

Table S1. Blind docking/virtual screening as Perl configuration and GRID box parameters.

Perl configuration	<pre>#!/usr/bin/perl print "Ligand_file: \t"; \$ligfile=<STDIN>; chomp \$ligfile; open (FH,\$ligfile) die "Cannot open file\n"; @arr_file=<FH>; for(\$i=0;\$i<@arr_file;\$i++) { print "@arr_file[\$i]\n"; @name=split(/\.\/,@arr_file[\$i]); } for(\$i=0;\$i<@arr_file;\$i++) { chomp @arr_file[\$i]; print "@arr_file[\$i]\n"; system("vina.exe -config conf_vs.txt -ligand @arr_file[\$i] -log @arr_file[\$i]_log.log"); }</pre>
GRID box parameters	<ul style="list-style-type: none"> • center_x = 2.863, center_y = 33.906, center_z = 116.625 • size_x = 54, size_y = 86, size_z = 54 • num_modes = 10; energy_range = 4