ALAGAPPA UNIVERSITY

(A State University Established in 1985)

Karaikudi - 630003. Tamil Nadu, India

2017 Accredited with A+ Grade by NAAC (CGPA: 3.64)

2018 MHRD Govt. of India Graded as Category - I & Granted Autonomy

2018 Swachh Campus Rank : 4

2021 nirf Rank : 33

2021 QS UNIVERSITY RANKINGS Asia Rank : 199

FACULTY OF SCIENCE

DEPARTMENT OF BIOINFORMATICS

M.Phil., BIOINFORMATICS

REGULATIONS AND SYLLABUS

(For the candidates admitted from the Academic Year 202 - 2023)

DEPARTMENT OF BIOINFORMATICS

M.PHIL. BIOINFORMATICS

REGULATIONS AND SYLLABUS

[For the candidates admitted from the Academic Year 2022 – 2023 onwards]

ALAGAPPA UNIVERSITY

(A State University Accredited with "A+" grade by NAAC (CGPA: 3.64) in the Third Cycle andGraded as Category-I University by MHRD-UGC)

Karaikudi - 630003, Tamil Nadu

The panel of Members-Broad Based Board of Studies

Name: Dr. J. Jeyakanthan
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Educational Qualification

- ✓ Ph.D (Crystallography and Biophysics) from CAS in Crystallography & Biophysics, University of Madras, Tamil Nadu, India (2000).
  Title: X-ray crystallographic studies on some organic compounds of medical and biological importance.
  Mentor: Prof. D. Velumurugan, Professor Emeritus, Former UGC-BSR faculty and Head, CAS in Crystallography & Biophysics, University of Madras, Tamil Nadu, India
- ✓ M.Phil (Physics) from M.K. University, Madurai (1995)
- ✓ M.Sc (Physics) from M.K. University, Madurai (1993)
- ✓ B.Ed (Physics) from University of Madras (1991)
- ✓ P.G. Diploma (Computer Application) from MIT, Anna University(1999)

Professional Experience

- ✓ Professor and Head in Department of Bioinformatics, Alagappa University, Karaikudi (Mar 2010-till date)
- ✓ Research Scientist, Spring-8, Japan (May2007-Mar2010)
- ✓ Researcher, RIKEN Harima Institute, Spring-8, Japan (Jun 2003-May2007)
- ✓ PDF, Indian Institute of Science, Bangalore (Jan 2000-May 2003)

Honours and Awards

- ✓ **Tamil Nadu Scientist Award (TANSA-2018)**Tamil Nadu State Council for Science and Technology in 2020
- ✓ **LEAP 2019** from the MHRD, Govt of India for training Senior Professors to next level academicians.
- ✓ **Research Award 2016** from the University Grants Commission, New Delhi, India (plus two year's salary)
- ✓ **Elected** Fellow for **The Academy of Sciences, Chennai**, India (**FASCh)** in 2015.
- ✓ **UGC-SAP Nominee** from the University Grants Commission, New Delhi to monitor and assess the effective implementation of SAP programme in Punjab University, Punjab (2015).
- ✓ **Vice-President –** Bioinformatics and Drug Discovery Society **(BIDDS), from** 2017 for three years.
- ✓ **Cited in "Marquis"-** Who's Who Scientific Directory (2007)
- ✓ **IRPHA, DST & DBT - Post Doctoral Fellowship** (2000-2003)
- ✓ **Young Scientist travel Grants** from **DST & UNESCO** (1999) and **IUCr Young Scientist Fellow** (1999)
- ✓ **CSIR - Senior Research Fellowship** (1997-2000)

Recent Publications

- ✓ Alexpandi, R., Gendrot, M., Abirami, G., Delandre, O., Fonta, I., Mosnier, J., & Veera Ravi, A. Repurposing of doxycycline to hinder the viral replication of SARS-CoV-2: From in silico to in vitro validation. *Frontiers in Microbiology* (2022). **(I.F. - 5.64)**
- ✓ Mohanrasu, K., Guru Raj Rao, R., Dinesh, G. H., Zhang, K., Sudhakar, M., Pugazhendhi, A., **Jeyakanthan, J.,** Ponnuchamy, K., Govarthanan, M., & Arun, A. Production and characterization of biodegradable polyhydroxybutyrate by Micrococcus luteus isolated from marine environment. *Int J Biol Macromol,* (2021),*186*, 125–134. **(I.F. -6.953)**
- ✓ Kanumuri, R., Chelluboyina, A. K., Biswal, J., Vignesh, R., Pandian, J., Venu, A., Vaishnavi, B., Leena, D. J., **Jeyaraman, J.,** Ganesan, K., Aradhyam, G. K., Venkatraman, G., & Rayala, S. K. Small peptide inhibitor from the sequence of RUNX3 disrupts PAK1-RUNX3 interaction and abrogates its phosphorylation-dependent oncogenic function. *Oncogene*. (2021), 40(34):5327-5341. **(I.F. -9.867)**
- ✓ Sankar, M., Ramachandran, B., Pandi, B., Mutharasappan, N., Ramasamy, V., Prabu, P. G., Shanmugaraj, G., Wang, Y., Muniyandai, B., Rathinasamy, S., Chandrasekaran, B., Bayan, M. F., **Jeyaraman, J.,** Halliah, G. P., & Ebenezer, S. K. *In silico* Screening of Natural Phytocompounds Towards Identification of Potential Lead Compounds to Treat COVID-19. *Front Mol Biosci*. (2021), *8*, 637122. **(I.F. -5.246)**
- ✓ Premnath, N., Mohanrasu, K., Guru Raj Rao, R., Dinesh, G. H., Siva Prakash, G., Pugazhendhi, A., **Jeyakanthan, J.,** Govarthanan, M., Kumar, P., & Arun, A. Effect of C/N substrates for enhanced extracellular polymeric substances (EPS) production and Poly Cyclic Aromatic Hydrocarbons (PAHs) degradation. *Environ Pollut*. (2021). *275*, 116035. **(I.F. - 5.246)**
- ✓ Murugan, N. A., Kumar, S., **Jeyakanthan, J.,** & Srivastava, V. Searching for target-specific and multi-targeting organics for Covid-19 in the Drugbank database with a double scoring approach. *Sci Rep*, (2020), *10*(1), 19125. **(I.F. -5.133)**
- ✓ Murugan, N. A., Muvva, C., Jeyarajpandian, C., **Jeyakanthan, J.,** & Subramanian, V. Performance of Force-Field- and Machine Learning-Based Scoring Functions in Ranking MAO-B Protein-Inhibitor Complexes in Relevance to Developing Parkinson's Therapeutics. *Int J Mol Sci*, (2020), *21*(20), 7648. **(I.F. -5.923)**
- ✓ Chaudhary, S. K., Elayappan, M., **Jeyakanthan, J.,** & Kanagaraj, S. Structural and functional characterization of oligomeric states of proteins in RecFOR pathway. *Int J Biol,* (2020), *Macromol.163*, 943-953. **(I.F. -6.953)**
- ✓ Boomi, P., Ganesan, R., Prabu Poorani, G., Jegatheeswaran, S., Balakumar, C., Gurumallesh Prabu, H., Anand, K., Marimuthu Prabhu, N., **Jeyakanthan, J.,** & Saravanan, M. Phyto-Engineered Gold Nanoparticles (AuNPs) with Potential Antibacterial, Antioxidant, and Wound Healing Activities Under in vitro and in vivo Conditions. *Int J Nanomedicine*, (2020), *15*, 7553–7568. **(I.F. -6.40)**

Cumulative Impact Factor: 650.77, Citations: 2361, h-index: 25, i10 index-68

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Educational Qualification

- ✓ Ph. D in Applied Chemistry from CSJM University, Kanpur from the period 2000 – 2004.
  Title : Quantum pharmacological studies on HIV-1 RT inhibitors
  Mentor : Dr. Arpita Yadav, Associate Professor, CSJM UNiveristy, Kanpur.
- ✓ M.Sc (Life Sciences) from the institute of Life Sciences, CSJM University, Kanpur during the period 1998 – 2000.
- ✓ B.Sc (Zoology, Botany, Chemistry) from Chirst Church College, CSJM University, Kanpur, Uttar Pradesh (1998).

Professional Experience

- ✓ Professor (20.03.2015 – till date)
- ✓ Associate Professor (20.03.2012 – 19.03.2015) ~3 years
- ✓ Reader (20.03.2009 – 19.03.2012) ~3 years
  Dept of Bioinformatics, Alagappa University, Karaikudi -630003, Tamilnadu, India
- ✓ Lecturer in CoE in Bioinformatics, School of Biotechnology, Madurai Kamaraj University (March, 2006 – March, 2009)
- ✓ Scientist II – Pharmacoinformatics Division, NIPER, Mohali (June, 2004 – March, 2006)

Honours and Awards

- ✓ **Biotech Research Society, India (BRSI) Fellow Award – 2018** from the Biotech Research Society, India.
- ✓ **ICMR Lala Ram Chand Kandhari Award**-2014 from the Indian council of Medical Research (ICMR), New Delhi, India.
- ✓ **Senior Scientist Award-2017** from the Association of Biotechnology and Pharmacy (ABAP), Hyderabad, Telangana, India.
- ✓ Elected Member for **The National Academy of Sciences, Allahabad**, India (**MNASc)** in May 2017.
- ✓ **Dr. P. Daisy Oration Award-2017** from Department of Zoology, Biotechnology and Bioinformatics, Holy Cross College, Tiruchirapalli, Tamil Nadu, India.
- ✓ Travel Awards from **CSIR, DBT, DST, and ICMR (Funding)**.
- ✓ **Fellow of Academy of Sciences- 2020-**The Academy of Sciences, Chennai, Tamil Nadu, India.
- ✓ **Vallal Alagappar Research Recognition Award 2020** for excellence in teaching and research-Alagappa University, Tamil Nadu, India.
- ✓ **DST Fast Track grant for Young Scientist-2010** in Chemical Sciences.

