

# **CURRICULUM VITAE**

## **NIKOLAY V. DOKHOLYAN**

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### **Education**

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| 1999-2002 | National Institutes of Health Postdoctoral Fellow, Department of Chemistry and Chemical Biology, Harvard University, USA.<br>Area of research: Biophysics |
| 1999      | Ph.D., Boston University, USA. Physics  |
| 1994      | M.S., Moscow Institute of Physics and Technology, Russia.<br>Physics  |
| 1992      | B.S., Moscow Institute of Physics and Technology, Russia.<br>Physics  |

### **Professional Experience**

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| 2017-present | Adjunct Professor, Joint Department of Biomedical Engineering, University of North Carolina at Chapel Hill and North Carolina State University     |
| 2014-present | Michael Hooker Distinguished Professor, Department of Biochemistry and Biophysics, University of North Carolina at Chapel Hill, School of Medicine |
| 2013         | Founder of the CFold, Inc  |
| 2013-present | Adjunct Professor, Division of Chemical Biology and Medicinal Chemistry, University of North Carolina at Chapel Hill, Eshelman School of Pharmacy  |

## Curriculum Vitae

Nikolay V. Dokholyan

2011-present	Professor, Department of Biochemistry and Biophysics, University of North Carolina at Chapel Hill, School of Medicine
2010-present	Member of The North Carolina Translational and Clinical Sciences Institute
2010-present	Faculty 1000 member
2009-present	Center for Neurosensory Disorders Faculty
2009-present	Cystic Fibrosis and Pulmonary Research & Treatment Center Faculty
2009-2014	Director, Center for Computational and Systems Biology, University of North Carolina at Chapel Hill
2008-2011	Associate Professor, Department of Biochemistry and Biophysics, University of North Carolina at Chapel Hill, School of Medicine
2008-present	Founder and President of the Molecules in Action, LLC
2007-2014	Graduate Director of the Program in Cellular and Molecular Biophysics
2006-present	Lineberger Comprehensive Cancer Center Faculty
2005-present	Neuroscience Center Faculty
2002-present	Carolina Center for Genome Sciences Faculty
2002-present	Molecular and Cellular Biophysics Program Faculty
2002-present	Bioinformatics and Computational Biology Training Program Faculty
2002-2008	Assistant Professor, Department of Biochemistry and Biophysics, University of North Carolina at Chapel Hill, School of Medicine
1999	Research Associate, Physics Department, Boston University
1988-1989	Teacher of Physics and Mathematics, Specialized Physics and Mathematics High School (at Moscow Institute of Physics and Technology), Moscow, Russia

## Honors & Awards

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2014-present	Michael Hooker Distinguished Professorship
2013	American Physical Society Fellow
2011-present	Book Series Editor, Series in Computational Biophysics
2011-2016	Editor-in-Chief, Research and Reports in Biochemistry
2004-2006	March of Dimes Basil O'Connor Starter Scholar Research Award
2004	The University of North Carolina at Chapel Hill IBM Junior Faculty Development Award
2003	Recipient of a UNC Research Council Award
1999-2002	NIH postdoctoral fellowship
1998-1999	NIH Molecular Biophysics Predoctoral Traineeship
1995,1998,2001	NSF Young Scientist Travel Award
1994	"Red Diploma" (equivalent to <i>summa cum laude</i> in USSR)
1990-1994	Recipient of Honorary Stipend, Moscow Institute of Physics and Technology

## Patents

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**N. V. Dokholyan** and J. R. Riordan, "Methods of treating lung disease" U.S. Patent Application No. 61/706,967 September 28, 2012

L. Diatchenko, W. Maixner, **N. V. Dokholyan**, F. Ding, A. W. R. Serohijos, S. Yin, "Mu-opioid receptor binding compounds" International Patent Application PCT/US12/40168 May 31, 2012 claiming the benefit of priority of U.S. Provisional Patent Application No. 61/491,828 filed May 31, 2011 in the names of L. Diatchenko, W. Maixner, **N. V. Dokholyan**, F. Ding, A. W. R. Serohijos, S. Yin for "Mu-opioid receptor binding compounds"

## Bibliography

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### A. Books and chapters

19. M. Convertino and **N. V. Dokholyan**, "Computational modeling of small molecule ligand binding interactions and affinities." *Methods in Molecular Biology: Computational Design of Ligand Binding Proteins* 1414: 23-32 (Chapter 2) Editor: Stoddard, Barry L. (2016)
18. C. Zhu, D. D. Mowrey and **N. V. Dokholyan**, "Computational protein design through grafting and stabilization." *Methods in Molecular Biology: Computational Protein Design* Volume 1529 pp. 227-241 (Chapter 11) Editor: Ilan Samish (2017)
17. A. Krokhotin, and **N. V. Dokholyan**, "Computational methods toward accurate RNA structure prediction using coarse-grained and all-atom models." *Methods in Enzymology* Vol. 553: pp. 65-89 (Chapter 3) *Macromolecular crystallography D*. Editors: D. H. Burke and S.-J. Chen (2015)
16. F. Ding, and **N. V. Dokholyan**, "RNA three-dimensional structure determination using experimental constraints." In "RNA Nanotechnology and Therapeutics" Editors: P. Guo and F. Haque. Taylor and Francis. pp. 159–176 (2013)
15. E. A. Kotelnikova, R. Redler, M. A. Pyatnitskiy, and **N. V. Dokholyan**, "Role of  $\text{Ca}^{2+}$ -mediated signaling in ALS pathology." In "From knowledge networks to biological models" Editors: A. Yuryev and N. Daraselia. Bentham Science Publishers. pp. 24-72 (2012)
14. P. A. Chong, P. Kota, **N. V. Dokholyan**, and J. D. Forman-Kay, "Dynamics intrinsic to CFTR function and stability." In "*Cystic Fibrosis: Molecular Basis, Physiological Changes, and Therapeutic strategies*." Editors: J. R. Riordan, R. C. Boucher, and P. M. Quinton. Cold Spring Harbor Press. 3: a009522 (2013)
13. **N. V. Dokholyan** (Editor), "*Computational Modeling of Biological Systems: From Molecules to Pathways*." Springer. (2012)
12. S. Ramachandran, and **N. V. Dokholyan**, "Homology modeling: Generating structural models to understand protein function and mechanism." in "*Computational Modeling of Biological Systems: From Molecules to Pathways*." Editor: **N. V. Dokholyan**. Springer. pp. 97-116 (2012)
11. F. Ding, and **N. V. Dokholyan**, "Discrete molecular dynamics simulation of biomolecules." in "*Computational Modeling of Biological Systems: From Molecules to Pathways*." Editor: **N. V. Dokholyan**. Springer. pp. 55-74 (2012)
10. M. Betnel, **N. V. Dokholyan**, and B. Urbanc, "From disordered amyloid  $\beta$ -proteins to soluble oligomers and protofibrils using Discrete Molecular Dynamics." in "Alzheimer's disease: Molecular Basis of Amyloid-beta protein aggregation and fibril formation - Insights into low molecular weight and cytotoxic aggregates from computer simulations." Editor: P. Derreumaux. Imperial College Press. vol. 7: pp 333-357 (2013)

