Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Higher-order interfiber interactions in the self-assembly of Benzene-1,3,5-tricarboxamide-based peptides in water

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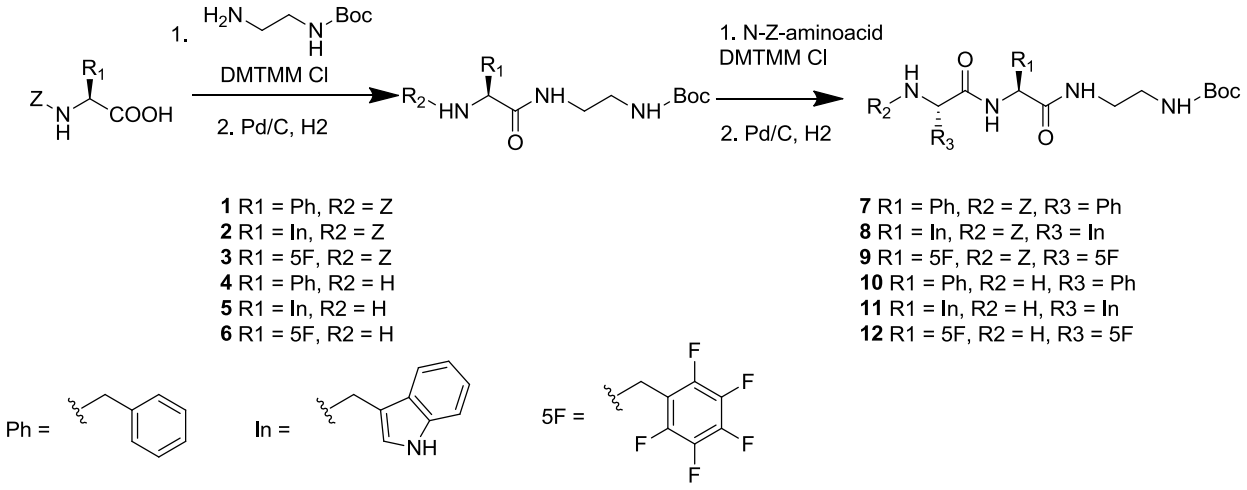
SI-1. Synthesis of Dipeptide-ethylenediamine-Boc Derivatives



Scheme SI-1. Synthesis of Dipeptide-ethylenediamine-Boc Derivatives

Synthesis of Z-L-pentafuorophenylalanine

L-pentafluorophenylalanine was synthesized as was described previously.[1] In a round bottom flask, L-2,3,4,5,6-pentafluorophenylalanine (4.950 g, 19.4 mmol) was dissolved in an acetone: water (50:50) mixture (100 mL). pH was adjusted to 7 using a saturated $NaHCO_3$ solution. Z-OSu (4.239 g, 19.4 mmol) was added, and the reaction was left overnight. Acetone was evaporated and the aqueous solution was washed with dichloromethane (100 mL x2). The aqueous layer was then acidified to pH 2.5 using hydrochloric acid and extracted with ethyl acetate (100 mL x 3). The combined organic layers were washed with water (150 mL), dried using magnesium sulfate and filtered. The solution was concentrated and further dried with a deep vacuum. Product - white powder. Product - white solid. Yield: 7.08 g (94 %).

^{1}H NMR (300 MHz, DMSO-d6): 7.75 (d, 1H), 7,42-7.22 (m, 5H), 4.24 (qd, 1H), 3.24-2.98 (m, 3H). ^{19}F NMR (300 MHz, DMSO-d6): -142.5 (dd, 2F), -157.2 (t, 1F), -161.2 (td, 2F).

*Synthesis of Compounds **1-3***

In a round bottom flask, Z-protected amino acid (1 eq.) and DMTMM*Cl (1.2 eq.) were dissolved in methanol. After 10 minutes, N-BOC-diaminoethane (1.1 eq.) was added, and the reaction left to continue overnight. The product was precipitated in water and filtered and then dried in a vacuum pump.

Z-F-EDA-Boc (1). Product - white powder. Global yield: 12.7 g (92%). ^{1}H-NMR (300 MHz.DMSO-d6): 1.37 (s, 9H), 2.68-3.21 (m, 6H), 7.45 (d, 1H), 4.17 (m, 1H), 7.1-7.37 (m, 10H), 8.03 (t, 1H), 4.94 (s, 2H), 6.72 (t, 1H).

Z-W-EDA-Boc (2). Product - yellowish solid. Global yield: 1.47 g (95 %). ^{1}H NMR (300 MHz, DMSO-d6): 10.88 (s, 1H), 8.02 (t, 2H), 7.61 (d, 1H), 7.37-7.20 (m, 7 H), 7.13 (d, 1H), 7.00 (ddt, 1H),6.73 (t, 1H), 4.94 (s, 2H), 4.21 (m, 1H), 3.17-2.82 (m, 6H), 1.37 (s, 9H).

Z-Ф-EDA-Boc (3). Product - white solid. Global yield: 1.31 g (95 %). ^{1}H NMR (300 MHz, DMSO-d6): 8.03 (t, 2H), 7.55 (d, 1H), 7.39-7.20 (m, 5 H), 6.73 (t, 1H), 5.06-4.86 (m, 2H), 4.31-4.21 (m, 1H), 3.17-2.87 (m, 6H), 1.36 (s, 9H); ^{19}F NMR (300 MHz, DMSO-d6): -142.83 (dd, 2F), -157.42 (t, 1F), -163.7 (td, 2F)

*Synthesis of Compounds **4-6***

In a round bottom flask, Z-X-EDA-Boc was dissolved in methanol (150 mL). The solution was mixed with a palladium (Pd) catalyst (150 mg) and purged (3 x N_2/vacuum cycle) to remove moisture and oxygen. The system was then placed under hydrogen. After the reaction was completed (evaluated with a ninhydrin test), the solution was filtered over a celite pad and dried using a rotary evaporator (Heidolph, Schwabach, Germany).

H-F-EDA-Boc (4). Product - white powder. Global yield: 8.67 g (87%). ^{1}H NMR (300 MHz. DMSO-d6): 1.37 (s, 9H), 6.74 (t, 1H), 2.86-3.12 (m, 5H), 7.04-7.39 (m, 5H), 3.36 (m, 1H), 7.87 (t, 1H).

H-W-EDA-Boc (5). Product - yellowish viscous liquid. Global yield: 1.01 g (88 %).^{1}H NMR (300 MHz, DMSO-d6): 1.37 (s, 9H), 2.74 (dd, 1H), 3.13-2.91 (m, 6H), 3.43 (dd, 1H), 6.77 (t, 1H), 7.00 (ddt, 1H), 7.14 (d, 1 H), 7.33 (d, 1H), 7.55

(d, 1H), 7.93 (t, 1H), 10.83 (s, 1H).

H-Φ-EDA-Boc (6). Product - white solid. Global yield: 920 mg (86 %).^{1}H NMR (300 MHz, DMSO-d6): 1.29 (s, 11H), 3.11-2.80 (m, 7H), 6.68 (t, 1H), 7.84 (t, 1H). ^{19}F NMR (300 MHz, DMSO-d6): -142.83 (dd, 2F), -158.36 (t, 1F), -163.7 (td, 2F). *m/z:* 397.2 Da (Expected: 397 Da).

*Synthesis of Compounds **7-9***

In a round bottom flask, the corresponding Z-L-amino acid (1.1 eq.) and DMTMM*Cl (1.2 eq.) were dissolved in methanol. After 10 minutes, H-X-EDA-Boc (1.0 eq) dissolved in methanol was added, and the reaction proceeded overnight. An excess amount of water was then added to the flask, and then the mixture was filtered, washed with water, and dried.

Z-FF-EDA-Boc (7). Product - white powder. Global yield: 8.14 g (94%). ^{1}H NMR (300 MHz. DMSO-d6): 1.36 (s, 9H), 2.56-3.15 (m, 8H), 4.23 (h, 1H), 4.45 (q, 1H), 4.94 (s, 2H), 6.96 (t, 1H), 7.14-7.36 (m, 15H), 7.44 (d, 1H), 7.94 (t, 1H), 8.08 (d, 1H).

Z-WW-EDA-Boc (8). Product - white to pinkish powder. Global yield: 1.40 g (79 %).^{1}H NMR (300 MHz, DMSO-d6): 1.36 (s, 9H), 3.18-2.80 (m, 8H), 4.29 (m, 1H), 4.50 (m, 1H), 4.94 (s, 2H), 6.70 (t, 1H), 7.39-6.91 (m, 15 H), 7.57 (d, 1H), 7.60 (d, 1H), 7.92 (t, 1H), 8.02 (d, 1H), 10.78(s, 1H), 10.81(s, 1H).

Z-ΦΦ-EDA-Boc (9). Product - white powder. Global yield: 2.54 g (91%). ^{1}H NMR (300 MHz, DMSO-d6): 1.37 (s, 9H), 2.73-2.64 (m, 8H), 4.53 (m, 1H), 4.34 (m, 1H), 4.89 (s, 2H), 6.69 (m, 1H), 7.45-6.76 (m, 5 H), 7.59 (m, 1H), 8.13 (t, 1H), 8.31 (m, 1H). ^{19}F NMR (300 MHz, DMSO-d6): -142.4 (dd, J = 25.29, 7.33 Hz, 2F), -143.1 (dd, J = 8.17, 24.47Hz, 2F), -156.0 (t, J = 22.84 Hz, 1H), -157.3 (t, J = 21.21 Hz, 1F), -161.5 - -163.3 (m, 4F).

*Synthesis of compounds **10-12***

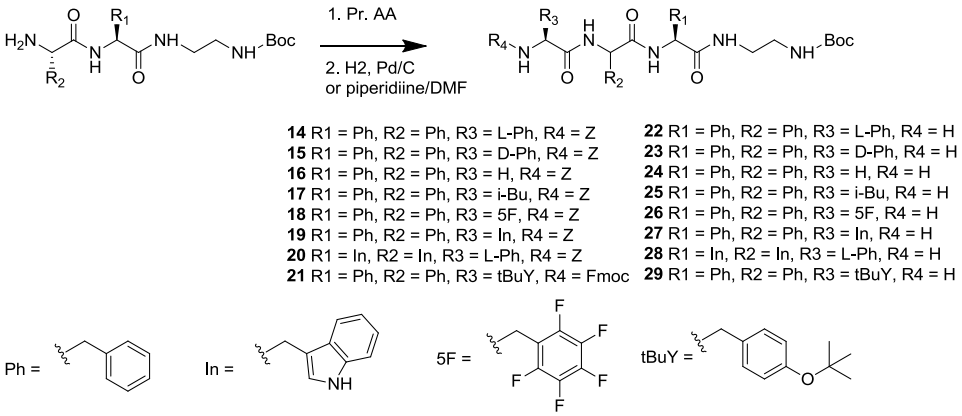
Directly after filtration, compound Z-XX-EDA-Boc was mixed in a flask together with a Pd/C catalyst (150 mg) in methanol (100 mL) and water (10 mL). After purging the flask (three cycles of N2/vacuum) of moisture and oxygen, the system was placed under hydrogen pressure and allowed to react for 2 h. The solution was filtered through a celite pad, and the filtrate was dried on a rotary evaporator, followed by a deep vacuum.

H-FF-EDA-Boc (10). Product - white powder. Global yield: 6.3 g (86%). 1H-NMR (300 MHz. DMSO-d6): δ 1.37 (s, 9H), 2.71-3.22 (m, 8H), 4.47 (q, 1H), 6.72 (t, 1H), 7.09-7.29 (m, 10H), 7.96 (t, 1H), 8.03 (d, 1H).

H-WW-EDA-Boc (11). Product - white powder. Global yield: 744 mg (85 %). **^{1}**H NMR (300 MHz, DMSO-d6): 1.36 (s, 9H), 2.66 (dd, 1H), 3.07-2.85 (m, 7H), 3.47 (dd, 1H), 4.50 (m, 1H), 6.72 (t, 1H), 7.15-6.86 (m, 6 H), 7.30 (d, 1H), 7.33 (d, 1H), 7.41 (d, 1H), 7.53 (d, 1H), 7.92 (t, 1H), 8.02 (d, 1H), 10.78(d, 1H), 10.84(d, 1H).

H-ΦΦ-EDA-Boc (12). Purification of the compound was carried out by column chromatography with ethyl acetate: dichloromethane (9:1) as the mobile phase. Two fractions eluted shortly after each other with the last eluted fraction containing the deprotected dipeptide. Product - white powder. Global yield after two steps: 1.33 g (68 %). **^{1}**H NMR (300 MHz, DMSO-d6): 1.37 (s, 9H), 2.75-2.61 (m, 1), 3.21-2.78 (m, 7H), 4.51 (m, 1H), 6.71 (m, 1H), 8.11 (t, 1H), 8.26 (m, 1H). **^{19}**F NMR (300 MHz, DMSO-d6): **-**141.87 (dd, J = 25.29, 7.33 Hz, 2F), -142,57 (dd, J = 8.17, 24.47Hz, 2F), -157.48 (t, J = 22.84 Hz, 1H), -158.36 (t, J = 21.21 Hz, 1F), -163.54 - -164.13 (m, 4F). *m/z:*783.3 Da

H-^{D}FF-EDA-Boc (13). Compound with D-phenylalanine residue was synthesized in a comparable manner to compound **10**. Product - white powder. Global yield: 1.25 g (80 %).^{1}H NMR (300 MHz, DMSO-d6): 1.37 (s, 9H), 1.54 (br.s, 2H), 2.42 (dd, 1H), 3.20-2.70 (m, 7H), 3.37 (dd, 1H), 4.46 (m, 1H), 6.72 (t, 1H), 7.30-7.03 (m, 10H), 8.00 (t, 1H), 8.12 (d, 1H).



Scheme SI-2. Synthesis of Tripeptide-ethylenediamine-Boc Derivatives

*Synthesis of Compounds **14-21***

In a round bottom flask, a corresponding Z-amino acid (1.1 eq.) and DMTMM*Cl (1.2 eq) were dissolved in methanol. After 10 minutes, H-XX-EDA-Boc (1.0 eq) dissolved in methanol was added, and the reaction proceeded overnight.

Z-FFF-EDA-Boc (14). Product - white powder. Global yield: 4.47 g (89 %). ^{1}H (DMSO-d6): 1.37(s, 9H), 2.58-3.10(m, 10H), 4.22(dt, 1H), 4.44(dt, 1H), 4.53(dt, 1H), 4.92(s, 2H), 6.68(t, 1H), 7.12-7.33(m, 20H), 7.43(d, 1H), 7.86(t, 1H), 8.03(d, 1H), 8.16(d, 1H).

Z-F^{D}FF-EDA-Boc (15). Product - white powder. Global yield: 2.01 g (93 %).^{1}H NMR (300 MHz, DMSO-d6): 1.37 (s, 9H), 3.10-2.22 (m, 8H), 4.21 (m, 1H), 4.55 (m, 2H), 4.89 (s, 2H), 6.74 (t, 1H), 7.36-6.98 (m, 20H), 8.11 (t, 1H), 8.20 (d, 1H), 8.46 (d, 1H).

Z-GFF-EDA-Boc (16). Product - white powder. Global yield: 1.76 g (71 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.36 (s, 9H), 3.12-2.67 (m, 10H), 3.56 (m, 2H), 4.11 (m, 1H), 4.42 (m, 1H), 4.49 (m, 1H), 5.01 (d, 2H), 6.67 (t, 1H), 7.43-7.11 (m,16H), 7.82 (t, 1H), 7.94 (d, 1H), 8.16 (d, 1H).

Z-LFF-EDA-Boc (17). Product - white powder. Global yield: 1.91 g (93 %).^{1}H NMR (300 MHz, DMSO-d6): 0.81 (dd, 6H), 1.59-1.81 (m, 11H), 3.14-2.70 (m, 8H), 3.97 (m, 1H), 4.41 (m, 1H), 4.50 (m, 1H), 5.01 (d, 2H), 6.67 (t, 1H), 7.39-7.10 (m,16H), 7.83 (m, 2H), 8.11 (d, 1H).

Z-ΦFF-EDA-Boc (18). An excess amount of water was added to the flask. The solution was filtered and washed with water. Product - white powder. Global yield: 1.29 g (63 %). ^{1}H NMR (300 MHz, DMSO-d6): 8.19 (d, 1H), 8.04 (d, 1H),7.83 (t, 1H), 7.49 (d, 1H),7.38-7.09 (m,15H), 6.66 (t, 1H), 4.96 (q, 2H), 4.54 (m, 1H), 4.43 (m, 1H), 4.31 (m, 1H), 3.97 (m, 1H), 3.13-2.70 (m, 12H), 1.36 (s, 9H). ^{19}F NMR (300 MHz, DMSO-d6): -141.9 (dd, J = 24.4, 6.7 Hz, 2F), -157.4 (t, J = 22.3 Hz, 1F), -163.5 (ddd, J =6.7 Hz, 22.3 Hz, 2F).

Z-WFF-EDA-Boc (19). Product - yellowish powder. Global yield: 1.71 g (91 %).^{1}H NMR (300 MHz, DMSO-d6): 1.37 (s, 9H), 3.08-2.67 (m, 10H), 4.52 (m, 1H), 4.45 (m, 1H), 4.54 (m, 1H), 4.92 (s, 2H), 6.69 (t, 1H), 7.31 (d, 1H), 7.46-6.83 (m,19H), 7.49 (t, 2H), 7.58 (d, 1H), 7.87 (t, 1H), 8.16 (d, 1H), 10.77 (s, 1H).

