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
   Highlight of the paper: The work is focused on designing ML derived peptides which targeted ATG8 in host autophagy and thus made a significant contribution towards studying host-pathogen interaction.
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
   Highlight of the paper: We are the first group to identify sleepy macrophages during leishmaniasis infection which is a path breaking finding in macrophage associated infectious diseases.
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
   Highlight of the paper: We demonstrated the effect of ML derived peptides during reciprocity of cytokines which govern the macrophage phenotypic plasticity in infection model under high salt stress.
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
   Highlight of the paper: We used biophysical experiments and molecular dynamics simulation studies to study the target protein and druggability of infection model genome.
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
   Highlight of the paper: We demonstrated the cytokines precision therapeutics and its axis in NSCLC model. The paper received accolades as it's the first model demonstrating tunability and robustness.
6. 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
   Highlight of the paper: We for the first time deciphered the cytokine axis with the lipid metabolism of the parasite which is of paramount importance as far as designing therapeutics is considered.
7. 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
   Highlight of the paper: We focused on Bio-AI which is important to answer the mechanistic insight dealing with the reciprocity of cytokines.
8. 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
   Highlight of the paper: We did virtual screening and churned out benzimidazole as a potential lead molecule to treat an important parasitic disease which has co-infection with

TB and HIV.

9. 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
   Highlight of the paper: We for the first time advocated the non-coding RNA which is important for impacting sphingolipid metabolism in NSCLC.
10. 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.
    Highlight of the paper: Using interdisciplinary approaches, we for the first time demonstrated allostericity in infection model using peptide based therapeutics.

https://pubmed.ncbi.nlm.nih.gov/?term=shailza+singh&sort=date