CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

Folding and Anion-binding Properties of Fluorescent Oligoindole Foldamers

Uk-Il Kim, Jae-min Suk, Veluru Ramesh Naidu, and Kyu-Sung Jeong*[a]

[a] Center for Bioactive Molecular Hybrids and Department of Chemistry
Yonsei University
Seoul 120-149 (Korea)

1. Computer modeling

Energy-minimized structures of oligoindoles were generated using MacroModel 9.1 program[1] with MMFF force field[2] in the gas phase via 5000 search steps in Monte Carlo conformational search. The ester side chains have been replaced with hydrogen atoms for convenience.

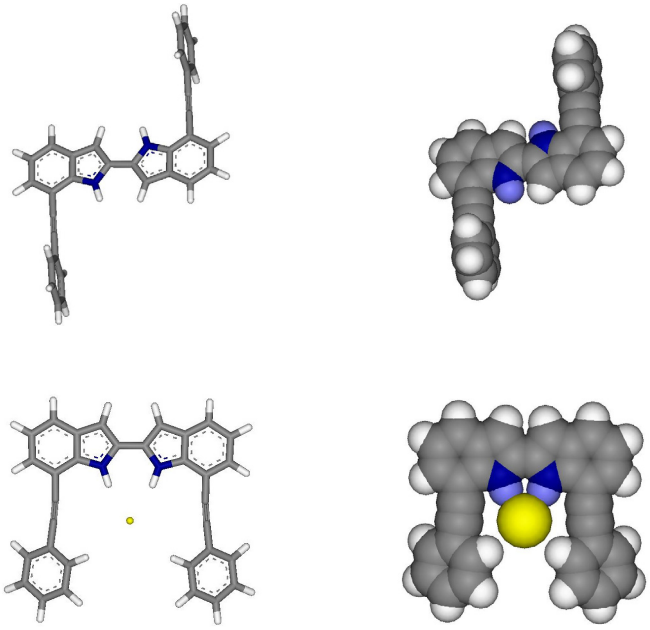


Figure S1. Stick (left) and CPK (right) representations for an energy-minimized structure of dimer **1a** (top) and its complex **1a** + Cl^- (bottom).

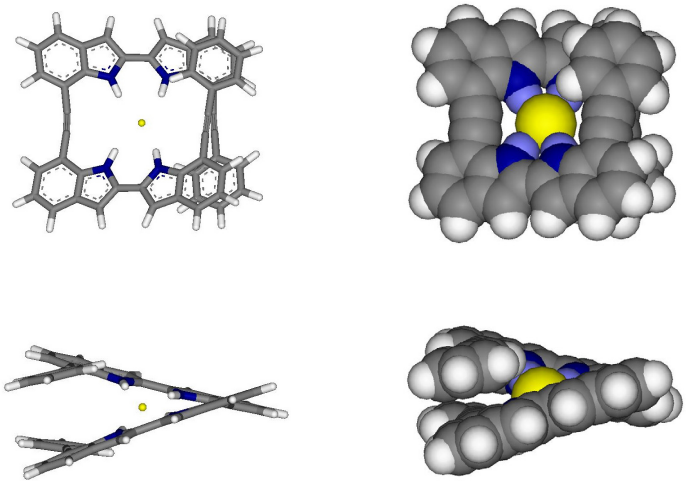


Figure S2. Stick (left) and CPK (right) representations for an energy-minimized structure of complex **1b** + Cl^-.

[1] F. Mohamedi, N. G. T. Richards, W. C. H. Liskamp, M. Lipton, C. Caufield, G. Chang, T. Hendrickson, W. C. Still, *J. Comput. Chem.* **1990**, *11*, 440–467.

[2] a) T. A. Halgren, *J. Comput. Chem.* **1996**, *17*, 490–519; b) T. A. Halgren, *J. Comput. Chem.* **1996**, *17*, 520–552; c) T. A. Halgren, *J. Comput. Chem.* **1996**, *17*, 553–586; d) T. A. Halgren, R. B. Nachbar, *J. Comput. Chem.* **1996**, *17*, 587–615; e) T. A. Halgren, *J. Comput. Chem.* **1996**, *17*, 616–641; f) T. A. Halgren, *J. Comput. Chem.* **1999**, *20*, 720–729; g) T. A. Halgren, *J. Comput. Chem.* **1999**, *20*, 730–748.

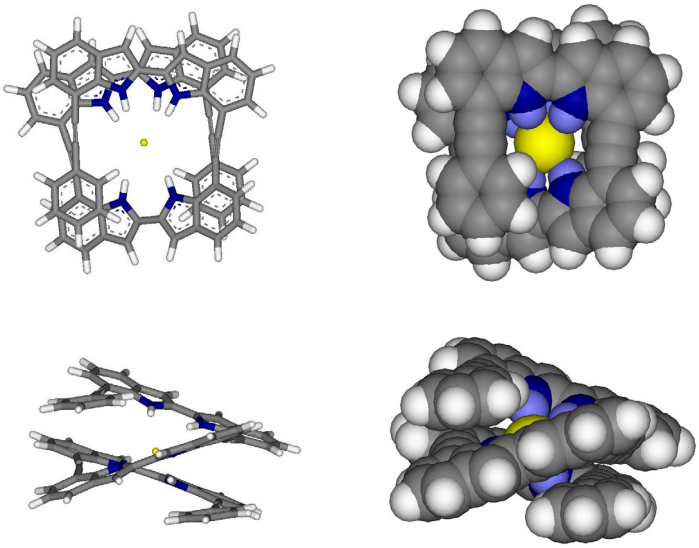


Figure S3. Stick (left) and CPK (right) representations for an energy-minimized structure of complex **1c** + Cl^-.

