

**National Institute of Pharmaceutical Education and Research (NIPER)
SAS Nagar – 160 062**



1. Name : Prasad V. Bharatam

2. Address with telephone/Fax/
e-mail:

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Professor
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website: www.niper.gov.in/pvbharatam.pdf

3. Date of Birth: 12 October 1962
Place of Birth: Rajahmundry, Andhra Pradesh

4. Nationality Indian

5. Nominee's field
of specialization Medicinal Chemistry

6. Academic qualifications:

<i>S. No.</i>	<i>Degree</i>	<i>Subject</i>	<i>Class</i>	<i>Marks %</i>	<i>Year</i>	<i>University</i>
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
1.	B.Sc	Chemistry, Maths, Physics	I class	72%	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)

7. Positions held earlier:

<i>S. No.</i>	<i>Period</i>	<i>Place of Employment</i>	<i>Designation</i>	<i>Scale of Pay</i>
5.	June 2006 – continuing	N.I.P.E.R.	Professor	Rs. 55360-10500
4.	June 2001 – June 2006	N.I.P.E.R.	Assoc. Prof.	Rs. 16400-450-20900
3.	Aug. 2000 – June 2001	G.N.D. University, Amritsar	Reader	Rs. 12000-250-16000
2.	Jan. 2000 – Aug. 2000	G.N.D. University, Amritsar	Sr. Lecturer	Rs. 3000-100-4500
1.	Dec. 1993 – Dec. 1999	G.N.D. University, Amritsar	Lecturer	Rs. 2200-75-3000

8. Significant Foreign Assignments:

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

9. Research Experience :

Medicinal chemistry of anti-malarial agents – Design and Synthesis	2005-current
Medicinal chemistry of anti-diabetic agents -- Design and Synthesis	2001-current
Organosulfur chemistry using computational methods	1994-2001
Tautomerism in high-energy material	1991-1993
Carbyne bridged metals and hydrocarbation reactions	1985-1990

10. Teaching Experience : *NIPER* 10 years.
G.N.D. Univ. 7.5 years – integrated M.Sc. (5 yr. course)

11. **Fields of Specialization:** Quantum Medicinal Chemistry, Pharmacoinformatics
Synthesis of computationally designed molecules.

12. **Publications:**

Scientific articles published	132
Science Education articles	10
Presentations at conferences	125
h-index (scopus)	18
No. of citations	1250

13. **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, London	-- 2007
IBM Faculty Award	-- 2007
Fellowship of Alexander von Humboldt Stiftung, Bonn	-- 2002
Council Member, Chemical Research Society of India	2008-2010
Member Editorial Advisory Board – Indian Journal of Chemistry A.	2008-2010
Member Editorial Advisory Board – Current Comput Aided Drug Design	2007-2009

14. Research Supervision:

A. Ph.D.	– 11 completed; 8 on going.
B. M.Sc. Research Projects	-- 16 completed
C. M.S. Pharm (Med. Chem.) research projects	– 45 completed, 12 on going.
D. Research Fellows (Non-Ph.D.)	– 9
E. Visiting Fellows / students	– 54

15. 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
8. Research Fellow grant	Rs. 5,84,000/-	2002-2005
9. DST project on Nitric Oxide donors	Rs. 16,10,000/-	2004-2007
10. DST project on Pharmacoinformatics	Rs. 1,50,00,000/-	2005-2008
11. CSIR project on Dual activators	Rs. 10,00,000/-	2005-2008
12. DST project – Nano Mission	Rs. 50,00,000/-	2009-2012
13. DST project on S-oxidation	Rs. 35,00,000/-	2009-2012
14. DBT grant on CYP metabolism	Rs. 40,00,000/-	2012-2015
15. CSIR grant on Y-shaped agonists	Rs. 16,00,000/-	2012-2015

