Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supplementary Information

Imprinted Micelles for Chiral Recognition in Water: Shape, Depth, and Number of Recognition Sites

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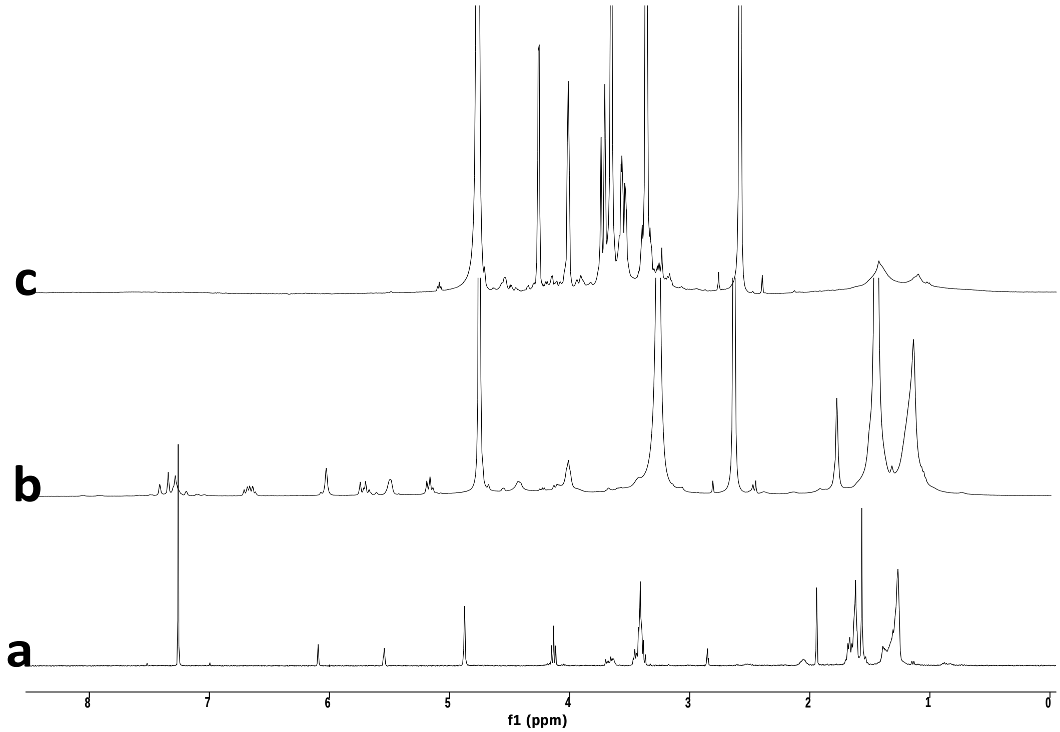


Figure S1. ^{1}H NMR spectra of: (a) **1** in $CDCl_3$, (b) alkynyl-SCM in D_2O, and (c) MINP(**4**) in D_2O.

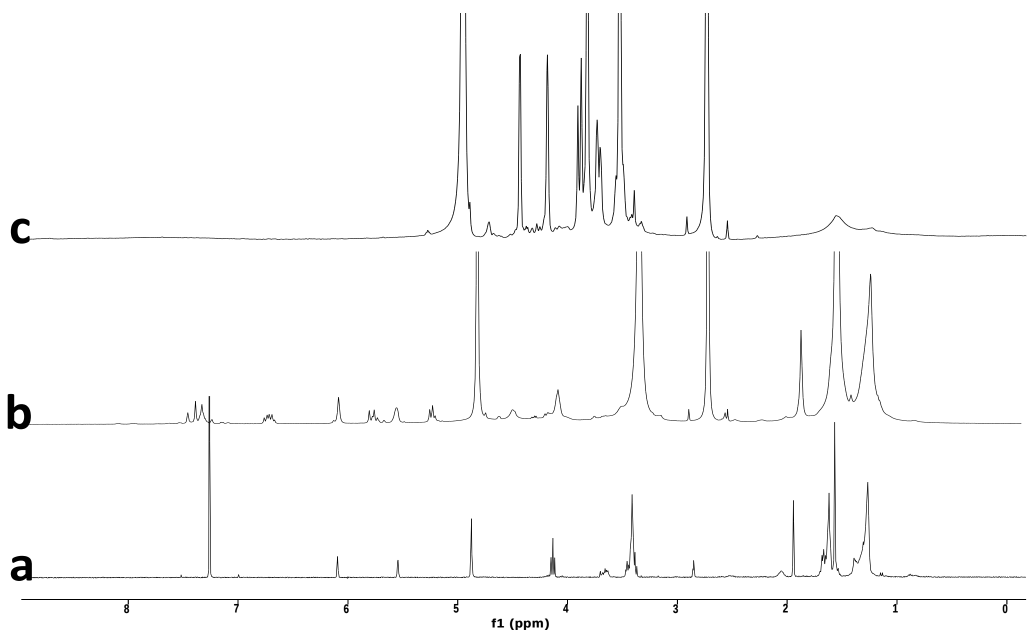


Figure S2. ^{1}H NMR spectra of: (a) **1** in $CDCl_3$, (b) alkynyl-SCM in D_2O, and (c) MINP(**6**) in D_2O.

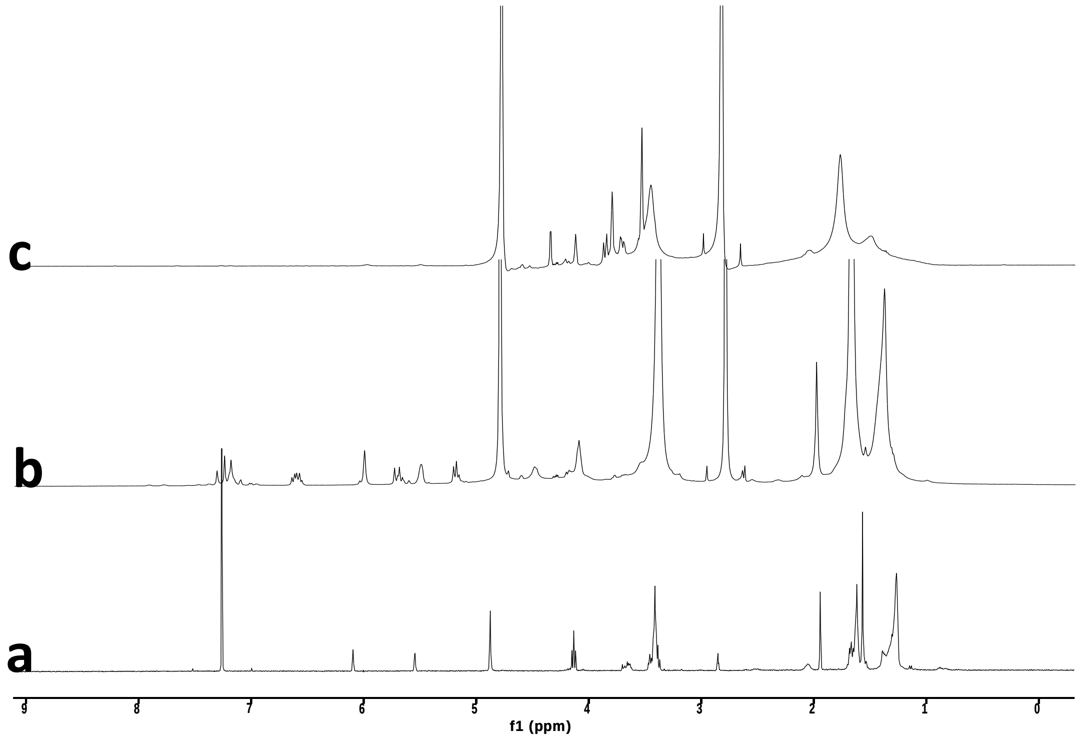


Figure S3. [1]H NMR spectra of: (a) **1** in $CDCl_3$, (b) alkynyl-SCM in D_2O, and (c) MINP(**7**) in D_2O.

