C-Terminal Functionalization of Nylon-3 Polymers: Effects of C-Terminal Groups on Antibacterial and Hemolytic Activities

Supporting Information Part 2

MALDI-TOF, GPC, ^{1}H NMR, Bioassay and CAC data

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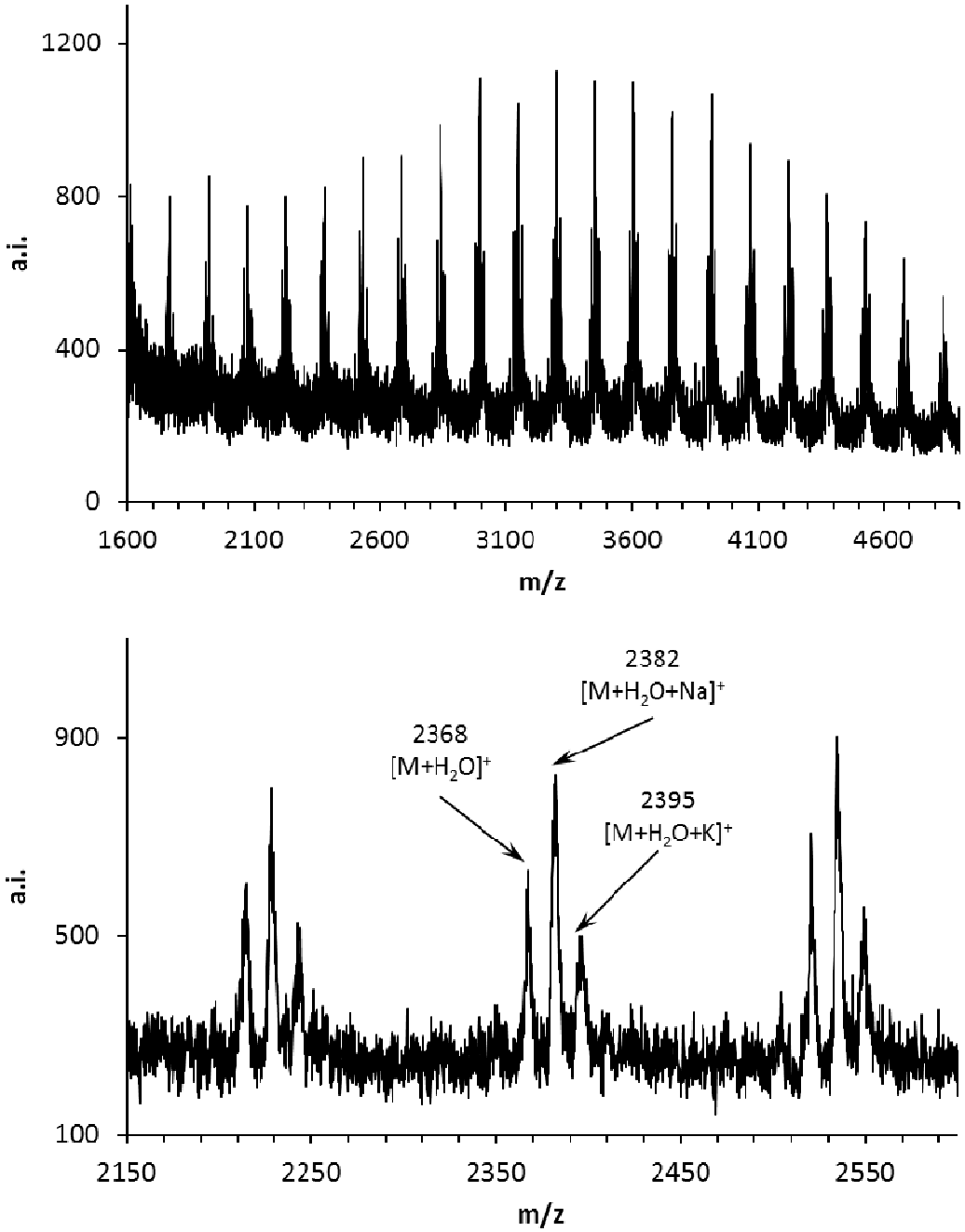
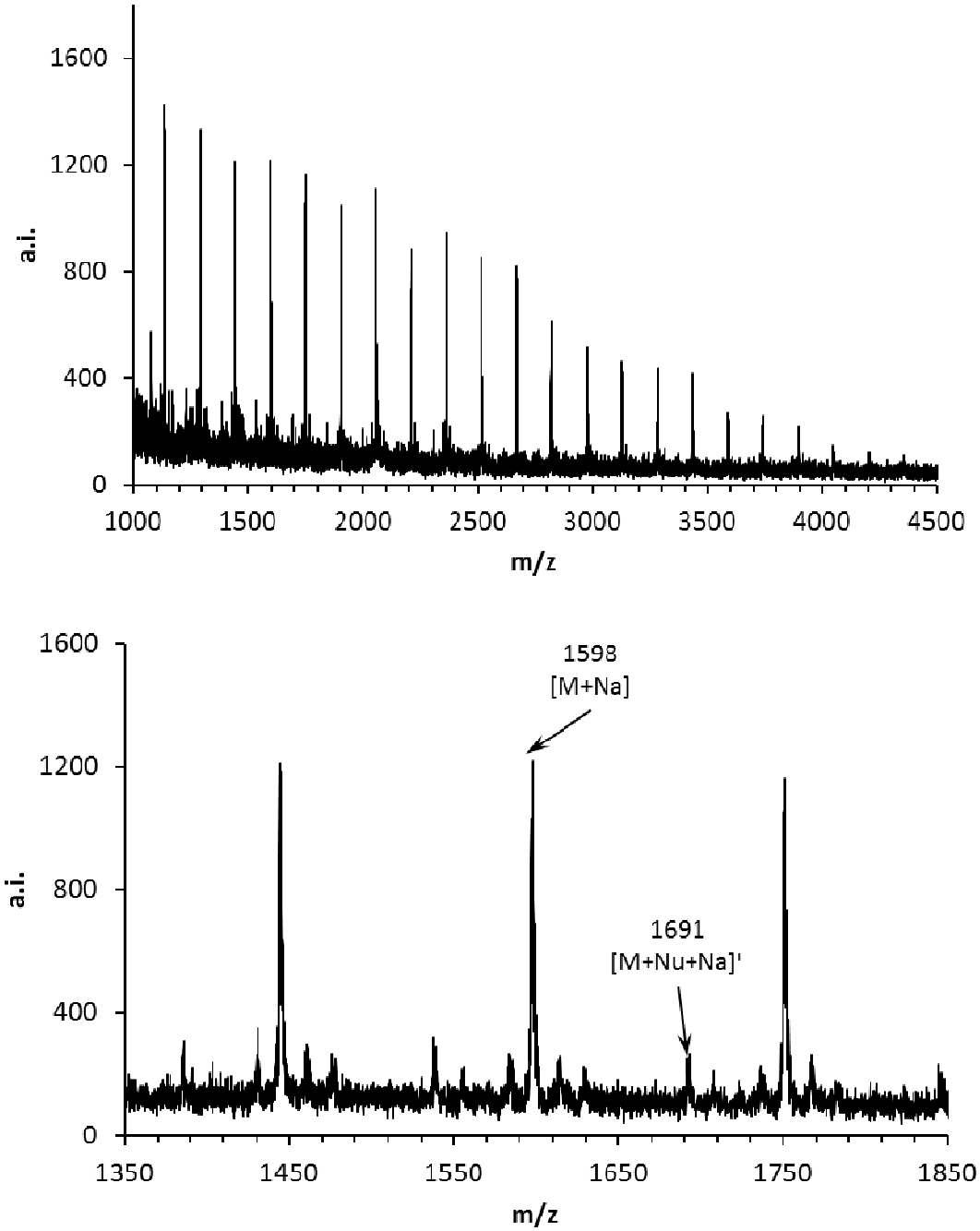
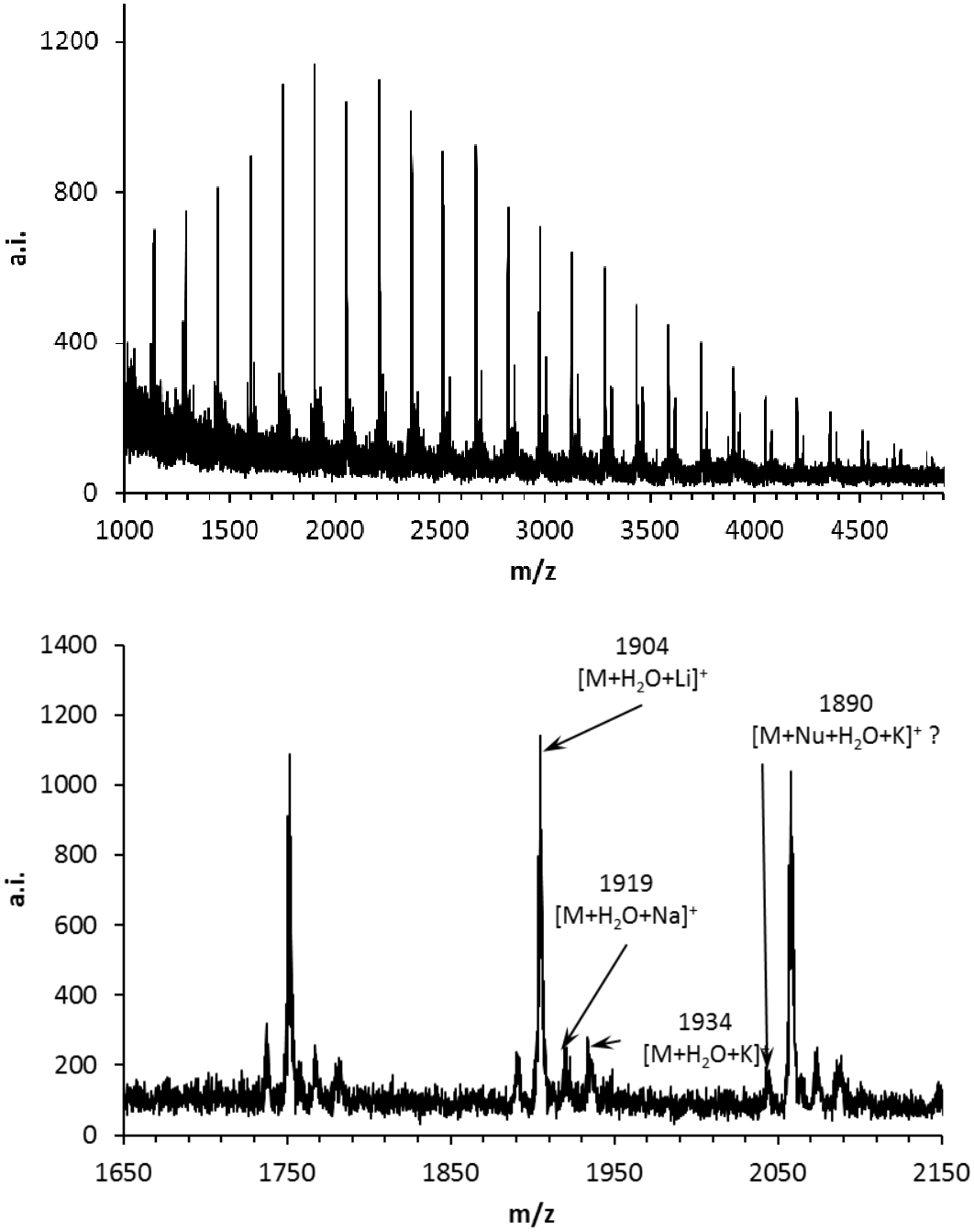
1 MALDI-TOF data samples generated during efforts to achieve *C*-terminal functionalization of poly(CO)



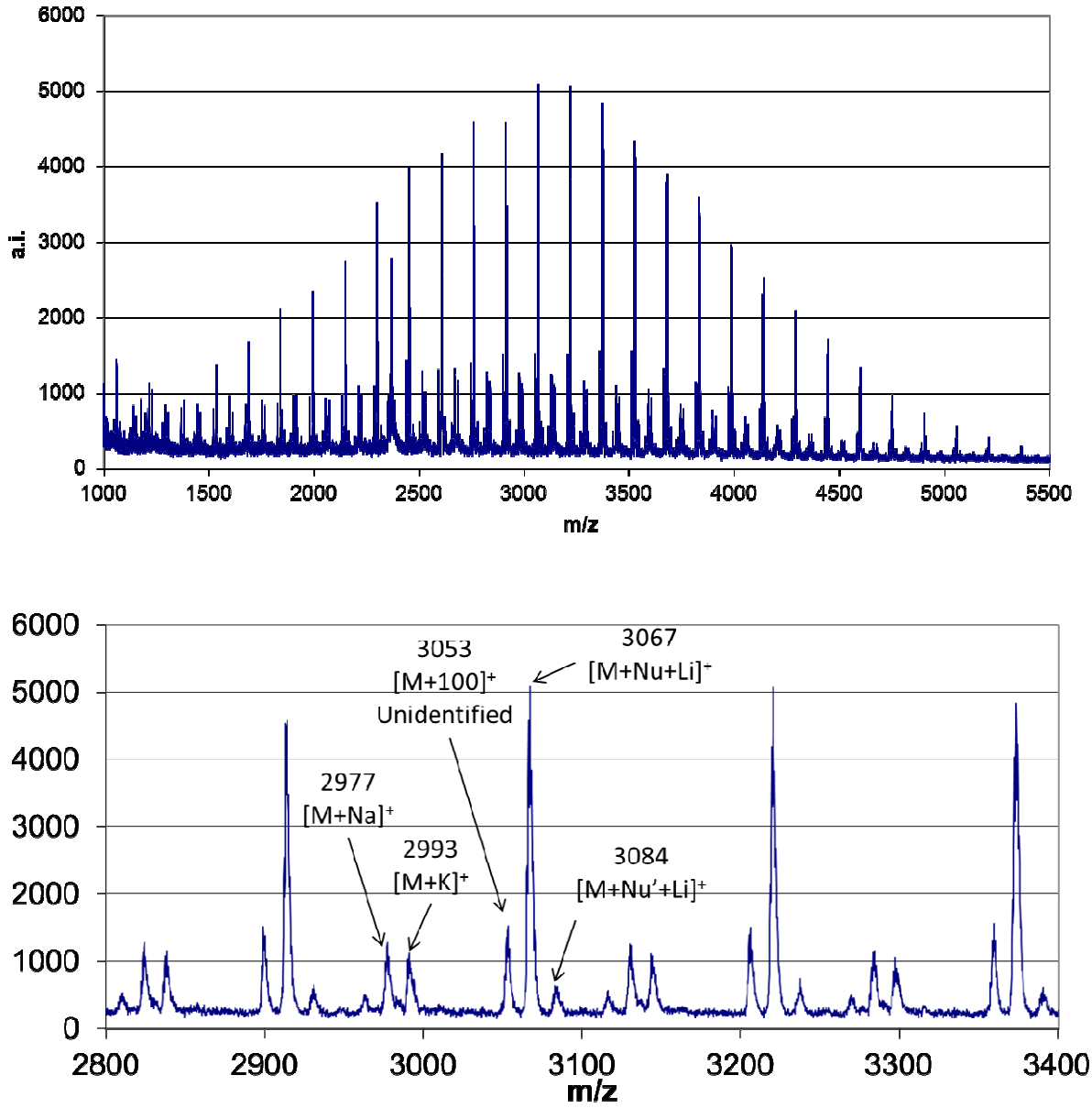
MALDI-TOF spectrum of the product from Table S1, entry 1. M refers to poly(**CO**) containing 15 units with an acetyl *N*-terminus and an imide *C*-terminus.



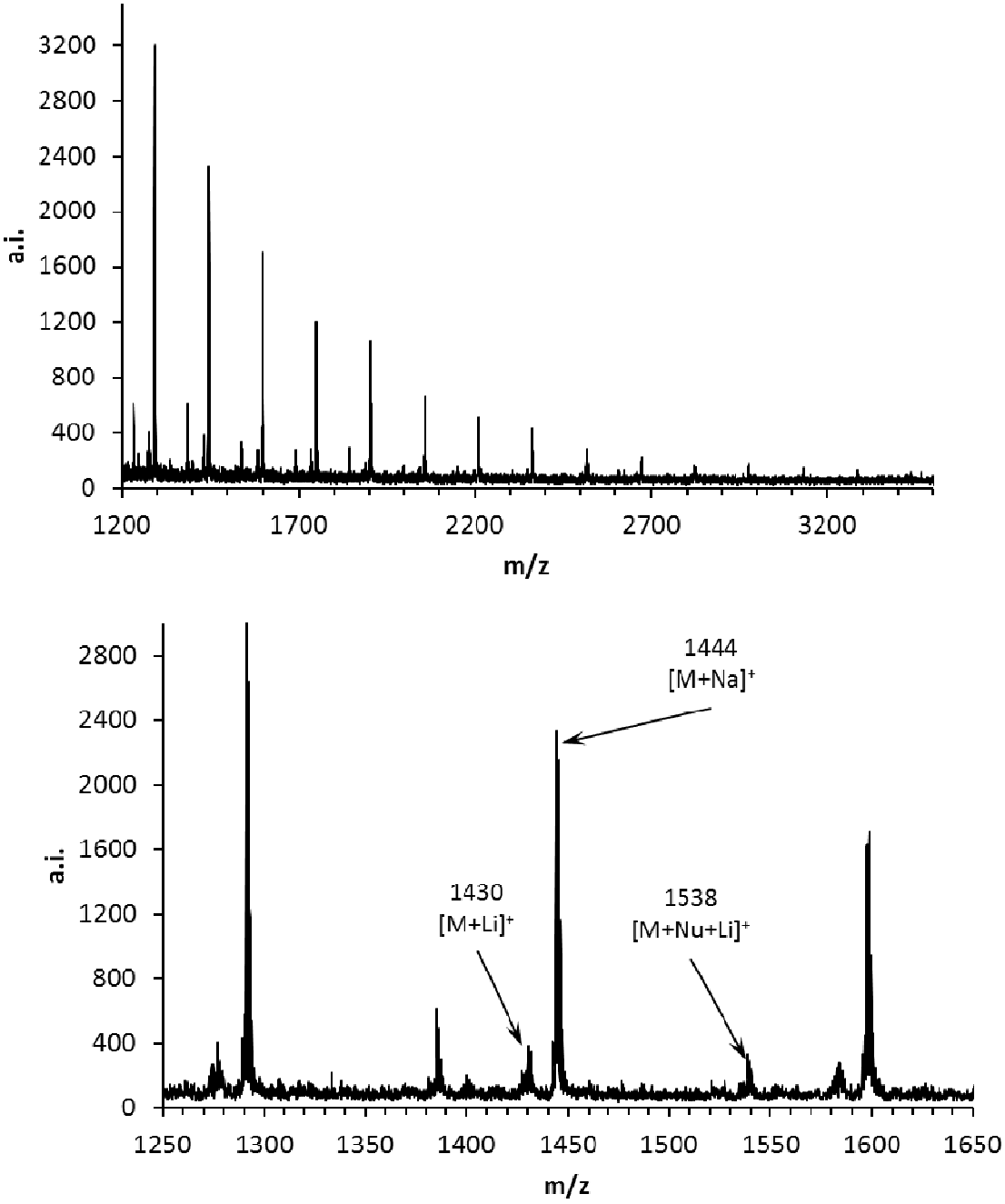
MALDI-TOF spectrum of the product from Table S1, entry 2. M refers to poly(**CO**) containing 10 subunits with an acetyl *N*-terminus and an imide *C*-terminus. Nu = benzylamine.



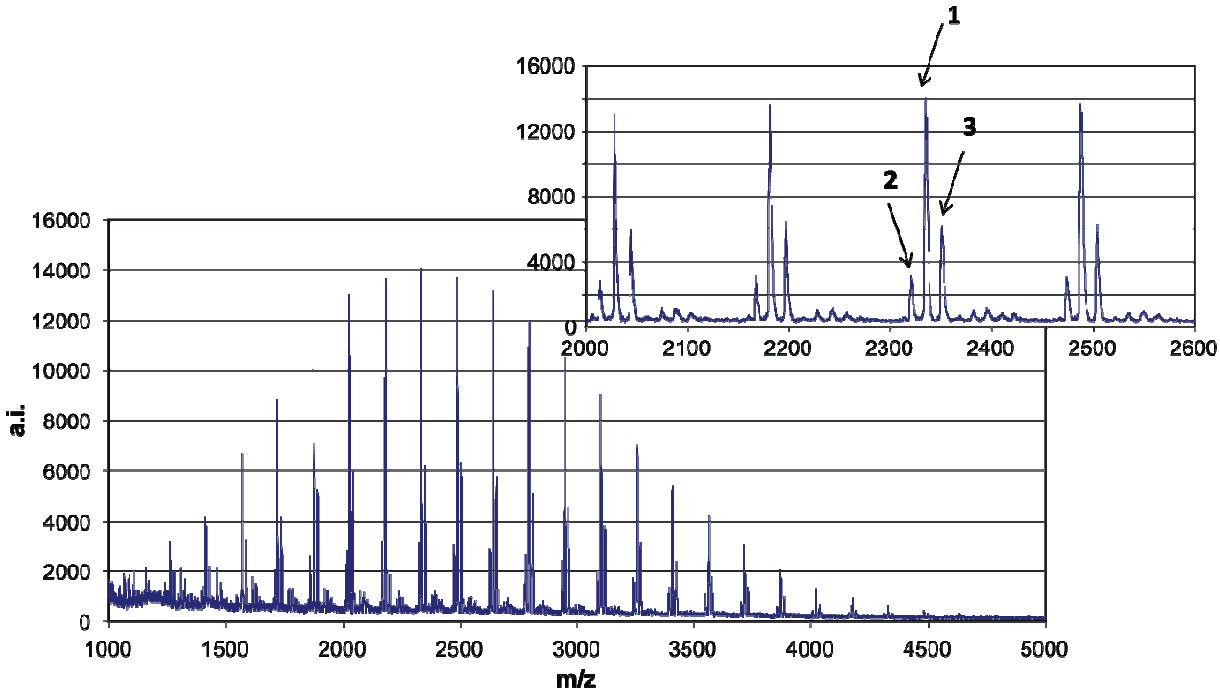
MALDI-TOF spectrum of the product from Table S1, entry 3. M refers to poly(**CO**) containing 12 subunits with an acetyl *N*-terminus and an imide *C*-terminus. Nu = benzylamine.



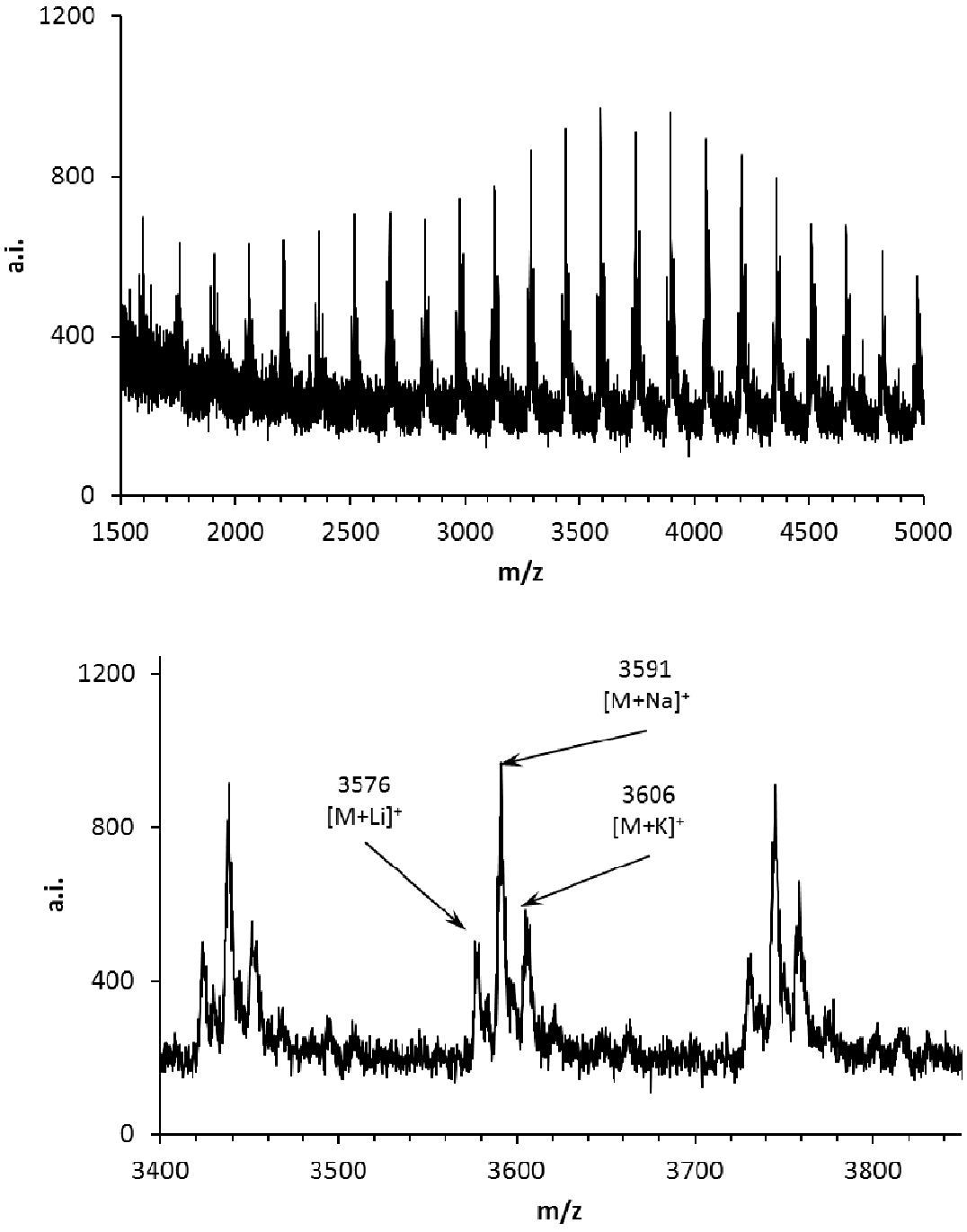
MALDI-TOF spectrum of the product from Table S1, entry 4. M refers to poly(**CO**) containing 19 subunits with an acetyl *N*-terminus and an imide *C*-terminus. Nu = benzylamine, Nu' = benzyl mercaptan.



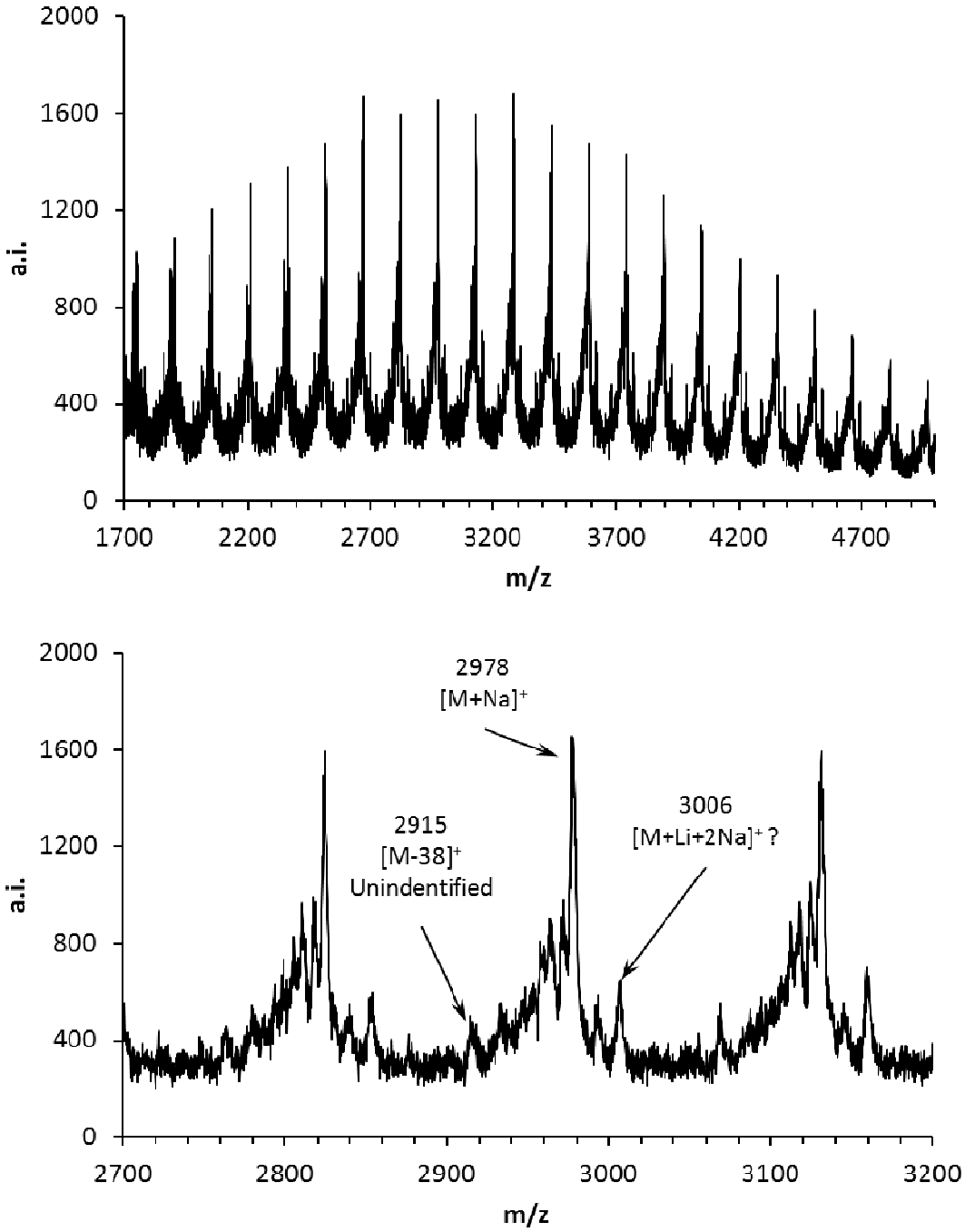
MALDI-TOF spectrum of the product from Table S1, entry 5. M refers to poly(**CO**) containing 9 subunits with an acetyl *N*-terminus and an imide *C*-terminus. Nu = benzylamine.



