Supporting Information

Inhibition of *Acinetobacter baumannii* Biofilm Formation on Methacrylate Polymer Containing a 2-Aminoimidazole Subunit

Lingling Peng,[&] Joseph DeSousa,[&] Zhaoming Su, Bruce M. Novak, Alexander A. Nevzorov, Eva R. Garland, and Christian Melander

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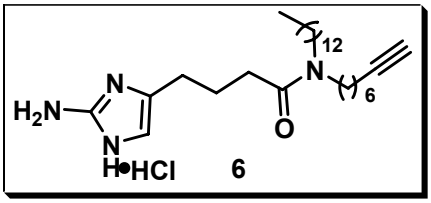
General Experimental: All reagents used for chemical synthesis were purchased from commercially available sources and used without further purification. Chromatography was performed using 60 Å mesh standard grade silica gel from Sorbtech. NMR solvents were obtained from Cambridge Isotope Labs and used as is. ^{1}H NMR (300 MHz or 400 MHz) and ^{13}C NMR (75 MHz or 100 MHz) spectra were recorded at 25ºC on Varian Mercury spectrometers. Chemical shifts (δ) are given in ppm relative to the respective NMR solvent; coupling constants (*J*) are in hertz (Hz). Abbreviations used are s = singlet, bs = broad singlet, d = doublet, dd = doublet of doublets, t = triplet, q = quartet, td = doublet of triplets, qd = doublet of quartets, m =

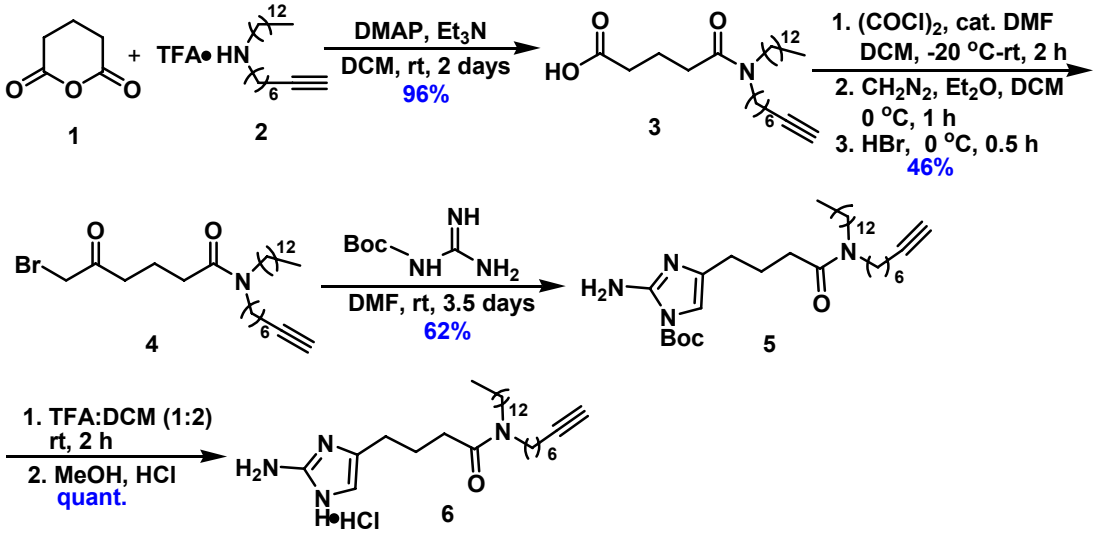
multiplet. Mass spectra were obtained at the NCSU Department of Chemistry Mass Spectrometry Facility. Funding was obtained from the North Carolina Biotechnology Center and the NCSU Department of Chemistry.

Acinetobacter baumannii (ATCC # 19606) was purchased from ATCC. Mechanically difibrinated sheep blood (DSB100) was obtained from Hemostat Labs. All other supplies were purchased from commercially available sources. Stock solutions (100, 10, 1 mM) of all compounds assayed for biological activity were prepared in DMSO and stored at 5 ^{o}C in frig. The amount of DMSO used in inhibition assay did not exceed 1% (by volume).

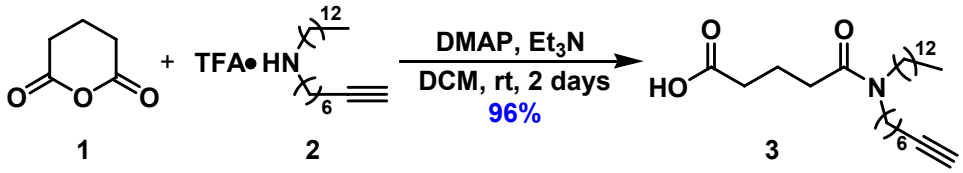
Synthesis:

Synthesis of **6**:

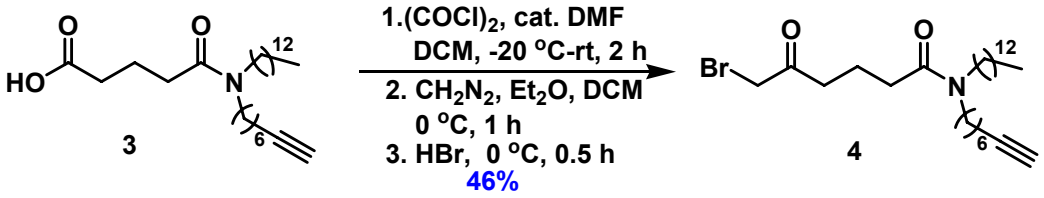




Scheme 1. Synthesis of **6**

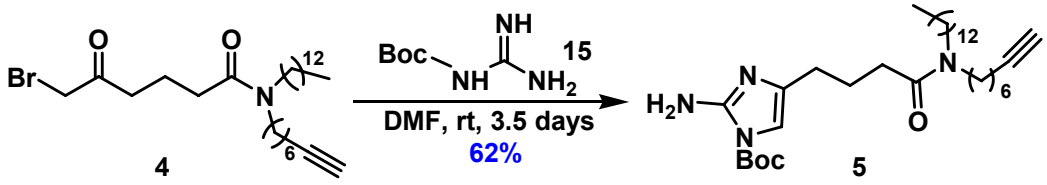


4-(*N*-(oct-7-ynyl)-*N*-tridecylcarbamoyl)butanoic acid (3):
Glutaric anhydride **1** (1.93 g, 16.9 mmol, 1.0 eq), dichloromethane (30 mL) and **2** (7.11 g, 16.9 mmol, 1.0 eq). Triethylamine (5.2 mL, 37.2 mmol, 2.2 eq) and then DMAP (41 mg, 0.34 mmol, 0.02 eq) were added at 0 ^{o}C. The stirring solution was allowed to warm to room temperature and continued stirring for two days. Volatiles were evaporated under reduced pressure. The crude oil was purified by flash column chromatography (Hexanes/ethyl acetate 1:1 to 1:3 to ethyl acetate) to obtain the titled compound **3** (6.83 g, 96 %) as a slight yellow oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.28-3.24 (m, 2H), 3.21-3.16 (m, 2H), 2.73 (t, J = 6.8 Hz, 2H), 2.43-2.36 (m, 4H), 2.16 (qd, J = 6.8, 2.4 Hz, 2H), 2.30-1.90 (m, 3H), 1.58-1.34 (m, 6H), 1.34-1.18 (m, 22H), 0.85 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.15, 172.40, 172.35, 84.79, 84.56, 68.63, 68.42, 48.34, 48.19, 46.36, 46.25, 33.62, 33.59, 32.13, 32.10, 30.16, 29.86, 29.81, 29.76, 29.64, 29.56, 29.29, 29.15, 28.66, 28.57, 28.47, 27.94, 27.79, 27.26, 27.10, 26.71, 26.57, 22.89, 20.71, 18.52, 18.50, 16.56, 14.33; HRMS (ESI) calcd for $C_{26}H_{48}NO_3$ (M+H)+ m/z 422.3629, found 422.3620.

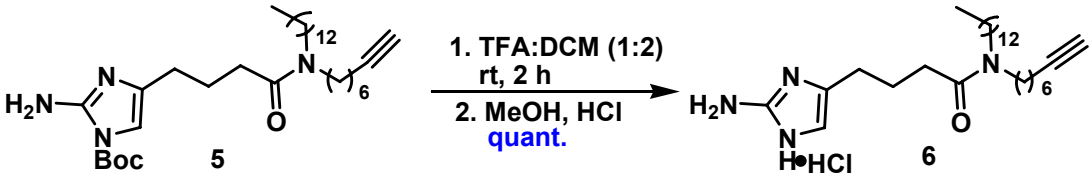


6-Bromo-*N*-(oct-7-ynyl)-5-oxo-*N*-tridecylhexanamide (4): Under N_2 protection, **3** (4.5 g, 10.7 mmol, 1.0 eq) was dissolved in anhydrous dichloromethane (40 mL) at -20 ^{o}C and a catalytic amount of DMF (5 drops) was added. To this solution was added oxalyl chloride (2.9 mL, 32.1 mmol, 3.0 eq) dropwise. The solution was continued stirring at -20 ^{o}C and was then slowly warmed to room temperature. After 2 h, volatiles were evaporated under reduced pressure. The residue was dissolved in 30 mL DCM again and then concentrated, repeated the process for 3 times to remove excess oxalyl chloride. The residue was dried under high vacuum for 2 h. The obtained crude acid chloride was dissolved in anhydrous dichloromethane (20 mL) and added dropwise to a 0 ^{o}C solution of CH_2N_2 (32.1 mmol, 3.0 eq, generated from Diazald®–KOH) in diethyl ether (150 mL). This solution was stirred at 0 ^{o}C for 1.5 h. Then the reaction was quenched *via* the dropwise addition of 48 % HBr (4.9 mL, 4.0 eq) at 0 ^{o}C. Continued to stir 0.5 h, then $NaHCO_3$ (aq) (70 mL) was added at 0 ^{o}C. After 20 min, the reaction mixture was diluted with EtOAc, washed with $NaHCO_3$ (aq) then Brine, dried over Na_2SO_4. Filtered and concentrated. The crude oil was purified by flash column chromatography (Hexanes/ethyl acetate 5:1 to 2:1 to 1:1) to obtain the titled compound **4** (2.44 g, 46 %) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ3.83 (s, 2H), 3.22-3.17 (m, 2H), 3.14-3.09 (m, 2H), 2.69 (t, *J* = 6.8 Hz, 2H), 2.26 (t, *J* = 6.8 Hz, 2H), 2.12-2.09 (m, 2H), 1.90-1.85 (m, 3H), 1.46-1.30 (m, 8H), 1.30-1.17 (m, 22H), 0.80 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.14, 171.69, 171.64, 84.80, 84.57, 68.60, 68.41, 48.16, 48.01, 46.17, 46.07, 39.24, 39.13, 34.55, 32.14, 31.80, 29.86, 29.78, 29.66, 29.58, 29.57, 29.31, 29.16, 28.70, 28.60, 28.51, 28.04, 27.88, 27.32, 27.13, 26.76, 26.62, 22.90, 19.66, 18.54, 14.33; HRMS (ESI) calcd for $C_{27}H_{49}BrNO_2$ (M+H)+ m/z 498.2941, found 498.2933.



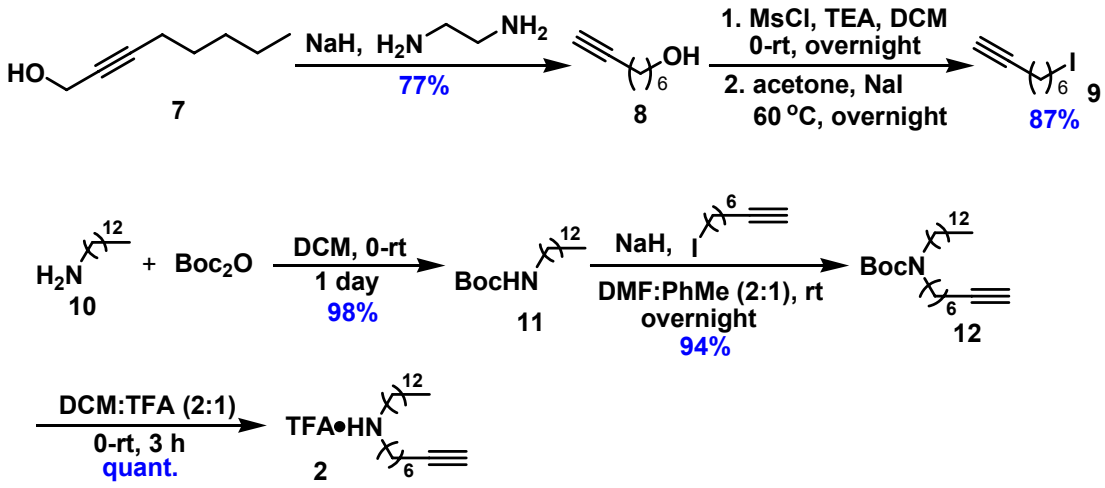
***tert*-Butyl 4-(3-(*N*-(oct-7-ynyl)-*N*-tridecylcarbamoyl)propyl)-2-amino-imidazole -1-carboxylate (5): 4** (2.4 g, 4.8 mmol, 1.0 eq) and Boc-guanidine **15** (2.3 g, 14.4 mmol, 3.0 eq) were dissolved in DMF (10 mL) and allowed to stir at room temperature. After 3.5 days the reaction mixture was diluted with EtOAc (120 mL), washed with H_2O (3×25 mL) and Brine (25 mL), dried over Na_2SO_4. Filtered and concentrated. The crude oil was purified by flash column chromatography (Hexanes/ethyl acetate 1:1 to ethyl acetate to ethyl acetate/MeOH 20:1) to obtain the titled compound **5** (1.7 g, 62 %) as a yellow oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.51 (s, 1H), 5.82 (s, 2H), 3.27-3.23 (m, 2H), 3.17-3.12 (m, 2H), 2.39 (t, *J* = 7.2 Hz, 2H), 2.30 (t, *J* = 7.2 Hz, 2H), 2.17-2.12 (m, 2H), 1.94-1.88 (m, 3H), 1.60-1.35 (m, 17H), 1.35-1.20 (m, 22H), 0.84 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.50, 172.45, 150.29, 149.68, 138.80, 106.97, 84.81, 84.67, 84.69, 84.54, 68.61, 68.37, 48.21, 48.06, 46.10, 45.99, 32.66, 32.12, 29.85, 29.83, 29.77, 29.66, 29.58, 29.55, 29.38, 29.23, 28.70, 28.59, 28.49, 28.20, 28.05, 27.91, 27.30, 27.11, 26.75, 26.59, 24.27, 22.89, 18.53, 18.50, 14.33; HRMS (ESI) calcd for $C_{33}H_{59}N_4O_3$ (M+H)+ m/z 559.4582, found 559.4574.



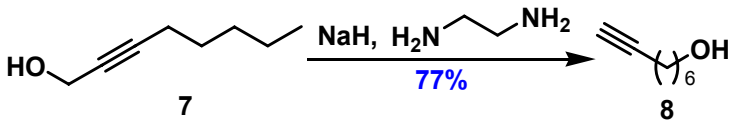
4-(2-Amino-imidazol-4-yl)-*N*-(oct-7-ynyl)-*N*-tridecylbutanamide hydrochloride (6): 5 (200 mg, 0.36 mmol) was dissolved in 2 mL anhydrous DCM, TFA (1 mL) was then added dropwise and the reaction was stirred for 2 h at room temperature. After

this time, the reaction was evaporated to dryness and DCM (2 mL) was added. Again the mixture was concentrated and the process was repeated for 3 times. The resulting residue was dried under high vacuum for 2 h. The obtained TFA salt was dissolved in methanol (2 mL), and 4 drops of HCl (conc.) was added. This solution was evaporated to dryness directly. The residue was dissolved in methanol (2 mL) and filtered to remove any precipitate by syringe filter (13 mm Diameter, 0.2 μm Pore Size, catalog No. 6788-1302, Whatman Inc.). Then concentrated and dried under high vacuum to yield the titled compound **6** (178 mg, quant.) as a slight brown oil.
^{1}H NMR (400 MHz, CD_3OD) δ 6.52 (s, 1H), 3.31-3.30 (m, 4H), 2.54 (t, J = 6.8 Hz, 2H), 2.43 (t, J = 6.8 Hz, 2H), 2.19-2.14 (m, 3H), 1.94-1.84 (m, 2H), 1.56-1.41 (m, 10H), 1.28 (bs, 20H), 0.89 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CD_3OD) δ 174.30, 148.67, 128.56, 110.07, 85.08, 69.77, 69.64, 47.41, 47.36, 33.21, 32.99, 30.93, 30.90, 30.83, 30.62, 30.22, 30.08, 29.74, 29.68, 29.63, 29.58, 28.87, 28.75, 28.19, 28.01, 27.66, 27.46, 25.31, 25.12, 23.88, 19.09, 14.62; HRMS (ESI) calcd for $C_{28}H_{51}N_4O$ (M+H)+ m/z 459.4057, found 459.4050.

Synthesis of **2**:

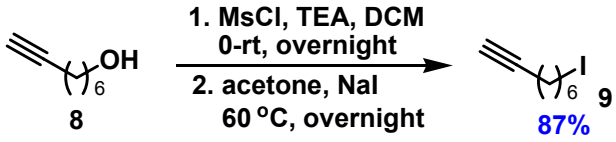


Scheme 2. Synthesis of **2**

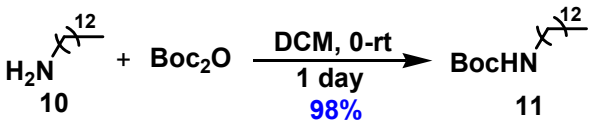


Oct-7-yn-1-ol (8)[1]**:** Under N_2 protection, ethane-1, 2-diamine (350 mL) was added to a 1 L round-bottomed flask equipped with a strong magnetic stir bar. The reaction was cooled to 0 °C and NaH (39.7g, 990 mmol, 5.0 eq) (60 % in mineral oil) was added in portion carefully. The reaction was continued to stir for 15 min at 0 °C and

then allowed to warm to 25 °C for 1 h and to 60 °C for 1 h. The reaction was cooled to 40 °C and oct-2-yn-1-ol **7** (25.0 g, 198.0 mmol, 1.0 eq) was added dropwise then continued to stir for 1 h under this temperature. Then the reaction was allowed to stir at 60 °C for 1h. After this time, the reaction was cooled to 0 °C and quenched *via* the dropwise addition of H_2O (100 mL) then 2 N HCl (100 mL). Extracted with Et_2O (500 mL) then EtOAc (500 mL). All organic phase was combined and washed with H_2O then brine, dried over Na_2SO_4. Filtered and concentrated. The crude oil was purified by flash column chromatography (Hexanes to Hexanes/ethyl acetate 5:1 to 3:1) to obtain the titled compound **8** (19.2 g, 77 %) as a brown oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.60 (t, *J* = 6.8 Hz, 2H), 2.16 (td, *J* = 7.2, 2.8 Hz, 2H), 1.92 (t, *J* = 2.8 Hz, 1H), 1.84 (s, 1H), 1.56-1.49 (m, 4H), 1.42-1.34 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 84.75, 68.37, 62.91, 32.71, 28.63, 28.52, 25.39, 18.46.

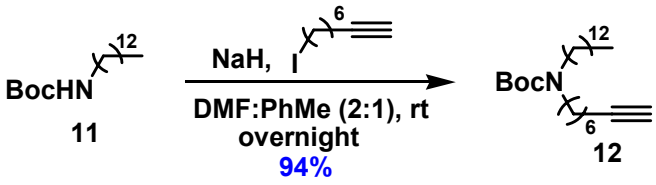


8-Iodooct-1-yne (9)[2]: Under N_2 protection, oct-7-yn-1-ol **8** (15.3g, 121.2 mmol, 1.0 eq) was dissolved in anhydrous dichloromethane (100 mL). Et_3N (33.8 mL, 242.5 mmol, 2.0 eq) followed by MsCl (14.2 mL, 181.9 mmol, 1.5 eq) were added dropwise at 0 °C. The reaction was allowed to warm to room temperature and continued to stir overnight. After this time, volatiles were evaporated under reduced pressure. The residue was added H_2O and EtOAc then extracted with EtOAc. The organic layer was washed with brine then concentrated under reduced pressure. The obtained crude oct-7-ynyl methanesulfonate was dissolved in acetone (250 mL), NaI (90.9g, 606.2 mmol, 5.0 eq) was added at room temperature. The reaction was continued to stir at 60 °C overnight. Then the reaction was cooled down and concentrated, the residue was diluted with EtOAc and H_2O, extracted with EtOAc. All organic phase was combined and washed with $Na_2S_2O_3$ (5%) then brine, dried over Na_2SO_4. Filtered and concentrated. The crude oil was purified by flash column chromatography (Hexanes to Hexanes/ethyl acetate 10:1) to obtain the titled compound **9** (24.8 g, 87 %) as a yellow oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.18 (t, *J* = 7.2 Hz, 2H), 2.18 (td, *J* = 7.2, 2.8 Hz, 2H), 1.94 (t, *J* = 2.8 Hz, 1H), 1.86-1.79 (m, 2H), 1.57-1.49 (m, 2H), 1.46-1.38 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 84.56, 68.52, 33.49, 30.14, 28.35, 27.75, 18.49, 7.24.