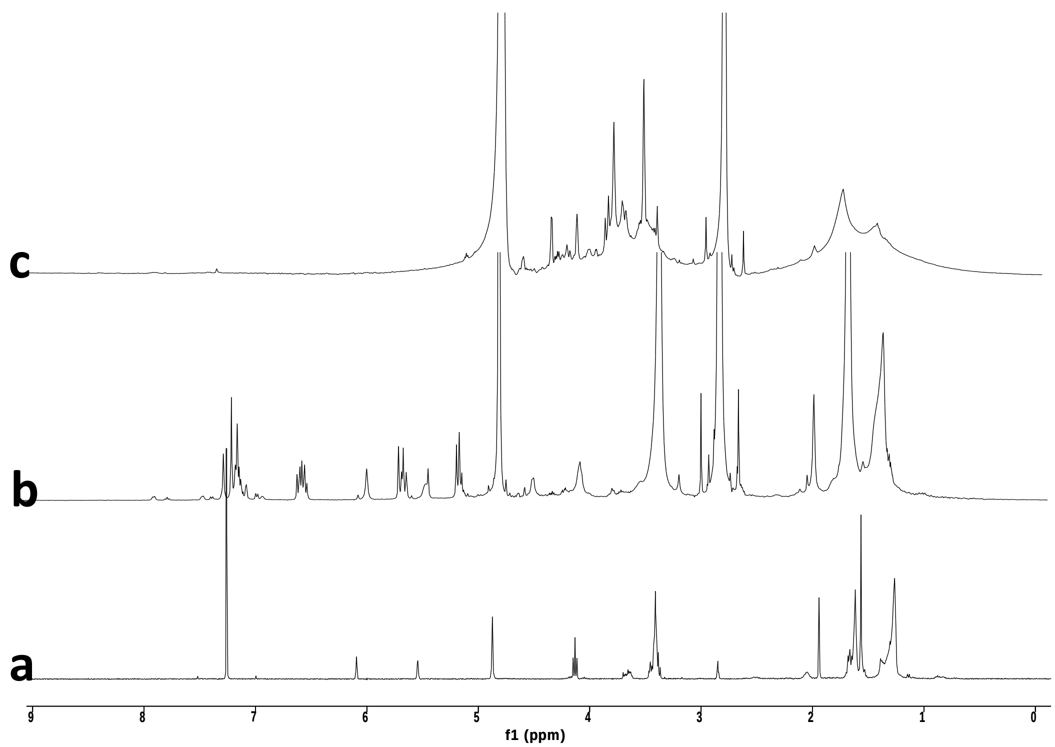


Figure S4. [1]H NMR spectra of: (a) **1** in $CDCl_3$, (b) alkynyl-SCM in D_2O, and (c) MINP(**10**) in D_2O.

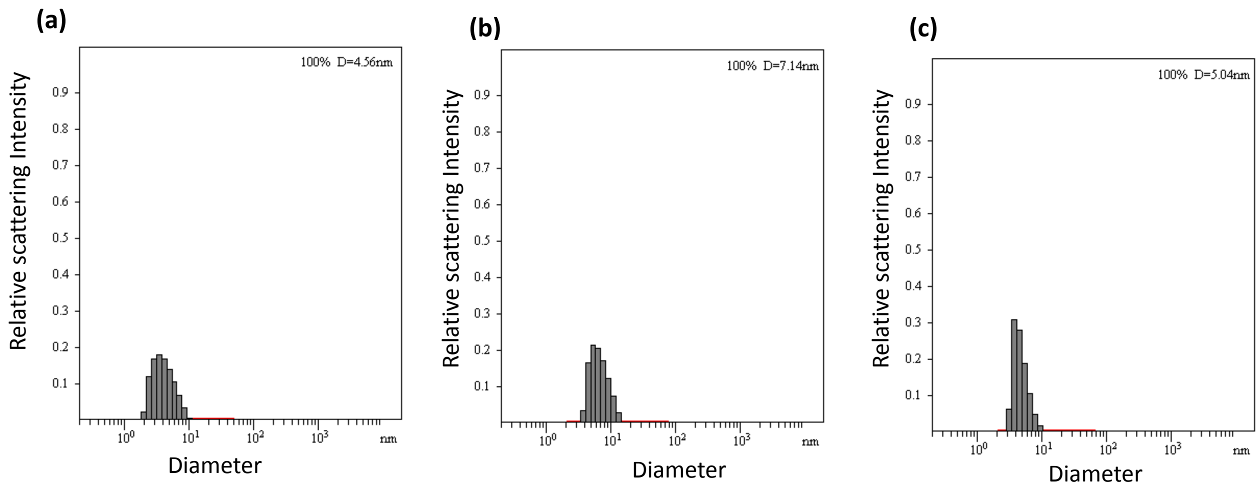


Figure S5. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM and (c) MINP(**4**) after purification.

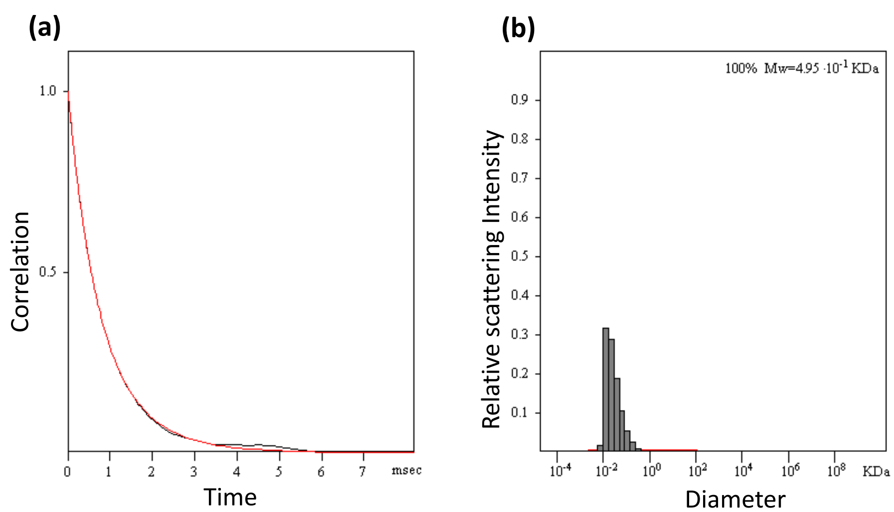


Figure S6. Distribution of the molecular weights and the correlation curves for MINP(**4**) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP is assumed to contain one molecule 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 0.04 molecules of 4-vinylphenylboronic acid (MW = 148 g/mol), the molecular weight of MINP translates to 49 [= 49500 / (465 + 1.2×172 + 130 + 0.8×264 + 0.04×148)] of such units.

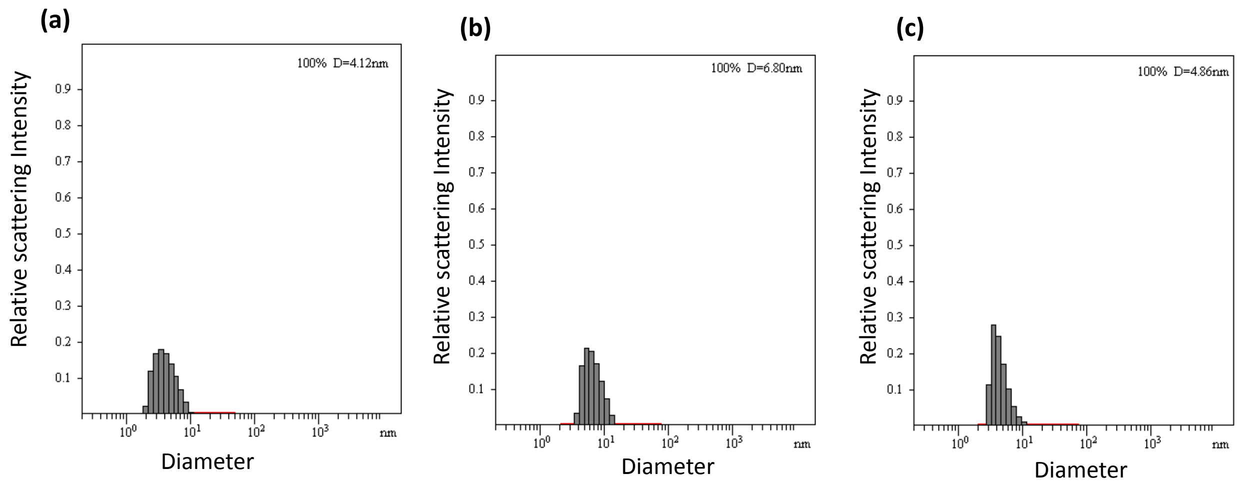


Figure S7. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM and (c) MINP(**6**) after purification.

