Supporting information

Probing the self-assembly and anti-glioblastoma efficacy of a cinnamoyl-capped dipeptide hydrogelator

E. D. Sitsanidis,[a/b] P. M. Kasapidou, [a/c] J. R. Hiscock,[d] V. Gubala,[a] H. Castel,[e] P. Poopla,[d] A. J. Hall[a] and A. A. Edwards[a*]

[a.] Medway School of Pharmacy, Universities of Kent and Greenwich at Medway, Central Avenue, Chatham Maritime, Kent, ME4 4TB, UK.

[b.] Department of Chemistry, Nanoscience Centre, P.O. Box 35, FI-40014, University of Jyväskylä, Finland.

[c.] Melville Laboratory for Polymer Synthesis, Yusuf Hamied Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, UK.

[d.] Supramolecular, Interfacial and Synthetic Chemistry Group, School of Physical Sciences, University of Kent, Canterbury, Kent, CT2 7NZ, UK.

[e.] Normandie Univ, UNIROUEN, INSERM U1245, CBG, 76000 Rouen, France.

List of figures

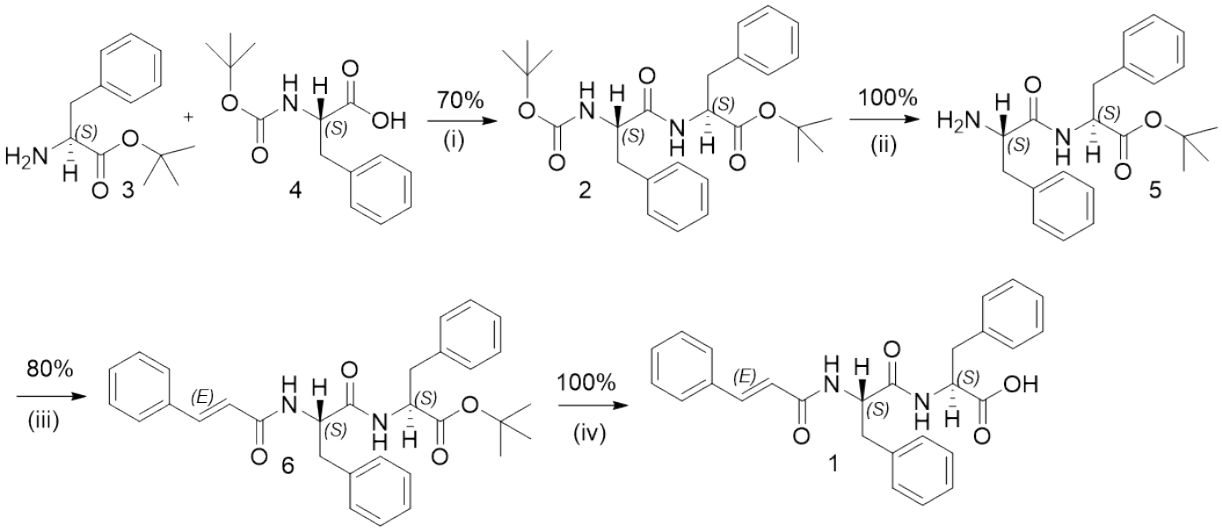

Figure S1. Synthesis of Cin-L-F-L-F **1**. Reagents and conditions: (i) anhydrous DMF, TBTU (1 eq.), $NaHCO_3$ (2.1 eq), RT; (ii) *tert*-Butyl acetate, conc. H_2SO_4 (3 eq), RT; (iii) anhydrous DMF, TBTU (1.5 eq), $NaHCO_3$ (2.5 eq), cinnamic acid (6 eq), RT; (iv) DCM, TFA (20 eq), RT.

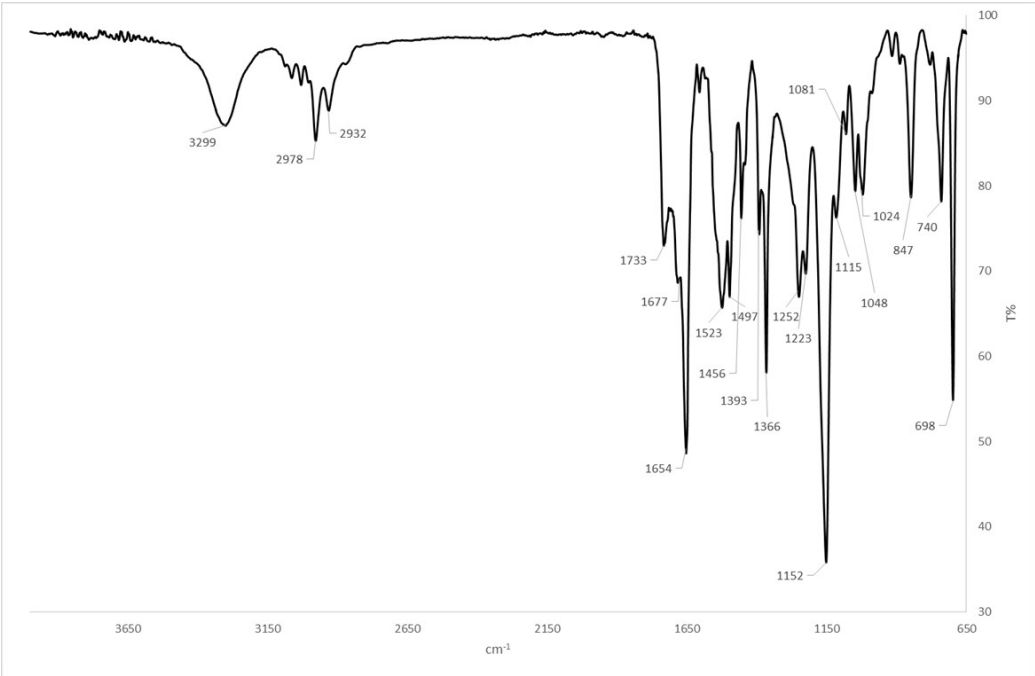

Figure S2. FT-IR spectrum of *Boc*-L-F-L-FO*t*Bu **2**.

