Supplementary Materials and Methods

The relative ratios for $K_d^{3'SL}/K_d^{6'SL}$ are inversely proportional to the ratio of STD signals in the competition experiment. Briefly, for the equilibria:

HA + 3'SL <-> HA-3'SL and HA + 6'SL <-> HA-6'SL

$K_d^{3'SL}$ = [HA][3'SL]/[HA-3'SL] and $K_d^{6'SL}$ = [HA][6'SL]/[HA-6'SL]

[HA-3'SL] = [HA][3'SL]/ $K_d^{3'SL}$ and [HA-6'SL] = [HA][6'SL]/ $K_d^{6'SL}$

In the concentration range [SL] < 3X K_d, STD intensity is proportional to HA bound to SL (Meyer B, Peters T (2003) NMR spectroscopy techniques for screening and identifying ligand binding to protein receptors. Angewantde Chemie International Edition 42: 864-890). Accordingly,

$STD^{3'SL}/STD^{6'SL}$ ~ [HA-3'SL]/ [HA-6'SL] = ([HA][3'SL]/ $K_d^{3'SL}$)/ ([HA][6'SL]/ $K_d^{6'SL}$)

Since [3'SL] ~ [6'SL] ~ 3 mM, $STD^{3'SL}/STD^{6'SL} \sim K_d^{6'SL}/K_d^{3'SL}$