Electronic Supplementary Information

Effects of Nano-Confinement and Conformational Mobility on Molecular Imprinting of Cross-Linked Micelles

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Data Analysis for Fluorescence Titrations

The binding constant was obtained by nonlinear least squares curving fitting of the emission intensity to the 1:1 binding isotherm according to equation 7, in which **S** is the host to be titrated by ligand **L**, X_{obs} is a observable spectroscopic property of **S** and **SL** such as absorbance or fluorescence.[1] In this particular work, because the size (and molecular weight) of MINP changed with the 1st-stage cross-linker level (Table 1), the true number of binding sites per nanoparticle differed for different MINPs. For comparison purposes, a nominal molecular weight of 50,000 was used for all the MINPs, based on ~50 units of cross-linked monomer, with each unit (MW 959.7) defined as 1 × **1** (MW 464.5), 1.2 × **2** (MW 172.1), 0.6 × **3** (MW 264.1), and 1 × DVB (MW 130.2). Since a 50:1 ratio of surfactant/template was used in all the MINP preparations, the 1:1 binding model for the curve fitting was for the binding between the guest and a nominal MINP consisting of 50 units of the cross-linked monomer.

$$\mathbf{S} + \mathbf{L} \leftrightarrows \mathbf{SL} \quad \text{(eq 1)}$$

$$K_a = 1/K_D = [\mathbf{SL}]/([\mathbf{S}][\mathbf{L}]) \quad \text{(eq 2)}$$

$$\text{Total concentration } [\mathbf{S}]_t = [\mathbf{S}] + [\mathbf{SL}] \quad \text{(eq 3)}$$

$$\text{Total concentration } [\mathbf{L}]_t = [\mathbf{S}] + [\mathbf{SL}] \quad \text{(eq 4)}$$

$$\text{Observed spectroscopic signal } X_{obs} = x_s[\mathbf{S}] + x_{sL}[\mathbf{SL}] \quad \text{(eq 5)}$$

$$\Delta x = x_{sL} - x_s - x_L \quad \text{(eq 5)}$$

$$X_{obs} = x_s[\mathbf{S}]_t + x_L[\mathbf{L}]_t + 0.5\Delta x([\mathbf{S}]_t + [\mathbf{L}]_t + K_D - \{([\mathbf{S}]_t + [\mathbf{L}]_t + K_D)^2 - 4[\mathbf{S}]_t[\mathbf{L}]_t\}^{1/2}) \quad \text{(eq 6)}$$

When the ligand used to titrate **S** des not contribute to X_{obs} (i.e., nonfluorescent in our case), x_L is zero and equation 6 becomes

$$X_{obs} = x_s[\mathbf{S}]_t + 0.5\Delta x([\mathbf{S}]_t + [\mathbf{L}]_t + K_D - \{([\mathbf{S}]_t + [\mathbf{L}]_t + K_D)^2 - 4[\mathbf{S}]_t[\mathbf{L}]_t\}^{1/2}) \quad \text{(eq 7)}$$

[1] Schneider, H. J.; Yatsimirsky, A. K. *Principles and methods in supramolecular chemistry*; New York: J. Wiley, 2000; pp 137-146.

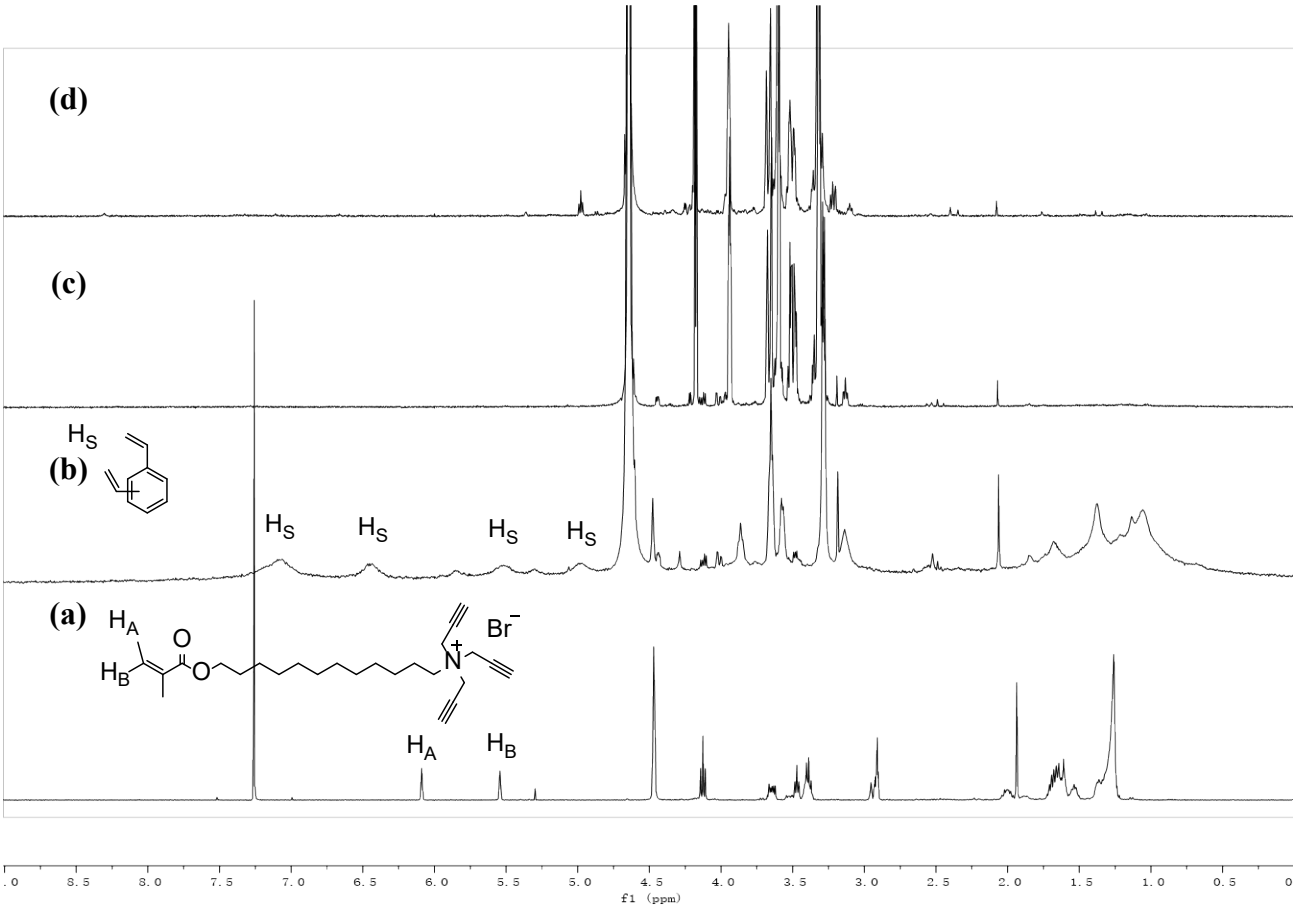

Figure S1. ^{1}H NMR spectra of (a) surfactant **1** in $CDCl_3$, (b) alkynyl-SCM in D_2O, (c) surface-functionalized SCM in D_2O. (d) core cross-linked SCM in D_2O.

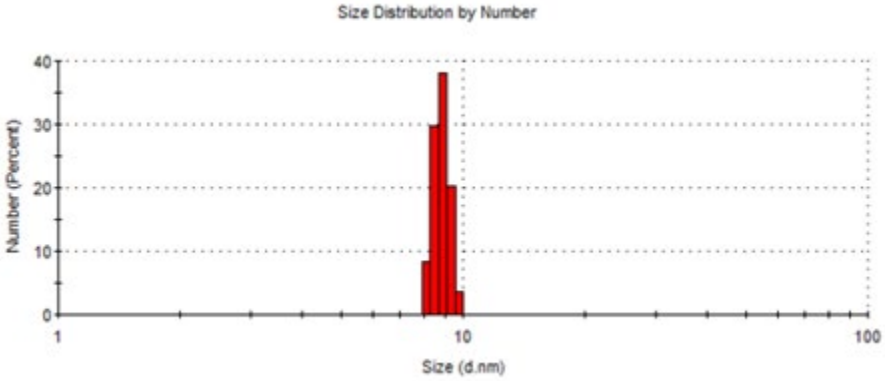

Figure S2. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for MINP with 0 equiv. of **2** in the 1st-stage cross-linking in water. D = 8.84 ± 0.40 nm.

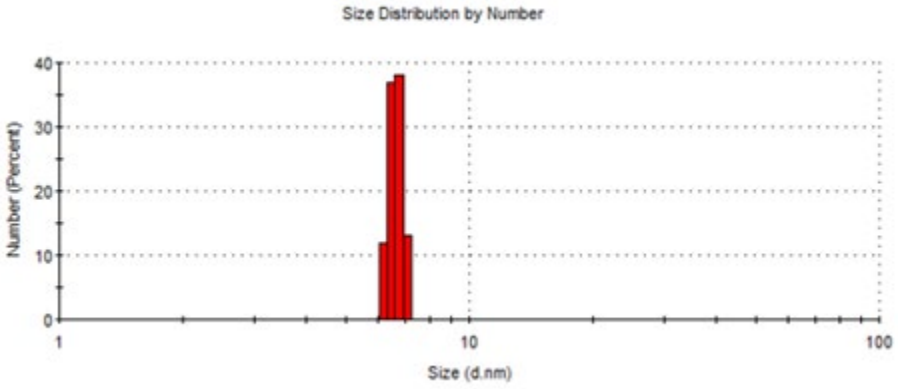

Figure S3. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for MINP with 0.4 equiv. of **2** in 1st-stage cross-linking in water (1CLL). D = 6.61 ± 0.26 nm.

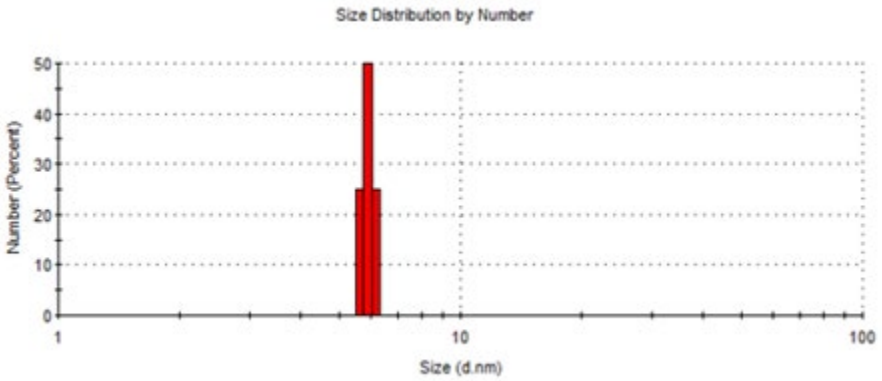

Figure S4. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for MINP with 0.6 equiv. of **2** in 1st-stage cross-linking in water (1CLL). D = 5.89 ± 0.19 nm.

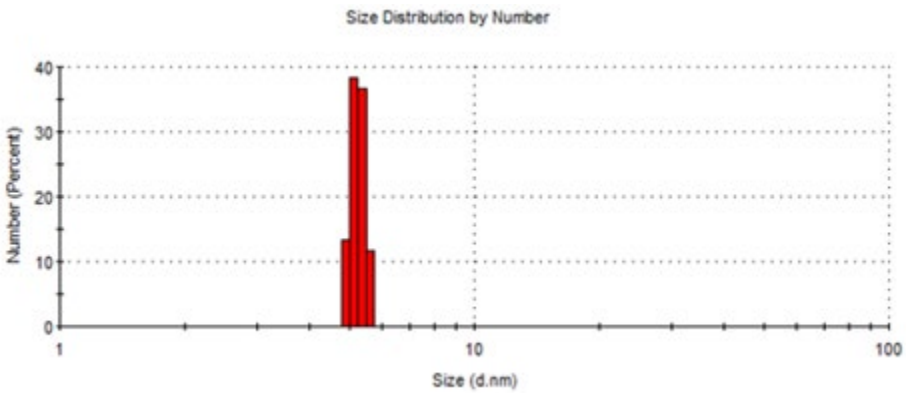

Figure S5. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for MINP with 0.8 equiv. of **2** in 1st-stage cross-linking in water (1CLL). D = 5.23 ± 0.21 nm.

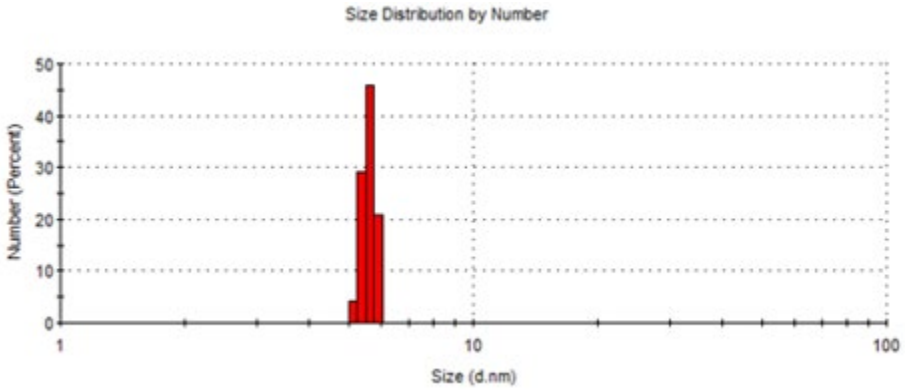

Figure S6. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for MINP with 1.2 equiv. of **2** in 1st-stage cross-linking in water (1CLL). D = 5.57 ± 0.21 nm.

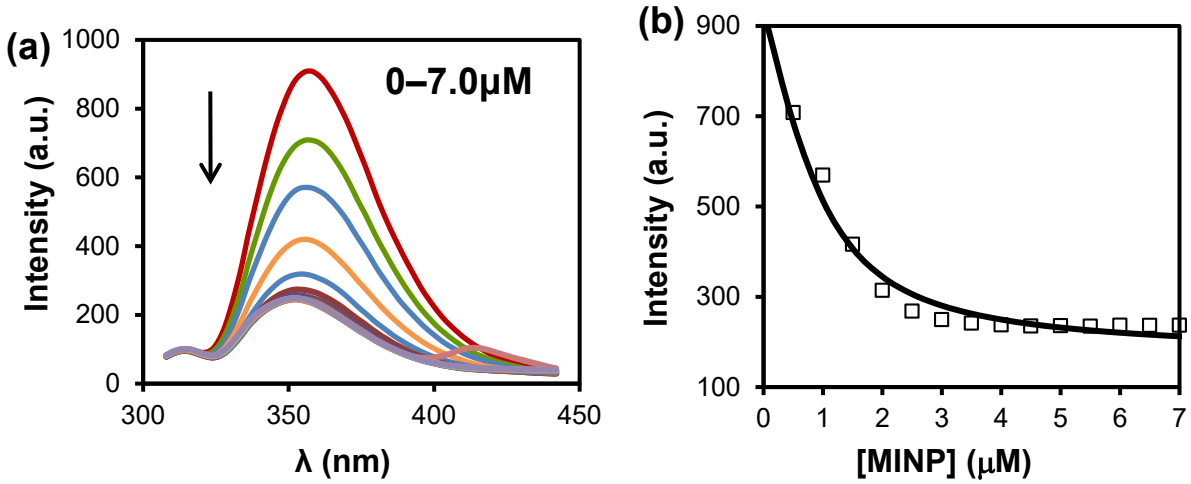

Figure S7. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **4** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **4** at 360 nm to a 1:1 binding isotherm.

