



# Twenty Years of the Rule of Five

## Synopsis

It has been over twenty years since Lipinski published his work determining the properties of drug molecules associated with good solubility and permeability. Since then, there have been a number of additions and expansions to these "rules". There has also been keen interest in the application of these guidelines in the drug discovery process and how these apply to new emerging chemical structures such as macrocycles.

This symposium will bring together researchers from a number of different areas of drug discovery and will provide a historical overview of the use of Lipinski's rules, as well as looking to the future and how we use these rules in the changing drug compound landscape.

## Programme

09:30 Registration and refreshments

Session 1: History to Present Day

Session chair: **Mary Wheldon**, University of Dundee, UK

10:00 *The rule of five and the pursuit of compound quality*

**Paul Leeson**, Paul Leeson Consulting, UK

10:30 *Do we need to change the definition of drug-like properties?*

**Michael Shultz**, Novartis, USA

11:00 Refreshments and posters

11:30 *Molecule properties: how relevant are aromatic and aliphatic descriptors?*

**Tim Ritchie**, Zerlavan Consulting UK, UK

12:00 *BET PROTACs: investigating the effects of linker functionality on physicochemical properties*

**John Priestner**, GlaxoSmithKline, UK

12:30 Discussion panel, facilitated by **Chris Swain**, Cambridge MedChem Consulting

13:00 Lunch and posters

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## Programme (continued)

Session 2: Beyond the Rule of Five and the Future

Session chair: **Jonathan Goodman**, University of Cambridge, UK

14:00 *Structure property relationships in the Ro5 space and beyond*  
**Elisabetta Chiarparin**, AstraZeneca, UK

14:30 *Investigating the chameleonic properties of  $\alpha$ VB6 integrin antagonists for the treatment of IPF*

**James Thompson**, GlaxoSmithKline, UK

15:00 *Chemical space adventures below and beyond Lipinski*  
**Jean-Louis Reymond**, University of Bern, Switzerland

15:30 Refreshments and posters

16:00 *Defining known drug space using DFT*  
**Jóhannes Reynisson**, Keele University, UK

16.30 *Property-based drug design Beyond Ro5- lessons learned from AbbVie's drugs and compound collection*  
**Phil Cox**, AbbVie, USA

17:00 Panel discussion, facilitated by **Mihiro Sunose**, Sygnature Discovery

17:30 Drinks reception

18:30 Close (latest)

### Call for Poster Abstracts

Applications for poster presentations are invited. Posters will be displayed throughout the day. The closing date is 6th October.