

## 6th RSC / SCI symposium on GPCRs in Medicinal Chemistry

### Overview

The conference programme will cover:

- First disclosures of clinical candidates
- Case studies in GPCR drug discovery and development
- New structural biology and drug design
- Allosteric modulation & biased signalling
- Structural and medicinal chemistry aspects of multiple GPCR drug targets

Also included are: evening networking reception - poster session - conference dinner - vineyard visit and dinner - trade exhibition opportunities - accommodation for direct booking

### Venue and Travel

Aptuit, Verona, Italy is a 7.5-mile taxi ride from the Verona Villafranca airport, and a 3.5 mile taxi ride from Verona Porta Nuova railway station. Aptuit is 3.5 miles from Verona city centre depending on hotel.

A coach service will be provided gratis between central Verona and Aptuit at the beginning and end of each day. Registered attendees will be contacted nearer the time regarding their requirements.

### Exhibitors

Contact the Secretariat for details of exhibitor opportunities.

### Accommodation and Conference Dinners

Please see our website for hotel details.

The registration fees include two dinners and a vineyard visit. Please opt in whilst registering.

### Registration and Students

Registration fee payments received:

	Up to 9 Mar	from 10 Mar to 11 May
RSC or SCI member	£360	£420
Non-member	£440	£500
RSC or SCI student* member	£150	£170
Student* non-member	£190	£215

£30 late payment fee will be added to the above standard rates from 12th May onwards.

\* Student is undergraduate or post-graduate, not post-doc

Some student bursaries are available, and the closing date for applications is 29th April 2016. Discounted rates are offered to RSC and SCI student members.

### Sponsors

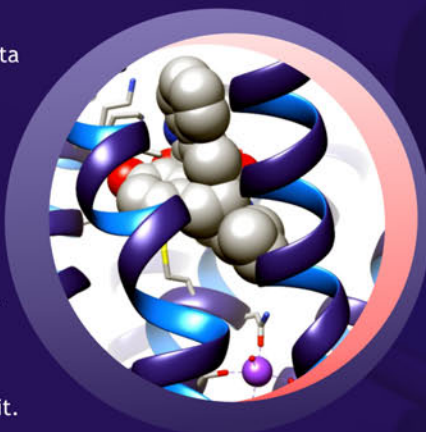
Special thanks to Aptuit for supporting this event. We are grateful to Takeda and Heptares for sponsoring the event, and additional sponsors would be welcomed.

### Secretariat Contact

Maggi Churchouse, 3 East Barn, Market Weston Road, Theltham, Diss IP22 1JJ, UK  
telephone +44 (0)1359 221004, maggi@maggichurchousevents.co.uk

