Supporting Information

Peptide-Binding Nanoparticle Materials with Tailored Recognition sites for Basic Peptides

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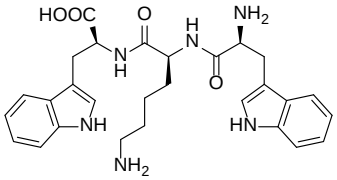
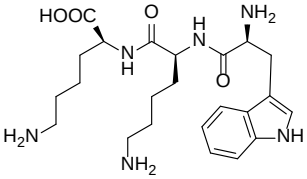
General Method

Biological peptides PKKKRKV, KKALRRQETVDAL, RVLSFIKGTK and LRRASLG were purchased from GenScript USA Inc., and reconstituted according to the instructions. Other oligopeptides were purchased from GL Biochem (Shanghai) Ltd. All organic solvents and reagents were of ACS-certified grade or higher grade, and were purchased from commercial suppliers. ^{1}H and ^{13}C NMR spectra were recorded on a Varian VXR-400 spectrometer. ESI-MS mass was recorded on Shimadzu LCMS-2010 mass spectrometer. Dynamic light scattering (DLS) data were recorded at 25 °C using PDDLS/CoolBatch 90T with PD2000DLS+ instrument. Transmission electron microscopy (TEM) was carried out using a TECNAI G2 F20 operated at 200 kV. Fluorescent titrations and Job's plot experiments were taken at ambient temperature on a Varian Cary Eclipse Fluorescence spectrophotometer. The binding constants were calculated by curve fitting using KaleidaGraph. Isothermal titration calorimetry (ITC) was performed using a MicroCal VP-ITC Microcalorimeter with Origin 7 software and VPViewer2000 (GE Healthcare, Northampton, MA). For the TEM imaging, 5 mg of MINP (KWW) was dissolved in 1 mL of Millipore water and the solution was ultrasonicated for 1 min. A microsyringe was used to load one small drop of the above solution onto a TEM copper grid covered with carbon film. The sample was left to dry at room temperature overnight. The sample was analyzed on a TECNAI G2 F20 instrument, operating at 200 kV.

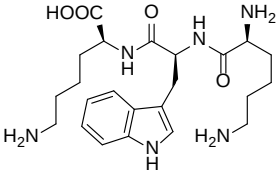
Chart S1. Structures of other oligopeptides used in study.



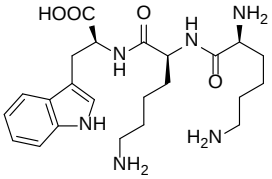
WKW



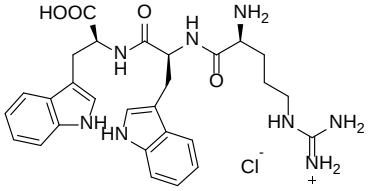
WKK



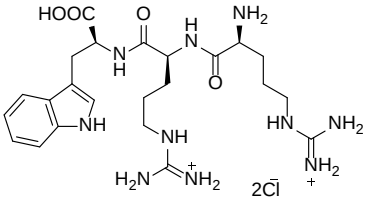
KWK



KKW



RWW



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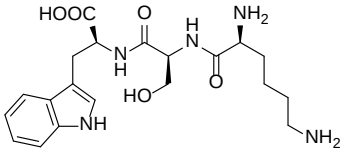

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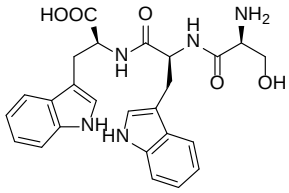

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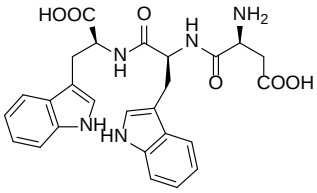

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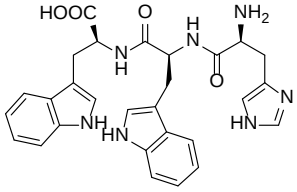

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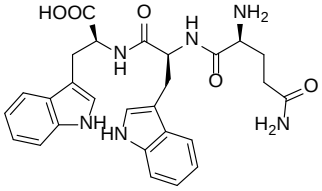

QWW

Characterization of MINPs

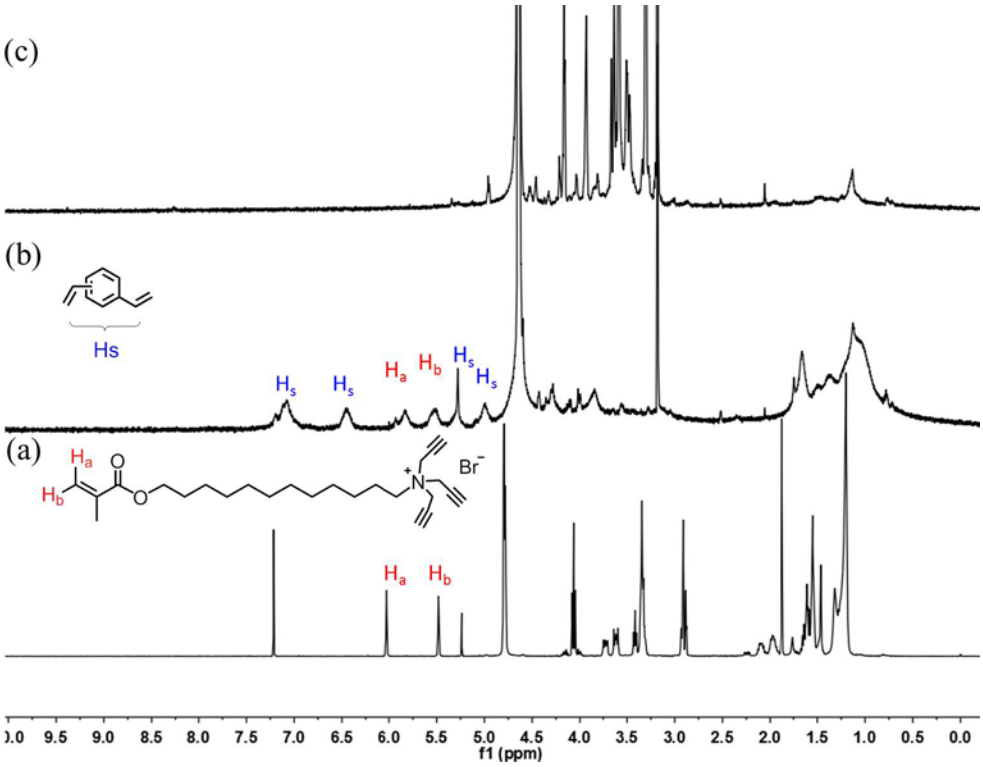

Figure S1. ^{1}H NMR spectra of (a) **1** in $CDCl_3$, (b) alkynyl-SCM in D_2O, and (c) MINP(KWW) without functional monomer in D_2O.

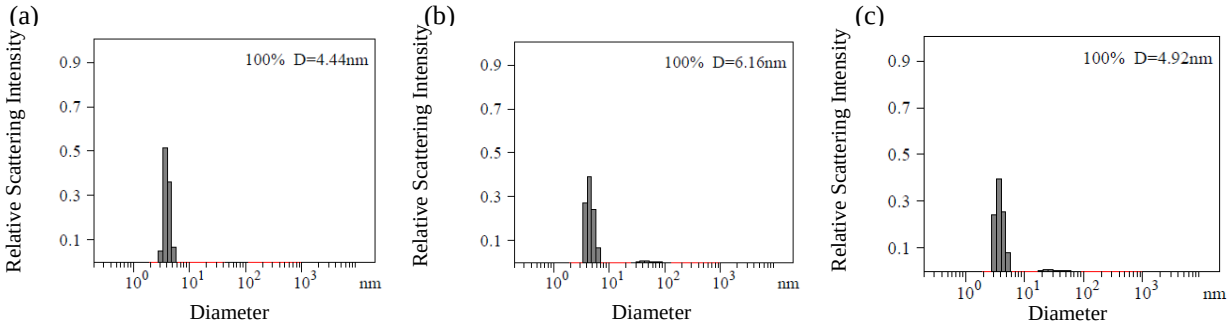

Figure S2. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM, and (c) MINP(KWW) without functional monomer in water.

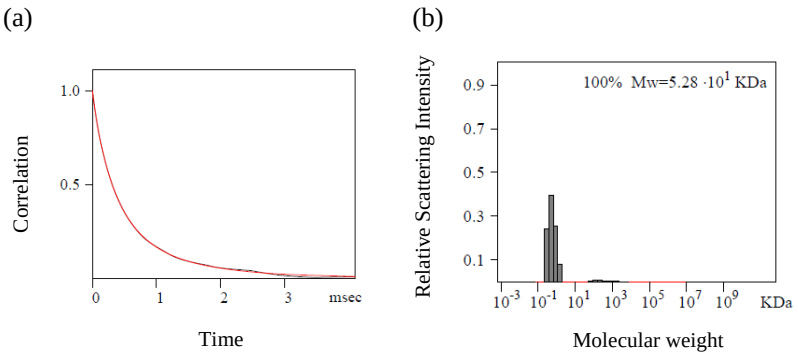

Figure S3. The correlation curve and the distribution of the molecular weight for MINP(KWW) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP(KWW) is assumed to contain one molecule of compound **1** (MW = 465 g/mol), 1.2 molecules of compound **2** (MW = 172 g/mol), one molecule of DVB (MW = 130 g/mol) and 0.8 molecules of compound **3** (MW = 264 g/mol), the molecular weight of MINP(KWW) translates to 52 [= 52800 / (465 + 1.2×172 + 130 + 0.8×264)] of such units.

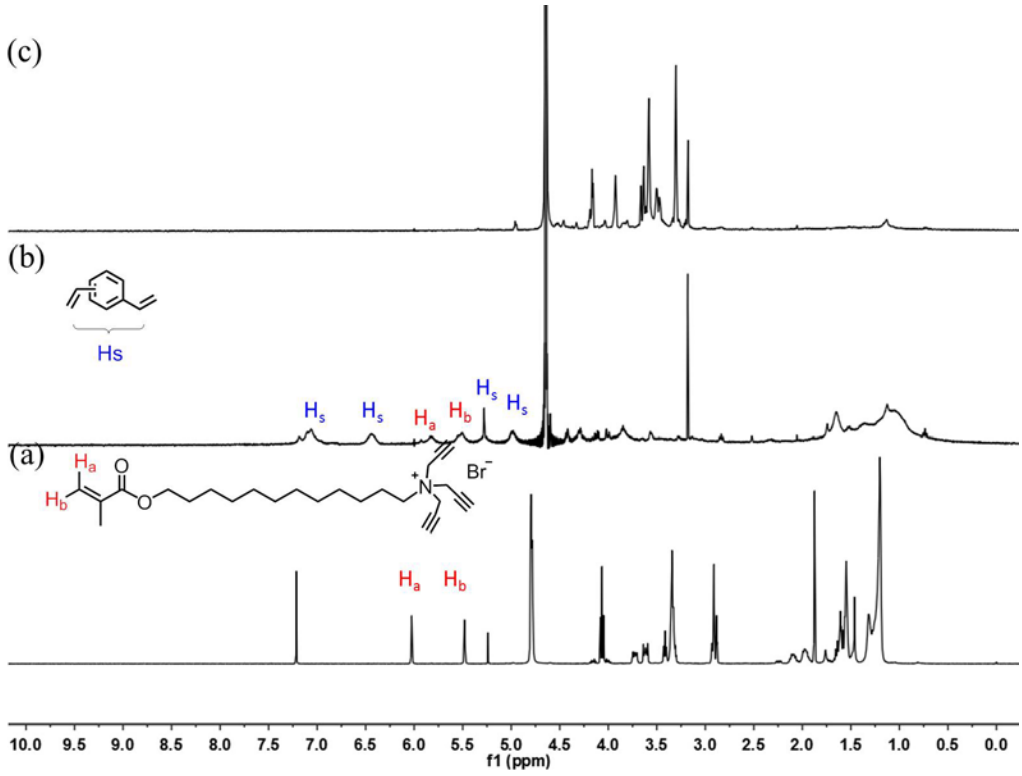

Figure S4. ^{1}H NMR spectra of (a) **1** in $CDCl_3$, (b) alkynyl-SCM in D_2O, and (c) MINP(KWW) with FM **4** (1:1) in D_2O.

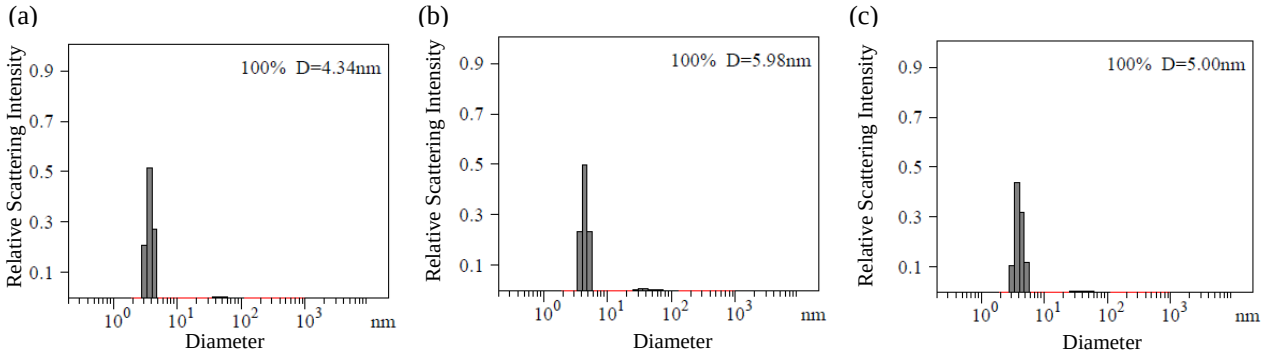

Figure S5. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM, and (c) MINP(KWW) with FM **4** (1:1) in water.

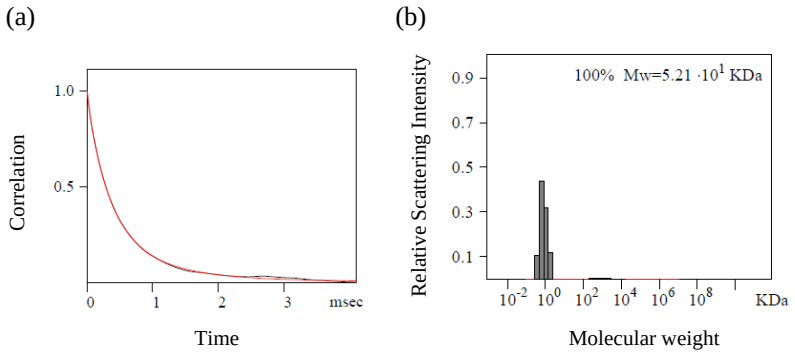

Figure S6. The correlation curve and the distribution of the molecular weight for MINP(KWW) with FM **4** (1:1) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP(KWW) with FM **4** (1:1) is assumed to contain one molecule of compound **1** (MW = 465 g/mol), 1.2 molecules of compound **2** (MW = 172 g/mol), one molecule of DVB (MW = 130 g/mol), 0.8 molecules of compound **3** (MW = 264 g/mol), and 0.02 molecules of FM **4** (MW = 595 g/mol), the molecular weight of MINP(KWW) with FM **4** (1:1) translates to 51 [= 52100 / (465 + 1.2×172 + 130 + 0.8×264 + 0.02×595)] of such units.

