

## Scientist Profile

Name	Dr.V.Umashankar
Designation	Scientist E
Date of Joining:	12-03-2020
Date of joining present post:	11-10-2021
Discipline	Bioinformatics
Address (off.) including Contact Number*	D3, FF, Eden Apartments, Mel Ayanambakkam, Chennai 600095.
Email address*	<a href="mailto:umashankar.v@icmr.gov.in">umashankar.v@icmr.gov.in</a>

\* **Mandatory**

Educational Qualifications <i>(begin with descending order)</i>			
DEGREE	INSTITUTION AND LOCATION	YEAR(s)	FIELD OF STUDY
Ph.D Zoology (Specialized in Computational Genomics and Drug Target Mining)	University of Madras	2008	Automation of Codon usage genomics and Drug Target Identification
M.Phil Genetics	University of Madras	2000	Genomic instability and Genotoxicity studies
M.Sc Zoology	University of Madras	1999	Zoology
P.G.Diploma in Bioinformatics	University of Mysore	2003	Bioinformatics
S-Star Certification in Bioinformatics	S-Star alliance, National University of Singapore	2004	Bioinformatics

### 1. Research Experience

I graduated my 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; M.Sc Zoology from Pachaiappas college, University of Madras in 1999. I also did my PG Diploma in Bioinformatics from University of Mysore in 2003; S-Star Certification in Bioinformatics awarded by National University of Singapore in 2004. I have got 19 years of experience in Research & mentoring in Bioinformatics. I am was serving earlier as Scientist-E at ICMR-NITM, Belagavi. Prior to that, I was working as HOD & Principal Scientist (10 years), Centre for Bioinformatics (established), Vision Research Foundation, a unit of Sankara Nethralaya. I also formerly worked as HOD, Department of Bioinformatics, School of Biosciences, SRM University and held positions like Academic Head, Research consultant, Senior Research Analyst in leading Research and Academic Organizations. I have been

appointed as member “Board of Studies in Bioinformatics” by University of Madras & SASTRA University. I have so far mentored 14 M.Phil, 3 PhD students and many post graduate students for their project works. My area of expertise includes, Drug design and drug target mining, Microbial genome analysis, peptide therapeutics, structural bioinformatics, design of databases and computational pipelines. I am 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 served as Investigator in many of the funded grants from ICMR, CSIR, DST and DBT. I have extensively worked on projects involving Genome sequencing and assembly of ***Mycobacterium tuberculosis* strains (XDR and MDR) and *Pseudomonas aeruginosa* (Ocular infective)**, Chennai wellington foundation and ICMR funded projects, respectively. These studies have led to significant publications featuring antibiotic resistance patterns and genome organization. As a principal investigator, I have also designed and developed peptide inhibitors targeting Carbonic Anhydrase IX to modulate pH homeostasis in cancer cells (findings published in ACS Omega). In another study, I have co-developed corneal penetrating peptides with antifungal activity (patent filed, data published in International Journal of nanomedicine). Currently, involved in Covid genomics (Published two whole genomes) and drug discovery studies. Also working on Covid metagenomics project funded (Indo-UK GCRF grant). I was also engaged in deciphering transcriptomic changes in the context of Hyperglycemia in Retinal cells by applying NGS technologies (as PI in ICMR funded project). I have published 103 Research papers in peer reviewed international journals (JBSD, BBRC, PLoS One, ACS, JCB etc) and have also written three chapters on Molecular modeling, Cheminformatics and Computational Epigenomics for a book published by John Wiley & Sons. I also serve as reviewer for many of the leading peer reviewed journals like PLOS One, Bioinformatics (OUP), Human Molecular Genetics, GENE, Nature scientific reports and RSC Advances etc. Also serving as associate editor in BMC Bioinformatics. I have delivered many lectures at various National and International conferences as an invited speaker. I also recently presented my research work on Drug target mining in *Chlamydia trachomatis* at ARVO-2018 international conference held at Honolulu, Hawaii, USA. I have authored Bioinformatics tools & Databases namely, KinomeRun, PepVis, PocketPipe, POAP, ACUA, OpenDiscovery, Nitrosoft, Readmol and Indian Plant Anticancer Compound Database (InpacDB), Polycystic Ovary syndrome database, respectively. Many of these tools are used by scientists worldwide and are cited in peer-reviewed journals. 'Theoretical model of human ghrelin precursor' (PDB ID: 1p7x)

predicted by me is printed and cited on the cover-page 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. I hold membership in American Chemical Society, Indian Bioinformatics Society, Society of Toxicology and Bioclues. I have also organized and convened many National Level Conferences and Workshops in Bioinformatics funded by Government bodies.

