Rahul Jain, PhD

Professor

National Institute of Pharmaceutical Education and Research (NIPER), Sector 67, S. A. S. Nagar, Punjab - 160 062, India

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Education

Doctor of Philosophy (Organic Chemistry), Central Drug Research Institute, Lucknow, India (**1991**)
Master of Science (Organic Chemistry), University of Lucknow, Lucknow, India (**1984**)

Professional Experience

2024 – Present

Head, Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research, S. A. S. Nagar, Punjab 160 062, India

2007 – Present

Professor, Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research, S. A. S. Nagar, Punjab 160 062, India

2019 – 2023

In-charge, Center of Infectious Diseases, National Institute of Pharmaceutical Education and Research, S. A. S. Nagar, Punjab 160 062, India

2018 – 2021

Dean, National Institute of Pharmaceutical Education and Research, S. A. S. Nagar, Punjab 160 062, India

2011 – 2020

Chairman and In-charge, Central Instrumentation Laboratory (CIL), National Institute of Pharmaceutical Education and Research, S. A. S. Nagar, Punjab 160 062, India

2018 – 2019

In-charge, Pharmaceutical Heritage Center, National Institute of Pharmaceutical Education and Research, S. A. S. Nagar, Punjab 160 062, India

2016 – 2019

Chairman, Student Placement committee, National Institute of Pharmaceutical Education and Research, S. A. S. Nagar, Punjab 160 062, India

2016 – 2017

Associate Dean of Academics Affairs, National Institute of Pharmaceutical Education and Research, S. A. S. Nagar, Punjab 160 062, India

2002 – 2007

Associate Professor, Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research, S. A. S. Nagar, Punjab 160 062, India

1997 – **2002**

Assistant Professor, Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research, S. A. S. Nagar, Punjab 160 062, India

1996 – **1997**

Assistant Professor, Peptide Research Laboratories, Department of Medicine, Tulane University Medical Center, New Orleans, LA 70112, USA

1990 – **1996**

Fogarty International Visiting Fellow, Laboratory of Bioorganic Chemistry, NIDDK, National Institutes of Health, Bethesda, MD 20892, USA

1989 – **1990**

Robert A. Welch Post-Doctoral Research Fellow, Department of Molecular Genetics, University of Texas, Southwestern Medical School, Dallas, TX 75235, USA

1984 – **1989**

Research Fellow, Division of Medicinal Chemistry, Central Drug Research Institute, Lucknow, 226 001, India

Research Expertise

Areas of interest: Medicinal chemistry, Peptide chemistry

•Synthesis and mechanistic studies of ultra-short neuropeptides, antimicrobial peptides, and antiplasmodial peptides; •C-H and C-N functionalization of natural and unnatural amino acids; •Backbone and late-stage

modification of peptides; •Sustainable peptide synthesis; •Synthesis of new structural classes of antiplasmodial and anti-tuberculosis agents.

Research Publications – 170

Representative Publications:

(i) Peptide hydrogen-bonded organic frameworks. *Chem Soc. Rev*. **2024**, *53*, 3640; (ii) Direct access to α,β-alkynylamides via Pd-catalyzed carbonylation of terminal alkynes with amines using chloroform as the CO surrogate. *J. Org. Chem.* **2023**, *88*, 7219; (iii) Design, synthesis, and applications of ring-functionalized histidines in peptide-based medicinal chemistry and drug discovery. *Med. Res. Rev*. **2023**, *43*, 775; (iv) Peptide-based drug discovery: current status and recent advances. *Drug Discov. Today*, **2023**, *28*, 103464; (v) Exploring helical peptides and foldamers for the design of metal helix frameworks: Current trends and future perspectives. *Angew. Chem. Int. Ed.* **2023**, *62*, e202214583; (vi) New structural classes of antimalarials. *Eur. J. Med. Chem.* **2022**, *242*, 114653; (vii) Palladium-catalyzed aminocarbonylation of hetero(aryl) iodides with α-amino acid esters as nucleophiles. *J. Org. Chem.* **2022**, *87*, 8005-8016; (viii) A modified histidine containing amphiphatic ultrashort antifungal peptide, His[2-*p*-(*n*-butyl)phenyl]-Trp-Arg-OMe that exhibits potent anticryptococcal activity *Eur. J. Med. Chem.* **2021**, *223*, 113635; (ix) Structural and mechanistic insights into the inhibition of amyloid-β aggregation by $A\beta_{39-42}$ fragment derived synthetic peptides. *Eur. J. Med. Chem.* **2021**, *212*, 113126; (x) New structural classes of anti-tuberculosis agents. *Med. Res. Rev*. **2018**, *38*, 684; (xi) Bioengineered PLGA-chitosan nanoparticles for brain targeted intranasal delivery of antiepileptic TRH analogues. *Chem. Eng. J*. **2018**, *346*, 630; (xii) Discovery of a membrane-active, ring-modified histidines containing ultra-short amphiphilic peptide that exhibits potent inhibition of *Cryptococcus neoformans*. *J. Med. Chem.* **2017**, *60*, 6607; (xiii) Regioselective access to 1,2-diarylhistidines through the copper-catalyzed N1-arylation of 2-arylhistidines. *Eur. J. Org. Chem.* 2017, 984; (xiv) C-Terminal fragment, $A\beta_{32-37}$ analogues protect against Aβ aggregation-induced toxicity. *ACS Chem. Neurosci*. **2016**, *7*, 615; (xv) Regioselective copper-catalyzed N(1)-(hetero)arylation of protected histidine. *Org. Biomol. Chem.* **2016**, *14*, 8937; (xvi) Metal-free synthesis of *N*-fused heterocyclic iodides via C-H functionalization mediated by *tert*-butylhydroperoxide. *Chem. Commun.* **2015**, *51*, 15129; (xvii) Discovery of short peptides exhibiting high potency against *Cryptococcus neoformans*. *ACS Med. Chem. Lett.* **2014**, *5*, 315; (xviii) Palladium-catalyzed regiospecific C-5 arylation of protected L-histidine: Microwave-assisted C-H activation adjacent to donor arm. *J. Org. Chem.* **2013**, *78*, 10954; (xix) Molecular mechanistic insights into the PepT1-mediated intestinal transport of a novel antiepileptic, NP-647. *Mol. Pharmaceutics* **2012**, *9*, 2458; (xx) Discovery of Trp-His and His-Arg analogues as new structural classes of short antimicrobial peptides. *J. Med. Chem.* **2009**, *52*, 7421; (xxi) Recent advances in antimalarial drug development. *Med. Res. Rev*. **2007**, *27*, 65. (xxii) Low affinity analogs of thyrotropin-releasing hormone are super-agonists. *J. Biol. Chem.* **2006**, *281*, 13103; (xxiii) Thyrotropin-releasing hormone (TRH) analogues that exhibit selectivity to TRH receptor subtype 2. *J. Med. Chem.* **2005**, *48*, 6162; (xxiv) Discovery of a bulky *tert*-butyl group containing primaquine analogue that exhibits potent blood-schizontocidal antimalarial activities and complete elimination of methemoglobin toxicity. *J. Med. Chem.* **2004**, *47*, 285; (xxv) Highly potent cyclic disulfide antagonists of somatostatin. *J. Med. Chem.* **1999**, *42*, 1863; (xxvi) Potent antagonists of somatostatin: Synthesis and biology. *J. Med. Chem.* **1998**, *41*, 1146; (xxvii) Synthesis of ring-halogenated histidines and histamines. *Tetrahedron* **1998**, *54*, 3235; (xxviii) Synthesis of novel ring-substituted histidines and histamines. *Tetrahedron* **1997**, *53*, 4539; (xxix) Regiospecific alkylation of histidines and histamines at C-2. *Tetrahedron* **1997**, *53*, 2365; (xxx) Regiospecific alkylation of histidines and histamines at N-1(τ). *Tetrahedron* **1996**, *52*, 5363; (xxxi) Lactam acetals Part XXIV: Reaction with activated haloalkyl compounds with and without zinc. *Tetrahedron Lett.* **1994**, *35*, 2951; (xxii) A new synthesis of di-(1-methylazacycloalkano)[2,3-*b*:2',3'-*d*]pyridines through annulation on lactam acetals. *Tetrahedron Lett.* **1990**, *31*, 131.

Patents – 20 (IN, EU, US)

Invited Talks and Research Presentations – 116

Mentoring – MS (154); Ph. D. (27); PDFs/RA (4)