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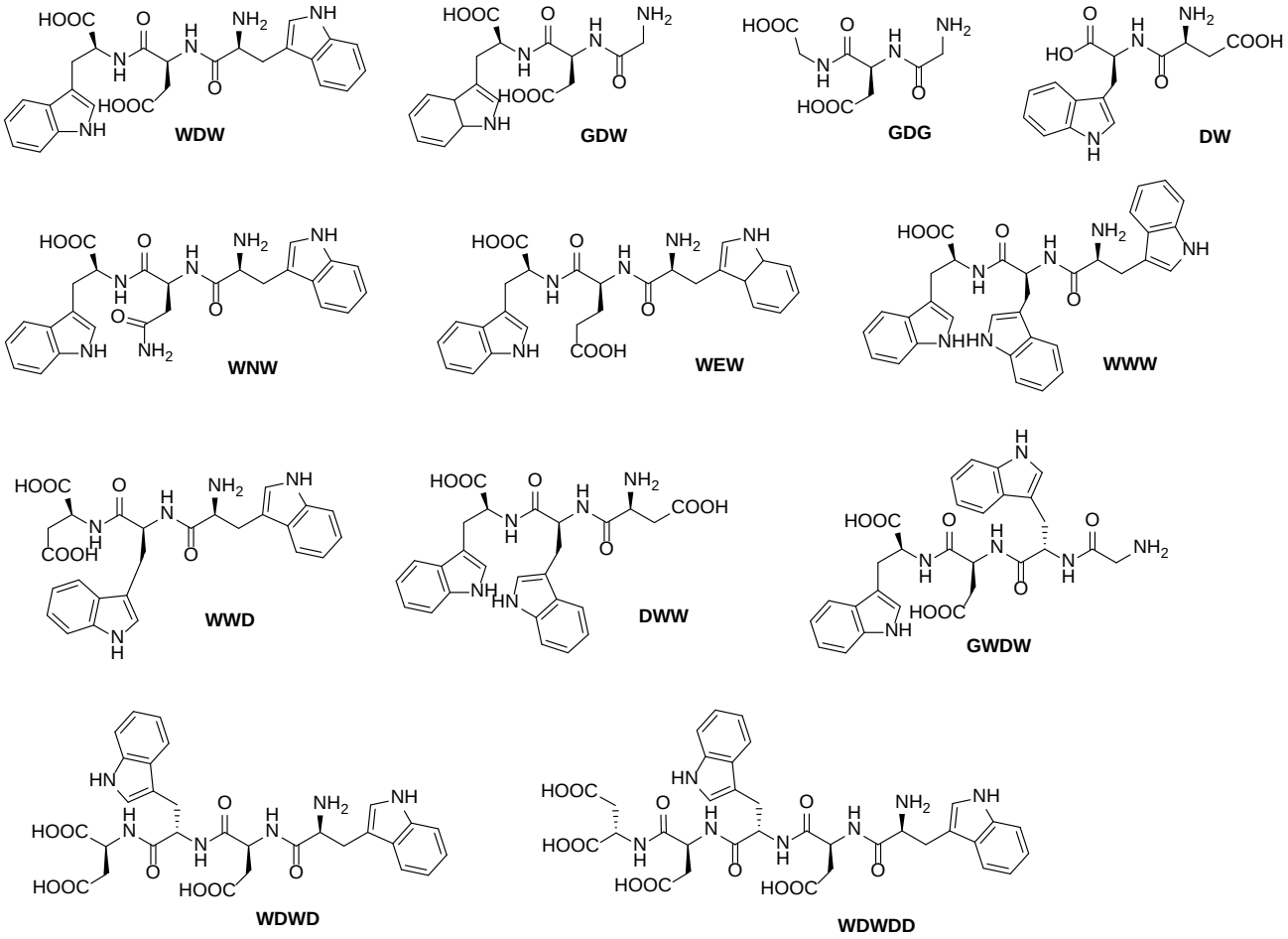
General Method

α2β1 integrin ligand peptide (DGEA), c-Myc peptide, DYKDDDDK peptide and HIF-1 alpha (556-574) peptide 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 Bruker DRX-400, on a Bruker AV III 600 or 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

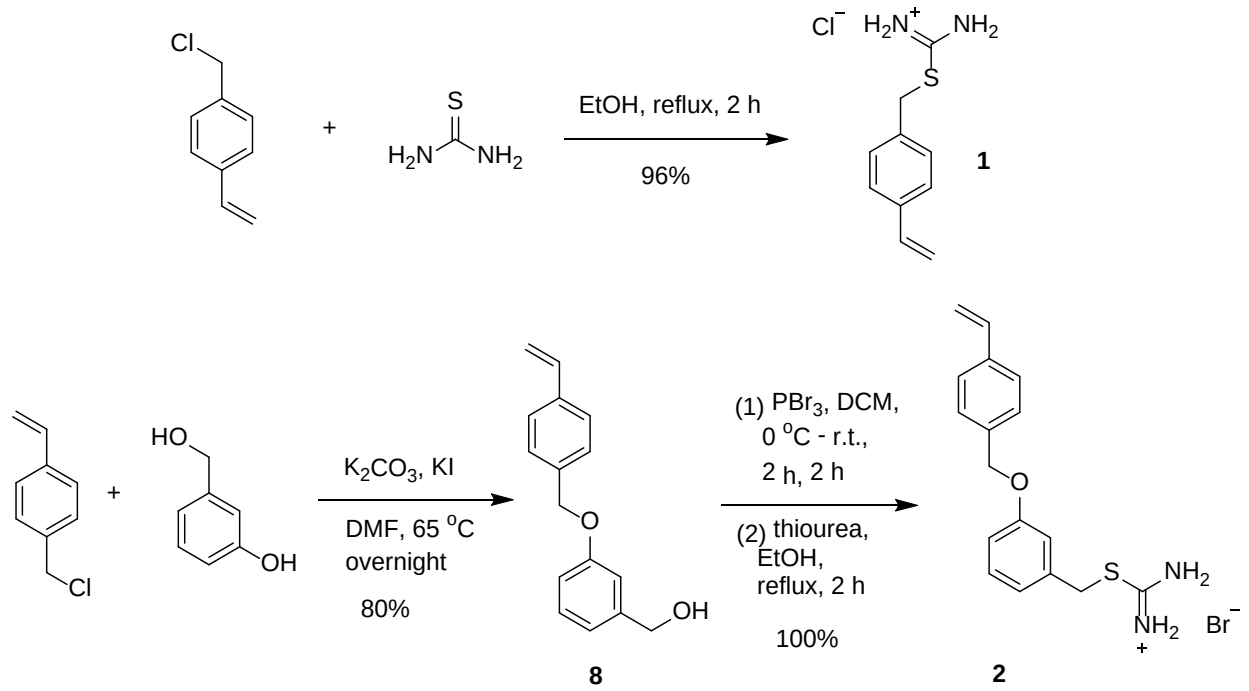
temperature on a Varian Cary Eclipse Fluorescence spectrophotometer. The binding constants were calculated by curve fitting using KaleidaGraph to the binding equation $F_{obs} = f_0 \times C_0 + 0.5 \times (f_{saturated} - f_0) \times (C_0 + C_{MINP} + 1/K_a - ((C_0 + C_{MINP} + 1/K_a)^2 - 4 \times C_0 \times C_{MINP})^{0.5})$, in which F_{obs} is the observed fluorescence intensity of the peptide during titration, f_0 the molar emission intensity of the peptide in the absence of the MINP receptor, $f_{saturated}$ the molar emission intensity of the peptide upon saturation by the MINP receptor, C_0 the total concentration of the peptide, and C_{MINP} the concentration of MINP added. [1] Isothermal titration calorimetry (ITC) was performed using a MicroCal VP-ITC Microcalorimeter with Origin 7 software and VPViewer2000 (GE Healthcare, Northampton, MA).

Chart S1. Structures of peptides used in study.



[1] Schneider, H.-J.; Yatsimirsky, A. K.: *Principles and Methods in Supramolecular Chemistry*; Wiley: New York, 2000.

Scheme S1



Syntheses

Syntheses of compounds **3**–**5**[2] and **6**–**7**[3] were previously reported.

Compound 1. 4-Vinylbenzyl chloride (3.66 g, 24 mmol) and thiourea (1.52 g, 20 mmol) in ethanol (10 mL) were heated to reflux for 2 h. Ethanol was removed under reduced pressure and the resulting yellow solid was washed with ether (3 × 30 mL). The resulting off-white solid was dissolved in methanol and crystallized from a methanol/methylene chloride mixture to get the pure product as a white solid (4.38 g, 96%).[4] ^{1}H NMR (400 MHz, CD_3OD, δ): 7.48 (d, J = 8.4 Hz, 2H), 7.42 (d, J = 8.4 Hz, 2H), 6.77 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1H), 5.84 (dd, J_1 = 17.6 Hz, J_2 = 0.8 Hz, 1H), 5.30 (dd, J_1 = 10.8 Hz, J_2 = 0.8 Hz, 1H), 4.91 (s, 4H), 4.46 (s, 2H) ppm. ^{13}C NMR (100 MHz, CD_3OD, δ): 171.8, 139.4, 138.7, 137.5, 131.9, 129.1, 117.4, 36.5 ppm. ESI - HRMS calcd for $C_{10}H_{13}N_2SCl$ (*m/z*): $[M - Cl]^+$, 193.0794; found, 193.0791.

[2] Awino, J. K.; Zhao, Y. *J. Am. Chem. Soc.* **2013**, *135*, 12552.
[3] Arifuzzaman, M. D.; Zhao, Y. *J. Org. Chem.* **2016**, *81*, 7518.
[4] Ingham, R. J.; Rive, E.; Nikbin, N.; Baxendale, I. R.; Ley, S. V. *Org. Lett.*, **2012**, *14*, 3920.

Compound 8. To a solution of 4-vinylbenzyl chloride (1.53 g, 10 mmol) in DMF (20 mL), potassium carbonate (2.76 g, 20 mmol), potassium iodide (166 mg, 1 mmol) and 3-(hydroxymethyl)phenol (1.24 g, 10 mmol) were added slowly. The reaction mixture was stirred at 65 °C overnight, then poured into water (50 mL) and extracted with EA (3 × 30 mL). The organic phase was combined and washed with brine (2 × 30 mL), dried over sodium sulfate, filtered, and concentrated by rotary evaporation. The residue was purified by column chromatography over silica gel using 1: 30 methanol/ methylene chloride as eluent to afford compound **8** as a colorless oil (1.93 g, 80 %). ^{1}H NMR (400 MHz, CCl_3D, δ): 7.44 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.27 (t, *J* = 8.0 Hz, 1H), 7.01 (s, 1H), 6.95 (d, *J* = 7.2 Hz, 2H), 6.91 (dd, J_1 = 8.0 Hz, J_2 = 2.4 Hz, 1H), 6.73 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1H), 5.77 (dd, J_1 = 17.6 Hz, J_2 = 1.2 Hz, 1H), 5.27 (dd, J_1 = 10.8 Hz, J_2 = 1.2 Hz, 1H), 5.06 (s, 2H), 4.65 (s, 2H) ppm. ^{13}C NMR (100 MHz, CCl_3D, δ): 159.0, 142.6, 137.3, 136.5, 136.4, 129.6, 127.7, 126.4, 119.4, 114.11, 114.10, 113.2, 69.7, 65.2 ppm. ESI - HRMS calcd for $C_{16}H_{16}O_2$ (*m/z*): $[M - H]^-$, 239.1078; found, 239.1081.

Compound 2. To a solution of **8** (721 mg, 3 mmol) in dry methylene chloride (15 mL) at 0 °C, phosphorus tribromide (313 μL, 3.3 mmol) was added dropwise. The reaction mixture was stirred at 0 °C for 2 hours, and warmed to room temperature. After stirred for another 2 hours, the reaction mixture was quenched by the addition of crushed ice. The bi-phasic mixture was transferred into a 100 mL separatory funnel. The layers were separated and the aqueous layer was extracted with ethyl ether (3 × 20 mL). The organic phase was combined, dried over sodium sulfate, filtered, and concentrated by rotary evaporation to give the benzyl bromide as a colorless oil (828 mg, 91 %). This oil (152 mg, 0.5 mmol) was dissolved in ethanol (10 mL), and thiourea (46 mg, 0.6 mmol) was added. The reaction mixture was heated to reflux for 2 hours. Ethanol was removed under reduced pressure. The resulting yellow solid was washed with ether (3 × 10 mL) and crystallized from a methanol/methylene chloride mixture to get the pure product as a white solid (189 mg, 100%). ^{1}H NMR (400 MHz, DMSO-d_6, δ): 9.12 (br, 4H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.29 (t, *J* = 8.0 Hz, 1H), 7.10 (s, 1H), 7.03-6.93 (m, 2H), 6.74 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1H), 5.85 (d, *J* = 17.6 Hz, 1H), 5.27 (d, *J* = 10.8 Hz, 1H), 5.09 (s, 2H), 4.47 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6, δ): 169.4, 158.9, 137.2, 137.0, 136.9, 136.7, 130.4, 128.5, 126.7, 121.8, 116.1, 115.0, 114.5, 69.4, 34.6 ppm. ESI - HRMS calcd for $C_{17}H_{19}BrN_2OS$ (*m/z*): $[M - Br]^+$, 299.1213; found, 299.1214.

Typical procedure for the synthesis of Functionalized MINPs.

(a) Preparation of the functional monomer-template complex: functional monomer **1** in methanol (75 μL of a 7.3 mg/2 mL solution, 0.0012 mmol**)** and template **WDW** in methanol (25μL of an 8.1

mg/mL solution, 0.0004 mmol) were added in a small vial with 100 μL of methylene chloride. The mixture was stirred for 2 hours, and then the solvent was evaporated under *vacuo*.

(b) Preparation of MINP: a micellar solution of surfactant **3** (9.3 mg, 0.02 mmol) in H_2O (2.0 mL) was added to the above complex, followed by the addition of DVB (2.8 μL, 0.02 mmol), and DMPA in DMSO (10 μL of a 12.8 mg/mL solution, 0.0005mmol). The mixture was subjected to ultrasonication for 10 min before cross-linker **4** (4.1 mg, 0.024mmol), $CuCl_2$ in H_2O (10 μL of 6.7 mg/mL solution, 0.0005 mmol), and sodium ascorbate in H_2O (10 μL of 99 mg/mL solution, 0.005 mmol) were added. After the reaction mixture was stirred slowly at room temperature for 12 hours, linear sugar **5** (10.6 mg, 0.04 mmol), $CuCl_2$ in H_2O (10 μL of 6.7 mg/mL solution, 0.0005 mmol), and sodium ascorbate in H_2O (10 μL of 99 mg/mL solution, 0.005 mmol) were added. The mixture was stirred at room temperature for another 6 hours, purged with nitrogen for 15 min, sealed with a rubber stopper, and irradiated in a Rayonet reactor for 12 hours. The progress of reaction could be monitored by ^1H NMR spectroscopy and dynamic light scattering (DLS). The reaction mixture was poured into acetone (8 mL). The precipitate collected by centrifugation was washed with a mixture of acetone/water (5 mL/1 mL) three times, followed by methanol/acetic acid (5 mL/0.1 mL) three times. The solid was then rinsed two times with acetone (5 mL) and dried in air to afford the final MINPs. Typical yields were >80%.

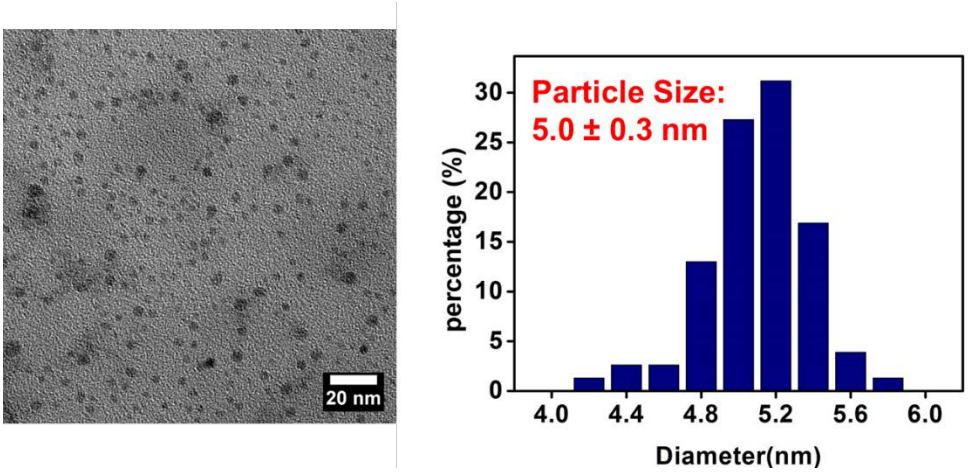


Figure S1. TEM image of typical MINPs and the distribution of size.

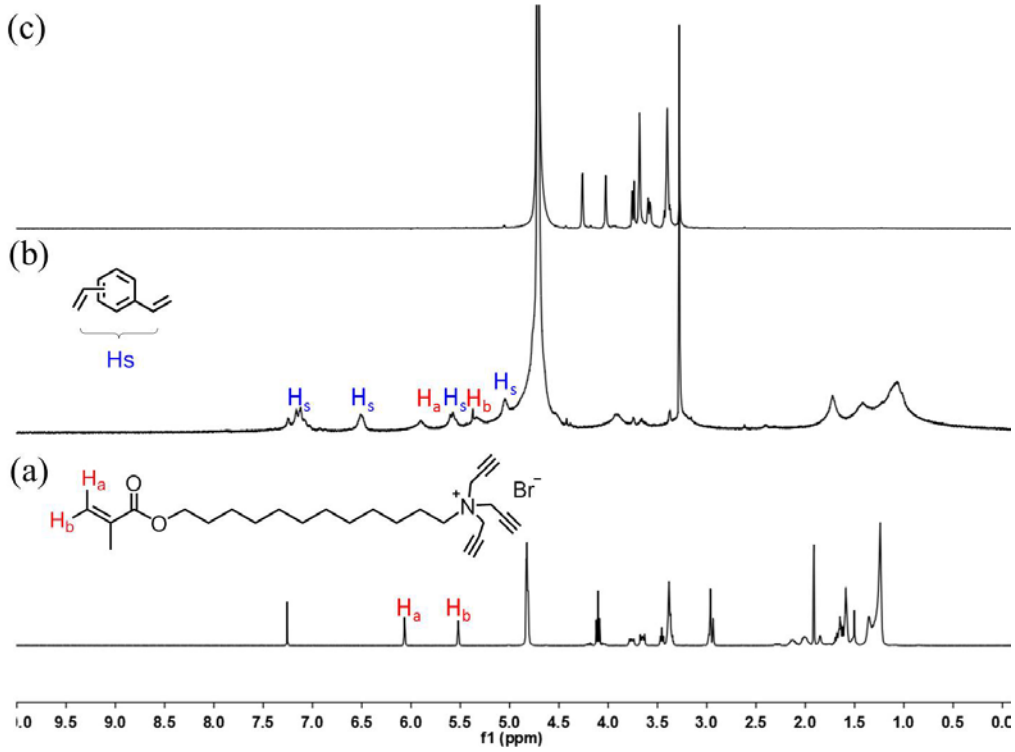


Figure S2. ^{1}H NMR spectra of (a) **3** in $CDCl_3$, (b) alkynyl-SCM in D_2O, and (c) MINP(WDW) without functional monomer in D_2O.

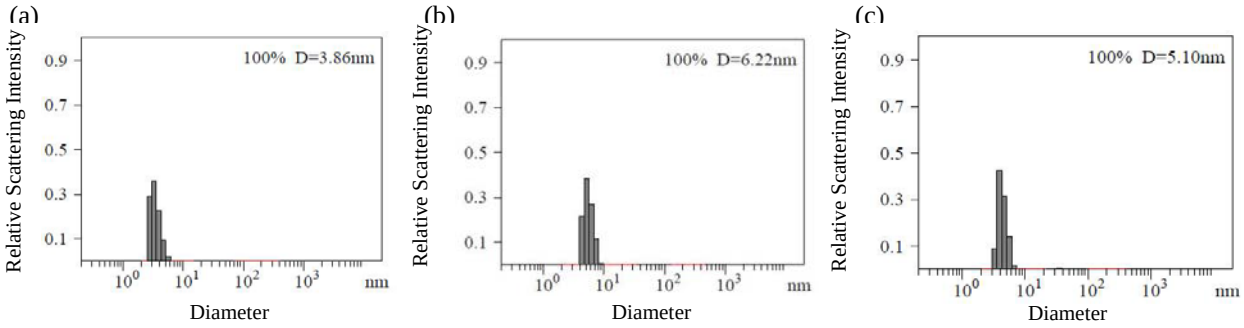


Figure S3. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM, and (c) MINP(WDW) without functional monomer in water.

