

Beatrice Vallone – Curriculum Vitae

Address	Dip. Di Scienze Biochimiche, Università di Roma “La Sapienza”. P.le A. Moro, 5 00185 - Roma Italy
Telephone(s)	[REDACTED] [REDACTED] [REDACTED]
	[REDACTED] [REDACTED]
Nationality	[REDACTED]
Gender	[REDACTED]
Work experience	
Dates	<p>03/2017-05/2017 Visiting Professor at Columbia University (New York USA)</p> <p>01/2016-06/2016 Alexander Bodini Research Fellow at the Italian Academy for Advanced Studies in America – Columbia University (USA)</p> <p>07/2014 - 06/2015 Research Scholar at Columbia University (New York USA)</p> <p>2009-present Full Professor - Sapienza University of Rome</p> <p>2000-2007 Associate Professor - Sapienza University of Rome</p> <p>1991-1999: Staff Scientist - Sapienza University of Rome</p>
Teaching Experience	<p>2000-Present Course of Chemistry and Biochemistry for the Degree in Medicine and Surgery at Sapienza (taught in Italian)</p> <p>2010-Present Course of Chemistry and Introduction to Biochemistry for the International Medical School of Sapienza University (taught in English)</p> <p>2020- Present Course of Biochemistry for the Course in Applied Pharmacological Sciences at Sapienza (taught in Italian)</p>
Occupation or position held	<p>Full Professor, BIO10 (Italian Ministry Discipline Group: Biochemistry and Biophysics).</p> <p>Appointed to teach Courses on Biochemistry, Molecular Biology, Chemistry for Medical Sciences, Biophysics, Protein Engineering</p>
Main activities and responsibilities	<p>-Director of the H2CU Interuniversity Center for International Training</p> <p>-Head of the Sapienza Structural Biology Group</p> <p>-Teaching chair of Biochemistry, Sapienza Faculty of Pharmacy and Medicine and Sapienza International Medical School</p> <p>-Member of the Advisory Committee for the CNR Cryo-EM Facility, 2018</p> <p>-Member of the PSI-FELLOW program II 3i Advisory Board</p> <p>-Member of the Biological Macromolecules Commission of the International Union of Crystallography 2017-present</p> <p>-Chair of the committee “Biological Macromolecules” for the Italian Elettra Synchrotron 2017-Present</p> <p>-Member of the Executive Committee of the Italian Society for Synchrotron Light (SILS) 2013-2017</p> <p>-Head of the CNR Biocrystal Facility (www.biocrystalfacility.it) 2012-2016</p> <p>-Teaching panel of the Doctorate School in Biochemistry, 2013-present</p> <p>-Teaching panel of the Doctorate School in Biophysics, 2007-2013</p> <p>-Member of the ESRF User Organization Committee 2010-2014</p> <p>-Member of the “Accademia Medica Romana” 2010-present</p> <p>-Editorial Board “AIMS Biophysics” 2017-present</p> <p>-Review Editor Frontiers in Molecular Biosciences – Structural Biology 2014-present</p>
Name and address of employer	Università di Roma “La Sapienza”, P.le A. Moro, 5. 00185, Rome, Italy.
Sector	Academic, research.
Education and training	
Title of qualification awarded	<p>PhD in Biochemistry, 1991</p> <p>Degree in Biology, 1987</p>
Name and type of organisation providing education and training	University of Rome “La Sapienza”, Academic

Honors:

Schaefer Research Scholar at Columbia Medical Center (2014).

"Alexander Bodini" Research Fellow at the Italian Academy for Advanced Studies at Columbia (2016)

Short Fellowships.

1988 Geneva University (CH) sponsored by EMBO- Dept. of Biochemistry (Prof.S.J. Edelstein)

1990 LMB-MRC, Cambridge (UK) sponsored by EMBO (Dr. K. Nagai)

1991 LMB-MRC, Cambridge (UK) sponsored by FEBS (Dr. G. Fermi).

1997 York University, Dept. of Biochemistry (UK) sponsored by FEBS (Prof. J. Tame)

2004 Cambridge University, Dept. of Biochemistry, (UK) sponsored by EMBO (Prof. B. Luisi)

Appointments

Coordinates the Structural Biology group of the Department of Biochemical Sciences "A. Rossi Fanelli" (Sapienza-DSB), (PO Biochemistry, BIO / 10). Author of around 90 scientific publications in the field of biochemistry and structural biology, she worked at the Molecular Biology Laboratory of the Medical Research Council (LMB-MRC, Cambridge, UK), the University of York (UK), Cambridge (UK), the University of Geneva (CH) and Columbia University (NY, USA) where he received the prestigious Schaefer Scholarship in 2014.

Member of the "Macromolecules" commission of the International Union of Crystallography and was elected member of the European Organization for Molecular Biology (EMBO) in 2020. She coordinated two European projects (ITN-MSCA and RISE-MSCA) focused on structural biology, leading two consortia of 10 international partners including universities, research institutions, large pharmaceutical industries (AstraZeneca) and SMEs.

Since 1 November he has been Director of the H2CU "Honors Center of Italian Universities" Interuniversity Center for International Training, which brings together 21 Italian Universities and 3 CNR institutes for the development of joint academic and research programs abroad.

Research.

Main research fields: structural biology, biochemistry and protein engineering.

H-Index 32. Citations 3549 Papers 101 (source Scopus)

The mechanism of action of proteins was investigated by using protein crystallography and biochemical characterization. This included the structure-function relationship of enzymes and transporters as well as their role within signalling networks that involves protein-protein recognition and complex formation.

