1st ICIQ High-Throughput Experimentation Symposium

Accelerating Synthetic Development: HTE, AI/ML and the Future of Autonomous Labs

ICIQ
Institute of Chemical Research of Catalonia

11-12 February 2025
Institut Català d'Investigació Química

The **1st ICIQ-HTE Symposium** will convene scientists from both industry and academia to delve into the latest advancements and applications of High-Throughput Experimentation (HTE), Lab Automation, and AI/ML in the realm of chemical synthesis. Participants will gain insights into HTE methodologies, Automated Synthesis, and engage in discussions on their integration with AI/ML.

Topics Covered

- HTE Application Examples
- HTE Methodology and Techniques
- AI/ML applied to Synthetic Chemistry
- Instrumentation for HTE Labs
- Lab Automation
- Establishing an HTE laboratory

Participant's profile

- Academy and Industry scientists.
- Scientists with or without experience in HTE techniques.
- AI/ML scientists looking for new applications of their knowledge.
- Scientists considering establishing their own HTE laboratory and looking for advice and ideas.
- Scientists looking for partners in the HTE field to complement and advance their research.
- HTE Experienced scientists looking for top scientific discussion opportunities with other scientists already working in HTE and related fields.

Day #1

Start	Finish	
13.00	14.30	**Registration**
14.30	15.00	**Xisco Caldentey (ICIQ).** HTE at ICIQ: Current capabilities and future directions.
15.05	15.35	**Fernando Bravo (ICIQ).** HTE applied to ICIQ's valorization and development activities.
15.40	16.10	**Alexander Dömling (Palacký University Olomouc).** HTE: From parallel mg to nanoscale synthesis, analytics, screening, to data capture, integration, and analysis.
16.15	16.25	**Carles Bo (ICIQ).** ioChem-BD: accelerating research in computational materials design
16.30	17.40	**Coffee & poster session.**
17.45	18.00	**Don Nguyen (Dotmatics Virscidian).** Analytical studio: From building experiments to analytical results.
18.05	18.45	**Laurent Lefort (J&J Innovative Medicine).** HTE and predictive models in process R&D at J&J. Plenary session sponsorized by Dotmatics Virscidian
18.50	19.20	**Catherine Holden (Exscientia).** From molecules to medicines: The automated synthesis revolution.
21.00	23.00	**Dinner**

Day #2

Start	Finish	
9.00	9.30	**Antonio M. Echavarren (ICIQ).** Discovering gold(I)-catalysis by HTE.
9.35	10.05	**Benjamin J. Deadman (Open Reaction Database, ORD).** Making your reaction data machine actionable with the Open Reaction Database.
10.10	10.40	**Philipp Holstein (Bayer Pharma).** Faster, higher, smaller: Continuous improvement of chemical HTE routines.
10.45	11.00	**Diego Esteban Fernández (Izasa Scientific).** Challenges and new tools in analytical instrumentation for HTE.
11.05	11.45	**Anat Milo (Ben-Gurion University of the Negev).** Data science strategies for designing and analysing experimental results. Plenary session
12.00	13.00	**Coffee & lunch**
13.05	14.05	**Santiago Cañellas & Harriet Fenton (J&J Innovative Medicine).** Automated high-throughput chemistry workflows in drug discovery at J&J. Plenary session
14.10	14.15	**Emilio Palomares (ICIQ Director)** Closing ceremony

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Agència de Gestió d'Ajuts Universitaris i de Recerca, AGAUR

Through the ioChemBD-EXPAND project (Ajuts innovadors 2022 INNOV 00019)

Carles Bo
Group Leader at ICIQ

Prof. Carles Bo graduated in Chemical Sciences from the University of Barcelona in 1986, and completed a Master's degree in Homogeneous Catalysis in 1988 at the Chemistry Faculty in Tarragona. He obtained his PhD from the Rovira i Virgili University in 1992 for the development and implementation of computational codes for the Topological Analysis of Electronic Density under the supervision of Prof. J. M. Poblet. He obtained a Profesor Titular de Universidad position in 1995. Later, he did a postdoctoral secondment in the group of Prof. Baerends in Amsterdam, during which he actively contributed to the development of the ADF program, the leader in the implementation of the Density Functional Theory. He joined the Catalan Institute for Chemical Research (ICIQ) as a Group Leader in 2004. His research has been mainly characterized by the application and development of modern computational chemistry methods to the study of the electronic structure and properties of systems with transition metals (organometallic complexes and polyoxometalates), placing special emphasis on their applications in homogeneous catalysis and the solving of specific problems in close collaboration with experimental chemists. Since 2015 he has led the development of the ioChem-BD platform.

