

## CURRICULUM VITÆ

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### **Education**

1979 Degree in Pharmaceutical Chemistry, 110/110 cum laude Universita' di Firenze, Italy

### **Professional Career:**

1980-82 Post doc., Istituto Chimica Fisica, U. di Firenze, Italy  
1983-92 Assistant Professor, Physical Chemistry, Dip. Chimica, U. Firenze, Italy  
1992-2001 Associate Professor, Biophysical Chemistry, Dip. Chimica, U. Firenze, Italy.  
2001-present Professor, Physical Chemistry, Dip. Chimica, U. Firenze, Italy.  
2003-2008 External Professor, Dept. of Life Sciences, Aalborg University (DK).

### **Previous Positions**

1981 Visiting Researcher, Chemistry Dept., Tel-Aviv U., Israel  
1984-85 Italian CNR fellowship, Chemistry Dept, Princeton U., Princeton, N.J., U.S.A..  
1985-1992 Visiting Researcher Staff Member, Chemistry Dept, Princeton U., Princeton, N. J., U.S.A.  
1988 Visiting Professor, Chemistry Dept, Rutgers U., New Brunswick, N.J., U.S.A.  
1990 Visiting Professor, Chemistry and Biochemistry Dept, Concordia U., Montreal, Canada

### **Involvement in Scientific Journals (member of boards)**

Editorial Board: "Biospectroscopy", 1995- 2003.  
Editorial Board: "Journal of Raman Spectroscopy", 2000-2009  
Editorial Board: "Biopolymers", 2004-present  
Editorial Board: "Journal of Inorganic Biochemistry", 2004-2008  
Associate Editor: "Journal of Raman Spectroscopy", 2008-present

### **Professional Activities and Services to the Community**

European Committee "European Conference on the Spectroscopy of Biological Molecules", 1995-2001  
Int. Steering Committee of "International Conference of Raman Spectroscopy", 1996-2002, 2008-present  
Coordinator of COST programme "Natural, engineered peroxidases, and synthetic Heme model compounds with peroxidase-like activity", 2001-2006

### **Professional Society Memberships:**

American Chemical Society  
American Biophysical Society  
Italian Chemical Society  
Society of Biological Inorganic Chemistry  
Society of Porphyrins and Phthalocyanine

**Research area:** Biophysical Chemistry

### **Current research interests:**

- Structure-function relationships in heme proteins: spectroscopic characterization of novel heme proteins via electronic (UV-Vis), vibrational (IR absorption and resonance Raman, (RR)) and Electron Paramagnetic Resonance (EPR) spectroscopies, carried out in collaboration with various leading Italian, European, Japanese and North-American groups.

The combination of different spectroscopic techniques, especially when applied to a study incorporating native, recombinant and mutant proteins of key residues, give detailed information at the molecular level of the active site. In particular, the combined study of native and mutant enzymes, at different pH and temperature, in the presence of various exogenous ligands, in solution and single crystal forms, has enabled the role of the key residues in the heme cavity to be defined and their structure-function properties to be elucidated.

- Development and validation of easy and fast spectroscopic methods to detect residuals of contaminants in food. In particular, UV-Vis, Raman, RR, and SER[R]S (Surface Enhanced [Resonance] Raman Scattering) spectroscopies have been applied.

Carbon monoxide can be used to treat fresh meat and fish in order to retain its 'fresh' red colour appearance for a longer period of time. The use of carbon monoxide, which reacts with the oxy-myoglobin to form a fairly stable cherry red CO-myoglobin complex, may mask spoilage because the CO-complex can be stable beyond the microbiological shelf life of the meat. Recently, we developed a rapid method, based on the combined analysis of electronic absorption spectra in their normal and second derivative modes, to unmask the presence of CO in frozen or fresh fish. The method represents a useful screening procedure for determining the presence of CO in food products, which are not labelled as such.