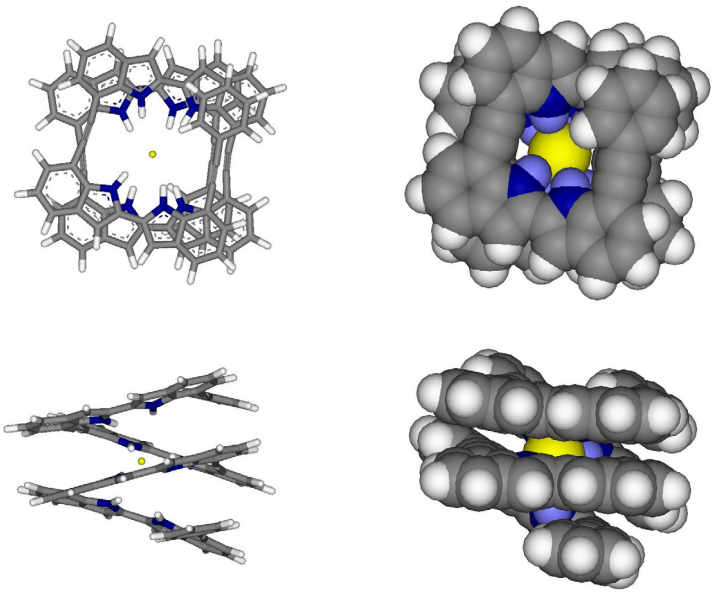


Figure S4. Stick (left) and CPK (right) representations for an energy-minimized structure of complex **1d** + Cl^-.

2. ^{1}H NMR spectra of **1b**, **1c** and **1d** in the presence of tetrabutylammonium chloride (TBA^+Cl^-)

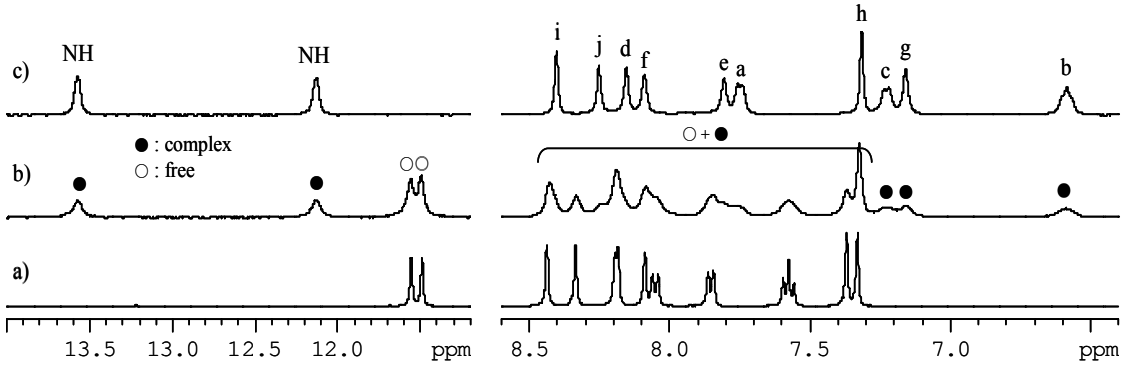


Figure S5. Partial ^{1}H NMR (400 MHz, acetone-d_6, 25°C) spectra of tetramer **1b** (0.5 mM) in the presence of TBA^+Cl^-; a) none, b) ~ 0.4 equiv, and c) 1 equiv.

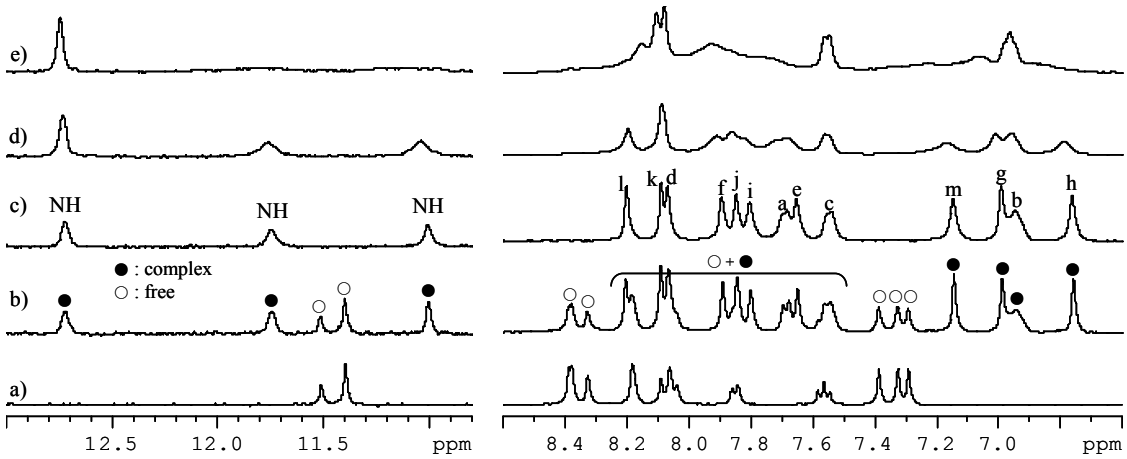


Figure S6. Partial ^{1}H NMR (400 MHz, acetone-d_6, 25°C) spectra of hexamer **1c** (0.3 mM) in the presence of TBA^+Cl^-; a) none, b) ~ 0.6 equiv, c) 1 equiv, d) 2 equiv, and e) 5 equiv.