as a co-Principal Investigator

1. CSIR Project	Rs. 6,50,000/-	2002-2005
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16. Industrial Projects

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

- (a) Guest editor Theo. Chem. Accounts -- Jan. 2012
- (b) Member of the National Academy of Sciences, Allahabad, -- Mar. 2006
- (c) Guest editor for Indian J. Chem. Section A. -- Jan. 2006
- (d) Subject Expert – Board of control, Biotechnology, GNDU, Amritsar -- 2007-2009
- (e) Subject Expert – Board of Research, Sciences, GNDU, Amritsar -- 2008-2011
- (f) A reviewer in many journals including,
 - Indian J. Chem.;
 - J. Phys. Chem.;
 - Chemistry, A European Journal;
 - J. Med. Chem.;
 - Inorg. Chem.;
 - Bioorg. Med. Chem. etc.
- (g) Evaluator of project proposals submitted to CSIR, DST, DBT, New Delhi.
- (h) Invited to the Gordon Research Conference on Computer Aided Drug Design in July 2005, Tilton School, Tilton, NH, USA.
- (i) Invited to the Keystone conference on Computer Aided Drug Design in April 2008, USA
- (j) Invited for Plenary lecture at Medicinal Chemistry Intl. conf. Aug. 2009, Bandung, Indonesia.
- (k) Coordinator for Indo-German Conference MCBR3 -- 2012

18. Organisational experience:

- 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 4 international symposia on DMPK, Feb. 2009, 2010, 2011, 2012.
- 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 organizing committees of several workshops and conferences (National, International) at GNDU (1994-2001).

19. Collaborators

The 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) Dr. Damanjit Kaur, Guru Nanak Dev University, Amritsar

20. 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 |

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

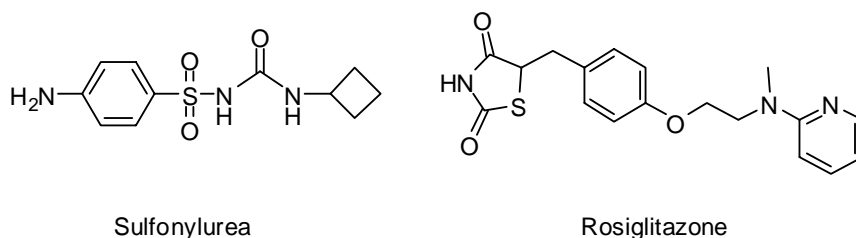
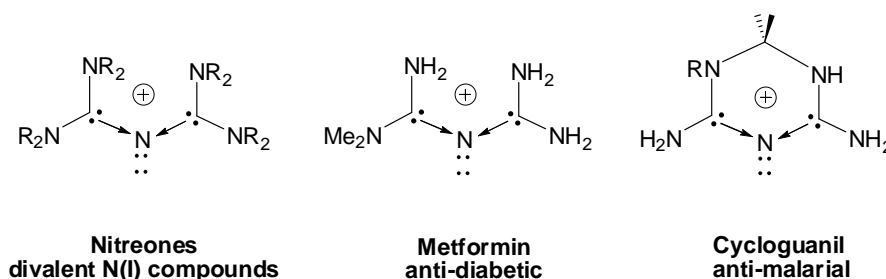
Dr. Bharatam has been working in the fields of Quantum Medicinal Chemistry, Design and synthesis of medicinally important molecules for the past 17 years. His initial contributions were in the area of studies on the electronic structure and reaction of organosulfur compounds with potential drug applications. (*Tet. Lett.* 2002, 43, 8289, *Tetrahedron*, 2004, 60, 4801). During this period he identified that some of these organosulfur compounds carry S-N bonds with hypervalent sulphur atoms and low valent nitrogen atoms. These nitrogen atoms carry two lone pairs of electrons. Continuing his efforts, he 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. Comm.* 2009, 1064; *J. Phys. Chem.* 2011, in print) 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 carbones, 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. Two of the synthesized guanylthiourea derivatives show anti-malarial activity, one in nano molar region. 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.

