Supporting Information

Fmoc-conjugated dipeptides-based hydrogels and their pH-tuneable behaviour

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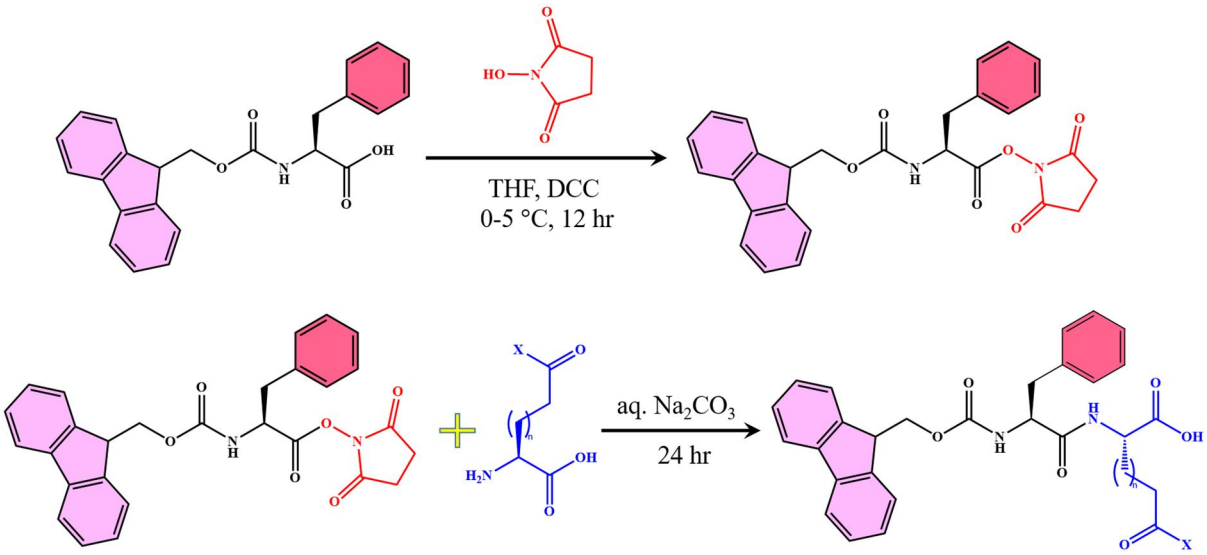

Figure S1. The general synthetic procedure of synthesis of Fmoc-protected dipeptides from Fmoc-Phe-OH. Here, the –COOH end is activated by coupling with N-hydroxy succinamide (NHS) in the presence of coupling agent DCC in THF medium at 0-5 °C. As formed Fmoc-Phe-NHS adduct in THF reacted with various hydrophilic amino acids (dissolved in Na_2CO_3) to give desired dipeptides.

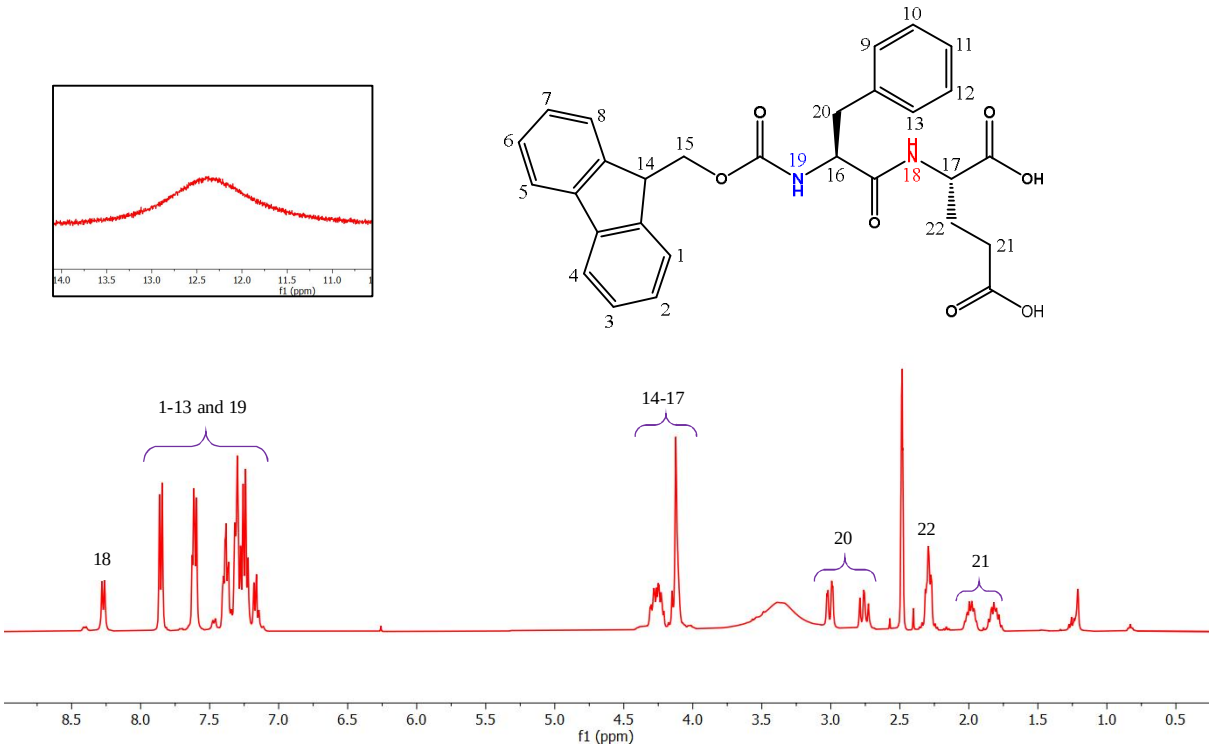

Figure S2.[1]H NMR (400 MHz) Spectrum of Fmoc-Phe-Glu-OH (FE) in DMSO-d_6 (0.5 to 8.5 ppm). Carboxylic acid peak is shown in inset.

