ALAGAPPA UNIVERSITY

DST-FIST LEVEL I SCHEME (2018-*)

DEPARTMENT OF BIOINFORMATICS

1. **File No:** SR/FST/LSI-667/2016 (C) dated 25.10.2018
2. **Amount Sanctioned:** 40.12 Lakhs –Level I

Duration-2018-* DST-FIST Project Co-Ordinator	**Period**
Dr. J. Jeyakanthan, Senior Professor & Head Department of Bioinformatics	**2018-***

3. **Brief Report:**

DBI has received numerous grants from DBT - BIC & NNP, DST-FIST Level-I, DST-PURSE and UGC-Innovative Schemes. Additionally, DBI have been supported for the research activities by various National (UGC, DBT, DST, ICMR, CSIR), State (TNSCST) and University start-up grant (AURF). Moreover, the faculty members are expecting to attract more than 2510.99 lakhs through research projects. We have also been collaborating with other reputed Institutions and Inter-Departmental projects were carried out that will prove to have a beneficiary outcome for the society. The novel research findings emerged from the coordination of the faculty members and scholars are reflected more than 700 research publications in highly reputed journals with h-index of 42. Since 2018, 22 Research Scholars have successfully completed and was awarded Ph.D degree and currently 33 Ph.D students are pursuing. (**More Details:** http://www.bioinfoau.org/)

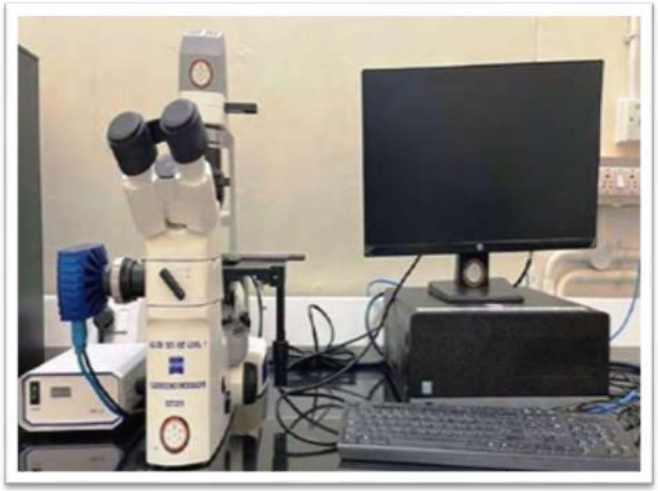
4. Infrastructure Facilities

ELISA reader and washer
(29th May, 2019)

Biosafety Cabinet
(09th June, 2019)

CO2 Incubator
(12th June, 2019)

Gel documentation system
(12th October, 2019)



Fluorescence microscope
(09th October 2019)

5. DST-FIST Level I Scheme Research Outcomes

S. No	Title of the Paper	Authors	Journal (Issue, Period, ISSN, page, etc.)	Impact factor	Natl.(N)/ Intl.(I)
1.	Investigation of translation initiation factor through protein–protein interactions And molecular dynamics approaches.	Jayaprakash, P., Biswal, J., Pandian, C. J., Kingsley, J., & **Jeyakanthan, J.**	*Molecular Simulation*, 2023 49:11, 1104-1116	**2.346**	**(I)**
2.	Combination of bendamustine-azacitidine against Syk target of breast cancer: an in silico study	Muthumanickam, S., Ramachandran, B., Boomi, P., **Jeyakanthan, J.,** Prabu, H. G., Jegatheswaran, S., & Premkumar, K.	*Journal of Biomolecular Structure and Dynamics, 2023 1-13.*	**5.235**	**(I)**
3.	Biochemical, Genotoxic and Histological Implications of Polypropylene Microplastics on Freshwater Fish *Oreochromis mossambicus*: An Aquatic Eco-Toxicological Assessment.	Jeyavani, J., Sibiya, A., Stalin, T., Vigneshkumar, G., Al-Ghanim, K. A., Riaz, M. N., Govindarajan, M., & Vaseeharan, B	*Toxics*, 2023 *11*(3), 282.	**4.48**	**(I)**
4.	Purification, crystallization and X-ray diffraction analysis of succinyl-diaminopimelate desuccinylase from Wolbachia endosymbiont of Brugia malayi.	Sruthi, S., Saritha, P., Yen- Chieh, H., Amala, M., **Jeyakanthan, J.,** Chen, CJ.	*Journal of the Chinese Chemical Society*, 2023 70, 5, 2192-6549, 1228-1236	**1.74**	**(I)**
5.	Computational exploration of molecular flexibility and interaction of meropenem analogs with the active site of oxacillinase-23 in *Acinetobacter baumannii*.	Ramachandran, B., Muthupandian, S., **Jeyaraman, J.,** & Lopes, B. S.	*Frontiers in chemistry*, 2023, *11*, 1090630.	**5.545**	**(I)**
6.	An integrated bioinformatics approach to identify candidate biomarkers and the evaluation of drugs for pheochromocytoma.	Javali, P. S., **Jeyakanthan, J.,** Chen, C. J., & Arumugam, M.	*bioRxiv, 2023-02.*	**Peer review**	
7.	Functional Characterization, Mechanism, and Mode of Action of Putative Streptomycin Adenylyltransferase from Serratia marcescens.	Prabhu, D., Rajamanikandan, S., Amala, M., Saritha, P., **Jeyakanthan, J.,** & Ramasamy, P.	*Antibiotics*, 2022,*11(12),1722.*	**4.94**	**(I)**
8.	Dietary consumption of polypropylene microplastics alter the biochemical parameters and histological response in freshwater benthic mollusc Pomacea	Jeyavani, J., Sibiya, A., Gopi, N., Mahboob, S., Riaz, M. N., & Vaseeharan, B.	*Environmental research*, 2022,212(Pt C), 113370**.**	**8.431**	