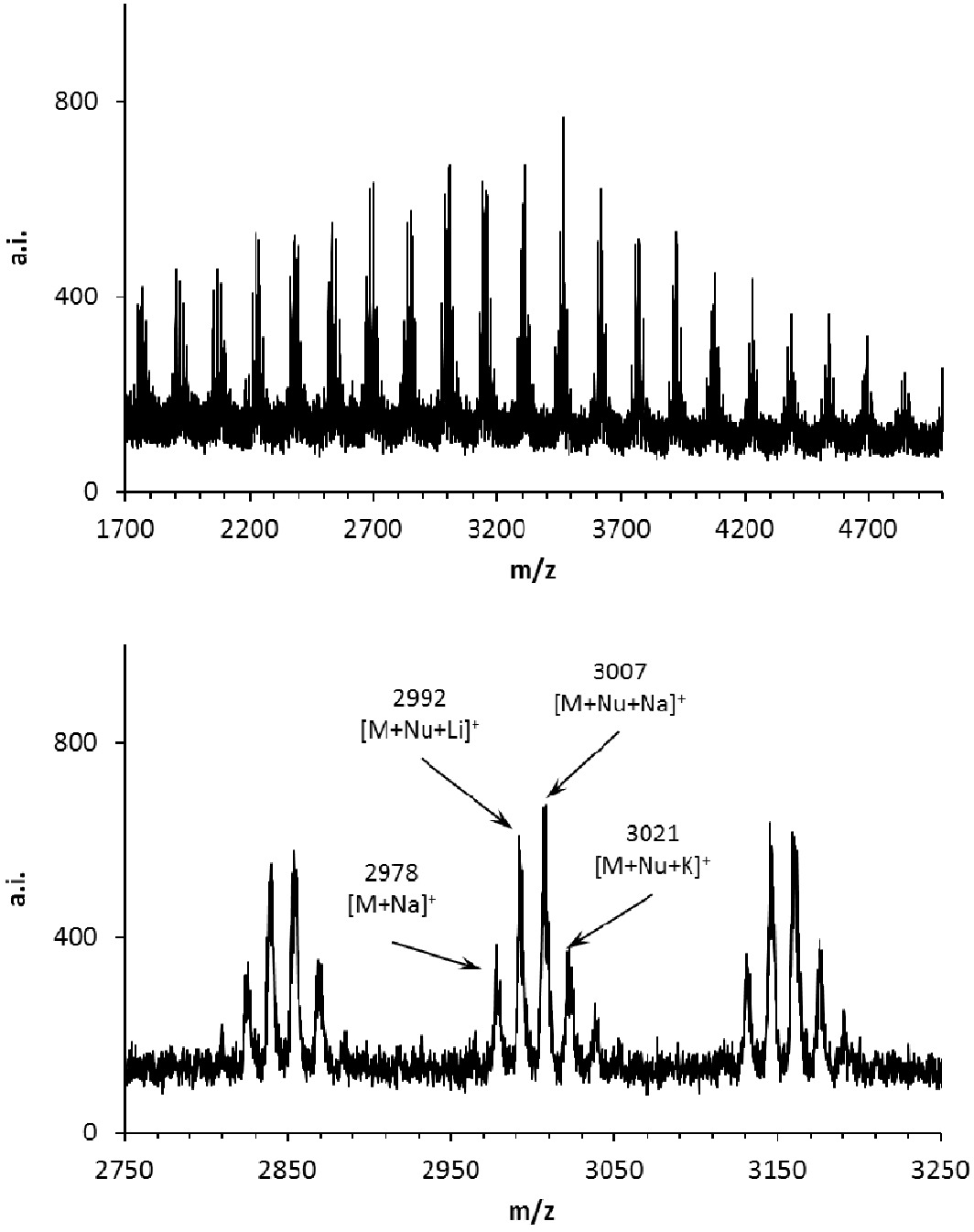
MALDI-TOF spectrum of the product from Table S1, entry 6. The labels 1, 2 and 3 indicate $[M+Nu+Li]^+$ (2165), $[M+Nu+Na]^+$ (2181) and $[M+Nu+K]^+$ (2197) peaks, respectively, where M refers to poly(**CO**) containing 13 subunits with an acetyl *N*-terminus and an imide *C*-terminus. Nu = benzyl mercaptan.



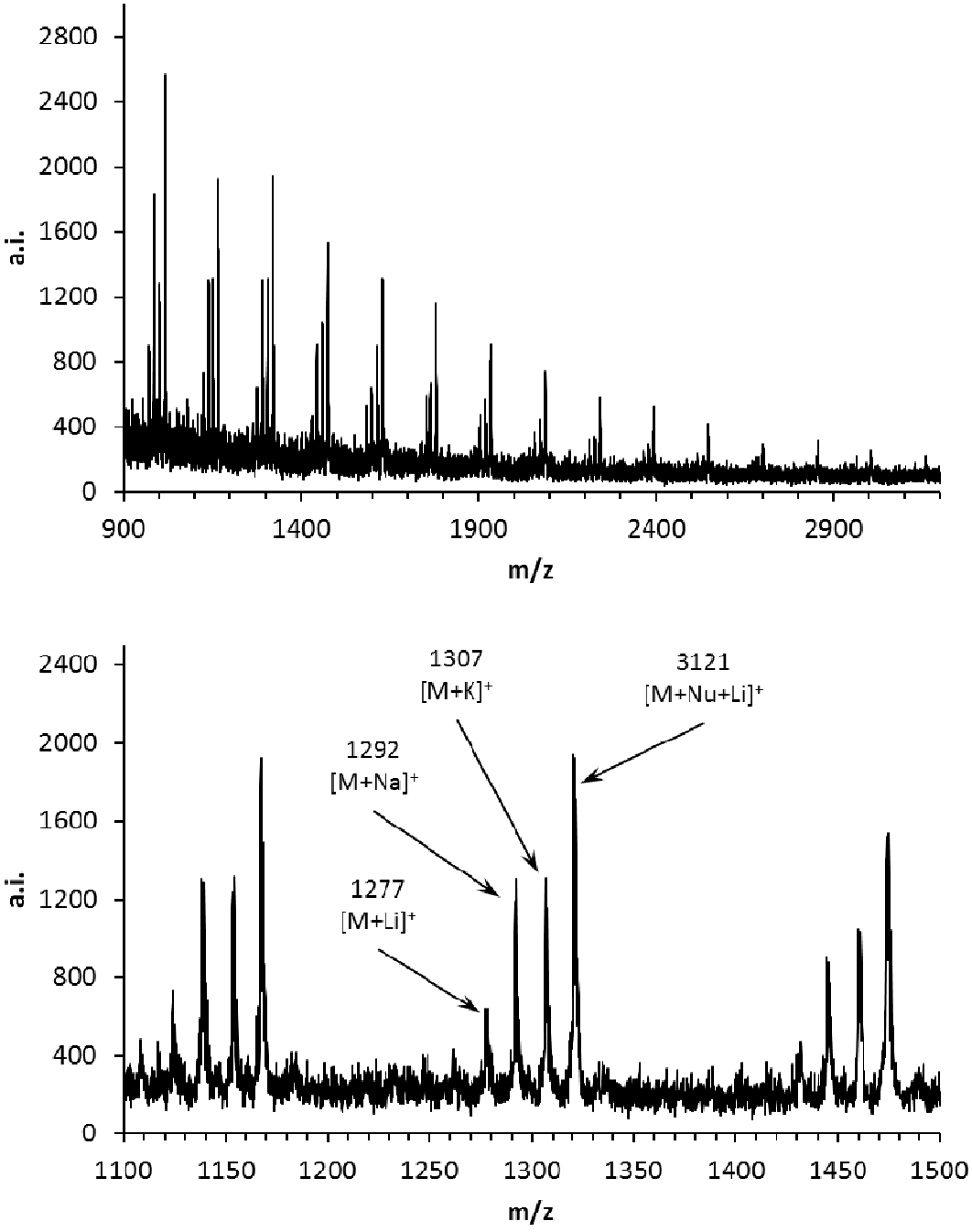
MALDI-TOF spectrum of the product from Table S1, entry 7. M refers to poly(**CO**) containing 23 subunits with an acetyl *N*-terminus and an imide *C*-terminus.



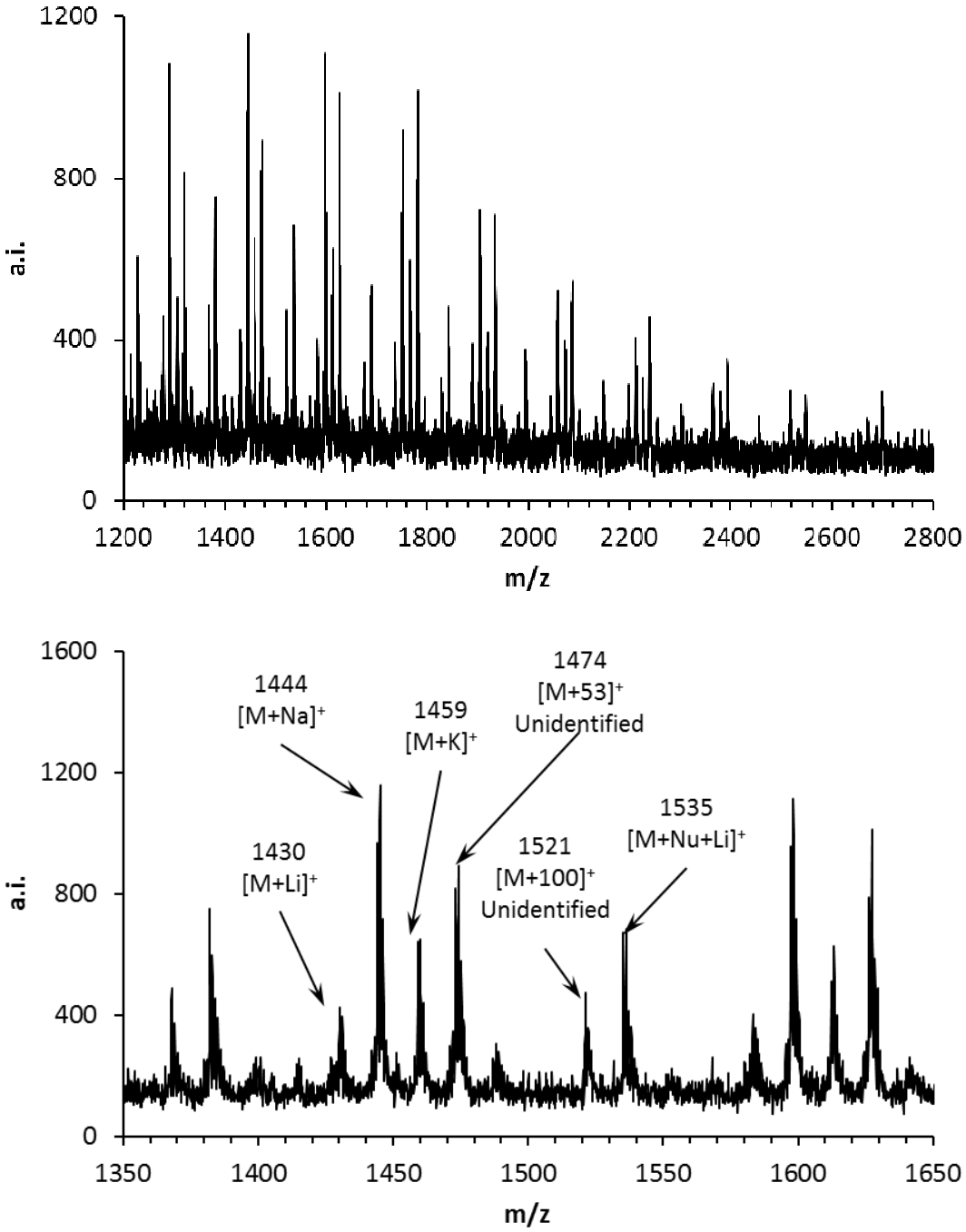
MALDI-TOF spectrum of the product from Table S1, entry 8. M refers to poly(**CO**) containing 19 subunits with an acetyl *N*-terminus and an imide *C*-terminus.



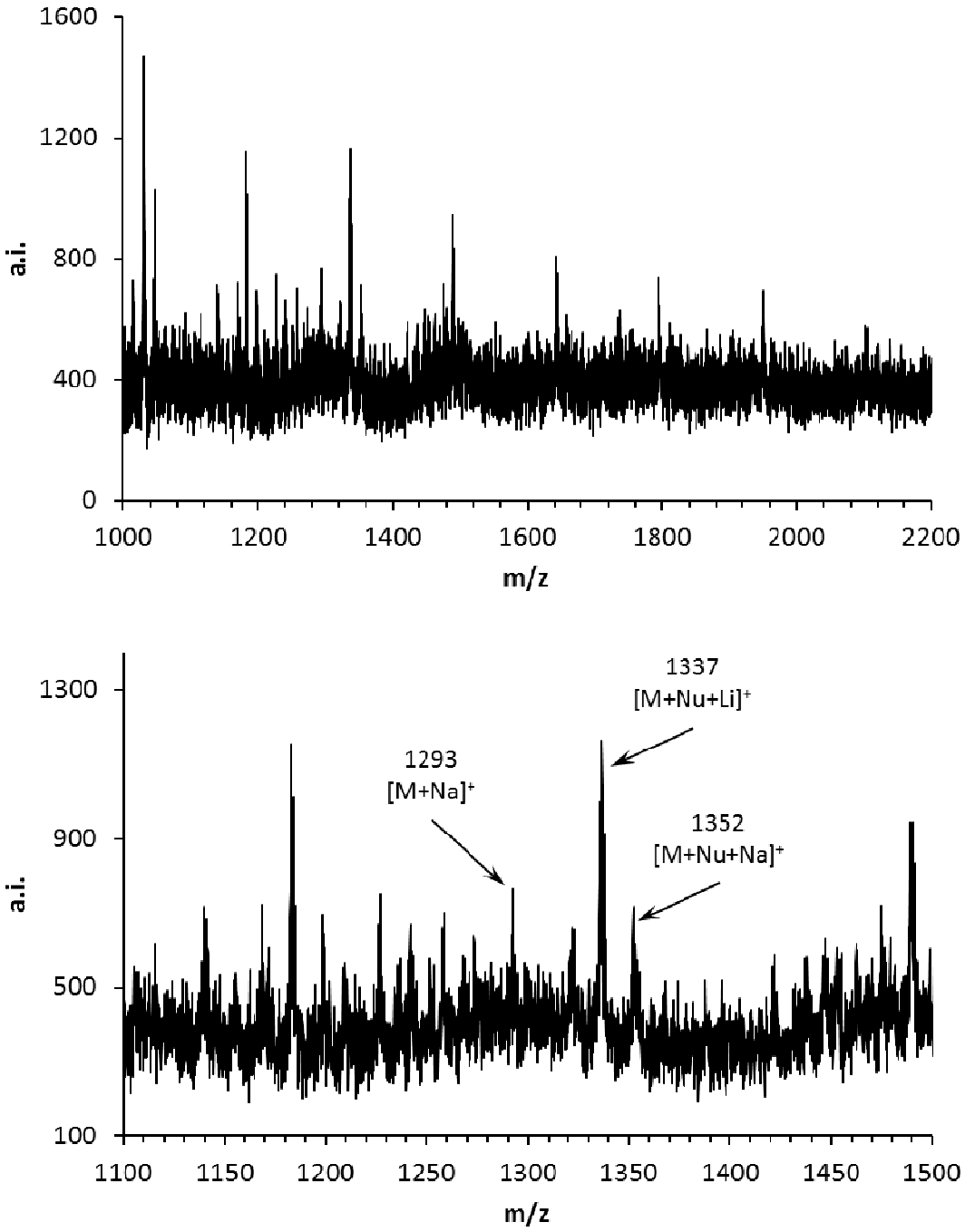
MALDI-TOF spectrum of the product from Table S1, entry 10. M refers to poly(**CO**) containing 19 subunits with an acetyl *N*-terminus and an imide *C*-terminus. Nu = MeOH.



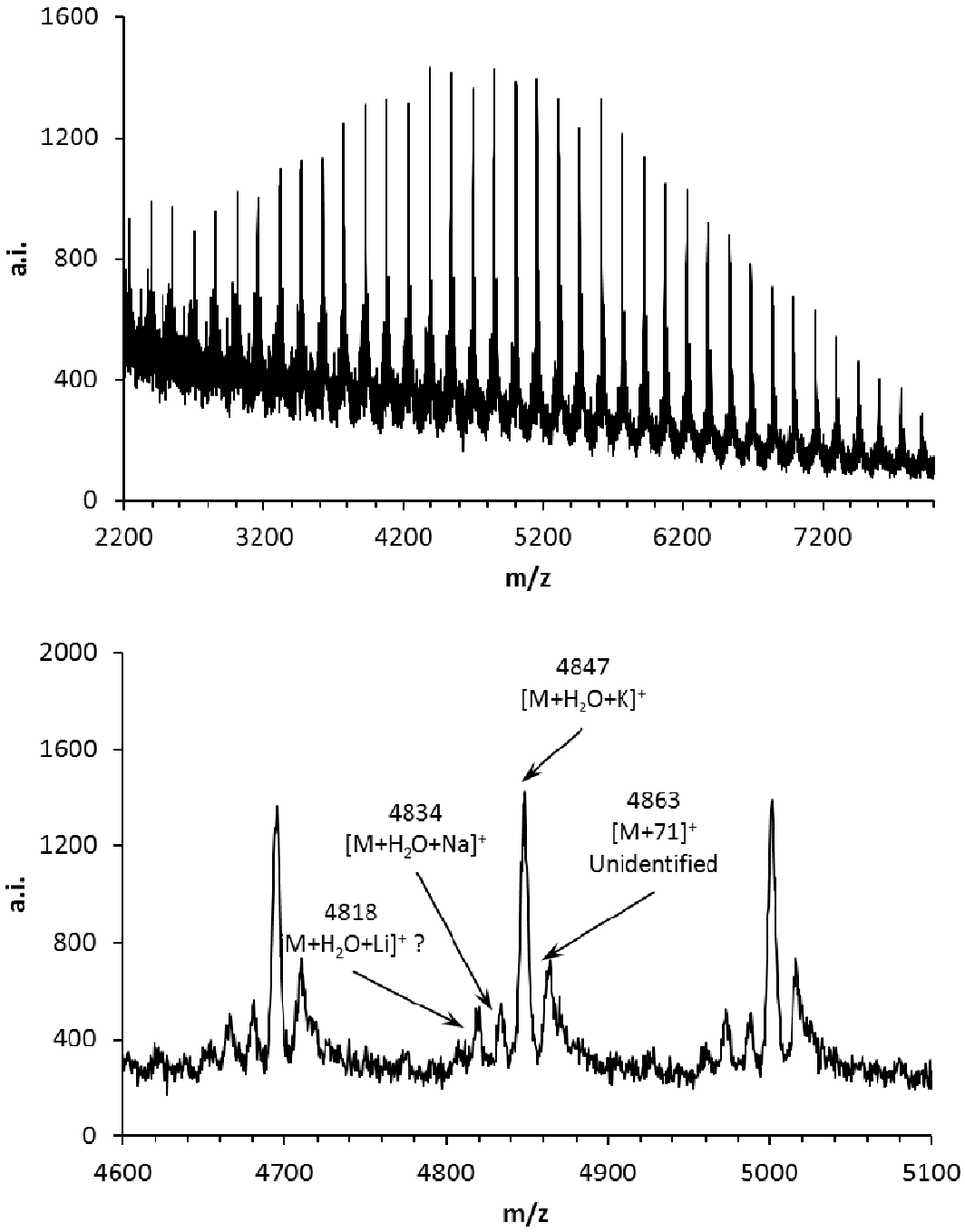
MALDI-TOF spectrum of the product from Table S1, entry 11. M refers to poly(**CO**) containing 8 subunits with an acetyl *N*-terminus and an imide *C*-terminus. Nu = EtOH.



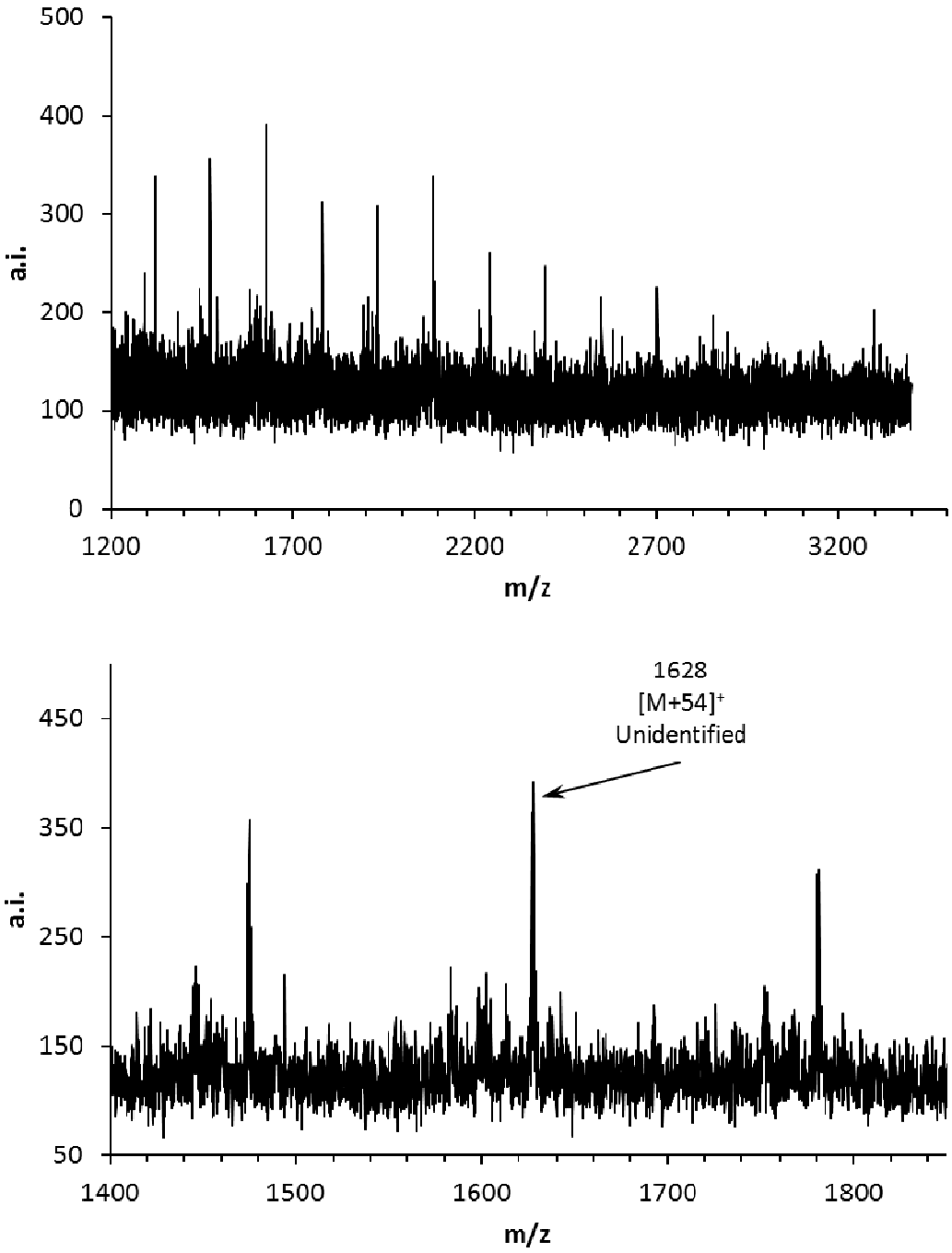
MALDI-TOF spectrum of the product from Table S1, entry 12. M refers to poly(**CO**) containing 9 subunits with an acetyl *N*-terminus and an imide *C*-terminus. Nu = BnOH.



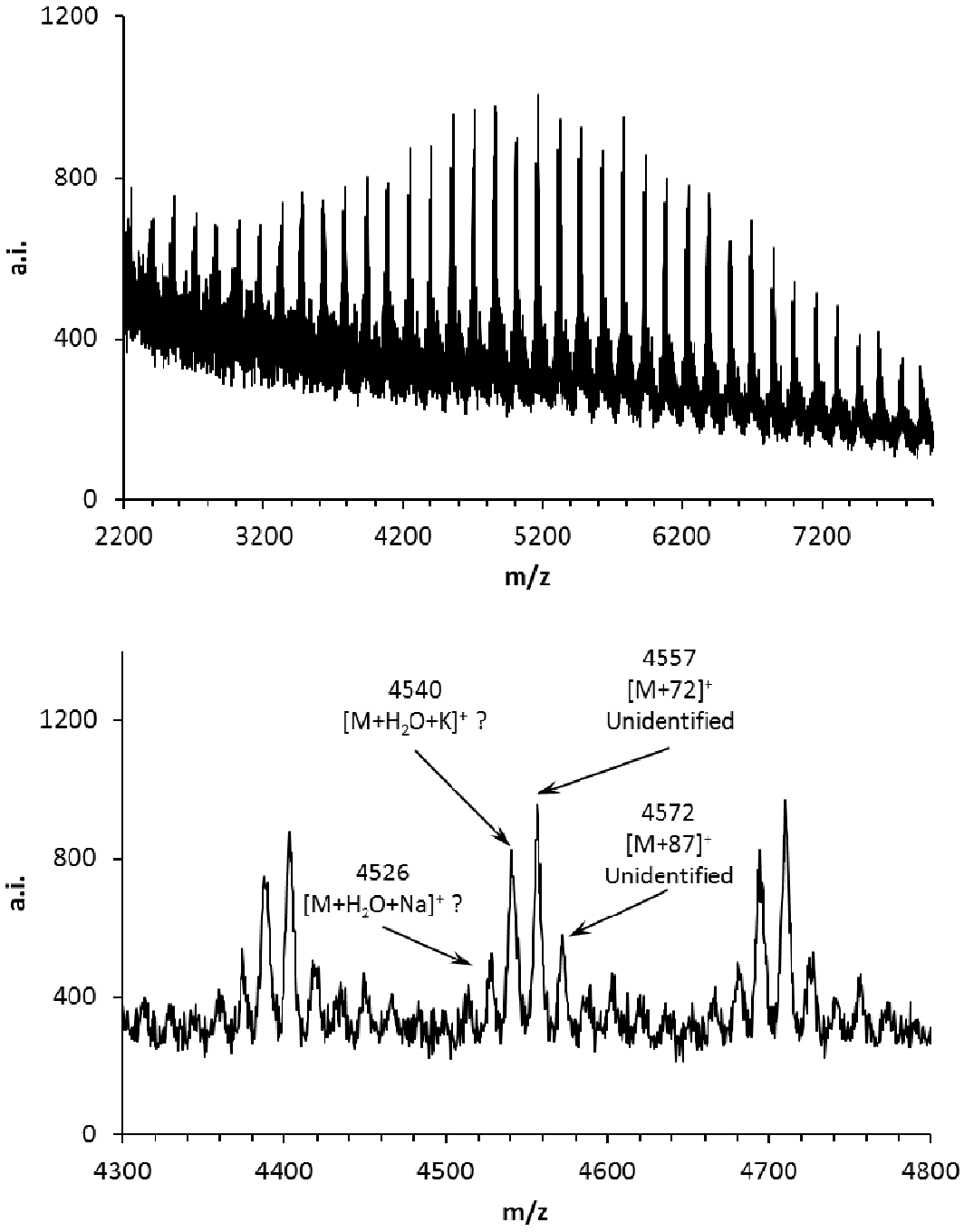
MALDI-TOF spectrum of the product from Table S1, entry 13. M refers to poly(**CO**) containing 8 subunits with an acetyl *N*-terminus and an imide *C*-terminus. Nu = $HOCH_2CH_2NH_2$.



MALDI-TOF spectrum of the product from Table S1, entry 14. M refers to poly(**CO**) containing 31 subunits with an acetyl *N*-terminus and an imide *C*-terminus.

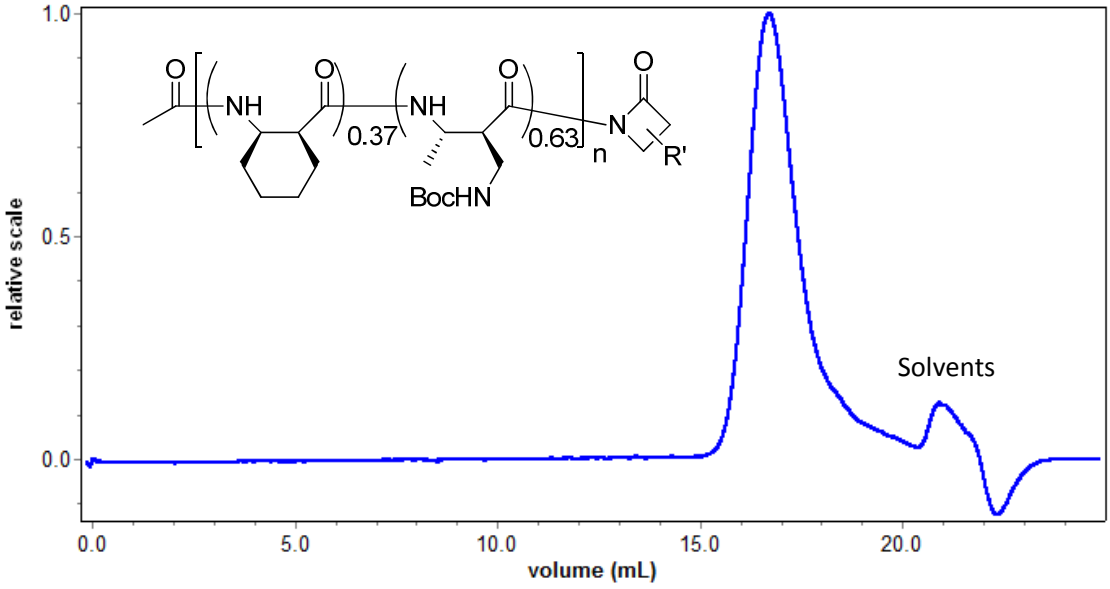


MALDI-TOF spectrum of the product from Table S1, entry 15. M refers to poly(**CO**) containing 10 subunits with an acetyl *N*-terminus and an imide *C*-terminus.

