

Curriculum Vitae et Studiorum

Dr. Daniele Dell'Orco

PERSONAL INFORMATION

Born on May 21st 1978 in Modena, Italian citizen, not married.

Present address:

Department of Life and Reproduction Sciences, Section of Biological Chemistry, University of Verona.

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SPOKEN LANGUAGES

- **Italian:** mother-tongue; **English:** Fluent; **Spanish:** Beginner; **German:** Beginner

EDUCATION/OCCUPATION

- **December 2011 – present:** Assistant Professor of Biochemistry, University of Verona, Italy. Adjunct Professor of Bioinformatics, Faculty of Natural and Mathematical Sciences, University of Verona, Italy
- **August 2009 – December 2011:** Alexander von Humboldt Research fellow at the Department of Biology and Environmental Sciences, University of Oldenburg, Germany. Member of the Biochemistry of Neurosensory Processes Group (head Prof. Karl-Wilhelm Koch). Main Project: Unravelling dynamic processes in vertebrate rods phototransduction: integrating biochemical/biophysical experiments with computational modelling at a systems-level
- **March 2009- June-2009:** FEBS Research Fellow (short visit grant) at the Department of Biophysical Chemistry, Lund University (Sweden). Project on: 1) Calcium binding proteins in vision and their dynamics; 2) Modeling the time evolution of protein corona-nanoparticle interaction in biological fluids
- **February 2007 – February 2009:** Post-Doc position at the Department of Chemistry and Dulbecco Telethon Institute, University of Modena and Reggio Emilia, Computational Biochemistry and Biophysics Group (Prof. Francesca Fanelli). Project on: multiscale modeling of protein networks involved in signal transduction
- **March-May 2008:** Visiting Scientist at the Systems Biology and Bioinformatics group, Dept. of Computer Science, University of Rostock (Prof. O. Wolkenhauer)
- **April – May 2007:** Visiting Scientist at the Fraunhofer Chalmers Research Centre – Department of Systems Biology, Gothenburg, Sweden. Host: Dr. Henning Schmidt
- **January 2004- January 2007:** PhD in Biotechnology and Molecular Medicine at the University of Modena and Reggio Emilia, Department of Chemistry and Dulbecco Telethon Institute. Work on computational modeling of point mutation effects on protein-protein binding and on structural features of key-proteins involved in the visual cascade signaling. Thesis title “Computational simulations of protein-protein recognition: predicting mutational effects on the binding thermodynamics”. Supervisor: Prof. Francesca Fanelli
- **July 2003:** “Laurea in Fisica” corresponding to B.Sc. degree in Physics and M.Sc. degree in Biophysics, obtained at University of Parma, Italy, with final grade 110/110 *summa cum laude*. Thesis Project about “Electrostatic contributions to the reconstitution and the stability of Calbindin D9k: *Surface Plasmon Resonance* studies”. Supervisors: Prof. Sara Linse (Lund University, Sweden); Prof. R. Favilla (University of Parma)
- **August 2002- June 2003:** Research activity at the Department of Biophysical Chemistry of Lund University (Sweden) concerning new approaches to protein stability and kinetics as measured by Surface Plasmon Resonance spectroscopy and computational methods (Monte Carlo simulations of the affinity for reconstitutions of fragment-complementation proteins).

ACADEMIC TEACHING

- **2012-present:** Teacher in charge for the basic course in Bioinformatics and Biological Databases, Biotechnology and Bioinformatics Bachelor program, University of Verona
- **2010-2011:** Theoretical and practical tutorial on “Concepts in Computational Systems Biology” for Master students, Practical course of Biochemistry, University of Oldenburg
- **2008:** Lecturer in biophysical chemistry for the specialization school in clinical biochemistry, medical school of University of Modena and Reggio Emilia
- **2008:** cycle of seminars on introductory systems biology for Bs and Ms students in Medical, Pharmaceutical and Industrial Biotechnology, University of Modena and Reggio Emilia
- **2004-2007:** assistant in undergraduate courses of biophysical chemistry and structural biology, University of Modena and Reggio Emilia

