Dr. D.Y. Patil Vidyapeeth's
Dr. D. Y. Patil Biotechnology and Bioinformatics Institute
Mumbai-Bangalore Express High way, Tathawade, Pune 411033
Mail: info.biotech@dpu.edu.in, **Website:** http://biotech.dpu.edu.in

Dr. Goldsmith

Designation: Assistant Professor

Email ID: g.goldsmith@dpu.edu.in ; ggoldsmith.gs@gmail.com

Qualification: M. Sc (Biophysics), Ph.D.

Profile Summary: Computational structural biologist with research experience in working on Protein, Nucleic acids (*DNA, RNA, DNA.RNA hybrid duplexes, DNA triple helices, G-quadruplex*) and Protein-Nucleic acid complex structures by integrating molecular modelling and molecular dynamics simulation methods. Familiar with protein-ligand as well as protein-nucleic acid and protein-protein docking techniques.

Area of Specialization: Computational Structural Biology, Molecular Biophysics; Molecular Modelling; MD simulation; Free Energy calculation; *In silico* Mutational studies; Protein-Nucleic Acid Docking; Computer Aided Drug Design (CADD)

Research focus: Understand the Biomolecular structure, dynamics and its function through molecular modelling, molecular dynamics simulation, *in-silico* docking and structural bioinformatics methods. Current interests include (i) examining the conformational flexibility of a DNA repair enzyme and its interaction with its nucleic acid substrate, relevant in antisense strategy of gene regulation (ii) Rational design of species-specific small molecule inhibitors against proteins implicated to be critical in disease and therapeutics and (iii) Development of computational tools to aid conformational analysis of macromolecule structures.

Professional experience

- **Aug 2024–** Present: *Assistant Professor* (Teaching & Research)

Dr. D.Y.Patil Biotechnology and Bioinformatics Institute, Dr. D. Y. Patil Vidyapeeth, Tathawade, Pune, India.

https://biotech.dpu.edu.in/faculty.aspx

- Lecturer and research guide in subjects like *Structural Biology*, Molecular Modeling and Drug design and Bioinformatics (*Theory and practicals*)

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- **Dec 2022– March 2024** NyBerMan Bioinformatics, Europe
  Computational Scientist, Tutor, research consultant

- Executed client research projects from planning to closure related to computational structural biology.
- Tutored post graduate students/industry professionals on concepts of structural biology/stereochemistry/molecular dynamics simulation.
- Acted as a scientific advisory committee member of the organization.

Research experience

Sep 2020–Mar 2021; IBAB, Bangalore, India
Post-doctoral Fellow; *Supervisor*: Prof. N. Yathindra

- Developed MD trajectory analysis pipeline for analyzing protein-nucleic acid complex interactions.
- Identified potential small molecule inhibitor molecules against RNase HI, an enzyme critical in antisense method of gene regulation.
- Authored internal reports and prepared manuscript for publication.

Nov 2010–Aug 2020; IBAB, Bangalore, India
Bioinformatician & Doctoral researcher (Ph.D.)

- Taught courses on Molecular modelling, MD simulation, docking, bioinformatics techniques (theory & hands-on) for M. Sc. students under UGC-IGNOU and University of Mysore, India. Framed syllabus, question paper & graded examination answer script for above mentioned course.
- Conducted workshop/training programs in computational structural biology and CADD catering to academicians & industry personnel.
- Guided post graduate students (M.Sc.) in end-semester research projects.
- Assisted in lectures on 'Stereochemistry of macromolecule (proteins, nucleic acids and carbohydrate) structures' and also evaluated internal & university semester examination answer scripts of this subject.
- Conceived & developed a computational tool for structural analysis.
- Liaised with multi-disciplinary scientists within and outside the organization on various collaborative projects.

