Dr. Kartikey Singh, Ph.D.

Post-Doctoral Fellow
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EDUCATION

Ph.D. in Medicinal Chemistry, Oct. 2018
Medicinal & Process Chemistry Division, Central Drug Research Institute, Uttar Pradesh, Lucknow, India
Thesis: *Synthesis and Bioevaluation of Sugar and Heterocycle Derived Hybrids asNew Chemotherapeutic Agents*
Advisor: Dr. Rama P. Tripathi
M.Sc. in Organic Chemistry, Jun.2012,
University of Lucknow, Lucknow
First Division (70.31%)
B.Sc. in Chemistry & Biology, Jun. 2010,
Lucknow Christian Degree College, Lucknow
First Division (69.44%)

PROFESSIONAL EXPERIENCE

Post Doctoral Fellow, Department of Chemistry
Wayne State University, Detroit, MI, USA| *Sept. 2022 to Present*

- Designed and synthesized heparan sulfate trisaccharide derivatives to target hyperphosphorylated tau protein, a key feature of Alzheimer's disease.
- Leading design and multi-step synthesis of glycopolymer-based heparanase inhibitors mimicking glycosaminoglycan for cancer therapeutics with SAR studies and *in cellulo* evaluation.
- Synthesizing and investigating the impact of hydrophobic functionalities on the computationally designed heparan sulfate trisaccharide mimetic and their relative biological activities *in silico* and *in vitro* and *in cellulo*.
- Collaborating with interdisciplinary teams for compound validation and biological assessment.
- Collaborative experiments with Indiana University on flow chemistry process development and scale-up.
- Mentoring junior researchers and managing compound libraries for biological screening.
- Authored several publications in high-impact journals, contributing to the advancement of glyco-medicine and drug discovery.

Post Doctoral Fellow, Department of Chemistry
Indian Institute of Technology Bombay, India| *Apr. 2019 to Apr. 2022*

- Synthesized conjugate-ready trisaccharide units of bacterial cell walls for vaccine development, focusing on *Acinetobacter baumannii* and *Pseudomonas aeruginosa*.
- Investigated, and synthesized rare bacterial D and L amino sugar by utilizing commercially available monosaccharides.
- Developed stereoselective glycosylation strategies to create bacterial oligosaccharides.
- Authored several peer-reviewed publications in high-impact journals, contributing to the advancement of glyco-medicine and infectious-disease drug discovery.

Research Associate, Defence Materials and Stores Research and Development Establishment
DMSRDE – DRDO Kanpur, India| *Dec. 2018 to Mar. 2019*

- Investigated nanomaterial science for defense applications, synthesizing graphene-based nanocomposites for enhanced material properties.
- Contributed to the advancement of nanoparticle science with potential applications in both defense and biomedical fields.
- Contributed to a limited number of peer-reviewed publications focused on nanocomposites for defense materials.

Ph.D. Research, Medicinal and Process Chemistry Division
CSIR- Central Drug Research Institute| *Jan. 2013 to Oct. 2018*

- Synthesized a range of bioactive molecules, including glyco-macrocycles and nucleoside analogs, as potential GPCR inhibitors, anti-cancer, anti-malarial and anti-infective agents.
- Proficient in organic synthesis, structure-activity relationship (SAR) studies.
- Published multiple peer-reviewed papers in leading journals, contributing to the understanding of carbohydrate derivatives in drug discovery.

Teaching Experience

Laboratory & Teaching Assistant, Department of Chemistry,
Indian Institute of Technology Bombay| *Apr. 2019 to Apr. 2022*

- Led organic chemistry experiments for undergraduate and graduate students, developing educational material and lectures.

Assistant Professor, Temporary Faculty
Lucknow Christian Degree College, Lucknow, India| *Jul. 2012 to Dec. 2012*

- Designed and delivered organic chemistry courses for undergraduate students, focusing on experimental and theoretical learning.

KEY STRENGTHS

- **Synthesis**: Expertise in glycosylation, glycomimetics, glycoconjugates, oligosaccharides, and new chemical entities (NCEs).
- **Bioassays:** Experience in TR-FRET, BLI, cytotoxicity assays, and cell culture techniques for drug efficacy evaluation.
- **Handling:** Proficient in multi-step synthesis, large-scale reactions, air- and moisture-sensitive reactions, and project management.
- **Computational Drug Design:** Actively developing skill in molecular docking, molecular dynamics simulations, and structure-based drug design for lead optimization using tools such as AutoDock and PyMOL.
- **Technical:** Skilled in NMR, FT-IR, UV-Vis, LCMS, HPLC, automated flow chemistry, microwave chemistry, chromatography (normal, reverse-phase, size-exclusion), and crystallization.
- **Scientific Tools:** Experienced with ChemOffice, Topspin, Mestrenova, Reaxys, SciFinder for data analysis and research

AWARDS & RECOGNITIONS

- **Invited Talk** Carbohydrates Gordon Research Seminar, 2025
- **Incentive Research Publication Award**, CSIR-CDRI, India, *Feb. 2020*
- **Institute Post-Doctoral Fellowship**, IIT Bombay, India, *Apr. 2019*
- **Research Associate Fellowship**, DMSRDE-DRDO, India, *Dec. 2018*
- **Best Poster Award**, ACCTI (CARBO-XXX), Pondicherry University, India, *Dec. 2015*
- **Gold Medal Award (B.Sc.)**, LCDC-Lucknow, First Rank, *Nov. 2010*

MEMBERSHIP

- Lifetime member of the Association of Carbohydrate Chemists and Technologists (ACCTI), India, 2014-Present.

