



DISCOVERY TECHNOLOGIES 2021

EARLY DRUG DISCOVERY
STRATEGIES

9TH & 10TH NOVEMBER
ALDERLEY PARK CONFERENCE CENTRE,
CHESHIRE

#ELRIG

#ELRIGDT21

#DISCOVERYTECHNOLOGIES

 elrig.org

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ABOUT ELRIG

The European Laboratory Research & Innovation Group (ELRIG) is a leading European not-for-profit organization that exists to provide outstanding scientific content to the life science community. The foundation of the organisation is based on the use and application of automation, robotics and instrumentation in life science laboratories, but over time, we have evolved to respond to the needs of biopharma by developing scientific programmes that focus on cutting-edge research areas that have the potential to revolutionize drug discovery.

Comprising a global community of over 12,000 life science professionals, participating in our events, whether it be at one of our scientific conferences or one of our networking meetings, will enable any of our community to exchange information, within disciplines and across academic and biopharmaceutical organisations, on an open access basis, as all our events are free-of-charge to attend!

OUR VALUES

Our values are to always ensure the highest **quality of content** and that content will be made readily **accessible to all**, and that we will always be an **inclusive** organisation, serving a **diverse scientific network**. In addition, ELRIG will always be a **volunteer led** organisation, run by and for **the life sciences community**, on a **not-for-profit** basis.

OUR PURPOSE

ELRIG is a company whose purpose is to bring the life science and **drug discovery** communities together to **learn, share, connect, innovate and collaborate**, on an **open access** basis. We achieve this through the provision of world class conferences, networking events, webinars and digital content.

GOVERNANCE

ELRIG's board is comprised of volunteers from it's community, who either work in biopharma, CRO's, academia or with vendor companies. The board is steered by the General Committee, who act as a direct connection to the community and thus is comprised of a diverse group of people. The board delegates its tasks to a series of work groups, who work with the Operational Team to ensure ELRIG achieves its objectives. Current work groups are:

- Early Career Professionals
- Marketing Communications
- Networking & Webinars
- People & Culture
- Publications
- Science Strategy
- Vendor Outreach

STRATEGIC PILLARS



EVENTS

Deliver UK leading events, showcasing cutting edge science and technology, that are accessible to all.



EQUALITY, DIVERSITY & INCLUSIVITY

Promote inclusivity, engagement and collaboration, in our diverse community.



PRESENCE & AWARENESS

Expand and enhance our digital presence.



SUSTAINABILITY

Drive an open and transparent organisation, with a focus on delivery excellence and financial sustainability.

WELCOME TO DISCOVERY TECHNOLOGIES 2021

As Scientific Program Chairs it is our great pleasure to welcome you to Alderley Park, Alderley Edge for an in-person Discovery Technologies 2021 meeting.

With the rapid advancement of new technologies, the potential for developing life changing therapeutic interventions has never been so promising. With these possibilities new challenges arise, not least how to prosecute drug discovery campaigns against new and novel targets and those previously deemed intractable. This conference will explore evolving early drug discovery technologies to overcome these obstacles by focusing on three core themes:

- **Emerging Discovery Strategies:** Historically drug discovery efforts largely focused on traditional target classes such as enzymes, GPCRs and nuclear receptors and aimed to modulate them via binding of small molecules or monoclonal antibodies. Whilst largely successful and still extremely relevant, it's believed a large proportion of the human proteome, whilst may present valid targets, may be undruggable by these traditional approaches. Other valid targets are difficult to prosecute discovery campaigns against with the current technologies available. To continue to address unmet medical need, the discovery process needs to unrelentingly evolve and innovate. Emerging Discovery Strategies will focus on these developing areas showcasing examples of identifying and utilising new target classes, drug modalities and the parallel development of novel screening strategies. We'll also consider how exploitation of big data integrated with machine learning can help drive discovery efforts to new heights.
- **Mass Spectrometry & Biophysical Approaches in Early Drug Discovery:** Recent years have seen increasing use of mass spectrometry (MS) and other biophysical methods alongside more traditional high throughput screening technologies in the search for target modulators and binders. They provide a direct assay readout, often with no labels or other reporters, and are therefore less susceptible to artefacts that can adversely affect other technologies. These methods can detect formation of covalent and non-covalent protein-ligand complexes and are not necessarily reliant on enzyme activity. As such they offer a route to screen targets that are catalytically inert, and are also able to detect ligand binding to regions of a protein other than the active site. They are therefore applicable to screen for novel therapeutic modalities such as PROTACs and RNA binding, as well as providing a means to directly screen covalent libraries. There are an increasing number of proteins emerging from genomics initiatives with strong rationale as drug targets for which biophysical screening approaches are desirable, so the demand for them is likely to grow. In this session application of various MS and biophysical methods for biochemical screening including covalent and non-covalent binding strategies will be discussed.
- **Hit Triage:** Small molecule screening has been a mainstay of hit identification and lead generation efforts for decades. Success is ultimately driven by a triumvirate of factors: reagents, chemistry and technology. Whether a cellular or biochemical approach is applied all reagents utilised need to be of high calibre and relevant for the disease target. The compound collection needs to be suitably diverse and of high quality. Finally the assay technology needs to be fit for purpose. Different technologies are impacted by varying assay artefacts that can result in false positive or negative results. If any of these three broad factors is suboptimal the potential success of the endeavour is diminished. This track will concentrate on the pitfalls that may arise due to the compounds tested and the assay technologies used. Many undesirable mechanisms exist to deleteriously enrich hit outputs and obscure the chemistry that projects should be focusing on. The content will include novel approaches for identifying metal contaminated and redox cycling compounds, the behaviour of nuisance compounds in cell painting studies and working examples of effective triage strategies.

As this event will take place face-to-face at Alderley Park, Alderley Edge, there will also be ample networking opportunities as well as an exhibition show-casing the technologies and their applications.

Our thanks go to all the Track Chairs and Speakers for their contribution, as well as the vendors who will be exhibiting; without their sponsorship, ELRIG would be unable to host events on an open access basis, ensuring they are free of charge to attend, for all. And a huge thank you to the ELRIG Operational Team. Clare Cockerham, Emma Zsadanyi, Sanj Kumar and Tara Shanks, who have ensured that this meeting happens in a timely and professional manner. And finally our thanks to you, the delegate, for attending, participating and contributing to this exciting area of drug discovery.

CONFERENCE DIRECTORS



Jarrod Walsh
AstraZeneca



Finn Holding
AstraZeneca



Gareth Davies
AstraZeneca



David Cronk
Domainex

ELRIG'S EQUALITY DIVERSITY AND INCLUSION AIMS AND GUIDING PRINCIPLES

OUR AIMS

- ELRIG will strive for cultural change, both for itself and the ELRIG community
- Rather than a policy we have developed the ELRIG Community's Guiding Principles
- We will communicate the journey and the conclusions
- The process and implementation of outcomes will be transparent
- Data and the ELRIG community will guide action
- Mechanisms will be put in place to ensure that accessibility is maximised at all events
- Guiding principles will be embedded in governance and all Work Groups daily activities

OUR GUIDING PRINCIPLES

We will promote equality, by welcoming all to all our events and will be inclusive, by removing barriers to access, and that our events will represent the diversity of the ELRIG community.

OUR EQUALITY PRINCIPLE IS:

We will ensure that all are welcome by: profiling the demographics of attendees by segment, age, ethnicity, disability and gender, monitoring and ensuring that no one group is favoured nor excluded and act to ensure equal outcomes and opportunities for the entire ELRIG community.

OUR DIVERSITY PRINCIPLE IS:

We will strive for gender balance at our events, by ensuring that the diversity mix of our speakers represents the diversity of our delegates, and that the diversity mix of our delegates represents the diversity of the ELRIG community, as well as ensuring that scientific content reflects the diversity of the ELRIG community.

OUR INCLUSIVITY PRINCIPLE IS:

We will ensure that accessibility is maximised at all events, by removing barriers to those with disabilities, limits on finances, caring and parental responsibilities, religious needs, geographical location and other requirements. To ensure our principles remain relevant, we will solicit, monitor, and report to the ELRIG community and act upon relevant feedback during and after events to maintain accessible and safe spaces in which to collaborate.

