

Andrea Carotti, PhD

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Education

February 00: Degree in Medicinal Chemistry at the University of Bari (Italy), with full marks and laude discussing the thesis: "Central benzodiazepinic receptor ligands: 3-D QSAR models and prediction of the intrinsic activity". Supervisor Prof. Cosimo Altomare.

March 03: Ph.D. thesis: "Innovative Computer-Assisted Approaches In Lead Finding And Optimization Of Neurological And Antithrombotic Drugs ". Supervisor Prof. Cosimo Altomare.

April 04: Appointed as post-doc fellow at the University of Bari.

September 06: Visiting period at the University of Perugia.

March 07: participant of the European Project FP6 PRIORITY LSH-2005-2.2.0-8: "Small-ligand libraries: improved tools for exploration and prospective antitumour therapy. DePPICT Project (Designing Therapeutic Protein- Protein Inhibitors for Brain Cancer Treatments)" Contract number: LSHC-CT-2007- 037834 (<http://www.deppict.eu/home.jsp>).

Apr 08: Appointed as Assistant Professor at the University of Perugia.

Teaching

Academic year 08-09: Appointed as teacher of "Introduzione alla Bioinformatica Genomica e Laboratorio di Bioinformatica" of the Corso di Laurea in Biotecnologie in the Facoltà di Scienze MM.FF.NN of the University of Perugia.

Academic year 10-11 and 11-12: Appointed as teacher of "Applicazioni computazionali per lo studio di biomacromolecole" of the Corso di Laurea in Biotecnologie in the Facoltà di Scienze MM.FF.NN of the University of Perugia.

Academic year 11-12: Appointed as teacher of "Analisi dei Medicinali II" of the Corso di Laurea in Farmacia in the Faculty of Pharmacy of the University of Perugia.

Academic years 12-13 until now: Appointed as teacher of "Analisi dei Medicinali I" of the Corso di Laurea in Farmacia in the Faculty of Pharmacy of the University of Perugia.

Awards

Dicember 11: Winner of 250000 hours of calculation in the ISCRA C calls of the CINECA Italian Institute.

Skills & Activities

Skills Computer Science, Virtual Screening, Docking Studies, Docking, Protein Dynamics, Molecular Docking, Molecular Dynamics, QSAR, Molecular Dynamics Simulation, Molecular Modeling, Clustering, Structure-based Drug Design, Drug Discovery

Languages English, Italian

Scientific Memberships

Interests Sports, music

Journal Publications

Stefano Giovagnoli, Donatella Pietrella, Lanfranco Barberini, Claudio Santi, Andrea Carotti, Alessandro di Michele, Maurizio Ricci: *Reshaping antibiotics through hydrophobic drug-bile acid ionic complexation enhances activity against Staphylococcus aureus biofilms*. International Journal of Pharmaceutics 06/2017;, DOI:10.1016/j.ijpharm.2017.06.008

Giuseppe Felice Mangiatordi, Domenico Alberga, Leonardo Pisani, Domenico Gadaleta, Daniela Trisciuzzi, Roberta Farina, Andrea Carotti, Gianluca Lattanzi, Marco Catto, Orazio Nicolotti: *A rational approach to elucidate human monoamine oxidase molecular selectivity*. European journal of pharmaceutical sciences: official journal of the European Federation for Pharmaceutical Sciences 02/2017; 101., DOI:10.1016/j.ejps.2017.02.008

Andrea Carotti, Federica Ianni, Emidio Camaioni, Lucia Pucciarini, Maura Marinozzi, Roccaldo Sardella, Benedetto Natalini: *N-Decyl-S-trityl-(R)-cysteine, a new chiral selector for "green" ligand-exchange chromatography applications*. Journal of pharmaceutical and biomedical analysis 02/2017;, DOI:10.1016/j.jpba.2017.02.009

