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## Relevant Research Experience and Education

<b>October 2022 –</b>	Research Associate, Weill Institute for Cell and Molecular Biology, Cornell University Advisor: Dr. Haiyuan Yu, Professor <b>Development of robust computational methods for data processing and quality control for large-scale proteomics studies</b>
<b>October 2016 – September 2022</b>	Postdoctoral Associate, Weill Institute for Cell and Molecular Biology, Cornell University Advisor: Dr. Haiyuan Yu, Professor <b>Development of robust computational methods for data processing and quality control for large-scale proteomics studies.</b>
<b>July 2016 – September 2016</b>	Bridging Postdoctoral Fellow, National Centre for Biological Sciences (NCBS-TIFR) Bangalore, India Advisor: R. Sowdhamini, Professor <b>Setup computational framework to better understand evolutionary importance of bacterial proteins</b>
<b>September 2015 – February 2016</b>	Pre-postdoctoral fellow, Department of Biotechnology, Indian Institute of Technology Madras Advisor: Dr. M. Michael Gromiha, Professor <b>Prioritization of malarial host-pathogen protein-protein interactions for drug discovery using their binding affinities</b>

**July 2011 – August 2015**

Ph.D. Computational Biology and Bioinformatics, Indian Institute of Technology Madras

Advisor: Dr. M. Michael Gromiha, Professor

**Thesis title: Binding Specificity of Protein-Protein Complexes: Development of Algorithms and Applications**

**July 2008 – April 2010**

M. Sc. Bioinformatics, University of Madras

Additional subjects: Biophysics and Biostatistics

### Research Areas of Interest

- Computational Biology and Bioinformatics
- Proteomics

### Patent(s)

1. Large-scale mapping of protein-protein interactions from crosslinking mass spectrometry. 2022, US Patent granted, US11215621B2. (**Contribution: Inventor**)

**Publications (citations: 823, h-index: 11, i10-index: 14)**

### AS FIRST AUTHOR

1. **Yugandhar K<sup>#</sup>**, Zhao Q<sup>#</sup>, Gupta S<sup>#</sup>, Xiong D<sup>#</sup>. and Yu H. (2021) Progress in methodologies and quality-control strategies in protein cross-linking mass spectrometry. *Proteomics*, 21, 2100145 (#Equal Contribution).
2. Lanz M.C<sup>#</sup>, **Yugandhar K<sup>#</sup>**, Gupta S, Sanford E, Faça V, Vega S, Joiner A, Fromme C, Yu H. and Smolka M.B. (2021) In-depth and 3-Dimensional Exploration of the Budding Yeast Phosphoproteome. *EMBO Reports*, 22, e51121 (#Equal Contribution).
3. **Yugandhar K**, Wang Ting-Yi, Wierbowski S.D, Shayhidin E.E. and Yu H. (2020) Structure-based validation can drastically underestimate error rate in proteome-wide cross-linking mass spectrometry studies. *Nature Methods*, 17, 985-988.
4. **Yugandhar K<sup>#</sup>** Wang Ting-Yi.<sup>#</sup>, Leung A.K.Y., Lanz, M.C., Motorykin, I., Liang, J., Shayhidin, E.E., Smolka, M.B., Zhang, S. and Yu, H. (2020) MaXLinker: proteome-wide cross-link identifications with high specificity and sensitivity. *Mol. Cell. Proteomics*, 19, 554-568 (#Equal Contribution).

5. Jemimah S<sup>#</sup>, **Yugandhar K<sup>#</sup>** and Gromiha MM. (2020) Binding affinity of protein-protein complexes: experimental techniques, databases and computational methods. Book chapter in ‘Protein interactions: Computational methods, analysis and applications’, *World Scientific*, 87-108 (#Equal Contribution).
6. **Yugandhar K<sup>#</sup>**, Gupta S<sup>#</sup> and Yu H. (2019) Inferring protein-protein interaction networks from mass spectrometry-based proteomic approaches: a mini-review. *Comput. Struct. Biotechnol. J.*, 17, 805-811 (#Equal Contribution).
7. Nikam R<sup>#</sup>, **Yugandhar K<sup>#</sup>** and Gromiha MM. (2018) Discrimination and prediction of protein-protein binding affinity using deep learning approach. *International Conference on Intelligent Computing, Springer*, 809-815 (#Equal Contribution).
8. **Yugandhar K.** and Gromiha MM. (2017) Computational approaches for predicting binding partners, interface residues and binding affinity of protein-protein complexes. *Methods Mol. Biol.*, 237-253.
9. **Yugandhar K.** and Gromiha MM. (2016) Analysis of protein-protein interaction networks based on binding affinity. *Curr. protein Pept. Sci.*, 17, 72-81.
10. **Yugandhar K.** and Gromiha MM. (2014) Protein-protein binding affinity prediction from amino acid sequence. *Bioinformatics*, 30, 3583–3589.
11. **Yugandhar K.** and Gromiha MM. (2014) Feature selection and classification of protein-protein complexes based on their binding affinities using machine learning approaches. *Proteins*, 82, 2088–2096.

