

Prof. Prasad V. Bharatam, FASc, FRSC

Department of Medicinal Chemistry
National Institute of Pharmaceutical Education and Research (NIPER),
Sector-67, S.A.S. Nagar (Mohali) – 160 062, Punjab, India
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Website: https://www.niper.gov.in/sites/default/files/profile-resume/2024_Bhartam.pdf



- 1. Fields of Specialization:**
- (i) Organic Synthesis
 - (ii) Medicinal Chemistry: Anti-bacterial
 - (iii) Chemical bonding: Nitreones, Nitrinium ions
 - (iv) Quantum Medicinal Chemistry
 - (v) Pharmacoinformatics: Programing, AI, Ayurinformatics
 - (vi) Drug Metabolism, Drug Toxicity, Drug delivery -- computational

2. Honors and Awards:

| | |
|---|---------|
| Fellowship of Indian Academy of Sciences | -- 2020 |
| Fellowship of Andhra Pradesh Akademi of Sciences | -- 2011 |
| Fellowship of Telangana Academi of Sciences | -- 2011 |
| OPPI Scientist Award | -- 2009 |
| Ranbaxy Research Award | -- 2008 |
| Chem. Research Society of India – Medal | -- 2008 |
| Fellowship of Royal Society of Chemistry (FRSC), London | -- 2007 |
| IBM Faculty Award | -- 2007 |
| Fellowship of Alexander von Humboldt Stiftung, Bonn | -- 2002 |

3. Research Experience:

| | |
|---|--------------|
| Chemical bonding novel concepts – divalent N(I) compounds | 2005-current |
| Bio-inorganic chemistry of drugs | 2004-current |
| Tautomerism in drugs | 1991-current |
| Carbynes, carbenes, carbones and related reactive intermediates | 1985-current |
| Ayurinformatics | 2022-current |

4. Teaching Experience:

| | | |
|-------------------------------|---|---|
| <i>NIPER, Mohali</i> | 24 years-- | Medicinal & Bioorg. Chemistry Bio-inorganic chemistry Chemoinformatics Pharmacoinformatics |
| <i>G.N.D. Univ., Amritsar</i> | 7 years – integrated M.Sc. (5 yr. course) | Quantum chemistry Physical Chemistry Computational Chemistry |

5. Adminstrative experience:

| | |
|---|--------------|
| Dean, NIPER, SAS Nagar | -- 2016-2018 |
| Associate Dean, NIPER, SAS Nagar | -- 2015-2016 |
| Head, Department of Medicinal Chemistry | -- 2019-2024 |
| Incharge, Departement of Pharmacoinformatics, NIPER, SAS Nagar | -- 2010-2021 |
| Officiating Director, NIPER, SAS Nagar (temporary: Jan, Feb. 2017, Sept.2018, March-May 2021) | |

| | | |
|-------------------------------|---|-------|
| 6. Publication record: | Original Scientific articles published (foreign journals) | 303 |
| | Original Scientific articles published (Indian Journals) | 19 |
| | Patent Filed | 03 |
| | Reviews (peer reviewed) | 21 |
| | Book Chapters (peer reviewed) | 10 |
| | Science Education articles | 18 |
| | Total | 374 |
| | Citations (Google Scholar) | ~8432 |
| | h-index (Google Scholar) | 48 |

7. Positions held:

| S. No. | Period | Place of Employment | Designation | Scale of Pay |
|--------|------------------------|-----------------------------|--------------|------------------------|
| 4. | June 2006 – continuing | N.I.P.E.R., Mohali | Professor | Rs. 2,22,000 GP 10,500 |
| 3. | June 2001 – June 2006 | N.I.P.E.R., Mohali | Assoc. Prof. | Rs. 16,400-450-20,900 |
| 2. | Aug. 2000 – June 2001 | G.N.D. University, Amritsar | Reader | Rs. 12,000-250-16,000 |
| 1. | Dec. 1993 – Aug. 2000 | G.N.D. University, Amritsar | Lecturer | Rs. 2,200-75-3,000 |

8. National / International Assignments:

- (xxiv) Member Senate, NIT, Kurukhetra -- 2022-2024
- (xxiii) Member DST PAC-International -- 2022-2024
- (xxii) Member DST-FIST -- 2022-2024
- (xxi) Member RAC, IISER, Mohali -- 2021-2025
- (xx) Member CSIR-CDRI – Research council -- 2020-2023
- (xix) Member syllabus forming : Punjabi Univ. – Physical Sci. 5 year integrated course -- 2021-2024
- (xviii) Member GNDU – Chemistry – Research council -- 2020-2022
- (xvii) Member CSIR-Chemistry-HRDG-committee -- 2019-2021
- (xvi) Member DBT (Bioinformatics) PAC -- 2019-2021
- (xv) Member DST WOS(Chem) PAC -- 2016-2019
- (xiv) Member of DST Organic Chemistry PAC -- 2015-2018
- (xiii) Member DST fast track PAC -- 2012-2015
- (xii) Member faculty selection committees, Central Univ. Punjab (2015), Pujab Univ., Chd. (2010, 2011, 2013, 2014, 2017, 2018), G.N.D. Univ., Amritsar (2012), BITS, Pilani (2018), IITR, Lucknow (2012, 2016), NIPER (2012-2020)
- (xi) Member committee on syllabus framing, Central Univ. Punjab -- 2013-2014
- (x) Subject Expert – Board of control, Biotechnology, GNDU, Amritsar -- 2007-2009
- (ix) Subject Expert – Board of Research, Sciences, GNDU, Amritsar -- 2008-2011
- (viii) Council Member, Chemical Research Society of India -- 2008-2010
- (vii) A reviewer in many journals including, Nature Chemistry; J. Med. Chem.; J. Org. Chem.; J. Am. Chem. Soc. J. Phys. Chem.; Inorg. Chem.; Chemistry, A Eur. J.; etc.
- (vi) Evaluator of project proposals submitted to CSIR, DST, DBT, UGC, ICMR, New Delhi.
- (v) Invited to the Gordon Research Conference on Computer Aided Drug Design in July 2005, Tilton, NH, USA.
- (iv) Invited to the Keystone conference on Computer Aided Drug Design in April 2008, USA
- (iii) Invited for Plenary lecture at Medicinal Chemistry Intl. conf. Aug. 2009, Bangdung, Indonesia.
- (ii) Invited for the Gordon Research Conference on Drug Metabolism, August 2013, USA.
- (i) Member: National Academy Sciences, Allahabad

9. Editorial Experience :

- (a) Guest editor Theo. Chem. Accounts -- Jan. 2012
- (b) Guest editor for Indian J. Chem. Section A. -- Jan. 2006
- (c) Edited a Festschrift on “Prof. E.D. Jemmis”, Springer -- 2012
- (d) Member Editorial Advisory Board – Indian Journal of Chemistry A. 2008-2010

- (e) Member Editorial Advisory Board – Current Comput Aided Drug Design 2007-2009
 (f) Editor, CRIPS, published by NIPER -- 2012- onward

10. Research Supervision:

- A. Ph.D. – 37 completed; 13 on going.
 B. M.Sc. Research Projects – 16 completed
 C. M.S. Pharm (Med. Chem.) research projects – Aprox.220 completed 16 on going.
 D. Research Fellows (Non-Ph.D.) – 13 completed
 E. Long-term visiting fellows – 20
 F. Short-term visiting Fellows / students – 60

Ph.D. Students:

