LORENZO DI RIENZO
Curriculum Vitae
ai fini della pubblicazione

Part I – General Information

Full Name	Lorenzo Di Rienzo
Spoken Languages	Italian, English

Part II – Education

Type	Year	Institution	Notes (Degree, Experience,…)
Ph.D. in Life Sciences	2019	Sapienza University of Rome	Thesis Title: “A moments-based analysis of shape and electrostatics in molecular recognition: the case of antibodies” (Mark: Ottimo)
M. Sc. in Physics	2015	Sapienza University of Rome	Curriculum: “Physics of biosystems”. Thesis Title: “Approccio meccanico-statistico alla regolazione genica post-trascrizionale basata su RNA” (Mark: summa cum laude)
Bachelor in Physics	2012	Sapienza University of Rome	Thesis Title: “Analisi degli spetti di emissione ed assorbimento di un eccitone in un semiconduttore”

Part III – National Scientific Habilitation

- National Scientific Habilitation for the function of 2nd level professor in SC 05/E1 from 03/07/2024 to 03/07/2035 (SSD BIOS-07/A)
- National Scientific Habilitation for the function of 2nd level professor in SC 05/E2 from 01/07/2024 to 01/07/2035 (SSD BIOS-08/A)

Part IV – Appointments

Start	End	Institution	Position
01-09-2025	ongoing	Saint Camillus International University of	Associate Professor (GSD 05/BIOS-07

		Health and Medical Sciences	Biochimica)
16-03-2020	31-08-2025	Center for Life Nano and Neuro Science - Istituto Italiano di Tecnologia	Post-doc
01-11-2018	15-03-2020	Department of Physics - Sapienza University of Rome	Post-doc

Part V – Teaching experience

Year	Institution	Lecture/Course
Jun 2025	University of Udine	Professor of "Computational methods in Protein Structural Biophysics" [3 CFU], PhD Course in Mathematics and Physics, Department of Mathematics, Computer Science and Physics
2024/25	Campus Bio-Medico University of Rome	Professor of Physics Course (60 h), Foundation Year programme
2024/25	Campus Bio-Medico University of Rome	Advanced Physics, degree program in Biomedical Engineering [1 CFU].
2024/25	Campus Bio-Medico University of Rome	General Physics 2, shared by the degree program in MedTech and Biomedical Engineering [3 CFU].
2024/25	Campus Bio-Medico University of Rome	Fisica Medica, degree program in Odontoiatria e Protesi Dentaria [1 CFU]
2023/24	Campus Bio-Medico University of Rome	Advanced Physics, degree program in Biomedical Engineering [1 CFU].
2023/24	Campus Bio-Medico University of Rome	General Physics 2, shared by the degree program in MedTech and Biomedical Engineering [2 CFU].
2023/24	Campus Bio-Medico University of Rome	Teaching assistant of General Physics 1 and General Physics 2, shared by the degree program in MedTech and Biomedical Engineering.
2022/23	Campus Bio-Medico University of Rome	General Physics 2, shared by the degree program in MedTech and Biomedical Engineering [2 CFU].
2022/23	Campus Bio-Medico University of Rome	Teaching assistant of General Physics 1 and General Physics 2, shared by the degree program in MedTech and Biomedical Engineering.
2022	Sapienza University of Rome	Professor of Physics Course (40 h), Sapienza Foundation Year

Part VI – Student Supervision

2021/25	The Open University, Doctoral School in Health, Sustainable and Human Technologies	Tutoring Ph.D Student [Fausta Desantis]: “Refining proteins interactions to tackle aggregation in AL amyloidosis via the computational design of inhibitory peptides”
2020/21	Sapienza University of Rome, Department of Physics	Tutoring Master Thesis Student [Alfredo De Lauro]: “Antibody Design through geometric optimization based on Zernike Polynomials and Monte Carlo Simulations”