Federica Lanni, Andrea Carotti, Roccaldo Sardella, Antonio Macchiarulo, Lucia Pucciarini, Benedetto Natalini: *Computational Studies For The Elucidation Of The Enantiomer Elution Order In Chiral Chromatography Systems*. Mini Reviews in Medicinal Chemistry 10/2016; 16(999)., DOI:10.2174/1389557516666161018143629

Roberto Pellicciari, Daniela Passeri, Francesca De Franco, Serena Mostarda, Paolo Filipponi, Carolina Colliva, Raffaella Maria Gadaleta, Placido Franco, Andrea Carotti, Antonio Macchiarulo, Aldo Roda, Antonio Moschetta, Antimo Gioiello: *Discovery of 3 α ,7 α ,11 β -Trihydroxy-6 α -ethyl-5 β -cholan-24-*oic Acid (TC-100), a Novel Bile Acid as Potent and Highly Selective FXR Agonist for Enterohepatic Disorders*. Journal of Medicinal Chemistry 09/2016; 59(19)., DOI:10.1021/acs.jmedchem.6b01126*

- Francesco Antonio Greco, Answald Bournique, Alice Coletti, Chiara Custodi, Daniela Dolciami, Andrea Carotti, Antonio Macchiarulo: *Docking Studies and Molecular Dynamic Simulations Reveal Different Features of IDO1 Structure*. *Molecular Informatics* 07/2016; 35(8-9), DOI:10.1002/minf.201501038
- Serkan Levent, Jana Gerstmeier, Abdurrahman Olgaç, Felix Nikels, Ulrike Garscha, Andrea Carotti, Antonio Macchiarulo, Oliver Werz, Erden Banoglu, Burcu Çalıřkan: *Synthesis and biological evaluation of C(5)-substituted derivatives of leukotriene biosynthesis inhibitor BRP-7*. *European Journal of Medicinal Chemistry* 07/2016; 122., DOI:10.1016/j.ejmech.2016.07.004
- Andrea Carotti, Federica Ianni, Stefano Sabatini, Alessandro Di Michele, Roccaldo Sardella, Glenn W. Kaatz, Wolfgang Lindner, Violetta Cecchetti, Benedetto Natalini: *The "racemic approach" in the evaluation of the enantiomeric NorA efflux pump inhibition activity of 2-phenylquinoline derivatives*. *Journal of pharmaceutical and biomedical analysis* 07/2016; 129., DOI:10.1016/j.jpba.2016.07.003
- Nóra Grecsó, Michal Kohout, Andrea Carotti, Roccaldo Sardella, Benedetto Natalini, Ferenc Fülöp, Wolfgang Lindner, Antal Péter, István Ilisz: *Mechanistic considerations of enantioselectivity on novel Cinchona alkaloid-based zwitterionic chiral stationary phases from the aspect of the separation of trans-paroxetine enantiomers as model compounds*. *Journal of Pharmaceutical and Biomedical Analysis* 05/2016; 124:164 - 173., DOI:10.1016/j.jpba.2016.02.043
- Erden Banoglu, Erřan Çelikođlu, Susanna Völker, Abdurrahman Olgaç, Jana Gerstmeier, Ulrike Garscha, Burcu Çalıřkan, Ulrich S. Schubert, Andrea Carotti, Antonio Macchiarulo, Oliver Werz: *4,5-Diarylisoaxazol-3-carboxylic acids: A new class of leukotriene biosynthesis inhibitors potentially targeting 5-lipoxygenase-activating protein (FLAP)*. *European Journal of Medicinal Chemistry* 02/2016; 113., DOI:10.1016/j.ejmech.2016.02.027
- Francesco Antonio Greco, Alice Coletti, Emidio Camaioni, Andrea Carotti, Maura Marinozzi, Antimo Gioiello, Antonio Macchiarulo: *The Janus-faced nature of IDO1 in infectious diseases: Challenges and therapeutic opportunities*. *Future medicinal chemistry* 12/2015; 8(1), DOI:10.4155/fmc.15.165
- Federica Ianni, Roccaldo Sardella, Andrea Carotti, Benedetto Natalini, Wolfgang Lindner, Michael Lämmerhofer: *Quinine-Based Zwitterionic Chiral Stationary Phase as a Complementary Tool for Peptide Analysis: Mobile Phase Effects on Enantio- and Stereoselectivity of Underivatized Oligopeptides*. *Chirality* 10/2015; 28(1), DOI:10.1002/chir.22541
- Daniela Passeri, Emidio Camaioni, Paride Liscio, Paola Sabbatini, Martina Ferri, Andrea Carotti, Nicola Giacchè, Roberto Pellicciari, Antimo Gioiello, Antonio Macchiarulo: *Concepts and Molecular Aspects in the Polypharmacology of PARP-1 Inhibitors*. *ChemMedChem* 10/2015; 11(12), DOI:10.1002/cmdc.201500391
- Federica Ianni, Andrea Carotti, Maura Marinozzi, Gloria Marcelli, Alessandro Di Michele, Roccaldo Sardella, Wolfgang Lindner, Benedetto Natalini: *Analytica Chimica Acta*. *Analytica chimica acta* 07/2015; 885:174-182., DOI:10.1016/j.aca.2015.06.001
- Maura Marinozzi, Gloria Marcelli, Andrea Carotti: *N-Aryl-5-aminopyrazole: A Versatile Architecture in Medicinal Chemistry*. *Mini Reviews in Medicinal Chemistry* 03/2015; 15(4), DOI:10.2174/1389557515666150312154536
- Andrea Carotti, Maura Marinozzi, Chiara Custodi, Bruno Cerra, Roberto Pellicciari, Antimo Gioiello, Antonio Macchiarulo: *Beyond Bile Acids: Targeting Farnesoid X Receptor (FXR) with Natural and*

