

Supplementary Material

VSpice, an Integrated Resource for Virtual Screening and Hit Selection: Applications to Protein Tyrosine Phosphatase Inhibition

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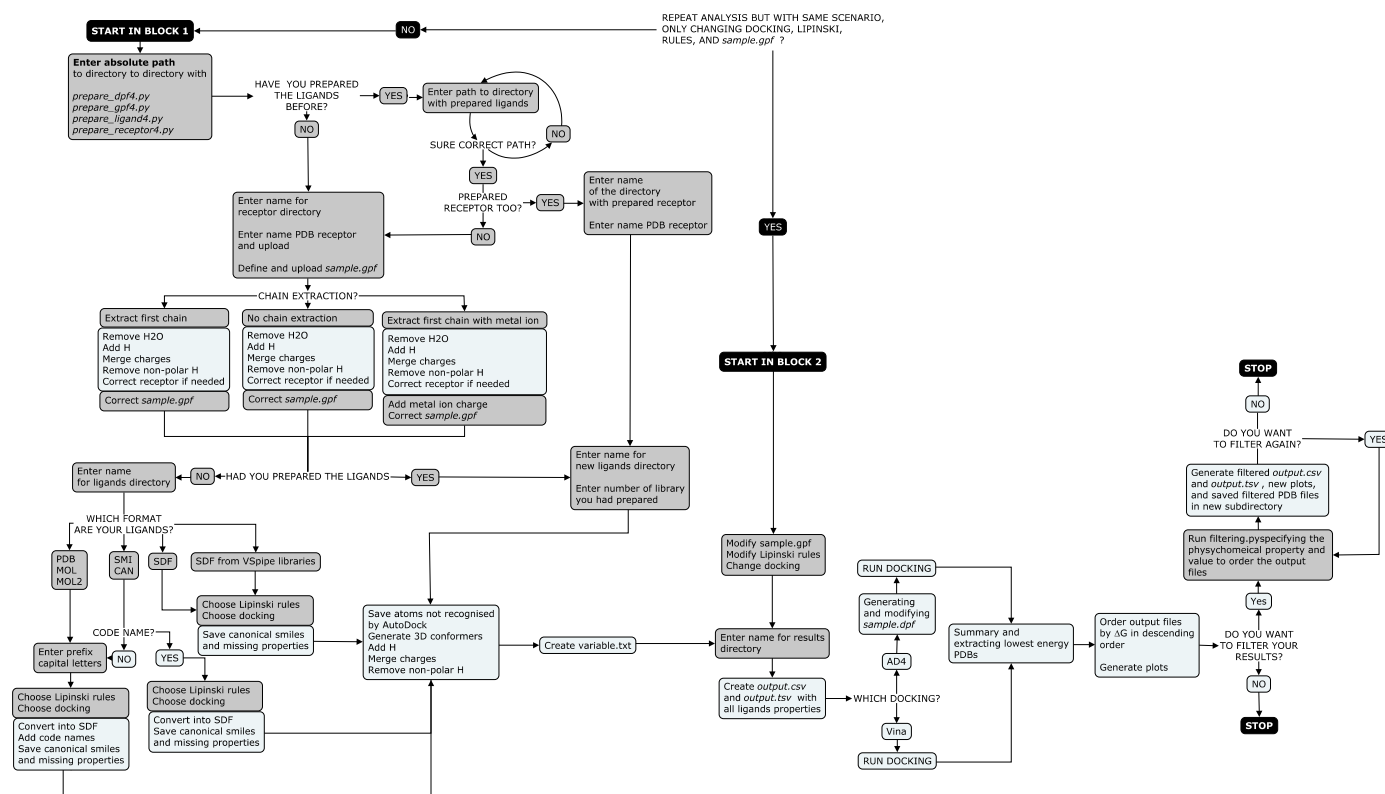


Figure S1. Workflow of VSpice-local. This workflow diagram shows all possible user choices from the preparation of input files to the output summary of results. All user choices are saved as global variables and then written in the *variables.txt* file. The black boxes show the start and the end of each block and of VSpice, the grey boxes show the information that users enter in the terminal or the tasks manually performed according to the instructions by VSpice. Blue boxes show the tasks VSpice performs after reading the information entered by the users.

