Stefano Artin SERAPIAN

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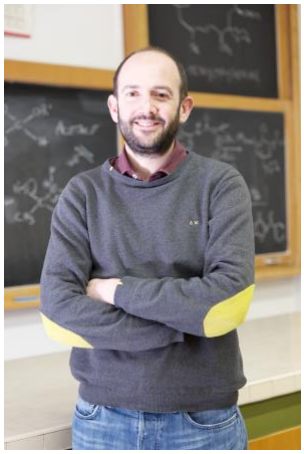

Section 1 of 7: Summary

Scientific and Academic Experience
(details: Sections 3 – 5)

University of Pavia, Italy
July 2025 – present

Biomolecular Simulations Group (group of Prof. Giorgio Colombo)
Associate Professor
- **Day-to-day research supervision and management** in Prof. Giorgio Colombo's laboratory (currently 1 undergraduate student, 4 postgraduate students, 2 postdocs)
- **Extension of my main research activity** (see below) to study chaperone protein Hsp60 and oncogene K-Ras4B; machine learning applications in biosimulations
- **Independent research collaborations**: Structural and mechanistic (TD-)DFT studies on: supramolecular cages to capture CO_2; hydroxyketone reduction; photocatalysts
- **Over 140h of frontal lecturing per full academic year**. Organic and computational chemistry courses across various departments, for Master's and Ph.D. degrees
- **Undergraduate thesis cross-examination**; participation in graduation committees
- **Membership of the Chemistry Department Teaching Committee**. Main focuses: innovation in teaching; setting up a double MSci degree with Tufts University, USA

July 2022 – June 2025

Senior Researcher (*RTDb*)

April 2019 – June 2022

Postdoctoral Fellow (*Assegnista di Ricerca*)
- *In silico* studies on chaperone proteins Hsp90, Trap1, and several oncogenes
  * Identification of allosteric binding sites and virtual design of allosteric modulators
  * Determination of such modulators' effects on reactivity (semiempirical QM/MM MD, DFT cluster models)
- Investigations on key SARS-CoV-2 proteins to identify potential immunogenic regions

University of Bristol, UK
Sep. 2017 – Mar. 2019

Research Associate – Computational Enzymology (group of Dr. Marc W. van der Kamp)
- Studies on enzymatic stereoselectivity (*e.g.* actinorhodin ketoreductase and mutants)
- Approaches employed include: classical and QM/MM MD; free energy methods (umbrella sampling, *WaterSwap*, MM/PBSA); protein- and ligand-protein docking

***Mind the Byte* S. L. Barcelona, Spain**
Nov. 2016 – Mar. 2017

Business Developer
- Start-up company providing software as a service and consultancy for drug design
- Responsible for finding and managing new customers in Germany, UK, Italy, Austria

Catalan Institute of Chemical Research (*ICIQ*) Tarragona, Spain
Sep. 2014 – Oct. 2016

Post-Doc – Funded by a Marie Curie (*COFUND*) **Grant** (group of Prof. Carles Bo)
- Six distinct collaborations in the fields of homogeneous catalysis (polyoxometalates) and supramolecular chemistry (encapsulated Ir^{I} complexes; fullerenes)
- Methods used include: DFT; TD-DFT; QM/MM (*ONIOM*); all-atom MM MD simulations

Imperial College London
Apr. 2010 – Feb. 2014

Ph.D. (Computational Chemistry): *Simulating Self-Assembly of Organosulfur Species on Gold Nanoparticles* (Supervisors: Prof. Michael J. Bearpark, Prof. Fernando Bresme)

Oct. 2008 – Apr. 2010

Predoctoral Project (Bioinformatics): *Investigating the Proteomic Code* (Supervisor: Prof. Andrew D. Miller) — *[Interrupted due to unexpected resignation of supervisor]*

***Italfarmaco* S.p.A. Cinisello Balsamo, Italy**
Jan. – Oct. 2008

Computational Medicinal Chemist (industrial R&D)
- Virtual design of effective HDAC inhibitors. Techniques employed include: molecular modelling; virtual screening, QSAR, pharmacophore models, and docking; *de novo* design; MD simulations of enzyme/substrate; semiempirical QM methods.

Education

Imperial College London
Sep. 2003 – Aug. 2007

MSci in Chemistry with Research Abroad (First Class Honours):
- **Literature Report:** *Is it a Small RNA World After All?* (Supervisor Prof. A. D. Miller)

Swiss Federal Institute of Technology (*ETH*), Zürich
May – Dec. 2006

Erasmus Project (part of MSci) – Faculty of Chemistry and Applied Biosciences:
- **MSci Dissertation (Experimental):** *The Mechanism of Tyrosyl Radical Repair by Glutathione and Selenocysteine* (Supervisor: Dr. Thomas Nauser)

Strengths and Skills

Chemistry and Biochemistry

- Extensive expertise with many (bio)chemical *in silico* approaches including:
  * Molecular modelling (incl. materials), cheminformatics, computer-aided drug design
  * QM simulations (DFT, TD-DFT, MP2, CCSD(T), HF, and semiempirical)
  * Classical MD simulations and forcefield manipulation
  * QM/MM simulations (both additive and *ONIOM*)
  * Free energy methods (*e.g.*, umbrella sampling, MM/PBSA)
- Expertise with relevant software, including: *GROMACS*; *AMBER*; *Schrödinger Maestro*; *PyMOL*; *VMD*; *BUDE Docking Engine*; *Gaussian*; *ADF*.
- Working knowledge of the software packages *AutoDock VINA*; *ClustalW*; *ORCA*
- Familiarity with online databases such as *ChEMBL*, *PDB*, *UniProtKB*, *Pfam*
- Familiarity with machine learning approaches and Markov State Models

IT and Programming

- Excellent knowledge of the programming languages *PHP* and *bash*
- Hands-on experience with *Python* and relevant biosimulation libraries

Personal Strengths and Teaching
(see also Sections 3 – 5)

- **Teaching and leadership skills**, consolidated through full-time supervision and co-supervision of undergraduates during my doctorate, in Bristol, and (especially) Pavia; yearly lectures and tutoring in Pavia; laboratory demonstrations at *Imperial College*
- **Positive attitude to teamwork and collaborations**, consolidated through joint international projects at *ICIQ* and Pavia; proactivity in my work as a Teaching Committee Member in Pavia; in a multidisciplinary medicinal chemistry team at *Italfarmaco*; and at *Mind the Byte*, as part of a 3-member Business Development team
- **Determination and adaptability** to any kind of situation: these were vital in mustering the motivation to start a new Ph.D. project upon my supervisor's resignation; to dare explore a different aspect of chemistry as a business developer; and to return to academia with the firm intention of broadening my skills in computational chemistry
- **Advanced communication skills**, developed by speaking at scientific conferences; cold-calling and managing customers at *Mind the Byte*; partaking in musical performances, and high school acting
- **Global mindset**, facilitated by linguistic skills, innate curiosity, 13-year attendance at an international school, and life in six locations across four different countries

Languages

Italian (mother tongue), **English** (bilingual proficiency), **Spanish** (excellent proficiency), **French** (good proficiency), **German** (good working knowledge), **Western Armenian** (limited working knowledge), **Catalan** (basic proficiency)

Publications
(details: Section 2)

56 peer-reviewed publications since 2012 (more in preparation); at least **1 for every stage of my academic career** since November 2008

Conferences
(details: Section 6)

35 interventions since 2010: **13 distinct oral presentations** and **8 distinct posters**

Qualifications and Prizes

- **Italian Scientific Qualification (ASN)** *(Oct. 2022)* as Associate Professor in: Organic Chemistry; Fundamentals of Chemistry & Inorganic Systems; General Biochemistry
- *Thomas Young Centre Postgraduate Students Day 2012:* **1st prize** (best talk)
- *Imperial College Postgraduate Symposium 2012* (physical chemistry talks)*:* **2nd prize**
- *Imperial College London 2006:* ***GlaxoSmithKline Pharmaceuticals*** **Prize** for excellence in practical physical chemistry

External Courses

2019 *New Approaches in Molecular Modelling* (Schrödinger Workshop, University of Milan)
2012 *National Training School in Theoretical Chemistry* (University of Oxford)
2011 *Advanced OpenMP* (University of Edinburgh); *Methods in Molecular Simulation* (CCP5 Summer school, Queen's University, Belfast); *Fortran95* (King's College London)

Additional Skills and Interests

- Piano (ABRSM Grade 8); Choral Singing (since age 11)
- Politics; Travelling, Languages and Geography; Gastronomy; Hiking and Skiing
- Italian **driving licence** (cat. *B*, private vehicles)

Section 2 of 7: Peer-reviewed Publications

Sorted by **descending impact factor (IF) available at the time of publication.**
***** denotes corresponding authorship (joint or individual)

(1) Corti, V.; Simionato, G.; Rizzo, L.; Serapian, S. A.; Pelosi, G.; Natali, M.; Dell'Amico, L., Triplet State Reactivity of Iminium Ions in Organocatalytic Asymmetric [2 + 2] Photocycloadditions. *Nat. Chem.* **2026**, *18* (1), 189.
IF: 20.200; **DOI:** 10.1038/s41557-025-01960-3

(2) Krishnan, C. G.; Cormier, G.; Serapian, S. A.; Bortolus, M.; Dell'Amico, L., Phosphoryl Radicals from Trivalent Iminyl Phosphines: A Photocatalytic Approach to *N*-Phosphoryl Azetidines. *Angew. Chem., Int. Ed.* **2026**, *65* (29), e9986925.
IF: 17.000; **DOI:** 10.1002/anie.9986925

(3) Masgras, I.; Laquatra, C.; Cannino, G.; Serapian, S. A.; Colombo, G.; Rasola, A., The Molecular Chaperone TRAP1 in Cancer: From the Basics of Biology to Pharmacological Targeting. *Semin. Cancer Biol.* **2021**, *76*, 45.
IF: 15.707; **DOI:** 10.1016/j.semcancer.2021.07.002

(4) Woodford, M. R.; Baker-Williams, A. J.; Sager, R. A.; Backe, S. J.; Blanden, A. R.; Hashmi, F.; Kancherla, P.; Gori, A.; Loiselle, D. R.; Castelli, M.; Serapian, S. A.; Colombo, G.; Haystead, T. A.; Jensen, S. M.; Stetler-Stevenson, W. G.; Loh, S. N.; Schmidt, L. S.; Linehan, W. M.; Bah, A.; Bourboulia, D.; Bratslavsky, G.; Mollapour, M., The Tumor Suppressor Folliculin Inhibits Lactate Dehydrogenase A and Regulates the Warburg Effect. *Nat. Struct. Mol. Biol.* **2021**, *28*, 662.
IF: 15.369; **DOI:** 10.1038/s41594-021-00633-2

(5) Castelli, M.; Marchetti, F.; Osuna, S.; Oliveira, A. S. F.; Mulholland, A. J.; Serapian, S. A.;* Colombo, G., Decrypting Allostery in Membrane-Bound K-Ras4B Using Complementary *In Silico* Approaches Based on Unbiased Molecular Dynamics Simulations. *J. Am. Chem. Soc.* **2024**, *146* (1), 901.
IF: 15.000; **DOI:** 10.1021/jacs.3c11396

