MUTHUKUMARASAMY KARTHIKEYAN Ph.D.

Principal Scientist, (Chemoinformatics)
http://in.linkedin.com/in/karthincl
Digital Information Resource Center(DIRC) and
Centre of Excellence Scientific Computing (CoESC)
National Chemical Laboratory, Pune – 411 008, INDIA
Ph: +91-020 2590 2483 Mobile: +91-**976 742 7981** (Res: 020-25889566)
e-mail: m.karthikeyan@ncl.res.in / karthincl@gmail.com
WEB: http://moltable.ncl.res.in/

Working in Molecular Informatics for the past 20 years (Application of HPC tools using distributed and cloud computing architecture) to handle large scale molecular data ~100 millions+ defining virtual chemical space of selected protein targets or therapeutic category. We are currently developing tools for exploring organic reactions using QM & QC tools and extending them to biological systems. Development of predictive QSAR (properties, toxicity, activity) , artificial neural networks and other machine learning tools, textmining. Recently we developed Visual computing tools for molecular informatics (ChemRobot) and their application in drug design, lead optimization, materials in addition to Education, Research and Management. We developed portals to manage Inventory and automation for chemical sample tracking system. With the in-house developed tools, currently millions of molecular docking is performed in a HPC environment (30+ million) to understand protein-ligand interactions by Insilco studies. Recent book Practical Chemoinformatics (from Springer) highlights the power of programming computers for chemoinformatics applications.

JOB EXPERIENCE

Apr 2010 – till date	Pr. Scientist,	National Chemical Laboratory (CSIR) , Pune, India
Apr 2005 – Mar 2010	Sr Scientist	National Chemical Laboratory (CSIR) , Pune, India
Apr 2000 – Mar 2005	Scientist C,	National Chemical Laboratory (CSIR) , Pune, India
Mar '98 – Mar '2000	Scientist B,	ARDE, Pune

POST-DOCTORAL RESEARCH EXPERIENCE

Visiting Scientist (DBT Overseas Associate) **2007-08** Univ. North Carolina, Chapel Hill, USA
Post-doctoral Fellow (DST BOYSCAST Fellow) **2003-04** Univ. North Carolina, Chapel Hill, USA

AWARDS & Scientific Recognitions

- ✓ Long term Overseas Associate (2007-08) Dept of Bio Tech - New Delhi
- ✓ BOYSCAST Fellow (2003-04) Dept of Science & Tech-New Delhi
- ✓ **Commendation Certificate** 1999 DRDO (1998-2000) & ChemInt'99 -Washington (CSA Award)
- ✓ Chem. Str. Association. Trust & CSIR (1996) (4th Intl. Conf. Chem. Str. Netherlands)
- ✓ Travel Grant : 2011 ACS meeting (Intl Year of Chemistry) Denver, Oral Presentation (ChemRobot)

EDUCATIONAL QUALIFICATION

MSc Computer Science	2012-**14**	Anna University, Chennai	First Class
MBA (DIM, PGDIMM)	2010-**12**	IGNOU, New Delhi	First Class
Ph. D. Chemistry	1992-**98**	Pune University (NCL)	
M.Sc. Chemistry	1989-**91**	Pondicherry University	First Class
B.Sc. Chemistry	1986-**89**	Pondicherry University	First Class

Research Fellowship Qualification

Research Scholar & Associate (Jan 92 to Feb 98) National Chemical Laboratory (CSIR) , Pune, India

Copyright / Patents

1. Interactive Chemical Information System ICIS © 1995 CSIR NewDelhi, L-15256 / 95, Govt. of India.
2. Computer Generated – Automatic Chemical Structure- Database: CG-ACS-DB (C) S-00061/99 dt 12/11/99, DRDO, New Delhi Govt of India
3. Internet compatible Bar-coding ICBC © 2001 NCL-CSIR No.23/2000 dt 13/11/2000 NewDelhi Govt of India,:
4. **CHEMICAL STRUCTURE RECOGNITION TOOL, M KARTHIKEYAN, WO Patent 2013/3/8 Pub. No.: WO/2013/030850 International Application No.:PCT/IN2012/000567 Publication Date:07.03.2013 International Filing Date: 27.08.2012** http://www.google.com/patents/WO2013030850A2?cl=en