Jan 2005-Sep 2010: **IBAB, Bangalore, India: *Senior research fellow and Tutor***

- Trained Post graduate diploma in Bioinformatics (PGDB) students (7 batches) on aspects of molecular modelling through usage of computational structural biology software's.
- Performed MD simulation of few antiparallel DNA triple helices followed by analyses of their trajectories.
- Conducted multiple workshop/training programs in structural bioinformatics and drug discovery process (docking, QSAR concept) catering to academicians & industry personnel in cooperation with Accelrys Inc & faculty members from premier institutes like IISc, NCBS, IGIB etc.

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Publications

- **Goldsmith G**, Raja S, N Yathindra (2003) ***Journal of Biomol. Struc. and Dynamics***, 20, 929.
- Nambiar M, **Goldsmith G**, Moorthy BT, Joshi MV, Hosur RV, Raghavan SC. (2011) ***Nucleic Acids Research***, 39, 936.
- Srivastava M, Nambiar M, Sharma S, **Goldsmith G**, Karki S, Pandey M, Singh RK, Ray P, Kelkar M, Choudhary B, Raghavan SC. (2012) ***Cell.*** , 151, 1474.

- Ananth P, **Goldsmith G**, N Yathindra. (2013) ***RNA***. 19, 1038.
- M Srivastava, M Nambiar, S Sharma, SS Karki, **Goldsmith G**, M Hegde (2013), ***Cancer discovery***, 3,135.
- **Goldsmith G** and Yathindra N (2015) ***Journal of Proteins and Proteomics*** 6 (1), 38.
- **Goldsmith G**, Rathinavelan T, N. Yathindra (2016) ***PLoS One***. 11, *e0152102.*
- Iyer D[#], Vartak SV[#], **Goldsmith G****, Mishra A*, Kumar S, Hegde M, Velusamy M, Choudhary B, Karki S, Surolia A, Raghavan SC (2016). ***FEBS J***. 283, 3408. **#** Equal first authorship *******Equal 2nd author*
- Lilian Olivieri, **Goldsmith G**, N. Yathindra (2015) ***Journal of Proteins and Proteomics*** 6 (1), 98.
- Pandey M, **Goldsmith G**, Kumar S, Srivastava M, Elango S, Shameem M, Bannerjee D, Choudhary B, Karki S, Raghavan SC (2017) ***Mol. Carcinog***. 56, 550.
- Vartak SV, Iyer D, S kumar, Sharma S, **Goldsmith G**, Srivastava S, Karki S, Surolia, Choudhary B, Raghavan SC (2017) ***Biochem Pharmacol.*** 131, 16.
- Vadivel K, Schreuder HA, Liesum A, Schmidt AE, **Goldsmith G**, Bajaj SP. (2019) ***J. Thromb Haemost***. 17, 574.
- **Goldsmith G****, Ayesha SP, Rujula SD, Isha Zafar, Soumya Basu, Satish Sasikumar* (2025); "Targeting unique histone deacetylases: A therapeutic strategy for idiopathic pulmonary fibrosis. ***IEEE Xplore*** (*manuscript accepted for publication*) ***corresponding author**
- **Goldsmith G****, Rujula SD, Vishaka Choube, Shuchi Nagar, Nilay Mitash* (2025) Inhibition of TEAD2 to combat pulmonary fibrosis; ***IEEE Xplore*** (*manuscript accepted for publication*) ***corresponding author**
- **Goldsmith G**** (2025) 'Mechanistic influence of the hybrid binding domain on substrate recognition in full-length *Halalkalibacterium halodurans* RNase HI'***; IEEE Xplore*** (*manuscript accepted for publication*) ***corresponding author**

Total Number of Citations: 786

https://scholar.google.com/citations?user=kAisfB8AAAAJ&hl=en

Scientific Patent

Co-inventor of an Indian patent (No: **386398**) titled "*Novel inhibitors of antiapoptotic BCL-2 protein*". **Grant date:11/01/2022**

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Selected Poster/Oral presentations in Conferences and Symposia