INFORMATION FOR PARTICIPANTS

REGISTRATION

To help keep Discovery Technologies 2021 COVID safe we will require you to observe the following registration process:

1. Pre-registration for the meeting is essential. Please register at elrig.org and enter our EventFlo registration system *(new for Discovery Technologies 2021, if you wish to, you may choose a pro-noun, which will be printed on your badge and don't forget to pre-register for our workshops, as spaces are limited)*
2. Print out your badge at home
3. To ensure we minimize the risk of spreading COVID, please have available one of the following:
 - Your COVID passport, which is a document issued by your local government showing you have been double vaccinated, for example for a UK resident, this is available via the NHS app. Either an electronic or paper QR code is acceptable and the passport must have your name printed on it and will be matched with your registration ticket.
 - A certificate showing that you have been tested in the last 72 hours and that you are negative for COVID infection. The certificate must have your name printed on it and will be matched with your registration ticket.
 - If you have neither of these we will direct you to a test center close by the venue.
4. Once you have entered the venue, you may wear a mask if you wish, but this is not compulsory. Also please choose a coloured lanyard to visibly demonstrate your comfort level.
 - Green - I am comfortable shaking your hand
 - Yellow - I am being cautious with social contact
 - Red - I am keeping my distance

WIFI

Wi-Fi is freely available throughout the venue and may be found by following the bellow instructions:

1. Enable the wireless function on your device
2. Connect to the APCC (wireless network)

ELRIG MOBILE APP

Download the free ELRIG app and access all our conference information, programme and more from your phone or tablet.

- View the event programme
- View presentation and poster abstracts
- View speaker profiles
- View the exhibitor guide
- View the delegate and exhibitor list
- Organise your day with your own favourites list
- Share your profile as vCard and QR Code and scan exhibitor QR code information tags
- Network – contact delegates, other exhibitors and speakers easily through opt-in directories and integration with Linked-In, Twitter and Facebook

You can download the ELRIG app by visiting the app store appropriate to your tablet or smart phone, scanning the QR code below or visiting the ELRIG website:

elrig.org/mobile-app



Please note that ELRIG authorised photographs and videos will be taken throughout the duration of the meeting, which may then be used for promotional purpose after the event. If you do not wish your image to be used, please let the organisers know. The taking of your own

photographs or making your own recordings is strictly forbidden, unless it is needed to help your accessibility to the presentations. The event is cashless and free! All beverages and food served at ELRIG's Discovery Technologies meeting is freely available to all who attend.

TRACK SUMMARY

EMERGING DISCOVERY STRATEGIES

9th November 2021
The Auditorium

Historically drug discovery efforts largely focused on traditional target classes such as enzymes, GPCRs and nuclear receptors and aimed to modulate them via binding of small molecules or monoclonal antibodies. Whilst largely successful and still extremely relevant, it's believed a large proportion of the human proteome, whilst may present valid targets, may be undruggable by these traditional approaches. Other valid targets are difficult to prosecute discovery campaigns against with the current technologies

SESSION CHAIRS

Emily Offer
Medicines Discovery Catapult
Graeme Walker
Sygnature Discovery

available. To continue to address unmet medical need, the discovery process needs to unremittingly evolve and innovate. Emerging Discovery Strategies will focus on these developing areas showcasing examples of identifying and utilising new target classes, drug modalities and the parallel development of novel screening strategies. We'll also consider how exploitation of big data integrated with machine learning can help drive discovery efforts to new heights.

09.15-09.20	Alderley Park Welcome - Kath Mackay, Bruntwood SciTech
09.20-09.25	Conference Welcome and Keynote Introduction - Jarrod Walsh, AstraZeneca
09.25-10.15	Plenary Keynote - Advances in Phenomics Drug Discovery: Combining high content and pathway profiling technologies with multiparametric data analysis tools to discover novel and effective drug mechanisms-of-action - Neil Carragher, University of Edinburgh
10.15-10.30	Industry Insider Presentation - Craig Malcolm, Promega
10.30-11.15	Refreshment Break
11.15-11.20	Session Chair Introduction - Emily Offer, Medicines Discovery Catapult & Graeme Walker, Sygnature Discovery
11.20-11.50	An update on the JUMP-CP Consortium: insights from pilot experiments and outlook - Paula Marin-Zapata, Bayer
11.50-11.55	Bronze Sponsorship - Jon Stone, Benchling
11.55-12.25	Exploring natural product library (venoms) as novel sources of chemistry - Elaine Duncan, Charles River & Steven Trim, Venomtech Ltd
12.25-14.00	Refreshment Break - with poster session
14.00-14.30	Fragment-based screening coupled to chemical proteomics as an emerging paradigm for early drug discovery in ER+ breast cancer - Stephanie Constantinou, AstraZeneca & Aarti Kawatkar, AstraZeneca
14.30-14.35	Bronze Sponsorship - Tamsin Lamont, Collaborative Drug Discovery
14.35-15.05	The concept of G-quadruplex ligands as novel gene regulators and potential anticancer drugs - Stephen Neidle, UCL School of Pharmacy
15.05-15.35	Refreshment Break
15.35-16.05	Right assay, right hit, right time. Identify "more physiological hits" earlier in drug discovery - Kathy Dodgson, Aurelia Bioscience Ltd
16.05-16.35	Patient-derived cell models as a clinically-relevant drug discovery strategy - Gareth Griffiths, Imagen Therapeutics
16.35-18.30	Networking