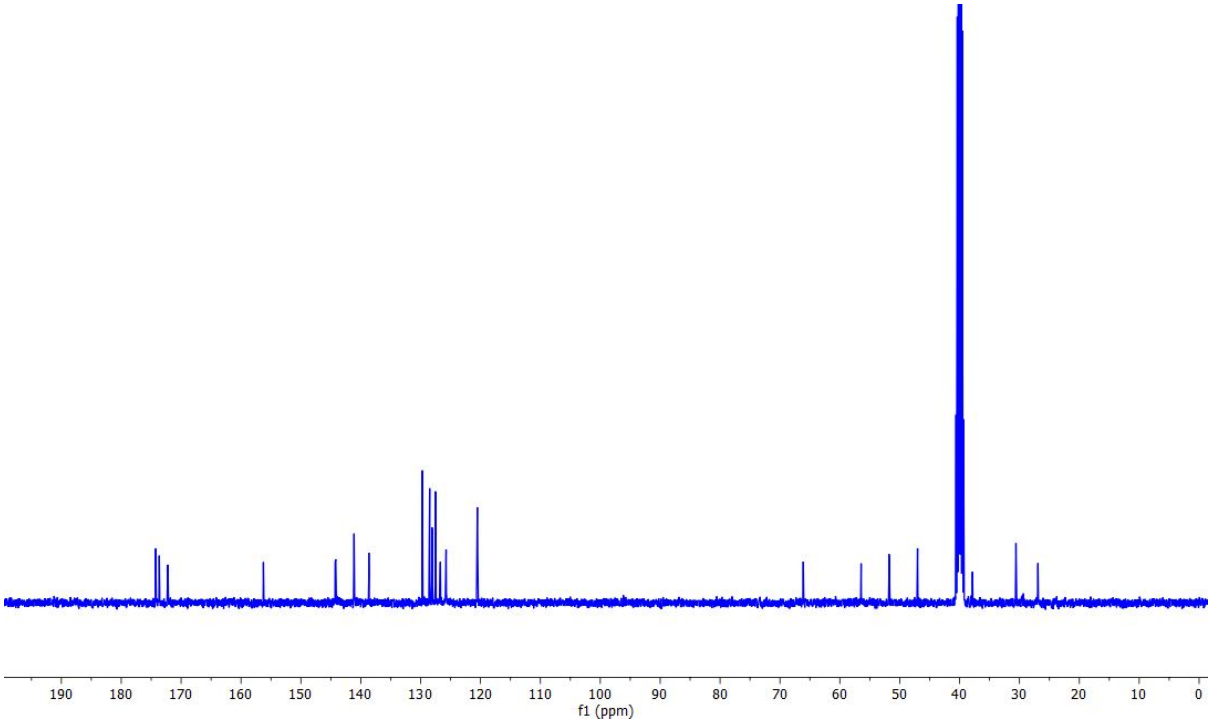

Figure S3. [13]C-NMR (100 MHz) spectrum of Fmoc-Phe-Glu-OH (FE) in DMSO-d_6 solvent.

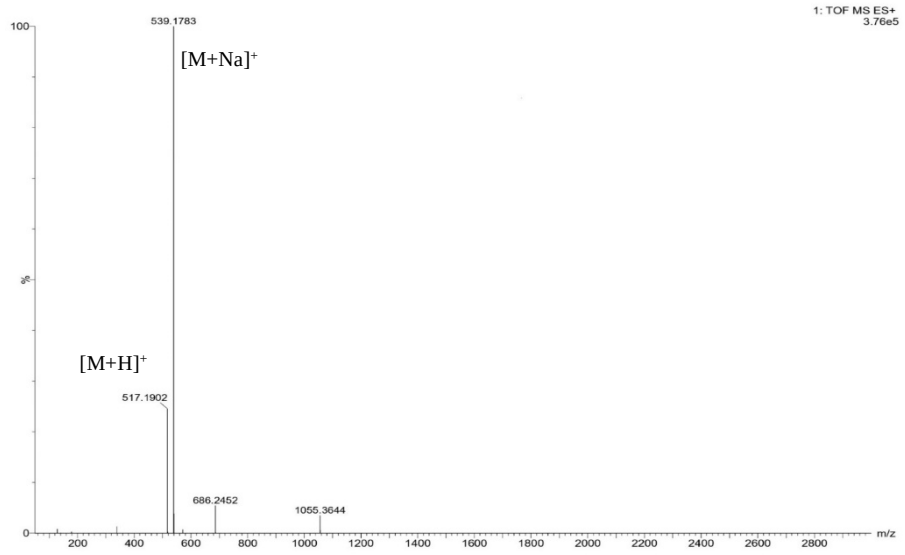

Figure S4. HRMS spectrum of Fmoc-Phe-Glu-OH (FE).

