

Prof. Prasad V. Bharatam

Department of Medicinal Chemistry
National Institute of Pharmaceutical Education and Research
NIPER, Sector-67, S.A.S. Nagar (Mohali)– 160 062, Punjab, India
Ph. +91-172-2292018
Fax. +91-172-2214692
e-mail: pybharatam@niper.ac.in
website: www.niper.gov.in/pybharatam.pdf



1. Fields of Specialization

Medicinal Chemistry
Organic Synthesis
Quantum Medicinal Chemistry
Pharmacoinformatics
Divalent N(I) compounds

2. Honors and Awards:

Fellowship of Andhra Pradesh Akademi 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	2005-current
Medicinal chemistry of anti-malarial agents – Design and Synthesis	2005-current
Medicinal chemistry of anti-diabetic agents -- Design and Synthesis	2001-current
Tautomerism in high-energy material	1991-current
Carbyne, carbenes, carbones and related reactive intermediates	1985-current

4. Teaching Experience

:	NIPER, Mohali	15 years --	Medicinal Chemistry Bio-inorganic chemistry Chemoinformatics Pharmacoinformatics
	G.N.D. Univ.	7.5 years – integrated M.Sc. (5 yr. course)	Quantum chemistry Physical Chemistry Computational Chemistry

5. Administrative experience:

Dean, NIPER, SAS Nagar	-- 2016-2019
Associate Dean, NIPER, SAS Nagar	-- 2015-2016
Incharge, Departement of Pharmacoinformatics, NIPER, SAS Nagar	-- 2010-continuing
Member, Computer Centre Committee, NIPER, SAS Nagar	-- 2010-continuing

6. Publication record:	Original Scientific articles published (foreign journals)	185
	Original Scientific articles published (Indian Journals)	16
	Reviews (peer reviewed)	9
	Book Chapters (peer reviewed)	4
	Science Education articles	<u>13</u>
	Total	<u>227</u>
	Citations	~2650
	h-index	26

7. Positions held:

<i>S. No.</i>	<i>Period</i>	<i>Place of Employment</i>	<i>Designation</i>	<i>Scale of Pay</i>
4.	June 2006 – continuing	N.I.P.E.R.	Professor	Rs. 55360-10500
3.	June 2001 – June 2006	N.I.P.E.R.	Assoc. Prof.	Rs. 16400-450-20900
2.	Aug. 2000 – June 2001	G.N.D. University, Amritsar	Reader	Rs. 12000-250-16000
1.	Dec. 1993 – Aug. 2000	G.N.D. University, Amritsar	Lecturer	Rs. 2200-75-3000

9. National / International Assignments:

- (a) Member of DST Organic Chemistry PAC -- 2015-2018
- (b) Member DST fast track project evaluation committee -- 2012-2015
- (c) Member selection committee, Central Univ. Punjab -- 2015
- (d) Member committee on syllabus framing, Central Univ. Punjab -- 2013-2014
- (e) Subject Expert – Board of control, Biotechnology, GNDU, Amritsar -- 2007-2009
- (f) Subject Expert – Board of Research, Sciences, GNDU, Amritsar -- 2008-2011
- (g) Council Member, Chemical Research Society of India -- 2008-2010
- (h) A reviewer in many journals including,

Indian J. Chem.;	J. Med. Chem.;
J. Phys. Chem.;	Inorg. Chem.;
Chemistry, A European Journal;	Bioorg. Med. Chem. etc.
- (i) Evaluator of project proposals submitted to CSIR, DST, DBT, UGC, New Delhi.
- (j) Invited to the Gordon Research Conference on Computer Aided Drug Design in July 2005, Tilton School, Tilton, NH, USA.
- (k) Invited to the Keystone conference on Computer Aided Drug Design in April 2008, USA
- (l) Invited for Plenary lecture at Medicinal Chemistry Intl. conf. Aug. 2009, Bandung, Indonesia.
- (m) Invited for the Gordon Research Conference on Drug Metabolism, August 2013, USA.
- (n) Member : American Chemical Society
- (o) Member : Royal Chemical Society
- (p) Member : National Academy Sciences, Allahabad

9. Editorial Experience :

- (a) Editor, CRIPS, published by NIPER -- 2012- onwards
- (b) Guest editor Theo. Chem. Accounts -- Jan. 2012
- (c) Guest editor for Indian J. Chem. Section A. -- Jan. 2006
- (d) Edited a book on “Prof. E.D. Jemmis”, Springer, -- 2012
- (e) Member Editorial Advisory Board – Indian Journal of Chemistry A. 2008-2010
- (f) Member Editorial Advisory Board – Current Comput Aided Drug Design 2007-2009

10. Research Supervision:

A. Ph.D.	– 20 completed; 11 on going.
B. M.Sc. Research Projects	– 16 completed
C. M.S. Pharm (Med. Chem.) research projects	– 120 completed, 12 on going.
D. Research Fellows (Non-Ph.D.)	– 11 completed
E. Long term visiting fellows	-- 11
F. Short term visiting Fellows / students	– 44

Ph.D. Students :

