Dial-a-Molecule

An EPSRC Grand Challenge Network

NETWORK UPDATE

Autumn 2012

A very warm welcome to this edition of the Dial-a-Molecule newsletter. The newsletter has been intermittent in the last few months but this is no reflection on network activities. Most notably after submission to EPSRC in November last year, the Dial-a-Molecule Roadmap has been published and network funding has been extended by 3 years. Also covered in this newsletter are funding opportunities, the first Annual Dial-a-Molecule meeting and the Using Synthetic Biology to Dial-Molecule meeting.

HAVE YOUR SAY: *If you wish to include an item in a future edition of this newsletter please contact the Network Coordinator Susanne.*

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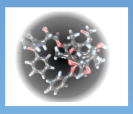

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New Coordinator for Dial-a-Molecule Network

The eagle-eyed will have noticed a slight change in the look of the newsletter – an indication of a more significant change for the network: On 1st September the new coordinator, Dr Susanne Coles, started work at the University of Southampton. Susanne takes over from Bogdan Ibanescu, who left for a job at AkzoNobel at the end of April. Our best wishes go to Bogdan in his new job and we thank him to for his efforts over the past two years. Unfortunately it has proven impossible to maintain our main website and Susanne is currently working on implementing the needed changes. In the interim please refer to our _Connect web presence, reachable via http://www.dial-a-molecule.org.

Dial-a-Molecule Roadmap: The Grand Challenge defined

On 2nd July 2012 the Dial-a-Molecule Roadmap was formally published as the result of a true community effort derived from many discussion meetings and community consultations throughout most of 2011. The outcome of this consultative process is a 52-page technical description of the Dial-a-Molecule Grand Challenge, which identifies key objectives and actions to be taken. It also details the steps required in the three theme areas to overcome the challenges. There has been a strong industry presence at many of the theme meetings which have shaped the roadmap and an industry "Focusing our Efforts" group has been convened several times to steer and direct some of the key outputs of the roadmap.

It is hoped that the roadmap will act as a stimulus to research and development in areas that will enable huge economic and scientific benefits.

This is reflected in the objectives for the second round of funding of Dial-a-Molecule. The aim is to establish a sustainable Grand Challenge community until March 2015 and raise the profile of Dial-a-Molecule in all areas of society. Through delivering some of the 'near term' objectives of the Dial-a-Molecule Roadmap it is hoped that economic and societal impact from the Grand Challenge can be achieved.

Further information on the roadmap is available on the website. If you are interested in becoming involved or are looking for collaborations in the Grand Challenge area, please contact the network coordinator Susanne Coles.

In 20 to 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.

Dial-a-Molecule Grand Challenge – key challenges

Lab of the Future/Synthetic Route Selection				A Step Change in Molecular Synthesis		Catalytic Paradigms for Efficient Synthesis		
Optimum Reaction and Route Design	The Smart Laboratory	Next Generation Reaction Platforms	Rapid Reaction Analysis	Stepwise perfection (1000 Click Reactions)	Holistic approach to molecular synthesis	New reactivity: target-driven catalysis	Intervention-free synthesis	Engineering control through understanding
Need for high quality reaction data	Electronic Laboratory Notebooks	Reactor Platforms	Equipment development – into the lab.	Establish criteria for 'perfection'	Tandem & telescoped reactions: generalising the concept	Efficient transformations across chemical space	Phase-separated catalysts	Rapid (self)-optimisation of reactions
New ways to analyse reaction data to predict unknown outcomes	Automated and high throughput equipment for synthesis	Intelligent Feedback Control	Software development – automation of expert tasks.	Establish an inventory of reactions required & with potential for automisation	Rational design & implementation of catalysts for multicompo-nent reactions	Complexity-building reactions	Mutually compatible catalysts	Full elucidation of catalytic mechanisms
Planning of synthetic routes subject to constraints	The intelligent fume cupboard	Microfluidics and Lab-on-a-chip	Equipping academia – overcoming the cost barrier.	Reagentless "*zero-emissions*" transformations (energy driven & catalytic)	Determining the reactions needed and priorities in targeting new chemical space	Sustainability: feedstocks	Switchable catalysts	Theoretical chemistry: through understanding to prediction
Theoretical prediction of reaction outcomes		Networks of reactors	Automatic identification of components of reactions	Understanding compatibility in complex systems	A framework to design redox-neutral processes	Sustainability: catalysts	Separation technology	
Active Study [illegible] isation of		Purification						

