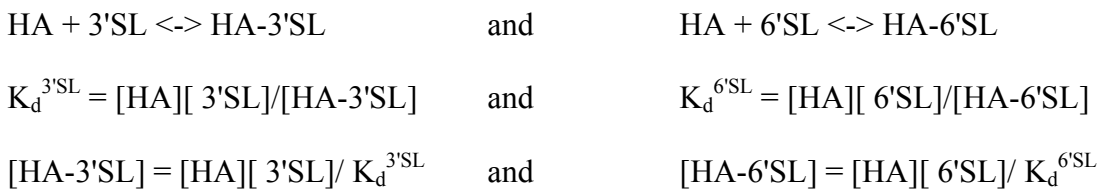


## Supplementary Materials and Methods

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:



In the concentration range  $[\text{SL}] < 3X K_d$ , 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. Angewandte Chemie International Edition 42: 864-890). Accordingly,

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

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