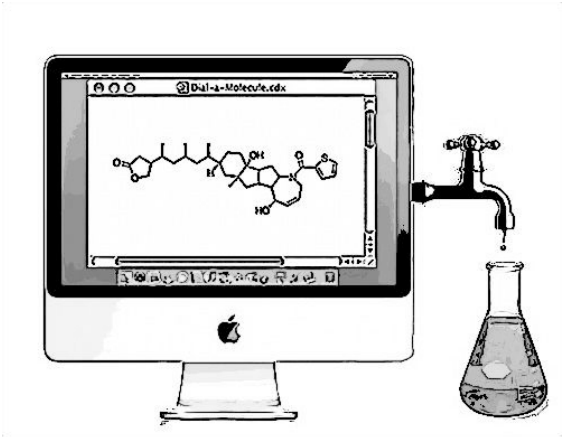
Dial-a-Molecule Grand Challenge

Vision: That 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.



Chemical Sciences and Engineering Grand Challenges

EPSRC Engineering and Physical Sciences Research Council

RSC | Advancing the Chemical Sciences

IChemE heart of the process

Chemistry Innovation Knowledge Transfer Network

Consultation: June 2008: 132 Proposals.

GC Workshop, Manchester, Nov. 2008: 13 areas.

GC Proposals, Jan 2009: 4 selected.

GC Network proposals, Sept 2009: 2 funded so far.

Start date Feb 2009. Running for 2 years.

Dial-a-Molecule

Aims of the network:

•To form new research communities directed at the 'Dial a Molecule' GC that extend beyond Chemistry and Chemical Engineering, and which involve academia, industry and users.

•To identify research priorities for the GC and the major barriers associated with them.

•To develop community driven research agendas in the area of the GC.

•To identify the major societal and economic benefits associated with the GC and widely disseminate the information in an accessible way.

•To drive a step change in the ambition of scientists involved in molecular synthesis encouraging highly innovative approaches with the potential to transform the subject.

•To encourage and facilitate grant applications in the area of the GC.

•To provide routes to maximize U.K. commercial benefit from the GC.

Dial-a-Molecule

Justification

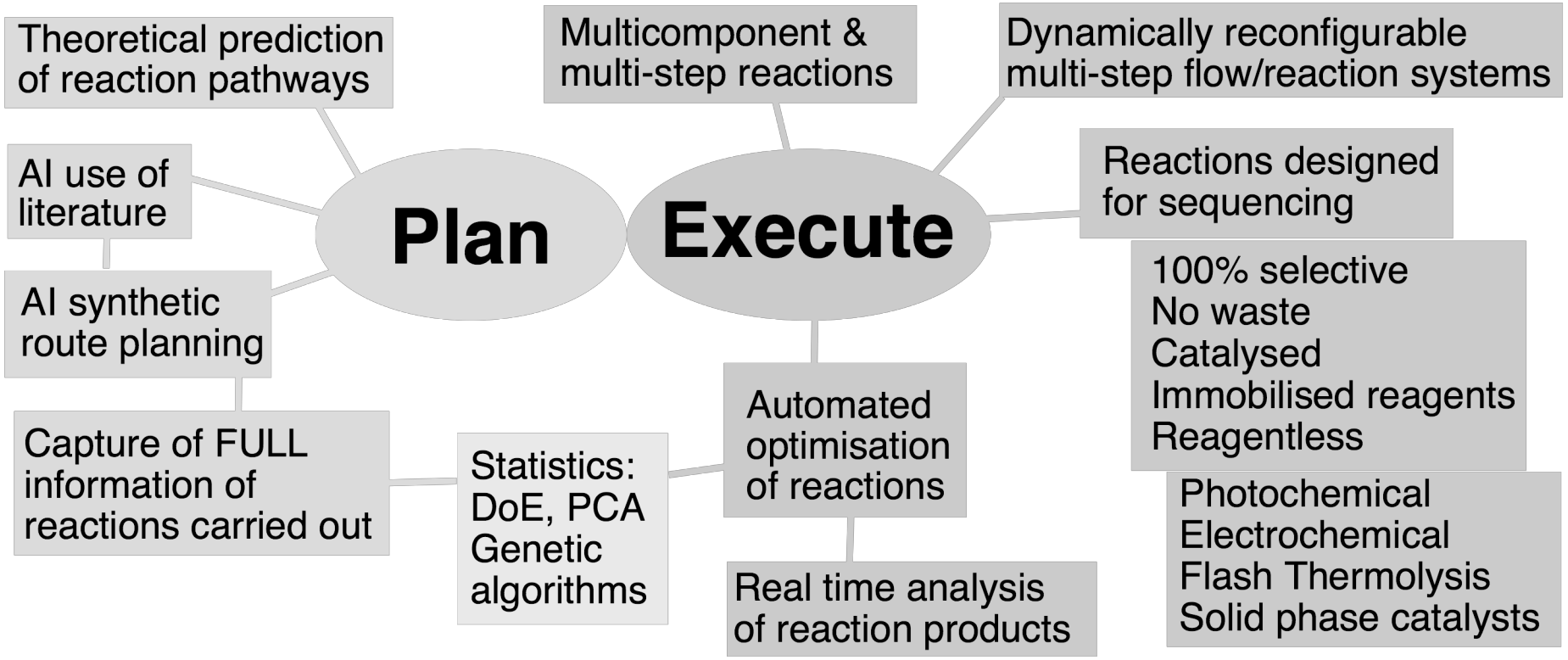
Drugs selective for one target.