	paludosa.				
9.	Post-acute sequelae of SARS-CoV-2 Delta variant infection: A report of three cases in a single family.	Jeyaraj Pandian, C., **Jeyaraman, J.,** & SM, R.	*Indian Journal of Biochemistry and Biophysics (IJBB),* 2022, *59(7),777-785.*	**1.918**	**(N)**
10.	Functional significance of mouse seminal vesicle sulfhydryl oxidase on sperm capacitation in vitro.	Balu, R., Ramachandran, S. S., Mathimaran, A., **Jeyaraman, J.,** & Paramasivam, S. G.	*Molecular human reproduction,* 2022, *29*(9), gaac025.	**4.518**	**(I)**
11.	Designing of potent anti-diabetic molecules by targeting SIK2 using computational approaches.	Jayaprakash, P., Biswal, J., Rangaswamy, R., & **Jeyakanthan, J.**	*Molecular Diversity (2022): 1-21.*	**2.943**	**(I)**
12.	Deciphering the conformational transitions of LIMK2 active and inactive states to ponder specific druggable states through microsecond scale molecular dynamics simulation.	Nagarajan, H., Samdani, A., Umashankar, V., & **Jeyakanthan, J.**	*Journal of computer-aided molecular design*, 2022, *36*(6), 459–482.	**3.686**	**(I)**
13.	Structural Modeling of Drosophila Melanogaster Gut Cytochrome P450s and Docking Comparison of Fruit Fly Gut and Human Cytochrome P450s.	Nirusimhan, V., Andrew Gideon, D., Parashar, A., Jeyachandran, S., **Jeyaraman, J.,** Subbaraj, G., & Kulanthaivel, L.	*Current drug metabolism*, 2022, *23*(4), 299–316.	**3.731**	**(I)**
14.	Quercetin-induced apoptosis in HepG2 cells and identification of quercetin derivatives as potent inhibitors for Caspase-3 through computational methods	Ramachandran, B., Jeyarajpandian, C., Jeyaseelan, J. M., Prabhu, D., Rajamanikandan, S., Boomi, P., ... & **Jeyakanthan, J.**	*Structural Chemistry*, 2022,33(6), 1867-1893.	**1.795**	**(I)**
15.	Computational identification of potential lead molecules targeting rho receptor of *Neisseria gonorrhoeae*	Rajamanikandan, S., Soundarya, S., Paramasivam, A., Prabhu, D., **Jeyakanthan, J.,** & Ramasamy, V	*Journal of Biomolecular Structure and Dynamics*, 2022 *40(14), 6415-6425.*	**5.235**	**(I)**
16.	Characterization of putative transcriptional regulator (PH0140) and its distal homologue.	Mariadasse, R., Rajmichael, R., Dwivedy, A., Amala, M., Ahmad, M., Mutharasappan, N., Biswal, B. K., & **Jeyakanthan, J.**	*Cellular signalling, 84,2021, 110031.*	**4.315**	**(I)**
17.	Small peptide inhibitor from the sequence of RUNX3 disrupts PAK1–RUNX3 interaction and abrogates its phosphorylation-dependent oncogenic function	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.	*Oncogene, 40(34), 2021, 5327–5341.*	**9.867**	**(I)**

18.	Modelling studies reveal the importance of the C-terminal inter motif loop of NSP1 as a promising target site for drug discovery and screening of potential phytochemicals to combat SARS-CoV-2.	Prabhu, D., Rajamanikandan, S., Sureshan, M., **Jeyakanthan, J.,** & Saraboji, K.	*Journal of Molecular Graphics and Modelling, ,2021 106, 107920.*	**2.079**	**(I)**
19.	Interpretations on the interaction between protein tyrosine phosphatase and E7 oncoproteins of high and low-risk HPV: A computational perception.	Aarthy, M., & **Singh, S. K.**	*ACS omega, ,2021 6(25), 16472-16487.*	**3.51**	**(I)**
20.	E-pharmacophore based screening to identify potential HIV-1 gp120 and CD4 interaction blockers for wild and mutant types.	Chandra, I., S. V. Prabhu, C. Nayak, and **S. K. Singh.**	*SAR and QSAR in Environmental Research, ,2021, 32(5):353-77, 1062-936X*	**3.00**	**(I)**
21.	Spectroscopic and molecular docking studies for the binding and interaction aspects of curcumin-cysteine conjugate and rosmarinicacid with human telomeric G-quadruplex DNA.	Dwivedi, A., Kumari, A., Aarthy, M., **Singh, S.K.,** Ojha,M., Jha,S., Jha, S.K. and Jha, N.S	*International journal of biological macromolecules, 2021, 182, 1463-1472.*	**6.95**	**(I)**
22.	Structure Based Virtual Screening, Molecular Docking, and Molecular Dynamics Simulation of VEGF inhibitors for the clinical treatment of Ovarian Cancer	Mukherjee, S., Abdalla, M., Yadav, M., Madhavi, M., Bhrdwaj, A., Khandelwal, R., ... & **Singh, S.K.**	*Journal of Molecular Modeling,2022 28(4),*1-21	**2.17**	**(I)**
23.	α-bisabolol β-D-fucopyranoside inhibits β-amyloid (Aβ) 25-35 induced oxidative stress in Neuro-2a cells via antioxidant approaches(**2022**)	Jeyakumar, M., Sathya, S., Gandhi, S., Tharra, P., Aarthy, M., Balan, D. J., ... **Singh, S.K.,** & Devi, K. P	*Process Biochemistry, 2022, 121, pp.*493-503	**4.88**	**(I)**
24.	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	Yadav, M., Abdalla, M., Madhavi, M., Chopra, I., Bhrdwaj, A., Soni, L., Shaheen, U., Prajapati, L., Sharma, M., Sikarwar, M.S., Albogami, S., Hussain, T., Nayarisseri, A., **Singh, S.K.**	*Molecular Simulation,2022, pp.*1-21	**2.34**	**(I)**