Fernando Bravo
Head of Knowledge and Technology Transfer at ICIQ

Head of the Knowledge and Technology Transfer and Industrial Projects Area of ICIQ since 2023. Dr. Bravo completed his PhD at the Rovira i Virgili University (1997-2000). After a postdoctoral stage at Emory University (2001-2003), Dr. Bravo was hired as a synthetic chemist in the chemical development department at GlaxoSmithKline Verona (Italy; 2003-2010), where he participated in various projects at different stages of development (from preclinical to registration and launch), and coordination of teams of development chemists. Dr. Bravo joined ICIQ in 2010 with the goal of creating and leading the CSOL unit until the year 2023, focusing on valorization of ICIQ's own technologies, as well as managing contract research projects with industry. In this role, he has supervised and formed part of the development team of about 40 valorization projects. Dr. Bravo has been the principal investigator in various regional, national, and international projects and has coordinated contract research projects with industrial partners, particularly related to the pharmaceutical sector. In particular, Dr. Bravo has applied his expertise in designing, optimizing, and scaling up synthetic routes in optimization and on-demand synthesis projects for pharmaceutical companies. He counts with > 30 publications, and 8 patent applications. Dr. Bravo holds the R3 accreditation from the AEI. Currently, he is the Head of Knowledge and Technology Transfer Department at ICIQ.

Xisco Caldentey
High-Throughput Experimentation Unit Manager at ICIQ

Dr. Xisco Caldentey obtained his PhD in Organic Chemistry from the University of Barcelona in 2010, focusing on Asymmetric Catalysis under the supervision of Prof. Miquel A. Pericàs. Following his doctoral studies, he worked as a project researcher at ICIQ contributing to the early stages of new drug development. In 2014 he assumed his current role as the Head of the CELLEX-ICIQ-HTE Unit within ICIQ's Scientific Core Facilities. In this role, he provides scientific and technical support to both ICIQ researchers and industry in implementing HTE for synthetic development. He has been involved in the development of microscale HTE platforms tailored to a diverse range of chemical experimental setups. These include platforms for photocatalysis, asymmetric catalysis, organocatalysis, transition metal catalysis, and reactions involving reactant gases. Furthermore, Dr. Caldentey has actively participated in numerous industrial and technology development projects in the pharmaceutical and agrochemical sectors.

Santiago Cañellas
Scientific manager at Johnson&Johnson Innovative Medicines

Dr. Santiago Cañellas currently leads the Parallel Medicinal Chemistry team at J&J Innovative Medicines in Toledo, Spain. Embedded within Therapeutics Discovery, his team focuses on accelerating medicinal chemistry programs through AI/ML-driven library design and automated high-throughput chemical synthesis. He also leads the Automated Chemistry initiatives for the Global CCCAP team (Chemistry Capabilities, Analytical, and Purification). Before joining J&J Innovative Medicines, he conducted academic research at the University of the Balearic Islands, the Institute of Chemical Research of Catalonia, and the University of Michigan, where he focused on developing new synthetic transformations and creating novel catalytic systems using continuous flow chemistry and high-throughput experimentation.

Benjamin J. Deadman
Program Manager and Reaction Data Evangelist, Open Reaction Database (ORD)

Dr. Benjamin J. Deadman is the Program Manager and Reaction Data Evangelist for the Open Reaction Database (ORD). He works closely with the synthetic and digital chemistry communities to support and encourage the sharing of organic reaction data in a structured format that enables downstream applications in computer-aided synthesis planning, reaction prediction, and other predictive chemistry tasks.

In addition to his role with the ORD, Ben also provides independent consultation and advanced training services in modern synthetic chemistry methods such as High-

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Throughput Experimentation (HTE), flow chemistry, in-situ reaction analysis and kinetics, and Design of Experiments (DOE).