| <i>Name</i> | <i>Current position</i> |
|-----------------------|--|
| 1. Punam Uppal | School management, Amritsar |
| 2. R. Senthil Kumar | Runs a CRO |
| 3. Amita Mahajan | Assoc. Prof. Eng. College, Gurdaspur, Punjab |
| 4. Rajnish Moudgil | Assoc. Prof., Hoshiarpur, Punjab |
| 5. Punita Sharma | Asst. Prof., ILS University, Jaipur |
| 6. Smriti Khanna | Sr. Scientist, Nicholas Piramal, Mumbai |
| 7. P. Senthil Kumar | Sr. Scientist, Orchids Research Laboratories, Chennai |
| 8. Sandeep Sundriyal | Faculty, Pharm. Sci. BITS, Pilani |
| 9. Amit Mittal | Asst. Prof., Lovely Professional Univ., Jalandhar |
| 10. Adane Leggesse | Assoc. Prof. Jimma University, Southwestern Ethiopia |
| 11. Dhilon Patel | Research Associate, Carneige-Millon Univ. Pennsylvania, USA |
| 12. Y. Kasetti | Scientist-cum-patent attorney, Hyderabad |
| 13. Vaibhav A. Dixit | Faculty, Pharm. Sci. BITS, Pilani |
| 14. Ramesh M. | Postdoc, South Africa |
| 15. Devendra Dhaked | Faculty, NIPER, Kolkata |
| 16. Nikhil Taxak | Associate Consultant, ZS, Gurgaon |
| 17. Vaibhav Jain | Manager, Sun Pharma Advanced Research Co. Ltd., Vadodara, |
| 18. Rajendra Kumar | Post doc, Umea Univ., Sweden |
| 19. Sonam Bhatia | Asst. Prof., Sam Higginbottom Inst., Allahabad |
| 20. Minhazul Arfeen | Asst. Prof. Qassim University, Buraydah |
| 21. Sheenu Abbat | Lecturer, Pharmacy College, Nasik |
| 22. Neha Tripathi | Post doc – University of Nantes, France |
| 23. C.K. Jaladanki | Senior Post doc– Bio-Informatics Institute, BII, A*STAR, Singapore |
| 24. S.S. Chourasiya | Group Leader, R & D, IOL Chemicals and Pharmaceuticals Ltd. |
| 25. Neha Patel | Marie Curie Postdoc. Friedrich-Alexander Univ., Germany |
| 26. Vishnu K. Sharma | Scientific Officer, NIPER. |
| 27. Shweta Bhagat | Postdoc, Chicago |
| 28. Deepika Kathuria | Asst. Prof., Chandigarh University |
| 29. Firdoos A. Sofi | Dr. D.S. Kothari Postdoc. fellow at DOPS Univ. Kashmir, Srinagar |
| 30. Tejender Singh | TIFR, Hyderabad |
| 31. Gurudutt Dubey | Postdoc, Valencia, Spain |
| 32. Aabid Wani | Postdoc – ETH, Zurich |
| 33. Mohammad Ovais | Asst. Prof., MM Univ. Mullana-Ambala, Haryana |
| 34. Kshitij Sharma | Industrial job in Jaipur |
| 35. Nirjhar Saha | RA, IACS, Kolkata |
| 36. P. Wanjari | Technical Officer, NIPER, SAS Nagar |
| 37. Kausar Jahan | Asst. Prof., |
| 38. Kriti Mehta | continuing 4 th year |
| 39. Kanika Manchanda | continuing 4 th year |
| 40. Astha Gupta | continuing 4 th year |
| 41. Joy Mukhopadhyay | continuing 3 rd year |
| 42. Nabajyoti Patra | continuing 3 rd year |
| 43. Mehak Sood | continuing 3 rd year |
| 44. Shivkanya Bhujbal | continuing 3 rd year |

| | |
|------------------------|---------------------------------|
| 45. Govinddas Vaishnav | continuing 2 nd year |
| 46. Lahu Dayare | continuing 2 nd year |
| 47. Sanjeev Ranjan | continuing 2 nd year |
| 48. Akash Kendre | continuing 2 nd year |
| 49. Anand Kumar Dubey | continuing 1 st year |
| 50. Rupal Kushwah | continuing 1 st year |

Other significant members:

| | |
|-----------------------|--|
| 51. D. Kaur | Retired Professor, Dept. Chem., G.N.D.U. |
| 52. Alka Marwaha | Asst. Prof., Lovely Professional Univ., Jalandhar |
| 53. M.E. Sophia | Assoc. Prof., NIPER, Mohali |
| 54. Pansy Iqbal | Sr. R&D Chemist, PPG Industries, Pennsylvania, USA |
| 55. S.K. Singh | Assoc. Prof., Alagappa University |
| 56. Mymoona Akhtar | Prof., Jamia Hamdard |
| 57. Prakash C. Rathi | Astra Zeneca, UK |
| 58. Jagmohan Saini | Lupin Pharma, Pune |
| 59. Harish Jangra | Post Doc. Fellow, LMU, Germany |
| 60. Subhash Agarwal | Scientist, ICMR-Inst. of Cytology and Preventive Oncology, Noida |
| 61. Sourav Kalra | JRF, IMTECH |
| 62. Venkata Krishnan | Ph.D. student France |
| 63. Pritika Gupta | JRF, USA |
| 64. Samima Zaman | JRF |
| 65. Sumi Isha | JRF |
| 66. Prajwal Nandrekar | Scientist, Schrodinger Inc., India |
| 67. Rohit Sathe | NPDF |
| 68. Kaushik | Proj. Assoc. |
| 69. Pratik Prasher | Postdoc Fellow |
| 70. Prajanya | RA |

11. Project supervision as Principal Investigator

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|---|--------------------|-----------|
| 1. UGC Interdisciplinary grant, GNDU | Rs. 4,000/- | 1994-1995 |
| 2. DST Young Scientist Project: | Rs. 2,60,000/- | 1996-1998 |
| 3. DST grant : | Rs. 6,60,000/- | 1999-2002 |
| 4. Research Fellow grant, GNDU | Rs. 1,20,000/- | 2000-2002 |
| 5. CSIR Project | Rs. 9,60,000/- | 2001-2004 |
| 6. NMITLI project | Rs. 12,20,000/- | 2002-2004 |
| 7. DST project on Nitric Oxide donors | Rs. 16,10,000/- | 2004-2007 |
| 8. DST project on Pharmacoinformatics | Rs. 1,50,00,000/- | 2005-2009 |
| 9. CSIR project on Dual activators | Rs. 10,00,000/- | 2005-2008 |
| 10. DST project – Nano Mission | Rs. 50,00,000/- | 2009-2012 |
| 11. DST project on S-oxidation | Rs. 35,00,000/- | 2009-2012 |
| 12. CSIR project on PPAR γ | Rs. 19,60,000/- | 2012-2015 |
| 13. DBT project of MBI | Rs. 40,00,000/- | 2012-2015 |
| 14. DST project on divalent N(I) compds | Rs. 45,00,000/- | 2013-2016 |
| 15. CSIR-OSDD chemoinformatics | Rs. 5,00,000/- | 2013-2014 |
| 16. DST nanomission- Dendrimers | Rs. 65,00,000/- | 2015-2018 |
| 17. DST-DAAD Indo-German Project | Rs. 8,00,000/- | 2018-2019 |
| 18. DBT-BMBF Indo-German Project | Rs. 52,00,000/- | 2019-2020 |
| 19. CSIR-Azines project | Rs. 20,00,000/- | 2019-2022 |
| 20. DBT – Bioinformatics Centre | Rs. 1,50,00,000/- | 2021-2025 |
| 21. DST- Pincer Complex | Rs. 50,00,000/- | 2022-2025 |
| 22. Indo-Swiss project | Personnel Exchange | 2023 |

as a co-Principal Investigator

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|-----------------|----------------|-----------|
| 1. CSIR Project | Rs. 6,50,000/- | 2002-2005 |
|-----------------|----------------|-----------|

12. Industrial Projects

1. Project with Eli Lilly, USA US \$ 44,000/- 2008-2010

13. Organisational experience:

- Coordinated online symposium cum workshop on Ayurinformatics- Nov 2024
- Coordinated symposium on Ayurinformatics-March 2024
- Coordinated national symposium on RABMC –Nov 2022
- Coordinated a symposium on theoretical chemistry and biology-Aug 2022
- Coordinated INDO-US conference in M2ID2 – Nov. 2015
- Coordinated Int. Symp. Recent Adv. Medicinal Chemistry – Sept. 2015
- Coordinated an Indo-German conference in Molecular Modeling – Feb. 2013.
- Coordinated 4 workshops on Pharmacoinformatics (2002, 2004, 2004, 2005)
- Coordinated an SERC summer School in Modeling and Informatics in Drug Design, June-July 2008
- Coordinated the 3rd mid-year symposium of CRSI, July 2008.
- Coordinated 5 international symposia on DMPK, Feb. 2009, 2010, 2011, 2012, 2013
- Active member of the organizing committees of several conferences and workshops at NIPER
- Established a National Centre for Pharmacoinformatics (DST) (2.5 crores)
- Established a PharmaGrid at NIPER (2008-2012) (14 crores)
- Member of Board of Research Studies, Chemistry, - GuruNanakDevUniversity. 2001-2002
- Member of several faculty selection committees, NIPER, IITR, GNDU, PU, etc.
- Chairman of several selection committees at NIPER.
- Established Bioinformatics Infrastructure facility (DBT) at NIPER, Mohali.
- Established computational chemistry research lab at G.N.D.Univ., Amritsar.
- Member of org. committees of several workshops and conf. (National, International) at GNDU (1994-2001).