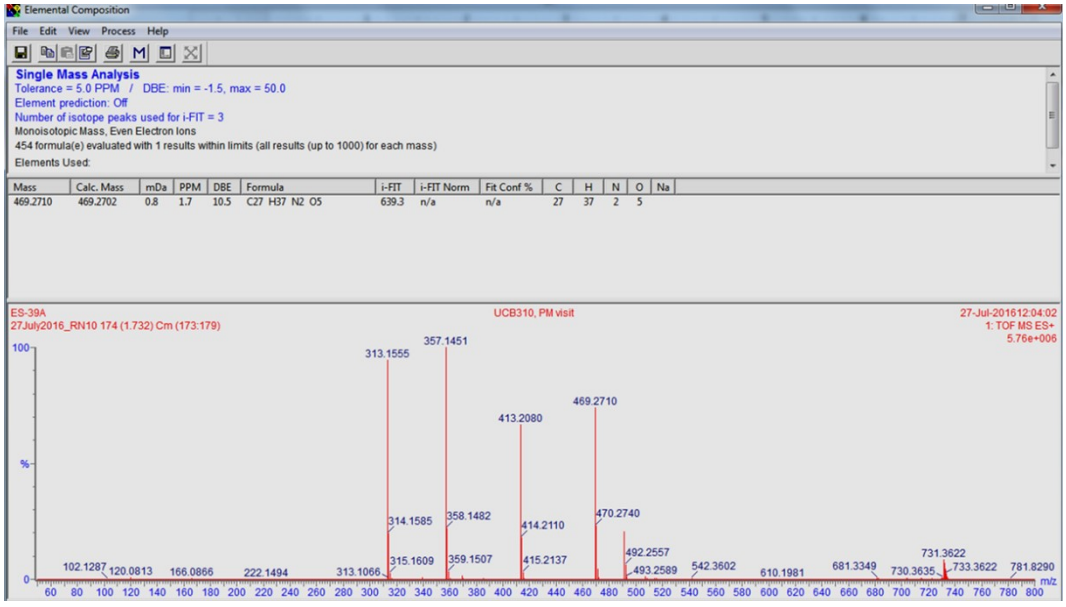

Figure S3. HRMS $[M+H]^+$ of *Boc*-L-F-L-FO*t*Bu **2**.

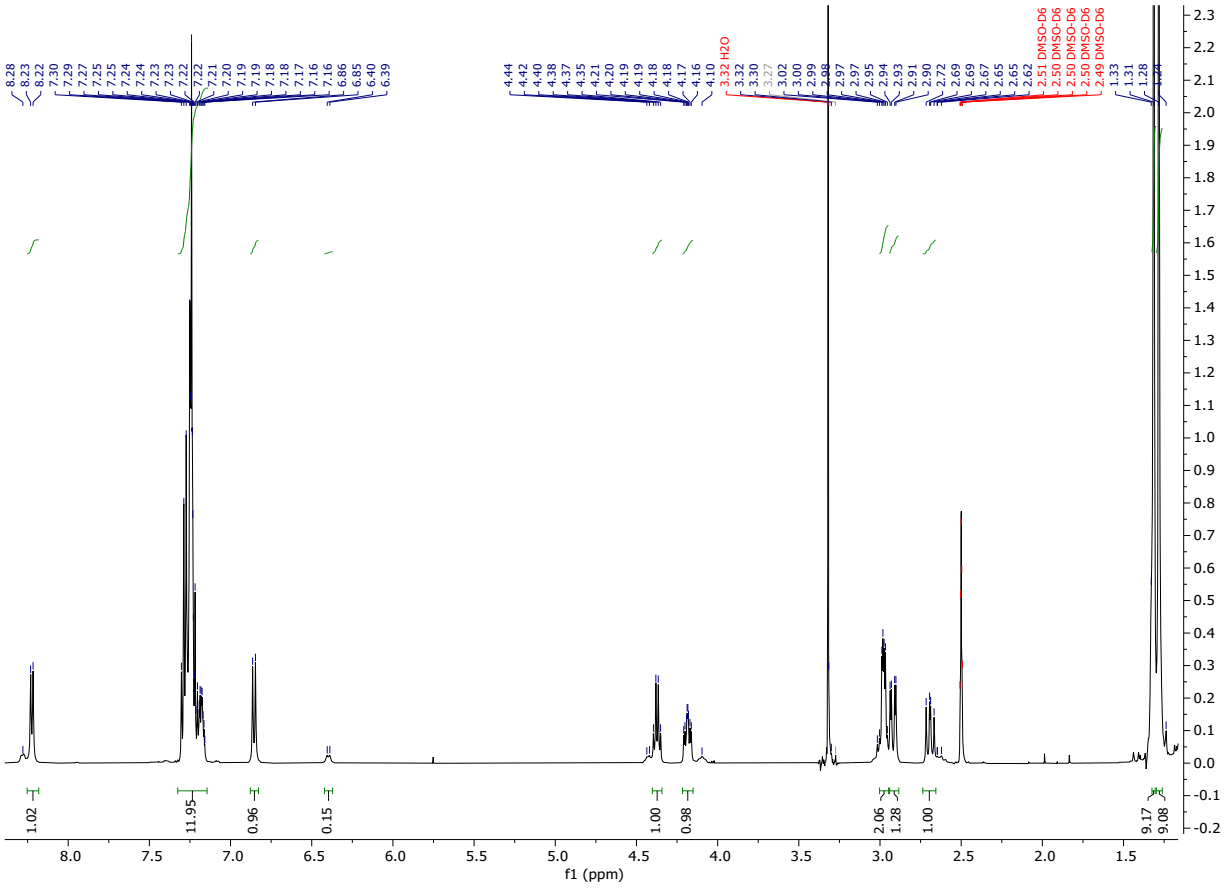

Figure S4. ^{1}H NMR (500 MHz, D_6-DMSO) spectrum of *Boc*-L-F-L-FO*t*Bu **2**.

