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# Created by Arjun Batra 08/02/2022
# Final Edits by Arjun Batra 08/02/2022
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import fnmatch
from Bio.SeqUtils import seq1

def get_receptor_residues(contact_file_str):
    contact_file = open(contact_file_str)
    r_residues = []
    for line in contact_file:
        line_list = line.split()
        receptor_aa = str(seq1(line_list[0]))
        receptor_pos = str(line_list[1])
        r_res = receptor_aa + receptor_pos
        if r_res not in r_residues:
            r_residues.append(r_res)
    return r_residues

summary = open("binding_affinities.txt")
files = [line.split()[0] + ".ic" for line in summary]

for complex_num in [1, 10, 11, 12, 13, 14, 15, 16, 17, 18]:
    pat_alpha = "colabfold_complex%i_ste2-alpha_factor*.ic" %(complex_num)
    pat_cystatin = "colabfold_complex%i_ste2-cystatin*.ic" %(complex_num)
    file_alpha = fnmatch.filter(files, pat_alpha)[0]
    file_cystatin = fnmatch.filter(files, pat_cystatin)[0]
    res_alpha = get_receptor_residues(file_alpha)
    res_cystatin = get_receptor_residues(file_cystatin)
    common_res = list(set(res_alpha) & set(res_cystatin))
    print("colab_complex" + str(complex_num) + ": " + str(common_res))

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