Curriculum Vitae

Personal Information

- **Family name, First name:** Khan, Kabiruddin Ikramuddin
- **ORCID ID:** orcid.org/0000-0003-4849-4516
- **Date of birth:** 10/06/1991
- **Nationality:** Indian
- **URL for the website:**
  https://sites.google.com/view/kk-research-blog/about-me?authuser=0
  https://nanosens.ug.edu.pl/

Current Profile

Dr. Kabiruddin Khan (Webpage, ORCID, Google Scholar, ResearchGate), associated with/handling several scientific projects in various well-established companies as part of their core scientific team.

My expertise lies in developing computational methods/models for designing safer chemicals (i.e., pharmaceuticals, personnel care products, endocrine disruptor chemicals, organic chemicals, nanomaterials, ionic liquids, etc.) that are safe for human health and the environment. Additionally, my performed research has attracted significant audiences across the globe mainly from Europe, and US, and Asia (>450 citations). My developed model on the mutagenicity of nitro and amino aromatic compounds against *Salmonella typhimurium* species has been incorporated into a commercial software AlvaRunner Project developed by the AlvaScience group based in Milan, Italy.

Education

2018-2022 **Ph.D. (17th May 2022),** Department of Pharmaceutical Technology, Jadavpur University, Kolkata, India. Thesis: "**Ecotoxicological modeling of pharmaceuticals and cosmetics using QSAR approaches**" (Supervisor: Prof. Kunal Roy).

2017-2018 **Project Fellow,** Department of Pharmaceutical Technology, Jadavpur University, Kolkata, India (Project Supervisor: Prof. Kunal Roy).

2015-2017 **M.S (Pharm):** National Institute of Pharmaceutical Education and Research Kolkata, India. Thesis: "**Ecotoxicological modeling of cosmetics for aquatic organisms: A QSTR approach**" (Project Supervisor: Prof. Kunal Roy). (CGPA 8.08 out of 10.00)

2011-2015 **Bachelor of Pharmacy (B. Pharm),** Goa College of Pharmacy, Panaji, Goa.

Academic Positions (From 01/01/2018 – 30/06/2019)

Guest Faculty Department of Pharmaceutical Technology, Jadavpur University, Kolkata, India. Subjects Taught: Pharmaceutical Chemistry-VII (Advance Organic), Pharmaceutical Chemistry-IV (Physical), Pharmaceutical Chemistry-III (Organic), and Medicinal Chemistry-II.

International Collaborations

Within the conducted collaborative projects include research institutions from India (**1**), **Saudi Arabia** (1), **Europe** (2), and the **US** (2).

Publication Record Summary

I am the main author or co-author of 7 book chapters, 13 full research papers for peer-reviewed journals, and 2 short papers published as conference abstracts in Mol2Net. I have published my research in internationally recognized peer-reviewed journals such as Green Chemistry (I.F = >11), Journal of Hazardous Materials (I.F = >14), Environment International (I.F = 11.8), Chemosphere (I.F = >8.5), Ecotoxicology and environmental safety (I.F = >7.5), Aquatic Toxicology (I.F = >5), Molecular Informatics (I.F = >4), Toxicology in vitro (I.F = >3.5), and SAR QSAR in Environmental Research (I.F = >3.5). My contributions have been cited >450 times; h-index = 9 (Excluding Self Citations). Google Scholar

List Of Publications In Peer-Reviewed Scientific Journals

1- **Khan, Kabiruddin**, Jillela Gopala Krishna, Agnieszka Gajewicz-Skretna. "Integrated Modeling of Organic Chemicals in Tadpole Ecotoxicological Assessment: Exploring QSTR, q-RASAR, and Intelligent Consensus Prediction Techniques." Chemosphere (communicated CHEM136060)

2- **Khan, Kabiruddin**, Supratik Kar, and Kunal Roy. "Are we ready to combat the ecotoxicity of COVID-19 pharmaceuticals? An in silico aquatic risk assessment." Aquatic Toxicology (2023): 106416.

3- **Khan, Kabiruddin**, Vinay Kumar, Erika Colombo, Anna Lombardo, Emilio Benfenati, and Kunal Roy. "Intelligent consensus predictions of bioconcentration factor of pharmaceuticals using 2D and fragment-based descriptors." Environment International 170 (2022): 107625.

4- **Khan, Kabiruddin,** and Kunal Roy. "Ecotoxicological Risk Assessment of Organic Compounds Against Various Aquatic and Terrestrial Species: Application of Interspecies i-QSTTR and Species Sensitivity Distributions Techniques" *Green Chemistry* (2022).

5- Jillella, Gopala Krishna, **Kabiruddin Khan**, and Kunal Roy. "Application of QSARs in identification of mutagenicity mechanisms of nitro and amino aromatic compounds against Salmonella typhimurium species." *Toxicology in Vitro* 65 (2020): 104768.

