# Curriculum Vitae et Studiorum

Daniele Narzi

***Affiliation:***

University of L'Aquila
Department of Physical and Chemical Sciences
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Nationality: Italian

## Education and working experience

***October 2019 – October 2024*** Researcher (RTD-A) at University of L'Aquila (Italy)

***April 2018 – February 2020 –*** Leader of the component ID C1698 within Human Brain Project:

*SGA2 - T6.1.1 - Multi scale simulations of protein dynamics and complexation*

***May 2016 – July 2019 –*** PostDoc position in the LCBC lab of Prof. Dr. Ursula Roethlisberger, EPFL (Switzerland)

***January 2012 – April 2016 –*** PostDoc position in the CBBC group of Prof. Dr. Leonardo Guidoni, University of L'Aquila and University of Rome "La Sapienza" (Italy)

***November 2011 –*** PhD (Dr. Rer. Nat.) Universität Erlangen-Nürnberg (Germany)
Thesis: "*Nanodynamics and Protonation State Characterization of Major Histocompatibility Complex Molecules and Thioredoxins*" Supervisor: Prof. Dr. Rainer A. Böckmann

***March/July 2005 –*** Collaboration contract with the group of Prof. Alfredo Di Nola, Chemistry Department, University of Rome "La Sapienza" (Italy)

***May 2004 –*** Degree (*Laurea*) in Chemistry - Summa cum laude, University of Rome "La Sapienza" (Italy)
Thesis: "*Studio del folding di proteine mediante simulazioni di Dinamica Molecolare*"
Supervisor: Prof. Alfredo Di Nola

## Research interests

● Simulations of molecular and macromolecular systems with methods based on classical mechanics.
● Characterization of catalytic mechanisms in enzymes by means of QM and QM/MM calculations.
● Computational analysis of dissociation constants of titratable sites of proteins based on the solution of the Poisson-Boltzmann equation.
● Binding free energy calculations of protein/ligand complexes.
● Investigation of protein/membrane interactions and membrane properties by means of classical MD simulations.
● Study of the molecular determinants behind autoimmune diseases.
● Study of the function of biological photosynthetic systems.
● Characterization of endogenous ligands and design of drugs binding to G protein-coupled receptors.
● Investigation of the molecular mechanisms and theoretical modeling of signal transduction pathways.

## Teaching

● Since 2021/2022 teacher in charge of the course of Chemistry, Industrial Engineering, University of L'Aquila.
● Since 2019/2020 teacher in charge of the course "Computer Modelling and Simulations of Biomolecules", Chemistry and Materials, University of L'Aquila.
● Teaching Assistant of "Physical Chemistry I", University of L'Aquila (Second Semester 2019/2020)
● Exam committee member of "General Chemistry" for Biotechnologies, University of L'Aquila (2015-2016)
● Lecturer for the Poisson-Boltzmann equation module in "Computer Modelling and Simulations of Chemical and Biological Systems", University of L'Aquila (November 2014)
● Adjunct Professor of "Computer Modelling and Simulations of Biomolecules", University of L'Aquila (First Semester 2013/2014)
● Lecturer for the Poisson-Boltzmann equation module in "Computer Modelling and Simulations of Chemical and Biological Systems", University of L'Aquila (December 2011)
● Teaching Assistant of "Structural Biology & Crystallography", Universität Erlangen-Nürnberg (March 2011)
● Teaching Assistant of "Lab training Computer Simulation of Biomolecular Systems", Universität des Saarlandes (October 2008)
● Teaching Assistant of "Computational Immunology", Universität des Saarlandes (April 2006, November 2007)

## Officially supervised students

● Ganesh Sivaraman
● Marco Manzoli
● Kwame Atta Gyamfi
● Adnan Gulzar
● Mario Frezzini (Master and PhD Student)
● Gianluca Parisse (Master and PhD Student)
● Noemi Di Stefano
● Emilia Piccirilli
● Cristina De Santis
● Giovanna Nuccetelli

## Publications

(*) Contributed equally (‡) Corresponding author

Scopus Author ID: 23100931600
http://www.scopus.com/authid/detail.uri?authorId=23100931600