(6) Serapian, S. A.; Sánchez-Martín, C.; Moroni, E.; Rasola, A.; Colombo, G., Targeting the Mitochondrial Chaperone TRAP1: Strategies and Therapeutic Perspectives. *Trends Pharmacol. Sci.* **2021**, *42* (7), 566.
IF: 14.819; **DOI:** 10.1016/j.tips.2021.04.003

(7) Torielli, L.; Guarra, F.; Shao, H.; Gestwicki, J. E.; Serapian, S. A.;* Colombo, G., Pathogenic mutation impairs functional dynamics of Hsp60 in mono- and oligomeric states. *Nat. Commun.* **2025**, *16*, 3158.
IF: 14.700; **DOI:** 10.1038/s41467-025-57958-5

(8) Serapian, S. A.;***** Moroni, E.; Ferraro, M.; Colombo, G., Atomistic Simulations of the Mechanisms of the Poorly Catalytic Mitochondrial Chaperone Trap1: Insights into the Effects of Structural Asymmetry on Reactivity. *ACS Catal.* **2021**, *11* (14), 8605.
IF: 13.086; **DOI:** 10.1021/acscatal.1c00692

(9) Korom, S.; Martin, E.; Serapian S. A.; Bo, C.; Ballester, P., Molecular Motion and Conformational Interconversion of Ir^{I}•COD Included in Rebek's Self-Folding Octa-amide Cavitand. *J. Am. Chem. Soc.* **2016**, *138* (7), 2273.
IF: 12.113; **DOI:** 10.1021/jacs.5b12646

(10) Izzet, G.; Abecassis, G.; Brouri, D.; Piot, M.; Matt, B.; Serapian, S. A.; Bo, C.; Proust, A., Hierarchical Self-assembly of Polyoxometalate-Based Hybrids Driven by Metal Coordination and Electrostatic Interactions: From Discrete Supramolecular Species to Dense Monodisperse Nanoparticles. *J. Am. Chem. Soc.* **2016**, *138* (15), 5093.
IF: 12.113; **DOI:** 10.1021/jacs.6b00972

(11) Parrot, A.; Bernard, A.; Jacquart, A.; Serapian, S. A.; Bo, C.; Derat, E.; Oms, O.; Dolbecq, A.; Proust, A.; Métivier, R.; Mialane, P.; Izzet, G., Photochromism and Dual-Color Fluorescence in a Polyoxometalate-Benzospiropyran Molecular Switch. *Angew. Chem., Int. Ed.* **2017**, *56* (17), 4872.
IF: 11.709; **DOI:** 10.1002/anie.201701860

(12) Guerriere, T. B.; Vancheri, A.; Ricotti, I.; Serapian, S. A.; Eggerichs, D.; Tischler, D.; Colombo, G.; Mascotti, M. L.; Fraaije, M. W.; Mattevi, A., Dehydrogenase versus Oxidase Function: The Interplay between Substrate Binding and Flavin Microenvironment. *ACS Catal.* **2025**, *15* (2), 1046.
IF: 11.700; **DOI:** 10.1021/acscatal.4c05944

(13) Serapian, S. A.; van der Kamp, M. W., Unpicking the Cause of Stereoselectivity in Actinorhodin Ketoreductase Variants with Atomistic Simulations. *ACS Catal.* **2019**, *9* (3), 2381.
IF: 11.384; **DOI:** 10.1021/acscatal.8b04846

(14) Longhi, E.; Magni, A.; Torielli, L.; Lodigiani, G.; Carlessi, E.; Borsotti, P.; Doria, F.; Pirota, V.; Serapian, S. A.; Arrigoni, C.; Lolicato, M.; Moroni, E.; Bergamaschi, G.; Taraboletti, G.; Colombo, G., Hijacking Client Instability to Selectively Disrupt HSP90-driven Glucocorticoid Receptor Activation. *Pharmacol. Res.* **2026**, *228*, 108205.
IF: 10.500; **DOI:** 10.1016/j.phrs.2026.108205

(15) Serapian, S. A.; Crosby, J.; Crump, M. P.; van der Kamp, M. W., Path to Actinorhodin: Regio- and Stereoselective Ketone Reduction by a Type II Polyketide Ketoreductase Revealed in Atomistic Detail. *JACS Au* **2022**, *2* (4), 972.
IF: 8.600 (first assigned 2023); **DOI:** 10.1021/jacsau.2c00086

(16) Chiara, R.; Morana, M.; Folpini, G.; Olivati, A.; Albini, B.; Galinetto, P.; Chelazzi, L.; Ciattini, S.; Fantechi, E.; Serapian, S. A.; Petrozza, A.; Malavasi, L., The Templating Effect of Diammonium Cations on the Structural and Optical Properties of Lead Bromide Perovskites: A Guide to Design Broad Light Emitters. *J. Mater. Chem. C* **2022**, *10*, 12367.
IF: 8.067; **DOI:** 10.1039/d2tc02113g

(17) Casali, E.; Serapian, S.A.; Gianquinto, E.; Castelli, M.; Bertinaria, M.; Spyrakis, F.; Colombo, G., NLRP3 Monomer Functional Dynamics: From the Effects of Allosteric Binding to Implications for Drug Design. *Int. J. Biol. Macromol.* **2023**, *246*, 125609.
IF: 8.025; **DOI:** 10.1016/j.ijbiomac.2023.125609

(18) Castelli, M.; Magni, A.; Bonollo, G.; Pavoni, S.; Frigerio, F.; Oliveira, A. S. F.; Cinquini, F.; Serapian, S. A.; Colombo, G., Molecular Mechanisms of Chaperone Directed Protein Folding: Insights from Atomistic Simulations. *Protein Sci.* **2024**, *33* (3), e4880.
IF: 8.000; **DOI:** 10.1002/pro.4880

(19) Frasnetti, E.; Magni, A.; Castelli, M.; Serapian, S. A.; Moroni, E.; Colombo, G., Structures, dynamics, complexes, and functions: From classic computation to artificial intelligence. *Curr. Opin. Struct. Biol.* **2024**, 87, 102835.
IF: 6.800; **DOI:** 10.1016/j.sbi.2024.102835

(20) Serapian, S. A.;* Bearpark, M. J.; Bresme, F., The Shape of Au_8: Gold Leaf or Gold Nugget? *Nanoscale* **2013**, *5* (14), 6445.
IF: 6.739; **DOI:** 10.1039/c3nr01500a

(21) Serapian, S. A.; Marchetti, F.; Triveri, A.; Morra, G.; Meli, M.; Moroni, E.; Sautto, G. A.; Rasola, A.; Colombo, G., The Answer Lies in the Energy: How Simple Atomistic Molecular Dynamics Simulations may Hold the Key to Epitope Prediction on the Fully Glycosylated SARS-CoV-2 Spike Protein. *J. Phys. Chem. Lett.* **2020**, *11* (19), 8084.
IF: 6.710; **DOI:** 10.1021/acs.jpclett.0c02341

(22) Triveri, A.; Casali, E.; Frasnetti, E.; Doria, F.; Frigerio, F.; Cinquini, F.; Pavoni, S.; Moroni, E.; Marchetti, F.; Serapian, S. A.; Colombo, G., Conformational Behavior of SARS-Cov-2 Spike Protein Variants: Evolutionary Jumps in Sequence Reverberate in Structural Dynamic Differences. *J. Chem. Theor. Comput.* **2023**, *19* (7), 2120.
IF: 6.578; **DOI:** 10.1021/acs.jctc.3c00077

(23) Torielli, L.; Serapian, S. A.; Mussolin, L.; Moroni, E.; Colombo, G., Integrating Protein Interaction Surface Prediction with a Fragment-Based Drug Design: Automatic Design of New Leads with Fragments on Energy Surfaces. *J. Chem. Inf. Model.* **2022**, *63* (1), 343.
IF: 6.162; **DOI:** 10.1021/acs.jcim.2c01408

(24) Castelli, M.; Bhattacharya, K.; Abboud, E.; Serapian, S. A.; Picard, D.; Colombo, G., Phosphorylation of the Hsp90 Co-chaperone Hop Changes its Conformational Dynamics and Biological Function. *J. Mol. Biol.* **2023**, *435* (3), 167931.
IF: 6.151; **DOI:** 10.1016/j.jmb.2022.167931

(25) Triveri, A.; Sánchez-Martín, C.; Torielli, L.; Serapian, S. A.; Marchetti, F.; D'Acerno, G.; Pirota, V.; Castelli, M.; Moroni, E.; Ferraro, M.; Quadrelli, P.; Rasola, A.; Colombo, G., Protein Allostery and Ligand Design: Computational Design Meets Experiments to Discover Novel Chemical Probes. *J. Mol. Biol.* **2022**, *434* (17), 167468.
IF: 6.151; **DOI:** 10.1016/j.jmb.2022.167468

(26) Scietti, L.; Moroni, E.; Mattoteia, D.; Fumagalli, M.; De Marco, M.; Negro, L.; Chiapparino, A.; Serapian, S. A.; De Giorgi, F.; Faravelli, S.; Colombo, G.; Forneris, F., A Fe^{2+}-Dependent Self-inhibited State Influences the Druggability of Human Collagen Lysyl Hydroxylase (LH/PLOD) Enzymes. *Front. Mol. Biosci.* **2022**, *9*, 876352.
IF: 6.113; **DOI:** 10.3389/fmolb.2022.876352

(27) Huerta, E.; Serapian, S. A.; Santos, E.; Cequier, E.; Bo, C.; de Mendoza, J., Molecular Basis for the Recognition of Higher Fullerenes into Ureidopyrimidinone-Cyclotriveratrylene Self-Assembled Capsules. *Chem. – Eur. J.* **2016**, *22* (38), 13496.
IF: 5.731; **DOI:** 10.1002/chem.201601690[1,2]
[1] Selected as "Hot Paper"
[2] Cover picture

(28) Frasnetti, E.; Cucchi, I.; Pavoni, S.; Frigerio, F.; Cinquini, F.; Serapian, S. A.; Pavarino, L. F.; Colombo, G., Integrating Molecular Dynamics and Machine Learning Algorithms to Predict the Functional Profile of Kinase Ligands. *J. Chem. Theor. Comput.* **2024**, *20* (20), 9209.
IF: 5.700; **DOI:** 10.1021/acs.jctc.4c01097

(29) Scantamburlo, F.; Masgras, I.; Ciscato, F.; Laquatra, C.; Frigerio, F.; Cinquini, F.; Pavoni, S.; Triveri, A.; Fransetti, E.; Serapian, S. A.; Colombo, G.; Rasola, A.; Moroni, E., Design and Test of Molecules that Interfere with the Recognition Mechanisms between the SARS-CoV-2 Spike Protein and Its Host Cell Receptors. *J. Chem. Inf. Model.* **2024**, *64* (21), 8274.
IF: 5.600; **DOI:** 10.1021/acs.jcim.4c01511

(30) Rodríguez-Santos, G.; Bonollo, G.; Sciva, C.; Colombo, G.; Pérez-Melero, C.; Serapian, S. A.,* Molecular Dynamics Simulations Provide Further Insights into the Allosteric Regulation of the Kinesin-5 Motor Domain by Loop 5. *J. Chem. Inf. Model.* **2026**, *66* (7), 4101.
IF: 5.300; **DOI:** 10.1021/acs.jcim.5c02999