The knowledge of the molecular mechanism exploited by proteins to carry out their function and involved in pathological processes is the starting point to design novel, targeted therapeutic strategies. In this contest, the main endeavour has been the determination of protein structures by protein crystallography and, more recently by single particle cryo-electron microscopy. Protein biochemical and biophysical characterization was carried out using a wide array of methods (kinetics, protein engineering, spectroscopy).

The most relevant results have been:

1. The study by single particle cryo-electron microscopy of engineered ferritins and of the complex between human ferritin and the CD71 receptor.
2. Structural and functional analysis of enzymes involved in antibiotic biosynthesis, that led to the determination of the structure of a new type of monooxygenase involved in the biosynthesis of aromatic polyketids and of P450 cytochromes involved in the biosynthesis of macrolide antibiotics, erythromycin and oleandomycin.
3. The determination of the structure of murine neuroglobin in different ligation states where a novel mechanism for ligand affinity regulation (heme sliding) was described and the characterization of its reactivity towards nitric oxide.
4. The study by time-resolved crystallography/wide angle X-ray scattering and molecular dynamics of myoglobin, hemoglobin and neuroglobin structural dynamics, that contributed to the description by direct detection of the pathway of ligands within the protein matrix and to the unveiling of a complex sub-nanosecond structural dynamics triggered by ligand dissociation.

Ongoing projects: integrative structural biology, biochemical characterization and engineering of i) ferritins as theranostics nanoparticles ii) Steroid 5- α dihydrogenases as oncotargets and pivotal membrane enzymes in neurosteroid biosynthesis iii) interaction between the oncosuppressor HIPK2 kinase and its target, p53.

Ongoing research is focussed on the structure-function relationship of proteins involved in human pathologies, also for theranostics designs:

1. SARS-COV-2 antibodies for diagnostics and therapy in collaboration with Takis Biotech with the support of grants from Regione Lazio .
2. Antibody-based therapeutics and diagnostics in collaboration with Takis Biotech.
3. Complex of plasma proteins with their receptors (haptoglobin, ferritin and LDL-receptor related protein)
4. Steroid 5- α dehydrogenase membrane enzymes
5. Alsln ALS-2 GEF in collaboration with the Politecnico of Turin, with the support of a Telethon Grant

Grants

- Regione Lazio Bando “Coronavirus ed oltre” Project Generas (GENERazione di proteine Ricombinanti e Anticorpi e per lo studio di mutanti del virus SARS-CoV-2) in collaboration with Takis Biotech.

- Regione Lazio Bandi Dottorato Industriale progetto “Anticorpi anti ErbB3 studi strutturali e funzionali mirati al disegno di farmaci oncologici”.

- In collaborazione con CNR-IBPM e Takis Biotech Dottorato Industriale Confindustria progetto “Anticorpi per diagnosi e terapia di varianti del SARS-Cov2”

-EU H2020 (2018-23) Marie Skłodowska-Curie Research And Innovation Staff Exchange (RISE) “ProMeTeus - Membrane protein integrated technologies development for drug design” **(Coordinator)**.

-EU H2020 (2014-18) Innovative Training Network “X-Probe” on frontier methods in protein structural dynamics **(Coordinator)**.

-Fondazione Cenci-Bolognietti/Pasteur Institute Grant (2013-16) “Bacterial P450 Cytochromes as tools for designing novel antimicrobial agents” **(PI)**

-University of Rome “La Sapienza” (2012) “Espansione multidisciplinare della biologia strutturale verso una dimensione di facility: sistema di imaging per screening di cristallizzazione di proteine.” **(PI)**

-CNR, Life Sciences Dept. “Biocrystal Facility of the CNR” (2012-15) **(Coordinator)**.

-VII Framework Program (2008)– EU – “CryoEm structure of gamma secretase: a key component in Alzheimer neurodegenerative disease”- Scientist in Charge.

As Unit Member:

EuroBlood - European Framework Program VI in Blood Substitutes

PRIN 2007 Proteine redox in azione: dinamica strutturale, meccanismi e fisiopatologia

FIRB 2003 Biologia Strutturale PostGenomica, sviluppo di infrastrutture per la cristallografia di proteine.

Reviewer Activity.

MSCA Actions

European research Council

Swiss Excellence Program

French CNRS

Italian Ministry of Education and Research (MIUR) Young Researchers Excellence Program

Deutsche Forschungsgemeinschaft Excellence Projects

French Fondation pour la Recherche Medicale - Structural Biology Infrastructures

Selected publications

1. Montemiglio LC, Testi C, Ceci P, Falvo E, Martina M, Savino C, Arcovito A, Peruzzi G, Baiocco P, Mancina F, Boffi A, des Georges A, Vallone B. Cryo-EM structure of the human Ferritin-Transferrin Receptor 1 complex. Nat Commun. 2019 Mar 8;10(1):1121.
2. Exertier, C., Milazzo, L., Freda, I., Montemiglio, L.C., Scaglione, A., Cerutti, G., Parisi, G., Anselmi, M., Smulevich, G., Savino, C., Vallone, B. Proximal and distal control for ligand binding in neuroglobin: role of the CD loop and evidence for His64 gating (2019) Scientific Reports, 9 (1), art. no. 5326.
3. Scaglione A, Monteonofrio L, Parisi G, Cecchetti C, Siepi F, Rinaldo C, Giorgi, A, Verzili D, Zamparelli C, Savino C, Soddu S, Vallone B, Montemiglio LC. Effects of Y361-auto-phosphorylation on structural plasticity of the HIPK2 kinase domain. Protein Sci. (2018) Vol 27 pp725-737.
4. Scaglione A, Celeste Montemiglio L, Parisi G, Asteriti IA, Bruni R, Cerutti G, Testi C, Savino C, Mancina F, Lavia P and Vallone B. Biochimie Open (2017) Subcellular localization of the five members of the human steroid 5 α -reductase family. Vol. 4 pp. 99-106.

