Scipion-chem: an open platform for Virtual Drug Screening

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INTRODUCTION

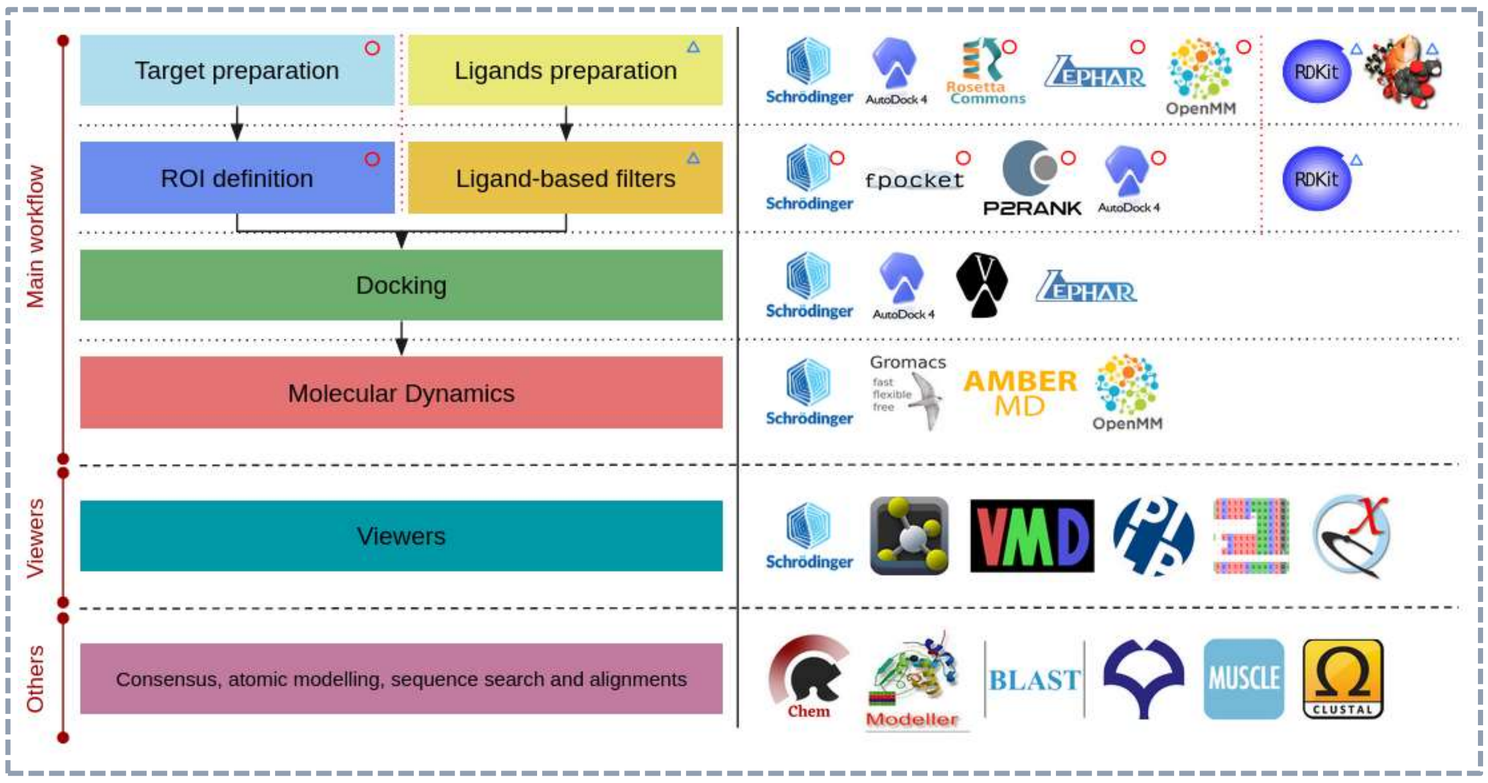
Virtual Drug Screening (VDS) tackles the problem of Drug Discovery by computationally **reducing the number of potential pharmacological molecules** which need to be tested experimentally in order to find a new drug. To do so, several approaches have been developed through the years, typically focusing either on the physicochemical characteristics of the receptor structure **(Structure Based Virtual Screening)** or those of the potential ligands **(Ligand Based Virtual Screening).**

Scipion[1] is a workflow engine particularly well-suited for **structural studies** of biological macromolecules. Here, we present **Scipion-chem**, a new branch oriented to VDS. A total of **11 plugins** have already been integrated from the most common programs used in the field **(Shcrödinger[2], AutoDock[3] and Rosetta[4]** among others). They can be used through the Scipion **Graphic User Interface (GUI)** to execute and analyse typical VDS tasks. In addition, we have developed several **consensus protocols**, which combine results from the different integrated programs in order to generate more robust predictions. On the backstage, Scipion also facilitates the interoperability of those different software, while tracking all the intermediate files, parameters and user decisions.