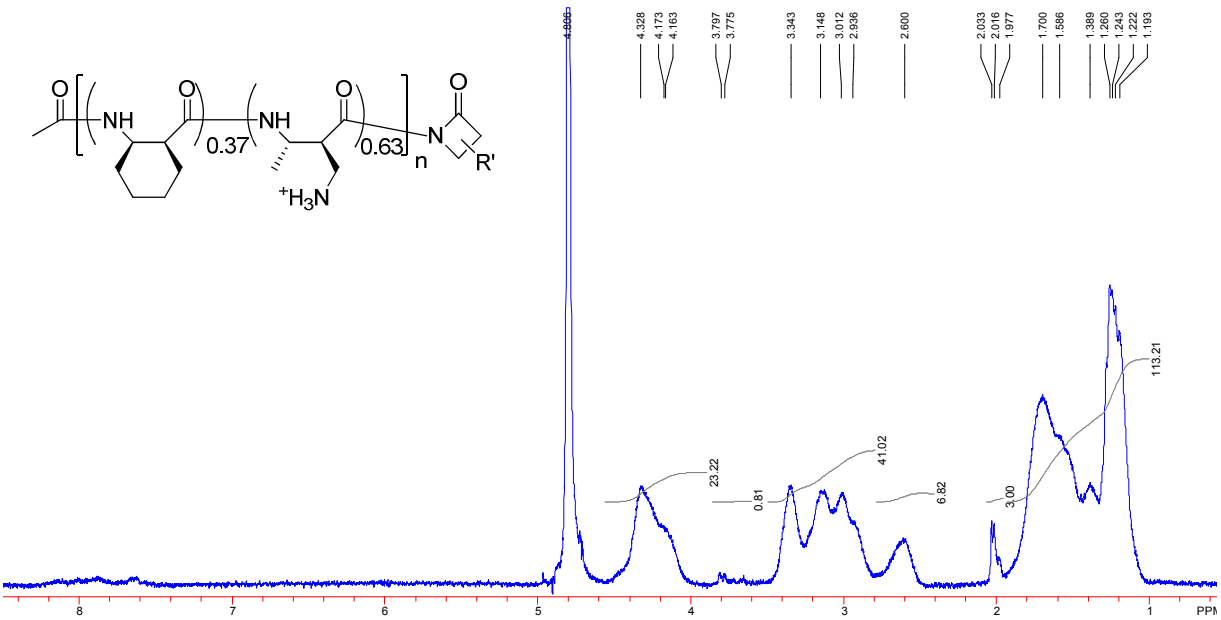


MALDI-TOF spectrum of the product from Table S1, entry 16. M refers to poly(**CO**) containing 29 subunits with an acetyl *N*-terminus and an imide *C*-terminus.

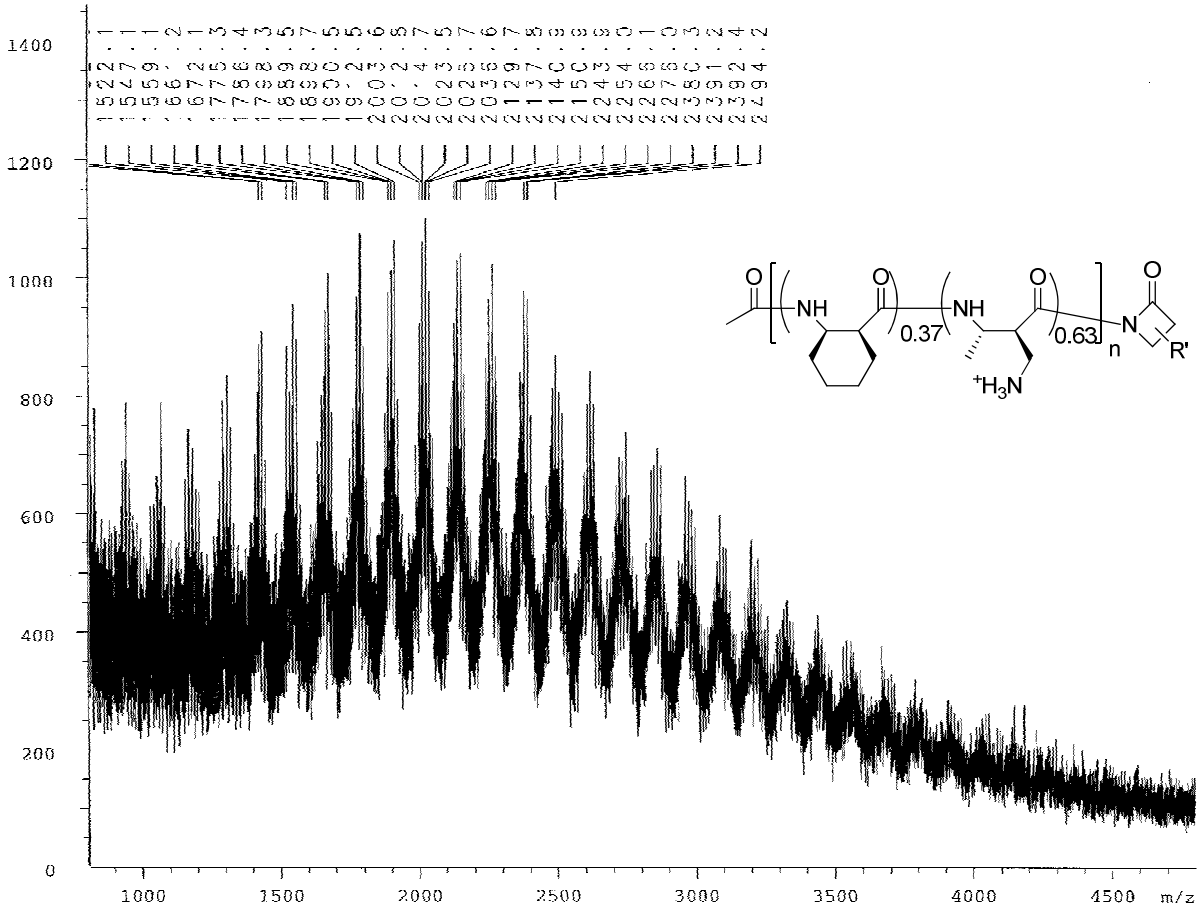
2 GPC, ^{1}H NMR and MALDI-TOF characterization data for *C*-terminal imide and *C*-terminal functionalized 37:63 CH:MM nylon-3 random copolymers (R' = side chain of either CH or MM)



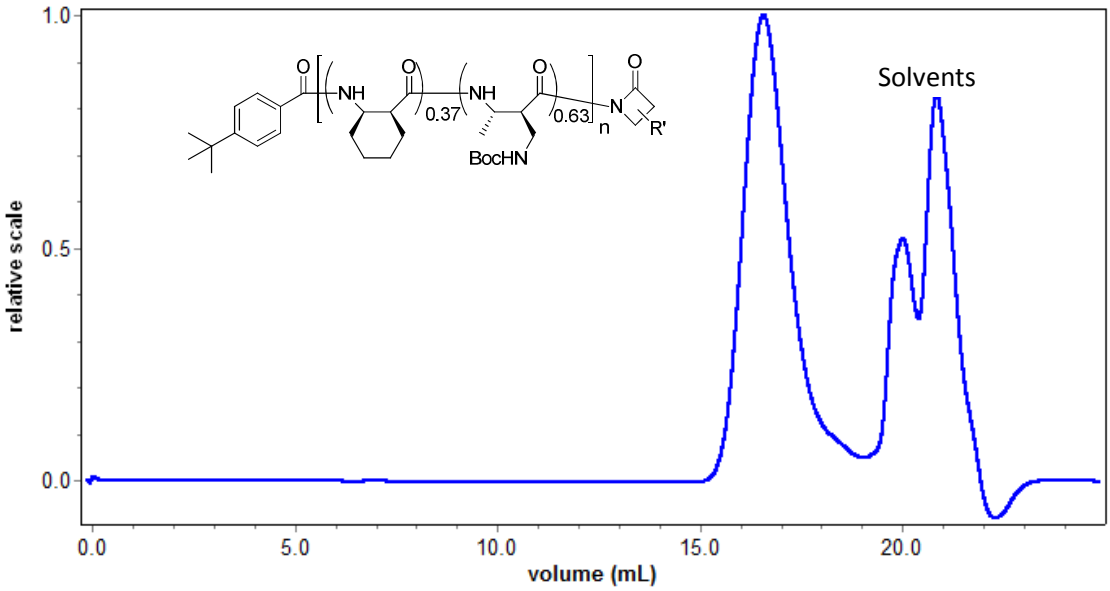
GPC trace (RI detection) of Boc-protected **1** in THF. M_n = 4627, PDI = 1.10, dn/dc = 0.1.



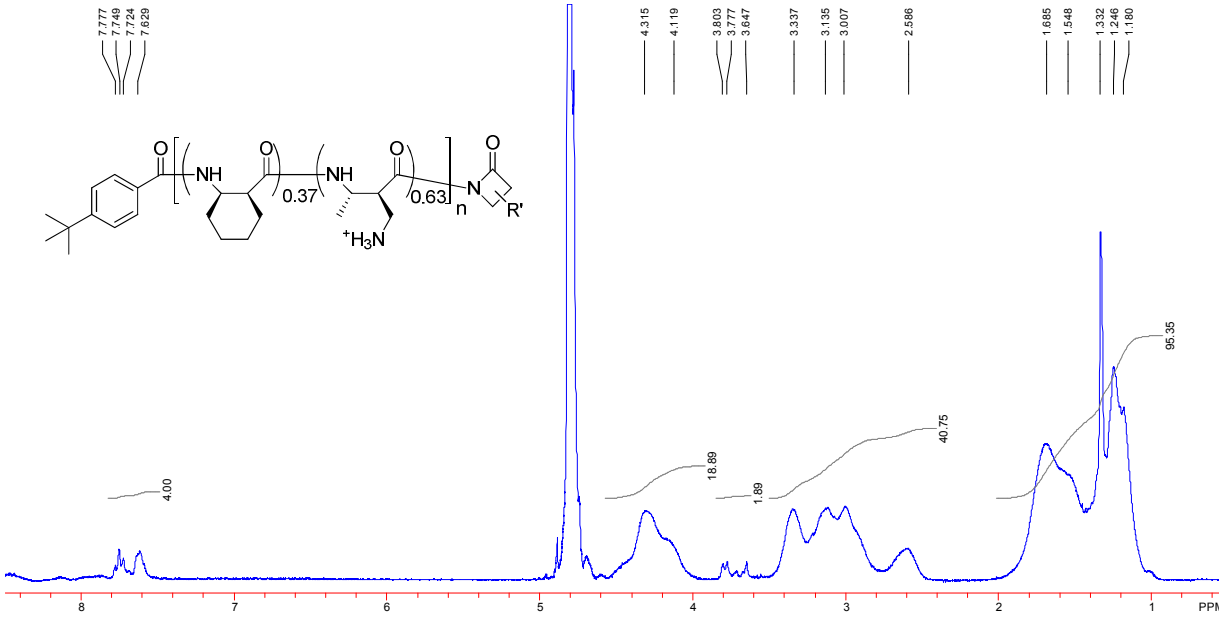
^{1}H NMR of **1** in D_2O at 10 mg/mL.



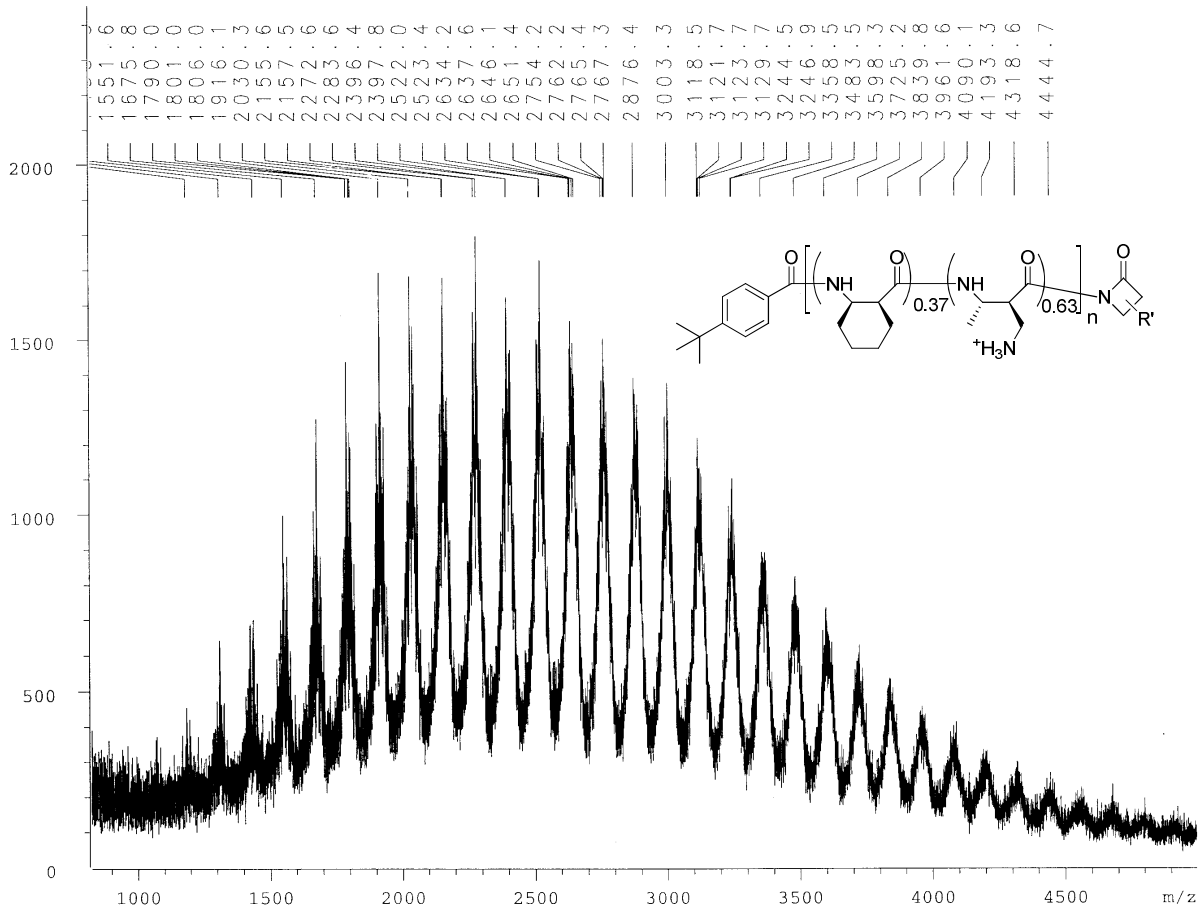
MALDI-TOF spectrum of **1.**



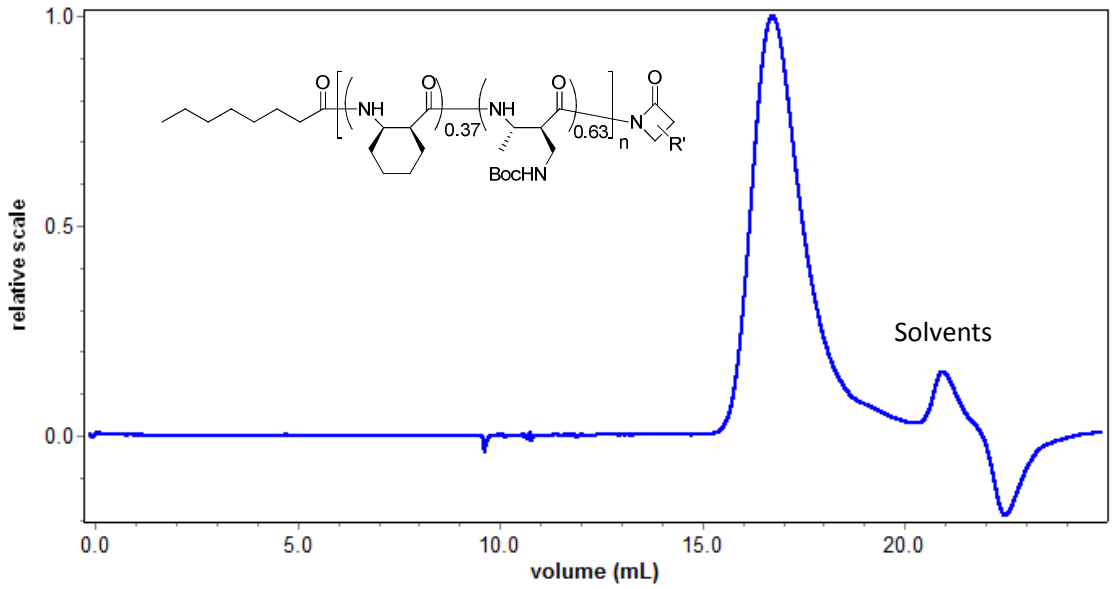
GPC trace (RI detection) of Boc-protected **2** in THF. M_n = 4749, PDI = 1.13, dn/dc = 0.1.



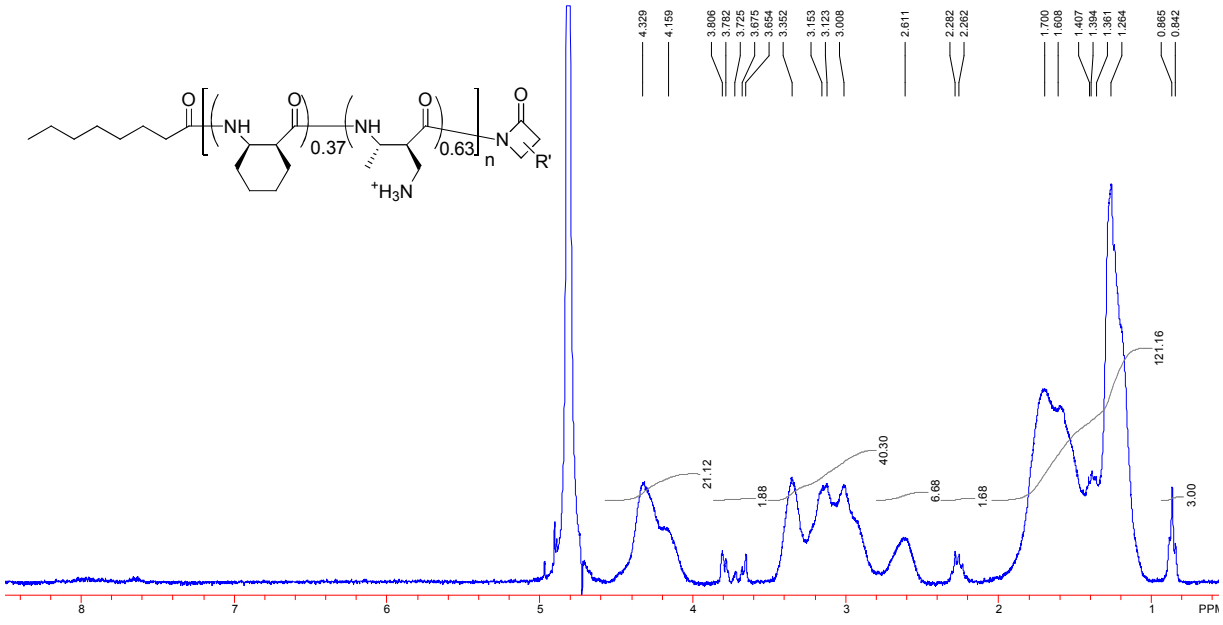
^{1}H NMR of **2** in D_2O at 10 mg/mL.



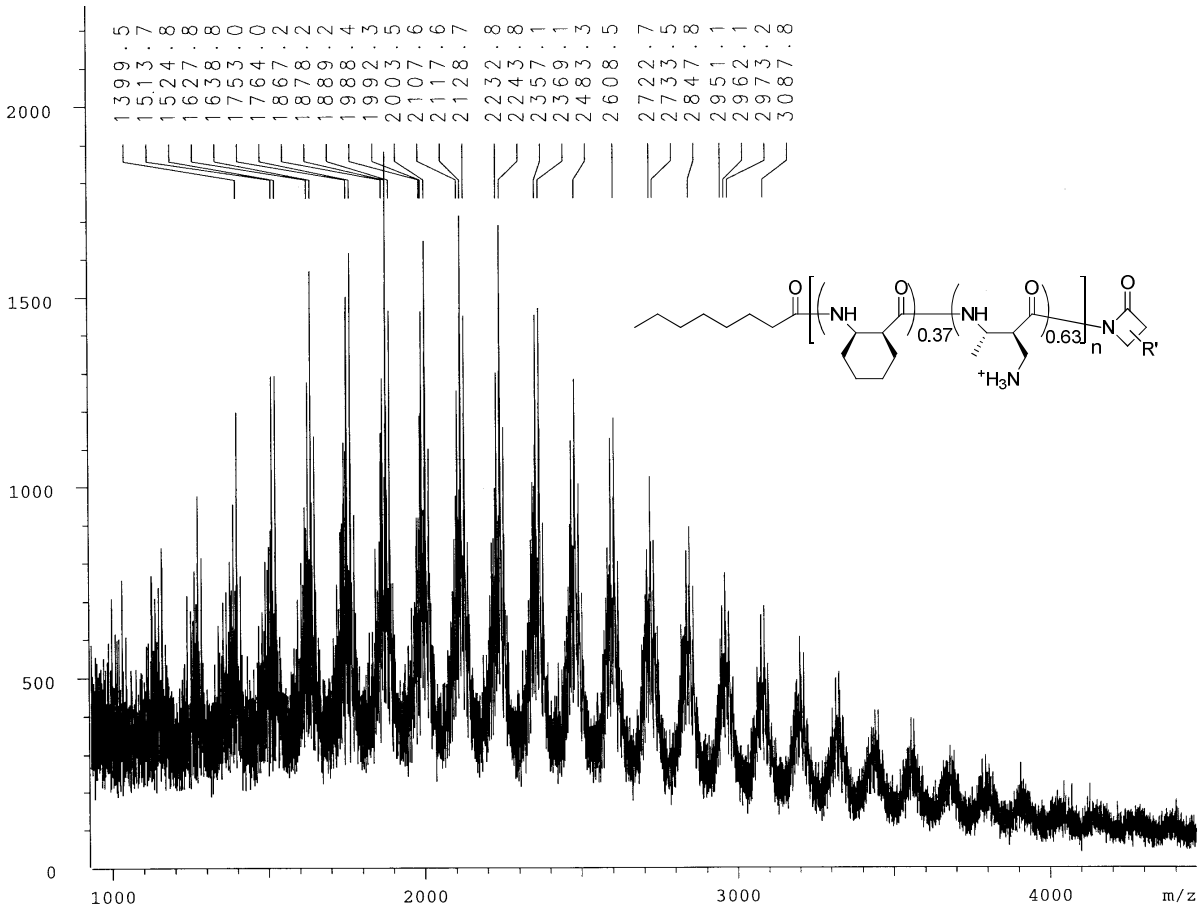
MALDI-TOF spectrum of **2.**



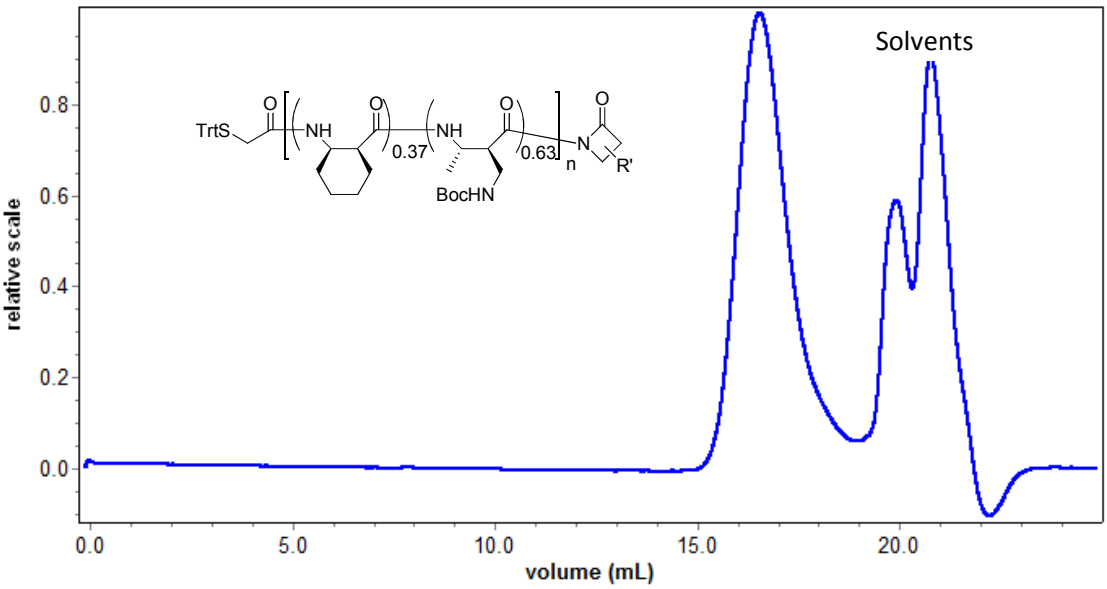
GPC trace (RI detection) of Boc-protected **3** in THF. M_n = 5845, PDI = 1.15, dn/dc = 0.1.



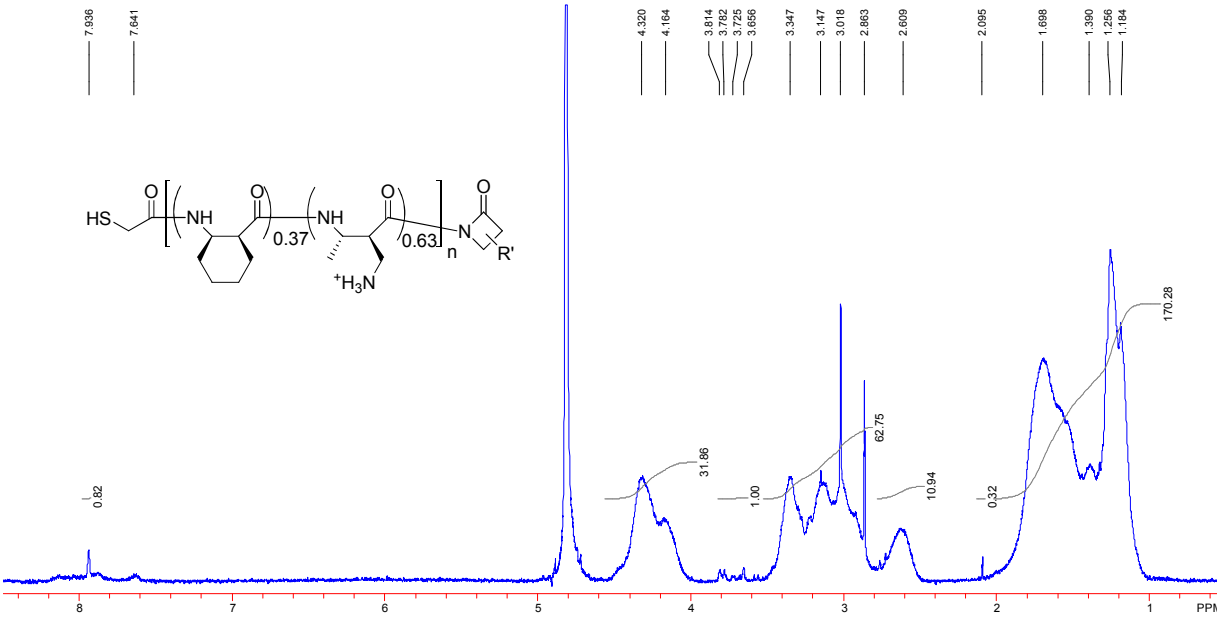
^{1}H NMR of **3** in D_2O at 10 mg/mL.