Synthetic Ligands. Current Topics in Medicinal Chemistry 11/2014; 14(19):2129-2142., DOI:10.2174/1568026614666141112094058

Roccaldo Sardella, Andrea Carotti, Giuseppe Manfroni, Daniele Tedesco, Alma Martelli, Carlo Bertucci, Violetta Cecchetti, Benedetto Natalini: *Enantioresolution, stereochemical characterization and biological activity of a chiral large-conductance calcium-activated potassium channel opener*. Journal of Chromatography A 10/2014; 1363:162-168., DOI:10.1016/j.chroma.2014.06.020

Maura Marinozzi, Gloria Marcelli, Andrea Carotti, Benedetto Natalini: *ChemInform Abstract: One-Pot, Telescoped Synthesis of N-Aryl-5-aminopyrazoles from Anilines in Environmentally Benign Conditions..* ChemInform 10/2014; 4(14):7019-7023., DOI:10.1039/C3RA47541G

Paride Liscio, Andrea Carotti, Stefania Ascutti, Martina Ferri, Maira M Pires, Sara Valloscuro, Jacob Ziff, Neil R Clark, Antonio Macchiarulo, Stuart A Aaronson, Roberto Pellicciari, Emidio Camaioni: *Scaffold hopping approach on the route to selective tankyrase inhibitors*. European Journal of Medicinal Chemistry 10/2014; 87:611., DOI:10.1016/j.ejmech.2014.10.007

Jean-Rémy Marchand, Andrea Carotti, Daniela Passeri, Paolo Filipponi, Paride Liscio, Emidio Camaioni, Roberto Pellicciari, Antimo Gioiello, Antonio Macchiarulo: *Investigating the Allosteric Reverse Signalling of PARP Inhibitors with Microsecond Molecular Dynamic Simulations and Fluorescence Anisotropy*. Biochimica et Biophysica Acta (BBA) - Proteins & Proteomics 10/2014; 1844(10)., DOI:10.1016/j.bbapap.2014.07.012

