Stefano Artin SERAPIAN

20131 Milan, ITALY
Date of Birth: 14/03/1985 **Nationality:** Italian

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Professional Experience

University of Pavia, Italy
May 2019 – present

Research Fellow (Biomolecular Simulation; group of Prof. Giorgio Colombo)
- *In silico* studies on chaperone proteins Hsp90 and 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 – May 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

Marie Curie (*COFUND*) **Research Fellow** (group of Prof. Carles Bo)
- Application of my expertise in computational chemistry to six distinct experimental collaborations, in the fields of homogeneous catalysis (polyoxometalates) and supramolecular chemistry (encapsulated Ir^{I} complexes and fullerenes)
- Methods applied include: DFT (reaction profile maps, structural optimisation); TD-DFT (spectral properties); QM/MM (*ONIOM*); large-scale all-atom MM MD simulations

***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
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

Partly Completed Ph.D. (Computational Biochemistry): *Investigating the Proteomic Code* (Supervisor: Prof. Andrew D. Miller)
[Forcibly interrupted due to unexpected resignation of supervisor]

Sep. 2003 – Aug. 2007

MSci in Chemistry (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)
- **Humanities Project** (in German): *Föderalismus und Mehrsprachigkeit in der Schweiz* (*Federalism and Multilingualism in Switzerland*; Supervisor: Prof. Charmian Brinson)

Sir James Henderson British School of Milan
Sep. 2002 – Jun. 2003

- **A-level** examinations in Chemistry, Biology, Mathematics, and Music (all grade A)
- **AS-Level** examination in French (grade A)
- **Italian *Maturità***: integrative examination in History and Literature (passed; no grade)

Strengths and Skills

Chemistry and Biochemistry

- Expertise with several *in silico* approaches in chemistry and biochemistry including:
  * Standard methods in computer-aided drug design and cheminformatics
  * All aspects of molecular modelling (materials and biomolecules)
  * QM simulations (DFT, TD-DFT, MP2, CCSD(T), HF, and semiempirical)
  * Classical MD simulations and forcefield handling
  * QM/MM simulations (both additive and *ONIOM*)

    * Free energy methods (umbrella sampling, MM/PBSA, free energy perturbation)
- Expertise with relevant software, including: *GROMACS*; *AMBER*; *Biovia Discovery Studio*; *Schrödinger Maestro*; *PyMOL*; *VMD*; *BUDE Docking Engine*; *Gaussian*; *ADF*.
- Working knowledge of the software packages *AutoDock VINA*; *SireMol*; *ClustalW*; *Accord*; *MOPAC*; *GAMESS-US*
- Familiarity with online databases such as *ChEMBL*, *PDB*, *UniProtKB*, *Pfam*

IT and Programming

- Excellent knowledge of the programming languages *PHP* and *bash*
- Hands-on experience with *Python* and relevant biosimulation libraries
- Extensive experience with the *Windows, MAC* and *Linux* operating systems
- Working knowledge of the programming languages *C,* and *Fortran77*

Personal Strengths

- **Positive attitude to teamwork**, consolidated whilst working at *Italfarmaco* in a multidisciplinary group of theoreticians and experimentalists; through collaborations at *ICIQ*; 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 biomolecular simulation
- **Leadership and didactic skills**, consolidated through full-time supervision of undergraduates during my doctorate, in Bristol, and particularly in Pavia; and demonstrating in undergraduate laboratories at *Imperial College*
- **Advanced communication skills**, developed over many years of speaking at scientific conferences; cold-calling and managing customers at *Mind the Byte*; as well as partaking in musical performances, and acting in the high school years
- **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)

External Courses

2011 – 2012 *National Training School in Theoretical Chemistry* (Univ. of Oxford); *Advanced Open MP* (Univ. of Edinburgh); *Methods in Molecular Simulation* (CCP5 Summer school, Queen's Univ., Belfast); *Fortran95* (King's College London)

