# Antonella Ciancetta

Via G. Amendola 138, 64020, Bellante - Teramo, Italy

antonella.ciancetta +39-3929256622 antonella.ciancetta@unipd.it

## Profile

- ✓ Proficiency in dealing with a broad variety of methods and software packages
- ✓ Experience with ADME/Tox predictions, Docking and QM calculations
- ✓ Personal attributes of enthusiasm to learn new methods and eagerness to work on innovative projects

## Education and Training

**Ph.D. Degree in Drug Sciences, "Doctor Europaeus"** (15th Dec 2010)
School of advanced studies "G. d'Annunzio", Chieti – Italy
Thesis: "Density Functional Theory and combined QM/MM studies on selected transition metal based anticancer complexes" *Theoretical studies of: i) Carboplatin reactions with relevant biological nucleophiles; ii) the binding of RAPTA analogues to Cathepsin B.*

**Master's Degree in Pharmaceutical Chemistry and Technology** (17th Oct 2007)
Final mark : 110/110 with honours, University "G. d'Annunzio", Chieti – Italy
Thesis: "Modelling of ADMET properties using QM descriptors" *Investigation of three ADMET properties: i) permeation through the Blood Brain Barrier; ii) interaction with P-Glycoprotein; iii) mutagenic properties of a set of aromatic anilines.*

**Training as pharmacist** (Jan – Apr 2007)
Apotheke Dr. Mack, Zeppelinring 7, 88400 Biberach an der Riss – Germany

**High School Diploma** (17th Jul 2002)
Final mark : 100/100, Liceo Scientico "A. Einstein", Teramo – Italy

## Research Experience

**PostDoc** (Apr 2012 - )
Molecular Modeling Section (MMS), University of Padova, Padua – Italy
Project: Developing a novel GPCR/kinase multitargeting approach in cancer therapy using an integrated in silico strategy

**PostDoc** (Feb – Oct 2011 )
Computational Chemistry Group, University "G. d'Annunzio", Chieti – Italy
Project: Theoretical study of the in vivo activation mechanism of Pt-based complexes with anticancer activity

**Visiting Scientist** (Aug 2011)
Institut für Chemie, Humboldt Universität zu Berlin – Germany
Project: Effective potential energy surfaces scans for transition states searches

**Visiting Ph.D. student**

- ✓ Department of Theoretical Chemistry, Lund University – Sweden (Mar – May 2010)
  Project: QM/MM study of the binding of Ruthenium(II)-arene compounds with Cathepsin B
- ✓ Abteilung für Theoretische Chemie, Universität Tübingen – Germany (Sep – Oct 2009)
  Project: Interaction of Ruthenium(II)-arene (RAPTA) compounds with Cathepsin B
- ✓ Molecular Modelling Section (MMS), University of Padova – Italy (Oct 2008 – Mar 2009)
  Project: In Silico Modelling of Volume of Distribution using MEP 3D autocorrelated descriptors

**Research Fellowship as undergraduate student** (Nov 2006 – Apr 2007)
Department of Lead Discovery, Boehringer Ingelheim Pharma, Biberach and der Riss – Germany
Project: Modelling of ADMET properties using QM descriptors

## Skills

**Languages**: Fluent in Italian (mother tongue), German and English

**Software Packages**:
- ✓ Visualization Tools: Maestro, MOE, Molden, Rasmol
- ✓ QM/MM: Qsite, ComQum
- ✓ Quantum Mechanics: Jaguar, Gaussian, Turbomole, Q-chem, Spartan, VAMP
- ✓ 3D structure generator: CoRiNa
- ✓ Descriptors calculation: ADRIANACode, VolSurf, ParaSurf, ADC/Labs
- ✓ Multivariate Data Analysis: SIMCA-P, The Unscrambler
- ✓ Molecular Mechanics: MOE, Macromodel, Impact
- ✓ Docking and Scoring: Autodock, PLANTS, Glide, Gold, MOE, Molegro
- ✓ Homology modelling: MOE, Prime
- ✓ Pharmacophore modelling: Phase
- ✓ Programming languages: Basics of Fortran95
- ✓ Molecular Dynamics Simulation: Amber

## List of Publications

**1)** A. Casini, F. Edafe, M. Erlandsson, L. Gonsalvi, **A. Ciancetta**, N. Re, A. Ienco, L. Messori, M. Peruzzini, and P. J. Dyson, "Rationalization of the inhibition activity of structurally related organometallic compounds against drug target cathepsin B by DFT", *Dalton Transactions* (2010), **39**, 5556-5563

**2)** **A. Ciancetta**, C. Coletti, A. Marrone and N. Re, "Activation of Carboplatin by Chloride ions: A Theoretical Investigation", *Theoretical Chemistry Accounts* (2011), **129**, 757-769

**3)** **A. Ciancetta**, S. Genheden and U. Ryde, "QM/MM study of the binding of RAPTA ligands to cathepsin B", *Journal of Computer-Aided Molecular Design* (2011), **25**, 729-742