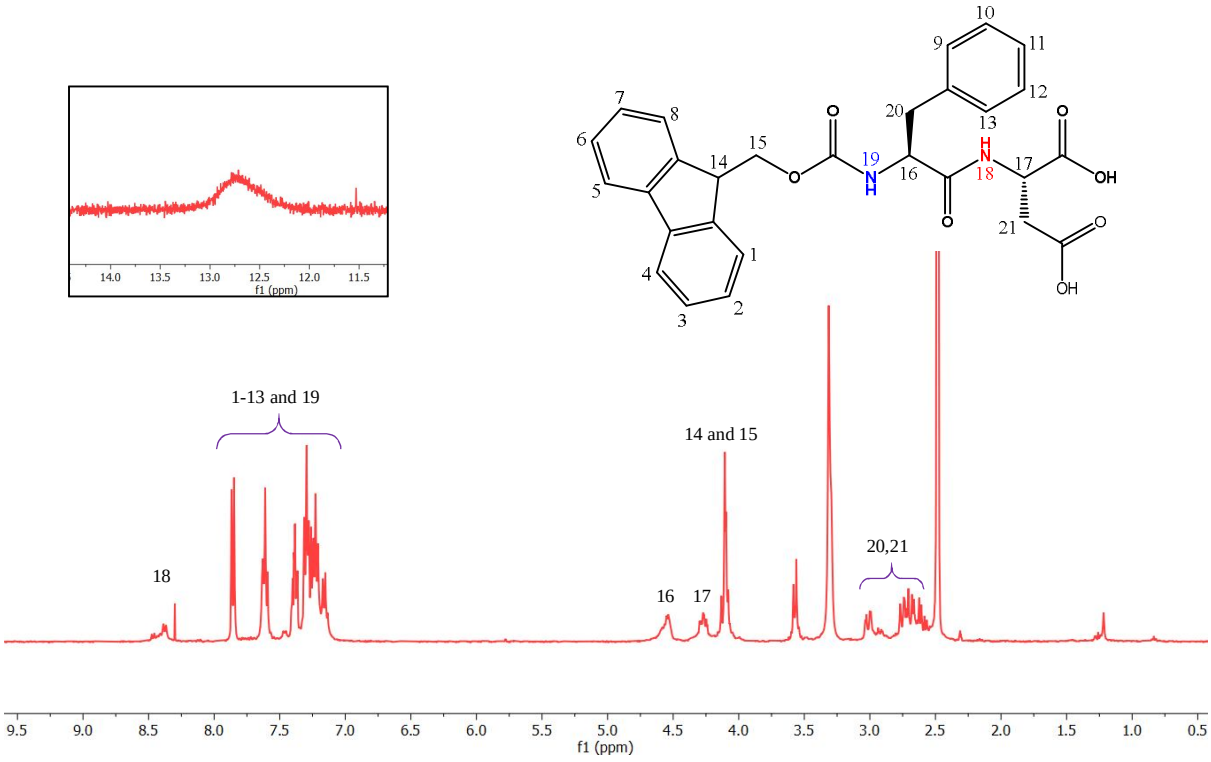

Figure S5.[1]H NMR (400 MHz) Spectrum of Fmoc-Phe-Asp-OH (FD) in DMSO-d_6 (0.5 to 9.5 ppm). Carboxylic acid peak is shown in inset.

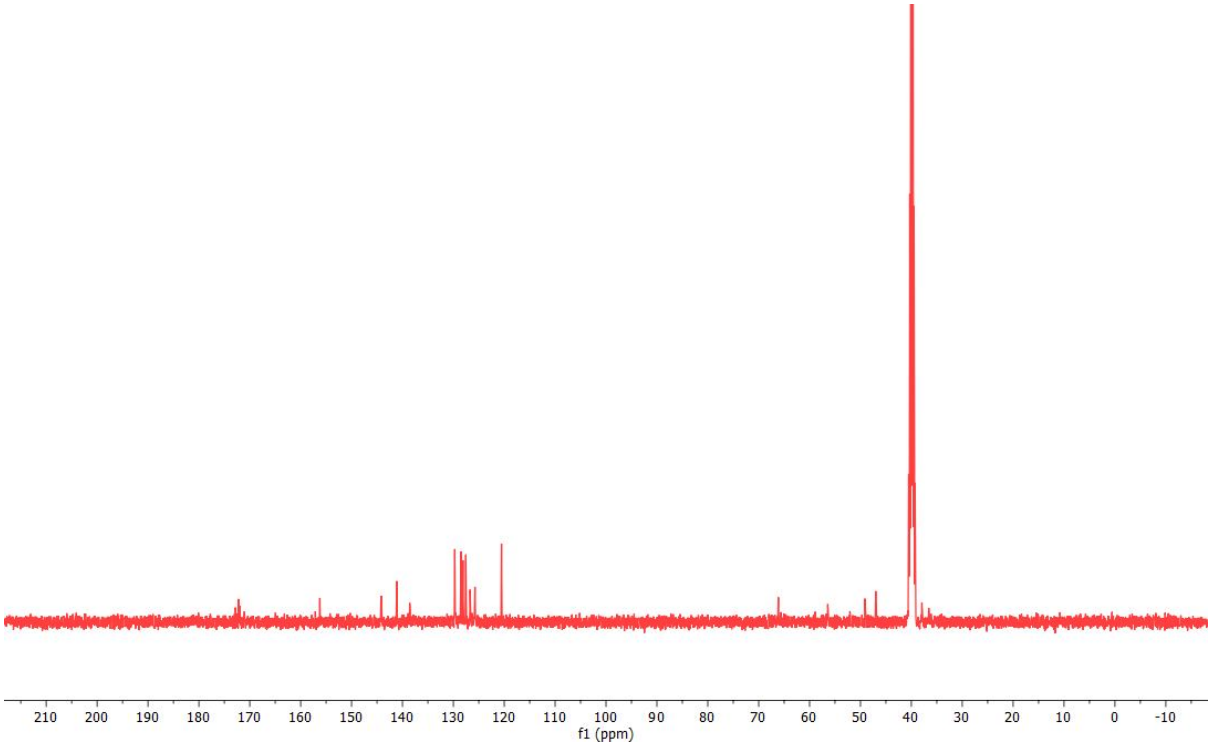

Figure S6. ^{13}C-NMR (100 MHz) spectrum of Fmoc-Phe-Asp-OH (FD) in DMSO-d_6 solvent.