25.	Structure-Based Virtual Screening, Molecular Docking, Molecular Dynamics Simulation of EGFR for the Clinical Treatment of Glioblastoma	Bhrdwaj, A., Abdalla, M., Pande, A., Madhavi, M., Chopra, I., Soni, L., ... & Singh, S. K. & **Singh, S.K.**	*Applied Biochemistry and Biotechnology, 2023,* 1-26	**3.09**	**(I)**
26.	Promoter–motif extraction from co-regulated genes and their relevance to co-expression using E. coli as a model	Nayarisseri, A., Bhrdwaj, A., Khan, A., Sharma, K., Shaheen, U., Selvaraj, C.,Khan, M. A.,Abhirami, R., Pravin, M. A., Shri, G. R. & **Singh, S.K.,**	*Briefings in Functional Genomics,2023,* elac043	**4.84**	**(I)**
27.	Mechanistic insights on nsSNPs on binding site of renin and cytochrome P450 proteins: A computational perceptual study for pharmacogenomics evaluation.	Loganathan, L., Kuriakose, B. B., Mushfiq, S., & Muthusamy, K.	*Journal of Cellular Biochemistry,* 122(10), 2021, 1460-1474.	**4.429**	**(I)**
28.	Targeting renin receptor for the inhibition of renin angiotensin aldosterone system: An alternative approach through in silico drug discovery.	Loganathan, L., Kuriakose, B. B., Sampayan, E. L., & Muthusamy, K.	*Computational and Theoretical Chemistry,* 2020, 1208, 113541.	**1.926**	**(I)**
29.	Modelling studies reveal the importance of the C-terminal inter motifloop of NSP1 as a promising target sitefor drug discovery phytochemicals to combat SARS-CoV-2.	Prabhu D, Rajamanikandan S, Sureshan M, **Jeyakanthan J**, Saraboji K.	*Molecular Graphics and Modelling, 2021,Jul 1;106:107920 ISSN: 1093-3263*	**2.079**	**(I)**
30.	*In silico* Screening of Natural Phytocompounds Towards Identification of Potential Lead Compounds to Treat COVID-19	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.	*Frontiers in molecular biosciences,* 2021, 8, 637122.	**6.113**	**(I)**
31.	*In-silico* protein-ligand docking studies against the estrogen protein of breast cancer using pharmacophore based virtual screening approaches	Sahayarayan, J. J., Rajan, K. S., **Vidhyavathi, R.,** Nachiappan, M., Prabhu, D., Alfarraj, S. Arokiyaraj & Daniel, A. N.	*Saudi journal of biological sciences, 2021, 28(1), 400–407.*	**4.05**	**(I)**

32.	*In Silico* mechanistic intervention of medicinal plants derived inhibitors against ABLkinase targeting cervical cancer: A novel approach.	Soundarya, S., **Vidhyavathi, R.M.**, Joseph Sahayarayan, J., Langeswaran, K., & Biruntha,M.	*Biomedical Research,2021 32(1). 0970-938X.*	-	**(I)**
33.	Computational identification of potential lead molecules targeting rho receptor of *Neisseria gonorrhoeae*	Rajamanikandan, S., Soundarya, S., Paramasivam, A., Prabhu, D., **Jeyakanthan, J.,** & Ramasamy, V	*Journal of Biomolecular Structure and Dynamics,2022, 40(14),6415-6425.*	**3.31**	**(I)**
34.	In-silico protein-ligand docking studies against the estrogen protein of Breast cancer using pharmacophore based virtual screening approaches	**Sahayarayan, J. J.,** Rajan, K. S., Vidhyavathi, R., Nachiappan, M., Prabhu, D., Alfarraj, S., Arokiyaraj, S., & Daniel, A. N.	*Saudi journal of biological sciences, 2021, 28(1), 400–407.*	**4.052**	**(I)**
36.	Structural Modeling of Drosophila melanogaster Gut Cytochrome P450s and Docking Comparison of Fruit Fly Gut and Human Cytochrome P450s	Nirusimhan, V., Andrew Gideon, D., Parashar, A., Jeyachandran, S., **Jeyaraman, J.,** Subbaraj, G., & Kulanthaivel, L.	*Current drug metabolism, 23*(4), 299–316. (2022)	**3.731**	**(I)**
37.	In silico mechanistic intervention of medicinal plants derived inhibitors against ABL Kinase targeting Cervical Cancer - A Novel Approach.	Soundarya, S., Vidhyavathi, R.M., **LANGESWARAN,** K., & Brindha, M.	*Biomedical Research,2021 32(1): 1-5.*	-	**(I)**
38.	Spectroscopic, Solvent Effect, Molecular Docking and Molecular Dynamics Investigations on Phytocompounds from *Elettaria cardamomum* against Covid-19.	Sangeetha, R., Premkumar, R., Maithili, S. S., Kirubhanand, C., Gowtham Kumar, S., Sangavi, P., & **Langeswaran, K.** .	*Polycyclic Aromatic Compounds, 2021,* 43(5), 4184-4202.	**2.195**	**(I)**
39.	Combination of bendamustine-azacitidine against Syk target of breast cancer: an in silico study	Muthumanickam, S., Ramachandran, B., **Boomi, P.,** Jeyakanthan, J., Prabu, H. G., Jegatheswaran, S., & Premkumar, K.	*Journal of Biomolecular Structure and Dynamics,2023, 1-13.*	**5.235**	**(I)**