#### AS CONTRIBUTING AUTHOR

12. Nikam R, Ridha F, Jemimah S, Yugandhar K and Gromiha MM. (2025) Binding affinity changes upon mutation in protein–protein complexes. Book chapter in PROTEIN MUTATIONS: Consequences on Structure, Functions, and Diseases. Pages: 105-122.
13. Nikam R, **Yugandhar K.** and Gromiha M.M. (2023) Deep learning-based method for predicting and classifying the binding affinity of protein-protein complexes. *BBA - Proteins and Proteomics*, 1871, 14098.

14. Nikam R, **Yugandhar K.** and Gromiha M.M. (2022) DeepBSRPred: deep learning-based binding site residue prediction for proteins. *Amino Acids*, <https://doi.org/10.1007/s00726-022-03228-3>.
15. Furman CM, Wang TY, Zhao Q, **Yugandhar K.** Yu H. and Alani E. (2021) Handcuffing intrinsically disordered regions in Mlh1-Pms1 disrupts mismatch repair. *Nucleic Acids Res.*, 49, 9327-9341.
16. Joiner A.M.N, Phillips B.P, **Yugandhar K.** Sanford E.J, Smolka M.B, Yu H, Miller E.A. and Fromme J.C. (2021) Structural basis of TRAPPIII-mediated Rab1 activation. *The EMBO Journal*, 40:e107607.
17. Jemimah S, **Yugandhar K.** and Gromiha MM. (2017) PROXiMATE: a database of mutant protein-protein complex thermodynamics and kinetics. *Bioinformatics*, doi: 10.1093/bioinformatics/btx312
18. Gromiha MM, **Yugandhar K.** and Jemimah S. (2017) Protein-protein interactions: scoring schemes and binding affinity. *Curr. Opin. Str. Biol.*, 44, 31-38.
19. Gromiha MM. and **Yugandhar K.** (2017) Integrating computational methods and experimental data for understanding the recognition mechanism and binding affinity of protein-protein complexes. *Prog. Biophys. Mol. Biol.*, 128, 33-38.
20. Kulandaisamy A, Lathi V, ViswaPoorani K, **Yugandhar K.** and Gromiha MM. (2017) Important amino acid residues involved in folding and binding of protein-protein complexes. *Int. J. Biol. Macromolec.*, 94, 438-444.

#### Citation List (partial) in highly reputed journals

- Burke et al. (2023) Nat. Struct. Mol. Biol. 1-10
- Matzinger et al. (2022) Nat. Commun. 13, 3975.
- Chavez et al. (2021) Chem. Rev. 122, 7647-7689.
- Lenz et al. (2021) Nat. Commun. 12, 1-11.
- Glick (2021) EMBO J. 40, e108537.
- Singh A. (2020) Nat. Methods, 17, 129.
- Beveridge et al. (2020) Nat. Commun. 11, 742.
- Donovan et al. (2020) Cell. 183, 1714-1731

