

Curriculum Vitae

Dr. M. Sivanandam

Assistant Professor (Sr. G)
Department of Physics
Centre for Research and Development (CFRD)
KPR Institute of Engineering and Technology
Arasur – 641 407
Coimbatore, Tamil Nadu, India



ORCID ID – 0000-0003-1123-8009

Web of Science Researcher ID - S-6266-2018

Carrier objective

A skilled and hardworking researcher with one year teaching experience and ten years of research experience. Looking, challenging and innovation position that will ameliorate and utilize my knowledge. I wish to collaborate with scientists from different disciplines in the field of computational and experimental biophysics to develops new ideas and solve critical problems.

Education and Research

Current Position - Assistant Professor (Sr. G) – Department of Physics, Centre for Research and Development (CFRD), KPR Institute of Engineering and Technology, Arasur – 641 407, Coimbatore, Tamil Nadu, India. From 2.9.2022 – On going

Postdoctoral Fellow – Laboratory of Biological Physics, Institute of Physics, Polish Academy of Sciences, Poland. (Adviser – Prof. Marek Cieplak). (3.4.2021 – 2.4.2022)

Research Title – The analysis of phase transition of some disordered proteins using coarse grained model.

Ph. D – Department of Physics, Periyar University, Salem – – Highly Commented – (Adviser – Prof. P. Kumaradhas). (26.2.2014 - 25.2.2019)

Research title - Investigation of binding mechanism of some synthetic and plant derived molecules with p300 histone acetyltransferase (HAT) enzyme via Molecular docking, Molecular dynamics simulation and Binding free energy studies.

Research Assistant - Bioinformatics Centre, Department of Physics, Manonmanium Sundaranar University, Tirunelveli – 627 012, Tamil Nadu, India. DBT, New Delhi, Government of India. (1.4.2013 – 30.11.2013)

M.Phil. – Department of Physics, Bharathiar University, Coimbatore - (2010-2012)

Thesis title - Study of Hydrogen bonding under vacuum and water environments- QM and MD studies.

Teaching Experience

I worked as a Guest Lecturer in the Department of Physics, Periyar University, Salem, Tamil Nadu, India (From 8.8.2019 to 20.3.2020 and 1.10.2020 to 28.2.2021).

Fellowships and Travel grant

Received Travel grant to attend the Bioexcel and PRACE joint course on “Hands-on Introduction to HPC for Life Scientists” organized by European Bioinformatics Institute, European Molecular Biology Laboratory, Cambridgeshire, UK.

Reviewer

1. Molecular Simulation – Taylor and Francis
2. Informatics in medicine unlocked – Elsevier.
3. Biomass Conversion and Biorefinery - Springer

Member

1. Indian Crystallographic Association (ICA)
2. Centre for Development of Advanced Computing (C-DAC), Pune.

Publications

1. Insights into Intermolecular interactions, electrostatic properties and the stability of C646 in the binding pocket of p300 Histone acetyltransferase enzyme: A combined molecular dynamics and charge density study. **M. Sivanandam**, K. Saravanan and P. Kumaradhas*, *J. Biomol. Struct. Dyn.*, 2017, 36(12), 3246-3264. doi: 10.1080/07391102.2017.1384761.
2. Investigation of activation mechanism and conformational stability of N-(4-chloro-3-trifluoromethyl-phenyl)-2-ethoxybenzamide and N-(4-chloro-3-trifluoromethyl-phenyl)-2-ethoxy-6-pentadecyl-benzamide in the active site of p300 histone acetyl transferase enzyme by molecular dynamics and binding free-energy studies. **M. Sivanandam**, S. Manjula and P. Kumaradhas*, *J. Biomol. Struct. Dyn.*, 2019, 37(15), 4006-4018. doi:10.1080/07391102.2018.1533497.
3. Investigation of Intermolecular interactions and Stability of Verubecestat in the active site of BACE1: Development of First model from QM/MM based Charge density and MD Analysis. K. Saravanan, **M. Sivanandam**, G. Hunday, L. Mathiyalagan and

