VSpipe-GUI, an Interactive Graphical User Interface for Virtual Screening and Hit Selection

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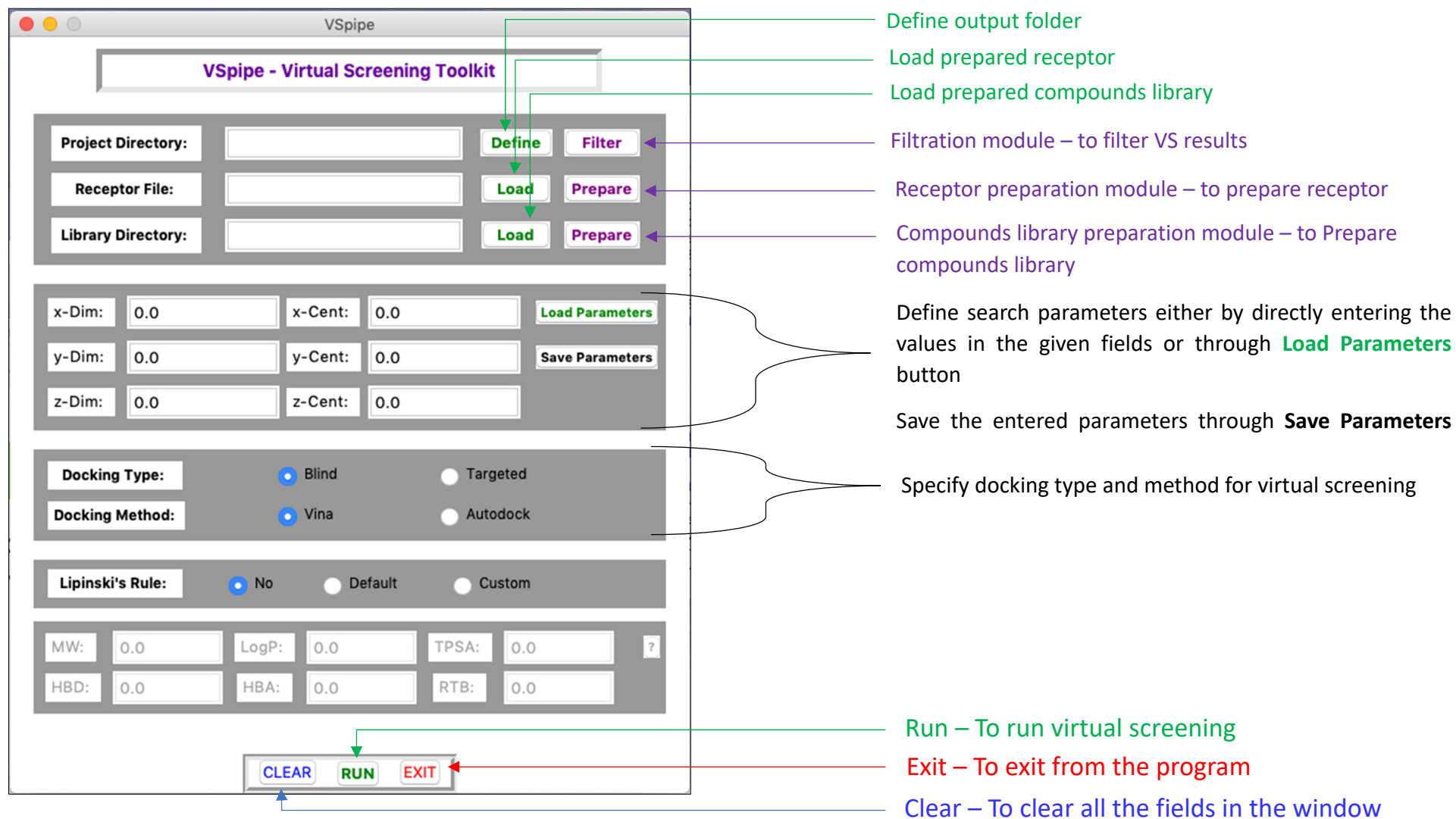*   Correspondence: sandra.ac93@gmail.com; lydia.tabernero@manchester.ac.uk.

Figure S1. Overview of Main GUI Window

Define physico-chemical parameters to filter the compounds library further based of Lipinski's rule of five.

No – No filter is applied.

