

# Shamrat Kumar Paul

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🌐 <http://paulshamrat.github.io/>

🌐 Sex: Male | Birth Year: 1996 | Nationality: Bangladeshi



## Education

- 2020 – 2022 **MS, Biochemistry and Molecular Biology** Bangabandhu Sheikh Mujibur Rahman Science and Technology University, Gopalganj 8100, Bangladesh.  
Thesis title: *Physicochemical role and potential inhibitor screening for the candidate biomarkers overexpressed in EAE mice*. Supervisor: Mahbub Hasan, PhD  
CGPA: Result not yet published
- 2016 – 2019 **BSc, Biochemistry and Molecular Biology**,  
Bangabandhu Sheikh Mujibur Rahman Science and Technology University, Gopalganj 8100, Bangladesh.  
Project title: *Advanced molecular dynamics simulation for studying peptide structures in OPLS-aa force field*.  
CGPA: 3.79 (in the scale of 4)

## Employment

- 2020 **Research Intern, Prof. D Karunagaran's Cancer Biology Lab**  
Dept. of Biotechnology, Indian Institute of Technology Madras, Chennai 600036, Tamil Nadu India.  
Project title: "Microarray Data Analysis Using GEO2R to Identify Differentially Expressed Genes in Ovarian Cancer after NSC319726 Treatment and Pathway Analysis"; Retrieved three RNA-seq datasets, performed the statistical and DEGs analysis; data analysis: Excel and R.
- 2019 **Trainee, Dept. of Analytical Chemistry and Environmental Science**  
Training Institute for Chemical Industries, Narsingdi 1611, Bangladesh.  
Training title: "Chemical Analysis and Quality Control"; Experience: HPLC, GC-MS, ICP-OES, FTIR and EDXRF.

## Research Skills

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|--------------|---|
| Biophysics   | ■ Molecular Dynamics simulation, Peptide Modeling, Molecular Docking, Microarray and NGS data analysis; elementary, Force-Fields: OPLS-aa.  |
| Applications | ■ GROMACS, VMD, SWISS-MODEL, MODELLER, PyRx, Discovery Studio, PyMol, UCSF-Chimera, Gaussian9 (DFT study; elementary), Bioconda, sra-tools, FastQC, gnuPlot.  |
| Molecular    | ■ Plasmid/DNA/RNA/Protein extraction, Cell culture, Differential/Special Stain, rt-qPCR   |
| Analytical   | ■ Spectroscopic techniques, HPLC, GC-MS, ICP-OES, FTIR and EDXRF; Elementary.   |
| Computing    | ■ Basic Programming languages: Biopython, R; MS Office: Word, Excel, PowerPoint, LibreOffice; Scientific Drawing: Inkscape, GIMP, Photoshop, Illustrator; Typing: 50 WPM: English; 35 WPM: Bengali. |
| OS           | ■ Windows, Linux (Ubuntu 20.04 Distro).   |
| Misc.        | ■ Teaching, training, consultation in molecular modeling and simulation.  |

## Grants and Awards

- 2022 ■ MS thesis Intern Scholarship at Indian Institute of Technology Palakkad, Kanjikkode, Kerala 678623, India (F. No: IITPKD/Acad.Rsch/Internship/2021/001).
- 2021 ■ National Science and Technology (NST) Fellowship for supporting computation facility of MD simulation study of proteins associated with EAE and MS progression. (Code No: 120005100-3821117).
- 2020 ■ Global Research Internship in Engineering Science Humanities and Management (GRIESHMA) awardee at Indian Institute of Technology Madras, Chennai 600036, India; (Internship Period: Mar 2020 - Sep 2020).
- 2018 ■ 2nd Runner up in Idea Contest for In Silico Drug Design (Poster Presentation) at BAUET Tech Fair 2K18, Bangladesh Army University of Engineering and Technology, Natore 6431, Bangladesh.

## Publications

## Articles

- 1 Ahmed, K. A., Hasib, T. A., **Paul, S. K.**, Saddam, M., Mimi, A., Saikat, A. S. M., ... Kim, B. et al. (2021). Potential role of ccn proteins in breast cancer: Therapeutic advances and perspectives. *Current Oncology*, 28(6), 4972–4985.
- 2 Seo, S.-H., **Paul, S. K.**, Shikder, M., Khanam, M., Ghosh, P., Hasib, T. A., ... Kwon, Y. (2021). An insight into pathophysiological features and therapeutic advances on ependymoma. *Cancers*, 13(13), 3221.
- 3 **Paul, S. K.**, Khalipha, A. B. R., Kabir, L., Ray, P., Mina, M. A., & Masum, H. M. (2020). In silico design and homology modeling of helicase c-terminal domain of nonstructural protein ns3 of west nile virus (strain ny-99), 723–732.
- 4 **Paul, S. K.**, Al Hasib, T., Ray, P., Kabir, L., & Khalipha, A. B. R. (2019). Structure prediction and functional characterization of uncharacterized protein rv1708 of mycobacterium tuberculosis (strain atcc 25618/h37rv), 179–184.

