Supplementary Material (ESI) for Soft Matter

The Influence of Side-Chain Halogenation on the Self-Assembly and Hydrogelation of Fmoc-Phenylalanine Derivatives

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ELECTRONIC SUPPORTING INFORMATION

Contents:

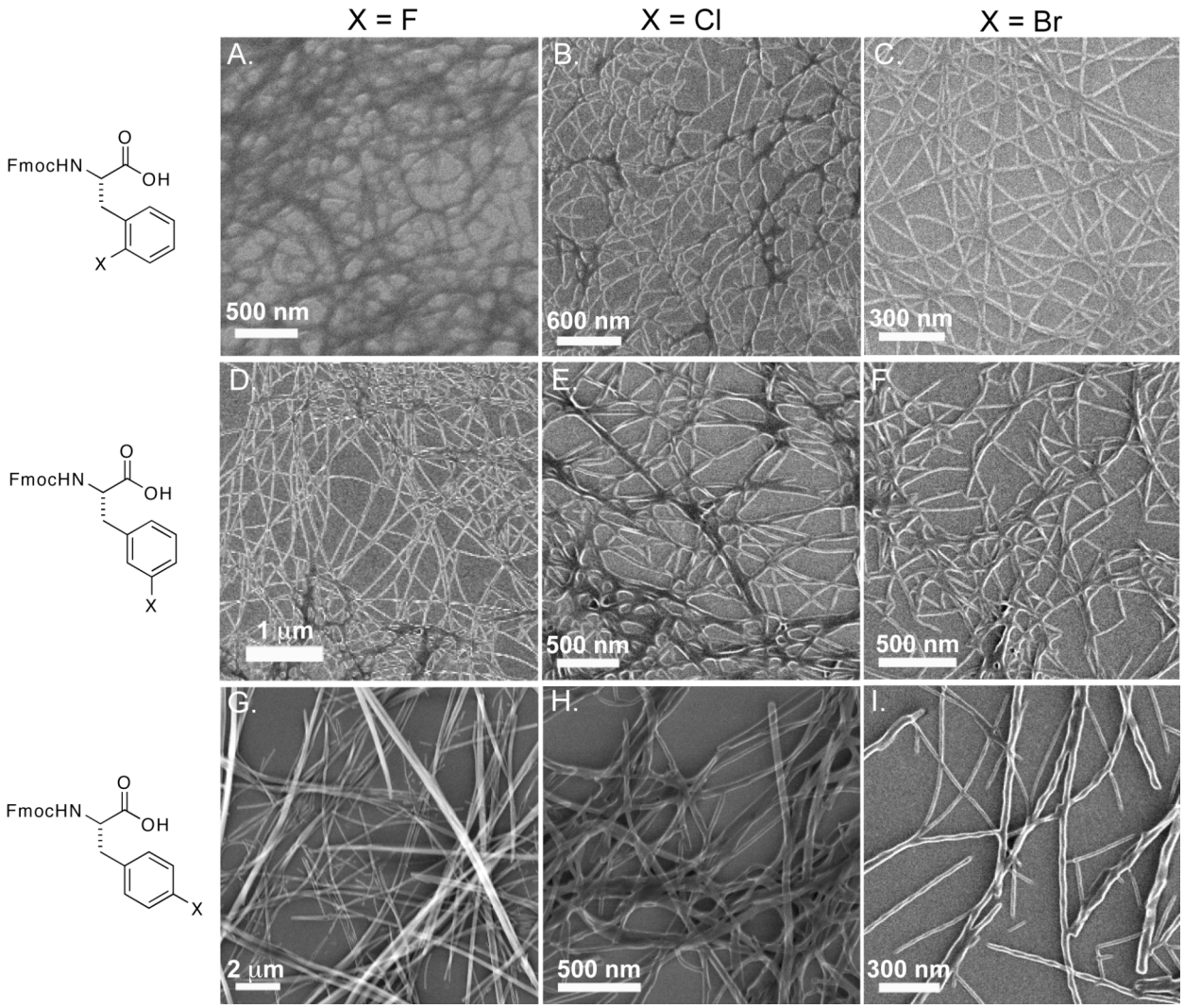

Figure S1. SEM images of Fmoc-n-X-Phe amino acids after a 3 day maturation period. A) Fmoc-2-F-Phe; B) Fmoc-2-Cl-Phe; C) Fmoc-2-Br-Phe; D) Fmoc-3-F-Phe; E) Fmoc-3-Cl-Phe; F) Fmoc-3-Br-Phe; G) Fmoc-4-F-Phe; H) Fmoc-4-Cl-Phe; I) Fmoc-4-Br-Phe.