PUBLICATIONS

Publications in Medicinal & Carbohydrate Science

- **Singh, K.**, et al. Heparanase-Inhibiting Polymeric Heparan Sulfate Mimetic Attenuates Myeloma Tumor Growth and Bone Metastasis. *ACS Appl. Bio Mater.* **2025** (*Just accepted*). Link
- Abdulsalam, H.; Hix, M. A.; Philip, L.; **Singh, K.** et al. From Docking and Molecular Dynamics to Experimental Discovery: Exploring the Hydrophobic Landscapes of Heparanase to Design Potent Inhibitors. *J. Chem. Info. Model.* **2025**, *65 (13)*, 6899-6912. Link
- Abdulsalam, H.; Philip, L.; **Singh, K.**, et al. Design of Paromomycin and Neomycin as Sulfated and Hydrophobic Glycans to Target Heparanase-Driven Tumor Progression and Metastasis. *J. Med. Chem.* **2025**, *68 (11),* 12058-12084. Link
- Philip, L.; Abdulsalam, H.; **Singh, K.** et al. Investigation into the binding domains of platelet factor 4 unlocks new avenues for the design and synthesis of selective sulfated pseudo-tetrasaccharide aminoglycoside ligands. *Eur. J. Med. Chem.* **2025**, *295*, 117792. Link
- Zhang, J.; **Singh, K.** et al. Effects of Heparan Sulfate Trisaccharide Containing Oleanolic Acid in Attenuating Hyperphosphorylated Tau-Induced Endoplasmic Reticulum Stress Apoptosis and Pro-inflammation Associated Alzheimer's

Disease. *J. Med. Chem.* **2025**, *68*,3356-3372. Link, (Co-First Author).

- **Singh, K.**; Tripathi, R. P. Carbohydrate derivatives fight against malaria parasite as anti-plasmodial agents, *Carbohydr. Res.* **2023**, *531*, 108887. Link
- **Singh, K.**; Kulkarni, S. S. Small Carbohydrate Derivatives as Potential Antibiofilm Agents, *J. Med. Chem.* **2022**, *65,* 8525-8549. Link
- **Singh, K.**; Tripathi, R. P. An Overview on Glyco-Macrocycles: Potential New Lead and their Future in Medicinal Chemistry. *Curr. Med. Chem.* **2020**, 27, 3386-3410. Link
- **Singh, K.**, et al. Metal and Phenol-free Synthesis of Biaryl Ethers: Access to Dibenzobistriazolo-1,4,7-oxadiazonines and Vancomycin-like Glyco-Macrocycles as Antibacterial Agents, *J. Org. Chem.* **2018**, *83*, 14882- 14893. Link
- **Singh, K.**, et al. Synthesis and Antiplasmodial Activity of Purine-Based *C*-Nucleoside Analogues, *Med. Chem. Comm.* **2018**, 7, 1232-1238. Link
- **Singh, K.**, et al. Identification of Dual Role of Phenyl Cyclopropyl Methanone-Linked N- Heterocycle as Positive Allosteric Modulator of 5-HT2C and Negative Allosteric Modulator of 5-HT2B Receptors, *Eur. J. Med. Chem.* **2019**, *164*, 499-516. Link
- **Singh, K.**, et al. Synthesis of β- C-Linked 2-Arylaminopyrimidines and β-Cyclohexenone C-Glycosides as H3 Receptor Antagonists, *Trends Carbohydr. Res.* **2017**, *9*, 26-33. Link
- Thakur, R.; Joshi, P.; Upadhyaya, K.; **Singh, K.**, et al. Synthesis of Isatin Based N1-alkylated 3-β-C-Glycoconjugated-Oxopropylidene Oxindoles as Potent Antiplasmodial Agents, *Eur. J. Med. Chem.* **2019**, 162, 448-454. Link
- Kumar, A.; Pasam, V. R.; Thakur, R. K.; Singh, M.; **Singh, K.**, et al. Novel Tetrahydroquinazolinamines as Selective Histamine 3 Receptor Antagonists for the Treatmentof Obesity. *J. Med. Chem.* **2019,** 62, 4638-4655. Link
- Upadhyaya, K.; Hamidullah; **Singh, K.**, et al. Identification of gallic acid-based glycoconjugates as a novel tubulin polymerization inhibitors, *Org. Biomol. Chem.* **2016**, 14, 1338-1358. Link
- Devender, N.; Gunjan, S.; Chhabra, S.; **Singh, K.**, et al. Identificationof β-amino alcohol grafted 1,4,5 trisubstituted 1,2,3-triazoles as potent antimalarial agents, *Eur. J. Med. Chem.* **2016**, 109, 187-198. Link
- Tripathi, R. P.; Upadhyaya, K.; **Singh, K.**, et al. Recent developments on carbohydrate-based anti-infective agents, *Trends Carbohydr. Res.* **2015**, 4, 1-21. Link

