AI Aided Drug Design-Make-Test-Analyse Feedback Loop in Selvita

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Selvita integrates cutting-edge AI and machine learning (ML) techniques to improve the drug discovery process, focusing on an optimisation of Design-Make-Test-Analyze (DMTA) feedback loop. In the design phase, our AI&CDD department combines traditional computational chemistry with advanced algorithms, including our in-house generative model SLOT, to rapidly design optimized, highly synthesizable molecules. Tools like infiniSee and TADAM enhance lead identification and multi-target activity prediction, while bioinformatics expertise strengthens biological evaluation. For the 'Make' phase, we employ AI-driven retrosynthesis and parallel synthesis strategies to streamline compound production, ensuring high synthesizability and efficient purification through automation. AI/ML models in the 'Test' phase predict ADMET properties and facilitate virtual docking, alongside automated analysis for false active discovery in HTS triaging. Finally, in the 'Analyze' phase, ML algorithms analyze complex datasets to optimize SAR and predict efficacy, enabling data-driven decisions. By integrating these AI/ML initiatives across the DMTA loop, Selvita accelerates timelines, enhances efficiency, and improves the selection of promising drug candidates, ultimately driving project success in drug discovery.