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[18] Structural Biology and Interaction Analysis in Drug Discovery

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Along the discovery process, structural biology and biophysical analyses of drug target interactions inform medicinal chemists how to transform an extremely large space of unselective chemical matter into a potent medicine. The established workflows support target proteins which express in large quantities and can be purified at high quality. Therefore, the access to recombinant proteins constrains the experimental space that can profit from structurally informed optimization processes.

Innovative technologies are reaching our horizon. Very tempting is a microfluidic preparation robot, which houses a magnetic bead purification trap to extract and represent minute amounts of proteins for structure determination with cryo-EM. Such data can be complemented with binding data gathered with focal molography (FM), a next generation optical biosensor, which enables researchers to record binding curves of drug target interactions directly in lysates and serum.

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