

Electronic Supporting Information

Lightly congested amino terminal dendrimers. Amide-based stable structures with large-scale synthesis.

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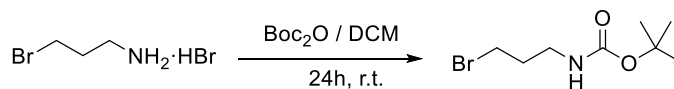
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1.- Synthetic protocols

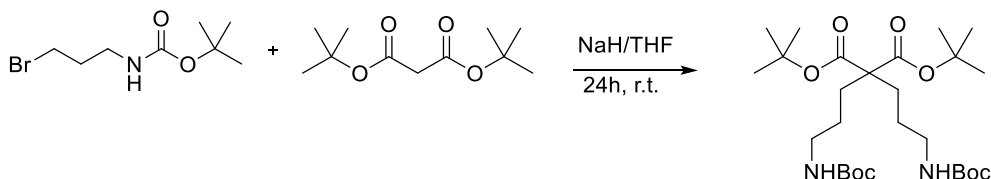
Synthesis of *tert*-butyl (3-bromopropyl)carbamate



This compound was synthesized as previously described.¹ 3-Bromopropylamine hydrobromide (15.00 g, 68.52 mmol, 1 eq) was dissolved in CH₂Cl₂ (60 mL). To this mixture di-*tert*-butyl dicarbonate (22.43 g, 102.78 mmol, 1.5 eq) dissolved in CH₂Cl₂ (40 mL) and triethylamine (10.46 mL, 75.37 mmol, 1.1 eq) were added. After the addition, the reaction was stirred overnight. The organic layer was then separated, washed with 1 M sodium bicarbonate (2 x 50 mL), and Brine (50 mL), dried over anhydrous MgSO₄ and the solvent removed under vacuum. Purification by silica gel column chromatography (ethyl acetate:n-hexane; 1:9) gave the desired compound as a colorless oil (15.25 g, 64.35 mmol, 94 %).

The reaction was monitored by TLC (eluent ethyl acetate:n-hexane; 1:9). **R_f**: 0.8. **¹H-NMR** (400 MHz, CDCl₃) δ ppm: 4.65 (bs, 1H), 3.44 (t, *J* = 6.5 Hz, 2H), 3.30 – 3.20 (m, 2H), 2.10 – 1.99 (m, 2H), 1.44 (s, 9H). **¹³C-NMR** (100 MHz, CDCl₃) δ ppm: 156.1, 79.6, 39.1, 32.8, 30.9, 28.5.

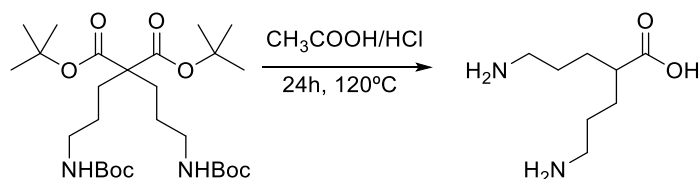
Synthesis of di-*tert*-butyl 2,2-bis(3-((*tert*-butoxycarbonyl)amino)propyl)malonate



This compound was synthesized as previously described.² NaH (60% in mineral oil (3.09 g, 77.23 mmol, 3 eq)) was dissolved in dry THF (20 mL) under nitrogen atmosphere. Di-*tert*-butyl malonate (5.77 mL, 25.74 mmol, 1 eq) was added and stirred for 15 minutes. To this, freshly prepared *N*-Boc-3-bromopropylamine (15.25 g, 64.35 mmol, 2.5 eq) in THF dry (20 mL) was added dropwise. The solution was stirred overnight. The solvent was then removed under vacuum and the residue was dissolved in H₂O (50 mL). The compound was extracted from the aqueous layer with ethyl acetate (3 x 30 mL), dried over MgSO₄ anhydrous and the solvent removed under vacuum. Purification by silica gel column chromatography (ethyl acetate:n-hexane; 2:8) gave the desired compound as a w solid (12.58 g, 23.73 mmol, 92 %).

The reaction was monitored by TLC (eluent ethyl acetate:n-hexane; 2:8). **R_f**: 0.4. **¹H-NMR** (400 MHz, CDCl₃) δ ppm: 4.58 (bs, 2H), 3.18 – 3.05 (m, 4H), 1.86 – 1.71 (m, 4H), 1.44 (s, 18H), 1.43 (s, 18H), 1.40 – 1.30 (m, 4H). **¹³C-NMR** (100 MHz, CDCl₃) δ ppm: 170.8, 156.0, 81.5, 79.2, 57.9, 40.8, 29.5, 28.5, 28.0, 24.6. **ESI-POS** calc. for C₂₇H₅₀N₂O₈Na⁺, 553.3460, [M + Na]⁺, found, 553.3462.

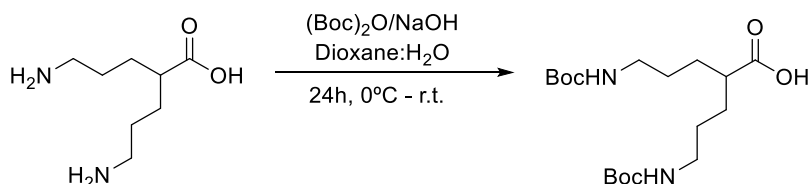
Synthesis of 5-amino-2-(3-aminopropyl)pentanoic acid



This compound was synthesized as described.² Di-*tert*-butyl 2,2-bis(3-((*tert*-butoxycarbonyl)amino)propyl)malonate (12.58 g, 23.73 mmol) was dissolved in acetic acid (20 mL) and 3 N hydrochloric acid (20 mL) and refluxed overnight. Evaporation of the solvent gave the compound as a sticky colorless solid (5.86 g, 23.73 mmol) in a quantitative way.

¹H-NMR (400 MHz, D_2O): δ ppm: 8.13 (bs, 4H), 2.81 – 2.65 (m, 4H), 2.27 (bs, 1H), 1.67 – 1.34 (m, 8H). **¹³C-NMR** (400 MHz, D_2O): δ ppm = 176.2, 43.8, 38.3, 28.4, 24.7. **ESI-POS** calc. for $\text{C}_8\text{H}_{18}\text{N}_2\text{O}_2$, 174.1368, $[\text{M} + \text{H}]^+$, found 175.1440.

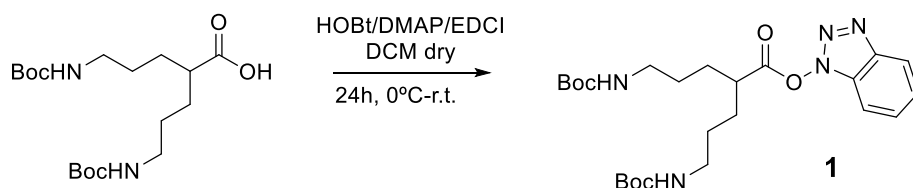
Synthesis of 5-((*tert*-butoxycarbonyl)amino)-2-(3-((*tert*-butoxycarbonyl)amino)propyl)pentanoic acid



A mixture of 5-amino-2-(3-aminopropyl)pentanoic acid (5.86 g, 23.70 mmol, 1 eq) and NaOH (2.84 g, 71.10 mmol, 3 eq) in dioxane: H_2O (2:1, 30 mL) was stirred and cooled in an ice bath (0°C). Di-*tert*-butyl dicarbonate (11.07 g, 52.14 mmol, 2.2 eq) in dioxane: H_2O (2:1, 15 mL) was added dropwise. After the addition was complete, the mixture was allowed to warm to room temperature and was stirred until reaction was finished. The solvent was then removed under vacuum and the residue was dissolved in H_2O (50 mL). The compound was extracted from the aqueous layer with ethyl acetate (2 x 30 mL). The aqueous layer was acidified to pH 1-2 with 1M HCl and extracted with ethyl acetate (3 x 50 mL). The organic layers were combined, dried over MgSO_4 anhydrous and the solvent removed under vacuum. The compound desired was obtained as a colorless oil (8.34 g, 22.31 mmol, 94 %).

The reaction was monitored by TLC (eluent ethyl acetate:n-hexane; 9:1). **R_f**: 0.7. **¹H-NMR** (400 MHz, CDCl_3) δ ppm: 4.75 (bs, 2H), 3.16 – 2.95 (m, 4H), 2.33 (bs, 1H), 1.73 – 1.55 (m, 2H), 1.52 – 1.30 (m, 24H). **¹³C-NMR** (100 MHz, CDCl_3) δ ppm: 180.4, 156.2, 79.3, 44.8, 40.4, 29.4, 28.5, 27.9. **ESI-POS** calc. for $\text{C}_{18}\text{H}_{34}\text{N}_2\text{O}_6\text{Na}^+$, 397.2310, $[\text{M} + \text{Na}]^+$, found, 397.2309.

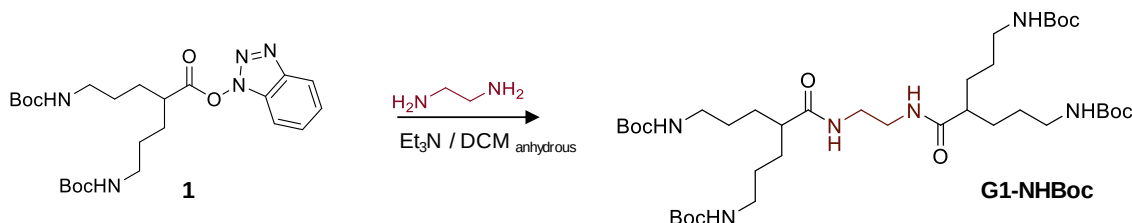
Synthesis of compound 1



5-((*tert*-butoxycarbonyl)amino)-2-(3-((*tert*-butoxycarbonyl)amino)propyl)pentanoic acid (8.34 g, 22.31 mmol, 1 eq) was dissolved in dry CH₂Cl₂ (50 mL) under nitrogen atmosphere and EDCI (4.70 g, 24.53 mmol, 1.1 eq) was added over a 10 min period. The reaction mixture was cooled in an ice bath (0 °C) and stirred for 10 minutes. After that HOBt (9.03 g, 69.90 mmol, 3 eq) and DMAP (218 mg, 1.78 mmol, 0.08 eq), previously dissolved in dry CH₂Cl₂, were added. After 5 minutes at 0 °C the ice bath was removed, and the reaction mixture was stirred at room temperature until reaction is finished. The reaction mixture was diluted with CH₂Cl₂ (50 mL) and washed with H₂O (50 mL), 0.5M HCl (2 x 50 mL) and with a saturated solution of NaHCO₃ (2 x 50 mL). The organic layer was dried over MgSO₄ and was concentrated under reduced pressure. Compound **1** was obtained as a colorless solid (9.86 g, 20.08 mmol, 90 %).

The reaction was monitored by TLC (eluent ethyl acetate:n-hexane; 8:2). **R_f**: 0.6. ¹H-NMR (400 MHz, CDCl₃) δ ppm: 8.06 (d, *J* = 8.6 Hz, 1H), 7.80 – 7.50 (m, 1H), 7.46 – 7.38 (m, 2H), 4.70 (bs, 2H), 3.28 – 3.17 (m, 4H), 2.97 (bs, 1H), 1.96 – 1.83 (m, 2H), 1.83 – 1.75 (m, 2H), 1.75 – 1.65 (m, 4H), 1.44 (s, 18H). **ESI-POS** calc. for C₂₄H₃₇N₅O₆Na⁺, 514.2637, [M + Na]⁺, found, 514.2627.

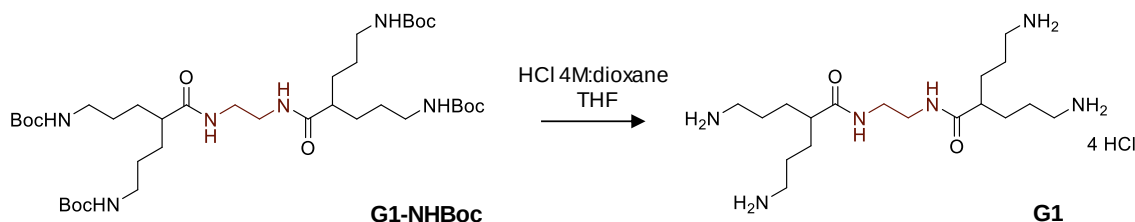
Synthesis of G1-NHBoc



Compound **1** (4.71 g, 9.60 mmol, 2.2 eq), ethylenediamine (290 μL, 4.36 mmol, 1 eq) and triethylamine (1.82 mL, 13.08 mmol, 3 eq) were dissolved in dry dichloromethane (30 mL) under anhydrous conditions. The reaction mixture was stirred at room temperature overnight. Then, it was washed with 0.5M HCl (2 x 30 mL) and with a saturated solution of NaHCO₃ (2 x 30 mL). The organic layer was dried over MgSO₄ and was concentrated under reduced pressure. **G1-NHBoc** was obtained as a colorless solid (3.03 g, 3.92 mmol, 90 %) with no need of purification.

The reaction was monitored by TLC (eluent ethyl acetate:n-hexane; 7:3). **R_f**: 0.5. ¹H-NMR (400 MHz, DMSO-*d*₆) δ ppm: 7.86 (bs, 2H), 6.74 (m, 4H), 3.10 – 3.03 (m, 4H), 2.89 – 2.80 (m, 8H), 2.03 (bs, 2H), 1.40 – 1.33 (m, 40 H), 1.30 – 1.20 (m, 12 H). ¹³C-NMR (100 MHz, DMSO-*d*₆) δ ppm: 174.8, 155.6, 77.3, 45.3, 39.8, 38.3, 29.8, 28.3, 27.6. **ESI-POS** calc. for C₃₈H₇₂N₆O₁₀Na⁺, 795.5203, [M + Na]⁺, found, 795.5201.

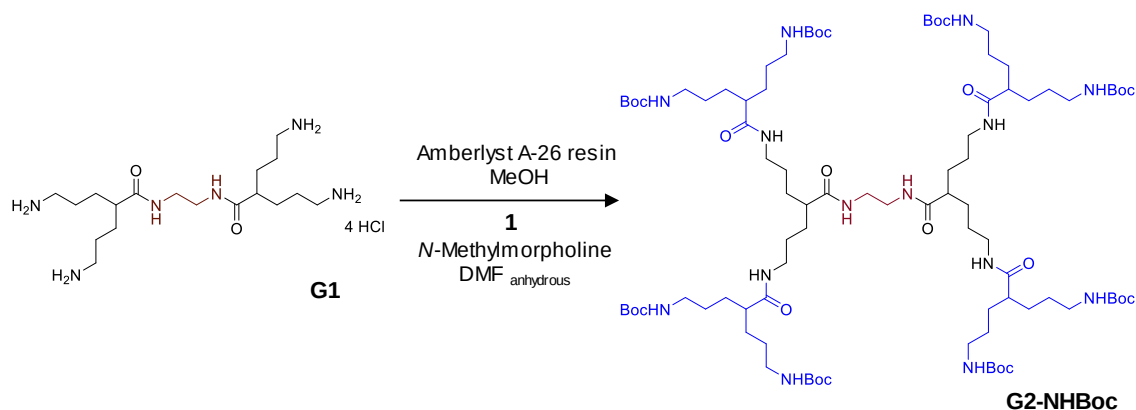
Synthesis of G1



The deprotection of **G1-NHBoc** (2.05 g, 2.65 mmol) gave **G1** (1.35 g, quantitative) as a yellow pale foamy solid.

¹H-NMR (400 MHz, DMSO-*d*₆) δ ppm: 8.46 (bs, 2H), 8.10 (bs, 8H), 3.13 (bs, 4 H), 2.85 – 2.66 (m, 8 H), 2.38 (bs, 2H), 1.59 – 1.43 (m, 12H), 1.41 – 1.26 (m, 4 H). **¹³C-NMR** (100 MHz, DMSO-*d*₆) δ ppm: 174.4, 43.9, 39.5 (with DMSO-*d*₆ signal), 38.5, 29.3, 24.8. **ESI-NEG** calc. for C₁₈H₄₀N₆O₂Cl[−], 407.2982, [M + Cl][−], found, 407.2893.

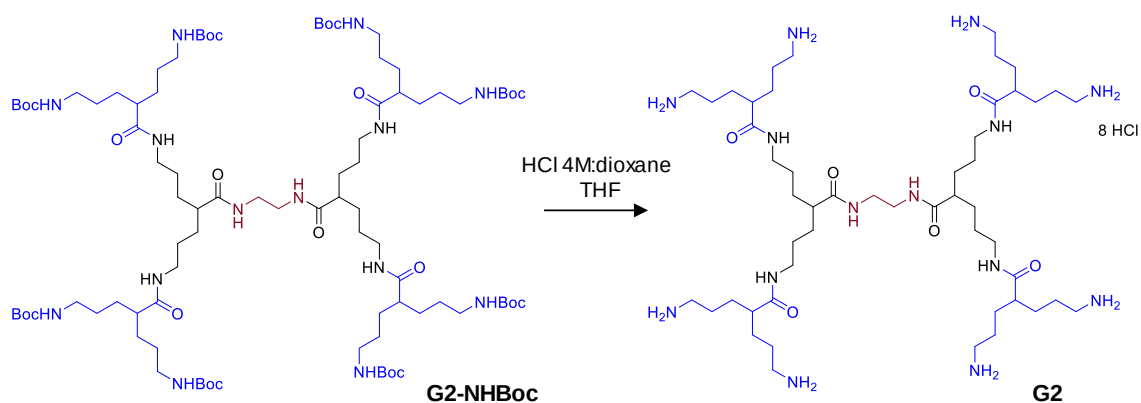
Synthesis of G2-NHBoc



G1 (1.80 g, 3.47 mmol) in methanol (10 mL) was treated with Amberlyst A-26 resin (7 g) for one hour. The obtained compound, **1** (7.46 g, 15.20 mmol, 4.4 eq) and *N*-methylmorpholine (2.28 mL, 20.70 mmol, 6 eq) were solved in anhydrous DMF (60 mL) under nitrogen atmosphere and stirred at room temperature overnight to obtain **G2-NHBoc** (5.62 g, 3.12 mmol, 90 %) as a colorless solid.

The reaction was monitored by TLC (eluent ethyl acetate:n-hexane; 7:3). **R_f**: 0.4. **¹H-NMR** (400 MHz, DMSO-*d*₆) δ ppm: 7.97 – 7.89 (m, 2 H), 7.83 – 7.75 (m, 4 H), 6.82 – 6.70 (m, 8 H), 3.13 – 3.05 (m, 4 H), 3.05 – 2.93 (m, 8 H), 2.91 – 2.80 (m, 16 H), 2.13 – 2.00 (m, 6 H), 1.42 – 1.17 (m, 120 H). **¹³C-NMR** (100 MHz, DMSO-*d*₆) δ ppm: 174.9, 174.5, 155.6, 77.3, 45.1, 39.5 (with DMSO-*d*₆ signal), 38.3, 30.0, 29.8, 28.3, 27.6, 27.2. **MALDI**: *m/z* calc. for C₉₀H₁₆₈N₁₄O₂₂Na⁺ 1821.2; exp. 1822.6 (M+Na⁺).

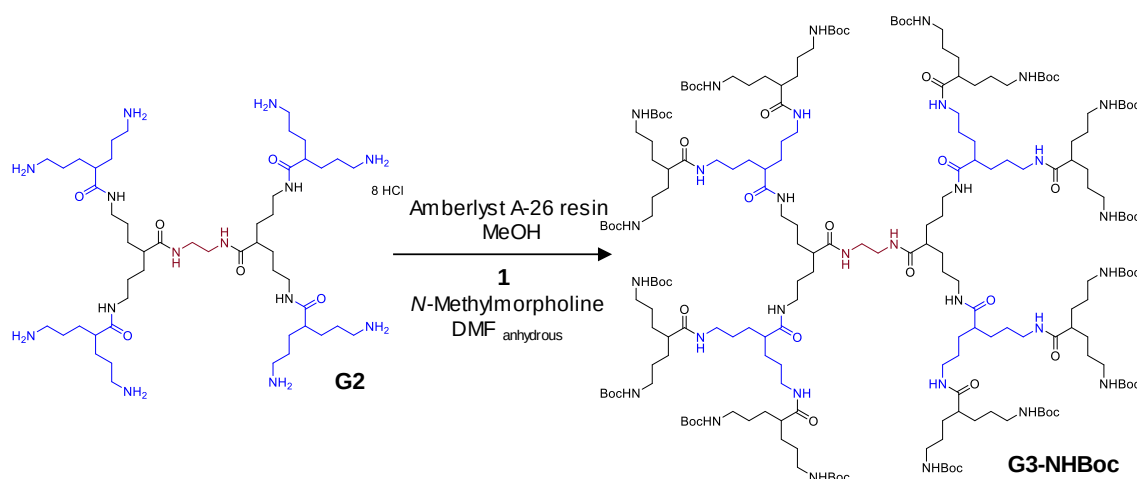
Synthesis of G2



This compound was obtained from **G2-NHBoc** (5.39 g, 3.00 mmol) to obtain the desired product (3.85 g, quantitative) as a yellow pale foamy solid.

¹H-NMR (400 MHz, DMSO-*d*₆) δ ppm: 8.53 – 7.96 (m, 22 H), 3.11 – 2.90 (m, 12 H), 2.84 – 2.65 (m, 16 H), 2.32 – 2.15 (m, 6 H), 1.56 – 1.22 (m, 48 H). **¹³C-NMR** (100 MHz, DMSO-*d*₆) δ ppm: 175.4, 174.0, 45.2, 44.1, 39.5 (with DMSO-*d*₆ signal), 38.6, 38.4, 30.1, 29.3, 27.3, 24.8. **MALDI**: *m/z* calc. for C₅₀H₁₀₄N₁₄O₆Na⁺ 1020.5; exp. 1020.5 (M+Na⁺).

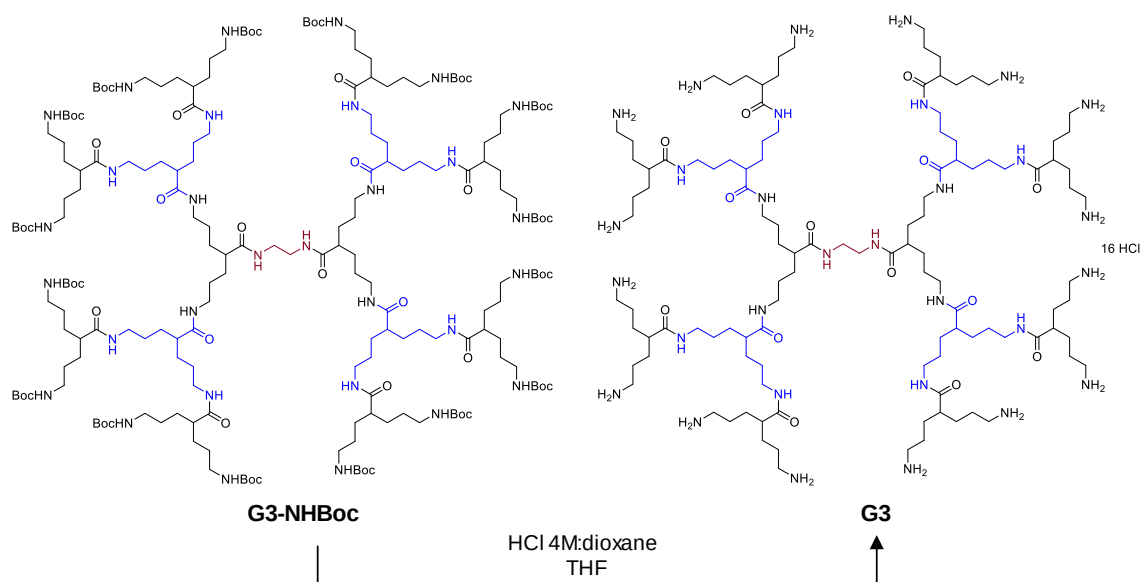
Synthesis of G3-NHBoc



G2 (1.73 g, 1.34 mmol) in methanol (10 mL) was treated with and Amberlyst A-26 resin (5.4 g) for one hour. The obtained compound, **1** (5.79 g, 11.80 mmol, 8.8 eq) and *N*-methylmorpholine (1.76 mL, 16.08 mmol, 12 eq) were solved in anhydrous DMF (60 mL) under nitrogen atmosphere and stirred overnight to obtain **G3-NHBoc** (4.68 g, 1.22 mmol, 91 %) as a colorless solid after precipitation (product was dissolved in the minimum amount of dichloromethane and precipitated in hexane).

¹H-NMR (400 MHz, DMSO-*d*₆) δ ppm: 8.12 – 7.67 (m, 14 H), 6.87 – 6.58 (m, 16 H), 3.13 – 2.77 (m, 60 H), 2.17 – 1.98 (m, 14 H), 1.48 – 1.17 (m, 246 H). **¹³C-NMR** (100 MHz, DMSO-*d*₆) δ ppm: 174.9, 174.5, 155.6, 77.3, 45.1, 39.5 (with DMSO-*d*₆ signal), 38.3, 30.0, 29.8, 28.3, 27.6, 27.3. **MALDI**: *m/z* calc. for C₁₉₄H₃₆₀N₃₀O₄₆Na⁺ 3871.7; exp. 3873.7 (M+Na⁺).

Synthesis of G3

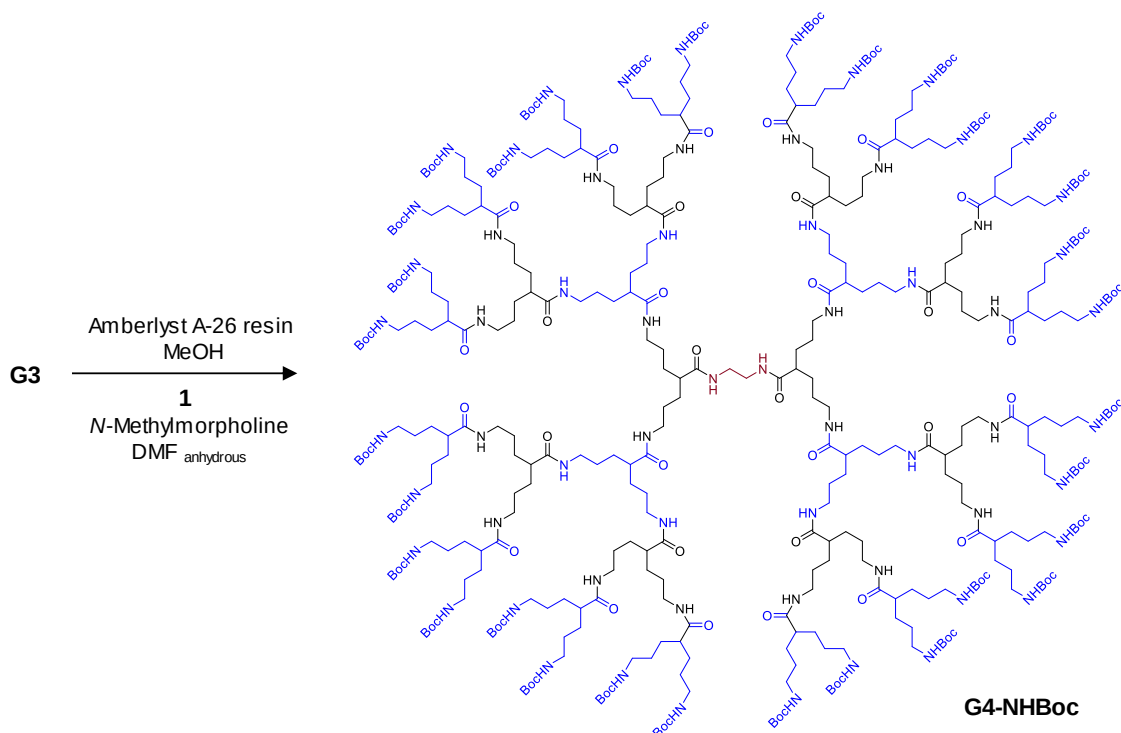


This compound was obtained from **G3-NHBoc** (4.68 g, 1.22 mmol) to obtain the product (3.43 g, quantitative) as a yellow pale foamy solid.

¹H-NMR (400 MHz, DMSO-*d*₆) δ ppm: 8.40 – 8.05 (m, 56 H), 3.18 – 2.89 (m, 28 H), 2.84 – 2.67 (m, 32 H), 2.35 – 2.12 (m, 14 H), 1.57 – 1.20 (m, 102 H). **¹³C-NMR** (100

MHz, DMSO-*d*₆) δ ppm: 175.3, 175.2, 174.1, 45.1, 44.1, 39.5 (with DMSO-*d*₆ signal), 38.6, 30.2, 29.3, 27.3, 24.8.

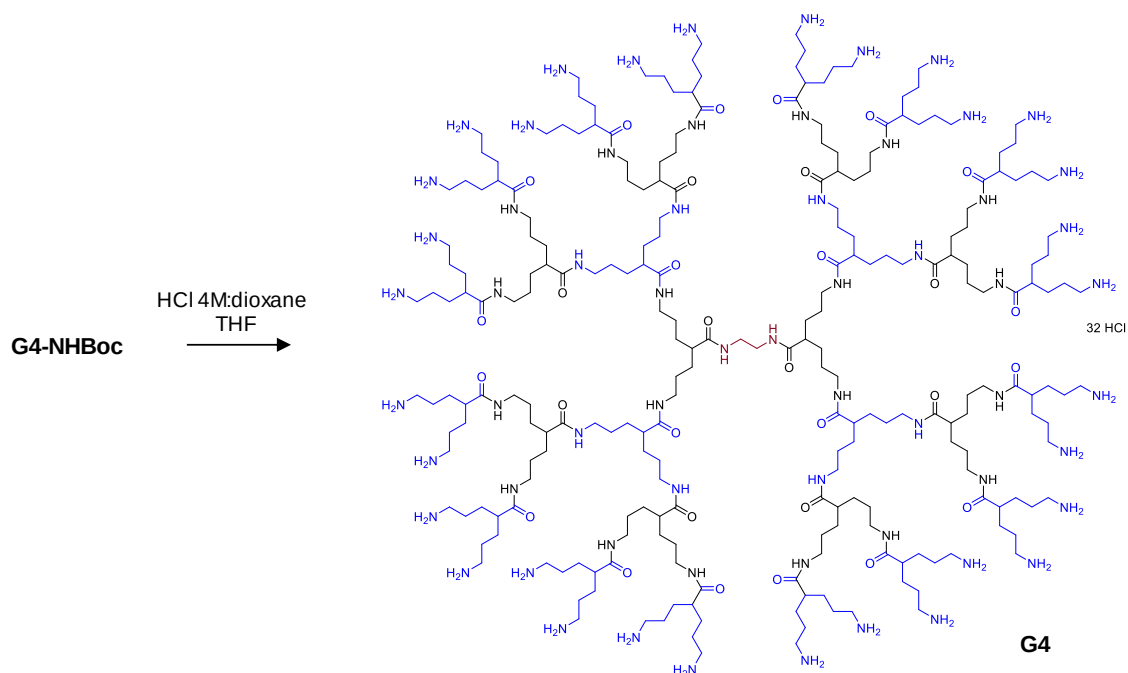
Synthesis of G4-NHBoc



G3 (831 mg, 0.30 mmol) in methanol (10 mL) was treated with and Amberlyst A-26 resin (2.40 g) in methanol for one hour. The obtained compound, **1** (2.45 g, 5 mmol, 17.6 eq) and *N*-methylmorpholine (740 μ L, 6.72 mmol, 24 eq) were dissolved in anhydrous DMF (60 mL) under nitrogen atmosphere and the mixture was stirred at room temperature for eight days. After four days, the reaction was refreshed with the same amount of **1** and *N*-methylmorpholine. **G4-NHBoc** (2.00 g, 0.25 mmol, 90 %) was obtained as a colorless solid after precipitation (product was dissolved in the minimum amount of dichloromethane and precipitated in hexane).

¹H-NMR (400 MHz, DMSO-*d*₆) δ ppm: 7.20 – 7.80 (m, 30H), 6.90 – 6.30 (m, 32H), 3.20 – 2.70 (m, 124H), 2.20 – 2.00 (m, 30H), 1.40 – 1.20 (m, 318 H). **¹³C-NMR** (100 MHz, DMSO-*d*₆) δ ppm 174.5, 155.6, 77.3, 45.1, 39.5 (with DMSO-*d*₆ signal), 38.3, 29.9, 28.2, 27.6, 27.3.

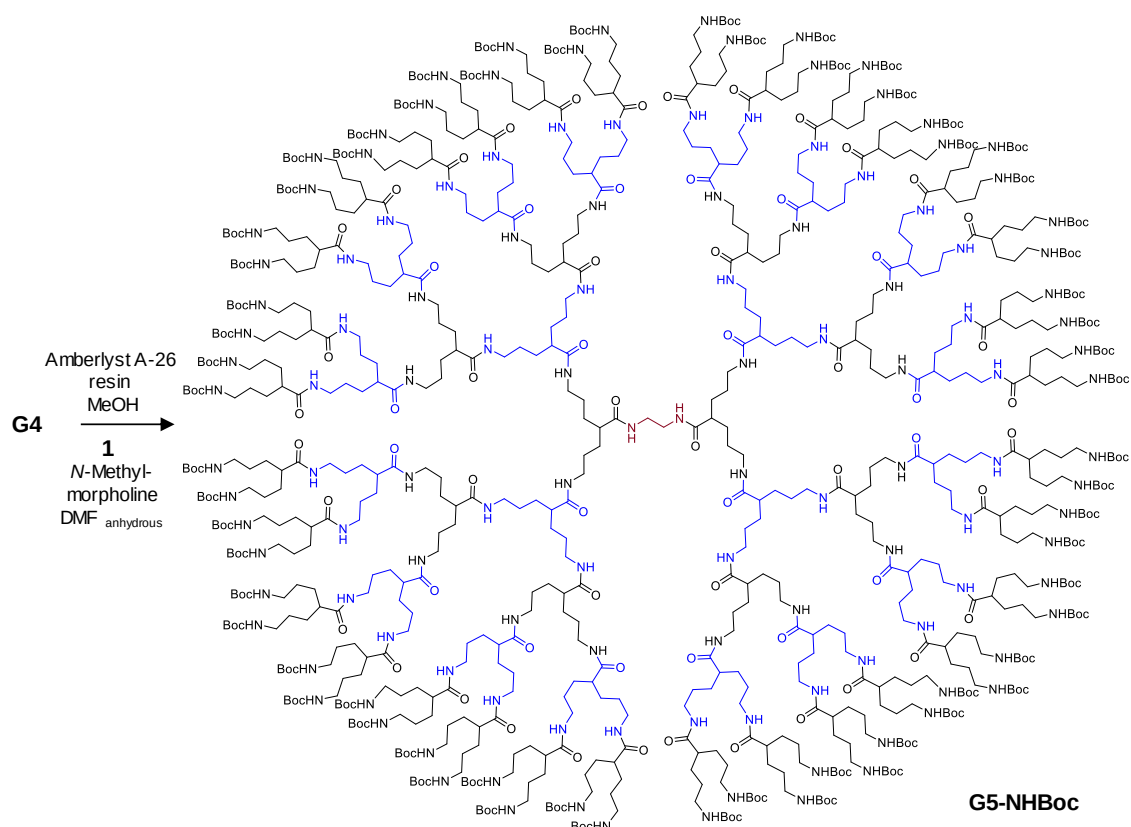
Synthesis of G4



The deprotection of amine groups of **G4-NHBoc** (2.00 g, 0.25 mmol) gave **G4** (1.45 g, quantitative) as a yellow pale foamy solid.

¹H-NMR (400 MHz, DMSO-*d*₆) δ ppm: 8.49 – 7.28 (m, 94 H), 3.17 – 2.90 (m, 60 H), 2.82 – 2.69 (m, 64 H), 2.34 – 2.16 (m, 30 H), 1.60 – 1.21 (m, 240 H). ¹³C-NMR (100 MHz, DMSO-*d*₆) δ ppm: 176.5, 175.2, 174.1, 45.0, 44.1, 39.5 (with DMSO-*d*₆ signal), 38.5, 30.2, 29.3, 27.3, 24.8.

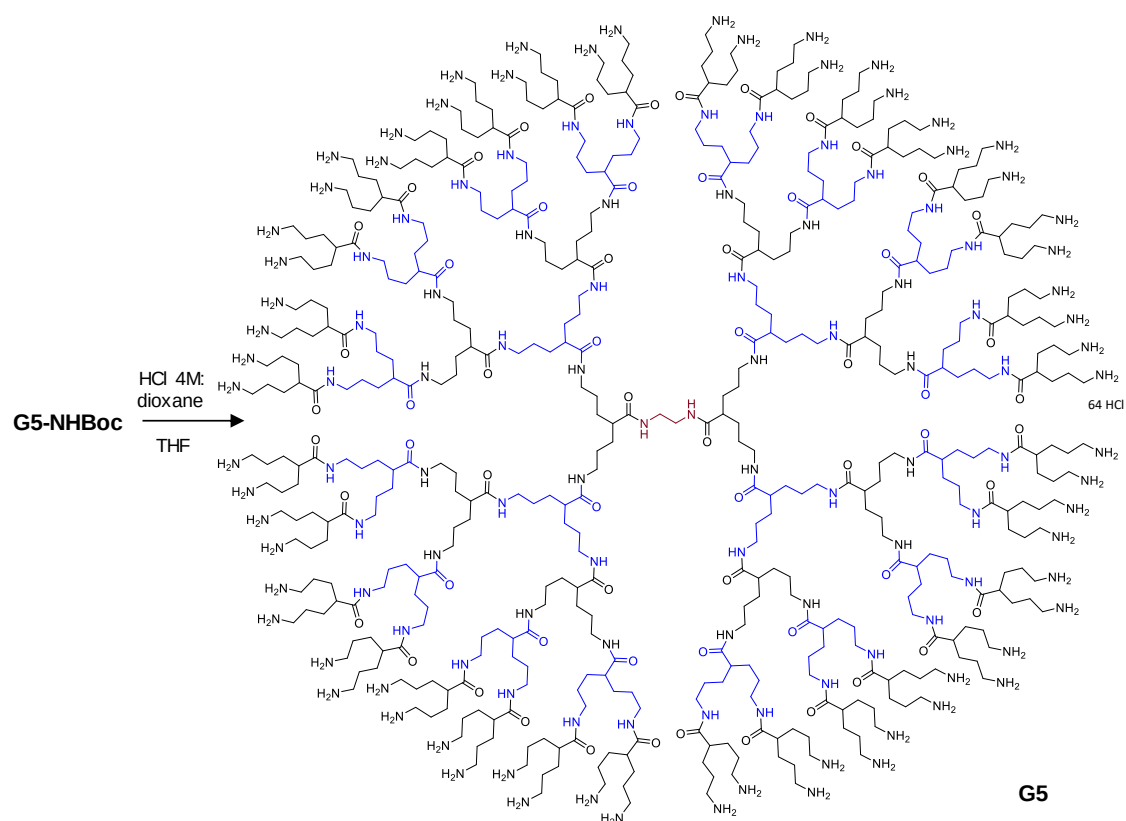
Synthesis of G5-NHBoc



G4 (600 mg, 0.10 mmol) in methanol (10 mL) was treated with Amberlyst A-26 resin (1.60 g) for one hour. The obtained compound, **1** (1.73 g, 3.52 mmol, 35.2 eq) and *N*-methylmorpholine (529 μ L, 4.80 mmol, 48 eq) were solved in anhydrous DMF (60 mL) under nitrogen atmosphere. The mixture of reaction was stirred at room temperature for fourteen days. After four and eight days, the reaction was refreshed with the same amount of **1** and *N*-methylmorpholine. **G5-NHBoc** (1.44 g, 0.09 mmol, 90 %) was obtained as a yellow pale solid after precipitation (product was dissolved in the minimum amount of dichloromethane and precipitated in hexane).

¹H-NMR (400 MHz, DMSO-*d*₆) δ ppm: 8.05 – 7.67 (m, 64 H), 6.81 – 6.68 (m, 62 H), 3.11 – 2.93 (m, 124 H), 2.90 – 2.81 (m, 128 H), 2.15 – 2.01 (m, 62 H), 1.39 – 1.16 (m, 1072 H). **¹³C-NMR** (100 MHz, DMSO-*d*₆) δ ppm: 174.6, 174.5, 155.6, 77.3, 45.2, 39.5 (with DMSO-*d*₆ signal), 38.3, 29.9, 28.3, 27.7, 27.3.

Synthesis of G5



The deprotection of amine groups of **G5-NHBoc** (1.77 g, 0.11 mmol) gave the product (1.30 g, quantitative) as a yellow pale foamy solid.

¹H-NMR (400 MHz, DMSO-*d*₆) δ ppm: 8.42 - 8.02 (m, 190 H), 3.17 – 2.86 (m, 124 H), 2.86 – 2.66 (m, 128 H), 2.36 – 2.13 (m, 62 H), 1.64 – 1.10 (m, 496 H). **¹³C-NMR** (100 MHz, DMSO-*d*₆) δ ppm: 175.1, 174.5, 174.0, 45.0, 44.5, 44.0, 39.5 (with DMSO-*d*₆ signal), 38.6, 29.9, 29.2, 27.2, 24.7, 22.6.

2.- NMR spectra

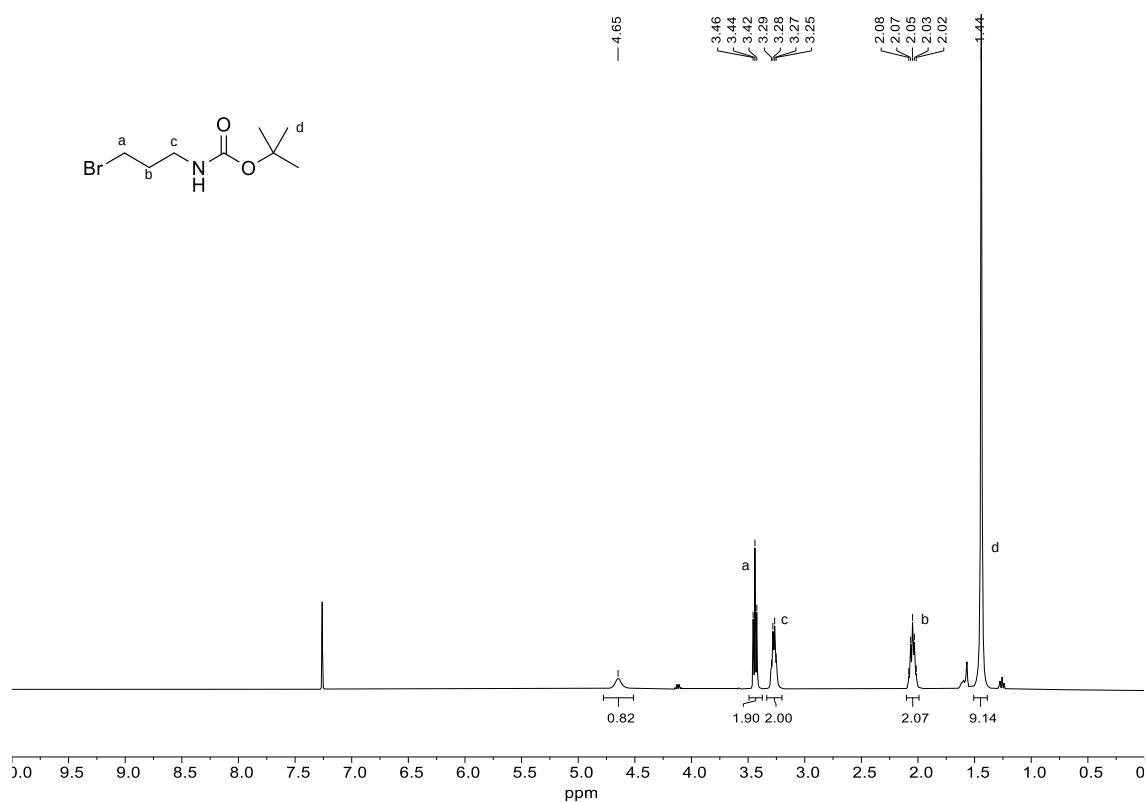


Figure S1. ¹H NMR spectrum of *tert*-butyl (3-bromopropyl)carbamate in CDCl₃.

