



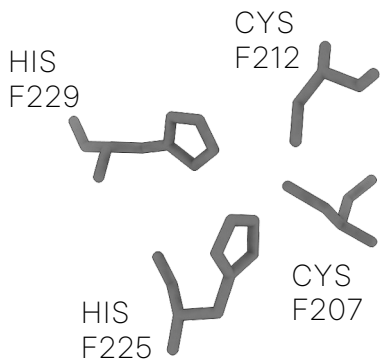
Searching protein structural motifs with Folddisco

Hyunbin Kim

Seoul National University
SteineggerLab

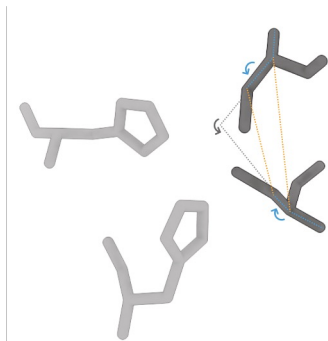
How to find structural motifs?

Structural motif



C2H2-type zinc finger
PDB: 1G2F

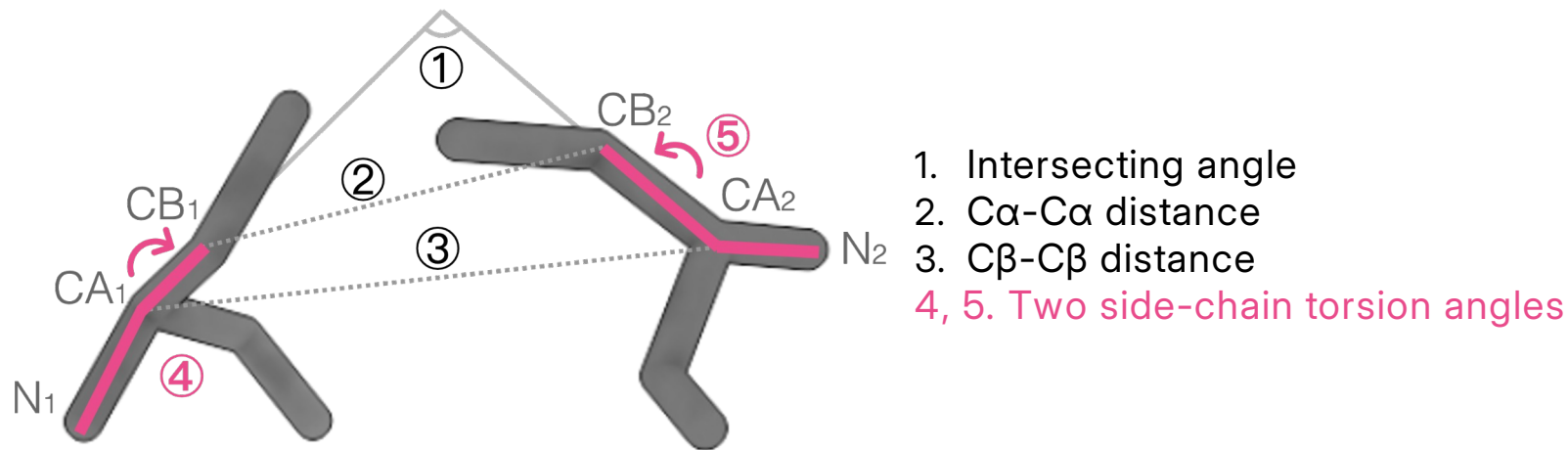
Pairwise interaction



Solution

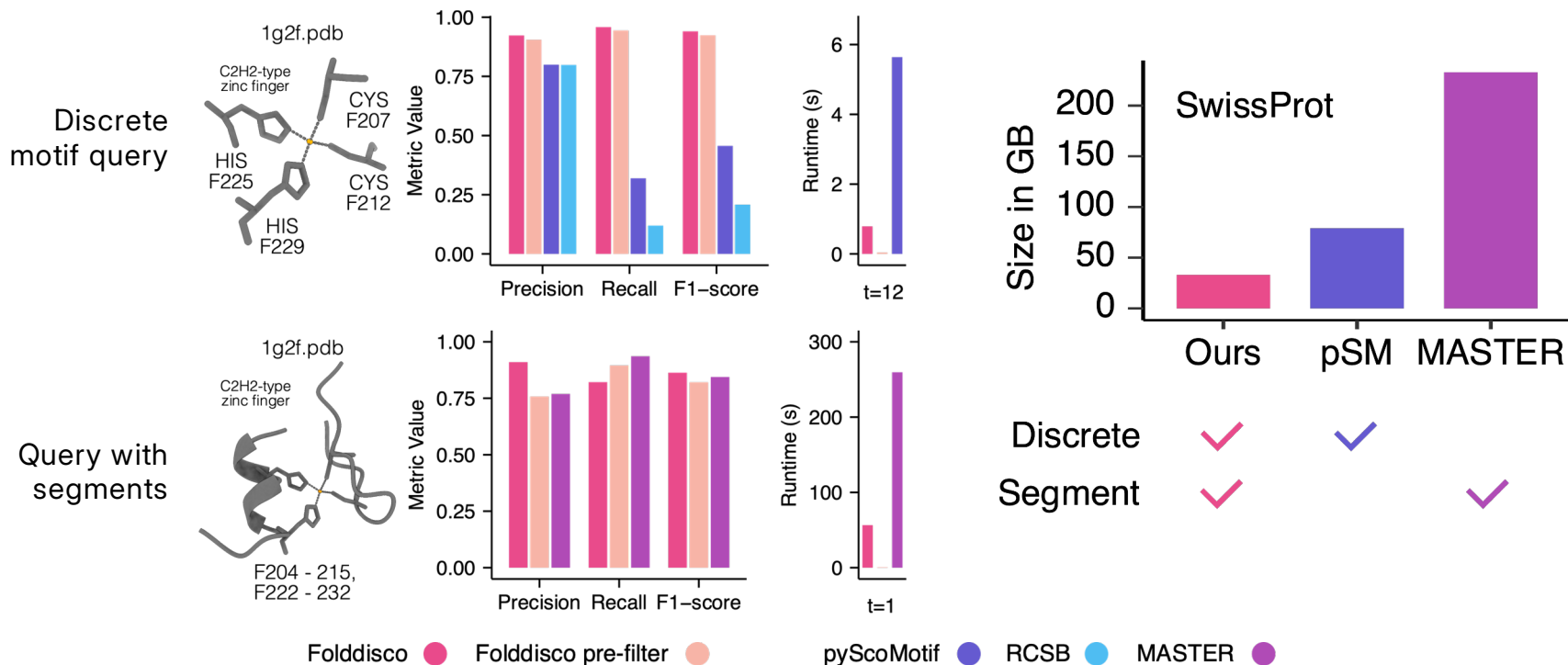
1. Store all pairwise interaction of given structures in an index
2. Disassemble motif into pairwise interactions and search against the index

We introduced a new pairwise-feature with side-chain orientation encoding