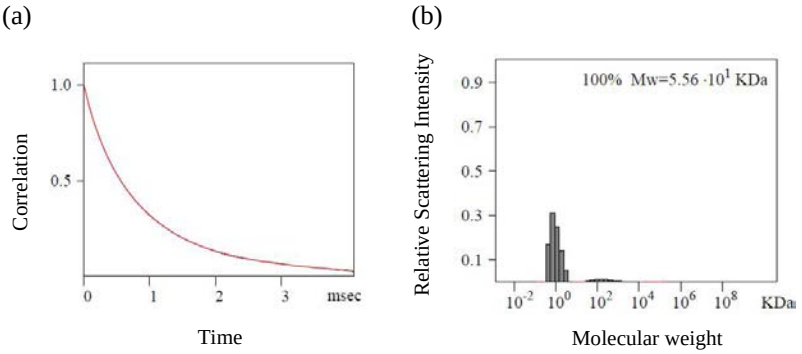


Figure S4. The correlation curve and the distribution of the molecular weight for MINP(WDW) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP(WDW) is assumed to contain one molecule of compound **3** (MW = 465 g/mol), 1.2 molecules of compound **4** (MW = 172 g/mol), one molecule of DVB (MW = 130 g/mol) and 0.8 molecules of compound **5** (MW = 264 g/mol), the molecular weight of MINP(WDW) translates to 55 [= 55600 / (465 + 1.2×172 + 130 + 0.8×264)] of such units.

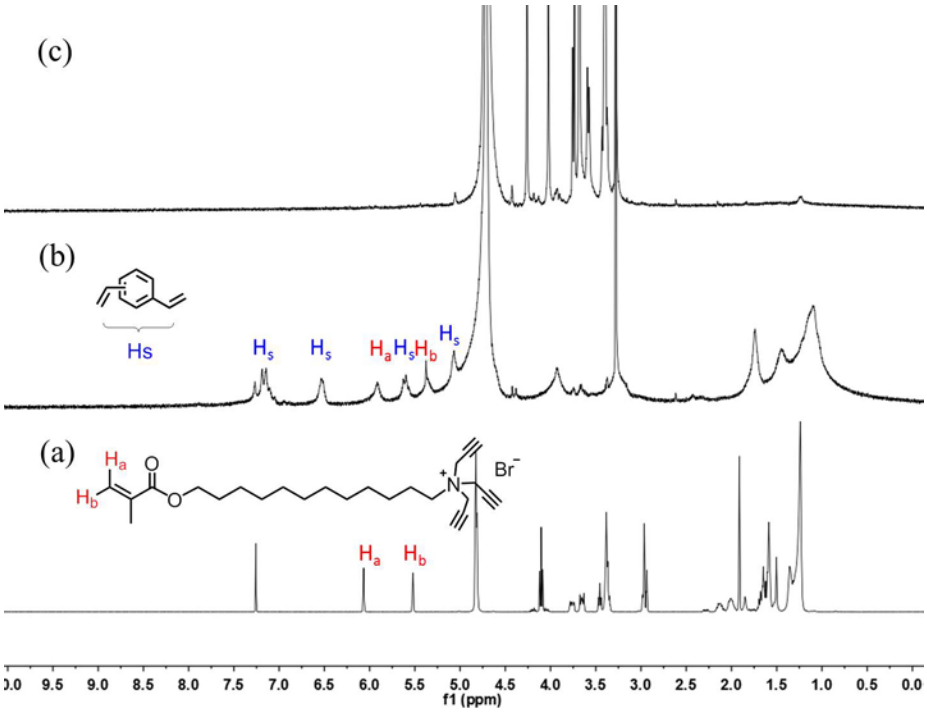


Figure S5. ^{1}H NMR spectra of (a) **3** in $CDCl_3$, (b) alkynyl-SCM in D_2O, and (c) MINP(WDW) with FM **1** (1:3) in D_2O.

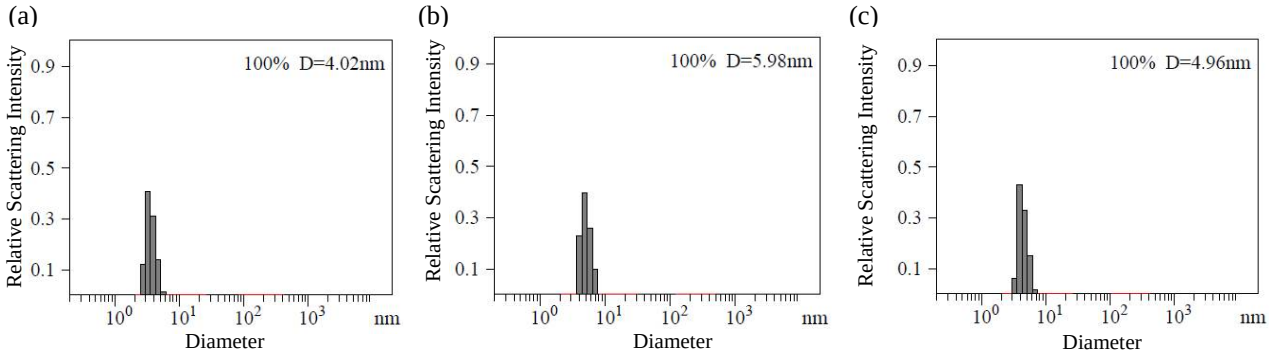


Figure S6. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM, and (c) MINP(WDW) with FM **1** (1:3) in water.

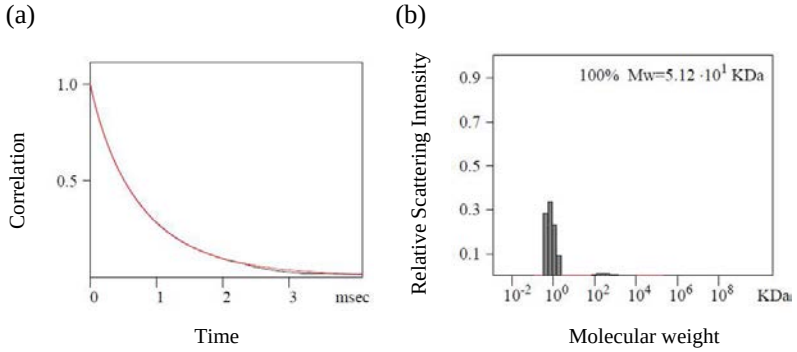


Figure S7. The correlation curve and the distribution of the molecular weight for MINP(WDW) with FM **1** (1:3) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP(WDW) with FM **1** (1:3) is assumed to contain one molecule of compound **3** (MW = 465 g/mol), 1.2 molecules of compound **4** (MW = 172 g/mol), one molecule of DVB (MW = 130 g/mol), 0.8 molecules of compound **5** (MW = 264 g/mol), and 0.06 molecules of FM **1** (MW = 228 g/mol), the molecular weight of MINP(WDW) with FM **1** (1:3) translates to 50 [= 51200 / (465 + 1.2×172 + 130 + 0.8×264 + 0.06×228)] of such units.

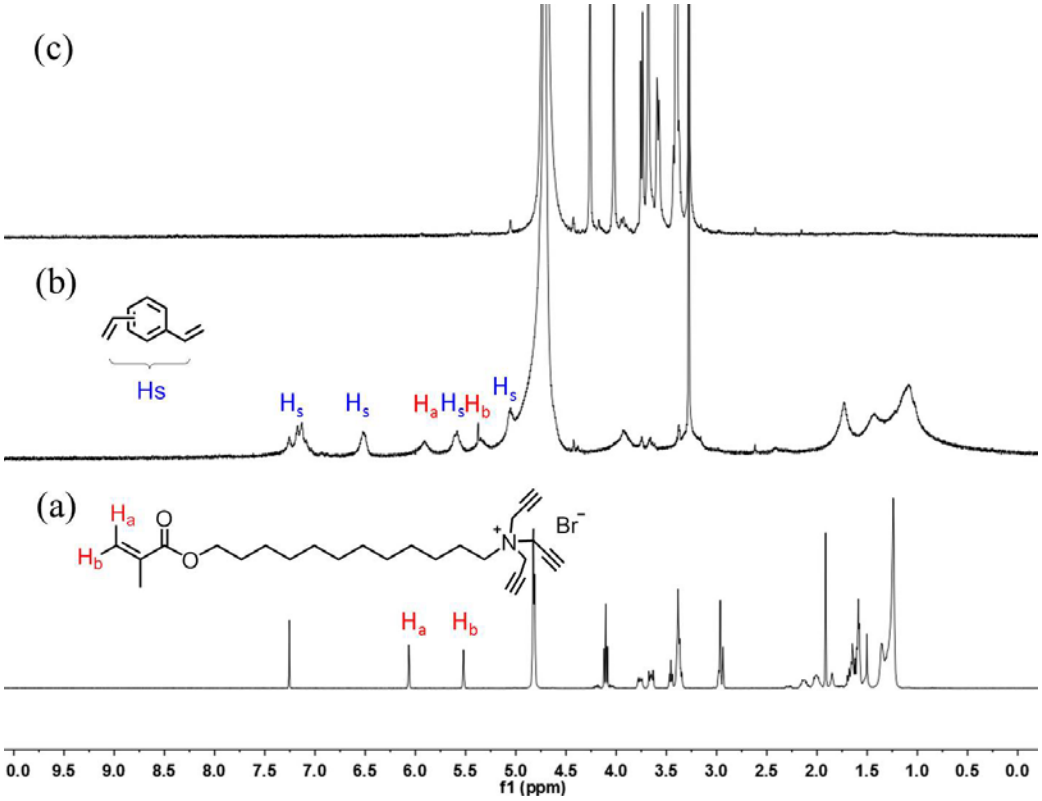


Figure S8. ^{1}H NMR spectra of (a) **1** in $CDCl_3$, (b) alkynyl-SCM in D_2O, and (c) MINP(WDW) with FM **2** (1:3) in D_2O.

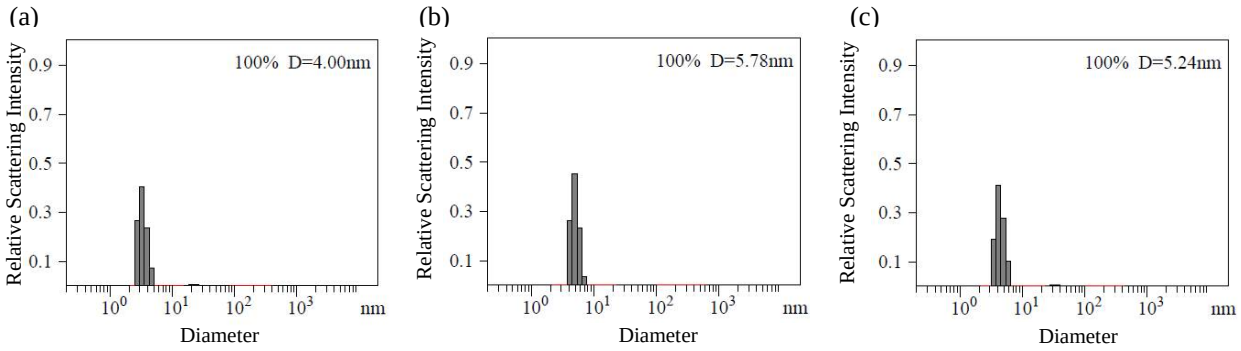


Figure S9. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM, and (c) MINP(WDW) with FM **2** (1:3) in water.

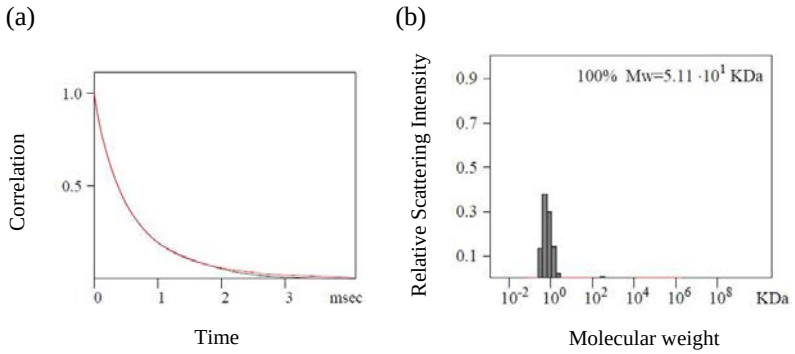


Figure S10. The correlation curve and the distribution of the molecular weight for MINP(WDW) with FM **2** (1:3) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP(WDW) with FM **2** (1:3) is assumed to contain one molecule of compound **3** (MW = 465 g/mol), 1.2 molecules of compound **4** (MW = 172 g/mol), one molecule of DVB (MW = 130 g/mol), 0.8 molecules of compound **5** (MW = 264 g/mol), and 0.06 molecules of FM **2** (MW = 379 g/mol), the molecular weight of MINP(WDW) with FM **2** (1:3) translates to 49 [= 51100 / (465 + 1.2×172 + 130 + 0.8×264 + 0.06×379)] of such units.

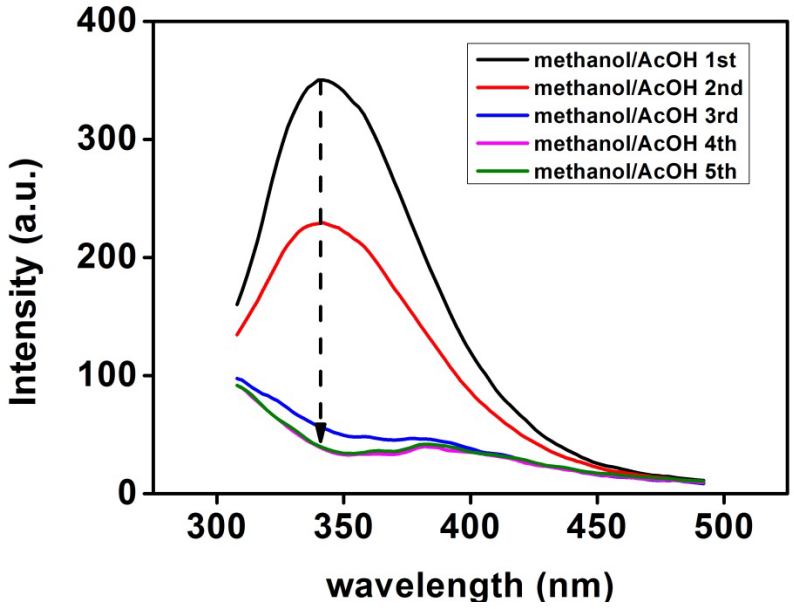


Figure S11. The template removing process of MINP(WDW) with FM **2** (1:3) by washing with methanol/acetic acid (5:0.1, v/v). The washing was monitored by fluorescence.

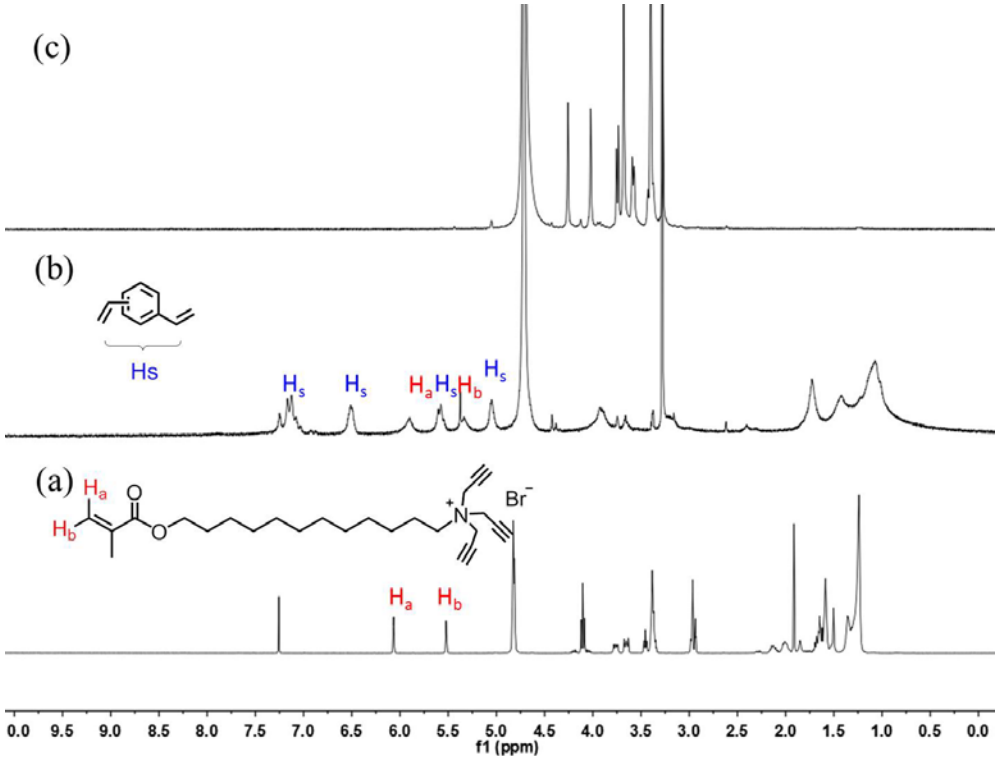


Figure S12. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM, and (c) MINP(c-Myc) with FM **2** (1:7.5) in water.

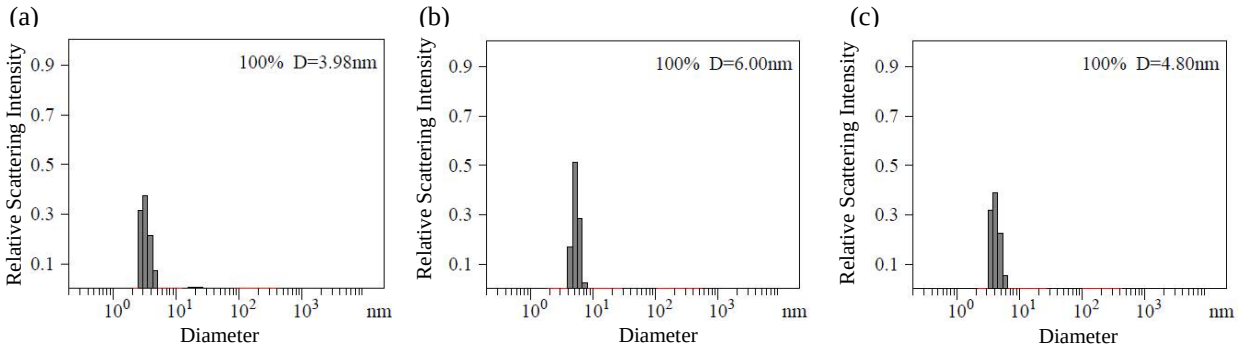


Figure S13. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM, and (c) MINP(c-Myc) with FM **2** (1:7.5) in water.