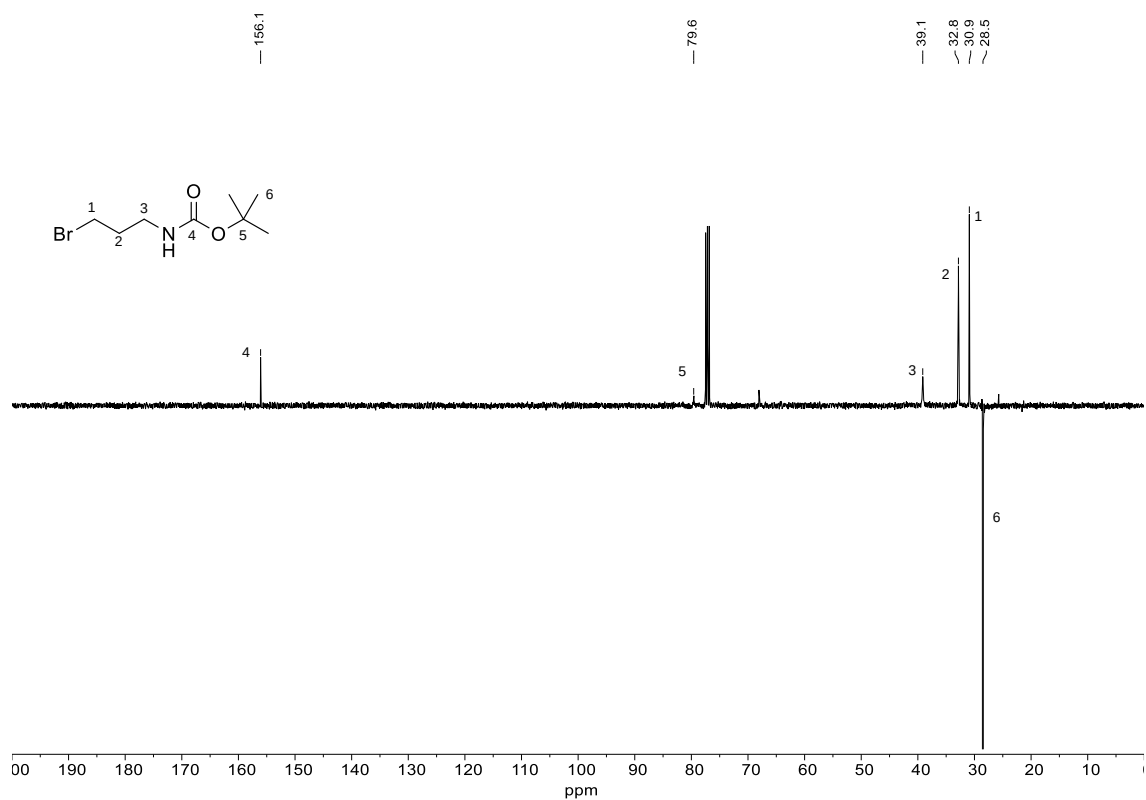
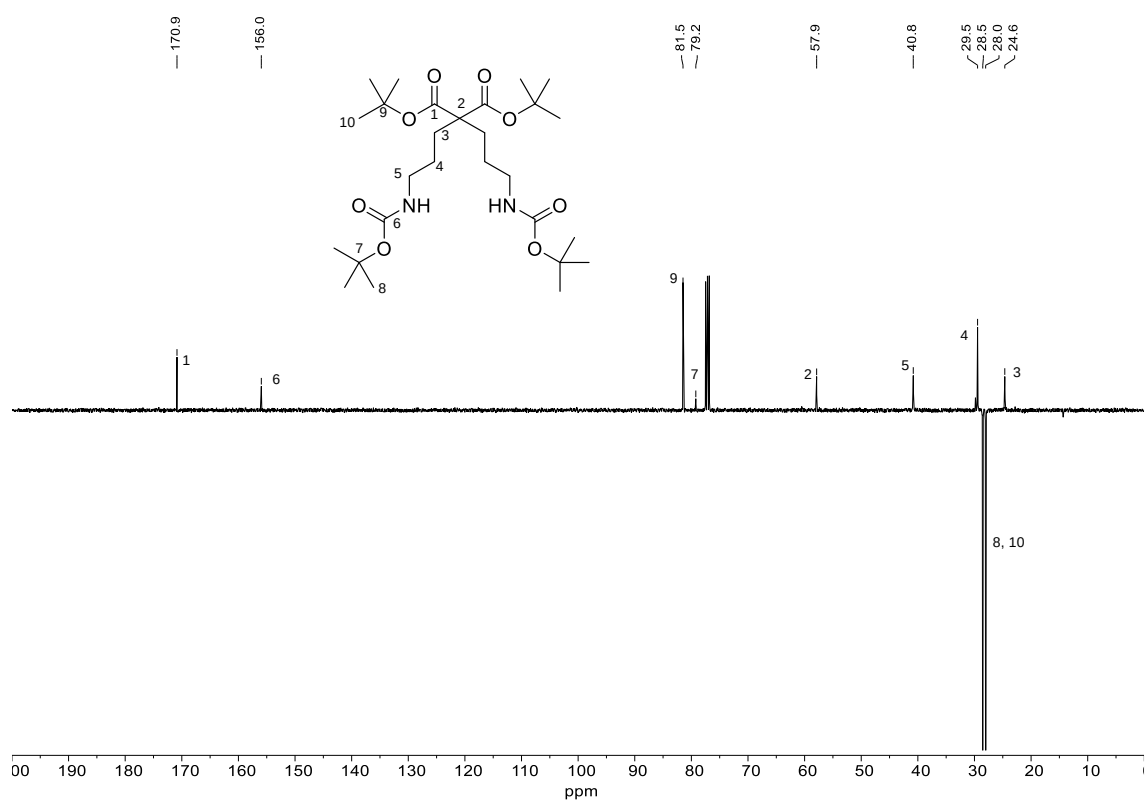
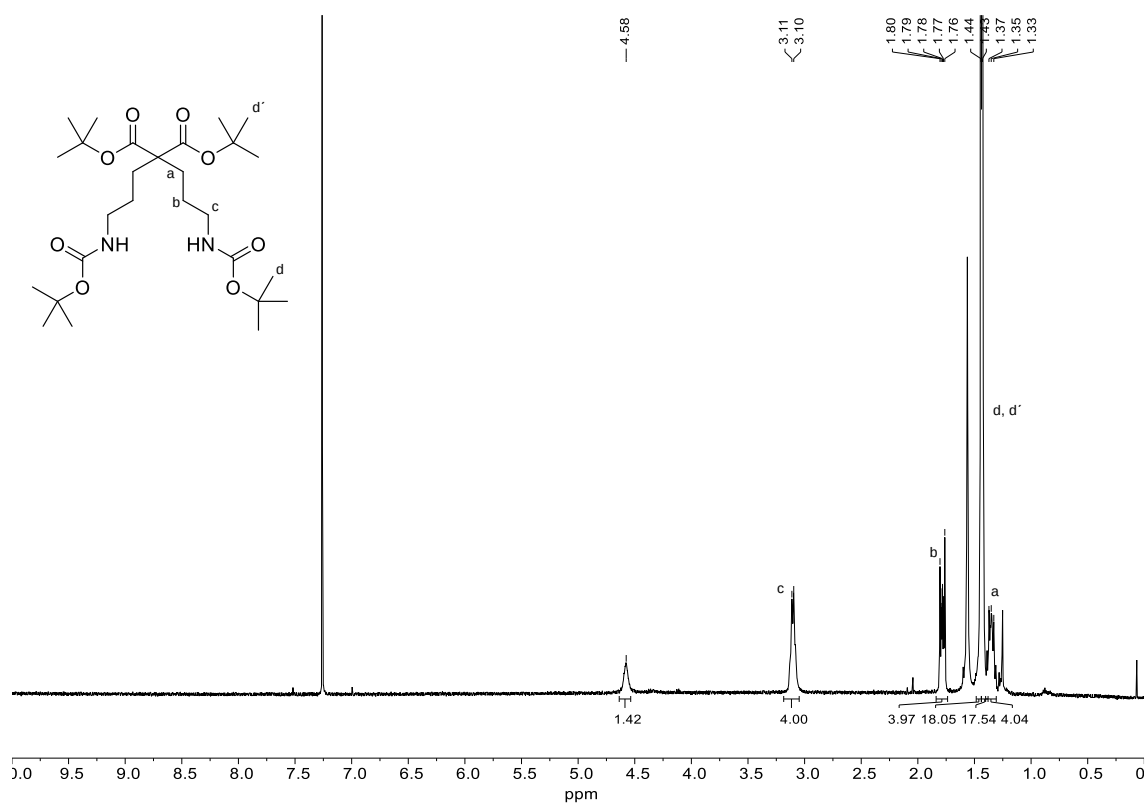


Figure S2. ¹³C NMR (SEFT) spectrum of *tert*-butyl (3-bromopropyl)carbamate in CDCl₃.



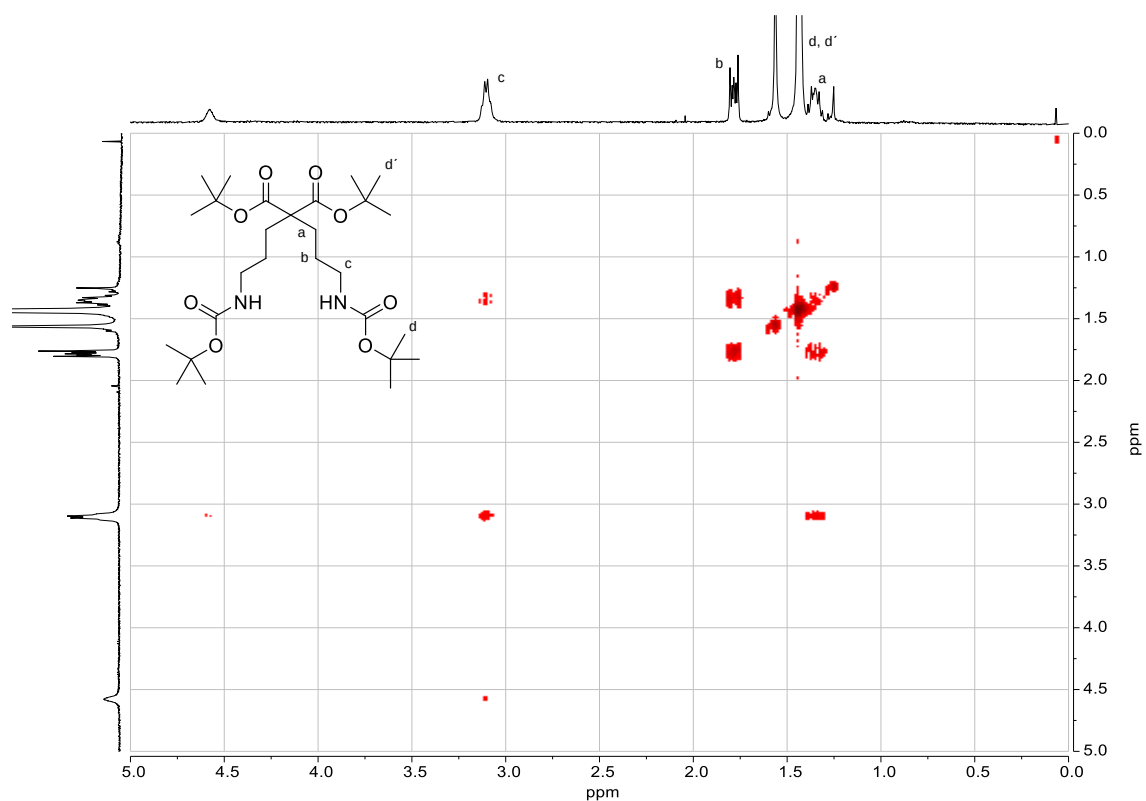


Figure S5. COSY spectrum of **di-*tert*-butyl 2,2-bis(3((*tert*-butoxycarbonyl)amino)propylmalonate** in CDCl_3

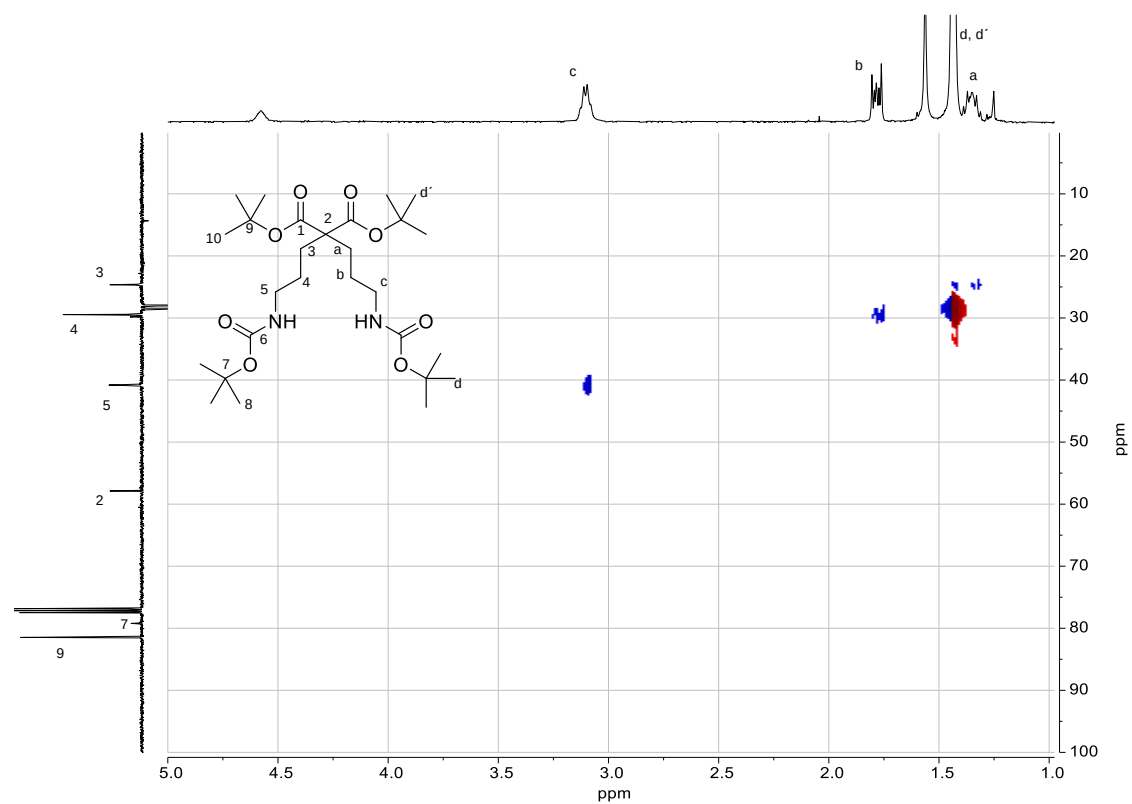


Figure S6. HSQC spectrum of **di-*tert*-butyl 2,2-bis(3((*tert*-butoxycarbonyl)amino)propylmalonate** in CDCl_3

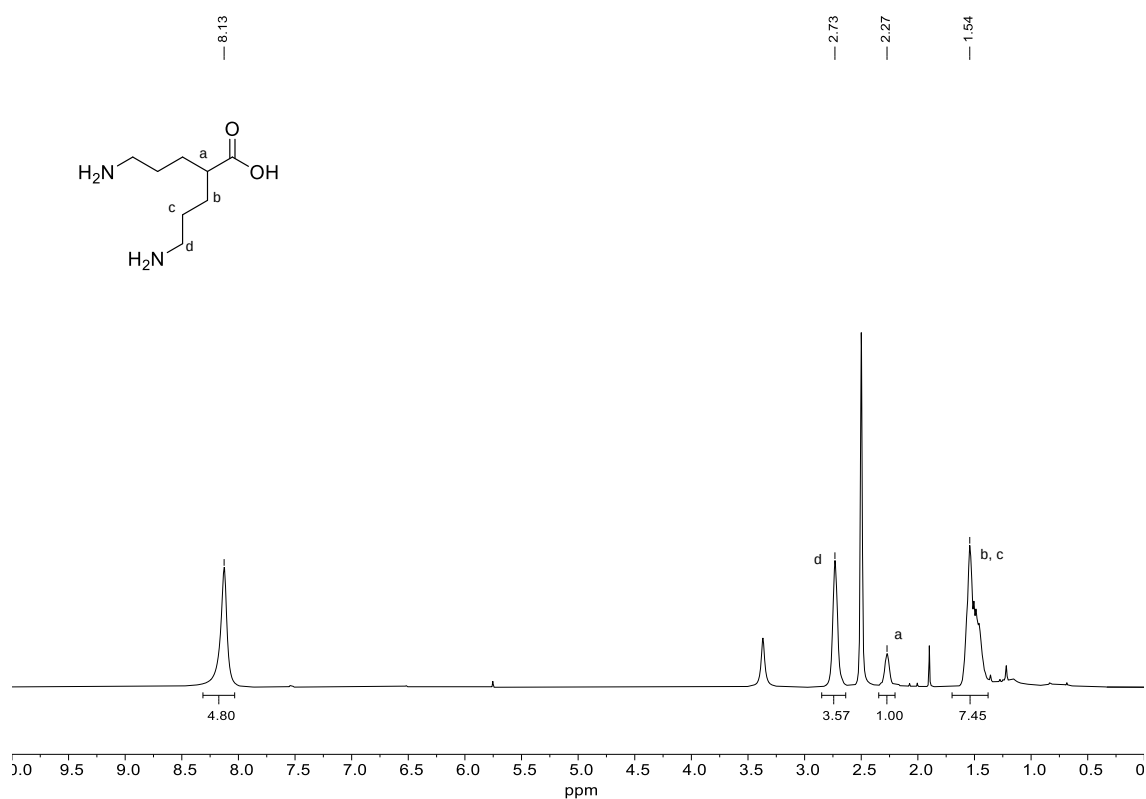


Figure S7. ¹H NMR spectrum of 5-amino-2-(3-aminopropyl) pentanoic acid in DMSO-*d*₆.

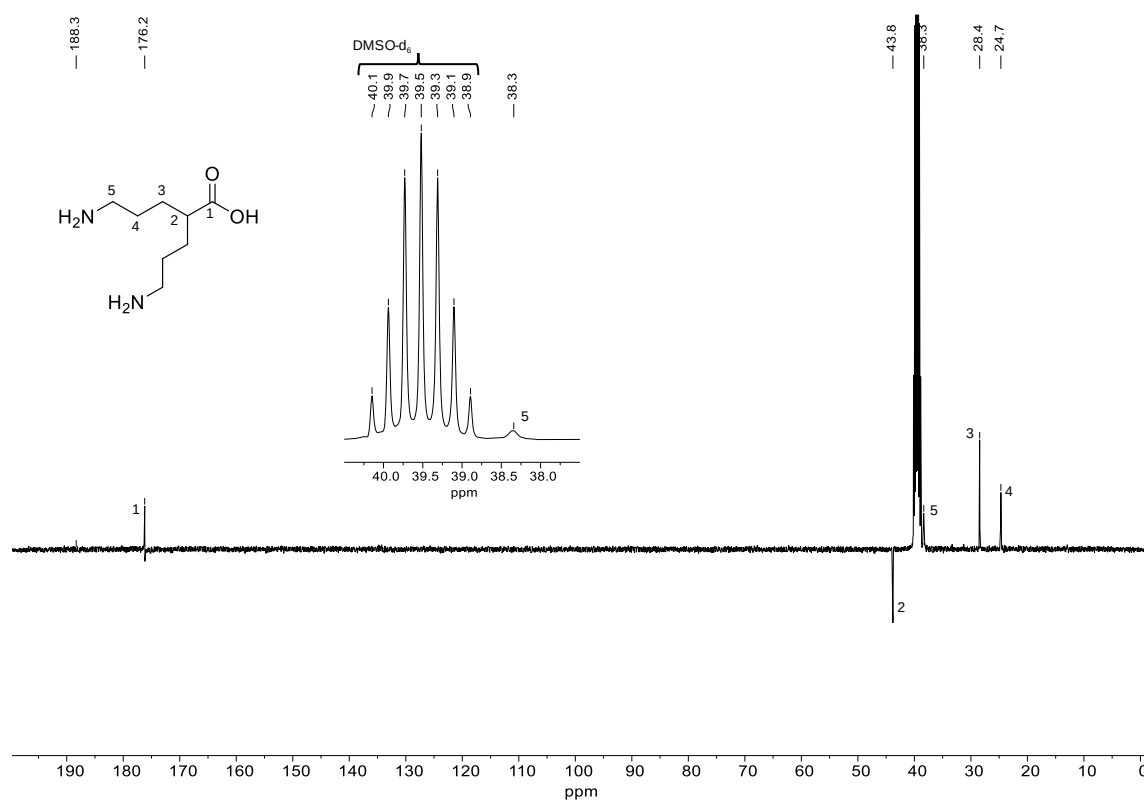


Figure S8. ¹³C NMR (SEFT) spectrum of 5-amino-2-(3-aminopropyl) pentanoic acid in DMSO-*d*₆.

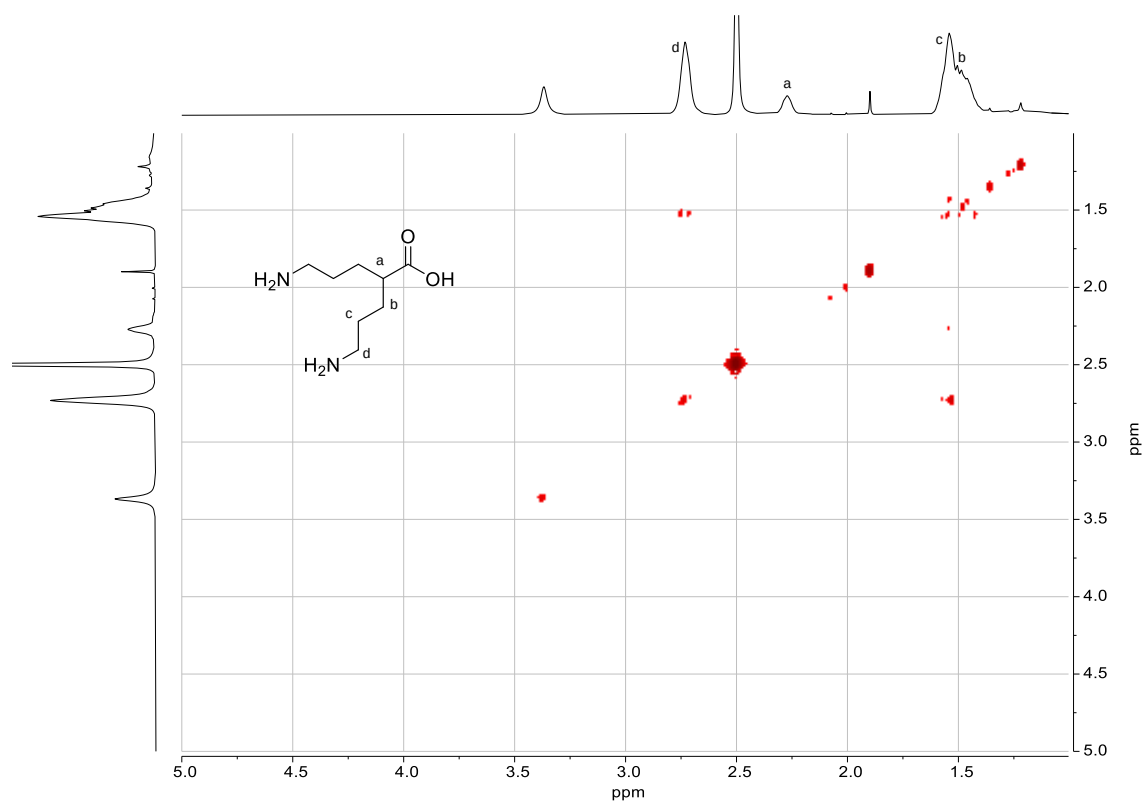


Figure S9. COSY spectrum of 5-amino-2-(3-aminopropyl) pentanoic acid in DMSO- d_6 .

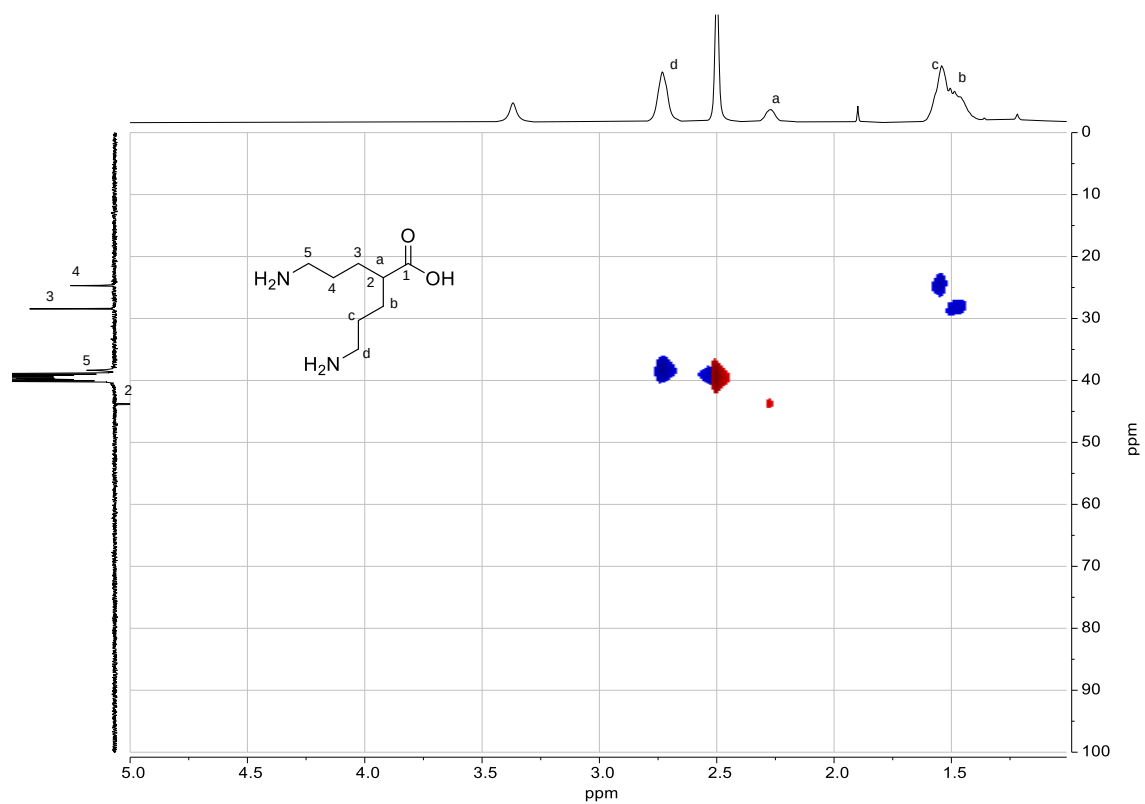


Figure S10. HSQC spectrum of 5-amino-2-(3-aminopropyl) pentanoic acid in DMSO- d_6 .

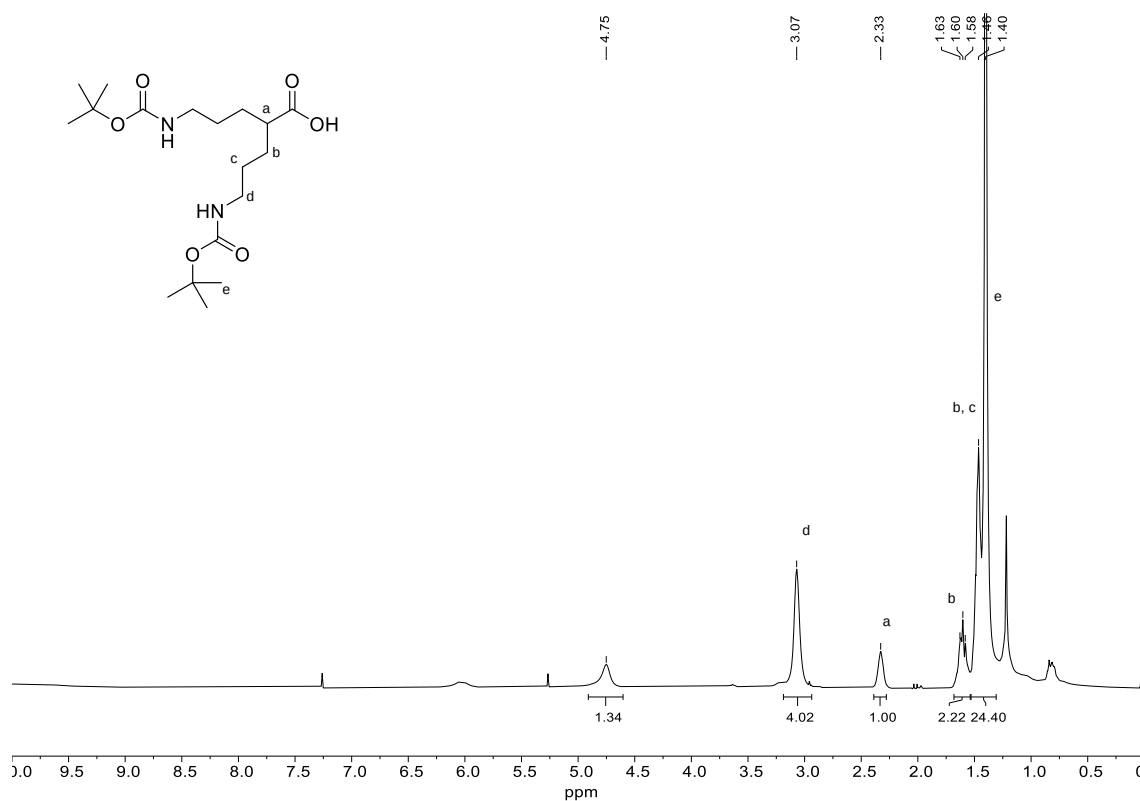


Figure S11. ¹H NMR spectrum of 5-((*tert*-butoxycarbonyl)amino)-2-(3-(*tert*-butoxycarbonyl)amino)propylpentanoic acid in CDCl₃.

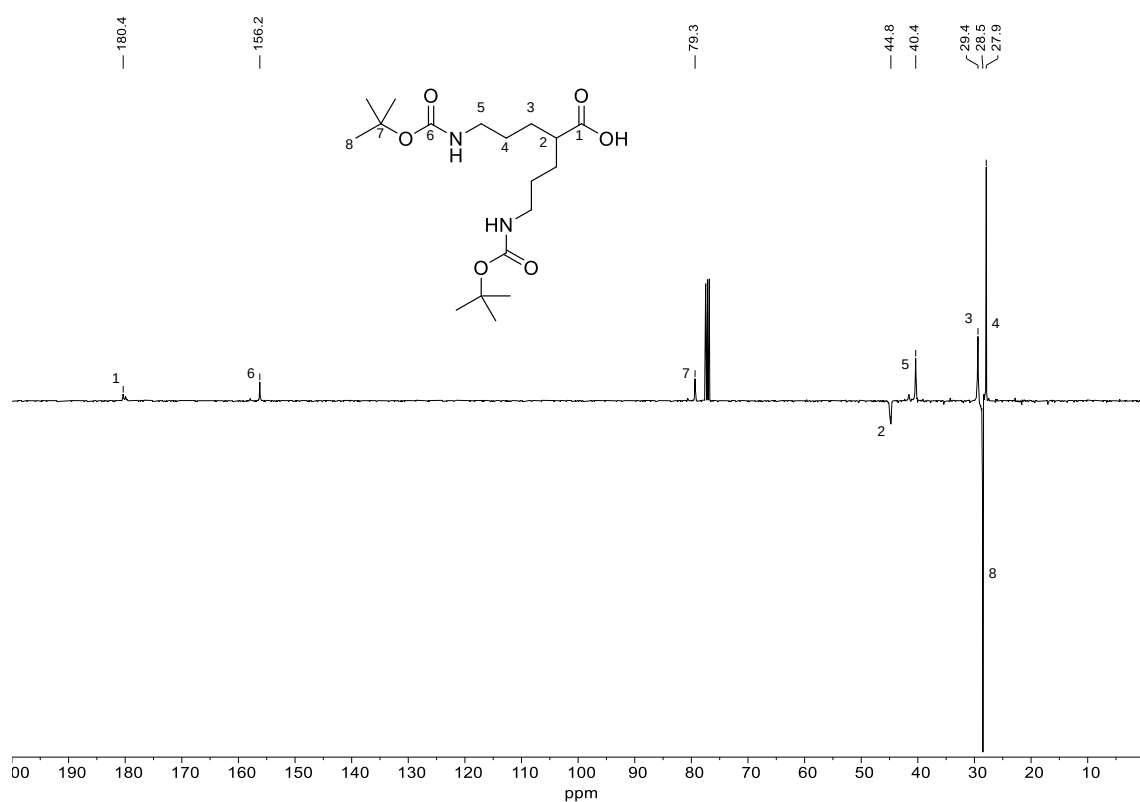


Figure S12. ¹³C NMR (SEFT) spectrum of 5-((*tert*-butoxycarbonyl)amino)-2-(3-(*tert*-butoxycarbonyl)amino)propylpentanoic acid in CDCl₃.

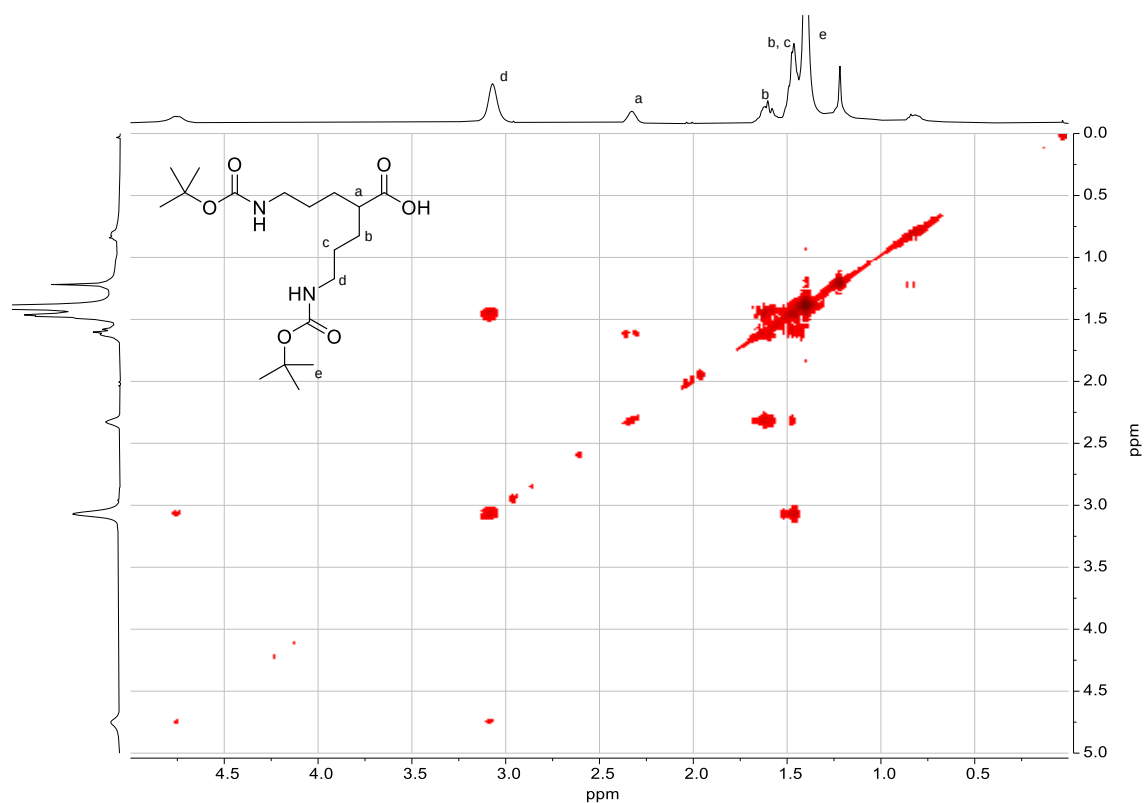


Figure S13. COSY spectrum of 5-((*tert*-butoxycarbonyl)amino)-2-(3-(*tert*-butoxycarbonyl)amino)propyl)pentanoic acid in CDCl₃.

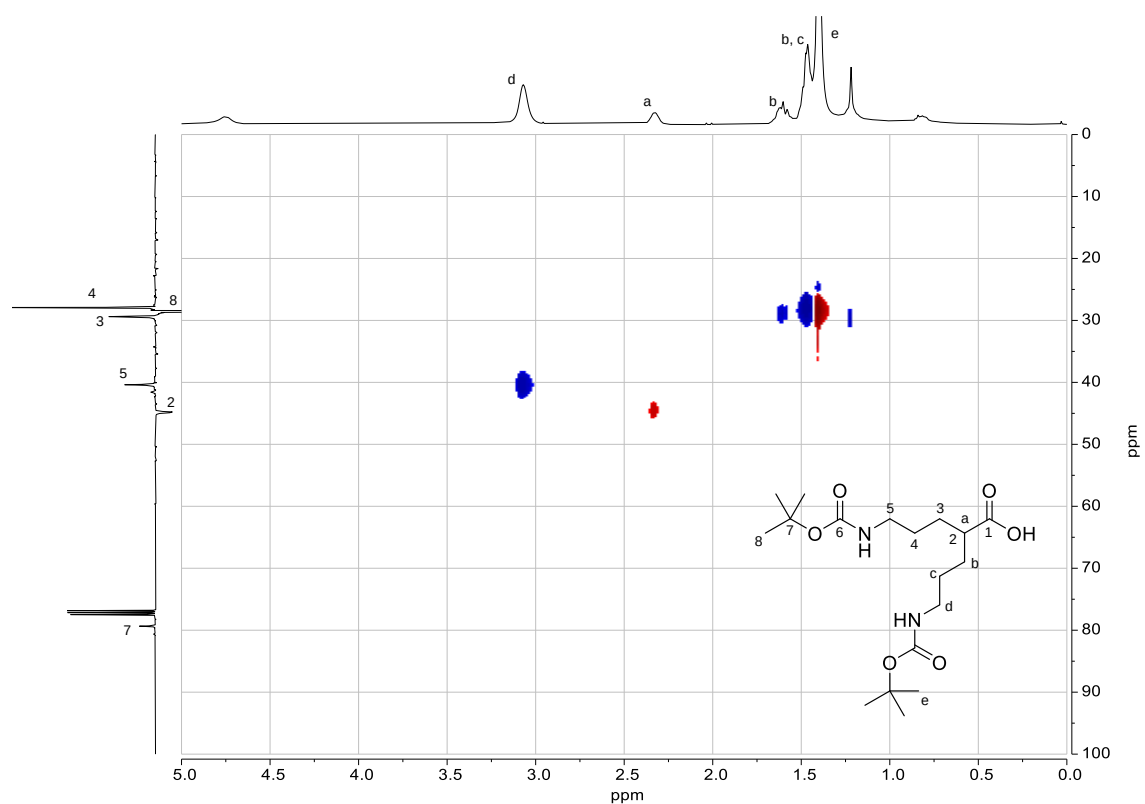


Figure S14. HSCQ spectrum of 5-((*tert*-butoxycarbonyl)amino)-2-(3-(*tert*-butoxycarbonyl)amino)propyl)pentanoic acid in CDCl₃.

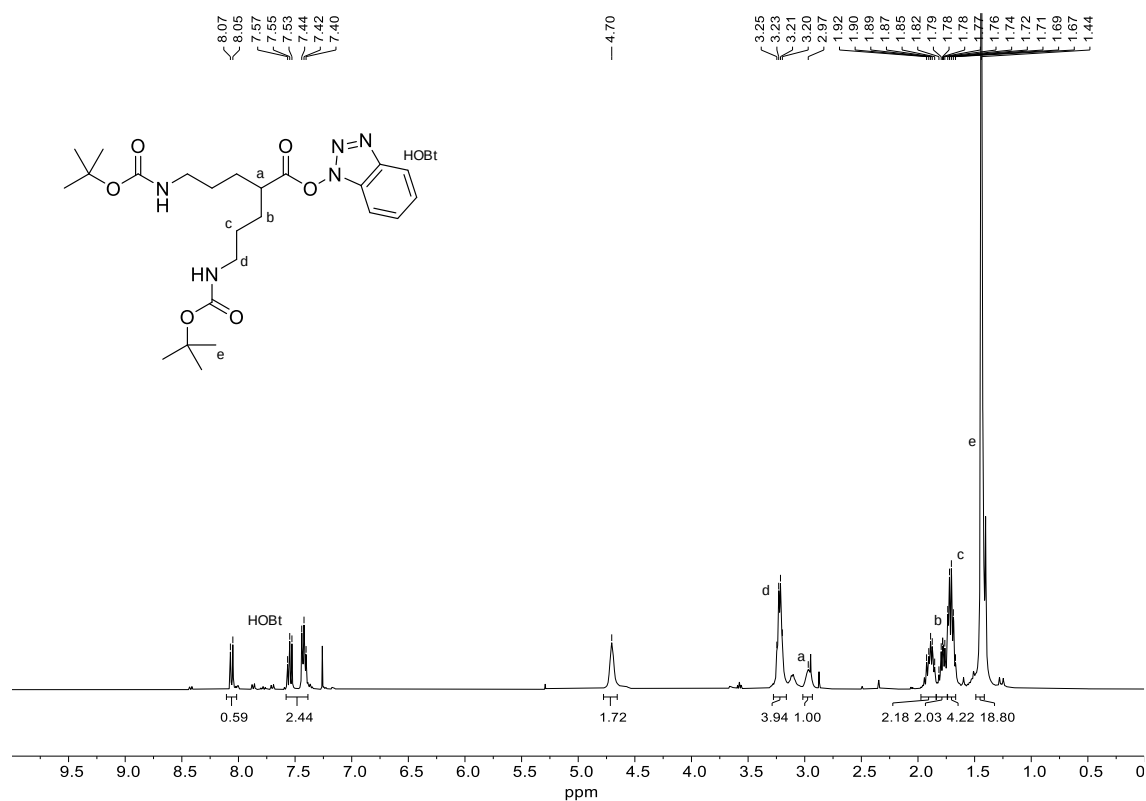


Figure S15. ¹H NMR spectrum of **1** in CDCl₃.

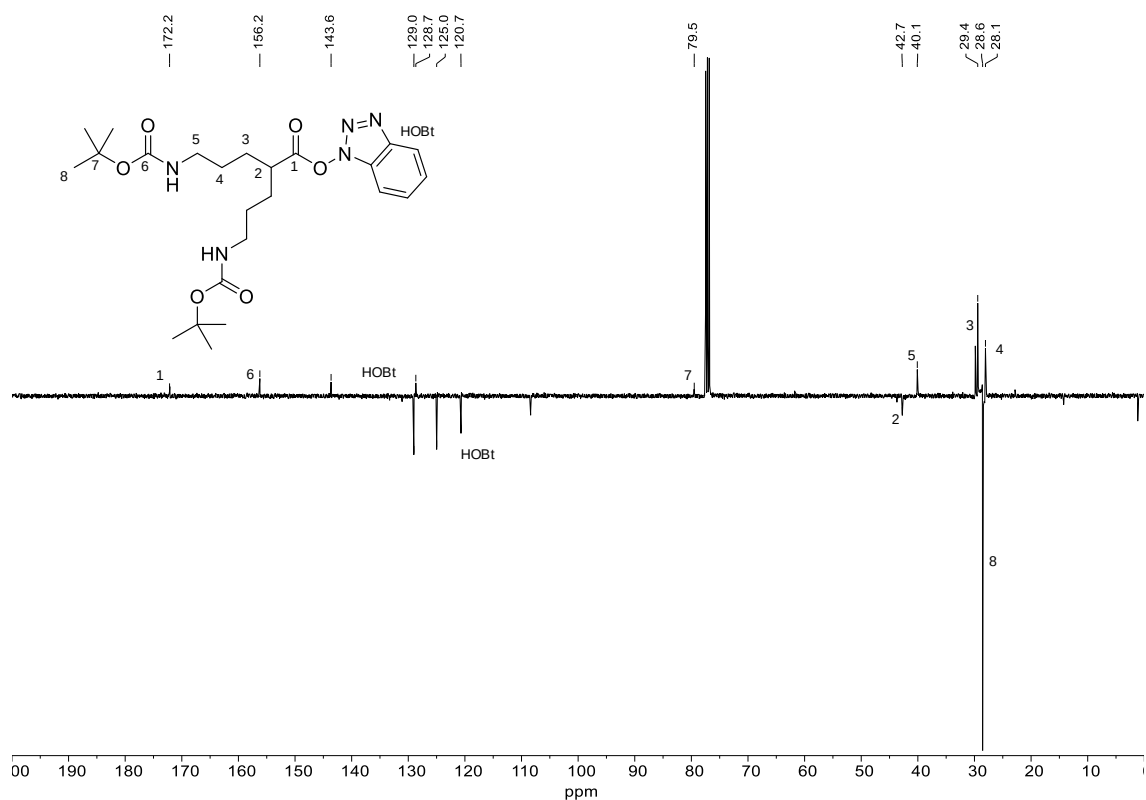
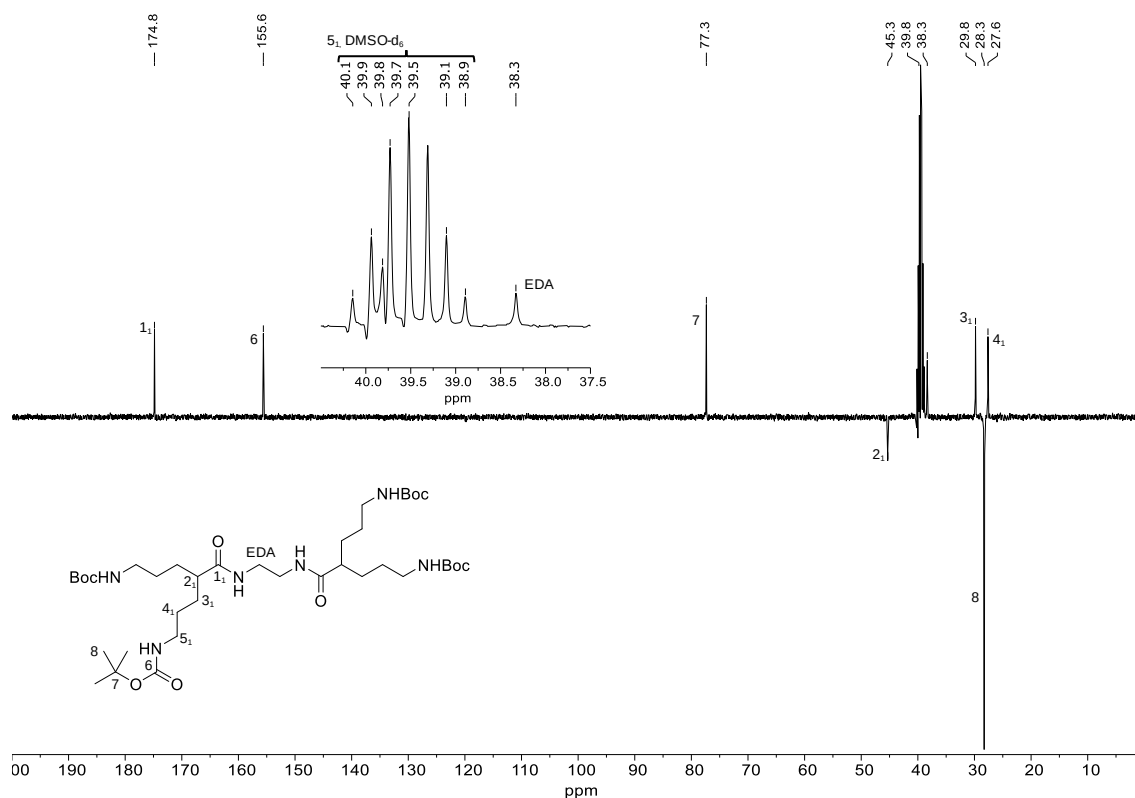
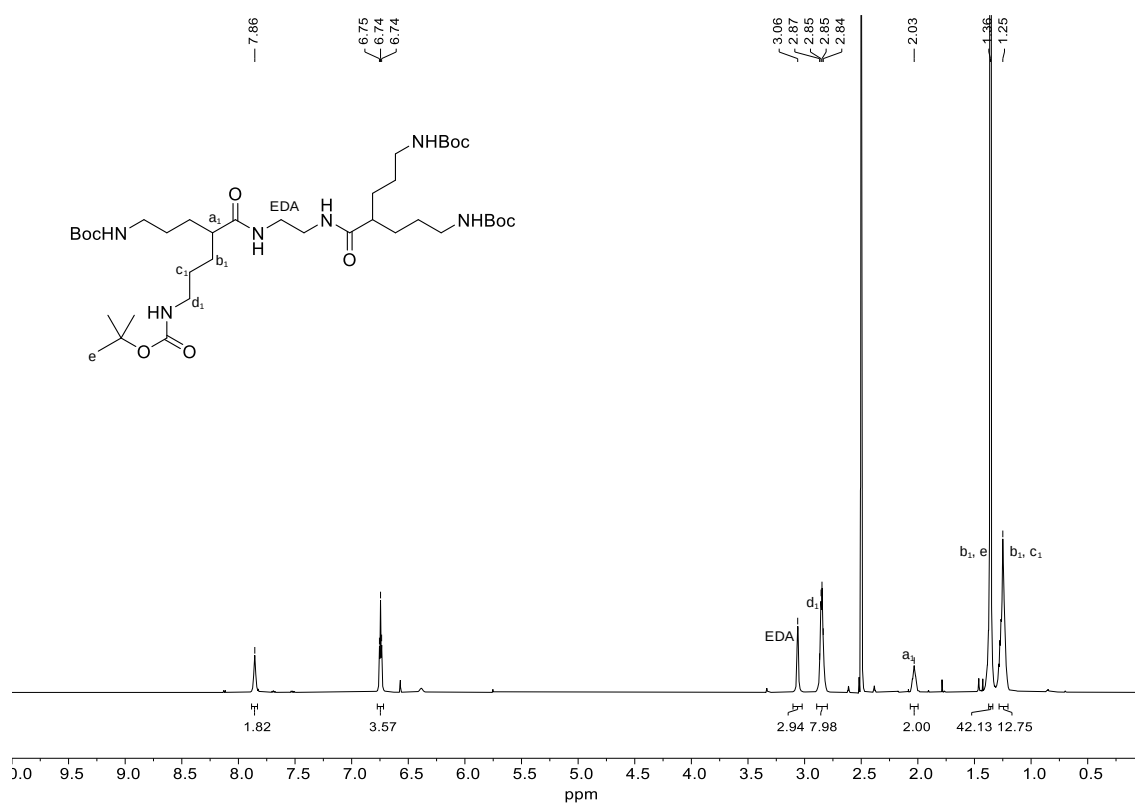


Figure S16. ¹³C NMR (SEFT) spectrum of **1** in CDCl₃.