Recent Publications

- ✓ Nayak, C., & **Singh, S. K***. (2022). Integrated Transcriptome Profiling Identifies Prognostic Hub Genes as Therapeutic Targets of Glioblastoma: Evidenced by Bioinformatics Analysis. ACS omega, 7(26), 22531–22550. **(I.F-4.13)**
- ✓ Selvaraj, C., Shri, G. R., Vijayakumar, R., Alothaim, A. S., Ramya, S., & **Singh, S. K***. (2022). Viral hijacking mechanism in humans through protein–protein interactions. Advances in Protein Chemistry and Structural Biology. **(I.F-5.4)**
- ✓ Yadav, M., Abdalla, M., Madhavi, M., Chopra, I., Bhrdwaj, A., Soni, L., & **Singh, S. K***. (2022). Structure-Based Virtual Screening, Molecular Docking, Molecular Dynamics Simulation and Pharmacokinetic modelling of Cyclooxygenase-2 (COX-2) inhibitor for the clinical treatment of Colorectal Cancer. Molecular Simulation, 1-21. **(I.F-2.3)**
- ✓ Mukherjee, S., Abdalla, M., Yadav, M., Madhavi, M., Bhrdwaj, A., Khandelwal, R., & **Singh, S. K***. (2022). Structure-Based Virtual Screening, Molecular Docking, and Molecular Dynamics Simulation of VEGF inhibitors for the clinical treatment of Ovarian Cancer. J. Mol. Mod. 28(4), 1-21. **(I.F-2.1)**
- ✓ Selvaraj, C., Rudhra, O., Alothaim, AS., Alkhanani, M., and **Singh, S.K***. (2022). Structure and Chemistry of Enzymatic Active Sites that play a role in the Switch and Conformation Mechanism. Advances in Protein Chemistry and Structural Biology, 130, 59-83. **(I.F-5.4)**
- ✓ Selvaraj, C., Abhirami, R., Vijayakumar, R., Alfaiz, FA., **Singh, S. K***. (2022). Immunological insights of selectins in human disease mechanism. Advances in Protein Chemistry and Structural Biology, 129, 163-188. **(I.F-5.4)**
- ✓ Selvaraj, C., Chandra, I., & **Singh, S. K***. (2022). Artificial intelligence and machine learning approaches for drug design: challenges and opportunities for the pharmaceutical industries. Molecular diversity, 26(3), 1893–1913. **(I.F-3.3)**
- ✓ Selvaraj, C., Dinesh, D. C., Krafcikova, P., Boura, E., Aarthy, M., Pravin, M. A., & **Singh, S. K***. (2022). Structural Understanding of SARS-CoV-2 Drug Targets, Active Site Contour Map Analysis and COVID-19 Therapeutics. Current molecular pharmacology, 15(2), 418–433. **(I.F-3.8)**

Cumulative Impact Factor: 550, Citations: 3423, h-index: 32, i10 index-102

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Educational Qualification

- ✓ Ph. D in (Biomedical Genetics) from Department of Genetics, Dr. ALMPGIBMS, University of Madras, Taramani Campus, Chennai, Tamil Nadu, India (Sep1999 - Oct 2006).
  Title : ANGIOTENSINOGEN (AGT) gene polymorphisms in South Indian Hypertensives.
  Mentor : Prof. G. JAYARAMAN, Coordinator (Molecular Biology Programme) & Former Director IBMS.
  Department of Genetics, Dr. ALM PGIBMS, University of Madras, Chennai – 600 113, Tamil Nadu, India.
- ✓ M.Sc (Biomedical Genetics) from Department of Genetics, Dr. ALMPGIBMS, University of Madras, Taramani Campus, Chennai, Tamil Nadu, India (May1999)
- ✓ B.Sc (Zoology) from Jamal Mohamed College, Bharathidasan University, Tiruchirappalli, Tamilnadu (April 1996).
- ✓ PG Diploma in Computer Applications (PGDCA) From Bishop Heber College, Bharathidasan University, Tiruchirappalli, Tamil Nadu, India (April 1999).

Professional Experience

- ✓ Assistant Professor (18.08.2008 – till date)
  Dept of Bioinformatics, Alagappa University, Karaikudi -630003, Tamilnadu, India
- ✓ Scientist in- charge (March 08 – August 08)
- ✓ Post doctoral Research Associate and Instructor (March 07 – August 07)
  College of Pharmacy, Nova South-eastern University, Florida, USA-33328
- ✓ Lecturer (July 05 –February 07)
  Department of Biotechnology, Vels College of Science, Pallavaram, Chennai- 600117, Tamilnadu, India

Honours and Awards

- ✓ Lady TATA Memorial Trust Junior scholarship (JRF) award 2001- 2003.
- ✓ Defense Research & Development Organization / Defense Institute of Physiology & Allied Sciences Senior Research Fellow (SRF) 2004 -2005.
- ✓ Qualified SLET (State Level Educational Testing) examination in the year of 1999 conducted by Bharathidasan University, Tiruchirappalli, Tamil Nadu.
- ✓ Best Paper Award in Pharmaceutical & Medicinal Synthetic Chemistry by The Indian Pharmaceutical Association's Prof. M. L. Khorana Memorial Indian Journal of Pharmaceutical Sciences in the year 2013.
- ✓ Received Best Poster award in National Conference on Recent Innovations in Biotechnology (18th April, 2016) Organized by Department of Biotechnology, Aarupadai Veedu Institute of Technology (AVIT), Kanchipuram, Tamil Nadu, India for the Poster Entitled "Identification of potential CYP24A1 inhibitors through E-Phamacophore mapping and Molecular docking and Dynamics study".
- ✓ Member (Basic Medical Scientist – Internal), Institute Ethics Committee (Human Studies), Alagappa University.
- ✓ Member, Institutional BioSafety Committee (IBSC), Alagappa University
- ✓ Assistant Director for International Relations of Alagappa University, Karaikudi, India.
- ✓ Best Paper Award in Pharmaceutical & Medicinal Synthetic Chemistry by The Indian Pharmaceutical Association's Prof. M. L. Khorana Memorial Indian Journal of Pharmaceutical Sciences in the year 2017.
- ✓ Received best poster award in National Conference on "Recent Trends in Plant Sciences"(01-02, March, 2017), organized by Department of Botany, ST. Xavier's College, Palayamkottai, Tamil Nadu, India.
- ✓ Recipient of Alagappa University prestigious research award "Alagappa Excellence Research Award for the year of 2018".
- ✓ Appointed as a Distinguished Adjunct Faculty by invitation at Saveetha Dental College and Hospitals, Chennai from 10th January 2019.

Recent Publications

- ✓ Singh, Khuraijam Dhanachandra, and Karthikeyan Muthusamy. "Molecular modeling, quantum polarized ligand docking and structure-based 3D-QSAR analysis of the imidazole series as dual AT1 and ETA receptor antagonists." Acta Pharmacologica Sinica 34.12 (2013): 1592-1606.
- ✓ Kirubakaran, Palani, Pitchaimani Arunkumar, Kumpati Premkumar, and Karthikeyan Muthusamy. "Sighting of tankyrase inhibitors by structure-and ligand-based screening and in vitro approach." Molecular BioSystems 2014.
- ✓ John Marshal Jayaraj, Beena Briget Kuriakose, Amani Hamad Alhazmi, Karthikeyan Muthusamy*. Structural and functional insights on vitamin D receptor and CYP24A1 deleterious single nucleotide polymorphisms: A computational and pharmacogenomics perpetual approach. Cell Biochemistry and Function, July 2021, Doi: 10.1002/cbf.3658.
- ✓ Loganathan, Lakshmanan, Beena Briget Kuriakose, Sakeena Mushfiq, and Karthikeyan Muthusamy. "Mechanistic insights on nsSNPs on binding site of renin and cytochrome P450 proteins: A computational perceptual study for pharmacogenomics evaluation." Journal of Cellular Biochemistry 122, no. 10 (2021): 1460-1474.
- ✓ Jayaraj, John Marshal, Muralidharan Jothimani, Chella Perumal Palanisamy, Olli T. Pentikäinen, Mehboobali Pannipara, Abdullah G. Al-Sehemi Karthikeyan Muthusamy, and Krishnasamy Gopinath. "Computational Study on the Inhibitory Effect of Natural Compounds against the SARS-CoV-2 Proteins." Bioinorganic chemistry and applications 2022 (2022).

Cumulative Impact Factor: 187.26; Total Citations: 1044; h-Index: 18; i10-index: 32

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Email : rmvbioinfo@gmail.com,vidhyamiss@gmail.com

Educational Qualification

- ✓ Ph. D in (Computer science) from Department of Computer Science and Engineering,Alagappa University,Karaikudi, Tamil Nadu, India (Feb 2008-Feb 20014).
  Title : A New Technique On Automatic Ontology Generation For Semantic Search System Using Data Mining Techniques.
  Mentor : Prof.E.Ramraj,Head of the Department.
  Department of Computer Science, Alagappa University, Karaikudi– 630003, Tamil Nadu, India.
- ✓ M.Tech(Information Technology)from,Department Information Technology,Sathyabama University,Chennai. (April 2010).
- ✓ M.Phil(Computer Science) form Department of Computer Science,alagappan University, Karaikudi– 630003, Tamil Nadu, India.(April 2007).
- ✓ M.Sc (Computer Science) from Department of Computer Science , S.R.M Arts & Science College,Kattankulathur, University of Madras, Chennai, Tamil Nadu, India (May2005).
- ✓ B.Sc (Computer Science) from Sri Saratha Niketan College for Women,Amaravathipudhur, Madhurai Kamaraj University, Madhuraii, Tamilnadu (April 2002).