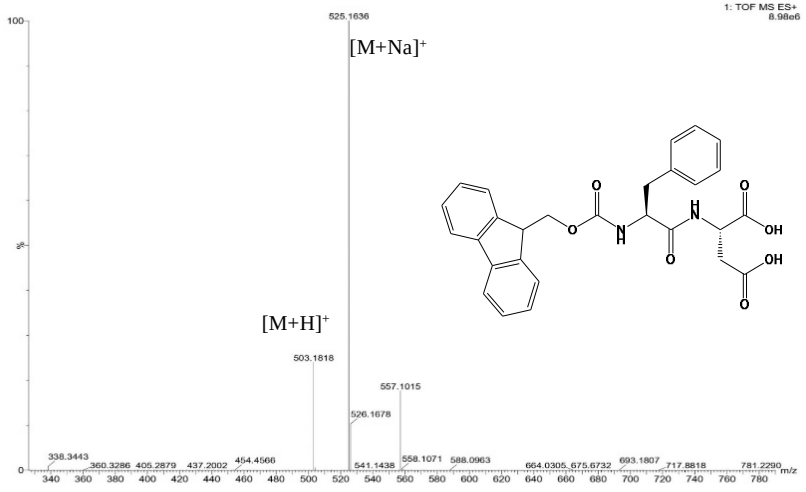

Figure S7. HRMS spectrum of Fmoc-Phe-Asp-OH (FD).

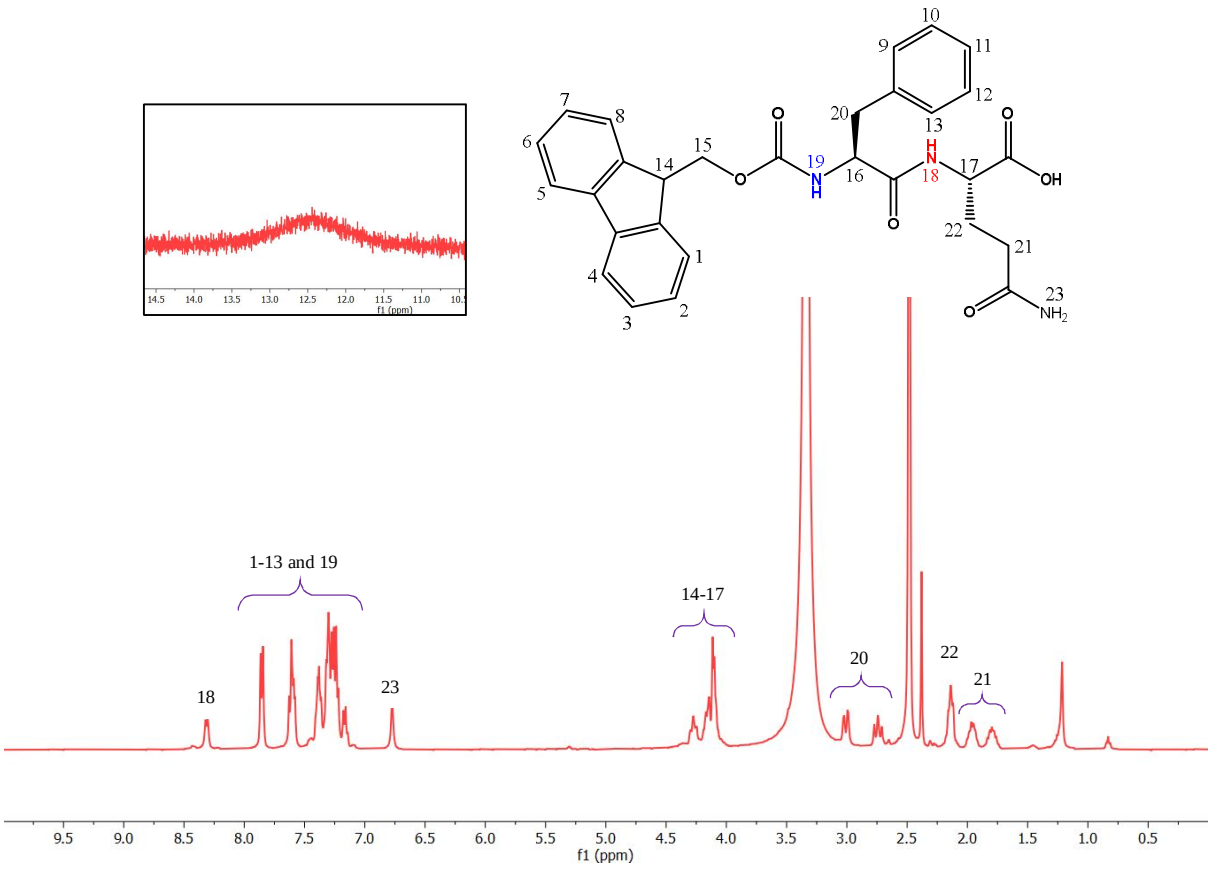

Figure S8.[1]H NMR (400 MHz) Spectrum of Fmoc-Phe-Gln-OH (FQ) in DMSO-d_6 (0.5 to 9.5 ppm). Carboxylic acid peak is shown in inset.

