

Dr.V.Umashankar, M.Sc.,M.Phil., PGDBI., Ph.D.,
HOD & Principal Scientist/Associate Professor,
Centre for Bioinformatics,
Vision Research Foundation,
SankaraNethralaya, Chennai -600006.
drvus@snmail.org

Dr.V.Umashankar completed his PhD. from School of Genomics, Dept. of Zoology, Loyola College, University of Madras, Chennai in 2008; M.Phil Genetics from Dr.ALMPGIBMS, University of Madras in 2000; Qualified SLET. He did his PG Diploma in Bioinformatics from University of Mysore in 2003; S-Star Certification in Bioinformatics awarded by National University of Singapore in 2004. He has 17 years of experience in Research & mentoring in Bioinformatics. He is currently HOD & Principal Scientist, Centre for Bioinformatics, Vision Research Foundation, a unit of Sankara Nethralaya since Jan 2010. He was formerly, HOD, Department of Bioinformatics, School of Biosciences, SRM University. He also held positions as Academic Head, Research consultant, Senior Research Analyst in leading Research and Academic Organizations. He has been appointed as member “Board of Studies in Bioinformatics” by University of Madras & SASTRA University. He is also an examiner and advisor for PhD, B.Tech, M.Tech, M.Sc courses offered by leading universities in India. He has mentored 14 M.Phil graduates. Dr.Umashankar is a recipient of RGYI (Rapid Grant for Young Investigators) grant awarded by DBT (for Anti-toxoplasmosis Drug Development) and Early Career Research Award from SERB-DST (for Drug target mining and Systems Biology studies towards targeting ocular Chlamydial Infections) and also serving as Investigator in many of the funded grants from ICMR, CSIR, DST and DBT.

Areas of Interest: Ocular Therapeutics and drug development by implementation of Bioinformatics techniques. Major focus in design and development of Peptide/Chemical Inhibitors targeting Ocular angiogenesis, Ocular infections and pH Homeostasis in Cancer cells. He has extensively worked on genome assembly and annotation of microbial Pathogens like *Mycobacterium tuberculosis* and *Pseudomonas aeruginosa* towards identification of drug targets.

He is also engaged in deciphering transcriptomic changes in the context of Hyperglycemia in Retinal cells by applying NGS technologies.

He has published 72 Research papers in peer reviewed International and national journals and has also written three chapters on Molecular modeling, Cheminformatics and Computational Epigenomics for a book published by John Wiley & Sons (click the underlined links for publications indexed in [Pubmed](#) and [Google Scholar](#)). He is also a reviewer for many of the leading peer reviewed journals like PLOS One, Bioinformatics (OUP), Human Molecular Genetics, GENE and RSC Advances etc. He has delivered many lectures at various National and International conferences as an invited speaker. He recently presented his research work on Drug target mining in *Chlamydia trachomatis* at ARVO-2018 international conference held at Honolulu, Hawaii, USA. He is the author of Bioinformatics tools & Databases namely, POAP, ACUA, OpenDiscovery, Nitrosoft, Readmol and Indian Plant Anticancer Compound Database (InpacDB), respectively. Many of these tools are used by scientists worldwide and are cited in peer-reviewed journals. Currently involved in the development of NGS and Drug discovery computational pipelines. 'Theoretical model of human ghrelin precursor' (PDB ID: 1p7x) predicted by him is printed and cited on the coverpage of 77th volume of the prestigious book 'Vitamins and Hormones' first published in 1943, and is the longest-running serial book published by Elsevier Academic/Press.

Membership of professional bodies in Indian Bioinformatics Society, Society of Toxicology and Bioclues. He has organized many National Level Conferences and Workshops on Bioinformatics funded by Government bodies. He was awarded with best faculty award in view of his teaching and research by Vels Academy.

