


NAME	Mukesh Chourasia	
DESIGNATION	Assistant Professor-II	
EMAIL ID	mchourasia@gmail.com	
CONTACT NUMBER	+91-9576161682	

RESEARCH INTERESTS

The main objective of my research is to build concepts which are based on Quantum Mechanics (QM), Molecular Mechanics (MM) and QM/MM and can guide experiments in new directions. I integrate all these three methods to study mechanisms and phenomenon governing pharmaceutically important bio-macromolecules. My three main research areas are:

1. Reaction mechanisms of therapeutic targets
2. Computer Aided Drug Design
3. Dynamics and signaling mechanism of proteins

EDUCATIONAL QUALIFICATIONS:

Name of College / University	Degree	Year
CSIR-Indian Institute of Chemical Technology, Hyderabad, India.	Ph.D. in Biochemistry (Computational Biology)	2010
Bioinformatics Institute of India, Noida.	Post Graduate Diploma in Bioinformatics	2003
College of Life Sciences, Cancer Hospital and Research Institute, Jiwaji University, Gwalior.	Masters in Applied Biochemistry	2001
Science College, Jiwaji University, Gwalior.	Bachelors in Environmental Science	1999

Title of Ph.D. thesis : Modelling Biomolecules: Studies on P-Type ATPases, DNA-ligand Interactions and π - π Networks in Proteins.

EXPERIENCE (in chronological order)

Designation	Type of post held (teaching/ research)	Name of the Institute	Year (From – To)
Assistant Professor	Teaching and research	Center for Computational Biology and Bioinformatics, Amity Institute of Biotechnology, Amity University, Noida	2018-Present
Senior Lecturer	Teaching and research	Department of Pharmacoinformatics, National Institute of Pharmaceutical Research and Education - Hajipur	2014-2018
Post-doctoral fellow	Research	Institute for Drug Research, School of Pharmacy, Faculty of Medicine, The Hebrew University of Jerusalem, Israel.	2012-2014
Post-doctoral fellow	Research	The Lise Meitner-Minerva Center for Computational Quantum Chemistry, Institute of Chemistry, The Hebrew University of Jerusalem, Israel.	2010-2012

No. of Ph.D. students supervised	Awarded: (no. only)
	Ongoing: (no. only)
<p>PUBLICATIONS (16)</p>	<ol style="list-style-type: none"> 1. Anil Singh, Sabrina Fechtner, Mukesh Chourasia, Jerry Sicalo, and Salahuddin Ahmed. Critical role of IL-1a in IL-1b–induced inflammatory responses: cooperation with NF-kBp65 in transcriptional regulation. <i>FASEB J.</i>, 2018 (Accepted) (IF: 5.498) 2. Sabrina Fechtner, Anil K. Singh, Mukesh Chourasia, Salahuddin Ahmed. Molecular insights into the differences in anti-inflammatory activities of green tea catechins on IL-1β signaling in rheumatoid arthritis synovial fibroblasts. <i>Toxicol Appl Pharmacol.</i> 2017; 329:112-120.(IF: 4.006) 3. Ranu Agrawal, Nazia Tarannum, Mukesh Chourasia and Rakesh Kumar Soni. Chemical Degradation of Poly(ethylene terephthalate) for Potential Antimicrobial Activity Evaluation and Molecular Docking Study. <i>Journal of Polymers and the Environment.</i> 2017; 1-11. (IF: 1.877) 4. Akbar Pathan, Bhavana Panthi, Zahid Khan, Purushotham Reddy Koppula, Mohammed Saud Alanazi, Narasimha Reddy Parine, Sachchidanand, Mukesh Chourasia*. Lead Identification for the K-Ras Protein: Virtual Screening and Combinatorial Fragment Based Approaches. <i>OncoTargets and Therapy.</i> 2016; 9: 2575-2584. (IF: 2.711) 5. Ewa Kozelaa, Christeene Haj, Lumir Hanuš, Mukesh Chourasia, Avital Shurki, Ana Juknat, Nathali Kaushansky, Raphael Mechoulam, Zvi Vogel. HU-446 and HU-465, derivatives of the non-psychoactive cannabinoid cannabidiol, decrease the activation of encephalitogenic T cells. <i>Chem. Biol. Drug. Des.</i> 2016; 87: 143-153. (IF: 2.396) 6. Anil K. Singh, Sadiq Umar, Sharayah Riegsecker, Mukesh Chourasia, Salahuddin Ahmed. Regulation of TAK1 activation by epigallocatechin-3-gallate in RA synovial fibroblasts: suppression of K63-linked autoubiquitination of TRAF6. <i>Arthritis Rheumatol.</i>, 2016; 68: 347-358. (IF: 7.764) [<i>Published as cover page article and cited in many National and International news papers</i>] 7. Reem Smoum, Saja Baraghithy, Mukesh Chourasia, Aviva Breuer, Naama Mussai, Malka Attar-Namdar, Natalya M. Kogan, Bitya Raphael, Daniele Bolognini, Maria G. Cascio, Pietro Marini, Roger G. Pertwee, Avital Shurki, Raphael Mechoulam, and Itai Bab. CB2 cannabinoid receptor agonist enantiomers HU-433 and HU-308: An inverse relationship between binding affinity and biological potency. <i>Proc. Natl. Acad. Sci. U S A.</i> 2015; 112: 8774-8779. (IF: 9.661) 8. Tamar Ansbacher, Mukesh Chourasia, Avital Shurki.

