Supporting Information

Heat-set supramolecular polymer gel and decomposition by guests

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Figure S1:Transformation from GelAto sol to GelB.

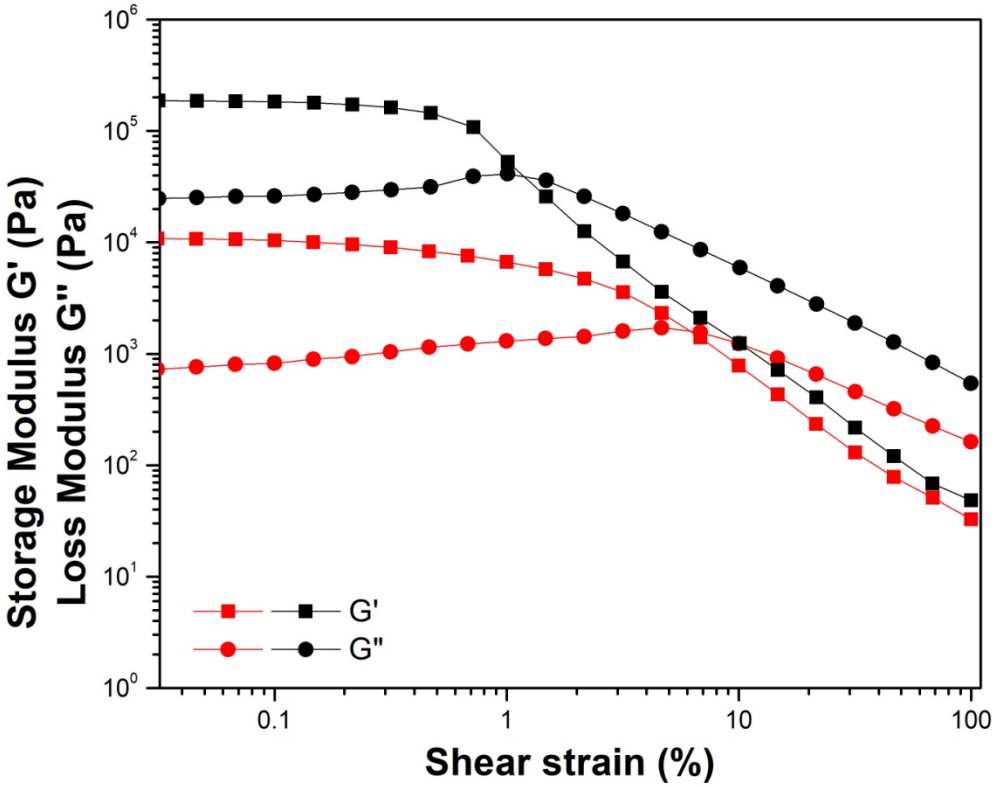


Figure S2: Comparism of modulus ofgelA (red colour) and gelB (black colour).