RESEARCH

Ongoing projects

Principal Investigator: Dr.V.Umashankar

Project	Funding Agency
Insilco drug target identification in Chlamydia species through systems biology and molecular modelling approaches pertaining to the development of potential drug molecules	DST-SERB
Genome wide Transcriptome profiling of Human Retinal Cells under diabetic milieu under the context of Egr-1 expression towards deciphering alternative pathways mediating Retinal Angiogenesis.	ICMR
<i>In silico</i> Design and Development of novel peptide inhibitors targeting CD147 through virtual screening and biopanning of peptide libraries and <i>in vitro</i> validation of anticancer efficacies.	DBT

Completed Projects

S.No	Project Name	Funding Agency
1	Design and development of novel Anti-Angiogenic molecules by targeting polysaccharide binding domain of Carbonic Anhydrase IX through structural bioinformatics methods and studies on cell culture models	ICMR - PI
2.	Molecular modelling and Docking, simulation studies of functional domains of Toxoplasma gondii RON4, RON2 & RON5 to understand the moving junction complex formation towards design of novel peptide and chemical inhibitors and validation through invitro studies	DBT-RGYI

As Co-Investigator

3	Development of therapeutic molecules for diabetic retinopathy from studies on structure/function relationship of PON2 by cloning	CSIR
4	Peripheral Blood Gene Expression Profiling In Eales Disease	ICMR
5	Regulation of Lysyl Oxidase expression in Lens Epithelial Cells and trabecular endothelium	ICMR
6	Molecular modelling and Docking, simulation studies of functional domains of Toxoplasma gondii RON4, RON2 & RON5 to understand the moving junction complex formation towards design of novel peptide and chemical inhibitors and validation through <i>in vitro</i> studies	DBT-RGYI
7	Development of modulators Ornithine decarboxylase (ODC) for the therapeutic application in retinoblastoma	CSIR
8	Application of Next Generation Sequencing technique to determine the whole genome sequence of laboratory isolates of Enterococcus fealias, P.aeruginosa, B.cervus (both sensitive and resistant strains) And application of bioinformatics approaches to identify the vulnerable area of drug targets in genome	ICMR
9	Biomarker pattern discovery of graded changes in the opacity of human lens in age-onset cataract: a proteomic approach	ICMR
10	Fuch's endothelial corneal Dystrophy (FCD)– Fine mapping and identifying candidate gene for the novel loci 20p12.1- q13.2 in early onset family and study the association of TCF4 gene in sporadic late onset FCD cases in our population	ICMR
11	FASN Structure and inhibition: Design of catalytic domains. Identification of novel inhibitors and characterisation of enzyme-inhibitor dynamics using insilico tools and experimental validation in Y79 retinoblastoma cells.	DBT

12	Development of therapeutic peptide from proteoglycan LRR-angiogenesis	DBT
13	Identification of novel interacting partners for PEDF in angiogenesis and obesity	DST

Collaborative research as a Core Facility serving other Departments

- Design of peptide carrier molecules targeting fungal keratitis (Nanobiotechnology)
- Structure Function relationship studies of PRR4 protein (Biochemistry)
- Binding mode analysis of Fatty acids with therapeutically important proteins (Biochemistry)
- Molecular modeling and Simulation studies of Aptamers and its molecular interactions (Nanobiotechnology& Pathology)
- NGS based Variant Analysis of different ocular genetic disorders (Genetics)
- Structure-function relationship studies of mutational impact on Retinoschisin- 1 (Genetics)
- NGS Data Analysis of Ocular Pathogens& Mycobacterium tuberculosis (Microbiology)
- Structure prediction of Lysyl oxidase using Insilico modeling techniques (Biochemistry)
- Comparative study of LOX and other amine oxidases (Biochemistry)
- Insilico mutation impact analysis in UL54 gene of hCMV (Microbiology)
- Diabetic Retinopathy Microarray Analysis Project (Genetics)
- Glaucoma Genome-wide Association Studies (GWAS) (Genetics)
- Structural studies on proteins of Ocular therapeutic interest(Biochemistry)
- Structure-function studies of the impact of mutations in Mycobacterium tuberculosis proteins (microbiology)
- Rule based siRNA&Primer design of SPARC and Copper Transporter Receptor 1.(Biochemistry)