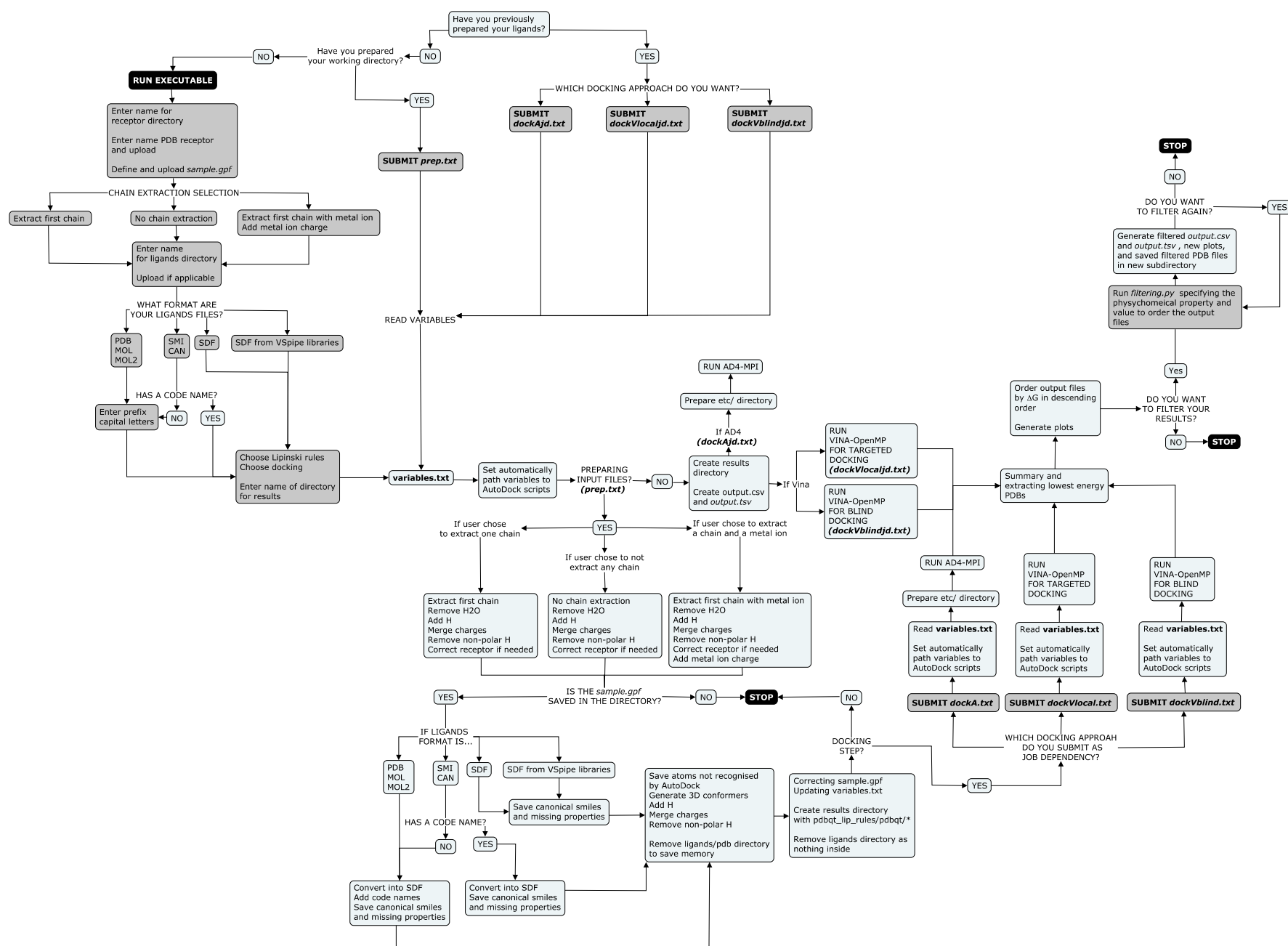


Figure S2. Workflow of VSpice-cluster. The diagram includes the different bash scripts the users can submit in the cluster mode. If the users have not run any previous VS before, VSpice starts with the executable file to prepare the working directory. Once the input files are in the directories created by this script, the users submit the script *prep.txt* to the cluster to prepare the receptor and the ligands. Afterwards, a job dependency script is used to perform the docking. The users have to decide which docking approach to use submitting either *dockADjd.txt*, *dockVblindjd.txt* or *dockVlocaljd.txt*. If users have previously prepared the ligands VSpice skips the preparation step and goes directly to the docking. In this instance, there are no job dependencies as there is no other script to run before. The *dockAD.txt*, *dockVblind.txt*, and the *dockVlocal.txt* scripts perform the docking in the same way than the other scripts submitted as job dependencies. The black boxes show the start or the end of VSpice, the grey boxes show the tasks that they have to be manually performed according to the instructions, and the blue boxes show the tasks VSpice performs after reading the information entered by the users.