TRACK SUMMARY

HIT TRIAGE

9th November 2021
The Helix Room

Small molecule screening has been a mainstay of hit identification and lead generation efforts for decades. Success is ultimately driven by a triumvirate of factors: reagents, chemistry and technology. Whether a cellular or biochemical approach is applied all reagents utilised need to be of high calibre and relevant for the disease target. The compound collection needs to be suitably diverse and of high quality. Finally the assay technology needs to be fit for purpose. Different technologies are impacted by varying assay artefacts that can result in false positive or negative results. If any of these three broad factors is suboptimal

SESSION CHAIRS

Gareth Davies
AstraZeneca
Kirsty Winn
Medicines Discovery Catapult

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11.15-11.20	Session Chair Introduction - Gareth Davies, AstraZeneca & Kirsty Winn, Medicines Discovery Catapult
11.20-11.50	Application of Acoustic Mist Ionisation MS to rapidly identify hits with undesirable mechanisms of action in HTS outputs - Rachel Moore, AstraZeneca
11.50-11.55	Bronze Sponsorship - Sharon Barnard, Integra Biosciences Ltd
11.55-12.25	Case studies in cellular nuisance compounds - Jayme Dahlin, NCATs
12.25-14.00	Refreshment Break - with poster session
14.00-14.30	Developing assay development tools to make screening less PAINS-full - Stuart McElroy, BioAscent
14.30-14.35	Bronze Sponsorship - Martin Main, Medicines Discovery Catapult
14.35-15.05	Computational and Empirical Strategies to Triage Nuisance Compounds in HTS - Sarah Martin, Charles River & Scott Maidment, Charles River
15.05-15.35	Refreshment Break
15.35-16.05	Hit or Miss? The Importance of Triage in the Active to Hit Transition - Alexandra Stowell, Sygnature Discovery
16.05-16.35	Pragmatic screening collection refinement to facilitate hit progression - Kristian Birchall, LifeArc
16.35-18.30	Networking

TRACK SUMMARY

EMERGING DISCOVERY STRATEGIES

10th November 2021
The Auditorium

Historically drug discovery efforts largely focused on traditional target classes such as enzymes, GPCRs and nuclear receptors and aimed to modulate them via binding of small molecules or monoclonal antibodies. Whilst largely successful and still extremely relevant, it's believed a large proportion of the human proteome, whilst may present valid targets, may be undruggable by these traditional approaches. Other valid targets are difficult to prosecute discovery campaigns against with the current technologies

SESSION CHAIRS

Peter Coombs
LifeArc
Kirsten Tschapalda
Roche

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09.00 - 09.10	Day 2 Welcome and Keynote Introduction - Jarrod Walsh, AstraZeneca
09.10 - 10.00	Plenary Keynote - Using DiBT-MS for high throughput and novel biocatalyst pharmaceutical discovery - Perdita Barran, University of Manchester
10.00 - 10.30	Refreshment Break
10.30 - 10.35	Session Chair Introduction - Peter Coombs, LifeArc & Kirstin Tschapalda, Roche
10.35 - 11.05	Modernising Drug Design and Prioritisation with AI - Simon Richards, Exscientia
11.05 - 11.35	Getting started with high-throughput mass spectrometry in early drug discovery - Martin Bachmann, Medicines Discovery Catapult
11.35 - 12.05	Development of BromoTag: A "Bump-and-Hole"-PROTAC System to Induce Potent, Rapid, and Selective Degradation of Tagged Target Proteins - Adam Bond, University of Dundee
12.05 - 13.30	Refreshment Break
13.30 - 14.00	Accelerating the validation of endogenous on-target engagement and assessment of in-cellulo kinetics for covalent inhibitors in early drug discovery - Vasudev Kantae, AstraZeneca
14.00 - 14.30	New way of screening: A case study comparing an iterative screening approach to conventional HTS campaigns - Markus Hierl, Roche
14.30 - 15.00	A MALDI-TOF assay identifies nilotinib as an inhibitor of inflammation in acute myeloid leukaemia - Matthias Trost, Newcastle University
15.00 - 15.20	Conference Close and Awards - David Cronk, Domainex

