

Dr. Narahari Sastry G

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Bibliography

Dr. G. Narahari Sastry has obtained his B.Sc. and M.Sc. from Osmania University and Ph.D. from University of Hyderabad (under the guidance of Professor E.D. Jemmis). After a couple of Post-Doctoral stints with Professor Sason Shaik (Hebrew Univ., Jerusalem) and Professor Thomas Bally (Univ. of Fribourg, Switzerland), he started his independent research career in 1997 at Pondicherry University. After spending five years at Pondicherry, he moved to IICT, Hyderabad to head the Molecular Modelling Group. Thus, from Nov., 2002 onwards he has been working as the Head of Molecular Modelling Group, at the Indian Institute of Chemical Technology, Hyderabad. Dr. Sastry's research interests are computational chemistry and computer aided drug design. With more than 210 publications to his credit, Dr. Sastry has contributed significantly in the fields of non-bonded interactions, buckybowl chemistry, hetero-aromaticity, designing structures that defy conventional bonding patterns, pericyclic reactions, biomolecular modeling and computer aided drug design (PDE4, p38kinase, aromatase, membrane proteins, etc). Several of his computational predictions have seen experimental realization. Noteworthy contributions are in the field of understanding the structural and energetic aspects of cation- π interactions and their relevance in chemistry and biology. His current interests are computational chemistry, computational biology and computer aided drug design.

He has successfully guided 12 Ph.D. students, and several M.Tech., M.Pharm., and M.Sc. students. 6 researchers spent time as Post-Doctoral colleagues in the group. Currently about 10 students are pursuing their Ph.D. under his guidance. He has organized and participated in many national and international conferences, and delivered about 150 invited/plenary lectures. His publications have so far received more than 2850 citations, and have an h-index of 28.

He has been awarded prestigious Shanthi Swarup Bhatnagar Prize in chemical sciences (2011), Swarnajayanthi Fellowship 2005 (DST), Alexander von Humboldt (AvH) Fellowship, B.C. Deb Memorial Award (Indian Science congress), National Bioscience Award (DBT) 2009, B.M. Birla Young Scientist Award for 2001, CRSI Medal 2011, etc. He was also elected as a Fellow of National Academy of Sciences (FNASc) and Andhra Pradesh Academy of Sciences (FAPASc).

Research Interests

Multi-disciplinary research programmes including organic synthesis, medicinal, combinatorial and green chemistry including chemical biology and biocatalysis. Non-Bonded Interactions, Computer Aided Drug Design, Theoretical Organic Chemistry, Multiscale Modeling & Dynamics.

Publications

- Analyzing Coordination preferences of Mg^{2+} complexes: Insights from computational and database study. Y. Indra Neela, A. Subha Mahadevi, G. N. Sastry, Struct. Chem., 2012, 00, 000.
 - Contrasting preferences of N and P substituted heteroaromatics towards metal binding: Probing the regioselectivity of Li^+ and Mg^{2+} binding to $(CH)_6$ -m-nNmPn. Bhaskar Sharma, D. Umadevi, G. N. Sastry, Phys. Chem. Chem. Phys., 2012, 00, 000.