

A Free and bound states	Free energy ΔG^i (kcal/mol)
BC	ΔG^{BC}
EC	ΔG^{EC}
EO	0
inhibitor bound BC	$\Delta G^{BC} - RT \ln(C_{\text{inhibitor}} / K_{d, \text{inhibitor}}^C)$
inhibitor bound EC	$\Delta G^{EC} - RT \ln(C_{\text{inhibitor}} / K_{d, \text{inhibitor}}^C)$
inhibitor bound EO	$-RT \ln(C_{\text{inhibitor}} / K_{d, \text{inhibitor}}^C)$

Statistical weight for each state: $S^i = \text{Exp}(-\Delta G^i / RT)$

Partition function of the system: $Q = \sum S^i$

Population of the extended states: $P^{\text{extended}} = (S^{EC} + S^{EO} + S^{\text{inhibitor bound EC}} + S^{\text{inhibitor bound EO}}) / Q$

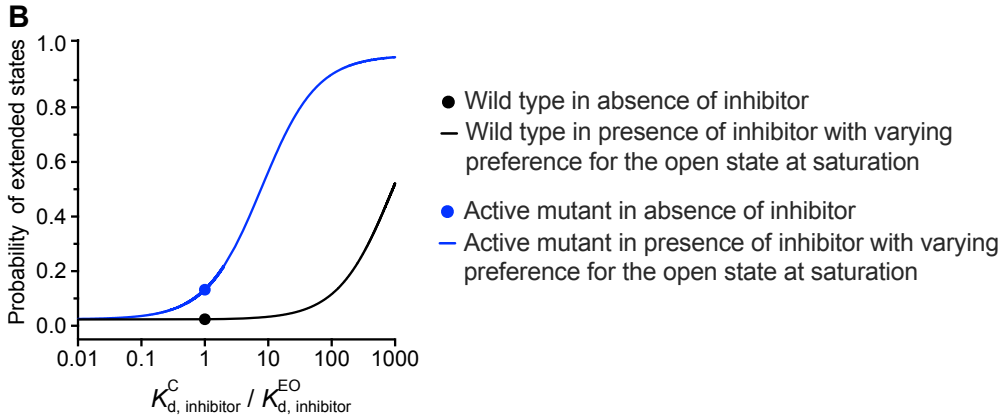


Figure S7. Called in Discussion. Related to Figs. 5, 6, and 7. Influence of inhibitors with varying preference for the open state on extension-stabilizing antibody epitope exposure.

(A) Equations for calculating the population of extended states of integrin in presence of inhibitors with different binding affinities to the closed and EO states. (B) A scenario to explain why wild type and active mutant integrin $\alpha 1 \text{Ib} \beta 3$ show different sensitivities in inhibitor-induced LIBS antibody epitope exposure assays. Free energy values used for the BC, EC and EO states of wild type $\alpha 1 \text{Ib} \beta 3$ are -4, -1.8 and 0 kcal/mol, respectively; free energy values used for the BC, EC and EO states of active mutant are -1.2, -1.0 and 0 kcal/mol, respectively, representing a 2.8 kcal/mol destabilization of the closed states by the mutation.

Any conformation-specific antibody can be a LIBS reporter. However, antibodies must be used at concentrations near their EC50 values to be good LIBS reporters. It appears that many useful, high-affinity, conformation-specific antibodies are not used in the literature because the typical antibody concentrations investigators use are too high for these antibodies to report epitope exposure. All LIBS antibodies must be titrated to find the optimal concentration.