CURRICULUM VITAE

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Current position

Assistant Professor in Organic Chemistry (CHIM/06)

Education

1991 Master Degree (*Laurea*) in Agricultural Science at the University of Bologna, with a thesis in insect biology titled: ***In vitro* rearing of *Pseudogonia rufifrons*.**

2001 Doctor of Philosophy in Chemistry at the University of York with the thesis: **Structure and Function Relationships of Urease and Cytochrome c-553 from *Bacillus pasteurii*** (examiners Doctor Phil Evans and Professor Guy Dodson). My research studies (from October 1996 to April 2000) were carried out at the **European Molecular Biology Laboratory (E.M.B.L.)** based at the synchrotron site in Hamburg under the supervision of Professor Keith Wilson and Professor Wojciech Rypniewski. I solved the crystal structure of urease native and in complex with several inhibitors thus providing the best characterisation of the urease active site to date and proposed a new reaction mechanism. I solved the structures of cytochrome c-553 from *Bacillus pasteurii,* Hipip from *Rhodoferax fermentans*, and cytochrome c' from *Rubrivivax gelatinosus.*

Academic experience

1992-1996 research assistant in the group of Professor Stefano Ciurli working on the purification and characterisation of proteins from different sources (plants and bacteria) and supervising undergraduate students.

1996-2000 PhD student in protein crystallography at the European Molecular Biology Laboratory (Hamburg)-University of York, see education section.

2000-2002 Post Doctoral Research Assistant (PDRA) at the **International Centre for Genetic Engineering and Biotechnology (ICGEB)** Trieste (Italy) in the group of Professor Arturo Falaschi working on the human DNA binding protein KU. I was responsible for the purification and refolding of KU for structural studies as well as the supervision of graduate students.

2002-2005 PDRA in the group of Professor Keith Wilson **York Structural Biology Laboratory (YSBL)** on structural and functional genomics of *Mycobacterium tuberculosis* (MTB) from target selection to structure solution. Despite the solubility problems of MTB proteins I was able to clone several genes and to solve the crystal structures of the FMN binding protein Rv2991 (2.0 Å), and the inorganic pyrophosphatase Rv3628 at pH 5.0 (1.3 Å) and 7.0 (1.5 Å).

2005-2007 PDRA in the group of Doctor Alfred Antson **(YSBL)** on the determination of the crystal structure of G1P and G2P. These two proteins are involved in the recognition, processing and insertion of the viral DNA into the capsid of *Bacillus subtilis* bacteriophages SPP1 and SF6. I solved the structure of the DNA binding domain of G1P at 1.58 Å and obtained crystals of the nuclease domain of G2P diffracting to 1.9 Å. I was responsible for the supervision of a technician and of graduate students.

Extra-academic experience

2007-2009 Protein crystallographer in the pharmaceutical company *AstraZeneca* in the group lead by Doctor Richard Pauptit. My work involved crystal structure determination of complexes between selected kinases and chemical compounds obtained either by soaking or co-crystallisation. The work included providing structural support for two programs:

- Compound Collection Enhancement
- Fragment Based Lead Generation

Responsible for the development and improvement of co-crystallisation and soaking protocols and the supervision of postdocs from protein crystallisation to structure solution.

Research activity

1. Areas of scientific interest

My main area of interest is the study of organic macromolecules of biological interest (hence Bio-Organic Chemistry) such as proteins. The technique I use to investigate the structure and function relationship of proteins is called protein crystallography (see my personal homepage http://pro.unibz.it/staff2/sbenini/). The work involves cloning of the genes of interest and expression and purification of the protein under investigation. The pure protein is then crystallized and irradiated with X-ray providing structural information.

2. Research projects

I am currently involved in three research projects:

- Sustainable chain for the use of biomass in south-tyrol
- Molecular basis of chemicals and odorants recognition in the insect model organism *Tribolium castaneum* by structural biology of chemoreceptor proteins
- A structural genomics approach for the study of *Erwinia amylovora* virulence and pathogenesis

List of publications

1. S. Benini, W. R. Rypniewski, K. S. Wilson, and S. Ciurli. **High Resolution Crystal Structure of *Rubrivivax gelatinosus* cytochrome *c'*.** *J. Inorg. Bioch.* (2008), **102**, 1322-1328.

2. M. Tammenkoski, S. Benini, N. N. Magretova, A. A. Baykov, and R. Lahti. **An Unusual, His-dependent Family I Pyrophosphatase from *Mycobacterium tuberculosis*.** *J. Biol. Chem.* (2005), **280**, 41819-41826.

3. S. Benini, W. R. Rypniewski, K. S. Wilson, S. Mangani and S. Ciurli. **Molecular Details of Urease Inhibition by Borate: Insights into the catalytic Mechanism.** *J. Am. Chem Soc.* (2004), **126**, 3714-3715.

4. A. González, S. Benini, and S. Ciurli. **Crystal Structure of *Rhodoferax fermentans* High Potential Iron-sulfur Protein Solved by MAD.** *Acta Cryst.* (2003), D**59**, 1582-1588.

5. S. Benini, W. R. Rypniewski, K. S. Wilson, S. Ciurli and S. Mangani. **Structure-Based Rationalization of Urease Inhibition by Phosphate: Novel Insights into the Enzyme Mechanism.** *J. Biol. Inorg. Chem.* (2001), **6**, 778-790.

6. S. Benini, A. González, W.R. Rypniewski, K.S. Wilson, J.J. Van Beeumen, S. Ciurli. **Crystal Structure of Oxidized *Bacillus pasteurii* Cytochrome c_{553} at 0.97-Å Resolution.** *Biochemistry*. (2000), **39**, 13115-13126.

