

PERSONAL INFORMATION

Maria Zappalà



 [Redacted] y

 +39 090 6766411  + [Redacted]

 mzappala@unime.it

Sex Female | Date of birth 07/04/1961 | Nationality Italian

POSITION

Professor of Medicinal Chemistry, University of Messina, Italy

WORK EXPERIENCE

September 2002 - present

Professor

Dept. of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina (Italy), Viale Annunziata, 98168 Messina – www.unime.it

- Teacher of Medicinal Chemistry I and Medicinal Chemistry II, Master Course in Pharmacy and in Pharmaceutical Chemistry and Technology
- Research activity mainly focused on the following themes: 1) Design, synthesis and pharmacological evaluation of peptidomimetics inhibitors of both human and protozoan proteases; 2) Design, synthesis and SAR of noncompetitive AMPA-receptor antagonists; 3) design and synthesis of RT or integrase inhibitors as anti-AIDS drugs

Business or sector Medicinal Chemistry (CHIM/08)

November 1998 -September 2002

Associate Professor

Pharmaco-Chemical Department, Faculty of Pharmacy, University of Messina (Italy) Viale Annunziata, 98168 Messina – www.unime.it

- Teacher of Medicinal Chemistry II, Master Course in Pharmacy and Analysis of drugs, Master Course in Pharmaceutical Chemistry and Technology
- Research activity mainly focused on the following themes: 1) design and synthesis of RT inhibitors as anti-AIDS drugs; 2) design and synthesis of new anticonvulsant agents.

Business or sector Medicinal Chemistry (CHIM/08)

September 1987 - November 1998

Assistant Professor

Pharmaco-Chemical Department, Faculty of Pharmacy, University of Messina (Italy) Viale Annunziata, 98168 Messina – www.unime.it

- Teacher of Analysis of drugs, Master Course in Pharmacy
- Research activity mainly focused on the following themes: 1) design and synthesis of new anti-tumor drugs; 2) design and synthesis of new anticonvulsant agents.

Business or sector Medicinal Chemistry (CHIM/08)

EDUCATION AND TRAINING

Nov 1990

Master Degree in Pharmaceutical Chemistry and Technology (*cum laude*)

Master

University of Messina, Italy (Viale Annunziata, 98168 Messina – www.unime.it)

July 1983 **Master Degree in Pharmacy (*cum laude*)**
University of Messina, Italy

Master

PERSONAL SKILLS

Mother tongue(s) Italian

Other language(s)	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	B2	B2	B2	B2	B2

Levels: A1/A2: Basic user - B1/B2: Independent user - C1/C2 Proficient user

Communication skills ▪ Good communication skills gained through my experience as Teacher at University and several Congresses and Meetings

Organisational / managerial skills ▪ President of the Degree Course in Pharmacy (2008-2013)
▪ Head of the Department of Drug Sciences and Health Products (2014-2015) and Member of the Academic Senate (2014-2015)
▪ President of the Degree Course in Pharmaceutical chemistry and technology (2021-2024)

Job-related skills ▪ Good experience on methods for drug design and discovery, lead individuation and optimization. Good experience on the synthesis of biologically active compounds

Digital skills

SELF-ASSESSMENT				
Information processing	Communication	Content creation	Safety	Problem solving
INDEPENDENT USER	INDEPENDENT USER	INDEPENDENT USER	INDEPENDENT USER	INDEPENDENT USER

Levels: Basic user - Independent user - Proficient user
[Digital competences - Self-assessment grid](#)

Replace with name of ICT-certificates

▪ good command of office suite (word processor, spread sheet, presentation software)

Other skills ▪

Driving licence B

ADDITIONAL INFORMATION

Publications
last ten years

Carla Di Chio, Josè Starvaggi, Noemi Totaro, Santo Previti, Benito Natale, Sandro Cosconati, Marta Bogacz, Tanja Schirmeister, Jenny Legac, Philip J. Rosenthal, Maria Zappalà, Roberta Ettari (2024). Development of novel peptidyl nitriles targeting rhodesain and falcipain-2 for the treatment of sleeping sickness and malaria. *International Journal of Molecular Sciences*, 25, 4410.