9. F. Ding, and **N. V. Dokholyan**, "Multiscale modeling of RNA structure and dynamics." in "RNA 3D Structure Analysis and Prediction" Editors: N. Leontis and E. Westhof. Series "Nucleic Acids and Molecular Biology" (Series Editor: J. Bujnicki). Springer. Volume 27, Chapter 9, pp. 167-184 (2012)
8. A. W. R. Serohijos, P. H. Thibodeau, and **N. V. Dokholyan**, "Molecular modeling tools and approaches for CFTR and cystic fibrosis." in "Cystic Fibrosis: Methods and Protocols" Editors: M. D. Amaral and K. Kunzelmann. Series "Methods in Molecular Biology", Springer Science+Business Media, LLC and Humana Press 741: 347-363 (2011)
7. S. Yin, F. Ding, and **N. V. Dokholyan**, "Modeling mutations in proteins using Medusa and discrete molecule dynamics." in "Protein Structure Prediction: Method and Algorithms" Editors: H. Rangwala and G. Karypis. Wiley (2010)
6. S. Yin, F. Ding, and **N. V. Dokholyan**, "Computational evaluation of protein stability change upon mutations using Eris." in "*In Vitro* Mutagenesis Protocols" 3<sup>rd</sup> Edition. Editor: J. Braman. Humana Press (*Methods in Molecular Biology*) 634: 189-201 (2010)
5. S. G. Chaney, S. Ramachandran, S. Sharma, **N. V. Dokholyan**, B. Temple, D. Bhattacharyya, Y. Wu and S. Campbell, "Differences in conformation and conformational dynamics between cisplatin and oxaliplatin DNA adducts." In "Platinum and Other Heavy Metal Compounds in Cancer Chemotherapy: Molecular Mechanisms and Clinical Applications (Cancer Drug Discovery and Development)" Editors: A. Bonetti, R. Leone, F. M. Muggia and S. B. Howell. pp. 157-169. Humana Press (2009)
4. **N. V. Dokholyan**, "Protein designability and engineering." in "Structural Bioinformatics" Editors: P. Bourne and J. Gu. pp. 961-982. Wiley-Blackwell (2009)
3. **N. V. Dokholyan** and E. I. Shakhnovich, "Towards unifying protein evolution theory." in "Structural approaches to sequence evolution: Molecules, networks, populations" Editors: U. Bastolla, M. Porto, H. E. Roman, and M. Vendruscolo. pp. 113-126. Springer, Berlin (2007)
2. **N. V. Dokholyan** and E. I. Shakhnovich, "Scale-free evolution: from proteins to organisms." in "Power Laws, Scale-free Networks and Genome Biology" Editors: E. V. Koonin, Y. I. Wolf, and G. P. Karev. pp. 86-105. Eureka.com and Springer (2006)
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*B. Original research*

227. Y. Zhang, M. Hashemi, Z. Lv, B. Williams, K. Popov, **N. V. Dokholyan**, and Yu. L. Lyubchenko, "High-speed atomic force microscopy reveals structural dynamics of alpha-synuclein monomers and dimers" *submitted* (2017)
226. G. Kaur, K. Guruprasad, B. R. S. Temple, D. G. Shirvanyants, **N. V. Dokholyan**, and P. K. Pati, "Structural complexity and functional diversity of plant NADPH oxidases" *Amino Acids*, *in press* (2017)
225. B. Williams II, B. Zhao, A. Tandon, F. Ding, K. M. Weeks, Q. Zhang, and **N. V. Dokholyan**, "Structure modeling of RNA using sparse NMR constraints" *Nucleic Acids Research*, *in press* (2017)
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223. R. Dronamraju, S. Ramachandran, D. K. Jha, A. T. Adams, J. V. DiFiore, M. A. Parra, **N. V. Dokholyan**, and B. D. Strahl, "Redundant functions for Nap1 and Chz1 in H2A.Z deposition" *Scientific Reports*, 7: 10791 (2017)
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201. S. E. Allen, **N. V. Dokholyan**, and A. A. Bowers, "Dynamic docking of conformationally constrained macrocycles: methods and applications", *ACS Chemical Biology*, 11: 10-24 (2016)
200. E. A. Proctor, L. Fee, Y. Tao, R. L. Redler, J. M. Fay, Y. Zhang, Z. Lv, I. P. Mercer, M. Deshmukh, Y. L. Lyubchenko, and **N. V. Dokholyan**, "Non-native SOD1 trimer is toxic to motor neurons in a model of amyotrophic lateral sclerosis" *Proceedings of the National Academy of Sciences USA*, 113: 614-619 (2016)
199. E. A. Proctor and **N. V. Dokholyan**, "Applications of discrete molecular dynamics in biology and medicine", *Current Opinion in Structural Biology*, 37: 9-13 (2016)
198. R. L. Redler, J. Das, J. R. Diaz, and **N. V. Dokholyan**, "Protein destabilization as a common factor in diverse inherited disorders", *Journal of Molecular Evolution*, 82: 11-16 (2016)
197. A. Samoshkin, M. Convertino, C. T. Viet, J. S. Wieskopf, O. Kambur, J. Marcovitz, P. Patel, L. Stone, E. Kalso, J. S. Mogil, B. L. Schmidt, W. Maixner, **N. V. Dokholyan\***, and L. Diatchenko\*, "Structural and functional interactions



between six-transmembrane  $\mu$ -opioid receptors and  $\beta$ 2-adrenoreceptors modulate opioid signaling", *Scientific Reports*, 5: 18198 (2015)

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potential therapeutic target for new effective opioids" *Progress in Neuro-Psychopharmacology & Biological Psychiatry*, 62: 61-67 (2015)

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185. S. S. Hasan, E. A. Proctor, E. Yamashita, **N. V. Dokholyan**, and W. A. Cramer, "Traffic within the cytochrome b6f lipoprotein complex: Gating of the quinone portal" *Biophysical Journal*, 107: 1620-1628 (2014)

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8. R. H. R. Stanley, **N. V. Dokholyan**, S. V. Buldyrev, S. Havlin, and H. E. Stanley, "Clumping of identical oligonucleotides in coding and noncoding DNA sequences." *Journal of Biomolecular Structure & Dynamics* 17: 79-87 (1999)
7. **N. V. Dokholyan**, S. V. Buldyrev, H. E. Stanley, and E. I. Shakhnovich, "Molecular dynamics studies of folding of a protein-like model." *Folding & Design* 3: 577-587 (1998)
6. **N. V. Dokholyan**, Y. Lee, S. V. Buldyrev, S. Havlin, H. E. Stanley, and P. King, "Scaling of the distribution of shortest paths in percolation." *Journal of Statistical Physics* 93: 603-613 (1998)
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4. S. V. Buldyrev, **N. V. Dokholyan**, A. L. Goldberger, S. Havlin, C.-K. Peng, H. E. Stanley, and G. M. Viswanathan, "Analysis of DNA sequences using methods of statistical physics." *Physica A* 249: 430-438 (1998)
3. **N. V. Dokholyan**, S. V. Buldyrev, S. Havlin, and H. E. Stanley, "Model of unequal chromosomal crossing over in DNA sequences." *Physica A* 249: 594-599 (1998)
2. **N. V. Dokholyan**, S. V. Buldyrev, S. Havlin, and H. E. Stanley, "Distribution of base pair repeats in coding and noncoding DNA sequences." *Physical Review Letters* 79: 5182-5185 (1997)
1. **N. V. Dokholyan**, G. V. Jikia, "Single top quark production and  $V_{tb}$  CKM matrix element measurement in high energy  $e^+e^-$  collisions." *Physics Letters B* 336: 251-256 (1994)