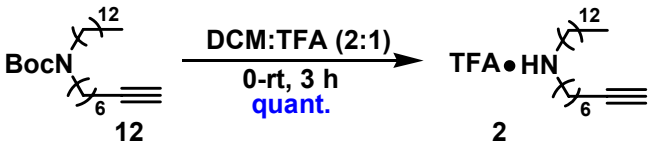
***tert*-Butyl tridecylcarbamate (11):** Tridecylamine **10** (10.0 g, 50.0 mmol, 1.0 eq) was dissovled in dichloromethane (100 mL). Boc_2O (10.9 g, 50.0 mmol, 1.0 eq) was then added in portion at 0 °C. Lots of white precipitate formed immediately. The reaction was allowed to warm to room temperature slowly and continued to stir overnight. Volatiles were evaporated under reduced pressure. The crude oil was purified by flash column chromatography (Hexanes to Hexanes/ethyl acetate 5:1) to obtain the titled compound **11** (14.7 g, 98 %) as a white solid.

^{1}H NMR (300 MHz, $CDCl_3$) δ 4.54 (s, 1H), 3.08 (q, J = 6.6 Hz, 2H), 1.42 (bs, 11H), 1.23 (bs, 20H), 0.86 (t, J = 6.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.23, 79.14, 40.85, 32.14, 30.29, 29.89, 29.87, 29.81, 29.58, 29.53, 28.64, 27.03, 22.91, 14.34; HRMS (ESI) calcd for $C_{18}H_{37}NNaO_2$ (M+Na)+ m/z 322.2717, found 322.2714.



***tert*-Butyl oct-7-ynyltridecylcarbamate (12): 11** (5.5 g, 18.4 mmol, 1.0 eq) was dissovled in anhydrous DMF (22 mL) and anhydrous toluene (11 mL). NaH (1.1 g, 27.6 mmol, 1.5 eq) (60 % in mineral oil) was then added portionwise at 0 °C. The suspension was continued to stir for 1 h under this temperature. Then 8-iodooct-1-yne (5.21g, 22.08 mmol, 1.2 eq) was added at 0 °C dropwise. The reaction was allowed to warm to room temperature and continued stirring overnight. Then the reaction was quenched *via* the dropwise addition of NH_4Cl (aq) at 0 °C. The reaction mixture was diluted with Et_2O, washed with H_2O then Brine, dried over Na_2SO_4. Filtered and concentrated. The crude oil was purified by flash column chromatography (Hexanes to Hexanes/ethyl acetate 20:1 to 10:1) to obtain the titled compound **12** (6.99 g, 94 %) as a slight yellow oil.

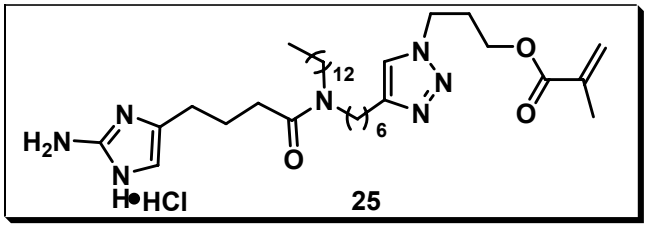
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.10 (bs, 4H), 2.15 (td, J = 6.9, 2.4 Hz, 2H), 1.90 (t, J = 2.4 Hz, 1H), 1.52-1.36 (m, 17H), 1.29-1.22 (m, 22H), 0.84 (t, J = 6.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.75, 84.67, 79.02, 68.34, 47.20, 47.06, 32.08, 29.84, 29.81, 29.76, 29.58, 29.52, 29.47, 28.64, 28.57, 27.06, 26.54, 22.85, 18.48, 14.28; HRMS (ESI) calcd for $C_{26}H_{49}NNaO_2$ (M+Na)+ m/z 430.3656, found 430.3654.



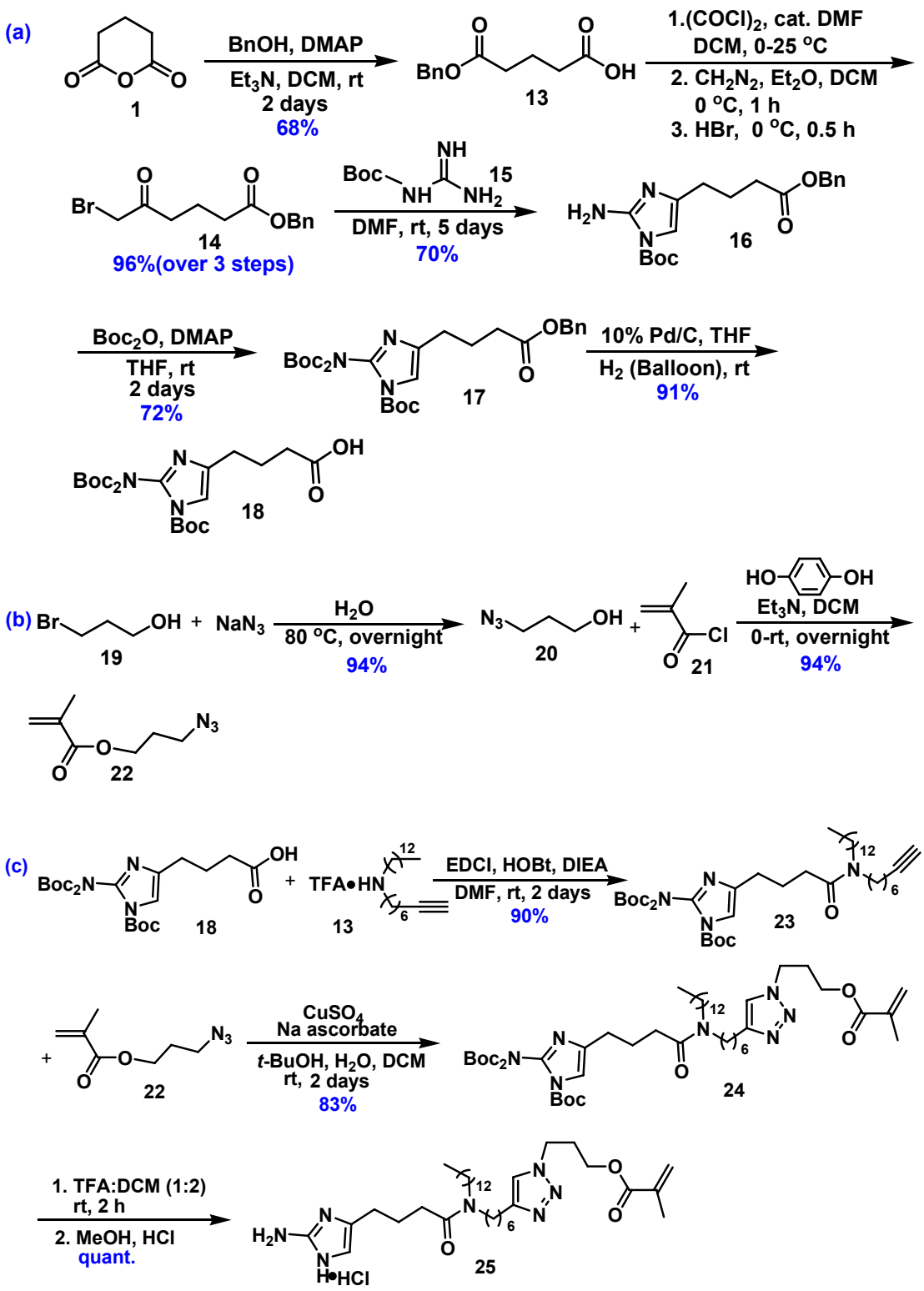
***N*-(Oct-7-ynyl)tridecan-1-amine trifluoroacetate (2): 12** (6.9 g, 17.0 mmol) was dissovled in 20 mL dichloromethane. TFA (10 mL) was then added dropwise at 0 ^{o}C. The reaction was allowed to warm to room temperature slowly and continued to stir for 3 h. Volatiles were evaporated under reduced pressure. The residue was dissolved in 30 mL DCM again and then concentrated, the process was repeated for 3 times to remove excess TFA. The crude solid was purified by flash column chromatography (DCM to DCM/MeOH 20:1 to 10:1) to obtain the titled compound **2** (7.1 g, quant.) as a slight brown solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.93 (bs, 4H), 2.17 (td, *J* = 6.8, 2.4 Hz, 2H), 1.92 (t, *J* = 2.4 Hz, 1H), 1.72-1.60 (m, 4H), 1.54-1.24 (m, 26H), 0.87 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.27, 161.89, 161.51, 161.14, 84.25, 68.69, 48.28, 48.14, 32.13, 29.87, 29.85, 29.81, 29.71, 29.56, 29.21, 28.20, 28.16, 26.72, 26.22, 26.17, 26.03, 22.90, 18.38, 14.32; HRMS (ESI) calcd for $C_{21}H_{42}N$ (M+H)+ m/z 308.3312, found 308.3313.

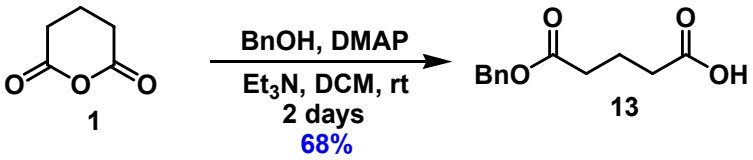
Synthesis of **25**:



We used the following protocol (Scheme 3) to synthesize a relative bigger scale of monomer **25** for the yield to form **4** from **3** is low in the above synthetic route (Scheme 1). And it could get higher yield to do the click reaction from a *tri*-Boc protected 2-aminoimidazole precursor (the reaction of **23** and **22** to form **24**).

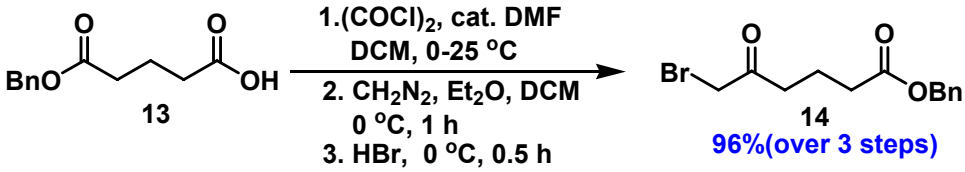


Scheme 3. Synthesis of **25**



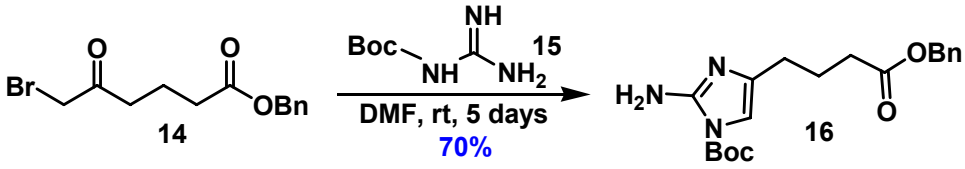
4-((Benzyloxy)carbonyl)butanoic acid (13)[3]: To a 250 mL round-bottomed flask equipped with a magnetic stir bar was added Glutaric anhydride **1** (20.0 g, 175.0 mmol, 1.0 eq), dichloromethane (120 mL) and BnOH (20.0 ml, 192.5 mmol, 1.1 eq). Triethylamine (27.0 ml, 192.5 mmol, 1.1 eq) and then DMAP (320 mg, 2.62 mmol, 0.015 eq) were added at 0 ^{o}C. The stirring solution was allowed to warm to room temperature and continued stirring for two days. Volatiles were evaporated under reduced pressure. The resulting residue was dissolved in Et_2O (150 mL), washed with $NaHCO_3$ (aq) three times (50 mL×3). Acidified the H_2O phase with 1M HCl to PH = 2.0. Then this solution was extracted with Et_2O, washed with Brine, dried over Na_2SO_4. Filtered and concentrated to get **13** (26.6 g, 68 %) as a colorless oil (turned to white solid when stored at 5 ^{o}C), it could be used for the next step without further purification.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.31 (m, 5H), δ 5.11 (s, 2H), 2.46-2.40 (m, 4H), 2.00-1.92 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.49, 173.03, 136.06, 128.84, 128.55, 128.50, 66.63, 33.38, 33.22, 20.00.



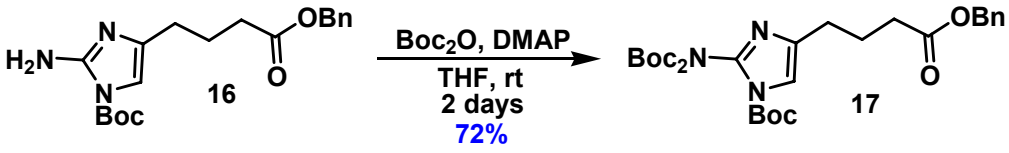
6-Bromo-5-oxo-hexanoic acid benzyl ester (14)[3]: Under N_2 protection, 4-((benzyloxy) carbonyl)butanoic acid **13** (4.0 g, 18.0 mmol, 1.0 eq) was dissolved in anhydrous dichloromethane (30 mL) at 0 ^{o}C and a catalytic amount of DMF (5 drops) was added. To this solution was added oxalyl chloride (4.7mL, 54.0 mmol, 3.0 eq) dropwise. The solution was stirred for 15 min at 0 ^{o}C and was then warmed to room temperature. After 1.5 h, volatiles were evaporated under reduced pressure. The residue was dissolved in 30 mL DCM again and then concentrated, repeated the process for 3 times to remove excess oxalyl chloride. The residue was dried under high vacuum for 2 h. The obtained crude acid chloride was dissolved in anhydrous dichloromethane (20 mL) and added dropwise to a 0 ^{o}C solution of CH_2N_2 (54.0 mmol, 3.0 eq, generated from Diazald®–KOH) in diethyl ether (180 mL). This solution was stirred at 0 ^{o}C for 1.5 h. Then the reaction was quenched *via* the dropwise addition of 48 % HBr (8.2 mL, 4.0 eq) at 0 ^{o}C. Continued to stir 0.5 h, then $NaHCO_3$ (aq) (100 mL) was added at 0 ^{o}C. After 20 min, the reaction mixture was diluted with EtOAc, washed with $NaHCO_3$ (aq) then Brine, dried over Na_2SO_4. Filtered and concentrated. The crude oil was purified by flash column chromatography (Hexanes/ethyl acetate 20:1 to 10:1 to 5:1 to 3:1) to obtain the titled compound **14** (5.14 g, 96 %) as a slight yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.31 (m, 5H), 5.11 (s, 2H), 3.84 (s, 2H), 2.71 (t, *J* = 7.2 Hz, 2H), 2.40 (t, *J* = 7.2 Hz, 2H), 1.98-1.91 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.54, 172.98, 136.11, 128.84, 128.55, 128.51, 66.54, 38.76, 34.45, 33.15, 19.16.



***tert*-Butyl 4-(3-(benzyloxycarbonyl)propyl)-2-amino-imidazole-1-carboxylate (16):** 6-Bromo-5-oxo-hexanoic acid benzyl ester **14** (2.45 g, 8.19 mmol, 1.0 eq) and Boc-guanidine **15** (3.9 g, 24.57 mmol, 3.0 eq) were dissolved in DMF (15 mL) and allowed to stir at room temperature. After 5 days the reaction mixture was diluted with EtOAc (150 mL), washed with H_2O (3×30 mL) and Brine (30 mL), dried over Na_2SO_4. Filtered and concentrated. The crude oil was purified by flash column chromatography (Hexanes/ethyl acetate 2:1 to 1:1 to 1:2) to obtain the titled compound **16** (2.05 g, 70 %) as a yellow oil.

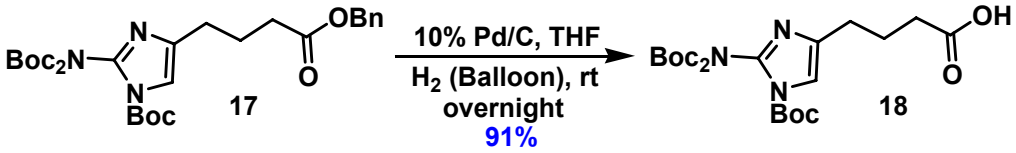
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.31 (m, 5H), 6.50 (s, 1H), 6.04 (s, 2H), 5.10 (s, 2H), 2.41-2.37 (m, 4H), 1.95-1.91 (m, 2H), 1.56 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.58, 150.60, 149.65, 138.18, 136.33, 128.75, 128.40, 128.36, 107.00, 84.72, 66.32, 33.82, 28.20, 27.63, 23.77; HRMS (ESI) calcd for $C_{19}H_{26}N_3O_4$ (M+H)+ m/z 360.1918, found 360.1924.



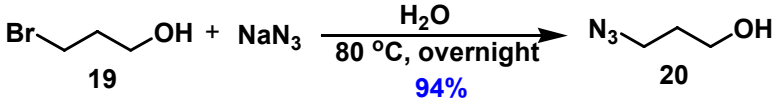
***tert*-Butyl 4-(3-((benzyloxy)carbonyl)propyl)-2-((di-*tert*-butoxycarbonyl)amino) -imidazole-1-carboxylate (17): 16** (2.1 g, 5.84 mmol, 1.0 eq) and DMAP (71 mg, 0.58 mmol, 0.1 eq) were mixed in anhydrous THF (10 mL), Boc_2O (3.82 g, 17.52 mmol, 3.0 eq) was then added in portion. This solution was continued to stir at room temperature for 2 days. After this time, volatiles were evaporated under reduced pressure. The crude oil was purified by flash column chromatography (Hexanes/ethyl acetate 5:1 to 3:1) to obtain the titled compound **17** (2.35 g, 72 %) as an orange oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.28 (m, 5H), 7.06 (s, 1H), 5.06 (s, 1H), 2.53 (t, *J* = 7.2 Hz, 2H), 2.33 (t, *J* = 7.2 Hz, 2H), 1.99-1.94 (m, 2H), 1.53 (s, 9H), 1.35 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.19, 149.45, 146.45, 139.17, 137.82, 136.07, 128.57, 128.22, 114.45, 85.67, 83.36, 66.14, 33.27, 27.90, 27.23, 23.97;

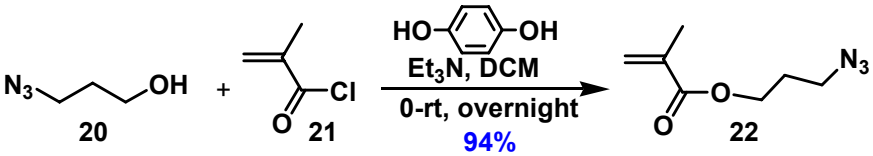
HRMS (ESI) calcd for $C_{29}H_{42}N_3O_8$ (M+H)+ m/z 560.2966, found 560.2972.



4-(1-(*tert*-Butoxycarbonyl)-2-((di-*tert*-butoxycarbonyl)amino)-imidazol-4-yl)butanoic acid (18): 17 (3.7 g, 6.62 mmol, 1.0 eq) and 10 % Pd/C (288 mg, 0.27 mmol, 0.04 eq) were mixed in 25 mL anhydrous THF. Air was removed from the system by water pump and the reaction was back flushed with hydrogen. This process was repeated three times before setting the reaction under a hydrogen balloon at atmospheric pressure. This black suspension was continued to stir overnight under room temperature. After this time the reaction was filtered through a Celite pad and the filter cake was washed with THF (5×20 mL). The filtrate was concentrated under reduced pressure to afford the titled compound **18** (2.8 g, 91 %) as a white solid, it could be used for the next step without further purification.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10 (s, 1H), 5.06 (s, 1H), 2.57 (t, J = 7.2 Hz, 2H), 2.32 (t, J = 7.2 Hz, 2H), 1.98-1.90 (m, 2H), 1.54 (s, 9H), 1.37 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.60, 149.45, 146.45, 139.09, 137.90, 114.60, 85.97, 83.62, 33.17, 27.98, 27.02, 23.96; HRMS (ESI) calcd for $C_{22}H_{36}N_3O_8$ (M+H)+ m/z 470.2497, found 470.2500.

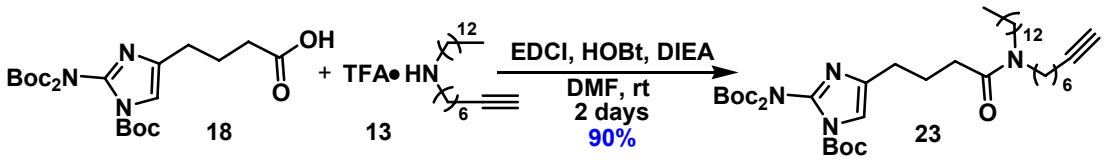


3-Azidopropan-1-ol (20)[4]: 3-bromopropan-1-ol **19** (10.0 g, 72.0 mmol, 1.0 eq) and NaN_3 (11.7 g, 180.0 mmol, 2.5 eq) were mixed in 50 mL H_2O at room temperature. The reaction was continued stirring at 80 °C overnight. Then the reaction was cooled down and extracted with DCM, washed with Brine, dried over Na_2SO_4. Filtered and concentrated to get **20** (6.85 g, 94 %) as a colorless oil, it could be used for the next step without further purification.
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.71-3.66 (m, 2H), 3.40 (t, J = 6.6 Hz, 2H), 2.62 (t, J = 4.2 Hz, 1H), 1.83-1.74 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 59.84, 48.59, 31.62.