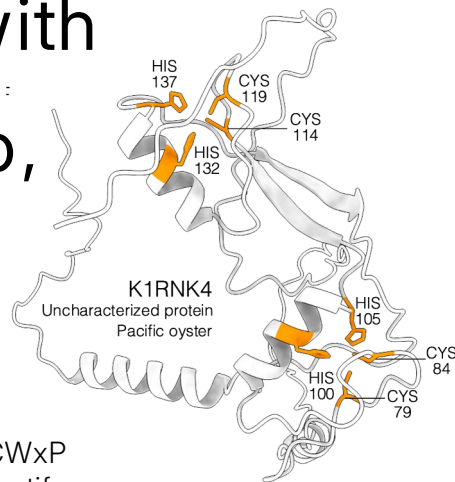
With this feature, we could reduce index size by not saving position while keeping accuracy.

Folddisco uniquely supports both discrete and segment-based motif queries while maintaining a small index size



Folddisco can retrieve GPCR structures with specific conformational states

Also,



Activated

Inactivated

PDB:6LFO
CXCR2
activated by
interleukin-8

PDB:6LFL
Inactivated
CXCR2

PDB:7XJI
Solabegron-activated
beta3 adrenergic
receptor

PDB:6PS5
Beta2 adrenergic
receptor bound to
propranolol

CWxP
motif

NPxxY motif

DRY motif

