

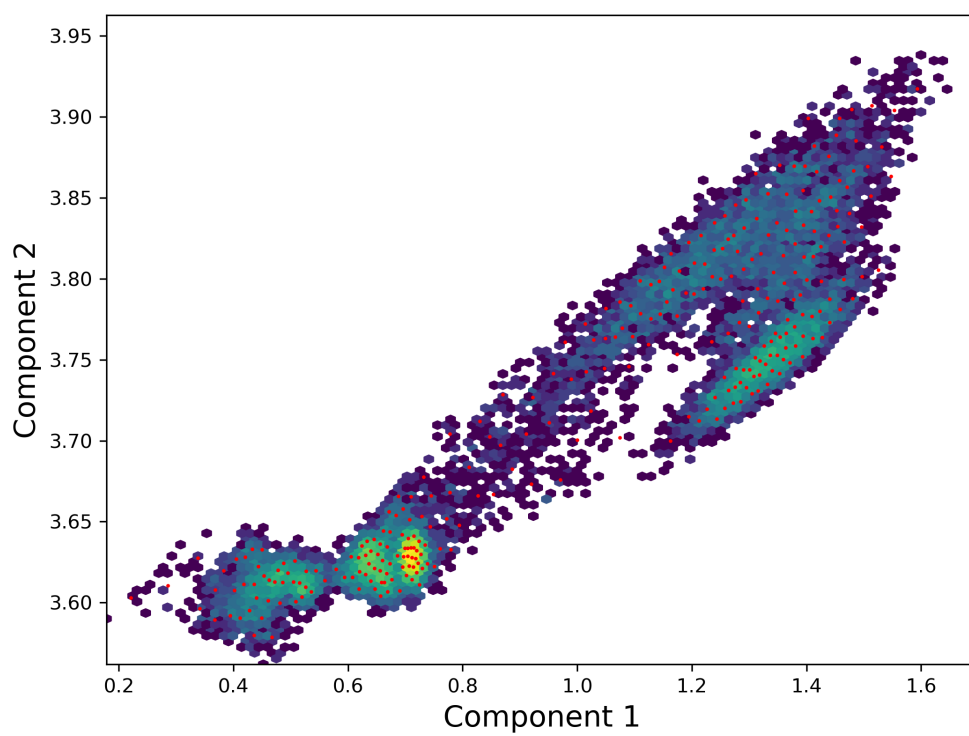
# **Deciphering the Protein Motion of S1 Subunit in SARS-CoV-2 Spike Glycoprotein Through Integrated Computational Methods**

Hao Tian and Peng Tao\*

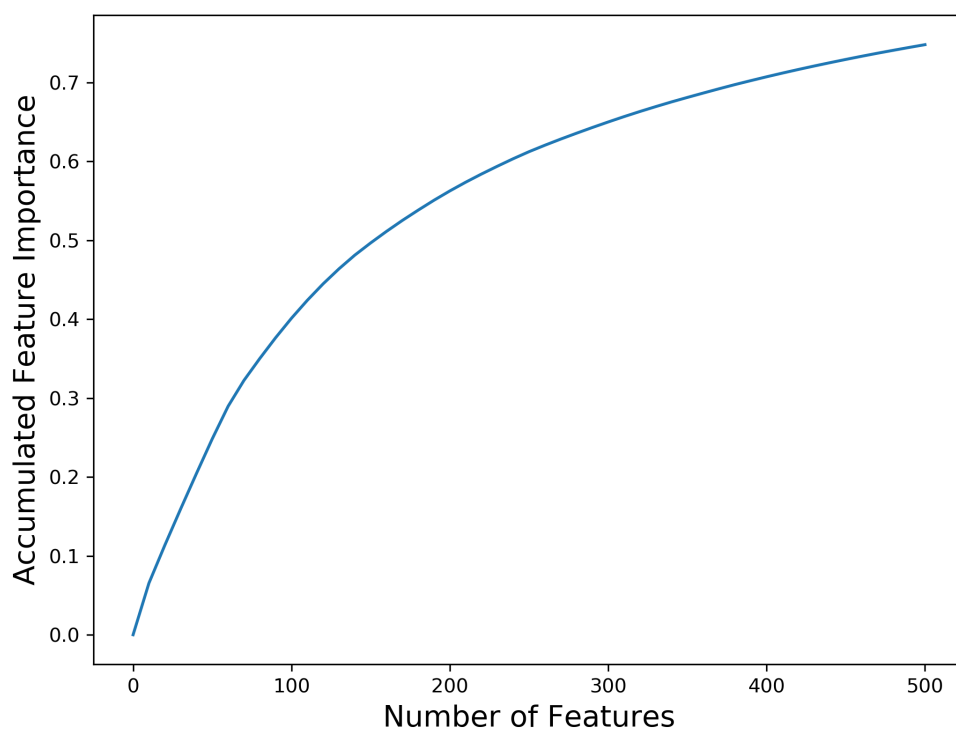
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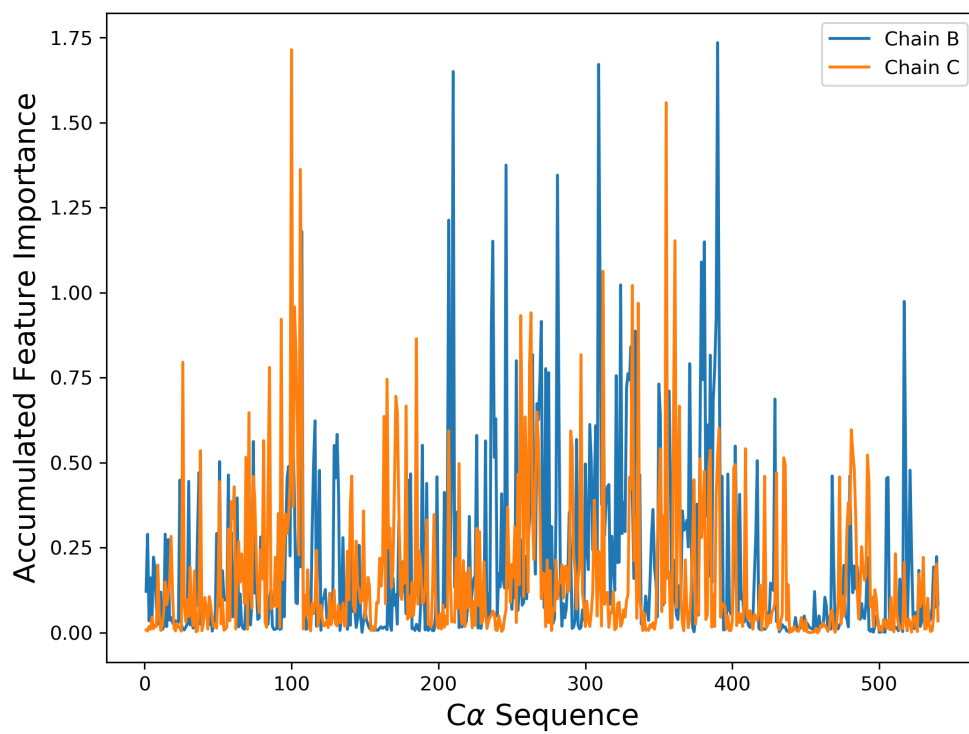
**Supporting Information Available**



**Figure S1:** MiniBatch k-means clustering results of 300 microstates shown in red dots.



**Figure S2:** Accumulated feature importance of the top 500  $C\alpha$  distances.



**Figure S3:** Accumulated residue importance in chain B (blue) and C (orange), respectively.