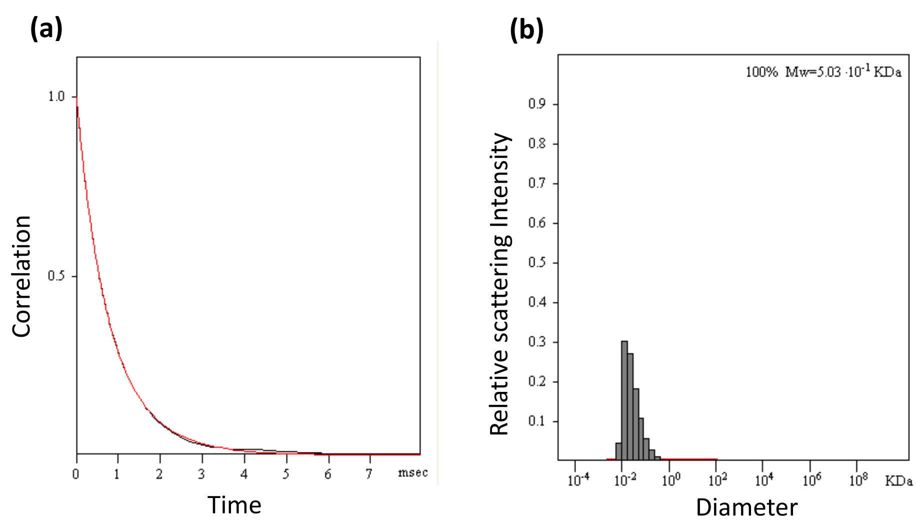


Figure S8. Distribution of the molecular weights and the correlation curves for MINP(**6**) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP is assumed to contain one molecule 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 translates to 50 [= 50300 / (465 + 1.2×172 + 130 + 0.8×264)] of such units.

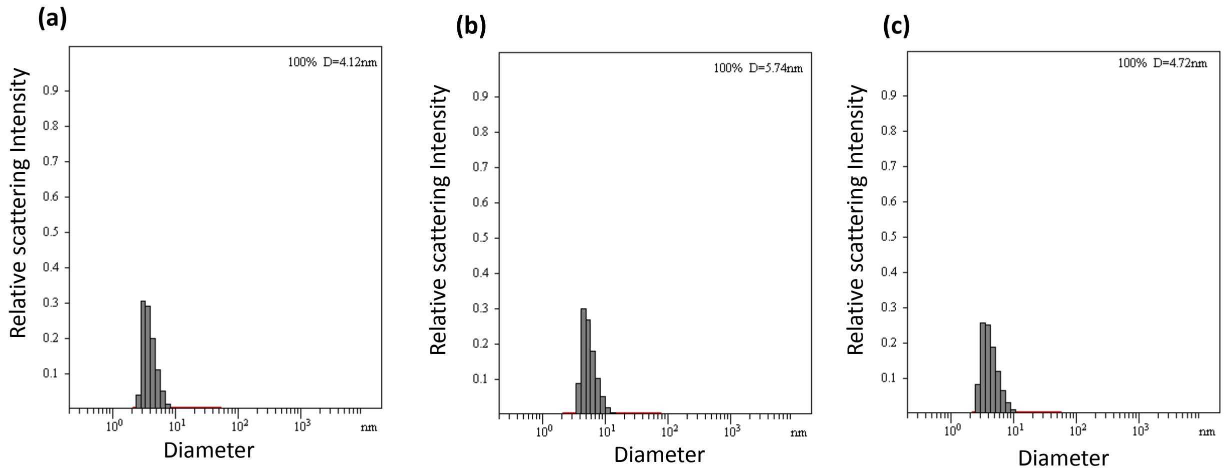


Figure S9. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM and (c) MINP(**7**) after purification.

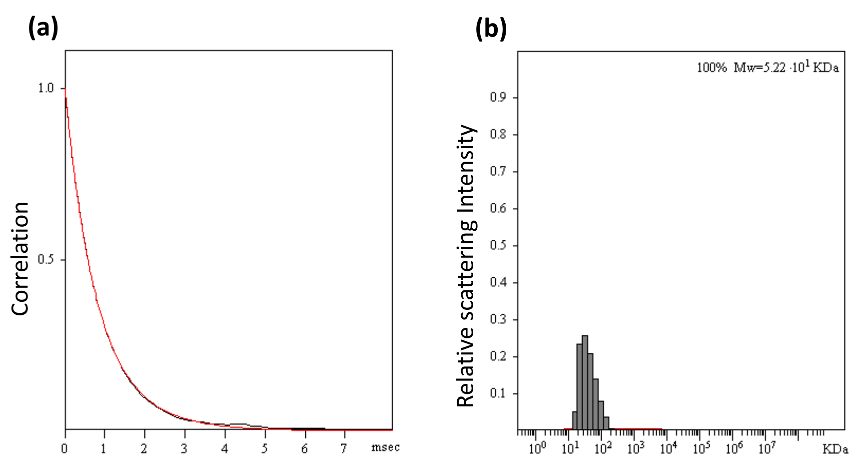


Figure S10. Distribution of the molecular weights and the correlation curves for MINP(**7**) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP is assumed to contain one molecule 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 0.04 molecules of 4-vinylphenylboronic acid (MW = 148 g/mol), the molecular weight of MINP translates to 52 [= 52200 / (465 + 1.2×172 + 130 + 0.8×264)] of such units.

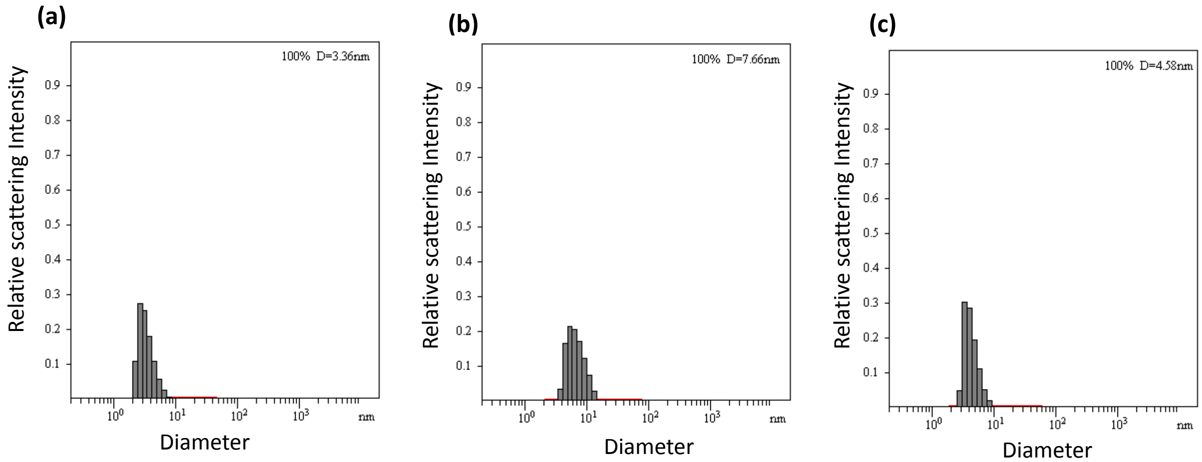


Figure S11. Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for (a) alkynyl-SCM, (b) surface-functionalized SCM and (c) MINP(**10**) after purification.

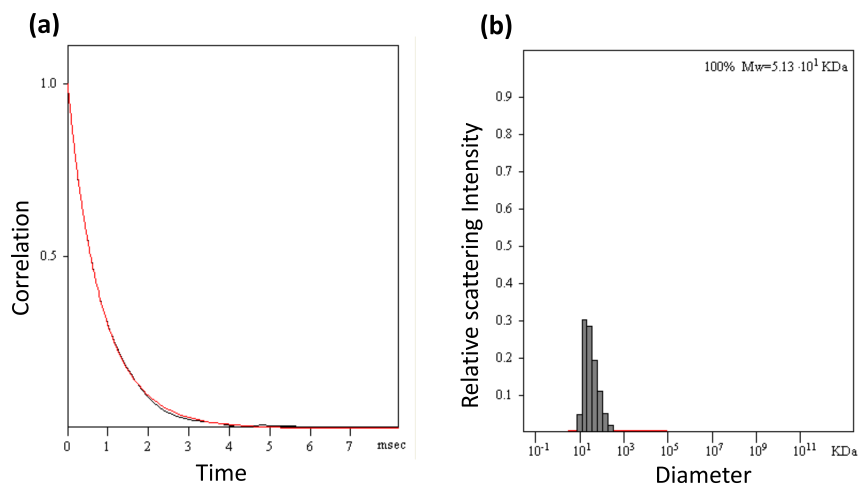


Figure S12. Distribution of the molecular weights and the correlation curves for MINP(**10**) from the DLS. The PRECISION DECONVOLVE program assumes the intensity of scattering is proportional to the mass of the particle squared. If each unit of building block for the MINP is assumed to contain one molecule 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 0.04 molecules of 4-vinylphenylboronic acid (MW = 148 g/mol), the molecular weight of MINP translates to 51 [= 51300 / (465 + 1.2×172 + 130 + 0.8×264)] of such units.

