Vlad Cojocaru, Ph.D., Habil.

Principal Investigator / Computational biochemist

Born on 15.07.1976 in Arad, Romania; Nationality: Romanian, German
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About me

I am an enthusiast senior research scientist with strong expertise in computational biochemistry. I have a broad interdisciplinary knowledge and experience across chemistry, physics, and biology. I dedicated my scientific career from Ph.D. student to research group leader to decode the link between the three dimensional structure and dynamics of molecules and their function in cells. I discovered how proteins influence the folding of RNA molecules, how drug metabolizing enzymes embed in lipid membranes and channel drug molecules from and to their active sites, and how specialized proteins that regulate gene expression engage and reshape DNA in different contexts. For these discoveries, I used diverse molecular modeling and simulation methods and established or self designed analysis tools. Through my research, I gained experience with computer architectures, unix, several programming languages and a variety of molecular modeling software. I have always been ambitious and enjoyed challenges, especially in designing and leading projects in highly interdisciplinary teams. Since 2012 I am leading a research team and I am guiding students towards successful completion of internships or Ph.D. studies. Currently, my research team is part of the STAR-UBB Institute of the Babeş-Bolyai University in Cluj-Napoca, Romania. Throughout my career, I have published appreciated collaborative research articles in prestigious scientific journals, gave invited lectures at prestigious international conferences and obtained third-party funding for my research. At the same time, I dedicated part of my career to developing innovative teaching programs for undergraduate and graduate students at different universities. The success of these programs was confirmed by the venia legendi (habilitation) I was awarded and by the positive evaluations received from students Currently, I am leading courses on structural bioinformatics/computational structural biology at the Babeş-Bolyai University and at the West University of Timişoara, Romania

Goals

I am enthusiastic about further developing my own research lines with challenging projects at a prestigious academic institution and about coagulating communities of scientific excellence in Romania. I am particularly excited about inter-disciplinary projects that involve state-of-the-art technologies at which I excel and novel technologies which I am looking forward to use and develop. I will continue fostering the intensive exchange between computational modelers and experimenters.

Moreover, I am dedicated to the development of new interactive teaching programs for undergraduate as well as graduate students.

Research keywords

Computational Biochemistry, Molecular Biophysics, Structural Biology, Structural Bioinformatics, Biomolecular Recognition, Biomolecular Dynamics, Computer Aided Drug Design, Transcription Factors, Chromatin Dynamics, Gene Regulation, Cell Fate Determination, Stem Cell Biology

Areas of expertise

Structural biology	Visualizing, analysing, and manipulating three dimensional structures of molecules, including proteins, nucleic acids, lipid bilayers, chemicals; applying methods to determine structures, to build structural models and to perform computer simulations of biomolecules.
Computer/IT skills	Using specialized software for structural biology and molecular modeling; basic computer programming in different languages; managing high end workstations and small computer clusters.
Management	Managing projects and a small research team; coordinating collaborative projects (attended management and coaching courses provided by the Max Planck Society)
Communication	Publishing and presenting research to specialized and non-specialized audiences; teaching (my lectures and practical courses have always been positively evaluated by students).

Work experience

Principal Investigator 2022-present	STAR-UBB Institute, Babes-Bolyai University, Cluj-Napoca, Romania
Senior Scientist 2022-2024	Utrecht University, the Netherlands
Guest scientist 2018-present	Utrecht University / Max Planck Institute (Münster, GE)
Group leader 2018-2021	Hubrecht Institute, Utrecht, NL
Project group leader 2010-2018	Max Planck Institute for Molecular Biomedicine, Münster, Germany
Research associate 2005-2010	Heidelberg Institute for Theoretical Studies, Heidelberg, Germany
Research fellow/associate 2001-2005 (Ph.D. studies)	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Education and degrees

Habilitation (2017)	Theoretical Chemistry, University of Münster, Germany
Ph.D. (2005)	Molecular Biology, University of Göttingen
M.Sc./Ph.D. International School (2000-2001)	Molecular Biology, Göttingen, Germany
B.Sc. (1999, 4 years)	Physics/Chemistry, Physics Faculty, West University of Timişoara, Romania
Romanian Baccalaureat (1995-1999)	Moise Nicoara High School, Arad, Romania