14. Collaborators

Developed strong collaboration with some colleagues. Such groups are headed by

- (a) Prof. S.V. Kessar, Panjab University, Chandigarh.
- (b) Prof. A.K. Chakraborti, NIPER, Mohali
- (c) Prof. P. Rama Rao, NIPER, Mohali
- (d) Prof. M.P. Mahajan, G.N.D.Univ., Amritsar
- (e) Prof. Damanjit Kaur, G.N.D. Univ., Amritsar
- (f) Prof. S.S. Chimni, G.N.D. Univ. Amritsar
- (g) Dr. S.K. Guchhait, NIPER, Mohali
- (h) Prof. Vibha Tandon, Delhi University, Delhi
- (i) Prof. A.K. Verma, Delhi University, Delhi
- (j) Dr. S.K. Mandal, IISER, Mohali
- (k) Dr. Parthasarathi Das, IIM, Jammu
- (l) Dr. S. Bharate, IIM, Jammu
- (m) Prof. A.K. Madan, MDU, Rohtak
- (n) Prof. RajKumar, Central University of Punjab, Bhatinda
- (o) Prof. A.T. Khan, IIT, Guwahati
- (p) Prof. A.K. Sahoo, Univ. of Hyderabad
- (q) Prof. Uwe Beifuss, Hohenheim Univ., Stuttgart, Germany
- (r) Prof. H. Gholke, Heinrich-Heine Univ., Dusseldorf, Germany
- (s) Prof. Arvind K. Bansal, NIPER, Mohali
- (t) Prof. D.W. Rawat, Delhi Univ., Delhi
- (u) Dr. Ramadas Maganti, SDACH, Chandigarh
- (v) Prof. Dulal Panda, IIT Bombay
- (w) Prof. SD Sawant, IIM Jammu
- (x) Prof. Srivastava Naidu, IIT Ropar
- (y) Prof. Joydev Laha, NIPER Mohali

15. References

1. Prof. E.D. Jemmis
Inorg. Phys. Chem., IISc., former Director, IISER, TVM
Bangalore – 560 012
e-mail : jemmis@ipc.iisc.ernet.in
2. Prof. N. Sathyamurthy
former Director, IISER
Mohali
e-mail: nsath@iitk.ac.in
2. Prof. K. Lammertsma
Vrije Universiteit
De Boelelaan 1083
1081, HV Amsterdam, The Netherlands
e-mail: lammert@chem.vu.nl
4. Prof. G. Frenking
Philips Universitat
Marburg
Germany
e-mail: frenking@chemie.uni-marburg.de

16. Personal details:

Full name: Bharatam Venkata Rama Surya Subrahmanya Visweswara Prasad
(As in official records, surname underlined)

Date of Birth: 12 October 1962

Place of Birth: Rajahmundry, Andhra Pradesh

Nationality: Indian

Permanent address: C/o Sri Bharatam Srimannarayana, Telugu and Sanskrit Poet, Principal (Sanskrit College), Retired
A.P.H.B. Colony, Tadepalligudem – 534 101, Andhra Pradesh, India

Academic qualifications:

| S. No. | Degree | Subject | Class Marks % | Year | University |
|--------|--------|----------------------------------|------------------|------|---|
| 4. | MS* | Computer Science | 87% | 1993 | Univ. Alabama at Birmingham (USA) |
| 3. | Ph.D. | Applied Theoretical Chemistry | | 1990 | Univ. of Hyderabad, India |
| 2. | M.Sc. | Organic Chemistry | I class 67% | 1984 | Visva-Bharati, Santiniketan, India UGC Net cleared in 1984 |
| 1. | B.Sc. | Chemistry, Maths, Physics | I class 70% | 1982 | Andhra University, Waltair, India |

* Non-degree

Title of the Ph.D. Thesis: **Electronic Structure and Reactivity of
Carbyne Bridged Bimetallic Complexes**
(August 1990)
(Supervisor: Prof. E.D. Jemmis, University of Hyderabad)

Significant Foreign Assignments:

| S. No. | Period of visit | Institute/ Country visited | Purpose of visit |
|--------|---------------------|--|----------------------|
| | From To | | |
| 5. | 2017 2019 | University of Düsseldorf, Germany | Visiting fellow |
| 4. | 2016 2018 | University of Hohenheim, Germany | Visiting fellow |
| 3. | Oct. 2002 Jan. 2003 | Phillips Universitat, Marburg, Germany | AvH Fellow |
| 2. | Apr. 1999 Aug. 1999 | Univ. Alabama at Birmingham, USA | Visiting Fellow |
| 1. | Jan. 1991 Dec. 1993 | Univ. Alabama at Birmingham, USA | Post Doctoral Fellow |

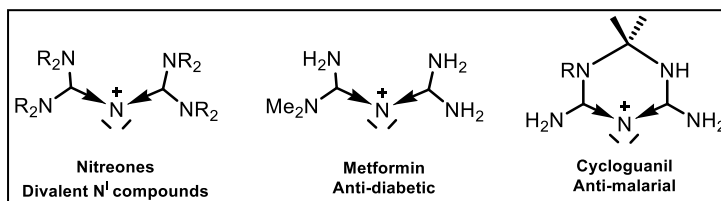
17. Scientific contributions of Prof. Prasad V. Bharatam (three-page summary)

Prof. Bharatam is a medicinal chemist with strong focus on theoretical and synthetic organic chemistry. His work involves rational methods of designing compounds and establishing the experimental proof for the concepts generated using theoretical methods. Members of his research group

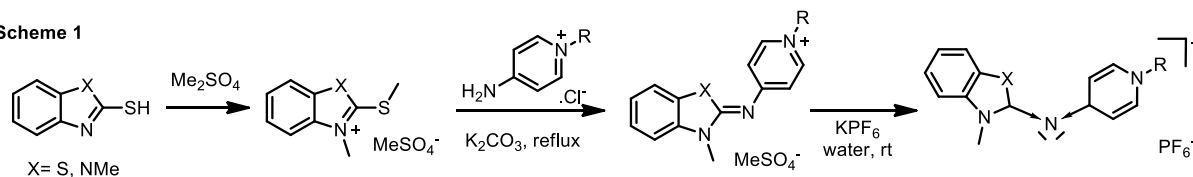
- synthesize the computationally designed species to provide proof of the concept;
- use quantum chemistry to design molecules with novel chemical bonding;
- use the CADD methods (QSAR, Molecular Docking, Mol. Dynamics, etc.) to design new entities;
- focus on the therapeutic areas -- diabetes, malarial, Leishmania and cancer.

This group identified a novel class of nitrogen species with divalent N(I) state and labelled them as nitreones. Nitreones are $::N(\leftarrow L)_2^+$ species (*Chem. Rev.* 2018, 118, 8770; *Chem. Eur. J.* 2018, 24, 6418) in which the central nitrogen (i) is found in the oxidation

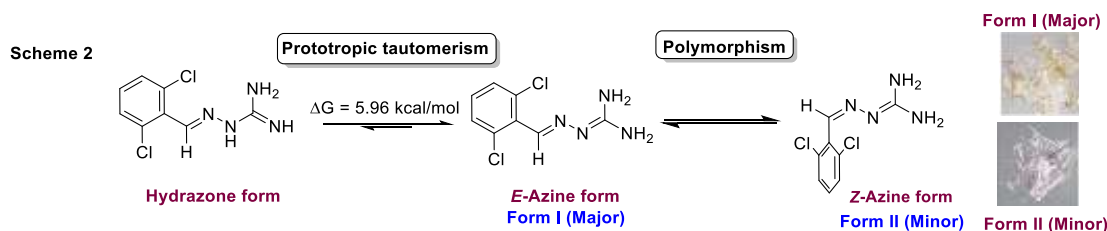
state one, (ii) carries two lone pairs of electrons, (iii) accept electron density from electron donating ligands and (iv) low nucleophilicity of nitreones makes them useful drugs. This novel environment has been identified in the blockbuster drug Metformin. Several new compounds were designed, synthesized (Scheme 1), and experimentally proven to possess this novel divalent N^I character. Many biguanide containing drugs such as Cycloguanil, Proguanil, Famotidine, Chlorhexidine, etc.) have been shown to carry nitreone type electronic features and thus play important role in biological interactions. The electronic, structural analyses and molecular electronic surface potential analysis of biguanides showed that the preferred structure is a tautomer of a generally considered structure. Hence, this study provided an opportunity for exploring the biomolecular target for metformin with renewed vision (*J. Med. Chem.* 2005, 48, 7615).



