Giulia Palermo – Curriculum Vitae

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Education and professional experience

2018/07–present	**University of California Riverside**. Assistant Professor of Biophysics
2016/02–2018/06	**University of California San Diego**. Swiss National Science Foundation (SNSF) Advanced post-doctoral fellow in biophysics. Advisor: Prof. J. Andrew McCammon
2013/10–2015/12	**École Polytechnique Fédérale de Lausanne, EPFL** (CH). Postdoctoral scientist in Computational Biochemistry and Chemistry. Advisor: Prof. Ursula Rothlisberger
2013/04	**Italian Institute of Technology** and **University of Genova** (IT). PhD in Computational Drug Discovery and Development, Doctoral School of Life and Human Technologies. Advisor: Dr. Marco De Vivo
2009/03	**University of Salerno** (IT). Master Degree summa cum laude (110/110 con lode) in Chemistry and Pharmaceutical Technologies

Honors and awards

2018/02	Nominee for the *"Future of Biophysics Burroughs Wellcome Fund Symposium"* at the 62nd Biophysical Society Meeting, San Francisco (USA).
2017/11	Best Use of High Performance Computing (HPC) in Life Sciences 2017. HPCwire (https://www.hpcwire.com)
2017/02	First place prize at the Art and Science image contest to the 61st Biophysical Society meeting, New Orleans, USA ($500).
2014–2015	Travel awards from: (1) Biophysical Society's Committee for Professional Opportunities for Women, Biophysical Society National Meeting, Baltimore, USA ($500); (2) Institute of Pure and Applied Mathematics (IPAM, $1,500); (3) Centre Européen de Calcul Atomique et Molécolaire (CECAM), Lausanne, CH.

Funding

2015/12	Advanced post-doc mobility fellowship. Swiss National Science Foundation (SNSF). (~$110,000) and gender equality grant for the participation to the EMBO Course: Communication & Negotiation for Female Leaders (09/2016, Mannheim, DE) (~$4,000).
2011/03	PhD mobility grant (~12,000 €) from the Italian National Science Foundation (MIUR)
2010/01	Graduate student fellowship from the Italian National Science Foundation (MIUR) (~50,000 €).

Grants for computational resources

2019/03	Awarded 885,000 Service Units (~$30,000) on CPUs by the National Science Foundation (NSF) Extreme Science and Engineering Discovery Environment (XSEDE).
2017/09	Awarded 30,110 Service Units (~$7,000) on GPUs by the National Science Foundation (NSF) Extreme Science and Engineering Discovery Environment (XSEDE).
2016/11	Awarded 225,000 Simulation Units (~$190,000) on ANTON-2, the specialized supercomputer for millisecond molecular dynamics.
2016/07	Awarded 1,573,193 Service Units (~$130,000) on CPUs by the National Science Foundation (NSF)
2015/07	Awarded 6,300,000 core hours on CPUs by the Partnership for Advanced Computing in Europe (PRACE).

List of Publications

Summary: 28 peer-reviewed papers, 20 papers as first-author, 8 papers as the corresponding author.

† Corresponding author *Equally contributed first author

1. **G. Palermo**.† Structure and Dynamics of the CRISPR-Cas9 Catalytic Complex. ***J. Chem. Inf. Model.*** **2019**, *In press*, DOI: 10.1021/acs.jcim.8b00988
2. **G. Palermo**† C. G. Ricci and J. A. McCammon. The invisible dance of CRISPR-Cas9. Molecular simulations unveil the molecular side of the gene-editing revolution. ***Physics Today*** **2019**, *72*, 4, 30-36.
3. C. G. Ricci, J. S. Chen, Y. Miao, M. Jinek, J. A. Douna, J. A. McCammon & **G. Palermo**,† Deciphering off-target effects in CRISPR-Cas9 through accelerated molecular dynamics. ***ACS Cent. Sci.*** **2019** *In press,* DOI: 10.1021/acscentsci.9b00020
4. **G. Palermo**,† L. Casalino, A. Magistrato and J. A. McCammon. Understanding the mechanistic basis of non-coding RNA through molecular dynamics simulations. ***J. Struct. Biol.*** **2019**. *In Press*, DOI: doi.org/10.1016/j.jsb.2019.03.004
5. S. J. Wodak, E. Paci, N. V. Dokholyan, N. I. Berezovsky, A. Horovitz, J. Li, ... **G. Palermo**, … T. McLeish. Allostery in its many disguises: from theory to applications. ***Structure*** **2019***, 4*, 566-578
6. **G. Palermo**,† J. S. Chen, C. G. Ricci, I. Rivalta, M. Jinek, V. S. Batista, J. A. Doudna, J. A. McCammon Key role of the REC lobe during CRISPR-Cas9 activation by "sensing", "regulating" and "locking" the catalytic HNH domain. ***Quarterly Rev. Biophys.*** **2018**, 51, e9.
7. L. Casalino, **G. Palermo**, A. Spinello, U. Rothlisberger and A. Magistrato. All-Atom Simulations Disentangle the Functional Dynamics Underlying Gene Maturation in the Intron Lariat Spliceosome. ***Proc. Natl. Acad. Sci. USA*** **2018**, 115, 6584-6589.

