

Dr. K.V Swamy

Designation: Associate Professor

E mail ID : k.swamy@dpu.edu.in

Qualification: M.Sc., Ph.D.



Area of Specialization: Structural Bioinformatics, Protein - Drug interaction, drug design, Protein modeling, Molecular modeling, Molecular dynamics and simulations

Academic Qualification

Ph.D. (Biochemistry) (2010) Sri Krishnadevaraya University, Anantapur, Andhra Pradesh, India Thesis Title: “*Computer aided Drug (CADD) design studies on Human histamine H2 Receptor*”

M.Sc. (Biochemistry.) (2003) Sri Krishnadevaraya University, Anantapur, Andhra Pradesh, India

B.S.c. (Biochemistry.) (2000) Sri Krishnadevaraya University, Anantapur, Andhra Pradesh, India

Professional Experience:

Associate Professor (15th July 2016 to Present) Dr. D. Y. Patil Biotechnology and Bioinformatics Institute, Dr. D. Y. Patil Vidyapeeth, Pune

Asst. Professor (Jan 2015 to 14th July, 2016): Dr. D. Y. Patil Biotechnology and Bioinformatics Institute, Dr. D. Y. Patil Vidyapeeth, Pune.

Officer, Lab Administration (Nov, 2013 Aug 2014) Thyrocare Technologies Limited, Navi Mumbai, India

Head and Asst. Professor (June, 2007 to October, 2013).Department of Biotechnology and Bioinformatics, Dr.D.Y.Patil Biotechnology and Bioinformatics Institute, Dr. D. Y. Patil Vidyapeeth, Pune

Visiting faculty: Jaffna University, Sri Lanka

Awards: Young Scientist Award, by ICMPHP, George Washington, USA on September 8, 2012

Academic Memberships at Dr.D.Y.PatilVidayapeeth, Pune

1. Curriculum committee member for Bioinformatics
2. Board of studies (BOS) Member for Bioinformatics
3. Board of Faculty (BOF) Member for Biotechnology and Bioinformatics

Reviewer for International Journals

1. Journal of Molecular modeling.
2. Interdisciplinary Sciences: Computational Life Sciences
3. Journal of Molecular modeling and Graphics

Research projects guided to students: 58

Protein structures deposited to Protein Model Data Base: 32

Joint Research collaborations for publications and Research projects

- 1) Department of Pathology, Barbara Ann Karmanos Cancer Institute, Wayne State University School of Medicine, 740Hudson Webber Cancer Research Center, USA
- 2) Department of Pharmacology, Pharmacology Core Services at Karmanos Cancer Center, Wayne State University, USA
- 3) D. Y. Patil Institute of Pharmaceutical Sciences, Pune, 411018, India.
- 4) Department of Bioinformatics, Pad. Dr.D.Y.PatilVidyapeeth, Mumbai. India
- 5) Department of Biochemistry, Sri Krishnadevaraya University, India
- 6) Department of Biotechnology, Sri VenkateswaraUniversity, India

Publications: 28

International: 22

National: 03

Conference Proceeding: 03

International Publications: 22

- 1) Pulakuntla Swetha Reddy, Kiran Bharat Lokhande, Shuchi Nagar, Vaddi Damodara Reddy, P. Sushma Murthy, **K. Venkateswara Swamy**. Molecular Modeling, Docking, Dynamics and simulation of Gefitinib and its derivatives with EGFR in Non-Small Cell Lung Cancer. *Current Computer-Aided Drug Design*. (2018), 14. (**Impact factor 0.732**).
- 2) Gadamsetty Saayi Krushna, Vutharadhi Leela Shivaranjani, Jolapuram Umamaheswari, Cheemanapalli Srinivasulu, Shaik Althaf Hussain, Mohammed Abdul Kareem, Vaddi Damodara Reddy, Daoud Ali, Kiran Bharat Lokhande, **K. Venkateswara Swamy**, Lakshmi Devi Kodidhela. *In vivo* and molecular docking studies using whole extract and phytocompounds of Aegle marmelos fruit protective effects against Isoproterenol-induced Myocardial infarction in rats. *Biomedicine & Pharmacotherapy*. (2017), 91:880–889. (**Impact factor 2.759**).
- 3) DhafirLatiefFayadh, **K Venkateswara Swamy** (2016) Molecular Docking Studies of Human Ubiquitin Conjugating Enzyme Rad6: A Systematic in Silico Approach. *International journal of science and research* vol5:3, 636-641(**ISSN (Online): 2319-7064**).
- 4) Prasad Dandawate, KiranmayiVemuri, **K. Venkateswara Swamy**, Ejazuddin M. Khan, ManjulaSriharan, SubhashPadhye (2014) Synthesis, characterization, molecular docking and anti-tubercular activity of Plumbagin-Isoniazid Analog and its β -cyclodextrin