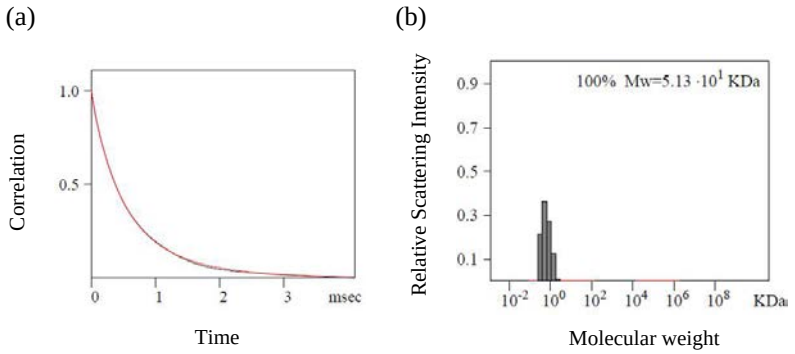


Figure S14. The correlation curve and the distribution of the molecular weight for MINP(c-Myc) with FM **2** (1:7.5) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP(c-Myc) with FM **2** (1:7.5) is assumed to contain one molecule of compound **3** (MW = 465 g/mol), 1.2 molecules of compound **4** (MW = 172 g/mol), one molecule of DVB (MW = 130 g/mol), 0.8 molecules of compound **5** (MW = 264 g/mol), and 0.15 molecules of FM **2** (MW = 379 g/mol), the molecular weight of MINP(c-Myc) with FM **2** (1:7.5) translates to 48 [= 51300 / (465 + 1.2×172 + 130 + 0.8×264 + 0.15×379)] of such units.

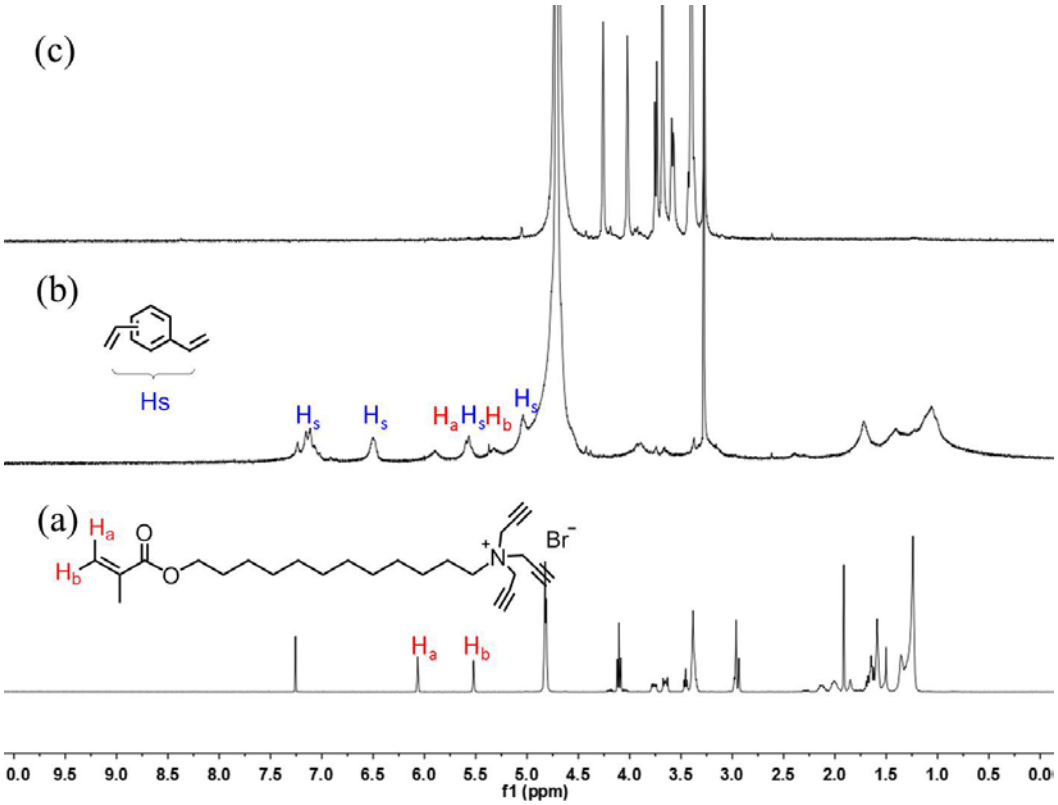


Figure S15. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM, and (c) MINP(DYKDDDDK) with FM **2** (1:9) in water.

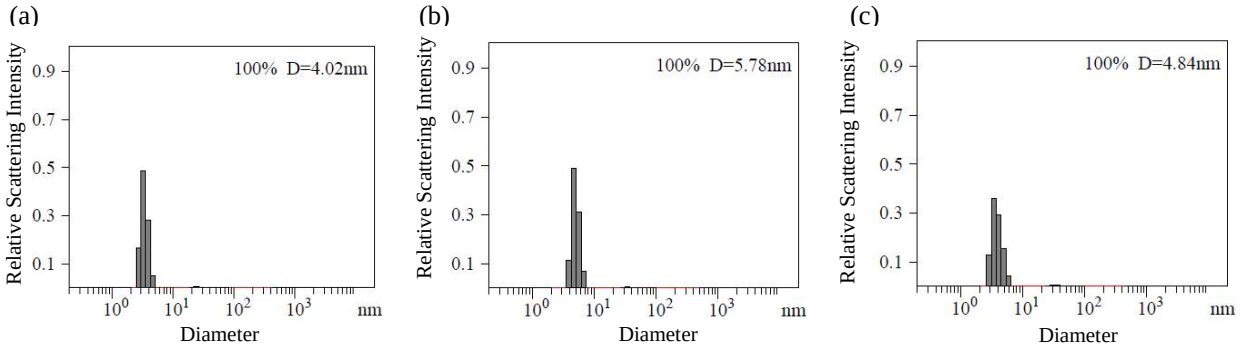


Figure S16. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM, and (c) MINP(DYKDDDDK) with FM **2** (1:9) in water.

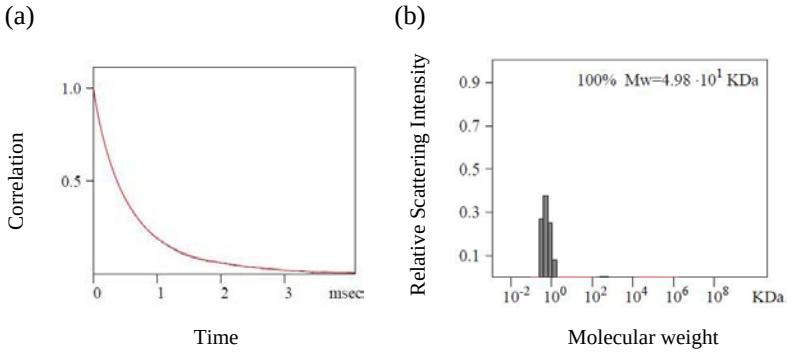


Figure S17. The correlation curve and the distribution of the molecular weight for MINP(DYKDDDDK) with FM **2** (1:9) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP(DYKDDDDK) with FM **2** (1:9) is assumed to contain one molecule of compound **3** (MW = 465 g/mol), 1.2 molecules of compound **4** (MW = 172 g/mol), one molecule of DVB (MW = 130 g/mol), 0.8 molecules of compound **5** (MW = 264 g/mol), and 0.18 molecules of FM **2** (MW = 379 g/mol), the molecular weight of MINP(DYKDDDDK) with FM **2** (1:9) translates to 46 [= 49800 / (465 + 1.2×172 + 130 + 0.8×264 + 0.18×379)] of such units.

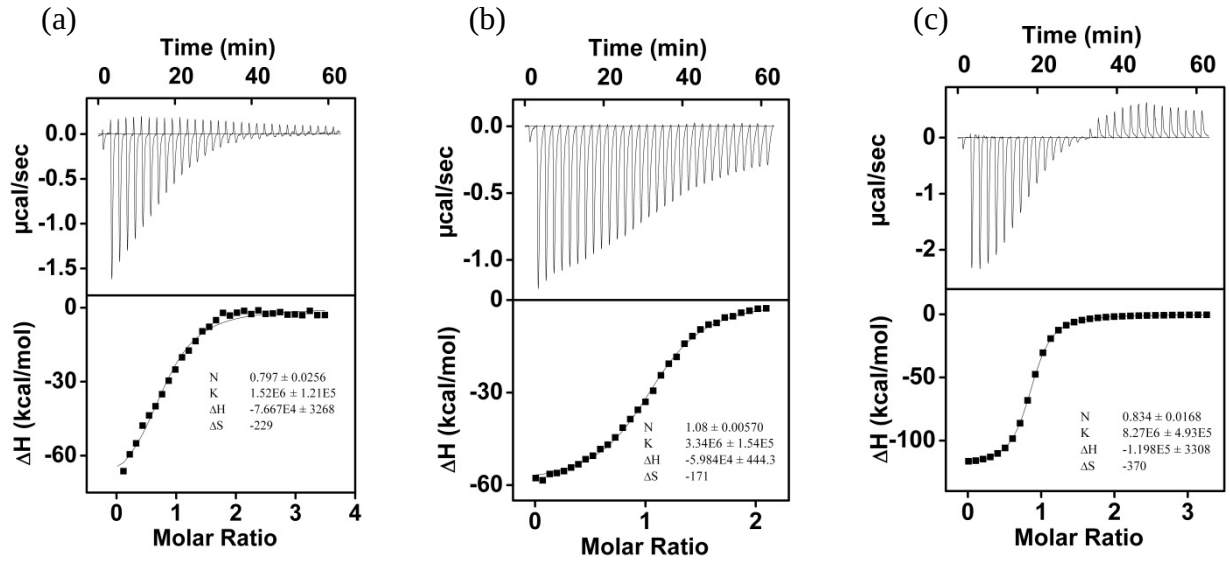


Figure S18. ITC titration curves obtained at 298 K for the titration of 5 μM of (a) MINP(WDW) without functional monomer, (b) MINP(WDW) with FM **1** (1:3) and (c) MINP(WDW) with FM **2** (1:3) by peptide WDW in Millipore water. The guest concentrations are (a) 75 μM, (b) 45 μM and (c) 70 μM, respectively. The data correspond to entries 1, 3, 6, respectively, in Table 1.

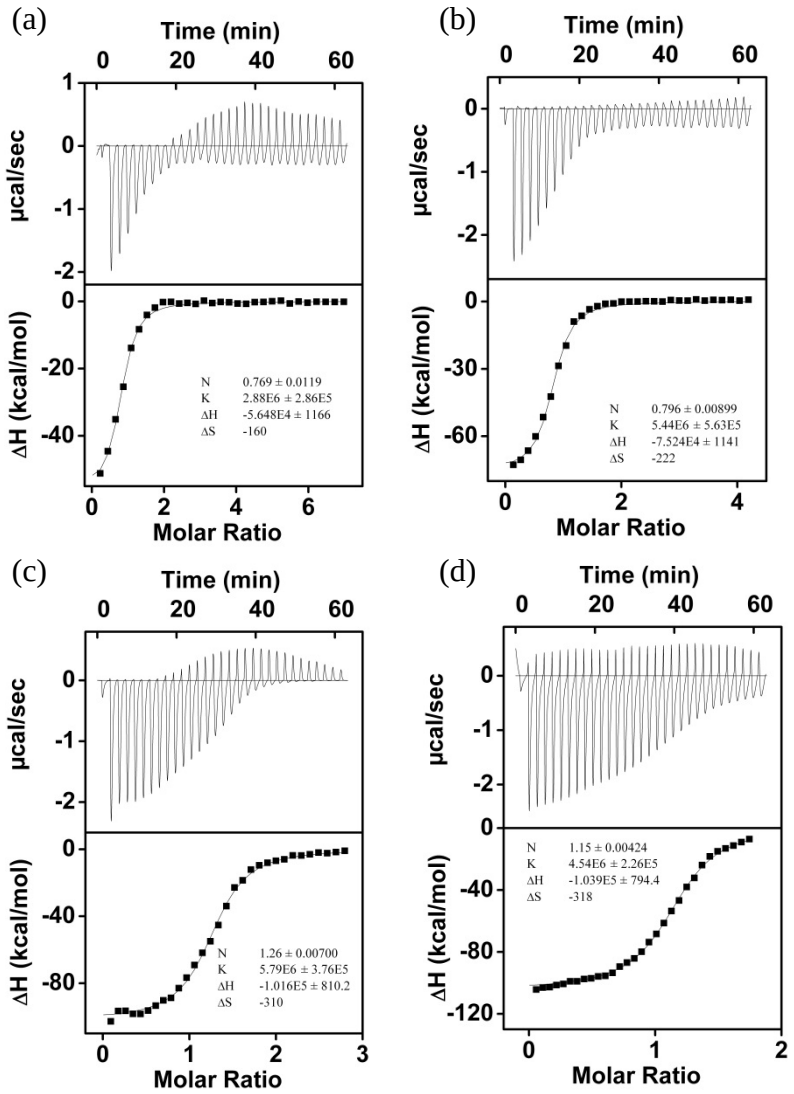


Figure S19. ITC titration curves obtained at 298 K for the titration of 5 μM of (a) MINP(WDW) with FM **2** (1:1), (b) MINP(WDW) with FM **2** (1:2), (c) MINP(WDW) with FM **2** (1:4) and (d) 8 μM of MINP(WDW) with FM **2** (1:5) by peptide WDW in Millipore water. The guest concentrations are (a) 150 μM, (b) 90 μM and (c) 60 μM and (d) 60μM, respectively. The data correspond to entries 4, 5, 8, 9, respectively, in Table 1.

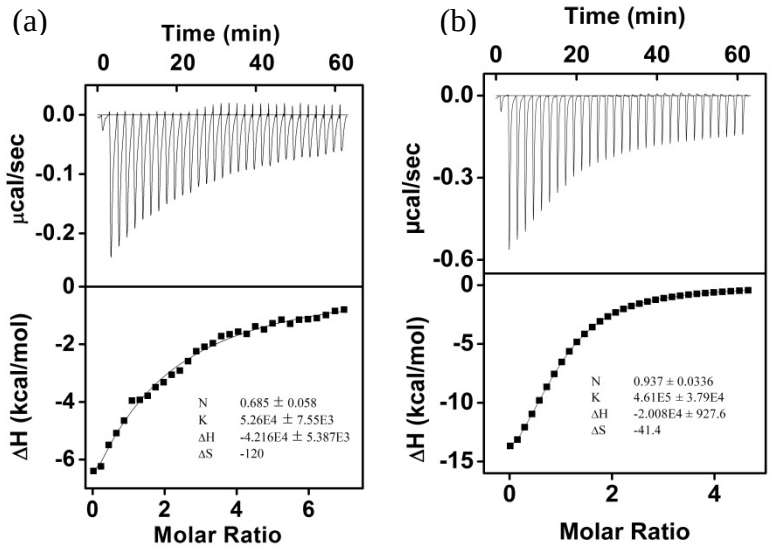


Figure S20. ITC titration curves obtained at 298 K for the titration of 5 μM of (a) MINP(GDG) without FM and (b) MINP(GDG) with FM **2** (1:3) by peptide GDG in Millipore water. The guest concentrations are (a) 150 μM and (b) 100 μM, respectively. The data correspond to entries 1, 2, respectively, in Table 2.

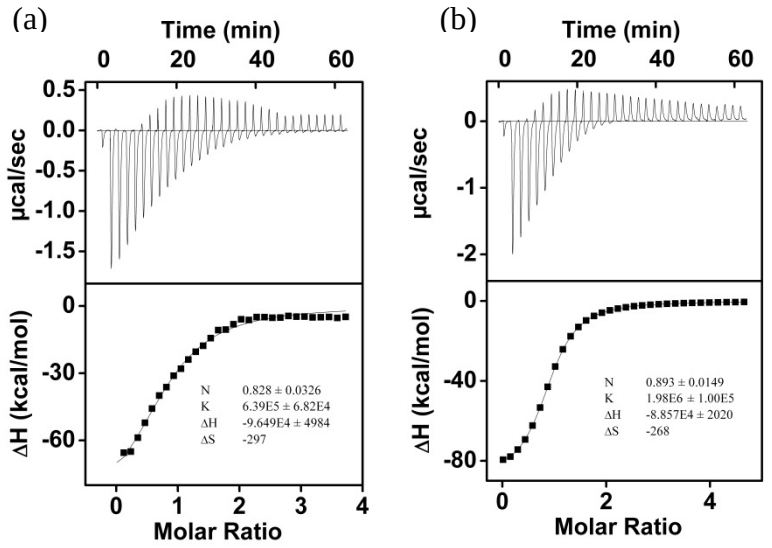


Figure S21. ITC titration curves obtained at 298 K for the titration of 5 μM of (a) MINP(GDW) without FM and (b) MINP(GDW) with FM **2** (1:3) by peptide GDW in Millipore water. The guest concentrations are (a) 80 μM and (b) 100 μM, respectively. The data correspond to entries 3, 4, respectively, in Table 2.

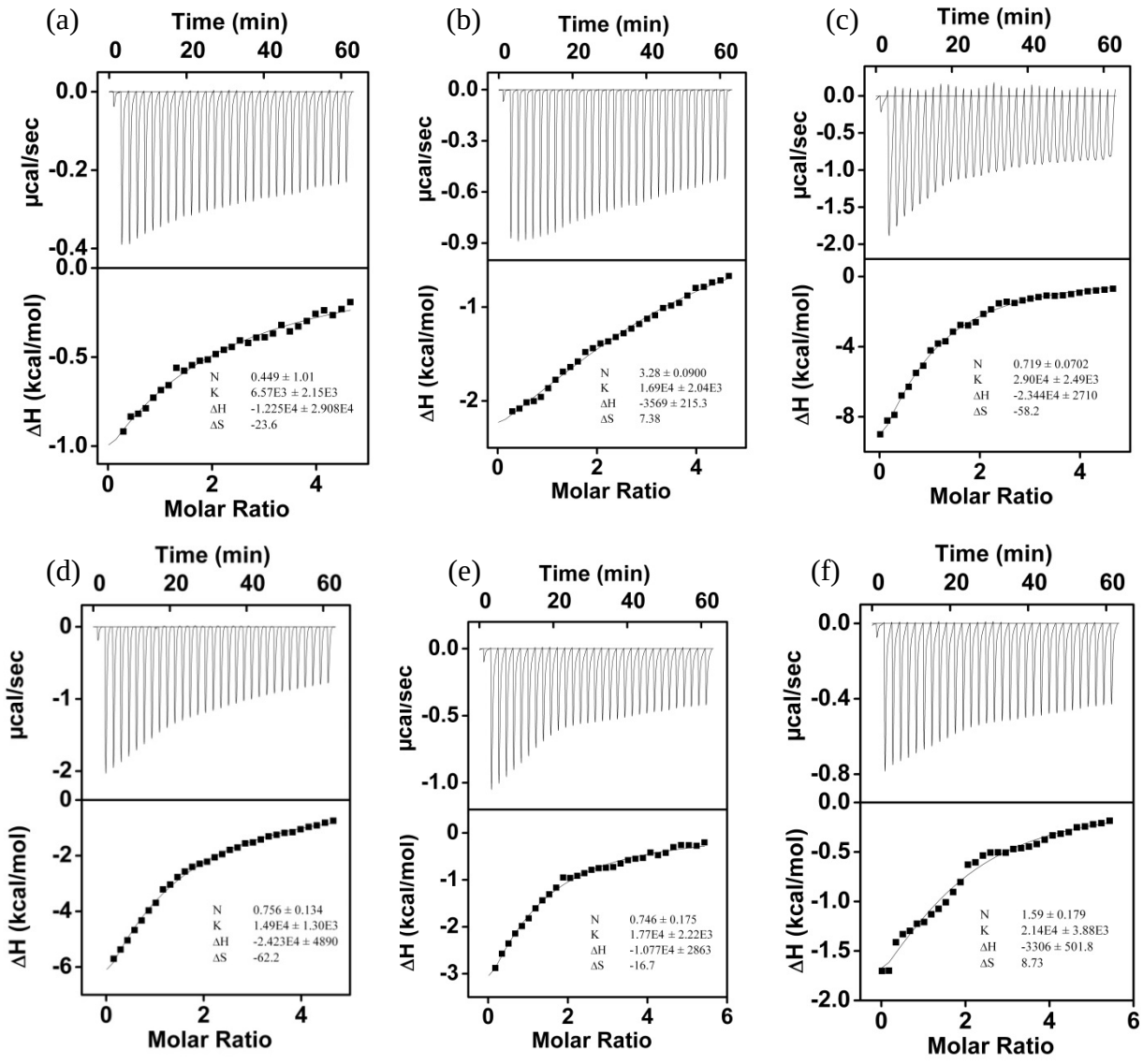


Figure S22. ITC titration curves obtained at 298 K for the titration of 30µM of MINP(WDW) (a,c,e) without FM and (b,d,f) with FM **2** (1:3) by peptide (a,b) DWW, (c,d) WWD and (e,f) WWW in Millipore water. The guest concentrations are (a-d) 600 µM and (e,f) 700 µM, respectively. The data correspond to entries 6, 14, 7, 15, 8, 16, respectively, in Table S1.

