Name: Dr. Shailza Singh

DOB: 17th March 1978

Present Designation: Scientist F, National Centre for Cell Science, Pune

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Details of employment including current employment:

No.	Institution/ Place	Position	From (Date)	To (date)
1	NCCS, Pune	Scientist-C	2010-2014 (25.3.2010)	24.3.2014
2.	NCCS, Pune	Scientist-D	2014 – 2018(25.3.2014)	24.3.2018
3.	NCCS, Pune	Scientist-E	25.3.2018	30.6.2023
4.	NCCS, Pune	Scientist- F	1.7.2023	Till date

Professional recognition, awards, fellowships received.

- Serving as Member of Board of Studies in Bioinformatics at D.Y. Patil University, Pune 2013-2017
- Serving as Chancellor's Nominee at Dr. B.R. Ambedkar Marathwada University, Aurangabad since 2017.
- Rapid Grant for Young Investigator 2012
- Selected by INSA for Bilateral Exchange Programme in "Chemometrics and Drug Delivery" 2012
- Nominated by DBT for SAKURA EXCHANGE PROGRAMME IN SCIENCE, TOKYO 2018
- DBT and CSIR Travel Award

- Life Member-Indian Biophysical Society
- Life Member -Biotechnology Society of India
- Life Member-Society of Biological Chemists, India
- Life Member-Association of Microbiologists of India (AMI)
- Life Member-Association for DNA Fingerprinting and Diagnostics
- Life Member-Proteomics Society of India (PSI)
- Life Member-Indian Immunology Society (IIS)
- Member-Molecular Immunology Forum (MIF 2023)
- FRSC-Fellow of Royal Society of Chemistry 2024

2.1 Details of Projects under Implementation:

S.No.	Title	Duration	Role as PI/Co-PI	Agency
1.	Systems regulatory network of autophagy proteins in Leishmania: Implications towards drug design 58/39/2020/PHA/BMS	2022-2025	PI	ICMR

2.2 Details of the projects completed during the last five years:

S.No.	Title	Duration	Role as PI/Co-PI	Agency
1.	Drug Target Identification in *L.major* and *S.mansoni* through Biochemical Network Modeling (BT/PR3140/BID/7/379/2011)	(2012-15) 20/6/2012-19/6/2015	PI	DBT
2.	Systems Biology of Metabolic Network of *L.major:* Therapeutic Implications (RGYI)(BT/PR6037/GBD/27/372/2012)	(2012-15) 11/09/2012-10/9/2015	PI	DBT
3.	Systems and Synthetic Biology in Leishmania : A Bioinformatics Approach(SB/FT/LS400/2012)	(2013-2016) 24/07/2013-23/07/2016	PI	DST
4.	Molecular motors as nanocircuits in Leishmaniasis : System cues guiding syntheticbiology device construction (BT/PR10286/BRB/10/1258/2013)	(2016-2019) (18.5.2016-17.5.2019)	PI	DBT
5.	Understanding the mechanism of ABC-typemetal sequestering proteins: structure-basednovel drug development against human pathogens (BT/PR16065/NER/95/61/2015)	(2017-2020) 20.1.2017-19.7.2020)	Collaborating Institute PI	DBT-Twinning Program for NE
6.	Delineating the relationship between mir146,lipid metabolism and autophagy in Leishmania : A Systems Perspective 2019-3999/CMB/BMS	(2019-2022) 16.8.2019-15.8.2022	PI	ICMR

LIST OF SELECTED PAPERS

1. Guhe V, Singh S*. (2024) Targeting peptide based therapeutics: Integrated computational and experimental studies of autophagic regulation in host-parasite interaction. **ChemMedChem.** 2024 Feb 5:e202300679. doi: 10.1002/cmdc.202300679. Online ahead of print. PMID: 38317307
2. Khandibharad S, Singh S*. (2024) Single-cell ATAC sequencing identifies sleepy macrophages during reciprocity of cytokines in L. major infection. **Microbiol Spectr.** 2024 Feb 1:e0347823. doi: 10.1128/spectrum.03478-23. Online ahead of print. PMID: 38299832
3. Khandibharad S, Singh S*. (2024) Mechanistic study of inhibitory peptides with SHP-1 in

hypertonic environment for infection model. **Biochim Biophys Acta Gen Subj.** 2024 Jul 10;1868(9):130670. doi: 10.1016/j.bbagen.2024.130670. Online ahead of print.PMID: 38996989