- P. Kumaradhas*. *J. Biomol. Struct. Dyn.*, 2019, 37(9), 2339-2354. doi: 10.1080/07391102.2018.1479661.
4. Probing the “fingers” domain inhibition—a new allosteric site of Hepatitis C virus NS5B RdRp via Docking and Molecular Dynamics simulation. S. Manjula, **M. Sivanandam** and P. Kumaradhas*. *J. Biomol. Struct. Dyn.* 2019, 37(9), 2440-2456 doi: 10.1080/07391102.2018.1491419.
 5. Exploring the different environments effect of Piperine via combined Crystallographic, QM/MM and Molecular dynamics simulation study. Kandasamy Saravanan, **Magudeeswaran Sivanandam**, Govindasamy Hunday, Mysore S Pavan and Poomani Kumaradhas*. *J Mol Graph Model.* 2019, 92, 280-295. <https://doi.org/10.1016/j.jmkgm.2019.07.019>
 6. Binding mechanism of spinosine and venenatine molecules with p300 HAT enzyme – Molecular screening, molecular dynamics and free-energy analysis. **M. Sivanandam** and P. Kumaradhas*. *J. Cell. Biochem.* 2020 Feb; 121(2): 1759-1777. doi: 10.1002/jcb.29412. Epub 2019 Oct 21. 2019.
 7. Identification of a Novel flavonoid Inhibitor of Catechol-O Methyltransferase enzyme by Computational Screening - through the analysis of Binding, Molecular dynamics simulations and Quantum mechanics/Molecular mechanics. Govindasamy Hunday, **Magudeeswaran Sivanandam** and Poomani Kumaradhas*. *J. Biomol. Struct. Dyn.* 2020 Nov; 38(18): 5307-5319. doi: 10.1080/07391102.2019.1699446.
 8. Insights of inhibition mechanism of Sifuvirtide and MT-Sifuvirtide against wild and mutant 2 HIV-1 envelope glycoprotein41 via molecular dynamics simulation and binding free energy studies. Ancy Iruthayaraj, **Sivanandam Magudeeswaran**, Kalaivani Raju and Poomani Kumaradhas*. *Mol. Simul.* 2020, 46(6), 429-439, doi: 10.1080/08927022.2020.1716978
 9. Binding mechanism, conformation and stability of diflunisal and mycophenolic acid with p300 HAT enzyme using molecular dynamics simulation and binding free energy analysis. **M. Sivanandam** and P. Kumaradhas*. *Med. Chem. Res.* 2020, 29, 504–518, doi.org/10.1007/s00044-020-02500-z.
 10. Design and Molecular dynamic Investigations of 7,8-Dihydroxyflavone Derivatives as Potential Neuroprotective Agents Against Alpha-synuclein. Mohankumar Thangavel, Vivek Chandramohan, Lalithamba Haralur Shankaraiah, Richard L Jayaraj, Kumaradhas Poomani, **Sivanandam Magudeeswaran**, Hunday Govindasamy, Rajendran Vijayakumar, Balakrishnan Rangasamy, Manimaran Dharmar, Elangovan Namasivayam*, *Nature, Sci. Rep.* 2020, 10:599, doi: 10.1038/s41598-020-57417-9.