40.	Quercetin-induced apoptosis in HepG2 cells and identification of quercetin derivatives as potent inhibitors for Caspase-3 through computational methods	Ramachandran, B., Jeyarajpandian, C., Mercy, J., Jeyaseelan, J., Prabhu, D., Rajamanikandan, S., Boomi, P. Venkateswari, R., & Jeyakanthan, J.	*Structural Chemistry,2022,* 33(6), 1867-1893.	**1.795**	**(I)**
41.	Biochemical evaluation and molecular docking studies on encapsulated astaxanthin for the growth inhibition of Mycobacterium tuberculosis	Vasudevan, S., Venkatraman, A., Yahoob, S. A. M., Jojula, M., Sundaram, R., & **Boomi, P.**	*Journal of Applied Biology and Biotechnology*,2021, 9(1), 31-39.	-	**(I)**
42.	*In silico* Screening of Natural Phytocompounds Towards Identification of Potential Lead Compounds to Treat COVID-19	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.,	*Frontiers in molecular biosciences, 2021, 8, 637122.*	**5.246**	**(I)**
43.	Characterization of putative transcriptional regulator (PH0140) and its distal homologue.	Richard M, Raji R, Abhisek D, Amala M, Ahmad M, Nachiappan M, Bichitra K. Biswal and **J Jeyakanthan.**	*Cellular Signalling, 2021 Aug 1;84:110031, ISSN: 0898-6568*	**4.315**	**(I)**
44.	Small peptide inhibitor from the sequence of RUNX3 disrupts PAK1-RUNX3 interaction and abrogates its phosphorylation-dependent oncogenic function	Rahul K, Aruna Kumar C, Jayashree Biswal, Vignesh R, Jaishree P, Akkanapally V, B Vaishnavi, DJ Leena, **Jeyakanthan J,** Kumaresan G, Gopala Krishna A, Ganesh V, Suresh K Rayala	*Oncogene. 2021 Jul 12:1-15.*	**9.867**	**(I)**
45.	Modelling studies Reveal the importance of the C- terminal inter motif loop of NSP1 as a promising target site for drug discovery phytochemicals to combat SARS-CoV-2.	Prabhu D, Rajamanikandan S, Sureshan M, **Jeyakanthan J,** Saraboji K.	*Molecular Graphics and Modelling, 2021 Jul 1;106:107920, ISSN: 1093-3263*	**2.079**	**(I)**
46.	Water Mapping and Scoring approaches to predict the role of Hydration sites in Binding Affinity of PAK1 inhibitors.	Jayashree Biswal, Prajisha J, Suresh Kumar Rayala, Ganesh V, Raghu R, Saritha P and **Jeyakanthan J.**	*Combinatorial Chemistry & High Throughput Screening, 2020; 23: 0-0. ISSN: 1386-2073*	**1.195**	**(I)**

47.	Discovery of potent Camkkl kinase inhibitors through e-pharmacophore and molecular screening approaches.	Prajisha J, Biswal J, **Jeyakanthan J.**	*Journal of Biomolecular Structure and Dynamics, 2020, Nov 4:1-7. ISSN:0739-1102*	**3.310**	**(I)**
48.	Molecular evolution, binding site interpretation and functional divergence of aspartate semi-aldehyde dehydrogenase.	M Amala, M Richard, P Saritha, D Prabhu, M Veerapandiyan, K Surekha, **J Jeyakanthan.**	*Journal of Biomolecular Structure and Dynamics, 2020, Nov 16:1-9. ISSN:0739-1102*	**3.310**	**(I)**
49.	Evolutionary Significance and Functional Characterization of Streptomycin adenylyltransferase from *Serratia Marcescens*	Prabhu D, Rajamanikandan S, Saritha P, **Jeyakanthan J**.	*Journal of Biomolecular Structure and Dynamics, 2020 Oct 12;38(15):4418-31. ISSN:0739-1102*	**3.310**	**(I)**
50.	Structural and functional insights of STAT2-NS5 interaction for the identification of NS5 antagonist - An approach for restoring interferon signaling.	Choubey SK, Nachiappan M, Richard M, Chitra JP, **Jeyakanthan J**	*Computational Biology and Chemistry, 2020 Oct 1;88:107332. ISSN:1476-9271*	**1.85**	**(I)**
51.	Molecular Docking, Dynamics and Free energy analyses of Acinetobacter baumannii OXA class enzymes with Carbapenems investigating their hydrolytic mechanisms.	Balajee R, **Jeyakanthan J**& Lopez BS.	*Journal of Medical Microbiology, 2020 Aug 1;69(8):1062-78. ISSN:0022-2615*	**2.156**	**(I)**
52.	In silico functional annotation and characterization of hypothetical proteins from Serratia marcescens FGI94	D. Prabhu, S. Rajamanikandan, S. Baby Anusha, M. Sushma Chowdary, M. Veerapandiyan & **J. Jeyakanthan**.	*Biology Bulletin,2020 Jul;47(4):319- 31. ISSN:1062-3590*	**0.45**	**(I)**
53.	Structural and functional analysis of Glutaminyl-tRNA synthetase (TtGlnRS) from Thermus thermophilus HB8 and its complexes	Surekha K, Prabhu D, Nachiappan M, Choubey SK, Prajisha J , Biswal J, **Jeyakanthan J**.	*Journal of Biomolecular Structure and Dynamics, 2021 Jun 13;39(9):3144 57. ISSN:0739-1102*	**3.310**	**(I)**
54.	IMRPS: Inserted and Modified Residues in Protein Structures: A Database.	Santhosh R, Bankoti N, Gurudarshan M, **Jeyakanthan J** & Sekar K.	*Journal of Applied Crystallography, 2020 Apr 1;53(2):569-73. ISSN:0021-8898*	**3.161**	**(I)**

