2-CS-4 Company-Organized Symposium

Towards a system combining ADMET prediction AI and de novo structure generation AI

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To efficiently drive drug discovery process, it is essential to improve the profile of ADMET, which is a collective term for endpoints related to pharmacokinetics and toxicity, as well as enhancing the activity and efficacy on a target protein. In this presentation, we will give an overview of the current status of ADMET prediction AI and de novo structure generation AI that are being promoted through AMED "drug discovery informatics project" and the activities of LINC (Life INtelligence Consortium), an AI drug discovery consortium on all Japan scale headed by Prof. Okuno in Kyoto University. Also, issues toward a new drug design AI system that combines above mentioned two types of AI models will be discussed.