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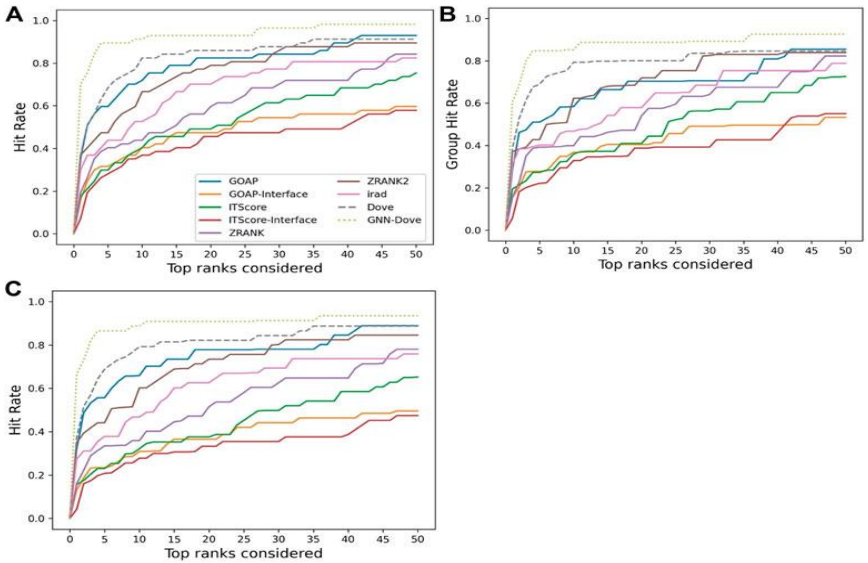
1. Feature Residue 추가

```
def residueproperty(rname):
    hydrophobic = ['ALA', 'VAL', 'LEU', 'ILE', 'MET', 'PHE', 'TRP', 'PRO', 'TYR']
    ionic = ['ARG', 'LYS', 'HIS', 'ASP', 'GLU']
    if rname in hydrophobic:
        return 1
    elif rname in ionic:
        return 2
    else:
        return 0


def atom_feature(m, atom_i):
    atom = m.GetAtomWithIdx(atom_i)
    ar = atom.GetPDBResidueInfo()
    rname = ar.GetResidueName()
    return np.array(one_of_k_encoding_unk(atom.GetSymbol(),
                                          [ 'C', 'N', 'O', 'S', 'F', 'P', 'Cl', 'Br', 'B', 'H']) +
                    one_of_k_encoding_unk(atom.GetDegree(), [0, 1, 2, 3, 4, 5]) +
                    one_of_k_encoding_unk(atom.GetTotalNumHs(), [0, 1, 2, 3, 4]) +
                    one_of_k_encoding_unk(atom.GetImplicitValence(), [0, 1, 2, 3, 4, 5]) +
                    [atom.GetIsAromatic()] +
                    one_of_k_encoding(residueproperty(rname),[0,1, 2]))    # (10, 6, 5, 6, 1, 3) --> total 31
# hydrophobic residues: ALA, VAL, LEU, ILE, MET, PHE, TRP, PRO, and TYR
# ionic residues: ARG, LYS, HIS, ASP, and GLU
```

2. 평가



Performance on the Dockground dataset.
Dockground 데이터셋으로 성능 평가를 진행함.

A) 58 complexes in the benchmark set
B) first within each of the 29 groups
C) TM-Score로 평가 된 거로 한 46 group
(interface area similarity를 고려한 그룹)
A scoring function to assess the similarity of protein structures
0.0 < TM-score < 0.17, random structural similarity
0.5 < TM-score < 1.00, in about the same fold

2. 평가에 필요한 것 - figure4

The best value among the top 10 ranked decoys was plotted.

interface root mean square deviation (iRMSD)
ligand RMSD (lRMSD)
the fraction of native contacts (fnat).

The iRMSD is the Cα RMSD of interface residues with respect to the native structure.
Interface residues in a complex are defined as all the residues within 10.0 Å from any residues of the other subunit.

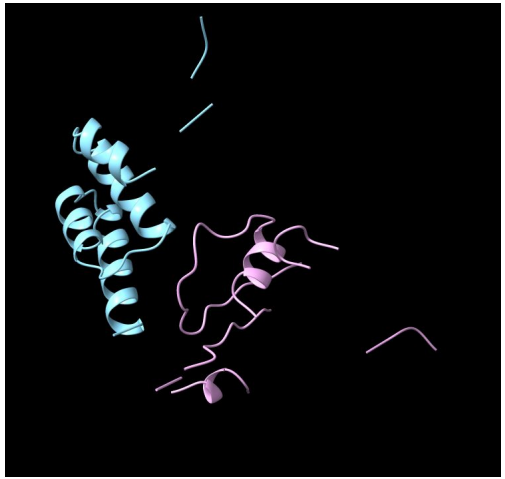
lRMSD is the Cα RMSD of ligands when receptors are superimposed, and

fnat is the fraction of contacting residue pairs, that is, residue pairs with any heavy atom pairs within 5.0 Å, that exist in the native structure.

2. 평가에 필요한 것

1. 다른 방식의 결과
2. hit rate를 측정하는 방식
3. 2-C에서 TM -Score로 새로 그룹한 46그룹은 어떻게 되었는지
4. figure 4 The best value among the top 10 ranked decoys **가 어떤 것 인지**

3. 시각화 - incorrect



3. 시각화 - incorrect

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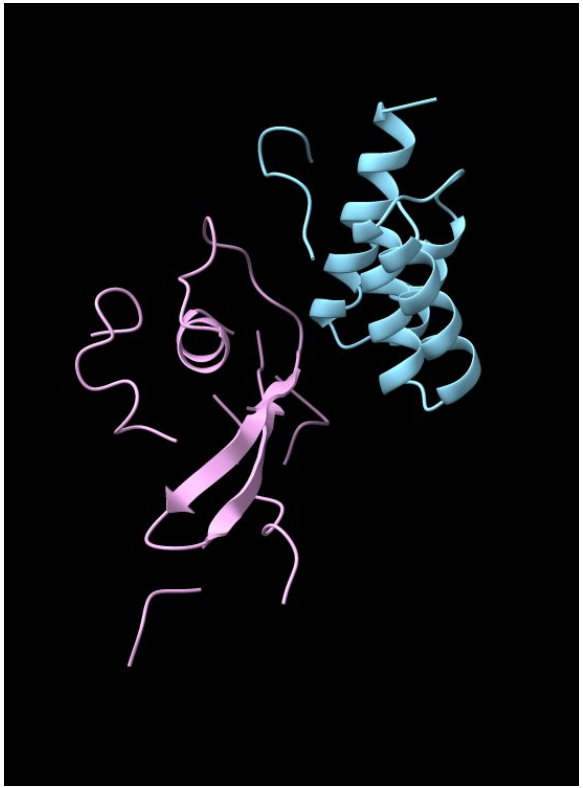

3. 시각화 - correct