



## Sunday May 13<sup>th</sup>, NH Carlton Hotel

17.00 – 19.00 Reception at NH Carlton for all Participants & Speakers

## Monday May 14<sup>th</sup>, Royal Tropical Institute

8.30 – 17.00 Registration

### Opening

9.00 – 9.05 Henk Timmerman, symposium chair

### Forum on the MedChem 2020 arena (chairs Henk Timmerman & Dave Swinney)

- 9.05 – 9.15 Introduction by **Dave Swinney** (iRND3, USA)
- 9.15 – 9.45 **Gerhard Müller** (Mercachem, NL)  
*Medicinal Chemistry Services within “small pharma”: from molecular understanding to complex chemistry*
- 9.45 – 10.15 **Anthony Wood** (Pfizer, US)  
*Challenges and Opportunities for Medicinal Chemistry*
- 10.15 – 10.30 **György Kesuru** (Gideon Richter, Hungary)  
*Finding the sweet spot: the role of nature and nurture in Medicinal Chemistry*
- 10.30 – 11.00 Discussion with **Gerhard Müller, Anthony Wood, Mike Hann, György Kesuru** and the audience - moderated by **Henk Timmerman & Dave Swinney**

11.00 – 11.30	Coffee break
---------------	--------------

### Session 1: New synthetic technologies for medicinal chemistry (chair: F. Rutjes, NL)

- 11.30 – 11.35 Introduction by **Floris Rutjes** (Radboud University Nijmegen, NL)
- 11.35 – 12.15 Keynote lecture: **Alex Gouliaev** (Nuevolution, Danmark)  
*Billion member DNA-tagged screening libraries. From theory to practical application in medicinal chemistry.*
- 12.15 – 12.45 **Floris Rutjes** (Radboud University Nijmegen, NL)  
*Recent advances in flow chemistry*
- 12.45 – 13.15 **Daniel Obrecht** (Polyphor, Switzerland)  
*Medium-sized macro cyclic PEM molecules: synthetic challenges and evaluation for targeting challenging and therapeutically relevant GPCRs*

13.15 – 14.15	Lunch break & poster viewing
---------------	------------------------------

## Session 2: Fragment-based drug discovery (chairs D. Rees, UK, I. De Esch, NL),

- 14.15 – 14.55      Keynote lecture: **David Rees** (Astex, UK)  
*The Rise of Fragment Based Drug Discovery*
- 14.55 – 15.25      **Mike Hann** (GSK, UK)  
*Molecular Obesity, potency and other addictions in medicinal chemistry.*
- 15.25 – 15.55      **Herbert Nar** (Boehringer Ingelheim, Germany)  
*Linking HTS-based and fragment-based approaches to a productive lead identification process using structural biology and biophysics*
- 15.55 – 16.10      **Carol Austin** (Selcia, UK)  
*Fragment screening using capillary electrophoresis*
- 16.10 – 16.25      **Gregg Siegal** (Leiden University, NL)  
*Effective structure determination of protein-fragment complexes using NMR*

20.15	Social program – <b>Concert</b> (ticket required) in <b>Royal Concert Hall</b>
-------	--

## Tuesday May 15<sup>th</sup>, Royal Tropical Institute

9.00 - 17.00 Registration

9.15 – 9.55 **Special lecture: Anette Beck-Sickinger** (Univ. Leipzig, Germany)  
*Peptide Drugs – State of the Art and Innovative Applications*

### Session 3: Structural biology of membrane proteins (chair: Fiona Marshall, UK)

9.55 – 10.35 Keynote lecture: **Fiona Marshall** (Heptares, UK)  
*Structure and fragment based drug discovery applied to G-protein coupled receptors*

10.35 – 11.05 **So Iwata** (UCL, UK)  
*Structural studies on G-protein coupled receptors*

11.05 – 11.30	Coffee break
---------------	--------------

11.30 – 12.00 **Gebhard Schertler** (Paul Scherrer Institute, Switzerland)  
*Structures of constitutively active G-Protein Coupled Receptors*

