

Fragments 2017

Pre-conference workshop

The pre-conference workshop will offer to those new to the area of FALG/FBLG an introduction into the fundamental principles governing fragment-based drug discovery approaches. A series of five short presentations with opportunities for discussions is scheduled. The pre-conference workshop is offered free-of-charge to conference attendees (opt-in required).

Bursaries and Sponsorship

Bursaries are available based on sponsorship of the event. If you wish to sponsor students to expand their knowledge in this area please contact the secretariat for further information.

Call for posters

Abstract deadline was 20th January 2017 although there are a few places for posters on FBDD remaining. Selected student speakers have been invited to present at the flash presentation session prior to the poster session.

Exhibitors

Those companies wishing to have a trade stand should apply early to avoid disappointment as these are limited. Details of fees may be found on the event website.

Registration

Registration is open, and rates for payments received by 3rd February are:

£436 RSC member	£224 RSC student* member
£544 Non-member	£278 Student* non-member

The late booking fee of £55 will be added to the above for payments received after 3rd February. Member is paid-up member of the RSC.

* Student is undergraduate or post-graduate, not post-doc, and does not apply to students in paid employment.

Venue and Travel

Austria Trend Parkhotel Schönbrunn, Hietzinger Hauptstrasse 10-14, 1130 Vienna, Austria. Austria has an excellent public transport system, and distances from the venue are: railway station 4.5 miles, city centre 5.5 miles, and airport 15 miles.

Accommodation and Dinner

The delegate accommodation package at the Parkhotel Schönbrunn includes two nights' B&B accommodation (Sunday and Monday) in a deluxe or executive en-suite bedroom. The conference dinner (included in the registration fee) will be held in the glorious Ballroom at the Parkhotel Schönbrunn.

Organising Committee

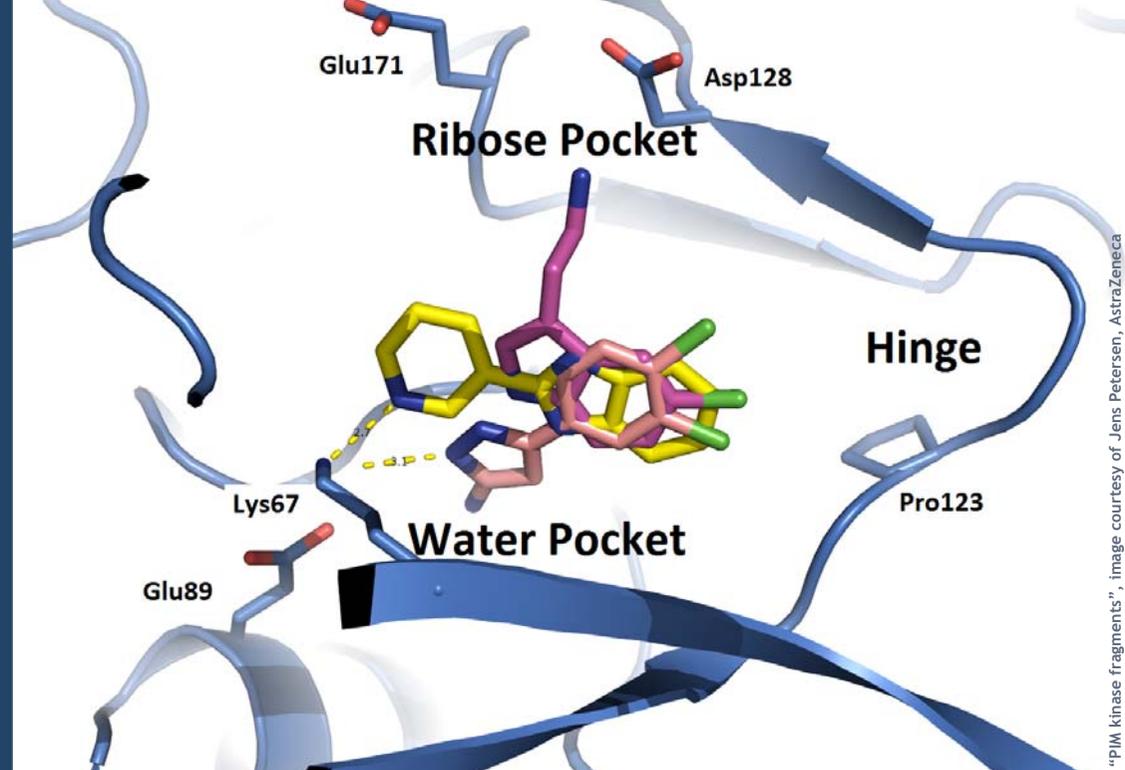
Mike Hann, GlaxoSmithKline
Samantha Hughes, AstraZeneca
Darryl McConnell, Boehringer Ingelheim
Thorsten Nowak, C4X Discovery
Gordon Saxty (chair), Fidelta
Mark Whittaker, Evotec

