## **CURRICULUM VITAE**

#### DR. PRADEEP KUMAR NAIK

Associate Professor Department of Biotechnology Guru Ghasidas Vishwavidyalaya, Bilaspur-495009 Chhattisgarh

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### **EDUCATION:**

- Post Doctorate (July 2010 to July 2011)
  - Emory University School of Medicine, Atlanta, Georgia, USA
- Advanced P.G. Diploma in Bioinformatics (2003)
  - Jawaharlal Nehru University, New Delhi, India
- Doctor of Philosophy (Ph. D) in Life Science (2001)
  - Sambalpur University, Jyoti Vihar, Orissa, India
  - Thesis title: Role of ethylene in spikelet development of rice.
- Master of Philosophy (M. Phil.) in Life Science (1995)
  - Sambalpur University, Jyoti Vihar, Orissa, India
- Master of Science (M. Sc.) in Life Science (1994)
  - Sambalpur University, Jyoti Vihar, Orissa, India
- Bachelor of Science (B. Sc.) (1992)
  - Sambalpur University, Jyoti Vihar, Burla, Sambalpur, Orissa, India

### PRESENT POSITION:

Associate Professor, Department of Biotechnology & Bioinformatics, Jaypee University of Information Technology, Solan, Himachal Pradesh, India, 1<sup>st</sup> August 2011 to present

### **POSITIONS HELD:**

- Assistant Professor, Department of Biotechnology & Bioinformatics, Jaypee University of Information Technology, Solan, Himachal Pradesh, India July 2008 – July 2011
- Senior Lecturer, Department of Biotechnology & Bioinformatics, Jaypee University of Information Technology, Solan, Himachal Pradesh, India July 2005 – June 2008
- Lecturer, Department of Biotechnology & Bioinformatics, Jaypee University of Information Technology, Waknaghat, Solan, Himachal Pradesh, India July 2003 June 2005
- Senior Research Fellow, CSIR, Sambalpur University, Orissa, India Dec 2000 Dec 2001
- Research Associate, ICAR, Sambalpur University, Orissa, India Dec 1997 Sept 1999
- Junior Research Fellow, ICAR, Sambalpur University, Orissa, India Nov 1996 Dec 1997

### **HONORS/AWARDS:**

- BOYSCAST Fellowship from Govt. of India, Department of Science and Technology, 2009
- CSIR-UGC Junior Research Fellowship and Eligibility for Lectureship- 2001
- ASRB National eligibility test for Assistant Professorship -1998 & 2001
- Graduate Aptitude Test for Engineering, Life Sciences 1996
- Sarojini G. Panigrahi Young Scientist Award, Orissa Botanical Society, 1997
- Senior Research Fellowship Award, CSIR Dec 2000 Dec 2001

### PROFESSIONAL EXPERIENCE:



### TEACHING:

Associate Professor, Department of Biotechnology, Guru Ghasidas Vishwavidyalaya, Bilaspur 7 <sup>th</sup> Feb 2014.

Associate Professor, Department of Biotechnology and Bioinformatics, Jaypee University of Information Technology, Himachal Pradesh August 2011 – 5<sup>th</sup> Feb 2014.

- Taught Advanced Bioinformatics (both lecture and lab) to Ph.D Biotechnology and Bioinformatics students.
- Taught Modelling and Simulation of Biological System (both lecture and lab) to M.Tech Computational Biology students.
- Taught Advanced Chemoinformatics (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Computer Aided Drug Design Techniques (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Molecular Modelling (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Highthroughput Screening Techniques (lecture) to B.Tech Bioinformatics students.

Assistant Professor, Department of Biotechnology and Bioinformatics, Jaypee University of Information Technology, Himachal Pradesh **July 2008 - July 2011** 

- Taught Modelling and Simulation of Biological System (both lecture and lab) to M.Tech Computational Biology students.
- Taught Advanced Chemoinformatics (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Computer Aided Drug Design Techniques (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Molecular Modelling (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Highthroughput Screening Techniques (lecture) to B.Tech Bioinformatics students.
- Taught System Biology (lecture) to B.Tech Bioinformatics students.

Senior Lecturer, Department of Biotechnology and Bioinformatics, Jaypee University of Information Technology, Himachal Pradesh **July 2005 - June 2008** 

- Taught Advanced Chemoinformatics (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Computer Aided Drug Design Techniques (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Molecular Modelling (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Highthroughput Screening Techniques (lecture) to B.Tech Bioinformatics students.
- Taught System Biology (lecture) to B.Tech Bioinformatics.
- Taught Computational Biology (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Molecular Biology (both lecture and lab) to B.Tech Bioinformatics students.

Lecturer, Department of Biotechnology and Bioinformatics, Jaypee University of Information Technology, Himachal Pradesh July 2003 - June 2005

- Taught Computational Biology (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Structural Biology (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Computer Aided Drug Design Techniques (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Biochemistry (both lecture and lab) to B.Tech Bioinformatics students.
- Taught Molecular Biology (both lecture and lab) to B.Tech Bioinformatics students

### SUPERVISORY TEACHING:

## • Ph.D. students directly supervised: 5

- ❖ Dr. Afroz Alam: Study of genetic variations in *Podophyllum hexandrum* and computational screening of podophyllotoxin analogues (**Nov 2009**).
- ❖ Dr. Mani Srivastava: Computational modeling of artemisinin and its structural derivatives: mechanism, interaction and predictive activity (Feb 2011).
- ❖ Dr. Jitendra Kumar: Assessment of genetic diversity and artemisinin content among genotypes of *Artemisia annua* and related species from the Ladakh region, India (March 2012).
- ❖ Dr. Manish S. Bhoyar: Molecular and phytochemical characterization and optimization of dormancy breaking treatment in *Capparis spinosa* L. from the Trans Himalayan region of Ladakh, India (**April 2012**)
- ❖ Dr. Shruti Jain: Communication of signals and responses leading to cell survival/cell death using engineered regulatory networks, (May 2012).