M. Capone, G. Parisse, **D. Narzi**, and L. Guidoni "Unravelling $Mn_4Ca$ cluster vibrations in the $S_1$, $S_2$ and $S_3$ states of the Kok-Joliot cycle of photosystem II" ***Phys. Chem. Chem. Phys.*** 26 (2024) 20598 - 20609

G. Parisse, **D. Narzi**, B. D. Belviso, V. Capriati, R. Caliandro, M. Trotta, and L. Guidoni "Unveiling the Influence of Hydrated Deep Eutectic Solvents on the Dynamics of Water-Soluble Proteins" ***J. Phys. Chem. B*** 127 (2023) 6487-6499

P. Greife, M. Schönborn, M. Capone, R. Assunção **D. Narzi**, L. Guidoni, and H. Dau "The electron-proton bottleneck of photosynthetic oxygen evolution" ***Nature*** 617 (2023) 623-628

G. Pascarella, L. Antonelli, **D. Narzi**‡, T. Battista, A. Fiorillo, G. Colotti, L. Guidoni, V. Morea, and A. Ilari "Investigation of the Entry Pathway and Molecular Nature of σ1 Receptor Ligands" ***Int. J. Mol. Sci***. 24 (2023) 6367

M. Frezzini, A. Scortica, M. Capone, **D. Narzi**‡, M. Benedetti, F. Angelucci, B. Mattei, and L. Guidoni "Molecular dynamics simulations and kinetic measurements provide insights into the structural requirements of substrate size-dependent specificity of oligogalacturonide oxidase 1 (OGOX1)" ***Plant Physiol. Biochem***.194 (2023) 315-325

S. Pascarella, M. Bianchi, M. Giovannetti, **D. Narzi**, R. Cauda, A. Cassone, and M. Ciccozzi "The SARS-CoV-2 Mu variant should not be left aside: It warrants attention for its immuno-escaping ability" ***J. Med. Virol.*** 94 (2022) 2479 - 2486

**D. Narzi**, and L. Guidoni "Structural and dynamic insights into $Mn_4Ca$ cluster-depleted Photosystem II" ***Phys. Chem. Chem. Phys.*** 23 (2021) 27428-27436

A. Scortica, M. Capone, **D. Narzi**‡, M. Frezzini, V. Scafati, M. Giovannoni, F. Angelucci, L. Guidoni, B. Mattei, M. Benedetti "A molecular dynamics-guided mutagenesis identifies two aspartic acid residues involved in the pH-dependent activity of OG-OXIDASE 1" ***Plant Physiol. Biochem.*** 169 (2021) 171-182

M. Capone, **D. Narzi**‡ and L. Guidoni "Mechanism of Oxygen Evolution and Mn4CaO5 Cluster Restoration in the Natural Water-Oxidizing Catalyst" ***Biochemistry*** 60 (2021) 2341–2348

**D. Narzi**, S.C. van Keulen and U. Roethlisberger "Gαi1 Inhibition Mechanism of ATP-bound Adenylyl Cyclase Type 5" ***PLoS ONE*** 16 (2021) e0245197

M. Frezzini, **D. Narzi**, A.M. Sciolari, L. Guidoni and S. Pascarella "Molecular dynamics of an asymmetric form of GabR, a bacterial transcriptional regulator" ***Biophys. Chem***. 262 (2020) 106380

M. Capone, L. Guidoni, and **D. Narzi**‡ "Structural and dynamical characterization of the $S_4$ state of the Kok-Joliot's cycle by means of QM/MM Molecular Dynamics Simulations" ***Chem. Phys. Lett.*** 742 (2020) 137111

S. Nakamura, M. Capone, **D. Narzi**, and L. Guidoni "Pivotal role of the redox-active tyrosine in driving the water splitting catalyzed by photosystem II" ***Phys. Chem. Chem. Phys.*** 22 (2020) 273-285

N. Bruce*, **D. Narzi***, D. Trpevski*, S.C. van Keulen*, A. Nair, P. Vidossich, U. Roethlisberger, R. Wade, P. Carloni and J.H.Kotaleski "Regulation of adenylyl cyclase 5 in striatal neurons confers the ability to detect coincident neuromodulatory signals" ***PLoS. Comp. Biol.*** 15 (2019) e1007382