Table S1. Binding data obtained from fluorescence titrations and ITC titrations. [a]

Entry	template	Guest	FM	K_a ($\times 10^5$ M^{-1})	K_{rel}
1	WDW	WDW	none	15.7 ± 1.4	1
2	WDW	WNW	none	28.8 ± 3.9	1.83
3	WDW	GDW	none	2.1 ± 0.1	0.13
4	WDW	DW	none	2.6 ± 0.1	0.17
5	WDW	GWDW	none	10.4 ± 0.7	0.66
6	WDW	DWW	none	(0.07 ± 0.02)	0.004
7	WDW	WWD	none	(0.29 ± 0.02)	0.018
8	WDW	WWW	none	(0.18 ± 0.02)	0.011
9	WDW	WDW	**2**	80.8 ± 7.2	1
10	WDW	WNW	**2**	32.3 ± 3.6	0.40
11	WDW	GDW	**2**	23.1 ± 2.4	0.29
12	WDW	DW	**2**	16.2 ± 0.7	0.20
13	WDW	GWDW	**2**	59.1 ± 5.7	0.73
14	WDW	DWW	**2**	(0.17 ± 0.02)	0.002
15	WDW	WWD	**2**	(0.15 ± 0.01)	0.002
16	WDW	WWW	**2**	(0.21 ± 0.04)	0.003

[a] The titrations were performed in Millipore water at 298 K, and the MINPs were prepared by using surfactant **3**. The K_a values in the parentheses are those determined by ITC and those without the parentheses from fluorescence titration. The FM/carboxylate ratio was kept 1.5:1 in the cases with FM2. K_{rel} is the binding constant of other guests to that of WDW with the MINP prepared by WDW.

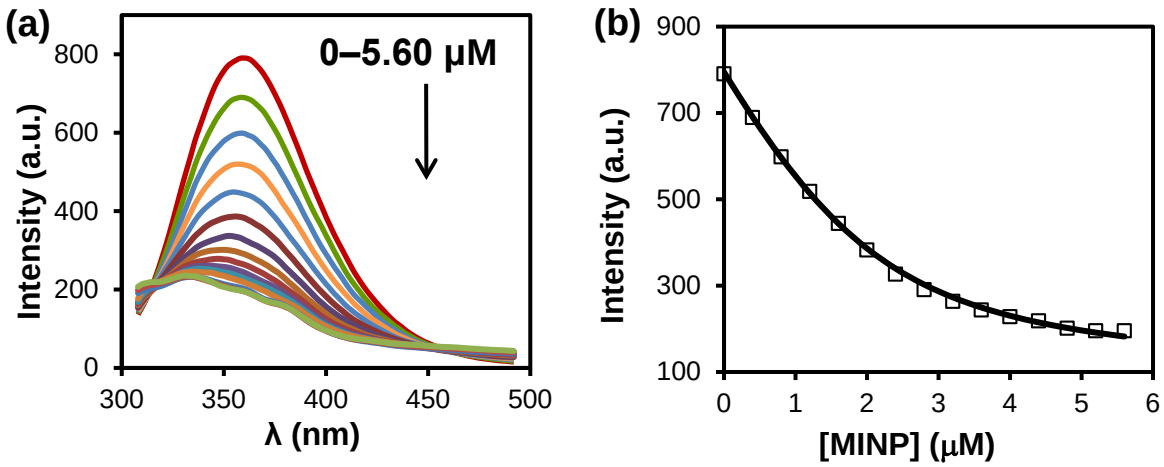


Figure S23. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 1 in Table 1.

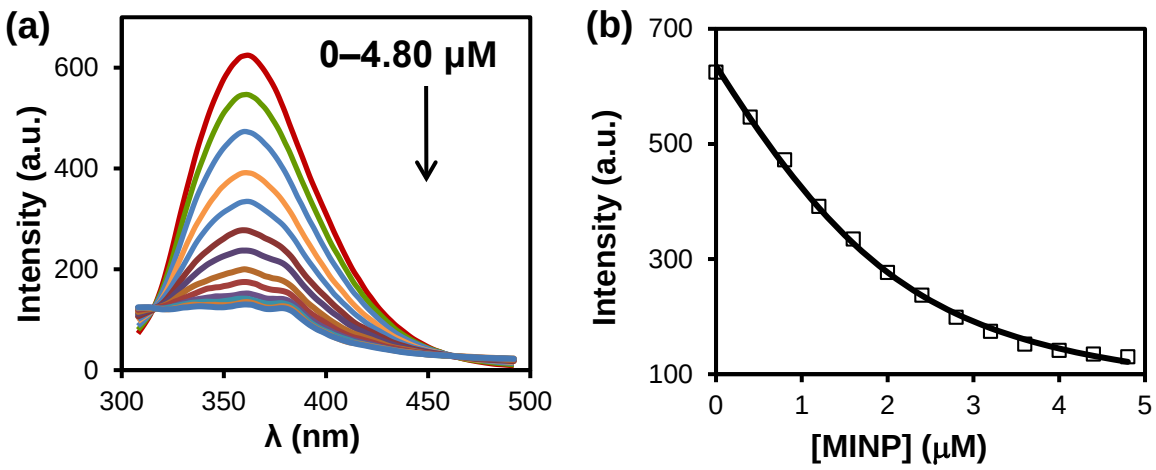


Figure S24. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) without functional monomer in 25 mM HEPES buffer at pH 7.4. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 2 in Table 1.

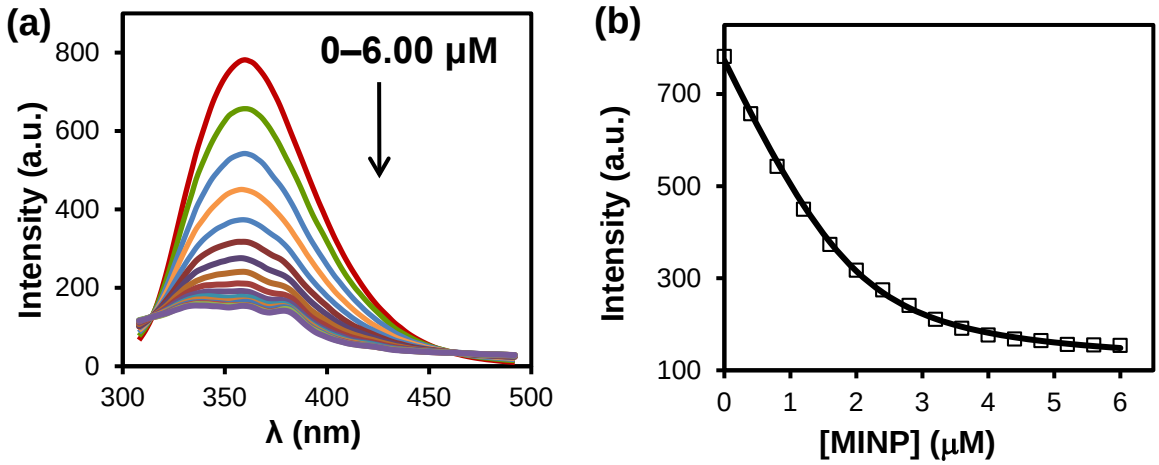


Figure S25. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **1** (1:3) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 3 in Table 1.

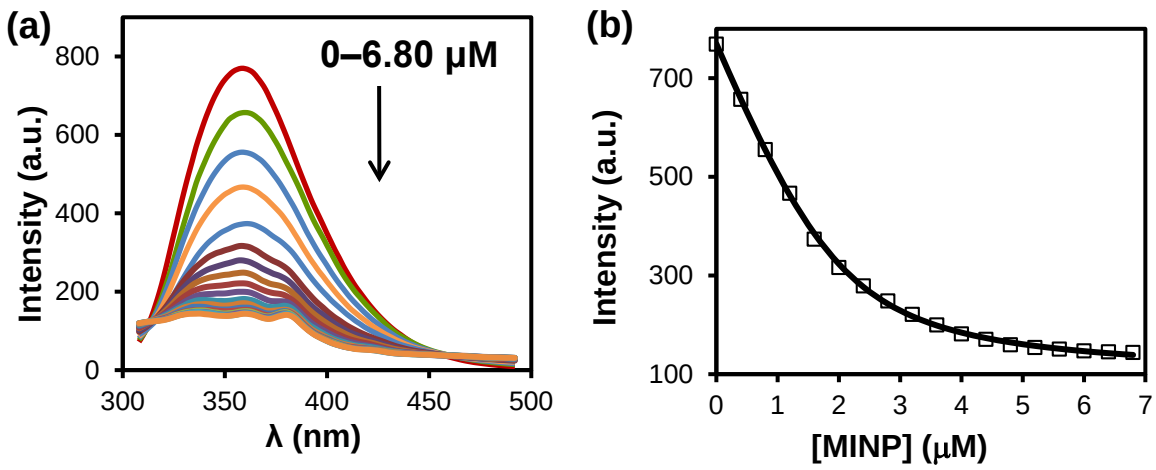


Figure S26. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:1) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 4 in Table 1.

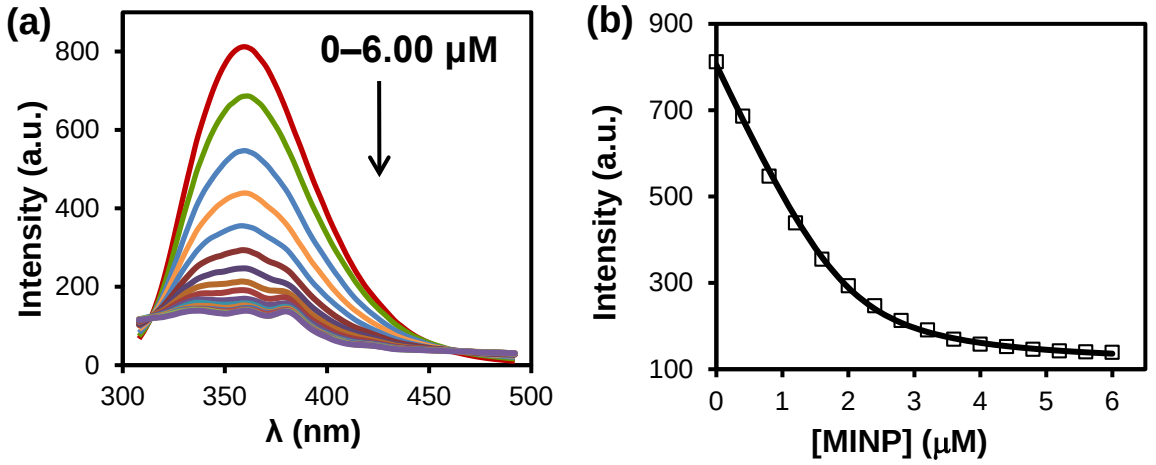


Figure S27. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:2) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 5 in Table 1.

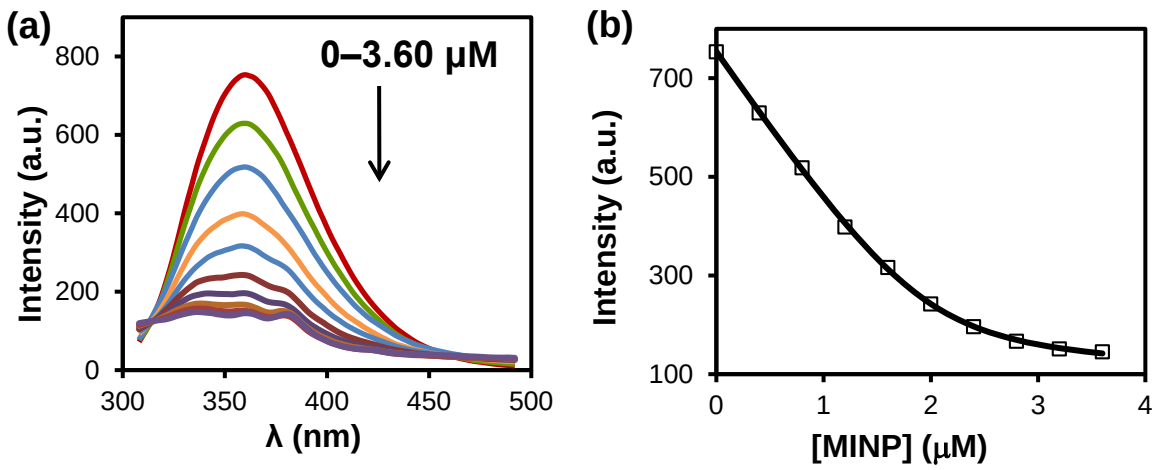


Figure S28. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:3) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 6 in Table 1.

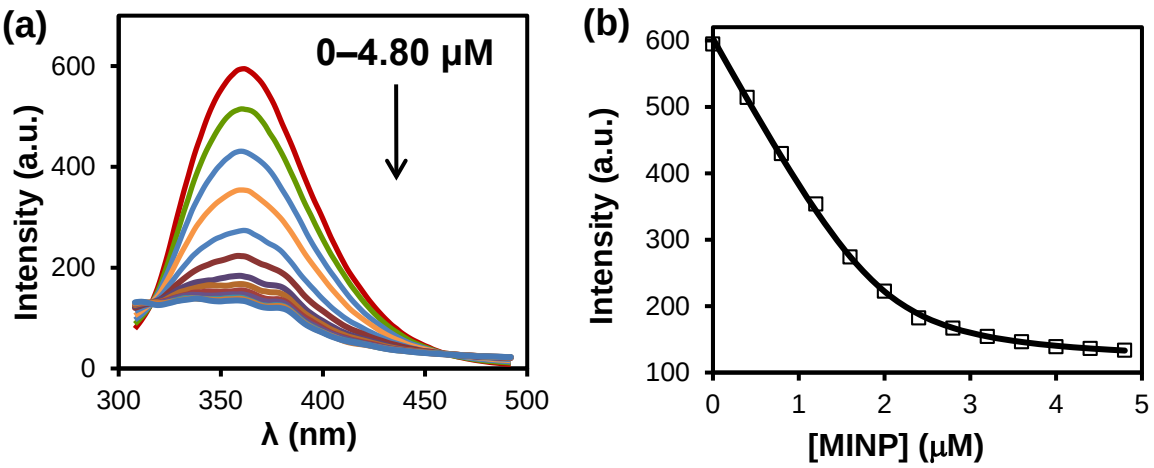


Figure S29. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:3) in 25 mM HEPES buffer at pH 7.4. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 7 in Table 1.

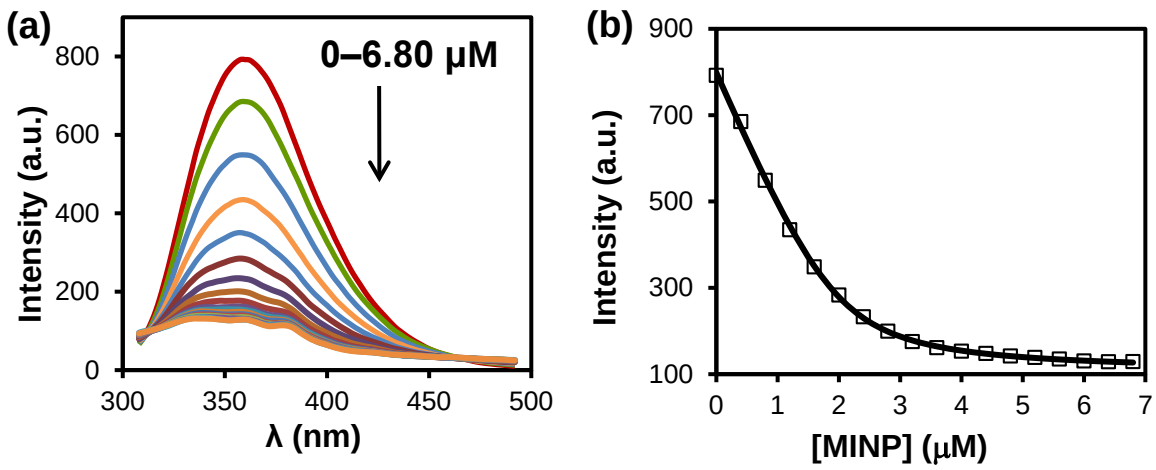


Figure S30. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:4) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 8 in Table 1.

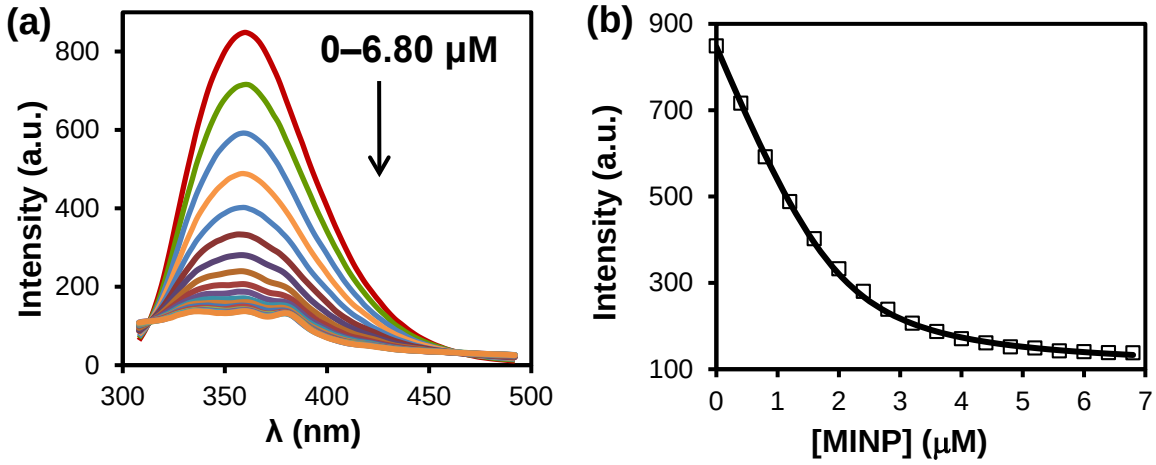


Figure S31. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:5) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 9 in Table 1.

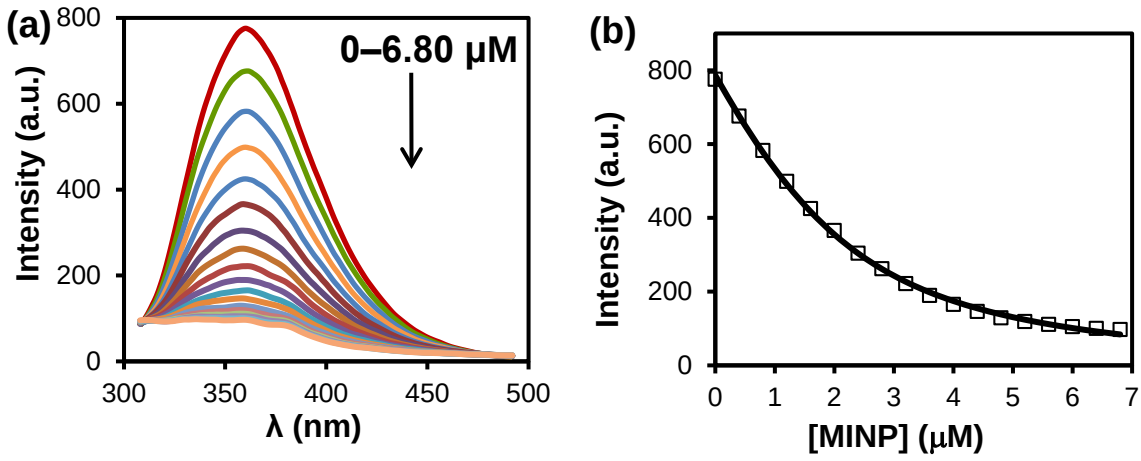


Figure S32. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) without functional monomer in water. The MINP was prepared by surfactant **6**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 10 in Table 1.