Name	Current position
1. R. Senthil Kumar	Owns a company
2. Amita Mahajan	Assoc. Prof. Eng. College, Gurdaspur, Punjab
3. Rajnish Moudgil	Assoc. Prof., Hoshiarpur, Punjab
4. Punita Sharma	Asst. Prof., ILS University, Jaipur
5. Smriti Khanna	Sr. Scientist, Nicholas Piramal, Mumbai
6. P. Senthil Kumar	Sr. Scientist, Orchids Research Laboratories, Chennai
7. Sandeep Sundriyal	Post doctoral fellow, Univ. of Oklahoma, USA
8. Amit Mittal	Asst. Prof., Lovely Professional Univ., Jalandhar
9. Adane Leggesse	Assoc. Prof. Jimma University, Southwestern Ethiopia
10. Dhilon Patel	Post Doc., Univ. Maryland, USA
11. Y. Kasetti	Scientist,
12. Vaibhav A. Dixit	Assoc. Prof., NMIMS, Shirpur, Maharashtra
13. Ramesh M.	Post Doc, South Africa
14. Devendra Dhaked	Research Associate, University of Hyderabad
15. Nikhil Taxak	e-Value serve, Gurgoan
16. Vaibhav Jain	Advinous Therapeutics, Pune
17. Rajendra Kumar	Post doc, France
18. Sonam Bhatia	Asst. Prof., LPU, Jalandhar
19. Minhazul Arfeen	Research Associate, NIPER
20. Sheenu Abbat	Thesis submitted
21. Neha Trivedi	continuing 5 th year
22. C.K. Jaladanki	continuing 5 th year
23. S.S. Chourasia	continuing 4 th year
24. Neha Patel	continuing 4 th year
25. Shweta Bhagat	continuing 3 rd year
26. Deepika Kathuria	continuing 3 rd year
27. Vishnu K. Sharma	continuing 3 rd year
28. Tejinder Singh	continuing 2 nd year
29. Firdos A. Soofi	continuing 2 nd year
30. P. Wanjari	continuing 1 st year
31. Gurudutt Dubey	continuing 1 st year

Other significant members :

30. D. Kaur	Professor, Dept. Chem., G.N.D.U.
31. Poonam Uppal	Principal, Sr. Sec. School, Amritsar
32. Alka Marwaha	Asst. Prof., Lovly Prof. Univ., Jalandhar
33. M.E. Sophia	Asst. Prof., NIPER, Mohali
34. Pansy Iqbal	Scientist, Gaussian Inc.
35. S.K. Singh	Assoc. Prof., Alagappa University
36. Mymoona Akhtar	Assoc. Prof., Jamia Hamdard
37. Prakash C. Rath	Astra Zeneca, UK
38. Jagmohan Saini	Lupin Pharma, Pune
39. Harish Jangra	Ph.D. student, Germany
40. Subhash Agarwal	Scientist, ICMR-Inst. of Cytology and Preventive Oncology, Noida
41. Sourav Kalra	JRF, IMTECH
42. Venkata Krishnan	Ph.D. student France
43. Pritika Gupta	Ph.D. student NIPER

11. Project supervision

as Principal Investigator

1. UGC Interdisciplinary grant :	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/-	2005-2008
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

as a co-Principal Investigator

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 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, - Guru Nanak Dev University. 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, IIIM, Jammu
- (l) Dr. S. Bharate, IIIM, Jammu
- (m) Prof. A.K. Madan, MDU, Rohtak
- (n) Prof. K.R.P. Kartha, NIPER, SAS Nagar
- (o) Dr. D. Mukherjee, IIIM, Jammu

15. References

- | | |
|--|---|
| 1. Prof. E.D. Jemmis
Director, IISER
Transit Campus, CET
Thiruvananthapuram 695 016
e-mail : jemmis@ipc.iisc.ernet.in | 2. Prof. N. Sathyamurthy
Director, IISER
Sector 81
Mohali - 160 026
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:
(August 1990)

**Electronic Structure and Reactivity of
Carbyne Bridged Bimetallic Complexes**
(Supervisor : Prof. E.D. Jemmis, University of Hyderabad)

Significant Foreign Assignments:

S. No.	Period of visit		Institute/ Country visited	Purpose of visit
	From	To		
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

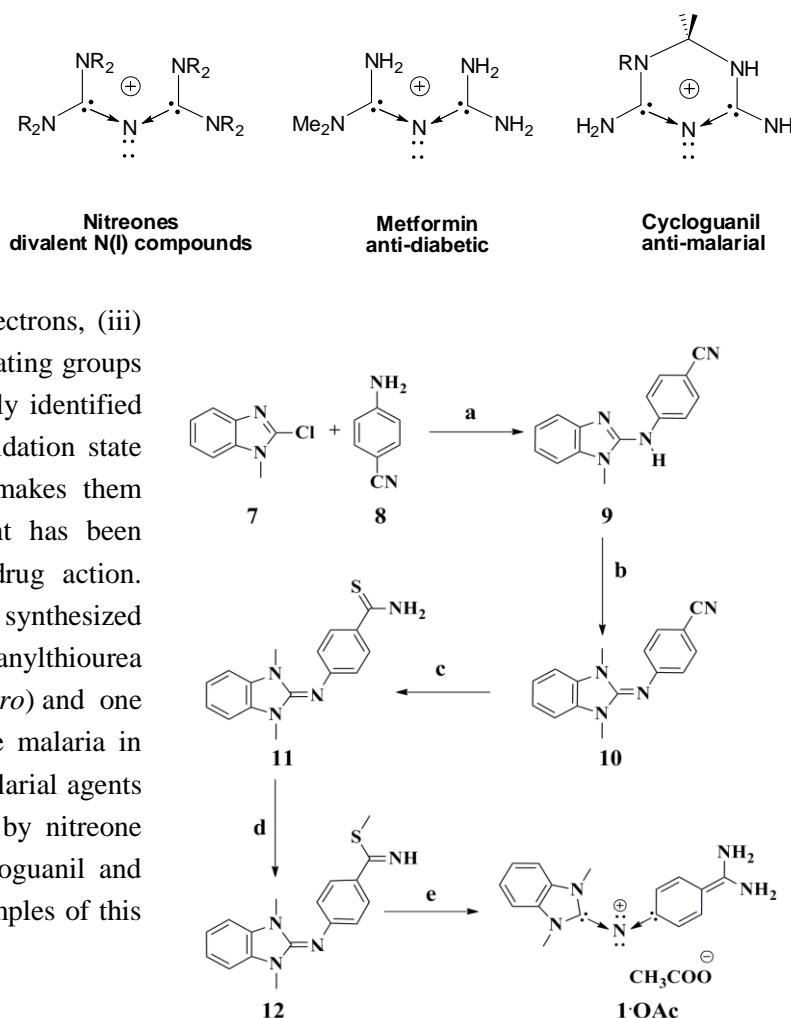
17. Two-page summary of the work done in India during last 10 years.