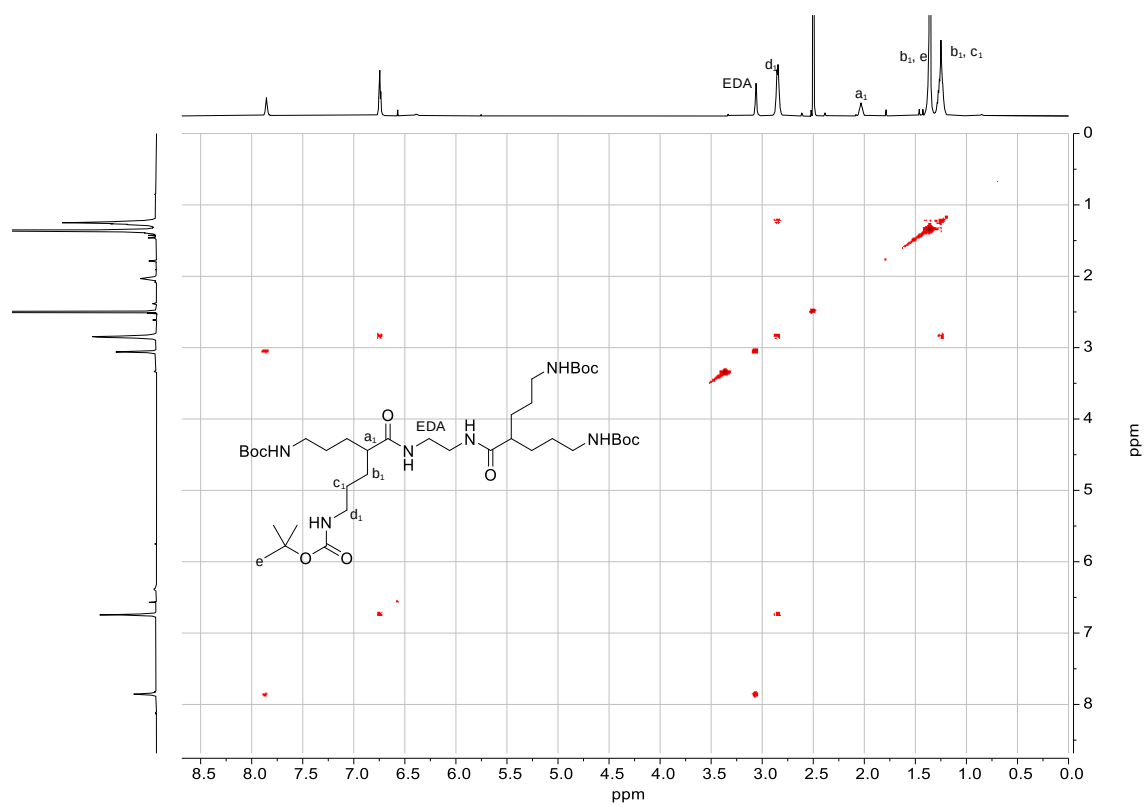


Figure S19. COSY spectrum of **G1-NHBoc** in DMSO- d_6 .

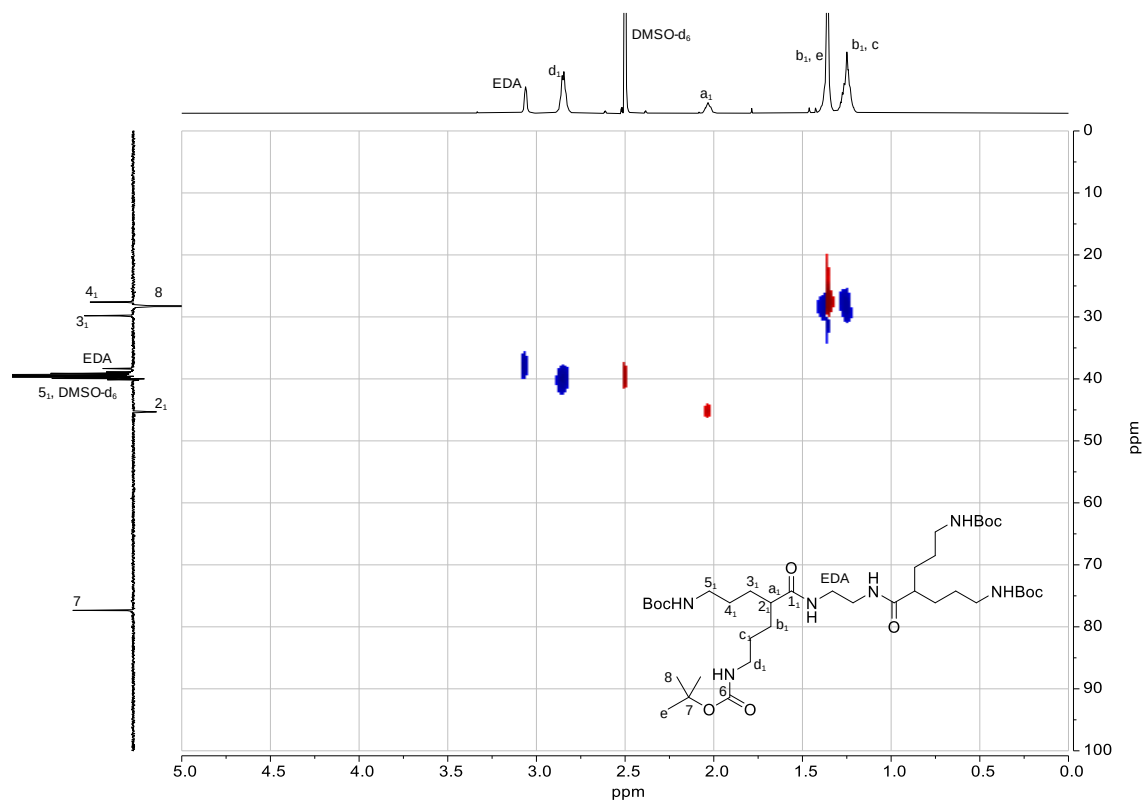
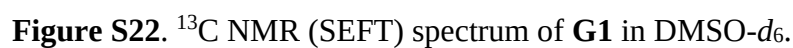


Figure S20. HSQC spectrum of **G1-NHBoc** in DMSO- d_6 .



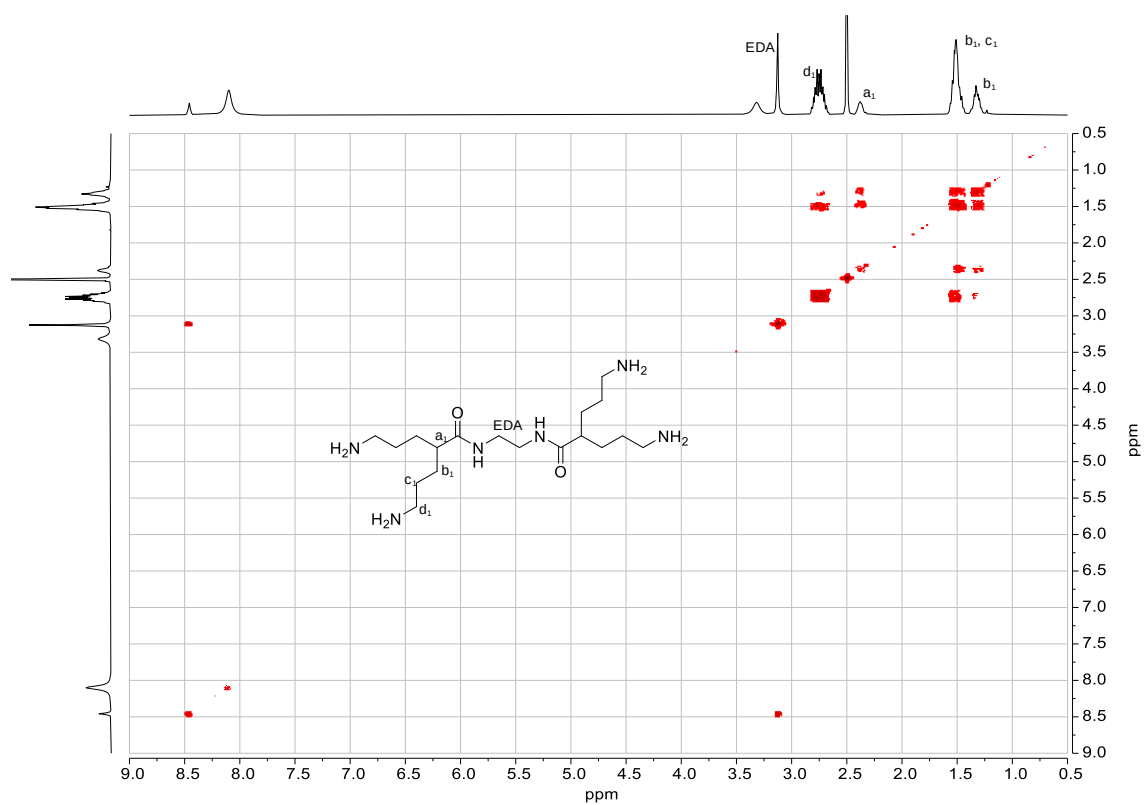


Figure S23. COSY spectrum of **G1** in DMSO- d_6 .

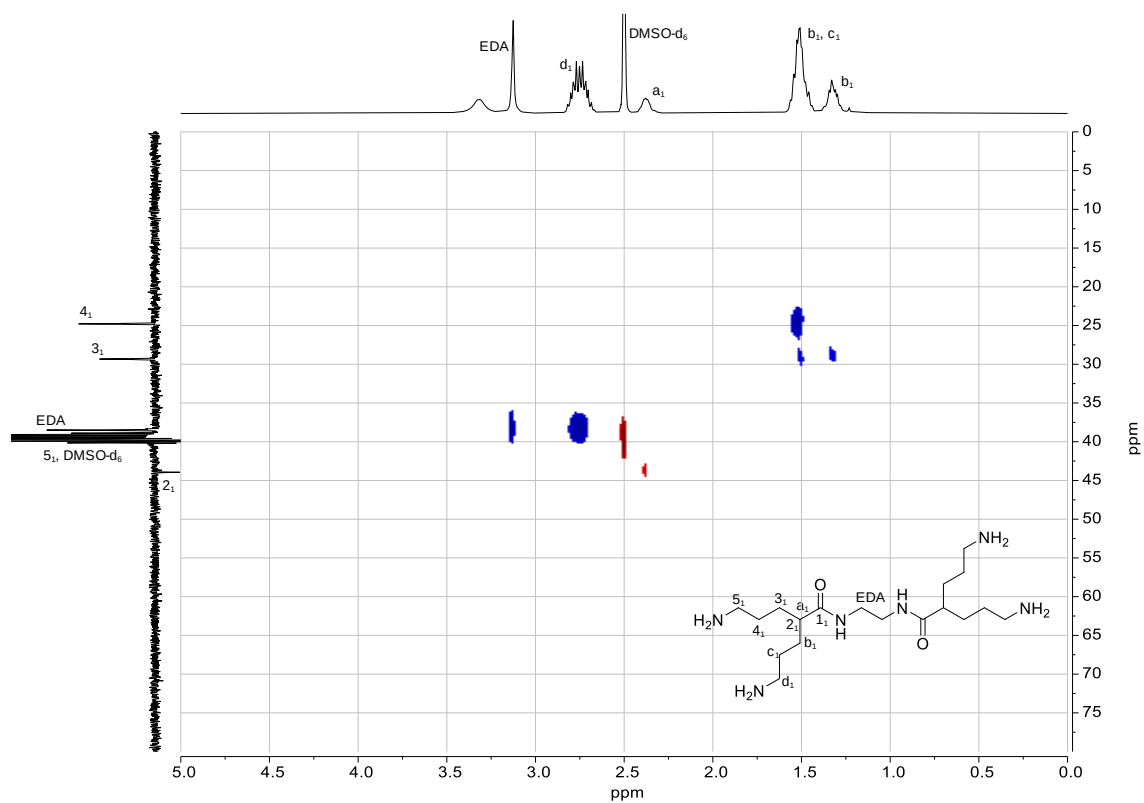


Figure S24. HSQC spectrum of **G1** in DMSO- d_6 .

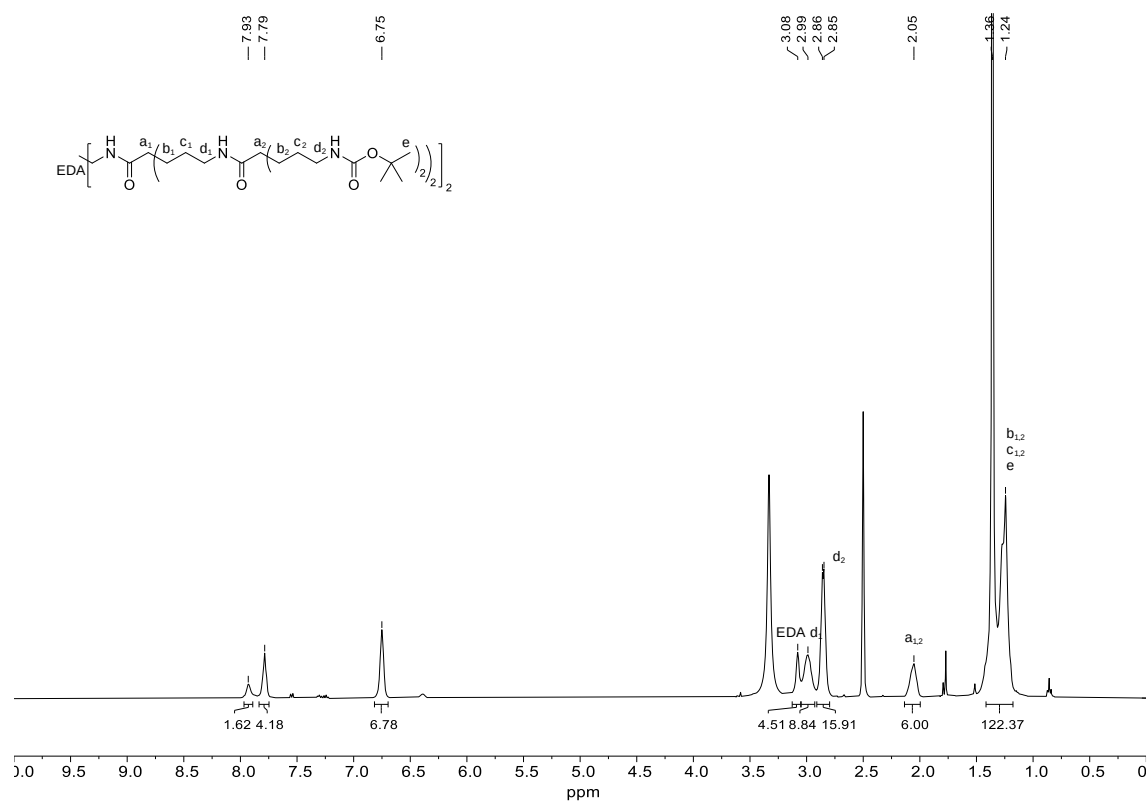


Figure S25. ¹H NMR spectrum of **G2-NHBoc** in DMSO-d₆.

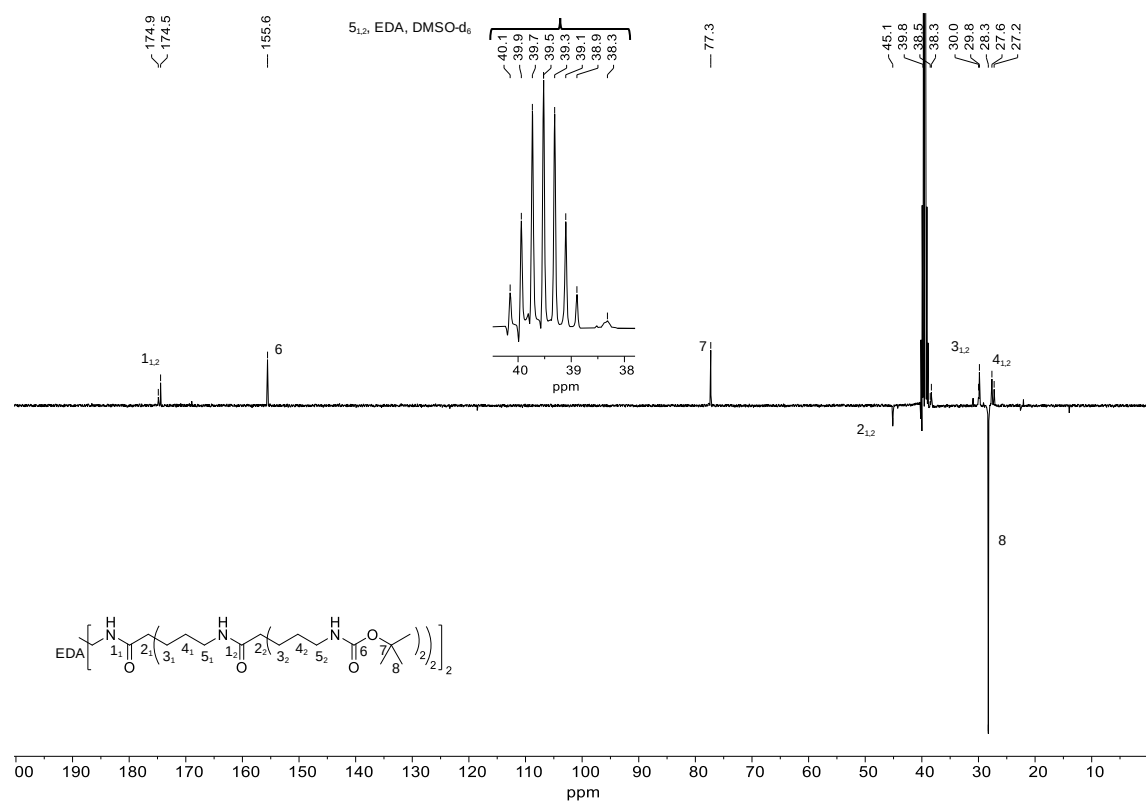


Figure S26. ¹³C NMR (SEFT) spectrum of **G2-NHBoc** in DMSO-d₆.

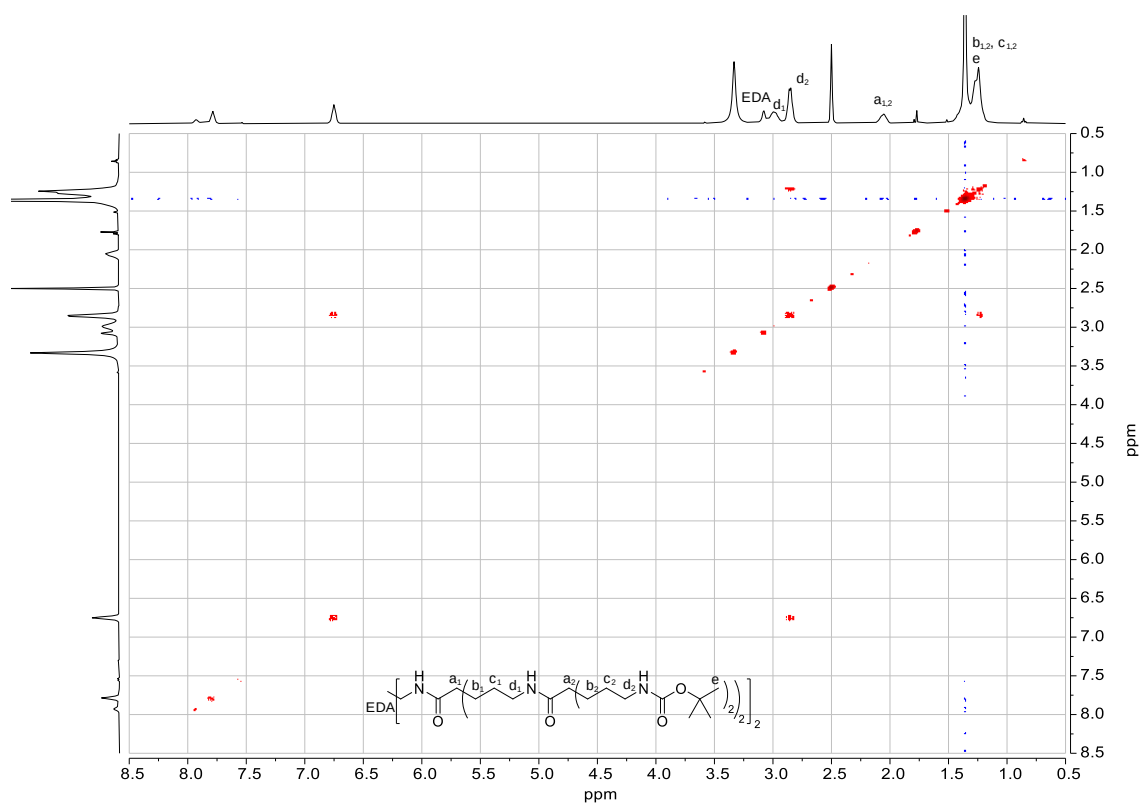


Figure S27. COSY spectrum of **G2-NHBoc** in DMSO- d_6 .

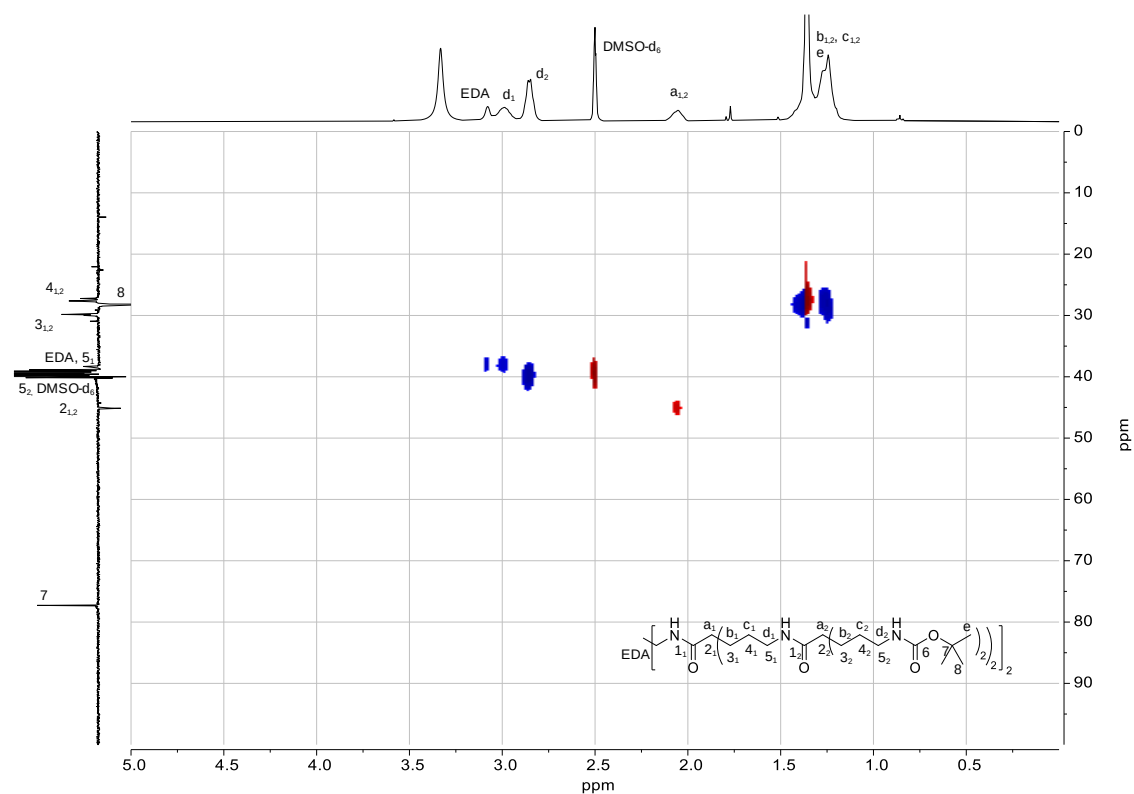


Figure S28. HSQC spectrum of **G2-NHBoc** in DMSO- d_6 .

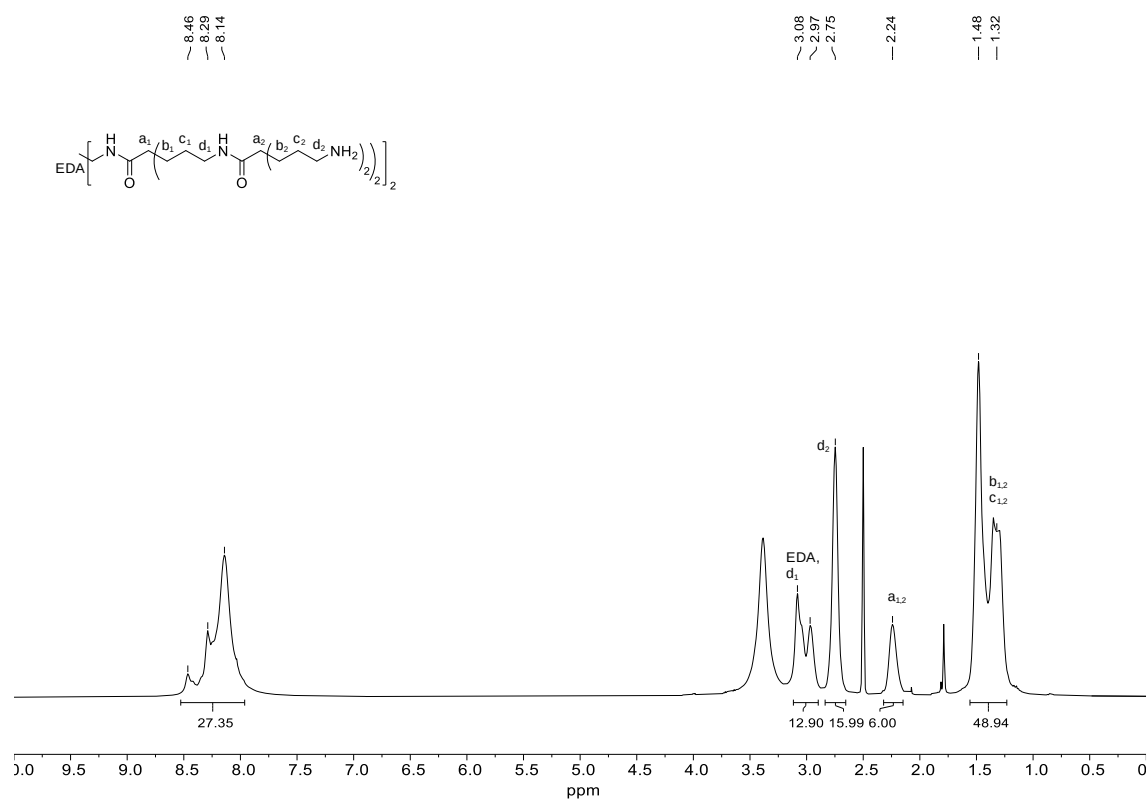


Figure S29. ^1H NMR spectrum of G2 in DMSO- d_6 .

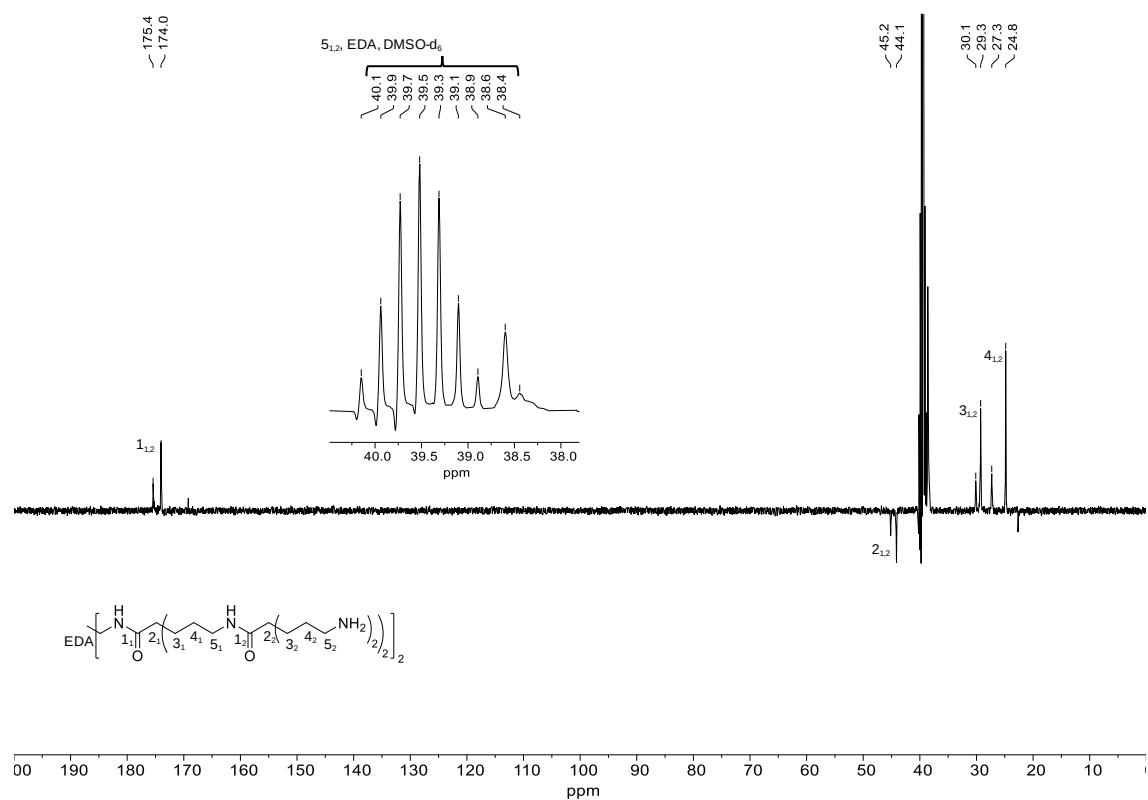


Figure S30. ^{13}C NMR (SEFT) spectrum of G2 in DMSO- d_6 .

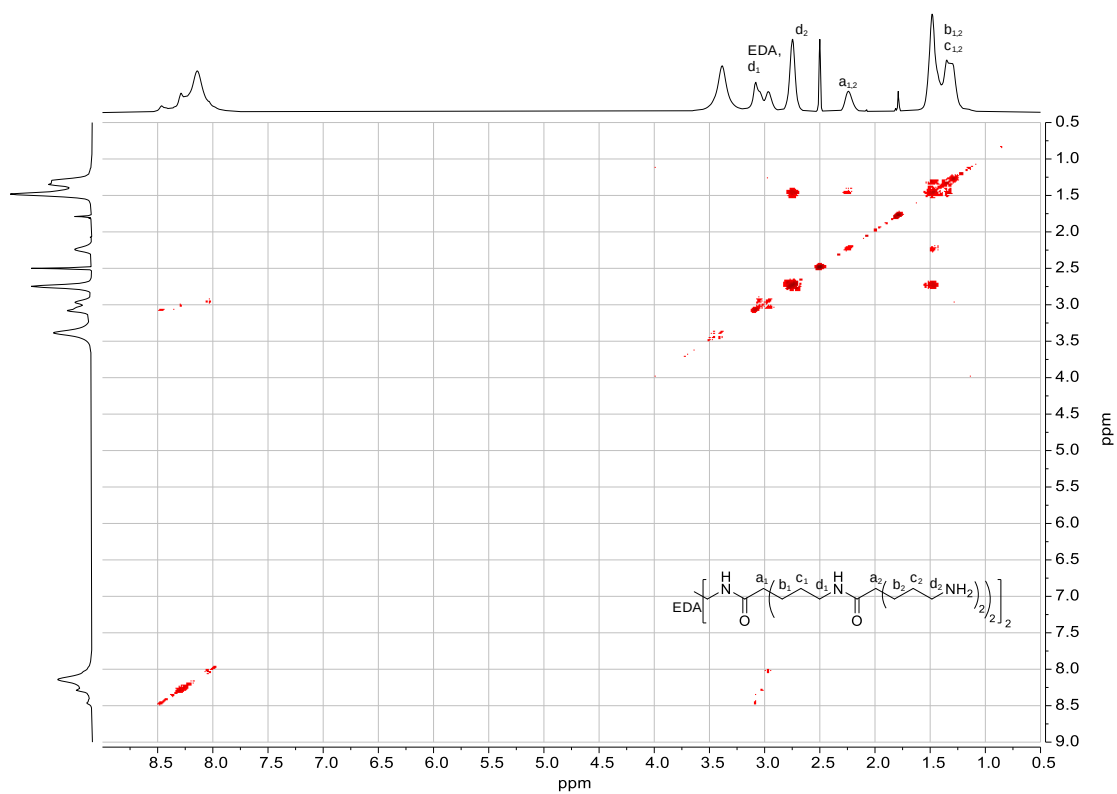


Figure S31. COSY spectrum of **G2** in DMSO- d_6 .

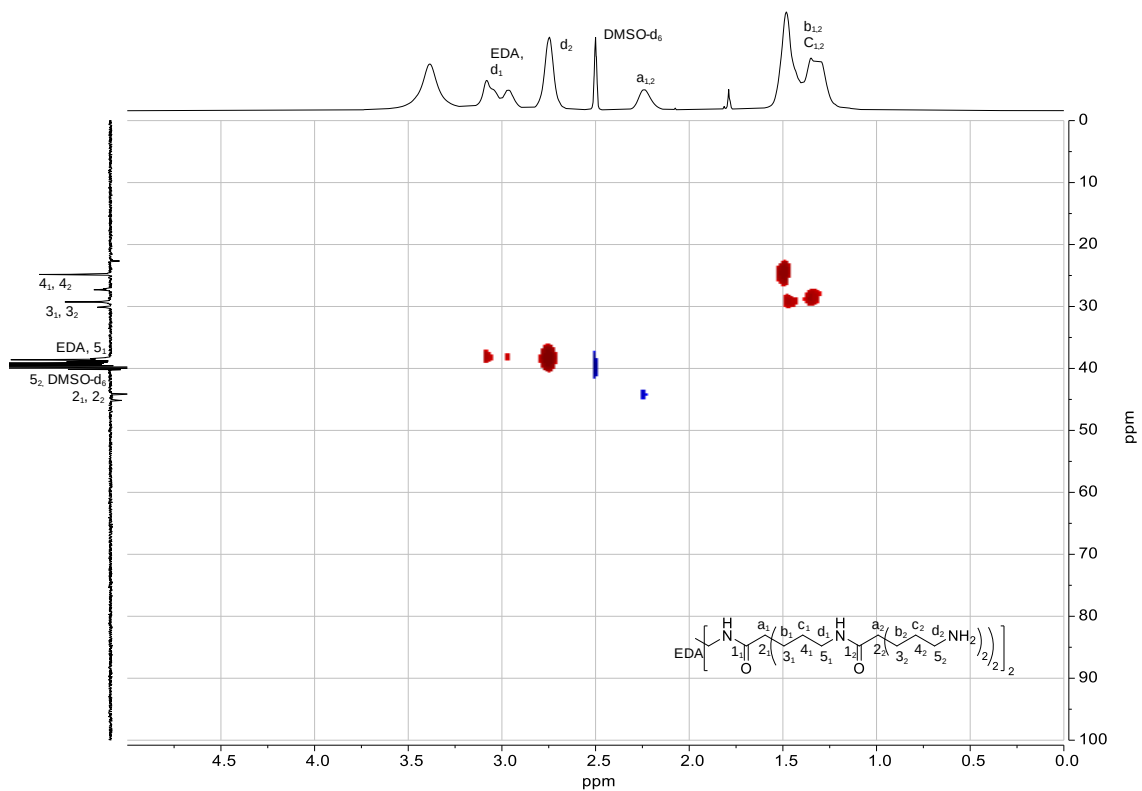


Figure S32. HSQC spectrum of **G2** in DMSO- d_6 .

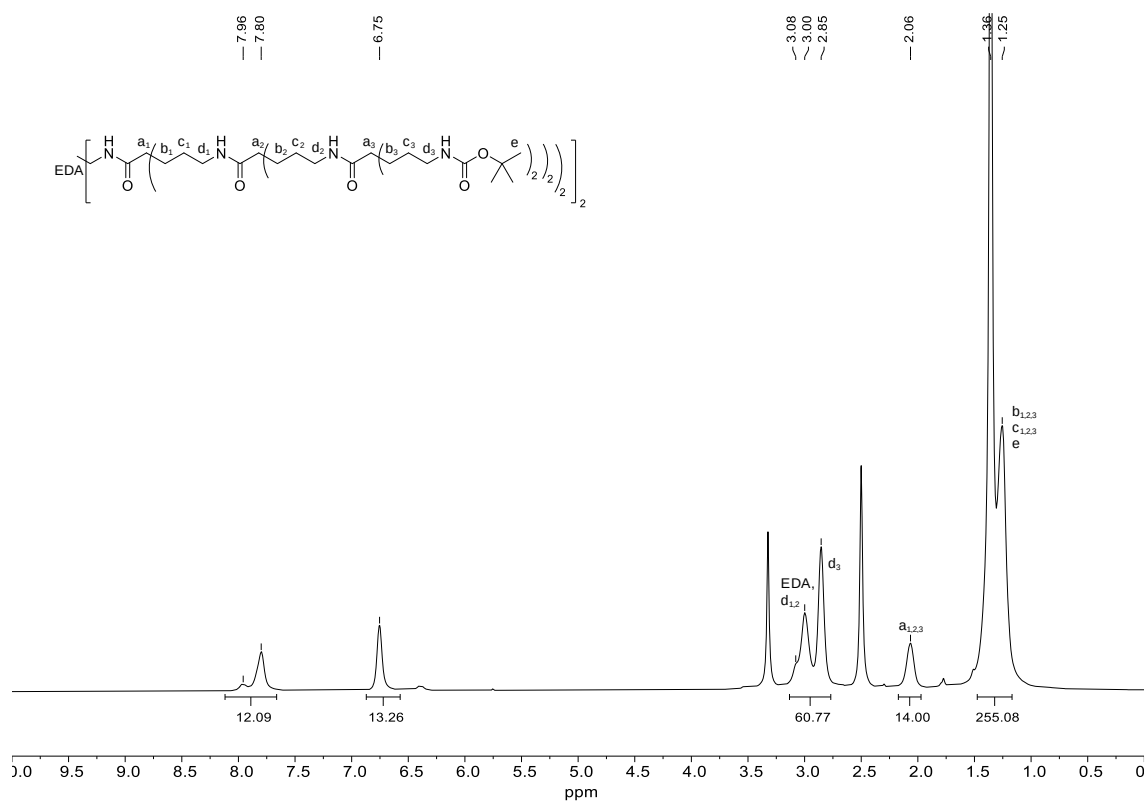


Figure S33. ^1H NMR spectrum of **G3-NHBoc** in DMSO- d_6 .

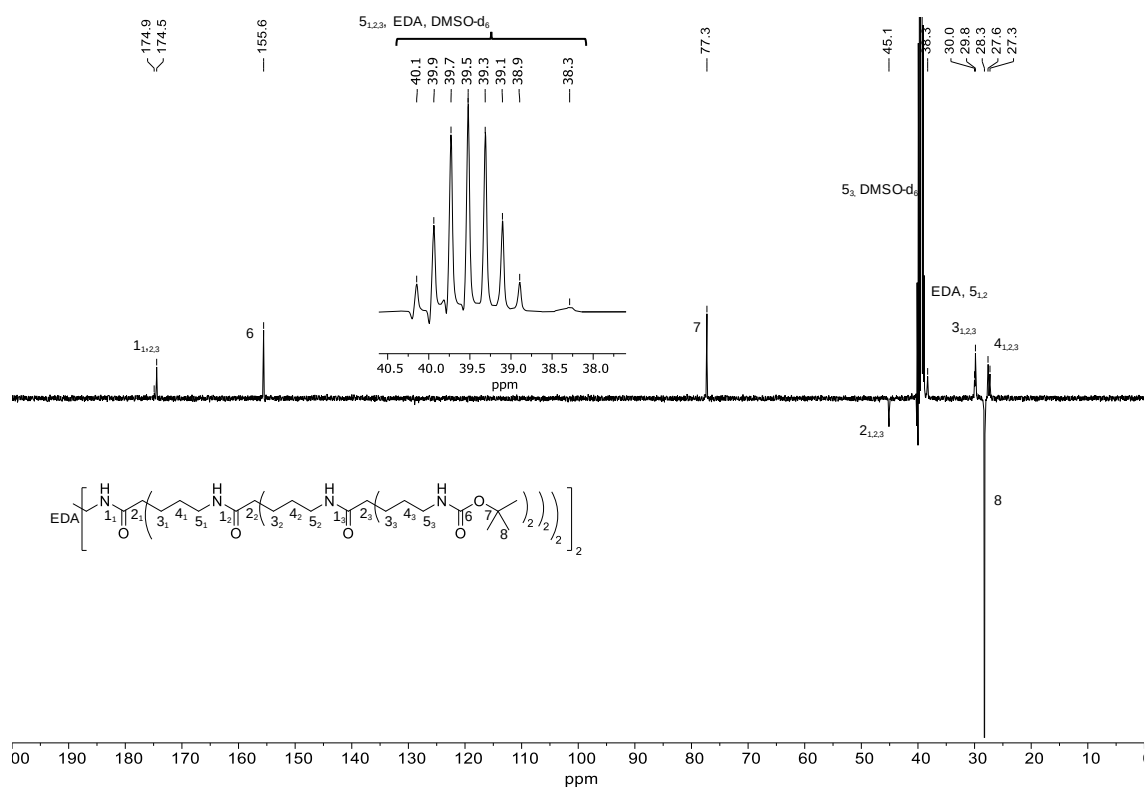


Figure S34. ^{13}C NMR (SEFT) spectrum of **G3-NHBoc** in DMSO- d_6 .

