BT1051 计算生物学 2024-2025-2

Project 4. AlphaFold3 Hands On

BT1051 | Project 4 | ddl 2025.5.20

1) Use AF3 to select/determine substrate.

PurA, PurZ and PurZ0 utilize ATP or GTP as one of their substrates. Please use AlphaFold3 to "cofold" ATP or GTP with a PurA, a PurZ and a PurZ0, and use proper evaluation method to tell which NTP is the right substrate for each enzyme.

Please upload the UniProt accessions for the PurA, PurZ, PurZ0 you picked and the 3 correct complex structures as your answer.

2）Use AF3 to discover novel viral proteins that can inhibit host immunity.

Read the paper "Structure-guided discovery of viral proteins that inhibit host immunity"（https://www.sciencedirect.com/science/article/pii/S0092867424014788） and then use AlphaFold3 to predict the following 7 complex structures.

(a) ThsB + Tad3/Tad4/Tad5/Tad6/Tad7 (Fig. 1 & Fig.2)

(b) ThsA + Tad8, CD-NTase + Abc3 (Fig. 2)

Please upload the 7 complex structures as your answer.

3) Use AF3 to find ligand binding pockets and poses.

Read the paper "Structured Odorant Response Patterns across a Complete Olfactory Receptor Neuron Population" (https://www.cell.com/neuron/fulltext/S0896-6273(18)31150-4#fig3), and then use AlphaFold3 to predict the complex structure of the top 5 sensitive ligand-receptor pairs in Fig 3B.

Please upload the 5 complex structures as your answer.