6- **Khan, Kabiruddin**, and Probir Kumar Ojha. "Ecotoxicological Modeling of Organic Chemicals for Their Acute Toxicity in Algae Using Classification and Toxicophore-Based Approaches." *International Journal of Quantitative Structure-Property Relationships (IJQSPR)* 5, no. 2 (2020): 17-72.

7- **Khan, K**., and K. Roy. "Ecotoxicological QSAR modelling of organic chemicals against Pseudokirchneriella subcapitata using consensus predictions approach." *SAR and QSAR in Environmental Research* 30, no. 9 (2019): 665-681.

8- **Khan, Kabiruddin**, Pathan Mohsin Khan, Giovanna Lavado, Cecile Valsecchi, Julia Pasqualini, Diego Baderna, Marco Marzo, Anna Lombardo, Kunal Roy, and Emilio Benfenati. "QSAR modeling of Daphnia magna and fish toxicities of biocides using 2D descriptors." *Chemosphere* 229 (2019): 8-17.

9- **Khan, Kabiruddin**, Supratik Kar, Hans Sanderson, Kunal Roy, and Jerzy Leszczynski. "Ecotoxicological modeling, ranking and prioritization of pharmaceuticals using QSTR and i-QSTTR approaches: Application of 2D and fragment based descriptors." *Molecular Informatics* 38, no. 8-9 (2019): 1800078.

10- **Khan, Kabiruddin**, Diego Baderna, Claudia Cappelli, Cosimo Toma, Anna Lombardo, Kunal Roy, and Emilio Benfenati. "Ecotoxicological QSAR modeling of organic compounds against fish: Application of fragment based descriptors in feature

analysis." *Aquatic Toxicology* 212 (2019): 162-174.

11- **Khan, Kabiruddin**, Kunal Roy, and Emilio Benfenati. "Ecotoxicological QSAR modeling of endocrine disruptor chemicals." *Journal of hazardous materials* 369 (2019): 707-718.

12- **Khan, Kabiruddin**, Emilio Benfenati, and Kunal Roy. "Consensus QSAR modeling of toxicity of pharmaceuticals to different aquatic organisms: ranking and prioritization of the DrugBank database compounds." *Ecotoxicology and environmental safety* 168 (2019): 287-297.

13- **Khan, K.**, and K. Roy. "Ecotoxicological modelling of cosmetics for aquatic organisms: A QSTR approach." *SAR and QSAR in Environmental Research* 28, no. 7 (2017): 567-594.

List Of Book Chapters

1- Sanderson, Hans, **Kabiruddin Khan**, Anna M. Brun Hansen, Kristin Connors, Monica W. Lam, Kunal Roy, and Scott Belanger. "Environmental Toxicity (Q) SARs for Polymers as an Emerging Class of Materials in Regulatory Frameworks, with a Focus on Challenges and Possibilities Regarding Cationic Polymers." In *Ecotoxicological QSARs*, pp. 681-705. Humana, New York, NY, 2020.

2- **Khan, Kabiruddin**, Hans Sanderson, and Kunal Roy. "Ecotoxicological QSARs of Personal Care Products and Biocides." In *Ecotoxicological QSARs*, pp. 357-386. Humana, New York, NY, 2020.

3- Aher, Rahul Balasaheb, **Kabiruddin Khan**, and Kunal Roy. "A Brief Introduction to Quantitative Structure-Activity Relationships as Useful Tools in Predictive Ecotoxicology." In *Ecotoxicological QSARs*, pp. 27-53. Humana, New York, NY, 2020.

4- Mohammed Kaleem, Mahmoud Alhosin, **Kabiruddin Khan**, ….., Epigenetic Basis of Polyphenols in Cancer Prevention and Therapy. In Polyphenols-based Nanotherapeutics for Cancer Management, pp. 189-238. Springer, Singapore, 2021.

5- **Kabiruddin Khan**, and Kunal Roy*. "Chemometric modeling of toxicity of chemicals to Tadpoles." Chemometrics and Cheminformatics in Aquatic Toxicology (2021): 331-357.

6- **Kabiruddin Khan**, and Kunal Roy*. "Chemometric Modeling of Toxicity of Chemicals to Marine Bacteria." Chemometrics and Cheminformatics in Aquatic Toxicology, pp.359-376.

7- **Kabiruddin Khan**, and Kunal Roy*. In silico modeling of environmental toxicity of drugs. In *Contemporary Chemical Approaches for Green and Sustainable Drugs*, Elsevier (in press).

Oral/Poster Presentation in Recognized International Conferences (Selected)

1- Invited to present a research paper at International Conferencia Chemometrica (CC 2023) organized by Karoly Heberger, in Sopron, Hungary from 10/09/2023 – 13/09/2023. (Oral Presentation).