Part VII – Conferences and Workshops

Sep 2025	Fifth DiSVA-MaSBiC Symposium Advances in Biomolecular Sciences: Perspectives on Structure, Function and Dynamics, Ancona, Italy	Scientific Committee Member
Jul 2025	15th European Biophysics Congress, Roma, Italy	Selected Oral Presentation
Sep 2024	IV DiSVA-MaSBiC Symposium, Advances in Biomolecular Science: Perspectives on Structure, Function and Complexity, Ancona, Italy	Local Organizer
Apr 2024	Seminar cycle organized at Campus Bio-Medico University of Rome by Unità di Ricerca di Fisica Non Lineare e Modelli Matematici	Invited Seminar
Feb 2024	VIII Workshop in Physics of Biomolecules: Structure, Dynamics and Function, Bressanone (BZ), Italy	Selected Oral Presentation
Sep 2023	III DiSVA-MaSBiC Symposium, advances in Protein Science: Exploring Structure, Function, and Beyond, Ancona, Italy	Chairman of a conference session
Mar 2023	XVI International Workshop on Complex Systems, Andalo (TN), Italy	Selected Oral Presentation
Sep 2022	II DiSVA-MaSBiC Symposium, Protein structure and function in Biology, Medicine and Nanotechnology, Ancona, Italy	Selected Oral Presentation
Jun 2022	XVIII annual meeting of Italian Society	Selected Oral Presentation

	of Bioinformatics, Verona, Italy	
Apr 2021	From Information to Function: a system biology view of the processes of life – A tribute to Anna Tramontano, online	Selected Oral Presentation
Jun 2019	XVI annual meeting of Italian Society of Bioinformatics, Palermo, Italy	Selected Oral Presentation
Nov 2018	V annual meeting of International Society of Computational Biology - LatinoAmerica, Vina del Mar, Chile	Selected Oral Presentation
Sep 2017	XIII Basel Computational Biology Conference, Basel, Switzerland	Selected Oral Presentation

Part VII - Society memberships and Editorial Service

Year	Title
2024 - on going	Member of the Italian society of pure and applied biophysics
2024 - on going	Associate Editor for BMC bioinformatics
2021 - on going	Review editor for Frontiers in Molecular Bioscience in section Protein Biochemistry for Basic and Applied Sciences and Biological Modeling and Simulation

Part VII - Funding Information [grants as PI-principal investigator or I-investigator]

Year	Title	Program	Grant value
2023	"Coexistence between Ordered and DIsordered Regions in proteins: a multiscale overview on the mechanisms regulating aggregate-associated diseases", CODIR	Progetti di Ricerca di Interesse Nazionale - PRIN - Investigator	€ 294762
2023	"Structure-based Assessment of Protein-Protein Human InteRactomE", SAPPHIR3	Italian SuperComputing Resource Allocation - ISCRA B - Investigator	960000 GPU hours / equivalent to 57600 euros
2022	"AntiBody Conformational changes upon binding through MOlecular DYNamics simulations" , ABCMODYN	Italian SuperComputing Resource Allocation – ISCRA C - Principal Investigator	64000 GPU hours / equivalent to 3840 euros
2019	"Investigation of antibody changes upon binding"	NVIDIA Academic Hardware Grant Program -	Nvidia Titan V GPU/ equivalent

	Principal Investigator	to 3000 euros

Part IX – Research Activities

Keywords	Brief Description
Computational Biology	My research is primarily focused on the in-silico investigation of fundamental interactions between biological molecules. The aim is to develop computational protocols to address challenging tasks in computational biology. Specifically, my work centers on the quantitative characterization of the physical mechanisms underlying molecular recognition, achieved through the analysis of the structural and dynamic features of biomolecules. The outcomes of this research are intended to support the development of predictive algorithms and methods with significant biomedical relevance
Protein-Protein Interactions	
Protein Design	
Molecular Dynamics	
Structural Bioinformatics	

Part X – Summary of Scientific Achievements

Scientific Publications

Product type	Number	Data Base	Start	End
Papers [international]	39	Scopus	2017	2025

Total Impact factor	241,1
Total Citations	711
Average Citations per Product	18,2
Hirsch (H) index	16
Normalized H index*	2

*H index divided by the academic seniority (8 years starting from the first publication until today).

Part XI– Selected Publications

List of the publications selected for the evaluation.