Professional Experience

- ✓ Assistant Professor (31.08.2015– till date) ~4 years
  Dept of Bioinformatics, Alagappa University, Karaikudi -630003, Tamilnadu, India
- ✓ Teaching Assistant (August 2013 – April 2015) ~2 Years
  Dept of Alagappa University,Karaikudi-630003,Tamilnadu,India.
- ✓ Seniour Lecturer (June 2010–Jan 2011)~6Months
  Dept of Information Technology,Madha Institute of Engineering & Technology, Sadhanadhapuram,Chennai.
- ✓ Seniour Lecturer (August 2006–April 2010)~3.9 Years.
  Dept of Computer Science and Engineering, Jaya Engineering College, Thiruninravur, Chennai, Tamilnadu, India

Recent Publications

- ✓ Muthumanickam Sankar, Balajee Ramachandran, Boomi Pandi, Nachiappan Mutharasappan, Vidhyavathi Ramasamy, Poorani Gurumallesh Prabu, Gowrishankar Shanmugaraj, Yao Wang, Brintha Muniyandai, Subaskumar Rathinasamy, Balakumar Chandrasekaran, Mohammad F. Bayan, Jeyakanthan Jeyaraman, Gurumallesh. In silico Screening of Natural Phytocompounds towards Identification of Potential Lead Compounds to Treat COVID-19. J. Frontiers in Molecular Biosciences. DOI.org/10.3389/fmolb.2021.637122,2021.
- ✓ Sundararaj Rajamanikandan, Soundarapandian Soundarya, Anandhi Paramasivam, Dhamodharan Prabhu, Jeyaraman Jeyakanthan & Vidhyavathi Ramasamy," Computational identification of potential lead molecules targeting rho receptor of Neisseria gonorrhoeae, Journal of Bimolecular Structure and Dynamics. DOI.org/10.1080/07391102.2021.1885491,2021.
- ✓ Jesudass Joseph Sahayarayan, Kulanthaivel Soundar Rajan, Ramasamy Vidhyavathi, Mutharasappan Nachiappan, Dhamodharan Prabhu, Saleh Alfarraj, Selvaraj Arokiyaraj, Amalorpavanaden, Nicholas Daniel, Antifungal activity and molecular docking of phenol, 2,4-bis(1,1-dimethylethyl) produced by plant growth-promoting actinobacterium Kutzneria sp. strain TSII from mangrove sediments",Saudi Journal of Biological Sciences. DOI.org/10.1016/j.sjbs.2020.10.023,2021.
- ✓ Thangarasu Suganya Devi, Karuppiah Vijay, R M Vidhyavathi, Ponnuchamy Kumar, Muthusamy Govarthanan, Thangavel Kavitha Antifungal activity and molecular docking of phenol, 2,4-bis(1,1-dimethylethyl) produced by plant growth-promoting actinobacterium Kutzneria sp. strain TSII from mangrove sediments, Archives of Microbiology, May 2021,(0302-8933) (IF:2.55).

Cumulative Impact Factor: 24.69; Total Citations: 405; h-Index:07; i10-index: 07

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Educational Qualification

- ✓ Ph. D in (Biotechnology) , Department of Biotechnology, Bharathidasan University,Truchirappalli,Tamil Nadu, India - (November -2010).
  - Title : *In vitro* Regeneration, Hairy Root Culture and *Agrobacterium tumefaciens* - Mediated Transformation in West Indian Gherkin (*Cucumis anguria* L.).
  - Mentor: Prof.A.Ganapathi, Professor and Head, Department of Biotechnology, Bharathidasan University, Truchirappalli, Tamil Nadu, India.
- ✓ M.Sc (Biotechnology), Department of Biotechnology, Bishop Heber College, Bharathidasan University, Truchirappalli,Tamil Nadu, India - (April – 2004).
- ✓ B.Sc (Biochemistry), Department of Biochemistry, Arputha College, Bharathidasan University, Truchirappalli,Tamil Nadu, India - (April – 2002).

Professional Experience

- ✓ Assistant Professor, Department of Bioinformatics, Alagappa University, Karaikudi -630003, Tamilnadu, India -(04.12.2015 – till date).
  Assistant Professor, Department of Biochemistry & Microbiology, RVS College of Arts and Science, Karaikkal, Pondicherry, India - (June -2010 to March - 2012)
- ✓ Assistant Professor, Department of General Engneering, St. Joseph's Group of Institution, Dar Es Salaam, Tanzania -(May -2012 to March - 2013).

Honours and Awards

1.Bharathidhasan university research fellowship (2006 – 2009)
2.Key Note Speaker Award –Gauhati University, Guwahati, India- 2019

Recent Publications

- ✓ Sukanya Panikar, Gunasekaran Shoba, Muthukrishnan Arun, **Jesudass Joseph Sahayarayan**, A. Usha Raja Nanthini, Arunachalam Chinnathambi, Sulaiman A. Alharbi, Omaima Nasif, Hak-Jae Kim, Essential oils as an effective alternative for the treatment of COVID-19: Molecular interaction analysis of protease (Mpro) with pharmacokinetics and toxicological properties, *Journal of Infection and Public Health,* 2021, 14, 601-610
- ✓ **Jesudass Joseph Sahayarayan**, Kulanthaivel Soundar Rajan, Ramasamy Vidhyavathi, Mutharasappan Nachiappan, Dhamodharan Prabhu, Saleh Alfarraj, Selvaraj Arokiyaraj, Amalorpavanaden Nicholas DanielIn-silico protein-ligand docking studies against the estrogen protein of breast cancer using pharmacophore based virtual screening approaches, *Saudi Journal of Biological Sciences,* 2021, 28, 400-407
- ✓ **Jesudass Joseph Sahayarayan**, Kulanthaivel Soundar Rajan, Mutharasappan Nachiappan, Dhamodharan Prabhu, Ravi Guru Raj Rao, Jeyaraman Jeyakanthan, Ahmed Hossam Mahmoud, Osama B Mohammed, Abubaker MA Morgan, Identification of potential drug target in malarial disease using molecular docking analysis, *Saudi Journal of Biological Sciences*, 2020, 27,3327-3333
- ✓ Abubaker M.A. Morgan, **Jesudass Joseph Sahayarayan**, Rajangam Udayakumar, Muthukrishnan Arun, Andy Ganapathi, Mona S. Alwahibi, Norah Salim Aldosari Effect of different Agrobacterium rhizogenes strains for in-vitro hairy root induction, total phenolic, flavonoids contents, antibacterial and antioxidant activity of (Cucumis anguria L.),Saudi Journal of Biological Sciences, 2020,27,2972-2979

Cumulative Impact Factor: 25; Total Citations: 221; h-Index: 07; i10-index: 06

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Educational Qualification

- ✓ Ph.D –Chemistry, Alagappa University, Karaikudi, September, 2014.
  Title: Studies on Polyaniline with Mono and Bimetal Nanocomposites for Antibacterial and Anticancer Applications.
  Mentor: Prof. H. Gurumallesh Prabu, Professor, Department of Industrial Chemistry, Algappa Universisty, Karaikudi– 630 004, Tamil Nadu, India.
- ✓ M.Phil-Industrial Chemistry, Alagappa University, Karaikudi, 2008.
- ✓ M.Sc-Chemistry, Alagappa University, Karaikudi, 2007.
- ✓ B.Sc, Chemistry, Madurai Kamaraj University, 2003.

Professional Experience

- ✓ Assistant Professor (04.12.2015– till date) ~4 years
  Dept of Bioinformatics, Alagappa University, Karaikudi -630003, Tamilnadu, India
- ✓ Research Associate-HRDG-CSIR, New Delhi, CECRI-Karaikudi (01.10.2015 to 03.12.2015).

Honours and Awards

- ✓ **JRF-Project Assistant** -CSIR, CECRI, Karaikudi (06.04.2009 to 05.10.2009)
- ✓ **Best research paper Award** presented in seminar on Application of Nanotechnology, in current agricultural practices, Dr.Zahir Husain College, Ilayankudi (2011).
- ✓ **Junior Research Fellow**- (UGC-BSR, New Delhi)-Alagappa University, Karaikudi (08.02.2011 to 08.02.2013)
- ✓ **Senior Research Fellow**- (UGC-BSR, New Delhi)-Alagappa University, Karaikudi, (09.02.2013 to 26.09.2014)
- ✓ **Young Researcher Award with Rs.25000 Cash Prize**, Anyang Institute of Technology,China
- ✓ **Vallal Alagappar Research Recognition Award 2020** for excellence in teaching and research-Alagappa University, Tamil Nadu, India