2- Invited to present a research paper at International Conferencia Chemometrica (CC 2019) organized by Karoly Heberger, in Karcag, Budapest, Hungary from 08/09/2019 – 12/09/2019. (Oral Presentation).

3- Invited to present a research paper at an international conference entitled "Current Trends in Pharmaceutical and Medical Sciences (CTPMS-2020)" organized by Dr. Sisir Nandi in Kashipur-244713, Uttarakhand, India from 26/02/2020 – 29/02/2020. (Oral Presentation).

4- Attended International Conferencia Chemometrica (CC 2019) organized by Karoly Heberger, in Karcag, Budapest, Hungary from 08/09/2019 – 12/09/2019. (Poster Presentation).

5- Attended 10th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2019) organized by James Devillers, Athina Geronikaki in Ioannina, Greece from 23/06/2019 – 27/06/2019. (Oral Presentation).

6- Attended EuroQSAR 2018 jointly organized by the Turkish and Greece research committee in Thessaloniki Greece from 16/09/2018 – 20/09/2018. (Poster presentation).

7- Attended National Symposium on Recent Advances in Chemistry and Industry (2017) organized by Indian Chemical Society at IIEST, Shibpur W.B (Oral Presentation).
8- Attended India-Russia Conference on "re-positioning of drug / natural products for healthcare" on 30th October 2017 in Goa.
9- Attended 9th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2017) Bogmallo Beach Resort Goa from 27/09/2017 – 30/09/2017. (Oral presentation).
10- Attended International Conference on Drug Design' (ICDD) 2017 jointly organized by **Schrodinger** and **JNU** Delhi from 7/04/2017 - 09/04/2017 (Poster presentation)**.**

Research Projects

2023 - 2025	**Principal investigator:** NanoSens: Towards multi-evidence approach for the risk assessment of a diverse group of nanoparticles and advanced materials funded by POLONEZ BIS 2 grant of MSCA-CoFund scheme. Budget: 1,44,000 Euros. Website
2022 - 2023	**Scientific Lead:** "OpenTox SSDM - A Novel Framework for Species Sensitivity Distribution Modelling". Budget: 40000$
2018 - 2021	**Principal investigator**: "Cheminformatic Modeling of PBT profile and Aquatic Ecotoxicity of Pharmaceuticals and Cosmetic Ingredients for the Design of Environmentally Safer and Greener Alternatives". Budget: 18,42,866.00 ₹
2017 - 2018	**Research Fellow:** "Natural Products and Drug Delivery", Budget: 1,58,946₹~1849 €
2015 - 2017	**Graduate Pharmacy Aptitude Test (GPAT) Scholarship**: For pursuing M.S (Pharm). Budget: 2,97,600 ₹

Competitive Exams Cracked	Type	Rank
Graduate Pharmacy Aptitude Test (GPAT) 2015	National Level	844
NIPER JEE 2015	National Level	648

Prizes and Awards

1. Travel Grant provided by Rashtriya Uchchatar Shiksha Abhiyan (RUSA) 2.0 for attending an international conference entitled "Current Trends in Pharmaceutical and Medical Sciences (CTPMS-2020)" held in Kashipur Uttarakhand, India. (20,000₹)
2. Travel Grant provided by RUSA 2.0 for attending an international conference entitled "Conferencia Chemometrica 2019" held in Karcag, Hungary. (80,000 ₹)
3. Conference bursary awarded from the organizing committee of the international conference "Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI) 2019" to attend the international conference held in Ioannina Greece. (600 €)
4. Travel Grant provided by International Travel Scheme of Science engineering and Research Board (ITS-SERB), Department of Science and Technology, Govt. of India for attending the international conference "Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI) 2019" held in Ioannina, Greece. (87,000 ₹)

Present/former employment

From	*To*	*Name of employer*	*Job*

10/07/2017	02/04/2018	Jadavpur University, Kolkata, India	UPE-II Research Fellow
01/01/2018	30/06/2019	Jadavpur University, Kolkata, India	Guest Faculty
03/04/2018	02/09/2021	Jadavpur University, Kolkata, India	ICMR-Senior Research Fellow
01/01/2022	31/07/2022	QSAR LAB, Gdansk, Poland (Remote)	Sr. R&D Specialist
03/08/2022	31/12/2022	QSAR LAB, Gdansk, Poland (Onsite)	Sr. R&D Specialist
01/03/2022	31/05/2023	Edelweiss Connect, Switzerland (Freelance)	SaferWorldbyDesign Intern
01/08/2022	31/05/2023	OpenTox Association, Switzerland (Freelance)	Research Scientist
01/06/2023	31/05/2025	University of Gdańsk	Assistant Professor (MSCA-CoFund Scientist