Dileep Vijayan. M.Sc., Ph.D.

Current position :

Scientist D and NRI/OCI/PIO fellow (DHR, Govt. of India)
Laboratory for Computational and Structural Biology,
Jubilee Centre for Medical Research,
Jubilee Mission Medical College & Research Institute,
Thrissur, Kerala- 680005,
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Career objectives and Research focuses :

My primary research focus is performing chemical biology research to propose lead molecules majorly for the drug targets in neurodegenerative disorders, epigenetics, cancer and inflammatory-related diseases by combining multiscale computational approaches with x-ray crystallography and other biophysical methods.

I am also interested to study the structure, function and dynamics of various biological macromolecules using my expertise in computational and structural biology and efficiently customize them for various purposes ranging from drug discovery to nanotechnology. In addition to that, I am interested to study the structure, dynamics and catalysis of the various chemical systems by means of classical molecular dynamics simulations coupled with QM/MM simulations and free energy estimation.

Skills :

- Protein designing and engineering.
- X-ray crystallography and structural analysis of biological macromolecules.
- Computer aided drug design and chemi-informatics
- Performing multi scale computational approaches like molecular dynamics, free energy perturbations, high throughput virtual screening.
- Expression, purification and biophysical characterization of protein ligand interactions.
- *In vitro* cell culture and cytotoxicity analysis.
- Other basic computational skills.

Professional Experiences :

- **Scientist D and NRI/OCI/PIO fellow : 22.11.21 to till date**
  Jubilee Center for Medical Research, JMMCRI, Thrissur, India.

- **Scientist D : 01.06.21 to 21.11.21**
  Jubilee Center for Medical Research, JMMCRI, Thrissur, India.

- **Research Scientist : 01.12.2018 to 31.05.2021**
  Laboratory for Structural Bioinformatics, RIKEN, Yokohama, Japan.

- **Visiting Researcher (JSPS Postdoctoral Fellowship) : 30.11.2016 to 29.11.2018**
  Laboratory for Structural Bioinformatics, RIKEN, Yokohama, Japan.

- **International postdoctoral Fellow (Takeda Science Foundation) : 09.05.2016 to 15.11.2016**
  Laboratory for Structural Bioinformatics, RIKEN, Yokohama, Japan.

- **Institute Postdoc Fellow : 22.12.2014 to 26.04.2016**
  School of Chemistry, IISER - Thiruvananthapuram, Kerala, India.

- **Junior Scientist : 01.07.2014 to 20.12.2014**
  Dept. of Computational Biology and Bioinformatics, University of Kerala, India.

- **Senior Research Fellow (ICMR Fellowship) : 28.11.2011 to 30.06.2014**
  Dept. of Biotechnology and Microbiology, Kannur University, India.
- **Research Fellow : 18.11.2008 to 19.02.2014**
  Dept. of Biotechnology and Microbiology, Kannur University, India.
- **Research Assistant : 19.04.2008 to 30.09.2010**
  Bioinformatics Infrastructure Facility, Dept. of Biotechnology and Microbiology, Kannur University, India.
- **Research Associate : 11.10.2007 to 18.04.2008**
  Bioinformatics Centre (DIC), Kerala Agricultural University, Kerala, India.
- **Senior Research Fellow : 01.03.2007 to 10.10.2007**
  Bioinformatics Centre (DIC), Kerala Agricultural University, Kerala, India.
- **Technical Assistant : 26.06.2006 to 28.02.2007**
  Kerala Forest Research Institute, Kerala, India.
- **Research Fellow : 06.02.2006 to 24.06.2006**
  Kerala Forest Research Institute, Kerala, India.
- **Project Assistant : June 2005 to February 2006**
  Kerala Forest Research Institute, Kerala, India.

Professional Affiliations :

- **Visiting scientist -** Laboratory for Structural Bioinformatics, RIKEN, Yokohama, Japan.
- **Molecular modeling consultant –** Evestra Inc., 14805 Omicron Dr #100, San Antonio, TX 78245, United States.
- **Founder and CEO –** Smart leads, at seed-stage.

