Atul Kumar

Personal Information

Date of Birth: 8th April 1990

Nationality: Indian
Gender: Male
Permanent Address: Rakwalla Padder Trilokpur, Gole Gujral Camp, Jammu, J&K, India, 180002
Mother Tongue : Hindi
Other Languages: English
Contact: +919906303166

Contact Details

Department of Chemistry
Indian Institute of Technology, Bombay, India (IIT-B)

E---mail: atulrana8490@gmail.com

Objective

To succeed in an environment of growth and excellence which provides me work satisfaction, self development and help me to achieve personal as well as organizational goals?

Academic Profile

IPDF July 2021 to till date Department of Chemistry, Indian Institute of Technology, Bombay, India (IIT-B)

NPDF (National Postdoctoral Fellow) Dec. 2019 to July 2021 (Dept. of Chemistry and Chemical Sciences, Central University of Jammu, India

Ph.D 2015---2019 (α-Carbonyl Assisted Unconventional Applications of 2-Oxoaldehydes & 2-Oxoesters and Medicinal Chemistry around Ciprofloxacin)

Supervisor Dr. Qazi Naveed Ahmed, Senior Scientist
Indian Institute of Integrative Medicine, Jammu, India

M. Sc. Chemistry 2011---13, Specialization in Organic Chemistry,
Department of Chemistry, University of Jammu, J&k, India.

Research Experience

- Postdoctoral Research Experience (Dec. 2019 to till date).
- Senior Research Fellow from Jan. 2017 to Nov. 2019.
- Junior Research Fellow from Jan. 2015---Jan.2017.

Fellowships and Awards

- Qualified GATE in Feb. 2014.
- Qualified Joint CSIR---UGC Test for Junior Research Fellowship and Eligibility of Lectureship (NET) in Aug 2014.

Research expertise

- Development of new synthetic methodologies around 2-Oxoaldehydes to generate new biologically important scaffolds.
- Synthesis of biologically active molecules involving multi-step synthesis and diversity-oriented synthesis for drug development.
- Multi-step organic synthesis in organic chemistry, as well as carbohydrate chemistry.
- Synthesis and performing air, moisture and light sensitive reactions.
- Structure elucidation by analyzing spectral data ^{1}H-NMR, ^{13}C-NMR, COSEY, NOESY, HMBS, HSQC, IR, LC-MS, etc.
- Able to identify experimental problems and resolve them independently.
- Capable of both collaborative and independent research.
- Possession of good communication and management skill.
- Computer skills and chemistry tools such as Chem. draw, Mestrenova, SciFinder Scholar etc.

Conferences attended

- Attended and presented a paper in an International conference ICGTS 2017 held in Ghaziabad India.
- Delivered oral presentation in 53rd ACC 2016 held at Gitam University, Visakhapatnam, India.
- Attended and presented a paper in 24th ISCB International Conference (ISCBC-2018) held at Jaipur, India.
- Presented paper in International Conference on "Pharmacology and Drug Discovery" with the theme, "Pharmacology for Future: Towards Translational Approach for Next Generation Pharmacologists" during October 4-6, 2018 at Baddi, Himachal Pradesh, India.
- Presented paper in SWEET-18 International Conference on “New Frontiers in Carbohydrate Chemistry and Biology” in 2018 at IISER Kolkata, India.
- Attended and presented a paper in “Recent Advances on Interdisciplinary Sciences” to be held in the University of Jammu from 11th to 12th January 2019. India.
- Attended and presented a paper in Two-day National Conference on “Emerging Trends in Chemical Sciences (ETCS-2019)” during 14-15 March 2019. at Central University Jammu. India.
- Attended and presented a paper in Recent Advances in Organic & Bio-organic Chemistry (RAOBC) 22–24 March 2019, IISER Mohali held, India.