Table S1. Tabulation of CD absorptions for each Fmoc-n-X-Phe derived hydrogel (min = minimum, max = maximum).

Amino acid	Major absorptions (nm)
Fmoc-2-F-Phe	200 (min), 224 (max), 275 (max), 293 (max), 307 (max)
Fmoc-2-Cl-Phe	207 (min), 225 (max), 278 (max), 296 (max), 307 (max)
Fmoc-2-Br-Phe	211 (min), 268 (min), 294 (min), 307 (min)
Fmoc-3-F-Phe	201 (min), 220 (max), 274 (max), 295 (max), 307 (max)
Fmoc-3-Cl-Phe	207 (min), 226 (max), 276 (max), 295 (max), 307 (max)
Fmoc-3-Br-Phe	210 (min), 228 (max), 279 (max), 296 (max), 309 (max)
Fmoc-4-F-Phe	229 (min), 289 (min), 298 (min), 310 (min)
Fmoc-4-Cl-Phe	209 (min), 231 (min), 279 (min), 296 (min), 309 (min)
Fmoc-4-Br-Phe	213 (min), 232 (max), 284 (max), 296 (max), 309 (max)

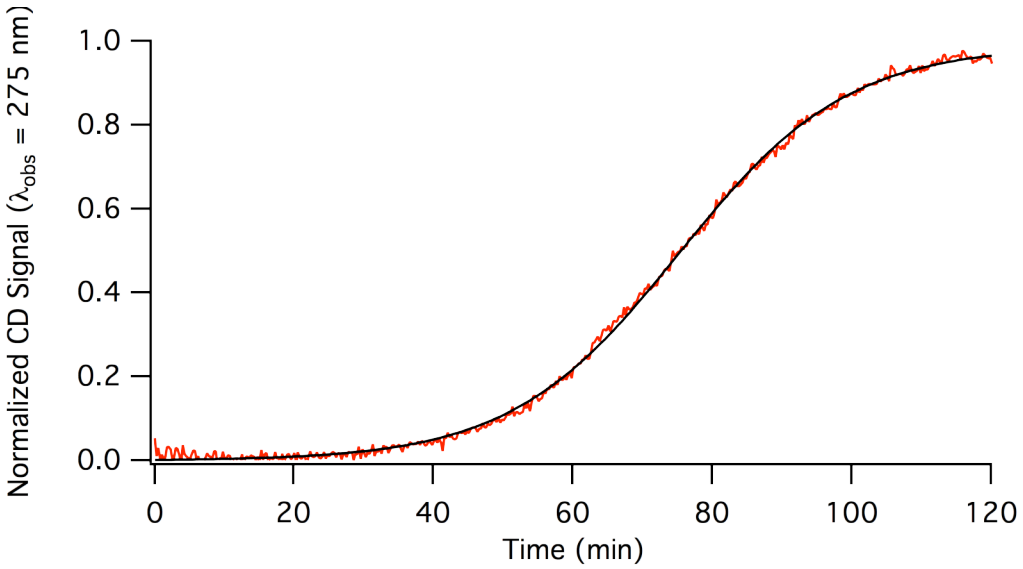

Figure S2. Representative empirical curve fit for Fmoc-2-F-Phe self-assembly kinetics ($t_{1/2}$ = 75 ± 5 min, k = 0.08 ± 0.02 min^{-1}).