Default – Default parameters are applied defined by Lipinski.

Custom – User-defined parameters.

Figure S2. Lipinski's rule of five GUI Window

Figure S3. Receptor Preparation GUI Window

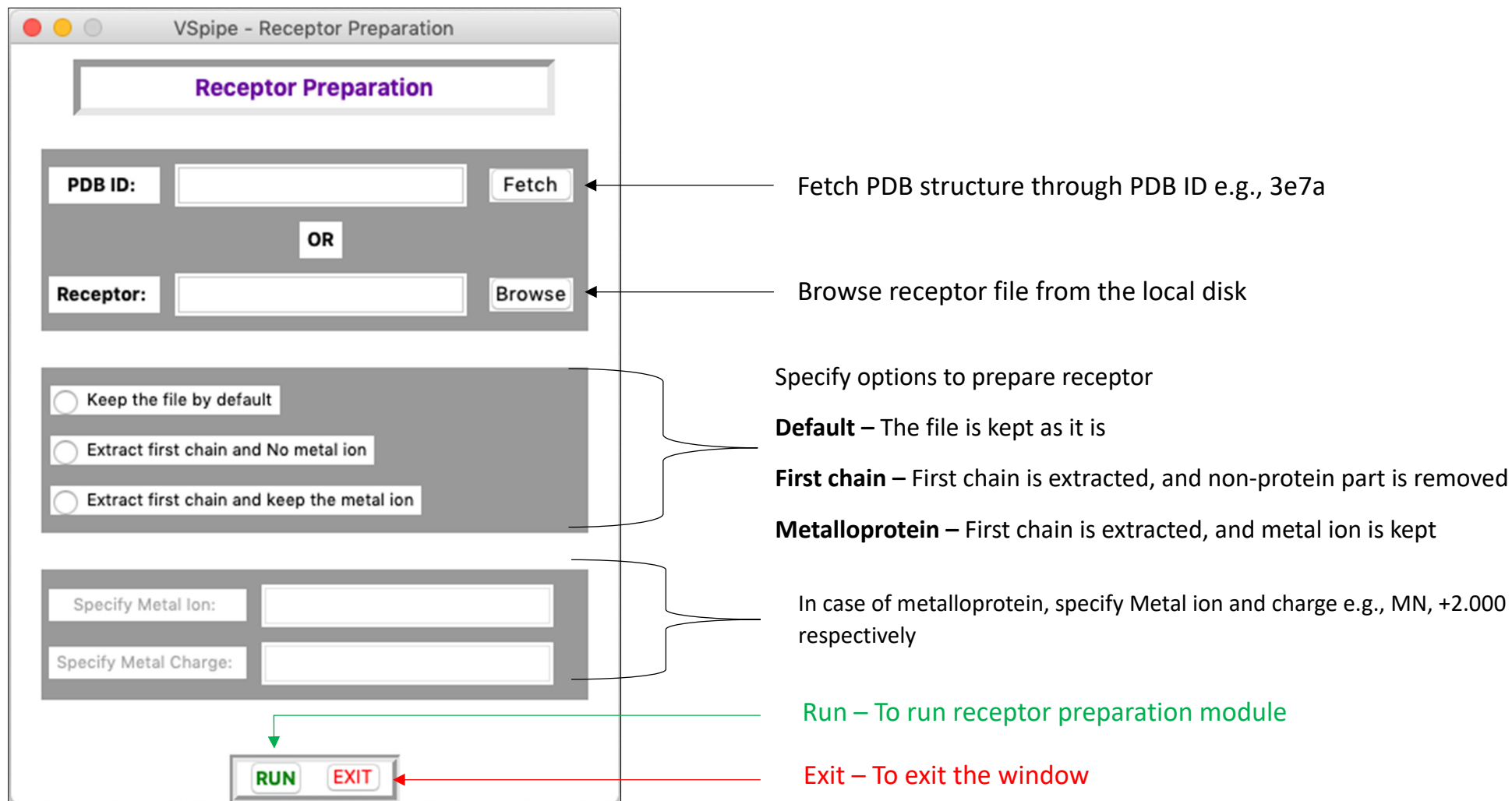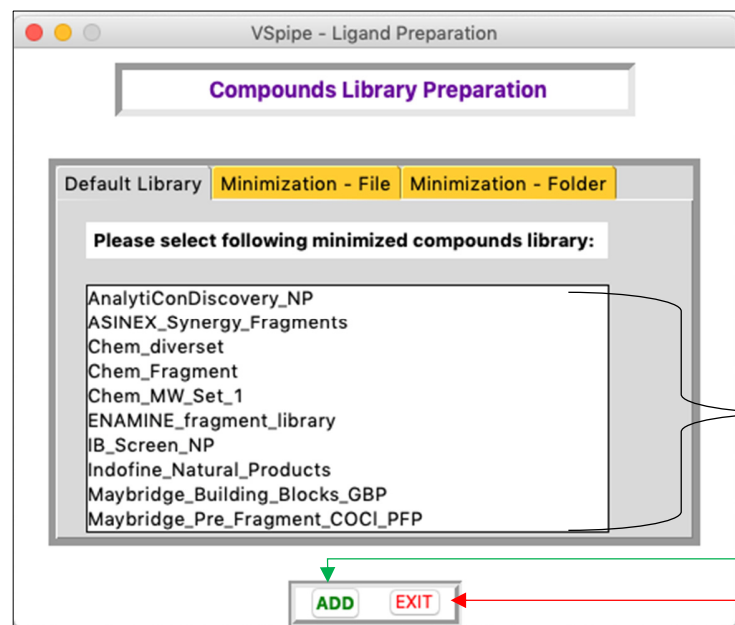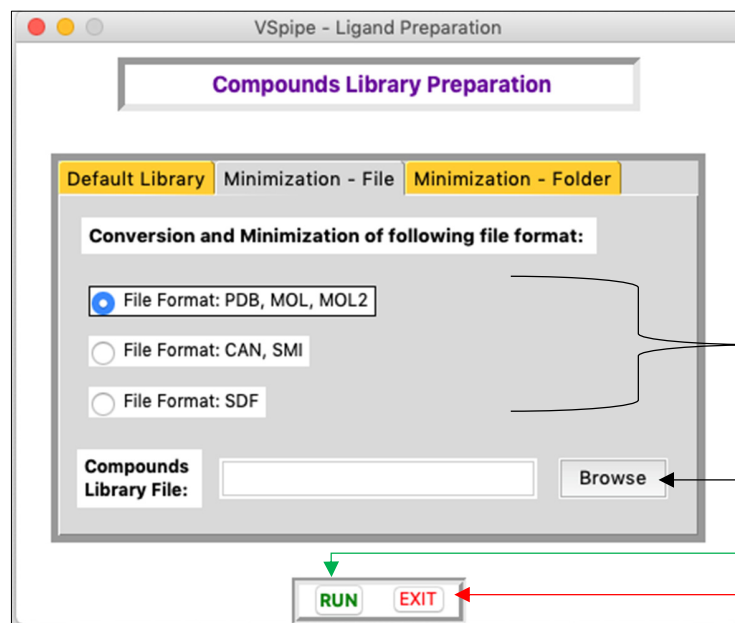**Figure S4**. Compounds Library Preparation GUI Window