Recent Publications

- ✓ S. Muthumanickam, A. Kamaladevi, **P. Boomi*,** S. Gowrishankar, S. Karutha Pandian, Indian ethnomedicinal phytochemicals as promising inhibitors of RNA binding domain of SARS-CoV-2 nucleocapsid phosphoprotein: an in silico study, Frontiers in Molecular Biosciences, Molecular Diagnostics and Therapeutics, (2021), 8, 637329 **(I.F-6.133).**
- ✓ S. Muthumanickam, **P. Boomi***, M. Nachiappan, R. Balajee, R. Vidhyavathi G. Poorani, S. Gowrishankar, Y. Wang, M. Biruntha, R. Subaskumar C. Balakumar, M. F. Bayan, J. Jeyaraman, H.G. Prabu K. Solomon, In Silico Screening of Natural Phytoconstituents Towards Identification of Potential Lead Compounds to Treat COVID-19, Frontiers in Molecular Biosciences, Molecular Diagnostics and Therapeutics, (2021), 8. 637122. **(I.F-6.133)**
- ✓ V. Karthik, S. Poornima, H. Barabadi, V. Arumugam, D. Daniel Raj, S. Manikandan, S. Ramasamy, K. Anand, P. Boomi, C. Balakumar, A. Selvaraj, M. Saravanan, Emerging Therapeutic Approaches to Combat COVID-19: Present status and future perspectives, Frontiers in Molecular Biosciences, Molecular Diagnostics and Therapeutics, (2021), 8, 604447, **(I.F- 6.133).**
- ✓ S. Gowrishankar, S. Muthumanickam, A. Kamaladevi, C. Karthika, R. Jothi, **P. Boomi**, D. Maniazhagu, S. Karutha Pandian, Promising phytochemicals of traditional Indian herbal steam inhalation therapy to combat COVID-19 – An in silico study, Food and Chemical Toxicology, (2021), 148, 111966, **(I.F-6.023).**
- ✓ K. Anand, S. Abdul Naeem, T. Ghazi, R, Muthusamy, G. Gupta, M. Tambuwala, H. Dureja, S. Sachin Kumar, D. Chellappan, D. Kamal, **P. Boomi**, M. Saravanan, Anil Chuturgoon, Induction of caspase-mediated apoptosis in HepG2 liver carcinoma cells using mutagen-antioxidant conjugated self-assembled novel carbazole nanoparticles and in silico modeling studies, ACS Omega, (2020), 6, 265–277. **(I.F-4.132)**
- ✓ K. Shanmugapriya, S. Palanisamy, **P. Boomi***, R. Subaskumar, S. Ravikumar, T. Thayumanavan, An eco-friendly Gnaphalium polycaulon mediated silver nanoparticles: Synthesis, characterization, antimicrobial, wound healing and drug release studies, Journal of Drug Delivery Science and Technology, (2020), 102202. **(I.F-5.062)**
- ✓ M. Karunakaran, K. Kasirajan, M. Balaji, **P. Boomi**, S. Mahalingam, S. Balamurugan, Cyclodextrin functionalized multi-layered MoS2 nanosheets and its biocidal activity against pathogenic bacteria and MCF-7 breast cancer cells: Synthesis, characterization and in-vitro biomedical evaluation, Journal of Molecular Liquids, October, (2020), 114631. **(I.F-6.633).**
- ✓ Muthumanickam, T. Indhumathi, **P. Boomi***, R. Balajee, J. Jeyakanthan, K. Anand, S. Ravikumar, P. Kumar, A. Sudha, Z. Jiang, In silico approach of naringin as potent phosphatase and tensin homolog (PTEN) protein agonist against prostate cancer, Journal of Biomolecular Structure and Dynamics, October, (2020), 9, 1-10. **(I.F-3.392)**

Cumulative Impact Factor: 175; Total Citations: 1191; h-Index: 19; i10-index: 28

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Educational Qualification

- ✓ Ph.D – Genetics Dr. ALM PG Inst of Basic Medical Sciences, Chennai, University of Madras, 2002.
- ✓ M.Sc- Bio-Medical Science Dr. ALM PG Inst of Basic Medical Sciences, Chennai, University of Madras, India- 1996
- ✓ B.Sc, Zoology Vivekananda College, Chennai. University of Madras1994.

Professional Experience

- ✓ Professor (2019-till date)
  Department of Biomedical Science, Bharathidasan University (BDU)
- ✓ Visiting Researcher, Michigan Centre for Translational Pathology, University of Michigan, Ann Arbor, MI. USA. (2016-2017)~1year
- ✓ Associate Professor(2016-2019) ~3years
  Department of Biomedical Science, BDU, Tiruchirappalli, Tamilnadu, India
- ✓ Assistant Professor (2006-2016) ~10 years
  Department of Biomedical Science, BDU, Tiruchirappalli, Tamilnadu, India

Honours and Awards

- ✓ 2019 Elected Executive Member of Indian Association of Biomedical Scientists (IABMS)
- ✓ 2019 Nominated as Member of National Academy of Sciences India (NASI)
- ✓ 2019 Nominated as Fellow of National Academy of Biological Sciences (NABS)
- ✓ 2018 Nominated as Fellow of Indian Association of Biomedical Scientists (IABMS)
- ✓ 2017 ICMR Award for Biomedical Research by Indian Council for Medical Research, New Delhi.
- ✓ 2017 Radio-Oration "AchamillaAathisayaMaruthuvam" Live, All India Radio Trichy
- ✓ 2016 RAMAN Post-Doctoral Fellowship, by University Grants Commission (UGC), New Delhi.
- ✓ 2016 RAMAN Post-Doctoral Fellowship, by University Grants Commission (UGC), New Delhi.

Recent Publications

- ✓ G Siva, S Venkatesh, G Prem Kumar, M Muthukumar, T Senthil Kumar, KPremkumar, N Jayabalan (2021) Rapid bio-reduction of Trivalent aurum using in vitroBabchi leaf powder and its cytotoxicity against breast cancer MCF-7 cell lines. Applied Nanoscience 1-9
- ✓ M Murugesan, P Kumpati. (2021) Integrative miRNA–mRNA functional analysis identifies miR- 182 as a potential prognostic biomarker in breast cancer. Molecular Omics. 17(4), 533-543.
- ✓ M Murugesan, P Kumpati. (2021) Systemic Multi-Omics Analysis Reveals Amplified P4HA1Gene Associated with Prognostic and Hypoxic Regulation in Breast Cancer. Frontiers in Genetics 12, 189
- ✓ M Murugesan, P Kumpati. (2020) Discovery of Aminoglycoside Derivatives as a Potent Inhibitor for the Prognostic P4HA1 gene in Breast Cancer: A Holistic Genomic and Virtual Screening Approach. European Journal of Molecular & Clinical Medicine 7 (6), 920-941
- ✓ K Sivakumar, G Parinamachivayam, M Murali Krishnan, V Ragavendran, T Stalin, K Premkumar, Sujay Chakravarty, A Bharathi. (2020) Reinforcement of 'imine- hydroxyl chelation pocket'by encapsulating into the β-CD cavity for the sterically protective detection of Al3+. Journal of Molecular Liquids. 114949
- ✓ R Vanajothi, H Vedagiri, MM Al-Ansari, LA Al-Humaid, P Kumpati. (2020) Pharmacophore based virtual screening, molecular docking and molecular dynamic simulation studies for finding ROS1 kinase inhibitors as potential drug molecules. Journal of Biomolecular Structure and Dynamics, 1-15
- ✓ M Sampath, A Pichaimani, P Kumpati, B Sengottuvelan. (2020) The remarkable role of emulsifier and chitosan, dextran and PEG as capping agents in the enhanced delivery of curcumin by nanoparticles in breast cancer cells. International Journal of Biological Macromolecules 162, 748-761
- ✓ R Vanajothi, V Hemamalini, J Jeyakanthan, K Premkumar. (2020) Ligand-based pharmacophore mapping and virtual screening for identification of potential discoidin domain receptor 1 inhibitors. Journal of Biomolecular Structure & Dynamics 38(9), 2800-08
- ✓ Hemamalini V, Velayutham DPM, Lakshmanan L, Muthusamy K, Sivaramakrishnan S, Premkumar K. (2020) Inhibitory potential of Hydroxychavicol on Ehrlich ascites carcinoma model and in silico interaction on cancer targets. Nat Prod Res. 34(11), 1591-1596
- ✓ P Boomi, GP Poorani, S Selvam, S Palanisamy, S Jegatheeswaran, K Anand, C Balakumar, K Premkumar, HG Prabu. (2020) Green biosynthesis of gold nanoparticles using Croton sparsiflorus leaves extract and evaluation of UV protection, antibacterial and anticancer applications. Applied Organometallic Chemistry 34 (5), e5574
- ✓ S Mehnath, M Arjama, M Rajan, K Premkumar, K Karthikeyan, M Jeyaraj. (2020) Mineralization of bioactive marine sponge and electrophoretic deposition on Ti-6Al- 4V implant for osteointegration. Surface and Coatings Technology, 125727

Cumulative Impact Factor: 300; Total Citations: 3873; h-Index: 29; i10-index: 58

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Educational Qualification

- ✓ Ph. D in (Biotechnology) , Department of Biotechnology, Bharathidasan University,Truchirappalli,Tamil Nadu, India - (November -2010).
  - Title : *In vitro* Regeneration, Hairy Root Culture and *Agrobacterium tumefaciens* - Mediated Transformation in West Indian Gherkin (*Cucumis anguria* L.).
  - Mentor: Prof.A.Ganapathi, Professor and Head, Department of Biotechnology, Bharathidasan University, Truchirappalli, Tamil Nadu, India.
- ✓ M.Sc (Biotechnology), Department of Biotechnology, Bishop Heber College, Bharathidasan University, Truchirappalli,Tamil Nadu, India - (April – 2004).
- ✓ B.Sc (Biochemistry), Department of Biochemistry, Arputha College, Bharathidasan University, Truchirappalli,Tamil Nadu, India - (April – 2002).

Professional Experience

- ✓ Assistant Professor, Department of Bioinformatics, Alagappa University, Karaikudi -630003, Tamilnadu, India -(04.12.2015 – till date).
  Assistant Professor, Department of Biochemistry & Microbiology, RVS College of Arts and Science, Karaikkal, Pondicherry, India - (June -2010 to March - 2012)
- ✓ Assistant Professor, Department of General Engneering, St. Joseph's Group of Institution, Dar Es Salaam, Tanzania -(May -2012 to March - 2013).