Research Interests

1. Development of new synthetic methodologies
2. Drug design and development
3. Catalysis
4. Asymmetric Total synthesis
5. Carbohydrate Chemistry

List of Publications

1. Introducing Oxo-Phenylacetyl (OPAc) as a Protecting Group for Carbohydrates; **A. Kumar**, V. Gannedi, S. A. Rather, R. A. Vishwakarma, Q. N. Ahmed, *J. Org. Chem*. 2019, 84, 4131−4148. (**IF = 4.335**)
2. Iodine-DMSO Promoted Divergent Reactivities of Arylacetylenes; S. A. Rather, **A. Kumar**, Qazi Naveed Ahmed, *Chem. Commun.*, 2019, **55**, 4511-4514. (**IF = 5.996**)
3. The Ritter Reaction of 2-Oxoaldehydes at Room Temperature: Divergent Behaviour towards Acid Strength; S. Khan, **A. Kumar**, R. Gupta, Q. N. Ahmed, *ChemistrySelect* **2017**, 2, 11336 – 11340. (**IF = 1.811**)
4. Base-Controlled Reactions through an Aldol Intermediate Formed between 2- Oxoaldehydes and Malonate Half Esters; **A. Kumar**, S. Khan, Q. N. Ahmed, *Org. Lett*. **2017**, 19, 4730 −4733. (**IF = 6.091**)
5. A Benzoquinone Imine Assisted Ring-Opening/Ring-Closing Strategy of the RCOCHN1N2 System: Dinitrogen Extrusion Reaction to Benzimidazoles; **A Kumar**, Q. N. Ahmed, *Eur. J. Org. Chem.* **2017**, 2751–2756. (**IF = 2.889**)
6. Air-Assisted 2-Oxo-Driven Dehydrogenative α, α-Diamination of 2-Oxo Aldehydes to 2-Oxo Acetamidines; **A. Kumar**, N. Battini, R. R. Kumar, S. Athimoolam, Q. N. Ahmed, *Eur. J. Org. Chem.* **2016**, 3344–3348. (**IF = 2.889**)
7. Metal-free oxidative cleavage of the C–C bond in α-hydroxy-β-oxophosphonates; S. Battula, **A. Kumar**, Q. N. Ahmed, *Org. Biomol. Chem.*, **2015**, 13, 9953–9956. (**IF = 3.412**)
8. 2-Oxo-Driven N_2 Elimination Induced Decarbonylative Cyclization Reaction in Benzotriazoles to 6-Aminophenanthridines; S. Battula, **A. Kumar**, A. P. Gupta, Q. N. Ahmed, *Org. Lett.*, **2015**, 17, 5562–5565. (**IF = 6.091**)
9. Selenium dioxide promoted dinitrogen extrusion/direct selenation of arylhydrazines and anilines; M. Y. Bhat, **A. Kumar**, Q. N. Ahmed, *Tetrahedron*, **2020**, 76, 131105. (**IF = 2.645**)
10. Javeed Ur Rasool, **Atul Kumar**, Asif Ali, Qazi Naveed Ahmed, An Efficient, Mild and Selective method for the removal of OPAc in saccharides. *Org. Biomol. Chem.*, **2021**, 19, 338-347 (Both authors contributed equally) (**IF = 3.412**)
11. **A. Kumar**, V. Sridharan, Transition Metal-Catalyzed Synthesis of 1,2-Diketones: An Overview, *Asian J. Org. Chem. **2021**, 10, 1619–1637* **(IF = 3.130)**
12. T. Vivekanand, **A. Kumar**; J. C. Menéndez; R. S. Kumar; A. I. Almansour; N. Arumugam, V. Sridharan, Synthesis of fused quinoline derivatives from easily accessible N-(2-aminobenzylidene)-4-methylanilines under catalyst-free conditions in water, *Chemistryselect*, **2021**, 6, 10436-10439. (**IF = 2.1**)

13. D. Rajput, **A. Kumar**, T. Jandial, M. Karuppasamy, N. Bhuvanesh, R. S. Kumar, A. I. Almansour, and V. Sridharan. Microwave-Assisted Copper (II)-Catalyzed Cascade Cyclization of 2-Propargylamino/Oxy-Arylaldehydes and O-Phenylenediamines: Access to Densely Functionalized Benzo[f]Imidazo[1,2-d][1,4]Oxazepines and Benzo[f]Imidazo[1,2-d][1,4] Diazepines. *J. Org. Chem.* **2022**, 87, 8956−8969. (**IF = 4.198**).
14. G. Jan, **A. Kumar**, M. Karuppasamy, D. Rajput, N. Slathia, K. K. Kapoor and V. Sridharan. Microwave-assisted one-pot two-step imine formation–hetero-Diels–Alder–detosylation/aromatization sequence: direct access to dibenzo [b,h][1,6]naphthyridines. *Org. Biomol. Chem.***,** 2022, 20**,** 7472-7482.
15. Rodney A. Fernandes, **A. Kumar**, Ramdas S. Pathare, Asymmetric Total Synthesis of (+)-Dihydroitomanallene B and Formal Synthesis of (-)-Kumausallene. *Chem. Commun.***,** *2022*, 58, *11921-11924.*

Book and Book Chapters

1. **Atul Kumar**, Javeed Rasool, Qazi Naveed Ahmed, "**Chemistry of 2-Oxoaldehydes and 2-Oxoacids**" **ISBN:** 9780128242858.

