

Fabio Polticelli, Ph.D.
Full Professor of Biochemistry

Theoretical Biology and Bioinformatics Lab
Department of Sciences, University of Roma Tre
Viale Marconi 446, 00146 Roma
Tel. 06-57336362
Fax 06-57336321
E-mail fabio.polticelli@uniroma3.it
Lab website <http://www.computationalbiology.it>



Curriculum vitae et studiorum

- 2021-present** Coordinator of the Ph.D. Program in Biomedical Sciences and Technologies - Department of Sciences - University Roma Tre.
- 2020-present** Full Professor of Biochemistry - Department of Sciences - University Roma Tre.
- 2011- 2019** Associate Professor of Biochemistry - Department of Sciences - University Roma Tre.
- 2004-present:** Head of the Theoretical Biology and Bioinformatics Lab – Department of Sciences – University Roma Tre
- 2000-2010:** Research Scientist - Department of Biology - University Roma Tre.
- 1998-2000:** Post-doctoral fellow - Department of Biochemistry and Molecular Biophysics, Columbia University (New York, USA)
- 1996-1998:** Research Scientist - Department of Biology - University Roma Tre.
- 1995:** Research fellow - Italian National Institute of Physics of the Matter (IT)
- 1994:** "Scientist" - Radiobiology Unit of the Medical Research Council (Chilton, Didcot, UK)
- 1993:** Post-doctoral fellow - Technobiochip Industrial Consortium (IT)
- 1993:** Ph.D. degree in Biochemistry.

- 1989-1992:** Ph.D. student - Department of Biochemical Sciences, University of Rome "La Sapienza"
- 1988:** Degree "cum laude" in Biology - University of Rome "La Sapienza"

Research interests

- Development of software tools for protein structure analysis and function recognition.
- Ab initio prediction of the three-dimensional structure and function of proteins from bacterial pathogens.
- Study of substrate specificity and catalytic mechanism of (metallo)enzymes and membrane transporters (molecular modelling and dynamics, computational chemistry and protein engineering).

Prof. Polticelli is the author of 200 papers on international peer-reviewed scientific journals (*h*-index=37, total number of citations >4400; source Scopus). His research has been funded by grants from the Human Frontier Science Program, from the MIUR PRIN and FIRB programs and from the European Commission FP4 and FP6 programs. He is currently the Head of the Theoretical Biology and Bioinformatics Lab of the University of Roma Tre, in which he coordinates the activity of one Ph.D. student, one Post-doc, one software engineer and several undergraduate students.

List of publications on peer reviewed international journals

1. Calabrese, L., **Polticelli, F.**, O'Neill, P., Galtieri, A., Barra, D., Schinina', E., Bossa, F. (1989). Substitution of arginine for lysine 134 alters electrostatic parameters of the active site in shark Cu,Zn superoxide dismutase. *FEBS Lett.*, 250, 49-52.
2. Capo, R.C., **Polticelli, F.**, Calabrese, L., Schinina', M.E., Carri', M.T., Rotilio, G. (1990) The Cu, Zn Superoxide Dismutase isoenzymes from Xenopus laevis. Purification, identification