11. Isolation of hesperetin - A flavonoid from Cordia sebestena flower extract through antioxidant assay guided method and its antibacterial, anticancer effect on cervical cancer via in vitro and in silico molecular docking studies. Shanmugam Prakash, Nagaraj Elavarasan, Kasivisvanathan Subashini, Selvaraj Kanaga, Ramamurthy Dhandapani, **Magudeeswaran Sivanandam**, Poomani Kumaradhas, Chinnasamy Thirunavukkarasu, Venugopal Sujatha. *J. Mol. Struct.* 2020, 1207, 127751, doi.org/10.1016/j.molstruc.2020.127751
12. Experimental and Theoretical charge density, Intermolecular interactions and Electrostatic properties of Plumbagin. Chinnasamy Kalaiarasi, **Magudeeswaran Sivanandam**, Suganya Suresh, George Christy, Rajesh G Gonnade, Venkatesha R Hathwar and Poomani Kumaradhas. *J. Mol. Struct.* 1220 (2020) 128714.
13. Possibility of HIV-1 protease inhibitors-clinical trial drugs as repurposed drugs for SARS- 2 CoV-2 main protease: A Molecular docking, Molecular dynamics and Binding free energy 3 simulation study. Iruthayaraj Ancy, **Magudeeswaran Sivanandam** and Poomani Kumaradhas. *J. Biomol. Struct. Dyn.* 2021, 39(15), 5368-5375, Doi: 10.1080/07391102.2020.1786459.
14. Synthesis and characterization of novel bioactive azo compounds fused with benzothiazole and their versatile biological applications. Shanmugam Prakash, Govindharaj Somiya, Nagaraj Elavarasan, Kasivisvanathan Subashini, Selvaraj Kanaga, Ramamurthy Dhandapani, **Magudeeswaran Sivanandam**, Poomani Kumaradhas, Chinnasamy Thirunavukkarasu and Venugopal Sujatha. *J. Mol. Struct.* 1224 (2020) 129016.
15. Strong binding of Leupeptin with TMPRSS2 protease may be an alternative to Camostat and Nafamostat for SARS-CoV-2 repurposed drug: Evaluation from Molecular docking and Molecular dynamics simulations, Jaganathan Ramakrishnan, Saravanan Kandasamy, Ancy Iruthayaraj, Sivanandam Magudeeswaran, Kalaiarasi Chinnasamy and Kumaradhas Poomani. *Appl. Biochem. Biotech.* 2021, **193(6)**, **1909-1923**. doi: 10.1007/s12010-020-03475-8.
16. Binding mechanism of naringenin with monoamine oxidase – B enzyme: QM/MM and molecular dynamics perspective. Govindasamy Hunday, **Magudeeswaran Sivanandam** Kandasamy Saravanan and Poomani Kumaradhas. *Heliyon*, 2021, 7, e06684, Doi-<https://doi.org/10.1016/j.heliyon.2021.e06684>.
17. Investigation of intermolecular interactions and binding mechanism of PU139 and PU141 molecules with p300 HAT enzyme via molecular docking, molecular dynamics simulations and binding free energy analysis. Jaganathan Ramakrishnan, Sivanandam

Conference/Seminar/Colloquium/Symposium/Workshops (Participation/Presentation)

1. Participated in the “International Seminar on Nanostructures for Electronics and Biomedical Applications” organized by Department of Nanoscience and Technology, Bharathiar University, during 09th January 2009 at Coimbatore, Tamil Nadu, India.
2. Participated in the one day Seminar on “Nuclear Energy for National Development”, (NEND) organized by Bhabha Atomic Research Centre, Mumbai and NGM Collage Department of Physics, Pollachi, during 3rd December 2009 at NGM Collage, Pollachi, Tamil Nadu, India.
3. Participated in the two-day national seminar on “Concepts of Quantum Mechanics” in commemoration of “National Science Day” organized by Department of Physics, Sri Ramakrishna Mission Vidyalaya Collage of Arts and Science, Coimbatore, Tamil Nadu, India, during 2nd and 3rd March 2010.
4. Participated in the one day Workshop program on “Preparation of Winning Project Proposal” organized by Project Preparation Club, Bharathiar University Students and Clubs (Initiative by BUSTAS) at Bharathiar University, Coimbatore, Tamil Nadu, on 4th March, 2011.
5. Participated in the “National Seminar on Radiation Technology in Health Care and its Safety (RADTECHS-2011)” on 16th & 17th, March 2011 organized by Department of Medical Physics, Bharathiar University, Coimbatore, Tamil Nadu, India.
6. Participated in the “National Seminar on Structural Bioinformatics-2013” (NSSB-2013) Funded by DBT on 15th March, 2013 held at Bioinformatics centre, Department of Physics, Manonmanium Sundaranar University, Tirunelveli, Tamil Nadu, India.
7. Participated in the Workshop on “Scientific Usage of Electron Microscopes: SEM and TEM” organized by Centre for Instrumentation and Maintenance Facility (CIMF), Periyar University, Periyar Palkalai Nagar, Salem-636 011 held on 6th January, 2014.
8. Participated in the 6th International Symposium on “Recent Trends in Macromolecular Structure and Function (ISRTMSF-2014)” organized by CAS in Crystallography and Biophysics, University of Madras, Maraimalai (Guindy) Campus, Chennai-600025, Tamil Nadu, India, held on January 22-24, 2014.
9. Participated in the Seminar on “Materials for Advanced Technology (SMAT-2014)” organized by Department of Physics, Periyar University, Periyar Palkalai Nagar, Salem-636011, Tamil Nadu, India, held on 21st February 2014.
10. Participated in the National Conference on “Recent Advances in New and Renewable Energy (RANRE-2014)” organized by Centre for new and Renewable Energy Studies