The Dial-a-Molecule Roadmap is available for download via the website.

"Dial-a-Molecule represents a fantastic opportunity for the UK's scientific community to come together and really understand how synthesis related opportunities can be understood, explored and exploited. The improvement in profile that Dial-a-Molecule gives the community for its capability, successes and challenge is crucial and as momentum builds this profile will grow. Dial-a-molecule will give the UK funding bodies confidence to fund in the key areas and equally importantly will improve the UK's European profile, to allow European funding to be secured by members of the network. The network strongly benefits both academia and industry and will allow strong, collaborative relationships to develop."
Dr Stephen Hillier, CIKTN

Opportunity: Funding available through Dial-a-Molecule

Dial-a-Molecule network members wishing to develop collaborations and grant applications in the Grand Challenge area can now apply for funding from the network. Four different types of support are available as detailed below. In order to quality for funding the applicant must be UK based and the application must be clearly aligned with the aims of Dial-a-Molecule as defined in the Roadmap. Normally the application is also expected to promote collaboration between two or more disciplines and/or institutions.

Interdisciplinary mobility fund.

This fund is aimed at promoting inter-disciplinary and academic-industry collaborations by funding travel and accommodation for short term visits and exchanges. These may involve several people and more than one visit. We expect a typical award to be £1-2000 and we aim to fund up to 40 exchanges over 3 yrs. Applications may be made at any time and we aim to turn-around in < 1 month. Payment will normally be made retrospectively on the submission of receipts and/or invoices and a short report.

Funded proof of concept studies.

The activity aims at providing seed funding for novel, early stage research critical for the development of the Grand Challenge, which cannot be funded in a timely manner from other sources, but will lead directly to grant applications. We will fund up to 3 months PDRA time (at 80% of FEC including indirect costs). Applications which leverage additional funding from other sources are particularly welcome, and the network will actively assist in looking for such additional support. We expect to make around 6 of these awards. Generally applications will be reviewed by the steering group in batches received by quarterly deadlines. The first deadline is Sept 30th 2012.

Funding for meetings.

We welcome proposals for meetings to fund, or co-fund. These may range from very small 'sandpit' type meetings of a selected group aimed at producing a specific grant application, to large 'open' meetings aimed at generating ideas and developing new collaborations in a defined area. Where needed we will also organise the meetings. Please discuss your proposal with the network coordinator.

Bursaries for Early Career Researchers (ECRs)

These will cover travel expenses and accommodation costs to allow ECRs to attend Dial-a-Molecule events. ECRs are defined as post-doctoral research fellows and academic staff in the first three years of their first academic appointment. Applications will be via meeting application forms.

Conditions of funding.

On completion of the funded exercise a short report on the work undertaken and the outputs suitable for public dissemination must be provided.
The applicant must identify themselves as a member of the EPSRC Dial-a-Molecule Network in any publicity, publication or further grant application arising from research supported by the funds.
We emphasize that Early Career Researchers are welcome to apply for funds in their own right.
Applications will be assessed through a light-touch peer-review system, managed by the network coordinator.

Dial-a-Molecule furthermore supports the development and delivery of educational activities at school, undergraduate and postgraduate level. Please contact the network coordinator for further details.

Further details and application forms are available from the Dial-a-Molecule website. For any queries on the Dial-a-Molecule funding opportunities please contact the network coordinator Susanne Coles.