- Mutational analysis of Pyrazinamide (PZA) of Mtb using structural bioinformatics approaches (Microbiology)
- Structural analysis of CYP4V2 mutations (Genetics)
- Structural analysis of SLC4A11 mutations (Genetics)
- Functional characterization of novel mutations in UL54 of ganciclovir resistant HCMV strain using structural analysis (Microbiology)
- Design of SiRNA for copper binding proteins using Bioinformatics tools (Biochemistry)
- Structure function analysis of 88KDa protein (Biochemistry)
- Characterization of Hypothetical proteins present in tear (Biochemistry)
- Insilico modeling and docking studies of Glutamate cysteine ligase (Biochemistry)
- Identification of various binding regions/ residues in Osteonectin, PEDF and Decorin (Biochemistry)
- Structural and functional analysis of Serum paraoxonase 2 using Insilico strategies (Biochemistry)
- Identification of anti-angiogenic peptides in small Leucine rich repeats (Biochemistry)
- Identification of Transcription factor Binding sites (CellBiology)
- Structural Domain analysis of RIM protein (Genetics)
- Structural analysis of RPE 65 mutations(Genetics)

PUBLICATIONS

INVITED BOOK CHAPTERS:



- *Insilico Tools of Molecular Modeling, in Handbook of Systems Toxicology*, **V.Umashankar** and S.Gurunathan, edited by Daniel A. Casciano and Saura C.Sahu. Chichester, **UK: John Wiley & Sons, Ltd**, pp 579-590. (2011)
- *Cheminformatics and its Applications, in Handbook of Systems Toxicology*, edited by Daniel A. Casciano and Saura C.Sahu. Chichester, **V.Umashankar** and S.Gurunathan, **UK: John Wiley & Sons, Ltd**,pp 347-360. (2011)
- *Databases and Tools for Computational Epigenomics for Computational Epigenomics, Toxicology and Epigenetics*, Edited by Saura C.Sahu. Chichester, **V. Umashankar** and S. Gurunathan, **UK: John Wiley & Sons, Ltd**,pp. 595-614. (2011)

LIST OF RESEARCH PUBLICATIONS

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- Umashankar Vetrivel, Nagarajan H. Deciphering ophthalmic adaptive inhibitors targeting RON4 of *Toxoplasma gondii*: An integrative in silico approach. *Life Sciences*. 2018 Oct 13. pii: S0024-3205(18)30639-8. doi: 10.1016/j.lfs.2018.10.022. PubMed PMID: 30326220.
- Sadhasivam A, Vetrivel U. Identification of potential drugs targeting L,L-diaminopimelate aminotransferase of *Chlamydia trachomatis*: An integrative pharmacoinformatics approach. *Journal of Cellular Biochemistry* 2018 Oct 10. doi:10.1002/jcb.27553. PubMed PMID: 30302805.
- Nagarajan H, Vetrivel U. Demystifying the pH dependent conformational changes of human heparanase pertaining to structure-function relationships: an in silico approach. *Journal of Computer Aided Molecular Design*. 2018 Jul 6. doi: 10.1007/s10822-018-0131-0. PubMed PMID: 29980923.
- Sudha D, Neriyanuri S, Sachidanandam R, Natarajan SN, Gandra M, Tharigopala A, Sivashanmugam M, Alameen M, Vetrivel U, Gopal L, Khetan V, Raman R, Sen P, Chidambaram S, Arunachalam JP. Understanding variable disease severity in X-linked retinoschisis: Does RS1 secretory mechanism determine disease severity? *PLoS One*. 2018 May 31;13(5):e0198086. doi: 10.1371/journal.pone.0198086. eCollection 2018. PubMed PMID: 29851975; PubMed Central PMCID: PMC5978886.
- Samdani, A., and Umashankar Vetrivel. "POAP: A GNU Parallel based multithreaded pipeline of Open Babel and AutoDock suite for boosted High Throughput Virtual Screening." *Computational Biology and Chemistry* (2018).
- Muthukumaran S, Sulochana KN, Umashankar V. Virtual screening of Natural inhibitors targeting Ornithine Decarboxylase with pharmacophore scaffolding of DFMO and

validation by molecular dynamics simulation studies. J Biomol Struct Dyn. 2018 Feb 13:1-30. doi: 10.1080/07391102.2018.1439772. [Epub ahead of print] PubMed PMID: 29436980.

