

Imperial College  
London

**Centre for  
Rapid Online Analysis  
of Reactions (ROAR)**

The Dial-a-Molecule Grand Challenge Institute

Based at Imperial College's Molecular Science Research Hub in White City, **ROAR** offers **state-of-the-art facilities** to enable **data-centric research in synthesis**.

**ROAR** supports both **fundamental** and **translational research**, by providing protocols and tools to enable rapid execution and analysis of reactions, delivering effective solutions to **optimise reaction efficiency, selectivity, and robustness**.

## Our Mission

- Provide critical equipment and expertise to the synthesis community
- Pave the way for Synthesis 4.0
- Discover and develop the next generation of (automated) synthesis and analytical technologies
- Enable the UK to take leadership in the Molecular Sciences

# The Dial-a-Molecule Grand Challenge



**DIAL-A-MOLECULE**  
An EPSRC Grand Challenge Network

Advances in healthcare, agrochemicals, molecular electronics, smart materials and other chemistry-driven emerging fields are often limited by the **slow speed** and **inefficiencies** of molecular synthesis .

Implementation of **computing and automation** in chemical synthesis is an important and necessary tool to accelerate the rate at which we can synthesise target molecules.

**ROAR** is a centralised facility which provides the Dial-a-Molecule network with the **equipment and expertise**, including robotic platforms, continuous flow reactions, *in situ* and high-throughput analytical instrumentation, which are needed to achieve the goals of the Dial-a-Molecule Grand Challenge.

***‘How can we make molecules in days not years?’***

**Robotic reaction platforms for high-throughput parallel experimentation and screening**

**Online, *in situ*, data-rich kinetic experimentation platforms**

**Equipment and Expertise**

**Continuous flow reaction platforms**

**Advanced analytical suite for rapid orthogonal analysis of reactions**

## A Central Resource for the UK Chemistry Community

**ROAR** was created for the benefit of the UK's Dial-a-Molecule community. **50% of the facility time is dedicated to external projects received through open calls**, and selected by an internationally leading Scientific Advisory Group. Under the auspices of a £4.7 M investment from EPSRC, Imperial College London, and our industrial partners, the **ROAR** facility is fully-funded for the first 3 years, allowing us to reduce the access charges.

Calls for proposals will be released in phases as equipment is commissioned.

**Join our mailing list to receive invitations to our future calls!**

## Future-Proofing Chemists

Providing skills and training in data-intensive synthesis, including analytical science, automation/robotics, reaction engineering and mathematical/data analysis.

### Analysis

Analytical Tools, sensors, controllers, programming synthesis, data collection and curation

### Optimization

Data-mining, design-of-experiments, parallel experimentation, statistical and multivariate analysis, machine learning

### Technology

Reactor design, flow and batch chemistry, kinetic analysis, transfer processes, process intensification, LCA

### Understanding

Kinetic analysis and modelling, identify reactive intermediates, theoretical modelling of reaction pathways

## MRes in Advanced Molecular Synthesis

Our MRes in Advanced Molecular Synthesis trains students in designing molecules and synthesising them in an efficient manner on a meaningful timescale. This multidisciplinary programme combines a **9-month project of original research** with **courses and training** in the latest approaches designed to automate, analyse and understand synthetic processes. Through **ROAR** our students have access to **world leading facilities**, and an **expert training programme**.

Students gain a strong understanding of the rational design and efficient synthesis of organic and inorganic compounds alongside the knowledge needed to bridge the current technological gap between academic and industrial research laboratories.

## Partnering with Industry to Develop Next Generation Reaction Technologies: **Synthesis 4.0**

**ROAR** brings the academic and industrial communities together to develop the next generation of technologies in chemical synthesis, reaction analysis, laboratory automation and optimisation.

- A platform where equipment vendors and academic scientists can work together on product development.
- Closely linked with the Advanced Hackspace to enable researchers to turn their concepts into technologies by supporting feasibility studies and prototyping activities.
- A network of multidisciplinary researchers from chemistry, chemical engineering, bioengineering, mechanical engineering, mathematics and computing.

## Robotic Reactor Platforms

Three **Freeslate Junior** platforms for a wide range of automated laboratory operations.



### Dispensing Robot

- Automated dispensing and weighing of solids and liquids
- Up to 12 solid dispensing source vials for screening multiple solids
- Positive displacement liquid dispensing
- Analytical balance (0.1 mg resolution)
- Integrated camera for inspection of dispensed materials
- Static minimised by an ioniser
- In a purge box for inert atmosphere

### Optimisation Sampling Reactor Robot

- 8 parallel reactors (5-25 mL working volume) with overhead stirring
- Reaction sampling under pressurised conditions
- Independent temperature control from  $-20$  to  $200$  °C
- Independent gas pressure control from 30 to 400 psi
- Gas selection manifold
- In a purge box for inert atmosphere



### Screening Reactor Robot

- Six independent temperature zones capable of  $-20$  to  $180$  °C
- Magnetic tumble stirring in 96 well or vial format
- Automated liquid dispensing/aspiration
- Automated preparation of samples for analysis
- Reactions in vials (96 x 1 mL), jars (<math><125 mL) and plate formats
- Pressurised reactor format for screening 48 vial reactions at up to 300 psi

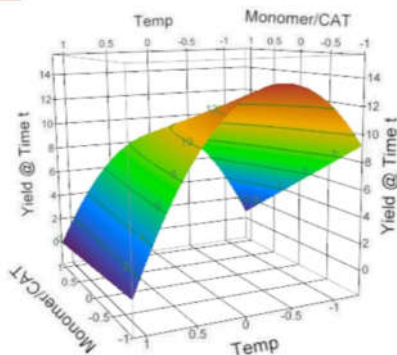
# High-Throughput Experimentation

## Optimisation of Continuous Variables

- Multivariate optimization using Design of Experiments (DoE)
- Solubility and crystallisation studies