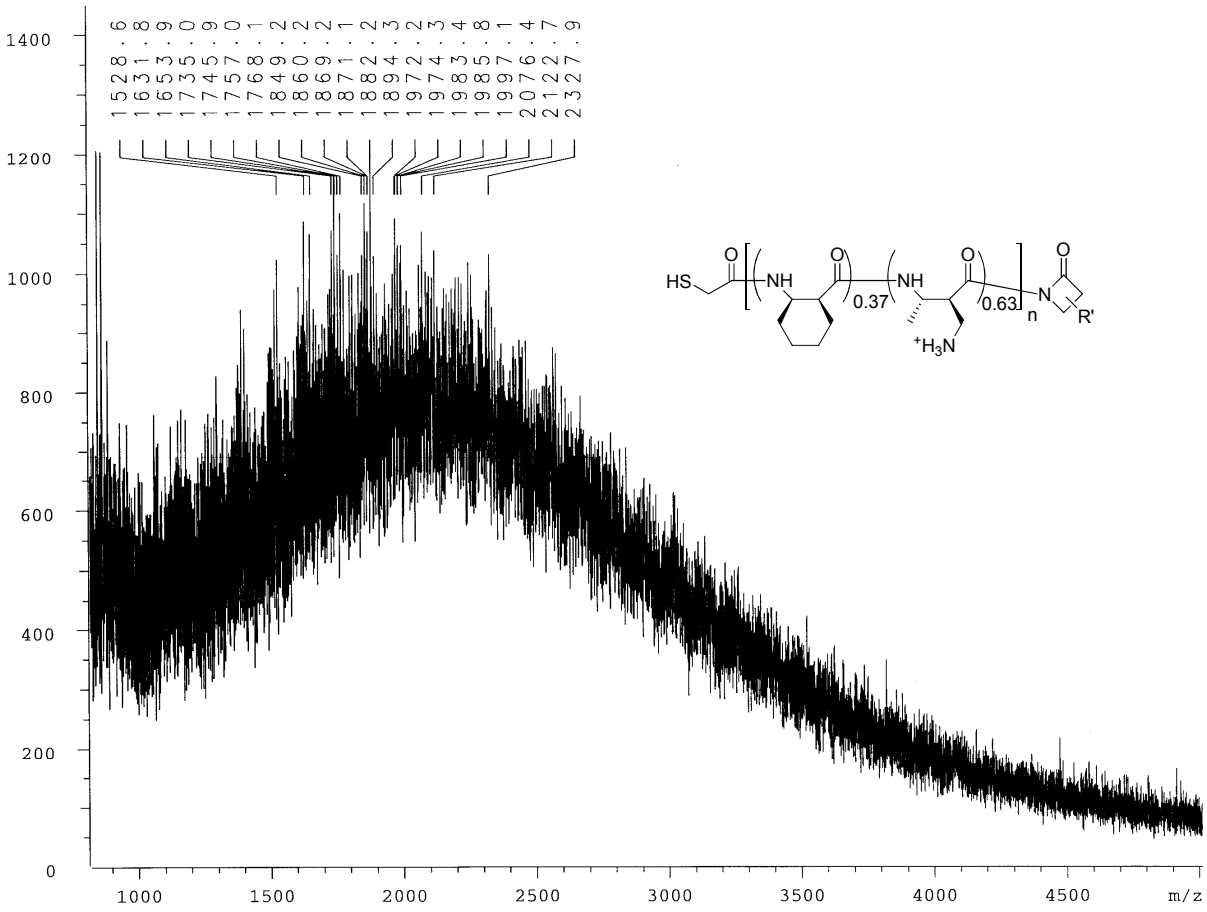
MALDI-TOF spectrum of **3.**



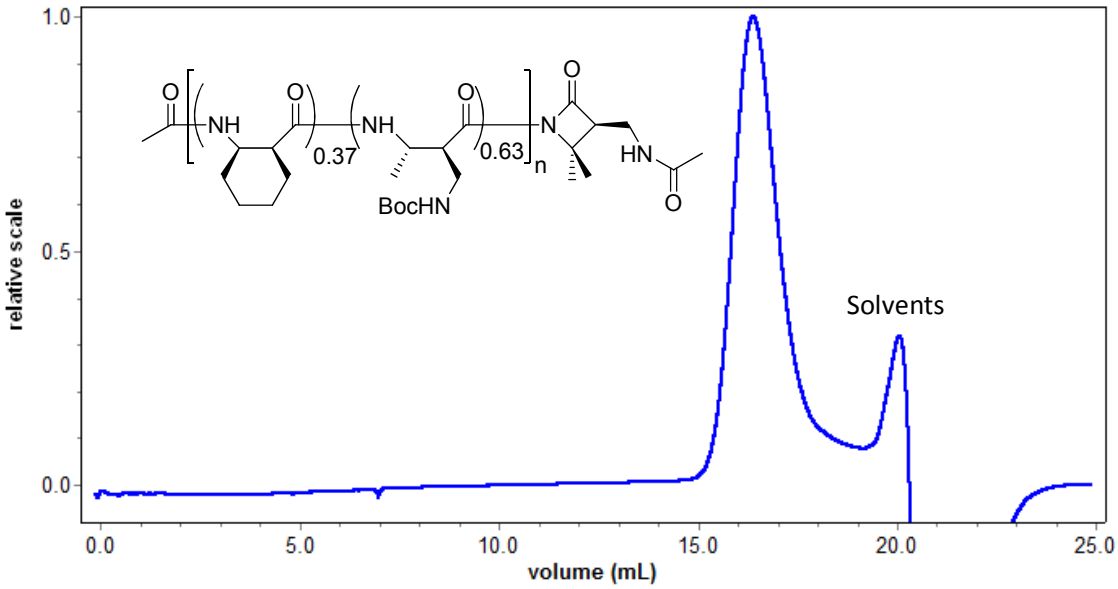
GPC trace (RI detection) of Boc-protected **4** (with trityl-proteced thiol) in THF. M_n = 5337, PDI = 1.07, dn/dc = 0.1.



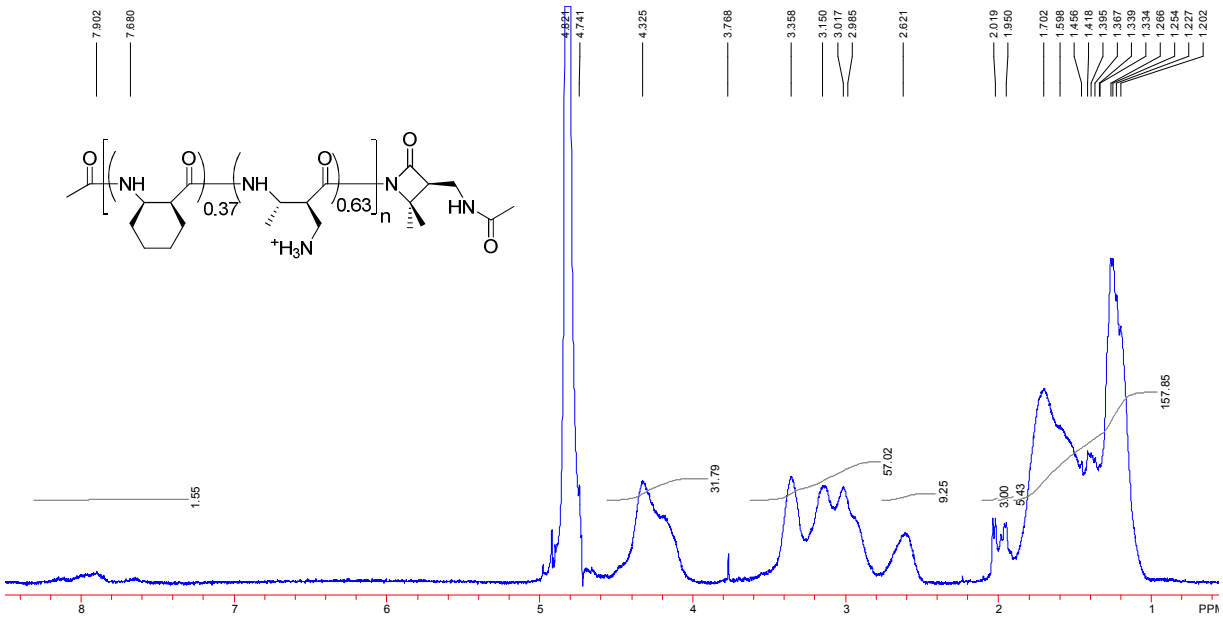
^{1}H NMR of **4** in D_2O at 10 mg/mL.



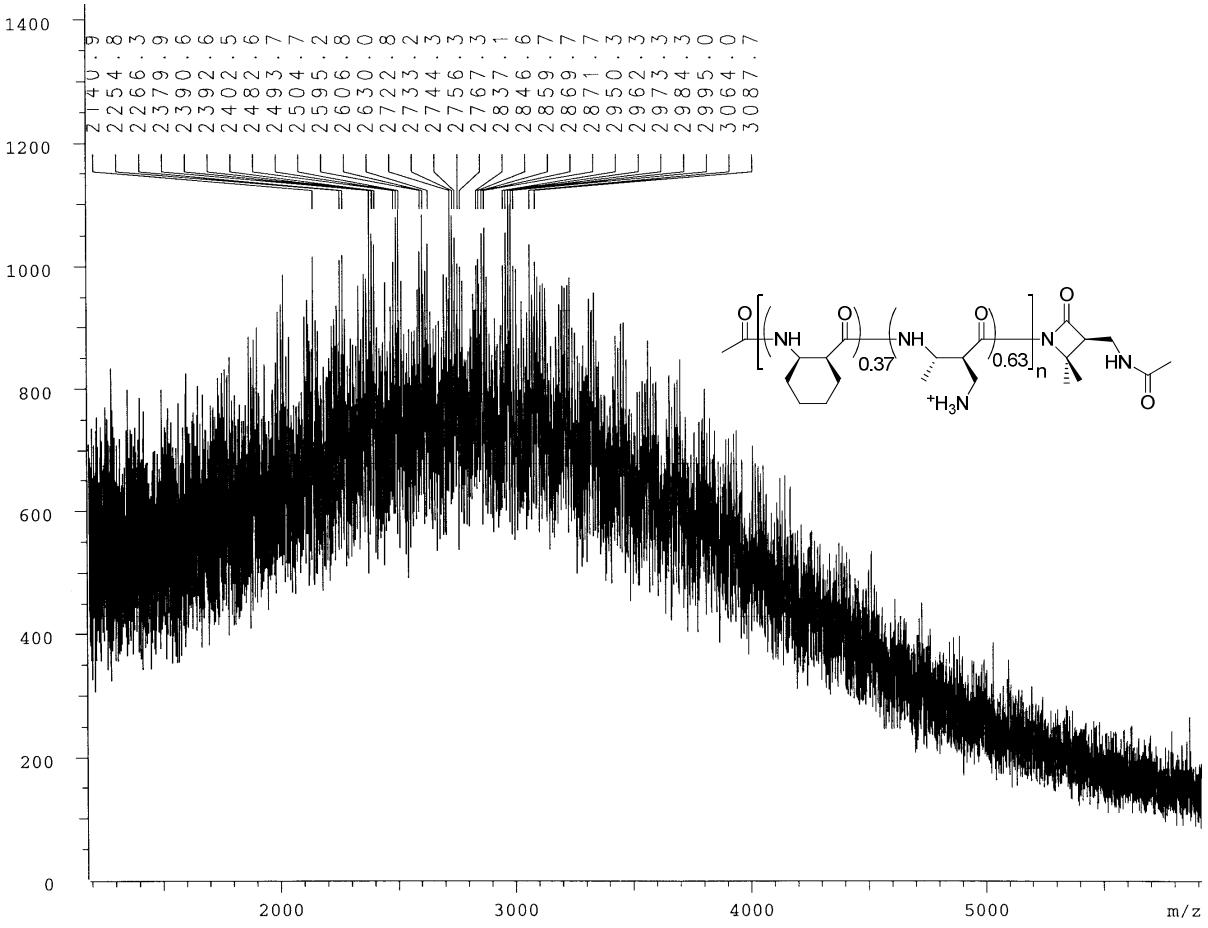
MALDI-TOF spectrum of **4.**



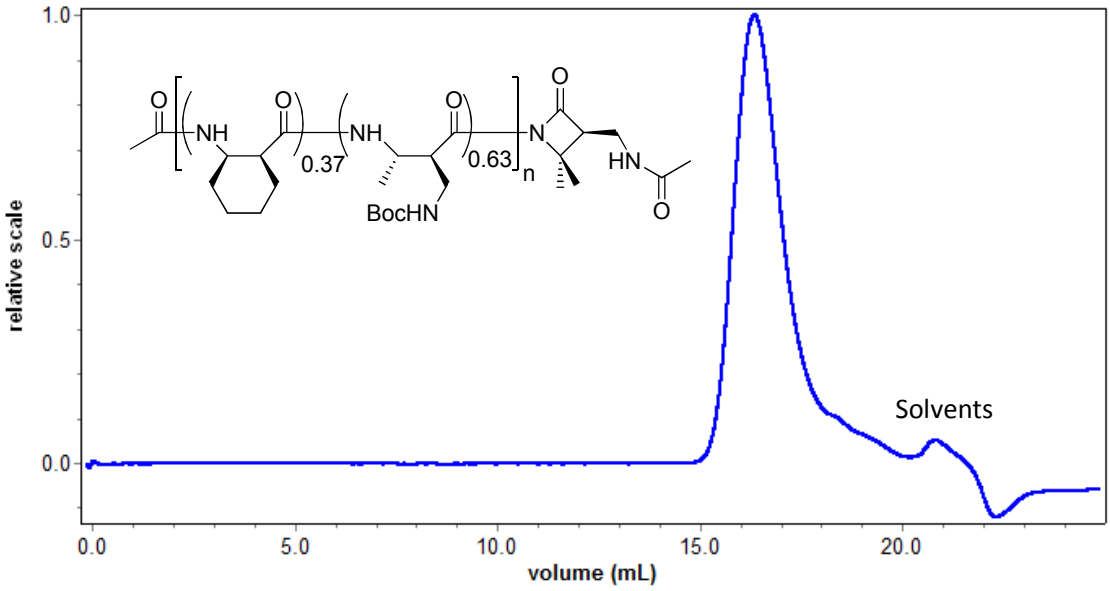
GPC trace (RI detection) of Boc-protected **1B-a** in THF. M_n = 4890, PDI = 1.13, dn/dc = 0.1.



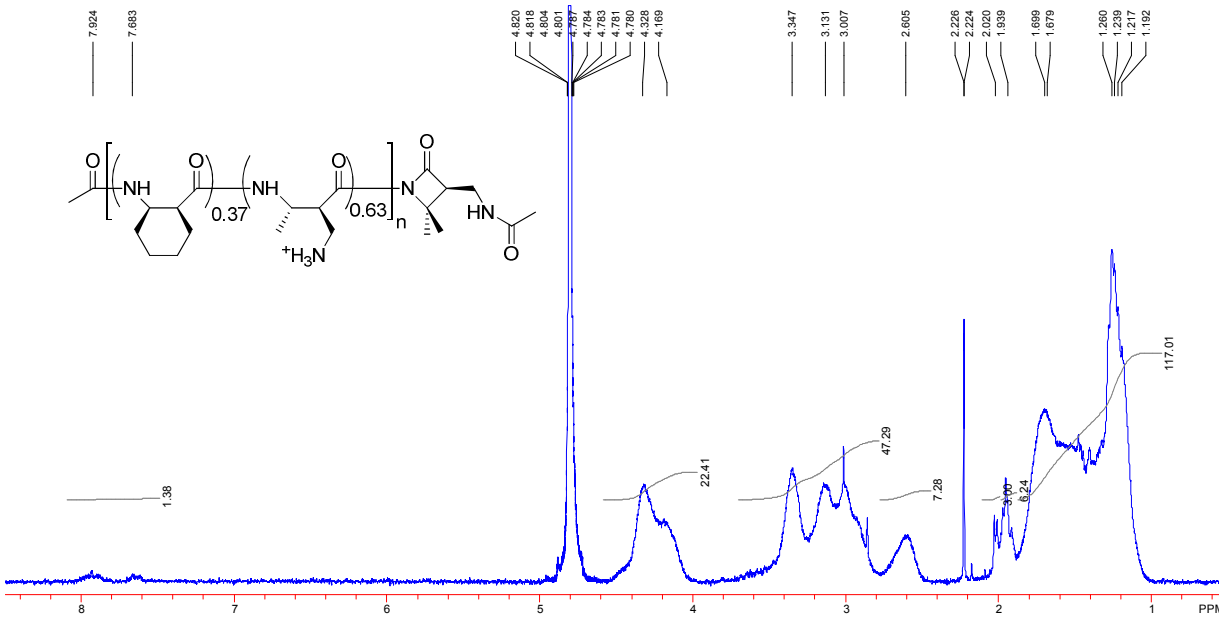
^{1}H NMR of **1B-a** in D_2O at 10 mg/mL.



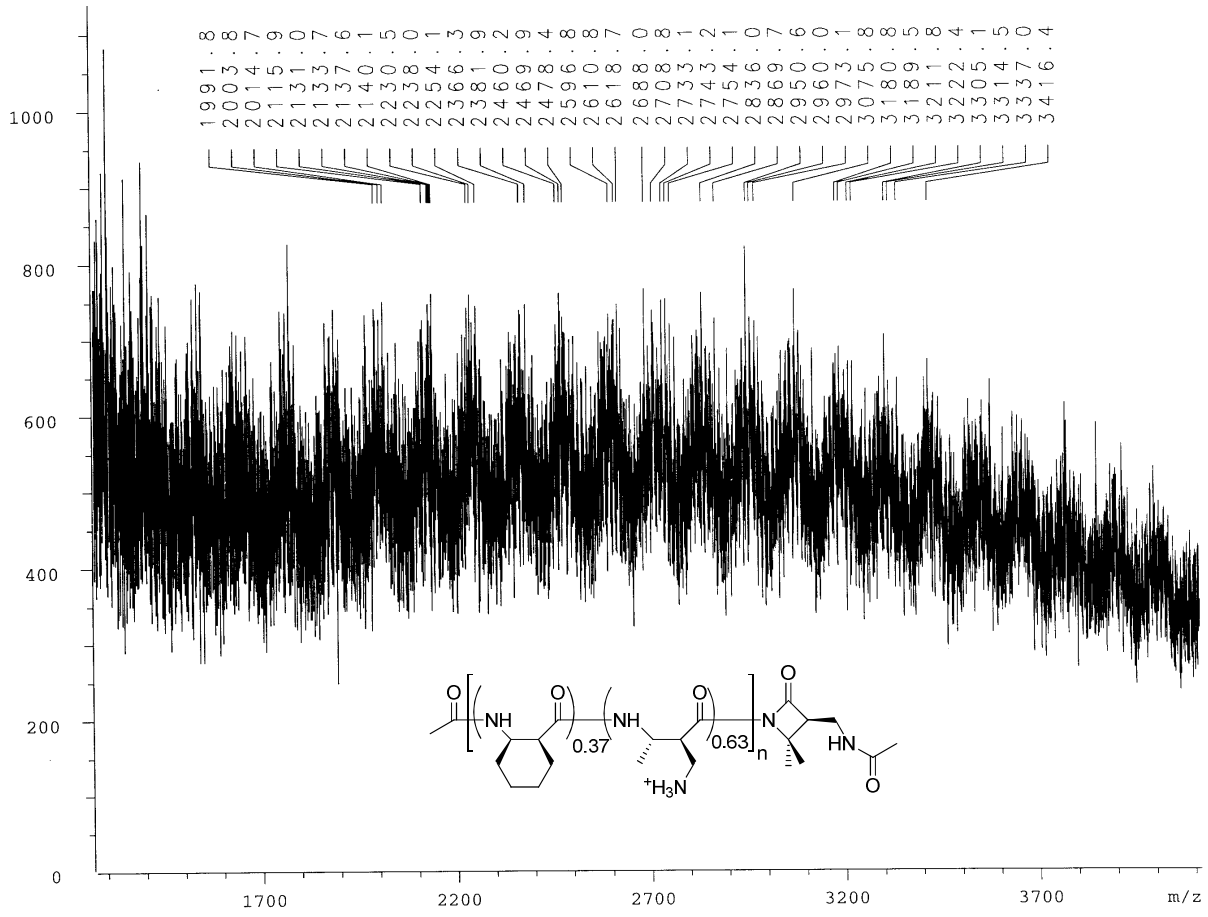
MALDI-TOF spectrum of **1B-a.**



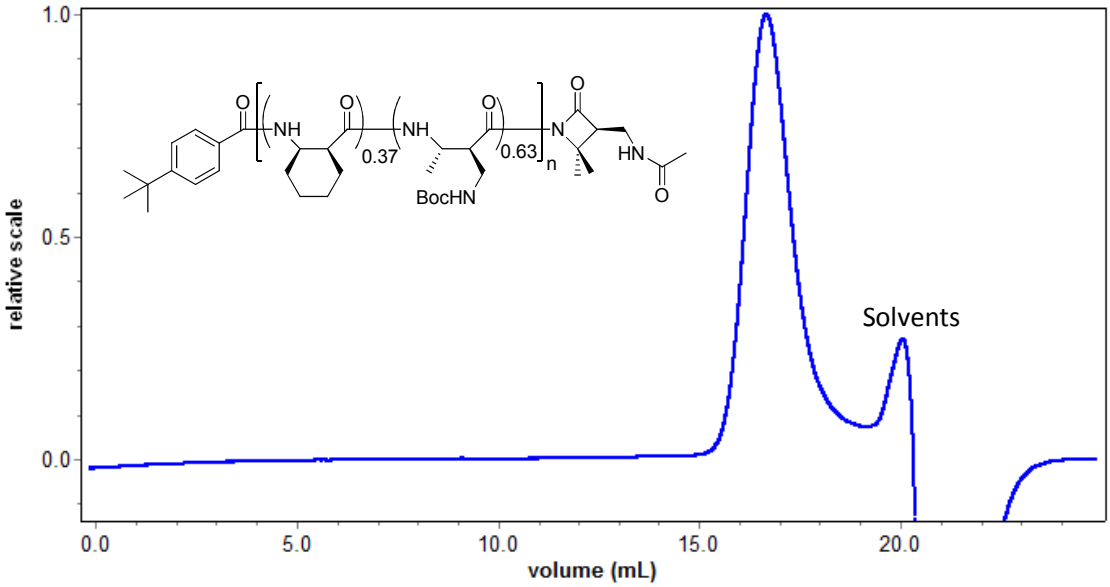
GPC trace (RI detection) of Boc-protected **1B-b** in THF. M_n = 5975, PDI = 1.07, dn/dc = 0.1.



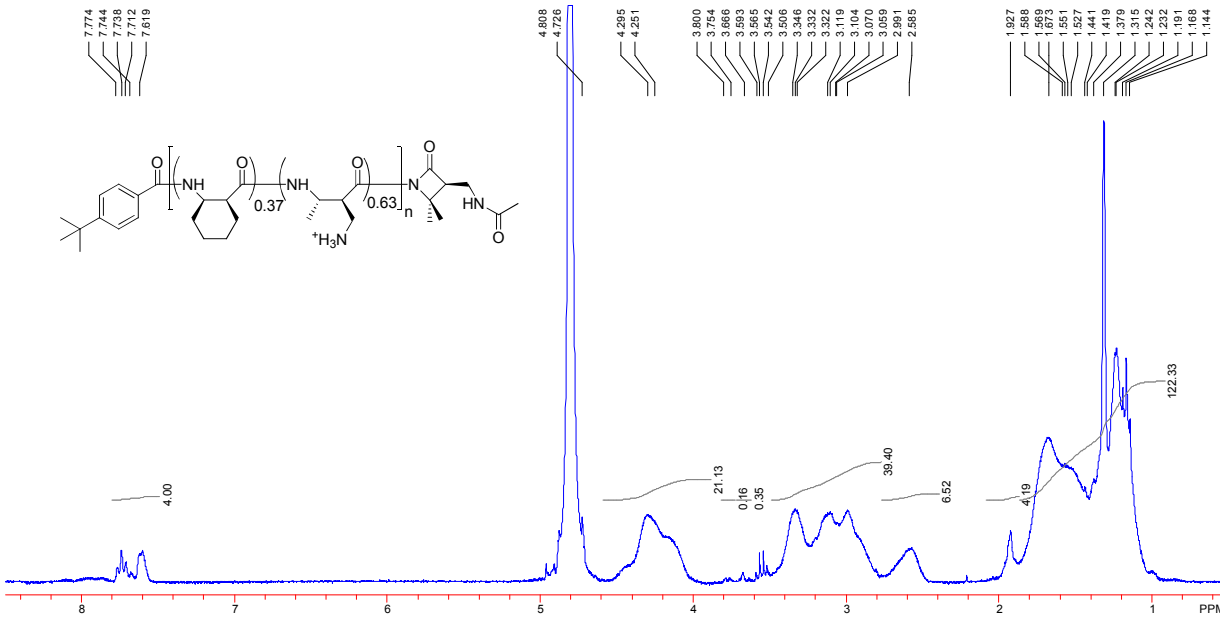
^{1}H NMR of **1B-b** in D_2O at 10 mg/mL.



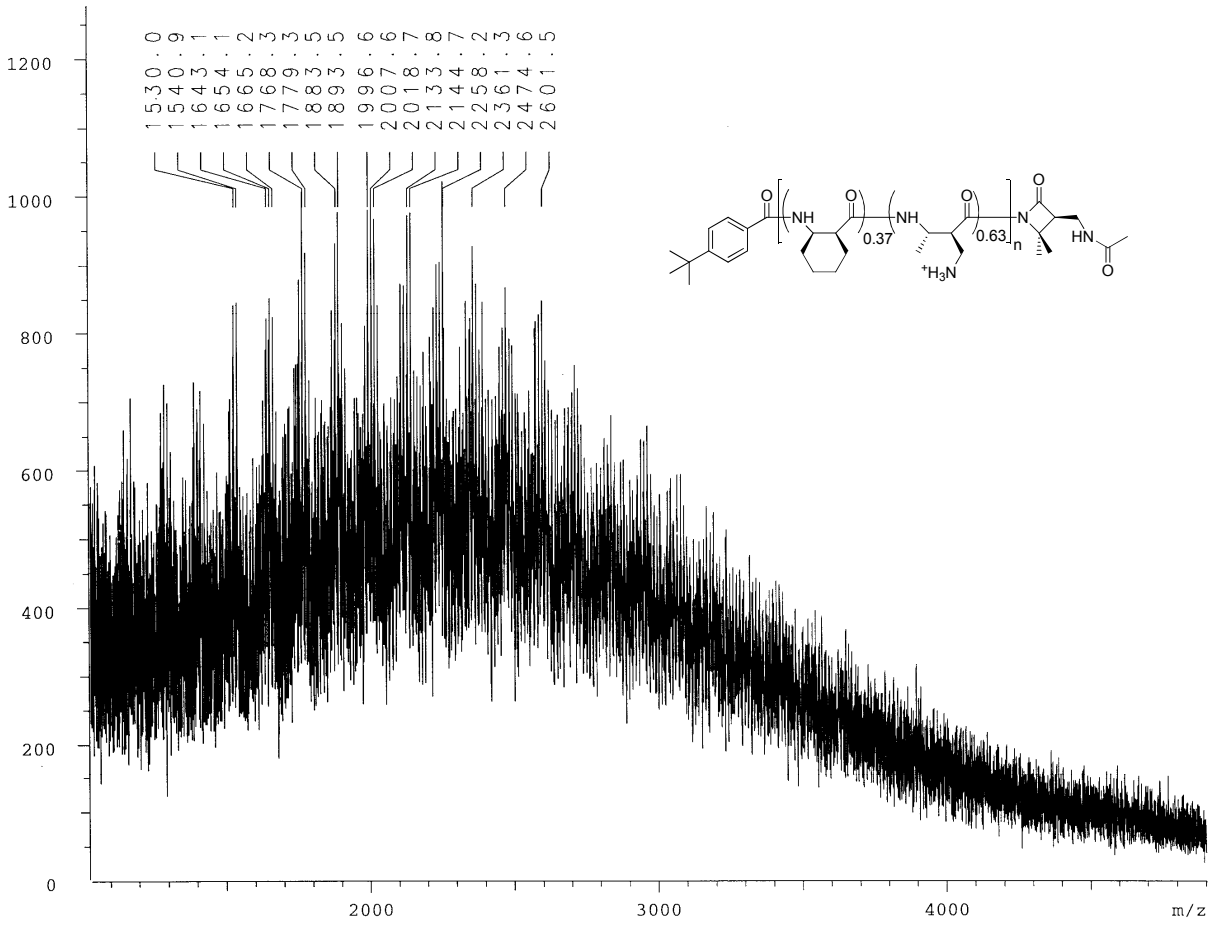
MALDI-TOF spectrum of **1B-b.**



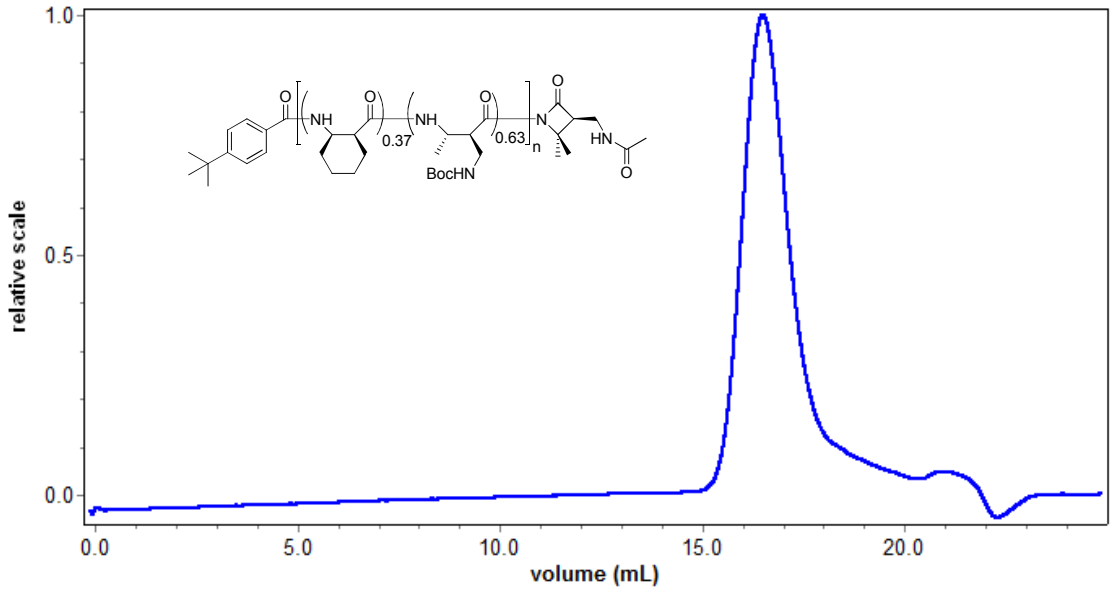
GPC trace (RI detection) of Boc-protected **2B-a** in THF. M_n = 3948, PDI = 1.13, dn/dc = 0.1.