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

- (i) use quantum chemistry to design molecules with novel chemical bonding
- (ii) use the CADD methods (QSAR, Mol. Dock., mol. Dynamics, etc.) to design new entities
- (iii) synthesize the computationally designed species to provide proof of the concept
- (iv) synthesize and biologically evaluate anti-diabetic potential of species
- (v) synthesize and biologically evaluate anti-malarial potential of species
- (vi) synthesize and biologically evaluate anti-leishmanial potential of the species

This group recently identified a novel class of nitrogen species with divalent N(I) state and labelled them as nitreones. Nitreones are $::N(\leftarrow L)_2^{\oplus}$ species (*Chem. Eur. J.* 2016, 22, 1088; *J. Org. Chem.* 2014, 79, 4852; *J. Phys. Chem.* 2011, 115, 7645; *Chem. Comm.* 2009, 1064) in which the central nitrogen (i) is found in the low oxidation state N(I), (ii) carries two lone pairs of electrons, (iii) forms coordination bonds with electron donating groups like carbenes (iv) isoelectronic to the newly identified carbenes, carbon compounds with C(0) oxidation state and (v) low nucleophilicity of nitreones makes them useful as drugs. This novel environment has been identified, analyzed to understand their drug action. Several new compounds were designed and synthesized (Scheme 1). A few of the synthesized guanylthiourea derivatives show anti-malarial activity (*in vitro*) and one of the compounds has been shown to cure malaria in mouse (*in vivo*). Anti-diabetic and anti-malarial agents with biguanidine moiety are characterized by nitreone type electronic structure. Metformin, cycloguanil and other related therapeutic agents are the examples of this class of compounds.

Compounds with biguanidine structure are effective drugs (metformin for anti-diabetic activity, pyrimethamine for anti-malarial activity). Electronic structure analysis and molecular electronic surface



Scheme 1. Reagents and conditions, (% Yield). (a) p-TsOH, i-PrOH, reflux, 5 h (80%), (b) CH₃I, TEA, acetone, 42 °C 12 h (60%), (c) P₄S₁₀, ethanol, rt, 10 h (65%), (d) CH₃I, reflux, 1 h (reaction mixture was directly used in the next step), (e) NH₄OAc, MeOH, reflux, 1.5 h (74%). (see supporting information for the chemical characterization data and details).

potential analysis (MESP, Fig. 1) 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. The protonated and deprotonated states of the systems have been shown to be possessing similar electrostatic surfaces. Further, metformin has been shown to possess, bent allenic character and is isoelectronic to carbodiarbenes. (*J. Med. Chem.* 2005, 48, 7615; *J. Org. Chem.* 2011, 76, 2558).

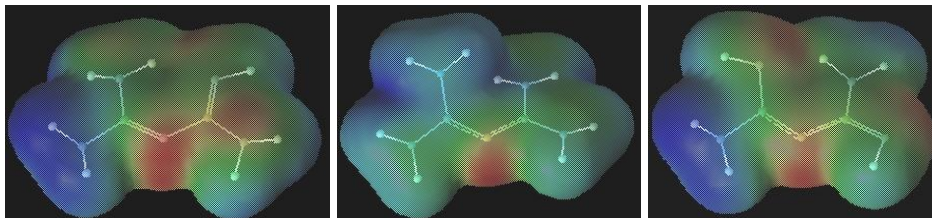


Fig. 1. MESP of biguanide, protonated biguanide and deprotonated biguanide.

Glitazones produce their insulin sensitivity by acting on the biological target PPAR γ (Peroxisome Proliferator Activating Receptors). 3D QSAR (Quantitative Structure Activity Relationships) studies performed on the PPAR γ agonists like glitazones, tyrosine derivatives have provided clues for the pharmacophoric properties of this series of compounds. Modulating the pharmacophoric features using the Comparative Molecular Field Analysis (CoMFA) has lead to the design of several new chemical entities with improved therapeutic potential in terms of their predicted IC₅₀ values. This further lead to the work on identifying the pharmacophoric features related to the dual PPAR γ and PPAR α activity to achieve the synergistic effect of anti-hyperglycemia and anti-triglyceridemia. To achieve this goal, a concept of ‘additivity of molecular fields’ was introduced. The steric and electrostatic contour maps (Fig. 2) of the three models have been employed to design new leads with improved therapeutic potential in both PPAR γ and PPAR α . The newly designed molecules have been validated to be effective compounds by estimating the binding affinity of these systems with the help of molecular docking analysis. The nominee 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. (*J. Med. Chem.* 2005, 48, 3015; *Bioorg. Med. Chem.* 2007, 15, 1547, *Bioorg. Med. Chem. Lett.* 2008, 15, 4959). Research work of the 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. IEE*, 2008, 47, 4703, *Scientific Reports (Nature)*, 2016, doi:10.1038/srep20600).

