# Scipion-Chem: a traversal tool for the development of antiviral drugs

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**Background:** Virtual screening (VS) is a powerful and efficient tool to identify in an efficient way new antiviral drugs from chemical libraries and a detailed knowledge of the structure of the target. VS allows to save time and money since the experimental work is only focused on the most promising ligands. In this communication we present a computational platform for virtual drug screening that combines several widely used software suites for this purpose.

**Methods**:

Scipion-chem: Scipion is a workflow engine [1] particularly well-suited for structural studies of biological macromolecules (Fig. 1 top). It includes structure determination by single-particle analysis in CryoEM, atomic modelling, and now, virtual drug screening using a library of candidate compounds. We have integrated the most common programs used in the field for this task: Shcrödinger, AutoDock4, AutoDock Vina, P2Rank, FPocket, OpenBabel, RDKit, Amber, and Rosetta (Fig. 1 bottom). We have also integrated some tools to design drugs based on ligand properties.

**Results**:

Scipion-chem: We show that by combining the output of various programs we are able to reduce the computational requirements in the virtual drug screening and the number of compounds to be experimentally tested in the wet laboratory.

**Conclusions**: In this abstract we show how this computational tool, SCipion-Chem, can be beneficial for the design of antiviral drugs.

**References**

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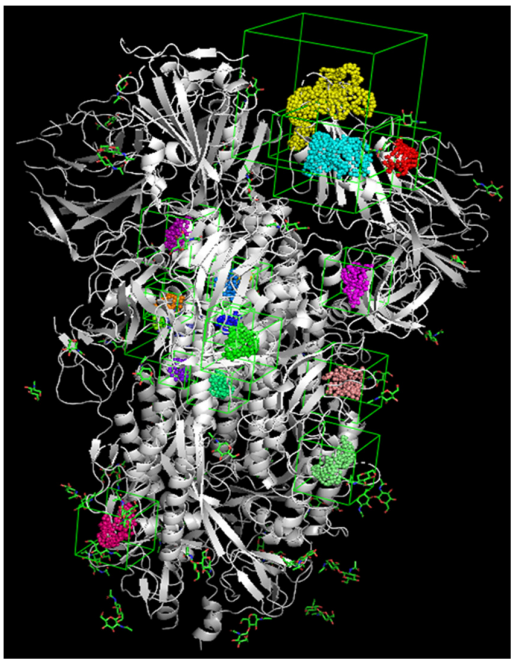

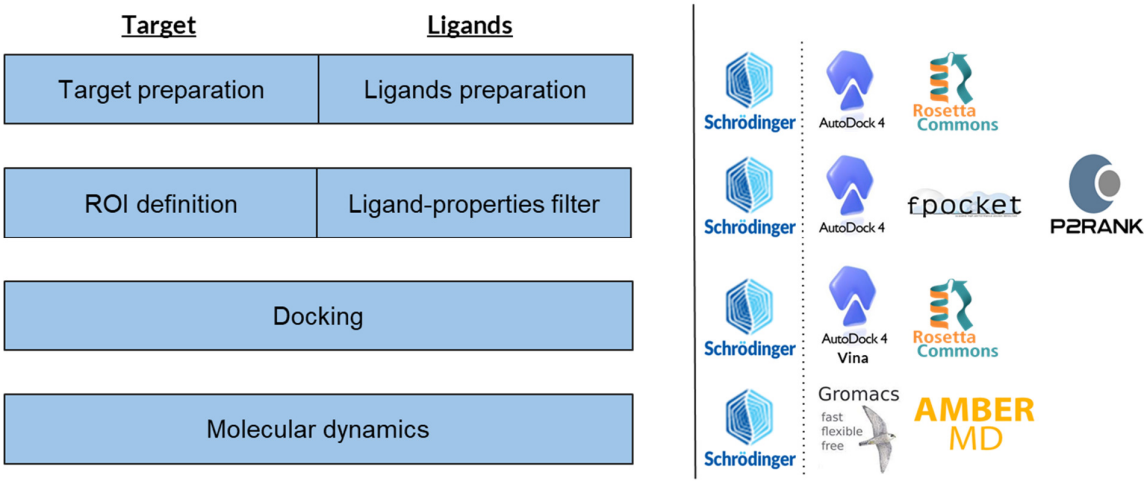


Fig. 1: (Top) Example of the structural analysis of SARS-CoV2 Protein S, in particular, its known variants are represented in the structure. These variants have been collected from Uniprot using Scipion-Chem. (Bottom) Schematic representation of the different steps needed for computational drug screening and some of the programs integrated for each step.