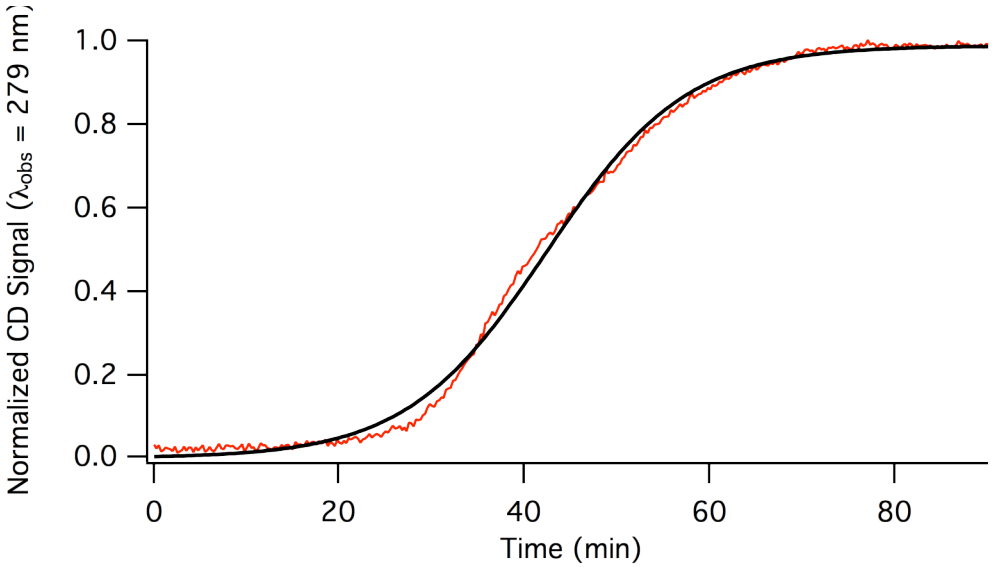

Figure S3. Representative empirical curve fit for Fmoc-2-Cl-Phe self-assembly kinetics ($t_{1/2}$ = 41 ± 4 min, k = 0.2 ± 0.1 min^{-1}).

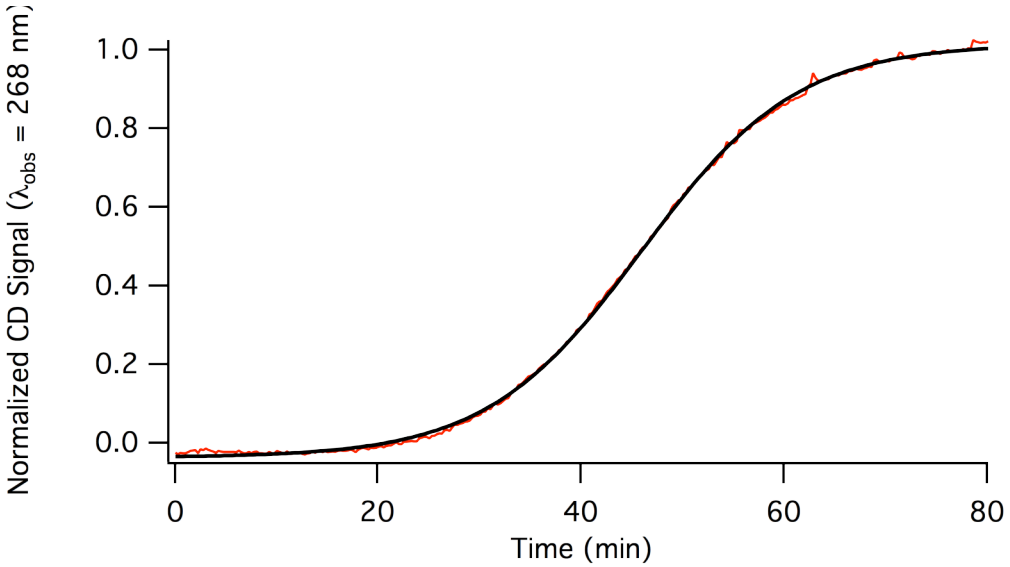

Figure S4. Representative empirical curve fit for Fmoc-2-Br-Phe self-assembly kinetics ($t_{1/2}$ = 47 ± 3 min, k = 0.12 ± 0.03 min^{-1}).