Z-FWW-EDA-Boc (20). Product - yellowish powder. Global yield: 2.15 g (73 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.36 (s, 9H), 2.64 (dd, 1H), 3.88-2.82 (m, 9H), 4.25 (m, 1H), 4.57 (m, 1H), 4.46 (m, 1H), 4.92 (q, 2H), 6.68 (t, 1H), 7.36-6.92 (m, 21H), 7.42 (d, 1H), 7.55 (d, 1H), 7.59 (d, 1H), 7.80 (t, 1H), 8.04 (d, 1H), 8.13 (d, 1H), 10.78 (s, 1H), 10.81 (s, 1H).

Fmoc-Y(OtBu)FF-EDA-Boc (21). Product - white powder. Global yield: 1.03 g (50 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.17 (s, 9H), 1.36 (s, 9H), 3.15-2.57 (m, 10H), 4.27-3.92 (m, 4H), 4.48 (m, 1H), 4.55 (m, 1H), 5.75 (s, 4H), 6.69 (t, 1H), 6.77 (d, 2H), 7.33-6.97 (m,15H), 7.41 (t, 2H), 7.52 (d, 1H), 7.63 (d, 2H), 7.88 (m, 3H), 8.04 (d, 1H), 8.17 (d, 1H).

*Synthesis of compounds **22-28***

In a round bottom flask, compound **14-20** was dissolved in methanol (150 mL). The solution was mixed with a Pd catalyst (10% w/w) and purged (3 x N2/ vacuum cycle). The system was then placed under hydrogen pressure and allowed to react for several hours. After the reaction was completed, the solution was filtered over a celite pad and dried under vacuum.

H-FFF-EDA-Boc (22). Product - white powder. Global yield: 3.1 g (90%). 1H-NMR (300 MHz. DMSO-d6): 1.37 (s, 9H), 2.45 (dd, 1H), 2.70-3.17 (m, 9H), 3.34 (dd, 1H), 4.43 (dt, 1H), 4.54 (m, 1H), 6.70 (t, 1H), 7.03-7.29 (m, 15H), 7.90-8.10 (m, 2H), 8.25 (d, 1H).

H-F^{D}FF-EDA-Boc (23). Product - white powder. Global yield: 1.37 g (86 %).^{1}H NMR (300 MHz, DMSO-d6): 1.37 (s, 9H), 1.51 (br. s, 2H), 3.21-2.31 (m, 8H), 3.39 (dd, 1H), 4.45 (m, 1H), 4.55 (m, 1H), 6.77 (t, 1H), 7.31-6.90 (m, 15H), 8.08 (m, 2H), 8.47 (d, 1H).

H-GFF-EDA-Boc (24). Product - white powder. Global yield: 1.34 g (87 %).^{1}H NMR (300 MHz, DMSO-d6): 1.36 (s, 9H), 1.69 (br.s, 2H), 3.19-2.69 (m, 12H), 4.43 (m, 1H), 4.51 (m, 1H), 6.70 (t, 1H), 7.31-7.08 (m, 11H), 7.91 (d, 1H), 8.22 (d, 1H).

H-LFF-EDA-Boc (25). Product - white powder. Global yield: 1.55 g (90 %).^{1}H NMR (300 MHz, DMSO-d6)*:* 0.79 (dd, 6H), 1.27-0.98 (m, 2H), 1.37 (s, 9H), 1.60 (m, 2H), 3.15-2.70 (m, 9H), 4.43 (m, 1H), 4.50 (m, 1H), 6.70 (t, 1H), 7.30-7.08 (m, 11H), 7.93 (m, 2H), 8.19 (d, 1H).

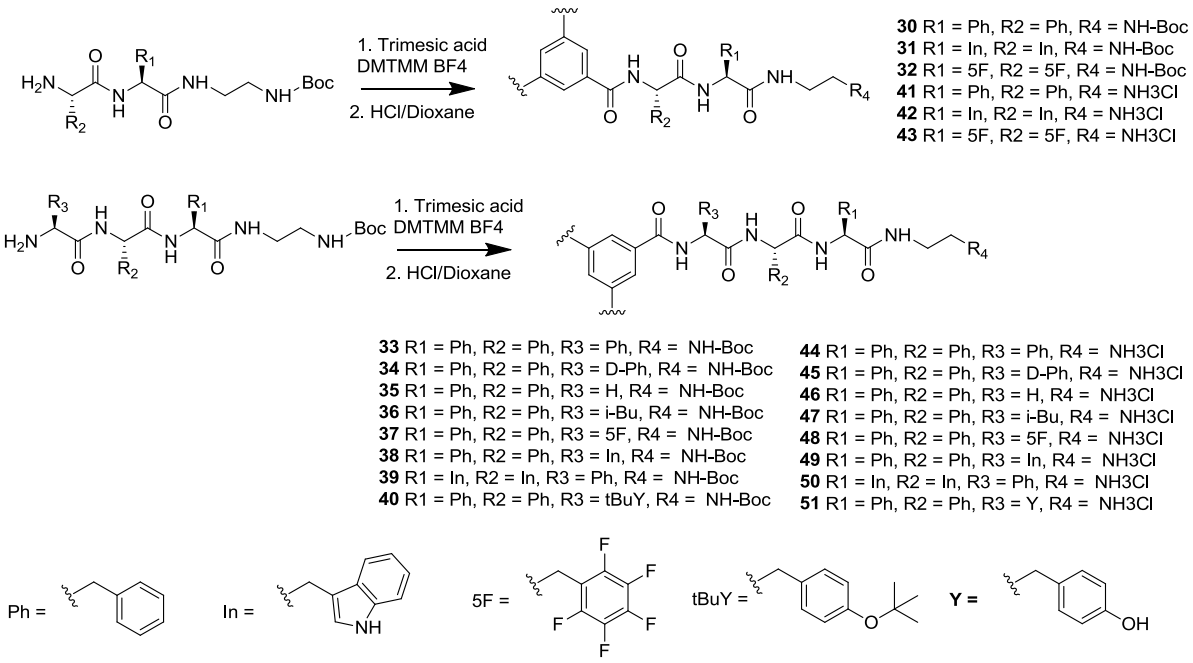
H-ΦFF-EDA-Boc (26). Product - white powder. Global yield: 0.92 g (87 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.36 (s, 9H), 1.73 (br.s, 2H), 2.57 (dd, 1H), 3.13-2.66 (m, 11H), 4.43 (m, 1H), 4.52 (m, 1H), 6.69 (t, 1H), 7.30-7.09 (m, 10H), 7.88 (t, 1H), 8.03 (d, 1H), 8.23 (d, 1H). ^{19}F NMR (300 MHz, DMSO-d6): -142.2 (dd, J = 24.0, 2F), -158.4 (t, 1F), -163.8 (ddd, 2F).

H-WFF-EDA-Boc (27). Product - yellowish powder. Global yield: 1.03 g (85 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.37 (s, 9H), 1.16 (br.s, 2H), 3.15-2.58 (m, 12H), 3.40 (dd, 1H), 4.44 (m, 1H), 4.54 (m, 1H), 6.71 (t, 1H), 7.29-6.94 (m,15H), 7.33 (d, 1H), 7.52 (d, 1H), 7.96 (t, 1H), 8.28 (d, 1H), 10.85 (d, 1H).

H-FWW-EDA-Boc (28). Product - yellowish powder. Global yield: 1.67 g (83 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.36 (s, 9H), 3.12-2.81 (m, 10H), 3.40 (m, 1H), 4.47 (m, 1H), 4.58 (m, 1H), 6.71 (t, 1H), 7.33-6.89 (m,12H), 7.42 (d, 1H), 7.50 (d, 1H), 7.55 (d, 1H), 7.86 (t, 1H), 8.09 (m, 2H), 10.79 (s, 2H).

*Synthesis of compound **29***

H-Y(OBoc)FF-EDA-Boc (29). Compound was treated with 10 % piperidine in DMF for 30 min and precipitated in diethyl ether. Product - white powder. Global yield: 0.44 g (95 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.25(s, 9H), 1.37 (s, 9H), 1.60 (br.s, 2H), 2.42 (dd, 1H), 2.69-3.17 (m, 11H), 4.44 (m, 1H), 4.54 (m, 1H), 6.70 (t, 1H), 7.41-6.99 (m, 16H), 7.68 (d, 1H), 7.86 (d, 1H), 8.00-7.89 (m, 2H), 8.23 (d, 1H).



Scheme SI-3. General scheme of synthesis of BTA-derivatives of di- and tripeptides**.**

*Synthesis of compounds **30-40***

Corresponding amine-terminated peptide (4.5 eq.) was dissolved in DMF. The solution was added to a mixture of DMTMM*BF4 (4.5 eq.) and trimesic acid (1.0 eq) and stirred for 48 hours. This was followed by

precipitation in 50 mL of diethyl ether. The solids were collected by filtration and washed with diethyl ether, and the product was further dried under vacuum.

BTA-FF-EDA-Boc (30). Product - white powder. Global yield: 1.25 g (86 %). ^{1}H NMR (DMSO-d6): 1.36 (s, 27H), 2.8-3.16 (m, 24H), 4.49 (ddd, 3H), 4.78 (ddd, 3H), 6.70 (t, 3H), 7.0-7.32 (m, 30H), 7.96 (t, 3H), 8.22 (t, 3H), 8.23 (s, 3H), 8.73 (d, 3H).

BTA-WW-EDA-Boc (31). Product - yellowish powder. Global yield: 417 mg (83 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.36 (s, 27H), 3.27-2.83 (m, 24H), 4.52 (m, 3H), 4.84 (m, 3H), 6.67 (t, 3H), 7.98 (ddt, 12H), 7.13 (m, 6H), 7.27 (m, 6H), 7.56 (d, 3H), 7.66 (d, 3H), 7.90 (t, 3H), 8.23 (d, 3H), 8.30 (s, 3H), 8.69 (d, 3H), 10.68 (d, 3H), 10.77 (d, 3H).

BTA-ΦΦ-EDA-Boc (32). Product - white powder. Global yield: 520 mg (70 %). **¹**H NMR (300 MHz, DMSO-d6): 1.37 (s, 27H), 2.95-2.69 (m, 27H), 4.75 (m, 3H), 8.42-8.22 (m, 6H), 8.71 (d, 1H). ^{19}F NMR (300 MHz, DMSO-d6): -141.93 (dd, J = 20.67, 6F), -157,79 (dd, 3F), - 163.70 (m, 6F).

BTA-FFF-EDA-Boc (33). Product - white powder. Global yield: 2.15 g (79 %). ^{1}H (DMSO-d6): 1.36 (s, 27H), 2.70-3.18 (m, 30H), 4.46 (dt, 3H), 4.57 (dt, 3H), 4.75 (dt, 3H), 6.68 (t, 3H), 7.00-7.31 (m, 45H), 7.88 (t, 3H), 8.08-8.25 (m, 9H), 8.67 (d, 3H).

BTA-F^{D}FF-EDA-Boc (34). Product - white powder. Global yield: 902 mg (85 %).^{1}H NMR (300 MHz, DMSO-d6): 1.35 (s, 27H), 3.22-2.33 (m, 30H), 4.54 (m, 3H), 4.52 (m, 3H), 4.68 (m, 3H), 6.72 (t, 3H), 7.31-6.99 (m, 45H), 8.12 (m, 6H), 8.48 (d, 3H), 8,52 (d, 3H).

BTA-GFF-EDA-Boc (35). Product - white powder. Global yield: 830 mg (77 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.36 (s, 27H), 3.16-2.70 (m, 30H), 4.44 (m, 3H), 4.54 (m, 3H), 4.87 (ddd, 6H), 6.66 (t, 3H), 7.30-7.08 (m, 30H), 7.84 (t, 3H), 8.07 (d, 3H), 8.18 (d, 3H), 8.48 (s, 3H), 8.83 (t, 3H).

BTA-LFF-EDA-Boc (36). Product - white powder. Global yield: 955 mg (89 %). ^{1}H NMR (300 MHz, DMSO-d6): 0.87 (t, 18H), 1.36 (s, 27H), 1.60 (m, 6H), 3.14-2.70 (m, 27H), 4.42 (m, 3H), 4.55 (m, 6H), 6.67 (t, 3H), 7.28-7.03 (m, 33H), 7.84 (t, 3H), 8.02 (d, 3H), 8.08 (d, 3H), 8.39 (s, 3H), 8.61 (d, 3H).

BTA-ΦFF-EDA-Boc (37). Product - white powder. Global yield: 470 mg (70 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.36 (s, 27H), 3.12-2.74 (m, 30H), 4.44 (m, 3H), 4.56 (m, 3H), 4.85 (m, 3H), 6.65 (t, 3H), 7.28-6.93 (m, 30H), 7.83 (t, 3H), 7.95 (s, 3H), 8.15 (d, 3H), 8.30 (s, 3H), 8.81 (d, 3H).

BTA-WFF-EDA-Boc (38). Product - white powder. Global yield: 715 mg (87 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.37 (s, 27H), 3.20-2.75 (m, 30H), 4.45 (m, 3H), 4.57 (m, 3H), 4.80 (m, 3H), 6.68 (t, 3H), 7.31-6.90 (m, 45H), 7.64 (d, 3H), 7.87 (t, 3H), 8.14 (d, 3H), 8.29 (s, 3H), 8.67 (d, 3H), 10.65 (d, 3H).

BTA-FWW-EDA-Boc (39). Product - yellowish powder. Global yield: 1.05 g (65 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.35 (s, 27H), 3.20-2.82 (m, 30H), 3.40 (m, 3H), 4.47 (m, 3H), 4.61 (m, 3H), 4.78 (m, 3H), 6.67 (t, 3H), 7.33-6.88 (m, 36H), 7.56 (m, 6H), 7.82 (t, 3H), 8.03 (d, 3H), 8.17 (s, 3H), 8.32 (d, 3H), 8.66 (d, 3H), 10.77 (s, 6H).

BTA-YFF-EDA-Boc (40). Product - white powder. Global yield: 140 mg (34 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.21 (s, 27H), 1.36 (s, 27H), 2.62 (dd, 3H), 3.13-2.75 (m, 33H), 4.26 (m, 3H), 4.44 (m, 3H), 4.49 (m, 3H), 6.27 (d, 3H), 6.66 (t, 3H), 6.74(d, 6H), 6.99(d, 6H), 7.27-7.08 (m, 36H), 7.80 (t, 3H), 8.00 (d, 3H), 8.12 (d, 3H).

*Synthesis of compounds **41-51***

Corresponding Boc-protected BTA derivatives were suspended in methanol (to reach a final concentration of 100 mg/ml). After 5 minutes, a hydrogen chloride solution in dioxane (1 ml per 1ml of methanol solution) was added, and the reaction proceeded for 3-5 hours. The compound mixture was precipitated in diethyl ether, followed by filtration, washing with diethyl ether and drying under vacuum.

FF (41): Product - white powder. Global yield: 1.05 g (98 %). ^{1}H NMR (500 MHz, DMSO-d6): 2.69-3.14 (m, 21H), 3.28 (dd, 3H), 4.48 (ddd, 3H), 4.76 (ddd, 3H), 7.06-7.34 (m, 30H), 7.92 (br.s (or badly resolved t), 9H), 8.23 (t, 3H), 8.29 (t, 3H), 8.31 (s, 3H), 8.86 (d, 3H). ^{13}C NMR (500 MHz, DMSO-d6): 36.9 (CH2), 37.5 (CH2), 38.0 (CH2), 38.7 (CH2), 54.8 (CH_{aliph}), 55.5 (CH_{aliph}), 126.9 (CH_{arom}), 128.4 (CH_{arom}), 129.7 (CH_{arom}), 134.6 (C), 136.5 (C), 138.7 (C), 165.9 (C=O), 171.9 (C=O), 171.8 (C=O). MS (EI): calcd. for $C_{69}H_{78}N_{12}O_9$ $[M+3H]^{+3}$: 406.9, found 406.8.

WW (42): Product - pinkish powder. Global yield: 300 mg (90 %). ^{1}H NMR (500 MHz, DMSO-d6): 2.73 (m, 6H), 3.27-2.99 (m, 18H), 4.52 (m, 3H), 4.84 (m, 3H), 6.98 (ddt, 12H), 7.17 (dd, 6H), 7.28 (dd, 6H), 7.56 (d, 3H), 7.66 (d, 3H), 7.82 (br. t, 9H), 8.09 (t, 3H), 8.34 (d, 3H), 8.38 (s, 3H), 8.83 (d, 3H), 10.72 (d, 3H), 10.82 (d, 3H). ^{13}C NMR (500 MHz, DMSO-d6): 28.1 (CH2), 36.9 (CH2), 38.7 (CH2), 54.4 (CH_{aliph}), 55.0 (CH_{aliph}), 110.3 (C_{ind}), 110.8 (C_{ind}), 111.8 (CH_{ind}), 118.7 (CH_{ind}), 118.8 (CH_{ind}), 121.3 (CH_{ind}), 124.2 (CH_{ind}), 127.7 (CH_{ind}), 127.8 (C_{ind}), 129.7 (CH_{ind}), 134.7 (C),

136.5 (C), 165.9 (C=O), 171.9 (C=O), 172.3 (C=O). MS (EI): calcd. for $C_{81}H_{84}N_{18}O_9$ $[M+3H]^{+3}$: 485.9, found 485.8.

ΦΦ (43). Product - yellow powder. Global yield: 395 mg (98 %). ^{1}H NMR (500 MHz, DMSO-d6): 2.85-2.74 (m, 6H), 3.35-3.15 (m, 12H), 4.70 (m, 6H), 8.42 (t, 3H), 9.10 (d, 3H). ^{19}F NMR (500 MHz, DMSO-d6): -142.10 (qd, J = 6.66, 23.69 Hz, 18F), -157.76- -158.01 (m, 9F), -163.48- -163.90 (m, 18F). MS (EI): calcd. for $C_{69}H_{48}N_{12}O_9F_{30}$ $[M+3H]^{+3}$: 587.8, found 587.7.

