



## Joint Annual COST Action meeting – Porto (PT), September 22–24 2017

Auditorium of the Portuguese Oncology Institute of Porto (IPO Porto)

Rua Dr. António Bernardino de Almeida – 4200–072 Porto, Portugal

[www.epichembio.eu](http://www.epichembio.eu)

*A bridge between EpiChemBio and MuTaLig COST Actions*

[www.mutalig.eu](http://www.mutalig.eu)

Friday September 22<sup>nd</sup> 2017

8:15 Registration and poster setup

8:45 **Introduction to the Joint COST Action annual meeting**

**José LARANJA PONTES** – President of Portuguese Oncology Institute, Porto (Portugal)

**A Fernando SILVA** – Dean of Faculty of Sciences, University of Porto (Portugal)

**Arminda ALVES** – LEPABE – University of Porto (Portugal)

**Fernanda BORGES** – University of Porto (Portugal)

**Carmen JERONIMO** – Portuguese Oncology Institute, Porto (Portugal)

**A GANESAN** (CA1406 Chair) – University of East Anglia, Norwich (UK)

**Stefano ALCARO** (CA15135 Chair) – Università “Magna Græcia” di Catanzaro (Italy)

### Session I “EpiChemBio: DNA and epigenetics”

**Moderator: Maria Berdasco MENENDEZ (Spain)**

9:30 SCE1 **Non-B DNA structures, as G-quadruplex and R loops, interact with each other regulating basic DNA functions and genome instability in human cancer cells**

**Giovanni CAPRANICO** – University of Bologna (Italy)

9:45 SCE2 **Molecular tools for targeted covalent functionalization and light-induced activation of biopolymers**

**Saulius KLIMASUSKAS** – University of Vilnius (Lithuania)

10:00 SCE3 **Direct and indirect targeting of DNA methylation in cancers**

**Marie LOPEZ** – CNRS, Toulouse (France)

10:15 SCE4 **Anti-Neoplastic Activity of Newly Synthesized DNMT inhibitors in Renal Tumors**

**Ines GRACA** – Portuguese Oncology Institute of Porto (Portugal)

10:30 SCE5 **Targeted DNA demethylation in human cells by 5-methylcytosine excision**

**Jara Teresa PARILLA-DOBLAS** – University of Cordoba (Spain)

10:45 SCE6 **Epigenetic and antitumor effects of platinum(IV)-octanoato conjugates**

**Viktor BRABEC** – Czech Academy of Sciences, Brno (Czech Republic)

11:00 SCE7 **The relation between famine exposure and schizophrenia explained by cross-chromosome regulation of DUSP22 promotor hypermethylation**

**Marco BOKS** – University of Utrecht (Netherlands)

11:15 *Coffee break and poster session*

### Session II “MuTaLig on CNS part A”

**Moderator: Fernanda BORGES (Portugal)**

11:45 PLM1 **Multi-target ligands: more effective and sustainable drugs for Alzheimer’s disease?**

**Maria Laura BOLOGNESI** – “Alma Mater” Università di Bologna (Italy)

12:15 PLM2 **Development of donecopride as a potential multi-target directed ligand for the treatment of Alzheimer’s**

**Christophe ROCHAIS** – CERMN, Université de Caen Normandie (France)

12:45 SCM1 **The role of the chromone scaffold in the development of novel multitarget agents in Alzheimer’s disease**

**Joana REIS** – University of Porto (Portugal)

13:00 *Lunch*

### Session III “EpiChemBio: Histone acylation and deacylation”

**Moderator: Philippe BERTRAND (France)**

14:00 SCE8 **Targeting protein lysine acetylation in inflammatory lung diseases**

**Frank DEKKER** – University of Groningen (Netherlands)

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- 14:15 SCE9 **Challenges in targeting histone acetyltransferases – A KAT8 case story**  
**Hannah WAPENNAAR** – University of Groningen (Netherlands)
- 14:30 SCE10 **In silico identification of isoform–selective HDAC inhibitors**  
**Kemal YELEKCI** – Kadir Has University, Istanbul (Turkey)
- 14:45 SCE11 **Revisiting non–ribosomal macrocyclic peptides: Discovery of class I HDAC inhibitors with pM affinities**  
**Christian OLSEN** – University of Copenhagen (Denmark)
- 15:00 SCE12 **Erasing the eraser: Treating parasitic disease with epigenetics**  
**Remy NAROZNY** – University of East Anglia, Norwich (UK)
- 15:15 SCE13 **Design and synthesis of novel Histone Deacetylase 6 zinc binding groups**  
**Leandro AVELAR** – University of Düsseldorf (Germany)
- 15:30 SCE14 **Double life of the multifunctional disordered TPPP/P25: physiological function**  
**Adél SZABÓ** – Hungarian Academy of Sciences, Budapest (Hungary)
- 15:45 *Coffee break and poster session*