**Websites:** [www.maggichurchousevents.co.uk/bmcs](http://www.maggichurchousevents.co.uk/bmcs)

**Also:** [www.rsc.org/bmcs](http://www.rsc.org/bmcs) and [www.soci.org/events](http://www.soci.org/events)



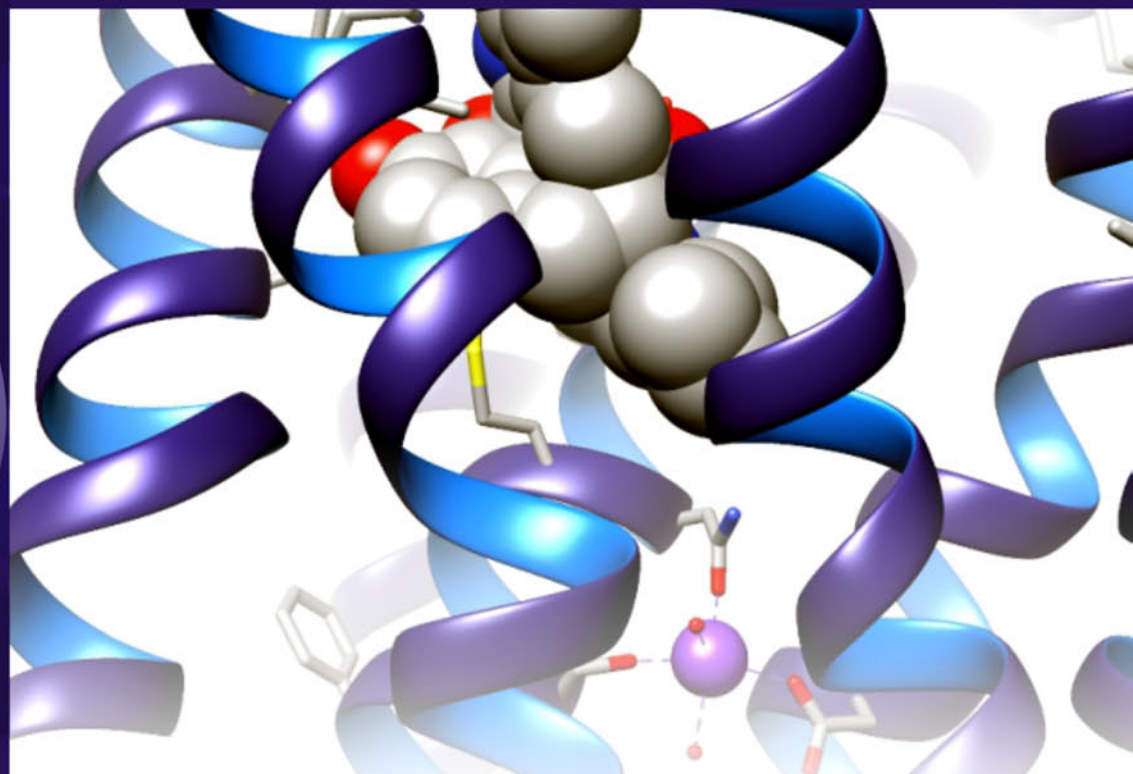
### Organising Committee

Adrian Hall (co-chairman), UCB  
Caroline Low, Consultant  
Jon Mason, Heptares  
Fabrizio Micheli, Aptuit  
David Miller (co-chairman),  
Takeda Cambridge Ltd  
Simon Peace, GlaxoSmithKline

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## Second announcement and call for posters



## 6<sup>th</sup> RSC / SCI symposium on GPCRs in Medicinal Chemistry

Monday-Wednesday, 13th-15th June 2016

Aptuit, Verona, Italy

Organised by

RSC's Biological and Medicinal Chemistry Sector, and  
SCI's Fine Chemicals Group



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# Introduction and Programme

## Synopsis

The key role of G-protein coupled receptors (GPCRs) in human disease underpins their importance to modern medicine. We are pleased to announce that Aptuit, Italy will support the sixth meeting in this series on GPCR drug discovery, which will combine cutting edge medicinal chemistry with innovative structural biology and novel drug design approaches.

## Call for Posters

Posters are invited for display throughout the meeting, and for flash presentation. Please download a template and send a one-page abstract to the secretariat by **29th April 2016**.