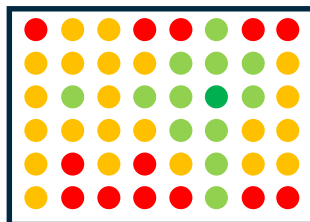
## Categorical Variable Screening

- Ligand, solvent and additive screening
- Full factorial screening
- 9 heated and stirred plate positions allowing up to 3,000 conditions to be screen in 384 well plates.
- Sparse arrays for larger experimental space
- Single or multiple substrate screening



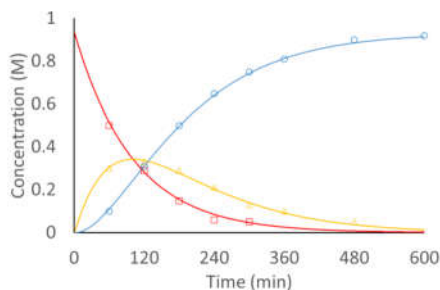
## High-Throughput Synthesis

- Diverse product sets preparation
- Large substrate scope studies
- Testing of multiple reaction conditions in substrate scope
- Reaction robustness screening
- Automation of individual operations (e.g. dispensing solids) to accelerate your research



## Small Scale Kinetics Investigations

- Streamlined initial kinetics in 8 parallel reactors with independent temperature and pressure control
- Automated sampling under pressure
- Possibility of gas uptake measurement



## What Do You Want to Automate?

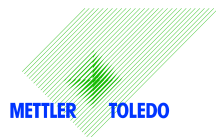
Our automation experts work with you to accelerate your research. We are there to support and teach you, from the initial planning of high-throughput experiments, right through to processing and understanding your results.

**Contact us to find out more about our automation capabilities!**

# Reaction Kinetics Platforms

**ROAR** has a suite of Mettler Toledo batch reactors and analytical tools which allow for orthogonal in-situ analysis of chemical processes, across scales (0.5 mL to 1 L). All our reactors have advanced temperature control (-40 to 180 °C) and automated dosing pump, can be operated with magnetic or mechanical stirring, and are compatible with multiple analysis techniques including:

- Automated sampling, quench and dilution with EasySampler probes
- In Situ IR spectroscopy with ReactIR 15 probes
- Heat flow calorimetry with the EasyMax 102 and OptiMax reactors
- Possibility of recording data from pH and other electrochemistry probes



## Two EasyMax 102 Reactors



## OptiMax Reactor



## Two EasySampler Probes



## Three ReactIR 15 Systems



## Example Experiments:

- Optimise and scale-up reactions, with full record of procedure and data
- Study reaction progression and measure kinetic parameters
- Investigate reaction intermediates and process impurities
- Monitor hazardous reaction species, and exothermic processes
- Operando studies of homogeneous and heterogeneous catalytic systems
- Collect high quality, synchronised data from a range of probes to maximise understanding of your reaction process

## Continuous Flow Reaction Platforms



- Commercial and custom-made flow reactors
- ThalesNano H-Cube Pro™ and Phoenix high temperature flow reactors
- Vapourtec R-Series automated flow reactor system
- Reaction scale up in flow
- Homogeneous and heterogeneous flow systems
- High temperature (< 450 °C) and pressure (< 200 bar) reaction conditions
- Photochemistry in flow
- Low temperature reaction conditions (> -40 °C)
- Fully Automated injection and fraction collection
- In-line analytics for the study of reaction intermediates and hazardous processes

vapourtec

### Phoenix



### R-Series



## Advanced Analytical Suite

**ROAR** is supported by a dedicated suite of analytical instrumentation for rapid orthogonal analysis of reactions, including two high-throughput LCMS systems.



### Agilent 1290II with 6530 QTOF MS

- Rapid UHPLC analysis
- High resolution accurate mass analysis
- 8 thermostated columns
- Multisampler with cooling (up to 6144 samples)
- DAD and QTOF MS detection

### Agilent 1260II Hybrid SFC/UHPLC with 6250 MS

- Automated switching between SFC and UHPLC
- Orthogonal method screening in a single system
- Multisampler with cooling (up to 6144 samples)
- DAD and MS detection

**ROAR** is also equipped with a **range of spectroscopy options** for the *in situ* analysis of processes. Please refer to the previous page for information about these *in situ* analysis tools.

Further analytical capabilities, including NMR spectroscopy, mass spectrometry and X-ray crystallography, are available within the Department of Chemistry Measurement Suite and the new Agilent Measurement Suite. Please contact us to discuss your analysis requirements.

## Get Involved

- Apply for access to the facilities at ROAR through a call for proposals
- Priority access to instruments is available to industrial users for a charge
- Check out our website for upcoming training and technology showcase events
- Want to showcase your technology to the chemistry community? Talk to us about hosting a training event

## Partners of ROAR

- Dial-a-Molecule Network
- Directed Assembly Network
- Institute of Process Research & Development (iPRD), Leeds
- Centre for Process Analytics & Control Technology (CPACT), Strathclyde
- EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing & Crystallisation (CMAC)

## Funding & Industrial Sponsors

**EPSRC**

Engineering and Physical Sciences  
Research Council

**Innovate UK**  
Knowledge Transfer Network

**syngenta**

**Dr.Reddy's**

**AstraZeneca**

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GlaxoSmithKline

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**Agilent**

**UNCHAINED  
LABS**

**THALESNano**

**vapourtec**

**jmp**

## Join Our Mailing List!

Join the ROAR mailing list to receive news of events and calls for proposals to access ROAR:

<http://eepurl.com/duaxZf>



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