

Sri Sai Ram Engineering College

Department Of Humanities And Sciences

Name : **Dr. C. MEGANATHAN**



Designation :

Associate Professor

Qualification :

Ph.D, PDF

Area of Specialisation :

Molecular modeling and Molecular Spectroscopy

Experience :

Teaching : UG : 12 years 6 months

PG : 5 Years

Industry : Nil

*No. of Workshop / Conferences / FDP
attended*

4/5/1

Publication :

Journal

National : 1

International : 38

Conference

National : 6

International : 7

Research Guidance :

3 Ph.D awarded

Supervising: 1 Ph.D Candidate

<i>General :</i>	<i>Postdoctoral Fellowship completed</i> <i>Gyeongsang National University, Jinju, South Korea 20-4-09 to 20-01-12 (2 years 9 month)</i>
<i>Staff Achievements</i>	<i>Keynote address in National Level workshop,</i> <i>Invited talk in National and International level conferences</i> <i>Produced more number of s-grade both Engineering physics I & II in Anna University Exam</i> <i>Stimulate the students creativity</i> <i>Encourage the student to do the research</i>

Educational Qualification:

Category	Name of the Degree	Specialization	Year of Passing	Name of the College	Name of the University	% of Marks / Grades obtained	Class obtained
<i>UG</i>	<i>B.Sc</i>	<i>Physics</i>	<i>1999</i>	<i>Govt. Arts & Science College</i>	<i>University of Madras</i>	<i>59.5</i>	<i>II</i>
<i>PG</i>	<i>M.Sc</i>	<i>Physics</i>	<i>2002</i>	<i>Annamalai University</i>	<i>Annamalai University</i>	<i>6.74</i>	<i>I</i>
	<i>M.Phil</i>	<i>Physics</i>	<i>2004</i>	<i>Annamalai University</i>	<i>Annamalai University</i>	<i>7.74</i>	<i>I</i>
	<i>Ph.D.</i>	<i>Physics</i>	<i>2008</i>	<i>Annamalai University</i>	<i>Annamalai University</i>	<i>Highly Commented</i>	

Academic Experience: (as on 30.09.2022)

Name of the College	Designation	Joining Date	Relieving Date	Experience		
				Years	Months	Days
<i>Dr M G R Polytechnic College</i>	<i>Lecturer</i>	<i>16.08.2004</i>	<i>26.11.2005</i>	<i>1</i>	<i>2</i>	<i>11</i>
<i>Dr Pauls Engineering College, Tindivanam</i>	<i>Lecturer</i>	<i>23.01.2008</i>	<i>11.06.2008</i>	<i>-</i>	<i>4</i>	<i>19</i>
<i>G K M College of Engg. & Tech</i>	<i>Assistant Professor</i>	<i>22.07.08</i>	<i>10.04.09</i>	<i>-</i>	<i>8</i>	<i>20</i>
<i>G K M College of Engg. & Tech</i>	<i>Assistant Professor</i>	<i>08.02.12</i>	<i>05.09.17</i>	<i>5</i>	<i>6</i>	<i>27</i>
<i>Central Institute of Petrochemical Engg. & Tech</i>	<i>Assistant Professor</i>	<i>06.09.17</i>	<i>05.06.21</i>	<i>3</i>	<i>8</i>	<i>30</i>
<i>Sri Sairam Engineering College</i>	<i>Associate Professor</i>	<i>15.11.21</i>	<i>Till Date</i>	<i>1</i>	<i>3</i>	<i>20</i>
Total				12	11	07

PUBLICATIONS

WORKSHOP:

Key Note Address 'National Level Workshop on "Computational Drug Discovery-2018 jointly organized by the Department of Physics and Biotechnology, 16.02.2018, P G Extension centre, Periyar University, Dharmapuri

JOURNAL:

I have published 39 International articles in reputed Journals, and Reviewer for 8 International journals

