

VIPUL KUMAR

PhD student
DAILAB, Department of Biochemical Engineering and
Biotechnology, Indian Institute of Technology (IIT)
Delhi
New Delhi 110016

Contact Details:

+91-7986787044, +91-9592036780

Email: vipul2732@gmail.com
vipul.kumar@dbeb.iitd.ac.in

Website:

vipul2732.wixsite.com/kumar-vipul

Education

Degree	Institution	year	CGPA
PhD in Computational Biology	Indian Institute of Technology Delhi (IIT Delhi)	July 2018 - present	8.045
MS(Research)* Biochemical Eng. And Biotechnology	Indian Institute of Technology Delhi (IIT Delhi)	July 2018 - December 2018	8.062
B.Tech in Biotechnology	Lovely Professional University, Punjab	July 2014-May 2018	8.82

MS(R) degree converted to PhD w.e.f. 2nd semester 2018-2019 based on IIT Delhi internal academic criteria.*

Relevant Experience

1. **Teaching Experience:** (Jan 2019 – May 2020) Teaching Assistant (TA) in Department of Biochemical Engineering and Biotechnology, Indian Institute of Technology Delhi. As a TA, led group discussions and lab sessions of undergraduate students in subject of Bioinformatics and Computational Structural Biology.

2. Professional training received

Duration	Nature of Training	Organization
June 2017-July 2017	Microbial Limit Test: Undergone four weeks of Industrial training at Capsule Healthcare Pvt. Ltd. as a trainee microbiologist under department of quality control where I have learnt about microbial limit testing of different In-Process and hard gelatin capsule shells according to standard of Indian Pharmacopeia	Capsugel Healthcare Pvt. Ltd. (A Lonza Group)

3. Students Co-mentored during PhD:

- I. **Pallavi Rao** (Amity University, Noida) 1ST Feb 2019 to 8th April 2019
Project title: Evaluating the potential of natural compounds on inhibiting the activity Of wild type and mutant form of EGFR.

II. **Aditya Rathi** (IIT Delhi)

1ST Sep 2020 to 8th May 2021

Project title: Identification of withanolides with potential as phosphodiesterase-4 (PDE4D) inhibitor.

Skills and Expertise

Computational Biology (Expertise)	Computational tools and techniques	Experimental Techniques (Basic)
Biomolecular modelling, Computational drug discovery (Virtual screening, QSAR, ADMET, ligand-based drug designing), Molecular Dynamic Simulations and Analysis, and bioinformatics tools and databases.	Schrodinger (Small molecule discovery), Desmond, Gromacs, Autodock, PyRx virtual screening, Pymol, VMD, Discovery Studio, Charmm-GUI, Windows/Linux command line, Python scripting.	Microscopy, AGE, HPLC(Basics), Centrifugation, Cell culturing, DNA extraction

Academic Achievements

1. **Best oral presentation** award in Sakura Science Program Workshop, AIST, Japan, October 2019.
2. **All India Rank 41 in GATE** Biotechnology (BT) in 2018.

Scientific Community Membership

1. **Member of Sakura Science Club, Japan.**
2. **American Chemical Society, USA.**

Presentation in Conferences/Webinars

1. Oral presentation in the webinar series 2020 **“COVID 19 Pandemic: The Road Map to Recovery”** on topic *Natural molecules against SARS-CoV-2 : A molecular modelling study*, organized by Sukshmjeev society , Bhaskaracharya college of applied sciences, University of Delhi (July 7, 2020).
2. Poster presentation at **“International Conference on Drug Discovery 2020, BITS Pilani, Hyderabad campus, India”** on topic entitled *Mechanistic Insights into Withanolides Action Against Cancer* (29th Feb – 2nd March 2020).

3. Oral presentation at “**Research on Mol. Biology of stress, aging and cancer using cell culture-based assays - interventions by natural compounds workshop, AIST, Tsukuba, Japan**” on topic entitled *DNA Methyltransferase Inhibitors: Natural Drugs for An Epigenetic Cancer Therapy* (Oct. 10, 2019)

Symposiums/Seminars/Workshop Attended

1. Regular participant of **DAILAB-Café series** at DAILAB, IIT Delhi.
2. “*Research on Mol. Biology of stress, aging and cancer using cell culture-based assays - interventions by natural compounds workshop*” **DAILAB, AIST, Biomedical Research Institute, Tsukuba, Japan**, Oct. 2019.
3. “*2nd DAICENETR-SHIMADZU Analytical Workshop*”, by **Shimadzu Analytical India Pvt. Ltd., Mumbai**, October 2019.
4. “*Drug Discovery Technology*” by DAILAB IIT Delhi and AIST Japan in collaboration with Schrodinger, at **IIT Delhi**, Feb 2019.

