Протонирование при PH 7.4

obabel mol.mol -O mol.mol -p

Конвертация форматов

obabel mol.mol -O mol.mol2

[Smiles to sdf](https://novoprolabs.com/tools/smiles2pdb)

Запуск докинга  
smina -r receptor.pdbqt -l ligand.sdf –autobox\_ligand box.sdf -o docking.sdf –log log.log  
  
--randomize\_only generate random poses, attempting to avoid clashes  
--minimize energy minimization  
--minimize\_early\_term Stop minimization before convergence conditions

are fully met.  
  
--atom\_terms arg optionally write per-atom interaction term values

--atom\_term\_data embedded per-atom interaction terms in output sd data

create S-RBD, chain E and polymer

sed -i -e 's/\r$//' script.sh