The work on sulfonamides lead to research in anti-hyperglycemic sulfonyl ureas and other related anti-diabetic agents. Glitazones are compounds which act as insulin sensitisers and can be used to reduce insulin resistance. Pioglitazone and rosiglitazone are drugs which are being used to prolong the

period of insulin resistance (before the onset of frank diabetes). These compounds are found to show rapid racemisation, which has been shown to be due to the keto-enol tautomerism in the thiazolidinedione acidic head group of these systems. However, studies by the nominee showed that the keto-enol tautomerism is a less favoured process in the thiazolidinediones. The reasons for the rapid racemisation have been found to be the *in vivo* reversible sulfoxidation of the thiazolidinedione rings, this work also explained the absence of rapid racemisation in the oxazolidinediones. (*J. Phys. Chem.* 2004, 108, 3784, *J. Phys. Chem.B*, 2010, 114, 11603).

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

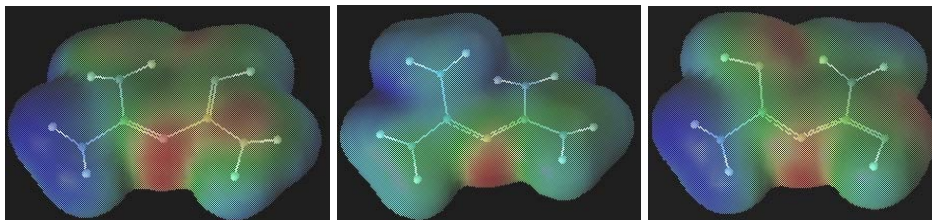


Fig. 1. MESP of biguanide, protonated biguanide and deprotonated biguanide.

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).

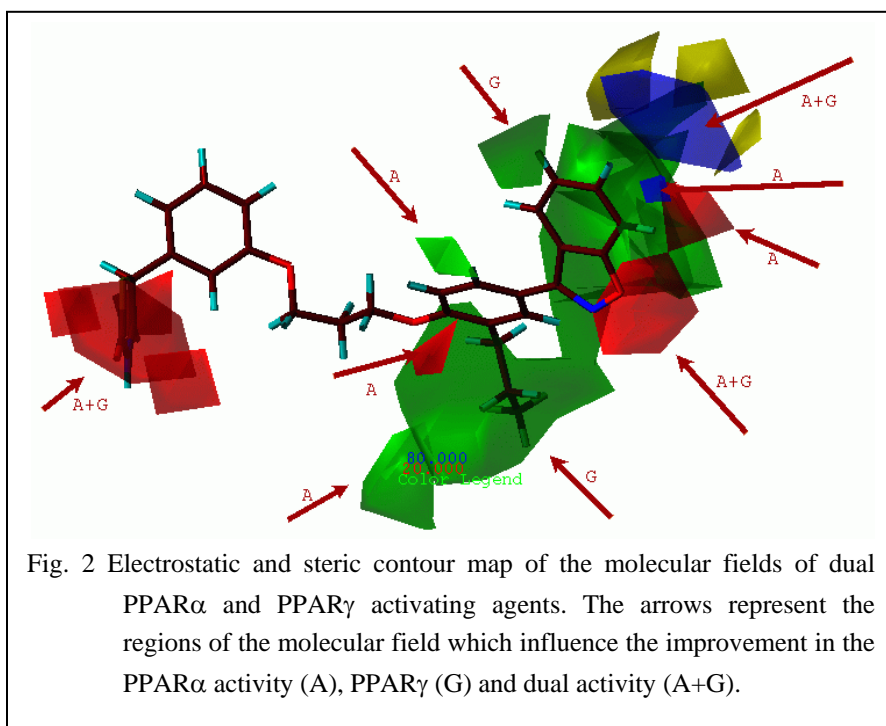


Fig. 2 Electrostatic and steric contour map of the molecular fields of dual PPAR α and PPAR γ activating agents. The arrows represent the regions of the molecular field which influence the improvement in the PPAR α activity (A), PPAR γ (G) and dual activity (A+G).

Research work of the nominee 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).