Previti, S.; Ettari, R.; Calcaterra, E.; Roggia, M.; Natale, B.; Weldert, A. C.; Müller-Ruttloff, C.; Salisch, F.; Irto, A.; Cigala, R.M.; Ziebuhr, J.; Schirmeister, T.; Cosconati, S.; Zappalà, M. Identification of Dual Inhibitors Targeting Main Protease (Mpro) and Cathepsin L as Potential Anti-SARS-CoV-2 Agents. *ACS Medicinal Chemistry Letters*, 2024, 15, 602.

J. Starvaggi, S. Previti, M. Zappalà, R. Ettari (2024). The inhibition of NS2B/NS3 protease: a new therapeutic opportunity to treat Dengue and Zika virus infection. *International Journal of Molecular Sciences*, 25, 4376.

Chiara Imbesi, Roberta Ettari, Natasha Irrera, Maria Zappalà, Giovanni Pallio, Alessandra Bitto, Federica Mannino. Blunting Neuroinflammation by Targeting the Immunoproteasome with Novel Amide Derivatives. *International Journal of Molecular Sciences*, 2023, 24(13), 10732

Culetta, G.; Tutone, M.; Ettari, R.; Perricone, U.; Di Chio, C.; Almerico, A.M.; Zappalà, M. Virtual screening strategy and in vitro tests to identify new inhibitors of immunoproteasome. *International Journal of Molecular Sciences*, 2023, 24(13), 10504

Carla Di Chio, Santo Previti, Noemi Totaro, Fabiola De Luca, Alessandro Allegra, Tanja Schirmeister, Maria Zappalà, Roberta Ettari. Dipeptide nitrile CD34 with curcumin: a new improved combination strategy to synergistically inhibit rhodesain of *Trypanosoma brucei rhodesiense*. *International Journal of Molecular Sciences*, 2023, 24(10), 8477

Fabiola De Luca, Alessandro Allegra, Carla Di Chio, Santo Previti, Maria Zappalà, Roberta Ettari. Monoclonal Antibodies: The Greatest Resource to Treat Multiple Myeloma. *International Journal of Molecular Sciences*, 2023, 24(4), 3136

S. Previti, R. Ettari, C. Di Chio, J. Legac, M. Bogacz, C. Zimmer, T. Schirmeister, P. J. Rosenthal, M. Zappalà. Influence of amino acid size at the P3 position of N-Cbz-tripeptide Michael acceptors targeting falcipain-2 and rhodesain for the treatment of malaria and human african trypanosomiasis. *Bioorganic Chemistry*, 2023, 137, 106587

Previti, S.; Ettari, R.; Calcaterra, E.; Di Maro, S.; Hammerschmidt, S. J.; Muller, C.; Ziebuhr, J.; Schirmeister, T.; Cosconati, S.; Zappalà, M. Structure-based lead optimization of peptide-based vinyl methyl ketones as SARS-CoV-2 main protease inhibitors. *European Journal of Medicinal Chemistry* 2023, 247, 115021.

Giulia Culetta, Marco Tutone, Maria Zappalà, Anna Maria Almerico. Sulfonamide moiety as "molecular chimera" in the design of new drugs. *Current Medicinal Chemistry*, 2023, 30(2), 128-163

Fabiola De Luca, Carla Di Chio, Roberta Ettari, Maria Zappalà. Dihydrochalcones as antitumor agents. *Current Medicinal Chemistry*, 2022, 29(30), 5042-5061

Di Chio, C.; Previti, S., Amendola, G., Ravichandran, R., Wagner A., Cosconati S., Hellmich, U.A., Schirmeister, T.; Zappalà, M., Ettari, R. (2022). Development of novel dipeptide nitriles as inhibitors of rhodesain of *Trypanosoma brucei rhodesiense*. *European Journal of Medicinal Chemistry* 234, 114328.