Honours and Awards

- ✓ Awarded in the Summer Research Fellowship **Sponsored by INSA** to work at **National Centre for Cell Science under the guidance of Dr. Musti. V. Krishnasastry**, for two months (14th May 2018 to 8th July 2018).
- ✓ Best Poster Presentation Award for the work presented in the "**International Conference on Recent Advances in Modern Medicine: molecular signaling scenarios in tissues and diseases",** at Bharath University, 3rd to 4th September 2016.
- ✓ Selected as Best Abstract and received a grant to present the work in the **"Indo-US Workshop on Biocomputing"** at National Institute of Technology, 12th -13th September 2011.
- ✓ Best Poster Presentation Award for the work presented in **"International conference on System Biology and Bioinformatics"** at Annamalai University, 16th -17th February 2011.

Recent Publications

- ✓ S Parthasarathy, P Soundararajan, N Krishnan, K Mala, V Devadasan, D Prabhu, **S Rajamanikandan**, P Velusamy, SCB Gopinath, P Raman. Detection of adulterants from common edible oils by GC-MS. *Biomass Conversion and Biorefinery*. (IF: 4.987).
- ✓ S Mani, SB Bhatt, V Vasudevan, D Prabhu, **S Rajamanikandan**, P Velusamy, P Ramasamy, P Raman. The updated review on plant peptides and their applications in human health. *International Journal Peptide Research and Therapeutics*. (IF: 1.931).
- ✓ P Ramasamy, G Dakshinamoorthy, S Jayashree, D Prabhu, **S Rajamanikandan**, P Velusamy, G Dayanithi, REB Hanna. A novel prototype biosensor array electrode system for detecting the bacterial pathogen Salmonella typhimurium. *Biosensors*. (IF: 5.75)
- ✓ ST Peter, P Adikesavan, B Muniyandi, **S Rajamanikandan**, D Prabhu, S Chellaiyan. Environmental impact assessment of algal bloom Noctiluca scintillans in the Mandapam Group of Islands, Gulf of Mannar Biosphere Reserve, Southeast coast of India. *Environmental Monitoring and Assessments*. (IF: 3.061)
- ✓ B Ramachandran, C Jeyarajpandian, JM Jeyaseelan, D Prabhu, **S Rajamanikandan**, P Boomi, R Venkateswari, J Jeyakanthan. Quercetin-induced apoptosis in HepG2 cells and identification of quercetin derivatives as potent inhibitors for caspase-3 through computational methods. *Structural Chemistry*. (IF: 1.887)
- ✓ V Ramesh, SA Kulkarni, V Palaniyandi, V Devadasan, P Devaraju, KN Rajnish, T Madhavan, P Anbu, P Ramasamy, **R Sundarraj**. Current Update of Phytotherapeutic Agents in the Treatment of Covid-19: *In-Silico* Based Virtual Screening Approach for the Development of Antiviral Drug. *Frontiers in Bioscience Landmarks*. (IF: 4.009)
- ✓ M Sureshan, **S Rajamanikandan**, S Srimari, D Prabhu, J Jeyakanthan, K Saraboji. Designing specific inhibitors against dihydrofolate reductase of W. bancrofti towards drug discovery for lymphatic filariasis. *Structural Chemistry*. (IF: 1.887)
- ✓ H Hadiatullah, Y Zhang, A Samurkas, Y Xie, **S Rajamanikandan**, H Zuilhof, J Qiao, Z Yuchi. Recent progress in the structural study of ion channels as insecticide targets. *Insect Science*. (IF: 3.4).

Cumulative Impact Factor: 40; Total Citations: 221; h-Index: 07; i10-index: 06

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Educational Qualification

- ✓ Ph.D. Department of Crystallography, University of Pittsburgh, U.S.A. 1994~1999
- ✓ M.S. Institute of Life Sciences, National Tsing Hua University, Taiwan, 1989~1991
- ✓ B.S. Department of Physics, National Tsing Hua University, Taiwan. 1985~1989

Professional Experience

- ✓ 2001~ Biophysics, Department of Physics, National Tsing Hua University, Taiwan
- ✓ 2001~X-ray Diffraction and Application, Department of Physics, National Tsing Hua University, Taiwan
- ✓ 2021~ Scientist, Life Science Group, Scientific Research Division, NSRRC
- ✓ 2019~Joint Professor, Dept. of Biological Science & Technology, National Yang Ming Chao Tung University
- ✓ 2011~Joint Professor, Dept. of Physics, National Tsing Hua University
- ✓ 2011~ Joint Professor, Dept. of Biotechnology and Industrial Sciences, National Cheng Kung University
- ✓ 2004~2010 Associate Scientist, Life Science Group, Scientific Research Division, NSRRC
- ✓ 2008~2011 Joint Associate Professor, Inst. of Biotechnology, National Cheng Kung Univ.
- ✓ 2005~2011 Joint Associate Professor, Dept. of Physics, National Tsing Hua University
- ✓ 2002~2005 Joint Assistant Professor, Dept. of Physics, National Tsing Hua University
- ✓ 2001~2002 Part-time Assistant Professor, Dept. of Physics, National Tsing Hua Univ.
- ✓ 2001~2003 Assistant Scientist, Life Science Group, Research Division, NSRRC
- ✓ 1999~2000Post-doc., Dept. of Biochemistry & Molecular Biology, Univ. of Georgia, U.S.A.

Honours and Awards

- ✓ NSC/MOST Outstanding Young Scholar Research Project (2012 ~ 2016)
- ✓ NSRRC Outstanding Paper Award (2012, 2013, 2014, 2015, 2016, 2017, 2018)
- ✓ Supervise a Post-doc researcher to receive the Post-doc Research Award of MOST (2014).
- ✓ Lam Research Award (2016)
- ✓ Award of Future Tech of MOST (2017, 2019)
- ✓ Researches on press & media: Grouper virus GNNV (2015), Outer membrane protein of Typhoid (2015), human hepatoma-derived growth factor (2018), Shrimp nodavirus (2019), virus study on space (2021)

Recent Publications

- ✓ Chan, S. I.*, Chuankhayan, P., Nareddy, Pavan K., Tsai, I-K., Tsai, Y.-F., Chen, K. H.-C., Yu, S. S.-F.*, **Chen, C-J.*** (2021) "The mechanism of PQQ-dependent hydride transfer chemistry from spectroscopic and high-resolution X-ray structural studies of the methanol dehydrogenase from *Methylococcus capsulatus* (Bath)" *J. Am. Chem. Soc.* 143, 9, 3359-3372.
- ✓ Shih, T.-W., Hsu, C.-L., Chen, L.-Y., Huang, Y.-C., **Chen, C.-J.**, Inoue, Y., Sugiyama, T.* (2021) "Optical Trapping-Induced New Polymorphism of β-Cyclodextrin in Unsaturated Solution" *Cryst. Growth Des.* 21, 6913-6923.
- ✓ Guan, H. H., Huang, Y. H., Lin, E. S., **Chen, C.-J.***, & Huang, C. Y.* (2021) "Plumbagin, a natural product with potent anticancer activities, binds to and inhibits dihydroorotase, a key enzyme in pyrimidine biosynthesis" *Intl. J. Mol. Sci.* 22(13), 6861.
- ✓ Guan, H. H., Huang, Y. H., Lin, E. S., **Chen, C.-J.***, & Huang, C. Y.* (2021) "Complexed Crystal Structure of Saccharomyces cerevisiae Dihydroorotase with Inhibitor 5-Fluoroorotate Reveals a New Binding Mode" *Bioinorg. Chem. Appl.* 2021.
- ✓ Guan, H. H., Huang, Y. H., Lin, E. S., **Chen, C.-J.***, & Huang, C. Y.* (2021) "Structural Analysis of *Saccharomyces cerevisiae* Dihydroorotase Reveals Molecular Insights into the Tetramerization Mechanism" *Molecules,* 26, 7249.
- ✓ Guan, H.-H., Huang, Y.-H. Lin, E.-S., **Chen, C.-J.***, Huang, C.-Y.* (2021) "Structural basis for the interaction modes of dihydroorotase with the anticancer drugs 5-fluorouracil and 5-aminouracil" *Biochem. Biophys. Res. Commun.* 551, 33-37.
- ✓ Chen, S.-K. Guan, H.-H., Wu, P.-H., Lin, L.-T., Wu, M.-C., Chang, H.-Y., Chen, N.-C., Lin, C.-C., Chuankhayan, C., Huang, Y.-C., Lin, P.-J., **Chen, C.-J.*** (2020) "Structural insights into histidine-containing phosphotransfer protein and receiver domain of sensor histidine kinase suggest a complex model in two-component regulatory system in *Pseudomonas aeruginosa" IUCrJ,* 7, 934-948.
- ✓ Astani, E. K., Ersali, S., Lee, Y.-C., Lin, P.-J., Huang, Y.-C., Huang, P.-Y., Jafarian, V., Hosseinkhani, S.*, **Chen, C.-J.*** (2020) "Determination and Evaluation of Secondary Structure Content Derived from Calcium-Induced Conformational Changes in Wild-Type and Mutant Mnemiopsin 2 by Synchrotron-based Fourier-Transform Infrared Spectroscopy" *Biochim. Biophys. Acta (BBA)-Proteins and Proteomics,* 1868 (12), 140528.
- ✓ Songsiriritthigul, C.*, Narawongsanont, R., Tantitadapitak, C., Guan, H.-H., **Chen, C.-J.** (2020) "Structural-function study of AKR4C14, an aldo-keto reductase from Thai Jasmine rice (*Oryza satica* L. ssp. *Indica* cv. KDML105)" *Acta Cryst.* D76, 472-483.

