

# FOURIER POWER SPECTRUM OF HYDROPHOBICITIES REVISITED: APPLICATION TO SARS-COV-2 SPIKE PROTEIN AND ACE-2



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## Introduction

The search of amphipathic structures in proteins has awakened especial interest since they are usually found on surface regions, which can participate in active centers or binding domains. Thus, one of the most powerful methods for their detection is the Fourier power spectrum of hydrophobicities. It is a predictive aminoacidic sequence-based method which allows the identification of recurrent properties of sequences using the periodic variation in hydrophobicity, being characteristic of their secondary structure. We apply this method on the SARS-CoV-2 Spike protein and human Angiotensin-converting enzyme 2 (ACE2) to show the potential application of this technique, which may help finding antigenic epitopes or binding sites being relevant for biomedical uses.

## Method

### Principles of Fourier power spectrum

Calculates the square of this amplitude of the Fourier transform (Power spectrum) :

$$I(k, \nu) = \left| \sum_{j=k-\frac{n}{2}}^{k+\frac{n}{2}} [h_j - \bar{h}(k)] \exp(2\pi i \cdot j \cdot \nu) \right|^2$$

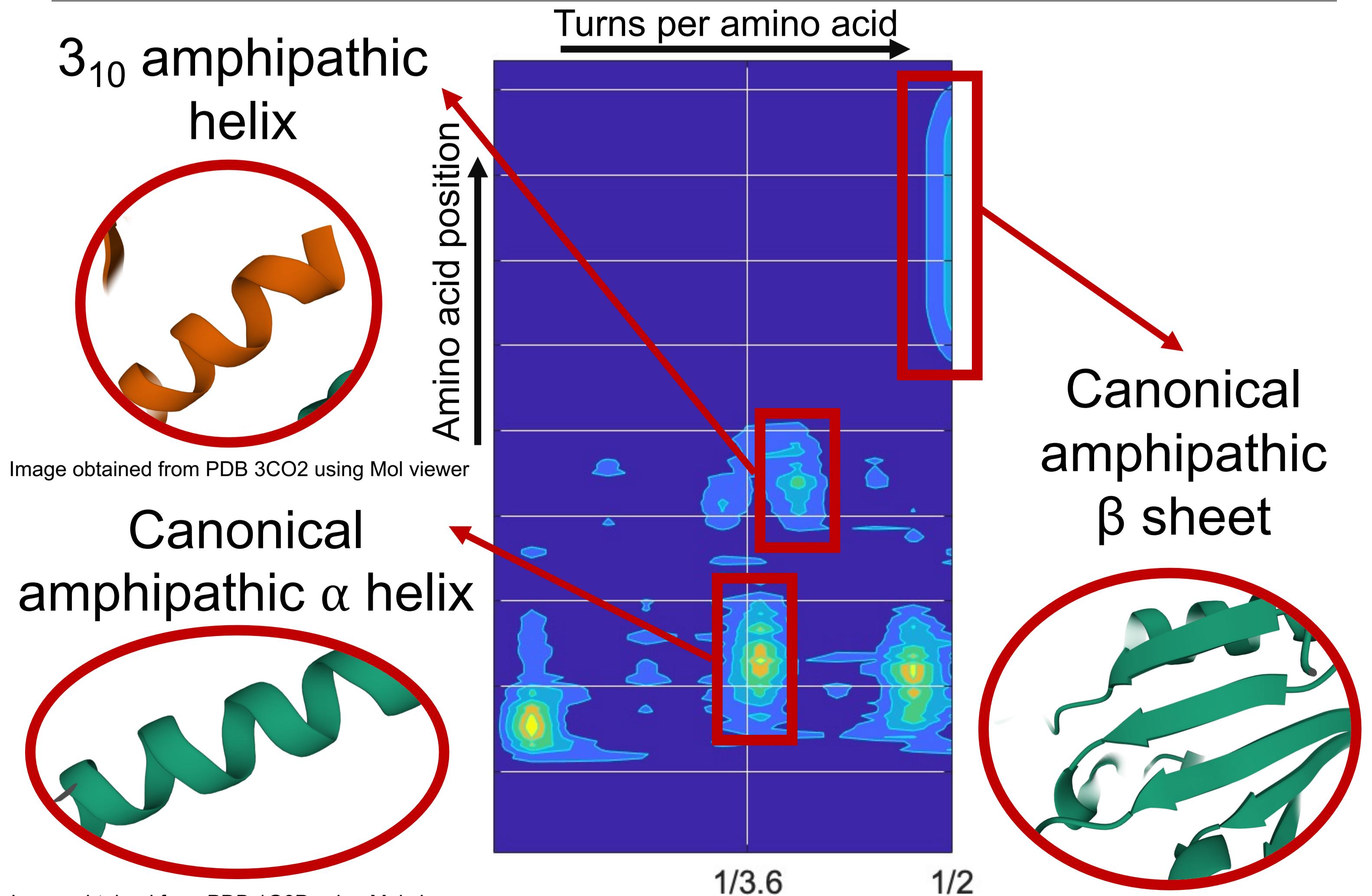
$k$  – residue number

$\nu$  – frequency

$h_j$  – hydrophobicity of residue  $j$

$\bar{h}(k)$  – average hydrophobicity (25 aa window)