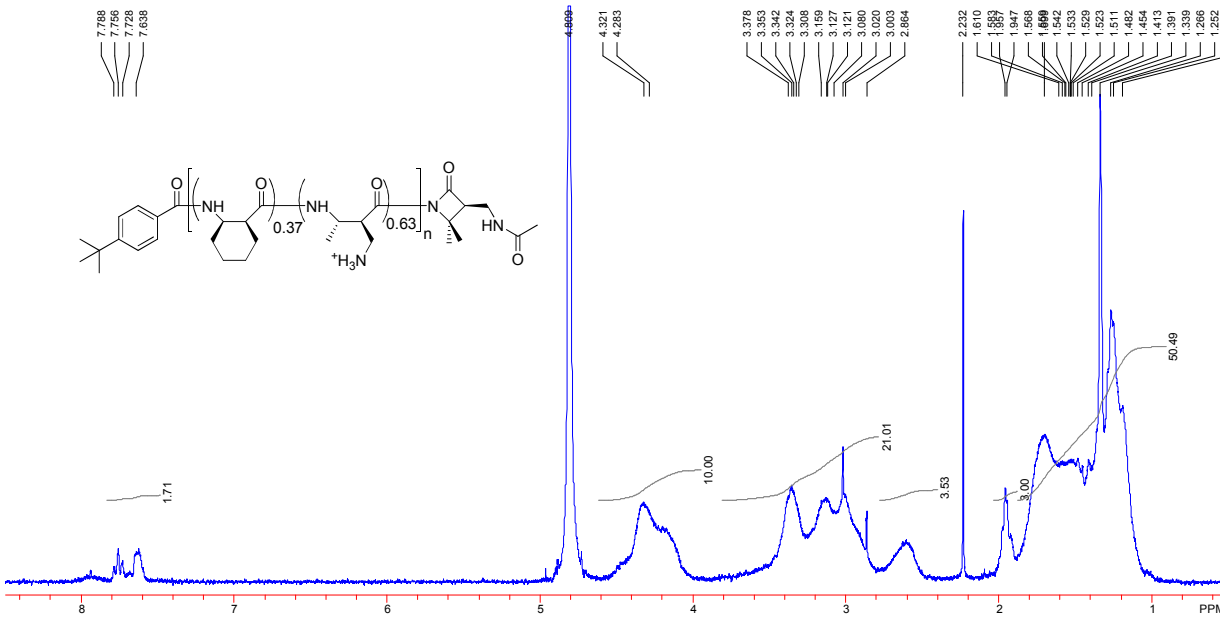
^{1}H NMR of **2B-a** in D_2O at 10 mg/mL.



MALDI-TOF spectrum of **2B-a.**

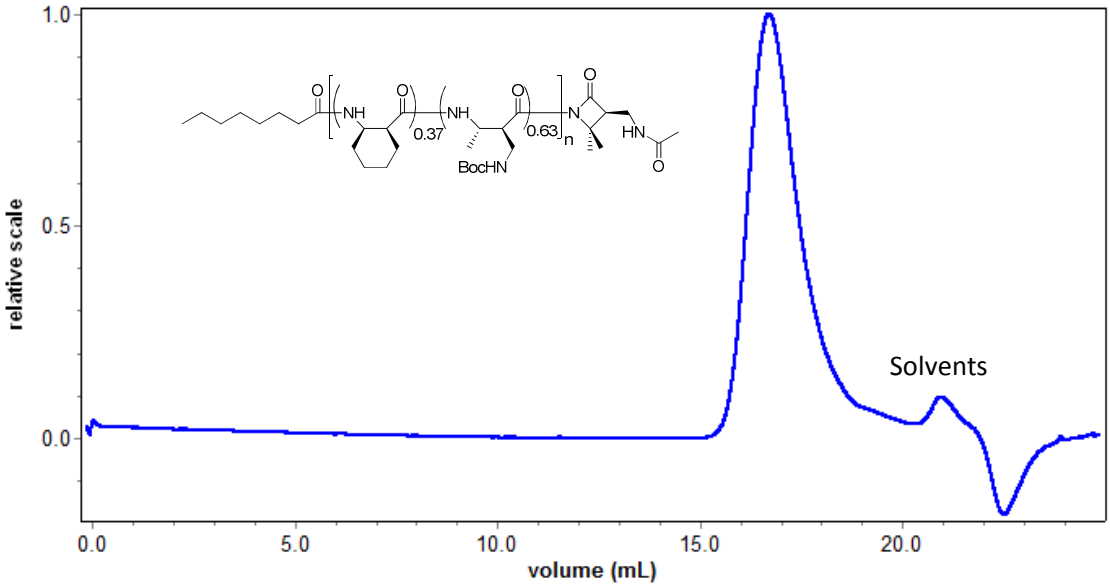


GPC trace (RI detection) of Boc-protected **2B-b** in THF. M_n = 4837, PDI = 1.12, dn/dc = 0.1.

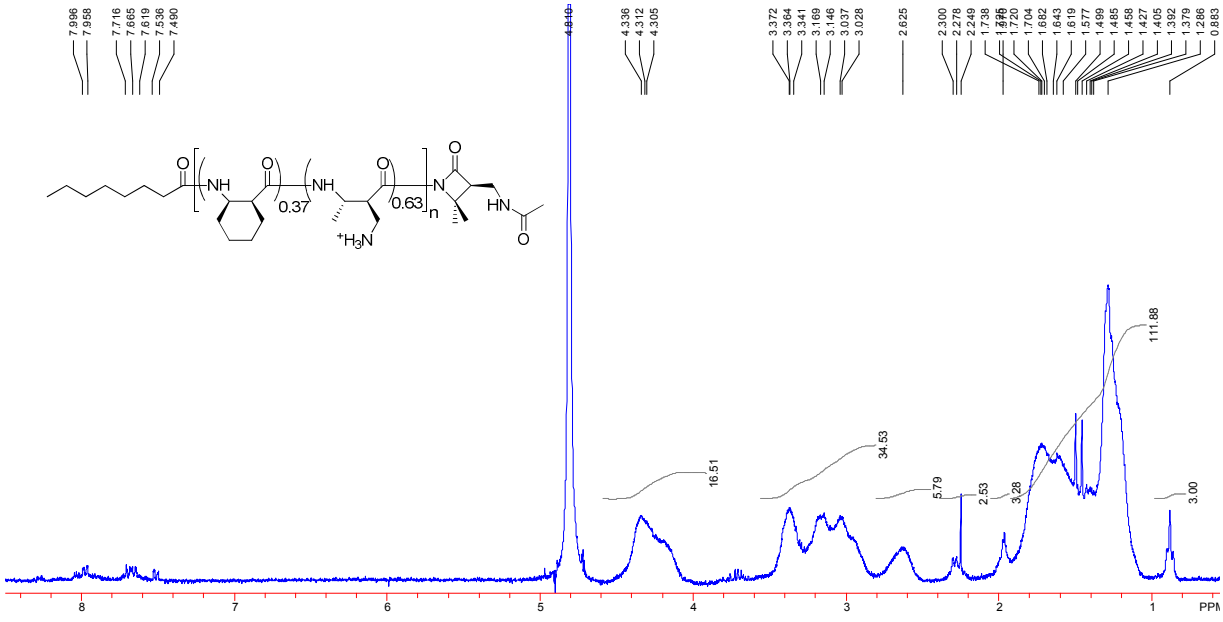


^{1}H NMR of **2B-b** in D_2O at 10 mg/mL.

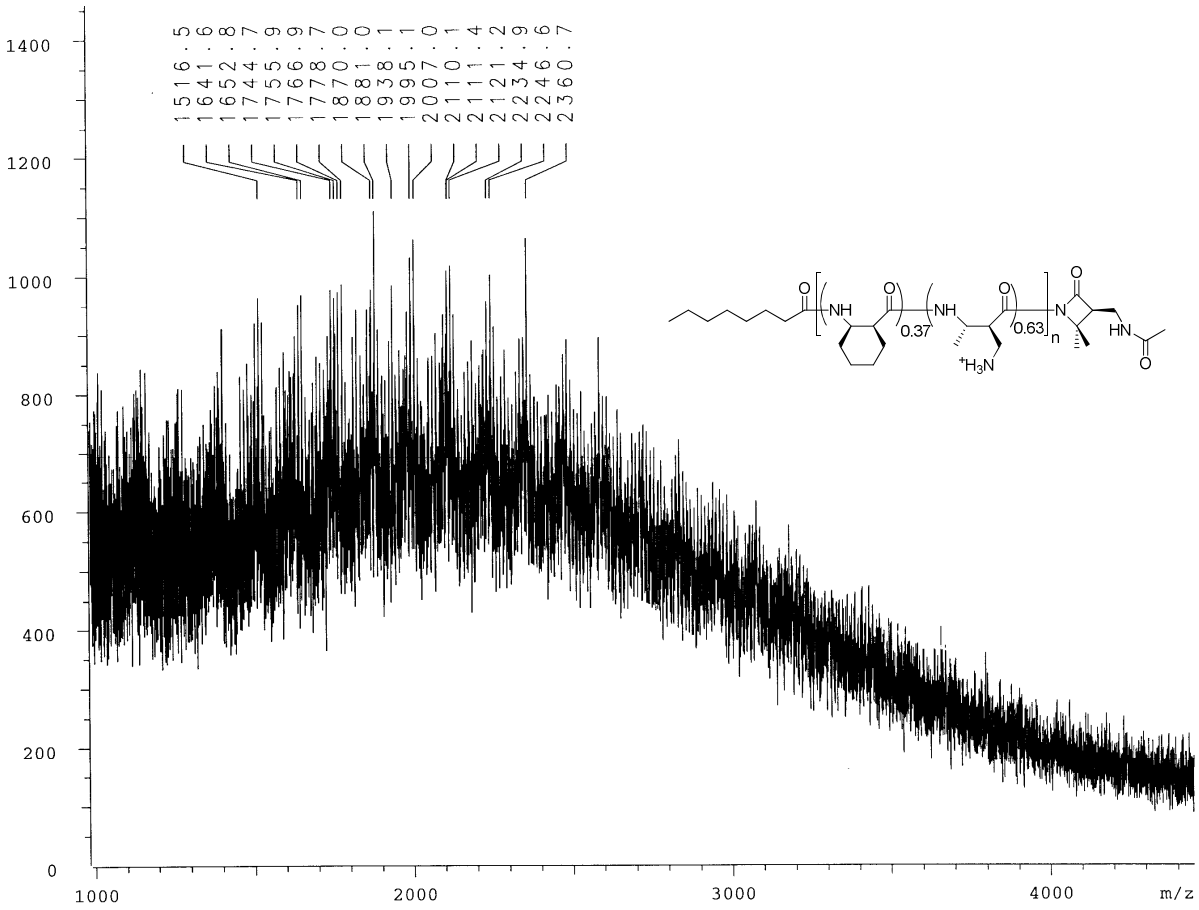
Polymer **2B-b** does not produce a MALDI-TOF spectrum.



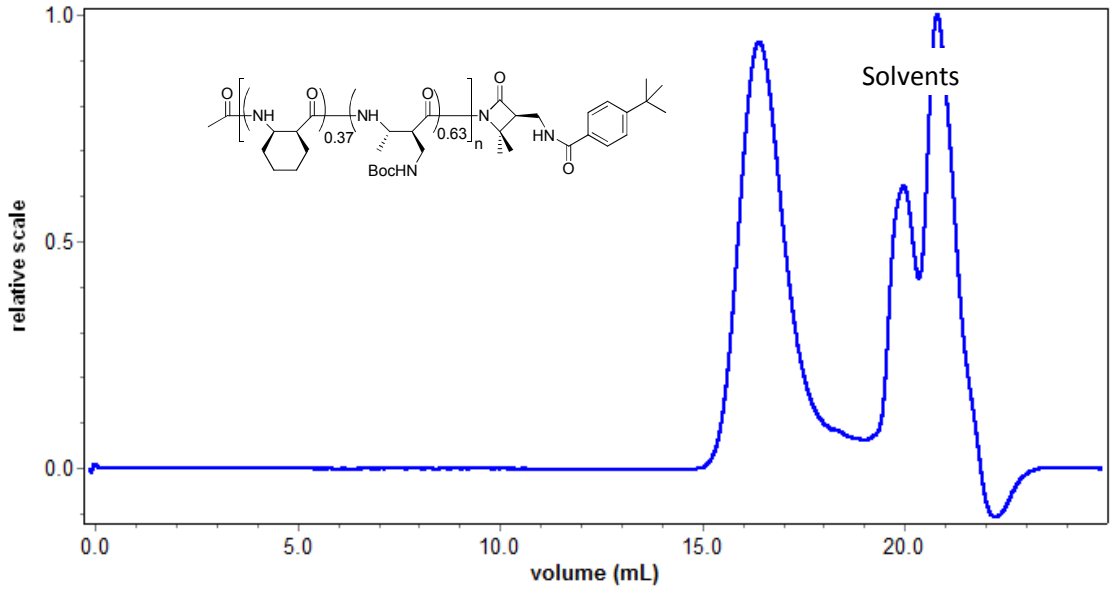
GPC trace (RI detection) of Boc-protected **3B** in THF. M_n = 4112, PDI = 1.12, dn/dc = 0.1.



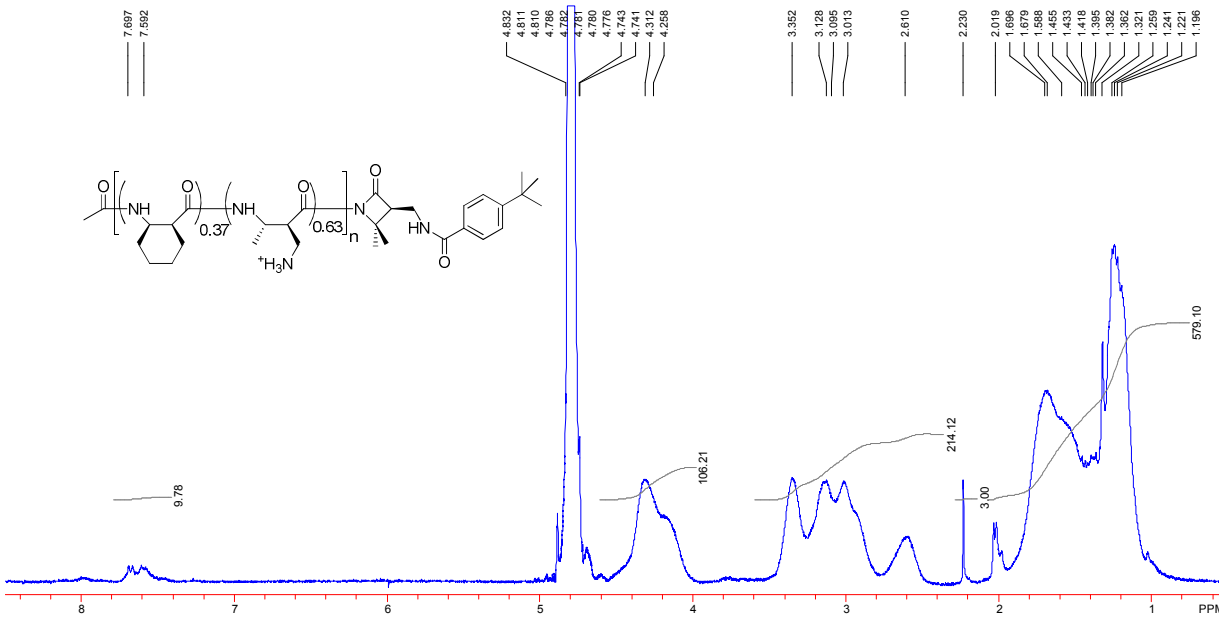
^{1}H NMR of **3B** in D_2O at 10 mg/mL.



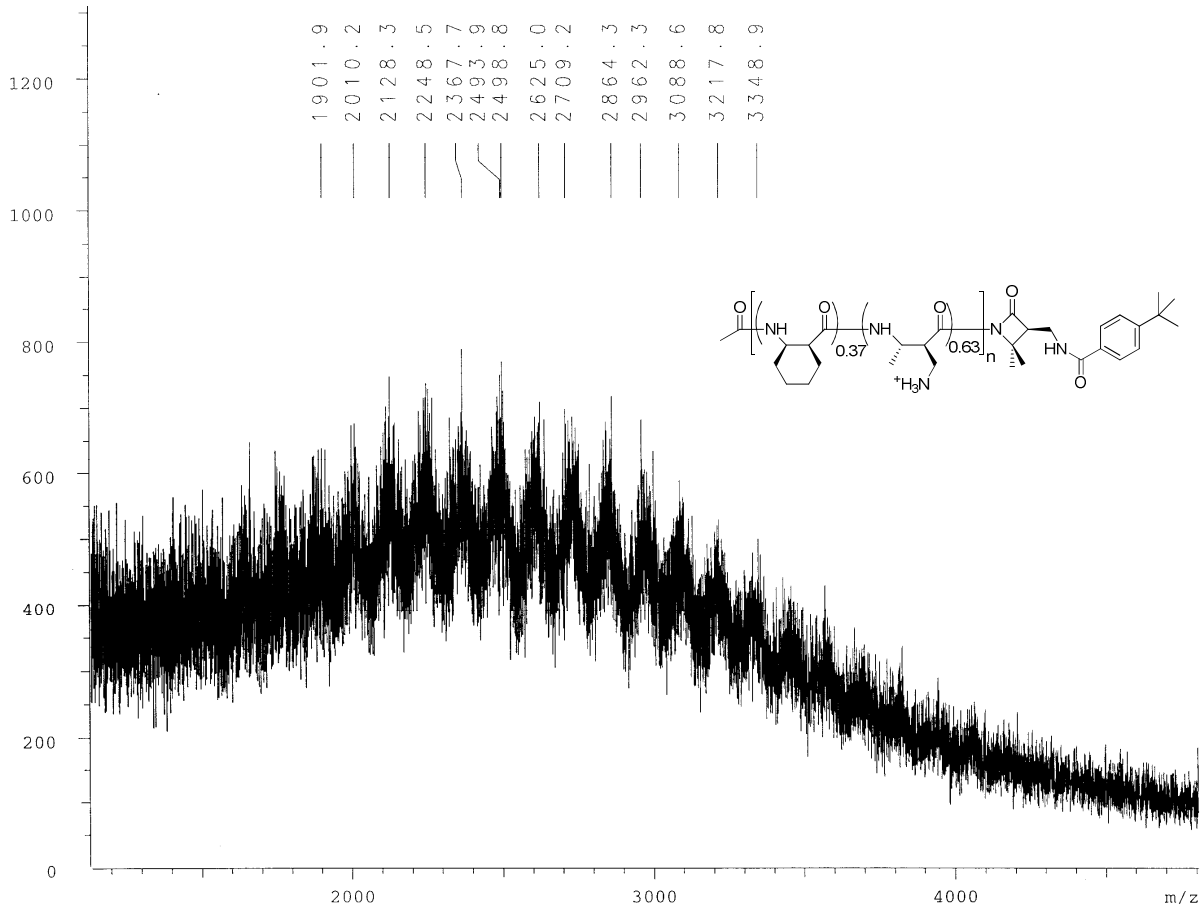
MALDI-TOF spectrum of **3B.**



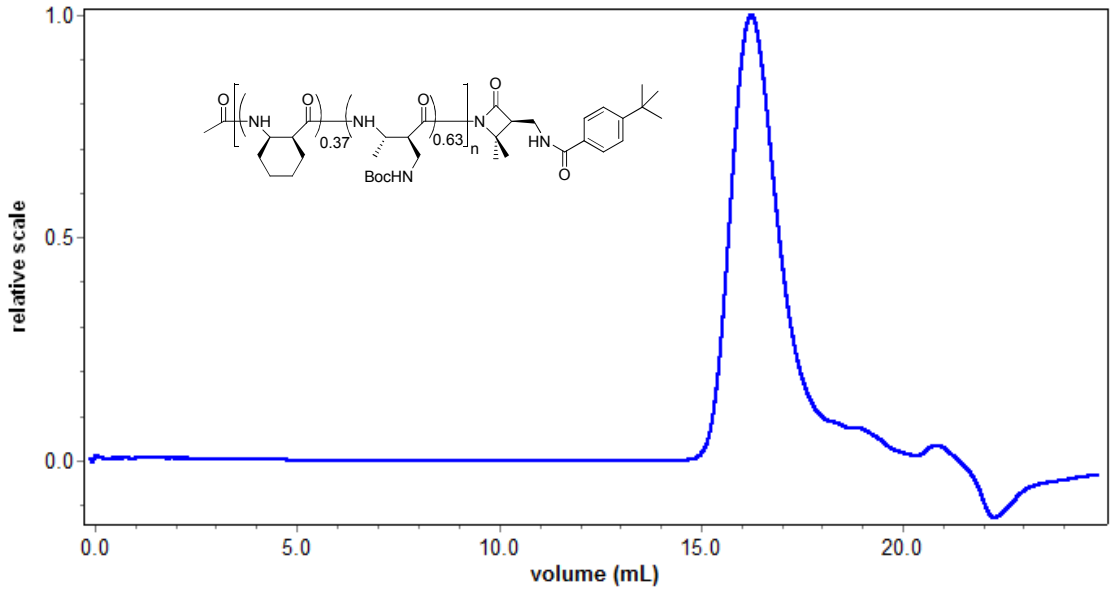
GPC trace (RI detection) of Boc-protected **1C-a** in THF. M_n = 5072, PDI = 1.09, dn/dc = 0.1.



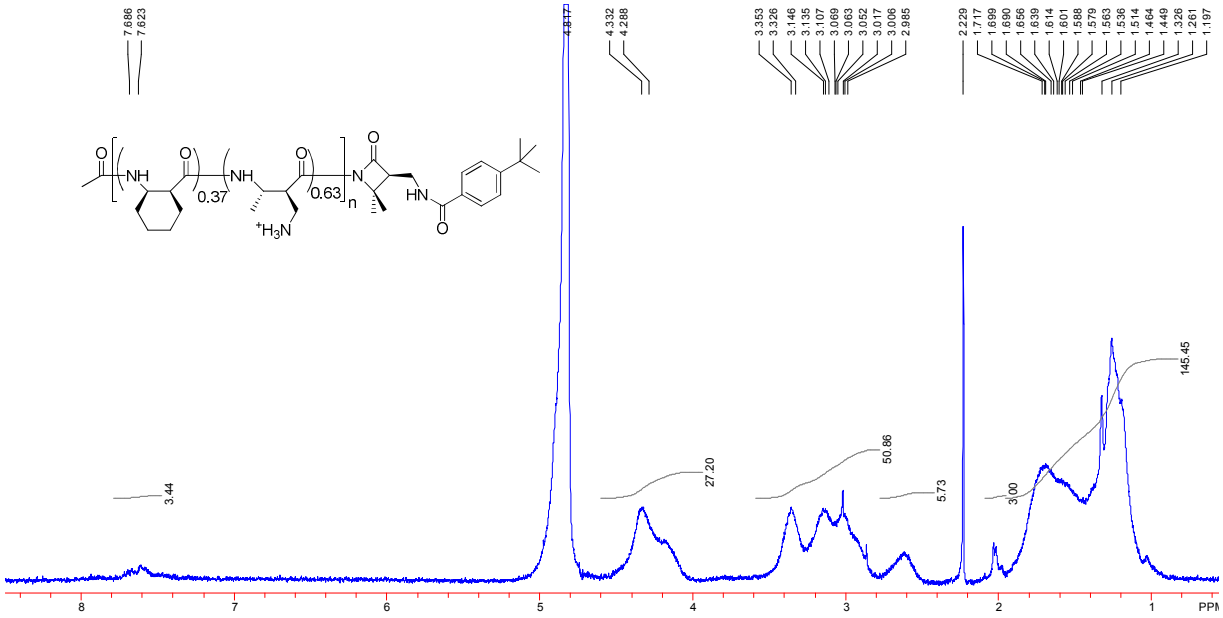
^{1}H NMR of **1C-a** in D_2O at 10 mg/mL.



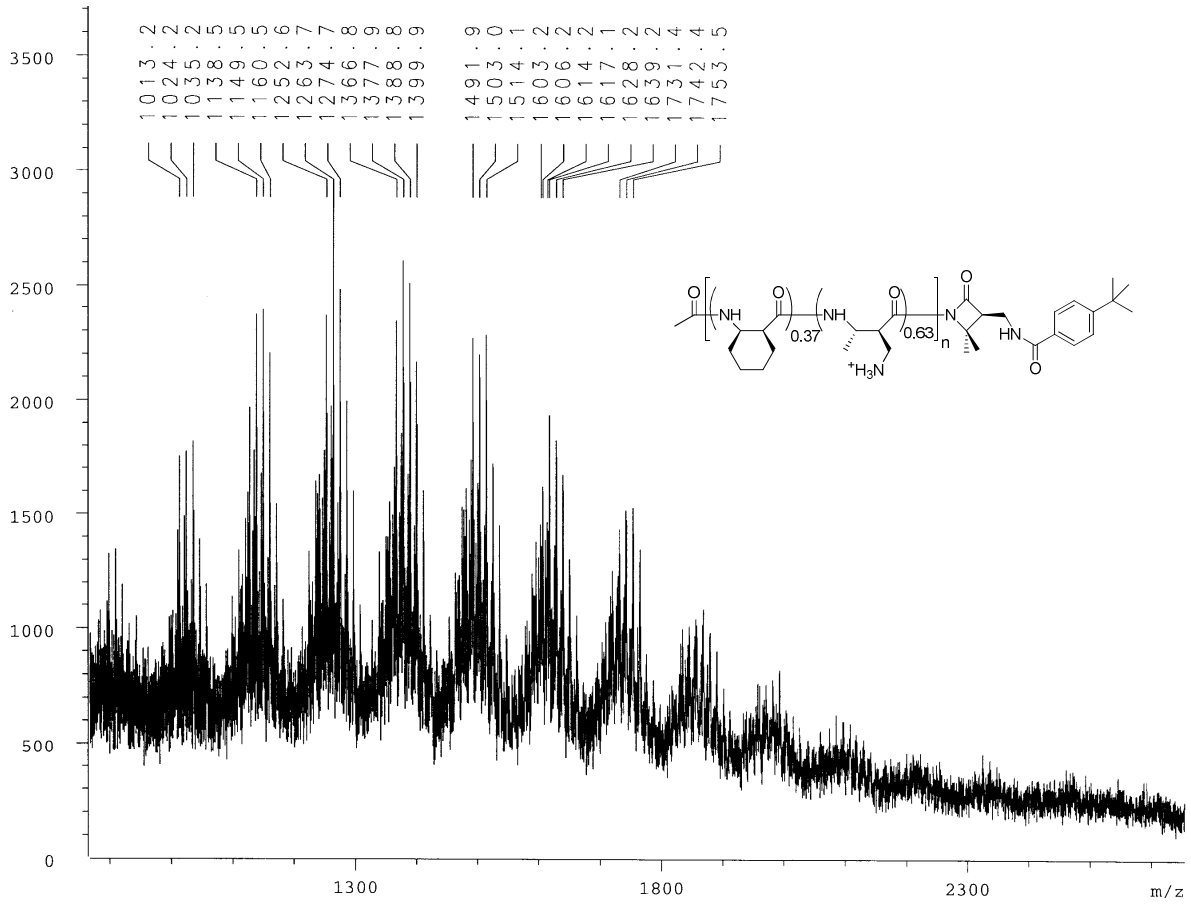
MALDI-TOF spectrum of **1C-a.**



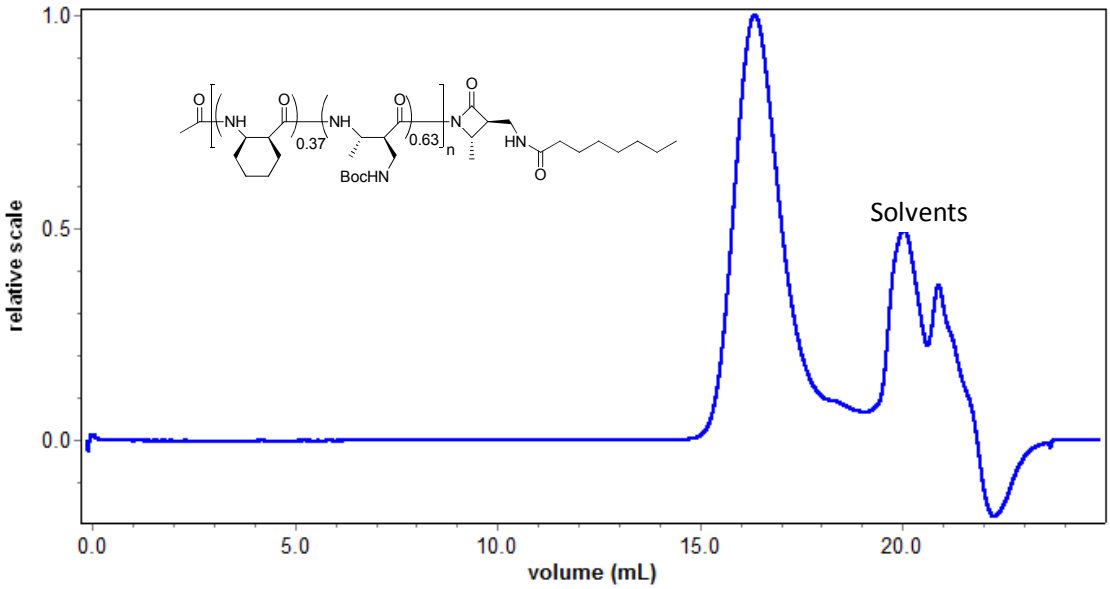
GPC trace (RI detection) of Boc-protected **1C-b** in THF. M_n = 6135, PDI = 1.12, dn/dc = 0.1.



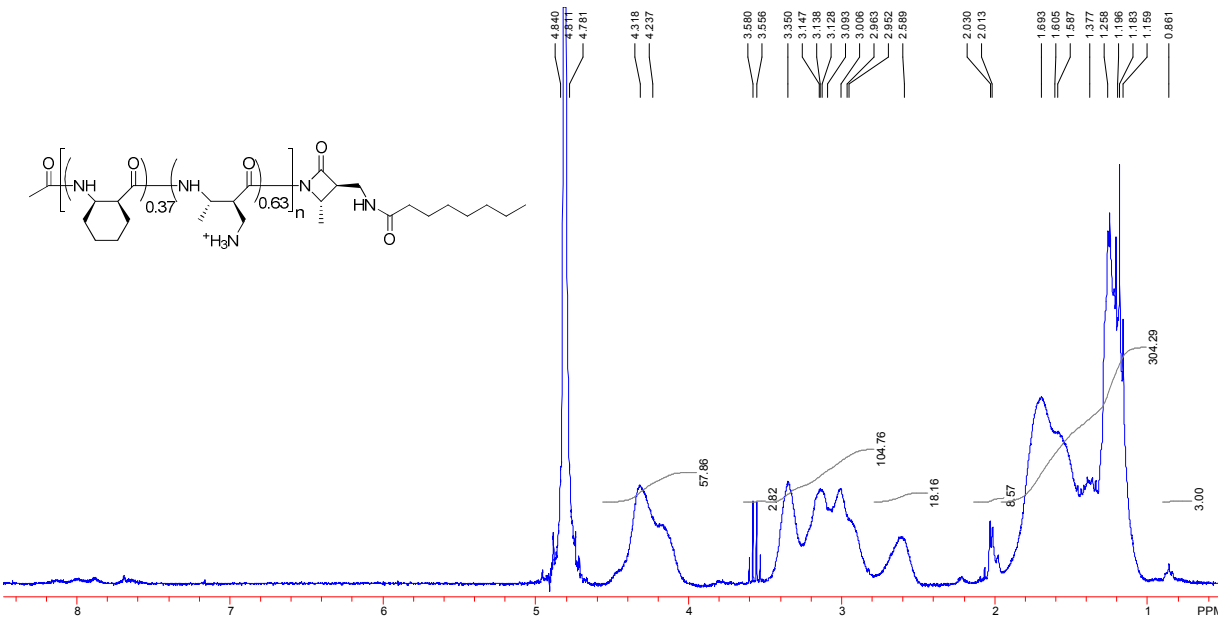
^{1}H NMR of **1C-b** in D_2O at 10 mg/mL.