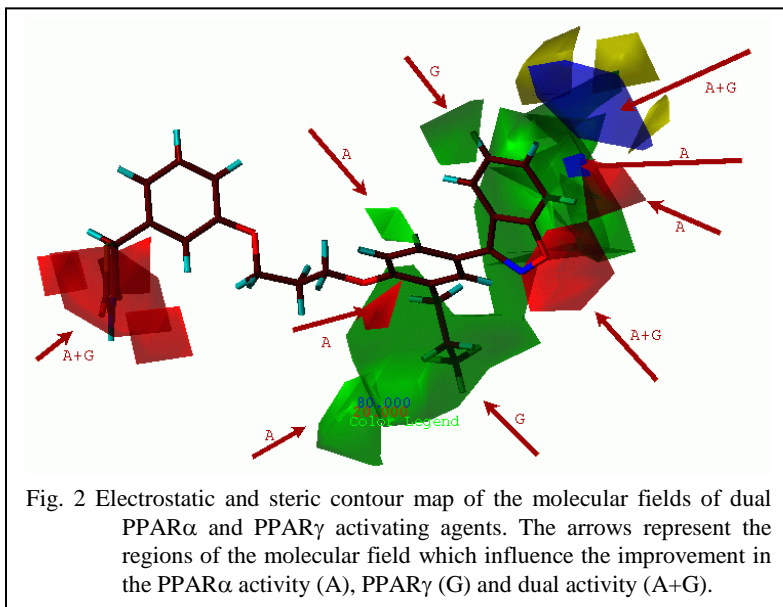


Fig. 2 Electrostatic and steric contour map of the molecular fields of dual PPAR α and PPAR γ activating agents. The arrows represent the regions of the molecular field which influence the improvement in the PPAR α activity (A), PPAR γ (G) and dual activity (A+G).

18. Fifty best publications at a glance

<i>Authors</i>	<i>Journal</i>	<i>Year</i>	<i>Vol.</i>	<i>Pages</i>
50. ...V. Jain....P.V. Bharatam	J. Chem. Phys.	2016		in print
49. ...N. Trivedi....P.V. Bharatam	Oncotarget	2016		in print
48. S. Chourasiya P.V. Bharatam	J. Org. Chem.	2016	81	in print
47. ... P.V. Bharatam, A. Goswami	J. Org. Chem.	2016	81	10.1021/acs.joc.6b00671
46. ...P.V. Bharatam, C.N. Kundu	Scientific Reports (Nature)	2016		10.1038/srep20600
45. P.V. Bharatam, ...M. Arfeen	Chem. Eur J.	2016	22	1088-1096
44. ..P.V Bharatam... S. Bharate	Chem. Commun.	2016		1009-1012
43. J. Chaitanya ... P.V. Bharatam	Chem. Res. Toxicol.	2015	28	2364-2376
42. S. Chourasiya... P.V. Bharatam	RSC Advances	2015	5	80027-80038
41. G.K. Rastogi, ... Bharatam, Tandon	ACS Med. Chem. Letts.	2015	6	1065-1070
40. A. Kusunuru, ... Bharatam, Mukherjee	Org. Letts.	2015	17	3742-3745
39. A. Bhaviskar, ... P.V. Bharatam	ACS Med. Chem. Lett.	2015	6	481-485
38. K.A. Kumar...P.V. Bharatam	J. Org. Chem.	2015	80	1746-1753
37. ... P.V. Bharatam ... S. Bharate	Chem. Commun.	2014		12076-12079
36. ... P.V. Bharatam, R. Kishore	J. Phys. Chem. B.	2014	118	9199-208
35. S. Bhatia P.V. Bharatam	J. Org. Chem.	2014	79	4852-4862
34. ... P.V. Bharatam. .. K.R.P. Kartha	J. Org. Chem.	2014	79	3427-3439
33. V. JainP.V. Bharatam	Nanoscale	2014	6	2476-2501
32. L Adane P.V. Bharatam	Bioorg. Med. Chem. Letts.	2014	24	613-617
31. N. Taxak P.V. Bharatam	Inorg. Chem.	2013	52	13496-13508
30. N. TaxakP.V. Bharatam	Inorg. Chem.	2013	52	5097-5109
29. V. Jain... ..P.V. Bharatam ...	Med. Chem. Comm.	2013	4	1257-1266
28. N. Taxak P.V. Bharatam	J. Phys. Chem. A.	2012	116	10441-10450
27. S.K. Guchhait .. P.V. Bharatam	J. Org. Chem.	2012	77	8321-8328
26. N. Anand P.V. Bharatam....	J. Org. Chem.	2011	76	5999-6006
25. A. Baviskar, ... P.V. Bharatam...	J. Med. Chem.	2011	54	5013-5030
24. D.S. Patel P.V. Bharatam	J. Org. Chem.	2011	76	2558-2567
23. L.S. Moon,PV. Bharatam	J. Org. Chem.	2010	75	5487-5498
22. N. PatelP.V. Bharatam	J. Phys. Chem. B.	2010	114	11603-11611
21. L.S. Moon, P.V. Bharatam	Chem. Commun.	2009		1067-1069
20. D.S. Patel,P.V. Bharatam	Chem. Commun.	2009		1064-1066
19. S. Sundriyal, ...P.V. Bharatam	Bioog. Med. Chem. Letts.	2008	15	4959-4962
18. S.V. Kessar,... P.V. Bharatam, ...	Angew. Chem. Int. Ed. Engl.	2008	47	4703-4706
17. S.V. Kessar,P.V. Bharatam	J. Am. Chem. Soc.	2007	129	4506-4507
16. R. Kumar P.V. Bharatam....	Bioorg. Med. Chem.	2007	15	1547-1555
15. T.S. Lobana, P. V. Bharatam	Inorg. Chem.	2006	45	1535-1542
14. P. V. Bharatam, D.S. Patel, P. Iqbal.	J. Med. Chem.	2005	48	7615-7622.
13. S. Khanna, P. V. Bharatam	J. Med. Chem.	2005	48	3015-3025
12. P. V. Bharatam, P. Iqbal, R. Tiwari	J. Phys. Chem. A	2004	108	10509-10517
11. P. V. Bharatam, S. Khanna	J. Phys. Chem. A	2004	108	3784-3788
10. P. V. Bharatam, ... D. Kaur.	Inorg. Chem.	2003	42	4743-4749
9. Nancy, P. V. Bharatam ... S. Trehan.	Chem. Commun.	2003		1420-1421
8. P. V. Bharatam, D. Kaur	Organometallics	2002	21	3683-3690
7. P. V. Bharatam, M.P. Mahajan.	Org. Letters	2000	2	2725-2728
6. K. Lammertsma and P. V. Bharatam	J. Org. Chem.	2000	65	4622-4670
5. B.V. Prasad P.S. Bassi	Chem. Phys. Lett.	1997	276	31-38
4. K. Lammertsma BharatamV. Prasad	J. Am. Chem. Soc.	1994	116	642-650
3. K. Lammertsma, BharatamV. Prasad	J. Am. Chem. Soc.	1993	115	2348-2351
2. E.D. Jemmis, Bharatam V. Prasad ...	Angew. Chem., Int. Ed. Engl.	1993	32	865-867
1. E.D. Jemmis, Bharatam V. Prasad	J. Am. Chem. Soc.	1987	109	2560-2563