BOOK CHAPTER

- *"Studies on Dual Inhibitors of HIV Reverse Transcriptase and Integrase", Subramanian Karunakaran, Ramanathan Shylaja and Chandrasekaran Meganathan "Nova Science Publishers, Inc". Hauppauge, NY 11788 USA*

CORRESPONDING AUTHOR

1. *Ramanathan Shylaja, Chandrasekaran Loganathan, SenthamaraiKannan Kabilan, T Vijayakumar and Chandrasekaran Meganathan "Synthesis and evaluation of the antagonistic activity of 3-acetyl-2H-benzo[g]chromen-2- one against mutant Y537S estrogen receptor alpha via E-Pharmacophore modeling, molecular docking, molecular*

dynamics, and in-vitro cytotoxicity studies" (Accepted in Journal of Molecular Structure Sep'2020)

2. Subramanian Karunagaran, Rengarajan Kavitha, Muthu Vadivelu, Keun woo Lee, Chandrasekaran Meganathan, Insight mechanism of the selective Lanosterol synthase inhibitor: Molecular modeling, docking and density functional theory approaches, **Current computer aided drug design** 13(4) (2017) 275-293. (IF:1.639)
3. Ramanathan Shylaja, Rengarajan Kavitha, and Chandrasekaran Meganathan, "Atom based 3D-QSAR, molecular docking and density functional theory approaches to identify novel JNK-1 inhibitors", *Journal molecular modeling*, 19 (2016) 771-797.(IF:2.172)
4. Subramanian Karunagaran, Subramanian Subaschandraboese, Keun woo Lee, **Chandrasekaran Meganathan**, "Investigation on the isoform selectivity of novel kinesin-like protein1 (KIF11) inhibitor using chemical feature based pharmacophore, molecular docking, and quantum mechanical studies" **Computational biology and chemistry** 61, (2016) 47-61 (IF: 3.737)
5. Rengarajan Kavitha, Subramanian Karunagaran, Subramaniyan Subhash Chandrabose, Keun Woo Lee, **Chandrasekaran Meganathan**, "Pharmacophore modeling, virtual screening, molecular docking studies and density functional theory approaches to identify novel ketohexokinase (KHK) inhibitors" **BioSystems**,138, (2015), 39–52 (IF: 1.957)
6. C. Loganathan, S. Sugunadevi, Keun Woo Lee, S. Kabilan, **C. Meganathan*** "Pharmacophore design, virtual screening, molecular docking and optimization approach to design potent inhibitors for Thrombin" **Combinatorial Chemistry & High Throughput Screening**, 16(9), (2013) 702-20, (IF: 1.714)

FIRST AUTHOR

1. **Chandrasekaran Meganathan**, Sugunadevi Sakkiah, Yuno Lee, Keun Woo Lee, "Discovery of potent inhibitors for Interleukin-2-inducible T-cell kinase: Structure-based virtual screening and Molecular dynamics simulation approaches", **Journal of Molecular Modeling** 19(2) 715-726 (2013)(IF: 2.172)
2. **Meganathan Chandrasekaran**, Sugunadevi Sakkiah, Keun Woo Lee, "Combined Chemical Feature Based Assessment and Bayesian Model Studies to identify Potential Inhibitors for Factor Xa" **Medicinal Chemistry Research** 21(12), 4083-4099 (2012) (IF:2.351).
3. **C. Meganathan**, S. Sebastian, I. Sivanesan, Keun Woo Lee, Byoung Ryong Jeong, Halil Oturak, N. Sundaraganesan. "Structural, vibrational (FT-IR and FT-Raman) and UV-Vis spectral analysis of 1-phenyl-3-(1,2,3- thiadiazol-5-yl) urea by DFT method", **Spectrochim Acta Part A: Molecular and Biomolecular Spectroscopy**, 95, 331-340(2012) (IF:4.831)
4. **Meganathan Chandrasekaran**, Sugunadevi Sakkiah, and Keun Woo Lee, "Combined Ligand Based Pharmacophore Modeling, virtual screening methods to identify critical

chemical features of novel Potential inhibitors for Phosphodiesterase-5" **Journal of the Taiwan Institute of Chemical Engineers**, 42 (5) 709-718 (2011) (IF: 5.477).