	<p>Copper-chaperones with di-coordinated Cu(I) - unique protection mechanism. <i>Proteins: Structure, Function, and Bioinformatics</i>. 2013; 81:4011-4019. (IF: 2.289)</p> <p>9. Usha Dandamudi, Costantino Zazza, Wenzhen Lai, Mukesh Chourasia, Lucy Waskell, Sason Shaik. A Single Site mutation (F429H) Converts the Enzyme CYP 2B4 into a Heme Oxygenase: A QM/MM Study. <i>J. Am. Chem. Soc.</i> 2012; 134:4053–4056. (IF: 13.858)</p> <p>10. Mukesh Chourasia, G. Narahari Sastry. The Nucleotide, Inhibitor, and Cation Binding Sites of P-type II ATPases. <i>Chem. Biol. Drug. Des.</i> 2012; 79:617–627. (IF: 2.396) <i>[Published as cover page article]</i></p> <p>11. Mukesh Chourasia, G. Madhavi Sastry, G. Narahari Sastry. Aromatic – Aromatic Interactions Database, A²ID: An Analysis of Aromatic π-Networks in Proteins. <i>Int. J. Biol. Macromol.</i> 2011; 48:540–552. (IF: 3.671)</p> <p>12. Hemant Kumar Srivastava, Mukesh Chourasia, Devesh Kumar, G. Narahari Sastry. Comparison of Computational Methods to Model DNA Minor Groove Binders. <i>J. Chem. Inf. Model.</i> 2011; 51:558–571. (IF: 3.760)</p> <p>13. Ahmed Kamal, Rajesh V. C. R. N. C. Shetti, M. Janaki Ramaiah, P. Swapna, K. Srinivasa Reddy, A. Mallareddy, M. P. Narasimha Rao, Mukesh Chourasia, G. Narahari Sastry, Aarti Juvekar, Surekha Zingde, Pranjal Sarma, S. N. C. V. L. Pushpavalli, Manika Pal-Bhadra. Carbazole-pyrrolo[2,1-c][1,4]benzodiazepine conjugates: design, synthesis, and biological evaluation. <i>Med. Chem. Commun.</i> 2011; 2:780–788. (IF: 2.608)</p> <p>14. Ahmed Kamal, K. Srinivasa Reddy, Chatla Srinivas, Manika Pal-Bhadra, Mukesh Chourasia, G. Narahari Sastry, <i>et. al.</i> Synthesis, DNA-binding affinity and anticancer activity of benzothiazole/benzoxazole-pyrrolo[2,1-c][1,4]benzodiazepine hybrids. <i>Bioorg. Med. Chem.</i> 2010; 18:4747–4761. (IF: 2.930)</p> <p>15. Ahmed Kamal, Rajender, D. Rajasekhar Reddy, MK. Reddy, G. Balakishan, TB Shaik, Mukesh Chourasia, G. Narahari Sastry. Remarkable enhancement in the DNA-binding ability of C2-fluoro substituted pyrrolo[2,1-c][1,4]benzodiazepines and their anticancer potential. <i>Bioorg. Med. Chem.</i> 2009; 17:1557–1572. (IF: 2.930)</p> <p>16. Mukesh Chourasia, G. Madhavi Sastry, G. Narahari Sastry. Proton binding sites and conformational analysis of H⁺K⁺-ATPase. <i>Biochem. Biophys. Res. Commun.</i> 2005; 336:961–966. (IF: 2.466)</p>
PATENTS (<i>total no.</i>)	<i>Details:</i>

RESEARCH PROJECTS Completed: <i>(total no.)</i> Ongoing: <i>(total no.)</i>	<i>Details:</i>
AWARDS & HONOURS/ DISTINCTIONS	<ol style="list-style-type: none"> 1. PBC Fellowships for Outstanding Post-doctoral Researchers, The Hebrew University of Jerusalem, Israel, 2012-2014. 2. Boehringer Ingelheim Fonds (BIF) funding, Germany, 2007 3. Qualified CSIR/UGC-NET (Life Sciences) held in June 2003. 4. Accelrys Certified Professional course in “Protein Modeling and Rational Drug Designing” from BioCampus, GVK Bio Sciences Pvt. Ltd, Hyderabad in 2003.
MEMBERSHIP with Professional/ Academic bodies	