1) Parisi G., Piacentini R., Incocciati A., Bonamore A., Macone A., Rupert J., Zacco E., Miotto M., Milanetti E., Tartaglia G. G., Ruocco G., Boffi A., Di Rienzo L. (2024). Design of protein-binding peptides with controlled binding affinity: the case of SARS-CoV-2 receptor binding domain and angiotensin-converting enzyme 2 derived peptides. FRONTIERS IN MOLECULAR BIOSCIENCES, vol. 10, ISSN: 2296-889X, doi: 10.3389/fmolb.2023.1332359
2) Fausta Desantis, Mattia Miotto, Edoardo Milanetti, Giancarlo Ruocco, Lorenzo Di Rienzo (2024).Computational evidences of a misfolding event in an aggregation-prone light chain preceding the formation of the non-native pathogenic dimer. PROTEINS, ISSN: 1097-0134, doi: 10.1002/prot.26672
3) Lorenzo Di Rienzo, Mattia Miotto, Edoardo Milanetti, Giancarlo Ruocco (2023). Computational structural-based GPCR optimization for user-defined ligand: Implications for the development of

biosensors. COMPUTATIONAL AND STRUCTURAL BIOTECHNOLOGY JOURNAL, ISSN: 2001-0370, doi: 10.1016/j.csbj.2023.05.004

4) Miotto M., Di Rienzo L., Gosti G., Bo' L., Parisi G., Piacentini R., Boffi A., Ruocco G., Milanetti E. (2022). Inferring the stabilization effects of SARS-CoV-2 variants on the binding with ACE2 receptor. COMMUNICATIONS BIOLOGY, vol. 5, ISSN: 2399-3642, doi: 10.1038/s42003-021-02946-w
5) Di Rienzo L., De Flaviis L., Ruocco G., Folli V., Milanetti E. (2022). Binding site identification of G protein-coupled receptors through a 3D Zernike polynomials-based method: application to C. elegans olfactory receptors. JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN, vol. 36, p. 11-24, ISSN: 0920-654X, doi: 10.1007/s10822-021-00434-1
6) Di Rienzo L., Miotto M., Bo L., Ruocco G., Raimondo D., Milanetti E. (2021). Characterizing hydropathy of amino acid side chain in a protein environment by investigating the structural changes of water molecules network. FRONTIERS IN MOLECULAR BIOSCIENCES, vol. 8, ISSN: 2296-889X, doi: 10.3389/fmolb.2021.626837
7) Di Rienzo L., Monti M., Milanetti E., Miotto M., Boffi A., Tartaglia G. G., Ruocco G. (2021). Computational optimization of angiotensin-converting enzyme 2 for SARS-CoV-2 Spike molecular recognition. COMPUTATIONAL AND STRUCTURAL BIOTECHNOLOGY JOURNAL, vol. 19, p. 3006-3014, ISSN: 2001-0370, doi: 10.1016/j.csbj.2021.05.016
8) Milanetti E., Miotto M., Di Rienzo L., Nagaraj M., Monti M., Golbek T. W., Gosti G., Roeters S. J., Weidner T., Otzen D. E., Ruocco G. (2021). In-Silico Evidence for a Two Receptor Based Strategy of SARS-CoV-2. FRONTIERS IN MOLECULAR BIOSCIENCES, vol. 8, ISSN: 2296-889X, doi: 10.3389/fmolb.2021.690655
9) Di Rienzo L., Milanetti E., Testi C., Montemiglio L. C., Baiocco P., Boffi A., Ruocco G. (2020). A novel strategy for molecular interfaces optimization: the case of ferritin-transferrin receptor interaction. COMPUTATIONAL AND STRUCTURAL BIOTECHNOLOGY JOURNAL, vol. 18, p. 2678-2686, ISSN: 2001-0370, doi: 10.1016/j.csbj.2020.09.020
10) Di Rienzo, Lorenzo, Milanetti, Edoardo, Alba, Josephine, D'Abramo, Marco (2020). Quantitative characterization of binding pockets and binding complementarity by means of Zernike descriptors. JOURNAL OF CHEMICAL INFORMATION AND MODELING, vol. 60, p. 1390-1398, ISSN: 1549-9596, doi: 10.1021/acs.jcim.9b01066
11) Miotto, Mattia, Olimpieri, Pier Paolo, Di Rienzo, Lorenzo, Ambrosetti, Francesco, Corsi, Pietro, Lepore, Rosalba, Tartaglia, Gian Gaetano, Milanetti, Edoardo (2019). Insights on protein thermal stability: a graph representation of molecular interactions. BIOINFORMATICS, vol. 35, p. 1-9, ISSN: 1367-4803, doi: 10.1093/bioinformatics/bty1011
12) Di Rienzo, Lorenzo, Milanetti, Edoardo, Lepore, Rosalba, Olimpieri, Pier Paolo, Tramontano, Anna (2017). Superposition-free comparison and clustering of antibody binding sites: implications for the prediction of the nature of their antigen. SCIENTIFIC REPORTS, vol. 7, ISSN: 2045-2322, doi: 10.1038/srep45053