#### Peer-reviewed primary articles, Last five years (151 total).

1. G. Smulevich, E. Droghetti, C. Focardi, C. Ciaccio, M. Coletta, and M. Nocentini  
*A rapid spectroscopic method to detect the fraudulent treatment of tuna fish with carbon monoxide.*  
Food Chemistry 101 (2007) 1071-1077 **I.F. 3.458**
2. S. Bruno, S. Faggiano, F. Spyrakis, A. Mozzarelli, S. Abbruzzetti, E. Grandi, C. Viappiani, A. Feis, S. Mackowiak, G. Smulevich, E. Cacciatori, P. Dominici  
*The reactivity with CO of AHb1 and AHb2 from Arabidopsis thaliana is controlled by the distal His E7 and internal hydrophobic cavities.*  
J. Am. Chem. Soc., 129 (2007) 2880-2889 **I.F. 9.019**
3. M. Zederbauer, P. G. Furtmuller, S. Brogioni, C. Jakopitsch, G. Smulevich, and C. Obinger  
*Heme to protein linkages in human peroxidases: Impact on spectroscopic, redox and catalytic properties.*  
Nat. Prod. Rep., 2007, 24, 571-584. **I.F. 8.881**
4. A. Feis, L. Tofani, G. De Sanctis, M. Coletta, and G. Smulevich  
*Multiphasic Kinetics of Myoglobin/SDS Complex Formation.*  
Biophys. J. (2007) 92, 4078-4087 **I.F. 4.218**
5. G. De Sanctis, G. Petrella, C. Ciaccio, A. Feis, G. Smulevich, and M. Coletta  
*A comparative study on axial coordination and ligand binding in ferric mini myoglobin and horse heart myoglobin.*  
Biophys. J. (2007) 93, 2135-2142 **I.F. 4.390**
6. E. Droghetti, B. D. Howes, A. Feis, P. Dominici, M. Fittipaldi and G. Smulevich  
*The quantum mechanically mixed-spin state in a non symbiotic plant hemoglobin: the effect of distal mutation on AHb1 from Arabidopsis thaliana.*  
J. Inorg. Biochem. (2007), 101, 1812-1819 **I.F.3.317**
7. B.D. Howes, L. Guerrini, S. Sanchez-Cortes, M.P. Marzocchi, J.V. Garcia-Ramos, and G. Smulevich  
*The influence of pH and anions on the adsorption mechanism of rifampicin on silver colloids.*  
J. Raman Spectroscopy (2007), 38, 859-864 **I.F.3.137**
8. A. Feis, A. Lapini, B. Catachio, S. Brogioni, P. Foggi, E. Chiancone, A. Boffi, and G. Smulevich  
*Unusually Strong H-Bonding to the Heme Ligand and Fast Geminate Recombination Dynamics of the Carbon Monoxide Complex of Bacillus subtilis Truncated Hemoglobin.*  
Biochemistry (2008), 47, 902-910 **I.F. 3.226**
9. G. Bonente, B. D. Howes, S. Caffarri, G. Smulevich, and R. Bassi  
*Interactions between the photosystem II subunit PsbS and xanthophylls studied in vivo and in vitro.*  
J. Biol. Chem. (2008), 283, 8434-8445, **I.F. 5.328**
10. S. Brogioni, J. Stamper, P.G. Furtmüller, A. Feis, C. Obinger and G. Smulevich  
*The role of the sulfonium linkage in the stabilization of the ferrous form of myeloperoxidase: a comparison with lactoperoxidase.*  
Biochim. Biophys. Acta, Proteins and Proteomics (2008), 1784, 843-849 **I.F. 2.773**
11. L. Vitagliano, A. Vergara, G. Bonomi, A. Merlino, C. Verde, G. di Prisco, B. D. Howes, G. Smulevich, L. Mazzarella  
*Spectroscopic and crystallographic characterization of a tetrameric hemoglobin oxidation reveals structural features of the functional intermediate R/T state.*  
J. Am. Chem. Soc. (2008), 130, 10527-10535 **I.F. 9.019**
12. F. Nicoletti, B.D. Howes, M. Fittipaldi, G. Fanali, M. Fasano, P. Ascenzi and G. Smulevich  
*Ibuprofen Induces an Allosteric Conformational Transition in the Heme Complex of Human Serum Albumin with Significant Effects on Heme Ligation.*  
J. Am. Chem. Soc. (2008), 130 11677-11688 **I.F. 9.019**
13. E. Droghetti, S. Sumithran, M. Sono, M. Antalík, M. Fedurco, J. H. Dawson, G. Smulevich  
*Effects of urea and acetic acid on the heme axial ligation structure of ferric myoglobin at very acidic pH.*  
Arch. Biochem. Biophys. (2009), 489, 68-75. **I.F.3.022**
14. A. Merlino, L. Vitagliano, B. D. Howes, C. Verde, G. di Prisco, G. Smulevich, F. Sica, A. Vergara  
*Combined Crystallographic and Spectroscopic Analysis of Trematomus bernacchii Hemoglobin Highlights Analogies and Differences in the Peculiar Oxidation Pathway of Antarctic Fish Hemoglobins.*  
Biopolymers (2009), 91, 1117-1125. **I.F.2.572**
15. P. Ascenzi, A. di Masi, M. Coletta, C. Ciaccio, G. Fanali, F.P. Nicoletti, G. Smulevich, and M. Fasano  
*Ibuprofen impairs allosterically peroxynitrite isomerization by ferric human serum heme-albumin.*  
J. Biol. Chem. (2009) 284, 31006-31017. **I.F. 5.328**