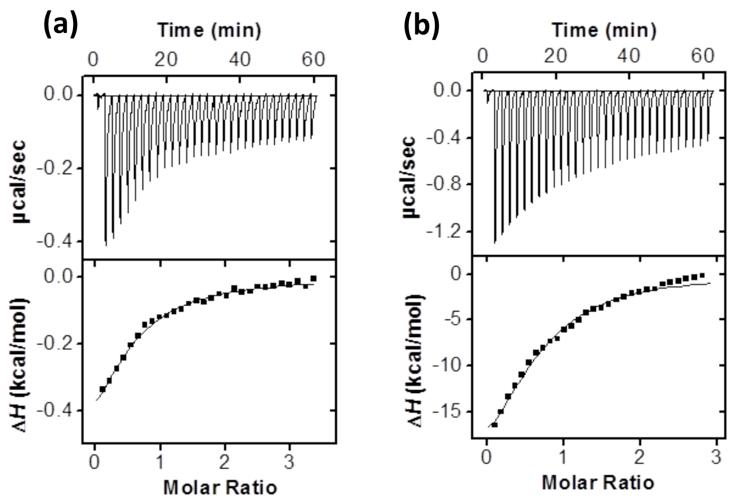


Figure S13. ITC titration curves obtained at 298 K for the binding of (a) **5** (3.0 mM) by MINP(**4**) (0.2 mM) and (b) **6** (0.15 mM) by MINP(**4**) (12 µM) in Millipore water. The data correspond to entries 3 and 4, respectively, in Table 1.

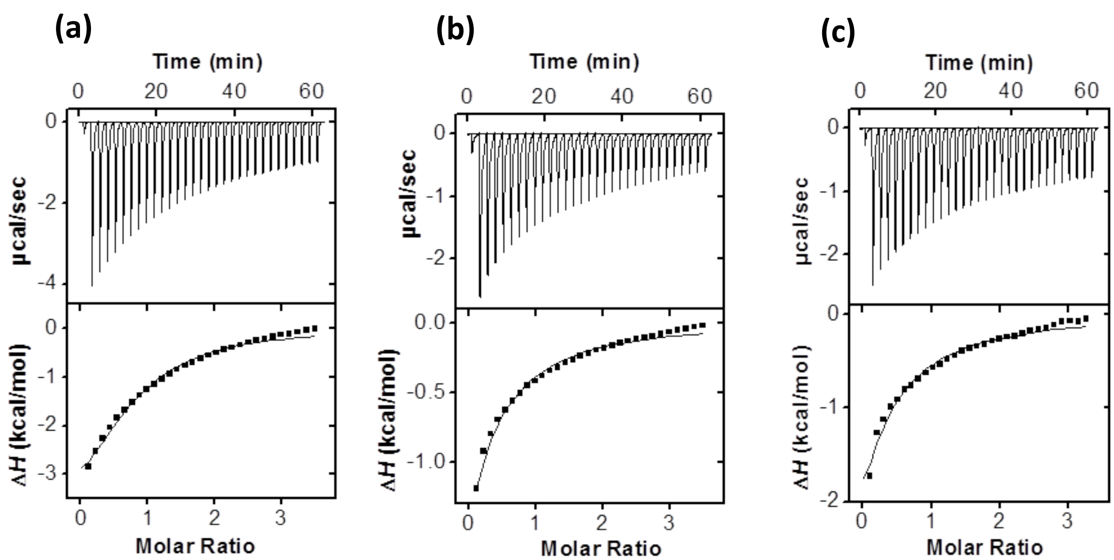


Figure S14. ITC titration curves obtained at 298 K for the binding of (a) **7** (3.0 mM) by MINP(**4**) (0.2 mM), (b) **8** (3.0 mM) by MINP(**4**) (0.2 mM) and (c) **9** (3.5 mM) by MINP(**4**) (0.25 mM). The data correspond to entries 5, 6, and 7, respectively, in Table 1.

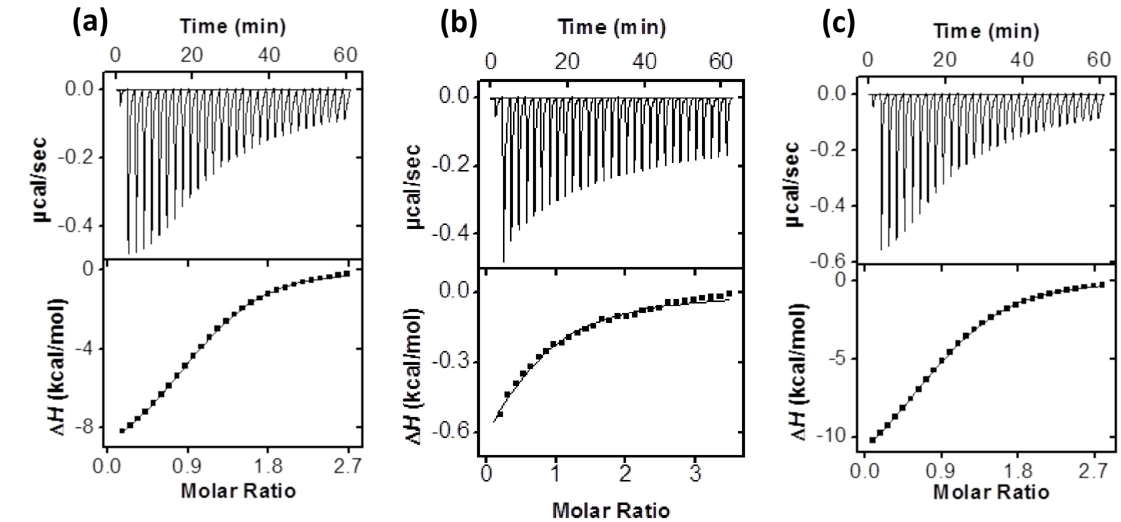


Figure S15. ITC titration curves obtained at 298 K for the binding of (a) **4** (0.12 mM) by MINP(**6**) (10 µM), (b) **5** (3.0 mM) by MINP(**6**) (0.2 mM), and (c) **6** (2.4 mM) by MINP(**6**) (0.2 mM). The data correspond to entries 8, 9, and 10, respectively, in Table 1.

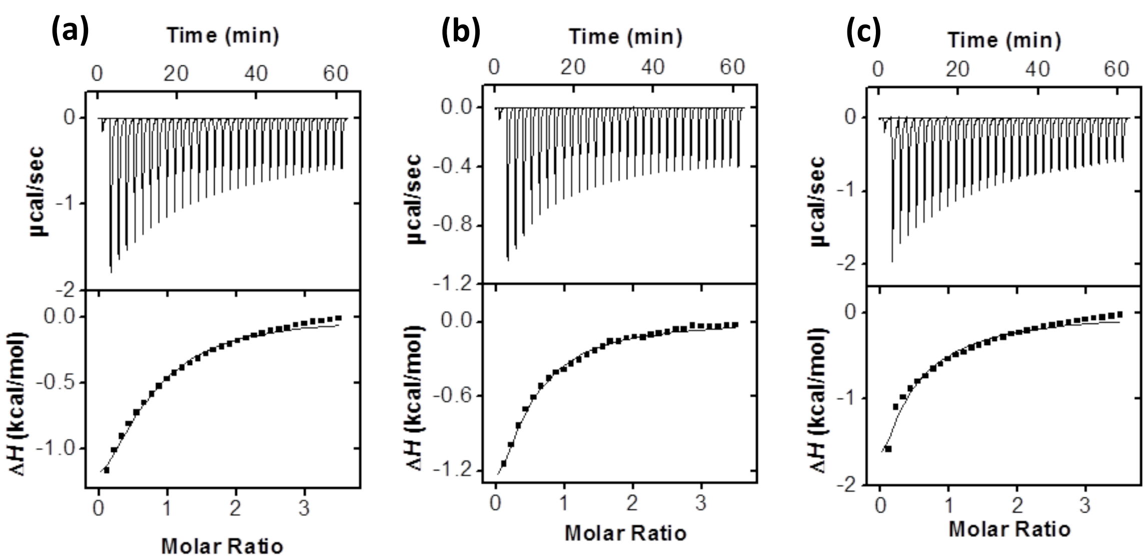


Figure S16. ITC titration curves obtained at 298 K for the binding of (a) **7** (3.0 mM) by MINP(**6**) (0.2 mM), (b) **8** (3.0 mM) by MINP(**6**) (0.2 mM) and (c) **9** (3.0 mM) by MINP(**6**) (0.2 mM). The data correspond to entries 11, 12, and 13, respectively, in Table 1.