2017

- Muthukumar S, Bhuvanasundar R, Umashankar V, Sulochana KN. Insights on ornithine decarboxylase silencing as a potential strategy for targeting retinoblastoma. Biomed Pharmacother. 2018 Feb;98:23-28. doi:10.1016/j.biopha.2017.12.030. Epub 2017 Dec 11. PubMed PMID: 29241071.
- Vetrivel U, Nagarajan H, Thirumudi I. Design of inhibitory peptide targeting Toxoplasma gondii RON4-human β -tubulin interactions by implementing structural bioinformatics methods. J Cell Biochem. 2017 Nov 1. doi: 10.1002/jcb.26480. [Epub ahead of print] PubMed PMID: 29091310.
- Genome-wide codon usage profiling of ocular infective Chlamydia trachomatis serovars and drug target identification. Anupriya Sadhasivam & Umashankar Vetrivel. Article in Journal of Biomolecular Structure and Dynamics. Published online on Jul 4 2017, page number 1-25. PMID: 28627970 DOI: 10.1080/07391102.2017.1343685
- Polymorphism of the PAI-1 gene (4G/5G) may be linked with Polycystic Ovary Syndrome and associated pregnancy disorders in South Indian Women. Maniraja Jesintha Mary, Lakshmanan Saravanan, Munuswamy Deecaraman, Melantharu Vijayalakshmi, Vetrivel Umashankar, Jaigopal Sailaja. Article in Bioinformation. 13(5): 149-153 May 2017. <http://www.bioinformation.net / 013 /97320630013149.htm>.
- *Ornithine and its role in metabolic diseases: An appraisal.* Muthukumar S, Sivashanmugam, Jaidev Ja, **Umashankar V.**, Sulochana K.N. Article in **Biomedicine & Pharmacotherapy** 86:185–194 · February 2017 DOI: 10.1016/j.biopha.2016.12.024

- *Inhibition of IKK β by celastrol and its analogues – an in silico and in vitro approach.* Karpagam Veerappan, Sathishkumar Natarajan, Purushoth Ethiraj, **Umashankar Vetrivel** & Shila Samuel. Article in **Pharmaceutical Biology** 55(1): 368-373 · January 2017. DOI: 10.1080/13880209.2016.1241809
- *Virulence genome analysis of Pseudomonas aeruginosa VRFPA10 recovered from patient with scleritis.* Murugan N, Malathi J, **Umashankar V**, Madhavan HN. **Genom Data.** 2017 Feb 6;12:1-3. doi: 10.1016/j.gdata.2017.02.007. eCollection 2017 Jun. PubMed PMID: 28217443; PubMed Central PMCID: PMC5302140.
- *Probing the intermolecular interactions of PPAR γ -LBD with polyunsaturated fatty acids and their anti-inflammatory metabolites to infer most potential binding moieties.* Shalini Muralikumar, **Umashankar Vetrivel**, Angayarkanni Narayanasamy and Undurti N. Das. Lipids Health Dis. 2017; 16: 17. DOI: 10.1186/s12944-016-0404-3.