4. Guhe V, Tambekar A, Singh S*. (2024) Computational and Experimental Approaches Towards Understanding the Role of ATG8 in Autophagy: A Therapeutic Paradigm in Leishmaniasis. **Protein J.** 2024 Jul 9. doi: 10.1007/s10930-024-10213-0. Online ahead of print. PMID: 38980535
5. Khilwani R, Singh S*. (2024) Traversing through the Mechanistic Event Analysis in IL-6 and IL-17 Signaling for a New Therapeutic Paradigm in NSCLC. **Int J Mol Sci.** 2024 Jan 19;25(2):1216. doi: 10.3390/ijms25021216.PMID: 38279220
6. Khandibharad S, Singh S*. (2023) Immuno-metabolic signaling in leishmaniasis: insights gained from mathematical modeling. **Bioinform Adv.** 2023 Sep 14;3(1):vbad125. doi: 10.1093/bioadv/vbad125. PMID: 37799190; PMCID: PMC10548086.
7. Jawale D, Khandibharad S, Singh S*. (2023) Decoding systems immunological model of sphingolipids with IL-6/IL-17/IL-23 axes in L. major infection. **Biochim Biophys Acta Mol Cell Biol Lipids**. 2023 Feb;1868(2):159261. doi: 10.1016/j.bbalip.2022.159261. Epub 2022 Dec 7.PMID: 36494028
8. Khandibharad S, Singh S*. (2022) Artificial intelligence channelizing protein-peptide interactions pipeline for host-parasite paradigm in IL-10 and IL-12 reciprocity by SHP-1. **Biochim Biophys Acta Mol Basis Dis**. 2022 1868(10):166466. doi: 10.1016/j.bbadis.2022.166466. Epub 2022 Jun 21. PMID: 35750267
9. Kumar A, Nimsarkar P, Singh S*. (2022) Systems pharmacology aiding benzimidazole scaffold as potential lead compounds against leishmaniasis for functional therapeutics. **Life Sci.** 2022 Sep 15:120960. doi: 10.1016/j.lfs.2022.120960. Online ahead of print. PMID: 36116527
10. Anurag Kumar, Prajakta Nimsarkar and Shailza Singh (2022) Probing the interactions responsible for the structural stability of Trypanothione reductase through Computer Simulation and Biophysical Characterization. **Protein J.** PMID: 35364760
11. Gulhane P, Nimsarkar P, Kharat K, Singh S*. (2022) Deciphering miR-520c-3p as a probable target for immunometabolism in non-small cell lung cancer using systems biology approach. **Oncotarget.** 2022; 13:725-746. doi: 10.18632/oncotarget.28233. eCollection 2022. PMID: 35634241.
12. Gulhane P, Singh S*. (2022) MicroRNA-520c-3p impacts sphingolipid metabolism mediating PI3K/AKT signaling in NSCLC: Systems perspective**. J Cell Biochem**. 2022 Aug 17. doi: 10.1002/jcb.30319. Online ahead of print. PMID: 35977046
13. Khandibharad S, Singh S*. (2022) Computational System Level Approaches for Discerning Reciprocal Regulation of IL10 and IL12 in Leishmaniasis. **Front Genet.** 2022 Jan 19;12:784664. doi: 10.3389/fgene.2021.784664. eCollection 2021. PMID: 35126456
14. Samarth N, Kabra R, **Singh S*.** (2021) Anthraquinolone and quinolizine derivatives as an alley of future treatment for COVID-19: an *in silico* machine learning hypothesis. **Sci Rep**. 2021 Sep 9; 11(1):17915. doi: 10.1038/s41598-021-97031-x. PMID: 34504128
15. Kabra R, Singh S*. (2021) Evolutionary artificial intelligence based peptide discoveries for effective Covid-19 therapeutics. **Biochim Biophys Acta Mol Basis Dis**. 2021 Jan 1; 1867(1):165978. doi: 10.1016/j.bbadis.2020.165978. Epub 2020 Sep 24.PMID: 32980462
16. Soni B, Singh S*. (2021) Synthetic Perturbations in IL6 Biological Circuit Induces Dynamical Cellular Response. **Molecules**. 2021 Dec 26; 27(1):124. doi: 10.3390/molecules27010124. PMID: 35011356
17. Soni B, **Singh S*.** (2021) COVID-19 co-infection mathematical model as guided through signaling structural framework. **Comput Struct Biotechnol J.** 2021; 19:1672-1683. doi: 10.1016/j.csbj.2021.03.028. Epub 2021 Mar 26.PMID: 33815692.
18. Kabra R, Ingale P, **Singh Shailza***. Computationally designed synthetic peptides for transporter proteins impart allostericity in Miltefosine resistant *L. major*. **Biochem J**. 2020 May 29; 477(10):2007-2026. Doi: 10.1042/BCJ20200176. PMID: 32391551.
19. Guhe V, Soni B, Ingale P, **Singh S*.** (2020) Autophagy proteins and its homeostasis in cellular environment. **Adv Protein Chem Struct Biol**. 123:73-93. doi: 10.1016/bs.apcsb.2019.12.002. Epub 2020 Jan 10.PMID: 33485489.
20. Chauhan N, **Singh Shailza*.** (2020) Multiscale Process Modeling in Translational Systems Biology of *L.major :* A Holistic View. **Scientific Reports** DOI: 10.1038/s41598-020-57640-4
21. Chauhan N, **Singh Shailza*** (2019) Integrative Computational framework for Understanding

