

# Shourya Sonkar ROY BURMAN

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## PROFESSIONAL EXPERIENCE

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- 2019-PRESENT Research Fellow in CANCER BIOLOGY  
**Dana-Farber Cancer Institute**, Boston, MD  
&  
BIOLOGICAL CHEMISTRY & MOLECULAR PHARMACOLOGY  
**Harvard Medical School**, Boston, MD
- 2018-2019 Postdoctoral Fellow in CHEMICAL & BIOMOLECULAR ENGINEERING  
**Johns Hopkins University**, Baltimore, MD

## EDUCATION

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- 2012-2018 Ph.D. in CHEMICAL & BIOMOLECULAR ENGINEERING  
**Johns Hopkins University**, Baltimore, MD
- 2008-2012 B. Tech. in BIOLOGICAL SCIENCES & BIOENGINEERING  
**Indian Institute of Technology Kanpur**, India

## AWARDS & HONORS

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- 2020-2023 Cancer Research Institute Irvington Postdoctoral Fellowship  
2011, 2009 Certificate of Merit for Academic Excellence at IIT Kanpur  
2010-2011 Mona and Paramjit Singh Scholarship  
2008-2010 Baljit and Nirmal Dhindsa Scholarship  
2008-2009 Nitish Thakor Scholarship

## RESEARCH EXPERIENCE

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- PRESENT Research Fellow at DANA-FARBER CANCER INSTITUTE  
PI: *Dr. Eric S. Fischer, Department of Cancer Biology*
- Designing synthetic tag proteins that get selectively degraded or stabilized with small molecule drugs.
  - Determining endogenous target proteins of two E3 ligase substrate receptors, cereblon and DCAF15 through large-scale computational simulations.
  - Developing a computational pipeline for rational design of hetero-bifunctional compounds called proteolysis inducing chimeras (PROTACs) using RosettaDock.
- 2013-2018 Graduate Research Assistant at JOHNS HOPKINS UNIVERSITY  
Thesis: *Modeling Interactions of Flexible Proteins*  
Advisor: *Dr. Jeffrey J. Gray, Department of Chemical & Biomolecular Engineering*
- Developed RosettaDock 4.0, a computational tool that efficiently predicts the structure of protein complexes. Tested this tool on a benchmark of flexible proteins to verify a high accuracy on proteins with difficult-to-predict conformational changes. Presently, modeling induced fit in the encounter complex to further improve docking accuracy.

- Developed Rosetta SymDock2 that enhanced global docking performance of high-order symmetric homomeric complexes by five-fold.
- Led the Gray Lab team in the blind prediction experiment, Critical Assessment of PRediction of Interactions (CAPRI) to predict structures of protein, peptide and oligosaccharide in complex in blind challenges for two years.
- Modeled putative interactions of a drug to demonstrate that it can simultaneously inhibit histone deacetylase and histone demethylase in the CoREST complex in collaboration with *Dr. Philip Cole*.

2010-2012 Undergraduate Student at INDIAN INSTITUTE OF TECHNOLOGY, KANPUR  
 Advisor: *Dr. Amitabha Bandyopadhyay, Department of Biological Sciences & Bioengineering*

- Investigated the origin of limb tendons and the genetic cues, which lead to the homing and attachment of tendons in chicken. Characterized the mechanism by which the tendons and the ligaments make spatially accurate connections with the bones.