Part XI– All Publications

1) Grassmann, G., Di Rienzo, L., Ruocco, G., Milanetti, E., & Miotto, M. (2025). Exploring neural networks to uncover information-richer features for protein interaction prediction. European Biophysics Journal, 1-12.
2) Di Rienzo, L.*, Miotto, M., Milanetti, E., & Ruocco, G. (2025). Ligand specificity in Saccaromices cerevisiae G-Protein coupled receptor binding site design. Philosophical Magazine, 1-17.
3) Grassmann, G., Di Rienzo, L., Ruocco, G., Miotto, M., & Milanetti, E. (2025). Compact assessment of molecular surface complementarities enhances neural network-aided prediction of key binding residues. *Journal of Chemical Information and Modeling*, *65*(5), 2695-2709.

4) Testi, C., Piacentini, R., Perrone, A., Bartoli, C., Leso, D., Pavia, D., ... & Di Rienzo, L*. (2025). Exploring the NANOG-TET2 interaction interface. Effects of a selected mutation and hypothesis on the clinical correlation with anemias. Frontiers in Chemical Biology, 3, 1517163.
5) Miotto, M., Di Rienzo, L., Bo', L., Ruocco, G., & Milanetti, E. (2025). Zepyros: a webserver to evaluate the shape complementarity of protein–protein interfaces. *Bioinformatics Advances*, *5*(1), vbaf051.
6) Panei, F. P., Di Rienzo, L., Zacco, E., Armaos, A., Tartaglia, G. G., Ruocco, G., & Milanetti, E. (2024). Synchronized motion of interface residues for evaluating protein–RNA complex binding affinity: Application to aptamer‐mediated inhibition of TDP‐43 aggregates. Protein Science, 33(12), e5201.
7) Grassmann, G., Miotto, M., Desantis, F., Di Rienzo, L., Tartaglia, G. G., Pastore, A., ... & Milanetti, E. (2024). Computational Approaches to Predict Protein–Protein Interactions in Crowded Cellular Environments. *Chemical Reviews*, *124*(7), 3932-3977.
8) Desantis, F., Miotto, M., Milanetti, E., Ruocco, G., & Di Rienzo, L.* (2024). Computational evidences of a misfolding event in an aggregation‐prone light chain preceding the formation of the non‐native pathogenic dimer. Proteins: Structure, Function, and Bioinformatics.
9) Monti, M., Milanetti, E., Frans, M. T., Miotto, M., Di Rienzo, L., Baranov, M. V., ... & Roeters, S. J. (2024). Two Receptor Binding Strategy of SARS-CoV-2 Is Mediated by Both the N-Terminal and Receptor-Binding Spike Domain. The Journal of Physical Chemistry B, 128(2), 451-464.
10) Parisi, G., Piacentini, R., Incocciati, A., Bonamore, A., Macone, A., Rupert, J., ... & Di Rienzo, L.* (2024). Design of protein-binding peptides with controlled binding affinity: the case of SARS-CoV-2 receptor binding domain and angiotensin-converting enzyme 2 derived peptides. *Frontiers in Molecular Biosciences*, *10*, 1332359.
11) Kalia, M., Miotto, M., Ness, D., Opie-Martin, S., Spargo, T. P., Di Rienzo, L., ... & Project MinE ALS Sequencing Consortium. (2023). Molecular dynamics analysis of superoxide dismutase 1 mutations suggests decoupling between mechanisms underlying ALS onset and progression. Computational and Structural Biotechnology Journal, 21, 5296-5308.
12) Grassmann, G., Di Rienzo, L., Gosti, G., Leonetti, M., Ruocco, G., Miotto, M., & Milanetti, E. (2023). Electrostatic complementarity at the interface drives transient protein-protein interactions. Scientific Reports, 13(1), 10207.
13) Di Rienzo, L.*, Miotto, M., Milanetti, E., & Ruocco, G. (2023). Computational structural-based GPCR optimization for user-defined ligand: Implications for the development of biosensors. *Computational and Structural Biotechnology Journal*, *21*, 3002-3009.
14) Di Rienzo, L.*, Miotto, M., Desantis, F., Grassmann, G., Ruocco, G., & Milanetti, E. (2023). Dynamical changes of SARS‐CoV‐2 spike variants in the highly immunogenic regions impact the viral antibodies escaping. *Proteins: Structure, Function, and Bioinformatics*, *91*(8), 1116-1129.
15) Miotto, M., Di Rienzo, L., Grassmann, G., Desantis, F., Cidonio, G., Gosti, G., ... & Milanetti, E. (2023). Differences in the organization of interface residues tunes the stability of the SARS-CoV-2 spike-ACE2 complex. *Frontiers in Molecular Biosciences*, *10*, 1205919.
16) Milanetti, E., Miotto, M., Di Rienzo, L., & Ruocco, G. (2023). Investigating the competition between ACE2 natural molecular interactors and SARS-CoV-2 candidate inhibitors. *Chemico-Biological Interactions*, *374*, 110380.
17) Desantis, F., Miotto, M., Di Rienzo, L., Milanetti, E., & Ruocco, G. (2022). Spatial organization of hydrophobic and charged residues affects protein thermal stability and binding affinity. *Scientific Reports*, *12*(1), 12087.
18) De Lauro, A.^, Di Rienzo, L.^*, Miotto, M., Olimpieri, P. P., Milanetti, E., & Ruocco, G. (2022). Shape complementarity optimization of antibody–antigen interfaces: the application to SARS-CoV-2 spike protein. *Frontiers in Molecular Biosciences*, *9*, 874296.

