

CV Francesca Fanelli

Education

1989: Master degree in Medicinal Chemistry with full marks from the University of Bari.

1994: PhD in Medicinal Chemistry in the area of Computational Medicinal and Biophysical Chemistry from the University of Bari. Almost two years were spent at the Department of Chemistry, University of Modena, Italy.

Employment and Research Experience

1994-2001: postdoctoral fellow at the University of Modena and Reggio Emilia (UNIMORE) supported by the Pharmaceutical Company Recordati S.p.A. During the eight post-doctoral years she made frequent visits at the University of Lausanne (Switzerland) in the context of a scientific collaboration.

2000-2005: external consultant of Seroxo Pharmaceutical Research Institute (Geneva, Switzerland) on structure-based optimization of selected GPCR ligands.

2002-2006: Assistant Scientist of the Dulbecco Telethon Institute (DTI), hosted by the Department of Chemistry, UNIMORE. DTI is a program of personal awards conceived to avoid "Brain Drain" or allow "Brain Gain".

2007-2011: Associate Scientist of DTI hosted by the Department of Chemistry, UNIMORE.

2007-November 2019: Associate Professor of Biochemistry, Department of Life Sciences, UNIMORE.

December 2019-present: Professor of Biochemistry, Department of Life Sciences, UNIMORE.

2002-present: FF leads a research laboratory of Computational Structural Biology (<https://www.csbl.unimore.it/>).

Awards

Dulbecco Telethon Institute Career award, Call 2001

Editorial Boards and Scientific Committees

-Member of the Editorial Boards of *Receptors and Signal Transduction Research* (<https://www.tandfonline.com/loi/irst20>);

-January and April 2019: guest Editor of PLOS Computational Biology;

-2015-2017: member of the Technical Scientific AIRC Fellowship Committee;

-Member of the Scientific Committee of the Internazionale dell'International Center for Translational Eye Research (ICTER), Warsaw (Poland).

Faculty member in PhD Programs

2007-2014: PhD Program in Neuroscience, UNIMORE;

2015-present: PhD Program in Molecular and Regenerative Medicine, UNIMORE.

Institutional roles

January 2013-October 2018: member of the Life Science Department Council (Giunta del Dipartimento);

September 2014-present: member and coordinator (since January 2019) of the departmental Research Committee;

Since December 2019: member of UNIMORE Research Observatory;

Since January 2020: member of UNIMORE Research Committee.

Since March 2022: member of the departmental Quality Committee

Reviewer activity

FF served as a reviewer for a number of granting agencies and journals (several times for each agency/journal, a selection of which is listed below in alphabetic order).

Granting agencies:

BBSRC (Biotechnology and Biological Sciences Research Council, UK); ISCRA (Italian SuperComputing Resource Allocation); NDP (National Development Plan) & European Union

Structural Funds; National Science Centre (Poland); NWO (Netherlands Organisation for Scientific Research); SFI (Science Foundation of Ireland); Swiss National Science Foundation.

Journals:

ACS Chemical Neurosci., BMC Biochemistry, Biochemistry, Bioinformatics, Bioorg. Med. Chem., Biophysical J., Curr. Med. Chem., Curr. Pharm. Des., Expert Opin. Drug Discov., FASEB J., FEBS J., Frontiers Pharmacol., J. Am. Chem. Soc., J. Biol. Chem., J. Biomol. Struct. Dyn., J. Chem. Inf. Model., J. Chem. Theory Comput., J. Comput. Aided Mol. Des., J. Med. Chem., J. Mol. Model., J. Phys. Chem. B, Mol. Endocrinol., Mol. Pharmacol., Nature Communications, Nature Struct. Mol. Biol., Pharmacol. Rev., PLoS Comput. Biol., PLoS One, J. Recept. Signal Transduct. Res., Proteins, Sci Reports.