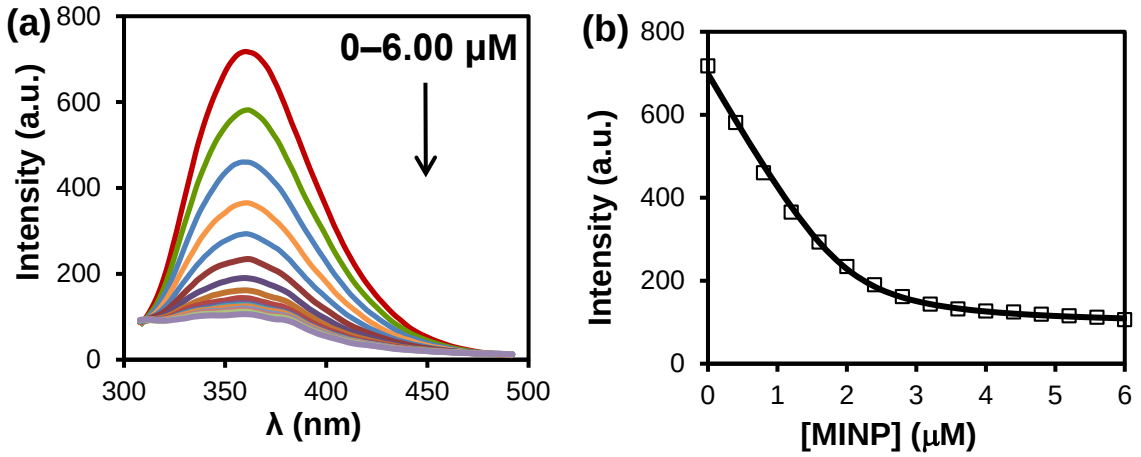


Figure S33. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:3) in water. The MINP was prepared by surfactant **6**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 11 in Table 1.

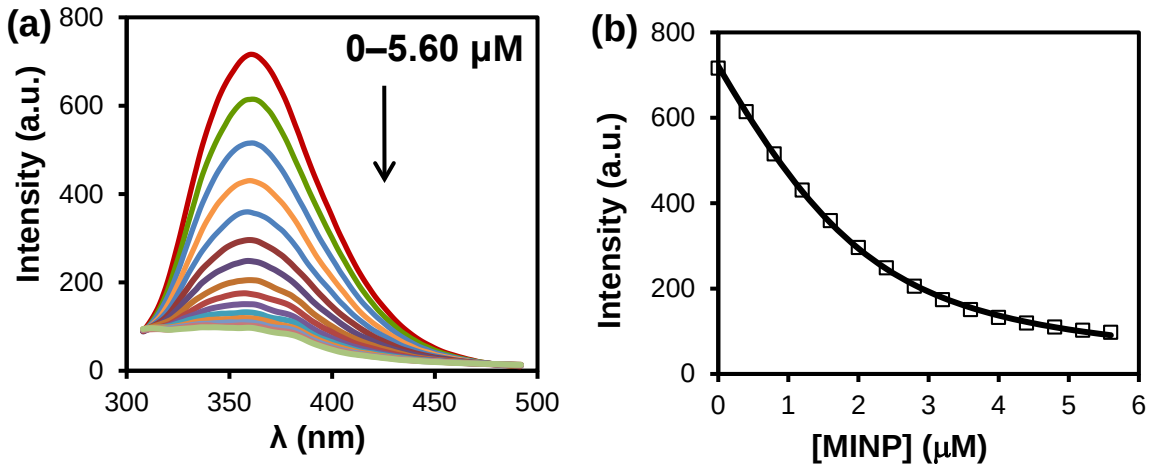


Figure S34. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) without functional monomer in water. The MINP was prepared by surfactant **7**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 12 in Table 1.

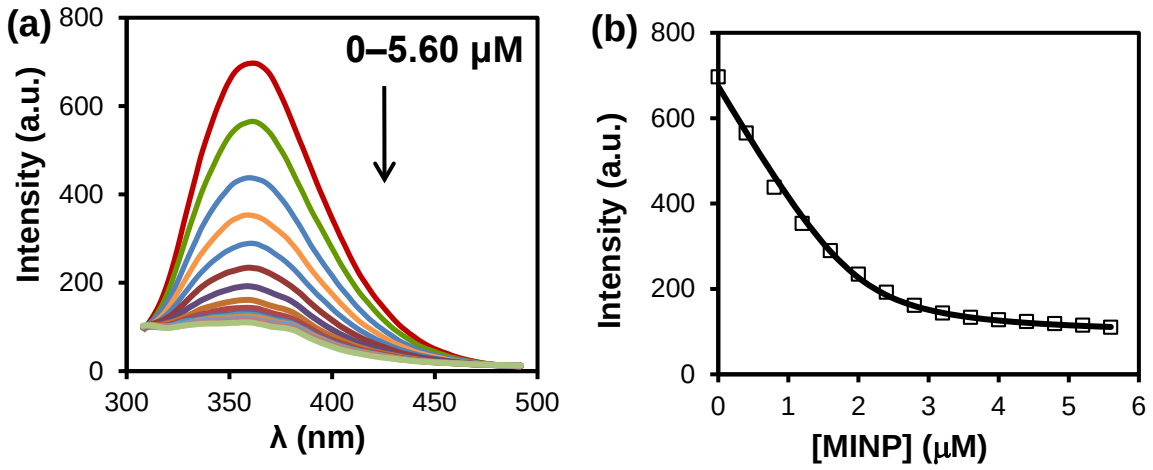


Figure S35. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:3) in water. The MINP was prepared by surfactant **7**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 13 in Table 1.

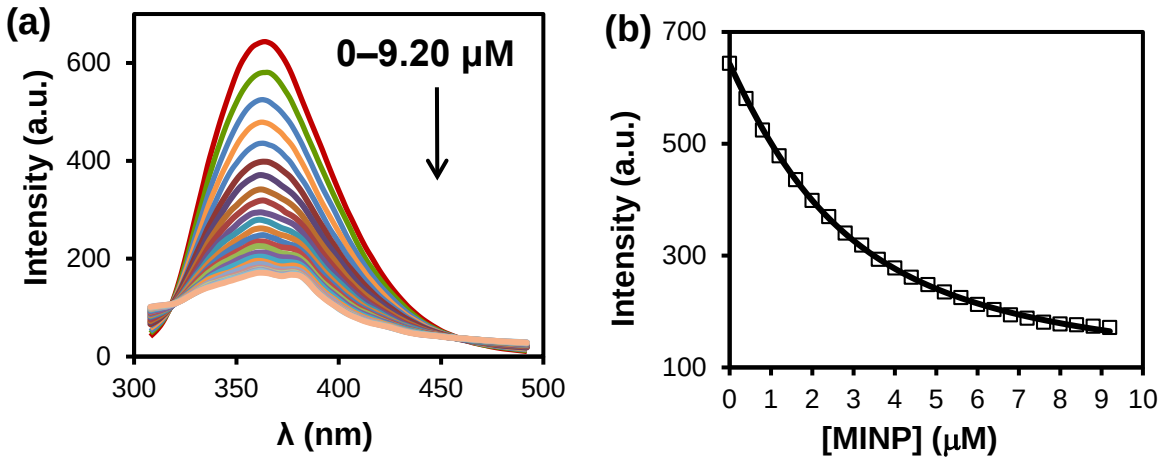


Figure S36. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide GDW (2.0 μM) upon addition of different concentrations of MINP(GDW) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide GDW at 364 nm to a 1:1 binding isotherm.

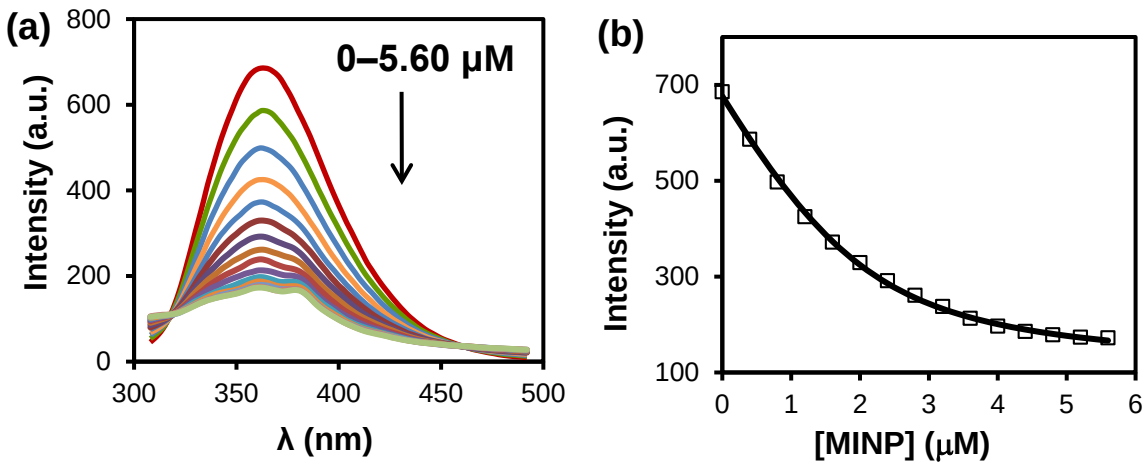


Figure S37. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide GDW (2.0 μM) upon addition of different concentrations of MINP(GDW) with FM **2** (1:3) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide GDW at 364 nm to a 1:1 binding isotherm.

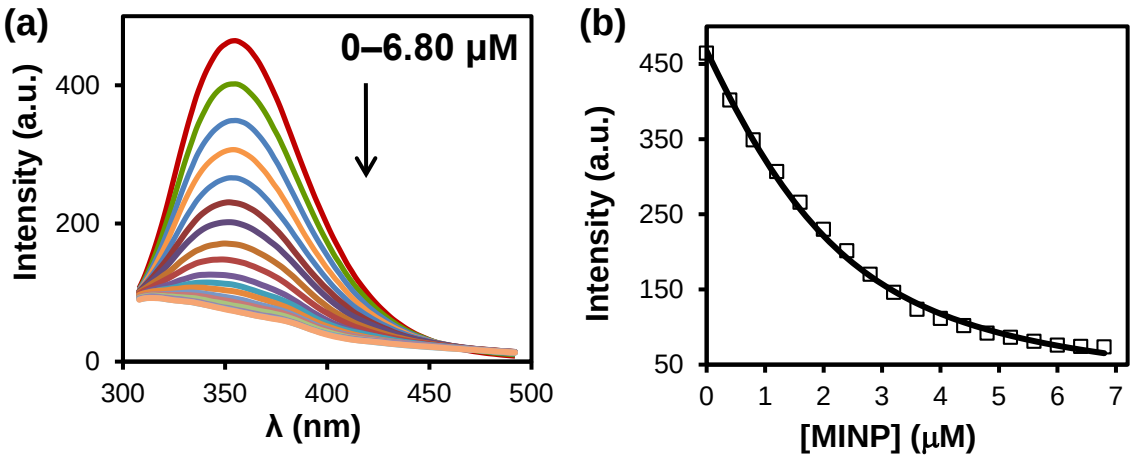


Figure S38. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDWD (2.0 μM) upon addition of different concentrations of MINP(WDWD) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDWD at 354 nm to a 1:1 binding isotherm. The data correspond to entry 3 in Table 3.

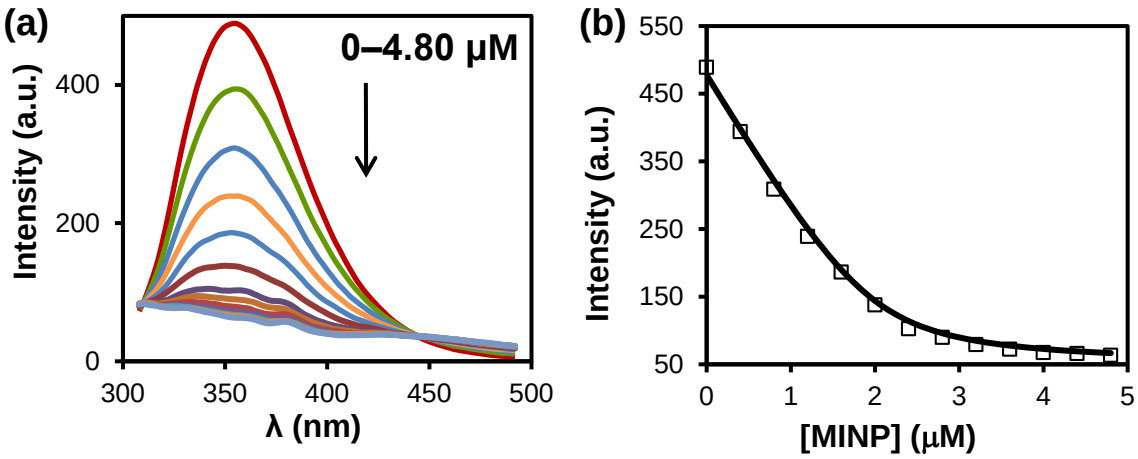


Figure S39. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDWD (2.0 μM) upon addition of different concentrations of MINP(WDWD) with FM **2** (1:3) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDWD at 354 nm to a 1:1 binding isotherm. The data correspond to entry 4 in Table 3.

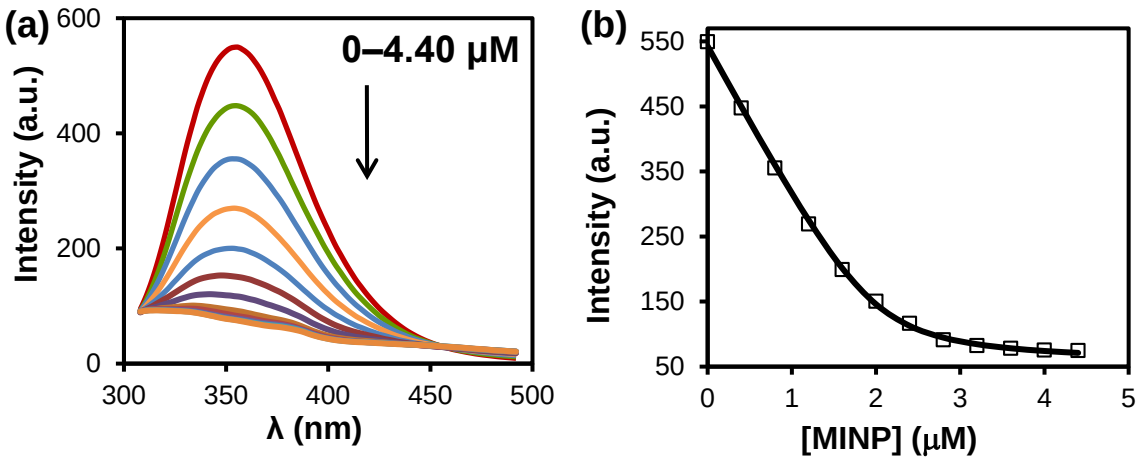


Figure S40. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDWD (2.0 μM) upon addition of different concentrations of MINP(WDWD) with FM **2** (1:4.5) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDWD at 354 nm to a 1:1 binding isotherm. The data correspond to entry 5 in Table 3.

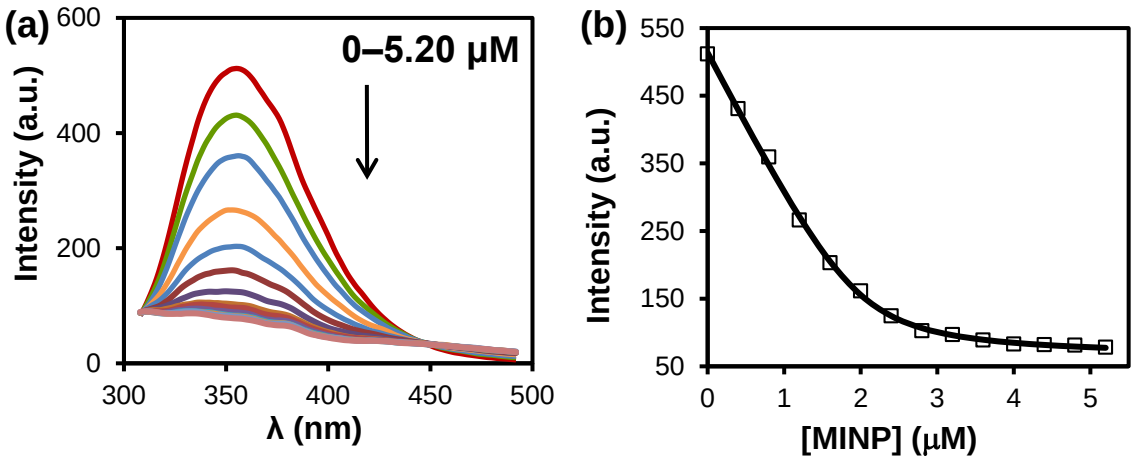


Figure S41. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDWD (2.0 μM) upon addition of different concentrations of MINP(WDWD) with FM **2** (1:6) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDWD at 354 nm to a 1:1 binding isotherm. The data correspond to entry 6 in Table 3.

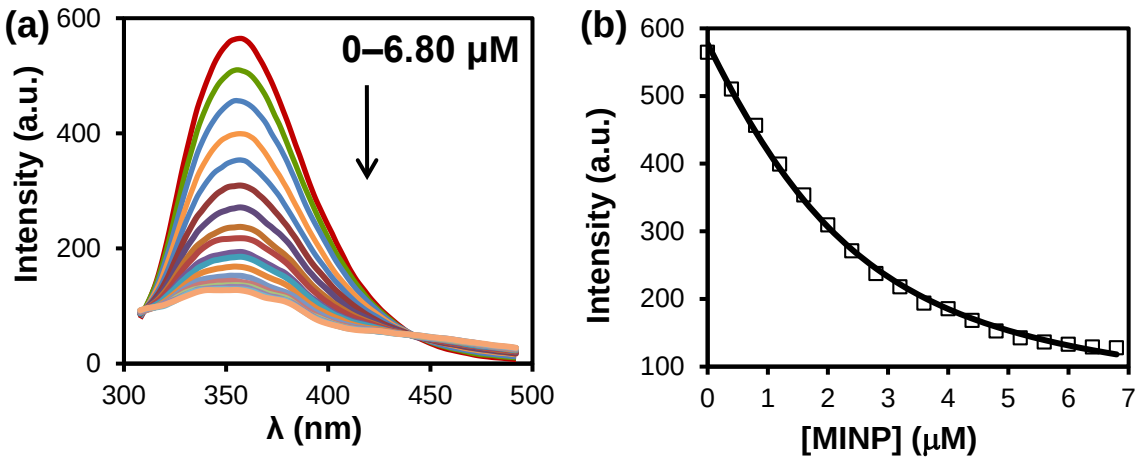


Figure S42. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDWDD (2.0 μM) upon addition of different concentrations of MINP(WDWDD) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDWDD at 356 nm to a 1:1 binding isotherm. The data correspond to entry 7 in Table 3.

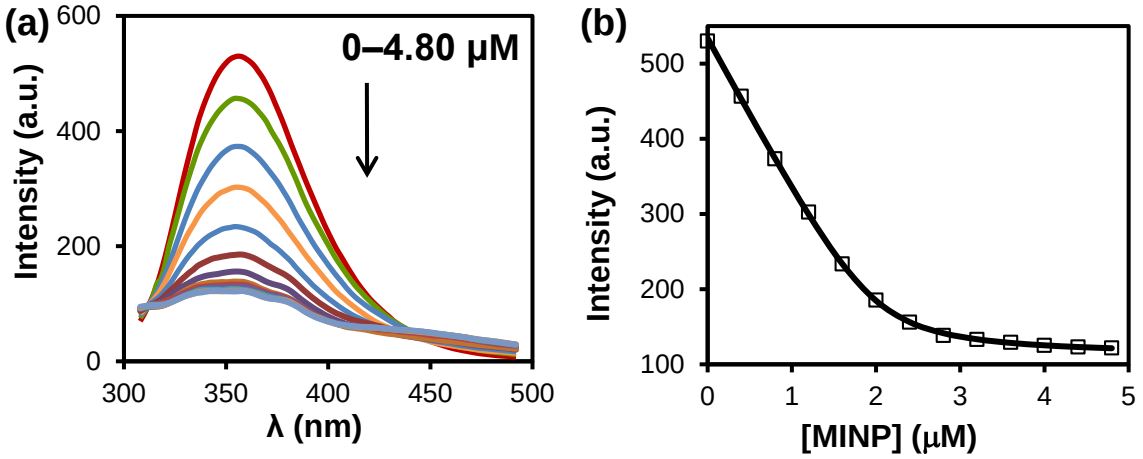


Figure S43. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDWDD (2.0 μM) upon addition of different concentrations of MINP(WDWDD) with FM **2** (1:6) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDWDD at 356 nm to a 1:1 binding isotherm. The data correspond to entry 8 in Table 3.