Ben began his chemistry career in New Zealand with an MSc in Analytical Chemistry from the University of Waikato. In 2009 he moved to the University of Cambridge (UK) as a Commonwealth Scholar to pursue research in flow chemistry under the supervision of Prof. Steven Ley. After the completion of his PhD in 2013, he then moved to University College Cork (Ireland) to work with Prof. Anita Maguire as a Postdoctoral Research Associate of the Synthesis and Solid-State Pharmaceutical Centre (SSPC). 2015 saw Ben relocate to Imperial College London (UK) to do postdoctoral research with Prof. King Kuok (Mimi) Hii and Prof. Klaus Hellgardt on the application of electrochemically generated oxidants in organic synthesis. Then in 2018 he established the Centre for Rapid Online Analysis of Reactions (ROAR), a shared state-of-the-art facility providing the UK chemical R&D community with the tools and protocols needed to perform data-rich experimentation in chemistry. As the founding Facility Manager of ROAR, Ben used his experience in reaction automation and reaction analysis to support the facility users throughout their adventures in data-rich chemical synthesis experimentation.

Alexander Dömling

Professor at Palacký University Olomouc (UPOL)

Professor Alexander Dömling studied Chemistry and Biology at the Technical University of Munich, where he was profoundly influenced by his PhD advisor, Ivar Ugi, and his postdoctoral mentor, double Nobel Laureate Barry Sharpless. His dynamic career has spanned several countries and esteemed institutions, including academic positions at the Technical University of Munich in Germany, the University of Pittsburgh in the USA, the University of Groningen in the Netherlands, and most recently at Palacký University Olomouc (UPOL) in the Czech Republic. His current research endeavors are supported, i.a., by two of the most prestigious EU grants: the ERA Chair ACCELERATOR and the ERC Advanced Grant AMADEUS.

As a serial entrepreneur, Professor Dömling has founded several startup companies, including his latest venture, AMADTEUS GmbH. His lifelong scientific interests center on multicomponent reaction (MCR) chemistry and its applications, particularly in innovative drug discovery. In 2018, he introduced the use of acoustic droplet ejection (ADE) technology in synthetic organic chemistry to automatically synthesize thousands of novel molecules per day at the nanoscale. He is now building a comprehensive technological framework around ADE to automate and miniaturize synthetic chemistry, leveraging big data to accelerate the pace of scientific discoveries.

Antonio M. Echavarren

Group Leader at ICIQ

Prof. Antonio M. Echavarren obtained his PhD from the Universidad Autónoma de Madrid (UAM, 1982). After a postdoctoral stay at Boston College, he joined the UAM as an Assistant Professor in 1984. Following a two year period as a NATO-fellow at Colorado State University, he joined the Institute of Organic Chemistry of the CSIC in Madrid. He returned in 1992 to the UAM as a Professor of Organic Chemistry. He is also Professor of Research of the CSIC since 2004. He moved in 2004 to Tarragona as a Group Leader at the Institute of Chemical Research of Catalonia (ICIQ). He has published more than 315 papers and has supervised 66 Doctoral Thesis, 48 Master Thesis and 70 Postdocs. He has been awarded with the Gold Medal of the RSEQ (2010), the Arthur C. Cope Scholar Award (2015), the Enrique Moles National Award in Chemical Science and Technology (2022), the 2023 RSC Organic Chemistry Pedler Prize, and the 2023 Rei Jaume I Award in Basic Research. He received two ERC Adv.Grants (2013 and 2019) and is President of the Spanish Royal Society of Chemistry.

Diego Esteban

Chromatography and Mass Spectrometry Specialist at Izasa Scientific.

Dr. Esteban studied Chemistry and carried out his PhD in Universidad Complutense de Madrid. After working as scientist in the Spanish National Laboratory for the Analysis of Food, he worked as post-doctoral researcher in Humboldt Universitaet zu Berlin. From 2016 he works in Izasa Scientific as Chromatography and Mass Spectrometry specialist.