### How to interpretate Fourier power spectrum



## Results

### Analysis SARS-CoV-2 spike protein (P0DTC2)

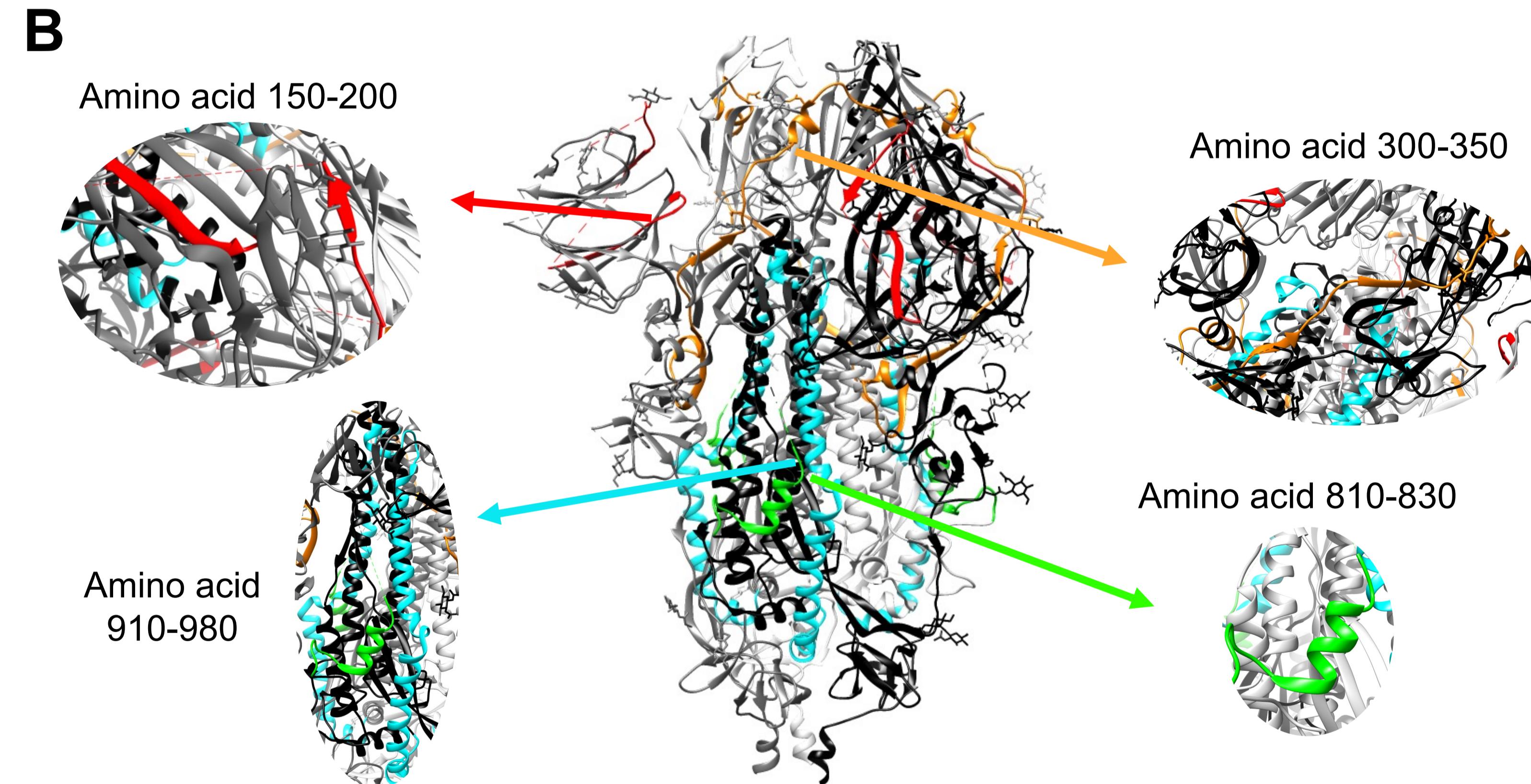
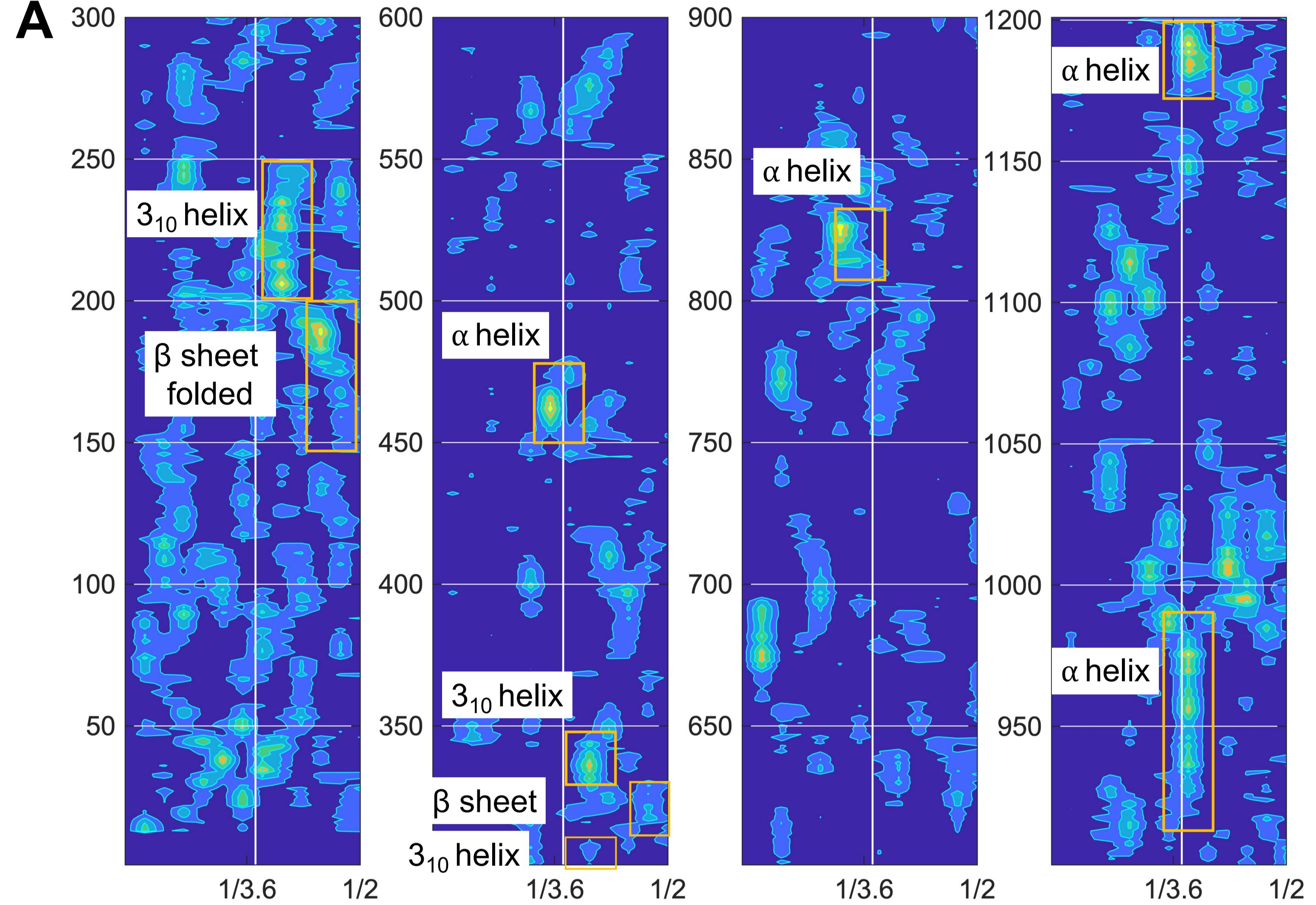


