RESEARCH TOPICS

The studies have been focused on different nuclear receptors (FXR, PXR, TGR5, RXR, LXR), The kynurenine pathway, the DAF-12 nematodes’ nuclear receptor, tumorigenic proteins (MDM2, MDMX, p53), coagulation proteins such as thrombin and factor Xa, analysis of the molecular interactions displayed during the chromatographic separation process involving enantiomeric/diastereoisomeric analytes.

COLLABORATIONS

Strict collaboration with the synthesis group guided by the Prof. Cosimo Altomare of the Dipartimento di Scienze del Farmaco of the University of Bari.

National and international relationships of the computational modeling research together with the Prof. Antonio Macchiarulo.

PUBLICATIONS


COMMUNICATIONS


2. “Targeting the FXR nuclear receptor through a virtual screening approach” TUMA 30 June - 1 July 2011, Perugia, Italy.

3. “Study of the micelle formation process of bile acids through molecular dynamics simulations” CDDD, 21-23 November 2011, Aquila, Italy.

4. “Effects of Molecular Dynamics and Replica Exchange Molecular Dynamics in Sampling the Conformational Space of PARP-1” CDDD, 4-6 February 2013, Genova, Italy.

5. “Therapeutic Potential of a Novel Poly(ADP-ribose) Polymerase Inhibitor, Hydamtiq, in Human Pancreatic and Colon Cancers” at DDW2013, 18-21 May 2013, Orlando, USA.

6. “Environmentally friendly, sequential, one-pot synthesis of N-aryl-5-aminopyrazoles from anilines” at 13th SAYCS, 28-30 October 2013, Riccione, Italy.

7. “Insights in the PARP1 poisoning effect” at 1st High-Throughput Molecular Dynamics Workshop, 7-8 November 2013, Barcelona, Spain.

8. “1µs Molecular Dynamics Simulations to study the poisoning effect of the PARP-1 full length enzyme” CDDD, 4-6 March 2014, Verona, Italy.

TEACHING
Academic year 13-14: Appointed as teacher of “Analisi dei Medicinali I” of the Corso di Laurea in Farmacia in the Department of Pharmaceutical Sciences of the University of Perugia.