Sukrit Singh

Email: sukrit.singh@choderalab.org | **Twitter**: @sukritsingh92 | **Website**: https://sukritsingh.github.io

Positions and Education

Postdoctoral Research Fellow 2021 – present
Memorial Sloan-Kettering Cancer Center
- NCI K99/R00 Pathway to Independence Award Fellow
- Damon Runyon Quantitative Biology Fellow
- Team member of the Folding@home consortium
- Advisors**:** Dr. John Chodera; Joint-mentorship from Dr. Markus Seeliger (Stony Brook University)

2020

Ph.D., Computational and Molecular Biophysics
Washington University in St. Louis
- Thesis**:** *Understanding and exploiting protein allostery & dynamics using molecular simulations*
- Team member of the Folding@home consortium
- Advisor**:** Dr. Gregory R. Bowman

2014

B.A., Chemistry and Biology
Washington University in St. Louis
- Undergraduate thesis*: Synthesizing an amide bond nitroxide for improving intermolecular distance measurements.*
- Research advisor: Dr. Garland R. Marshall & Dr. Jay Ponder

Undergraduate Researcher Dec. 2012 – June 2014
Lab of Dr. Garland R. Marshall & Dr. Jay Ponder
- WUSTL Career Center Fellowship

Undergraduate Research Assistant Nov. 2010 – Nov. 2012
Lab of Dr. Joseph D. Dougherty
- HHMI Undergraduate Research Fellow

Teaching Experience

Teaching Assistant for General Biochemistry Aug 2015 – Dec 2015
Dept. of Biology, Washington University in St. Louis

Teaching Assistant for Modern Medicinal Chemistry Jan. 2014 – June 2014
Dept. of Chemistry, Washington University in St. Louis

Lab instructor for Introductory Organic Chemistry June 2014 – Aug. 2014
Dept. of Chemistry, Washington University in St. Louis June 2013 – Aug. 2013

Teaching assistant for Introduction to Computer Science Aug. 2010 – Dec 2011
Dept. of Computer Science, Washington University in St. Louis

Awards & Fellowships

NCI Pathway to Independence Award for Outstanding Early Stage Postdoctoral Researchers (K99/R00) June 2024 – present
National Cancer Institute, USA

Best Talk – NCI Junior Investigators 2023 meeting August 2023
National Cancer Institute, Junior Investigators meeting 2023

Damon Runyon Quantitative Biology Fellowship May 2022 – present
Damon Runyon Cancer Research Foundation

Community Ambassador Jan. 2022 – present
eLife journal

Millipore-Sigma Fellowship March 2019 – 2020
WUSM Dept. of Biochemistry and Molecular Biophysics

Best Poster – Runner up September 2016
Biochemistry and Molecular Biophysics Department Retreat

MCC Travel Award September 2015
Materials Computation Center at Univ. Illinois Urbana-Champaign

WU Career Center Summer Internship Award June – August 2013
Washington University in St. Louis
- Design & synthesis of novel peptidomimetics of antibacterials

HHMI Summer Undergraduate Research Fellowship June – August 2011
Washington University in St. Louis
- Investigation of glucocorticoid-induced cerebellar apoptosis

Mr. and Mrs. Nicolas M. Georgitsis Scholar June 2010 – May 2014
Washington University in St. Louis
- 4-year scholarship providing full tuition and room & board

Publications (by year)

*** denotes co-first authorship**
⁺ denotes corresponding or co-corresponding authorship
† denotes lead-computational authorship

