Siddhartha Kundu, MD, PhD (Associate Professor)

Address:	3023, Department of Biochemistry, AIIMS, New Delhi – 110029
Email:	siddhartha_kundu@yahoo.co.in; siddhartha_kundu@aiims.edu
Telephone:	+91-11-26546514
Public profiles:	Orcid || Exaly || GoogleScholar || ResearchGate
	Orcid [https://orcid.org/0000-0003-3962-776X] Exaly [https://exaly.com/author/9078290/siddhartha-kundu] GoogleScholar [https://scholar.google.co.in/citations?user=gBl-tT0AAAAJ&hl=en] ResearchGate [https://www.researchgate.net/profile/Siddhartha_Kundu3]
Research:	**Mathematical and Computational Biochemistry** • Mathematical analyses of biochemical reactions & networks • Mathematical modelling of complex biochemical systems • Algorithms for molecular biology

Positions held

Institution/Organization
Faculty (Biochemistry) • Associate Professor: All India Institute of Medical Sciences (AIIMS), New Delhi 110029 (*2023-*) • Assistant Professor: All India Institute of Medical Sciences (AIIMS), New Delhi 110029 (*2019-2023*) • Associate Professor: Army College of Medical Sciences (ACMS), New Delhi 110010 (*2018-2019*); Dr. Baba Saheb Ambedkar Medical College and Hospital (BSAMCH), GNCTD, Delhi 110085 (*2015-2018*) • Assistant Professor: Army College of Medical Sciences (ACMS), New Delhi 110010 (*2009-2014*)
Consultancy/Program officer Indian Council of Medical Research (ICMR), New Delhi 110029 (*2019*); Digital India Corporation, Ministry of Electronics and Information Technology (ITRA), New Delhi 110030 (*2016-2017*); India Research Labs (IRL) IBM (*2002-2003*)
Postdoctoral work International Center for Genetic Engineering and Biotechnology (ICGEB) (*2014*); National Institute of Immunology (NII) (*2005-2008*); ICMR-National Institute of Pathology (NIOP) (*2003-2004*); Indian Institute of Technology Delhi (IITD) (*2002*)

Servers/Software developed

Hyperlink	Description
“ReDirection” http://doi.org//10.3389/fmolb.2023.1206502 https://cran.r-project.org/package=ReDirection	**Kundu S#***. ReDirection: an R-package to compute the probability dissociation constant for every reaction of a user-defined biochemical network. ***Front Mol Biosci.*** 2023, 10. PMID: 37942290 [FMBI2023]. (https://www.frontiersin.org/articles/10.3389/fmolb.2023.1206502)
“TemporalGSSA” http://doi.org//10.1142/S0219720022500184 https://cran.r-project.org/package=TemporalGSSA	**Kundu S#***. TemporalGSSA: a numerically robust R-wrapper to facilitate computation of a metabolite-specific and simulation time-dependent trajectory from stochastic simulation algorithm (SSA)-generated datasets. ***Jour Bioinf. Comp. Biol.*** 2022, 20(4):2250018. PMID: 35941839 [JBCB2022]. (https://www.worldscientific.com/doi/10.1142/S0219720022500184)
“ProTG4” http://doi.org//10.1177/11779322211045878 http://178.63.18.214/ProTG4.html	**Kundu S#***. ProTG4: A Web Server to Approximate the Sequence of a Generic Protein From an in Silico Library of Translatable G-Quadruplex (TG4)-Mapped Peptides. ***Bioinform Biol Insights.*** 2021, 15:11779322211045878. PMID: 34602814. [BBI2021]. (https://journals.sagepub.com/doi/10.1177/11779322211045878)
“Fe2OG” http://doi.org/10.1186/s13104-021-05477-z http://178.63.18.214/Fe2OG.html	**Kundu S#***. Fe(2)OG: An integrated HMM profile-based web server to predict and analyze putative non-haem iron(II)- and 2-oxoglutarate-dependent dioxygenase function in protein sequences. ***BMC Res Notes.*** 2021, 14(1):80. PMID: 33648553. [BMRN2021]. (https://bmcresnotes.biomedcentral.com/articles/10.1186/s13104-021-05477-z).