5. de Turris V, Cardoso Trabuco M, Peruzzi G, Boffi A, Testi C, Vallone B, Celeste Montemiglio L, Georges AD, Calisti L, Benni I, Bonamore A, Baiocco P. *Nanoscale*. (2017) Humanized archaeal ferritin as a tool for cell targeted delivery. Vol. 9 pp.647-655.
6. Savino C, Montemiglio LC, Sciara G, Miele AE, Kendrew SG, Jemth P, Gianni S, Vallone B. (2009). Investigating the structural plasticity of a cytochrome P450: three-dimensional structures of P450 EryK and binding to its physiological substrate. *J. Biol. Chem.*, Vol. 284; p. 29170-9-29179.
7. Renzi F, Caffarelli E, Laneve P, Bozzoni I, Brunori M, Vallone B. (2006). The structure of the endoribonuclease XendoU: From small nucleolar RNA processing to severe acute respiratory syndrome coronavirus replication. *Prof. Natl. Acad. Sci. USA*, vol. 103; p. 12365-12370.
8. Brunori M, Giuffrè A, Nienhaus K, Nienhaus GU, Scandurra FM, Vallone B. (2005). Neuroglobin, nitric oxide, and oxygen: functional pathways and conformational changes. *Prof. Natl. Acad. Sci. USA*, Vol. 102; p. 8483-8488.
9. Vallone B., Nienhaus K, Matthes A, Brunori M, Nienhaus GU. (2004). The structure of carbonmonoxy neuroglobin reveals a heme-sliding mechanism for control of ligand affinity. *Prof. Natl. Acad. Sci. USA*, Vol. 101; p. 17351-17356.
10. Bourgeois D, Vallone B., SchotteF, Arcovito A, Miele AE, Sciara G, Wulff M, Anfinrud P, Brunori M. (2003). Complex landscape of protein structural dynamics unveiled by nanosecond Laue crystallography. *Prof. Natl. Acad. Sci. USA*, Vol. 100; p. 8615-8617.

Recent Invited Talks

- Conference of the Italian Society of Biochemistry, Lecce Sept 2019 “Key interactions for iron uptake are exploited by infectious agents as revealed by the cryo-EM structure of the Ferritin-CD71 complex”
- ICCP450 (International Conference on P450) Brisbane (Australia) June 2019 Structural Plasticity in Macrolide Biosynthetic P450s
- International Colloquium on Protein and Biointerface Engineering ,Catania, Italy, Sept. 2017
“Single Particle Cryo-EM structure of the complex between human Ferritin and Transferrin Receptor: a gateway for targeted delivery and theranostics”.
- International Conference on Nanoinnovation Rome, Italy, July 2018 – Keynote Session.
“Single Particle Cryo-EM structure of the complex between human Ferritin and Transferrin Receptor: a gateway for targeted delivery and theranostics”.
- International Conference on “High-Resolution Protein Structures: Understanding Human Diseases”, Ben Gurion University, March 2018 Israel “Ferritin exploits virus-like site on transferrin receptor for cell binding and entry”.
- XXI School of Pure and Applied Biophysics on “Time Resolved Methods in Biophysics” Venice, Italy January 2017 “Time-resolved studies of protein structures”
- 1st COMPPA Meeting, New York Structural Biology Center, USA, May 2017 “Srd5 α Reductases”
- 50th Anniversary of the Italian Crystallographic Association Rome, Italy, Jan. 2017 “Molecular Beauty: Crystallography and Life Sciences”.
- APRE Meeting on 20 years of MSCA Actions, Rome, Italy, Jan. 2017 “Impact of the MSCA-ITN X-Probe Project on PhD training and educational programs”.
- Biochemical Colloquium, Hamburg University, Germany, Oct. 2016 “Time Resolved Methods in Biophysics: the biochemists’s point of view”.
- Structural Biology for the Next Millennium Meeting, Rome, Italy, Sept. 2016 “Past and Perspectives of time-resolved structural studies”.
- 1st NYMaSBiC International Meeting, Ancona, Italy, Feb. 2015 “Protein Crystallization and Structural Analysis”
- Fondazione Cenci Bolognetti – Pasteur Institute “Aperitivo Scientifico”, Rome, Italy, May 2014 “Grandi macchine e piccole molecole: i sincrotroni e le scienze della vita”
- Biophysics PhD School Seminar, Palermo, Italy, Dec. 2013 “Investigating the Structural Plasticity of a Cytochrome P450: Three Dimensional Structures of Eryk and Binding Kinetics”
- XX Italian Society for Synchrotron Meeting, Arcavacata, Italy, July 2012 “Studies on myoglobin, neuroglobin and hemoglobin by combined synchrotron methods”
- Accademia Nazionale dei Lincei, Centennial of X-ray Diffraction Symposium, Rome, Italy, May 2012 “Time-resolved crystallography for Protein Structures: devices and desires”.
- ESRF User Meeting, Grenoble, France, March 2011 “Structural dynamics of neuroglobin, from ligand binding to signalling”
- International Meeting on Allostery, Bari, Italy, 2010 “Structural dynamics of neuroglobin, from ligand binding to signalling”

- European Conference on the Spectroscopy of Biological Molecules, Palermo, Italy 2009 "Will biophysical studies on Neuroglobin provide clues for novel therapies of neuronal death and degeneration?"
- XVth International Conference on Oxygen Binding and Sensing Proteins, Aug. 2008 Aarhus, Denmark "Neuroglobin: clues to mechanism from structure and kinetics"
- BCA 2005 Loughborough
- ECM22 2004
- June 2006 Leiden Blood Substitutes
- Parma 2006 Blood Substitutes
- Naples 2006 International Conference on Oxygen Binding and Sensing Proteins,
- Pozzuoli 2010
- Sparx-FEL 2011 Tor Vergata