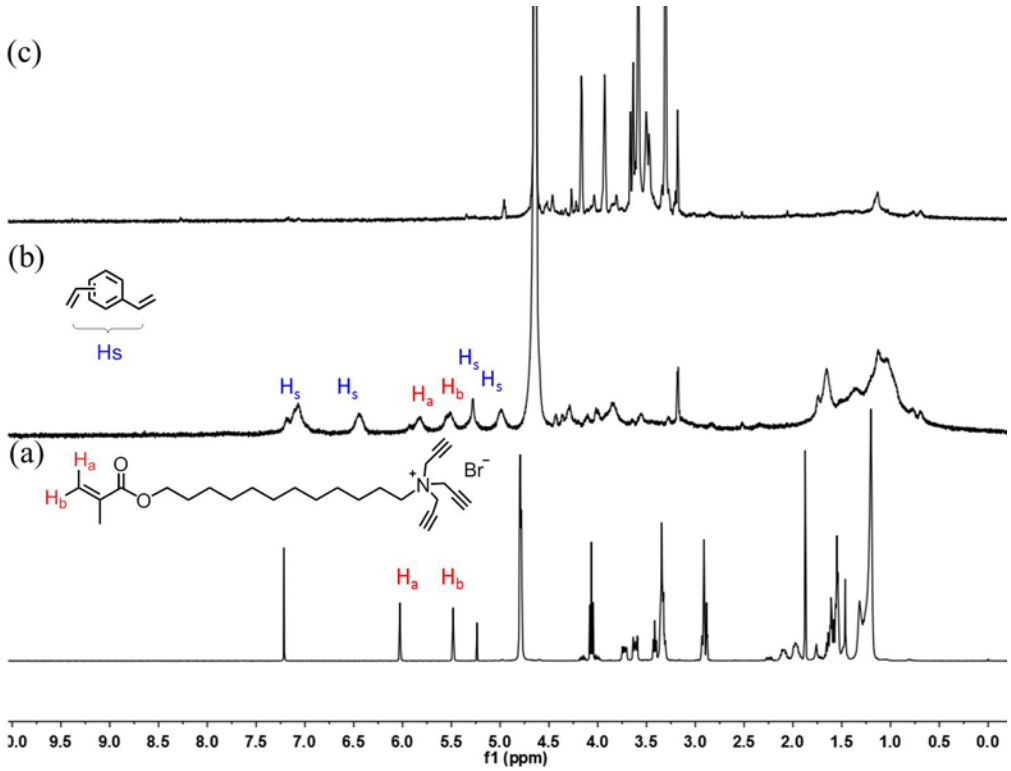

Figure S7. ^{1}H NMR spectra of (a) **1** in $CDCl_3$, (b) alkynyl-SCM in D_2O, and (c) MINP(KWW) with FM **4** (1:2) in D_2O.

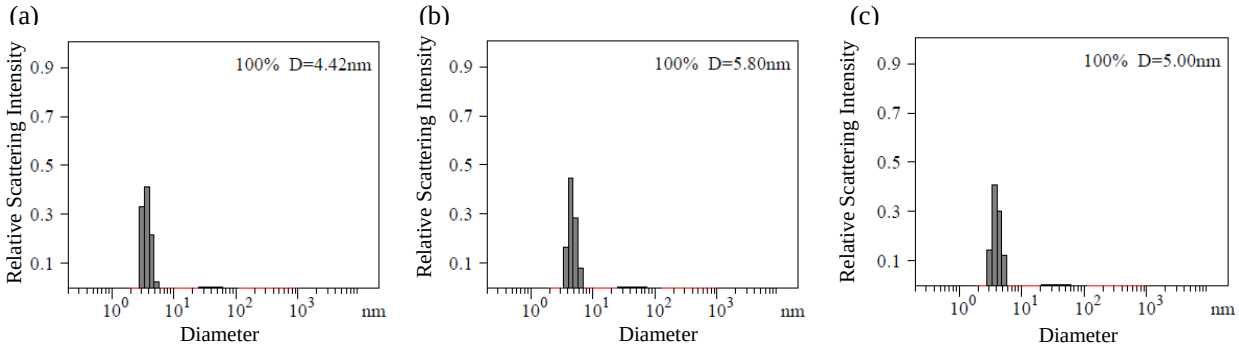

Figure S8. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM, and (c) MINP(KWW) with FM **4** (1:2) in water.

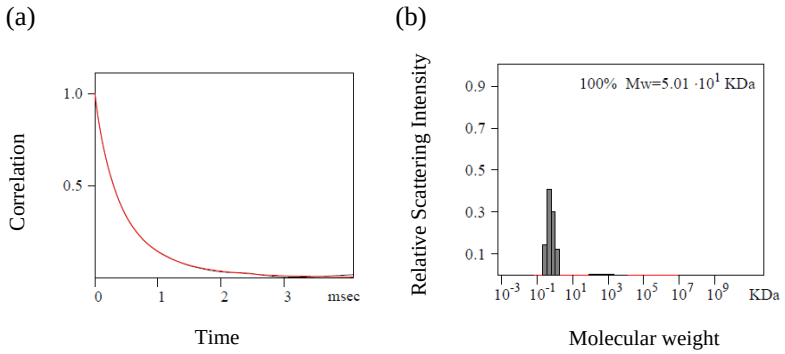

Figure S9. The correlation curve and the distribution of the molecular weight for MINP(KWW) with FM **4** (1:2) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP(KWW) with FM **4** (1:2) is assumed to contain one molecule of compound **1** (MW = 465 g/mol), 1.2 molecules of compound **2** (MW = 172 g/mol), one molecule of DVB (MW = 130 g/mol), 0.8 molecules of compound **3** (MW = 264 g/mol), and 0.06 molecules of FM **4** (MW = 595 g/mol), the molecular weight of MINP(KWW) with FM **4** (1:2) translates to 48 [= 50100 / (465 + 1.2×172 + 130 + 0.8×264 + 0.04×595)] of such units.

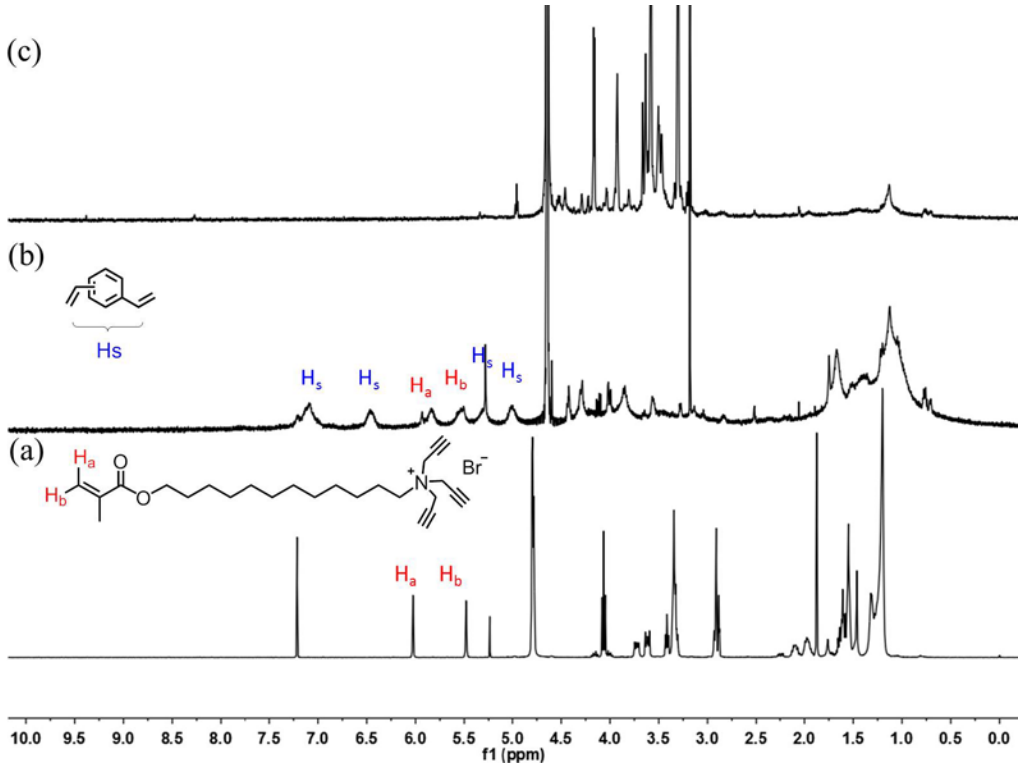

Figure S10. ^{1}H NMR spectra of (a) **1** in $CDCl_3$, (b) alkynyl-SCM in D_2O, and (c) MINP(KWW) with FM **4** (1:3) in D_2O.

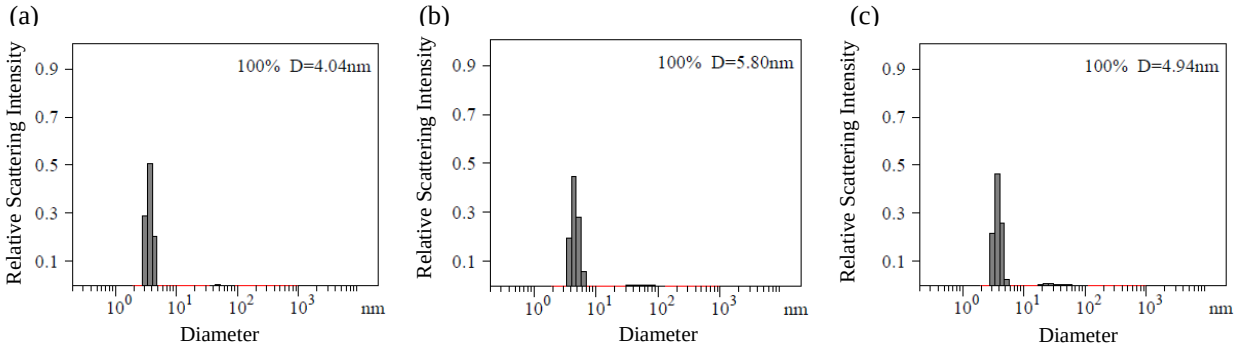

Figure S11. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM, and (c) MINP(KWW) with FM **4** (1:3) in water.

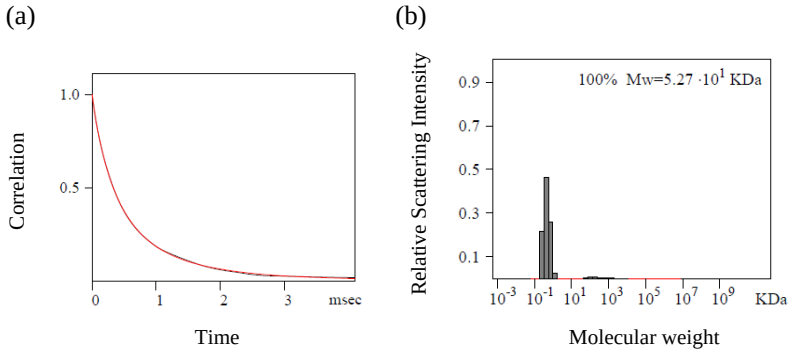

Figure S12. The correlation curve and the distribution of the molecular weight for MINP(KWW) with FM **4** (1:3) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP(c-Myc) with FM **2** (1:7.5) is assumed to contain one molecule of compound **1** (MW = 465 g/mol), 1.2 molecules of compound **2** (MW = 172 g/mol), one molecule of DVB (MW = 130 g/mol), 0.8 molecules of compound **3** (MW = 264 g/mol), and 0.06 molecules of FM **4** (MW = 595 g/mol), the molecular weight of MINP(KWW) with FM **4** (1:3) translates to 50 [= 52700 / (465 + 1.2×172 + 130 + 0.8×264 + 0.06×595)] of such units.

Fluorescence titration experiments

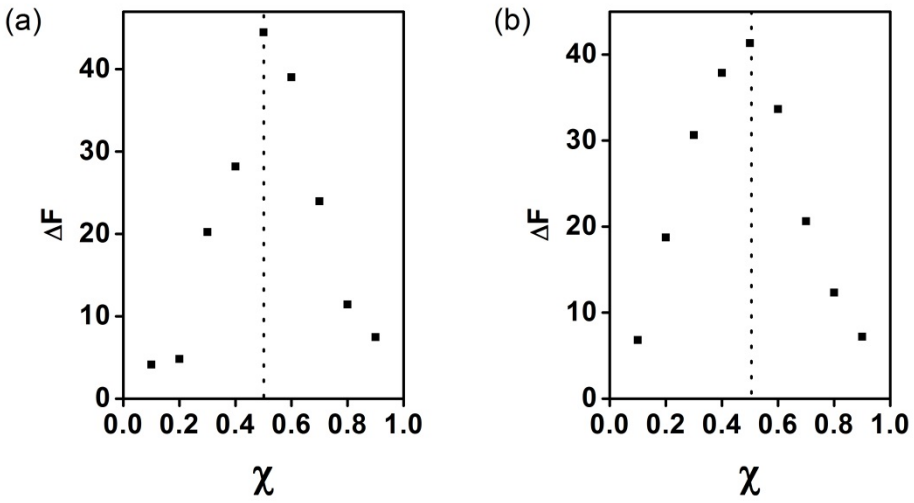

Figure S13. Job's plots for KWW with MINP(KWW) prepared (a) without FM and (b) with 2 equiv FM **4**. The total concentration of MINP and the guest was 10 μM. χ = [Host]/{[Host] + [Guest]}

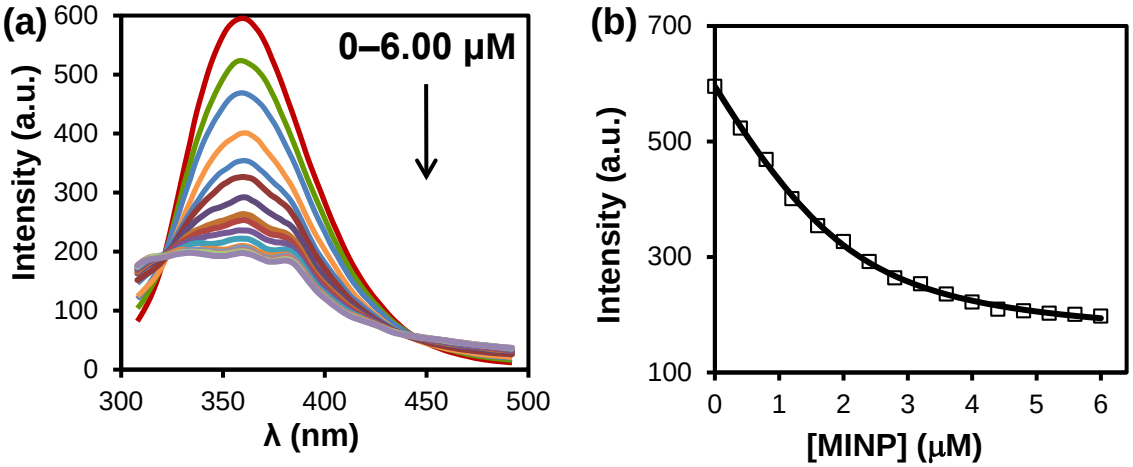

Figure S14. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KWW (2.0 μM) upon addition of different concentrations of MINP(KWW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 1 in Table 1.