Select an already minimized library to use in virtual screening

Add – To add library in main window
Exit – To exit the window

Specify file format to get minimized

Browse batch file/folder from local disk

Run – To run single file/folder minimization
Exit – To exit the window
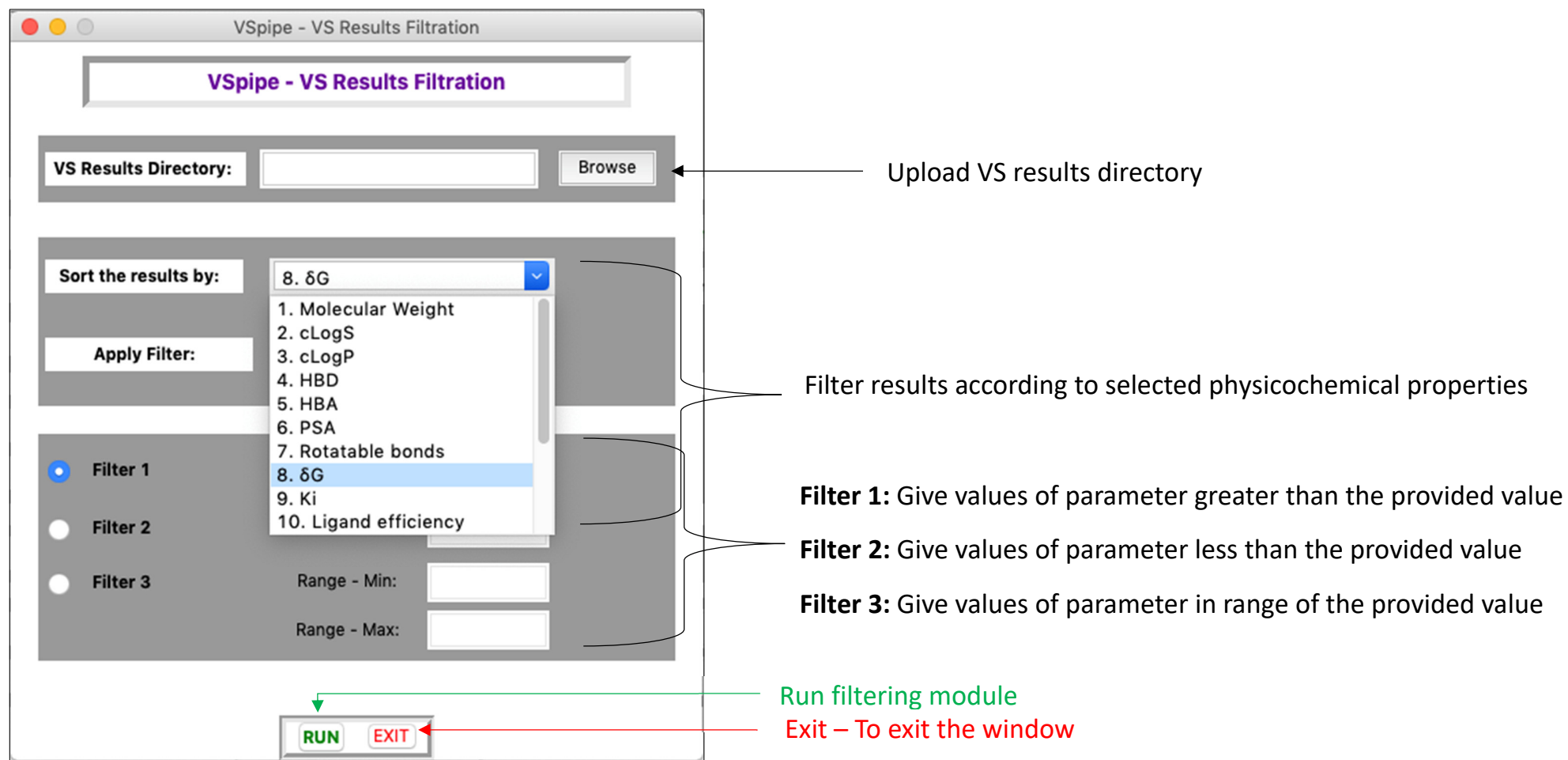
Figure S5. Filtration GUI Window for Filtering Screening Results   \

Define VSpipe Lowest Energy PDB folder

Define VSpipe Output.csv file

Enter name for results folder

Select ligand from Lowest energy PDB folder or enter XYZ coordinates for pocket centre

Select number of closest ligands or all ligands with X to be copied to output folder