TRACK SUMMARY

MS & BIOPHYSICAL APPROACHES IN EARLY DRUG DISCOVERY

10th November 2021
The Helix Room

SESSION CHAIRS

Trevor Askwith
Domainex
Finn Holding
AstraZeneca

Recent years have seen increasing use of mass spectrometry (MS) and other biophysical methods alongside more traditional high throughput screening technologies in the search for target modulators and binders. They provide a direct assay readout, often with no labels or other reporters, and are therefore less susceptible to artefacts that can adversely affect other technologies. These methods can detect formation of covalent and non-covalent protein-ligand complexes and are not necessarily reliant on enzyme activity. As such they offer a route to screen targets that are catalytically inert, and are also able to detect ligand binding to regions

of a protein other than the active site. They are therefore applicable to screen for novel therapeutic modalities such as PROTACs and RNA binding, as well as providing a means to directly screen covalent libraries. There are an increasing number of proteins emerging from genomics initiatives with strong rationale as drug targets for which biophysical screening approaches are desirable, so the demand for them is likely to grow. In this session application of various MS and biophysical methods for biochemical screening including covalent and non-covalent binding strategies will be discussed.

10.30 - 10.35	Session Chair Introduction - Trevor Askwith, Domainex & Finn Holding, AstraZeneca
10.35 - 11.05	Building a high-throughput MS workflow for covalent Hit Finding - Sarah Hewitt, AstraZeneca
11.05 - 11.35	Utilizing biophysics to kick start drug discovery projects - Jana Wolf, Domainex
11.35 - 12.05	MALDI-TOF AS-MS – a label-free hit validation strategy in early drug discovery - Roman Simon, Boehringer
12.05 - 13.30	Refreshment Break
13.30 - 14.00	Revolutionizing Screening: MALDI-ToF Mass Spectrometry in a Fully Automated HTS System - Steven van Helden, Pivot Park Screening Centre
14.00 - 14.30	Reactive fragment screening for expansion of the liganded proteome - Jacob Bush, GSK
14.30 - 15.00	Identification of allosteric binders of an active GPCR : Screening of EDELIRIS Keychemical Space™ by Affinity Selection-Mass Spectrometry - Renaud Prudent, Edelris
15.00 - 15.20	Conference Close and Awards - David Cronk, Domainex - taking place in The Auditorium

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ELRIG EVENTS 2022

KEY EVENTS

ELRIG organises up to 6 scientific conferences and 6 networking meetings per year, that will have anywhere between 40 to 1500 attendees. Meetings may be an afternoon only to 2 days in length and have a very narrow focus or contain a broad range of topics, applicable to many research areas within the drug discovery community. All events are free-to-attend, simply register at elrig.org. Remaining events for 2021 and future events for 2022 are:



EVENTS 2021

PHARMACEUTICAL FLOW CYTOMETRY & IMAGING

Circle Square, Manchester
November 30th - December 1st 2021

EVENTS 2022

CRISPR IN DRUG DISCOVERY 2022

Babraham Research Campus, Cambridge
March 1st - 2nd 2022

RESEARCH & INNOVATION 2022

The Kings Centre, Oxford
March 29th - 30th 2022

CELL BASED ASSAY 2022

Astra Zeneca, Gothenburg
May 10th - 12th 2022

TRANSLATING IDEAS INTO THERAPIES

The Crick, London
July 4th - 5th 2022

DRUG DISCOVERY 2022

ExCeL, London
October 4th - 5th 2022

PROTEIN SCIENCES IN DRUG DISCOVERY 2022

Astra Zeneca, Cambridge
November 2nd - 3rd 2022

ROBOTICS & AUTOMATION 2022

Festo, Esslingen, Stuttgart
November 2022



ELRIG plans to run its future events face-to-face, so we will continue to observe government guidelines for the current global COVID-19 pandemic. In the event that we are unable to host those events in person or social distancing is required, they will take place virtually or as a hybrid.