Metabolic Modulation in Leishmania. **Front. Bioeng. Biotechnol** doi: 10.3389/fbioe.2019.00336 PMID: 31803732

22. Kumar A, Chauhan N, **Singh Shailza*.** (2019) Understanding the Cross-Talk of Redox Metabolism and Fe-S Cluster Biogenesis in Leishmania through Systems Biology Approach. **Front Cell Infect Microbiol.** 2019 Feb 4; 9:15. doi: 10.3389/fcimb.2019.00015. eCollection 2019. PMID: 30778378
23. Mol M, Kosey D, Boppana R, **Singh Shailza***. (2018) Transcription Factor Target Gene Network governs the Logical Abstraction Analysis of the Synthetic Circuit in Leishmaniasis. **Sci Rep.** 2018 Feb 22; 8(1):3464. doi: 10.1038/s41598-018-21840-w. PMID: 29472639
24. Pruthvi Raj B and **Shailza Singh*** (2018) Engineering riboswitch in *L.major:* From prediction to conceptualization. **International Journal of Biological Macromolecules** https://doi.org/10.1016/j.ijbiomac.2018.04.031PMID: 29655887
25. Sonar K, Kabra R, **Singh Shailza*** (2018) TryTransDB: A web-based resource for transport proteins in Trypanosomatidae. **Sci Rep.** 2018 Mar 12; 8(1):4368. doi: 10.1038/s41598-018-22706-x. PMID: 29531295
26. Soni B, Saha B, **Singh Shailza*.** (2017) Systems cues governing IL6 signaling in leishmaniasis. **Cytokine.** 2017 Nov 8. pii: S1043-4666(17)30343-5. doi: 10.1016/j.cyto.2017.11.001. [Epub ahead of print] PMID: 29128405
27. Vineetha Mandlik, Sohan Patil, Ramanamurthy Bopanna, Sudipta Basu and **Shailza Singh*** (2016) Biological activity of coumarin derivatives as antileishmanial agents. **Plos One** 10.1371/journal.pone.0164585
28. **Singh Shailza*,** Mandlik V, Shinde S. (2015) Molecular dynamics simulations and statistical coupling analysis of GPI12 in *L. major*: functional co-evolution and conservedness reveals potential drug-target sites. **Mol Biosyst**. 2015 Mar 17; 11(3):958-68. doi: 10.1039/c4mb00649f. Epub 2015 Jan 22. PMID: 25609494
29. **Singh Shailza***, Mandlik V. (2015) Structure based investigation on the binding interaction of transport proteins in leishmaniasis: insights from molecular simulation. **Mol Biosyst.** 2015 Mar 12. [Epub ahead of print] PMID: 25761976 [PubMed - as supplied by publisher]
30. Bejugam P.R and **Singh Shailza*(**2016) Computing molecular devices in *L.major* through transcriptome analysis: Structured Simulation Approach. **Plos One.** DOI: 10.1371/journal.pone.0148909
31. Mandlik V, Shinde S, **Singh Shailza***. (2014) Molecular evolution of the enzymes involved in the sphingolipid metabolism of Leishmania: selection pressure in relation to functional divergence and conservation. **BMC Evol Biol**. 2014 Jun 21; 14(1):142. [Epub ahead of print] PMID: 24951280 [PubMed - as supplied by publisher]
32. Shinde S, Mol M, Jamdar V, **Singh Shailza***. (2014) Molecular modeling and molecular dynamics simulations of GPI 14 in *Leishmania major*: Insight into the catalytic site for active site directed drug design. **J Theor Biol**. 2014 Feb 25; 351C:37-46. doi: 10.1016/j.jtbi.2014.02.017. [Epub ahead of print] PMID: 24583312 [PubMed - as supplied by publisher]
33. Shinde S, Mol M, **Singh Shailza*.** (2014) Regulatory networks, genes and glycerophospholipid biosynthesis pathway in schistosomiasis: a systems biology view for pharmacological intervention. **Gene** 2014 Oct 25; 550(2):214-22. doi: 10.1016/j.gene.2014.08.031. Epub 2014 Aug 19. PMID: 25149020 [PubMed - in process]
34. Mol M, Patole MS, **Singh Shailza***. (2014) Immune signal transduction in leishmaniasis from natural to artificial systems: role of feedback loop insertion. **Biochim Biophys Acta**. 2014 Jan; 1840(1):71-9. doi: 10.1016/j.bbagen.2013.08.018. Epub 2013 Aug 30. PMID: 23994140 [PubMed - indexed for MEDLINE]
35. Mandlik V, Shinde S, Chaudhary A, **Singh Shailza***. (2012) Biological network modeling identifies IPCS in Leishmania as a therapeutic target. **Integr Biol (Camb).** 2012 Sep;4(9):1130-42. doi: 10.1039/c2ib20037f. Epub 2012 Jul 30. PMID: 22842708 [PubMed - indexed for MEDLINE]

