

# Rohit Farmer

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## Research Summary

Around ten years' experience in interdisciplinary research, applying computational methods at the intersection of biology, and chemistry. Currently, I am working on the application of deep learning to large-scale molecular data to understand drug bioactivation and toxicity. I have extensive experience in protein structure/complex prediction, modelling protein-protein interactions, molecular dynamics simulations, virtual screening, and sequence analysis.

## Teaching & Research Experience

2018- <i>now</i>	Postdoctoral Research Associate	Washington University in St. Louis, USA Department of Pathology and Immunology
2015-2018	Assistant Professor	Sam Higginbottom University of Agri., Tech. and Sci. (SHUATS), India Department of Computational Biology and Bioinformatics (CBBI)
2008-2011	Assistant Professor	SHUATS, India CBBI
2016-2018	Associate Editor	The Allahabad Journal of Science and Technology (Formerly The Allahabad Farmer)

## Administrative Experience

2015-2016	International Training Associate	SHUATS, India Directorate of International Education and Training
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## Teaching Assignments

2008	Molecular Genetics (UG, MBGE-441)	SHUATS, India
2009-2011	Biomolecular Modelling (UG, BI-605)	SHUATS, India
2012-2014	<i>Assisted in teaching</i> Physical Biochemistry (UG, Bio143)	University of Birmingham, UK
2015-2017	Concepts of Bioinformatics (UG, CBBI-502)	SHUATS, India
2015-2017	Structural Bioinformatics (UG, CBBI-601)	SHUATS, India
2015-2017	Fundamentals of Bioinformatics and Information Technology (PG, CBBI-701)	SHUATS, India
2015-2017	Computer Aided Drug Designing (PG, CBBI-803)	SHUATS, India

## Education

2011-2015	Doctor of Philosophy (Ph.D.) Biosciences	University of Birmingham, UK
2008-2010	Master of Technology (M.Tech.) Bioinformatics <i>CGPA 9.35/10; Silver Medal</i>	Sam Higginbottom Institute of Agri., Tech. and Sci. (SHIATS), India
2004-2008	Bachelor of Technology (B.Tech.) Biotechnology <i>CGPA 8.41/10</i>	Allahabad Agricultural Institute, India

## Certifications

2017	Algorithms for DNA Sequencing	Johns Hopkins University, USA Coursera
2017	Python for Genomic Data Science	Johns Hopkins University, USA Coursera

## Awards & Achievements

2014	Travel grant, 28 <sup>th</sup> Annual Symposium of The Protein Society, USA	Biochemical Society
2013	Travel grant, 15 <sup>th</sup> EMBL PhD Symposium, Germany	EMBL
2013	Travel grant, ISMB/ECCB'13, Germany	National Science Foundation
2013	George Parks travel grant, Molecular Perspectives On Protein-Protein Interactions, Poland	University of Birmingham
2012	Travel grant, ECCB'12, Switzerland	Swiss Foundation for Excellence and Talent in Biomedical Research
2011-2014	PhD scholarship	The Darwin Trust of Edinburgh
2010	Silver medal in M.Tech. Bioinformatics	SHIATS

## Key Scientific Skills

**Computational Biology:** Molecular structure prediction, molecular docking, molecular dynamics simulation, bioinformatics

**Experimental Biology:** PCR, Gibson assembly, restriction digestion, plasmid transformation, microbiology techniques, HPLC

**Operating Systems:** Linux, Mac OS X, MS Windows

**Computer Languages (Proficient):** Python, Perl

**Computer Languages (Familiar):** C++, R,  $\text{\LaTeX}$ , HTML, CSS, Java Script

**Data Science and ML Tools:** NumPy, Pandas, SciPy, Matplotlib, Seaborn, Plotly, Scikit Learn, Keras, TensorFlow

**Database:** SQLite, Neo4J

**HPC:** SLURM, PBS

**Containers & VMs:** Docker, Singularity, Oracle Virtual Box

**VCS:** Git, Mercurial

## Transferable Skills Training

2018	Mentorship Training Program	Washington University in Saint Louis, USA
2018	Mentoring Undergraduate Research	Washington University in Saint Louis, USA
2012	Leading Academics, Leadership development program	University of Birmingham, UK
2012	One day course on Poster Presentations: Planning the Content	University of Birmingham, UK
2012	Talent Pool, Training program on entrepreneurship	University of Birmingham, UK
2012	One day course on Speed Reading	University of Birmingham, UK
2011	One day course on Time Management	University of Birmingham, UK