1. Vithani, N., Todd, T.D., **Singh, S.,** Blumer, K.J., Bowman, G.R., *G protein activation occurs via a largely universal mechanism*., **J. Phys. Chem. B.**, 2024, 128, 15, 3554-3562, Available online at: https://doi.org/10.1021/acs.jpcb.3c07028
2. Todd, T.D., Vithani, V., **Singh, S.,** Bowman, G.R., Blumer, K.J., Soranno, A., *Stabilization of interdomain closure by a G protein inhibition*, **Proc. Nat. Acad. Sci.**, In Press, 2023
3. Eastman P., Galvelis, R., Peláez, R.P., Abreu, C.R.A., Farr, S.E., Gallicchio, E., Gorenko, A., Henry M.M., Hu, F., Huang, J., Krämer, A., Michel, J., Mitchell, J.A., Pande, V.S., Rodrigues, J.P.G.L.M, Rodriguez-Guerra, J., Simmonett, A.C., **Singh, S.,** Swails, J., Turner, P., Wang, Y., Zhang, I., Chodera, J.D., De Fabritiis, G., Markland, T.E., *OpenMM 8: Molecular dynamics simulation with machine learning potentials*, **J. Phys. Chem. B**, 2024, 128, 1, 109-116, Available online at: https://doi.org/10.1021/acs.jpcb.3c06662
4. Nigam A., Hurley, M.F.D., Li, F., Konkolova, E., Klíma, M., Trylčová, J., Pollice R., Çinaroglu, S.S., Levin-Konigsberg, R., Handjaya, J., Schapira, M., Chau, I., Perveen, S., Ng, H.L, Kaniskan, H.Ü, Han, Y., **Singh, S.**, Gorgulla, C., Kundaje, A., Jin, J., Voelz, V.A., Weber, J., Nenca R., Boura E., Vedadi, M., Aspuru-Guzik, A., *Application of established computational techniques to identify potential SARS-CoV-2 Nsp14-MTase inhibitors in low data regimes*, **Digital Discovery**, 2024, Available online at: https://doi.org/10.1039/D4DD00006D

5. Zhang, I., Rufa, D.A., Pulido, I., Henry, M.M., Rosen, L.E., Hauser, K., **Singh, S.**[+], Chodera, J.D.[+], *Identifying and overcoming the sampling challenges in relative binding free energy calculations of a model protein:protein complex*., **J. Chem. Theory Comput.**, July 2023, https://doi.org/10.1021/acs.jctc.3c00333

6. The COVID Moonshot Consortium, [..] **Singh, S.,** [..], *Open Science Discovery of Oral Non-Covalent SARS-CoV-2 Main Protease Inhibitor Therapeutics*. **Science,** 382 (6671), 2023, https://www.science.org/doi/10.1126/science.abo7201

7. Perner, F., Stein, E.M., Wenge, D.V., **Singh, S.**[†]**,** Kim, J., Apazidis, A., Rahnamoun, H., Anand, D., Marinaccio, C., Hatton, C., Wen, Y., Stone, R.M., Schaller, D., Mowla, S., Xiao, W., Gamlen, H.A., Stonestrom, A.J., Persaud, S., Ener, E., Cutler, J.A., Doench, J.G., McGeehan, G.M., Volkamer, A., Chodera, J.D., Nowak, R.P., Fischer, E.S., Levine, R.L., Armstrong, S.A., Cai, S.F., *MEN1 mutations mediate clinical resistance to Menin inhibition*. **Nature**, 2023. https://doi.org/10.1038/s41586-023-05755-9

8. Outhwaite, I.R., **Singh, S.,** Berger, B.-T., Knapp, S., Chodera J.D., Seeliger, M.A., *Death by a thousand cuts – Combining kinase inhibitors for selective target inhibition and rational polypharmacology*. **eLife**, 2023, Available online at: https://doi.org/10.7554/eLife.86189

9. Cruz, M.A., Frederick, T.E., Mallimadugula, U. L., **Singh, S.,** Vithani, N., Zimmerman, M.I., Porter, J.R., Moeder, K.E., Amarasinghe, G.K., Bowman, G.R., *Discovery of a cryptic allosteric site in Ebola's 'undruggable' VP35 protein using simulations and experiments*. **Nature Communications**, 2022, Accessible online at: https://doi.org/10.1038/s41467-022-29927-9

