Marcello Miceli

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Research Profile

Marcello Miceli (Italy, born in 1994) is currently a Research Fellow in University of Modena (UNIMORE). He was a Research Fellow at the Department of Mechanical and Aerospace Engineering of Politecnico di Torino under the supervision of Prof. Marco Agostino Deriu within the Mechanistic and Machine Learning-driven Modelling in Bioengineering (M3B) group (https://m3b.it/). Marcello's research is dedicated to the employment of computational methods, including molecular modelling and machine learning methods, to unravel the molecular mechanisms and features at the basis of physiological and pathological phenomena. With his expertise initiated during his PhD, his primary area of specialization involves the molecular characterization of proteins related to neurodegenerative disease. The central goal of his research is the investigation at the base of the onset of protein related neurodegenerative pathologies. In detail, the mechanistic approach employs molecular modelling and dynamics techniques to unveil the structure-to-function relationships of proteins. Marcello has also some experience in wet lab for protein expression and purification.

Research Experience

15/05/2024 - Today	**Research Fellow** University of Modena, Modena (ITALY)
01/12/2022 - 15/05/2024	**Research Fellow** Politecnico di Torino, Turin (ITALY)
01/12/2020 – today	**PhD Student** Politecnico di Torino, Turin (ITALY)
02/12/2019 – 01/12/2020	**Undergraduate University Intern** Politecnico di Torino, Turin (ITALY)

Education and qualifications

2024	**Doctor of Philosophy (PhD)** Politecnico di Torino, Turin (ITALY) **Thesis title**: *Insights Into the Molecular Mechanisms Driving Rare Neurodegenerative Diseases and Therapeutic Strategies Aided By In Silico Modelling*

Supervisors: Prof. Marco A. Deriu, Prof. Umberto Morbiducci, Dr Gianvito Grasso

Thesis Referees: Prof. Travis Craddock, Dr. Francesco Gentile

PhD Defence Date: 11/07/2024

2019 **Licensing to practice as "Industrial Engineering"**

Politecnico di Torino, Turin (ITALY)

2016 - 2019 **Master's Degree in Biomedical Engineering (LM-21)**

Politecnico di Torino, Turin (ITALY)
Final degree: 110/110 cum laude
Thesis title: *Prediction of ultrasonic wave driven conformational dynamics of amyloid protein assemblies by molecular modelling*
Supervisors: Prof. Marco Agostino Deriu, Prof.

2013 - 2016 **Bachelor's Degree in Biomedical Engineering (L-9)**

Politecnico di Torino, Turin (ITALY)
Final degree: 106/110

Awards

2019 **Master thesis award: "Margherita and Antonio Poletto 2019"** from Collegio Universitario di merito "Luigi Einaudi" di Torino for "Best thesis in the field of Medical and Biomedical Science"

2021 **Cover Art:** Journal of Medicinal Chemistry, Vol. 64 N. 21, related to the publication "Noncovalent Interactions with PAMAM and PPI Dendrimers Promote the Cellular Uptake and Photodynamic Activity of Rose Bengal: The Role of the Dendrimer Structure"

Publications

The following table reports some metrics concerning scientific publications.

Citations	Documents	H-index	Source
64	14	5	Google Scholar
47	9	4	Scopus

Regarding the Scopus database, indexed publications relating to Marcello Miceli include 6 original articles and 1 reviews. He is the first author of 3 of these publications.

Additional information regarding the scientific publications is available at the following links:

- Google Scholar: https://scholar.google.com/citations?user=FYfIduIAAAAJ&hl=it&oi=ao
- Scopus:
- https://www.scopus.com/authid/detail.uri?authorId=57212757169
- ORCID: https://orcid.org/0000-0002-2763-5407

The total publications, summarized in the following, include **9 papers in peer-reviewed journals, 1 conference papers and 2 journal proceedings**.

Peer-reviewed Scientific Publications

Marcello Miceli published **9 papers** in peer-reviewed scientific journals.