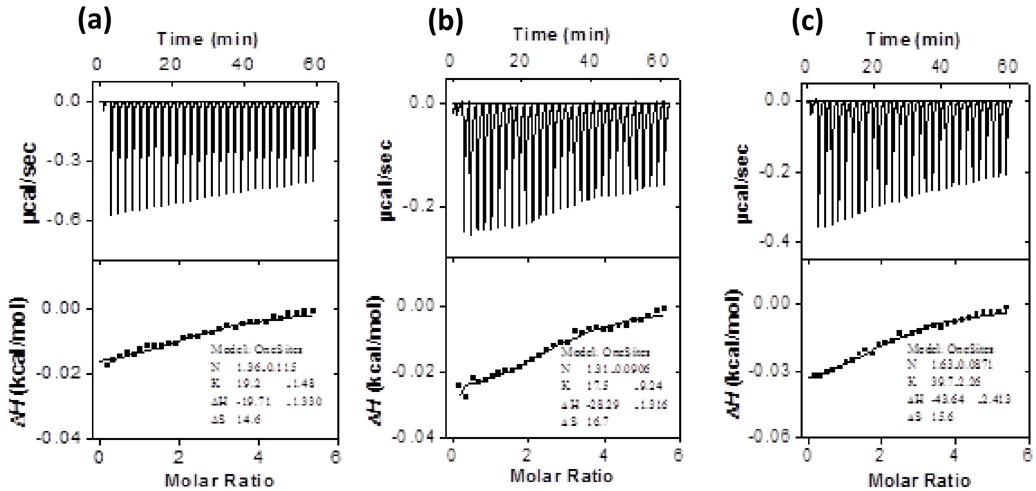


Figure S17. ITC titration curves obtained at 298 K for the binding of (a) **4,** (b) **5,** and (c) **6** MINP(**7**) (0.2 mM). The concentration of each guest was 6.0 mM. The data correspond to entries 14, 15, and 16, respectively, in Table 1.

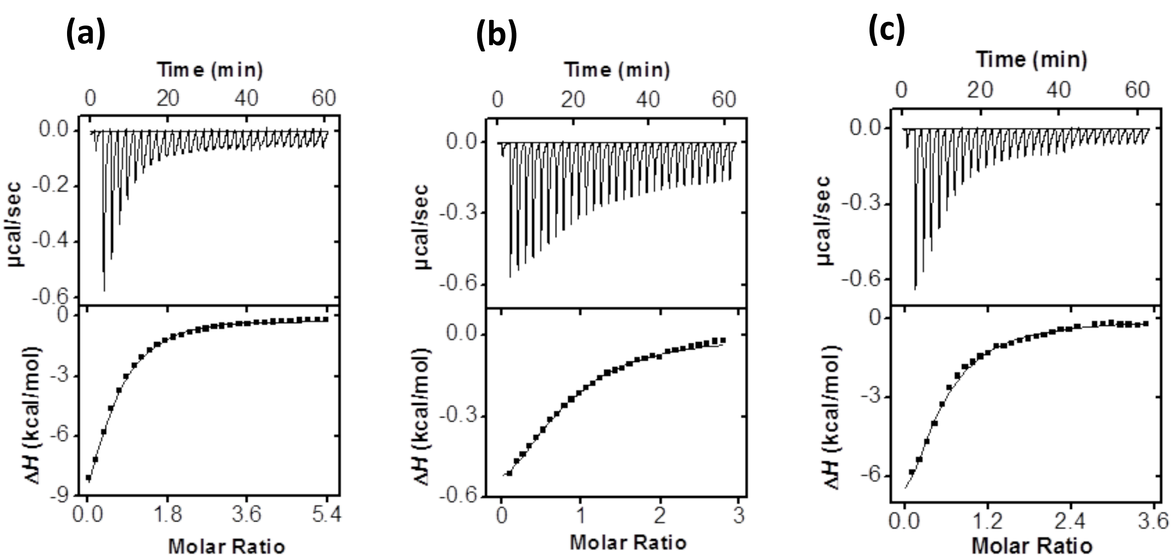


Figure S18. ITC titration curves obtained at 298 K for the binding of (a) **7** (0.24 mM) by MINP(**7**) (10 µM), **8** (2.4 mM) by MINP(**7**) (0.2 mM), and (b) **9** (0.3 mM) by MINP(**7**) (20 µM). The data correspond to entries 17, 18, and 19, respectively, in Table 1.

