Name	**MUTHUKUMARASAMY KARTHIKEYAN**
Address	Principal Scientist Information Division, Digital Information Resource Center, National Chemical Laboratory, Pune – 411 008, INDIA
Phone	**91-20-2590 2483** (Preferred) / +91-(0) **97 67 427 981**
Email	m.karthikeyan@ncl.res.in
URL	http://moltable.ncl.res.in
Date of Birth	07-12-1968 (dd-mm-yyyy)
Specialization:	Organic Chemistry (Synthesis) and Chemoinformatics-Bioinformatics for Drug Discovery Research, Computer Science, Robotics (Embedded systems with chemical Sensors for IoT Applications)

EDUCATIONAL BACKGROUND

B.Sc (Chemistry)	**1989**	Pondicherry University, India	**First Class**
MSc (Chemistry)	**1991**	Pondicherry University, India	**First Class**
PhD (Chemistry)	**1998**	CSIR-National Chemical Laboratory, Pune University	Synthetic Organic Chemistry & Photo Induced Electron Transfer Reactions (Supervisor: Dr Ganesh Pandey) 1992-1998
MSc(Computer Sci)	**2014**	Anna University	**First Class**
MBA (Marketing)	**2015**	IGNOU (School of Management)	**First Class** (DIM), PGDIM, PGDMM
PGDIPR **(IPR)**	**2017**	IGNOU (School of Law)	**In Progress**

(b) WORK EXPERIENCE

1998-2000	Scientist B Armament Research Development Establishment (DRDO), Pune – 411 021, INDIA
2000-2005	Scientist C CSIR-National Chemical Laboratory, Pune – 411 008, INDIA
2005-2010	Senior Scientist (Scientist E-1) CSIR-National Chemical Laboratory, Pune – 411 008, INDIA
2010-	Principal Scientist (Scientist E2) CSIR-National Chemical Laboratory, Pune – 411 008, INDIA

Awards/Fellowships

1. 1992-93 Junior Research Fellow (CSIR-National Chemical Laboratory) Dr Ganesh Pandey (PhD Supervisor)
2. 1994-1997 Senior Research Fellow (CSIR-National Chemical Laboratory) Dr Ganesh Pandey (PhD Supervisor)
3. 2003-04 **BOYSCAST** Award (Department of Science and Technology- New Delhi)
4. 2007-08 **Long term Overseas Associate** (Department of Biotechnology- New Delhi)
5. **2015 Codex Innovation Award**, Stanford University, Thomson & Reuters. (Innocentive)

Research Publications

1. Application of Genetic Programming (GP) Formalism for Building Disease Predictive Models from Protein-Protein Interactions (PPI) Data Published in: IEEE/ACM **Transactions on Computational Biology and Bioinformatics (Volume: PP, Issue: 99) Date of Publication: 26 October 2016 Print ISSN: 1545-5963**
2. Building and analysis of protein-protein interactions related to diabetes mellitus using support vector machine, biomedical text mining and network analysis Renu Vyasa, , ,Sanket Bapatb,Esha Jainb,Muthukumarasamy Karthikeyanb,Sanjeev Tambec,Bhaskar D. Kulkarnic **doi.org/10.1016/j.compbiolchem.2016.09.011**
3. **CHEMENGINE:** harvesting 3D chemical structures of supplementary data from PDF files Muthukumarasamy karthikeyanemail authorview ORCID ID profile and Renu Vyas **Journal of Cheminformatics 2016** 8:73 **DOI: 10.1186/s13321-016-0175-x**
4. Spirochromone-chalcone conjugates as antitubercular agents: synthesis, bio evaluation and molecular modeling studies M Muthukrishnan, Mohammad Mujahid, Perumal Yogeeswari, Sriram Dharmarajan, Murali Basavanag, Erik Díaz-Cervantes, Luis Bahena, Juvencio Robles, Rajesh G. Gonnade, Karthikeyan M and Renu Vyas, **RSC Adv**., **2015, DOI: 10.1039/C5RA21737G**
5. Role of Open Source Tools and Resources in Virtual Screening for Drug Discovery,**Combinatorial chemistry & high throughput screening** 18(6): 528 – 543 **(2015)** Muthukumarasamy Karthikeyan and Renu Vyas. **DOI: 10.2174/138620731866615070311191**1
6. **CHEMSCREENER:** A Distributed Computing Tool for Scaffold based Virtual Screening,Combinatorial chemistry & high throughput screening 18(6): 544 – 561 **(2015)** Muthukumarasamy Karthikeyan, Deepak Pandit and Renu Vyas. **DOI: 10.2174/138620731866615070311224**2
7. Prediction of Bioactive Compounds Using Computed NMR Chemical Shifts,**Combinatorial chemistry & high throughput screening** 18(6): 562 – 576 **(2015)** Muthukumarasamy Karthikeyan, Pattuparambil Ramanpillai Rajamohanan and Renu Vyas. **DOI: 10.2174/138620731866615070311331**2
8. Protein Ligand Complex Guided Approach for Virtual Screening,**Combinatorial chemistry & high throughput screening** 18(6): 577 – 590 **(2015)** Muthukumarasamy Karthikeyan, Deepak Pandit and Renu Vyas. **DOI: 10.2174/138620731866615070311262**0
9. Megaminer: A Tool for Lead Identification Through Text Mining Using Chemoinformatics Tools and Cloud Computing Environment,**Combinatorial chemistry & high throughput screening** 18(6): 591 – 603 **(2015)** Muthukumarasamy Karthikeyan, Yogesh Pandit, Deepak Pandit and Renu Vyas. **DOI: 10.2174/138620731866615070311352**5
10. Design and Development of cheminfocloud: An Integrated Cloud Enabled Platform for Virtual Screening,**Combinatorial chemistry & high throughput screening** 18(6): 604 – 619 (2015) Muthukumarasamy Karthikeyan, Deepak Pandit, Arvind Bhavasar and Renu Vyas. **DOI: 10.2174/138620731866615070311365**6
11. Pharmacophore and Docking Based Virtual Screening of Validated Mycobacterium tuberculosis Targets,**Combinatorial chemistry & high throughput screening** 18(7): 624 – 637 (2015) Renu Vyas, Muthukumarasamy Karthikeyan, Ganesh Nainaru and Murugan Muthukrishnan. **DOI: 10.2174/138620731866615070311275**9
12. Role of Chemical Reactivity and Transition State Modeling for Virtual Screening,**Combinatorial chemistry & high throughput screening** 18(7): 638 – 657