### • Ph.D. students co-supervised: 1

Dr. Rajani Kant Mahapatra: Computational study of histo-aspartic protease (HAP) and artemisinin-quinine hybrid: interaction, mechanism and antimalarial activity (Feb 2013)

## • Ph.D students currently supervising: 3

- ❖ Mr. Dipankar Sengupta: Translational and highend computing of clinical data in India (Thesis Submitted, **16 December 2013**).
- ❖ Miss. Seneha Santoshi: Computer aided design of novel noscapinoids and their experimental evaluation as tubulin binding anti-cancer agents (since July 2010).
- ❖ Miss. Charu Suri: Elucidating molecular basis of microtubule nucleation: a combined molecular dynamics simulation, free-energy calculation and computational alanine scanning study (since **July 2011**).
- M.Tech students supervised: 6
- Undergraduates supervised: 94

### *ACTIVE GRANT SUPPORT:*

- 1. *In vitro* and *in vivo* evaluation of synergistic effect of novel microtubule-interfering agent, amino-noscapine and taxotere for prostate cancer therapy. **Principal Investigator**, Indian Council of Medical Research (ICMR), Total costs: 42.35 lakhs (Approved for funding 2013).
- 2. Identification of intermediate metabolites for linking missing links in the biosynthetic pathways of desired chemical constituents in target plant species. **Principal Investigator**, Department of Biotechnology (**DBT**), India, Total costs: **68.65 lakhs** (**Sept. 2010 Sept. 2015**).
- 3. Toxicological evaluation of herbal formulations: (a) herbal performance enhancing capsules (PerfoMax), (b) herbal adaptogenic appetizer, (c) herbal tea and (d) seabuckthron oil based

- soft gel capsule. **Principal Investigator**, Defence Institute of High Altitude Research, **DRDO**, India, Total costs: **8.49 lakhs** (**Dec. 2012 Dec. 2013**).
- 4. Genetic characterization, chemical profiling and optimization of parameters for artemisinin yield in *Artemisia annua* from the Ladakh region. **Principal Investigator**, Defence Institute of High Altitude Research, **DRDO**, India, Total costs: **9.50 lakhs** (**April 2009 April 2011**).
- 5. Study of population structure of *Podophyllum hexandrum* using biochemical and molecular markers. **Principal Investigator**, Department of Science and Technology (**DST**), India, Total costs: **10.32 lakhs** (**Feb. 2006 Feb. 2009**).
- 6. Development of business intelligence model of army personnel's at higher altitude. Co-Investigator, Defence Institute of High Altitude Research, DRDO, India, Total costs: 9.90 lakhs (July 2012 July 2014).
- 7. Genetic analysis to avoid inbreeding of the endangered Western Tragopan in the aviaries of Himachal Pradesh. Co-Investigator, Department of Science and Technology (DST), India, total costs: 11.5 lakhs (April 2012 March 2015).
- 8. Fabrication of energy harvesting prototypes using piezoelectric materials. Co-Investigator, Defence Institute of High Altitude Research, DRDO, India, Total costs: 9.68 lakhs (Sept. 2012 Sept. 2014).
- 9. Establishment of an assay using human embryonic stem cell derived cardiac precursors from KIND2 cells for cytotoxicity testing. Co-Investigator, Department of Biotechnology (DBT), India, Total costs: 45.0 lakhs (April 2013 Sept. 2014).
- **10.** Chemical profiling of turmeric from different agroclimatic regions and optimization of environmental parameters for high curcumin yield. **Co-Investigator**, Department of Biotechnology (**DBT**), India, Total costs: **34.52 lakhs** (**Feb. 2013 Feb. 2016**).
- **11.** Development of a standardized herbal product for urolithiasis from *Tribulus terrestris* and *Achyranthes aspera*, **Co-Investigator**, Department of Biotechnology (**DBT**), India, Total costs: **26.2 lakhs** (**May 2008 May 2011**).
- 12. Development of candidate gene markers (SNPs & SSRs) for Jatropha (*Jatropha curcas*) by utilizing genome resources of Castor Bean (*Ricinus communis*). **Co-Investigator**, Department of Biotechnology (**DBT**), India, Total costs: **41.92 lakhs** (**July 2007 July 2010**).