Before the University of California Riverside

8. **G. Palermo**,† C. Ricci, R. Basak, A. Fernando, M. Jinek, I. Rivalta, V. Batista, J. A. McCammon. PAM-induced allostery activates CRISPR-Cas9. ***J. Am. Chem. Soc.*** **2017**, *139*, 16028–16031. Cover Art. **Featured in the 2018 *J. Am. Chem. Soc*. Young Investigators Virtual Issue**.
9. N. Ashari Astani, S. Meloni, A. H. Salavati, **G. Palermo**, M. Graetzel, U. Rothlisberger. Computational Characterization of the Dependence of Halide Perovskite Effective Masses on Chemical Composition and Structure. ***J. Phys. Chem. C.*** **2017**, 121, 23886–23895.
10. **G. Palermo**,† Y. Miao, R. C. Walker, M. Jinek, J. A. McCammon. CRISPR-Cas9 conformational activation as elucidated from enhanced molecular simulations. ***Proc. Natl. Acad. Sci. USA*** **2017**, *114*, 7260-7265.
11. Adhireksan,* **G. Palermo,*** T. Riedel,* Z. Ma,* R. Muhammad, P. J. Dyson, U. Rothlisberger, C. A. Davey. Allosteric cross-talk in chromatin can mediate drug-drug synergy. ***Nat. Commun.*** **2017**, *8*, 14860.
12. L. Casalino, **G. Palermo**, N. Abdurakhmonova, U. Rothlisberger, A. Magistrato. Development of Site-specific Mg-RNA Force Field Parameters: A Dream or Reality? Guidelines from Combined Molecular Dynamics and Quantum Mechanics Simulations. ***J. Chem. Theory Comput.*** **2017**, *13*, 340–352.
13. **G. Palermo,**† Y. Miao, R. C. Walker, M. Jinek, J. A. McCammon. Striking plasticity of CRISPR-Cas9 and key role of non-target DNA, as revealed by molecular simulations. ***ACS Cent. Sci.*** **2016**, *2*, 756–763.
14. Z. Ma,* **G. Palermo,*** Z. Adhireksan,* B. S. Murray, T. von Erlach, P. J. Dyson, U. Rothlisberger, C. A. Davey. An Organometallic Compound Displays a Unique One-Stranded Intercalation Mode that is DNA Topology-Dependent. ***Angew. Chem. Int. Ed.*** **2016**, *128*, 7441–7444.
15. L. Casalino, **G. Palermo**, U. Rothlisberger, A. Magistrato. Who Activates the Nucleophile in Ribozyme Catalysis? An Answer from the Splicing Mechanism of Group II Introns. ***J. Am. Chem. Soc.*** **2016**, *138*, 10374–10377. Cover Art.
16. S. Meloni, **G. Palermo**, N. Ashari Astani, M. Graetzel, U. Rothlisberger. Valence and conduction bands tuning in halide perovskites for solar cell applications. ***J. Mater. Chem. A.*** **2016**, *4*, 15997–16002.
17. **G. Palermo**, A. Magistrato, T. Riedel, T. von Erlach, C. A. Davey, P. J. Dyson, U. Rothlisberger. Fighting cancer with organometallic compounds: from naked DNA to protein and chromatin targeting strategies. ***ChemMedChem*** **2016**, *11*, 1199-1210. Special Issue Polypharmacology and Multitarget Drugs.
18. **G. Palermo**, A. D. Favia, M. Convertino, M. De Vivo. The molecular basis for dual Fatty Acid Amide Hydrolase (FAAH) / Cyclooxygenase (COX) inhibition. ***ChemMedChem*** **2016**, *11*, 1252–1258.
19. **G. Palermo**, A. Cavalli, M. L. Klein, M. Alfonso-Prieto, M. Dal Peraro, M. De Vivo. Catalytic metal ions and enzymatic processing of DNA and RNA. ***Acc. Chem. Res.*** **2015**, 48, 220–228.
20. **G. Palermo**, E. Minniti, M. L. Greco, L. Riccardi, E. Simoni, M. Convertino, C. Marchetti, M. Rosini, C. Sissi, A. Minarini, M. De Vivo. An optimized polyamine moiety boosts potency of human type II

