

Dr G Narahari Sastry

Dr G Narahari Sastry has obtained his early education in Khammam, Telangana and obtained his B.Sc. and M.Sc. from Osmania University (campus), Andhra Pradesh and Ph.D from University of Hyderabad. After a couple of post-doctoral stints, he started his independent research career in 1997 at Pondicherry University, and moved to CSIR-IICT in 2002, to head centre for molecular modeling. He is a professor of AcSIR in chemistry and lifesciences disciplines. Dr Sastry's research interests are theoretical and computational chemistry, computational biology, computer aided molecular design and chemoinformatics. Dr Sastry has made fundamental contributions in the area of non-covalent interactions and developed several important concepts in this area. His group is interested to apply the data science approaches, and also developing indigenous software, Molecular Property Diagnostic Suite. Several of his computational predictions have seen experimental realization. Besides publishing independently, the group also has active collaboration with several experimentalists and strongly believe that 'theory-experiment interplay is indispensable' for the progress of science. He has successfully guided 21 Ph.D students and published more than 275 papers. Currently 12 members are doing Ph.D and postdoctoral studies in the group. These publications received over 8700 citations, with an h-index of 47.

Dr Sastry is a J C Bose National Fellow (2015). He was awarded with Shanthi Swarup Bhatnagar Prize in Chemical Sciences (2011), considered as one of the highest prize for science and engineering in India, National Bioscience award (DBT) 2009, one of the highest for Lifesciences in India, Swarnajayanthi Fellowship 2005 (DST), B.M. Birla award for 2001, B C Deb Memorial award (2009), CRSI Medal 2011, and AvH Fellowship. He has delivered more than 300 invited lectures which include talks in national and international conferences. He was a visiting professor at IMS, Japan; LMU, Munich, Germany; Jackson State University, USA, and Kyushu University, Japan. He was elected as a Fellow of National Academy of Sciences (FNASc), Fellow of the Indian Academy of Sciences (FASc), Fellow of Association of Biotechnology and Pharmacy, Telangana State Academy of Sciences (Founder Fellow) and Andhra Pradesh Academy of Sciences (FAPAS). He is a regular reviewer to some prestigious journals and also in the editorial board of some journals.

G N Sastry's major research contributions to science: a) developing of indigenous software for drug discovery; b) fundamental contributions to the concept of cooperativity of non-covalent interactions; c) several important contributions in the areas of buckyball chemistry, aromaticity, pericyclic reactions, hypervalent structures, electron transfer reactions, organic reaction mechanisms and reactive intermediates; d) design of selective and efficient enzyme inhibitors on a number of targets, and also developing QSAR, pharmacophore and structure based models for selectivity, permeability and efficacy. Currently, his main focus is on employing artificial intelligence (AI) and machine learning (ML) methods to integrate with cheminformatics, bioinformatics, electronic structure calculations, and molecular dynamics simulations. This integrated approach will be employed in developing disease specific webportals, delineating disease biology and working in the area of healthcare.