Educations :

- **Ph.D :** ("Studies on interactions of selected indole derivatives with their target proteins associated with alzheimers disease and neuroinflammation"). Dept. of Biotechnology and Microbiology, Kannur University, India. 2015. Research supervisor. Prof. C. Sadasivan
- **Master of Science in Bioinformatics :** KSR college of Arts and Science, Thiruchengode, Tamil Nadu, India. 2005.
- **Bachelor in Chemistry :** St. Thomas College, Thrissur, Kerala, India. 2003.

Awards and Honours :

- **DHR-NRI/PIO/OCI re-entry fellowship.** 2021-2024 by Department of Health Research (DHR), Govt. of India.
- **Japan Society of the Promotion of Science (JSPS) Postdoctoral Fellowship for Overseas Researchers.** 2016-2018 by Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan.
- **International postdoctoral fellowship, (Takeda Science Foundation).** 24-02-2016.
- **Institute postdoctoral Fellowship, IISER, Thiruvananthapuram, Kerala, India.** 12-05-2014.
- **Best poster award.** "New Horizons and Challenges in Biotechnology and Bioinformatics". National seminar during 9-10 October 2014 held at Central Plantation Crops Research Institute, Kerala, India.

- **Best poster award.** "Bioinformatica Indica 2014". International Conference on 9-14 January 2014 held at Kerala University, India.
- **1st prize.** "Perspectives and issues in structural biology (PISB-2012) Motif '12". National Symposium on 14th September 2012 held at Bharathiar University, Tamil Nadu. India.
- **2nd prize.** "Perspectives and issues in structural biology (PISB-2012) Motif '12". National Symposium on 14th September 2012 held at Bharathiar University, Tamil Nadu, India.
- **Senior Research Fellowship (ICMR).** 28th November 2011.
- **1st prize.** "Bio Revolutions-04".National Symposium on 13th and 14th September 2004 held at Kongunadu College of arts and science, Tamil Nadu India

Research Grants :

- **Research grant for the Alzheimer's diseases** – Project Number MKT-PD&R/003/2021-Marketing. **5,008,000 INR.** Project title: Elucidating the role of spices as preventive and therapeutic agents for Alzheimer's disease
- **Research grant for the Ayurbiology project** – Institutional research grant. **600,000 INR.** Project title: Study on the phenotypic-genotypic relations of Ayurveda prakriti through a multi-disciplinary approach.
- **Research grant for the DHR-NRI/PIO/OCI re-entry fellows –** Project number NRIPIO/2020/000004/PRCNRI. **9,244,910 INR**. Project title: Non-invasive treatment of uterine fibroids through rationally designed selective progesterone receptor modulators.
- **Research grant for the JSPS - Postdoctoral Fellows –** Project number 16F16385. **2,400,000 JPY (approx. 1,600,000 INR)**. Project title: Discovery of human Glutaminyl Cyclase inhibitors for the treatment of Alzheimer's disease.

Publications in peer reviewed journals : *Corresponding author, #Equal contribution