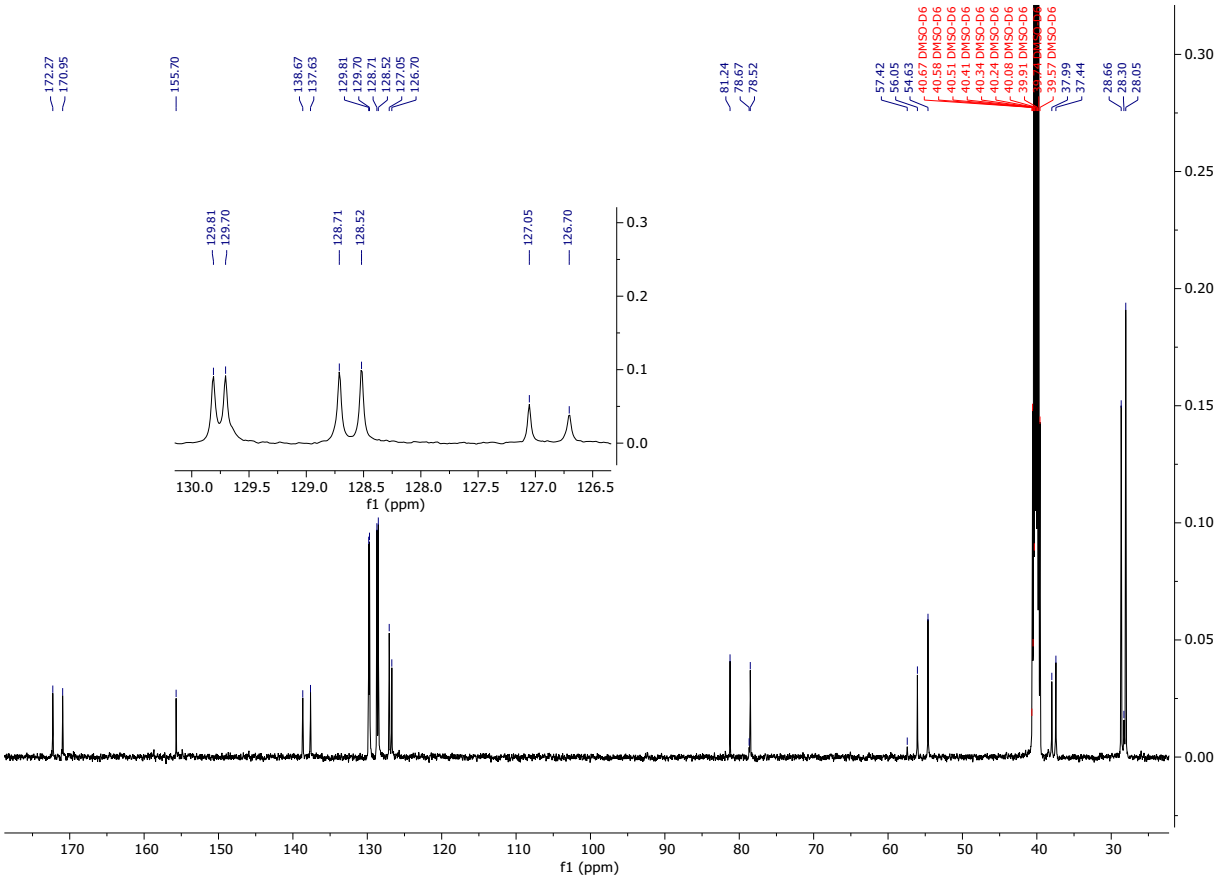

Figure S5. ^{13}C NMR (126 MHz, D_6-DMSO) spectrum of *Boc*-L-F-L-FO*t*Bu **2**.

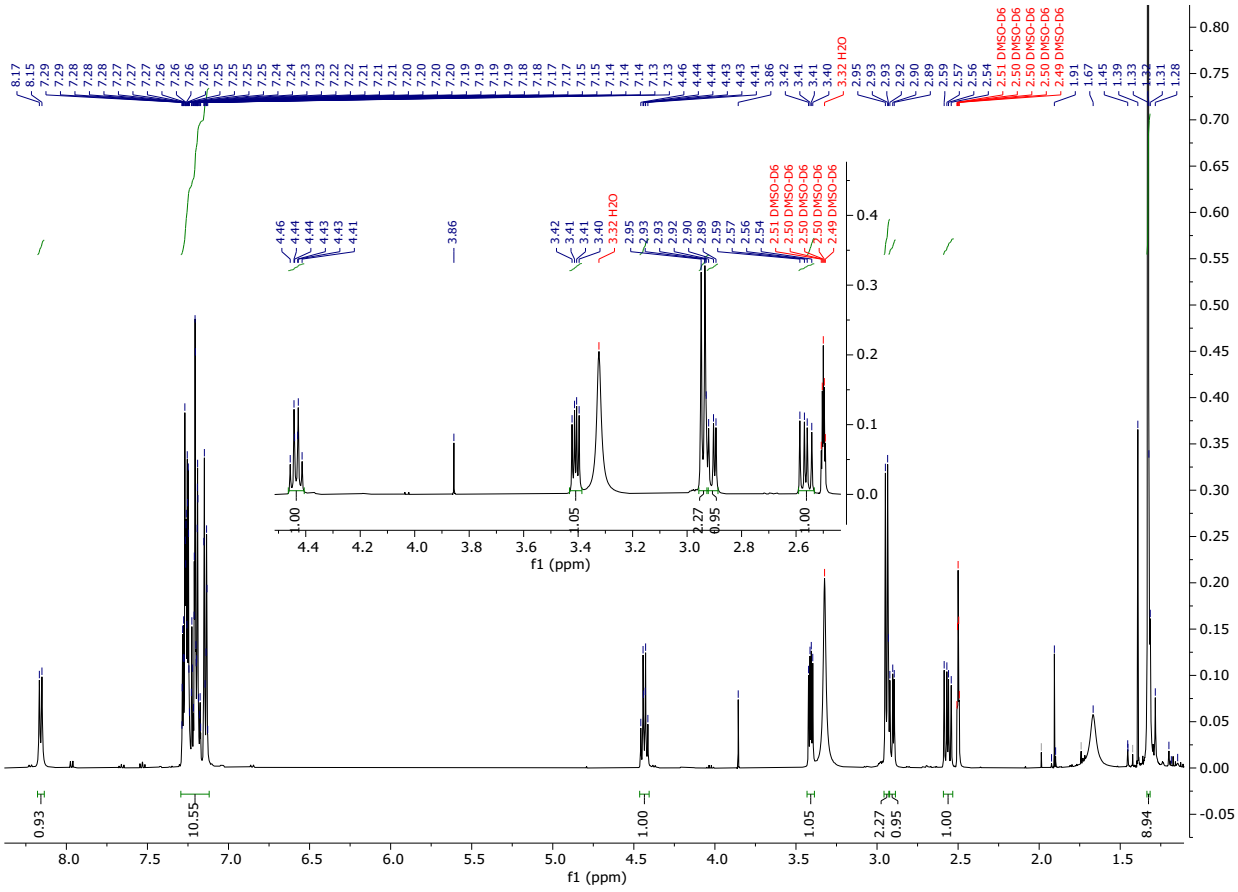

Figure S6. ^{1}H NMR (500 MHz, D_6-DMSO) spectrum of L-F-L-FO*t*Bu **5**.