## 2. Membership/Fellowship of Professional Societies/Associations:

Society of Toxicology  
Indian Bioinformatics Society (InBios)  
International Society for Computational Biology (ISCB)  
American Chemical Society

## 3. Workshops/Conferences/Symposiums:

### **Invited Talks Delivered & Training:**

- “Ocular Bioinformatics” at INAE-NATF Workshop on Technology and Health-Care with emphasis on Affordable Healthcare & Bioinformatics (2015).
- “Insilico tools for Bioinformatics” at National Workshop on Recent Trends in Computer Aided Drug Design on conducted by Sri Venkateswara Engineering of College (2014)
- “Bioinformatics & Molecular Diagnostics, VRR Institute of Biomedical Sciences, Chennai (2014).
- “Bioinformatics & Open-source tools” at National Level Bioinformatics Workshop held at Tamilnadu Veterinary University (2013).
- “Bioinformatics” in a Seminar on Bioinformatics at Sathyabama University (2013).
- “CME programme on Next Generation Sequencing” at MicroLabs, coimbatore on (2013).
- “Bioinformatics and bioactive compounds” at the National Level Conference on Bioactive compounds held at Meenakshi college, Chennai (2013).
- Introduction to Sequence Analysis and Biological Databases” at the CME program on Biomedical Informatics conducted by Aravind Eye Hospital, Madurai (2013).
- “Bioinformatics and Data Analysis Challenges” and also chaired a technical session at the International Conference on “Recent Advances on High Dimensional Data Analysis” conducted by International biometry society and National Institute for Tuberculosis Research (2013)
- “Bioinformatics and Open Source Tools” at Tamilnadu Veterinary University, Chennai. (2013).
- “Opensource tools for Bioinformatics at National conference on mathematical computing at Vellore Institute of technology, Chennai (2012).
- “Genotype to Phenotype SNPs annotation –an *insilico* approach” at IERG (Indian Eye Research Group) (2011), Hyderabad
- “Recent Trends Bioinformatics Research” at Sri Ramachandra Medical University (2011)
- “Open-source Software for Bioinformatics” at National Level Conference on Statistical Methods for Bioinformatics (2011) conducted by National Institute

- “Advances in Bioinformatics”, Valliammal College for Women, Chennai (2010)
- “Protein fold recognition” at National level seminar sponsored by DST, in Stella Mary’s College, Chennai(2003)

**Events Chaired:** Invited as Judge for paper presentation event for National Level Conference, “National Conference on Recent Trends in Environmental Biotechnology” at SRM University, to 18th October 2008”

#### **Conferences Organized:**

- National Level Symposium on Career prospects for lifescience students- METAMORPH – Head & Convener of the event, held at SRM University, Ramapuram Campus, Chennai – 600 089.
- ONE DAY SEMINAR CUM DEMONSTRATION ON MICROARRAY ANALYSIS – Head & Convener of the event, held at SRM University, Ramapuram Campus, Chennai – 600089.
- GENOMICS, PROTEOMICS AND COMPUTATIONAL BIOLOGY- Served as a resource person for conducting National Level Symposium cum workshop funded by DST, CSIR AND TNSCST, on 15th-17th February 2006.
- DNA-DRUG DESIGN – Organized a National Level Symposium funded by CSIR, TNSCST, on 7th and 8th of sep 2004.
- BIOINFORMATICA 2003 - Served as a resource person for conducting National Level Seminar on Bioinformatics jointly conducted by Bioinsilico Research Team and Dept. of Bioinformatics, Stella Marys College, Chennai.
- VIBS 2003 - Served as one of the core Organiser for the Inter-collegiate symposium conducted by Vel’s institute of Biological sciences.

#### **Conferences & Workshops Attended:**

- Certification in cybersecurity, trained by Information Security Education and Awareness (ISEA) Project, Centre for Development of Advanced Computing, Govt. of india
- Indian Eye Research Group Conference conducted by LVPEI & CCMB 30 to 31 July 2011
- Symposium on Approaches to Understanding the Biology of Diseases, July 29, 2011, LVPEI, Hyderabad
- Sankara Nethralya -ARVO, Sep 2010
- BIO-GEOINFORMATICS 2005 – National Level Symposium, School of Genomics, Department of Zoology, Loyola College, Chennai -34. Date: 28<sup>th</sup> February to March 1st 2005.
- State level symposium on hi-tech and instrumentation in medical laboratory technology for diagnosis of human diseases, Loyola College, Chennai -600034.
- Attended the workshop on Next Generation Sequencing Data Analysis conducted by European Molecular Biology Laboratory (EMBL) and National Centre for Biological Sciences on 13-01-2103 at Centre for Cellular and Molecular Platforms(C-CAMP) Bangalore
- Faculty Improvement Programme 2005, Vel’s College of Science, Chennai – 600117.

#### 4. Awards/Achievements:

- **Associate Editor of BMC Bioinformatics**
- **Sep 2007 to till date:** Appointed as Member, **Board of studies in Bioinformatics, University of Madras.**
- **Biography included (28th) Edition of Who's Who in the World**
- **'Vitamins and Hormones'** was first published in 1943, and is the longest-running serial book published by **Elsevier Academic/Press.** **'Theoretical model of human ghrelin precursor'(PDB ID: 1p7x)** predicted by me is printed and cited on the cover page of 77th volume of the above-mentioned prestigious book.
- **OpenDiscovery:** The Bioinformatics Linux Distro developed by my team under my guidance is being used worldwide and it has been cited in **EMBLNet Journal** released by **EMBL**
- **ACUA:** The codon usage analysis software developed by me has been cited in peer-reviewed international Journals from Springer link, SGM journals etc., and as been adopted by many of the academic organizations for teaching codon usage analysis.
- **Jul 2004 to till date:** Serving as external examiner for the following courses: **B.Tech & M.Tech** in Bioinformatics, **B.Tech** in Biomedical Engineering at **Sathyabama University, Chennai.**
- **M.Sc., Bioinformatics** at **Sri Ramachandra Medical University, Chennai**
- **B.Tech** Biotechnology at **Dr.MGR, University, Chennai**
- **Doctoral Committee member for Bioinformatics** in **Sathyabama University, Dr.MGR. University**
- **Reviewer for the many of the Peer-reviewed Journals: (listing a few)**

