

**Report of the second Training School of COST Action CA15135**  
**Certosa di Pontignano (Siena, Italy) 21-26 May 2017**

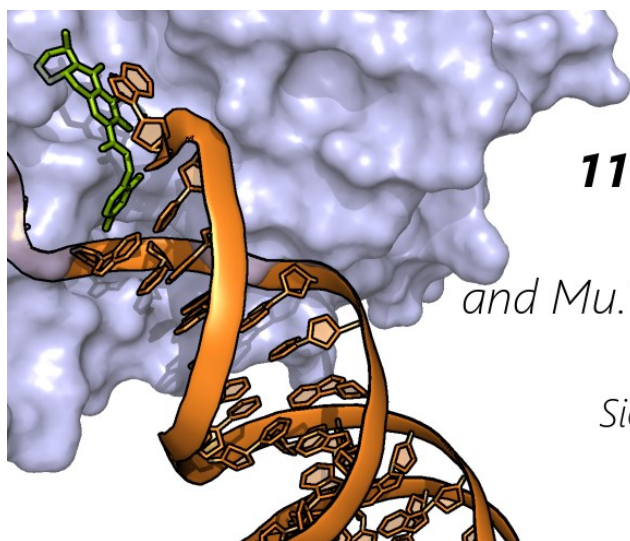
The first event of the second grant period of the COST Action CA15135 was performed as second Training School (TS) “11<sup>th</sup> European Workshop in Drug Design and MuTaLig Training School” from May 21 to 26 2017. The location chosen for this event is the extraordinary Certosa of Pontignano (Siena, Italy), that hosts from several decades high quality schools and congresses in all scientific fields at international level. The idea to join the EWDD event, started in its former edition more than 20 years ago, was to allow young investigators of all over the MuTaLig network to be educated on the most advanced techniques related to the computational area, that is the core of the COST Action CA15135 linking field. Actually, a consistent number of grants (30) were put in the budget of this second training school for young investigators, applying for this opportunity. Even if not all countries of the MuTaLig network applied, the assignment of all available grants was successfully performed and all participants were included in the theoretical and practical sessions organized in the week of May at the Certosa of Pontignano.

The training school setup was carried out by the team of Prof. Maurizio Botta, CA15135 MC member of Italy and EWDD organizer from the former edition. The faculty board of event was composed by renewed scientists working in the computational chemistry area in academic as well as industrial institutions, coming from Italy (Andrea Cavalli, Gabriele Costantino, Gabriele Cruciani, Stefano Moro and Francesco Ortuso), Europe (Zoe Cournia, Roderick Guigò, Gerhard Ecker, Dusanka Janezic, Hugo Kubinyi, Thierry Langer, Klaus Liedl, Elena Lo Piparo and Christian Ottmann), Israel (Idit Buch and Hanoch Senderowitz) and USA (Ruben Abagyan, Joanna Jansen, William Jorgensen, Dennis Liotta and Kenneth Merz). During the introduction a special reminder was dedicated to the memory of two scientists, Jim Snyder and Anna Tramontano, that gave important contributions to the success of the previous EWDD edition. A special session, strictly related to the MuTaLig COST Action, was organized during the third day of the meeting, introduced and moderated by the COST Action Chair Prof. Stefano Alcaro. During such a session, the Chemotheca, the web-based cheminformatics tool developed by Francesco Ortuso, associate professor at the Università Magna Græcia di Catanzaro, was presented in its updated version. This tool, accessible at the link [chemotheca.unicz.it](http://chemotheca.unicz.it), allows any participant to register and to insert his/her set of compounds in order to create and enrich a common molecular database, useful to speed up the identification of multi-targeting compounds within the MuTaLig scientific community of COST Action CA15135. More than 100 participants, mostly young researchers, were registered in the TS from 12 different COST countries (Austria, Czech Republic, France, Germany, Greece, Israel, Italy, Slovenia, Spain, Sweden, Switzerland and UK) and other 6 (Egypt, India, Morocco, Netherlands, Russian Federation and United States). The gender balance was quite good: 57,14 % (male) vs 42,86 % (female). Four working groups were respectively divided into computer rooms, respectively dedicated to following tools: Schrödinger (Maestro suite and much more), Inte:Ligand (LigandScout, not only Pharmacophores), Molecular Discovery & BiKi Technologies (Bioinformatics softwares and Molecular dynamics simulations) and Protein-Protein Interaction (Molecular modeling applied to 14-3-3 proteins). The TS activities ended with the summary and the selection of five best poster contributions, prepared by young investigator trainees. The atmosphere was friendly and appropriate for exchanging ideas and information about all TS topics among industrial and academic participants.

Catanzaro, May 30<sup>th</sup> 2017

Prof. Stefano Alcaro

Chair of COST Action CA15135



**XI EWDD**  
**11<sup>th</sup> European Workshop**  
**in Drug Design**  
**and Mu.Ta.Lig. Training School**

Siena, Certosa di Pontignano  
21 - 26 May 2017



TS logo

## Remembering Jim Snyder and Anna Tramontano



**James P. Snyder**  
(1939 - 2016)



**Anna Tramontano**  
(1957 - 2017)

Pictures of the remebered scientists

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Group Photo



Iuni Trist, ECI from the University of Siena, local organizer of 11<sup>th</sup> European Workshop in Drug Design and MuTaLig Training School

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Opening session by Prof. Francesco Frati, Rector of the University of Siena



Lectures and discussions in the conference hall (Sala Bracci)

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Case study "Molecular modeling tools applied to 14-3-3 proteins" (Sala Veranda)



Case study "LigandScout, Not only Pharmacophores" (Sala Focolare)

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Case study "Maestro suite and much more" (Sala Caratelli)



Case study "Bioinformatics softwares and Molecular dynamics simulations" (Sala Palio)

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Prof. Maurizio Botta, organizer of the meeting and MC member CA15135 for Italy, and Prof. Francesco Frati, Rector of the University of Siena.



Prof. Maurizio Botta, organizer of the meeting and MC member CA15135 for Italy, and Prof. Hanoch Senderowitz, WG2 leader.



Social moments among participants.



Social moments among participants.



Social dinner at Piazza del Campo (Siena).



Mu.Ta.Lig. COST Action speeds up the  
European Drug Discovery process