INTERNATIONAL WORKSHOP



CosmoCaixa, BARCELONA October 18-20, 2017

PRESENTATION:

The aim of this workshop is to review the state-of-the-art and broaden the knowledge on highthroughput analytical methods, data integration and modelling in Environmental Omics and Toxicology.

The main workshop topics will be the following:

- Transcriptomic and Genomic studies
- Metabolomic and Lipidomic studies
- Development of Chemometrics and Analytical Tools
- Data Integration and Modelling

We are pleased to invite you to participate in this workshop that will promote knowledge exchange and creation of new relationships and future collaborations.

ORGANIZING COMMITTEE:

This workshop is organized by researchers from the Institute of Environmental Assessment and Water Research (IDAEA-CSIC) under the scope of the ERC Advanced Grant (320737-CHEMAGEB) that aims to develop new chemometric and high-throughput analytical methods for Environmental Omics and Toxicology.

This act is also organized as part of the commemorative acts of the Research and Development Center (CID) 50th anniversary.

Carmen Bedia Bruno Campos Cristian Gomez-Canela Joaquim Jaumot Igor Marín de Mas Laia Navarro Martin Romà Tauler Website: <u>wenvomics2017.info</u>

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PRELIMINARY PROGRAM

Wednesday 18th

• 15.00-15.30 Workshop presentation and Opening (Romà Tauler, IP of the ERC Advanced Grant CHEMAGEB project, and Joan Grimalt, IDAEA and CID director)

• SESSION 1: GENOMICS AND TRANSCRIPTOMICS

PLENARY LECTURES

▶ 15.30-16.00

<u>James B. Brown.</u> University of California, Berkeley (California, USA). Research Interests: Genomics, Ecotoxicology, Statistical Machine Learning, Molecular Ecosystems Biology.

▶ 16.00-16.30

"Environmental Genomics in a Variable World: Defining the issues". <u>Christopher J. Martyniuk</u>. Center for Environmental and Human Toxicology & Department of Physiological Sciences (Florida, USA). Research Interests: Toxicology, Neuroendocrinology, Neurogenic Hypertension, Transcriptomic

Research Interests: Toxicology, Neuroendocrinology, Neurogenic Hypertension, Transcriptomics, Proteomics, Endocrine Disruption.

SHORT COMMUNICATIONS

▶ 16.30-16.50

"Methylation sensitive high resolution melting as a high throughput technique to detect DNA methylation alterations after exposures to endocrine disruptors" <u>Laia Navarro-Martín</u>. IDAEA-CSIC, Barcelona

16.50-17.20 Coffee break

▶ 17.20-17.40

"Development of microbial indicators of anaerobic digestion inhibition with omics" <u>Olivier Chapleur</u>. IRSTEA, Antony, France

▶ 17.40-18.00

"RNA-seq analysis of oysters exposed to different types of contaminants in the Brazilian coast" <u>Alfonso C. Dias Bainy</u>. Universidade Federal de Santa Catarina, Florianópolis, SC, Brazil

▶ 18.00-18.20

"Transcriptomic responses to temperature shifts in a mediterranean keystone sea urchin" <u>Rocío Pérez-Portela</u>. CEAB-CSIC, Blanes, Spain

FLASH-POSTER PRESENTATIONS

▶ 18.20-18.25 P01

"The human early life exposome (HELIX) project : Molecular Mechanisms. " <u>Marta Vives-Usano.</u> Centre for Genomic Regulation (CRG), Universitat Pompeu Fabra (UPF), Barcelona, Spain

▶ 18.25-18.30 P02

"Untargeted liquid chromatography coupled with high resolution mass spectrometry analysis of rice lipidome under hydric and heat stress"

<u>Meritxell Navarro-Reig.</u> Institute of Environmental Assessment and Water Research, CSIC, Barcelona, Spain

▶ 18.30-18.35 P03

"Assessment of endocrine disruptors effects on zebrafish embryos by untargeted metabolomics"

<u>Elena Ortiz-Villanueva.</u> Institute of Environmental Assessment and Water Research, CSIC, Barcelona, Spain

18.35-18.40 P04

"Phenotypic and lipidomic changes of green bean plants exposed to chlorpyrifos" <u>Carmen Bedia</u>. Institute of Environmental Assessment and Water Research, CSIC, Barcelona, Spain

> 18.40-18.45 P05

"Phenotypic and lipidomic changes of green bean plants exposed to chlorpyrifos" <u>Núria Dalmau.</u> Institute of Environmental Assessment and Water Research, CSIC, Barcelona, Spain

> 18.45-18.50 P06

"ROIMCR: a powerful data analysis strategy for LC-MS metabolomic data sets" <u>Eva Gorrochategui.</u> Institute of Environmental Assessment and Water Research, CSIC, Barcelona, Spain

