PERSONAL INFORMATION

Rita Casadio



- Via Capramozza 3, 40123 Bologna (Italy)
- 0039-3495577461
- x rita.casadio@unibo.it
- 1 http://www.biocomp.unibo.it

Nationality Italian

WORK EXPERIENCE

Senior Researcher and Honorary Group Leader Biocomputing Group, University of Bologna, Bologna (Italy)

Academical Positions

2019 (11/1)-ongoing Professor Alma Mater and Lecturer, University of Bologna.

2011-2019. Joint Professor of the Shanghai Jiao Tong University, Shanghai China

2005-2015 (1/29). President of the International Bologna Master in Bioinformatics. University of Bologna, Italy

2001(10/1)-2019 (11/1). Full Professor of Biochemistry. University of Bologna, Italy

1987 - 2001 Associate Professor of Biophysics. University of Bologna, Italy

1981 - 1987 Permanent Researcher, Physics of Matter. University of Bologna, Italy

1978 - 1979 Assistant Research Biochemistry I, Cardiovascular Research Institute, University of California, San Francisco

1974 - 1981 Assegnista Ministeriale, University of Bologna, Italy.

Consulting Activity

2017-2019. Elected Vice Chair of the Elixir Europe Board, which includes scientific representatives of 23 European countries.

2008-2010 Coordinator of the Project Bioinformatics and Computational Biology at the Life Science Department of the Italian CNR

EDUCATION AND TRAINING

EQF level 8

- 1) Certificato di Studiosita' in Biofisica (Universita' degli Studi di Bologna)
- 2) Perfezionamento in Teoria e Applicazione delle Macchine Calcolatrici
- 3) Degree in Physics (Universita' degli Studi di Bologna)
- Maturità classica

Special courses and Fellowships

1983- Introduzione alla Scienza della Complessita': Processi Stocastici e Autoorganizzazione nei Sistemi Complessi (Istituto di Aggiornamento e formazione dell'ENI-TEMA, Castelgandolfo)

1982- International School on Biothermokinetics (Biozentrum, Basel)

1981- Short Term Embo Fellowship at the Department of Biophysics, University of Osnabruck (Germany)

1980- Corso Avanzato di NMR applicata in Chimica Organica e Biologia (Universita' della Calabria, Rende)

1980- International Course on Bacteriorhodopsin (Science Academy, Szeged, Ungheria)

1978- Human Biology (Medical Center, University of California, San Francisco)

1977- 2nd International Course on the Bioenergetics of Biological Membranes (Gruppo Italiano di Bioenergetica ed Accademia dei Lincei, Roma)



1976- FEBS Advanced Course n.41 on the Biochemistry of Cellular Membranes (Politecnico Federale Svizzero, Zurigo)

1973- Advanced Course on Computer Science (Universita' degli Studi di Bologna)

PERSONAL SKILLS

Mother tongue(s)

Italian

Foreign language(s)

UNDERSTANDING		SPEAKING		WRITING
Listening	Reading	Spoken interaction	Spoken production	
C1	C1	C1	C1	C1

English

Levels: A1 and A2: Basic user - B1 and B2: Independent user - C1 and C2: Proficient user

Common European Framework of Reference for Languages

Communication skills

RC integrate herself with her own research group and teaching classes, acting as a group leader and a professor (during her working life)

Organisational / managerial skills

RC organised the activities of her working group, acting as a group leader, doing fund raising and getting results. Presently she is working actively within the group.

(RC acquired this experience during her working life)

Job-related skills

Life Science; Biotechnology; Information Technology

More specifically Bioinformatics; Computational Biology; Genomics; Proteomics; Interomics; Metabolomics; NGS data analysis (Full Professor of Biochemistry and Bionformatics)

Digital skills

The Biocomputing Group counts on a computer network, comprising several servers (some 500 cores, 300 TB disk space and up to 1000 GB of RAM memory) and routinely develops algorithms for problem solving in Computational Biology/Bioinformatics. Our activities include: Genome and Proteome Annotation, Single Nucleotide Polymorphism Annotation, Protein Structure and Function prediction, Protein Stability Prediction upon mutations, Multiscale Modelling. We run several public servers (www.biocomp.unibo.it) and several platforms for genome annotation. Our tools are mainly based on machine and deep learning.

ADDITIONAL INFORMATION

Honor

2020-Distinctive honor of **FELLOW** from The International Society for Computational Biology (ISCB Fellow) in recognition of significance contributions and service to the field of computational biology.

Recent scientific appointments

2019-ongoing- Appointed Editor of Journal of Molecular Biology

2019-ongoing- Appointed Editor of NAR Bioinformatics and Genomics

2019-ongoing- Appointed member of the FEBS (Federation of the European Biochemical Societies) Fellowship Committee

2018-2019-Appointed member of PRIN 2017 evaluation panel LS2

2018-ongoing-Appointed Associate Professor of the CNR-IBIOM (Istituto di Biomembrane, Bioenergetica e biotecnologie Molecolari)

2018-2019- Appointed member of ERC (European Research Council) evalution panel LS2 (Genomics and Bioinformatics)

2017-ongoing-Representative of the Italian Ministry of Education, University and Research in the European ELIXIR Board (www.Elixir-Europe.org), the largest European Bioinformatics infrastructure

2016-2017 Invited member of HFSP (Human Frontiers Science Program) review committee for Fellowships

2015-2019. Italian representative in the NGP-Net (BMBS COST Action BM1405)

2014 (8/5)- 2018. Appointed Vice-chair (2014-2016) and Chair (2016-2018) of the Gordon Conference



on Human Single Nucleotide Polymorphisms & Disease

2013 - 2019. Representative of the University of Bologna in ELIXIR ITALIA, node of the largest European Bioinformatics infrastructure coordinated by the European Bioinformatics Institute.