1. S. Hima, C. Remya, C. Sadasivan, **K.V. Dileep.** 2023. Carboxylic acid derivatives suppress the growth of Aspergillus flavus through the inhibition of fungal alpha-amylase. J. Biomol. Struct. Dyn., pp.1-5.
2. A. Babu, M. John, M. J. Liji, E. Maria, S. J. Bhasker, B. K. Binukumar, A. M. Sajith, E. K. Reddy, **K.V. Dileep**, K. Sunil. Sub-pocket-focused designing of tacrine derivatives as potential acetylcholinesterase inhibitors. 2023. https://doi.org/10.1016/j.compbiomed.2023.106666.
3. F. Saritha, N. Aiswarya, R. Aswath Kumar, **K. V. Dileep**. Structural analysis and ensemble docking revealed the binding modes of selected progesterone receptor modulators. J. Biomol. Struct. Dyn. 2023. https://doi.org/10.1080/07391102.2023.2166999.
4. N. Aiswarya, C. Remyaa, A.B. Remashree, C. Sadasivan, **K.V. Dileep**. Binding of rosmarinic acid curcumin and capsaicin with PLA2: A comparative study. Biochem. Biophys. Res. Commun. 626 (2022) 187-191.
5. **K.V. Dileep**, K. Ihara, C. Mishima-Tsumagari, M. Kukimoto-Niino, M. Yonemochi, K. Hanada, M. Shirouzu, K.Y.J Zhang. Crystal structure of human acetylcholinesterase in complex with tacrine: Implications for drug discovery. Int. J. Biol. Macromol. 210 (2022) 172-181.
6. P. Gupta, I.P. Kadamberi, S. Mittal , S.W. Tsaih, J. George , S. Kumar, **D.K. Vijayan**, A. Geethadevi, D. Parashar, P. Topchyan, L. McAlarnen, B.F. Volkman, W. Cui, K.Y.J. Zhang, D. Di Vizio, P.C. Raghavan, S. Pradeep. Tumor Derived Extracellular Vesicles Drive T Cell Exhaustion in Tumor Microenvironment through Sphingosine Mediated Signaling and Impacting Immunotherapy Outcomes in Ovarian Cancer. Adv Sci (Weinh). 9 (2022) 2104452 (1-15).
7. C. Remya, **K.V. Dileep**. Exploring the binding mode of PQ912 against secretory glutaminyl cyclase through systematic exploitation of conformational ensembles. Chem. Biol. and Drug Des. 2021. (In press)
8. C. Remya, **K.V. Dileep**, E.K. Reddy, K. Mantosh, K. Lakshmi, R.S. Jacob, A.M. Sajith, E.J. Variyar, S. Anwar, K.Y.J. Zhang, C. Sadasivan, R.V. Omkumar. Neuroprotective derivatives of tacrine that

target NMDA receptor and acetyl cholinesterase - Design, synthesis and biological evaluation. Comput. Struct. Biotechnol. 2021. (Accepted)