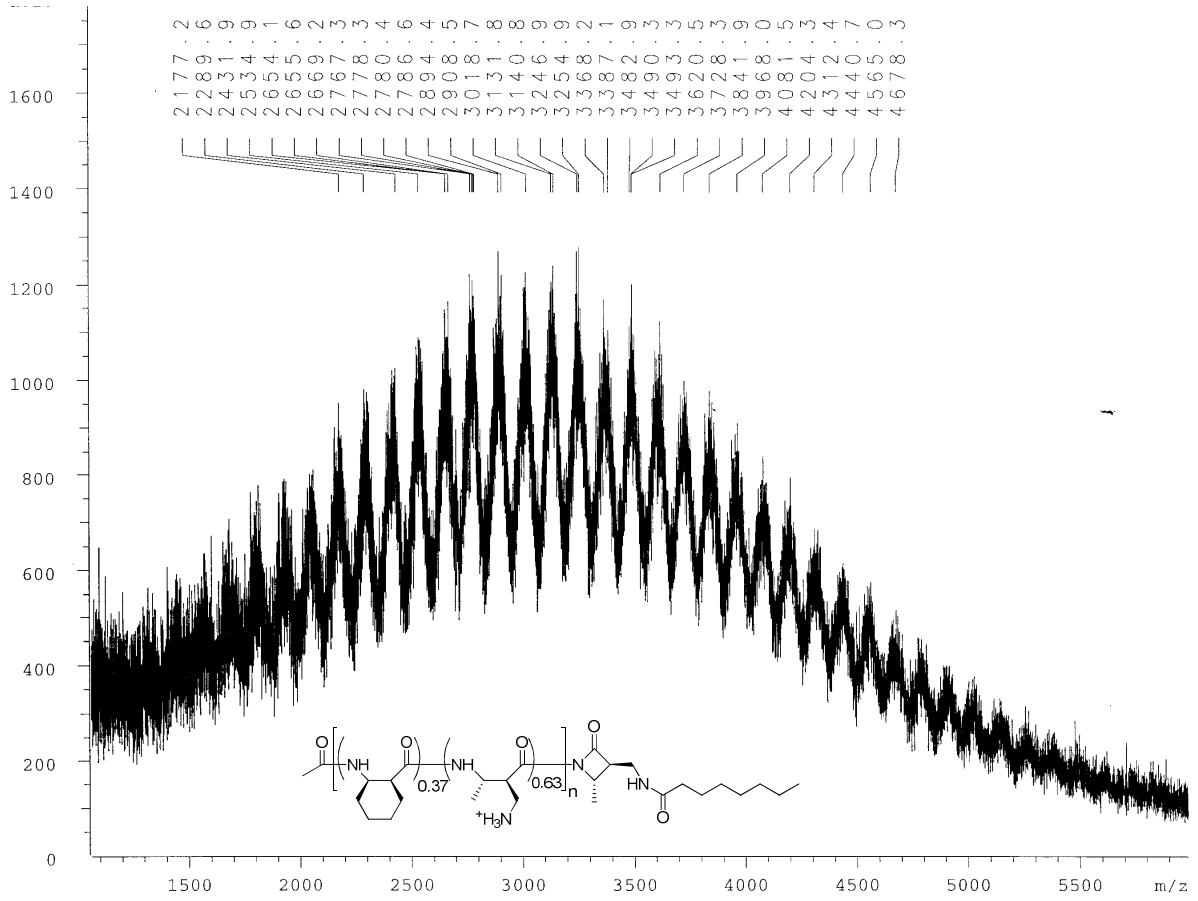
MALDI-TOF spectrum of **1C-b.**



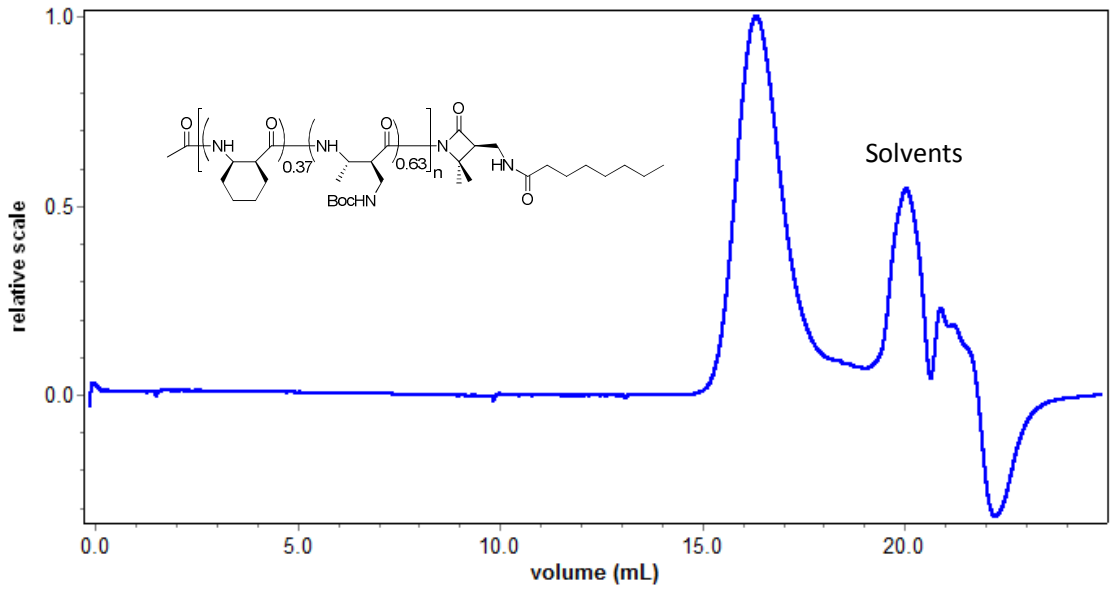
GPC trace (RI detection) of Boc-protected **2D** in THF. M_n = 5753, PDI = 1.11, dn/dc = 0.1.



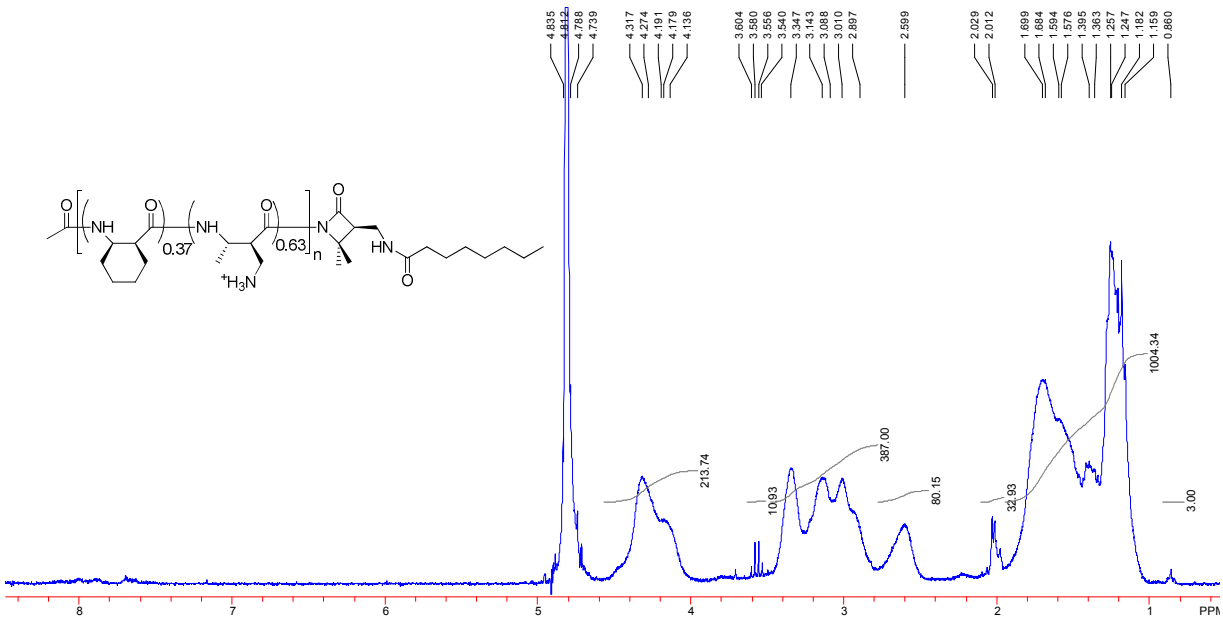
^{1}H NMR of **1E** in D_2O at 10 mg/mL.



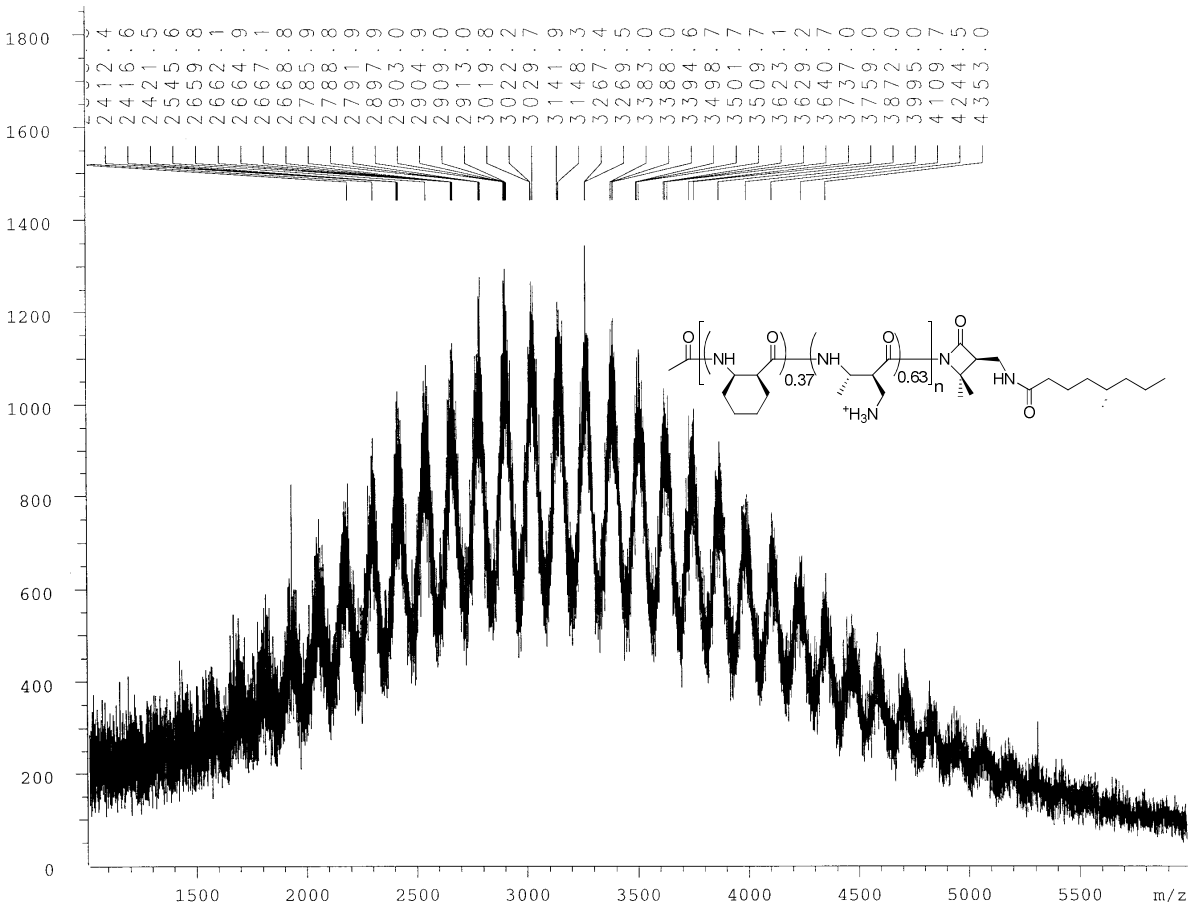
MALDI-TOF spectrum of **1E.**



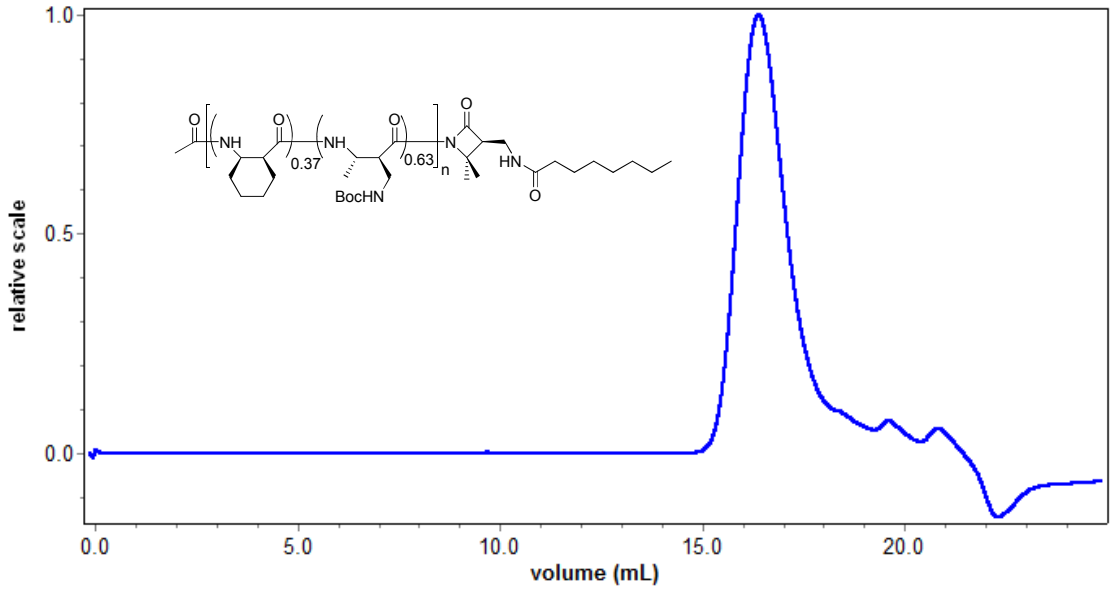
GPC trace (RI detection) of Boc-protected **1D-a** in THF. M_n = 5676, PDI = 1.06, dn/dc = 0.1.



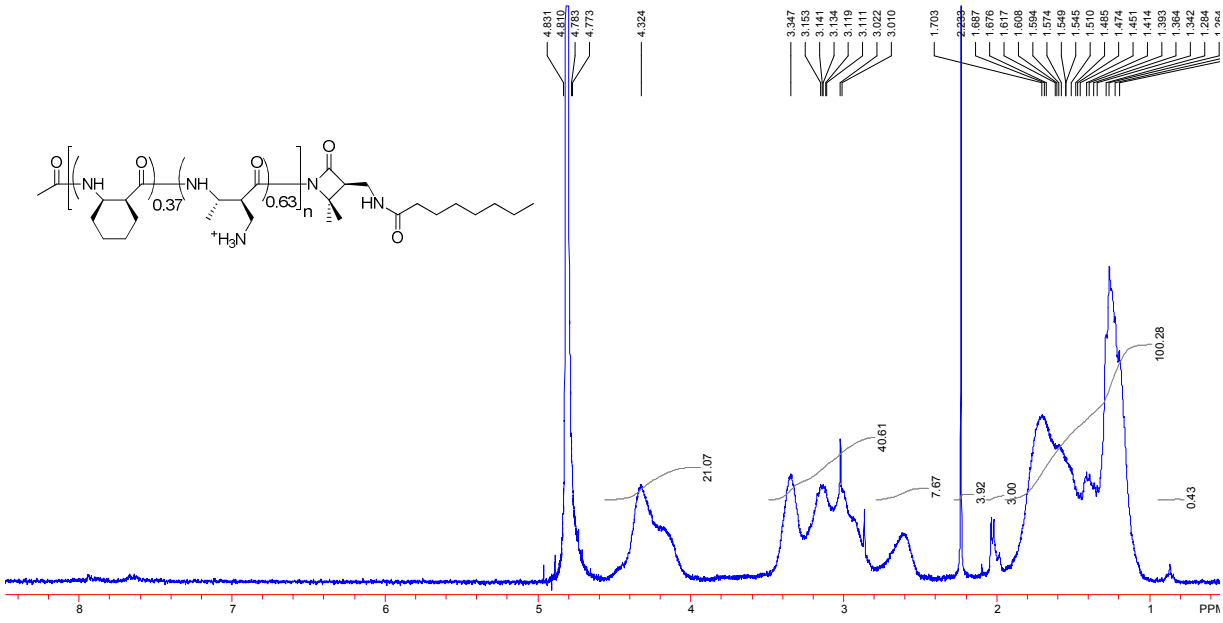
^{1}H NMR of **1D-a** in D_2O at 10 mg/mL.



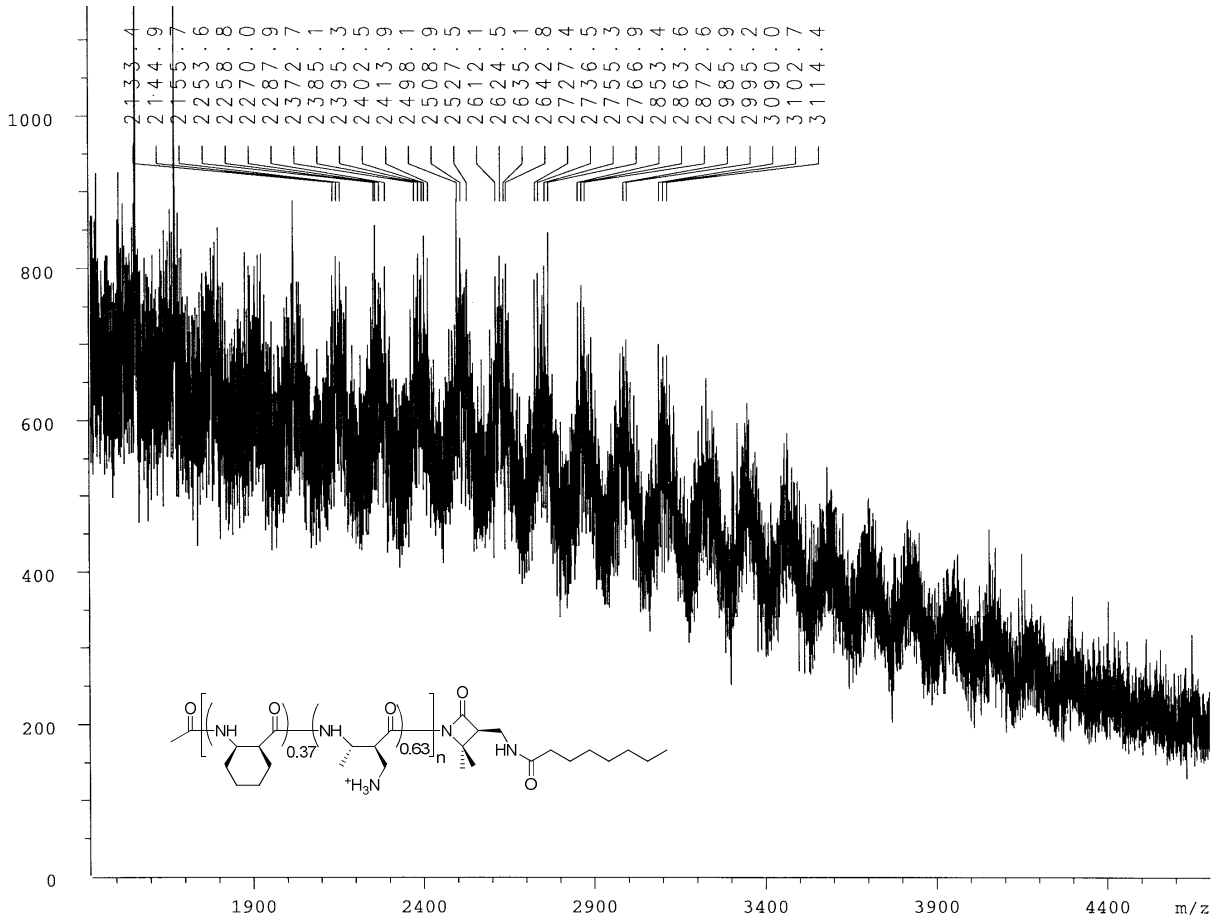
MALDI-TOF spectrum of **1D-a.**



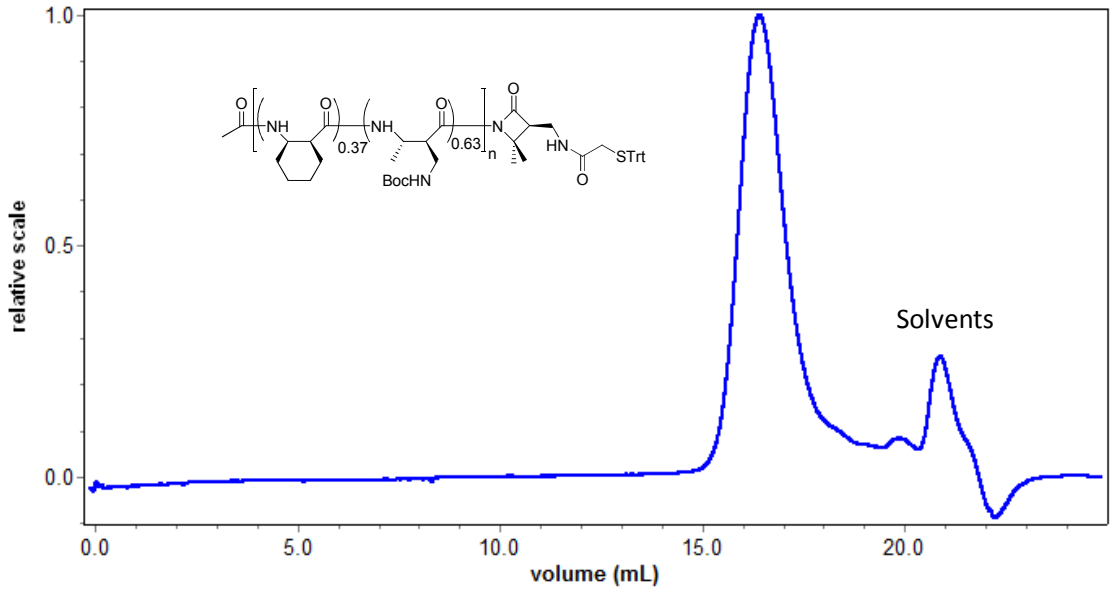
GPC trace (RI detection) of Boc-protected **1D-b** in THF. M_n = 5544, PDI = 1.09, dn/dc = 0.1.



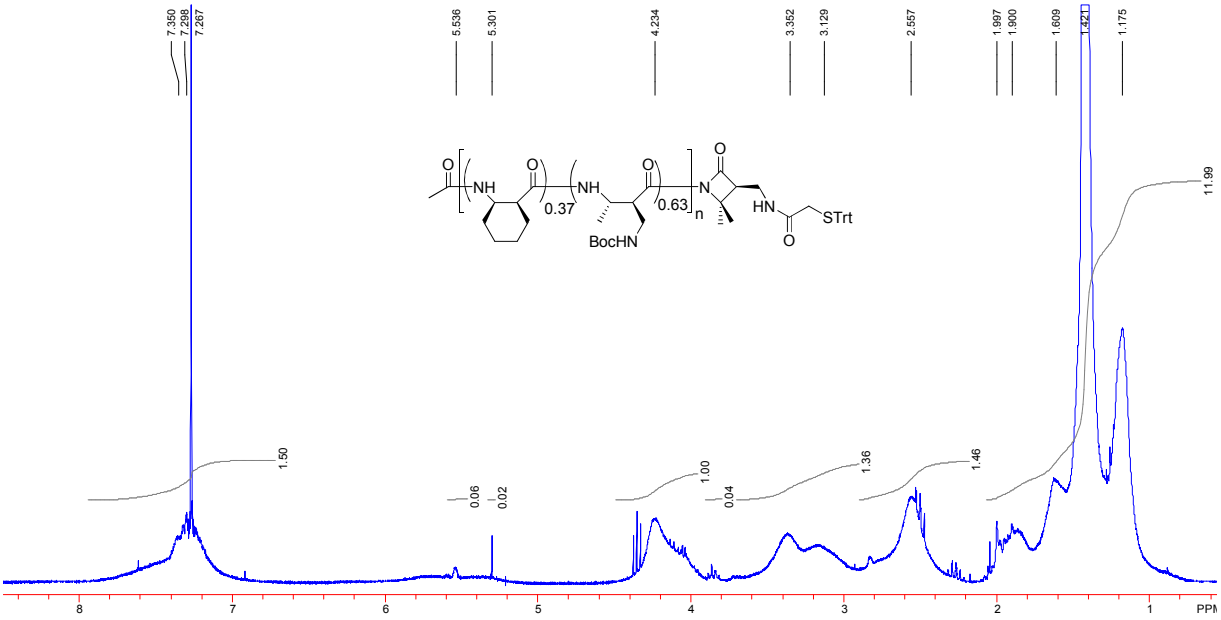
^{1}H NMR of **1D-b** in D_2O at 10 mg/mL.



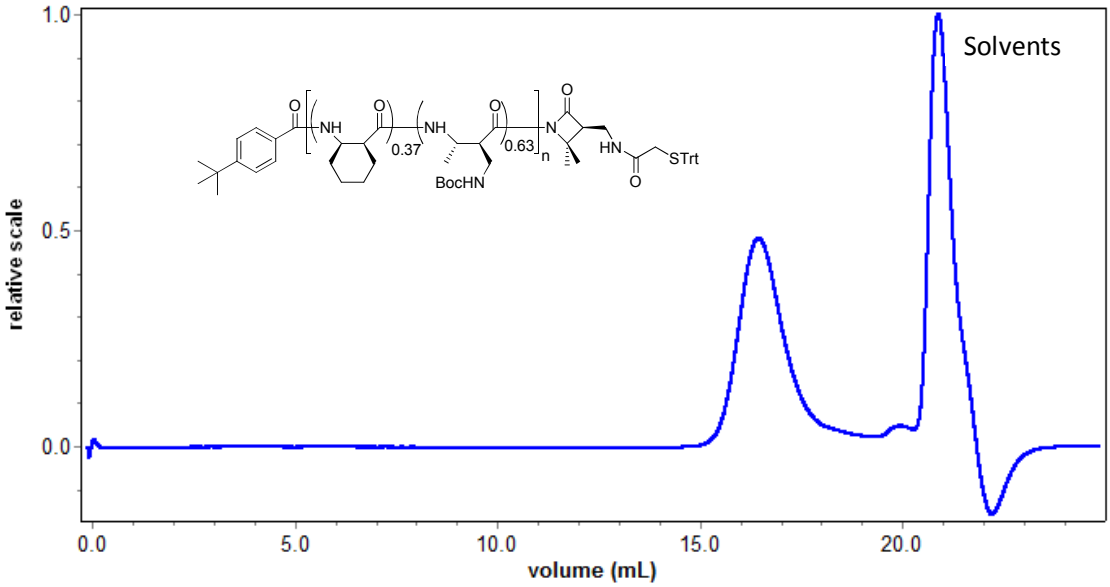
MALDI-TOF spectrum of **1D-b.**



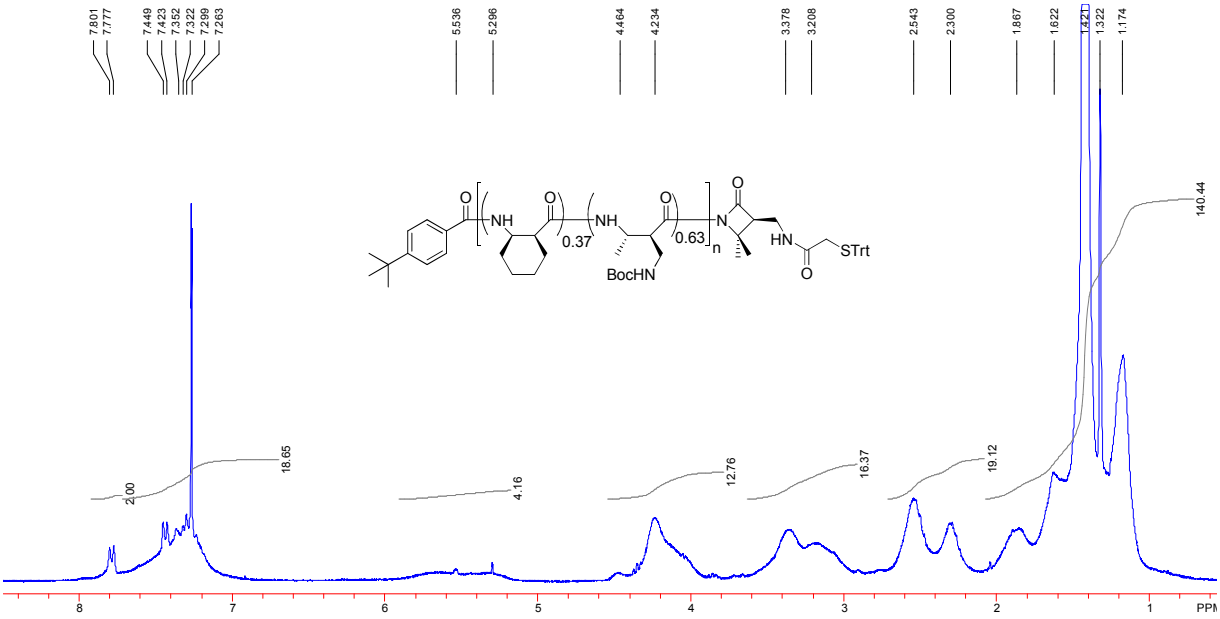
GPC trace (RI detection) of Boc-protected **1F** (with trityl-proteced thiol) in THF. M_n = 5449, PDI = 1.11, dn/dc = 0.1.