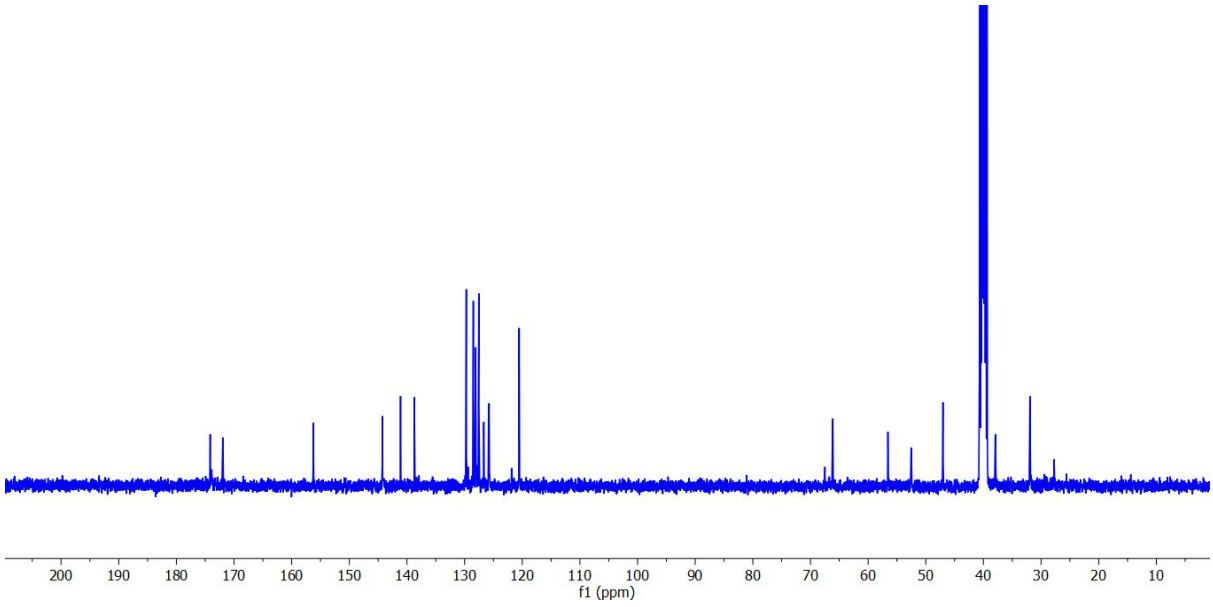

Figure S9. [13]C-NMR (100 MHz) spectrum of Fmoc-Phe-Gln-OH (FQ) in DMSO-d_6 solvent.

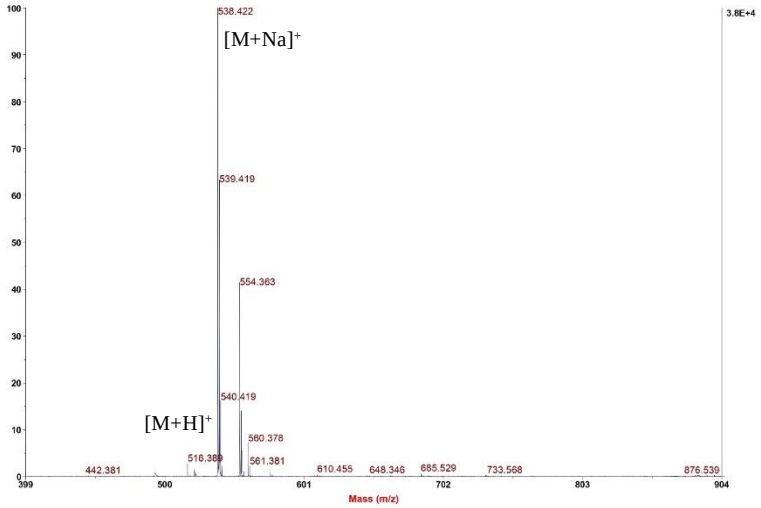

Figure S10. HRMS spectrum of Fmoc-Phe-Gln-OH (FQ).

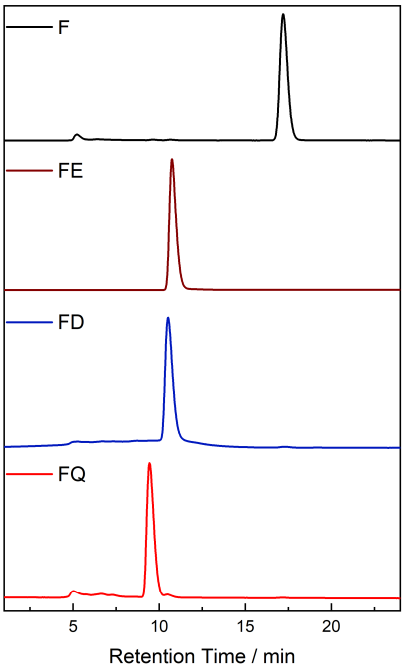

Figure S11. Comparison of HPLC traces of three dipeptides with Fmoc-Phe-OH (F).