SUPERVISION

- **2013:** supervisor of 2 BSc students in Bioinformatics (Michela Cecchin, Monica Marchetto) and 1 BSc Biotechnology (Giuditta dal Cortivo); supervisor of the Ms degree in Medical Biotechnology and Bioinformatics of Luca Barbon, University of Verona
- **2012-2013:** supervisor of the Ms degree in Medical Biotechnology and Bioinformatics of Valerio Marino, University of Verona
- **2012 :** co-tutor for the PhD Thesis in Biomedical Sciences of Marco Aquila, University of Ferrara (European PhD Program)
- **2011:** co-supervisor of the Bs Thesis in Chemistry of Stefan Sulmann, University of Oldenburg
- **2009:** co-supervisor of the Ms Thesis in Biology of Simona Mariani, University of Modena and Reggio Emilia

RESEARCH TOPICS AND EXPERTISE

- Protein-protein and protein-ion interactions studied by experimental techniques (surface plasmon resonance, isothermal titration calorimetry, fluorescence and absorption spectroscopy, circular dichroism);
- Thermodynamic and kinetic analysis of protein-protein and protein-ion interactions
- Bioinformatics and computational approaches to build structural models of single proteins and protein complexes (protein modeling and protein-protein docking simulations);
- Simulation of protein interactions and prediction of binding constants; effects of point mutations on the kinetics and thermodynamics of binding;
- Quantitative structure-function/structure-activity relationships of enzymes involved in the visual cascade and other signaling pathways
- Network-level analysis of signal transduction pathways, especially vertebrate phototransduction; computational modeling of protein networks time-evolution in normal and disease-associated conditions;
- Biochemical analysis of pathogenic states in vertebrate rods (Leber congenital amaurosis, cone dystrophy);
- Monte Carlo simulations of peripheral and integral membrane proteins involved in vertebrate phototransduction;
- Experimental and computational characterization of interactions between biological fluids and artificial nanoparticles; applications in nanobiotechnology and nanomedicine

RNNING SCIENTIFIC COLLABORATIONS

National

- Dr. Lorenzo Cangiano, Dipartimento di Ricerca Traslazionale e delle nuove Tecnologie in Medicina e Chirurgia, Università di Pisa
- Prof. Francesca Fanelli, Dipartimento di Scienze della Vita, Università di Modena e Reggio Emilia
- Prof. Giorgio Rispoli, Dipartimento di Biologia ed Evoluzione, Università di Ferrara
- Prof. Mario Buffelli, Dipartimento di Scienze Neurologiche, Neuropsicologiche, Morfologiche e Motorie, Università di Verona
- Dr. Fabio Piccinelli, Dipartimento di Biotecnologie, Università di Verona
- Dr. Alessandra Astegno, Dipartimento di Biotecnologie, Università di Verona

International

- Prof. Sara Linse, Department of Biochemistry, Chemical Center, Lund University, Sweden

- Prof. Pere Garriga, Department of Chemical Engineering, Polytechnic University of Catalonia, Barcelona, Spain
- Prof. Karl-Wilhelm Koch, Department of Biology and Environmental Sciences, University of Oldenburg, Sweden