Run – To run spatial filtering module

Exit – To exit from the program

Clear – To clear all the fields in the window

Figure S6. Spatial Filtering GUI window – Pocket-based Filtering
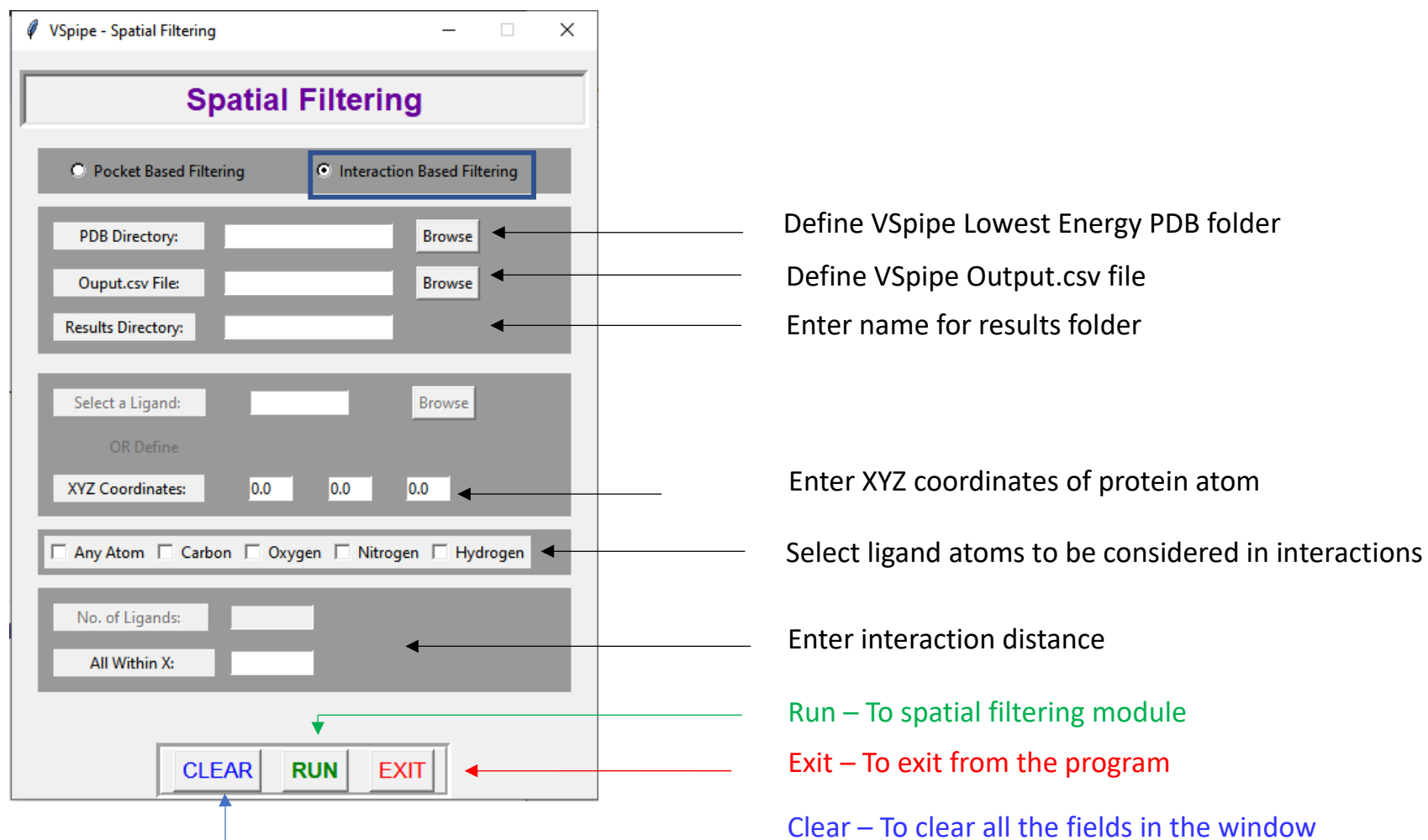
Figure S7. Spatial Filtering GUI window – Interaction-based Filtering.
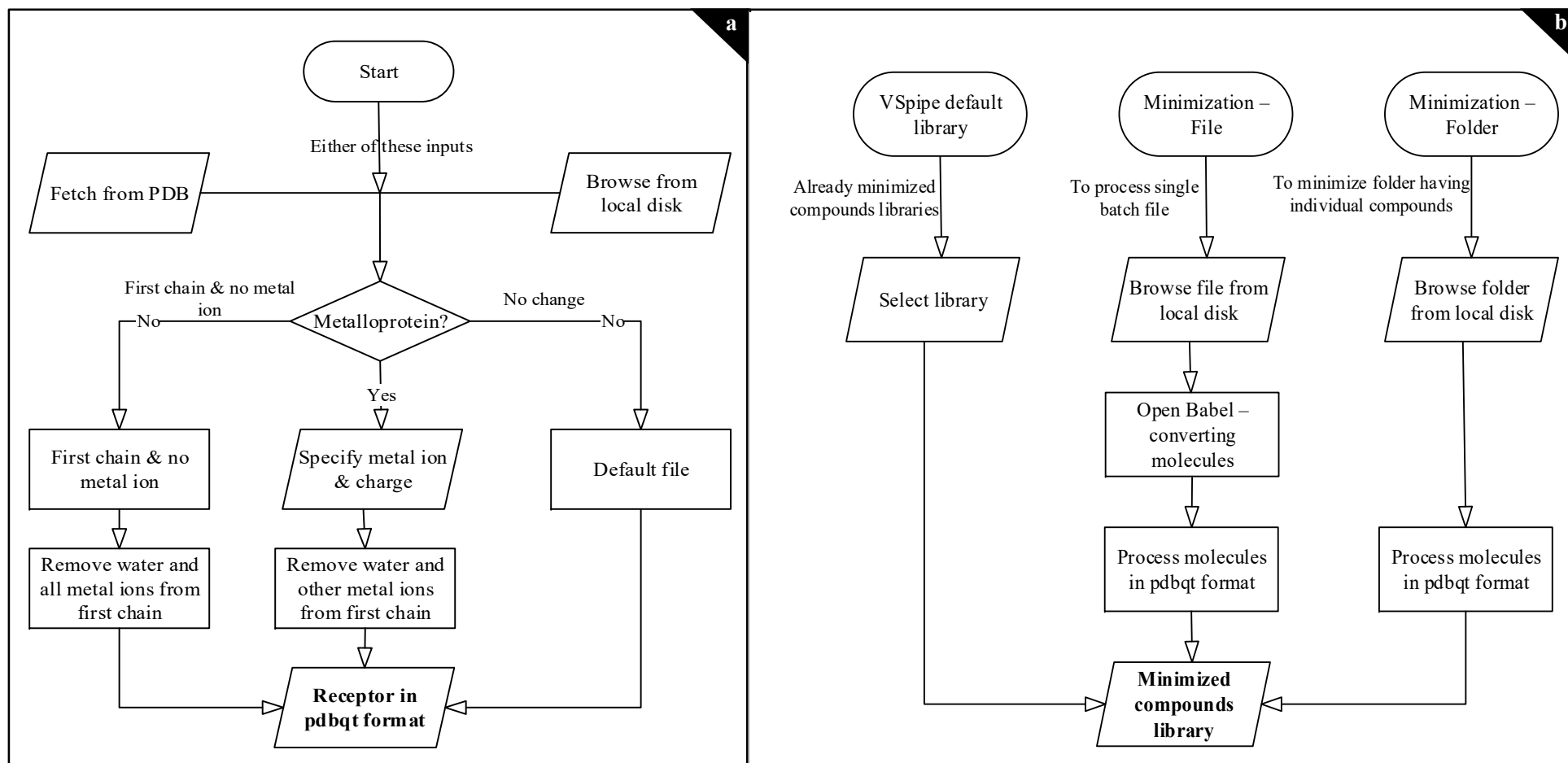
Figure S8. a) Receptor Preparation: module that processes the target protein as the receptor onto which the ligands will be later docked. b) Compounds Library Preparation: module used to prepare the ligands to be docked onto the receptor in which users can either select one of the already minimized libraries included in VSpipe-GUI, select one of their already minimized libraries, or minimize an external library if provided in PDB, mol2, or SDF format.