SELECTED LIST OF PUBLICATIONS (PEER REVIEWEED JOURNALS)

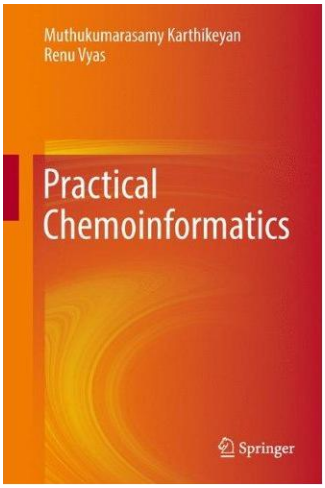
Organic Chemistry:

1. Intramolecular Nucleophilic Addition of Silylenol Ether to Photosensitized Electron Transfer (PET) Generated Arene Radical Cations: A Novel Non-Reagent Based Carboannulation Reaction: M. Karthikeyan , G Pandey (1993) Tetrahedron Letters, Vol.34, No.(41), pp.6631-6634 [IF*: 2.660]
2. A New Intramolecular Alpha-Arylation Strategy of Ketones by the reaction of Silylenol ethers to PET Generated Arene Radical Cations: Construction of Benzannulated and Benzospiroannulated Compounds. M. Karthikeyan, G Pandey (1998), J. Org. Chem. Vol 63. No.(9), pp-2867-2872 [IF*: **4.564**]
3. EPZ-10 catalyzed regioselective transformation of alkenes into -iodo ethers, iodohydrins and 2-iodomethyl-2,3-dihydrobenzofurans Green Chem., (2002), 4, 325 - 327, DOI: 10.1039/b202725a (IF*: **6.828**)

Chemoinformatics:

4. Chemoinformatics – A tool for modern drug discovery, M. Karthikeyan, Krishnan,S, (2002) Intl. J. Inf. Tech Mgmt. 1, (1), 69-82 :http://chemvista.molecularsociety.org/ijitm.pdf (Downloadble)
5. PharmTree 2.1: M Karthikeyan (2003) J. Chem.Inf.Comp.Sci, vol. 43, No.6, 2194-2195 [IF*: **4.675**]
6. Encoding and Decoding Graphical Chemical Structures as Two-Dimensional (PDF417) Barcodes (2005) J. Chem. Inf. Model.; 45(3) pp 572 - 580 [Click Here] [IF*: **4.675**]
7. 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.[Click Here] [IF*: **4.675**]
8. Harvesting Chemical Information from the Internet Using a Distributed Approach: ChemXtreme (**2006**) J. Chem. Inf. Model., 46 (2), 452 -46 1.[Click Here] [IF*: **4.675**]
9. Tryptophan residue in substrate binding of penicillin G acylase from Kluyvera citrophila: evidence from biochemical and modeling studies." (**2007**) Enzyme and Microbial Technology 40, 1389-97 [IF*: **2.638]**
10. 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.[Click Here] (Pubchem 12 million molecules with computed data!) [IF*: **4.675**]
11. Chemical structure representations and applications in computational toxicity. Karthikeyan, Muthukumarasamy; Vyas, Renu. 10.1007/978-1-62703-050-2_8 Methods Mol. Biol. (N. Y., NY, U. S.) 929 Computational Toxicology, Volume I 167-192 **2012**

Text Book : Practical Chemoinformatics , **M Karthikeyan** and **Renu Vyas**. Springer **2014** (ISBN: 978-81-322-1779-4) http://www.springer.com/chemistry/book/978-81-322-1779-4



- Enables the readers to practice chemoinformatics with open source tools and open source data
- Includes numerous step-by-step tutorials that help the reader to grasp the topics quickly
- Provides exposure to open source based computer programs for chemoinformatics

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.

