

International Conference on Pure and Applied Chemistry (ICPAC- 2016)

18th-22nd July 2016

Hotel Sofitel, Impérial Resort & Spa, Mauritius

Mauritius Drug Discovery Workshop: How to progress small molecule hits from screening efforts

MMV-UCT-MRC

Description of Workshop:

The purpose of this symposium aimed at researchers from disease endemic countries is to enhance and build scientific research capacity in integrated drug discovery. Specifically the symposium will focus on how to progress small molecule chemical matter (hits) from screening efforts (both from primary screens, and particularly from the use of the Malaria and Pathogen Box to deliver leads suitable for optimization and selection as pre-clinical drug development candidates. A key outcome will be to raise awareness of existing drug discovery activities in the continent in an attempt to foster new collaborations between attendees.

Participants targeting:

Medicinal chemists or natural products chemists from Africa and other disease endemic countries, biologists interested in developing in vitro assays involved in drug discovery networks, particularly for infectious diseases beyond TB HIV and Malaria.

Day 1:

9:00 Introduction from the organisers – *Tim Wells, Richard Gordon, Kelly Chibale*

9:15 Drug Discovery – the challenges from screen to Candidate Drug – *Peter Sjö (AstraZeneca)*

9:45 The power of Open access compounds – from the Malaria to Pathogen boxes – *Benoît Laleu (MMV)*

10:15 Discussion

10:30 *Coffee*

Workshop with Case studies

Assay Development and Screening

11:00 How to build an assay and conduct screening – *Wes Van Voorhis (University of Washington)*

11:30 Screening the Malaria Box against toxoplasma – *Fabrice Boyom (Cameroon)*

11:45 Screening the Malaria Box against gametocytes – *Dalu Mancama (CSIR)*

12:00 Discussion

12:15 *Lunch*

Medicinal Chemistry, DMPK, Computer Aided Drug Design and early Safety

13:30 What makes a molecule ‘attractive’? Introduction to medicinal chemistry – *Greg Basarab (H3D/UCT)*

14:00 What the body can do to a molecule and why this is important: DMPK – *Collen Masimirembwa (Harare)*

14:30 How can computers help with Drug Discovery? An introduction to Computer Aided Drug Design – *Joe Eyermann (H3D/UCT)*

15:00 Discussion

15:15 *Coffee*

Learnings from the Malaria Box

15:45 Four 15 mins talks (10mins + 5 mins questions) given by endemic region scientists who have completed studies with the Malaria Box

16:45 Plenary case study: Transforming ‘hits’ into ‘leads’ – *Tanya Paquet (H3D/UCT)*

17:15 *Poster session*

Day 2:

Overcoming obstacles to maximize the chance of success

9:15 The challenge of Drug Discovery for Neglected and Tropical Diseases – Tim Wells (MMV)

9:45 The importance of collaboration in successful drug discovery – Rich Gordon (MRC)

10:15 Discussion

10:30 *Coffee*

Oral posters - discussion

11:00 Five 10 mins talks (5mins + 5 mins questions) given by recipients of the MMV Fellowships

12:00 *Lunch*

13:30 Five 10 mins talks (5mins + 5 mins questions) given by recipients of the MMV Fellowships

14.30 Interactive case study led by David Waterson (MMV)

All workshop participants to be presented with an interactive challenge to cement learnings from the symposium

16:30 *Coffee*

17:00 Closing Plenary: First African Candidate drug – the Discovery of MMV390048 – Kelly Chibale (H3D/UCT)

17:30 Workshop ends