Roccaldo Sardella, Antonella Lisanti, Andrea Carotti, Paolo Blasi, Wolfgang Lindner, Benedetto Natalini: *Ketoprofen enantioseparation with a Cinchona-alkaloid-based stationary phase: Enantiorecognition mechanism and release studies*. Journal of Separation Science 10/2014; 37(19):2696., DOI:10.1002/jssc.201400630

Emiliano Rosatelli, Andrea Carotti, Mariangela Ceruso, Claudiu T Supuran, Antimo Gioiello: *Flow synthesis and biological activity of aryl sulfonamides as selective carbonic anhydrase IX and XII inhibitors*. Bioorganic & Medicinal Chemistry Letters 06/2014; 24(15)., DOI:10.1016/j.bmcl.2014.05.086

Roccaldo Sardella, Andrea Carotti, Antimo Gioiello, Antonella Lisanti, Federica Ianni, Wolfgang Lindner, Benedetto Natalini: *Chromatographic separation of free dafachronic acid epimers with a novel triazole click quinidine-based chiral stationary phase*. Journal of Chromatography A 04/2014; 1339., DOI:10.1016/j.chroma.2014.02.080

Paride Liscio, Andrea Carotti, Stefania Ascutti, Tobias Karlberg, Daniele Bellocchi, Laura Llacuna, Antonio Macchiarulo, Stuart A Aaronson, Herwig Schüler, Roberto Pellicciari, Emidio Camaioni: *Design, Synthesis, Crystallographic Studies, and Preliminary Biological Appraisal of New Substituted Triazolo[4,3-b]pyridazin-8-amine Derivatives as Tankyrase Inhibitors*. Journal of Medicinal Chemistry 02/2014; 57(6)., DOI:10.1021/jm401356t

Paride Liscio, Emidio Camaioni, Andrea Carotti, Roberto Pellicciari, Antonio Macchiarulo: *From Polypharmacology to Target Specificity: The Case of PARP Inhibitors*. Current topics in medicinal chemistry 10/2013; 13(23)., DOI:10.2174/15680266113136660209

Modesto de Candia, Filomena Fiorella, Gianfranco Lopopolo, Andrea Carotti, Maria Rosaria Romano, Marcello Diego Lograno, Sophie Martel, Pierre Alain Carrupt, Benny D Belviso, Rocco Caliandro, Cosimo Altomare: *Synthesis and Biological Evaluation of Direct Thrombin Inhibitors Bearing 4-(Piperidin-*

1-yl)pyridine at the P1 Position with Potent Anticoagulant Activity. *Journal of Medicinal Chemistry* 10/2013; 56(21)., DOI:10.1021/jm401169a

Albert A Antolin, Andrea Carotti, Roberto Nuti, Aydie Hakkaya, Emidio Camaioni, Jordi Mestres, Roberto Pellicciari, Antonio Macchiarulo: *Exploring the effect of PARP-1 flexibility in docking studies*. *Journal of molecular graphics & modelling* 09/2013; 45C:192-201., DOI:10.1016/j.jmgm.2013.08.006

Maura Marinozzi, Andrea Carotti, Roccaldo Sardella, Federica Buonerba, Federica Ianni, Benedetto Natalini, Daniela Passeri, Giovanni Rizzo, Roberto 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*. *Bioorganic & medicinal chemistry* 04/2013; 21(13)., DOI:10.1016/j.bmc.2013.04.038

Antonio Macchiarulo, Andrea Carotti, Marco Cellanetti, Roccaldo Sardella, Antimo Gioiello: *Navigations of chemical space to further the understanding of polypharmacology in human nuclear receptors*. *Medicinal Chemistry Communication* 01/2013; 4(1):216-227., DOI:10.1039/c2md20157g

Roccaldo Sardella, Antonio Macchiarulo, Andrea Carotti, Federica Ianni, Maria Eugenia García Rubiño, Benedetto Natalini: *Chiral mobile phase in ligand-exchange chromatography of amino acids: Exploring the copper(II) salt anion effect with a computational approach*. *Journal of Chromatography A* 08/2012; 1269., DOI:10.1016/j.chroma.2012.08.018