Beatrice Vallone - Full list of publications

- 1) Exertier C, Sebastiani F, Freda I, Gugole E, Cerutti G, Parisi G, Montemiglio LC, Becucci M, Viappiani C, Bruno S, Savino C, Zamparelli C, Anselmi M, Abbruzzetti S, Smulevich G, Vallone B. Probing the Role of Murine Neuroglobin CDloop-D-Helix Unit in CO Ligand Binding and Structural Dynamics. *ACS Chem Biol*. 2022 17(8):2099-2108.
- 2) Exertier C, Montemiglio LC, Freda I, Gugole E, Parisi G, Savino C, Vallone B. Neuroglobin, clues to function and mechanism. *Mol Aspects Med*. 2022 84:101055.
- 3) Miceli M, Exertier C, Cavaglià M, Gugole E, Boccardo M, Casaluci RR, Ceccarelli N, De Maio A, Vallone B, Deriu MA. ALS2-Related Motor Neuron Diseases: From Symptoms to Molecules. *Biology (Basel)*. 2022 11(1):77.
- 4) Montemiglio LC, Gugole E, Freda I, Exertier C, D'Auria L, Chen CG, Nardi AN, Cerutti G, Parisi G, D'Abramo M, Savino C, Vallone B. Point Mutations at a Key Site Alter the Cytochrome P450 OleP Structural Dynamics *Biomolecules*. 2021 Dec 31;12(1):55.
- 5) The Nuts and Bolts of SARS-CoV-2 Spike Receptor-Binding Domain Heterologous Expression Maffei M, Montemiglio LC, Vitagliano G, Fedele L, Sellathurai S, Bucci F, Compagnone M, Chiarini V, Exertier C, Muzi A, Roscilli G, Vallone B, Marra E. *Biomolecules*. 2021 11(12):1812. doi: 10.3390/biom11121812.
- 6) Exertier C, Montemiglio LC, Freda I, Gugole E, Parisi G, Savino C, Vallone B. Neuroglobin, clues to function and mechanism *Mol Aspects Med*. 2022 Apr;84:101055.
- 7) Cerutti G, Gugole E, Montemiglio LC, Turbé-Doan A, Chena D, Navarro D, Lomascolo A, Piumi F, Exertier C, Freda I, Vallone B, Record E, Savino C, Sciara G. Crystal structure and functional characterization of an oligosaccharide dehydrogenase from *Pycnoporus cinnabarinus* provides insights into fungal breakdown of lignocellulose *Biotechnol Biofuels*. 2021 Jul 22;14(1):161. doi: 10.1186/s13068-021-02003-y.
- 8) Parisi G, Freda I, Exertier C, Cecchetti C, Gugole E, Cerutti G, D'Auria L, Macone A, Vallone B, Savino C, Montemiglio LC. Dissecting the Cytochrome P450 OleP Substrate Specificity: Evidence for a Preferential Substrate *Biomolecules*. 2020 Oct 6;10(10):1411. doi: 10.3390/biom10101411.
- 9) Milazzo L, Exertier C, Becucci M, Freda I, Montemiglio LC, Savino C, Vallone B, Smulevich G. Lack of orientation selectivity of the heme insertion in murine neuroglobin revealed by resonance Raman spectroscopy *FEBS J*. 2020 Feb 8. doi: 10.1111/febs.15241. Online ahead of print.
- 10) Parisi G, Montemiglio LC, Giuffrè A, Macone A, Scaglione A, Cerutti G, Exertier C, Savino C, Vallone B. Substrate-induced conformational change in cytochrome P450 OleP. *FASEB J*. 2019 Feb;33(2):1787-1800. doi: 10.1096/fj.201800450RR.
- 11) Ardicioni C, Arcovito A, Della Longa S, van der Linden P, Bourgeois D, Weik M, Montemiglio LC, Savino C, Avella G, Exertier C, Carpentier P, Prangé T, Brunori M, Colloc'h N, Vallone B. Ligand pathways in neuroglobin revealed by low-temperature photodissociation and docking experiments *IUCrJ*. 2019 Jul 10;6(Pt 5):832-842
- 12) Exertier, C., Milazzo, L., Freda, I., Montemiglio, L.C., Scaglione, A., Cerutti, G., Parisi, G., Anselmi, M., Smulevich, G., Savino, C., Vallone, B. Proximal and distal control for ligand binding in neuroglobin: role of the CD loop and evidence for His64 gating (2019) *Scientific Reports*, 9 (1), art. no. 5326.
- 13) Montemiglio LC, Testi C, Ceci P, Falvo E, Martina M, Savino C, Arcovito A, Peruzzi G, Baiocco P, Mancina F, Boffi A, des Georges A, Vallone B. Cryo-EM structure of the human Ferritin-Transferrin Receptor 1 complex. *Nat Commun*. 2019 Mar 8;10(1):1121. doi: 10.1038/s41467-019-09098-w.
- 14) Parisi G, Montemiglio LC, Giuffrè A, Macone A, Scaglione A, Cerutti G, Exertier C, Savino C, Vallone B. Substrate-induced conformational change in cytochrome P450 OleP. *FASEB J*. 2018 Sep 12:fj201800450RR. doi:10.1096/fj.201800450RR. [Epub ahead of print].
- 15) Scaglione A, Monteonofrio L, Parisi G, Cecchetti C, Siepi F, Rinaldo C, Giorgi, A, Verzili D, Zamparelli C, Savino C, Soddu S, Vallone B, Montemiglio LC. Effects of Y361-auto-phosphorylation on structural plasticity of the HIPK2 kinase domain. *Protein Sci*. 2018 Vol 27 pp725-737.
- 16) Scaglione,A., Fullone,M.R., Montemiglio,L.C., Parisi,G., Zamparelli,C., Vallone,B., Savino,C. and Grgurina, I. "Structure of the adenylation domain Thr1 involved in the biosynthesis of 4-chlorothreonine in *Streptomyces* sp. OH-5093: protein flexibility and molecular bases of substrate specificity" *FEBS Journal* (2017) Vol. 284, pp. 2981-2999.
- 17) Colloc'h N, Sacquin-Mora S, Avella G, Dhaussy AC, Prangé T, Vallone B, Girard E. Determinants of neuroglobin plasticity highlighted by joint coarse-grained simulations and high pressure crystallography. *Sci Rep*. (2017) Vol. 7 pp. 1858.