AWARDS AND GRANTS

- **2011:** Visiting Fellow (Host of the Rector), Hanse-Wissenschaftskolleg (HWK) Institute for Advanced Study Delmenhorst – Germany
- **2010:** European Science Foundation – Short Visit Grant (Lund, Sweden).
- **2009:** Alexander von Humboldt Research Fellowship for 24 month-project in Germany. Project Title: Unravelling dynamic processes in vertebrate rods phototransduction: integrating biochemical/biophysical experiments with computational modelling at a systems-level
- **2009:** European Science Foundation – Short Visit Grant (Lund, Sweden). Project title: Mathematical model of nanoparticle-protein interaction dynamics in biological fluids and environments
- **2009:** FEBS-Short Term Fellowship (Lund, Sweden): Project Title: Ca^{2+} signalling in vision: biophysical characterization of Ca^{2+} -dependent conformational changes in the neuronal calcium sensors guanylate cyclase-activating proteins (GCAPs) and determination of the protein-ion binding constants
- **2009:** Blancefor Boncompagni Ludovisi Grant (Stockholm, Sweden) for support of research expenses (170,000 SEK)
- **2008:** Italian Bioinformatics Society (BITS) award for the best italian PhD thesis in Bioinformatics; international reviewing committee

INVITED LECTURES AND SEMINARS

- **2013:** 38th FEBS Congress, Saint Petersburg, Russia. Invited lecture in the session “Biochemistry of Vision”. “Rhodopsin organization and phototransduction: reconciling classical and novel perspectives”.
- **2013:** 18th International Conference on Calcium Binding Proteins and Calcium Function in Health and Disease, Kiruna, Sweden. Invited lecture entitled: “Dynamics of conformational transitions in calcium sensors investigated by surface plasmon resonance”.
- **2012:** “Rhodopsin, transducin and dynamic scaffolding: rethinking the early steps in vertebrate vision”, invited seminar, Department of Physiology, University of Pisa, Italy
- **2011:** “Rhodopsin, transducin and dynamic scaffolding: rethinking the early steps in vertebrate vision”, invited seminar, Department of Pharmacology, Vanderbilt Medical School, Nashville, USA
- **2011:** “Early molecular events in vertebrate vision: the phototransduction cascade from a systems perspective”, invited seminar, Focused Meeting DYNAMO, Center for experimental Ophthalmology, Eye Clinic, University of Tuebingen, Germany
- **2011:** “Early molecular events in vertebrate vision: the phototransduction cascade from a systems perspective”, invited seminar, Department of Molecular Evolution, University Pompeu Fabra, Barcelona, Spain
- **2010:** “Systems biochemistry approaches to vertebrate phototransduction: toward a molecular understanding of disease”, Systems Biochemistry- Linked Focus Meeting, York, UK
- **2009:** “Light adaptation in rod cells under normal and altered conditions: a computational network-level analysis”, European Retina Meeting, Oldenburg, Germany
- **2008:** “Bridging the gap between systems and structural biology: protein-protein interaction as a starting point”, Dipartimento di Biologia ed Evoluzione, University of Ferrara
- **2008:** “Molecular Systems Biology approaches to phototransduction in vertebrate rods: from single photon response to light adaptation”, XIC congerence of Societa’ Italiana di Biofisica Pura ed Applicata (SIBPA), Rome
- **2007:** “Computational simulations of protein-protein recognition: predicting mutational effects on the binding thermodynamics”, Department of Physics, University of Parma
- **2007:** “Mutation-induced modulation of protein-protein interactions: fast computational screening of kinetic and thermodynamic effects”, 5th Dulbecco Telethon Institute Scientific Retreat, Foligno
- **2007:** “Computational simulations of protein-protein recognition: predicting mutational effects on the binding thermodynamics”, Department of Systems Biology – FCC Centre, Gothenburg, Sweden
- **2007:** “Computational screening of mutational effects on protein-protein and protein-DNA interactions: a fast docking-based approach”, Bologna Winter School 2007 in *Bioinformatics for Systems and Synthetic Biology*, Bologna

- **2006:** “Computational screening of mutational effects on protein-protein and protein-DNA interactions: a fast docking-based approach”, VI Convegno Nazionale Gruppo Interdivisionale di Chimica Computazionale, Isola di San Servolo, Venezia
- **2006:** “In Silico Screening of Mutational Effects on Enzyme- Inhibitor Affinity: a Docking-based approach.”, workshop *From Computational Biophysics to Systems Biology*, Jülich, Germany
- **2005:** “Fragment complementation and rigid-body docking: a combined approach to protein domain assembly”, Department of Biophysical Chemistry, Lund, Sweden