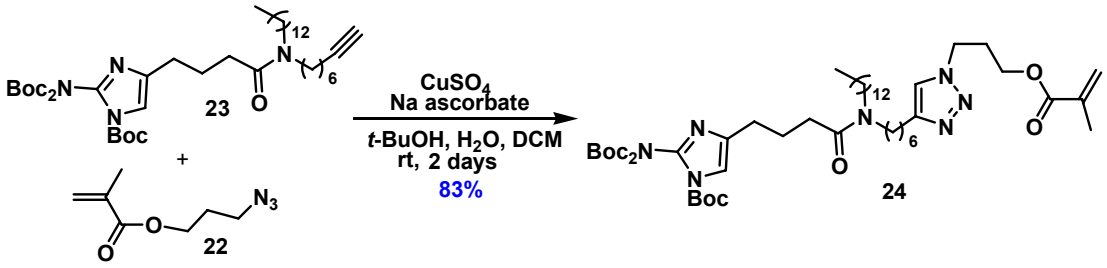
3-Azidopropyl methacrylate (22)[5]: Under N_2 protection, 3-azidopropan-1-ol **20** (3.0 g, 29.7 mmol, 1.0 eq) and hydroquinone (12 mg, 0.4g/mol) were mixed in anhydrous DCM (35 mL). Et_3N (6.2 mL, 44.6 mmol, 1.5 eq) followed by methacryloyl chloride **21** (3.2 mL, 32.7 mmol, 1.1 eq) were then added dropwise at 0 ^oC. The reaction was continued to stir for 1 h under this temperature. Then the reaction was allowed to warm to room temperature and continued stirring overnight (better to wrap the reaction flask with an aluminium foil to avoid light). Then volatiles were evaporated under reduced pressure. The residue was purified by flash column chromatography (Hexanes to Hexanes/ethyl acetate 10:1 to 5:1 to 3:1) to obtain the titled compound **22** (4.68 g, 94 %) as a slight yellow oil. This product was stored with additional hydroquinone (0.4 g/mol).

^1H NMR (400 MHz, $CDCl_3$) δ 6.11-6.10 (m, 1H), 5.58-5.57 (m, 1H), 4.24 (t, J = 6.0 Hz, 2H), 3.41 (t, J = 6.4 Hz, 2H), 2.00-1.94 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.41, 136.35, 125.91, 61.73, 48.46, 28.36, 18.50.

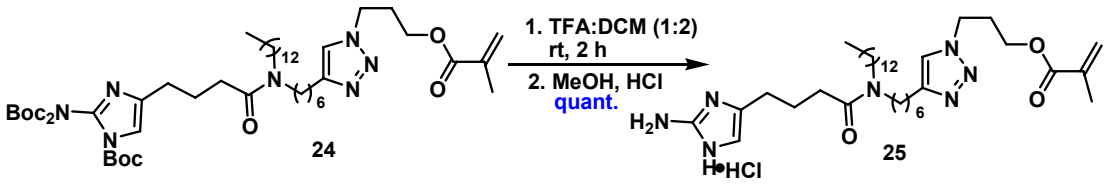


***tert*-Butyl 4-(3-(*N*-(oct-7-ynyl)-*N*-tridecylcarbamoyl)propyl)-2-((di-*tert*-butoxy carbonyl)amino)-imidazole-1-carboxylate (23): 18** (2.0 g, 4.26 mmol, 1.0 eq), EDCI (1.32 g, 8.52 mmol, 2.0 eq), HOBt (1.15 g, 8.52 mmol, 2.0 eq) and diisopropylethylamine (4.45 mL, 25.56 mmol, 6.0 eq) were mixed in anhydrous DMF (16 mL). The reaction was allowed to stir for 15 min at room temperature. Then **13** (2.33 g, 5.54 mmol, 1.3 eq) was added and the solution was continued to stir at room temperature for 2 days. After that time, H_2O (30 mL) and EtOAc (150 mL) were added. The organic layer was successively washed with water (2×30 mL) and brine (30 mL), dried over Na_2SO_4. Filtered and concentrated. The crude oil was purified by flash column chromatography (Hexanes/ethyl acetate 5:1 to 2:1 to 1:1) to obtain the titled compound **23** (2.9 g, 90 %) as an orange oil.

^1H NMR (400 MHz, $CDCl_3$) δ 7.09 (s, 1H), 3.28-3.23 (m, 2H), 3.18-3.13 (m, 2H), 2.54 (t, J = 7.6 Hz, 2H), 2.31 (t, J = 7.6 Hz, 2H), 2.15 (qd, J = 7.2, 2.4 Hz, 2H), 1.99-1.89 (m, 3H), 1.53 (s, 9H), 1.50-1.42 (m, 8H), 1.38 (s, 18H), 1.24-1.20 (m, 22H), 0.84 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.21, 172.16, 149.68, 146.57, 140.03, 137.76, 114.26, 85.59, 84.71, 84.46, 83.42, 68.55, 68.31, 48.12, 47.96, 46.04, 45.94, 32.45, 32.42, 32.05, 29.77, 29.72, 29.55, 29.49, 29.32, 29.17, 28.63, 28.56, 28.52, 28.43, 28.03, 28.00, 27.90, 27.82, 27.24, 27.05, 26.68, 26.53, 24.72, 22.82, 18.46, 18.44, 14.34, 14.26; HRMS (ESI) calcd for $C_{43}H_{75}N_4O_7$ (M+H)+ m/z 759.5630, found 759.5626.



3-(4-(6-(4-(2-(di-*tert*-Butoxycarbonyl)amino-1-(*tert*-butoxycarbonyl)imidazol-4-yl)-*N*-tridecylbutanamido)hexyl)-1*H*-1,2,3-triazol-1-yl)propyl methacrylate (24): **23** (2.7 g, 3.56 mmol, 1.0 eq) and **22** (726.0 mg, 4.27 mmol, 1.2 eq) were mixed in DCM (4 mL), H_2O (8 mL) and *t*-BuOH (8 ml). $CuSO_4$ (85.0 mg, 0.53 mmol, 0.15 eq) and then Na ascorbate (282.0 mg, 1.42 mmol, 0.4 eq) were added. This suspension was continued to stir at room temperature for 2 days (better to wrap the reaction flask with an aluminium foil to avoid light). After this time, H_2O (30 mL) and EtOAc (30 mL) were added. The reaction was extracted with EtOAc, washed with brine, dried over Na_2SO_4. Filtered and concentrated. The crude oil was purified by flash column chromatography (Hexanes/ethyl acetate 1:1 to Ethyl acetate to Ethyl acetate/MeOH 20:1) to obtain the titled compound **24** (2.74 g, 83 %) as a yellow oil. This product was stored with additional hydroquinone (0.4 g/mol).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29, 7.28 (s, s, 1H), 7.09 (s, 1H), 6.07 (s, 1H), 5.56 (s, 1H), 4.40 (td, *J* = 7.2, 2.4 Hz, 2H), 4.16 (t, *J* = 6.0 Hz, 2H), 3.26-3.23 (m, 2H), 3.17-3.12 (m, 2H), 2.69-2.64 (m, 2H), 2.54 (t, *J* = 7.2 Hz, 2H), 2.33-2.26 (m, 4H), 1.97-1.91 (m, 5H), 1.66-1.59 (m, 2H), 1.53 (m, 9H), 1.51-1.44 (,m, 4H), 1.37 (s, 18H), 1.32-1.21 (m, 24H), 0.84 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.20, 172.16, 167.27, 149.68, 148.53, 148.31, 146.56, 140.03, 140.01, 137.76, 136.10, 126.12, 120.99, 120.97, 114.26, 85.61, 83.44, 61.40, 61.37, 48.10, 48.01, 47.15, 46.03, 45.95, 32.48, 32.40, 32.04, 29.76, 29.72, 29.70, 29.64, 29.60, 29.55, 29.48, 29.31, 29.24, 29.18, 29.11, 28.02, 27.99, 27.88, 27.81, 27.23, 27.05, 26.93, 26.86, 25.70, 25.67, 24.76, 24.67, 22.81, 18.44, 14.26; HRMS (ESI) calcd for $C_{50}H_{86}N_7O_9$ (M+H)+ m/z 928.6482, found 928.6489.

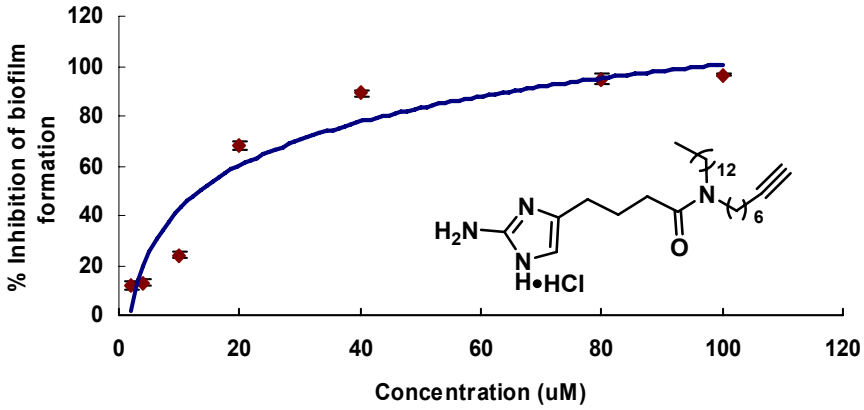


3-(4-(6-(4-(2-Amino-imidazol-4-yl)-*N*-tridecylbutanamido)hexyl)-1*H*-1,2,3-triazol-1-yl)propyl methacrylate hydrochloride (25): **24** (2.08 g, 2.24 mmol) was dissolved in 20 mL anhydrous DCM, TFA (10 mL) was then added dropwise and the reaction was stirred for 2 h at room temperature. After this time, the reaction was evaporated to dryness and DCM (20 mL) was added. Again the mixture was concentrated and the process was repeated for 3 times. The resulting residue was dried

under high vacuum for 2 h. The obtained TFA salt was dissolved in methanol (20 mL), and 0.6 mL of HCl (conc.) was added. This solution was evaporated to dryness directly. The residue was dissolved in methanol (20 mL) and filtered to remove any precipitate by syringe filter (13 mm Diameter, 0.2 μm Pore Size, catalog No. 6788-1302, Whatman Inc.). Then concentrated and dried under high vacuum to yield the titled compound **25** (1.49 g, quant.) as a slight brown solid.
^{1}H NMR (400 MHz, CD_3OD) δ 8.63, 8.62 (s, s, 1H), 6.53 (d, *J* = 2.8 Hz, 1H), 6.04 (s, 1H), 5.64 (s, 1H), 4.76 (t, *J* = 6.0 Hz, 2H), 4.25 (t, *J* = 6.0 Hz, 2H), 3.34-3.30 (m, 4H), 2.93-2.87 (m, 2H), 2.55 (t, *J* = 7.2 Hz, 2H), 2.48-2.40 (m, 4H), 1.91-1.84 (m, 5H), 1.82-1.72 (m, 2H), 1.66-1.50 (m, 4H), 1.50-1.28 (m, 24H), 0.89 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CD_3OD) δ 174.54, 168.46, 148.65, 145.92, 137.59, 128.50, 126.68, 116.92, 110.11, 62.58, 52.12, 52.07, 47.60, 47.36, 33.22, 32.92, 30.94, 30.91, 30.86, 30.62, 30.18, 30.04, 29.91, 29.73, 29.61, 29.28, 29.17, 28.83, 28.55, 28.21, 28.03, 27.60, 25.45, 25.36, 25.12, 24.23, 24.20, 23.88, 18.56, 14.60; HRMS (ESI) calcd for $C_{35}H_{62}N_7O_3$ (M+H)+ m/z 628.4909, found 628.4904.

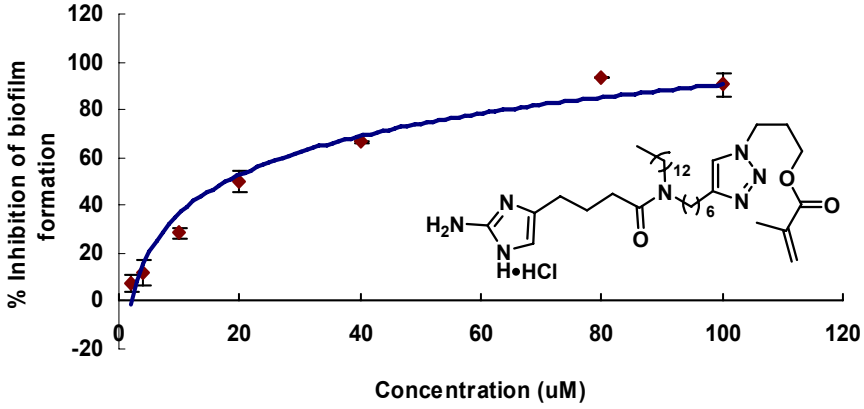
General Procedure to Determine the Inhibitory Effect of Test Small Compounds On *Acinetobacter baumannii* Biofilm Formation: An overnight culture of *A. baumannii* (ATCC # 19606) was subcultured at an OD_{600} of 0.01 into LB media along with a predetermined concentration of the small molecule to be tested for biofilm inhibition. Samples were then aliquoted (100 μL for each well) into the wells of a 96-well PVC microtiter plate. Sample plates were then wrapped in GLAD Press'n Seal® followed by incubation under stationary conditions for 24 h at 37 °C. After incubation, the media was discarded from the wells and the plates were rinsed thoroughly with water. The wells were then stained with a 0.1% aqueous solution of crystal violet (110 μL for each well) and incubated at ambient temperature for 30 min. The wells were rinsed thoroughly with water again and the remaining stain was solubilized with 95 % ethanol (200 μL for each well). A sample of 125 μL of solubilized CV stain from each well was transferred to the corresponding wells of a polystyrene microtiter dish. Biofilm inhibition was quantitated by measuring the OD_{540} of each well in which a negative control lane wherein no biofilm was formed served as a background and was subtracted out.

A. baumannii



IC_{50} = 13.4 ± 0.8 µM

A. baumannii



IC_{50} = 16.5 ± 0.6 µM

General Procedure to Determine the Inhibitory Effect of Test Polymer Strips On *Acinetobacter baumannii* Biofilm Formation: An overnight culture of *A. baumannii* (ATCC # 19606) was subcultured at an OD_{600} of 0.01 into LB media. The resulting bacterial suspension was then aliquoted (600 µL) into culture tubes. Blank polymer strips (20 mm × 8 mm) and 4 % sample polymer strips (20 mm × 8 mm) were added separately, one strip in one tube. All strips were soaked in corresponding solvent (2 mL for each strip) for 24 h at ambient temperature before use. When the soaked solvent was Hexane or MeOH, strips were dried under high vacuum overnight after the soak. Samples were then placed in an incubator for 24 h at 37 °C and shaken at 200 rpm. After incubation, the strips were taken out by a tweezers and rinsed carefully with water there times. The stips were then stained with a 0.1 % aqueous solution of crystal violet (1 mL for each strip) in culture tube and incubated at ambient

temperature for 30 min. Strips were rinsed carefully with water again and the remaining stain was solubilized with 95% ethanol (1.5 mL for each strip) in culture tube. A sample of 125 μL×8 of solubilized CV stain from each tube was transferred to the corresponding wells of a polystyrene microtiter dish. Biofilm inhibition was quantitated by measuring the OD_{540} of each well in which a lane of 95 % ethanol was served as a background and was subtracted out.

Scanning Electron Microscope: One blank polymer strip and one 4 % sample polymer strip (20 mm × 8 mm, both strips were soaked in distilled H_2O for 24 h at ambient temperature before use, 2 mL for each strip) were grown *A. baumannii* biofilm by the above procedure. Then strips were carefully rinsed three times with phosphate-buffered saline (PBS), and the cells were fixed with 2.5 % (vol/vol) glutaraldehyde solution in phosphate-buffered saline (PBS) at room temperature for 1 h. This was followed by a series of sequential ethanol dehydration steps (30%, 50%, 70%, 95% and 100% ethanol, 2mL solvent for each strip and 5-10 min for each step). Samples were dried under high vacuum overnight. The samples were examined using a JEOL 6400F Field Emission SEM with the aid of the North Carolina State University Analytical Instrumentation Facility.

Red Blood Cell Hemolysis Assay: Hemolysis assays were performed on mechanically difibrinated sheep blood (Hemostat Labs: DSB100). 1.5 mL of blood was placed into a microcentrifuge tube and centrifuged at 10,000 rpm for ten minutes. The supernate was removed and then the cells were resuspended with 1 mL of phosphate-buffered saline (PBS). The suspension was centrifuged, the supernate was removed and cells resuspended two more times. The final cell suspension was diluted twentyfold with PBS. The twentyfold suspension dilution was then aliquoted (1 mL) into 4 culture tubes. One culture tube was added one blank polymer strip (20 mm × 8 mm) and one culture tube was added one 4% sample polymer strip (20 mm × 8 mm). Both strips were soaked in distilled H_2O (2 mL for each strip) for 24 h at ambient temperature before use. One culture tube was added 1%v Triton®-X-100 which was used as a positive control and the 100% lysis marker. The last culture tube with the blood PBS solution only was employed as a negative control and as a zero hemolysis marker. Samples were then placed in an incubator at 37 ◦C and shaken at 200 rpm. After 1 hour, the samples were transferred to microcentrifuge tubes and then centrifuged at 10000 rpm for ten minutes. The resulting supernate was diluted by a factor of 40 in distilled water. The absorbance of the supernate was measured with a UV spectrometer at a 540 nm wavelength.

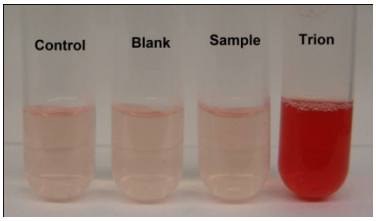


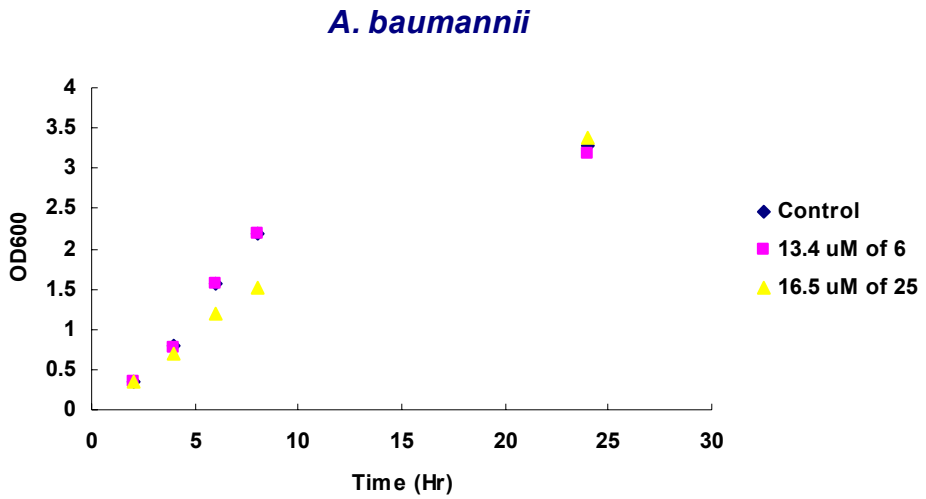
Fig. 1. The final resulting supernate for UV spectrometer reading
Blank: Supernate after incubation with blank strip
Sample: Supernate after incubation with sample strip

Table 1. The absorbance data (dilute by 40) of all supernate measured with a UV spectrometer at a 540 nm wavelength.

$OD_{540}/40$	Control	Blank	Sample	Trion
1	0.025	0.025	0.022	0.095
2	0.028	0.024	0.021	0.096

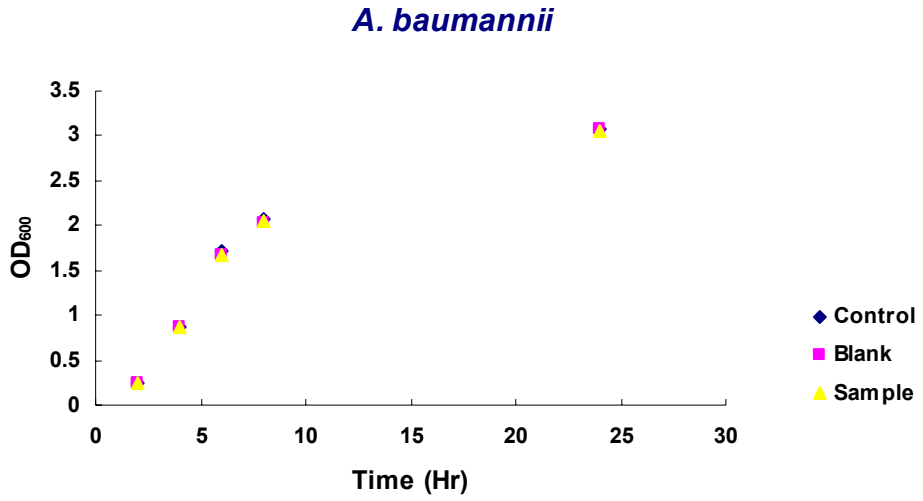
0% lysis for both blank strip and sample strip

Procedure to Determine the Effect of Compound 6 and 25 on *Acinetobacter baumannii* via Growth Curve Analysis: An overnight culture of *A. baumannii* (ATCC # 19606) was subcultured at an OD_{600} of 0.01 into LB media. The resulting bacterial suspension was then aliquoted (3.0 mL) into 3 culture tubes. One culture tube was added 13.4 μM of **6**, one culture tube was added 16.5 μM of **25**. The last culture tube was employed as control in which no compound was added. Samples were then placed in an incubator at 37 °C and shaken at 200 rpm. The OD_{600} of all samples was measured after 2 hours, 4 hours, 6 hours, 8 hours and 24 hours.



Procedure to Determine the Effect of Test Polymer Strips on *Acinetobacter baumannii* via Growth Curve Analysis: An overnight culture of *A. baumannii*

(ATCC # 19606) was subcultured at an OD_{600} of 0.01 into LB media. The resulting bacterial suspension was then aliquoted (3.0 mL) into 3 culture tubes. One culture tube was added one blank polymer strip (20 mm × 8 mm), one culture tube was added one 4% sample polymer strip (20 mm × 8 mm). Both strips were soaked in distilled H_2O (2 mL for each strip) for 24 h at ambient temperature before use. The last culture tube was employed as control in which no strip was added. Samples were then placed in an incubator at 37 °C and shaken at 200 rpm. The OD_{600} of all samples was measured after 2 hours, 4 hours, 6 hours, 8 hours and 24 hours.