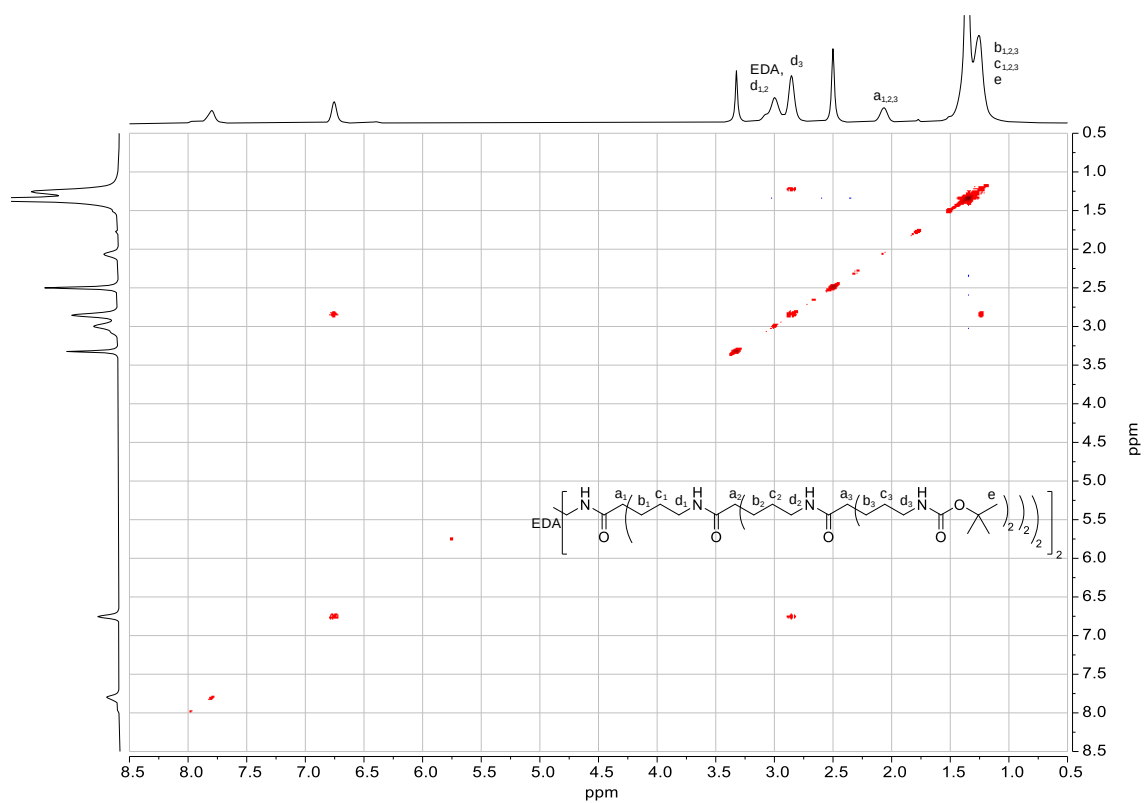


Figure S35. COSY spectrum of G3-NHBoc in DMSO- d_6 .

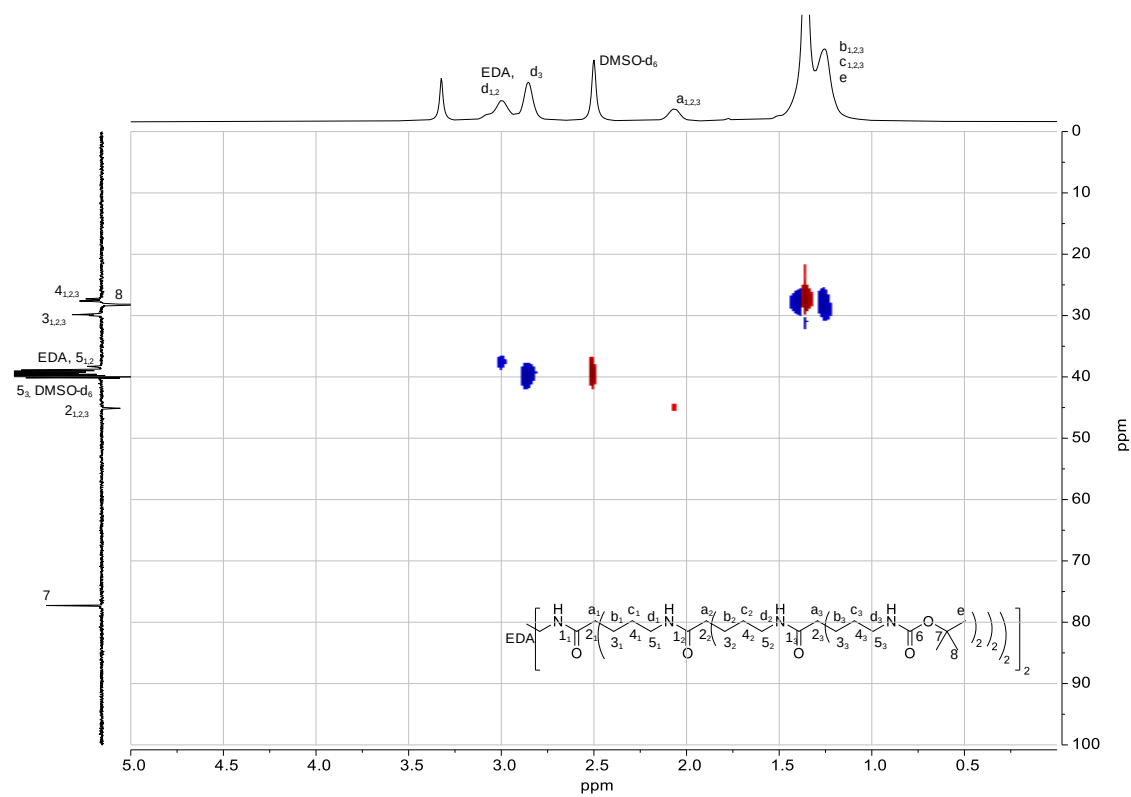


Figure S36. HSQC spectrum of G3-NHBoc in DMSO- d_6 .

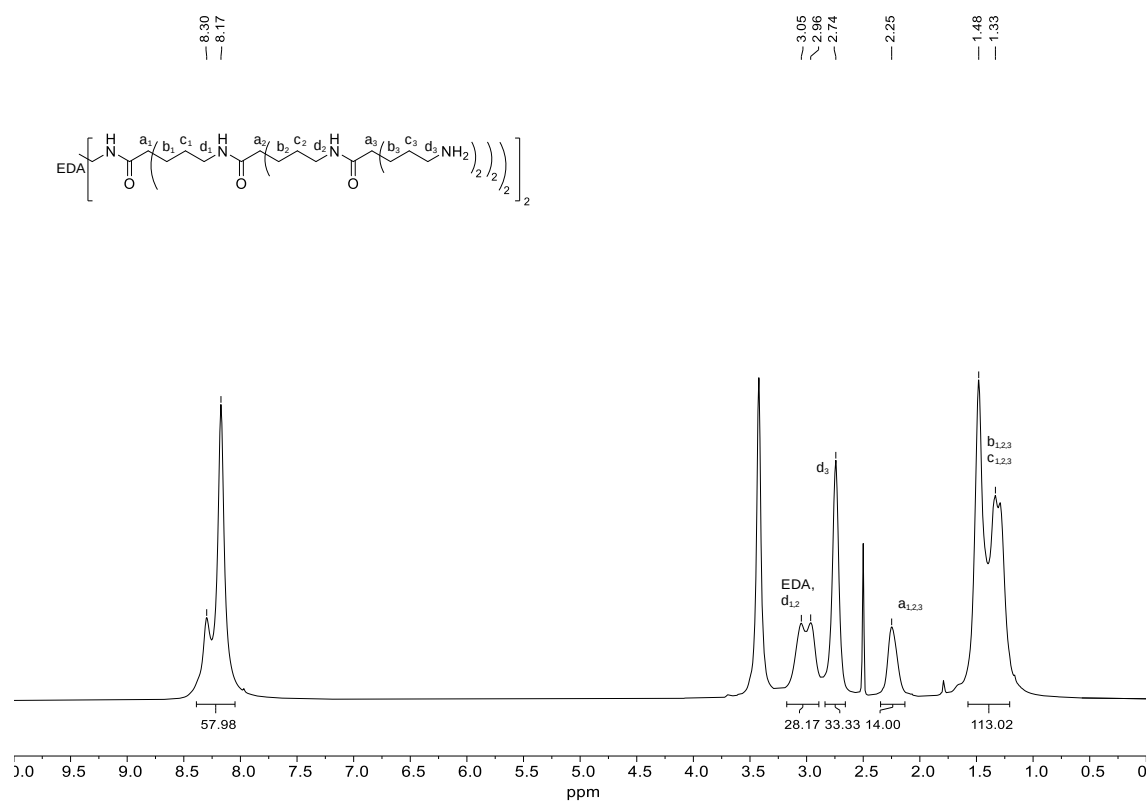


Figure S37. ^1H NMR spectrum of **G3** in $\text{DMSO}-d_6$.

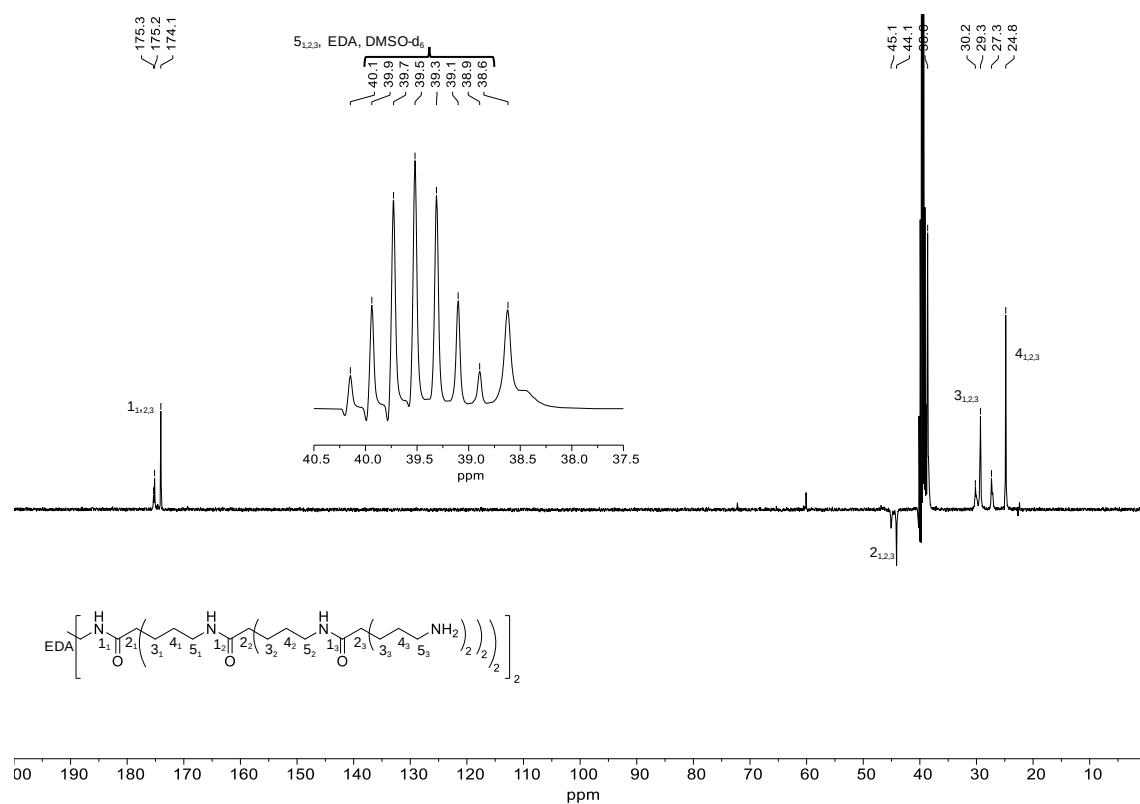


Figure S38. ^{13}C NMR (SEFT) spectrum of **G3** in $\text{DMSO}-d_6$.

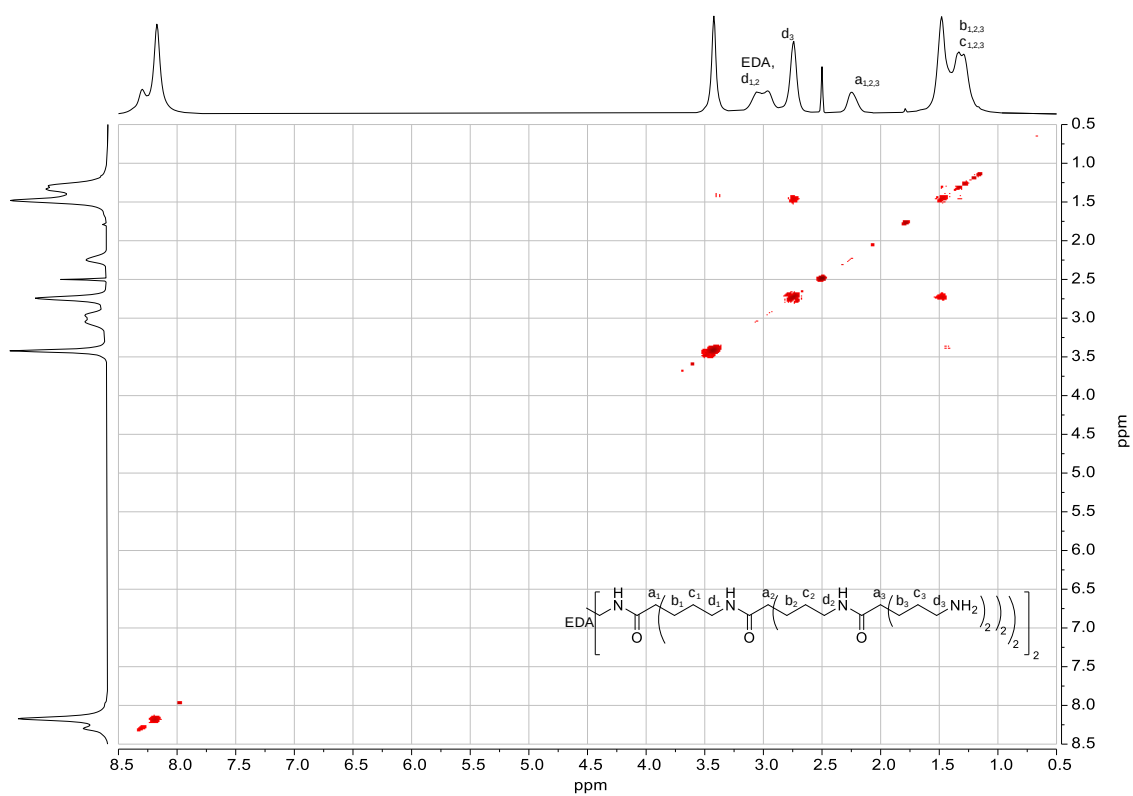


Figure S39. COSY spectrum of **G3** in DMSO- d_6 .

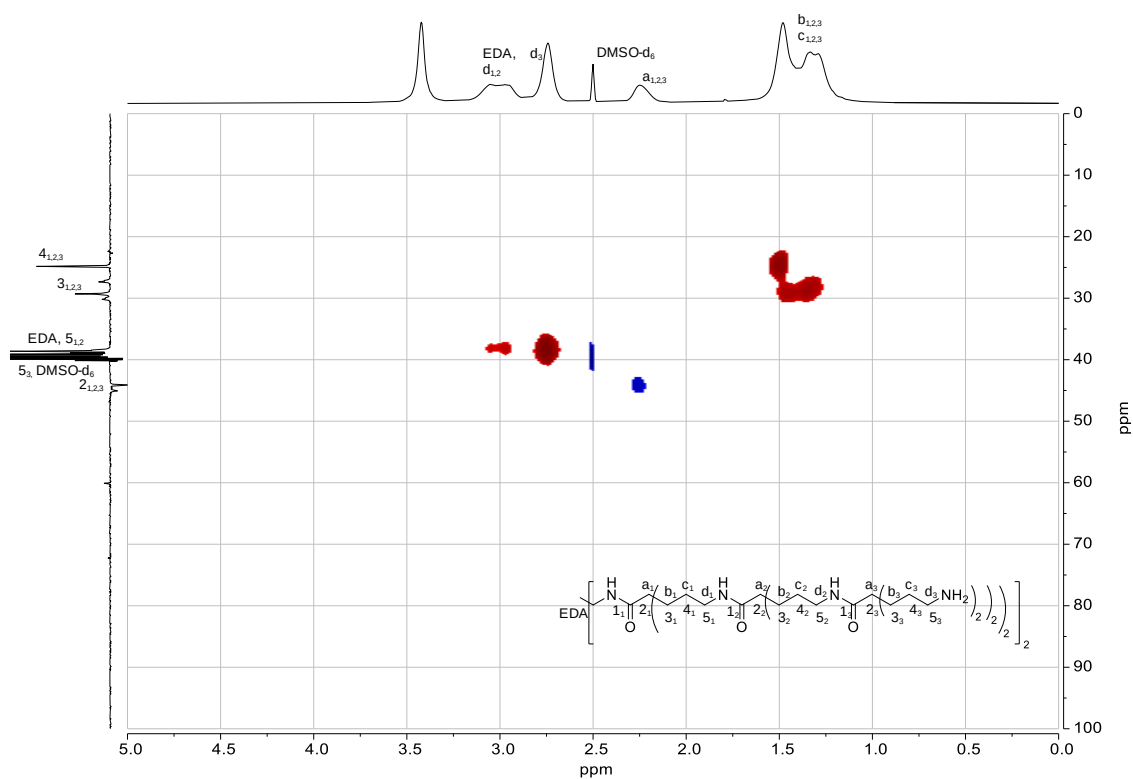
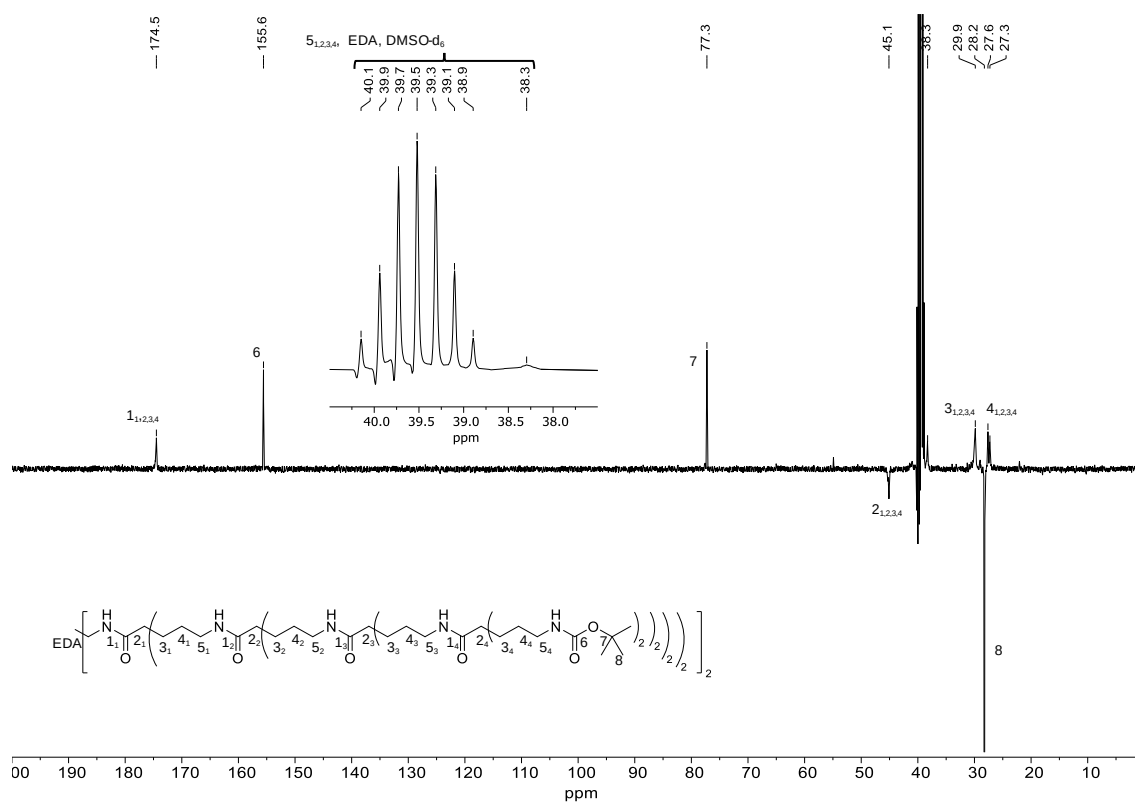
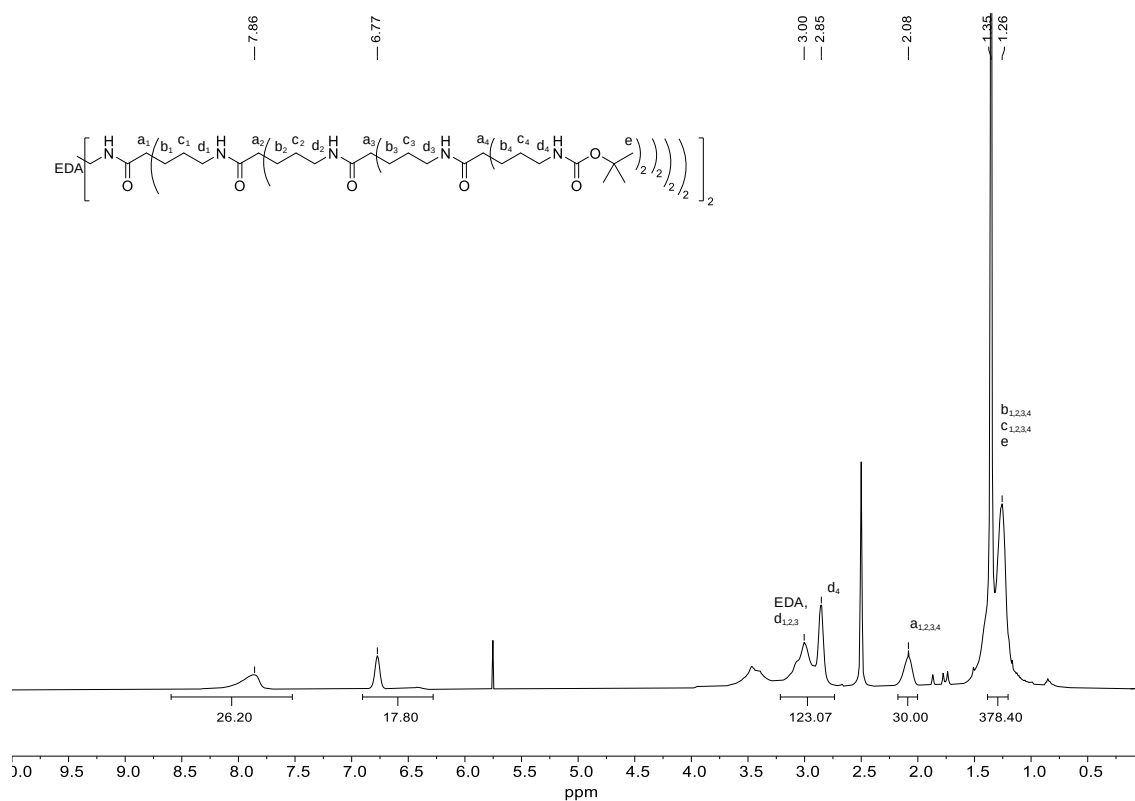


Figure S40. HSQC spectrum of **G3** in DMSO- d_6 .



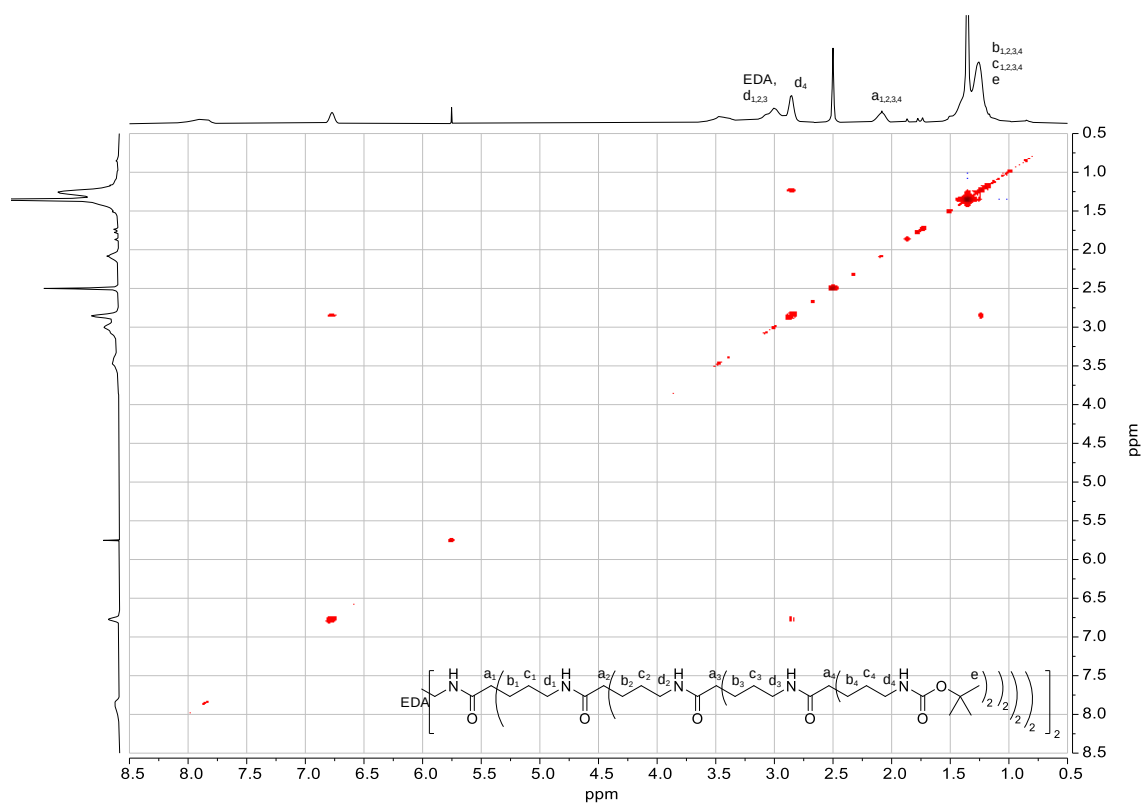


Figure S43. COSY spectrum of G4-NHBoc in DMSO- d_6 .

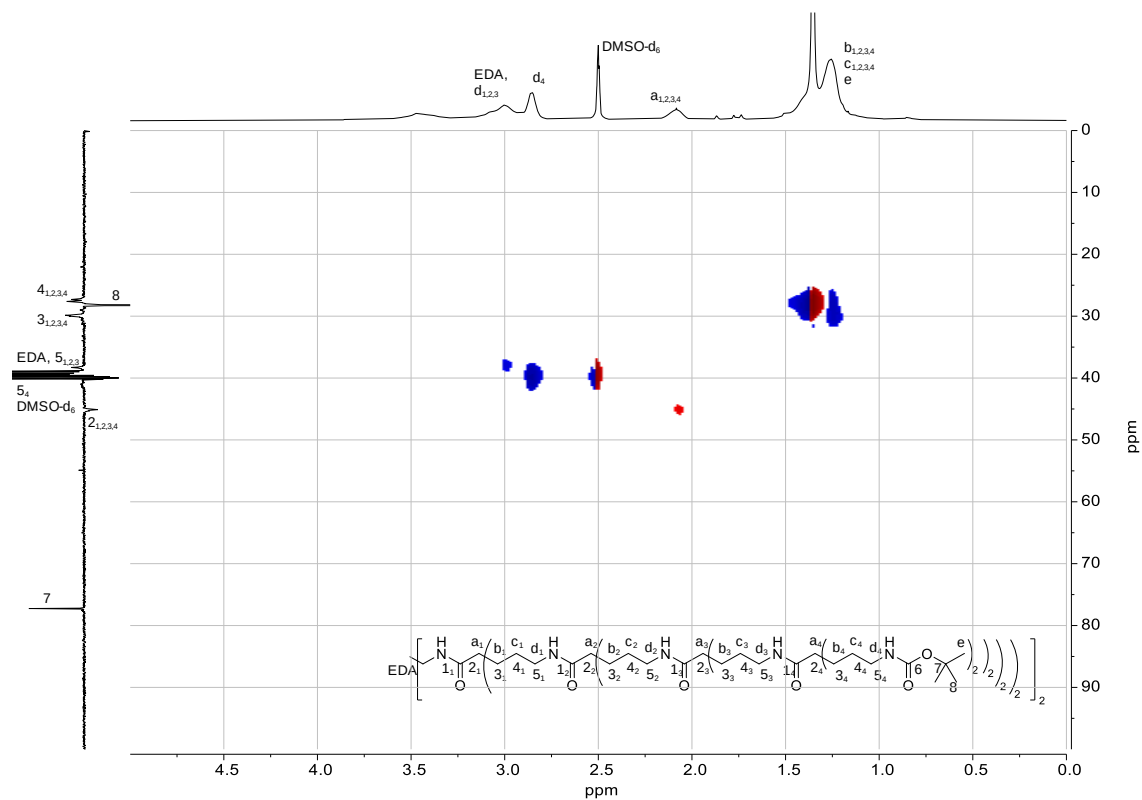
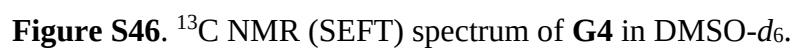


Figure S44. HSQC spectrum of G4-NHBoc in DMSO- d_6 .



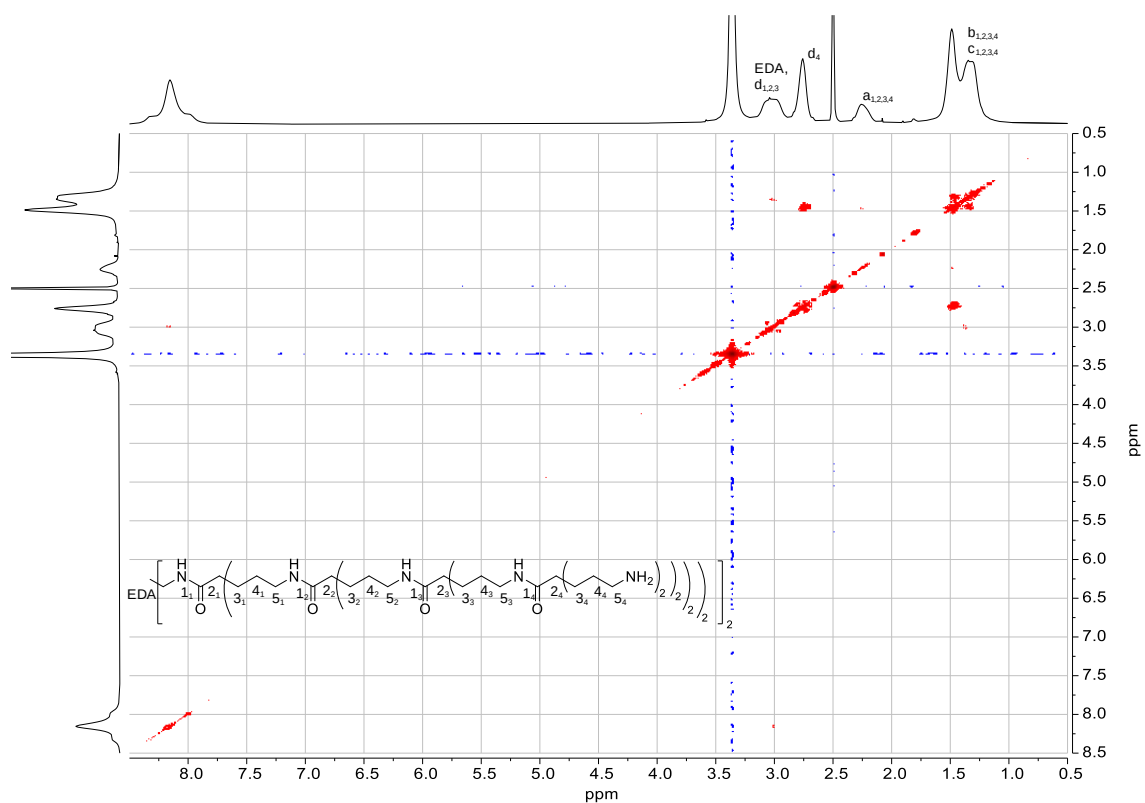


Figure S47. COSY spectrum of **G4** in DMSO- d_6 .

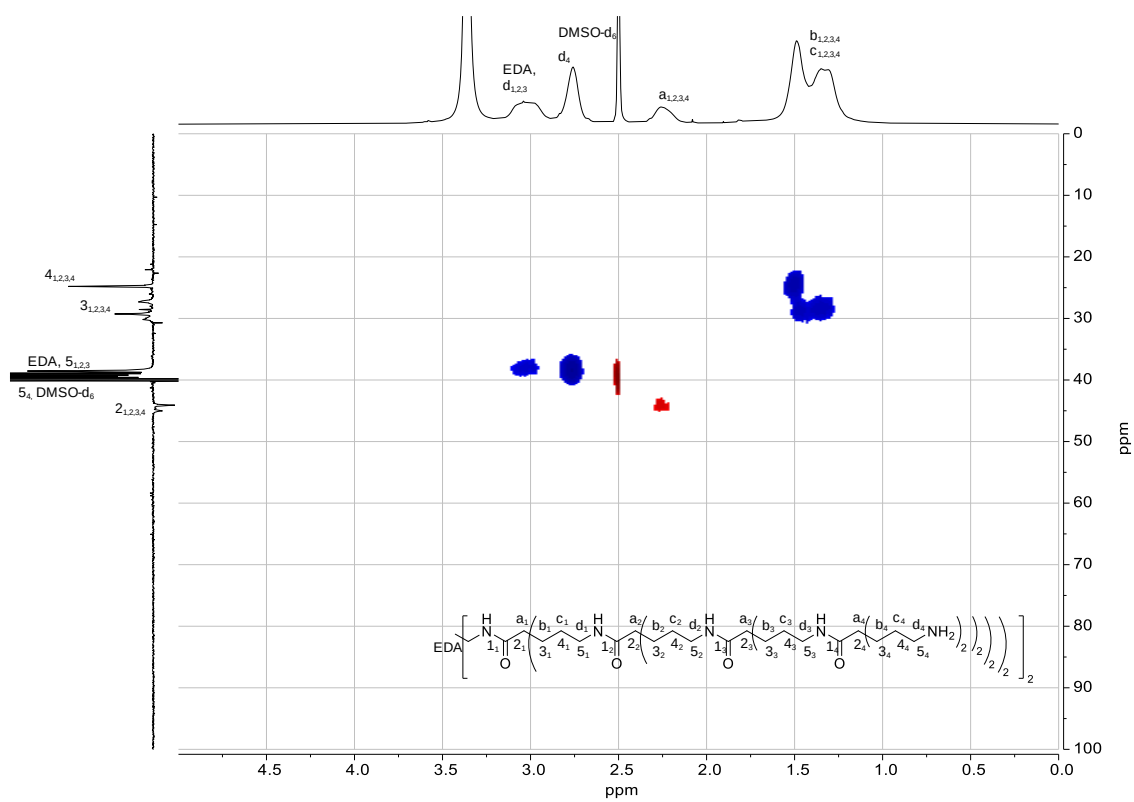


Figure S48. HSQC spectrum of **G4** in DMSO- d_6 .

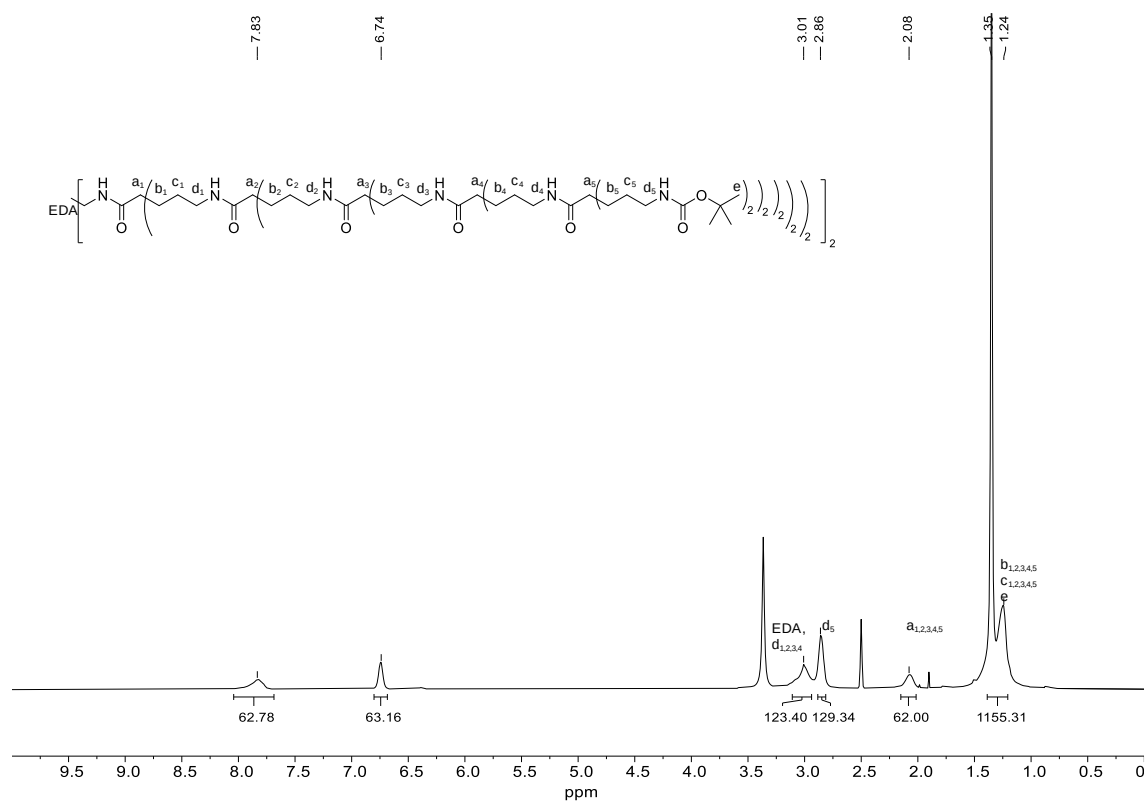


Figure S49. ^1H NMR spectrum of **G5-NHBoc** in $\text{DMSO}-d_6$.

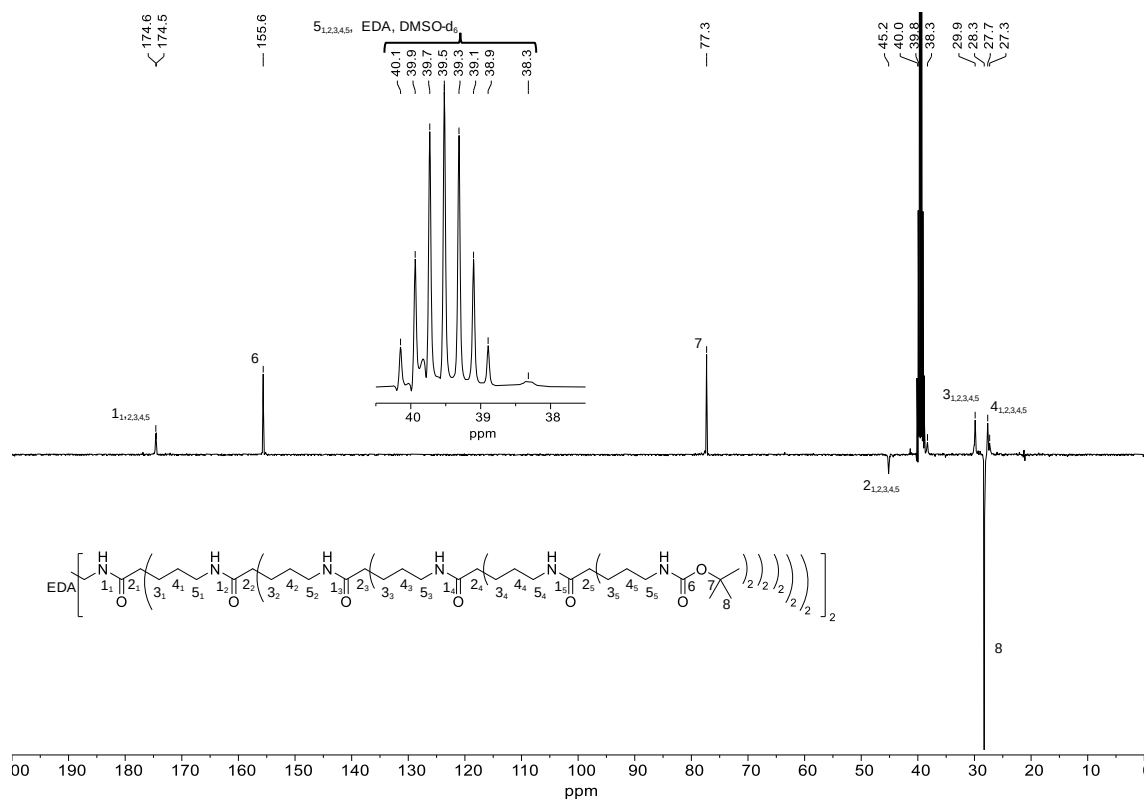


Figure S50. ^{13}C NMR (SEFT) spectrum of **G5-NHBoc** in $\text{DMSO}-d_6$.

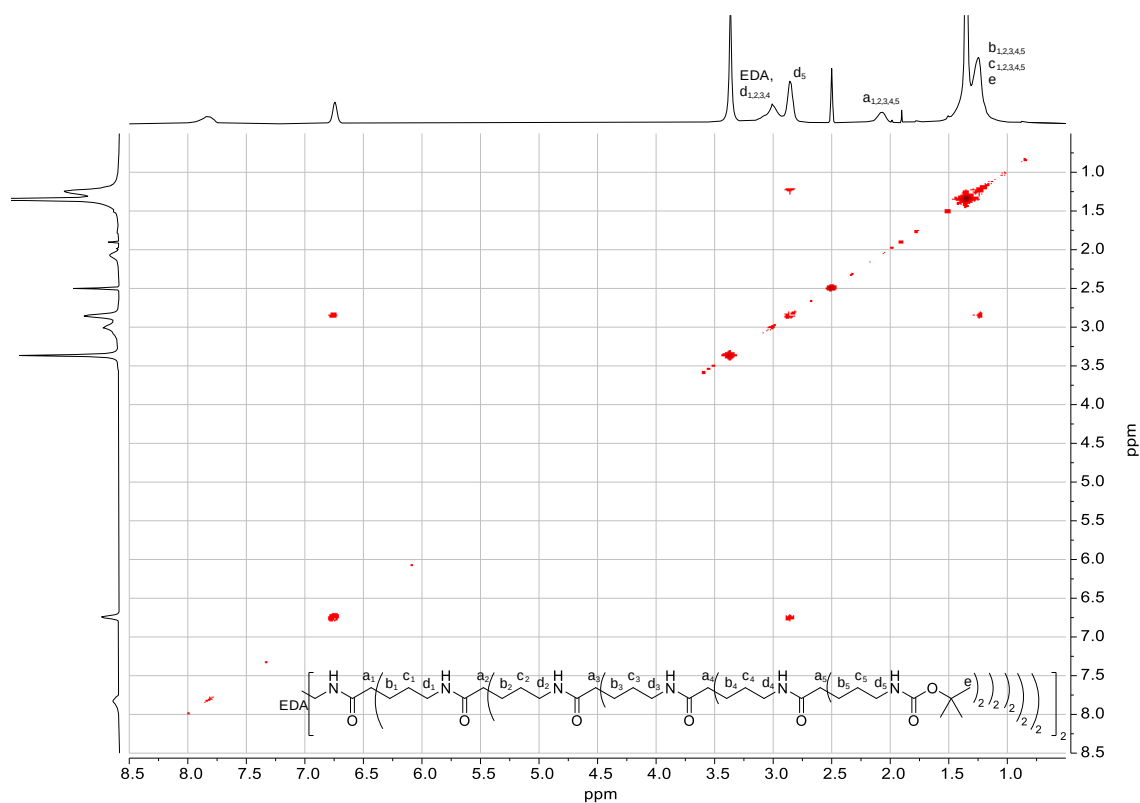


Figure S51. COSY spectrum of **G5-NHBoc** in DMSO- d_6 .

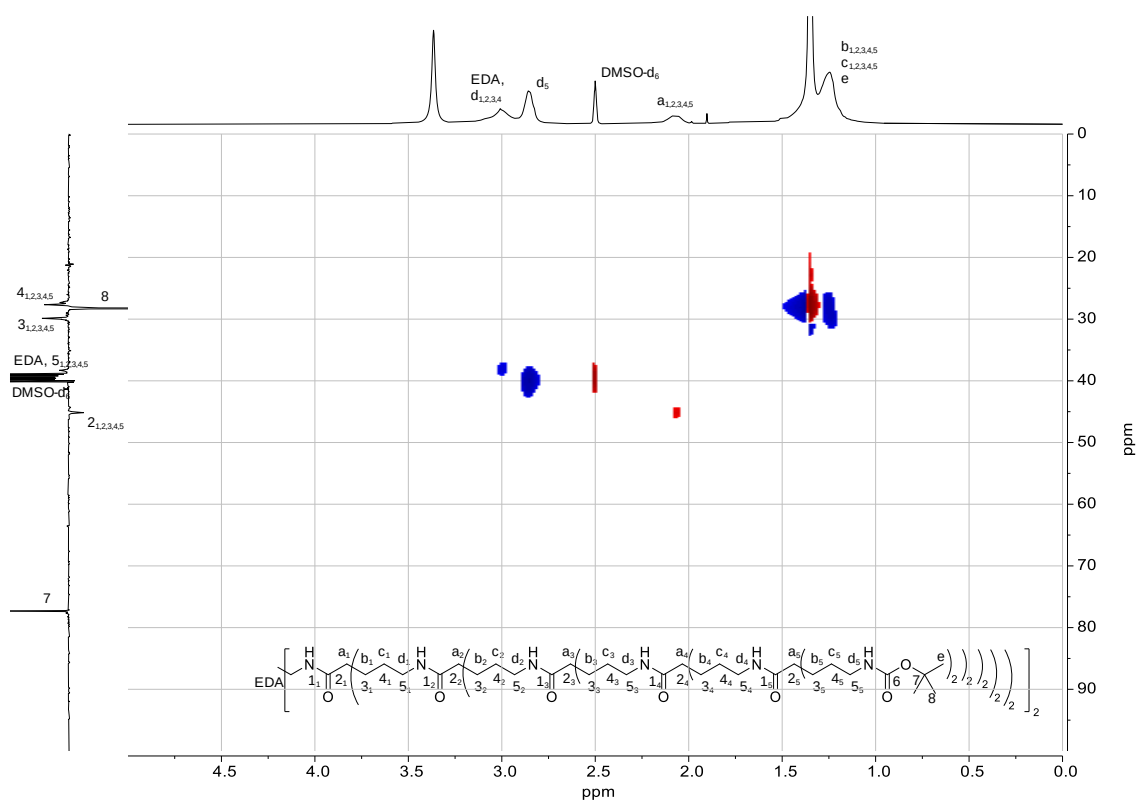


Figure S52. HSQC spectrum of **G5-NHBoc** in DMSO- d_6 .