## **PUBLICATIONS:**

#### **Year 2013**

- 92. Dipankar Sengupta and Pradeep Kumar Naik (2013). SN algorithm: analysis of temporal clinical data for mining periodic patterns and impending augury. *Journal of Clinical Bioinformatics*, 3(14): 1-7. [20439113, IF: 2.09]
- 91. Naresh Kumar Manchukonda, **Pradeep Kumar Naik\***, Seneha Santoshi, Manu Lopus, Silja Joseph, Balasubramanian Sridhar, Srinivas Kantevari (2013). Rational design, synthesis and biological evaluation of third generation α-noscapine analogues as potent tubulin binding anticancer agents. *PLoS One*, 8(10): e77970. [ISSN: 1932-6203, IF: 3.730]
- 90. Kanu Priya Aggarwal, Simran Tandon, **Pradeep Kumar Naik**, Shrawan Kumar Singh and Chanderdeep Tandon (2013). Peeping into human renal calcium oxalate stone matrix: characterization of novel proteins involved in the intricate mechanism of urolithiasis. *PLoS One*, 8(7): e69916. [ISSN: 1932-6203, IF: 3.730]
- 89. Kanu Priya Aggarwal, Simran Tandon, **Pradeep Kumar Naik**, Shrawan Kumar Singh, Chanderdeep Tandon (2013). Novel antilithiatic cationic proteins from human calcium oxalate renal stone matrix identified by MALDI-TOF-MS endowed with cytoprotective potential: An insight into the molecular mechanism of urolithiasis. *Clinica Chimica Acta*, 415: 181-190. [ISSN: 0009-8981, IF: 2.850]
- 88. Dipankar Sengupta, Priyanka Arora, Shradha Pant, **Pradeep Kumar Naik\*** (2013). Design of dimensional model for clinical data storage and analysis. *Applied Medical Informatics*, 32(2): 47-53. [ISSN: 1224-5593]
- 87. Kar B, Nanda S, **Naik P. K**, Nayak S and Joshi R.K (2013). Molecular characterization and functional analysis of CzR1, a coiled-coil nucleotide binding site leucine rich repeat R-gene from *Curcuma dezoaria* (Loeb.) that confers resistance to *Pythium aphanidermatum*. *Physiological and Molecular Plant Pathology*, 83: 59-68. [ISSN: 0885-5765, IF: 1.506]
- 86. Manya Sharma and **Pradeep Kumar Naik\*** (2013). To study the mode and mechanism of interaction of Angiopoietin II with receptor tyrosine kinase (Tie-2) using molecular mechanics and molecular dynamics approach. *Int. J. Fundamental Applied Science*, 2(1): 8-11. [ISSN: 2278-1404]
- 85. N.B. Singh, M.K. Singh, **P.K. Naik**, S. Thakur and J.P. Sharma (2013). Analysis of genetic diversity in female, male and half sibs willow genotypes through RAPD and SSR markers. *African Journal of Biotechnology*, 12(29):4578-4587. [ISSN: 1684-5315]
- 84. Joshi R.K, Nanda S, Rout E, Kar B, **Naik P. K** and Nayak S (2013). Molecular modeling and docking characterization of CzR1, a CC-NBS-LRR gene from *Curcuma dezoaria* (Loeb.) that confers resistance to *Pythium aphanidermatum*. *Bioinformation* 9(11): 560-564. [ISSN: 0973-2063, IF: 1.0]
- 83. Dipankar Sengupta, Meemansa Sood, Poorvika Vijayvargia, Sunil Hota, **Pradeep K. Naik\*** (2013). Association rule mining based study for identification of clinical parameters akin to occurrence of brain tumor. *Bioinformation*, 9(11): 555-559. [ISSN: 0973-2063, IF: 1.0]

#### **Year 2012**

82. **Pradeep K. Naik\***, Manu Lopus, Ritu Aneja, Surya N. Vangapandu and Harish C. Joshi (2012). In silico inspired design and synthesis of a novel tubulin-binding anti-cancer drug: folate conjugated noscapine (Targetin). *Journal Computer aided molecular design*, 26(2): 233-247. [ISSN: 0920-654X, IF: 3.172]