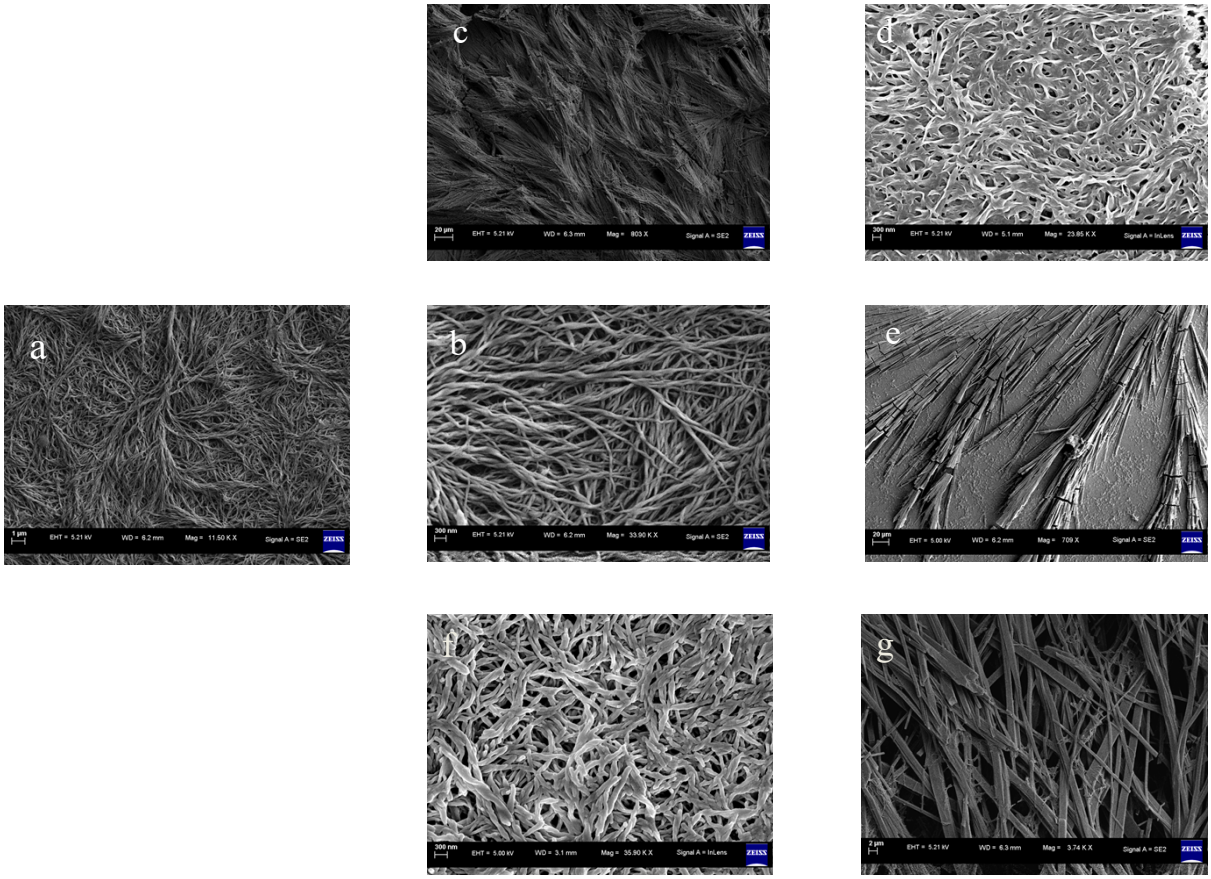


Figure S3: FE-SEM image of all gel and solution (a) FE-SEM image of xerogelformed by low-molecular-weight gelator 1 in DMF (b) FE-SEM image of DMF solutionformed by low-molecular-weight gelator 1 (c) FE-SEM image xerogel formed by compound 1with β-CD (d) FE-SEM image of sol at 85°C without K_2CO_3. (e) FE-SEM image of xerogelB formed with β-CD and K_2CO_3 (f) FE-SEM image of xerogelA. (g) FE-SEM image of solution form by gelAat 58 °C.

Procedure of sample preparation for ^{1}H-NMR: At first we have prepared a gel (gelA) in NMR tube by compound **1** with β-CD/α-CD/γ-CD and K_2CO_3in DMF-D_7 at room tempareture,then we have taken NMR data. After that we have heated these gels around 90°C and taken NMR.

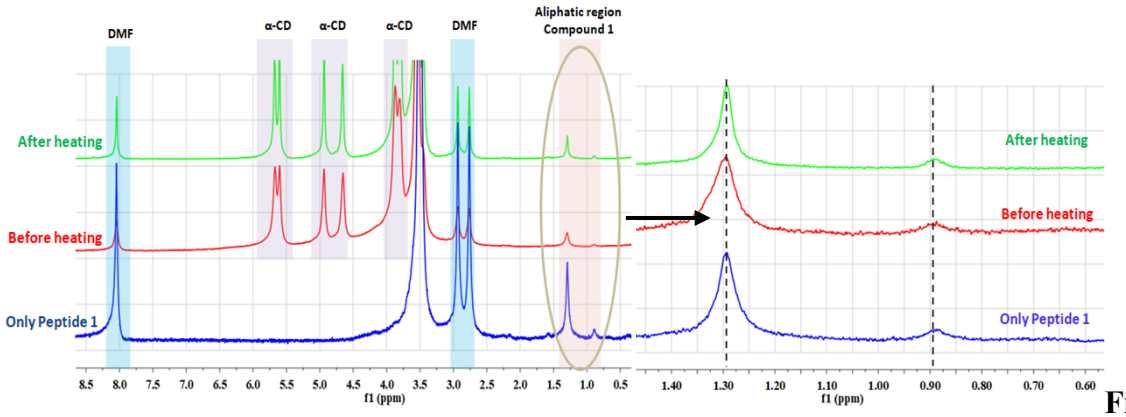


Figure S4: ^{1}H-NMR (500 MHz, DMF-D_7, δ in ppm)of Peptide **1**, before and after heating with α-CD.