(31) Magni, A.; Bonollo, G.; Trèves, G.; Frigerio, F.; Cinquini, F.; Pavoni, S.; Oliveira, A. S. F.; Mulholland, A. J.; Serapian, S. A.;* Colombo, G., Ligand-driven modulation of chaperone–cochaperone networks shapes proteostasis outcomes. *Protein Sci.* **2026**, *35* (5), e70543.
IF: 5.200; **DOI:** 10.1002/pro.70543

(32) Serapian, S. A.; Colombo, G., Designing Molecular Spanners to Throw in the Protein Networks. *Chem. – Eur. J.* **2020**, *26* (21), 4656.
IF: 5.160; **DOI:** 10.1002/chem.201904523[3]
[3] Appearing in "Showcased Reviews" section

(33) Colombo, G.; Paladino, A.; Woodford, M. R.; Backe, S. J.; Sager, R. A.; Kancherla, P.; Daneshvar, M. A.; Chen, V. Z.; Bourboulia, D.; Ahanin, E. F.; Prodromou, C.; Bergamaschi, G.; Strada, A.; Cretich, M.; Gori, A.; Veronesi, M.; Bandiera, T.; Vanna, R.; Bratslavsky, G.; Serapian, S. A.; Mollapour, M., Chemical Perturbation of Oncogenic Protein Folding: from the Prediction of Locally Unstable Structures to the Design of Disruptors of Hsp90-Client Interactions. *Chem. – Eur. J.* **2020**, *26* (43), 9459.
IF: 5.160; **DOI:** 10.1002/chem.202000615[1]
[1] Selected as "Hot Paper"

(34) Triveri, A.; Serapian, S. A.; Marchetti, F.; Doria, F.; Pavoni, S.; Cinquini, F.; Moroni, E.; Rasola, A.; Frigerio, F.; Colombo, G., SARS-CoV-2 Spike Protein Mutations and Escape from Antibodies: A Computational Model of Epitope Loss in Variants of Concern. *J. Chem. Inf. Model.* **2021**, *61* (9), 4687.

IF: 4.956; **DOI:** 10.1021/acs.jcim.1c00857

(35) Gaiaschi, L.; De Luca, F.; Serapian, S. A.; Lugli, E.; Maraschi, F.; Bini, A.; Merli, D.; Bottone, M. G., In Vitro Anti-Glioblastoma Activity of a Novel Pt(IV)-Ganoderic Acid A Conjugate. *Int. J. Mol. Sci.* **2026**, *27* (6), 2760.
IF: 4.900; **DOI:** 10.3390/ijms27062760

(36) Sánchez-Martín, C.; Serapian, S. A.; Colombo, G.; Rasola, A., Dynamically Shaping Chaperones. Allosteric Modulators of Hsp90 Family as Regulatory Tools of Cell Metabolism in Neoplastic Progression. *Front. Oncol.* **2020**, *10*, 1177.
IF: 4.848; **DOI:** 10.3389/fonc.2020.01177

(37) Naeem, S.; Serapian, S. A.; Toscani, A.; White, A. J. P.; Hogarth, G.; Wilton-Ely, J. E. D. T., Ring-Closing Metathesis and Nanoparticle Formation Based on Diallyldithiocarbamate Complexes of Gold(I): Synthetic, Structural, and Computational Studies. *Inorg. Chem.* **2014**, *53* (5), 2404.
IF: 4.762; **DOI:** 10.1021/ic402048a

(38) Torielli, L.; Guarra, F.; Serapian, S. A.;* Colombo, G., Density Functional Theory Calculations to Investigate the Role Played by an Aspartate Dyad in Hsp60-Catalyzed ATP Hydrolysis. *J. Phys. Chem. Lett.* **2025**, *16* (42), 10879.
IF: 4.600; **DOI:** 10.1021/acs.jpclett.5c02351

(39) Bonollo, G.; Roncati, B.; Torielli, L.; Wang, S.; Pasala, C.; Pavoni, S.; Frigerio, F.; Cinquini F.; Chiosis, G.; Serapian, S. A; Colombo, G., Post-Translational Modification as an Allosteric Switch in Hsp90: How Dual Phosphorylation Locks Chaperone Complexes into Hyperstabilized States. *J. Phys. Chem. Lett.* **2026**, *17* (28), 8098.
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(40) Sures, D. J.; Serapian, S. A.; Kozma, K.; Molina, P. I.; Bo, C.; Nyman M., Electronic and Relativistic Contributions to Ion-Pairing in Polyoxometalate Model Systems. *Phys. Chem. Chem. Phys.* **2017**, *19* (13), 8715.
IF: 4.449; **DOI:** 10.1039/c6cp08454k

(41) Mobili, R.; La Cognata, S.; Monteleone, M.; Longo, M.; Fuoco, A.; Serapian, S. A.; Vigani, B.; Milanese, C.; Armentano, D.; Jansen, J. C.; Amendola, V., Gas Permeation through Mechanically Resistant Self-Standing Membranes of a Neat Amorphous Organic Cage. *Chem. – Eur. J.* **2023**, *29* (56), e202301437.
IF: 4.300; **DOI:** 10.1002/chem.202301437

(42) Torielli, L.; Castelli, M.; Milani, F.; Heritz, J. A.; Cayaban, S. J.; Hernandez, J.; Serapian, S. A.; Magni, A.; Frasnetti, E.; Doria, F.; Pirota, V.; Wengert, L. A.; Woodford, M. R.; Lodigiani, G.; Bergamaschi, G.; Veronesi, M.; Bandiera, T.; Girotto, S.; Paladino, A.; Prodromou, C.; Backe, S. J.; Bourboulia, D.; Canciani, A.; Arrigoni, C.; Lolicato, M.; Gestwicki, J. E.; Mollapour, M.; Colombo, G., Design of Multi-Target Peptide Modulators for Protein Chaperone Networks. *Structure* **2025**, *33* (11), 1944.
IF: 4.300; **DOI:** 10.1016/j.str.2025.07.021

(43) Montefiori, M.; Pilotto, S.; Marabelli, C.; Moroni, E.; Ferraro, M.; Serapian, S. A.; Mattevi, A.; Colombo, G., Impact of Mutations on NPAC Structural Dynamics: Mechanistic Insights from MD Simulations. *J. Chem. Inf. Model.* **2019**, *59* (9), 3927.
IF: 3.966; **DOI:** 10.1021/acs.jcim.9b00588

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[5] Special Issue dedicated to Prof. Giovanni Ciccotti (by invitation only)

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(56) Magni, A.; Bonollo G.; Guarra, F.; Torielli, L.; Moroni, E.; Serapian, S. A.; Colombo, G., Investigating Allostery with Atomistic Biomolecular Simulations. In *Reference Collection in Life Sciences*; Elsevier, 2025, *In press*.
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Section 3 of 7: Teaching and Examinations (including abroad)

Frontal Lecturing

University of Pavia, Italy

a. yr. 2022/23 – present **Ph.D. Degree** in *Chemical and Pharmaceutical Sciences and Industrial Innovation*
- Molecular simulations in Chemical Biology (in Italian)
  * 24 hours (out of 24)
  * 6 credits (out of 6)

a. yr. 2022/23 – present **Master's degree** in *Pharmacy*
- Organic Chemistry (in Italian)
  * 24 hours (out of 72)
  * 3 credits (out of 9)

a. yr. 2023/24 – present **Master's degree** in *Medical and Pharmaceutical Biotechnologies*
- Computational Biology for Drug Design (in English)
  * 24 hours (out of 24)
  * 3 credits (out of 3)

a. yr. 2024/25 – present **Master's degree** in *Conservation and Restoration of Cultural Heritage*
- Foundation Chemistry (Organic Chemistry module; in Italian)
  * 6 hours (out of 18)
  * 1 credit (out of 3)

a. yr. 2025/26 – present **Master's degree** in *Chemistry*
- Introduction to Molecular Computational Chemistry (in English)
  * 48 hours (out of 48)
  * 6 credits (out of 6)

a. yrs. 2023/24 – 2024/25 **Master's degree** in *Conservation and Restoration of Cultural Heritage*
- Organic Chemistry (in Italian)
  * 12 hours (out of 36)
  * 2 credits (out of 6)

a. yr. 2025/26 – present **Bachelor's degree** in *Safety Skills for the Environment and the Workplace*
- Chemistry and Biochemistry (Organic Chemistry module; in Italian)
  * 16 hours (out of 55)
  * 2 credits (out of 6)

Internal Thesis Cross-Examination

University of Pavia, Italy

All cross-examined theses were written by Bachelor or Master graduands in **Chemistry**

2026
- Ms. Greta Armelin
  * *Sintesi di un Radiotracer per ^{19}F: Sviluppo di Procedure Radiochimiche Compatibili con Applicazioni di Medicina Nucleare*

2025
- Ms. Anastassya Udalova
  * *Impact of Storage Conditions on the Therapeutic Potential of Amniotic Mesenchymal Stromal Cell (ASMC)-Derived Secretome and Small Extracellular Vesicles: A Comparative* In Vitro *Analysis on Cardiovascular Cell Lines*
- Mr. Alessandro Galli
  * Machine Learning Applied to Asymmetric Diels-Alder Reaction Catalyzed by Rare Earth Metals

2024
- Mr. Umberto Sangalli
  * *Integration of Photocatalysis and Flow Chemistry in the Synthesis of Sulfinamides*
- Mr. Emanuele Bosetti
  * *Sviluppo di Eterogiunzioni* g-C_3N_4/$CsPbCl_3$ *come Nuovi Catalizzatori Eterogenei per Condurre Reazioni di Foto-ossidazione dei Substrati Benzilici*
- Ms. Alessia Corbo
  * *Uso di Compositi Graphitic Carbon Nitride – Perovskite come Fotocatalizzatori Eterogenei per Reazioni ATRA (Atom Transfer Radical Addition)*

2023
- Mr. Andrea Murgia
  * *Funzionalizzazione di Biopolimeri Mediante la Chimica del Legame Covalente Dinamico*

- Ms. Elena Cassera
  * *Generazione di Alchil Radicali Iniziata da* Photo-*HAT su Idrogeni Formilici*
- Mr. Ismaele Barbetta
  * *Sviluppo di Nuovi Gruppi Dyedauxiliary per Reazioni Fotochimiche Mediate da Luce Visibile*

External Ph.D. Thesis Examination

***Rovira i Virgilii* University Tarragona, Spain**
January 2025

- Mr. Marco Nicaso
  * *Development of Systems for Artificial Photosynthesis: A Combined Experimental and Computational Approach*

University of Salamanca, Spain
September 2023

- Mr. Pablo Ortega-Álvarez
  * *Intersystem Crossing in Systems Lacking Metal Cofactors*

External Examination Committees

***New Technologies of Life* Higher Education Institute, Bergamo, Italy**
July 2025

President of a 5-member examination committee overseeing final year written and oral examinations for three different courses: *Industrial Chemistry*, *Polymers*, *Pharmaceutical Plants and Production*. Nominated by the Italian Minister for Education and Merit.