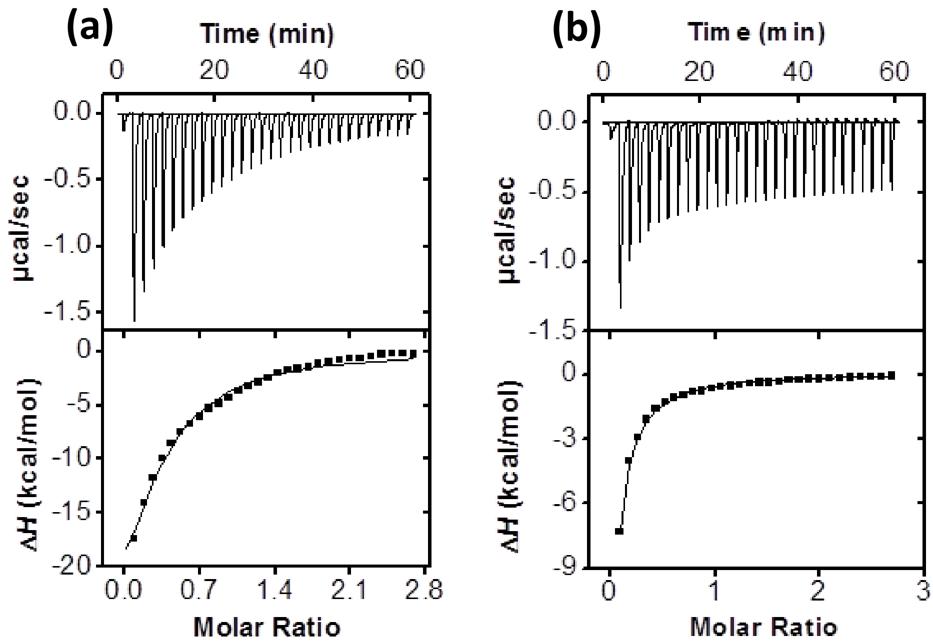
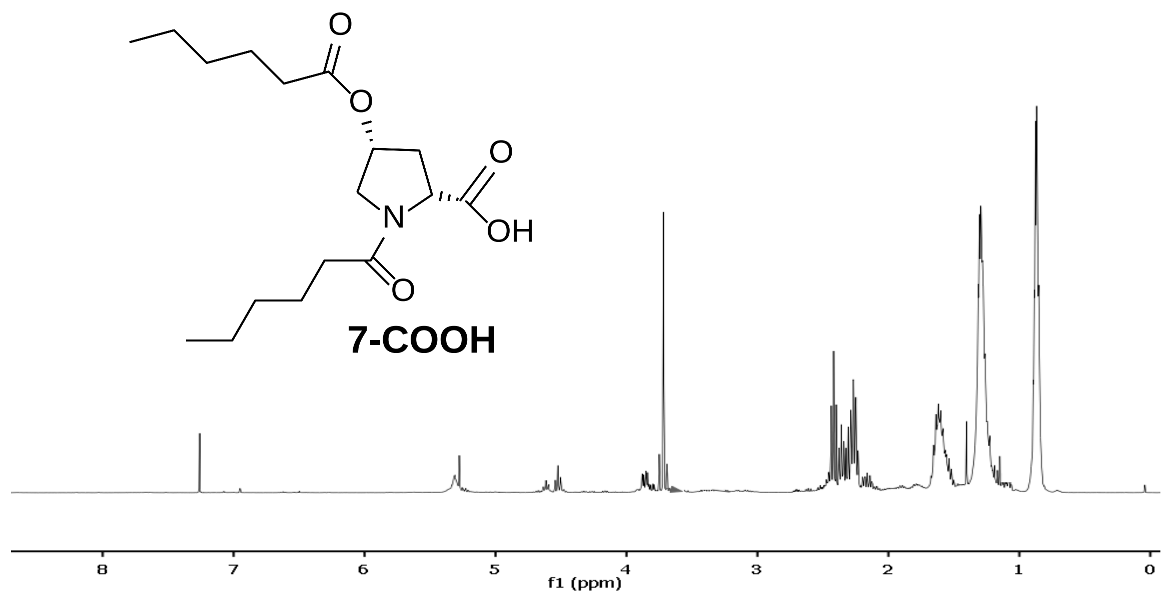
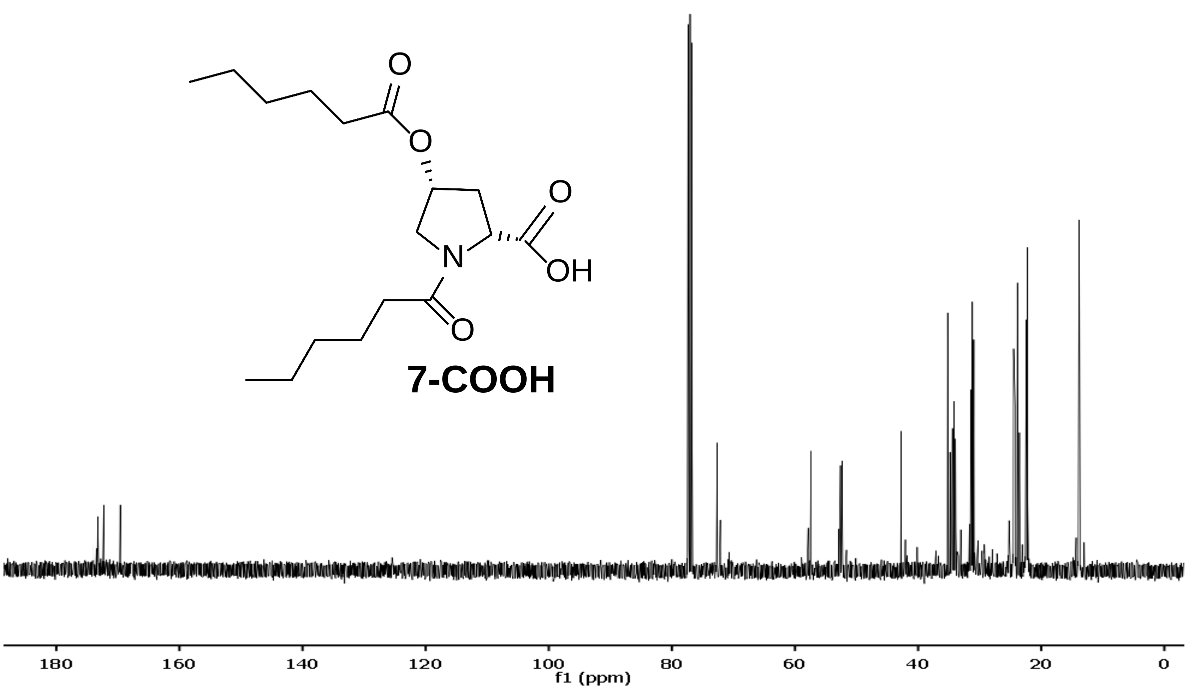
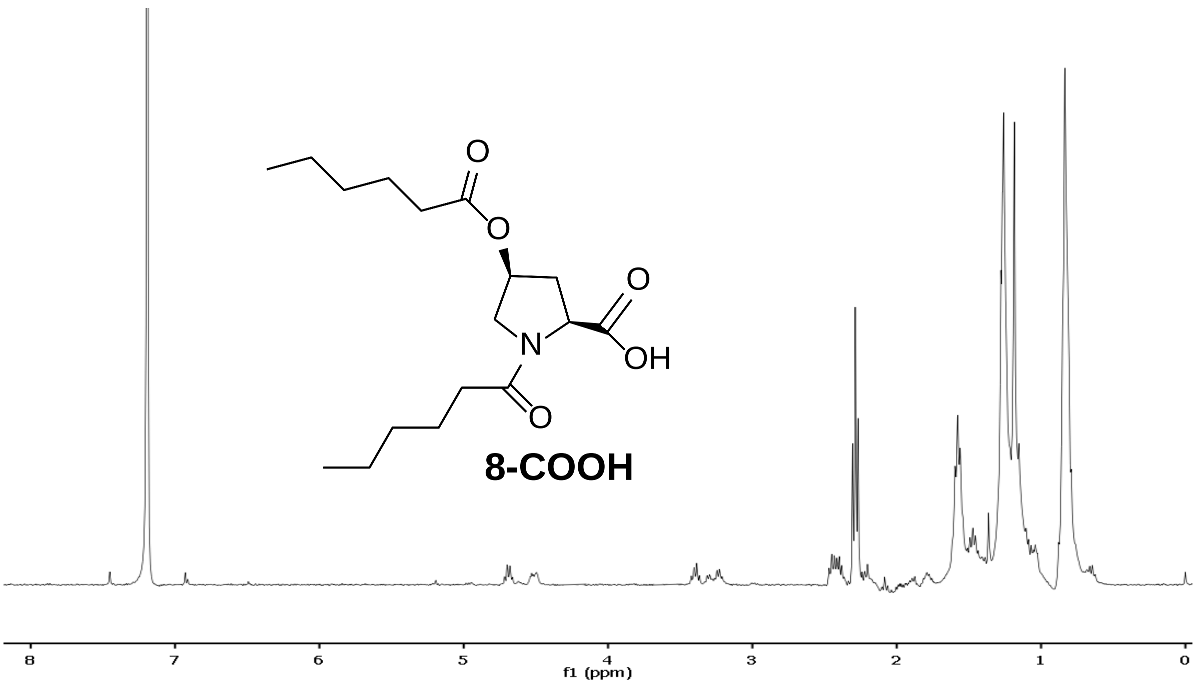


Figure S19. ITC titration curves obtained at 298 K for the binding of (a) **10** (0.12 mM) by MINP(**10**) (10 µM) and (b) **11** (0.12 mM) by MINP(**10**) (10 µM). The data correspond to entries 20 and 21, respectively, in Table 1.

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







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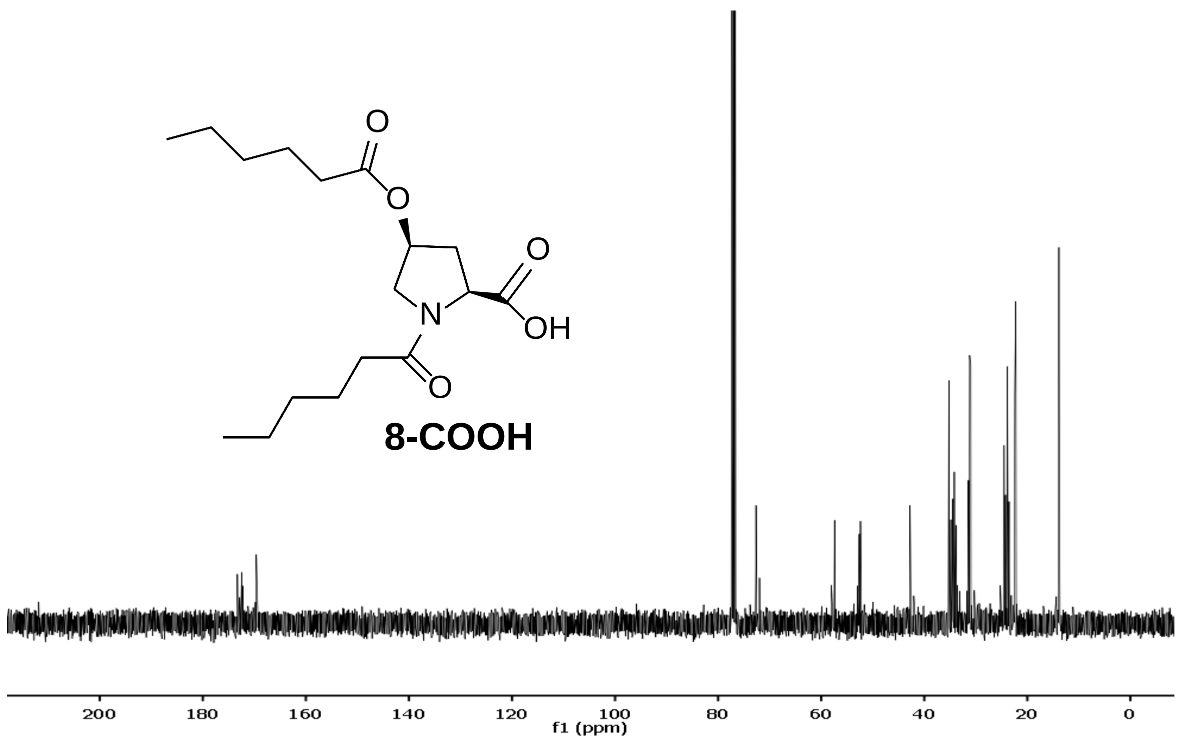
f1 (ppm)