conjugate. *Bioorganic & Medicinal Chemistry Letters*, 24(21):5070-5075 (**Impact factor 2.65**)

- 5) Prasad Dandawate, Aamir Ahmad, Jyoti Deshpande, **K Venkateswara Swamy**, Ejazuddin M Khan, Madhukar Khetmalas, Subhash Padhye, Fazlul Sarkar (2014). Anticancer phytochemical analogs 37: Synthesis, characterization, molecular docking and cytotoxicity of novel plumbagin hydrazones against breast cancer cells. *Bioorganic & Medicinal Chemistry Letters*, 24:2900-2904 (**Impact factor 2.65**)
- 6) P Sharma, P Patil, N Rao, **K V Swamy**, M.B khetmalas, G D Tandon (2014). Mapping Biodiversity of Indigenous Freshwater Chlorophytes. *Research Journal of Pharmaceutical, Biological and Chemical Sciences* 5(3): 1632-1639 (**Impact factor 0.35**).
- 7) Shihnath Ghataka, Alok Vyas, Suniti Misra, Paul O'Brien, Ajit Zambre, Victor M. Fresco, Roger R. Markwald, **K. Venkateshwara Swamy**, Zahra Afrasiabif, Amitava Choudhury, Madhukar Khetmalas, Subhash Padhye. (2013) Novel di-tertiary-butyl phenylhydrazones as dual cyclooxygenase-2/5-lipoxygenase inhibitors: synthesis, COX/LOX inhibition, molecular modeling, and insights into their cytotoxicities. *Bioorganic & Medicinal Chemistry Letters*, 24:317-324 (**Impact factor 2.65**).
- 8) Siddiqui A, Dandawate P, Rub R, Padhye S, Aphale S, Moghe A, Jagyasi A, **Venkateswara Swamy K**, Singh B, Chatterjee A, Ronghe A, Bhat HK. (2013) Novel Aza-resveratrol analogs: Synthesis, characterization and anticancer activity against breast cancer cell lines. *Bioorganic & Medicinal Chemistry Letters*, 23: 635–640 (**Impact factor 2.978**).
- 9) Yusufi M, Banerjee S, Mohammad M, Khatal S, **Venkateswara Swamy K**, Khan EM, Aboukameel A, Sarkar FH, Padhye S. (2013) Synthesis, characterization and anti-tumor activity of novel thymoquinone analogs against pancreatic cancer. *Bioorg Med Chem Lett*. 15;23(10):3101-3104. (**Impact factor 2.978**).
- 10) Misra S, Ghatak S, Patil N, Dandawate P, Ambike V, Adsule S, Unni D, Venkateswara Swamy K, Padhye S. (2013) Novel dual cyclooxygenase and lipoxygenase inhibitors targeting hyaluronan-CD44v6 pathway and inducing cytotoxicity in colon cancer cells. *Bioorg Med Chem*. 1;21(9):2551-2559 (**Impact factor 2.978**).
- 11) Y. Nanda Kumar, K. Kalpana, **K. Venkateswara Swamy**, P.V.G.K.Sarma, M. Bhaskar (2012) Molecular dynamics simulations of mody2 mutated glucokinase structures revealed significant conformational variations explaining reasons for hyperglycemic condition, *International Journal of Pharma and Bio Sciences*, 493 - 499.
- 12) Dipti Shingnapurkar, Prasad Dandawate, Christopher E. Anson, Annie K. Powell, Zahra Afrasiabi, Ekkehard Sinn, Sheetal Pandit, **K. Venkateswara Swamy**, Scott Franzblau, Subhash Padhye (2012) Synthesis and Characterization of Pyruvate-Isoniazid Analogs and their Copper Complexes as Potential ICL Inhibitors. *Bioorganic & Medicinal Chemistry Letters*, 22: 3172–3176 (**Impact factor 2.978**).
- 13) Prasad Dandawate, Ejazuddin Khan, Subhash Padhye, Himanshi Gaba, Swati Sinha, Jyoti Deshpande, **K. Venkateswara Swamy**, Madhukar Khetmalas, Aamir Ahmad, Fazlul Sarkar (2012) Synthesis, Characterization, Molecular Docking and Cytotoxic Activity of Novel

