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## Effect of Dendrimer in HIV-1 inhibition

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The polyamidoamine (PAMAM) dendrimer prevents HIV-1 entry into target cells in vitro. Its mechanism of action, however, remains unclear and precludes the design of potent dendrimers targeting HIV-1 entry. We employed steered molecular dynamics simulations to examine whether the HIV-1 gp120-CD4 complex is a target of PAMAM. We found that the complex dissociates via complex pathways and defies the standard classification of adhesion molecules as catch and slip bonds. Our simulations reveal that PAMAM targets the gp120-CD4 complex at two levels: it weakens the complex and also alters its dissociation pathway, potentially inhibiting HIV-1 entry (JCP 2013). Recently, we have also demonstrated that anionic SPL7013 dendrimer binds to gp120 in complex with CD4, destabilizes the complex and expedites its dissociation. The number of stable gp120-CD4 complexes across a virus-cell pair is thus lowered, preventing viral entry.

(work done in collaboration with B. Nandy, Sourav Purohit, Anil Sahoo, D Hima Bindu and Narendra Dixit)

### References:

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