*Nature Scientific Reports*

*Frontiers in Medicine*

*International Journal of Biological and Chemical Sciences*

*Journal of Human and Experimental Toxicology*

*Indian Journal of Science and Technology*

*Journal of Medicinal Plants Research*

*International Journal of Integrative Biology*

*International journal food & chemical toxicology* (Elsevier)

*International Journal of Human Genetics*

*Journal of Biomolecular structure & dynamics*

*Journal of molecular Liquids*

*International Journal of Biological Macromolecules*

*Human Molecular Genetics*

*PLOS ONE*

*BMC Bioinformatics*

*Computers in Biology & Medicine* (Springer)

*Bioinformatics* (OUP)

*GENE*

*RSC ADVANCES*

**Certifications:** **Good Governance and Transparency through RTI Act 2005,**  
National Productivity Council (NPC) India (2021)  
Credential ID N307I14P596150W866

**Data Science in Stratified Healthcare and Precision Medicine,**

The University of Edinburgh, Jul 2020  
Credential ID XQHYYEV8DGLD

**Metagenomics applied to surveillance of pathogens and Antimicrobial Resistance**, DTU - Technical University of Denmark, Credential ID 34QRFGWFMBTP

**Foundation course on Cyber Security**, CDAC, Feb 2021

**Projects (handled):**

**Ongoing Funded grants :**

**As Principal investigator (PI):**

1. Local evaluation of RT-PCR vs NGS for early detection, surveillance and prevention of communicable viral diseases in Central India: a wastewater-based epidemiological study (Co-I) (**Indo-UK Extramural grant funded by GCRF jointly with University of Nottingham**)
2. Whole genome sequencing of SARS-CoV2 patient isolates from Belagavi district to infer the mutational spectrum (PI) (**Intramural ICMR-NITM**)
3. Developing herbal solutions for COVID-19, based on TM leads (Co-PI) (Intramural ICMR-NITM)

**As Co- Principal Investigator (Co-PI):**

1. Functional Characterization of Lacrimal Proline rich 4 protein (LPRR4) (EMR/2016/000929) - **SERB-DST**
2. Unravelling the genetic architecture of Diabetic Retinopathy in South Indian population (No.BT/PR22701/MED/15/166/2016) - **DBT (INDO-US)**
3. Self-assembling peptide nanofiber matrix as implants for fungal keratitis drug delivery system (BT/PR14690/MED/32/496/2015) -**DBT**
4. Intervention of ciliopathy genes in the molecular pathology of BBS in Indian population (File No. 54/17/2012-HUM-BMS) -**ICMR**
5. Whole Exome sequencing in Leber Congenital amaurosis (LCA) to identify novel gene(s) (BT/PR10766/MED/12/643/2014 dated 22-12-2015) - **DBT**
6. Development of therapeutic molecules for diabetic retinopathy from studies on structure/function relationship of PON2 by cloning. (CSIR/27(0310)14/EMR-II) -**CSIR**

**Completed Funded Grants:**

**As Principal investigator (PI):**

1. *Insilico* Design and Development of novel peptide inhibitors targeting CD147 through virtual screening and biopanning of peptide libraries and in vitro validation of anticancer efficacies (No.BT/PR21490/MED/30/1773/2016) - **DBT**
2. Insilco drug target identification in Chlamydia species through systems biology and molecular modelling approaches pertaining to the development of potential drug molecules (YSS/2014/000282/DT20.10.15)- **DST-SERB**

3. 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. (No. BIC/12(7)/2012) – **ICMR**
4. 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. (BT/PR6476/GBD/27/496/2013)- **DBT-RGYI**
5. Rational Design of novel peptide inhibitors targeting DNA-Topoisomerase-II-Beta through virtual screening of combinatorial peptide libraries and in vitro validation of anticancer efficacies (ISRM/12(25)2019) – **ICMR** (Transferred to Co-PI)
6. 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 (5/4/08/OPH/2015/NCD-II) – **ICMR** (Transferred to Co-PI)