*C. Other un-refereed works*

8. **N. V. Dokholyan** and K. M. Hahn, “Stealthy control of proteins and cellular networks in live cells”, *Cell Systems* 4:5 (2017)

7. **N. V. Dokholyan**, “Dr\_Dokholyan, r/Science, Science AMA Series: I am Dr. Nikolay Dokholyan, professor at the University of North Carolina School of Medicine in Chapel Hill, N.C., here to talk about a major development toward understanding ALS”, *The Winnower* 3:e145493.34392 (2016). DOI: [10.15200/winn.145493.34392](https://doi.org/10.15200/winn.145493.34392)

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4. **N. V. Dokholyan**, C. Glabe, D. Holtzman, A. Koudinov, A. Lomakin, N. Oyler, N. Paganini, D. Teplow, D. Thirumalai, and R. Tycko, “Live discussion: Protein folding and neurodegeneration: Biophysics to the rescue?”, *Journal of Alzheimer's Disease*, 6: 99–105 (2004)

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2. **N. V. Dokholyan**, S. V. Buldyrev, H. E. Stanley, and E. I. Shakhnovich, “Kinetics of the protein folding transition.” *AIP Proceedings of the Third Tohwa University Conference on Statistical Physics, November 8-12, 1999* 419-425 (2000)

1. **N. V. Dokholyan** and E. I. Shakhnovich, “Two models of amino acid conservation in proteins.” *Proceedings of the International School of Physics “Enrico Fermi” Course CXLV: “Protein folding, evolution and design”, Varenna, Italy* p. 227-245 (2000)

*D. Presentations*

- |      |  |
|------|--|
| 2017 | Purdue University (invited)  |
| 2017 | 4th International Conference on Protein and RNA Structure Prediction organized in Montego Bay, Jamaica (invited) |
| 2017 | 2nd Forum of Armenian Diaspora Scientists, Yerevan, Armenia (invited)  |

## Curriculum Vitae

Nikolay V. Dokholyan

- 2017 International workshop “Boyajayan readings”, Yerevan, Armenia (invited)
- 2017 CECAM conference “Computational approaches to investigating allostery”, Lausanne, Switzerland (organizer)
- 2017 University of Michigan, Ann Arbor (invited)
- 2017 Pennsylvania State University, Hershey Medical Center (invited)
- 2017 Bioinformatics Summer School, Dolgoprudnyi, Russia (invited)
- 2017 Advances in Complex Systems 2017, Lago Como, Italy (invited)
- 2017 University of Illinois Urbana-Champaign, Illinois (invited)
- 2017 Pennsylvania State University, Pennsylvania (invited)
- 2017 Computational Aspects of Biomolecular NMR Gordon Research Conference, Sunday River, Maine (invited)
- 2017 253 American Chemical Society National Meeting, San Francisco, California (invited)
- 2017 University of Pittsburg, Pennsylvania (invited)
- 2017 University of Massachusetts, Amherst, Massachusetts (invited)
- 2016 The Third International Conference on Computational Science and Engineering, Ho Chi Minh City, Vietnam (invited)
- 2016 The Sixth Symposium on Structural Proteomics, Dortmund, Germany (invited)
- 2016 University of North Carolina Charlotte, Charlotte, North Carolina (invited)
- 2016 University of North Carolina at Chapel Hill, Biochemistry & Biophysics, Chapel Hill, North Carolina (invited)
- 2016 North Carolina State University, Raleigh, North Carolina (invited)
- 2016 University of North Carolina at Chapel Hill, MD/PhD Program, Chapel Hill, North Carolina (invited)
- 2016 Common Mechanisms of Neurodegeneration, Keystone, Colorado (poster)

## Curriculum Vitae

Nikolay V. Dokholyan

- 2016            4th Prague Protein Spring, Prague, Czech Republic (invited)
- 2016            Masaryk University, Department of Experimental Biology, Brno, Czech Republic (invited)
- 2016            Stony Brook University, The Louis and Beatrice Laufer Center for Physical and Quantitative Biology (invited)
- 2016            Duke University, Department of Anesthesiology, Center for Translational Pain Medicine (invited)
- 2016            Experimental Biology 2016, San Diego (contributed)
- 2016            UNC Pathology and Laboratory Medicine Grand Rounds (invited)
- 2016            University of Milano, Center for Complexity & Biosystems, Milano Italy (invited)
- 2016            University of Milano, Department of Physics, Milano Italy (invited)
- 2016            UNC BBSP (invited)
- 2015            3rd International Conference of Protein & RNA Structure Prediction, Punta Cana, Dominican Republic (invited)
- 2015            26th International Symposium on ALS/MND, Orlando, Florida (poster)
- 2015            North American Cystic Fibrosis Conference, Phoenix, Arizona (poster)
- 2015            Nizhniy Novgorod State University, Neuroscience Institute, Russia (invited)
- 2015            Northeastern University, Physics Department, Boston USA (invited)
- 2015            Boston University, Physics Department, Boston USA (invited)
- 2015            ASBMB 2015 Annual Meeting/Experimental Biology, EB2015, Boston USA (poster)
- 2015            12th European Cystic Fibrosis Society Basic Science Conference, Albufeira, Portugal (session chair)
- 2015            UNC BBSP (invited)

2015	McGill University, Montreal, Canada (invited)
2014	EU-US Frontiers of Engineering Symposium (FoE), Seattle (invited)
2014	Molecular Modeling and Informatics in Drug Design, NIPER, India (invited)
2014	University of North Carolina, Program in Bioinformatics and Computational Biology (invited)
2014	Biomolecular Systems Interactions, Dynamics, and Allostery: Bridging Experiments and Computations, Istanbul, Turkey (invited)
2014	Gordon Research Conference: Biopolymers Gordon Research Conference, Newport, Rhode Island (invited)
2014	Structure and dynamics of RNA interactions, Montreal, Canada (invited)
2014	UNC RCAC symposium 2014, Chapel Hill (invited)
2014	3rd Prague Protein Spring, Prague, Czech Republic (invited)
2014	6th SIMPAR International Meeting, Rome, Italy (invited)
2014	Indiana University School of Medicine, Indianapolis (invited)
2014	East Carolina University, Greenville, North Carolina (invited)
2014	Biophysical Society Meeting, San Francisco (invited)
2013	CCS2011 Lake Arrowhead Reunion Conference II, Lake Arrowhead, California (invited)
2013	Barcelona BioMed Conference on “Frontiers in dynamics simulations of biological molecules”, Barcelona, Spain (invited)
2013	North American Cystic Fibrosis Conference, Salt Lake City, Utah
2013	University of Toronto, Department of Biochemistry (invited)
2013	Iowa State University, Laurence H. Baker Center for Bioinformatics and Biological Statistics (invited)

