

**Dr. R. Narayanan**

***Principal Scientist***

***TCS Research & Innovation***

### **Education**

- M.Sc (Bio-Chemistry), University Of Madras, 1986
- Ph D (Organic Chemistry-Bio-Chemistry-Interdisciplinary) University of Madras (1993).

### **Research Interests**

- Pharmacokinetic & Pharmacodynamic data analyses
- New approaches for the prediction of absorption, distribution, metabolism, excretion and toxicity of drug candidates.
- New Approaches for drug repurposing using gene expressions, target-drug interactions, side-effects etc.
- Realizing the value of Pharma R&D data using advanced data analytics.

### **Patent Details**

1. Viswajanani Sattigeri, Mohammad Salman, Ramamurthi Narayanan, Subhendu Seth, Simi Sarin, Abhijit Ray, Sunanda Dastidar, Triazines derivatives as cell adhesion inhibitors, WO2005030735A1, (2005).
2. Viswajanani Jitendra Sattigeri, Sudershan K Arora, Mohammad Salman, Venkata P Palle, Gyan Chand Yadav, Madan Pal Tanwar, Ashis Mukherjee, Ramamurthy Narayanan, Abdul Rehman, Abdul Rauf, Keshav Prabhakar Naik, Ajay Soni, Abhijit Ray, Raj Kumar Shirumalla, Kasim Abbas Mookhtiar, Monosaccharide derivatives as anti-cancer and anti-inflammatory agents, WO2005092907A3 (2005).
3. R. Narayanan et al, MYCOBACTERIAL INHIBITORS, WO 1999/065483, (1999).
4. Nishant Kumar Agrawal, Manoj Karunakaran Nambiar, R Narayanan, Shyam Sundar Das, Rihab Abdulrazak, 'Parallel Implementation of Grid search method on GPU and its application for initial PK-PD parameter estimation', 21/03/2014, India, US-14/663,968, 24/09/2015, USA.
5. R Narayanan, Geervani K, 'SYSTEMS AND METHODS FOR SELECTING OPTIMAL VARIABLES USING MODIFIED TEACHING LEARNING BASED SEARCH

- OPTIMIZATION TECHNIQUE', IN-201621035471, 17/10/2016, India, EP17163520.4, 29/03/2017, Europe, US-15/474,389, 30/03/2017, USA.
6. R. Narayanan, Geervani K, 'Parallelization Approaches of Modified Teaching Learning Based Search Optimization Technique For Variable Selection', IN-201621039514, 19/11/2016, India, EP-17 162 466.1, 23/03/2017, Europe, US 15/469,045, 24/03/2017, USA.
  7. R. Narayanan, Geervani. K, 'Parallelization Techniques For Variables Selection And Predictive Models Generation and its Applications', IN-201621020879, 15/06/2017, India, EP17176197.6, 15/06/2017, Europe, US-15/625,383, 16/06/2017, USA.
  8. R. Narayanan, Shyam Sundar Das, Geervani K, 'Systems and Methods for Generating Optimized Set Of Pharmacokinetic (PK) and Pharmacodynamic (PD) Parameters', IN-201921029215, 19/07/2019, India, EP-20 186 478.2, 17/07/2020, Europe, US-16/932,659, 17/07/2020, USA.
  9. R.Narayanan, Dipayan Ghosh, Geervani K, 'Automated Prediction of Biological Response of Chemical Compounds Based on Chemical Information', IN-201921011056, 22/03/2019, India, EP-19189669.5, 01/08/2019, Europe, US 16/535,025, 07/08/2019, USA.

### **Conference & Journal Publications**

1. Narayanan R and Swaminathan S 1990, Indian J. Chem. B29 1401.
2. Rearrangement Reactions of (Hydroxyphenyl)carbenes, Anil Kumar, Ramamurthi Narayanan, and Harold Shechter, The Journal of Organic Chemistry 1996 61 (13), 4462-4465, DOI: 10.1021/jo952269k.
3. Rajagopal, D., Narayanan, R. & Swaminathan, S. Enantioselective solvent-free Robinson annulation reactions. J Chem Sci 113, 197-213 (2001). <https://doi.org/10.1007/BF02704070>.
4. D. Rajagopal, R. Narayanan, S. Swaminathan, Asymmetric one-pot Robinson annulations, Tetrahedron Letters, Volume 42, Issue 29, 16 July 2001, Pages 4887-4890.
5. Akash Khandelwal 1, Ramamurthi Narayanan, Bulusu Gopalakrishnan, 3-D-QSAR CoMFA and CoMSIA studies on tetrahydrofuroyl-L-phenylalanine derivatives as VLA-4 antagonists, Bioorg Med Chem. 2003 Sep 15;11(19):4235-44.
6. Sitarama Brahmam Gunturi, R. Narayanan, January 2005, 'In silico ADME modelling: prediction models for blood-brain barrier permeation using a systematic variable selection method ', Bioorganic and Medicinal Chemistry, vol. 13, no. 8, pp. 3017-3028.