10. Knoverek, C.R., Mallimadugula, U.L., **Singh, S.**[†]**,** Rennella, E., Frederick T.E., Yuwen, T., Raavicharla, S., Kay, L.E., Bowman, G.R., *Opening of a cryptic pocket in β-lactamase increases penicillinase activity*, **Proc. Nat. Acad. Sci.,** Nov 2021, 118 (47) e2106473118 https://doi.org/10.1073/pnas.2106473118

11. Vithani, N., Ward, M.D., Zimmerman, M.I, Novak B., Borowsky J.H., **Singh, S.,** Bowman, G.R., *SARS-CoV-2 Nsp16 activation mechanism and a cryptic pocket with pan-coronavirus antiviral potential*, **Biophysical Journal**, 2021, Available online at: https://doi.org/10.1016/j.bpj.2021.03.024

12. Zimmerman, M.I., Porter, J.R., Ward, M.D., **Singh, S.**, Vithani, N., Meller, A., Mallimadugula, U.L, Kuhn, C. E., Borowsky, J.H., Wiewiora, R.P., Hurley, M.F.D., Harbison, A.M., Fogarty, C.A., Coffland, J.E., Fadda, E., Voelz, V.A., Chodera, J.D., Bowman, G.R. *SARS-CoV-2 Simulations Go Exascale to Capture Spike Opening and Reveal Cryptic Pockets Across the Proteome*, **Nature Chemistry,** 2021, Available online at: https://doi.org/10.1038/s41557-021-00707-0

13. Cubuk, J., Alston, J.J., Incicco, J.J., **Singh S.,** Stuchell-Brereton, M.D. , Ward, M.D., Zimmerman, M.I., Vithani, N., Griffith, D., Wagoner, J.A., Bowman, G.R., Hall, K.B., Soranno, A., Holehouse A.S., *The SARS-CoV-2 nucleocapside protein is dynamic, disordered, and phase separates with RNA*. **Nature Communications**, 12**,** 1936 (2021). Available online at: https://doi.org/10.1038/s41467-021-21953-3

14. Brown, C.A., Hu, L., Sun, Z., Patel, M.P., **Singh, S.**[†]**,** Porter, J.R., Sankaran, B., Prasad, B.V.V., Bowman, G.R., Palzkill, T.M., *Antagonism between substitutions inβ-Lactamase explains a path not taken in the evolution of bacterial drug resistance*., **Journal of Molecular Biology** (2020). doi: 10.1074/jbc.RA119.012489

15. **Singh, S.*,** Sun, X.*, Blumer, K.J., Bowman, G.R., *Simulation of spontaneous G protein activation reveals a new intermediate driving GDP unbinding*, **eLife** (2018). 7, e38465 doi: 10.7554/eLife.38465.

16. Reddy, D.N., **Singh, S.†,** Ho, C.M.W., Patel, J., Schlesinger, P., Rodgers, S., Doctor, A., Marshall, G.R., *Design, synthesis, and biological evaluation of stable β6.3-Helices: Discovery of non-hemolytic antibacterial peptides.* **Eur. J. Med. Chem.** (2018). 149, 193–210

17. Patrick, G.J., Fang, L., Schaefer, J., **Singh, S.†,** Bowman, G.R., Wencewicz, T.A., *Mechanistic Basis for ATP-Dependent Inhibition of Glutamine Synthetase by Tabtoxinine-β-Lactam.* **Biochemistry** (2017). 57(1), 117-135

18. **Singh S.** & Bowman, G.R., *Quantifying allosteric communication via both concerted structural changes and conformational disorder with CARDS.* **J. Chem. Theory Comput.** (2017). 13(4), 1509-1517

19. Cascella, B., Lee, S. G., **Singh, S.†**, Jez, J. M. & Mirica, L. M. *The small molecule JIB-04 disrupts O2 binding in the Fe-dependent histone demethylase KDM4A/JMJD2A.* **Chem. Commun.** (2017). 53**,** 2174–2177