20. Citations : Total citations as on June 2016 are 2750

List of articles and their number of citations leading to h-index 27 are given below

	<i>Authors</i>	<i>Journal</i>	<i>Year</i>	<i>Vol.</i>	<i>Pages</i>	<i>No. of citations</i>
1.	A. Baviskar, ... P.V. Bharatam...	J. Med. Chem.	2011	54	5013-5030	108
2.	S. Agrawal, P. V. Bharatam....	Eur. J. Pharma. Sciences	2004	22	127-144	99
3.	T.S. Lobana, P. V. Bharatam	Inorg. Chem.	2006	45	1535-1542	91
4.	K. Lammertsma Bharatam V. Prasad	J. Am. Chem. Soc.	1994	116	642-650	86
5.	K. Lammertsma, Bharatam V. Prasad	J. Am. Chem. Soc.	1993	115	2348-2351	67
6.	P. V. Bharatam, D.S. Patel, P. Iqbal.	J. Med. Chem.	2005	48	7615-7622	61
7.	S. Khanna, P. V. Bharatam	J. Med. Chem.	2005	48	3015-3025	57
8.	P. V. Bharatam, P. Uppal, ... D. Kaur,	J. Chem. Soc., Perkin Trans. 2	2000		43-50	56
9.	P.D. Dey, P.V. Bharatam ...	Tetrahedron	1997	53	13829-13840	48
10.	P. V. Bharatam, D. Kaur.	Tetrahedron	2002	58	1759-1764	45
11.	P. V. Bharatam, P. Iqbal, R. Tiwari	J. Phys. Chem. A	2004	108	10509-10517	39
12.	P.V. Bharatam, D.S. Patel.	Curr. Pharm. Design	2007	13	3518-3530	39
13.	N. Dessalew, D.S. Patel, P. V. Bharatam.	J. Mol. Graph Model.	2007	25	885-895	39
14.	K. Lammertsma and P. V. Bharatam	J. Org. Chem.	2000	65	4622-4670	39
15.	P. V. Bharatam, ... D. Kaur.	J. Phys. Chem. A	2003	107	1627-1634	38
16.	K. Singh, H. Kaur, ... P.V. Bharatam	Eur. J. Med. Chem.	2012	52	82-97	36
17.	N. Dessalew, P. V. Bharatam.	Eur. J. Med. Chem.	2007	42	1014-1027	35
18.	S.K. Singh, N. Dessalew, P. V. Bharatam	Eur. J. Med. Chem.	2006	41	1310-1319	32
19.	D.S. Patel, P.V. Bharatam	Chem. Commun.	2009		1064-1066	31
20.	S.V. Kessar, P.V. Bharatam, ...	Angew. Chem. Int. Ed. Engl.	2008	47	4703-4706	31
21.	P. V. Bharatam, Amita, D. Kaur.	J. Phys. Org. Chem.	2002	15	197-203	31
22.	E.D. Jemmis, Bharatam V. Prasad ...	J. Phys. Chem.	1990	94	5530-5535	31
23.	P. V. Bharatam, D. Kaur	Organometallics	2002	21	3683-3690	31
24.	D.S. Patel, P. V. Bharatam.	Curr. Protein & Peptide Sci.	2007	8	352-364	31
25.	Y.D. Aher, ... P. V. Bharatam....	J. Mol. Mod.	2007	13	519-529	29
26.	S.V. Kessar, ... P.V. Bharatam	J. Am. Chem. Soc.	2007	129	4506-4507	30
27.	L.S. Moon, ... P.V. Bharatam	J. Org. Chem.	2010	75	5487-5498	29
28.	Bharatam V. Prasad, ... P.S. Bassi	Chem. Phys. Lett.	1997	276	31-38	26

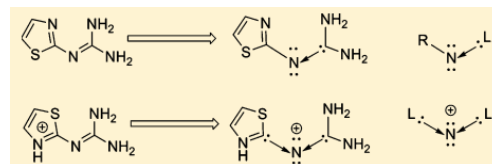
Full details will be provided when required.