(2015) Muthukumarasamy Karthikeyan, Renu Vyas, Sanjeev S. Tambe, Deepthi Radhamohan and Bhaskar D Kulkarni.**DOI: 10.2174/138620731866615070311313 5**

13. A Study of Applications of Machine Learning Based Classification Methods for Virtual Screening of Lead Molecules,**Combinatorial chemistry & high throughput screening** 18(7): 658 – 672 (2015) Renu Vyas, Sanket Bapat, Esha Jain, Sanjeev S. Tambe, Muthukumarasamy Karthikeyan and Bhaskar D Kulkarni. **DOI: 10.2174/138620731866615070311244 7**
14. Chemoinformatics Approach for Building Molecular Networks from Marine Organisms,**Combinatorial chemistry & high throughput screening** 18(7): 673 – 684 (2015) Muthukumarasamy Karthikeyan, Deepika Nimje, Rakhi Pahujani, Kushal Tyagi, Sanket Bapat, Renu Vyas and Krishna Pillai Padmakumar. **DOI: 10.2174/138620731866615070311295 0**
15. Pharmacokinetic Modeling of Caco-2 Cell Permeability Using Genetic Programming (GP) Method Renu Vyas, Purva Goel, M. Karthikeyan, S.S. Tambe, B.D. Kulkarni **Letters in Drug Design & Discovery** VOLUME: 11 ISSUE: 9 **2014** Page: [1112 - 1118] Pages: 7 **DOI: 10.2174/15701808116661406102134 38**
16. **M Karthikeyan**, S Krishnan, Anil Kumar Pandey, Andreas Bender, Alexander Tropsha Distributed Chemical Computing Using **CHEMSTAR:** Open Source Java RMI Architecture applied to Large Scale Molecular Data from pubchem. (2008) **J. Chem. Inf. Model.,** 48 (4), 691-703.
17. **M Karthikeyan,** S Krishnan, Anil Kumar Pandey, Andreas Bender Harvesting Chemical Information from the Internet Using a Distributed Approach: **CHEMXTREME** (2006**) J. Chem. Inf. Model.,** 46 (2), 452 -46 1.
18. **M Karthikeyan,** Robert C Glen, Andreas Bender General Melting Point Prediction Based on a Diverse Compound Data Set and Artificial Neural Networks. (2005) **J. Chem. Inf. Model.;** 45(3) pp 581 - 590.
19. **M Karthikeyan,** Andreas Bender Encoding and Decoding Graphical Chemical Structures as Two-Dimensional (PDF417) Barcodes M. (2005) **J. Chem. Inf. Model.;** 45(3) pp 572 - 580
20. **Muthukumarasamy Karthikeyan,** Subramanian Krishnan Chemoinformatics A tool for modern drug discovery, (2002) **Intl. J. Inf. Tech Mgmt**. 1, (1), 69-82. **[DOI: 10.1504/IJITM.2002.001188]**