2013 - 2017. Member of the Steering Committee of the IRT Alma-Seq of the University of Bologna.

2011-2015. Italian representative in the RGB-Net (COST Action TD1101)

Other appointments

2020-ongoing. Cochair of the ISCB-ECCB 2021 conference, the largest and most high profile annual meeting of scientists working in computational biology.

2017-2019. Appointed Vice Chair of the Elixir Europe Scientific Board

2017-2019. Appointed Vice Director of the Giorgio Prodi Cancer Research center at the University of Bologna

2015-2018. Elected member of the Executive Board of the Italian Society of Biochemistry and Italian representative at the Federation of European Biochemical Societies Board

2012-2016. Elected member of the Coordinating Board of the Italian full Professors of Biochemistry.

2012-2013- Evaluating Expert (GEV 05) for the Italian Agency evaluating Universities and Researches (ANVUR) on the behalf of the Italian Ministry for Education, University and Research.

2003-20013- Member of the board of directors of I.N.B.B, the Italian InterUniversity Consortium for Researches in Biostructures and Biosystems, acting also as a representative of the Italian Minister of Education, University and Research.

Research Activities

RC started her career in the fields of membrane and protein Biophysics (particularly with bacteriorhodopsin from Halobacterium Halobium and F1F0 ATPases from mesophilic organisms), both experimentally and theoretically, including mechanisms of energy conservation in bacteria. After that, she became interested in Bioinformatics and Computational Biology, developing computer modelling of relevant biological processes, such as protein folding, protein-protein and protein-DNA/RNA interactions. Her researches have been/are devoted mainly to the application of Artificial Intelligence methods to different aspects of protein modelling, including prediction of structure to function relationship with deep and neural networks, hidden Markov models and labbeling techniques, suited to analyse large volume of data. One activity is the functional annotation of biosequences and their variants, also related to human diseases. Drug Design and molecular docking are among her interests (for details see http://www.biocomp.unibo.it). One major field of research has been/is the implementation and developments of tools out of machine-learning approaches for the prediction of secondary and tertiary structure of proteins from their aminoacid residue sequences, particularly of membrane proteins and their transmembrane topology. Projects focused on the prediction of contact maps, of protein-protein and protein-DNA interaction, of the bonding state of cysteines and their topology. Presently her researches are mainly devoted to the specific development of tools based on machine and deep learning for problem solving of relevant biomedical and biotechnological problems for large scale analysis of genomic, proteomic and interactomic data (for details see http://biocomp.unibo.it) with specific focus among other topics on the implementation and developments of tools for the prediction subcellular localisation of proteins, particularly of membrane proteins, for genome and variant annotation, the prediction of variation effect on protein stability and interaction, and mutiscale modelling of data derived from Next Generation sequencing data. Recently natural langiage protein models are adopted for specific implementations. Tools developped by the group are compliant with the standards required by ELIXIR Europe (https://www.elixir-europe.org/) and integrated in the largest distributed european bioinformatic infrastructure. Projects are devoted to the analysis of interactomes, their relation with protein-protein interaction at the molecular levels and modelling of the biological complexity.

As to RC qualifications: RC is the author of over 300 publications in the field of Computatonal Biology/Bioinformatics/Biophysics and presented (invited, oral, selected oral) the work of her group at more than 300 international and national meetings. On several occasions RC gave invited lectures and/or seminars in Europe, Cina, Turkey, Oman, Equador, and USA.

RC total IF is > 1500, with some 14.744 total citations, h-index of 60 according to SCOPUS, 70 according to Google Scholar, and g- index > 110). For details: https://www.biocomp.unibo.it, https://orcid.org/0000-0002-7462-7039.

The list of her recent publications is available at www.biocomp.unibo.it and a selection (last five years) is also appended



Reviewing Activities

RC is currently acting as JMB editor, and included in the Associate Editor board of several Journals in the field of Bioinformatics, Computational Biology, Genomics and Information Technology. RC acted/acts as reviewer for several Italian, EU and extraEU funding agencies (such as FSRI, European Commission, NIH, Israelian Science Fundation, DFG, ERC, CNR, MIUR, Regione Toscana) and is often contacted for writing evaluation letters during promotion selection procedures by foreign universities.

RC acted/acts as a referee for scientific journals such as Proteins, Protein Science, Bioinformatics, FEBS Lett, Proteomics, European Journal Biochemistry, EMBO J, NAR, and for PRIN, NIH and EC research projects. She is also regularly included in the reviewing committee of several international meeting such as ISMB, WABI (co-chaired in 2005), BIRD, BBIM all devoted to different computational aspects of Bioinformatics and Computational Biology.

Presently she is a member of the Editorial Board of JMB, BMC Bioinformatics; BioDataMining; Advances inBioinformatics; BMC Research Notes; Journal of Biomedicine and Biotechnology, Advanced Studies in Biology, The Open Chemical and Biomedical Methods Journal; she has been Guest Editor to the Special Section on Computational Biology and Bioinformatics (WABI) -- Part 1 and 2 on Lecture Notes in Bioinformatics (Lecture Notes in Computer Science).