A brief summary of Ph. D Research

During my Ph.D. I have worked on α- carbonyl assisted reactions around 2-oxoaldehydes in presence of various nucleophiles such as Secondary amines, Primary amines, 4-azidophenol, azoles and malonate acid half esters for the synthesis of biologically important products. Also I have worked in multi-step reactions in carbohydrate chemistry and introduce a new protecting group (OPAc). In addition, I have also developed a new protocol for the synthesis of α-ketoamide based analogues of Ciprofloxacin and checked their activity against different bacterial strains. I have good experience of column chromatography and NMR interpretation (1H, 13C, COSY, HMBC, HSQC and NOESY).

Section A: Air-assisted 2-Oxo-driven dehydrogenative α, α-diamination of 2-Oxo aldehydes to 2-Oxoacetamidines. *Eur. J. Org. Chem.* **2016**, 3344–3348.

This section describes the dehydrogenative α, α-Diamination approach for the synthesis of 2-Oxoacetamidines. The said protocol demonstrate air-assisted, functional-group-driven, mild, additive-free, three-component synthetic approach to different 2- oxo acetamidines from 2-oxo aldehydes, secondary amines, and anilines. (Figure 1).

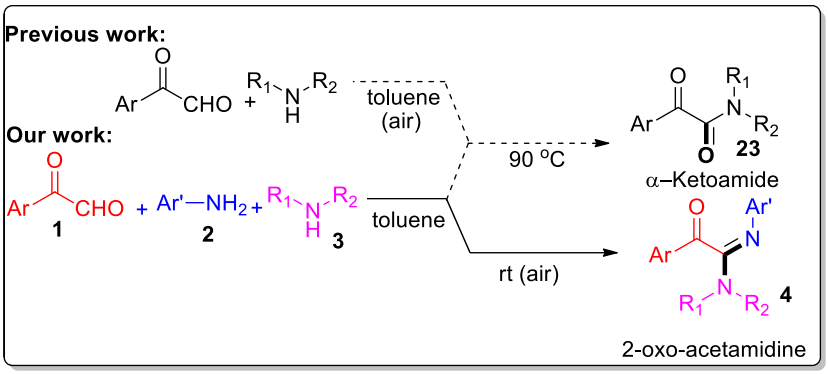


Figure 1: Dehydrogenative α, α-Diamination approach for the synthesis of 2-Oxoacetamidines.

Section B: A Benzoquinone imine assisted Ring-Opening/Ring-Closing strategy of the RCOCHN1N2 system: dinitrogen extrusion reaction to Benzimidazoles. *Eur. J. Org. Chem.* **2017**, 2751–27.

This section deals with the novel strategy for the synthesis of 1,2-disubstituted benzimidazoles from 2-oxoaldehydes, 4-azidophenol, and benzotriazoles. (Figure 2).