Results of Leaching experiments:

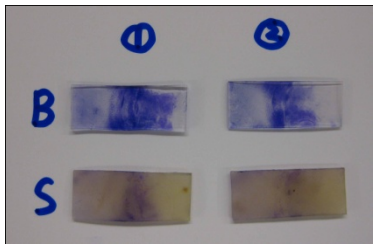


Fig. 2. Polymer strips after *Acinetobacter baumannii* biofilm formation assay. All strips were soaked with DI-H_2O for 2 weeks before use. B = control polymer, S = polymer was incorporated with 4% of **25**. Inhibition: 74%.

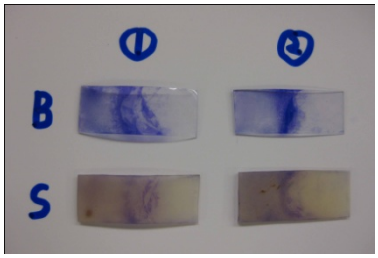


Fig. 3. Polymer strips after *Acinetobacter baumannii* biofilm formation assay. All strips were soaked with Hexane for 24 h before use. B = control polymer, S = polymer was incorporated with 4% of **25**. Inhibition: 80%

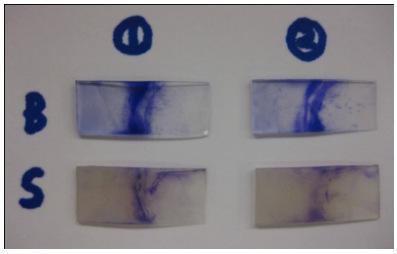


Fig. 4. Polymer strips after *Acinetobacter baumannii* biofilm formation assay. All strips were soaked with MeOH for 24 h before use. B = control polymer, S = polymer was incorporated with 4% of **25**. Inhibition: 72%.

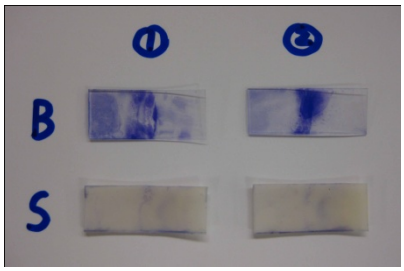


Fig. 5. Polymer strips after *Acinetobacter baumannii* biofilm formation assay. All strips were soaked with DI-H_2O for 24 h before use. B = control polymer, S = polymer was incorporated with 4% of **6**. Inhibition: 83%.

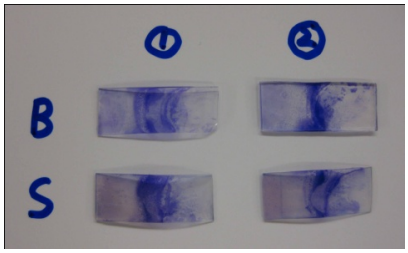
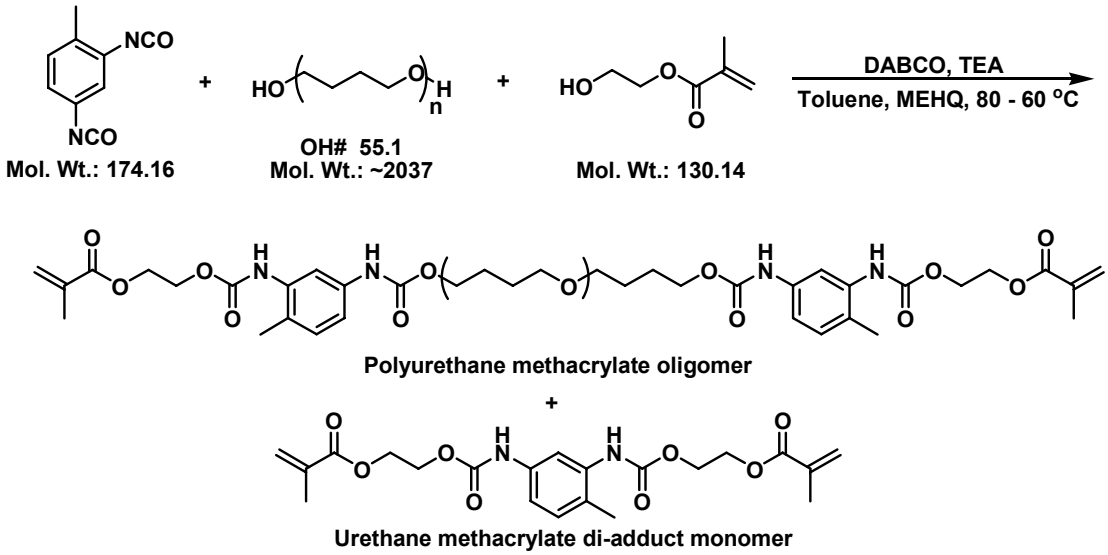


Fig. 6. Polymer strips after *Acinetobacter baumannii* biofilm formation assay. All strips were soaked with MeOH for 24 h before use. B = control polymer, S = polymer was incorporated with 4% of **6**. Inhibition: -6%

Polyurethane Methacrylate Oligomer Cross-linking Synthesis:

All reagents were purchased from Sigma Aldrich Inc. and were used without further purification. Infrared Spectra were collected from a Jasco FT/IR 410 Fourier Transform Infrared Spectrophotometer using KBr salt plates for liquid samples and KBr pellet for the powder samples. X-ray Photoelectron Spectra were collected using Riber XPS with the aid of the North Carolina State University Analytical Instrumentation Facility.



Scheme 4. Polyurethane methacrylate oligomer synthesis

Polyurethane Methacrylate Oligomer (PUMA): Prior to starting reaction poly(tetrahydrofuran) polyether polyol was placed in an 80 °C oven for two hours to facilitate use. To a clean, dry 250 mL three neck round bottom flask, 50 mL toluene was added with a magnetic stir bar, fitted thermometer, and placed over an oil bath. The reaction vessel was connected to a nitrogen stream and to the solution 10.0 mL (12.1 g, 69.5 mmol, 2.2 eq.) of 2,4-toluene diisocyanate was added via a syringe. In one addition 64.3 g (31.6 mmol, 1 eq.) of melted poly(tetrahydrofuran) polyether polyol is added to reaction mixture in one addition. The reaction solution was heated to 80 °C; once the reaction temperature reached 60 °C, 86 mg (1000 ppm based on the polyol) of 1,4-diazabicyclo[2.2.2]octane (DABCO) was added to catalyze the reaction, this resulted an immediate increase in temperature to 80 °C. Following two hours at 80 °C, the solution was air cooled to 60 °C and the remaining reagents were added; 9.9 g (75.8 mmol, 1.2 eq.) of 2-hydroxyethyl methacrylate and 43 mg (500 ppm based on the oligomer) 4-methoxyphenol. The reaction was kept at 60 °C and covered with aluminum foil to block ambient light for an additional 8 hours. Toluene was removed via reduced pressure evaporation followed by 2 hours under high vacuum. Yield: 86 g of a yellow, viscous liquid, quantitative yield. FTIR (thinfilm): 3301.5, 3023.8, 2940.9, 2858.0, 2796.3, 1727.9, 1621.8, 1602.6, 1535.1, 1226.5, 1110.8 cm^{-1}.

Table 2. UV polymerization of formulations.

	Bio-assay polymer films	
	Control (wt. %) **Form. A**	Sample (wt. %) **Form. B**
Methacrylic oligomer	59	59
Isobornyl methacrylate	39	35
25	-	4
Photoinitiator	2	2

Photoinitiator: 4-(2-hydroxyethoxy)phenyl-(2-hydroxy-2-propyl)ketone

Polymerization procedure: The polymer films were prepared by thoroughly mixing the components in a 20 mL vial followed by degassing under vacuum for two hours. Once degassed, formulation was poured on clean aluminum foil attached to the bottom of an inverted, glass Petri dish. A second clean, glass Petri dish wish placed on top of the viscous formulation to form a laminated film. The set up was placed under a 450 W, submersion broad-spectrum UV lamp for 6 minutes for photo-polymerization. The polymerized film was removed by peeling the aluminum foil from one side followed by removing the film from the glass.

X-ray Photoelectron Spectroscopy:
Sample preparation: polymer films were soaked in deionized water for 24 hours at ambient temperature followed by drying under high vacuum prior to experiment.

Table 3. XPS data for **Form. A** and **Form. B**.

	% Oxygen (1s)	% Carbon (1s)	% Nitrogen (1s)	% Chlorine (2p)
Form. A	24.1	74.4	1.4	~ 0.0
Form. B	18.9	72.9	7.5	0.7

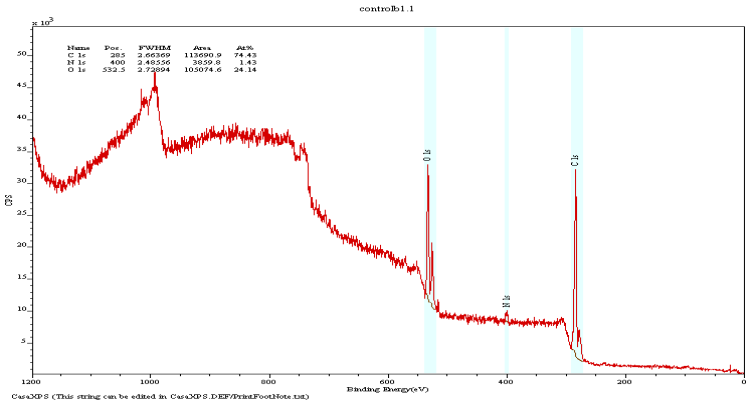


Fig. 7. XPS of Formulation A

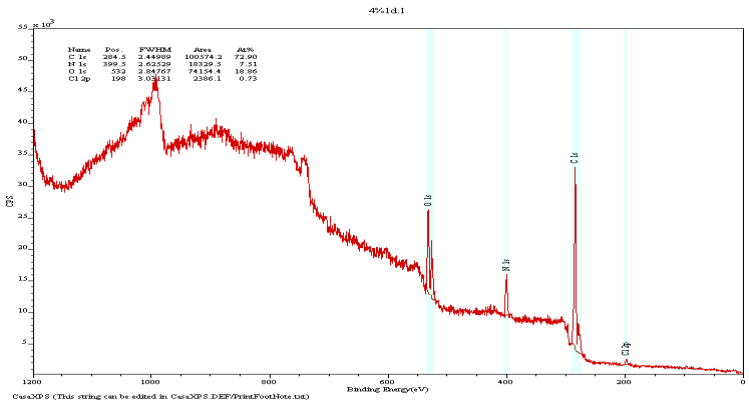
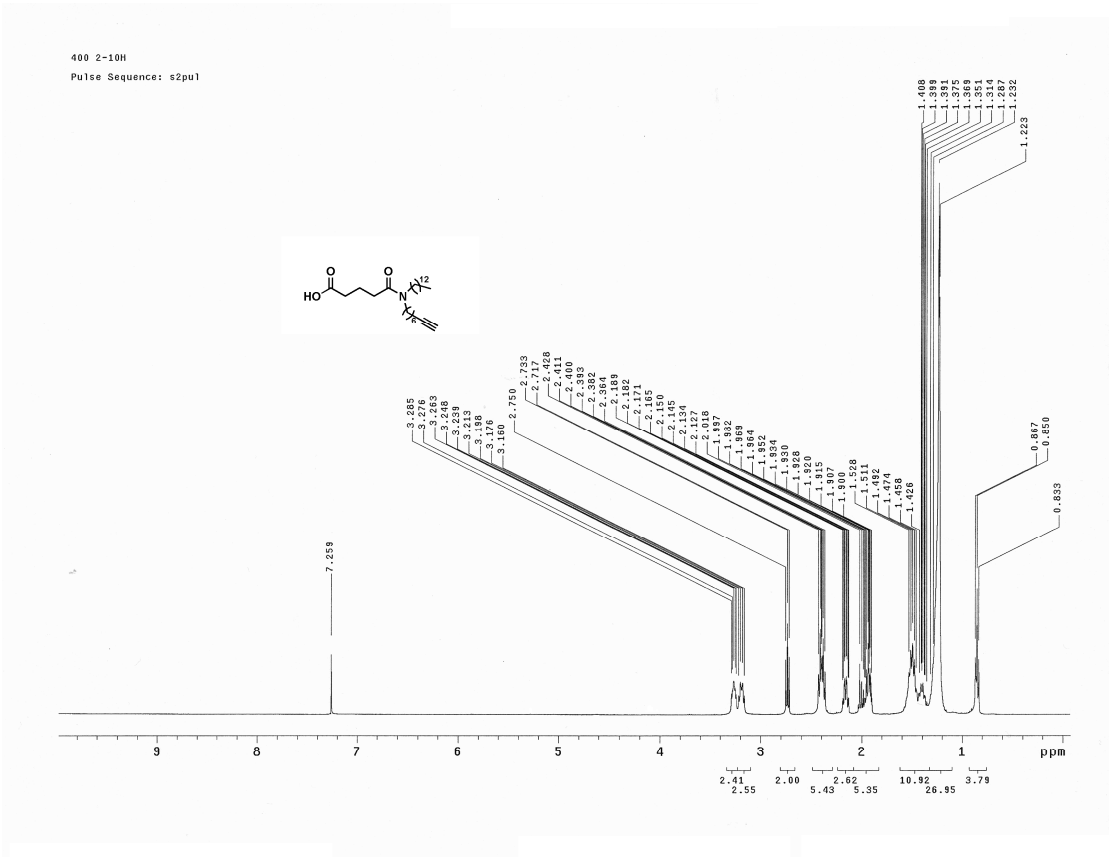
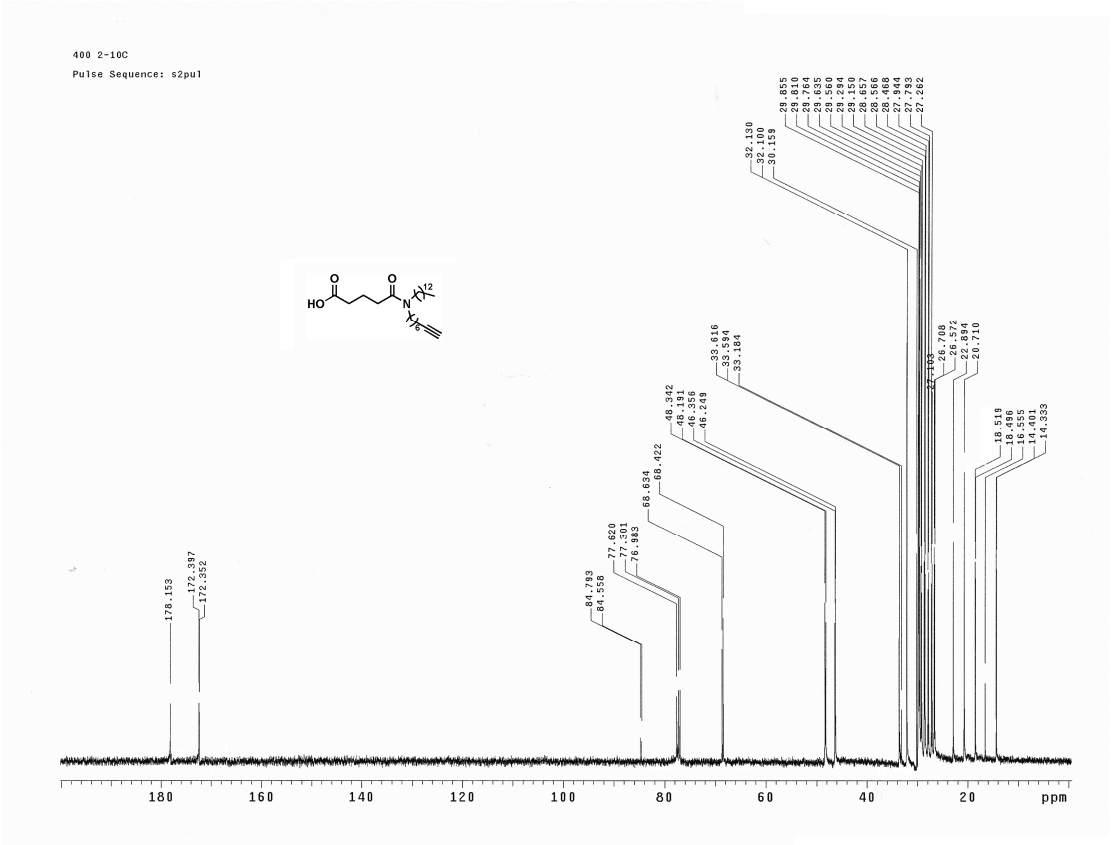


Fig. 8. XPS of Formulation B

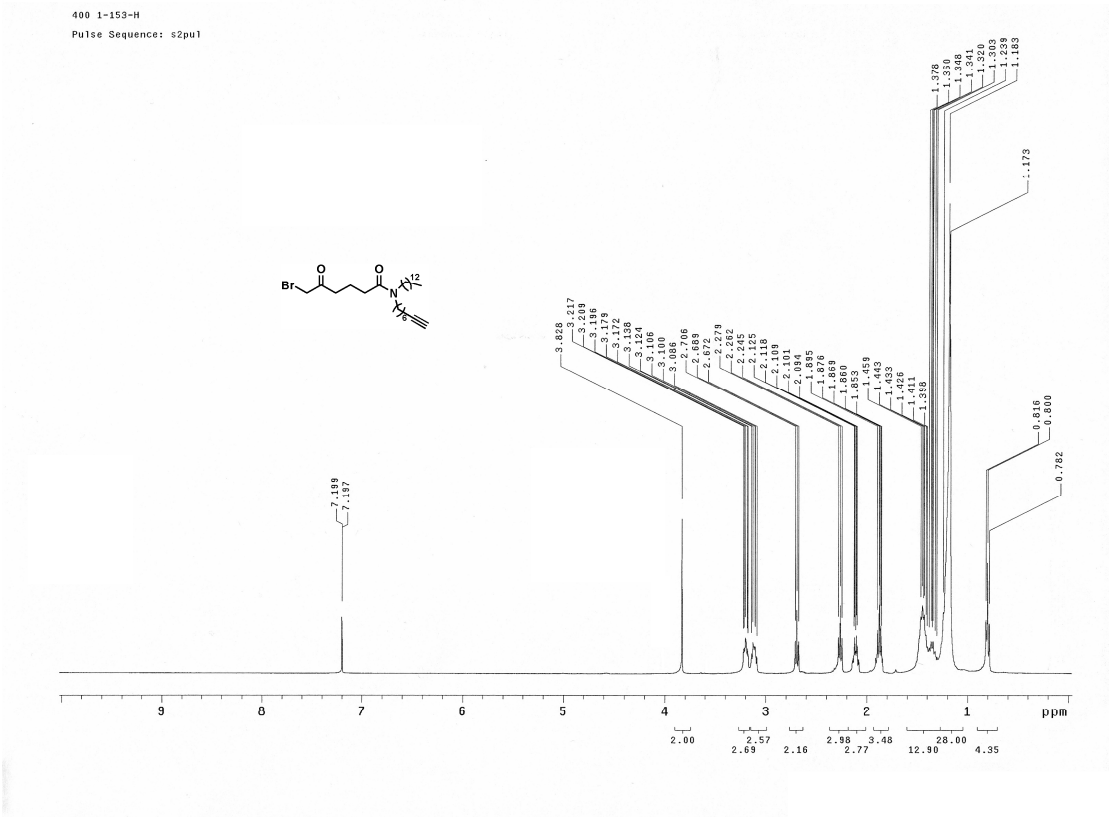
NMR Spectra:

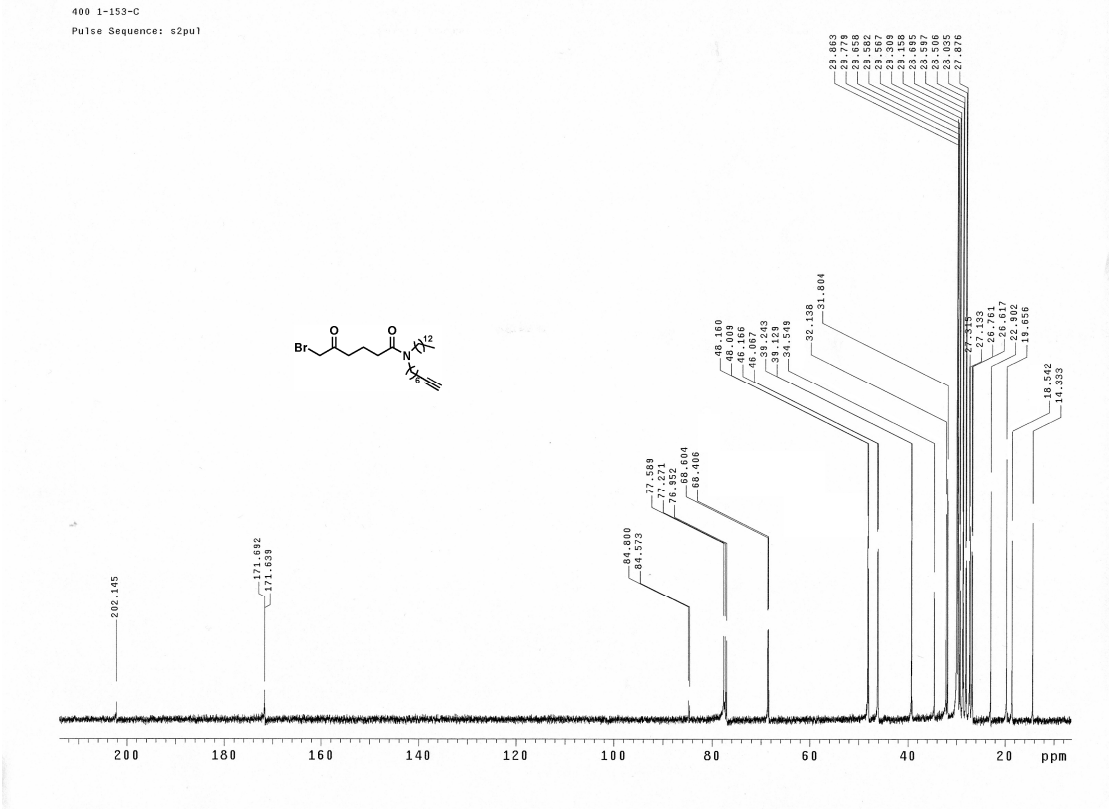
4-(*N*-(oct-7-ynyl)-*N*-tridecylcarbamoyl)butanoic acid (3)