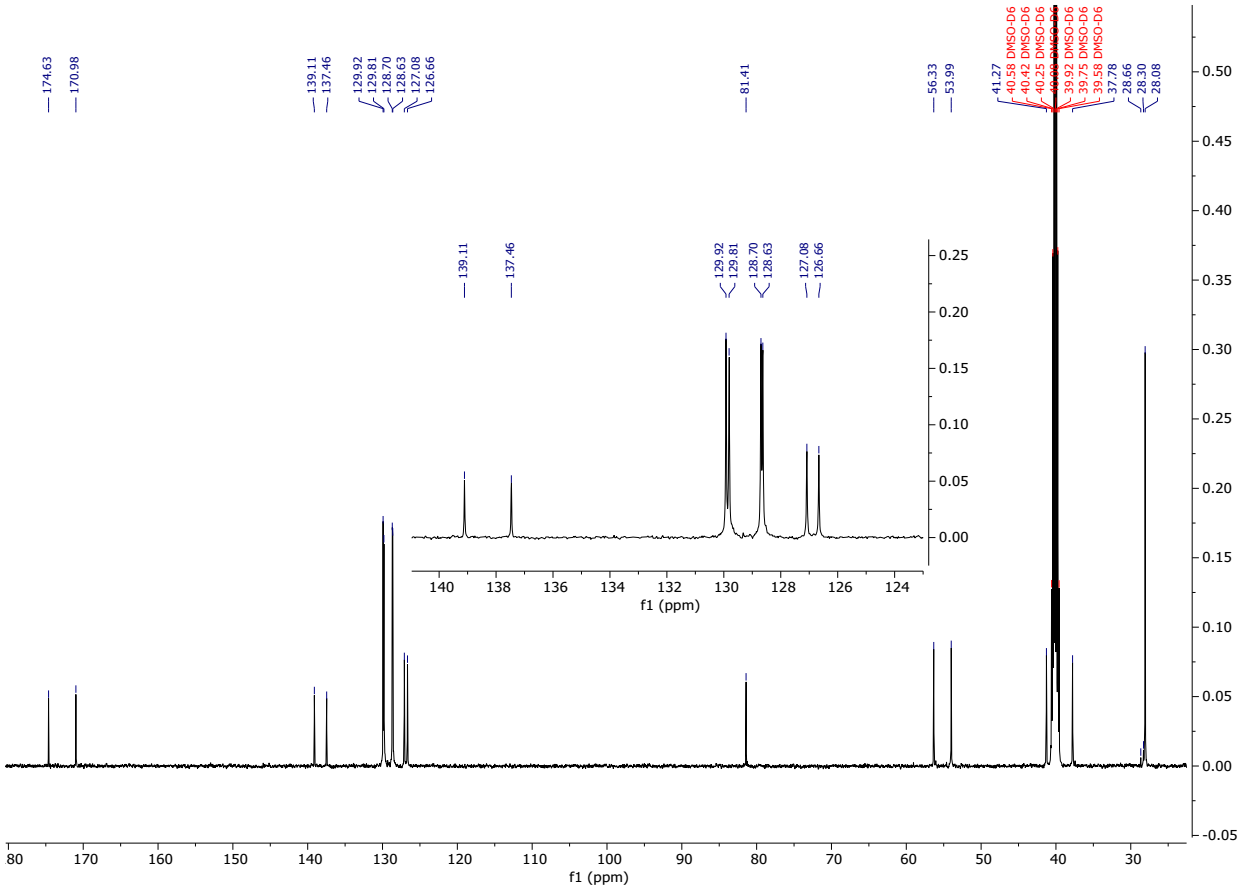

Figure S7. ^{13}C NMR (126 MHz, D_6-DMSO) spectrum of L-F-L-FO*t*Bu **5**.

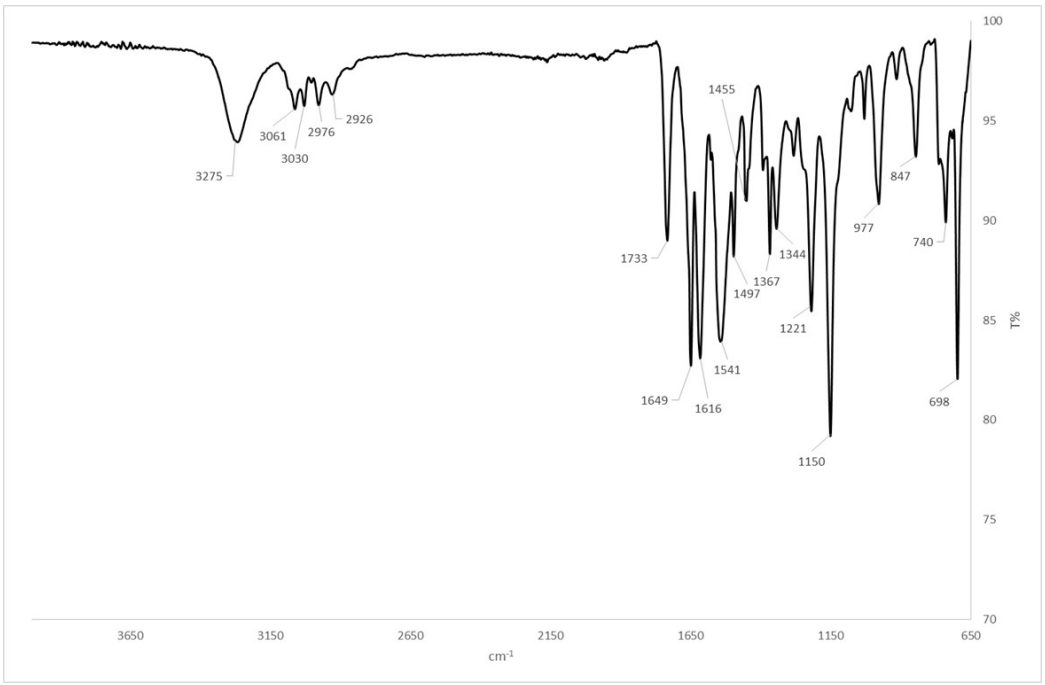

Figure S8. FT-IR spectrum (neat) of Cin-L-F-L-FO*t*Bu **6**.

