

SUPPLEMENTAL INFORMATION

In silico analysis and experimental verification of OSR1 kinase - peptide interaction

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Rosetta command line for relax:

```
rosetta/rosetta_source/bin/relax.default.linuxgccrelease -s PDB.pdb -database rosetta/rosetta_database/  
ex1 ex2 use_input_sc relax:quick -nstruct 100
```

Rosetta command line for docking:

```
rosetta/rosetta_source/bin/rosetta_scripts.default.linuxgccrelease -s PDB.pdb -database  
rosetta/rosetta_database/ -ex1 -ex2 -use_input_sc -parser:protocol dock.xml -unboundrot  
PDB_unbound.pdb -nstruct 1000
```

RosettaScripts XML script for relax (dock.xml):

```
<dock>  
  <SCOREFXNS>  
  </SCOREFXNS>  
  <TASKOPERATIONS>  
  </TASKOPERATIONS>  
  <FILTERS>  
  </FILTERS>  
  <MOVERS>  
  
  <FlexPepDock name=flex_pep_dock min_only=0 pep_refine=1 lowres_abinitio=0  
  peptide_chain=B receptor_chain=A ppk_only=0 scorefxn=score12 extra_scoring=0/>  
  
  <ddG name=ddg jump=1 per_residue_ddg=1 repack=1 scorefxn=score12 />  
  
  </MOVERS>  
  <APPLY_TO_POSE>  
  </APPLY_TO_POSE>  
  <PROTOCOLS>  
    <Add mover_name=FlexPepDock/>  
    <Add mover=ddg />  
  </PROTOCOLS>  
</dock>
```

Rosetta command line for design:

```
rosetta/rosetta_source/bin/rosetta_scripts.default.linuxgccrelease -s PDB.pdb -database  
rosetta/rosetta_database/ -ex1 -ex2 -use_input_sc -parser:protocol design.xml -unboundrot  
PDB_unbound.pdb -nstruct 1000
```

RosettaScripts XML script for relax (design.xml):

```
<dock_design>
  <SCOREFXNS>
  </SCOREFXNS>
  <TASKOPERATIONS>

    <InitializeFromCommandline name=ifcl />

    <RestrictChainToRepacking name=rctr1 chain=1 />

  </TASKOPERATIONS>
  <FILTERS>
  </FILTERS>
  <MOVERS>

    <FlexPepDock name=flex_pep_dock min_only=0 pep_refine=1 lowres_abinitio=0
      peptide_chain=B receptor_chain=A ppk_only=0 scorefxn=score12 extra_scoring=0/>.

    <ddG name=ddg jump=1 per_residue_ddg=1 repack=1 scorefxn=score12 />

    <PackRotamersMover name=soft_des scorefxn=soft_rep task_operations=rctr1,ifcl />

  </MOVERS>
  <APPLY_TO_POSE>
  </APPLY_TO_POSE>
  <PROTOCOLS>
    <Add mover=soft_des />
    <Add mover=FlexPepDock />
    <Add mover=soft_des />
    <Add mover=ddg />
  </PROTOCOLS>
</design>
```