

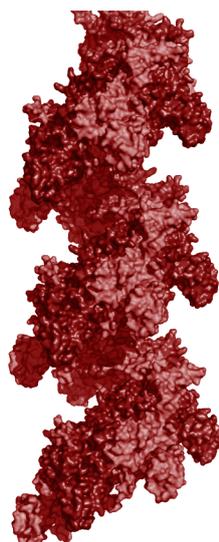
Practical session #3 & 4 - interface comparison, families of oligomeric forms

In this session, we will compare interfaces by simultaneously loading two sets of binding geometries in the server. The aim is to relate the global form to the interface similarity. Similarity is measured by the f_{NAT} value (see below).

During this session, you will also be able to use your protein structures and we will do our best to provide help for constructing filaments.

Interfaces

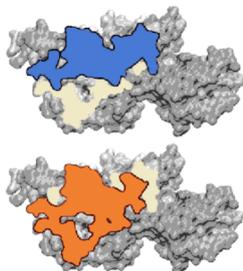
A binding geometry can be characterized by a set of pairs of amino-acid in contact across the interface. Oligomers are considered to participate to a same family in terms of interface if they share a sufficient ratio of contact pairs. This ratio is called f_{NAT} (fraction of native contacts) due to its historical definition in folding studies, but it can be used with profit to characterize the similarity of alternative interfaces.



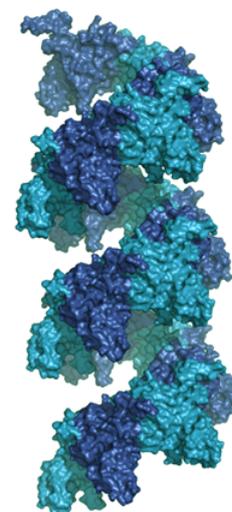
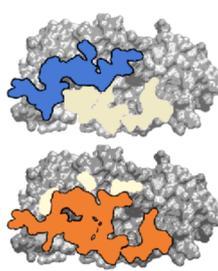
extended

Example of the RecA filament forms: the f_{NAT} value between the two interfaces is 0 (when the Nter domain, residues 1-36, is omitted) but the interfaces of the compressed form (blue) and the stretched form (orange) overlap both for the "upper" and the "lower" interfaces (each monomer binds a "upper" and a "lower" monomer)

upper interface



lower interface



compressed

f_{NAT} values vary between 0 (no similarity) and 1 (identical interfaces). Values above 0.5 indicate reasonably close interfaces, that can be considered as belonging to the same family of assemblies. During molecular dynamics simulations of protein assemblies, f_{NAT} values typically vary between 0.5 and 0.8 as a result of thermal agitation.

RecA - comparison between the stretched and compressed form

RecA_AB_ATP.pdb

RecA_AB_ADP.pdb

the fNAT value will be calculated for the whole structure residue 1-333

or for truncated structures, without the N-terminal domain (helix_linker): residues 38-333

PDB: 2REC

calculate FNAT values between each helical form and the hexameric form 2REC

RecA - binding geometries and filament forms

compare the following sets of oligomeric assemblies of the RecA protein

a_RecA_AB_formATP.pdb with a_RecA_AB_formADP.pdb

g_RecA_AB_formATP.pdb with g_RecA_AB_formADP.pdb

j_RecA_AB_formATP.pdb with j_RecA_AB_formADP.pdb

Dmc1 - comparison between the binding geometries in the octameric ring and in two helical forms — one generated by docking simulations, the other one obtained in 2021 by CryoEM, with bound DNA

Dmc1_AC_R.pdb

Dmc1_AB_H_Docking.pdb

Dmc1_AB_H_7C9C.pdb

parM (actin family)

6izr.pdb

generate and compare the protomers obtained from chains:

B,A E,D H,G K,J N,M Q,P (N.B. the order is important)

b,c e,f h,i k,l n,o q,r t,u w,x

Y,Z

visualize together all generated .pdb files with vmd