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 in *doi of the paper*.

**Keywords**

AlphaFold, UCSF ChimeraX, VPS13C, ASAPCRN

**Steps**

A. Structure prediction

1. Full-length VPS13C and truncation mutant are separated 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 VPS13CΔ1235-1748.

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

1. AlphaFold 2.0, installed on the Yale Farnam high performance computer cluster, is used for structural prediction of each segment.

Note: 5 pTM models are used to generate five structures. The one with highest confidence score, shown in rankings.json file, is used for subsequent analysis.

B. Combination of segments

1. Open UCSF ChimeraX software and import pdb files of segments.
2. The fragments with overlapping regions are aligned with “mmaker” command.
3. The overlapping regions from adjacent fragments are deleted with “delete” command.
4. At the connection point, a carbon–nitrogen bond is formed with “build join peptide” command to connect two amino acid residues from two fragments.