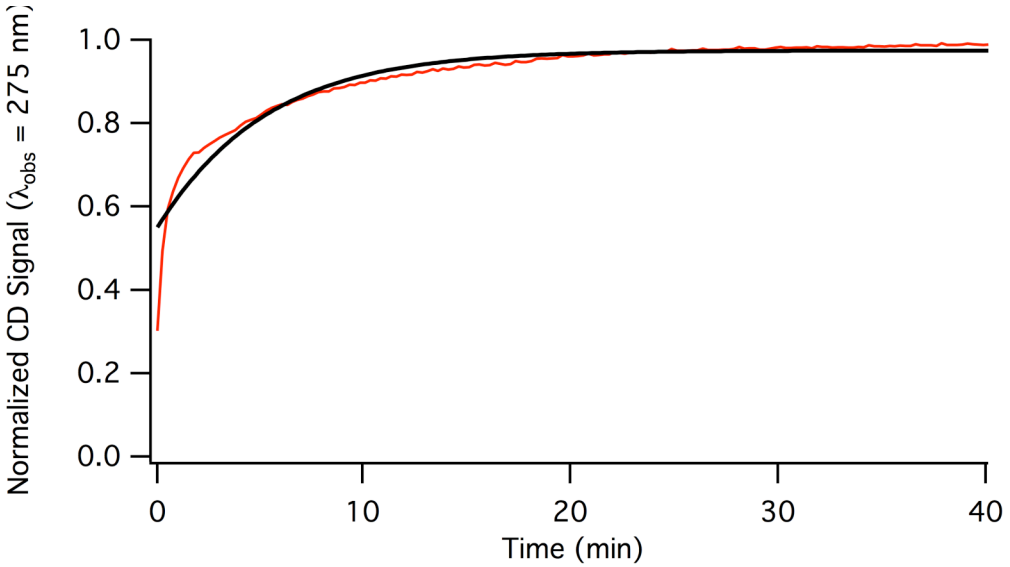

Figure S5. Representative empirical curve fit for Fmoc-3-F-Phe self-assembly kinetics (reliable $t_{1/2}$ and k values could not be obtained to the lack of an observable lag phase).

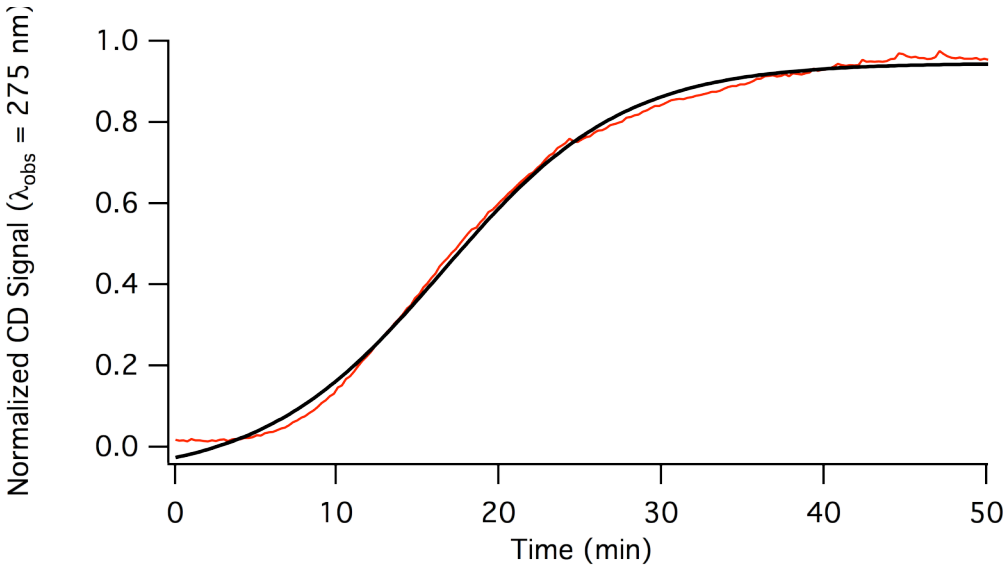

Figure S6. Representative empirical curve fit for Fmoc-3-Cl-Phe self-assembly kinetics ($t_{1/2}$ = 18 ± 2 min, k = 0.23 ± 0.03 min^{-1}).

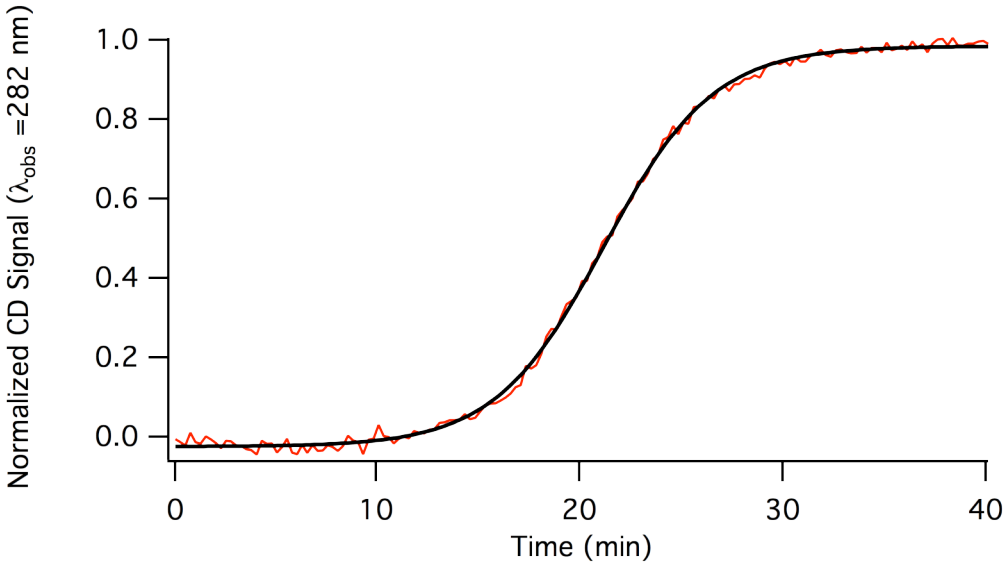

Figure S7. Representative empirical curve fit for Fmoc-3-Br-Phe self-assembly kinetics ($t_{1/2}$ = 21 ± 1 min, k = 0.6 ± 0.3 min^{-1}).