Integrative Teaching

University of Pavia, Italy
January and June 2020

Two problem classes (2 + 2 hours) intended for students attending the *Organic Chemistry and Biochemistry* course (*Chimica Organica e Biochimica*), part of the Bachelor's degree in *Science and Technology for the Environment and Nature* (*Scienze e Tecnologie per l'Ambiente e la Natura*)

Imperial College London
2009 – 2010

Demonstration in organic teaching laboratories (40 hours in total)

Day-to-day Student Supervision

Undergraduates and Interns

University of Pavia, Italy

Graduated in 2026
- Mr. Fabrizio Marullo (Master student in *Molecular Biology & Genetics*)
  * *Computational investigations on the dynamics and aggregation of five mammalian serum albumins*

Graduated in 2025
- Mr. Benedetto Roncati (Master student in *Chemistry & Pharmaceutical Technologies*)
  * *Using Molecular Dynamics simulations to model the allosteric effects induced by phosphorylation of two serines in Hsp90β*

Graduated in 2024
- Mr. Alessandro Vancheri (Master student in *Advanced Biotechnologies*)
  * *Come può la semplice mutazione P151L trasformare la Vanillil alcool deidrogenasi in ossigenasi? Studi di diffusione dell'ossigeno mediante approcci di dinamica molecolare*

Internship 2024
- Ms. Ilaria Ricotti (Master student in *Industrial Nanobiotechnologies for Pharmaceuticals*)
  * *Using MD simulations to model oxygen diffusion in EugO and VAD*

Graduated in 2022
- Mr. Andrea Magni (Master student in *Chemistry*)
  * *Targeting the Hsp90:p23:GR maturation complex* in silico*: from the study of the internal dynamics to the design of modulators of interactions*
- Ms. Elena Frasnetti (Master student in *Chemistry*)
  * *Investigation of a conserved cryptic site in the SARS-CoV-2 Spike Protein among Variants of Concern: computational methods to design new active ligands*

Graduated in 2021
- Mr. Luca Torielli (Master student in *Chemistry & Pharmaceutical Technologies*)
  * *Approcci Computazionali alla Perturbazione delle Interazioni di Hsp90*

University of Bristol, UK

Graduated in 2019
- Mr. Kelvin Chu, BSc student in Medicine (visiting Dr. Van der Kamp's group from *Imperial Colllege London*)
  * In Silico *Studies on Stereoselectivity in* N-*acetylneuraminic Acid Lyase Variants*

Graduated in 2018
- Mr. Nigel Foo, BSc student in Biochemistry
  * In Silico *Studies on Stereoselectivity in Limonene Epoxide Hydrolase Variants*

Imperial College London

Graduated in 2012
- Mr. Tommy Vayron, Master student in Chemistry (visiting Prof. Bresme's group from *Paris-Tech*)
  * *Auto-assemblage de Thiols Autour de Nanoparticules d'Or* (*Self-assembly of Thiols around Gold Nanoparticles*)

Postgraduates (Ph.D.)

University of Pavia, Italy

ongoing
- Mr. Giorgio Bonollo (3rd year)
  * *Development of biochemical and biophysical computational methods to investigate protein complexes*
- Mr. Gauthier Trèves (1st year)
  * *Design of molecules with biological activities using computers*
- Mr. Fabrizio Marullo (1st year)
  * *Studying and Allosterically Targeting PTM-Regulated Hsp90 Networks with Molecular Simulations*

Sep. 2024 – Nov. 2024
- Mr. Gabriel Rodríguez-Santos (2nd year), **visiting Ph.D. student from the University of Salamanca, Spain**
  * *Diseño, Obtención, y Actividad Biológica de Inhibidores de Quinesinas Mitóticas como Potenciales Agentes Antiproliferativos (Design, Obtainment, and Biological Activity of Inhibitors of Mitotic Kinesins as Potential Antiproliferative Agents)*

Graduated in 2026
- Ms. Elena Frasnetti
  * *Predicting the biology of small molecules* via *an integrated structural and chemoinformatic approach*
- Mr. Andrea Magni
  * *Studying and targeting networks in chemical biology with* in silico *simulations*

Graduated in 2025
- Mr. Luca Torielli
  * *Computational Studies of Protein Dynamics and Interactions: Implications for Molecular Design*

Graduated in 2023
- Ms. Alice Triveri
  * *Novel Approaches for the Development of Pan-coronavirus Antiviral Molecules*
- Mr. Matteo Castelli
  * *Protein-protein Interactions: New Approaches to the Design of Selective Modulators*

Section 4 of 7:
Research

University of Pavia, Italy
Apr. 2019 – present

Positions: *Group of Prof. Giorgio Colombo*
(July 2022 – present) **Senior Researcher (RTDb)**
(Apr. 2019 – June 2022) **Postdoctoral Fellow (*Assegnista di Ricerca*)**

Project Title: *Studying Reactivity and Interactions of Hsp90 for the Development of Novel Anticancer Molecules*
Years: *2018-2022*
Funding Body: Italian Cancer Research Association (*Associazione Italiana per la Ricerca sul Cancro*)
Funding: € 27 190 / yr.
Awardees: Prof. Giorgio Colombo

Project Title: *TRAPping tumor growth: designing molecules to perturb the chaperone TRAP1, from enzymatic activities to cell-cell interaction*
Years: *2022-2025*
Funding Body: Italian Ministry of Higher Education and Research (*MUR*) – PRIN program
Funding: € 82 486 / yr. (for the entire laboratory)
Awardees: Prof. Giorgio Colombo

Project Title: *Immuno-HUB*
Years: *2022-2026*
Funding Body: Italian Ministry of Health (*Ministero della Salute*)
Funding: € 50 000 / yr.
Awardees: Prof. Giorgio Colombo, Prof. Filippo Doria

Project Title: *Targeting the Chaperone-Mediated Folding of CDK4 in Kidney Cancer*
Years: *2022-2023*
Funding Body: United States Department of Defense (Defence) – US Army Medical Research Acquisition Activity
Funding: US$ 70 000 (for the entire laboratory)
Awardees: Prof. Giorgio Colombo

Main lines of Research:

(A) *In silico* identification of allosteric binding sites (and other allosteric routes) on known disease targets. Subsequent virtual design of allosteric modulators.
(B) Computational modelling of the effects of allosteric ligands and client proteins binding to such targets, and of post translational modifications. Aspects analysed include variations: in reactivity / catalytic activity; at orthosteric interface(s); within active site(s); and in conformational equilibria.
(C) Extension of methods and concepts used in (A) and (B) to the realm of biocatalysis: investigations on enzymatic reactivity, reaction mechanisms, stereoselectivity, and their dependence on allostery.
(D) Identification of potential epitopes on key SARS-CoV-2 proteins and other immunogenic proteins through detection of regions with weaker energetic coupling.
(E) Application of artificial intelligence and stochastic methods (*e.g.*, Markov State Models) to process molecular dynamics simulations of large proteins and protein-protein complexes involved in cancers and other pathologies. Aims are, *e.g.*, activity prediction of potential ligands, the continued detection of allosteric hotspots, stability prediction, and the kinetically correct reproduction of conspicuous conformational changes.
(F) Gradual diversification of my lines of research with the prospect of setting up external collaborations of my own, and an autonomous research group that—without severing links to my current laboratory: (a) retains its focus on classical MD simulations and QM / QM/MM calculations; and (b) extends its scope beyond nonbiological systems.
    (F1) *In silico* structural and spectroscopic investigations on supramolecular systems using QM approaches.
    (F2) Modelling the excited states of simple organic photochemical systems in collaboration with experimentalists.
    (F3) Modelling the reaction mechanisms of simple (photo)organocatalysed and metal-catalysed transformations in organic synthesis in collaboration with experimentalists.

Description of work and techniques:

My work in Prof. Colombo's research group has mainly consisted in applying my research skills as a computational chemist to model (glyco)proteins and protein complexes, if necessary with their natural substrate(s), in order to pave the way for the design of small molecule modulators. Starting off as a *Postdoctoral Fellow* and conducting most research activities on my own, my subsequent transition to the position of *Senior Researcher* has necessarily entailed gradually relinquishing my direct research activities, and delegating them to a sizeable team of valid collaborators, who come from the most diverse backgrounds and academic levels, and whom it is a pleasure to supervise each day.

The starting point for most of the protein systems modelled is virtually always a series of μs-long, independent molecular dynamics (MD) replicas (in *AMBER*, *Desmond*, or *GROMACS*). This is typically followed by trajectory analysis to extract key properties and conformational information. Amongst the aspects that I'm most interested in exploring are the allosteric pathways present within the simulated systems and how they are altered by a perturbation (such as a pathogenic mutation or the arrival of a specific therapeutic allosteric ligand). Through inter-residue cross-talk, allosteric pathways typically interconnect distal interfaces as well as ortho- and allosteric binding sites, regulating their formation and/or opening; however, allosteric information is typically difficult to assess at timescales accessible by ordinary MD simulations, and therefore requires a combination of specific detection methods. One of my main achievements was to compare the performance of four such methods—in collaboration with their developers—on the notorious oncotarget K-Ras4B, and publishing the findings in the *Journal of the American Chemical Society*.

Over the years, I have published further allosteric investigations on a series of protein complexes and pathogenic variants: *e.g.*, oncotargets lactate dehydrogenase A and NPAC; anti-inflammatory target NLRP3 in the presence of an allosteric inhibitor; antiproliferative target kinesin-5; fully glycosylated SARS-CoV-2 variant Spike proteins; chaperone protein Hsp60 and its complexes with Hsp10; chaperone protein Hsp90 and its complexes; and Hsp90 mitochondrial equivalent Trap1.

Indeed, one of the most relevant advantages of mapping allostery in protein and protein complexes is that one can use traditional drug discovery tools (*e.g.*, *Schrödinger*'s *Maestro* suite) to identify potential binding pockets involving allosterically relevant residues, and virtually design *ad hoc* allosteric modulators targeting these allosteric binding sites; *e.g.*, with various flavours of docking, virtual screening on structure-based pharmacophores, and 2D and 3D similarity searches in common drug databases. Indeed, this is what we managed to achieve for Trap1, with proposed allosteric inhibitors actually being tested *in vitro* and *in vivo*. Along similar lines, in collaboration with the University of Salamanca, MD simulations of kinesin-5 have served as the starting point for the identification of a modified allosteric pocket for which ligands are being designed. Finally, exploiting the latest advances in artificial intelligence, we have reported a machine learning model that can adequately predict the degree of activation/inhibition of potential kinase ligands *before* they are even synthesised.

On a different front, the MD simulations that I ran on fully glycosylated SARS-CoV-2 spike protein variants were analysed with in-house tool—rewritten by me so that it processes glycans and executes more rapidly—that analyses individual energetic contributions (calculated with MM/GBSA) to identify possible immunogenic or client-binding regions. Application of this method was able to demonstrate a progressive loss of immunogenicity in areas that were initially immunogenic in early SARS-CoV-2 spike variants.

My other main interest, in line with my previous experience with nonbiological systems, is to explore the reactivity of proteins / enzymes in general using quantum mechanical (QM) and hybrid quantum/classical (QM/MM) calculations. Of course, protein reactivity is another property on which allostery and allosteric perturbations can have a big effect. Along these lines, using QM/MM MD simulations with umbrella sampling on (homodimeric) Trap1, started from classical MD simulations, were able to identify the causes of 'asymmetric' ATPase reactivity in the two protomers: in the less reactive protomer, allosteric effects bring a tyrosine further inside the active site, whence it is able to sequester the nucleophilic water and hinder its ability to hydrolyse ATP. We furthermore proved that the presence of one of our allosteric inhibitors could further alter reactivity through a similar principle.

