

```
1  #!/bin/bash
2
3  for file in /*; do tmp=${file%.pdbqt}; name="${tmp##*/}"; \
4  ./vina-w --receptor 5c5a_clean.pdbqt --ligand "$file" --out $name.pdbqt --log $name.log
5  --cpu 20 --exhaustiveness 256 \
6  --num_modes 10 --center_x -14.768 --center_y 3.77996 --center_z -23.8846 --size_x 25.0 --
7  size_y 25.0 --size_z 20.0; \
8  awk '/^[-+]+$/ {getline; print FILENAME, $0}' $name.log >> temp; done; sort temp -nk 3 > 5
9  c5a_redocking.txt; rm temp; \
10 mkdir logs; mv *.log logs; mkdir outputs; mv *.pdbqt outputs
```