

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 Timișoara, 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

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| 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

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| 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

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| 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 Timișoara, Romania |
| Romanian Baccalaureat (1995-1999) | Moise Nicoara High School, Arad, Romania |

Grants

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| German Research Foundation (DFG) | “In silico approaches to untangle the structural mechanisms of the 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

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| 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 | Thematic 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 Thematic meeting “Multiscale modeling of chromatin: bridging experiment and theory”, Les Houches, France (2019)

Teaching

Babeş-Bolyai University Supervisor/Mentor (M.Sc. and Ph.D. students)
Cluj-Napoca, Romania Course on Integrative Structural Bioinformatics, Doctoral School for
(2022-present) 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 Supervisor/Mentor (M.Sc. and Ph.D. students)
Timișoara, Romania Course on Advanced Computational Methods for Biomolecular
(2018-present) Dynamics, M.Sc. Program in Bioinformatics (Faculty of
Informatics)

University of Münster Supervisor/Mentor (M.Sc. and Ph.D. students)
Germany Advanced practical courses, M.Sc. Programs (Biology Department)
(2012-2020) 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)

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| 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. 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. *BioRxiv*, <https://doi.org/10.1101/2024.09.16.613212>
2. 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>
3. 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>
4. 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>
5. 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>
6. Guni F, Krishuns T, Schreiber JA, Henschel L, Wahrenburg M, Drexler HCA, Leidel SA, Cojocaru V, Seeböhm 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>
7. 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>
8. 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>

9. 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>
10. 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>
11. 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>
12. 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>
13. 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>
14. 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>
15. 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>
16. 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>
17. 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>
18. Öztürk M, Pachov G, Wade RC, Cojocaru V (2016). Conformational selection and dynamic adaptation upon linker histone binding to the nucleosome. *Nucleic Acids Research* 44(14):6599-6613 (featured on issue cover), <https://doi.org/10.1093/nar/gkw514>
19. 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>

20. 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>
21. 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>
22. 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>
23. 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>
24. 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>
25. 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.bbagr.2013.10.001>
26. Esch D, Vahokoski J, Groves MR, Pogenberg V, Cojocaru V, Vom Bruch H, Han D, Drexler HC, Arauzo-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>
27. 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>
28. 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>
29. 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>
30. Tapia N, Reinhardt P, Duemmler A, Wu G, Arauzo-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>

31. 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.org/10.2174/138920012798918462>
32. 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>
33. 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>
34. 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>
35. 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>
36. 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>
37. 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>)