

Curriculum Vitae



Personal information

Isabella Romeo

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E-mail Isabella.romeo@unicz.it; Isabella.romeo@unical.it
Nationality Italian
Date of birth 07/09/1989
Gender Female

Work experience

Date	January 2020 - Present
Occupation or position held	Adviser of Società Chimica Italiana – Sezione Calabria 2020-2023
Name and address of employer	Sezione Calabria– Società Chimica Italiana
Dates	December 2019 –Present
Occupation or position held	Tutor of Inorganic Chemistry CHIM/03
Name and address of employer	Department of Pharmacy and Health and Nutrition Sciences - University of Calabria, Italy
Date	October 2019
Occupation or position held	Visiting Assistant in Research
Main activities and responsibilities	Project MX18MO10: Development of computational methodologies for the investigation and characterization of antioxidant in Italian and Mexican natural products. 2 nd year
Name and address of employer	Department of Chemistry - Universidad Autónoma Metropolitana-Iztapalapa (Mexico) Supervisor: Prof. Annia Galano
Dates	June 2019 – present
Occupation or position held	Post-doctoral research
Main activities and responsibilities	Project FORESTCOMP- “PON ricerca e innovazione 2014-2020”: Study and realization of new sustainable polymeric materials starting from renewable resources
Name and address of employer	Department of Chemistry and Chemical Technologies – University of Calabria, Italy Laboratory of Computational and Theoretical Chemistry
Date	March 2019 - Present
Occupation or position held	Member of Communication Team
Main activities and responsibilities	Spreading the Medicinal Chemistry culture on the web and using social medias. Design of novel strategies of People Engagement and Brand Awareness.
Name and address of employer	Divisione Chimica Farmaceutica – Società Chimica Italiana
Dates	8 th -19 th December 2018
Occupation or position held	Visiting Assistant in Research
Main activities and responsibilities	Project MX18MO10: Development of computational methodologies for the investigation and characterization of antioxidant in Italian and Mexican natural products.
Name and address of employer	Department of Chemistry - Universidad Autónoma Metropolitana-Iztapalapa (Mexico) Supervisor: Prof. Annia Galano
Dates	February 2018 - Present
Occupation or position held	Post-doctoral research
Main activities and responsibilities	Project RESIFAC: Realization and testing of pilot plants for fast composting of organic and industrial waste
Name and address of employer	Department of Chemistry and Chemical Technologies – University of Calabria, Italy

Laboratory of Computational and Theoretical Chemistry

Dates	May 2017 – August 2017
Occupation or position held	Visiting Assistant in Research
Main activities and responsibilities	Lead optimization – Free Energy Perturbation (FEP)
Name and address of employer	Department of Chemistry - Yale University, New Haven, USA Supervisor: Prof. William Jorgensen
Dates	April 2016 – June 2016
Occupation or position held	Teaching for the Integrated Course: Operative Management Tools, clinical and therapeutic and economic 1
Name and address of employer	Postgraduate school in Hospital pharmaceuticals – University Magna Graecia of Catanzaro, Italy Pharmaeconomic module
Dates	2014 –2015
Occupation or position held	Tutor of Analytical Chemistry 1 and 2
Name and address of employer	University Magna Graecia of Catanzaro, Italy
Dates	January 2014 – March 2014
Occupation or position held	Teaching in Trichology and Hygiene
Name and address of employer	ECIPA, Crotone, Italy
Dates	2010 – 2011
Occupation or position held	Part-time contract as University secretariat
Name and address of employer	University Magna Graecia of Catanzaro, Italy.

Education and training

Dates	2014 - 2017
Title of qualification awarded	PhD in Life Sciences
Principal subjects/occupational skills covered	Thesis: “ <i>Computational studies on antiviral targets: drug resistance mechanism and rational drug design</i> ”.
Name and type of organisation providing education and training	Department of Health Sciences – University Magna Graecia of Catanzaro, Italy Supervisor: Dr. Anna Artese
Dates	2013
Title of qualification awarded	Qualified Pharmacist
Name and type of organisation providing education and training	University Magna Graecia of Catanzaro, Italy
Dates	2007 - 2013
Title of qualification awarded	Degree in Pharmacy with highest honours
Principal subjects/occupational skills covered	Thesis: “ <i>Identification of natural compounds against HIV-1 Protease by means of virtual screening techniques</i> ”.
Name and type of organisation providing education and training	University Magna Graecia of Catanzaro, Italy Supervisor: Dr. Anna Artese

