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Dr. Jayaram joined IIT Delhi as a faculty in the Chemistry Department in 1990. Prior to this, he obtained his Ph.D. in Chemistry from the City University of New York (1986) under the guidance of Prof. David L. Beveridge, a renowned quantum chemist and one of the world's leading experts in DNA modeling. Dr.Jayaram's thesis work was concerned with developing methodologies to model nucleic acid constituents at atomic level under aqueous conditions on what was then one of the largest computer installations of IBM in mid-town Manhattan. After his Ph.D., he took up a Post Doctoral assignment with Prof. Barry Honig, a pioneer in Biomolecular Electrostatics and Bioinformatics, at Columbia University, USA. Dr. Jayaram's contributions on electrostatics of DNA have eventually found their way into Delphi software of what was formerly Biosym, subsequently Accelrys etc.. Later, he worked as a Senior Research Associate with Prof. Beveridge at Wesleyan University where he developed methodologies to help understand the energetics of Biomolecular recognition.

At IIT Delhi, he started building the infrastructure to carry out biomolecular modeling and creating the necessary science and software pursuing the dream of developing *in silico* solutions for personalized medicine (individual specific drugs with no side effects). A result of these efforts is the Supercomputing Facility for Bioinformatics & Computational Biology (SCFBio) at IIT Delhi which currently hosts over 1000 cores with a compute capacity close to 65 Tera Flops and 200 terabytes of storage, and the Gene to Drug suite of softwares (www.scfbio-iitd.res.in).The SCFBio website is accessed by over 20,000 users per day from more than 30 countries (www.scfbio-iitd.res.in/usage). *Dhanvantari* ("A comprehensive automated computer-aided discovery pipeline from genomes to hit molecules", *Chemical Engineering Science*, 2020. https://doi.org/10.1016/j.ces.2020.115711) incorporates some very significant original scientific contributions of Prof. Jayaram and his students (http://www.scfbio-iitd.res.in/BJ_SCFBio_Web_Nov_2019.pdf).

Dhanvantari includes

(1) deciphering the language of DNA and identifying the various genomic elements from a physico-chemical perspective:
(Chemgenome:

(i) *J. Chem. Inf. Model.*, 2006, *46*, 78-85.
http://pubs.acs.org/doi/abs/10.1021/ci050119x,
(ii) *Biophys J.*, 2008, *94*, 4173-4183;
doi: 10.1529/biophysj.107.116392,
(iii) *Biophys. J.*, 2014, 106 (11), 2465-73.
DOI:10.1016/j.bpj.2014.04.029.

(iv) *Nucleic Acids Research*, 2016, 45 (7), e47. *doi:10.1093/nar/gkw1236,*
(v) *Biophysical Journal*, 2018,115(7): 1180-1189. *DOI:10.1016/j.bpj.2018.08.002,*
(vi) *Nucleic Acids Research*, 2021. *https://doi.org/10.1093/nar/gkab098);*

(2) force field based approaches to protein structure prediction (*Bhageerath*:

(i) *Phys. Chem. Chem. Phys., 2005,* 7, *2364-2375.* *http://pubs.rsc.org/en/content/articlelanding/2005/CP/b502226f,*
(ii) *Nucl. Acids Res.*, 2006, 34, *6195-6204* *http://nar.oxfordjournals.org/content/34/21/6195.long,*
(iii) *BMC* Bioinformatics, *2014,15 (Suppl16):S7* *http://www.biomedcentral.com/1471-2105/15/S16/S7),*

(3) and binding free energy based methodologies for protein/DNA target directed lead molecule discovery (*Sanjeevini*:
(i) *Ind. J. Chem.*, 2006, *45A*, 21-33, *Bioinformatics*, 2012**,** *13*, S7. http://www.biomedcentral.com/1471-2105/13/S17/S7).

(ii) *Sanjeevini*, a complete drug design software suite, boasts of delivering molecules against

HAV
(The FEBS Journal, 2018, 286 (2019), pg. 765 -787. *DOI: https://doi.org/10.1111/febs.14707),*

HBV
(J AntimicrobChemother, 2022, 77(8):2120-2124. doi: 10.1093/jac/dkac148.,&*Scientific Reports*, 2021, https://doi.org/10.1038/s41598-021-91196-1),

CHIKV
(*Virology*, 2020, DOI: 10.1016/j.virol.2020.05.010),

Breast cancer
(*Chemical Biology & Drug Design*, 2017, DOI: 10.1111/cbdd.13126),

Fungal infections
(*Nature*, 2016, doi:10.1038/nature16963),

Malaria
(*Journal of Molecular Graphic and Modelling*, 2016, 71, 96-103. doi: 10.1016/j.jmgm.2016.10.022) and so on.