Maura Marinozzi, Andrea Carotti, Emanuele Sansone, Antonio Macchiarulo, Emiliano Rosatelli, Roccaldo Sardella, Benedetto Natalini, Giovanni Rizzo, Luciano Adorini, Daniela Passeri, Francesca De Franco, Mark Pruzanski, Roberto Pellicciari: *Pyrazole[3,4-e][1,4]thiazepin-7-one derivatives as a novel class of Farnesoid X Receptor (FXR) agonists*. *Bioorganic & medicinal chemistry* 04/2012; 20(11):3429-45., DOI:10.1016/j.bmc.2012.04.021

Roberto Pellicciari, Emidio Camaioni, Adam M. Gilbert, Antonio Macchiarulo, Jack A. Bikker, Falgun Shah, Joel Bard, Gabriele Costantino, Antimo Gioiello, Graeme M. Robertson, Paola Sabbatini, Francesco Venturoni, Paride Liscio, Andrea Carotti, Daniele Bellocchi, Andrea Cozzi, Andrew Wood, Cathleen Gonzales, Margaret M. Zaleska, John W. Ellingboe, Flavio Moroni: *Discovery and characterization of novel potent PARP-1 inhibitors endowed with neuroprotective properties: From TIQ-A to HYDAMTIQ*. *Medicinal Chemistry Communication* 06/2011; 2(6):559-565., DOI:10.1039/C1MD00021G

Antimo Gioiello, Antonio Macchiarulo, Andrea Carotti, Paolo Filipponi, Gabriele Costantino, Giovanni Rizzo, Luciano Adorini, Roberto Pellicciari: *Extending SAR of bile acids as FXR ligands: Discovery of 23-N-(carbocinnamyloxy)-3 α ,7 α -dihydroxy-6 α -ethyl-24-nor-5 β -cholan-23-amine*. *Bioorganic & medicinal chemistry* 04/2011; 19(8):2650-8., DOI:10.1016/j.bmc.2011.03.004

Antonio Macchiarulo, Nicola Giacch, Andrea Carotti, Fabiola Moretti, Roberto Pellicciari: *Expanding the horizon of chemotherapeutic targets: From MDM2 to MDMX (MDM4)*. *Medicinal Chemistry Communication* 02/2011; 2(6-2040-25031):455-465., DOI:10.1039/C0MD00238K

R. Pellicciari, A. Macchiarulo, A. Gioiello, C. Thomas, E. Rosatelli, P. Filipponi, A. Carotti, R. Nuti, D. Shapiro, G. Rizzo, A. Roda, L. Adorini, M. Prusaski, K. Schoonjans, J. Auwerx: *Deconstructing bile acid signaling pathways*. *ACS National Meeting Book of Abstracts* 01/2011; 241.

R. Pellicciari, A. Gioiello, E. Camaioni, A. Macchiarulo, A. Gilbert, J. Bikker, G. Costantino, G. M. Robertson, F. Venturoni, A. Carotti, D. Bellocchi, A. Cozzi, A. Wood, C. Gonzales, M. Zaleska, J.

Ellingboe, M. Flavio: *HYDAMTIQ: A new, potent PARP-1 inhibitor with neuroprotective properties*. ACS National Meeting Book of Abstracts 01/2011; 241.