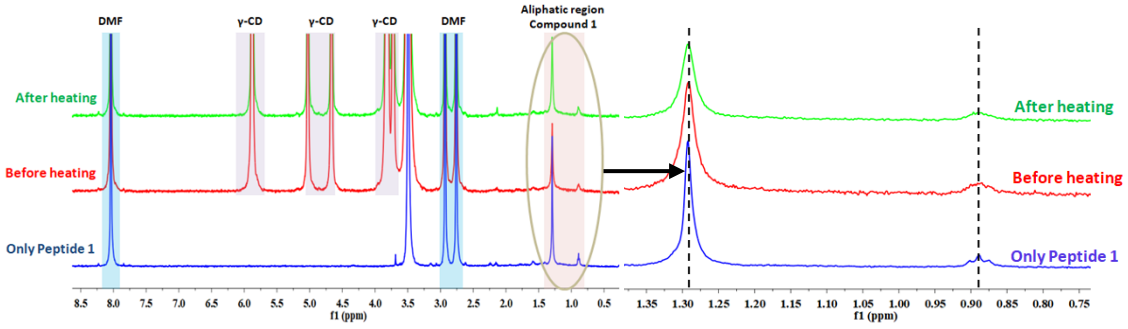


Figure S5: ^{1}H-NMR (500 MHz, DMF-D_7, δ in ppm)of Peptide **1**, before and after heating with γ-CD.

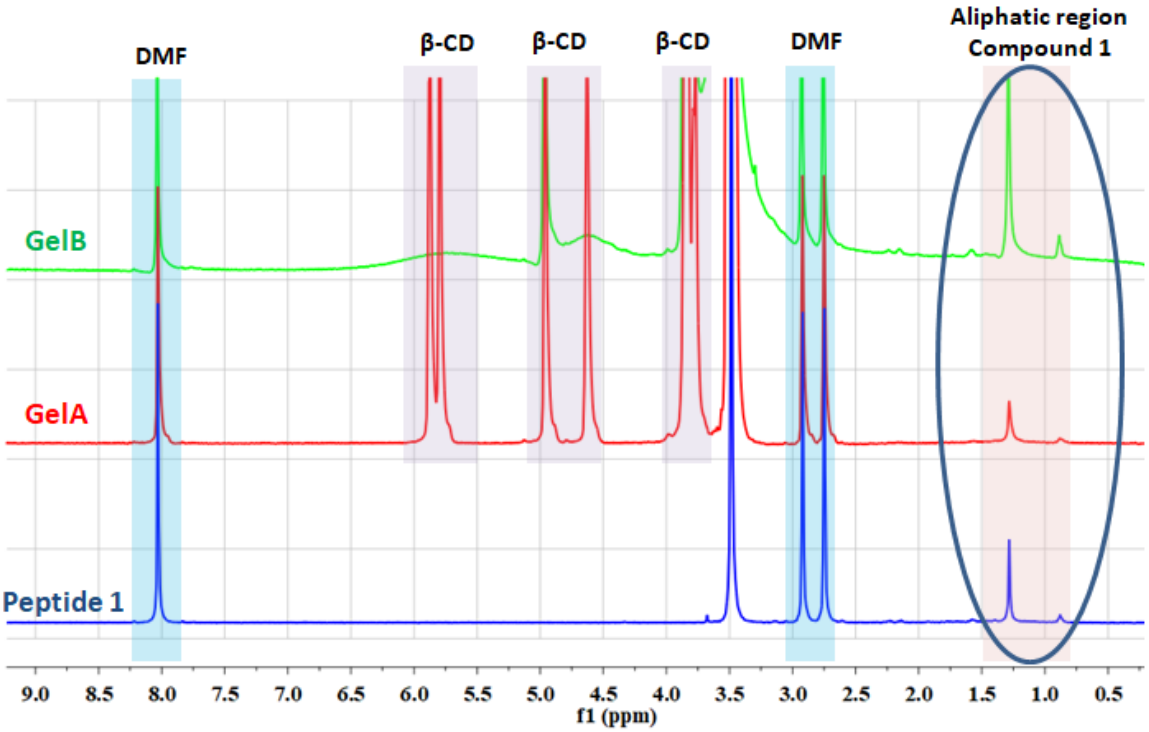


Figure S6:[1]H-NMR(500 MHz, DMF-D_7, δ in ppm)of Peptide **1**, GelA, GelB with β-CD.