S. Previti, R. Ettari, E. Calcaterra, C. Di Chio, R. Ravichandran, C. Zimmer, S. Hammerschmidt, A. Wagner, M. Bogacz, S. Cosconati, T. Schirmeister, M. Zappalà (2022). Development of Urea-Bond-Containing Michael Acceptors as Antitrypanosomal Agents Targeting Rhodesain. *ACS Medicinal Chemistry Letters*, 13, 1083-1090

Ettari R., Iraci N., Di Chio C., Previti S., Danzè M., Zappalà M (2022). Development of isoquinolinone derivatives as immunoproteasome inhibitors. *Bioorganic & Medicinal Chemistry Letters*, vol. 55, p. 1-4.

Santo Previti, Roberta Ettari, Carla Di Chio, Rahul Ravichandran, Marta Bogacz, Ute A. Hellmich, Tanja Schirmeister, Sandro Cosconati, Maria Zappalà (2022). Development of reduced peptide bond pseudopeptide Michael acceptors for the treatment of Human African Trypanosomiasis. *Molecules*, 27, 3765

Carla Di Chio, Santo Previti, Fabiola De Luca, Alessandro Allegra, Maria Zappalà, Roberta Ettari (2022). Drug combination studies of PS-1 and quercetin against rhodesain of *Trypanosoma brucei rhodesiense*. *Natural Product Research*, vol. 36, p. 4282-4286

C. Di Chio, S. Previti, F. De Luca, M. Bogacz, C. Zimmer, A. Wagner, T. Schirmeister, M. Zappala, R. Ettari (2022). Drug combination studies of the dipeptide nitrile CD24 with curcumin: a new strategy to synergistically inhibit rhodesain of trypanosoma brucei rhodesiense. *International Journal of Molecular Sciences*, 23, 14470

S Previti, C Di Chio, R Ettari, M Zappalà (2022). Dual inhibition of parasitic targets: a valuable strategy to treat malaria and neglected tropical diseases. *Current Medicinal Chemistry*, 29, 2952-2978

C. Di Chio, M. Zhou, T. Efferth, T. Schirmeister, M. Zappalà, R. Ettari (2022). Synthesis and cytotoxicity of diarylpentanoids against sensitive CCRF-CEM and multidrug-resistant CEM/ADR5000 leukemia cells. *Chemistry & Biodiversity*, 18, 1-8.

Archimede Rotondo, Maria Zappala', Santo Previti, Carla Di Chio, Alessandro Allegra, Roberta Ettari (2021). Design and NMR conformational analysis in solution of β 5i-selective inhibitors of immunoproteasome. *Journal of Molecular Structure*, 1230, 129633

R. Ettari, S. Previti, C. Di Chio, M. Zappalà (2021). Falcipain-2 and Falcipain-3 inhibitors as promising antimalarial agents. *Current Medicinal Chemistry*, 28, 3010-3031

G. Culetta, M. Zappalà, R. Ettari, A. M. Almerico, M. Tutone (2021). Immunoproteasome and Non-Covalent Inhibition: Exploration by Advanced Molecular Dynamics and Docking Methods. *Molecules*, 26, 4046-4064

Amendola, G., Ettari, R., Previti, S., Di Chio, C., Messere, A., Di Maro, S. Hammerschmidt, S., Zimmer, C., Zimmermann, R., Schirmeister, T., Zappalà, M., Cosconati, S. Lead Discovery of SARS-CoV-2 Main Protease Inhibitors Through Covalent Docking-Based Virtual Screening. *Journal of Chemical Information and Modeling*, 2021, 61, 4, 2062-2073.

