BIOGRAPHICAL SKETCH

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NAME: BRINDA VALLAT

eRA COMMONS USER NAME (credential, e.g., agency login): bkvallat

POSITION TITLE: Associate Research Professor

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows as necessary.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	Start Date MM/YYYY	Completion Date MM/YYYY	FIELD OF STUDY
Women's Christian College, Affiliated to the University of Madras, Chennai, Tamil Nadu, India	B.S.	1994	1997	Chemistry
Department of Chemistry, University of Pune, Pune, Maharashtra, India	M.S.	1997	1999	Biochemistry
Molecular Biophysics Unit, Indian Institute of Science, Bangalore, Karnataka, India	Ph.D.	1999	2006	Biophysics

A. Personal Statement

I am a computational biologist and a data scientist interested in understanding biological processes from the perspective of macromolecular structure and function. I am intrigued by the complexities of biomolecular structures and how they control and coordinate biological function at the cellular level. I have extensive experience in developing computational tools that analyze and predict the structures of biomolecules from experimental and theoretical data. I am currently working on enabling data science in structural biology through the development of a repository for archiving structures determined using integrative modeling methods. These emerging methods integrate information from various experimental and computational techniques to derive the structures of complex macromolecular assemblies. The inherent complexities of the different data types involved in integrative modeling provide challenging opportunities for data acquisition, standardization, archiving, validation and dissemination. My current focus is on developing a comprehensive infrastructure for archiving integrative structures through the PDB-Dev prototype system (https://pdb-dev.wwpdb.org). Following the FAIR (Findable, Accessible, Interoperable, and Reusable) principles of scientific data management, PDB-Dev ensures that the results of integrative structure determinations are freely accessible to everyone.

Ongoing and recently completed projects that I would like to highlight include:

NSF - 1756248 (Vallat -PI) 09/2018-08/2022
Title: Collaborative Research: ABI Development: Building a Pipeline for Validation, Curation and Archiving of Integrative/Hybrid Models
Role: PI

NSF - 2112966 (Vallat -PI) 09/2021-08/2024
Title: Collaborative Research: Creating mechanisms to make integrative structures of large macromolecular assemblies available from the Protein Data Bank
Role: PI

NIH – R01GM079429 (Chiu -PI) 02/2018-01/2022
Title: Unified Data Resource for 3DEM
Role: Scientific Software Developer

NIH – R01GM085328 (Zirbel -PI) 09/2020-08/2024
Title: Integrated Resource for Nucleic Acid Structures
Role: Scientific Software Developer

B. Positions, Scientific Appointments and Honors

2021-current Associate Research Professor, Institute for Quantitative Biomedicine, Rutgers, The State University of New Jersey, Piscataway, NJ

2019-2021 Assistant Research Professor, Institute for Quantitative Biomedicine, Rutgers, The State University of New Jersey, Piscataway, NJ

2015-2018 Research Associate, Institute for Quantitative Biomedicine, Rutgers, The State University of New Jersey, Piscataway, NJ

2011-2015 Postdoctoral Fellow, Department of Systems and Computational Biology, Albert Einstein College of Medicine, Bronx, NY

2008-2011 Postdoctoral Research Associate, Institute for Computational Engineering and Sciences, University of Texas, Austin, TX

2006-2007 Postdoctoral Research Associate, Department of Computer Science, Cornell University, Ithaca NY

Academic and Professional Honors

2009 Indian National Science Academy young scientist award (https://www.insaindia.res.in/aa4young1.php)
2007-2010 Human Frontier Science Program (http://www.hfsp.org) long-term postdoctoral fellowship (Award number: LT00469/2007-L)
2005-2006 R.K. Maller memorial medal for the best thesis in the biological sciences division, at the Indian Institute of Science, Bangalore, India (https://iisc.ac.in/)
1999-2004 Junior and senior research fellowships awarded by the Council of Scientific and Industrial Research, India (https://www.csir.res.in/)
1997-1999 Fellowship awarded by the National Chemical Laboratory (https://www.ncl-india.org/), Pune, to pursue masters degree in the Department of Chemistry at the University of Pune (http://www.unipune.ac.in/dept/science/chemistry/default.htm)

C. Contributions to Science

1. Creating data standards and a prototype system for archiving integrative structures

Recent advances in the field of structural biology have led to the development of integrative/hybrid modeling methods, where data from a variety of experimental and computational techniques are combined to determine the structures of complex macromolecular assemblies. I have developed a standalone prototype system for archiving integrative structures, called PDB-Dev (https://pdb-dev.wwpdb.org). The PDB-Dev infrastructure is supported by an automated data harvesting system, as well as mechanisms for curation, visualization, validation, and dissemination of integrative structures to the broader scientific community. The data standards for PDB-Dev are provided by the IHM-dictionary (https://github.com/ihmwg/IHM-dictionary), which is an extension of the PDBx/mmCIF dictionary (https://mmcif.wwpdb.org) used by the wwPDB to archive experimentally derived structures of macromolecules. In addition to the IHM-dictionary, I have also worked on developing extensions of PDBx/mmCIF for representing and archiving computed structure models (https://github.com/ihmwg/ModelCIF) and for describing the details of Fluorescence/FRET experiments (https://github.com/ihmwg/FLR-dictionary).