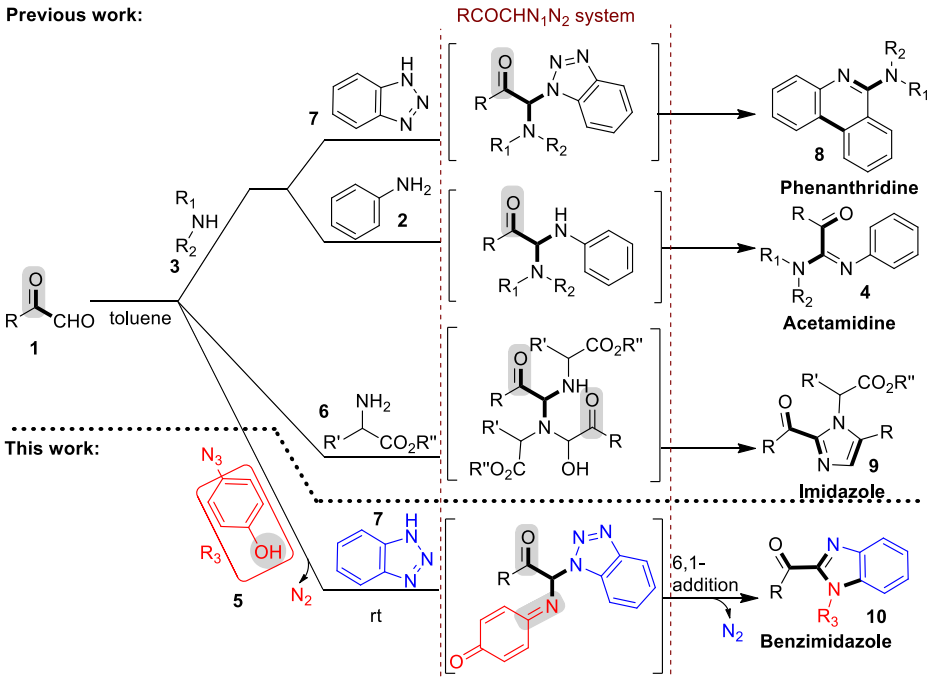


Figure 2: Synthesis of 1,2-disubstituted benzimidazoles.

Section C: Base-Controlled Reactions through an Aldol Intermediate Formed between 2- Oxoaldehydes and Malonate Half Esters. Org. Lett. 2017, 19, 4730 −4733.

A practical, atom-economical, base-directed, and highly efficient method for the generation of different selective products through a common aldol intermediate of 2-oxoaldehydes and malonate half esters is successfully developed. The addition of a strong

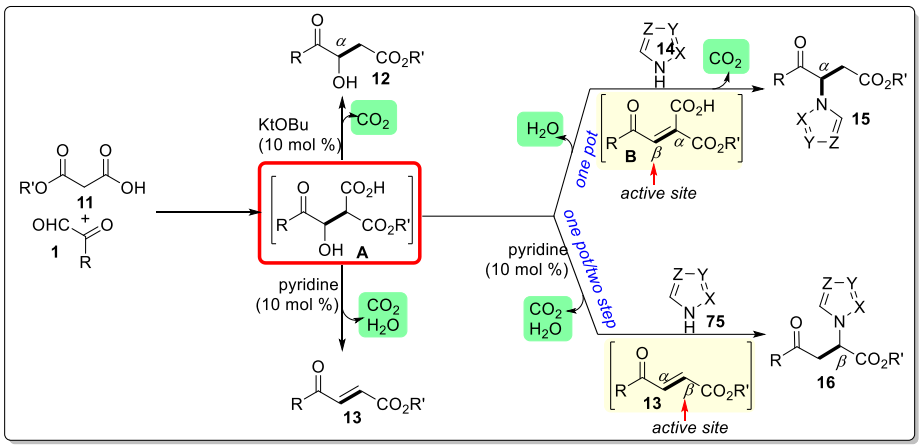


Figure 3: Base-Controlled Reactions between 2- Oxoaldehydes and Malonate Half Esters.

basic environment (potassium tert-butoxide) catalyzed the synthesis of stable decarboxylative aldol products (α-hydroxy ketones), while the Doebner modification procedure resulted in decarboxylativeelimination to (E)-α,β-unsaturated esters in good yields. The application of this method in one pot and one pot/two steps with azoles helped to develop regioselective α- and β-azolatedproducts in appreciable yields. (Figure 3).

Chapter 3: Introducing Oxo-Phenylacetyl (OPAc) as a Protecting Group for Carbohydrates.

A series of oxo-phenylacetyl (OPAc) protected saccharides, with divergent base sensitivity profiles against benzoyl (Bz) and acetyl (Ac), were synthesized and KHSO5/AcCl in methanol was identified as an easy, mild, selective and efficient deprotecting reagent for their removal in the perspective of carbohydrate synthesis. Timely monitoring of AcCl reagent was supportive in both sequential as well as simultaneous deprotecting of OPAc, Bz and Ac. The salient feature of our method is the orthogonal stability against different groups, its ease to generate different valuable acceptors using designed monosaccharides and use of OPAc as a glycosyl donar (Figure 4).

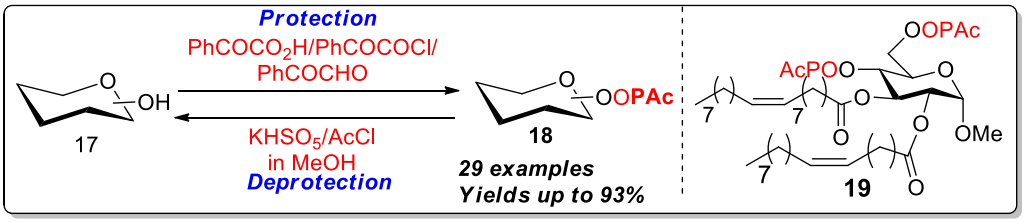


Figure 4. Oxo-Phenylacetyl (OPAc) as a new Protecting Group.