**4)** A.P. Martins, A. Marrone, **A. Ciancetta**, A.G. Cobo, M. Echevarría, T.F. Moura, N. Re, A. Casini and G. Soveral, "Targeting Aquaporin Function: Potent Inhibition of Aquaglyceroporin-3 by a Gold-based Compound", *PLoS ONE* (2012), **7**, art. n° e37435

**5)** F. Heims, V. Mereacre, **A. Ciancetta**, S. Mebs, A.K. Powell, C. Greco and K. Ray "Synthesis, characterisation and reactivity of a heterodinuclear iron(III)-copper(II) complex based on an asymmetric dinucleating ligand system", *European Journal of Inorganic Chemistry* (2012), **29**, 4565-4569

**6)** **A. Ciancetta**, C. Coletti, A. Marrone and N. Re, "Activation of Carboplatin by Carbonate", *Dalton Transactions* (2012) , **41**, 12960-12969

**7)** S. Federico, **A. Ciancetta**, D. Sabbadin, S. Paoletta, G. Pastorin, B. Cacciari, K.N. Klotz, S. Moro, and G. Spalluto "Exploring the Directionality of 5 Substitutions in a New Series of 5- Alkylaminopyrazolo[4,3-*e*]1,2,4-triazolo[1,5-*c*]pyrimidine as a Strategy To Design Novel Human $A_3$ Adenosine Receptor Antagonists", *Journal of Medicinal Chemistry*(2012), **55**, 9654-9668

**8)** L. Squarcialupi, V. Colotta, D. Catarzi, F. Varano, G. Filacchioni, K. Varani, C. Corciulo, F. Vincenzi, P. A. Borea, C. Ghelardini, L. Di Cesare Mannelli, **A. Ciancetta**, and S. Moro "2-Arylpyrazolo[4,3-*d*]pyrimidin-7-amino Derivatives As New Potent and Selective Human $A_3$ Adenosine Receptor Antagonists. Molecular Modeling Studies and Pharmacological Evaluation", *Journal of Medicinal Chemistry*(2013), **56**, 2256-2269

**9)** A. P. Martins, **A. Ciancetta**, A. de Almeida, A. Marrone, N. Re, G. Soveral, and A. Casini "Aquaporin Inhibition by Gold(III) Compounds: New Insights", *ChemMedChem*(2013), 8, 1086-1092

**10)** M. Bacilieri, **A. Ciancetta**, S. Paoletta, S. Federico, S. Cosconati, B. Cacciari, S. Taliani, F. Da Settimo, E. Novellino, K. N. Klotz, G. Spalluto, and S. Moro "Revisiting a receptor-based pharmacophore hypothesis for human $A_{2A}$ adenosine receptor antagonists" *Journal of Chemical Information and Modeling* (2013), 53, 1620-1637

**11)** D. Sabbadin, **A. Ciancetta**, S. Moro "Bridging molecular docking to membrane molecular dynamics to investigate GPCR-ligand recognition: the human $A_{2A}$ adenosine receptor as a key study" *Journal of Chemical Information and Modeling* (2013), submitted

**12)** L. Calderan, S. Castellano, A. M. Balzano, D. Saggioro, C. Milite, G. Deganutti, **A. Ciancetta**, G. Sbardella, C. R. Rossi, S. Moro and L. Quintieri "Design, Synthesis and Preliminary Biological Evaluation of Salycylbenzoimidazoles Structurally Related to Sulfasalazine as Inhibitors of Human Glutathione Trasferase P1-1" *In preparation*

**13)** A. Ciancetta and S. Moro, "The umane adenosine $A_{2A}$ receptor: a docking benchmark study" *In preparation*

## References

These persons are familiar with my professional qualifications:


**Prof. Stefano Moro** Molecular Modeling Section (MMS), Via Marzolo 5 35131- Padova, Italy
Phone: +39 049 827 5704
E-mail: stefano.moro@unipd.it

**Prof. Ulf Ryde** Department of Theoretical Chemistry, Lund University, Chemical Centre, P. O. Box 124 S-221 00, Lund - Sweden
E-mail: Ulf.Ryde@teokem.lu.se

**Dr. Franco Lombardo** Novartis Institutes for Biomedical Research, Building 600, 1B-123, 250 Massachusetts Avenue, Cambridge, MA 02139 – USA
E-mail: franco.lombardo@novartis.com

**Dr. Jan Kriegl** Boehringer Ingelheim Pharma GmbH & Co. KG, Birkendorferstrasse 65, D-88397, Biberach and der Riss - Germany
E-mail: jan.kriegl@boehringer-ingelheim.com

**Prof. Nazzareno Re** Dipartimento di Scienze del Farmaco, Università "G. d'Annunzio", Via dei Vestini 31 66100 Chieti – Italy
Phone : +39 0871 3554603
E-mail: nre@unich.it