Ettari, R., Previti, S., Di Chio, C., Maiorana, S., Allegra, A., Schirmeister, T., Zappala, M. Drug synergism: Studies of Combination of RK-52 and Curcumin against Rhodesain of Trypanosoma brucei rhodesiense. (2020) *ACS Medicinal Chemistry Letters*, 11 (5), pp. 806-810.

G. Culetta, M. R. Gulotta, U. Perricone, M. Zappalà, A. M. Almerico, M. Tutone (2020). Exploring the SARS-CoV-2 proteome in the search of potential inhibitors via structure-based pharmacophore modeling/docking approach. *Computation*, 8, 1-16.

S. Maiorana, R. Ettari, S. Previti, G. Amendola, A. Wagner, S. Cosconati, U. A. Hellmich, T. Schirmeister, M. Zappalà (2020). Peptidyl Vinyl Ketone Irreversible Inhibitors of Rhodesain: Modifications of the P2 Fragment. *CHEMMEDCHEM*, vol. 15, p. 1552-1561

Ettari, R., Previti, S., Maiorana, S., Allegra, A., Schirmeister, T., Grasso, S., Zappalà, M. Evaluation of curcumin irreversibility (2020) *Natural Product Research*, vol. 34, p. 3159-3162

Di Chio, C., Previti, S., Amendola, G., Cosconati, S., Schirmeister, T., Zappalà, M., Ettari, R. Development of Novel Benzodiazepine-Based Peptidomimetics as Inhibitors of Rhodesain from Trypanosoma brucei rhodesiense. (2020) *ChemMedChem*, vol. 15, p. 995-1001

Ettari, R., Previti, S., Maiorana, S., Allegra, A., Schirmeister, T., Grasso, S., Zappalà, M. Drug combination studies of curcumin and genistein against rhodesain of Trypanosoma brucei rhodesiense. (2019) *Natural Product Research*, 33 (24), pp. 3577-3581.

Ettari, R., Previti, S., Maiorana, S., Amendola, G., Wagner, A., Cosconati, S., Schirmeister, T., Hellmich, U.A., Zappalà, M. Optimization Strategy of Novel Peptide-Based Michael Acceptors for the Treatment of Human African Trypanosomiasis. (2019) *Journal of Medicinal Chemistry*, 62, 10617-10629

Ettari, R., Cerchia, C., Maiorana, S., Guccione, M., Novellino, E., Bitto, A., Grasso, S., Lavecchia, A., Zappalà, M. Development of novel amides as noncovalent inhibitors of immunoproteasomes. (2019) *ChemMedChem*, 14 (8), pp. 842-852.

Ettari, R., Pallio, G., Pizzino, G., Irrera, N., Zappalà, M., Maiorana, S., Di Chio, C., Altavilla, D., Squadrito, F., Bitto, A. Non-covalent immunoproteasome inhibitors induce cell cycle arrest in multiple myeloma MM.1R cells (2019) *Journal of Enzyme Inhibition and Medicinal Chemistry*, 34, 1307-1313.

Maccari, R., Ettari, R., Adomato, I., Naß, A., Wolber, G., Bitto, A., Mannino, F., Aliquò, F., Bruno, G., Nicolò, F., Previti, S., Grasso, S., Zappalà, M., Ottanà, R. Identification of 2-thioxoimidazolidin-4-one derivatives as novel noncovalent proteasome and immunoproteasome inhibitors. (2018) *Bioorganic and Medicinal Chemistry Letters*, 28 (3), pp. 278-283.

Ettari, R., Zappalà, M., Grasso, S., Musolino, C., Innao, V., Allegra, A. Immunoproteasome-selective and non-selective inhibitors: A promising approach for the treatment of multiple myeloma. (2018) *Pharmacology and Therapeutics*, 182, pp. 176-192.