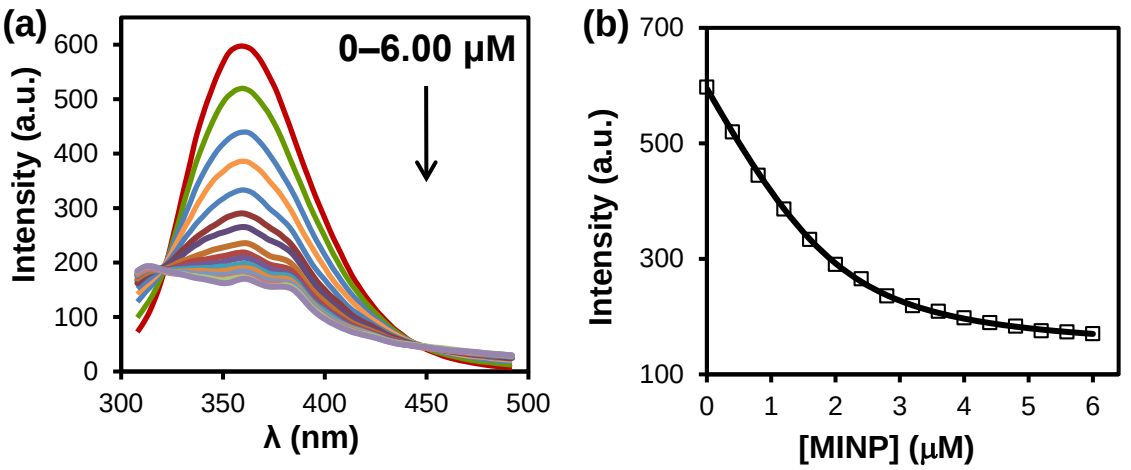

Figure S15. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KWW (2.0 μM) upon addition of different concentrations of MINP(KWW) with FM **4** (1:1) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 2 in Table 1.

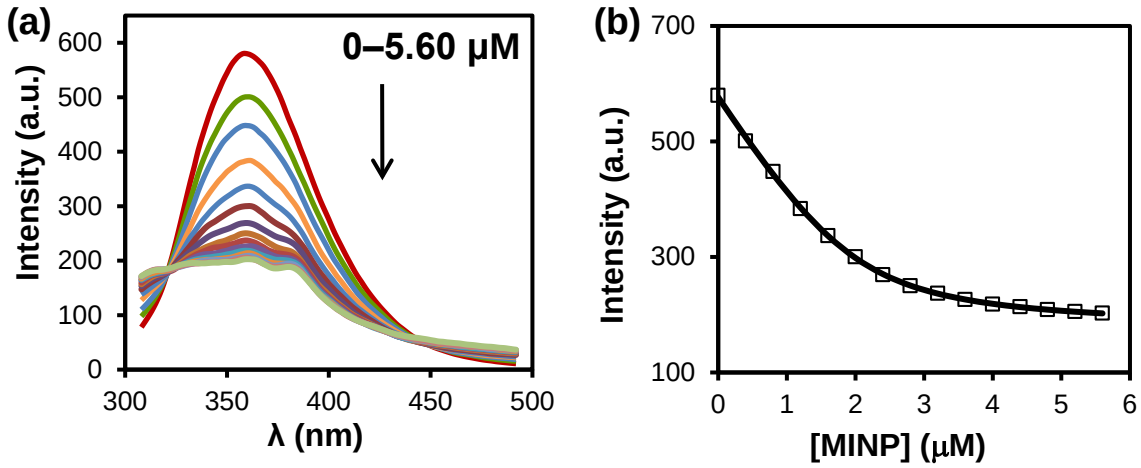

Figure S16. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KWW (2.0 μM) upon addition of different concentrations of MINP(KWW) with FM **4** (1:2) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 3 in Table 1.

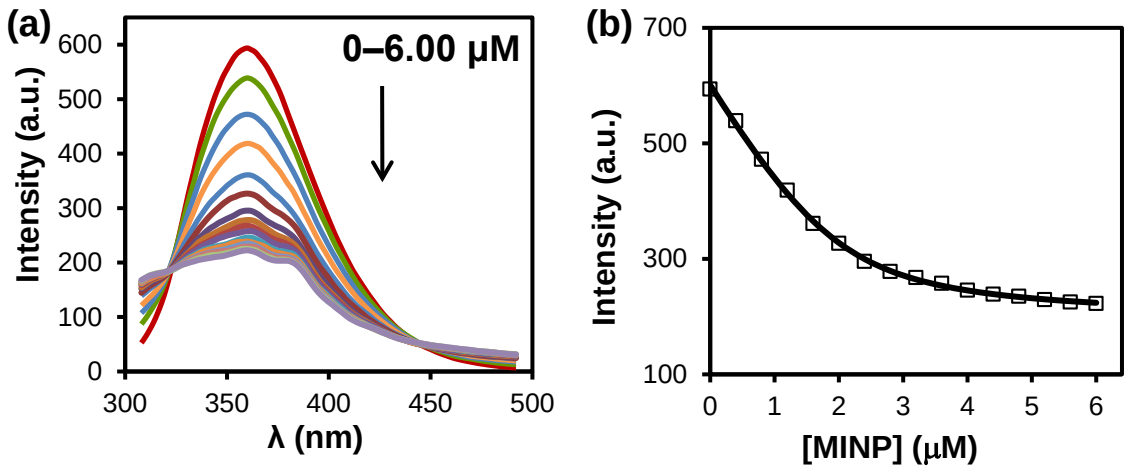

Figure S17. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KWW (2.0 µM) upon addition of different concentrations of MINP(KWW) with FM **4** (1:3) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 4 in Table 1.

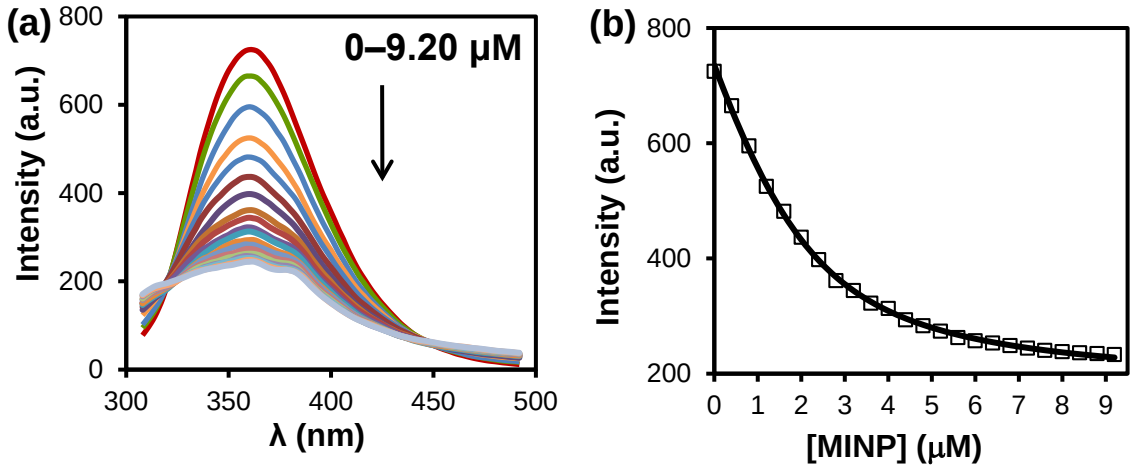

Figure S18. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WKW (2.0 µM) upon addition of different concentrations of MINP(WKW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide WKW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 11 in Table 1.

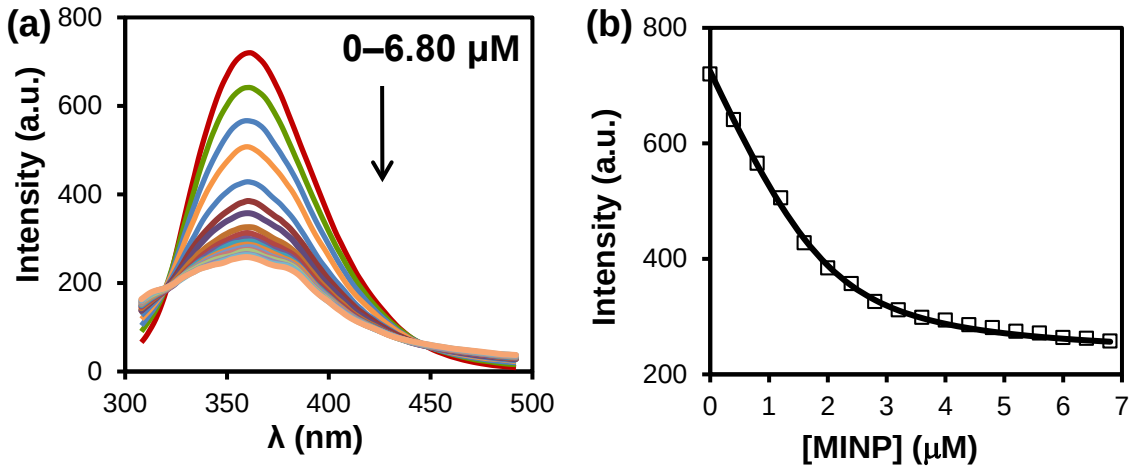

Figure S19. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WKW (2.0 μM) upon addition of different concentrations of MINP(WKW) with FM **4** (1:2) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide WKW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 12 in Table 1.

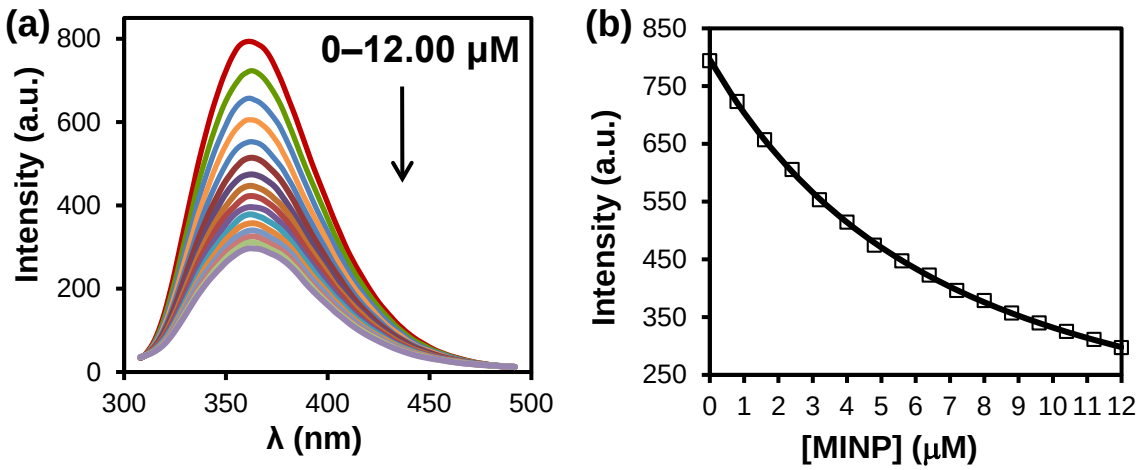

Figure S20. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KKW (2.0 μM) upon addition of different concentrations of MINP(KKW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KKW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 13 in Table 1.

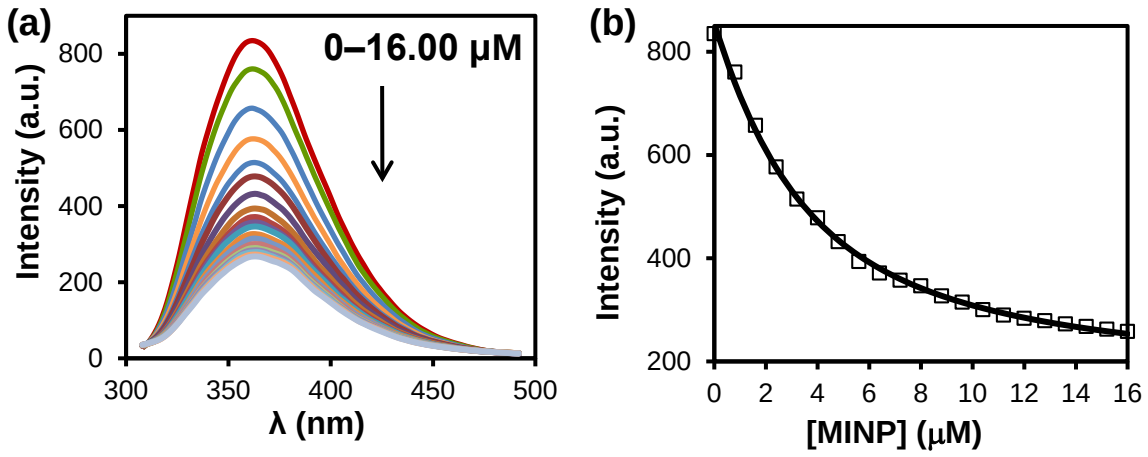

Figure S21. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KKW (2.0 μM) upon addition of different concentrations of MINP(KKW) with FM **4** (1:3) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KKW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 14 in Table 1.