Recently RC acted as a reviewer for the research activities of CRG (Centre for Genomic Regulation), Barcelona-Spain and partecipates/ed to selection panels both in Europe and Italy.

Teaching and Assessment Activities

RC has been founder and coordinator (2005-2015) of the International Bologna Master in Bioinformatics, a two year 2nd level course at the Bologna University. She has been giving and gives courses of Molecular Theoretical Biophysics, Bioinformatics, Systems and Computational Biology.

She is routinely invited to give lectures to undergraduate and graduate students in different Master and PHD courses in Italy, Europe and Extra EU countries.

RC organised and gave one week courses on Bioinformatics at:

- Sultan Quaboos University-College of Medicine and Health (Oman, January 12-26 20012)
- Shanghai Jiao Tong University-Department of Automation, China (April 16-26, 2012; October 25-November 1, 2014)

She partecipated into final PHD evaluation sections in different occasions, recently including a joint doctorate program between LMU Munich, Technische Universität München and Moscow State University (2011); Stockholm University (2011); CNIO, Madrid (2012)

She is often acting as a remote assessor for competing positions in EU and extra EU countries. She is/has been partecipating to several national selection committees and also member of the evaluation committee of a CNR call for a research position in Genetics/Bioinformatics.

RC with the Biocomputing Unit of Bologna is active in organizing International Schools on Bioinformatics (www.biocomp.unibo.it) and the Bologna Master in Bioinformatics.

RC has been involved in several PHD programs of the Bologna University, all related to Computational Biology and Bioinformatics for about some 30 theses through the years. She is now a faculty member of the PHD program in Data Science and Computation. She is teaching and routinely involved in other PHD programs in Europe, partecipating to the final exams of PHD Evaluation.

Memberships

RC is presently member of:

- the Academy of Science of the Bologna Institute (elected full honorary member since 2009 and Vice President, President of the Physical Classes for a three year term, since 1-11-2018)
- the Italian Society of Biochemistry (where she has been coordinating the group of Bioinformatics/Computational Biology (2011-2014)),
- the International Society of Computational Biology (ISCB, since 1999)*,
- the Italian Society of Bioinformatics (since 2003, founder member)

*RC has been a member of the board of directors of ISCB, the International Society of Computational Biology, comprising over 800 researchers, in the period 2003-2009.

RC has been also member of the American Biophysical Society, of the Protein Society, and of the Italian Society of Biophysics.





The Biocomputing group of the Bologna University

About the Biocomputing Unit of the University of Bologna.

Since 1995 Rita Casadio has been the group leader of the Biocomputing Unit of the University of Bologna. The group became officially active in 1995, when the Interdepartmental Center for the Biotechnological Research of the University of Bologna (CIRB) supported the establishment of a Biocomputing Center. Since then research interests focus on different aspects of protein sequence analysis, mainly the development and implementation of predictive algorithms based on methods of machine and deep learning. The results of these works have been selected several times for presentation at the International Forum of Bioinformatics "Intelligent Systems for Molecular Biology (ISMB)". A method (CORNET) developed in the lab for the prediction of contact maps of proteins (a relevant step for the ab initio prediction of protein 3D structure) was scored the best of its category in the Critical Assessment of Techniques for Protein Structure Prediction (CASP) No 4 and No 5 (Asimolar, California, 2000 and 2002). A method for predicting the topography of outer membrane proteins based on HMM and sequence profile was acknowledged with the SGI best award at ismb02 (Edmonton, Canada, August 3-7, 2002).

More recently the group has been/is active in International Competitions to assess the validity of its computational tools (all available for end users at www.biocomp.unibo.it) for annotation of desease related variants (CAGI, Critical Assessment of Genome Interpretation, since 2011-ongoing) and annotation of functions from protein sequences (CAFA, Critical Assessment of Function Annotation, since 2010-ongoing). The results of the group always scored among the highest and were/are reported in co-outhered publications with other emerging groups known at international level.

The group is member of the European Bioinformatics Community (ECBB), and is active in organizing international training courses since 1999 (**Bologna Winter Schools**) on Bioinformatics (<u>www.biocomp.unibo.it</u>), focusing on different aspects of the analysis of biological data.

In 2006 the Group organized in Bologna BITS, the Annual Conference of the Italian Society of Bioinformatics and more recently, workshops on Computational Biology (2016, 2017, 2018) with the sponsorship of the Italian Society of Biochemistry. Occasionally, the group hosted training activities of EIIXIR Europe (2017), and special workshops on Bioschemas, sponsered by Elixir Italy and Europe (2018).

The Biocomputing group has been a node of a network of excellence (BIOSAPIENS) within the VIth European Community framework (2004-2009) and a node of the National platform LIBI for Bioinformatics (2003-2011). It was involved in two European Cost Action activities for the Rabbit Genome (2011-2016) and NGP-NET in Biomedicine (2015-ongoing) and two Italian National projects for operative research in animal genetics. RC and the Biocomputing group had/have contacts and collaborations with some of the major research groups working in Bioinformatics and Computational Biology in Europe.