Figure 1. Fourier power spectrum applied on SARS-CoV-2 Spike protein. A) Amphipathic map highlighting possible secondary structure zones. B) 3-D representation of the protein (PDB: 6VXX) marking predicted amphipathic structures.

### Analysis ACE-2 (Q9BYF1)

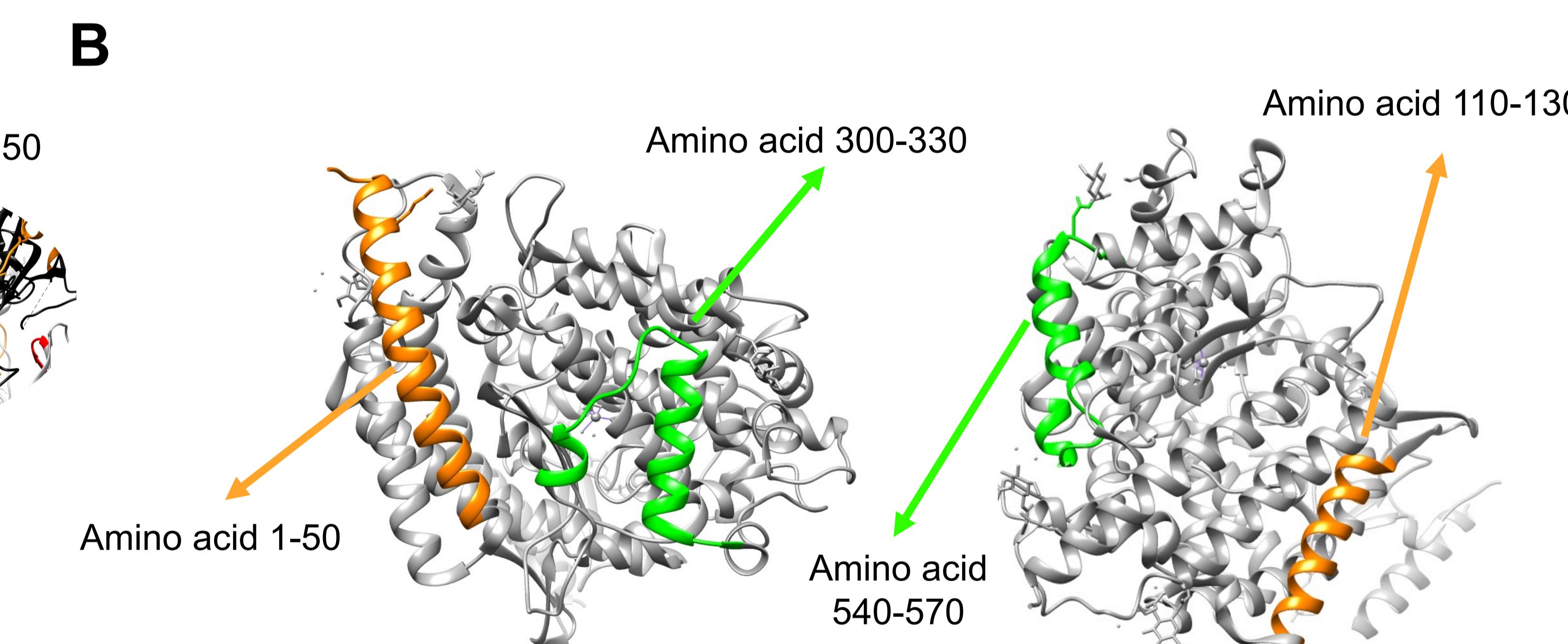
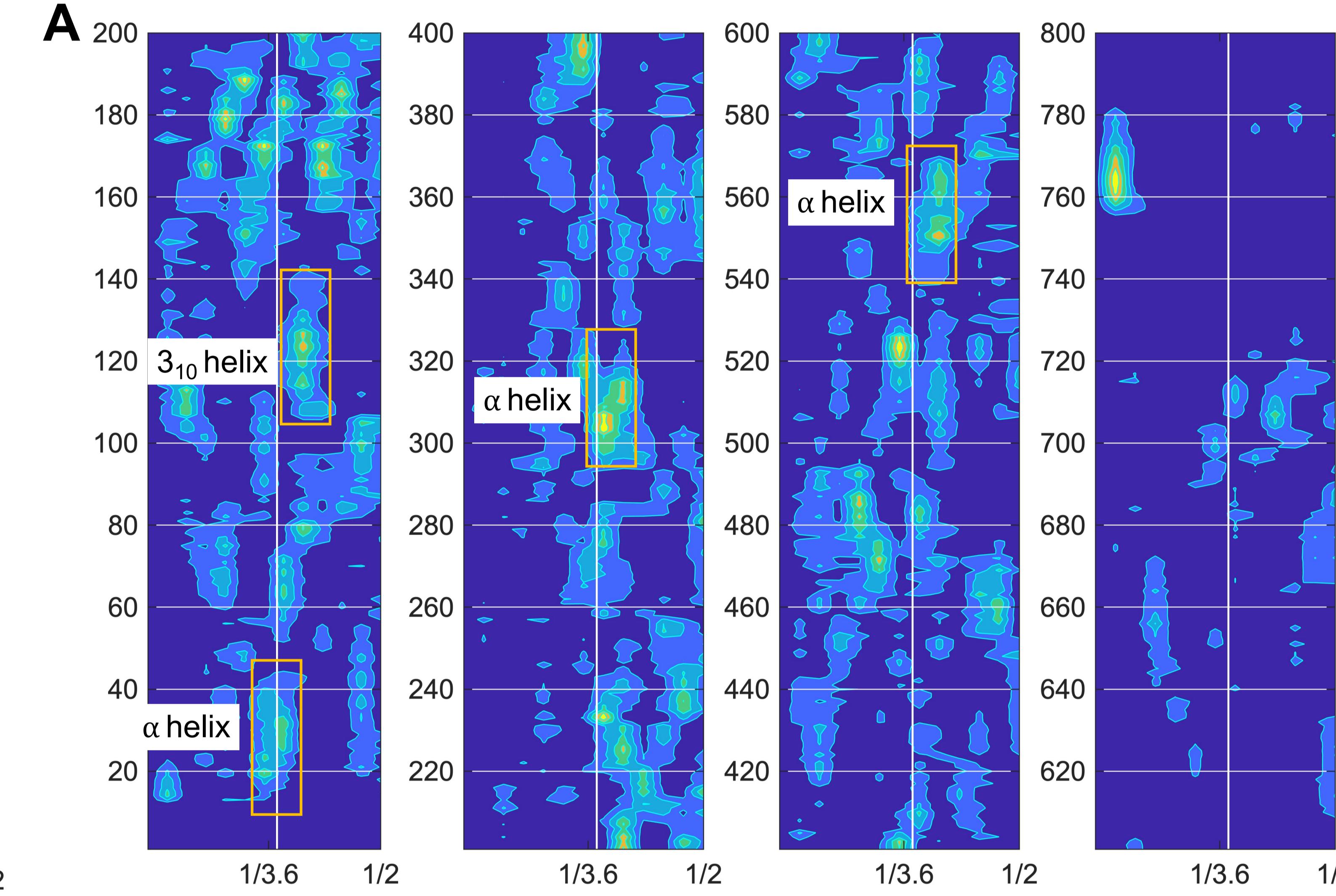


Figure 2. Fourier power spectrum applied on human ACE2. A) Amphipathic map highlighting possible secondary structure zones. B) 3-D representation of the protein (PDB: 1R42) marking predicted amphipathic structures.

## Conclusions

- Amphipathic secondary structures by the Fourier power spectra is an unusual method with a strong mathematical foundation that could be useful for the detection of interesting structural features.
- Fourier power spectrum is a predictive method which provides an approximate idea of the proteins' amphipathic structure from their sequence.
- In combination with other predictive methods, it could help to complete the information obtained.