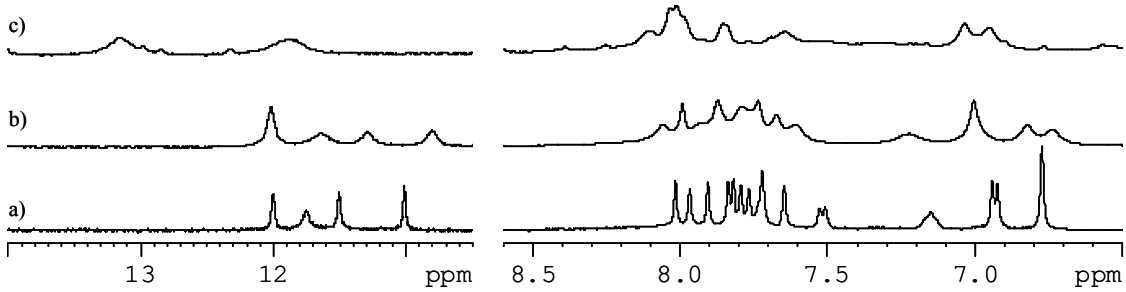


Figure S7. Partial ^{1}H NMR (400 MHz, acetone-d_6, 25°C) spectra of octamer **1d** (0.1 mM) in the presence of TBA^+Cl^-; a) 1 equiv, b) 2 equiv, and c) 5 equiv.

3. 2D ^{1}H-^{1}H TOCSY and ROESY spectra of **1b** and **1c**

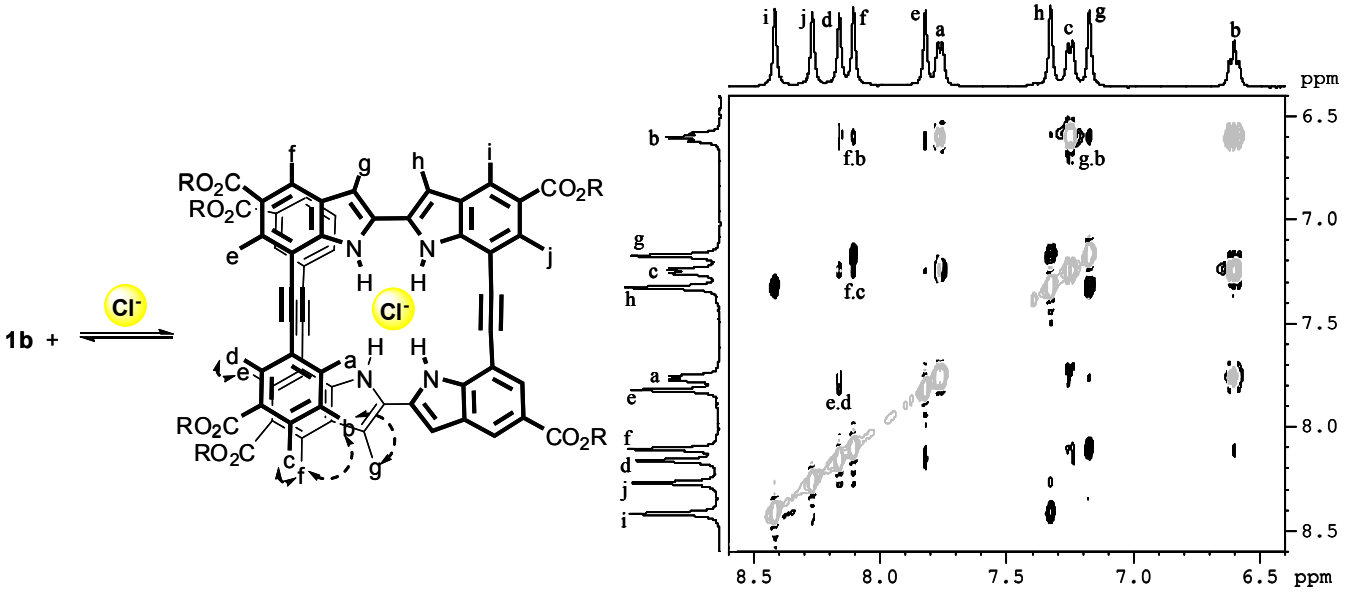


Figure S8. 2D ^{1}H - ^{1}H ROESY spectrum of tetramer **1b** + TBA^{+}Cl^{-} (1 equiv) (400 MHz, 25°C, 4 mM in acetone-d_6).