Publication in Nanomaterial and Biomedical Applications

- **Singh K.**, et al. Emergence of Fluorescent Glycodots for Biomedical Applications **2025**, *11*, 742-773. Link
- **Singh K.**, et al. Polymer-based nanocomposites as defence material, *Bull. Mater. Sci.* **2023**, *46,* 1-15. Link
- Yadav, G.; Gupta, S. K.; **Singh K.**, et al. High Thermally Stable Polyurethane Nanocomposite Foam Containing Polydimethyl Siloxane and Carbonaceous Nanofillers, *Silicon* **2023**, *15,* 2869-2878. Link
- Mandal T.; Mishra S. R.; **Singh K.**, et al. Fluorescent carbon nanomaterials from coal and its derivatives: structure, properties, and applications, **2023**, *25*, 125. Link

CONFERENCE PRESENTATIONS

- **"Computational-Driven Rational Design and Modular Synthesis of Heparan Sulfate Trisaccharide Mimetics Conjugated with Oleanolic Acid Linkers for Targeted Modulation of Heparanase Enzymatic Activity".** Gordon Research Conference on Carbohydrates held 06/15/2025 - 06/20/2025 at Holderness School in Holderness, New Hampshire, United States.
- **"Heparan sulfate trisaccharide mimetics conjugated with oleanolic acid methyl ester as heparanase inhibitors"**. 19th Midwest Carbohydrate & Glycobiology Symposium, Washington University, USA, Sept. 2024.
- **"Effects of Heparan Sulfate Trisaccharide Containing Oleanolic Acid in Alzheimer's Disease"**. 18th Midwest Carbohydrate & Glycobiology Symposium, Purdue University, USA, Sept. 2023.
- **"Glyco-Macrocycles: Potential New Lead and their Future in Medicinal Chemistry"**. Lucknow University, Mar. 2019
- **"Synthesis of β-C-Linked 2-Arylaminopyrimidines as H3 Receptor Antagonists"**. 10th NIPER-R Symposium on Nano-Based Therapy, Raebareli, India, Mar. 2018.
- **"Synthesis of β-C-Linked 2-Arylaminopyrimidines and β-Cyclohexenone C-Glycosides as H3 Receptor Antagonists".** 24th ISCB International Conference (ISCBC), Department of Chemistry, Manipal University Jaipur, India, Jan. 2018
- **"Carbohydrate-Based Small Molecule in Chemotherapeutics".** National Seminar on Paradigm Shift in Chemical Sciences, Lucknow Christian Post-Graduate College, Lucknow, India, Nov. 2017
- **"Synthesis of Glycomimetics as Chemotherapeutic Agents"**. XIIth J-NOST Conference for Research Scholars (J-NOST), CSIR-CDRI, Lucknow, India, Nov. 2016
- **"Identification of β-amino alcohol grafted 1,4,5 trisubstituted 1,2,3- triazoles as potent antimalarial agents".** 6th International Symposium on Current Trends in Drug Discovery & Research (CTDDR), CSIR-CDRI, Lucknow, India, Feb. 2016
- **"A Strategy for the Synthesis of Anthraquinone-Based Aryl-C-glycosides".** 30th Carbohydrate Conference CARBO-XXX, Pondicherry University, Puducherry, India, Dec. 2015
- **"A Strategy for the Synthesis of Anthraquinone-Based Aryl-C-glycosides".** National Symposium on Interfacing Chemical Biology & Drug Design, Amity University Lucknow, India, Feb. 2015
- **"A strategy to access fused triazoloquinoline and related nucleoside analogues".** 29th Carbohydrate Conference CARBO XXIX, Center of Innovative andApplied Bioprocessing (CIAB), Mohali, India, Dec. 2014
- **"Convergent Synthesis of Carbohydrate-Based Novel Macrocyclic Compounds".** Emerging Trends in Glycoscience & Glycotechnology (A satellite symposiumof ICS-27), Indian Institute of Technology Delhi, India, Jan. 2014
- **"Taxol".** National Seminar on Natural Products & Organic Synthesis(NPOS), Department of Chemistry University of Lucknow, India, March 2012
- **"Wacker Process".** National Seminar on Supramolecular andOrganometallic Chemistry, Department of Chemistry University of Lucknow, India, March 2011
- **"Spectacular Experiment of Chemistry and Research Showcase".** Convocation Week of Lucknow University, Department of Chemistry University of Lucknow, India, Nov. 2010