

# List of Publications

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**This thesis is partly based on the following original communications:**

1. **Sarma, H.** and Mattaparthi, V. S. K. Structure based virtual screening of high-affinity ATP competitive inhibitors against Human Lemur Tyrosine Kinase-3 (LMTK3) domain- a novel therapeutic target for breast cancer. *Interdisciplinary sciences computational life sciences*, 2018, DOI: 10.1007/s12539-018-0302-7.
2. **Sarma, H.** and Mattaparthi, V. S. K. Salient Structural Features of Human Lemur Tyrosine Kinase 3 (LMTK3) Domain from Molecular Dynamics Simulation Study. *Current Biotechnology*, 7: 2018. DOI: 10.2174/2213529404666180125161856
3. **Sarma, H.** and Mattaparthi, V. S. K. Unveiling the transient Protein-Protein interactions that regulate the activity of Human Lemur Tyrosine Kinase-3 (LMTK3) domain by Cyclin-dependent kinase 5 (CDK5) in breast cancer: An *in silico* study. *Current Proteomics*, 15: 62-70, 2018.
4. **Sarma, H.** and Mattaparthi, V. S. K. Effect of activation loop phosphorylation on Lemur Tyrosine Kinase 3(LMTK3) activity: A Molecular Dynamics Simulation Study. *Biological Forum: An International Journal*, 9(1): 01-13, 2017.
5. **Sarma, H.** and Mattaparthi, V. S. K. Unveiling the transient Protein-Protein interactions that modulate the activity of Estrogen Receptor (ER)- $\alpha$  by Human Lemur Tyrosine Kinase-3 (LMTK3) domain: An *in silico* study. *Current Proteomics*, 14: 1-8, 2017.

## Other publications

1. Pradhan, S. and **Sarma, H.** Bharadwaz, B., and Mattaparthi V. S. K. Comparative Study on the Binding Affinity of Methimazolean Propylthiouracil to Thyroid Peroxidase as an Anti-Thyroid Drug: An *In silico* Approach. *Journal of Molecular Imaging and Dynamics*, 7(1):1000131, 2017.
2. Pradhan, S. and **Sarma, H.**, Mattaparthi V. S. K. Investigation of the probable homo-dimer model of the *Xeroderma pigmentosum* complementation group A (XPA) protein to represent the DNA binding core. *Journal of Biomolecular Structure and Dynamics*, 2018. DOI: 10.1080/07391102.2018.1517051
3. Book Chapter “Phylogenetic Analysis: Early Evolution of Life” has been published in “Encyclopedia of Bioinformatics and Computational Biology” doi:10.1016/B978-0-12-809633-8.20171-4. (ELSEVIER Publishers).

**In addition, this thesis also contains unpublished data.**

# Conference Proceedings

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- Organized and **Attended lecture series and hands on training** on International Seminar cum Workshop on “Computer Aided Drug Design for Human Pathogen” at Department of Molecular Biology and Biotechnology, Tezpur University, Tezpur, Assam, India, held on 12<sup>th</sup> – 17<sup>th</sup> February 2018
- **Sarma, H., and Mattaparthi V. S. K.** Unveiling the transient Protein-Protein interactions that modulate the activity of Estrogen Receptor(ER)- $\alpha$  by Human Lemur Tyrosine Kinase-3 (LMTK3) domain: An in silico study. International conference on “Emerging Trends in Chemical Sciences” (ETCS-2018) held at Department of Chemistry, Dibrugarh University, Assam, India, held on 26<sup>th</sup> - 28<sup>th</sup> March 2018. (Poster presentation)
- **Sarma, H., and Mattaparthi V. S. K.** Structure based virtual screening of novel high-affinity ATP competitive inhibitors against Human Lemur Tyrosine Kinase-3 (LMTK3) domain. Research conclave on “Recent Innovations in Science and Engineering 2017” at NIT Silchar, Assam, India held on 24<sup>th</sup> - 26<sup>th</sup> March 2017. (Oral Presentation)
- **Sarma, H., and Mattaparthi V. S. K.** Effect of activation loop phosphorylation on Lemur Tyrosine Kinase 3 (LMTK3) activity: A Molecular Dynamics Simulation Study. Symposium on “Accelerating Biology” at C-DAC, Pune, Maharashtra, India, held on 17<sup>th</sup> - 19<sup>th</sup> January 2017 (Poster presentation)
- **Sarma, H., and Mattaparthi V. S. K.** Human LMTK3 domain: Modelling, Structural Dynamics and Virtual Screening of Novel High Affinity Inhibitors. At National Network for Mathematical and Computational Biology (NNMCB), National Meeting at IISER Pune, Maharashtra, India, held on 27<sup>th</sup> - 30<sup>th</sup> December 2015, (Oral and Poster Presentation)
- **Attended** a National conference on “Recent Advance in Cancer Biology and Therapeutics” held on 5<sup>th</sup> Dec 2014, organized by IIT Guwahati, Dept of Biotechnology.