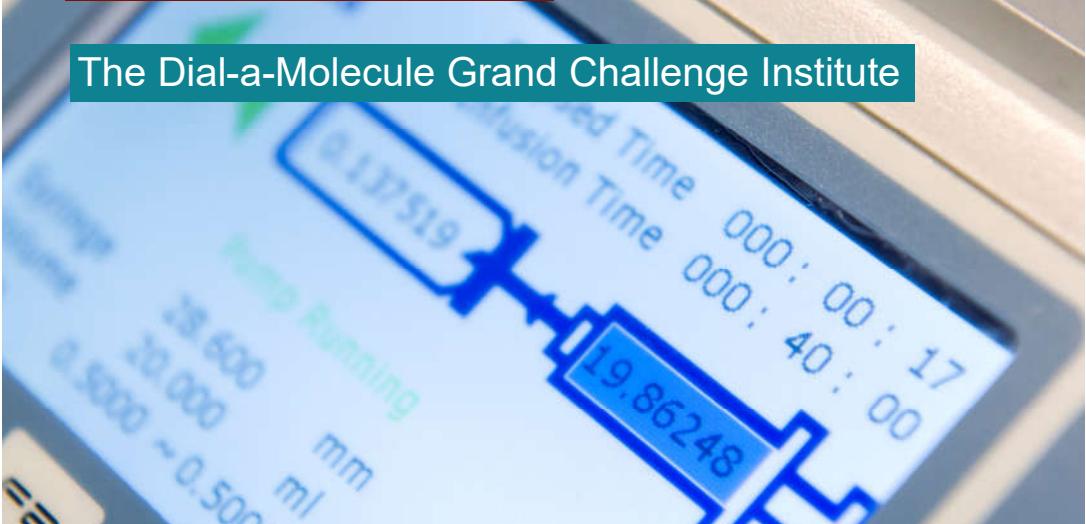


Centre for Rapid Online Analysis of Reactions (ROAR)

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



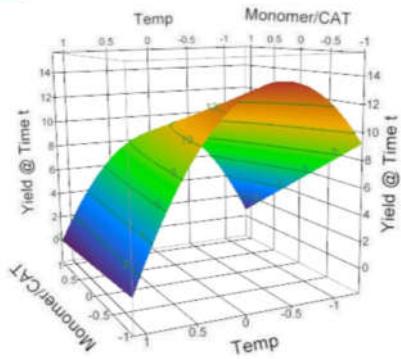
Screening Reactor Robot

- 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 (<125 mL) and plate formats
- Pressurised reactor format for screening 48 vial reactions at up to 300 psi

High-Throughput Experimentation

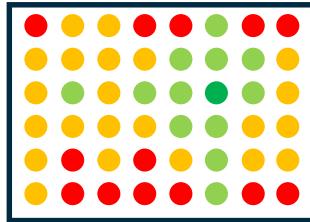
Optimisation of Continuous Variables

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



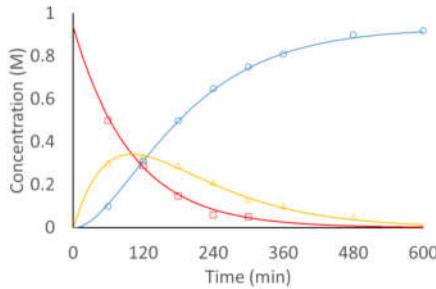
Categorical Variable Screening

- 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?

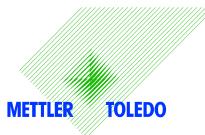
Our automation experts work with you to accelerate your research. We are there to support and teach you, from the initial planning of high-throughput experiments, right through to processing and understanding your results.

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



THALESNano

- 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



Engineering and Physical Sciences
Research Council



Knowledge Transfer Network



Procter&Gamble



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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