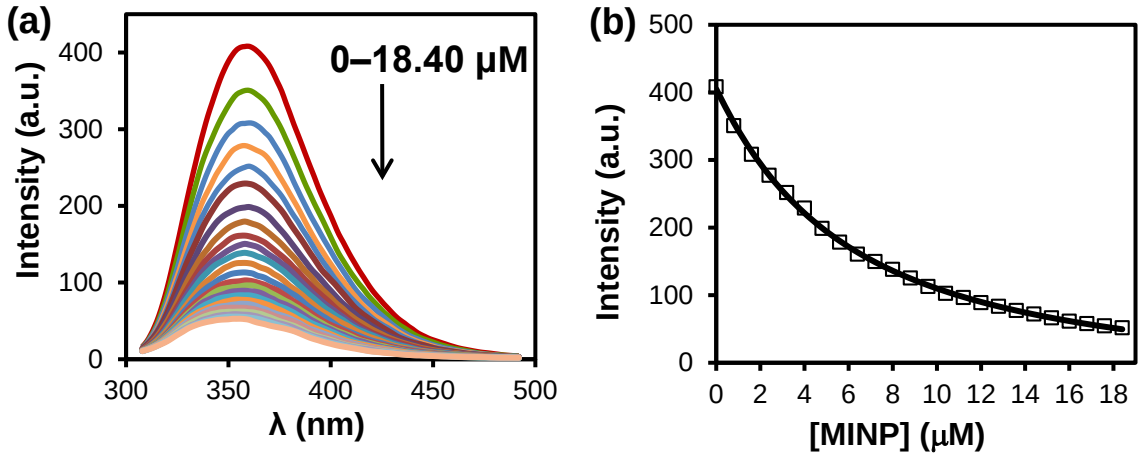

Figure S22. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WKK (2.0 μM) upon addition of different concentrations of MINP(WKK) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide WKK at 360 nm to a 1:1 binding isotherm. The data correspond to entry 15 in Table 1.

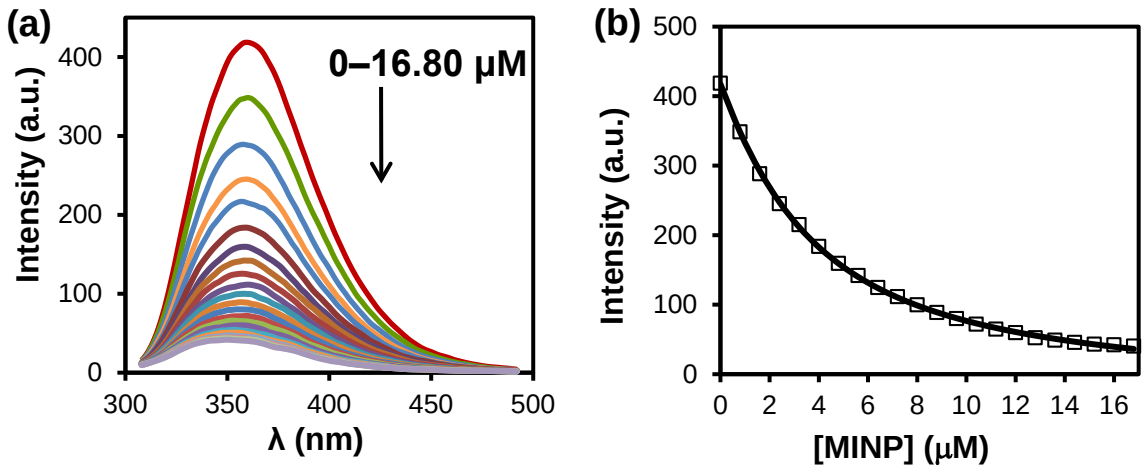

Figure S23. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WKK (2.0 μM) upon addition of different concentrations of MINP(WKK) with FM **4** (1:3) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide WKK at 360 nm to a 1:1 binding isotherm. The data correspond to entry 16 in Table 1.

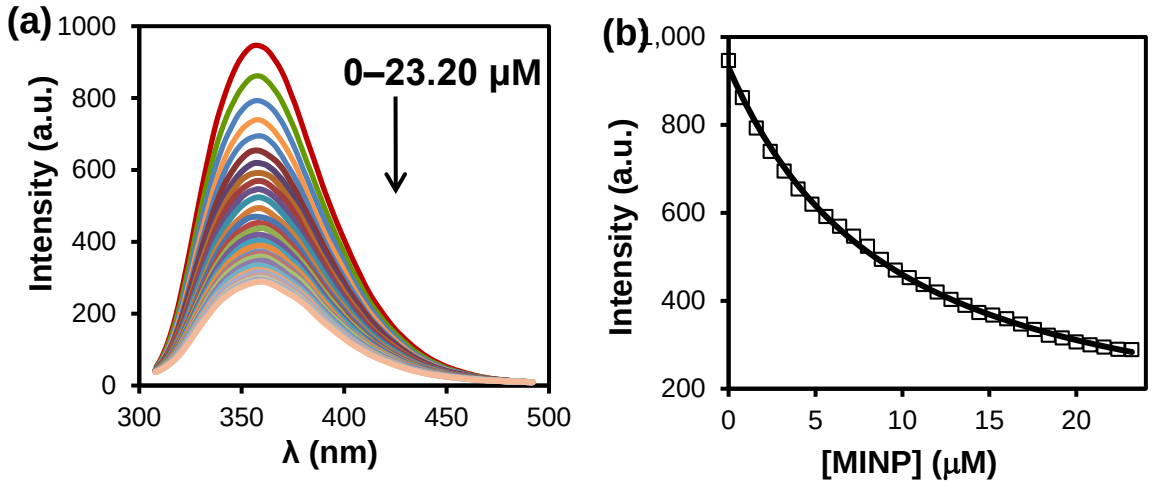

Figure S24. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KWK (2.0 μM) upon addition of different concentrations of MINP(KWK) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KWK at 358 nm to a 1:1 binding isotherm. The data correspond to entry 17 in Table 1.

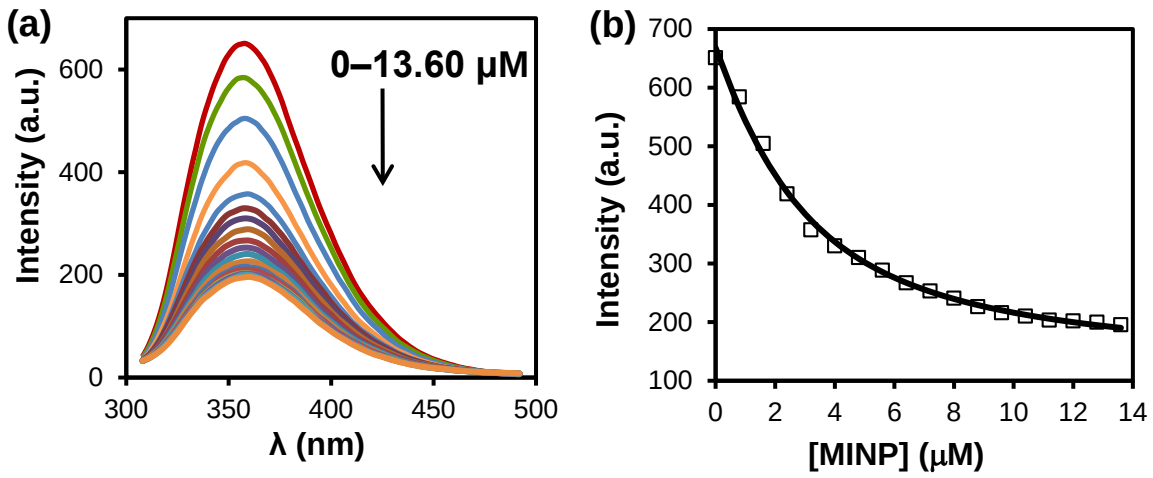

Figure S25. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KWK (2.0 μM) upon addition of different concentrations of MINP(KWK) with FM **4** (1:3) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KWK at 358 nm to a 1:1 binding isotherm. The data correspond to entry 18 in Table 1.

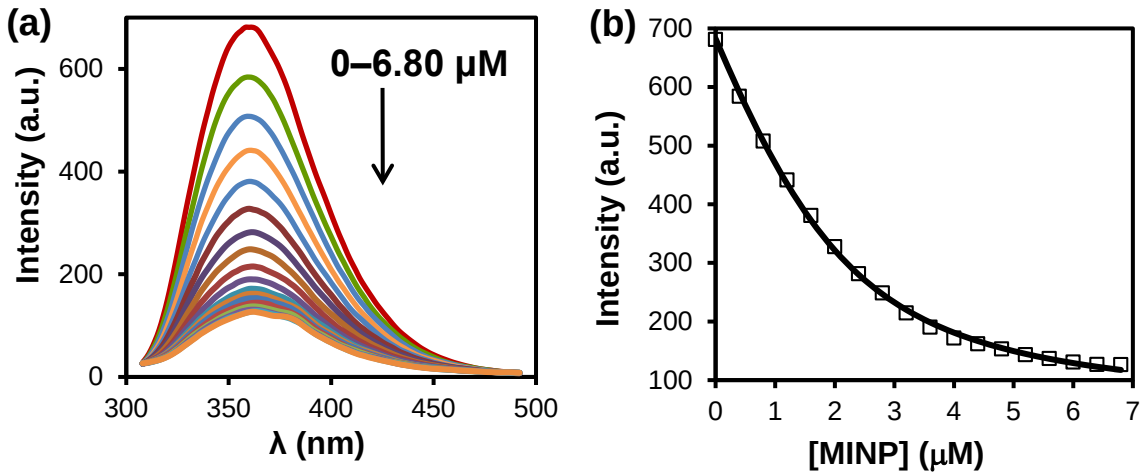

Figure S26. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide RWW (2.0 μM) upon addition of different concentrations of MINP(RWW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide RWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 19 in Table 1.

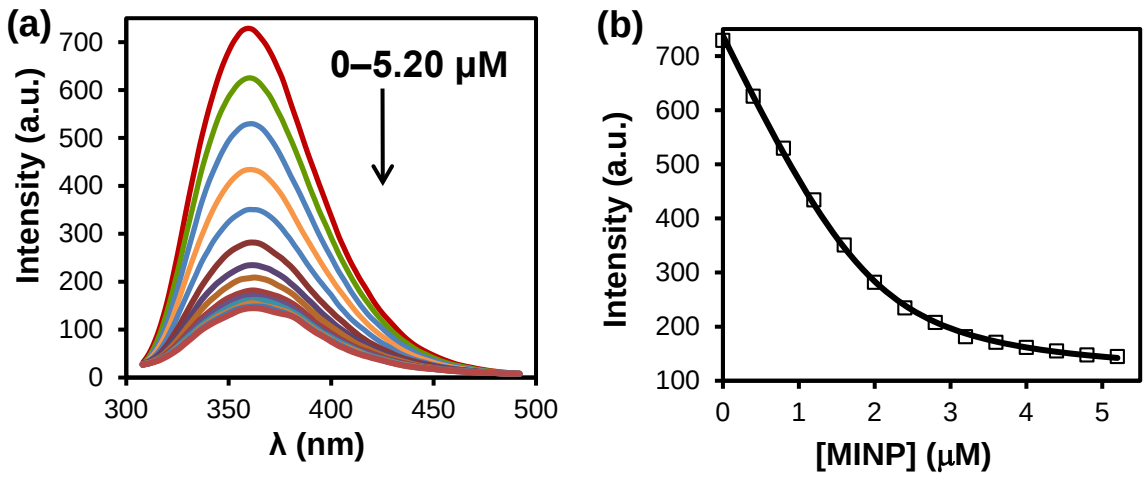

Figure S27. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide RWW (2.0 μM) upon addition of different concentrations of MINP(RWW) with FM **4** (1:2) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide RWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 20 in Table 1.

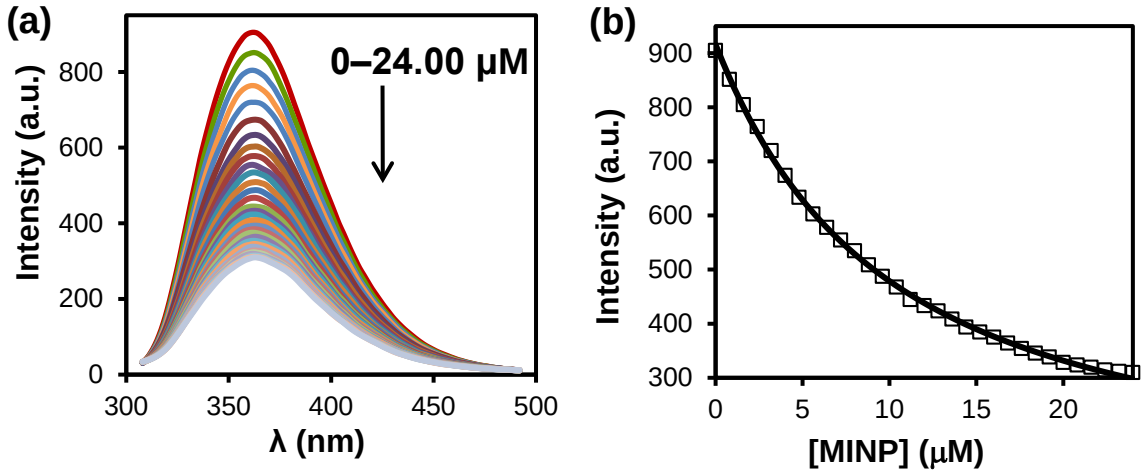

Figure S28. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide RRW (2.0 μM) upon addition of different concentrations of MINP(RRW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide RRW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 21 in Table 1.

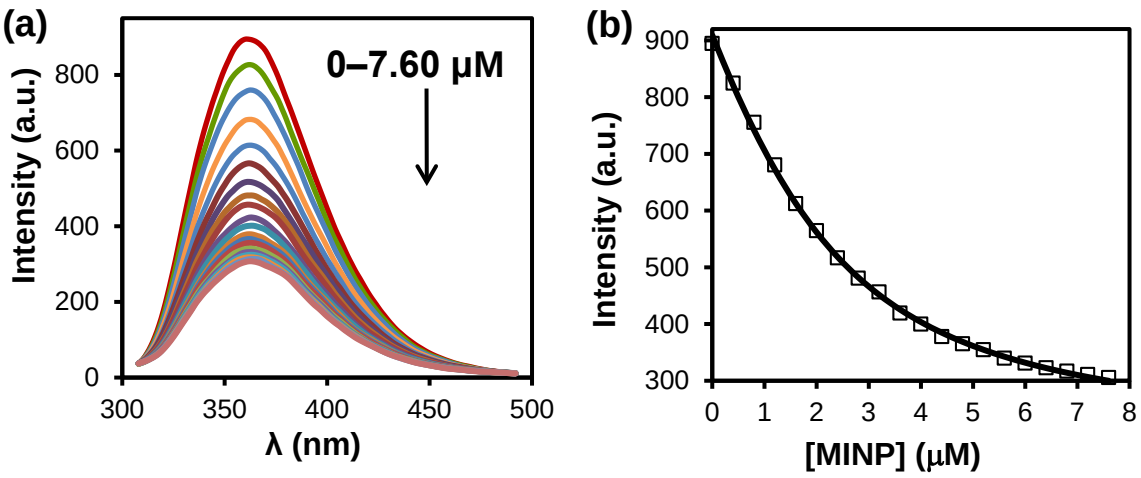

Figure S29. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide RRW (2.0 μM) upon addition of different concentrations of MINP(RRW) with FM **4** (1:3) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide RRW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 22 in Table 1.