#### **As Co- Principal Investigator (Co-PI):**

1. To elucidate the role of Cystathionine beta synthase enzyme and hydrogen sulphide in retinal cells exposed to thiol compounds (BT/PR8244/BRB/10/1219/2013)- **DBT**
2. Peripheral Blood Gene Expression Profiling In Eales Disease. (5/4/6/2/OPH/12-NCD-II – ICMR) - **ICMR**
3. Regulation of Lysyl Oxidase expression in Lens Epithelial Cells and trabecular endothelium. (52/15/2011-BMS) - **ICMR**
4. Application of Next Generation Sequencing technique to determine the whole genome sequence of laboratory isolates of *Enterococcus faecalis*, *P.aeruginosa*, *B.cervus* (both sensitive and resistant strains) And application of bioinformatics approaches to identify the vulnerable area of drug targets in genome. (AMR/10/2011- ECD-I) - **ICMR**
5. Biomarker pattern discovery of graded changes in the opacity of human lens in age-onset cataract: a proteomic approach. (54/16/CFP/GER/2011-NCD-II) - **ICMR**
6. 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. (53/10//2011-BMS) - **ICMR**
7. 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. (BT/01/CEIB/11/V/16; Dt: 08-05-2012)- **DBT**
8. Development of therapeutic peptide from proteoglycan LRR-angiogenesis (DST-SR/50/JS/0099) - **DBT**
9. Identification of novel interacting partners for PEDF in angiogenesis and obesity. (DST-SR/50/JS/0099) – **DST**
10. Development of modulators Ornithine decarboxylase (ODC) for the therapeutic application in retinoblastoma. (No.02(0105)/12/EMR-II) - **CSIR**

## Other research projects involved

**2010- March 2020**  
**Vision Research Foundation,**  
**Sankara Nethralaya**  
**Chennai**

Presently engaged in Ocular Bioinformatics studies which involves Microarray Analysis, SNP analysis, NGS data analysis, RNA-Seq, Molecular modelling, Drug Design, Dynamics, etc. Also working on siRNA design and Peptide inhibitor design for Angiogenesis studies:

1. Whole Genome Assembly and Analysis of Bacterial Genomes (ICMR –grant)
2. Leurich Rich Repeats based Peptide inhibitor design for TGF-Beta targeting angiogenesis
3. SiRNA design for CTR1 targeting angiogenesis
4. In silico studies on Adiponection and angiogenesis

**2008-2009**  
**School of Biosciences,**  
**Department of Bioinformatics,**  
**SRM University,**  
**Ramapuram Campus**

**Indian Plant Anticancer Compound Database:** This project is an initiative to collate the Comprehensive details of Anticancer compounds arising from Indian Plant origin. [www.inpacdb.org](http://www.inpacdb.org), (published in Bioinformation)

**OpenDiscovery:** This project was conceptualized and guided by me towards creation of high-performance Live Linux for Molecular Modelling applications accessible via Flash Drive. This Live distribution can be downloaded from [www.opendiscovery.org.in](http://www.opendiscovery.org.in) (published in Bioinformation)

**Axon ROCKS Super Computing Unit:** Established High Performance Biocomputing Unit with 44 GigaFlops capacity, capable of running MPI Programs

**2004-2007**  
**School of Genomics,**  
**Dept. of Zoology,**  
**Loyola College Chennai**

**ACUA:** developed a robust automated pipeline tool for Codon usage genomics as part of Doctoral work

**2001-2002**  
**Gemeiosys Research**  
**Labs-Chennai**

**Toxin Database:** This project was done for a Client at Gemeiosys Research Labs. I was involved in the design, 3D modelling, identification of novel ligands and Functional annotation of different toxin protein sequences.

**Bioweave:** This project involved the development of comprehensive sequence Annotation tool. I was involved in schema designing, paramatrical analysis and software testing

Presented research work on Chlamydia trachomatis drug target prediction by multiomics methods at ARVO 2018 held at Honolulu, Hawaii, USA, (Apr 29 to May 3rd 2018)



5. Publications (Mention your Orchid/PubMed/Google Scholar profile link here, if available)

#### Invited Chapters in Books:

1. Insilico Tools of Molecular Modeling, in *Handbook of Systems Toxicology*, V.Umashankar and S.Gurunathan,(2011) edited by Daniel A. Casciano and Saura C.Sahu. Chichester, UK: John Wiley & Sons, Ltd, pp 579-590
2. Cheminformatics and its Applications, in *Handbook of Systems Toxicology*, V.Umashankar and S.Gurunathan, (2011) edited by Daniel A. Casciano and Saura C.Sahu. Chichester, UK: John Wiley & Sons, Ltd, pp 347-360
3. Tools and data bases for computational epigenomics, *Toxicology and Epigenetics*, John Wiley & Sons, Ltd.