- 81. Manchukonda NK, Sridhar B, **Pradeep K. Naik**, Harish C. Joshi, Srinivas Kantevari (2012). Copper(I) mediated facile synthesis of potent tubulin polymerization inhibitor, 9-amino-αnoscapine from natural α-noscapine. *Bioorganic Medicinal Chemistry Letter*, 22(8): 2983-2987. [ISSN: 0960-894X, IF: 2.338]
- 80. **Pradeep K. Naik\***, Seneha Santoshi and Harish C. Joshi (2012). Noscapinoids with anti-cancer activity against human acute lymphoblastic leukemia cells (CEM): a three dimensional chemical space pharmacophore modeling and electronic feature analysis. *Journal of Molecular Modeling*, 18(1): 307-318. [ISSN: 1610-2940, IF: 1.984]
- 79. Nidhi Gupta, **Pradeep K. Naik** and Rajinder Singh Chauhan (2012). Differential transcript profiling through cDNA-AFLP showed complexity of rutin biosynthesis and accumulation in seeds of a nutraceutical food crop (Fragopyrum spp.). *BMC Genomics*, 13(1): 231, PMID: 22686486. [ISSN: 1471-2164, IF: 4.40]
- 78. Saurabh Pandit, Kirti Shitiz, Hemant Sood, **Pradeep K. Naik** and Rajinder S. Chauhan (2012). Expression pattern of fifteen genes of non-mevalonate (MEP) and mevalonate (MVA) pathways in different tissues of endangered medicinal herb Picrorhiza kurroa with respect to picrosides content. *Molecular Biology Report*, 40(2): 1053-1063. [ISSN: 0301-4851, IF: 2.506]
- 77. Rajani K. Mahapatra, Niranjan Behera and **Pradeep K. Naik\*** (2012). Molecular modeling and evaluation of binding mode and affinity of artemisinin-quinine hybrid and its congeners with Fe-protoporphyrin-IX as a putative receptor. *Bioinformation*, 8(8): 369-380. [ISSN: 0973-2063, IF: 1.0]
- 76. Sunil Gupta, Manish S. Bhoyar, Jitendra Kumar, Ashish R. Warghat, Prabodh K. Bajpai, Muzamil Rasool, Gyan P. Mishra, **Pradeep K. Naik** and Ravi B. Srivastava (2012). Genetic diversity among natural populations of *Rhodiola imbricata* Edgew. from trans- Himalayan cold arid desert using random amplified polymorphic DNA (RAPD) and inter simple sequence repeat (ISSR) markers. *Journal of Medicinal Plant Research*, 6(3): 405-415. [ISSN: 1996-0875]
- 75. Chandan Singh, Ritesh K. Baboota, **Pradeep K. Naik** and Harvinder Singh (2012). Biocompatible synthesis of silver and gold nanoparticles using leaf extract of *Dalbergia sissoo*. *Advanced Materials Letters*, 3(4):279-285. [ISSN: 0976-3961]
- 74. Rajani K. Mahapatra, Niranjan Behera and **Pradeep K. Naik\*** (2012). Molecular modelling and prediction of binding mode and relative binding affinity of Art-Qui-OH with *P. falciparum* Histo-Aspartic Protease (HAP). *Bioinformation*, 8(17): 827-833. [ISSN: 0973-2063, IF: 1.0]
- 73. Manish S Bhoyar, Gyan P. Mishra, **Pradeep K Naik\***, Ashutosh A Murkute and R. B. Srivastava (2012). Genetic variability studies among natural populations of *Capparis spinosa* from cold arid desert of trans-Himalayas using DNA markers. *National Academic Science Letter*, 35(6): 505-515. [ISSN: 0250-541X, IF: 0.067]
- 72. Anil Kumar, Ravinder Kumar, Vikas Beniwal, Sheo Narain Kala, Anamika Mishra, Ashwin Ashok Raut, **Pradeep Kumar Naik\*** and Vinod Chhokar (2012). Molecular differentiation of Peroxysome proliferator activated receptor coactivator-1 among different breeds of *Bubalus bubalis*. *Bioinformation*, 8(13): 600–606. [ISSN: 0973-2063, IF: 1.0]
- 71. Sankalp Jain, Piyush Ranjan, Dipankar Sengupts and **Pradeep K. Naik\*** (2012). TpPred: A tool for hierarchical prediction of transport proteins using cluster of neural networks and sequence derived features. *International Journal of Computational Biology*, 1(1): 46-60. [ISSN: 2278-8115]
- 70. Shruti Jain, **Pradeep K. Naik\*** and Sunil V. Bhooshan (2012). Compendium model of AKT for cell survival/death and its equivalent bio-circuit. *International Journal of soft Computing and Engineering*, 2(3): 91-97. [ISSN: 2231-2307, IF: 1.0]

- 69. Shruti Jain and **Pradeep K. Naik\*** (2012). System modelling of cell survival and cell death: A deterministic model using Fuzzy system. *International Journal of Pharma and Bio Sciences*, 3(4): 358-373. [ISSN: 0975-6299, IF: 0.67]
- 68. Shruti Jain, Sunil V. Bhooshan and **Pradeep K. Naik\*** (2012). Communication of signals and responses leading to cell death using Engineered Regulatory Networks. *Research Journal of Pharmaceutical, Biological and Chemical Sciences*, 3(3): 492-508. [ISSN: 0975-8585]
- 67. Jitendra Kumar, Gyan P. Mishra, Ashutosh A. Murkute, G. Phani Kumar, **Pradeep K. Naik\*** and R. B. Srivastava (2012). Exploring genetic relationships in *Artemisia* species growing in trans-Himalayan cold arid desert using RAPD markers. *Indian Journal of Horticulture*, 69(2):239-245. [ISSN: 0972-8538, IF: 0.229]
- 66. Jitendra Kumar, Prasad Bajaj, Harvinder Singh, Gyan P. Mishra, Shashi Bala Singh and **Pradeep K. Naik\*** (2012). Utilization of Intron-flanking EST-specific Markers in the genetic characterization of *Artemisia annua* genotypes from the trans-Himalayan region of Ladakh, India. *Journal of Environmental Biology*, 33, 991-997. [ISSN: 0254-8704, IF: 0.64]
- 65. Anil Kumar, Vinod Chhokar, Ravinder Kumar, Vikas Beniwal, S. N. Kala, Anamika Mishra, Ashwin Ashok Raut and **Pradeep K. Naik** (2012). Molecular differentiation of mitochondrial glycerol-3-phosphate acyltransferase among different breeds of *Bubalus bubalis*. *International Journal of Pharma and Bio Sciences*, 3(4): (B) 685-694. [ISSN: 0975-6299, IF: 0.67]
- 64. Seneha Santoshi and **Pradeep Kumar Naik\*** (2012). A field based 3D QSAR model of novel anti-microtubule agent noscapine and its derivatives. *International Journal of Fundamental & Applied Sciences*, 1(2): 81-87. [ISSN: 2278-1404]
- 63. Charu Suri and **Pradeep Kumar Naik\*** (2012). Elucidating the precise interaction of reduced and oxidized states of neuroglobin with Ubc12 and Cop9 using molecular mechanics studies. *International Journal of Fundamental & Applied Sciences*, 1(2): 74-77. [ISSN: 2278-1404]