2019 *New Approaches in Molecular Modelling* (Schrödinger Workshop, Univ. of Milan)

Prizes and Achievements

- *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

Overview of Publications

37 peer-reviewed publications since 2012 (3 more in preparation), including:

- in ***Nature Structural & Molecular Biology***; ***Trends in Pharmacological Sciences***; ***Journal of the American Chemical Society***; ***Angewandte Chemie***; ***ACS Catalysis***
- 10 as **first author**, comprising 3 as **corresponding author**
- An up-to-date list is available at https://orcid.org/0000-0003-0122-8499

Recent Conferences

31 interventions since 2010: **10 distinct oral presentations** and **7 distinct posters**

2023

- **14th European Conference on Computational and Theoretical Chemistry**, Thessaloniki, GR

2022

- **National Conference of the Organic Chemistry Division of the Italian Chemical Society (40th CDCO)**, Palermo, IT
- **CECAM Workshop – Present and Future of Hybrid QM/MM Simulations**, Lecco, IT
- **Invited Talk – Prof. Adrian J. Mulholland's Group**, Univ. of Bristol, UK (online)
- **Invited Talk – Prof. Iñaki Tuñón's Group**, Univ. of Valencia, ES

2021

- **ISQBP – President's Meeting**, Strasbourg, FR (online)
- **Invited Workshop – Institut Català d'Investigació Química**, Tarragona, ES (online)

Additional Skills and Interests

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

Annex 1: Peer-reviewed journal articles

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

(1) 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; **Latest IF:** 17.012; **DOI:** 10.1016/j.semcancer.2021.07.002

(2) 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; **Latest IF:** 18.361; **DOI:** 10.1038/s41594-021-00633-2

(3) 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; **Latest IF:** 15.000; **DOI:** 10.1021/jacs.3c11396

(4) 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; **Latest IF:** 17.638; **DOI:** 10.1016/j.tips.2021.04.003

(5) 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; **Latest IF:** 13.700; **DOI:** 10.1021/acscatal.1c00692

(6) 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; **Latest IF:** 15.000; **DOI:** 10.1021/jacs.5b12646

(7) 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; **Latest IF:** 15.000; **DOI:** 10.1021/jacs.6b00972

(8) 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; **Latest IF:** 16.823; **DOI:** 10.1002/anie.201701860

(9) 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; **Latest IF:** 13.700; **DOI:** 10.1021/acscatal.8b04846

(10) 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; **Latest IF:** 8.067; **DOI:** 10.1039/d2tc02113g

(11) 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; **Latest IF:** 8.025; **DOI:** 10.1016/j.ijbiomac.2023.125609

(12) 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; **Latest IF:** 8.000; **DOI:** 10.1002/pro.4880

(13) 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; **Latest IF:** 6.800; **DOI:** 10.1016/j.sbi.2024.102835

(14) 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; **Latest IF:** 8.307; **DOI:** 10.1039/c3nr01500a

(15) Serapian, S. A.; Marchetti, F.; Triveri, A.; Morra, G.; Meli, M.; Moroni, E.; Sautto, G.; 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; **Latest IF:** 6.888; **DOI:** 10.1021/acs.jpclett.0c02341

(16) 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; **Latest IF:** 6.578; **DOI:** 10.1021/acs.jctc.3c00077

(17) 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; **Latest IF:** 6.162; **DOI:** 10.1021/acs.jcim.2c01408

(18) 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; **Latest IF:** 6.151; **DOI:** 10.1016/j.jmb.2022.167931

(19) 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; **Latest IF:** 6.151; **DOI:** 10.1016/j.jmb.2022.167468

(20) 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; **Latest IF:** 6.113; **DOI:** 10.3389/fmolb.2022.876352

(21) 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; **Latest IF:** 4.300; **DOI:** 10.1002/chem.201601690[1,2]
[1] Selected as "Hot Paper"
[2] Cover picture

