

## Short CV of Giorgio Colombo

Giorgio Colombo (born 24<sup>th</sup> June 1971) received his M.Sc. Degree in chemistry in the academic year 1994/1995 from the University of Milano. After that, he continued his studies obtaining a Ph.D. in chemical sciences from the University of Milano in 2000. He spent one year (1998) as a visiting scientist in the laboratory of Prof. Ken Merz at the Pennsylvania State University, working on computational and theoretical approaches to study enzymatic and protein properties. He then moved to the University of Groningen (1999-2001) as a postdoctoral fellow to work on the molecular dynamics simulations of the folding and stability of proteins and peptides.

Dr. Giorgio Colombo joined the Institute for Molecular Recognition Chemistry, Italian National Research Council, in 2001 where he founded the biocomputing group. Since December 2017, he is Full Professor of Organic Chemistry at the University of Pavia. His interests focus on the development of computational approaches to study the relationships among protein structure, dynamics and function and to translate this knowledge in new methods to design biologically active chemical tools. He is the author or coauthor of more than 200 scientific publications with an H-index of 55 (Google Scholar, 2023)

### Honors

1999-2000 TMR Fellowship from the European Community  
2000-2001 Marie Curie Fellowship from the European Community  
2004 Young Investigator Award, Division of Biological Systems of the Italian Chemical Society  
2008 Career Development Research Award from the Presidency of the Lombardy Region  
2011 **PERSONAL AWARD FROM THE CARIPLO-UNESCO CALL** "*Exploration of new research frontiers – Award 2011*". Title of the project: Chemical control of signalling pathways by modulation of hub proteins (**Checosp**), **230 K€**. Special call for funding dedicated to International year of Chemistry 2011. The selection committee was composed by: - **Aaron Ciechanover**, Technion- Israel Institute of Technology, Nobel Laureate for Chemistry 2004; - **Gerhard Ertl**, Fritz-Haber Institut Max-Planck, Nobel Laureate for Chemistry 2007 - **Oliver Guthmann**, Investment Manager of BASF Venture - **Krzysztof Matyjaszewski**, Carnegie Mellon University, Wolf Prize for Chemistry 2011- **Phillip Szuromi**, Supervisor Senior Editor of Science Magazine.

### Main Grants

#### Main Ongoing Research Support

**G. Colombo** 2023-2027 Amount of Grant: 600000€  
Italian Association for Cancer Research (AIRC)  
*Integrative approaches to target Hsp90 networks in cancer*  
Role: Principal Investigator

**G. Colombo** 2022-2025 Total Amount of Grant: 662400€, for the Colombo  
Lab: 247458€  
Italian Ministry of Research  
*TRAPping tumor growth: designing molecules to perturb the chaperone TRAP1, from enzymatic activities to cell-cell interaction.*  
Role: Principal Investigator, Coordinator

**G. Colombo** 2021-2023 Total Amount of Grant: 112500K€  
European Commission – Human Brain Project P1-EBRAINS  
*BRAVE - Protecting the brain from COVID-19-mediated neurodegeneration through inflammasome inhibition*  
Role: Co-Principal Investigator

#### Main Completed Research Support

**G. Colombo** 2015-2018 Amount of Grant: 296K€  
Italian Association for Cancer Research (AIRC)  
*Discovery of selective modulators of the functional dynamics of Hsp90 family members as novel anticancer compounds*  
Role: Principal Investigator

**G. Colombo** 2012-2015 Amount of Grant: 230 K€  
**PERSONAL AWARD FROM THE CARIPLO-UNESCO CALL** "*Exploration of new research frontiers – Award 2011*". Title of the project: *Chemical control of signalling pathways by modulation of hub proteins*  
Role: Principal Investigator

## Selected indexed publications:

- 1) Castelli, M.; Marchetti, F.; Osuna, S.; Oliveira, 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), 901–919
- 2) Castelli, M.; Yan, P.; Rodina, A.; Digwal, C.S.; Panchal, P.; Chiosis, G.; Moroni, E.; Colombo, G. How aberrant N-glycosylation can alter protein functionality and ligand binding: An atomistic view. *Structure* **2023**, 31(8), 987-1004
- 3) Gonzalez-Teran, B.;... **Colombo, G.**; Conklin, B.R.; Black, B.L.; Bruneau, B.G.; Krogan, N.J.; Pollard, K.S.; Srivastava, D. Transcription factor protein interactomes reveal genetic determinants in heart disease. *Cell* **2022**, S0092-8674(22)00079-4
- 4) 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. *Journal of Chemical Information and Modeling* **2021**, 61 (9), 4687-4700
- 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 Catalysis* **2021**, 11 (14), 8605-8620
- 6) Sanchez-Martin, C.; Moroni, E.; Ferraro, M.; Laquatra, C.; Cannino, G.; Masgras, I.; Negro, A.; Quadrelli, P.; Rasola, A.; **Colombo, G.**, Rational Design of Allosteric and Selective Inhibitors of the Molecular Chaperone TRAP1. *Cell Reports* **2020**, 31 (3), 107531
- 7) 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. *The Journal of Physical Chemistry Letters* **2020**, 8084-8093
- 8) 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.; **Colombo, G.** Chemical Perturbation of Oncogenic Protein Folding: from the Prediction of Locally Unstable Structures to the Design of Disruptors of Hsp90–Client Interactions. *Chemistry – A European Journal* **2020**, 26 (43), 9459-9465
- 9) Taylor, I.R.; Assimon, V.A.; Rinaldi, S.; Kuo, S.Y.; Li, X.; Young, Z.T.; Morra, G.; Green, K.; Nguyen, D.; Shao, H.; Garneau-Tsodikova, S.; **Colombo, G.\***; Gestwicki, J.E. Tryptophan Scanning Mutagenesis as a Way to Mimic the Compound-Bound State and Validate the Selectivity of Allosteric Inhibitors in Cells. *Chemical Science*, **2020**, 11, 1892-1904
- 10) Moroni, E.; Agard, D.A.; **Colombo, G.** The structural asymmetry of mitochondrial Hsp90 (Trap1) determines fine tuning of functional dynamics. *J. Chem. Theor. Comput.* **2018**, 14(2), 1033-1044.
- 11) Gourlay, L.; Peri, C.; Bolognesi, M.; **Colombo, G.** Structure and Computation in Immunoreagent Design: From Diagnostics to Vaccines. *Trends Biotechnol.* **2017** pii: S0167-7799(17)30167-1. doi: 10.1016/j.tibtech.2017.06.018
- 12) Gourlay, L.J.; Peri, C.; Ferrer-Navarro, M.; Conchillo-Solé, O.; Gori, A.; Rinchai, D.; Thomas, R.J.; Champion, O.L.; Mitchell, S.L.; Kewcharoenwong, C.; Nithichanon, A.; Lassaux, P.; Perletti, L.; Longhi, R.; Lertmemongkolchai, G.; Titball, R.W.; Daura, X.; **Colombo, G.\***; Bolognesi, M. Exploiting the *Burkholderia pseudomallei* Acute Phase Antigen BPSL2765 for Structure-Based Epitope Discovery/Design in Structural Vaccinology. *Chem Biol* **2013**, 20(9), 1147-1156