- 2013 Chemical and Biological Defense Program Enzyme Colloquium, Falls Church, VA (invited)
- 2013 University of North Carolina at Chapel Hill, Department of Biochemistry and Biophysics (invited)
- 2013 Federation of European Biochemical Societies Congress "Mechanisms in Biology", St. Petersburg, Russia
- 2013 RNA Nanotechnology, Kentucky 2013, USA (invited)
- 2013 American Physical Society Meeting, Baltimore, USA (contributed)
- 2013 Yeshiva University, Physics Department (invited)
- 2013 University of Maryland, Biophysics Program (invited)
- 2013 Rutgers University (invited)
- 2012 UCLA Institute for Pure and Applied Math, Arrowhead conference (invited)
- 2012 Society for Neuroscience Annual Meeting, New Orleans, LA (invited)
- 2012 Chemical and Biological Defense Program Enzyme Colloquium, Falls Church, VA (invited)
- 2012 Allosteric Regulation of Cell Signaling, Madrid Spain (invited)
- 2012 American Chemical Society 244th National Meeting, Philadelphia USA (invited)
- 2012 Biodynamics in Buffalo, Buffalo (invited)
- 2012 Lund University, Lund, Sweden (invited)
- 2012 Virginia Bioinformatics Institute, VirginiaTech, Blacksburg (invited)
- 2012 Stockholm University, Sweden (invited)
- 2012 NORDITA program on "Dynamics of biomolecular processes: from atomistic representations to coarse-grained models", Stockholm, Sweden (invited)
- 2012 The 2nd workshop "Physics of protein folding and aggregation", Bressanone, Italy (invited)

- 2011            The 22nd international symposium on ALS/MND, Sydney, Australia (invited)
- 2011            "Perspectives and challenges in statistical physics and complex systems for the next decade: A conference in honor of Eugene Stanley and Liacir Lucena", Natal, Brazil (invited)
- 2011            25th Annual North American Cystic Fibrosis Conference, Anaheim, CA (contributed)
- 2011            3D CFTR Structure Consortium (invited)
- 2011            Pfizer Inc., Cambridge, MA (invited)
- 2011            NESCent meeting, "Modeling protein structural and energetic constraints on sequence evolution", Durham, NC (invited)
- 2011            Computer Integrated Systems for Microscopy and Manipulation Center meeting, Chapel Hill, NC (invited)
- 2011            Chemical and Biological Defense Program Enzyme Colloquium, Falls Church, VA (invited)
- 2011            Colorado Protein Stability Conference, Breckenridge, Colorado (invited)
- 2011            "Macromolecular Crowding" workshop, Telluride, Colorado (invited)
- 2011            UCLA Institute for Pure and Applied Math, Arrowhead conference (invited)
- 2011            UCLA Institute for Pure and Applied Math (invited)
- 2011            Wesleyan University, Physics Department (invited)
- 2011            Vanderbilt University, Department of Chemistry (invited)
- 2011            Symposium and Gala "Horizons in Emergence & Scaling", Boston University (advisory committee)
- 2011            Symposium "New Era of Biosimulations with Supercomputers", Osaka, Japan (invited)
- 2011            University of North Carolina at Chapel Hill, Department of Physics and Astronomy (invited)



## Curriculum Vitae

Nikolay V. Dokholyan

- 2010            University of North Carolina at Chapel Hill, Department of Biochemistry and Biophysics (invited)
  
- 2010            Conference on "RNA Nanotechnology and Therapeutics", Cleveland, OH USA (invited)
  
- 2010            CECAM Workshop on "Protein Folding Dynamics: Bridging the Gap between Theory and Experiment", Lausanne, Switzerland (invited)
  
- 2010            Chemical and Biological Defense Program Enzyme Colloquium, Falls Church, VA (invited)
  
- 2010            American Chemical Society 240th National Meeting, Boston MA USA (invited)
  
- 2010            Summer School in Biophysics at UT/ORNL: "Computational and Experimental Challenges", Knoxville, TN USA (plenary talk)
  
- 2010            Bioinformatics & Computational Molecular Biology Undergraduate Summer Research Program, University of Wyoming, WY USA (invited)
  
- 2010            "From Computational Biophysics to Systems Biology (CBSB)", Traverse City, MI USA (invited)
  
- 2010            Washington University St. Louis, MO USA (invited)
  
- 2010            Biophysical Society Meeting, RNA modeling group, San Francisco USA (invited)
  
- 2009            State University of New York at Buffalo and Hauptman-Woodward Medical Research Institute, Buffalo USA (invited)
  
- 2009            The 20th International Symposium on ALS MND, Berlin Germany (invited)
  
- 2009            Expanding the frontiers of molecular dynamics simulations in biology, Barcelona Spain (invited)
  
- 2009            University of North Carolina Department, Cystic Fibrosis Center (invited)
  
- 2009            American Chemical Society 238th National Meeting, Washington DC USA (invited)
  
- 2009            Moscow Conference on Computational Molecular Biology, Russian Federation (invited)

## Curriculum Vitae

Nikolay V. Dokholyan

- 2009            NCTS Workshop on Critical Phenomena and Complex Systems, Taipei Taiwan (2 talks) (invited)
  
- 2009            DARPA Protein Design Processes Meeting, Palm Beach Gardens USA (invited)
  
- 2009            University of Arizona, Tucson USA (invited)
  
- 2009            Memorial workshop in memoriam of Angel R. Ortiz “Structural Bioinformatics and Beyond”, Madrid Spain (invited)
  
- 2008            National Central University, Taipei Taiwan (invited)
  
- 2008            NCTS December Workshop on Critical Phenomena and Complex Systems, Taipei Taiwan (3 talks) (invited)
  
- 2008            University of Texas Southwestern Medical Center, Dallas USA (invited)
  
- 2008            University of Texas Health Science Center at San Antonio USA (invited)
  
- 2008            DARPA Protein Design Processes Meeting, Seattle USA (invited)
  
- 2008            University of North Carolina Department of Applied Mathematics (invited)
  
- 2008            American Chemical Society 236th National Meeting, Philadelphia USA (invited)
  
- 2008            Cystic Fibrosis Foundation’s annual Williamsburg Conference, Williamsburg USA (invited)
  
- 2008            From Computational Biophysics to Systems Biology, Julich Germany
  
- 2008            Institute of Enzymology of the Hungarian Academy of Sciences, Budapest, Hungary (invited)
  
- 2008            ABC Proteins-From Multidrug Resistance to Genetic Diseases, Innsbruck Austria (plenary speaker)
  
- 2008            Rice University (invited)
  
- 2008            Clemson University (invited)

- 2007 DARPA Protein Design Processes Meeting, Islamorada USA (invited)
- 2007 Meeting in honor of Eugene Shakhnovich, Cambridge USA (invited)
- 2007 SymBioSys: A Virtual High-Throughput Screening and Docking Workshop, Chapel Hill (invited)
- 2007 Los Alamos National Laboratory, Center for Nonlinear Studies (invited)
- 2007 Drexel University (invited)
- 2007 American Chemical Society 234th National Meeting, Boston USA (invited)
- 2007 Colorado Protein Stability Conference, Breckenridge USA (invited)
- 2007 DARPA Protein Design Processes Meeting, Santa Fe USA (invited)
- 2007 Trends in Transient Interactions between Biological Macromolecules, Sevilla Spain
- 2007 Bennett College (educational presentation)
- 2007 Columbia University (invited)
- 2007 University of North Carolina at Chapel Hill, Cystic Fibrosis Center (invited)
- 2007 University of North Carolina at Chapel Hill, Chemistry Department (invited)
- 2007 North Carolina State University, Department of Biochemistry (invited)
- 2007 DARPA Protein Design Processes Meeting, Los Angeles USA (invited)
- 2006 PASI2006 "From Disordered systems to Complex Systems", Mar del Plata Argentina (invited)
- 2006 7th Spanish Symposium on Bioinformatics and Computational Biology (JdB06), Zaragoza Spain (invited)
- 2006 University of California Santa Barbara (invited)