9. S. Balan, Y. Iwayama, T. Ohnishi, M. Fukuda, A. Shirai, A. Yamada, S. Weirich, M.S. Schuhmacher, **K.V. Dileep**, T. Endo, Y. Hisano, K. Kotoshiba, T. Toyota, T. Otowa, H. Kuwabara, M. Tochigi, A. Watanabe, M. Ohba, M. Toyoshima, T. Sasaki, K. Nakamura, M. Tsujii, H. Matsuzaki, K.Y.J. Zhang, A. Jeltsch, Y. Shinkai, T. Yoshikawa. A loss of function variant in SUV39H2 identified in autism spectrum disorder causes altered H3K9-trimethylation and dysregulation of protocadherin β cluster genes in the developing brain. Molecular Psychiatry. 2021. (doi: 10.1038/s41380-021-01199-7)
10. S. Viswanadhapalli, **K.V. Dileep**, KYJ Zhang, HB Nair, RK Vadlamudi. Targeting LIF/LIFR signaling in cancer. Genes & Diseases. 2021. (https://doi.org/10.1016/j.gendis.2021.04.003).
11. M. Janezic, **K.V. Dileep**, KYJ. Zhang. A multidimensional computational exploration of congenital myasthenic syndrome causing mutations in human choline acetyltransferase. J Cell Biochem. 122 (8) (2021) 787-800.
12. C. Remya, **K.V. Dileep**, E.J. Variyar, K.Y.J. Zhang, R.V. Omkumar, C. Sadasivan. Chemical Similarity assisted search for acetylcholinesterase inhibitors: Molecular modeling and evaluation of their neuroprotective properties. Int. J. Biol. Macromol. 174 (2021) 466-476.
13. **K.V. Dileep**, S. Naoki, K. Ihara, M.K. Murayama, A. Nakata, A. Ito, D.M. Sivaraman, J.W. Shin, M. Yoshida, M. Shirouzu, K.Y.J. Zhang. Piperidine-4-carboxamide as a new scaffold for designing secretory glutaminyl cyclase inhibitors. Int. J. Biol. Macromol. 170 (2021) 415–423.
14. M. Aditi, **K.V. Dileep**, K Mukesh, P Mukta, P Kavita, K.Y.J. Zhang, S. Vinod[*], B.K. Binukumar[*]. ATP7A Clinical Genetics Resource – a comprehensive clinically annotated database and resources for genetic variants in ATP7A gene, Comput Struct Biotec. 18 (2020) 2347-2356.
15. X. Yue, F. Wu, J. Wang, K. Kim, B. Santhamma, **K.V. Dileep**, K.Y.J. Zhang, S. Viswanadhapalli, R.K. Vadlamudi, G. Ahmed, Z. Feng, K. Nickisch, W. Hu[*], EC330, a small-molecule compound, is a potential novel inhibitor of LIF signaling, J Mol Cell Biol 12(6) (2020) 477-480.
16. **D. Vijayan**[*], R. Chandra, Amyloid Beta Hypothesis in Alzheimer's Disease: Major Culprits and Recent Therapeutic Strategies, Curr Drug Targets 21(2) (2020) 148-166.
17. H. Shabeer Ali, K. Ajesh, **K.V. Dileep**, P. Prajosh, K. Sreejith[*], Structural characterization of Kannurin isoforms and evaluation of the role of beta-hydroxy fatty acid tail length in functional specificity, Sci Rep 10(1) (2020) 2839.
18. N. Krishnan, D. Perumal, S. Atchimnaidu, K.S. Harikrishnan, M. Golla, N.M. Kumar, J. Kalathil, J. Krishna, **D.K. Vijayan**, R. Varghese[*], Galactose-Grafted 2D Nanosheets from the Self-Assembly of Amphiphilic Janus Dendrimers for the Capture and Agglutination of Escherichia coli, Chem. Eur. J. 26(5) (2020) 1037-1041.
19. **K.V. Dileep**[*], S. Ashok, C. Remya, K.Y. Dharmendra, H. Perez-Sanchez[*], C. Sadasivan[*], Indole fragments for the design of lead molecules against pancreatitis, J. Biomol. Struct. Dyn 38(1) (2020) 263-267.
20. S. Viswanadhapalli, Y. Luo, G.R. Sareddy, B. Santhamma, M. Zhou, M. Li, S. Ma, R. Sonavane, U.P. Pratap, K.A. Altwegg, X. Li, A. Chang, A. Chavez-Riveros, **K.V. Dileep**, K.Y.J. Zhang, X. Pan, R. Murali, M. Bajda, G.V. Raj, A.J. Brenner, V. Manthati, M.K. Rao, R.R. Tekmal, H.B. Nair[*], K.J. Nickisch, R.K. Vadlamudi[*], EC359: A First-in-Class Small-Molecule Inhibitor for Targeting Oncogenic LIFR Signaling in Triple-Negative Breast Cancer, Mol Cancer Ther 18(8) (2019) 1341-1354.
21. **D.K. Vijayan**, K.Y.J. Zhang[*], Human glutaminyl cyclase: Structure, function, inhibitors and involvement in Alzheimer's disease, Pharmacol Res 147 (2019) 104342.
22. H.B. Nair[*], B. Santhamma, **K.V. Dileep**, P. Binkley, K. Acosta, K.Y.J. Zhang, R. Schenken, K. Nickisch, EC313-a tissue selective SPRM reduces the growth and proliferation of uterine fibroids in a human uterine fibroid tissue xenograft model, Sci Rep 9(1) (2019) 17279.
23. **K.V. Dileep**[*], C. Remya, I. Tintu, P.K. Mandal, P. Karthe, M. Haridas, C. Sadasivan[*], Crystal structure of phospholipase A2 in complex with 1-naphthaleneacetic acid, IUBMB Life 70(10) (2018) 995-1001. Selected as - Highlight of the issue and Cover page. https://doi.org/10.1002/iub.1938.
24. **K.V. Dileep**[*], K. Nithiyanandan, C. Remya, Binding of acarbose, an anti-diabetic drug to lysozyme: a combined structural and thermodynamic study, J Biomol Struct Dyn 36(13) (2018) 3354-3361.

