

|  |  |                            |                 |
|--|--|----------------------------|-----------------|
| <b>Name:</b><br><br><b>DR C MEGANATHAN</b> |   |                            |                 |
| <b>Designation:</b>                        | <b>Associate Professor</b>   |                            |                 |
| <b>Qualification:</b>                      | M.Sc., M.Phil., Ph.D., Post Doc (South Korea)  |                            |                 |
| <b>Area of specialization:</b>             | Molecular spectroscopy and Drug Designing  |                            |                 |
| <b>Experience:</b>                         | <b>Industrial Experience</b>   | <b>Teaching Experience</b> |                 |
|  | <b>3 years Post Doc</b>  |                            | <b>15</b>       |
| <b>Number of workshops / FDP attended:</b> | <b>Number of Workshops</b>   | <b>Number of FDPs</b>      |                 |
|  | <b>12</b>  | <b>10</b>                  |                 |
| <b>Publications:</b>                       | <b>Conference</b>  | <b>Journal</b>             |                 |
|  | <b>National</b>  | <b>International</b>       | <b>National</b> |
|  | <b>6</b>   | <b>6</b>                   | <b>1</b>        |
| <b>Books / Book Chapters</b>               |  |                            |                 |
| <b>Patents:</b>                            | <b>National</b>  | <b>International</b>       |                 |
|  | <b>1</b>   | <b>1</b>                   |                 |
| <b>Professional Body Membership</b>        | 1. The Institute of Electrical and Electronics Engineers (IEEE. No. 98741359)<br>2. Member of IEEE Nuclear Plasma science society<br>3. Member of IEEE Photonics Society<br>4. Member of IEEE Magnetic society<br>5. Member of IEEE instrumentation measurement<br>6. Member of IEEE Ultrasonics, Ferroelectrics, and Frequency Control Society<br>7. Member IEEE engineering in medicine<br>8. Member IEEE electron devices<br>9. Member IEEE engineering in medicine<br>10. Member IEEE Circuits and systems |                            |                 |

|                           |  |
|---------------------------|--|
| <b>Staff Achievements</b> | <ol style="list-style-type: none"> <li>1. Dr K RAMASWAMY Endowment award for highest publication in Annamalai University (2007)</li> <li>2. Keynote address given for workshop (national level)</li> <li>3. Invited talk both national and international conference</li> </ol> |
|---------------------------|--|

## 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 |
|-----------|--------------------|----------------|-----------------|---|------------------------|------------------------------|----------------|
| UG        | B.SC.,             | Physics        | 1999            | Govt Arts and Science college, Tiruvannamalai | University of Madras   | 59.5                         | II             |
| PG        | M.Sc.,             | Physics        | 2003            | Annamalai University                          | Annamalai University   | 67.8                         | I              |
|           | M.Phil.,           | Physics        | 2004            | Annamalai University                          | Annamalai University   | 74.5                         | I              |
| Doctorate | Ph.D.,             | Physics        | 2008            | Annamalai University                          | Annamalai University   | Highly commented             |                |

| Name of the College                         | Designation         | Joining Date | Relieving Date | Experience |          |           |
|---|---------------------|--------------|----------------|------------|----------|-----------|
|   |                     |              |                | Years      | Months   | Days      |
| Sri Sai Ram Engineering College             | Associate Professor | 01.09.2023   | Till Date      | 1          | 2        | 18        |
| Sri Sai Ram Engineering College             | Assistant Professor | 15.11.2021   | 31.08.2022     | 1          | 9        | 29        |
| CIPET                                       | Assistant Professor | 06.09.2017   | 05.06.2021     | 3          | 9        | 0         |
| G K M College of Engineering and Technology | Assistant Professor | 08.02.2012   | 05.09.2017     | 5          | 7        | 04        |
| G K M College of Engineering and Technology | Assistant Professor | 22.07.2008   | 31.03.2009     | 0          | 8        | 8         |
| <b>Total</b>                                |                     |              |                | <b>13</b>  | <b>0</b> | <b>29</b> |