2024 Veneziani G., Luciani F., **Miceli M.**, Spallaccini S., Galli F., Pezzuti L., Lai C., Inside the gamer's mind: How violent video games and emotional dysregulation affect EEG interbrain synchronization, Computers in Human Behavior Reports, doi: 10.1016/j.chbr.2024.100509

2024 **Miceli M**., Cannariato M., Tortarolo, R.;Pallante, L.;Zizzi, E. A.;Deriu, M. A. Conformational Dynamics and Molecular Characterization of Alsin MORN Monomer and Dimeric Assemblies. Proteins: structure, functions bioninformatics. Doi: doi.org/10.1002/prot.26728

2023 Cannariato M, Zizzi EA, Pallante L, **Miceli M,** Deriu MA. Mechanical communication within the microtubule through network-based analysis of tubulin dynamics. Biomech Model Mechanobiol. doi:10.1007/s10237-023-01792-5

2022 **Miceli, M**., Deriu, M. A. & Grasso, G. Toward the design and development of peptidomimetic inhibitors of the Ataxin-1 aggregation pathway. Biophysical Journal 121, 4679–4688 (2022).

2022 Cannariato M**, Miceli M.**, Cavaglià M, Deriu MA (2022). Prediction of Protein–Protein Interactions Between Alsin DH/PH and Rac1 and Resulting Protein Dynamics. *Front. Mol. Neurosci.* 14:772122. Doi: 10.3389/fnmol.2021.772122.

2022 Cannariato M, **Miceli M**, Deriu MA (2022). *In silico* investigation of Alsin RLD conformational dynamics and phosphoinositides binding mechanism. *PLoS ONE* 17(7): e0270955. doi: 10.1371/journal.pone.0270955.

2022 **Miceli, M.,** Exertier, C., Cavaglià, M., Gugole, E., Boccardo, M., Casaluci, R.R., Ceccarelli, N., De Maio, A., Vallone, B., Deriu, M.A. (2022). ALS2-Related Motor Neuron Diseases: From Symptoms to Molecules. *Biology, 11 (1), art. no. 77*. doi: 10.3390/biology11010077.

2021 Sztandera K, Gorzkiewicz M, Dias Martins AS, **Miceli M.**, et al. Noncovalent Interactions with PAMAM and PPI Dendrimers Promote the Cellular Uptake and Photodynamic Activity of Rose Bengal: The Role of the Dendrimer Structure. J Med Chem. 2021:acs.jmedchem.1c01080. doi:10.1021/acs.jmedchem.1c01080

2020 **Miceli** M., Muscat S., Morbiducci M, Cavaglià M., Deriu M.A.,Ultrasonic waves effect on S-shaped β-amyloids conformational dynamics by non-equilibrium molecular dynamics,Journal of Molecular Graphics and Modelling, Doi: 10.1016/j.jmgm.2019.107518

Conference Papers

2021 **Miceli, M.,** Exertier, C., Vallone, B., Cavaglià, M. & Deriu, M. A. Elucidating molecular connetion between IAHSP onset and Alsin protein by means of Homology Modelling and

Molecular Dynamics. Biomedical Science and Engineering 4, (2021). Doi: https://doi.org/10.4081/bse.183

Conference Proceedings

2021 Zizzi E.A., Pallante L., **Miceli M.**, Tuszynski J.A., Deriu M.A. PAMAM and PPI dendrimers as potential anti-cancer drug carriers: a computational investigation. CancerTO - Nanoscience in Cancer Immunotherapy. Frontiers Event Abstracts, p.120. doi: 10.3389/978-2-88966-543-3

2021 Pallante L**.**, Zizzi E.A., **Miceli M.**, Grasso G., Huczynski A, Tuszynski J.A., Deriu M.A. Understanding the molecular binding mechanism of colchicine derivatives targeting βIII human tubulin isotype. CancerTO - Nanoscience in Cancer Immunotherapy. Frontiers Event Abstracts, p.120. doi: 10.3389/978-2-88966-543-3

Manuscripts submitted or under review

Marcello Miceli is also the author of 1 **additional works** already submitted or under review in peer-reviewed journals and available as preprints.

2024 Cannariato M., Fanunza R., Zizzi E.A., **Miceli M.**, Di Benedetto G., Deriu M.A and Pallante L., Molecular Biomechanics of the TAS2R46 Bitter Taste Receptor through Network-based Investigation, Under review in Frontiers in Molecular Biosciences.