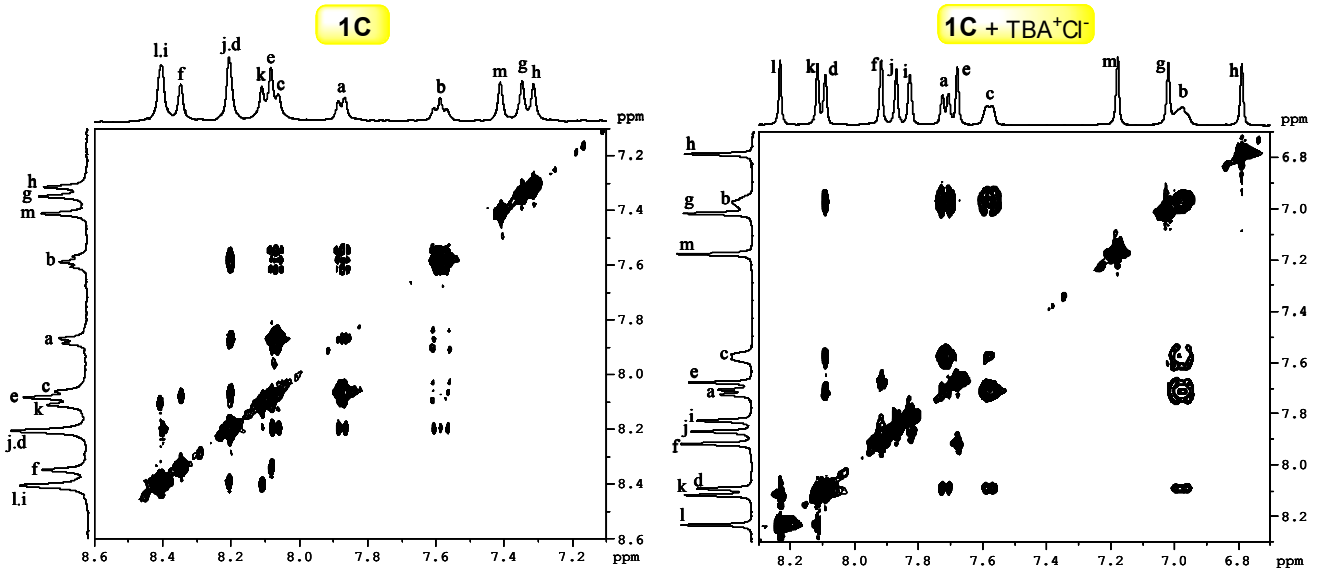


Figure S9. 2D ^{1}H - ^{1}H TOCSY spectra of **1c** (400 MHz, 25°C, ~ 1 mM in acetone-d_6) (left) and **1c** + TBA^{+}Cl^{-} (1 equiv) (400 MHz, 25 °C, 5 mM in acetone-d_6) (right).

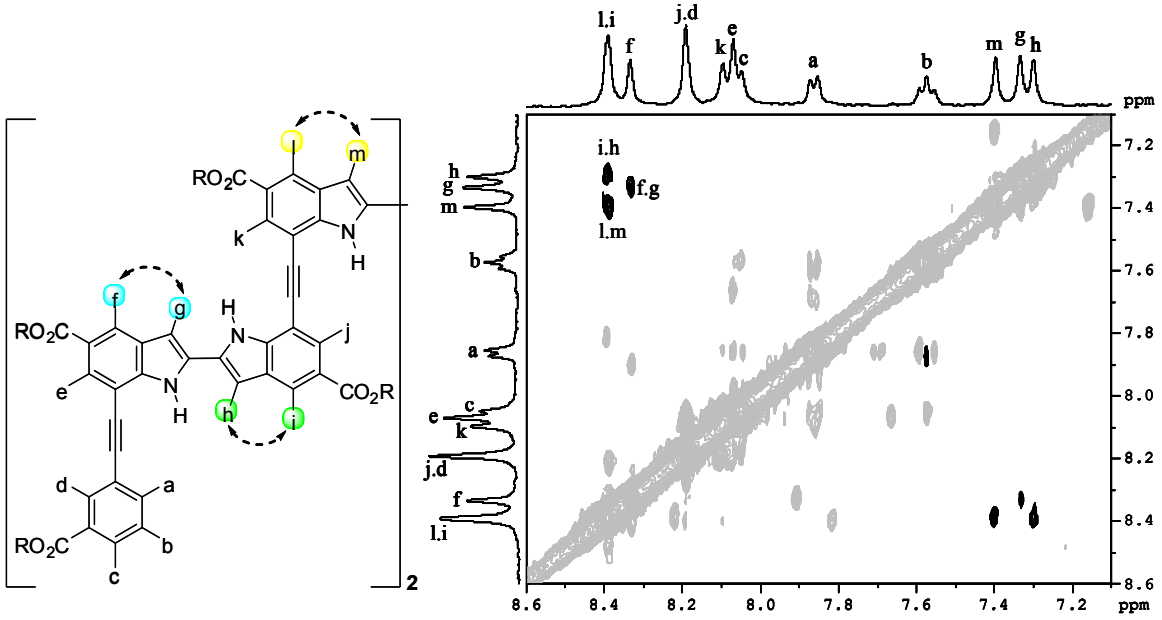


Figure S10. 2D ^{1}H - ^{1}H ROESY spectrum of **1c** (400 MHz, 25°C, ~1 mM in acetone-d_6).