25. P. Haris, V. Mary, P. Aparna, **K.V. Dileep**, C. Sudarsanakumar[*], A comprehensive approach to ascertain the binding mode of curcumin with DNA, Spectrochim Acta A Mol Biomol Spectrosc 175 (2017) 155-163.
26. C. Remya, **K.V. Dileep**, E.J. Variayr, C. Sadasivan[*], An in silico guided identification of nAChR agonists from Withania somnifera, Front Life Sci 9(3) (2016) 201-213.
27. E.K. Reddy, C. Remya, A.M. Sajith, **K.V. Dileep**, C. Sadasivan, S. Anwar[*], Functionalised dihydroazo pyrimidine derivatives from Morita-Baylis-Hillman acetates: synthesis and studies against acetylcholinesterase as its inhibitors, Rsc Adv 6(81) (2016) 77431-77439.
28. H.B. Nair[*], B. Santhamma, N.K. Krishnegowda, **K.V. Dileep**, K.J. Nickisch, Effects of Combination of Estradiol with Selective Progesterone Receptor Modulators (SPRMs) on Human Breast Cancer Cells In Vitro and In Vivo, Plos One 11(3) (2016).
29. **K.V. Dileep**[*], V. Vijeesh, C. Remya, Rational design and interaction studies of combilexins towards duplex DNA, Mol Biosyst 12(3) (2016) 860-867.
30. M.J. Tomy, C.S. Sharanya, **K.V. Dileep**, S. Prasanth, A. Sabu, C. Sadasivan, M. Haridas[*], Derivatives Form Better Lipoxygenase Inhibitors than Piperine: In Vitro and In Silico Study, Chem Biol Drug Des 85(6) (2015) 715-721.
31. **K.V. Dileep**, C. Remya, I. Tintu, M. Haridas, C. Sadasivan[*], Binding of NDGA and morin with phospholipase A(2): experimental and computational evidences, Mol Simulat 41(4) (2015) 281-286.
32. **K.V. Dileep**, C. Remya, J. Cerezo, A. Fassihi, H. Perez-Sanchez, C. Sadasivan[*], Comparative studies on the inhibitory activities of selected benzoic acid derivatives against secretory phospholipase A(2), a key enzyme involved in the inflammatory pathway, Mol Biosyst 11(7) (2015) 1973-1979.
33. S.R. Aravind, M.M. Joseph, S.K. George, **K.V. Dileep**, S. Varghese, A. Rose-James, P. Balaram, C. Sadasivan, T.T. Sreelekha[*], TRAIL-based tumor sensitizing galactoxyloglucan, a novel entity for targeting apoptotic machinery, Int J Biochem Cell B 59 (2015) 153-166.
34. M.J. Tomy[#], **K.V. Dileep**[#], S. Prasanth, D.S. Preethidan, A. Sabu, C. Sadasivan, M. Haridas[*], Cuminaldehyde as a Lipoxygenase Inhibitor: In Vitro and In Silico Validation, Appl Biochem Biotech 174(1) (2014) 388-397. ([#]Equal contribution)
35. I. Tintu[#], J. Abhilash[#], **K.V. Dileep**[#], A. Augustine, M. Haridas, C. Sadasivan[*], A Lectin from Spatholobus parviflorus Inhibits Aspergillus flavus -Amylase: Enzyme Kinetics and Thermodynamic Studies, Chem Biol Drug Des 84(1) (2014) 116-122. ([#]Equal contribution)
36. C. Remya, **K.V. Dileep**, I. Tintu, E.J. Variyar, C. Sadasivan, Flavanone Glycosides as Acetylcholinesterase Inhibitors: Computational and Experimental Evidence, Indian J Pharm Sci 76(6) (2014) 567-570.
37. **K.V. Dileep**, C. Remya, I. Tintu, C. Sadasivan[*], Interactions of selected indole derivatives with COX-2 and their *in silico* structure modifications towards the development of novel NSAIDs, Journal of Biomolecular Structure & Dynamics 32(11) (2014) 1855-1863.
38. **K.V. Dileep**, C. Remya, I. Tintu, M. Haridas, C. Sadasivan[*], Inhibitory activity of IAA and IBA against lipoxygenase: in silico and in vitro validation, Mol Simulat 40(5) (2014) 418-422.
39. C. Remya, **K.V. Dileep**, I. Tintu, E.J. Variyar, C. Sadasivan[*], In vitro inhibitory profile of NDGA against AChE and its in silico structural modifications based on ADME profile, J Mol Model 19(3) (2013) 1179-1194.
40. **K.V. Dileep**, C. Remya, I. Tintu, C. Sadasivan[*], Inhibition, ADME and structure-based modification of IAA and IBA against acetylcholinesterase: an attempt towards new drug development for Alzheimer's disease, Front Life Sci 7(3-4) (2013) 164-173.
41. **K.V. Dileep**, C. Remya, I. Tintu, C. Sadasivan[*], Designing of multi-target-directed ligands against the enzymes associated with neuroinflammation: an in silico approach, Front Life Sci 7(3-4) (2013) 174-185.
42. **K.V. Dileep**, C. Remya, I. Tintu, M. Haridas, C. Sadasivan[*], Interactions of selected indole derivatives with phospholipase A(2): in silico and in vitro analysis, J Mol Model 19(4) (2013) 1811-1817.
43. S. Bhaskaran, **K.V. Dileep**, S.S. Deepa, C. Sadasivan, M. Klausner, N.K. Krishnegowda, R.R. Tekmal, J.L. VandeBerg, H.B. Nair[*], Gossypin as a Novel Selective Dual Inhibitor of v-raf Murine Sarcoma Viral Oncogene Homolog B1 and Cyclin-Dependent Kinase 4 for Melanoma, Molecular Cancer Therapeutics 12(4) (2013) 361-372.
44. V. Aparna, **K.V. Dileep**, C. Sadasivan, M. Haridas[*], Computational and thermodynamic analyses of the phospholipase A(2) inhibition by erucic acid and linoleic acid, Med Chem Res 22(3) (2013) 1102-1106.