Of course, the study of the links between allostery and reactivity is also important in the field of biocatalysis (which I retain a keen interest on from my years in Bristol; *vide infra*). On this front, we recently published in *ACS Catalysis* classical MD simulations of flavoenzyme vanillyl alcohol dehydrogenase (VAD) in the presence of O_2: it is known that the P151L mutation is enough to turn the enzyme into an oxidase, and we were able to show, in full accordance with experiment, that this is due to allosteric effects that make the (correct) *re* face of the flavin more accessible to O_2 through a secondary diffusion route, and the *si* face less accessible. To assess O_2 diffusion routes we also employed a pocket detection method (*MD pocket*) normally used in drug design.

In the future, subject to time and funding, I would definitely like to continue to perform QM studies on (metallo)enzymes of therapeutic and biocatalytic interest. Time-dependent-DFT (TD-DFT) investigations on O_2 reactivity of P151L VAD—for which I have already hypothesised a mechanism—would be a natural continuation of the MD study just published. Another example would be reactivity in the ferroenzyme lysyl hydroxylase, which I have contributed to model in 2022, and for which my QM calculations were essential to confirm the quintet spin state of both Fe^{2+} centres. In the meantime, we are already using QM cluster models of the Hsp60 active site, excided from our classical MD simulations, to prove that a forcibly juxtaposed, unprotonated catalytic aspartate dyad (which the V72I Hsp60 mutant is better poised to achieve) lowers the barrier necessary for ATP hydrolysis by increasing aspartate basicity.

Other current work on biosimulations includes focusing on how to design allosteric disruptors of Hsp90 complexes with the glucocorticoid receptor (a hallmark of certain cancers).

Finally, with the perspective of broadening my scientific independence within the organic chemistry sector, I have also sought to build active collaborations (including with synthetic organic chemists) in Italy and abroad, reextending my studies back to nonbiological systems. For example, with Prof. Luca dell'Amico from the University of Padua, we have submitted a paper in which TD-DFT calculations, organic synthesis, and spectroscopy came together to prove that [2+2] photocycloadditions in iminium-based photocatalysts must proceed through a T_1 state. With Prof. Valeria Amendola, at the University of Pavia, I have resumed my work with supramolecular systems: my DFT calculations, with predicted NMR spectra, were able to definitively prove that imine-organic cages for CO_2 capture adopted egg shapes instead of the suspected disc shapes.

Past and present collaborations during my experience in Pavia are listed in the next section.

Ongoing studies that are still in the early stages are the TD-DFT exploration of the photocatalytic breakup of simple arylazosulfone compounds—in collaboration with the University of Pavia's *PhotoGreen Lab*, and the investigation of the sources of stereoselectivity in DIBALH-catalysed reduction of a bicyclic hydroxyketone.

Publications:

(1) Montefiori, M.; Pilotto, S.; Marabelli, C.; Moroni, E.; Ferraro, M.; Serapian, S. A.; Mattevi, A.; Colombo, G., *J. Chem. Inf. Model.* **2019**, *59* (9), 3927
(2) Serapian, S. A.; Colombo, G., *Chem. – Eur. J.* **2020**, *26* (21), 4656
(3) Colombo, G.; Paladino, A.; Woodford, M. R.; Backe, S. J.; Sager, R. A.; Kancherla, P.; Daneshvar, M. A.; Chen, V. Z.; Bourboulia, D.; Ahanin, E. F.; Prodromou, C.; Bergamaschi, G.; Strada, A.; Cretich, M.; Gori, A.; Veronesi, M.; Bandiera, T.; Vanna, R.; Bratslavsky, G.; Serapian, S. A.; Mollapour, M., *Chem. – Eur. J.* **2020**, *26* (43), 9459
(4) Sánchez-Martín, C.; Serapian, S. A.; Colombo, G.; Rasola, A., *Front. Oncol.* **2020**, *10*, 1177
(5) Serapian, S. A.; Marchetti, F.; Triveri, A.; Morra, G.; Meli, M.; Moroni, E.; Sautto, G. A.; Rasola, A.; Colombo, G., *J. Phys. Chem. Lett.* **2020**, *11* (19), 8084
(6) Serapian, S. A.; Castelli, M.; Marchetti, F.; Triveri, A.; Colombo, G., *ChemMedChem* **2021**, *16* (10), 1593
(7) Serapian, S. A.; Colombo, G., *Biophys. J.* **2021**, *120* (6), 977
(8) Serapian, S. A.; Sánchez-Martín, C.; Moroni, E.; Rasola, A.; Colombo, G., *Trends Pharmacol. Sci.* **2021**, *42* (7), 566
(9) Serapian, S. A.;***** Moroni, E.; Ferraro, M.; Colombo, G., *ACS Catal.* **2021**, *11* (14), 8605
(10) Castelli, M.; Serapian, S. A.; Marchetti, F.; Triveri, A.; Pirota, V.; Torielli, L.; Collina, S.; Doria, F.; Freccero, M.; Colombo G., *RSC Med. Chem.* **2021**, *12* (9), 1491
(11) Masgras, I.; Laquatra, C.; Cannino, G.; Serapian, S. A.; Colombo, G.; Rasola, A., *Semin. Cancer Biol.* **2021**, *76*, 45
(12) Woodford, M. R.; Baker-Williams, A. J.; Sager, R. A.; Backe, S. J.; Blanden, A. R.; Hashmi, F.; Kancherla, P.; Gori, A.; Loiselle, D. R.; Castelli, M.; Serapian, S. A.; Colombo, G.; Haystead, T. A.; Jensen, S. M.; Stetler-Stevenson, W. G.; Loh, S. N.; Schmidt, L. S.; Linehan, W. M.; Bah, A.; Bourboulia, D.; Bratslavsky, G.; Mollapour, M., *Nat. Struct. Mol. Biol.* **2021**, *28*, 662
(13) Triveri, A.; Serapian, S. A.; Marchetti, F.; Doria, F.; Pavoni, S.; Cinquini, F.; Moroni, E.; Rasola, A.; Frigerio, F.; Colombo, G., *J. Chem. Inf. Model.* **2021**, *61* (9), 4687
(14) Triveri, A.; Sánchez-Martín, C.; Torielli, L.; Serapian, S. A.; Marchetti, F.; D'Acerno, G.; Pirota, V.; Castelli, M.; Moroni, E.; Ferraro, M.; Quadrelli, P.; Rasola, A.; Colombo, G., *J. Mol. Biol.* **2022**, *434* (17), 167468
(15) Chiara, R.; Morana, M.; Folpini, G.; Olivati, A.; Albini, B.; Galinetto, P.; Chelazzi, L.; Ciattini, S.; Fantechi, E.; Serapian, S. A.; Petrozza, A.; Malavasi, L., *J. Mater. Chem. C* **2022**, *10*, 12367
(16) Scietti, L.; Moroni, E.; Mattoteia, D.; Fumagalli, M.; De Marco, M.; Negro, L.; Chiapparino, A.; Serapian, S. A.; De Giorgi, F.; Faravelli, S.; Colombo, G.; Forneris, F., *Front. Mol. Biosci.* **2022**, *9*, 876352
(17) Castelli, M.; Bhattacharya, K.; Abboud, E.; Serapian, S. A.; Picard, D.; Colombo, G., *J. Mol. Biol.* **2022**, *435* (3), 167931
(18) Torielli, L.; Serapian, S. A.; Mussolin, L.; Moroni, E.; Colombo, G., *J. Chem. Inf. Model.* **2023**, *63* (1), 343
(19) Capelli, R.; Serapian, S. A.; Colombo G., In *Computer-Aided Antibody Design*; Methods in Molecular Biology, Vol. 2552; Humana, New York, NY, 2023; pp 255-266
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(41) Frasnetti, E.; Frigerio, F.; Cinquini, F.; Serapian, S. A.; Pavoni, S.; Colombo, G., *ChemBioChem* **2026**, *27* (8), e70350
(42) Longhi, E.; Magni, A.; Torielli, L.; Lodigiani, G.; Carlessi, E.; Borsotti, P.; Doria, F.; Pirota, V.; Serapian, S. A.; Arrigoni, C.; Lolicato, M.; Moroni, E.; Bergamaschi, G.; Taraboletti, G.; Colombo, G., *Pharmacol. Res.* **2026**, *228*, 108205
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(44) Bonollo, G.; Roncati, B.; Torielli, L.; Wang, S.; Pasala, C.; Pavoni, S.; Frigerio, F.; Cinquini F.; Chiosis, G.; Serapian, S. A; Colombo, G., *J. Phys. Chem. Lett.* **2026**, *17* (28), 8098

Scientific skills: Consolidation of the methods learnt in Bristol. Further MD and trajectory analysis (*AMBER*, *GROMACS, Desmond,* in-house tools). Familiarisation with *GLYCAM* forcefields and forcefields for phosphorylated amino acids. Bioinformatics skills. Docking calculations. General experience with *Schrödinger* software packages. Familiarisation with the construction of Markov State Models. Familiarization with Machine Learning algorithms. Consolidation of programming skills with *Python*. Practice with grid-based pocket detection methods in proteins. Modelling of excited states with TD-DFT, beyond simulation of UV-Vis spectra.

Personal skills: Consolidation of teaching skills (see relevant section). Improvement of my personal organisation skills and the ability to delegate research activities, given the substantial increase in the amount of time dedicated to administrative and teaching commitments, and consequent progressive abandonment of first-hand research in favour of supervised research.

University of Bristol, UK
Sep. 2017 – May 2019

Position: **Research Associate**, *Group of Dr. Marc W. van der Kamp*
Project Title: *Multi-scale Simulation of Biocatalysts*

Funding Body: UK Biotechnology and Biological Sciences Research Council (Dr. van der Kamp's *David Phillips* Fellowship)
Funding: £ 32 004 / yr.
Awardees: Dr. Marc W. van der Kamp
Research: Research in computational enzymology / biocatalysis using state-of-the-art *in silico* techniques (*vide infra*), aiming to develop a reliable approach for the smart design of novel, more catalytically efficient enzyme mutants.

Description of work and techniques: Rationalisation of stereoselectivity in actinorhodin ketoreductase and two mutants, all catalysing reduction of small ketones to chiral alcohols. Methods included: classical MD (*AMBER*); QM/MM MD with umbrella sampling of the reduction process (*AMBER*) after benchmarking with *Gaussian* (DFT); *WaterSwap* and MM/PBSA calculations to probe substrate binding affinity; and protein-protein docking (*BUDE*), to explore interaction with the protein bearing the natural substrate (in collaboration with Prof. Matthew P. Crump). More enzymes were tentatively explored with a similar approach.

