Fragments 2024

9th RSC-BMCS Fragment-based Drug Discovery Meeting

3rd – 5th March, 2024 Hinxton Hall, Cambridge, UK



ANNOUNCEMENT



Synopsis

The aim of the 9th RSC-BMCS Fragment-based Drug Discovery meeting will be to continue the focus on case studies in Fragment-based Drug Discovery that have delivered compounds to late stage medicinal chemistry, preclinical or clinical programmes. The Fragment series was started in 2007 and continues with this theme in having over three-quarters of the presentations focused on case studies. This will be complemented by technology progress in high concentration, NMR, SPR and X-ray screening.

Meet the Experts Session

On Sunday 3rd March there will be "Meet the Experts" interactive session and it is included in your delegate package. The Meet the Experts in Fragment-Based Drug Discovery (FBDD) is designed to provide participants with an understanding of the principles and applications of FBDD in drug discovery. The session leaders Anna Hirsch, Dan Erlanson, and David Rees will present and discuss FBDD's approach that focuses on identifying small, low molecular weight fragments as starting points for drug design, leading to the discovery of launched drugs. The session will encourage questions and answers from the audience in an informal atmosphere. After the interactive session, a buffet dinner will be served in the Hinxton Hall conference centre.



Emma Grant GSK



Iva Lukac Charnwood Discovery

Organising Committee



Gordon Saxty NS-MC Consulting LTD (Chair)



Marianne Schimpl AstraZeneca



Mary Wheldon University of Dundee (Treasurer)



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https://www.rscbmcs.org/events/fragments24

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Programme

Sunday 3rd March

- 15:00- Meet the Experts session: with Anna Hirsch, 17:20 Dan Erlanson, and David Rees
- 19:00 Buffet Dinner

Monday 4th March

- 09:00 Registration and Refreshments
- 10:20 Opening remarks
- 10:30 Leveraging fragment-based drug discovery (FBDD) to inform other screening platforms: How to describe, inventory, and incorporate fragment pharmacophores into picks from other platforms Justin Dietrich, Abbvie, US
- 11:00 Automation, automation: Application of automated synthesis to off-DNA PAC-FragmentDEL hits and crude reaction screens for rapid fragment elaboration Lucie Guetzoyan, Vernalis, UK
- 11:30 New Oncology targets from Fragment Leads John Spencer, University of Sussex, UK
- 12:00 Flash poster presentations
- 12:30 Lunch, exhibition, posters (odd-numbers) and networking
- 13:30 Late Breaking Talk
- 14:00 An NMR Toolbox for Drug Design Gerald Platzer, University of Vienna, Austria
- 14:30 Current and emerging opportunities for fragment-based drug design assisted with molecular simulations Julien Michel, University of Edinburgh, UK
- 15:00 Refreshments, exhibition and networking
- 15:30 RSC-BMCS Hall of Fame Winner talk Andrew Hopkins, Excientia, UK
- 16:15 Pannel Discussion
- 17:15 Drinks Reception, exhibition, posters (even-numbers) and networking
- 19:00 Conference Dinner

Tuesday 5th March

- 09:00 Structure-based fragment merging and linking affording potent and selective inhibitors of Pseudomonas aeruginosa elastase LasB Anna Hirsch, Helmholtz Institute for Pharmaceutical Research Saarland, Germany
- 09:30 Discovery of inhibitors targeting wild-type and a drug-resistant mutant of c-MET lacovos Michaelides and Gavin Collie, AstraZeneca, UK
- 10:00 Fragment Based Drug Discovery of Allosteric SH2 Domain-Containing Protein Tyrosine Phosphatase-2 (SHP2) Inhibitors Nicola Wilsher, Astex, UK
- 10:30 Refreshments, exhibition and networking
- 11:00 Deconstruction of HTS hits into fragments as a route to discover potent BCL6 inhibitors and degraders Rob Van Monfort, Institute of Cancer Research, UK
- 11:30 Discovery of potent SOS1 inhibitors through complementary use of FBDD and HTS Martina Schaefer, Nuvisan, Germany
- 12:00 Fragment based drug design approaches applied to IL-1β: from hit identification to cellular proof of concept Anna Vulpetti, Novartis, Switzerland
- 12:30 Lunch, exhibition, all posters and networking
- 13:30 Reversible Dual-Covalent Molecular Locking of the 14-3-3/ERRγ Protein–Protein Interaction as a Molecular Glue Drug Discovery Approach Peter Cossar, Eindhoven University of Technology, Netherlands
- 14:00 From fragment to allosteric activator targeting a novel metabolic regulator using FBDD Matthew Calabrese, Pfizer, UK
- 14:30 Refreshments, exhibition and networking
- 15:00 Reactive fragments in Chemical Biology at GSK Jonathan Pettinger, GSK, UK
- 15:30 Covalent fragment-based drug discovery Dan Erlanson, Frontier Medicines, US
- 16:15 Closing Remarks