45. J. Abhilash[#], **K.V. Dileep**[#], M. Palanimuthu, K. Geethanandan, C. Sadasivan, M. Haridas[*], Metal ions in sugar binding, sugar specificity and structural stability of Spatholobus parviflorus seed lectin, J Mol Model 19(8) (2013) 3271-3278. ([#]Equal contribution)
46. **K.V. Dileep**, M. Kelly, E. Hardin, C. Sadasivan, H.B. Nair[*], Approaches in the chemoprevention of breast cancer, J Cancer Sci Ther 5(8) (2013) 282-288.
47. I. Tintu, **K.V. Dileep**, C. Remya, A. Augustine, C. Sadasivan[*], 6-Gingerol inhibits fungal alpha amylase: Enzyme kinetic and molecular modeling studies, Starch-Starke 64(8) (2012) 607-612.
48. I. Tintu, **K.V. Dileep**, A. Augustine, C. Sadasivan[*], An Isoquinoline Alkaloid, Berberine, Can Inhibit Fungal Alpha Amylase: Enzyme Kinetic and Molecular Modeling Studies, Chem Biol Drug Des 80(4) (2012) 554-560.
49. C. Remya, **K.V. Dileep**, I. Tintu, E.J. Variyar, C. Sadasivan[*], An in silico approach for the identification of inhibitors against Acetylcholinesterase, Med Chem Res 21(10) (2012) 2779-2787.
50. C. Remya, **K.V. Dileep**, I. Tintu, E.J. Variyar, C. Sadasivan[*], Design of potent inhibitors of acetylcholinesterase using morin as the starting compound, Front Life Sci 6(3-4) (2012) 107-117.
51. **K.V. Dileep**, I. Tintu, C. Remya, M. Haridas, C. Sadasivan[*], Studies of IAA and IBA as fungal a-amylase inhibitors using enzyme kinetics, molecular modeling and thermodynamics, Starch-Starke 64(12) (2012) 991-995.
52. **K.V. Dileep**, I. Tintu, P.K. Mandal, P. Karthe, M. Haridas, C. Sadasivan[*], Binding to PLA2 May Contribute to the Anti-Inflammatory Activity of Catechol, Chem Biol Drug Des 79(1) (2012) 143-147.
53. V. Aparna[#], **K.V. Dileep**[#], P.K. Mandal, P. Karthe, C. Sadasivan, M. Haridas[*], Anti-Inflammatory Property of n-Hexadecanoic Acid: Structural Evidence and Kinetic Assessment, Chem Biol Drug Des 80(3) (2012) 434-439. ([#]Equal contribution)
54. **K.V. Dileep**, I. Tintu, N.V. Vinod, P.P. Saliha, C. Sadasivan[*], Role of invariant water molecules in retaining the active site geometry of beta-lactamase: a molecular dynamics simulation study, Mol Simulat 37(15) (2011) 1234-1238.
55. **K.V. Dileep**, I. Tintu, C. Sadasivan[*], Molecular Docking Studies of Curcumin Analogs with Phospholipase A2, Interdiscip Sci 3(3) (2011) 189-197.
56. **K.V. Dileep**, I. Tintu, P.K. Mandal, P. Karthe, M. Haridas, C. Sadasivan[*], Crystal structure of porcine pancreatic phospholipase A(2) in complex with 2-methoxycyclohexa-2-5-diene-1,4-dione, Front Life Sci 5(3-4) (2011) 135-139.
57. N.V. Vinod, R. Shijina, **K.V. Dileep**, C. Sadasivan[*], Inhibition of Beta-Lactamase by 1,4-Naphthalenedione from the Plant Holoptelea integrifolia, Appl Biochem Biotech 160(6) (2010) 1752-1759.