7. S. Benini, W.R. Rypniewski, K.S. Wilson, S. Miletti, S. Ciurli, S. Mangani. **The Complex of *Bacillus pasteurii* Urease with Acetohydroxamate Anion from X-Ray Data at 1.55 Å Resolution.** *J. Biol. Inorg. Chem.* (2000), **5**, 110-118.

8. I.H.M. Vandenberghe, Y. Guisez, S. Ciurli, S. Benini, J.J. Van Beeumen. **Cytochrome *c*-553 from the Alkalophilic Bacterium *Bacillus pasteurii* has the Primary Structure Characteristics of a Lipoprotein.** *Biochem. Biophys. Res. Commun.* (1999), **264**, 380-387.

9. A. González, J-D. Pédelacq, M. Solà, F.X. Gomis-Rüth, M. Coll, J-P.Samama, S. Benini. **Two-Wavelength MAD Phasing: in Search of the Optimal Choice of Wavelengths.** *Acta Cryst.* (1999), D**55**, 1449-1458.

10. S. Ciurli, S. Benini, W. R. Rypniewski, K. S. Wilson, S. Miletti, S. Mangani. **Structural Properties of the Nickel Ions in Urease: Novel Insights into the Catalytic and Inhibition Mechanism.** *Coord. Chem. Rev*. (1999), **190**, 331-355.

11. S. Benini, W. R. Rypniewski, K. S. Wilson, S. Miletti, S. Ciurli , S. Mangani. **A New Proposal for Urease Mechanism Based on the Crystal Structures of the Native and the Inhibited**

Enzyme from *Bacillus pasteurii*: Why Urea Hydrolysis Costs Two Nickels. *Structure*, (1999), **7**, 205-216.

12. S. Benini, M. Borsari, S. Ciurli, A. Dikiy, M. Lamborghini. **Modulation of *Bacillus pasteurii* Cytochrome c_{553} Reduction Potential by Structural and Solution Parameters.** *J. Bio. Inorg. Chem.,* (1998), **3**, 371-382.

13. S. Benini, S. Ciurli, W. R. Rypniewski, K. S. Wilson, S. Mangani. **The Complex of *Bacillus pasteurii* Urease with β-Mercaptoethanol from X-ray Data at 1.65 Å Resolution.** *J. Bio. Inorg. Chem.,* (1998), **3**, 268-273.

14. S. Benini, S. Ciurli, W. R. Rypniewski, K. S. Wilson, S. Mangani. **Crystallization and Preliminary High-Resolution X-Ray Diffraction Analysis of Native and β-Mercaptoethanol-Inhibited Urease from *Bacillus pasteurii*.** *Acta Cryst.*, (1998), D**54**, 409-412.

15. S. Benini, W. R. Rypniewski, K. S. Wilson, S. Ciurli. **Crystallization and Preliminary X-ray Diffraction Analysis of Cytochrome *c'* from *Rubrivivax gelatinosus* at 1.3 Å Resolution.** *Acta Cryst.* (1998), D**54**, 284-287.

16. S. Benini, S. Ciurli, W. R. Rypniewski, K. S. Wilson. **Crystals of Cytochrome *c*-553 from *Bacillus pasteurii* Show Diffraction to 0.97 Å Resolution.** *Proteins: Struc., Func., Genet.*, (1997), **28**, 580-585

17. M. Cremonini, O. Francioso, S. Benini, S. Ciurli. **Quantification of *Bacillus pasteurii* Urease Secondary Structure by Factor Analysis of FT-IR Spectra**. *P. Carmona et al. (eds.) Spectroscopy of Biological Molecules: Modern trends*, 173-174. 1997 *Kluwer Academic Publisher. Printed in the Netherlands.*

18. M. Borsari, S. Benini, D. Marchesi, S. Ciurli. **Cyclic Voltammetry and Spectroelectrochemistry of Cytochrome *c*8 from *Rubrivivax gelatinosus*. Implications in Photosynthetic Electron Transfer.** *Inorg. Chim. Acta* (1997), **263**, 379-384.

19. S. Benini, S. Ciurli, S. Mangani, H. F. Nolting. **X-ray Absorption Spectroscopy Study of Native and Phenylphosphorodiamidate-Inhibited *Bacillus pasteurii* Urease.** *Eur. J . Biochem.*, (1996), **239**, 61-66.

20. S. Ciurli, C. Marzadori, S. Benini, S. Deiana, C. Gessa. **Urease from the Soil Bacterium *Bacillus pasteurii*. Immobilization on Ca-polygalacturonate.** *Soil Biol. Biochem.*, (1996), **28**, 811-817.

21. S. Benini, C. Gessa, S. Ciurli. ***Bacillus pasteurii* Urease: a Heteropolimeric Enzyme with a Binuclear Nickel Active Site.** *Soil Biol. Biochem.*, (1996), **28**, 819-821.

22. S. Benini, S. Ciurli, C. Luchinat. **Oxidized and reduced [Fe_2Q_2] (Q=S,Se) Cores of Spinach Ferredoxin: a Comparative Study Using ^{1}H NMR Spectroscopy.** *Inorg. Chem.*, (1995), **34**, 417-420.

23. A. Bratti, S. Benini. **Allevamento «in vitro» delle larve di *Pseudogonia rufifrons* Wied. (Dipt. Tachinidae). Prove su diete subnaturali e meridiche.** *Boll. Ist. Ent. "G. Grandi"* (1992), **46**, 71-85.