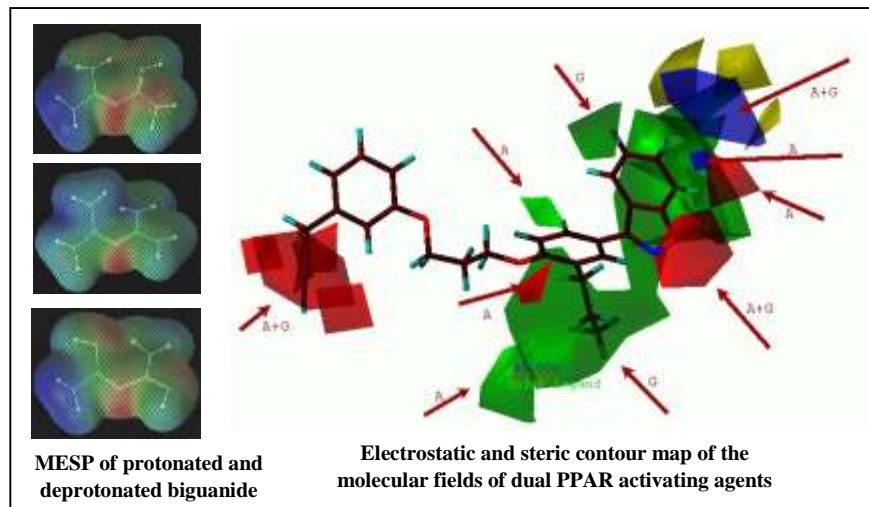
Scheme 1



In the past five years, his research group extensively explored tautomerism, in drugs and its importance in chemical and biological environments. His research group has shown Azine \rightleftharpoons hydrazone tautomersim in the antihypertensive drug Guanabenz and proved its preference to existence in azine form using theoretical and experimental methods such as variable temperature NMR and XRD (*RSC Adv.*, 2015, 5, 55938, *J. Org. Chem.*, 2016, 81, 7574). The effect of tautomerism on the chemical reactivity has been explored which suggested that the azine tautomer prefers to undergo intermolecular instead of intramolecular cyclization (*Org. Biomol. Chem.*, 2019, 17, 4129-4138). Recently, the polymorphic form of Guanabenz has been identified which may play crucial role in modulating the pharmacokinetic properties of this anti-hypertensive drug (*Cryst. Growth Des.*, 2019, 19, 3183). Currently, his research group is exploring the applications of 1,1-Diaminoazines in catalysis: organocatalysis and organometallic catalysis. This moiety acts as abifunctional organocatalyst and facilitates different types of Michael Addition reactions (*Chem. Comm.* 2021, 57, 11717; *New J. Chem.*, 2023, 47, 1998; *Tetrahedron Lett.*, 2023, 122, 154505; *ChemistrySelect.*, 2024, 9, e202405002). These azines also form a bench-stable, robust tridentate complex with different transition metals like Pd, Mn, Fe etc. The pincer complexes generated fromazines have been successfully employed in the synthesis of different heterocycles like benzimidazoles, quinolines etc (*Org. Biomol. Chem.*, 2025, 23, 343).



Prof. Bharatam's research group has also generated remarkable results in the field of medicinal chemistry of anti-malarial, anti-diabetic and antibacterial agents with the aid of *in silico* methods. Modulating the pharmacophoric features using the CoMFA has led to the design of several new chemical entities with improved therapeutic potential. To achieve this goal, the concept of 'additivity of molecular fields' was introduced (*J Med Chem.* 2005, 48, 3015). Prof. Bharatam is also involved in carrying out synthesis of theoretically designed compounds to provide proof of concept. Synthesis and radio ligand binding analysis studies provided the proof of concept as

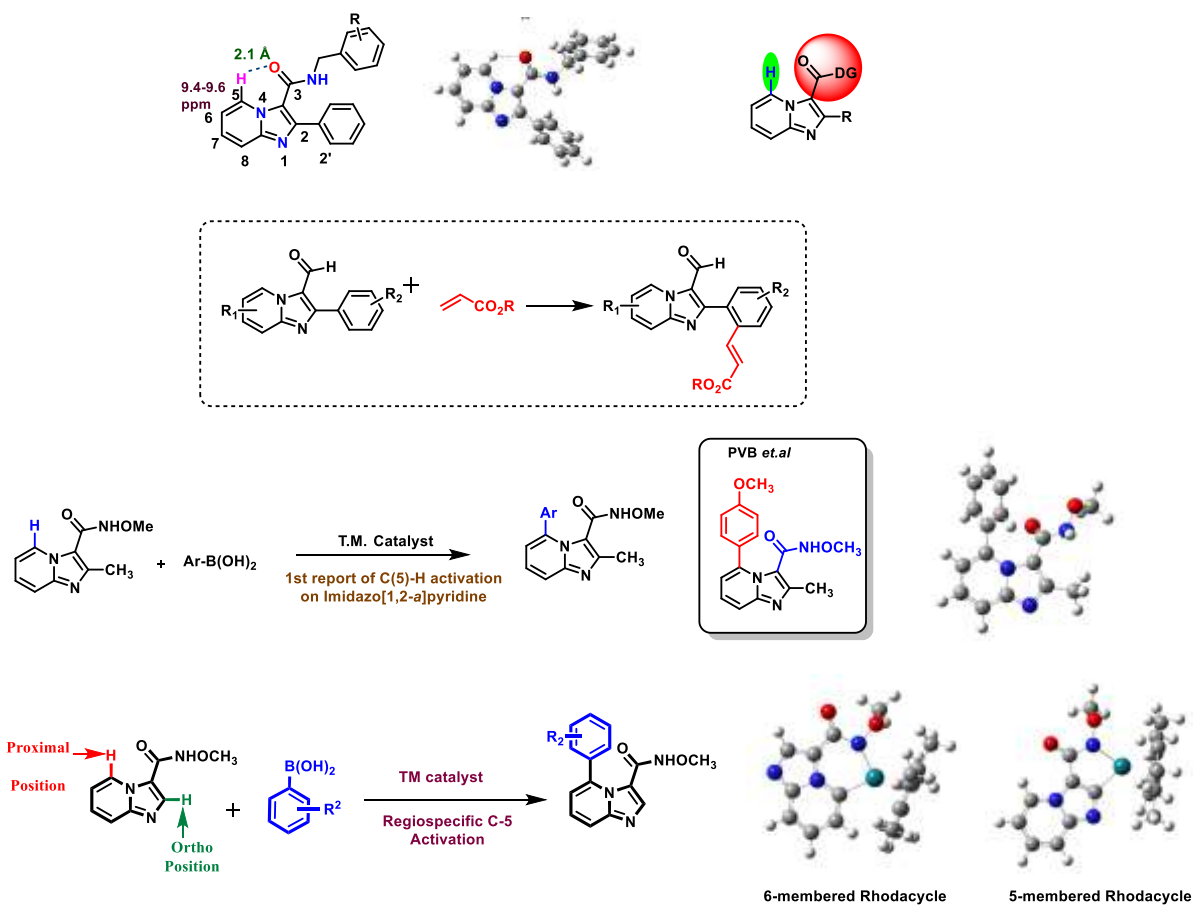


30% of the compounds showed activity, about 10% of them showing better biological activity than the existing drug. (*Bioorg. Med. Chem.* 2007, 15, 1547, *Bioorg. Med. Chem. Lett.* 2008, 15, 4959). A few of guanythiourea derivatives have shown to possess potential antimalarial activity (*in vitro*) and one of the compounds has been tested to cure malaria in mouse (*in vivo*) (*Eur. J. Med. Chem.*, 2017, 135, 339). Prof. Bharatam is also involved in rational design and synthesis of antibacterial compound for FtsZ protein inhibition. One compound of the series found active against FtsZ protein (*Eur. J. Med. Chem.*, 2024, 116196).

Prof. Bharatam's group recently identified that the peri-H in fused bicyclic aromatic ring systems, particularly in imidazo[1,2-*a*]pyridine heterocycles, exhibits unusual deshielding due to intramolecular hydrogen bonding, particularly when a proximal carbonyl-containing directing group is present (*Tetrahedron* 2020, 76, 131060-131068). This finding triggered their exploration into activating the C-5 proton of imidazo[1,2-*a*]pyridine using a proximal directing group approach.

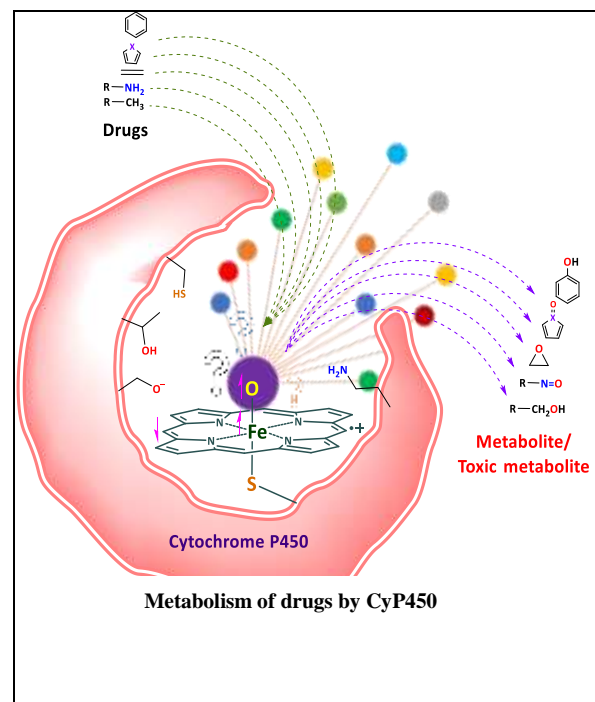
In their initial attempt with 2-phenyl-imidazo[1,2-*a*]pyridine-3-carbaldehyde, they observed activation at the C-2' position instead of the intended C-5 position. This shift was attributed to the strong coordinating nature of the N-1 center in the imidazo[1,2-*a*]pyridine ring, which was favored over the C-5 activation. (*Tetrahedron* 2022, 122, 132956).