18.50-18.55 P07

"Untargeted metabolomic processing of blood samples from preterm infants stored with RNA stabilization reagent" José David Piñeiro-Ramos. Instituto de Investigación Sanitaria La Fe (IIS La Fe), Valencia, Spain

▶ 18.55-19.00 P08

"Analysis of neurobehavioural data by chemometric methods in ecotoxicological studies" <u>Cristian Gómez-Canela.</u> Institute of Environmental Assessment and Water Research, CSIC, Barcelona, Spain

Thursday 19th

SESSION 2: METABOLOMICS AND LIPIDOMICS

PLENARY LECTURES

▶ 9.00-9.30

"Environmental Metabolomics: New Tools and Techniques to Measure the Exposome". <u>David Wishart</u>. Departments of Computing Science and Biological Sciences, University of Alberta (Edmonton, Canada).

Research Interests: Bioinformatics, Metabolomics, Structural Biology, Nanobiology, Synthetic Biology and Prion Biology.

▶ 9.30-10.00

"Metabolomics and Systems Biology in studies on Endocrine Disruptors". <u>Daniel Zalko</u>. Institut national de la recherche agronomique, INRA (Toulouse, France). Research Interests: Metabolism of Xenobiotics, Metabolic Networks, Metabolism, Genotoxicity of Xenobiotics.

▶ 10.00-10.30

"Efficacy of spectrochemical biomarkers to identify sublethal stress in environmental settings". <u>Francis L Martin</u>. Pharmacy and Biomedical Sciences, University of Central Lancashire (Preston, UK).

Research Interests: Genetic toxicology, bio-imaging and biospectroscopy.

10.30-11.00 Coffee break

SHORT COMMUNICATIONS

▶ 11.00-11.20

"Metabolomics reveals metabolic disorders in mice exposed to thirdhand tobacco smoke" <u>Noelia Ramírez</u>. University Rovira i Virgili, Tarragona, Spain

▶ 11.20-11.40

"Re-thinking ecotoxicology paradigms in the omics era" <u>Steven D. Melvin</u>. Griffith University, Southport, Australia

▶ 11.40-12.00

"Environmental effects of cyanobacterial blooms on fish: a metabolomic approach from experimental fish to natural population"

Marie Benjamin. Muséum National d'Histoire Naturelle, Paris, France

▶ 12.00-12.20

"Hybrid target/non-target profiling of biological samples for human metabolomics & exposomics studies"

James J. Harynuk. University of Alberta, Edmonton / Canada

▶ 12.20-12.40

"Identifying markers of lung cancer and cardiovascular disease with adductomics"

Sonia Dagnino. Imperial College London, London, UK

FLASH-POSTER PRESENTATIONS

▶ 12.40-12.45 P09

"The hide-and-seek challenge of 1H-13C HSQC NMR Metabolomics " <u>Francesc Puig-Castellví</u>. Institute of Environmental Assessment and Water Research, CSIC, Barcelona, Spain

▶ 12.45-12.50 P10

"Muscle lipids of fish may be affected by environmental pollution ?" <u>Maria Blanco.</u> Institute of Environmental Assessment and Water Research, CSIC, Barcelona, Spain

▶ 12.50-12.55 P11

" GPCA for improved multivariate analysis interpretation in lipidomics" <u>Sara Tortorella.</u> Molecular Horizon, Perugia, Italy

> 12.55-13.00 P12

"Mercury effects in salt marsh plants: alterations in the metabolome of *Halimione portulacoides* from a highly contaminated system"

Célia Fernandes. Department of Biology, University of Aveiro, Aveiro, Portugal

▶ 13.00-13.05 P13

"Metabolic flux analysis of glucose-lactate concomitant consumption in cho cell cultures" <u>Iván Martínez-Monge</u>. Universitat Autònoma de Barcelona, Bellaterra, Spain.

▶ 13.05-13.10 P14

"Bacterial volatiles as plant growth promoters-detection by the combined application of HS-SPME, GC-MS and MCR-ALS analysis " Paulo Cardoso. Department of Biology and CESAM, University of Aveiro, Portugal

• SESSION 3: CHEMOMETRICS

PLENARY LECTURES

▶ 15.00-15.30

"Common and Distinct Components in HeteroFusion". <u>Age Smilde</u>. Biosystems Data Analysis, Swammerdam Institute for Life Sciences, University of Amsterdam (Netherlands). Research Interests: Multiset data analysis and implementation in fields of biology.

▶ 15.30-16.00

"Approaches for the analysis of designed metabolomic data". <u>Federico Marini</u>. Dept. of Chemistry, University of Rome "La Sapienza" (Rome, Italy). Research Interests: Analytical Chemistry, Chemometrics.

▶ 16.00-16.30

"Multivariate analysis and integration of multi-OMICS data". Johan Trygg. Kemiska institutionen Umeå universitet, (Umeå, SE). Research Interests: Chemometrics in Metabolomics, Systems biology and Process Analytical Technologies.

