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In silico study of anti-HIV and anticoagulant properties of coumarin and p-coumaric acid, fullerenes and their respective conjugates

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Coumarin and p-coumaric acid have been implicated to alleviate multiple disease conditions and nanoparticles have been known to inhibit key proteins, individually but in this study we are interested in assessing the anti-HIV and anticoagulant properties of coumarin and p-coumaric acid along with their synthesized fullerene conjugates and fullerene. We isolated coumarin and p-coumaric acid from endophytic fungi, alternaria species-1 from crotalaria pallida leaf and characterized by UV, XRD, FTIR, and C13 NMR. Subsequently, we synthesized the fullerene nanoparticles using coumarin and p-coumaric acid separately. Two coagulant proteins and nine HIV-1 proteins were selected using iGEMDOCK. We report that p-coumaric acid has greater interaction with coagulant proteins followed by coumarin and fullerenes. Among HIV-1 proteins higher interaction was observed with p-coumaric acid especially, HIV-1gp120. However, upon conjugating fullerene to coumarin and p-coumaric acid, coumarin-fullerene showed significantly greater interaction with coagulant proteins and all HIV-1 proteins, compared to p-coumaric acid-fullerene and fullerene. Our in silico study, thus identifies nanoparticles synthesized by fullerene conjugated to naturally occurring coumarin and p-coumaric acid as a safe and cost effective alternative strategy to treating HIV or its use as an anticoagulant.

Keywords: Alternaria species-1, coumarin, p-coumaric acid, molecular docking, anticoagulant, anti-HIV

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