Realizing the need to block or modify the C-2' position to prevent this side reaction, they replaced the phenyl group with a methyl group and then H. This modification enabled the desired activation regioselectively at the C-5 position of imidazo[1,2-*a*]pyridine, marking the first successful C(5)-H activation and functionalization of this heterocyclic system (*Org. Biomol. Chem.* 2024, 22(35), 7121–7127, Patent application no: 202311004031).



Apart from the above topics he also contributed in the toxicity study of drugs and pharmacophoric moieties using quantum chemical methods. These studies help in understanding of CYP450-catalyzed toxic reactions and identification of structural alerts for toxic metabolites (*Inorg. Chem.*, 2013, 52, 13496; *Chem. Res. Tox.* 2015, 28, 2364). The importance of cytochrome in the cyclization of proguanil (inactive-drug) to cycloguanil (active metabolite) was also identified by his group (*J. Comput. Chem.*, 2014, 35, 2047). The molecular dynamics approach has been used to understand the complexation of drugs with dendrimeric nanoparticles (*Soft Matt.*, 2013, 9, 6482; *Nanoscale*, 2014, 6, 2476).

Research work of Prof. Bharatam in collaborative projects in theoretical organic chemistry and organometallic chemistry also yielded significant results (*Chem. Commun.* 2003, 1420; *Inorg. Chem.* 2006, 45, 1535; *J. Am. Chem. Soc.* 2007, 129, 4506; *Angew. Chem. Int. Ed.* 2008, 47, 4703, *Chem. Commun.*, 2009, 1067; *Scientific Reports (Nature)*, 2016, 6, 20600). The bicyclic *N*-fused aminoimidazoles were identified as topoisomerase II inhibitors (using of molecular modeling studies) and proven



to be potent using *in vitro* methods (*J. Med. Chem.*, 2011, 54, 5013).

18. Fifty best publications at a glance

| <i>Authors</i> | <i>Journal</i> | <i>Year</i> | <i>Vol.</i> | <i>Pages</i> |
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| 50. A Gupta, ... P.V. Bharatam | Chem. Commun. | 2025 | 61 | 105-108 |
| 49. S. Faraz... P.V. Bharatam, A. Khan | J. Org. Chem. | 2024 | 89 | 17362-17373 |
| 48. K. Jahan ...P. V. Bharatam, D. Panda | Eur. J. Med. Chem. | 2024 | | 116196 |
| 47. P.V Bharatam | Drug Discovery Today | 2023 | 28 | 4-8 |
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| 41. D. Kathuria P.V. Bharatam | Cryst. Grow. Des. | 2019 | 19 | 3183-3191 |
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| 36. S. Chourasiya P.V. Bharatam | J. Org. Chem. | 2016 | 81 | 7574-7583 |
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| 32. K.A. Kumar...P.V. Bharatam | J. Org. Chem. | 2015 | 80 | 1746-1753 |
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| 4. K. Lammertsma BharatamV. Prasad | J. Am. Chem. Soc. | 1994 | 116 | 642-650 |
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| Original Scientific articles published (<i>foreign journals</i>) | 303 |
| Original Scientific articles published (<i>Indian journals</i>) | 19 |
| Reviews (<i>peer reviewed</i>) | 21 |
| Book Chapters | 10 |
| Patents | 03 |
| Science Education articles | 18 |
| Total | <u>374</u> |
| Citations (Google Scholar) | ~8432 |
| h-index (Google Scholar) | 48 |

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|------|--|--------------------------------------|------|------|-------------|----|
| 13. | SS Chourasiya, ...P.V. Bharatam | Org. Biomol. Chem. | 2019 | 17 | 8486-8521 | 69 |
| 14. | D.S. Patel, P.V. Bharatam | J. Phys. Chem. A | 2011 | 115 | 7645-7655 | 68 |
| 15. | A.K. Kusunuru...P.V. Bharatam | Organic Letters | 2015 | 17 | 3742-3745 | 68 |
| 16. | P.V. Bharatam, D.S. Patel. | Curr. Pharm. Design | 2007 | 13 | 3518-3530 | 68 |
| 17. | K. Lammertsma and P. V. Bharatam | J. Org. Chem. | 2000 | 65 | 4662-4670 | 66 |
| 18. | V. Jain ... P.V. Bharatam | Soft Matter | 2013 | 9 | 6482-6496 | 61 |
| 19. | D Kathuria, P.V. Bharatam | J. Mol. Struct. | 2018 | 1152 | 61-78 | 59 |
| 20. | D. Swain P.V. Bharatam, | J. Pharm. Biomed. Anal. | 2016 | 120 | 352-363 | 59 |
| 21. | AS Reddy.... P.V. Bharatam | Org. Biomol. Chem. | 2017 | 15 | 801-806 | 57 |
| 22. | S.K. Singh, N. Dessalew, P. V. Bharatam | Eur. J. Med. Chem. | 2006 | 41 | 1310-1319 | 57 |
| 23. | N Taxak, PV Bharatam | Resonance | 2014 | 19 | 259-282 | 57 |
| 24. | A Nayak, ... PV Bharatam, ... | Scientific Reports | 2016 | 6 | 1-16 | 56 |
| 25. | D Das, ...P.V. Bharatam. | DNA repair | 2014 | 24 | 15-25 | 56 |
| 26. | V. Jain, P.V. Bharatam | Nanoscale | 2014 | 6 | 2476-2501 | 56 |
| 27.. | N. Dessalew, D.S. Patel, P. V. Bharatam. | J. Mol. Graph Model. | 2007 | 25 | 885-895 | 56 |
| 28. | P. V. Bharatam, P. Uppal, ... D. Kaur, | J. Chem. Soc., Perkin Trans.2 | 2000 | | 43-50 | 56 |
| 29. | L.S. Moon, ... P.V. Bharatam | J. Org. Chem. | 2010 | 75 | 5487-5498 | 54 |
| 30. | D. Kathuria,...P.V. Bharatam ... | Eur. J. Med. Chem. | 2021 | 219 | 113378 | 53 |
| 31. | M. Arfeen, P.V. Bharatam | Eur. J. Med. Chem. | 2016 | 121 | 727-736 | 53 |
| 32. | D.S. Patel, P.V. Bharatam | J. Org. Chem. | 2011 | 76 | 2558-2567 | 53 |
| 33. | P.D. Dey, P.V. Bharatam ... | Tetrahedron | 1997 | 53 | 13829-13840 | 53 |
| 34. | N. Dessalew, P. V. Bharatam. | Eur. J. Med. Chem. | 2007 | 42 | 1014-1027 | 52 |
| 35. | P. V. Bharatam, ... D. Kaur. | J. Phys. Chem. A | 2003 | 107 | 1627-1634 | 52 |
| 35. | P. V. Bharatam, P. Iqbal, R. Tiwari | J. Phys. Chem. A | 2004 | 108 | 10509-10517 | 51 |
| 36. | N Sanghai, P.V. Bharatam | MedChemComm | 2014 | 5 | 766-782 | 51 |
| 37. | N Taxak, B Patel, PV Bharatam | Inorganic Chemistry | 2013 | 52 | 5097-5109 | 50 |
| 38. | T. Aggarwal P.V. Bharatam... | J. Org. Chem. | 2012 | 77 | 8562-8573 | 50 |
| 39. | M Arfeen, PV Bharatam | J. Biomol. Struct. Dynam. | 2015 | 33 | 2578-2593 | 49 |
| 40. | V. Kumar, PV Bharatam | J. Org. Chem. | 2014 | 79 | 3427-3439 | 49 |
| 41. | S.S. Chimni....P.V. Bharatam | Tetrahedron | 2010 | 66 | 3042-3049 | 49 |
| 42. | P. V. Bharatam, D. Kaur | Organometallics | 2002 | 21 | 3683-3690 | 48 |
| 43. | DS Patel, PV Bharatam | Chemical Communications | 2009 | | 1064-1066 | 48 |
| 44. | N. Kumar,.... P.V. Bharatam, ... | Med. Chem. Res. | 2016 | 25 | 1175-1192 | 46 |
| 45. | M Arfeen, PV Bharatam | Curr. Pharm. Design | 2013 | 19 | 4755-4775 | 46 |
| 46. | S.K. Guchhait.... P.V. Bharatam, ... | J. Org. Chem. | 2012 | 77 | 8321-8328 | 46 |
| 47. | S. Sundriyal, ...P.V. Bharatam | Bioorg. Med. Chem. Letts. | 2008 | 18 | 4959-4962 | 46 |
| 48. | S. Sharma. P.V. Bharatam, | ACS Omega | 2019 | 4 | 18520-18529 | 45 |
| 49. | S.V. Kessar,.... P.V. Bharatam, ... | Angew. Chem. Int. Ed. Engl. | 2008 | 47 | 4703-4706 | 45 |
| 50. | SS. Chourasiya,.... P.V. Bharatam, ... | J. Org. Chem. | 2016 | 81 | 7574-7583 | 44 |
| 51. | E.D. Jemmis, Bharatam V. Prasad ... | J. Phys. Chem. | 1990 | 94 | 5530-5535 | 43 |

Full details will be provided when required.