16.30-17.00 Coffee break

SHORT COMMUNICATIONS

▶ 17.00-17.20

"A new omics for the environment: algal single-cell fingerprinting with flow cytometry" <u>Jeroen Jansen</u>. Institute for Molecules and Materials (IMM), Nijmegen, The Netherlands

▶ 17.20-17.40

"Regularized MANOVA for analysis of untargeted multi-factor metabolomics data" Jasper Engel. Institute for Molecules and Materials (IMM), Nijmegen, The Netherlands

▶ 17.40-18.00

"Urinary metabolome changes in preterm newborns fed with breast milk or donor breast milk" <u>Julia Kuligowski</u>. Instituto de Investigación Sanitaria La Fe (IIS La Fe), Valencia, Spain

▶ 18.00-18.20

"Hyperspectral imaging and chemometrics for environmental –omics" <u>Anna de Juan</u>. Universitat de Barcelona, Barcelona, Spain.

FLASH-POSTER PRESENTATIONS

▶ 18.20-18.25 P15

"Combined use of chemometrics and hyperspectral images for enviromental –omics studies applied to rice plants"

<u>Silvia Concolino</u>. Department of Chemical Engineering and Analytical Chemistry, University of Barcelona, Barcelona, Spain.

▶ 18.25-18.30 P16

"Assessment of the effect of time exposure of chlorpyrifos-oxon on different phenotypes of zebrafish embryos by hyperspectral imaging and chemometric methods" <u>Víctor Olmos</u>. Department of Chemical Engineering and Analytical Chemistry, University of

<u>Victor Olmos</u>. Department of Chemical Engineering and Analytical Chemistry, University Barcelona, Barcelona, Spain.

▶ 18.30-18.35 P17

"Assessment of rotational ambiguities effects in the resolution of sparse matrices: the case of mass spectrometry metabolomic data"

Joaquim Jaumot. Dept. of Environmental Chemistry, IDAEA-CSIC, Barcelona, Spain.

▶ 18.35-18.40 P18

"Modelling the duration of hypoxia: a plasma metabolite score<u>.</u>" <u>Ángel Sánchez-Illana</u>. Health Research Institute Hospital La Fe, Valencia, Spain

> 18.40-18.45 P19

"Evaluation of batch effect elimination using quality control replicates in LC-MS metabolite profiling"

Guillermo Quintás. Leitat Technological Center, Valencia, Spain

▶ 18.45-18.50 P20

"Outfitting the factory of the future with on-line analysis" <u>André van den Doel</u>. Institute of Molecules and Materials, Radboud University, The Netherlands

GALA DINNER

Friday 20th

SESSION 4: DATA INTEGRATION AND MODELLING

PLENARY LECTURES

▶ 9.00-9.30

"Multiomics data integration to unravel local gene regulatory networks". <u>Ana Conesa</u>. Intituto Principe Felipe (Valencia, Spain). Research Interests: Integration of multi-omics data, Genomics of gene expression.

> 9.30-10.00

"A systems medicine approach to target metabolic reprogramming associated to metastasis". <u>Marta Cascante</u>. Department of Biochemistry and Molecular Biology, Facultad de Biología, Universitat de Barcelona (Barcelona, Spain).

Research Interests: Integrative Systems Biology, Metabolomics and Cancer.

▶ 10.00-10.30

"Kinetic modelling within our GRASP: new strategies for fitting accurate network kinetic models".

Lars Keld Nielsen. Novo Nordisk Foundation Center for Biosustainability, Technical University of Denmark (Lyngby, Denmark).

Research Interests: Systems and Synthetic Biology.

- 10.30-11.00 Coffee break
- ▶ 11.00-11.30

"Enhancing integrative omics analysis with biological knowledge". <u>Alex Sánchez-Pla</u>. Genetics Microbiology & Statistics Department, University of Barcelona and Statistics and Bioinformatics Unit, Vall d'Hebron Institut de Recerca. Research Interests: Integrative Omics Analysis and Biomarker discovery.

SHORT COMMUNICATIONS

▶ 11.30-11.50

"Study of the effects of chronic exposure to aldrin in prostate cancer via multi-level approaches".

Igor Marín de Mas. Danmarks Tekniske Universitet. Lyngby, Denmark.

▶ 11.50-12.10

"Rexposome: a bioinformatic tool for characterizing multiple environmental factors and its association with different omics biomarkers and disease" <u>Carles Hernandez-Ferrer</u>. CREAL, UPF, CIBERESP, Barcelona, Spain

▶ 12.10-12.30

"Multidataset: an R package for encapsulating multiple data sets with application to omic data integration"

Juan R. González. CREAL, UPF, CIBERESP, Barcelona, Spain

- 12.30-12.50 Vendor Seminars
- 12.50-13.00 CLOSING REMARKS