# Editorial

## Design and Development of New Chemoinformatics Tools for Virtual Screening

**M. Karthikeyan**

**R. Vyas**

Chemoinformatics is an ever-growing inter-disciplinary field poised to meet the challenges and promises in the area of drug design. Virtual Screening (VS) is the backbone of computational drug discovery workflow, an indispensable component in all drug design programs. The computational model driven research can minimize cost, time and energy and complement the experimental efforts of medicinal chemists in the pharmaceutical industry. Any new invention or development in chemoinformatics is bound to impact virtual screening in a significant way. The pharmaceutical industry has benefited tremendously in the past by applying the chemoinformatics techniques for designing focused virtual libraries of small organic molecules with desired properties/ affinities.

It is therefore timely and pertinent to compile a set of two special issues highlighting the importance of new tools, data and emerging methods in chemoinformatics to fully comprehend their role and applications in virtual screening. The core objective of these special issues is to disseminate the state of art knowledge on open source chemoinformatics tools, data and evince research interest for further advancement of this field. The emphasis is on the use of emerging cloud computing (PAAS, SAAS, IAAS), distributed computing, multicore GPU computing, text analytics, barcoding technologies, etc. which have not only enhanced the computation speed many fold but also revolutionized the subject of chemoinformatics. It has been our constant endeavour to contribute to this subject and demonstrate its vast potential in solving problems in biology and chemistry [1,2]. Virtual screening has always been a topic of current interest as amply demonstrated in recent general reviews [3-5]. It involves a host of modelling techniques from simple similarity search methods to advanced algorithms for finding the accurate bioactive conformation of a molecule to bind to its corresponding target. Virtual screening assists drug discovery at every stage from conceptualization to searching for novelty, safety profiles and any known information about molecules at the abstract level from the pool of scientific literature for the discovery of a new molecular entity.

The first set of articles is focused on various aspects of chemoinformatics tools and their applications for virtual screening. It is composed of overall six peer reviewed papers wherein we have highlighted the role of chemical informatics in drug discovery in the context of virtual library design, analysis, tools, data and screening methods demonstrated by selected case studies in active areas of research. The tools are related to computational handling of chemical structures, properties and development of integrated workflows and application of high performance computing platform as a problem solving environment for major chemoinformatics tasks. The virtual screening tools presented, possess logically integrated modules for similarity searching, diversity selection, scaffold analysis, virtual library generation, annotation and pharmacophore mapping to explore diverse chemotypes from the vast chemical space.

It is sincerely hoped that this collection of carefully selected articles will enhance interest in the subject and the tools will aid in performing virtual screening experiments efficiently and encourage readers towards development of their own customized tools specifically tailored to their needs.

It is our pleasure to thank the authors and co-authors of all the papers in this issue. We are grateful to the esteemed members of the referee panel for reviewing the manuscripts. Their critical comments and thorough review process helped in enhancing the quality of the papers. Editorial assistance provided by the Bentham Science team, especially Ms. Mehjabeen and Dr. Samina Khan is greatly acknowledged. Sincere thanks are due to Editor-in-Chief Dr. Rathnam Chaguturu and Section Editor for Chemoinformatics Dr. Gerald Lushington and for their offer to compile a special issue and providing continuous support throughout the entire process of its successful completion.

## EDITORS BIOGRAPHIES

**Dr. Muthukumarasamy Karthikeyan** obtained Ph.D. (Chemistry) from University of Pune, India in the area of Organic Synthesis (National Chemical Laboratory). He developed interest in chemoinformatics in early 90s and supported by Chemical Structure Association Trust and CINF Division of American Chemical Society. He began his career as a scientist in ARDE, Pune later joined as a senior scientist CSIR-National Chemical Laboratory, Pune and since then he is pursuing his active research career in Chemoinformatics especially in the area of high performance computing (Cloud, GPU computing) for molecular informatics. His current interest includes development of open-source tools for virtual screening in drug discovery. He is the recipient of BOYSCAST Fellowship from Department of Science and Technology, and Long term Overseas Associateship from Department of Biotechnology in the area of molecular informatics and structure-activity relationship studies at University of North Carolina at Chapel Hill, USA. He is a member in the executive advisory board of journal of Molecular Informatics from Wiley and also recently joined the editorial board of the Journal, *Combinatorial Chemistry and High Throughput Screening* (CCHTS)

**Dr. Renu Vyas** is a scientist (DST) in Artificial Intelligence (AI) and Molecular Modeling group, in Chemical Engineering and Process Development Division at National Chemical Laboratory (NCL) Pune, India since 2011. She obtained her Ph.D (Chemistry) from NCL in 2002 and pursued post doctoral fellowship from University of Knoxville, Tennessee, USA. Her multi-disciplinary background enabled her to excel at all levels in academia, research and industry. She has served in various capacities as chemical information scientist, manager- chemoinformatics, domain consultant, etc. in the IT industry. As Head of Department, Bioinformatics and Computer Sciences, at Dr. D.Y. Patil Institute of Biotechnology and Bioinformatics, Pune she conducted chemistry, chemoinformatics and bioinformatics courses. Her research career includes several international publications, patents, awards, fellowships, invited talks, book chapters and a book. Currently, she is involved in research related to application of machine learning methods in biology and chemistry.

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**Muthukumarasamy Karthikeyan**
(***Guest Editor***)
Digital Information Resource Centre (DIRC) &
Centre of Excellence in Scientific Computing (CoESC)
CSIR-National Chemical Laboratory
Pune - 411008
India
E-mail: m.karthikeyan@ncl.res.in

**Renu Vyas**
(***Guest Editor***)
Chemical Engineering Division
CSIR-National Chemical Laboratory
Pune - 411008
India
E-mail: vyasrenu@yahoo.com