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Molecular docking and pharmacokinetics studies of *Curcuma longa* (Curcumin) potency against Ebola virus

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Abstract. The Ebola virus disease causing hemorrhagic fever in human, has been known for nearly about 40 years, with the most recent outbreak being in West Africa creating humanitarian crisis, where over 11,308 deaths were recorded as reported in 30th March, 2016 (World Health Organization). Till now, Ebola virus drugs have been far from achieving regulatory FDA approval, and coupled with toxicity of these drugs, it is become imperative to appraise the available trail drugs, as well as looking into alternative natural resources of tackling menace. Therefore, *in silico* methods were used to assess the potency of the bioactive phytochemical, Curcumin from Turmeric and results compared with those obtained for some selected trial drugs in use for the treatment of Ebola virus. This study is focused on molecular docking of Curcumin and eight commercially available drugs (Amodiaquine, Apilimod, Azithromycin, Bepridil, Pyronaridine, Remedesivir and Tilorone) against Ebola transcription activator **VP30** proteins (PDB: 2I8B, 4Z9P and 5T3T) and their ADMET profiling. The results showed that binding affinity (ΔG kJ/mol) ranged from -5.8 (Tilorone) to -7.3 (Remdesivir) for 218B, -6.4 (Tilorone) to -8.2 (Pyronaridine, Remedesivir) and -5.8 (Bepridil) to -7.4 (Pyronaridine). Curcumin could be more desirable as inhibitor for than Tilorone, Dronedarone and Bepridil in the treatment of Ebola virus; the ADMET profile revealed that Curcumin presents attractive pharmacokinetic properties than the trial drugs.

***Keywords*:** curcumin; docking; pharmacokinetics; Ebola virus.

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