Publications in book chapters :

1. **K.V. Dileep,** Venom as a Drug – pp: 197-204, Trends in Bioinformatics. Pointer publishers, Jaipur. ISBN 81-7132- 461-4.
2. **K.V. Dileep,** J Abhilash, A Sabu, C Sadasivan and M Haridas. Modeling of Tannin acyl hydrolase – pp: 188-199, Chemistry of Polyphenols. CiBET Publishers. ISBN 978-81-920782-0-5.

Protein Databank entries :

1. **KV Dileep**, G Tintu, P Karthe, PK Mandal, M Haridas and C Sadasivan. Crystal structure of porcine pancreatic phospholipase A2 in complex with 2-methoxycyclohexa-2-5-diene-1, 4-dione. PDB ID: 3HSW.
2. **KV Dileep**, G Tintu, P Karthe, PK Mandal, M Haridas and C Sadasivan. Crystal structure of porcine pancreatic phospholipase A2 in complex with 1,2-dihydroxybenzene. PDB ID: 3O4M.
3. V Aparna, **KV Dileep**, P Karthe, PK Mandal, C Sadasivan and M Haridas. Crystal structure of porcine pancreatic phospholipase A2 in complex with n-hexadecanoic acid. PDB ID: 3QLM.
4. **KV Dileep**, C Remya, G Tintu, P Karthe, PK Mandal, M Haridas and C Sadasivan. Crystal structure of Porcine Pancreatic Phospholipase A2 in complex with 1-Naphthaleneacetic acid. PDB ID: 4O1Y.
5. **KV Dileep**, K Ihara, N Sakai, M Shirozu, K.Y.J. Zhang. Crystal Structure of double mutant Y115E Y117E human Secretory Glutaminyl Cyclase. PDB ID: 7CP0.
6. **KV Dileep**, K Ihara, N Sakai, M Shirozu, K.Y.J. Zhang. Crystal Structure of double mutant Y115E Y117E human Secretory Glutaminyl Cyclase in complex with LSB-41. PDB ID: 7COZ.

7. **KV Dileep**, K Ihara, N Sakai, M Shirozu, K.Y.J. Zhang. Crystal Structure of double mutant Y115E Y117E human Secretory Glutaminyl Cyclase in complex with LSB-09. PDB ID: 7D8E.
8. **KV Dileep**, K Ihara, C Mishima-Tsumagari, M Kukimoto-Niino, M Yonemochi, K Hanada, M Shirozu, K.Y.J. Zhang. Crystal structure of human acetylcholinesterase. PDB ID: 7E3D
9. **KV Dileep**, K Ihara, C Mishima-Tsumagari, M Kukimoto-Niino, M Yonemochi, K Hanada, M Shirozu, K.Y.J. Zhang. Crystal structure of human Acetylcholinesterase in complex with donepezil. PDB ID: 7E3H
10. **KV Dileep**, K Ihara, C Mishima-Tsumagari, M Kukimoto-Niino, M Yonemochi, K Hanada, M Shirozu, K.Y.J. Zhang. Structure of human acetylcholinesterase in complex with tacrine. PDB ID: 7E3I

Other interests :

- Reading, Teaching, Cooking and Sports.

References :

1. Dr. C. Sadasivan, Professor, Department of Biotechnology and Microbiology, Thalassery Campus, Kannur University, Kerala, India.
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