#### Research Articles Published (selected):

##### [Google scholar link](#)

1. Deciphering the structural and functional impact of missense mutations in Egr1-DNA interacting interface: an integrative computational approach.Nagarajan, H., & Vetrivel, U. (2021). **Journal of Biomolecular Structure & Dynamics**, 1–13.
2. Retinoschisis and Norrie disease: a missing link,Rahini Rajendran, Dhandayuthapani Sudha, Subbulakshmi Chidambaram, Hemavathy Nagarajan, Umashankar Vetrivel, Jayamuruga Pandian Arunachalam,**BMC Research Notes**,(2021) 14:204
3. Umashankar Vetrivel, Deshpande S, Hegde HV, Singh I, Chattopadhyay D. 2021. Phytochemical moieties from Indian traditional medicine for targeting dual hotspots on SARS-CoV-2 spike protein: an integrative in-silico approach. **Frontiers in Medicine** 8:545.
4. Singh I & Umashankar vetrivel, Harish, Chattopadhyay D. 2021. Coding-Complete Genome Sequences of NITMA1086 and NITMA1139, Two SARS-CoV-2 Isolates from Belagavi District, Karnataka State, India, Harboring the D614G Mutation. **Microbiology Resource Announcements** 10.
5. samdani ansar, Umashankar Vetrivel. 2021. Structure-based design of small molecule and peptide inhibitors for selective targeting of ROCK1: an integrative computational approach. **Journal of Biomolecular Structure and Dynamics**:1–19.
6. Nagarajan H, Vetrivel U. 2021. Membrane dynamics simulation and virtual screening reveals potential dual natural inhibitors of endothelin receptors for targeting glaucomatous condition. **Life Sciences**:119082.
7. Nagarajan H, Vetrivel U. 2020. Microsecond scale sampling of Egr-1 conformational landscape to decipher the impact of its disorder regions on structure–function relationship. **Molecular Simulation**:1–10.

8. Nagarajan H, Lakshmi PD, Vetrivel U. 2020. Deciphering potential inhibitors targeting THI4 of *Fusarium solani* sp. To combat fungal keratitis: An integrative computational approach. **Computational Biology and Chemistry**:107350.
9. Muthukumaran S, Sulochana KN, Umashankar V. 2020. Structure based design of inhibitory peptides targeting ornithine decarboxylase dimeric interface and in vitro validation in human retinoblastoma Y79 cells. **Journal of Biomolecular Structure and Dynamics**:1–15.
10. Jonnalagadda B, Arockiasamy S, Vetrivel U, PA A. 2020. In silico docking of phytocompounds to identify potent inhibitors of signaling pathways involved in prostate cancer. **Journal of Biomolecular Structure and Dynamics**:1–27.
11. Chatterjee A, Nagarajan H, Padmanabhan P, Vetrivel U, Therese KL, Janakiraman N. 2020. Understanding the Uptake Mechanism and Interaction Potential of the Designed Peptide and Preparation of Composite Fiber Matrix for Fungal Keratitis. **ACS Omega**.
12. PocketPipe: A computational pipeline for integrated Pocketome prediction and comparison”, Samdani Ansar, Anupriya Sadhasivam & **Umashankar Vetrivel**. **Bioinformatics** 15(4): 295-298 (2019)
13. Structure-based drug target prioritization and rational drug design for targeting *Chlamydia trachomatis* eye infections, Sadhasivam A, Nagarajan H, **Umashankar V**. **Journal of Biomolecular structure & dynamics** (2019) Aug 5:1-18. doi:10.1080/07391102.2019.1652691. PubMed PMID: 31380730.
14. Deciphering ophthalmic adaptive inhibitors targeting RON4 of *Toxoplasma gondii*: An integrative in silico approach, **Vetrivel U**, Nagarajan H. **Life Sciences**. 2018. 213:82-93. DOI: 10.1016/j.lfs.2018.10.022. PubMed PMID: 30326220
15. Demystifying the pH dependent conformational changes of human heparanase pertaining to structure-function relationships: an in-silico approach, Nagarajan H, **Vetrivel U**. **Journal of Computer Aided Molecular Design**, 32 (2018) 821–840. 2018. DOI: 10.1007/s10822-018-0131-0. PubMed PMID: 29980923.
16. POAP: A GNU Parallel based multithreaded pipeline of Open Babel and AutoDock suite for boosted High Throughput Virtual Screening, Samdani, A., and **Umashankar Vetrivel**. **Computational Biology and Chemistry** (2018).74:39-48. DOI: 10.1016/j.compbiolchem.2018.02.012. PubMed PMID: 29533817.
17. Genome-wide codon usage profiling of ocular infective *Chlamydia trachomatis* serovars and drug target identification, Anupriya Sadhasivam & **Umashankar Vetrivel**, **Journal of Biomolecular Structure and Dynamics**, Taylor & Francis, 2017, 0739-1102.
18. Inhibition of IKK $\beta$  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.
19. 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.
20. *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