Ch 1. **Open-Source Tools, Techniques, and Data in Chemoinformatics .** M Karthikeyan and Renu Vyas. Pages 1-92 . DOI 10.1007/978-81-322-1780-0_1

Ch 2. **Chemoinformatics Approach for the Design and Screening of focused virtual libraries** M Karthikeyan and Renu Vyas. Pages 93-131 DOI 10.1007/978-81-322-1780-0_2

Ch 3. **Machine Learning Methods in Chemoinformatics for Drug Discovery** M Karthikeyan and Renu Vyas..Pages 133-194 DOI 10.1007/978-81-322-1780-0_3

Ch 4. **Docking and pharmacophore modeling for virtual screening** M Karthikeyan and Renu Vyas. Pages 195-269 DOI 10.1007/978-81-322-1780-0_4

Ch 5. **Active site directed pose prediction programs for efficient filtering of molecules** M Karthikeyan and Renu Vyas..Pages 271-316 DOI 10.1007/978-81-322-1780-0_5

Ch 6. **Representation, fingerprinting and modeling of chemical reactions.** M Karthikeyan and Renu Vyas..Pages 317-374 DOI 10.1007/978-81-322-1780-0_6

Ch 7. **Predictive methods for Organic Spectral data Simulation.** M Karthikeyan and Renu Vyas. Practical Pages 375-414 DOI 10.1007/978-81-322-1780-0_7

Ch 8. **Chemical Text mining for Lead Discovery**. M Karthikeyan and Renu Vyas. Chemoinformatics.Pages 415-449. DOI 10.1007/978-81-322-1780-0_8

Ch 9. **Integration of Automated Work flow in Chemoinformatics for drug discovery.** M Karthikeyan and Renu Vyas..Pages 451-499. DOI 10.1007/978-81-322-1780-0_9

Ch 10. **Cloud computing Infrastructure development for Chemoinformatics.** M Karthikeyan and Renu Vyas. Pages 501-528 .DOI 10.1007/978-81-322-1780-0_10

Other General Articles

1. Artificial Intelligence in Chemical Synthesis. M. Karthikeyan, NCL Bulletin, vol. XVIII, No.2: Jul 1993 - Mar 1994, pp-43-58.
2. Electronic Conferences: Wired Meetings. M. Karthikeyan, Science Reporter, (CSIR) Vol.33, No.8, Aug 1996, pp-60, ISSN 0036-8512.
3. ICIS (Interactive Chemical Information System) M. Karthikeyan, 4th Intl Conf. on Chem. Str., June 2-6, 1996, (CSA)
4. Internet and Chemical Information in India: M. Karthikeyan, CSA (Chemical Structure Association) Newsletter. Issue - 45 Feb 1997

Webportals (Open Access)

An Open Access Molecular Informatics Portal http://moltable.ncl.res.in
Open Access Portal Dspace@NCL: http://dspace.ncl.res.in

Members Advisory Board / Committees

- ✓ Editorial Advisory Board (Wiley's Molecular Informatics 2010-)
- ✓ Editorial Advisory Board (QSAR World)
- ✓ American Chemical Society (Member)
- ✓ Scientific Advisory Board [DrugInfoMeet]
- ✓ Chemical Structure Association (The Netherlands)

Research Expertise: Chemoinformatics, Bioinformatics and Computational Chemistry

- ✓ Research, Teaching, Training and Consulting Services in Chemoinformatics
- ✓ Standards and Efficiency in Chemical Structure Representation
- ✓ Building Large Molecular structure database with associated data
- ✓ Technology Development (Distributed Computing, Textmining, Datamining, Encoding systems)
- ✓ Design of knowledge based in-silico libraries for drug discovery
- ✓ Building Chemoinformatics portals to access molecular information (http://moltable.ncl.res.in)
- ✓ High Performance Environment for Distributed Computing applications in chemistry
- ✓ Protein Databank Analysis for drug discovery
- ✓ Machine Learning and Statistical Techniques for QSAR / QSPR / QSTR
- ✓ Design and development of Electronic Laboratory Notebooks
- ✓ Chemical Literature and Patent Analysis, Text based Mining & Information Harvesting
- ✓ Open Access / Archive Initiatives (Chemical Information Analysis)
- ✓ Training program in Chemoinformatics and Bioinformatics

Meetings / International Conferences Organized:
Convener: International Conference on chemoinformatics [22-24 January 2007] http://moltable.ncl.res.in/