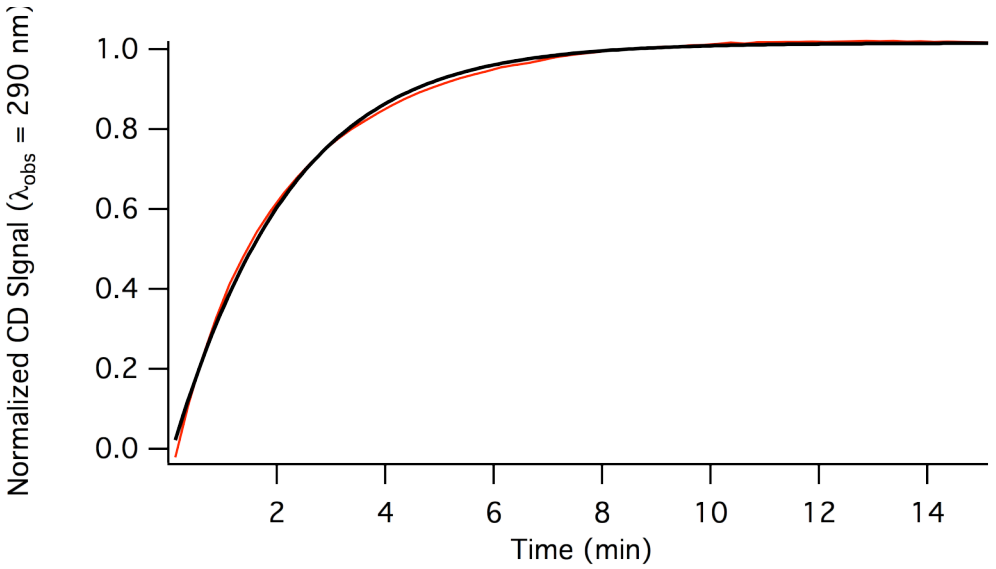

Figure S8. Representative empirical curve fit for Fmoc-4-F-Phe self-assembly kinetics (reliable $t_{1/2}$ and k values could not be obtained to the lack of an observable lag phase).

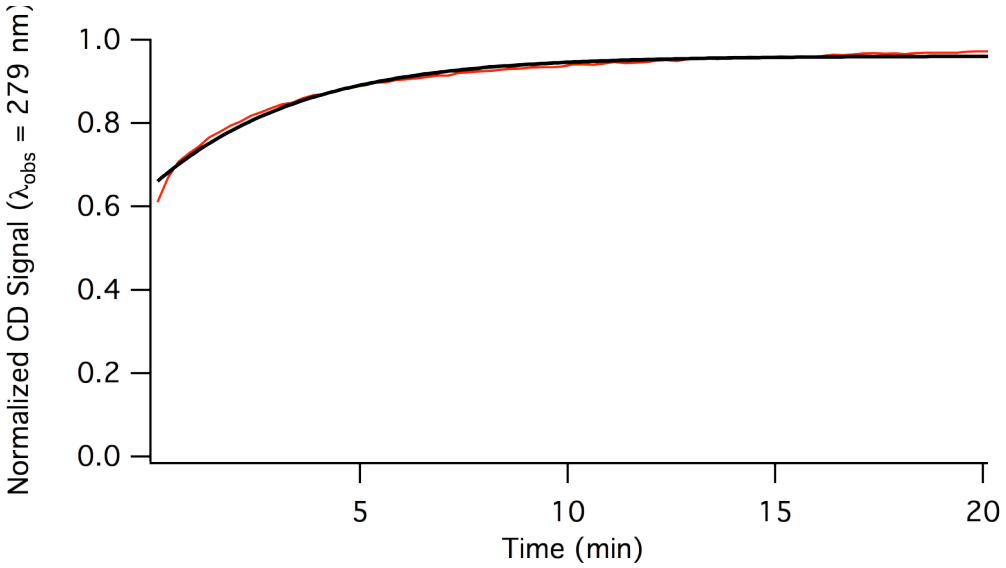

Figure S9. Representative empirical curve fit for Fmoc-4-Cl-Phe self-assembly kinetics (reliable $t_{1/2}$ and k values could not be obtained to the lack of an observable lag phase).