a

Docking result files Output.tsv Summary files Lowest energy pdb files

Docking by Autodock AD4

Define x,y,z coordinates size & dimensions

Minimized compounds library

Start

Receptor in pdbqt format

Browse gpf file from local disk

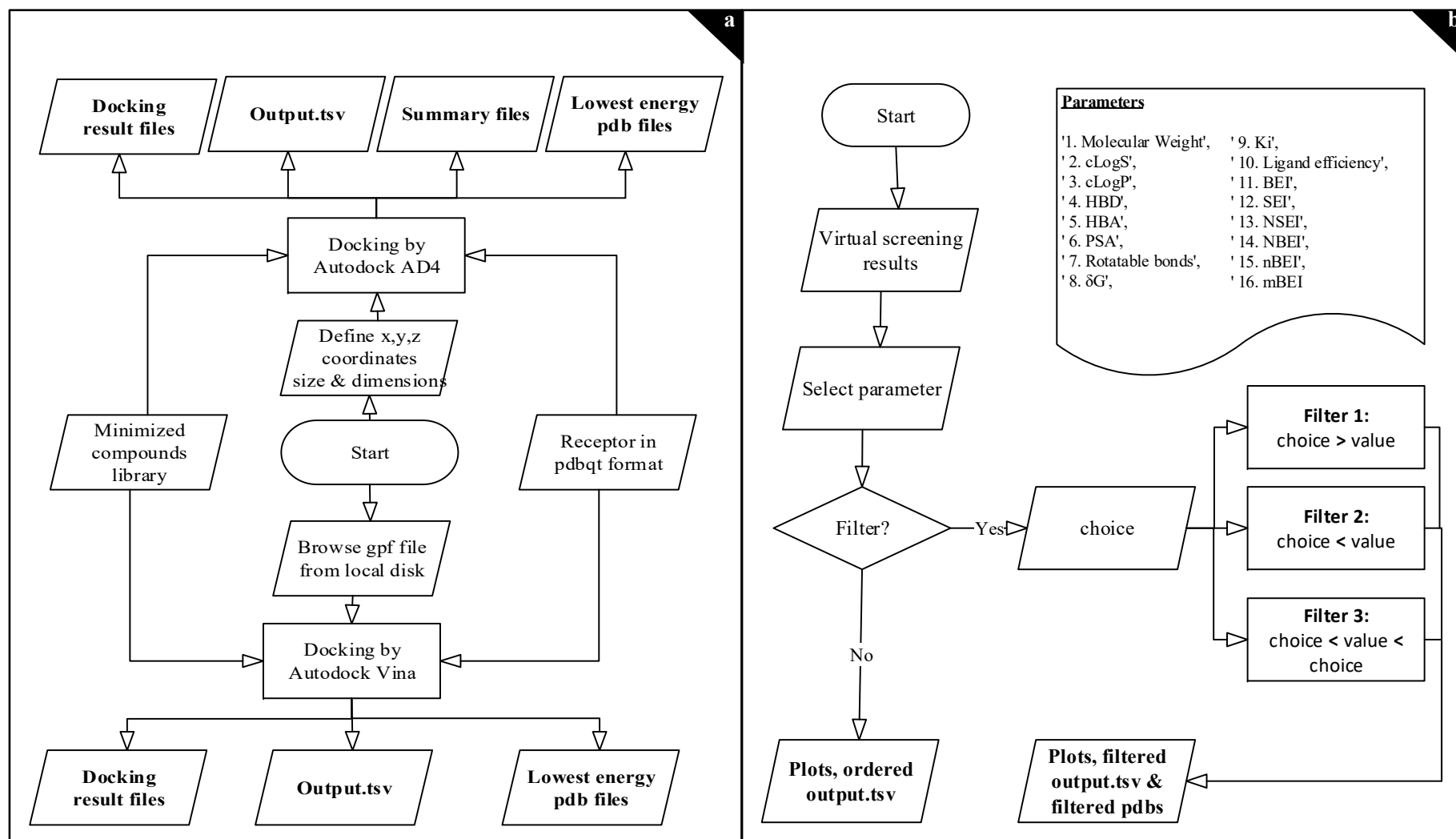Docking by Autodock Vina

Docking result files Output.tsv Lowest energy pdb files

b

Start

Virtual screening results

Select parameter

Filter? —Yes→ choice

No

Plots, ordered output.tsv

Filter 1: choice > value

Filter 2: choice < value

Filter 3: choice < value < choice

Plots, filtered output.tsv & filtered pdbs

Parameters

'1. Molecular Weight',   ' 9. Ki',
' 2. cLogS',   ' 10. Ligand efficiency',
' 3. cLogP',   ' 11. BEI',
' 4. HBD',   ' 12. SEI',
' 5. HBA',   ' 13. NSEI',
' 6. PSA',   ' 14. NBEI',
' 7. Rotatable bonds',   ' 15. nBEI',
' 8. δG',   ' 16. mBEI

Figure S9. a) Docking: this module requires the 3D coordinates that define the grid box in which the docking will take place, which can be provided by either entering the coordinate values (i.e., values for coordinates x, y, and z) on VSpipe-GUI or by uploading the GPF file on the tool (the coordinates will be extracted from this file). In addition, users need to select the software that will be used for the docking, either AD4 or Vina. b) Filtering: this module allows for the docking results to be filtered according to a given threshold by the user for one of the 16 physicochemical properties the screened ligands have had calculated during the virtual screening.