Personal skills and competences

Mother tongue(s) **Italian**
Other language(s)

Self-assessment

European level (*)

English

French

Understanding				Speaking				Writing	
Listening		Reading		Spoken		Spoken			
	B1		B2		B1		B1		B2
	B2		B2		B2		B2		B2

(*) [Common European Framework of Reference for Languages](#)

Social skills and competences Good communication skills gained during my experience as Commercial Promoter. I am an ambitious and diligent worker willing to take responsibility and learn fast.

Proficient user of Office Suite
Proficient user of UNIX Operating System
Basic user of Python.

Organisational skills and competences

Good team-leading skills gained as project creator for the “ILove Research Project” at the University Magna Graecia of Catanzaro.
I am goal oriented and can handle deadlines and pressure while taking responsibility for different projects at the same time.

Technical skills and competences

Expertise in computational techniques in the drug discovery process, both *hit identification* and *lead optimization* and data mining (Molecular Dynamic simulations, Coarse-Grained simulations, docking programs, Free Energy Perturbation (FEP), Density Function Theory (DFT), ONIOM, QM/MM, Principal Component Analysis, Pharmacophoric models) acquired during my degree and doctoral program at the University Magna Graecia of Catanzaro, meanwhile FEP was acquired during my abroad stage at Yale University (USA).

DFT and QM/MM have been learned at the University of Calabria during the post-doc research.

Programs: Schrodinger Suite, Desmond, Glide, AMBER, GROMACS, Gaussian, LigandScout, Autodock, Autodock Vina.

Topics: HIV, HCV, radical activity, CD98, artificial enzyme.

Computer skills and competences

Proficient user of Office Suite
Proficient user of UNIX Operating System
Basic user of Python.
Experience using High Performance Computing techniques (CUDA, MPI).

Driving licence

Driving license B

Additional information**Publications
and related Impact
Factor (IF)**

Romeo, I.; Parise, A.; Galano, A.; Russo, N.; Alvarez-Idaboy, J. R.; Marino, T. The antioxidant capability of higenamine: Insights from theory. 2020. *Antioxidants*, 9. doi.org/10.3390/antiox9050358

Bagetta, D.; Maruca, A.; Lupia, A.; Mesiti, F.; Catalano, R.; Romeo, I.; Moraca, F.; Ambrosio, F.A.; Costa, G.; Artese, A.; Ortuso, F.; Alcaro, S. Rocca, R. Mediterranean products as promising source of multi-target agents in the treatment of metabolic syndrome, 2020. *Eur. J. Med. Chem.* 186: 111903. doi: 10.1016/j.ejmech.2019.111903

Beneduci, A.; Corrente, G. A.; Marino, T.; Aiello, D.; Bartella, L.; Di Donna, L.; Napoli, A.; Russo, N.; Romeo, I.; Furia, E. Insight on the chelation of aluminum(III) and iron(III) by curcumin in aqueous solution, 2019. *Journal of Molecular Liquids.* 296: 111805. doi:10.1016/j.molliq.2019.111805.

Esposito, F.; Ambrosio, F.A.; Maleddu, R.; Costa, G.; Rocca, R.; Maccioni, E.; Catalano, R.; Romeo, I.; Eleftheriou, P.; Karia, D.C.; Tsirides, P.; Godvani, N.; Pandya, H.; Corona, A.; Alcaro, S.; Artese, A.; Geronikaki, A.; Tramontano, E. Chromenone derivatives as a versatile scaffold with dual mode of inhibition of HIV-1 reverse transcriptase-associated Ribonuclease H function and integrase activity. 2019. *Eur. J. Med. Chem.* 182:111617. doi: 10.1016/j.ejmech.2019.111617

Maruca, A.; Catalano, R.; Bagetta, D.; Mesiti, F.; Ambrosio, F.A.; Romeo, I.; Moraca, F.; Rocca, R.; Ortuso, F.; Artese, A.; Costa, G.; Alcaro, S.; Lupia, A. The Mediterranean Diet as source of bioactive compounds with multi-targeting anti-cancer profile. 2019. *Eur. J. Med. Chem.* 181:111579. Doi: 10.1016/j.ejmech.2019.111579.