FFF (44). Product - white powder. Global yield: 1.2 g (98 %). ^{1}H NMR (500 MHz, DMSO-d6): 2.66-3.12(m, 24H), 8.67(d, 3H), 3.27(m, 6H), 4.44 (dt, 3H), 4.55(dt, 3H), 4.74(dt, 3H), 7.00-7.33(m, 45H), 7.91(br.s, 9H), 8.14(t, 3H), 8.21 (d, 3H), 8.24-8.33 (m, 6H), 8.80 (d, 3H). ^{13}C NMR (500 MHz, DMSO-d6): 37.5 (CH_2), 38.0 (CH_2), 38.4 (CH_2), 54.3 (CH_{aliph}), 54.5 (CH_{aliph}), 55.0 (CH_{aliph}), 126.6 (CH_{arom}), 126.7 (CH_{arom}), 126.75 (CH_{arom}), 128.4 (CH_{arom}), 128.5 (CH_{arom}), 128.52 (CH_{arom}), 129.55 (CH_{arom}), 129.6 (CH_{arom}), 129.7 (CH_{arom}), 134.7 (C), 137.9 (C), 138.0 (C), 138.6 (C), 165.7 (C=O), 170.9 (C=O), 171.0 (C=O), 171.4 (C=O). MS (EI): calcd. for $C_{96}H_{105}N_{15}O_{12}$ $[M+3H]^{+3}$: 554.8, found 554.9.

F^{D}FF (45): Product - white powder. Global yield: 170 mg (98 %). ^{1}H NMR (500 MHz, DMSO-d6): 3.34-2.40 (m, 30H), 4.57 (m, 6H), 4.68 (m, 3H), 7.31-7.03 (m, 45H), 8.02 (br. t, 9H), 8.21 (s, 3H), 8.43 (m, 6H), 8.57 (d, 3H), 8.64 (d, 3H). ^{13}C NMR (500 MHz, DMSO-d6): 36.9 (CH_2), 38.3 (CH_2), 38.5 (CH_2), 54.2 (CH_{aliph}), 54.5 (CH_{aliph}), 55.4 (CH_{aliph}), 126.6 (CH_{arom}), 126.8 (CH_{arom}), 128.3 (CH_{arom}), 128.4 (CH_{arom}), 128.5 (CH_{arom}), 129.6 (CH_{arom}), 129.78 (CH_{arom}), 129.8 (CH_{arom}), 134.6 (C), 138.1 (C), 138.2 (C), 138.6 (C), 165.5 (C=O), 171.3 (C=O), 171.4 (C=O), 172.0 (C=O). MS (EI): calcd. for $C_{96}H_{105}N_{15}O_{12}$ $[M+3H]^{+3}$: 554.8, found 554.9.

GFF (46). Product - white powder. Global yield: 695 mg (93 %). ^{1}H NMR (500 MHz, DMSO-d6): 3.11-2.66 (m, 30H), 3.90 (ddd, 6H), 4.46 (m, 6H), 7.08-7.30 (m, 30H), 7.92 (br. t, 9H), 8.08 (t, 3H), 8.18 (d, 3H), 8.30 (d, 3H), 8.53 (s, 3H), 8.92 (t, 3H). ^{13}C NMR (500 MHz, DMSO-d6): 36.4 (CH_2), 37.2 (CH_2), 37.4 (CH_2), 38.3 (CH_2), 54.2 (CH_{aliph}), 54.3 (CH_{aliph}), 64.9 (CH_{aliph}), 126.2 (CH_{arom}), 126.3 (CH_{arom}), 128.0 (CH_{arom}), 128.1 (CH_{arom}), 129.2 (CH_{arom}), 134.3 (C), 137.6 (C), 137.7 (C), 165.6 (C=O), 168.9 (C=O), 170.8 (C=O), 171.2 (C=O). MS (EI): calcd. for $C_{75}H_{87}N_{15}O_{12}$ $[M+3H]^{+3}$: 464.5, found 464.6.

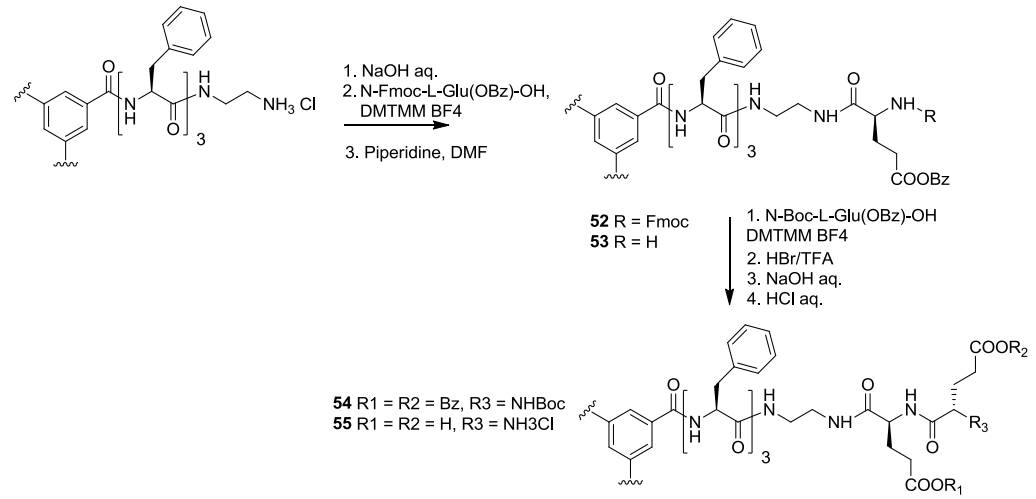
LFF (47): Product - white powder. Global yield: 810 mg (95 %). ^{1}H NMR (500 MHz, DMSO-d6): 0.86 (dd, 18H), 1.71-1.37 (m, 9H), 3.05-2.68 (m, 24H), 4.42 (m, 3H), 4.53 (m, 6H), 7.28-7.03 (m, 36H), 7.88 (br.t, 9H), 8.09 (m, 6H), 8.18 (d, 3H), 8.49 (s, 3H), 8.75 (d, 3H). ^{13}C NMR (500 MHz, DMSO-d6): 36.8 (CH_2), 37.7 (CH_2), 37.9 (CH_2), 38.6 (CH_2), 52.4 (CH_{aliph}), 54.3 (CH_{aliph}), 54.6 (CH_{aliph}), 126.2 (CH_{arom}), 126.8 (CH_{arom}), 128.4 (CH_{arom}), 128.6 (CH_{arom}), 129.6 (CH_{arom}), 129.7 (CH_{arom}), 134.8 (C), 138.0 (C), 166.0 (C=O), 171.2 (C=O), 171.6 (C=O), 172.3 (C=O). MS (EI): calcd. for $C_{87}H_{111}N_{15}O_{12}$ $[M+3H]^{+3}$: 520.9, found 520.9, $[M+2H]^{+2}$: 778.4, found 778.4.

ΦFF (48). Product - white powder. Global yield: 410 mg (94 %). ^{1}H NMR (500 MHz, DMSO-d6): 3.14-2.69 (m, 24 H), 4.48 (dt, 3H), 4.75 (dt, 3H), 7.32-7.04 (m, 36H), 7.88 (s, 9H), 8.21 (t, 3H), 8.31 (s, 3H), 8.85 (d, 3H). ^{13}C NMR (500 MHz, DMSO-d6): 36.8 (CH_2), 38.0 (CH_2), 38.7 (CH_2), 54.3 (CH_{aliph}), 54.5 (CH_{aliph}), 121.0 (C), 126.5 (CH_{arom}), 126.7 (CH_{arom}), 128.3 (CH_{arom}), 128.5 (CH_{arom}), 129.6 (CH_{arom}), 129.7 (CH_{arom}), 134.3 (C), 137.8 (C), 137.9 (C), 165.6 (C=O), 169.6 (C=O), 170.7 (C=O), 171.5 (C=O). ^{19}F NMR (500 MHz, DMSO-d6): -141.0 (q, 2F), -156.3 (t, 1F), -163.2 (dt, 2F). MS (EI): calcd. for $C_{96}H_{90}N_{15}O_{12}F_{15}$ $[M+3H]^{+3}$: 644.8, found 644.9.

WFF (49). Product - yellow powder. Global yield: 670 mg (99 %). ^{1}H NMR (500 MHz, DMSO-d6): 3.18-2.67 (m, 30H), 4.44 (m, 3H), 4.56 (m, 3H), 4.79 (m, 3H), 7.35-6.88 (m, 45H), 7.64 (d, 3H), 7.85 (br. s, 9H), 8.12 (t, 3H), 8.22 (m, 6H), 8.36 (s, 3H), 8.78 (d, 3H), 10.66 (s, 3H). ^{13}C NMR (500 MHz, DMSO-d6): 36.8 (CH_2), 37.9 (CH_2), 38.7 (CH_2), 54.4 (CH_{aliph}), 54.6 (CH_{aliph}), 63.5 (CH_{aliph}), 110.8 (C_{ind}), 111.8 (CH_{ind}), 118.9 (CH_{ind}), 121.4 (CH_{ind}), 124.1 (CH_{ind}), 126.7 (CH_{arom}), 126.8 (CH_{arom}), 127.7 (C_{ind}), 128.4 (CH_{arom}), 128.6 (CH_{arom}), 129.7 (CH_{arom}), 134.6 (C), 136.5 (C), 138.0 (C), 165.7 (C=O), 171.2 (C=O), 171.7 (C=O), 171.9 (C=O). MS (EI): calcd. for $C_{102}H_{108}N_{18}O_{12}$ $[M+3H]^{+3}$: 593.9, found 593.9.

FWW (50). Product - brownish powder. Global yield: 423 mg (91 %). ^{1}H NMR (500 MHz, DMSO-d6): 2.72 (m, 6H), 3.28-2.88 (m, 24H), 4.45 (m, 3H), 4.60 (m, 3H), 4.77 (m, 3H), 7.35-6.88 (m, 36H), 7.54 (d, 6H), 7.58 (d, 6H), 7.88 (br. t, 3H), 7.99 (t, 3H), 8.14 (d, 3H), 8.31 (s, 3H), 8.40 (d, 3H), 8.83 (d, 3H), 10.85 (s, 6H). ^{13}C NMR (500 MHz, DMSO-d6): 27.5 (CH_2), 36.4 (CH_2), 38.3 (CH_2), 53.7 (CH_{aliph}), 53.8 (CH_{aliph}), 55.0 (CH_{aliph}), 109.7 (C_{ind}), 109.9 (C_{ind}), 111.3 (CH_{ind}), 118.2 (CH_{ind}), 120.8 (CH_{ind}), 123.6 (CH_{ind}), 123.7 (CH_{ind}), 126.1 (CH_{arom}), 127.27 (C_{ind}), 127.33 (C_{ind}), 128.0 (CH_{arom}), 129.2 (CH_{arom}), 134.2 (C), 136.0 (C), 138.2 (C), 165.5 (C=O), 171.3 (C=O), 171.4 (C=O), 171.7 (C=O). MS (EI): calcd. for $C_{108}H_{111}N_{21}O_{12}$ $[M+3H]^{+3}$: 623.9, found 623.9.

YFF (51). Product - white powder. Global yield: 120 mg (91 %). ^{1}H NMR (500 MHz, DMSO-d6): 3.00-2.57 (m, 30H), 4.11 (m, 3H), 4.37 (m, 6H), 6.20 (d, 3H), 6.51 (d, 6H), 6.79 (d, 6H), 7.22-7.03 (m, 36H), 7.70 (br. t, 9H), 7.92 (m, 6H), 8.07 (d, 3H), 9.04 (s, 3H). ^{13}C NMR (500 MHz, DMSO-d6): 36.3 (CH_2), 37.31 (CH_2), 37.35 (CH_2), 38.2 (CH_2), 54.0 (CH_{aliph}), 54.2 (CH_{aliph}), 114.8 (C_{arom}), 126.2 (CH_{arom}), 126.3 (CH_{arom}), 127.4 (CH_{arom}), 128.0 (CH_{arom}), 128.1 (CH_{arom}), 129.15 (CH_{arom}), 129.16 (CH_{arom}), 130.2 (CH_{arom}), 137.5 (C), 155.7 (C-O), 170.7 (C=O), 171.7 (C=O), 172.0 (C=O). MS (EI): calcd. for $C_{96}H_{105}N_{15}O_5$ $[M+3H-3H2O]^{+3}$: 531.7, found 531.6.



Scheme SI-4. General scheme of synthesis of **F3E2.**

*Synthesis of compound **52***

N-Fmoc-L-Glu(OBz)-OH (540.4 mg, 1.176 mmol) was dissolved in DMF, and DMTMM tetrafluoroborate was added (414 mg, 1.264 mmol). After 10 minutes, a solution of **44** (500 mg, 0.301 mmol) in DMF was added, and the reaction proceeded for 48 h. The product was precipitated in acetone, filtered, and washed with acetone and diethyl ether.

Product - white powder. Global yield: 914 mg (87 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.73-2.05 (m, 6H), 2.37 (t, 6H), 2.68-3.18 (m, 30H), 3.97(dt, 3H), 4.14-4.36 (m, 9H), 4.45 (dt, 3H), 4.58 (dt, 3H), 4.76 (dt, 3H), 5.07 (s, 6H), 6.99-7.43 (m, 72H), 7.51 (d, 3H), 7.70 (t, 6H), 7.82-7.97 (m, 12H), 8.11-8.23 (m, 9H), 8.65 (d, 3H).

*Synthesis of compound **53***

Compound **52** (370 mg) was dissolved in DMF (15 ml), and piperidine (0.75 ml) was added. After 20 minutes, the solution was precipitated in methanol, filtered, and washed with methanol and diethyl ether.

Product - white powder. Global yield: 315 mg (94 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.55-1.94 (m, 6H), 2.40 (t, 6H), 2.69-3.20 (m, 30H), 3.32 (m, 3H), 4.45 (dt, 3H), 4.57 (dt, 3H), 4.75 (dt, 3H), 5.06 (s, 6H), 6.99-7.40 (m, 60H), 7.86 (t, 3H), 7.93 (t, 3H), 8.08-8.26 (m, 9H), 8.66 (d, 3H).

*Synthesis of compound **54***

N-Boc-L-Glu(OBz)-OH (151 mg, 0.445 mmol) was dissolved in DMSO, and DMTMM tetrafluoroborate (170 mg, 0.514 mmol) was added. After 10 minutes, a solution of **53** (265 mg, 0.114 mmol) in DMSO was added, and the reaction proceeded for 48 h. The product was precipitated in acetone, filtered, and washed with acetone and diethyl ether.

Product - white powder. Global yield: 305 mg (92 %). ^{1}H NMR (300 MHz, DMSO-d6): 1.34 (s, 27H), 1.69-2.03 (m, 12H), 2.30-2.43 (m, 12H), 2.70-3.16 (m, 30H), 3.93 (dt, 3H), 4.24 (dt, 3H), 4.45 (dt, 3H), 4.58 (dt, 3H), 4.76 (dt, 3H), 5.05 (s, 6H), 5.07 (s, 6H), 6.99-7.39 (m, 75H), 7.79-7.99 (m, 9H), 8.08-8.23 (m, 9H), 8.65 (d, 3H).

*Synthesis of compound **F3E2 (55)***

Compound **54** (240mg) was dissolved in TFA (2.5 ml), and after 15 min, 48% hydrobromic acid was added, and the reaction proceeded for 6 hours. The product was precipitated in diethyl ether, filtered, and washed with diethyl ether.

Product - white powder. Global yield: 160 mg (76 %). ^{1}H NMR (500 MHz, DMSO-d6): 1.70-2.02 (m, 12H), 2.21-2.42 (m, 12H), 2.74-3.20 (m, 36H), 3.90 (m, 3H), 4.26 (dt, 3H), 4.45 (dt, 3H), 4.58 (dt, 3H), 4.75 (dt, 3H), 7.00-7.36 (m, 45H), 7.95 (t, 3H), 8.03-8.23 (m, 21H), 8.57-8.72 (m, 6H). ^{13}C NMR (500 MHz, DMSO-d6): 26.9 (CH2), 27.9 (CH2), 29.5 (CH2), 30.5 (CH2), 37.5 (CH2), 38.0 (CH2), 38.3 (CH2), 38.5 (CH2), 38.6 (CH2), 51.9 (CH_{aliph}), 52.7 (CH_{aliph}), 54.2 (CH_{aliph}), 54.5 (CH_{aliph}), 55.0 (CH_{aliph}), 126.6 (C_{arom}), 126.7 (CH_{arom}), 126.8 (CH_{arom}), 128.4 (CH_{arom}), 128.5 (CH_{arom}), 128.6 (CH_{arom}), 129.6 (CH_{arom}), 129.66 (CH_{arom}), 134.7 (C), 137.9 (CH_{arom}), 138.0 (CH_{arom}), 138.6 (C), 165.7 (C=O), 168.5 (C=O), 171.0 (C=O), 171.2 (C=O), 171.4 (C=O), 173.9 (C=O), 174.3 (C=O). MS (EI): calcd. for $C_{126}H_{147}N_{21}O_{31}$ H^{+}:2435.1, found 2435.0.