12.00 – 12.30 **Chris de Graaf** (VU University Amsterdam, NL)  
*Fragments, Fits, Fingerprints: Structure-based virtual screening for fragment-like GPCR ligands*

12.30 – 13.00 **Marijn Sanders** (Radboud University Nijmegen, NL)  
*Snooker: Multiple sequence alignment derived pharmacophores and its application in drug design*

13.00 – 14.00	Lunch break
---------------	-------------

14.00– 14.30 **Werner Sieghardt** (University of Vienna, Austria)  
*GABAA receptor subtypes – exciting targets for the development of clinically important drugs*

14.30 – 15.00 **Chris Ulens** (University of Leuven, Belgium)  
*Structural principles of agonist and modulator recognition in a bacterial GABA-gated ion channel*

15.00 – 15.15 **Rogier Smits** (Griffin Discoveries, NL)  
*Long receptor residence time and H<sub>4</sub>R antagonism*

15.15 – 15.30 **Fabio Del Bello** (University of Camerino, Italy)  
*Might Allyphenyline and cyclomethyline become profitable multifunctional tools in the opioid addiction management?*

15.30 – 15.45 **Maikel Wijtmans** (VU University Amsterdam, NL)  
*Bisaryl-type Ligands: a Thin Line Between Antagonism and Agonism at Chemokine Receptor CXCR3*

15.45 – 17.00	Drinks & poster discussions with presenters (please be present at your poster!!)
---------------	--

## Wednesday May 16<sup>th</sup>, Royal Tropical Institute

9.00 – 17.00	Registration
9.15 – 9.55	<b>Special lecture: Martine Smit</b> (VU University Amsterdam) <i>Therapeutic targeting of chemokine receptors with Nanobodies (VHH immunoglobulin-based single variable domains)</i>

### Session 4: Target tumor therapy via antibody-drug conjugates (chair: R. Jautelat, Ger)

9.55 – 10.00	Introduction by chair <b>Rolf Jautelat</b> (Bayer, Germany)
10.00 – 10.40	Keynote lecture: <b>Hans-Georg Lerchen</b> (Bayer, Germany) <i>Antibody Drug Conjugates: Challenges in the interface between proteins and small molecules</i>

10.40 – 11.15	Coffee break
---------------	--------------

11.15 – 11.45	<b>Vincent de Groot</b> (Synthon, NL) <i>Preclinical Development Progress of ADCs based on Novel Potent Payload Linker-Drug Technology</i>
11.45 – 12.15	<b>David Satijn</b> (Genmab, Denmark) <i>Development of antibody drug conjugates against Tissue Factor for the treatment of solid tumors.</i>

12.15 – 13.15	Lunch break
---------------	-------------

#### Late breaking topics

13.15 – 13.45	<b>Eelco de Ruijter</b> (AIMMS, VU University Amsterdam, NL) <i>Multicomponent reactions – opportunities for medicinal chemistry</i>
13.45 – 14.15	<b>Thierry Langer</b> (Prestwick, Chemical SAS France) <i>3D Chemical Feature-based Pharmacophores: Efficient Tools In Lead Optimization and Profiling</i>
14.15 – 14.30	<b>Kristina Orrling</b> (TI Pharma consortium T4-302 Swe) <i>From fragments to trypanocidals – PDE inhibitors as potential new treatment of African Sleeping Sickness</i>

14.30 – 15.00	Coffee break
---------------	--------------

### Session 5: Epigenetics: from chemical biology to new therapeutics (chair: M. Hann, UK)

15.00 – 15.05	Introduction by chair <b>Mike Hann</b> (GSK, UK)
15.05 – 15.45	Keynote lecture by <b>John Trzupek</b> (Pfizer, USA) <i>Chemical Probes for Epigenetics</i>
15.45 – 16.15	<b>Jian Jin</b> (University of North Carolina, USA) <i>Discovery of Chemical Probes for Methyl Writers of the Histone Code</i>
16.15 – 16.45	<b>Chun-wa Chung</b> (GSK, USA) <i>Hedging your BETs: from phenotypic screening to fragment based drug discovery</i>