Google Scholar citations: https://scholar.google.co.in/citations?hl=en&user=33_LekMAAAAJ&view_op=list_works

8. Contributions in Theoretical Organic Chemistry

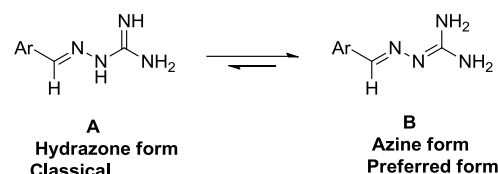
Chemical bonding

Chem. Eur. J.	2015		accepted
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



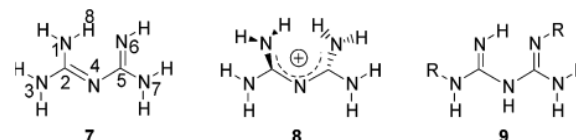
Tautomerism

RSC Advances	2015	5	55938
RSC Advances	2013	3	25268
J. Comput. Chem.	2013	34	1577
Int. J. Quant. Chem.	2008	108	1277
J. Org. Chem.	2000	65	4622
J. Am. Chem. Soc.	1994	116	642
J. Am. Chem. Soc.	1993	115	2348



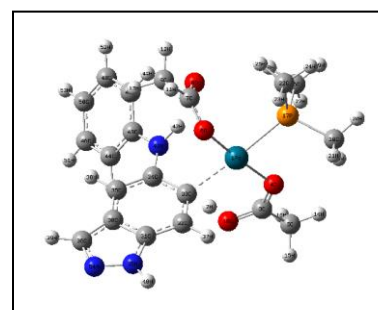
Electron delocalization / resonance

RSC Advances	2014	4	4533
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



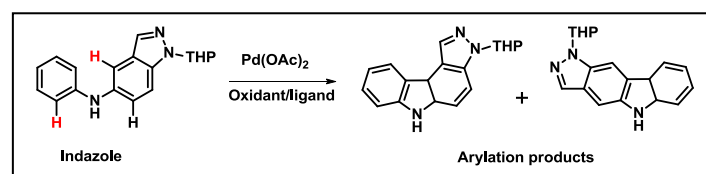
C-H bond activation

Org. Letts.	2015	17	3742
Org. Biomol. Chem.	2015	13	7790
Tetrahedron Letts	2015	56	4057
Org. Biomol. Chem.	2015	13	5235
J. Org. Chem.	2015	80	1746
Org. Biomol. Chem.	2015	13	1481
Chem. Commun.	2014		12076
J. Org. Chem.	2012	77	8321



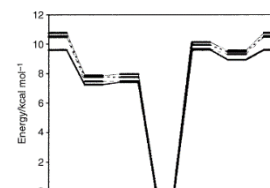
Reaction Mechanisms

Chem. Commun.	2016		in print
RSC Advances	2015	5	88353
J. Phys. Chem. B	2014	118	9199
J. Org. Chem.	2014	79	3427
Crystal Growth Design	2013	13	2004
RSC Advances	2012	2	11366
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

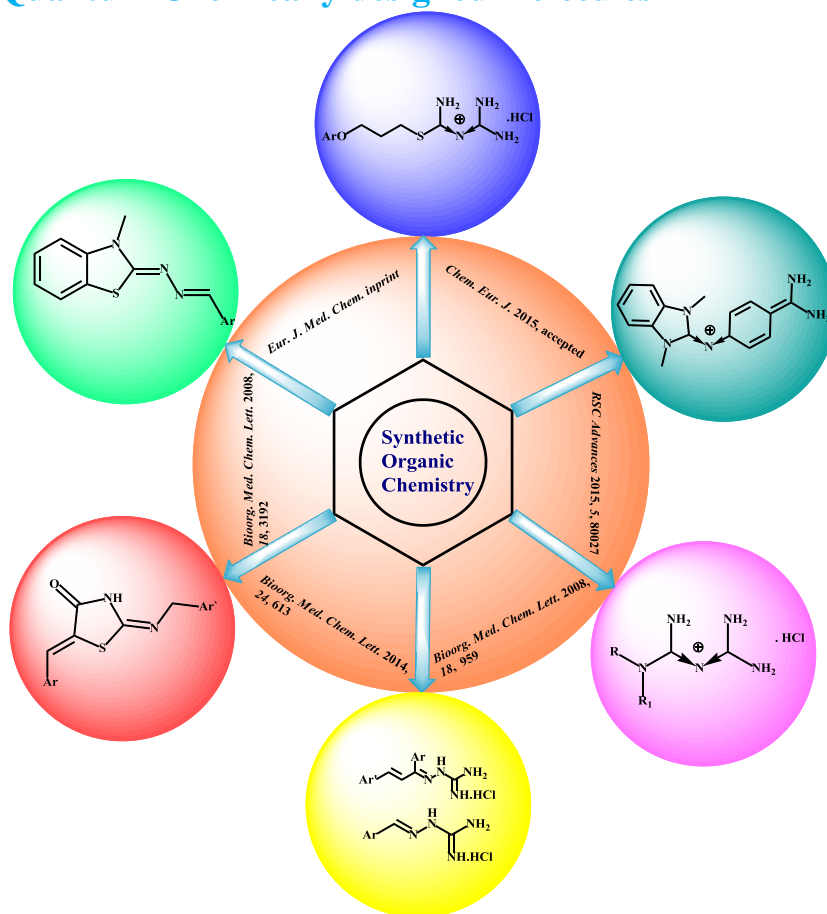


Conformational analysis

J. Phys. Chem. A	2014	118	187
Tetrahedron	2005	61	5633
Tet. Lett.	2002	43	8289
J. Chem. Soc., Perkin Trans.	2000		2469
J. Chem. Soc., Perkin Trans.	2000		43