Personalised Heath care

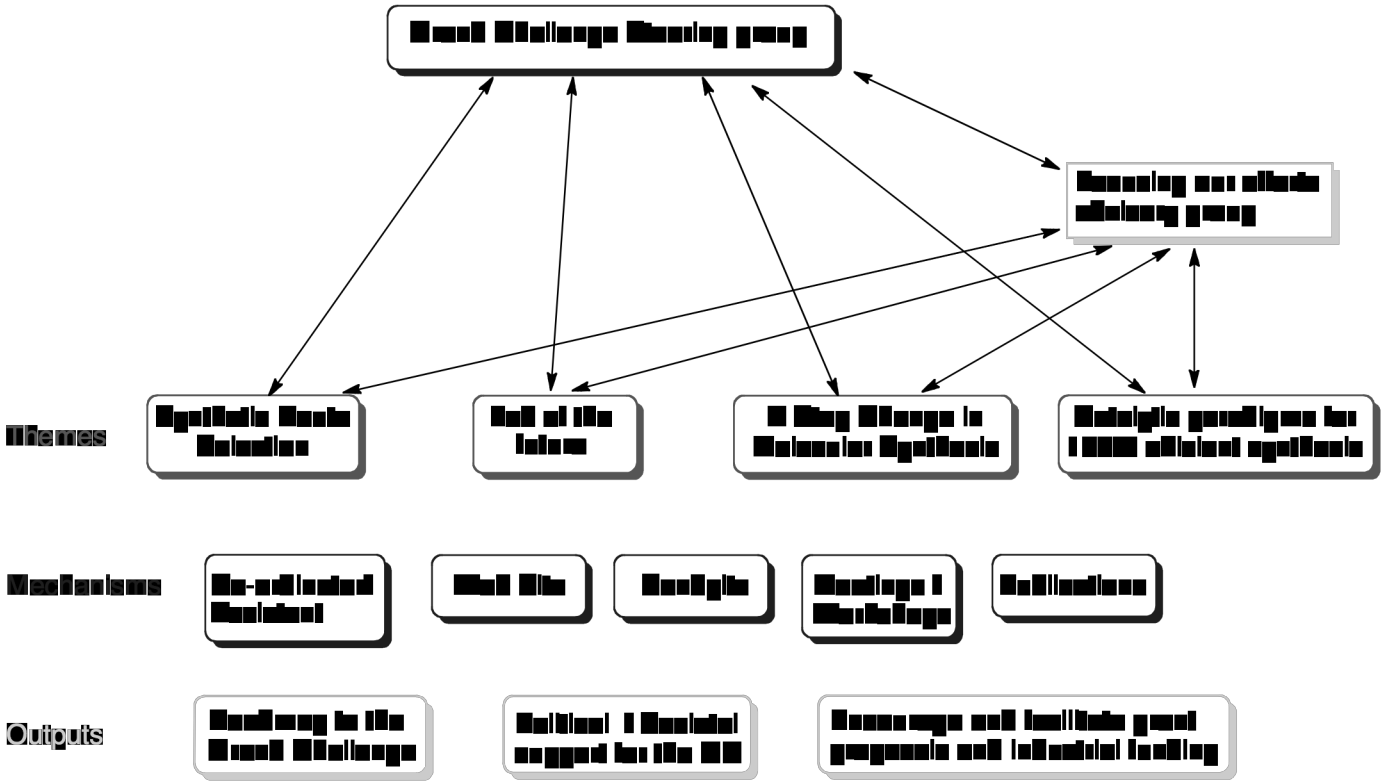
Molecular computers and nanobots

And a myriad of other applications

Dial-a-Molecule



Dial-a-Molecule



Dial-a-Molecule

Synthetic route selection

Reliable prediction of reaction outcomes
CAD of optimum Synthetic routes

Better ways of abstracting past data.
Capture full reaction information (ELN's).
Application of theoretical methods to real systems.
Common description of reactions.

Core Group: PI, Peter Murray-Rust (Unilever centre, Cambridge), Sophia Ananiadou (Manchester, National Centre for Text Mining), Jonathan Goodman (Cambridge), Stuart Macgregor (Heriot-Watt), Natalio Krasnogor (Nottingham), Jon Essex (Southampton DTC in Complex Systems Simulation).
Jeremy Frey, Simon Coles.

Computer science, mathematics (operational research, statistics), complexity, data mining, systems engineering, neuroscience, bioinformatics …

Dial-a-Molecule

Lab of the future

Carrying out reactions repeatably with full capture of information (ELN integration)

Auto optimisation of reactions:

Real time reaction composition analysis.

Sequencing reactions: flow, linked batch, in-line purification.

Modular reconfigurable / adaptable reaction systems.

Modelling - integration of reaction and reactor design

Core group: PI, Harris Makatsoris (Brunel), Asterios Gavriilidis and Giota Angeli (UCL), Sven Schroeder (Manchester), Ahmed al-Shamma'a (Engineering, Liverpool John Moores), Sue Lewis (Southampton Statistical Sciences Research Institute), Malcolm Berry (GSK), Chris Hayes (Nottingham).