## PUBLICATIONS

1. Koehler Leman J\*, Lyskov S\*, Lewis S\*, Adolf-Bryfogle J, Alford RF, Barlow K, Ben-Aharon Z, Farrell D, Fell J, Hansen WA, Harmalkar A, Jeliaskov J, Kuenze G, Krys JD, Ljubetic A, Loshbaugh AL, Maguire J, Moretti R, Mulligan VK, Nguyen PT, Ó Conchúir S, **Roy Burman SS**, Smith ST, Teets F, Tiemann JKS, Watkins A, Woods H, Yachnin BJ, Bahl CD, Bailey-Kellogg C, Baker D, Das R, DiMaio F, Khare SD, Kortemme T, Labonte JW, Lindorff-Larsen K, Meiler J, Schief W, Schueler-Furman O, Siegel J, Stein A, Yarov-Yarovoy V, Kuhlman B, Leaver-Fay A, Gront D, Gray JJ & Bonneau R (2021) "Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks." *Under Review*. Pre-print: <https://doi.org/10.1101/2021.04.04.438423>
2. Le KH, Adolf-Bryfogle J, Klima JC, Lyskov S, Labonte J, Bertolani S, **Roy Burman SS**, Leaver-Fay A, Weitzner B, Maguire J, Rangan R, Adrianowycz MA, Alford RF, Adal A, Nance ML, Wu Y, Willis J, Kulp D, Das R, Dunbrack RL Jr, Schief W, Kuhlman B, Siegel JB & Gray JJ (2021) "PyRosetta Jupyter Notebooks Teach Biomolecular Structure Prediction and Design." *The Biophysicist*. Accepted; Pre-print: [www.preprints.org/manuscript/202002.0097/v1](http://www.preprints.org/manuscript/202002.0097/v1)
3. Slabicki M\*, Yoon H\*, Koeppel J\*, Nitsch L, **Roy Burman SS**, Di Genua CA, Donovan KA, Sperling AS, Hunkeler M, Tsai JM, Sharma R, Guirguis A, Zou C, Chudasama P, Gasser JA, Miller PG, Scholl C, Fröhling S, Nowak RP, Fischer ES & Ebert BL (2020) "Small molecule-induced polymerization triggers degradation of BCL6." *Nature*. 588, 164–168
4. Koehler Leman J, Weitzner BD, Lewis SM, Adolf-Bryfogle J, Alam N, Alford RF, Aprahamian M, Baker D, Barlow KA, Barth P, Basanta B, Bender BJ, Blacklock K, Bonet J, Boyken S, Bradley P, Bystroff C, Conway P, Cooper S, Correia BE, Coventry B, Das R, De Jong RM, DiMaio F, Dsilva L, Dunbrack R, Ford A, Frenz B, Fu DY, Geniesse C, Goldschmidt L, Gowthaman R, Gray JJ, Gront D, Guffy S, Horowitz S, Huang P-S, Huber T, Jacobs TM, Jeliaskov JR, Johnson DK, Kappel K, Karanickolas J, Khakzad H, Khar KR, Khare SD, Khatib Firas, Khramushin A, King IC, Kleffner R, Koepnick B, Kortemme T, Kuenze G, Kuhlman B, Kuroda D, Labonte JW, Lai JK, Lapidoth G, Leaver-Fay A, Lindert S, Linsky T, London N, Lubin JH, Lyskov S, Maguire J, Malmström L, Marcos E, Marcu O, Marze NA, Meiler J, Moretti R, Mulligan VK, Nerli S, Norn C, Ó'Conchúir S, Ollikainen N, Ovchinnikov S, Pacella MS, Pan X, Park H, Pavlovicz RE, Pethe M, Pierce BG, Pilla KB, Raveh B, Renfrew PD, **Roy Burman SS**, Rubenstein A, Sauer MF, Scheck A, Schief W, Schueler-Furma O, Sedan Y, Sevy AM, Sgourakis NG, Shi L, Siegel J, Silva D-A, Smith S, Song Y, Stein A, Szegedy M, Teets FD, Thyme SB, Wang RY-R, Watkins A, Zimmerman L & Bonneau R (2020) "Macromolecular modeling and design in Rosetta: new methods and frameworks." *Nature Methods*. 17, 665–680
5. **Roy Burman SS**, Jeliaskov JR, Labonte JW, Nance ML, Lubin JH, Biswas N & Gray JJ (2020) "Novel sampling strategies and a coarse-grained score function for docking homomers, flexible heteromers, and oligosaccharides using Rosetta in CAPRI Rounds 37–45." *Proteins*. 88(8), 973–985
6. **Roy Burman SS**, Yovanno RA & Gray JJ (2019) "Flexible backbone assembly and refinement of symmetrical homomeric complexes." *Structure*. 27, 1041–1051

