Workflow Applications

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We chemists have a mind-boggling amount of software available to help us in our research tasks. For all this software we hardly can do our work in the lab anymore. Instead of learning many programs, we can let a few gurus select programs and develop workflows. Then we chemists can push one button to get the results. Even if it is more than one button that we have to push many tasks can be automated. In general most things that we do are part of workflows.

A project starts with a literature search. Today, we cannot exclude Internet anymore and for this we have developed CWM Global Search, the Internet search engine for chemists. This would be the perfect place to start collecting ligand-protein complexes to define our target.

Sometimes we have specific problems, like finding the perfect binding site (pose) for a ligand. Molegro's Virtual Docker could predict in a study 87% of 77 compound perfectly. The results of other docking programs are shown below.

Docking Product	Accuracy (RMDS < 2Å)
MVD	87.0%
Glide	81.8%
Surflex	75.8%
FlexX (76)	57.9%
GOLD (55)	78.2%

Very often we want to find lead compounds and want to decide which compounds have the highest chance of success. Why start with 1000, or 100'000 compound? Download the whole PubChem database and start whittling down the huge number to a manageable number of compounds for testing. A workflow program like KNIME can help you to filter by fragments (no NO_2 groups, no metals, etc.), a PASS node can reduce the millions to thousand using a knowledge base, at the same time you already can set flags for toxicity. Using a MVD node supporting graphical processing units (GPU) you can dock accurately ligands in less than a second. Knowing the target you can reduce the final list to hundreds, and with automatic substructure matches against a database like Toxicity and Metabolite you can weed out unfavorable leads. All of this, and much more can be combined into one workflow.

We will shortly present CWM Global Search, KNIME client, PASS, Molegro's Virtual Docker, and Data Modeller.