Lab members:

	Senior residents, Visitors (Ad hoc, informal)

	Dr. Sachin S Desh completed his M.D. in Biochemistry from AIIMS, New Delhi (2024) and has joined as an SR (senior resident). Dr. Sachin had previously completed his M.B.B.S. and internship from Govt. Medical College, Thiruvananthapuram, Kerala in 2020. Dr. Sachin has utilized stochastic modelling and simulation studies to investigate the role of early metabolic changes in the polarization of M1-competent macrophages.
	Registered students
	Dr. Syed Mohammed Turab Ul Haq completed his M.B.B.S from Shadan Institute of Medical Sciences, Hyderabad, Telangana. Dr. Turab is currently pursuing his M.D. in Biochemistry (2nd year) and is working on an agent-based model (ABM) to explore the molecular basis of microgravity-based generalized immunosuppression.
	Dr. Dhanshree Bakhru completed her M.B.B.S from Lady Hardinge Medical College (LHMC), New Delhi, Delhi and pursuing her M.D. in Biochemistry (1st year). Dr. Dhanshree is interested in interdisciplinary fundamental research and is working on gene regulatory network analysis of neutrophil transcriptomes in liver disease. Dr. Dhanshree would also like to understand the underlying philosophy of the scientific method used in biomedical research.

Educational qualifications

Degree	Subject	University/Institution	Year
Ph.D.	Computational Biology & Bioinformatics	School of Computational and Integrative Sciences (SCIS-JNU), New Delhi 110067	2014-2018
M.D.	Biochemistry	All India Institute of Medical Sciences (AIIMS), New Delhi 110029	1999-2001
M.B.B.S.	Pre-&Para-/Medical/ Surgical subjects	University College of Medical Sciences (UCMS), New Delhi 110095	1992-1996

Memberships

1. American Mathematical society (AMS): Life member (ID: 2991607513)
2. Society for Mathematical Biology (SMB): Life member (ID:36503496)
3. European Society for Mathematical and Theoretical Biology (ESMTB): Life member (ID: 50143836)
4. Elected member Sigma Xi society (Scientific Research Honors Society)

Awards/recognition:

AIIMS excellence research award (certificate of commendation): 2022, 2021

Research publications/Preprints (complete citations)

[2020,)	**1.** **(Preprint) Kundu S#*.** Construction, analysis and assessment of relevance of an algebraic model for a class of biochemical networks. (https://doi.org/10.1101/2024.03.07.583960) **2.** **Kundu S#*.** A mathematically rigorous algorithm to define, compute and assess relevance of the probable dissociation constants in characterizing a biochemical network. ***Scientific Reports*** 2024, 14. PMID: 38347039 **[SCIR2024].** (https://doi.org/10.1038/s41598-024-53231-9.) **3.** **Kundu S#***. ReDirection: an R-package to compute the probability dissociation constant for every reaction of a user-defined biochemical network. ***Front Mol Biosci.*** 2023, 10. PMID: 37942290 [FMBI2023]. (https://www.frontiersin.org/articles/10.3389/fmolb.2023.1206502) **4.** **Kundu S$^{\#}$***. Modeling ligand-macromolecular interactions as eigenvalue-based transition-state dissociation constants may offer insights into biochemical function of the resulting complexes. ***Math Biosci Eng.*** 2022, 19(12): 13252-275. [MBE2022]. (https://www.aimspress.com/article/10.3934/mbe.2022620) **5.** **Kundu S$^{\#}$***. TemporalGSSA: a numerically robust R-wrapper to facilitate computation of a metabolite-specific and simulation time-dependent trajectory from stochastic simulation algorithm (SSA)-generated datasets. ***Jour Bioinf. Comp. Biol.*** 2022, 20(4):2250018. PMID: 35941839 [JBCB2022]. (https://www.worldscientific.com/doi/10.1142/S0219720022500184) **6.** **Kundu S$^{\#}$***. ProTG4: A Web Server to Approximate the Sequence of a Generic Protein From an in Silico Library of Translatable G-Quadruplex (TG4)-Mapped Peptides. ***Bioinform Biol Insights.*** 2021, 15:11779322211045878. PMID: 34602814. [BBI2021]. (https://journals.sagepub.com/doi/10.1177/11779322211045878) **7.** **Kundu S$^{\#}$***. Mathematical modeling and stochastic simulations suggest that low-affinity peptides can bisect MHC1-mediated export of high-