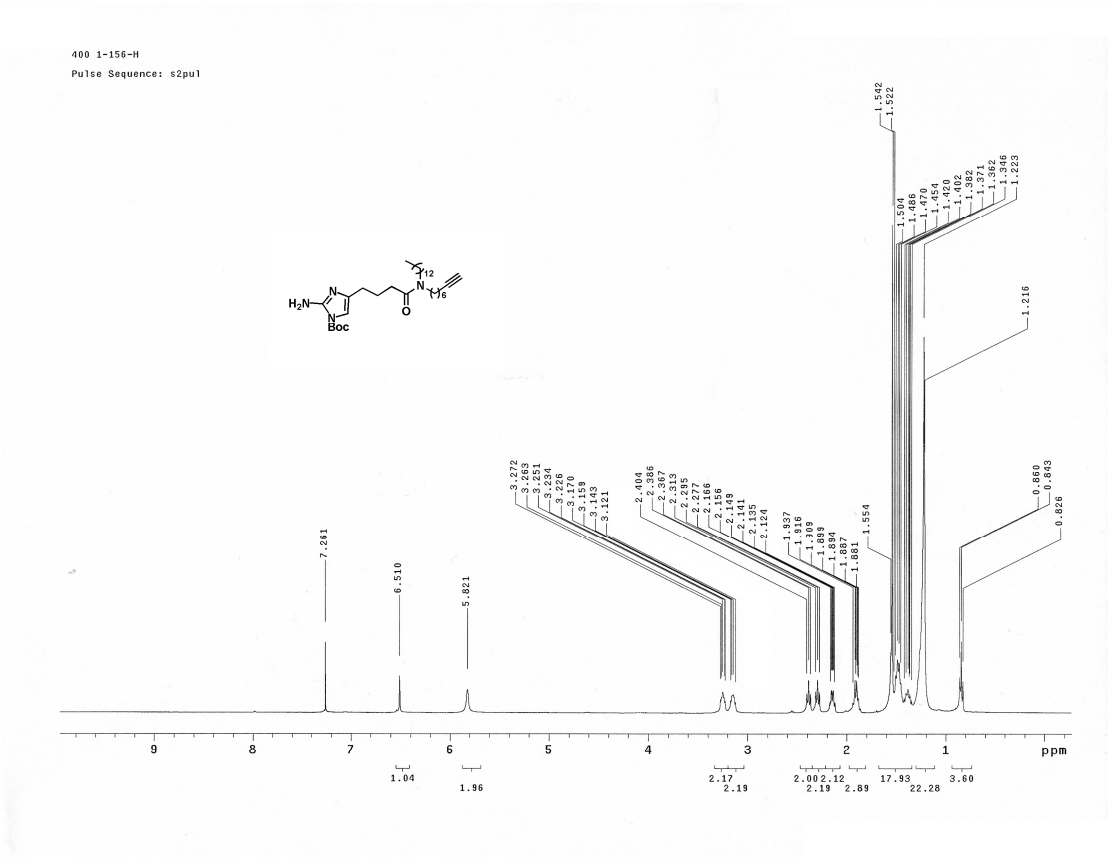


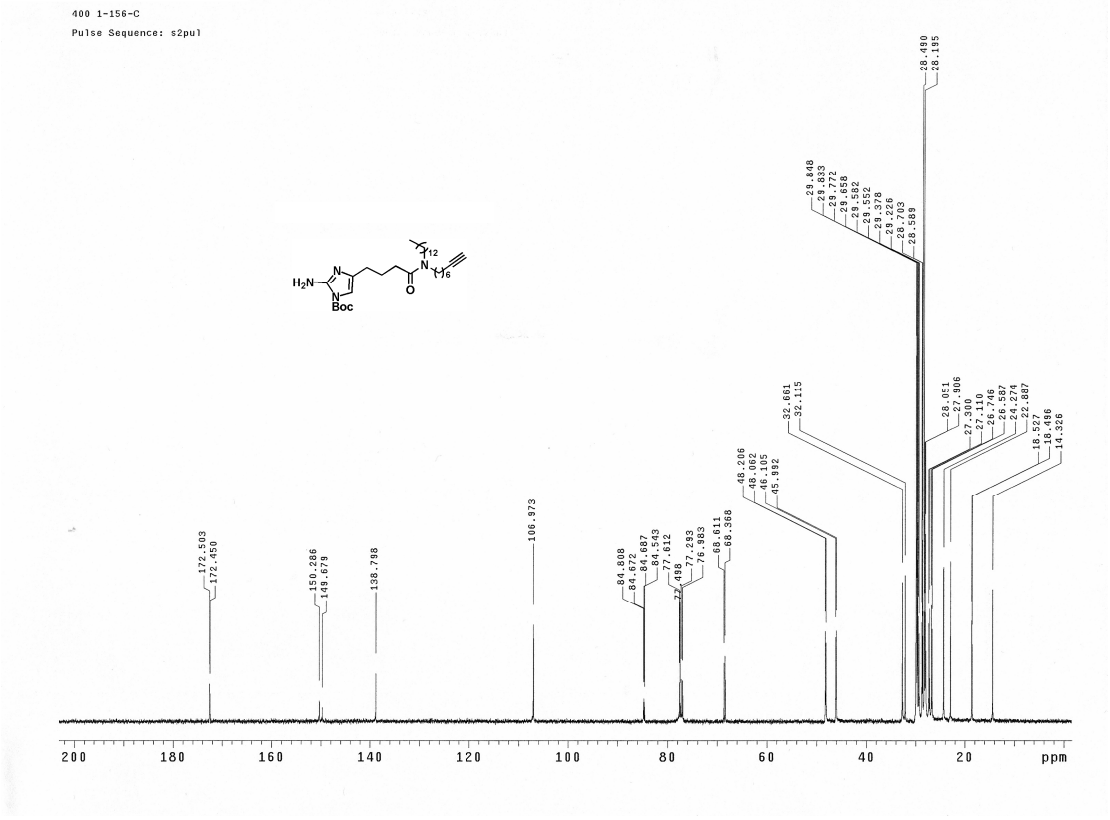
6-Bromo-*N*-(oct-7-ynyl)-5-oxo-*N*-tridecylhexanamide (4)



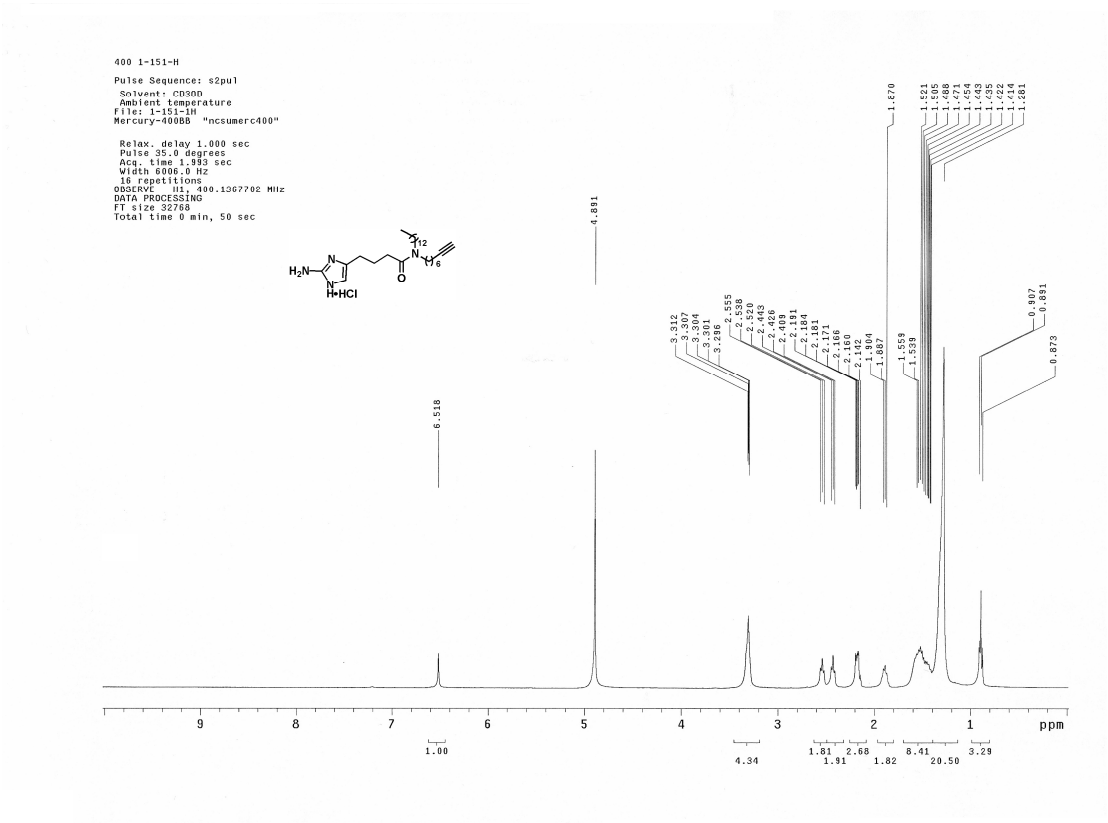


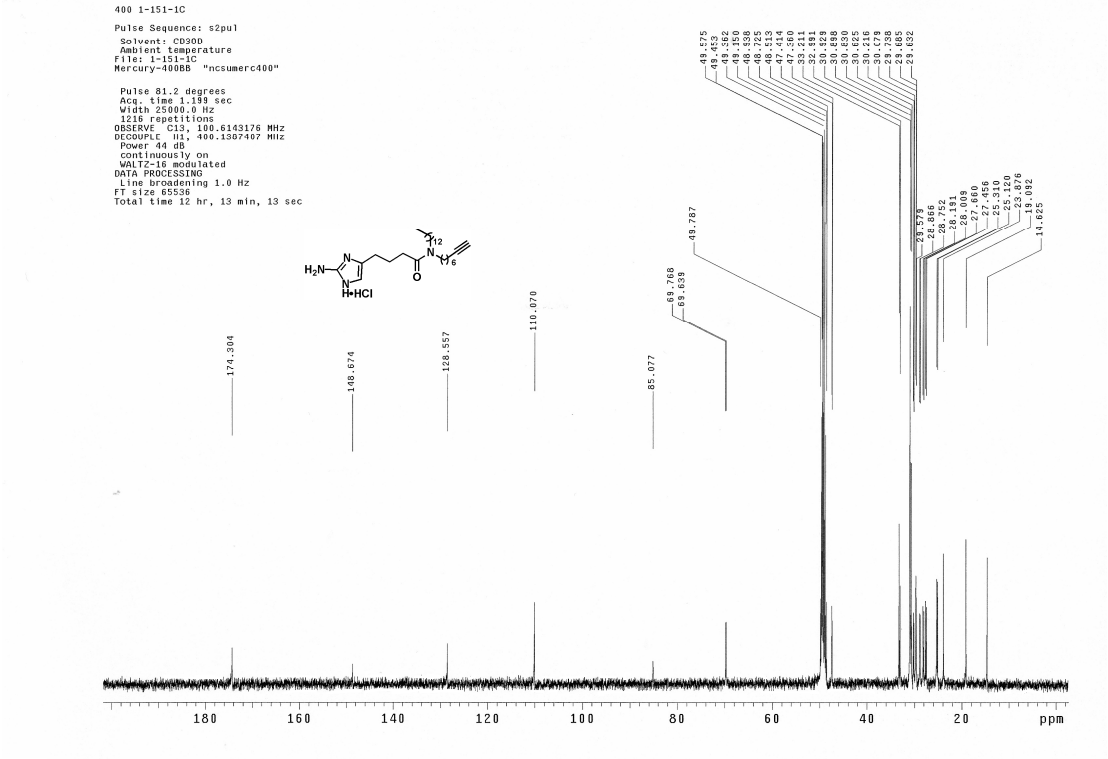
tert-Butyl 4-(3-(*N*-(oct-7-ynyl)-*N*-tridecylcarbamoyl)propyl)-2-amino-imidazole -1-carboxylate (5)



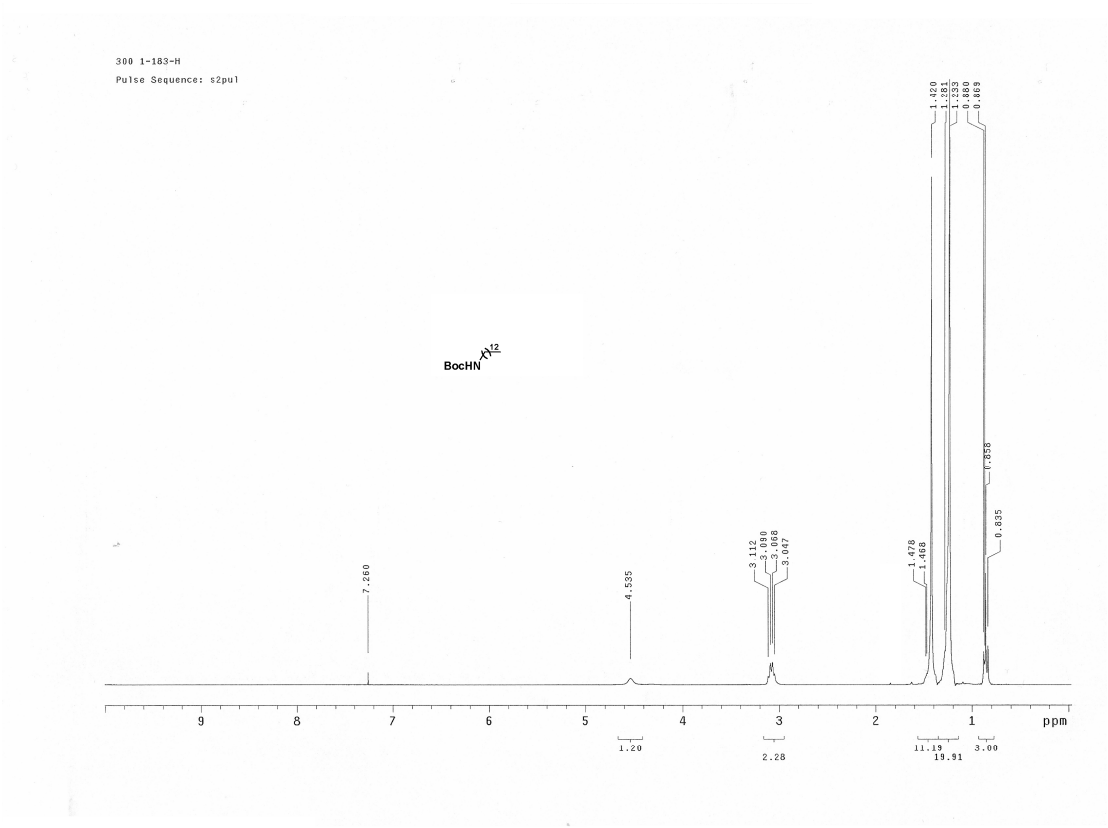


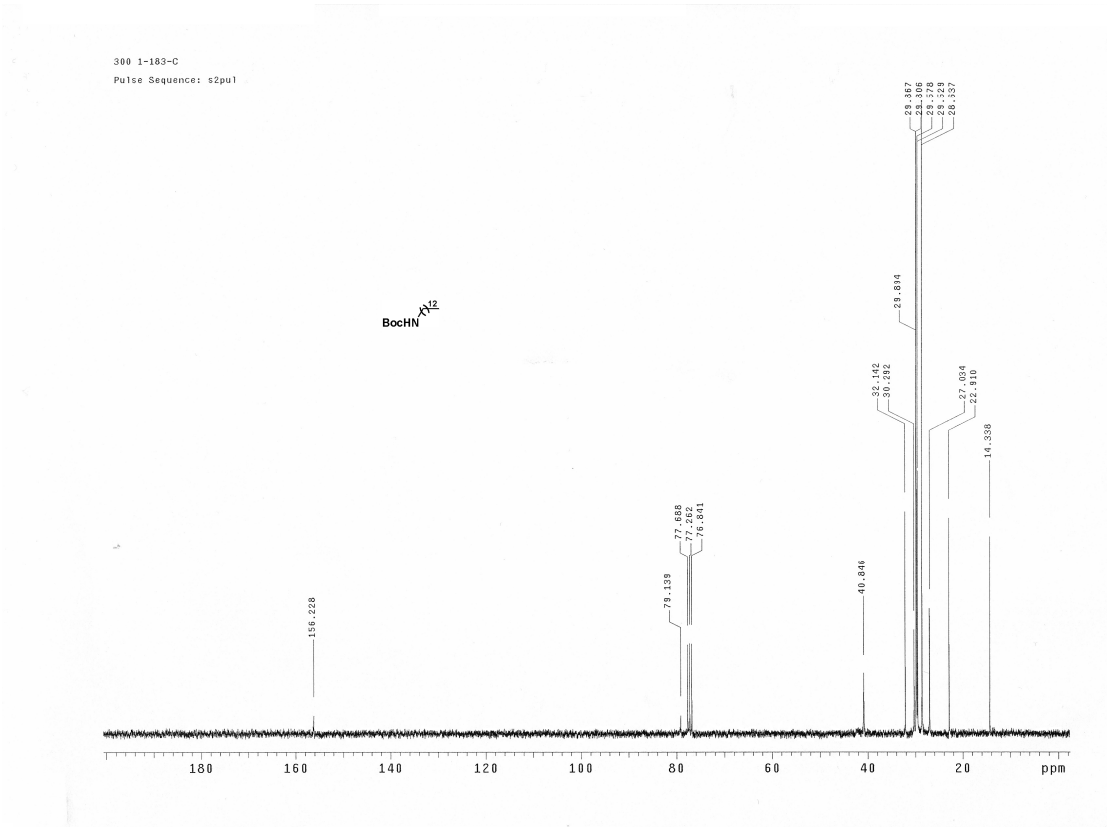
4-(2-Amino-imidazol-4-yl)-*N*-(oct-7-ynyl)-*N*-tridecylbutanamide hydrochloride (6)



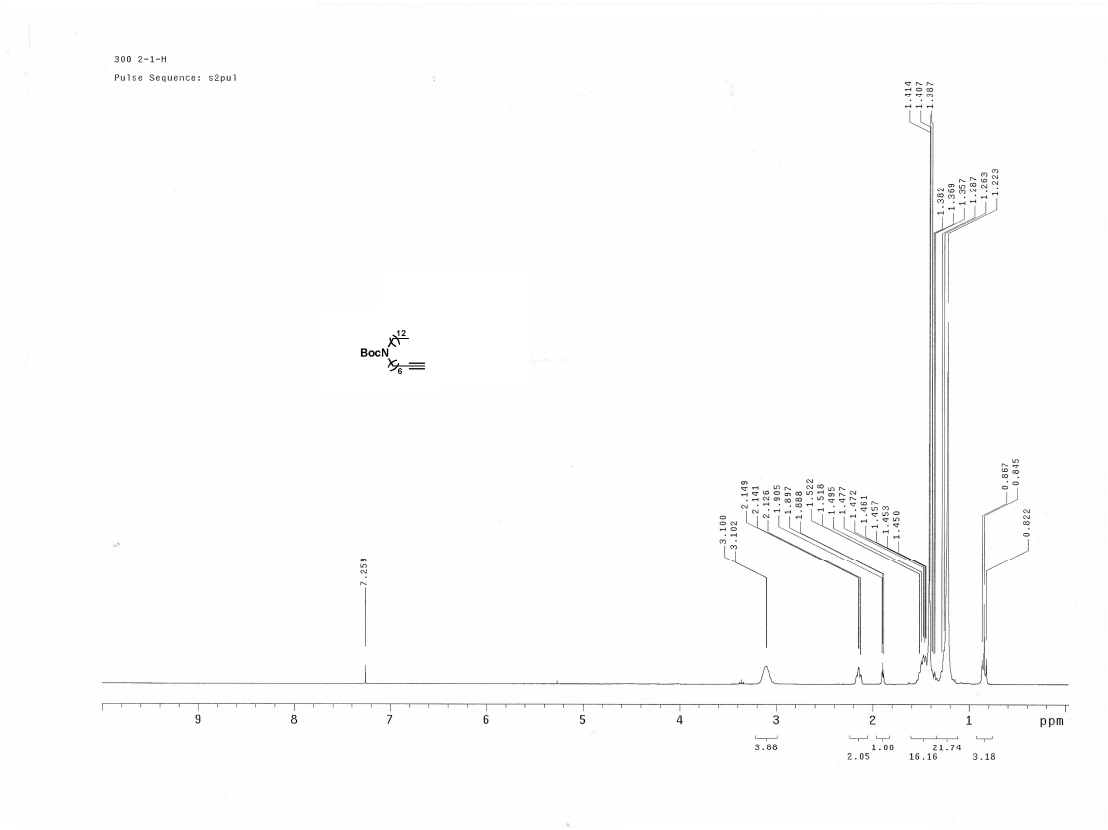


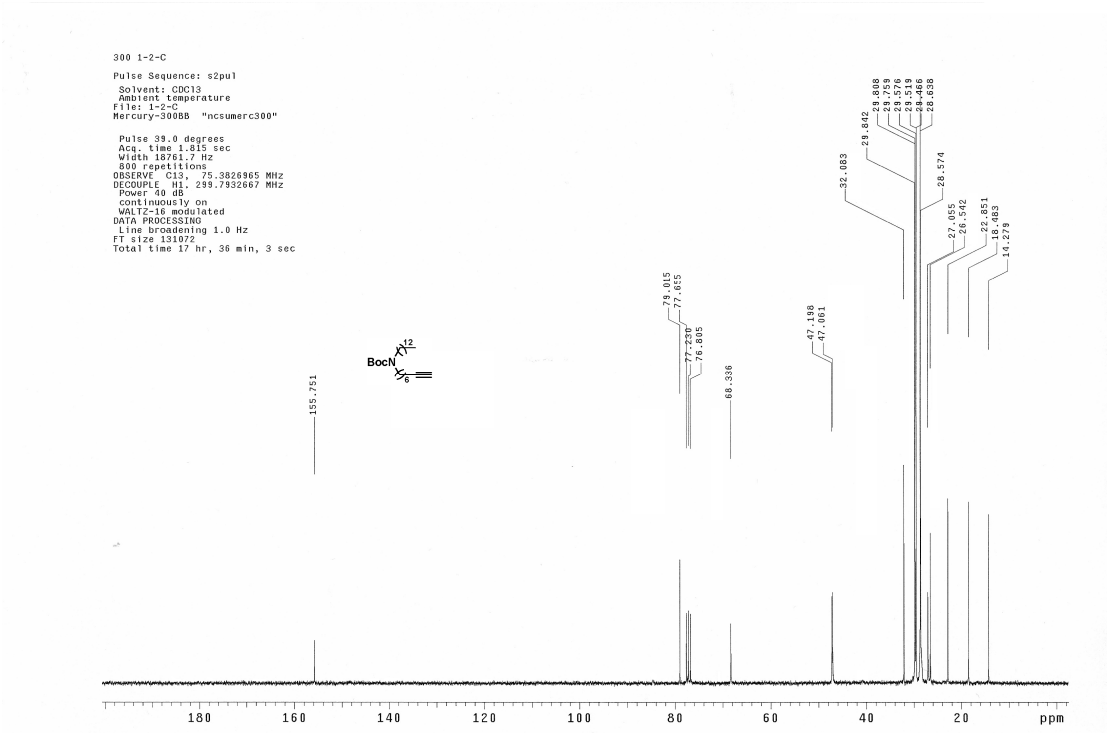
tert-Butyl tridecylcarbamate (11)