The Group through the years hosted several Professors (two of them ISA Fellows) and PhD students for collaborations (https://www.biocomp.unibo.it)

Special recognitions to the Biocomputing Group work are listed below:

- 1) SGI Best Paper Award at the International Conference on Intelligent Systems for Molecular Biology 2002, (ISMB2002) Edmonton (Canada) August 3-7, 2002:Martelli PL, Fariselli P, Krogh A, Casadio R —A sequence-profile-based HMM for predicting and discriminating beta barrel membrane proteins-Bioinformatics 18: S46-S53 (2002)
- 2) Selection for the Human Mutation Virtual Issue "Evaluating Mutation Patogenicity"; Tavtigian SV and Greenblatt MS, eds; May 2010: Calabrese R, Capriotti E, Fariselli P, Martelli PL, Casadio R Functional annotations improve the predictive score of human disease-related mutations in proteins-Hum Mutat 30:1237-1244 (2009) (Selected for the Human Mutation Virtual Issue "Evaluating Mutation Patogenicity"; Tavtigian SV and Greenblatt MS, eds; May 2010)
- 3) Evaluated as Recommended by Faculty of 1000, Biology reports: Fariselli P, Finelli M, Marchignoli D, Martelli PL, Rossi I, Casadio R -MaxSubSeq: an algorithm for segment-length optimization. The case study of the transmembrane spanning segments- Bioinformatics 19:500-505 (2003)
- 4) Evaluated as Recommended by Faculty of 1000, Biology reports: Martelli PL, Fariselli P, Krogh A, Casadio R-A sequence-profile-based HMM for predicting and discriminating beta barrel membrane proteins-Bioinformatics 18: S46-S53 (2002)

Patents:

1) Antonio Facchiano, Francesco Facchiano, Ivan Rossi, Rita Casadio

"Molecole non peptidiche analoghe al peptide RGD con effetto inibitorio sulla adesione, la migrazione e la proliferazione cellulare" Domanda n. RM2001A000089 depositata il 21.02.2001 a ROMA per Brevetto Nazionale (Italy)



2) Antonio Facchiano, Francesco Facchiano, Ivan Rossi, Rita Casadio

"RGD-analog non-peptidic molecules having anti-adhesive, Anti-migration anti-proliferative effects" Domanda n. WO 02/066421A1 depositata il 29.08.2002 a Agente: SARPI Maurizio, Studio Ferrario, Via Collina 36 00187 ROMA ITALIA per Brevetto "Europeo" in ARIPO PATENT, EUASIAN PATENT,

EUROPEAN PATENT, OAP PATENT (European Patent) Assegnatari: Istituto Dermopatico dell'Immacolata, Roma

3) Antonio Facchiano, Francesco Facchiano, Ivan Rossi, Rita Casadio

"RGD-analog non-peptidic molecules having anti-adhesive, anti-migration anti-proliferative effects" Domanda n. US20020119932A1 depositata il 29.08.2002 a YOUNG & THOMPSON, 745 South 23rd Stren 2nd Floor, Arlington, VA, 22202 per Brevetto Nazionale (United States of America) in United States of America

Selected Publications (in the last 4 years, www.biocomp.unibo.it)

