

Alberto Massarotti

Curriculum vitae

PERSONAL DATA

Address Novara, Italy

BIO AND EDUCATION

He received his Degree in Biotecnologie Mediche e Farmaceutiche in 2006 at the Università del Piemonte Orientale. In the same year he began a Ph.D. under the supervision of Prof. Giovanni Sorba. In 2007 he spent six months in the laboratory of Prof. Roberto Pellicciari (Dipartimento di Chimica e Tecnologia del Farmaco, Perugia, Italy), working on 3DQSAR of bile acids as agonist of farnesoid X receptor. Between 2008 and 2009 he has spent one year in the laboratory of Dr. Andrea Brancale (Cardiff University), working on new methodologies in *de novo* drug design. He received his doctoral degree in 2009. After a post-doc period, he became Assistant Professor and he is now Associate Professor in Medicinal Chemistry at the Dipartimento di Scienze del Farmaco of the Università del Piemonte Orientale.

UNIVERSITY CAREER

2019-	Associate professor, Università del Piemonte Orientale
2016-2019	Assistant professor, Università del Piemonte Orientale
2015-2016	Post-doctoral fellow, Università del Piemonte Orientale
2012-2015	Assistant professor, Università del Piemonte Orientale
2009-2012	Post-doctoral fellow, Università del Piemonte Orientale

MAIN FIELDS OF INTEREST

1. Computer aided drug design
2. Cystic fibrosis
3. Tubulin

CURRENT ISSUES OF RESEARCH

1. Computer aided drug design

Computer aided drug design will be able to predict affinity of compounds before been synthesized saving time and cost. This project includes the development and application of novel computational methodologies to discover new lead compounds.

2. Cystic fibrosis

Cystic fibrosis (CF) is the most common autosomal recessive genetic disease of the Caucasian population in the United States and Europe. The most affected target is the respiratory system, in which the reduced activity of the channel results in obstruction of small airways that, together with airway inflammation and infections, eventually lead to respiratory failure and death in 80% of CF patients. The ultimate goal of this project is to validate the therapeutic benefits of a small-molecule peptidomimetic activator. This would eventually open new therapeutic horizons for the vast majority of CF patients.

3. Tubulin

Combretastatin A-4 is a well-known lead compounds acting as inhibitors of tubulin. Despite their interesting biological properties, it has shown to possess some weak points which might stop its use in clinic. In particular, the double bond is configurationally unstable and under the influence of light, heat and protic media can isomerize to give origin to the inactive trans isomer. The goal of this project is to design analogues of combretastatin A-4 using molecular modelling techniques. All the synthesized compounds will be biologically evaluated on different tumoral cell lines to evaluate their cytotoxicity.

CURRENT FUNDED PROJECTS

PROGRAMME	FUNDED PROJECT
Cariplo Foundation research grant "Biomedical research conducted by young researchers 2015".	<p><u>"Discovery of new PI3Kgamma scaffold activity disruptor via molecular dynamics, virtual screening and click chemistry to identify novel treatments for cystic fibrosis"</u> http://www.fondazionecariplo.it</p> <p><i>Cystic fibrosis (CF) is the most common autosomal recessive genetic disease of the Caucasian population in USA and Europe, affecting 70000 people worldwide. CF patients have severe clinical complications that affect several organs. The underlying cause of CF is a mutation in the gene encoding a protein kinase A (PKA)-stimulated chloride channel, the CFTR. The ultimate goal of this project is to validate the therapeutic benefits of a small-molecule peptidomimetic activator of PKA in CF models.</i></p>

TOP FIVE PAPERS

1. Levré D., Arcisto C., Mercalli V., **Massarotti A.*** ZINClick v.18: Expanding Chemical Space of 1,2,3-Triazoles. *J. Chem. Inf. Model*, **2019**, *59*, 1697-1702. DOI: 10.1021/acs.jcim.8b00615
2. Opassi G.,[§] Gesù A.,[§] **Massarotti A.*** The hitchhiker's guide to the chemical-biological galaxy. *Drug Discovery Today*, **2018**, *23*, 565-574. DOI: 10.1016/j.drudis.2018.01.007
3. **Massarotti A.**,[§] Coluccia A.^{§,*} An in-silico approach aimed to clarify the role of Y181C and K103N HIV-1 reverse transcriptase mutations versus Indole Aryl Sulphones. *J. Mol. Graph. Model.*, **2016**, *63*, 49-56. DOI: 10.1016/j.jmglm.2015.11.013
4. **Massarotti A.***, Aprile S.,* Mercalli V., Del Grosso E., Grosa G., Sorba G., Tron G.C. Are 1,4- and 1,5-disubstituted-1,2,3-triazoles good pharmacophoric groups? *ChemMedChem*, **2014**, *9*, 2497-2508. DOI: 10.1002/cmdc.201402233
5. **Massarotti A.***, Brunco A., Sorba G., Tron G.C.* ZINClick: a database of 16 million novel, patentable and readily synthesizable 1,4-disubstituted triazoles *J. Chem. Inf. Model*, **2014**, *54*, 396-406. DOI: 10.1021/ci400529h

AWARDS

1. "Divisione di Chimica Farmaceutica" Prize of the Italian Chemical Society, for the year 2019
2. GiovedìScienza Prize 2015 (fourth edition)
3. Best Young Researcher under 38 in natural sciences, for the year 2014, at the University of Piemonte Orientale