Grants

Marie Skłodowska-Curie Doctoral Networks	**“**Enhanced VAccines DEsign against antimicrobial Resistance” Resistance “EVADERE” (HORIZON-MSCA-2024-DN-01-01, prdicted 2026-2030)
Romanian Research Council (UEFISCDI)	“How do transcription factors interplay with histone tails to unravel genomic nucleosomes ?” (240.000 EUR, 2025-2027, PCE PN-IV-P1-PCE-2023-1458
German Research Foundation (DFG)	“In silico approaches to untangle the structural mechanisms of he combinatorial regulation of transcription by the pluripotency marker Oct4”, (SPP1356 Program “Pluripotency and Cellular Reprogramming”) (168.000 EUR, 2011-2014)
Gauss Center for Supercomputing	“Characterizing the structural basis for the nucleosome recognition by pioneer transcription factors” (high performance computing resources, 40 million core hours)
PRACE European Research Infrastructure	“Large scale molecular simulations of protein-DNA recognition in the combinatorial control of transcription (LASIPROD)” (high performance computing resources)
PRACE European Research Infrastructure	“Large scale molecular simulations of protein-DNA recognition in the combinatorial control of transcription (MUSIPROL)” (high performance computing resources)

Invited Talks

CECAM	Workshop on the dynamics of biomolecular interfaces Paris, France (2024)
ISQBP	President’s meeting Athens, Greece (2024), Strasbourg, France (2021, virtual), Bergen, Norway (2016)

Erwin Schroedinger Institute	ESI workshop on chromatin modelling, Vienna, Austria (2024),
Biophysical Society	**T**hematic meeting “Biophysics at the dawn of exascale computers”, Hamburg, Germany (2022)
Biophysical Society	2022 Annual Meeting, San Francisco, USA Multiscale Genome Organization subgroup (failed to attend)
Albany Conversation	20th edition (2019), Albany, USA
Biophysical Society	**T**hematic meeting “Multiscale modeling of chromatin: bridging experiment and theory”, Les Houches, France (2019)

Teaching

Babeş-Bolyai University Cluj-Napoca, Romania (2022-present)	Supervisor/Mentor (M.Sc. and Ph.D. students) Course on Integrative Structural Bioinformatics, Doctoral School for Integrative Biology (Faculty of Biology and Geology) Course on Integrative Structural Bioinformatics, M.Sc. Program in Bioinformatics (Faculty of Biology and Geology)
West University of Timişoara, Romania (2018-present)	Supervisor/Mentor (M.Sc. and Ph.D. students) Course on Advanced Computational Methods for Biomolecular Dynamics, M.Sc. Program in Bioinformatics (Faculty of Informatics)
University of Münster Germany (2012-2020)	Supervisor/Mentor (M.Sc. and Ph.D. students) Advanced practical courses, M.Sc. Programs (Biology Department) Lecture series “Current aspects in theoretical chemistry” , M.Sc. program (Chemistry Department) Lectures on Quantum Mechanics, B.Sc. Program (Chemistry Department)

Distinctions, memberships, awards, fellowships

ISQBP	President (2024-2026) Vicepresident (2022-2024)
University of Münster	Habilitation (Venia Legendi in Theoretical Chemistry, 2017)
Klaus Tschira Foundation	Postdoctoral fellowship (2005-2008)
Max Planck Society	Ph.D. fellowship (2001-2004)

Article and Research Proposal Reviews

Nature Communications, Nucleic Acids Research, PLoS Computational Biology, Journal of Chemical Theory and Computation, Proteins, Biophysical Journal, Biochemistry, Scientific Reports, Journal of

Chemical Information and Modeling, Gauss Supercomputer Center (Germany), Polish National Science Center

Skills

Technical	Molecular modeling and simulation methods and software (e.g. VMD, NAMD, Chimera, Modeller, Pymol, Amber), Unix/Linux, Programming languages (Perl, Tcl, Bash, Python)
Soft	Science communication (publications, presentations, teaching), Project and team leading, Mentoring and guidance, Conference organization, Team working and building
Languages	Romanian (mother language), English, German (fluent), Spanish (good), French, Italian (understanding level)

Also about me

I have two daughters (10 and 13 years old); I am sociable, passionate about science and nature, outdoor activities (mountaineering, skiing, football, running, trail biking) and rock music and I enjoy cooking