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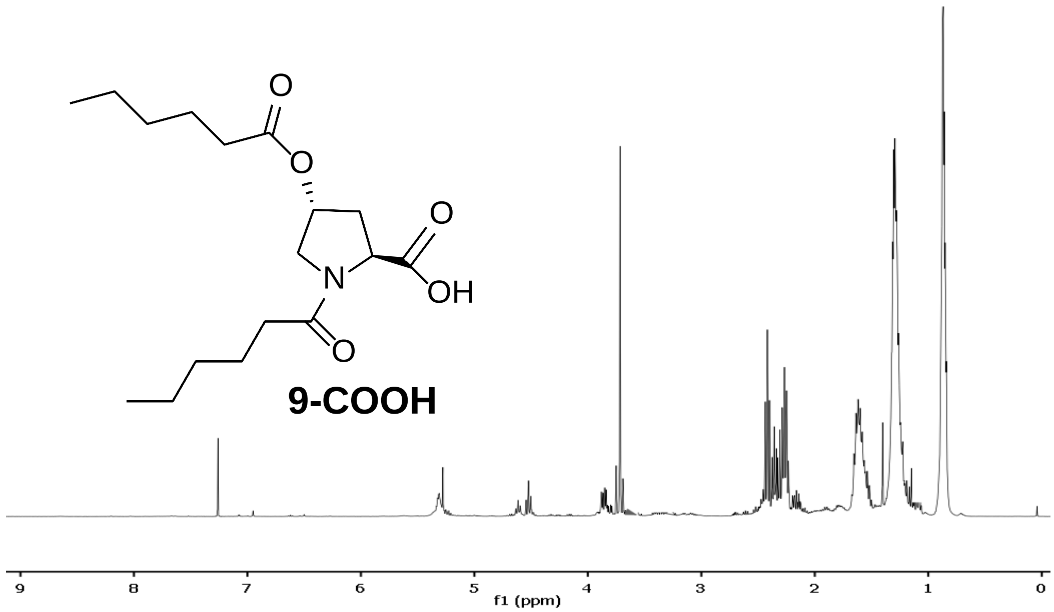

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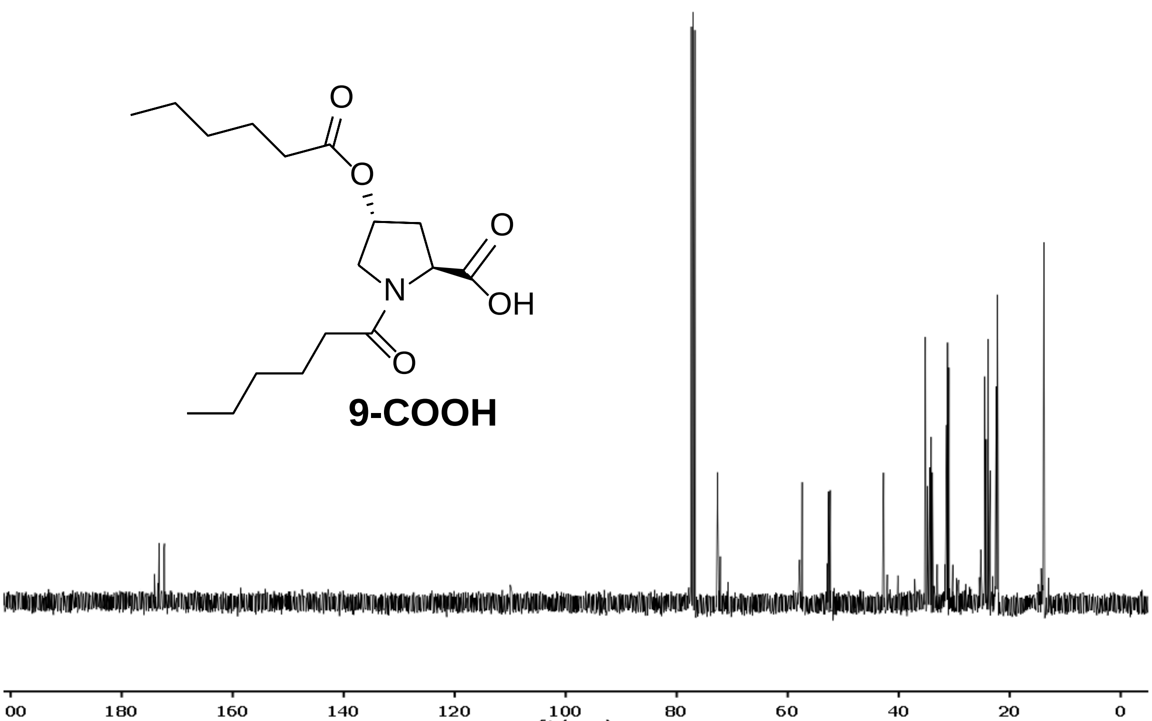