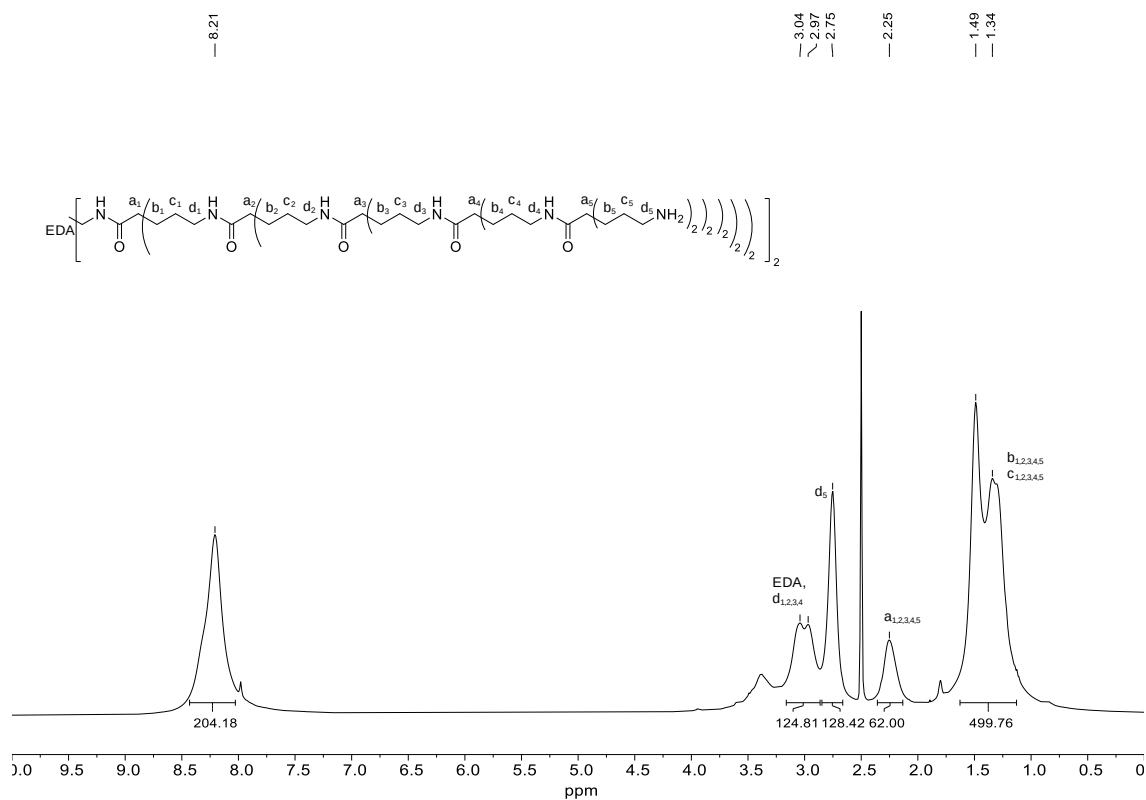


Figure S53. ^1H NMR spectrum of **G5** in $\text{DMSO-}d_6$.

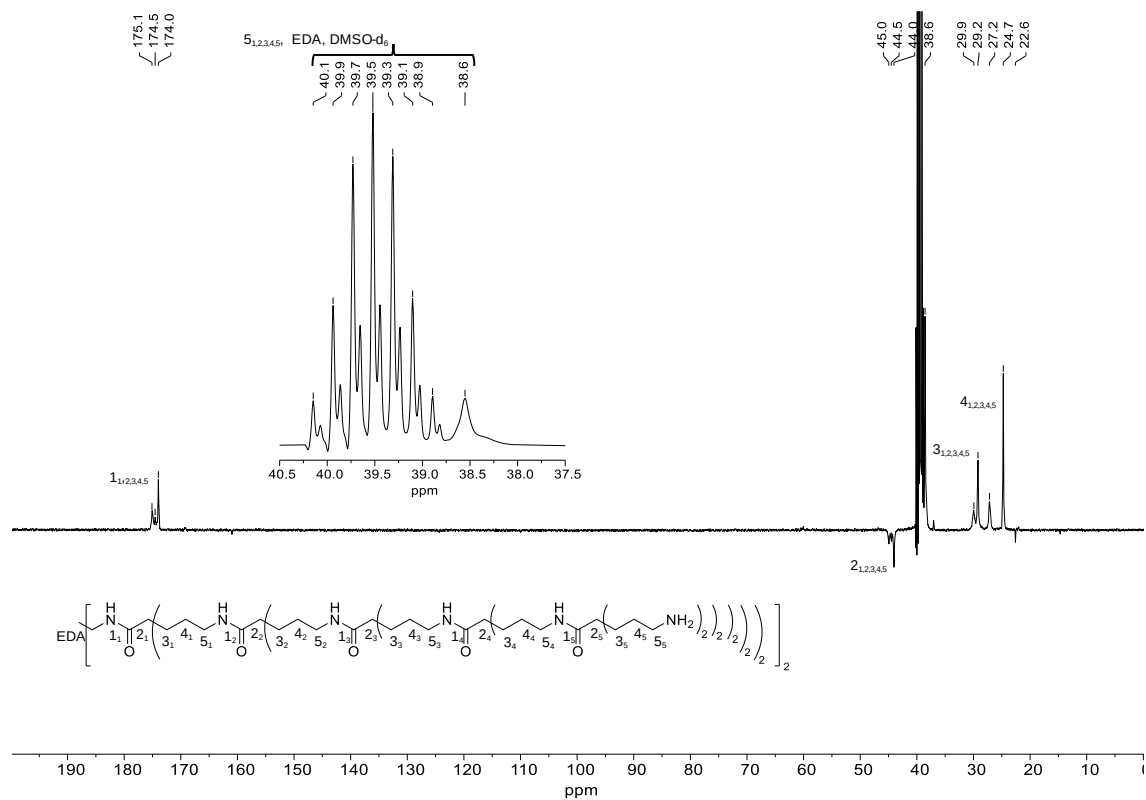


Figure S54. ^{13}C NMR (SEFT) spectrum of **G5** in $\text{DMSO-}d_6$.

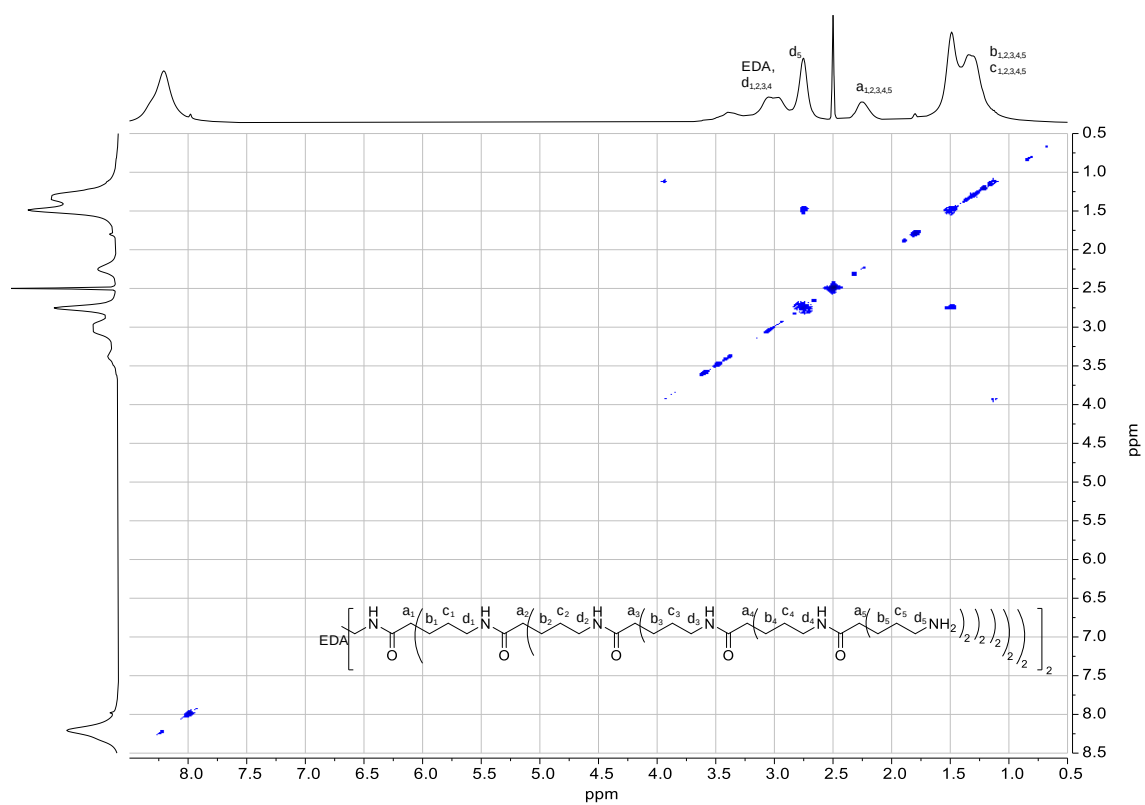


Figure S55. COSY spectrum of G5 in DMSO- d_6 .

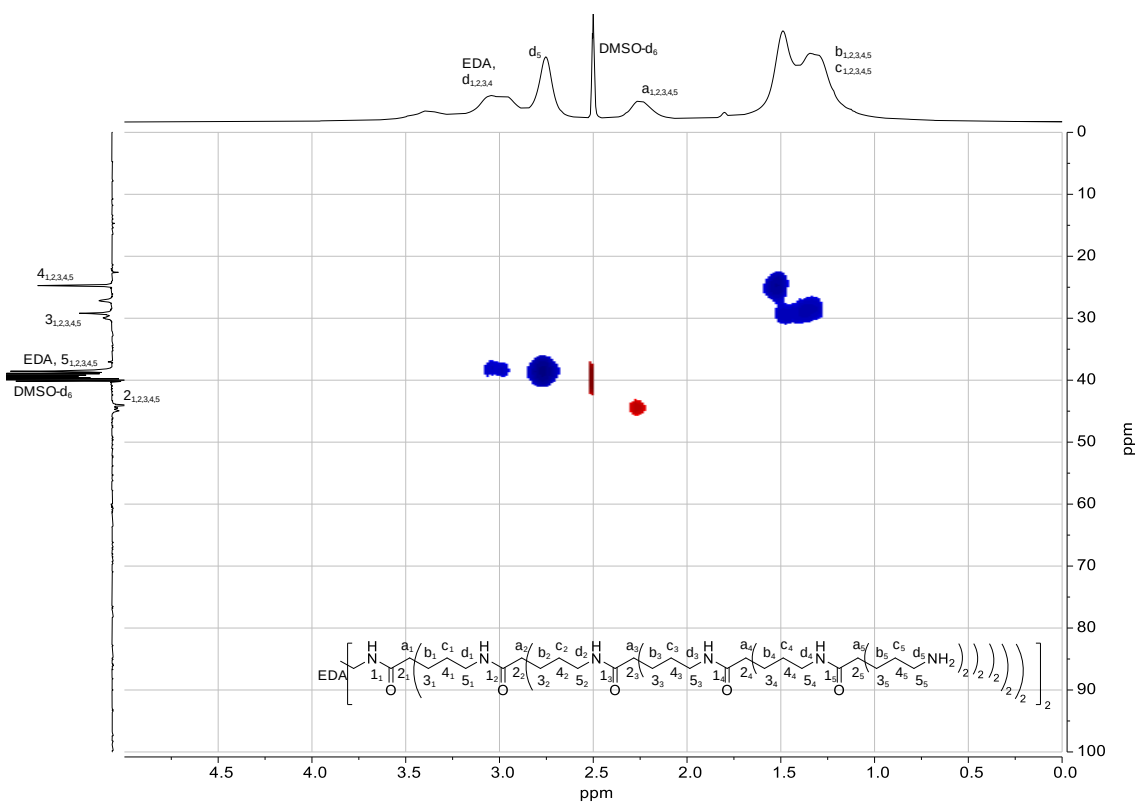


Figure S56. HSQC spectrum of G5 in DMSO- d_6 .

3.- Stability studies

NMR Studies were performed to evaluate the stability of **G5** in aqueous solution. Sample was prepared in D₂O and kept at 37 °C.

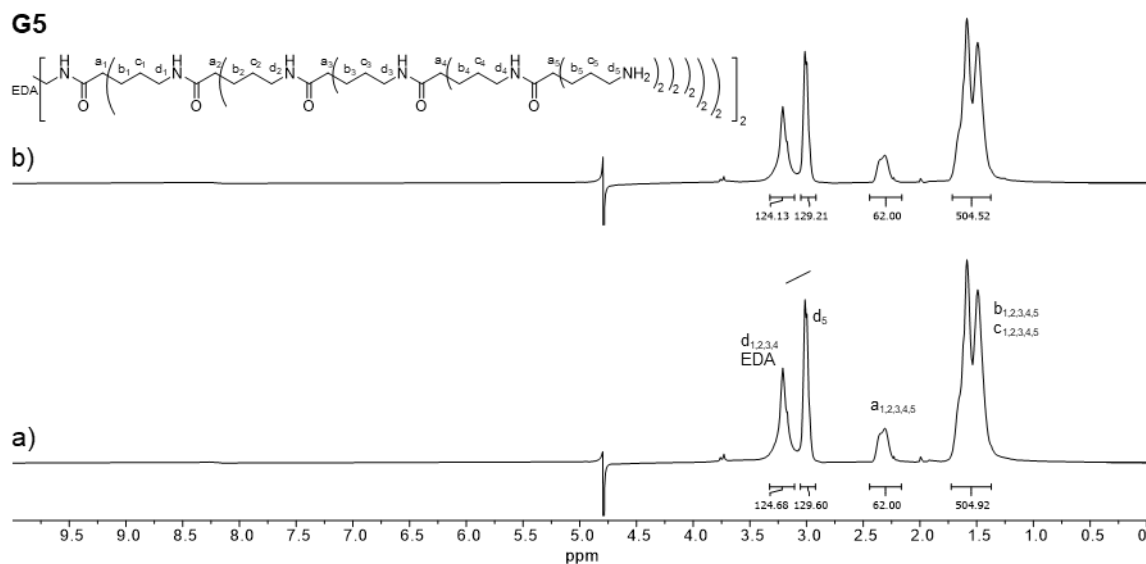


Figure S57. ¹H-NMR spectra of **G5** in D₂O a) freshly prepared and b) after 7 days at 37°C.

4.- MALDI-TOF spectra

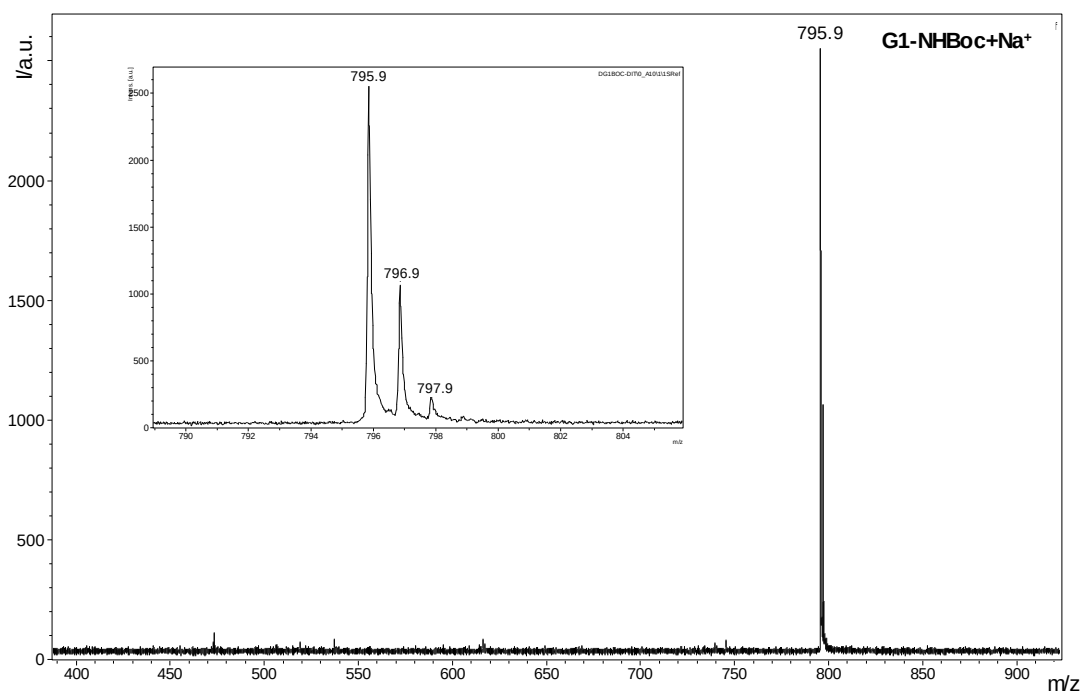


Figure S58. MALDI-TOF spectra of compound **G1-NHBoc** in dithranol (DIT) matrix. Values: m/z calc. 795.5; exp. 795.9 (M+Na⁺).

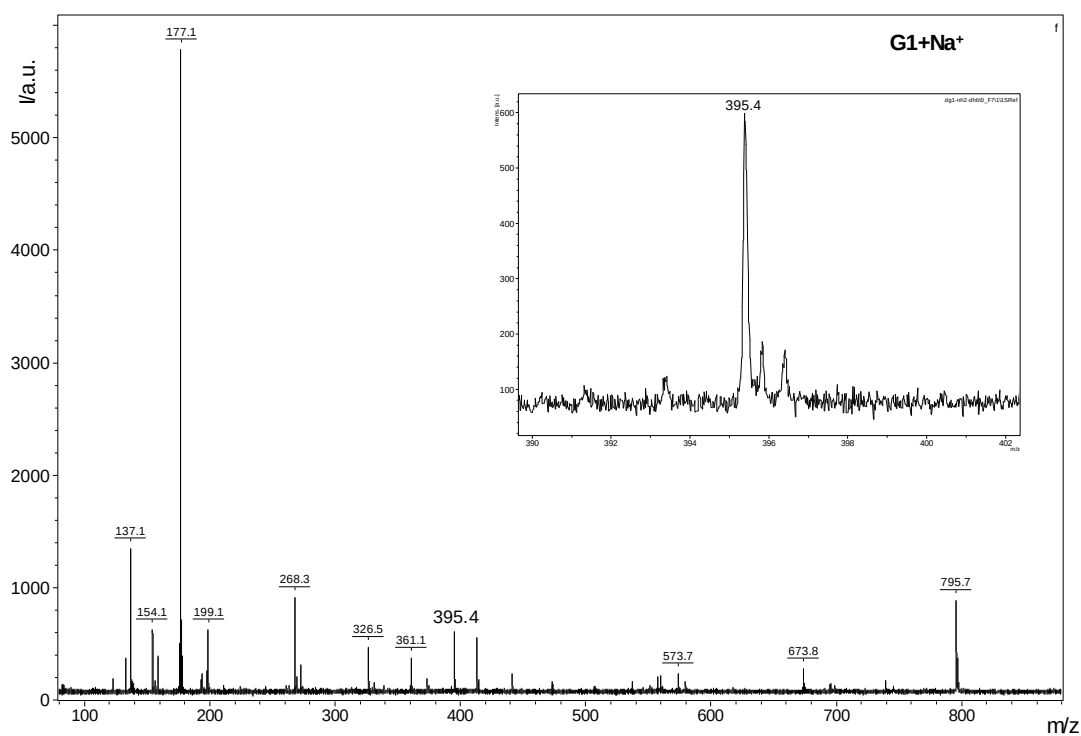


Figure S59. MALDI-TOF spectra of compound **G1** in 2,5-dihydroxybenzoic acid (DHB) matrix. Values: m/z calc. 395.5; exp. 395.4 ($M+Na^+$).

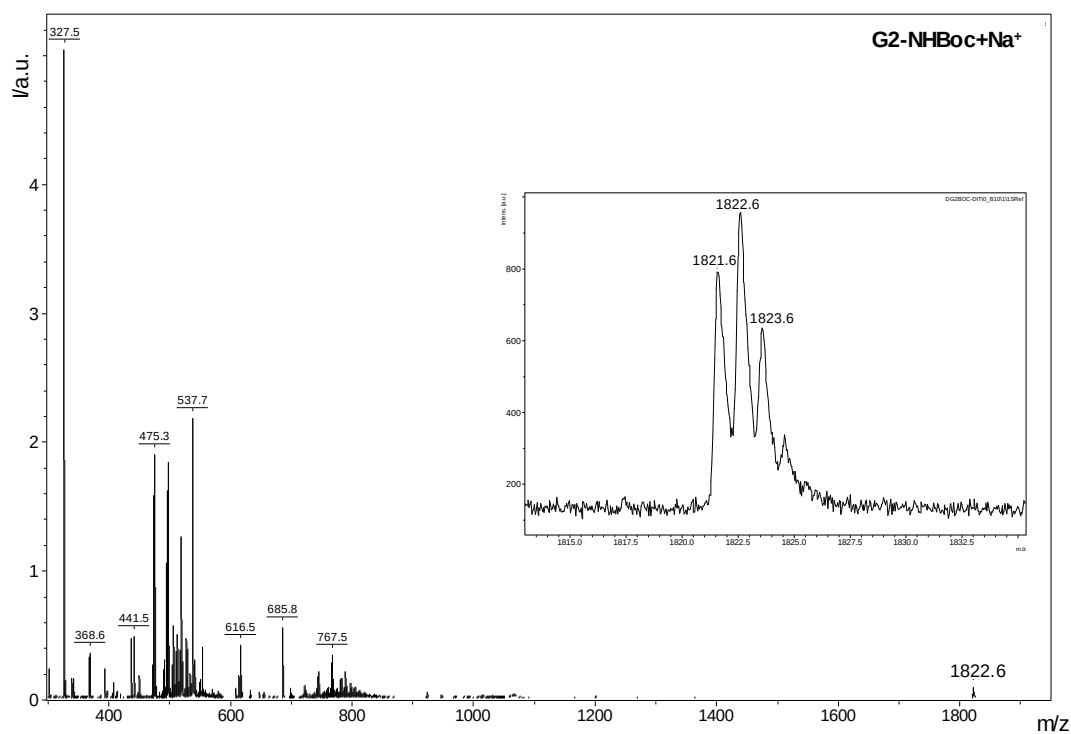


Figure S60. MALDI-TOF spectra of compound **G2-NHBoc** in dithranol (DIT) matrix. Values: m/z calc. 1821.2; exp. 1822.6 ($M+Na^+$).

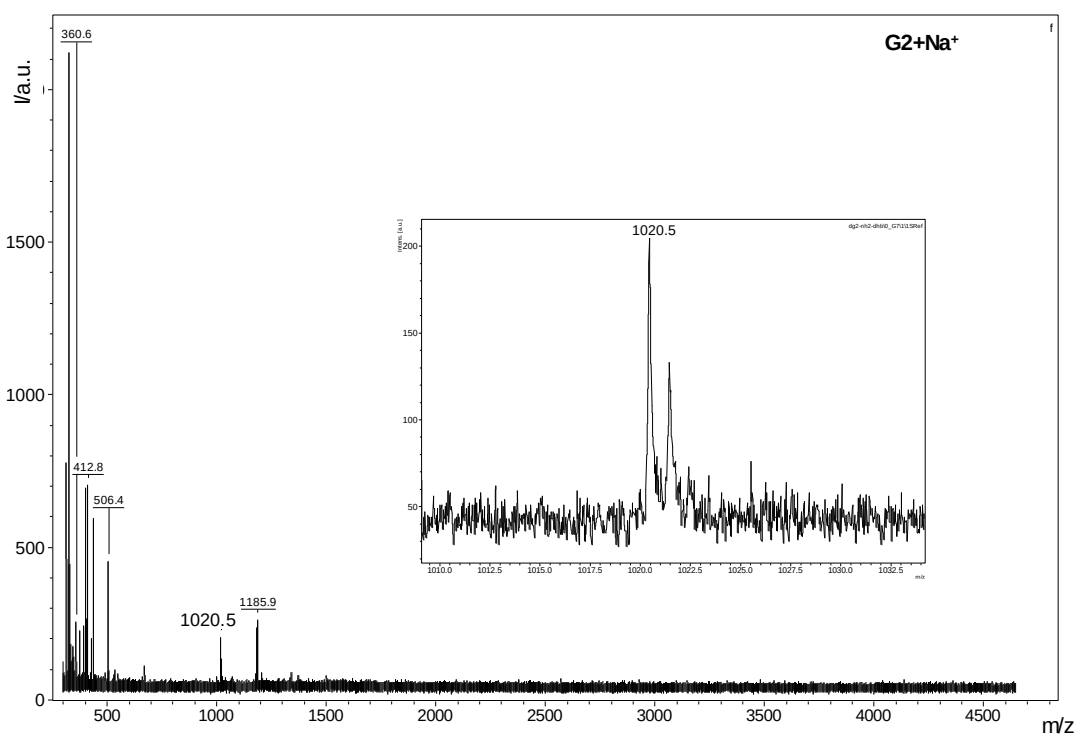


Figure S61. MALDI-TOF spectra of compound **G2** in 2,5-dihydroxybenzoic acid (DHB) matrix. Values: m/z calc. 1020.5; exp. 1020.5 ($M+Na^+$).

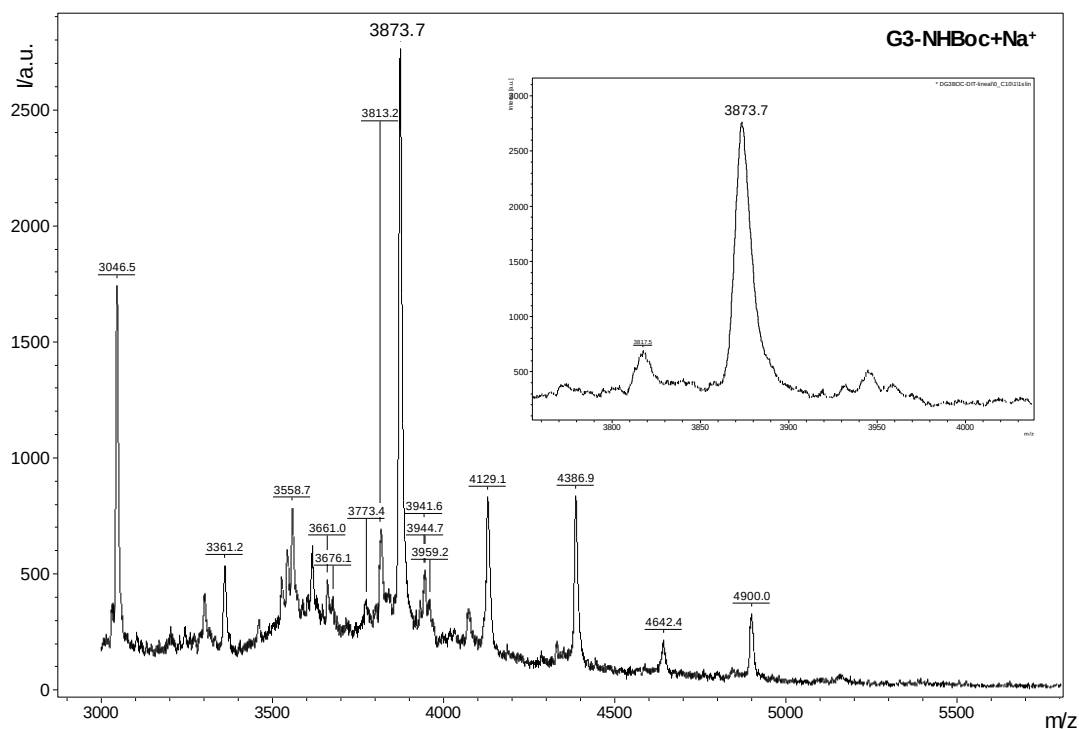


Figure S62. MALDI-TOF spectra of compound **G3-NHBoc** in dithranol (DIT) matrix. Values: m/z calc. 3871.7; exp. 3873.7 ($M+Na^+$).

5.- DOSY NMR Experiments

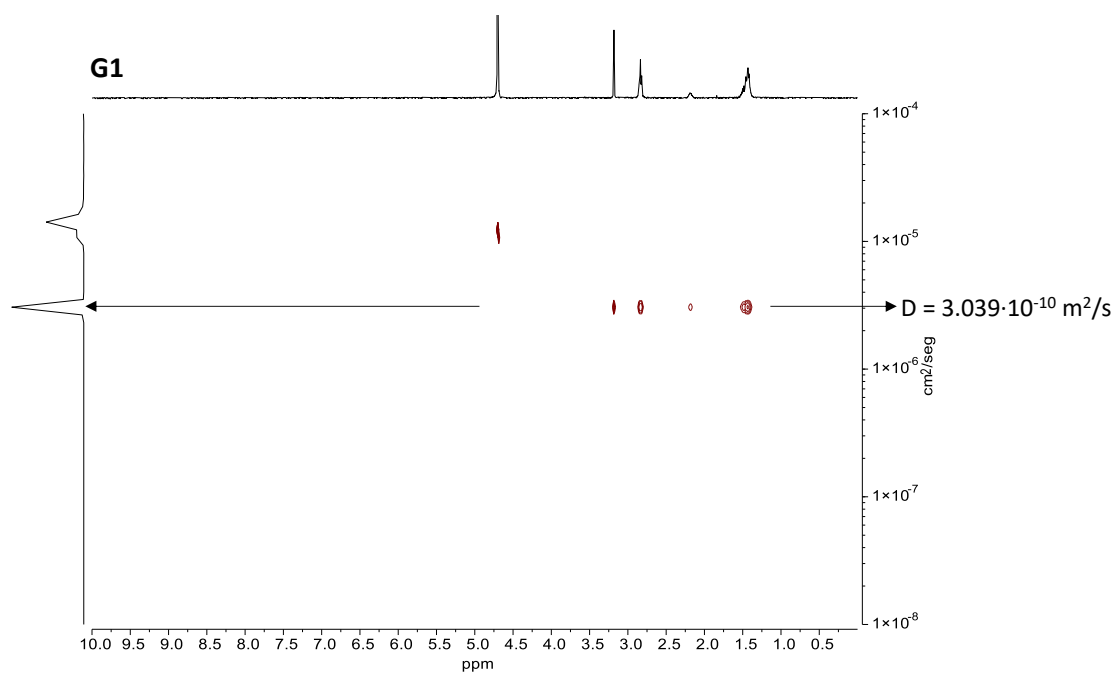


Figure S63. DOSY NMR experiment of **G1** in D₂O.

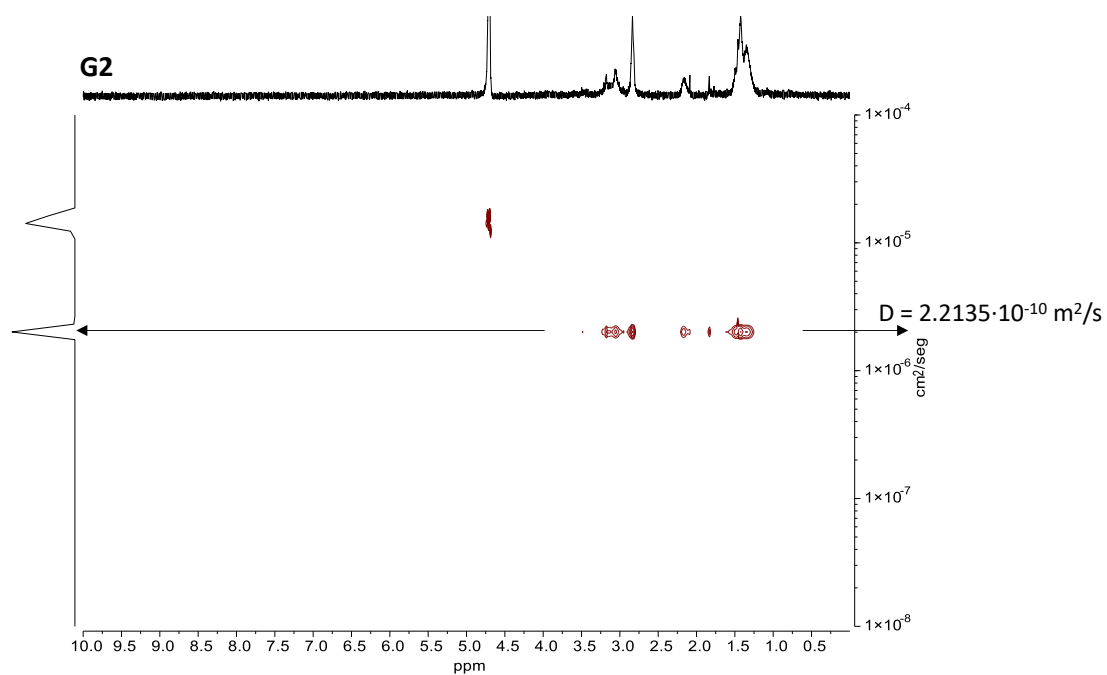


Figure S64. DOSY NMR experiment of **G2** in D₂O.

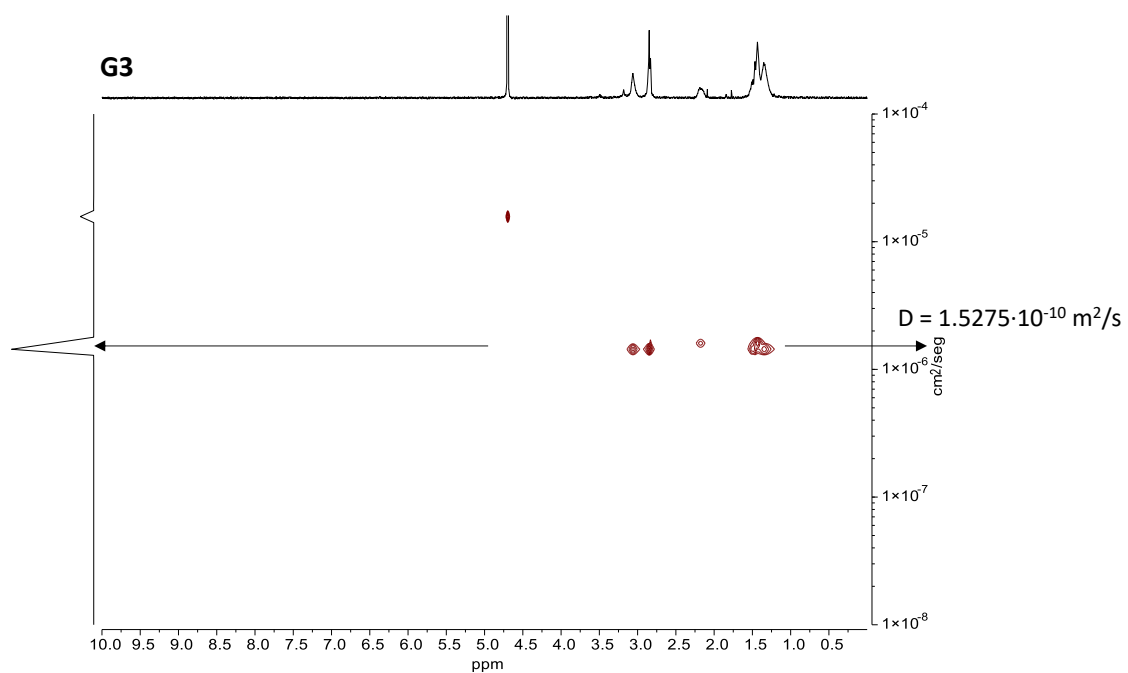


Figure S65. DOSY NMR experiment of **G3** in D₂O.

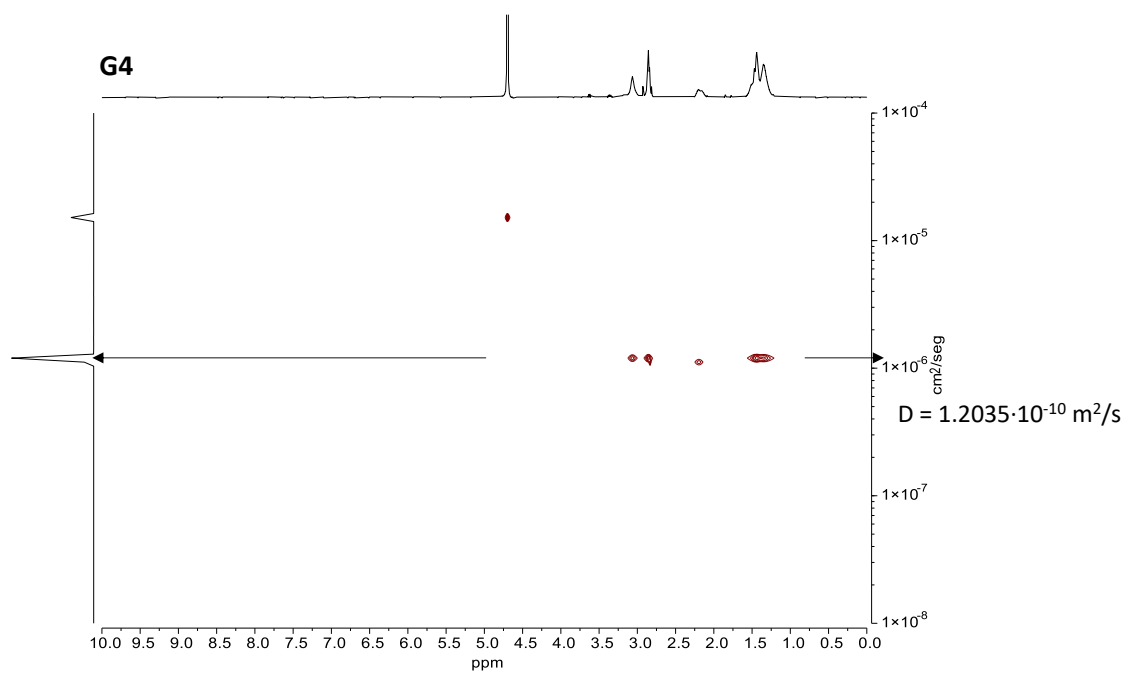


Figure S66. DOSY NMR experiment of **G4** in D₂O.

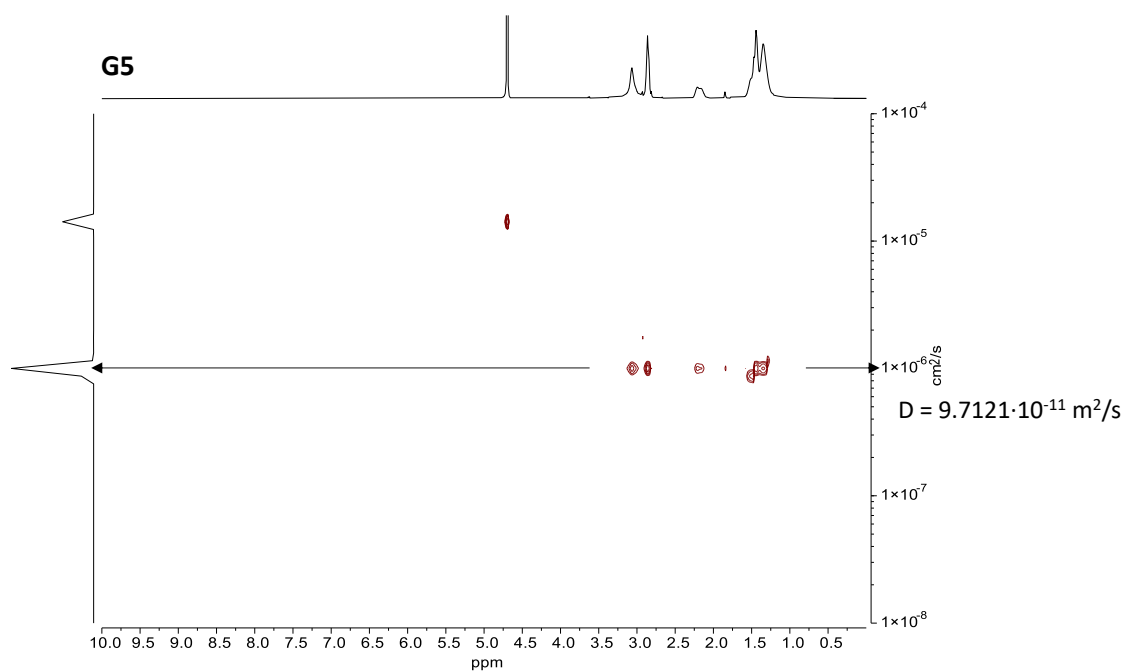


Figure S67. DOSY NMR experiment of **G5** in D_2O .

6.- AFM experiments

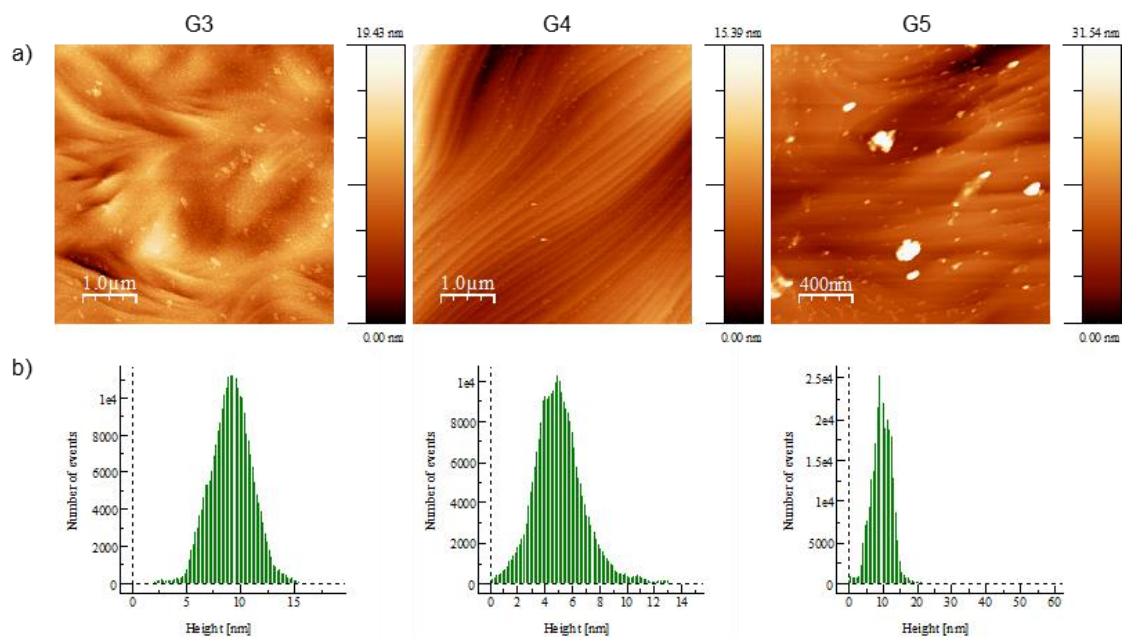


Figure S68. a) representative AFM images of dendrimers **G3**, **G4** (low magnification), and **G5** deposited on (111) gold substrates, and b) the corresponding height histograms showing particle size distributions in the samples, including dendrimer aggregates.

7.- Molecular Dynamic Simulations

Dendrimer Building. The dendrimers were built based on three capped-residues: the cap-core (cap-COR): *N,N'*-(ethane-1,2-diyl)diacetamide; the cap-repetitive units (cap-REP): *N,N'*-(4-(methylcarbamoyl)heptane-1,7-diyl)diacetamide, and the cap-terminal unit (cap-TAM): 4-(methylcarbamoyl)heptane-1,7-diaminium group (Figure S69).

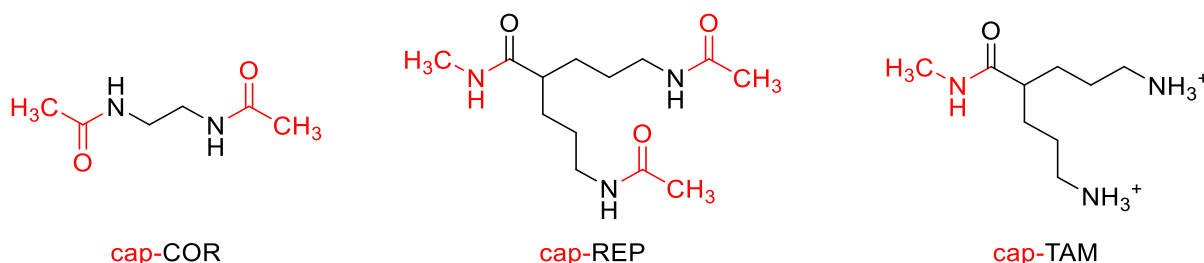


Figure S69. Residues selection for the dendrimers. Cap atoms are in red.