List of publications

1. Gao Y, Tan DS, Girbig M, Hu H, Zhou X, Xie Q, Yeung SW, Lee KS, Ho SY, Cojocaru V, Yan J, Hochberg GKA, de Mendoza A, Jauch R (2024). The emergence of Sox and POU transcription factors predates the origins of animal stem cells. *Nat Commun* **15**, 9868. https://doi.org/10.1038/s41467-024-54152-x
2. Reyes V, Giulini M, Cojocaru V, Engel A, Xu X, et al. (2024). Integrative modeling in the age of machine learning: a summary of HADDOCK strategies in CAPRI rounds 47-55. *Proteins,* https://doi.org/10.1002/prot.26789
3. Orsetti A, van Oosten D, Vasarhelyi RG, Danescu TM, Huertas J, van ingen H, Cojocaru V (2024). Structural dynamics in chromatin unraveling by pioneer transcription factors. Biophysical Reviews 16: 365-382. https://doi.org/10.1007/s12551-024-01205-6
4. MacCarthy CM, Wu G, Malik V, Menuchin-Lasowski Y, Velychko T, Keshet G, Fan R, Bedzhov I, Church GM, Jauch R, Cojocaru V, Schöler HR, Velychko S (2024). Highly cooperative chimeric super-SOX induces naive pluripotency across species. *Cell Stem Cell* 31(1): 127-147. https://doi.org/10.1016/j.stem.2023.11.010
5. Tan DS, Cheung SA, Gao Y, Weinbuch M, Hu H, Shi L, Ti AC, Hutchins AP, Cojocaru V, Jauch R (2023). The homeodomain of Oct4 is a dimeric binder of methylated CpG elements. *Nucleic Acids Research* 51(3):1120-1138. https://doi.org/10.1093/nar/gkac1262

6. MacCarthy CM, Huertas J, Ortmeier C, vom Bruch H, Tan DA, Reinke D, Sander A, Bergbrede T, Jauch R, Schöler HR, Cojocaru V (2022). OCT4 interprets and enhances nucleosome flexibility. *Nucleic Acids Research* 50(18):10311-10327. https://doi.org/10.1093/nar/gkac755
7. Guni F, Krishuns T, Schreiber JA, Henschel L, Wahrenburg M, Drexler HCA, Leidel SA, Cojocaru V, Seebohm G, Mellmann A, Schwemmle M, Ludwig S, Brunotte L (2023). The ubiquitination landscape of the influenza A virus polymerase. *Nature Communications* 14(787). https://doi.org/10.1038/s41467-023-36389-0
8. Huertas J, Schöler HR, Cojocaru V (2021). Histone tails cooperate to control the breathing of genomic nucleosomes. *PLoS Computational Biology* 17(6): e1009013 (featured on issue cover), https://doi.org/10.1371/journal.pcbi.1009013
9. Huertas J, Cojocaru V (2021). Breaths, twists, and turns of atomistic nucleosomes. *Journal of Molecular Biology* 433:166744, https://doi.org/10.1016/j.jmb.2020.166744
10. Huertas J, MacCarthy CM, Schöler HR, Cojocaru V (2020). Nucleosomal DNA Dynamics Mediate Oct4 Pioneer Factor Binding. *Biophysical Journal* 118(9):2280-2296 (featured on issue cover), https://doi.org/10.1016/j.bpj.2019.12.038
11. Öztürk MA, De M, Cojocaru V, Wade RC (2020). Chromatosome Structure and Dynamics from Molecular Simulations. *Annual Review of Physical Chemistry* 71:101-119, https://doi.org/10.1146/annurev-physchem-071119-040043
12. Viplav A, Saha T, Huertas J, Selenschik P, Ebrahimkutty MP, Grill D, Lehrich J, Hentschel A., Biasizzo M, Mengoni S, Ahrens R, Gerke V, Cojocaru V, Klingauf J, Galic M (2019). ArhGEF37 assists dynamin 2 during clathrin-mediated endocytosis. *Journal of Cell Science* 132(9):jcs226530, https://doi.org/10.1242/jcs.226530
13. Srivastava Y, Senna Tan D, Malik V, Weng M, Javed A, Cojocaru V, Wu G, Veerapandian V, Cheung LWT, Jauch R (2019). Cancer-associated missense mutations enhance the pluripotency reprogramming activity of OCT4 and SOX17. *FEBS Journal* 287(1):122-144, https://doi.org/10.1111/febs.15076
14. Wang C, Srivastava Y, Jankowski A, Malik V, Wei Y, del Rosario R, Cojocaru V, Prabhakar S, Jauch R (2018). DNA mediated dimerization on a compact sequence signature controls enhancer engagement and regulation by FOXA1. *Nucleic Acids Research* 46(11):5470-5486, https://doi.org/10.1093/nar/gky259
15. Öztürk MA, Cojocaru V, Wade RC (2018). Towards an ensemble view of the linker histone - nucleosome complex structure: A paradigm shift from one to many. *Structure* 26(8):1050-1057, https://doi.org/10.1016/j.str.2018.05.009
16. Öztürk MA, Cojocaru V, Wade RC (2018). Dependence of chromatosome structure on linker histone sequence and post-translational modifications. *Biophysical Journal* 114(10):2363-2375, https://doi.org/10.1016/j.bpj.2018.04.034
17. Jerabek S, Ng CKL, Wu G, Arauzo-Bravo MJ, Kim KP, Esch D, Malik V, Chen Y, Velychko S, Yang X, Cojocaru V, Schöler HR and Jauch R (2017). Changing POU dimerization