It is a matter of immense satisfaction that the National Supercomputing Mission of India, commissioned a project for implementation of *Sanjeevini* on its petaflop machines for free use by the student and scientific community.

Some of Prof.Jayaram's other significant scientific contributions include,

(A) discovery of the rule of conjugates which provides a molecular basis for wobble hypothesis (*J. Mol. Evol.*, 1997, *45*, 704-705, https://doi.org/10.1007/PL00013144);

(B) discovery of stoichiometry and universalities in protein structures (*J. Biomol. Struc. Dyn.*, 2010, *28*, 133-142.doi/abs/10.1080/07391102.2010.10507349);

(C) discovery of a new stereochemical classification and a new chemical logic of amino acids which unravels the hidden similarities in protein sequences and pushes the accuracies of homology modeling and function prediction (*Biochemistry*, 2018, 55(5): 503-505.DOI: 10.1021/acs.biochem.7b01073&*Proteins: Structure, Function, and Bioinformatics* , 2021.https://doi.org/10.1002/prot.26069);

(D) discovery that protein folding is a convergent problem (*Biochemical and Biophysical Research Communications*, **2016**, 480 (4), 741-44. doi: http://dx.doi.org/10.1016/j.bbrc.2016.10.119),

(E) and that experimental Higher order Ramachandran maps even at the tripeptide level have sufficient information to generate tertiary structures of small proteins (*J. Phys. Chem. B , **2015** . 119 (34), pp 11136 - 11145. DOI: 10.1021/acs.jpcb.5b02999);*

(F) development of proteome wide structural databases (*Database*, 2018. https://doi.org/10.1093/database/bay021);

(G) invention of Symmetric DNA (*J BiomolStructDyn.* 2019, https://doi.org/10.1080/07391102.2019.1585292);

(H) accurate mapping of Electrostatics of DNA (*Biopolymers*, 1989, *28*, 975-993, https://doi.org/10.1002/bip.360280506);

(I) molecular view of counterion condensation around DNA (*Macromolecules*, 1990, *23*, 3156-3165, https://doi.org/10.1021/ma00214a021 & *J. Am. Chem. Soc.* 1997, *119*, 59-69, https://doi.org/10.1021/ja960459m);

(J) reaction field versus Refraction field in interaction and binding (*J. Phys. Chem.*, 1994, *98*, 5773-5777, https://doi.org/10.1021/j100073a034);

(K) dielectric continuum theories for solvation (*J. Phys. Chem.*, 1990, *94*, 4666-4671,

DOI: 10.1021/j100374a055&*Biopolymers*, 1988, *27*, 617-627,doi.org/10.1002/bip.360270406);

(L) Statistical Mechanics on the unit interval
(*J. Phys. Chem.*, 1990, *94*, 7288-7293,https://doi.org/10.1021/j100381a061) and so on.

Jay as he is known, believes that language of DNA is close to being deciphered, that the protein folding problem, the holy grail of molecular biology, unsolved for the last 70 years, would find a solution soon and that computers would generate reliable lead molecules to fight disease. He is proud of being instrumental in creating Children's parks in IIT Delhi. A flutist by passion and a long distance runner, he intends to participate in New York Marathon and dreams of climbing Mt. Everest one of these years.

Prof. Jayaram published and presented over 150 papers in refereed international journals of high impact and presented over 300 talks in national and international conferences. He has supervised 29 Ph.D. students (27 completed, 2 in progress) and over 125 M.Tech., M.Sc. and B. Tech. Project students (http://www.scfbio-iitd.res.in/training/training.htm). Prof. Jayaram was awarded the CRSI (Chemical Research Society of India) medal in 2000 for contributions to research in Chemistry and was a Recipient of IBM Faculty Award (2014-2015). He was Head of Chemistry (2006-2009), Founder Coordinator of Kusuma School of Biological Sciences (2008-2014), Founder Coordinator of SCFBio (2002-2019) and, a member of several Governmental professional bodies (http://www.scfbio-iitd.res.in/scfbiogroup/biocomputinggroup.htm)

Prof.Jayaram is currently an Emeritus Professor in the Department of Chemistry, IITD and a Co-PI & mentor for SCFBIO, IITD.