- of a heterodimer and differential heat sensitivity. *Biochem. Biophys. Res. Commun.*, 173, 1186-1193.
3. Galtieri, A., Lania, A., **Polticelli, F.**, Calabrese, L. (1990) The effect of phenylglyoxal on Cu,Zn superoxide dismutase from the shark *Prionace glauca*. *Ital. J. Biochem.* 39, 207A-208A
 4. Galtieri, A., Lania, A., **Polticelli, F.**, Calabrese, L. (1990) The inactivation of shark Cu,Zn superoxide dismutase by hydrogen peroxide. *Ital. J. Biochem.* 39, 206A-207A.
 5. Calabrese, L., **Polticelli, F.**, Capo, C., Musci, G. (1991). Involvement of the copper in the inhibition of Cu,Zn superoxide dismutase activity at high pH. *Free Rad. Res. Commun.*, 12-13, 305-312.
 6. Desideri, A., Falconi, M., **Polticelli, F.**, Bolognesi, M., Djinovic, K., Rotilio, G. (1992). Evolutionary conservativeness of electric field in the Cu,Zn superoxide dismutase active site. Evidence for coordinated mutations of charged amino acid residues. *J. Mol. Biol.*, 223, 337-342..
 7. Desideri, A., **Polticelli, F.**, Falconi, .M. (1992). An electrostatic enzyme-substrate recognition: the case of Cu,Zn superoxide dismutase. *J. Mol. Structure (Teochem)*, 256, 153-160.
 8. Desideri, A., **Polticelli, F.**, Falconi, M., Sette, M., Ciriolo, M.R., Paci, M., Rotilio, G. (1993) Electrostatic recognition in redox copper proteins. A ¹H NMR study of the protonation behaviour of His19 in oxidized and reduced Cu,Zn superoxide dismutase. *Arch. Biochem. Biophys.* 301, 244-250.
 9. Djinovic Carugo, K., Collyer, C., Coda, A., Carri', M.T., Battistoni, A., Bottaro, G., **Polticelli, F.**, Desideri, A., Bolognesi, M. (1993) Crystallisation and preliminary analysis of recombinant *Xenopus laevis* Cu,Zn superoxide dismutase B. *Biochem. Biophys. Res. Commun.* 194, 1008-1011.
 10. Galtieri, A., Lania, A., Costanzo, S., **Polticelli, F.**, Calabrese, L., Desideri, A. (1993) A comparative study on Cu, Zn superoxide dismutase from *Bos taurus* and shark *Prionace glauca*. *Ital. J. Biochem.*, 42, 320-321.
 11. Lo Bello, M., Parker, M.W., Desideri, A., **Polticelli, F.**, Falconi, M., Del Boccio, G., Pennelli, A., Federici, G., Ricci, G. (1993) Peculiar spectroscopic and kinetic properties of Cys47 in human placental glutathione transferase. Evidence for an atypical thiolate ion pair near the active site. *J. Biol. Chem.* 268, 19033-19038.
 12. **Polticelli, F.**, Falconi, M., O'Neill, P., Petruzzelli, R., Galtieri, A., Lania, A., Calabrese, L., Rotilio, G., Desideri A. (1994) Molecular modelling and electrostatic potential calculations

- on chemically modified Cu,Zn superoxide dismutases from *Bos taurus* and *Prionace glauca*. Role of Lys134 in electrostatically steering the substrate to the active site.. *Arch. Biochem. Biophys.*, 312, 22-30.
13. **Polticelli, F.**, Battistoni, A., Bottaro, G., Carri', M.T., O'Neill, P., Desideri, A., Rotilio, G. (1994) Mutation of Lys120 and Lys134 drastically reduces the catalytic rate of Cu,Zn superoxide dismutase. *FEBS Lett.* 352, 65-68.
 14. Djinovic-Carugo, K., **Polticelli, F.**, Desideri, A., Rotilio, G., Wilson, K.S., Bolognesi, M. (1994) Crystallographic study of azide-inhibited bovine Cu, Zn superoxide dismutase. *J. Mol. Biol.* 240, 179-183.
 15. Djinovic-Carugo, K., Battistoni, A., Carri', M.T., **Polticelli, F.**, Desideri, A., Rotilio, G., Coda, A., Bolognesi, M. (1994) Crystal Structure of the Cyanide-Inhibited *Xenopus laevis* Cu, Zn Superoxide Dismutase at 98 K. *FEBS Lett.* 349, 93-98.
 16. Sergi, A., Ferrario, M., **Polticelli, F.**, O'Neill, P., Desideri, A. (1994) Simulation of superoxide-superoxide dismutase association rate for six natural variants. Comparison with the experimental catalytic rate. *J. Phys. Chem.* 98, 10554-10557.
 17. Cupane, A., Leone, M., Militello, V., Stroppolo, M.E., **Polticelli, F.**, Desideri, A. (1994) Low temperature optical spectroscopy of native and azide-reacted bovine Cu,Zn superoxide dismutase. A structural dynamics study. *Biochemistry*, 33, 15103-15109.
 18. Stroppolo, M.E., **Polticelli, F.**, Costanzo, S., Lania, A., Galtieri, A., Polizio, F., Petruzzelli, R., Desideri, A. (1994) A comparative study of the anion binding properties of *Bos taurus* and *Prionace glauca* Cu,Zn superoxide dismutases native and chemically modified at lysines. *Comp. Biochem. Physiol.*, 109C, 141-145.
 19. Costanzo, S., Fanara, P. Lania, A., Galtieri, A., Capo, C, Petruzzelli, R., **Polticelli, F.**, Desideri, A. (1994) A comparative study of Cu,Zn-superoxide dismutase from the sea squirt *Styela plicata* and the mesopelagic fish *Lampanichtus crocodilus*. *Ital. J. Biochem.*, 43, 228.
 20. **Polticelli, F.**, Bottaro, G., Battistoni, A., Carri', M.T., Djinovic-Carugo, K., Bolognesi, M., O'Neill, P., Rotilio, G., Desideri, A. (1995) Modulation of the catalytic rate of Cu,Zn superoxide dismutase in single and double mutants of conserved positively and negatively charged residues. *Biochemistry*, 34, 6043-6049.
 21. **Polticelli, F.**, O'Neill, P., Costanzo, S., Lania, A., Rotilio, G., Desideri, A. (1995) Identification of the residues responsible for the alkaline inhibition of the activity of Cu,Zn superoxide dismutase. A study of native and chemically modified enzymes. *Arch. Biochem. Biophys.*, 321, 123-126.