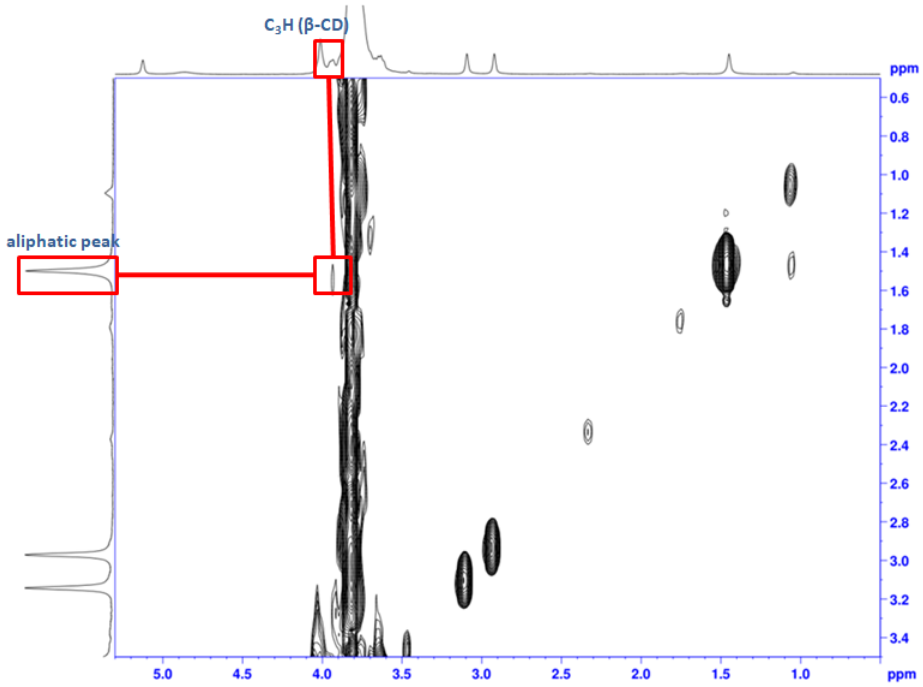


Figure S7: 2D COSY NMR spectrum of heat set gelB (500 MHz, DMF-D_7, δ in ppm). cross peak between the inner protons C(3)-H of βCD and peptide 1.

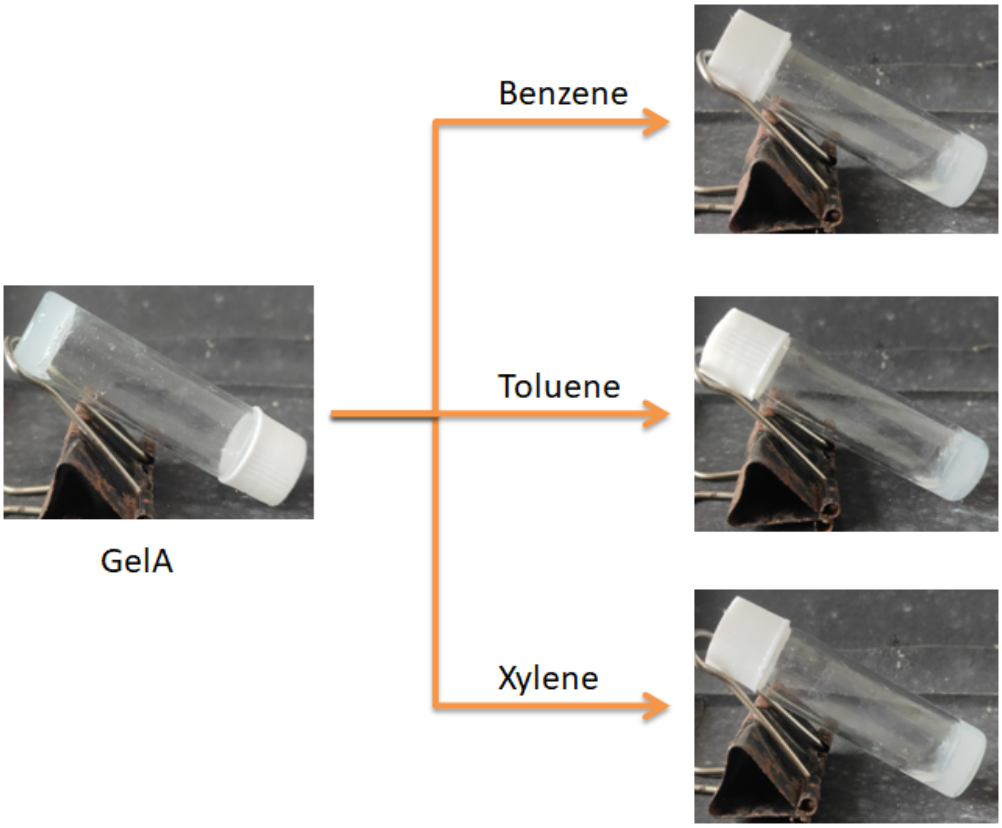


Figure S8: Theguest molecules like benzene, toluene, xylene do not have effect on gelA. No sol to gel conversion on addition of these guests.