## Programme

### Day 1 Monday, 13th June

- 08:30 Registration and refreshments  
Session Chair: **Fabrizio Micheli**, Aptuit
- 09:20 Opening remarks  
**Jonathan Goldman**, Aptuit, and **Adrian Hall**, UCB
- 09:30 Plenary: *The seventh millennium of GPCR drug discovery*  
**Fiona Marshall**, Heptares Therapeutics, UK
- 10:20 *Insights into chemistry and biology of GPCRs from molecular modelling*  
**Irina Tikhonova**, Queen's University Belfast, UK
- 10:55 Refreshments and exhibition
- 11:25 *Biased agonism @ FPR2*  
**Olivier Corminboeuf**, Actelion, Switzerland
- 12:00 *TAAR1 agonists - a new approach for the treatment of psychiatric disorders*  
**Roger Norcross**, Roche Pharma Research & Early Development, Switzerland
- 12:30 *Binding of anticholinergics to the M3 receptor: explaining kinetics by mutagenesis and molecular dynamics simulations*  
**Christofer Tautermann**, Boehringer Ingelheim, Germany
- 13:00 Lunch and exhibition  
Session Chair: **Simon Peace**, GlaxoSmithKline
- 14:00 *High-resolution structure of the human GPR40 receptor bound to allosteric agonist TAK-875*  
**Gyorgy Snell**, Takeda California, USA
- 14:40 *Design, synthesis and pharmacological profile of the GPR40 receptor agonist MK-8666*  
**Ravi Nargund**, Merck, USA
- 15:10 Refreshments and exhibition
- 15:40 *Universal mechanism of activation of G proteins by GPCRs*  
**Madan Babu**, Medical Research Council LMB, UK
- 16:25 Close
- 16:30 Coaches depart for visit to Vineyard (Cantina Sociale di Soave - Soave and Valpolicella) and evening meal
- 20:00 Coaches leave Vineyard for Verona city centre

## Programme continued

### Day 2 Tuesday 14th June

- Session Chair: **Adrian Hall**, UCB
- 09:30 *Recent computational trends in exploring G protein-coupled receptor (GPCR) ligand recognition pathways*  
**Stefano Moro**, University of Padova, Italy
- 10:00 *Discovery of small molecule modulators of PAR-2*  
**Roland Bürli**, AstraZeneca and MedImmune, UK
- 10:30 Refreshments, exhibition and posters
- 11:00 *Nutrient sensing GPCR FFAR1 (GPR40): allosteric agonist binding mode and physical properties influence agonist pharmacology*  
**Bruce Ellsworth**, Bristol-Myers Squibb, USA
- 11:30 *Roles of waters to predict binding affinity, selectivity and kinetics: a key component of high end GPCR SBDD*  
**Jonathan Mason**, Heptares Therapeutics, UK
- 12:15 Lunch, exhibition and posters  
Session Chair: **Caroline Low**, Consultant
- 13:15 *Design and synthesis of highly selective 5-HT<sub>2C</sub> receptor agonists as potential novel treatment for neuropsychiatric diseases*  
**Andreas Haupt**, AbbVie, Germany
- 13:50 *Dopamine D<sub>3</sub>/D<sub>2</sub> antagonist PF-04363467 attenuates drug-seeking behaviour without concomitant D<sub>2</sub> side effects*  
**Travis Wager**, Pfizer, USA
- 14:25 *Discovery of mGluR2 negative allosteric modulators for the treatment of neuropsychiatric disorders*  
**Michiel Van Gool**, Janssen, Belgium
- 15:00 Refreshments, exhibition and posters
- 15:30 *Acquired resistance to smoothened inhibitors in cancer patients*  
**Hayley Sharpe**, Genentech, USA
- 16:05 Plenary: *Are we there yet? How many unique GPCR structures needed?*  
**Vsevolod (Seva) Katritch**, University of Southern California, USA
- 16:55 Flash poster presentations
- 17:30 Poster session
- 19:00 Conference dinner at Aptuit

### Day 3 Wednesday 15th June

- Session Chair: **David Miller**, Takeda Cambridge
- 09:00 *What happens when you thermostabilise a GPCR?*  
**Bernadette Byrne**, Imperial College London, UK
- 09:40 *Rationalising activity cliffs at the adenosine A<sub>2a</sub> receptor via crystallography*  
**Zara Sands**, UCB, Belgium
- 10:15 Refreshments
- 10:45 *Mas-1 receptor inverse agonists for cardiovascular disease*  
**Graeme Semple**, Arena Pharmaceuticals, USA
- 11:20 *LPARs - recent progress and medchem approach towards LPAR5*  
**Werngard Czechtizky**, Sanofi
- 12:00 Closing remarks  
**David Miller**, Takeda Cambridge, UK
- 12:05 Close

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