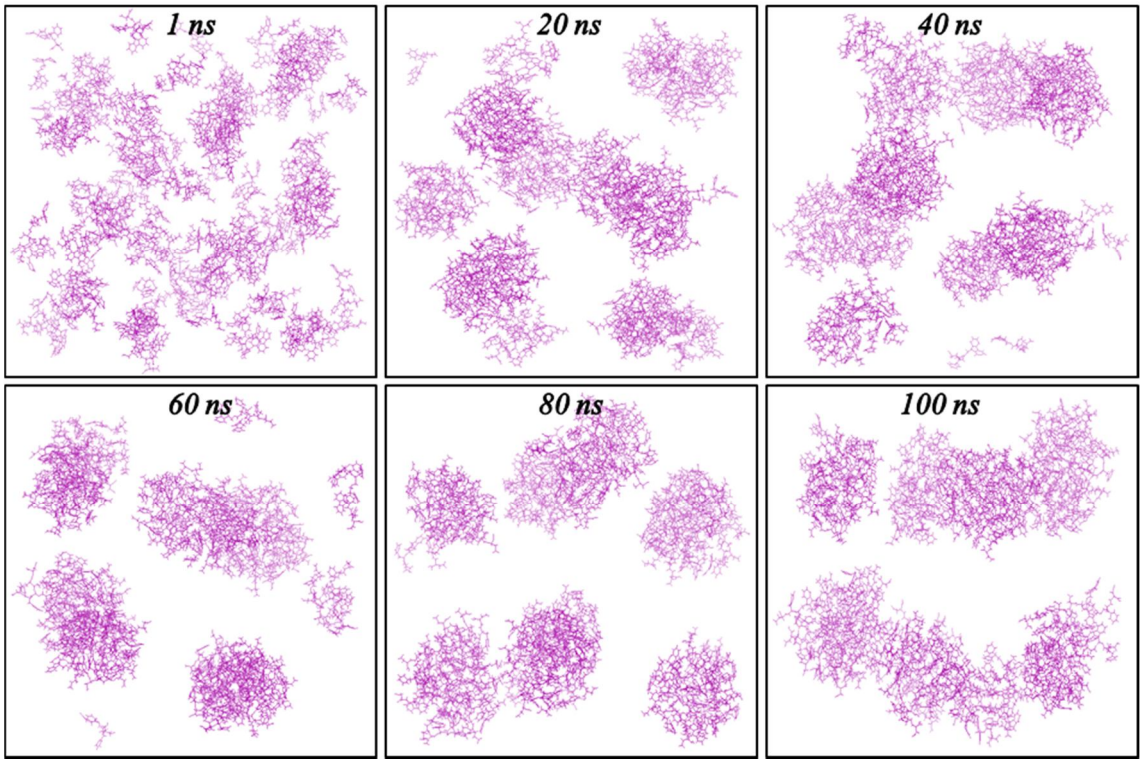

Figure S12. Time-dependent aggregation of FD.

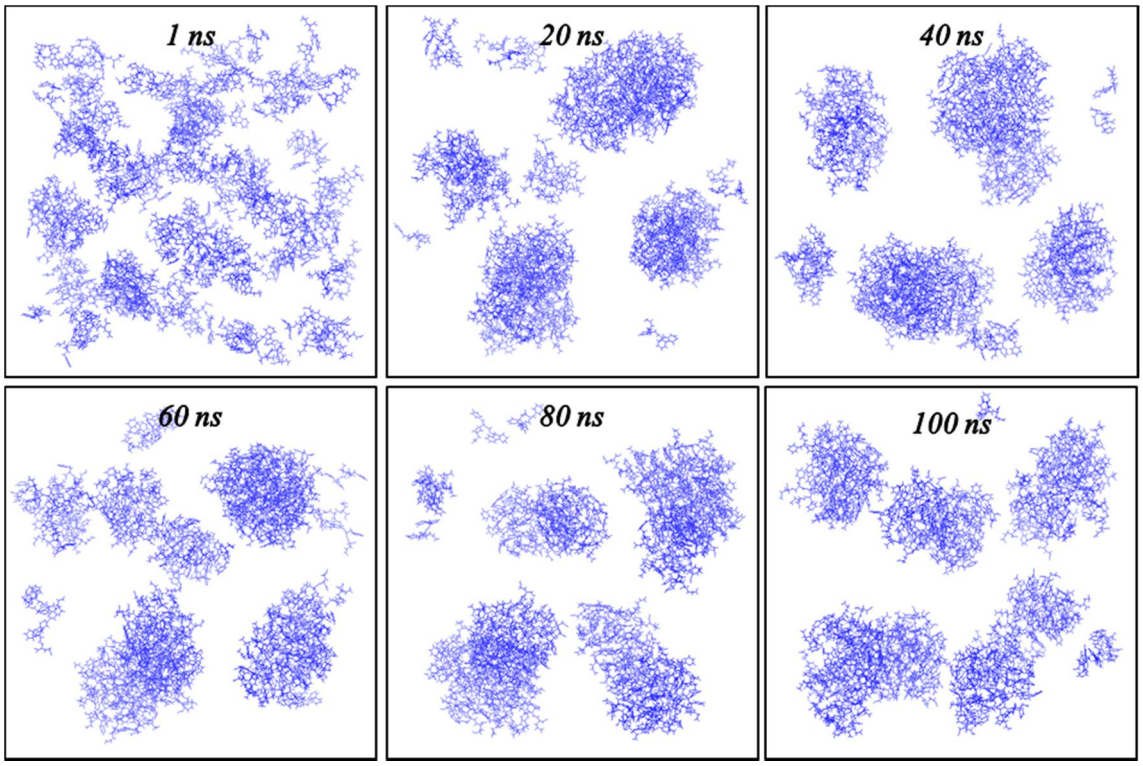

Figure S13. Time-dependent aggregation of FE.