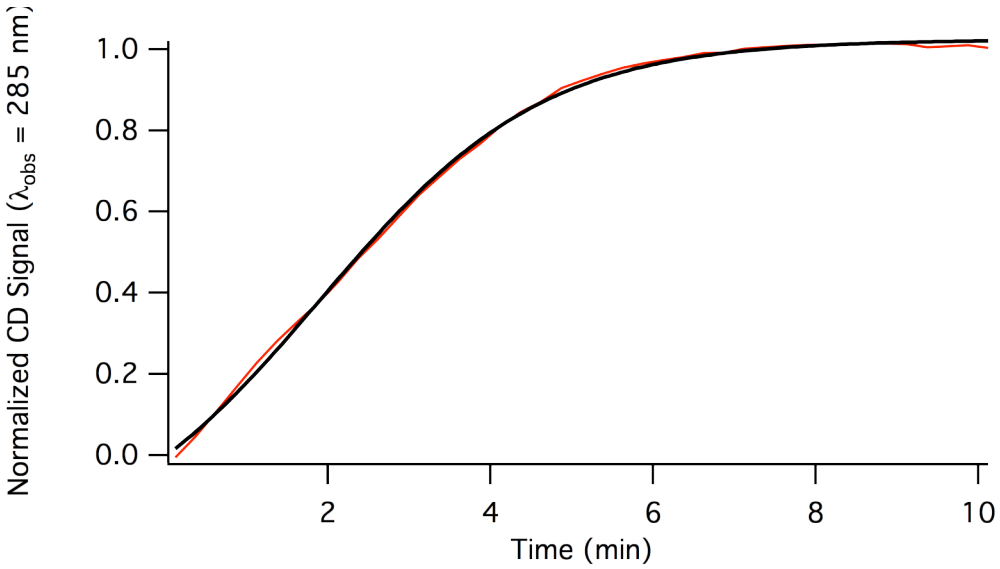

Figure S10. Representative empirical curve fit for Fmoc-4-Br-Phe self-assembly kinetics (reliable $t_{1/2}$ and k values could not be obtained to the lack of an observable lag phase).

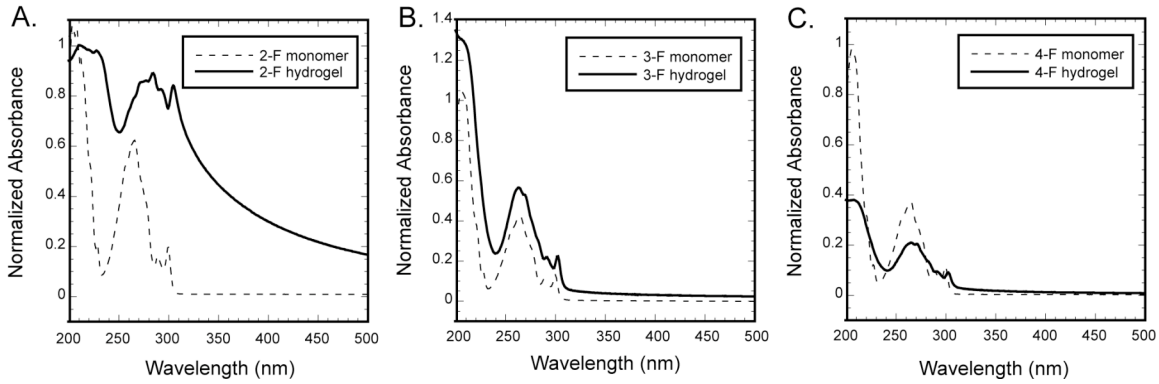

Figure S11. Normalized UV-Vis absorbance of monomeric Fmoc-n-F-Phe derivatives (4.94 mM in MeOH) and assembled Fmoc-n-F-Phe derivatives (4.94 mM in 2% MeOH/H_2O). A) Fmoc-2-F-Phe; B) Fmoc-3-F-Phe; C) Fmoc-3-Cl-Phe.