22. Organic Synthesis of computationally designed molecules



Azines

| | | | |
|---------------------|------|----|-------|
| Tetrahedron Letters | 2023 | 77 | |
| J. Org. Chem. | 2021 | 86 | 7659 |
| Chem. Commun. | 2021 | 57 | 11717 |
| Cryst. Growth Des. | 2019 | 19 | 3183 |
| Org. Biomol. Chem. | 2019 | 17 | 4129 |
| Tetrahedron | 2018 | 74 | 2857 |
| J. Org. Chem. | 2016 | 81 | 7574 |
| RSC Advances | 2015 | 5 | 80027 |

Divalent N(I) compounds

| | | | |
|---------------------------|------|-----|--------|
| Chem Select | 2023 | 7 | 3613 |
| J. Comput. Chem. | 2022 | 44 | 346 |
| Int. J. Quantum Chem. | 2022 | 122 | e26907 |
| Phys. Chem. Chem. Phys. | 2021 | 24 | 629 |
| Chem. Eur. J. | 2018 | 24 | 6418 |
| Eur. J. Med. Chem. | 2017 | 135 | 339 |
| Chem. Eur. J. | 2016 | 22 | 1088 |
| Bioorg. Med. Chem. Letts. | 2014 | 24 | 613 |
| Med. Chem. Res. | 2015 | 24 | 1974 |

Heterocycles

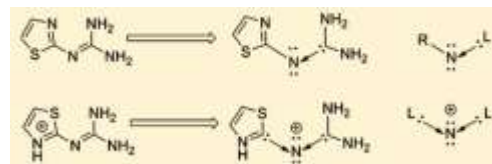
| | | | |
|--------------------|------|-----|----------|
| Tetrahedron | 2022 | 122 | 132965 |
| Chem Select | 2023 | 8 | 4845 |
| New J. Chem. | 2021 | | accepted |
| Tetrahedron | 2020 | 76 | 131060 |
| Tetrahedron | 2020 | 76 | 131482 |
| Eur. J. Org. Chem. | 2019 | 34 | 5887 |
| Tetrahedron | 2019 | 75 | 130536 |
| Org. Biomol. Chem. | 2019 | 17 | 4129 |

| | | | |
|----------------------------------|-------------|------------|-------------|
| New J. Chem. | 2019 | 43 | 4013 |
| Eur. J. Med. Chem. | 2016 | 121 | 727 |
| Eur. J. Med. Chem. | 2016 | 108 | 423 |
| Bioorg. Med. Chem. Letts. | 2008 | 18 | 959 |
| Bioorg. Med. Chem. Letts. | 2008 | 18 | 3192 |
| Sulfonamides | | | |
| Tetrahedron | 2018 | 74 | 3634 |
| New J. Chem. | 2017 | 41 | 8118 |

23. Contributions in Theoretical Organic Chemistry

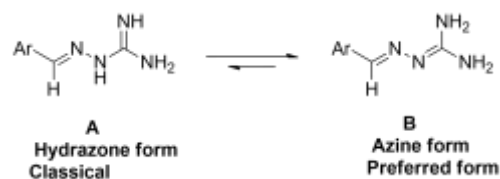
Chemical bonding

| | | | |
|------------------|------|----------|------|
| J. Mol. Mod. | 2023 | accepted | |
| J. Comput. Chem. | 2020 | 41 | 2624 |
| J. Comput. Chem. | 2019 | 40 | 2207 |
| Chem. Rev. | 2018 | 118 | 8770 |
| Chem. Eur. J. | 2018 | 246418 | |
| Chem. Eur. J. | 2016 | 221088 | |
| J. Org. Chem. | 2014 | 79 | 4852 |
| J. Phys. Chem. A | 2012 | 116 | 9071 |
| J. Phys. Chem. A | 2011 | 115 | 7645 |
| J. Org. Chem. | 2011 | 76 | 2558 |
| Chem. Commun. | 2009 | | 1064 |
| J. Med. Chem. | 2005 | 48 | 7615 |



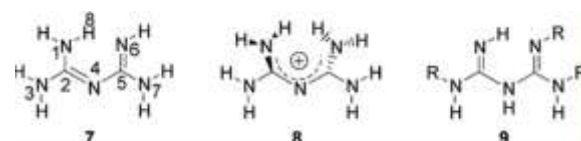
Tautomerism / Isomerism

| | | | |
|-------------------|------|-----|------|
| Cryst Growth Des. | 2019 | 19 | 3183 |
| J. Org. Chem. | 2016 | 81 | 7574 |
| J. Comput. Chem. | 2013 | 34 | 1577 |
| J. Org. Chem. | 2000 | 65 | 4622 |
| J. Am. Chem. Soc. | 1994 | 116 | 642 |
| J. Am. Chem. Soc. | 1993 | 115 | 2348 |



Electron delocalization / resonance

| | | | |
|--------------------|------|------|-------|
| Eur. J. Org. Chem. | 2019 | 2019 | 2481 |
| J. Org. Chem. | 2014 | 79 | 4852 |
| J. Comput. Chem. | 2010 | 31 | 1259 |
| J. Comput. Chem | 2006 | 27 | 334 |
| J. Phys. Chem. A | 2004 | 108 | 10509 |
| J. Phys. Chem. A | 2003 | 107 | 1627 |
| J. Org. Chem. | 2000 | 65 | 4622 |
| Chem. Phys. Lett. | 1997 | 276 | 31 |



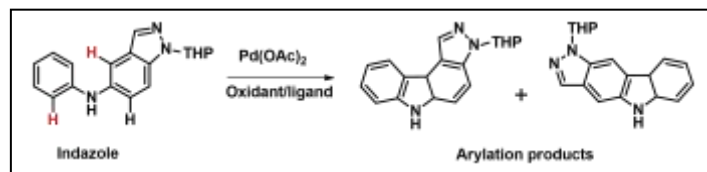
C-H bond activation

| | | | |
|--------------------|------|-----|--------|
| Tetrahedron | 2022 | 122 | 132965 |
| J. Org. Chem. | 2020 | 85 | 4951 |
| Adv. Synth. Cat. | 2018 | 360 | 1876 |
| J. Org. Chem. | 2017 | 82 | 7234 |
| J. Org. Chem. | 2017 | 82 | 10077 |
| Org. Letts. | 2015 | 17 | 3742 |
| Org. Biomol. Chem. | 2015 | 13 | 5235 |
| J. Org. Chem. | 2015 | 80 | 1746 |
| Chem. Commun. | 2014 | | 12076 |
| J. Org. Chem. | 2012 | 77 | 8321 |



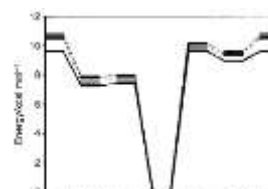
Reaction Mechanisms

| | | | |
|-----------------------|------|-----|-------|
| ACS Omega | 2019 | 4 | 18520 |
| ACS Omega | 2019 | 4 | 4604 |
| J. Org. Chem | 2018 | 83 | 9667 |
| J. Org. Chem. | 2016 | 81 | 5120 |
| Chem. Commun. | 2016 | 52 | 1009 |
| J. Phys. Chem. B | 2014 | 118 | 9199 |
| J. Org. Chem. | 2014 | 79 | 3427 |
| J. Org. Chem. | 2012 | 77 | 8562 |
| J. Org. Chem. | 2011 | 76 | 5999 |
| J. Org. Chem. | 2010 | 75 | 5487 |
| Chem. Commun. | 2009 | | 1067 |
| Angew. Chem. Int. Ed. | 2008 | 47 | 4703 |
| J. Am. Chem. Soc. | 2007 | 129 | 4506 |
| J. Phys. Chem. A | 2004 | 108 | 784 |
| Chem. Commun. | 2003 | | 1420 |
| Org. Letters | 2000 | 2 | 2725 |