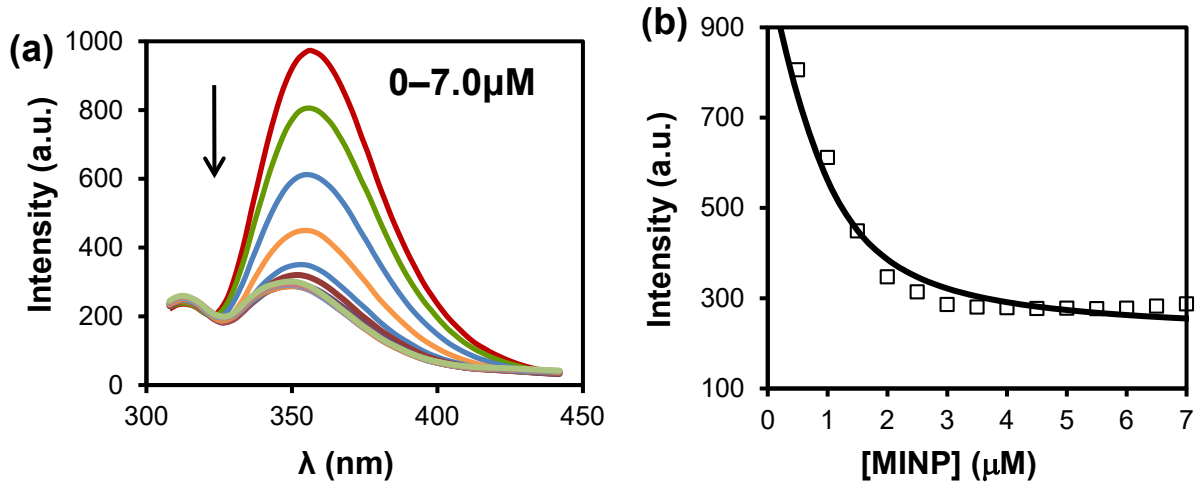

Figure S8. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **4** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.4 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **4** at 360 nm to a 1:1 binding isotherm.

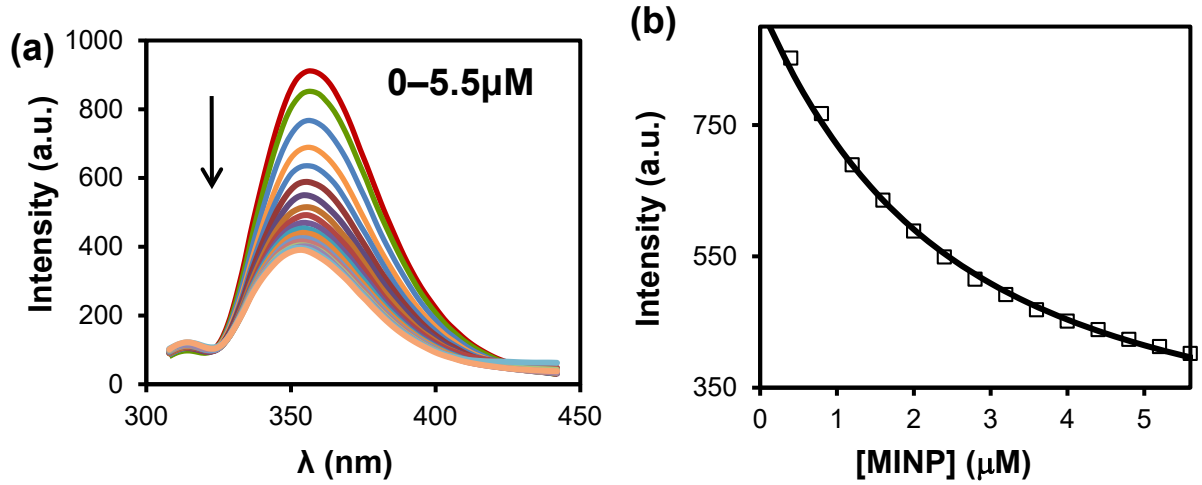

Figure S9. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **4** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **4** at 360 nm to a 1:1 binding isotherm.

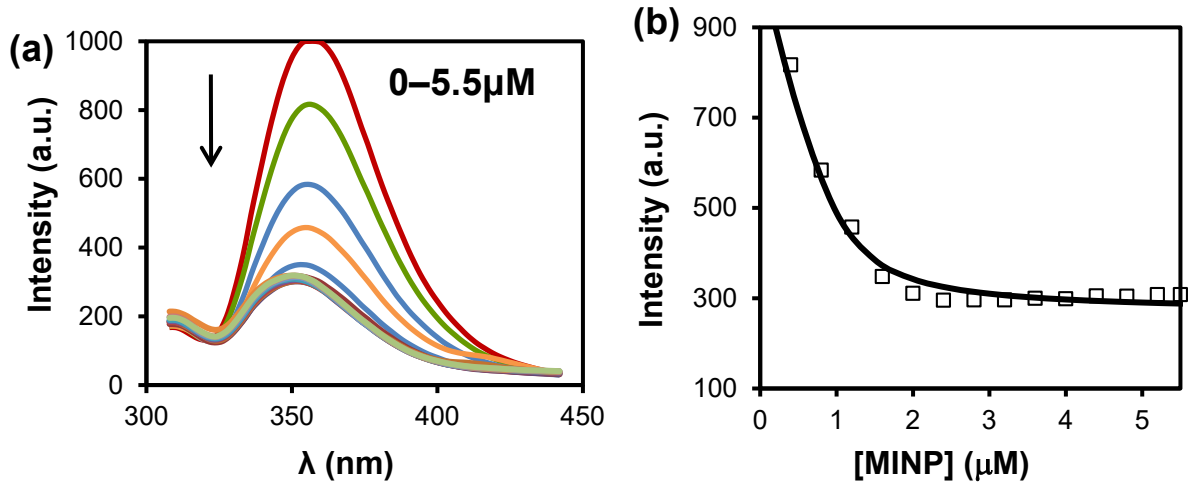

Figure S10. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **4** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **4** at 360 nm to a 1:1 binding isotherm.

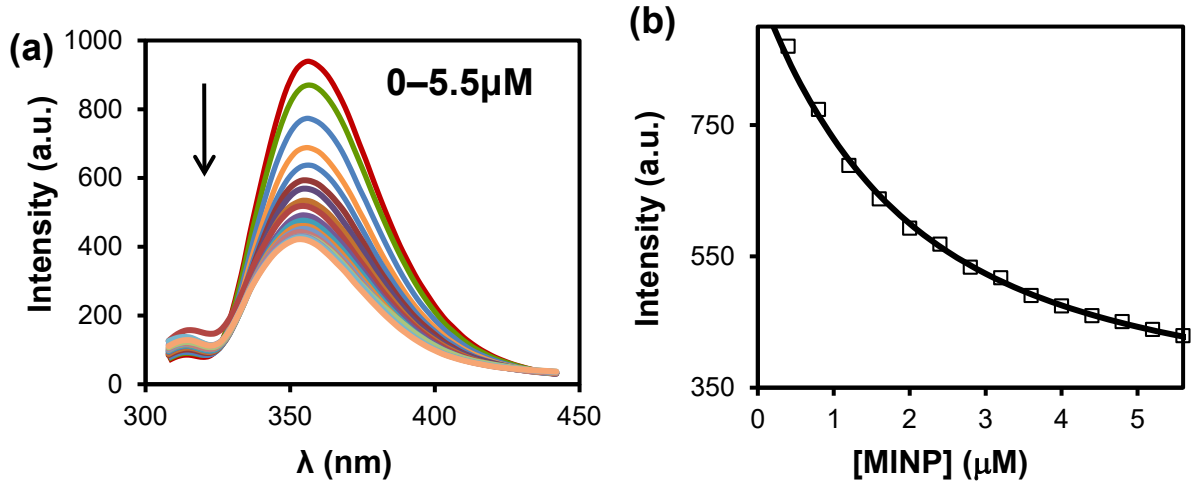

Figure S11. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **4** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **4** at 360 nm to a 1:1 binding isotherm.

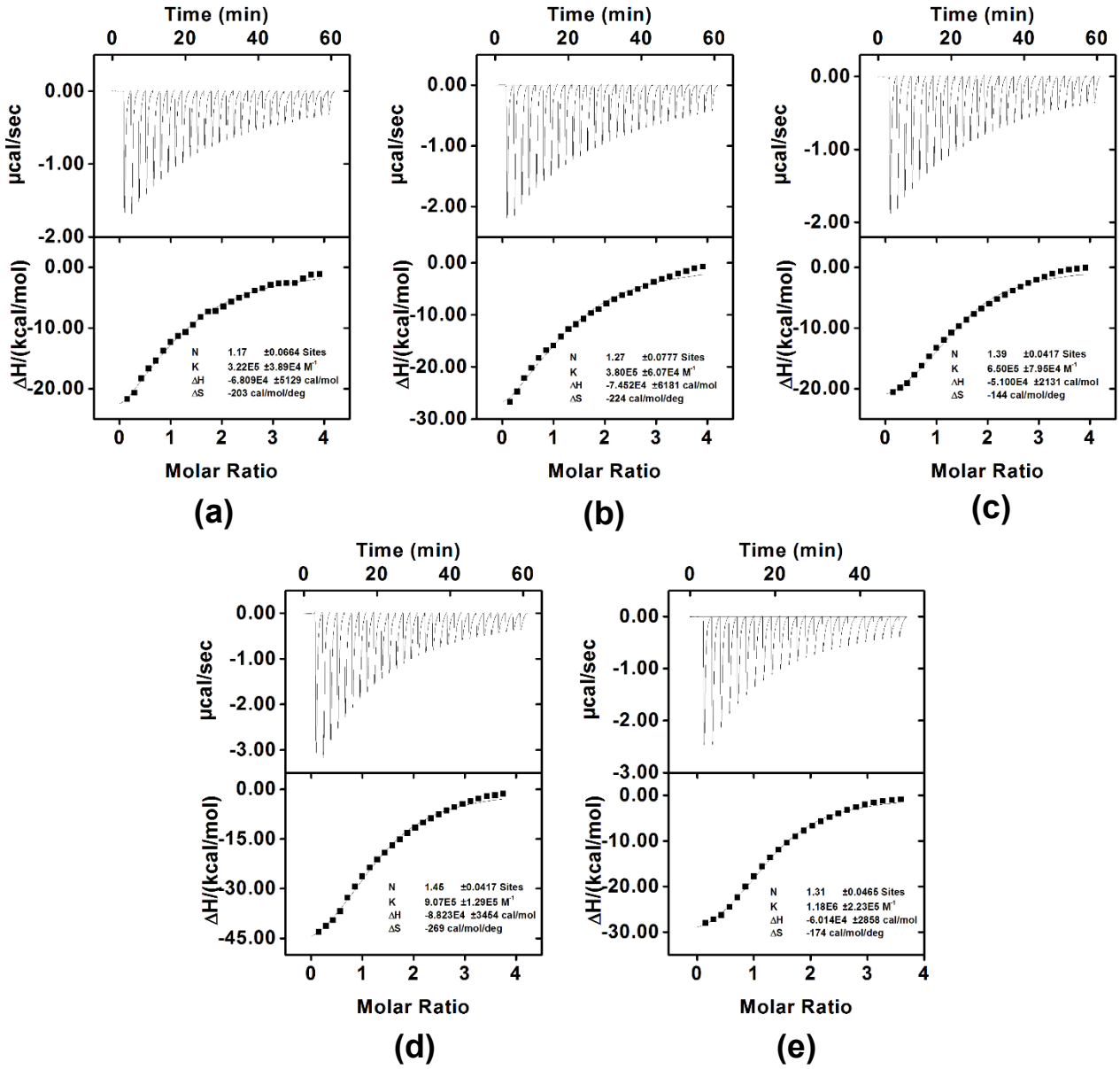

Figure S12. ITC titration curves obtained at 298 K for the titration of guest **4** with (a) MINP prepared with 0 equiv. of **2** in the 1st-stage cross-linking, (b) MINP prepared with 0.4 equiv. of **2** in the 1st-stage cross-linking, (c) MINP prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking, (d) MINP prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking, and (e) MINP prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking in 10 mM HEPES (pH 7.0). The top panel shows the raw calorimetric data. The area under each peak represents the amount of heat generated at each ejection and is plotted against the molar ratio of MINP to the substrate. The solid line is the best fit of the experimental data to the sequential binding of *N* equal and independent binding sites on the MINP. The heat of dilution for the substrate, obtained by adding the substrate to the buffer, was subtracted from the heat released

during the binding. Binding parameters were auto-generated after curve fitting using Microcal Origin 7.

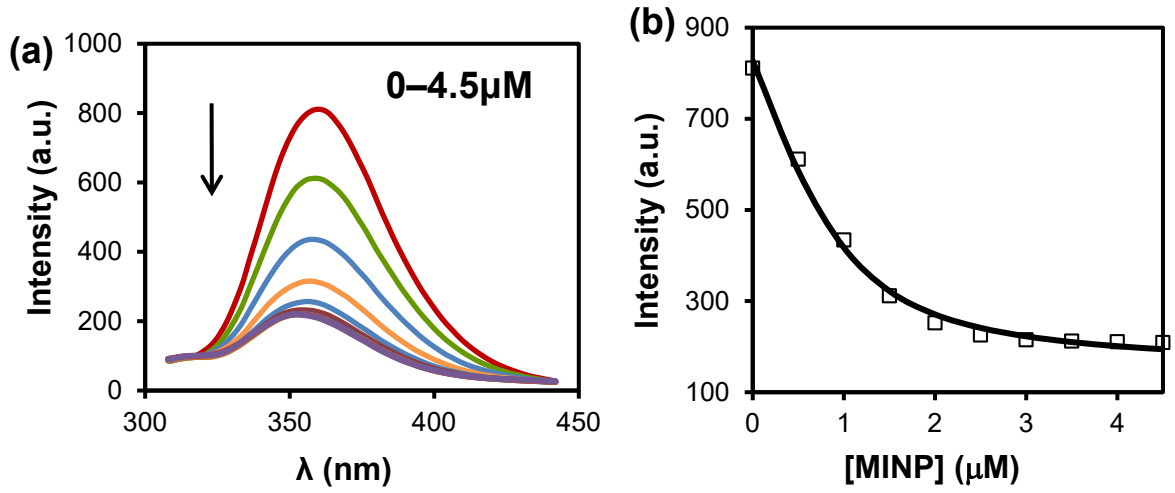

Figure S13. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **5** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **5** at 360 nm to a 1:1 binding isotherm.

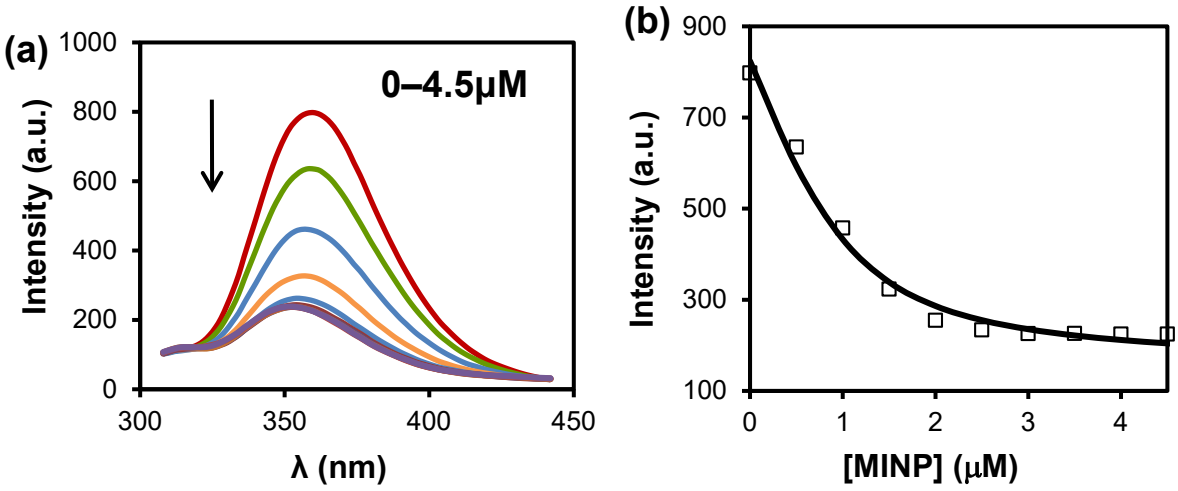

Figure S14. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **5** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.4

equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **5** at 360 nm to a 1:1 binding isotherm.