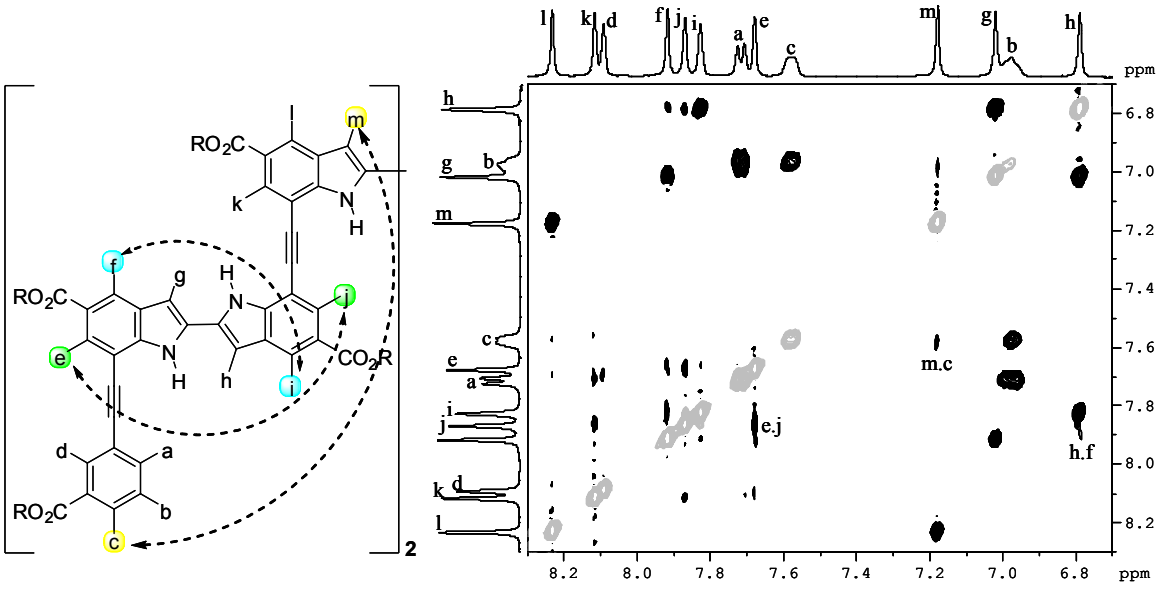
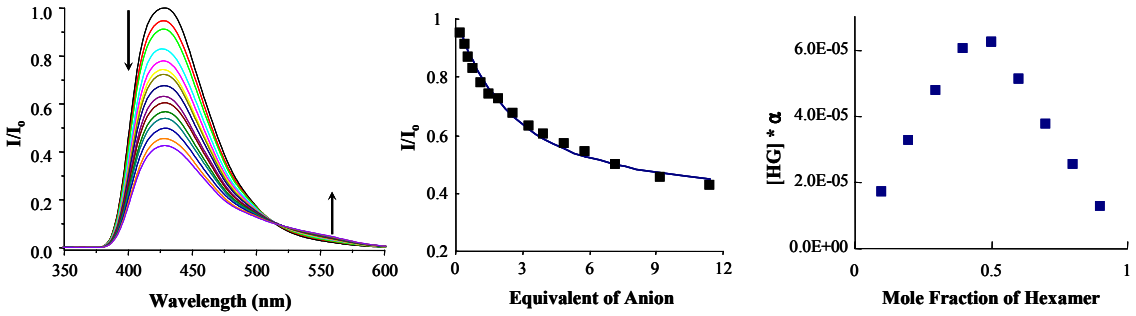


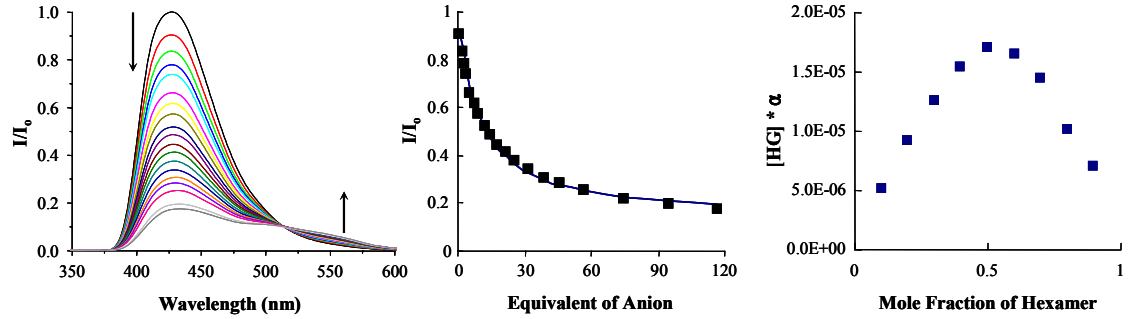
Figure S11. 2D ^{1}H - ^{1}H ROESY spectrum of **1c** + $TBA^{+}Cl^{-}$ (1 equiv) (400 MHz, 25°C, 5 mM in acetone-d_6)