- 62. **Pradeep K. Naik\***, Biswa Prasun Chatterji, Surya N. Vangapandu, Ritu Aneja, Ramesh Chandra, Srinivas Kanteveri and Harish C. Joshi (2011). Rational design, synthesis and biological evaluations of amino-noscapine: A high affinity tubulin-binding noscapinoid. *Journal Computer Aided Drug Design*, 25(5): 443-454. [ISSN: 0920-654X, IF: 3.386]
- 61. **Pradeep K. Naik\***, Seneha Santoshi, Ankit Rai and Harish C. Joshi (2011). Molecular modelling and competition binding of Br-noscapine and colchicine provides insight into noscapinoid-tubulin binding site. *Journal of Molecular Graphics and Modeling*, 29(7): 947-955. [ISSN: 1093-3263, IF: 2.325]
- 60. Seneha Santoshi, **Pradeep K. Naik\*** and Harish C. Joshi (2011). Rational design of novel antimicrotubule agent (9-azido-noscapine) from quantitative structure activity relationship (QSAR) evaluation of noscapinoids. *Journal of Biomolecular Screening*, 16(9):1047-1058. [ISSN: 1087-0571, IF: 2.207]
- 59. **Pradeep K. Naik\***, Mani Srivastava, Prasad Bajaj, Sankalp Jain, Abhishek Dubey, Piyush Ranjan, Rishay Kumar and Harvinder Singh (2011). The Binding modes and binding affinities of artemisinin derivatives with *Plasmodium falciparum* Ca<sup>2+</sup>-ATPase (PfATP6). *Journal of molecular modeling*, 17(2): 333-357. [ISSN: 1610-2940, IF: 1.797]
- 58. Priyadarshini Pathak, **Pradeep K. Naik**, Dipankar Sengupta, Shrawan K. Singh, Chanderdeep Tandon (2011). Mode of interaction of calcium oxalate crystal with human phosphate cytidylyltransferase 1: a novel inhibitor purified from human renal stone matrix. *J. Biomedical Science and Engineering*, 4: 591-598. [ISSN: 1937-6871]

- 57. Pani A, Mahapatra RK, Behera N, **Naik PK** (2011). Computational identification of sweet wormwood (*Artemisia annua*) microRNA and their mRNA targets. *Genomics Proteomics Bioinformatics*, 9(6): 200-210. [ISSN: 1672-0229]
- 56. **Pradeep K. Naik\***, Piyush Ranjan, Pooja Kesari and Sankalp Jain (2011). MetalloPred: A tool for hierarchical prediction of metal ion binding proteins using cluster of neural networks and sequence derived features. *Journal of Biophysical Chemistry*, 2(2): 112-123. [ISSN: 2153-036X]
- 55. Chandan Singh, Vineet Sharma, **Pradeep K. Naik**, Vikas Khandelwal and Harvinder Singh (2011). A green biogenic approach for synthesis of gold and silver nanoparticles using *Zingiber officinale*. *Digest Journal of Nanomaterials and Biostructures*, 6(2): 535-542. [ISSN: 1842-3582, IF: 2.078]
- 54. Jitendra Kumar, Gyan P. Mishra, **Pradeep K. Naik\***, Ashutosh A. Murkute and Ravi B. Srivastava (2011) Genomic DNA isolation from *Artemisia* species grown in cold desert high altitude of India. *African Journal of Biotechnology*, 10(37): 7303-7307. [ISSN: 1684-5315]
- 53. Manish S Bhoyar, Gyan P. Mishra, **Pradeep K Naik\*** and R.B. Srivastava (2011). Estimation of antioxidant activity and total phenolics among natural populations of *Capparis spinosa* leaves collected from cold arid desert of trans-Himalayas. *Australian Journal of Crop Sciences*, 5(7): 912-919. [ISSN: 1835-2693, IF: 1.632]
- 52. Jitendra Kumar, Harvinder Singh, Gyan P. Mishra, Ravi B. Srivastava and **Pradeep K. Naik\*** (2011). Genetic analysis of *Artemisia annua* genotypes using RAPD and ISSR molecular markers from the trans-Himalayan (Ladakh, India) region. *Journal of Medicinal Plant Research*, 5(23):5568-5576. [ISSN: 1996-0875]
- 51. Shruti Jain, Sunil V. Bhoosan and **Pradeep K. Naik**\* (2011). Mathematical modeling deciphering balance between cell survival and cell death using insulin. *Network Biology*, 1(1): 46-58. [ISSN: 2220-8879]
- 50. Shruti Jain, Sunil V. Bhooshan and **Pradeep K. Naik\*** (2011). Mathematical modeling deciphering balance between cell survival and cell death using tumor necrosis factor α. *Research Journal of Pharmaceutical, Biological and Chemical Sciences*, 2(3): 574-583. [ISSN: 0975-8585]
- 49. Shruti Jain, **Pradeep K. Naik**\* and Sunil V. Bhooshan (2011). A computational model for cell survival/death using petrinets. *International Journal of Applied Engineering Research*, 6(5): 545-552. [ISSN: 0973-4562]

- 48. Kunal Jaiswal, Chandan Kumar and **Pradeep K. Naik\*** (2010). Prediction of EF-hand calciumbinding proteins and identification of calcium-binding regions using machine learning techniques. *Journal of Cell and Molecular Biology*, 8(2): 41-49. [ISSN: 1303-3646]
- 47. **Pradeep K. Naik\***, Abhishek Dubey, Komal Soni, Rishay Kumar and Harvinder Singh (2010). The binding modes and binding affinities of epipodophyllotoxin derivatives with human topoisomerase IIα. *Journal of Molecular Graphics and Modeling*, 29(4): 546-564. [ISSN: 1093-3263, IF: 2.033]
- 46. Komal Soni, Shruti Rawat, Ankit Gupta, Karma Yangzom, Saurabh Pandit, **Pradeep K. Naik** and Harvinder Singh (2010). Genetic characterization of *Rhodiola rosea* using gene specific SSR and CAPS molecular markers. *Genetic Engineering and Biotechnology Journal*, GEBJ-11. [ISSN: 2150-3516]
- 45. **Pradeep K. Naik\***, Abhishek Dubey and Rishay Kumar (2010). Development of predictive quantitative structure activity relationship models of epipodophyllotoxin derivatives. *Journal of Biomolecular Screening*, 15(10): 1194-1203. [ISSN: 1087-0571, IF: 2.5]