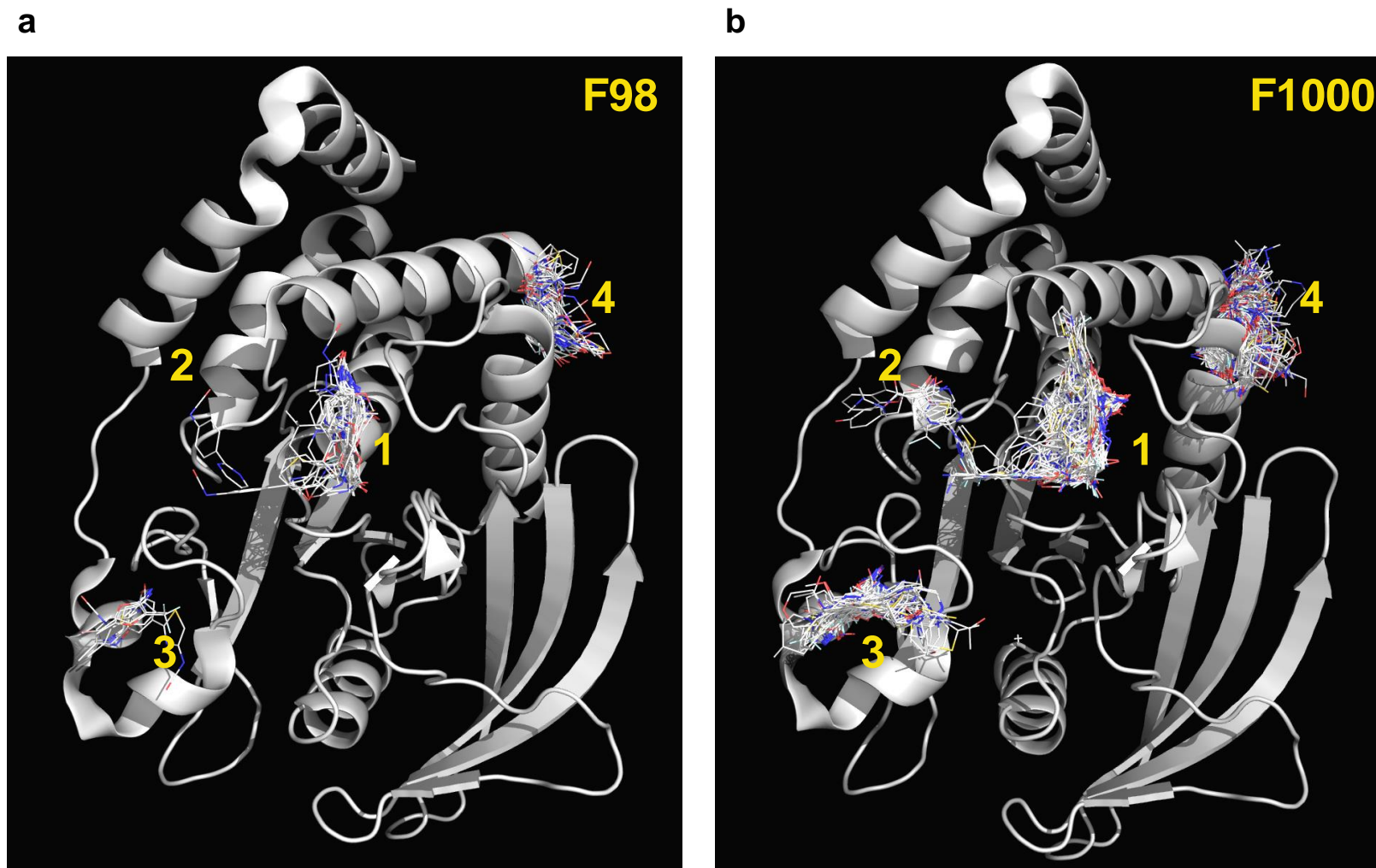


Figure S3. Cluster distribution from VS with fragment libraries. Blind docking results from VSpice using PTP1B (PDB ID: 1T4J) and the **a)** Maybridge pre-fragment (NCO) library (F98) or **b)** the Maybridge R03 1000 fragment library (F1000). The structure of PTP1B is shown as a grey cartoon with compounds shown as lines. Clusters match sites of functional importance: 1) active site, 2) secondary pTyr site, 3) centred on L41 4) allosteric binding site.