55.	Conformational changes in Glutaminyl-tRNA synthetases upon binding of the substrates and analogs using molecular dockingand molecular dynamics approaches	Nachiappan M, Jain V, Sharma A, Yogavel M & **Jeyakanthan J**.	*Journal of Biomolecular Structure and Dynamics, 2019 May 30 38(6):1575- 1589. ISSN:0739-1102*	**3.310**	**(I)**
56.	Conformational insights into the inhibitory mechanism of phyto-compounds against SRC Kinase familymembers implicated in psoriasis.	Sudharsana S, MadhanaPriya N, Prabhu D, **Jeyakanthan J** & Mohanapriya Arumugam.	Journal of Biomolecular Structure and Dynamics, 2020 Mar 23;38(5):1398-414. ISSN:0739-1102	**3.310**	**(I)**
57.	MRPC: MissingRegions in Polypeptide Chains - AKnowledgebase.	Santhosh R, Bankoti N, Malgonnavar PA, Michael D, **Jeyakanthan J** & Sekar K.	*Journal of Applied Crystallography,2019 Dec 1;52 (6):1422-6. ISSN:1600-5767*	**3.161**	**(I)**
58.	Insights into Exogenous Tryptophan- Mediated Allosteric communication and Helical Transition of TRP Protein for Transcription Regulation.	Richard M, Choubey SK& **Jeyakanthan J**.	*Journal of chemical information and modeling, 2019 Nov 19;60 (1):175-91. ISSN:1549-9596*	**3.966**	**(I)**
59.	Identification of Pak1 inhibitors Using water thermodynamic analysis.	Biswal J, Prajisha J, Rayala SK, Ganesh V, Saritha P,Raghu R & Jeyakanthan J.	*Journal of Biomolecular Structure and Dynamics,2019 Feb 17:1-19, ISSN:0739-1102*	**3.310**	**(I)**
60.	Exploration of N5-CAIR Mutase Novel Inhibitors from Pyrococcus horikoshii OT3: A Computational Study.	Ravi GR, Biswal J, Kanagarajan S, **Jeyakanthan J**.	*Journal of Computational Biology, 2019 May 1;26(5):457-72. ISSN:1066-5277*	**1.479**	**(I)**
61.	Identification of Anti-filarial leads against Aspartate semialdehyde Dehydrogenase of *Wolbachia* endosymbiont of *Brugia malayi*: Combined Molecular Docking and Molecular Dynamics Approaches.	Amala. M, Rajamanikandan. S, Prabhu. D, Surekha, K &**J Jeyakanthan.**	Journal of Biomolecular Structure and Dynamics, 2019 Jan 22;37(2):394-410. ISSN:0739-1102	**3.310**	**(I)**
62.	Structural and functional analysis of Glutaminyl-tRNA synthetase (TtGlnRS) from Thermus thermophilus HB8 and its complexes.	Nachiappan M, Jain V, Sharma A, Yogavel M & **Jeyakanthan J.**	*International journal of biological macromolecules, 2018 Dec 1;120:1379-86. ISSN:0141-8130*	**3.909**	**(I)**
63.	Molecular dynamicsand Quantum chemistry based Approaches to identify isoform	Sanjay K Choubey & **J Jeyakanthan**	*Journal of Receptors and Signal Transduction, 2018 May 4;38(3):266-78. ISSN:1079-9893*	**1.775**	**(I)**

	selective HDAC2 inhibitor – A novel target to prevent Alzheimer's disease.				
64.	E-pharmacophore based screening to identify potential HIV-1 gp120 and CD4 interaction blockers for wild and mutant types.	Chandra, I., Prabhu, S.V., Nayak, C. and **Singh, S.K***	*SAR and QSAR in Environmental Research, 2021 May 4;32(5):353-77 ISSN:1062-936X*	**3.00**	**(I)**
65.	Interpretations on the Interaction between Protein Tyrosine Phosphatase and E7 Oncoproteins of High and Low-Risk HPV: A Computational Perception.	Aarthy, M. and **Singh, S.K***	*ACS Omega 2021 Jun 17 6(25) 16472–16487 ISSN:2470-1343*	**3.51**	**(I)**
66.	Spectroscopic and molecular docking studies for the binding and interaction aspects of curcumin- cysteine conjugate and rosmarinic acid with human telomeric G-quadruplex DNA.	Dwivedi, A., Kumari, A., Aarthy, M., **Singh, S.K**., Ojha, M., Jha, S., Jha, S.K. and Jha, N.S	*International Journal of Biological Macromolecules,2021 Jul 1;182:1463-72. ISSN:0141-8130*	**6.95**	**(I)**
67.	A Multi-Target Drug Designing for BTK, MMP9, Proteasome And TAK1 for the clinical treatment of Mantle Cell Lymphoma.	Qureshi, S., Khandelwal , R., Madhavi, M., Khurana, N., Gupta, N., Choudhary, S.K., Suresh, R.A., Hazarika, L., Srija, C.D., Sharma, K., Hindala, M.R., Hussain, T., Nayarisseri, A., **Singh, S.K*.**	*Current Topics in Medicinal Chemistry,2021 Mar 1;21(9):790-818. ISSN:1568-0266*	**3.29**	**(I)**
68.	Artificial Intelligence, Big data and Machine Learning approaches in Precision Medicine & Drug Discovery.	Nayarisseri, A., Khandelwal, R., Tanwar, P.,Madhavi, M., Sharma, D., Thakur, G., Speck-Planche,A., **Singh, S.K***	*Current drug targets 2021 Apr 1;22(6):631-55 ISSN:1389-4501*	**3.46**	**(I)**
69.	Atom-based 3D-QSAR, molecular docking, DFT, and simulation studies of acylhydrazone, hydrazine, and diazene derivatives as IN-LEDGF/p75 inhibitors.	Panwar, U. and **Singh, S.K***	*Structural Chemistry 2021 Feb;32(1):337-52 ISSN:1040-0400*	**1.88**	**(I)**