Selection of invited talks

1. First European Congress of Pharmacology, June 16-19, 1995 - Milano, Italy; talk entitled: "Computer simulation of signal transduction mechanism in a α 1b-adrenergic and m3-muscarinic receptors".
2. Advanced graduate course in receptor research: Structure and Function of G-protein Coupled Receptors, August 31-September 2, 1995 - BioCity, Turku Finland; talk entitled: "Computer simulations of ligand- and mutation-induced activation of G protein coupled receptors".
3. International Society of Quantum Biology and Pharmacology President's meeting: Molecular Structure and Dynamics in Biology, September 8-11, 1998 - Elba, Italy; talk entitled: "Theoretical study on receptor/G protein recognition: new insights into the mechanism of the α 1b-adrenergic receptor activation"
4. Seminar entitled: "*Methods for predicting protein structure. Modeling and computer simulation of GPCR activation*", February 5, 1998 - Department of Pharmacology, University of Milano, Milano, Italy.
5. Seminar entitled: "*Protein structure predictions*", April 2, 1998 - Institut of Pharmacology and Toxicology, University of Lausanne, Lausanne, Switzerland.
6. Seminar entitled: "*Molecular Modeling of the LH receptor*", March 25, 1999 - Faculty of Medicine and Health Sciences, Erasmus University Rotterdam, The Netherlands.
7. Symposium on: "G-Protein Coupled Receptors: Structure and Interaction with Partners", April 3, 2001 - College de France, Paris, France; talk entitled: "GPCR Function: Insights from Natural, Engineered and Computer-Simulated Mutations".
8. X Convention Scientifica Telethon, November 18-20, 2001 - Riva del Garda, Italy; "Understanding the activation of the lutropin receptor from natural, engineered and computer-simulated mutations".
9. Meeting on: "Biophysics & Modeling of the 7-Trans-Membrane Receptor Gene Family, December, 13-15, 2001 - St. Cetherine's College, Oxford, England; lecture entitled: "Understanding GPCR activation by molecular modeling of natural and engineered receptor mutation".
10. 12th European Workshop on Molecular and Cellular Endocrinology of the Testis, April 6-10, 2002 - Doorwerth, The Netherlands; plenary lecture entitled: "Understanding the mutation-induced activation of the lutropin receptor from computer simulation".
11. Congresso Nazionale SIE, September 24-27, 2003 - Milano, Italy; lecture entitled: "Anatomia molecolare" within the Symposium on "Recettori accoppiati alle G-proteine".
12. Workshop on: "Proteins from Pathology to Therapy", December, 19, 2003 - Department of Pharmaceutical Sci., Milano, Italy; talk entitled: "Insights into GPCR function from Computational modeling".
13. 12th International Congress of Endocrinology, August 31-September 4, 2004 - Lisbon, Portugal; lecture entitled: "LH receptor modeling"
14. International Conference on Gonadotropins & Receptors, April 12-17, 2005 - Athens, Georgia, USA; lecture entitled: "Hormone-Independent Active States and Supramolecular Organization of the LH Receptor: Insights from Computational Modeling".
15. Workshop on: "Recettori: dal silicio al laboratorio", June 17, 2005 - Department of Pharmaceutical Sci., Milano, Italy; talk entitled: "Integrazione di modellistica computazionale