(CNRES), Periyar University, Periyar Palkalai Nagar, Salem-636 011 held on 27th February, 2014.

11. Participated in the International Seminar on “Nanobiotechnology in Cancer Research (NCR-2014)” organized by Department of Biotechnology, Periyar University, Salem-636 011, TN, India held on 21th July, 2014.
12. Participated in the National Symposium on “X-ray Diffraction and Recent Advances in Crystallography (XDRAC-2015)” organized by Department of Physics, School of Sciences, Periyar University, Salem-636 011, TN, India held on 27-28th February, 2015.
13. Participated in the National workshop on “Technical Aspects of High Speed Computers and Applications (THSCA 2015)” organized by Centre for Instrumentation and Maintenance Facility (CIMF), Periyar University, Periyar Palkalai Nagar, Salem- 636 011 held on 27th March, 2015.
14. Participated in the “Interaction programme on DST SCHMES FOR RESEARCHERS” organized by the Centre for Nanoscience and Nanotechnology, Periyar University, Salem-636 011, TN, India held on 12th June, 2015.
15. Participated in the IQAC Seminar on “Smartphone Application in teaching, Learning: Pros and Cons” held at Periyar University, Periyar Palkalai Nagar, Salem on 21st December 2015.
16. Participated in the workshop on “Solar photovoltaic (PV) Based Power Generation Technologies” organized by Department of Energy Studies, Periyar University, Salem-636011 on 22nd February 2016.
17. Participated in the International seminar on “PERSPECTIVE IN MODERN BIOLOGY” held on 2nd September, 2016 at Periyar University, Salem- 636011, Tamil Nadu, India.
18. Participated in the Quiz competition and won Second Prize in the “National Science Day Celebrations – 2017” organized by Periyar University, Salem.
19. Participated in the workshop on “Mathematica and its Applications” held at the Department of Mathematics, Periyar University, Salem-636011 on 6th March 2017.
20. Participated in the workshop on “Technical Aspects of Internet of Things (TAIOT 2017) organized by Centre for Instrumentation and Maintenance Facility (CIMF), Periyar University, Periyar Palkalai Nagar, Salem – 636 011 held on 23 March, 2017. Mathematica and its Applications” held at the Department of Mathematics, Periyar University, Salem-636011 on 6th March 2017.
21. Presented a paper entitled “Analysis of intermolecular interactions and Electrostatic properties of C646 of C646 in the binding pocket of p300 HAT enzyme”, in the TEQIP II Sponsored international conference on advances in Biological, Chemical and Physical Sciences (ABCPS’2017) jointly organized by the Department of Biotechnology,

Chemistry and Physics, held at Bharathidasan Institute of Technology (BIT) Campus, Anna University, Tiruchirapalli- 620 024 during March 13th – 15th, 2017.