S.C. van Keulen, **D. Narzi**, U. Roethlisberger "Association of Both Inhibitory and Stimulatory Gα Subunits Implies Adenylyl Cyclase 5 Deactivation" ***Biochemistry*** 58 (2019) 4317-4324

M. Capone, **D. Narzi**, A. Tychengulova and L. Guidoni "On the comparison between differential vibrational spectroscopy spectra and theoretical data in the carboxyl region of Photosystem II" ***Physiologia Plantarum*** 166 (2019) 33-43

**D. Narzi***,‡, M. Capone*, D. Bovi and L. Guidoni "Evolution from $S_3$ to $S_4$ state of the oxygen evolving complex in Photosystem II monitored by QM/MM dynamics" ***Chem. – Eur. J.*** 24 (2018) 10820-10828

T. Milano, A. Gulzar, **D. Narzi**, L. Guidoni and S. Pascarella "Molecular dynamics simulation unveils the conformational flexibility of the interdomain linker in the bacterial transcriptional regulator GabR from *Bacillus subtilis* bound to pyridoxal 5'-phosphate" ***PLoS ONE***. 12 (2017) e0189270

**D. Narzi**‡, E. Coccia, M. Manzoli and L. Guidoni "Impact of molecular flexibility on the site energy shift of chlorophylls in Photosystem II" ***Biophys. Chem.*** 229 (2017) 93-98

**D. Narzi***,‡, G. Mattioli*, D. Bovi and L. Guidoni "A Spotlight on the Compatibility between XFEL and *Ab Initio* Structures of the Oxygen Evolving Complex in Photosystem II" ***Chem. – Eur. J.*** 23 (2017) 6969-6973

D. Bovi, M. Capone, **D. Narzi**, and L. Guidoni "Vibrational fingerprints of the $Mn_4CaO_5$ cluster in Photosystem II by mixed quantum-classical molecular dynamics" ***Biochim. Biophys. Acta - Bioenergetics*** 1857 (2016) 1669-1677

M. Capone, **D. Narzi**, D. Bovi, and L. Guidoni "Mechanism of water delivery to the active site of Photosystem II along the S2 to S3 transition" ***J. Phys. Chem. Lett.*** 7 (2016) 592-596

**D. Narzi,** D. Bovi, P. De Gaetano and L. Guidoni, "Dynamics of the Special Pair of Chlorophylls of Photosystem II" ***J. Am. Chem. Soc.*** 138 (2016) 257-264

M. Capone, D. Bovi, **D. Narzi** and L. Guidoni, "Reorganization of substrate waters between the closed and open cubane conformers during the $S_2$ to $S_3$ transition in the Oxygen Evolving Complex" ***Biochemistry***. 54 (2015) 6442

F. Pitari, D. Bovi, **D. Narzi** and L. Guidoni, "Characterization of $Sr^{2+}$ and $Cd^{2+}$ substituted Oxygen Evolving Complex of Photosystem II by QM/MM calculations" ***Biochemistry***. 54 (2015) 5959

**D. Narzi***, D. Bovi* and L. Guidoni. "Pathway for Mn-cluster oxidation by tyrosine-Z in the $S_2$ state of photosystem II" ***Proc. Natl. Ac. Sci. USA*** 111 (2014) 8723 – 8728

D. Bovi, **D. Narzi** and L. Guidoni. "Magnetic interactionsin the catalyst used by nature to split water: a DFT+U multiscale study on the $Mn_4CaO_5$ core in photosystem II" ***New J. Phys***. 16 (2014) 015020

D. Bovi*, **D. Narzi*** and L. Guidoni. "The S2 state of the Oxygen-Evolving Complex of Photosystem II explored by QM/MM dynamics: spin surfaces and metastable states suggest a reaction path towards the S3 state" ***Ang. Chem. Int. Ed***. 52 (2013) 11744–11749

**D. Narzi**, C. M. Becker, M. T. Fiorillo, A. Ziegler and R. A. Böckmann. "Dynamical characterization of two differentially disease-associated MHC Class I proteins in complex with viral- and self-antigenes" ***J. Mol. Biol***. 415 (2012) 429-442.