- 18) Scaglione A, Celeste Montemiglio L, Parisi G, Asteriti IA, Bruni R, Cerutti G, Testi C, Savino C, Mancina F, Lavia P and Vallone B. *Biochimie Open* (2017) Subcellular localization of the five members of the human steroid 5 α -reductase family. Vol. 4 pp. 99-106.
- 19) de Turreis V, Cardoso Trabuco M, Peruzzi G, Boffi A, Testi C, Vallone B, Celeste Montemiglio L, Georges AD, Calisti L, Benni I, Bonamore A, Baiocco P. *Nanoscale*. (2017) Humanized archaeal ferritin as a tool for cell targeted delivery. Vol. 9 pp.647-655.
- 20) Montemiglio LC, Parisi G, Scaglione A, Sciara G, Savino C, Vallone B (2016) Functional analysis and crystallographic structure of clotrimazole bound OleP, a cytochrome P450 epoxidase from *Streptomyces antibioticus* involved in oleandomycin biosynthesis. *Biochim Biophys Acta*. Vol. 1860 pp.465-75.
- 21) Abraini JH, Marassio G, David HN, Vallone B, Prangé T, Colloc'h N (2014) Crystallographic studies with xenon and nitrous oxide provide evidence for protein-dependent processes in the mechanisms of general anesthesia. *Anesthesiology*. Vol. 121 pp.1018-27
- 22) Avella G, Ardiccioni C, Scaglione A, Moschetti T, Rondinelli C, Montemiglio LC, Savino C, Giuffrè A, Brunori M, Vallone B. Engineering the internal cavity of neuroglobin demonstrates the role of the haem-sliding mechanism. (2014) *Acta Crystallogr D Biol Crystallogr*. Vol. 70 pp 1640-8.
- 23) Yang Y, Allemand F, Guca E, Vallone B, Delbecq S, Roumestand C. 1H, 15N and 13C Backbone resonance assignments of murine met-neuroglobin, free and in complex with cyanide. (2014) May 16. [Epub ahead of print].
- 24) Guca E, Roumestand C, Vallone B, Royer CA, Dellarole M. Low-cost equilibrium unfolding of heme proteins using 2 μ l samples. (2013) *Anal Biochem*. Vol 443 pp.13-5.
- 25) Montemiglio LC, Macone A, Ardiccioni C, Avella G, Vallone B, Savino C. Redirecting P450 EryK Specificity by Rational Site-Directed Mutagenesis. *Biochemistry*. (2013) Vol 52, pp 3678–3687
- 26) van der Linden P, Vitoux H, Steinmann R, Vallone B, Ardiccioni C. (2013) An open flow helium cryostat for synchrotron X-ray diffraction experiments. *Journal of Physics: Conference Series*, Vol. 425, p. 12015-12018.
- 27) Vallone B. (2013) Time-resolved crystallography for protein structure: the case of heme proteins. *Rend. Lincei* Vol. 24; p. 101-107.
- 28) Levantino M, Spilotros A, Cammarata M, Schiro G, Ardiccioni C, Vallone B, Brunori M, Cupane A. (2012) The Monod-Wyman-Changeux allosteric model accounts for the quaternary transition dynamics in wild type and a recombinant mutant human hemoglobin. *Proc Natl Acad Sci U S A* Vol. 109; p. 14894-14899.
- 29) Palladino P, Scaglione GL, Arcovito A, Maria Vitale R, Amodeo P, Vallone B, Brunori M, Benedetti E, Rossi F. (2011) Neuroglobin-prion protein interaction: what's the function? *J. Pept Sci.* 10.1002/psc.1333.
- 30) Montemiglio LC, Gianni S, Vallone B., Savino. Azole Drugs Trap Cytochrome P450 EryK in Alternative Conformational States. (2010) *Biochemistry*, Vol. 49; p.9199-206.
- 31) Arcovito A, Ardiccioni C, Cianci M, D'Angelo P, Vallone B., Della Longa S (2010). Polarized X-ray absorption near-edge structure spectroscopy of neuroglobin and myoglobin single crystals. *J. Phys. Chem. B*, vol. 114; p. 36415-36423.
- 32) Moschetti T, Giuffrè A, Ardiccioni C, Vallone B., Modjtahedi N, Kroemer G, Brunori M (2009). Failure of apoptosis-inducing factor to act as neuroglobin reductase. *Biochem. Biophys. Res. Commun.*, vol. 390; p. 121-124.
- 33) Moschetti T, Mueller U, Schultze J, Brunori M, Vallone B. (2009). The structure of neuroglobin at high Xe and Kr pressure reveals partial conservation of globin internal cavities. *Biophys. J.*, vol. 97; p. 1700-1708.
- 34) Pedotti M, Rosini E, Molla G, Moschetti T, Savino C, Vallone B., Pollegioni L (2009). Glyphosate resistance by engineering the flavoenzyme glycine oxidase. *J. Biol. Chem.*, vol. 284; p. 15-23.
- 35) Savino C, Miele A.E, Draghi F, Johnson K.A, Sciara G, Brunori M, Vallone B. (2009). Pattern of cavities in globins: The case of human hemoglobin. *Biopolymers*, vol. 91; p. 1097-1107.
- 36) Savino C, Montemiglio LC, Sciara G, Miele AE, Kendrew SG, Jemth P, Gianni S, Vallone B. (2009). Investigating the structural plasticity of a cytochrome P450: three-dimensional structures of P450 EryK and binding to its physiological substrate. *J. Biol. Chem.*, vol. 284; p. 29170-9-29179.
- 37) Anselmi M, Brunori M, Vallone B., Di Nola A (2008). Molecular dynamics simulation of the neuroglobin crystal: comparison with the simulation in solution. *Biophys. J.*, vol. 95; p. 4157-4162.
- 38) Arcovito A, Moschetti T, D'Angelo P, Mancini G, Vallone B., Brunori M, Della Longa S (2008). An X-ray diffraction and X-ray absorption spectroscopy joint study of neuroglobin. *Arch. of Biochem. Biophys.*, vol. 475; p. 7-13.
- 39) Brunori M, Bourgeois D, Vallone B. (2008). Structural dynamics of myoglobin. *Methods Enzymol.*, vol. 437; p. 397-416.
- 40) Giuffrè A, Moschetti T, Vallone B., Brunori M (2008). Is neuroglobin a signal transducer?. *IUBMB Life*, vol. 60; p. 410-413.
- 41) Giuffrè A, Moschetti T, Vallone B., Brunori M (2008). Neuroglobin: enzymatic reduction and oxygen affinity. *Biochem. Biophys. Res. Commun.*, vol. 367; p. 893-898.