9. Synthesis of Quantum Chemically designed molecules



Divalent N(I) compounds

Chem. Eur. J.	2015		accepted.
Eur. J. Med. Chem.	2015		accepted.
Bioorg. Med. Chem. Letts.	2014	24	613
Med. Chem. Res.	2015	24	1974

Guanythioureia derivatives

Bioorg. Med. Chem. Letts.	2014	24	613
---------------------------	------	----	-----

Azines

J. Org. Chem.	2016		in print
RSC Advances	2015	5	80027

Barbituric acid derivatives

Eur. J. Med. Chem.	2016		accepted.
Bioorg. Med. Chem. Letts.	2008	18	959
Bioorg. Med. Chem. Letts.	2008	18	3192

10. Contributions in Medicinal Chemistry

Anti-diabetic agent design and synthesis

Eur. J. Med. Chem.	2016	<i>in print</i>	
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. Biomol. Struct. Dyn.	2015	33	1913
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
J. Med. Chem.	2005	48	7615



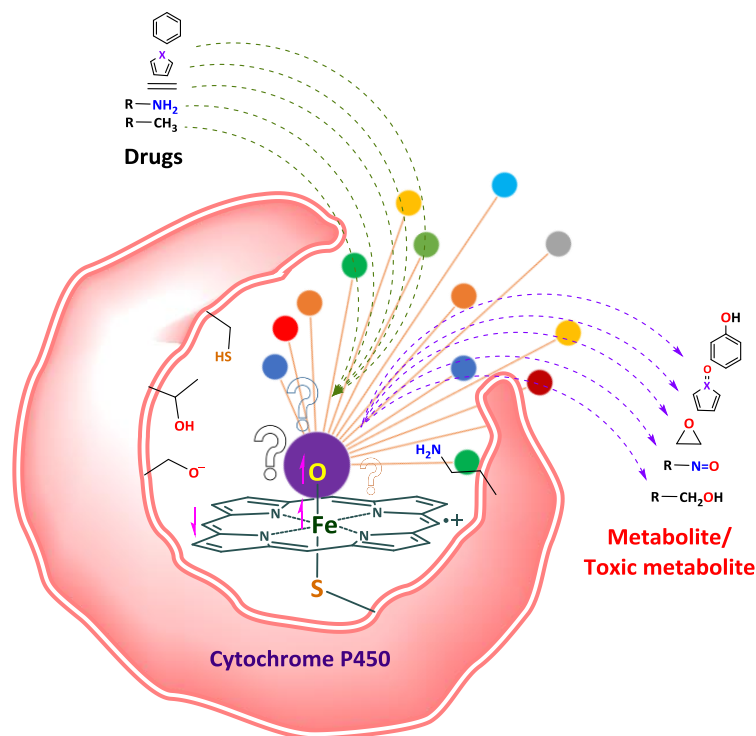
Anti-cancer agent design and synthesis

Oncotarget	2016	<i>in print</i>	
Scientific Reports	2016		
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

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

11. Contributions in Pharmaceutical Sciences



Drug Metabolism

J. Comput. Chem.	2014	35	2047
Eur. J. Med. Chem.	2014	71	15
Inorg. Chem.	2013	52	13496
Drug Metabolism Letters	2013	6	221
Inorg. Chem.	2013	52	5097
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.

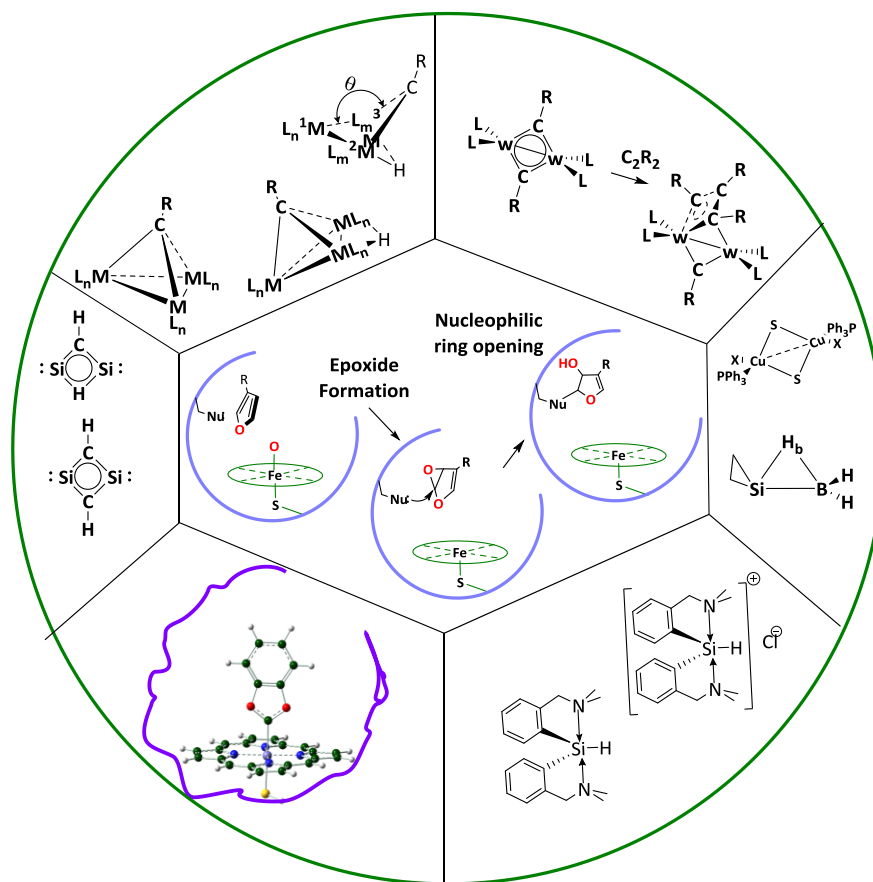
Drug toxicity

Chem. Res. Tox.	2015	28	2364.
Drug Metabolism Letters	2013	6	221
Chem. Res. Tox.	2011	24	1113