*Corresponding author

List of papers as co-authors:

1. Kumari S, Bodhale N, Sarode A, Jha MK, Bhadange S, Pandey SP, Selvaraj S, Chande AG, Mukhopadhyaya R, Ghosh SK, **Singh S**, Mukherjee D, Duffin R, Andrews P, Saha B. (2024) *Leishmania major* MAPK4 intercepts and redirects CD40 signaling promoting infection. **Int Immunopharmacol.** 2024 Jun 15;134:112100. doi: 10.1016/j.intimp.2024.112100. Epub 2024 May 9.PMID: 38728877
2. Roy PK, Paul A, Khandibharad S, Kolhe SD, Farooque QSS, Singh S, **Singh S.** (2024) Mechanistic and structural insights into vitamin B2 metabolizing enzyme riboflavin kinase from *Leishmania donovani.* Int J Biol Macromol. 2024 Aug 7;278(Pt 1):134392. doi: 10.1016/j.ijbiomac.2024.134392. Online ahead of print.PMID: 39098675
3. Choppara S, Ganga S, Manne R, Dutta P, **Singh S**, Santra MK. (2018) The SCF^{FBXO46} ubiquitin ligase complex mediates degradation of the tumor suppressor FBXO31 and thereby prevents premature cellular senescence. **J Biol Chem**. 2018 Oct 19; 293(42):16291-16306. doi: 10.1074/jbc.RA118.005354. Epub 2018 Aug 31. PMID: 30171069
4. Bandyopadhyay S, Chandel HS, **Singh S**, Roy S, Krishnasastry MV, Saha B. (2015) Counteractive functions are encrypted in the residues of CD154. **Hum Immunol.** 2015 Sep;76(9):673-80. doi: 10.1016/j.humimm.2015.09.019. Epub 2015 Sep 30. PMID: 26429321
5. Gangalum PR, de Castro W, Vieira LQ, Dey R, Rivas L, **Singh S**, Majumdar S, Saha B. (2015) Platelet-activating factor receptor contributes to antileishmanial function of miltefosine. **J Immunol**. 2015 Jun 15;194(12):5961-7. doi: 10.4049/jimmunol.1401890. Epub 2015 May 15. PMID: 25980013
6. Chakraborty S, Srivastava A, Jha MK, Nair A, Pandey SP, Srivastava N, Kumari S, **Singh S**, Krishnasastry MV, Saha B. (2015) Inhibition of CD40-induced N-Ras activation reduces leishmania major infection. **J Immunol**. 2015 Apr 15;194(8):3852-60. doi: 10.4049/jimmunol.1401996. Epub 2015 Mar 18. PMID: 25786685
7. Naiyer MM, Saha S, Hemke V, Roy S, **Singh S**, Musti KV, Saha B. (2013) Identification and characterization of a human IL-10 receptor antagonist. **Hum Immunol.** 2013 Jan;74(1):28-31. doi: 10.1016/j.humimm.2012.09.002. Epub 2012 Sep 19. PMID: 23000375