4. Titrations and Job's plots

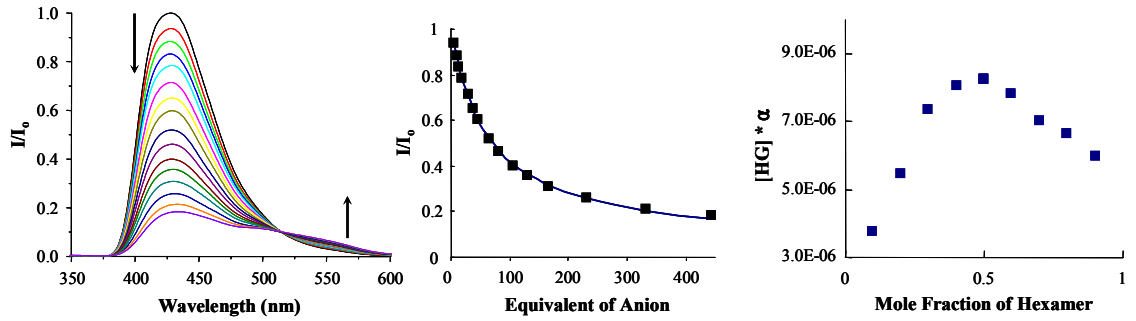
1c + TBA^+F^-



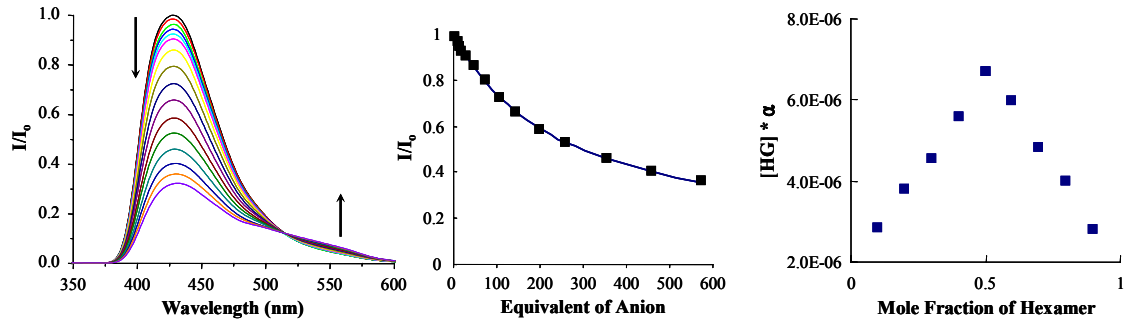
1c + TBA^+Cl^-



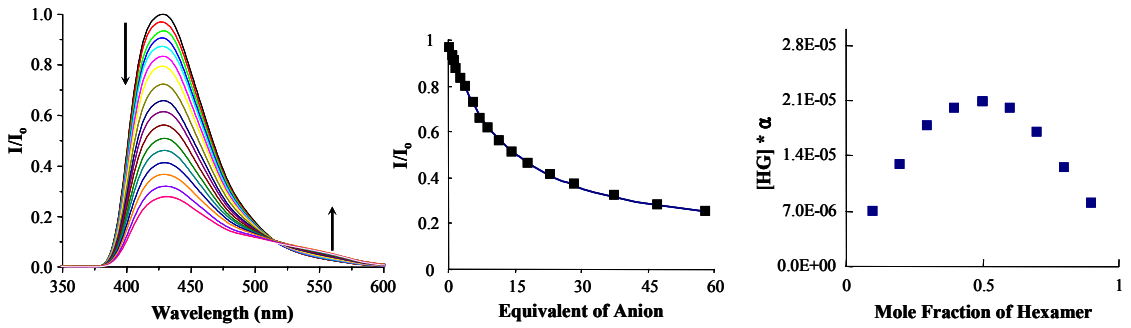
1c + TBA^+Br^-



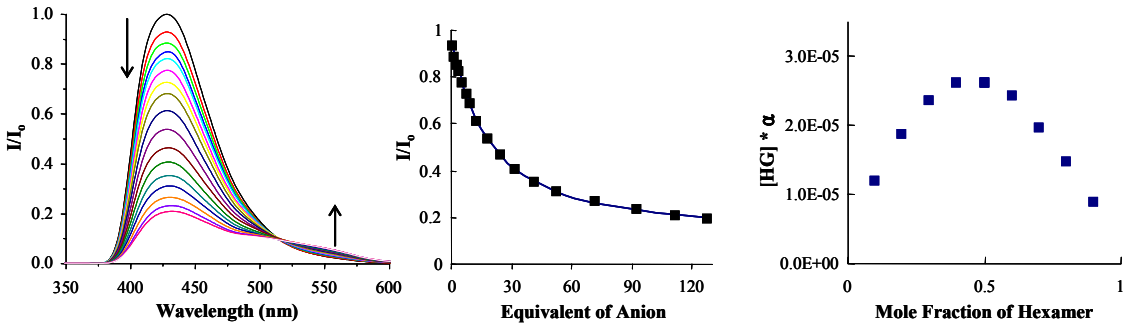
1c + TBA^+I^-



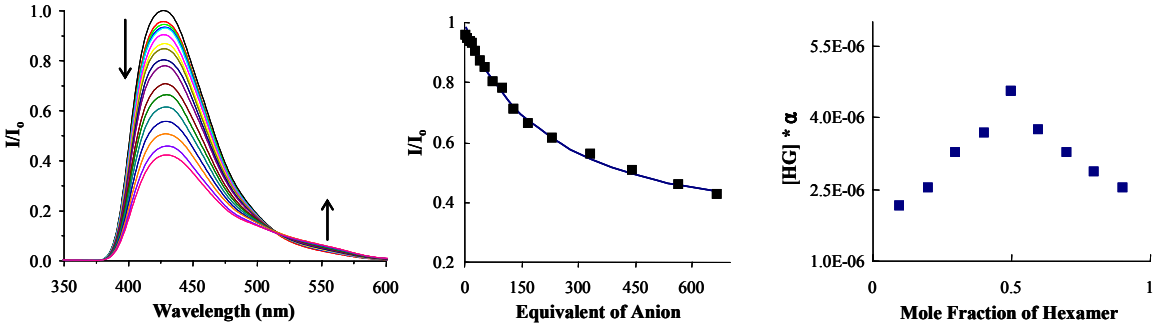
