Combination of structure- and ligand-based AI methods for molecular design for future medicinal chemistry DMT platforms

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Automated molecular design is a central component of future closed-loop DMT platforms for medicinal chemistry applications. Two projects towards such automated design concepts will be presented combining information on target structure and ligand activities from iterative DMT cycles. The use of such combined information aims to reduce the number of required optimization cycles. In the first project, active learning combined with physics-based structure-based design methods are used for reducing the number of optimization cycles for peptide design. In the second project, physics-inspired deep neural networks are being developed for improved structure-based lead identification and optimization.