Figure S9.(a) Sol in presence of α-CD at high temperature (we heated upto 100 ˚C); (b) Sol in presence of γ-CD at high temperature (we heated upto 100 ˚C); (c) gelB form with β-CD at 86 ˚C.

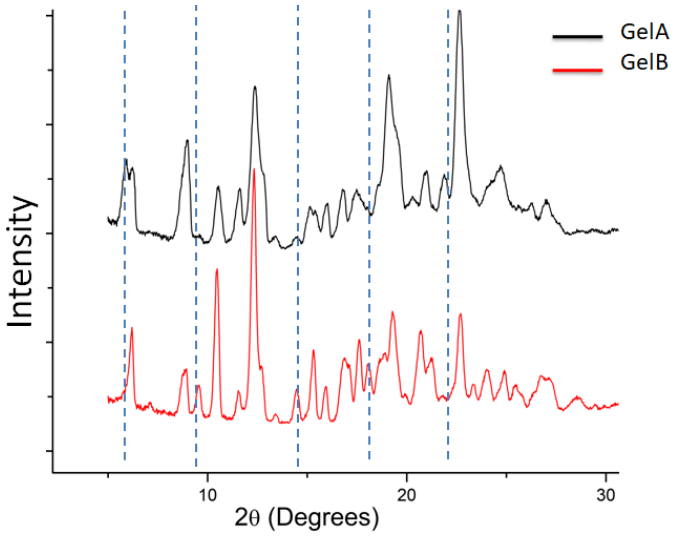


Fig. S10: Comparable PXRD pattern of gelA and gelB

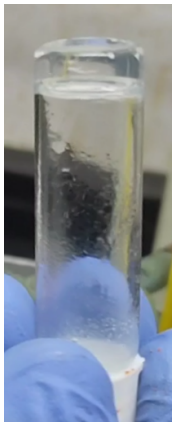


Fig. S11: Image of transparent gel form by only compound 1.

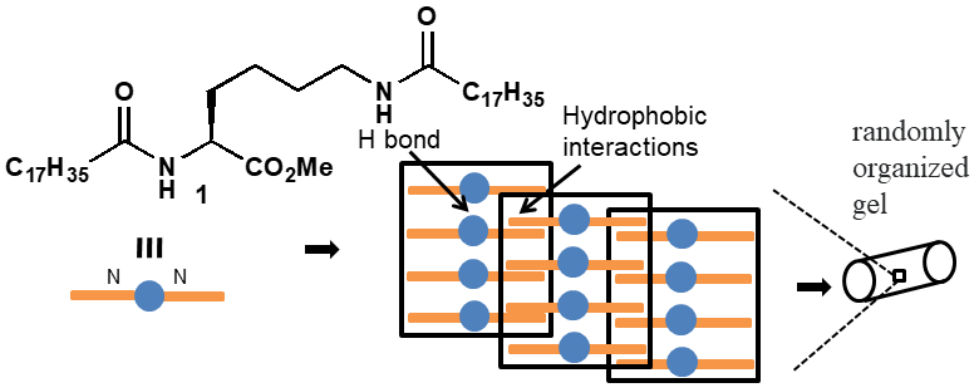
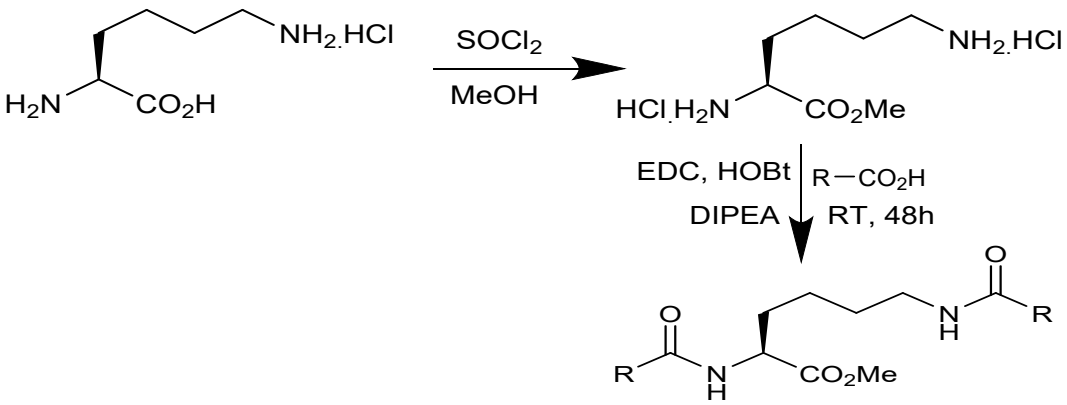


Fig. S12: Tentative model for the structureof randomly organized gelA of compound **1**.