Patents filed

1. **Muthukumarasamy Karthikeyan ; Vyas Renu +**An automated remote computing method and system by email platform for molecular analysis **WO2017072794** (a1) - council scient ind res [in] + application number: wo2016 in 50367 20161028 priority number(s): in2015 del 3527 20151030
2. **Muthukumarasamy Karthikeyan** and Deepak Pandit Method for encoding and decoding large scale molecular virtual libraries into a barcode **WO 2016181412** A3 " 2014-INV-0018 . CSIR-NCL, Pune. 2014.
3. **Muthukumarasamy Karthikeyan** 2013040366488 Development Of Nmr Chemical Shift Fingerprints And Applications 2013-Ncl-0049 2013-Nf-0124 In 1874/Del/2013
4. **Muthukumarasamy Karthikeyan** 2012092596056 Rapid Recognition And Prediction Of Objects Using Visual Computing And Machine Learning Methods 2013-Ncl-0035 2013-Nf-0090 In
5. **Muthukumarasamy Karthikeyan** 201304227151 Automatic Harvesting Of Molecular Information Raster Graphics 2011-Ncl-0031 2011-Nf-0140 Wo Pct/In2012/000567 &

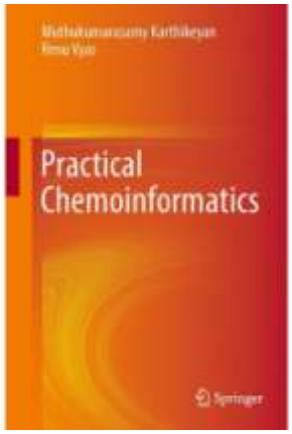
2011-Ncl-0031 2011-Nf-0140 In 2420del2011

6. **Muthukumarasamy Karthikeyan** 2013052198317 Development Of Visual Imaging Device And Compatible Materials To Recognize Masked Patterns
7. **Muthukumarasamy Karthikeyan** 2012061564523 Apparatus For Digital Vision To Recognize Chemical Objects From Physical Models
8. **Muthukumarasamy Karthikeyan** US PATENT: Chemical Structure Recognition Tool (2014)

Copyright

1) **Muthukumarasamy Karthikeyan** 2011042887039 I C B C (Internal Compatible Bar Code Generator) 2000-Ncl-0052 In L-19372/2001
2) **Muthukumarasamy Karthikeyan** ICIS Interactive Chemical Information System (1995) CSIR-New Delhi

Text Book :



Practical Chemoinformatics , Springer 2014 (ISBN: 978-81-322-1779-4) http://www.springer.com/chemistry/book/978-81-322-1779-4

Chemoinformatics is equipped to impact our life in a big way mainly in the fields of chemical, medical and material sciences. This book is a product of several years of experience and passion for the subject written in a simple lucid style to attract the interest of the student community who wish to master chemoinformatics as a career. The topics chosen cover the entire spectrum of chemoinformatics activities (methods, data and tools). The algorithms, open source databases, tutorials supporting theory using standard datasets, guidelines, questions and do it yourself exercises will make it valuable to the academic research community. At the same time every chapter devotes a section on development of new software tools relevant for the growing pharmaceutical, fine chemicals and life sciences industry. The book is intended to assist beginners to hone their skills and also constitute an interesting reading for the experts.

List of Book Chapters

1. Open Source Tools, Techniques and Data in Chemoinformatics . **Muthukumarasamy Karthikeyan** and Renu Vyas. Practical Chemoinformatics © Springer India 2014 . DOI 10.1007/978-81-322-1780-0_1
2. Chemoinformatics Approach for the Design and Screening of focused virtual libraries **Muthukumarasamy Karthikeyan** and Renu Vyas. Practical Chemoinformatics © Springer India 2014 . DOI 10.1007/978-81-322-1780-0_2
3. Machine Learning Methods in Chemoinformatics for Drug Discovery **Muthukumarasamy Karthikeyan** and Renu Vyas. Practical Chemoinformatics © Springer India 2014 . DOI 10.1007/978-81-322-1780-0_3

4. Docking and pharmacophore modeling for virtual screening **Muthukumarasamy Karthikeyan** and Renu Vyas. Practical Chemoinformatics © Springer India 2014 . DOI 10.1007/978-81-322-1780-0_4

5. Active site directed pose prediction programs for efficient filtering of molecules **Muthukumarasamy Karthikeyan** and Renu Vyas. Practical Chemoinformatics © Springer India 2014 . DOI 10.1007/978-81-322-1780-0_5

6. Representation, fingerprinting and modeling of chemical reactions. **Muthukumarasamy Karthikeyan** and Renu Vyas. Practical Chemoinformatics © Springer India 2014 . DOI 10.1007/978-81-322-1780-0_6