Previti, S., Ettari, R., Cosconati, S., Amendola, G., Chouchene, K., Wagner, A., Hellmich, U.A., Ulrich, K., Krauth-Siegel, R.L., Wich, P.R., Schmid, I., Schirmeister, T., Gut, J., Rosenthal, P.J., Grasso, S., Zappalà, M. Development of Novel Peptide-Based Michael Acceptors Targeting Rhodessin and Falcipain-2 for the Treatment of Neglected Tropical Diseases (NTDs). (2017) *Journal of Medicinal Chemistry*, 60, 6911-6923.

Espahbodinia, M., Ettari, R., Wen, W., Wu, A., Shen, Y.-C., Niu, L., Grasso, S., Zappalà, M. Development of novel N-3-bromoisoxazolin-5-yl substituted 2,3-benzodiazepines as noncompetitive AMPAR antagonists (2017) *Bioorganic and Medicinal Chemistry*, 25 (14), pp. 3631-3637.

Ettari, R., Previti, S., Tamborini, L., Cullia, G., Grasso, S., Zappalà, M. The inhibition of cysteine proteases rhodessin and TbCatB: A valuable approach to treat human african trypanosomiasis. (2016) *Mini-Reviews in Medicinal Chemistry*, 16 (17), pp. 1374-1391.

Ettari, R., Previti, S., Cosconati, S., Kesselring, J., Schirmeister, T., Grasso, S., Zappalà, M. Synthesis and biological evaluation of novel peptidomimetics as rhodessin inhibitors. (2016) *Journal of Enzyme Inhibition and Medicinal Chemistry*, 31 (6), pp. 1184-1191.

Di Giovanni, C., Ettari, R., Sarno, S., Rotondo, A., Bitto, A., Squadrito, F., Altavilla, D., Schirmeister, T., Novellino, E., Grasso, S., Zappalà, M., Lavecchia, A. Identification of noncovalent proteasome inhibitors with high selectivity for chymotrypsin-like activity by a multistep structure-based virtual screening. (2016) *European Journal of Medicinal Chemistry*, 121, pp. 578-591.

Guccione, M., Ettari, R., Taliani, S., Da Settimo, F., Zappalà, M., Grasso, S. G-protein-coupled receptor kinase 2 (GRK2) inhibitors: Current trends and future perspectives. (2016) *Journal of Medicinal Chemistry*, 59, 9277-9294

Ettari, R., Previti, S., Bitto, A., Grasso, S., Zappalà, M. Immunoproteasome-selective inhibitors: A promising strategy to treat hematologic malignancies, autoimmune and inflammatory diseases. (2016) *Current Medicinal Chemistry*, 23, 1217-1238.

Ettari, R., Previti, S., Cosconati, S., Maiorana, S., Schirmeister, T., Grasso, S., Zappalà, M. Development of novel 1,4-benzodiazepine-based Michael acceptors as antitrypanosomal agents. (2016) *Bioorganic and Medicinal Chemistry Letters*, 26, 3453-3456.

Ettari, R., Pinto, A., Previti, S., Tamborini, L., Angelo, I.C., La Pietra, V., Marinelli, L., Novellino, E., Schirmeister, T., Zappalà, M., Grasso, S., De Micheli, C., Conti, P. Development of novel dipeptide-like rhodessin inhibitors containing the 3-bromoisoxazoline warhead in a constrained conformation. (2015) *Bioorganic and Medicinal Chemistry*, 23, 7053-7060.

Rotondo, A., Ettari, R., Grasso, S., Zappalà, M. NMR conformational analysis in solution of a potent class of cysteine proteases inhibitors. (2015) *Structural Chemistry*, 26 (4), art. no. 597, pp. 943-950.

Rotondo, A., Ettari, R., Zappalà, M., De Micheli, C., Rotondo, E. NMR characterization and conformational analysis of a potent papain-family cathepsin L-like cysteine protease inhibitor with different behaviour in polar and apolar media (2014) *Journal of Molecular Structure*, 1076, 337-343.