5. **Meganathan Chandrasekaran**, Sugunadevi Sakkiah, Sundarapandian Thangapandian, Sundaraganesan Namadevan, Hyong-Ha Kim, Youg Seong Kim, Keun Woo Lee, "Pharmacophore Design for Anti-inflammatory Agent Targeting Interleukin-2 Inducible Tyrosine Kinase (Itk)" **Bull. Korean Chem. Soc.** 31 (11) (2010) 3333-3340 (IF:1.241)
6. **C.Meganathan**, S.Sebastian, Mutafa Kurt, Keun Woo Lee, N.Sundaraganesan, "Molecular structure, spectroscopic (FTIR, FTIR gas phase, FT-Raman) first-order hyperpolarizability and HOMO-LUMO analysis" **Journal of Raman Spectroscopy** 41(10) (2010) 1369-1378. (IF: 2.727).

CO AUTHOR

7. S. Subashchandrabose, **C. Meganathan**, Y. Erdođdu, H. Saleem, C.Jajkumar, P. Latha "Vibrational and Conformational Analysis on N1-N2- Bis ((Pyridine-4-yl) Methylene) Benzene-1, 2-Diamine", **Journal of Molecular Structure** 1042, 37-44 (2013) (IF: 1.634)
8. Sugunadevi Sakkiah, **Chandrasekaran Meganathan**, Yuno Lee, Sogmi Kim, Keun Woo Lee, "Molecular Modeling Study for Conformational Changes of Sirtuin; 2 Due to Substrate and Inhibitor Binding" **Journal of Biomolecular Structure and Dynamics**, 30(3), 235-254 (2012) (IF:4.986)
9. Sugunadevi Sakkiah, **Chandrasekaran Meganathan**, Young-sik shon, Sundaraganesan Namadevan, Keun Woo Lee, "Identification of important chemical features of 11 β -Hydroxysteroid dehydrogenase type1 inhibitors: Application of ligand based virtual screening and density function theory" **International Journal of Molecular Science**, 13 (4), 5138-5162 (2012)(IF: 2.279)
10. Venketesh Arulalapperumal, Sugunadevi Sakkiah, Sundarapandian Thangapandian, Yuno Lee, **Meganathan Chandrasekaran**, Suwon Hwang, Keun Woo Lee, "Ligand Based Pharmacophore Identification and Molecular Docking Studies for Grb2 Inhibitors." **Bulletin of The Korean Chemical Society** 33(5), 1707-1714 (2012) (IF: 0.871).
11. P. Lazar, Y. Lee, S. Kim, **Meganathan Chandrasekaran**, K. W. Lee, "Molecular Dynamics Simulation Study for Ionic Strength Dependence of RNA-host factor Interaction in Staphylococcus aureus Hfq" **Bull. Korean Chem. Soc.**31 (6) (2010) 1519-1526 (IF: 0.871).
12. N.Sundaraganesan, G.Elango, **C.Meganathan**, B.Karthikeyan, M.Kurt, "Molecular Structure and Vibrational Spectra and HOMO, LUMO analysis of 4-piperidone by density functional theory and ab initio Hartree-Fock calculations" **Molecular Simulation** 35(9) (2009) 705-713 (IF: 1.215).