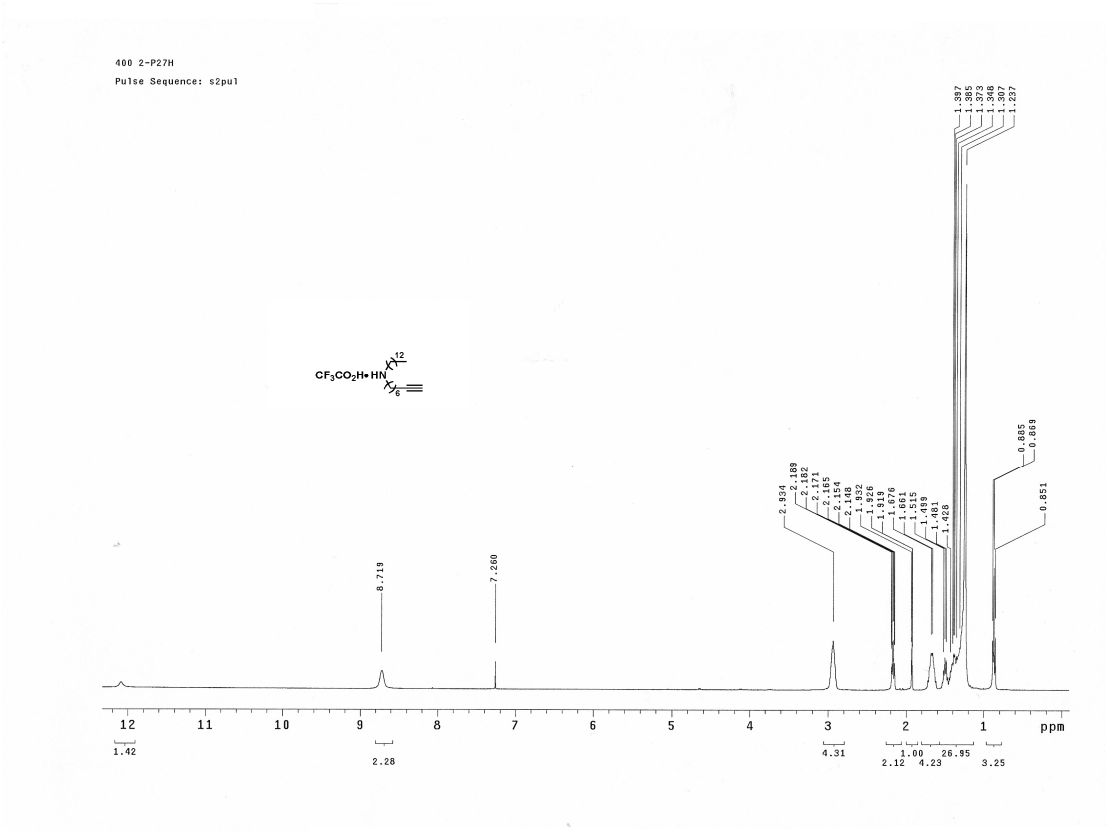


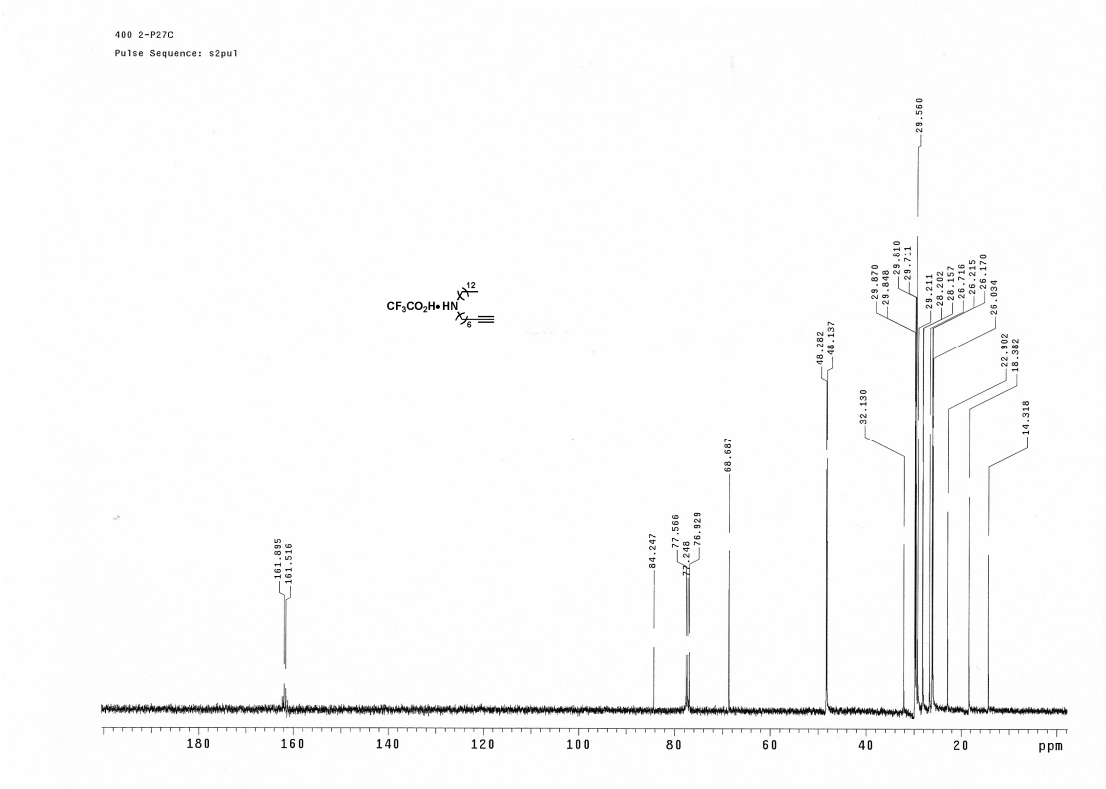
tert-Butyl oct-7-ynyltridecylcarbamate (12)



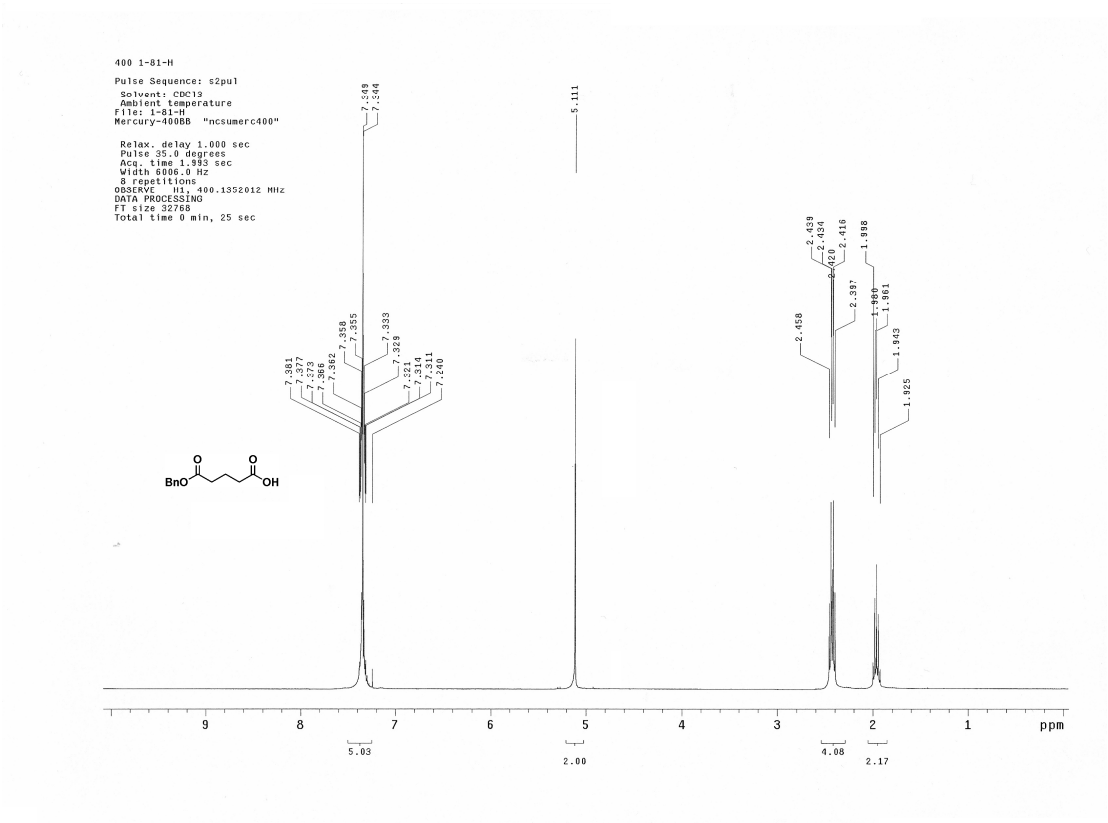


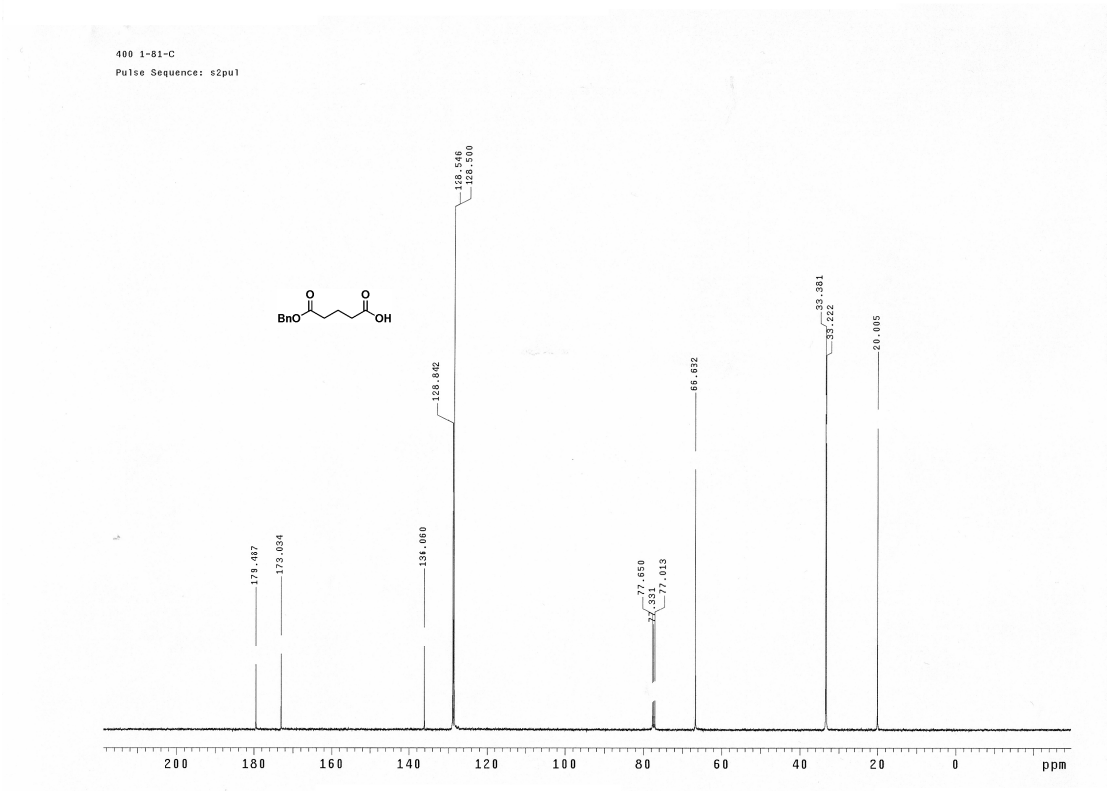
N-(oct-7-ynyl)tridecan-1-amine trifluoroacetate (2)



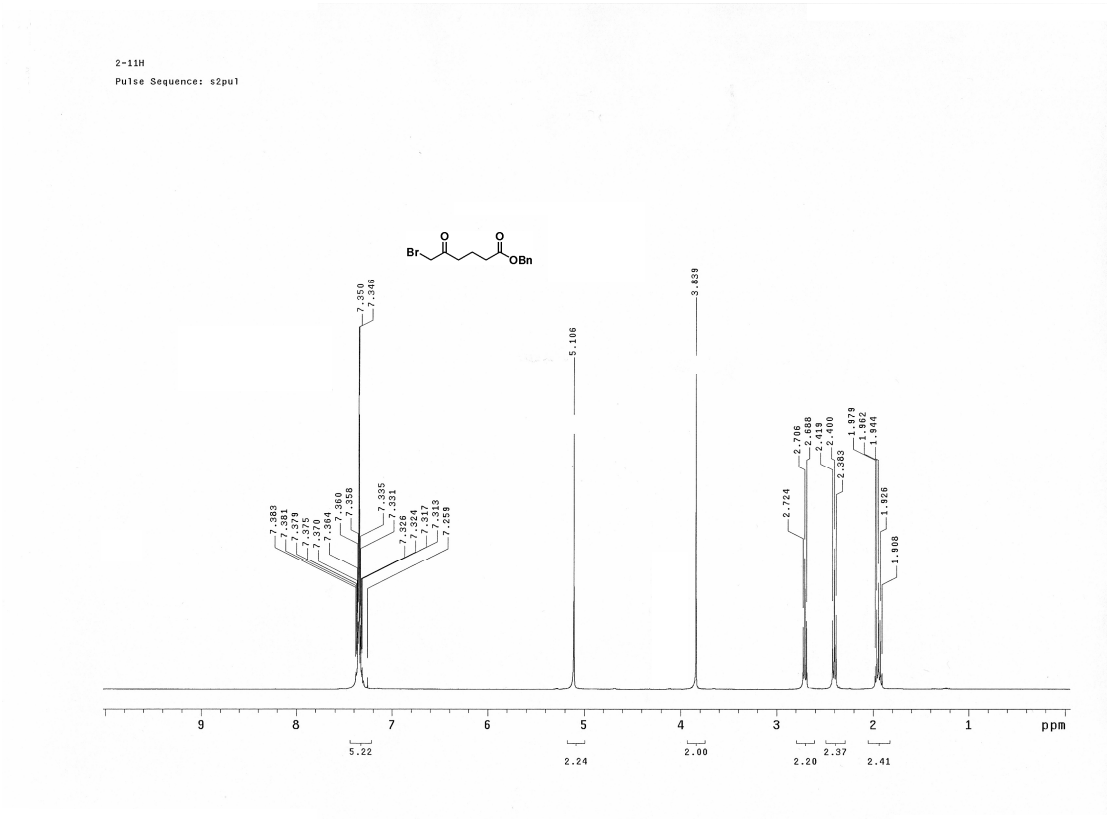


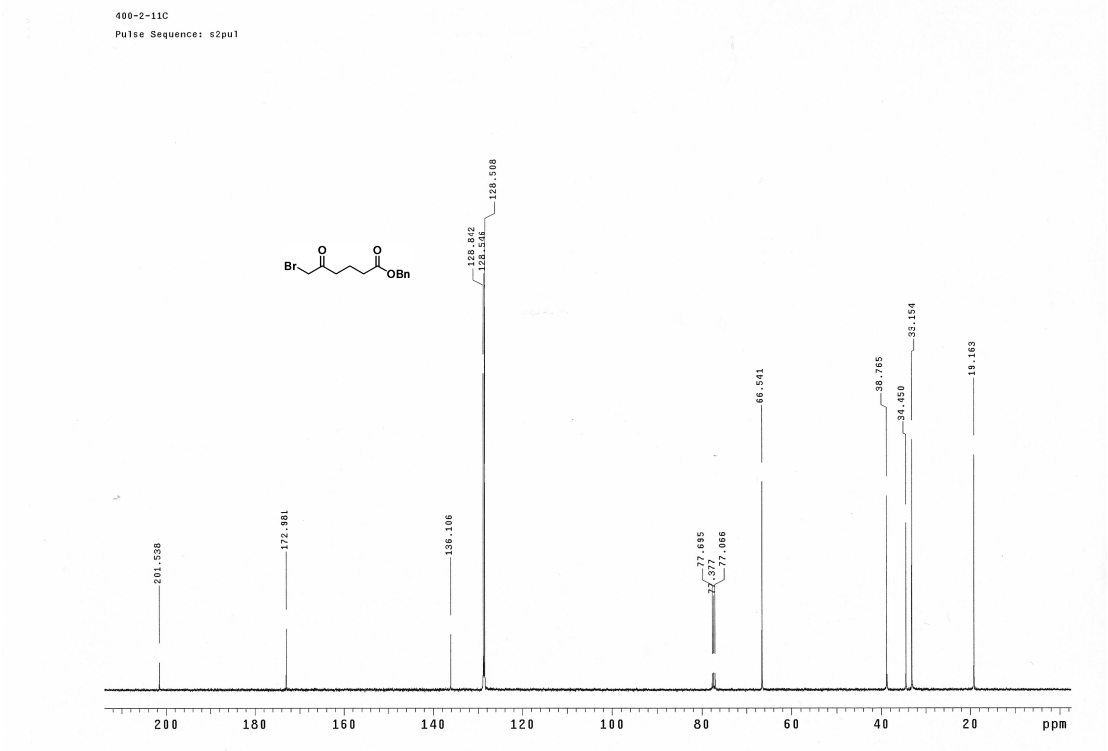
4-((Benzyloxy)carbonyl)butanoic acid (13)