20. Brosey, C. A., Ho, C.M.W., Long, W.Z., **Singh**, **S.,** Burnett, K., Hura, G.L., Nix, J.C., Bowman, G.R., Ellenberger, T.E., Tainer, J.A., *Defining NADH-Driven Allostery Regulating Apoptosis-Inducing Factor.* **Structure** (2016). 24, 2067-2079

21. O'Connor, S.D., Cabrera, O.H, Dougherty, J.D., **Singh, S.**, Swiney, B.S., Salinas-Contreras, P., Farber, N.B., Noguchi, K.K, *Dexmedetomidine protects against glucocorticoid induced progenitor cell apoptosis in neonatal mouse cerebellum.* **J. Matern. Fetal. Neonatal. Med.** (2017). 30**,** 2156–2162

22. Nelson, C.A., Epperson, M.L., **Singh**, **S.†**, Elliott, J.I., Fremont, D.H., *Structural Conservation and Functional Diversification within the Poxvirus Immune Evasion (PIE) Domain Superfamily.* **Viruses**, (2015). 7, 4878-4898

23. Cabrera, O.H., Dougherty, J.D., **Singh, S.,** Swiney, B.S., Farber, N.B, Noguchi, K.K, *Lithium protects against glucocorticoid induced neural progenitor cell apoptosis in the developing cerebellum.* **Brain Research**, (2014). 1545, 54-63

Invited Talks

1. **Gordon Research Seminar on "Phosphorylation and G-protein mediated signaling networks"** June 2024
   Parsing Kinase Drug Resistance Mechanisms using Distributed Computing
   Waterville Valley, NH, USA (location of GRC/GRS)

2. **Illinois Institute of Technology – Dept. of Chemistry**
   Mechanism-based parsing of cancer drug resistance using protein dynamics May 2024
   Chicago, IL, USA

3. **American Chemical Society COMP division invited seminar (Invited session: Markov state modeling of conformational dynamics in the wake of machine learning)** Mar. 2024
   Mechanism-based parsing of mutations in cancer drug resistance
   New Orleans, LA, USA

4. **New York University Dept of Chemistry Teaching Seminar**
   Generating and analyzing ultra-large molecular dynamics datasets Nov. 2023
   New York, NY, USA

5. **National Cancer Institute Junior Investigators Meeting** — Aug. 2023
Biophysical parsing of drug resistance using exascale supercomputing
University of Pennsylvania, Philadelphia, PA, USA

6. **School of Chemistry, University of Edinburgh** — July 2023
Parsing drug resistance using exascale supercomputing
U. of Edinburgh, Edinburgh, UK,

7. **CCPBioSim 2023 – Biomolecular Simulations for a Better World** — July 2023
Parsing drug resistance using exascale supercomputing
U. of Leeds, Leeds, UK

8. **Single Cell Analysis and Innovation Lab, MSKCC** — Feb. 2022
Studying drug resistance and therapeutic opportunities in COVID and cancer using exascale computing
New York, NY, USA

9. **RockEDU Teacher's Summit** — Jan. 2023
Crowd-sourced scientific discovery and opportunities in education
New York, NY, USA

10. **SciLifeLab, Sweden** — Oct. 2022
Meta-sampling of enhanced sampling methods to explore kinase dynamics
SciLifeLab, Stockholm, Sweden

11. **Loyola High School, New York, NY** — Apr. 2021
Folding@home: Science at the exascale
An educational presentation presented to high school chemistry and biology classes at Loyola High School in Manhattan, NY.

12. **Folding@SiliconValley Educational Presentation** — Nov. 2020
Folding@home: Science at the exascale
An educational seminar given to high-schoolers interested in learning more about Folding@home and computational biophysics.

