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Computer-aided drug design and pharmacophore modelling towards the discovery of novel anti-ebola agents

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Ebolavirus is a genus of the Filoviridae viral family, containing six known species (de La Vega *et al.*, 2015). Four species of this viral family (Ebola, Sudan, Taï Forest, and Bundibugyo viruses) cause human disease in the form of viral hemorrhagic fevers, with frequent outbreaks that reach epidemic scale in the African continent, exhibiting high numbers of casualties (Rugarabamu *et al.*, 2020). The Ebola virus (EBOV) genome is a linear, single-stranded, non-segmented, negative-sense RNA containing seven genes, which code for structural and non-structural proteins (Mühlberger, 2007). Among these proteins is the viral glycoprotein (GP), the only virally expressed protein on the virion surface, critical for attachment to host cells and catalysis of membrane fusion (Lee and Saphire, 2009). The viral glycoprotein (GP) is produced through proteolytic cleavage of the precursor (pre-GP) and is comprised of two subunits (GP1 and GP2), connected by a disulfide bond (Ning *et al.*, 2017). As a result of its critical role in the virus life cycle and replication, the EBOV GP is a crucial component in vaccine development and an essential target in the research for neutralising antibodies and inhibitors of attachment and fusion (Hoenen *et al.*, 2019). In addition to standard approaches, the study of possible post-translational modifications concerning the EBOV GP can provide new insight into the efforts of developing new anti-ebola agents (Cook and Lee, 2013).

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