preferences converts Oct6 into a pluripotency inducer. *EMBO Reports* 18(2):319-333, https://doi.org/10.15252/embr.201642958

18. Hu C, Malik V, Chang YK, Veerapandian V, Srivastava Y, Huang YH, Hou L, Cojocaru V, Stormo GD, Jauch R (2017). Coop-Seq Analysis Demonstrates that Sox2Evokes Latent Specificities in the DNARecognition by Pax6. *Journal of Molecular Biology* 429:3626-3634, https://doi.org/10.1016/j.jmb.2017.10.013
19. Öztürk M, Pachov G, Wade RC, Cojocaru V (2016). Conformational selection and dynamic adaptation upon linker histone binding to the nucleosome. *Nucleic Acids Research* 19;44(14):6599-613 (featured on issue cover), https://doi.org/10.1093/nar/gkw514
20. Yu X, Nandekar P, Mustafa G, Cojocaru V, Lepesheva GI, Wade RC (2015). Ligand tunnels in *t. brucei* and human CYP51: Insights for parasite-specific drug design. *Biochimica Biophysica Acta* 1:67-78, https://doi.org/10.1002/jmr.2412
21. Tapia N, MacCarthy C, Esch D, Marthaler AG, Tiermann U, Arauzo-Bravo MJ, De Miguel MP, Jauch R, Cojocaru V, and Schöler HR (2015). Dissecting the role of distinct OCT4-SOX2 heterodimer configurations in pluripotency. *Scientific Reports* 5:13533, https://doi.org/10.1038/srep13533
22. Merino F, Bouvier B, Cojocaru V (2015). Cooperative DNA recognition modulated by an interplay between protein-protein interactions and DNA-mediated allostery. *PLoS Computational Biology* 11(6): e1004287, https://doi.org/10.1371/journal.pcbi.1004287
23. Yu X, Cojocaru V, Mustafa G, Salo-Ahen OM, Lepesheva GI, Wade RC (2015). Dynamics of CYP51: implications for function and inhibitor design. *Journal of Molecular Recognition* 28(2):59-73, https://doi.org/10.1002/jmr.2412
24. Narasimhan K, Pillay S, Huang YH, Jayabal S, Udayasuryan B, Veerapandian V, Kolatkar P, Cojocaru V, Pervushin K, Jauch R (2015). DNA-mediated cooperativity facilitates the co-selection of cryptic enhancer sequences by SOX2 and PAX6 transcription factors. *Nucleic Acids Research* 43(3):1513-28, https://doi.org/10.1093/nar/gku1390
25. Merino F, Ng CKL, Veerapandian V, Schöler HR, Jauch R, Cojocaru V (2014). Structural basis for the SOX-dependent genomic redistribution of OCT4 in stem cell differentiation. *Structure* 22(9):1274-86, https://doi.org/10.1016/j.str.2014.06.014
26. Jerabek S, Merino F, Schöler HR, Cojocaru V (2014). OCT4: dynamic DNA binding pioneers stem cell pluripotency. *Biochimica Biophysica Acta* 1839(3):138-54, https://doi.org/10.1016/j.bbagrm.2013.10.001
27. Esch D, Vahokoski J, Groves MR, Pogenberg V, Cojocaru V, Vom Bruch H, Han D, Drexler HC, Araúzo-Bravo MJ, Ng CK, Jauch R, Wilmanns M, Schöler HR (2013). A unique Oct4 interface is crucial for reprogramming to pluripotency. *Nature Cell Biology* 15(3):295-301, https://doi.org/10.1038/ncb2680