21. Virtual Screening, Molecular dynamics and binding free energy calculations on Human Carbonic Anhydrase IX catalytic domain for deciphering potential leads. Arun John, Muthukumaran Sivashanmugam, **Vetrivel Umashankar**, Sulochana Konerirajapuram Natarajan. **Journal of Biomolecular Structure & Dynamics**. 2016; DOI:10.1080/07391102.2016.1207565. PMID: 27373313
22. 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.
23. 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.
24. 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.
25. Resistome and pathogenomics of multidrug resistant (MDR) *Pseudomonas aeruginosa* VRFPA03, VRFPA05 recovered from alkaline chemical keratitis and post-operative endophthalmitis patient. Murugan N, Malathi J, **Umashankar V**, Madhavan H. **Gene**. 2016; 578(1):105-111. PMID: 26692145.
26. Bio-conjugation of antioxidant peptide on surface-modified gold nanoparticles: a novel approach to enhance the radical scavenging property in cancer cell. Kalmudia S, Vandhana S, Tejaswini Rama B, Jayashree B, Sreenivasan Seethalakshmi T, **Umashankar V** et al., **Cancer Nanotechnology**. 2016; 7(1). PMID: 26900409.
27. Probing the biophysical interaction between Neocarzinostatin toxin and EpCAM RNA aptamer. Athyala PK, Kanwar JR, Alameen M, Kanwar RK, Krishnakumar S, Watson J, Vetrivel U, Narayanan J. **Biochem Biophys Res Commun**. 2016; 469(2):257-62. PMID: 26642954.
28. Homozygosity mapping in Leber congenital amaurosis and autosomal recessive retinitis pigmentosa in South Indian families. Sundaramurthy Srilekha, Tharigopala Arokiasamy, Natarajan N. Srikrupa, **Vetrivel Umashankar**, Swaminathan Meenakshi, Parveen Sen, Suman Kapur, Nagasamy Soumitra. **PLOS ONE**. 2015. PMID: 26147992.
29. Draft genome sequence of blaVeb-1, bla<sub>oxa</sub>-10 producing multi-drug resistant (MDR) *Pseudomonas aeruginosa* strain VRFPA09 recovered from bloodstream infection. Nandagopal Murugan, Jambulingam Malathi, **Vetrivel Umashankar**, Hajib Narahari Rao Madhavan. **Brazilian Journal of Microbiology**. 2015; vol.46, n.3, pp. 639-640. PMID: 26413042.
30. Comparative Modeling and Molecular Dynamics Simulation of Substrate Binding in Human Fatty Acid Synthase: Enoyl Reductase and  $\beta$ -Ketoacyl Reductase Catalytic Domains. Arun John, **Vetrivel Umashankar**, Subramanian Krishnakumar, and Perinkulam Ravi Deepa. **Genomics & Informatics**. 2015; 13(1): 15-24. PMID: 25873848.
31. Insights on Drug Targeting of *Toxoplasma gondii* Host Invasion Proteins: A Review. Indhuja Thirumudi, **Umashankar Vetrivel**, Mahalakshmi B, Lily Therese K, Madhavan HN. **Asian Journal of Pharmaceutical and Clinical Research**. 2015; 8:3.

32. Drug Discovery: an appraisal. **Umashankar, V.**, and S. Gurunathan. **International Journal of Pharmacy and Pharmaceutical Sciences**. 2015; 7.4..
33. Virtual screening studies of seaweed metabolites for predicting potential ppar $\gamma$  agonists. Gurula, H., Loganathan, T., Krishnamoorthy, T., **Vetrivel, U.**, & Samuel, S. **International Journal of Pharmacy and Pharmaceutical Sciences**. 2015 7(11).
34. 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.
35. *In Silico* analysis and prioritization of drug targets in *Fusarium solani*. Muthukumaran Sivashanmmugam, Hemavathy Nagarajan, **Umashankar Vetrivel**, Gayathri Ramasubban, KL therese, Madhavan HN. **Medical Hypotheses, Elsevier**. 2014; 84(2). **PMID**: 25555413.
36. 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
37. 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, Lakshmi pathy D, Ramasubban G, **Vetrivel U**, Rao MH, Rathinam S, Narasimhan M.. **Genome Announcements, American Society of Microbiology**. 2014; 2(6). **PMCID**: PMC4241668.
38. Whole genome sequence of polyresistant *Mycobacterium tuberculosis* CWCFVRF PRTB 19 sputum isolate from Chennai, India, closely clustering with East African Indian 5 genogroup. Lakshmi pathy 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.
39. 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 Lakshmi pathy, **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.
40. Importance of ABC transporters in different tissues. **Umashankar Vetrivel** and Gurunathan Subramanian. **Drug metabolism and drug interactions** 29.2 2014; 65-66.
41. Comparative genomic analysis of multidrug-resistant *Pseudomonas aeruginosa* clinical isolates VRFPA06 and VRFPA08 with VRFPA07. Murugan, Nandagopal, Jambulingam Malathi, **Vetrivel Umashankar**, and Hajib Narahari Rao Madhavan. **Genome announcements, American Society of Microbiology**. 2014; no. 2 (2014): e00140-14. **PMCID**: PMC3945505.
42. Whole-Genome Sequencing of Streptomycin-Resistant *Mycobacterium tuberculosis* Isolate VRFCWCF MRTB 180 Reveals Novel and Potential Mutations for Resistance. Gayathri Ramasubban, Dhanurekha Lakshmi pathy, **Umashankar Vetrivel**, Lily Therese Kulandai, Hajib Narahari Madhavan, R. Sridhar, N. Meenakshi. **Genome announcements, American Society of Microbiology**. 2014 2(5): pii: e00919-14. **PMID**: 25212629.