Publications:
(1) Serapian, S. A.; van der Kamp, M. W., *ACS Catal.* **2019**, *9* (3), 2381
(2) Serapian, S. A.; Crosby, J.; Crump, M. P.; van der Kamp, M. W., *JACS Au* **2022**, *2* (4), 972

Skills: Additive QM/MM methods, classical and QM/MM MD with *AMBER*, DFT, free energy techniques (MM/PBSA, *WaterSwap*, umbrella sampling), Docking, Programming (initial approach to *Python*), Didactic skills (supervision of two Master's students), Adaptability (switching back to academia after a brief stint in a start-up company, to acquire more expertise with biosimulation).

Catalan Institute of Chemical Research (ICIQ)
Tarragona, Spain
Sep. 2014 – Oct. 2016

Position: **Post-Doc**, *Group of Prof. Carles Bo Jané*
Project Title: *Computational Modelling of the Properties and Reactivity of Molecular Systems in Confined Spaces*
Funding Body: European Union (*Marie Curie COFUND* scholarship)
Funding: € 29 000 / yr. + € 1 100 / yr. bonus + € 20 000 / yr. conferences
Awardees: Prof. Carles Bo Jané
Research: Research on six independent projects in homogeneous catalysis (functionalised polyoxometalates) and supramolecular chemistry, involving collaborations with experimental research groups, and relying on QM, MM, and QM/MM methods.

Description of work and techniques: Each project is separately discussed in the following paragraphs (***1a***-***1f***), with associated publications at the end of each paragraph.

1a ***Explaining the different aggregative behaviour of plenary and lacunary Keggin anions in aqueous solution*** (based on data by Prof. Ira Weinstock, Ben-Gurion University of the Negev, Israel).
Large scale, all-atom classical MD simulations of voluminous aqueous solutions of Keggin anion salts $Li_5AlW_{12}O_{40}$ and $Li_9AlW_{11}O_{39}$ (*ca.* 39000 atoms; TIP4P water) were conducted with *GROMACS* using an *ad hoc* forcefield, and point charges fitted with *Gaussian09* (CHelpG method).

Publications: (1) Serapian, S. A.; Bo, C., *J. Phys. Chem. B* **2016**, *120* (50), 12959

1b ***Investigating the rotation of an Ir^{I}•(cyclooctadiene) complex encapsulated inside Rebek's cavitand*** (collaboration with Prof. Pau Ballester, ICIQ, Spain).
By running a series of DFT optimisations and transition state searches with *Gaussian09* (BP86/LANL2DZ/6-311G(d,p)), it was possible to produce a full energetic map of the 90° anticlockwise spin of a THF-complexed Ir^{I}•(cyclooctadiene)$(THF)_2$, encapsulated within Rebek's cavitand.

Publications: (1) Korom, S.; Martin, E.; Serapian S. A.; Bo, C.; Ballester, P., *J. Am. Chem. Soc.* **2016**, *138* (7), 2273

1c ***Characterising a novel Fe^{II}-co-ordinated polyoxometalate-organic hybrid oligomer*** (collaboration with Prof. Anna Proust, Univ. Pierre et Marie Curie, France).
In order to elucidate whether a polyoxometalate-organic hybrid oligomer, co-ordinated by Fe^{II}, is likely to coexist as a "molecular triangle" and a "molecular square", structural optimisations of these putative structures were carried out with *Gaussian09* and *ADF2014*. QM/QM approaches used in both cases.

Publications: (1) Izzet, G.; Abecassis, G.; Brouri, D.; Piot, M.; Matt, B.; Serapian, S. A.; Bo, C.; Proust, A., *J. Am. Chem. Soc.* **2016**, *138* (15), 5093

1d ***Justifying the energetic preference of* ad hoc *dimeric supramolecular capsules for C_{70} and C_{84}*** (collaboration with Prof. Javier de Mendoza, ICIQ, Spain).
In order to corroborate experimental work featuring supramolecular dimeric capsules for the extraction of higher fullerenes, full capsules, empty capsules, and dissociated capsule monomers were structurally optimised with *ADF2014* using DFT (BP86/TZP).

Publications: (1) Huerta, E.; Serapian, S. A.; Santos, E.; Cequier, E.; Bo, C.; de Mendoza, J., *Chem. – Eur. J.* **2016**, *22* (38), 13496

1e ***Ion-Pairing Studies on aqueous Cs^+ salts of the polyoxometalates $[Ta_6O_{19}]^{8-}$ and $[Nb_6O_{19}]^{8-}$*** (collaboration with Prof. May Nyman, Oregon State University, USA).

In order to rationalise odd solubility trends in $Cs_8Ta_6O_{19}$ and $Cs_8Nb_6O_{19}$, these were studied with a series of DFT structural optimisations at the PBE0/SDD/D95 level, in *Gaussian09*, followed by single-point calculations at the PBE0/def2-TZVP level.

Publications: (1) Sures, D. J.; Serapian, S. A.; Kozma, K.; Molina, P. I.; Bo, C.; Nyman M., *Phys. Chem. Chem. Phys.* **2017**, *19* (13), 8715

1f ***Understanding the Photochromic and Fluorescent Properties of a Benzospiropyran-polyoxometalate Molecular Switch*** (collaboration with Prof. Anna Proust, Univ. Pierre et Marie Curie, France).

The centrepiece of this study were: a benzospiropyran "molecular switch", its lacunary Keggin-anion-conjugate, and its tolylated equivalent. Spectral studies on these species were corroborated by TD-DFT calculations at the PBE0-D3(BJ)/def2-TZVP level, after prior DFT optimisation (PBE0-D3(BJ)/SDD/D95(d) level).

Publications: (1) Parrot, A.; Bernard, A.; Jacquart, A.; Serapian, S. A.; Bo, C.; Derat, E.; Oms, O.; Dolbecq, A.; Proust, A.; Métivier, R.; Mialane, P.; Izzet, G., *Angew. Chem., Int. Ed.* **2017**, *56* (17), 4872

Skills (*1a-f*): DFT, Time-dependent DFT, Large-scale MD simulations, Positive attitude to teamwork, Ability to work independently, Improved ability to redact scientific texts, Organisation, Global mindset (conferences)

Imperial College London, UK
Apr. 2010 – Feb. 2014

Position: **Doctoral degree in Computational and Theoretical Chemistry**, *Profs. Fernando Bresme and Michael J. Bearpark*
Thesis Title: *Simulating Self-Assembly of Organosulfur Species on Gold Nanoparticles*
Funding Body: UK Engineering and Physical Sciences Research Council
Funding: £ 1 382 / yr.
Research: Develop an accurate, efficient simulation strategy for thiol self-assembly on gold nanoparticles.

Description of work and techniques: Adaptation of available computational techniques and software (*Gaussian*; *GROMACS*) to a successful two-stage strategy. The first stage entailed classical molecular dynamics simulations (forcefield: *OPLS-AA*) to reproduce the initial physisorption. For the second stage, thiolated nanoparticles resulting from the previous stage were structurally optimised, using QM/MM (*ONIOM*).

Publications: (1) Serapian, S. A.;* Bearpark, M. J.; Bresme, F., *Nanoscale* **2013**, *5* (14), 6445
(2) Naeem, S.; Serapian, S. A.; Toscani, A.; White, A. J. P.; Hogarth, G.; Wilton-Ely, J. E. D. T., *Inorg. Chem.* **2014**, *53* (5), 2404

Skills: Large-scale MD, forcefield manipulation, DFT, QM/MM, Creativity in research, Programming (*C*, *Fortran*, *Bash*), Working with high-performance computing environments, Didactic skills (Successful supervision of a MSci student from *ParisTech*)

Imperial College London, UK
Oct. 2008 – Apr. 2010

Position: **Pre-doctoral project in Bioinformatics‡**, *Group of Prof. Andrew D. Miller* – ‡Interrupted due to supervisor's unexpected resignation
Thesis Title: *Investigating the Proteomic Code*
Funding Body: Self- funded
Research: Computational investigation on a hypothesised epigenetic *Proteomic Code*, whereby specific 'complementary' residue pairs would be directed at key sites to mediate binding at protein-protein interfaces, and functional folding within proteins themselves.

Description of work and techniques: Development of my own *PHP* program able to: (1) detect interacting residue pairs in mono- and dimeric protein crystal structures; (2) verify whether they sustain the hypothesis of a *proteomic code* (as compared to multiple sequence alignments of homologous proteins); (3) verify the statistical significance of the code (as compared to randomised mutations); and (4) display results in *PyMOL*.

Publications: (1) Illingworth, C. J. R.; Chintapalli, S. V.; Serapian, S. A.; Miller, A. D.; Veverka, V.; Carr, M. D.; Reynolds, C. A., *J. Comput. Chem.* **2012,** *33* (16), 1440
(2) Pullen, J. R.; Dalmaris, J.; Serapian, S. A.; Miller, A. D., *Bioorg. Med. Chem. Lett.* **2013**, *23*, 496

Skills: Better understanding of structural biology, Programming (*PHP*), Adaptability following unexpected changes (supervisor's resignation), Didactic skills (80 hr. demonstration in organic teaching labs)

Italfamaco S.p.A.
Cinisello Balsamo, Milan, Italy
Jan. – Oct. 2008

Position: **Computational Medicinal Chemist (Industrial R&D)**

Research: Computer-aided design of selective inhibitors of histone deacetylases.
Skills: MD simulations, Semi-empirical QM, Computer-aided drug design (*BIOVIA Discovery Studio*), Communication and interpersonal skills, Positive attitude to teamwork

Section 5 of 7: Collaborations

University of Pavia, Italy
Apr. 2019 – present

Past and present Collaborations:

- **Prof. Luca Dell'Amico**, University of Padua, Italy
  * Corti, V.; Simionato, G.; Rizzo, L.; Serapian, S. A.; Pelosi, G.; Natali, M.; Dell'Amico, L., *Nat. Chem.* **2026**, *18* (1), 189
  * Krishnan, C. G.; Cormier, G.; Serapian, S. A.; Bortolus, M.; Dell'Amico, L., *Angew. Chem., Int. Ed.* **2026**, *65* (29), e9986925

- **Prof. Gabriela Chiosis**, Memorial Sloan Kettering Cancer Center, New York, U.S.A.
  * Bonollo, G.; Roncati, B.; Torielli, L.; Wang, S.; Pasala, C.; Pavoni, S.; Frigerio, F.; Cinquini F.; Chiosis, G.; Serapian, S. A; Colombo, G., *J. Phys. Chem. Lett.* **2026**, *17* (28), 8098

- **Prof. Concepción Pérez-Melero**, University of Salamanca, Spain
  * Rodríguez-Santos, G.; Bonollo, G.; Sciva, C.; Colombo, G.; Pérez-Melero, C.; Serapian, S. A.,* *J. Chem. Inf. Model.* **2026**, *66* (7), 4101

- **Prof. Adrian J. Mulholland**, University of Bristol, UK
  * Castelli, M.; Marchetti, F.; Osuna, S.; Oliveira, A. S. F.; Mulholland, A. J.; Serapian, S. A.;* Colombo, G., *J. Am. Chem. Soc.* **2024**, *146* (1), 901
  * Balega, B.; Beer, M.; Spencer, J.; Colombo, G.; Serapian, S. A.; Oliveira, A. S. F.; Mulholland, A. J., *Mol. Phys.* **2024**, 123, 7-8, e2428350
  * Magni, A.; Bonollo, G.; Trèves, G.; Frigerio, F.; Cinquini, F.; Pavoni, S.; Oliveira, A. S. F.; Mulholland, A. J.; Serapian, S. A.;* Colombo, G., *Protein Sci.* **2026**, *35* (5), e70543