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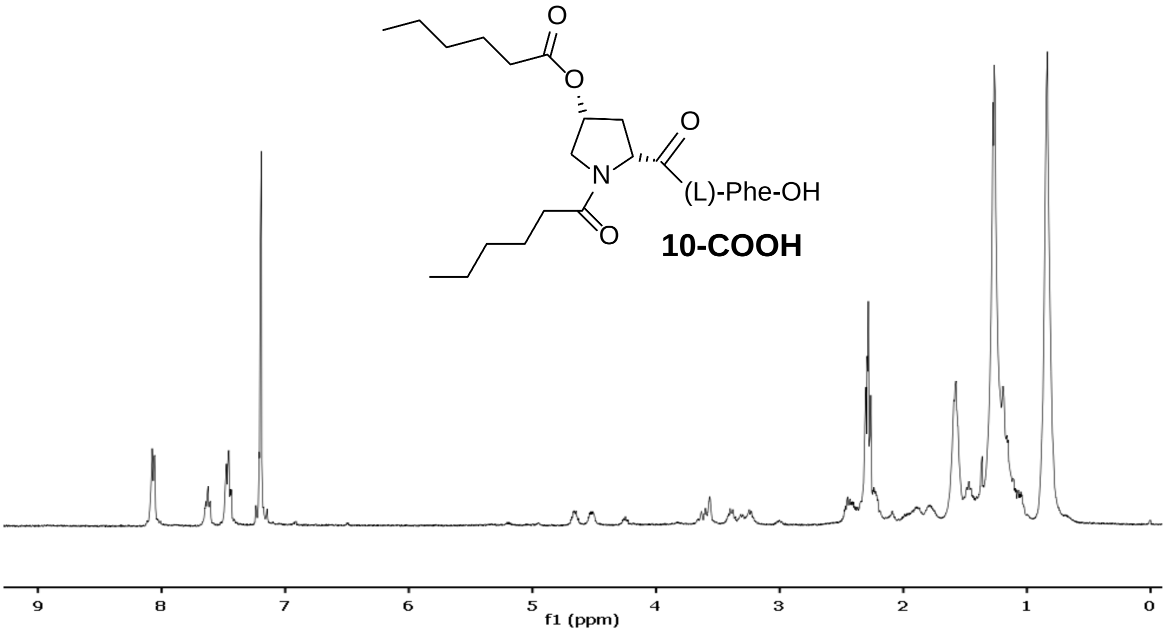
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O
10-COOH
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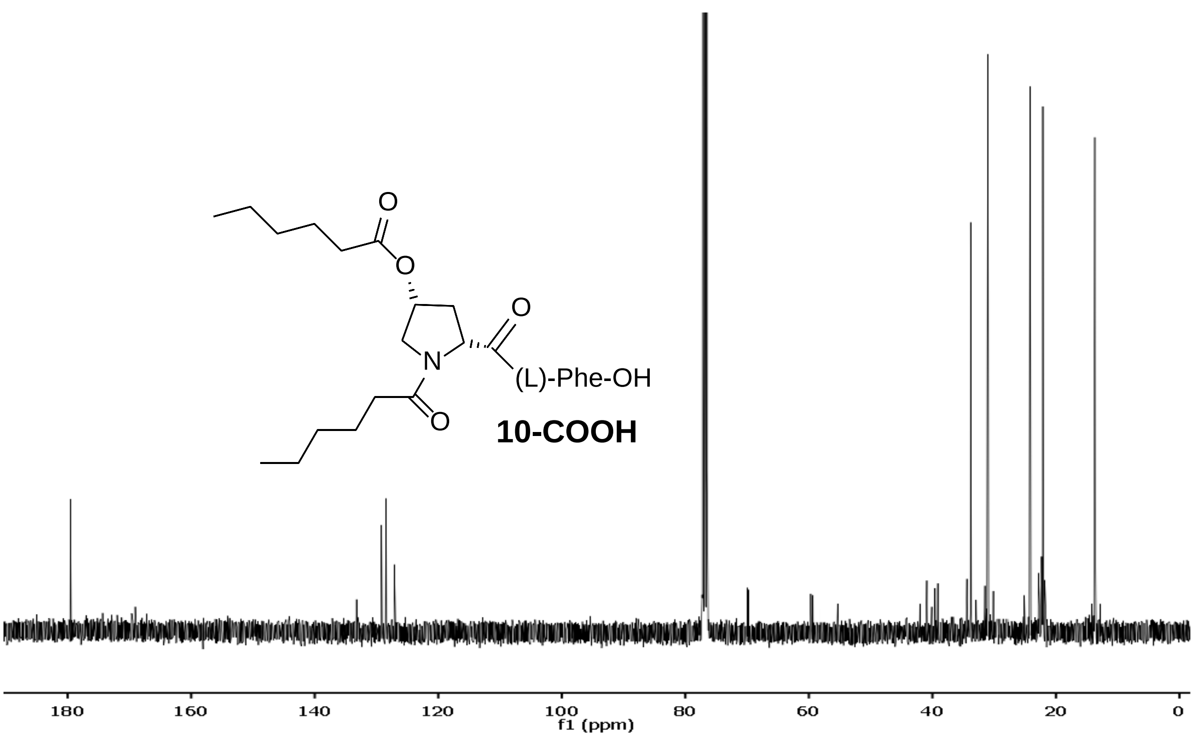
f1 (ppm)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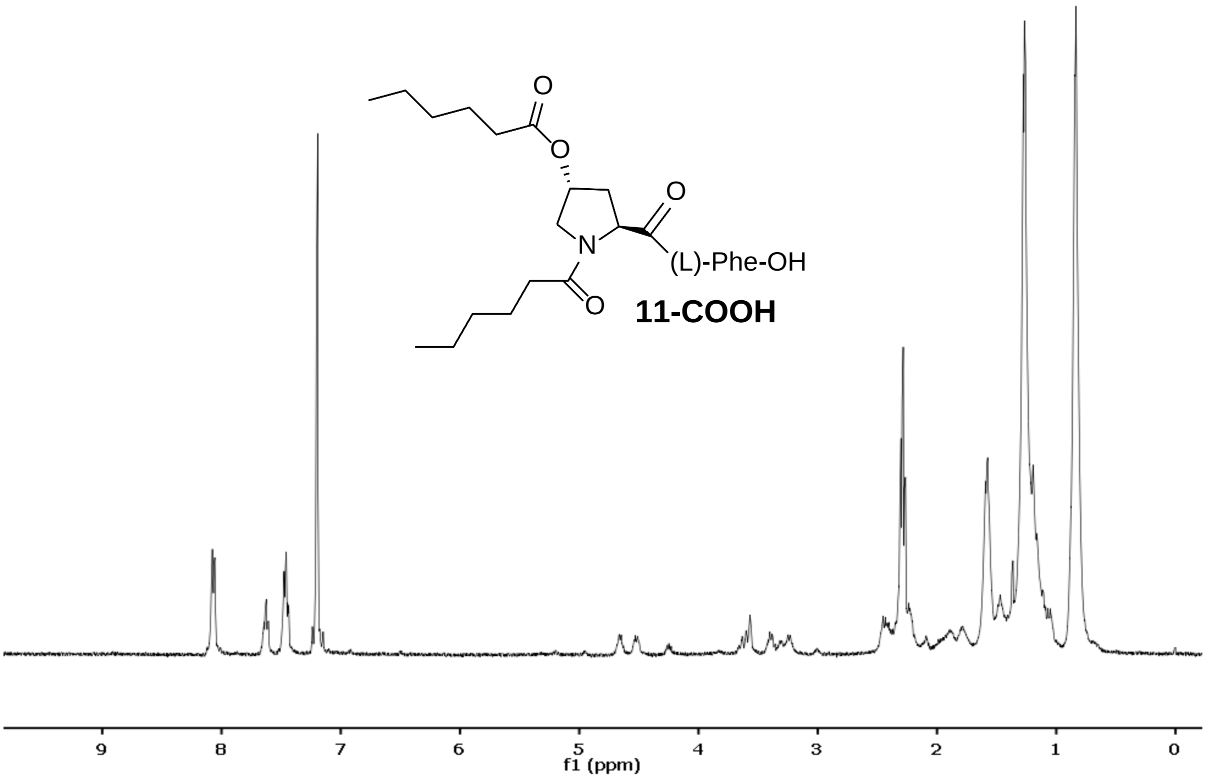
O
O
N
(L)-Phe-OH
O
10-COOH
180 160 140 120 100 80 60 40 20 0
f1 (ppm)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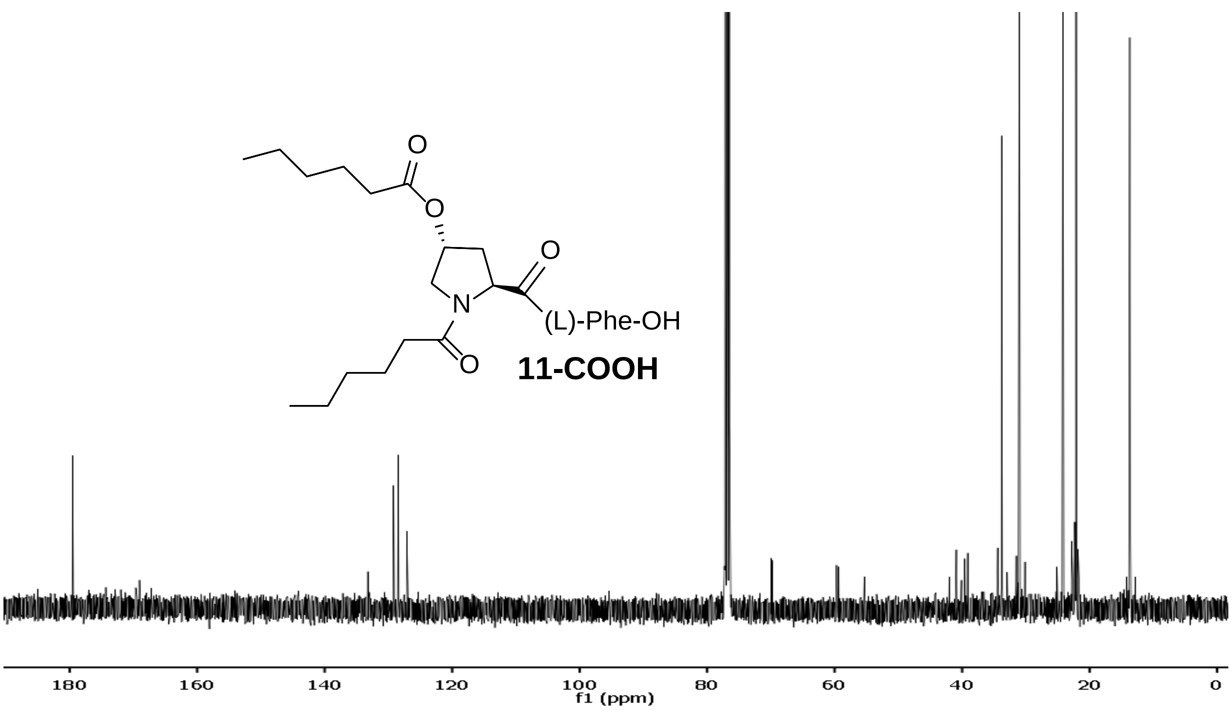
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f1 (ppm)