In summary, in this communication we present Scipion-chem, an **accessible, interoperable and traceable** platform which provides the user all the tools needed for carrying out a successful **VDS workflow.** Scipion-chem is openly available at **https://github.com/scipion-chem**

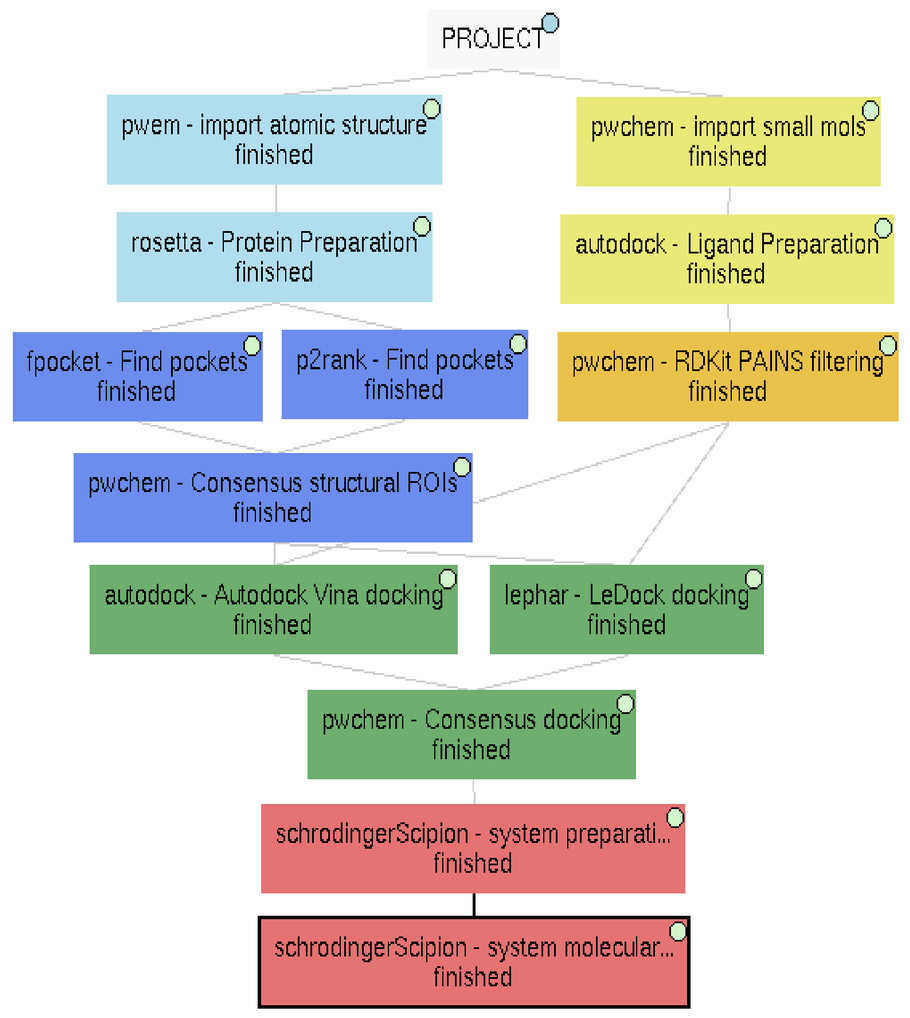
RESULTS

1. VDS stages and corresponding tools



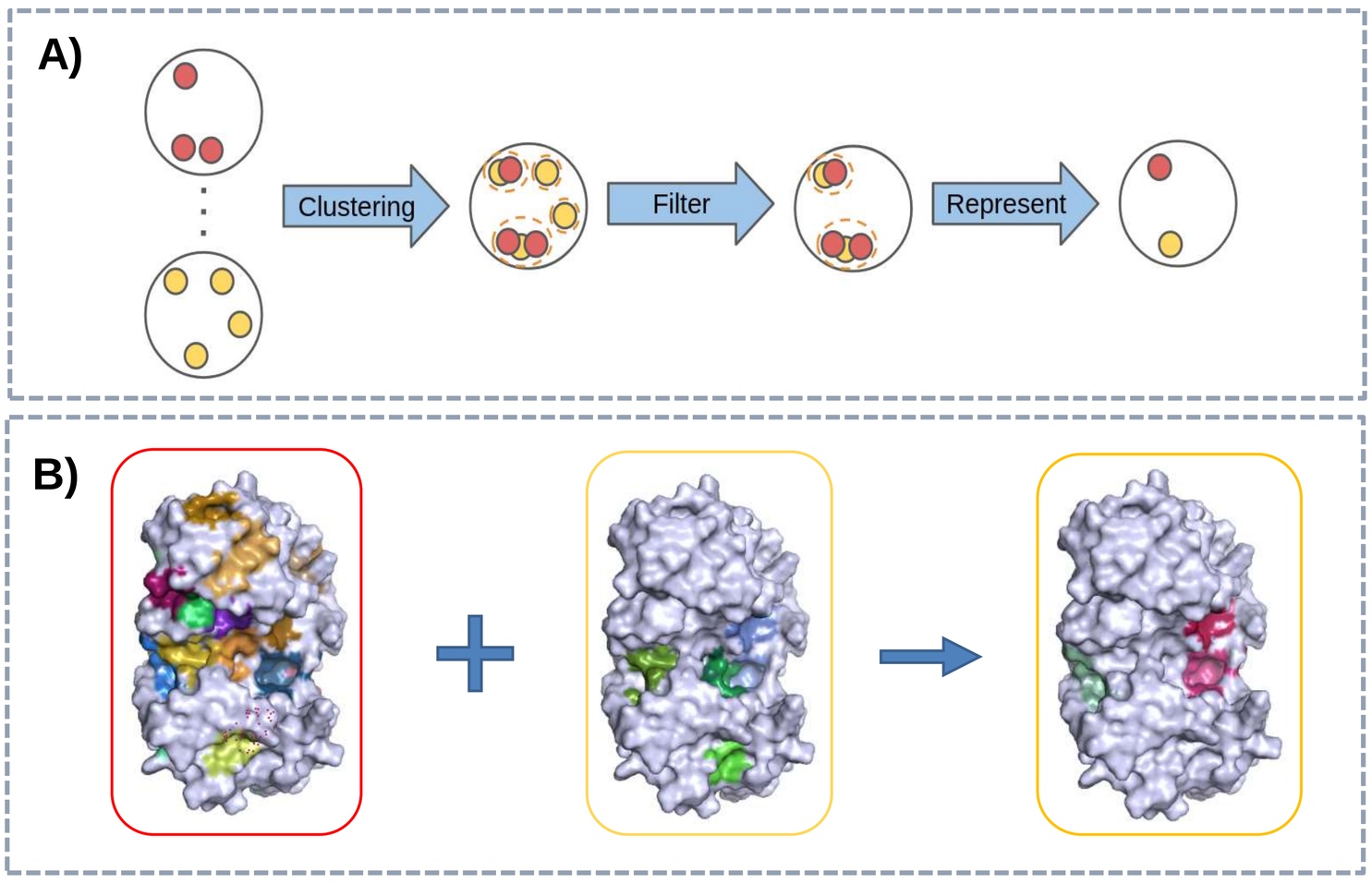
Typical VDS stages and tools dedicated in Scipion-chem for each of them. The core VDS functionalities integrated in Scipion-chem can be classified on the stages on the left graph. On the right side, some of the different tools which are able to address each of these stages are shown.

2. Workflow



Example of a VDS workflow. Example of workflow built within Scipion-chem following the stages on Figure 1. Consensus protocols for the structural ROIs and the docking stages are also included.

3. Scipion-chem consensus protocols



A) Schematic representation of consensus protocols: Results of structural ROIs (1) or docking poses (2) from different software are clustered based on surface overlap (1) or RMSD (2). Clusters are filtered, keeping only those with a minimum size to gain robustness. Finally, a representative is chosen based on the struct. ROI area or volume (1); or from the docking score or energy (2).

B) Example of consensus struct. ROIs: struct. ROIs predicted on **1cm8** PDB structure with FPocket (red) and P2Rank (yellow) and the correspondant consensus struct. ROIs (orange).

CONCLUSIONS

1) **Scipion-chem** provides an **open platform** with an **intuitive GUI** for designing, running and analyzing **VDS workflows,** using a **wide variety of tools** from different software.

2) **Consensus tools** are available to **combine and filter** the results from different software, yielding an output more robust than single programs

3) **Scipion-chem** provides **traceability** to your projects by storing the parameters, choices and results obtained in a workflow.

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