Novel Hydrazide-Based Quadruply Hydrogen Bonded Heterodimers.  
Structure, Assembling Selectivity and Supramolecular Substitution

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Supporting Information
NOESY spectrum of the 1:1 solution of 1 and 2 (10 mM) in CDCl₃.
Partial NOESY spectrum of the 1:1 solution of 1 and 11 (10 mM) in CDCl₃.
Partial NOESY spectrum of the 1:1 solution of 1 and 12 (10 mM) in CDCl₃.
Partial NOESY spectrum of the 1:1 solution of 19 and 2 (10 mM) in CDCl$_3$. 

19 and 2 chemistries: 

- 19: 
  - O$_2$C$_{12}$H$_{25}$O
  - N

- 2: 
  - C$_{12}$H$_{25}$O
  - N
  - H
  - H

The spectrum shows cross-peaks indicating NOE interactions between the protons of the molecules.
Partial NOESY spectrum of the 1:1 solution of 19 and 11 (10 mM) in CDCl₃.
NOESY spectrum of the 1:1 solution of 19 and 12 (10 mM) in CDCl3.

![Diagram of 19 and 12 molecules and NOESY spectrum graph.](image-url)
NOESY spectrum of the 1:1 solution of 1 and 23 (10 mM) in CDCl₃.
Partial NOESY spectrum of the 1:1 solution of 19 and 23 (10 mM) in CDCl₃.
Calculation for the binding constant of complex 23-25:

\[ [23] + [25] \xrightleftharpoons{\Delta G_1} [23] \cdot [25] \]  
(equ. 1)

\[ [1] + [23] \xrightleftharpoons{\Delta G_2} [1] \cdot [23] \]  
(equ. 2)

(equ. 3)

(equ. 4)

\[ \Delta G_1 = 0.5 (2 \Delta G_2 + \Delta G_3 - \Delta G_4) \]

Since \( \Delta G_2, \Delta G_3, \) and \( \Delta G_4 \) are available, \( \Delta G_1 \) could be obtained from the above equation. The corresponding binding constant \( K_{[23][25]} \) was then derived from the Eyring equation.