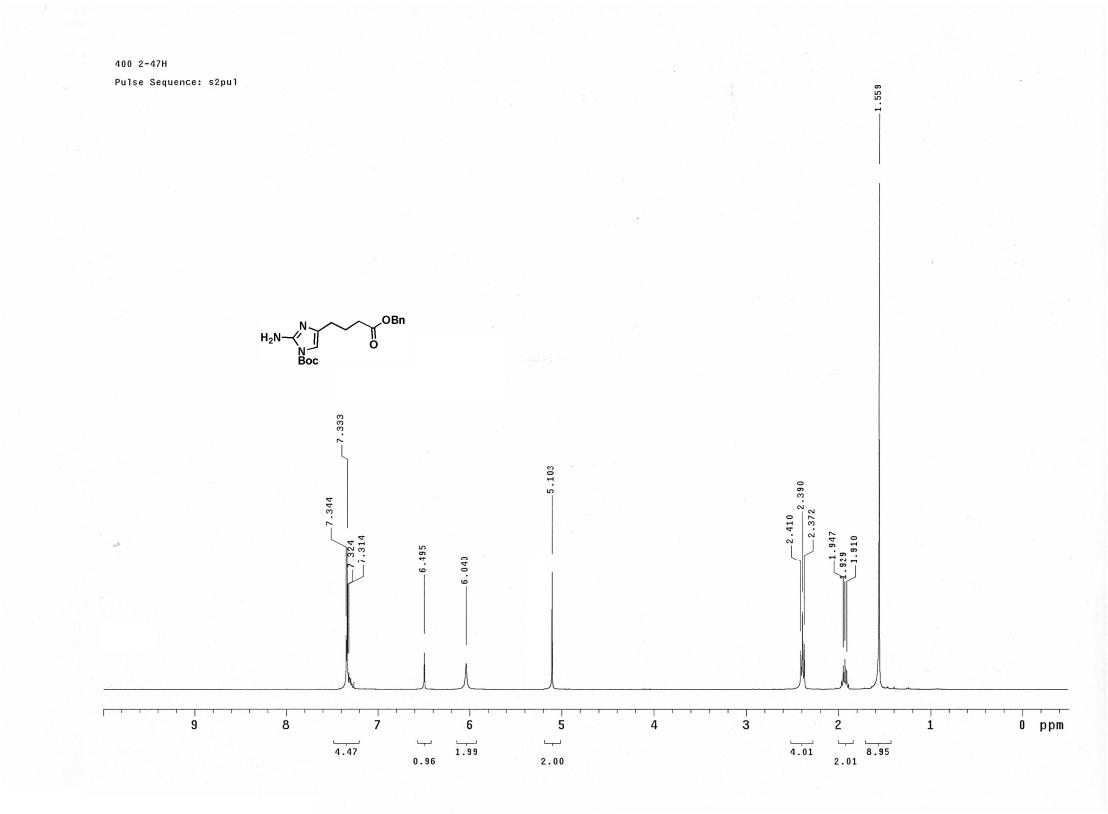


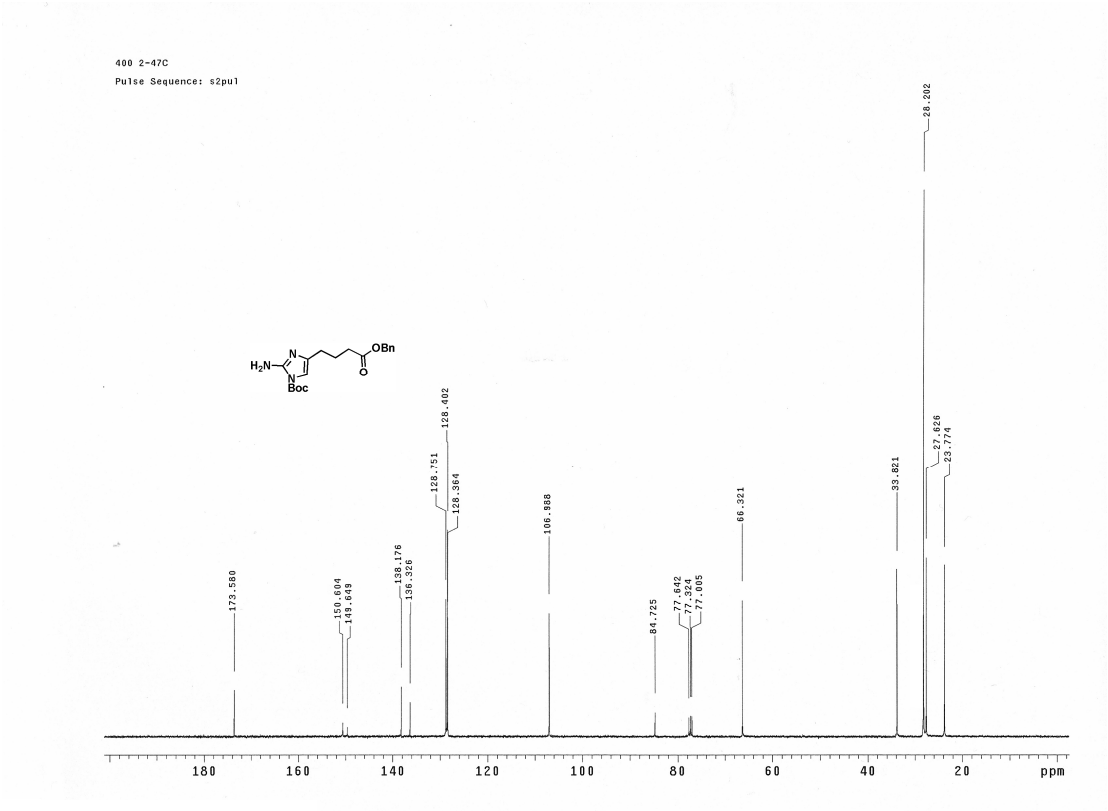
6-Bromo-5-oxo-hexanoic acid benzyl ester (14)



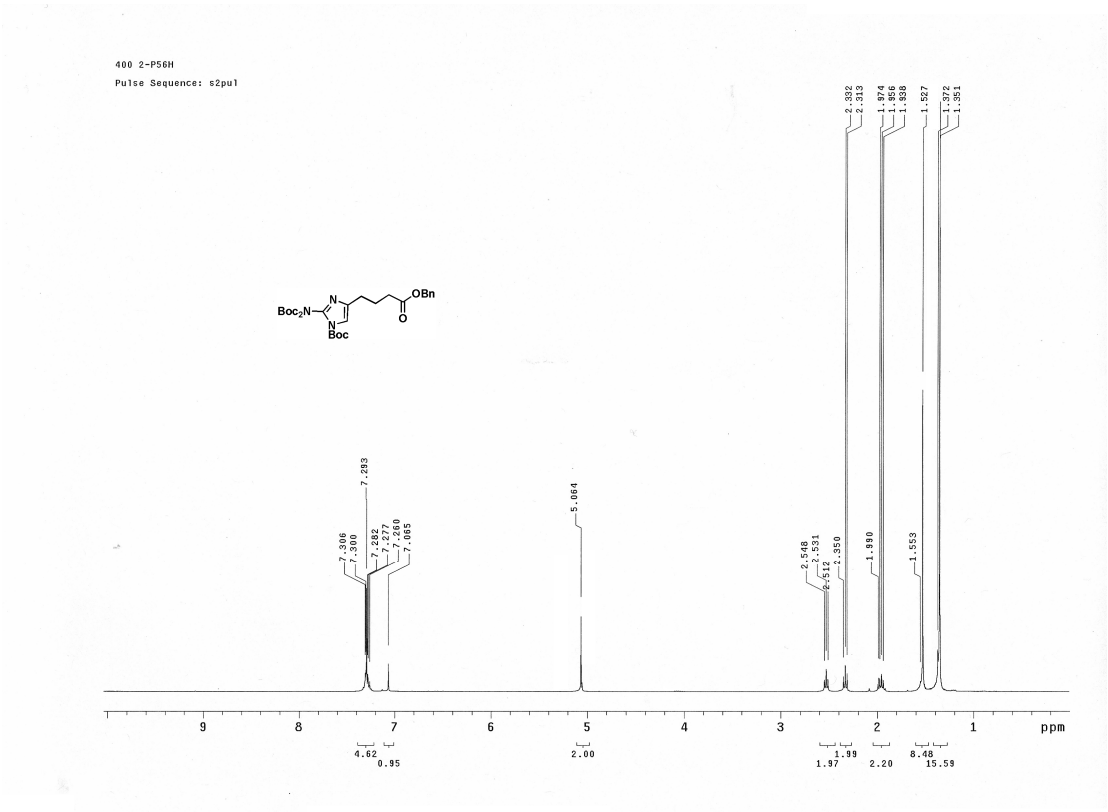


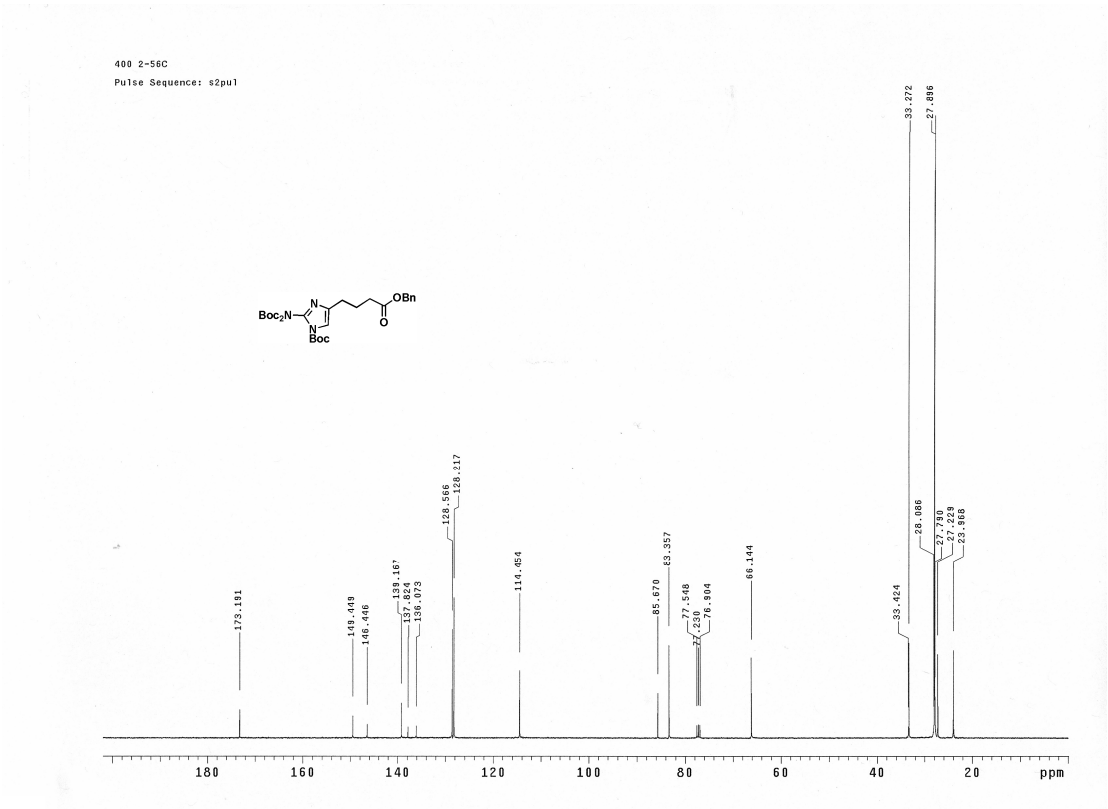
tert-Butyl 4-(3-(benzyloxycarbonyl)propyl)-2-amino-imidazole-1-carboxylate (16)



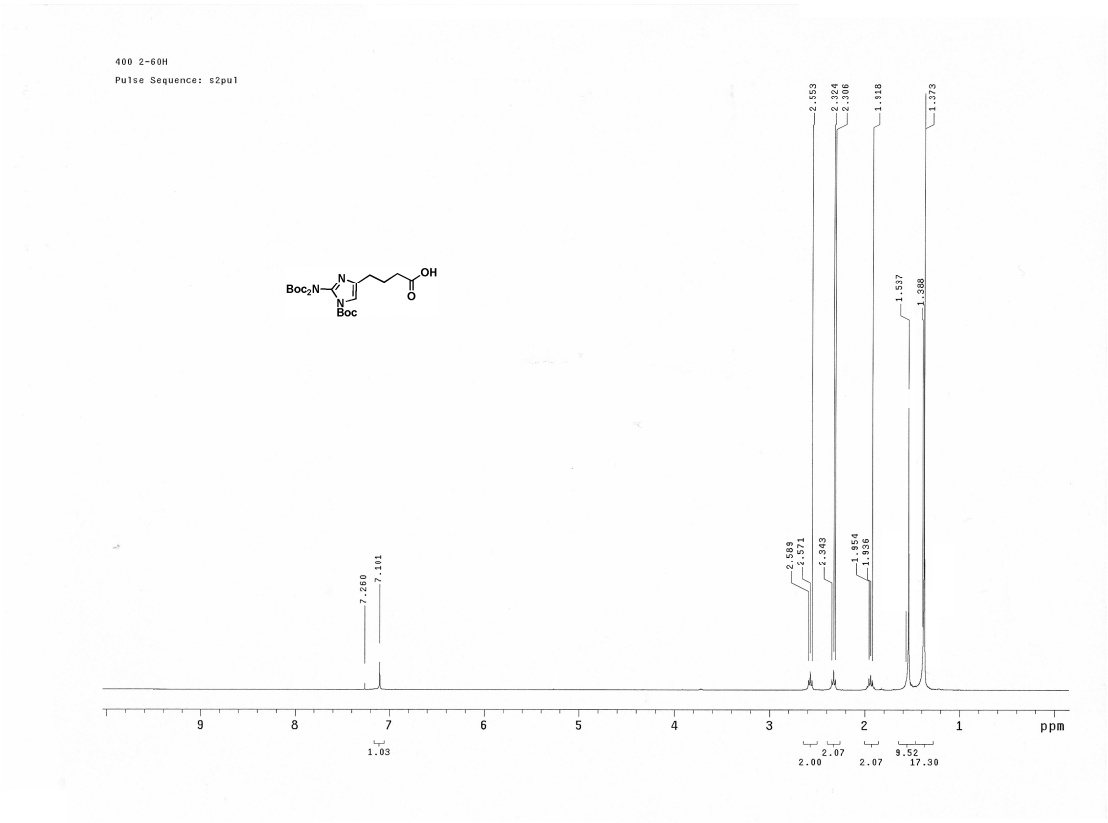


tert-Butyl 4-(3-((benzyloxy)carbonyl)propyl)-2-((di-*tert*-butoxycarbonyl)amino) -imidazole-1-carboxylate (17)

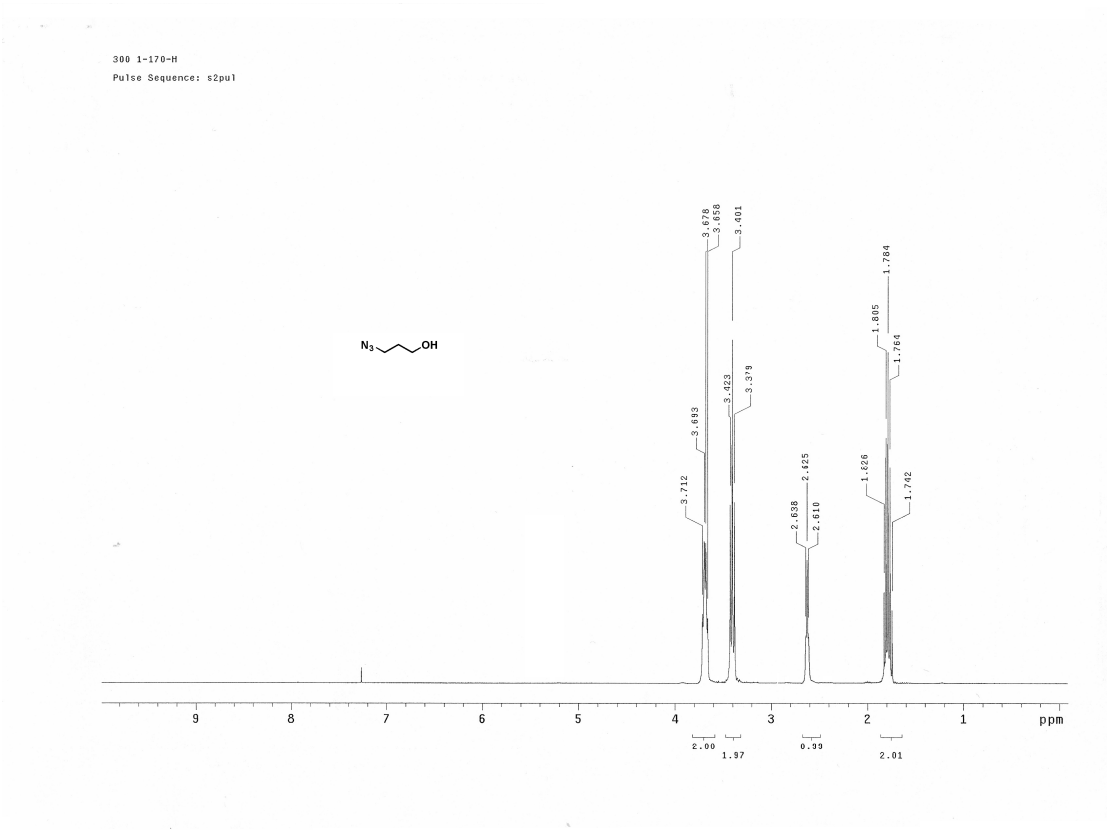


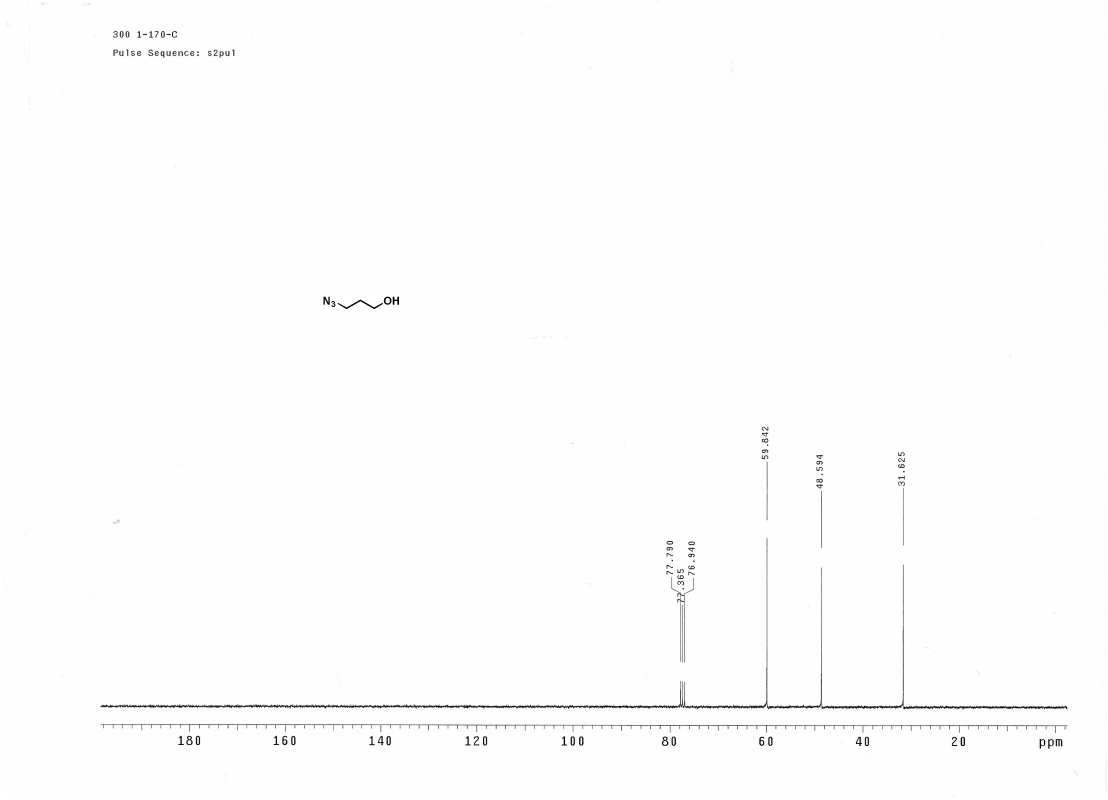


4-(1-(*tert*-Butoxycarbonyl)-2-((di-*tert*-butoxycarbonyl)amino)-imidazol-4-yl)butanoic acid (18)