Costa, G.; Carta, F.; Ambrosio, F.A.; Artese, A.; Ortuso, F.; Moraca, F.; Rocca, R.; Romeo, I.; Lupia, A.; Maruca, A.; Bagetta, D.; Catalano, R.; Vullo, D.; Alcaro, S.; Supuran, C.T. A computer-assisted discovery of novel potential anti-obesity compounds as selective carbonic anhydrase VA inhibitors. 2019. *Eur. J. Med. Chem.* 181: 111565. doi: 10.1016/j.ejmech.2019.111565

Maruca, A.; Ambrosio, F. A.; Lupia, A.; Romeo, I.; Rocca, R.; Moraca, F.; Talarico, C.; Bagetta, D.; Catalano, R.; Costa, G.; Artese, A. (2018). Computer-based techniques for lead identification and optimization I: Basics. *Physical Sciences Reviews.* 2018.

Prejanò, M.; Romeo, I.; Sgrizzi, L.; Russo, N.; Marino, T. Why hydroxy-proline improves the catalytic power of the peptidoglycan: N -deacetylase enzyme: Insight from theory. 2019. *Phys. Chem. Chem. Phys.* 21, 23338-23345. doi: 10.1039/c9cp03804c

Costa, G.; Rocca, R.; Corona, A.; Grandi, N.; Moraca, F.; Romeo, I.; Talarico, C.; Gagliardi, M.G.; Ambrosio, F.A.; Ortuso, F.; Alcaro, S.; Distinto, S.; Maccioni, E.; Tramontano, E.; Artese, A. Novel natural non-nucleoside inhibitors of HIV-1 reverse transcriptase identified by shape- and structure-based virtual screening techniques. 2018. *Eur. J. Med. Chem.* 161, 1-10. DOI: 10.1016/j.ejmech.2018.10.029

Pouga, L.; Santoro, M.M.; Charpentier, C.; Di Carlo, D.; Romeo, I.; Artese, A.; Alcaro, S.; Antinori, A.; Wirden, M.; Perno, C.F.; Ambrosio, F.A.; Calvez, V.; Descamps, D.; Marcelin, A.G.; Ceccherini-Silberstein, F.; Lambert-Niclot, S. New Resistance Mutations to Nucleoside Reverse Transcriptase Inhibitors at Codon 184 of HIV-1 Reverse Transcriptase (M184L and M184T). 2018. *Chemical Biology and Drug Design.* 93, 50-59. DOI: 10.1111/cbdd.13378.

Romeo, I.; Marascio, N.; Pavia, G.; Talarico, C.; Costa, G.; Alcaro, S.; Artese, A.; Torti, C.; Liberto, M.C.; Focà, A. Structural Modeling of HCV Polymerase Novel Natural Polymorphism Clusters Isolated in Direct-Acting Antiviral Naïve Patients: Focus on Dasabuvir and Setrobuvir Binding Affinity. *ChemistrySelect*, 2018. DOI: 10.1002/slct.201800649.

Marascio, N.; Pavia, G.; Romeo, I.; Talarico, C.; Di Salvo S.; Reale, M.; Marano, V.; Barreca, G.S.; Fabiani, F.; Perrotti, N.; De Siena, M.; Giancotti, F.; Gravina, T.; Alcaro, S.; Artese, A.; Torti, C.; Liberto, M.C.; Focà, A. Real-life 3D therapy failure: Analysis of NS5A 93H RAS plus 108K polymorphism in complex with ombitasvir by molecular modeling. *Journal of Medical Virology*, 2018. DOI: 10.1002/jmv.25073.

Molinaro, R.; Evangelopoulos, M.; Hoffman, J.R.; Corbo, C.; Taraballi, F.; Martinez, J.O.; Hartman, K.A.; Cosco, D.; Costa, G.; Romeo, I.; Sherman, M.; Paolino, D.; Alcaro, S.; Tasciotti, E. Design and Development of Biomimetic Nanovesicles using a Microfluidic Approach. 2018. *Advanced Materials.* DOI: 10.1002/adma.201702749.