7. Sitarama Brahmam Gunturi, R. Narayanan, May 2005, 'In silico ADME modeling: QSPR models for the binding of lactams to human serum proteins using genetic algorithms', ARKIVOC, vol. 11, pp. 102-103.
8. R.Narayanan, October 2005, 'ADME in Children and The Elderly People: Clinical Challenges and Opportunities', D and MD Publications.
9. Sitarama Brahmam Gunturi, R. Narayanan, June 2006, 'In silico ADME modelling 2: Computational models to predict human serum albumin binding affinity using ant colony systems', Bioorganic and Medicinal Chemistry, vol. 14, no.12, pp. 4118-4129.
10. Sitarama Brahmam Gunturi, R. Narayanan, May 2007, 'In Silico ADME Modeling 3: Computational Models to Predict Human Intestinal Absorption Using Sphere Exclusion and kNN QSAR Methods', QSAR & Combinatorial Science, vol. 26, no. 5, pp. 653-668.
11. Sitarama Brahmam Gunturi, R. Narayanan, September 2008, 'Prediction of hERG Potassium Channel Blockade Using kNN-QSAR and Local Lazy Regression Methods ', QSAR & Combinatorial Science (QSARCS), vol. 27, no. 11-12, pp. 1305-1317.
12. Gunturi, S. B., Theerthala, S. S., Patel, N. K., Bahl, J., & Narayanan, R., February 2010, 'Prediction of Skin Sensitization Potential Using D-Optimal Design and GA-kNN Classification Methods', SAR and QSAR in Environmental Research (SARQSAR ER), vol. 21, no. 3-4, pp. 305-335.
13. R. Narayanan, Sitrama Brahmam Gunturi, November 2011, 'Quantitative prediction of aqueous toxicity using spline based regression methods', Drug Metabolism and Reviews, vol. 43, pp. 135-136.
14. R. Narayanan, Sitrama Brahmam Gunturi, November 2011, 'A novel approach to generate robust predictive developmental toxicity classification', Drug Metabolism and Reviews, vol. 43, pp. 131-132.
15. R. Narayanan, Sitrama Brahmam Gunturi, January 2013, 'Prediction of hERG Potassium Channel Blockade using spline based approximation method', Drug Metabolism and Reviews, vol. 44, pp. 100-101.
16. R. Narayanan, Sitrama Brahmam Gunturi, January 2013, 'Prediction of Liver Related Toxicity effect using logistic regression and support vector machines', Drug Metabolism and Reviews, vol. 44, pp. 100-101.
17. Sitarama Brahmam Gunturi, R. Narayanan, September 2013, 'Novel Algorithm to select basis functions in Spline Regressions: Applications in QSAR studies', Journal of Chemometrics, vol. 26, no.3-4, pp. 85-94.

18. R. Narayanan, Sitrama Brahmam Gunturi, Vijay Singh Punia, October 2013, 'Prediction of Plasma Protein Binding Using Genetic Algorithms and Local Lazy Regressions ', Drug Metabolism and Reviews, vol. 45, pp. 159-159.
19. R. Narayanan, Sitrama Brahmam Gunturi, Vijay Singh Punia, October 2013, 'Development of classification models to predict Carcinogenic potency Using Ant Colony Optimization and Decision Trees ', Drug Metabolism and Reviews.
20. Sitarama Brahmam Gunturi, R. Narayanan, May 2014, 'A Novel Approach to Generate Robust Classification Models to Predict Developmental Toxicity from Imbalanced Data Sets', SAR and QSAR in Environmental Research, vol. 25, no. 9, pp. 711-727.
21. R. Narayanan, Sitrama Brahmam Gunturi, 'In silico ADME Modeling: Computational models to Predict Human Intestinal Absorption using Sphere Exclusion and kNN QSAR methods', International Symposium on Medicinal Chemistry, 29/08/2006 - Istanbul, Turkey.
22. R. Narayanan, Sitrama Brahmam Gunturi, 'In silico ADME Modeling: Computational models to Predict Human Serum Albumin Binding Affinity Using Ant Colony Systems', International Symposium on Medicinal Chemistry, 21/09/2006 - Istanbul, Turkey.
23. R. Narayanan, Sitrama Brahmam Gunturi, 'Computational Risk Assessment and Classification of Skin Sensitization- Understanding the Limitations', International ISSX Meeting, 04/09/2010 - Istanbul, Turkey.
24. Sitarama Brahmam Gunturi, R. Narayanan, 'Novel Algorithm to select basis functions in Spline Regression: Applications in QSAR studies', Conferentia Chemometrica, 18/09/2011 - Sumeg, Hungary.
25. Sitarama Brahmam Gunturi, R. Narayanan, 'Quantitative Prediction of Aqueous Toxicity using Spline Based Regression Methods', North American Regional ISSX Meeting, 16/10/2011 - Atlanta, USA.
26. Sitarama Brahmam Gunturi, R. Narayanan, 'A novel approach to generate robust predictive developmental toxicity classification models from highly unbalanced dataset and benchmarking with the reported models', North American Regional ISSX Meeting, 16/10/2011 - Atlanta, USA.
27. Sitarama Brahmam Gunturi, R. Narayanan, Theerthala Siva Rama Sarma, 'Prediction of Liver Related Toxicity Effects Using Logistic Regression and Support Vector Machines', North American Regional ISSX Meeting, 15/10/2012 - Dallas, USA.
28. Sitarama Brahmam Gunturi, R. Narayanan, 'Prediction of hERG Potassium Channel Blockage Using Spline Based Approximation Methods', North American Regional ISSX Meeting, 15/10/2012 - Dallas, USA.