Synthesis of Compound 1.

Synthesis of stearic acid appended L-lysine: 1.194 g (4.2 mmol) of stearic acid dissolved in minimum DMF and 30 ml DCM and kept in an ice bath and 0.466 g (2 mmol) of Lyn-OMe.HCl (which was isolatedfrom acid protection reaction of L-lysine by $SOCl_2$, MeOH) was added followed by 0.802 g (4.2 mmol) EDC.HCl and 0.567 g(4.2 mmol) HOBt and 2 ml DIPEA. The reaction mixture was kept at room temperature and stirred for 2 days. Then DCM evaporated and the residue was dissolved in ethyl acetate (60 mL); organic layer washed with 2 M HCl (3 × 50 mL) and 1 M Na_2CO_3 (3 × 50 mL), then collected the precipitated.

The synthetic procedure of stearic acid appended L-lysine:



R= $C_{17}H_{35}$

Figure S13: The proposed scheme for the synthesis of stearic acid appended L-lysine 1.

Characterization of stearic acid appended L-lysine 1:

^{1}H NMR (400 MHz, CDCl3, δ in ppm, 298K): 6.20(d,1H, NH), 5.71(s, 1H, NH), 4.55(m, 1H, Cα-H), 3.72(s, 3H, OCH_3), 3.22(m, 2H, C_β-H), 2.21(t, 2H, CH_2), 2.14(t, 2H, CH_2), 1.87(m, 2H, CH_2), 1.71-1.13(m, 64H, aliphatic proton) 0.849(t, 6H, CH_3 proton). ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 173.63, 173.42, 173.20, 52.49, 51.74, 38.79, 38.96, 36.67, 36.96, 32.05, 29.81, 29.49, 28.97, 25.96, 25.76, 22.80, 22.41, 14.24 ESI-MS (MeOH): m/z (Calc): C43H84N2O4Na [M+Na]+ 715.64; found: 715.63. Yield: 55%. white colour solid.

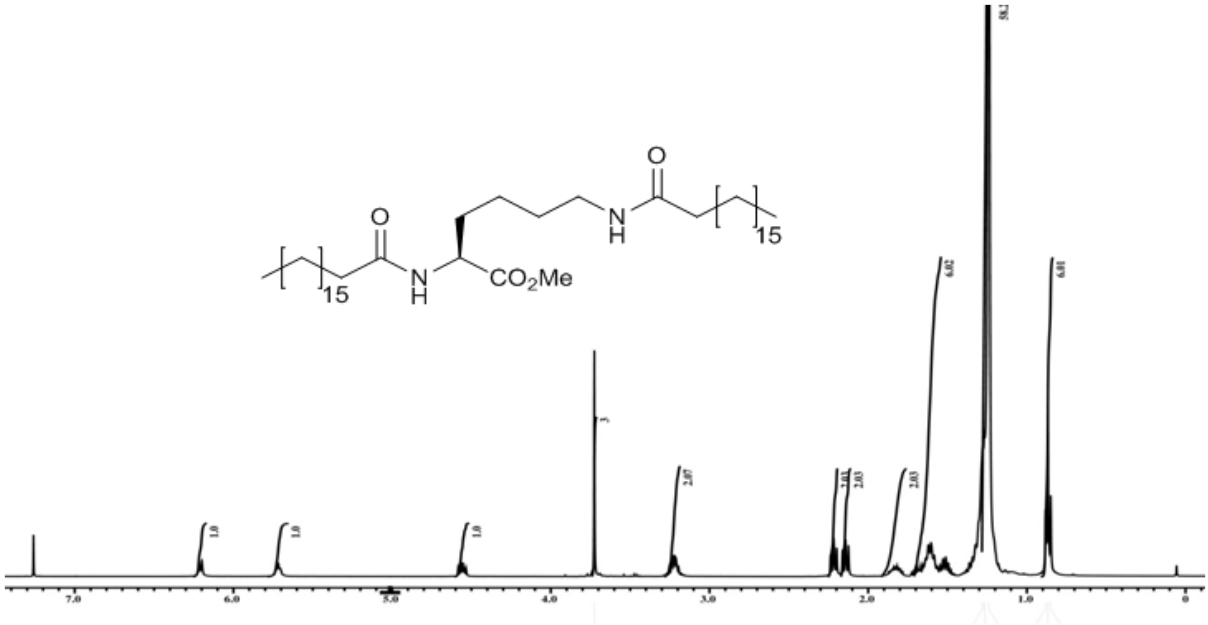


Figure S14:^{1}H NMR (400 MHz, CDCl3, δ in ppm, 298K) spectra of stearic acid appended lysine **1**.

