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. G. Goldsmith

**Designation:** Assistant Professor

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

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

**Area of Specialization**: Computational Structural Biology

**Research Interest**: Molecular Biophysics; Biomolecular Structure, Dynamics, and interactions; Molecular Modelling; MD simulation; Free Energy calculation; *In silico* Mutational studies; Protein- Nucleic Acid Docking; Computer Aided Drug Design (CADD)

## Professional experience

**Aug 2024-** present 📌 Dr. D.Y.Patil Biotechnology and Bioinformatics Institute, Dr. D. Y. Patil Vidyapeeth, Tathawade, Pune, India.

**Assistant Professor (Teaching & Research)**

- Lecturer in subjects like Bioinformatics, Structural Biology and Molecular Modeling and Drug design (Theory & practical's)

**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.
- Supervised academic dissertation of master degree and doctoral students.
- 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

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**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.

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- 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 tool 'IntScan' to catalogue all intra molecular and inter molecular interactions within a protein and protein-complexes from MD trajectories. (Coded in Python by my project trainee)
- Liaised with multi-disciplinary scientists within and outside the organization on various collaborative projects.

**Jan 2005-Sep 2010 IBAB, Bangalore, India; *Junior Research Fellow***

● 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.

## 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.
- **G Goldsmith**, N Yathindra (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, **G. Goldsmith**, 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); ***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
- Gunaseelan Goldsmith* (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

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## Scientific Patent

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

### 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*, Aarti Nakat, Ridhi D, Sneha B, Sejuti N, Shuchi Nagar* (2025) 'Protein structure prediction using a comparative modeling approach' (communicated) *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)

## 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.

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## Education

- **Ph.D.** in Computational Structural Biology from *IBAB, Bangalore* & Manipal Academy of Higher Education (MAHE), Manipal, India. (2020).

- **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. PGDB: 5
3. Postdoctoral: 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.