(22) Serapian, S. A.; Colombo, G., Designing Molecular Spanners to Throw in the Protein Networks. *Chem. – Eur. J.* **2020**, *26* (21), 4656.
IF: 5.160; **Latest IF:** 4.300; **DOI:** 10.1002/chem.201904523[3]
[3] Appearing in "Showcased Reviews" section

(23) 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; **Latest IF:** 4.300; **DOI:** 10.1002/chem.202000615[1]
[1] Selected as "Hot Paper"

(24) 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; **Latest IF:** 6.162; **DOI:** 10.1021/acs.jcim.1c00857

(25) 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; **Latest IF:** 5.738; **DOI:** 10.3389/fonc.2020.01177

(26) 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; **Latest IF:** 5.436; **DOI:** 10.1021/ic402048a

(27) 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; **Latest IF:** 3.945; **DOI:** 10.1039/c6cp08454k

(28) 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; **Latest IF:** 4.300; **DOI:** 10.1002/chem.202301437

(29) 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; **Latest IF:** 6.162; **DOI:** 10.1021/acs.jcim.9b00588

(30) Illingworth, C. J. R.; Chintapalli, S. V.; Serapian, S. A.; Miller, A. D.; Veverka, V.; Carr, M. D.; Reynolds, C. A., The Statistical Significance of Selected Sense-Antisense Peptide Interactions. *J. Comput. Chem.* **2012**, *33* (16), 1440.
IF: 3.835; **Latest IF:** 3.672; **DOI:** 10.1002/jcc.22977

(31) Serapian, S. A.; Colombo, G., Bow to the Enemy: How Flexibility of Host Protein Receptors Can Favor SARS-CoV-2. *Biophys. J.* **2021**, *120* (6), 977.
IF: 3.665; **Latest IF:** 3.699; **DOI:** 10.1016/j.bpj.2021.01.029

(32) Serapian, S. A.; Castelli, M.; Marchetti, F.; Triveri, A.; Colombo, G., Exploiting the Folding and Degradation Machineries to Target Undruggable Proteins: What can the Computational Approach Tell Us? *ChemMedChem* **2021**, *16* (10), 1593.
IF: 3.466; **Latest IF:** 3.540; **DOI:** 10.1002/cmdc.202000960[4]
[4] Selected as "VIP Paper"

(33) Serapian, S. A.; Bo, C., Simulating the Favourable Aggregation of Monolacunary Keggin Anions. *J. Phys. Chem. B* **2016**, *120* (50), 12959.
IF: 3.187; **Latest IF:** 3.466; **DOI:** 10.1021/acs.jpcb.6b10387

(34) Pullen, J. R.; Dalmaris, J.; Serapian, S. A.; Miller, A. D., Assessing the Preferred Solution Conformation of an Interacting Sense-Antisense (Complementary) Peptide Pair. *Bioorg. Med. Chem. Lett.* **2013**, *23*, 496.
IF: 2.338; **Latest IF:** 3.461; **DOI:** 10.1016/j.bmcl.2012.11.038

(35) Castelli, M.; Serapian, S. A.; Marchetti, F.; Triveri, A.; Pirota, V.; Torielli, L.; Collina, S.; Doria, F.; Freccero, M.; Colombo G., New Perspectives in Cancer Drug Development: Computational Advances with an Eye to Design. *RSC Med. Chem.* **2021**, *12* (9), 1491.
IF: Pending; **Latest IF:** 3.470 (partial for 2021); **DOI:** 10.1039/D1MD00192B

(36) 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: Pending; **Latest IF:** Pending; **DOI:** 10.1021/jacsau.2c00086

(37) Capelli, R.; Serapian, S. A.; Colombo G., Computational Epitope Prediction and Design for Antibody Development and Detection. In *Computer-Aided Antibody Design*; Methods in Molecular Biology, Vol. 2552; Humana, New York, NY, 2023; pp 255-266.
IF: 1.37; **Latest IF:** 1.37; **DOI:** 10.1007/978-1-0716-2609-2_13