SI-2. Additional data

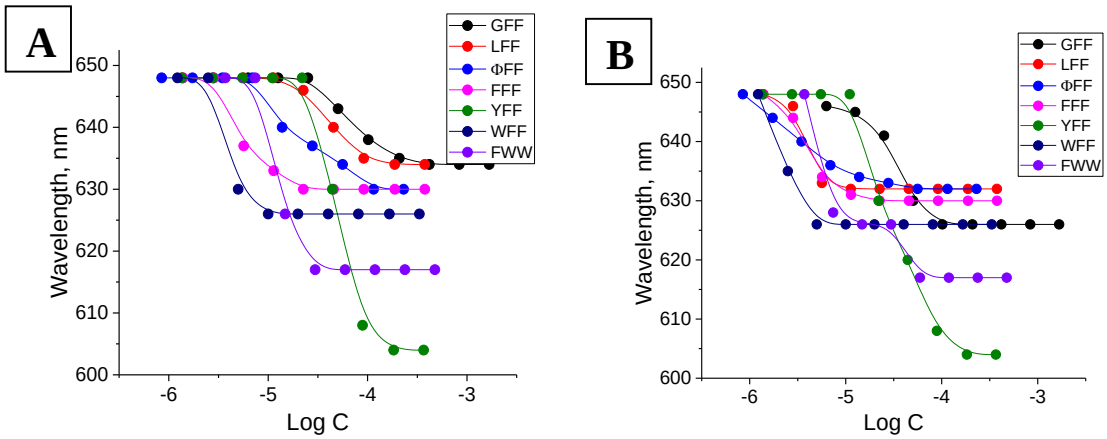


Figure S1. NR peak maximum dependence on the concentration of BTA-tripeptide derivatives in water (A) and 150 mM NaCl (B)

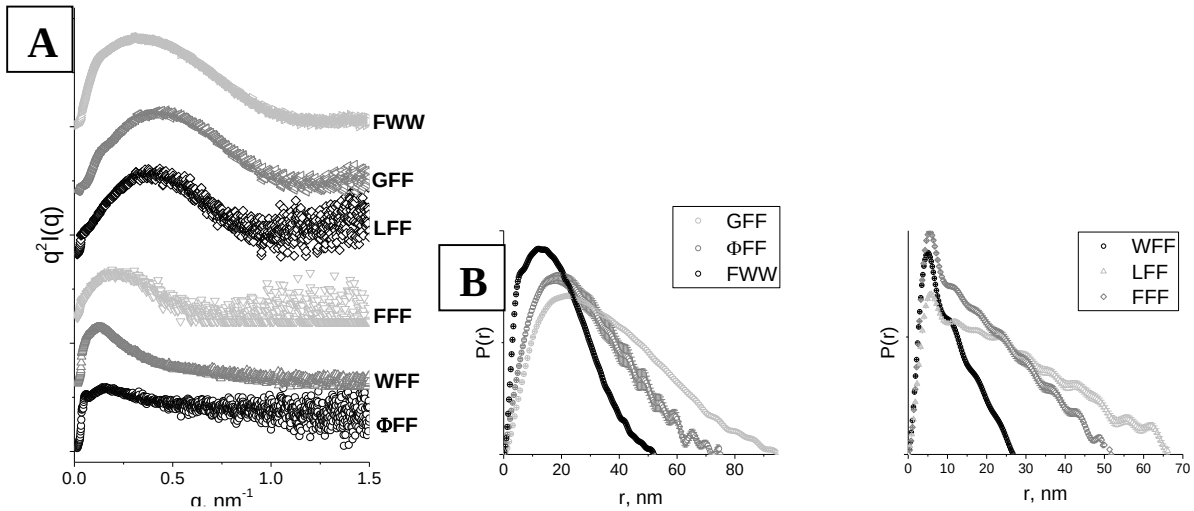


Figure S2. Kratky plots (A) and P(r) functions (B) of BTA-based tripeptides

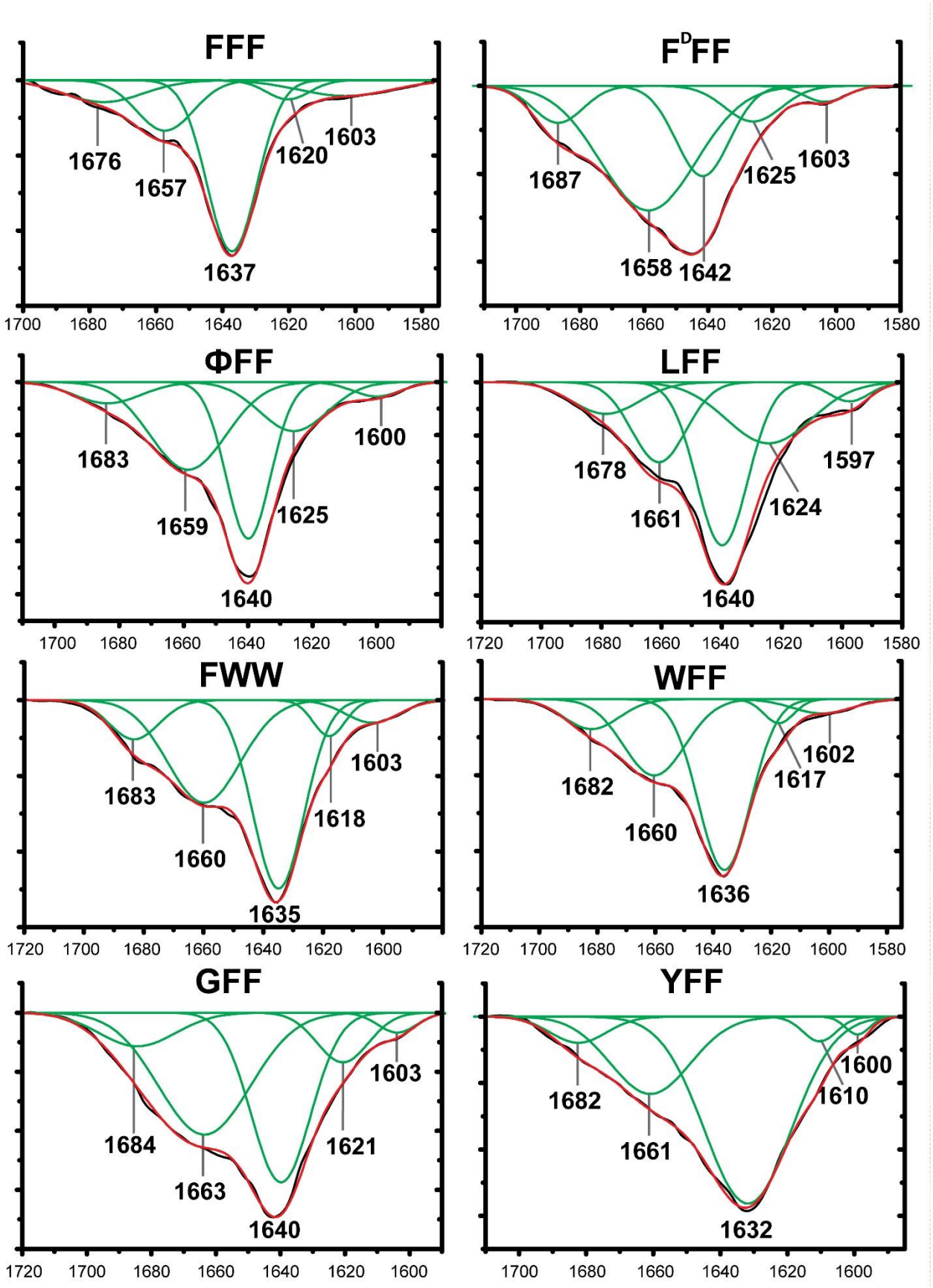


Figure S3. Deconvolutions of Amide I region of FT-IR spectra of BTA-tripeptide derivatives. Black line correspond to original spectrum, red line to fitting and deconvoluted peaks are shown in green.

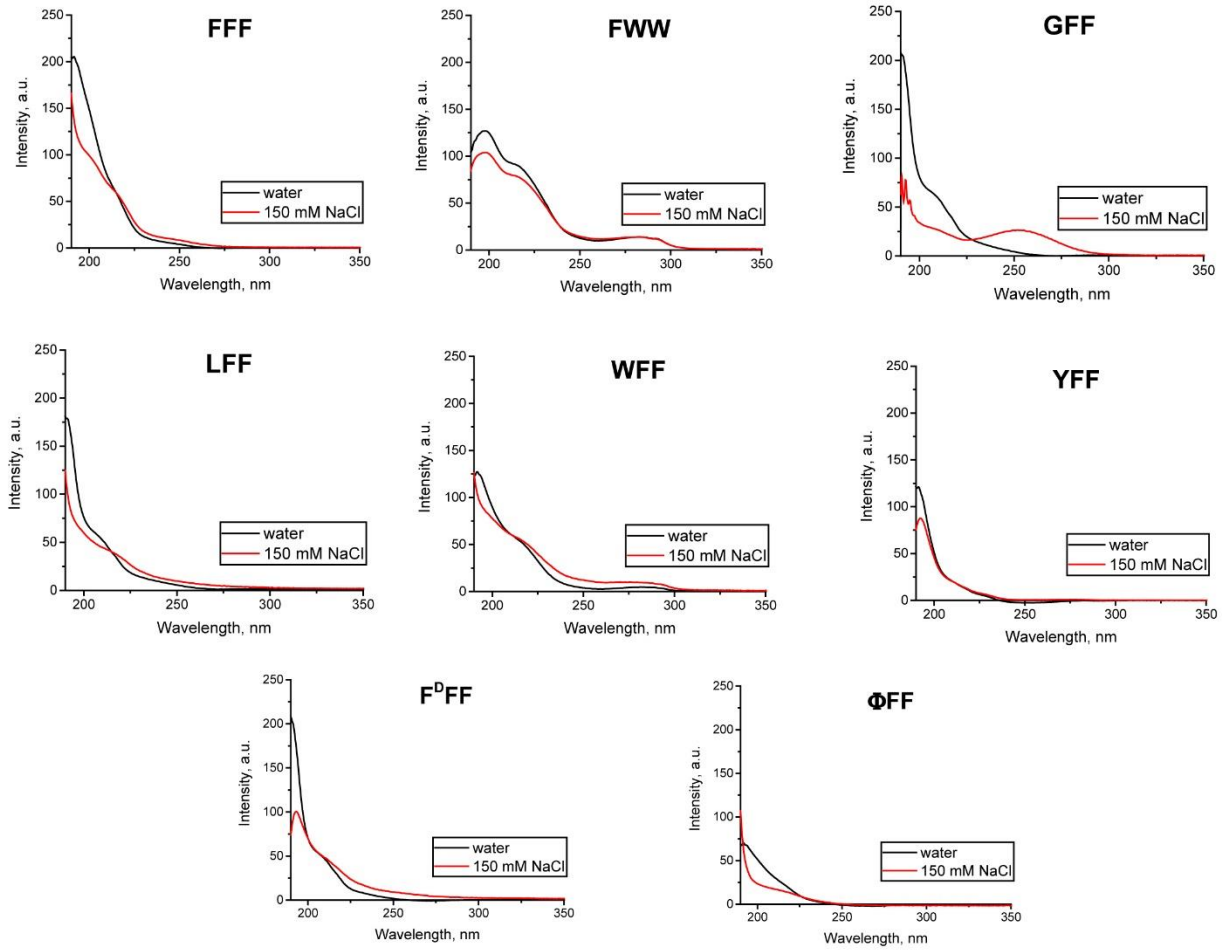


Figure S4. HT curves corresponding to the CD curves of BTA-tripeptide derivatives.

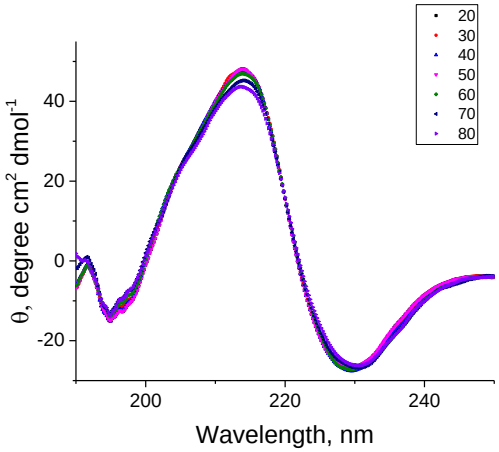


Figure S5. CD spectra of 0.03 mM solution of **FWW** at temperatures from 20 to 80 °C