	affinity peptides into “early”- and “late”-phases. ***Heliyon***. 2021, 7(7):e07466. PMID: 34286133 [HEON2021]. (https://doi.org/10.1016/j.heliyon.2021.e07466) **8.** **Kundu S**[#]*. Fe(2)OG: An integrated HMM profile-based web server to predict and analyze putative non-haem iron(II)- and 2-oxoglutarate-dependent dioxygenase function in protein sequences. ***BMC Res Notes.*** 2021, 14(1):80. PMID: 33648553. [BMRN2021]. (https://bmcresnotes.biomedcentral.com/articles/10.1186/s13104-021-05477-z). **9.** **Kundu S**[#]*. Mathematical model of a short translatable G-quadruplex and an assessment of its relevance to misfolding-induced proteostasis. ***Math Biosci Eng.*** 2020, 17(3): 2470-2493. PMID: 32233549. [MBE2020]. (https://www.aimspress.com/article/10.3934/mbe.2020135).
[2002,2019]	• **Kundu S**[#]*. Insights into the mechanism(s) of digestion of crystalline cellulose by plant class C GH9 endoglucanases. ***J Mol Model.*** 2019, 25(8):240. PMID: 31338614. [JMM2019]. (https://link.springer.com/article/10.1007%2Fs00894-019-4133-1). • **Kundu S**[#]*. Mathematical basis of predicting dominant function in protein sequences by a generic HMM-ANN algorithm. ***Acta Biotheor.*** 2018, 66(2):135-148. PMID: 29700659 [ACBI2018]. (https://link.springer.com/article/10.1007/s10441-018-9327-x). • **Kundu S***, Sharma R*. Origin, evolution, and divergence of plant class C GH9 endoglucanases. ***BMC Evol. Biol.*** 2018, 18(1):79. PMID: 29848310. [BMEB2018]. (https://bmcevolbiol.biomedcentral.com/articles/10.1186/s12862-018-1185-2). • **Kundu S**[#]*. Mathematical basis of improved protein subfamily classification by a HMM-based sequence filter. ***Math Biosci.*** 2017, 293:75-80. doi:10.1016/j.mbs.2017.09.001. PMID: 28916136. (https://www.sciencedirect.com/science/article/abs/pii/S0025556416303017?via%3Dihub) • **Kundu S***, Sharma R*. In silico Identification and Taxonomic Distribution of Plant Class C GH9 Endoglucanases. ***Front Plant ci.*** 2016, 7:1185. PMID: 27570528. [FPS2016]. (https://www.frontiersin.org/articles/10.3389/fpls.2016.01185/full). • **Kundu S**[#]*. Stochastic modelling suggests that an elevated superoxide anion-hydrogen peroxide ratio can drive extravascular phagocyte transmigration by lamellipodium formation. ***J Theor Biol.*** 2016, 407:143-54. PMID: 27380944. (https://www.sciencedirect.com/science/article/abs/pii/S0022519316301734?via%3Dihub). • **Kundu S**[#]*. Co-operative intermolecular kinetics of 2-oxoglutarate dependent dioxygenases may be essential for system-level regulation of plant cell physiology. ***Front Plant Sci.*** 2015, 6:489. PMID: 26236316. [FPS2015a]. (https://www.frontiersin.org/articles/10.3389/fpls.2015.00489/full). • **Kundu S**[#]*. Unity in diversity, a systems approach to regulating plant cell physiology by 2-oxoglutarate-dependent dioxygenases. ***Front Plant Sci.*** 2015, 6:98. PMID: 25814993. [FPS2015b]. (https://www.frontiersin.org/articles/10.3389/fpls.2015.00098/full). • **Kundu S**[#]*. Distribution and prediction of catalytic domains in 2-oxoglutarate dependent dioxygenases. ***BMC Res Notes.*** 2012, 5:410. PMID: 22862831. [BMRN2012]. (https://bmcresnotes.biomedcentral.com/articles/10.1186/1756-0500-5-410). o **Kundu S***, Subodh S. Gradient sensing in vectorial chemotaxis – a novel role for Reactive Oxygen Species. ***International Journal of Trends in Medicine.*** 2011 1; 54-59. [IJTM2011]

	- Singh N, Khanna N, Sharma H, **Kundu S**, Azmi S. Insights into the molecular mechanism of apoptosis induced by TNF-alpha in mouse epidermal JB6-derived RT-101cells. ***Biochem Biophys Res Commun.*** 2002, 295(1):24-30. PMID:12083761.
	(#) Single author; (*) Corresponding author;