2006	California Institute of Technology (invited)
2006	Georgia Institute of Technology (invited)
2006	University of North Carolina Bioinformatics Colloquium (invited)
2006	University of California Los Angeles (invited)
2006	CECAM Workshop on “Protein Folding and Misfolding”, Lyon France (invited)
2006	Wake Forest University (invited)
2006	CECAM Workshop on “Protein Aggregation”, Lyon France (invited)
2006	"Isolated Biomolecules and Biomolecular Interactions: Theory and Experiment" Conference, Trest Czech Republic (invited)
2006	DARPA Protein Design Processes Meeting, Islamorada USA (invited)
2006	EMBO-FEBS Workshop on “Amyloid Formation”, Florence Italy
2006	Gordon Research Conference, “Protein Folding Dynamics”, Ventura USA
2005	Workshop on “Enabling Petascale Science and Engineering Applications”, Georgia Tech, Atlanta USA (invited)
2005	North Carolina Central University (invited)
2005	“Bridging Knowledge Gaps in Computational Biology”, Cary USA (invited)
2005	DARPA Protein Design Processes, Seattle USA
2005	Protein Society Annual Meeting, Boston USA (contributed)
2005	University of North Carolina at Chapel Hill, Department of Neuroscience (invited)
2005	American Crystallographic Society Annual Meeting, Orlando USA (invited)
2005	University of North Carolina at Chapel Hill, Chemistry Department (invited)

- 2005 Yeshiva University (invited)
- 2005 Cambridge Healthtech Institute "Protein Folding Disorders", San Diego, CA USA (invited)
- 2004 "Electrons to Proteins: Coupling and Linkage in Biology", The Fifth Biannual Triangle Biophysics Symposium, Chapel Hill, USA (invited)
- 2004 The eCheminfo 2004 virtual conference "Applications of Cheminformatics and Chemical Modeling to Drug Discovery" (invited)
- 2004 Workshop on the Structural approaches to sequence evolution: Molecules, networks, populations, Dresden, Germany (invited)
- 2004 Symposium on the Evolution of Biomolecular Structure, Michigan State University, Michigan, USA (invited)
- 2004 American Mathematical Society Meeting, Rider University, Lawrenceville, USA (invited)
- 2003 Gordon Research Conference, "Proteins", Holderness, USA (contributed)
- 2003 Alzforum Live Discussion: Protein Folding and Neurodegeneration: Biophysics to the Rescue? (invited)
- 2003 Bioinformatics Symposium, UNC at Chapel Hill, USA (invited)
- 2002 An Interdisciplinary School, "Protein Aggregation", Les Houches, France (invited)
- 2002 Cornell University, Genomics Initiative (invited)
- 2002 Northeastern University, Physics Department (invited)
- 2002 University of North Carolina at Chapel Hill, Department of Physics and Astronomy (invited)
- 2002 University of North Carolina at Chapel Hill, Department of Biochemistry and Biophysics (invited)
- 2002 Computational Biophysics: Integrating Theoretical Physics and Biology, San Feliu de Guixols, Spain (invited)
- 2002 Physics and Computation on Protein Structure, The Fourth Biannual Triangle Biophysics Symposium, Chapel Hill, USA (invited)

- 2001 International Conference in Honor of the 60th Birthday of H. E. Stanley, "Horizons in Complex Systems", Messina, Italy (invited)
- 2001 International Workshop on Protein Folding, Structure and Design, Trieste, Italy (invited)
- 2001 Third Annual Greater Boston Area Statistical Mechanics Meeting, Brandeis University (contributed)
- 2001 Statphys XXI, Cancun, Mexico (contributed)
- 2000 Harvard University, Department of Chemistry and Chemical Biology, Whitesides group (invited)
- 2000 International School of Physics "Enrico Fermi" Course CXLV: "Protein folding, evolution and design", Varenna, Italy (contributed)
- 1999 International Workshop on Dynamics of Non-Equilibrium Systems, Trieste, Italy (invited)
- 1999 The 3rd Tohwa University International Conference on Statistical Physics, Fukuoka, Japan (invited)
- 1999 Boston University Science Day (invited)
- 1999 American Physical Society Centennial Meeting, Atlanta, USA (contributed)
- 1998 Harvard University, Department of Chemistry and Chemical Biology (invited)
- 1998 Boston University, Physics Department (invited)
- 1998 Conference on Protein folding and structure prediction, Torino, Italy (contributed)
- 1998 Conference on Percolation and Disordered Systems: Theory and applications, Giessen, Germany (contributed)
- 1997 Conference on Statistical Mechanics, Rutgers University (contributed)
- 1997 Conference on Complex Systems, Bar Ilan University, Israel (contributed)
- 1996 International School of Physics "Enrico Fermi", Varenna, Italy (contributed)

1996	Patterns in Nature '96. Two-week summer Institutes to introduce teachers in the use of advanced technology materials, Boston University (lecturer, educational presentation)
1995	Patterns in Nature '95. Two-week summer Institutes to introduce teachers in the use of advanced technology materials, Boston University (lecturer, educational presentation)
1995	Statphys XIX, Xiamen, China (contributed)
1993	The Physics Institute, Tbilisi, Georgia (invited)

## Teaching Record

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### A. Classroom teaching

2006,2012-2015	BCH 712: "Scientific writing". (~15 students, assisting with the course)
2006-present	BIOC 652: " <i>Macromolecular Equilibria: Conformation Change and Binding</i> ". (~15 students)
2006-2013	BCH 715: "Scientific presentation". (~15 students, ~2-3 contact hours)
2012	BIOC 649: " <i>Essentials of Macromolecular Science</i> ". (~15 students, 1 contact hour)
2010	BIOCH 901: "Advanced biochemistry of human diseases" (~7 students, 2 contact hours)
2003-2005	BIOC 146: " <i>Macromolecular Equilibria: Conformation Change and Binding</i> ". (~15 students)
2005	BIOC 145: " <i>Applications of statistical mechanics: molecular mechanics and binding equilibria</i> ". (~15 students)
2003	BIOC 154: " <i>Principles of and Simulation of Macromolecular Dynamics</i> ". Offered in even years. (~4-6 students)
1994-1998	Teaching Assistant for a number of beginning and advanced undergraduate courses, Boston University. (~15-25 students)

## Curriculum Vitae

Nikolay V. Dokholyan

1988-1989 Teacher of Physics and Mathematics, Specialized Physics and Mathematics High School (at Moscow Institute of Physics and Technology), Moscow, Russia.

