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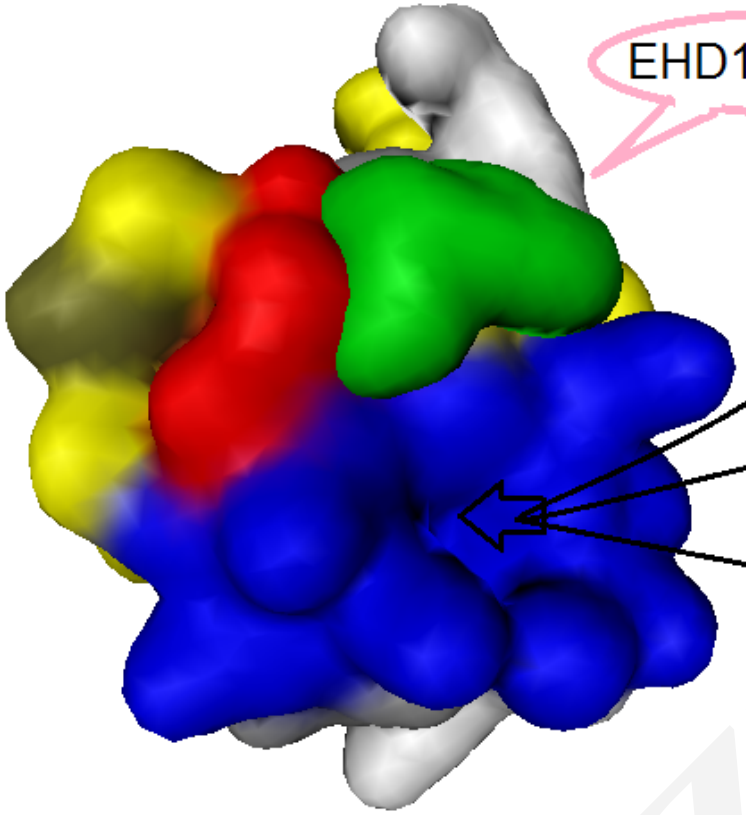
Molecular dynamics simulation of the interactions between EHD1 EH domain and multiple peptides

Key words: EHD1 EH domain, Peptide, Molecular dynamics simulation, Inhibitor design, Binding affinity



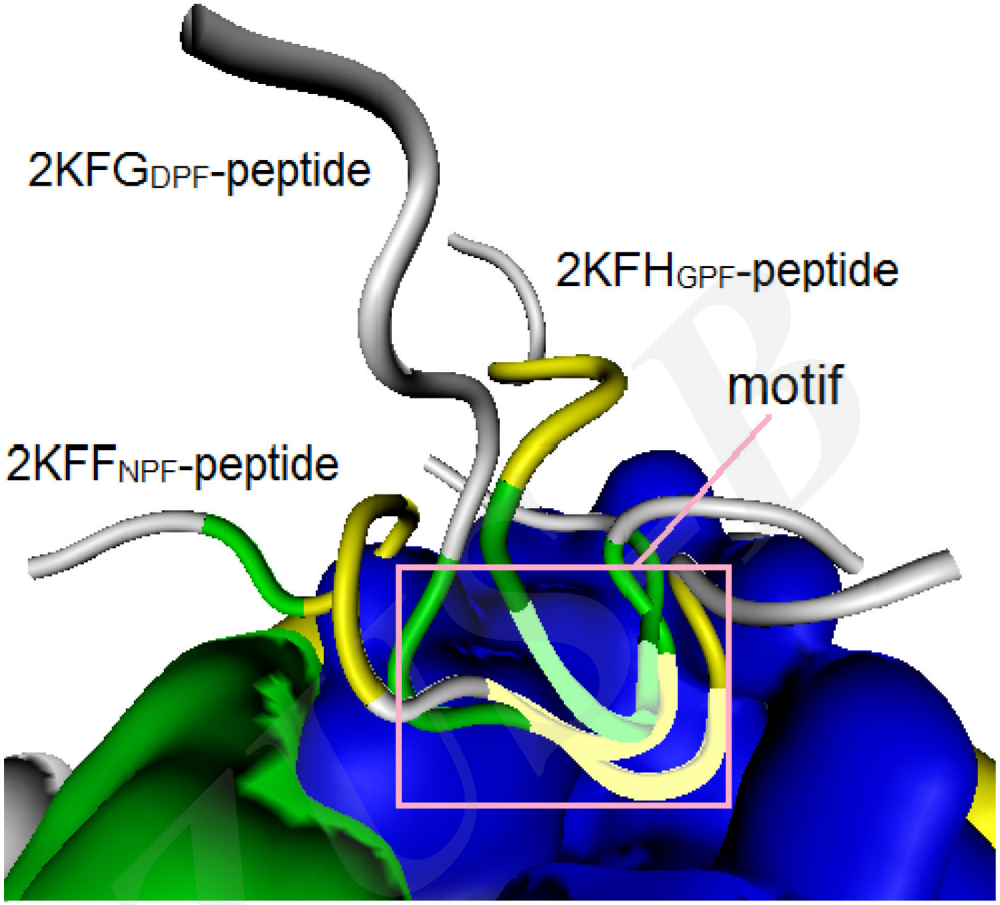
EHD1 EH domain

peptide	disassociation constant
FNYEST**NPF**TAK	245 μM
FNYEST**DPF**TAK	1.2 mM
FNYEST**GPF**TAK	2.4 mM

Only one residue is different while their disassociation constants differ a lot.

Why?

Results



In Terms of Structure

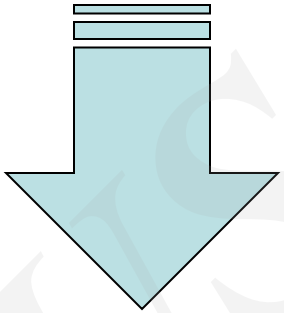
- Proteins are very similar while peptide structures differ from each other especially for the flanking residues (peptide residues except for the motif).
- Intermolecular hydrogen bonds of the flanking residues provide the structure basis of their van der Waals interactions.

In Terms of Key Energy

- van der Waals interactions of both the motif and the flanking residues

Significance

Provide essential information for peptide inhibitor design



- van der Waals interactions
- Intermolecular hydrogen bonds of the flanking residues