16. S. Faggiano, S. Abbruzzetti, F. Spyraakis, E. Grandi, C. Viappiani, S. Bruno, A. Mozzarelli, P. Cozzini, A. Astegno, P. Dominici, S. Brogioni, A. Feis, G. Smulevich, O. Carrillo, P. Schmidtke, B. C. Axel, and F. J. Luque  
*Structural Plasticity and Functional Implications of Internal Cavities in Distal Mutants of Type 1 Non-Symbiotic Hemoglobin AHb1 from Arabidopsis thaliana.*  
J. Phys. Chem. B (2009), 113, 16028–16038. **I.F. 3.603**
17. F.P. Nicoletti, M. Thompson, B.D. Howes, S. Franzen, and G. Smulevich  
*New Insights into the role of distal histidine flexibility in ligand stabilization of dehaloperoxidase-hemoglobin from Amphitrite ornata.*  
Biochemistry (2010), 49, 1903-1912. **I.F.3.226**
18. F.P. Nicoletti, A. Comandini, A. Bonamore, L. Boechi, F. M. Boubeta, A. Feis, G. Smulevich, and A. Boffi  
*Sulfide binding properties of truncated hemoglobins.*  
Biochemistry (2010), 49, 2269-2278. **I.F.3.226**
19. F. Sinibaldi, B.D. Howes, M.C. Piro, F. Polticelli, C. Bombelli, T. Ferri, M. Coletta, G. Smulevich, and R. Santucci  
*Extended cardiolipin anchorage to cytochrome c: a model for protein-mitochondrial membrane binding.*  
J. Biol. Inorg. Chem. (2010), 15, 689–700. **I.F.3.287**
20. M. K. Thompson, M. F. Davis, V. de Serrano, F. P. Nicoletti, B. D. Howes, G. Smulevich, S. Franzen  
*Two-site competitive inhibition in dehaloperoxidase-hemoglobin*  
Biophysical Journal (2010), 99, 1586–1595. **I.F. 4.218**
21. G. Bartolucci, E. Droghetti, C. Focardi, M. Bambagiotti-Alberti, M. Nocentini, and G. Smulevich  
*High throughput headspace GC-MS quantitative method to measure the amount of carbon monoxide treated tuna fish.*  
J. Mass. Spectrom. 2010, 45, 1041–1045 **I.F. 3.289**
22. A. Merlino, L. Vitagliano, A. Balsamo, F. Nicoletti, B. Howes, D. Giordano, D. Coppola, G. di Prisco, C. Verde, G. Smulevich, L. Mazzarella and A. Vergara  
*Crystallization, preliminary X-ray diffraction studies and Raman microscopy of the major hemoglobin from the sub-Antarctic fish *Eleginops maclovinus* in the carbomonoxy form.*  
Acta Cryst. (2010) F66, 1536-1540. **I.F. 0.551**
23. Enrica Droghetti, Francesco Paolo Nicoletti, Alessandra Bonamore, Leonardo Boechi, Pau Arroyo Mañez, Dario A. Estrin, Alberto Boffi, Giulietta Smulevich, and Alessandro Feis  
*Heme pocket structural properties of a bacterial truncated hemoglobin from *Thermobifida fusca*.*  
Biochemistry 2010, 49, 10394–10402 **I.F.3.226**
24. G. Smulevich, A. Feis, B.D. Howes, and A. Ivancich  