List of patents granted:

(a) Number of Indian patents–with details on each patent

"A CHIMERIC PROTEIN KINASE C AS AN IMMUNOMODULATOR" Indian Patent Application No. 201821005856

1) The chimeric protein kinase C is a novel designed protein constructed through synthetic device to act against infections caused by *Leishmania*.

2) The chimeric PKC of the present invention is capable of immune modulation via activation of NFκB signal transduction pathway in infected macrophages.

(b) Number of international patents–with brief details on each patent

PCT filed for "A novel chimeric protein kinase C as an immunomodulator"

OBJECT OF THE INVENTION

An object of the invention is to provide a novel designed protein, in particular, chimeric protein kinase C (PKC) to act as an immunomodulator in infections caused by *Leishmania* species.

SUMMARY OF THE INVENTION

The present invention relates to a novel designed protein to act against infections caused by *Leishmania* species. More specifically, the present invention pertains to a novel, chimeric protein kinase C for immune modulation by targeting NFκB pathway in leishmaniasis.

The present invention relates to a method of producing the chimeric protein comprising the steps:

i) selection of the template for modeling of chimeric protein;
ii) building of the model based on the template of step (i) using homology modeling optimization protocol to obtain the chimeric protein;
iii) sequencing and synthesis of the chimeric protein obtained in step(ii);
iv) analyzing effect of the chimeric protein as an immunomodulator in cells infected with *Leishmania.*

The present invention further discloses a composition comprising the chimeric protein kinase C and at least one pharmacologically acceptable carrier. The present invention also discloses the utility of novel chimeric protein kinase C in leishmaniasis.

Edited Books

- Systems Biology Application in Synthetic Biology (Edited Volume 1) Springer Publishers DOI: 10.1007/978-81-322-2809-7 ISBN :978-81-322-2807-3 (2016)
- Synthetic Biology: Omics Tools and their Application (Edited), Springer Nature ISBN: 978-981-10-8692-2 (2018)
- Systems and Synthetic Immunology (Edited Volume with Springer Nature Publishers) ISBN 978-981-15-3349-5 (2020)
- Metagenomic Systems Biology (Edited), Springer Nature ISBN:978-981-15-8562-3 (2020)
- Machine Learning and Systems Biology in Genomics and Health(Edited), Springer Nature ISBN: 9789811659928
- Systems Biomedicine Approaches in Cancer Research (Edited), Springer Singapore ISBN: 978-981-19-1952-7

Book Chapters

- Kabra R, Soni B, Kumar A, Chauhan N, Ingale P, **Singh S*** (2018). Integrated Systems and Chemical Biology Approach for Targeted Therapies. In Synthetic Biology 2018 (pp. 1-19). Springer Nature Singapore.
- Milsee Mol, Vineetha Mandlik and **Shailza Singh*** (2016) Microbial Chassis assisting Retrosynthesis in book titled "Systems Biology application in Synthetic Biology", Springer Publishers DOI: 10.1007/978-81-322-2809-7.
- Vineetha Mandlik, Pruthvi Raj Bejugam and **Shailza Singh*** (2014) "Application of ANN in Drug Discovery" in book titled "Artificial Neural Network for Drug Design, Delivery and Disposition", Elsevier Inc.
- Milsee Mol and **Shailza Singh*** (2013) "*In silico* Approaches for dealing with Gene Regulatory Network to understand the Molecular Mechanisms of Immunity in Infectious Disease" in Post Genomics Approaches in Drug Discovery, River Publishers.
- Milsee Mol and **Shailza Singh*** (2013) "Computational Design of Biological Systems: From Systems to Synthetic Biology" in "Frontiers in Computational Chemistry", Bentham Science Publishers
- Vineetha, Mandlik, Milsee, Mol., Sonali, Shinde and **Shailza Singh*** (2013). Gene Regulatory Network: A New Paradigm in Bioinformatics. Biotechnology, 6, Studium Press LLC, USA.
- Sonali Shinde, Vineetha Mandlik and **Shailza Singh*** (2012) Chapter on Integrating Bioinformatics and Systems Biology for exploring novel lipid pathways in infectious Diseases for Bentham Science Publisher E-book titled "Advances in mathematical chemistry"
- **Shailza Singh*** and Shinde, S. (2012) Chapter 16- Stochastic Simulation for Biochemical Reaction Networks in Infectious Disease. Medicinal Chemistry and Drug Design ISBN 978-953-51-0513-8. DOI: 10.5772/38245