Table S1. Binding selectivity of MINP(KWW) prepared without and with FM **4**.[a]

Entry	template	Guest	FM	K_a ($\times 10^5$ M^{-1})	K_{rel}
1	KWW	KWW	none	20.7 ± 1.7	1
2	KWW	KSW	none	3.52 ± 0.22	0.17
3	KWW	KKW	none	0.94 ± 0.03	0.05
4	KWW	KWK	none	1.01 ± 0.05	0.05
5	KWW	SWW	none	13.4 ± 0.71	0.65
6	KWW	DWW	none	9.44 ± 0.53	0.46
7	KWW	HWW	none	5.39 ± 0.26	0.26
8	KWW	QWW	none	7.38 ± 0.35	0.36
9	KWW	RWW	none	10.5 ± 0.5	0.51
10	KWW	KWW	**4**	36.7 ± 2.4	1
11	KWW	KSW	**4**	8.19 ± 0.79	0.22
12	KWW	KKW	**4**	1.92 ± 0.04	0.05
13	KWW	KWK	**4**	1.71 ± 0.09	0.05
14	KWW	SWW	**4**	8.32 ± 0.71	0.23
15	KWW	DWW	**4**	3.63 ± 0.17	0.10
16	KWW	HWW	**4**	0.69 ± 0.03	0.02
17	KWW	QWW	**4**	1.44 ± 0.02	0.04
18	KWW	RWW	**4**	34.1 ± 2.1	0.93

[a] The titrations were performed in Millipore water at 298 K. The K_a values are determined by fluorescence titration. The FM/amino group ratio was kept 1:1 in the cases with FM**4**. K_{rel} is the binding constant of other guests to that of KWW with the MINP prepared by KWW.

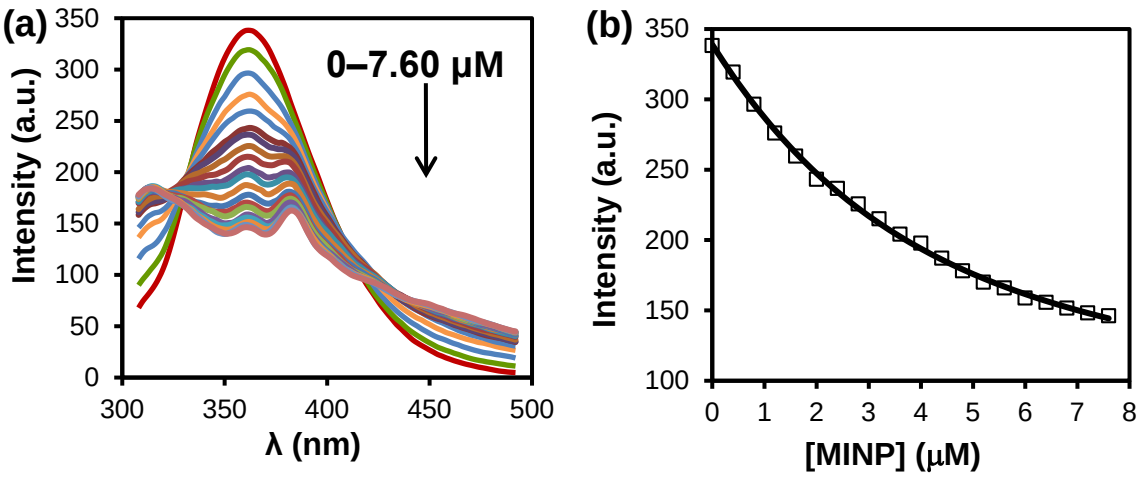

Figure S30. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KSW (2.0 μM) upon addition of different concentrations of MINP(KWW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KSW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 2 in Table S1.

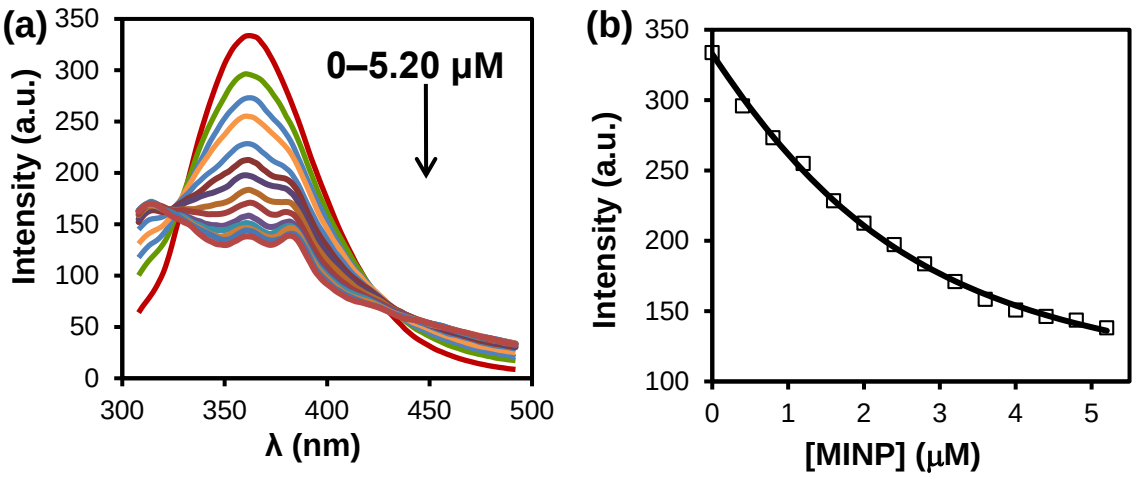

Figure S31. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KSW (2.0 μM) upon addition of different concentrations of MINP(KWW) with FM **4** (1:2) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KSW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 11 in Table S1.

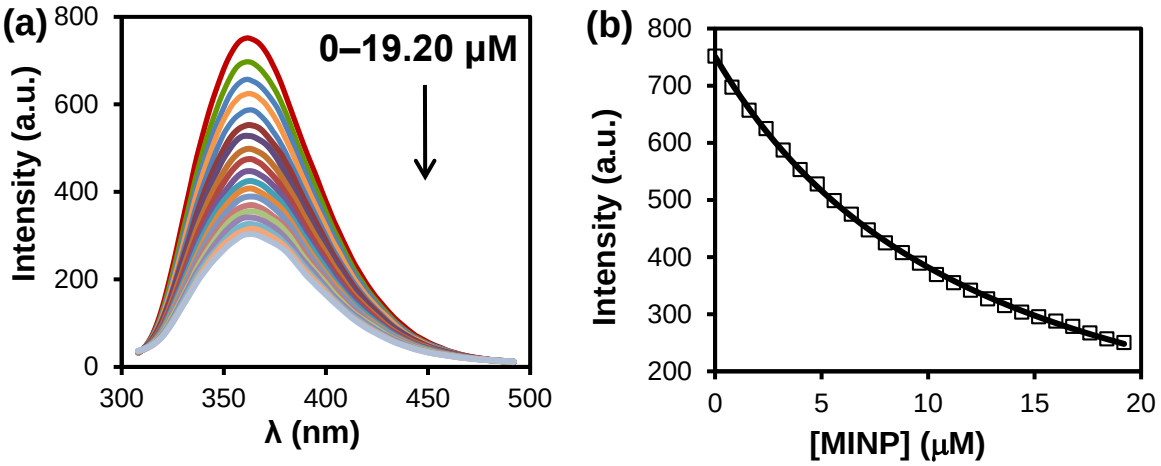

Figure S32. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KKW (2.0 μM) upon addition of different concentrations of MINP(KWW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KKW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 3 in Table S1.

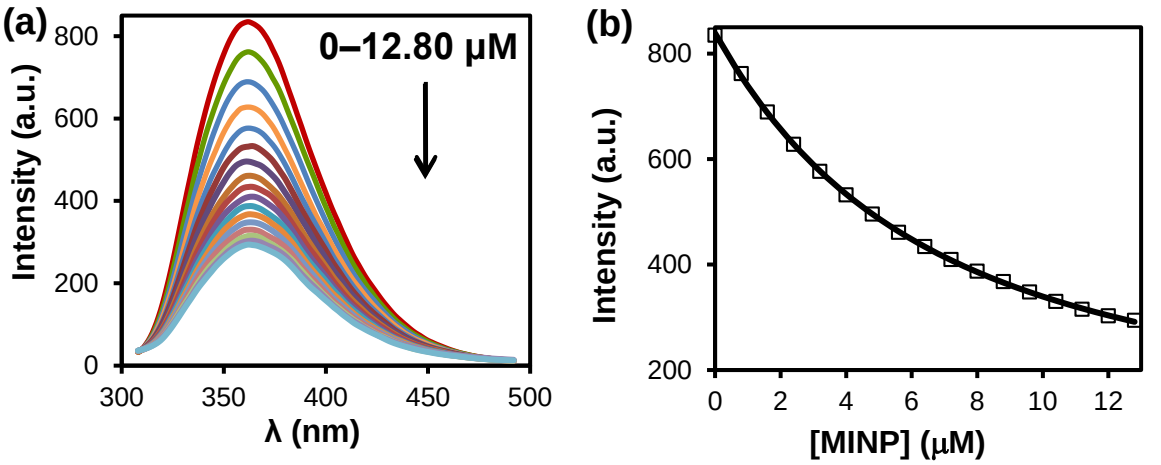

Figure S33. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KKW (2.0 μM) upon addition of different concentrations of MINP(KWW) with FM **4** (1:2) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KKW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 12 in Table S1.

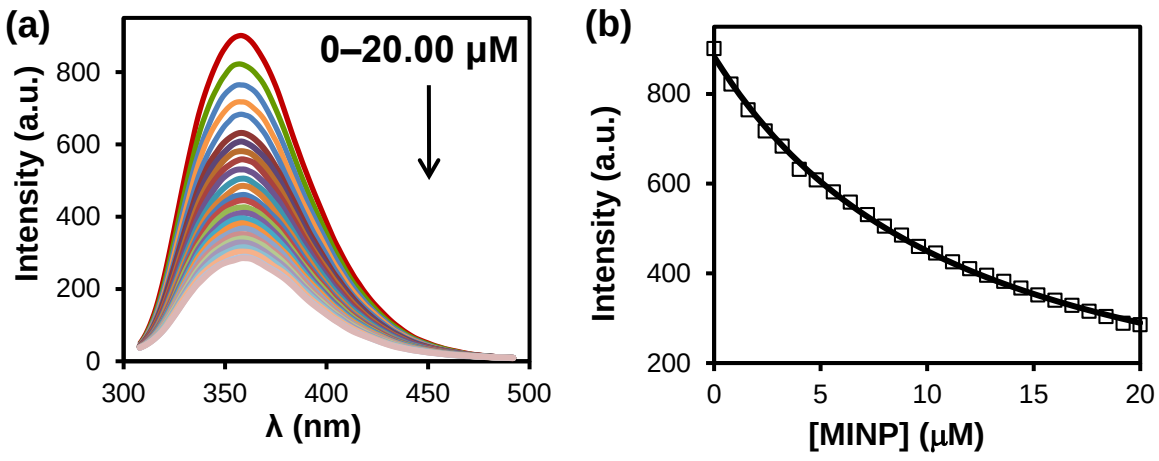

Figure S34. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KWK (2.0 μM) upon addition of different concentrations of MINP(KWW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KWK at 358 nm to a 1:1 binding isotherm. The data correspond to entry 4 in Table S1

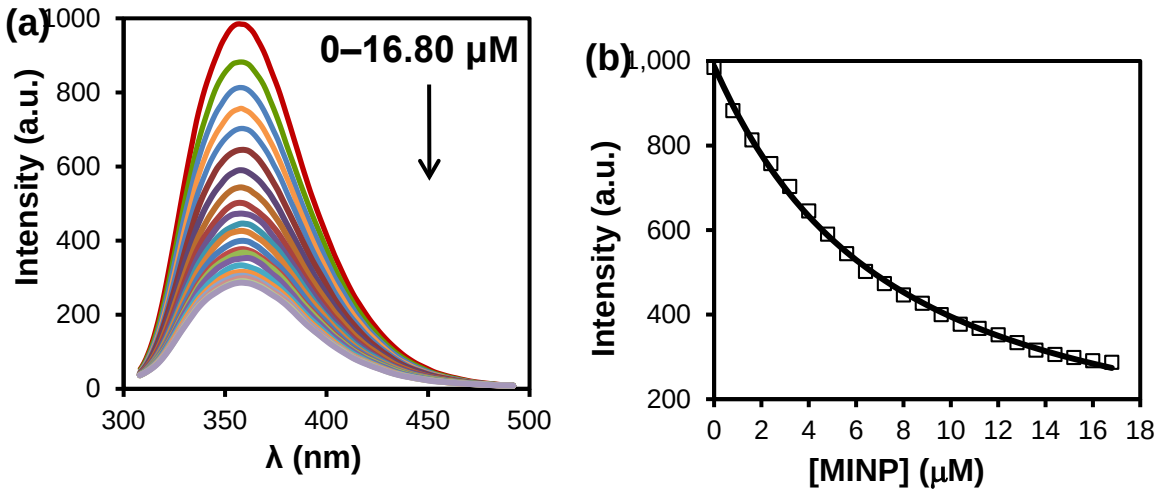

Figure S35. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KWK (2.0 μM) upon addition of different concentrations of MINP(KWW) with FM **4** (1:2) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide WNW at 358 nm to a 1:1 binding isotherm. The data correspond to entry 13 in Table S1.

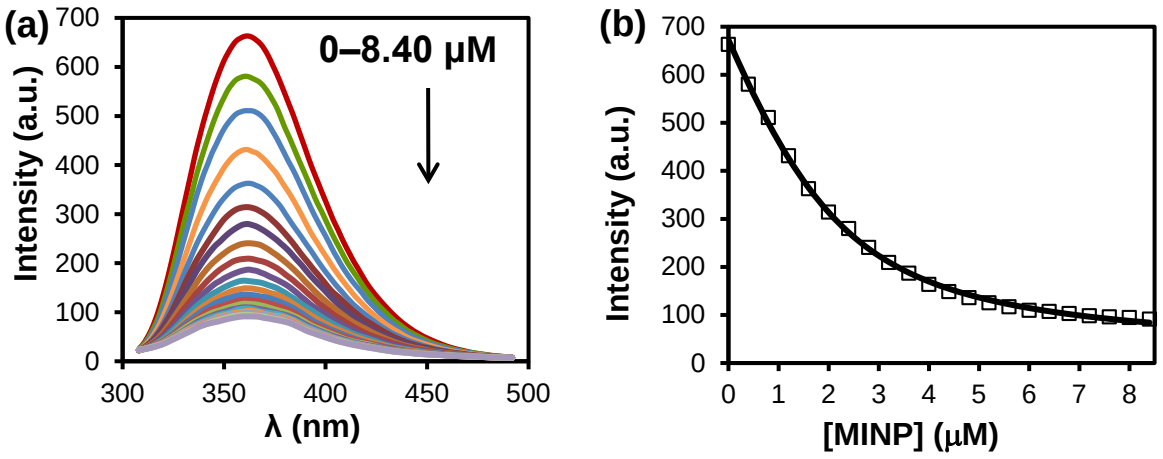

Figure S36. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide SWW (2.0 μM) upon addition of different concentrations of MINP(KWW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide SWW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 5 in Table S1.