70.	Identification and characterization of Lipopeptide biosurfactant producing Micro bacterium *sp* isolated from brackish river water.	Nayarisseri, A., Khandelwal, R. and **Singh,S.K***	*Current Topics in Medicinal Chemistry 2020 Sep 1;20(24):2221-34, ISSN:1568-0266*	**3.29**	**(I)**
71.	Computational analysis identifiesdruggable mutationsin human rBAT mediated Cystinuria.	Pandey, B., Aarthy, M., Sharma, M., **Singh, S.K.** and Kumar, V	*Journal of Biomolecular Structure and Dynamics 2020 Jun 29:1-0 ISSN:0739-1102*	**3.54**	**(I)**
72.	Structural Insights into the MolecularDesign of ROS1inhibitor for the treatment of Non- Small Cell Lung Cancer (NSCLC).	Adhikary, R., Khandelwal, R., Madhavi, M., Khurana, N., Sharma, K., Hussain T., Nayarisseri, A. and **Singh, S.K***	*Current computer aided drug designing 2021 Jun 1; 17(3):387-401. ISSN:0739-1102*	**1.60**	**(I)**
73.	Investigating into the molecular interactionsof flavonoids targeting NS2B-NS3 protease from ZIKA virus through *in-silico* Approaches	Yadav, R., Selvaraj, C., Aarthy, M., Kumar, P., Kumar, A., **Singh, S.K**. and Giri, R	*Journal of Biomolecular Structure and Dynamics 2021 Jan 2;39(1):272-84ISSN:0739-1102*	**3.54**	**(I)**
74.	Targeting the NTPase site of Zika virus NS3 helicase for inhibitor discovery.	Kumar, D., Aarthy, M., Kumar, P., **Singh, S.K,** Uversky, V.N. and Giri, R	*Journal of Biomolecular Structure and Dynamics 2020 Nov 1;38(16):4827-37, ISSN:0739-1102*	**3.54**	**(I)**
75.	*In silico* insights on Disialoganglioside GD2: A Potential forPediatric Neuroblastoma.	Limaye, A., Sweta, J., Mudgal, U., Mukherjee, S., Sharma, S., Hussain, T., Nayarisseri, A. and **Singh, S.K***	*Current topics in medicinal chemistry 2019 Nov 1;19(30):2766-81.ISSN:1568-0266*	**3.29**	**(I)**
76.	Identification of Dual negative allosteric modulators of Group I mGluR family: A shape based screening, ADME Prediction, Induced Fit Docking and Molecular Dynamics approach against Neurodegenerative Diseases.	Prabhu, S.V. and **Singh, S.K**	*Current topics in medicinal chemistry 2019 Nov 1;19(29):2687-707. ISSN:1568-0266*	**3.29**	**(I)**
77.	Current Computational Approaches for the Development of Anti-HIV Inhibitors: An Overview.	Panwar, U., Chandra, I., Selvaraj, C. and **Singh, S.K***	*Current pharmaceutical design 2019 Sep 1;25(31):3390-405. ISSN:1381-6128*	**3.11**	**(I)**

78.	*In silico* insights on IL-6: A Potential targetfor Multicentric Castleman Disease	Aher, A., Udhwani, T., Khandelwal, R., Limaye, A., Hussain, T., Nayarisseri, A. and **Singh, S.K***	*Current computer-aided drug design 2020 Oct 1;16(5):641-53 ISSN:1573-1102*	**0.93**	**(I)**
79.	Energetically optimized pharmacophore modeling to identify dual negative allosteric modulators against group I mGluRs in neurodegenerative diseases	Prabhu, S.V. and **Singh, S.K***	*Journal of Biomolecular Structure and Dynamics 2020 May 23; 38(8):2326-37. ISSN:0739-1102*	**3.54**	**(I)**
80.	A Computer-Aided Drug Designing for Pharmacological Inhibition of Mutant ALK for the Treatment of Non-small Cell Lung Cancer.	Sharda, S., Khandelwal, R., Abhikary, R., Sharma, D., Majhi, M., Hussain, T., Nayarisseri, A. and **Singh, S.K***	*Current topics in medicinal chemistry 2019 May 1;19(13):1129-44. ISSN:1568-0266*	**3.29**	**(I)**
81.	Identification of High affinity small molecules targetingGamma Secretase for the treatment ofAlzheimer's Disease	Ali, M.A., Vuree, S., Goud, H., Hussain, T., Nayarisseri, A. and **Singh, S.K***	*Current Topics in Medicinal Chemistry 2019 May 1;19(13):1173-87. ISSN:1568-0266*	**3.29**	**(I)**
82.	α-bisabolol β-D-fucopyranoside as a potential modulator ofβ-Amyloid peptideinduced neurotoxicity:an *in vitro* & *in silico* study	Jeyakumar, M., Sathya, S., Gandhi, S., Tharra, P., Suryanarayanan, V., **Singh, S.K.,** Baire,B. and Devi, K.P	*Bioorganic Chemistry2019 Jul 1;88:102935ISSN:0045-2068*	**5.27**	**(I)**
83.	Functional Inhibition of VEGF and EGFR Suppressors in Cancer Treatment	Nayarisseri, A. and **Singh,S.K***	*Current Topics in Medicinal Chemistry 2019 Jan 1(3):178-9. ISSN:1568-0266*	**3.29**	**(I)**
84.	Identification of Potent VEGF Inhibitors for the Clinical Treatment of Glioblastoma, A Virtual Screening Approach.	Yadav, M,, Khandelwal, R., Mudgal, U., Srinitha, S., Khandekar, N., Nayarisseri, A., Vuree, S., **Singh, S.K***	*Asian Pacific Journal of Cancer Prevention 2019;20(9):2681-2692. ISSN:1513-7368*	**1.77**	**(I)**
85.	Identification of High-Affinity SmallMolecule TargetingIDH2 for the Clinical Treatment of Acute Myeloid Leukemia.	Sweta, J., Khandelwal, R., Srinitha, S., Pancholi, R., Adhikary, R., Ali, M.A., Nayarisseri, A., Vuree, S., **Singh, S.K***	*Asian Pacific Journal of Cancer Prevention 2019;20(8):2287-229. ISSN:1513-7368*	**1.77**	**(I)**
86.	An *in silico* approach to identify highaffinity small moleculetargeting m-TORinhibitors for the clinical treatment of	Patidar, K., Panwar, U., Nayarisseri, A., **Singh, S.K***	*sian Pacific Journal of Cancer Prevention 2019;20(4):1229-1241. ISSN:1513-7368*	**1.77**	**(I)**