7. Marze NA\*, Roy Burman SS\*, Sheffler W & Gray JJ (2018) "Efficient flexible backbone protein-protein docking for challenging targets." *Bioinformatics*. 34(20), 3461-3469
8. Kalin JH\*, Wu M\*, Gomez AV\*, Song Y\*, Das J, Hayward D, Adejola N, Wu M, Panova I, Chung HJ, Kim E, Roberts HJ, Roberts JM, Prusevich P, Jeliaskov JR, Roy Burman SS, Fairall L, Milano C, Eroglu A, Proby CM, Dinkova-Kostova AT, Hancock WW, Gray JJ, Bradner JE, Valente S, Mai A, Anders NM, Rudek MA, Hu Y, Ryu B, Schwabe J, Mattevi A, Alani RM & Cole PA (2018) "Targeting the CoREST complex with dual histone deacetylase and demethylase inhibitors" *Nature Communications*. 9(1), 53
9. Marze NA\*, Jeliaskov JR\*, Roy Burman SS, Boyken SE, DiMaio F & Gray JJ (2017) "Modeling oblong proteins and water-mediated interfaces with RosettaDock in CAPRI rounds 28–35" *Proteins*. 85(3), 479-486
10. Lensink MF, Velankar S, Kryshchuk A, Huang SY, Schneidman-Duhovny D, Sali A, Segura J, Fernandez-Fuentes N, Viswanath S, Elber R, Grudinin S, Popov P, Neveu E, Lee H, Baek M, Park S, Heo L, Rie Lee G, Seok C, Qin S, Zhou HX, Ritchie DW, Maigret B, Devignes MD, Ghoorah A, Torchala M, Chaleil RA, Bates PA, Ben-Zeev E, Eisenstein M, Negi SS, Weng Z, Vreven T, Pierce BG, Borrmann TM, Yu J, Ochsenbein F, Guerois R, Vangone A, Rodrigues JP, van Zundert G, Nellen M, Xue L, Karaca E, Melquiond AS, Visscher K, Kastiris PL, Bonvin AM, Xu X, Qiu L, Yan C, Li J, Ma Z, Cheng J, Zou X, Shen Y, Peterson LX, Kim HR, Roy A, Han X, Esquivel-Rodriguez J, Kihara D, Yu X, Bruce NJ, Fuller JC, Wade RC, Anishchenko I, Kundrotas PJ, Vakser IA, Imai K, Yamada K, Oda T, Nakamura T, Tomii K, Pallara C, Romero-Durana M, Jiménez-García B, Moal IH, Fernández-Recio J, Jöng JY, Kim JY, Joo K, Lee J, Kozakov D, Vajda S, Mottarella S, Hall DR, Beglov D, Mamonov A, Xia B, Bohnuud T, Del Carpio CA, Ichiishi E, Marze N, Kuroda D, Roy Burman SS, Gray JJ, Chermak E, Cavallo L, Oliva R, Tovchigrechko A & Wodak SJ (2016) "Prediction of homo- and hetero-protein complexes by ab-initio and template-based docking: a CASP-CAPRI experiment" *Proteins*. 84(Suppl 1), 323-48

\* These authors contributed equally.

