Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Internal Webinar

Data Driven Drug Discovery

Soham Choudhuri

IIIT, Hyderabad

The traditional drug discovery process is both slow and costly, leading to the emergence of computer-aided drug discovery (CADD). Deep learning algorithms significantly enhance these processes by enabling the selection of drug targets and the generation of drug molecules from various data sources including molecular and transcriptomic data. This discussion will focus on how machine learning and network analysis contribute to identifying drug targets from single-cell transcriptomics data, alongside our innovative peptide design framework, HYDRA. HYDRA, a generative hybrid diffusion model, designs peptides based on specific target binding sites. Comparative analysis with the benchmark RFdiffusion demonstrates that our model excels in most aspects crucial to therapeutic peptide generation.

Wednesday, Jun 26th 2024

11:00 Hrs