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from pymol import stored

# Command to mutate receptor at ligand position
# Note: new amino acid has to be in three letter code
def mutate (old_struc, res_num, new_aa):

    cmd.delete("enabled")

    cmd.load(old_struc)

    receptor = ""
    ligand = ""
    arr = cmd.get_chains()
    sel1 = "chain " + arr[0]
    sel2 = "chain " + arr[1]
    if (cmd.count_atoms(sel1) >= cmd.count_atoms(sel2)):
        receptor = sel1
        ligand = sel2
    else:
        receptor = sel2
        ligand = sel1
    residue = receptor + " and resi " + str(res_num)


    cmd.wizard("mutagenesis")
    # for i in dir(cmd.get_wizard()): print(i) # Gets list of commands that
     can be performed in wizard
    cmd.get_wizard().set_mode(new_aa) # Selects amino acid to mutate to
    cmd.get_wizard().do_select(residue) # Selects residue to mutate
    cmd.get_wizard().apply() # Applies mutation
    cmd.wizard() # Exits wizard

    cmd.clean(residue + " expand 5.0")

    cmd.show("lines", residue)
    cmd.zoom(residue)

    new_struc = str(old_struc) + "_mutant_res" + str(res_num)+ "_to_" + new_aa
     + ".pdb"
    cmd.save(new_struc)

    cmd.delete("enabled")

cmd.extend("mutate", mutate)
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