## Session IV “MuTaLig on CNS part B” Moderator: **Rona RAMSAY (UK)**

- 16:15 PLM3 **Pain and Depression. Can be treated together?**  
**Dariusz MATOSIUK** – Medical University, Lublin (Poland)
- 16:45 PLM4 **Histamine H3 receptor antagonists acting as monoamine oxidase a/b inhibitors**  
**Holger STARK** – Heinrich Heine University Düsseldorf (Germany)
- 17:15 SCM2 **Novel multi–target ligands of aminergic GPCRS as potential antipsychotics**  
**Agnieszka KACZOR** – University of Lublin (Poland)
- 17:30 *Social program (optional)*

**Saturday September 23<sup>rd</sup> 2017**

## Session V “MuTaLig on Cancer and other targets” Moderator: **Danijel KIKELJ (Slovenia)**

- 8:45 PLM5 **Kinetic, structural and biochemical characterization of asparagine synthetase inhibitors**  
**Nigel RICHARDS** – University of Cardiff (UK)
- 9:15 SCM3 **From cholinesterase inhibitors to multifunctional anti–Alzheimer’s agents with anti–aggregating properties**  
**Barbara MALAWSKA** – Jagiellonian University Collegium Medicum, Kraków (Poland)
- 9:30 SCM4 **Targeting A<sub>1</sub> or/and A<sub>2A</sub> adenosine receptors and MAO–B to treat neurodegenerative diseases**  
**Katarzyna KIEĆ-KONONOWICZ** – Jagiellonian University Collegium Medicum, Kraków (Poland)
- 9:45 SCM5 **Crosstalk between PDK1 and aurora kinase A: development of small multi–target agents**  
**Simona SESTITO** – Università di Pisa (Italy)
- 10:00 SCM6 **Diindolylmethanes (DIMs) as novel anti–cancer agents targeting GPR84 and cannabinoid receptors**  
**Thanigaimalai PILLAIYAR**, University of Bonn (Germany)
- 10:15 SCM7 **ABAD (17β–HSD10) inhibitors and their effect on key mitochondrial enzymes in the research of neurodegenerative diseases or cancer treatment**  
**Kamil MUSILEK** – University of Hradec Kralove (Czech Republic)
- 10:30 SCM8 **Development of an Antibody Radiolabeled Drug Conjugate (ARDC) using 195mPt–Carboplatin for Theranostic Approach in Ovarian Cancer**  
**Lisa–Maria REČNIK** – CNRS & Université de Montpellier (France)
- 10:45 SCM9 **Resveratrol analog induces hydrogen sulfide formation and vasorelaxation**  
**Gunay YETIK-ANACAK**, Ege University, Izmir (Turkey)
- 11:00 *Coffee break and poster session*

## Session VI “EpiChemBio: Histone Methylation” Moderator: **A. GANESAN (UK)**

- 11:30 PLE1 **Regulatory elements and function of new lysine acylation pathways**  
**Yiming ZHAO** – University of Chicago, IL (USA)

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- 12:00 SCE15 **From DNA methyltransferase transition state analogues to chemical scaffolds for the inhibition of PRMT4**  
Paola ARIMONDO – CNRS, Toulouse (France)
- 12:15 SCE16 **The quinazoline ring as a privileged scaffold in epigenetic (poly)pharmacology: from dual G9a methyltransferase/LSD1 demethylase inhibitors to selective LSD1 inhibitors**  
Dante ROTILI – University La Sapienza, Roma (Italy)
- 12:30 SCE17 **The Clinically Used Iron Chelator Deferasirox is an Inhibitor of Epigenetic JumonjiC Domain-Containing Histone Demethylases**  
Martin ROATSCH – University of Leipzig (Germany)
- 12:45 SCE18 **Histone H3K27 Demethylase JMJD3 as a Therapeutic Target in Cancer**  
Patrick PERRIGUE – Polish Academy of Sciences, Poznan (Poland)
- 13:00 SCE19 **BLIMP1 and EZH2 in antibody secreting malignancies**  
Erna MAGNUSDOTTIR – University of Reykjavik (Iceland)
- 13:15 *Lunch*

## Session VII “MuTaLig on in silico methods”

Moderator: Maurizio BOTTA (Italy)

EpiChemBio MC meeting in room 7

- 14:15 SCM10 **Updates about the Chemotheca tool: status of implementation and use**  
Stefano ALCARO – Università “Magna Græcia” di Catanzaro (Italy)  
Fernanda BORGES – University of Porto (Portugal)
- 14:30 PLM6 **Selective 3D-Pharmacophore models Targeted for Aldose Reductase: Medicinal Chemistry Decision Support and Activity Profiling**  
Sharon BRYANT – Inte:Ligand GmbH, Vienna (Austria)
- 15:00 SCM11 **Carbonic Anhydrase VA for the treatment of obesity: in silico identification of new inhibitors and prediction of anti-obesity side effects of FDA-approved drugs**  
Isabella ROMEO – Università “Magna Græcia” di Catanzaro (Italy)
- 15:15 SCM12 **Pharmacophore models for identification of DNA gyrase and topoisomerase IV inhibitors and evaluation of their off-target binding**  
Tihomir TOMAŠIČ – University of Ljubljana (Slovenia)
- 15:30 SCM13 **Identification of G-quadruplex DNA/RNA binders: structure-based virtual screening and biophysical characterization**  
Carmine TALARICO – Università “Magna Græcia” di Catanzaro (Italy)
- 15:45 SCM14 **BitterPredict- A Tool for Predicting Bitterness of Drug candidate from its Chemical Structure**  
Ayana DAGAN WIENER – The Hebrew University of Jerusalem (Israel)
- 16:00 *Coffee break and poster session*