International Conferences

Marcello Miceli participated in **7 national and international conferences** as (invited) speaker, poster presenter or listener attendee.

2024 **Emerging Theoretical Approaches to Compliment Single-Particle Cryo-Electron Microscopy**

Biophysical society, Trieste (Italy)

Title *Understanding the molecular consequences of the R1611W mutation in alsin's vps9 domain: experimental and computational perspectives*

Type: Poster

2023 **GGMM 2023**

Young Modellers conference, Toulouse (France)

Title *Investigate the mechanisms of onset for Alsin-related pathology by means of molecular modelling*

Type: Poster

2022 **Virtuous Transfer of Knowledge (ToK) - Second Workshop**

First Workshop of the EU-funded VIRTUOUS project (GA: 872181)
Lugano, Switzerland
Type: Listener attendee

2022 **CCPBioSim 2022**

8th Annual CCPBioSim Conference Frontiers in Biomolecular Simulation 2022
Edinburgh, Scotland
Type: Poster & flash talk
Title: *Elucidating structure to functions relationship of Alsin domains by means of Homology Modelling and Molecular Dynamics*

2021 **ESB 2021**

26th Congress of the European Society of Biomechanics
Milan, Italy (Online)
Type: Oral presentation
Title: *Ultrasound driven amyloid fibril unfolding investigated by molecular modelling.*

2021 **III Annual Conference Centro 3R**

"The 3R era: in silico, in vitro, and in vivo models to promote translational research", Turin (online)

Type: *Invited Speaker*

Title: *"Elucidating molecular connection between IAHSP onset and Alsin protein by means of Homology Modelling and Molecular Dynamics"*

2020 **Virtuous Transfer of Knowledge (ToK) - First Workshop**

First Workshop of the EU-funded VIRTUOUS project (GA: 872181)
Patras, Greece (Online)
Type: Listener attendee

Peer-Review Activities

Marcello Miceli is regular reviewer for the following scientific journals:

1. Scientific Reports (Nature)
2. Frontiers in Molecular Biosciences

Teaching Expertise

As master thesis student Marcello Miceli participate as teaching assistant for the following Master's Degree course in Biomedical Engineering at Politecnico di Torino, and Bachelor Degree's courses in Aerospace Engineering and Computer Science Engineering

- Signal And Systems (ENG) 30 hrs -Tutoring
- Fondamenti di elettrotecnica (ITA) 60 hrs Tutoring
- Sensori e misure per la bioingegneria (ITA) 30 hrs Lab Tutoring and exam surveillance
- Informatica I – (ITA) 50 hrs Lab Tutoring and exam surveillance

The teaching activities listed below were carried out within the Master's Degree course in Biomedical Engineering at Politecnico di Torino during the PhD activity:

- Biomechanical Design (ENG) – 16 hrs.
- Rational Drug Design (ENG) – 11 hrs.
- Biomeccanica Multiscala (ITA) – 37 hrs.

In summary, Marcello Miceli contributed a total of 64 hours (comprising 31.5 hours of lectures and 32.5 hours of tutoring sessions) to teaching activities within the Biomedical Engineering Degree program at Politecnico di Torino.

Additionally, Marcello Miceli supervised the following Master's and Bachelor's thesis students at Politecnico di Torino:

- 4 Master Thesis Students (https://bit.ly/3oP63MW)
- 22 Bachelor Thesis Students

Professional Memberships

Editorial Board Member

2023 - Today **Review Editor** for *Biological Modeling and Simulation* (specialty section of *Frontiers in Molecular Biosciences* and *Frontiers in Applied Mathematics and Statistics*)

Membership of Scientific Societies

- European Society of Biomechanics (2020)
- Italian Chapter of the European Society of Biomechanics (2020)
- 'Centro 3R' (2022)
- Biophysical society (2024)

Involvement in Funded Projects

VIRTUOUS (PI: Marco Agostino Deriu, GA: 872181, https://virtuoush2020.com/). *"Virtual tongue to predict the organoleptic profile of mediterranean ingredients and their effect on human homeostasis by means of an integrated computational multiphysics platform"*, European H2020 project MSCA-RISE (2019-2023).