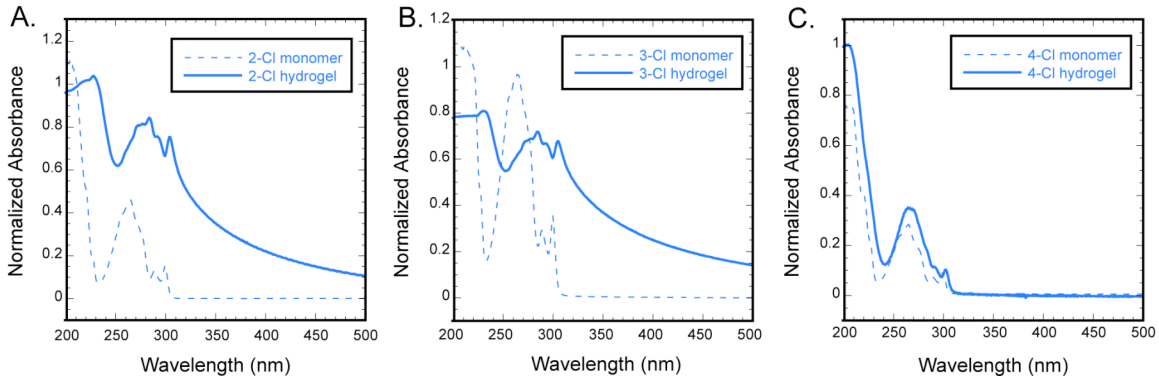

Figure S12. Normalized UV-Vis absorbance of monomeric Fmoc-n-Cl-Phe derivatives (4.94 mM in MeOH) and assembled Fmoc-n-Cl-Phe derivatives (4.94 mM in 2% MeOH/H_2O). A) Fmoc-2-Cl-Phe; B) Fmoc-3-Cl-Phe; C) Fmoc-4-Cl-Phe.

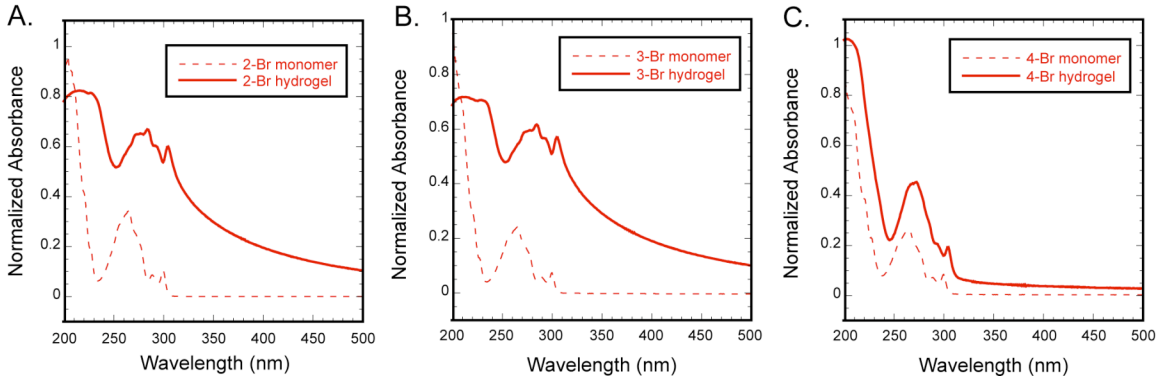

Figure S13. Normalized UV-Vis absorbance of monomeric Fmoc-n-Br-Phe derivatives (4.94 mM in MeOH) and assembled Fmoc-n-Br-Phe derivatives (4.94 mM in 2% MeOH/H_2O). A) Fmoc-2-Br-Phe; B) Fmoc-3-Br-Phe; C) Fmoc-4-Br-Phe.