29. Sitarama Brahmam Gunturi, R. Narayanan, Vijay Singh Punia, 'Prediction of Protein Binding using Genetic Algorithm and Local Lazy Regression', International ISSX Meeting, 01/10/2013 - Toronto, Canada.
30. Sitarama Brahmam Gunturi, R. Narayanan, Vijay Singh Punia, 'Classification Models to predict Carcinogenicity using Ant Colony Optimization and Decision Trees ', International ISSX Meeting, 02/10/2013 - Toronto, Canada.
31. Nishant Kumar Agrawal, R. Narayanan, Manoj Karunakaran Nambiar, Rihab Abdulrazak, 'PK-PD Parameter Estimation Using Parallelized Grid Search Method on GPU', GPU Technology Conference , 24/03/2014 - San Jose, USA
32. Sitarama Brahmam Gunturi, R. Narayanan, Shyam Sundar Das, 'Evaluation and Comparison of dissolution Models for different formulations of Metoprolol: A comprehensive study ', North American International ISSX Meeting, 21/10/2014 - San Francisco, USA.
33. Ms. Jyotsna Bahl, R. Narayanan, Shyam Sundar Das, 'Pharmacokinetic-Pharmacodynamic Parameter Estimation: Application ', North American International ISSX Meeting, 21/10/2014 - San Francisco, USA.
34. Nishant Kumar Agrawal, Payal Guha Nandy, Manoj Karunakaran Nambiar, R Narayanan, Shyam Sundar Das, 'Parallel Implementation of PK-PD Parameter Estimation on Xeon Phi Using Grid Search Method', HPCAC Swiss Workshop, 25/03/2015 - Switzerland.
35. Ms. Jyotsna Bahl, Shyam Sundar Das, Geervani K, R. Narayanan, 'Prediction Based Random Replacement Method: An application for efficient polynomial model building in Quantitative Structure Activity/Property Relationship studies', North American International ISSX Meeting, 18/10/2015 - Orlando, Florida, USA.
36. Geervani K, Ms. Jyotsna Bahl, Shyam Sundar Das, R Narayanan, 'Mutated Teaching Learning Based Algorithm: Applications to Predictive ADME Model Generation', North American International ISSX Meeting, 18/10/2015 - Orlando, Florida, USA.
37. Ms. Jyotsna Bahl, Shyam Sundar Das, R. Narayanan, 'Unsupervised Pharmacokinetic and Pharmacodynamics Parameter Estimation Using Modified Teaching Learning Based Optimization', AAPS Annual Meeting and Exposition, 25/10/2015 - Orlando, Florida, USA.
38. Geervani K, Dipayan Ghosh, R. Narayanan, 'Prediction of Renal Toxicity Using Chemical Information and Machine Learning Techniques: Scope and Limitations', AAPS Annual Meeting and Exposition, 12/11/2017 - San Diego, USA.



39. Geervani K, R Narayanan, 'Parallelized Variable Selection and Modeling based on Prediction algorithm on GPU for Feature Selection and ADMET Model Generation', Bioinformatics and Biomedicine, 13/11/2017 - Kansas, United States of America (USA).
40. Geervani K, R Narayanan, 'DEEP CONVOLUTION NEURAL NETWORKS ANALYSIS OF CHEMICAL IMAGES: APPLICATIONS IN DRUG DISCOVERY AND DEVELOPMENT', North American ISSX Meeting, 15/07/2018 - Montreal, Canada.
41. Geervani K, R Narayanan, 'GENERATION OF REPRODUCIBLE REGRESSION MODELS USING PARALLELIZED MODIFIED TEACHING LEARNING BASED SEARCH OPTIMIZATION METHOD AND ITS APPLICATIONS', North American ISSX Meeting, 15/07/2018 - Montreal, Canada
42. Dipayan Ghosh, Geervani K, R. Narayanan, 'PREDICTION OF RESPIRATORY TOXICITY USING CHEMICAL INFORMATION AND MACHINE LEARNING TECHNIQUES', North American ISSX Meeting, 15/07/2018 - Montreal, Canada.
43. Dipayan Ghosh, Geervani K, R. Narayanan, 'PREDICTION OF ADVERSE DRUG REACTIONS OF BIASED DATA USING BOOTSTRAP AGGREGATING AND MACHINE LEARNING TECHNIQUES', North American ISSX Meeting, 15/07/2018 - Montreal, Canada.