Recognition of HIV-Inactivating Peptide Triazoles by a recombinant soluble trimer, BG505 SOSIP.664

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Supplementary Information

Table S1. Percentage of contacts among **1**, **2** and **3** with subsite 1 and subsite 2 residues over their respective 50 ns MD trajectories.

PT	*Per-residue* contact %					
	Subsite 1		Subsite 2			
	T257	S375	I109	W112	F210	M426
1	31.7	1.4	71.0	99.3	99.1	99.9
2	97.6	0.1	41.4	99.8	76.9	66.3
3	11.6	0	99.7	99.0	48.8	97.8

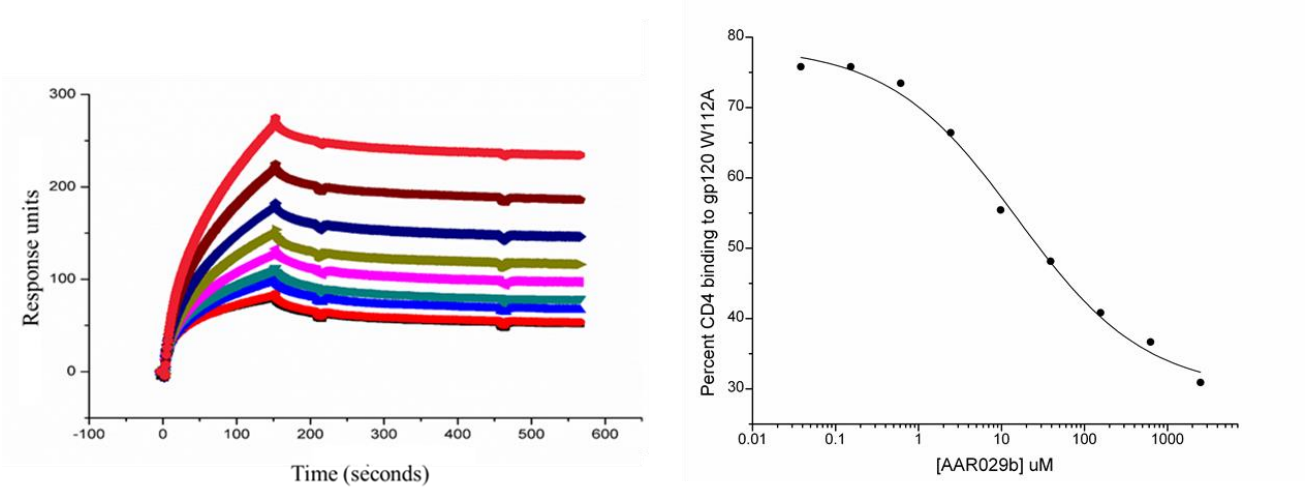

Figure S1. (Left) SPR sensograms resulting from dose dependent inhibition of CD4 binding to immobilized monomeric gp120 mutant protein W112A by peptide 2. The data show ~ 500-fold decrease in potency (IC_{50}: 15 μM) compared to the previously calculated[10] IC_{50} (32 nM) value with the wild-type monomeric gp120 protein. (Right) Dose response curve for gp120-W112A binding to CD4 in the presence of increasing concentrations of peptide **2**.