Drug delivery

J. Chem. Phys.	2016		<i>in print</i>
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

12. Contributions in theoretical Inorganic Chemistry



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

Bioinorganic Catalysis

Chem. Res. Tox.	2016	28	2364
J. Bio. Inorg. Chem.	2015	142	84
Inorg. Chem.	2013	52	13496
Inorg. Chem.	2013	52	5097

13. Computer programming and Pharmacoinformatics tool development

Drug likeness



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

Dendrimer builder

J. Comp. Chem.

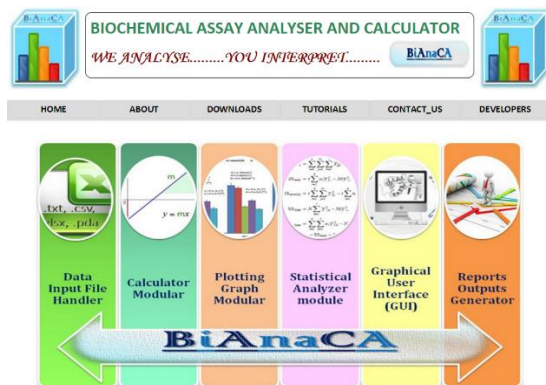
2012

33

1997

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

BiAnaca

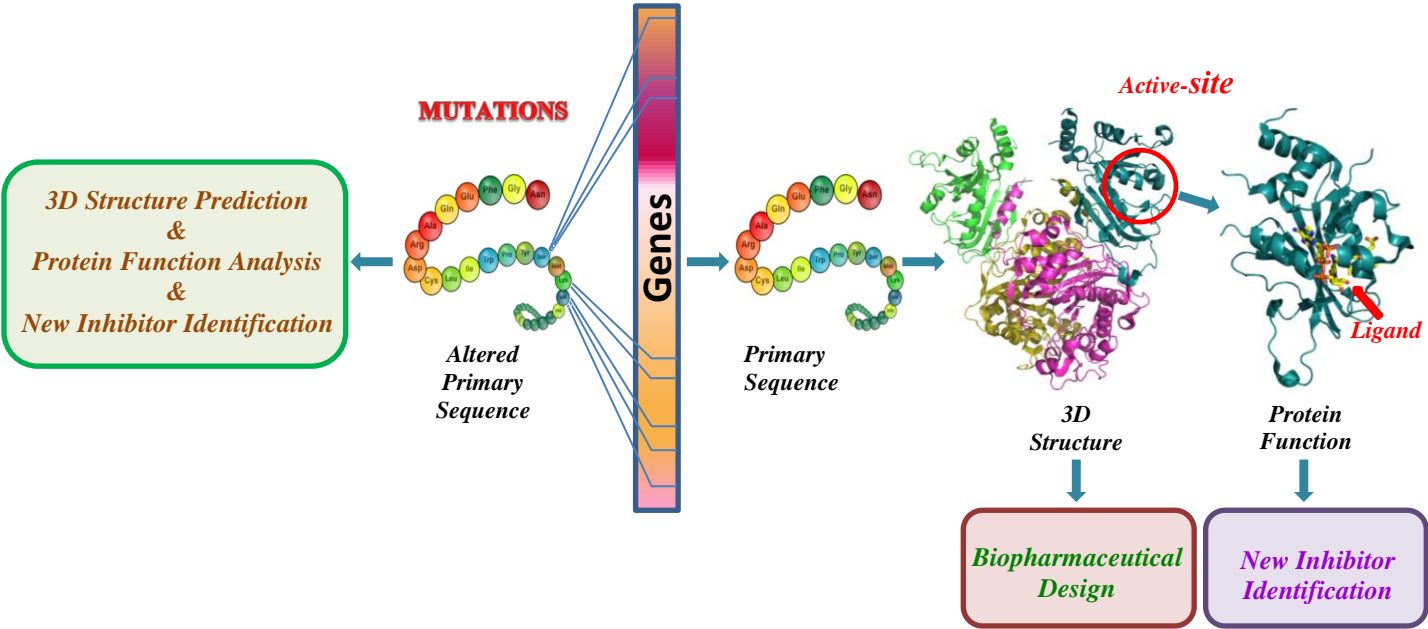


http://www.niper.ac.in/pi_dev_tools/BiAnaCA/ABOUT.html

Descriptor calculations

Int. J. Chem. Mod.	2016	accepted.	
Internet Ele. J. Mol. Design	2015	accepted.	
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

14. Contributions in Computational Biology



Computational mutational analysis

Science Reporter (Nature) 2016 DOI 10.1038/srep20600

Macromolecular structure and function prediction

J. Biomol. Struct. Dyn.	2015	1
J. Biomol. Struct. Dyn.	2015	DOI 10.1080/07391102.2015.1005137.
Appl. Biochem. Biotech.	2013	171 417
Curr. Protein & Peptide Sci.	2007	8 352
Enzyme and Microbial Tech.	2005	36 232

Biopharmaceutical design

PLOS One 2016 11 e0150764