Dr. Dandamudi Usharani, Principal Scientist
Department of Food Safety & Analytical Quality Control Laboratory, CSIR Central Food Technological Research Institute, Mysore, Karnataka.

Research Area Applied Chemistry, Computational Chemistry

Research Interests
Computational Bioinorganic Chemistry, Structural Biology, Chemical Biology, Spectroscopy, Molecular Modeling, Bio catalysis, Disease Mechanisms, Quality Assurance of Oils & Fats

Research Profile

A group leader of oils and fats developed several in-house mass spectrometric and chromatographic techniques to quantify antioxidants, vitamins, fatty acid profiling, and bioactive lipids that assist in nutritional profiling and lipidomics of food products. Understanding of food structure and analysis of lipids are of keen interest. Pursuing electronic structure bonding, and spectroscopic characterization of porphyrin compounds, the fats and oils, bioactive lipid species, active catalytic species and the organometallic complexes that are of biological interest through multiscale modeling. Elucidating disease mechanisms through structure-function relationships of the biomolecules and bioactive compounds of food. Phytochemical profiling, screening, pharmacokinetics of leads and structural basis for protein-ligand interactions assist for rationalizing the mechanism and selectivity and provide future directions for nutraceuticals and design of functional foods.

Professional appointments / Scientific career

2009 - 2014	Postdoctoral fellow at The Hebrew University of Jerusalem
2014 - 2017	Quick Hire Scientist at CSIR- Central Food Technological Research Institute
Since 2017	Principal Scientist at CSIR-Central Food Technological Research Institute

Education

2004 - 2009	Doctoral dissertation “Computational Structural Aspects of the Phosphorus Containing Clusters and Phosphodiesterases under the guidance of Prof. E. D. Jemmis, University of Hyderabad
1998 - 2004	Lecturer at MNR Degree College, Vignan Junior College and Guntur Vikas Junior College
1998	Master in Science, General Chemistry, University of Hyderabad

Memberships & Research Awards

- Mrs Vaidehi Kishan Rao Memorial Gold Medal from Osmania University, B.Sc., 1996
- Member of Scientific Panel on Oils and Fats, Food Safety and Standards Authority of India, Team member of *'Network for Scientific Co-operation for Food Safety and Applied Nutrition*' for Foods of Plant Origin
- Member of American Chemical Society, World Association of Theoretical and Computational Chemists, Chemical Research Society of India, Society of Biological Chemists (INDIA), Indian Science Congress Association and The Association of Analytical Communities (AOAC) International, India.

Selected list of publications (Out of 39 no of publications)

1. A. Lohithakshan, R. Naryanasamy, U. S. Potteth, S. Kishava, V. Nagaraja, D. Usharani, R. Kumar* Molecular insights into the mechanism of substrate binding and catalysis of bifunctional FAD synthetase from Staphylococcus aureus, ***Biochimie***, 2021, 182, 217-227.

2. S. Abduldileep, R. Narayanasamy, D. Usharani, A. Singh, R. Rajasekharan, R., A Bioactive Polypeptide from Sugarcane Selectively Inhibits Intestinal Sucrase. ***Int. J Biol. Macromo****l*., 2020, 156, 938-948.

3. K. C. Sahoo, M. S. Kumaraswami, D. Usharani,* H. Rath,* "Conformationally Rigid Ethynylene-Cumulene Conjugated Aromatic [30] Heteroannulenes with NIR Absorption: Synthesis, Spectroscopic and Theoretical Characterization***. J. Org. Chem***., 2019, 84, 5203 (*selected for ACS editor choice*)

4. J. Anusha, D. Usharani, M. Srinivasan, R. Rajasekharan, "Sesaminol diglucoside, a water-soluble lignin from sesame seeds induce brown fat thermogenesis in mice. ***Biochem. Biophys. Res. Comm***., 2018, 507, 155-160 (No of Citations: 4).

5. S. Ghosh, M. Sinha, A. Bhattacharyya, S. Sadhasivam, J. Megha, S. Reddy, S. Saini, S. Singh, D. Kumar, S. P. Kaur, M. Mishra, D. Usharani, S. Ghosh, S. Sengupta, "A Rationally Designed Multi-Functional Antibiotic For the Treatment of Drug-Resistant Acne", ***J. Investig. Dermatol.*** 2018, 138, 1400-1408.

6. J. Li, S. Zhou, J. Zhang, M. Schlangen, D. Usharani, S. Shaik, H. Schwarz, "Mechanistic Variants in Gas-phase Metal-oxide Mediated Activation of Methane at Ambient Conditions" ***J. Am. Chem. Soc.*** 2016, 138, 11368-11377 Selected for ***JACS Spotlights*** 2016, 138, 12003.

7. S. Shaik, Chemistry as A Game of Molecular Construction: The Bond-Click Way. (Contributors R. B-K. Wakshlak, D. Usharani, D. A. Sharon) Book In Press John Wiley & Sons Inc., 2016. ISBN: 978-1-119-00140-9.

8. D. Usharani, D. C. Lacy, A. S. Borovik, S. Shaik, "Dichotomous Hydrogen Atom Transfer vs. Proton Coupled Electron Transfer during Activation of X-H Bonds (X = C, N, O) by Nonheme Iron-Oxo Complexes of Variable Basicity." ***J. Am. Chem. Soc****.,* 2013, 135, 17090-17104.

Ongoing Projects:

1. FOCUS project on Understanding structure function relationships in enzymes critical for the survival of bacterial food pathogens---CSIR, New Delhi

2. Development of Process Know-how for the production of sunflower oil enriched with bioactive lipids and nutraceuticals for immune boosting --- Sponsored M/s Anagha Mangalore

3. Structural Characterization of Emulsifiers – In-house, CFTRI

Completed Projects

1. National Centre for Advanced Analytical Services Theme: Agriculture, Nutrition and Biotechnology, CSIR New Delhi
2. Consultancy on designing & Optimizing new structural scaffolds using computer software— Sponsored Vyome BioSciences, New Delhi

3. Understanding the affinity and efficacy of a few synthesized antibiotics using computer software –Sponsored Vyome BioSciences, New Delhi