Conformational analysis

| | | | |
|------------------------------|------|-----|------|
| Int. J. Quant. Chem. | 2016 | 116 | 1362 |
| J. Phys. Chem. A | 2014 | 118 | 187 |
| Tet. Lett. | 2002 | 43 | 8289 |
| J. Chem. Soc., Perkin Trans. | 2000 | | 2469 |
| J. Chem. Soc., Perkin Trans. | 2000 | | 43 |



24. Contributions in Medicinal Chemistry

Anti-diabetic agent design and synthesis

| | | | |
|---------------------------|------|-----|------|
| Eur. J. Med. Chem. | 2016 | 121 | 727 |
| Eur. J. Med. Chem. | 2016 | 108 | 423 |
| J. Biomol. Struct. Dyn. | 2015 | 33 | 2578 |
| Eur. J. Med. Chem. | 2009 | 44 | 3488 |
| Eur. J. Med. Chem. | 2009 | 44 | 42 |
| Bioorg. Med. Chem. Letts. | 2008 | 18 | 4959 |
| Eur. J. Med. Chem. | 2008 | 43 | 2784 |
| Eur. J. Med. Chem. | 2008 | 43 | 949 |
| Bioorg. Med. Chem. | 2007 | 15 | 3728 |
| Eur. J. Med. Chem. | 2007 | 42 | 1014 |
| Bioorg. Med. Chem. | 2007 | 15 | 1547 |
| J. Med. Chem. | 2005 | 48 | 7615 |
| J. Med. Chem. | 2005 | 48 | 3015 |
| Bioorg. Med. Chem. | 2005 | 13 | 2331 |
| Bioorg. Med. Chem. | 2004 | 12 | 2709 |

Anti-malarial agent design and

| | | | |
|---------------------------|------|-----|------|
| J. Mol. Gra. Mod | 2019 | 87 | 76 |
| Int. J. Quantum Chemistry | 2016 | 116 | 1362 |
| Eur. J. Med. Chem. | 2017 | 135 | 339 |
| J. Biomol. Struct. Dyn. | 2015 | 33 | 1913 |
| J. Compt. Chem. | 2014 | 35 | 2047 |
| Bioorg. Med. Chem. Letts. | 2014 | 24 | 613 |
| J. Mol. Mod. | 2011 | 17 | 657 |
| J. Enzy. Inhib Med. Chem. | 2010 | 25 | 635 |
| Chem. Biol. Drug Design | 2010 | 75 | 15 |
| J. Mol. Graph. Mod. | 2009 | 28 | 357 |
| Curr. Med. Chem. | 2008 | 15 | 1522 |



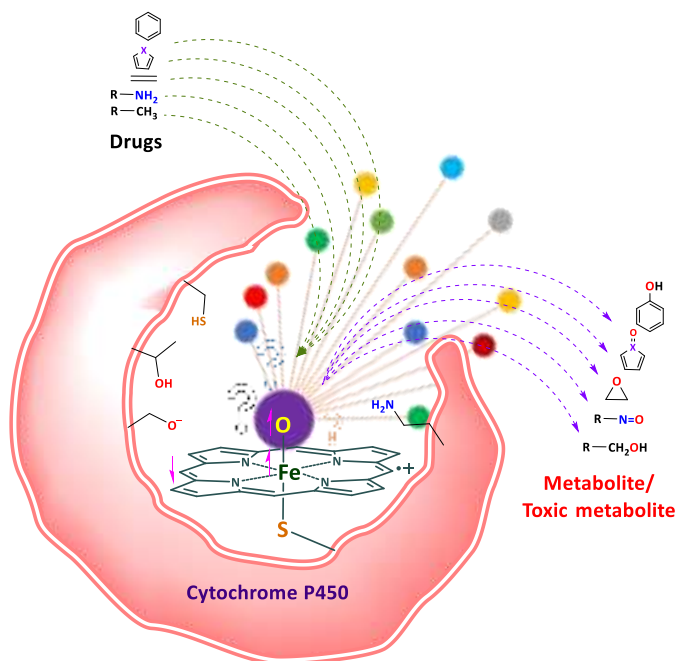
Anti-cancer agent design and synthesis

| | | | |
|----------------------|------|----|-------|
| Apoptosis | 2017 | 22 | 1205 |
| Oncotarget | 2017 | | 8248 |
| Scientific Reports | 2016 | 6 | 20600 |
| ACS Med. Chem. Lett. | 2015 | 6 | 481 |
| DNA Repair | 2014 | 24 | 15 |
| Anticancer Drugs | 2014 | 25 | 704 |
| Med. Chem. Comm. | 2014 | 5 | 766 |
| ChemMedChem. | 2013 | 8 | 1873 |
| MedChemComm | 2013 | 4 | 1257 |
| J. Med. Chem. | 2011 | 54 | 5013 |
| Eur. J. Med. Chem. | 2006 | 41 | 1310 |

Other therapeutic areas

| | | | |
|--------------------------|------|----|----------|
| ACS Chem. Neuro. | 2020 | 11 | 2303 |
| J. Mol. Gra. Mod. | 2019 | 86 | |
| App. Biochem. Biotech. | 2017 | | 1-21 |
| J Biomol. Struct. Dyn. | 2016 | 34 | 1-14 |
| PLOS one | 2016 | 11 | e0150764 |
| Scientific Reports | 2017 | 7 | 40097 |
| J. Biomol. Struct. Dyn. | 2015 | 33 | 1082 |
| RSC Advances | 2015 | 5 | 80027 |
| ACS Med. Chem. Letts. | 2015 | 6 | 1065 |
| Med. Chem. Res. | 2013 | 23 | 1819 |
| Medicinal Chemistry Res. | 2013 | 21 | 5654 |
| Eur. J. Med. Chem. | 2012 | 52 | 82 |

25. Contributions in Pharmaceutical Sciences



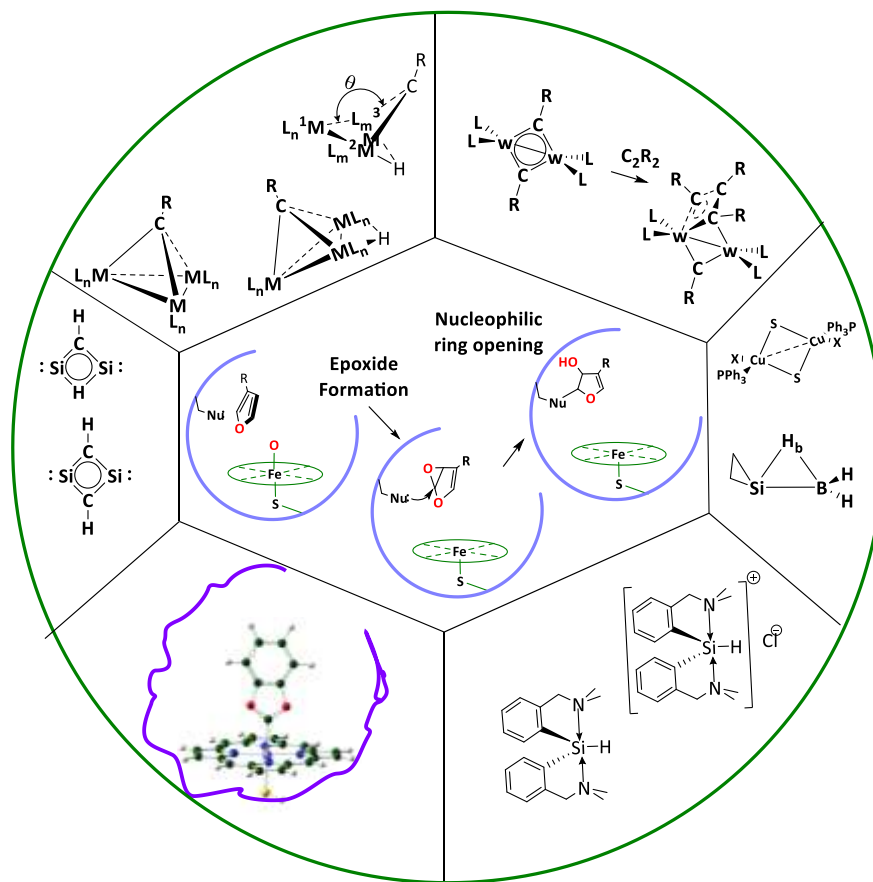
Drug Metabolism and Toxicity

| | | | |
|-------------------------|------|-----|-------|
| Drug Metabolism Reviews | 2020 | 52 | 366 |
| Drug Metabolism Letters | 2019 | 13 | 64 |
| J. Anal. Chem. | 2018 | 73 | 560 |
| Chem. Res. Tox. | 2017 | 30 | 2060 |
| Chem. Res. Tox. | 2015 | 28 | 2364 |
| J. Comput. Chem. | 2014 | 35 | 2047 |
| Eur. J. Med. Chem. | 2014 | 71 | 15 |
| Inorg. Chem. | 2013 | 52 | 13496 |
| Inorg. Chem. | 2013 | 52 | 5097 |
| Drug Metabolism Letters | 2013 | 6 | 221 |
| J. Phys. Chem. A | 2012 | 116 | 10441 |
| J. Comp. Chem. | 2012 | 33 | 1740 |
| J. Mol. Mod. | 2012 | 18 | 709 |
| J. Phys. Chem. A | 2011 | 115 | 891 |
| Chem. Res. Tox. | 2011 | 24 | 1113 |
| Theochem | 2010 | 962 | 97 |
| J. Phys. Chem. A | 2004 | 108 | 3784 |