22. Fifty important publications in a nutshell

<i>Authors</i>	<i>Journal</i>	<i>Year</i>	<i>Vol.</i>	<i>Pages</i>
50. V.A. Dixit ... P.V. Bharatam	Chem. Res. Tox.	2011	24	1113-1122
49. N. Anand P.V. Bharatam....	J. Org. Chem.	2011	76	5999-6006
48. A. Baviskar, ... P.V. Bharatam...	J. Med. Chem.	2011	54	5013-5030
47. D.S. Patel P.V. Bharatam	J. Org. Chem.	2011	76	2558-2567
46. D.S. Patel.... P.V. Bharatam	J. Phys. Chem. A.	2011	115	7645-7655
45. N. Taxak, P.V. Bharatam	J. Phys. Chem. A.	2011	115	891-898
44. L.S. Moon, PV. Bharatam	J. Org. Chem.	2010	75	5487-5498
43. N. Patel P.V. Bharatam	J. Phys. Chem. B.	2010	114	11603-11611
42. A. Medhi, ... P.V. Bharatam	J. Comput. Chem.	2010	31	1259-1267
41. L.S. Moon, P.V. Bharatam	Chem. Commun.	2009		1067-1069
40. D.S. Patel, P.V. Bharatam	Chem. Commun.	2009		1064-1066
39. S. Sundriyal,P.V. Bharatam	Bioorg. Med. Chem. Letts.	2008	15	4959-4962
38. S. Sundriyal, P.V. Bharatam	Bioorg. Med. Chem. Letts.	2008	15	3192-3195
37. L. Adane, P. V. Bharatam	Curr. Med. Chem.	2008	15	1522-1569
36. P. V. Bharatam, ... D.S. Patel.	Curr. Pharm. Design	2007	13	3518-3530
35. D.S. Patel, P. V. Bharatam	Curr. Protein & Peptide Sci.	2007	8	352-364
34. S.V. Kesar,... P.V. Bharatam, ...	Angew. Chem. Int. Ed. Engl.	2008	47	4703-4706
33. S.V. Kessar,P. V. Bharatam	J. Am. Chem. Soc.	2007	129	4506-4507
32. R. Kumar PV. Bharatam....	Bioorg. Med. Chem.	2007	15	1547-1555
31. P. V. Bharatam, S. Sundriyal	J. Nanosci. Nanotech.	2006	6	3277-3282
30. D.S. Patel, P. V. Bharatam	J. Comput. Aided Mol. Des.	2006	20	55-66
29. P. Iqbal, P. V. Bharatam	J. Comput. Chem	2006	27	334-343
28. T.S. Lobana, P. V. Bharatam	Inorg. Chem.	2006	45	1535-1542
27. P. V. Bharatam, D.S. Patel, P. Iqbal.	J. Med. Chem.	2005	48	7615-7622.
26. S. Khanna, P. V. Bharatam	J. Med. Chem.	2005	48	3015-3025
25. M.E. Sobhia, P. V. Bharatam	Bioorg. Med. Chem.	2005	13	2331-2338
24. P. V. Bharatam, P. Iqbal, R. Tiwari	J. Phys. Chem. A	2004	108	10509-10517
23. P. V. Bharatam, S. Khanna	J. Phys. Chem. A	2004	108	3784-3788
22. P. V. Bharatam, P. S. Kumar	Tetrahedron	2004	60	4801-4805
21. T.L. Aboye P. V. Bharatam	Bioorg. Med. Chem.	2004	12	2709-2715
20. S. Mittal, H.P.S. Chawla.	Bioorg. Med. Chem. Letts.	2004	14	979-982
19. P. V. Bharatam, ... D. Kaur.	Inorg. Chem.	2003	42	4743-4749
18. Nancy, P. V. Bharatam ... S. Trehan.	Chem. Commun.	2003		1420-1421
17. P. V. Bharatam, ... D. Kaur.	J. Phys. Chem. A	2003	107	1627-1634
16. P. V. Bharatam Amita.	Tet. Lett.,	2002	43	8289-8291
15. P. V. Bharatam, D. Kaur	Organometallics	2002	21	3683-3690
14. P. V. Bharatam, M.P. Mahajan.	Org. Letters	2000	2	2725-2728
13. K. Lammertsma and P. V. Bharatam	J. Org. Chem.	2000	65	4622-4670
12. P. V. Bharatam, ... D. Kaur.	J. Chem. Soc., Perkin Trans. 2	2000		2469-2474
11. P. V. Bharatam, D. Kaur	J. Chem. Soc., Perkin Trans. 2	2000		43-50
10. B.V. Prasad ... P.S. Bassi	Chem. Phys. Lett.	1997	276	31-38
9. E.D. Jemmis ... Bharatam V. Prasad.	Inorg. Chem.	1994	33	2046-2048
8. K. Lammertsma BharatamV. Prasad	J. Am. Chem. Soc.	1994	116	642-650
7. K. Lammertsma, BharatamV. Prasad	J. Am. Chem. Soc.	1993	115	2348-2351
6. E.D. Jemmis, Bharatam V. Prasad ...	Angew. Chem., Int. Ed. Engl.	1993	32	865-867
5. E.D. Jemmis, ... Bharatam V. Prasad	Organometallics	1993	12	4267-4268
4. E.D. Jemmis, Bharatam V. Prasad	Organometallics	1992	11	2528-2533
3. E.D. Jemmis, BharatamV. Prasad	Organometallics	1991	10	3613-3620
2. E.D. Jemmis, BharatamV. Prasad ...	J. Phys. Chem.	1990	94	5530-5535
1. E.D. Jemmis, Bharatam V. Prasad	J. Am. Chem. Soc.	1987	109	2560-2563

