

# Nuclear Receptors: From *in silico* modelling to *in vivo* experiments

September 21<sup>st</sup>, 2012

Aula Magna "L. Cavalca", Chemistry Building  
University of Parma, Parma, Italy



**University of Parma**  
**Parma, Italy**

Laboratory of Molecular Modeling  
Department of Food Science



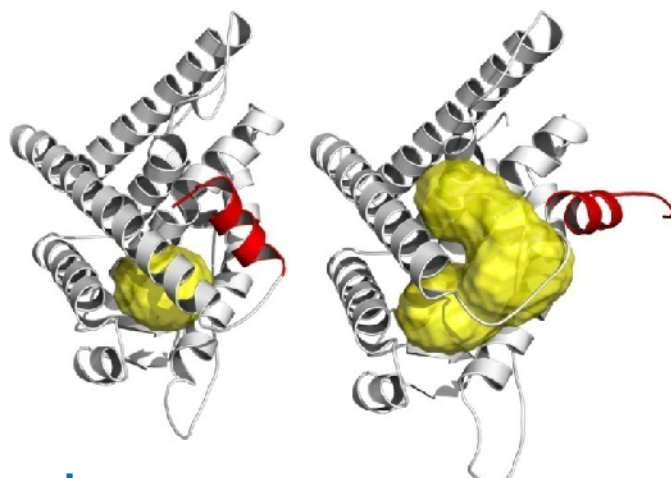
**University of Pisa**  
**Pisa, Italy**

Department of Medicinal Chemistry



**Virginia Commonwealth University**  
**Richmond, USA**

School of Pharmacy



**Universitat de Barcelona**  
**Barcelona, Spain**

Dept. Fisicoquímica,  
Facultat de Farmàcia

## PROGRAM

- |       |  |       |  |
|-------|--|-------|--|
| 8.00  | Registration   | 12.45 | Lunch time   |
| 9.30  | Welcome messages & Opening remarks   | 14.30 | <b>Structure network analysis to unveil the molecular communication in biological systems</b><br>F. Fanelli - University of Modena and Reggio Emilia, Italy                          |
| 10.00 | <b>Nuclear Receptors: Connecting Human Health to the Environment</b><br>Stefano Lorenzetti - Istituto Superiore di Sanita', Roma, Italy    | 15.00 | <b>Docking, screening and selectivity prediction for small molecule modulators of nuclear receptors</b><br>Ruben Abagyan - UCSD (University of California, San Diego), La Jolla, USA |
| 10.30 | <b>Pros and cons of structural data as base for computational investigations</b><br>Martin K. Safo - Virginia Commonwealth University, USA | 15.30 | Coffee Break   |
| 11.00 | Coffee Break   | 16.00 | <b>Fluorescent rats to test computational studies</b><br>Adriana Maggi - University of Milano, Italy   |
| 11.45 | <b>Protein Structure Prediction and Analysis with Constraint Logic Programming</b><br>Alessandro Dal Palu' - University of Parma, Italy    | 16.30 | <b>Estrogen Zearalenones &amp; Human Health Topics</b><br>Francesco Massart - St. Chiara University Hospital of Pisa, Italy  |
| 12.15 | <b>Molecular Dynamics: A Tool to Understand Nuclear Receptors</b><br>F. Javier Luque - Barcelona University, Spain                         | 17.00 | <b>Closing remarks</b><br>Glen E. Kellogg - Virginia Commonwealth University, USA  |