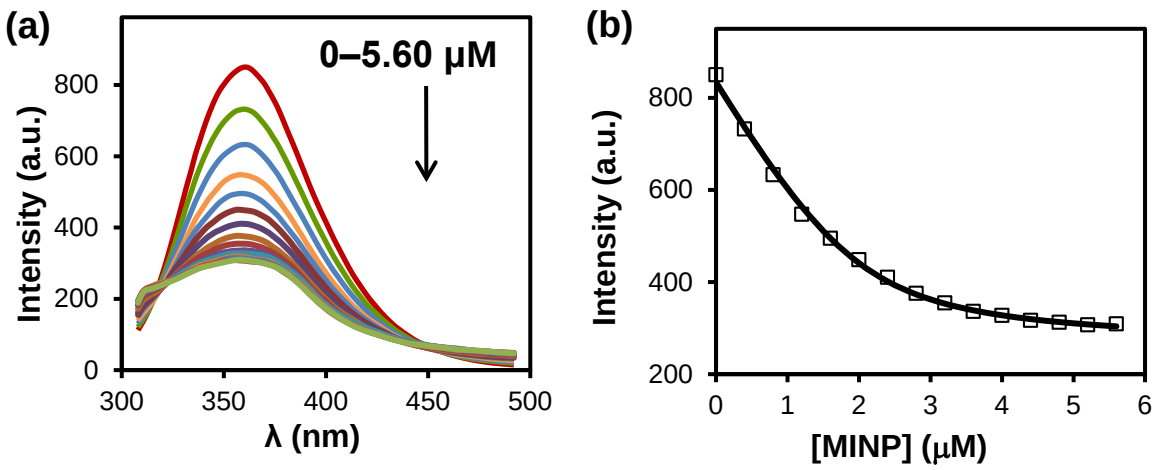


Figure S44. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WNW (2.0 μM) upon addition of different concentrations of MINP(WNW) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WNW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 1 in Table 4.

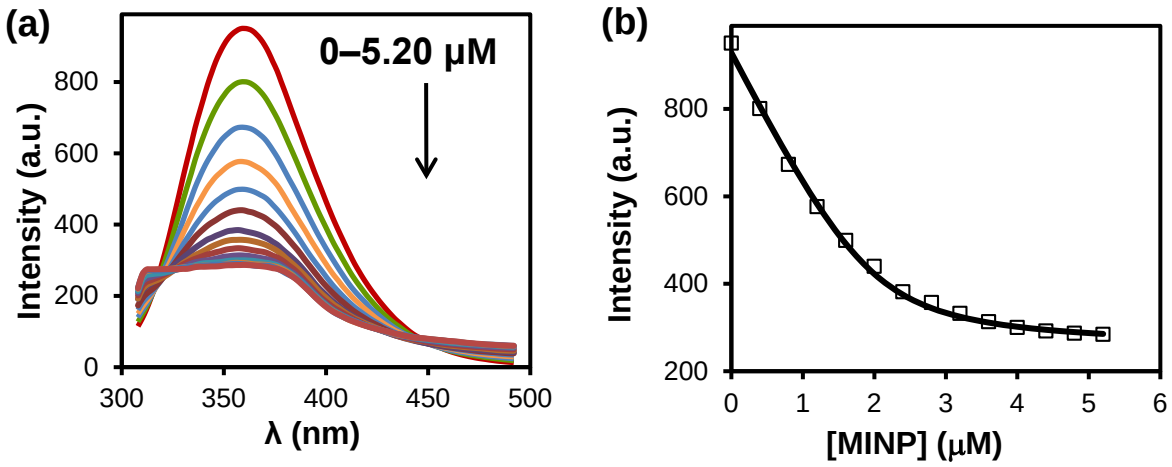


Figure S45. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WNW (2.0 μM) upon addition of different concentrations of MINP(WNW) with FM **2** (1:1.5) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WNW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 2 in Table 4.

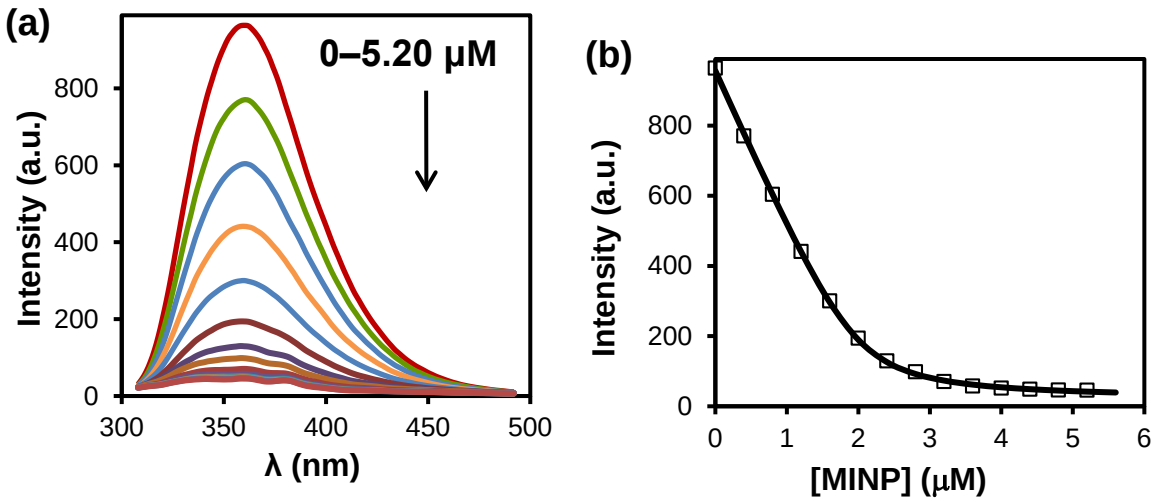


Figure S46. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WWW (2.0 μM) upon addition of different concentrations of MINP(WWW) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 3 in Table 4.

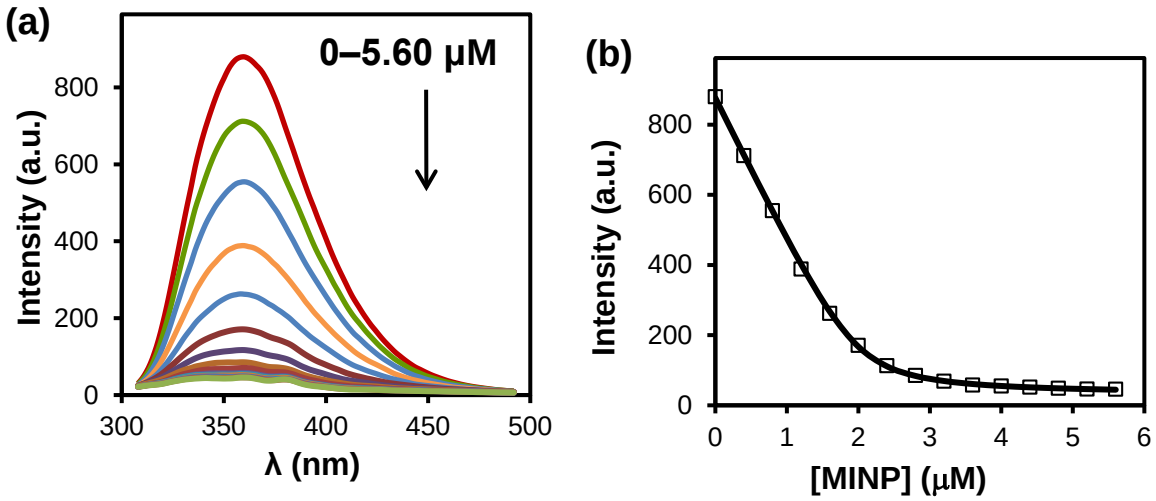


Figure S47. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WWW (2.0 μM) upon addition of different concentrations of MINP(WWW) with FM **2** (1:1.5) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WWW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 4 in Table 4.

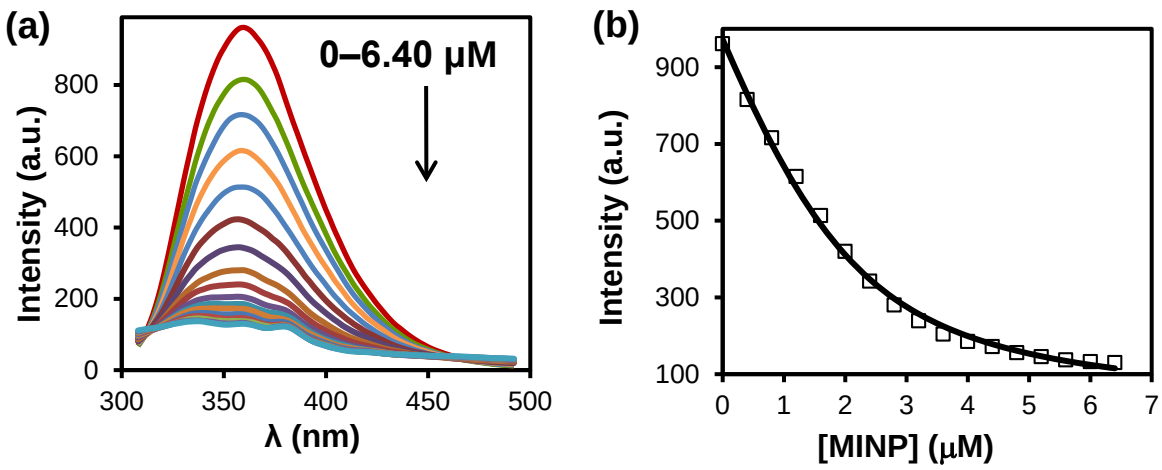


Figure S48. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WEW (2.0 μM) upon addition of different concentrations of MINP(WEW) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WEW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 7 in Table 4.

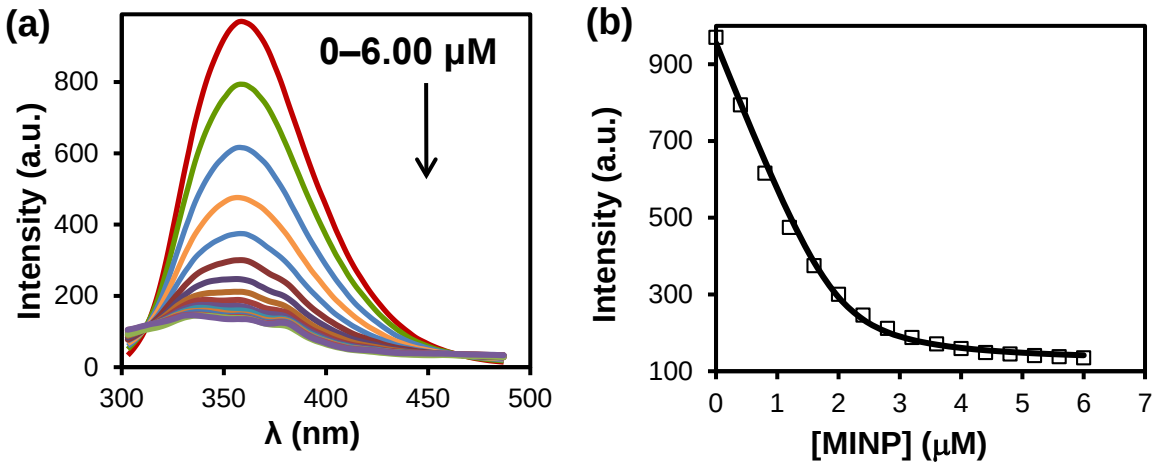


Figure S49. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WEW (2.0 μM) upon addition of different concentrations of MINP(WEW) with FM **2** (1:3) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WEW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 8 in Table 4.

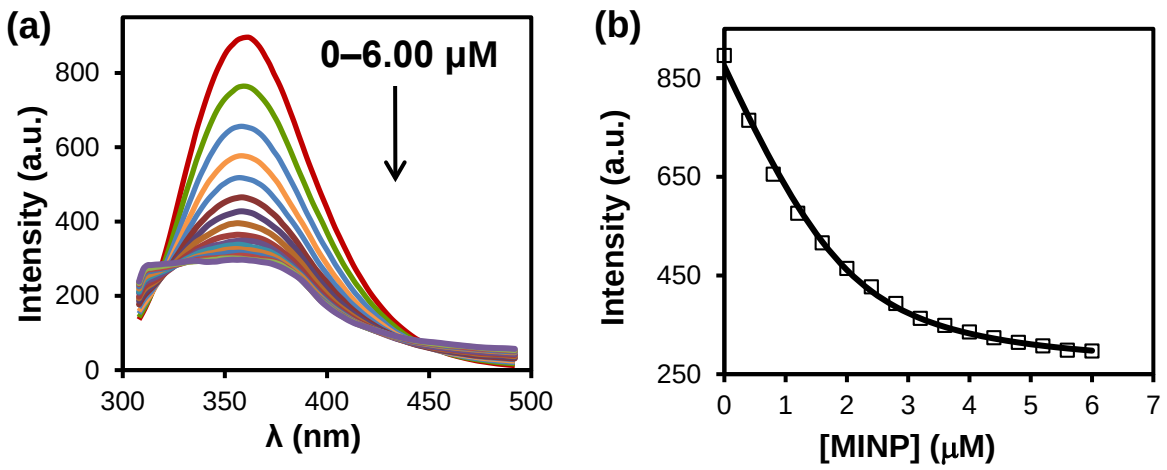


Figure S50. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WNW (2.0 μM) upon addition of different concentrations of MINP(WDW) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WNW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 2 in Table S1.

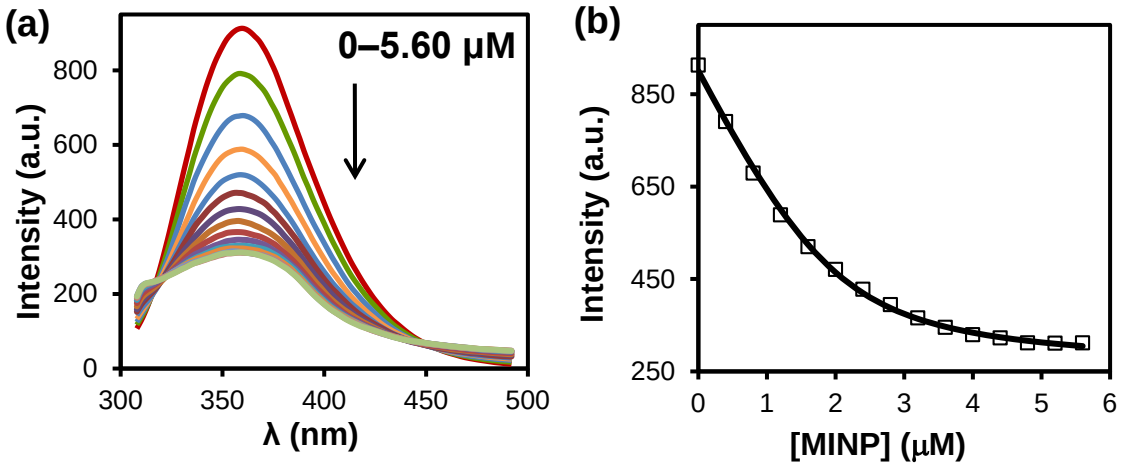


Figure S51. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WNW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:3) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WNW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 10 in Table S1.

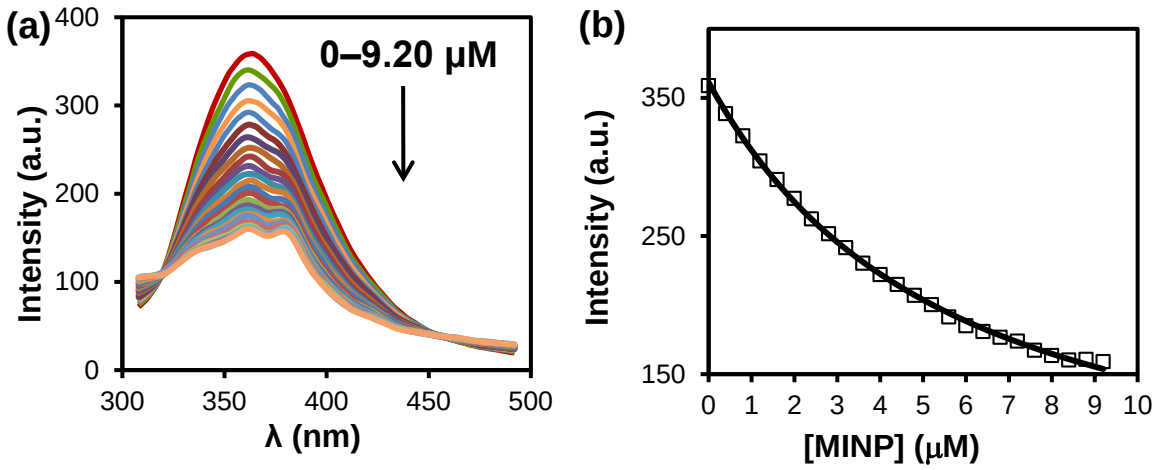


Figure S52. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide GDW (2.0 μM) upon addition of different concentrations of MINP(WDW) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide GDW at 364 nm to a 1:1 binding isotherm. The data correspond to entry 3 in Table S1.

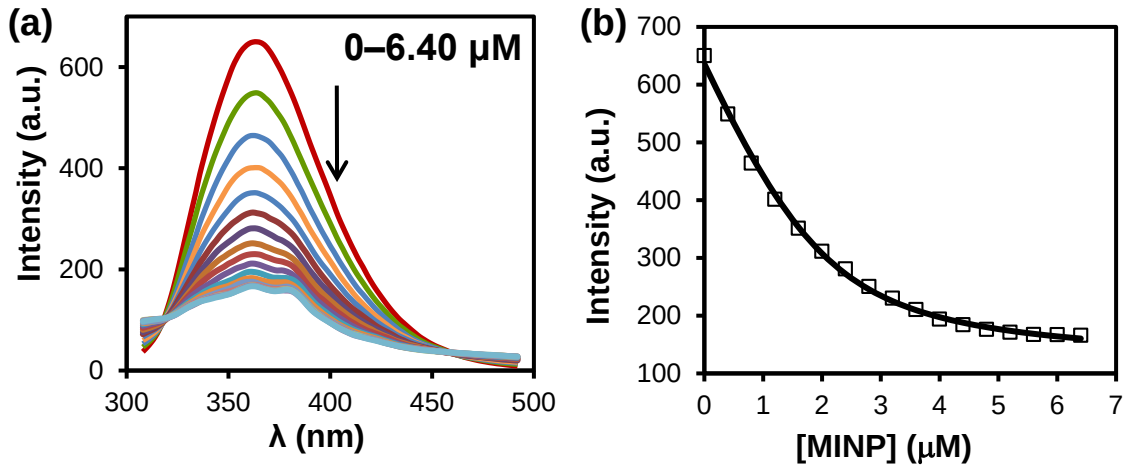


Figure S53 (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide GDW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:3) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide GDW at 364 nm to a 1:1 binding isotherm. The data correspond to entry 11 in Table S1.