## Conferences Attended & Organised

2015	National Conference on Bioinformatics Panorama in Agriculture and Health, India	Sponsor Liaison
2014	1 <sup>st</sup> RSG-UK Student Symposium on Computational Biology and Life Sciences, UK	Secretary
2014	Synthetic Biology of Antibiotic Production II, Spain	Short Talk
2014	The 28 <sup>th</sup> Annual Symposium of the Protein Society, USA,	Poster Presentation
2013	15 <sup>th</sup> EMBL PhD Symposium, Germany	Short Talk

2013	ISMB/ECCB'13, Germany	Poster Presentation
2013	Molecular Perspectives On Protein-Protein Interactions, Poland	Poster Presentation
2012	11 <sup>th</sup> European Conference on Computational Biology, Switzerland	Poster Presentation
2012	3 <sup>rd</sup> BEAR Postgraduate Conference on Research Computing, UK	Secretary and Sponsor Liaison
2010	The Eighth Asia Pacific Bioinformatics Conference, India	Poster Presentation
2009	National Workshop on Functional Genomics and Proteomics, India	Participant
2009	International Conference on Open Source for Computer Aided Drug Discovery, India	Poster Presentation

## Professional Memberships

2013-2014	The Protein Society
2012-2015	International Society for Computational Biology (ISCB)
2012-2015	Biochemical Society

## Extra Curricular Positions Held

2013-2014	Co-Founder and Secretary, Regional Student Group, UK	Student Council, ISCB
2011-2012	Secretary, Bharat Parivar, Guild of Students	University of Birmingham
2009-2010	Vice president for Society of Biotechnology	SHIATS

## Publications

**Rohit Farmer.** Modelling polyketide synthases and related macromolecular complexes. *PhD Thesis. University of Birmingham*, 2015. <http://etheses.bham.ac.uk/5909/>

## Book Chapter

**Farmer R.\***, Thomas C. M., and Winn P. J. Modelling Polyketide Synthases and Similar Macromolecular Complexes. In: Wadhwa G., Shanmughavel P., Singh A., Bellare J. (eds) *Current trends in Bioinformatics: An Insight*. Springer, Singapore, 2018, 121-144. [https://doi.org/10.1007/978-981-10-7483-7\\_7](https://doi.org/10.1007/978-981-10-7483-7_7)

## Refereed Journal Articles

Google Scholar: h-index 8, i10-index 7 <https://goo.gl/MrHXcA>

16. **Farmer R.**, Thomas C. M., and Winn P. J. Structure, Function and Dynamics in Acyl Carrier Proteins. *Under Review*, 2018.
15. Dhusia K., Yadav P. K., **Farmer R.**, and Ramteke P. W. Inhibition of polyamine biosynthesis for toxicity control in *Serratia marcescens* strain WW4 by targeting ornithine decarboxylase: A structure-based virtual screening study. *International Journal of Computational Biology and Drug Design*, 11(1-2), 2018.
14. Konda A. K., **Farmer R.**, Soren K. R., P. S. S., and Setti A. Structural modelling and molecular dynamics of a multi-stress responsive WRKY TF-DNA complex towards elucidating its role in stress signalling mechanisms in chickpea. *Journal of Biomolecular Structure and Dynamics*, 2017.
13. Khanim F., Davies N., Veliça P., Hayden R., Ride J., Pararasa C., Chong M. G., Gunther U., Veerapen N., Winn P. J., **Farmer R.**, Trivier E., Rigoreau L., Drayson M., and Bunce C. Selective AKR1C3 inhibitors do not recapitulate the anti-leukaemic activities of the pan-AKR1C inhibitor medroxyprogesterone acetate. *British Journal of Cancer*, 110(6), 2014.
12. Lodhi S. S., **Farmer R.**, Singh A. K., Jaiswal Y. K., and Wadhwa G. 3D structure generation, virtual screening and docking of human Ras-associated binding (Rab3A) protein involved in tumourigenesis. *Molecular Biology Reports*, 41(6), 2014.