43. A molecular model of human Lysyl Oxidase (LOX) with optimal copper orientation in the catalytic cavity for induced fit docking studies with potential modulators. Bhuvanasundar R, John A, Sulochana KN, Coral K, Deepa PR4, **Umashankar V. Bioinformatics.** 2014 10(7):406-412. **PMID:** 25187679.
44. Identification and In silico Analysis of Retinoblastoma Serum microRNA Profile and Gene Targets Towards Prediction of Novel Serum Biomarkers. Madhu Beta, Nalini Venkatesan, Madavan Vasudevan, **Umashankar Vetrivel**, Vikas Khetan, Subramanian Krishnakumar, **Bioinformatics and Biology Insights.** 2013; Vol 7, 21-34, **PMID:** 23400111.
45. 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.
46. *In silico* Analysis of Novel Mutation ala102pro Targeting pncA Gene of M. Tuberculosis. Dhanurekha Lakshmiopathy, 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.
47. Draft Genome Sequence of Multidrug-Resistant Pseudomonas aeruginosa Strain VRFP02, 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.
48. Elucidation Of IRON Binding Patterns Through Insilico Approaches In Human Iron Binding Proteins. Muthukumaran Sivashanmugam, Anusha Kuppaswamy, **Umashankar Vetrivel**, K.N. Sulochana. **International Journal of Therapeutic Applications**, Volume 10, 2013, 11-18.
49. Structural studies on AIPL1 and its functional interactions with NUB1 to identify key interacting residues in LCA4. S. Muthukumaran, V. **Umashankar**, Meena Revathi Valliappan. **Journal of Ocular Biology, Diseases, and Informatics.** 2013 April. Springer. **PMID:** 24596939.
50. Virtual screening studies reveal linarin as a potential natural inhibitor targeting cdk-4 in retinoblastoma. S. Muthukumaran & R. Chandana, V. **Umashankar.** **Journal of Pharmacology and Pharmacotherapeutics.** 2013. **PMID:** 24250202.
51. 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.
52. ICAM-1 K469E polymorphism is a genetic determinant for the clinical risk factors of T2D subjects with retinopathy in Indians: a population-based case-control study. Kumari Vinita1, Sarangapani Sriprya1, Krishnamurthy Prathiba, Kulothungan Vaitheeswaran, Ravichandran Sathyabaarathi, Mahendran Rajesh, John Amali, Vetrivel **Umashankar**, Govindasamy Kumaramanickavel, Swakshyar Saumya Pal, Rajiv Raman, Tarun Sharma, **British Medical Journal Open.** 2012; 2:e001036. **PMID:** 22904330.
53. Agonistic effect of polyunsaturated fatty acids (PUFAs) and its metabolites on brain-derived neurotrophic factor (BDNF) through molecular docking simulation. **Umashankar Vetrivel** et al., **BMC Lipids in Health and Disease.** 2012 11:109. **PMCID:** PMC3477081.
54. *In vitro* and *In silico* studies on inhibitory effects of curcumin on multi drug resistance associated protein (MRP1) in retinoblastoma cells. Seethalakshmi Sreenivasan, Sathyabaarathi Ravichandran, **Umashankar Vetrivel**, and Subramanian Krishnakumar, **Bioinformatics.** 2012; 8(1): 13-19. 2012. **PMID:** 22359429.