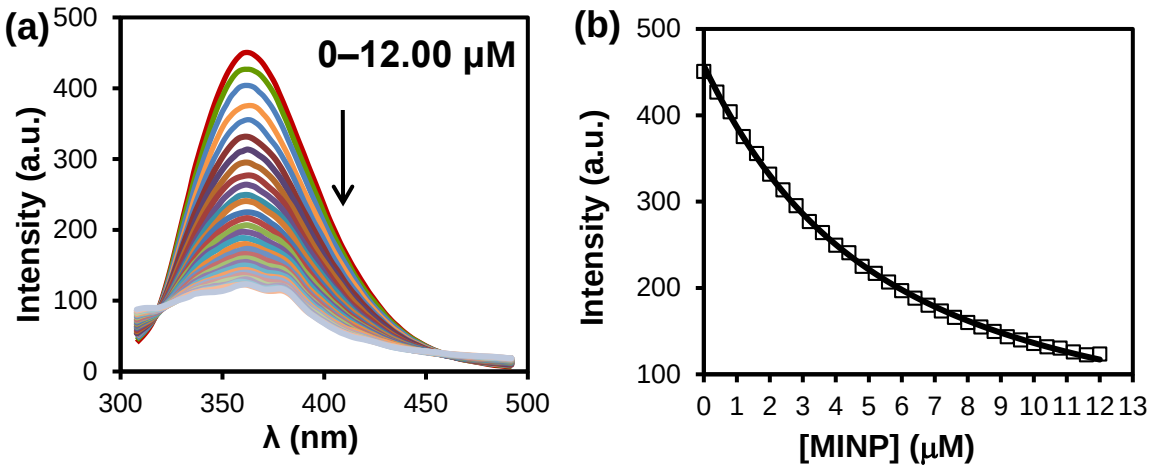


Figure S54. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide DW (2.0 μM) upon addition of different concentrations of MINP(WDW) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide DW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 4 in Table S1.

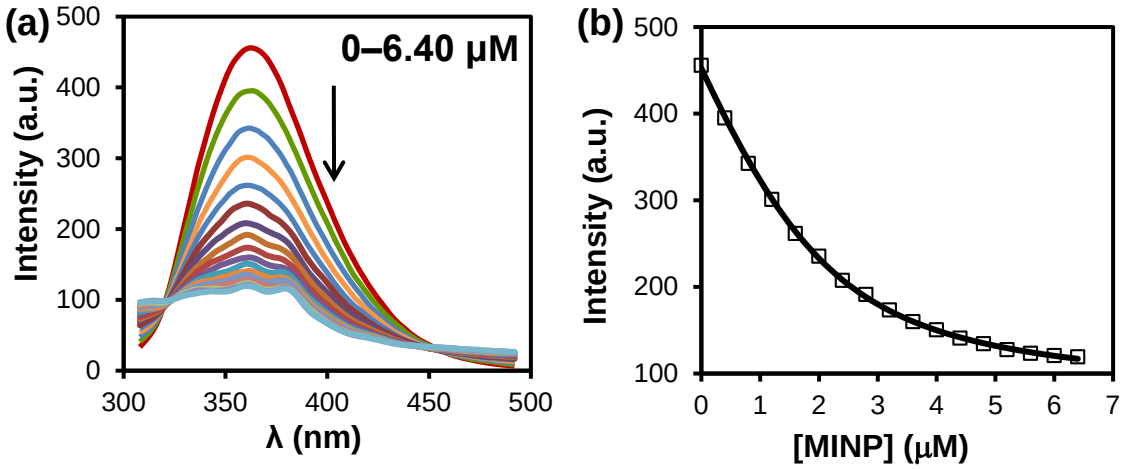


Figure S55. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide DW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:3) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide DW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 12 in Table S1.

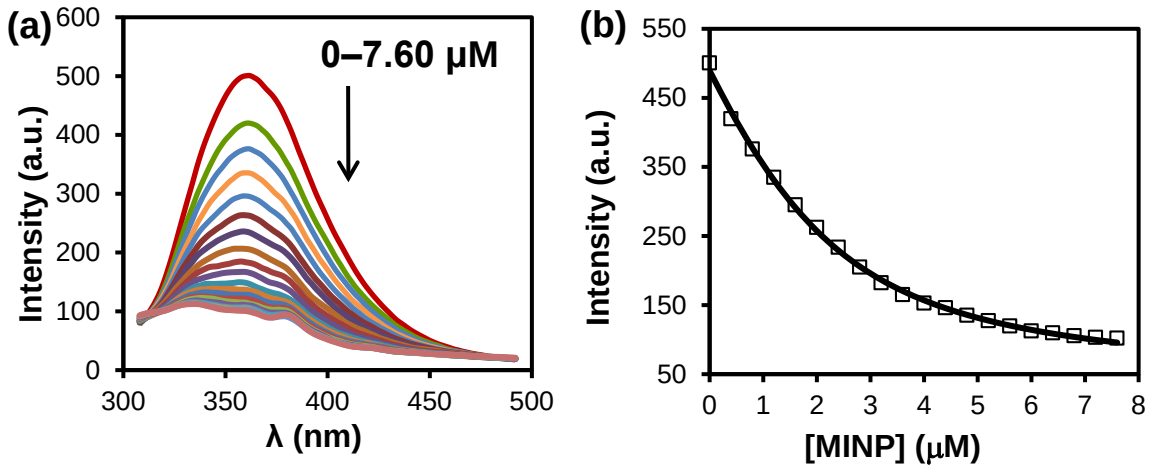


Figure S56. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide GWDW (2.0 μM) upon addition of different concentrations of MINP(WDW) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide GWDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 5 in Table S1.

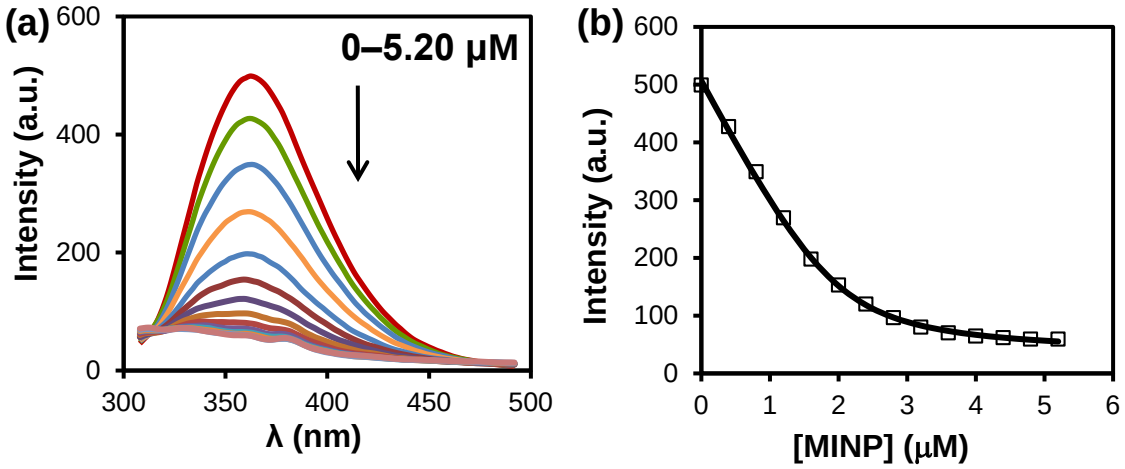


Figure S57. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide GWDW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:3) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide GWDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 13 in Table S1.

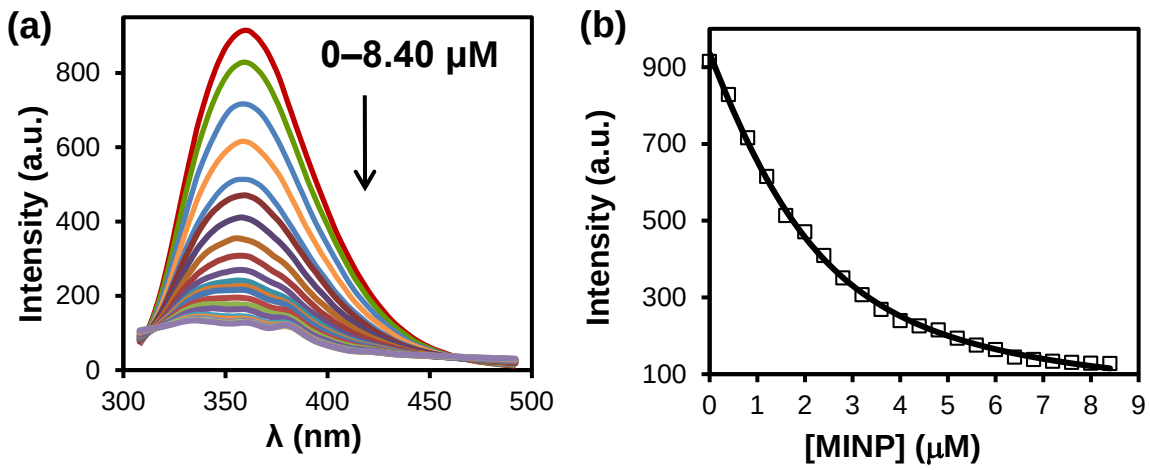


Figure S58. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WEW (2.0 μM) upon addition of different concentrations of MINP(WDW) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WEW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 2 in Table 5.

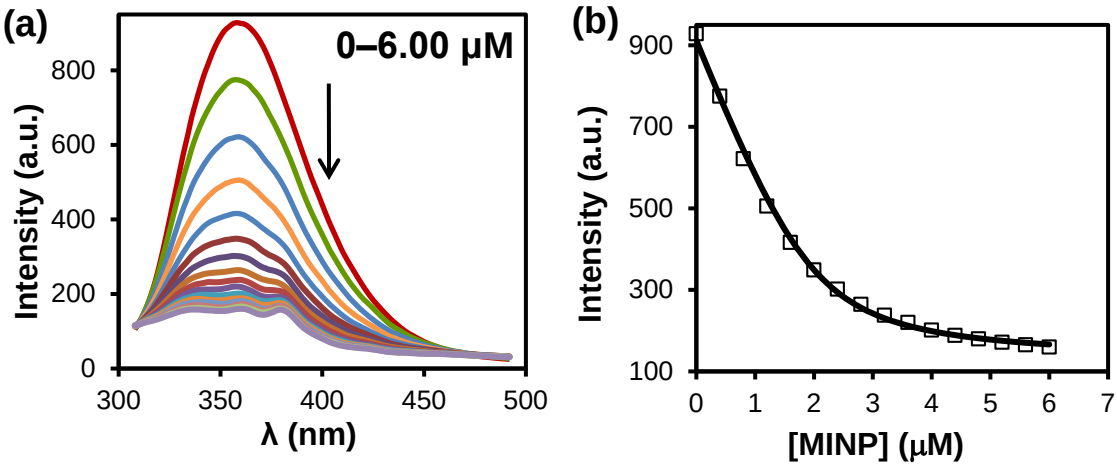


Figure S59. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WEW (2.0 μM) upon addition of different concentrations of MINP(WDW) with FM **2** (1:3) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WEW at 360 nm to a 1:1 binding isotherm. The data correspond to entry 6 in Table 5.

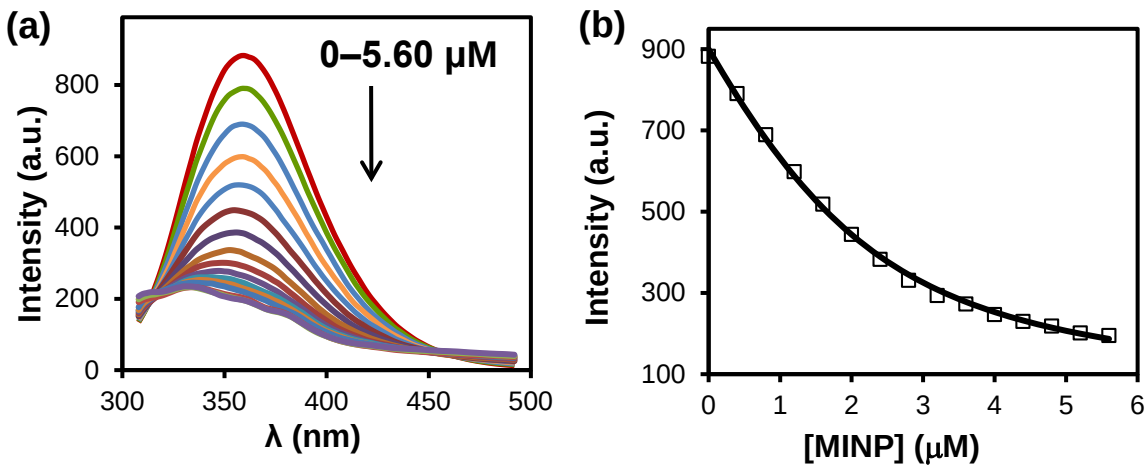


Figure S60. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WEW) without functional monomer in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 4 in Table 5.

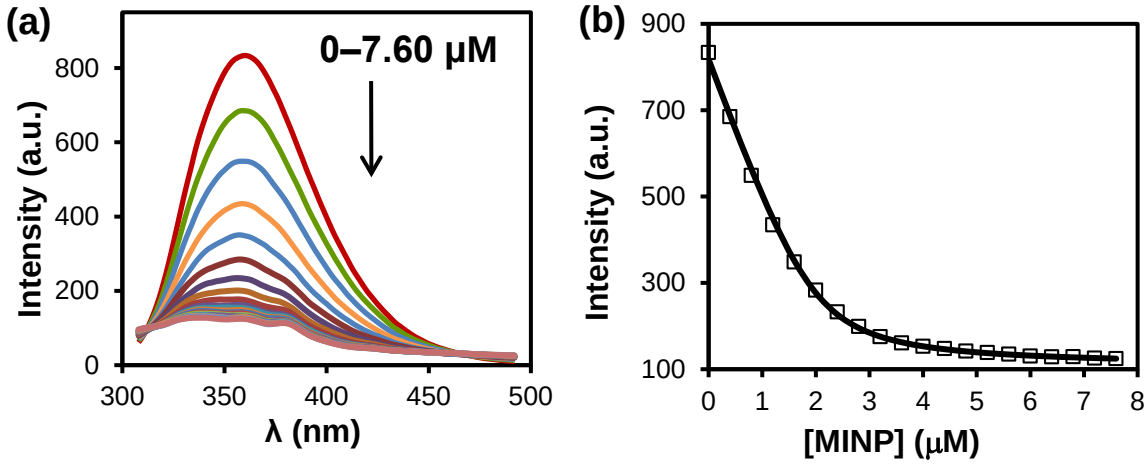


Figure S61. (a) Fluorescence emission spectra (λ_{ex} = 280 nm) of peptide WDW (2.0 μM) upon addition of different concentrations of MINP(WEW) with FM **2** (1:3) in water. The MINP was prepared by surfactant **3**. (b) Nonlinear least squares fitting of the emission intensity of peptide WDW at 362 nm to a 1:1 binding isotherm. The data correspond to entry 8 in Table 5.

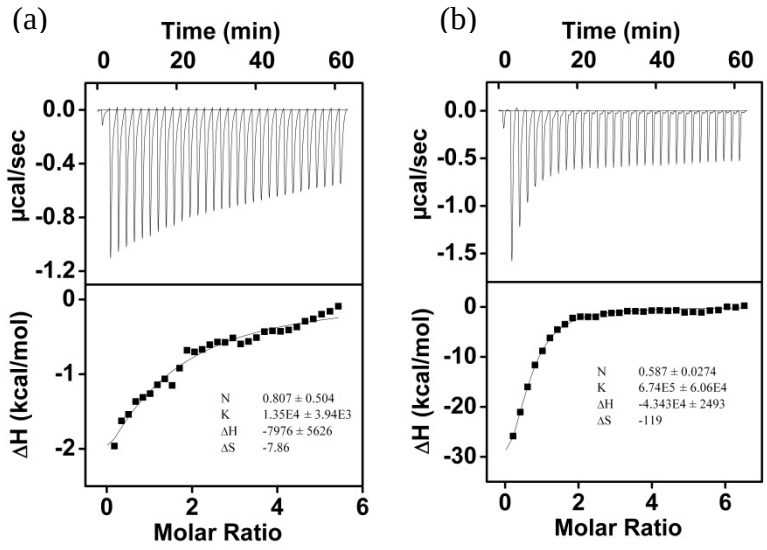


Figure S62. ITC titration curves obtained at 298 K for the titration of 30 µM of (a) MINP(DGEA) without FM and (b) MINP(DGEA) with FM **2** (1:4.5) by peptide DGEA in water. The guest concentrations are (a) 700 µM and (b) 840 µM, respectively.

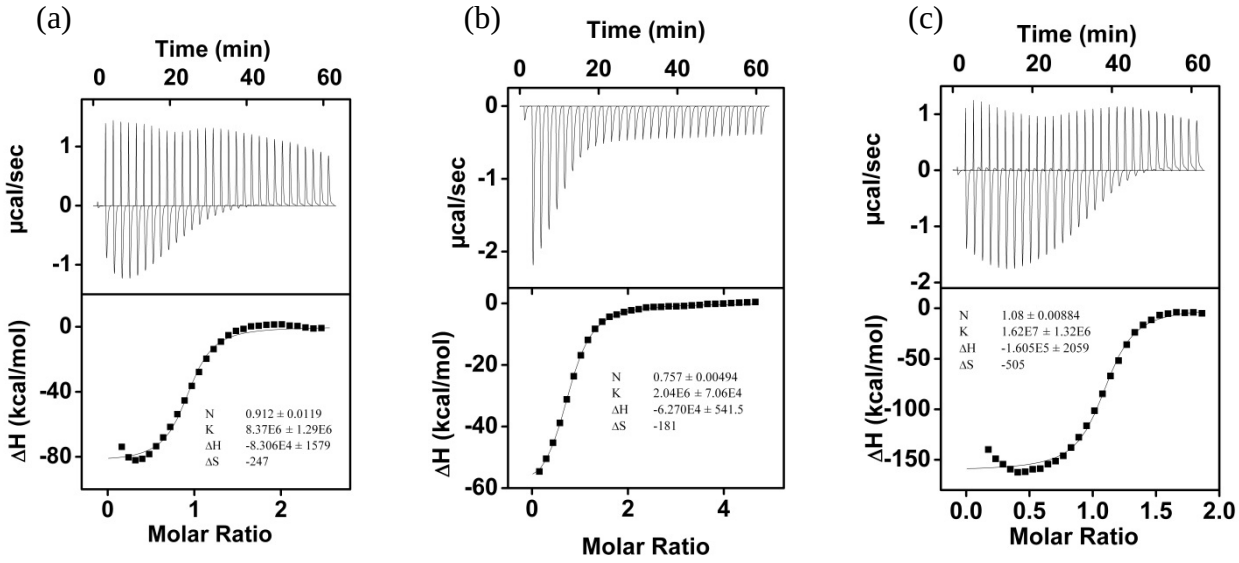


Figure S63. ITC titration curves obtained at 298 K for the titration of 5.0 µM of (a) MINP(c-Myc) with FM **2** (1:7.5) by peptide c-Myc (55 µM), (b) MINP(DYKDDDDK) with FM **2** (1:9) by peptide DYKDDDDK (100 µM) and (c) MINP(HIF-1 alpha) with FM **2** (1:10.5) by peptide HIF-1 alpha (40 µM) in water.