- 1: Jain S, Trinidad M, Nguyen TB, Jones K, Neto SD, Ge F, Glagovsky A, Jones C, Moran G, Wang B, Rahimi K, Çalıcı SZ, Cedillo LR, Berardelli S, Özden B, Chen K, Katsonis P, Williams A, Lichtarge O, Rana S, Pradhan S, Srinivasan R, Sajeed R, Joshi D, Faraggi E, Jernigan R, Kloczkowski A, Xu J, Song Z, Özkan S, Padilla N, de la Cruz X, Acuna-Hidalgo R, Grafmüller A, Barrón LTJ, Manfredi M, Savojardo C, Babbi G, Martelli PL, Casadio R, Sun Y, Zhu S, Shen Y, Pucci F, Rooman M, Cia G, Raimondi D, Hermans P, Kwee S, Chen E, Astore C, Kamandula A, Pejaver V, Ramola R, Velyunskiy M, Zeiberg D, Mishra R, Sterling T, Goldstein JL, Lugo-Martinez J, Kazi S, Li S, Long K, Brenner SE, Bakolitsa C, Radivojac P, Suhr D, Suhr T, Clark WT. Evaluation of enzyme activity predictions for variants of unknown significance in Arylsulfatase A. bioRxiv [Preprint]. 2024 May 19:2024.05.16.594558. doi: 10.1101/2024.05.16.594558. PMID: 38798479; PMCID: PMC11118473.
- 2: Manfredi M, Savojardo C, Iardukhin G, Salomoni D, Costantini A, Martelli PL, Casadio R. Alpha&ESMhFolds: A Web Server for Comparing AlphaFold2 and ESMFold Models of the Human Reference Proteome. J Mol Biol. 2024 May 6:168593. doi: 10.1016/j.jmb.2024.168593. Epub ahead of print. PMID: 38718922.
- 3: Stenton SL, O'Leary MC, Lemire G, VanNoy GE, DiTroia S, Ganesh VS, Groopman E, O'Heir E, Mangilog B, Osei-Owusu I, Pais LS, Serrano J, Singer-Berk M, Weisburd B, Wilson MW, Austin-Tse C, Abdelhakim M, Althagafi A, Babbi G, Bellazzi R, Bovo S, Carta MG, Casadio R, Coenen PJ, De Paoli F, Floris M, Gajapathy M, Hoehndorf R, Jacobsen JOB, Joseph T, Kamandula A, Katsonis P, Kint C, Lichtarge O, Limongelli I, Lu Y, Magni P, Mamidi TKK, Martelli PL, Mulargia M, Nicora G, Nykamp K, Pejaver V, Peng Y, Pham THC, Podda MS, Rao A, Rizzo E, Saipradeep VG, Savojardo C, Schols P, Shen Y, Sivadasan N, Smedley D, Soru D, Srinivasan R, Sun Y, Sunderam U, Tan W, Tiwari N, Wang X, Wang Y, Williams A, Worthey EA, Yin R, You Y, Zeiberg D, Zucca S, Bakolitsa C, Brenner SE, Fullerton SM, Radivojac P, Rehm HL, O'Donnell-Luria A. Critical assessment of variant prioritization methods for rare disease diagnosis within the rare genomes project. Hum Genomics. 2024 Apr 29;18(1):44. doi: 10.1186/s40246-024-00604-w. PMID: 38685113; PMCID: PMC11057178.
- 4: Manfredi M, Savojardo C, Martelli PL, Casadio R. CoCoNat: A Deep Learning-Based Tool for the Prediction of Coiled-coil Domains in Protein Sequences. Bio Protoc. 2024 Feb 20;14(4):e4935. doi: 10.21769/BioProtoc.4935. PMID: 38405078; PMCID: PMC10883893.
- 5: Critical Assessment of Genome Interpretation Consortium. CAGI, the Critical Assessment of Genome Interpretation, establishes progress and prospects for computational genetic variant interpretation methods. Genome Biol. 2024 Feb 22;25(1):53. doi: 10.1186/s13059-023-03113-6. PMID: 38389099; PMCID: PMC10882881.
- 6: Bertolini E, Babbi G, Savojardo C, Martelli PL, Casadio R. MultifacetedProtDB: a database of human proteins with multiple functions. Nucleic Acids Res. 2024 Jan 5;52(D1):D494-D501. doi: 10.1093/nar/gkad783. PMID: 37791887; PMCID: PMC10767882.
- 7: Casadio R, Babu MM. Editorial overview: Sequences and topology. Curr Opin Struct Biol. 2023 Oct;82:102677. doi: 10.1016/j.sbi.2023.102677. Epub 2023 Aug 16. PMID: 37595511.
- 8: Stenton SL, O'Leary M, Lemire G, VanNoy GE, DiTroia S, Ganesh VS, Groopman E,



O'Heir E, Mangilog B, Osei-Owusu I, Pais LS, Serrano J, Singer-Berk M, Weisburd B, Wilson M, Austin-Tse C, Abdelhakim M, Althagafi A, Babbi G, Bellazzi R, Bovo S, Carta MG, Casadio R, Coenen PJ, De Paoli F, Floris M, Gajapathy M, Hoehndorf R, Jacobsen JOB, Joseph T, Kamandula A, Katsonis P, Kint C, Lichtarge O, Limongelli I, Lu Y, Magni P, Mamidi TKK, Martelli PL, Mulargia M, Nicora G, Nykamp K, Pejaver V, Peng Y, Pham THC, Podda MS, Rao A, Rizzo E, Saipradeep VG, Savojardo C, Schols P, Shen Y, Sivadasan N, Smedley D, Soru D, Srinivasan R, Sun Y, Sunderam U, Tan W, Tiwari N, Wang X, Wang Y, Williams A, Worthey EA, Yin R, You Y, Zeiberg D, Zucca S, Bakolitsa C, Brenner SE, Fullerton SM, Radivojac P, Rehm HL, O'Donnell-Luria A. Critical assessment of variant prioritization methods for rare disease diagnosis within the Rare Genomes Project. medRxiv [Preprint]. 2023 Aug 4:2023.08.02.23293212. doi: 10.1101/2023.08.02.23293212. Update in: Hum Genomics. 2024 Apr 29;18(1):44. doi: 10.1186/s40246-024-00604-w. PMID: 37577678; PMCID: PMC10418577.