1st Annual Meeting of the Grand Challenge Network: Warwick, 2nd July 2012

The **Dial-a-Molecule Grand Challenge Network** held its First Annual meeting on **2nd July 2012** at **University of Warwick, UK**.
Around 65 people gathered to hear about the progress of the Grand Challenge network so far and the opportunities resulting from the recently announced renewal of funding. The meeting also saw the Dial-a-Molecule roadmap formally published on the day with a number of presentations outlining key outputs from the three theme areas as well as future perspectives. In addition to these, ten short presentations were included highlighting projects in the various focus areas. The afternoon was dedicated to group discussions and the participants were asked to share and discuss their thoughts on how to achieve progress in different focus areas and move them forward to the next level. Some areas proved particularly popular such as:

Towards a national Electronic Laboratory Notebook.
Developing automated, real time reaction analysis.
Self-optimising reactors, reactions and catalysts.
Non-precious metal catalysts or ultra low-loading precious-metal homo- and heterogeneous catalysts.
Engineering and chemical solutions and tools for efficient phase-separation.
Reactor/catalyst design for routine catalyst separations.
Predicting the outcome of novel reactions.
Predictable generation of useful complexity.
Establishing a national service and regional centres for the high-throughput study of reactions.
Developing chemistry industry needs and will use. Why is industry slow to embrace new chemical reactions?

Dial-a-Molecule is working towards organising workshops and sandpit meetings to facilitate turning these ideas into actual proposals.

If you would like to get involved or simply learn more then please contact the network coordinator Susanne Coles.

Presentations on the day

The Dial-a-Molecule Network. The first two years, renewal funding, and aims for today (***Richard Whitby***)
Key Roadmap outputs from the theme areas (***Richard Whitby, David Harrowven, Steve Marsden***)
Roadmap economic impact and funding opportunities (***Stephen Hillier***)
EPSRC perspective and funding opportunities (***Alex Berry***)
The 'National Electronic Laboratory Notebook' initiative (***Richard Whitby***)
Towards freely accessible data: Automated extraction of reaction and spectroscopic data from thesis (***Peter Murray-Rust***)
Dial-a-Molecule and Synthetic Biology (***Joe Sweeney & David Hollinshead***)
Next Generation Reaction Platforms (***Harris Makatsoris***)
Reagentless Synthesis (***Andrew Russell***)
Materials Science and Dial-a-Molecule (***Mike Shipman***)
Barriers to the uptake of new reactions by industry (***David Fox***)
Inventing new reactions with impact (***Anne Horan***)
The 3D-fragment consortium (***Andy Morley***)
National Centre for Reaction study (***Richard Whitby***)

The presentations are available for download from the website subject to permission.

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Dr David Fox *(RSC)*
Dr David Hollinshead *(Consultant)*
Prof John Leonard *(AstraZeneca)*
Dr Harris Makatsoris *(Brunel University)*
Dr Peter Murray-Rust
Dr Andrew Russell *(University of Reading)*
Dr Gillian Smith *(Consultant)*
Prof Joe Sweeney *(University of Huddersfield)*
Dr Matt Tozer *(Peakdale)*
Prof Nick Turner *(Manchester University)*

Meeting Report: Using Synthetic Biology to "Dial-a-Molecule"

On 19th June 2012 the **Dial-a-Molecule Grand Challenge Network** ran a theme meeting at GSK, Stevenage. Nearly 70 people from academia and industry came together to explore "*Using Synthetic Biology to Dial-a-Molecule*". The day, showcasing the diversity of the field, ultimately sparked the debate what Synthetic Biology actually encompasses. The discussion and networking sessions identified the need for a definition of the Synthetic Biology potential in terms of Dial-a-Molecule and how synthesis can achieve maximum impact in the Synthetic Biology sphere.