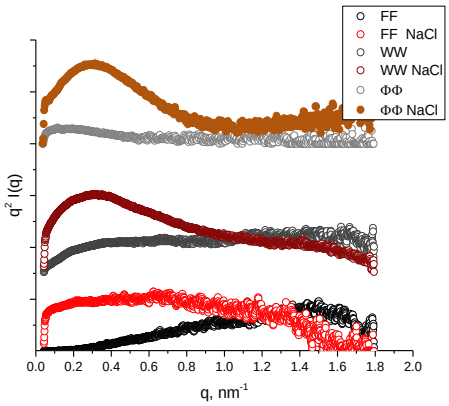


Figure S6. Kratky plots of BTA-based dipeptides

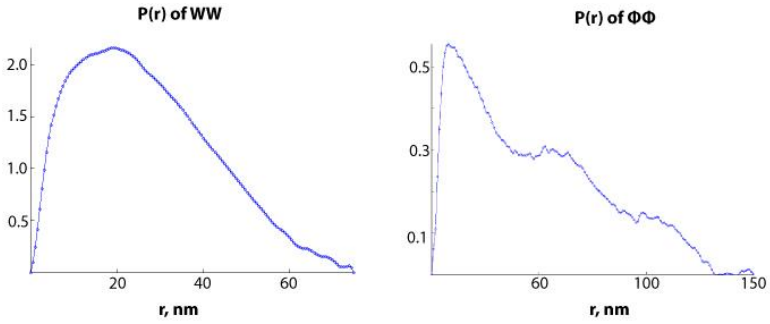


Figure S7. P(r) functions of **WW** and **ΦΦ**

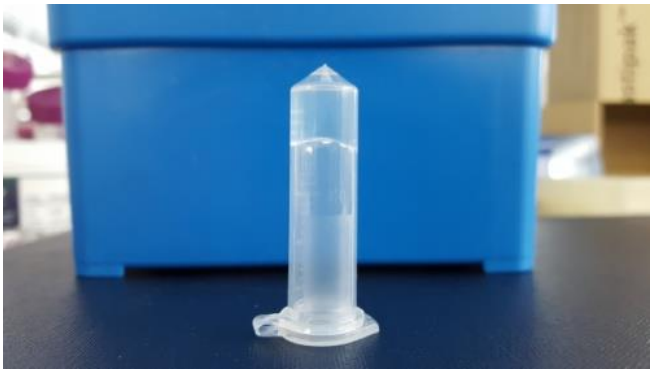


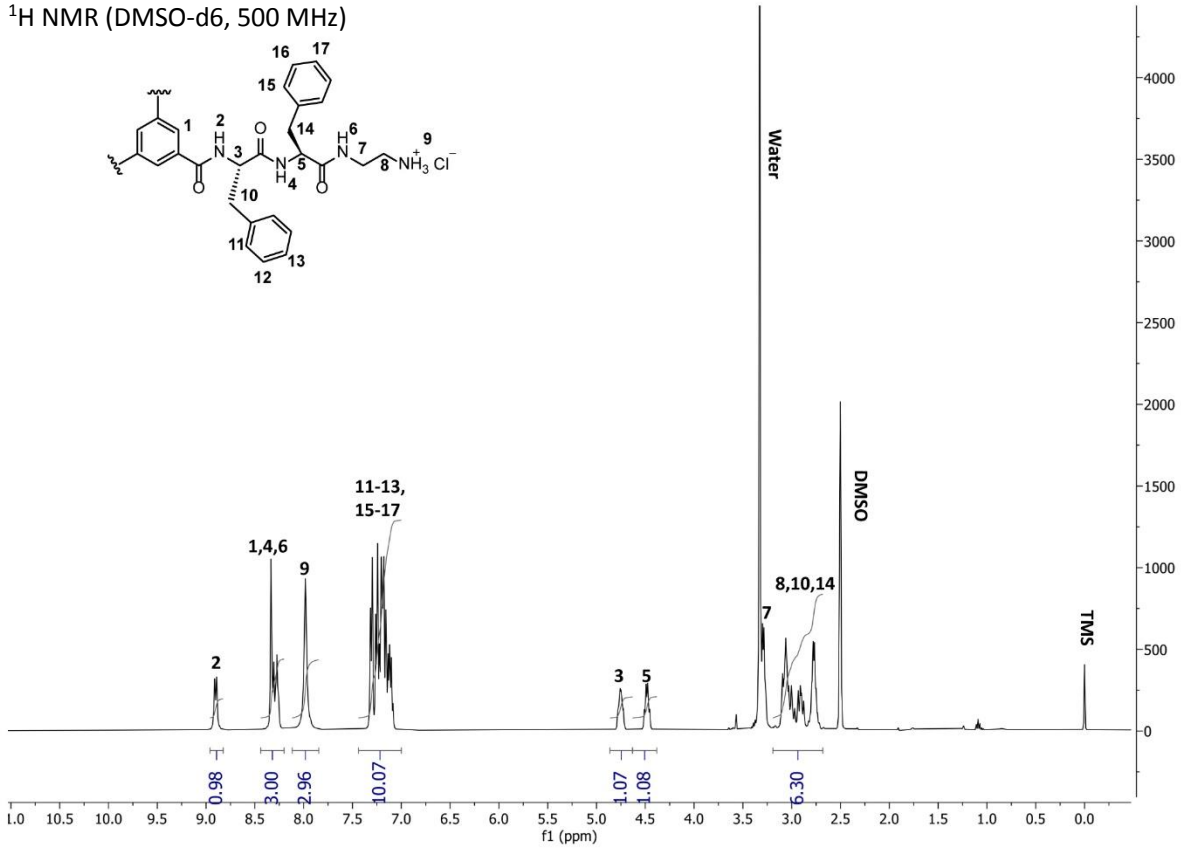
Figure S8. Photo of **FF-H** gel

SI-3. References

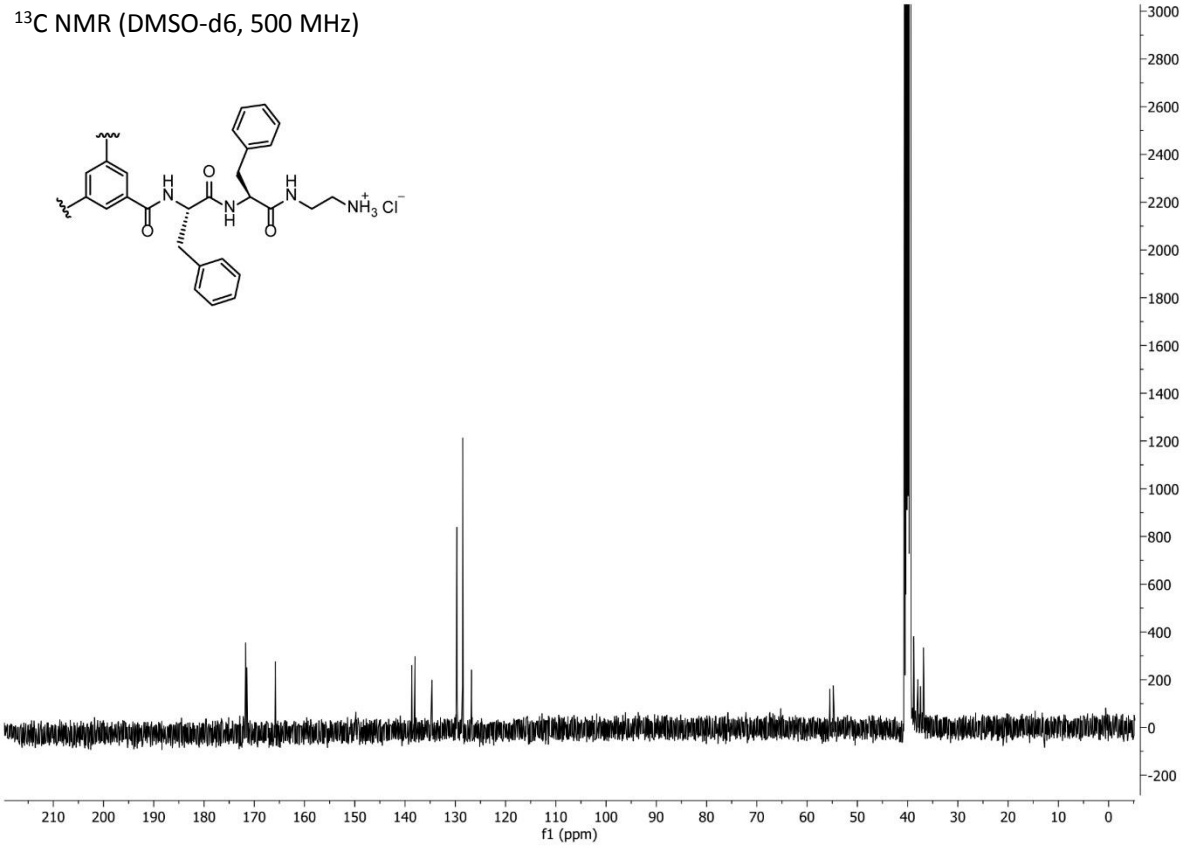
1. Park, H. *et al*. *Angew. Chem.*, **6**, 3162–3164 (2002).

SI-4. Attachment

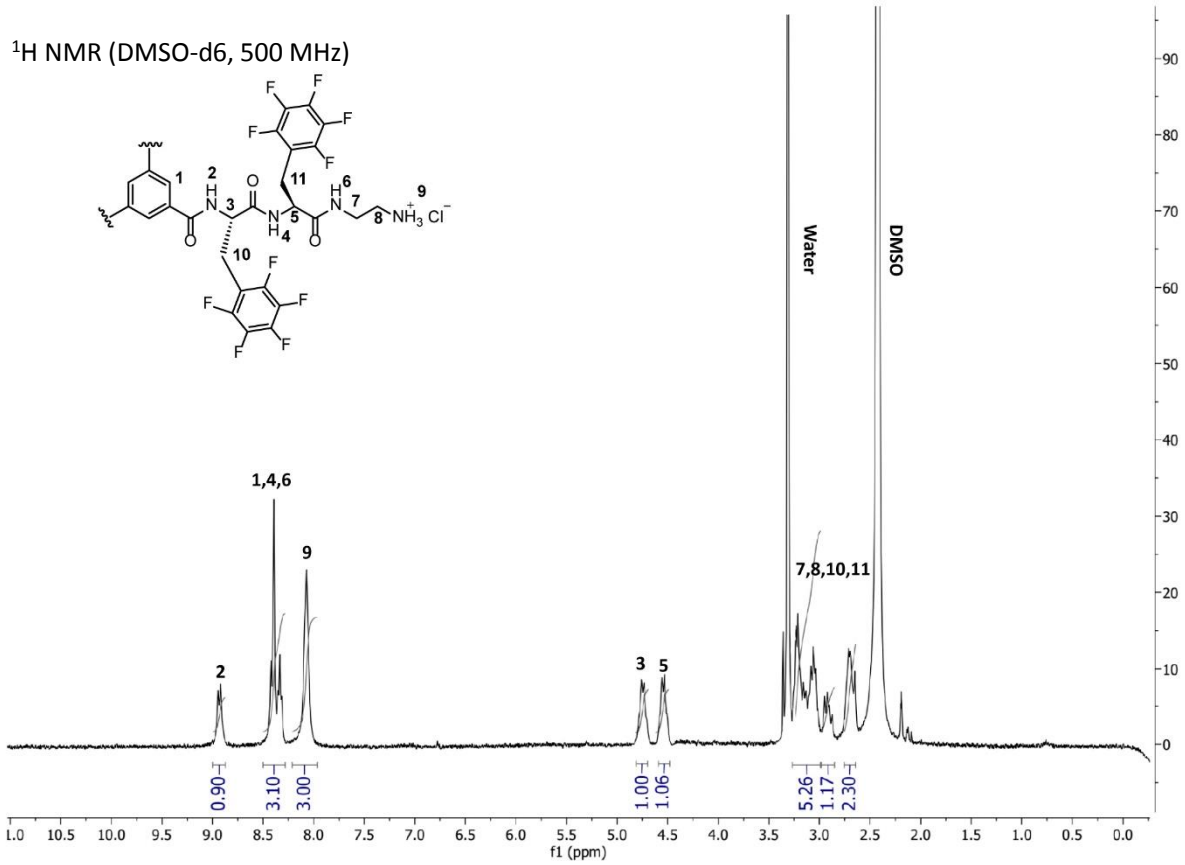
^{1}H NMR (DMSO-d6, 500 MHz)



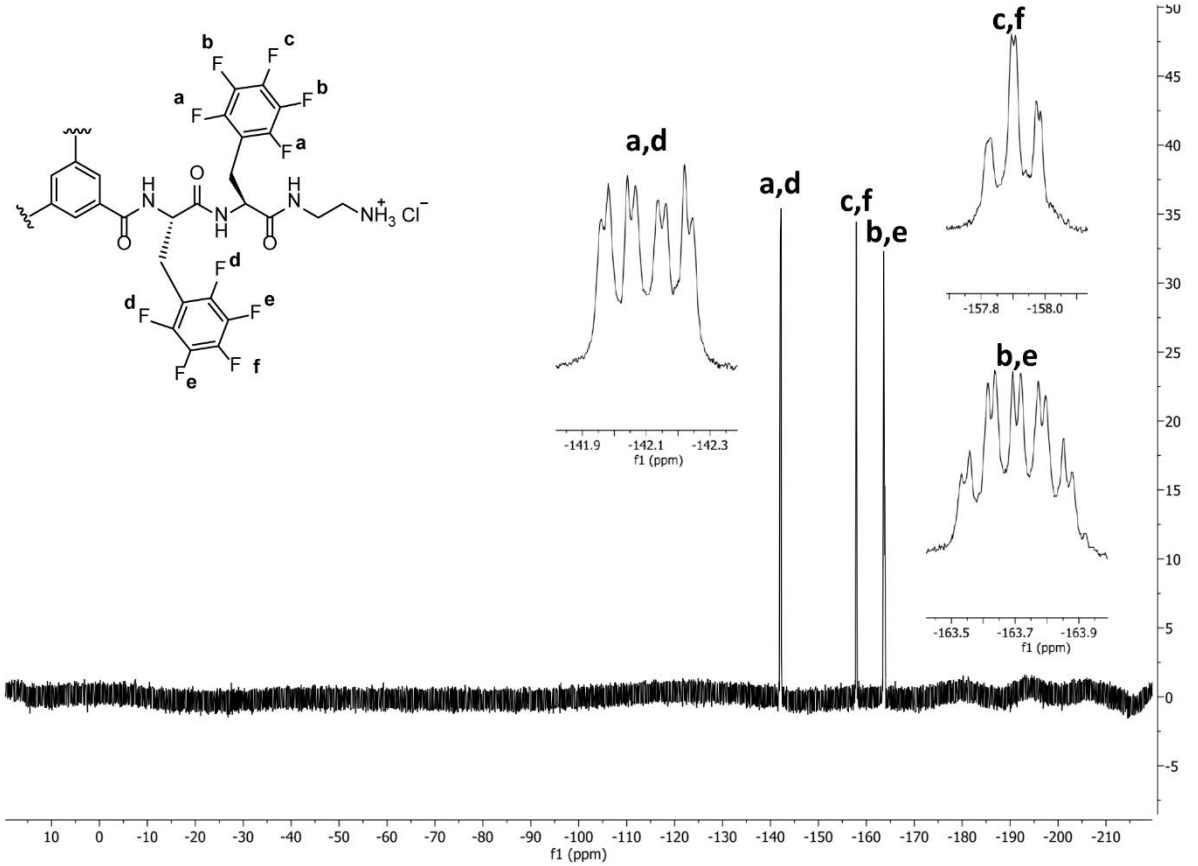
^{13}C NMR (DMSO-d6, 500 MHz)



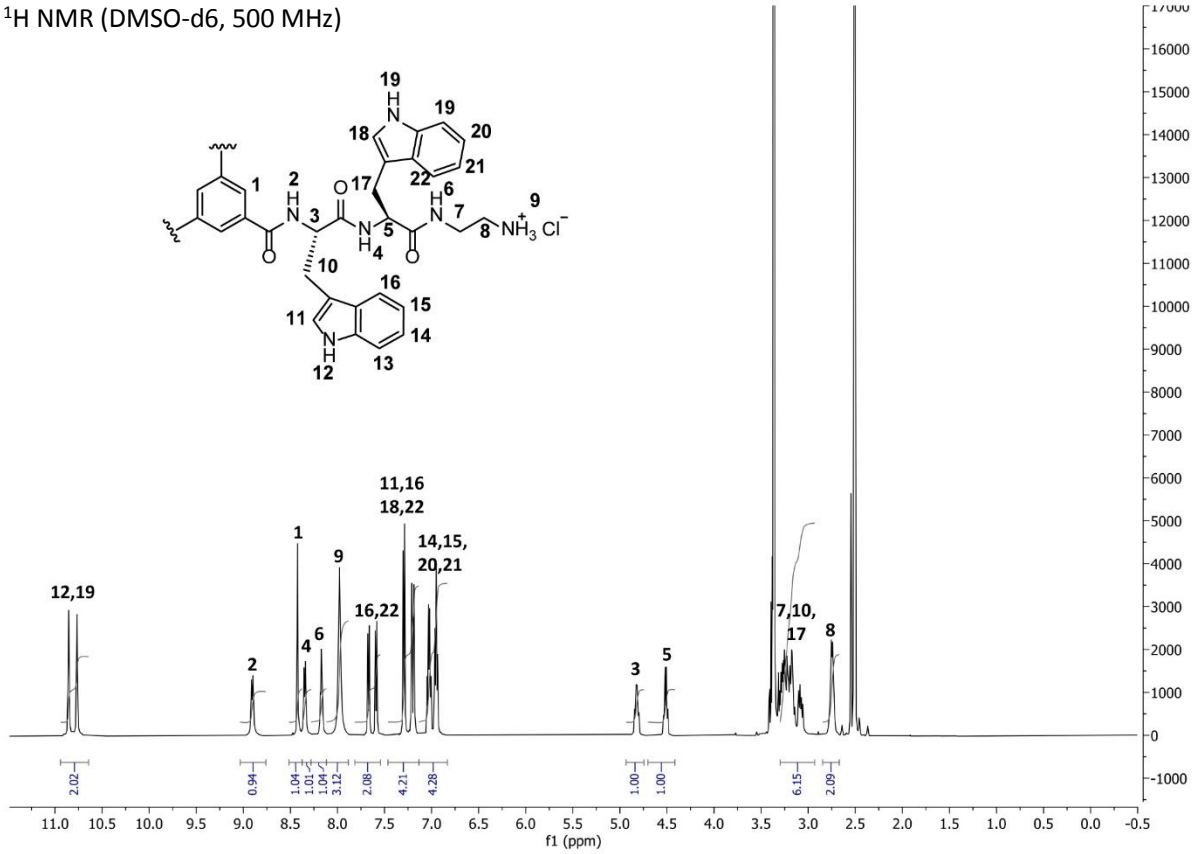
^{1}H NMR (DMSO-d6, 500 MHz)



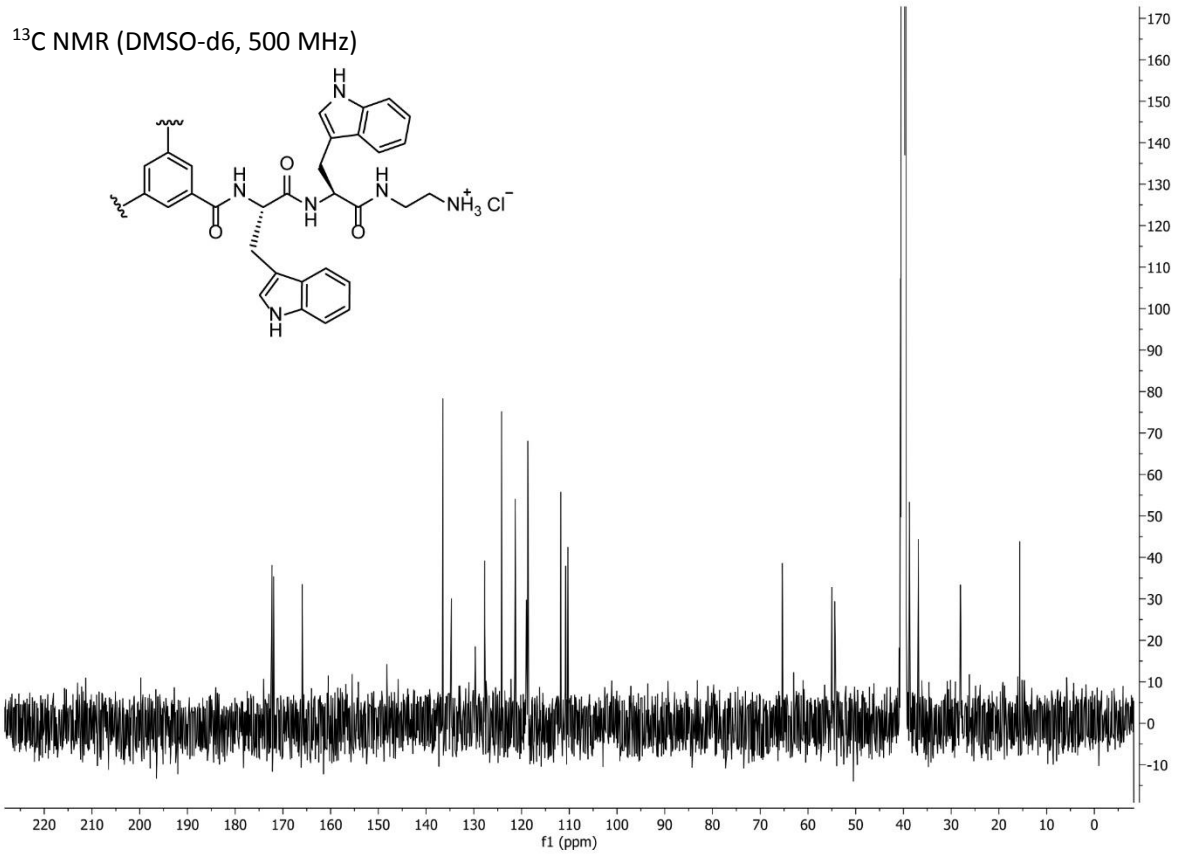
^{19}F NMR (DMSO-d6, 500 MHz)



