CURRICULUM VITAE

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/diasteroisomeric 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.

PUBBLICATIONS

1. M. De Candia, F. Liantonio, A. Carotti, R. De Cristofaro, C. Altomare, "Fluorinated Benzyloxyphenyl Piperidine-4-carboxamides with Dual Function against Thrombosis: Inhibitors of Factor Xa and Platelet Aggregation", *J. Med. Chem.,* **52** (2009), 1018-1028.

2. D. Bellocchi, A. Macchiarulo, A. Carotti, R. Pellicciari, "Quantum mechanics/molecular mechanics (QM/MM) modeling of the irreversible transamination of L-kynurenine to kynurenic acid: the round dance of kynurenine aminotransferase II", *Biochim Biophys Acta.,* 12 (2009), 1802-1812.

3. A. Carotti, A. Macchiarulo, N. Giacchè, R. Pellicciari, "Targeting the conformational transitions of MDM2 and MDMX: insights into key residues affecting p53 recognition", *Proteins*, **3** (2009), 524-535.

4. C. Dezi, A. Carotti, M. Magnani, M. Baroni, A. Padova, G. Cruciani, A. Macchiarulo, R. Pellicciari, "Molecular Interaction Fields and 3D-QSAR Studies of p53-MDM2 inhibitors Suggest Additional Features of Ligand-Target Interaction", *J. Chem. Inf. Model.*, **50** (2010),

1451-1465.

5. A. Macchiarulo, N. Giacchè, A. Carotti, F. Moretti, R: Pellicciari, "Expanding the horizon of chemotherapeutic targets: From MDM2 to MDMX (MDM4)", *MedChemComm*, **2** (2011), 455-465.

6. A. Gioiello, A. Macchairulo, A. Carotti, P. Filipponi, G. Costantino, G: Rizzo, L. Adorini, R. Pellicciari, "Extending SAR of bile acids as FXR ligands: Discovery of 23-N-(carbocinnamyloxy)-3a,7a-dihydroxy-6a-ethyl-24-nor-5b-cholan-23-amine", *Bioorg. Med. Chem.*, **19** (2011), 2650-2658.

7. R. Pellicciari, E. Camaioni, A. M. Gilbert, A. Macchiarulo, J. A. Bikker, F. Shah, J. Bard, G. Costantino, A. Gioiello, G. M. Robertson, P. Sabbatini, F. Venturoni, P. Liscio, A. Carotti, D. Bellocchi, A. Cozzi, A. Wood, C. Gonzales, M. M. Zaleska, J. W. Ellingboe, F. Moroni, "Discovery and characterization of novel potent PARP-1 inhibitors endowed with neuroprotective properties: From TIQ-A to HYDAMTIQ", *MedChemComm*, **2** (2011), 559-565.

8. M. Marinozzi, A. Carotti, E. Sansone, A. Macchiarulo, E. Rosatelli, R. Sardella, B. Natalini, G. Rizzo, L. Adorini, D. Passeri, F. De Franco, M. Pruzanski, R. Pellicciari, "Pyrazole[3,4-e][1,4]thiazepin-7-one Derivatives as a Novel Class of Farnesoid X Receptor (FXR) Agonists", *Bioorg. Med. Chem.,* **20** (2012), 3429-3445.

9. R. Sardella, A. Macchiarulo, A. Carotti, F. Ianni, M.E. Rubino, B. Natalini, "Chiral mobile phase in ligand-exchange chromatography of amino acids: exploring the copper(II) salt anion effect with a computational approach.", *J. Chromatogr. A.*, **1269** (2012), 316-324.

10. A. Macchiarulo, A. Carotti, M. Cellanetti, R. Sardella, A. Gioiello, "Navigations of Chemical Space to Further the Understanding of Polypharmacology in Human Nuclear Receptors", **4** (2013), 216-227.

11. M. Marinozzi, A. Carotti, R. Sardella, F. Buonerba, F. Ianni, B. Natalini, D. Passeri, G. Rizzo, R. Pellicciari, "Asymmetric Synthesis of the Four Diastereoisomers of a Novel Non-Steroidal Farnesoid X Receptor (FXR) Agonist: Role of the Chirality on the Biological Activity.", *Bioorg. Med. Chem.*, **21** (2013), 3780-3789.

12. A. A. Antolin, A. Carotti, R. Nuti, A. Hakkaya, E. Camaioni, J. Mestres, R. Pellicciari, A. Macchiarulo, "Exploring the effect of PARP-1 flexibility in docking studies.", *J. Mol. Graph. Model.*, **45C** (2013), 192-201.

13. P. Liscio, E. Camaioni, A. Carotti, R. Pellicciari, A. Macchiarulo, "From Polypharmacology to Target Specificity: The Case of PARP Inhibitors." *Curr. Top. Med. Chem.*,**13** (2013), 2939-

2954.

14. M. de Candia, F. Fiorella, G. Lopopolo, A. Carotti, M. R. Romano, M. D. Lograno, S. Martel, P. A.Carrupt, B. D. Belviso, R. Caliandro, C. Altomare, "Synthesis and Biological Evaluation of Direct Thrombin Inhibitors Bearing 4-(Piperidin-1-yl)pyridine at the P1 Position with Potent Anticoagulant Activity." *J. Med. Chem.,* **56** (2013), 8696-8711.

15. M. Marinozzi, G. Marcelli, A. Carotti, B. Natalini, "One-pot, telescoped synthesis of N-aryl-5-aminopyrazoles from anilines in environmentally benign conditions" *RSC Adv.*, **14** (2014), 7019-7023.

16. P. Liscio, A. Carotti, S. Asciutti, T. Karlberg, D. Bellocchi, L. Llacuna, A. Macchiarulo, S. A. Aaronson, H. Schüler, R. Pellicciari, E. Camaioni , "Design, Synthesis, Crystallographic Studies and Preliminary Biological Appraisal of New Substituted Triazolo[4,3-b]pyridazin-8-amine Derivatives as Tankyrase Inhibitors" *J. Med. Chem.*, DOI: 10.1021/jm401356.

COMMUNICATIONS

1. "Allosteric Modulations in Conditionally Permissive Nuclear Receptor Complexes: The Case of FXR/RXR Heterodimer" at EFMC- ISMC, 5-9 September 2010, Brussels, Belgium.

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.