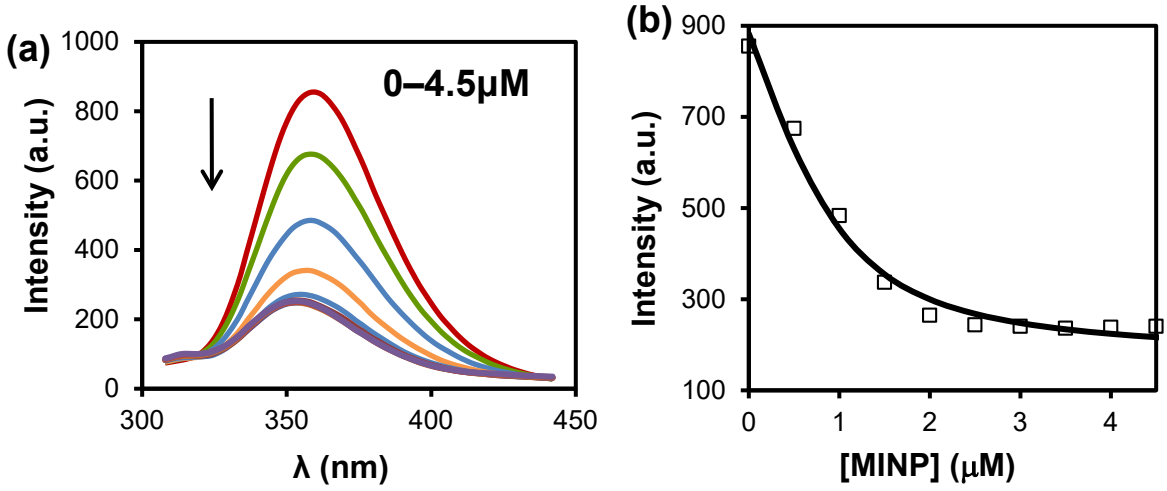

Figure S15. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **5** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **5** at 360 nm to a 1:1 binding isotherm.

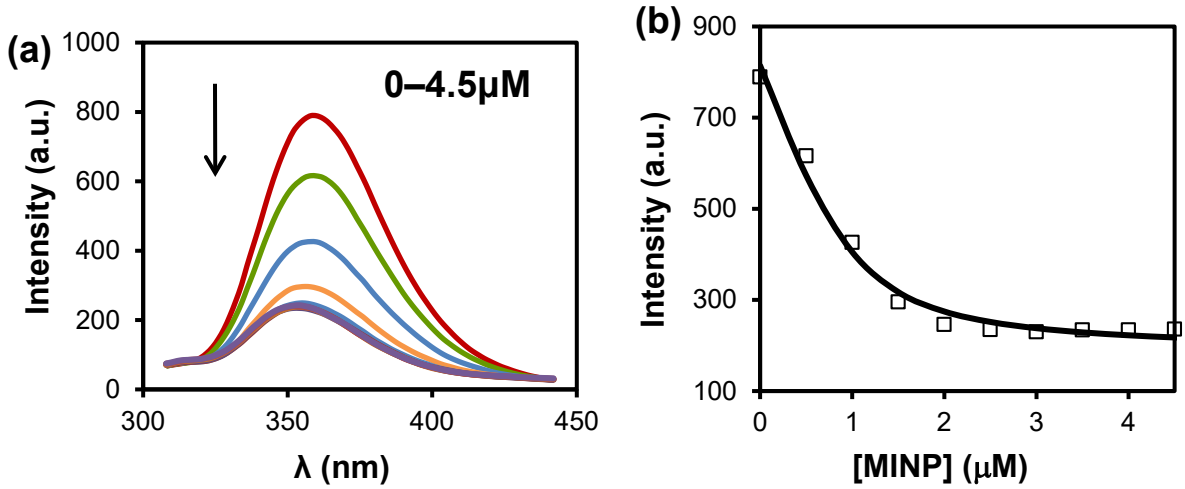

Figure S16. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **5** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **5** at 360 nm to a 1:1 binding isotherm.

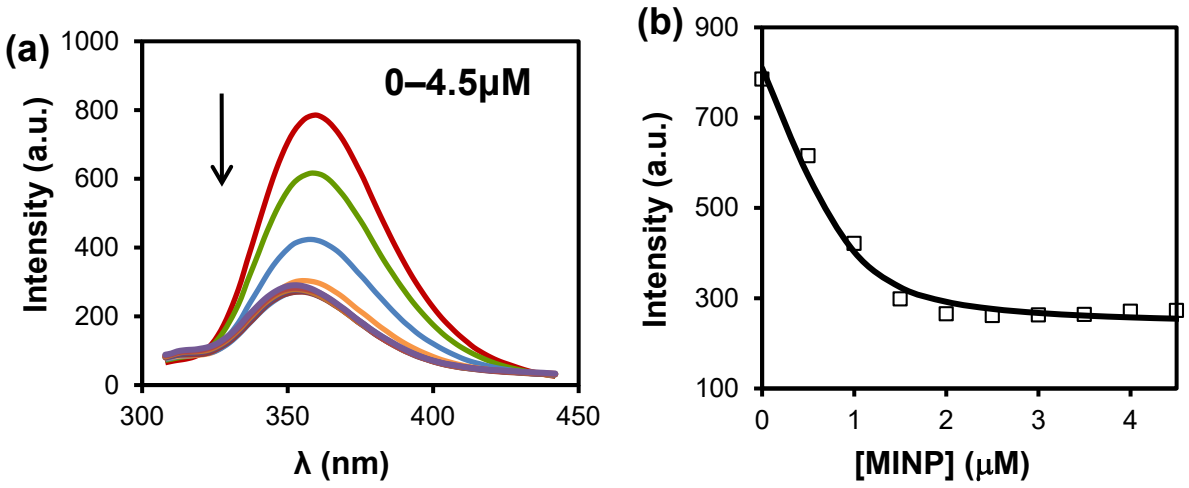

Figure S17. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **5** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **5** at 360 nm to a 1:1 binding isotherm.

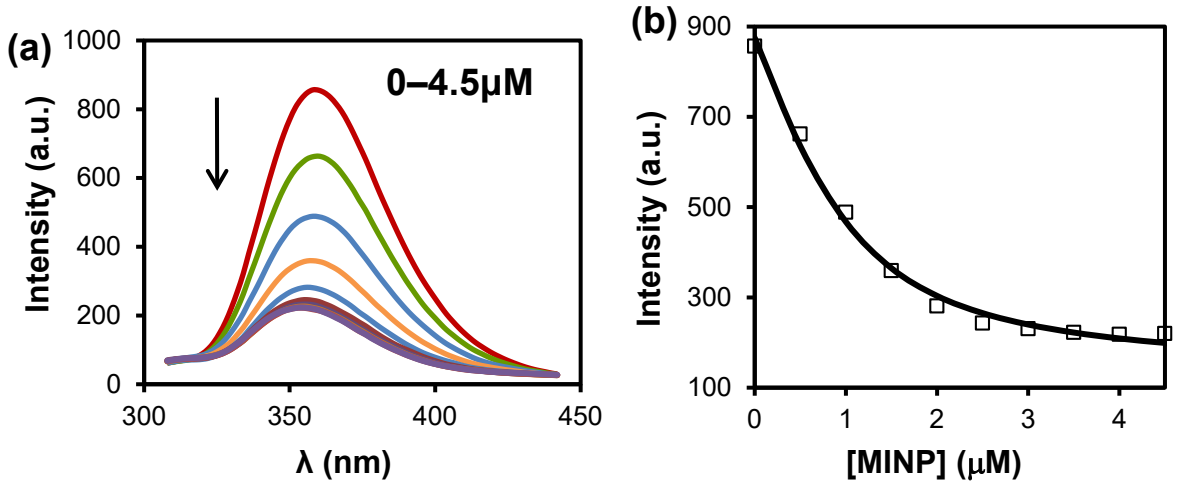

Figure S18. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **6** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **6** at 360 nm to a 1:1 binding isotherm.

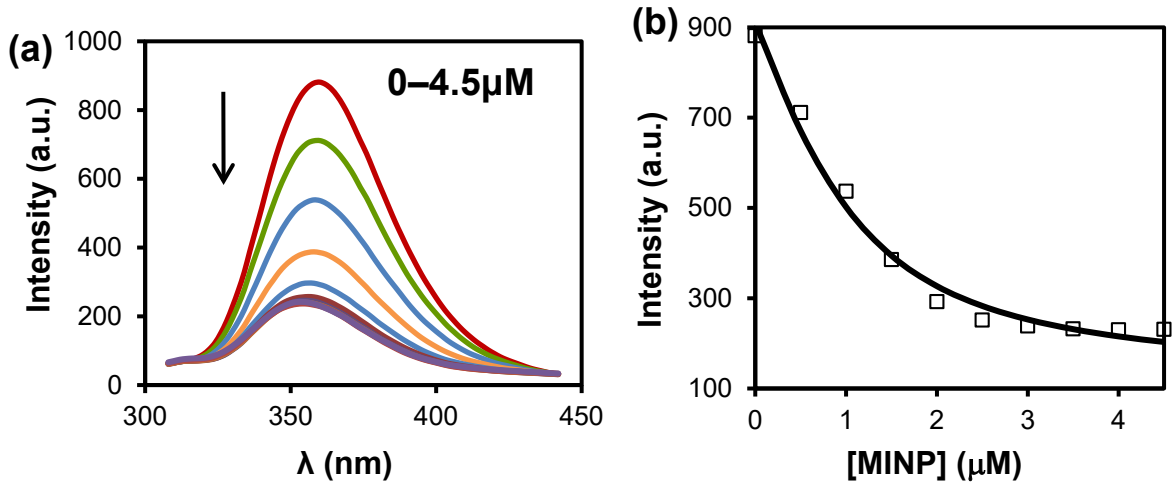

Figure S19. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **6** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.4 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **6** at 360 nm to a 1:1 binding isotherm.

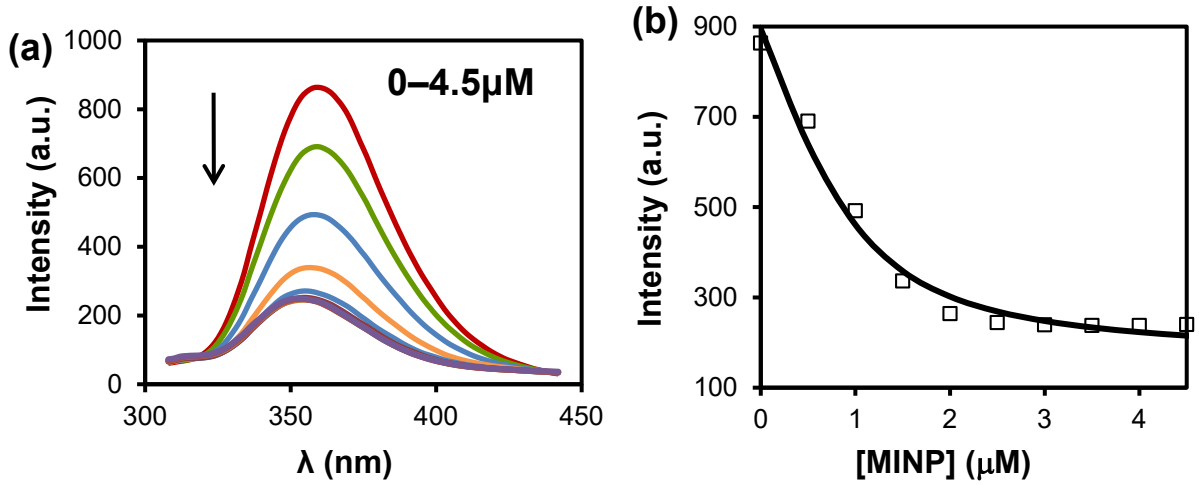

Figure S20. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **6** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **6** at 360 nm to a 1:1 binding isotherm.

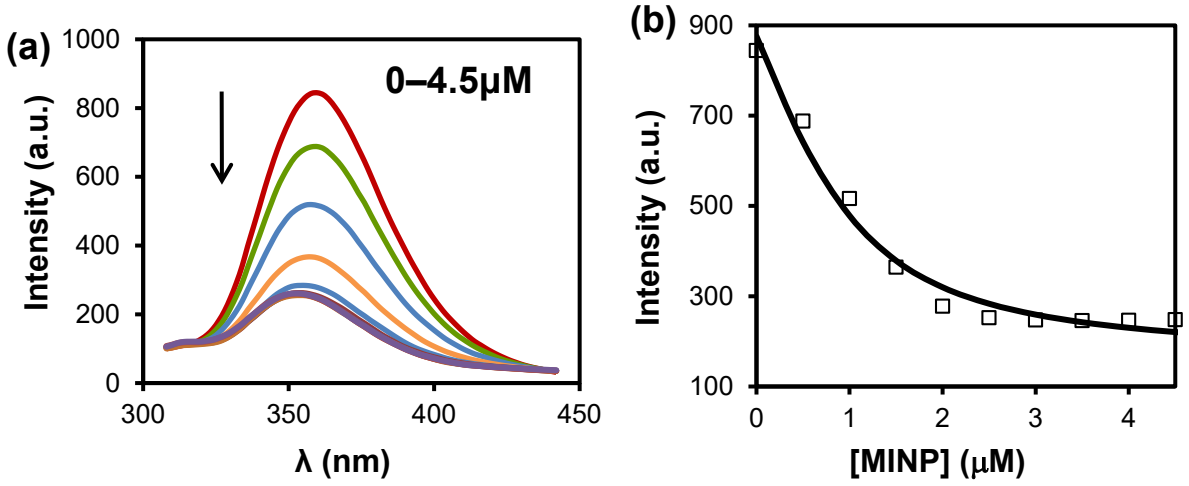

Figure S21. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **6** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **6** at 360 nm to a 1:1 binding isotherm.

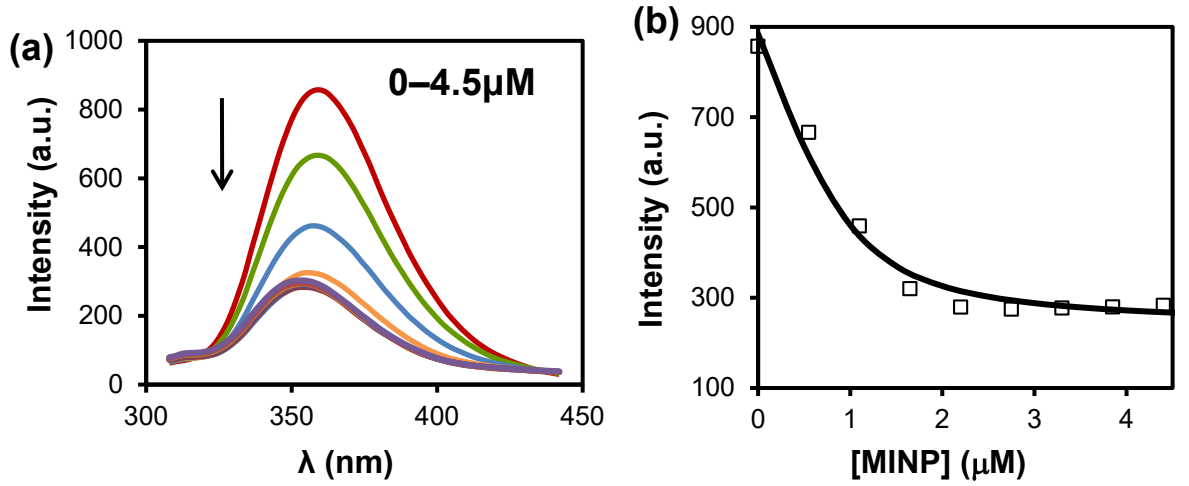

Figure S22. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **6** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **6** at 360 nm to a 1:1 binding isotherm.

