Graphical Abstract

Figure 1. Receptors 1, 2 and guanosine derivative, 3 used for binding studies; TIPS = triisopropylsilyl.
Figure 2. Dimers of 1 and 2, 1•1 and 2•2; respectively.

Figure 3. Curve fitting from NMR dilution of 2; $K_{2,2} = 340\pm 7$ M$^{-1}$.
Figure 4. Curve fitting from NMR dilution of 1 in CDCl₃; $K_{1+4} = 83\pm3$ M⁻¹.

Figure 5. Self-association model of lipophilic guanosine 3 in chloroform.
**Chemical shift (ppm)**

- **Concentration (M)**
  - 0.000
  - 0.010
  - 0.020
  - 0.030
  - 0.040
  - 0.050
  - 0.060
  - 0.070

**N3-H observed**

- Chemical shift: 11.99 - 12.09 ppm

**N3-H Calculated**

**H-8 observed**

- Chemical shift: 7.76 - 7.81 ppm

**H-8 Calculated**

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**Graph 1:**
- N3-H observed
- N3-H Calculated

**Graph 2:**
- H-8 observed
- H-8 Calculated
Figure 6. Curve fitting for NMR dilution of 3 in CDCl₃. The three titration curves (A) N3-H (B) H-8 and (C) NH₂ are fitted simultaneously to give $K_{3,3}$ of 370±72 and $K_{3,3,3,3}$ of 15±1 M⁻¹.

Figure 7. Complexation of receptors 1 or 2 with 3; TIPS = triisopropylsilyl.
Scheme 1. Equilibria in the binding studies between 2 and 3.
Figure 8. Curve fitting of NMR titration in CDCl₃ between 2 and 3. $K_{2\cdot3} \pm 8100 \pm 380$; $K_{2\cdot3\cdot3} \pm 1170 \pm 80 \text{ M}^{-1}$.

Figure 9. Speciation curve for receptor 2 upon addition of 3 in CDCl₃, showing monomeric 2, dimeric 2, 1:1 complex ($2\cdot3$) and 1:2 complex ($2\cdot3\cdot3$).
Figure 10. Curve fitting of NMR titration in CDCl$_3$ between 1 and 3. $K_{130} = 5180 \pm 210$, $K_{133} = 4800 \pm 170$ M$^{-1}$.

Figure 11. Speciation curve for 1 upon addition of 3 in CDCl$_3$. 
Figure 12. Summary of equilibria in deuteriochloroform for monoalkyne receptor 1.

Figure 13. Summary of equilibria in deuteriochloroform for dialkyn receptor 2.
Figure 14. C-P-K models of 1 at $E_{\text{min}}$ (left) dihedral $\approx 30^\circ$ showing interactions between TIPS groups and $E_{\text{max}}$ (right) dihedral $\approx 165^\circ$. 
Figure 15. Torsional energy vs. dihedral angle for monoalkyne 1
**Figure 16.** Torsional energy vs. dihedral angle for dialkyne 2