Publications

Malet, I.; Ambrosio, F.A.; Subra, F.; Herrmann, B.; Leh, H.; Bouger, M.; Artese, A.; Katlama, C.; Talarico, C.; Romeo, I.; Alcaro, S.; Costa, G.; Deprez, E.; Calvez, V.; Marcelin, A.; Delelis, O. Pathway involving the N155H mutation leads to dolutegravir resistance. *Journal of Antimicrobial Chemotherapy*, 2017. DOI:10.1093/jac/dkx529.

Rocca, R.; Talarico, C.; Moraca, F.; Costa, G.; Romeo, I.; Ortuso, F.; Alcaro, S.; Artese, A. Molecular recognition of a carboxy pyridostatin toward G-quadruplex structures: Why does it prefer RNA?. *Chemical biology and drug design*, 2017, 90, 919-925. doi: 10.1111/cbdd.13015.

Costa, G.; Rocca, R.; Moraca, F.; Talarico, C.; Romeo, I.; Ortuso, F.; Alcaro, S.; Artese, A. A Comparative Docking Strategy to Identify Polyphenolic Derivative as Promising Antineoplastic Binders of G-quadruplex DNA c-myc and bcl-2 Sequences. *Molecular Informatics*, 2016, 35, 391402. DOI:10.1002/minf.201501040.

Alteri, C.; Surdo, M.; Di Maio, V.C.; Di Santo, F.; Costa, G.; Parrotta, L.; Romeo, I.; Gori, C.; Santoro, M.M.; Fedele, V.; Carta, S.; Continenza, F.; Pinnetti, C.; Bellagamba, R.; Liuzzi, G.; Orchi, N.; Latini, A.; Bertoli, A.; Girardi, E.; Alcaro, S.; Giuliani, M.; Petrosillo, N.; Andreoni, M.; Antinori, A.; D'Arminio Monforte, A.; Ceccherini-Silberstein, F.; Artese, A.; Perno, C.F.; Svicher, V. The HIV-1 reverse transcriptase polymorphism A98S improves the response to tenofovir disoproxil fumarate+emtricitabine-containing HAART both in vivo and in vitro. *Journal of Global Antimicrobial Resistance*, 2016, 7, 1-7. DOI: 10.1016/j.jgar.2016.06.005.

Projects

Tutor for the "ILoveResearch – Catanzarorienta" project for a term of 20 hours, organized by the Foundation UMG of Catanzaro at the University Magna Graecia of Catanzaro.

Courses and Schools

- 1stMuTaLig COST Action Training School: Computational Approaches to Polypharmacology, 8-10 February, 2017 – Pharmaziezentrum UZA2, University of Wien.
- Course "High Performance Molecular Dynamics" in Cineca – Bologna from November 18th to 20th, 2015.
- Course ONE HEALTH Cibo, salute e "Prospettive future" at the University Magna Graecia of Catanzaro from March 26th to 27th, 2015.

Awards

Pietro Bucci medal 2018 – Young researcher award for the PhD thesis- (Palermo)

Award of excellence Paul Ehrlich MedChem Euro-PhD Network, July 2018, Portugal. Award refers to PhD Thesis with title "*Computational studies on antiviral targets: drug resistance mechanism and rational drug design*".

Award of excellence for the degree in Pharmacy, 2013, awarded by the Order of Pharmacists of Catanzaro.