Related publications

a. **Vallat B.,** Webb B., Fayazi M., Voinea S., Tangmunarunkit S., Ganesan S.J., Lawson C.L., Westbrook J.D., Kesselman C., Sali A., Berman H.M. 2021. New system for archiving integrative structures. *Acta Crystallogr D Struct Biol.*, 77(Pt 12), 1486-1496.
b. **Vallat B**, Webb B, Westbrook J, Sali A, Berman HM. 2019. Archiving and disseminating integrative structure models. *J Biomol NMR*, 73(6-7), 385-398.
c. **Vallat B**, Webb B, Westbrook JD, Sali A, Berman HM. 2018. Development of a prototype system for archiving integrative/hybrid structure models of biological macromolecules. *Structure*, 26(6), 894-904.
d. Berman HM, Trewhella J**, Vallat B,** Westbrook JD. 2018. Archiving of integrative/hybrid models. *Adv Exp Med Biol.*, 1105, 261-272.

2. Modeling of protein structures

During my postdoctoral studies, I worked on predicting protein structures from their amino acid sequences using computational tools. I developed a hybrid modeling method to predict protein structures using computational techniques combined with preliminary experimental data from nuclear magnetic resonance spectroscopy. The hybrid modeling software, SmotifCS, is publicly available at https://metacpan.org/dist/SmotifCS. The algorithm was further used to develop a template-free protein modeling method using a library of super-secondary structure motifs, which is publicly available at https://metacpan.org/dist/SmotifTF. I also developed a protein modeling method using machine-learning algorithms, and implemented the same as a protein structure prediction web server at https://clsbweb.oden.utexas.edu/loopp.html. The prediction server participated in community-wide assessment of protein structure prediction methods (https://predictioncenter.org/), with many successful predictions.

Related publications

a. **Vallat BK,** Madrid-Aliste C, and Fiser A. 2015. Modularity of protein folds as a tool for template-free modeling of structures. *PloS Comput. Biol.,* 11(8), e1004419.
b. Menon V, **Vallat BK**, Dybas JM, Fiser A. 2013. Modeling proteins using a super secondary structure library and NMR chemical shift information. *Structure*, 21(6), 891-9. (*Co-first author & Journal Cover Illustration*).
c. **Vallat BK**, Pillardy J, Májek P, Meller J, Blom T, Cao B and Elber R. 2009. Building and assessing atomic models of proteins from structural templates: Learning and benchmarks. *Proteins,* 76(4), 930-45.
d. **Vallat BK**, Pillardy J and Elber R. 2008. A template-finding algorithm and a comprehensive benchmark for homology modeling of proteins. *Proteins,* 72(3), 910-28.

3. Analysis of protein structures

The three-dimensional structures of proteins are complex in nature and the native folded state of a protein is critical for its function in the cell. Detailed analysis of protein structures can provide insights into their function and interactions with other biological molecules. During my graduate studies, I developed of a novel method to analyze three-dimensional protein structures using concepts from graph theory and systems biology. Application of the developed method provides valuable insights into protein stability and folding, protein-protein interactions and protein-DNA interactions. The method developed to study protein structures as connected networks has been implemented as a web server at http://vishgraph.mbu.iisc.ernet.in/GraProStr/index.html.

Related publications

a. Sathyapriya R., **Brinda K.V.** and Vishveshwara S. 2006. Correlation of side-chain hubs with the functional residues in DNA-binding protein structures. *J Chem Inf Model.*, 46(1), 123-9.
b. **Brinda K.V.** and Vishveshwara S. 2005. A network representation of protein structures: Implications to protein stability. *Biophys J.*, 89(6), 4159-70.
c. **Brinda K.V.** and Vishveshwara S. 2005. Oligomeric protein structure networks: Insights into protein-protein interactions. *BMC Bioinformatics*, 6, 296.
d. **Brinda K.V.**, Surolia A. & Vishveshwara S. 2005. Insights into the quaternary association of proteins through structure graphs: A case study of lectins. *Biochem J.*, 391, 1-15. *(Journal Cover Illustration)*.

Link to all publications

https://www.ncbi.nlm.nih.gov/myncbi/1tKeupbqykw52J/bibliography/public/