Reviews

- Samarth N, Gulhane P, **Singh S*.** Immunoregulatory framework and the role of miRNA in the pathogenesis of NSCLC - A systematic review. **Front Oncol.** 2022 Dec 21;12:1089320. doi: 10.3389/fonc.2022.1089320. PMID: 36620544; PMCID: PMC9811680.

- Gulhane P, **Singh S*.** Unraveling the Post-Translational Modifications and therapeutical approach in NSCLC pathogenesis. **Transl Oncol.** 2023 Jul;33:101673. doi: 10.1016/j.tranon.2023.101673. Epub 2023 Apr 14. PMID: 37062237; PMCID: PMC10133877.

- Guhe V, Ingale P, Tambekar A, **Singh S*.** Systems biology of autophagy in leishmanial infection and its diverse role in precision medicine. **Front Mol Biosci.** 2023 Apr 21;10:1113249. doi: 10.3389/fmolb.2023.1113249. PMID: 37152895; PMCID: PMC10160387.

- Khilwani R, **Singh S*.** Systems Biology and Cytokines Potential Role in Lung Cancer Immunotherapy Targeting Autophagic Axis. **Biomedicines.** 2023 Oct 5;11(10):2706. doi: 10.3390/biomedicines11102706. PMID: 37893079; PMCID: PMC10604646.

- Khandibharad S, Nimsarkar P and **Singh S*** (2022). Mechanobiology of immune cells: Messengers, Receivers and Followers in Leishmaniasis aiding Synthetic Devices. **Current Research in Immunology**. 2022 Aug 23;3:186-198. doi: 10.1016/j.crimmu.2022.08.007. eCollection 2022. PMID: 36051499

- Soni B, Kabra R and **Singh S*** (2021). Quantitative Insight into Immunopathology of SARS-CoV2 Infection. **J Interferon Cytokine Res**. 2021 2021 Jul;41(7):244-257. doi: 10.1089/jir.2020.0156. PMID: 34280026

- Kabra R, **Singh S*.** (2020) ABC Exporters in Pathogenesis: Role of Synthetic Anti-Microbial Peptides. **Protein J.** Dec; 39(6):657-670. doi: 10.1007/s10930-020-09931-y. Epub 2020 Oct 17.PMID: 33068233.

- Misra P, **Singh S*** (2019) Site Specific Microbiome of Leishmania Parasite and its Cross- talk with Immune Milieu. **Immunol Lett**. 2019 Oct 30. pii: S0165-2478(19)30388-8. doi: 10.1016/j.imlet.2019.10.004. [Epub ahead of print] Review. PMID: 31678358

- Soni, B and **Singh S*** (2019) Cytokine Milieu in Infectious Disease: A Sword or a Boon. **Journal of Interferon and Cytokine Research.** 2019 Sep 24. doi: 10.1089/jir.2019.0089. [Epub ahead of print] PMID: 31553263
- Misra P, **Singh S*.** (2019) Role of cytokines in combinatorial immunotherapeutics of non- small cell lung cancer through systems perspective. **Cancer Med.** 2019 Apr 17. doi: 10.1002/cam4.2112. [Epub ahead of print] PMID: 30997737
- Kabra R, Chauhan N, Kumar A, Ingale P, **Singh S*.** (2019) Efflux pumps and antimicrobial resistance: Paradoxical components in systems genomics. **Prog Biophys Mol Biol.** 2019 Jan; 141:15-24. doi: 10.1016/j.pbiomolbio.2018.07.008. Epub 2018 Jul 18. PMID: 30031023
- Mol M, Raj Bejugam P, Singh S. (2014) Synthetic biology at the interface of functional genomics. Brief Funct Genomics. 2015 May;14(3):180-8. doi: 10.1093/bfgp/elu031. Epub 2014 Sep 10. PMID: 25212484
- Mol M, Kabra R, **Singh S*.** (2018) Genome modularity and synthetic biology: Engineering systems. **Prog Biophys Mol Biol**. 2018 Jan; 132:43-51. doi: 10.1016/j.pbiomolbio.2017.08.002. Epub 2017 Aug 8. Review. PMID: 28801037
- Soni B, Nimsarkar P, Mol M, Saha B, **Singh S *** (2018) Systems-synthetic biology in understanding the complexities and simple devices in immunology. **Cytokine** 108, pp60-66.
- Mandlik V, Kabra R, **Singh S*.** (2017) System pharmacogenomics application in infectious diseases. **Brief Funct Genomics.** 2017 Mar 21. doi: 10.1093/bfgp/elx002. [Epub ahead of print] PMID: 28369182