topoisomerase poisons as quantified by comparative analysis centered on the clinical candidate F14512. ***Chem. Commun*. 2015**, *51*, 14310.

21. **G. Palermo**, I. Bauer, P. Campomanes, A. Cavalli, A. Armirotti, S. Girotto, U. Roethlisberger, M. De Vivo. Keys to lipid selection in FAAH catalysis: Structural flexibility, gating residues, and multiple binding pockets. 2015, ***PLoS Comput. Biol*. 2015**, *11*, e1004231. Cover Art.
22. **G. Palermo**, P. Campomanes, A. Cavalli, U. Roethlisberger, M. De Vivo. Anandamide hydrolysis in FAAH reveals a dual strategy for efficient enzyme-assisted amide bond cleavage via nitrogen inversion. ***J. Phys. Chem. B. 2015***, *119*, 789–801. W. L. Jorgensen Festschrift. Cover Art.
23. **G. Palermo**, A. Cavalli, U. Roethlisberger, M. De Vivo. Computational insights into function and inhibition of the Fatty Acid Amide Hydrolase (FAAH). ***Eur. J. Med. Chem*. 2015**, *91*, 15–26.
24. **G. Palermo**, M. Stenta, A. Cavalli, M. Dal Peraro, M. De Vivo. Molecular simulations highlight the role of metals in catalysis and inhibition of type II topoisomerase. ***J. Chem. Theory Comput*. 2013**, *9*, 857–862. Cover Art.
25. **G. Palermo**, P. Campomanes, M. Neri, D. Piomelli, A. Cavalli, U. Roethlisberger, M. De Vivo. Wagging the tail: essential role of substrate flexibility in FAAH catalysis. ***J. Chem. Theory Comput.* 2013**, *15*, 1202–1213.
26. **G. Palermo**, D. Branduardi, M. Masetti, A. Lodola, M. Mor, D. Piomelli, A. Cavalli, M. De Vivo. Covalent inhibitors of fatty acid amide hydrolase: a rationale for the activity of piperidine and piperazine aryl ureas. ***J. Med. Chem*. 2011**, *54*, 6612–6623.
27. E. Brunk, N. Ashari Astani, P. Athri, P. Campomanes, F. F. de Carvalho, B. F. Curchod, P. Diamantis, M. Doemer, J. Garrec, A. Laktionov, M. Micciarelli, M. Neri, **G. Palermo**, T. J. Penfold, S. Vanni, I. Tavernelli, U. Rothlisberger. ***Chimia (Aarau)* 2011**, *65*, 667–671.
28. **G. Palermo**, R. Riccio, G. Bifulco. Effect of Electronegative Substituents and Angular Dependence on the Heteronuclear Spin-Spin Coupling Constant $^{3}J_{C\text{-}H}$: An Empirical Prediction Equation Derived by Density Functional Theory Calculations. ***J. Org. Chem*. 2010**, *75*, 1982 –1991.

Submitted manuscripts.