*Structure–Function Relationships Among Heme Peroxidases: New Insights from Electronic Absorption, Resonance Raman, and Multifrequency Electron Paramagnetic Resonance Spectroscopies*  
in HANDBOOK OF PORPHYRIN SCIENCE With Applications to Chemistry, Physics, Materials Science, Engineering, Biology and Medicine, Vol 6: NMR and EPR Techniques. (K. M Kadish, K. M Smith, R. Guilard, Eds), World Scientific, 2010, 367-455
25. B.D. Howes, D. Giordano, L.Boechi, R. Russo, S. Mucciacciaro, C. Ciaccio, F. Sinibaldi, M. Fittipaldi, M.A. Martí, D.A. Estrin, G. di Prisco, M. Coletta, C. Verde, and G. Smulevich  
*The Peculiar Heme Pocket of the 2/2 Hemoglobin of Cold Adapted *Pseudoalteromonas haloplanktis* TAC125.*  
J. Biol. Inorg. Chem. (2011), 16, 299-311 **I.F.3.287**
26. F.P. Nicoletti, M. Thompson, S. Franzen, and G. Smulevich  
*Degradation of sulfide by Dehaloperoxidase-Hemoglobin from Amphitrite Ornata.*  
J. Biol. Inorg. Chem. (2011), 16, 611-619 **I.F.3.287**
27. F. Spyraakis, S. Faggiano, S. Abbruzzetti, P. Dominici, E. Cacciatori, A. Astegno, E. Droghetti, A. Feis, G. Smulevich, S. Bruno, A. Mozzarelli, P. Cozzini, C. Viappiani, C. Bidon, A. Chanal, F.J. Luque  
*Histidine E7 Dynamics Modulates Ligand Exchange between Distal Pocket and Solvent in AHb1 from Arabidopsis Thaliana.*  
J. Phys. Chem. B (2011), 115, 4128–4137 **I.F. 3.603**
28. E. Droghetti, G.L. Bartolucci, C. Focardi, M. Bambagiotti-Alberti, M. Nocentini and G. Smulevich  
*Development and validation of a quantitative spectrophotometric method to detect the amount of carbon monoxide in treated tuna fish.*  
Food Chemistry (2011), 128, 1143–1151 **I.F. 3.458**
29. A. Merlino, B.D. Howes, G. di Prisco, C. Verde, G. Smulevich, L. Mazzarella, A. Vergara  
*Occurrence and formation of endogenous histidine hexa-coordination in cold-adapted hemoglobins..*  
IUBMB Life (2011) 63, 295-303 **I.F. 4.251**
30. Daniela Giordano, Roberta Russo, Chiara Ciaccio, Barry D. Howes, Guido di Prisco, Michael C. Marden, Gaston Hui Bon Hoa, Giulietta Smulevich, Massimo Coletta, and Cinzia Verde  
*Ligand- and proton-linked conformational changes of the ferrous 2/2 hemoglobin of *Pseudoalteromonas haloplanktis* TAC125.*  
IUBMB Life (2011) 63, 566-573 **I.F. 4.251**
31. C. Iannuzzi, S. Adinolfi, B. D. Howes, R. Garcia-Serres, M. Clémancey, J.-M. Latour, G. Smulevich, A. Pastore  
*A Mössbauer and resonance Raman study of the role of CyaY in iron sulfur cluster assembly on the *E. coli* IscU scaffold protein.*  
PlosOne (2011) accepted **I.F. 4.411**