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\* Corresponding Author

11. Haines A. S., Dong X., Song Z., **Farmer R.**, Williams C., Hothersall J., Płoskoń E., Wattana-Amorn P., Stephens E.R., Yamada E., Gurney R., Takebayashi Y., Masschelein J., Cox R. J., Lavigne R., Willis C. L., Simpson T. J., Crosby J., Winn P. J., Thomas C. M., and Crump M. P. A conserved motif flags acyl carrier proteins for  $\beta$ -branching in polyketide synthesis. *Nature Chemical Biology*, 9(11), 2013.
10. Singh S., Sablok G., **Farmer R.**, Singh A. K., Gautam B., and Kumar S. Molecular dynamic simulation and inhibitor prediction of cysteine synthase structured model as a potential drug target for trichomoniasis. *BioMed Research International*, 2013, 2013.
9. Kumar S., **Farmer R.**, Turnbull A. P., Tripathy N. K., and Manjasetty B. A. Structural and functional conservation profiles of novel cathepsin L-like proteins identified in the *Drosophila melanogaster* genome. *Journal of Biomolecular Structure and Dynamics*, 31(12), 2013.
8. Paital B., Kumar S., **Farmer R.**, and Chainy G. B. N. In silico prediction of 3D structure of Mn superoxide dismutase of *Scylla serrata* and its binding properties with inhibitors. *Interdisciplinary Sciences: Computational Life Sciences*, 5(1), 2013.
7. Gautam B., Singh G., Wadhwa G., **Farmer R.**, Singh S., Singh A. K., Jain P. A., and Yadav P. K. Metabolic pathway analysis and molecular docking analysis for identification of putative drug targets in *Toxoplasma gondii*: novel approach. *Bioinformation*, 8(3):134–41, 2012.
6. Fazil M. H. U. T., Kumar S., **Farmer R.**, Pandey H. P., and Singh D. V. Binding efficiencies of carbohydrate ligands with different genotypes of cholera toxin B: Molecular modeling, dynamics and docking simulation studies. *Journal of Molecular Modeling*, 18(1), 2012.
5. Kumari S., Shridhar S., Singh D., Priya P., **Farmer R.**, Hundal J., Sharma P., Bavishi K., Schrick K., and Yadav G. The role of lectins and HD-ZIP transcription factors in isoprenoid based plant stress responses. *Proceedings of the Indian National Science Academy*, 78(4), 2012.
4. Lodhi S. S., **Farmer R.**, Singh A. K., Wadhwa M., Jaiswal Y. K., and Wadhwa G. Statistical analysis of differential gene expression profile for colon cancer. *Indian Journal of Biotechnology*, 11(4), 2012.
3. Paital B., Kumar S., **Farmer R.**, Tripathy N. K., and Chainy G. B. N. In silico prediction and characterization of 3D structure and binding properties of catalase from the commercially important crab, *Scylla serrata*. *Interdisciplinary Sciences: Computational Life Sciences*, 3(2), 2011.
2. Jeyakumar E., Lawrence R., **Farmer R.**, and Sahai S. *In vitro* and *In silico* analysis of xylanase produced by *Bacillus licheniformis*. *Applied Biological Research*, 13(1):17–27, 2011.
1. **Farmer R.**<sup>†</sup>, Gautam B., Singh S., Yadav P. K., and Jain P. A. Virtual screening of AmpC/ $\beta$ -lactamase as target for antimicrobial resistance in *Pseudomonas aeruginosa*. *Bioinformation*, 4(7):290–4, 2010.

## Preprint

Hassan M., Rahman F., **Farmer, R.**, Das S., and Vayani F. Highlights of the 1<sup>st</sup> Student Symposium of the ISCB RSG UK. *F1000Research*, 4, 2015. <https://doi.org/10.12688/f1000research.6616.1>

December 5, 2018

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