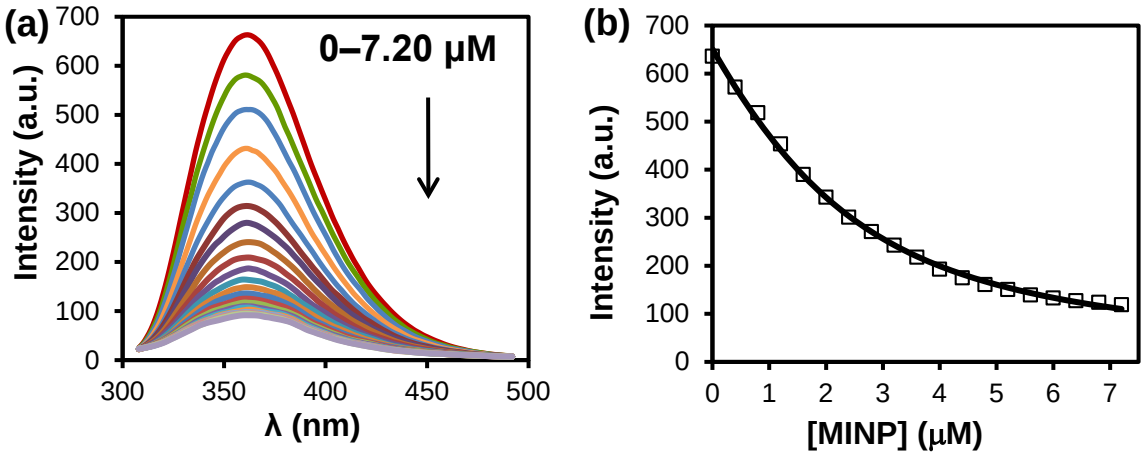

Figure S37. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide SWW (2.0 μM) upon addition of different concentrations of MINP(KWW) with FM **4** (1:2) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide SWW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 14 in Table S1.

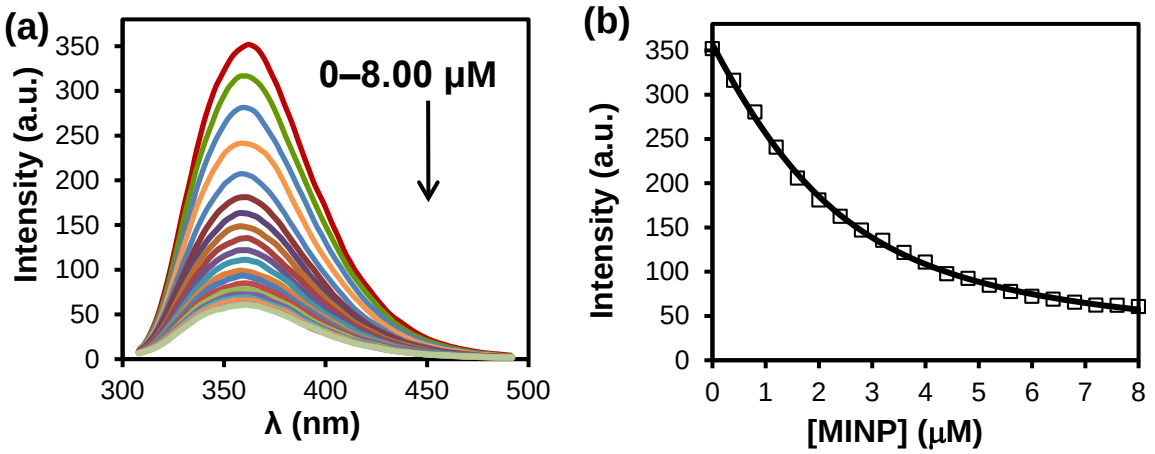

Figure S38. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide DWW (2.0 μM) upon addition of different concentrations of MINP(KWW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide DWW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 6 in Table S1.

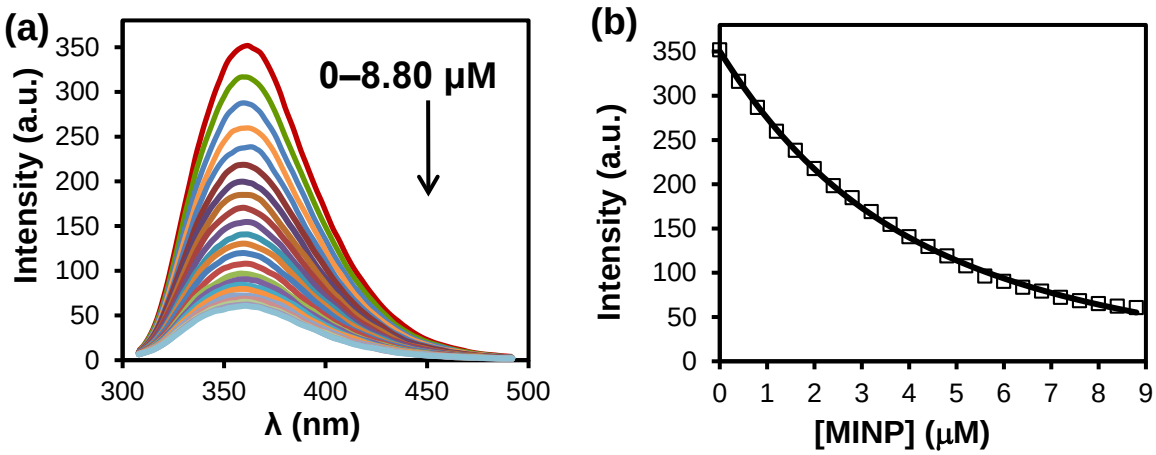

Figure S39. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide DWW (2.0 μM) upon addition of different concentrations of MINP(KWW) with FM **4** (1:2) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide DWW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 15 in Table S1.

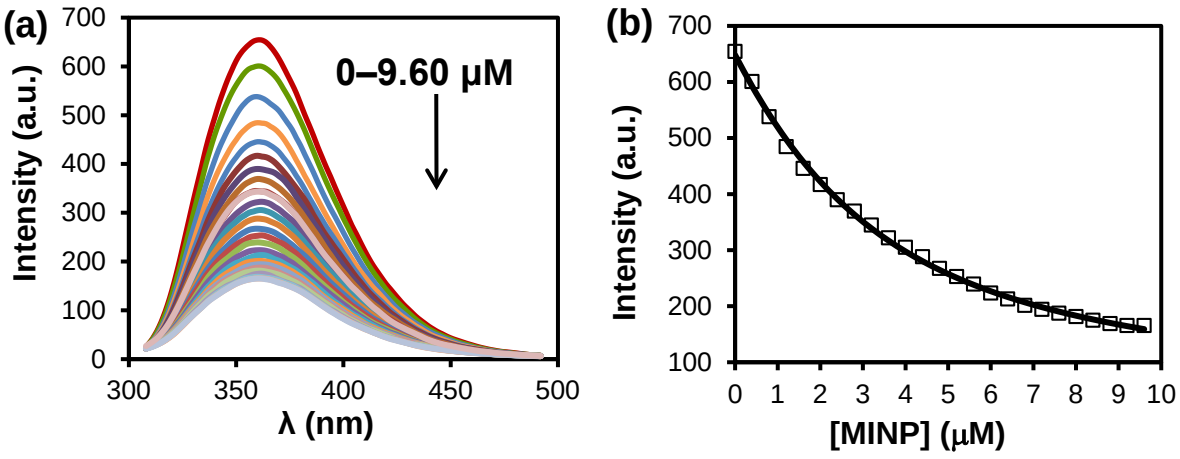

Figure S40. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide HWW (2.0 μM) upon addition of different concentrations of MINP(KWW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide HWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 7 in Table S1.

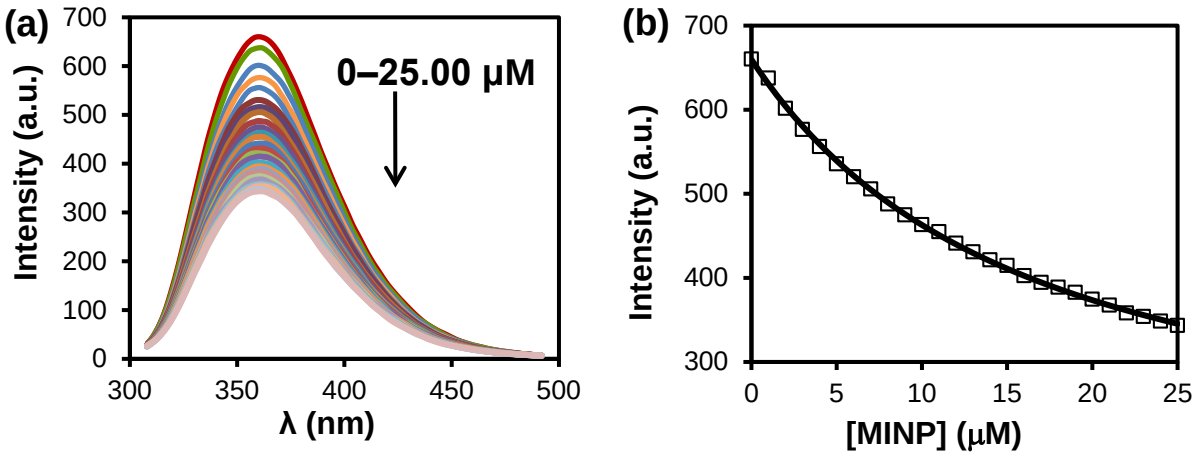

Figure S41. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide HWW (2.0 μM) upon addition of different concentrations of MINP(KWW) with FM **4** (1:2) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide HWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 16 in Table S1.

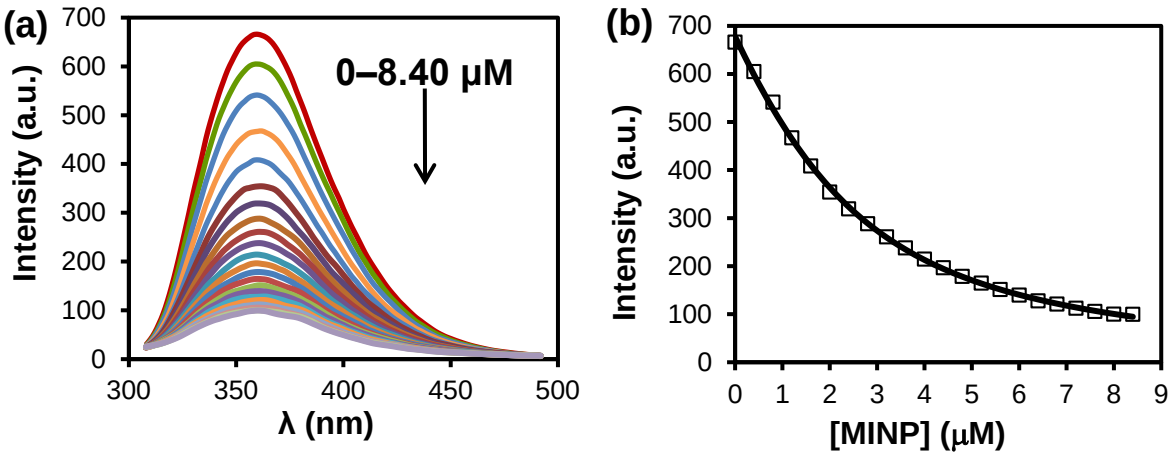

Figure S42. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide QWW (2.0 μM) upon addition of different concentrations of MINP(KWW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide QWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 8 in Table S1.

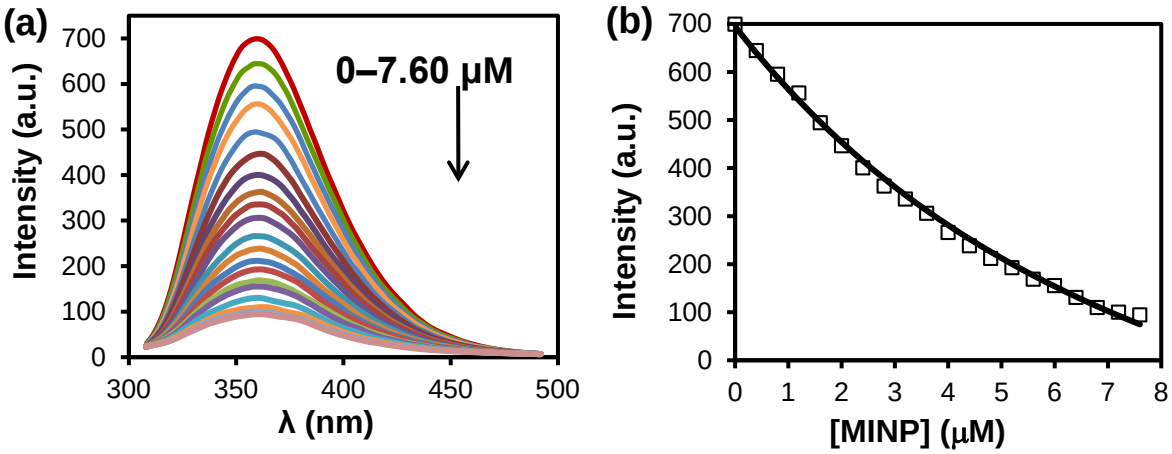

Figure S43. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide QWW (2.0 μM) upon addition of different concentrations of MINP(KWW) with FM **4** (1:2) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide QWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 17 in Table S1.

