DE NOVO MOLECULAR DESIGN WITH MACHINE INTELLIGENCE

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Artificial intelligence (AI) methods have emerged as transformative tools in drug discovery and automation. These systems not only mimic the chemist's pattern recognition but also leverage domain-specific data and associations to enhance model development. AI, particularly deep networks and jury methods, has revolutionized the field by producing accurate qualitative and quantitative prediction models for pharmacological activities and molecule properties. The allure of AI in drug design stems from its potential to navigate extensive datasets and prioritize alternatives through data-driven model building. The ultimate challenge is autonomous de novo generation of chemical entities with desired attributes, eliminating the need for costly experimental compound screening. In this presentation, we will showcase specific AI techniques for ligand- and structure-based de novo drug design, with a particular emphasis on chemical language models and graph neural networks. Through case studies ranging from targeted molecular design to fully automated design-make-test-analyse cycles, we will carefully evaluate the potential and constraints of these approaches.