COMPUTATIONAL BIOLOGY WEBINAR @ IMSc

STRUCTURAL AND DYNAMICAL INSIGHTS INTO MAMMALIAN CIRCADIAN CLOCK PROTEINS

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The physiology and behavior of almost all living organisms on earth is synchronized to a 24-hour solar cycle by a well-regulated molecular clock mechanism. This internal biological clock regulates a host of cellular responses to the environment, ranging from gene expression and cell division in cyanobacteria, to photosynthesis in plants and finally to the sleep/wake cycles in mammals (commonly referred as circadian rhythms). In this talk, I will present the work that we have been doing to not only enhance the understanding of molecular mechanisms regulating circadian clock [1] but also to develop therapeutic interventions to modulate the circadian rhythms in mammals [2, 3]. Using hybrid/integrative modeling, involving multiple experimental and computational methods, we have been able provide mechanistic insights into the role of cryptochromes – a core clock protein, in regulating circadian period length, thus directly relating protein structure and dynamics to in vitro and in vivo experimental observations [1].

1. Jennifer Fribourgh*, Ashutosh Srivastava*, Colby Sandate* et al. (2020); Dynamics at the serine loop underlie differential affinity of cryptochromes for CLOCK:BMAL1 to control circadian timing; eLife; 9:e55275 (*Equal Contribution)
2. Tsuyoshi Oshima, Yoshimi Niwa, Keiko Kuwata, Ashutosh Srivastava, et al.(2019); Cell-based screen identifies a new potent and highly selective CK2 inhibitor for modulation of circadian rhythms and cancer cell growth; Science Advances, 5, 1, eaau9060
3. Simon Miller, You Lee Son, Yoshiki Aikawa, Eri Makino, Yoshiko Nagai, Ashutosh Srivastava, et al. (2020); Isoform-selective regulation of mammalian cryptochromes. Nature Chemical Biology 16, 676-685.

GOOGLE MEET LINK:

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