Engineers (of all types – chemical, electrical/electronic, control, systems, microsystems), spectroscopists, computer scientists, synthetic chemists, statisticians, mathematicians, complexity scientists, biologists etc.

Dial-a-Molecule

A step change in molecular synthesis

Robust modular processes designed for sequencing.

Catalytic; Reagentless; No-work-up; 100% conversion.

Reactive fragments which can be ‘clicked’ together.

Holistic approaches to targets.

Chells as chemical factories

Dial-a-Molecule

Catalytic paradigms for 100% efficient synthesis

Highly selective catalysts with wide scope.

New approaches to selectivity.

Cross-compatibility in catalysts for multi-catalyst processing

Multifunctional catalysts for sequential reactions;

Forced chemocatalyst evolution.

Next generation Biocatalysts

Sequecing of catalysts (Chells as chemical factories)

Core Group: Steve Marsden, Graham Hutchings, Nick Turner, Mimi Hii, Paul Murray (AZ).

Dial-a-Molecule

The “Focusing our efforts” advisory group

Predominantly industrial representation and chaired by CIKTN.

Ensure that the long-term goals match societal and economic needs

Maximise early stage (commercial) return.

Route to industrial funding

Core group: Stephen Hillier (CIKTN, Chair), David Fox (Pfizer), David Lathbury (AstraZeneca), David Alker (SCI Fine Chemicals Group and RSC Industry and Technology Forum), Paul Raithby (from the “Directed Assembly of Extended Structures” Grand Challenge), John Carey (GSK), David Hollinshead (AZ) and Adam Russell (Syngenta).