Annex 2: Conferences and Seminars

31 interventions at 27 events, including **10 distinct oral presentations** (**5 invited**) and **7 distinct posters** (numbered 1 to 10 or 1 to 6, respectively, and listed chronologically)

2023
- **14th European Conference on Computational and Theoretical Chemistry (EuChemS CompChem 2023)**, Thessaloniki, GR
  * Talk 10: *Learning the Languages of Allostery in K-Ras4B*

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*

Annex 3:
Research

Università degli Studi di Pavia, Italy
May 2019 – present

Position: **Research Fellow**, *Group of Prof. Giorgio Colombo*
Project Title: *Studying Reactivity and Interactions of Hsp90 for the Development of Novel Anticancer Molecules*
Funding Body: Italian Cancer Research Association (*Associazione Italiana per la Ricerca sul Cancro*)
Funding: € 27 190 / yr.
Main Tasks: (1) *In silico* identification of allosteric binding sites on known disease targets (including members of the Hsp90 chaperone family, the oncogene Folliculin, the oncotarget K-Ras, and a DNA G-quadruplex sequestered by naphthalene diimide as a click-chemistry template). Subsequent virtual design of allosteric modulators. (2) Computational modelling of the effects of allosteric ligand and client protein binding to such sites. Aspects analysed include variations: in reactivity / catalytic activity; at orthosteric interface(s); within active site(s); and in conformational equilibria. (3) Identification of potential epitopes on key SARS-CoV-2 proteins through detection of regions with weaker energetic coupling.

Description of work and techniques: All-atom classical MD simulations of the (glyco)proteins under study (independent replicas in *AMBER* or *Desmond*), followed by trajectory analysis to identify key properties, such as the frequency of reactive poses (for further QM/MM calculations on reactivity), the degree of cross-talk between residues at potential allo- and orthosteric sites/interfaces, and how this is altered by (existing) allosteric ligands. MD simulations of oligopeptides derived from targets' endogenous protein substrates and application of stochastic methods to pinpoint potentially active substates on which to base the design of druglike allosteric modulators. Guidance of (pre)doctoral students in using *Schrödinger*'s *Maestro* suite to virtually design such modulators acting at the identified 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 with respect to simulated oligopeptides. Additional calculations with *WaterSwap*, as well as bioinformatics methods (coevolution analysis) to verify allosteric sites' isoform-specificity, and analysis of residues' individual energetic contribution (calculated with MM/GBSA) again to identify possible immunogenic or client-binding regions. Collaborators include Prof. Mehdi Mollapour (State University of New York, USA), Prof. Andrea Rasola (Univesity of Padua, Italy), Dr. Francesco Frigerio (ENI corporation, Italy)

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.; 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
(20) 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
(21) Casali, E.; Serapian, S.A.; Gianquinto, E.; Castelli, M.; Bertinaria, M.; Spyrakis, F.; Colombo, G., *Int. J. Biol. Macromol.* **2023**, *246*, 125609
(22) 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
(23) 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
(24) 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.
(25) Frasnetti, E.; Magni, A.; Castelli, M.; Serapian, S. A.; Moroni, E.; Colombo, G., *Curr. Opin. Struct. Biol.* **2024**, 87, 102835

Skills: Consolidation of the methods learnt in Bristol, further MD and trajectory analysis (*AMBER*, *Desmond,* in-house tools), Familiarisation with *GLYCAM* forcefields, Bioinformatics, Docking, General experience with *Schrödinger* software packages, Didactic skills (further supervision of 2 Ph.D. students and co-supervision of a student's final year Master's project), Organisation (in charge of several projects as the only post-doc in the laboratory until 2021), Expansion of *Python* coding skills, particularly with relevant biosimulation libraries, Familiarisation with stochastic methods (Markov State Models and time-lagged independent component analysis)

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

techniques:

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.
Main Task: 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
Main task: 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)**
Main task: 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