Chapter 3: Development of new α-ketoamide based analogues of ciprofloxacin against different resistant strains.

α-Ketoamides are important units in biologically active molecules, synthetic drugs, and drug candidates. They are well reported to have better stability than normal amides and due to the presence of 2-oxo group have polar nature. Previously, most of the fluoroquinolone

derivatives were synthesized by addition of an additional functional moiety on the N atom of the C-7 side chain in order to increase their lipophilicity, and some of them shows better antibacterial or anti-MTB activity than the corresponding parent FQs.17,18 These research studies intensified our interest to design and synthesize a series of novel α-Ketoamides derivatives by introduction of a lipophilic moiety to the N atom on the C-7 piperazine ring of Ciprofloxacin, and evaluate their antibacterial activity against different resistant strains (Figure 5).

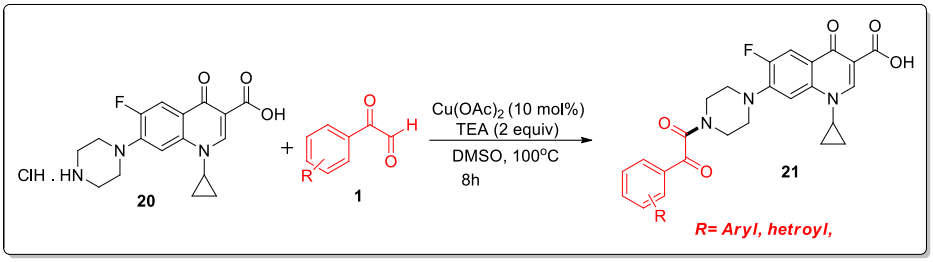


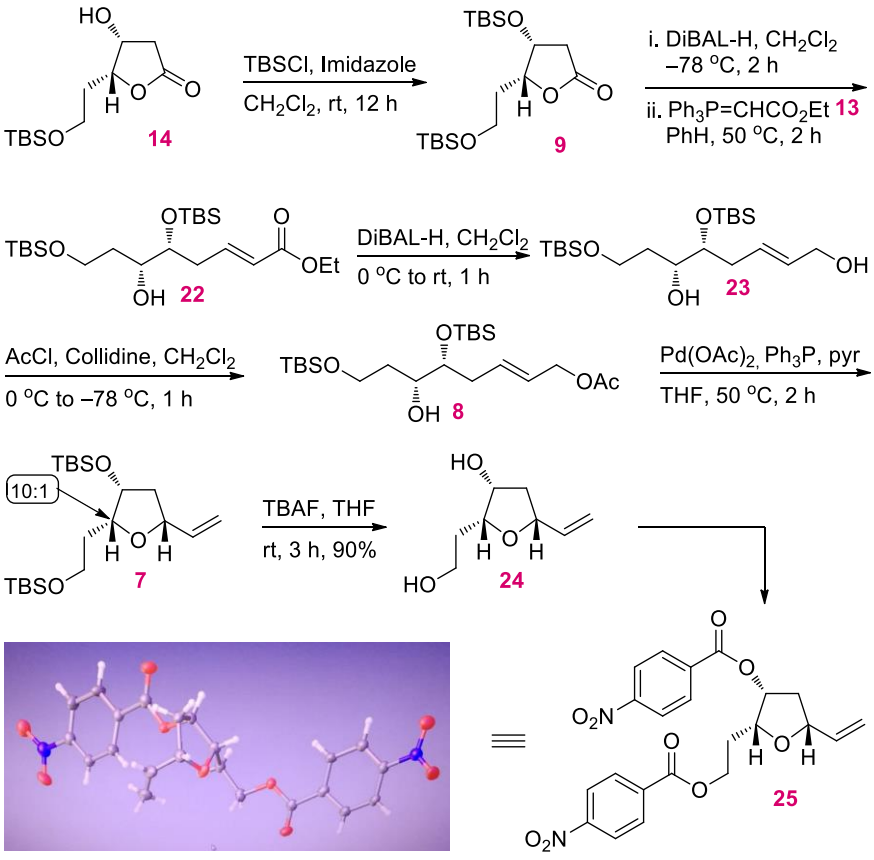
Figure 5. Synthesis of α-Ketoamides based analogues of Ciprofloxacin.