Seminars

- Invited talk on "Systems pharmacology strategies and discovery avenues in Bioactive Natural Products: (Re)-defining Lessons from the Past and Future" at GITAM University, Department of Biochemistry and Bioinformatics, Vizag, 26th-27th March 2015.

- Invited Talk on "Engineering signal transduction pathways through synthetic modular systems: Dissecting the puzzle in infectious disease" at 50th Indian Biophysical Society Conference, Jamia Millia Islamia, New Delhi, 14th-17th Feb 2015.

- Key Note Talk on "Systems engineering and the integration of mechanistic explanation in infectious disease through synthetic biology::A golden braid" at Pre-Science Congress, Aurangabad, 30th-31st December 2014

- Invited Talk on "Elucidating the interactome in Leishmania: Molecular insights with ligand pharmacophoric sites through combinatorial QSAR and Molecular Dynamics simulation" in a State-level Seminar titled "Recent Advances in Computational Medicinal Chemistry" on 14th November 2014 at Smt.Kashibai Navale College of Pharmacy, Singhad Technical Education Society, SP University of Pune, Pune.

- Invited Talk on "Rational Drug Design in the Bioinformatics Era: Navigating the translational challenges through an integrated approach" in the Bioinformatics Workshop, ACTREC, Navi Mumbai, Kharghar, 23rd-24th April 2015.

- Invited Talk on **"**Computational System Biology and Synthetic Biology : The Future of Infectious Disease" at Jamia Millia Islamia, 14th October 2015, Hall No.202, S Ramanujan Block, Mujeeb Bagh, JMI, New Delhi

- Invited Talk on "Systems and Synthetic Biology Approaches in Infectious Disease: Two sides of the same coin dealing with Validation and Variability" at TERI, New Delhi, 13th October 2015.

- Invited Talk on "Paradoxical components in Biological circuit and negative autoregulation of transcriptional factors: A systems theoretic model in Leishmaniasis" at 14th FAOBMB Congress and 84th Annual Meeting of SBC (I), Hyderabad, 27th-30th November 2015.

- Invited Talk on "Anti-leishmanial activity of coumarin derivatives: Network based drug design using mechanistic systems biology" at IIT Guwahati, Bioinformatics and Computer aided drug design conference, 7th December 2015.
- Invited Talk on "Structure based design of a new series of coumarins as anti-leishmanial inhibitors" at Department of Biochemistry, MGIMS, Wardha, 9th-10th March 2017.

- Invited talk on "Bioinformatics - Tool for Drug development of Natural products" at Garware College, 23rd March 2016, Pune.

- Invited Talk on "Structureomics of the sphingolipid metabolism of the parasite Leishmania", National Symposium on Omics to Structural Basis of Diseases, 30th September-1st October 2016, MSU Vadodara, Gujarat.

- Invited Lecture in DST Inspire Camp, Dayanand Science College, Latur, "Cells governing the Life in Science" (Four Lectures), 26th-27th September 2016.

- Invited talk on "Dissecting and Optimizing Druggability through Network Modeling and Liposomal formulations" at National Seminar on Drug Development and Diagnostic Approaches for Tuberculosis Infection, July 29-30, 2016, Bhanuben Nanawati College of Pharmacy, Vile Parle, Mumbai.

- Invited Talk on "Deciphering lipid metabolism in Leishmaniasis using systems perspective" Lipid Meet 2016, Amity University, Gurgaon, 14th-15th Dec 2016.

- Invited talk on " Synthetic Bioengineering for Neglected Tropical Disease: A Computational Pipeline" at Interdisciplinary Biotechnology Unit, AMU, Aligarh, 16th-17th March 2017.

