<ROSETTASCRIPTS>

<TASKOPERATIONS> You can control which parts you want to change from here

<ProteinInterfaceDesign name="pido" repack_chain1="1" repack_chain2="1" design_chain1="1" design_chain2="0" interface_distance_cutoff="10"/> task operation that designates which residues are designable and repackable at the interface

<ReadResfile name="rrf" filename="resfile" />

</TASKOPERATIONS>

<FILTERS> This part enables to output useful values for post-processing

<Ddg name="ddG" scorefxn="REF2015" threshold="-15" repeats="2"/> binding energy calculation; an average of two repeats is computed for better numerical accuracy

<Sasa name="sasa" threshold="100"/> Buried surface area upon complex formation

<Rmsd name="rmsd" confidence="0"/> confidence=0 means that the filter will be evaluated but not used as an acceptance criterion

<CompoundStatement name="ddg_sasa"> combine filters into a single logical statement

<AND filter_name="ddG"/>

<AND filter_name="sasa"/>

</CompoundStatement>

</FILTERS>

<MOVERS>

<Docking name="docking" score_high="soft_rep" fullatom="1" local_refine="1"/> Invokes RosettaDock local-refinement (in full-atom) with a soft potential

<BackrubDD name="backrub" partner1="1" partner2="0" interface_distance_cutoff="8.0" moves="1000" sc_move_probability="0.25" scorefxn="REF2015" small_move_probability="0.15" bbg_move_probability="0.25"/> perturb the backbone of chain2. Change moves to 1000 for real application

<RepackMinimize name="des1" scorefxn_repack="soft_rep" scorefxn_minimize="soft_rep" minimize_bb="0" minimize_rb="1"/>

```
    <RepackMinimize name="des2" scorefxn_repack="REF2015" scorefxn_minimize="REF2015" minimize_bb="0" minimize_rb="1"/> Design and minimization at the interface
    <RepackMinimize name="des3" minimize_bb="1"/>

     <ParsedProtocol name="design">
      <Add mover_name="des1"/>
      <Add mover_name="des2"/>
      <Add mover_name="des3"/>
      <Add mover_name="backrub"/>
      <Add mover_name="des3" filter_name="ddg_sasa"/>
    </ParsedProtocol>
    <GenericMonteCarlo name="iterate" scorefxn_name="REF2015" mover_name="design" trials="2"/> Iterate through design to find best solution. change trial numbers to higher for real application.
 </MOVERS>

 <PROTOCOLS>
    <Add mover="docking"/>
    <Add mover="iterate"/>
    <Add filter="ddG"/>
    <Add filter="sasa"/>
    <Add filter="rmsd"/>
  </PROTOCOLS>
</ROSETTASCRIPTS>
```

-s GJ_AB_mod.pdb

-debug

-ex1

-ex2

-extrachi_cutoff 5

-ignore_unrecognized_res

-nstruct 100

-jd2:ntrials 3

-parser:protocol flexbb_interfacedesign.xml

-docking:no_filters