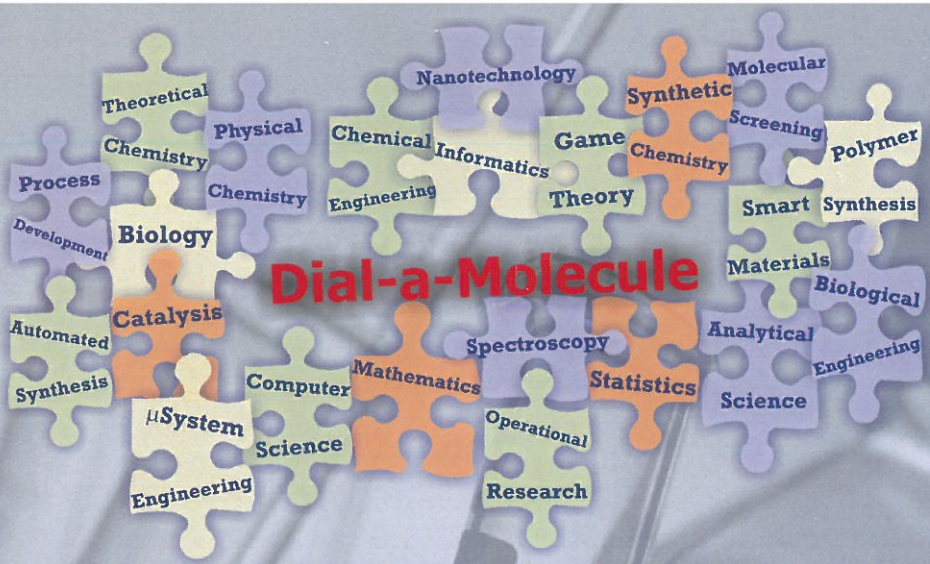
We hope that you will find it valuable to become a part of this network - it will provide you with opportunities for collaboration and knowledge exchange, creating new links between academia and industry. It will enable you to draw on shared knowledge to tackle problems and will use your input to drive the agenda for research funding.

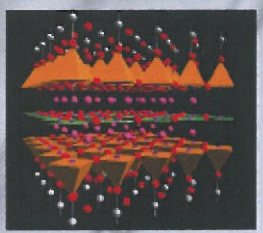
We have many planned activities to aid working together, from face-to-face meetings such as this, through to virtual interactions on the website we are creating. Working together in open meetings we will create our road map for taking the challenge forward and working in virtual space we will create a centre of excellence where ideas can be exchanged and collaborations fostered. Our research and its outcomes will be promoted through workshops with industry, through a series of Grand Challenge lectures delivered to universities and through outreach to the public and schools.

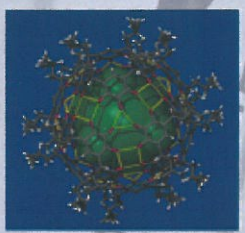
We look forward to meeting you at this launch event and working with you in future.

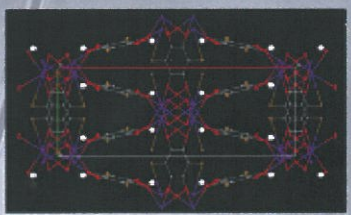
Paul Raithby
George Jackson
Matthew Rosseinsky
Sophia Yaliraki
Harris Makatsoris
Sally Price
Michael Ward
Neil Hunter
Kevin Roberts
Chick Wilson

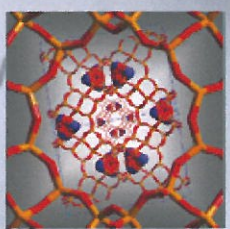
The Core Network Group

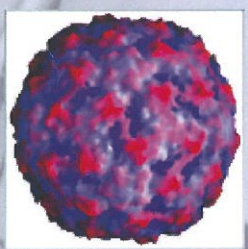












Enquiries and further information on the Networks

Dial-a-Molecule

Coordinators:

Prof. Richard Whitby
Prof. Steve Marsden
Prof. David Harrowven

Assistant: Dr. Bogdan Ibanescu

http://www.dial-a-molecule.org
dial-a-molecule@soton.ac.uk

DAESTP

Network Champions:

Prof. Paul Raithby
Dr. Harris Makatsoris

Network Coordinator: Dr. Jenny Woods

http://www.daestp.org.uk
enquiries@daestp.org.uk

Designed by Bogdan Ibanescu