22. Participated in the workshop on “Innovative Approaches on Herbal Products” held on 13th October, 2017 at the Department of Botany, School of Life Sciences, Periyar University, Salem.
23. Presented a poster entitled “p300 enzyme is a potential target for different malignant diseases – A Molecular docking, Molecular dynamics and QM/MM approach” in the Seventh All Indian Young Scientist Convention “Learning Science from Nature” held from 18-22 December, 2017 at Periyar University Salem, Tamil Nadu.
24. Presented a research paper entitled “Quantum chemical and molecular docking analysis of plumbagin and its derivatives with p300 HAT enzyme” in the 4th International young scientist congress (IYSC-2018) on 8th & 9th May 2018 held at Rashtriya Sanskrit Vidyapeetha, Tirupati, Andhra Pradesh, India.
25. Participated in the two day “workshop on Research Methodology” held on 27th and 28th August 2018 organized by the Department of English, Periyar University, Salem, Tamil Nadu.
26. Attended the science Academics Lecture Workshop on “Emerging Trends in Chemical Sciences” held during October 04-06, 2018 in the Department of Chemistry, Periyar University, Salem-636011.
27. Participated in the workshop on “Advances in Microscopic Techniques” held between 11th and 12th November, 2019 at the Department of Zoology, Periyar University, Salem – 636011, Tamil Nadu.
28. Participated in the “International Conference on Drug Discovery” held at BITS-Pilani Hyderabad Campus from 29th February to 2nd March and presented a poster entitled “Structural insights and Binding Mechanism of Synthetic Homo-Palmatine and Homo-Berberine molecules with p300 HAT enzyme- A Molecular Dynamics Simulation Study”.

Training Programme

1. Attended two days training Programme on “Computer Hardware: Assembling and Maintenance” conducted by Centre for Instrumentation and Maintenance Facility (CIMF), Periyar University, Periyar Palkalai Nagar, Salem- 636 011 held on 21-22nd March, 2014.
2. Attended two days training Programme on “Computer Hardware and Networking” conducted by Centre for Instrumentation and Maintenance Facility (CIMF), Periyar University, Periyar Palkalai Nagar, Salem-636 011 held on 28-29th March, 2014.

3. Participated in the five days training Programme on “Think Parallel: Parallel Programming for Engineers & Scientists” from 20th to 24th July 2015 at C-DAC Bangalore.
4. Attended two days program on “Application Training Course on Single Crystal XRD” held at Centre for Instrumentation and Maintenance Facility (CIMF), Periyar University, Salem, Tamilnadu-636011, India on April 15-16, 2019.
5. Attended ten days training Programme on BioTecNika Schrodinger joint workshop on “Computer - Aided Drug Discovery” organized by Biotechnika Info Labs Pvt Ltd on 22nd July to 2nd August 2019.
6. Attended Two days training Program on “National workshop on Bruker Single Crystal X-ray Diffraction & User Training” held at Department of Chemistry, Annamalai University, Annamalai Nagar, Tamil Nadu – 608002 on September 27-28th, 2019.

Tutor

1. Attended as a tutor in the two days national workshop on “Crystal and Molecular Structure Determination from X-ray Diffraction Measurements (CMSDX 2016)” organized by Centre for Instrumentation and Maintenance Facility (CIMF), Periyar University, Periyar Palkalai Nagar, Salem-636 011 held on 28-29th March, 2016.
2. Attended as a tutor in the five days program on “Periyar School of Crystallography (PSC-2020)” in association with Bruker India Scientific Pvt. Ltd held at Centre for Instrumentation and Maintenance Facility (CIMF), Periyar University, Salem – 636011, Tamil Nadu, India, From February 21-25, 2020.

