1161-00-239 **Q. S. Baldwin*** (qbaldwin8382@tuskegee.edu) and **Eleni Panagiotou** (eleni-panagiotou@utc.edu). *The local topological free energy of viral glycoproteins.*

Many viruses infect cells by using a mechanism that involves binding of a viral protein to the host cell. During this process, the three-dimensional conformation of the viral binding protein changes significantly and disruption of this process could be achieved by targeting key locations in the viral protein that are essential in this rearrangement. In this manuscript we propose to use the local geometry/topology of the crystal structure of the viral protein backbone alone to identify these essential locations. Our results show that the local Writhe, local Average Crossing Number and the local Torsion alone can identify "exotic" amino acids that are essential in the viral protein infection mechanism. We apply this method to the SARS-Cov-2 Spike protein to propose target amino-acids for drug discovery. (Received August 17, 2020)