Drug delivery & Pharm. Anal.

| | | | |
|--------------------------|------|-----|---------|
| J. Pharm. Sci. | 2020 | 109 | 1883 |
| J. Pharm. Biomed. Anal. | 2020 | 177 | 112881 |
| Eur. J. Pharm. Biopharm. | 2019 | 142 | 165 |
| Mol. Pharm. | 2019 | 16 | 2980 |
| Cryst. Growth Des. | 2019 | 19 | 3183 |
| J. Pharm. Biomed. Anal. | 2017 | 11 | 1600156 |
| J. Pharm. Biomed. Anal. | 2017 | 145 | 209 |
| J. Pharm. Biomed. Anal. | 2017 | 136 | 66 |
| J. Chem. Phys. | 2016 | 145 | 124902 |
| Nanoscale | 2014 | 6 | 2476 |
| Soft Matter | 2013 | 9 | 6492 |
| Structural Chem. | 2012 | 23 | 1857 |
| J. Phys. Org. Chem. | 2012 | 25 | 649 |
| J. Nanosci. Nanotechnol. | 2006 | 6 | 3277 |

26. Contributions in theoretical Inorganic Chemistry



Bioinorganic Catalysis

| | | | |
|----------------------|------|-----|-------|
| Chem. Res. Tox. | 2017 | 30 | 2060 |
| Chem. Res. Tox. | 2016 | 28 | 2364 |
| J. Bio. Inorg. Chem. | 2015 | 142 | 84 |
| Inorg. Chem. | 2013 | 52 | 13496 |
| Inorg. Chem. | 2013 | 52 | 5097 |

Organometallic chemistry

| | | | |
|------------------------------|------|-----|------|
| Inorg. Chem. | 2006 | 45 | 1535 |
| Inorg. Chem. | 2003 | 42 | 4743 |
| Organometallics | 2002 | 21 | 3683 |
| Inorg. Chem. | 1994 | 33 | 2046 |
| Chem. Phys. Lett. | 1994 | 217 | 296 |
| Organometallics | 1993 | 12 | 4267 |
| Angew. Chem., Int. Ed. Engl. | 1993 | 32 | 865 |
| Organometallics | 1991 | 10 | 3613 |
| Organometallics | 1992 | 11 | 2528 |
| J. Phys. Chem. | 1990 | 94 | 5530 |
| Inorg. Chim. Acta | 1989 | 162 | 281 |
| Polyhedron | 1988 | 7 | 871 |
| J. Organomet. Chem. | 1988 | 347 | 401 |
| J. Am. Chem. Soc. | 1987 | 109 | 2560 |

27. Computer programming and Pharmacoinformatics tool development

Drug likeness



http://www.niper.gov.in/pi_dev_tools/DruLiToWeb/DruLiTo_index.html

Dendrimer builder

<http://www.physics.iisc.ernet.in/~maiti/dbt/home.html>

BiAnaca

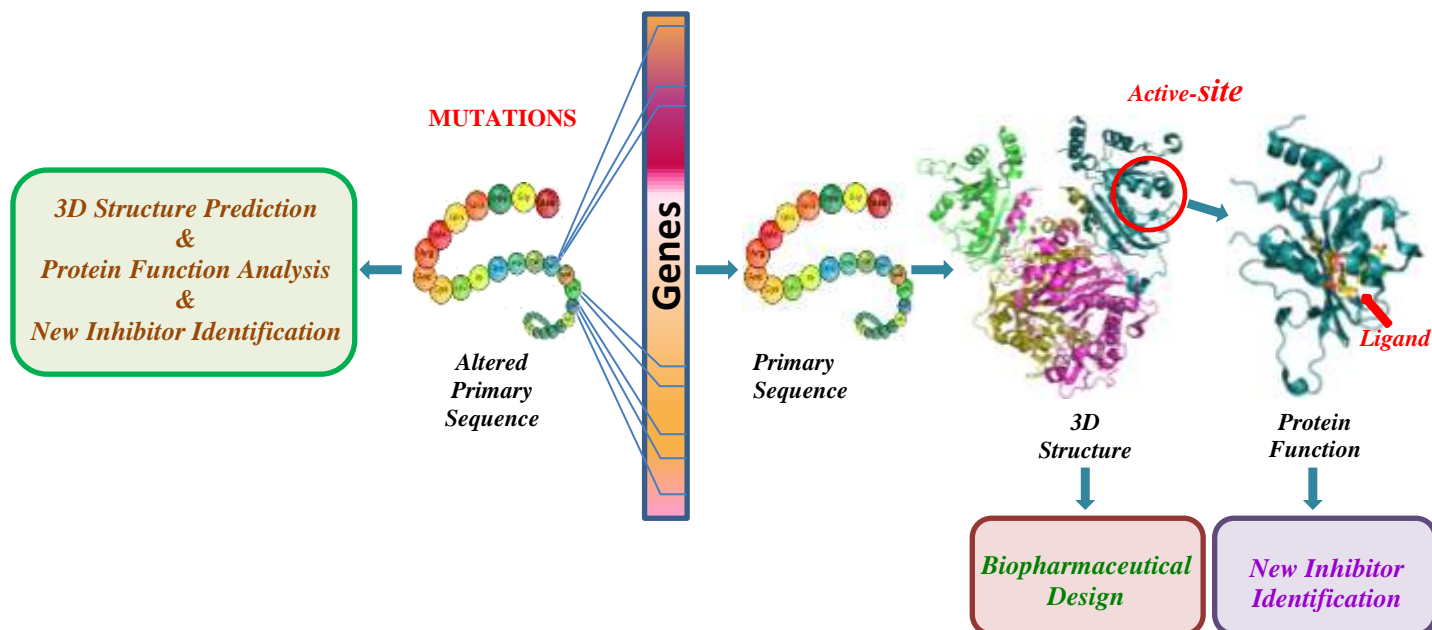


http://www.niper.ac.in/pi_dev_tools/BiAnaCA/ABOUT.html

Descriptor calculations

| | | | |
|--|-------------|----|----------|
| Mol. Info. | 2019 | 88 | 1800046 |
| J. Chem. Sci. | 2017 | | in print |
| Int. J. Chem. Mod. | 2016 | | |
| InternetEle. J. Mol. Design | 2015 | | |
| Lett. Drug Design Disc. | 2015 | 11 | 844 |
| ACS Comb. Sci. | 2014 | 16 | 101 |
| Int. J. Comput. Biol. Drug Des. | 2014 | 7 | 295 |
| Int. J. Comp. Biol. Drug Des. | 2012 | 5 | 335 |
| J. Comp. Chem. | 2012 | 33 | 1997 |

28. Contributions in Computational Biology



Macromolecular structure and function prediction

| | | | |
|------------------------------|------|-----|-----------|
| J. Biomol. Struct. Dyn. | 2020 | | in print. |
| ACS chemical neuroscience | 2020 | 11 | 2303 |
| Int. J. Biol. Macromol. | 2020 | 146 | 860 |
| Int. J. Biochem. Cell Biol. | 2020 | | 105682 |
| J. Mol. Gra. Mod. | 2019 | 87 | 76 |
| J. Mol. Gra. Mod. | 2019 | 86 | 1-18 |
| Mol. Inform. | 2019 | 38 | 1800046 |
| FEBS J | 2018 | 285 | 1791 |
| Applied Biochem. Biotech. | 2017 | | 1 |
| J. Biomol. Struct. Dyn. | 2016 | 34 | 1 |
| J. Biomol. Struct. Dyn. | 2015 | 33 | 1082 |
| J. Biomol. Struct. Dyn. | 2015 | 33 | 2578 |
| Appl. Biochem. Biotech. | 2013 | 171 | 417 |
| Curr. Protein & Peptide Sci. | 2007 | 8 | 352 |
| Enzyme and Microbial Tech. | 2005 | 36 | 232 |

Biopharmaceutical design

| | | | |
|---------------------------|------|----|----------|
| Apoptosis | 2017 | 22 | 1205 |
| Oncotarget | 2017 | 8 | 248 |
| PLOS One | 2016 | 11 | e0150764 |
| Science Reporter (Nature) | 2017 | 7 | 40097 |
| Science Reporter (Nature) | 2016 | 6 | 20600 |