29. J. Borišek, A. Saltalamacchia, **G. Palermo** and A. Magistrato. Disclosing the impact of carcinogenic SF3b mutations on pre-mRNA recognition via atomic-level simulations.
30. S. Vanni, L. Riccardi, **G. Palermo** and M. De Vivo. Structure and dynamics of the acyl chains in the membrane trafficking and enzymatic processing of lipids

Book chapters

31. **G. Palermo** and M. De Vivo. Computational Methods for Drug Discovery. Book chapter in Encyclopedia of Nanotechnology, 2nd Ed. Springer. **2015**, 1-15.

Conference organization and chairman activity

2019/03	Recipient of the Innovative Project Grant ($5000), awarded by the ACS for the organization of the *"Women make COMP"* symposium at the 258th ACS meeting in San Diego (CA, aimed at motivating young women in computational chemistry.
2019/02	Organizer of the workshop *"Multiscale Modeling from Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations"*, Lausanne (CH), funded by CECAM (~13,000 $), Schrödinger (~1,500 $) and by the Swiss industry consortium SISF (~5,000 CHF).
2018/08	Organizer of the symposium *"COMP meets CRYO: new frontiers in flexible fitting, image processing and refinement of cryo-EM data"* at the 256th ACS meeting, Boston.
2018/07	Organizer of the workshop *"Frontiers and challenges of computing metals for biochemical, medical and technological applications"* Paris (FR), funded by CECAM (~10,000 €).
2016/02	Co-chair with Prof. A. Dickson, at the 60th Biophysical Society meeting.

Professional service

2019-2021	Early career board member of the Journal of Chemical Information and Modeling.
2019/03	Guest editor of the Special Issue *"Multiscale Modeling from Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations"* in the Journal of Frontiers in Molecular Biosciences
Reviewing	Reviewer for the scientific journals: *(i)* ***Journal of Chemical Theory and Computation***, *(ii)* ***Nature Chemistry***, *(iii)* ***Journal of Chemical Information and Modeling***, *(iv)* ***PLoS One***, *(v)* ***Proteins: Structure, Function and Bioinformatics***, *(vi)* ***Computational Biology and Chemistry***, *(vii)* ***Physical Chemistry Chemical Physics,*** *(viii)* ***ACS Central Science,*** *(ix)* ***Nature Scientific Reports,*** *(x)* ***The Journal of Physical Chemistry,*** *(xi)* ***PNAS*** Reviewer for the European Funding agency ***PRACE***
Membership	American Chemical Society, Biophysical Society, RNA society, Member of the ACS COMP executive committee, American Hearth Association

Communications to Conferences (main)

2019/04	Two talks at the 257th ACS National Meeting, Boston (USA)
2019/03	Talk at the 63nd Biophysical Society Meeting, Baltimore (USA)
2018/08	Talk at the 2nd International conference on CRISPR technologies. San Diego (USA)
2018/08	Talk at the 256th ACS National Meeting, Boston (USA)
2018/07	Invited speaker at the workshop *"Challenges in RNA Structural Modeling and Design"* at the Telluride Science Research Center, Telluride (USA)
2018/05	Invited speaker at the CECAM workshop *"Physiological role of ions in the brain: toward a comprehensive understanding via molecular simulations"*, Scuola Normale Superiore, Pisa (IT)
2018/02	Nominee at the *"Future of Biophysics Burroughs Wellcome Fund Symposium"* at the 62nd Biophysical Society Meeting, San Francisco (USA)
2017/11	Invited speaker at the CECAM workshop *"Computational approaches to investigating allostery"*, Lausanne (CH)
2017/09	Talk at the conference *"Computational Advances in Drug Discovery"*, Lausanne (CH)
2017/04	Four talks at the 253th ACS National Meeting, San Francisco (USA)
2017/02	Poster at the 61th Biophysical Society meeting, New Orleans (USA)
2016/09	Two posters at the EMBO Meeting, Mannheim (DE)
2016/05	Talk at the CECAM workshop *"Structural and Functional Annotation of Bioinorganic Systems"* Scuola Normale Superiore (Pisa, IT)
2016/03	Two talks at the 251th ACS National Meeting, San Diego (USA)
2016/02	Talk and poster at the 60th Biophysical Society meeting, Los Angeles (USA)
2015/06	Talk at the CECAM workshop *"Modeling activity vs. selectivity in metalloproteins"* Chimie Paris Tech, Paris (FR)
2015/02	Talk and poster at the 59th Biophysical Society meeting, Baltimore (USA)
2014/11	Talk at the CECAM workshop *"Advanced modeling to investigate biomolecules"* Italian Institute of Technology, Genova (IT)
2014/04	Talk at the 245th ACS National Meeting, New Orleans (USA)