19) Piacentini, R., Centi, L., Miotto, M., Milanetti, E., Di Rienzo, L., Pitea, M., ... & Parisi, G. (2022). Lactoferrin inhibition of the complex formation between ACE2 receptor and SARS CoV-2 recognition binding domain. *International journal of molecular sciences*, *23*(10), 5436.
20) Miotto, M., Armaos, A., Di Rienzo, L., Ruocco, G., Milanetti, E., & Tartaglia, G. G. (2022). Thermometer: a webserver to predict protein thermal stability. *Bioinformatics*, *38*(7), 2060-2061.
21) Miotto, M., Di Rienzo, L., Gosti, G., Bo', L., Parisi, G., Piacentini, R., ... & Milanetti, E. (2022). Inferring the stabilization effects of SARS-CoV-2 variants on the binding with ACE2 receptor. *Communications biology*, *5*(1), 20221.
22) Grassmann, G., Miotto, M., Di Rienzo, L., Gosti, G., Ruocco, G., & Milanetti, E. (2022). A novel computational strategy for defining the minimal protein molecular surface representation. *Plos one*, *17*(4), e0266004.
23) Di Rienzo, L., De Flaviis, L., Ruocco, G., Folli, V., & Milanetti, E. (2022). Binding site identification of G protein-coupled receptors through a 3D Zernike polynomials-based method: application to C. elegans olfactory receptors. *Journal of Computer-Aided Molecular Design*, 1-14.
24) Grassmann, G., Miotto, M., Di Rienzo, L., Salaris, F., Silvestri, B., Zacco, E., ... & Milanetti, E. (2021). A computational approach to investigate tdp-43 rna-recognition motif 2 c-terminal fragments aggregation in amyotrophic lateral sclerosis. *Biomolecules*, *11*(12), 1905.
25) Di Rienzo, L., Milanetti, E., Ruocco, G., & Lepore, R. (2021). Quantitative description of surface complementarity of antibody-antigen interfaces. *Frontiers in molecular biosciences*, *8*, 749784.
26) Milanetti, E.^, Miotto, M.^, Di Rienzo, L.^, Nagaraj, M.^, Monti, M., Golbek, T. W., ... & Ruocco, G. (2021). In-silico evidence for a two receptor based strategy of SARS-CoV-2. *Frontiers in molecular biosciences*, *8*, 690655.
27) Di Rienzo, L.*, Monti, M., Milanetti, E., Miotto, M., Boffi, A., Tartaglia, G. G., & Ruocco, G. (2021). Computational optimization of angiotensin-converting enzyme 2 for SARS-CoV-2 Spike molecular recognition. *Computational and Structural Biotechnology Journal*, *19*, 3006-3014.
28) Calvo Galve, N., Abrishamkar, A., Sorrenti, A., Di Rienzo, L., Satta, M., D'Abramo, M., ... & Puigmartí‐Luis, J. (2021). Exploiting reaction‐diffusion conditions to trigger pathway complexity in the growth of a MOF. *Angewandte Chemie*, *133*(29), 16056-16063.
29) Miotto, M., Di Rienzo, L., Gosti, G., Milanetti, E., & Ruocco, G. (2021). Does blood type affect the COVID-19 infection pattern?. *Plos one*, *16*(5), e0251535.