- 42) Savino C, Sciara G, Miele AE, Kendrew SG, Vallone B. (2008). Cloning, expression, purification, crystallization and preliminary X-ray crystallographic analysis of C-12 hydroxylase EryK from *Saccharopolyspora erythraea*. *Protein Peptide Lett.*, vol. 15; p. 1138-1141.
- 43) Anselmi M, Brunori M, Vallone B., Di Nola A (2007). Molecular dynamics simulation of deoxy and carboxy murine neuroglobin in water. *Biophys. J.*, vol. 93; p. 434-441.
- 44) Arcovito A, Benfatto M, Cianci M, Hasnain SS, Nienhaus K, Nienhaus GU, Savino C, Strange RW, Vallone B., Della Longa S (2007). X-ray structure analysis of a metalloprotein with enhanced active-site resolution using in situ x-ray absorption near edge structure spectroscopy. *Prof. Natl. Acad. Sci. USA*, vol. 104; p. 6211-6216.
- 45) Bourgeois D, Schotte F, Brunori M, Vallone B. (2007). Time-resolved methods in biophysics. 6. Time-resolved Laue crystallography as a tool to investigate photo-activated protein dynamics. *Photochem. Photobiol Sci.*, vol. 6; p. 1047-1056.
- 46) Brunori M, Vallone B. (2007). Neuroglobin, seven years after. *Cell. Mol. Life Sci.*, vol. 64; p. 1259-1268.
- 47) Bellelli A, Brunori M, Miele AE, Panetta G, Vallone B. (2006). The allosteric properties of hemoglobin: insights from natural and site directed mutants. *Curr. Prot. Peptide Sci.*, vol. 7; p. 17-45
- 48) Bourgeois D, Vallone B., Arcovito A, Sciara G, Schotte F., Anfinrud PA, Brunori M (2006). Extended subnanosecond structural dynamics of myoglobin revealed by Laue crystallography. *Prof. Natl. Acad. Sci. USA*, vol. 103; p. 4924-4929.
- 49) Nienhaus G.U, Nienhaus K, Holzle A, Ivanchenko S, Renzi F, Oswald F, Wolff M, Schmitt F, Rocker C, Vallone B., Weidenmann W, Heilker R, NAR H, Wiedenmann J (2006). Photoconvertible fluorescent protein EosFP: biophysical properties and cell biology applications. *Photochem. Photobiol. Sci.*, vol. 82; p. 351-358.
- 50) Nienhaus K, Renzi F, Vallone B., Wiedenmann J, Nienhaus G.U (2006). Chromophore-protein interactions in the anthozoan green fluorescent protein asFP499. *Biophys. J.*, vol. 91; p. 4210-4220.
- 51) Nienhaus K, Renzi F, Vallone B., Wiedenmann J, Nienhaus G.U (2006). Exploring Chromophore-Protein Interactions in Fluorescent Protein cmFP512 from *Cerianthus membranaceus*: X-ray Structure Analysis and Optical Spectroscopy. *Biochemistry*, vol. 45; p. 12942-12953.
- 52) Renzi F, Caffarelli E, Laneve P, Bozzoni I, Brunori M, Vallone B. (2006). The structure of the endoribonuclease XendoU: From small nucleolar RNA processing to severe acute respiratory syndrome coronavirus replication. *Prof. Natl. Acad. Sci. USA*, vol. 103; p. 12365-12370
- 53) Renzi F, Panetta G, Vallone B., Brunori M, Arcenci M, Bozzoni I, Laneve P, Caffarelli E (2006). Large-scale purification and crystallization of the endoribonuclease XendoU: troubleshooting with His-tagged proteins. *Acta Crystallogr Sect F Struct Biol Cryst Commun.*, vol. 62; p. 298-301
- 54) Vallone B., Brunori, M (2006). A globin for the brain. *FASEB J.*, vol. 20; p. 2192-2197.
- 55) Bossa C, Amadei A, Daidone I, Anselmi M, Vallone B., Brunori M, Di Nola A. (2005). Molecular dynamics simulation of sperm whale myoglobin: effects of mutations and trapped CO on the structure and dynamics of cavities. *Biophys. J.*, vol. 89; p. 465-474.
- 56) Brunori M, Giuffrè A, Nienhaus K, Nienhaus GU, Scandurra FM, Vallone B. (2005). Neuroglobin, nitric oxide, and oxygen: functional pathways and conformational changes. *Prof. Natl. Acad. Sci. USA*, vol. 102; p. 8483-8488.
- 57) Wiedenmann J, Vallone B., Renzi F, Nienhaus K, Ivanchenko S, Rocker C, Nienhaus GU (2005). Red fluorescent protein eqFP611 and its genetically engineered dimeric variants. *J. Biomed. Opt.*, vol. 10; p. 14003.
- 58) Bossa C, Anselmi M, Roccatano D, Amadei A, Vallone B., Brunori M, Di Nola A. (2004). Extended molecular dynamics simulation of the carbon monoxide migration in sperm whale myoglobin. *Biophys. J.*, vol. 86; p. 3855-3862.
- 59) Brunori M, Bourgeois D, Vallone B. (2004). The structural dynamics of myoglobin. *J. of Struct. Biol.*, vol. 147; p. 223-234.
- 60) Savino C, Federici L, Johnson KL, Vallone B., Nastopoulos V, Rossi M, Pisani FM, Tsernoglou D Insights into DNA replication: the crystal structure of DNA polymerase B1 from the archaeon *Sulfolobus solfataricus*. *Structure*, vol. 12; p. 2001-2008.
- 61) Vallone B., Brunori M (2004). Roles for holes: are cavities in proteins mere packing defects?. *Ital. J. Biochemistry*, vol. 53; p. 46-52.
- 62) Vallone B., Nienhaus E, Brunori M, Nienhaus GU (2004). The structure of murine neuroglobin: novel pathways for ligand migration and binding. *Proteins*, vol. 56; p. 85-92.
- 63) Vallone B., Nienhaus K, Matthes A, Brunori M, Nienhaus GU. (2004). The structure of carbonmonoxy neuroglobin reveals a heme-sliding mechanism for control of ligand affinity. *Prof. Natl. Acad. Sci. USA*, vol. 101; p. 17351-17356.