Invited talks (main)

2019/04	University of Idaho, Invited by Prof. D. Stenkamp and Dr. J. Patel.
2018/02-03	Talk at: (i) Washington University St. Louis; (ii) California Institute of Technology; (iii) University of Rochester; (iv) University of Florida; (v) Max Plank Institute; Berlin; (vi) The Scripps Research Institute, La Jolla; (vii) University of California Riverside.
2017/06	Invited at the DEShaw women's forum, NYC (USA)
2016/09	University of Zürich (CH), invited by Prof. M. Jinek
2017/09	Heidelberg Institute for Theoretical Studies (DE), invited by Prof. R. Wade
2015/10	Selected talk for the ETH post-doc day 2015, ETH – Zürich
2015/03	Forschungszentrum Jülich (DE), Invited by Prof. P. Carloni
2015/02	University of Chicago, Invited by Prof. B. Roux
2014/12	International School of Advanced Studies, Trieste (IT)**,** invited by Prof. A. Laio

Teaching

2019-Spring	Teaching the course "Biomolecular Engineering" (BIEN165) at the University of California Riverside (undergraduate, upper division)
2018-Fall	Teaching the course "Biophysics and Biothermodynamics" (BIEN135) at the University of California Riverside (undergraduate, upper division)
2017	Teaching the seminar course "Integrative structural and computational biophysics" at the Thurgood Marshall College (UCSD)

Mentoring

2018–present	Brandon Mitchell, Dominic Biondo, Nasim Farajpour (PhD students, UCR)
2018–present	Marco Medrano, Ponmathi Jayaseelan (undergraduate students, UCR)
2016–2017	Ramces Gonzales, Yibei Jiang (undergraduate UCSD),
2015–2016	Lorenzo Casalino (SISSA, now at UCSD)
2014–2016	Thibaud von Erlach (undergraduate, now at EPFL)
2012–2013	Huan Francisco Bada (undergraduate at EPFL, now at Oxford University)

Collaborations

Present collaborators:

Martin Jinek – University of Zürich, CH (X-ray crystallography and biochemistry)
Jennifer Doudna – University of California Berkeley, USA (X-ray crystallography and biochemistry)
Samuel Sternberg – Columbia University, USA (biochemistry and biophysics)
Victor Batista – Yale University, USA (computational chemistry)
George P. Lisi – Brown University (NMR)
Navtej Toor – University of California San Diego (cryo-EM)

Collaborations at EPFL:

Paul J. Dyson – EPFL, CH (organometallic chemistry)
Curt A. Davey – NTU, Singapore (nucleosome crystallography)
Matteo Dal Peraro – EPFL, CH (computational biophysics)
Micheal Graetzel – EPFL (solar cells technology)
Alessandra Magistrato – SISSA/CNR, IT (computational biophysics)

Collaborations during graduate studies:

Andrea Cavalli – University of Bologna, IT (computational chemistry)
Claudia Sissi – University of Padua, IT (biochemistry)
Micheal L. Klein – Temple University, USA (computational chemistry)
Daniele Piomelli – UC Irvine, USA (pharmacology)

In the news (main)

2018/08	**JACS features Giulia Palermo in 2018 Young Investigators Virtual Issue**
2017/03	**Supercomputers reveal acrobatics of CRISPR-Cas9**
2017/03	**Anticancer drug gets a boost when combined with anti-rheumatic**
2016/07	**The RNA that snips and stitches RNA**

Science and Art

Art, Philosophy and Classical Music have been essential part of my training, giving me the opportunity to provide cover for many scientific journals (more information: https://palermolab.com/science-art/). The Biophysical Society has selected two of my paintings for the Art & Science Contest at the 59th and 61st annual meetings, where I have been awarded the 1st place prize.