30) Di Rienzo, L.^, Miotto, M.^, Bò, L., Ruocco, G., Raimondo, D., & Milanetti, E. (2021). Characterizing hydropathy of amino acid side chain in a protein environment by investigating the structural changes of water molecules network. *Frontiers in molecular biosciences*, *8*, 626837.
31) Miotto, M., Di Rienzo, L., Bò, L., Boffi, A., Ruocco, G., & Milanetti, E. (2021). Molecular mechanisms behind anti SARS-CoV-2 action of lactoferrin. *Frontiers in molecular biosciences*, *8*, 607443.
32) Milanetti, E., Miotto, M., Di Rienzo, L., Monti, M., Gosti, G., & Ruocco, G. (2021). 2D Zernike polynomial expansion: Finding the protein-protein binding regions. *Computational and structural biotechnology journal*, *19*, 29-36.
33) Sandomenico, A.^, Di Rienzo, L.^, Calvanese, L., Iaccarino, E., D'Auria, G., Falcigno, L., ... & Raimondo, D. (2020). Insights into the Interaction Mechanism of DTP3 with MKK7 by Using STD-NMR and Computational Approaches. *Biomedicines*, *9*(1), 20.
34) Alba, J., Di Rienzo, L., Milanetti, E., Acuto, O., & D'Abramo, M. (2020). Molecular dynamics simulations reveal canonical conformations in different pMHC/TCR interactions. *Cells*, *9*(4), 942.
35) Miotto, M.^, Di Rienzo, L^, Corsi, P., Ruocco, G., Raimondo, D., & Milanetti, E. (2020). Simulated epidemics in 3d protein structures to detect functional properties. *Journal of Chemical Information and Modeling*, *60*(3), 1884-1891.
36) Di Rienzo, L., Milanetti, E., Alba, J., & D'Abramo, M. (2020). Quantitative characterization of binding pockets and binding complementarity by means of zernike descriptors. *Journal of chemical information and modeling*, *60*(3), 1390-1398.

37) Di Rienzo, L.*, Milanetti, E., Testi, C., Montemiglio, L. C., Baiocco, P., Boffi, A., & Ruocco, G. (2020). A novel strategy for molecular interfaces optimization: the case of ferritin-transferrin receptor interaction. *Computational and structural biotechnology journal*, *18*, 2678-2686.
38) Miotto, M., Olimpieri, P. P., Di Rienzo, L., Ambrosetti, F., Corsi, P., Lepore, R., ... & Milanetti, E. (2019). Insights on protein thermal stability: a graph representation of molecular interactions. *Bioinformatics*, *35*(15), 2569-2577.
39) Di Rienzo, L.^, Milanetti^, E., Lepore, R., Olimpieri, P. P., & Tramontano, A. (2017). Superposition-free comparison and clustering of antibody binding sites: implications for the prediction of the nature of their antigen. *Scientific reports*, *7*(1), 45053.

Number of publications as (co-)first author: 13
Number of publications as corresponding author: 9
Number of publications as last author: 3