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- *Unraveling Genomic and Phenotypic nature of Multidrug-Resistant (MDR) Pseudomonas aeruginosa VRFPA04 Isolated from Keratitis Patient.* N. Murugan, J. Malathi, **V. Umashankar**, H.N. Madhavan. **Microbiological Research.** 2016; 193. DOI:10.1016/j.micres.2016.10.002. PMID: 27825482
- *In Silico Structure Prediction of Human Fatty Acid Synthase–Dehydratase: A Plausible Model for Understanding Active Site Interactions.* Perinkulam Ravi Deepa, John Arun, **Vetrivel Umashankar**, A Samdani, Manoharan Sangeetha, Subramanian Krishnakumar. **Bioinformatics and biology insights** 2016; DOI:10.4137/BBI.S38317.2016. PMID: 27559295
- *Virtual Screening, Molecular dynamics and binding free energy calculations on Human Carbonic Anhydrase IX catalytic domain for deciphering potential leads.* Arun John, Muthukumar Sivashanmugam, **Vetrivel Umashankar**, Sulochana Konerirajapuram

Natarajan. *Journal of Biomolecular Structure & Dynamics*. 2016; DOI:10.1080/07391102.2016.1207565. PMID: 27373313

- *Multilevel Precision-Based Rational Design of Chemical Inhibitors Targeting the Hydrophobic Cleft of Toxoplasma gondii Apical Membrane Antigen 1 (AMA1)*. **Umashankar Vetrivel**, Shalini Muralikumar, B Mahalakshmi, K Lily Therese, HN Madhavan, Mohamed Alameen, Indhuja Thirumudi. *Genomics & Informatics*. 2016; 14(2). DOI:10.5808/GI.2016.14.2.53. PMID: 27445648
- *Comparative docking of dual conformations in human fatty acid synthase thioesterase domain reveals potential binding cavity for virtual screening of ligands*. Arun John, **Umashankar Vetrivel**, Krishnakumar Subramanian, Perinkulam Ravi Deepa. *Journal of Biomolecular Structure & Dynamics* 2016; DOI:10.1080/07391102. PMID: 27145135
- *Targeting CD44, ABCG2 and CD133 markers using aptamers: in silico analysis of CD133 extracellular domain 2 and its aptamer*. Subramanian N, Akilandeswari B, Bhutra A, Alameen M, **Vetrivel U**, Khetan V et al.,. *RSC Advances*. 2016; 6(38): 32115-32123. DOI: 10.1039/C5RA27072C
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Vetrivel U, Narayanan J. *Biochem Biophys Res Commun*. 2016; 469(2):257-62. PMID: 26642954

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- *Drug Discovery: an appraisal*. **Umashankar, V.**, and S. Gurunathan. *International Journal of Pharmacy and Pharmaceutical Sciences*. 2015; 7.4.
- *Virtual screening studies of seaweed metabolites for predicting potential ppar γ agonists*. Gurula, H., Loganathan, T., Krishnamoorthy, T., **Vetrivel, U.**, & Samuel, S. *International Journal of Pharmacy and Pharmaceutical Sciences*. 2015 7(11).

2014

- *Mutation spectrum in BBS genes guided by homozygosity mapping in an Indian cohort.* Sathya Priya C, P. Sen, V. **Umashankar**, N. Gupta, M. Kabra, G. Kumaramanickavel, C. Stoetzel, H. Dollfus and S. Sripriya. ***Clin Genet.*** 2014. doi: 10.1111/cge.12342. **PMID:** 24400638
- *In Silico analysis and prioritization of drug targets in Fusarium solani.* Muthukumarar Sivashanmmugam, Hemavathy Nagarajam, **Umashankar Vetrivel**, Gayathri Ramasubban, KL therese, Madhavan HN, **Umashankar Vetrivel**. ***Medical Hypotheses, Elsevier.*** 2014; 84(2). **PMID:** 25555413
- *Computational docking studies reveal the potential inhibitory binding mode of Curcumin and its analogues on Lung Resistance Protein.* Seethalakshmi Sreenivasan, Mohamed al ameen, Subramanian Krishnakumar and **Umashankar Vetrivel**. ***International Journal of Pharmacy and Pharmaceutical Sciences.*** 2014
- *Whole-Genome Sequencing and Mutation Analysis of Two Extensively Drug-Resistant Sputum Isolates of Mycobacterium tuberculosis (VRFCWCF XDRTB 232 and VRFCWCF XDRTB 1028) from Chennai, India.* Kulandai LT, Lakshmipathy D, Ramasubban G, **Vetrivel U**, Rao MH, Rathinam S, Narasimhan M.. ***Genome Announcements, American Society of Microbiology.*** 2014; 2(6). **PMCID:** PMC4241668
- *Whole genome sequence of polyresistant Mycobacterium tuberculosis CWCFVRF PRTB 19 sputum isolate from Chennai, India, closely clustering with East African Indian 5 genogroup.* Lakshmipathy D, **Vetrivel U**, Ramasubban G, Kulandai LT, Madhavan HN, Sridhar R, Meenakshi N. ***Genome Announcements, American Society of Microbiology.*** 2014; 2(4):e00702-14. **PMCID:** PMC4102868