## ORAL PRESENTATIONS

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1. "Modeling interactions of flexible proteins." *Boston Protein Design and Modeling Club*, Cambridge, MA, March 2019
2. "Docking symmetric homomers with flexible-backbone refinement." *RosettaCON*, Leavenworth, WA, August 2018
3. "Flexible-backbone protein docking using motif scoring and large conformational ensembles." *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN, November 2017
4. "Flexible-backbone protein docking." *Lectures in Computational Biophysics* at Johns Hopkins University, Baltimore, MD, October 2017
5. "Flexible-backbone protein docking using motif scoring and efficient conformer sampling." *RosettaCON*, Leavenworth, WA, August 2017
6. "Efficient flexible-backbone protein docking." *Regional Computational Biophysics Symposium*, Baltimore, MD, June 2017

## SELECT POSTER PRESENTATIONS

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1. "Computational tools inform the design of protein degraders." *Harvard Structural Biology Retreat*, Cambridge, MA, June 2019
2. "Efficient flexible backbone protein-protein docking for challenging targets." *Biophysical Society Meeting*, San Francisco, CA, February 2018
3. "Efficient flexible protein-protein docking using a diverse ensemble of monomers." *RosettaCON*, Leavenworth, WA, August 2016
4. "Characterization of peptides designed to control calcite growth." *Gordon Research Conference on Biomineralization*, New London, NH, August 2014
5. "Identification of genes essential for attachment of tendons." *Summer Undergraduate Research Grant for Excellence Poster Session*, Kanpur, India, July 2010 (Awarded Best Poster)

## PEER-REVIEW ACTIVITIES

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Reviewer for *Journal of Chemical Information and Modeling* & *Computational and Structural Biotechnology Journal*

## TEACHING EXPERIENCE

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| 2019      | <b>Organizer &amp; Instructor, PYROSETTA CODE SCHOOL for RosettaCommons at Johns Hopkins University</b><br>Designed, organized, and co-taught a week-long workshop to train scientists from experimental backgrounds or with limited coding experience to write computational protocols in Rosetta. Participants had hands-on programming experience to write custom PyRosetta protocols and use a wide range of Rosetta objects. |
| 2015      | <b>Instructor, PROTEIN MISFOLDING DISEASES: A MOLECULAR PERSPECTIVE at Johns Hopkins University</b><br>Conceptualized and co-taught a one credit undergraduate course on molecular mechanisms of Alzheimer's, Huntington's and prion diseases. Students were encouraged to read, discuss and critique recent scientific literature in the field, and were evaluated based on it.  |
| 2013-2015 | <b>Fellow , PREPARING FUTURE FACULTY TEACHING ACADEMY at Johns Hopkins University</b><br>Participated in a professional development program to learn pedagogical theory and teach practice modules with feedback from the instructors. The program was designed to introduce course design, pedagogical models and methods, and develop evaluation skills.  |
| 2014      | <b>Teaching Assistant, COMPUTATIONAL PROTEIN STRUCTURE PREDICTION AND DESIGN</b><br><i>Instructor: Dr. Jeffrey J. Gray, Johns Hopkins University</i><br>Assisted the students during weekly lab sessions. Designed some exam questions and graded assignments and examinations.   |
| 2013      | <b>Teaching Assistant, INTRODUCTION TO CHEMICAL AND BIOLOGICAL PROCESS ANALYSIS</b><br><i>Instructor: Dr. Lise Dahuron, Johns Hopkins University</i><br>Conducted peer-led recitations sections, taught as a substitute instructor and graded examinations.   |

## ACTIVITIES & OUTREACH

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- Wrote [tutorials](#) for Rosetta Molecular Modeling Suite. (2016)
- Mentored students in Margaret Brent Elementary School to engineer toy solutions to local problems as a part of the [STEM Achievement in Baltimore Elementary Schools](#) Program. (2015)
- Provided one-on-one tutoring to local adults seeking a high school-equivalent degree as a part of [Johns Hopkins GED Prep](#). (2013-2015)
- Coordinated new student orientation, mentored students on academic probation, and organized mental health workshops as Assistant Coordinator of the [Counselling Service](#) at Indian Institute of Technology, Kanpur. (2010-2011)

## REFERENCES

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**Dr. Eric S. Fischer**

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