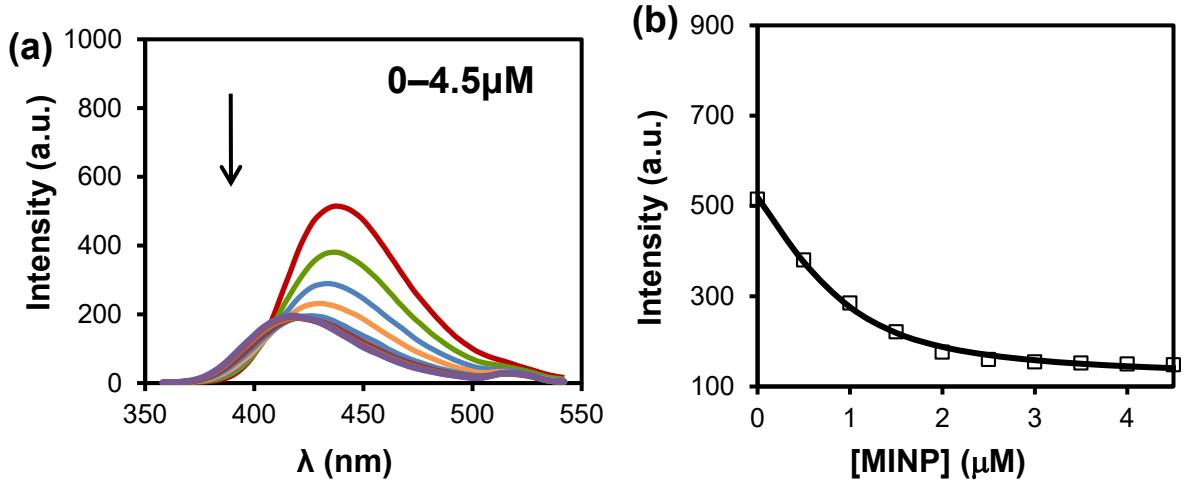

Figure S23. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **7** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **7** at 440 nm to a 1:1 binding isotherm.

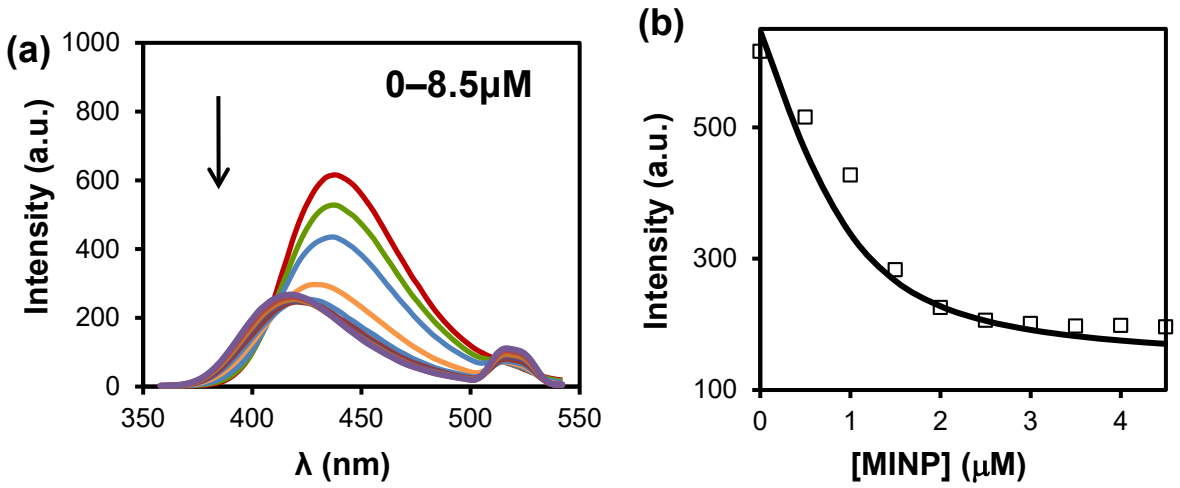

Figure S24. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **7** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.4 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **7** at 440 nm to a 1:1 binding isotherm.

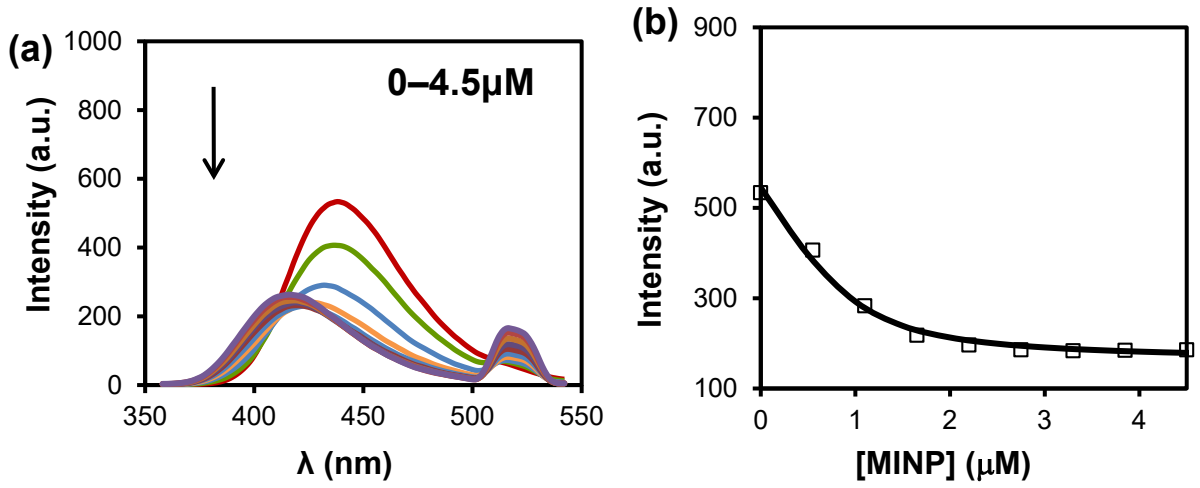

Figure S25. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **7** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **7** at 440 nm to a 1:1 binding isotherm.

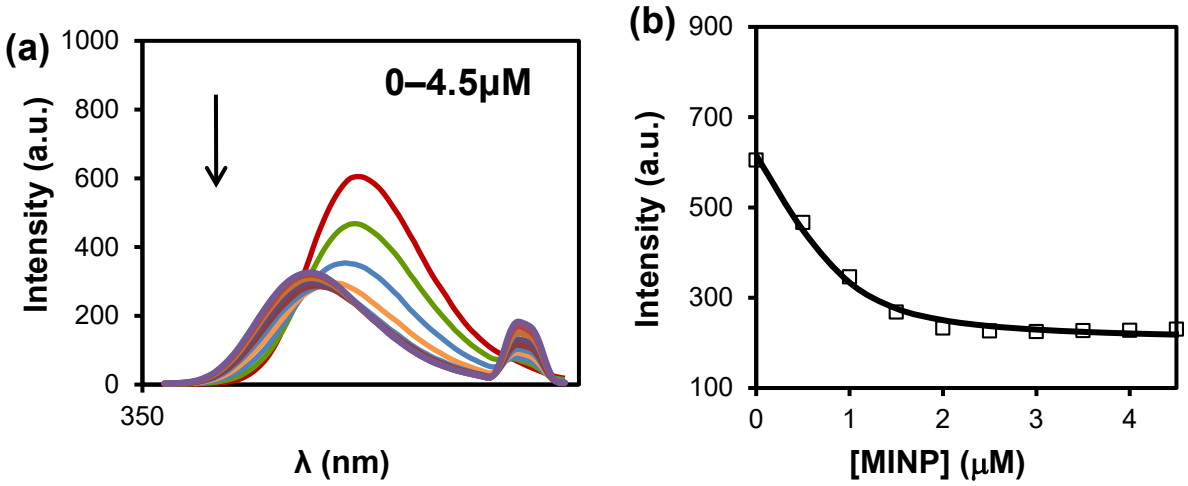

Figure S26. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **7** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **7** at 440 nm to a 1:1 binding isotherm.

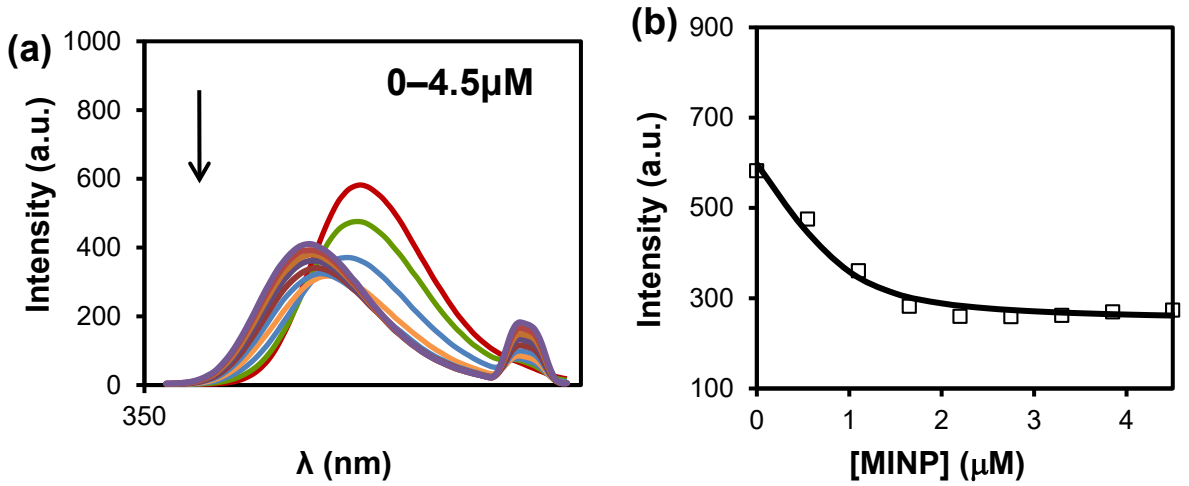

Figure S27. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **7** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **7** at 440 nm to a 1:1 binding isotherm.

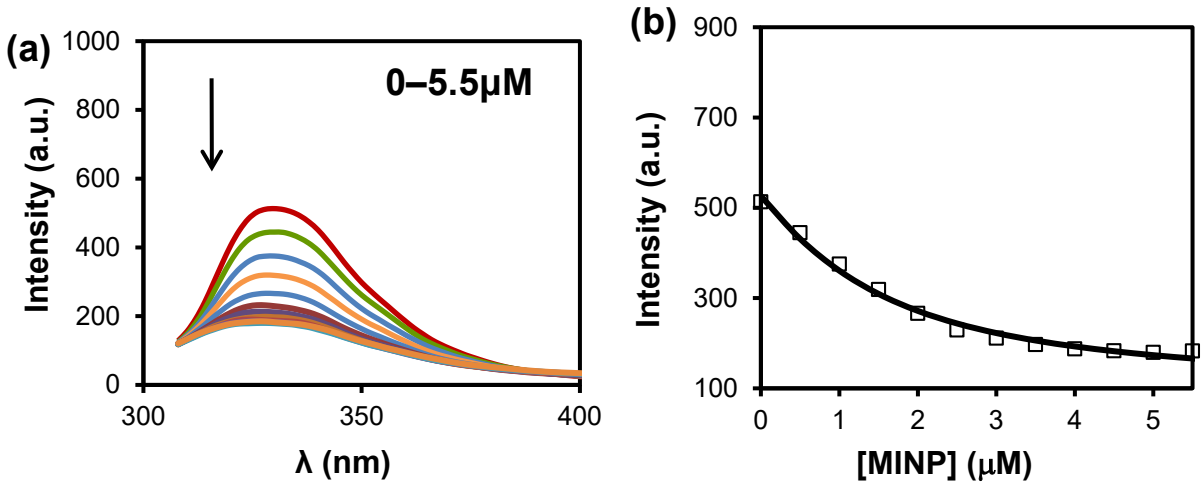

Figure S28. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **8** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **8** at 330 nm to a 1:1 binding isotherm.

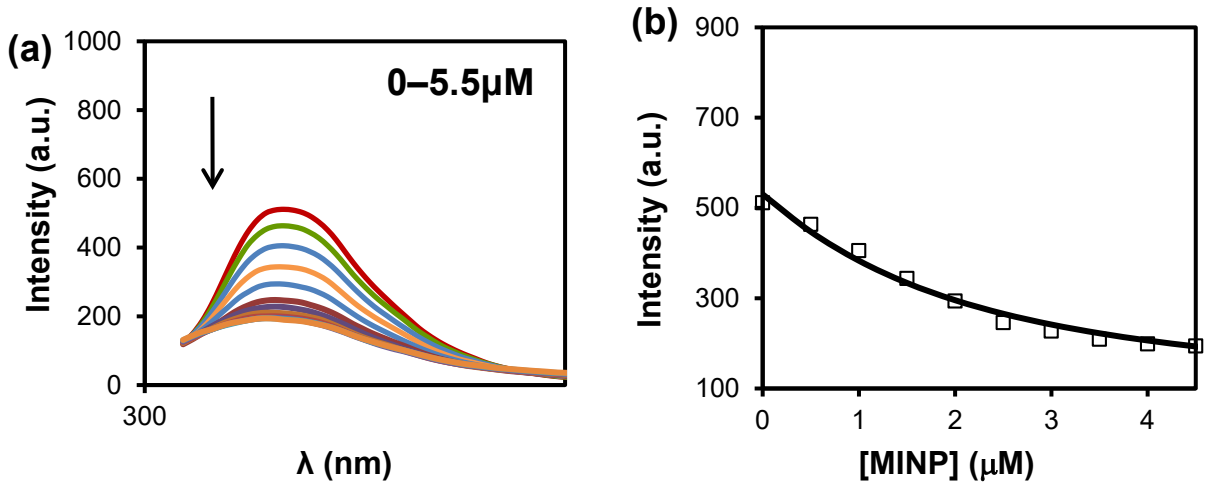

Figure S29. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **8** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.4 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **8** at 330 nm to a 1:1 binding isotherm.

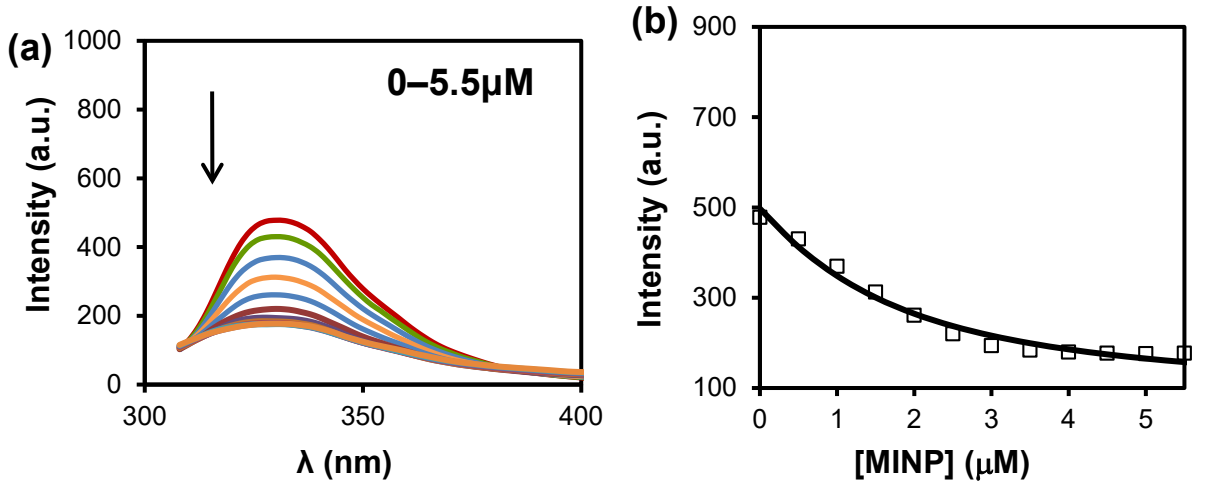

Figure S30. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **8** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **8** at 330 nm to a 1:1 binding isotherm.