The comments made at the meeting were subsequently taken into account in the production of the briefing document – a working group effort organised by Joe Adams (GSK) and Rebecca Goss (St-Andrews). The key aspects of this document are depicted below. Next is the incorporation of this document into the Dial-a-Molecule Roadmap: "*Nature has evolved to be capable of mediating many synthetic transformations and series of tranformations that synthetic chemistry alone is currently unable to achieve. By combining synthetic biology (in its broadest definition) with synthetic chemistry it will be possible to bring about a step change in accessing even complex designer molecules at will.*"

The efforts are certainly very timely with Synthetic Biology emerging as hot topic as reflected in the recent competition call "*Advancing the industrial application of synthetic biology*" by the Technology Strategy Board and a follow-up meeting is currently being organised for the beginning of next year.

If you would like to get involved in the Synthetic Biology initiative please contact the Network Coordinator Susanne Coles.

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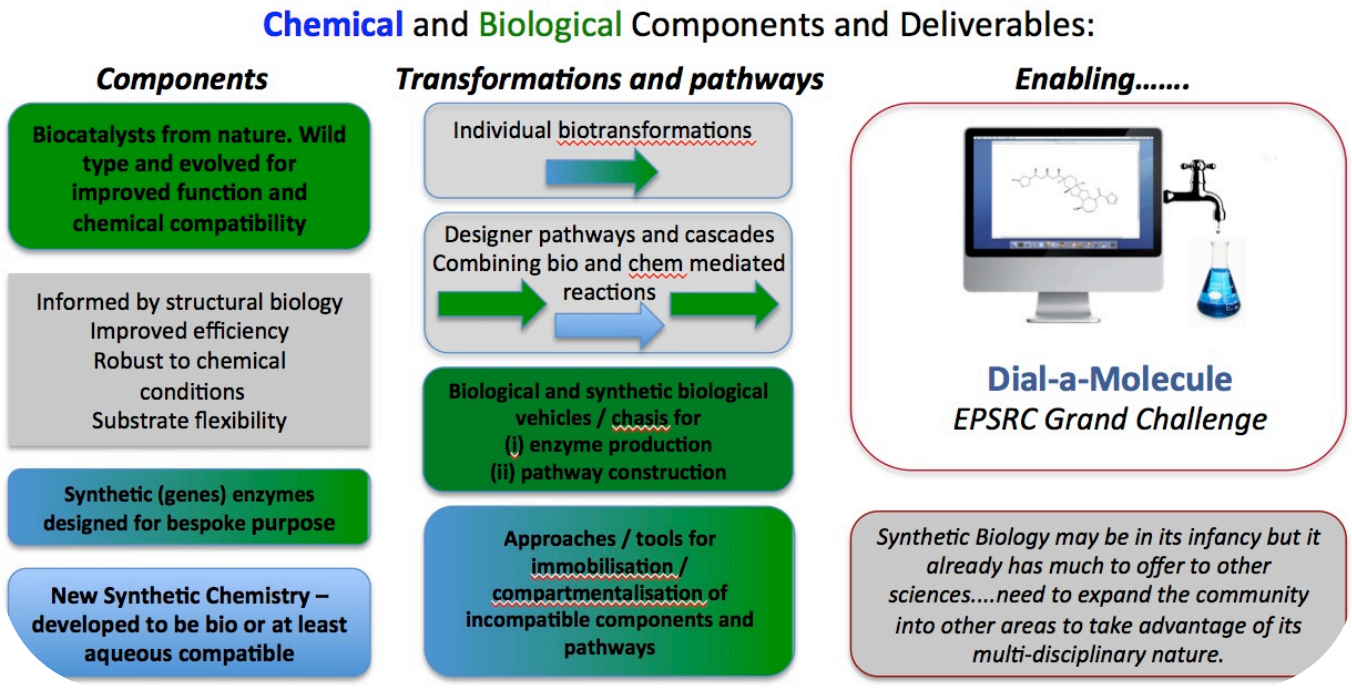

The meeting was realised with the generous support of EPSRC and GSK. The presentations are available for download from the website subject to permission.