13. N.Sundaraganesan, B.Dominic Joshua, **C.Meganathan**, S.Sebastian, "Vibrational spectroscopic studies supported by HF, DFT calculations of 2,4,6 - triaminopyrimidine" **Indian Journal of Chemistry** 47A, (2008), 821-829 (IF: 0.920).
14. N.Sundaraganesan, Umamaheswari, **C. Meganathan**, S. Sebastein, "Molecular Structure and Vibrational Spectra of 4-nitrobenzylchloride by ab initio Hartree-Fock and Density Functional Methods" **Molecular Simulation** 34(6), (2008), 619-630 (IF: 1.215). Cited by
15. N.Sundaraganesan, H.Umamaheswari, B.Dominic Joshua, **C.Meganathan**, M. Ramalingam, "Molecular Structure and Vibrational Spectra of indole and 5-aminoindole by Density Functional theory and ab initio Hartree fock calculations", **Journal of Molecular Structure (Theochem)** 850(1-3), (2008), 84-93 (IF: 1.220).
16. Sundaraganesan, **C. Meganathan**, Mustafa Kurt, "Molecular structure and vibrational spectra of 2-amino-5-methyl pyridine and 2-amino-6- methylpyridine by ab initio Hartree-Fock and Density Functional Methods" **Journal of Molecular Structure** 891(1-3),(2008), 284-291(IF: 1.599).
17. N. Sundaraganesan, B. Anand **C. Meganathan**, B. Dominic Joshua, H. Saleem, "Vibrational spectra and assignments of 3-aminobenzyl alcohol by ab initio Hartree-Fock and density functional method" **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 69(1), (2008), 198-204 (IF: 1.770)
18. N. Sundaraganesan, B. Anand, **C. Meganathan**, B. Dominic Joshua, "FT-IR, FT-Raman spectra and ab initio HF, DFT vibrational analysis of p-chlorobenzoic acid", **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 69(3), (2008), 871-879 (IF: 1.770).
19. N. Sundaraganesan, M. Priya, **C. Meganathan**, B. Dominic Joshua J.P. Cornard, "FT-IR, FT-Raman spectra and quantum chemical calculations of 3, 4-dimethoxyaniline" **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 70(1), (2008), 50-59 (IF:1.770).
20. N. Sundaraganesan, B. Dominic Joshua, **C. Meganathan**, R. Meenashi, J.P.Cornard, "Vibrational spectra and quantum chemical calculations of 3,4-diaminobenzoic acid" **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 70(2), (2008), 376-383 (IF: 1.770).
21. N. Sundaraganesan, **C. Meganathan**, B. Karthikeyan, "FT-IR, FT-Raman spectra and quantum chemical calculations of some chloro substituted phenoxy acetic acids", **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 70(2), (2008),430-438 (IF: 1.770).
22. N.Sundaraganesan, S.Kalaichelvan, **C.Meganathan**, B.Dominic Joshua, J.Cornard, "FT-IR, FT-Raman spectra and ab initio HF and DFT calculations of 4-N, N-dimethylamino

- pyridine”, **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 71(3) (2008), 898-906 (IF:1.770).
23. N. Sundaraganesan, **C. Meganathan**, B. Dominic Joshua, P. Mani, A. Jayaprakash, “Molecular structure and vibrational spectra of 3-chloro-4-fluorobenzonitrile by *ab initio* HF and density functional method” **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 71(3), (2008), 1134-1139 (IF: 1.770).
24. N. Sundaraganesan, **C. Meganathan**, B. Anand, Christine Lapouge, “FT-IR, FT-Raman spectra and *ab initio* DFT vibrational analysis of *p*-bromophenoxyacetic acid”, **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 66(3), (2007), 773-780 (IF:1.770).
25. N. Sundaraganesan, S. Illakiamani, **C. Meganathan**, B. Dominic Joshua, “Vibrational spectroscopy investigation using *ab initio* and density functional theory analysis on the structure of 3-aminobenzotrifluoride”, **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 67(1), (2007), 214-224 (IF:1.770).
26. N. Sundaraganesan, **C. Meganathan**, B. Anand, B. Dominic Joshua, Christine Lapouge, “Vibrational spectra and assignments of 2-amino-5-iodopyridine by *ab initio* Hartree-Fock and density functional methods”, **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 67(3-4), (2007), 830-836 (IF: 1.770).
27. N. Sundaraganesan, B. Anand, **C. Meganathan**, B. Dominic Joshua, “FT-IR, FT-Raman spectra and *ab initio* HF DFT vibrational analysis of 2,3-difluorophenol” **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 68(3), (2007), 561-566 (IF:1.770).
28. N. Sundaraganesan, **C. Meganathan**, H. Saleem, B. Dominic Joshua, “Vibrational spectroscopy investigation using *ab initio* and density functional theory analysis on the structure of 5-amino-*o*-cresol”, **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy** 68(3), (2007), 619-625 (IF:1.770).
29. N. Sundaraganesan, K. Sathesh Kumar, **C. Meganathan**, B. Dominic Joshua, “Vibrational spectroscopy investigation using *ab initio* and density functional theory analysis on the structure of 2-amino-4,6-dimethoxy pyrimidine” **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy** 65 (5), (2006), 1186-1196 (IF: 1.770).