M. Borisovska, Y. N. Schwarz, **D. Narzi**, S. W. I. Siu, J. Kesavan, R. Mohrmann, R. A. Böckmann and D. Bruns. "Membrane-proximal tryptophanes of Synaptobrevin II promote priming of secretory vesicles" ***J. Neur. Sci***. 32 (2012) 15983–15997

E. Nurzia*, **D. Narzi***, A. Cauli, A. Mathieu, V. Tedeschi, R. Sorrentino, R. A. Böckmann and M. T. Fiorillo. "Interaction pattern of Arg 62 in the A-pocket of differentially disease-associated HLA-B27 subtypes suggests distinct TCR binding modes" ***PLoS ONE*** 7 (2012) e32865

**D. Narzi**, S. W. I. Siu, C. U. Stirnimann, J. P. A. Grimshaw, R. Glockshuber, G. Capitani and R. A. Böckmann. "Evidence for proton shuffling in a thioredoxin-like protein during catalysis" ***J. Mol. Biol.*** 382 (2008) 978-986.

**D. Narzi***, K. Winkler*, J. Saidowski, R. Misselwitz, A. Ziegler, R. A. Böckmann and U. Alexiev. "Molecular determinants of MHC class I complex stability: shaping antigenic features through long-range electrostatic interactions" ***J. Biol. Chem.*** 283 (2008) 23093-23103.

H. Fabian, H. Huser, **D. Narzi**, R. Misselwitz, B. Loll, A. Ziegler, R. A. Böckmann, B. Uchanska-Ziegler and D. Naumann. "HLA-B27 Subtypes Differentially Associated with Disease Exhibit Conformational Differences in Solution" ***J. Mol. Biol.*** 376 (2008) 798-810.

**D. Narzi**, I. Daidone, A. Amadei and A. Di Nola. "Protein folding pathways revealed by essential dynamics sampling" ***J.Chem. Theory Comput.*** 4 (2008) 1940-1948.

## Approved Project Proposals *(as Principal Investigator)*

● "Exploring the molecular determinants of the bottleneck of photosynthetic oxygen evolution using MD simulations" within the ISCRA-B project 2023

● "Investigating the gating mechanism of the inner membrane urea channel UreI by MD simulations" within the ISCRA-C project 2023

● "Structural and dynamical insights into engineered T-cell receptors for cancer immunotherapy" within the ISCRA-C project 2022

● "*Exploring the effect of pathogenic mutations in Sigma-1 receptor by means of Classical MD simulations*" within the ISCRA-C project 2021

● "*Characterization of the protonation and the hydration states in the active site of apo Photosystem II*" within the ISCRA-C project 2020

● "*Exploring substrate specificity of BBE-like enzymes by means of MD simulations*" within the ISCRA-C project 2019

● "*Evolution of the oxidized $S_3$ state of the Kok cycle in Photosystem II explored by QM/MM Molecular Dynamics simulations*" within the ISCRA-C project 2015

● "*Multilevel theoretical investigation of the Photosystem II*" within the ISCRA-B project 2013

● "*Dynamical characterization of Photosystem II*" within the Standard HPC Grant 2012 call (CASPUR)

## Reviewer activity

● Nature Communications
● Photosynthesis Research
● Physical Chemistry Chemical Physics
● Journal of American Chemical Society
● Life
● Chemical Science
● Frontiers in Chemistry
● PNAS Nexus
● Chemical Physics Letters
● Catalysts
● European Biophysics Journal
● Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO)
● Review Editor for "Theoretical and Computational Chemistry" in the journal Frontiers in Chemistry