- **Prof. Andrea Rasola**, University of Padua, Italy
  * Sánchez-Martín, C.; Serapian, S. A.; Colombo, G.; Rasola, A., *Front. Oncol.* **2020**, *10*, 1177
  * Serapian, S. A.; Marchetti, F.; Triveri, A.; Morra, G.; Meli, M.; Moroni, E.; Sautto, G. A.; Rasola, A.; Colombo, G., *J. Phys. Chem. Lett.* **2020**, *11* (19), 8084
  * Serapian, S. A.; Sánchez-Martín, C.; Moroni, E.; Rasola, A.; Colombo, G., *Trends Pharmacol. Sci.* **2021**, *42* (7), 566
  * Masgras, I.; Laquatra, C.; Cannino, G.; Serapian, S. A.; Colombo, G.; Rasola, A., *Semin. Cancer Biol.* **2021**, *76*, 45
  * Triveri, A.; Serapian, S. A.; Marchetti, F.; Doria, F.; Pavoni, S.; Cinquini, F.; Moroni, E.; Rasola, A.; Frigerio, F.; Colombo, G., *J. Chem. Inf. Model.* **2021**, *61* (9), 4687
  * Triveri, A.; Sánchez-Martín, C.; Torielli, L.; Serapian, S. A.; Marchetti, F.; D'Acerno, G.; Pirota, V.; Castelli, M.; Moroni, E.; Ferraro, M.; Quadrelli, P.; Rasola, A.; Colombo, G., *J. Mol. Biol.* **2022**, *434* (17), 167468
  * Scantamburlo, F.; Masgras, I.; Ciscato, F.; Laquatra, C.; Frigerio, F.; Cinquini, F.; Pavoni, S.; Triveri, A.; Fransetti, E.; Serapian, S. A.; Colombo, G.; Rasola, A.; Moroni, E., *J. Chem. Inf. Model.* **2024**, *64* (21), 8274
  * Guarra, F.; Komarov, D.; Ciamarone, A.; Torielli, L.; Previtali, V.; Margaroli, N.; Romeo, E.; La Spina, M.; Sbuelz, F.; Laquatra, C.; Veronesi, M.; Lolicato, M.; Arrigoni, C.; Moroni, E.; Serapian, S. A.; Girotto, S.; Rasola, A.; Colombo, G., *Cell Stress Chaperones* **2026**, *31* (2), 100162

- **Dr. Francesco Frigerio**, ENI Corporation, Italy
  * Triveri, A.; Serapian, S. A.; Marchetti, F.; Doria, F.; Pavoni, S.; Cinquini, F.; Moroni, E.; Rasola, A.; Frigerio, F.; Colombo, G., *J. Chem. Inf. Model.* **2021**, *61* (9), 4687
  * Triveri, A.; Casali, E.; Frasnetti, E.; Doria, F.; Frigerio, F.; Cinquini, F.; Pavoni, S.; Moroni, E.; Marchetti, F.; Serapian, S. A.; Colombo, G., *J. Chem. Theor. Comput.* **2023**, *19* (7), 2120
  * Castelli, M.; Magni, A.; Bonollo, G.; Pavoni, S.; Frigerio, F.; Oliveira, A. S. F.; Cinquini, F.; Serapian, S. A.; Colombo, G., *Protein Sci.* **2024**, *33* (3), e4880
  * Frasnetti, E.; Cucchi, I.; Pavoni, S.; Frigerio, F.; Cinquini, F.; Serapian, S. A.; Pavarino, L. F.; Colombo, G., *J. Chem. Theor. Comput.* **2024**, *20* (20), 9209
  * Scantamburlo, F.; Masgras, I.; Ciscato, F.; Laquatra, C.; Frigerio, F.; Cinquini, F.; Pavoni, S.; Triveri, A.; Fransetti, E.; Serapian, S. A.; Colombo, G.; Rasola, A.; Moroni, E., *J. Chem. Inf. Model.* **2024**, *64* (21), 8274
  * Magni, A.; Bonollo, G.; Trèves, G.; Frigerio, F.; Cinquini, F.; Pavoni, S.; Oliveira, A. S. F.; Mulholland, A. J.; Serapian, S. A.;* Colombo, G., *Protein Sci.* **2026**, *35* (5), e70543
  * Frasnetti, E.; Frigerio, F.; Cinquini, F.; Serapian, S. A.; Pavoni, S.; Colombo, G., *ChemBioChem* **2026**, *27* (8), e70350

* Bonollo, G.; Roncati, B.; Torielli, L.; Wang, S.; Pasala, C.; Pavoni, S.; Frigerio, F.; Cinquini F.; Chiosis, G.; Serapian, S. A; Colombo, G., *J. Phys. Chem. Lett.* **2026**, *17* (28), 8098

- **Prof. Filippo Doria**, University of Pavia, Italy
  * Castelli, M.; Serapian, S. A.; Marchetti, F.; Triveri, A.; Pirota, V.; Torielli, L.; Collina, S.; Doria, F.; Freccero, M.; Colombo G., *RSC Med. Chem.* **2021**, *12* (9), 1491
  * Triveri, A.; Serapian, S. A.; Marchetti, F.; Doria, F.; Pavoni, S.; Cinquini, F.; Moroni, E.; Rasola, A.; Frigerio, F.; Colombo, G., *J. Chem. Inf. Model.* **2021**, *61* (9), 4687
  * Triveri, A.; Casali, E.; Frasnetti, E.; Doria, F.; Frigerio, F.; Cinquini, F.; Pavoni, S.; Moroni, E.; Marchetti, F.; Serapian, S. A.; Colombo, G., *J. Chem. Theor. Comput.* **2023**, *19* (7), 2120
  * Torielli, L.; Castelli, M.; Milani, F.; Heritz, J. A.; Cayaban, S. J.; Hernandez, J.; Serapian, S. A.; Magni, A.; Frasnetti, E.; Doria, F.; Pirota, V.; Wengert, L. A.; Woodford, M. R.; Lodigiani, G.; Bergamaschi, G.; Veronesi, M.; Bandiera, T.; Girotto, S.; Paladino, A.; Prodromou, C.; Backe, S. J.; Bourboulia, D.; Canciani, A.; Arrigoni, C.; Lolicato, M.; Gestwicki, J. E.; Mollapour, M.; Colombo, G., *Structure* **2025**, *33* (11), 1944
  * Longhi, E.; Magni, A.; Torielli, L.; Lodigiani, G.; Carlessi, E.; Borsotti, P.; Doria, F.; Pirota, V.; Serapian, S. A.; Arrigoni, C.; Lolicato, M.; Moroni, E.; Bergamaschi, G.; Taraboletti, G.; Colombo, G., *Pharmacol. Res.* **2026**, *228*, 108205

- **Prof. Marco G. Lolicato**, University of Pavia, Italy
  * Torielli, L.; Castelli, M.; Milani, F.; Heritz, J. A.; Cayaban, S. J.; Hernandez, J.; Serapian, S. A.; Magni, A.; Frasnetti, E.; Doria, F.; Pirota, V.; Wengert, L. A.; Woodford, M. R.; Lodigiani, G.; Bergamaschi, G.; Veronesi, M.; Bandiera, T.; Girotto, S.; Paladino, A.; Prodromou, C.; Backe, S. J.; Bourboulia, D.; Canciani, A.; Arrigoni, C.; Lolicato, M.; Gestwicki, J. E.; Mollapour, M.; Colombo, G., *Structure* **2025**, *33* (11), 1944
  * Guarra, F.; Komarov, D.; Ciamarone, A.; Torielli, L.; Previtali, V.; Margaroli, N.; Romeo, E.; La Spina, M.; Sbuelz, F.; Laquatra, C.; Veronesi, M.; Lolicato, M.; Arrigoni, C.; Moroni, E.; Serapian, S. A.; Girotto, S.; Rasola, A.; Colombo, G., *Cell Stress Chaperones* **2026**, *31* (2), 100162
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- **Prof. Jason E. Gestwicki**, University of California, San Francisco, USA
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- **Prof. Mehdi Mollapour**, State University of New York, USA
  * Colombo, G.; Paladino, A.; Woodford, M. R.; Backe, S. J.; Sager, R. A.; Kancherla, P.; Daneshvar, M. A.; Chen, V. Z.; Bourboulia, D.; Ahanin, E. F.; Prodromou, C.; Bergamaschi, G.; Strada, A.; Cretich, M.; Gori, A.; Veronesi, M.; Bandiera, T.; Vanna, R.; Bratslavsky, G.; Serapian, S. A.; Mollapour, M., *Chem. – Eur. J.* **2020**, *26* (43), 9459
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- **Prof. Andrea Mattevi**, University of Pavia, Italy
  * Montefiori, M.; Pilotto, S.; Marabelli, C.; Moroni, E.; Ferraro, M.; Serapian, S. A.; Mattevi, A.; Colombo, G., *J. Chem. Inf. Model.* **2019**, *59* (9), 3927

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- **Prof. Sílvia Osuna**, University of Girona, Spain
  * Castelli, M.; Marchetti, F.; Osuna, S.; Oliveira, A. S. F.; Mulholland, A. J.; Serapian, S. A.;* Colombo, G., *J. Am. Chem. Soc.* **2024**, *146* (1), 901

- **Prof. Valeria Amendola**, University of Pavia, Italy
  * Mobili, R.; La Cognata, S.; Monteleone, M.; Longo, M.; Fuoco, A.; Serapian, S. A.; Vigani, B.; Milanese, C.; Armentano, D.; Jansen, J. C.; Amendola, V., *Chem. – Eur. J.* **2023**, *29* (56), e202301437

- **Prof. Federico Forneris**, University of Pavia, Italy
  ***** Scietti, L.; Moroni, E.; Mattoteia, D.; Fumagalli, M.; De Marco, M.; Negro, L.; Chiapparino, A.; Serapian, S. A.; De Giorgi, F.; Faravelli, S.; Colombo, G.; Forneris, F., *Front. Mol. Biosci.* **2022**, *9*, 876352

- **Prof. Lorenzo Malavasi**, University of Pavia, Italy
  * Chiara, R.; Morana, M.; Folpini, G.; Olivati, A.; Albini, B.; Galinetto, P.; Chelazzi, L.; Ciattini, S.; Fantechi, E.; Serapian, S. A.; Petrozza, A.; Malavasi, L., *J. Mater. Chem. C* **2022**, *10*, 12367

- ***PhotoGreen Lab***, University of Pavia, Italy
  * *ongoing:* TD-DFT investigation on the photocatalytic breakup of arylazosulfones

- **Dr. Daniele Fiorito**, Polytechnic University of Milan, Italy
  * *ongoing:* Investigating the sources of stereoselectivity in DIBALH-catalysed reduction of a bicyclic hydroxyketone
  * *ongoing:* Modelling the asymmetric reduction mechanism of unsaturated boronic acids and related substrates in Old Yellow Enzymes.

- **Dr. Kirill Zinovjev**, University of Valencia, Spain
  * *ongoing:* Application of the Adaptive String Method in mechanistic enzyme studies.