- 9: Aspromonte MC, Conte AD, Zhu S, Tan W, Shen Y, Zhang Y, Li Q, Wang MH, Babbi G, Bovo S, Martelli PL, Casadio R, Althagafi A, Toonsi S, Kulmanov M, Hoehndorf R, Katsonis P, Williams A, Lichtarge O, Xian S, Surento W, Pejaver V, Mooney SD, Sunderam U, Srinivasan R, Murgia A, Piovesan D, Tosatto SCE, Leonardi E. CAGI6 ID-Challenge: Assessment of phenotype and variant predictions in 415 children with Neurodevelopmental Disorders (NDDs). Res Sq [Preprint]. 2023 Aug 2:rs.3.rs-3209168. doi: 10.21203/rs.3.rs-3209168/v1. PMID: 37577579; PMCID: PMC10418555.
- 10: Madeo G, Savojardo C, Manfredi M, Martelli PL, Casadio R. CoCoNat: a novel method based on deep learning for coiled-coil prediction. Bioinformatics. 2023 Aug 1;39(8):btad495. doi: 10.1093/bioinformatics/btad495. PMID: 37540220; PMCID: PMC10425188.
- 11: Savojardo C, Martelli PL, Casadio R. Finding functional motifs in protein sequences with deep learning and natural language models. Curr Opin Struct Biol. 2023 Aug;81:102641. doi: 10.1016/j.sbi.2023.102641. Epub 2023 Jun 28. PMID: 37385080.
- 12: Schweke H, Xu Q, Tauriello G, Pantolini L, Schwede T, Cazals F, Lhéritier A, Fernandez-Recio J, Rodríguez-Lumbreras LA, Schueler-Furman O, Varga JK, Jiménez-García B, Réau MF, Bonvin AMJJ, Savojardo C, Martelli PL, Casadio R, Tubiana J, Wolfson HJ, Oliva R, Barradas-Bautista D, Ricciardelli T, Cavallo L, Venclovas Č, Olechnovič K, Guerois R, Andreani J, Martin J, Wang X, Terashi G, Sarkar D, Christoffer C, Aderinwale T, Verburgt J, Kihara D, Marchand A, Correia BE, Duan R, Qiu L, Xu X, Zhang S, Zou X, Dey S, Dunbrack RL, Levy ED, Wodak SJ. Discriminating physiological from non-physiological interfaces in structures of protein complexes: A community-wide study. Proteomics. 2023 Sep;23(17):e2200323. doi: 10.1002/pmic.202200323. Epub 2023 Jun 27. PMID: 37365936; PMCID: PMC10937251.
- 13: Manfredi M, Savojardo C, Martelli PL, Casadio R. ISPRED-SEQ: Deep Neural Networks and Embeddings for Predicting Interaction Sites in Protein Sequences. J Mol Biol. 2023 Jul 15;435(14):167963. doi: 10.1016/j.jmb.2023.167963. Epub 2023 Jan 13. PMID: 37356906.
- 14: Mathews DH, Casadio R, Sternberg MJE. Computational Resources for Molecular Biology 2023. J Mol Biol. 2023 Jul 15;435(14):168160. doi: 10.1016/j.jmb.2023.168160. Epub 2023 May 25. PMID: 37244569.
- 15: Licata L, Via A, Turina P, Babbi G, Benevenuta S, Carta C, Casadio R, Cicconardi A, Facchiano A, Fariselli P, Giordano D, Isidori F, Marabotti A, Martelli PL, Pascarella S, Pinelli M, Pippucci T, Russo R, Savojardo C, Scafuri B, Valeriani L, Capriotti E. Resources and tools for rare disease variant interpretation. Front Mol Biosci. 2023 May 10;10:1169109. doi: 10.3389/fmolb.2023.1169109. PMID: 37234922; PMCID: PMC10206239.
- 16: Martelossi J, Forni G, Iannello M, Savojardo C, Martelli PL, Casadio R, Mantovani B, Luchetti A, Rota-Stabelli O. Wood feeding and social living: Draft genome of the subterranean termite Reticulitermes lucifugus (Blattodea; Termitoidae). Insect Mol Biol. 2023 Apr;32(2):118-131. doi: 10.1111/imb.12818. Epub 2022 Nov 21. PMID: 36366787.
- 17: Savojardo C, Baldazzi D, Babbi G, Martelli PL, Casadio R. Mapping human disease-associated enzymes into Reactome allows characterization of disease



groups and their interactions. Sci Rep. 2022 Oct 26;12(1):17963. doi: 10.1038/s41598-022-22818-5. PMID: 36289281; PMCID: PMC9605996.