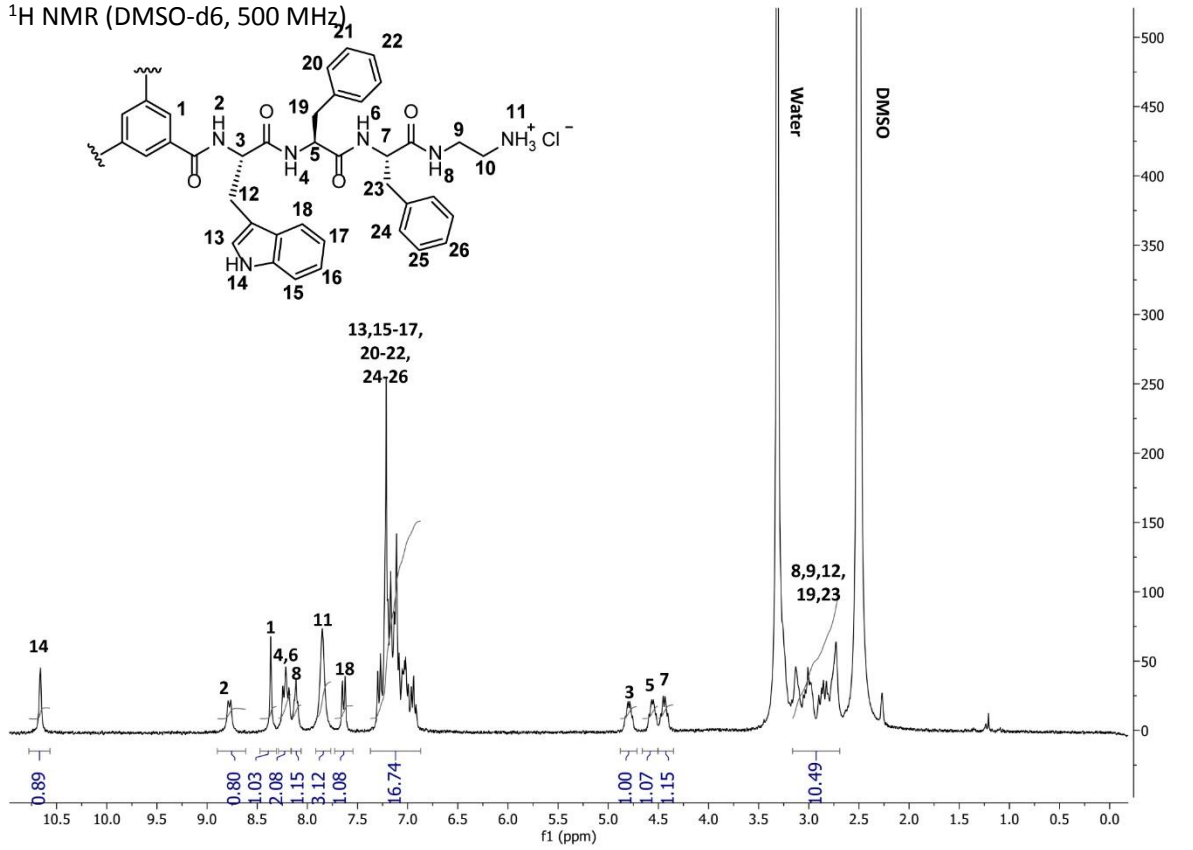
^{1}H NMR (DMSO-d6, 500 MHz)



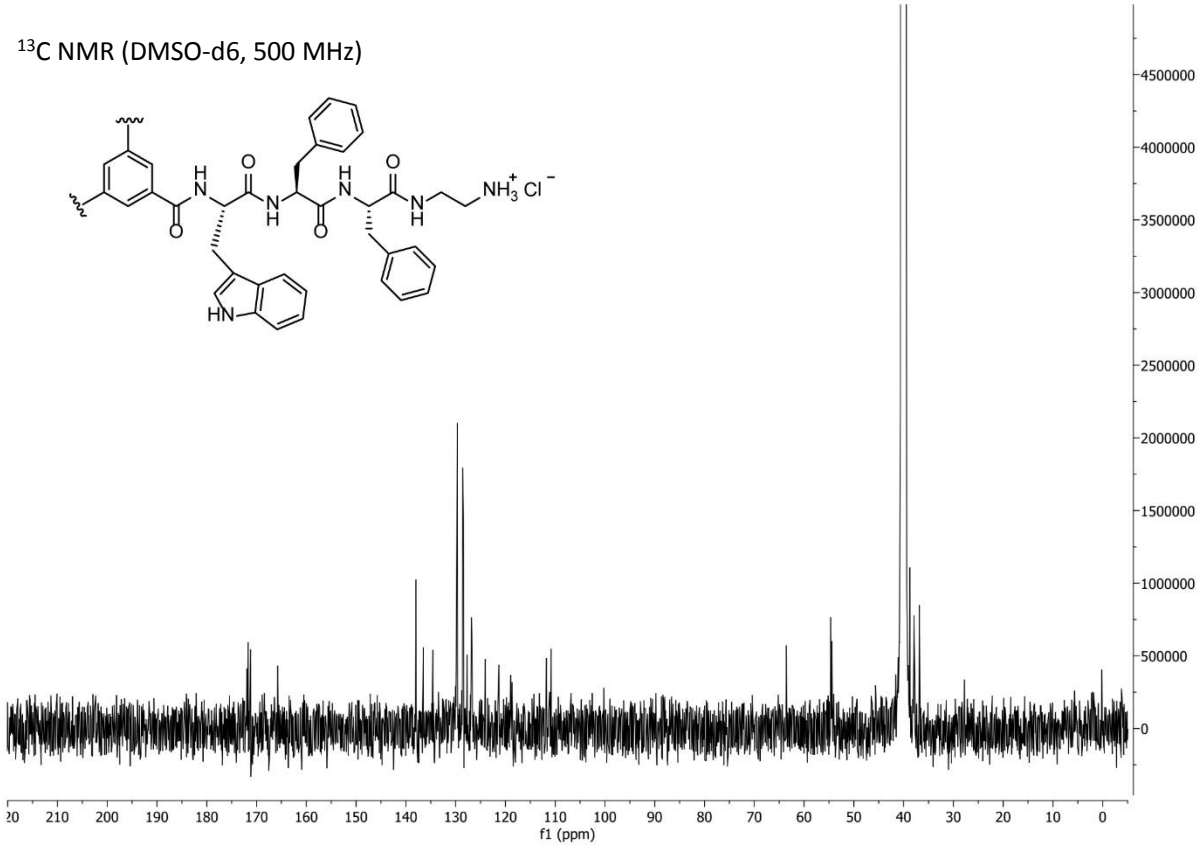
^{13}C NMR (DMSO-d6, 500 MHz)



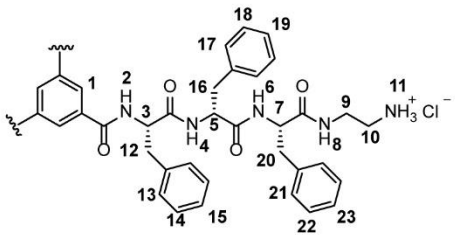
^{1}H NMR (DMSO-d6, 500 MHz)



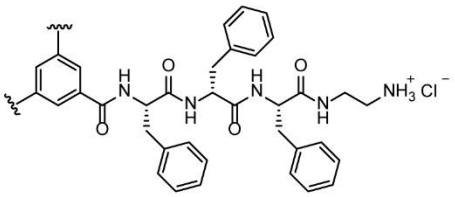
^{13}C NMR (DMSO-d6, 500 MHz)



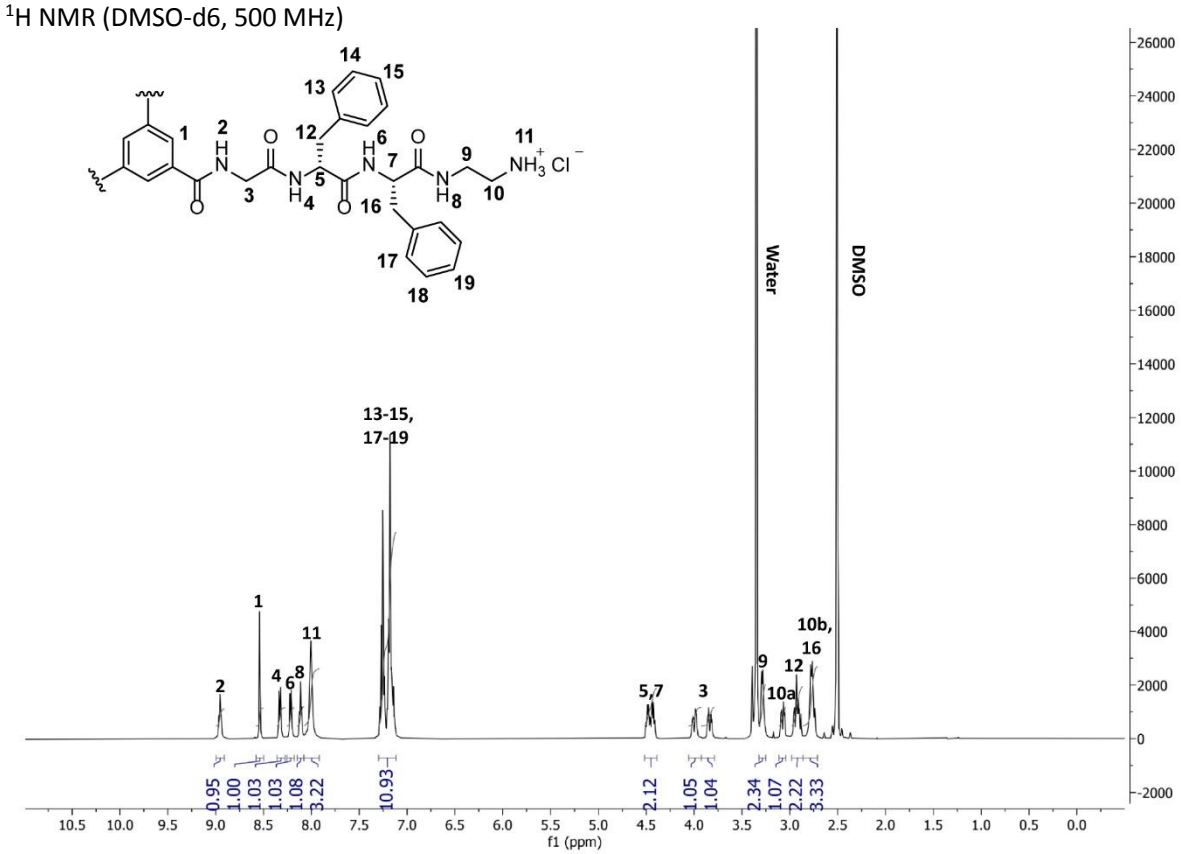
^{1}H NMR (DMSO-d6, 500 MHz)



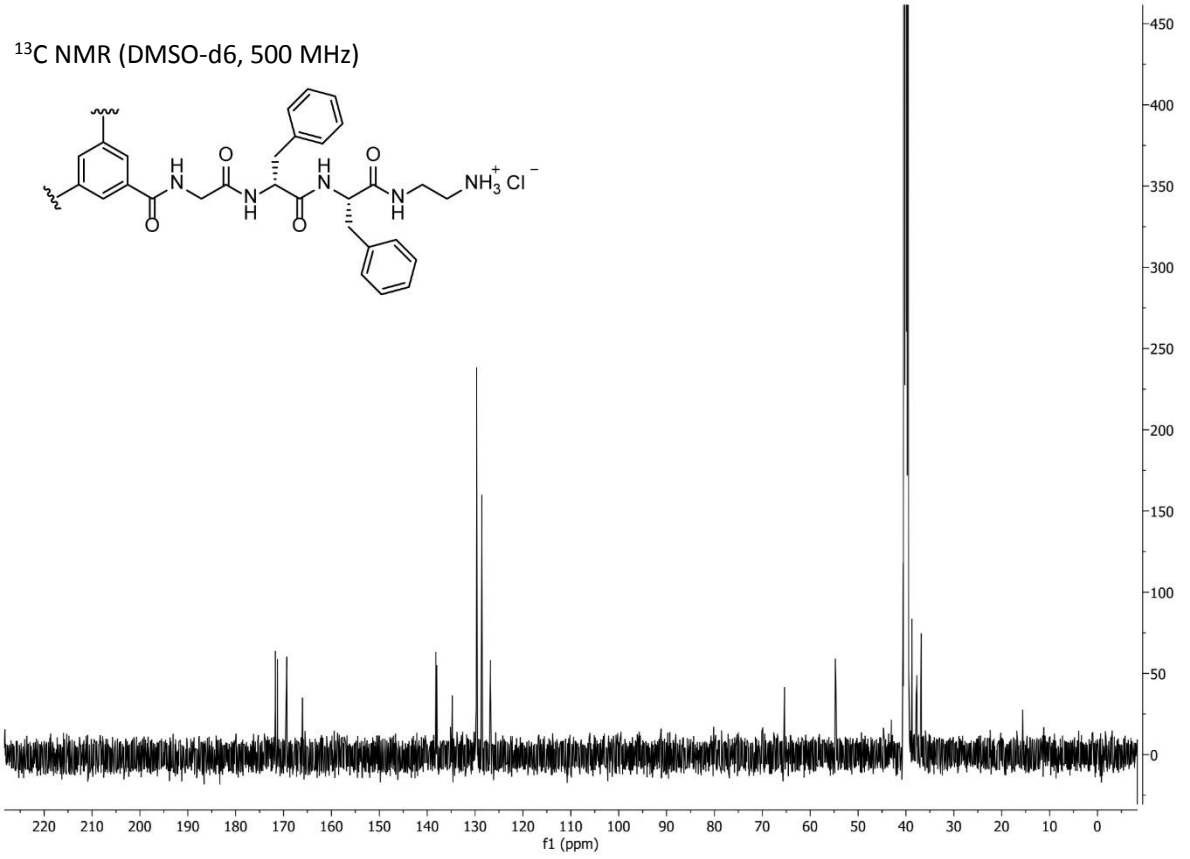
^{13}C NMR (DMSO-d6, 500 MHz)



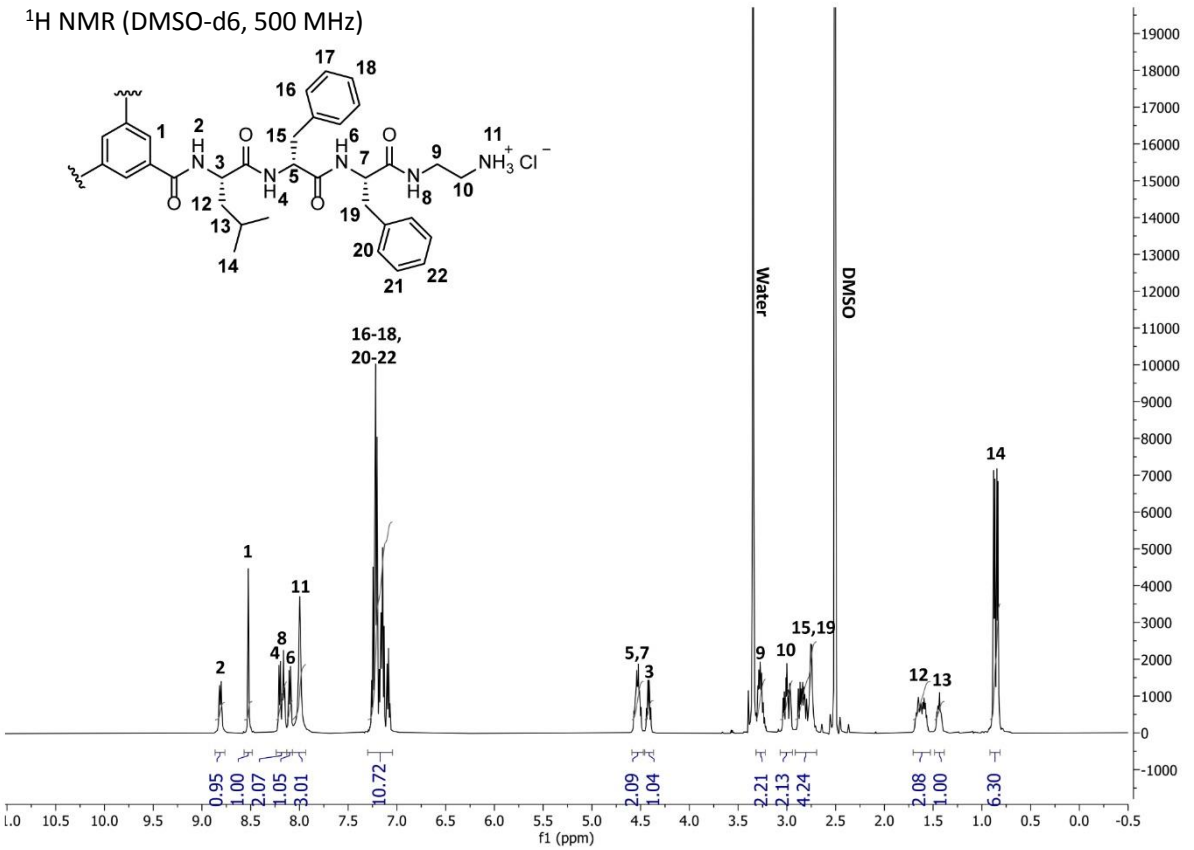
^{1}H NMR (DMSO-d6, 500 MHz)



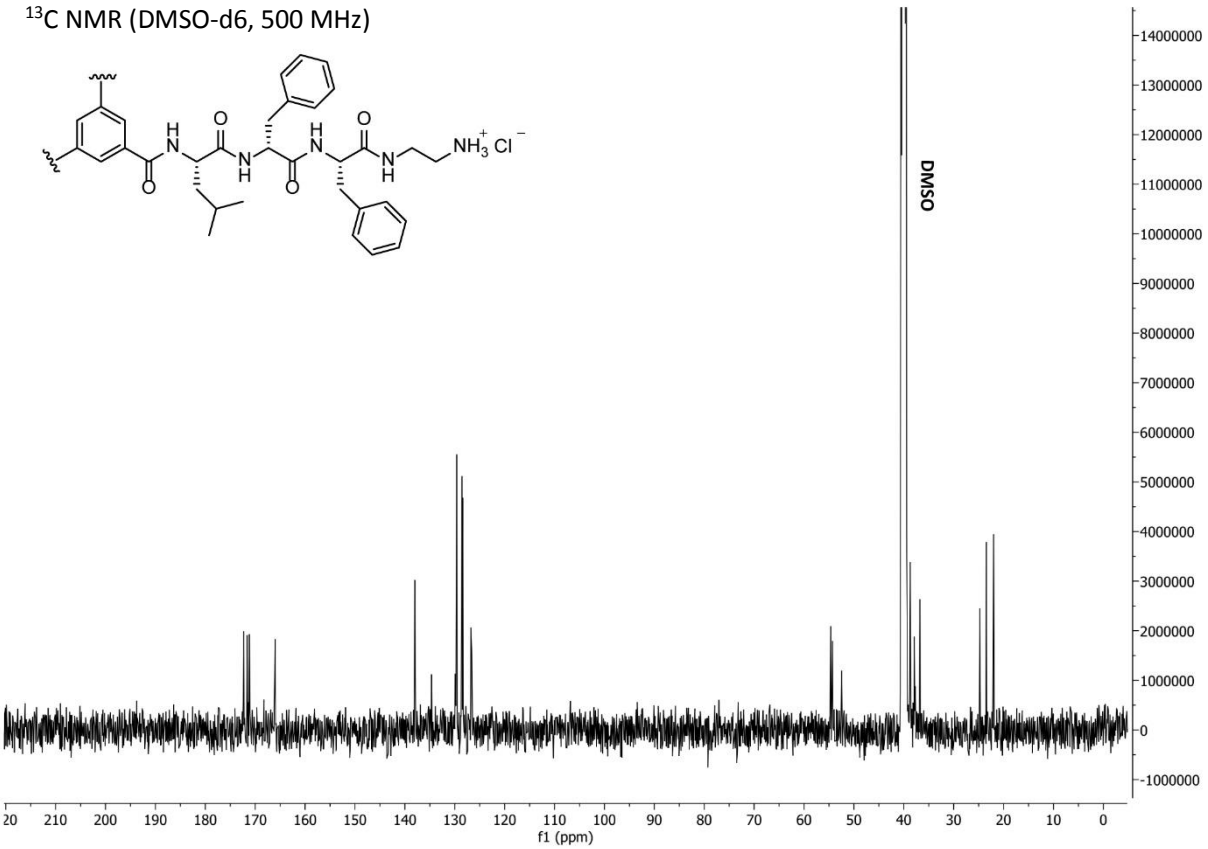
^{13}C NMR (DMSO-d6, 500 MHz)



