

# 5th EFMC Short Course on Medicinal Chemistry - Spring 2012

## Programme

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### Sunday April 1, 2012

**18:00**      **Dinner**

**Introduction to Course**

**19:30**      **Drug Discovery in the Century of Systems and Chemical Biology**

Dr Brian HARMS (MERRIMACK PHARMACEUTICALS, Cambridge, MA, United States)  
Dr Thomas KLABUNDE (SANOFI-AVENTIS, Frankfurt am Main, Germany)

**20:30**      **Close**

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## Programme

### Monday April 2, 2012

**07:30 Breakfast**

#### Session I: Understanding Disease Physiology

**08:30 Modelling of Physiological Processes to Understand Disease**

Dr Brian HARMS (MERRIMACK PHARMACEUTICALS, Cambridge, MA, United States)  
Dr Thomas KLABUNDE (SANOFI-AVENTIS, Frankfurt am Main, Germany)

**09:00 Lost in Translation (?)**

Dr Henning SCHMIDT  
(NOVARTIS PHARMA AG, Basel, Switzerland)

**09:45 Optimizing Lead Compound Selection Using Mechanistic Physiological Modeling**

Dr Christina FRIEDRICH  
(ROSA & CO, San Carlos, United States)

**10:30 Coffee Break**

**10:45 Physiological and Disease Modelling for Diabetes: Glucose/insulin Homeostasis**

Dr Thomas KLABUNDE  
(SANOFI-AVENTIS, Frankfurt am Main, Germany)

**11:00 Qualifying Mechanistic Physiological Models for Use in Pharmaceutical Discovery and Development, Part I**

Dr Christina FRIEDRICH  
(ROSA & CO, San Carlos, United States)

#### WORKSHOP/TUTORIAL

**13:00 Lunch**

**14:00 Qualifying Mechanistic Physiological Models for Use in Pharmaceutical Discovery and Development, Part II**

Dr Christina FRIEDRICH  
(ROSA & CO, San Carlos, United States)

**15:30 Coffee Break**

#### Session II: Understanding Complex Biological Systems

**16:00 Modelling of Cellular Systems: Helping you to Identify the Most Relevant Switches**

Dr Brian HARMS (MERRIMACK PHARMACEUTICALS, Cambridge, MA, United States)  
Dr Thomas KLABUNDE (SANOFI-AVENTIS, Frankfurt am Main, Germany)  
Prof. Julio SAEZ-RODRIGUEZ (EMBL-EBI, Heidelberg, Germany)

**16:45 Comparative Logical Models of Signalling Networks in Normal and Transformed Hepatocytes**

Prof. Julio SAEZ-RODRIGUEZ  
(EMBL-EBI, Heidelberg, Germany)

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17:30      End day-1, followed by a social event

# 5th EFMC Short Course on Medicinal Chemistry - Spring 2012

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**Tuesday April 3, 2012**

**07:30 Breakfast**

**09:00 Modelling of EGFR Signalling for Target Identification**

Dr Brian HARMS  
(MERRIMACK PHARMACEUTICALS, Cambridge, MA, United States)

**09:45 The Virtual Pancreatic Beta-cell: a Mod & Sim Approach in Diabetes Drug Discovery**

Dr Thomas KLABUNDE  
(SANOFI-AVENTIS, Frankfurt am Main, Germany)

**10:30 Coffee Break**

### WORKSHOP/TUTORIAL

**11:00 Models of Signalling Networks: from Coarse Boolean Approaches to Dynamic Models of Underlying Biochemistry**

Prof. Julio SAEZ-RODRIGUEZ  
(EMBL-EBI, Heidelberg, Germany)

**13:00 Lunch**

### Session III: Target Identification by Chemical Biology

**14:00 Chemical and Systems Biology Approaches for Target Identification**

Dr Uwe RIX  
(H. LEE MOFFITT CANCER CENTER & RESEARCH INSTITUTE, Tampa, FL, United States)

**14:45 Targets and Molecular Mechanisms: Charting Kinase Inhibitors in Malignant Diseases Using Chemical Proteomics**

Dr Uwe RIX  
(H. LEE MOFFITT CANCER CENTER & RESEARCH INSTITUTE, Tampa, FL, United States)

**15:30 Coffee Break**

### WORKSHOP/TUTORIAL

**16:00 Computational Approaches to Target Prediction**

Dr Thomas KLABUNDE  
(SANOFI-AVENTIS, Frankfurt am Main, Germany)

**17:00 End day-2**

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### Wednesday April 4, 2012

**07:30**      **Breakfast**

**Session IV: Understand Disease Mechanisms from Transcriptomics Data and Map Disease and Drug-response Signatures**

**09:00**      **Review Tools and Case Studies for Computational Drug Repositioning**

Dr Francesco IORIO  
(EMBL-EBI & WELLCOME TRUST SANGER INSTITUTE, Cambridge, United Kingdom)

**09:45**      **Review Computational Methods and Case Studies for Understanding Disease Mechanisms and Drug Responses**

Dr Francesco IORIO  
(EMBL-EBI & WELLCOME TRUST SANGER INSTITUTE, Cambridge, United Kingdom)

**10:30**      **Coffee Break**

#### **WORKSHOP/TUTORIAL**

**11:00**      **Using cMap and MANTRA to identify Drug Repositioning Opportunities**

Dr Francesco IORIO  
(EMBL-EBI & WELLCOME TRUST SANGER INSTITUTE, Cambridge, United Kingdom)

**12:30**      **Summary**

**13:00**      **Lunch and depart**