- **G. Goldsmith** and N. Yathindra. **Poster presentation** titled '*Mechanistic insights into the effects of nonisomorphic base triplets in DNA triplexes. Extreme effects of NBT render parallel GT TFO less suited for Triplex formation*' in "Conference on Informatics & Integrative Biology": Dec 14 -16, 2011 @ Bose institute, Kolkata. ***"Won best poster award"***

- **G. Goldsmith** and N. Yathindra. **Poster presentation** titled '*Insights into the conformational dynamics of RNase H enzymes and their role in substrate recognition*' in "International conference on Biomolecular forms and functions: A celebration of 50 years of Ramachandran map": Jan 8-11, 2013 @ IISc, Bangalore, India.

- **G. Goldsmith**: **Oral presentation** titled '***Rational drug design***' under the lecture series 'Relevance of computational studies in research & society (Bio-IT)' in "***Bangalore India Bio***": Feb 4-6,2013. Bangalore, India.

- **G. Goldsmith** and N. Yathindra. **Oral presentation** titled '*Substrate specificity of RNase H enzymes*'. in "National Symposium on Biophysics & Golden Jubilee Meeting of Indian Biophysical Society": Feb 14-17, 2015 @ Jamia Milia University, New Delhi.

- Ayesha SP, Dimple Davray, **Goldsmith G***, Satish Sasikumar* (2024) 'Exploring potential protein interactions of Grainyhead-like 2 transcription factor' International Conference on Advances in Biotechnology and Bioinformatics (ICABB 2024)" 26th-29th November 2024 at DYPBBI, DPU, Pune. ***Corresponding author**

Book Chapter

Goldsmith G*, Riddhi Deka, Dipshika Basangar, Aarti Nakat, Prakashini Nilgirwar, Vishakha Chobe, Dimple Davray, Shuchi Nagar* (2025) "Protein structure prediction using a comparative modeling approach" *Nova Publishers, India*. ***Corresponding author***

Technical Skills

- **Operating System**: Linux, Windows, Mac, Sgi-Irix
- **Platform:** Linux desktops, GPU, HPC
- **Programming languages**: Shell scripting, R (familiar)
- **Molecular Modelling:** Insight II, Discovery Studio, Cerius2, Chimera, PyMOL, Modeller, XPLOR, *Schrodinger*
- **MD Simulation:** AMBER, GROMACS. CHARMM-GUI
- **Sequence Analysis:** Clustal W, CLANS, MEGA EMBOSS & other online tools.
- **Molecular Docking:** Ligand-fit, AutoDock, AutoDockVina, DOCK, ZDOCK, OpenBabel
- **Machine Learning in CADD:** Weka (familiar)

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Recognition/Honour

- Received a grant of over **One crore Indian Rupees** for the institute IBAB, from the Govt. of Karnataka, India in recognition of my work on finding potential drug against anti-cancer target Ligase 4 (2013)
- Won the **best research poster** award on several occasions in scientific research Review Meet/conferences.
- College **Top rank holder** throughout the 3-year **B.Sc. Physics** degree course.

Education

- **Ph.D.** in ***Computational Structural Biology*** from *IBAB,* Bangalore and Manipal Academy of Higher Education (MAHE), Manipal, India.
- **M. Sc.** in ***Biophysics*** from the *Dept. of Crystallography and Biophysics*, **University of Madras**, Chennai, India.
- **B.Sc.** in ***Physics*** with Chemistry and Mathematics as ancillaries, New College, **University of Madras**, Chennai, India.

No. of Ph.D., Postdoctoral, B. Tech, M. Tech. /M.Sc. students Guided:

1. M.Sc**:** 6
2. PG. Diploma in Bioinformatics**:** 5
3. Postdoctoral student**:** 1

Institute Level Academic and Administrative Responsibility

- Local organizing committee member in "International Conference on Advances in Biotechnology and Bioinformatics (ICABB 2024)" 26th-29th November 2024 at Dr. D. Y. Patil Biotechnology & Biotechnology & Bioinformatics Institute, Pune.