All capped regions were removed before connecting to another residue. All capped-residues were optimized using the AMBER (parm99) force field, and the parameters not include in it were obtained from the general AMBER force field (GAFF).³ The minimum energy conformation was submitted to B3LYP/6-31G(d) basis set calculation using G09,⁴ (capped-COR and REP residues were optimized *in vacuum*, while capped TAM residue was optimized employing PCM-B3LYP/6-31G(d) with water as solvent).⁵ Total cap atom charge was set to zero during charge calculation and the overall full residue charge was also set to zero except for the protonated residue (TAM), which was kept at +2. Decapped residues were created using the Antechamber module of AmberTools12,⁶ and the restrained potential (RESP) method was used for charge fitting.⁷ Finally, the residues obtained were used to build the desired dendrimer generation with the Dendrimer Building Tool (DBT).⁸

Simulation Details. Simulations were performed in water as explicit solvent at neutral pH (7.4). All calculations were done with the AMBER 12 MD software.⁶ To preserve the overall charge, a proper number of Cl⁻ counterions were added. Then, water molecules were added using the TIP3P water model,⁹ in a truncated octahedral cell. In all cases, a minimum 10 Å solvation shell around the dendrimer structure were. Initial properties of the dendrimers are collected in Table S1.

Table S1. Initial properties of dendrimers and simulation details. N_{den} , N_{Cl^-} , N_{solvent} and N_{total} are, respectively, the number of dendrimer atoms, chloride ions, atoms in solvent molecules and the total number of atoms. V is the initial octahedral box volume.

Dendrimer	N_{den}	N_{Cl^-}	N_{solvent}	N_{total}	$V(\text{\AA}^3)$
G1	70	4	1423	1497	52445
G2	182	8	3497	3687	124257
G3	406	16	4318	4740	159319
G4	854	32	7948	8834	290099
G5	1750	64	13633	15447	501907

Solvated structures were minimized as described previously.¹⁰ The dendrimers were optimized using a conjugated gradient optimization keeping their starting conformation with a harmonic constraint force. Then, was followed by five periods of minimization decreasing the harmonic restraint force constant from 20 kcal/mol-Å² to zero.

The minimized dendrimers were heated from 0 to 300 K with three steps of 40 ps of MD, the first under (NVT) conditions and the rest under (NPT) conditions. Finally, we carried out an unconstrained MD simulation (2ns) in NPT ensemble to equilibrate the system at 300 K. The motion equation was solved using the Verlet leapfrog algorithm,¹¹ with an integration step of 2 fs. The bond lengths involving bonds to hydrogen were constrained with the SHAKE algorithm.¹² The equilibration of all system was confirmed using an autocorrelation function of the squared radius-of-gyration (Figure S70).

Finally, production runs of 20 ns trajectories were done under an NPT ensemble and the dynamic summary properties of the last nanosecond of the trajectory for all dendrimers are summarized in Tables S2-S6 and Figures S71-S75. Temperature regulation was achieved using the Berendsen weak coupling.¹³ The particle-mesh Ewald (PME) algorithm was employed to treat long-range electrostatic interactions,¹⁴ with a real space cut off of 9 Å. The same cutoff was used for van der Waals interactions. For the structural analyses (R_g , RDF, etc.) the last 1 ns equilibrated trajectory was used. Amber modules *ptraj* and *cpptraj* were used to accomplish these analyses. VMD software was used for the calculation of molecular surfaces.¹⁵

Autocorrelation function: Dendrimer relaxation was determined from the autocorrelation function of the squared radius-of-gyration, $C_{R_g^2}(t)$ which is evaluated from the expression:¹⁶

$$C_{R_g^2}(t) = \frac{\langle R_g^2(0)R_g^2(t) \rangle - \langle R_g^2 \rangle^2}{\langle R_g^4 \rangle - \langle R_g^2 \rangle^2}$$

The resulting graph is presented in Figure S64. In all cases $C_{R_g^2}(t)$ decays to 0 at time scales shorter than 1 ns, implying that the simulation times are sufficient to sample enough independent configurations in order to average static properties. The details of the five systems studied were listed before in Table S1.

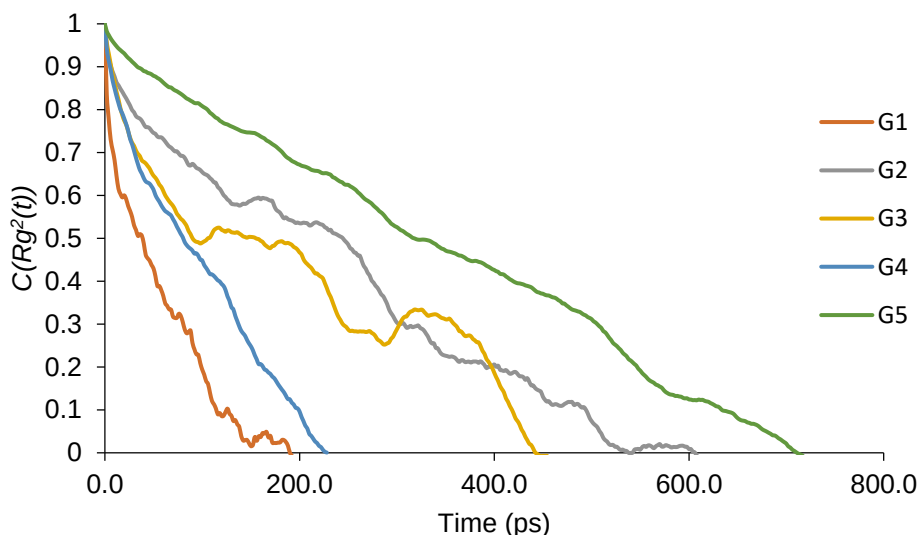


Figure S70. Correlation functions of the squared radius of gyration for **G1-5** dendrimers.

Dynamic summaries of Molecular Dynamic Simulations

Table S2. Dynamic summary of dendrimer **G1**

Dynamics summary	Final	Average (last nanosecond)	Std. Dev. (last nanosecond)
Total energy (kcal/mol)	-11519.084	-11518.017	11.987
Potential energy (kcal/mol)	-14092.714	-14110.652	32.924
Kinetic energy (kcal/mol)	2573.630	2592.635	29.977
Temperature (K)	297.280	299.477	3.463

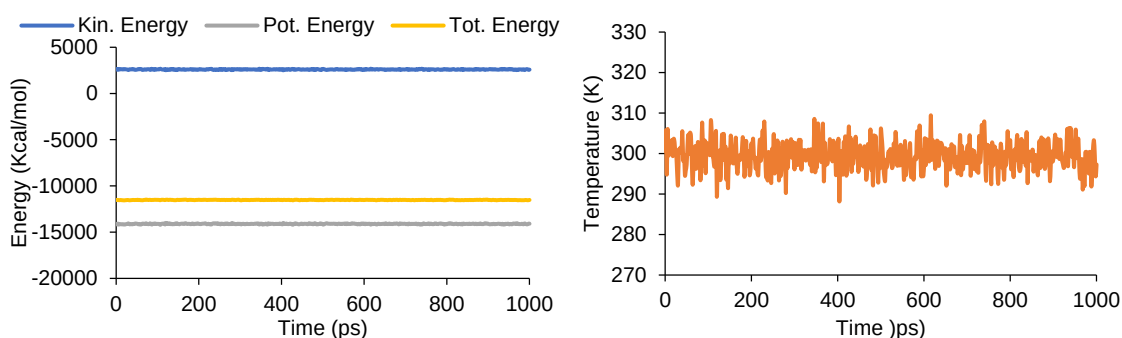


Figure S71. Energy and temperature profiles (last 1 ns) of the MD simulation on dendrimer **G1**.

Table S3. Dynamic summary of dendrimer **G2**

Dynamics summary	Final	Average (last nanosecond)	Std. Dev. (last nanosecond)
Total energy (kcal/mol)	-28053.857	-28027.128	18.120
Potential energy (kcal/mol)	-34543.196	-34415.169	50.818
Kinetic energy (kcal/mol)	6489.340	6388.040	47.658
Temperature (K)	304.670	299.912	2.237

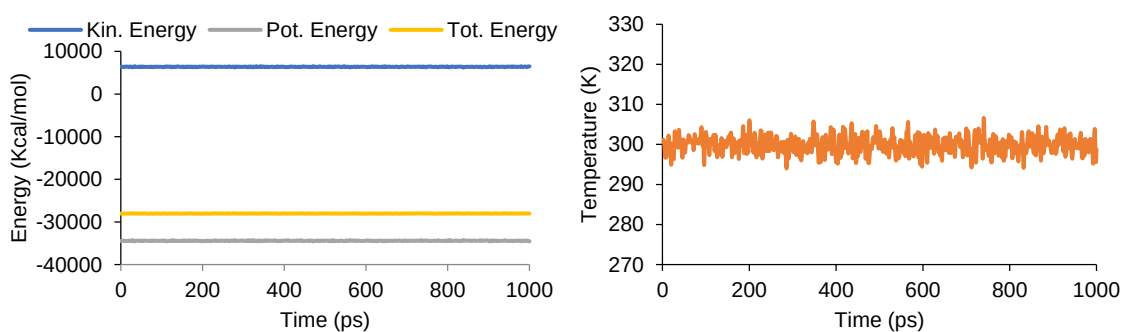
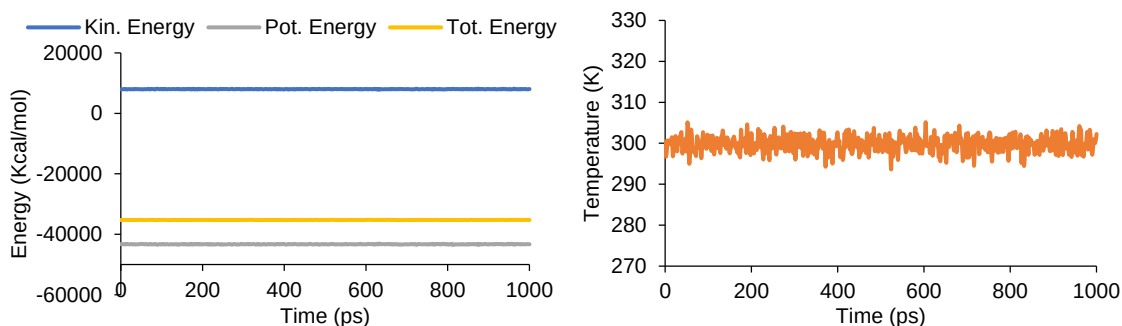


Figure S72. Energy and temperature profiles (last 1 ns) of the MD simulation on dendrimer **G2**.

Table S4. Dynamic summary of dendrimer **G3**

Dynamics summary	Final	Average (last nanosecond)	Std. Dev. (last nanosecond)
Total energy (kcal/mol)	-35240.416	-35261.286	23.845
Potential energy (kcal/mol)	-43283.292	-43281.639	60.632
Kinetic energy (kcal/mol)	8042.877	8020.353	53.739
Temperature (K)	300.660	299.820	2.009

**Figure S73.** Energy and temperature profiles (last 1 ns) of the MD simulation on dendrimer **G3**.**Table S5.** Dynamic summary of dendrimer **G4**

Dynamics summary	Final	Average (last nanosecond)	Std. Dev. (last nanosecond)
Total energy (kcal/mol)	-65111.453	-65125.955	32.420
Potential energy (kcal/mol)	-80071.810	-79975.663	83.090
Kinetic energy (kcal/mol)	14960.357	14849.708	74.318
Temperature (K)	302.210	299.971	1.501

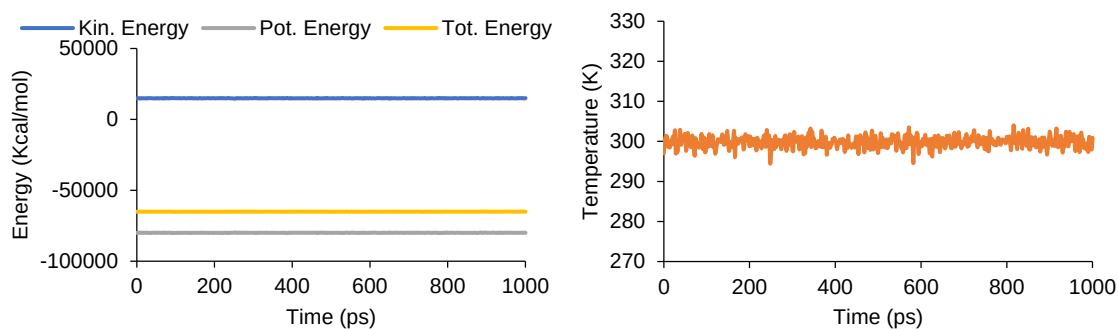
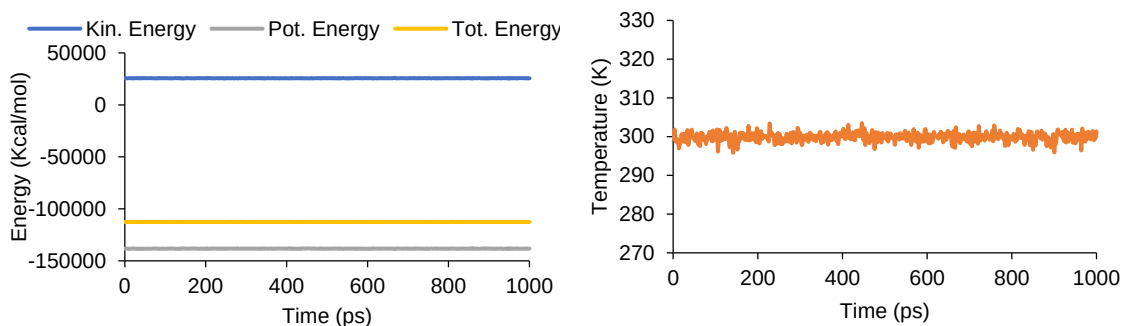
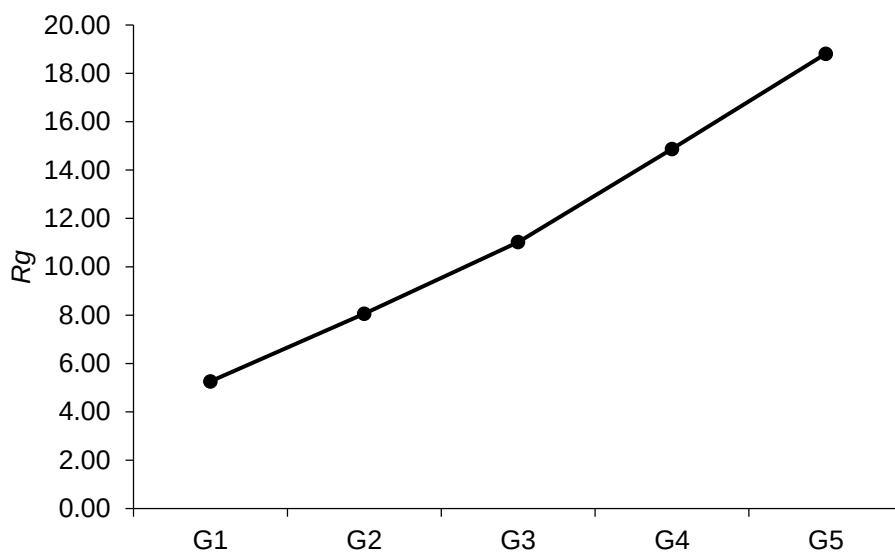
**Figure S74.** Energy and temperature profiles (last 1 ns) of the MD simulation on dendrimer **G4**.

Table S6. Dynamic summary of dendrimer **G5**

Dynamics summary	Final	Average (last nanosecond)	Std. Dev. (last nanosecond)
Total energy (kcal/mol)	-112657.992	-112630.954	42.671
Potential energy (kcal/mol)	-138240.236	-138305.153	111.838
Kinetic energy (kcal/mol)	25582.244	25674.199	101.397
Temperature (K)	298.780	299.858	1.184

**Figure S75.** Energy and temperature profiles (last 1 ns) of the MD simulation on dendrimer **G5**.

Radius of Gyration (R_g) for G_n

**Figure S76.** Radius of Gyration R_g values for G1-5 dendrimer generations.

Dendrimers shape: Considering the average values of the three principal moments of inertia I_x , I_y , I_z (in decreasing order) and the asphericity, a structure-persistent characteristic of these dendrimers can be obtained.

Molecular asphericity was calculated as defined:¹⁷

$$\delta = 1 - 3 \frac{\langle I_2 \rangle}{\langle I_1^2 \rangle}$$

where I_1 and I_2 are the first and second invariants of the radius of gyration tensor: $I_1 = I_x + I_y + I_z$, $I_2 = I_x I_y + I_y I_z + I_x I_z$. This quantity assumes values between 1 (for a linear array of atoms) and 0 (for shapes of high 3D similarity).

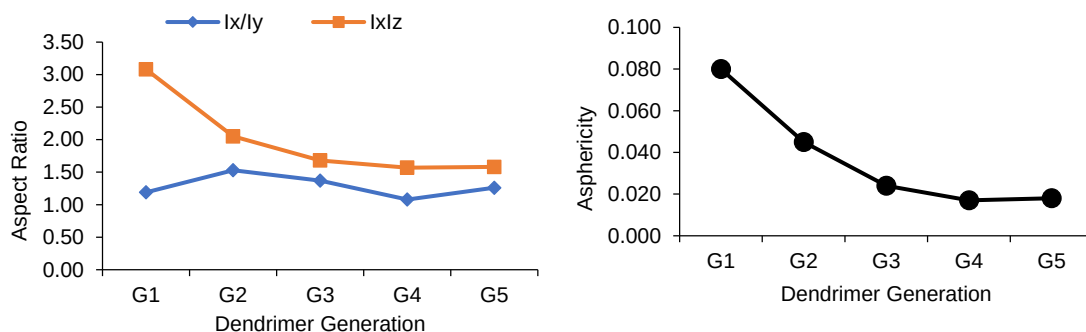
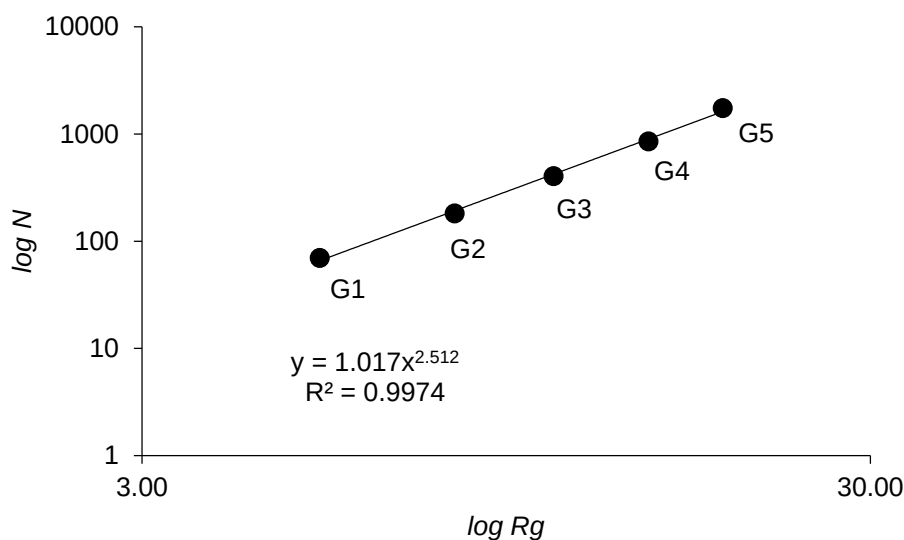


Figure S77. a) Aspect ratios and b) asphericity values for **G1-5** dendrimers as function of their generation.

Fractal dimension (d_f) for G_n



$$N \sim R_g^{2.51}$$

Figure S78. Relationship between the number of atoms (N) of the **G1-5** dendrimers and their R_g values.

Monomer radial distribution functions: The average radial distribution function $\rho(r)$ can be expressed conveniently the dendrimers conformations. This radial function can be defined by counting the number $N(r)$ of atoms whose centers of mass are located within the spherical shell of radius r and thickness Δr . Hence, integration over r yields the total number of atoms as: $N(r) = 4\pi \int_0^\infty r^2 \rho(r) dr$, where r is the distance from the dendrimer center of mass.

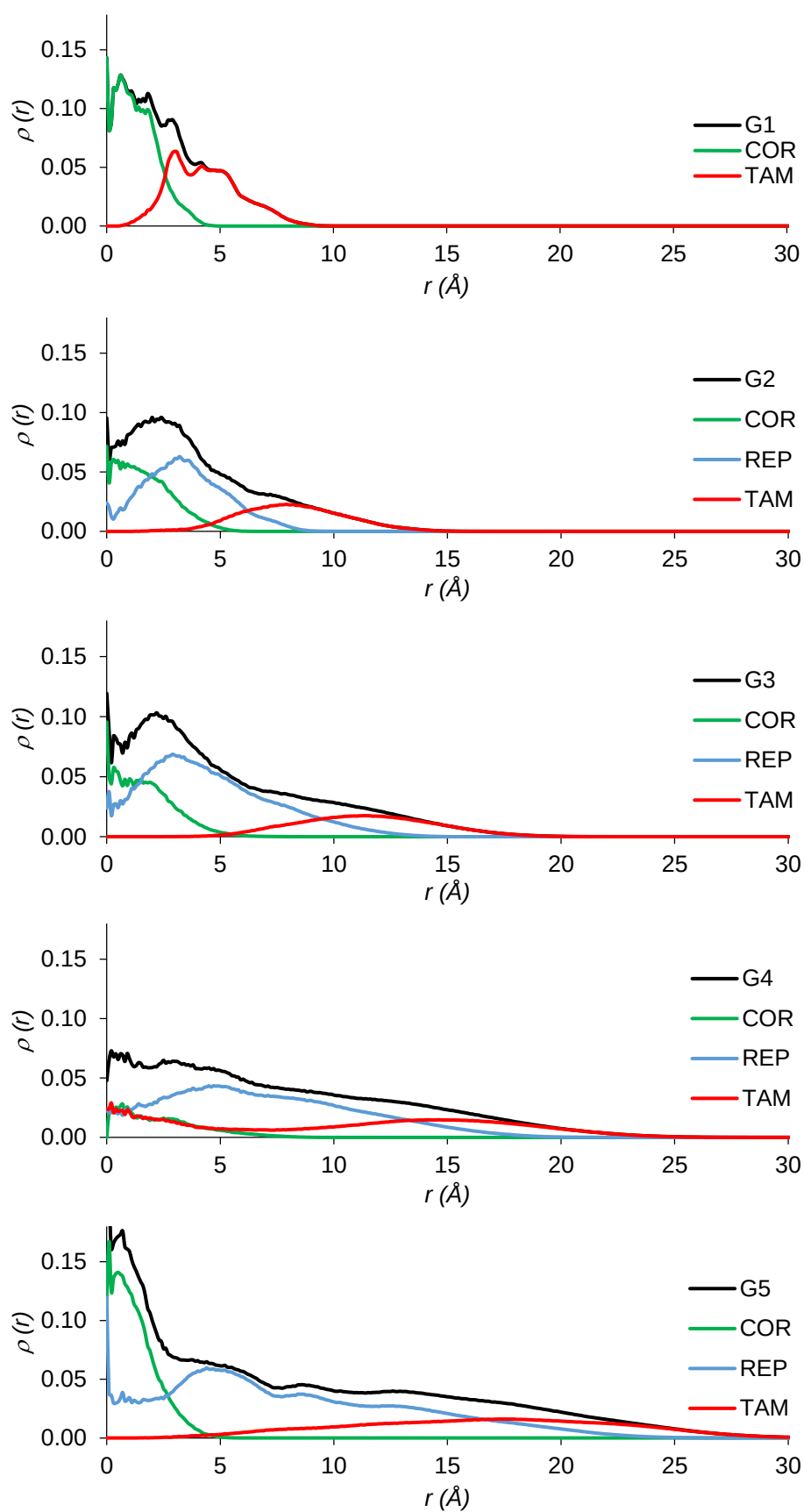


Figure S79. Radial distribution function of the **G1-5** dendrimers and its monomers using dendrimer center of mass as reference. The unit value for $\rho(r)$ is expressed in $\text{atoms}/\text{\AA}^3$.

8.- References

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9.- Optimized structures of cap-residues and optimized geometries of the dendrimers before MDS

Atomic coordinates for the optimized ground state (S_0) of **cap-COR** at B3LYP/6-31G(d)

Energy (Hartrees)	-492.8498150		
Imaginary freq.	0		
	Coordinates (Angstroms)		
Atom type	X	Y	Z
N	-1.828800	-0.359282	-0.000003
C	-0.618230	0.449288	0.000035
C	0.618261	-0.449343	-0.000033
N	1.828831	0.359226	0.000004
C	-3.066455	0.159608	-0.000042
C	-4.218473	-0.841668	0.000003
O	-3.301509	1.370485	0.000014
C	3.066425	-0.159561	-0.000032
C	4.218448	0.841693	0.000020
O	3.301484	-1.370460	0.000008
H	-1.715020	-1.362776	0.000064
H	-0.606200	1.080824	-0.889270
H	-0.606231	1.080774	0.889222
H	0.606262	-1.080830	-0.889221
H	0.606314	-1.080825	0.889279
H	1.715001	1.362779	0.000057
H	-4.154482	-1.472467	0.887277
H	-4.154447	-1.472616	-0.887155
H	-5.174082	-0.315961	-0.000080
H	5.174052	0.316008	0.000006
H	4.154478	1.472560	0.887157
H	4.154485	1.472628	-0.887225

Atomic coordinates for the optimized ground state (S_0) of **cap-REP** at B3LYP/6-31G(d)

Energy (Hartrees)	-900.4362899		
Imaginary freq.	0		
	Coordinates (Angstroms)		
Atom type	X	Y	Z
C	2.532950	3.169227	-1.102165
N	1.717474	2.042394	-0.664795
C	0.891111	2.083185	0.383716
C	0.092548	0.811626	0.703195
O	0.765138	3.084561	1.081815
C	0.877231	-0.041761	1.726464

C	0.477538	-1.530450	1.796176
C	0.756620	-2.349620	0.522006
N	2.188933	-2.463901	0.246328
C	2.862953	-1.683243	-0.607012
C	4.325041	-2.022731	-0.853429
O	2.352065	-0.717671	-1.169100
C	-1.332618	1.142439	1.216840
C	-2.206679	1.946724	0.231118
C	-2.588170	1.204751	-1.061416
N	-3.617585	0.195415	-0.814777
C	-3.379134	-1.097051	-0.564571
C	-4.585352	-2.014636	-0.435746
O	-2.246523	-1.547228	-0.426630
H	3.202943	3.475251	-0.296768
H	1.889791	4.011153	-1.364489
H	3.124443	2.884070	-1.973062
H	1.828109	1.158026	-1.151135
H	0.000683	0.245234	-0.220817
H	0.754285	0.400319	2.716936
H	1.941117	0.013355	1.493189
H	-0.586104	-1.604811	2.022651
H	1.015471	-1.992292	2.625565
H	0.243513	-1.908958	-0.333429
H	0.346598	-3.351564	0.660748
H	2.678080	-3.236455	0.671457
H	4.873344	-1.976425	0.086809
H	4.752233	-1.309062	-1.557862
H	4.399573	-3.027651	-1.267374
H	-1.242849	1.726627	2.134974
H	-1.854902	0.223341	1.475801
H	-1.682417	2.863631	-0.041625
H	-3.121436	2.248691	0.743741
H	-1.707093	0.751679	-1.518610
H	-2.986884	1.934032	-1.769179
H	-4.577706	0.489468	-0.907948
H	-5.221194	-1.668304	0.378088
H	-4.250594	-3.030801	-0.227603
H	-5.150431	-2.003953	-1.367089

Atomic coordinates for the optimized ground state (S_0) of **cap-TAM** at PCM(H_2O)/B3LYP/6-31G(d)

Energy (Hartrees)	-596.0253932		
Imaginary freq.	0		
	Coordinates (Angstroms)		
Atom type	X	Y	Z
C	-0.000564	3.478630	-0.222687
N	-0.000399	2.065716	-0.562275
C	0.000020	1.077562	0.344208
C	0.000074	-0.357159	-0.206522
O	0.000303	1.277202	1.559898
C	-1.258068	-1.130957	0.235419
C	-2.555439	-0.487740	-0.279099
C	-3.771020	-1.324250	0.133813
N	-5.026509	-0.724111	-0.347402
C	1.258245	-1.130810	0.235412
C	2.555539	-0.487512	-0.279080

C	3.771179	-1.324006	0.133613
N	5.026720	-0.723821	-0.347445
H	-0.890971	3.716024	0.360082
H	-0.001050	4.069980	-1.138252
H	0.890229	3.716311	0.359407
H	-0.000665	1.829224	-1.544078
H	0.000063	-0.321746	-1.298161
H	-1.200531	-2.148757	-0.153778
H	-1.290126	-1.181815	1.325103
H	-2.518048	-0.420763	-1.367608
H	-2.659146	0.515908	0.135690
H	-3.808241	-1.394590	1.221246
H	-3.677736	-2.327605	-0.282707
H	-5.127975	0.202144	0.042359
H	-5.006761	-0.664871	-1.355422
H	-5.806210	-1.297853	-0.059130
H	1.200788	-2.148689	-0.153832
H	1.290338	-1.181761	1.325106
H	2.659271	0.516049	0.135867
H	2.518062	-0.420402	-1.367567
H	3.678019	-2.327324	-0.283012
H	3.808396	-1.394546	1.221123
H	5.128057	0.202347	0.042490
H	5.006904	-0.664345	-1.355421
H	5.806429	-1.297569	-0.059299

Atomic coordinates for the optimized structure of **G1** with AMBER at MM level (parm99, gaff)

Energy (kcal/mol)	-18478		
	Coordinates (Angstroms)		
Atom type	X	Y	Z
N	18.184999	22.580999	18.549000
H	18.676001	22.103001	17.813999
C	18.735001	22.475000	19.903999
H	18.902000	23.479000	20.313000
H	18.017000	21.954000	20.547001
C	20.058001	21.701000	19.844999
H	20.782000	22.271999	19.252001
H	19.893000	20.737000	19.350000
N	20.638000	21.445999	21.167000
H	20.211000	21.886000	21.980000
C	17.091999	23.288000	18.215000
O	16.445000	23.892000	19.042999
C	16.747999	23.278000	16.732000
C	17.091000	24.653999	16.091999
C	18.615000	24.941999	16.136000
C	18.958000	26.346001	15.603000
N	20.431999	26.665001	15.663000
H	20.825001	26.500999	16.617001
H	20.996000	26.094999	15.001000
H	20.608000	27.664000	15.436000
H	18.444000	27.101000	16.205000
H	18.636000	26.454000	14.564000
H	19.148001	24.188999	15.550000
H	18.978001	24.875999	17.165001
H	16.752001	24.671000	15.052000

H	16.549999	25.444000	16.622000
C	15.256000	22.896999	16.520000
C	14.949000	21.474001	17.052000
C	13.467000	21.101000	16.865000
N	13.101000	19.764999	17.469999
H	13.401000	19.671000	18.464001
H	13.550000	18.971001	16.983999
H	12.080000	19.580000	17.417000
H	13.217000	21.065001	15.799000
H	12.836000	21.855000	17.341999
H	15.191000	21.414000	18.115999
H	15.574000	20.743000	16.531000
H	15.018000	22.941000	15.454000
H	14.615000	23.625999	17.023001
H	17.349001	22.517000	16.230000
C	21.737000	20.686001	21.334999
O	22.291000	20.155001	20.389000
C	22.233000	20.540001	22.764999
C	23.700001	21.049999	22.885000
C	23.884001	22.518000	22.413000
C	25.377001	22.902000	22.407000
N	25.688000	24.230000	21.760000
H	25.301001	24.296000	20.792999
H	25.332001	25.039000	22.311001
H	26.718000	24.353001	21.700001
H	25.941999	22.152000	21.847000
H	25.768999	22.936001	23.427999
H	23.325001	23.195000	23.065001
H	23.493999	22.639000	21.399000
H	24.031000	20.962000	23.924000
H	24.348000	20.402000	22.288000
C	22.143999	19.051001	23.214001
C	20.702000	18.479000	23.174000
C	20.707001	16.962000	23.459999
N	19.350000	16.299000	23.424999
H	18.847000	16.452999	22.523001
H	18.724001	16.625000	24.174000
H	19.448000	15.265000	23.535999
H	21.135000	16.764000	24.447001
H	21.322001	16.451000	22.714001
H	20.254999	18.643999	22.190001
H	20.079000	18.997999	23.909000
H	22.539000	18.955000	24.229000
H	22.787001	18.448000	22.566000
H	21.605000	21.141001	23.427999

Atomic coordinates for the optimized structure of **G2** with AMBER at MM level (parm99, gaff)

Energy (kcal/mol)	-45584		
	Coordinates (Angstroms)		
Atom type	X	Y	Z
N	26.924999	25.910000	25.434999
H	27.903000	26.141001	25.518000
C	26.021000	26.341999	26.511000
H	25.197001	26.926001	26.089001
H	25.603001	25.451000	26.995001

C	26.756001	27.183001	27.566999
H	27.018000	28.159000	27.143999
H	27.681999	26.673000	27.857000
N	25.929001	27.375999	28.770000
H	25.421000	28.250999	28.871000
C	26.555000	25.136000	24.395000
O	25.392000	24.809000	24.247000
C	27.679001	24.688000	23.471001
C	27.816999	23.142000	23.572001
C	29.219999	22.615000	23.180000
C	30.253000	22.792999	24.313999
N	30.072001	21.818001	25.412001
H	29.770000	20.874001	25.167000
H	30.214001	23.816999	24.704000
H	31.256001	22.656000	23.893999
H	29.572001	23.129000	22.283001
H	29.150000	21.554001	22.926001
H	27.065001	22.672001	22.933001
H	27.596001	22.816000	24.591999
H	28.612000	25.141001	23.812000
C	27.423000	25.136000	22.002001
H	26.534000	24.620001	21.628000
H	28.253000	24.819000	21.367001
C	27.200001	26.660000	21.816999
H	26.368999	26.985001	22.447001
H	26.889999	26.848000	20.785000
C	28.438000	27.532000	22.127001
H	28.865000	27.260000	23.097000
H	28.110001	28.576000	22.200001
N	29.483000	27.457001	21.084999
H	29.379999	28.070000	20.275999
C	25.878000	26.490000	29.785000
O	26.471001	25.430000	29.719000
C	25.052000	26.885000	30.996000
C	23.796000	25.975000	31.054001
C	22.719999	26.434999	32.067001
C	22.000999	27.740999	31.660999
N	21.149000	27.552000	30.469999
H	20.271000	27.055000	30.608000
H	22.726000	28.544001	31.490999
H	21.364000	28.063000	32.492001
H	23.166000	26.559999	33.056000
H	21.975000	25.642000	32.162998
H	24.104000	24.958000	31.309999
H	23.346001	25.914000	30.059999
H	24.729000	27.915001	30.870001
C	25.886999	26.789000	32.306999
H	26.025000	25.737000	32.566002
H	25.330999	27.243999	33.129002
C	27.289000	27.448000	32.234001
H	27.893999	26.938999	31.480000
H	27.802999	27.290001	33.186001
C	27.261000	28.959000	31.920000
H	26.641001	29.157000	31.039000
H	28.278000	29.278000	31.667999
N	26.799000	29.764999	33.064999
H	27.489000	29.961000	33.789001
C	30.420000	22.046000	26.695999

O	30.750999	23.153000	27.076000
C	30.379999	20.841000	27.625999
C	29.625000	21.139000	28.950001
C	28.209999	21.731001	28.789000
C	27.546000	21.784000	30.179001
N	26.395000	22.740999	30.290001
H	26.695999	23.716999	30.087000
H	25.635000	22.535000	29.610001
H	25.993999	22.743999	31.249001
H	28.282000	22.107000	30.921000
H	27.187000	20.791000	30.462999
H	27.608000	21.124001	28.108000
H	28.280001	22.740000	28.372000
H	29.552000	20.208000	29.517000
H	30.219999	21.830999	29.554001
C	31.816000	20.407000	28.021999
C	32.675999	19.830000	26.878000
C	34.062000	19.487000	27.462999
N	34.983002	18.695999	26.575001
H	35.324001	19.205999	25.732000
H	34.563000	17.802999	26.254000
H	35.833000	18.424000	27.114000
H	33.931000	18.891001	28.371000
H	34.587002	20.405001	27.743000
H	32.782001	20.556000	26.066999
H	32.202000	18.931000	26.475000
H	31.754999	19.652000	28.812000
H	32.333000	21.268999	28.451000
H	29.875999	20.011999	27.125000
C	30.608999	26.719000	21.173000
O	30.778999	25.951000	22.098000
C	31.658001	26.952000	20.090000
C	31.896999	25.674000	19.226999
C	30.908001	25.493999	18.049000
C	31.419001	24.360001	17.127001
N	30.832001	24.299999	15.735000
H	29.844999	23.972000	15.689000
H	30.855000	25.211000	15.259000
H	31.388000	23.657000	15.128000
H	31.268000	23.384001	17.597000
H	32.494999	24.490000	16.982000
H	30.856001	26.423000	17.478001
H	29.903999	25.268999	18.417999
H	32.903000	25.722000	18.799000
H	31.882999	24.785000	19.865999
C	33.019001	27.386000	20.712999
C	32.959000	28.671000	21.577000
C	34.395000	29.171000	21.858000
N	34.505001	30.379999	22.753000
H	34.459999	30.139999	23.767000
H	33.743999	31.063000	22.573000
H	35.404999	30.881001	22.601000
H	34.861000	29.450001	20.909000
H	34.992001	28.379000	22.318001
H	32.438999	28.466000	22.517000
H	32.403000	29.450001	21.049000
H	33.730000	27.554001	19.900000
H	33.417999	26.566999	21.320999

H	31.325001	27.761000	19.436001
C	21.437000	27.973000	29.224001
O	22.474001	28.562000	28.990000
C	20.381001	27.688999	28.158001
C	21.030001	27.247000	26.811001
C	21.702999	25.854000	26.848000
C	22.344000	25.558001	25.472000
N	22.886000	24.166000	25.285000
H	23.153000	23.711000	26.180000
H	22.219999	23.544001	24.777000
H	23.747000	24.184999	24.701000
H	23.181999	26.242001	25.313000
H	21.614000	25.715000	24.673000
H	20.955999	25.090000	27.082001
H	22.472000	25.822001	27.624001
H	20.260000	27.222000	26.035000
H	21.763000	27.997999	26.500000
C	19.514000	28.955999	27.900000
C	18.587000	29.348000	29.077000
C	17.805000	30.629999	28.716000
N	16.843000	31.122000	29.767000
H	17.275999	31.165001	30.712999
H	15.991000	30.535999	29.879999
H	16.514000	32.087002	29.554001
H	17.226000	30.476999	27.801001
H	18.514999	31.444000	28.542000
H	19.174999	29.528000	29.980000
H	17.889000	28.532000	29.290001
H	18.886000	28.788000	27.020000
H	20.174999	29.795000	27.660999
H	19.729000	26.882000	28.503000
C	25.587000	30.344000	33.178001
O	24.731001	30.179001	32.330002
C	25.407000	31.268000	34.382000
C	24.177000	30.860001	35.264000
C	24.556000	30.174000	36.606998
C	23.294001	29.902000	37.467999
N	23.544001	29.465000	38.896999
H	24.063999	28.568001	38.993000
H	24.104000	30.166000	39.424999
H	22.660000	29.362000	39.438999
H	22.677999	29.131001	36.995998
H	22.700001	30.818001	37.537998
H	25.233000	30.827000	37.164001
H	25.084000	29.237000	36.412998
H	23.587999	31.750999	35.499001
H	23.511999	30.204000	34.694000
C	25.264999	32.743999	33.901001
C	26.459000	33.238998	33.041000
C	26.344000	34.754002	32.764999
N	27.459999	35.337002	31.937000
H	27.388000	35.155998	30.915001
H	28.396000	34.998001	32.233002
H	27.507000	36.373001	32.034000
H	26.358999	35.292000	33.717999
H	25.407000	34.980999	32.248001
H	26.486000	32.698002	32.090000
H	27.398001	33.040001	33.564999

H	25.172001	33.391998	34.777000
H	24.341999	32.849998	33.323002
H	26.309000	31.216000	34.998001

Atomic coordinates for the optimized structure of **G3** with AMBER at MM level (parm99, gaff)

Energy (kcal/mol)	-56846		
	Coordinates (Angstroms)		
Atom type	X	Y	Z
N	30.606001	34.410999	29.278999
H	31.024000	34.726002	28.403999
C	31.537001	34.141998	30.392000
H	31.767000	35.082001	30.903999
H	31.052000	33.487999	31.115000
C	32.842999	33.486000	29.907000
H	33.483002	34.251999	29.455999
H	32.605999	32.762001	29.121000
N	33.583000	32.813999	30.997999
H	33.872002	33.397999	31.782000
C	29.263000	34.271999	29.358999
O	28.753000	33.842999	30.379000
C	28.445000	34.599998	28.108000
C	27.304001	33.550999	27.973000
C	26.417999	33.645000	26.702999
C	27.183001	33.643002	25.356001
N	28.142000	32.536999	25.125000
H	29.002001	32.793999	24.650999
H	27.731001	34.589001	25.271000
H	26.448999	33.638000	24.542000
H	25.802999	34.544998	26.750999
H	25.711000	32.814999	26.716999
H	26.646000	33.619999	28.843000
H	27.752001	32.557999	28.006001
H	29.086000	34.485001	27.238001
C	27.896999	36.056000	28.146000
H	27.403000	36.227001	29.106001
H	27.136999	36.196999	27.378000
C	28.975000	37.146999	27.930000
H	29.740000	37.063999	28.705999
H	28.513000	38.130001	28.054001
C	29.650000	37.084000	26.539000
H	30.115999	36.108002	26.385000
H	30.466999	37.816002	26.521999
N	28.740999	37.394001	25.414000
H	28.103001	38.187000	25.525000
C	33.903000	31.500000	31.017000
O	33.534000	30.766001	30.118000
C	34.702000	30.987000	32.216999
C	34.105000	29.618000	32.660999
C	34.629002	29.028999	33.998001
C	34.286999	29.858000	35.264000
N	32.863998	30.208000	35.474998
H	32.687000	31.156000	35.778999
H	34.865002	30.788000	35.223999
H	34.639999	29.312000	36.144001
H	35.709999	28.889000	33.945999

H	34.221001	28.023001	34.105999
H	34.294998	28.882000	31.875000
H	33.022999	29.712000	32.727001
H	34.598000	31.693001	33.042999
C	36.205002	30.833000	31.843000
H	36.283001	30.201000	30.955000
H	36.741001	30.309999	32.636002
C	36.946999	32.164001	31.563999
H	36.429001	32.721001	30.780001
H	37.941002	31.931000	31.173000
C	37.110001	33.061001	32.811001
H	36.123001	33.347000	33.195000
H	37.611000	33.990002	32.518002
N	37.905998	32.423000	33.882999
H	38.853001	32.106998	33.669998
C	28.031000	31.238001	25.483000
O	27.033001	30.775999	26.007000
C	29.218000	30.334999	25.188999
C	29.084999	29.763000	23.750999
C	29.766001	28.382000	23.556000
C	29.033001	27.219999	24.273001
N	27.660000	27.023001	23.761000
H	27.480000	27.296000	22.791000
H	29.021999	27.381001	25.354000
H	29.594999	26.296000	24.094999
H	30.802000	28.427999	23.899000
H	29.804001	28.160999	22.486000
H	29.510000	30.475000	23.038000
H	28.028000	29.672001	23.488001
H	29.129999	29.504000	25.881001
C	30.618000	30.975000	25.433001
H	30.853001	31.649000	24.607000
H	31.365999	30.183001	25.407000
C	30.799999	31.775000	26.750000
H	30.266001	32.717999	26.664000
H	31.855000	32.047001	26.847000
C	30.341999	31.063999	28.041000
H	29.327999	30.674999	27.924000
H	30.313000	31.798000	28.851999
N	31.264000	29.993999	28.448999
H	32.141998	30.275000	28.888000
C	28.913000	36.929001	24.156000
O	29.653999	35.986000	23.950001
C	28.170000	37.680000	23.052999
C	28.855000	39.066002	22.854000
C	28.010000	40.109001	22.077999
C	26.694000	40.507999	22.785000
N	26.893999	41.361000	23.973000
H	26.834000	42.355999	23.829000
H	26.112000	39.622002	23.058001
H	26.079000	41.057999	22.065001
H	27.773001	39.727001	21.084000
H	28.612000	41.007000	21.922001
H	29.801001	38.918999	22.327000
H	29.118000	39.500999	23.820000
H	27.146999	37.825001	23.400000
C	28.141001	36.882000	21.712000
H	29.152000	36.537998	21.480000