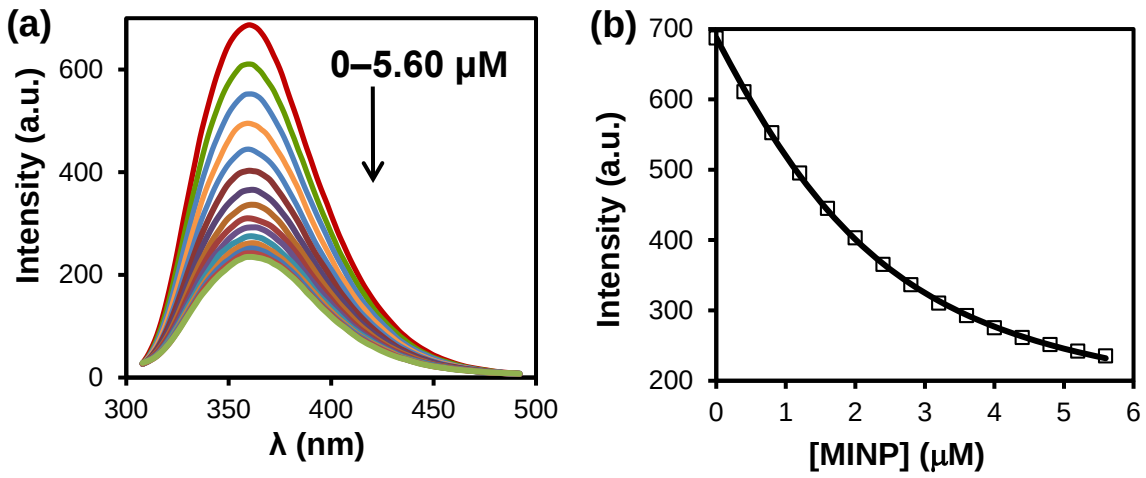

Figure S44. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide RWW (2.0 μM) upon addition of different concentrations of MINP(KWW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide RWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 9 in Table S1.

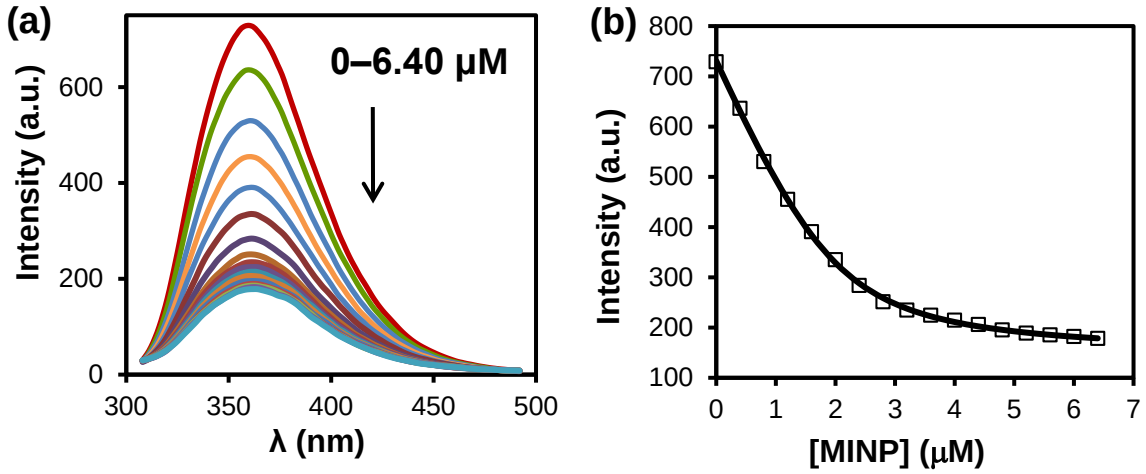

Figure S45. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide RWW (2.0 μM) upon addition of different concentrations of MINP(KWW) with FM **4** (1:2) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide RWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 18 in Table S1.

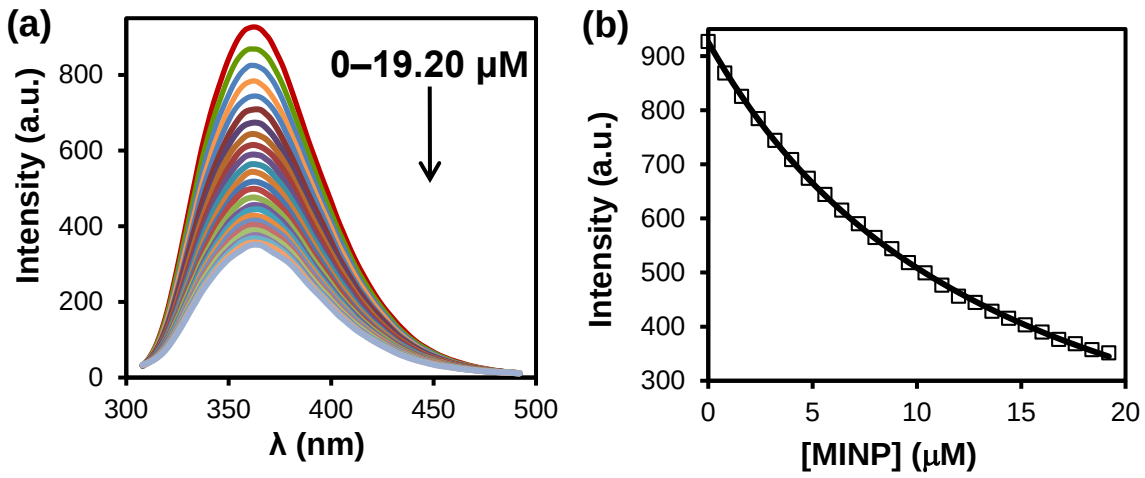

Figure S46. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide RRW (2.0 μM) upon addition of different concentrations of MINP(KKW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide RRWW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 2 in Table 3.

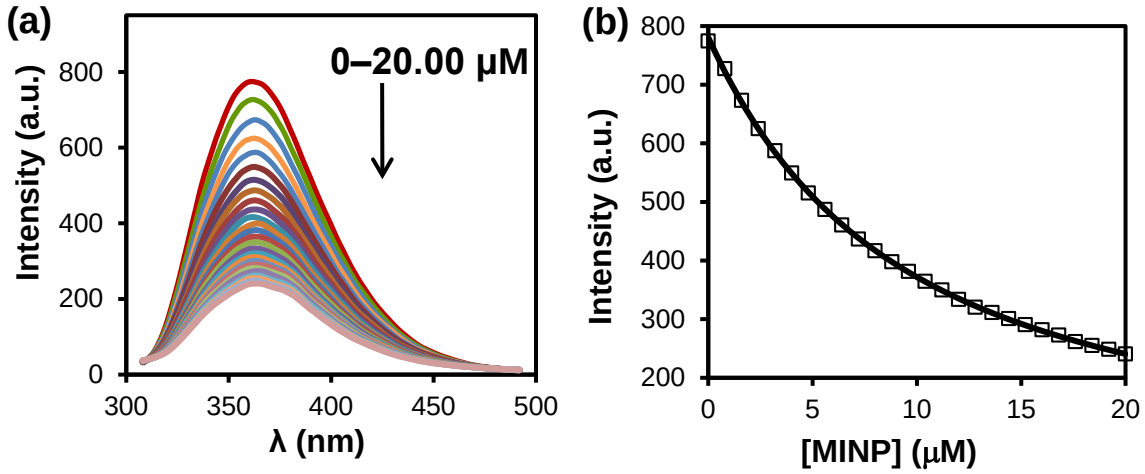

Figure S47. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KKW (2.0 μM) upon addition of different concentrations of MINP(RRW) in water. (b) Nonlinear least squares fitting of the emission intensity of peptide KKW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 4 in Table 2.

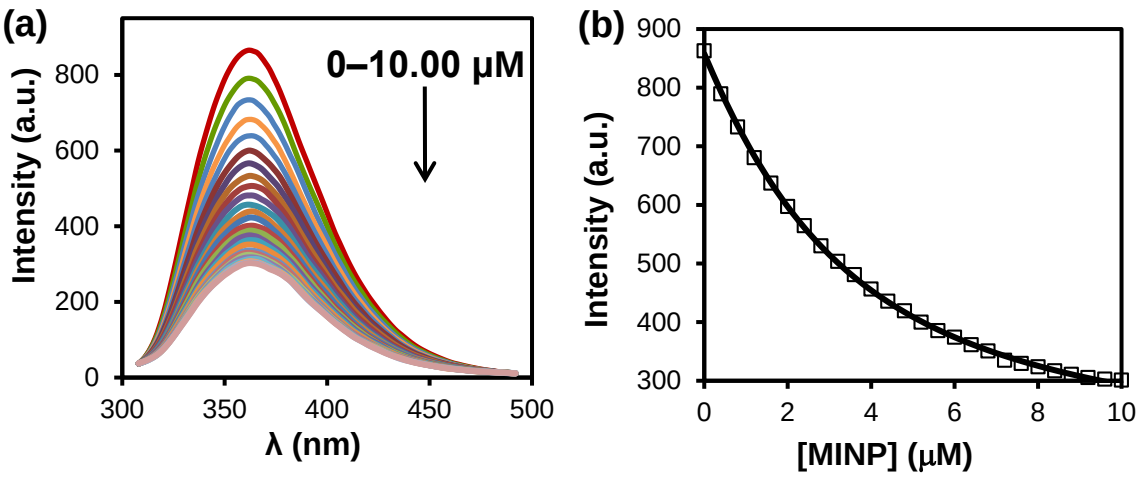

Figure S48. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide RRW (2.0 μM) upon addition of different concentrations of MINP(KKW) with FM **4** (1:3). (b) Nonlinear least squares fitting of the emission intensity of peptide RRW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 6 in Table 2.

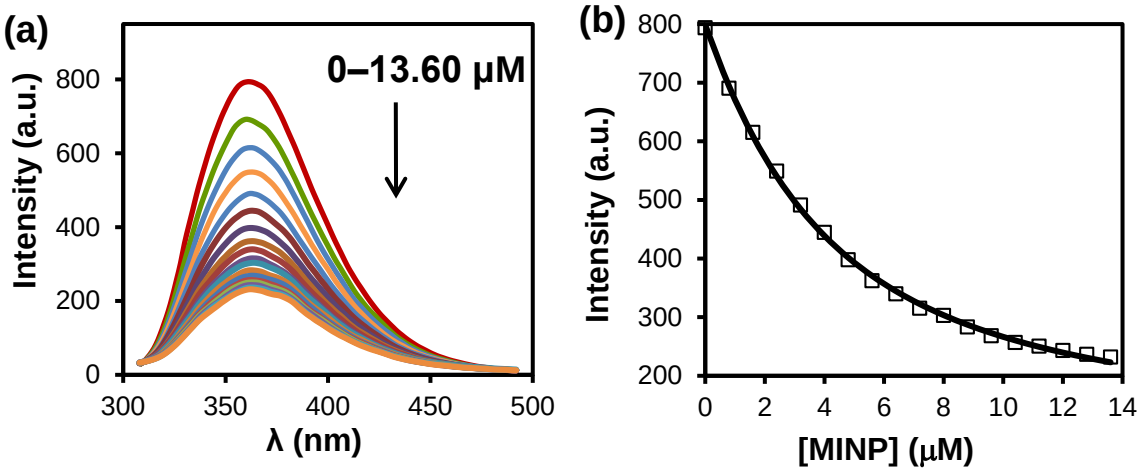

Figure S49. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide KKW (2.0 μM) upon addition of different concentrations of MINP(RRW) with FM **4** (1:3). (b) Nonlinear least squares fitting of the emission intensity of peptide KKW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 8 in Table 2.

ITC titration experiments

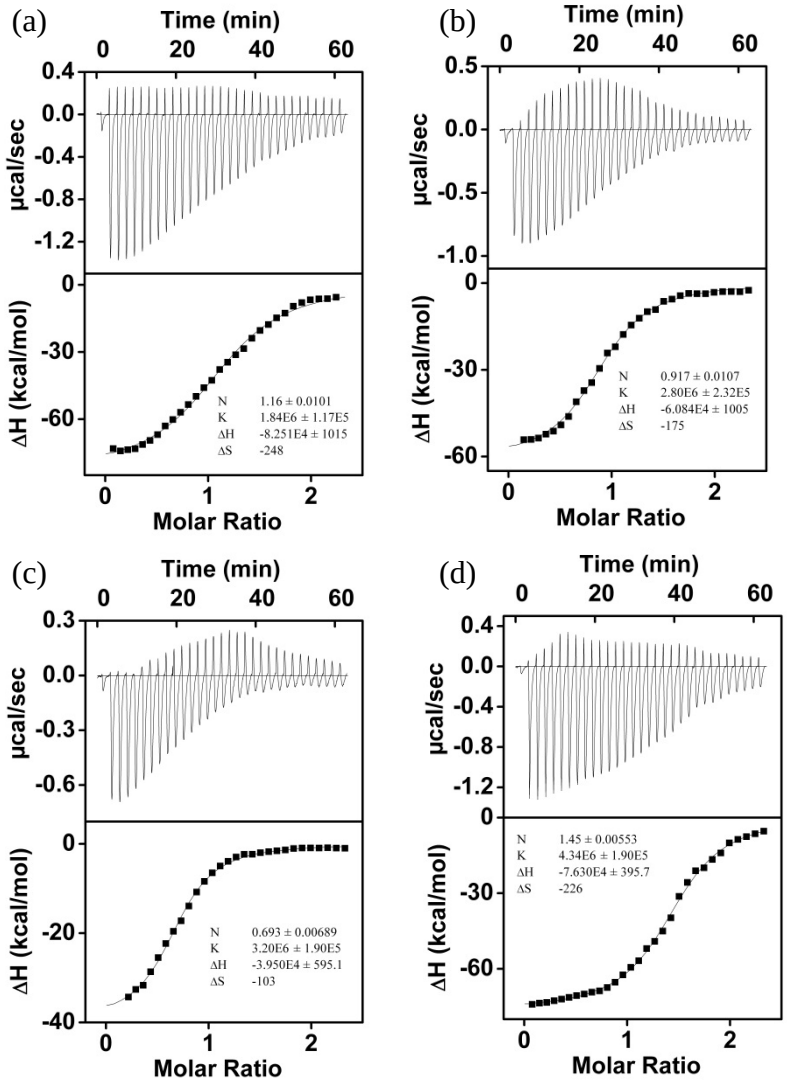

Figure S50. ITC titration curves obtained at 298 K for the titration of 5 μM of (a) MINP(KWW) without FM, (b) MINP(KWW) with FM **4** (1:1), (c) MINP(KWW) with FM **4** (1:2) and (d) MINP(KWW) with FM **4** (1:3) by peptide KWW (50 μM) in Millipore water.