## INVITED LECTURES (Last 5 years) (~ 90 total)

- 2007** \*Struttura-funzione di emoproteine mediante le tecniche Raman e micro-Raman risonante, Lezione Carlo Zauli 2007, Facoltà di Chimica Industriale, U. Bologna, Bologna, Italy  
\*Raman microscopy of heme proteins,  
3rd Serbian Congress for Microscopy, Belgrade, Serbia  
\*New bacterial and plant hemoglobins: structure-function relationships studied by optical spectroscopy, Dept. of Biological Sciences, Aarhus University, DK, 2  
\*Extraordinary effects of Ibuprofen binding to heme-HSA (Human Serum Albumin), Dept. of Life Sciences, Aalborg University, DK
- 2008** \*Insights into the heme pocket of bacterial truncated hemoglobins as revealed by RR spectra XXI ICORS, London, UK  
\*Ibuprofen binding to heme-Human Serum Albumin induces marked conformational changes: an allosteric modulation ICCP-5, Mosca, Russia  
\*Ligand binding properties of bacterial hemoglobins Workshop on "The intriguing world of protein structure", Naples, Italy
- 2009** \*Caratterizzazione spettroscopica del complesso emalbumina-ibuprofene: evidenza di una transizione conformazionale allosterica Dip. Biologia, Università degli Studi Roma Tre, Italy  
\*The intriguing world of truncated hemoglobins XXI CONGRESSO GNSR, Milano, Italy  
\*Heme pocket structural properties of bacterial truncated hemoglobins as revealed by RR spectroscopy XIII ECSBM, Palermo, Italy
- 2010** \*Heme cavity structure of truncated bacterial hemoglobins as envisaged by RR spectroscopy ICCP-6, New Mexico, USA  
\*Non-Symbiotic Hemoglobins from Arabidopsis thaliana and selected distal variants Dept. Biochemistry and cell Biology, Rice University, TX USA  
\*The heme cavity properties of truncated hemoglobins from unicellular organism Dept. Chemistry and Mol. Biol., North Dakota State U. USA  
\*Structural properties of truncated hemoglobins from unicellular organisms Dept. Biochemistry and Mol. Biol. Wayne State U., USA  
\*Ligand binding properties of truncated hemoglobins from unicellular organism Dept. Biochemistry Mol. Biol., Michigan State U., USA  
\*What have we learnt from the resonance Raman spectroscopy of heme proteins? Biochemistry Dept. Case Western Reserve U., USA  
\*High protein structural flexibility of a truncated hemoglobin from an antarctic cold-adapted bacterium XXII ICORS, Boston, USA  
\*Ligand binding properties of Thermobifida fusca truncated haemoglobin XVI Int. Conference on Oxygen Binding and Sensing Proteins Antwerp, Belgium  
\*Development and validation of a rapid spectroscopic method to detect the fraudulent treatment of tuna fish with carbon monoxide Workshop on specific methods for food safety and quality, Belgrade, Serbia  
\*Structural properties of truncated hemoglobins from unicellular organisms as revealed by RR Spectroscopy 10<sup>th</sup> Int. Conf. on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, Serbia
- 2011** \*Influence of cold-adaptation on the structural properties of an Antarctic 2/2 hemoglobin 3<sup>rd</sup> Georgian Bay International Conference on Bioinorganic Chemistry, Toronto, Canada