## Selected conferences with poster and/or oral presentation

● XLIX Congress of the Physical Chemistry Division of SCI (September 2023, Torino, Italy) (**Oral Presentation**)
● Principles of light-induced charge transfer for optogenetics (July 2023, Modena, Italy) (**Oral Presentation**)
● BUUR meeting 2022 (April 2022, Uppsala, Sweden) (**Oral Presentation**)
● SCI2021 (September 2021, on-line) (**Oral Presentation**)
● XII AICIng (September 2021, Reggio Calabria, Italy) (**Oral Presentation**)
● RENews - Renewable Energies News (March 2021, on-line) (**Oral Presentation**)
● CDP6 - Modeling for Drug Discovery 2018 (October 2018, Jülich, Germany) (**Oral Presentation**)
● BUR workshop 2017 (April 2017, Rome, Italy) (**Oral Presentation**)
● 79$^{th}$ Harden Conference 2016 (April 2016, Innsbruck, Austria) (**Oral Presentation**)
● BUUR meeting 2015 (November 2015, Uppsala, Sweden) (**Oral Presentation**)
● 10$^{th}$ European Biophysics Congress, (July 2015, Dresden, Germany)
● CMCB-2015 Conference (April 2015, Nanjing, China) (**Oral Presentation**)
● BUUR meeting 2014 (November 2014, Uppsala, Sweden) (**Oral Presentation**)
● WATOC 2014 (October 2014, Santigo de Chile, Chile)
● 4$^{th}$ Visegrad Symposium on Structural Systems Biology (June 2014, Nove Hrady, Czech Republic) (**Oral Presentation**)
● Interface between experimental and theoretical approaches to energy-related enzyme catalysis (June 2014, London, UK)
● Biophysics@Rome 2014 (May 2014, Rome, Italy) (**Oral Presentation**)
● The 16th International Congress on Photosynthesis (August 2013, St. Louis, US)
● BUUR meeting 2013 (April 2013, Berlin, Germany) (**Oral presentation**)
● Energy from the Sun: Computational Chemists and Physicists Take up the Challenge, (Sep. 2012, Cagliari, Italy)

● Annual Meeting of the German Biophysical Society, (October 2010, Bochum, Germany)
● The 45th Winterseminar, (January 2010, Klosters, Switzerland)
● Computer simulation and theory of macromolecules, (April 2009, Hünfeld, Germany) (**Oral Presentation**)
● 7th European Biophysics Congress, (July 2009, Genoa, Italy)
● 25th Molecular Model(l)ing Workshop, (September 2009, Erlangen, Germany) (**Oral Presentation**)
● VIII European Symposium of the Protein Society, (June 2009, Zurich, Switzerland)
● Deutschen Biophysikalischen Gesellschaft, (September 2008, Berlin, Germany)
● 6th European Biophysics Congress, (July 2007, London, England)
● Computer simulation and theory of macromolecules, (May 2007, Hünfeld, Germany) (**Oral Presentation**)

## Organization of workshops and schools

● International Workshop on Natural and Artificial Photosynthesis (September 2023, L'Aquila, Italy) (**Local and scientific organizer**)

● Summer School on ab initio molecular dynamics simulations for biomolecules (June 2013, Santo Stefano di Sessanio, Italy) (**Local organizer**)

## Computational skills

**Operating systems:** Unix/Linux, Windows, Macintosh

**Programming languages:** Shell, Awk, Python, IDL

**Scientific packages:**
Gromacs, LEaP (AMBER), CP2K, WHAT IF, MODELLER, Pymol, VMD *(Advanced)*
AMBER, Delphi, CPMD, GAUSSIAN *(Basic)*

**Drawing programs:** Xfig, Gnuplot, Power Point, Adobe Creative Suite.

**Word processor:** Latex and Word

## ASN (National Scientific qualification)

● National Scientific qualification as associate in the Italian higher education system, in the call 2021/2023 (Ministerial Decree n. 553/2021 and 589/2021) for the disciplinary field of 03/A2 - Models and methods for chemistry

● National Scientific qualification as associate in the Italian higher education system, in the call 2021/2023 (Ministerial Decree n. 553/2021 and 589/2021) for the disciplinary field of 03/B1 - Principles of chemistry and inorganic systems

● National Scientific qualification as associate in the Italian higher education system, in the call 2021/2023 (Ministerial Decree n. 553/2021 and 589/2021) for the disciplinary field of 03/B2 - Principles of chemistry for applied technologies

● National Scientific qualification as associate in the Italian higher education system, in the call 2021/2023 (Ministerial Decree n. 553/2021 and 589/2021) for the disciplinary field of 05/E1 - General biochemistry

● National Scientific qualification as associate in the Italian higher education system, in the call 2018/2020 (Ministerial Decree n. 2175/2018) for the disciplinary field of 05/E2 - Molecular biology

## Languages

**Italian** *(native speaker)*

**English** *(fluent)*

Date: 29th October 2024 Daniele Narzi