



Shamrat Kumar Paul

🌐 Mobarakpur, Rajganj, Manirampur, Jashore 7440, Bangladesh



✉ shamratpaul.bmb@gmail.com

🌐 <http://paulshamrat.github.io/>








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: 120005100-382117).
- 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 | <ul style="list-style-type: none"> ■ 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 | <ul style="list-style-type: none"> ■ 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 | <ul style="list-style-type: none"> ■ Physicochemical properties of MUNC18 and MUNC 13 protein. ■ Microarray data analysis to identify DEGs in ovarian cancer. |
| 2019 | <ul style="list-style-type: none"> ■ Investigation on mycobacterial ABC transporter. ■ PETase enzyme: investigation of tertiary structures. ■ Biophysics of WNV Helicase C-terminal. |
| 2018 | <ul style="list-style-type: none"> ■ Modification of Delafloxacin and Fenofibrate. |
| 2017 | <ul style="list-style-type: none"> ■ 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