- 44. **Pradeep K. Naik\***, Md. Afroz Alam, Ashutosh Malhotra and Owasis Rizvi (2010). Molecular Modeling and Structure-activity relationship of the podophyllotoxin and its congeners. *Journal of Biomolecular Screening*, 15(5): 528-540. [ISSN: 1087-0571, IF: 2.5]
- 43. **Pradeep K. Naik\***, Md. Afroz Alam, Harvinder Singh, Vinod Goyal, Swarup Parida, Sanjay Kalia and T. Mohapatra (2010). Assessment of genetic diversity through RAPD, ISSR and AFLP markers in *Podophyllum hexandrum*: a medicinal herb from the Northwestern Himalayan region. *Physiology and Molecular Biology of Plants*, 16(2): 1-14. [ISSN: 0971-5894]
- 42. **Pradeep K. Naik\***, Seneha Santoshi and Ashima Birmani (2010). Computational prediction of potent therapeutic targets of *Pseudomonas aeruginosa* and in silico virtual screening for novel inhibitors. *Internet Electronic Journal of Molecular Design*, 8: 42–62. [ISSN: 1538-6414]
- 41. Shruti Jain, Sunil V. Bhooshan, **Pradeep K. Naik\*** (2010). Model of Mitogen Activated Protein Kinases for Cell Survival/Death and its Equivalent Bio-Circuit. *Current Research Journal of Biological Sciences*, 2(1): 59-71. [ISSN: 2041-0778]
- 40. Mani Srivastava, Harvinder Singh and **Pradeep K. Naik\*** (2010). Molecular modeling evaluation of the antimalerial activity of artemisinin analogues: molecular docking and rescoring using Prime/MM-GBSA approach. *Current Research Journal of Biological Sciences*, 2(2): 83-102. [ISSN: 2041-0778]
- 39. **Pradeep K. Naik\***, Seneha Santoshi and Ashima Birmani (2010). Computational prediction of potent therapeutic targets of *Pseudomonas syringae* and *in silico* virtual screening for novel inhibitors. *International Journal of Pharma and Bio Sciences*, 1(2): 1- 23. [ISSN: 0975-6299, IF: 0.47]
- 38. Shruti Jain, **Pradeep K. Naik\*** and Sunil V. Bhooshan (2010). Petri net implementation of cell signaling for cell death. *International Journal of Pharma and Bio Sciences*, 1(2): 1-18. [ISSN: 0975-6299, IF: 0.47]
- 37. Shruti Jain, Sunil V. Bhooshan and **Pradeep K. Naik\*** (2010). Caspase: leads to apoptosis using VHDL and SPICE. *International Journal of Electronics and Computers*, 2(1): 9-17. [ISSN: 0975-3796]
- 36. Shruti Jain, **Pradeep K. Naik\*** and Sunil V. Bhooshan (2010). Computational modeling of cell survival/death using BiCMOS. *International Journal of Computer Theory and Engineering*, 2(4): 478-481. [ISSN: 1793-8201]
- 35. Shruti Jain and **Pradeep K. Naik\*** (2010). Computational modeling of cell survival using VHDL. *BVICAM,s International Journal of Information Technology*, 2: 47-51. [ISSN: 0973-5658]
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- 7. Seneha Santoshi and **Pradeep K. Naik** (2012). Evaluation of structure activity relationship of noscapinoids utilizing field based 3D QSAR modeling. National conference on Computational Biology, Pharmaceutics & Life Sciences, Bangalore, India, November 23-24.
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- 21. S. Marla, S. Nayak, **P.K. Naik** and R. Arrora (**2004**). Rights of farmers cultivating medicinal plants and some recommendations. Abstract published in National Seminar on Intelectual Property Rights in Horticultural Crops, Held in Dr. Y.S. Parmer University of Horticulture and Forestry, Solan, India.

### RESEARCH:

## Associate Professor, Jaypee University, Himachal Pradesh, India August 2011 – present

• Presently working on tubulin-binding anticancer drugs, noscapine, and its rationally-designed chemically-synthesized more potent analogs. Investigating the effect of these drugs on cellular proliferation (SRB, MTT), cell cycle using flow-cytometry, spindle architecture using