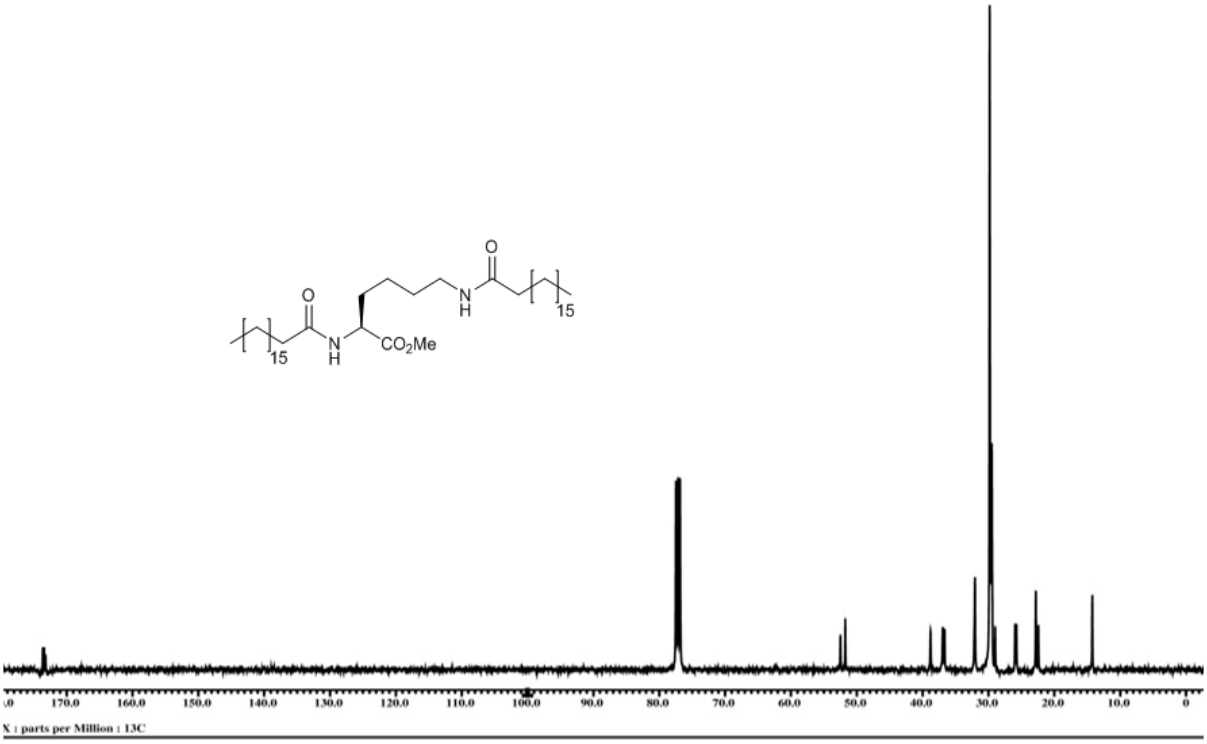


Figure S15:[13]C NMR (100 MHz, CDCl3, δ in ppm, 298K) spectra of stearic acid appended L-lysine **1**.