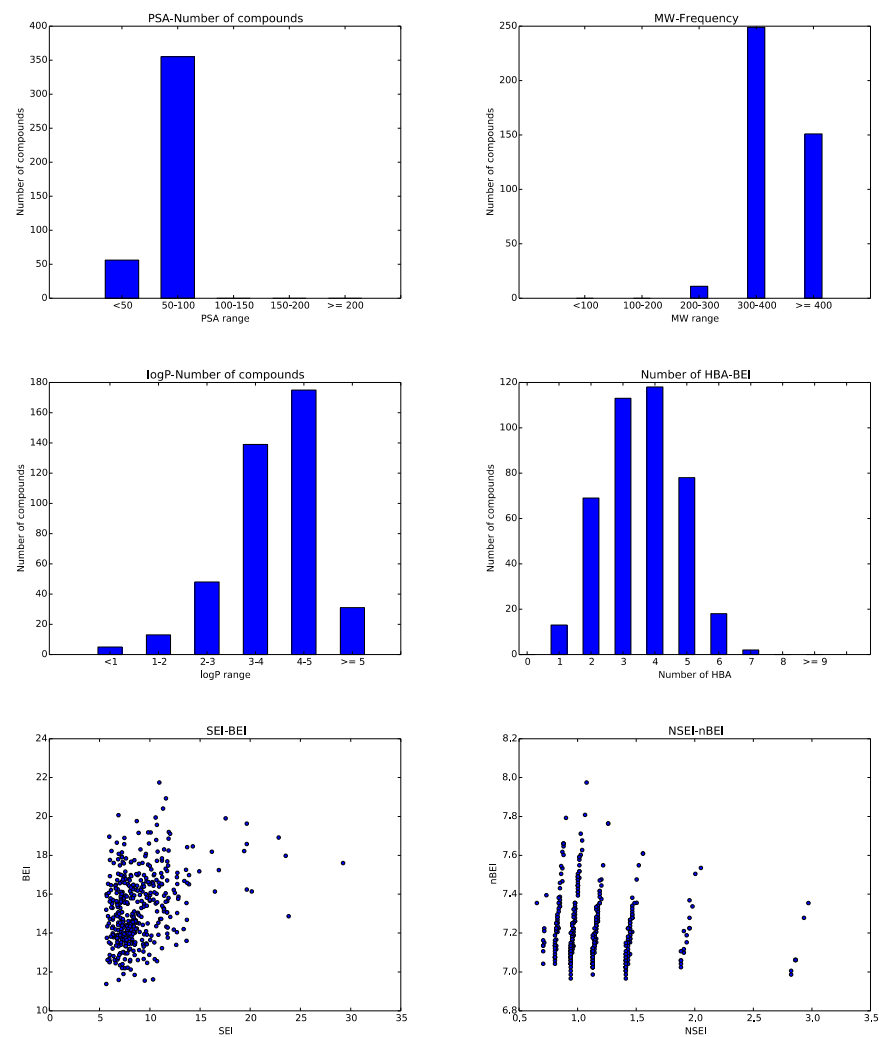


Figure S4. VSpice plots for the targeted VS at the PTP1B active site. Plots produced by the filtering script for the top 500 binders at the active site. PSA plot, Mw plot, logP plot, HBA plot, SEI-BE plot and NSEI-nBEI plot.