23. List of publications with complete bibliographic details

<i>Original Scientific articles published</i> (foreign journals)	110
<i>Original Scientific articles published</i> (Indian Journals)	15
<i>Reviews</i> (peer reviewed)	5
<i>Book Chapters</i> (peer reviewed)	2
<i>Science Education articles</i>	<u>10</u>
Total	<u>142</u>
<i>Citations</i>	1250
<i>h-index</i> (scopus)	18

Submitted (Peer reviewed foreign journals) (7)

Format: S.No., Title, Authors, **Journal**, **Year**, *vol.* pages. [Impact Factor] (Number of citations)

117. Unusual structural attributes of an unsubstituted non-proteinogenic γ -aminobenzoic-acid: A flat β -strand-like molecular template for designing non-covalent duplex β -sheet *mimics*"
M. Ramesh, Prasad V. Bharatam, P. Venugopalan, R. Kishore
2012, revision to be submitted
116. Path eccentric connectivity indices: Novel highly discriminating topological descriptors for QSAR/QSPR
Neelam Mahajan, Harish Jangra, Kinkar Ch.Das, P.V.Bharatam, S.S.Sambi and A.K. Madan
2012, submitted
115. Fourth generation detour matrix based topological indices for QSAR/QSPR part-1: development and evaluation
Rakesh K. Marwaha, Harish Jangra, P.V.Bharatam, Kinkar C. Das, Anil Kumar Madan
2012, submitted
114. 2-Aminopyrimidine Based 4-Aminoquinoline Antiplasmodial and Antimycobacterial Agents. Synthesis, Biological Activity, Structure-Activity Relationship and Mode of Action Studies
Kamaljit Singh, Hardeep Kaur, Kelly Chibale, Jan Balzarini, Susan Little, Scott Franzblau and Prasad V. Bharatam
2012, revision to be submitted.
113. Conformational and Synthon Polymorphism in Bicalutamide: A Quantum Chemical Study
Devendra K. Dhaked, Vaibhav Jain, Yoganjaneyulu Kasetti, Prasad V. Bharatam
Structural Chem. 2012, submitted.
112. Metabolic-intermediate Complex Formation with Cytochrome P450: Theoretical Studies in Elucidating the Reaction Pathway for the Generation of Reactive Nitroso Intermediate
Nikhil Taxak, Bhargav Patel, Prashant V. Desai, Michael Mohutsky, Valentine J. Klimkowski, Vijay Gombar, Prasad V. Bharatam
J. Comp. Chem. 2012, submitted
111. Pharmacophoric Features of Drugs with Guanylurea Moiety: An Electronic Structure Analysis
Yoganjaneyulu Kasetti and Prasad V. Bharatam,
Eur. J. Med. Chem. 2012, to be submitted.