- ed esperimenti in vitro nello studio delle relazioni struttura-funzione in recettori accoppiati a proteina G”.
16. XX Congress of the International Union of Crystallography, August 23-31, 2005 - Firenze, Italy; lecture entitled:” Computational modeling of GPCRs: insight into the function of the most privileged drug targets”.
 17. Congress of the Italian Society for Neurosciences, October 1-4, 2005 - Ischia, Italy; Lecture entitled: “Supramolecular assemblies of GPCRs and intracellular proteins: insights from computational modeling”.
 18. 232st ACS National Meeting, March 26-30, 2006 - Atlanta, GA, USA; Talk entitled:”Inactive and active states and supramolecular organization of GPCRs: insights from computational modeling”
 19. Course entitled:”From structural Genomics to Drug Discovery – Modeling the Flexibility”, September 20-21, 2007 - Parma, Italy; Talk entitled: Intra- and Inter-molecular Communication in GPCRs.
 20. Gordon Research Conference on Molecular Pharmacology: Recent Advances In Basic And Translational Research On G Protein-Coupled Receptors and Signaling, May 31-June 5, 2009 - Il Ciocco, Lucca (Barga), Italy; "Receptor impact on G protein dynamics"
 21. Seminar entitled: “*Structural aspects of rhodopsin function and their implication in genetic diseases*”, July 1th, 2009 - DIBIT, Milano, Italy.
 22. Symposium on: “Conversazioni tra molecole: metodi di intercettazione”, June 14, 2010 - Milano, Italy; talk entitled: “*Struttura e dinamica della rodopsina: simulazione molecolare di mutanti associati a retinite Pigmentosa*”.
 23. Conference on: “Proteine 2010”, April 8-10, 2010 - Parma, Italy; Structural determinants of rhodopsin function and their implications in genetic diseases
 24. Seminar entitled: “*Insights into Rhodopsin and Transducin Function from Dynamic Structure Network Analyses*”, April 5, 2011 - King’s College, London, England.
 25. Seminar entitled: “*Approcci simulativi allo studio di mutazioni patogenetiche della rodopsina*”, April 22, 2011 - CNR - University of Pisa, Italy.
 26. EPHAR Symposium on: “Molecular Pharmacology of G protein coupled receptors and signaling partners”, June 6-7, 2011 - Istanbul, Turkey; Insights into receptor-G protein communication from dynamic structure network analysis.
 27. Seminar entitled: “*Structural determinants of rhodopsin function and their implications in genetic diseases*”; October 28, 2011 - University of Oldenburg, Oldenburg, Germany;
 28. 15th International Congress of Endocrinology- 14th European Congress of Endocrinology, May 5-9, 2012 – Firenze, Italy; Light on the structural communication in Gonadotropin Hormone Receptors: implications in genetic diseases
 29. Workshop on “From Structural Genomics to Drug Discovery-Nuclear Receptors: From *in silico* modelling to *in vivo* experiments”, September 21, 2012- Parma, Italy; Structure network analysis to unveil the molecular communication in biological systems
 30. European Meeting on Phototransduction June 19-22, 2013 - Delmenhorst, Germany. Computational modeling of rhodopsin mutations associated with Retinitis Pigmentosa towards the discovery of therapeutic agents
 31. XVII Telethon Scientific Convention, March 11, 2013 - Riva Del Garda (TN), Italy; Talk entitled;”A computational strategy to discover pharmacological chaperones with therapeutic potential for Retinitis Pigmentosa”;
 32. PhD Programme in Complex Systems for Life Sciences, March 5-6, 2013 - Torino, Italy; Computational experiments to unveil the structural determinants of genetic retinal diseases
 33. Seminar entitled:”*Computational modeling of rhodopsin mutations associated with Retinitis Pigmentosa towards the discovery of therapeutic agents*” October 25th, 2013 - CBIO, Trento, Italy.
 34. Biochemical Society Focused Meeting: GPCRs: Beyond Structure Towards Therapy, September 16-18, 2015 - Prato (FI), Italy; lecture entitled *Structural determinants of misfolding diseases linked to GPCR mutations: rhodopsin as a paradigm*
 35. Annual Meeting of the European Neuroendocrine Association Milan 2016, 18-22 October, 2016 - Milano, Italy; Application of protein structure network analysis to uncover GPCR communication

36. International Congress on Gonadotropin Receptors (ICGR)-IV Modena 2017 & 12th International Symposium on GnRH, 20-23 September, Modena, Italy; Talk entitled: "In silico analyses of GPCR functions".
37. PhD course on Signaling pathways and their relevance for human pathology, October 26-27, 2017 – Milan Italy; talk entitled: Uncovering GPCR and G Protein Function by Protein Structure Network Analysis
38. Seminar entitled: "A small chaperone improves folding and routing of rhodopsin mutants linked to inherited blindness" February 12th, 2018 – CMR (Istituto di Biochimica delle Proteine), Napoli, Italy.
39. CECAM Meeting: "Network analysis to elucidate natural system dynamics, diversity and performance 2-4 May 2019, Lion, France; Talk entitled: "Uncovering Protein Function by Structure Network Analysis".