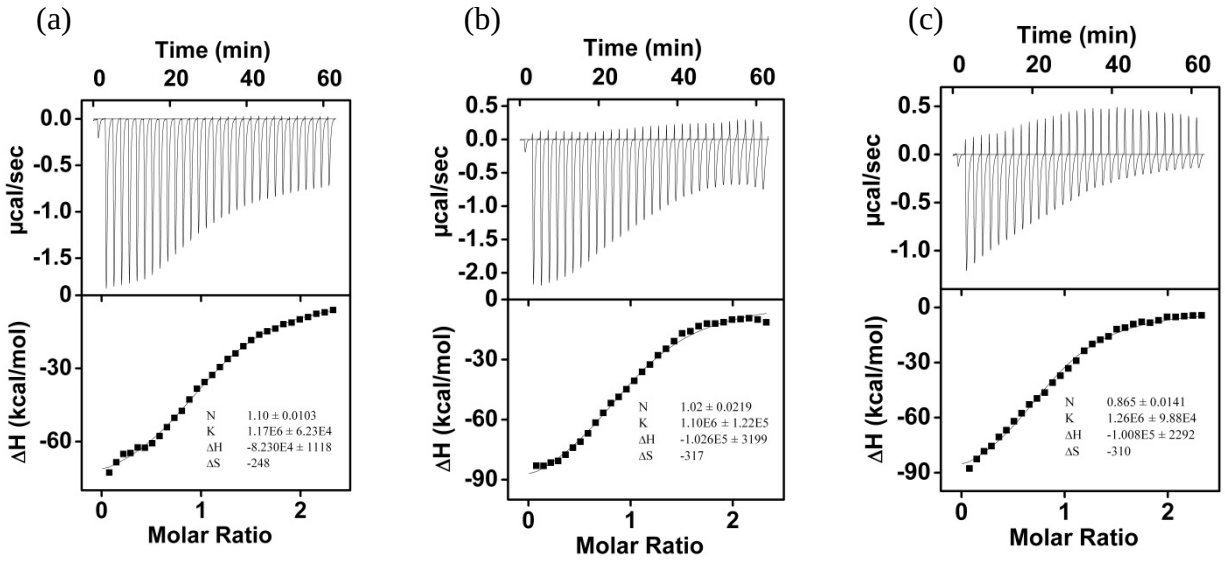


Figure S64. ITC titration curves obtained at 298 K for the titration of 5.0 µM of MINP(DYKDDDDK) with FM 2 (1:9) by peptide DYKDDDDK (50 µM) in (a) HEPES buffer (pH 7.4, 10 mM), (b) MES buffer (pH 6.0, 10 mM) and (c) Bicine buffer (pH 9.0, 10 mM), respectively.

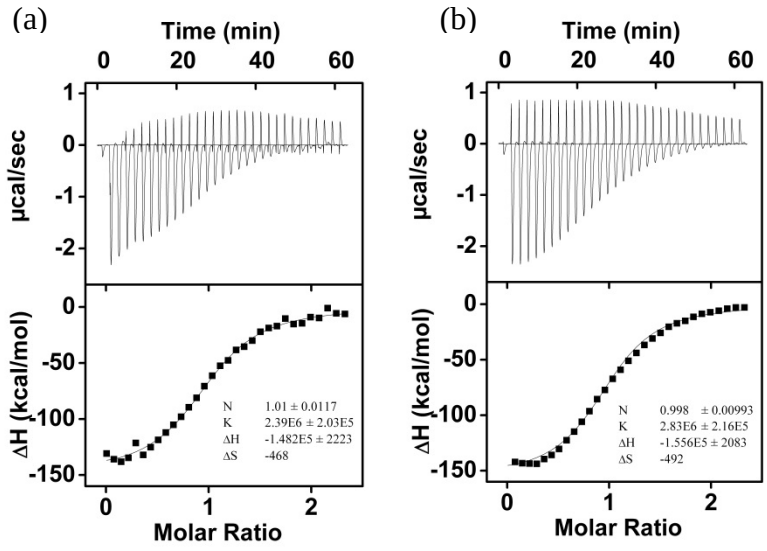
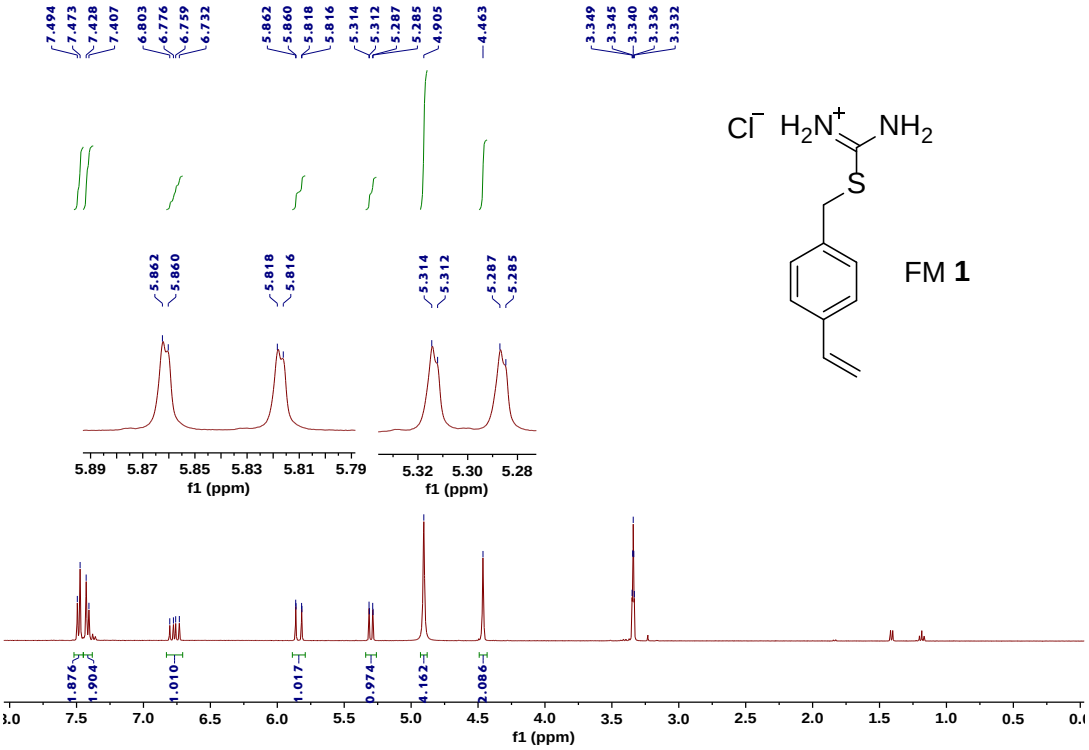
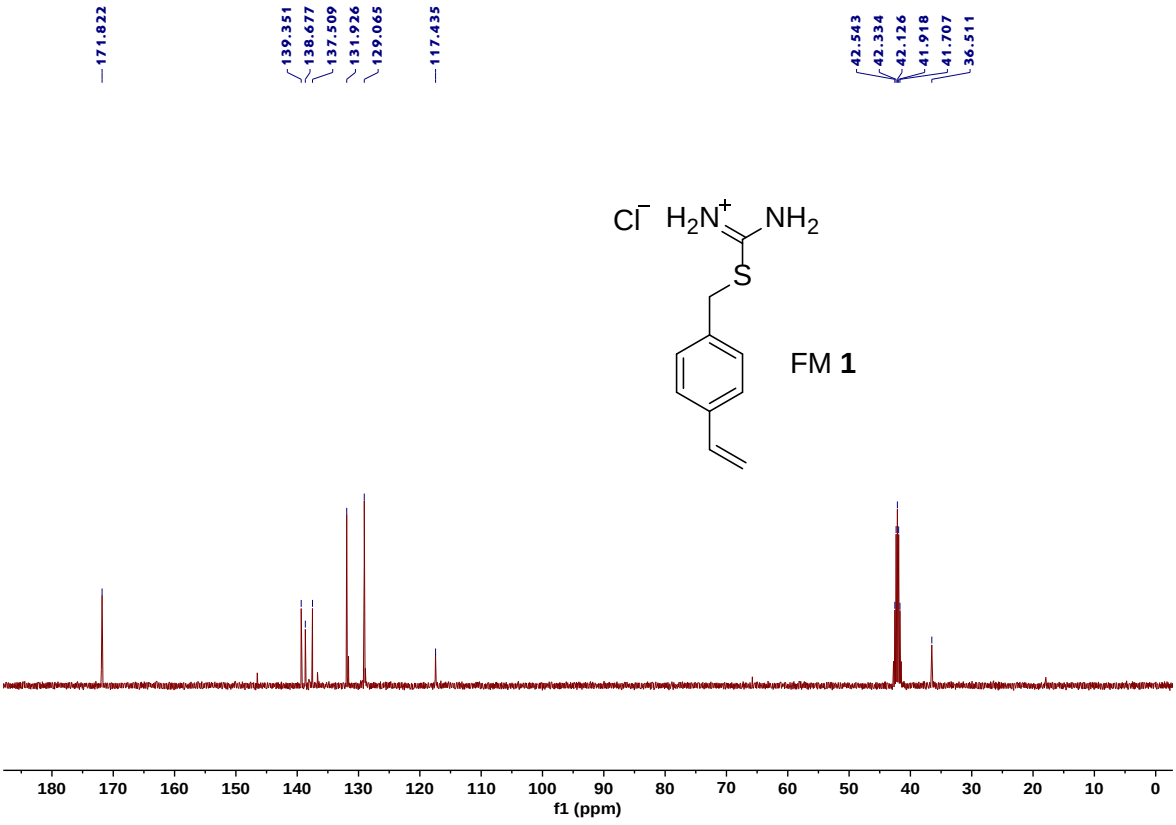
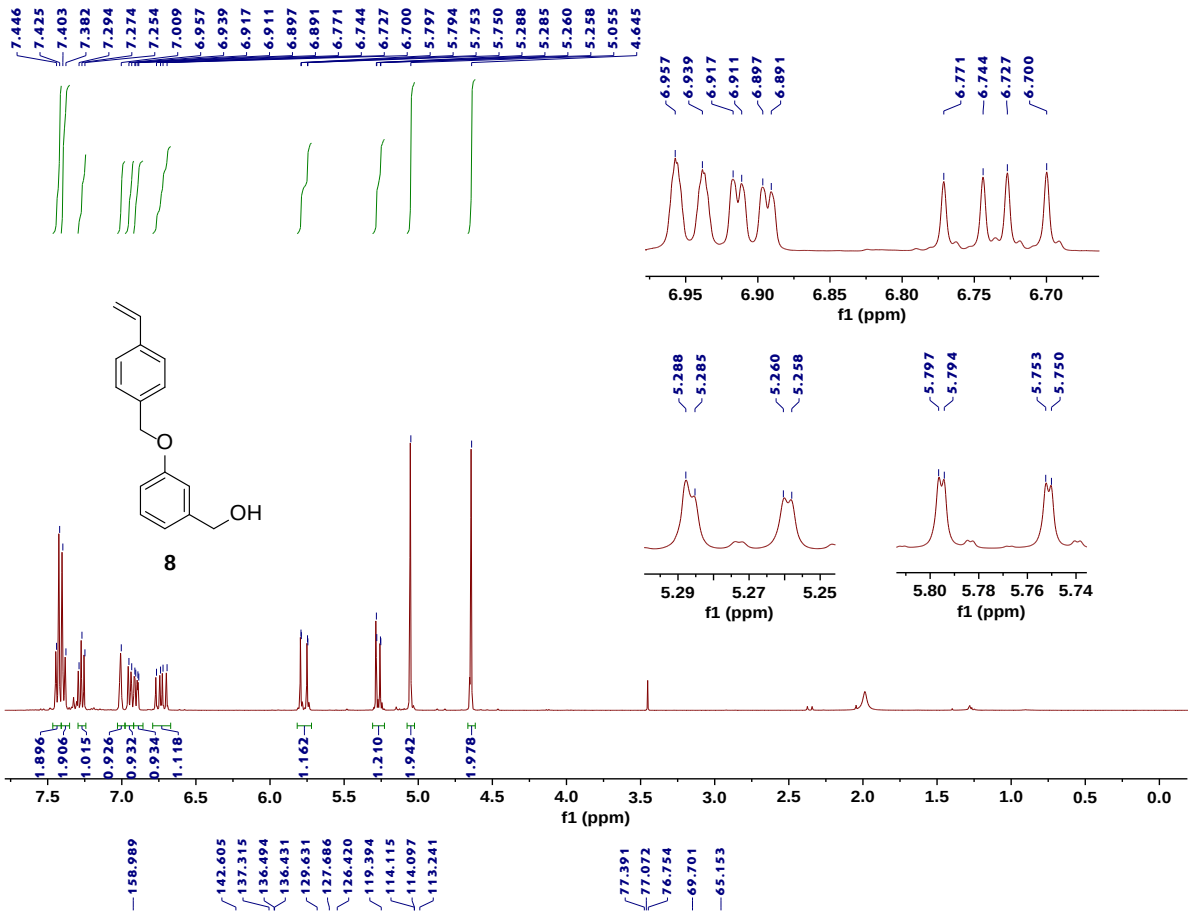


Figure S65. ITC titration curves obtained at 298 K for the titration of 5.0 µM of MINP(DYKDDDDK) with FM 2 (1:9) by peptide DYKDDDDK (50 µM) in (a) Tris buffer (pH 7.4, 10 mM) and (b) Tris buffer (pH 9.0, 10 mM), respectively.

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



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7.382
7.294
7.274
7.254
7.009
6.957
6.939
6.917
6.911
6.897
6.891
6.771
6.744
6.727
6.700
5.797
5.794
5.753
5.750
5.288
5.285
5.260
5.258
5.055
4.645
6.957
6.939
6.917
6.911
6.897
6.891
6.771
6.744
6.727
6.700
6.95
6.90
6.85
6.80
6.75
6.70
f1 (ppm)
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5.285
5.260
5.258
5.797
5.794
5.753
5.750
5.29
5.27
5.25
f1 (ppm)
5.80
5.78
5.76
5.74
f1 (ppm)
O
OH
8
1.896
1.906
1.015
0.926
0.932
0.934
1.118
1.162
1.210
1.942
1.978
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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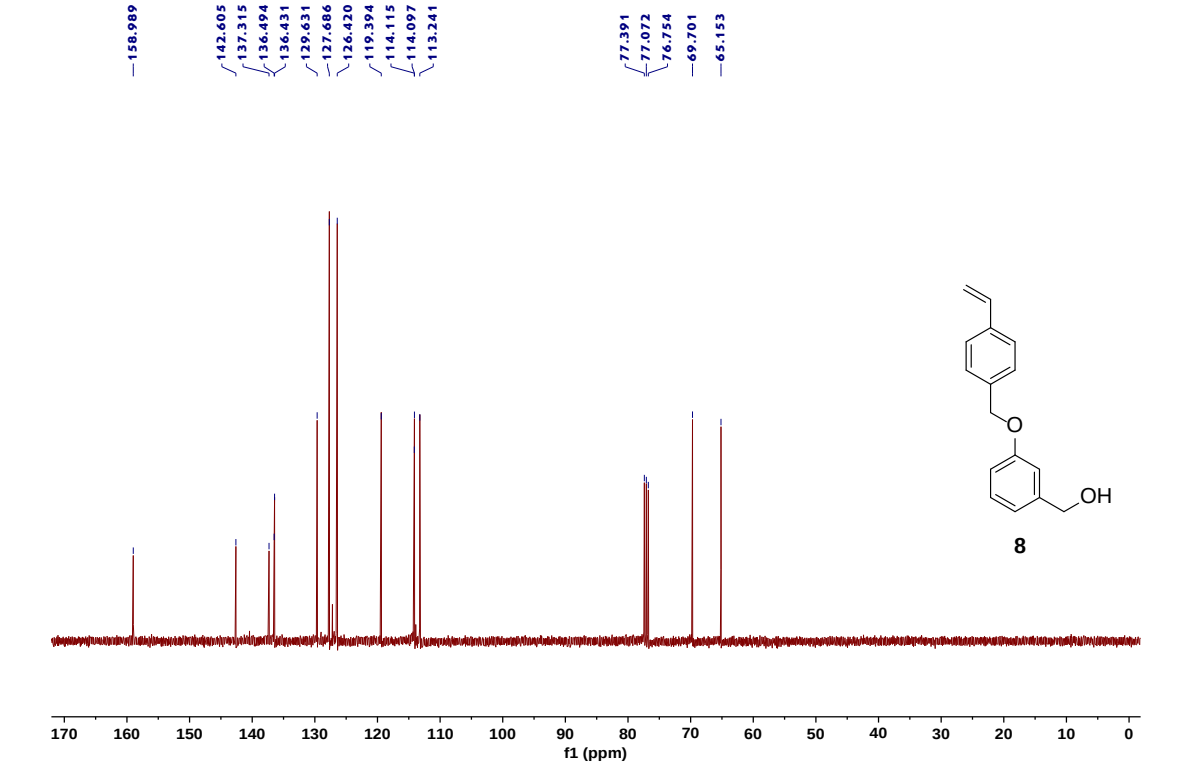
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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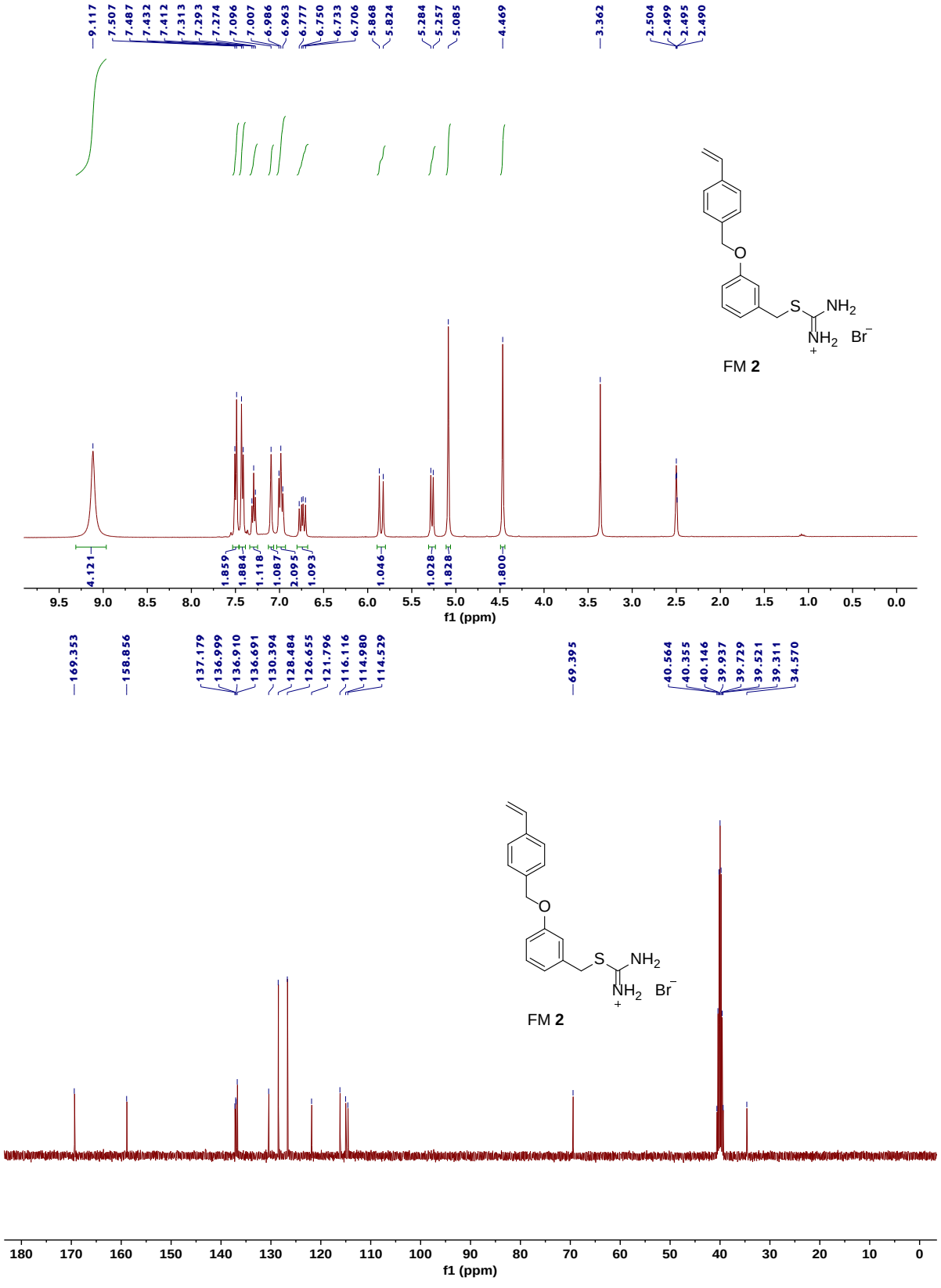
77.072
76.754
69.701
65.153
O
OH
8
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.706
5.868
5.824
5.284
5.257
5.085
4.469
3.362
2.504
2.499
2.495
2.490
O
S
NH2
NH2
Br−
FM 2
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1.118
1.087
2.095
1.093
1.046
1.028
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f1 (ppm)
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39.937
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39.521
39.311
34.570
f1 (ppm)