	Breast Cancer.				
87.	Identification of novel pancreatic lipase Inhibitors using structure based virtual screening, docking and simulations studies.	Panwar, U. and **Singh, S.K***	*Endocrine, metabolic & immune disorders drug targets 2019 Jun 1;19(4):449-57 ISSN:2212-3873*	**2.89**	**(I)**
88.	An *In silico* pharmacological approach towards the discovery of potent inhibitors to combatdrug resistance HIV-1 protease variants.	Nayak, C., Chandra, I. and **Singh, S.K***	*Journal of Cellular Biochemistry 2019 Jun; 120(6):9063-81, ISSN:0730-2312*	**4.42**	**(I)**
89.	Discovery of potent inhibitors for the inhibition of Dengue Envelope protein: An *In silico* Approach.	Aarthy, M. and **Singh, S.K***	*Current Topics in Medicinal Chemistry 2018 Jul 1;18 (18):1585-602. ISSN:1568-0266*	**3.29**	**(I)**
90.	Investigation of drug interaction potentials and binding modes on direct renin inhibitors.A computational modeling study	Lakshmanan Loganathan and **Karthikeyan Muthusamy***	*Letters in Drug Design and Discovery, 2019 Aug 1;16(8):919-38. ISSN:1570-1808*	**0.924**	**(I)**
91.	Structural insights on Vitamin D receptorand screening of new potent agonistmolecules: Structureand ligand-based approach	John Marshal Jayaraj, Everlyne Reteti, Chandrasekhar Kesavan,and **Karthikeyan Muthusamy***.	*Journal of Biomolecular Structure and Dynamics, 2020 Jun 8:1-2. ISSN:0739-1102*	**3.310**	**(I)**
92.	Mechanistic insightson nsSNPs on binding site of renin andcytochrome P450proteins: A computational perceptual study for pharmacogenomics evaluation	Lakshmanan Loganathan, Beena Briget Kuriakose, Sakeena Mushfiq, **Karthikeyan Muthusamy***.	*Journal of Cellular Biochemistry, 2021, doi:10.1002/jcb.30069 ISSN:0730-2312*	**4.429**	**(I)**
93.	In silico mechanistic intervention ofmedicinal plantsderived inhibitors against ABL kinase targeting cervical cancer: A novelapproach.	Soundarya S, **Vidhyavathi RM**, Joseph Sahayarayan J, Langeswaran K, Biruntha M	*Biomedical Research, 2021 Jan 1;32(1). ISSN 0970-938X.*	-	**(I)**
94.	Computational identification of potential lead molecules	Sundararaj Rajamanikandan, Soundarapandian Soundarya , Anandhi Paramasivam,	*Journal of Bimolecular Structure and Dynamics, 2021 Feb 5:1-1, ISSN:0739-1102*	**3.31**	**(I)**

	targeting rho receptor of Neisseria gonorrhoeae	Dhamodharan Prabhu, Jeyaraman Jeyakanthan & **Vidhyavathi Ramasamy**			
95.	Effect of different *Agrobacterium rhizogenes* strains forin-vitro hairy rootinduction, totalphenolic, flavonoids contents, antibacterial and antioxidant activity of(*Cucumis anguria* L.)	**Jesudass Joseph Sahayarayan**, Rajangam Udayakumar, Muthukrishnan Arun, Andy Ganapathi, Mona S. Alwahibi, NorahSalim Aldosari and Abubaker M.A. Morgan	*Saudi Journal of Biological Sciences, 2020 Nov 1; 27(11):2972-9. ISSN:1319-562X*	**2.802**	**(I)**
96.	Identification ofpotential drug target in malarial disease using molecular docking analysis	**Jesudass Joseph Sahayarayan**, Kulanthaivel Soundar Rajan, Mutharasappan Nachiappan, Dhamodharan Prabhu, Ravi Guru Raj Rao, Jeyaraman Jeyakanthan, Ahmed Hossam Mahmoud, Osama B. Mohammed and Abubaker M.A. Morgan	*Saudi Journal of Biological Sciences, 2020 Dec 1;27(12):3327-33, ISSN:1319-562X*	**2.802**	**(I)**
97.	*In-silico* protein-ligand docking studies against the estrogen protein of breast cancer using pharmacophore based virtual screening approaches	***Jesudass Joseph Sahayarayan,*** *Kulanthaivel Soundar Rajan, Ramasamy Vidhyavathi, Mutharasappan Nachiappan, Dhamodharan Prabhu, Saleh Alfarraj, Selvaraj Arokiyaraj and Amalorpavanaden Nicholas Daniel*	*Saudi Journal of Biological Sciences, 2021 Jan 1;28(1):400-7. ISSN:1319-562X*	**2.802**	**(I)**
98.	Screening of inhibitors as potential remedial against Ebolavirus infection: harmacophore-based approach.	S. Muthumanickam, **K.Langeswaran,** P. Sangavi, P. Boomi,	*Journal of Biomolecular Structure and Dynamics, 2021 Jan 22;39(2):395-408, ISSN: 0739-1102*	**3.310**	**(I)**
99.	Evaluation of Antibacterial and Anticancer Potentialof Polyaniline-Bimetal Nanocomposites Synthesized from Chemical Reduction Method	**P.Boomi**, H. Gurumallesh Prabu, G.Poorani, S. Palanisamy, S. Selvan, G. Ramanathan, S. Ravikumar,	*Journal of Cluster Science, 2019 May;30(3):715-26. ISSN: 1040-7278*	**3.061**	**(I)**
100.	Plant-Mediated Synthesis, Characterization and Bactericidal Potentialof Emerging Silver Nanoparticles Using Stem Extract of Phyllanthus pinnatus:A Recent Advance in Phytonanotechnology.	R.Balachandar, P.Gurumoorthy, N.Karmegam, H.Barabadi,R.Subbaiya, K.Anand, **P.Boomi**, M.saravanam	*Journal of Cluster Science, 2019 Nov;30(6):1481-8, ISSN: 1040-7278*	**3.061**	**(I)**