Cristina Dezi, Andrea Carotti, Matteo Magnani, Massimo Baroni, Alessandro Padova, Gabriele Cruciani, Antonio Macchiarulo, Roberto Pellicciari: *Molecular Interaction Fields and 3D-QSAR Studies of p53-MDM2 Inhibitors Suggest Additional Features of Ligand-Target Interaction*. Journal of Chemical Information and Modeling 08/2010; 50(8):1451-65., DOI:10.1021/ci100113p

Andrea Carotti, Antonio Macchiarulo, Nicola Giacchè, Roberto Pellicciari: *Targeting the conformational transitions of MDM2 and MDMX: Insights into key residues affecting p53 recognition*. Proteins Structure Function and Bioinformatics 11/2009; 77(3):524-35., DOI:10.1002/prot.22464

Daniele Bellocchi, Antonio Macchiarulo, Andrea Carotti, Roberto 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*. Biochimica et Biophysica Acta 09/2009; 1794(12):1802-12., DOI:10.1016/j.bbapap.2009.08.016

Modesto de Candia, Francesco Liantonio, Andrea Carotti, Raimondo De Cristofaro, Cosimo Altomare: *Fluorinated Benzyloxyphenyl Piperidine-4-carboxamides with Dual Function against Thrombosis: Inhibitors of Factor Xa and Platelet Aggregation*. Journal of Medicinal Chemistry 03/2009; 52(4):1018-28., DOI:10.1021/jm801141f

Roberto Pellicciari, Francesco Venturoni, Daniele Bellocchi, Andrea Carotti, Maura Marinozzi, Antonio Macchiarulo, Laura Amori, Robert Schwarcz: *Sequence Variants in Kynurenine Aminotransferase II (KAT II) Orthologs Determine Different Potencies of the Inhibitor S-ESBA*. ChemMedChem 08/2008; 3(8):1199-202., DOI:10.1002/cmdc.200800109

Orazio Nicolotti, Teresa Fabiola Miscioscia, Andrea Carotti, Francesco Leonetti, Angelo Carotti: *An Integrated Approach to Ligand- and Structure-Based Drug Design: Development and Application to a Series of Serine Protease Inhibitors*. Journal of Chemical Information and Modeling 07/2008; 48(6):1211-26., DOI:10.1021/ci800015s

Andrea Carotti, Marco Catto, Francesco Leonetti, Francesco Campagna, Ramón Soto-Otero, Estefanía Méndez-Alvarez, Ulrike Thull, Bernard Testa, Cosimo Altomare: *Synthesis and Monoamine Oxidase Inhibitory Activity of New Pyridazine-, Pyrimidine- and 1,2,4-Triazine-Containing Tricyclic Derivatives*. Journal of Medicinal Chemistry 12/2007; 50(22):5364-71., DOI:10.1021/jm070728r

Andrea Carotti, Modesto de Candia, Marco Catto, Tatiana N Borisova, Alexey V Varlamov, Estefanía Méndez-Alvarez, Ramón Soto-Otero, Leonid G Voskressensky, Cosimo Altomare: *Ester derivatives of annulated tetrahydroazocines: A new class of selective acetylcholinesterase inhibitors*. Bioorganic & Medicinal Chemistry 11/2006; 14(21):7205-12., DOI:10.1016/j.bmc.2006.06.055

Marco Catto, Orazio Nicolotti, Francesco Leonetti, Andrea Carotti, Angelo Danilo Favia, Ramón Soto-Otero, Estefanía Méndez-Alvarez, Angelo Carotti: *Structural Insights into Monoamine Oxidase Inhibitory Potency and Selectivity of 7-Substituted Coumarins from Ligand- and Target-Based Approaches*. Journal of Medicinal Chemistry 09/2006; 49(16):4912-25., DOI:10.1021/jm060183l

Raimondo De Cristofaro, Andrea Carotti, Sepideh Akhavan, Roberta Palla, Flora Peyvandi, Cosimo Altomare, Pier Mannuccio Mannucci: *The natural mutation by deletion of Lys9 in the thrombin A-chain*

affects the PKa value of catalytic residues, the overall enzyme's stability and conformational transitions linked to Na binding. FEBS Journal 02/2006; 273(1):159-69., DOI:10.1111/j.1742-4658.2005.05052.x