### *B. Graduate students*

2014-2017	Benfeard Williams, UNC-CH Biochemistry & Biophysics
2014-2015	Dominique Soroka, UNC-CH Pharmacology
2013-2017	Reed Jacob, UNC-CH Curriculum in Bioinformatics and Computational Biology
2013-2017	Mahmoud Shobair, UNC-CH Biochemistry & Biophysics
2012-2013	Gurpreet Kaur, Fulbright Foreign Student
2012-2014	Arpit Tandon, UNC-CH Biochemistry & Biophysics
2011-2016	Onur Dagliyan, UNC-CH Biochemistry & Biophysics
2009-2013	Elizabeth Proctor, UNC-CH Curriculum in Bioinformatics and Computational Biology (postdoctoral appointment with Prof. Douglas Lauffenburger, MIT) (NIH Predoctoral Fellow)
2009-2013	Rachel Redler, UNC-CH Biochemistry & Biophysics (postdoctoral appointment NYU) (NIH Predoctoral Fellow)
2008-2012	Pradeep Kota, UNC-CH Biochemistry & Biophysics (postdoctoral appointment NIH)
2007-2011	Douglas Tsao, UNC-CH Chemistry
2006-2011	Srinivas Ramachandran, UNC-CH Biochemistry & Biophysics (postdoctoral appointment Fred Hutchinson Cancer Research Center) (American Heart Association Predoctoral Fellow)
2007-2009	Barry Kesner, UNC-CH Cell & Developmental Biology (research specialist in the group of Prof. Jeannie T. Lee at HHMI and Harvard Medical School, Massachusetts General Hospital)
2006-2009	Adrian W. Serohijos, UNC-CH Physics & Astronomy (Assistant Professor at the University of Montreal) (American Heart Association Predoctoral Fellow)



## Curriculum Vitae

Nikolay V. Dokholyan

2005-2009	Shantanu Sharma, UNC-CH Biochemistry & Biophysics (Quantitative finance developer and algorithmic trading researcher at Mismi, New York)
2004-2009	Kyle C. Wilcox, UNC-CH Biochemistry & Biophysics (postdoctoral appointment with Prof. William L. Klein at Northwestern University)
2004-2007	Yiwen Chen, UNC-CH Physics & Astronomy (postdoctoral appointment with Prof. X. Shirley Liu at Harvard School of Public Health) (American Heart Association Predoctoral Fellow)
2004-2006	Peng Gong, UNC-CH Biomedical Engineering (MS)
2002-2005	Sagar D. Khare, UNC-CH Biochemistry & Biophysics (Assistant Professor at Rutgers University, Department of Chemistry and Chemical Biology)

## *C. Postdoctoral trainees*

2017-present	Jian Wang
2017-present	M. Ashhar Iqbal
2017-present	Venkat R. Chirasani
2014-2017	David Mowrey
2013-present	Cheng Zhu
2013-present	Andrey Krokhotin
2013-2015	Raul Mendez Giraldez
2013-2016	Marino Convertino
2012-2017	Jhuma Das
2012	Pradeep Kota
2011-2012	Srinivas Ramachandran
2010-2013	David Shirvanyants (Senior Director of Research and Development at Carbon3D, Inc.)
2006-2011	Shuangye Yin (research associate at the Broad Institute)

2003-2007	Feng Ding
2005-2007	Huifen Nie (financial analyst, Shanghai, China)
2003-2004	Jainab Khatun (currently a postdoctoral fellow with Prof. Morgan Giddings, UNC-CH)
2004	Peter Itskowitz (co-mentored with Prof. Alexander Tropsha; diseased)

*D. Research professors*

2015-present	Konstantin Popov
2016-2017	Marino Convertino
2008-2012	Feng Ding

*E. Rotation graduate students trained*

2017	Elizaveta Kulko
2017	Shu Zhang
2016	Brandon Price
2016	Alice Gabrielov
2016	James Fay
2015	Jessica Jean Hobson
2015	Jack Maguire
2015	Stephan T. Kudlacek
2015	Hanna Trzeciakiewicz
2015	Alex Carlson
2014	Frank D. Teets
2014	Aspen Gutsell
2014	Matt Satusky

2014	Dominique Soroka
2013	Benfeard Leechelle Williams
2013	Ardeshir Goliaei
2013	Kossi Agbeve
2012	Reed Jacob
2012	Rachel Cohen
2012	Mayukh Chakrabarti
2012	Mahmoud Shobair
2012	Kevin Houlihan
2012	Chanin B. Tolson
2012	Dylan Glatt-Dowd
2012	Doo Nam Kim
2012	Patrick McCarter
2011	Christine S. Kim
2011	Arpit Tandon
2011	Adam D. Friedman
2010	Greggory Rice
2010	Timothy Jacobs
2010	Srinivas Niranj Chandrasekaran
2010	Onur Dagliyan
2010	William Monteith
2009	Vinal Lakhani
2009	Bryan Der
2008	Elizabeth Proctor
2008	Stephen Bush

2008	Rachel Redler
2008	Sai Phanindra
2008	James A. Green (MD/PhD)
2007	Pradeep Kota
2007	Ben Stranges
2007	Oana Lungu
2007	Lauren Mitchell
2006	Lada Bendova (Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic)
2006	Alex Schlesinger
2006	Meng Jin
2006	Douglas Tsao
2006	Srinivas Ramachandran
2006	Daud Cole
2005	Charles Davis
2005	Ron Jacak
2005	Natsuki Tanaka
2005	Adrian Serohijos (with Prof. Timothy C. Elston)
2005	Tony Law
2004	Ramesh K. Jha
2004	Bruce E. Bondo
2004	Kun Wang
2004	Mariel L. Conlon
2003	Paul D. Renfrew
2003	David J. Bautz

2002                Deanne Sammond

2002                James M. Harris

*F. Undergraduate honor thesis students*

2017-present     Caroline Christine Folz

2017-present     Edgar M. Faison

2006-present     Faith Jarvis

2007-2010        Brittany Fotsch

2006-2009        Vinal Lakhani

2004-2005        Joshua J. Larocque

*G. Summer/Rotation undergraduate students*

2017                Skanda K. Sastry

2017                Ernesto Alva Sevilla

2017                Madeleine Nieto

2016                Rajeshree (Ria) Das

2016                Azira Rivera (Biophysics Summer Research Student)

2016-present     Faith Jarvis

2015-2016        Stephen L. Upton

2015-2016        Anthony Wu

2014-2016        Kenan Michaels

2014-2016        Cathy Anderson

2012-2013        Ian Mercer

2013-2014        Chris H. McMahon

2012-2014        Pooja Patel

2012-2013	Sainath Asokan
2012	Cameron Pinnock
2012	Juan R Diaz
2012- 2013	Jordan Texier
2012	Simon Menaker
2011-2014	Srinivas Saripalli
2011-2012	Chris Kao
2011-2012	Jimmy Fay
2010	Kalada Kienka (The Summer Research Experience for Undergraduates (SURE-REU) Program in Molecular Biosciences)
2010	Shayna Atkins (Biophysics Summer Research Student)
2009	Regis A. James (Biophysics Summer Research Student)
2009	Andrew D. A. Marshall (Biophysics Summer Research Student)
2008-2009	Kevin D'Auria
2007-2009	Brittany Fotsch
2006-2009	Vinal Lakhani
2007	Elvira Jasarevic
2006	Sunjay Barton (Partnership for Minority Advancement in the Biomolecular Sciences fellow)
2005	Tamara James (Partnership for Minority Advancement in the Biomolecular Sciences fellow)
2004, 2005	Joshua J. Larocque
2004	Justin Low (Kauffman fellow)
2004	Kenneth Nteh Gwanmesia (Summer Pre-Graduate Research Experience fellow)

*H. Research Technicians*

2015-present	Edgar M. Faison
2014-2016	Kenan Michaels
2014-2016	Yazhong Tao
2013-2015	Joseph N. Kousouros
2013-2016	Cathy Jeanette Anderson
2012-2015	Jimmy Fay
2009-2013	Lanette Fee
2007-2009	Joshua Jordon