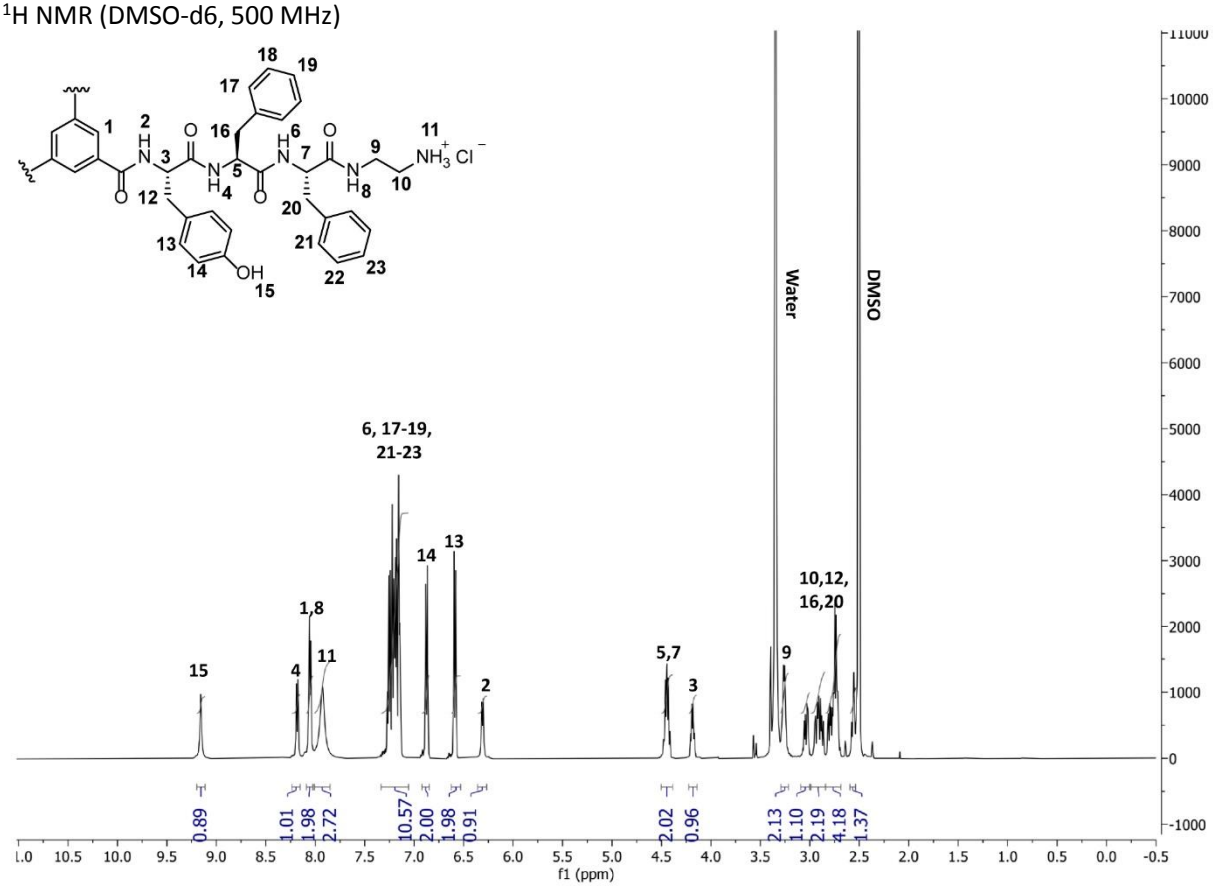
^{1}H NMR (DMSO-d6, 500 MHz)



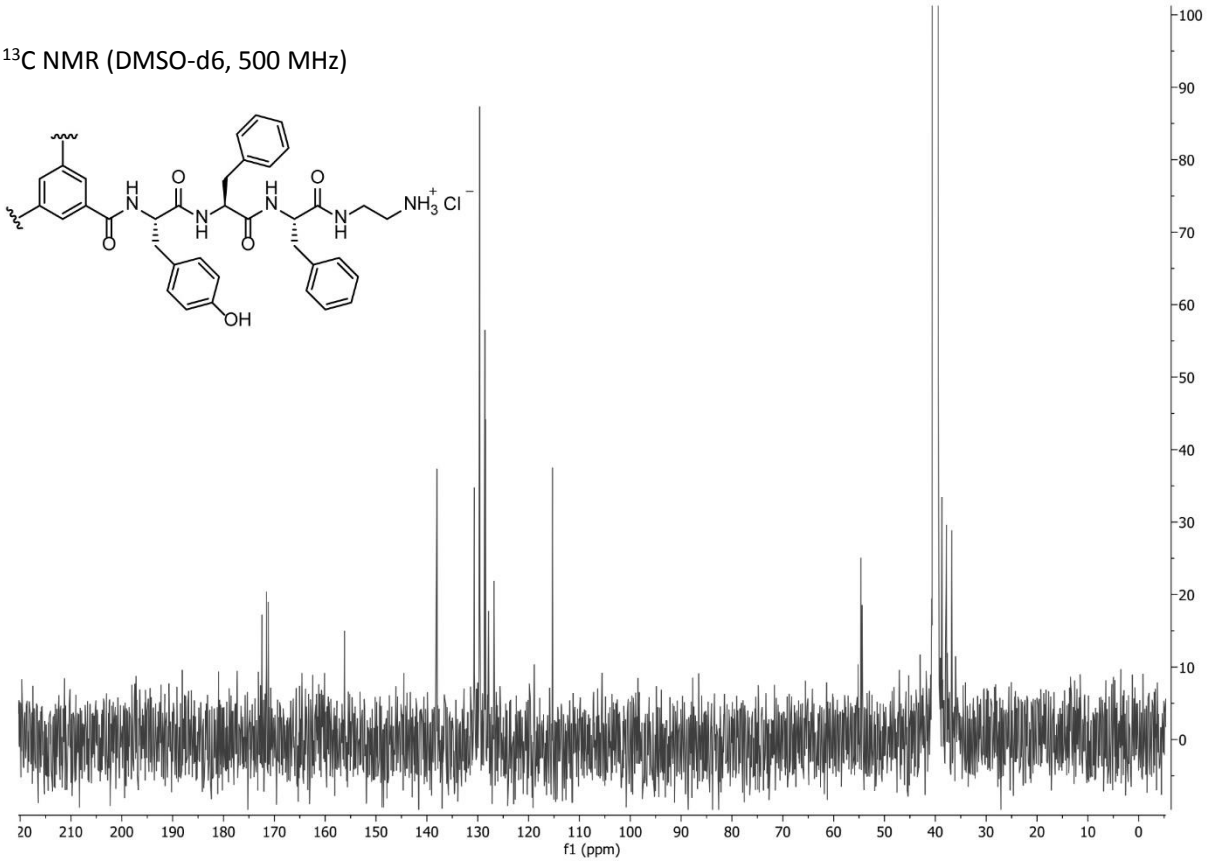
^{13}C NMR (DMSO-d6, 500 MHz)



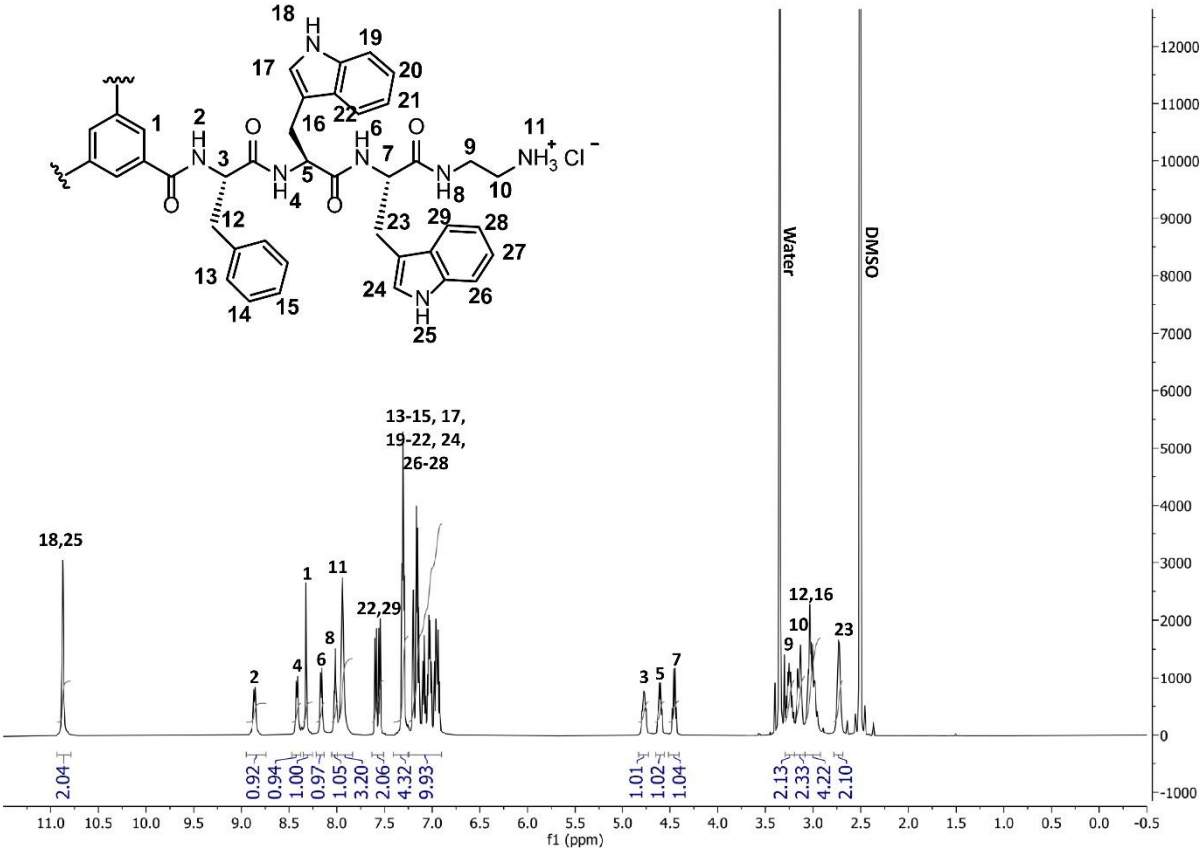
^{1}H NMR (DMSO-d6, 500 MHz)



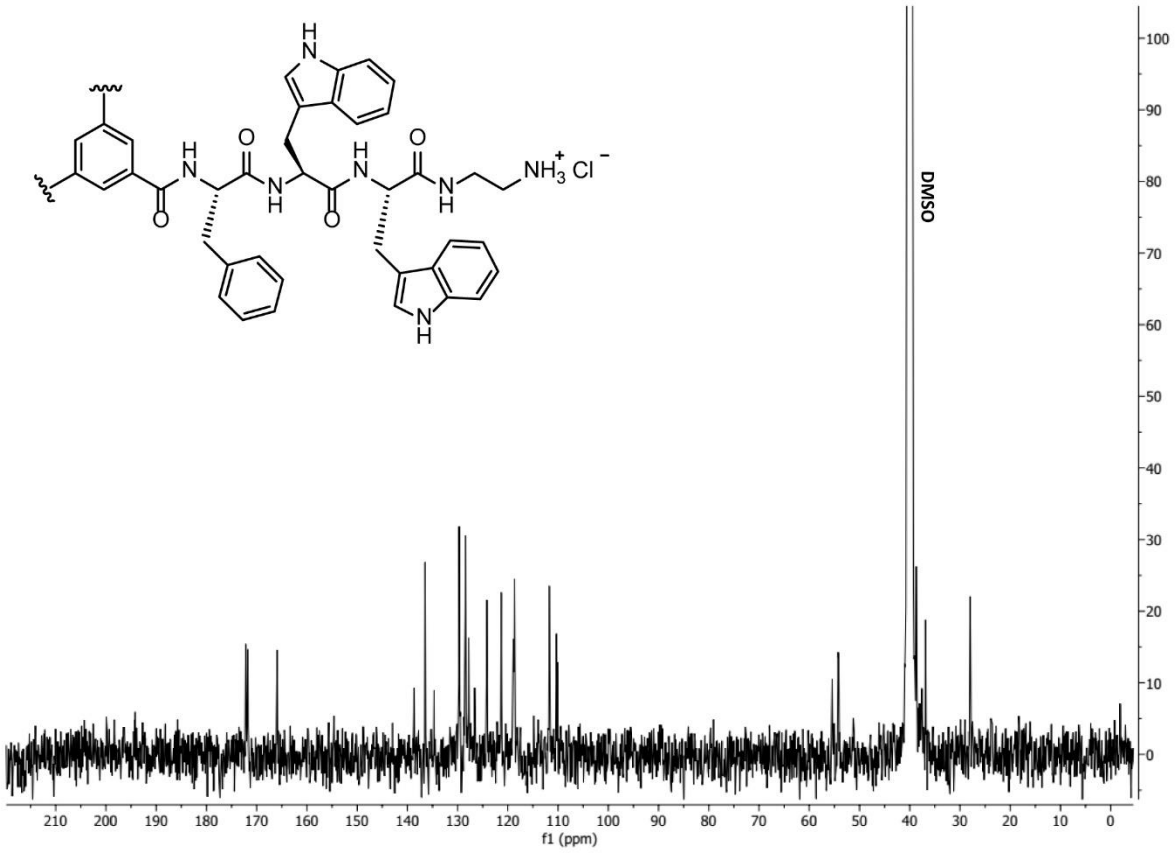
^{13}C NMR (DMSO-d6, 500 MHz)



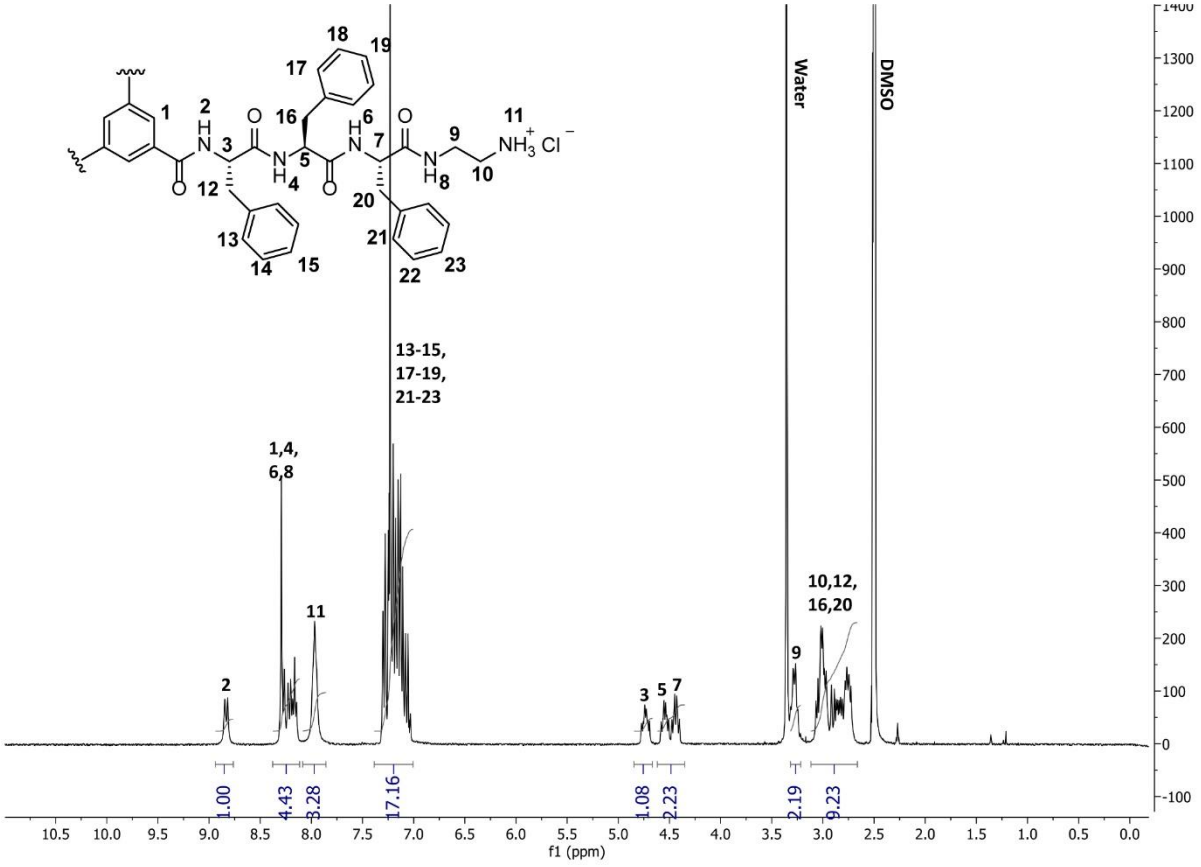
^{1}H NMR (DMSO-d6, 500 MHz)