- Invited talk on "Systems framework for Synthetic biology inspired therapy in Leishmaniasis" at Cross-Talk in Omics 2017, Centre for Bioinformatics, School of Life Sciences, Pondicherry University, Pondicherry, August 9, 2017.

- Plenary lecture on "Signaling framework for Synthetic circuit immuno-modulation in Leishmaniasis: A Structural Perspective for Drug Delivery Systems at SBCADD 2018, Alagappa University, Karaikudi, 20th-23rd February 2018.

Seminars/Conferences attended by Ph.D students:

- Pruthvi Raj Bejugam amd Shailza Singh (2014) Exploring Synthetic Biology in Leishmania through Autoregulatory RNA Elements: A Mechanistic Perspective, FEBS-EMBO 2014,30th August-4th September, Paris. (Poster presentation)
- Ritika Kabra and Shailza Singh (2017) Lipid trafficking through lipid transport proteins in leishmaniasis, Bharatiya Vigyan Sammelan, Fergusson College, Pune, 11th to 14th May 2017(Poster presentation)
- Bhavnita Soni and Shailza Singh (2017) Systems biology of IL6 in Leishmaniasis (2017) Bharatiya Vigyan Sammelan, Fergusson College, Pune, 11th to 14th May 2017
- Bhavnita Soni and Shailza Singh (2017) Systems Studies Unveil Role of IL6 in macrophage polarization during *L.major* infection. National Conference on Protein Structure and Dynamics in Health and Agriculture, New Delhi. 3/11/2017 to 4/11/2017. Journal of Proteins and Proteomics 2017, Volume 8:4, Pg: JPP27-28. (Poster presentation)
- Ritika Kabra and Shailza Singh (2017) Miltefosine resistance reversal in *Leishmania major* by a synthetic peptide. National Conference on Protein Structure and Dynamics in Health and Agriculture, New Delhi. 3/11/2017 to 4/11/2017. Journal of Proteins and Proteomics 2017, Volume 8:4, Pg: JPP66 (Bagged Second Prize in Poster presentation)

Teaching work such as:

Courses taught :Biostatistics, Computer Application, Bioinformatics,Practicals conducted: Computer Application and Bioinformatics

Theses completed under my supervision

1. Vineetha Mandlik (DBT-SRF)
2. Milsee Mol (CSIR-SRF)
3. PruthviRaj Bejugam (UGC-SRF)
4. Ritika Kabra (DBT-SRF)

5. Bhavnita Soni (DST-SRFInspire)
6. Prajakta Nimsarkar (DBT-JRF)
7. Anurag Kumar (UGC-JRF)
8. Vrushali Guhe (UGC-JRF)

Theses submitted: Subhajit Das (JGEEBILS)

Theses (to be) completed under my supervision:
1. Nikhil Samarth (UGC SRF)
2. Shweta Khandibharad (UGC-SRF)
3. Pooja Gulhane (DBT-JRF)
4. Diksha Jawale (DBT-JRF)
5. Riya Khilwani (CSIR-JRF)
6. Manasi Tukrul (UGC-JRF)

Guidance of Post-Doctoral Fellow:
Dr. Nutan Chauhan (DST SERB NPDF)
Dr. Pragya Misra (CSIR-SRA)
Dr. Nirupma Singh (DST-WISE)-
joining

Post graduate students under my supervision:
Dipali Kosey, Project JRF
Prajakta Ingale, Project JRF
Krushna Sonar, Project JRF (joined PhD in Australia)
Neelam Topno, Project JRF (tenure-completed)
Priyanka Patel, Project JRF (tenure-completed)
Deepika Bhujbal, Project Assistant (tenure-completed)
Sakshi Shambhavi Pandey, BHU Varanasi, (Project trainee)
P.L. Suganthi, Pandit Ravishankar Shukla University, Raipur(Project trainee)
Akanksha Pandey, AKS University, Satna(Project trainee)
Ankita Roy, Assam University, Silchar (INSA Summer Fellow)
Aastha Mathur, University Maharani's College,Jaipur (INSA Summer Fellow)
Baishali Sarmah, Tezpur University, Assam (Project trainee)
Ragini Tripathi, AKS University, Satna (Project trainee)
Akila Kannan, Bannari Amman Institute of Technology, Sathyamangalam Erode, Tamil Nadu (INSA Summer Fellow)
Dheeraj Joshi, University of Delhi (INSA Summer Fellow)