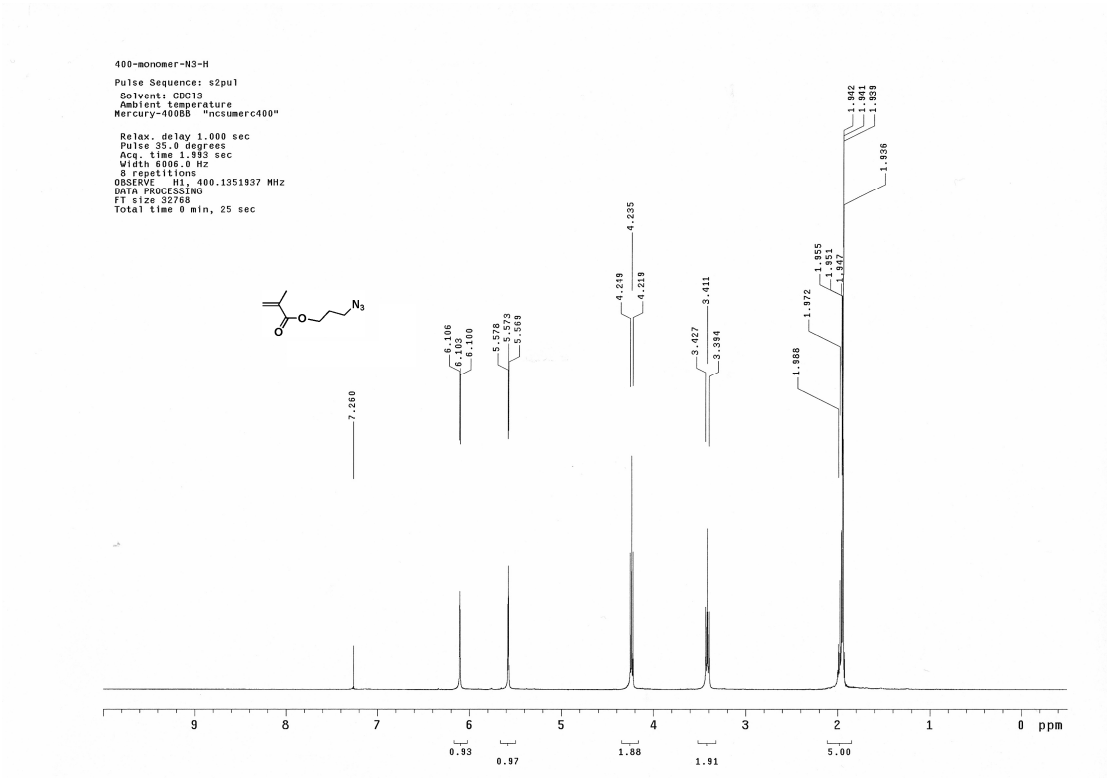


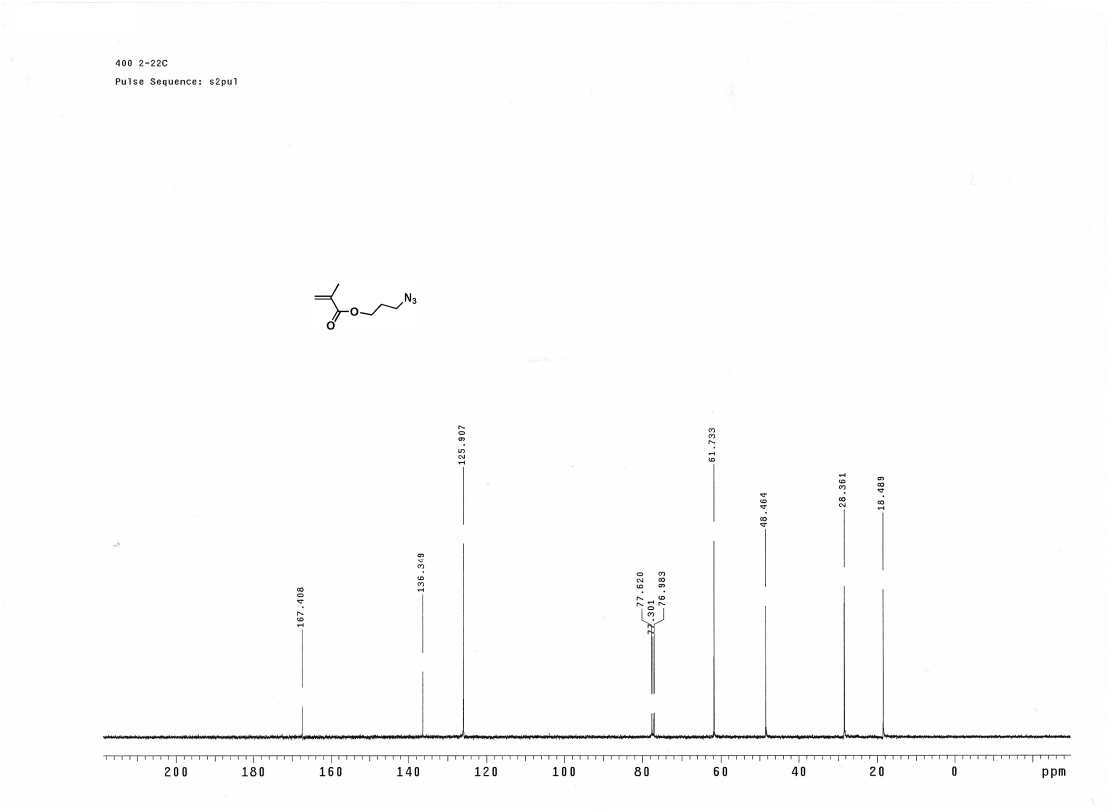
3-Azidopropan-1-ol (20)



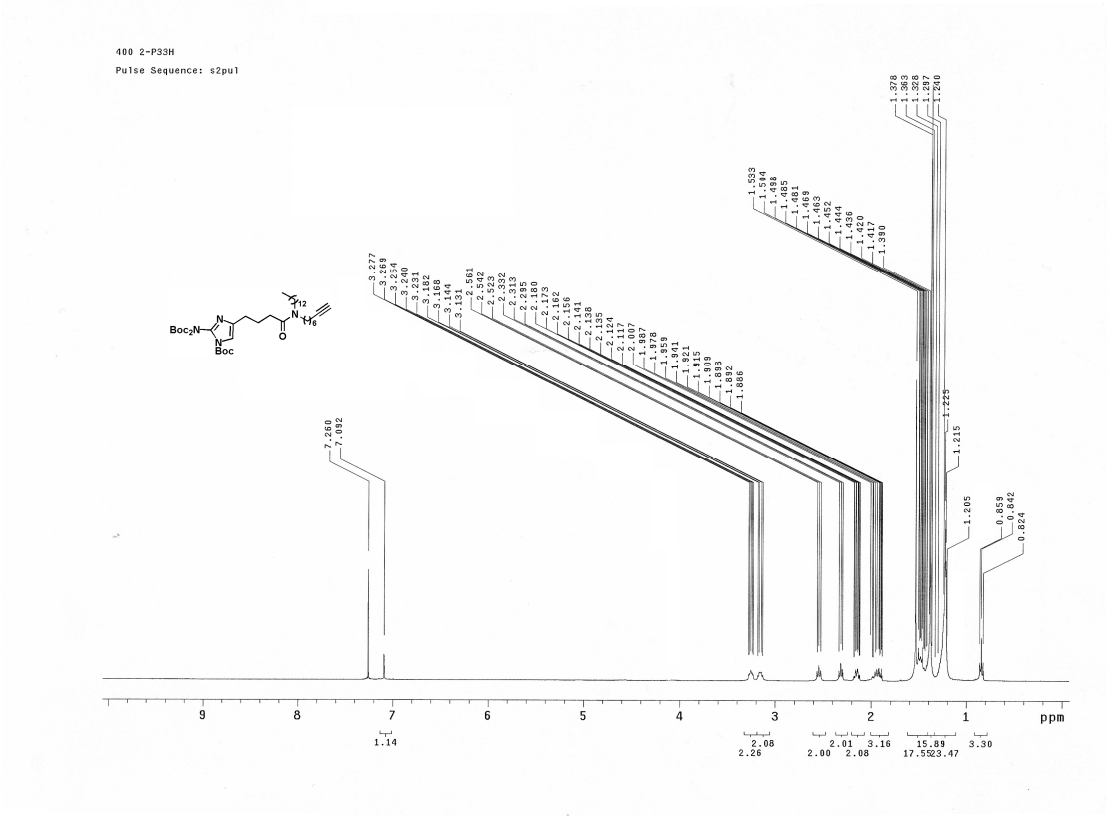


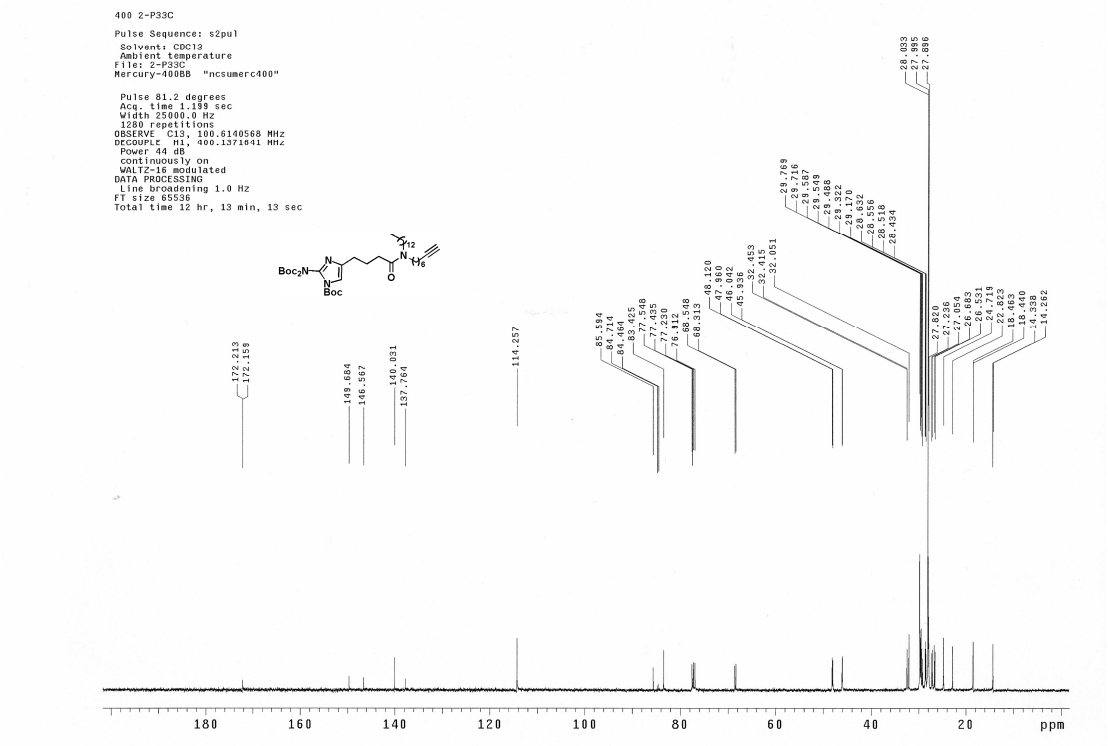
3-Azidopropyl methacrylate (22)



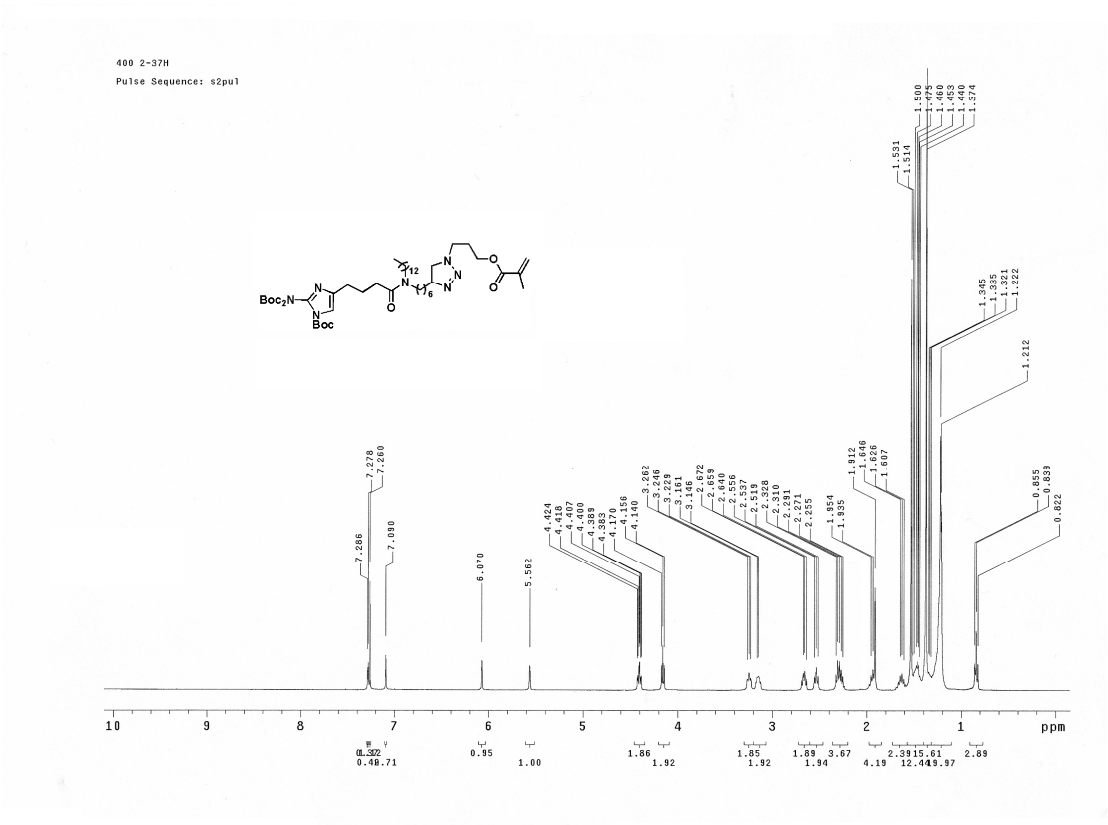


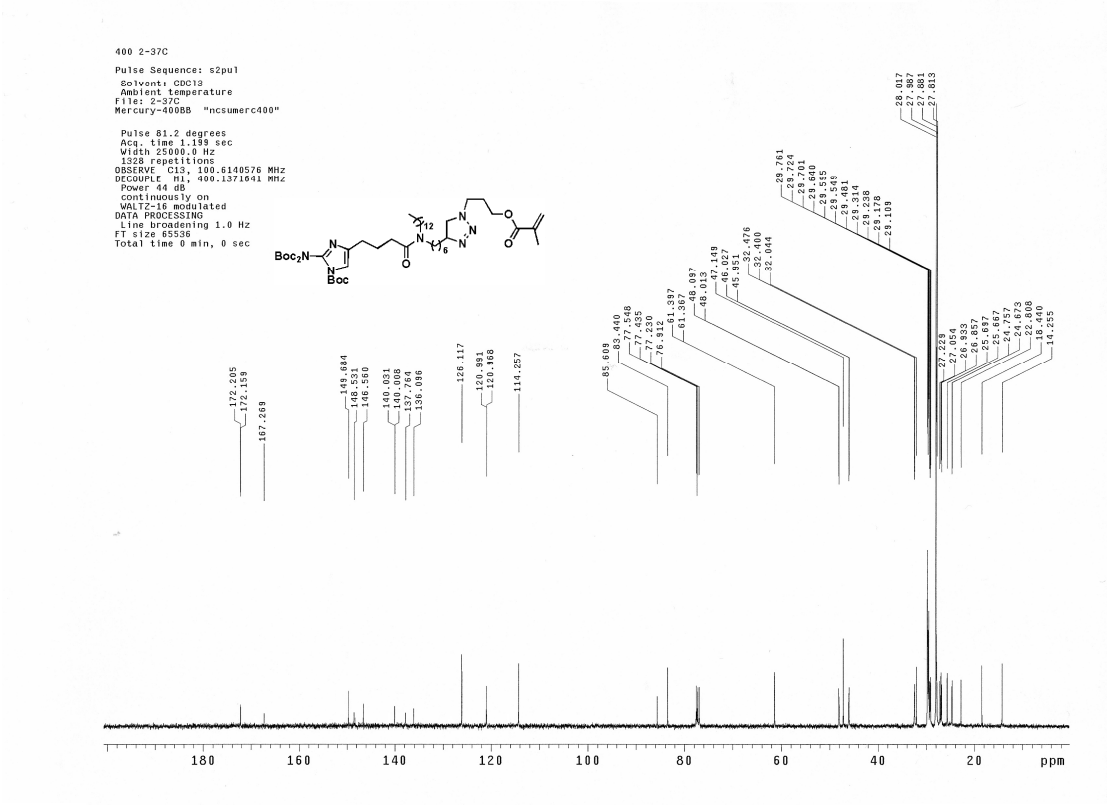
tert-Butyl 4-(3-(*N*-(oct-7-ynyl)-*N*-tridecylcarbamoyl)propyl)-2-((di-*tert*-butoxy carbonyl)amino)-imidazole-1-carboxylate (23)



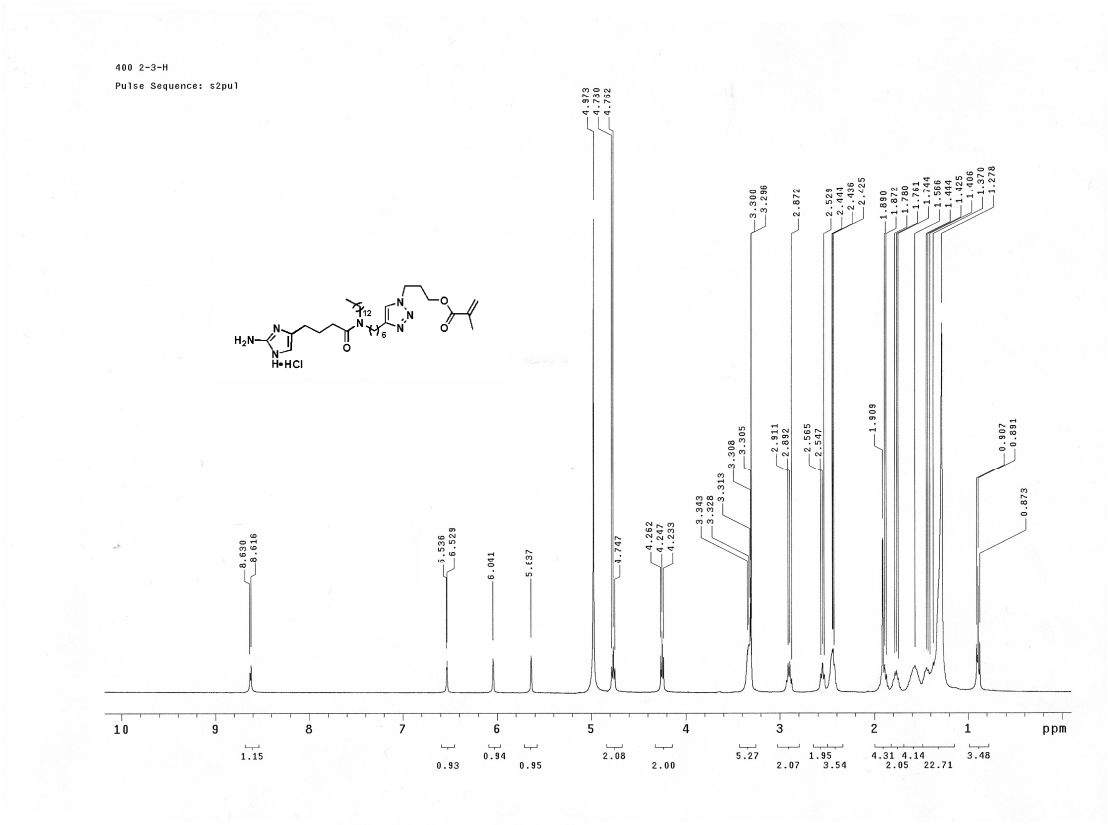


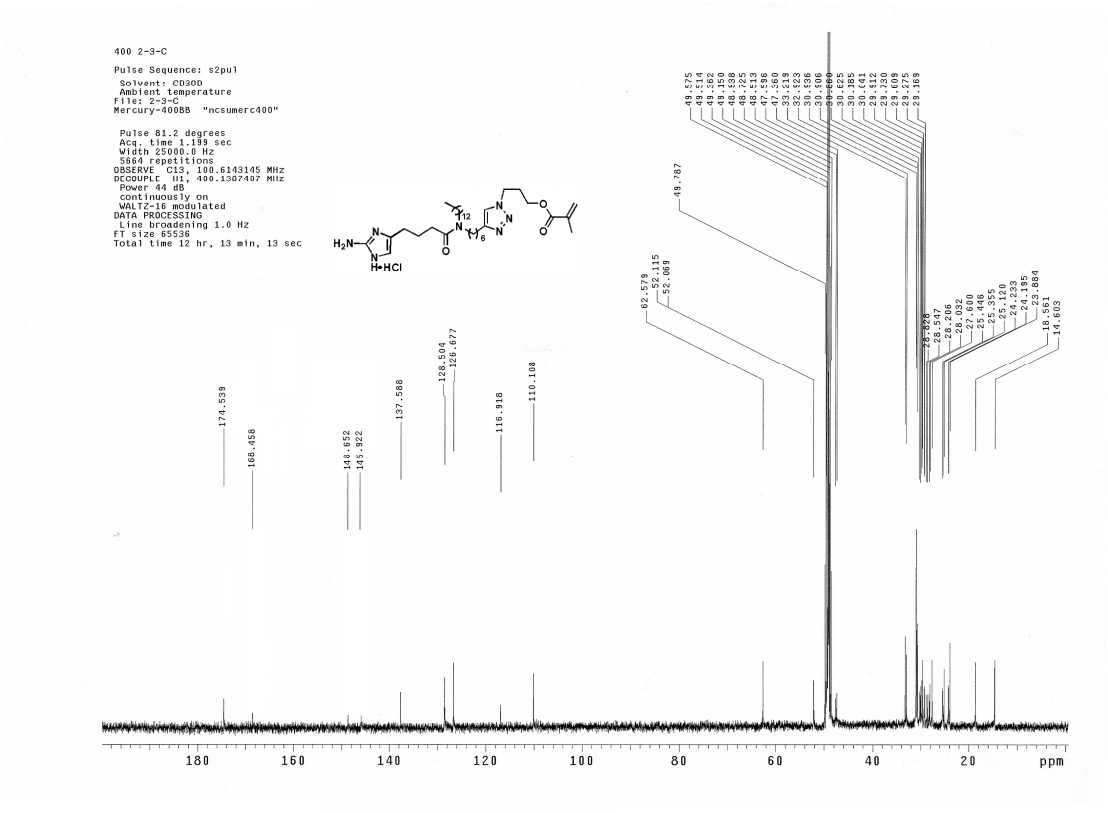
3-(4-(6-(4-(2-(di-*tert*-Butoxycarbonyl)amino-1-(*tert*-butoxycarbonyl)imidazol-4-yl)-*N*-tridecylbutanamido)hexyl)-1*H*-1,2,3-triazol-1-yl)propyl methacrylate (24)





3-(4-(6-(4-(2-Amino-imidazol-4-yl)-*N*-tridecylbutanamido)hexyl)-1*H*-1,2,3-triazol-1-yl)propyl methacrylate hydrochloride (25)





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2. F. F. Knapp, Jr., P. C. Srivastava, A. P. Callahan, E. B. Cunningham, G. W. Kabalka and K. A., R. Sastryt, ***J. Med. Chem.***, 1984**, 27,** 57-63.
3. (a) J. J. Richards, T. E. Ballard and C. Melander, *Org. Biomol. Chem.*, 2008, **6**, 1356-1363. (b) T. E. Ballard, J. J. Richards, A. L. Wolfe and C. Melander, *Chem. Eur. J.*, 2008, **14**, 10745 -1076.
4. V. Aucagne, K. D. Hänni, D. A. Leigh, P. J. Lusby and D. Barney Walker, *J. Am. Chem. Soc.*, 2006, **128**, 2186-2187.
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