Secretariat Contact

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Website Addresses

www.maggichurchousevents.co.uk/bmcs (also www.rsc.org/bmcs)



"PI3K kinase fragments", image courtesy of Jens Petersen, AstraZeneca

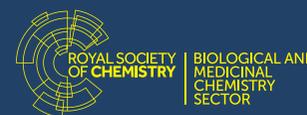
Second announcement and call for posters

Fragments 2017

6th RSC-BMCS Fragment-based Drug Discovery meeting

Sunday-Tuesday, 5th-7th March 2017

Parkhotel Schönbrunn, Vienna, Austria



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Synopsis

The aim of the 6th 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 the theme, having over three-quarters of the presentations focused on case studies. The conference will include successful examples from all types of fragment-based approaches, including high concentration, NMR, SPR and X-ray screening.

Who should attend

This conference is suitable for scientists including all chemists as well as other important disciplines including biophysics, structural biology, etc. This international meeting attracts delegates from the UK, several mainland European countries, as well as from the USA, Japan, China and South Korea.

Programme

Sunday, 5th March - optional pre-conference workshop

- 14:30 Registration opens
- 15:00 *Introduction to FBLG/FBDD - background*
Thorsten Nowak, C4X Discovery, UK and
- 15:30 *Fragment screening: some theory and what to expect in terms of quality of hits*
Mike Hann, GlaxoSmithKline, UK
- 16:00 *Fragment screening methods*
Samantha Hughes, AstraZeneca, UK
- 16:30 Refreshments
- 17:00 *Fragment optimisation*
Mark Whittaker, Evotec, UK
- 17:30 *Fragment optimisation and PPIs*
Darryl McConnell, Boehringer Ingelheim, Austria
- 18:00 Close
Buffet dinner

Monday, 6th March

- 09:15 Registration and refreshments
- 10:00 *Opening remarks*
Darryl McConnell, Boehringer Ingelheim, Austria
- Session chair: **Mike Hann**, GlaxoSmithKline, UK
- 10:10 *Targeting protein protein interactions in oncology using a fragment-based drug discovery approach*
Justin Bower, Beatson Institute, UK
- 10:55 *Novel inhibitors of iNOS Discovered through FBLG*
Fredrik Edfeldt, AstraZeneca, Sweden
- 11:40 Flash poster presentations
- 12:10 Lunch and posters



**Boehringer
Ingelheim**



astex
pharmaceuticals



AstraZeneca



evotec



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Programme (continued)

Monday, 6th March (continued)

- Session chair: **Samantha Hughes**, AstraZeneca, UK
- 13:00 *Finding better fragments faster with MST*
Dennis Breitsprecher, NanoTemper, Germany
- 13:45 *Addressing novel targets by crystallography with fragments and self-optimized inhibitors*
Gerhard Klebe, University of Marburg, Germany
- 14:30 *Scanning the protein surface to uncover new small molecule binding sites using fragments*
Gregg Siegal, ZoBio, The Netherlands
- 15:15 Refreshments
- 15:45 *Fragment optimization and structure based design of DNA gyrase inhibitors*
Dominic Ryan, formerly Cubist
- 16:30 *AbbVie's re-vamped fragment-based drug discovery platform*
Phil Cox, AbbVie, USA
- 17:15 Poster session and drinks reception
- 19:15 Conference dinner at Heurige 10er Marie Restaurant

Tuesday, 7th March

- Session chair: **Thorsten Nowak**, C4X Discovery, UK
- 09:00 *Fragment optimisation without co-crystal X-ray structures: from hits to nanomolar inhibitors of human PAICS*
Simon Osborne, MRC Technology, UK
- 09:45 *Leveraging iterative 3D-structure information while managing physicochemical properties: design of eFT508, an oral, potent and highly selective inhibitor of mitogen-activated protein kinase interacting kinase (MNK) 1 and 2*
Siegfried Reich, eFFECTOR, USA
- 10:30 Refreshments
- 11:00 *Computational approaches to fragment-based drug discovery*
Paul Mortenson, Astex Pharmaceuticals, UK
- 11:45 *Advances in fragment-based drug discovery applied to membrane protein drug targets*
Michael Hennig, leadXpro AG, Switzerland
- 12:30 Lunch and posters
- Session chair: **Mark Whittaker**, Evotec, UK
- 13:30 *Training early stage researchers in FBDD, two examples of European training networks*
Iwan de Esch, VU Amsterdam, and **Christian Ottmann**, University of Eindhoven, The Netherlands
- 14:15 *Innovating drug discovery by locking GPCRs in functional conformations*
Christel Menet, Confo Therapeutics, Belgium
- 15:00 Refreshments
- 15:30 *BCL6 Inhibitors - From micro-molar binders to nano-molar degraders*
Steffen Steurer, Boehringer Ingelheim, Austria
- 16:15 *Cancer drug discovery using fragment-based methods and structure-based design*
Stephen W Fesik, Vanderbilt University, USA
- 17:30 Closing remarks
Gordon Saxty, Fidelta, Croatia