Cumulative Impact Factor: 170; Total Citations: 1164; h-Index: 19; i10-index: 28

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Educational Qualification

- ✓ Ph.D (Biophysics)- University of Madras, Chennai, India (1984)
- ✓ M.Sc. (Biophysics & Crystallography)-University of Madras, Chennai, India (1982)

Professional Experience

- ✓ Professor (Structural Biology and Bio-computing), Computational and Data Sciences, Indian Institute of Science Bangalore (2016 till date)
- ✓ Associate Professor (Structural Biology and Bio-computing), Computational and Data Sciences
- ✓ Indian Institute of Science, Bangalore (2010-2016)
- ✓ Principal Research Scientist (Structural Biology and Bio-computing), Bioinformatics Centre, Indian Institute of Science, Bangalore (2004-2010)

Honours and Awards

- ✓ National Bioscience award (2004-2005)

Recent Publications

- ✓ Chandrasekaran Palaniappan, Rahul C. Narayanan and **K. Sekar**, Mutation-dependent Refolding of Prion Protein Unveils Amyloidogenic-related Structural Ramifications: Insights from Molecular Dynamics Simulations, ACS Chemical Neuroscience, (2021), 12, 2714-2952 **(I.F-4.5)**
- ✓ Gunalan Seshan, Somarathinam Kanagasabai, Sailapathi Ananthasri, Balaji Kannappan, A. Suvitha, S. M. Jaimohan, Gugan Kothandan and **K. Sekar**, Insights of structure-based pharmacophore studies and inhibitor design against Gal3 receptor through molecular dynamics simulations, Journal of Biomolecular Structure and Dynamics, (2020), 1-13. **(I.F-3.39)**
- ✓ SK Chaudhary, M Elayappan, J Jeyakanthan and **K. Sekar**, Structural and functional characterization of oligomeric states of proteins in RecFOR pathway, International Journal of Biological Macromolecules (2020), 5, 943-953 **(I.F-8.02)**
- ✓ D Mitra, N Bankoti, D Michael, TNG Row and **K. Sekar**, C-halogen… pi interactions in nucleic acids: a database study, Journal of Chemical Sciences, (2020), 132, 1-6 **(I.F-2)**
- ✓ Ananthasri Sailapathi, Gopinath Murugan, Kanagasabai Somarathinam, Seshan Gunalan, Rahul Jagadeesan, Niyaz Yoosuf, Gugan Kothandan and **K. Sekar**, Proposing the Promiscuous Protein Structures in JNK1 and JNK3 for Virtual Screening in Pursuit of Potential Leads, **ACS Omega** (2020), 5, 3969-3978 **(I.F-4.1)**
- ✓ Seshan Gunalan, Kanagasabai Somarathinam, Jayanti Bhattacharya, Shantkriti Srinivasan, S.M Jaimohan, Ravi Manoharan, Sowmya Ramachandran, Gugan Kothandan and **K. Sekar,** Understanding the dual mechanism of bioactive peptides targeting the enzymes involved in Renin Angiotensin System (RAS): An In-Silico Approach, Journal of Biomolecular Structure and Dynamics, (2019). 1-18. **(I.F-3.39)**
- ✓ Rajendran Santhosh, Namrata Bankoti, Padmashri Adgonda Malgonnavar, Daliah Michael, Jeyaraman Jeyakanthan and **K. Sekar,** MRPC: Missing Regions in Polypeptide Chains - A Knowledgebase, Journal of Applied Crystallography(2019). 52, 1422-1426. . **(I.F-3.3)**

Cumulative Impact Factor: 500; Total Citations: 4057; h-Index: 35; i10-index: 84

DEPARTMENT: BIOINFORMATICS

ALAGAPPA UNIVERSITY, KARAIKUDI

(A State University Accredited with "A+" grade by NAAC (CGPA: 3.64) in the Third Cycle and Graded as Category-I University by MHRD-UGC)

M. Phil BIOINFORMATICS

Choice Based Credit System (CBCS)

[For those who joined in July 2022 and after]

Objective

To make the students impart a great knowledge on worldly research and teaching qualities in Bioinformatics.

Curriculum

The study of M. Phil course of bioinformatics includes the advanced areas of development of new computational methods for studying Evolutionary Genomics, Computational approaches to Macromolecular structure, dynamics and simulation, Comparative evolutionary genomics, Drug design and discovery, Pharmacogenomics, Algorithm development, Data mining, and Prediction and analysis of structure etc.

Course Description

The Course extends for a period of one year under Semester Pattern (Two semesters). The major and recent advances in Bioinformatics and career in Research is the major prospective of this program.

Outcome

The course has been designed in a way to enable analytical and scientific facets of research methodology.

ALAGAPPA UNIVERSITY

(*A State University Accredited with 'A+' Grade by NAAC (CGPA:3.64)in the Third Cycle and Graded as Category-I University by MHRD-UGC)*

M. Phil BIOINFORMATICS

Choice Based Credit System (CBCS)

[For those who joined in July 2022 and after]

COURSE STRUCTURE

S. No	Course Code	Name of the Course	Credits	Marks		
		SEMESTER – I		**Int.**	**Ext.**	**Total**
1.	505101	Research Methodology in Bioinformatics	4	25	75	100
2.	505102	Advanced Topics in Bioinformatics	4	25	75	100
3.	505103	General Skills in Science	4	25	75	100
SEMESTER – II						
4.	505104	Research Area Specialization	4	25	75	100
5	505999	Dissertation and Viva Voice	8	50	150	200
		Total	**24**			**600**

SEMESTER I

Paper I Research Methodology in Bioinformatics

Paper II Advanced Topics in Bioinformatics

Paper III General Skills in Science

The Semester I examinations will be conducted during November/December and Semester II will be in April/May every Academic year.

SEMESTER II

Paper IV Research Area Specialization

Paper V Dissertation and Viva Voice

Candidates should choose a research problem in his/her area of research and submit a dissertation with the results of his /her Research, carried out under the supervision of a recognized supervisor.

Courses offered to other Departments: Research Area Specialization

ALAGAPPA UNIVERSITY

(*A State University Accredited with 'A+' Grade by NAAC(CGPA:3.64)in the Third Cycle and Graded as Category-I University by MHRD-UGC)*

M. Phil BIOINFORMATICS

Choice Based Credit System (CBCS)

[For those who joined the Course in July 2019 and after]

REGULATIONS

1. **Eligibility**

   Candidates for admission to Master of Philosophy (M. Phil) in Bioinformatics must have obtained 55% marks in M.Sc. Life Sciences (any branch) /Physics/Chemistry.

2. **Duration of the Course**

   The course period is of one year under Semester Pattern (two Semesters).

3. **Standards of Passing and award of Division.**

   a) The Minimum marks for passing in each theory paper / lab course is 50% of the marks prescribed for the theory paper/ lab course.

   b) A candidate who secure 50% - 59% of the aggregate marks prescribed for two semesters taken together, will be awarded **SECOND CLASS.**

   c) A candidates who secures 60% or more of the aggregate marks prescribed for two semesters taken together, will be awarded **FIRST CLASS.**

   d) Project shall be assessed by the two examiners, appointed by the University.

4. **Admission**

   Admission is based on Entrance Examination.

   i) A candidate can answer a maximum of 100 questions.

   ii) Duration of Examination will be two hours.

   iii) Government of Tamil Nadu/University norms may be followed for selection.

5. Attendance

Students must have earned 75% of attendance in each course for appearing for the examination. Students who have earned 74% to 70% of attendance to be applied for condonation in the prescribed form with the prescribed fee. Students who have earned 69% to 60% of attendance to be applied for condonation in the prescribed form with the prescribed fee along with the Medical Certificate.

Students who have below 60% of attendance are not eligible to appear for the examination. They shall re-do the semester(s) after completion of the programme.

6. Project

Each candidate shall be required to take up a Project Work; submit Project Report at the end of the second year. The Head of the Department shall assign the Guide who in turn will suggest the Project Work to the student in the beginning of the second year. One typed copy of the Project Report shall be submitted to the University through Head of the Department on or before the date fixed by the University.

The project report will be evaluated by an Internal Examiner and an External Examiner, nominated by the University. The candidate concerned will have to defend his project in a Viva– Voce examination.

7. **Examination Question Pattern**

Theory Courses:	**Max: 75 Marks**
Five questions (either or type) (One question from each Unit)	5 x 15= 75 marks
Project Viva-voce	

8. Fee structure

Fee for First Semester	Rs.7500/-
Fee for Second Semester	Rs.2500/-
Total Fee	Rs.10,000/-

Tuition Fees, Laboratory Fees, Special Fees and other fees is as prescribed by the University.

For Foreign Nationals opting for M.Phil programme the fees in **USD $ 300**

9. General Objectives of the Program

The general objective of the M.Phil program in Bioinformatics is to develop strong-minded graduates with high-quality skills in the field of Bioinformatics assisted with Computer Aided Drug Design, Structural Biology, Pharmacogenomics, and other varied disciplines from the faculty experts of Bioinformatics. The curriculum designed bridges the scholarly prospects of research and higher studies and hence this program facilitates to producea research student who gains the all-round knowledge of a specialization area with expertise and present a part of original research for a higher degree.

10. Specific Objectives of the Program

i. To strengthen teaching and research environment as a bridge course for scholars to provide the forefront of guidance in the field of Structural Biology, Computational Biology and Pharmacogenomics.

ii. To identify and perform Cloning, Expression, Purification and Crystallization techniques in order to solve crucial putative targets using X-ray Crystallography.

iii. To develop a proficient Structural Bioinformatics knowledgebase that is intended to provide with novel information of several targets and molecular signaling pathways which will further increase the innovative solutions from the growing scientific research community.

