Deep Docking – the AI-enabled platform for advanced virtual screening

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With the recent explosion of chemical libraries beyond billion molecules, more efficient virtual screening approaches are needed. The Deep Docking (DD) platform enables up to hundred-fold acceleration of structure-based virtual screening by docking only a subset of a chemical library, iteratively synchronized with a ligand-based prediction of the remaining docking scores. This method results in hundreds-to-thousands fold virtual hit enrichment (without significant loss of potential drug candidates) and hence, enables screening billion-sized chemical libraries without using extraordinary computational resources. Herein we present the generalized DD protocol that has been proven successful in a variety of computer-aided drug discovery (CADD) campaigns and can be applied in conjunction with any conventional docking program.