Troiano, V., Scarbaci, K., Ettari, R., Micale, N., Cerchia, C., Pinto, A., Schirmeister, T., Novellino, E., Grasso, S., Lavecchia, A., Zappalà, M. Optimization of peptidomimetic boronates bearing a P3 bicyclic scaffold as proteasome inhibitors. (2014) *European Journal of Medicinal Chemistry*, 83, 1-14.

Scarbaci, K., Troiano, V., Micale, N., Ettari, R., Tamborini, L., Di Giovanni, C., Cerchia, C., Grasso, S., Novellino, E., Schirmeister, T., Lavecchia, A., Zappalà, M. Identification of a new series of amides as non-covalent proteasome inhibitors. (2014) *European Journal of Medicinal Chemistry*, 76, pp. 1-9.

Micale, N., Scarbaci, K., Troiano, V., Ettari, R., Grasso, S., Zappalà, M. Peptide-Based Proteasome Inhibitors in Anticancer Drug Design (2014) *Medicinal Research Reviews*, 34 (5), pp. 1001-1069.

Scarbaci, K., Troiano, V., Ettari, R., Pinto, A., Micale, N., Di Giovanni, C., Cerchia, C., Schirmeister, T., Novellino, E., Lavecchia, A., Zappalà, M., Grasso, S. Development of novel selective peptidomimetics containing a boronic acid moiety, targeting the 20s proteasome as anticancer agents (2014) *ChemMedChem*, 9 (8), pp. 1801-1816.

Ettari, R., Pinto, A., Tamborini, L., Angelo, I.C., Grasso, S., Zappalà, M., Capodicasa, N., Yzeiraj, L., Gruber, E., Aminake, M.N., Pradel, G., Schirmeister, T., De Micheli, C., Conti, P. Synthesis and biological evaluation of papain-family cathepsin I-like cysteine protease inhibitors containing a 1,4-benzodiazepine scaffold as antiprotozoal agents (2014) ChemMedChem, 9 (8), pp. 1817-1825.

- Projects** Scientific Responsible of research projects financed by the Italian Ministry of Education FISR2020 COVID-19
 Scientific Responsible of research projects financed by the University of Messina (PRA2004, PRA2005, PRA2006/2007, PRA2008/2009, FABR2019, FFABR2020, FFABR2023)
 Member of research teams financially supported by Italian Ministry of Education (PRIN2004, PRIN2005, PRIN2008, PRIN2010-2011, FISR2019, PRIN 2022 PNRR)
 Member of research teams financially supported by Italian-German University (Vigoni Project 2008/09 and 2012/2013)
- Honours and awards** Winner of the 'XXIV Award Anassilaos' 'Raffaele Piria' for 'Arts, Culture, Economics, Sciences', 08/11/2014 Reggio Calabria, Italy
- Memberships** Member of The Italian Chemical Society, from 1987
 Member of the Executive Committee of the SICILY Section of The Italian Chemical Society from December, 2018-2021
 Member of the Scientific Committee of the PhD program in 'Pharmaceutical Sciences' (2002-2013)
 Member of the Scientific Committee of the PhD program in 'Chemical Sciences' (2013-present)
- Bibliometric Informations** Scopus (21/06/2024)
 Total Papers 173
 H-Index: 41
 Total Citations: 5615
- Journal Reviewing** Reviewer for the following journals:
 J. Med. Chem.
 ACS Med. Chem. Lett.
 European J. Med Chem.
 Bioorg. Med. Chem.
 Bioorg. Med. Chem. Lett.
 Bioorg. Chem.
 Medicinal Chemistry
 ChemMedChem
 Natural Product Research
 Chemistry Select



Firmato digitalmente
 da Maria Zappala
 Data: 21.06.2024
 07:03:44 CEST
 Organizzazione:
 UNIVERSITA' DEGLI
 STUDI DI
 MESSINA/80004070
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