11. Outcomes of the Program

i. To comprehend the scope and concepts of Structural Biology, CADD, Structural Pharmacogenomics and Structural Bioinformatics that will provide a profound impact on Scientific research.

ii. To build libraries of therapeutic interests for screening purposes after the target of interest has been identified (Structural and Functional aspects) thereon to propose a lead molecule with modifications that could enrich the drug-likeness for human uses which tend to be specific based on molecular fingerprints of human.

iii. Key information for one's research purposes can be obtained from the knowledgebase that is built using structured programming languages

iv. To understand and review the relative effectiveness among the different methods and techniques in Structural Biology, Drug Discovery and Pharmacogenomics

SEMESTER – I

Semester - I		
Course Code: 505101	**Research Methodology in Bioinformatics**	**Credits: 4**
Objectives	➢ Learn the statistical techniques such as measures of standard deviation, measures of dispersion and regression analysis. ➢ The knowledge of intellectual property rights and filing the patents.	
Unit - I	**Research Methodology:** Choosing of research problem/relevance to society, literature survey, research manuscript preparation, Dissertation/thesis preparation, writing of research project proposal, Intellectual Property Rights: Introduction, types and importance of Intellectual Property Rights (IPR) and patents, Organization – GATT-TRIPS, IPRs and ownership of traditional knowledge – IPR impacts on biological research in India	
Unit - II	**Mathematics and Bio-statistics**: Trigonometric Functions, Series Expansion, Inverse, General Values, Graphs, Vector Algebra, Vector Calculus, Basic Computations. Data Representation, Measures of central tendency, Measures of Dispersion, Linear Correlation: Types, Methods of studying Correlation, Karl Pearson's Coefficient of Correlation, Linear Regression: Regression line, Regression Equations, Regression Coefficients, Chi squared distribution, Students t distribution and ANOVA.	
Unit - III	**Sequence Alignment and Analysis**: Nucleic acids, central dogma of molecular biology DNA sequence analysis: Entrez, GenBank, EMBOSS, Artemis R11, Sequencher, DNAuser, jambw, GENSCAN, Glimmer. Amino acids, peptide bond, Protein sequence analysis: ExPASy Proteomics tools, AnthePro, PSAAM, Osprey, WinPep, SubMito, ProteinVis, and PSIPRED, Sequence alignment and Phylogeny: NetPrimer, PerlPrimer, SimVector, CGView, BioEdit, BioCococa, Readseq, PAUP, Phylip, ClustalW, Microarray analysis, ScanAnalyze, Cluster.	
Unit - IV	**Methods for Protein Structures:** Levels of protein structures, protein structure determination using X-ray crystallography, Ramachandran Plot, PDB. Homology modeling, Threading and *ab initio* method, Tools for Structure prediction; Protein structural visualization; Geometry optimization and Loop refinement; Structure validation tools etc.,	
Unit-V	**Genome Database and Resources:** Sequence and structural resources for bioinformatics – Genome Databases – The Human Genome Project – Genetic disease and Genomics –Comprehensive Microbial Resource of TIGR - Databases and webservers (PAM, BLOSSUM, PFAM, Uniprot/Swissprot, PDB, SCOP, CATH, DALI, PDBSum), (CSD/CCDC).	

Suggested Readings:-

Arthur M. L. (2017). *Introduction to Bioinformatics (2nd ed.)*. Oxford University Press, New Delhi.

Attwood, K.J., Parry-Simith, J.D. (2005). *Introduction to Bioinformatics.* Pearson Education Publisher.

Bourne, P.E., Weissig, H. (2003). *Structural Bioinformatics*, John-Wiley and sons.

Gromiha, M. (2010). *Protein Bioinformatics: From Sequence to Function (1st ed.),* Academic Press.

<table>
<tr><td colspan="2">Cengage Learning.
Mount, D. (2004). Bioinformatics: Sequence and Genome Analysis. Cold Spring Harbor Laboratory Press,
New York.
Zoe, L., Terence, C. (2003). Bioinformatics-Managing Scientific Data, Morgan Kaufman Publishers.</td></tr>
<tr><td>Outcomes</td><td>➢ Applying statistical techniques for data analysis: measurement of standard deviation, dispersion and regression analysis.
➢ Understand intellectual property rights and patent profiling.</td></tr>
</table>

Name of the Course Teacher: Dr. J. Jeyakanthan
Dr. Sanjeev Kumar Singh
Dr. M. Karthikeyan
Dr. RM. Vidhyavathi
Dr. J. Joseph Sahayarayan
Dr. V.K.Langeswaran

Semester I		
Course Code: 505102	**Advanced Topics in Bioinformatics**	**Credits: 4**
Objectives	• Familiarize Bioinformatics methods for managing, analyzing and interpreting data. • To create biological databases and network analysis will be helpful for inferring the underlying interaction of genes and gaining insights about the pathway structures with which the drug interacts. • Understand and detect the molecular bases for diseases and designing a molecule.	
Unit - I	**Introduction to Molecular Modeling**: Features of molecular mechanics, force fields; Bond structure and bending angles – electrostatic, van der Waals and non-bonded interactions, hydrogen bonding in molecular mechanics; Derivatives of molecular mechanics energy function; Calculating thermodynamic properties using force field; Transferability of force field parameters, treatment of delocalized pi system; Force field for metals and inorganic systems – Application of energy minimization. Molecular Dynamics Simulation Methods – using simple models; continuous potentials; constant temperature; pressure and time-dependent properties. Solvent effects and Conformational changes in Molecular Dynamics simulation.	
Unit - II	**Pharmacoinformatics and Drug Discovery**: Deriving and using 3D pharmacophore; Molecular Docking; Structure and ligand based methods to identify lead compounds; de novo ligand design; Applications of 3D Database Searching and Docking, Structure Activity Relationship - QSARs and QSPRs, QSAR Methodology, Various Descriptors used in QSARs: Electronic; Topology; Quantum Chemical based Descriptors. Use of genetic algorithms, neural networks and principle components analysis in the QSAR equations. Tools: Hex, Auto dock, Argus lab. RasMol, CN3D, DTMM, Swiss-PdbViewer, gopenmol, StrukEd, JMVC	
Unit - III	**Genome Mapping**: Introduction, Relationship between mapping and sequencing, Genome mapping elements, Types of maps, Comparative Maps, Uses of Mapping resources. Genomic databases: Introduction, Genome projects, Genome browsers, UCSC, NCBI, Ensemble.	
Unit - IV	**Protein-Protein Interaction Networks, databases and softwares**: DIP (Database of Interacting Proteins), PPI Server, BIND - Bimolecular Interaction Network Database, PIM – Hybrigenics, PathCalling Yeast Interaction Database, PROXiMATE - A database of mutant protein-protein complex thermodynamics and kinetics, PPA-Pred2-Protein-protein binding affinity prediction from amino acid sequence,MINT - a Molecular Interactions Database, GRID - The General Repository for Interaction Datasets, InterPreTS - protein interaction prediction through tertiary structure.	
Unit-V	Transcriptomics – Metabolomics - Microarray analysis – DNA Microarrays – Protein Microarrays – Gene / Protein expression-Application of Microarrays in Pharmacogenomics - Mass Spectrometry –	

	Systems Biology – biochemical / metabolic networks – small world networks – E-cell – Applications-Immunoinformatics, Artificial Intelligence, Neural networks and SVM

Suggested Readings:-

Lesk, A. M. (2014). *Introduction to Bioinformatics (4th ed.).* UK: Oxford University Press.

Mount, D. (2004). *Bioinformatics: Sequence and Genome Analysis.* New York: Cold Spring Harbor Laboratory Press, New York.

Roderick D.M. Page., Edward C. Holmes. (1998). *Molecular Evolution: A Phylogenetic Approach (1st ed.).* Wiley-Blackwell, ISBN-13: 978-0865428898.

Sung, W. (2010*). Algorithms in Bioinformatics: A Practical Introduction.* CRC press, ISBN: 9781420070330.

Outcomes	• Transform raw data into meaningful information by applying computational techniques. • Identify new, clinically relevant, molecular targets to the discovery of innovative drugs using computational methods. • Study the behavior and properties of molecular systems. Specifically, the techniques employed in the fields of computational biology and chemistry.

Name of the Course Teacher: Dr. J. Jeyakanthan
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SEMESTER-I		
Course Code: 505103	**General Skills in Science**	**Credits:4**
Objectives	➢ Attain Knowledge about introduction to Operating systems, Computer architecture, Hardware, Languages and creating Email, Website. ➢ To understand the principles, classes and structure of C++ Programming. ➢ Introduce students with basic MS office application operations like creating, saving, closing, renaming and deleting a document.	
Unit-I	**Communication Skills in English:** Understanding communication – greeting and introducing – making requests – asking for and giving permission – offering help – giving instruction and directions- art of small talk – participating in conversation – making a short formal speech –Describing the people, place, events and things. Telephone skill: understanding, handling calls, leaving message and making request. Written communication: report writing, note making - career skills: curriculum vitae and cover letters - Facing an interview and presentation skills – academic listening.	
Unit-II	**Introduction to Computers:** Computer Hardware: Input devices and media, magnetic device and media, output devices and media, storage device and media, computer architecture. **System software:** types, operating system and translators. **Application software:** types of language, application packages, **integrated software**: Introduction to operating system, Working with windows and office programs, Internet, Website and Email.	
Unit-III	**Computer Operating Skills:** Starting a program and opening a document, saving and naming the document, create file and folders, deleting and un-deleting a document, closing a document, renaming and moving a document, finding a document. **MS office**: Word, Excel, Access, power point, outlook and integrated office applications, C programming. Principles, classes and structure of C++ Programming.	
Unit-IV	**Pedagogical Skill for Science Teachers:** Science Teacher: Qualification, teacher competencies and professional growth. Theory and models of curriculum development: Concept and Technical scientific models of curriculum development - planning a science library – Handling of practical classes. Educational technology and classroom pedagogy: Educational Technology – Concept, Emerging technologies- New technologies on methodology of teaching, learning experiences and curriculum development. Micro-teaching: Meaning, teaching, skill of stimulus variation, questioning, explanation, reacting, linking and benefits.	
Unit-V	**Practical Training:** Preparation of charts and models for handling classes of science teacher - Creating management documents e.g. Curriculum Plan, Time Table scheduling, Evaluation- Strategies etc – Learning to write and draw on the blackboard - Preparation of over head projector presentations - Preparation of power point/LCD presentations – Preparation of micro-teaching skills — Preparation of teaching materials – seminar classes for PG students- Preparation of album.	