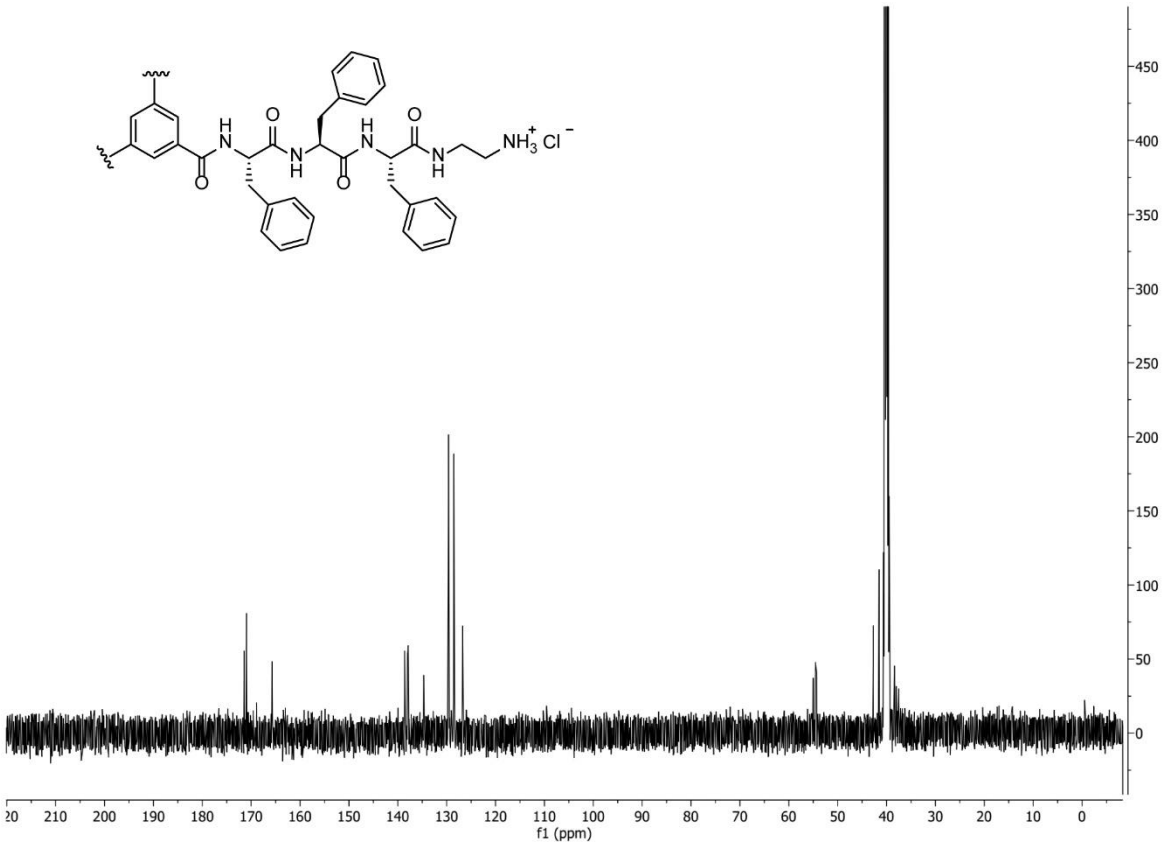
^{13}C NMR (DMSO-d6, 500 MHz)



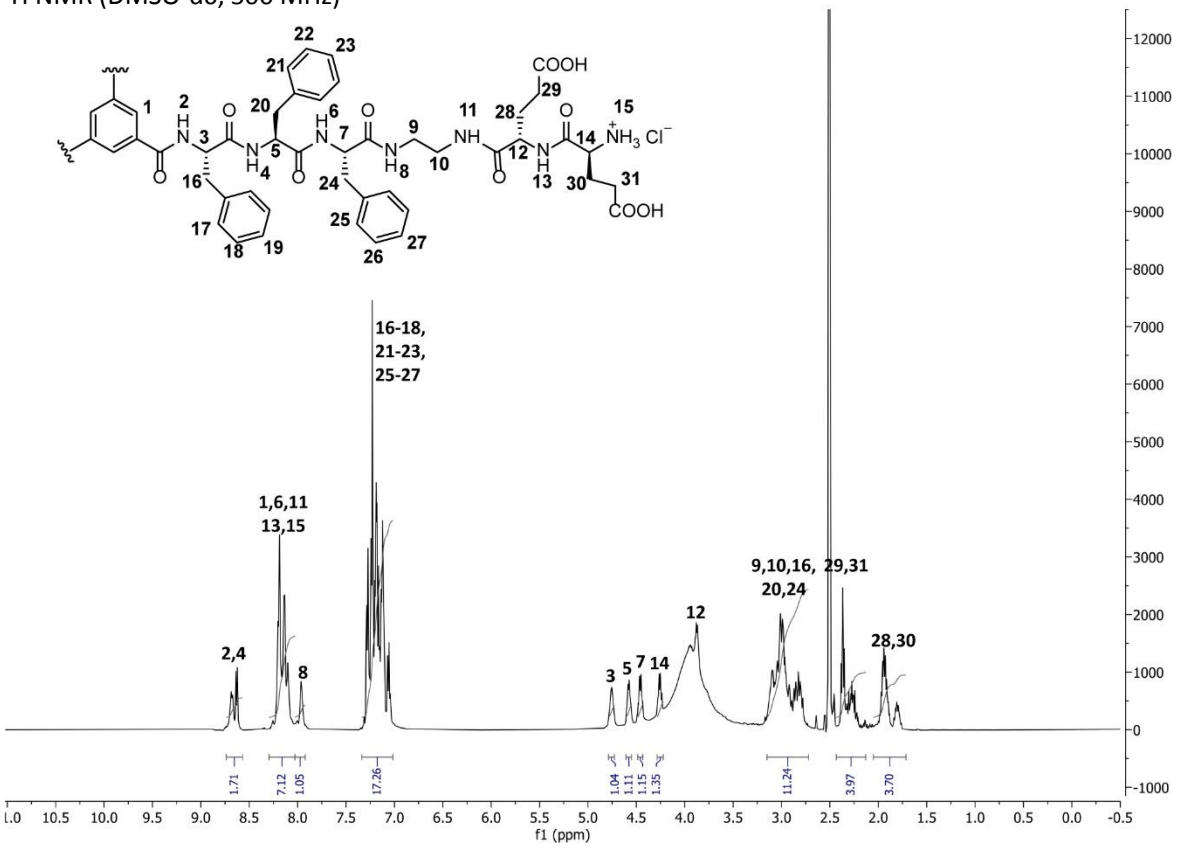
^{1}H NMR (DMSO-d6, 500 MHz)



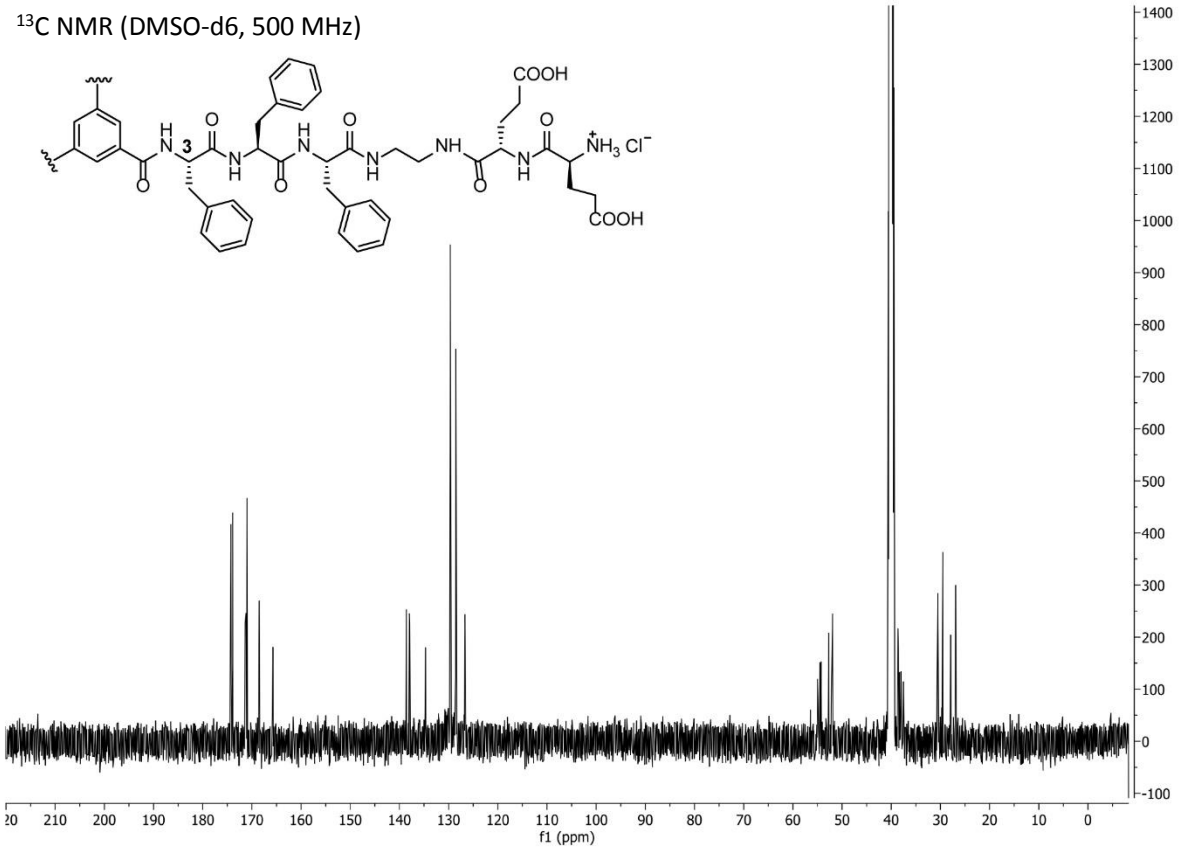
^{13}C NMR (DMSO-d6, 500 MHz)



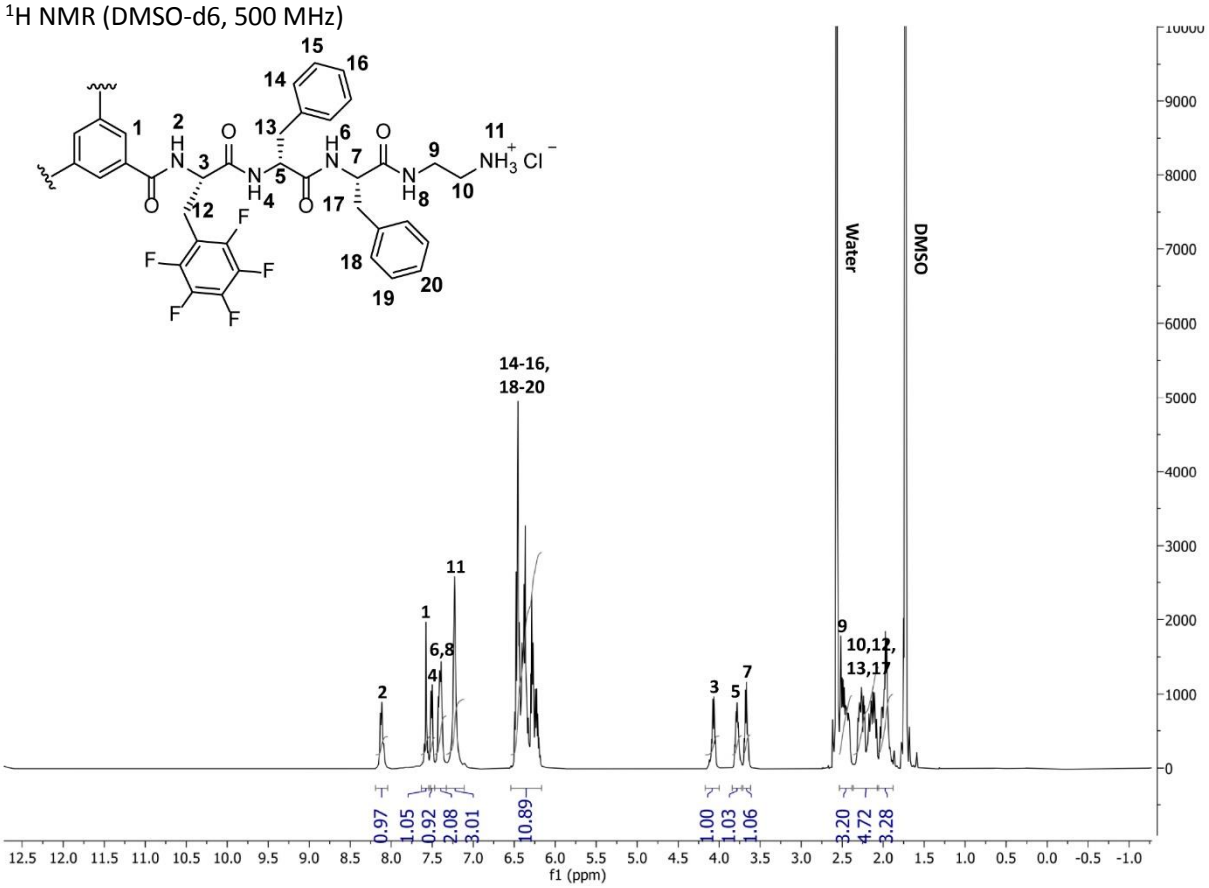
^{1}H NMR (DMSO-d6, 500 MHz)



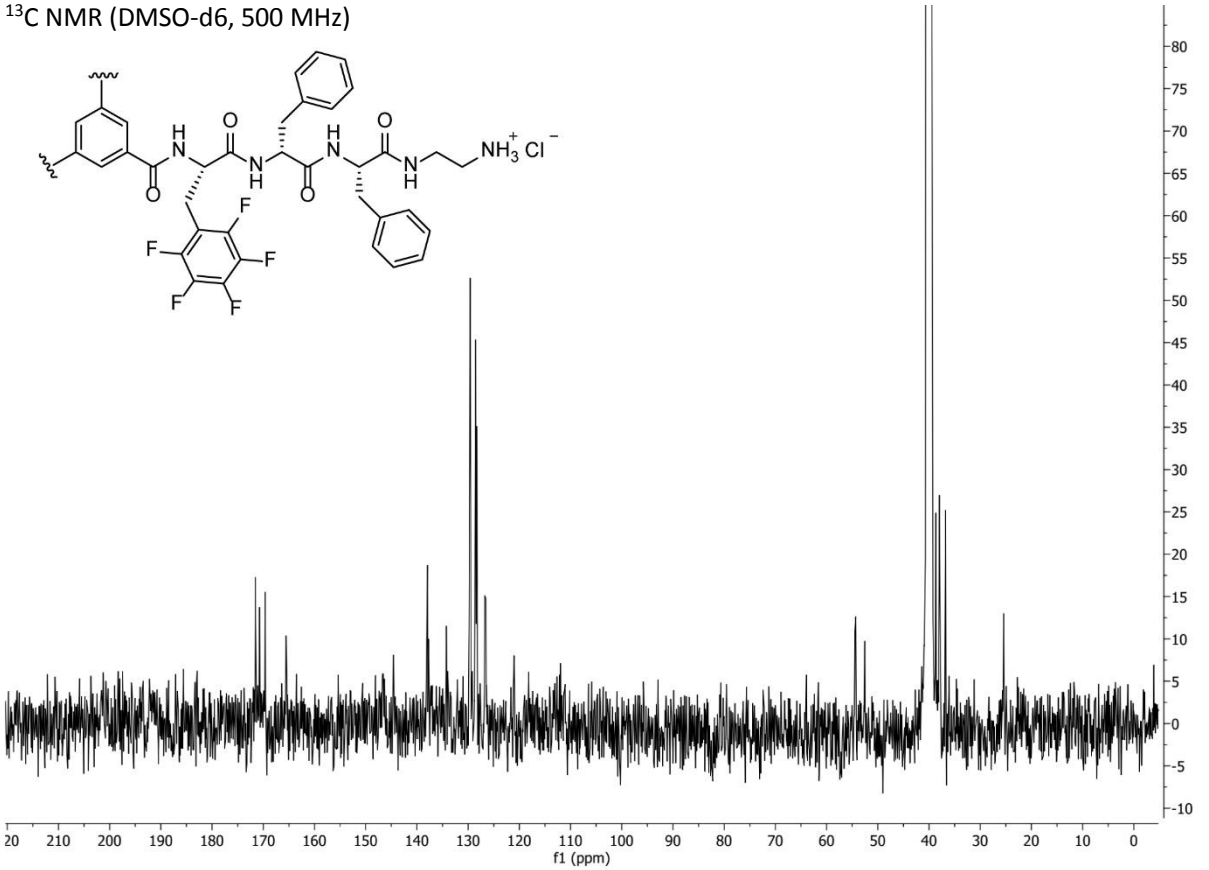
^{13}C NMR (DMSO-d6, 500 MHz)



^{1}H NMR (DMSO-d6, 500 MHz)



^{13}C NMR (DMSO-d6, 500 MHz)



^{19}F NMR (DMSO-d6, 500 MHz)