Poster and Oral communications

- Romeo, I. Mechanistic insights of hydrolytic activity into a de novo homo-heptameric design protein framework. VI Congresso della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana, 19th-20th September 2019, University of Calabria - Aula Magna "Beniamino Andreatta. *Oral communication*
- Romeo, I.; Artese, A.; Talarico, C.; Costa, G.; Ortuso, F.; Ambrosio, F.A.; Alcaro, S. Computational studies on antiviral targets: drug resistance mechanism and rational drug design. Congresso Congiunto Sicilia- Calabria, 1-2 March 2019, Palermo. *Oral communication*
- Romeo, I.; Prejanò, M.; Marino, T.; Russo, N. Mechanistic insights of hydrolytic activity into a de novo functional "Frankenstein" protein framework. Merck & Elsevier Young Chemists Symposium 2018 in Rimini (Italy), November 19th-21st, 2018.
- Marino, T.; Prejanò, M.; Romeo, I. Russo, N. De novo proteins: Insights from the theoretical investigations – DCTC 2018 QUINTA EDIZIONE – 19-21 September 2018 Università degli Studi di Trieste, Italy.
- Romeo, I.; Costa, G.; Stramandinoli, M.; Artese, A.; Supuran, CT.; Alcaro, S. Carbonic anhydrase VA for the treatment of obesity: in silico identification of new inhibitors and prediction of antiobesity side effects of FDA-approved drugs - 2nd Annual Meeting- MuTaLig Cost Action - 22-24 September 2017 Porto, Portugal. *Oral communication*
- Romeo, I.; Costa, G.; Stramandinoli, M.; Artese, A.; Alcaro, S. Identification of anti-obesity side effects of FDA-approved drugs through computer-aided repurposing techniques. MuTaLig COST Action Working Group meeting, Budapest, Hungary – 19th-20th November 2016.
- Romeo, I.; Talarico, C.; Costa, G.; Pavia, G.; Marascio, N.; Zicca, E.; Barreca, G.S.; Pisani, V.; Liberto, M.C.; Focà, A.; Alcaro, S.; Artese, A. In silico analysis of resistance mutations naturally occurring in Hepatitis C Virus NS5B polymerase. 3rd Innovative Approaches for Identification of Antiviral Agents Summer School, Cagliari, Italy – September 28th –October 3rd 2016.
- Costa, G.; Corona, A.; Distinto, S.; Maccioni, E.; Moraca, F.; Romeo, I.; Talarico, C.; Ortuso, F.; Rocca, R.; Alcaro, S.; Tramontano, E.; Artese, A. identification of natural non-nucleoside inhibitors of HIV-1 Reverse Transcriptase by a combined shape- and structure-based virtual screening approach. 21st EuroQSAR - 21st European Symposium on Quantitative Structure-Activity Relationship, Aptuit Conference Center, Verona, Italy - September 4th-8th 2016.
- Romeo, I.; Artese, A.; Costa, G., Ceccherini-Silberstein, F.; Di Maio, V.C.; Perno, C.F.; Alcaro, S. In silico analysis of the drug-resistance mechanism of HCV NS5A inhibitors in Hepatitis C Virus genotypes 1-4. 21st EuroQSAR - 21st European Symposium on Quantitative Structure-Activity Relationship, Aptuit Conference Center, Verona, Italy - September 4th-8th 2016.
- Pouga, L.; Santoro, M.M.; Charpentier, C.; Di Carlo, D.; Romeo, I.; Artese, A.; Alcaro, S.; Antinori, A.; Wirden, M.; Perno, C.F.; Calvez, V.; Descamps, D.; Marcelin, A.G.; Ceccherini-Silberstein, F.; Lambert-Niclot, S. New resistance Mutation to Nucleoside Reverse Transcriptase Inhibitors at Codon 184 of HIV-1 Reverse Transcriptase (M184T). 14th European Meeting on HIV & Hepatitis 2016 – Rome, Italy - 25th-27th May 2016.
- Romeo, I.; Costa, G.; Artese, A.; Parrotta, L.; Alcaro, S.; Alteri, C.; Bertoli, A.; Ceccherini-Silberstein, F.; Svicher, V.; Perno, CF.; Antinori, A.; Latini, A.; D'Arminio Monforte, A. – Structural modifications induced by the HIV-1 Reverse Transcriptase polymorphism at position 98 tightly modulate the viremia decay to Tenofovir and Emtricitabine – International Retreat of PhD Students in Immunology – 19-20 June 2015 – University "Magna Græcia" of Catanzaro, Catanzaro, Italy. *Oral communication*
- Romeo, I.; Artese, A.; Costa, G.; Ortuso, F.; Santoro, M.; Svicher, V.; Perno, C.F.; Alcaro, S. Analisi strutturale di nuove mutazioni della proteasi di HIV-1 correlate a bassi livelli di viremia in pazienti sottoposti a terapia HAART. Convegno Congiunto SCI Calabria-Sicilia 2015, Catanzaro, Italia – 3-4 Dicembre 2015.

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