CONFERENCE PUBLICATION

1. Rengarajan Kavitha, Chandrasekaran Meganathan, 3D-QSAR modeling, molecular docking and quantum mechanical approaches to identify Pleckstrin homology domain of new AKT1 inhibitors, AIP Conference proceedings cited as Proceedings 2117, 020015 (2019); <https://doi.org/10.1063/1.5114595>
2. Pharmacophore based virtual screening, molecular docking and density functional theory approaches to discover the potent beta-amyloid precursor protein (B-APP) inhibitor,

AIP Conference proceedings cited as Proceedings 2117, 020015 (2019); <https://doi.org/10.1063/1.5114595>

INVITED TALK:

- I have given "invited talk" in 2nd International Congress On The World Of Technology And Advanced Materials, 28 September – 02 October 2016 Kirsehir/Turkey
- I have given "invited talk" in International conference on nanomaterials and molecular research (ICNMR - 2016) ST. Joseph's College Of Arts and Science (Autonomous) Cuddalore, December 8-9, 2016.
- I have given "invited talk" International conference on Modern material research 2016 (ICMMR 2016) PG & Research department of physics Sri Vidya Mandir Arts and Science College, Uthangarai, December 19-20, 2016.
- I have given "invited talk" in "National conference On Recent Advances in Physics 2012" (NCRAP2012) organized by "Sri Vidya Mandir Arts and Science College" Uthangarai, INDIA (20-21 July 2012)

WORKSHOP KEY NOTE ADDRESS

- National Level Workshop on "Computational Drug Discovery-2018" jointly organized by the Department of Physics and Biotechnology, 16.02.2018, P G Extension centre, Periyar University, Dharmapuri

INTERNATIONAL CONFERENCE

1. International Virtual Conference on "Recent Trends in Clean Technologies for Sustainable Environment" on September 15 & 16 organized by CEWAR, SSN College of Engineering, Chennai.
2. C. Meganathan, presented "Combined Chemical Feature Based Assessment and Bayesian Model Studies to Identify Potential Inhibitors for Factor Xa." The 22nd International Conference on Genome Informatics, Haeundae Grand Hotel, Busan, Korea, Dec. 5-7, 2011.
3. C. Meganathan presented "Structure-based Pharmacophore Modeling and Molecular Dynamics Simulations Approaches to Design Potent Inhibitor for Interleukin-2-inducible T-cell Kinase." Translational Bioinformatics Conference, Seoul National University College of Medicine, Seoul, Korea, Nov. 10-11, 2011.
4. C. Meganathan, presented "Pharmacophore modeling, virtual screening approach to discover potent inhibitor for thrombin" in the 9th Asia Pacific Bioinformatics Conference of Korean Society for Bioinformatics and Systems Biology (KSBSB), Songdo Convensia, Incheon, Korea, Jan. 11-14, 2011.