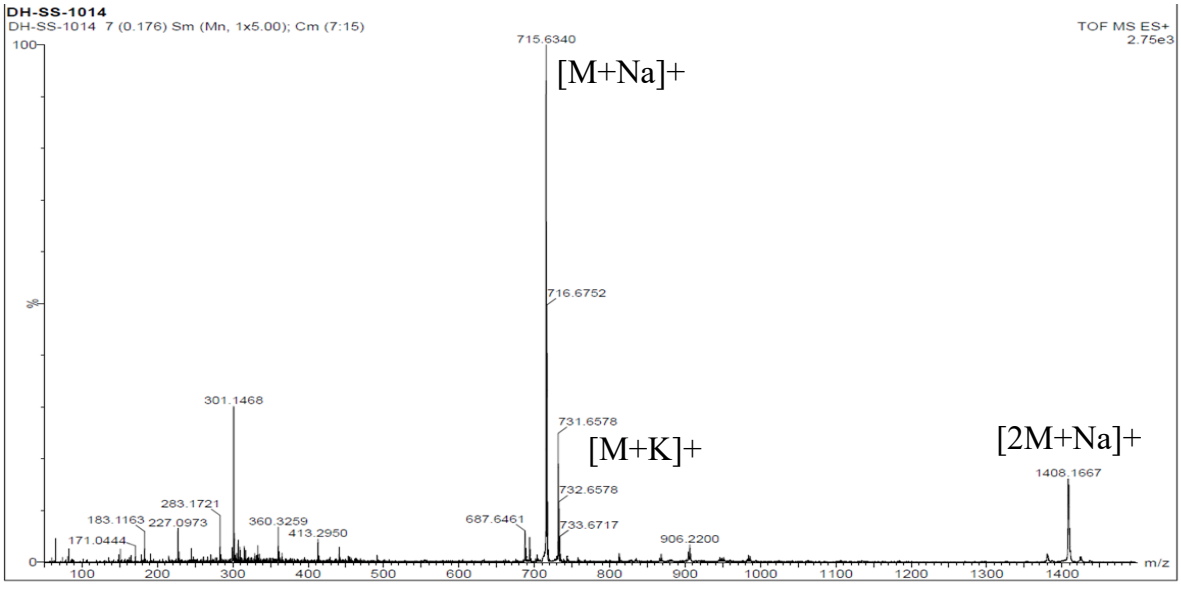


Figure S16: ESI-MS spectra of stearic acid appended L-lysine **1**.

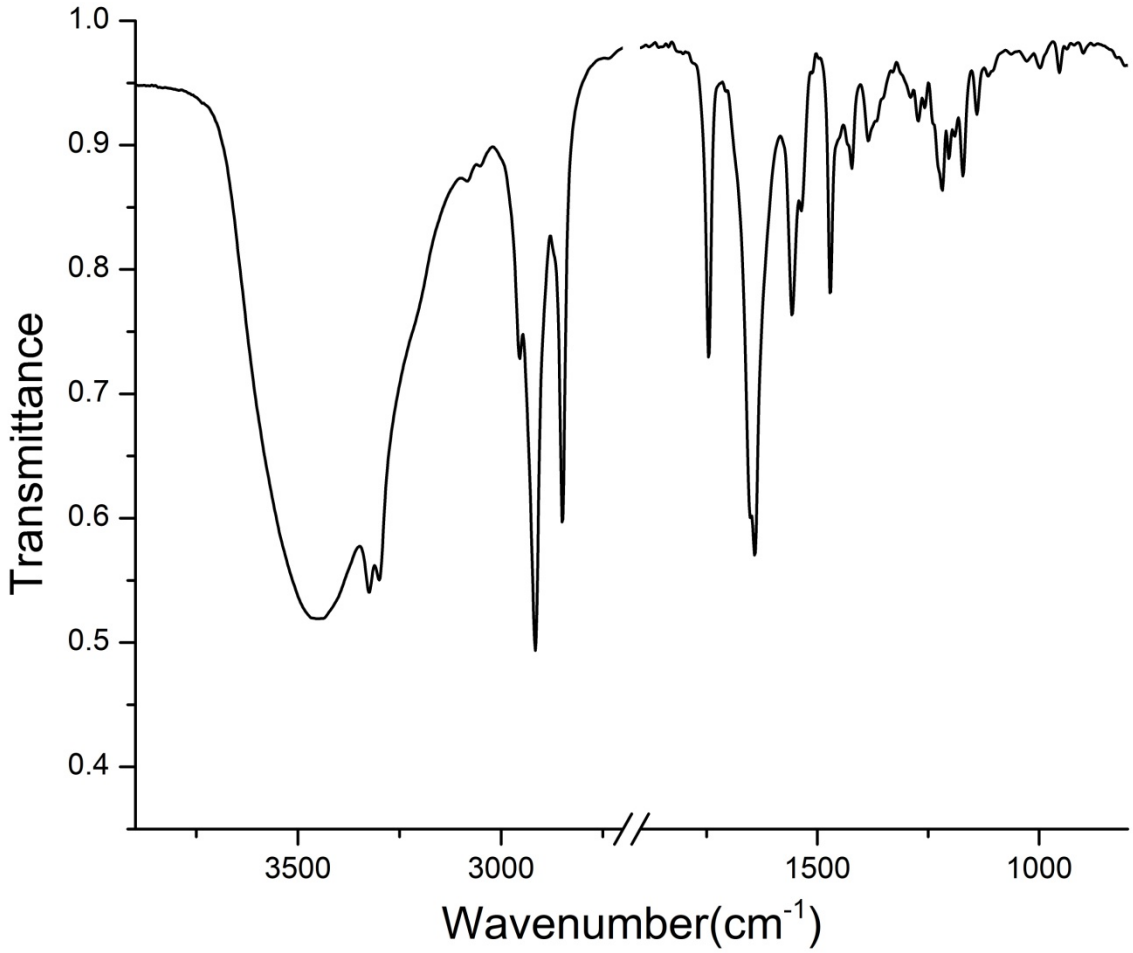


Figure S17: FT-IR spectra of stearic acid appended L-lysine **1**.