ORGANIZATION OF INTERNATIONAL CONFERENCES AND MEETINGS

- **2013:** Co-organizer, together with Karl-Wilhelm Koch, of the European Meeting on Phototransduction, to be held June 19-22, 2013 at the HWK Delmenhorst (Germany)
- **2013:** International organizing Committee, 8th International Conference on Calcium Binding Proteins and Calcium Function in Health and Disease 30 June – 4 July, 2013 in Kiruna (Sweden)

CONFERENCES AND WORKSHOPS – CONTRIBUTIONS

- **09/2012:** Biochemical Society Focused Meeting: G-protein-coupled-receptors: from structural insights to functional mechanisms, Pisa, Italy (**poster**)
- **06/2011:** FASEB Meeting “Biology and chemistry of vision”, Carefree, Arizona, USA (**poster**)
- **04/2011:** PRO RETINA Research Colloquium, Potsdam (**poster**)
- **03/2010:** Systems Biochemistry Focused Meeting, York, UK (**selected talk**)
- **10/2009:** European Retina Meeting, Oldenburg, Germany (**selected talk**)
- **10/2008:** 6th Dulbecco Telethon Institute Scientific Retreat, Bardolino, Italy (**poster**)
- **09/2008:** European Conference on Computational Biology, Cagliari, Italy (**invited talk**)
- **09/2008:** Italian Society of Pure and Applied Biophysics Conference, Rome, Italy (**invited talk**)
- **10/2007:** SysBioHealth 2007 Symposium and Tutorials, Milan, Italy
- **09/2007:** course From Structural Genomics to Drug Discovery – Modeling the Flexibility, Parma
- **05/2007:** 5th Dulbecco Telethon Institute Scientific Retreat, Foligno, Italy (**talk**)
- **02/2007:** Bologna Winter School – Bioinformatics for Syst. and Synthetic Biology, Bologna (**talk**)
- **12/2006:** VI Convegno Nazionale Gruppo Interdivisionale di Chimica Computazionale, Isola di San Servolo, Venezia (**talk**)
- **09/2006:** Second School in Computational Cell Biology - Computational methods in multiscale processes for protein interactions, Università di Modena e Reggio Emilia, Modena
- **10/2006:** Gordon Research Conference on Computational Chemistry, Les Diablerets, Switzerland (**poster**)
- **06/2006:** Workshop: From Computational Biophysics to Systems Biology, Jülich, Germany (**talk**)
- **05/2006:** 4th Dulbecco Telethon Institute Scientific Retreat, Terni, Italy (**poster**)
- **10/2005:** 1st European Conference on Chemistry for Life Sciences, Rimini, Italy (**2 posters**)
- **06/2005:** Corso Pratico di Determinazione Strutturale mediante Diffrazione dei raggi X su cristallo singolo, curatore prof. A. Cornia, CGIS Università di Modena e Reggio Emilia
- **05/2005:** 3rd Dulbecco Telethon Institute Scientific Retreat, Orvieto, Italy (**poster**)
- **06/2004:** XXXIII Congresso Nazionale Società di Chimica Italiana, Divisione di Chimica Fisica, Napoli (**poster**)
- **09/2004:** course From Structural Genomics to Drug Discovery, Parma
- **05/2004:** 2nd Dulbecco Telethon Institute Scientific Retreat, Piacenza, Italy

REFEERING

Referee for the following Peer-review journals:

- *BBA-Proteins and Proteomics*
- *Physical Chemistry Chemical Physics*
- *PLoS Computational Biology*
- *Journal of Physical Chemistry B*
- *Molecular BioSystems*
- *Integrative Biology*
- *BioSystems*
- *Cellular and Molecular Life Sciences*

- *Biomaterials*
- *ACS Nano*
- *PLoS One*

SCIENTIFIC EVALUATION PANELS

International evaluator for the 2012 project proposals for the Romanian National Council for Scientific Research