- 18: Manfredi M, Savojardo C, Martelli PL, Casadio R. E-SNPs&GO: embedding of protein sequence and function improves the annotation of human pathogenic variants. Bioinformatics. 2022 Nov 30;38(23):5168-5174. doi: 10.1093/bioinformatics/btac678. PMID: 36227117; PMCID: PMC9710551.
- 19: Babbi G, Savojardo C, Baldazzi D, Martelli PL, Casadio R. Pathogenic variation types in human genes relate to diseases through Pfam and InterPro mapping. Front Mol Biosci. 2022 Sep 16;9:966927. doi: 10.3389/fmolb.2022.966927. PMID: 36188216; PMCID: PMC9523224.
- 20: Madeo G, Savojardo C, Martelli PL, Casadio R. SVMyr: A Web Server Detecting Co- and Post-translational Myristoylation in Proteins. J Mol Biol. 2022 Jun 15;434(11):167605. doi: 10.1016/j.jmb.2022.167605. Epub 2022 Apr 26. PMID: 35662454.
- 21: Casadio R, Mathews DH, Sternberg MJE. Computational Resources for Molecular Biology 2022. J Mol Biol. 2022 Jun 15;434(11):167625. doi: 10.1016/j.jmb.2022.167625. Epub 2022 May 13. PMID: 35569508.
- 22: Casadio R, Savojardo C, Fariselli P, Capriotti E, Martelli PL. Turning Failures into Applications: The Problem of Protein $\Delta\Delta G$ Prediction. Methods Mol Biol. 2022;2449:169-185. doi: 10.1007/978-1-0716-2095-3_6. PMID: 35507262.
- 23: Calmet X, Casadio R, Hsu SDH, Kuipers F. Quantum Hair from Gravity. Phys Rev Lett. 2022 Mar 18;128(11):111301. doi: 10.1103/PhysRevLett.128.111301. PMID: 35362995.
- 24: Savojardo C, Babbi G, Baldazzi D, Martelli PL, Casadio R. A Glance into MTHFR Deficiency at a Molecular Level. Int J Mol Sci. 2021 Dec 23;23(1):167. doi: 10.3390/ijms23010167. PMID: 35008593; PMCID: PMC8745156.
- 25: Manfredi M, Savojardo C, Martelli PL, Casadio R. DeepREx-WS: A web server for characterising protein-solvent interaction starting from sequence. Comput Struct Biotechnol J. 2021 Oct 13;19:5791-5799. doi: 10.1016/j.csbj.2021.10.016. PMID: 34765094; PMCID: PMC8566768.
- 26: Luchetti A, Forni G, Martelossi J, Savojardo C, Martelli PL, Casadio R, Skaist AM, Wheelan SJ, Mantovani B. Comparative genomics of tadpole shrimps (Crustacea, Branchiopoda, Notostraca): Dynamic genome evolution against the backdrop of morphological stasis. Genomics. 2021 Nov;113(6):4163-4172. doi: 10.1016/j.ygeno.2021.11.001. Epub 2021 Nov 5. PMID: 34748900.
- 27: Andrews AJ, Puncher GN, Bernal-Casasola D, Di Natale A, Massari F, Onar V, Toker NY, Hanke A, Pavey SA, Savojardo C, Martelli PL, Casadio R, Cilli E, Morales-Muñiz A, Mantovani B, Tinti F, Cariani A. Ancient DNA SNP-panel data suggests stability in bluefin tuna genetic diversity despite centuries of fluctuating catches in the eastern Atlantic and Mediterranean. Sci Rep. 2021 Oct 20;11(1):20744. doi: 10.1038/s41598-021-99708-9. PMID: 34671077; PMCID: PMC8528830.
- 28: Walsh I, Fishman D, Garcia-Gasulla D, Titma T, Pollastri G; ELIXIR Machine Learning Focus Group; Harrow J, Psomopoulos FE, Tosatto SCE. Author Correction: DOME: recommendations for supervised machine learning validation in biology. Nat Methods. 2021 Nov;18(11):1409-1410. doi: 10.1038/s41592-021-01304-2. Erratum for: Nat Methods. 2021 Oct;18(10):1122-1127. doi: 10.1038/s41592-021-01205-4. PMID: 34556867.
- 29: Walsh I, Fishman D, Garcia-Gasulla D, Titma T, Pollastri G; ELIXIR Machine Learning Focus Group; Harrow J, Psomopoulos FE, Tosatto SCE. DOME: recommendations for supervised machine learning validation in biology. Nat Methods. 2021 Oct;18(10):1122-1127. doi: 10.1038/s41592-021-01205-4. Erratum in: Nat Methods. 2021 Nov;18(11):1409-1410. doi: 10.1038/s41592-021-01304-2. PMID: 34316068.
- 30: Martelli PL, Savojardo C, Fariselli P, Tartari G, Casadio R. Computer-Aided Prediction of Protein Mitochondrial Localization. Methods Mol Biol. 2021;2275:433-452. doi: 10.1007/978-1-0716-1262-0_28. PMID: 34118055.