55. Phylogenetic comparison of exonic US4, US7 and UL44 regions of clinical herpes simplex virus type 1 isolates showed lack of association between their anatomic sites of infection and genotypic/sub genotypic classification. Harishankar A, Jambulingam M, Gowrishankar R, Venkatachalam A, **Vetrivel Umashankar**, Ravichandran S, Yesupadam SM and Madhavan HN, **Virology Journal, BMC**. 2012; 9:65. **PMID**: 22416856.
56. Studies on New Delhi Metallo-Beta-Lactamase-1 producing *Acinetobacter baumannii* isolated from donor swab in a tertiary eye care centre, India and structural analysis of its antibiotic binding interactions. Murali Sowmiya, **Vetrivel Umashankar**, Sivashanmugan Muthukumaran, Hajib Narahari rao Madhavan, and Jambulingam Malathi, **Bioinformatics**. 2012; 8(10): 445–452. **PMID**: 22715297.
57. Elucidation Of Structure - Function Relationship In Families Of Copper Binding Proteins In Homo Sapiens – A Bioinformatics Approach. Mathangi Jayaraman & Sudarshana N, Vidya Natarajan, **Umashankar Vetrivel**, Sulochana. K.N. **International Journal of Pharma and Bio Sciences**. 2012 3(3): (B) 647 – 662.
58. A novel in silico approach to identify potential therapeutic targets in human bacterial pathogens. **Umashankar Vetrivel** Gurunathan Subramanian Sudarsanam Dorairaj. **HUGO Journal (Official Journal of Human Genome Organization)**. 2011; DOI 10.1007/s11568-011-9152-7. Springer. **PMID**: PMC3238024.
59. *In silico* Identification of Novel Inhibitors for Emphysema through Structure Based Drug Design Approaches. Raghavan rajashekar, Charanya muralidharan, Sathyabaarathi ravichandran, **Umashankar vetrivel**. **Journal of Biology and Life Sciences**. 2011; Vol 2, No 1.
60. Detection of novel coupled mutations in the katG gene (His276Met, Gln295His and Ser315Thr) in a multidrug-resistant *Mycobacterium tuberculosis* strain from Chennai, India, and insight into the molecular mechanism of isoniazid resistance using structural bioinformatics approaches. Gayathri Ramasubbana, Kulandai Lily Theresea, **Umashankar Vetrivel**, Muthukumaran Sivashanmugamb, Parvathy Rajanc, R. Sridhard, Hajib N. Madhavana, N. Meenakshie. **International Journal of Antimicrobial Agents. Elsevier**. 2011 **PMID**: 21330112
61. Functional characterization of novel mutations in UL54 of ganciclovir resistant HCMV strain using structural analysis. Jambulingam Malathi, **Vetrivel Umashankar**, Ravichandran Sathyabaarathi, Sivashanmugan Muthukumaran, Murali Ishwarya, Hajib Narahari Madhavan. **Bioinformatics**. 2011. **PMID**: 21383907.
62. Molecular screening of the CYP4V2 gene in Bietti crystalline dystrophy that is associated with choroidal neovascularization. Gandra Mamatha, Vetrivel **Umashankar**, Nachiappan Kasinathan, Tandava Krishnan, Ravichandran Sathyabaarathi, Thirumalai Karthiyayini,<sup>1</sup> John Amali,<sup>1</sup> Chetan Rao,<sup>3</sup> Jagadeesan Madhavan<sup>1</sup>. **Molecular Vision**. 2011; 17:1970-1977. **PMID**: 21850171.
63. Chemical inhibition of Fatty Acid Synthase: molecular docking analysis and biochemical validation in ocular cancer cells. P. R. Deepa, S. Vandhana, S. Muthukumaran, **V. Umashankar**, U. Jayanthi, S. Krishnakumar, **J Ocul Biol Dis Infor**. Springer, 2011. **PMID**: 23181152.
64. Comparative modeling of PON2 and analysis of its substrate binding interactions using computational methods. Subramanian Barathi & Muralidaran Charanya & Shivashanmugam Muthukumaran & Narayanasamy Angayarkanni & **Vetrivel Umashankar**. **J Ocul Biol Dis Infor**, springer. 2011; DOI 10.1007/s12177-011-9057-7. **PMID**: 22319641.

65. Ab initio model of HIV's Vif and simulation studies of APOBEC3G-Vif complex. **Umashankar Vetrivel. International Journal of Integrative Biology (IJIB)**. 2010, Vol. 10, No. 1, 29.
66. Indian Plant Anticancer Compound Database (InPACdb), **V.Umashankar**, Nanditha Subramaniam, Kalabharath, **Bioinformatics**, 4(2), 71-74 (2009).
67. Open discovery: An integrated live Linux Bioinformatics Platform, **Umashankar & Kalabharath Pilla**, **Bioinformatics**, 3(4), 144-146 (2008).
68. ACUA: A software tool for automated codon usage analysis, **Umashankar et al.**, **Bioinformatics**, 2(2): 62-63 (2007).

#### Reviews:

- Structural insights on druggable hotspots in CD147: A bull's eye view, Kumar D, Vetrivel U, Parameswaran S, Subramanian KK.. *Life Sciences*. 2019 May 1;224:76-87. doi: 10.1016/j.lfs.2019.03.044. Epub 2019 Mar 20. Review. PubMed PMID: 30904494.
- Ornithine and its role in metabolic diseases: An appraisal. Muthukumaran Sivashanmugam, Jaidev J, **Umashankar V.**, Sulochana K.N. Article in **Biomedicine & Pharmacotherapy** 86:185–194 · February 2017 DOI: 10.1016/j.biopha.2016.12.024
- Insights On Drug Targeting Of Toxoplasma gondii Host Invasion Proteins: A Review. Indhuja Thirumudi, **Umashankar Vetrivel**, Mahalakshmi B, Lily Therese K, Madhavan HN. **Asian Journal Of Pharmaceutical And Clinical Research** 2015; **8:3**
- DRUG DISCOVERY: AN APPRAISAL. Umashankar, V., and S. Gurunathan. *International Journal of Pharmacy and Pharmaceutical Sciences* 7.4 (2015).
- Microbial Informatics – Unraveling the Mysteries of Pathogens, K.Santhiya, T.Manoj, C.P.Anitha Devi, V Umashankar, Y Rajalakshmi, **Advanced Biotech. Vol.9. Issue 8,(2010)**
- Toxicoinformatics –Review- An Informatics talk on Toxicology, V.Umashankar et al., **Toxicology international**, Society of Toxicology, **Vol. 13 (2), 2006.**
- Pharmacogenomics: an appraisal, **Bioinformatics India journal. Vol 2. 27 – 32, (2003)**

#### Theoretical Protein Models:

- 3D model of Cyclophilin of *S.pombe* (Accession No: 1WVS)
- 3D model of Acyl Carrier Protein of *Pseudomonas aeruginosa* (Acc.No: 1OP7).
- 3D model of Ghrelin precursor of *Homo sapiens* (Acc. No:1P7X).
- 3D model of phosphomethyl pyrimidine kinase from *Leptospira* (Acc.No: 2G53).
- DBI 01 trehalose-6-phosphate synthase (tps) gene