Published (Peer reviewed foreign journals) (110)

Format: S.No., Title, Authors, **Journal**, **Year**, *vol.* pages. [Impact Factor] (Number of citations)

110. Complex Induced Proximity Effect in the Regioselective Lithiation of Pyridine Derivatives
Jaspreet S. Dhau, Amritpal Singh, Yoganjaneyulu Kasetti, P.V. Bharatam
Eur. J. Org. Chem. **2012**, **accepted**.
109. Tautomerism in drugs with Benzimidazole Carbamate Moiety: An Electronic Structure Analysis
Yoganjaneyulu Kasetti and Prasad V. Bharatam
Theor. Chem. Acc. **2012**, **accepted**.
108. Computational study on the conformational preferences in Nateglinide
Vaibhav Jain, Devendra Kumar Dhaked, Yoganjaneyulu Kasetti, P. V. Bharatam
J. Phys. Org. Chem. **2012**, DOI: 10.1002/poc.1956
107. CytochromeP450 Isoenzyme Specificity in the Metabolism of Anti-malarial Biguanides: Molecular Docking and Molecular Dynamics Analyses
Dhilon S. Patel, Ramesh M. and Prasad V. Bharatam
Medicinal Chemistry Research, **2012**, DOI 10.1007/s000444-011-9966-9
106. Toxic metabolite formation from Troglitazone (TGZ): New Insights from DFT study.
V.A. Dixit, P.V. Bharatam
Chem. Res. Tox. **2011**, 24, 1113-1122. [3.74]
105. Entrapment and Kinetic Resolution of Stabilized Axial and Equatorial Conformers of Spiro- β -Lactams,
N. Anand, B.A. Shah, M. Kapoor, R. Parshad, R.L. Sharma, M. S. Hundal, A.P. S. Pannu, P.V. Bharatam,
S.C. Taneja
J. Org. Chem. **2011**, 76, 5999-6006 [4.219]
104. N-Fused imidazoles as novel anticancer agents that inhibit catalytic activity of topoisomerase II α and induced apoptosis in G1/S phase.
A.T. Baviskar, C. Madaan, R. Preet, P. Mohapatra, V. Jain, S.K. Guchhait, C. N. Kundu, U.C. Banerjee,
P. V. Bharatam.
J. Med. Chem. **2011**, 54, 5013-5030 [4.802]
103. Divalent N(I) compounds with two lone pairs on nitrogen.
D.S. Patel, P.V. Bharatam.
J. Phys. Chem. A, **2011**, 7645-7655. [2.899]
102. CYP Isoform specificity towards drug metabolism: Analysis using common feature hypothesis.
Ramesh M., P.V. Bharatam.
J. Mol. Mod., **2011**, DOI: 10.1007/s00894-011-1105-5. [2.336]
101. To bend or not to bend! The dilemma of allenes.
D.S. Patel, P.V. Bharatam.
J. Org. Chem., **2011**, 76, 2558-2567. [4.219]

100. S-Oxidation of thiazolidinedione with hydrogen peroxide, peroxyntrous acid, and C4a-hydroperoxyflavin: A theoretical study.
N. Taxak, V. Parmar, D.S. Patel, A. Kotasthane, P.V. Bharatam.
J. Phys. Chem. A, **2011**, *115*, 891-898. [4.802]
99. Computer-aided molecular design of 1H-imidazole-2,4-Diamine derivatives as potential inhibitors of *plasmodium falciparum* DHFR enzyme.
L. Adane, P.V. Bharatam.
J. Mol. Mod., **2011**, *17*, 657-667. [2.336]
98. A new colorimetric chemodosimeter for Hg²⁺ based on charge-transfer compound of N-methylpyrrole with TCNQ.
P. Kaur, S. Kaur, Y. Kasetti, P.V. Bharatam, K. Singh.
Talanta, **2010**, *83*, 644-650. [3.29] (1)
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