

Features

- Historical look at the use of the Rule of Five
- New parameters used in drug discovery
- Look forward to the next 20 years
- Panel discussion in each session
- Poster session
- Drinks reception

Who should attend

Scientists from industry and academia, including medicinal and computational chemists.

Registration

Registration is open, and fees are:

£120 RSC member

£165 non-member

£50 RSC student* member

£80 student* non-member

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

A late fee of £30 will apply to payments received from 19th October onwards.

Venue and Travel

Innovation Building, Sygnature Discovery, BioCity, Pennyfoot Street, Nottingham NG1 1GR
East Midlands airport is just 20 minutes away, and regular trains run direct from London (journey time two hours). Sygnature Discovery is just over half-a-mile from the railway station.

Sponsorship

We are grateful to Sygnature Discovery for their generous support of this symposium.

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Secretariat Contact

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Also: www.rsc.org/bmcs and www.rsc.org/cicag

Call for Poster Abstracts

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

Twitter Hashtag

#RuleofFive2019

Students & Bursaries

A number of RSC-BMCS and RSC-CICAG student bursaries are available up to a value of £250, to support registration, travel and accommodation costs for PhD and post-doctoral applicants studying at European academic institutions. The closing date for bursary applications is 4th October.

Organising Committee

Chris Swain (chair)	Cambridge MedChem Consulting
Jonathan Goodman	University of Cambridge
Mihiro Sunose	Sygnature Discovery
Mary Wheldon	University of Dundee

Third Announcement and Call for Posters

beyond the rule of 5

rule of five

solubility

rotatable bond

bioavailability

cell permeable

Hydrogen bond

LipE

Lipinski

Molecular weight

molar refractivity

permeability

ionisation

LogD

HBA

bro5

HBD

1MW

pKa

Lipophilicity

LogP

TPSA

Polar surface area

Twenty Years of the Rule of Five

Wednesday, 20th November 2019

Sygnature Discovery, BioCity, Nottingham, UK

Hosted at



**SYGNATURE
DISCOVERY**



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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Twenty Years of the Rule of Five

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 αVβ6 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

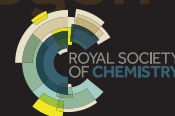
17:00 Panel discussion, facilitated by **Mihiro Sunose**, Sygnature Discovery

17:30 Drinks reception

18:30 Close (latest)

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