



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

“Portuguese Oncology Institute” of Porto (IPO Porto)

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

A bridge between EpiChemBio and MuTaLig COST Actions

www.epichembio.eu

www.mutalig.eu

Friday September 22nd 2017

8:30 Registration and poster setup

9:00 **Introduction to the Joint COST Action annual meeting**

Fernanda BORGES – University of 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 KLIMASIAUSKAS – 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, 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, Caen, (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 SCM2 **From cholinesterase inhibitors to multifunctional anti–Alzheimer’s agents with anti–aggregating properties**

Barbara MALAWSKA, Jagiellonian University Collegium Medicum, Kraków, (Poland)

13:15 *Lunch*

Session III “EpiChemBio: Histone acylation and deacylation”

Moderator: Philippe BERTRAND (France)

14:15 SCE8 **Targeting protein lysine acetylation in inflammatory lung diseases**

Frank DEKKER – University of Groningen (Netherlands)

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- 14:30 SCE9 **Challenges in targeting histone acetyltransferases – A KAT8 case story**
Hannah WAPENAAR – University of Groningen (Netherlands)
- 14:45 SCE10 **Exploring Conformational Space of Sirtuin 2– Molecular Dynamic Approach**
Katarina NIKOLIC – University of Belgrade (Serbia)
- 15:00 SCE11 **In silico identification of isoform–selective HDAC inhibitors**
Kemal YELEKCI – Kadir Has University, Istanbul (Turkey)
- 15:15 SCE12 **Revisiting non–ribosomal macrocyclic peptides: Discovery of class I HDAC inhibitors with picomolar affinities**
Christian OLSEN – University of Copenhagen (Denmark)
- 15:30 SCE13 **Erasing the eraser: Treating parasitic disease with epigenetics**
Remy NAROZNY – University of East Anglia (UK)
- 15:45 SCE14 **Design and synthesis of novel Histone Deacetylase 6 zinc binding groups**
Leandro AVELAR – University of Düsseldorf (Germany)
- 16:00 *Coffee break and poster session*

Session IV “MuTaLig on CNS part B”

Moderator: **Rona RAMSAY (UK)**

- 16:30 PLM3 **Pain and Depression. Can be treated together?**
Dariusz MATOSIUK, Medical University, Lublin (Poland)
- 17:00 PLM4 **Histamine H3 receptor antagonists acting as monoamine oxidase a/b inhibitors**
Holger STARK, Heinrich Heine University Düsseldorf, (Germany)
- 17:30 SCM3 **Novel multi–target ligands of aminergic GPCRS as potential antipsychotics**
Agnieszka KACZOR, University of Lublin (Poland)
- 17:45 SCM4 **Targeting A₁ or/and A_{2a} adenosine receptors and MAO–B to treat neurodegenerative diseases**
Katarzyna KIEĆ–KONONOWICZ, Jagiellonian University Collegium Medicum, Kraków, (Poland)

Saturday September 23rd 2017

Session V “MuTaLig on Cancer and other targets”

Moderator: **Danijel KIKELJ (Slovenia)**

- 9:00 PLM5 **Kinetic, structural and biochemical characterization of asparagine synthetase inhibitors**
Nigel RICHARDS, University of Cardiff (UK)
- 9:30 SCM5 **Crosstalk between PDK1 and aurora kinase A: development of small multi–target agents**
Simona SESTITO, Università di Pisa (Italy)
- 9:45 SCM6 **Diindolylmethanes (DIMs) as novel anti–cancer agents targeting GPR84 and cannabinoid receptors**
Thanigaimalai PILLAIYAR, University of Bonn (Germany)
- 10:00 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)
- 10:15 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)
- 10:30 SCM9 **Resveratrol analog induces hydrogen sulfide formation and vasorelaxation**
Gunay YETIK–ANACAK, Ege University, Izmir (Turkey)
- 10:45 *Coffee break and poster session*

Session VI “EpiChemBio: Histone Methylation”

Moderator: **A. GANESAN (UK)**

- 11:15 PLE1 **Title**
Name SURNAME – Affiliation (Country)
- 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 (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: Thierry LANGER (Austria)

- 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)

- 16:30 SCE20 **Induction of Antitumor and Antifungal agents by Epigenetic Modifiers in the endophytic fungal strain *Dimorphosporicola tragani***
Jose Ruben TORMO – MEDINA Foundation, Grenada (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 – University of 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 FIGUIREIDO – University of Lisbon (Portugal)

18:00 **SCE26 Epigenetic biomarkers for liquid biopsy–based testing of prostate cancer patients**
Sonia JARMALAITÉ, Vilnius University (Lithuania)

Sunday September 24th 2017

Session IX “EpiChemBio & MuTaLig common topics”

Moderator: Paola ARIMONDO (France)

9:00 **SCC1 Dual targeting with epigenetics**

A GANESAN, University of East Anglia (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, Rome (Italy)

10:00 **SCC5 Hybrid LSD1/JMJ Inhibitor As Therapeutic Option In Cancers With Deregulated Hormone–Receptor Signalling**

Rosaria BENEDETTI – University La Sapienza (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 Siena (Italy)

11:30 **SCC7 Click chemistry a tool for medicinal chemistry**

Christian CAVÉ, Université Paris Sud & CNRS, Châtenay–Malabry (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?**

Roman BART, Ghent University (Belgium)

12:15 **SCC10 TBC**

Maurizio BOTTA, Università di Siena (Italy)

Final Session: “EpiChemBio & MuTaLig round table and conclusions”

Moderators Marianne ROTS (Netherlands) and Maurizio BOTTA (Italy)

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)

13:15 *Lunch*

14:00 MC meetings EpiChemBio

15:00 MC meetings MuTaLig