CRYSTAL (PI: Marco Agostino Deriu, GA: **GSP20005_PAsIAHSP007**, https://crystal.m3b.it).

"Elucidating the Alsin structure to function relationships toward a better understanding of infantile-onset ascending hereditary spastic paralysis and possible therapeutic strategies", Telethon Funded Project (**GSP20005_PAsIAHSP007**), **CRYSTAL** (2020-2022)

Courses, Workshops and Schools

Marcello Miceli participated in the following national and international courses, workshops and school that have enhanced his skills in molecular modelling and machine learning methods.

2020	Computing@Polito Workshop – HPC/Big Data/Cloud for Research (**link**)
2021	Non-Extensive Statistical Mechanics (link)
2021	High-Performance Molecular Dynamics (link)
2021	Martini Workshop 2021
2022	AIDD 2022 Spring School - Lugano

2022 2022 Workshop on MDAnalysis/Machine Learning (link)

International and national Exchange Periods

During his master thesis Marcello Miceli participated in period abroad within the framework of ERASMUS+/ PROGRAMME COUNTRIES

Period	Host Institution	Place
1/2/2018 – 01/07/2018	Tampere University of Technology	Tampere, Finland

Marcello Miceli participated in periods abroad within the framework of the European H2020 project MSCA-RISE VIRTUOUS (PI: Marco Agostino Deriu, GA: 872181, https://virtuoush2020.com/).

Period	Host Institution	Place
1/1/2020 – 1/03/2020	Missing Tech Sagl.	Chiasso, Switzerland
5/10/2020 – 5/12/2020	Insybio PC	Patras, Greece
03/05/2022 –03/ 06/2022	Missing Tech Sagl.	Chiasso, Switzerland
18/11/2022 – 18/12/2022	Missing Tech Sagl.	Chiasso, Switzerland
30/08/2023 – 02/10/2023	Insybio PC	Patras, Greece

Marcello Miceli participated in period in a wet biochemistry lab, in the framework of his Phd research project

Period	Host Institution	Place
20/02/2023 – 01/05/2023	ValloneLAB	Rome, Italy

Community Involvement and Public Engagement

UNight – Researchers' night

Participation together with the entire M3B research group in two editions of Researchers' Night, 2022 and 2023. At these events, the group presented the activities of the PARENT, VIRTUOUS and CRYSTAL projects to the public through posters, interactive videos, and games for youngsters.

Just the Woman I Am

Participation together with the M3B group in the *Just the Woman I Am* event (two editions: 2020 and 2022). Just the Woman I Am is an event promoting cancer prevention in women. The research group participated by presenting the group's activities related to cancer research at a dedicated stand.

“Seralmente” Events

Marcello Miceli collaborated with the *QPP-Seralmente* association to promote the dissemination and communication of scientific achievements to a wider audience. The organized events involve experts from academic and industrial backgrounds. Marcello Miceli helped in the organization of a series of seminars and conferences at the Politecnico di Torino:

1. "*AI, Computation, Physical Law, and Consciousness*", Prof. Sir Roger Penrose, 27th September 2020 (around 600 participants).
2. "*7 affascinanti rompicapi della fisica moderna: dai buchi neri al gatto di Schroedinger*", Prof. Catalina Curceanu, Laboratori Nazionali di Frascati dell'INFN, 25th November 2021 (around 600 participants).
3. "*La coscienza è quantistica*", Giacomo D'Ariano (Università degli Studi di Pavia) and Federico Faggin (Cofondatore e CEO di Zilog, Cygnet Technologies e Synaptics), 12th May 2023 (around 700 participants).
4. "*Meccanica Quantistica e Realtà*", Prof. Angelo Bassi (Università di Trieste) and Prof. Federico Laudisa (Università di Trento), 1st December 2023 (around 600 participants).

Communication in the EU-funded VIRTUOUS project

Marcello collaborated in design, realization, and maintenance of the official site for the Telethon Funded Project (**GSP20005_PAsIAHSP007**), **CRYSTAL** (https://crystal.m3b.it).