H	27.862000	37.534000	20.885000
C	27.186001	35.660999	21.715000
H	27.301001	35.110001	22.650999
H	27.486000	34.980000	20.914000
C	25.698000	36.034000	21.510000
H	25.402000	36.799000	22.237000
H	25.080999	35.148998	21.702000
N	25.403999	36.508999	20.136999
H	25.253000	35.813000	19.408001
C	31.775000	29.451000	35.220001
O	31.864000	28.278999	34.908001
C	30.410999	30.118000	35.328999
C	29.809999	29.888000	36.741001
C	28.260000	29.811001	36.757000
C	27.693001	28.488001	36.189999
N	28.091000	27.309000	36.990002
H	28.160000	27.426001	38.001999
H	27.997999	28.362000	35.146999
H	26.598000	28.545000	36.193001
H	27.841999	30.653999	36.202999
H	27.914000	29.917999	37.786999
H	30.131001	30.701000	37.394001
H	30.214001	28.969000	37.173000
H	29.782000	29.583000	34.625999
C	30.372000	31.625000	34.925999
H	30.830999	32.223000	35.716999
H	29.327999	31.943001	34.870998
C	31.063000	31.999001	33.585999
H	32.146000	31.938999	33.695999
H	30.851999	33.049999	33.373001
C	30.643000	31.142000	32.374001
H	30.775999	30.080000	32.594002
H	31.298000	31.368999	31.528000
N	29.260000	31.410999	31.958000
H	29.066000	32.306000	31.504999
C	37.509998	32.312000	35.168999
O	36.404999	32.678001	35.520000
C	38.547001	31.739000	36.126999
C	39.508999	32.882999	36.560001
C	40.784000	32.425999	37.319000
C	41.654999	31.405001	36.550999
N	42.339001	31.975000	35.369999
H	43.284000	32.303001	35.512001
H	41.063000	30.533001	36.254002
H	42.422001	31.025999	37.237999
H	40.507000	31.996000	38.283001
H	41.389999	33.307999	37.544998
H	38.959999	33.591999	37.186001
H	39.825001	33.441002	35.674999
H	39.110001	30.989000	35.575001
C	37.882000	31.024000	37.337002
H	37.039001	31.614000	37.703999
H	38.578999	30.965000	38.167999
C	37.401001	29.593000	36.988998
H	37.054001	29.559999	35.955002
H	36.547001	29.341000	37.622002
C	38.500000	28.525999	37.195000
H	39.402000	28.797001	36.636002

H	38.146999	27.563000	36.801998
N	38.813000	28.364000	38.627998
H	38.021000	28.290001	39.266998
C	26.639000	26.462000	24.437000
O	26.750000	26.194000	25.618000
C	25.333000	26.288000	23.670000
C	24.268000	27.313000	24.157000
C	24.777000	28.774000	24.124001
C	23.646000	29.768999	24.445000
N	24.139999	31.141001	24.811001
H	24.587999	31.132999	25.750000
H	24.819000	31.509001	24.113001
H	23.351999	31.823999	24.843000
H	23.058001	29.414000	25.296000
H	22.987000	29.878000	23.579000
H	25.194000	29.010000	23.139999
H	25.576000	28.893999	24.857000
H	23.382000	27.229000	23.521999
H	23.959999	27.063999	25.176001
C	24.774000	24.839001	23.806000
C	25.559999	23.816999	22.951000
C	25.020000	22.379000	23.125000
N	25.530001	21.386999	22.103001
H	26.570999	21.326000	22.070999
H	25.240000	21.638000	21.146999
H	25.171000	20.423000	22.288000
H	23.930000	22.379000	23.042000
H	25.289000	21.997000	24.114000
H	26.620001	23.841000	23.219000
H	25.475000	24.108000	21.900999
H	23.731001	24.822001	23.480000
H	24.783001	24.534000	24.857000
H	25.518999	26.482000	22.610001
C	31.037001	28.677000	28.318001
O	29.992001	28.256001	27.851000
C	32.148998	27.775999	28.833000
C	32.898998	27.086000	27.663000
C	33.639999	28.099001	26.753000
C	34.466999	27.354000	25.690001
N	35.167999	28.222000	24.674999
H	34.512001	28.826000	24.136999
H	35.875999	28.864000	25.091000
H	35.678001	27.628000	23.992001
H	33.820000	26.676001	25.127001
H	35.240002	26.754000	26.179001
H	34.301998	28.729000	27.353001
H	32.919998	28.750999	26.256001
H	33.631001	26.384001	28.073999
H	32.193001	26.500999	27.066999
C	31.577000	26.733000	29.830000
C	31.011999	27.419001	31.096001
C	30.311001	26.410999	32.019001
N	29.777000	27.052000	33.268002
H	29.160000	27.858999	33.037998
H	30.552000	27.388000	33.872002
H	29.205999	26.391001	33.838001
H	31.002001	25.622000	32.321999
H	29.468000	25.952000	31.499001

H	30.291000	28.191999	30.820000
H	31.826000	27.903999	31.639000
H	32.366001	26.035000	30.128000
H	30.792999	26.146999	29.341999
H	32.879002	28.379999	29.378000
C	26.976999	40.924999	25.246000
O	27.077999	39.745998	25.518000
C	26.889999	42.012001	26.309000
C	28.181999	42.102001	27.164000
C	29.450001	42.346001	26.312000
C	30.597000	42.886002	27.191000
N	31.941000	42.900002	26.514000
H	32.342999	41.941002	26.504000
H	31.908001	43.285999	25.544001
H	32.627998	43.462002	27.055000
H	30.708000	42.272999	28.091000
H	30.375000	43.912998	27.493999
H	29.243999	43.071999	25.521000
H	29.752001	41.410000	25.834000
H	28.066999	42.921001	27.879999
H	28.309000	41.183998	27.746000
C	25.660000	41.776001	27.229000
C	24.327999	41.875999	26.451000
C	23.120001	41.658001	27.379999
N	21.805000	41.881001	26.688000
H	21.702999	41.250000	25.862000
H	21.742001	42.858002	26.350000
H	20.983999	41.720001	27.305000
H	23.158001	42.351002	28.226000
H	23.118999	40.633999	27.764000
H	24.299000	41.131001	25.650999
H	24.254999	42.862999	25.985001
H	25.657000	42.520000	28.031000
H	25.738001	40.792000	27.702999
H	26.754999	42.979000	25.816999
C	25.231001	37.800999	19.792000
O	25.266001	38.685001	20.625999
C	24.950001	38.083000	18.320999
C	26.134001	38.832001	17.646000
C	27.357000	37.926998	17.368000
C	28.431999	38.728001	16.601000
N	29.601000	37.922001	16.094999
H	30.124001	37.424999	16.843000
H	29.292000	37.214001	15.394000
H	30.268000	38.537998	15.581000
H	28.837000	39.518002	17.238001
H	27.981001	39.191002	15.718000
H	27.045000	37.070000	16.764000
H	27.771000	37.543999	18.304001
H	25.796000	39.237999	16.688000
H	26.430000	39.682999	18.266001
C	23.653000	38.924000	18.174000
C	22.400000	38.145000	18.625999
C	21.138000	39.007000	18.450001
N	19.867001	38.216000	18.565001
H	19.747000	37.768002	19.493999
H	19.853001	37.445000	17.870001
H	19.018000	38.786999	18.389000

H	21.132999	39.460999	17.455999
H	21.110001	39.805000	19.197001
H	22.490000	37.841999	19.673000
H	22.311001	37.235001	18.025999
H	23.521999	39.206001	17.125000
H	23.743000	39.851002	18.749001
H	24.797001	37.139000	17.792000
C	28.344999	26.082001	36.491001
O	28.306999	25.879000	35.292999
C	28.768999	25.016001	37.495998
C	30.242001	24.582001	37.250000
C	31.209999	25.782000	37.160000
C	32.665001	25.322001	36.971001
N	33.608002	26.459999	36.689999
H	33.282001	27.017000	35.876999
H	33.680000	27.086000	37.518002
H	34.563000	26.099001	36.473000
H	32.734001	24.638000	36.122002
H	33.026001	24.806999	37.867001
H	31.129000	26.398001	38.056999
H	30.933001	26.403000	36.310001
H	30.561001	23.920000	38.060001
H	30.302000	24.007000	36.320999
C	27.860001	23.756001	37.438999
C	26.393999	24.027000	37.849998
C	25.607000	22.698999	37.888000
N	24.157000	22.830999	38.278999
H	23.584999	23.348000	37.578999
H	24.031000	23.278999	39.208000
H	23.704000	21.898001	38.351002
H	26.068001	22.021000	38.612000
H	25.632000	22.219000	36.904999
H	25.927999	24.715000	37.139999
H	26.368999	24.493999	38.838001
H	28.273001	22.996000	38.108002
H	27.882000	23.334000	36.429001
H	28.707001	25.434999	38.502998
C	28.230000	30.566000	32.129002
O	28.388000	29.472000	32.643002
C	26.893999	31.061001	31.601000
C	25.982000	31.532000	32.764000
C	26.375000	32.945000	33.258999
C	25.548000	33.334999	34.495998
N	25.667000	34.782001	34.896999
H	26.649000	35.132999	34.882999
H	25.125999	35.403000	34.264999
H	25.257999	34.930000	35.839001
H	25.863001	32.737000	35.355000
H	24.485001	33.151001	34.316002
H	26.201000	33.669998	32.458000
H	27.437000	32.985001	33.511002
H	24.941999	31.563000	32.428001
H	26.032000	30.809999	33.584999
C	26.212000	29.955999	30.757999
C	27.051001	29.620001	29.507000
C	26.429001	28.483999	28.684999
N	27.209999	28.226999	27.429001
H	28.219000	28.073000	27.639999

H	27.146999	29.042999	26.791000
H	26.877001	27.386000	26.913000
H	25.403999	28.733000	28.396999
H	26.416000	27.559000	29.266001
H	28.063000	29.323999	29.795000
H	27.129999	30.511000	28.882999
H	25.230000	30.308001	30.438000
H	26.058001	29.059000	31.365000
H	27.062000	31.910999	30.936001
C	41.896000	31.902000	34.095001
O	40.756001	31.586000	33.823002
C	42.945999	32.179001	33.027000
C	42.397999	33.125000	31.920000
C	41.993999	34.515999	32.464001
C	41.410000	35.389000	31.336000
N	41.025002	36.771000	31.790001
H	40.331001	36.755001	32.567001
H	41.849998	37.312000	32.116001
H	40.598999	37.333000	31.025999
H	40.509998	34.921001	30.927000
H	42.141998	35.505001	30.530001
H	42.868000	35.007999	32.898998
H	41.244999	34.408001	33.254002
H	43.160999	33.252998	31.146000
H	41.532001	32.657001	31.441000
C	43.438999	30.844999	32.387001
C	43.813000	29.771999	33.443001
C	44.471001	28.528000	32.813999
N	44.508999	27.353001	33.761002
H	43.556000	26.937000	33.834999
H	44.801998	27.635000	34.721001
H	45.136002	26.591999	33.457001
H	45.497002	28.761999	32.516998
H	43.908001	28.207001	31.931999
H	42.908001	29.457001	33.970001
H	44.493000	30.202000	34.182999
H	44.304001	31.055000	31.750999
H	42.653000	30.441999	31.740000
H	43.804001	32.668999	33.497002
C	40.044998	28.346001	39.167999
O	41.049000	28.358000	38.480000
C	40.087002	28.329000	40.691002
C	40.488998	29.733999	41.237000
C	39.292000	30.716000	41.374001
C	39.764000	32.076000	41.942001
N	38.695000	33.120998	42.183998
H	38.168999	33.383999	41.326000
H	37.994999	32.841999	42.903999
H	39.139000	33.994999	42.539001
H	40.491001	32.523998	41.258999
H	40.257000	31.917000	42.904999
H	38.539001	30.287001	42.041000
H	38.819000	30.868000	40.403000
H	40.955002	29.620001	42.216999
H	41.254002	30.170000	40.588001
C	41.054001	27.233999	41.229000
C	40.720001	25.802000	40.731998
C	41.464001	24.750999	41.585999

N	41.556999	23.361000	41.000999
H	42.186001	23.377001	40.168999
H	40.640999	22.957001	40.716999
H	41.966000	22.686001	41.681000
H	40.984001	24.659000	42.563999
H	42.497002	25.077999	41.744999
H	41.014000	25.705000	39.682999
H	39.644001	25.617001	40.792000
H	41.012001	27.243999	42.320999
H	42.084000	27.478001	40.949001
H	39.092999	28.082001	41.069000

Atomic coordinates for the optimized structure of **G4** with AMBER at MM level (parm99, gaff)

Energy (kcal/mol)	-105380		
	Coordinates (Angstroms)		
Atom type	X	Y	Z
N	36.060001	39.166000	33.558998
H	36.416000	39.532001	32.675999
C	37.051998	38.719002	34.548000
H	37.926998	39.376999	34.516998
H	36.611000	38.785999	35.549000
C	37.474998	37.271000	34.257999
H	38.188999	37.256001	33.426998
H	36.591000	36.694000	33.965000
N	38.068001	36.618999	35.430000
H	38.057999	37.125999	36.299999
C	34.726002	39.106998	33.757000
O	34.263000	38.701000	34.806000
C	33.847000	39.534000	32.591999
C	32.777000	38.428001	32.362000
C	31.986000	38.542000	31.034000
C	32.846001	38.265999	29.784000
N	33.324001	36.872002	29.719000
H	33.064999	36.242001	30.464001
H	33.700001	38.952000	29.756001
H	32.243000	38.459999	28.889999
H	31.531000	39.529999	30.950001
H	31.160000	37.826000	31.056999
H	32.063999	38.445000	33.189999
H	33.261002	37.448002	32.396999
H	34.466999	39.612999	31.698999
C	33.185001	40.910000	32.889000
H	32.580002	40.825001	33.794998
H	32.500000	41.179001	32.084000
C	34.191002	42.073002	33.082001
H	34.882999	41.837002	33.894001
H	33.641998	42.965000	33.396000
C	34.993999	42.410999	31.808001
H	35.556999	41.535999	31.469999
H	35.734001	43.181999	32.055000
N	34.134998	42.917999	30.722000
H	33.520000	43.705002	30.934000
C	38.537998	35.355999	35.424000
O	38.605000	34.713001	34.394001
C	38.941002	34.801998	36.783001

C	38.161999	33.477001	37.021999
C	38.305000	32.855999	38.433998
C	37.772999	33.743000	39.581001
N	36.304001	33.907001	39.587002
H	35.759998	33.438000	38.877998
H	38.250999	34.729000	39.556999
H	38.055000	33.276001	40.532001
H	39.354000	32.619999	38.624001
H	37.772999	31.902000	38.452000
H	38.498001	32.736000	36.293999
H	37.099998	33.648998	36.825001
H	38.639000	35.514000	37.550999
C	40.481998	34.610001	36.852001
H	40.785999	33.900002	36.078999
H	40.764000	34.167999	37.810001
C	41.286999	35.923000	36.660999
H	41.002998	36.403999	35.721001
H	42.347000	35.675999	36.563000
C	41.120998	36.930000	37.821999
H	40.066002	37.162998	37.993999
H	41.615002	37.867001	37.535000
N	41.750000	36.441002	39.061001
H	42.706001	36.085999	38.987000
C	34.090000	36.388000	28.722000
O	34.466999	37.132999	27.836000
C	34.455002	34.905998	28.799000
C	33.666000	34.129002	27.697001
C	33.999001	32.618000	27.518999
C	33.612000	31.705999	28.709000
N	32.202000	31.240000	28.697001
H	31.502001	31.885000	29.021999
H	33.828999	32.209999	29.656000
H	34.269001	30.827000	28.679001
H	35.068001	32.507999	27.323999
H	33.498001	32.249001	26.621000
H	33.852001	34.617001	26.737000
H	32.595001	34.230999	27.889999
H	34.139999	34.514999	29.768000
C	35.999001	34.733002	28.688999
H	36.308998	34.959999	27.666000
H	36.263000	33.691002	28.872000
C	36.824001	35.629002	29.656000
H	36.639000	36.681000	29.427999
H	37.888000	35.466999	29.464001
C	36.543999	35.389000	31.158001
H	35.470001	35.348999	31.361000
H	36.945999	36.244999	31.709999
N	37.196999	34.171001	31.671000
H	38.105999	34.278000	32.109001
C	34.167000	42.500999	29.440001
O	34.839001	41.542000	29.096001
C	33.285999	43.303001	28.486000
C	33.902000	44.719002	28.270000
C	32.948002	45.763000	27.628000
C	31.691000	46.105000	28.468000
N	31.985001	46.841999	29.715000
H	31.920000	47.862000	29.693001
H	31.125999	45.199001	28.704000

H	31.038000	46.737999	27.856001
H	32.632999	45.415001	26.642000
H	33.511002	46.685001	27.457001
H	34.792000	44.623001	27.643000
H	34.248001	45.124001	29.223000
H	32.314999	43.411999	28.969000
C	33.081001	42.543999	27.143999
H	34.058998	42.306999	26.716000
H	32.577999	43.180000	26.414000
C	32.271000	41.231998	27.319000
H	32.512001	40.761002	28.271999
H	32.560001	40.520000	26.542000
C	30.750000	41.456001	27.242001
H	30.455999	42.313999	27.856001
H	30.239000	40.566002	27.625999
N	30.330999	41.668999	25.849001
H	31.056000	41.785000	25.153000
C	35.648998	34.588001	40.553001
O	36.284000	35.174000	41.410000
C	34.122002	34.575001	40.520000
C	33.634998	33.674999	41.702000
C	32.119999	33.703999	42.046001
C	31.188999	33.115002	40.964001
N	31.171000	31.636000	40.931999
H	31.826000	31.181000	40.320999
H	31.464001	33.506001	39.978001
H	30.170000	33.463001	41.169998
H	31.813000	34.729000	42.263000
H	31.962999	33.147999	42.974998
H	34.167000	33.980000	42.606998
H	33.933998	32.641998	41.507999
H	33.780998	34.127998	39.584000
C	33.573002	36.030998	40.598999
H	33.794998	36.437000	41.589001
H	32.487000	36.021999	40.502998
C	34.147999	37.008999	39.536999
H	35.237999	37.036999	39.609001
H	33.808998	38.021000	39.776001
C	33.745998	36.686001	38.078999
H	33.978001	35.643002	37.839001
H	34.344002	37.312000	37.403000
N	32.321999	36.963001	37.806999
H	32.068001	37.924999	37.639000
C	41.233002	36.535999	40.304001
O	40.116001	36.978001	40.507999
C	42.144001	36.014000	41.407001
C	43.223000	37.085999	41.733002
C	44.429001	36.568001	42.560001
C	45.277000	35.483002	41.853001
N	46.026001	35.984001	40.682999
H	46.991001	36.290001	40.826000
H	44.653999	34.636002	41.550999
H	46.006001	35.099998	42.574001
H	44.077000	36.178001	43.516998
H	45.077000	37.416000	42.797001
H	42.750999	37.910000	42.273998
H	43.606998	37.515999	40.805000
H	42.638000	35.124001	41.016998

C	41.324001	35.601002	42.664001
H	40.761002	36.466999	43.021000
H	41.988998	35.310001	43.479000
C	40.337002	34.438999	42.375999
H	39.869999	34.567001	41.400002
H	39.523998	34.452999	43.103001
C	41.007000	33.057999	42.430000
H	41.959999	33.064999	41.888000
H	40.347000	32.327000	41.948002
N	41.226002	32.632000	43.820999
H	41.040001	33.296001	44.563000
C	31.808001	29.958000	28.493000
O	32.598999	29.138000	28.063000
C	30.346001	29.610001	28.822001
C	30.049999	28.122000	28.429001
C	28.558001	27.701000	28.348000
C	27.768000	28.330999	27.177000
N	28.198000	27.823999	25.863001
H	28.322001	26.816000	25.780001
H	27.862000	29.417000	27.202999
H	26.711000	28.069000	27.301001
H	28.056999	27.919001	29.289000
H	28.514999	26.613001	28.240000
H	30.549000	27.469999	29.150999
H	30.502001	27.886999	27.471001
H	29.709999	30.261000	28.223000
C	30.018000	29.799000	30.340000
H	30.731001	29.212999	30.926001
H	29.038000	29.372999	30.555000
C	30.000999	31.245001	30.909000
H	31.011999	31.655001	30.936001
H	29.688000	31.184999	31.955000
C	29.056999	32.229000	30.180000
H	29.406000	32.389999	29.153999
H	29.098000	33.199001	30.688999
N	27.653000	31.768000	30.165001
H	27.204000	31.589001	31.052000
C	36.639000	32.943001	31.708000
O	35.481998	32.771999	31.379999
C	37.557999	31.813000	32.159000
C	37.256001	31.450001	33.634998
C	38.160999	30.350000	34.256001
C	39.669998	30.480000	33.924999
N	40.501999	29.719999	34.876999
H	41.082001	30.246000	35.528999
H	39.963001	31.535000	33.978001
H	39.868999	30.118999	32.909000
H	37.813999	29.365999	33.931999
H	38.026001	30.379999	35.341000
H	36.213001	31.136000	33.727001
H	37.356998	32.355999	34.235001
H	38.581001	32.189999	32.126999
C	37.441002	30.583000	31.209999
H	36.402000	30.245001	31.184000
H	38.027000	29.746000	31.591999
C	37.912998	30.872999	29.766001
H	37.339001	31.702999	29.351999
H	37.686001	30.006001	29.139000

C	39.424000	31.200001	29.679001
H	39.860001	31.337000	30.673000
H	39.549999	32.141998	29.132999
N	40.194000	30.157000	28.982000
H	40.436001	30.332001	28.004000
C	32.158001	46.278000	30.931000
O	32.155998	45.068001	31.066000
C	32.334000	47.263000	32.081001
C	30.936001	47.773998	32.535999
C	30.961000	49.049000	33.421001
C	31.547001	50.310001	32.735001
N	30.611000	50.959000	31.797001
H	30.127001	51.794998	32.119999
H	32.481998	50.077000	32.214001
H	31.808001	51.036999	33.513000
H	31.531000	48.848999	34.328999
H	29.938999	49.262001	33.740002
H	30.433001	46.974998	33.088001
H	30.308001	47.970001	31.665001
H	32.907001	48.103001	31.693001
C	33.120998	46.633999	33.270000
H	32.625999	45.709000	33.576000
H	33.091000	47.292000	34.138000
C	34.602001	46.324001	32.944000
H	34.668999	45.785000	31.996000
H	35.000000	45.652000	33.709000
C	35.494999	47.584000	32.879002
H	35.074001	48.308998	32.173000
H	36.476002	47.292000	32.485001
N	35.693001	48.217999	34.201000
H	36.310001	47.745998	34.848999
C	29.058001	41.632000	25.410000
O	28.138000	41.473999	26.191000
C	28.914000	41.740002	23.896999
C	29.041000	40.316002	23.284000
C	29.587000	40.310001	21.834999
C	31.084999	40.685001	21.743999
N	31.997000	39.652000	22.285999
H	31.673000	38.682999	22.297001
H	31.281000	41.644001	22.233999
H	31.334999	40.832001	20.687000
H	29.007000	41.006001	21.223000
H	29.444000	39.317001	21.402000
H	28.063000	39.827999	23.304001
H	29.702000	39.700001	23.899000
H	29.745001	42.346001	23.538000
C	27.594999	42.444000	23.462999
H	26.747000	41.903000	23.889999
H	27.482000	42.391998	22.378000
C	27.513000	43.928001	23.903000
H	27.757999	44.005001	24.965000
H	26.480000	44.273998	23.804001
C	28.438999	44.870998	23.098000
H	29.398001	44.390999	22.878000
H	28.648001	45.751999	23.715000
N	27.827000	45.347000	21.841999
H	27.167000	46.122002	21.910000
C	30.235001	30.854000	41.518002

O	29.450001	31.348000	42.308998
C	30.222000	29.357000	41.146999
C	28.822001	28.740999	41.490002
C	28.732000	27.188000	41.487000
C	29.493000	26.521000	42.652000
N	28.830999	26.736000	43.945999
H	27.851999	26.985001	43.933998
H	30.518999	26.896000	42.699001
H	29.534000	25.441999	42.473999
H	29.090000	26.775000	40.543999
H	27.677999	26.902000	41.550999
H	28.089001	29.132000	40.778999
H	28.495001	29.077999	42.473999
H	30.966000	28.867001	41.772999
C	30.545000	29.093000	39.632999
H	29.952999	29.775999	39.019001
H	30.212000	28.096001	39.353001
C	32.032001	29.174000	39.180000
H	32.363998	30.209999	39.112000
H	32.090000	28.789000	38.158001
C	33.025002	28.378000	40.054001
H	33.036999	28.785000	41.070999
H	34.035000	28.514000	39.647999
N	32.735001	26.929001	40.074001
H	32.632000	26.462000	39.178001
C	31.357000	36.023998	37.701000
O	31.615000	34.847000	37.855999
C	29.954000	36.530998	37.377998
C	29.646999	36.207001	35.889000
C	28.254000	36.632000	35.349998
C	27.914000	38.130001	35.542000
N	27.063999	38.661999	34.452000
H	27.469000	39.410999	33.890999
H	28.844000	38.709999	35.541000
H	27.431999	38.293999	36.509998
H	27.471001	36.020000	35.804001
H	28.239000	36.400002	34.282001
H	29.756001	35.131001	35.730999
H	30.410999	36.687000	35.271000
H	29.937000	37.617001	37.486000
C	28.910999	35.914001	38.355000
H	28.856001	34.837002	38.178001
H	27.919001	36.312000	38.143002
C	29.239000	36.141998	39.855999
H	30.211000	35.702000	40.077999
H	28.518999	35.594002	40.470001
C	29.261000	37.625999	40.292000
H	29.552000	38.286999	39.471001
H	30.021000	37.737999	41.075001
N	27.978001	38.078999	40.855000
H	27.922001	38.168999	41.870998
C	45.623001	35.907001	39.396000
O	44.511002	35.507999	39.101002
C	46.683998	36.320999	38.386002
C	47.594002	35.096001	38.078999
C	48.879002	35.415001	37.270000
C	49.723999	36.581001	37.834999
N	50.527000	36.243999	39.025002

H	51.522999	36.136002	38.855999
H	49.105999	37.453999	38.048000
H	50.421001	36.891998	37.049999
H	48.603001	35.653999	36.241001
H	49.497002	34.514999	37.212002
H	47.014000	34.342999	37.541000
H	47.897999	34.632000	39.021000
H	47.285000	37.068001	38.891998
C	46.096001	36.984001	37.105000
H	45.240002	36.403999	36.751999
H	46.825001	36.970001	36.294998
C	45.667000	38.456001	37.327000
H	45.016998	38.509998	38.203999
H	45.066002	38.783001	36.473999
C	46.859001	39.433998	37.508999
H	47.527000	39.091999	38.305000
H	46.456001	40.398998	37.839001
N	47.629002	39.667999	36.266998
H	47.098999	39.848999	35.425999
C	41.532001	31.372999	44.182999
O	41.733002	30.525999	43.334999
C	41.549000	31.113001	45.680000
C	40.095001	30.792000	46.133999
C	39.808998	31.129999	47.616001
C	39.792999	32.650002	47.900002
N	38.648998	33.368000	47.291000
H	37.762001	32.873001	47.206001
H	40.736000	33.113998	47.589001
H	39.736000	32.791000	48.985001
H	40.560001	30.653000	48.249001
H	38.841999	30.705999	47.898998
H	39.888000	29.733000	45.959999
H	39.381001	31.344000	45.518002
H	41.875999	32.032001	46.165001
C	42.542000	29.980000	46.076000
H	42.198002	29.039000	45.640999
H	42.527000	29.840000	47.159000
C	44.007999	30.215000	45.617001
H	44.039001	30.319000	44.530998
H	44.595001	29.323000	45.851002
C	44.692001	31.447001	46.254002
H	44.037998	32.323002	46.213001
H	45.587002	31.684000	45.667000
N	45.112000	31.202999	47.646000
H	46.001999	30.750999	47.789001
C	28.363001	28.559000	24.745001
O	28.011000	29.724001	24.695000
C	29.075001	27.839001	23.601000
C	30.570000	28.259001	23.524000
C	31.283001	28.006001	24.871000
C	32.813999	27.976000	24.764999
N	33.459000	27.360001	25.981001
H	33.266998	27.892000	26.854000
H	33.151001	26.375000	26.108000
H	34.495998	27.299000	25.889999
H	33.217999	28.983999	24.639999
H	33.112999	27.368000	23.907000
H	30.952999	27.042999	25.271000

H	30.997000	28.790001	25.575001
H	31.063000	27.674999	22.740000
H	30.657000	29.315001	23.249001
C	28.372999	28.052999	22.233000
C	27.177000	27.091999	22.059999
C	26.493000	27.270000	20.690001
N	25.483999	26.193001	20.392000
H	24.975000	25.903999	21.254999
H	25.915001	25.339001	19.978001
H	24.743999	26.525999	19.746000
H	27.230000	27.252001	19.882000
H	25.969000	28.230000	20.659000
H	26.448999	27.263000	22.857000
H	27.528000	26.059999	22.152000
H	29.086000	27.857000	21.430000
H	28.051001	29.091999	22.122999
H	29.062000	26.764999	23.809000
C	26.954000	31.468000	29.051001
O	27.447001	31.657000	27.957001
C	25.549000	30.900999	29.256001
C	25.611000	29.570000	30.070000
C	24.256001	29.165001	30.687000
C	24.406000	27.913000	31.573000
N	23.118999	27.539000	32.249001
H	22.639999	28.382000	32.626999
H	22.452000	27.127001	31.563999
H	23.230000	26.871000	33.035999
H	25.143999	28.094000	32.356998
H	24.726999	27.052000	30.978001
H	23.521000	28.962999	29.906000
H	23.875000	29.990000	31.294001
H	25.959999	28.760000	29.427999
H	26.329000	29.658001	30.888000
C	24.806000	30.666000	27.900999
C	24.551001	31.948999	27.063000
C	24.993999	31.759001	25.594999
N	26.479000	31.921000	25.385000
H	26.886999	31.209000	24.742001
H	26.989000	31.791000	26.282000
H	26.709999	32.875000	25.035000
H	24.502001	32.494999	24.952000
H	24.719000	30.757999	25.254000
H	25.047001	32.821999	27.495001
H	23.480000	32.167999	27.079000
H	23.834000	30.202000	28.087000
H	25.371000	29.941000	27.311001
H	24.987000	31.636999	29.837999
C	40.577000	28.375000	34.969002
O	40.042000	27.655001	34.145000
C	41.353001	27.853001	36.182999
C	41.250000	26.304001	36.339001
C	42.189999	25.521999	35.397999
C	42.214001	24.042000	35.831001
N	43.317001	23.225000	35.220001
H	43.126999	22.990000	34.223000
H	44.240002	23.702999	35.299000
H	43.398998	22.311001	35.713001
H	41.264999	23.556000	35.587002

H	42.362999	23.987000	36.912998
H	43.199001	25.936001	35.469002
H	41.861000	25.610001	34.359001
H	41.507999	26.018999	37.360001
H	40.216000	25.981001	36.187000
C	40.879002	28.535000	37.507999
C	41.898998	28.372999	38.660999
C	41.616001	29.386999	39.785000
N	42.221001	28.996000	41.103001
H	43.233002	28.768999	41.049999
H	41.765999	28.125000	41.445999
H	42.077999	29.698999	41.853001
H	40.537998	29.459999	39.952999
H	42.005001	30.371000	39.508999
H	42.917999	28.528000	38.297001
H	41.846001	27.358999	39.062000
H	39.910000	28.125999	37.810001
H	40.722000	29.603001	37.360001
H	42.396999	28.132000	36.020000
C	40.789001	29.105000	29.573000
O	40.624001	28.858999	30.752001
C	41.679001	28.271000	28.663000
C	41.812000	26.802999	29.163000
C	40.459000	26.041000	29.202999
C	40.166000	25.448000	30.598000
N	39.646999	26.437000	31.615000
H	40.203999	27.318001	31.639999
H	38.678001	26.715000	31.407000
H	39.657001	26.044001	32.581001
H	41.073002	24.999001	31.011999
H	39.407001	24.666000	30.513000
H	40.505001	25.219000	28.483999
H	39.626999	26.676001	28.886999
H	42.490002	26.256001	28.503000
H	42.280998	26.801001	30.150999
C	43.068001	28.959999	28.549999
C	43.876999	28.514999	27.309999
C	45.101002	29.434000	27.139000
N	45.855000	29.247000	25.851999
H	45.224998	29.261999	25.023001
H	46.361000	28.337000	25.797001
H	46.568001	29.990999	25.737000
H	45.810001	29.284000	27.959000
H	44.771999	30.476999	27.150999
H	43.248001	28.587999	26.419001
H	44.201000	27.475000	27.409000
H	43.646999	28.788000	29.461000
H	42.916000	30.041000	28.479000
H	41.213001	28.259001	27.673000
C	30.486000	50.653999	30.489000
O	31.099001	49.730999	29.983999
C	29.502001	51.527000	29.716999
C	28.091000	50.875000	29.770000
C	26.941000	51.865002	29.455000
C	25.584000	51.136002	29.510000
N	24.379999	52.020000	29.325001
H	24.202000	52.619999	30.155001
H	24.466000	52.646999	28.500999

H	23.521000	51.444000	29.202999
H	25.457001	50.639999	30.476999
H	25.538000	50.380001	28.724001
H	27.069000	52.305000	28.464001
H	26.947001	52.681999	30.184000
H	28.055000	50.025002	29.083000
H	27.921000	50.474998	30.775999
C	29.976000	51.744999	28.252001
C	31.247999	52.619999	28.170000
C	31.855000	52.539001	26.757000
N	32.834000	53.633999	26.441000
H	33.592999	53.709999	27.150000
H	32.380001	54.566002	26.379999
H	33.298000	53.490002	25.521999
H	31.066999	52.598000	26.003000
H	32.380001	51.588001	26.631001
H	31.999001	52.292999	28.895000
H	30.987000	53.655998	28.408001
H	29.191999	52.229000	27.665001
H	30.164000	50.771999	27.785999
H	29.452000	52.499001	30.214001
C	35.206001	49.424000	34.567001
O	34.463001	50.054001	33.841999
C	35.700001	49.958000	35.907001
C	34.601002	50.764000	36.667000
C	33.367001	49.937000	37.104000
C	32.355999	50.855999	37.830002
N	31.160000	50.160000	38.435001
H	30.530001	49.716000	37.736000
H	31.434000	49.428001	39.122002
H	30.552000	50.821999	38.958000
H	31.973000	51.609001	37.134998
H	32.862000	51.374001	38.650002
H	33.682999	49.133999	37.773998
H	32.889000	49.483002	36.233002
H	35.044998	51.210999	37.561001
H	34.266998	51.596001	36.039001
C	36.939999	50.886002	35.723000
C	38.049999	50.316002	34.806000
C	39.290001	51.231998	34.823002
N	40.340000	50.877998	33.800999
H	40.075001	51.178001	32.837002
H	40.561001	49.862999	33.778000
H	41.240002	51.368000	33.969002
H	39.766998	51.180000	35.806000
H	38.998001	52.268002	34.627998
H	37.678001	50.238998	33.780998
H	38.331001	49.313000	35.139000
H	37.363998	51.098999	36.708000
H	36.616001	51.842999	35.307999
H	35.995998	49.109001	36.528999
C	33.310001	39.876999	22.500000
O	33.742001	41.011002	22.514999
C	34.214001	38.657001	22.666000
C	35.394001	38.933998	23.648001
C	34.976002	39.284000	25.094999
C	36.242001	39.421001	25.971001
N	36.007000	39.519001	27.458000

H	35.615002	40.435001	27.761999
H	35.389999	38.751999	27.790001
H	36.915001	39.414001	27.957001
H	36.817001	40.301998	25.673000
H	36.874001	38.541000	25.826000
H	34.332001	38.493999	25.489000
H	34.416000	40.222000	25.108999
H	36.030998	38.044998	23.684000
H	36.013000	39.744999	23.250999
C	34.834000	38.278000	21.289000
C	33.861000	37.598000	20.299000
C	34.464001	37.620998	18.879000
N	33.752998	36.743000	17.879000
H	32.724998	36.707001	18.002001
H	34.069000	35.756001	17.975000
H	33.942001	37.026001	16.895000
H	35.507000	37.287998	18.908001
H	34.443001	38.645000	18.495001
H	32.897999	38.111000	20.278999
H	33.686001	36.567001	20.620001
H	35.682999	37.602001	21.434999
H	35.237000	39.186001	20.836000
H	33.626999	37.818001	23.048000
C	28.104000	44.889999	20.605000
O	28.837999	43.938999	20.434999
C	27.454000	45.654999	19.454000
C	26.445999	44.761002	18.681000
C	25.173000	44.405998	19.479000
C	24.274000	43.514000	18.599001
N	22.962999	43.115002	19.214001
H	23.055000	42.748001	20.184999
H	22.288000	43.901001	19.289000
H	22.495001	42.375000	18.650000
H	24.804001	42.588001	18.362000
H	24.038000	44.026001	17.660000
H	24.639999	45.319000	19.757000
H	25.437000	43.875999	20.399000
H	26.136000	45.279999	17.768000
H	26.951000	43.841999	18.368000
C	28.511999	46.167000	18.438999
C	29.544001	47.160999	19.020000
C	30.457001	47.623001	17.867001
N	31.658001	48.452000	18.239000
H	32.247002	47.988998	18.962999
H	31.414000	49.410000	18.562000
H	32.265999	48.535999	17.396999
H	29.879999	48.203999	17.142000
H	30.854000	46.742001	17.355000
H	30.141001	46.671001	19.794001
H	29.039000	48.020000	19.468000
H	27.993999	46.659000	17.610001
H	29.042999	45.308998	18.014999
H	26.920000	46.522999	19.846001
C	29.438000	26.649000	45.145000
O	30.606001	26.323999	45.237999
C	28.572001	27.010000	46.344002
C	28.709999	28.523001	46.689999
C	28.403000	29.436001	45.476002

C	28.323000	30.927999	45.838001
N	27.864000	31.760000	44.667999
H	28.566000	31.798000	43.901001
H	27.004000	31.353001	44.240002
H	27.600000	32.724998	44.948002
H	29.296000	31.306999	46.160999
H	27.601000	31.077999	46.646000
H	27.448999	29.135000	45.034000
H	29.180000	29.316999	44.716999
H	28.018000	28.763000	47.501999
H	29.719999	28.733000	47.054001
C	28.902000	26.128000	47.583000
C	28.731001	24.614000	47.298000
C	28.985001	23.768999	48.562000
N	28.857000	22.285000	48.327999
H	29.561001	21.938000	47.640999
H	27.914000	22.048000	47.958000
H	28.987000	21.737000	49.206001
H	28.261000	24.035999	49.338001
H	29.993999	23.950001	48.943001
H	29.427000	24.295000	46.518002
H	27.719000	24.424999	46.930000
H	28.240999	26.412001	48.407001
H	29.927999	26.323000	47.910999
H	27.528000	26.820999	46.080002
C	32.733002	26.155001	41.175999
O	32.960999	26.660999	42.258999
C	32.504002	24.650000	40.990002
C	31.292999	24.327999	40.060001
C	31.416000	22.931999	39.401001
C	30.330000	22.731001	38.327000
N	30.381001	21.386000	37.655998
H	31.275999	21.207001	37.155998
H	30.271999	20.611000	38.341000
H	29.625000	21.287001	36.945999
H	30.434999	23.485001	37.542999
H	29.336000	22.829000	38.771999
H	31.332001	22.148001	40.157001
H	32.397999	22.833000	38.929001
H	30.356001	24.395000	40.618000
H	31.224001	25.063000	39.258999
C	32.340000	23.921000	42.361000
C	33.667000	23.818001	43.157001
C	33.507999	24.214001	44.640999
N	33.247002	25.683001	44.848999
H	32.299999	25.865999	45.237000
H	33.270000	26.191000	43.944000
H	33.951000	26.143000	45.457001
H	34.425999	23.976999	45.186001
H	32.687000	23.656000	45.102001
H	34.446999	24.437000	42.705002
H	34.028000	22.788000	43.105999
H	31.969000	22.905001	42.209000
H	31.576000	24.431999	42.952000
H	33.403000	24.268999	40.500999
C	25.783001	38.330002	34.169998
O	25.176001	37.578999	34.910999
C	25.167000	38.936001	32.894001

C	23.945999	38.096001	32.389000
C	22.589001	38.486000	33.022999
C	21.458000	37.726002	32.294998
N	20.049999	38.070999	32.702999
H	19.851999	37.803001	33.687000
H	19.812000	39.074001	32.573002
H	19.377001	37.516998	32.127998
H	21.570000	36.648998	32.452999
H	21.517000	37.918999	31.221001
H	22.426001	39.562000	32.916000
H	22.582001	38.248001	34.090000
H	23.832001	38.206001	31.311001
H	24.138000	37.032001	32.555000
C	26.198999	39.091000	31.723000
C	25.709000	40.028999	30.587000
C	26.860001	40.401001	29.625999
N	26.381001	40.959000	28.311001
H	25.709999	41.747002	28.436001
H	25.860001	40.222000	27.792999
H	27.142000	41.271999	27.674999
H	27.448000	39.511002	29.388000
H	27.510000	41.146000	30.091999
H	25.290001	40.946999	31.009001
H	24.916000	39.543999	30.014000
H	26.440001	38.106998	31.313000
H	27.136000	39.506001	32.087002
H	24.830000	39.938000	33.167000
C	26.940001	38.561001	40.150002
O	26.924000	38.543999	38.932999
C	25.790001	39.098999	40.985001
C	24.434000	38.942001	40.241001
C	24.024000	37.464001	39.994999
C	23.663000	37.227001	38.514999
N	24.879999	37.221001	37.623001
H	25.531000	37.993000	37.882000
H	25.423000	36.353001	37.728001
H	24.662001	37.331001	36.608002
H	22.990999	38.019001	38.168999
H	23.155001	36.264999	38.393002
H	23.156000	37.226002	40.616001
H	24.815001	36.773998	40.299000
H	23.646000	39.422001	40.819000
H	24.476000	39.493999	39.298000
C	26.048000	40.590000	41.333000
C	25.263000	41.040001	42.584999
C	25.205000	42.571999	42.675999
N	24.577999	43.066002	43.945999
H	25.259001	43.021999	44.731998
H	23.746000	42.507000	44.213001
H	24.285000	44.060001	43.862999
H	24.612000	42.966999	41.847000
H	26.209999	43.000999	42.624001
H	25.735001	40.625000	43.480999
H	24.240999	40.665001	42.553001
H	25.787001	41.216000	40.473999
H	27.113001	40.750000	41.526001
H	25.747000	38.523998	41.916000
C	50.134998	36.323002	40.313999

O	48.978001	36.523998	40.630001
C	51.243999	36.126999	41.341000
C	51.188000	34.691002	41.931999
C	51.574001	33.616001	40.888000
C	51.613998	32.210999	41.520000
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H	51.791000	31.118000	39.698002
H	53.243000	31.426001	40.444000
H	52.263000	30.233999	41.078999
H	50.601002	31.871000	41.752998
H	52.199001	32.233002	42.443001
H	52.557999	33.855000	40.478001
H	50.863998	33.616001	40.056999
H	51.882000	34.620998	42.775002
H	50.185001	34.491001	42.323002
C	51.161999	37.187000	42.478001
C	51.502998	38.612999	41.981998
C	51.394001	39.645000	43.125999
N	51.919998	41.013000	42.771999
H	51.511002	41.355999	41.875999
H	52.945000	40.987000	42.596001
H	51.734001	41.727001	43.509998
H	51.962002	39.304001	43.994999
H	50.347000	39.764999	43.417000
H	50.827000	38.900002	41.172001
H	52.519001	38.620998	41.577999
H	51.866001	36.921001	43.271999
H	50.161999	37.174999	42.922001
H	52.212002	36.251999	40.847000
C	48.966000	39.856998	36.210999
O	49.685001	39.643002	37.167999
C	49.521000	40.381001	34.894001
C	50.576000	39.417999	34.287998
C	49.980999	38.195999	33.564999
C	51.130001	37.466000	32.841999
N	50.702000	36.504002	31.771000
H	50.148998	35.713001	32.166000
H	50.150002	36.966999	31.018999
H	51.542000	36.122002	31.292000
H	51.735001	36.909000	33.563000
H	51.772999	38.199001	32.346001
H	49.241001	38.530998	32.833000
H	49.483002	37.526001	34.271000
H	51.158001	39.969002	33.546001
H	51.280998	39.096001	35.061001
C	50.209999	41.754002	35.109001
C	49.236000	42.887001	35.485001
C	49.987000	44.224998	35.374001
N	49.117001	45.445000	35.467999
H	48.719002	45.558998	36.423000
H	48.316002	45.381001	34.806999
H	49.669998	46.292999	35.244999
H	50.484001	44.278000	34.403000
H	50.748001	44.299999	36.154999
H	48.852001	42.745998	36.499001
H	48.388000	42.886002	34.796001
H	50.708000	42.042000	34.181000
H	50.987999	41.669998	35.874001

H	48.708000	40.514999	34.174999
C	38.632000	34.709000	47.131001
O	39.667999	35.341000	47.132999
C	37.264999	35.375999	47.001999
C	37.294998	36.601002	46.037998
C	37.737999	36.273998	44.594002
C	37.650002	37.546001	43.723999
N	37.848999	37.342999	42.242001
H	38.830002	37.176998	41.950001
H	37.268002	36.557999	41.888000
H	37.523998	38.188000	41.723999
H	38.380001	38.289001	44.060001
H	36.655998	37.987000	43.840000
H	37.096001	35.491001	44.180000
H	38.765999	35.910000	44.603001
H	36.297001	37.047001	46.001999
H	37.964001	37.365002	46.445000
C	36.775002	35.888000	48.389999
C	36.573002	34.782001	49.453999
C	36.250999	35.409000	50.827000
N	36.167000	34.418999	51.960999
H	36.921001	33.703999	51.910999
H	35.284000	33.872002	51.970001
H	36.209000	34.896000	52.889000
H	35.303001	35.953999	50.792000
H	37.043999	36.113998	51.091000
H	37.486000	34.193001	49.555000
H	35.769001	34.106998	49.148998
H	35.828999	36.423000	48.264999
H	37.500999	36.613998	48.768002
H	36.548000	34.647999	46.613998
C	44.394001	31.528999	48.738998
O	43.291000	32.027000	48.646999
C	45.046001	31.208000	50.078999
C	44.408001	29.924999	50.681999
C	44.810001	28.634001	49.925999
C	43.957001	27.441999	50.400002
N	44.421001	26.100000	49.896000
H	44.747002	26.122999	48.903999
H	45.175999	25.705000	50.494999
H	43.651001	25.406000	49.983002
H	42.926998	27.575001	50.056000
H	43.950001	27.382999	51.491001
H	45.870998	28.427999	50.096001
H	44.665001	28.756001	48.849998
H	44.709000	29.820000	51.728001
H	43.320999	30.034000	50.674000
C	44.903999	32.389999	51.081001
C	45.549999	33.706001	50.581001
C	45.498001	34.782001	51.686001
N	46.000000	36.140999	51.270000
H	45.414001	36.561001	50.514999
H	46.966999	36.127998	50.884998
H	45.993000	36.812000	52.064999
H	46.097000	34.464001	52.543999
H	44.466999	34.916000	52.023998
H	45.019001	34.069000	49.695999
H	46.590000	33.528000	50.294998