PlumbaginHydrazones against Breast Cancer Cells.*Bioorganic & Medicinal Chemistry Letters*, 22: 3104–3108(**Impact factor 2.978**).

- 14) Dandawate PR, Vyas A, Ahmad A, Banerjee S, Deshpande J, **Swamy KV**, Jamadar A, Dumhe-Klaire AC, Padhye S, Sarkar FH. (2012) Inclusion Complex of Novel Curcumin Analogue CDF and β -Cyclodextrin (1:2) and Its Enhanced *in Vivo* Anticancer Activity against Pancreatic Cancer *Pharm Res*, 29:1775-1786 (**Impact factor 4.456**).
- 15) **K.Venkateswara swamy** , Jyothi Deshpande, Jasmine SoumyaPathageri ,VidyaKothekar, SubhashPadhye (2011) Molecular Docking Studies On Estrogen Receptor - α And Chalcone Derivatives. *International Journal of Advances in Pharmacy and Biological Sciences* (IJAPBS) 1(3): 87– 93.
- 16) Parul J, Sagar N, **Swamy K V** and Suresh Kumar C (2011) An insight into blood clotting disorders in humans. *Journal of Computational Biology and Bioinformatics Research*. 3(1): 8-14.
- 17) Padhye S, Ahmad A, Oswal N, Dandawate P, Deshpandye J, **Swamy K.V**, Farkar F.H (2010). Fluorinated 2'-Hydroxychalcones as Garcinol analogs with enhanced antioxidant and anticancer activities. *Bioorganic & Medicinal Chemistry Letters*1; 20(19):5818-21. (PMID: 20729081) (**Impact factor 2.65**)
- 18) Padhye S, chavan D, Pandey S, Deshpande J, **Swamy KV**, Sarkar (2010). Perspectives on chemopreventive and therapeutic potential of curcumin analogs in medicinal chemistry. *Medicinal chemistry*, 10, 1-16 (PMID:20370702) (**Impact factor.3.12**)
- 19) Subhash P, Sanjeev B, Deepak C, Shubhangini P, **Swamy K V**, Shadan A, Jing Li, Q. Fazlul H. Sarkar (2009) Fluorocurcumins as Cyclooxygenase-2 Inhibitor: Molecular Docking, Pharmacokinetics and Tissue Distribution in Mice. *Pharmaceutical Research*, 26(11):2438-2448(**Impact factor 4.5**) (PMID: 19714451).
- 20) Chitta Suresh Kumar, C.M. Anuradha, **K. Venkateswara Swamy**, Niamat Ali Khan. (2006) Structural and Functional Characterization of Cation-Transporting Atpase of *Mycobacterium tubeculosis* CDC 1551 By in Silico Methods Int. J. Genomics and Proteomics, Volume 2, Number 1. **ISSN:1540-260**.
- 21) Chittasuresh Kumar, C.M. Anuradha, K. Venkata Rao, **K. Venkateswara Swamy** (2006) In silico Characterization of Fatty acid synthase of *Mycobacterium tuberculosis* H37Rv. Int. J. Genomics and Proteomics, volume 2, Number 1 **ISSN:1540-260**.
- 22) Chitta Suresh Kumar, C. M. Anuradha, **K. Venkateswara Swamy** (2005), Genomic characterization of Chromosome 1 *Plasmodium falciparum* by computational Method. Int .J. Microbiology Volume 1 Number **ISSN: 1937-8289**.

