

POSTER PRESENTATION

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Automatic docking of a small number of ligands into a large number of binding sites

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Very fast docking programs [1] enable new applications. In predefined workflows we start with an SDF file, filter the structures by substructure queries, followed by PASS predictions [2]. The remaining few structures are docked into 100 binding sites chosen for predicting adverse effects. The results are good indicators if a lead compound should be considered risky.

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