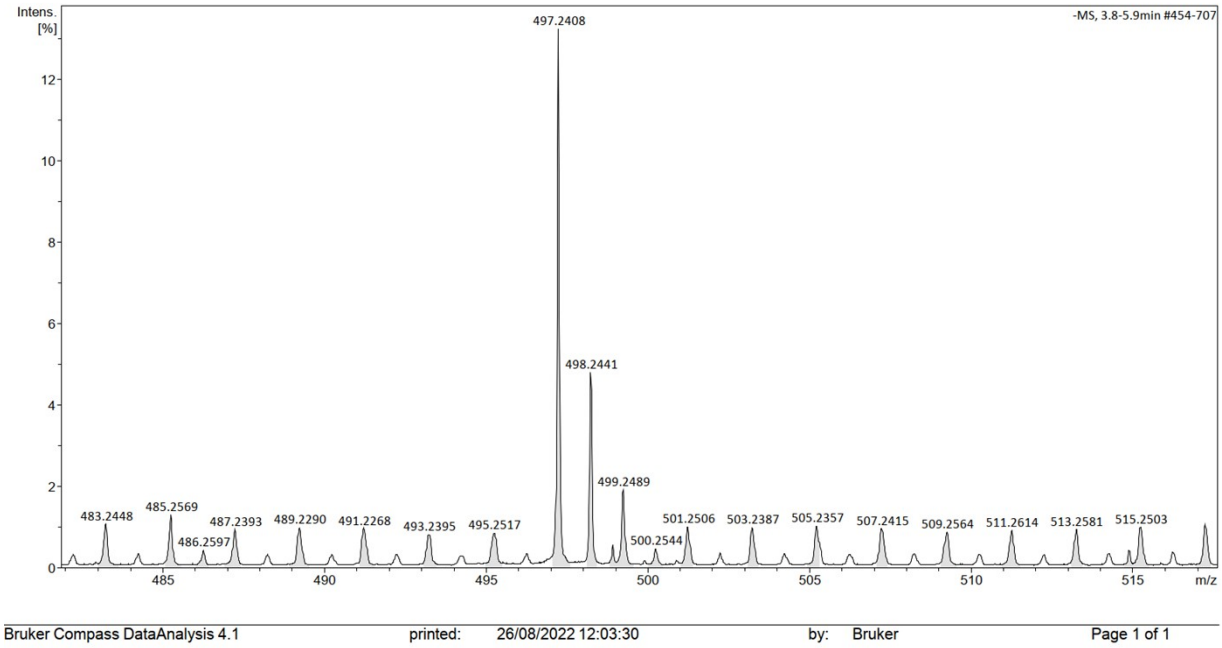

Figure S9. HRMS of Cin-L-F-L-FO*t*Bu **6**.

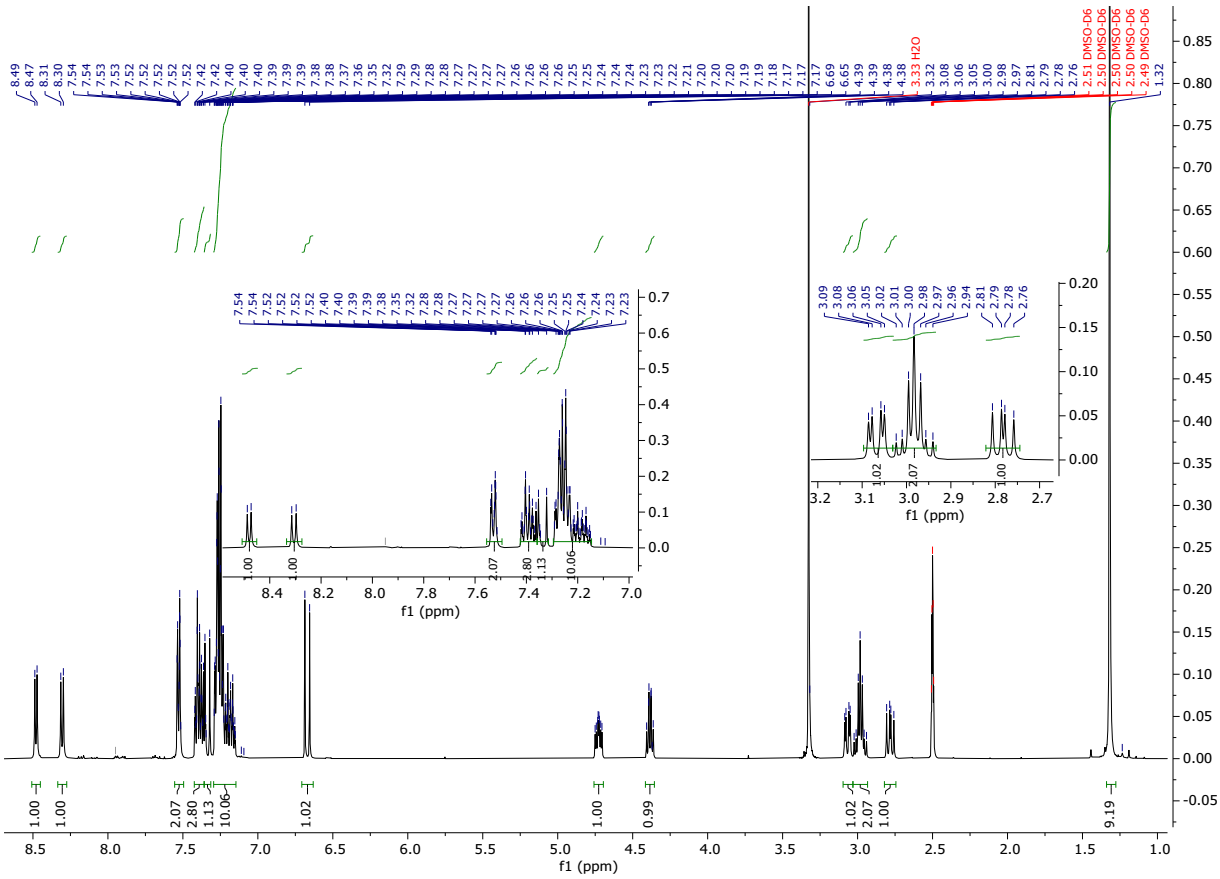

Figure S10. ^{1}H NMR (500 MHz, D_6-DMSO) spectrum of Cin-L-F-L-FO*t*Bu **6**.