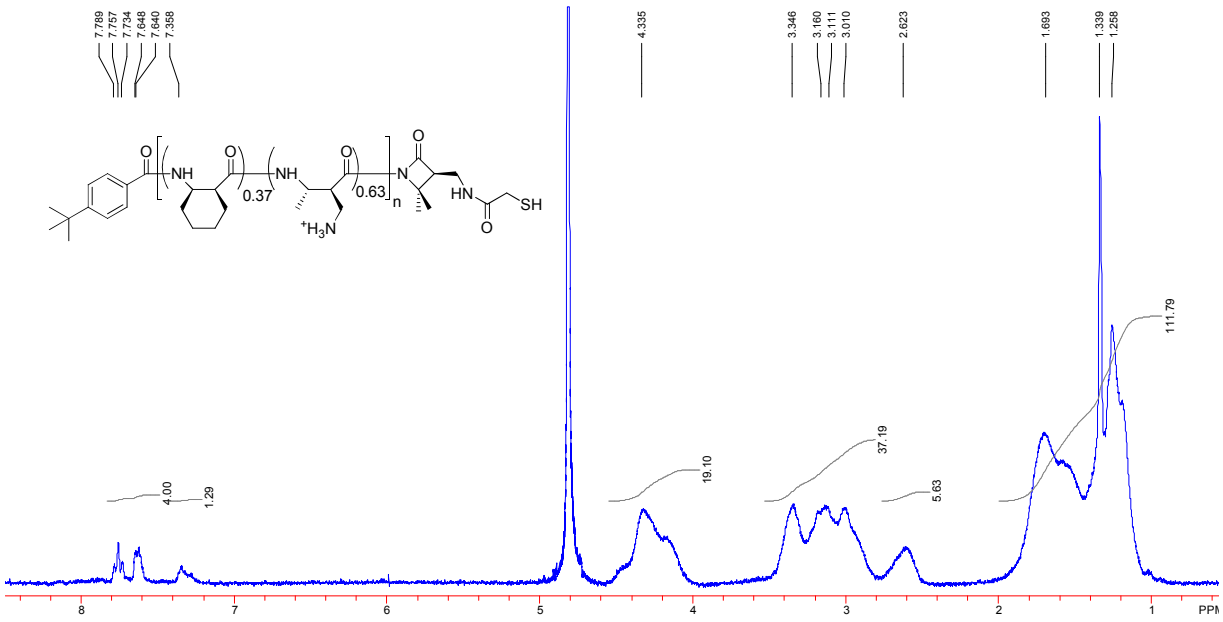
^{1}H NMR of Boc-protected **1F** (with trityl-proteced thiol) in $CDCl_3$ at 10 mg/mL.



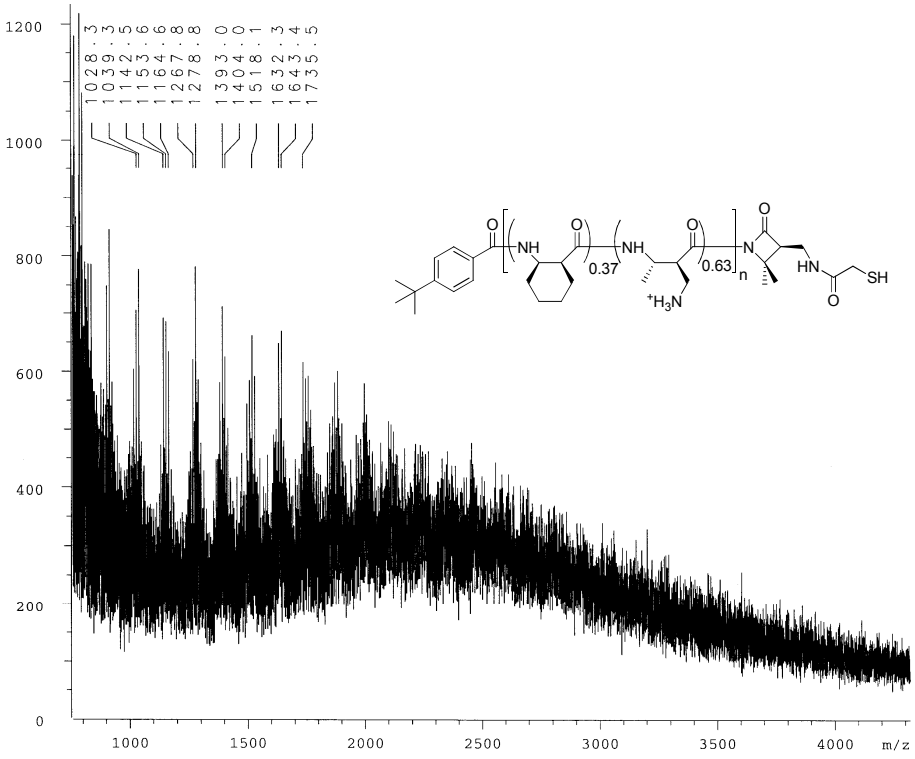
GPC trace (RI detection) of Boc-protected **2F** (with trityl-proteced thiol) in THF. M_n = 4917, PDI = 1.12, dn/dc = 0.1.



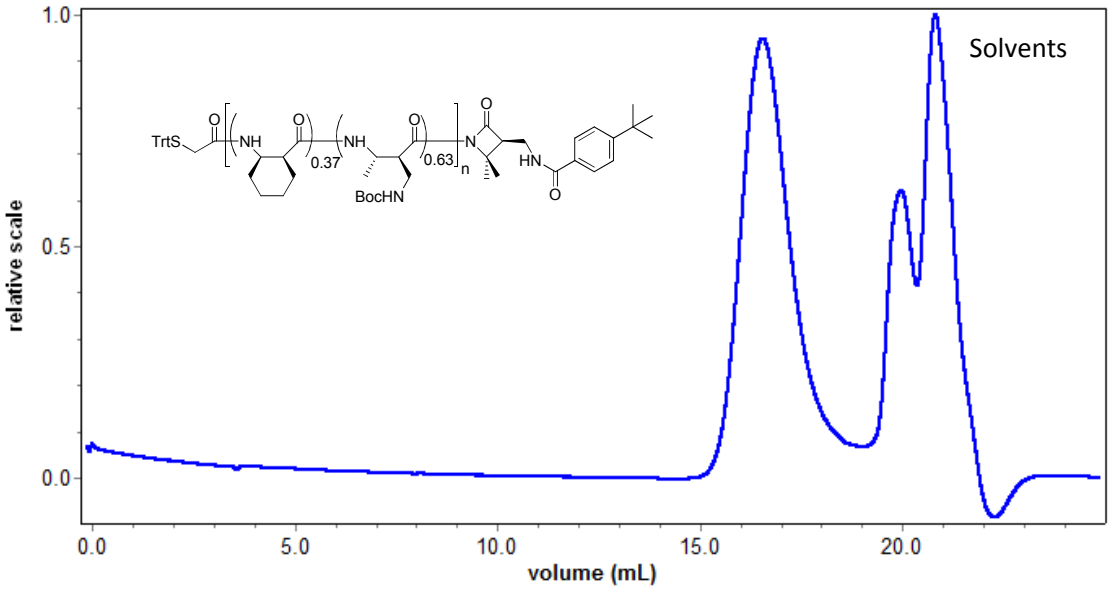
^{1}H NMR of Boc-protected **2F** (with trityl-proteced thiol) in $CDCl_3$ at 10 mg/mL.



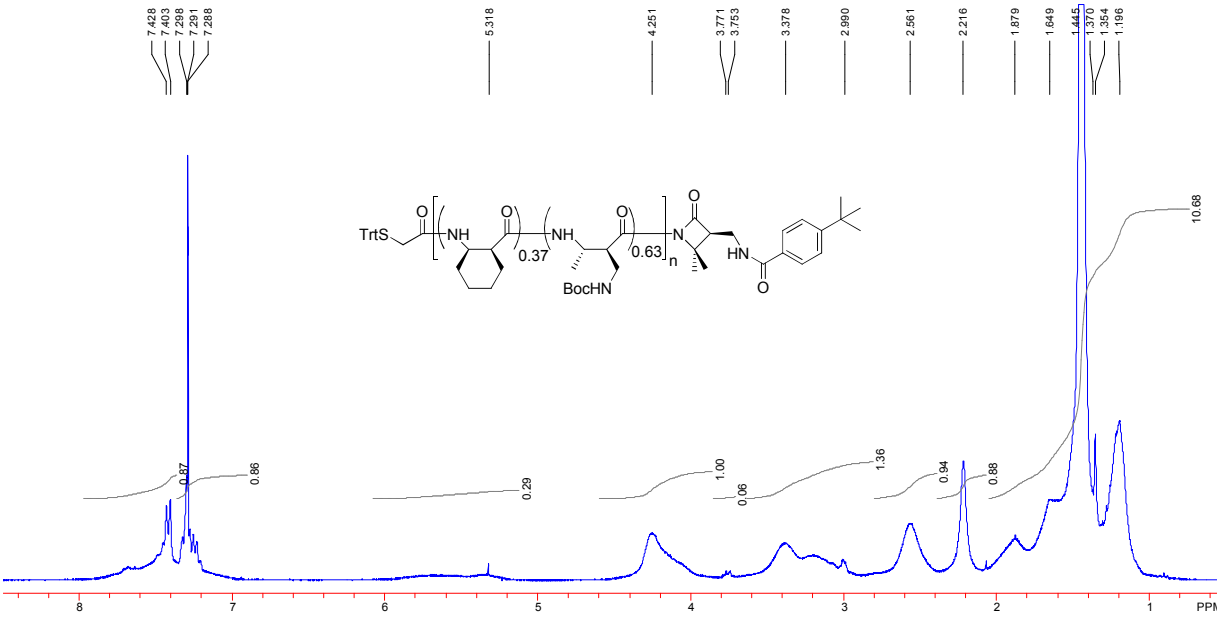
^{1}H NMR of **2F** D_2O at 10 mg/mL.



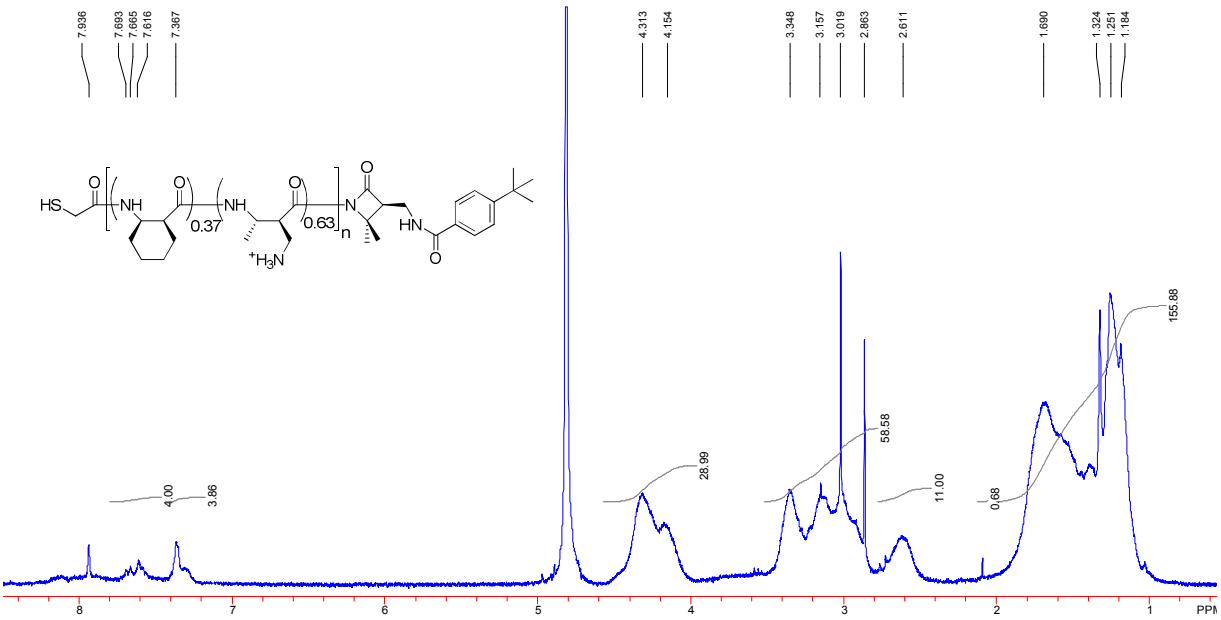
MALDI-TOF spectrum of **2F**.



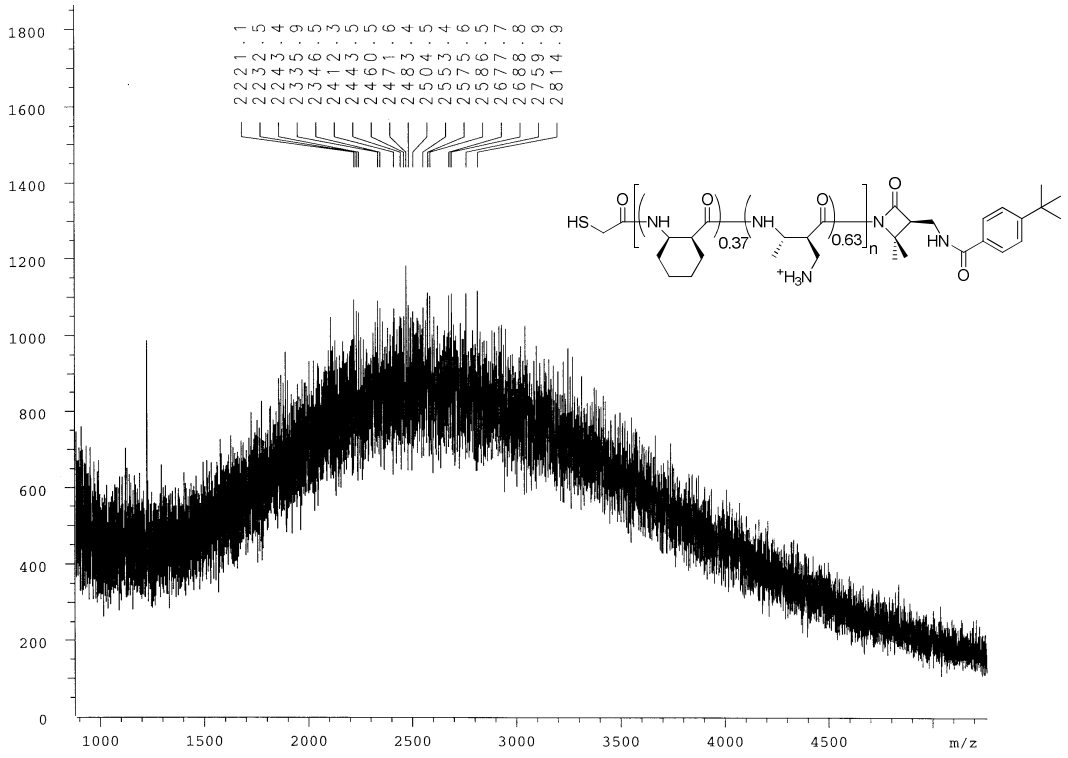
GPC trace (RI detection) of Boc-protected **4C** (with trityl-proteced thiol) in THF. M_n = 4573, PDI = 1.13, dn/dc = 0.1.



^{1}H NMR of Boc-protected **4C** (with trityl-proteced thiol) in $CDCl_3$ at 10 mg/mL.

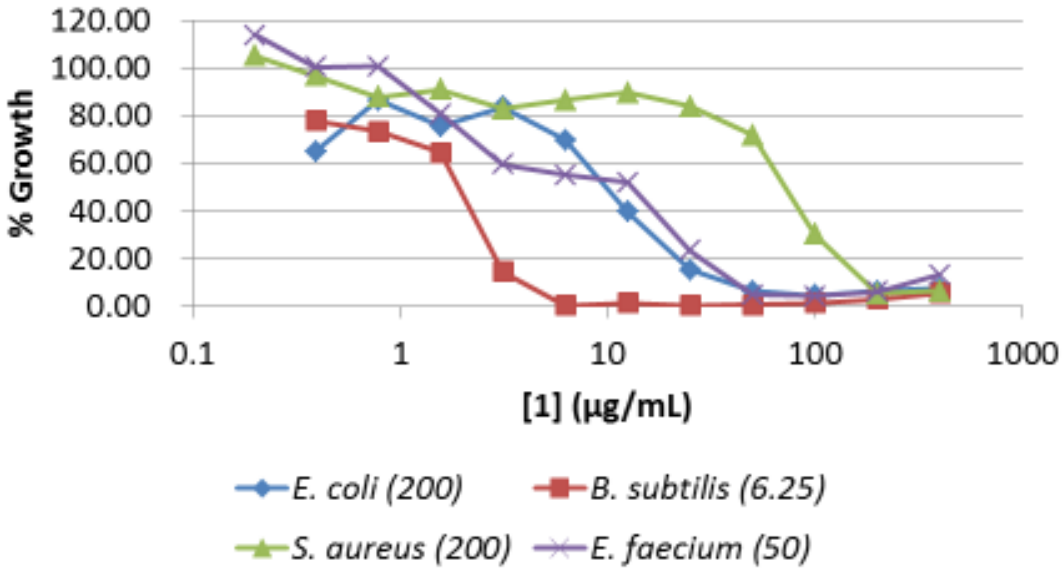


^{1}H NMR of **4C** D_2O at 10 mg/mL.

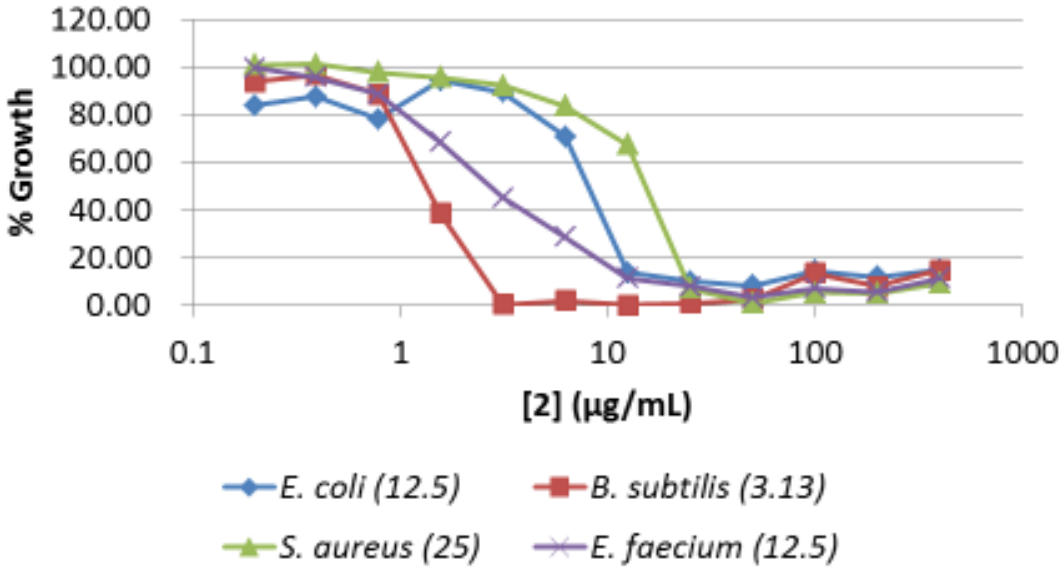


MALDI-TOF spectrum of **4C.**

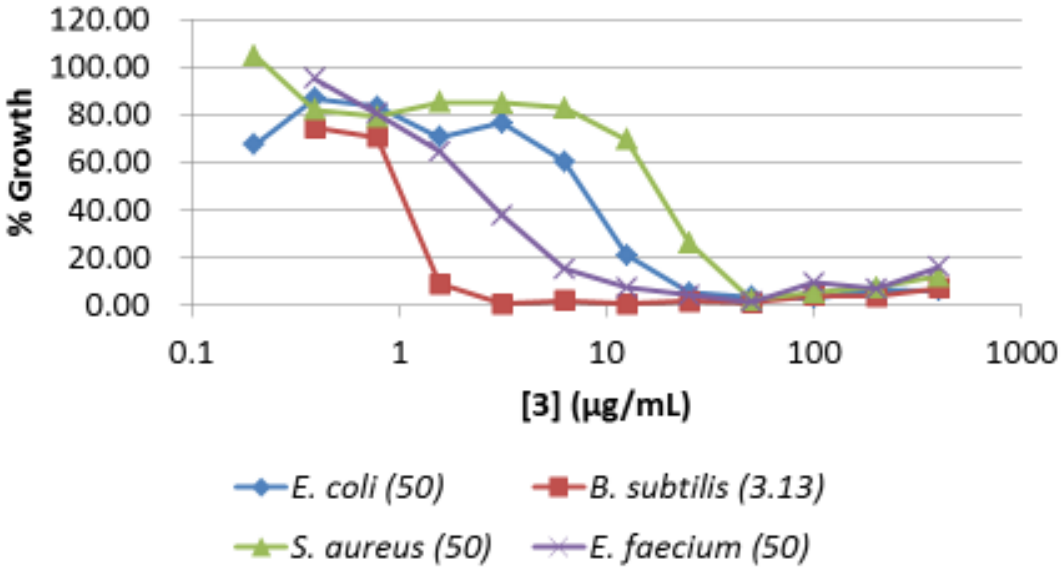
3 Antibacterial and hemolytic assays



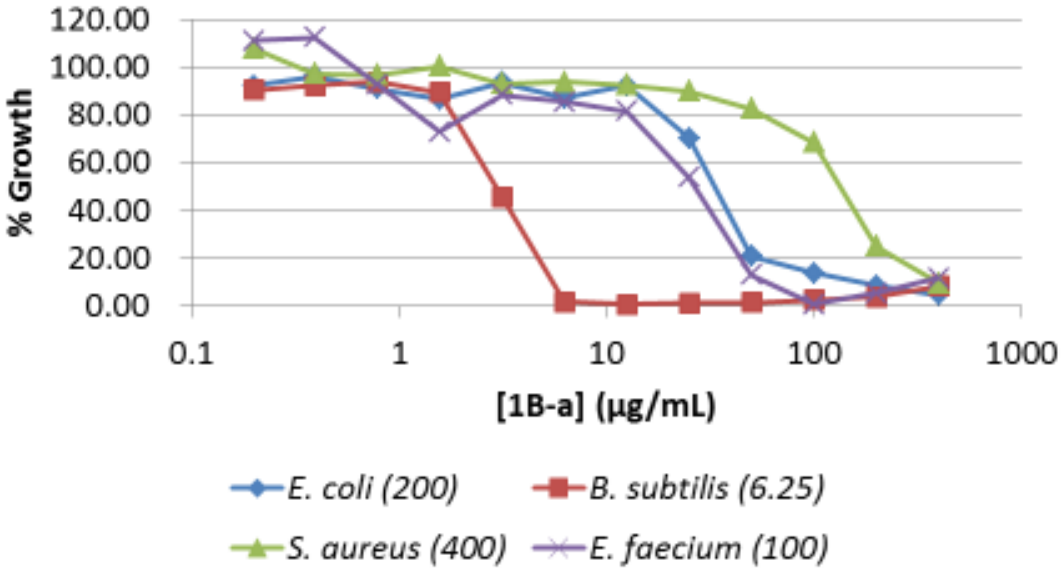
Dose-response curves of antibacterial activity of polymer **1**. Numbers in the parentheses are the MIC values (µg/mL) deduced from the corresponding curves. The lines simply connect the data points.



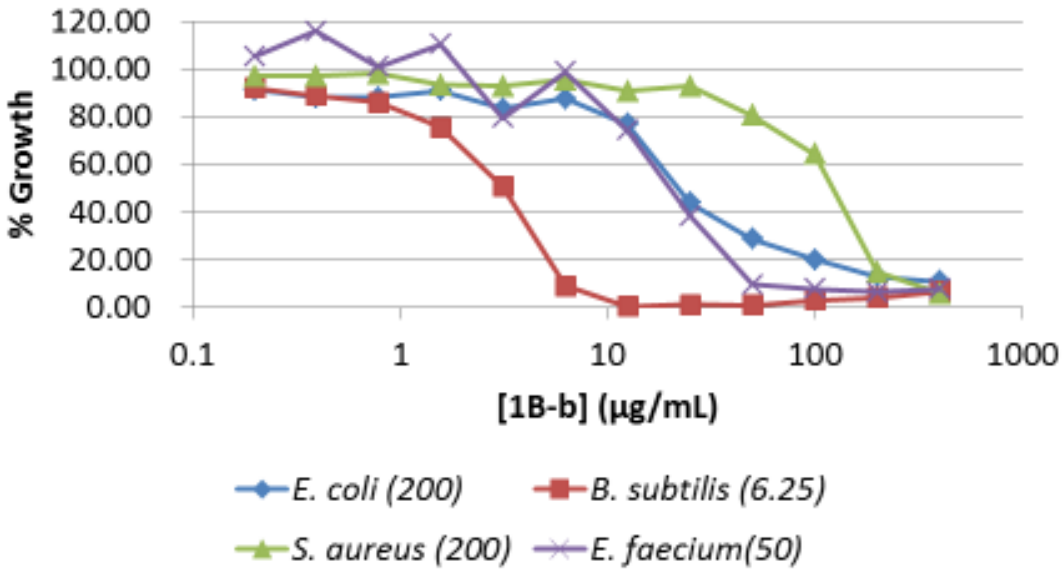
Dose-response curves of antibacterial activity of polymer **2**. Numbers in the parentheses are the MIC values (µg/mL) deduced from the corresponding curves. The lines simply connect the data points.



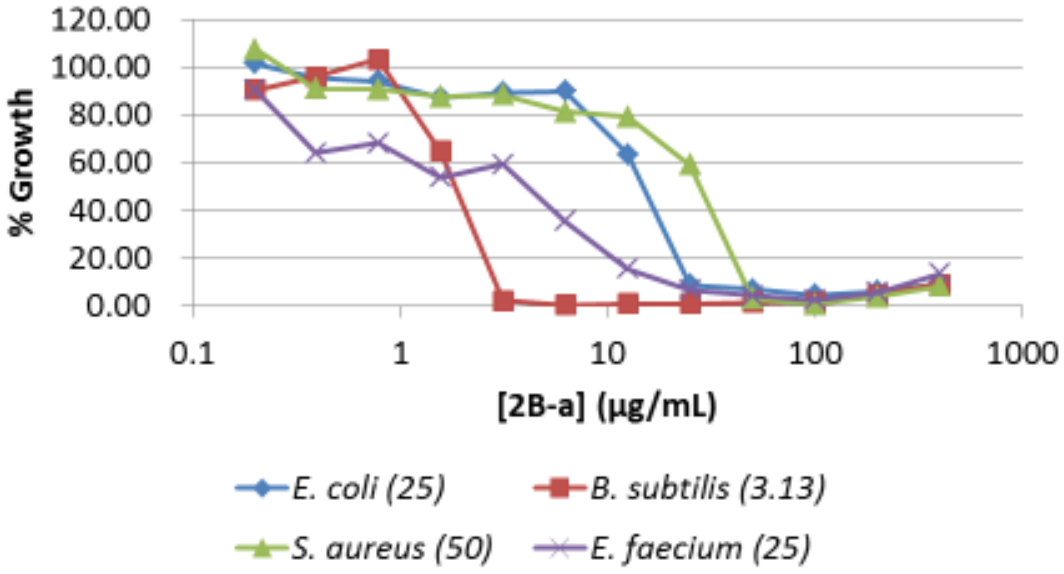
Dose-response curves of antibacterial activity of polymer **3**. Numbers in the parentheses are the MIC values (µg/mL) deduced from the corresponding curves. The lines simply connect the data points.



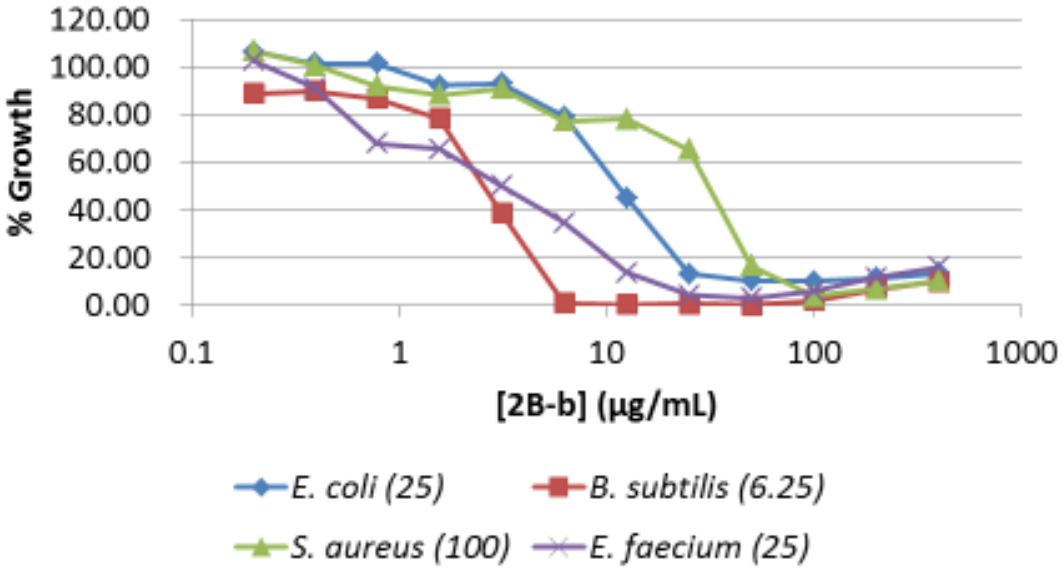
Dose-response curves of antibacterial activity of polymer **1B-a**. Numbers in the parentheses are the MIC values (µg/mL) deduced from the corresponding curves. The lines simply connect the data points.