- immunofluorescence confocal microscopy, apoptosis (Annexin-V, TUNEL assays), mitochondrial membrane potential using flow cytometry and confocal microscopy, tubulin binding assay and tubulin polymerization assay.
- Studying *in vivo* tumor inhibition and regression by more potent noscapine analogs utilizing xenograft models of various human cancers (breast, prostate, ovarian) in nude mice, and evaluation of toxicity by histopathology, immunohistochemical techniques as well as hematological toxicities using FACS analyses
- Studying the molecular basis of interactions between Tyrosine kinase receptor-2 (Tie2) and Activated protein C (APC) as well as Tie2 and Angiopoietin to investigate whether APC protects endothelial barrier function through angiopoietin/Tie2 axis leading to protective effect in sever sepsis and other disorders associated with vascular abnormalities. The possibility of interaction between Tie2 and APC has been studying based on protein-protein docking, molecular dynamic simulation, binding affinity calculation using MM-GBSA and MM-PBSA simulation, prediction of hot spot amino acids and alanine scanning mutations followed by experimental validation.
- Studying the molecular basis of interactions between Neuroglobin with UBC12 and COP9 to investigate the role of these proteins in regulating the process of protein neddylation and deneddylation. We are using protein-protein docking, molecular dynamic simulation, binding affinity calculation using MM-GBSA and MM-PBSA simulation, prediction of hot spot amino acids and alanine scanning mutations to identify the possibility of molecular interaction followed by experimental validation.
- Studying the molecular hallmarks in the nucleation of microtubules in the microtubule organizing center. To dissect the nucleation process we are investigating the molecular basis of interactions between Y-tubulin with  $\sigma$  and  $\beta$  tubulin as well as Y-tubulin with GCP4. We are using protein-protein docking, molecular dynamic simulation, binding affinity calculation using MM-GBSA and MM-PBSA simulation, prediction of hot spot amino acids and alanine scanning mutations to identify the possibility of molecular interaction followed by experimental validation.
- Studying the toxicity of herbal formulations such as: (a) herbal performance enhancing capsules (PerfoMAX), (b) herbal adaptogenic appetizer, (c) herbal tea and (d) Seabuckthorn oil based soft gel capsule developed by DIHAR, DRDO. We are performing the toxicological evaluation such as: (a) acute toxicity, (b) sub-acute toxicity, and (c) chronic toxicity of oral administration of above herbal formulations as per "The Organization for Economic Cooperation and Development (OECD) test guidelines" in rats. Hematological and histological examination of all the vital organs including liver, heart, kidney, lungs, large intestine, small intestine, stomach and brain are performing for any evidence of toxicity caused by herbal formulation.
- Designing a business intelligence model to store and analyze the diverse form of clinical data set for army personnel's and hospital patients. We are developing a clinical data warehouse (Kimball Model) using MySQL RDBMS, which can store the information for patients in temporal form i.e. for each visit to hospital or any diagnosis being conducted, the record will be stored uniquely corresponding to date and time dimension respectively. Also we are analyzing the various clinical parameters with respect to a specific disease and discover associative rules among it. Besides applying traditional data mining algorithms to deduce the hidden information from the warehouse, we are also developing new temporal mining algorithm, which would help to analyze a particular disease based on its associated clinical parameters at different time points and help to predict future state which can be augured with the disease.
- Studying on DNA profiling, mitogenomics and stress analysis of highly endangered Western Tragopan (state bird of Himachal Pradesh) and Cheer Pheasants in avoiding the inbreeding, increasing the hatchability of eggs in these birds and create DNA barcoding for conservation

breeding. We are establishing the parental lineage of the captive populations based on DNA barcoding of mitochondrial/nuclear genome sequences as well as DNA profiling using molecular markers (RAPD, ISSR and SSR). Furthermore, sequencing and annotating the entire mitochondrial genome of both the species to establish the syntenic relationship with available genomic resources of pheasant species. Determining the elemental composition of egg shells from both the bird species to understand the environmental contamination or nutrient deficiency if any to improve the life of both the pheasant species.

- Developed various online prediction servers for biological sequence (both protein and DNA) analysis and functional annotations.
  - MetalloPred: A tool for hierarchical screening of metal ion binding proteins from protein sequence using cluster of neural networks and sequence derived features.
  - TpPred: A tool for hierarchical screening of various transport proteins from protein sequence using cluster of neural networks and sequence derived features.

## BOYSCAST Fellow, Emory University School of Medicine, Georgia, USA July 2010-July 2011

The research work undertaken at Emory University School of Medicine as BOYSCAST Fellow includes rational design of potent noscapine derivatives, their chemical synthesis and biological evaluation as anti-cancer drugs. The outline of my research work was as follows.

- Rational design of potent noscapine derivatives (noscapinoids) based on *in silico* approaches such as quantitative structure activity relationship (QSAR) model, molecular docking, and molecular mechanics-generalize Born solvation area (MM-GBSA) and linear interaction energy method with a surface generalized Born (SGB) continuum solvation model.
- Developed a three dimensional chemical space pharmacophore model for anti-cancer activity against human acute lymphoblastoid leukaemia cells.
- Systematic synthesis of designed noscapinoids with high yield, purification (column chromatography and HPLC analysis) and chemical characterization (1D and 2D NMR).
- The biological evaluation of designed noscapinoids based on cell line assay to calculate the IC<sub>50</sub> value with various types of cancers, tubulin binding assay, microtubule polymer recovery assay, perturbation in microtubule dynamics, measuring apoptotic index, measuring mitotic cell cycle progression and sensitivity analysis of designed noscapinoids with the panel of 60 human cancer cell lines of various tissue origins.
- Elucidated the site of interaction and binding affinity of designed noscapinoids with tubulin and their experimental validation based on competition binding study with colchicine.

## Assistant Professor, Jaypee University, Himachal Pradesh, India July 2008 – June 2010

- Genetic variation among the *Podophyllum hexandrum* populations from the north-western Himalayas (Himachal Pradesh) was investigated using DNA profiling techniques such as RAPD, ISSR, AFLP, etc. and correlated with podophyllotoxin content. High genetic variation among the populations of *P. hexandrum* was revealed using above molecular markers reveals that any future conservation plans for this species should be specifically designed to include representative populations with the highest genetic variation for both *in situ* conservation and germplasm collection expeditions. Whereas the yield of podophyllotoxin is not related to the genetic variations but related to environmental factors.
- Studied the relationship between the environmental factors and podophyllotoxin yield in the diminishing wild populations of *P. hexandrum* in the north-western Himalayas, Himachal Pradesh and developed prediction model for selection of conservation area for commercial cultivation of *P. hexandrum* populations.