Evaluator

1. Attended as an Evaluator of 24th National Children’s Science Congress (District Level) -2016 held at Little Flower H.S. School Salem, Tamil Nadu, India.
2. Attended as an Evaluator of 24th National Children’s Science Congress (State Level) -2016 held at KPR Institute of Engg. & Tech – Coimbatore, Tamil Nadu, India.
3. Attended as an Evaluator of 25th National Children’s Science Congress (District Level) -2017 held at Periyar University, Salem, Tamil Nadu, India.
4. Attended as an Evaluator of 25th National Children’s Science Congress (State Level) -2017 held at Sathyabama Institute of Science and Technology, Chennai, Tamil Nadu, India.
5. Attended as an Evaluator of 26th National Children’s Science Congress (District Level) -2018 held at Periyar University, Salem, Tamil Nadu, India.
6. Attended as an Evaluator of 26th National Children’s Science Congress (State Level) -2018 held at KPR Institute of Engg & Tech – Coimbatore, Tamil Nadu, India.

7. Attended as an Evaluator of 27th National Children's Science Congress (District Level) -2019 held at Periyar University, Salem, Tamil Nadu, India.
8. Attended as an Evaluator of 27th National Children's Science Congress (State Level) -2019 held at ASMV College, Arcot, Tamil Nadu, India.

Field of interest

- ♣ Molecular modeling and Molecular dynamics simulation
- ♣ Protein- Ligand interactions
- ♣ Geometry optimization using quantum mechanics
- ♣ Molecular Docking Studies
- ♣ Small molecule Crystallization
- ♣ QM/MM and QM/MM MD calculations
- ♣ Homology Modeling
- ♣ Virtual Screening
- ♣ Pharmacophore and 3-D QSAR
- ♣ Theoretical Charge density studies of small molecules

List of software known to use

- ♣ **Molecular Dynamics:** AMBER, GROMACS
- ♣ **Molecular Modeling & Docking:** Discovery Studio, Schrodinger, DOCK, HEX, Arguslab, Autodock, Modeller.
- ♣ **Gaussian:** Gaussian, Gauss view and Chemcraft
- ♣ **Charge Density:** XD2006, SHELXL
- ♣ **Structure Determination** – APEX 3
- ♣ **Graphics:** Mercury, Chemdraw
- ♣ **Visualization software:** VMD, Pymol, RasMol, Photoshop, Maestro, Chimera
- ♣ **Others:** AIM2000, Moliso, Sirius, Ligplot, Origin, Matlap.

Technical skills

Operating Systems - All Windows and Linux Operating Systems

Supercomputers - SUN Fire X2200 m2 server – 5 node cluster

FUJITSU Server primergy RX2540 and RX2530 – 9 Node cluster

PARAM Yuva – II (C-DAC- Bangalore, India).

BioEmbryo HPC Cluster – C-DAC - Pune (BRAAF Facility)

X-ray Diffractometer – Bruker D8 Quest Eco (3-circle diffractometer)

Programming Knowledge – Python, FORTRAN (Beginner)

Extracurricular activities

- ♣ Type writing – English (Junior Grade)
- ♣ CLP (Computer Literacy Program)

Personal details

Father's name	:	Magudeeswaran. M
Mother's name	:	Amutha. M
Date of birth	:	10.05.1986
Nationality	:	Indian
Marital Status	:	Married
Languages known	:	English and Tamil

Projects Completed

♣ M.Sc. (Physics)

1. “Optical and Structural Properties of ZnO and Nickel doped ZnO thin film using Chemical bath Deposition” under the guidance of **Dr. A. Ali Fathima**, Assistant Professor, Department of physics, Government Arts College, Udumalpet, Tamil Nadu, India.
2. “Microscopy of Mn doped SnO₂ Nano powders prepared by sol-gel technique”, under the guidance of **Dr. K. Vadivel**, Assistant Professor, Department of Physics, Government Arts College, Udumalpet, Tamil Nadu, India.

♣ M.Phil. (Physics)

1. “Study of Hydrogen bonding under vacuum and water environments- QM and MD studies”, under the guidance of **Prof. P. Kolandaivel**, Department of physics, Bharathiar University, Coimbatore, Tamil Nadu, India.

References

1. **Prof. Anna Niedzwiecka**
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3. Dr. N. Elangovan, Ph.D.,

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DECLARATION

I hereby declare that the above information furnished by me is true to the best of my knowledge and belief.

November, 2022

yours faithfully,



(M. Sivanandam)