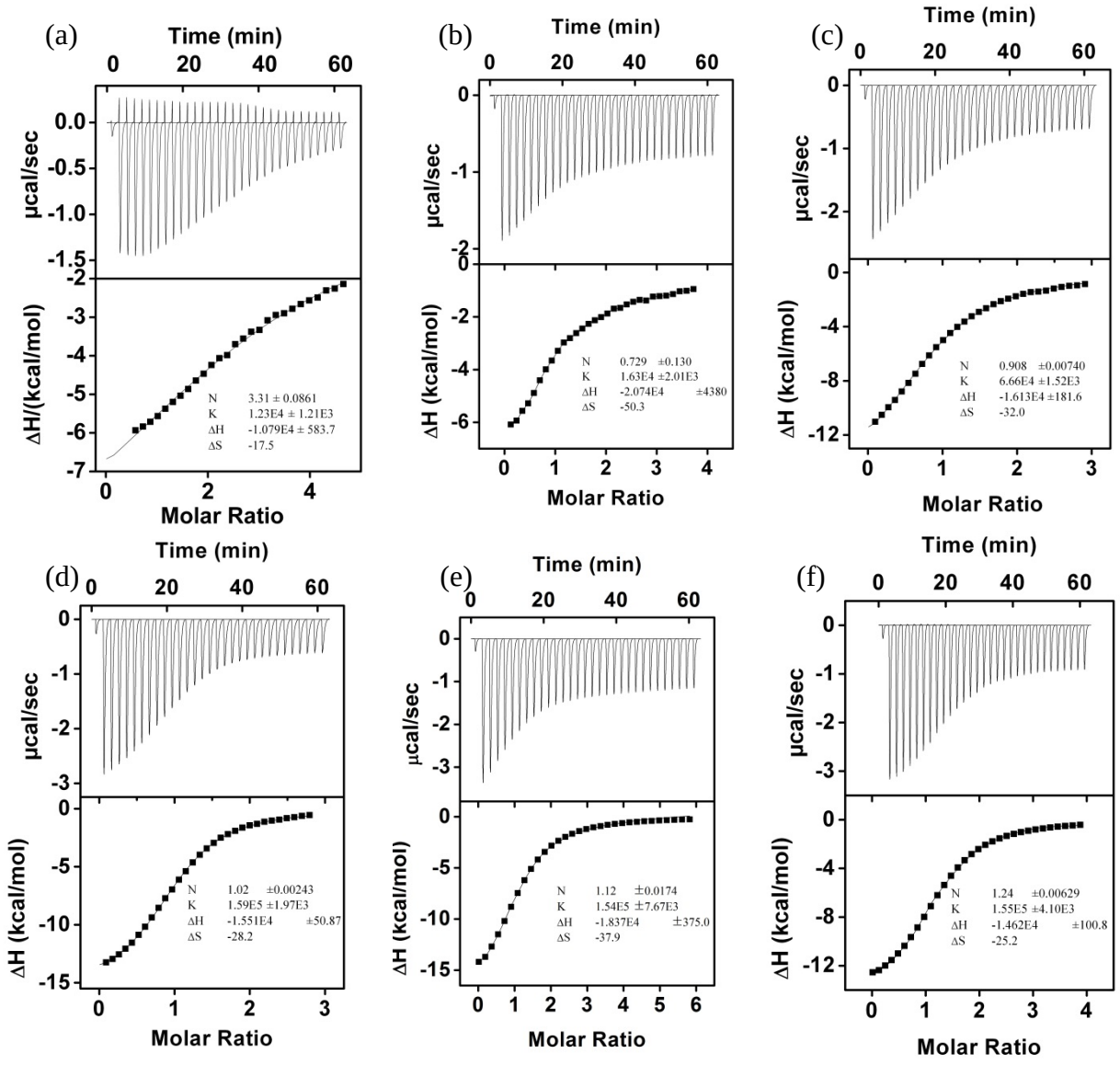

Figure S51. ITC titration curves obtained at 298 K for the titration of (a) MINP(KKK) without FM, (b) MINP(KKK) with FM **4** (1:2), (c) MINP(KKK) with FM **4** (1:3), (d) MINP(KKK) with FM **4** (1:4), (e) MINP(KKK) with FM **4** (1:5), and (f) MINP(KKK) with FM **4** (1:6) by peptide KKK in Millipore water. The concentration of MINP in all cases is 40 µM . The guest concentrations are (a) 800 µM, (b) 640 µM and (c) 500 µM, (d) 480 µM, (e) 1000 µM and (f) 670 µM, respectively. The data correspond to entries 5, 6, 7, 8, 9 10 in Table 1, respectively.

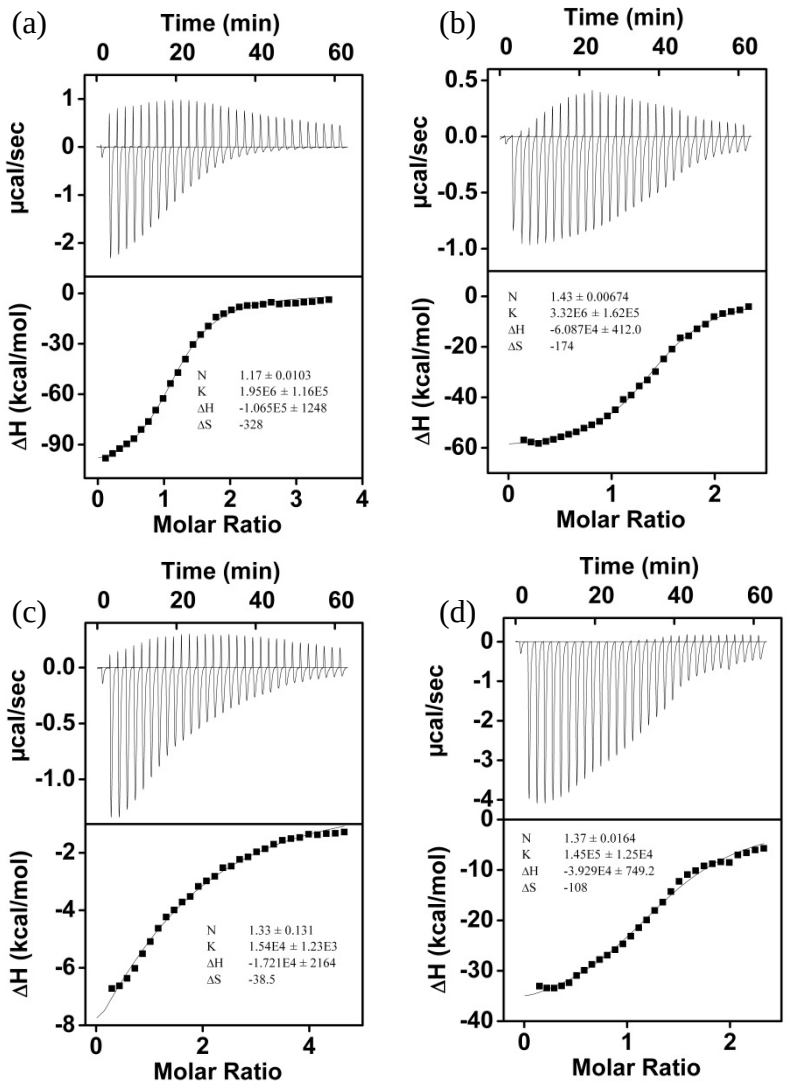

Figure S52. ITC titration curves obtained at 298 K for the titration of (a) MINP(KWW) without FM (5 μM) by peptide KWW (75 μM) , (b) MINP(KWW) with FM **4** (1:2) (5μM) by peptide KWW (50 μM), (c) MINP(KKK) without FM (40 μM) by peptide KKK (800 μM) and (d) MINP(KKK) with FM **4** (1:4) (40 μM) by peptide KKK (400 μM) in 25 mM HEPES buffer (pH 7.4).

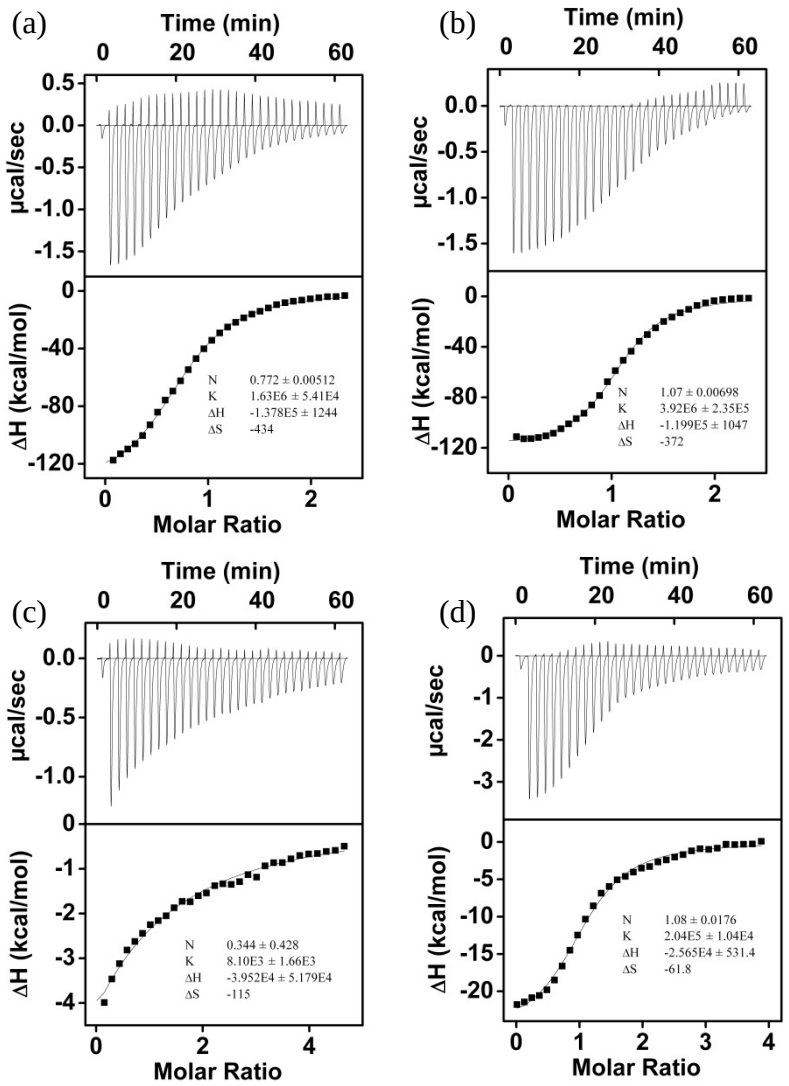

Figure S53. ITC titration curves obtained at 298 K for the titration of (a) MINP(KWW) without FM (5 μM) by peptide KWW (50 μM) , (b) MINP(KWW) with FM **4** (1:2) (5μM) by peptide KWW (50 μM), (c) MINP(KKK) without FM (40 μM) by peptide KKK (800 μM) and (d) MINP(KKK) with FM **4** (1:4) (30 μM) by peptide KKK (500 μM) in 25 mM HEPES buffer (pH 4.7).

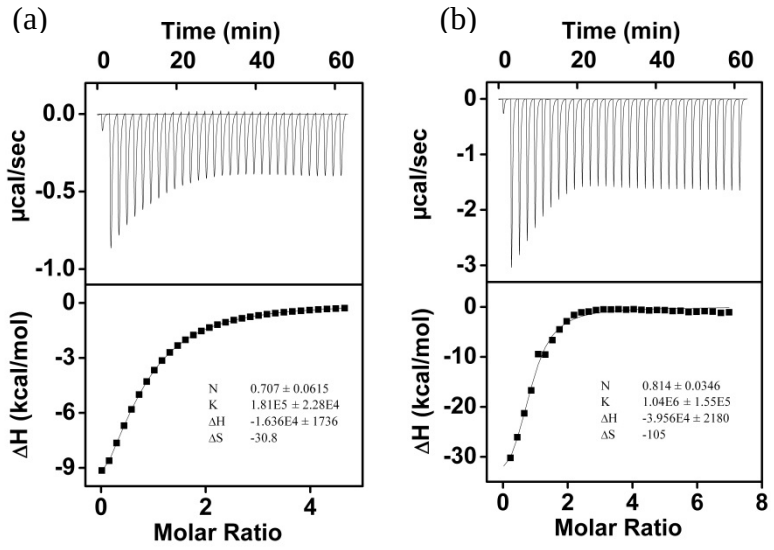

Figure S54. ITC titration curves obtained at 298 K for the titration of (a) MINP(PKKKRKV) without FM (10 µM) and (b) MINP(PKKKRKV) with FM **4** (1:6) (5µM) by peptide PKKKRKV in Millipore water. The guest concentrations are (a) 200 µM and (b) 150 µM, respectively.

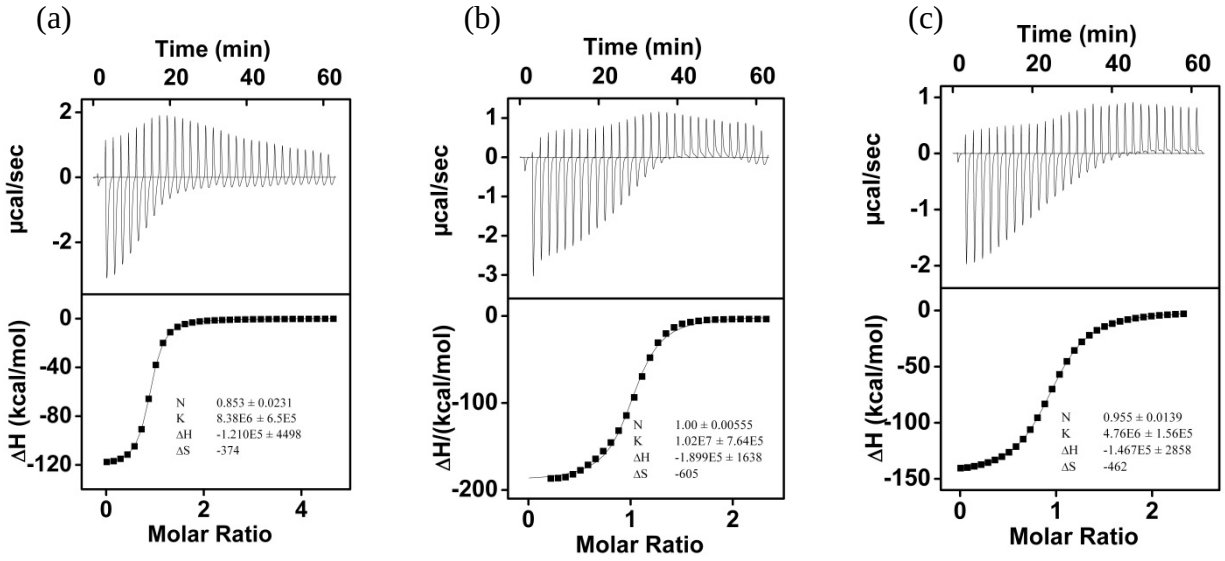

Figure S55. ITC titration curves obtained at 298 K for the titration of 5.0 µM of (a) MINP(KKALRRQETVDAL) with FM **4** (1:5) by peptide KKALRRQETVDAL (100 µM), (b) MINP(RVLSFIKGTK) with FM **4** (1:4) by peptide RVLSFIKGTK (50 µM) and (c) MINP(LRRASLG) with FM **4** (1:3) by peptide LRRASLG (50 µM) in Millipore water.

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