### Reference

D. Eisenberg, E. Schwarz, M. Komaromy, R. Wall, Analysis of membrane and surface protein sequences with the hydrophobic moment plot, Journal of Molecular Biology. 179 (1984) 125-142.

### Predictive method comparation

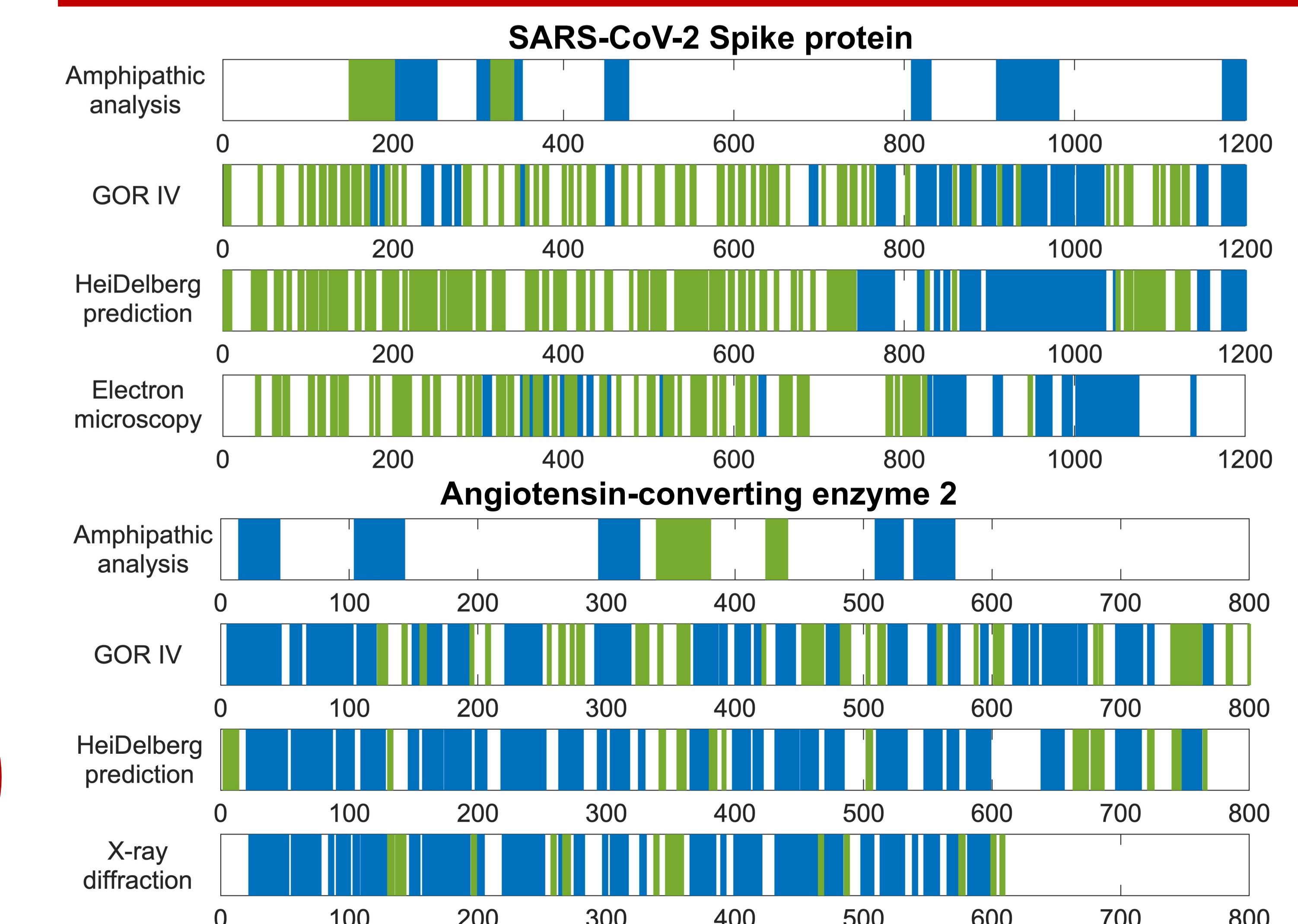


Figure 3. Comparison between different methods for the analysis of predictive or empirical secondary protein structures. In blue alpha helix and in green beta sheets.