13. **Folding@home online** — Nov. 2020
What happens when you run a Folding@home work unit on your PC?
Online presentation during Folding@home's 20th anniversary event: https://www.youtube.com/watch?v=1N0cZgcVFRE&t=2s

14. **Biophysical Society 2020 Annual Meeting** — Feb. 2020
Simulation of spontaneous G protein activation reveals a new intermediate driving GDP unbinding
San Diego, CA., USA

15. **MilliporeSigma Fellowship lecture** — July 2019
Allostery in cellular signaling: Capturing biological switches in action
St. Louis, MO., USA

16. **Protein Folding Consortium 2019** — June 2019
Identifying new intermediates in signaling proteins
St. Louis, MO., USA

17. **Wash. U. Biochemistry and Molecular Biophysics Retreat** — October 2017
Building an allosteric network of G protein activation via direct observation of GDP-Release
St. Louis, MO., USA

18. **Gibbs Conference in Biothermodynamics 2016** — October 2016
Quantifying allosteric communication via structure and disorder
Carbondale, IL., USA

19. **Biochemistry and Molecular Biophysics Science Friday Seminar** — August 2016
Quantifying allostery through structure and disorder: Reading the CARDS
St. Louis, MO., USA

20. **Department of Chemistry Capstone seminar** — May 2014
Synthesis of the Amide Bond Nitroxide and Design of Novel Heterochiral Peptide Mimetic
St. Louis, MO., USA

21. **Midstates Consortium of Math and Sciences** — October 2013
Synthesis of Amide Bond Nitroxide for Determination of Intermolecular Distances in HIV
Chicago, IL., USA

Leadership & Service

MDTraj open-source project — July 2023 – present
Maintainer and Admin
- Admin for MDTraj: an open source library for analysis of molecular dynamics simulations (https://github.com/mdtraj/mdtraj/) - a repository with over 1 million downloads
- Maintain repository upkeep and releases
- Manage community contributions for new features and updates

Folding@home consortium — Oct. 2018 – present
Managing director, Communications, Outreach, and Digital
- Manage social media (@foldingathome on twitter, ~32.0K followers) and outreach efforts
- Run twitch streams on the Folding@home twitch channel (https://www.twitch.tv/foldingathomedotorg)
- Help manage collaborations with consortium partners

Living Journal of Computational Molecular Sciences — Mar. 2021 – Mar. 2023
Trainee Advisory Committee member
- Member of committee advising the editorial board

Biochemistry and Molecular Biophysics Student Liason Committee
Chair — 2017 – 2018
- Organizing seminars and events for the department

Organizer — 2015 – 2019
- Schedule speakers and host the weekly Friday department seminar

Peer-Reviews conducted

eLife
Structural Biology and Molecular Biophysics

Proteins

PLoS One

Protein Science

Living Journal of Computational Molecular Sciences

Computational Biology and Chemistry Journal

Computational and Structural Biotechnology Journal

Media Appearances

Youtube – Folding@home Dec. 2020
A presentation explaining the basics of molecular dynamics and simulation and how Folding@home works.
Link: https://www.youtube.com/watch?v=1N0cZgcVFRE&t=2s

Bloomberg Government Oct. 15, 2020
Interview regarding the impact of COVID19 on academic research and careers
Link: https://about.bgov.com/news/creativity-is-simply-lost-as-covid-cripples-academic-research/

St. Louis Post Dispatch June 26, 2020
Interview regarding Folding@home and COVID19 efforts.
Link: https://www.stltoday.com/business/local/gamers-big-tech-even-la-liga-soccer-link-computers-to-fight-covid-19-in-washington/article_ea4a4485-89f6-5140-97e1-d04e5f6e7f4a.html

Association for Computing Machinery – SIGGRAPH May 28, 2020
Interview regarding Folding@home and COVID19 efforts.
https://blog.siggraph.org/2020/05/foldinghome-citizen-scientists-gain-insight-on-covid-19.html/