Conformational analysis of novel trimeric cross linking reagents

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Twelve potential cross-linking reagents for inhibitors of HIV fusion were characterized by classical mechanical conformational searching techniques using the Schrödinger software package. Mixed Low Mode and Monte Carlo searching techniques were performed to exhaustively sample the OPLS2005/GBSA(water) potential energy surfaces of C3 symmetric trisubstituted derivatives of cyclohexane, benzene, and triazacyclododecane. Geometric structure, molecular length, and hydrogen bonding patterns were analyzed for the compounds and compared to temperature dependent NMR and biological inhibition studies.