## Conference Presentation

- 1 **Paul, S. K.**, Hasib, T. A., & Rizvy, T. K. (2019). *Development and molecular modelling of petase enzyme for degradation of polyethylene terephthalate (pet)*. BUP Environmental Fest 2019, Dhaka 1216, Bangladesh; April 19, 2019. (Poster Presentation).
- 2 **Paul, S. K.**, Kabir, M. L., Mina, M. A., & Rizvy, T. K. (2019). *Molecular docking study of tetrabenazine for targeting huntingtin protein*. Biospectrum 2018, UEM, Kolkata 700156, India, July 27–28, 2018; (Poster Presentation).
- 3 **Paul, S. K.**, Khalipha, A. B. R., Hossain, S., & Islam, M. T. (2019). *In silico molecular docking study of delafloxacin against 4mq; the treatment of acute bacterial skin and skin structure infections*. BAUET Tech Fair 2K18, BAUET, Natore, Bangladesh; May 10, 2018; (Poster Presentation); Awarded Prize for the 3rd Best Poster.
- 4 **Paul, S. K.**, Khalipha, A. B. R., Kabir, M. L., Ray, P., Mina, M. A., & Masum, H. M. (2019). *In-silico design and homology modeling of helicase c-terminal domain of nonstructural protein ns3 of west nile virus (strain ny-99)*. ICCDC 2019, HIT, Kolkata 721657, India; 14–15 March 2019. (Oral Presentation).
- 5 **Paul, S. K.**, Mina, M. A., Noor, M. I., Singha, S., Hossain, M., Rima, S. A., & Halim, M. A. (2019). *Searching potential inhibitors for targeting toll-like receptor 4 (tlr4) protein by virtual screening*. 8th Annual Conference, BCS; Chittagong, Bangladesh; March 31, 2017; (Oral presentation).


## In-progress

- 1 Hasan, M., **Paul, S. K.**, Nidhan Chandra, and Paul, Saikat, A. S., Akter, H., Mandal, M., & Lee, S.-S. (n.d.). *Natural products-based potential therapeutic interventions of pulmonary fibrosis*.
- 2 **Paul, S. K.**, Metu, C. L. N., Sutihar, S. K., Hasib, T. A., Saddam, Kabur, L. M., ... Shihab, S. R. (n.d.). *Homology modeling and molecular dynamics simulation study on rhob: Modulator of cytoskeleton organization*.
- 3 **Paul, S. K.**, Saddam, M., Lee, S.-S., & Hasan, M. (n.d.). *Physicochemical, structural properties, and 100 nanoseconds molecular dynamics simulation of mouse grancalcin (gca) protein: An in-silico study*.

## Projects




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|------|--|
| 2022 | ■ MD simulation: via SSH@science outreach server; access: 12 Intel Xeon E5 cores, and an NVIDIA GTX 2080 GPU]    |
|      | ■ MD simulation on RhoB; modulator of cytoskeleton organization.   |
| 2021 | ■ Physicochemical role and potential inhibitor screening for the candidate biomarkers overexpressed in EAE mice. |
|      | ■ Role of CCN protein family in breast cancer.   |
|      | ■ Idiopathic pulmonary fibrosis; potential therapeutic advancements.   |
|      | ■ Ependymoma: therapeutics and it's advancements.  |
| 2020 | ■ Physicochemical properties of MUNC18 and MUNC 13 protein.  |
|      | ■ Microarray data analysis to identify DEGs in ovarian cancer.   |
| 2019 | ■ Investigation on mycobacterial ABC transporter.  |
|      | ■ PETase enzyme: investigation of tertiary structures.   |
|      | ■ Biophysics of WNV Helicase C-terminal.   |
| 2018 | ■ Modification of Delafloxacin and Fenofibrate.  |

## Projects (continued)



2017     Searching for potential inhibitors of TLR4 protein.

## Science Outreach









### Organizational role

- Jan 2021-     **Research Assistant**, ABEx Bio-Research Center, Dhaka 1230, Bangladesh.
- Mar 2020 -     **Project Mentor**, Bio-Science Research Initiative, Gopalganj 8100, Bangladesh.
- Jan 2018 -     **Research Assistant**, Evergreen Scientific Research Centre, Gopalganj 8100, Bangladesh.



### Training

- Mar 29, 2020     Training on CRISPR Cas-9 molecular biology tool conducted by Bio Bangla and Dept. of BMB, BSMRSTU, Gopalganj 8100 Bangladesh.
- Mar 08, 2019     Hands-on Training Workshop on Molecular Biological Tools used for DNA Barcoding and Basic Bioinformatics at Molecular Pathology Lab of CVASU, Chittagong 4225, Bangladesh.

### Workshops

- Apr 22, 2018     A journey to code and sequence 02 at BSMRSTU, Gopalganj 8100, Bangladesh.
- Apr 06, 2018     Code and sequence returns at BSMRSTU, Gopalganj 8100, Bangladesh.
- Feb 10, 2018     Training on bioinformatics at Rajshahi University, Rajshahi, Bangladesh.
- Jan 02, 2018     A journey to code and sequence (workshop) at BSMRSTU, Gopalganj 8100, Bangladesh.
- Oct 29, 2017     Workshop on Computational Chemistry at Red green research center Dhaka, Bangladesh.
- Sep 11, 2017     A Workshop on Synthetic Biology by Bio Bangla at NMST, Dhaka, Bangladesh.
- Aug 06, 2017     Workshop on Synthetic Biology by Bio Bangla at Software Technology Park, Dhaka, Bangladesh.
- Apr 11, 2017     Advance workshop on computational chemistry at Red Green Research Center Dhaka, Bangladesh.

## Language

- English     Professional Working Proficiency; Medium of instructions for both BSc and MSc Studies.
- Bengali     Native/Bilingual Proficiency

## References

Available on Request