MEMBERSHIP

- Member of the Biochemical Society (UK)
- Member of the Italian Society of Biochemistry and Molecular biology (SIB)
- Member of the Bioinformatics Italian Society (BITS)

EDITORIAL BOARDS MEMBERSHIP

Member of the editorial Board for the Journal of Nanomedicine and Biotherapeutic Discovery (2010-present)

PUBLICATIONS AND CONTRIBUTIONS

Starting from 2005, Dr. Dell'Orco has authored 28 articles appeared in international peer-reviewed journals. He is **first author** in **19** of these papers, and **corresponding author** in **12**. He has also co-authored a book chapter. To date, his papers have an **average number of citations of 9.4**, the **H-index is 11**.

PUBLICATIONS AND CONTRIBUTIONS

Peer-reviewed articles:

Underlined: *corresponding author*

1. **Dell'Orco D.** A physiological role for the supramolecular organization of rhodopsin and transducin in rod photoreceptors. *FEBS Letters* **2013**, in press, PMID: 23684654
2. Invergo BM, Montanucci L, Koch KW, Bertranpetit J, and **Dell'Orco D.** Exploring the rate-limiting steps in visual phototransduction recovery by bottom-up kinetic modeling. *Cell Commun Signal.* **2013**, in press, PMID: 23693153
3. Koch KW, **Dell'Orco D.** A Calcium-Relay Mechanism in Vertebrate Phototransduction. *ACS Chem Neurosci.* **2013**, in press. PMID: 23472635
4. Aquila M, Benedusi M, Koch KW, **Dell'Orco D.** and Rispoli G. Divalent cations modulate membrane binding and pore formation of a potent antibiotic peptide analog of alamethicin. *Cell Calcium* **2013**, 53(3):180-6
5. Cangiano L., **Dell'Orco D.** Detecting single photons: a supramolecular matter? *FEBS Letters* **2013**, 587(1):1-4.
6. **Dell'Orco D.** The Importance of the Protein Corona for Successful Nanodevice Design and Delivery. *J Nanomedic Biotherapeu Discover* **2012**, 2:1
7. **Dell'Orco D.** Sulmann, S., Linse, S., Koch KW. Dynamics of conformational Ca²⁺-switches in signaling networks detected by a planar plasmoni device. *Analytical Chemistry* **2012**, 84(6):2982-9
8. **Dell'Orco D.** Lundqvist M, Cedervall T, Linse S. Delivery succes rate of engineered nanoparticles in the presence of the protein corona: a systems-level screening. *Nanomedicine* **2012**, 8(8):1271-81
9. **Dell'Orco D.** Koch KW. A dynamic scaffolding mechanism for rhodopsin and transducin interaction in vertebrate vision. *Biochem J.* **2011** Dec 1; 440(2):263-271