- *Draft Genome Sequence of sputum isolate of Multidrug resistant Mycobacterium tuberculosis CWCFVRF MDRTB 670 strain from Chennai, India with Clinically Suspected Tuberculosis.* Gayathri Ramasubban, Dhanurekha Lakshmiopathy, **Umashankar Vetrivel**, Lily Therese Kulandai, Hajib Narahari Madhavan, R Sridhar, N Meenakshi. **Genome announcements, American Society of Microbiology.** 2014; Vol 2. Issue 3. **PMID:** 24855307
- *Importance of ABC transporters in different tissues.* **Umashankar Vetrivel** and Gurunathan Subramanian. **Drug metabolism and drug interactions** 29.2 2014; 65-66.
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Madavan Vasudevan, **Umashankar Vetrivel**, Vikas Khetan, Subramanian Krishnakumar, *Bioinformatics and Biology Insights*. 2013; Vol 7, 21-34, **PMID**: 23400111.

- *Modulation of MDR1 expression and function in retinoblastoma cells by curcumin*. Seethalakshmi Sreenivasan, Sathyabaarathi Ravichandran, **Umashankar Vetrivel**, Subramanian Krishnakumar, *Journal of Pharmacology and Pharmacotherapeutics*. 2013 doi: 10.4103/0976-500X.110882. **PMCID**: PMC3669568
- *In silico Analysis of Novel Mutation ala102pro Targeting pncA Gene of M. Tuberculosis*. Dhanurekha Lakshmipathy, Gayathri Ramasubban, Lily Therese*, **Umashankar Vetrivel**, Muthukumaran Sivashanmugam, Sunitha Rajendiran, Sridhar R, Madhavan HN, and Meenakshi N. *J Comput Sci Syst Biol*. 2013, 6:2.
- *Draft Genome Sequence of Multidrug-Resistant Pseudomonas aeruginosa Strain VRFPA02, Isolated from a Septicemic Patient in India*. Malathi J, Murugan N, **Umashankar V**, Bagyalakshmi R, Madhavan HN. *Genome Announc. American Society of Microbiology*. 2013; **1(4)**. **PMCID**: PMC3703595
- *Elucidation Of IRON Binding Patterns Through Insilico Approaches In Human Iron Binding Proteins*. Muthukumaran Sivashanmugam, Anusha Kuppuswamy, **Umashankar Vetrivel**, K.N. Sulochana. *International Journal of Therapeutic Applications*, Volume 10, 2013, 11-18.
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- *Novel Mutations in the thymidine kinase gene of ocular herpes simplex virus isolate responsible for acyclovir resistance by in silico analysis.* Samson Moses Y, Malathi J, **Umashankar V**, Sherlin and Madhavan H.N, *International Journal of Computational Bioinformatics and In Silico Modeling*. 2013 2(4): 158-165

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2011

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Contact

Dr. V. Umashankar, M.Sc., M.Phil., PGDBI., Ph.D.,

HOD & Reader,

Center for Bioinformatics

Vision Research Foundation,

Sankara Nethralaya,

18, College Road,

Chennai - 600 006.

Phone: 044-28271616 (Extn 1870)

Fax: 044-28254180

e-mail id: drvus@snmail.org