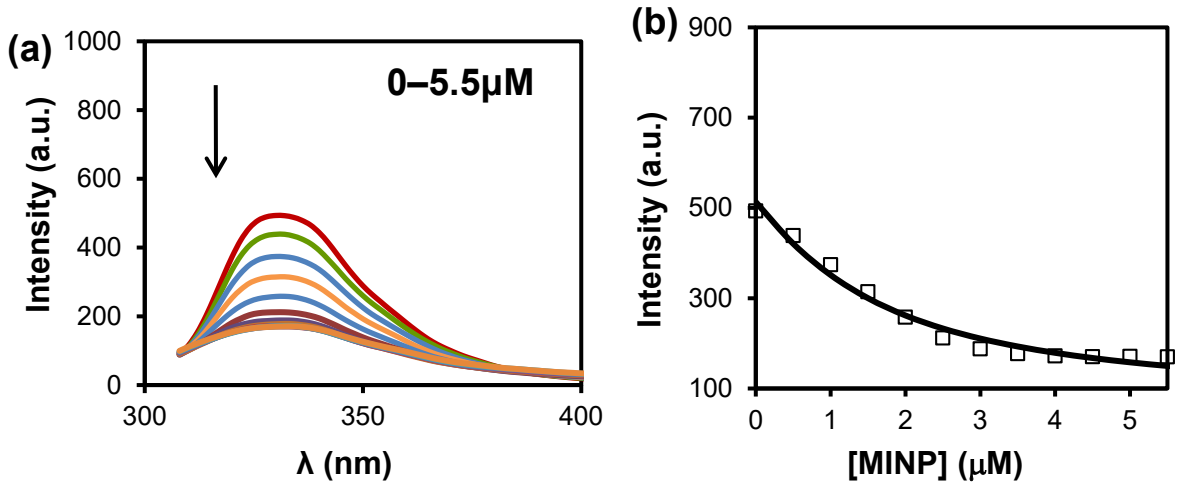

Figure S31. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **8** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **8** at 330 nm to a 1:1 binding isotherm.

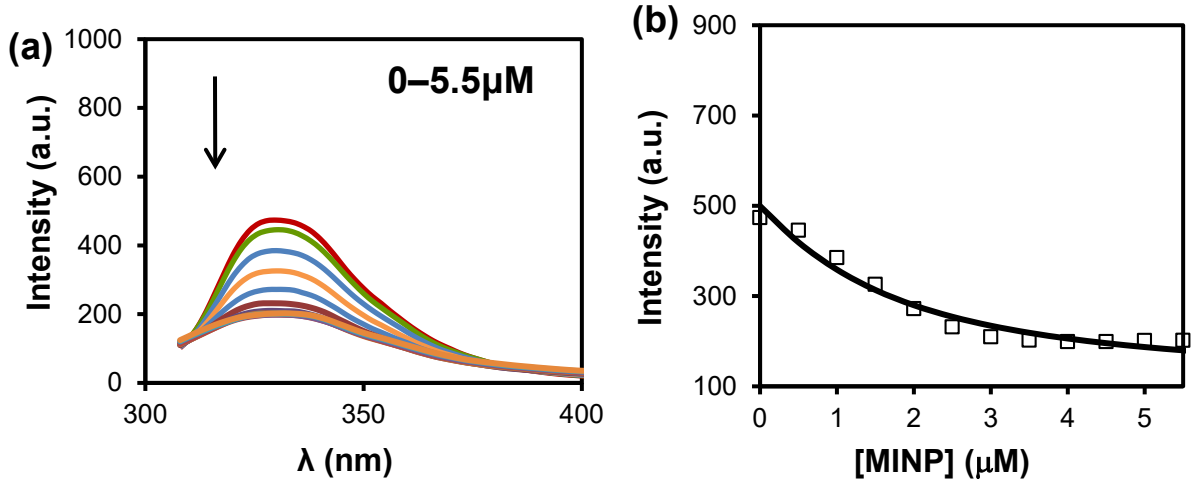

Figure S32. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **8** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **8** at 330 nm to a 1:1 binding isotherm.

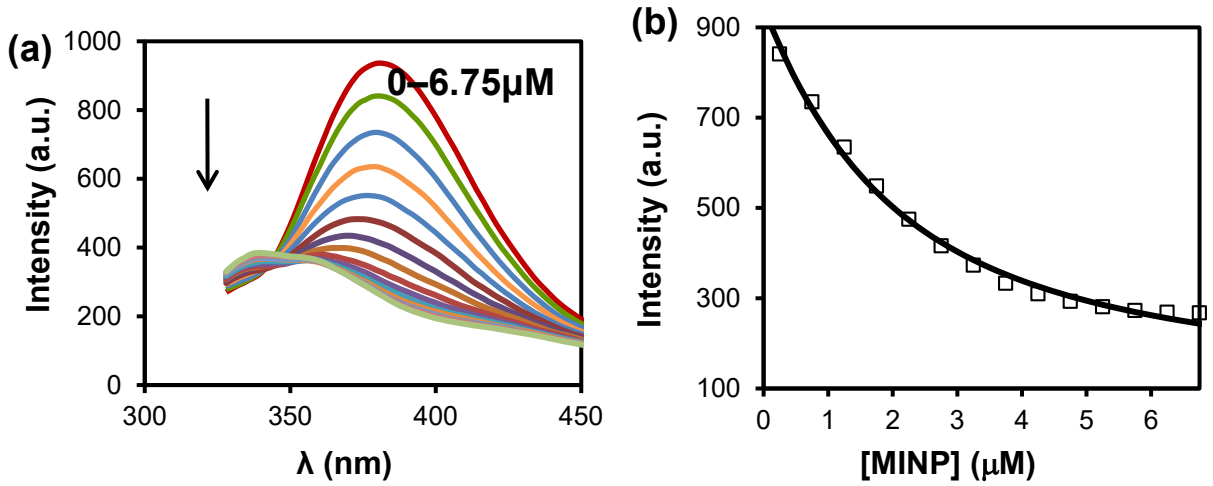

Figure S33. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **9** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **9** at 380 nm to a 1:1 binding isotherm.

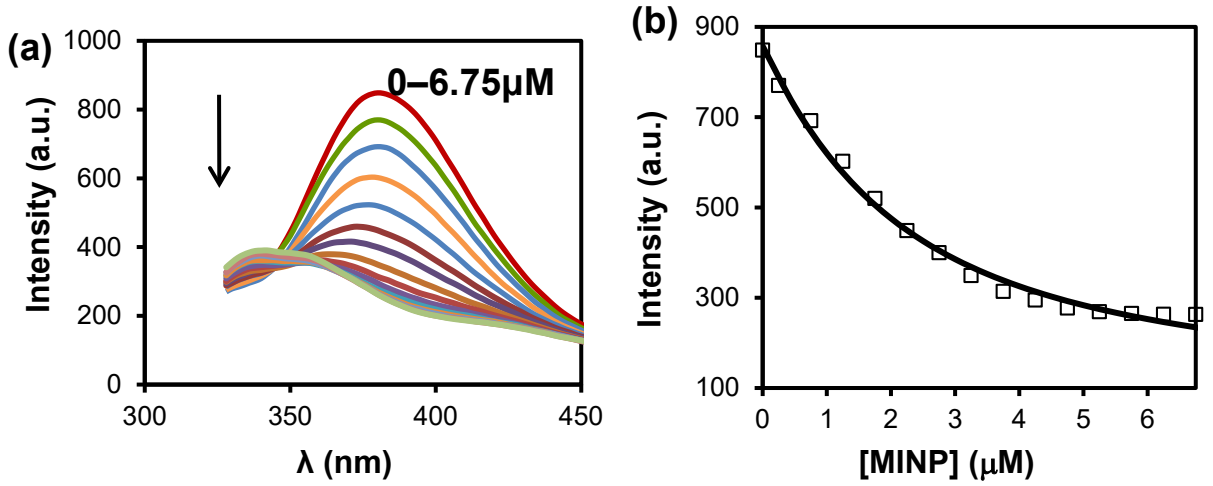

Figure S34. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **9** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.4 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **9** at 380 nm to a 1:1 binding isotherm.

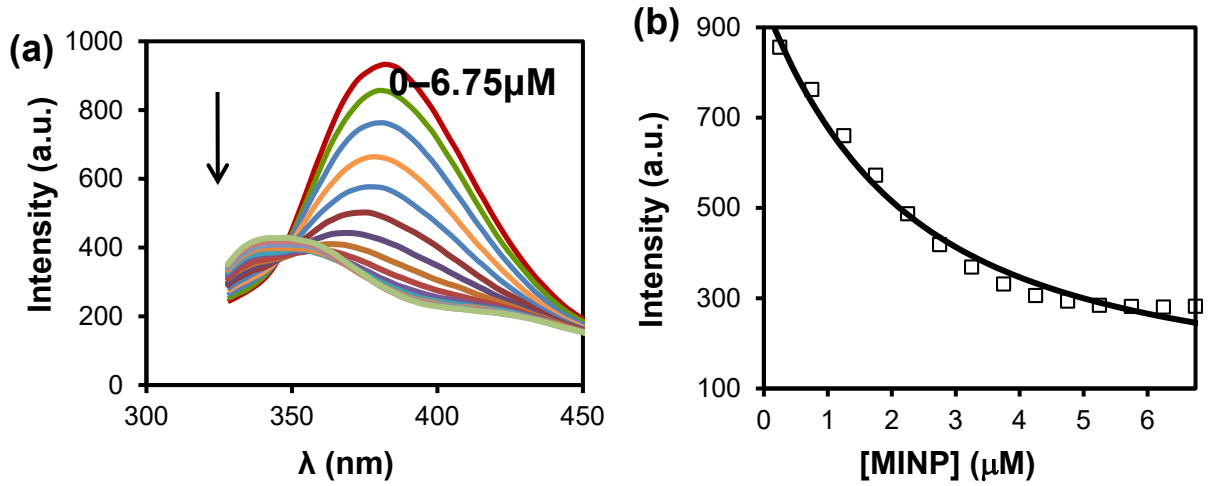

Figure S35. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **9** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **9** at 380 nm to a 1:1 binding isotherm.

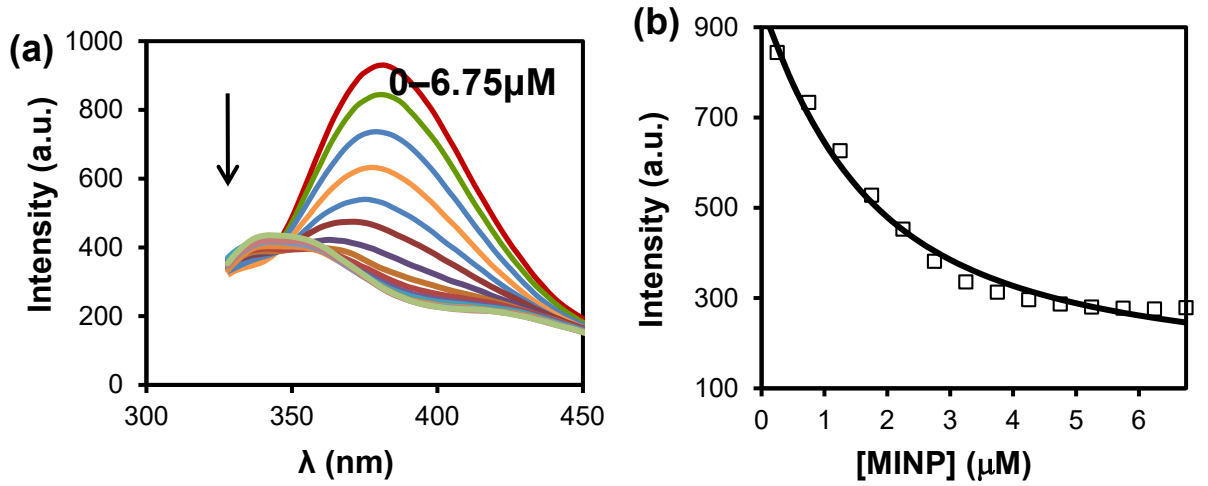

Figure S36. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **9** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **9** at 380 nm to a 1:1 binding isotherm.

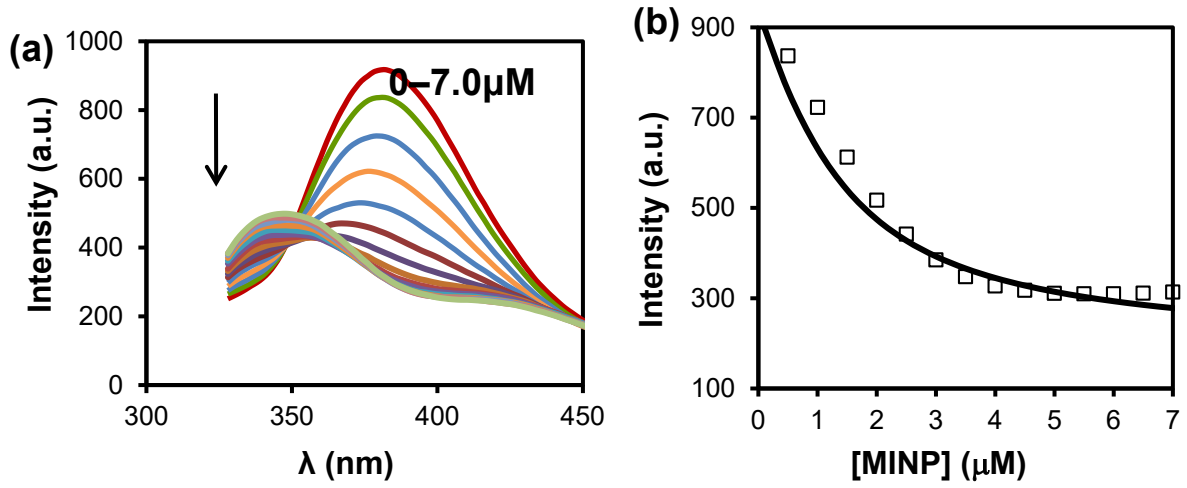

Figure S37. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **9** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **9** at 380 nm to a 1:1 binding isotherm.

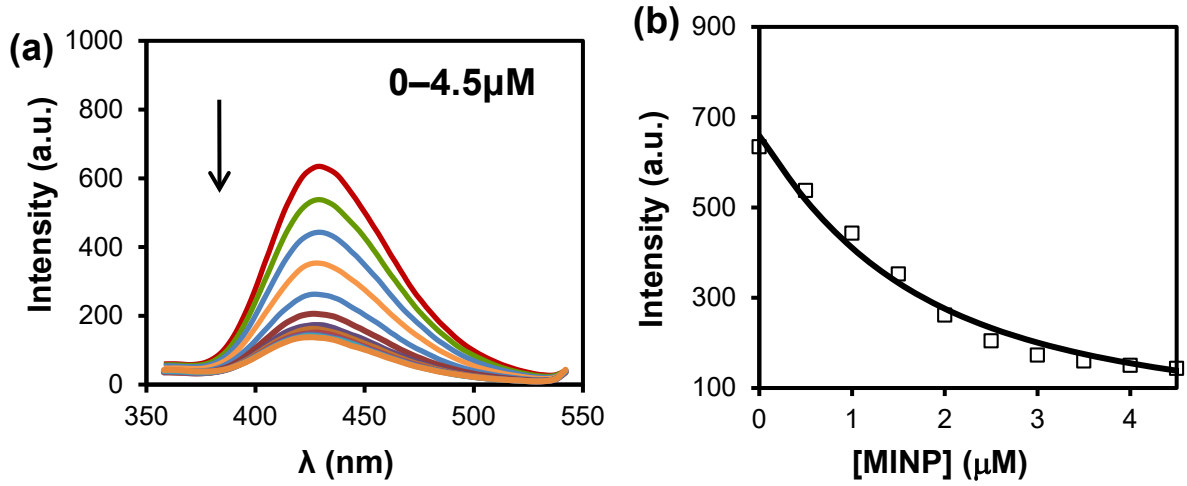

Figure S38. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **10** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **10** at 430 nm to a 1:1 binding isotherm.