National: 03

- 1) Rachna Pandey, **K V Swamy**, Madhukar B Khetmalas (2013) Indole: A novel signaling molecule and its applications. *Indian journal of Biotechnology*vol 12, 297-310(**Impact factor 0.36**)

- 2) P Sharma, P Patil, N Rao, **KV Swamy**, MB Khetmalas, GD Tandon (2013) Algal Database—Bioprospecting indigenous algae for industrial application. *Indian journal of Biotechnology* vol12, 548-549(**Impact factor 0.36**)
- 3) **Swamy KV**, SupriyaKore, Rachna Pandey, Madhukar Khetmalas (2011) Extraction, isolation, molecular modeling and optimization of antimicrobial agents from *Coriandrum sativum*. *Current Trends in Biotechnology and Pharmacy*. 4 (5):1033-1038.

Conference Proceeding: 03

- 1) **K Venkateswara Swamy** and Kiran Bharat Lokhande, Molecular modeling, docking, dynamics and simulation of deguelin and its derivatives with cyclin D1 and cyclin E in cancer cell signaling pathway. *J Proteomics Bioinform*, 10:11(Suppl), (2017).
- 2) Prachi Bhole, Kiran Bharat Lokhande, Shuchi Nagar, **K. Venkateswara Swamy**. Molecular Docking and Molecular Dynamics Simulation studies of DHFR inhibitors in Plasmodium falciparum. *Can J Biotech*, Volume 1, Special Issue, Page 23, (2017).
- 3) Rohit Singh Yadav, Kiran Bharat Lokhande, Vaddi Damodara Reddy, **K. Venkateswara Swamy**. Molecular Docking and Molecular Dynamic studies of Phytocompounds with HIF-1alpha, HIF-2alpha, and SREBP1c to explore its Inhibitory Effect on Metabolic disorders and in Cancer. *Can J Biotech*, Volume 1, Special Issue, Page 25, (2017).

Trainings

1. Workshop on “**Development of signaling pathways network**” at Rajiv Gandhi Centre for Biotechnology, Thiruvanthapuram, Kerala during January, 11-13, 2016.
2. SLI- International webcasting on **Basic aspects in Bioinformatics** organized by Department of Biochemistry, Sri Krishnadevaraya University Department of

Biochemistry, Sri Krishnadevaraya University, Anantapur, Andhra Pradesh during 19-20 March, 2011.

3. Two day National workshop on “**Python programming and Data visualization**” organized by Department of Bioinformatics, Dr.G.R. Damodaran College of Science, and Coimbatore during 17-18 March, 2007.
4. **Advanced Immunology** course organized by 8th FIMSA/IIS, New Delhi during 1-5 March, 2006.
5. National workshop on **molecular modeling and drug designing using tripos (sibyl software)** conducted by department of genetics, Osmania university, Hyderabad on 9 -02-2005.
6. Second National workshop on **Genome and Proteome analysis** conducted by Dept. of biochemistry, Sri Krishnadevaraya university, Anantapur, Andhra Pradesh on 21-03-2005.
7. National workshop on **Bio-computing tools** (Bioinformatics) conducted by Kuvempu university, shimoga, Karnataka on 25th Oct, 2004

Invited Speaker

1. National workshop on “**Molecular modeling and Drug designing**” organized by Department of Chemistry, Savitribai Phule Pune University during 25-30 March 2015.
2. Two day National Level seminar on “**Advanced Drug Design and Development: A Medicinal Chemistry Approach**” organized by PadmashreeDr .D.Y.Patil Institute of Pharmaceutical Sciences and Research, Pune on 27-09-2013
3. State level seminar on “**Drug Discovery, Development and Delivery**” organized by Pad.Dr.D.Y.Patil institute of Pharmaceutical Science and Research, Pimpri, Pune during 15-16 February 2008.
4. Second National Workshop on “**Genome and proteome Analysis**” organized by Department of Biochemistry, Sri Krishnadevaraya University, Anantapur, Andhra Pradesh during 21-23 March,2005.
5. Key note speaker at National workshop on “**Sequence annotations and Molecular modeling of Cancer targeted Proteins** “ organized by Dept of Biochemistry & Biotechnology, S. K. Univeristy, Anantapur, Andhra Pradesh, India on 27-03-2015
6. Invited speaker at 7th National workshop on “**Application of Structural Bioinformatics to Drug design and Discovery**” conducted by Department of Biochemistry, Sri Krishnadevaraya University, Anantapur, Andhara Pradesh, India on March 19-20th, 2011.
7. Invited speaker at National Seminar on “**Structural Bioinformatics**” conducted by Arts and Science College, Dandeli, Karnataka, India on Feb 12th, 2010.