Agostino De Marco, Modesto De Candia, Andrea Carotti, Saverio Cellamare, Erica De Candia, Cosimo Altomare: *Lipophilicity-related inhibition of blood platelet aggregation by nipecotic acid anilides.* European Journal of Pharmaceutical Sciences 07/2004; 22(2-3):153-64., DOI:10.1016/j.ejps.2004.03.003

Raimondo De Cristofaro, Sepideh Akhavan, Cosimo Altomare, Andrea Carotti, Flora Peyvandi, Pier Mannuccio Mannucci: *A Natural Prothrombin Mutant Reveals an Unexpected Influence of A-chain Structure on the Activity of Human -Thrombin.* Journal of Biological Chemistry 04/2004; 279(13):13035-43., DOI:10.1074/jbc.M312430200

Andrea Carotti, Cosimo Altomare, Luisa Savini, Luisa Chiasserini, Cesare Pellerano, Maria P Mascia, Elisabetta Maciocco, Fabio Busonero, Manuel Mameli, Giovanni Biggio, Enrico Sanna: *High affinity central benzodiazepine receptor ligands. Part 3: Insights into the pharmacophore and pattern recognition study of intrinsic activities of pyrazolo[4,3-c]quinolin-3-ones.* Bioorganic & Medicinal Chemistry 12/2003; 11(23):5259-72., DOI:10.1016/S0968-0896(03)00527-3

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Angelo Carotti, Antonio Carrieri, Stefano Chimichi, Marco Boccalini, Barbara Cosimelli, Carmela Gnerre, Andrea Carotti, Pierre Alain Carrupt, Bernard Testa: *Natural and synthetic geiparvarins are strong and selective MAO-B inhibitors. Synthesis and SAR studies.* Bioorganic & Medicinal Chemistry Letters 01/2003; 12(24):3551-5., DOI:10.1016/S0960-894X(02)00798-9

Antonio Carrieri, Andrea Carotti, M Letizia Barreca, Cosimo Altomare: *Binding models of reversible inhibitors to type-B monoamine oxidase.* Journal of Computer-Aided Molecular Design 12/2002; 16(11):769-78., DOI:10.1023/A:1023815426730

Oral Communications

Title: "Targeting the FXR nuclear receptor through a virtual screening approach". XXX Convegno Interregionale Toscana-Umbria-Marche-Abruzzo (TUMA), Perugia, Italia, 2011, 30 Giugno -1 Luglio.

Title: "Study of the micelle formation process of bile acids through molecular dynamics simulations" Computationally Driven Drug Discovery Meeting (CDDD), 21-23 Novembre, 2011, Aquila, Italia.

Title: "Effects of Molecular Dynamics and Replica Exchange Molecular Dynamics in Sampling the Conformational Space of PARP-1" Computationally Driven Drug Discovery Meeting (CDDD), 4-6 Febbraio, 2013, Genova, Italia.

Title: "1 μ s Molecular Dynamics Simulations to study the poisoning effect of the PARP-1 full length enzyme" Computationally Driven Drug Discovery Meeting (CDDD), 4-6 Marzo, 2014, Verona, Italia.

Title: "Investigating the Allosteric Reverse Signalling of PARP Inhibitors with Microsecond Molecular Dynamic Simulations and Fluorescence Anisotropy". Invited Speaker at Summer School in Biotechnology - Molecular Aspects of Chemotherapy, 25-26 Settembre, 2014, Danzica, Polonia.

Title: "PHARMACOINFORMATICS IN DRUG R&D PROCESS". GPSS - 1st International Gazi Pharma Symposium Series, 12-15 Novembre, 2015, Antalya, Turchia.

Title: "Successful rate gain by combination of multiple techniques". Invited Speaker at International Bioinformatics Summer School - Resources and Technique in Computational Drug Discovery, 23-26 Maggio, 2016, Tangeri, Marocco.

Title: "Computational Modeling Overview and Evolution". Invited Speaker at International Bioinformatics Summer School - Resources and Technique in Computational Drug Discovery, 23-26 Maggio, 2016, Tangeri, Marocco.