RESEARCH GRANTS

1. PRIN2017 (2019-2023) "*Hyponatremia and syndrome of inappropriate antidiuresis in cancer: integrated in silico, in vitro, and in vivo approaches towards the discovery of therapeutic agents targeting vasopressin signaling*" (FF is coordinator of a pentacentric grant and PI of a Research Unit);
2. Fondo di Ateneo per la Ricerca 2018 (2018-2021) "*Computational tools to infer the structural determinants of conformational diseases and discover/design small chaperones with therapeutic potential*" (FF was coordinator of two Research Units);
3. Fondazione Roma Grant (2015-2019) Genomic and pharmacological therapeutic approaches to target dominant mutations in Rhodopsin (FF was PI of a Research Unit);
4. AIRC grant N. IG14811 (2014-2018) "Structure-based development of anti-cancer agents inhibiting the oncogenic activity of AKAP-Lbc" (Single-Investigator grant);
5. Telethon Italy Grant N. GGP13227 (2013-2018) "Gain-of-function mutations of the V2 vasopressin receptor in nephrogenic syndrome of inappropriate antidiuresis (NSIAD): molecular characterization and in silico identification of potential therapeutic agents" (bi-centric grant, FF was PI of a Research Unit);
6. FP7-PEOPLE-2011-COFUND - 291778 - DTI-IMPORT, Dulbecco Telethon Institute-International mobility for postdoctoral research training (FF was one of the applicant PIs);
7. Telethon Italy Grant N. GGP11210 (2011-2014), "Integrated in Silico, in Vitro, and in Vivo Studies Towards the Design of Molecules with Therapeutic Potential for Retinitis Pigmentosa" (Bicentric grant; FF was both Coordinator and PI of a Research Unit);
8. AIRC grant N. IG10740 (2010-2013), "Structural investigation of Rho GTPase activation in cancer: implication for drug design" (Single-Investigator grant);
9. Telethon-Italy grant N. S00068TELU (2007-2011), "G protein-coupled receptors: structure-functional analysis of disease-causing mutations" (Single-Investigator grant);
10. NIH grant N. DK33973 (2003-2007), "*hCG-LH/CG Receptor Binding and Activation*" (PI: J. D. Puett, UGA University, Athens GA, USA; FF was a collaborator);
11. Compagnia S. Paolo grants N. S00068CSPA-D (2003-2007), "Role of G protein-coupled receptors (GPCRs) in the ontogenesis of hereditary diseases" (FF got support for four years as a PI of DTI);
12. Telethon-Italy grant N. S00068TELA (2002-2006), "G protein-coupled receptors: structure-functional analysis of disease-causing mutations" (Single-Investigator grant).

Computer facility projects: CINECA PROJECTS

1. CINECA ISCR_A_B – (V2RMUTS - HP10BNEE5A) 2017 "Structural determinants of inherited kidney diseases linked to V2 vasopressin receptor mutations"; Total core hours: 2000000 h;
2. CINECA ISCR_A_C - (RHOGF2 - HP10CC1RCO) 2014 "Untangling functional dynamics and structural communication in Rho GTPases and their associated Guanine Exchange Factors"; total core hours: 50000 h;

3. CINECA-ISCRA C (MDRHOGEF - HP10C0DWCB) 2013 "Untangling functional dynamics and structural communication in Rho GTPases and their associated Guanine Exchange Factors"; Total core hours: 50000 h;
4. CINECA-ISCRA A (HTVSIRLI - HP10AVFSWH) 2011-2012: "High-Throughput Virtual Screening of Inhibitors of RhoA-Lbc Interaction"; Total core hours: 200000 h.

Computer facility projects: EUROPEAN FACILITY PROJECTS

1. Res Española de Supercomputacion 2011-2012: BCV-2011-2-0011: "High-Throughput Virtual Screening of Inhibitors of RhoA-Lbc Interaction". Total core hours: 400000 h;
2. Res Española de Supercomputacion 2011: BCV-2011-3-0016: "Virtual Screening towards the Discovery of Pharmacological Chaperons with Therapeutic Potential for Retinitis Pigmentosa". Total core hours: 200000 h;
3. HPC-EUROPA2 2009 - (project number: 228398): "Large time scale simulations of Ras superfamily G proteins";
4. HPC-EUROPA 2008 - (project number: 1278): "Large time scale simulations of heterotrimeric G proteins".

The full list of publications and the relative citations can be found at <https://scholar.google.com/citations?user=tkFT9g4AAAAJ&hl=en>

Modena, October 13, 2022

Francesca Farelli