22. Marino, M., Galvano, M., Cambria, A., **Polticelli, F.**, Desideri, A. (1995) Modelling the three-dimensional structure and electrostatic potential field of two Cu,Zn superoxide dismutase variants from tomato leaves. *Protein Eng.*, 8, 551-556.
23. Cupane, A., Leone, M., Militello, V., Stroppolo, M.E., **Polticelli, F.**, Desideri, A. (1995) Low temperature optical spectroscopy of cobalt in Cu,Co superoxide dismutase. A structural dynamics study of the solvent-unaccessible metal site. *Biochemistry*, 34, 16313-16319.
24. Djinovic-Carugo, K., Battistoni, A., Carri', M.T., **Polticelli, F.**, Desideri, A., Rotilio, G., Wilson, K.S., Bolognesi, M. (1996) Three-dimensional structure of *Xenopus laevis* Cu,Zn superoxide dismutase b determined by X-ray crystallography. *Acta Crystallog.*, D52, 176-188.
25. Folcarelli, S., Battistoni, A., Carri', M.T., **Polticelli, F.**, Falconi, M., Nicolini, L., Stella, L., Rosato, N., Rotilio, G., Desideri,, A. (1996) Effect of Lys-Arg mutation on the thermal stability of Cu,Zn superoxide dismutase: influence on the monomer-dimer equilibrium. *Protein Eng.* 9, 323-325.
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33. **Polticelli, F.**, Ascenzi, P., Bolognesi, M., Honig, B. (1999) Structural determinants of trypsin affinity and specificity for cationic inhibitors. *Protein Sci.* 8, 2621-2629.
34. Persichini, T., Colasanti, M., Fraziano, M., Coalizzi, V., Medana, C., **Polticelli, F.**, Venturini, G., Ascenzi, P. (1999) Nitric oxide inhibits the HIV-1 reverse transcriptase activity. *Biochem. Biophys. Res. Commun.* 258, 624-627.
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36. Ascenzi, P., Balliano, G., Gallina, C., **Polticelli, F.**, Bolognesi, M. (2000) Serine proteinase inhibition by the active site titrant N- α -(N,N-dimethylcarbamoyl)- α -azaornithine *p*-nitrophenyl ester. A comparative study. *Eur. J. Biochem.* 267, 1239-1246.
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38. Trovato, M., Maras, B., **Polticelli, F.**, Costantino, P., Ascenzi, P. (2000) A chimeric mini-trypsin inhibitor derived from the oil rape proteinase inhibitor type III. *Biochem. Biophys. Res. Commun.* 275, 817-820.
39. Ascenzi, P., Colasanti, M., Persichini, T., Muolo, M., **Polticelli, F.**, Venturini, G., Bordo, D., Bolognesi, M. (2000) Re-evaluation of amino acid sequence and structural consensus rules for cysteine-nitric oxide reactivity. *Biol. Chem.* 381, 623-627.
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41. **Polticelli, F.**, Raybaudi-Massilia, G., Ascenzi, P. (2001) Structural determinants of mini-protein stability. *Biochem. Mol. Biol. Edu.* 29, 16-20.
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A handwritten signature in black ink, appearing to read "Fabio Polticelli".