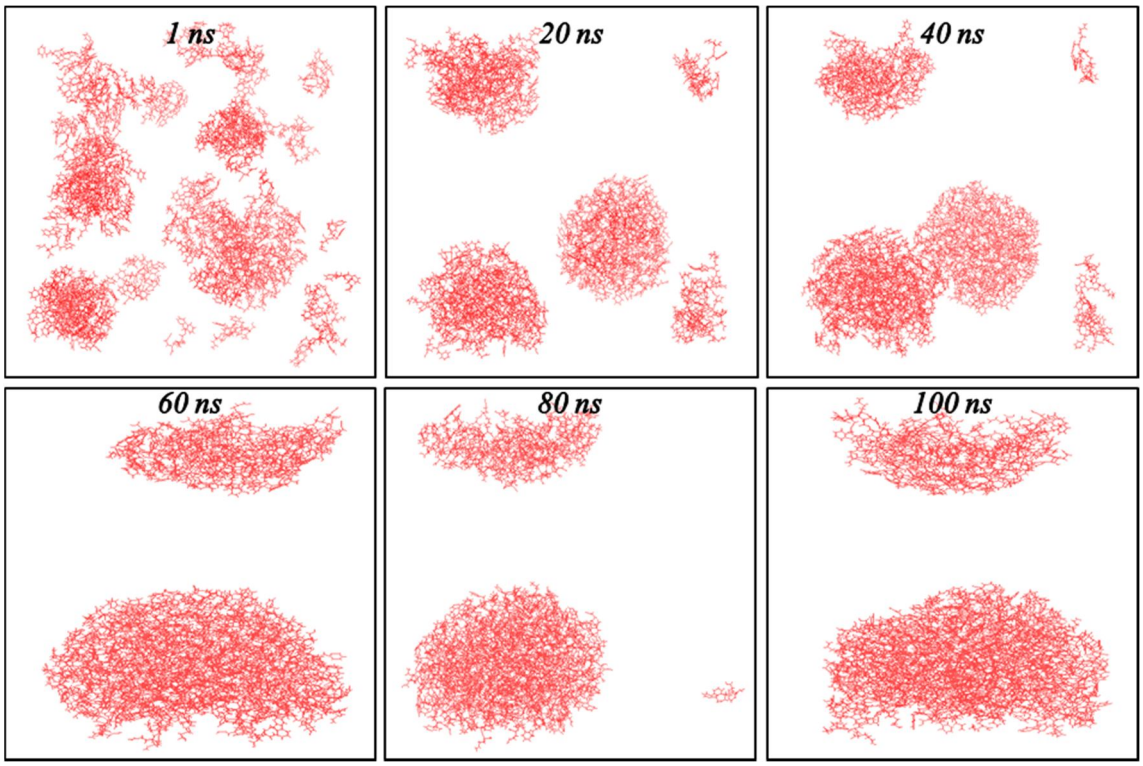

Figure S14. Time-dependent aggregation of FQ.

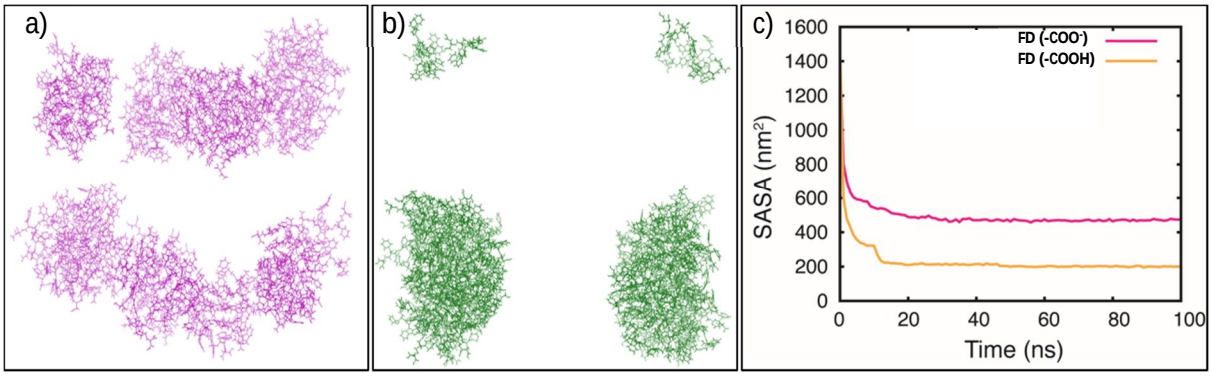

Figure S15. MD simulated self-assembled cluster of FD after 100 ns: a) both carboxylic acid end as -COO^- form, and b) both carboxylic acid end as –COOH form. c) Comparison of SASA value of FD when fully deprotonated and protonated state.

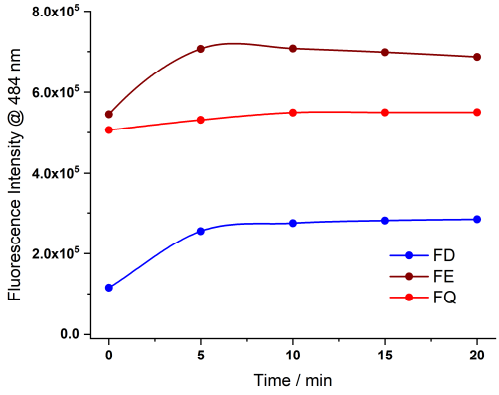

Figure S16. Changes in fluorescence intensity at 484 nm are plotted against time at pH 6.0.

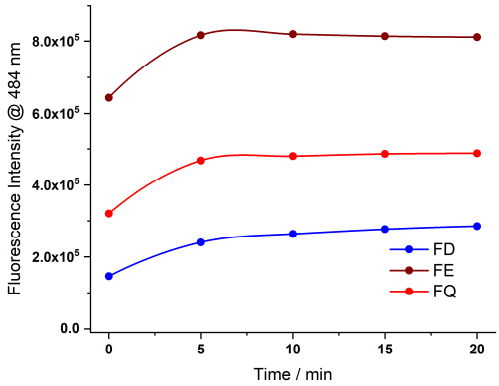

Figure S17. Fluorescence intensity changes at 484 nm are plotted against time at pH 5.0.