Conference Presentations

1. Application of GPU computing for analysis of implicit hydrogen based molecular descriptors in structure activity relationship studies. Karthikeyan, Muthukumarasamy; Pandit, Deepak. Abstracts of Papers, 247th ACS National Meeting & Exposition, Dallas, TX, United States, March 16-20, 2014 COMP-164 **2014**

2. Computer Vision based chemical information extraction from digital images and streaming videos. Karthikeyan, Muthukumarasamy. Abstracts of Papers, 242nd ACS National Meeting & Exposition, Denver, CO, United States, August 28-September 1, 2011 CINF-20 **2011**

3. Chemical datamining approach to scaffold based QSAR studies of NCI anti-tumor dataset. electronic Karthikeyan, M.; Sebastian, Letha; Tropsha, Alexander. Abstracts of Papers, 230th ACS National Meeting, Washington, DC, United States, Aug. 28-Sept. 1, **2005**

4. MOLTABLE: An open access intiative on molecular informatics. Karthikeyan, M.; Krishnan, S. Abstracts of Papers, 230th ACS National Meeting, Washington, DC, United States, Aug. 28-Sept. 1, **2005** CINF-024 2005

5. ChemXtreme: Harvesting chemical information from internet. M.Karthikeyan, S Krishnan International Conference on Chemical structures, The Netherlands. 4-9 June **2005**.

6. General Melting Point prediction based on a diverse compound dataset and artificial neural networks M. Karthikeyan and S Krishnan, Presented in Fourth Indo-US Workshop on Mathematical Chemistry with applications to Drug Discovery, Environmental Toxicology, Cheminformatics and Bioinformatics, January 8 - 12, (**2005**), Pune, Maharashtra, India

7. Chemoinformatics tools for combinatorial chemistry. Karthikeyan, M.; Krishnan, S.; Uzagare, Deepak. Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, **2003** CINF-060 200

8. Compressed Chemical Markup Language for compact storage and inventory applications. Karthikeyan, M.; Uzagare, Deepak; Krishnan, S. Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 CINF-030 **2003**

9. Text-based chemical information locator from the Internet using commercial barcodes. Karthikeyan, M.; Krishnan, S.; Steinbeck, Christoph. Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002 CINF-072 **2002**

10. Integration of computed molecular data with rendered images: Application of Steganography in chemical information retrieval, M. Karthikeyan, (6 International Conference on Chem. Str, The Netherlands, June2-6, **2002**)

11. Computer search for high energetic organic compounds from the automatically generated chemical structure database. Poster presentation in the Fifth Int. conf Chemical Structure, June 6-10, **1999**.

12. A Computational Approach in predicting the explosive properties using molecular mechanics force field calculations, M.Karthikeyan, PN Gadhikar; First Int. Seminar on Force Multiplier Technologies for Naval and Land Warfare, NewDelhi, October 13-15, **1999**

13. Algorithm for Compact Storage and Retrieval of Chemical Structures as Intelligent Pixels in M. Karthikeyan ChemInt'99, , September **1999**. Washington DC, USA

14. Molecular mechanics Force Field Calculations to predict properties of organic nitro compounds, Poster # 141, M. Karthikeyan 32 Annual Conference of ICT July 3-6,**2001**

15. Synthesis, Characterization of Modified PZT/PMN-PT for Sensor Applications, M. Karthikeyan, Proceedings of the Third IWSHM Technomic Publishing Company, Inc, 2001 September 11-14, Standford University, USA

16. Novel construction of the benzazocine framework through photoinduced electron transfer (PET) generated arene radical cation. Pandey, Ganesh; Karthikeyan, M. Electron. Conf. Heterocycl. Chem., [Proc.] [CD-ROM] **1997**

17. Intramolecular cyclization of silyl enol ethers to PET (photoinduced electron transfer) generated arene radical cation: a general spirocyclization strategy. Pandey, Ganesh; Karthikeyan, M. Electron. Conf. Trends Org. Chem. [CD-ROM] Paper 65 **1996**

18. Novel construction of benzazocine framework through photoinduced electron transfer (PET) generated arene radical cation. Ganesh Pandey and M. Karthikeyan, International Conference on Organic Synthesis (ICOS10), Bangalore, India, December 11-16, **1994**. pp-212.