Postdoctoral Work:

Total synthesis of Dihydroitomanallene B

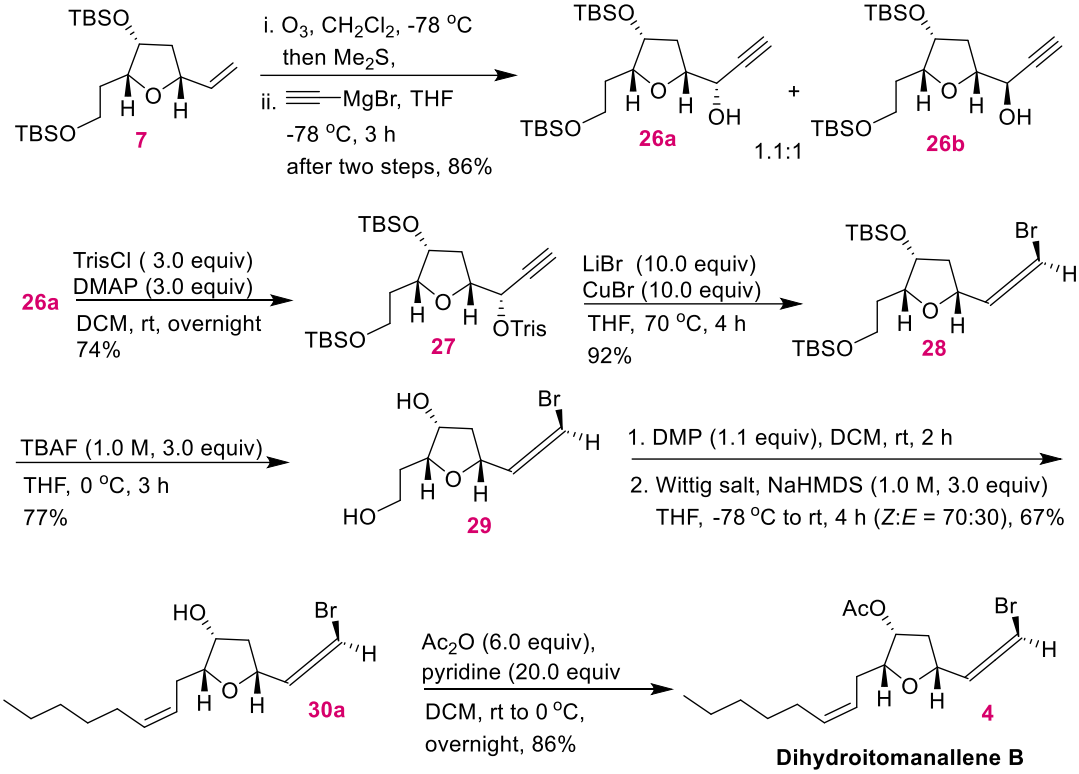
Recently, in 2012, Vairappan and coworkers isolated dihydroitomanallene B (4) from L. nangii from Tun Sakaran Marine Park, Sabah, Malaysia. The structure of dihydroitomanalle-

Synthesis of Compound 7



ne B (4) was thoroughly characterized based spectroscopic techniques like 1H, 13C NMR, COSY, HMBC, HSQC, IR and HRMS spectra.4 Till date, there is no report available for the synthesis of dihydroitomanallene B and this prompted us to envisage a convenient strategy for the synthesis of dihydroitomanallene B.

Synthesis of Dihydroitomanallene B



References

Dr. Qazi Naveed Ahmed

Senior Scientist

Medicinal Chemistry Division, CSIR-Indian Institute of Integrative Medicine

Canal Road, Jammu Tawi-180001

Email: naqazi@iiim.ac.in

Dr. Parvinder Pal Singh

Senior Scientist

Medicinal Chemistry Division, CSIR-Indian Institute of Integrative Medicine

Canal Road, Jammu Tawi-180001

Email: ppsingh@iiim.ac.in

Dr. Debaraj Mukherjee

Senior Scientist,
HOD Department of Natural Product Chemistry and Bio-Organic Chemistry,
CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu Tawi-180001
Email: dmukherjee@iiim.ac.in

Declaration

I hereby declare that all information given above is true to the best of my knowledge and belief that the document in the support of the information will be forwarded when required.

Atul Kumar