101.	Green Biosynthesis of gold nanoparticles Using Crotonsparsiflorus leavesextract and evaluationof UV protection, antibacterial and anticancer applications.	P. Boomi, G. Poorani, S. Selvam, S. Palanisamy, S. Jegatheeswaran, K. Anand, C. Balakumar, K. Premkumar, H. Gurumallesh Prabu,	*Applied Organometallic Chemistry. 2020 May;34(5):e5574. ISSN: 1099-0739*	**4.105**	**(I)**
102.	Phyto-engineered Gold Nanoparticles(AuNPs) with Potential Antibacterial, Antioxidant, and Wound HealingActivities under *invitro* and *invivo* Conditions	**P. Boomi**, R. Ganesan, G. Poorani, S. Jegatheeswaran, C. Balakumar, H. Gurumallesh Prabu, K. Anand, N. M. Prabhu, J. Jeyakanthan, M. Saravanan,	*International Journal of Nanomedicine. 2020;15:7553 ISSN: 1176-9114*	**6.400**	**(I)**
103.	*In silico* approach of naringin as potent phosphatase andtens in homolog (PTEN) protein agonist againstprostate cancer	S. Muthumanickam, T. Indhumathi, **P. Boomi**, R. Balajee, J. Jeyakanthan, K. Anand, S. Ravikumar, P. Kumar, A. Sudha, Z. Jiang,	*Journal of Biomolecular Structure and Dynamics. 2020Oct 8:1-0. ISSN: 0739-1102*	**3.310**	**(I)**
104.	*In Silico* Screening of Natural Phytoconstituents Towards Identification ofPotential Lead Compounds to Treat COVID-19	S. Muthumanickam, R. Balajee, **P. Boomi**, M. Nachiappan, R. Vidhyavathi, G. Poorani, S. Gowrishankar, W. Yao, M. Brintha, R. Subaskumar, C. Balakumar, M. F. Bayan, J. Jeyakanthan, H. Gurumallesh Prabu , K.E. Solomon.	*Frontiers in Molecular Biosciences. 2021;8. ISSN: 2296-889X*	**5.246**	**(I)**

RESEARCH PROJECT SANCTIONED AFTER THE DST-FIST LEVEL-I SCHEME (2018-*)

ON-GOING PROJECT					
S.NO	**PRINCIPAL INVESTIGATOR**	**PROJECT TITLE**	**PROJECT PERIOD**	**FUNDING AGENCY**	**TOTAL GRANT**
1.	**Dr. J. Jeyakanthan**	Design, Synthesis and in vitro anticancer activity of novel and potent p21 activated kinase 1 (Pak1) inhibitors	2018-21	DAE-BRNS	30.33
2.		Structural and functional insights of potential anti-malarial drug targets of G6PD and 6PGD from Plasmodium falciparum(3D7)	2020-24	DST INDO-TAIWAN	73.72
3.		Structural and functional characterization of phosphotransacetylase (PTA) and Acetate Kinase (ACKA) from Mycobacterium tuberculosis H3R7Rv using in silico and in vitro studies	2021-24	TANSCHE	29.805
4.	**Dr. Sanjeev Kumar Singh**	Identification of the vital targets of dengue and Chikungunya, an expanding threat to public health in Tamil Nadu: A potential drug discovery approach	2020-23	TANSCHE	20.10
5.	**Dr. M. Karthikeyan**	Molecular Insight and In Vitro Validation of novel lead molecules against SH3BP2 and KIT Protein	2023-26	ICMR	24.50
6.	**Dr. J. Joseph Sahayarayan**	Isolation, structural elucidation and biological properties of secondary metabolites from Mucuna pruriens and their In Silico studies	2018-20	AURF	1.00
7.	**Dr. P. Boomi**	Mechanistic Investigation Involved in the Development of Hybrid Self-Assembly Prodrug Targeting Breast Cancer.	2023-26	DST	27.90

RESEARCH SCHEMES AFTER DST-FIST LEVEL-I SCHEME (2018-*)

S.No	Research Schemes	Period	Amount in Lakhs
1.	DBT-National Network Project (NNP)	2023-2027	144. 56
2.	DBT–Bioinformatics and Computational Biology Center (BIC)	2022-2026	183.80
3.	MHRD – RUSA 2. 0 (2nd Installment)	2022-2023	58.00
4.	MHRD – RUSA 2. 0 (1st Installment)	2018-2020	64.54

PATENT FILED/PUBLISHED AFTER DST-FIST LEVEL-I SCHEME (2018-*)

S.No.	Patent App. No.	Inventor's Name	Title of the Patent	Patent filed on	Patent Published on
1.	202141046236	Dr. A. Sivaranjini, Dr. R. Subashkumar, Dr. P. Boomi, Dr. S. Santhosh Baboo, Dr. B. L. Shivakumar, A. Aswini, Dr. J. Jeyakanthan, Dr. H. Gurumallesh Prabu, Dr. P. Sagadevan	A Process For Extraction of Copper Oxide Nanoparticles Using Green Synthesis	11/1/2021	12/3/2021
2.	202241057508A	Dr. Dhamodharan Prabhu,Dr. Sundarraraj Rajamanikandan, Ramasamy palaniappan, Dr. Jeyaraman Jeyakanthan	Synergistic formulation for preventing antibiotic resistance effect of serratia marcescens	10/7/2022	14/10/2022