- Studied the genetic diversity among the genotypes and populations of *Artemisia annua* based on DNA profiling techniques utilizing dominant molecular markers such as RAPD and ISSR as well as co-dominant markers such as EST-derived SSRs and intron-flanking EST-specific markers in the Ladakh region, India. High genetic variation measured among the genotypes of *Artemisia annua* using above molecular markers reveals that any future conservation plans for this species should be specifically designed to include representative populations with the highest genetic variation for both *in situ* conservation and germplasm collection expeditions.
- Extracted and measured the artemisinin content at different developmental stages from *Artemisia annua* L. collected from Ladakh region. The artemisinin content of the plant varied significantly with respect to their geographical distribution. The artemisinin content of leaf was detected to be maximum during reproductive stage (in the month of August), whereas in the inflorescence it was detected to be highest at full flowering stages (in the month of September).
- A new and alternative source of artemisinin was screened out by screening other species of *Artemisia* growing in cold arid desert of trans-Himalayas (Ladakh, India). The species *A. tournefortiana* identified as an alternative source consists of even high artemisinin in the inflorescence in comparison to *A. annua* and therefore could be a great potential for artemisinin content.
- Investigated the rate of seed germination, genetic diversity, antioxidant activity and nutritional content of flower buds of the population of *Capparis spinosa* from the Ladhak region for commercial cultivation. *Capparis spinosa* has long been used by the natives of Ladakh as leafy vegetable, forage and used in cuisine as salad, pickle and condiments. Several types of medicinal preparations from *Capparis* are being used for the treatment of various ailments like gastrointestinal infection, diarrhoea and rheumatism. Very poor seed germination is the major problem in the wide scale cultivation of caper bush in the trans-Himalayan region. Seed germination was increased significantly by different types of treatments suggesting effective breaking of physical and physiological dormancy. High genetic variation was observed among the genotypes using RAPD and ISSR molecular markers. All the edible parts including leaves of *C. spinosa* contain significant amount of polyphenols and possess a strong antioxidant/free radical scavenging activity. Flower buds consist of more nutritional contents than the other parts of the world. Therefore it can be used as nutritional supplements.
- Studied the genetic variability among genotypes of Apricot and *Rhodiola rosea* collected from different regions of cold arid desert of Ladhak using different DNA markers such as RAPD, ISSR and SSR.
- Developed quantitative structure activity relationship models for the prediction of biological
  activity and screening of potent derivatives of podophyllotoxin, epipodophyllotoxin,
  artemisinin and insecticides. Further developed several structure based computational models
  based on molecular docking, MM-GBSA and LIE-SGB for prediction of binding affinity and
  cytotoxicity activity of podophyllotoxin analogs. Binding affinity of artemisinin derivatives
  with haeme were also computed based on developed structure based computational models.
  These techniques guided in development of more potent derivatives with better therapeutic
  outcome.
- Studied the binding modes and binding affinity of artemisinin derivatives with *Plasmodium falciparum* Ca<sup>2+</sup>-ATPase (PfATP6) to understand the anti-malarial activity of these compounds. Similarly studied the possible interaction of epipodophyllotoxin derivatives with human topoisomerase IIα pertaining to anti-cancer activity of these compounds.

- Developed various online prediction servers for biological sequence (both protein and DNA) analysis and functional annotations.
  - CalPred: A tool for screening of EF-hand calcium binding proteins and identification of calcium-binding regions from protein sequence using ANN and SVM machine learning techniques.
  - RetroPred: A tool for prediction, classification and extraction of non-LTR retrotransposons (LINEs and SINEs) from the genome sequence through pipelines of PALS, PILER, MEME and ANN.

## Senior Lecturer, Jaypee University, Himachal Pradesh, India July 2005 – June 2008

- Genetic characterization of different genotypes of *Jatropha curcas*, turmeric and ginger was performed using RAPD and ISSR molecular markers.
- Studied the mode of interaction and binding affinity of Nevirapine and its analogues as well as Delvardine and its analogues onto the HIV-1 reverse transcriptase for screening of potent derivatives pertaining to anti-HIV activity.
- Developed online prediction server for prediction of enzymes and non-enzymes from protein sequence based on sequence derived features and PSSM matrix using artificial neural network. Similarly developed a prediction model for the prediction of anticancer and non-anticancer drugs based on comparative molecular moment descriptors using artificial neural network and support vector machine.

## Ph.D research works, Sambalpur University, Orissa, India Nov 1996 - Dec2001

• The experiments conducted have revealed that the ethylene is the causal agent for poor development of basal spikelets of rice panicle, which affects grain yield and quality. Application of inhibitors of ethylene action and synthesis successfully overcome the problem and boost grain production from rice cultivars. Analyses of ethylene concentration and the dry matter partitioning processes of the spikelets from contrasting position of the panicle and the effect of inhibitors have confirmed this proposition.

#### **MANUSCRIPT REVIEWER FOR:**

Expert reviewer for various scientific journals (Molecular Pharmaceutics; PLoS ONE; BMC Bioinformatics; Industrial Crop and Products; Molecular Modeling; Current Chemical Biology; Molecular Diversity; SAR QSAR in Env. Research; Recent Patents on DNA and Gene Sequence; BMC Cancer Biology; Drug Design, Development and Therapy; Plant Omics Journal; Current Computer Aided Drug Design; Indian Journal of Biotechnology; Journal of Biophysical Chemistry)

# **Personal Details:**

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