protocols.io

⊕ Structural prediction of VPS13C with AlphaFold2

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ABSTRACT

This protocol describes the procedure of structural prediction of full-length human VPS13C and its truncation mutant with AlphaFold2 and the procedure to combine each segments into one structure.

ATTACHMENTS

442-930.docx

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Structure prediction

1 Separate Full-length VPS13C and truncation mutant into three pieces and two pieces, respectively, i.e., a.a. 1-1860, 1201-2340, 1801-3753 for full-length VPS13C and a.a. 1-1762, 1277-3240 for VPS13C$_{\Delta1235\text{-}1748}$.

> **Note**: prediction of the entire VPS13C sequence does not work because of sequence-length limitation of AlphaFold 2.0.

2 Install AlphaFold 2.0 on the Yale Farnam high performance computer cluster, used for structural prediction of each segment.

> **Note:** Use 5 pTM models to generate five structures. For subsequent analysis use the one with highest confidence score, shown in rankings.json file.

Combination of segments

3 Open UCSF ChimeraX software and import pdb files of segments.

4 Align the fragments with overlapping regions with "mmaker" command.

5 Delete the overlapping regions from adjacent fragments with "delete" command.

6   At the connection point, form a carbon–nitrogen bond with "build join peptide" command to connect two amino acid residues from two fragments.