*I. High School Students*

2017	Skanda Sastry
2013	Shyam Vasudevan
2007	J. J. Lang

*J. Thesis committees*Biochemistry

Jack Barton Maguire (2017-present)  
Jared T. Baisden (2015-present)  
Hyunna (Theresa) Lee (2015-present)  
Dominique Soroka (2014-2015)  
Benfeard Williams (2014-2017)  
Kevin Houlihan (2014-present)  
Mahmoud Shobair (2013-present)  
Srinivas Niranj Chandrasekaran (2012-2016)  
Onur Dagliyan (2011-2016)  
Kenneth Nesbitt (2010-2013)  
Shen Shen (2010-2013)  
Brian Der (2009-2013, chair)  
Katie Mayo (2009-2013)  
Rachel Redler (2009-2013)  
Ben Stranges (2009-2013, chair)  
Erin Toth (2009-2012)  
Steven Lewis (2008-2013)

Curriculum Vitae

Daud Cole (2008-2013)  
Anthony Law (2008-2013)  
Pradeep Kota (2008-2012)  
Monica Frazier (2007-2012)  
Charles Davis (2007-2010)  
Srinivas Ramachandran (2007-2011)  
Joshua Boyer (2006-2011)  
Matthew Whitley (PhD, 2006-2010)  
Yetian Chen (MS, 2006-2008)  
Natsuki Tanaka (MS, 2006-2008)  
Amanda Gates (PhD, 2005-2007)  
Stephen Roberts (PhD, 2005-2009)  
Shantanu Sharma (PhD, 2005-2009)  
Ziad Eletr (PhD, 2004-2007, chair)  
Xiaozhen Hu (PhD, 2004-2008)  
Sean Palmer (PhD, 2004-2008, chair)  
Douglas Renfrew (PhD, 2004-2010)  
Kyle C. Wilcox (PhD, 2004-2010)  
Dianne Sammond (PhD, 2003-2008)  
Sagar D. Khare (PhD, 2002-2005)

Bioinformatics and Computational Biology

Reed Jacob (2013-2017)  
Elizabeth Proctor (2009-2013)

Chemistry

Tom Christy (2015-present)  
Greggory Rice (2012-2015)  
Christine Hajdin (2010-2013)  
Christopher Lavender (2008-2013)  
Natalie Thompson (2008-2013)  
Douglas Tsao (2007-2011)  
Pavel Zhuravlev (PhD, 2007-2010)  
Denise Teotico (PhD, 2007-2008)

Computer Science

Luke Huan (PhD, 2005-2006)  
Xueyi Wang (PhD, 2007-2008)

Physics and Astronomy

Nathan Hudson (PhD, 2010-2012)  
Adrian W. Serohijos (PhD, 2006-2009)  
Yiwen Chen (PhD, 2004-2008)

Biomedical Engineering

Peng Gong (MS, 2004-2006)



Curriculum Vitae  
Department of Cell & Developmental Biology  
Kattie Wolfe (2009-2013)  
Daniel Summers (2007-2012)  
Peter Douglas (PhD, 2006-2008)

Nikolay V. Dokholyan

Department of Medicinal Chemistry  
Stephen Capuzzi (2015-present)  
Juihua Hsieh (2008-2011)

Technical University, Dresden  
Sergey A. Samsonov (PhD, 2009-2010)

Lund University, Sweden  
Iskra Staneva (PhD, 2012)

Guru Nanak Dev University, India  
Gurpreet Kaur (PhD, 2015)

University of Barcelona, Spain  
Pedro Sfriso (PhD, 2016)

## **Professional Service**

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### *To Discipline*

2017-present	Armenian Scientific Diaspora Association (ASDA) Coordination Committee
2017	<i>ad hoc</i> Reviewer, NIH Synapses, Cytoskeleton and Trafficking Study Section
2017	<i>ad hoc</i> Reviewer, NIH MSFB study section
2017	<i>ad hoc</i> Reviewer, Competitive Research Grants (KAUST)
2017	<i>ad hoc</i> Reviewer, 2017-10 ZGM1 RCB-X (SC) <u>Support of Competitive Research (SCORE)</u> program
2016	Ministry of Education and Science of the Russian Federation Advisory Committee member
2016	<i>ad hoc</i> Reviewer, NIH Synapses, Cytoskeleton and Trafficking Study Section

2016	<i>ad hoc</i> Reviewer, NIH/NIGMS BCMB
2015	SkolkovoTech Advisory Committee member
2015	<i>ad hoc</i> Reviewer, NIH/NIEHS ZES1 SET-J (R4) Cell Differentiation Assays
2014	<i>ad hoc</i> Reviewer, Department of Defense CDMRP Therapeutic Idea Award (TIA) 2014
2014	<i>ad hoc</i> Reviewer, ZGM1 TWD-3 (SC) Support of Competitive Research (SCORE)
2014	<i>ad hoc</i> Reviewer, Neurodegenerative Application Review Special Emphasis Panel ZES1 LWJ-K (R) 1
2013	<i>ad hoc</i> Reviewer, NIH NSD-B - Neurological Sciences and Disorders B
2013-present	Advisory Committee Member, Development Roadmap Program, Tomsk State University, Russia
2013	<i>ad hoc</i> Reviewer, NIH Pathway to Independence Award (K99/R00)
2013	<i>ad hoc</i> Reviewer, NIH MSFA
2012-present	Editor, <i>F1000 Research</i>
2012	Organizer, CECAM Workshop “Exploring Protein Interactions through Theory and Experiments”, Lausanne, Switzerland
2012	Reviewer, Polish Science Center
2012	Romanian National Council for Research and Development
2012	<i>ad hoc</i> Reviewer, NIH 05 ZNS1 SRB-J (01)
2012	<i>ad hoc</i> Reviewer, NIH MSFA
2011	<i>ad hoc</i> Reviewer, NIH ZRG1 MDCN-G (03)
2011	<i>ad hoc</i> Reviewer, NIH ZNS1 SRB-E (51)
2011-2013	Editorial Board Member, <i>Current Biotechnology</i>
2011-present	Book Series Editor, Series in Computational Biophysics

Curriculum Vitae	Nikolay V. Dokholyan
2011	French National Research Agency, "Interface Biology-Physics, Interface Biology-Chemistry and Biotechnology" Committee
2011-present	Editor-in-Chief, Research and Reports in Biochemistry
2011	<i>ad hoc</i> Reviewer, NIH ZRG1 BCMB
2011-2012	Editorial Board Member, <i>World Journal of Biological Chemistry</i>
2010	Reviewer, The Oak Ridge Associated Universities (ORAU)
2010	Reviewer, United Kingdom MRC NIMR Structural Biology & Biological NMR Division
2010	Organizing Committee, "Solvation and Ionic Effects in Biomolecules; Theory to Experiment", Tsakhkadzor, Armenia
2010-present	BSF Israel-USA
2010-present	Reviewer, James and Esther King Biomedical Research Program (Florida Department of Health)
2009	<i>ad hoc</i> Reviewer, NIH MABS
2009-present	Reviewer, AHA Bioengineering R1 Peer Review Study Group
2009	Reviewer, NSF MCB
2009-present	Reviewer, National Science Foundation (NSF)
2009	Reviewer, NSF Materials Research Science and Engineering Center (MRSEC) at University of Washington, Seattle
2009	Organizer, Mesilla Chemistry Workshop "Multi-Scale Modeling of Biological Molecules", Mesilla
2005-2008	Ad hoc Reviewer, NIH ZRG1 MDCN K51, ZRG1 MDCN G90S, MSFC
2008-present	Reviewer, Grant Agency, Academy of Sciences of the Czech Republic
2008-2012	Scientific Advisory Board, Prionet Canada
2007	UK-India Education and Research Initiative [UKIERI]
2007-present	Editorial Board Member, <i>Proteins: Structure, Function, and Bioinformatics</i>