Harriet Fenton

Associate Scientist at Johnson&Johnson Innovative Medicines

Harriet Fenton currently supports Medicinal Chemistry programs through library design, automated high-throughput chemical synthesis, and reaction optimization via high-throughput experimentation (HTE). Before joining J&J Innovative Medicines, she earned her Master's degree in Chemistry from Durham University in 2019 and completed an industrial placement at AkzoNobel Packaging Coatings. In 2020, she joined the High-Throughput Experimentation Team at Pfizer R&D, where she contributed to the design and optimization of synthetic routes in late-stage drug development. By using HTE and Bayesian optimization, she identified robust, high-yielding, and cost-effective processes. Harriet also developed and utilized advanced robotics to fully automate reaction screening, execution, and sampling, enabling continuous operations seven days a week.

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Catherine Holden

Associate Director of Automated Synthesis at Exscientia

Dr. Catherine Holden read chemistry at the University of Oxford and then pursued her PhD in organic chemistry at the University of Manchester under the supervision of Prof. Mike Greaney, focusing on innovative synthetic methodologies. Subsequently, she undertook postdoctoral research at the Institute of Chemical Research of Catalonia (ICIQ) in Spain with Prof. Melchiorre, specializing in photochemical synthesis technologies. A Marie Curie fellowship led to a pivotal industrial stay at Syngenta UK, after which Catherine advanced to lead teams in Crop Protection Research and Automation Chemistry. Catherine's professional endeavours are driven by a commitment to new technologies to enable molecular synthesis. Currently, as Associate Director of Automated Synthesis at Exscientia, Catherine is at the forefront of revolutionising drug discovery through encoding and automating chemical synthesis, embodying the company's vision of transforming the way the world discovers medicines.

Philipp Holstein

Medicinal Chemist and HTE lead, Catalyst Screening Laboratory at Bayer Pharma

Dr. Holstein obtained his PhD from Université Claude Bernard Lyon 1 in 2014, focusing on asymmetric Pd-catalyzed C(sp3)-H activation under the supervision of Professor Olivier Baudoin. Following his doctoral studies, he joined the group of Professor Antonio M. Echavarren at ICIQ (Spain). During his postdoctoral studies he investigated the mechanisms of Au-catalyzed cyclopropanation reactions. It was at that time at the ICIQ, that he was introduced to high-throughput screening for catalyst identification.

In December 2015, he joined Edelris in France, where he gained his first experience in medicinal chemistry. At Edelris, Dr. Holstein initiated the application of photocatalysis and implemented photo-flow chemistry for scale-up processes. In 2021, he returned to Germany and assumed his current role at Bayer Pharma as a medicinal chemist and HTE lead in the Catalyst Screening Laboratory. In this position, he supports organic chemists across all divisions and project stages at Bayer with HTE studies for identification of new synthetic routes and optimizing established reactions.

His interests include the development of new catalysts, rationalizing screening design, and catalyst selection based on physicochemical properties, as well as accelerating HTE using machine learning.

Laurent Lefort

Senior Principal Scientist in High-Throughput Experimentation at J&J Innovative Medicine

Dr. Lefort obtained his PhD at the University Henri Poincare in Nancy, France. Afterwards, he spent two years as post-doctoral research associate in Organometallic Chemistry in the group of Pr. William D. Jones at the University of Rochester, NY, USA – sponsored by a grant from Elf-Aquitaine, and a year as post-doctoral fellow in Surface Organometallic Chemistry in the group of Pr. Jean-Marie Basset, Laboratoire CPE-COMS, CNRS, Lyon, France – sponsored by a grant from BP Chemicals. From 1999 to 2003 he worked as research scientist at Symyx Technologies, a start-up specialized in high- throughput experimentation, located in the Silicon Valley, Santa Clara, California, USA. Later on, he worked during four years as Project leader/Senior R&D chemist (Small Molecules Synthesis) in DSM Pharma (The Netherlands). From 2019 until now he is Senior Principal Scientist in High-Throughput Experimentation (Chemical Process R&D - API Small Molecule Development) at J&J Innovative Medicine, Beerse, Belgium. He is author of more than 60 publications, 17 patents and 5 book chapters.