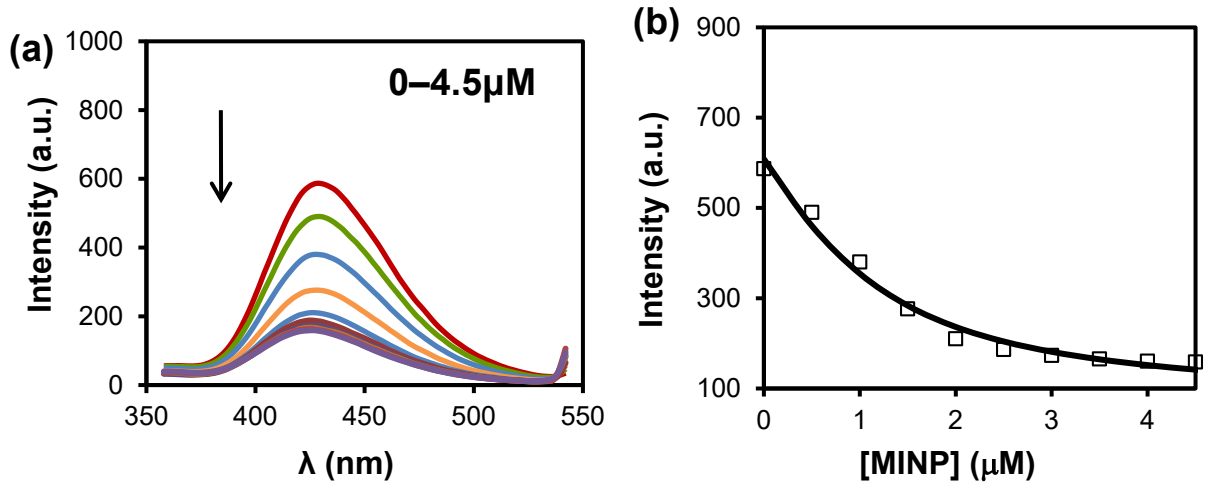

Figure S39. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **10** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.4 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **10** at 430 nm to a 1:1 binding isotherm.

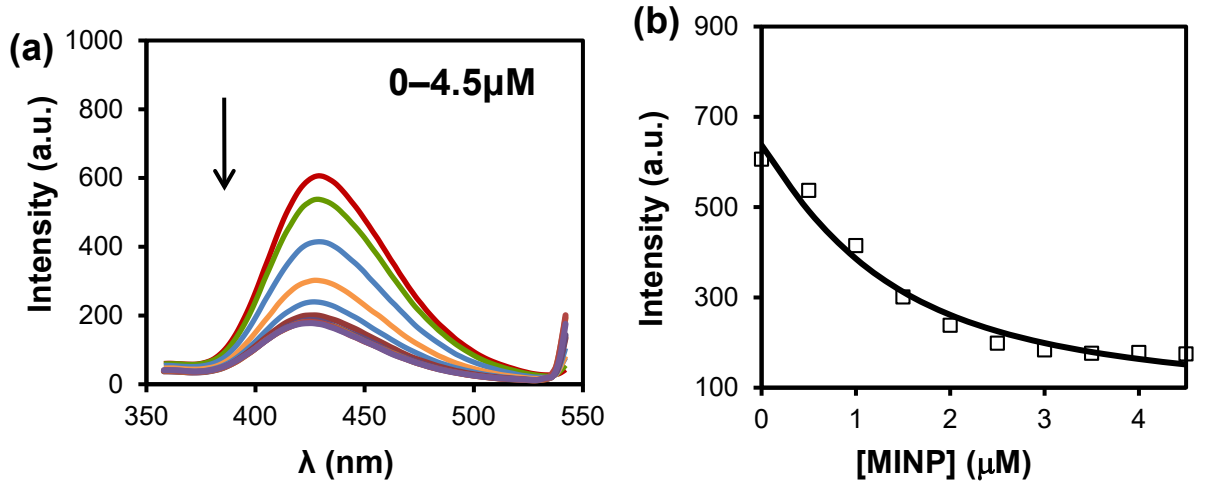

Figure S40. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **10** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **10** at 430 nm to a 1:1 binding isotherm.

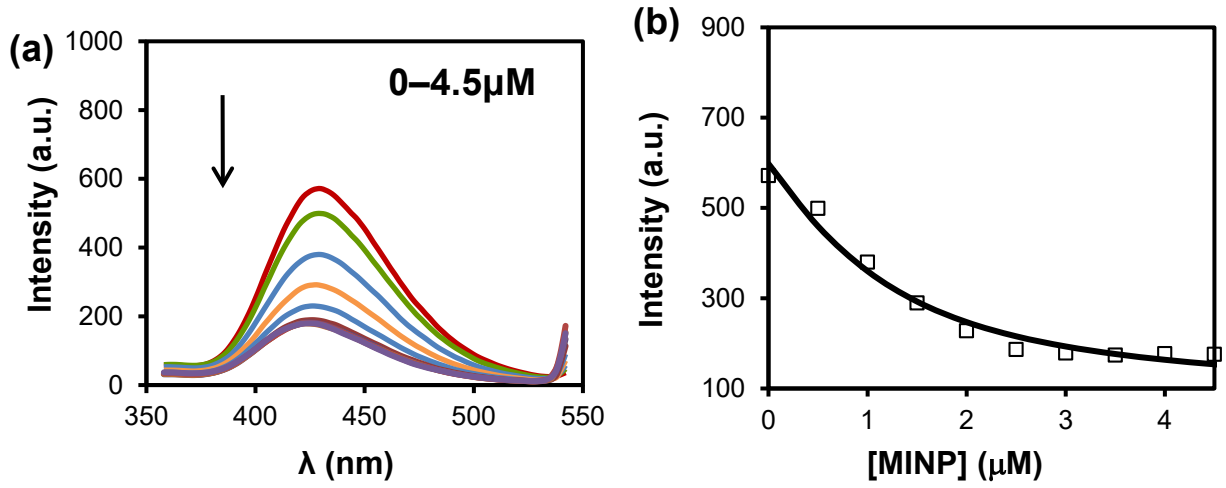

Figure S41. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **10** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **10** at 430 nm to a 1:1 binding isotherm.

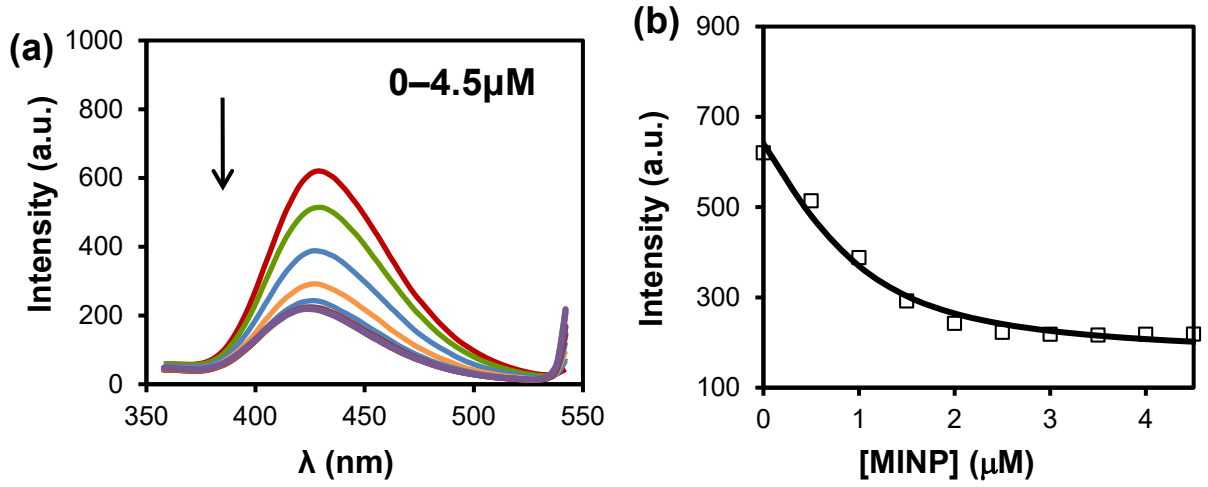

Figure S42. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **10** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **10** at 430 nm to a 1:1 binding isotherm.

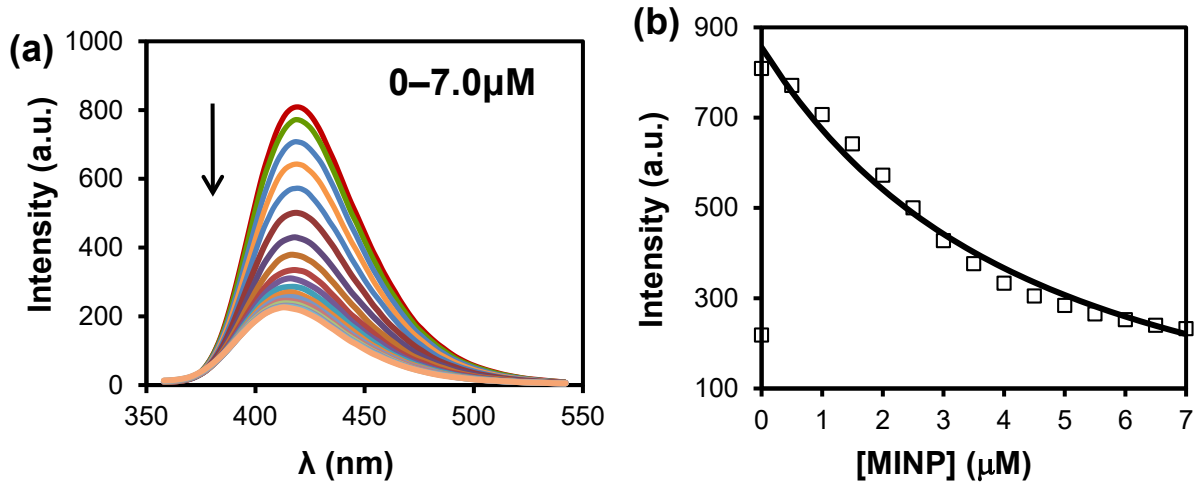

Figure S43. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **11** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **11** at 420 nm to a 1:1 binding isotherm.

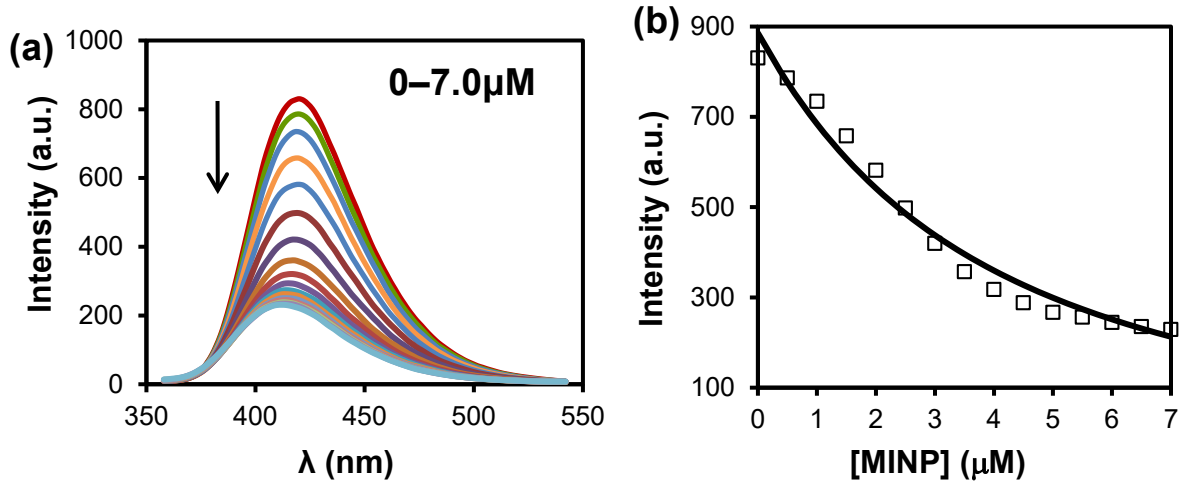

Figure S44. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **11** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.4 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **11** at 420 nm to a 1:1 binding isotherm.

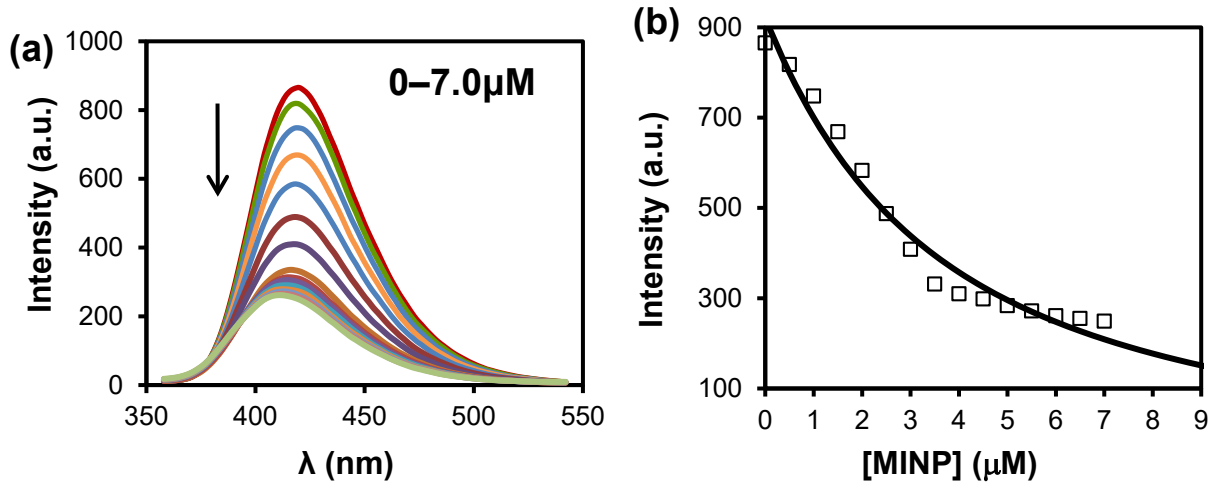

Figure S45. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **11** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **11** at 420 nm to a 1:1 binding isotherm.

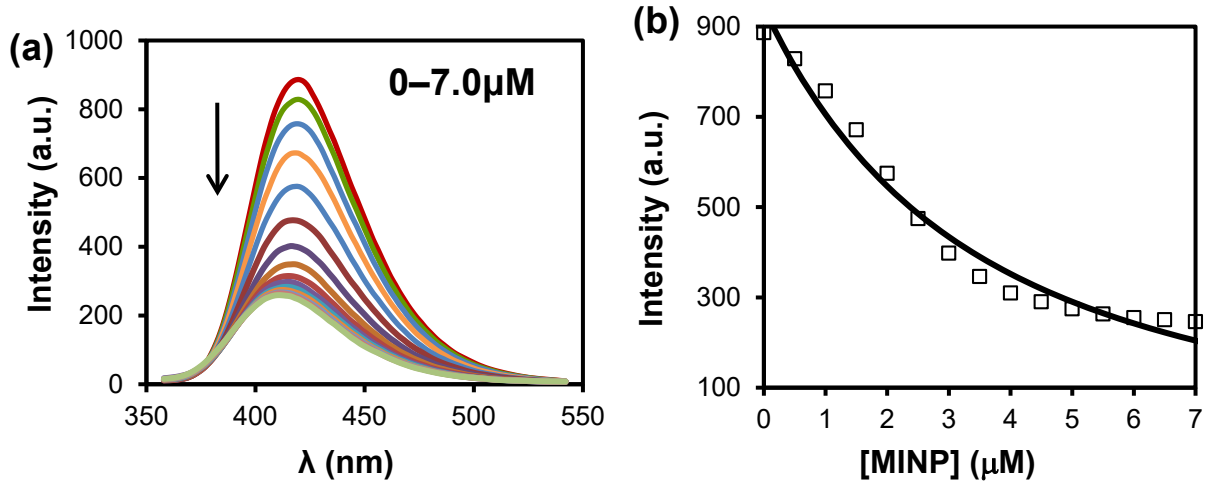

Figure S46. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **11** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **11** at 420 nm to a 1:1 binding isotherm.