7. Predictive methods for Organic Spectral data Simulation. **Muthukumarasamy Karthikeyan** and Renu Vyas. Practical Chemoinformatics © Springer India 2014 . DOI 10.1007/978-81-322-1780-0_7

8. Chemical Text mining for Lead Discovery. **Muthukumarasamy Karthikeyan** and Renu Vyas. Practical Chemoinformatics © Springer India 2014 . DOI 10.1007/978-81-322-1780-0_8

9. Integration of Automated Work flow in Chemoinformatics for drug discovery. **Muthukumarasamy Karthikeyan** and Renu Vyas. Practical Chemoinformatics © Springer India 2014 . DOI 10.1007/978-81-322-1780-0_9

10. Cloud computing Infrastructure development for Chemoinformatics. **Muthukumarasamy Karthikeyan** and Renu Vyas. Practical Chemoinformatics © Springer India 2014 . DOI 10.1007/978-81-322-1780-0_10

11. **Muthukumarasamy Karthikeyan1** , Renu Vyas Chemical Structure Representations and Applications in Computational Toxicity Computational Toxicology : Volume I Methods in Molecular Biology (2012) Volume: 929 , 167-192 | DOI: 10.1007/978-1-62703-050-2_8 (URL)

List of Research Projects Successfully Implemented

2002-2004 DSIR Encoding and Decoding Chemical Structures as Barcodes Rs 10 Lakhs
2004-2006 DSIR Establishing MOLTABLE an Open access scientific Portal Rs 10 Lakhs
2009-2013 DST Chemoinformatics Cloud Platform for design of new materials Rs. 16.0 Lakhs
2012-2017 CSIR GENESIS (Chemoinformatics, Drug Discovery) Rs. 80 Lakhs
2012-2017 CSIR INSPIRE (Chemoinformatics, Reaction Modeling) Rs. 40 Lakhs
2016-2019 DRDO Chemoinformatics portal for HEM 45.0 Lakhs Ongoing

Summary of the project Major Results/Highlights of the projects by PI (Dr. M Karthikeyan)

1. Barcoding Molecular Structure

This project is sponsored by DSIR (Department of Scientific and Industrial Research). The major objective of this project is to establish a mechanism to encode truly computable chemical structures as barcode for inventory and other automation processes. Build an automatic inventory system with chemical structure encoding (Fast encoding and Retrieval of electronic data on paper) Details of the major achievements cited in the biodata of Co-PI.

Encoding and Decoding Graphical Chemical Structures as Two-Dimensional (PDF417) Barcodes M. (2005) J. Chem. Inf. Model.; (American Chemical Society) 45(3) pp 572 - 580.

2. Building MOLTABLE (http://moltable.ncl.res.in/)

This project was sponsored by DSIR to build an open molecular data repository with computed / experimental data related to chemical structures. Moltable is established as an open access scientific data portal for molecular informatics. Currently host over 25 million molecules with computed data. (http://moltable.ncl.res.in/chemstar/) Details of the major achievements cited in the biodata of Co-PI.

Publication Distributed Chemical Computing Using ChemStar: Open Source Java RMI Architecture

applied to Large Scale Molecular Data from PubChem. (2008) J. Chem. Inf. Model.; (American Chemical Society) 48 (4), 691-703.

3) Design and Development of cheminfocloud: An Integrated Cloud Enabled Platform for Virtual Screening,**Combinatorial chemistry & high throughput screening** 18(6): 604 – 619 (2015) Muthukumarasamy Karthikeyan, Deepak Pandit, Arvind Bhavasar and Renu Vyas. **DOI: 10.2174/1386207318666150703113656**

Biography

Muthukumarasamy Karthikeyan is a Principal Scientist in the Chemical Engineering and Process Development Division at **CSIR-National Chemical Laboratory Pune**, India.

Dr Karthikeyan holds PhD in Organic Chemistry and working in the area of chemoinformatics its application in drug discovery and design of novel materials for the past 17 years. He has co-authored a text book on **Practical Chemoinformatics** (Springer 2014) and about 20 research papers and several international patents in the area of chemoinformatics handling large scale molecular data and developed open source tools for harvesting chemical information (http://moltable.ncl.res.in/). He is also the recipient of BOYSCAST Award by Department of science and Technology and Overseas Associate Award by Department of Biotechnology. He is selected for 2015 Open Innovation Challenge Award by Thomson Reuters and CodeX of Stanford University. Recently he published two special issues in **J. Combi. Chem. High Throughput Screening (2015)** containing articles on chemoinformatics tools for drug discovery. Currently he is working in the area of harvesting large scale molecular data associated with medicinal plants and their bioactivity.