

Vlad Cojocaru, Ph.D., Computational biochemist

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About me

I am an enthusiast senior research scientist with strong expertise in computational molecular biochemistry. I have a broad interdisciplinary knowledge and experience across physics, chemistry and biology. Throughout my scientific career from Ph.D. student to research group leader, I strove to discover how the three dimensional structure and dynamics of molecules impact on 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 bind to and explore DNA. For these discoveries, I used diverse molecular modeling and simulation methods and self built or established 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. Most recently, I have been leading a small research team and guided students towards successful completion of internships or Ph.D. studies. I have published appreciated collaborative research articles in prestigious competitive journals, gave invited lectures at prestigious international conferences and obtained third-party funding for my research.

Goals

My research is aimed at discovering how different factors modulate the dynamics of nuclear chromatin substructures using computational structural biology methods. Nuclear chromatin stores the genomic DNA and its dynamics are essential, among other processes, for gene regulation and cell identity determination. Different factors such as specialized proteins bind to DNA wrapped around histone proteins or to different regions on the histones modifying chromatin dynamics by mechanisms that are still largely unknown.

Keywords

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

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

Guest scientist 2018-present	Hubrecht Institute (Utrecht, NL) / Max Planck Institute (Münster, GE) I am finalizing and publishing research projects
Group leader 2018-2021	Hubrecht Institute, Utrecht, NL I continued my research lines established in Münster
Project group leader 2010-2018	Max Planck Institute for Molecular Biomedicine, Münster, Germany I discovered structural features and dynamics involved in DNA binding by a special class of proteins (transcription factors)
Research associate 2005-2010	Heidelberg Institute for Theoretical Studies, Heidelberg, Germany I discovered how cytochromes P450, a major class of drug metabolizing enzymes anchor in membranes and channel drug molecules to and from their active site
Research fellow/associate 2001-2005 (Ph.D. studies)	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany I discovered how proteins influence the folding of RNA molecules

Education and degrees

Habilitation (2017)	Theoretical Chemistry, University of Münster, Germany Official recognition to supervise/teach based on academic record
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 and Chemistry, West University of Timișoara, Romania

Grants

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

Biophysical Society	2022 Annual Meeting, San Francisco, USA Multiscale Genome Organization subgroup
ISQBP	President’s meeting Strasbourg, France (2021, virtual), Bergen, Norway (2016)
Albany Conversation Biophysical Society	20 th edition (2019), Albany, USA Thematic meeting “Multiscale modeling of chromatin: bridging experiment and theory”, Les Houches, France (2019)

Teaching

Babeş-Bolyai University Cluj-Napoca, Romania (starting 2021)	Courses/Seminars on Structural Bioinformatics, M.Sc. Program in Bioinformatics (Biology Department)
West University of Timișoara, Romania (2018-2021)	Advanced course on Structural Bioinformatics, M.Sc. Program in Bioinformatics (Informatics Department)
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, awards, fellowships

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, Awk, 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)

Selected publications

* A complete list of publications is attached below (page 6)

1. 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>
2. 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>
3. 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>
4. 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>
5. 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>

Also about me

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

Complete list of publications

Preprints, in peer review

1. MacCarthy CM, Huertas J, Ortmeier C, vom Bruch H, Reinke D, Sander A, Bergbrede T, Schöler HR, Cojocaru V (2021). OCT4 interprets and enhances nucleosome flexibility. *Biorxiv*, <https://doi.org/10.1101/2021.04.27.441583>

Peer-reviewed

1. 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>
2. 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>
3. 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>
4. Öztürk MA, De M, Cojocaru V, Wade RC (2020). Chromatosome Structure and Dynamics from Molecular Simulations. *Annual Review in Physical Chemistry* 71:101-119, <https://doi.org/10.1146/annurev-physchem-071119-040043>
5. Viplav A, Saha T, Huertas J, Selenschik P, Ebrahimkuty 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>
6. 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>
7. 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>
8. 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>

9. Öztürk MA, Cojocaru V, Wade RC (2018). Dependence of chromosome 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>
10. 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>
11. 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 Sox2 Evokes Latent Specificities in the DNA Recognition by Pax6. *Journal of Molecular Biology* 429:3626-3634, <https://doi.org/10.1016/j.jmb.2017.10.013>
12. 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>
13. 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>
14. 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>
15. 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>
16. 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>
17. 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>
18. 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>
19. 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>
20. 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>
21. 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>
 22. 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>
 23. 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>
 24. Tapia N, Reinhardt P, Duemmler A, Wu G, Araúz-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>
 25. 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>
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 27. 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>
 28. 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>
 29. 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>
 30. 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>
 31. 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>