1c + TBA^+CN^-



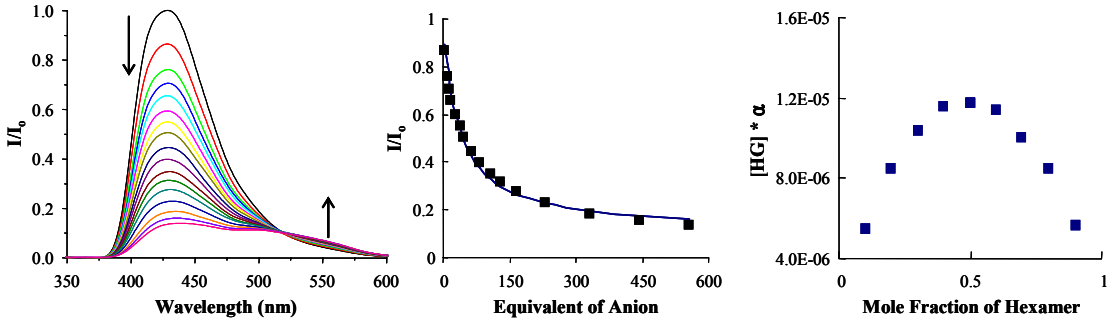
1c + $TBA^+N_3^-$



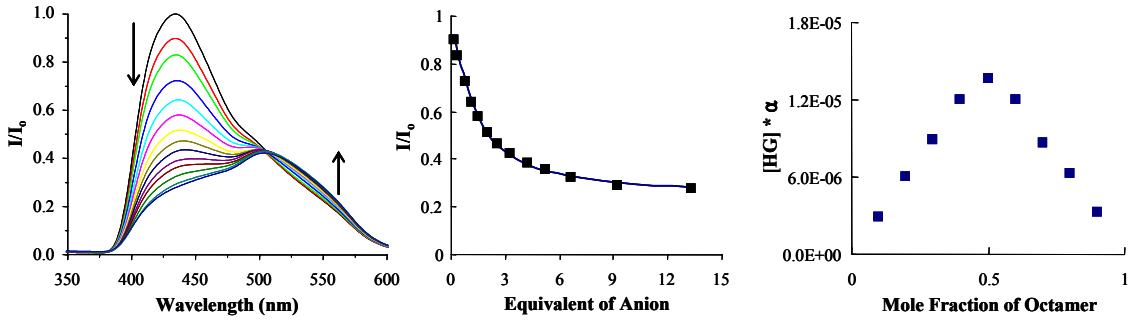
1c + $TBA^+NO_3^-$



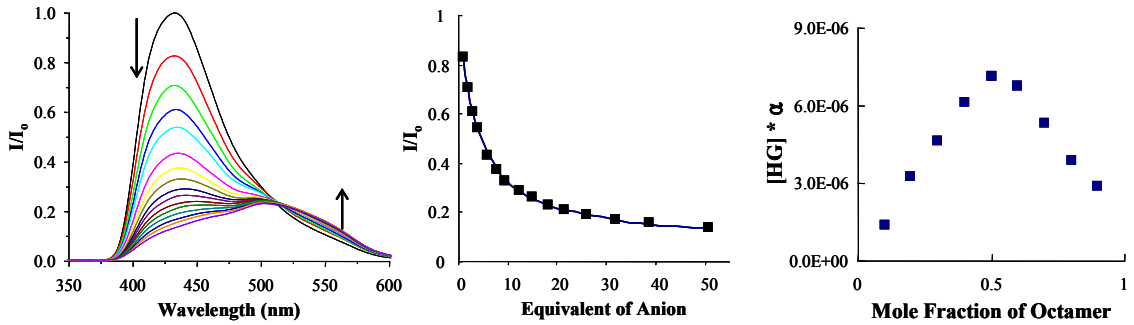
1c + TBA^+AcO^-



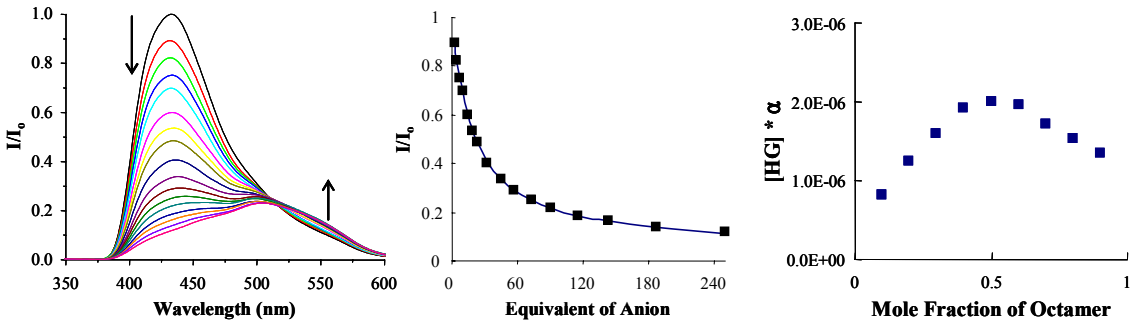
1d + $TBA^{+}F^{-}$



