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<ROSETTASCRIPTS>
  <SCOREFXNS>
    <ScoreFunction name="sfx_clean" weights="beta" symmetric="1"
  />
  </SCOREFXNS>

  <TASKOPERATIONS>
    <ReadResfile name="designed_identities"
filename="%%resfile%%" />
  </TASKOPERATIONS>

  <RESIDUE_SELECTORS>
    <Task name="resfile_muts" designable="true"
task_operations="designed_identities" /> // selects mutations from
resfile
    <Not name="not_resfile" selector="resfile_muts" /> //
everything else that isn't mutated

    <Neighborhood name="mutant_neighbor" selector="resfile_muts"
distance="10" include_focus_in_subset="false" /> // only operate on other
residues that are 10A from mutation
    <Or name="resfile_or_nbors"
selectors="resfile_muts,mutant_neighbor" />
    <Not name="not_res_or_nbors" selector="resfile_or_nbors"
  />
    <ResidueName name="cysteines" residue_name3="CYS" /> // will
be used to make sure that disulfides aren't repacked or minimized

  </RESIDUE_SELECTORS>

  <TASKOPERATIONS>
    <IncludeCurrent name="ic" /> // includes input pdb's rotamers
in packing operations
    <LimitAromaChi2 name="limitaro" chi2max="110" chi2min="70" />
// disallow extreme aromatic rotamers
    <RestrictToRepacking name="repack_only" /> //
for minimize/repack
    <ExtraRotamersGeneric name="ex1_ex2" ex1="1" ex2="1" />
// use ex1 ex2 rotamers

    <OperateOnResidueSubset name="repack_neighbor"
selector="mutant_neighbor" > // neighbors to mutations are only allowed
to repack
    <RestrictToRepackingRLT/> </OperateOnResidueSubset>

    <OperateOnResidueSubset name="lock_not_resfile_or_nbors"
selector="not_res_or_nbors" > // everything that isn't a mutation or
neighbor cannot move
    <PreventRepackingRLT/> </OperateOnResidueSubset>

    <OperateOnResidueSubset name="lock_cysteines"
selector="cysteines" > // freeze cysteines
    <PreventRepackingRLT/> </OperateOnResidueSubset>

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</TASKOPERATIONS>

<MOVERS>
  <Symmetrizer name="gen_docked_config" symm_file="%%symfile%%"
/>
  <SymPackRotamersMover name="design_from_resfile"
scorefxn="sfx_clean"
task_operations="designed_identities,repack_neighbor,lock_not_resfile_or_
nbors,limitaro,ic,ex1_ex2" /> // Adds mutation and repacks the mutation
and neighbors
  <TaskAwareSymMinMover name="rb_min_hard_bb"
scorefxn="sfx_clean" bb="%%bb%%" chi="1" rb="0"
task_operations="repack_neighbor,lock_not_resfile_or_nbors" /> //
minimizes sidechains, and also backbone if bb set to 1
  <SymPackRotamersMover name="repack_hard" scorefxn="sfx_clean"
task_operations="repack_only,repack_neighbor,lock_not_resfile_or_nbors,li
mitaro,ic,ex1_ex2" /> // repacks mutation and neighbors only

</MOVERS>

<FILTERS>
  <SaveResfileToDisk name="save_resfile"
task_operations="designed_identities" designable_only="0"
resfile_prefix="%%outpath%%" resfile_suffix="" resfile_name=""
resfile_general_property="NATRO" selected_resis_property=""
renumber_pdb="0" /> // save a resfile with mutations. Only gives useful
info if allowing Rosetta to make decisions

</FILTERS>

<PROTOCOLS>
  // generate docked configuration
  <Add mover_name="gen_docked_config" />

  // design and minimization
  <Add mover_name="design_from_resfile" />
  <Add mover_name="rb_min_hard_bb" />
  <Add mover_name="design_from_resfile" />
  <Add mover_name="rb_min_hard_bb" />

  // save resfile
  <Add filter_name="save_resfile" />

</PROTOCOLS>

</ROSETTASCRIPTS>

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