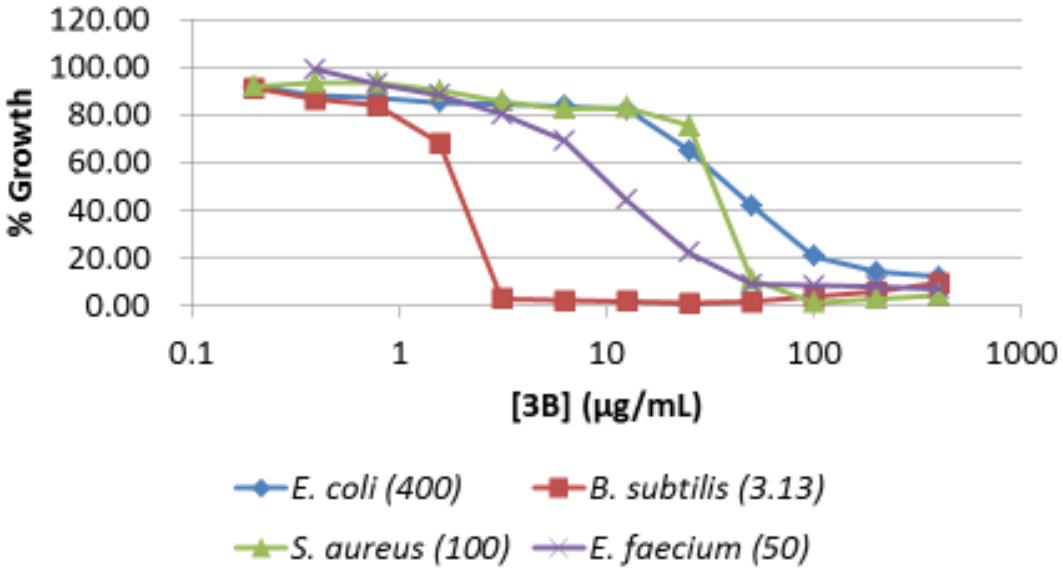
Dose-response curves of antibacterial activity of polymer **1B-b**. Numbers in the parentheses are the MIC values (µg/mL) deduced from the corresponding curves. The lines simply connect the data points.



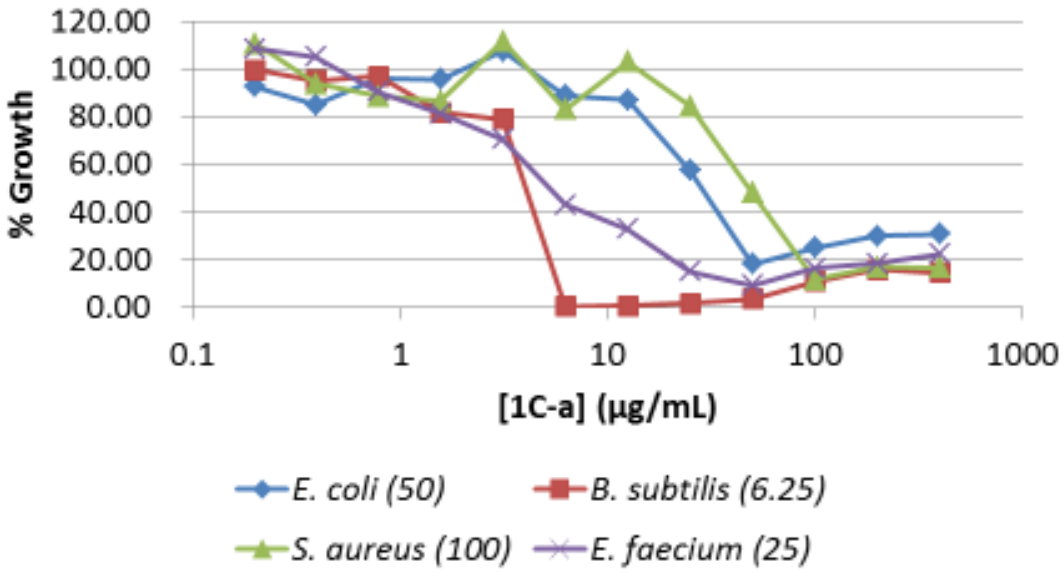
Dose-response curves of antibacterial activity of polymer **2B-a**. Numbers in the parentheses are the MIC values (µg/mL) deduced from the corresponding curves. The lines simply connect the data points.



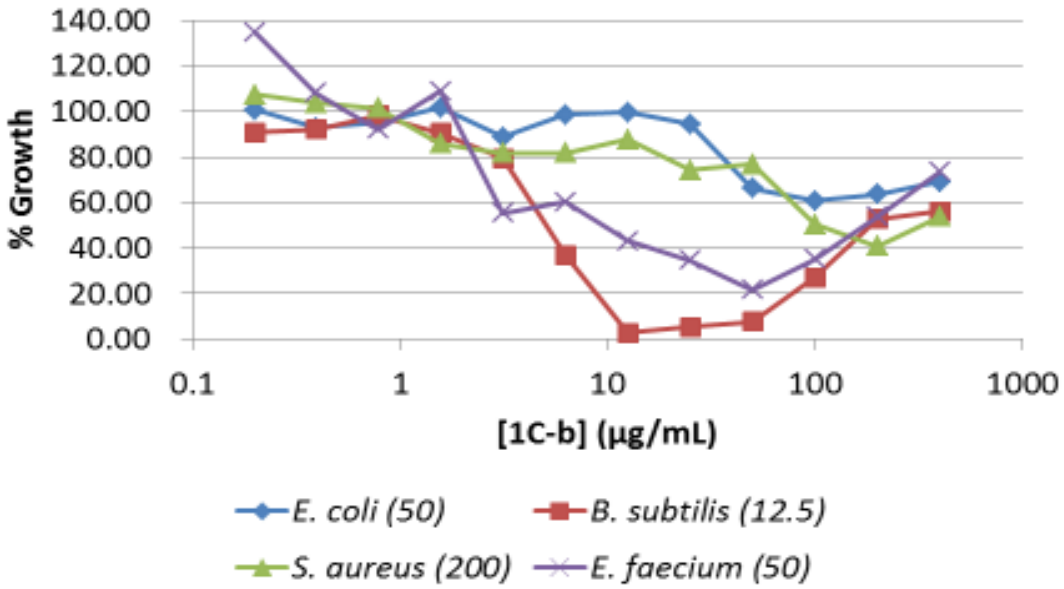
Dose-response curves of antibacterial activity of polymer **2B-b**. Numbers in the parentheses are the MIC values (µg/mL) deduced from the corresponding curves. The lines simply connect the data points.



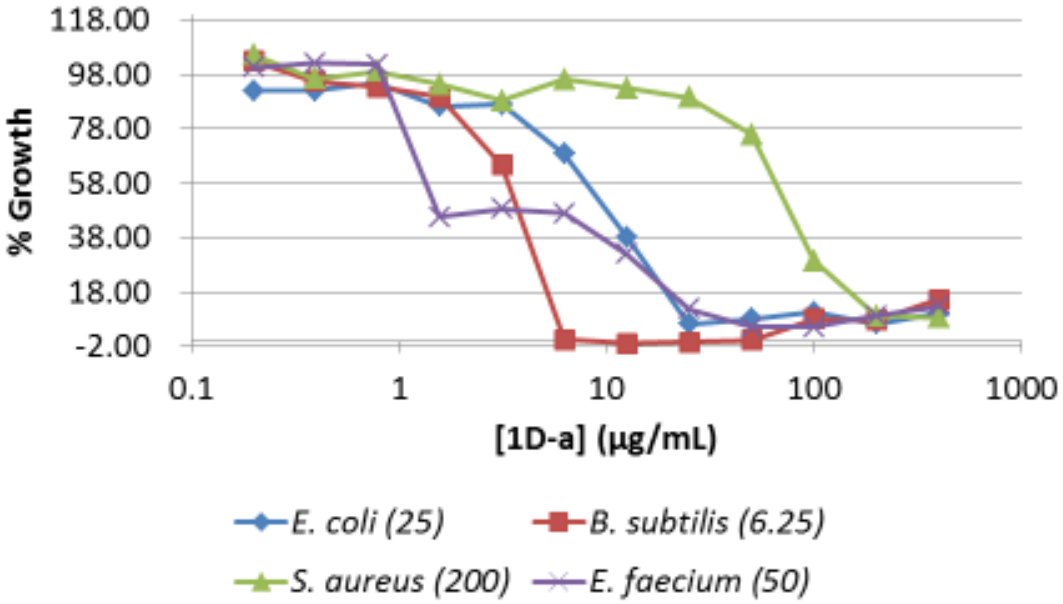
Dose-response curves of antibacterial activity of polymer **3B**. Numbers in the parentheses are the MIC values (µg/mL) deduced from the corresponding curves. The lines simply connect the data points.



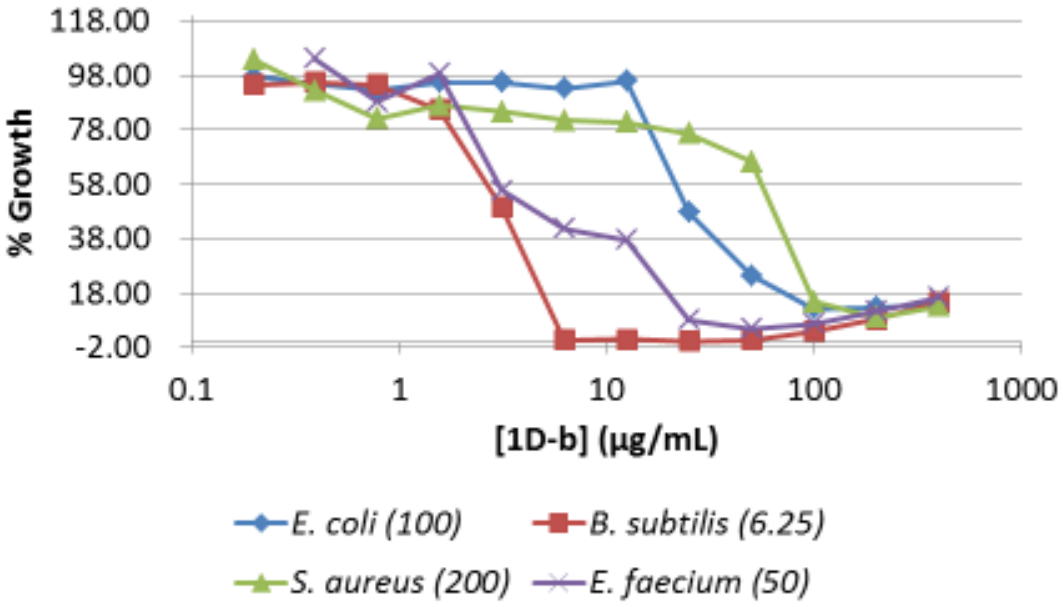
Dose-response curves of antibacterial activity of **1C-a**. Numbers in the parentheses are the MIC values (µg/mL) deduced from the corresponding curves. The lines simply connect the data points.



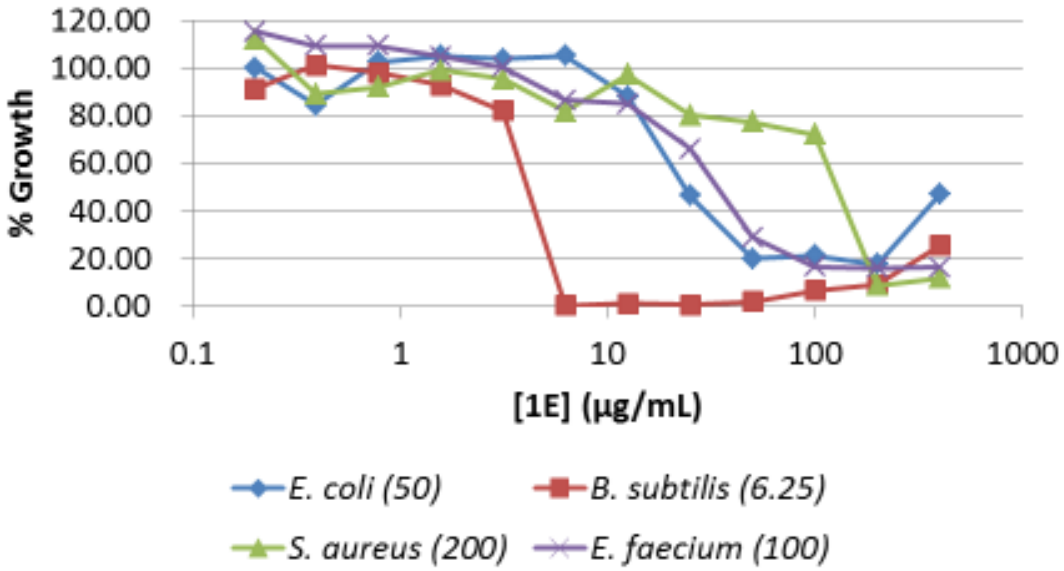
Dose-response curves of antibacterial activity of **1C-b**. Numbers in the parentheses are the MIC values (µg/mL) deduced from the corresponding curves. The lines simply connect the data points. The polymer is not fully soluble in BHI > 100 µg/mL.



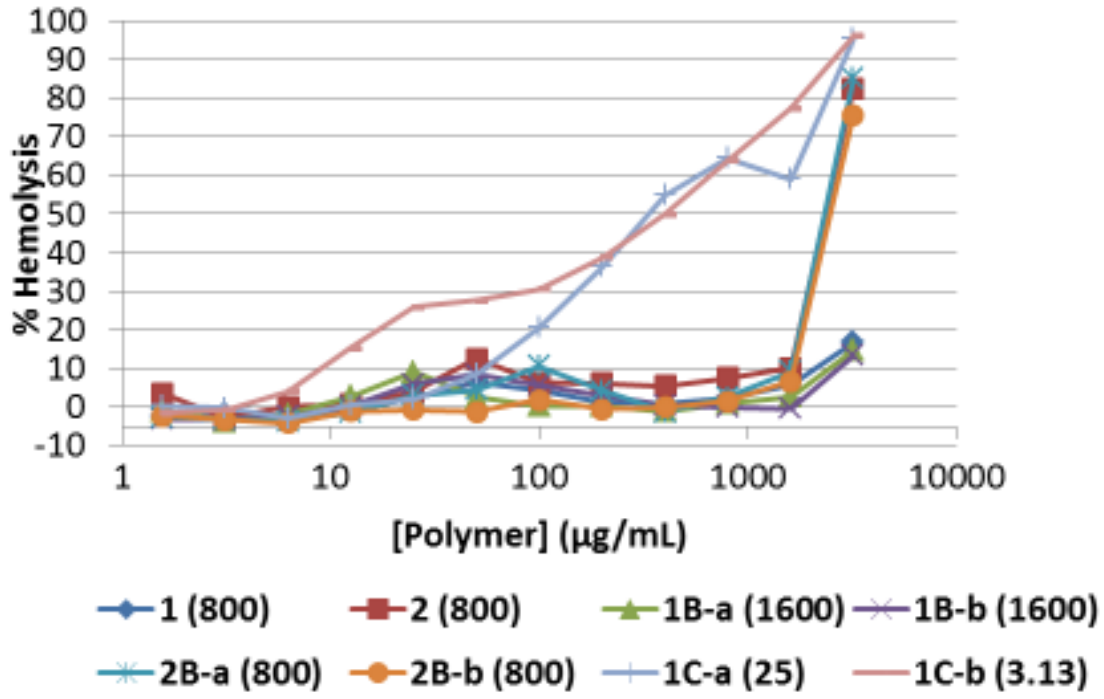
Dose-response curves of antibacterial activity of **1D-a**. Numbers in the parentheses are the MIC values (μg/mL) deduced from the corresponding curves. The lines simply connect the data points.



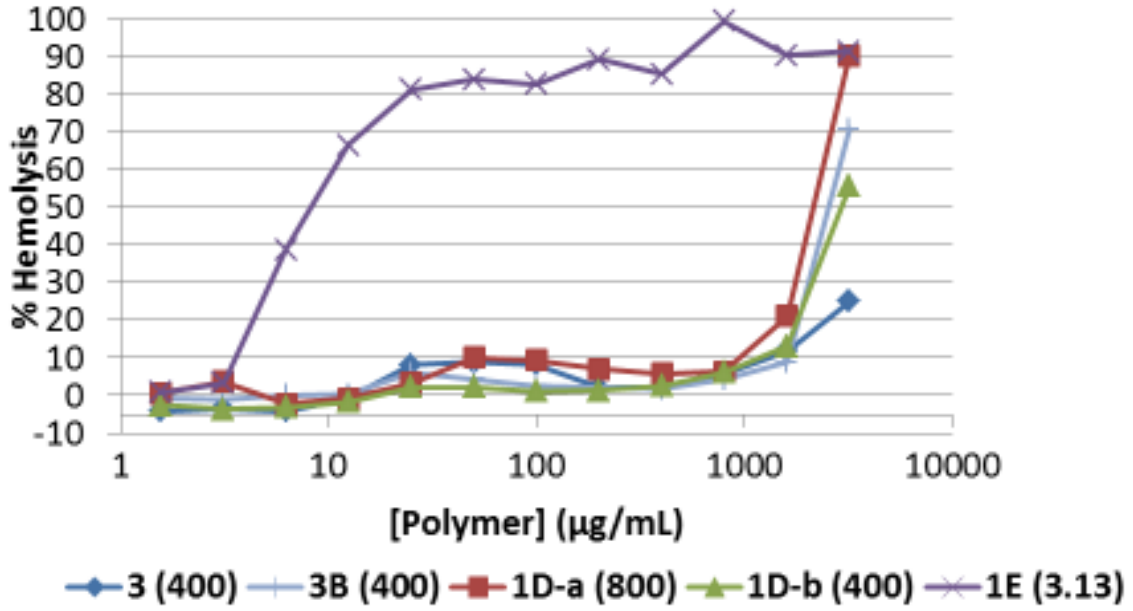
Dose-response curves of antibacterial activity of **1D-b**. Numbers in the parentheses are the MIC values (μg/mL) deduced from the corresponding curves. The lines simply connect the data points.



Dose-response curves of antibacterial activity of **1E**. Numbers in the parentheses are the MIC values (µg/mL) deduced from the corresponding curves. The lines simply connect the data points. The polymer is not fully soluble in BHI > 200 µg/mL.

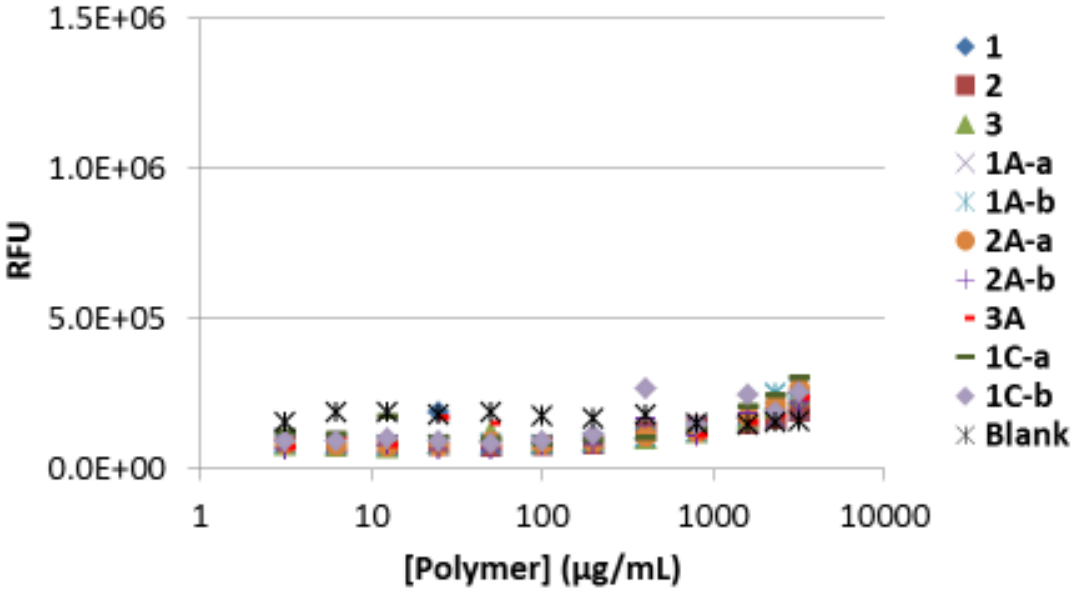


Dose-response curves of hemolytic activity. Numbers in the parentheses are the MHC values (μg/mL) deduced from the corresponding curves. The lines simply connect the data points.

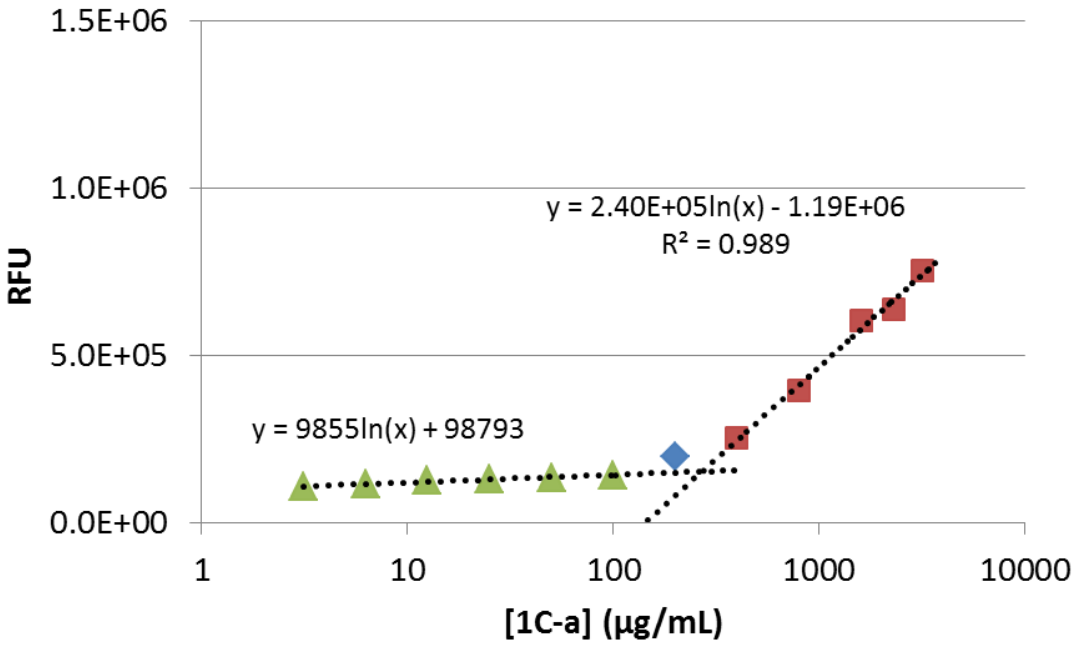


Dose-response curves of hemolytic activity. Numbers in the parentheses are the MHC (µg/mL) values deduced from the corresponding curves. The lines simply connect the data points.

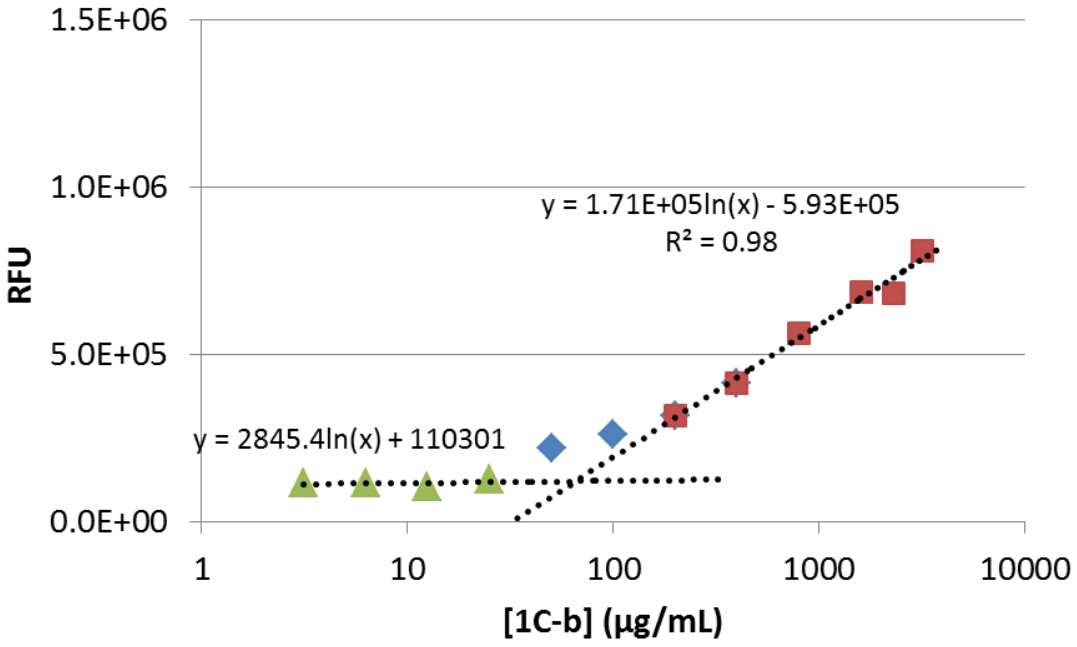
3 CAC measurements in Tris-buffered saline



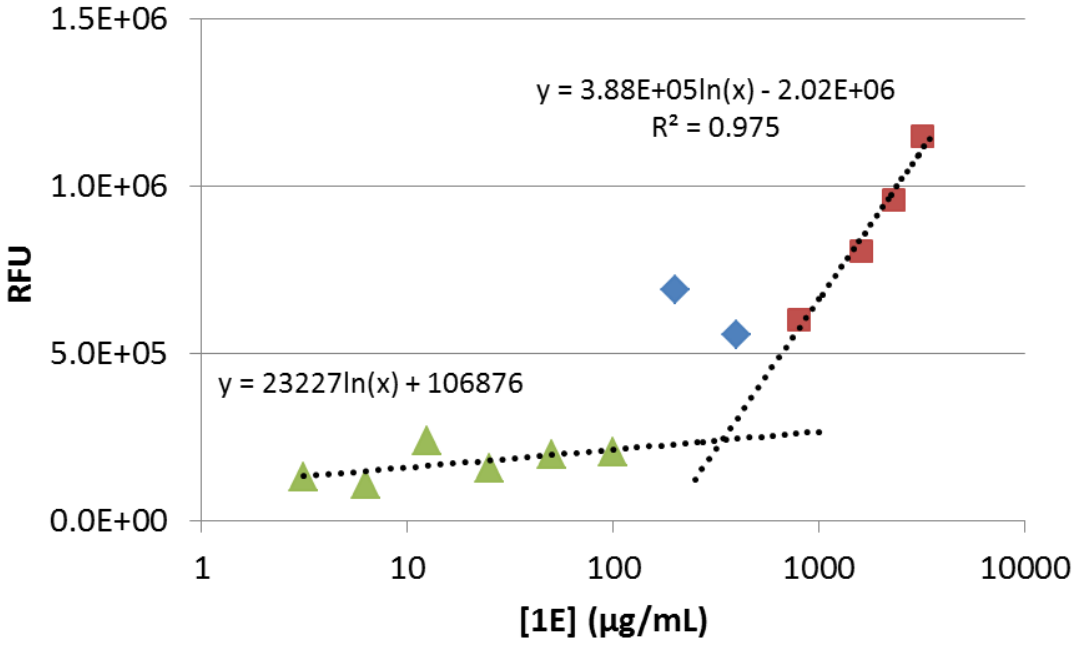
DPH fluorescence plot for the non-aggregating polymers



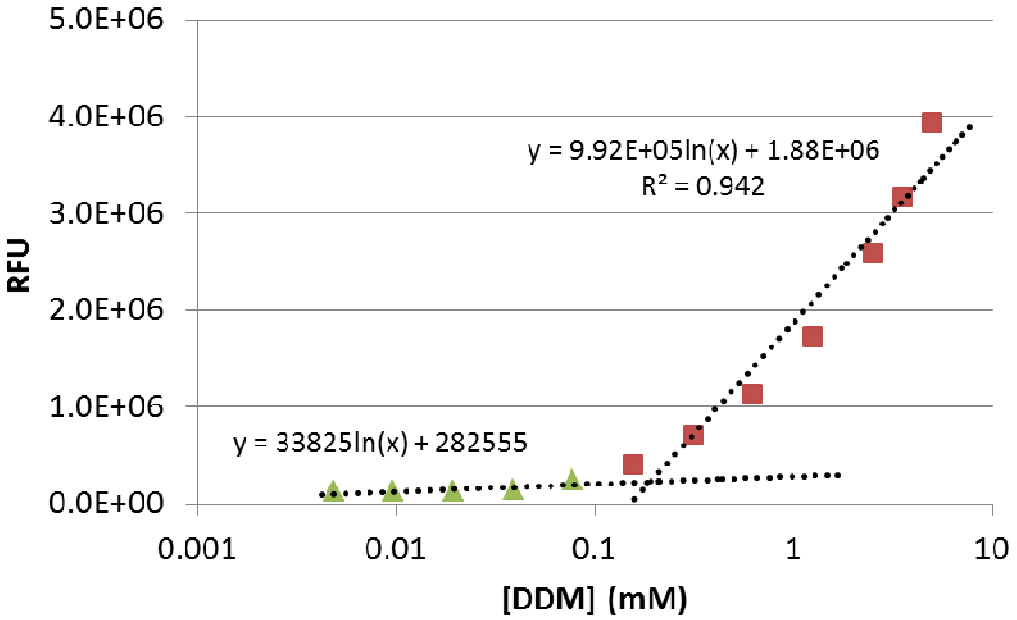
DPH fluorescence plot for **1C-a**. CAC = 220 µg/mL.



DPH fluorescence plot for **1C-b**. CAC = 70 µg/mL.



DPH fluorescence plot for **1E**. CAC = 360 µg/mL.



DPH fluorescence plot for **DDM**. CAC = 0.19 mM (lit. 0.17mM).