10. Zernii EY, Komolov KE, Permyakov SE, Kolpakova T, **Dell'Orco D**, Poetsch A, Knyazeva EL, Grigoriev II, Permyakov EA, Senin II, Philippov PP, Koch KW. Involvement of the recoverin C-terminal segment in recognition of the target enzyme rhodopsin kinase. *Biochem J*. **2011** Apr 15;435(2):441-50.
11. **Dell'Orco D**, Koch KW. Systems biochemistry approaches to vertebrate phototransduction: towards a molecular understanding of disease. *Biochem Soc Trans*. **2010** Oct;38(5):1275-80.
12. **Dell'Orco D**, Mueller M, Koch KW. Quantitative detection of conformational transitions in a calcium sensor protein by surface plasmon resonance. *Chem Commun*. **2010** Oct 21;46(39):7316-8.
13. **Dell'Orco D**, Lundqvist M, Oslakovic C, Cedervall T, Linse S. Modeling the time evolution of the nanoparticle-protein corona in a body fluid. *PLoS One*. **2010** Jun 3;5(6):e10949.
14. Behnen P, **Dell'Orco D**, Koch KW. Involvement of the calcium sensor GCAP1 in hereditary cone dystrophies. *Biol Chem*. **2010** Jun;391(6):631-7.
15. **Dell'Orco D**, Behnen P, Linse S, Koch KW. Calcium binding, structural stability and guanylate cyclase activation in GCAP1 variants associated with human cone dystrophy. *Cell Mol Life Sci*. **2010** Mar;67(6):973-84.
16. **Dell'Orco D**, Schmidt H, Mariani S, Fanelli F. Network-level analysis of light adaptation in rod cells under normal and altered conditions. *Mol Biosyst*. **2009** Oct;5(10):1232-46.12.
17. **Dell'Orco D**. Fast predictions of thermodynamics and kinetics of protein-protein recognition from structures: from molecular design to systems biology. *Mol Biosyst*. **2009** Apr;5(4):323-34
18. Casciari D, **Dell'Orco D**, Fanelli F. Homodimerization of neurotensin 1 receptor involves helices 1, 2, and 4: insights from quaternary structure predictions and dimerization free energy estimations. *J Chem Inf Model*. **2008** Aug;48(8):1669-78.
19. **Dell'Orco D**, Casciari D, Fanelli F. Quaternary structure predictions and estimation of mutational effects on the free energy of dimerization of the OMPLA protein. *J Struct Biol*. **2008** Aug;163(2):155-62.
20. **Dell'Orco D**, Schmidt H. Mesoscopic Monte Carlo simulations of stochastic encounters between photoactivated rhodopsin and transducin in disc membranes. *J Phys Chem B*. **2008** Apr 10;112(14):4419-26.
21. Fanelli F, **Dell'Orco D**. Dark and photoactivated rhodopsin share common binding modes to transducin. *FEBS Lett*. **2008** Mar 19;582(6):991-6.
22. **Dell'Orco D**, De Benedetti PG. Quantitative structure-activity relationship analysis of canonical inhibitors of serine proteases. *J Comput Aided Mol Des*. **2008** Jun-Jul;22(6-7):469-78.
23. **Dell'Orco D**, De Benedetti PG, Fanelli F. In silico screening of mutational effects on transmembrane helix dimerization: insights from rigid-body docking and molecular dynamics simulations. *J Phys Chem B*. **2007** Aug 2;111(30):9114-24.
24. **Dell'Orco D**, De Benedetti PG, Fanelli F. In silico screening of mutational effects on enzyme proteic inhibitor affinity: a docking-based approach. *BMC Struct Biol*. **2007** Jun 8;7:37.

25. **Dell'Orco D**, Seeber M, Fanelli F. Monomeric dark rhodopsin holds the molecular determinants for transducin recognition: insights from computational analysis. *FEBS Lett.* **2007** Mar 6;581(5):944-8.
26. Fanelli F, **Dell'Orco D**. Rhodopsin activation follows precoupling with transducin: inferences from computational analysis. *Biochemistry.* **2005** Nov 15;44(45):14695-700.
27. **Dell'Orco D**, Seeber M, De Benedetti PG, Fanelli F. Probing fragment complementation by rigid-body docking: in silico reconstitution of calbindin D9k. *J Chem Inf Model.* **2005** Sep-Oct;45(5):1429-38.
28. **Dell'Orco D**, Xue WF, Thulin E, Linse S. Electrostatic contributions to the kinetics and thermodynamics of protein assembly. *Biophys J.* **2005** Mar;88(3):1991-2002.

Book chapters:

1. **Dell'Orco, D.**, De Benedetti, P.G., and Fanelli F. Single Amino Acid Contributions to Binding Affinity in Enzyme-Inhibitor Interactions: a Docking-Based Screening of BPTI-Beta Trypsin interaction, *NIC Workshop 2006, From Computational Biophysics to Systems Biology*, 2006 34: 67-72.