Anat Milo

Associate Professor at Ben-Gurion University of the Negev

Anat Milo received her BSc/BA in Chemistry and Humanities from the Hebrew University of Jerusalem in 2001, her MSc from UPMC Paris in 2004 with Berhold Hasenknopf, and her PhD from the Weizmann Institute of Science in 2011 with Ronny Neumann. Her postdoctoral studies at the University of Utah with Matthew Sigman focused on developing physical organic descriptors and data analysis approaches for chemical reactions. At the end of 2015 she returned to Israel to join the Department of Chemistry at Ben-Gurion University of the Negev, where her research interests are focused on physical organic chemistry that combines experimental, computational, and statistical strategies to identify design principles behind molecular functionality, reactivity, and selectivity.

Don Nguyen

Senior Scientist at Dotmatics Virscidian

Dr. Nguyen graduated in Chemistry and carried out his PhD in University of California, San Diego, focused in mass spec tool and method development for natural products discovery, characterization, metabolomics, and genomics. As post-doctoral researcher at the European Molecular Biology Laboratory in Heidelberg, Germany, he worked combining traditional LC-MS approaches with high spatial resolution imaging mass spectrometry, subcellular metabolomics, and optical microscopy technologies. Later on, he took a position as Lab Head at Merck Healthcare, Darmstadt, Germany, working in automated and integrated high-throughput MS-based screening for small molecule drug discovery. Currently, he works as Senior Scientist with Dotmatics Virscidian, LLC, implementing automated analytical workflows.

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Poster submission

We encourage symposium participants to submit abstracts for posters related to the conference topics.

This is an excellent opportunity to showcase your research and engage with fellow attendees.

» **Poster Format:** Portrait, DIN A0 size.

» **Submission Deadline:** 1st February 2025.

Please, submit your poster abstact to: iciqhtesymposium@iciq.es

Registration

Regular participant:

» Dinner included: 120 €

» Without dinner: 80 €

ICIQ participant

» Dinner included: 100 €

» Without dinner: 60 €

Registration deadline: 1st February 2025

How to arrive

ICIQ is located in the Avinguda Països Catalans, nº 16, 43007 Tarragona

» **By Car**

ICIQ has a very small parking lot. For this reason, we recommend you to park in the adjacents streets.

» **By Taxi**

Tarragona has many taxi stands around the city. You can also get a taxi by calling to the following taxi companies: Taxi Tarraco (+34 642 269 752), Agrupació de Ràdio-Taxis de Tarragona (+34 977 221 414) and Tarragona City Taxi Service (+34 693 30 30 50).

» **By Bus**

Tarragona's bus station is at the Imperial Tarraco Square (for further information you can call +34 977 214 475). Plana company operates the route Barcelona-Tarragona (for information you can call +34 977 214 475).

» **By Train**

Trains from different origins stop at Tarragona's station. For more information visit RENFE's website.

» **By High Speed Train**

If you are coming from Barcelona, Madrid or Zaragoza you can take the AVE up to the Camp de Tarragona Station, which is 9 km far from the ICIQ. For further information you can visit RENFE's AVE website.

» **By Plane**

The nearest airport to ICIQ is Reus Airport, 7 km far from Tarragona. From there you can get to the ICIQ by taxi or bus. Barcelona's airport is 90 km far away. You can get to Tarragona from Barcelona airport by taxi or bus.

» **ICIQ transport**

There are different bus lines from the city centre (5, 41 and 54) that go to Sant Pere i Sant Pau, Sescelades Campus (where ICIQ is located). The nearest bus stops are the ones called "Educacional N-240" or "Joan Serra".

For further information check the "Empresa Municipal de Transports Públics de Tarragona" map or contact them at (+34) 977 549 480.

Accommodation

HOTEL PLAÇA DE LA FONT*

Plaça de la Font, 26, 43003 Tarragona
+34 977 240 882

HOTEL URBIS***

Plaça Corsini, 10, 43001, Tarragona
+34 977 240 116

HOTEL LAURIA***

Rambla Nova, 20 , 43001, Tarragona
+34 977 236 712

HOTEL SB EXPRESS TARRAGONA***

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AC HOTEL TARRAGONA****

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HOTEL SB CIUTAT DE TARRAGONA****

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