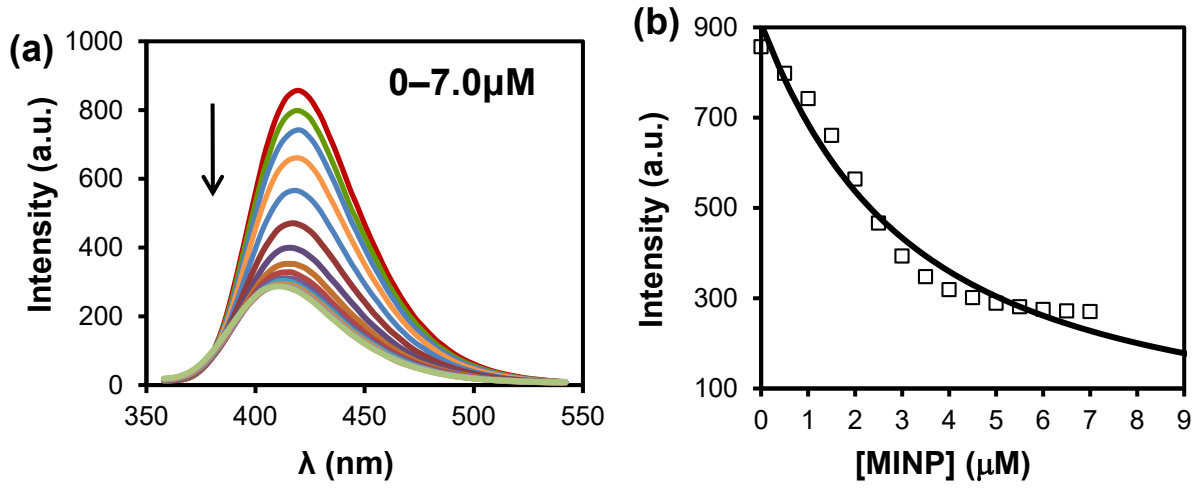

Figure S47. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **11** (1.0 μM) upon addition of different concentrations of MINP(**4**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **11** at 420 nm to a 1:1 binding isotherm.

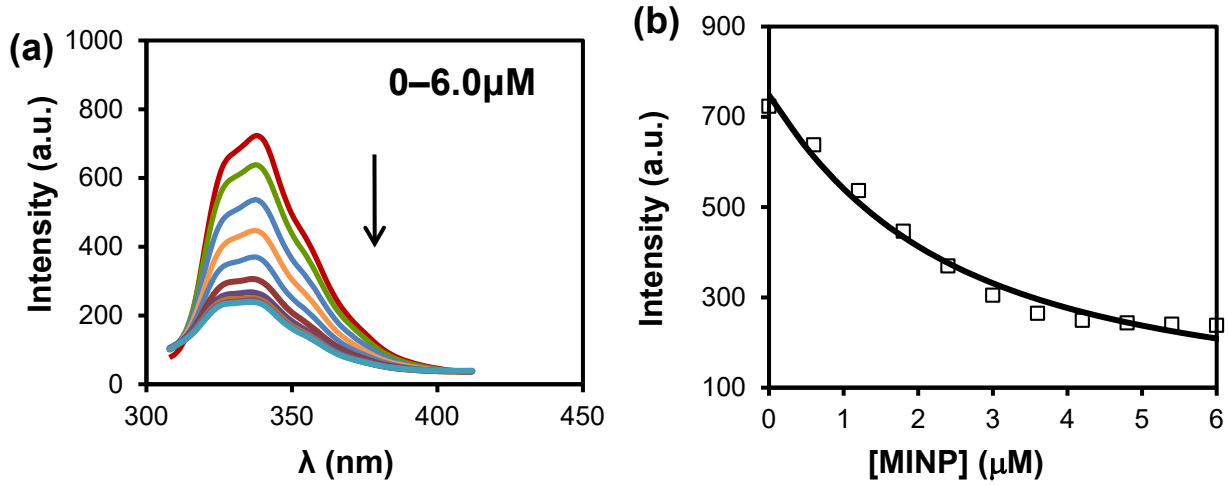

Figure S48. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **5** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **5** at 340 nm to a 1:1 binding isotherm.

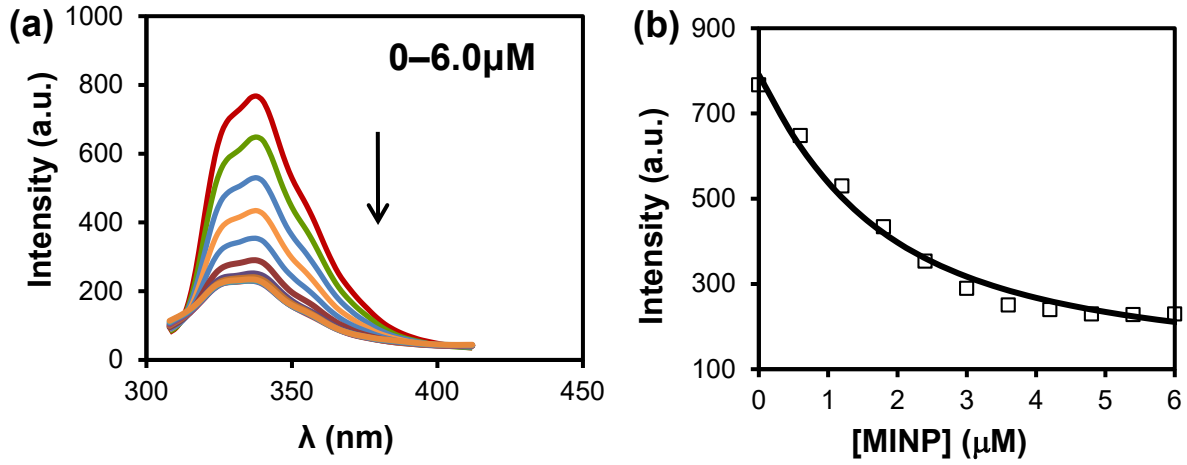

Figure S49. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **5** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.4 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **5** at 340 nm to a 1:1 binding isotherm.

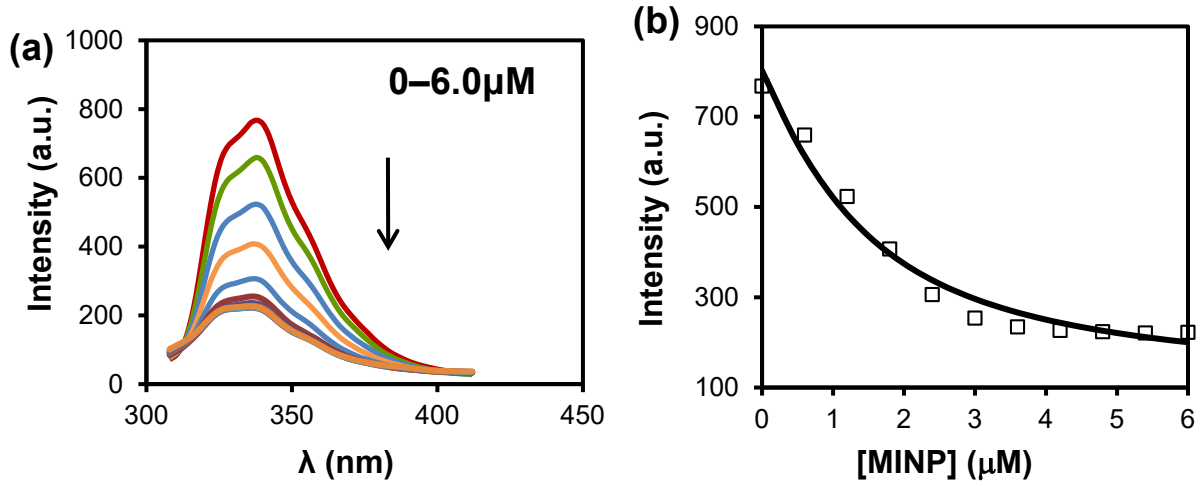

Figure S50. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **5** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **5** at 340 nm to a 1:1 binding isotherm.

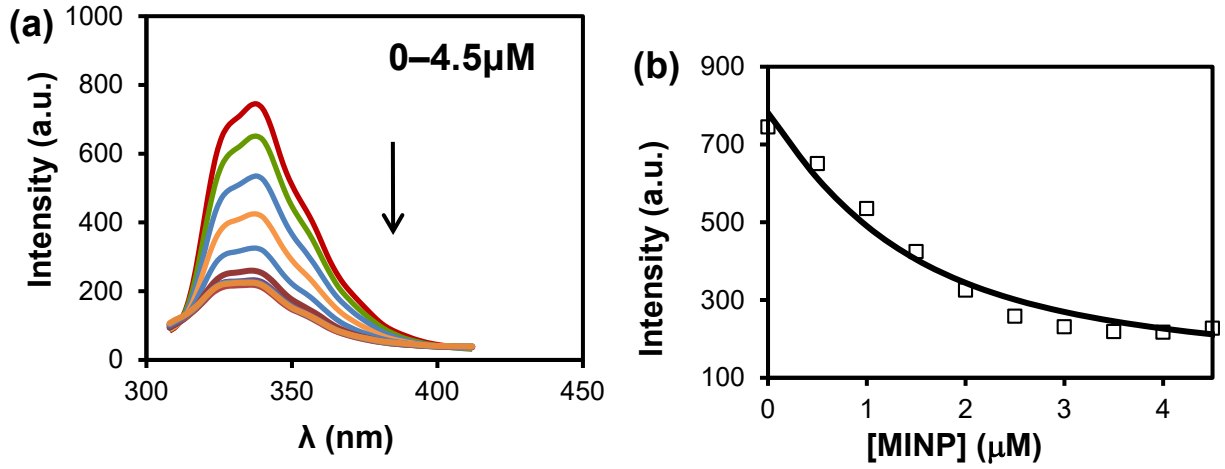

Figure S51. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **5** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **5** at 340 nm to a 1:1 binding isotherm.

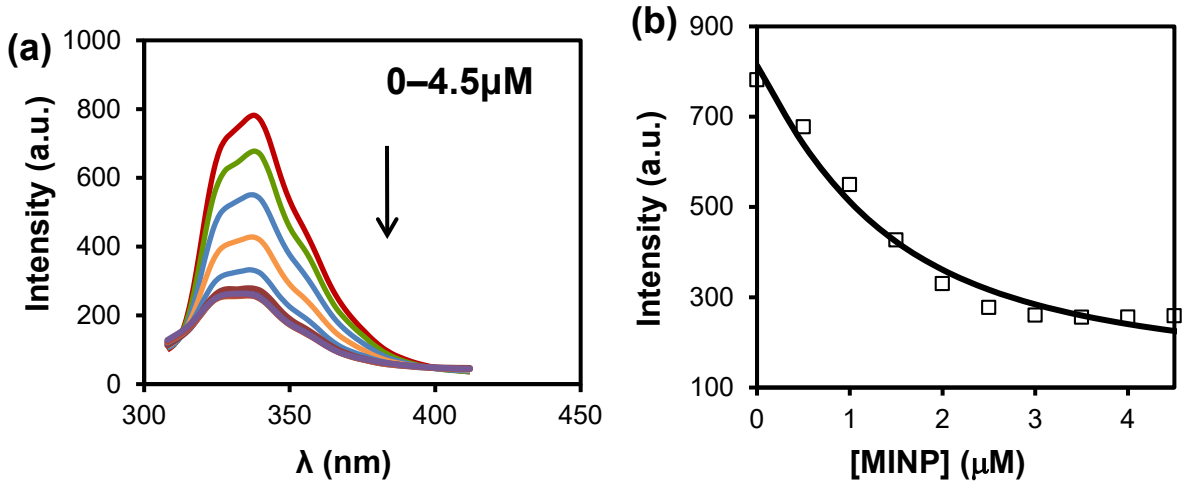

Figure S52. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **5** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **5** at 340 nm to a 1:1 binding isotherm.

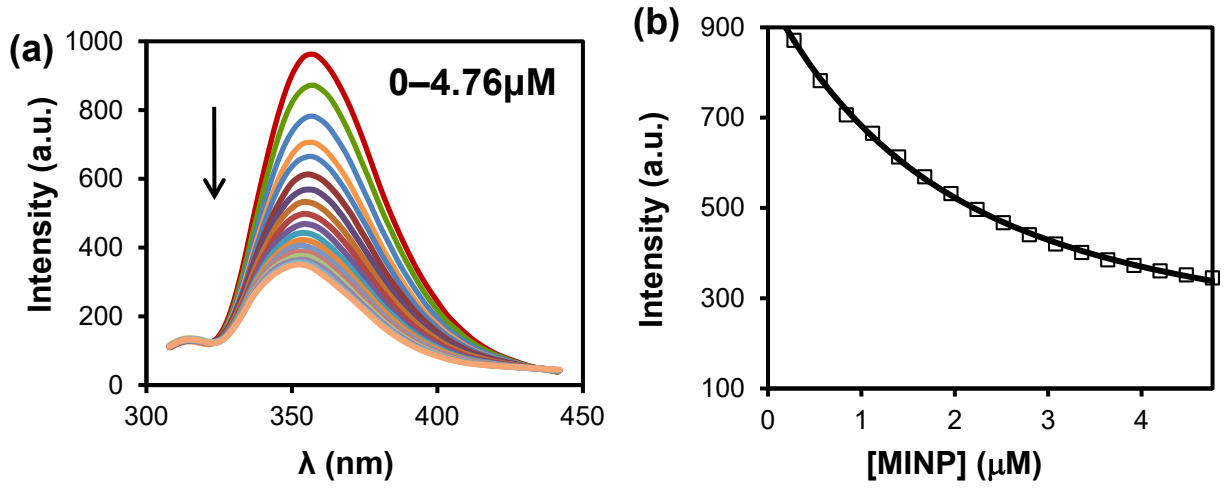

Figure S53. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **4** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **4** at 356 nm to a 1:1 binding isotherm.

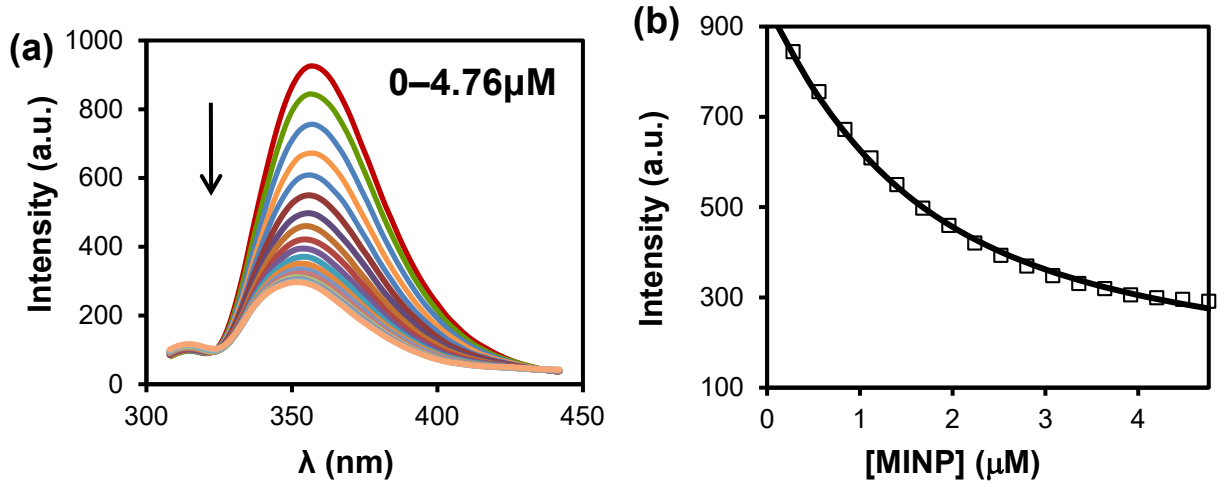

Figure S54. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **4** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.4 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **4** at 356 nm to a 1:1 binding isotherm.