Published Conference Abstracts

1. **Kumar, V.,** Sundar, D. (2020). Mechanistic Insights into Withanolides Action Against Cancer Proceedings of International Conference on Drug Discovery (ICDD) 2020. Available at SSRN: <https://ssrn.com/abstract=352798>

Peer Reviewed Publications

1. Rathi, A., **Kumar, V.** and Sundar, D. (2022). Insights into the potential of withanolides as as Phosphodiesterase-4 (PDE4D) inhibitors. *J. Biomolecular Structure and Dynamics*
2. **Kumar, V.,** Singh, J., Hasnain, S.E. and Sundar, D. (2021). Possible link between higher transmissibility of Alpha, Kappa and Delta variants of SARS-CoV-2 and increased structural stability of its spike protein and hACE2 affinity. *International Journal of Molecular Sciences* 22(17): 9131.
3. Dhanjal, J.K., **Kumar, V.,** Garg, S., Subramani, C., Agarwal, S., ...& Wadhwa, R. (2021). Molecular mechanism of anti-SARS-CoV2 activity of Ashwagandha-derived withanolides. *International journal of biological macromolecules*,184: 297-312.
4. Singh, J., Samal, J., **Kumar, V.,** Sharma, J., Agrawal, U., Ehtesham, N. Z., ... & Hasnain, S. E. (2021). Structure-Function Analyses of New SARS-CoV-2 Variants B. 1.1. 7, B. 1.351 and B. 1.1. 28.1: Clinical, Diagnostic, Therapeutic and Public Health Implications. *Viruses*, 13(3), 439.
5. Kalra RS, **Kumar V,** Dhanjal JK, Garg S, Li X, Kaul SC, Sundar D, Wadhwa R. (2021). COVID19-inhibitory activity of withanolides involves targeting of the host cell surface receptor ACE2:

- insights from computational and biochemical assays. *Journal of Biomolecular Structure and Dynamics*.
6. Sari, A. N., Elwakeel, A., Dhanjal, J. K., **Kumar, V.**, Sundar, D., Kaul, S. C., & Wadhwa, R. (2021). Identification and Characterization of MortaparibPlus—A Novel Triazole Derivative That Targets Mortalin-p53 Interaction and Inhibits Cancer-Cell Proliferation by Wild-Type p53-Dependent and-Independent Mechanisms. *Cancers*, 13(4), 835.
 7. Malik, V., **Kumar, V.**, Kaul, S. C., Wadhwa, R., & Sundar, D. (2021). Computational Insights into the Potential of Withaferin-A, Withanone and Caffeic Acid Phenethyl Ester for Treatment of Aberrant-EGFR Driven Lung Cancers. *Biomolecules*, 11(2), 160.
 8. **Kumar, V.**, Dhanjal, J. K., Bhargava, P., Kaul, A., Wang, J., Zhang, H., ... & Sundar, D. (2020). Withanone and Withaferin-A are predicted to interact with transmembrane protease serine 2 (TMPRSS2) and block entry of SARS-CoV-2 into cells. *Journal of Biomolecular Structure and Dynamics*, 1-13.
 9. **Kumar, V.**, Dhanjal, J. K., Kaul, S. C., Wadhwa, R., & Sundar, D. (2020). Withanone and caffeic acid phenethyl ester are predicted to interact with main protease (Mpro) of SARS-CoV-2 and inhibit its activity. *Journal of Biomolecular Structure and Dynamics*, 1-13.
 10. **Kumar, V.**, Chakraborty, A., Kaur, M., Pandey, S., & Jena, M. K. (2018). Comparative study on antimicrobial activity of tulsi (*Ocimum sanctum*) and neem (*Azadirachta indica*) methanol extract. *Asian Journal of Pharmaceutical and Clinical Research*, 11(12), 514-517.

References

Name	Dr. Durai Sundar	Dr. Renu Wadhwa	Dr. Ashok Kumar Patel
Position	Head and Professor, DBEB, Indian Institute of Technology Delhi, India	Group Head, National Institute of Advanced Industrial Science & Technology (AIST), Japan	Assistant Professor, Kusuma School of Biological Sciences, Indian Institute of Technology Delhi, India
Contact	sundar@dbeb.iitd.ac.in	Renu- wadhwa@aist.go.jp	ashokpatel@bioschool.iitd.ac.in