5. C. Meganathan, presented "Identify novel potential inhibitors for PDE5 using pharmacophore modeling and ligand-based virtual screening." in the 105th spring meeting of the Korean Chemical Society, Songdo Convensia, Incheon, Korea, Apr. 29-30, 2010
6. C. Meganathan, presented "Pharmacophore design for anti-inflammatory agent targeting interleukin inducible 2 tyrosine kinase (Itk)." in the Bioinfo 2009, The 10th International conference, Haeundae Grand Hotel, Busan, Korea, Nov. 4-6, 2009

NATIONAL CONFERENCE

1. C. Meganathan, participated "National seminar on New engineering materials and their applications" organized by the Department of Physics, Valliammai Engineering College, Kattankulathur, Chennai, Apr 27, 2015.
2. C. Meganathan, Participated DST-FIST & UGC-SAP sponsored National seminar on "Chemistry education and research & National convention of chemistry teachers (NCCT-13)" organized by the Department of Chemistry and the Association of Chemistry Teachers (ACT) Annamalai University, Chidambaram, Nov 8-10, 2013.
3. C. Meganathan, Presented " Drug design for Factor Xa" in the National conference on physics of new materials organized by Department of Physics, Noorul Islam University, Kumarakoil, Apr 20-21,2012.
4. C. Meganathan, presented "abintio and density functional theory studies on p-bromophenoxy acetic acid", in the CSIR &UGC sponsored National seminar on recent trends in heteroatom chemistry organized by Department of chemistry, Annamalai University, Chidambaram, Mar 28-29, 2007.
5. C. Meganathan, presented "Molecular vibrational studies on 2-amino-5-iodopyridine in the National conference on recent advances in Vibrational spectroscopy organized by Department of physics, Periyar University, Salem, Jan 29-30, 2007
6. C. Meganathan presented "Vibrational spectroscopy studies on 5-amino-o-cresol in the National seminar on advances in material sciences organized by Department of physics, Manonmaniam Sundaranar University, Tirunelveli, Mar 27-28, 2006.

WORKSHOP

1. Participated "Recent trends in structural bioinformatics and computer aided drug design" organized by Department of Bioinformatics, Alagappa University, Karaikudi, Feb 24-27, 2015.
2. Participated "Recent advances in computational drug design" organized by Schrodinger, held at Indian Institute of Science campus, Bangalore, Sep 16-17, 2013.
3. Participated "Research methodology workshop", organized by Department of Economics, Annamalai University, Chidambaram, Feb 9-12, 2012.

4. Participated "UGC-COSIP sponsored one day state level seminar on quantum chemistry and spectroscopy", organized by Department of chemistry, Rajah Serfoji Government College, Thanjavur, Feb 9, 2006.
5. Participated "CRSI seminar on recent advances in chemistry", organized by Department of Chemistry, Annamalai University, Chidambaram, Mar 10-11, 2006.

FDP:

1. I have participated "Faculty development program" conducted by Anna University, Chennai, 22nd to 30th Dec 2008 (Material Science)

REVIEWER FOR INTERNATIONAL JOURNALS

1. *Journal of Bio molecular structure and dynamics*
2. *Spectrochim Acta –Molecular and bio molecular spectroscopy*
3. *Journal Of Asian Ceramic Societies*
4. *Journal of Material Cycles and Waste Management*
5. *Computers in biology and medicine*
6. *BMC-Bioinformatics*
7. *Current computer aided drug designing*
8. *SAR and QSAR in environmental research*

Patents

1. *A novel nano crystal/silver difunctional composite nano material for cancer treatment and method thereof. (National Patent, No: 202231054139)*
2. *Method for preparation of Room Temperature stable photoactive Formamidium Lead Iodide Perovskite. (International Patent, No: 2021106454).*
3. *Method for Facile Synthesizing Heterostructure NiO-SnO₂ Nanocomposite for Selective Electrochemical Determination of L-Cysteine. (National Patent, No: 202141050557 A).*

Honors

- **"Best Paper Presentation award"** for the research work entitled "Synthesis, molecular docking, quantum mechanical calculation and anticancer activities of some curcumin analogues : 2,6-(Difurfurylidene) cyclohexanone and 2,6-Bis(2,6-Dichloro Benzylidene) cyclohexanone" presented at 3rd Virtual conference on Recent Trends in Clean Technologies for sustainable Environment (CTSE 2022) organised by Center of Excellence in Water Research, Sri Sivasubramaniya Nadar College of Engineering, Chennai on September 15th & 16th, 2022.