## Session VIII “EpiChemBio: Programming and Reprogramming ”

Moderator: Carmen JERONIMO (Portugal)

MuTaLig MC meeting in room 7

- 16:30 SCE20 **Induction of Antitumor and Antifungal agents by Epigenetic Modifiers in the endophytic fungal strain *Dimorphosporicola tragani***  
Jose Ruben TORMO – MEDINA Foundation, Granada (Spain)
- 16:45 SCE21 **Meta-analysis of commonly deregulated miRNAs in oral cancer**  
Katarina ZELJIC – University of Belgrade (Serbia)
- 17:00 SCE22 **RESPONSE project: Chromatin regulators as biomarkers and combinatorial drug targets in colorectal cancer therapy**  
Sonia FORCALES – Germans Trias i Pujol Research Institute, Badalona (Spain)
- 17:15 SCE23 **Studying the Epigenetic Mechanisms and Biomarkers in Neuropsychiatric Diseases**  
Roberto Carlos AGIS-BALBOA – Galicia Sur Health Research Institute – IISGS, Vigo (Spain)

- 17:30 **SCE24 Environmental programming of respiratory allergy: utility of a child's spit epigenome**  
**Sabine LANGIE** – Flemish Institute for Technological Research, Mol (Belgium)
- 17:45 **SCE25 May epigenetics explain the serine proteases involvement in grapevine resistance to *Plasmopara viticola*?**  
**Joana FIGUEIREDO** – University of Lisbon (Portugal)
- 18:00 **SCE26 Epigenetic biomarkers for liquid biopsy-based testing of prostate cancer patients**  
**Sonata JARMALAITÉ** – Vilnius University (Lithuania)
- 18:30 *Port wine & cheese*

**Sunday September 24<sup>th</sup> 2017**

**Session IX "EpiChemBio & MuTaLig common topics"**

**Moderator: Paola ARIMONDO (France)**

- 9:00 **SCC1 Dual targeting with epigenetics**  
**A GANESAN** – University of East Anglia, Norwich (UK)
- 9:15 **SCC2 Cross metathesis for the synthesis of HDAC inhibitors. Potential in multitarget drug design**  
**Philippe BERTRAND** – University of Poitiers (France)
- 9:30 **SCC3 Photoactivatable platinum(IV) complex targeting genomic DNA and histone deacetylases**  
**Jana KASPARKOVA** – Czech Academy of Sciences, Brno (Czech Republic)
- 9:45 **SCC4 New chalcone derivatives as HAT/HDAC modulators**  
**Leonardo PALAFERRI** – University La Sapienza, Roma (Italy)
- 10:00 **SCC5 Hybrid LSD1/JMJ Inhibitor As Therapeutic Option In Cancers With Deregulated Hormone-Receptor Signalling**  
**Rosaria BENEDETTI** – University of Campania "Luigi Vanvitelli", Napoli (Italy)
- 10:15 *Coffee break and poster session*

**Session X "EpiChemBio & MuTaLig common topics"**

**Moderator: Stefano ALCARO (Italy)**

- 10:45 **PLC1 Mitochondrial Toxicology in Drug Discovery and Development**  
**Paulo OLIVEIRA** – University of Coimbra (Portugal)
- 11:15 **SCC6 Naphthalene diimides and DNA: a variegated friendship**  
**Claudia SISSI** – Università di Padova (Italy)
- 11:30 **SCC7 Click chemistry a tool for medicinal chemistry**  
**Christian CAVÉ** – Université Paris Sud & CNRS (France)
- 11:45 **SCC8 Multi-level strategy for analysis of bioactive drug conformations**  
**Sanja ZIVANOVIC** – Institute for Research in Biomedicine, Barcelona (Spain)
- 12:00 **SCC9 Anticancer chalcones, selective or multitarget ligands?**  
**Bart ROMAN** – Ghent University (Belgium)
- 12:15 **SCC10 Smart screening libraries for academic use – General presentation – Building of an epigenetic library**  
**Marie Louise JUNG** – Prestwick Chemical, Strasbourg (France)

**Final Session: "EpiChemBio & MuTaLig round table and conclusions"**

**Moderators: Marianne ROTS (Netherlands) and Thierry LANGER (Austria)**

12:30

- A GANESAN** (CA1406 Chair) – University of East Anglia, Norwich (UK)  
**Stefano ALCARO** (CA15135 Chair) – Università "Magna Græcia" di Catanzaro (Italy)  
**Fernanda BORGES** – University of Porto (Portugal)  
**Lucia FORZI** – Science Officer CA1406 & CA15135 COST Actions, Brussels (Belgium)  
**Marie Louise JUNG** – Prestwick Chemical, Strasbourg (France)