- 64) Bourgeois D, Vallone B., Schotte F, Arcovito A, Miele AE, Sciara G, Wulff M, Anfinrud P, Brunori M. (2003). Complex landscape of protein structural dynamics unveiled by nanosecond Laue crystallography. *Proc. Natl. Acad. Sci. USA*, vol. 100; p. 8615-8617.
- 65) Miele AE, Federici L, Sciara G, Draghi F, Brunori M, Vallone B. (2003). Analysis of the effect of microgravity on protein crystal quality: the case of a myoglobin triple mutant. *Acta Cryst. D, Biol. Crystallogr.*, vol. 59; p. 982-988.
- 66) Nienhaus K, Vallone B., Renzi F, Wiedenmann J, Nienhaus GU. (2003). Crystallization and preliminary X-ray diffraction analysis of the red fluorescent protein eqFP611. *Acta Cryst. D, Biol. Crystallogr.*, vol. 59; p. 1253-1255.
- 67) Sciara G., Kendrew S.G., Miele A.E., Marsh N.G, Federici L., Malatesta F., Schimperia G., Savino L., Vallone B. (2003). The structure of ActVA-Orf6, a novel type of monooxygenase involved in actinorhodin biosynthesis. *EMBO J.*, vol. 22. p. 205-215.
- 68) Draghi F, Miele AE, Travaglini-Allocatelli C, Vallone B., Brunori M, Gibson QH, Olson JS. (2002). Controlling ligand binding in myoglobin by mutagenesis. *J. Biol. Chem.*, vol. 277; p. 7509-7519.
- 69) Miele A.E., Draghi F., Arcovito A., Bellelli A., Brunori M., Travaglini-Allocatelli C., Vallone B. (2001). Control of heme reactivity by diffusion: structural basis and functional characterization in hemoglobin mutants. *Biochemistry*, vol. 40; p. 14449-14458.
- 70) Brunori M., Vallone B., Cutruzzolà F., Travaglini-Allocatelli C., Berendzen J., Chu K., Sweet R.M., Schlichting I (2000). The role of cavities in protein dynamics: crystal structure of a photolytic intermediate of a mutant myoglobin. *Proc. Natl. Acad. Sci. USA*, vol. 97; p. 2058-2063.
- 71) Kendrew S.G., Federici L., Savino C., Miele A.E., Marsh E.N.G., Vallone B. (2000). Crystallization and preliminary diffraction studies of a monooxygenase from *S. coelicolor* A3(2) involved in the biosynthesis of the polyketide actinorhodin. *Acta Cryst. D, Biol. Crystallogr.*, vol. D56; p. 481-483.
- 72) Tame J.R.H., Vallone B. (2000). The structures of deoxy human hemoglobin and the mutant Hb Tyr α 42His at 120 K. *Acta Cryst. D, Biol. Crystallogr.*, vol. D56; p. 805-811.
- 73) Della Longa S., Arcovito A. Vallone B., Congiu-Castellano A., Kahn R., Vicat J., Soldo Y., Hazmann J.L. (1999) Polarized x-ray absorption spectroscopy of the low-temperature photoproduct of carbonmonoxy-myoglobin. *J. Synchrotron Rad.* 6, 1138-1147.
- 74) Brunori, M., Cutruzzolà, F., Savino, C., Travaglini-Allocatelli, C., Vallone, B., Gibson, QH. (1999) " Does picosecond protein dynamics have survival value?" *Trends Biochem Sci.* 24, 253-5.
- 75) M. Brunori, F. Cutruzzolà, C. Savino, C. Travaglini-Allocatelli, B. Vallone, Q.H. Gibson. (1999) Structural dynamics of ligand diffusion in the protein matrix: a study on a new myoglobin mutant Y(B10) Q(E7) R(E10) *Biophys. J.* 75, 1259-1269.
- 76) Miele AE, Santanchè S, Travaglini-Allocatelli C, Vallone B., Brunori M, Bellelli A (1999). Modulation of ligand binding in engineered human hemoglobin distal pocket. *J. Mol. Biol.* vol. 290; p. 515-524.
- 77) B. Vallone, A.E. Miele, P. Vecchini, E. Chiancone, M. Brunori. (1998) Free Energy of burying hydrophobic residues in the interface between protein subunits. *Proc. Natl. Acad. Sci. USA* 95, 6103-6107.
- 78) B. Vallone, A. Bellelli, A.E. Miele, M. Brunori, G. Fermi. (1996) Probing the $\alpha\beta$ interface of human hemoglobin by mutagenesis. *J. Biol. Chem.* 271, 12472-12480.
- 79) A. Amadei, B. Vallone. (1996) Identification of a pattern in protein structure based on statistical and energetical considerations. *Proteins* 24, 35-50.
- 80) M. Brunori, F. Cutruzzolà, B. Vallone. (1995) Haemoglobin Engineering. *Curr. Biol.*, 5, 462-465
- 81) C. Travaglini-Allocatelli, F. Cutruzzolà, A. Brancaccio, B. Vallone, M. Brunori (1994) Engineering Ascaris hemoglobin oxygen affinity in sperm-whale myoglobin: role of tyrosine B10. *FEBS Lett.* 352, 63-
- 82) B. Vallone, P. Vecchini, V. Cavalli, M. Brunori (1993) Site-directed mutagenesis in hemoglobin: effect of some mutations at protein interfaces. *FEBS Lett.* 324, 117-122.
- 83) O. Schaad, B. Vallone, S.J. Edelstein. (1993) Critical residues responsible for self association differences of hemoglobin α and β chains. *C. R. Acad. Sci. III, Vie* 316, 564-71.
- 84) E. Lendaro, R. Ippoliti, A. Brancaccio, A. Bellelli, B. Vallone, G. Ivaldi, G.V. Sciaratta, C. Castello, S. Tomova, M. Brunori, G. Amiconi. (1992) Hemoglobin Dallas (β 97(G4) Asn \rightarrow Lys): functional characterization of a high affinity natural mutant. *Biochim. Biophys. Acta* 1180, 15-20.
- 85) A. Alleyne, M.T. Wilson, G. Antonini, F. Malatesta, B. Vallone, P. Sarti, M. Brunori. (1992) Investigation of the electron-transfer properties of cytochrome oxidase covalently cross-linked to Fe- or Zn-containing cytochrome c. *Biochem. J.* 287, 951-956.
- 86) F. Malatesta, P. Sarti, G. Antonini, B. Vallone, M. Brunori. (1990) Electron transfer to the binuclear center in cytochrome c oxidase: Catalytic significance and evidence for an additional intermediate. *Proc. Natl. Acad. Sci. USA* 87, 7410-7413.

