

# Vlad Cojocaru, Ph.D., P.D. (Habil.)

## Computational biochemist / Leading research scientist

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. 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. 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.

### Goals

I am enthusiastic about further developing new research programs from a leading position in a prestigious academic institution. At the dawn of exascale computers, the application of molecular models and simulations will span longer times scales of increasingly larger biomolecular complexes. With these, we will be able to discover missing links between the structure, dynamics and biological function of large macromolecules and macromolecular assemblies. In turn, such discoveries will enable the development of novel therapeutic strategies for a range of debilitating diseases. Together with my future research group, I aim to make important contributions in this direction. In addition, I am enthusiastic about developing exciting teaching programs in life or natural sciences for graduate or undergraduate university curricula.

## Keywords

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

## Areas of expertise

<b>Structural biology</b>	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.
<b>Computer/IT skills</b>	Using specialized software for structural biology and molecular modeling; basic computer programming in different languages; managing high end workstations and small computer clusters.
<b>Management</b>	Managing projects and a small research team; coordinating collaborative projects (attended management and coaching courses provided by the Max Planck Society)
<b>Communication</b>	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

<b>Leading research scientist (C.S. I)</b>	The Institute for Advanced Studies in Science and Technology / Babeş-Bolyai University (Cluj-Napoca, Romania)
2022-present	Developing research programs/Establishing a research group
<b>Senior research scientist</b>	University of Utrecht (Utrecht, NL)
2022-present	Developing research programs
<b>Guest scientist</b>	Max Planck Institute (Münster, GE)
2018-present	Finalizing and publishing research projects
<b>Guest scientist</b>	Hubrecht Institute (Utrecht, NL)
2021-2022	Finalizing and publishing research projects
<b>Fellow group leader</b>	Hubrecht Institute, Utrecht, NL
2018-2021	I continued my research programs established in Münster
<b>Project group leader</b>	Max Planck Institute for Molecular Biomedicine, Münster, Germany
2010-2018	I discovered structural features and dynamics involved in DNA binding by a special class of proteins (transcription factors)
<b>Research associate</b>	Heidelberg Institute for Theoretical Studies, Heidelberg, Germany

2005-2010 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** Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

2001-2005 (Ph.D. studies) I discovered how proteins influence the folding of RNA molecules

## Education and degrees

**Habilitation** (2017) Theoretical Chemistry, University of Münster, Germany  
Degree based on academic record conferring official recognition as a university teacher/supervisor/mentor

**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 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

**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<sup>th</sup> edition (2019), Albany, USA  
Thematic meeting “Multiscale modeling of chromatin: bridging experiment and theory”, Les Houches, France (2019)

## Teaching

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

<b>University of Münster</b>	Habilitation (Venia Legendi in Theoretical Chemistry, 2017)
<b>Klaus Tschira Foundation</b>	Postdoctoral fellowship (2005-2008)
<b>Max Planck Society</b>	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

<b>Technical</b>	Molecular modeling and simulation methods and software (e.g. VMD, NAMD, Chimera, Modeller, Pymol, Amber), Unix/Linux, Programming languages (Perl, Tcl, Bash, Awk, Python)
<b>Soft</b>	Science communication (publications, presentations, teaching), Project and team leading, Mentoring and guidance, Conference organization, Team working and building
<b>Languages</b>	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 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/10.1101/2021.04.27.441583v2>

### 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, 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>
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 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>

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 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>
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* 19;44(14):6599-613 (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>
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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>
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## References

1. **Prof. Dr. Alexander van Oudenaarden**, Hubrecht Institute, Utrecht, The Netherlands
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