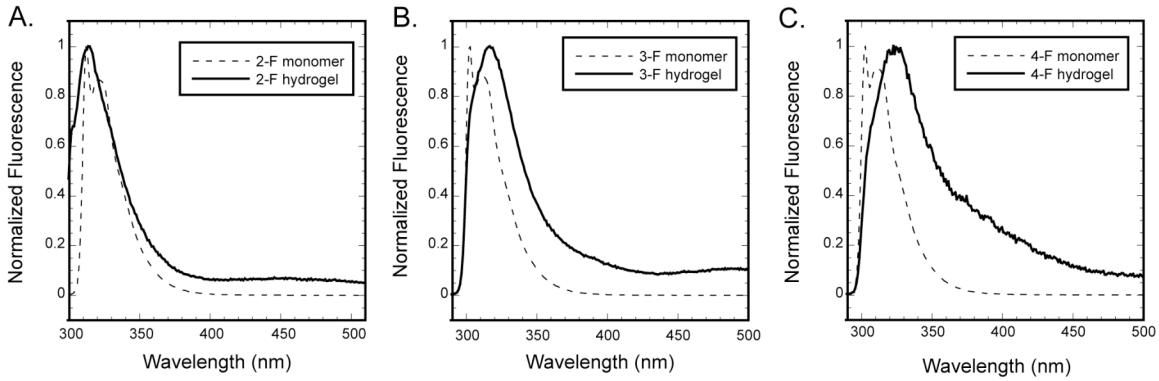

Figure S14. Normalized fluorescence emission spectra of monomeric Fmoc-n-Br-Phe derivatives (4.94 mM in MeOH) and assembled Fmoc-X-Br-Phe derivatives (4.94 mM in 2% MeOH/H_2O). A) Fmoc-2-Br-Phe; B) Fmoc-3-Br-Phe; C) Fmoc-4-Br-Phe.

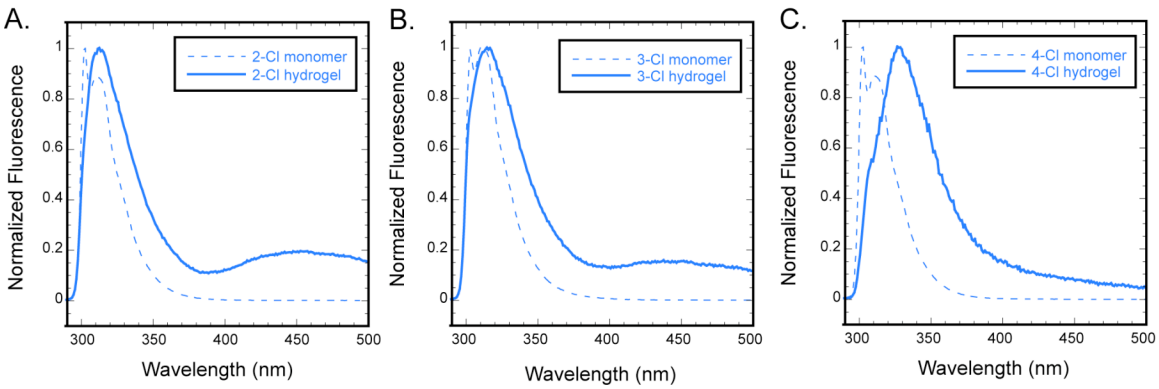

Figure S15. Normalized fluorescence emission spectra of monomeric Fmoc-n-Br-Phe derivatives (4.94 mM in MeOH) and assembled Fmoc-n-Br-Phe derivatives (4.94 mM in 2% MeOH/H_2O). A) Fmoc-2-Br-Phe; B) Fmoc-3-Br-Phe; C) Fmoc-4-Br-Phe.

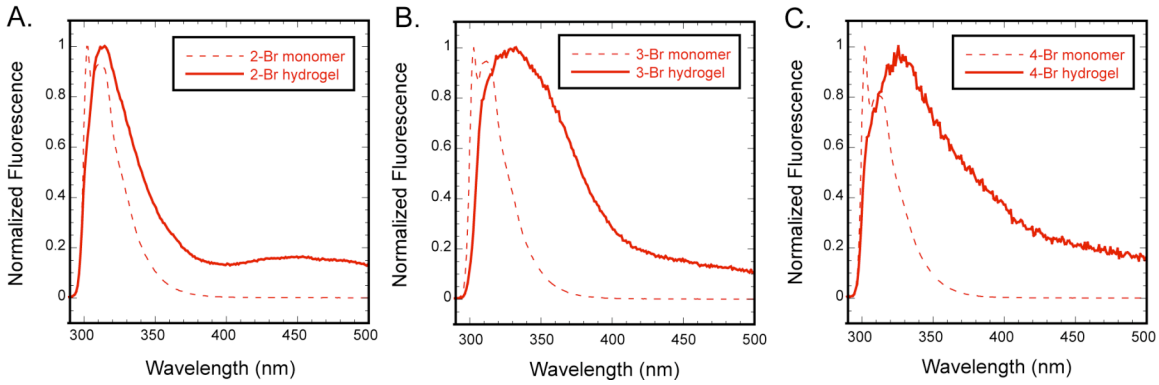

Figure S16. Normalized fluorescence emission spectra of monomeric Fmoc-n-Br-Phe derivatives (4.94 mM in MeOH) and assembled Fmoc-n-Br-Phe derivatives (4.94 mM in 2% MeOH/H_2O). A) Fmoc-2-Br-Phe; B) Fmoc-3-Br-Phe; C) Fmoc-4-Br-Phe.