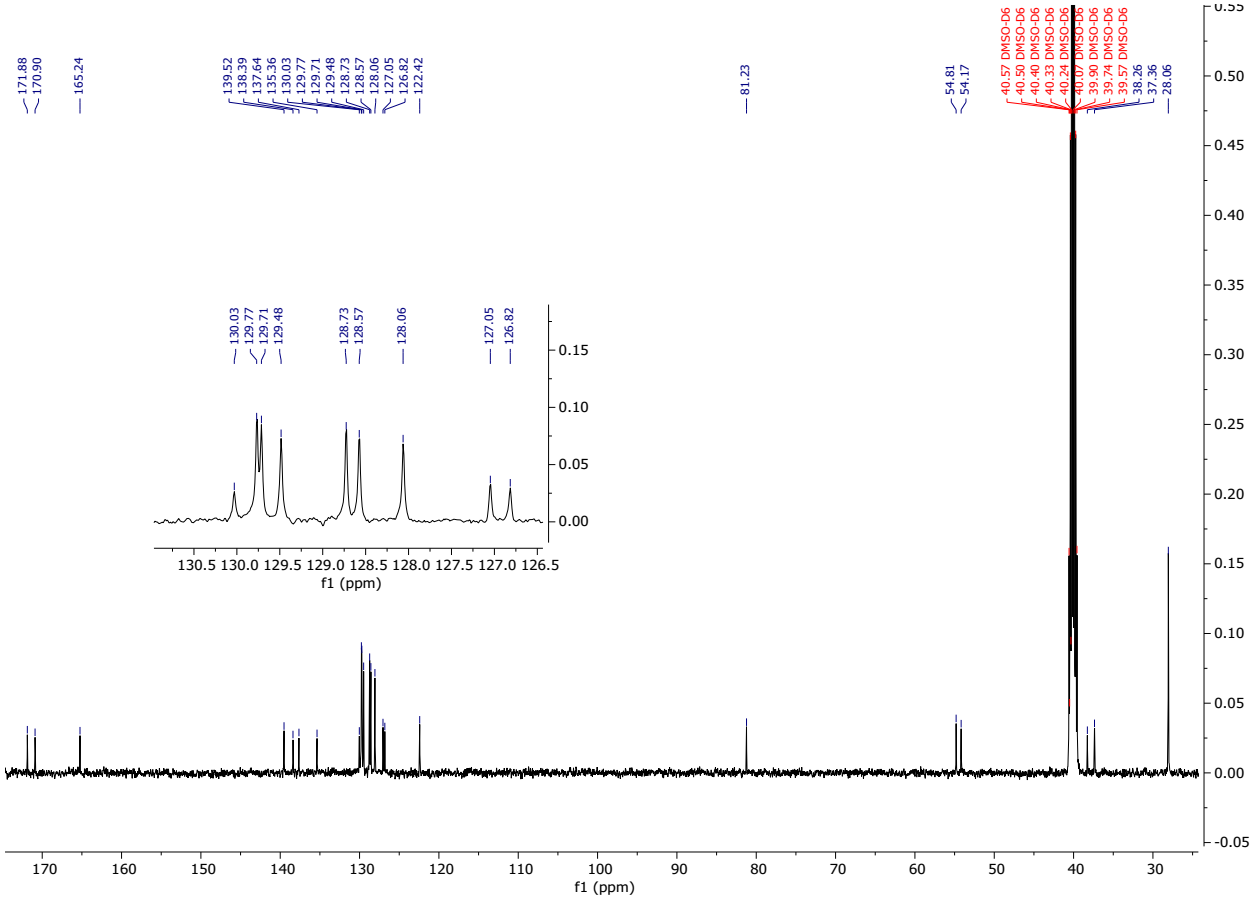

Figure S11. ^{13}C NMR (126 MHz, D_6-DMSO) spectrum of Cin-L-F-L-FO*t*Bu **6**.

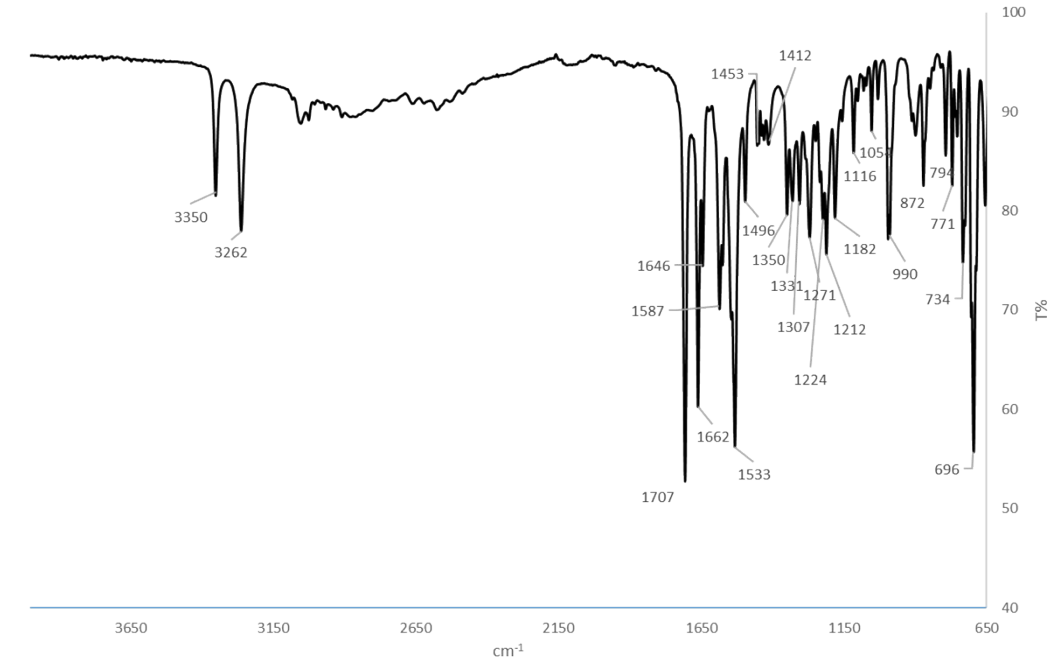

Figure S12. FT-IR (neat) of Cin-L-F-L-F **1**.