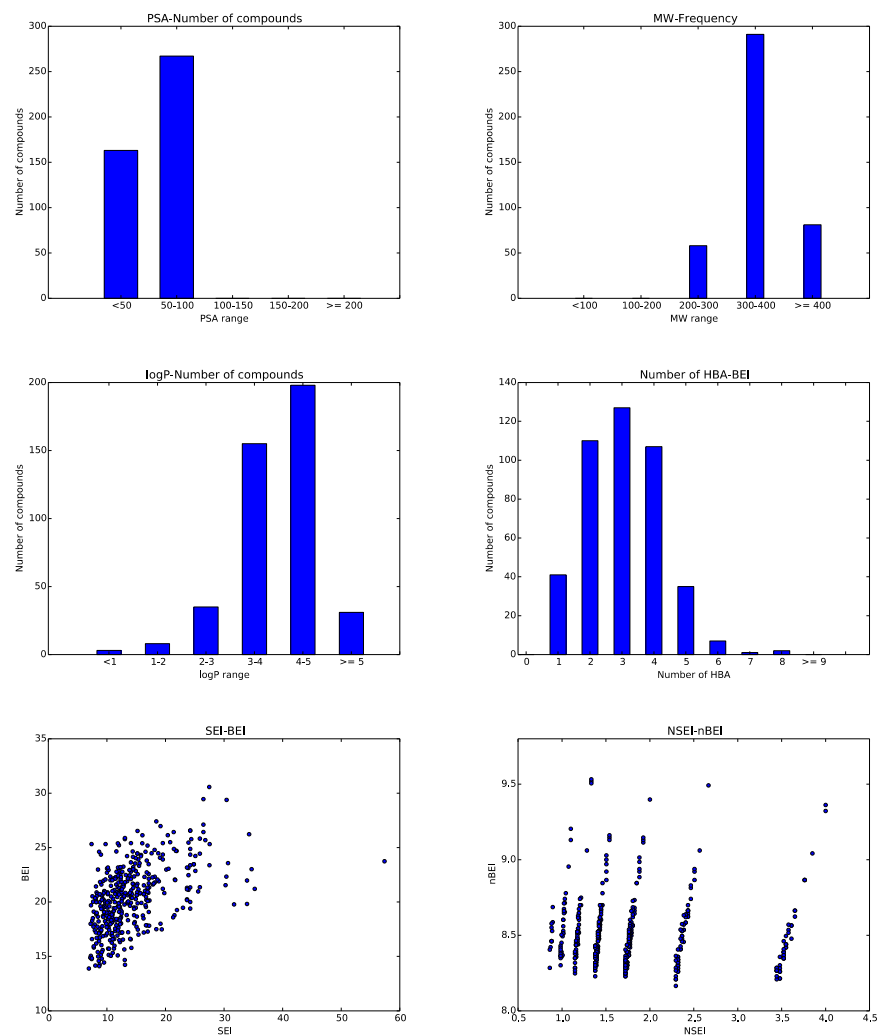


Figure S5. VSpice plots for the targeted VS at the PTP1B allosteric site. Plots produced by the filtering script for the top 500 binders at the allosteric site. PSA plot, Mw plot, logP plot, HBA plot, SEI-BEI plot and NSEI-nBEI plot.