H	45.370998	32.110001	52.029999
H	43.844002	32.568001	51.290001
H	46.113998	31.031000	49.925999

Atomic coordinates for the optimized structure of **G5** with AMBER at MM level (parm99, gaff)

Energy (kcal/mol)	-181690		
	Coordinates (Angstroms)		
Atom type	X	Y	Z
N	43.327000	46.195000	41.473000
H	43.787998	47.047001	41.199001
C	43.782001	45.518002	42.701000
H	42.977001	45.544998	43.444000
H	43.987000	44.466999	42.473999
C	45.049999	46.161999	43.287998
H	44.827000	47.186001	43.608002
H	45.827999	46.209000	42.518002
N	45.561001	45.402000	44.441002
H	45.157001	45.595001	45.356998
C	42.303001	45.749001	40.714001
O	41.702000	44.740002	41.020000
C	41.974998	46.557999	39.464001
C	42.000000	45.603001	38.237000
C	42.134998	46.301998	36.856998
C	43.501999	46.983002	36.599998
N	44.646000	46.119999	36.949001
H	45.096001	46.293999	37.834000
H	43.558998	47.910000	37.185001
H	43.568001	47.262001	35.542000
H	41.334000	47.033001	36.723000
H	41.988998	45.542000	36.084999
H	41.084000	45.007999	38.233002
H	42.811001	44.881001	38.348000
H	42.738998	47.326000	39.330002
C	40.581001	47.235001	39.591999
H	39.813999	46.457001	39.629002
H	40.376999	47.828999	38.699001
C	40.403000	48.130001	40.845001
H	40.598000	47.546001	41.748001
H	39.358002	48.441002	40.903999
C	41.293999	49.389999	40.851002
H	42.348000	49.109001	40.763000
H	41.180000	49.896000	41.817001
N	40.937000	50.342999	39.780998
H	40.088001	50.875000	39.890999
C	46.549000	44.483002	44.379002
O	47.053001	44.155998	43.320000
C	46.945999	43.862999	45.710999
C	46.724998	42.331001	45.632000
C	46.882999	41.580002	46.978001
C	46.074001	42.185001	48.153000
N	44.630001	42.293999	47.862999
H	44.272999	43.219002	47.627998
H	46.462002	43.182999	48.390999
H	46.216000	41.583000	49.055000
H	47.938999	41.535999	47.255001

H	46.564999	40.550999	46.811001
H	47.414001	41.898998	44.903000
H	45.716000	42.145000	45.251999
H	46.271999	44.245998	46.469002
C	48.403999	44.235001	46.109001
H	49.069000	44.025002	45.266998
H	48.745998	43.611000	46.936001
C	48.573002	45.715000	46.533001
H	48.168999	46.363998	45.750999
H	49.639000	45.948002	46.605999
C	47.889999	46.056999	47.880001
H	46.837002	45.762001	47.865002
H	47.895000	47.148998	47.993999
N	48.571999	45.484001	49.063999
H	49.571999	45.612999	49.118000
C	45.098999	45.071999	36.229000
O	44.644001	44.846001	35.118999
C	46.168999	44.174000	36.868999
C	47.290001	43.936001	35.813999
C	48.259998	42.749001	36.051998
C	47.722000	41.556999	36.879002
N	46.605999	40.713001	36.375000
H	46.320000	39.997002	37.032001
H	47.443001	41.925999	37.868999
H	48.570999	40.882999	37.046001
H	49.133999	43.138000	36.580002
H	48.630001	42.389000	35.088001
H	47.875999	44.852001	35.701000
H	46.838001	43.772999	34.841999
H	45.667000	43.227001	37.066002
C	46.791000	44.699001	38.209999
H	47.136002	45.724998	38.057999
H	47.687000	44.122002	38.448002
C	45.868000	44.662998	39.464001
H	44.931000	45.178001	39.269001
H	46.351002	45.223999	40.269001
C	45.535000	43.249001	39.986000
H	45.273998	42.584000	39.155998
H	44.647999	43.313000	40.627998
N	46.632000	42.671001	40.787998
H	46.988998	43.227001	41.564999
C	41.703999	50.623001	38.703999
O	42.745998	50.023998	38.526001
C	41.154999	51.714001	37.780998
C	41.223000	53.097000	38.502998
C	40.224998	54.153999	37.960999
C	38.757999	53.855999	38.362999
N	38.185001	54.862000	39.283001
H	38.547001	55.803001	39.233002
H	38.680000	52.867001	38.827999
H	38.139999	53.834999	37.458000
H	40.300999	54.221001	36.873001
H	40.518002	55.136002	38.342999
H	42.238998	53.490002	38.424000
H	41.029999	52.980999	39.571999
H	40.105000	51.477001	37.602001
C	41.889999	51.779999	36.403999
H	42.942001	52.013000	36.583000

H	41.488998	52.601002	35.806999
C	41.827999	50.487000	35.549999
H	42.185001	49.641998	36.137001
H	42.525002	50.580002	34.713001
C	40.421001	50.148998	35.013000
H	39.640999	50.571999	35.653999
H	40.292999	49.061001	35.039001
N	40.191002	50.591000	33.623001
H	40.886002	51.165001	33.173000
C	43.730999	41.294998	48.012001
O	44.130001	40.186001	48.328999
C	42.236000	41.605000	47.814999
C	41.506001	41.247002	49.139999
C	39.983002	41.546001	49.228001
C	39.124001	41.143002	48.005001
N	38.980000	39.714001	47.636002
H	38.657001	39.570000	46.683998
H	39.497002	41.673000	47.124001
H	38.115002	41.533001	48.179001
H	39.858002	42.620998	49.382999
H	39.570000	41.078999	50.120998
H	41.997002	41.770000	49.965000
H	41.660000	40.182999	49.319000
H	41.868999	40.912998	47.056999
C	41.931000	43.062000	47.333000
H	42.462002	43.771000	47.969002
H	40.879002	43.311001	47.463001
C	42.276001	43.313999	45.841000
H	43.299999	42.999001	45.631001
H	42.236000	44.388000	45.644001
C	41.318001	42.602001	44.859001
H	41.264000	41.530998	45.074001
H	41.727001	42.702000	43.846001
N	39.959999	43.183998	44.841000
H	39.886002	44.203999	44.863998
C	47.931999	45.176998	50.216999
O	46.726002	45.041000	50.210999
C	48.800999	45.053001	51.474998
C	49.380001	46.474998	51.780998
C	50.327000	46.601002	53.004002
C	51.698002	45.922001	52.804001
N	52.700001	46.783001	52.133999
H	52.668999	47.786999	52.310001
H	51.584999	44.983002	52.254002
H	52.095001	45.671001	53.792999
H	49.841999	46.195999	53.890999
H	50.488998	47.658001	53.227001
H	48.537998	47.153999	51.941002
H	49.916000	46.852001	50.905998
H	49.626999	44.377998	51.248001
C	48.012001	44.488998	52.709000
H	47.238998	45.213001	52.976002
H	48.675999	44.411999	53.570999
C	47.331001	43.099998	52.543999
H	46.726002	43.076000	51.638000
H	46.620998	42.967999	53.365002
C	48.305000	41.901001	52.520000
H	49.317001	42.237000	52.266998

H	47.984001	41.219002	51.726002
N	48.345001	41.148998	53.797001
H	48.245998	41.675999	54.653999
C	45.964001	40.675999	35.181000
O	46.145000	41.487000	34.293999
C	44.992001	39.512001	35.000000
C	45.807999	38.181000	34.951000
C	44.998001	36.856998	34.925999
C	44.000999	36.719002	33.757999
N	44.646999	36.769001	32.433998
H	45.653999	36.748001	32.398998
H	43.237999	37.499001	33.820999
H	43.487000	35.754002	33.865002
H	44.458000	36.740002	35.868999
H	45.702000	36.021000	34.882000
H	46.465000	38.127998	35.821999
H	46.466000	38.209000	34.078999
H	44.511002	39.636002	34.028000
C	43.869999	39.494999	36.083000
H	44.298000	39.187000	37.041000
H	43.132000	38.735001	35.820000
C	43.113998	40.835999	36.299999
H	43.778000	41.547001	36.798000
H	42.287998	40.653000	36.993000
C	42.548000	41.502998	35.025002
H	43.377998	41.868000	34.410999
H	41.960999	42.381001	35.323002
N	41.701000	40.609001	34.209999
H	42.172001	39.938999	33.619999
C	47.108002	41.416000	40.632999
O	46.637001	40.673000	39.793999
C	48.257000	40.991001	41.540001
C	47.820999	39.716999	42.323002
C	48.841999	39.236000	43.383999
C	48.325001	38.004002	44.161999
N	49.429001	37.366001	44.904999
H	50.153000	36.941002	44.346001
H	47.910999	37.272999	43.455002
H	47.521000	38.304001	44.842999
H	49.066002	40.043999	44.084999
H	49.776001	38.959000	42.894001
H	47.632000	38.903999	41.617001
H	46.873001	39.926998	42.827000
H	48.463001	41.782001	42.264999
C	49.527000	40.758999	40.667000
H	49.268002	40.116001	39.821999
H	50.290001	40.220001	41.228001
C	50.147999	42.077000	40.126999
H	49.431000	42.897999	40.201000
H	50.375000	41.959000	39.063999
C	51.445000	42.464001	40.875999
H	51.283001	42.429001	41.959000
H	51.719002	43.492001	40.613998
N	52.563999	41.577000	40.507999
H	52.491001	41.056000	39.630001
C	37.099998	54.636002	40.058998
O	36.619999	53.521999	40.132999
C	36.530998	55.828999	40.826000

C	35.203999	56.250999	40.122002
C	34.507999	57.519001	40.685001
C	35.188000	58.837002	40.257999
N	34.696999	59.331001	38.955002
H	33.785999	58.998001	38.627998
H	36.277000	58.723000	40.222000
H	34.956001	59.602001	41.006001
H	34.451000	57.476002	41.772999
H	33.470001	57.534000	40.340000
H	34.497002	55.419998	40.194000
H	35.391998	56.401001	39.056000
H	37.240002	56.658001	40.778000
C	36.294998	55.453999	42.324001
H	35.525002	54.679001	42.367001
H	35.903000	56.308998	42.875999
C	37.547001	54.926998	43.074001
H	38.110001	54.242001	42.436001
H	37.217999	54.332001	43.931000
C	38.492001	56.035999	43.587002
H	38.671001	56.780998	42.803001
H	39.459000	55.581001	43.832001
N	37.979000	56.707001	44.800999
H	37.002998	56.596001	45.028999
C	39.084000	50.234001	32.936001
O	38.213001	49.598000	33.492001
C	39.000999	50.613998	31.459999
C	38.903999	49.278000	30.657000
C	38.602001	49.372002	29.139000
C	39.667999	50.105000	28.302000
N	40.971001	49.407001	28.274000
H	41.188999	48.779999	29.032000
H	39.804001	51.125999	28.677999
H	39.282001	50.189999	27.278999
H	37.631001	49.848000	28.983000
H	38.495998	48.358002	28.746000
H	38.111000	48.664001	31.091000
H	39.832001	48.717999	30.799000
H	39.910000	51.138000	31.158001
C	37.778999	51.548000	31.226999
H	36.875000	51.028999	31.556000
H	37.647999	51.741001	30.162001
C	37.862000	52.910000	31.971001
H	38.132000	52.755001	33.018002
H	36.860001	53.345001	31.978001
C	38.825001	53.938000	31.330999
H	39.851002	53.556999	31.336000
H	38.816002	54.861000	31.924000
N	38.433998	54.252998	29.947001
H	37.672001	53.707001	29.541000
C	39.235001	38.588001	48.342999
O	39.653000	38.606998	49.487000
C	38.955002	37.269001	47.624001
C	37.423000	36.976002	47.709999
C	36.882000	35.804001	46.845001
C	37.391998	34.403000	47.238998
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H	38.479000	34.414001	47.373001

H	37.169998	33.730000	46.403999
H	37.134998	35.981998	45.798000
H	35.790001	35.806999	46.887001
H	36.882999	37.873001	47.396000
H	37.151001	36.806000	48.754002
H	39.474998	36.487000	48.181999
C	39.497002	37.217999	46.160000
H	38.765999	37.682999	45.492001
H	39.564999	36.169998	45.858002
C	40.868999	37.889999	45.869999
H	40.720001	38.966999	45.764000
H	41.213001	37.547001	44.889999
C	41.998001	37.660000	46.897999
H	41.729000	38.089001	47.866001
H	42.877998	38.212002	46.548000
N	42.369999	36.245998	47.080002
H	41.686001	35.535000	46.862999
C	38.841000	42.470001	44.587002
O	38.849998	41.257999	44.689999
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C	37.243999	42.791000	42.699001
C	36.181999	43.675999	41.994999
C	36.069000	43.313999	40.495998
N	34.978001	44.047001	39.825001
H	34.339001	44.561001	40.411999
H	35.884998	42.237000	40.396999
H	37.019001	43.539001	39.995998
H	36.457001	44.729000	42.091000
H	35.209000	43.542999	42.473999
H	36.901001	41.752998	42.715000
H	38.157001	42.813999	42.097000
H	37.856998	44.311001	44.091999
C	36.436001	43.041000	45.150002
H	36.509998	42.046001	45.595001
H	35.470001	43.067001	44.645000
C	36.433998	44.101002	46.278999
H	37.462002	44.308998	46.589001
H	35.917999	43.701000	47.157001
C	35.742001	45.412998	45.841999
H	36.069000	45.702999	44.837002
H	36.042999	46.213001	46.529999
N	34.269001	45.306999	45.887001
H	33.861000	44.686001	46.585999
C	53.778999	46.290001	51.485001
O	53.841999	45.105000	51.221001
C	54.900002	47.266998	51.127998
C	56.236000	46.689999	51.695000
C	57.426998	47.685001	51.727001
C	57.514999	48.494999	53.040001
N	58.300999	47.823002	54.104000
H	59.312000	47.749001	53.987999
H	56.506001	48.723000	53.405998
H	57.998001	49.453999	52.826000
H	57.360001	48.376999	50.887001
H	58.360001	47.131001	51.594002
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H	56.071999	46.308998	52.707001
H	54.709999	48.230000	51.605000

C	54.970001	47.453999	49.578999
H	55.053001	46.466999	49.118000
H	55.873001	47.995998	49.294998
C	53.743000	48.178001	48.960999
H	52.830002	47.865002	49.473999
H	53.627998	47.863998	47.919998
C	53.848000	49.720001	49.001999
H	54.202999	50.036999	49.987999
H	52.844002	50.137001	48.862000
N	54.733002	50.264999	47.948002
H	55.097000	49.613998	47.264999
C	48.629002	39.827000	53.881001
O	48.727001	39.167000	52.862999
C	48.820000	39.229000	55.280998
C	48.134998	37.824001	55.334999
C	48.416000	36.938000	56.582001
C	48.022999	37.564999	57.935001
N	46.581001	37.846001	58.020000
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H	48.293999	36.869999	58.740002
H	49.473999	36.664001	56.609001
H	47.869999	35.998001	56.466000
H	48.452999	37.238998	54.467999
H	47.056000	37.959999	55.229000
H	48.320000	39.868000	56.011002
C	50.334000	39.154999	55.641998
H	50.825001	38.476002	54.941002
H	50.465000	38.728001	56.638000
C	51.083000	40.512001	55.612999
H	50.945000	40.992001	54.641998
H	52.151001	40.308998	55.695000
C	50.679001	41.495998	56.736000
H	49.589001	41.569000	56.814999
H	51.036999	42.497002	56.472000
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C	43.971001	36.820999	31.267000
O	42.756001	36.755001	31.278000
C	44.810001	36.938999	29.995001
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H	43.247002	36.973000	28.483999
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H	45.738998	36.389000	30.150999
C	45.139999	38.426998	29.674000
H	44.199001	38.963001	29.521999
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H	45.396999	39.264000	31.672001
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C	47.365002	38.618999	31.025000
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H	47.856998	39.243999	31.778999
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C	40.351002	40.629002	34.125000
O	39.657001	41.386002	34.783001
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C	38.127998	39.049000	30.527000
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H	37.733002	38.488998	31.382999
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H	39.366001	37.495998	32.993999
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H	49.056999	34.942001	47.278999
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H	44.514999	29.569000	26.885000
H	44.779999	29.198999	29.316000
H	46.368999	29.934999	29.312000
H	43.903999	31.415001	28.319000
C	49.435001	37.973000	29.809999
O	49.923000	37.542999	30.837999
C	50.097000	37.821999	28.445000
C	49.747002	36.415001	27.882000
C	50.001999	36.264999	26.361000
C	49.945999	34.780998	25.955999
N	50.362000	34.500000	24.538000
H	49.674999	34.797001	23.816999
H	51.261002	34.971001	24.296000
H	50.541000	33.479000	24.415001
H	48.941002	34.375000	26.093000
H	50.634998	34.213001	26.589001
H	50.985001	36.654999	26.094000
H	49.261002	36.834999	25.796000
H	50.325001	35.664001	28.430000
H	48.693001	36.199001	28.072001
C	51.640999	38.014000	28.525000
C	52.068001	39.469002	28.813000
C	53.606998	39.542999	28.849001
N	54.166000	40.923000	29.046000
H	53.715000	41.412998	29.844000
H	54.087002	41.530998	28.204000
H	55.185001	40.889000	29.243000
H	54.032001	39.160000	27.917000
H	53.983002	38.930000	29.674000
H	51.658001	39.805000	29.768999
H	51.683998	40.130001	28.032000
H	52.105000	37.719002	27.583000
H	52.054001	37.348999	29.289000
H	49.682999	38.580002	27.778999
C	36.178001	40.590000	30.572001
O	35.400002	39.667999	30.632000
C	35.683998	42.021000	30.662001
C	35.888000	42.786999	29.327000
C	35.109001	42.108002	28.170000
C	35.189999	42.924999	26.868000
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H	34.645000	41.416000	25.452000
H	33.349998	42.286999	26.056000

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H	34.828999	43.943001	27.045000
H	34.056999	41.999001	28.452000
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H	35.526001	43.813000	29.444000
H	36.951000	42.841999	29.077000
C	36.277000	42.762001	31.896999
C	36.118999	41.917000	33.189999
C	36.473000	42.703999	34.465000
N	36.762001	41.814999	35.648998
H	37.765999	41.546001	35.654999
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H	36.533001	42.298000	36.544998
H	35.639000	43.358002	34.737999
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H	36.764999	41.039001	33.130001
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H	37.334999	42.984001	31.732000
H	34.604000	41.956001	30.827999
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O	35.738998	39.181999	35.181999
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C	33.862000	37.358002	33.709999
C	34.261002	37.172001	32.230000
C	33.172001	37.738998	31.292999
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H	34.419998	38.242001	29.652000
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H	32.791000	38.125999	29.230000
H	32.974998	38.784000	31.545000
H	32.245998	37.168999	31.405001
H	34.403000	36.109001	32.018002
H	35.216999	37.665001	32.048000
H	32.952999	36.776001	33.883999
H	33.601002	38.403000	33.901001
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C	33.861000	34.921001	35.888000
C	33.299999	34.422001	37.234001
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H	33.997002	32.417999	37.337002
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H	34.673000	34.264000	35.568001
H	33.077000	34.860001	35.129002
H	33.613998	37.041000	36.374001
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H	35.528999	36.078999	34.212002
C	56.534000	38.757000	46.118000
O	56.796001	37.581001	46.283001
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C	57.020000	42.615002	43.223999
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H	56.624001	44.374001	42.123001
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H	55.613998	41.584000	44.533001
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C	59.417000	38.862999	47.640999
C	60.958000	38.754002	47.717999
N	61.518002	38.127998	48.966999
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H	62.561001	38.148998	48.974998
H	61.396000	39.751999	47.636002
H	61.324001	38.152000	46.881001
H	58.956001	37.889999	47.830002
H	59.061001	39.564999	48.398998
H	59.737999	40.179001	45.998001
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H	57.380001	40.608002	46.798000
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O	51.521999	31.299000	47.592999
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C	54.019001	29.253000	47.473999
C	54.588001	28.149000	48.395000
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H	53.418999	26.535000	47.633999
H	55.013000	26.511000	47.087002
H	54.665001	26.051001	48.640999
H	54.104000	28.202000	49.375000
H	55.662998	28.295000	48.534000
H	54.504002	29.198999	46.497002
H	52.951000	29.091999	47.320000
H	55.333000	30.705000	48.341000
H	53.741001	30.719999	49.060001
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C	56.104000	33.139000	47.064999
C	56.943001	34.313999	47.615002
N	58.376999	34.278000	47.159000
H	58.491001	34.484001	46.143002
H	58.798000	33.338001	47.320000
H	58.992001	34.952999	47.653999
H	56.962002	34.271000	48.708000
H	56.526001	35.277000	47.301998
H	56.063999	33.206001	45.974998
H	56.609001	32.202999	47.306999
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H	54.183998	34.047001	47.323002
H	54.157001	31.620001	46.162998
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C	53.889999	44.084000	36.708000

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H	54.648998	44.132999	35.921001
H	54.361000	43.653999	37.594002
H	52.210999	43.706001	35.403000
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C	52.054001	41.077999	34.965000
C	52.487000	39.694000	34.418999
C	51.445000	39.147999	33.424999
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H	51.069000	37.486000	32.166000
H	51.379002	39.816002	32.561001
H	50.462002	39.092999	33.900002
H	52.610001	38.991001	35.248001
H	53.451000	39.778000	33.912998
H	51.735001	41.708000	34.129002
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O	55.438000	35.931000	38.407001
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C	59.983002	36.566002	37.995998
C	60.605999	37.627998	37.069000
N	62.112000	37.620998	37.074001
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H	62.523998	36.707001	36.792000
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H	60.285999	38.626999	37.377998
H	60.276001	37.469002	36.039001
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H	58.185001	37.728001	38.233002
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H	57.016998	31.322001	40.386002
H	58.632000	31.862000	39.911999
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H	57.139999	33.720001	40.632000
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H	57.556999	34.104000	37.637001
H	58.257000	35.908001	40.009998
C	31.695000	62.700001	39.243999
O	31.476999	61.505001	39.220001
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C	34.292000	63.034000	40.606998
C	35.547001	62.796001	41.465000
N	36.820000	62.773998	40.653000
H	36.827999	62.042999	39.911999
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H	37.653000	62.633999	41.259998
H	35.476002	61.840000	41.988998
H	35.657001	63.596001	42.203999
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H	34.219002	62.212002	39.900002
H	33.084999	63.772999	42.250999
H	32.797001	62.082001	41.844002
C	30.457001	63.342999	41.374001
C	29.198000	63.928001	40.688000
C	27.992001	63.773998	41.638000
N	26.731001	64.504997	41.241001
H	26.201000	64.054001	40.466999
H	26.927999	65.487999	40.952999
H	26.087000	64.555000	42.055000
H	28.273001	64.168999	42.617001
H	27.738001	62.716999	41.761002
H	28.997999	63.411999	39.744999
H	29.361000	64.986000	40.467999
H	30.593000	63.847000	42.334999
H	30.292000	62.283001	41.591999
H	31.882999	64.558998	40.297001
C	33.167999	59.900002	32.590000
O	33.939999	59.054001	32.193001
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C	33.139999	62.382000	31.923000
C	34.686001	62.479000	31.917000
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N	36.598000	64.188004	32.193001
H	36.981998	63.840000	33.097000
H	37.152000	63.744999	31.433001
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N	28.106001	62.106998	29.367001
H	27.872000	61.191002	28.931000
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H	27.200001	62.594002	29.528000
H	28.915001	62.877998	31.155001
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H	41.727001	57.207001	45.362999
H	42.882000	58.383999	45.542000
H	43.269001	57.032001	44.657001
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H	44.330002	57.012001	46.847000
H	42.548000	58.049000	48.250000
H	41.458000	56.710999	47.837002
H	44.113998	56.353001	49.318001
H	42.952000	55.087002	48.939999
C	42.839001	55.365002	51.576000
C	42.380001	55.589001	53.035999
C	42.952999	54.444000	53.896000
N	42.935001	54.626999	55.393002
H	41.993999	54.653000	55.839001
H	43.422001	55.497002	55.695999
H	43.459000	53.849998	55.837002
H	44.005001	54.303001	53.632999
H	42.425999	53.512001	53.675999
H	41.289001	55.603001	53.105000
H	42.755001	56.548000	53.398998
H	43.932999	55.373001	51.561001
H	42.528000	54.367001	51.252998
H	42.594002	57.410000	50.891998
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O	34.733002	57.376999	49.814999
C	34.021999	59.563999	50.495998
C	35.272999	59.866001	51.373001
C	35.073002	60.880001	52.526001
C	36.429001	61.108002	53.224998
N	36.382000	61.903999	54.501999
H	36.057999	62.882999	54.381001
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H	35.643002	58.928001	51.797001
H	36.058998	60.248001	50.716999
C	32.799999	59.109001	51.348999
C	31.573999	58.691002	50.499001
C	30.327000	58.543999	51.398998
N	29.055000	58.187000	50.674000
H	28.993999	57.196999	50.356998
H	28.910000	58.786999	49.839001
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H	30.492001	57.782001	52.165001
H	31.775000	57.747002	49.985001
H	31.382000	59.449001	49.736000
H	32.498001	59.933998	51.999001
H	33.091000	58.273998	51.993000

H	33.744999	60.477001	49.966000
C	42.768002	45.080002	25.209999
O	42.335999	44.542999	26.209000
C	42.067001	45.009998	23.857000
C	40.757000	45.842999	23.886999
C	41.012001	47.330002	24.211000
C	39.712002	48.139999	24.115999
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H	40.473000	49.819000	25.174000
H	40.409000	50.053001	23.528999
H	38.974998	50.070999	24.454000
H	39.001999	47.794998	24.872999
H	39.254002	48.015999	23.131001
H	41.752998	47.740002	23.518999
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H	40.264000	45.775002	22.913000
H	40.070000	45.421001	24.627001
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C	42.529999	41.479000	22.240999
N	43.660000	40.639999	21.716000
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H	43.523998	42.432999	23.933001
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C	49.183998	50.436001	28.611000
N	49.040001	51.903000	28.326000
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H	49.507000	48.201000	30.141001
H	48.261002	47.875999	28.947001
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N	45.478001	43.659000	32.601002
H	44.971001	44.180000	33.344002
H	46.092999	42.973000	33.085999
H	44.793999	43.098999	32.046001
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H	46.715000	46.212002	33.028999
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C	34.897999	54.664001	29.063000
O	35.777000	53.849998	29.264999
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C	36.640999	57.409000	32.122002
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H	36.611000	56.323002	30.292000
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H	35.284000	55.058998	31.927999
C	33.160999	54.029999	30.783001
C	32.257000	53.304001	29.764999
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N	30.690001	51.285000	29.587000
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H	32.839001	52.957001	28.907000
H	31.488001	53.986000	29.398001
H	32.536999	54.421001	31.591999
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C	38.366001	53.921001	23.556000
O	37.372002	53.306000	23.889999
C	38.390999	54.938999	22.413000
C	38.301998	56.373001	23.009001
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C	38.592999	58.859001	22.739000
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H	39.990002	60.105000	21.728001
H	38.514999	59.952999	20.952999
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H	39.161999	58.944000	23.669001
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H	38.324001	57.444000	21.117001
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H	37.264000	56.585999	23.278999
H	38.887001	56.424000	23.926001
C	37.233002	54.706001	21.398001
C	37.483002	53.506001	20.459000
C	36.180000	53.146000	19.722000
N	36.366001	52.390999	18.431999
H	37.094002	51.646999	18.507000
H	36.678001	53.011002	17.655001
H	35.491001	51.957001	18.110001
H	35.623001	54.054001	19.480000
H	35.558998	52.528000	20.375000

H	37.830002	52.636002	21.023001
H	38.264999	53.771000	19.740999
H	37.094002	55.591999	20.773001
H	36.294998	54.567001	21.941999
H	39.345001	54.837002	21.891001
C	34.334999	29.242001	48.720001
O	34.040001	30.382999	48.430000
C	34.612999	28.171000	47.667999
C	35.410000	28.771000	46.472000
C	36.756001	29.395000	46.901001
C	37.384998	30.214001	45.764000
N	38.610001	30.966999	46.206001
H	38.424999	31.528999	47.062000
H	39.386002	30.311001	46.431999
H	38.938000	31.607000	45.456001
H	36.666000	30.955000	45.402000
H	37.672001	29.566000	44.930000
H	37.443001	28.614000	47.236000
H	36.596001	30.077000	47.733002
H	35.601002	27.993000	45.727001
H	34.797001	29.535999	45.986000
C	33.298000	27.549000	47.122002
C	32.534000	26.677000	48.145000
C	31.297001	26.058001	47.459999
N	30.482000	25.117001	48.312000
H	30.089001	25.555000	49.171001
H	31.011999	24.268000	48.597000
H	29.666000	24.747999	47.780998
H	31.615999	25.489000	46.581001
H	30.625000	26.853001	47.126999
H	32.221001	27.281000	49.000999
H	33.188000	25.881001	48.512001
H	33.542000	26.923000	46.258999
H	32.644001	28.349001	46.759998
H	35.217999	27.379000	48.117001
C	32.339001	35.095001	51.984001
O	31.878000	35.680000	51.022999
C	31.497000	34.651001	53.172001
C	30.775999	33.323002	52.806000
C	30.333000	32.519001	54.050999
C	29.684999	31.188999	53.631001
N	29.273001	30.309999	54.778000
H	30.087999	29.999001	55.346001
H	28.615000	30.808001	55.410999
H	28.767000	29.466000	54.438999
H	30.375999	30.610001	53.013000
H	28.785000	31.386999	53.041000
H	29.624001	33.094002	54.650002
H	31.204000	32.311001	54.674000
H	29.915001	33.533001	52.164001
H	31.455999	32.695000	52.223000
C	30.476999	35.747002	53.599998
C	31.146999	36.958000	54.292999
C	30.069000	37.938000	54.806000
N	30.391001	38.659000	56.092999
H	31.049999	39.459000	56.000999
H	30.833000	38.021999	56.791000
H	29.528999	39.055000	56.521999

H	29.160999	37.368999	55.013000
H	29.829000	38.688000	54.048000
H	31.827999	37.472000	53.611000
H	31.738001	36.584999	55.132000
H	29.757999	35.318001	54.301998
H	29.900999	36.084000	52.733002
H	32.167999	34.455002	54.014000
C	46.160999	33.811001	51.063999
O	45.160999	34.069000	51.695000
C	47.504002	34.446999	51.414001
C	47.965000	33.984001	52.823002
C	48.339001	32.483002	52.831001
C	48.691002	31.983000	54.244999
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H	48.664001	29.927999	53.700001
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H	49.395000	30.194000	55.183998
H	47.796001	31.964001	54.873001
H	49.442001	32.629002	54.709000
H	49.193001	32.320999	52.167999
H	47.507999	31.884001	52.450001
H	48.837002	34.563999	53.138000
H	47.171001	34.173000	53.550999
C	47.403999	35.997002	51.353001
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C	46.806999	37.993999	49.873001
N	46.424999	38.452999	48.488998
H	45.693001	37.826000	48.096001
H	47.235001	38.410999	47.835999
H	45.997002	39.400002	48.471001
H	47.674000	38.576000	50.202000
H	45.963001	38.214001	50.530998
H	46.255001	35.948002	49.512001
H	47.970001	36.264999	49.272999
H	48.339001	36.445999	51.702000
H	46.613998	36.334999	52.028999
H	48.257999	34.130001	50.689999
C	46.935001	32.020000	44.450001
O	47.862999	32.790001	44.599998
C	47.071999	30.638000	43.823002
C	48.376999	29.910000	44.244999
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C	49.660999	28.819000	46.125000
N	50.029999	28.820000	47.583000
H	50.471001	29.723000	47.855000
H	49.202000	28.650999	48.195999
H	50.701000	28.048000	47.771000
H	49.390999	27.792999	45.855000
H	50.558998	29.096001	45.568001
H	47.577000	29.382999	46.202999
H	48.692001	30.753000	46.222000
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H	49.244999	30.447001	43.851002
C	46.971001	30.799000	42.279999
C	46.895000	29.464001	41.506001
C	46.542000	29.732000	40.030998
N	46.470001	28.500000	39.174000
H	45.879002	27.757999	39.603001

H	47.407001	28.080999	39.012001
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H	47.285000	30.393000	39.576000
H	45.561001	30.211000	39.970001
H	46.131001	28.820000	41.949001
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H	47.821999	31.382000	41.917000
H	46.070999	31.379999	42.054001
H	46.229000	30.028000	44.157001
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C	31.013000	49.659000	42.155998
C	32.500999	49.605999	42.575001
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H	34.714001	50.255001	44.157001
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H	32.275002	50.909000	44.292999
H	33.078999	50.367001	42.044998
H	32.923000	48.627998	42.327999
H	30.504000	50.349998	42.835999
H	30.535999	48.689999	42.326000
C	29.594999	51.129002	40.700001
C	29.319000	51.861000	39.370998
C	28.533001	53.154999	39.688000
N	27.480000	53.526001	38.688999
H	26.722000	52.811001	38.669998
H	27.865999	53.658001	37.733002
H	27.032000	54.431000	38.938999
H	29.215000	54.005001	39.776001
H	28.003000	53.037998	40.638000
H	28.745001	51.207001	38.708000
H	30.249001	52.122002	38.862000
H	29.822001	51.895000	41.445999
H	28.679001	50.630001	41.035000
H	31.650000	50.668999	40.327999
C	28.792999	42.494999	37.528999
O	28.632000	41.797001	38.513000
C	27.636999	42.930000	36.638000
C	27.584999	42.016998	35.376999
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H	24.231001	40.453999	33.373001
H	24.420000	41.945999	32.612999
H	24.899000	40.550999	31.841999
H	26.552999	40.148998	33.662998
H	26.896999	41.560001	32.633999
H	26.000000	43.090000	34.323002
H	25.433001	41.757999	35.325001
H	28.389999	42.289001	34.688000
H	27.764999	40.980999	35.681999
C	27.693001	44.436001	36.241001
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C	27.518000	46.849998	36.943001

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H	27.997000	47.966000	38.713001
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H	27.113001	48.814999	37.569000
H	26.674999	46.898998	36.247002
H	28.417000	47.167999	36.410000
H	28.608999	45.313999	38.021999
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H	28.570000	44.632000	35.619999
H	26.723000	42.765999	37.216000
C	31.958000	44.240002	49.117001
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H	34.826000	48.074001	53.283001
H	35.105000	46.424999	51.514999
H	34.771999	45.650002	53.081001
H	32.341999	45.410000	52.414001
H	32.710999	46.145000	50.863998
H	33.819000	43.500000	51.953999
H	34.367001	44.213001	50.443001
C	32.660000	41.987999	49.993999
C	31.433001	41.242001	49.414001
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N	30.610001	39.028000	48.478001
H	30.099001	39.518002	47.715000
H	29.920000	38.898998	49.245998
H	30.856001	38.073002	48.150002
H	32.240002	39.254002	49.784000
H	32.512001	39.859001	48.131001
H	31.027000	41.785999	48.556000
H	30.645000	41.195000	50.171001
H	33.008999	41.455002	50.882999
H	33.477001	41.977001	49.265999
H	31.468000	43.444000	51.050999
C	27.861000	43.112000	44.238998
O	28.139999	42.361000	45.152000
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C	25.353001	43.438999	44.633999
C	25.355000	44.859001	45.242001
C	24.054001	45.028999	46.049000
N	23.812000	46.375999	46.678001
H	24.475000	46.571999	47.463001
H	23.868999	47.169998	46.009998
H	22.861000	46.383999	47.090000
H	24.024000	44.298000	46.862999
H	23.197001	44.841999	45.396000
H	25.392000	45.609001	44.448002
H	26.225000	44.999001	45.889000
H	24.389000	43.287998	44.138000
H	25.409000	42.696999	45.436001
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C	26.712000	40.181000	41.040001
N	27.728001	39.601002	40.091000
H	28.547001	39.221001	40.609001
H	28.068001	40.303001	39.402000
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H	25.818001	40.416000	40.457001
H	26.461000	39.390999	41.752998
H	28.152000	41.223999	42.275002
H	27.346001	42.254002	41.084000
H	25.173000	41.939999	42.380001
H	26.066999	41.047001	43.598999
H	26.457001	43.986000	42.861000
C	62.318001	48.127998	54.603001
O	61.346001	47.514000	54.207001
C	63.215000	48.938000	53.673000
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C	61.778999	51.067001	53.766998
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N	60.800999	53.424999	53.681000
H	60.261002	53.290001	54.560001
H	61.695999	53.868999	53.980000
H	60.284000	54.113998	53.097000
H	60.106998	51.778000	52.563000
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H	62.592999	51.523998	54.333000
H	61.077999	50.644001	54.490002
H	63.002998	50.436001	52.110001
H	61.564999	49.443001	52.327000
C	64.021004	48.006001	52.719002
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C	66.082001	46.547001	52.370998
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H	67.936996	46.195000	53.422001
H	67.973000	47.516998	52.419998
H	68.040001	45.991001	51.766998
H	65.884003	46.883999	51.349998
H	65.749001	45.508999	52.462002
H	65.084999	46.884998	54.271999
H	65.954002	48.291000	53.655998
H	64.310997	48.564999	51.826000
H	63.383999	47.181999	52.381001
H	63.930000	49.511002	54.270000
C	59.143002	42.669998	59.209999
O	58.090000	42.068001	59.153999
C	60.124001	42.473999	60.360001
C	60.431000	43.806000	61.111000
C	59.154999	44.562000	61.573002
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H	57.806999	47.023998	61.609001
H	57.648998	46.473999	63.152000
H	58.660000	47.764999	62.828999
H	60.223999	46.449001	61.602001
H	60.002998	45.729000	63.207001
H	58.585999	43.943001	62.271999
H	58.508999	44.764999	60.715000
H	61.055000	43.591000	61.983002

H	61.015999	44.463001	60.460999
C	61.424000	41.779999	59.845001
C	62.126999	40.891998	60.903999
C	63.370998	40.196999	60.299000
N	63.863998	38.999001	61.074001
H	63.131001	38.263000	61.101002
H	64.134003	39.228001	62.049999
H	64.695000	38.560001	60.626999
H	64.202003	40.903999	60.223999
H	63.138000	39.826000	59.297001
H	61.422001	40.131001	61.251999
H	62.423000	41.487999	61.771999
H	62.124001	42.528999	59.463001
H	61.165001	41.136002	58.999001
H	59.626999	41.796001	61.061001
C	53.930000	53.660000	42.972000
O	54.032001	52.587002	42.409000
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C	51.667000	53.828999	44.070000
C	52.310001	53.747002	45.473999
C	51.325001	53.209999	46.518002
N	51.882999	53.188999	47.912998
H	52.817001	52.748001	47.976002
H	51.981998	54.145000	48.320000
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H	51.061001	52.181999	46.264999
H	50.412998	53.814999	46.535999
H	52.665001	54.735001	45.773998
H	53.167000	53.073002	45.448002
H	50.755001	54.429001	44.125999
H	51.375999	52.827000	43.745998
C	51.952000	54.542999	41.638000
C	52.747002	55.426998	40.652000
C	52.040001	55.480999	39.285000
N	52.613998	56.500999	38.341000
H	53.625999	56.339001	38.145000
H	52.512001	57.471001	38.707001
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H	50.986000	55.736000	39.419998
H	52.105999	54.507000	38.792999
H	53.758999	55.034000	40.521000
H	52.834000	56.438999	41.058998
H	50.946999	54.958000	41.750999
H	51.841999	53.537998	41.226002
H	52.854000	55.474998	43.349998
C	59.459999	51.928001	43.443001
O	58.729000	51.785999	42.486000
C	60.650002	52.879002	43.430000
C	60.154999	54.327000	43.155998
C	61.193001	55.411999	43.516998
C	60.563999	56.812000	43.395000
N	61.522999	57.924999	43.709999
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H	59.859001	54.426998	42.108002
H	59.259998	54.512001	43.750000
C	61.699001	52.429001	42.375999
C	62.264000	51.020000	42.673000
C	63.282001	50.612999	41.594002
N	63.889999	49.251999	41.793999
H	63.198002	48.478001	41.757000
H	64.416000	49.182999	42.691002
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H	61.457001	50.283001	42.698002
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H	61.118000	52.861000	44.416000
C	43.257000	35.243000	59.105000
O	44.152000	35.581001	58.352001
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C	44.681000	33.616001	60.506001
C	45.186001	34.632000	61.562000
C	45.964001	35.797001	60.923000
N	46.324001	36.904999	61.877998
H	46.632000	37.751999	61.362000
H	45.521000	37.200001	62.472000
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H	45.362999	36.250000	60.134998
H	46.894001	35.433998	60.476002
H	45.854000	34.117001	62.257999
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H	45.417000	33.505001	59.702999
C	42.769001	32.740002	59.069000
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C	40.716000	31.570999	58.034000
N	40.562000	30.332001	58.877998
H	40.013000	30.520000	59.743999
H	41.470001	29.924000	59.180000
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H	41.054001	33.695000	58.146999
H	40.692001	32.956001	59.699001
H	42.966999	31.813000	59.611000
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H	42.595001	34.062000	60.764000
C	42.113998	40.743999	55.749001
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C	40.938999	41.696999	55.556999
C	40.146000	41.905998	56.876999
C	40.891998	42.744999	57.931999
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N	40.478001	44.112000	60.049999
H	41.266998	43.709000	60.598000
H	40.812000	44.999001	59.618999
H	39.738998	44.384998	60.723000
H	39.591999	42.256001	59.608002

H	39.032001	43.622002	58.625000
H	41.292999	43.646000	57.467999
H	41.728001	42.183998	58.349998
H	39.210999	42.423000	56.641998
H	39.872002	40.937000	57.306000
C	39.926998	41.189999	54.487000
C	40.529999	40.824001	53.111000
C	41.012001	39.359001	53.073002
N	41.306999	38.831001	51.692001
H	42.041000	39.382999	51.223000
H	40.466999	38.865002	51.070000
H	41.610001	37.844002	51.723000
H	40.247002	38.709999	53.508999
H	41.924999	39.250000	53.664001
H	41.334999	41.514000	52.844002
H	39.738998	40.945999	52.368999
H	39.192001	41.984001	54.325001
H	39.370998	40.333000	54.880001
H	41.321999	42.665001	55.221001
C	54.609001	39.865002	58.796001
O	53.507999	39.387001	58.599998
C	55.581001	40.151001	57.660000
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C	54.529999	42.514000	57.534000
C	53.816002	43.577999	56.678001
N	52.966999	44.512001	57.509998
H	52.293999	44.014999	58.127998
H	53.543999	45.096001	58.150002
H	52.374001	45.153999	56.944000
H	53.141998	43.091000	55.969002
H	54.540001	44.182999	56.125999
H	55.335999	42.967999	58.116001
H	53.785000	42.158001	58.234001
H	55.855000	41.615002	56.058998
H	54.250000	40.904999	56.112000
C	55.859001	38.848000	56.852001
C	56.388000	37.692001	57.744999
C	56.546001	36.377998	56.952000
N	56.889999	35.187000	57.811001
H	56.172001	35.016998	58.549999
H	57.799999	35.282001	58.285999
H	56.932999	34.313000	57.244999
H	57.331001	36.477001	56.195999
H	55.608002	36.136002	56.444000
H	55.692001	37.506001	58.567001
H	57.347000	37.976002	58.188000
H	56.585999	39.057999	56.063000
H	54.935001	38.526001	56.362999
H	56.528000	40.479000	58.090000
C	49.624001	37.868000	63.686001
O	48.613998	37.257999	63.396999
C	50.189999	37.886002	65.098999
C	50.721001	39.299999	65.494003
C	50.980000	39.456001	67.013000
C	51.598000	40.828999	67.337997
N	51.912998	41.004002	68.799004
H	51.076000	40.966000	69.394997
H	52.568001	40.271000	69.152000

H	52.373001	41.923000	68.983002
H	50.918999	41.638000	67.049004
H	52.539001	40.951000	66.793999
H	51.667000	38.687000	67.370003
H	50.042000	39.334999	67.559998
H	51.638000	39.521000	64.943001
H	49.983002	40.051998	65.195999
C	51.269001	36.775002	65.252998
C	50.651001	35.361000	65.308998
C	51.743999	34.305000	65.563004
N	51.195000	32.957001	65.949997
H	50.611000	32.521999	65.204002
H	50.596001	33.004002	66.786003
H	51.943001	32.270000	66.190002
H	52.391998	34.632000	66.383003
H	52.356998	34.173000	64.666000
H	50.126999	35.130001	64.378998
H	49.917999	35.324001	66.120003
H	51.832001	36.918999	66.174004
H	51.990002	36.834000	64.431999
H	49.355000	37.660000	65.766998