COST ACTION CM1407

Challenging organic syntheses inspired by nature-from natural products chemistry to drug discovery

3rd Training School
La Laguna, Tenerife (Spain), 10-12 December, 2018

Computational modeling tools in drug discovery with natural products

Universidad de La Laguna

La Laguna, Tenerife (Spain)

Location and date	La Laguna, Tenerife (Spain), 10-12 December, 2018
Venue	Universidad de La Laguna
Participants	the Training School **is addressed to participants from all the Working Groups** (ECIs, PhDs, PhD students, graduate and undergraduate students).
Selection criteria	the Scientific Committee will select the Trainees according to geographical distribution (no more than one participant from a laboratory), multi-disciplinarily and gender. A Grant will be afforded to each selected Trainee.

Scientific Committee

Bruno Botta – Action Chair (Italy)
Juan I. Padron – IPNA – CSIC (Spain)
Ezequiel Quintana –IPNA – CSIC (Spain)
Ilza Pajeva – MC member (Bulgaria)
Petko Alov – (Inst. of Biophysics and Biomedical Engineering, Bulgaria)
Mattia Mori – MC member (Italy)

Local Organizing Committee

Juan Ignacio Padrón IPNA – CSIC
David Tejedor IPNA – CSIC
Fernando García-Tellado IPNA – CSIC
Víctor S. Martín ULL
Tomás Martín IPNA – CSIC
Romen Carrillo IPNA – CSIC
Fernando Pinacho-Crisóstomo ULL
Ezequiel Quintana IPNA – CSIC
Celina García ULL
Ignacio Brouard IPNA – CSIC

Sponsors

Cabildo de Tenerife
Universidad de La Laguna
Grupo especializado de Química Orgánica de la Real Sociedad Española de Química

Description

The main purpose of the Training School is:

- *to make effective use of computational modeling tools in the optimization of hit/leads up to pharmaceutically-relevant compounds, and to support the profiling phase defined in the Action objectives;*
- *to plan and to start the total synthesis of the most interesting hits/leads emerged by Action's collaborative projects and the Action screening;*
- *to train students to the challenging total syntheses.*

The Training School will focus on computational modeling and on the virtual screening, analysis, optimization and rational design of medicinally active agents. The topics addressed by the School will be: virtual library preparation, analysis, screening using both ligand- and structure-based methods, screening results analysis, chemical diversity, rational optimization in silico.