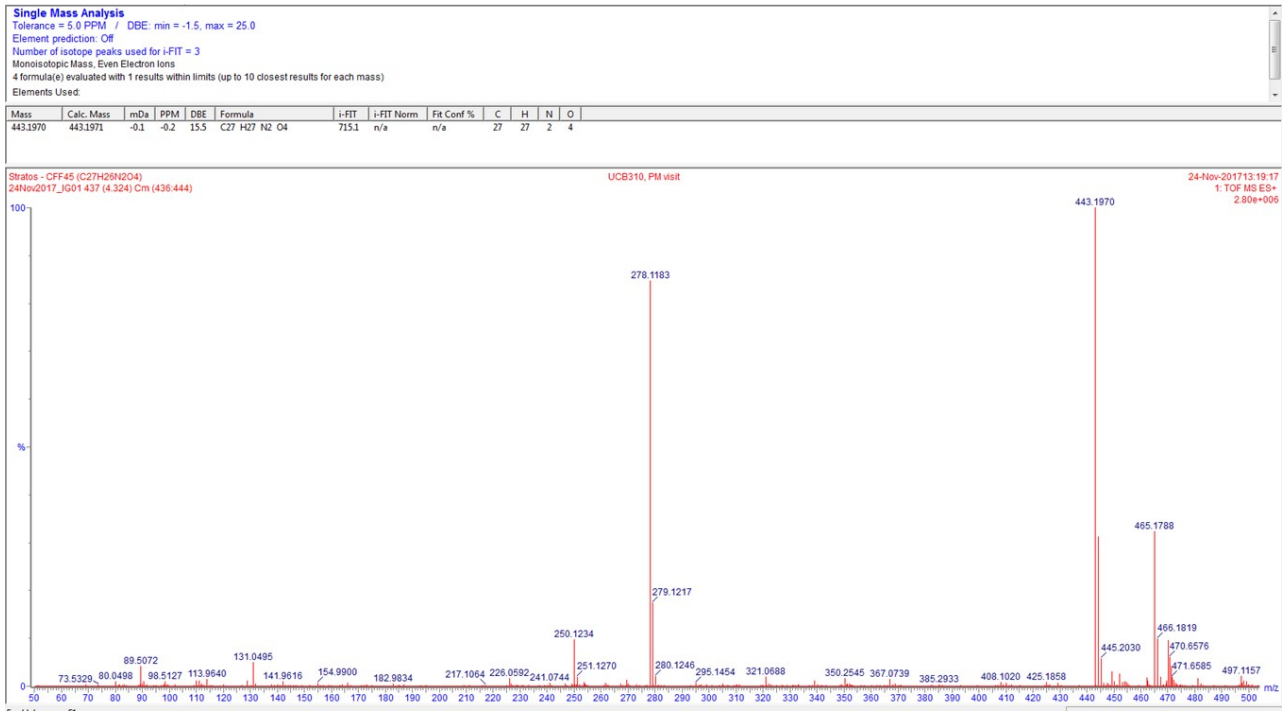

Figure S13. HR-MS of Cin-L-F-L-F **1**.

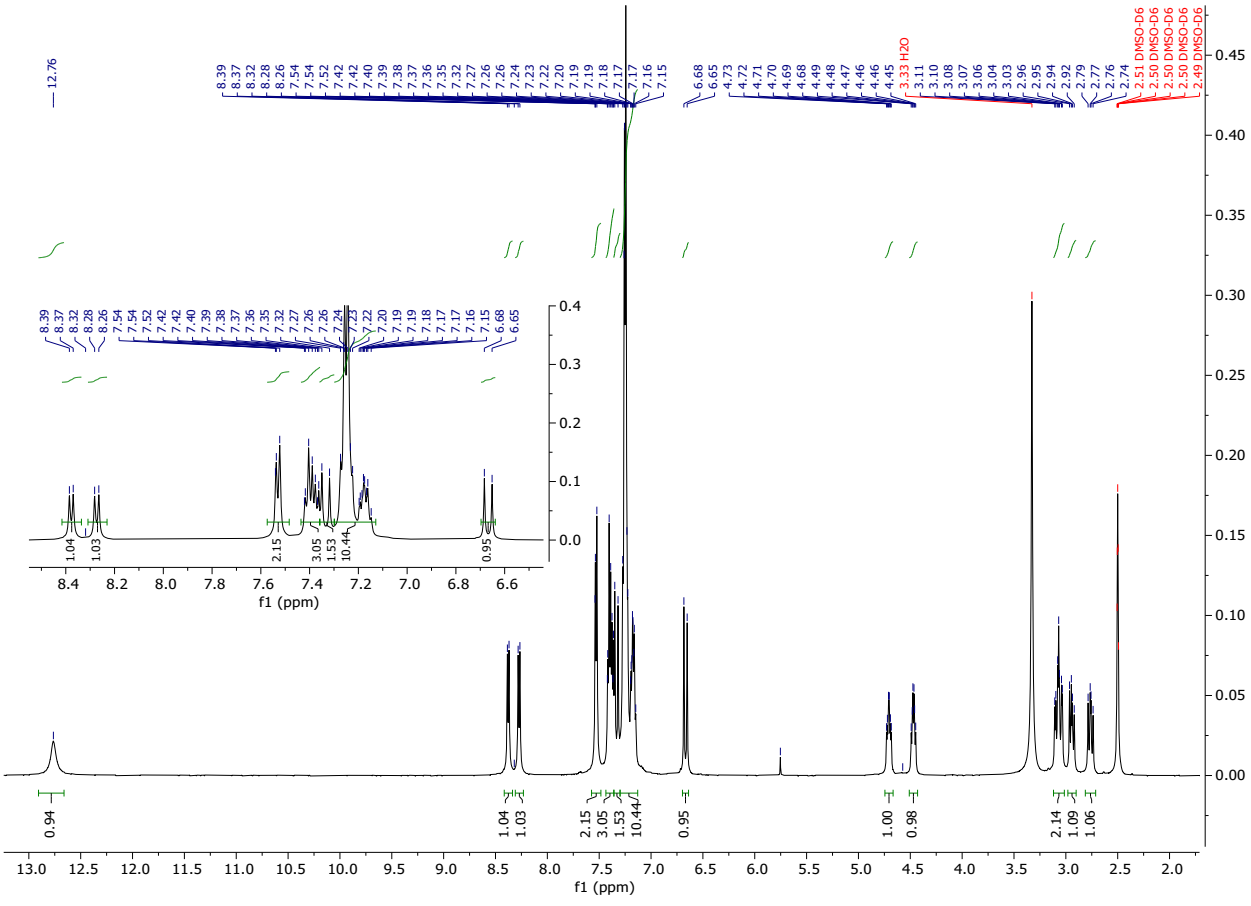

Figure S14. ^{1}H NMR (500 MHz, D_6-DMSO) spectrum of Cin-L-F-L-F **1**.