## Academic Experience:

| S.No | Book Chapter | Journal       |          | As a Corresponding author | First author | Co-author |
|------|--------------|---------------|----------|---------------------------|--------------|-----------|
|      |              | International | National |                           |              |           |
| 1    | 1            | 39            | 1        | 7                         | 6            | 24        |

| <b>Citation Indices</b> |            |                   |
|-------------------------|------------|-------------------|
|                         | <b>All</b> | <b>Since 2019</b> |
| <b>Citation</b>         | 1182       | 399               |
| <b>h-index</b>          | 20         | 12                |
| <b>i10-index</b>        | 24         | 14                |

#### **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
9. Journal of Molecular structure
10. Journal of molecular graphics and modelling
11. Scientific Reports
12. Results in Chemistry

#### **CONFERENCE**

| S.No | Conference    |          | Oral Presentation |          | Poster Presentation |          | Invited Talk  |          |
|------|---------------|----------|-------------------|----------|---------------------|----------|---------------|----------|
|      | International | National | International     | National | International       | National | International | National |
| 1    | 6             | 6        | 5                 | 4        | 1                   | 2        | 1*            | 4        |

\*I have given “invited talk” in 2ND INTERNATIONAL CONGRESS ON THE WORLD OF TECHNOLOGY AND ADVANCED MATERIALS, 28 SEPTEMBER -02OCTOBER 2016 KIRSEHIR/TURKEY

#### **WORKSHOP KEYNOTE 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’

#### **SUPERVISING**

| <b>S.No</b> | <b>No. of Ph.D.<br/>student</b> | <b>Ph.D.,<br/>Awarded</b> | <b>Thesis<br/>submitted</b> | <b>M.Tech<br/>Completed</b> |
|-------------|---------------------------------|---------------------------|-----------------------------|-----------------------------|
| 1           | 2                               | 3                         | -                           | 1                           |

## **SOFTWARE KNOWN FOR RESEARCH**

Gaussian  
Molvib  
Discovery studio  
Gromacs  
GOLD  
Molgro  
Wingx (To solve small molecules)  
Window and Linux  
Schrodinger  
Auto dock

## **FUNDED PROJECT**

“Drug design for ITK inhibitors” Funded by BK21 program, Gyeongsang National University, South Korea, 2009 (Completed 2010)

“Drug design for PDE-5 inhibitors” Funded by BK21 program, Gyeongsang National University, South Korea, 2010 (Completed 2011)

“Drug design for Thrombin inhibitors” Funded by BK21 program, Gyeongsang National University, South Korea, 2011 (Completed 2012)

## **BOOK CHAPTER**

1. “Studies on Dual Inhibitors of HIV Reverse Transcriptase and Integrase”, **Subramanian Karunagaran, Ramanathan Shylaja and Chandrasekaran Meganathan\*** “*Nova Science Publishers, Inc*”. *Hauppauge, NY 11788 USA*

## **CORRESPONDING AUTHOR**

1. Ramanathan Shylaja, Chandrasekaran Loganathan, Senthamarai Kannan 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:0.935)

3. Ramanathan Shylaja, Rengarajan Kavitha, and Chandrasekaran Meganathan, “Atom based 3D-QSAR, molecular docking and density functional theory approaches to identity novel JNK-1 inhibitors”, *Journal molecular modeling*, 19 (2016) 771-797.(IF:1.346)
4. Subramanian Karunagaran, Subramanian Subaschandrabose, 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: 1.1),
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: 1.5),
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: 1.7)

#### 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: 1.871)
- 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: 1.271).
- 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: 1.770)
- 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: 1.260).

- 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: 0.871).
- 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: 3.137). Cited by

#### CO AUTHOR

- 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 $\beta$ -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 Joshuva, **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-fluoro benzonitrile 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-difluoro phenol" **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**

30 Rengarajan Kavitha, Chandrasekaran Meganathan, 3D-QSAR modeling, molecular docking and quantum mechanical approaches to identify Pleckstrin homology domain of new AKT1inhibitors, AIP Conference proceedings cited as Proceedings 2117, 020015 (2019); <https://doi.org/10.1063/1.5114595>

31 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>