Accelerating drug discovery using Free Energy Perturbation

Identification of potential inhibitors for SARS-Cov-2 cystein proteases

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Cresset Discovery experts in Free Energy Perturbation (FEP) methods investigated the binding affinity of compounds with known experimental activity to the Mpro protein, a potential target for SARS-CoV2. Using FEP calculations and applying *de novo* design expertise to optimize bioisosteric replacement, we generated new designs predicted to be more active than the starting point.

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