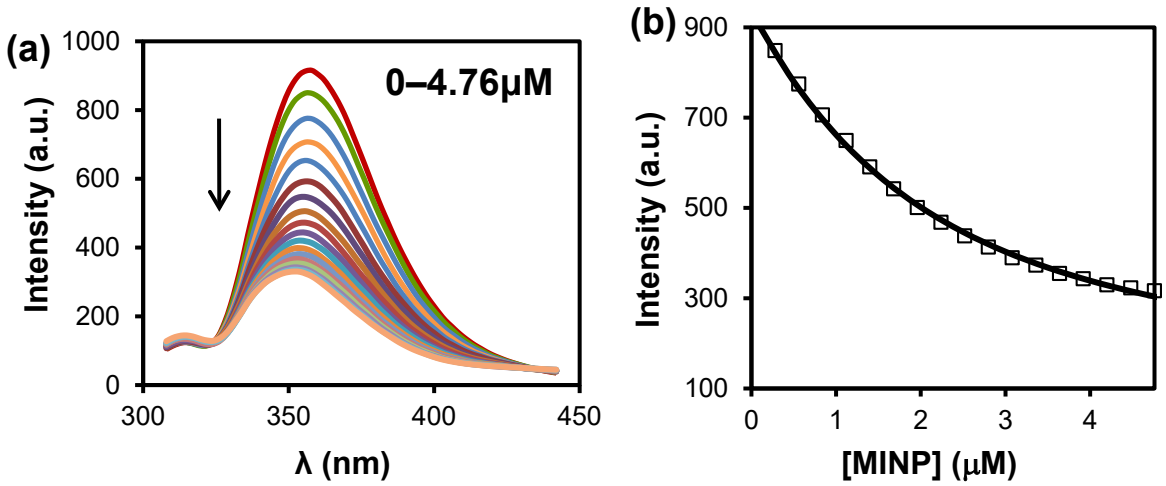

Figure S55. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **4** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **4** at 356 nm to a 1:1 binding isotherm.

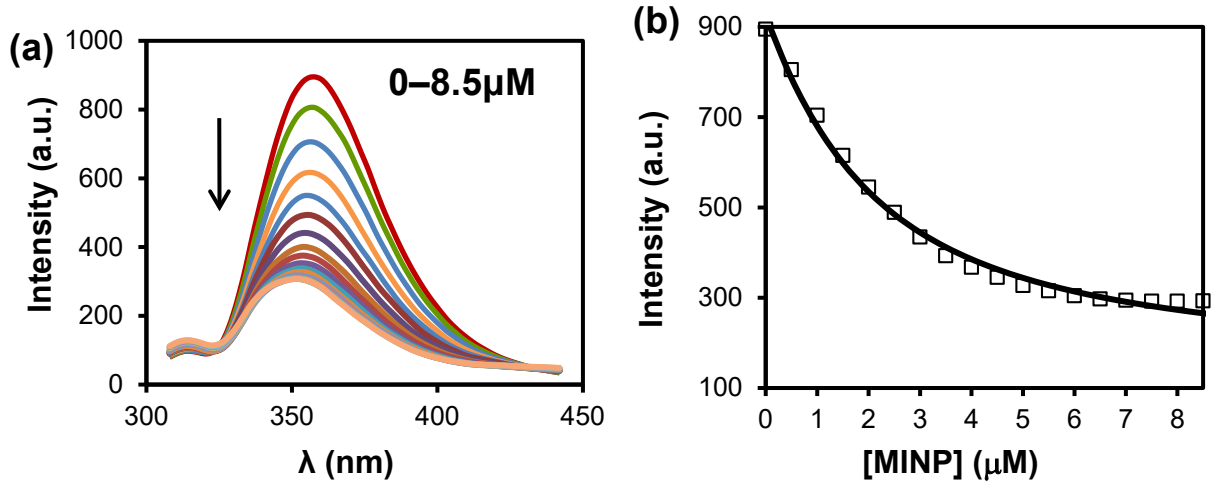

Figure S56. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **4** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **4** at 356 nm to a 1:1 binding isotherm.

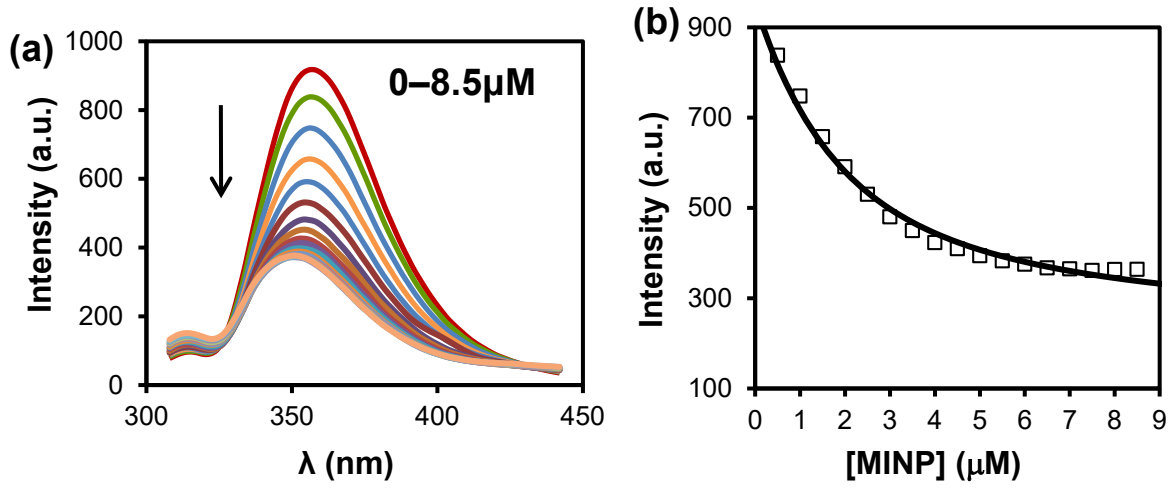

Figure S57. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **4** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **4** at 356 nm to a 1:1 binding isotherm.

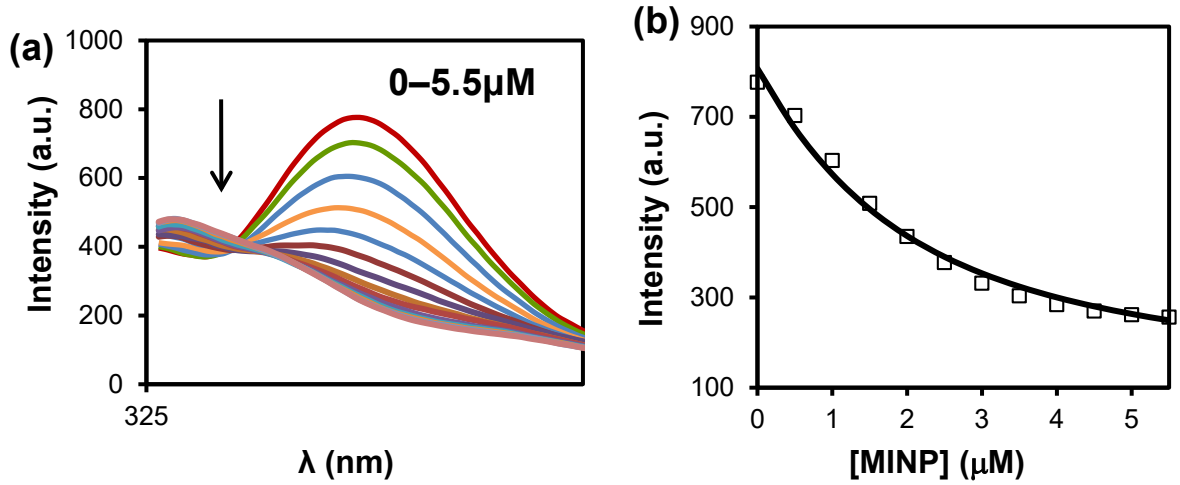

Figure S58. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **9** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **9** at 380 nm to a 1:1 binding isotherm.

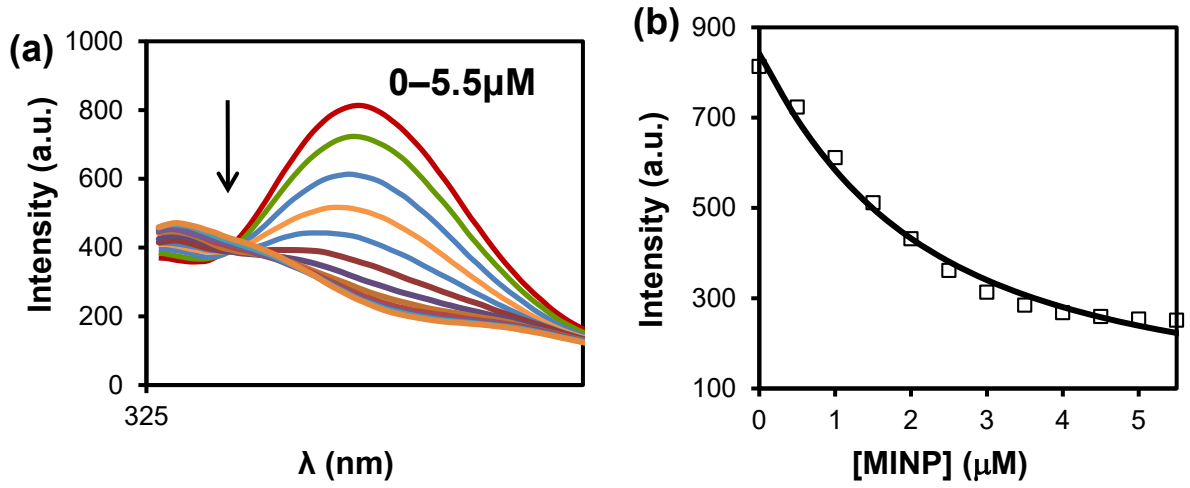

Figure S59. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **9** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.4 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **9** at 380 nm to a 1:1 binding isotherm.

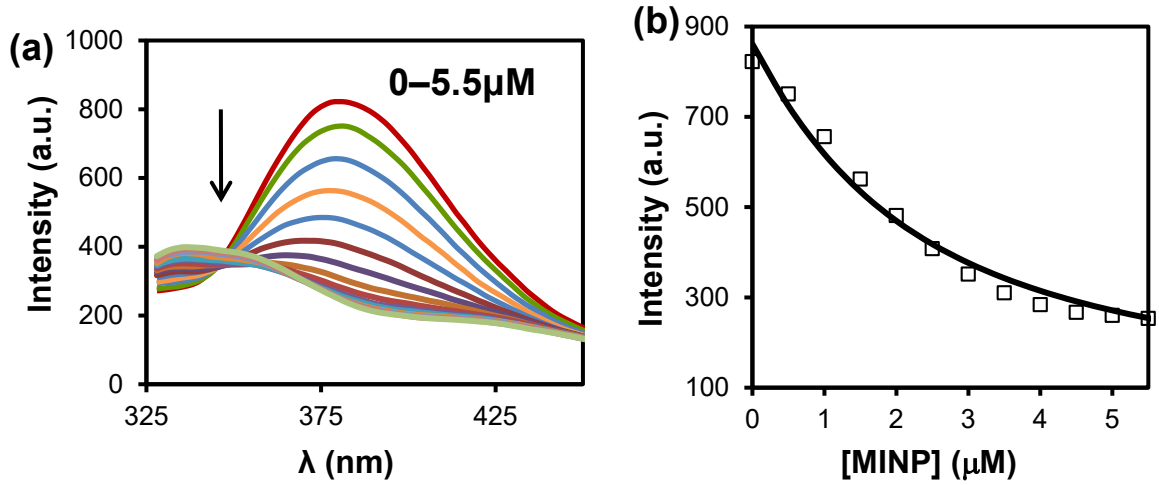

Figure S60. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **9** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.6 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **9** at 380 nm to a 1:1 binding isotherm.

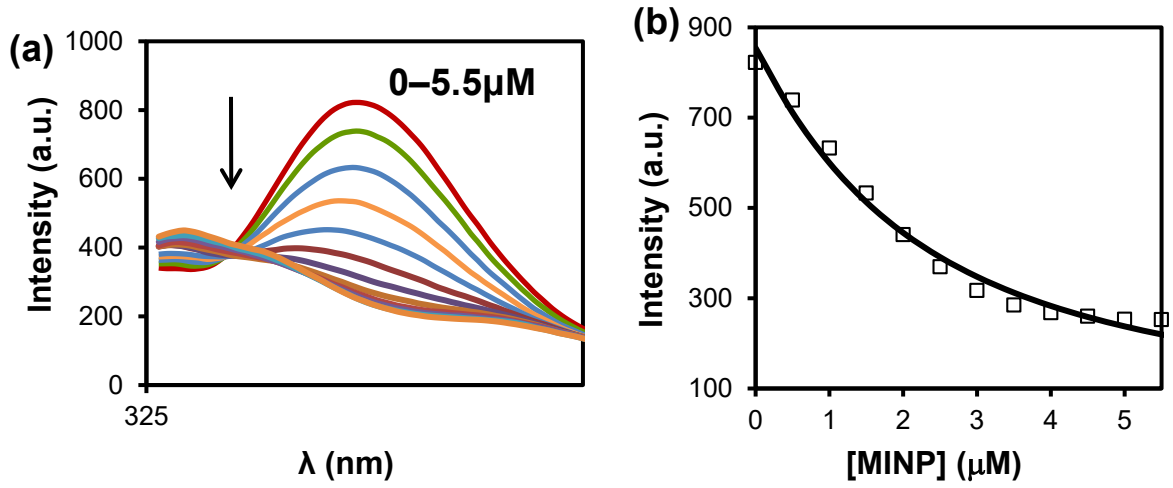

Figure S61. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **9** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 0.8 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **9** at 380 nm to a 1:1 binding isotherm.

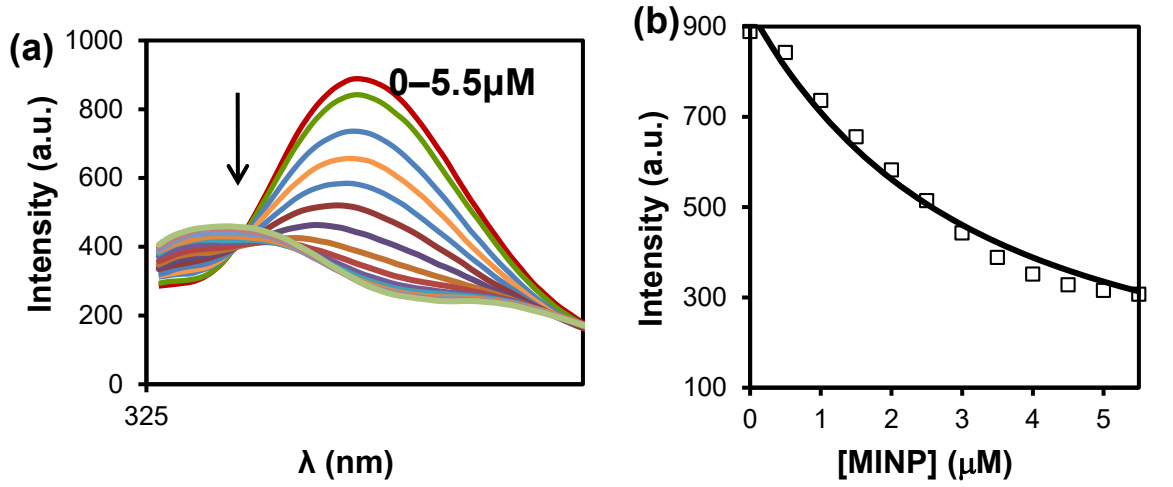

Figure S62. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of guest **9** (1.0 μM) upon addition of different concentrations of MINP(**5**) in 10 mM HEPES (pH 7.0). The MINP was prepared with 1.2 equiv. of **2** in the 1st-stage cross-linking. (b) Nonlinear least squares fitting of the emission intensity of guest **9** at 380 nm to a 1:1 binding isotherm.

^{1}H & ^{13}C NMR spectra