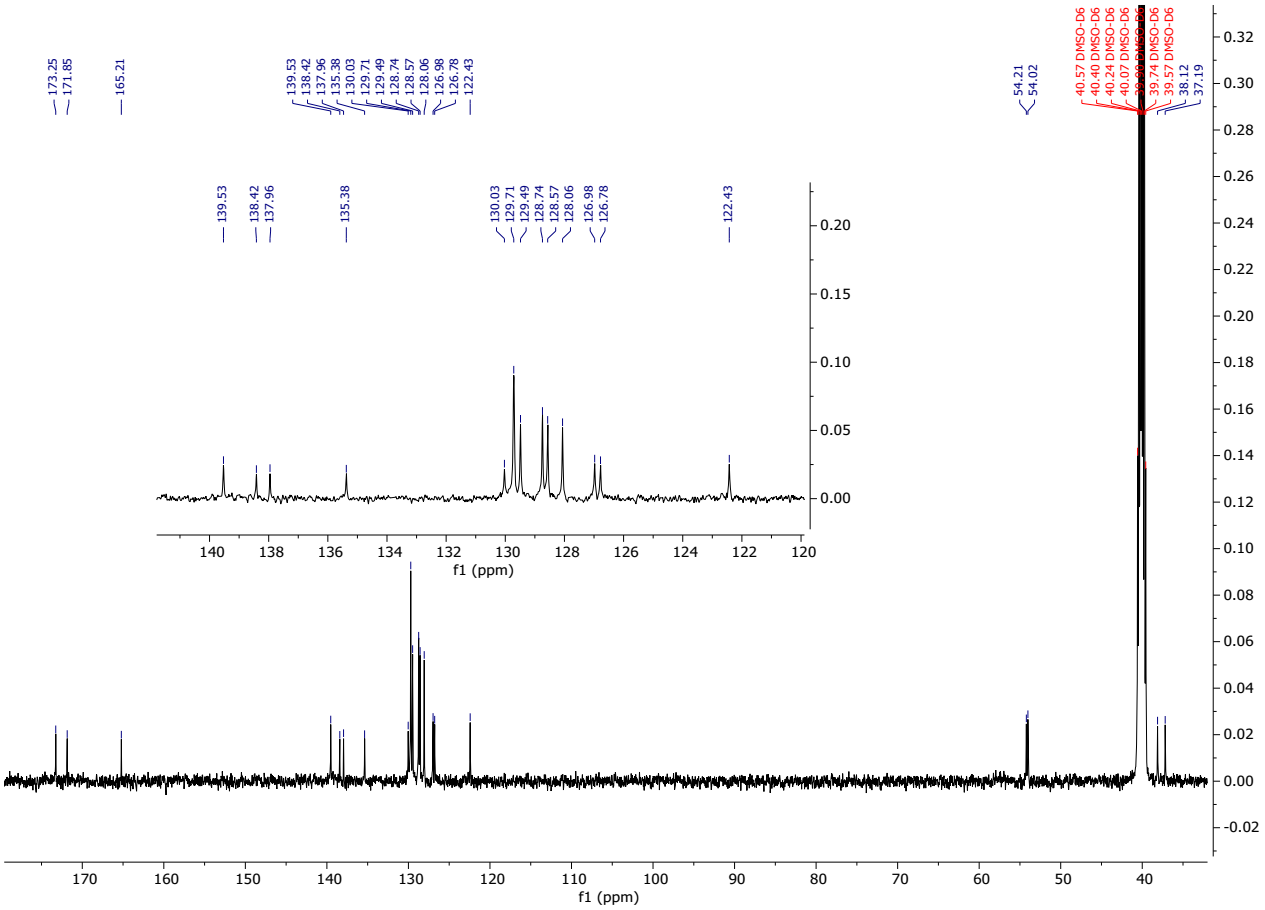

Figure S15. ^{13}C NMR (126 MHz, D_6-DMSO) spectrum of Cin-L-F-L-F **1**.

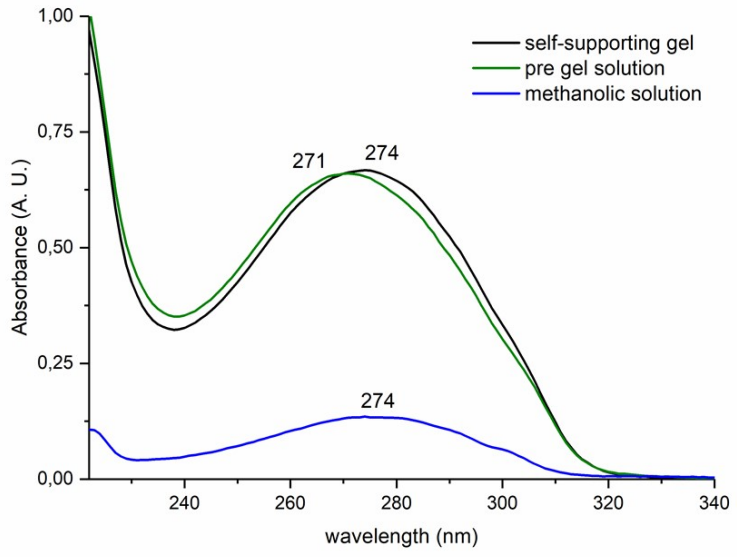

Figure S16. The absorbance of the gel, "pre gel" solution and methanolic solution of Cin-L-F-L-F. The spectra were obtained from the UV-vis channel of the Chirascan spectrophotometer while recording the CD spectra of the samples. The obtained CD spectra were truncated where the corresponding absorbance value exceeded 1.0 A.U.

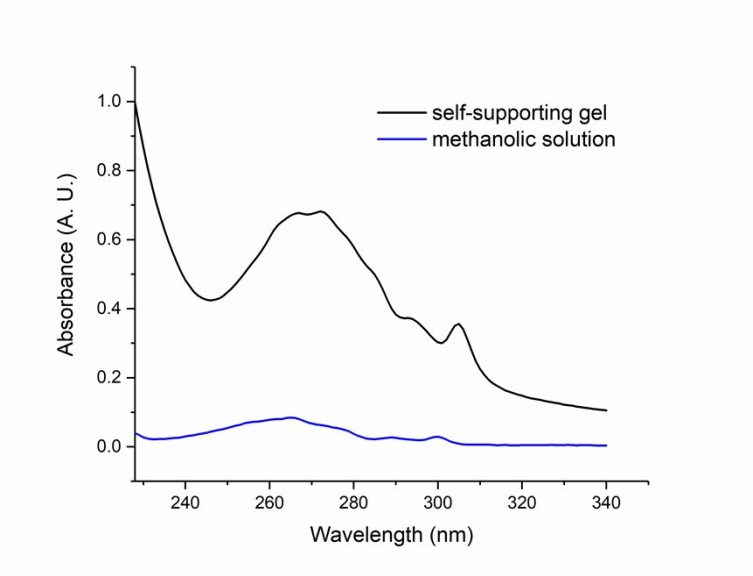

Figure S17. The absorbance of the gel and methanolic solution of Fmoc-L-F-L-F. The spectra were obtained from the UV-vis channel of the Chirascan spectrophotometer while recording the CD spectra of the samples. The obtained CD spectra were truncated where the corresponding absorbance value exceeded 1.0 A.U.