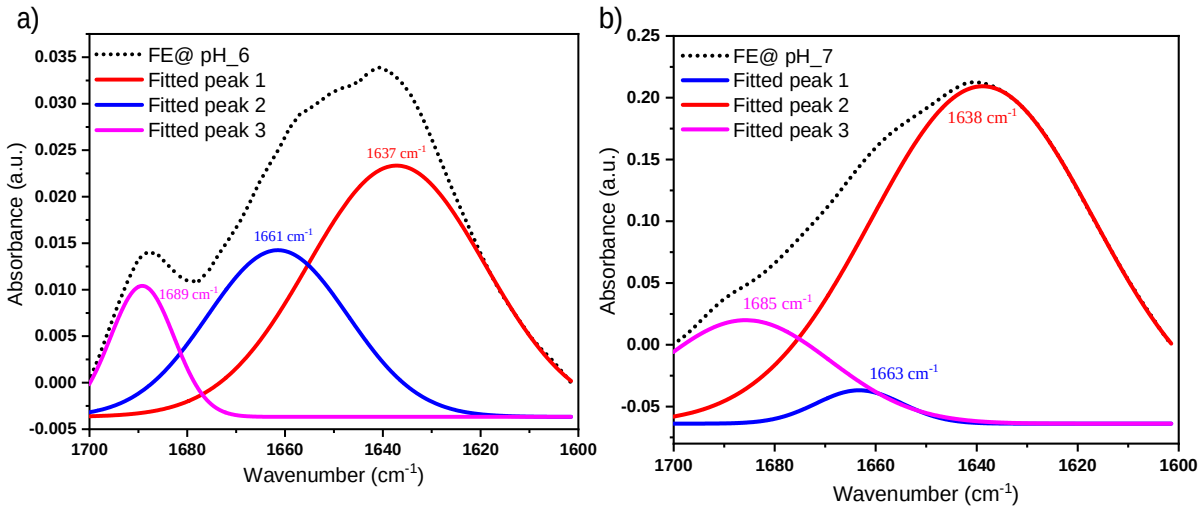

Figure S18. Deconvulated FT-IR data of FE a) at pH 6.0 and b) at pH 7.0 respectively. Deconvulated data showed that major contribution coming from β-sheet conformation.

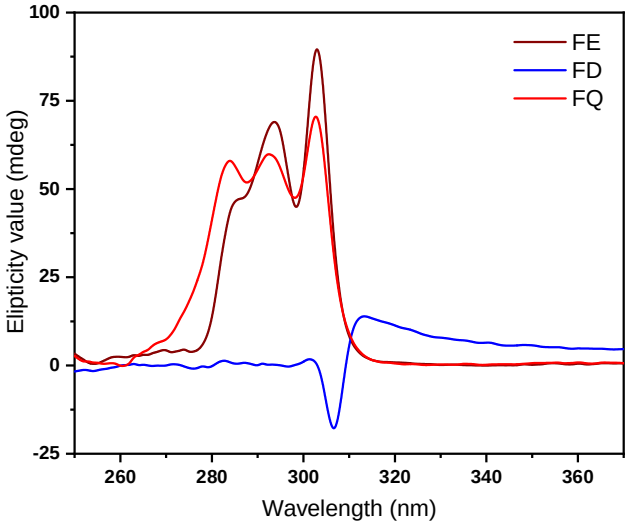

Figure S19. CD spectra of the three gelators at pH 6.0 with their corresponding MGC value.

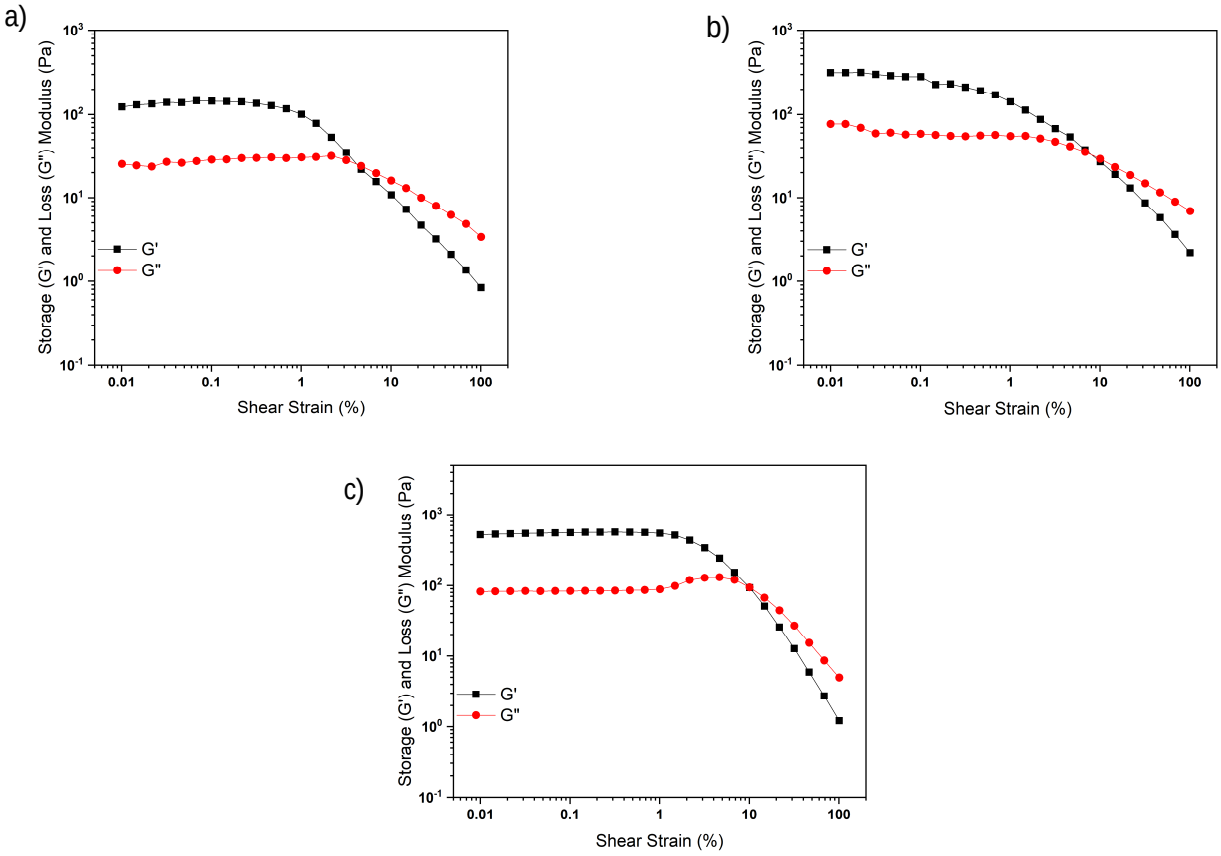

Figure S20. Strain sweep experiments of hydrogels were prepared from a) FE, b) FD and c) FQ at pH 7.0.