Curriculum Vitae	Nikolay V. Dokholyan
2007-2013	Editorial Board Member, <i>The Open Structural Biology Journal</i>
2007-2013	Editorial Board Member, <i>The Open Biotechnology Journal</i>
2007-2013	Editorial Board Member, <i>Open Biotechnology Letters</i>
2007-2013	Editorial Board Member, <i>Open Biotechnology Reviews</i>
2007-2008	Reviewer, AHA Bioengineering & Biotechnology 3 Peer Review Study Group
2006-present	Reviewer, Kansas University Medical Center
2006-present	Reviewer, Motor Neurone Disease Association
2005-present	Reviewer, Alberta Prion Research Institute
2005-present	Reviewer, High Q Foundation
2005-present	Reviewer, Alzheimer's Association
2005	Organizer, eChemInfo conference " <i>Protein Folding, Misfolding &amp; Aggregation: Applications to Disease</i> ", Philadelphia USA
2005	Organizer, eChemInfo conference " <i>Protein Folding &amp; Misfolding: Applications to Drug Discovery</i> "
2005-2007	Ad hoc Editor, <i>Proteins: Structure, Function, and Bioinformatics</i>
2004-2005	Reviewer, Louisiana Board of Regents Research and Development Grants
2004	Reviewer, US Army Medical Research and Materiel Command (USAMRMC)
2004	Co-organizer, Triangle Biophysics Symposium 2004
2003	Reviewer, Cooperative Grants Program, U.S. Civilian Research & Development Foundation
1995-present	Reviewer for over 90 scientific journals

*Within UNC-Chapel Hill*

2017–present Biochemistry & Biophysics strategic planning committee

## Curriculum Vitae

Nikolay V. Dokholyan

2016–present	Biochemistry & Biophysics comprehensive examination committee
2015	Rita Allen Foundation Scholars Program Committee
2015-present	Member, Service Enhancement Initiative (SEI), School of Medicine Human Resources Office
2014-present	Royster Society of Fellows Faculty Board
2014-present	UNC Center for Structural Biology Advisory Committee
2014-present	Department Speaker Series Committee
2014	Pew Scholars Program Committee
2013	Searle Scholars Program Committee
2013	Prof. Wolfgang Bergmeier Promotion Committee
2013-present	Prof. Qi Zhang Mentoring Committee
2012	UNC Faculty Nomination Committee for the 2013 Rita Allen Scholar Award
2011-2014	Associate Director of the Program in Cellular and Molecular Biophysics
2011	Mallinckrodt Award for Junior Faculty committee
2010-2013	The Biomedical Analysis and Simulation Supercomputer advisory board member
2010	Chemistry Department faculty search committee
2009-2014	Biochemistry & Biophysics Department Graduate Education Committee (GECO)
2009-2010	Biochemistry & Biophysics Department Retreat Committee
2008-present	UNC Research Computing Advisory Committee
2008-2010	Biochemistry & Biophysics Department faculty search committee
2007-2009	Center for Neuroscience faculty search committee
2007-2013	Biological & Biomedical Sciences Program Admissions Committee

2007-2010	Graduate Director of the Program in Cellular and Molecular Biophysics
2007-2009	Cancer Research and Treatment Taskforce
2006	Biochemistry & Biophysics Department space committee
2006	Beckman/Pew/Sloan Awards candidate selection committee
2006	Junior Faculty Awards candidate selection committee
2006–2009	Bioinformatics and Computational Biology Admissions Committee
2005–2007	Health Sciences Library Advisory Committee
2005–2007	Biochemistry & Biophysics comprehensive examination committee
2005,2006	Mathematics Department faculty search advisor
2004-2006	Bioinformatics RoadMap committee
2004	Packard Fellowship candidate selection committee

*Professional Associations*

2012-present	Society for Neuroscience
2006-present	International Society for Computational Biology
2006-present	American Chemical Society
2004-present	Biophysical Society
2001-present	American Association for the Advancement of Science
1994-present	American Physical Society

**Research Funding**

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*Current Research Support*

R01 GM115597 (Campbell, Dokholyan MPI) 04/01/2016-03/31/2020

1.73 calendar

NIH \$226,566.00

*Mechanisms of vinculin activation and force transmission*

This will be accomplished by generating and characterizing vinculin variants with specific defects in actin binding, actin-induced vinculin dimer formation and PIP2 association in vitro, and then expressing the full length wild type protein and mutants in vinculin null cells

R37 AR018687 (Meissner, PI) 05/01/1976 - 6/30/20

0.60 calendar

NIH \$249,364 (*Dokholyan direct: \$75,955*)*Ion Transport by Skeletal Muscle Ryanodine Receptor*

The goal of this project is to uncover the molecular basis of channel opening and  $\text{Ca}^{2+}$  permeability of the skeletal muscle  $\text{Ca}^{2+}$  release channel (ryanodine receptor, RyR1). RyR1 is a 2,200 kDa ion channel that releases  $\text{Ca}^{2+}$  ions in response to an action potential from the sarcoplasmic reticulum (SR), an intracellular  $\text{Ca}^{2+}$ -storing compartment in skeletal muscle.

R01GM114015 (Dokholyan, PI) 8/15/16 - 5/31/20

1.80

calendar

NIH \$196,619 (*Dokholyan direct: \$104,500*)*Integrating cheminformatics and molecular simulations for virtual drug screening*

This proposal advances an efficient and robust computational workflow for structure-based virtual screening of very large chemical libraries. The ultimate goal of this project is to arrive at a small number of candidate molecules with high predicted binding affinity to their biological targets, which will be tested in confirmatory experiments.

0044297(011606 (Dokholyan, PI)

08/01/2014-07/31/2017

0.6 calendar

NSF \$31,429.00

*Control of Protein Dimerization through Light-Regulated Rapamycin*

We will perform docking simulations of rapamycin analogs to proteins, molecular dynamics simulations of the complexes, and molecular modeling.

R01GM123247-01 (Dokholyan, PI) 5/1/17 - 3/31/21

2.40 calendar

NIH \$350,000 (*Dokholyan direct: \$241,500*)*Engineering allostery for in vivo protein control*

Curriculum Vitae

Nikolay V. Dokholyan

This project is focused on understanding if protein activity can be controlled through the modulation of the dynamics of distant but allosterically coupled regions by exploiting the interaction networks among protein residues.

R01 GM083059 (Lee, PI) 4/1/17 - 3/31/21 0.60  
calendar

NIH/NIGMS \$250,000 (*Dokholyan lab direct: \$40,000*)

*The Role of Dynamics in Enzyme Mechanism and Allostery*

The goal of this project is to determine the structural and dynamic mechanisms that enable the homodimeric enzyme thymidylate synthase, from *E. coli* and from human, to function.

Role: Co-Investigator