28. Yu X, Cojocaru V, Wade RC (2013). Conformational Diversity and Ligand Tunnels of Mammalian Cytochrome P450s. *Biotechnology and Applied Biochemistry* 60(1):134-45, https://doi.org/10.1002/bab.1074
29. Veith N, Feldman-Salit A, Cojocaru V, Henrich S, Kummer U, Wade RC (2013). Organism-adapted specificity of the allosteric regulation of pyruvate kinase in lactic acid bacteria. *PLoS Computational Biology* 9(7):e1003159, https://doi.org/10.1371/journal.pcbi.1003159
30. Feldman-Salit A, Hering S, Messiha HL, Veith N, Cojocaru V, Sieg A, Westerhoff HV, Kreikemeyer B, Wade RC, Fiedler T (2013). Regulation of the activity of lactate dehydrogenases from four lactic acid bacteria. *Journal of Biological Chemistry* 288(29):21295-306, https://doi.org/10.1074/jbc.m113.458265
31. Tapia N, Reinhardt P, Duemmler A, Wu G, Araúzo-Bravo MJ, Esch D, Greber B, Cojocaru V, Rascon CA, Tazaki A, Kump K, Voss R, Tanaka EM, Schöler HR (2012). Reprogramming to pluripotency is an ancient trait of vertebrate Oct4 and Pou2 proteins. *Nature Communications* 3:1279, https://doi.org/10.1038/ncomms2229
32. Cojocaru V, Winn PJ, Wade RC (2012). Multiple, ligand-dependent routes from the active site of cytochrome P50 2C9. *Current Drug Metabolism* 13(2):143-154, https://doi.org10.2174/138920012798918462
33. Cojocaru V, Balali-Mood K, Sansom MS, Wade RC (2011). Structure and dynamics of the membrane-bound cytochrome P450 2C9. PLoS Computational Biology 7(8):e1002152 (featured on issue cover), https://doi.org/10.1371/journal.pcbi.1002152
34. Slanchev K, Stebler J, Goudarzi M, Cojocaru V, Weidinger G, Raz E (2009). Control of Dead end localization and activity-implications for the function of the protein in antagonizing miRNA function. *Mechanisms of Development* 126:270-277, https://doi.org/10.1016/j.mod.2008.10.006
35. Cojocaru V, Winn PJ, Wade RC (2007) The ins and outs of cytochrome P450s. Biochimica et Biophysica Acta 770(3):390-401 (featured on issue cover), https://doi.org/10.1016/j.bbagen.2006.07.005
36. Cojocaru V, Klement R, Jovin TM (2005). Loss of G-A base pairs is insufficient for achieving a large opening of U4 snRNA K-turn motif. Nucleic Acids Research 33:3435-3446 (featured on issue cover), https://doi.org/10.1093/nar/gki664
37. Cojocaru V, Nottrott S, Klement R, Jovin TM (2005). The snRNP 15.5K protein folds its cognate K-turn RNA: A combined theoretical and biochemical study. RNA 11:197-209, https://doi.org/10.1261/rna.7149605
38. Stebler J, Spieler D, Slanchev K, Molyneaux KA, Richter U, Cojocaru V, Tarabykin V, Wylie C, Kessel M, Raz E (2004). Primordial germ cell migration in the chick and mouse embryo: the role of the chemokine SDF-1/CXCL12. Developmental Biology 272:351-61, https://doi.org/10.1016/j.ydbio.2004.05.009

Doctoral Thesis

1. Molecular motions at the 5' stem-loop of U4 snRNA: Implications for U4/U6 snRNP assembly. University of Göttingen, 2005 (https://ediss.uni-goettingen.de/bitstream/handle/11858/00-1735-0000-0006-B6C3-D/cojocaru.pdf)