## Selected Citations

- Matzinger et al. (2022) Nat. Commun. 13, 3975: highlighted my work on underestimation of error rates in cross-linking mass spectrometry (“Yugandhar et al. showed that this approach can lead to a significant underestimation ...”).
- Chavez et al. (2022) Chem. Rev. : Discussed about the superior performance of my MaXLinker algorithm (“... Yugandhar et al. developed a new search engine termed MaXLinker, which was found to outperform XlinkX ...”).
- Singh A. (2020) Nat. Methods: Associate editor from the Nature Methods journal highlighted my MaXLinker software in their ‘Research Highlights’ section (“... Yugandhar et al. have developed MaxLinker, an MS3-centric cross-link search approach that the authors demonstrate to have a significantly lower misidentification rate ...”).
- Beveridge et al. (2020) Nat. Commun. 11, 742.; Bartolec et al. (2019) Analytical Chemistry. 92, 1874-1882: Our study highlighting the underestimation of error rates in proteome-wide cross-linking studies has been discussed.
- Dutta et al. (2019) Biochim Biophys Acta. 1861, 958-977: Utilized my PPA-Pred affinity prediction web server to study implications of the interaction between snake pshospholipase 2 enzyme and a rat protein in venom-induced cytotoxicity.

## Web Servers/Algorithm/Methods/Databases Developed

- **SuperPhos:** A comprehensive database for yeast proteome-scale phosphorylation events along with mappings to 3D structures and interaction interfaces, 2021 ([superphos.yulab.org](https://superphos.yulab.org))
- **MaXLinker:** Software for protein cross-link identification from cross-linking mass spectrometry experiments with high specificity and sensitivity, 2020 (<https://www.yulab.org/resources/MaxLinker/>).
- **PPA-Pred:** Web server for binding affinity prediction between two interacting proteins, 2014 ([https://www.iitm.ac.in/bioinfo/PPA\\_Pred/](https://www.iitm.ac.in/bioinfo/PPA_Pred/)) (Accessed more than 32,000 times).

## Conferences, Workshops and Symposia

### Oral Presentations

- Invited talk at Protein Bioinformatics Lab, Indian Institute of Technology Madras (December, 2018).
- Biannual retreat of Weill Institute of Cell and Molecular Biology, Cornell University (August, 2018).
- Invited talk at Protein Bioinformatics Lab, Indian Institute of Technology Madras (January, 2018).
- Invited talk at Lineberger Comprehensive Cancer Center, University of North Carolina, Chapel Hill, North Carolina, USA (March, 2016).
- 3<sup>rd</sup> IITM-Tokyo Tech Joint Symposium on Algorithms and Applications of Bioinformatics held at IIT Madras, Chennai, India (November, 2015).

### Poster Presentations

- American Society for Mass Spectrometry (ASMS) annual conference held at Atlanta, Georgia, USA (June, 2019).
- 23<sup>rd</sup> annual meeting of Intelligent Systems for Molecular Biology (ISMB) and 14th European Conference on Computational Biology (ECCB) held at Dublin, Ireland (July, 2015).
- 2<sup>nd</sup> IITM-Tokyo Tech Joint Symposium on Techniques and Applications of Bioinformatics held at IIT Madras, Chennai, India (September, 2013).
- Biotech Meet of Research Scholars (BIOMERS) 2013 Symposium held at IIT Madras, Chennai, India (November, 2013).
- Biotech Meet of Research Scholars (BIOMERS) 2012 Symposium held at IIT Madras, Chennai, India (September, 2012).

## Manuscript Reviewer (reviewed 46 journal articles and 2 conference article in total so far)

- Scientific Reports (Nature Publishing Group)
- Review Editor for Frontiers in Bioinformatics (Frontiers)

- Journal of Proteomics (Elsevier)
- Methods (Elsevier)
- Amino Acids (Springer)
- Computational Biology and Chemistry (Elsevier)
- Microbial Pathogenesis (Elsevier)
- Bioinformatics Advances (Oxford)
- Biochemistry Research International (Wiley)
- Applied Biochemistry and Biotechnology (Springer)
- Journal of Biosciences (Springer)
- BioMed Research International (Wiley)
- Journal of Bioinformatics and Computational Biology (World Scientific)
- International Conference on Bioinformatics (InCoB)
- International Conference on Intelligent Computing (ICIC)

#### **Honors/Awards/Achievements**

- Sam and Nancy Fleming Trust Postdoctoral Fellowship Award, USA (2017-2020)
- Postdoctoral Leadership Certificate Program, Cornell University, USA (2018)
- Honorary Fellowship Award by IIT Madras for submission of PhD thesis within four years (2015)
- All India Rank 54 with UGC-JRF in CSIR/UGC/NET Examination (2011)
- All India Rank 42 with 99.7 percentile in GATE Biotechnology (2011)