

Task 2:

The nuclear protein Baf1 is reported to bind different nuclear and centromeric proteins Like EMD and CENP-C). Model the binding of BaF1 to EMD and CENP-C and determine which interaction is predicted to be the strongest. Baf1 and CENP-C are both dimers in solution.

References:

- J Cell Sci. 2014 Sep 15;127(Pt 18):3956-69. doi: 10.1242/jcs.148247. Epub 2014 Jul 22.
- bioRxiv 2023.09.25.559341; doi: <https://doi.org/10.1101/2023.09.25.559341>

BaF1

MTTSQKHRDFVAEPMGEKPVGSLAGIGEVLGKKLEERGFDKAYVVLGQFLVLKKDEDLFREWLK
DTCGANAKQSRDCFGCLREWCD AFL

EMD¹⁻¹⁸⁷

MDNYADLSDELTTLLRRYNIPHGPVVGSTRRLYEKKIFEYETQRRRLSPSSSAASSYSFSDLNS
TRGDADMYDLPPKEDALLYQSKGYND DYYEESYFTTRTYGEPESAGPSRAVRQSVTSFPDADAF
HHQVHDDDLLSSSEEECKDRERPMYGRDSAYQSITHYRPVSASRSSL DLSYYPTSSS

CENP-C^{600-C}

SGGIVGHDEISRCSLSEPLESDEADLAKKKNLDCSRSTRSSKNEDNIMTAQNVPLKPQTSGYTC
NIPTESNLDSGEHKTSVLEESGPSRLNNNYLMSGKNDVDDEEVHGSSDDSKQSKVIPKNRIHH
KLVLPSTPNVRRTRKRLKPLEYWRGERIDYQGRPSGGFVISGVLSPTISSKRKAKENIGKVNK
KSNKKRICLDNDERKTNL MVNLGIPLGDPLQPTRVKDPETREILMDLVRPQDTYQFFVKHGELK
VYKTLDPFFSTGKLILGPQEEKGKHVGQDILVFYVNF GDLLCTLHETPYILSTGDSFYVPSGNY
YNIKNLRNEESVLLFTQIKR