- 31: Savojardo C, Babbi G, Martelli PL, Casadio R. Mapping OMIM Disease-Related Variations on Protein Domains Reveals an Association Among Variation Type, Pfam Models, and Disease Classes. Front Mol Biosci. 2021 May 7;8:617016. doi: 10.3389/fmolb.2021.617016. PMID: 34026820; PMCID: PMC8138129.
- 32: Madeo G, Savojardo C, Martelli PL, Casadio R. BetAware-Deep: An Accurate Web Server for Discrimination and Topology Prediction of Prokaryotic Transmembrane β-barrel Proteins. J Mol Biol. 2021 May 28;433(11):166729. doi: 10.1016/j.jmb.2020.166729. Epub 2020 Dec 3. PMID: 33972021.
- 33: Baldazzi D, Savojardo C, Martelli PL, Casadio R. BENZ WS: the Bologna ENZyme Web Server for four-level EC number annotation. Nucleic Acids Res. 2021 Jul 2;49(W1):W60-W66. doi: 10.1093/nar/gkab328. PMID: 33963861; PMCID: PMC8262719.
- 34: Bonora E, Chakrabarty S, Kellaris G, Tsutsumi M, Bianco F, Bergamini C, Ullah F, Isidori F, Liparulo I, Diquigiovanni C, Masin L, Rizzardi N, Cratere MG, Boschetti E, Papa V, Maresca A, Cenacchi G, Casadio R, Martelli P, Matera I, Ceccherini I, Fato R, Raiola G, Arrigo S, Signa S, Sementa AR, Severino M, Striano P, Fiorillo C, Goto T, Uchino S, Oyazato Y, Nakamura H, Mishra SK, Yeh YS, Kato T, Nozu K, Tanboon J, Morioka I, Nishino I, Toda T, Goto YI, Ohtake A, Kosaki K, Yamaguchi Y, Nonaka I, Iijima K, Mimaki M, Kurahashi H, Raams A, MacInnes A, Alders M, Engelen M, Linthorst G, de Koning T, den Dunnen W, Dijkstra G, van Spaendonck K, van Gent DC, Aronica EM, Picco P, Carelli V, Seri M, Katsanis N, Duijkers FAM, Taniguchi-Ikeda M, De Giorgio R. Biallelic variants in LIG3 cause a novel mitochondrial neurogastrointestinal encephalomyopathy. Brain. 2021 Jun 22;144(5):1451-1466. doi: 10.1093/brain/awab056. PMID: 33855352.
- 35: Babbi G, Savojardo C, Martelli PL, Casadio R. Huntingtin: A Protein with a Peculiar Solvent Accessible Surface. Int J Mol Sci. 2021 Mar 12;22(6):2878. doi: 10.3390/ijms22062878. PMID: 33809039; PMCID: PMC8001614.
- 36: Ledwaba MB, Glover BA, Matle I, Profiti G, Martelli PL, Casadio R, Zilli K, Janowicz A, Marotta F, Garofolo G, van Heerden H. Whole Genome Sequence Analysis of <i>Brucella abortus</i> Isolates from Various Regions of South Africa. Microorganisms. 2021 Mar 11;9(3):570. doi: 10.3390/microorganisms9030570. PMID: 33799545; PMCID: PMC7998772.
- 37: Casadio R, Lenhard B, Sternberg MJE. Computational Resources for Molecular Biology 2021. J Mol Biol. 2021 May 28;433(11):166962. doi: 10.1016/j.jmb.2021.166962. Epub 2021 Mar 24. PMID: 33774035.
- 38: Savojardo C, Manfredi M, Martelli PL, Casadio R. Solvent Accessibility of Residues Undergoing Pathogenic Variations in Humans: From Protein Structures to Protein Sequences. Front Mol Biosci. 2021 Jan 7;7:626363. doi: 10.3389/fmolb.2020.626363. PMID: 33490109; PMCID: PMC7817970.
- 39: Savojardo C, Martelli PL, Tartari G, Casadio R. Large-scale prediction and analysis of protein sub-mitochondrial localization with DeepMito. BMC Bioinformatics. 2020 Sep 16;21(Suppl 8):266. doi: 10.1186/s12859-020-03617-z. PMID: 32938368; PMCID: PMC7493403.
- 40: Babbi G, Baldazzi D, Savojardo C, Martelli PL, Casadio R. Highlighting Human Enzymes Active in Different Metabolic Pathways and Diseases: The Case Study of EC 1.2.3.1 and EC 2.3.1.9. Biomedicines. 2020 Jul 29;8(8):250. doi: 10.3390/biomedicines8080250. PMID: 32751059; PMCID: PMC7459455.
- 41: Turri V, Latinovic OS, Bonafè M, Toyang N, Parigi M, Calassanzio M, Martelli PL, Vagheggini A, Abbati G, Sarnelli A, Casadio R, Ratti C, Massi P, Schoelz JE, Salvato MS, Piccinini F, Martinelli G. Cauliflower Mosaic Virus TAV, a Plant Virus Protein That Functions like Ribonuclease H1 and is Cytotoxic to Glioma Cells. Biomed Res Int. 2020 Mar 16;2020:7465242. doi: 10.1155/2020/7465242. PMID: 32258141; PMCID: PMC7102451.
- 42: Bovo S, Martelli PL, Di Lena P, Casadio R. NETGE-PLUS: Standard and Network-Based Gene Enrichment Analysis in Human and Model Organisms. J Proteome Res. 2020 Jul 2;19(7):2873-2878. doi: 10.1021/acs.jproteome.9b00749. Epub 2020 Feb 4.

Main funding

PMID: 31971806.



1. Coordinatore scientifico ESPRIT FP4-1998-DRUG: Supercomputing Drug Design for Industrial and Academic Partnership dal 16-01-1998 al 15-06-1999

- 2. Responsabile Unità PRIN 1997: Biocatalisi e Bioconversioni dal 15-02-1998 al 14-02-2000
- 3. Responsabile Unità PRIN 1999: Proprietà Strutturali e Funzionali, Aspetti Applicativi di Proteine Isolate da Termofili dal 26-11-1999 al 25-11-2001
- 4. Responsabile Unità FP5-IST BIOWULF: Speeding-up Biocomputing applications using a commodity-based parallel computer dal 01-12-2000 al 31-03-2002
- 5. Responsabile Unità PRIN 2001: Idrolasi da Microrganismi Termofili: Aspetti Strutturali, Funzionali ed Espressione Omologa ed Eterologa dal 12-12-2001 al 11-12-2003
- 6. Responsabile Unità PRIN 2002: Strumenti basati su apprendimento automatico per la genomica strutturale e funzionale dal 16-12-2002 al 15-12-2004
- 7. Responsabile Unità FIRB Progetti Negoziali 2001: Bioinformatica per la Genomica e la Proteomica dal 10-01-2003 al 10-07-2007
- 8. Responsabile Unità PRIN 2003: Idrolasi Termostabili e Termoattive da Archaea: Aspetti Strutturali e Funzionali dal 20-11-2003 al 19-11-2005
- 9. Responsabile unità locale FP6-2002-LIFESCIHEALTH: A European Network for Integrated Genome Annotation (BioSapiens) dal 01-01-2004 al 30-06-2009
- 10. Responsabile Unità FIRB Laboratori 2003: LIBI: Laboratorio Internazionale di BioInformatica dal 12-09-2005 al 12-09-2011
- 11. Responsabile Unità PRIN 2009: Analisi su larga scala dello splicing alternativo nel trascrittoma umano mediante approcci computazionali e sperimentali dal 17-10-2011 al 16-10-2013

Other grants

COST BMBS Action TD1101 and BM1405 (European Union RTD Framework Program) PON projects PON01_02249 and PAN Lab PONa3_00166 (Italian Miur) FARB-UNIBO 2012