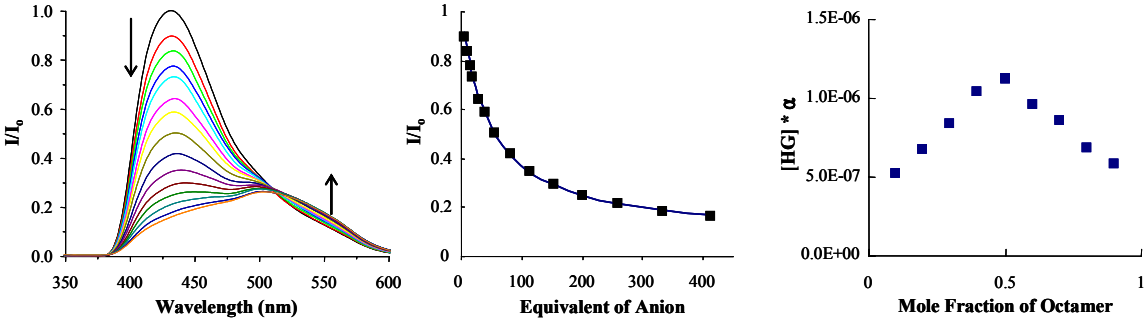
1d + $TBA^{+}Cl^{-}$



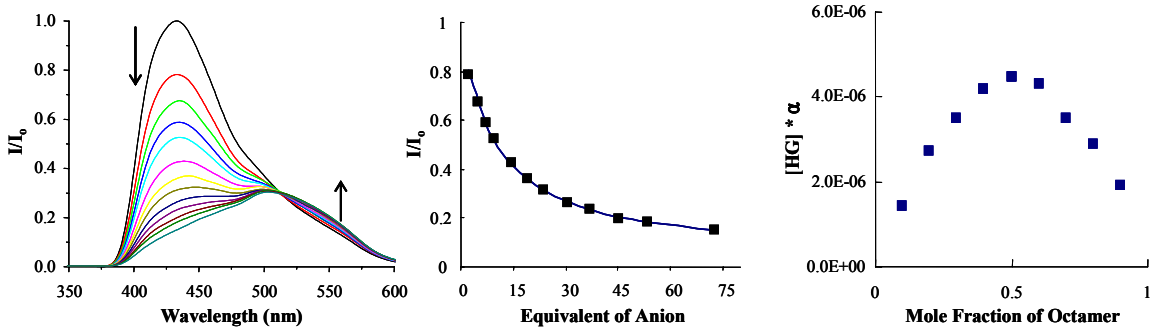
1d + $TBA^{+}Br^{-}$



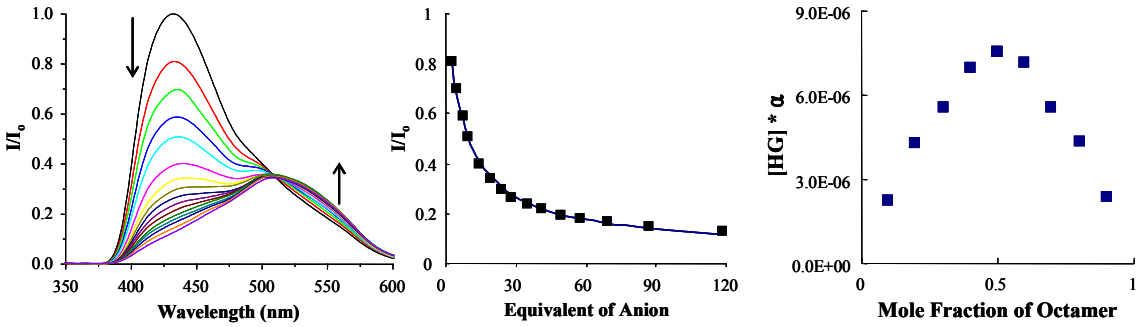
1d + $TBA^{+}I^{-}$



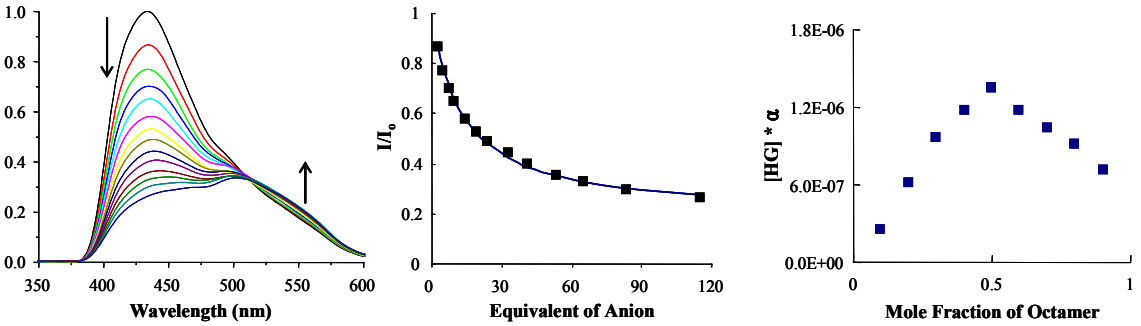
1d + TBA^+CN^-



1d + $TBA^+N_3^-$



1d + $TBA^+NO_3^-$



1d + TBA^+AcO^-