- 87) B. Vallone, E. D'Itri, G. Antonini, F. Malatesta, P. Sarti (1990) Reconstitution of cytochrome c oxidase into phospholipid vesicles: effect of detergents. *Bioelectroch. and Bioener.* 23, 265-270.
- 88) P. Sarti, G. Antonini, F. Malatesta, B. Vallone, M. Brunori, M. Masserini, P. Palestini, G. Tettamanti (1990) Effect of gangliosides on membrane permeability studied by enzymic and Fluorescence-spectroscopy techniques. *Biochem. J.* 267, 413-416.
- 89) P. Sarti, F. Malatesta, G. Antonini, B. Vallone, M. Brunori. (1990) Control of electron transfer by the electrochemical potential gradient in cytochrome oxidase reconstituted into phospholipidic vesicles. *J. Biol. Chem.* 265, 5554-5560.
- 90) Malatesta F, Antonini G, P. Sarti, Vallone B., Brunori M (1990). Structure and function of cytochrome c oxidase. *Gazzatta Chimica Italiana*, vol. 120; p. 475-484.
- 91) Sarti P, Antonini G, Malatesta F, Vallone B., Villaschi S, Brunori M, Hider RC, Hamed K (1989). Reconstitution of cytochrome c oxidase in phospholipid vesicles containing polyvinyl polymers. *Biochem. J.*, vol. 257; p. 783-787.
- 92) F. Malatesta, G. Antonini, P. Sarti, B. Vallone, M. Brunori. (1988) Modulation of cytochrome oxidase activity by an electrical transmembrane gradient. *Ann.N.Y.Acad.Sci.*, 550, 269-276.
- 93) G. Antonini, F. Malatesta, P. Sarti, B. Vallone, M. Brunori. (1988) ATP induced spectral perturbation in cytochrome oxidase. Kinetic aspects and role of calcium ions. *Ann. N.Y.Acad.Sci.*, 550, 118-123.
- 94) P. Sarti, G. Antonini, F. Malatesta, B. Vallone, M. Brunori. (1988) Is the internal electron transfer the rate limiting step in the catalytic cycle of cytochrome oxidase? *Ann.N.Y.Acad.Sci.*, 550, 161-166.
- 95) P. Sarti, G. Antonini, F. Malatesta, B. Vallone, S. Villaschi, M. Brunori, R.C. Hider, K. Hamed. (1989) Reconstitution of cytochrome c oxidase into vesicles containing polyvinyl polymers. *Biochem. J.* 257, 783-787.
- 96) G. Antonini, F. Malatesta, P. Sarti, B. Vallone, M. Brunori. (1988) ATP induced spectral changes in cytochrome c oxidase: a kinetic investigation. *Biochem. J.*, 256, 835-840