Suggested Readings:- Curtis Frye, (2004), *Microsoft office Excel 2003 step by step*; Microsoft press. Guy Hart-D Eavis, (2007), *How to do everything with Microsoft office word 2007;* Mac Graw-Hill professional. .Jim Boyce. (*2003. Absolute beginner's guide to Microsoft office 2003*. Que publishing.	
Outcomes	➢ Identifies hardware components, starts an application and create a document. Creates a simple slide show, recognizes the elements of a multi-media presentation. ➢ Understands the general structure of an email address. Use new technologies of teaching methods. Write scientific reports, note-making, journal paper, review etc.

Name of the Course Teacher: Dr. RM. Vidhyavathi,
Faculty of English and Skill Development

Course code: 505104	Research Area Specialization	Credit:4
Objective	➢ To improve the knowledge in the field of molecular modelling, drug design and crystallization techniques. ➢ To gain the knowledge about pharmacogenomics through it helps to utilize the personalized medicine.	
Unit-I	**Small and Macromolecular X-ray Crystallography:** X-ray generation, synchrotron radiation and applications, unit cell, atomic scattering factor and structure factor, diffraction theory, phase problem –methods of its solution – electron density function, anomalous scattering, intensity data collection and reduction, direct method of solving a small molecule, refinement of crystal structure, hydrogen bonding. Protein purification and crystallization methods, data collection and data reduction, protein structure determination-molecular replacement technique (MR); multiple isomorphous replacement method (MIR); multi wavelength anomalous diffraction method (MAD), Single wavelength anomalous diffraction method (SAD), Calculation and interpretation of electron density map, protein structure refinement and validation method (Ramachandran Plot).	
Unit-II	**Pharmaceutical Chemistry: Modern Pharmaceutical Techniques:** Basic principle and theory of advanced Spectroscopy techniques such as UV-Vis, FT-IR, XRD, MolD, ITC, DSC, Mass spectrometry, Circular dichroism (CD), Surface plasmon resonance (SPR) and NMR. Chromatography techniques-Principles, chromatographic parameters, factors affecting and applications of TLC, Column chromatography, Paper chromatography, Ion exchange chromatography, Fast protein liquid chromatography (FPLC) and High pressure liquid chromatography. Introduction and application of various thermal methods TGA/DTA and DSC.	
Unit-III	**Molecular Modeling and Drug Design:** Drug discovery process, Role of Bioinformatics in drug design, Target identification and validation, lead optimization and validation, Structure and ligand based drug design, Modeling of target-small molecule interactions, Molecular Simulations, Protein modeling. **Structure Activity Relationship** - QSARs and QSPRs, QSAR Methodology, Various Descriptors used in QSARs: Electronic; Topology; Quantum Chemical based Descriptors. Use of Genetic Algorithms, Neural Networks and Principle Components Analysis in the QSAR equations.	
Unit-IV	**Pharmacogenomics:** Overview; Basic Principles and Present status of Pharmacogenetics, Basic concepts about genetics diseases, mode of inheritance, population genetics concepts involved in Pharmacogenetics, Concepts of individualized medicine; Pharmacogenomics of genetic diseases e.g. hypertension and Cancer, role of bioinformatics in Pharmacogenomics; Approaches to Pharmacogenomics studies; Classical and non-Classical Pharmacogenomics, Advantage, Limitations and Ethical issues of Pharmacogenomics.	
Unit-V	**Synthetic Biology:** Introduction, foundation, component and applications of	

	synthetic biology in plant systems, Targeted plant genome editing - gene editing, ZFN, TALEN and CRISPR, Whole-genome sequencing, Exome sequencing, Transcriptome sequencing, DNA-Protein Interactions (CHIP-Seq), Epigenomics and DNA methylation analysis, Metagenome analysis.

Suggested Readings:-

Allinger LN, *"Molecular Structure : Understanding Steric And Electronic Effects From Molecular Mechanics",* Springer,

Mount, D. (2004*), Bioinformatics: Sequence and Genome Analysis;* Cold Spring Harbor Laboratory Press, New York.

Pevzner, P.A. (2004), *Computational Molecular Biology*; Prentice Hall of India Ltd, New Delhi.

Phillips,F. C. "*An Introduction to Crystallography*" Cambridge

Robert Lanza, Robert Langer, Joseph Vacanti, (2013) *"Principles of Tissue Engineering"* (4th Edition).

Russell S.J., Peter Norvig, (2015) *"Artificial Intelligence-A Modern Approach"*, 3rd edition, Pearson

Scott R. P.W. (1995) *"Techniques and Practice of Chromatography",* Vol-70, CRC Press.

Sepe M.P. (1997) *"Thermal Analysis of Polymers"*, iSmithers Rapra Publishing.

Stroud R, *"Computational and Structural Approaches to Drug Discovery ligand- Protein"*, Royal Society of Chemistry, Acc. No. 100217

Young Min Kwon, Steven C. Ricke, (2011) *"High-Throughput Next Generation Sequencing: Methods and Applications".* Springer Protocols.

Outcomes:	➢ Students can be able to know the macromolecules structure and function through the crystallization techniques. ➢ Students will be able to dothe furfure research in tissue engineering to overcome health hazards

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PAPER V: 505999 DISSERTATION AND VIVA-VOCE

Program: M.Phil.,	Semester: II (2022 Onwards) Credits-8
Course Title and Code: Dissertation Subject Code: 50599	Class Time: As per Time Table
Name of the Course Teacher	Prof. J. Jeyakanthan
Mobile: +91 - 97898 09245	E-mail: jjeyakanthan@alagappauniversity.ac.in
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Mobile: +91 - 94448 35869	E-mail: vidhyavathirm@alagappauniversity.ac.in
Name of the Course Teacher	Dr. J. Joseph Sahayarayan
Mobile: +91 - 90475 64087	E-mail: josephj@alagappauniversity.ac.in
Name of the Course Teacher	Dr. P. Boomi
Mobile: +91 -9486031423	E-mail: boomip@alagappauniversity.ac.inm

Major Research Areas

- Small and Macro molecule X-ray Crystallography.
- 3D Quantitative Structure - Activity Relationship (3D-QSAR).
- Human Molecular Genetics.
- Pharmacogenomics.
- Cheminformatics.
- Quantum Pharmacology.
- Computer Aided Drug Designing (CADD).
- Structural Bioinformatics
- Data mining, Data warehousing and Networking.
- Plant tissue Culture, Genetic Transformation, Plant Molecular Biology, Virology and Plant Pathology.
- Molecular Oncology, Pharmacology and Environmental Toxicology.

Course Brief:

The study of M.Phil course in Bioinformatics includes a six months project work in the thrust areas of specialization which is broadly classified into six categories keeping in mind the number of faculties present. First, is the Structural Biology and Bio - Computing where Molecular Biology concepts such as Protein Cloning, Expression, Purification and Crystallization are performed to work on the isolation of the desired protein where the structural and functional characteristics that are yet to be explored. Hence, through X-ray Crystallography one can deduce the same and collect the insight details. Based on the inputs from the X-ray crustallographic studies the computer aided drug designing techniques such as screening, molecular dynamics simulation, quantum based approaches, structure based drug design, QSAR etc (Drug Discovery and Design, CADD & Structural Bioinformatics) are performed to identify suitable leads from commercial/natural sources for a disease – associated targets. Either way, leads identified by targeting the molecular fingerprints of an

individual known as Personalized medicine (Pharmacogenomics & CADD) as this sought to be the most preferred, selected and specific approaches by the Pharma related Industries to further validate the compounds with the aid of assay to estimate its inhibitory potential against that target conferring to life-threatening diseases such as cancer, TB, Diabetes, HIV, Inference of Vitamin D – Deficiency on population through genetic studies, Implications of *Vibrio* species to the aquaculture residential species by the application of phage therapy. Additionally, these collected inputs such as the availability of different targets in association in many pathways (cross-talk), established compounds based on experimental evidences either commercially or from natural sources (Isolation from plants that is claimed to have therapeutic significance) is well collected, documented and maintained in the form of databases and also the information that are collected from several sources are also included. Thus, the scholars can frame their thesis based on these areas mentioned above along with updated working of methodologies within the stipulated period of time.

Reference/Text Books:

As per the area of study taken

Course Objectives: To make the students:

i. To strengthen teaching and research environment as a bridge course for scholars to provide the forefront of guidance in the field of Structural Biology, Computational biology and Pharmacogenomics.

ii. To identify and perform Cloning, Expression, Purification and Crystallization techniques in order to solve crucial putative drug targets using X-ray Crystallography

iii. To develop a healthy and proficient Structural Bioinformatics knowledgebase that is intended to provide with novel information of several targets and molecular signaling pathways which will further increase the innovative solutions from the growing scientific research community.

iv. To produce a research student to gain the good all-round knowledge of a specialization area with expert skills and present a part of original research for a higher degree.

Course Outcomes: The student shall be able to:

i. To comprehend the scope and concepts of Structural Biology, CADD, Structural Pharmacogenomics and Structural Bioinformatics that will provide a profound impact on scientific research.

ii. To build libraries of therapeutic interests for screening purposes after the target of interest has been identified (structural and functional aspects) thereon to propose a lead molecule with modifications that could enrich the drug-likeness for human use which tend to be specific based on molecular fingerprints of human.

iii. Key information for one's research purposes can be obtained from the knowledgebase that is built using structured programming languages.

iv. To understand and review the relative effectiveness among the different methods and techniques in Structural biology, Drug discovery and Pharmacogenomics.

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