University of Bristol, UK
Sep. 2017 – Mar. 2019

Collaborations:
- **Prof. Matthew P. Crump**, University of Bristol, UK
  * Serapian, S. A.; Crosby, J.; Crump, M. P.; van der Kamp, M. W., *JACS Au* **2022**, *2* (4), 972

Catalan Institute of Chemical Research (*ICIQ*) Tarragona, Spain
Oct. 2014 – Oct. 2016

Collaborations:
- **Prof. Anna Proust**, Univ. Pierre et Marie Curie, France
  ***** Izzet, G.; Abecassis, G.; Brouri, D.; Piot, M.; Matt, B.; Serapian, S. A.; Bo, C.; Proust, A., *J. Am. Chem. Soc.* **2016**, *138* (15), 5093
  ***** Parrot, A.; Bernard, A.; Jacquart, A.; Serapian, S. A.; Bo, C.; Derat, E.; Oms, O.; Dolbecq, A.; Proust, A.; Métivier, R.; Mialane, P.; Izzet, G., *Angew. Chem., Int. Ed.* **2017**, *56* (17), 4872

- **Prof. May Nyman**, Oregon State University, USA
  * Sures, D. J.; Serapian, S. A.; Kozma, K.; Molina, P. I.; Bo, C.; Nyman M., *Phys. Chem. Chem. Phys.* **2017**, *19* (13), 8715

- **Prof. Pau Ballester**, ICIQ, Spain
  * Korom, S.; Martin, E.; Serapian S. A.; Bo, C.; Ballester, P., *J. Am. Chem. Soc.* **2016**, *138* (7), 2273

- **Prof. Javier de Mendoza**, ICIQ, Spain
  * Huerta, E.; Serapian, S. A.; Santos, E.; Cequier, E.; Bo, C.; de Mendoza, J., *Chem. – Eur. J.* **2016**, *22* (38), 13496

Imperial College London
Oct. 2008 – Feb. 2014

Collaborations:
- **Prof. James Wilton-Ely**, Imperial College London, UK
  * Naeem, S.; Serapian, S. A.; Toscani, A.; White, A. J. P.; Hogarth, G.; Wilton-Ely, J. E. D. T., *Inorg. Chem.* **2014**, *53* (5), 2404

- **Prof. Christopher Reynolds**, University of Essex, UK
  * Illingworth, C. J. R.; Chintapalli, S. V.; Serapian, S. A.; Miller, A. D.; Veverka, V.; Carr, M. D.; Reynolds, C. A., *J. Comput. Chem.* **2012,** *33* (16), 1440

Section 6 of 7: Conferences and Seminars

35 interventions at 32 events, including **13 distinct oral presentations** (**6 invited**) and **8 distinct posters** (numbered 1 to 13 or 1 to 8, respectively, and listed chronologically)

2026
- **Invited Lecture – 14th IUPAC International Conference on Bioorganic Chemistry (ISBOC-14)**, Milan, IT
  * Talk 13: *Machine Learning to Boost Detection of Allosteric Fingerprints from Molecular Dynamics*
- **International Society of Quantum Biology and Pharmacology (ISQBP) – President's Meeting**, Cluj-Napoca, NO
  * Poster 8: *Allosteric Regulation in the Kinesin-5 Motor Domain Investigated by Molecular Dynamics Simulations Across 4 Catalytic States*

2025
- **13th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2025)**, Oslo, NO
  * Talk 12: *Multiscale Modelling of Allostery in Proteins*

2024
- **10th Annual CCPBiosim & MGMS Conference: Molecular modelling in structure-based drug design**, Newcastle, UK
  * Talk 11: *MD Simulations Map the Havoc Wreaked by One Mutation in* $[Hsp60]_{14}$

2023
- **Invited Seminar – Prof. Pablo García Jambrina's Research Group, University of Salamanca**, Spain
  * Talk 10: *Learning the Languages of Allostery in K-Ras4B and Speaking them Elsewhere* (version II)
- **14th European Conference on Computational and Theoretical Chemistry (EuChemS CompChem 2023)**, Thessaloniki, GR
  * Talk 10: *Learning the Languages of Allostery in K-Ras4B* (version I)

2022
- **40th National Conference of the Organic Chemistry Division of the Italian Chemical Society (XL CDCO)**, Palermo, IT
  * Talk 6: *Modelling Reactivity and Stereocontrol in Actinorhodin Ketoreductase* (version III)
- **Centre Européen de Calcul Atomique et Moléculaire (CECAM) – Workshop: Present and Future of Hybrid Quantum Chemical and Molecular Mechanical Simulations**, Lecco, IT
  * Poster 7: *Using QM/MM Molecular Dynamics to Model Reactivity in the Mitochondrial Chaperone Trap1*
  * Talk 8: *Using QM/MM Molecular Dynamics to Model Reactivity in the Mitochondrial Chaperone Trap1* (version IV)
- **Invited Seminar – Prof. Adrian J. Mulholland's Research Group, University of Bristol**, UK (online)
  * Talk 9: *Modelling Reactivity in Enzymes (with an Eye on Allostery): Two Recent Case Studies*
- **Invited Seminar – Prof. Iñaki Tuñón's Research Group, Univ. of Valencia,** ES
  * Talk 9: *Modelling Reactivity in Enzymes (with an Eye on Allostery): Two Recent Case Studies*

2021
- **International Society of Quantum Biology and Pharmacology (ISQBP) – President's Meeting**, Strasbourg, FR (online)
  * Talk 8: *Modelling the Peculiar Reactivity of the Molecular Chaperone Trap1* (version III)
- **Computationally Driven Drug Discovery (CDDD – 7th Meeting)**, Milan, IT (online)
  * Talk 8: *Modelling Asymmetric Reactivity in Trap1 to Guide the Design of Allosteric Modulators* (version II)
- **Invited Workshop – Institut Català d'Investigació Química**, Tarragona, ES (online)
  * Talk 8: *You Poor Asymmetric Catalyst:*

Modelling Reactivity in the Mitochondrial Chaperone Trap1 (version I)

2019 - **Computational Molecular Science 2019 (6th edition)**, Coventry, UK
* Talk 7: *Atomistic Simulations of the Catalytic Behaviour of a Keto-reductase Towards Small-molecule and Natural Substrates* (**Invited contributed talk**, one of 6 chosen out of 150 submitted)

2018 - **Invited Seminar – Istituto di Chimica del Riconoscimento Molecolare**, Milan, IT
* Talk 6: In Silico *Studies on Stereocontrol in Actinorhodin Ketoreductase* (version II)

- **EMBO - Enzymes, Biocatalysis, Chemical Biology: The New Frontiers**, Pavia, IT
* Poster 6: *Stereocontrol for Small Substrates in Actinorhodin Ketoreductase: A Computational Perspective* (version II)

- **Quantum Bioinorganic Chemistry (QBIC•IV)**, Bath, UK
* Talk 6: In Silico *Studies on Stereocontrol in Actinorhodin Ketoreductase* (version I)

- **3rd CCPBioSim/CCP5 Conference on Multiscale Modelling,** Manchester, UK
* Poster 6: *Stereocontrol for Small Substrates in Actinorhodin Ketoreductase: A Computational Perspective* (version I)

2016 - **251st National Meeting of the American Chemical Society**, San Diego, US
* Talk 5: *Huddling together when something is missing: Supramolecular Aggregation in Monolacunary Keggin Anions*
* Talk 4: *Catching the big fullerene: Selectivity of self-assembled molecular capsules towards C_{70} and C_{84}*
* Talk 3: *Supramolecular Rotation: The Fascinating motion of an Ir^{I} complex within Rebek's self-folding octaamide cavitand*
* Talk 2: *Of Triangles and Squares: Hierarchical Self-Assembly of Interlinked Polyoxometalates*

- **XXXII Ed. – Catalonian Theoretical Chemistry Reference Network**, Barcelona, ES
* Talk 2: *Of Triangles and Squares: Hierarchical Self-Assembly of Interlinked Polyoxometalates*

- **Fourth Meeting – Frontiers in Metal Oxide Cluster Science**, Newcastle, UK
* Poster 5: *That Organic Extra Something:* In Silico *Studies on Two Organic-Polyoxometalate Hybrids*

- **Theory and Applications of Computational Chemistry (TACC 2016)**, Seattle, US
* Poster 5: *That Organic Extra Something:* In Silico *Studies on Two Organic-Polyoxometalate Hybrids*

2015 - **EuCheMS 10th European Conference on Computational Chemistry**, Fulda, DE
* Poster 4: *Huddling Together When Something is Missing: Simulating the Aggregation of Lacunary Keggin Anions*

- **Congress of Theoretical Chemists of Latin Expression (CHITEL 2015)**, Turin, IT
* Poster 4: *Huddling Together When Something is Missing: Simulating the Aggregation of Lacunary Keggin Anions*

- **The 15th International Congress of Quantum Chemistry (ICQC)**, Beijing, PRC
* Poster 3: *DFT to the Rescue: The Rotation of an Ir^{I} Complex within Resorcin[4]arene*

2012 - **RSC Theoretical Chemistry Group Grad. Students Meeting**, King's College London
* Talk 1: *QM and QM/MM simulations of Pristine and Passivated Gold Nanoparticles*

- **Chemistry Department Postgraduate Symposium**, Imperial College London
* Talk 1: *QM and QM/MM simulations of Pristine and Passivated Gold Nanoparticles* (**Second prize**: Second-best Physical Chemistry Talk)

- **Thomas Young Centre Postgraduate Students Day**, Queen Mary Univ. of London
* Talk 1: *QM and QM/MM simulations of Pristine*

and Passivated Gold Nanoparticles
(**First prize**: Best Talk)

2011 - **Gold: Faraday Discussion 152**, Cardiff University, UK
* Poster 2: *A QM/MM Study on the Self-Assembly of Thiol Monolayers on Gold Surfaces*

- **Chemistry Department Postgraduate Symposium**, Imperial College London
* Poster 2: *A QM/MM Study on the Self-Assembly of Thiol Monolayers on Gold Surfaces*

2010 - **RSC Bioorganic Group Postgraduate Symposium**, Univ. of Nottingham, UK
* Poster 1: *A Study on Second Generation Mekler-Idlis Residue Pairs*

- **Chemistry Department Postgraduate Symposium**, Imperial College London
* Poster 1: *A Study on Second Generation Mekler-Idlis Residue Pairs*

Section 7 of 7: Peer Reviewing Activities

Journals

Peer reviewer for articles submitted to the following journals:

- *Computational and Structural Biotechnology Journal*
- *Journal of Chemical Information and Modelling*
- *Journal of Chemical Theory and Computation*
- *Journal of Physical Chemistry Letters*
- *Scientific Reports*

Ph.D. Theses (Reviewing)

Some jurisdictions require Ph.D. theses to be externally peer-reviewed.

November 2024

- Mr. Marco Nicaso, *Rovira i Virgilii* University, Tarragona, Spain
  * *Development of Systems for Artificial Photosynthesis: A Combined Experimental and Computational Approach*
    [For this Thesis, I also partook in the examination committee; see Section 3]

June 2025

- Ms. Anzhela Veselinova, University of Salamanca, Spain
  * *Theoretical Studies of Reactive and Inelastic Collisions in Systems of Astrochemical Interest: O + H_2 and C_2O / C_5N^- / C_7N^- + He*