Paper presentation

1. Oral Presentation on “Molecular modeling, docking, dynamics and simulation of Deguelin and its derivatives with cyclin D1 and cyclin E in cancer cell signaling pathway”, in 9th International Conference and Expo on Proteomics and Molecular Medicine & 9th International Conference on Bioinformatics, at France, Paris. 13th – 15th Nov., 2017.
2. Oral presentation on "*Molecular modeling and docking studies on curcumin and curcumin analogs with cyclooxygenase-2*" at 4th International conference on Medicinal plants and Medicinal herbs, Johns Hopkins University, Washington, USA, 6-8th September, 2012
3. Oral presentation on “*Structural and functional characterization of Fatty acid synthase Mycobacterium tuberculosis- insilico methods*” at three day National level seminar on “Structural Bioinformatics” organized by Department of Bioinformatics, Dr. G.R. Damodaran College of Science, Coimbatore during 18-20 August, 2005.
4. Oral presentation on "*Molecular modeling and docking studies on curcumin and curcumin analogs with cyclooxygenase-2*" at National conference on Recent trends in Biotechnology and Bioinformatics organized by Department of Biotechnology and Bioinformatics, Yogi Vemana University, Kadapa, Andhra Pradesh during 12-13 February, 2014.

Poster presentations at international level seminars

1. Poster presented on “**Molecular Modeling and Docking Studies of Aromatase Inhibitors with Aromatase for ERP Breast Cancer**” in 86th Conference of Society of Biological Chemists (SBC) - Emerging Discoveries in Health and Agricultural Sciences organized by School of Life Sciences, Jawaharlal Nehru University, New Delhi, during 16th – 19th Nov., 2017.
2. Poster presented on “**Molecular docking and Molecular Dynamics studies of phytochemicals with HIF-1 α , HIF-2 α and Srebp1c to explore its inhibitory effect on metabolic disorder in cancer**”, in 2017 NextGen Genomics, Biology, Bioinformatics and Technologies (NGBT) organized by SGRF, at Bhubaneswar, Odisha, India. 1st - 4th Oct, 2017.
3. Poster presented on “**Molecular Docking and Molecular Dynamics Simulation studies of DHFR inhibitors in Plasmodium falciparum**”, in 2017 NextGen Genomics, Biology, Bioinformatics and Technologies (NGBT) organized by SGRF, at Bhubaneswar, Odisha, India. 1st - 4th Oct, 2017.
4. Poster presented on “**Molecular Modeling, Docking, Dynamics and Simulation of Deguelin and Its Derivatives with Cyclin D1 and Cyclin E In Cancer Cell Signaling Pathway**” in International Conference on Drug Design, at Convention Centre, Jawaharlal

Nehru University, New Delhi, on 8th April, 2017.

5. Poster presentation at National Symposium on “**Molecular modeling and docking studies of deguelin with cyclin D, Cyclin E and PI3 γ proteins**” organized by CDAC, Pune during 19-21 January, 2016.
6. Poster presented on “**Homology modeling of Plasmodium Vivax protein phosphatase V and validation of the structure**’ at S.V. University, Tirupathi, Andhra Pradesh on 25th November, 2007.
7. Poster presented on “**Homology modeling of D-alanine D-alanine ligase of *M. tuberculosis* CDC 1551**” at Osmania university, Hyderabad, Andhra Pradesh on 9th January, 2006.
8. Poster presented on “**Homology modeling of Human histamine H2 receptor and Docking studies**” at AIIMS, New Delhi on 1st March, 2006.