Supporting Information:

Scalable Total Synthesis of Mycobactin T Analog Utilizing Novel Synthetic and Protection Strategy

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Table of contents:

1. Experimental procedure

Unless otherwise noted, commercially available materials were used without further purification. All NMR experiments were carried out on a Bruker Avance 400 MHz spectrometer. Chemical shifts were given in ppm (δ) relative to the residual solvent and coupling constants (J) in Hz. Melting points were determined without correction with a Yanaco micromelting point apparatus. HPLC-MS analysis was performed on a Thermo Finnigan LCQ Advantage mass spectrometer. The column was a Kromasil C18 column (4.6 μm, 4.6 mm × 50 mm). The eluent was a mixture of acetonitrile and water containing 0.05% HCOOH with a linear gradient from 5:95 (v/v) to 95:5 (v/v) of acetonitrile-H_2O within 5 min at a 1.0 mL/min flow rate. The UV wavelength was 254 nm. Mass spectra was electrospray ionization (ESI). High resolution LC-MS (HRMS) was carried out by Agilent LC/MSD TOF using a column of Agilent ZORBAX SB-C18 (rapid resolution, 3.5 μm, 2.1 mm × 30 mm) at a flow of 0.40 mL/min. The solvent was methanol/water = 75/25 (v/v) containing 5 mmol/L ammonium formate. The ion source was electrospray ionization (ESI). Flash column chromatography was performed with silica gel 60 (200-300 mesh) from Qingdao Haiyang Chemical Factory. The tested compounds were purified $\geqslant$ 95%.

Synthesis of (*S*)-2-(2-hydroxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid A

To a solution of salicylic acid **2** (1.38g, 10.0 mmol) and L-serine benzyl ester hydrochloride **3** (2.77g, 12.0mmol) in dry THF (20 ml) was added 1-hydroxybenzotriazole (HOBT) (2.03g, 15.0mmol), EDCI (2.87g, 15.0mmol) and triethylamine (Et_3N) (4.04g, 40.0mmol) at r.t. Then the mixture was stirred at r.t. for 20 hs. After PFBSF (15.06g, 30.0mmol) was added dropwise at r.t. The solvent was stirred for another 20 hs. The reaction was quenched with ice water (50.0 mL). The organic layer was evaporated in vacuo. The **4** was obtained as white powder after purification by silica gel column chromatography eluting with petroleum ether-ethyl acetate (3:1, v/v). Yield 75% (2.23g); mp 37-39 °C; $[a]_D^{25}$ = +64.62 (C=2.0, MeOH); ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.83 (s, 1H), 7.68-7.64 (m, 1H), 7.52-7.46 (m, 1H), 7.44-7.33 (m, 5H), 7.04-7.00 (d, J = 8.3 Hz, 1H), 6.99-6.93 (m, 1H), 5.25-5.18 (m, 3H), 4.75-4.65 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 170.6, 167.2, 159.6, 136.1, 134.8, 128.9, 128.7,

128.6, 128.4, 119.7, 117.1, 110.1, 69.7, 67.10, 67.08; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{17}H_{16}NO_4$ 298.1074; Found 298.1074.

To a solution of the intermediate **4** (1.5g, 5.0mmol) in methanol (70 mL) was added 5% Pd/C (0.3g, w/w, 20%) at r.t. The mixture was stirred under H_2 (gas) at r.t. for 20 hs. Then the solution was filtrated and evaporated in vacuo. The residue was purified by silica gel column chromatography eluting with dichloromethane-methanol (20:1, v/v) to get the building block **A**. Yield 85% (0.88g); White powder; mp 156-158 °C; $[a]_D^{25}$ = +66.00 (C=1.5, MeOH); ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.16 (br, 1H), 11.95 (br, 1H), 7.67-7.60 (m, 1H), 7.52-7.43 (m, 1H), 7.01 (d, J = 8.3 Hz, 1H), 6.96 (t, J = 7.5 Hz, 1H), 5.07-5.00 (m, 1H), 4.70-4.57 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.1, 166.7, 159.6, 134.6, 128.5, 119.6, 117.0, 110.2, 69.8, 67.2; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{10}H_{10}NO_4$ 208.0604; Found 208.0604.

Synthesis of (*S*)-tert-butyl- 6-(N-(benzoyloxy)palmitamido)-2-(((benzyloxy) carbonyl)amino)hexanoate 8

L-lysine **5** (5.6g, 20.0mmol) was dissolved in *tert*-butyl acetate (150 mL). Then perchloric acid (3.0g, 30.0mmol) was added dropwise at r.t. The mixture solution was stirred for 18 hs. The reaction was quenched with 1N HCL solution (50.0 mL). And the water layer was added saturated potassium carbonate solution to pH=8 followed by extraction with ethyl acetate (3×40 mL). The combined organic layer was washed with saturated NaCl solution, dried over anhydrous Na_2SO_4 and evaporated in vacuo. Colorless oil; The intermediate 6 was used directly in the next step without purification. To the solution of the intermediate 6 in pH 10.5 buffer solution (including 2.34g NaOH and 7.0g $NaHCO_3$ in 150 mL water) was added BPO solution (including 23.4 mmol in 100 mL dichlomethane) dropwise at r.t. Then the solution was stirred for another 3.5 hs and partitioned. The water layer was washed with DCM (2×40 mL). The combined organic layer was washed with saturated NaCl solution, dried over anhydrous Na_2SO_4 and evaporated in vacuo. The residue was purified by silica gel column chromatography eluting with petroleum ether-ethyl acetate (6:1, v/v) to get the intermediate **7**. Yield 74% (5.74g); Colorless oil; $[a]_D^{25}$ = -14.59 (C=1.6, MeOH); ^{1}H NMR (400 MHz, Acetone-d_6)

δ 8.14 (s, 1H), 8.02 (d, *J* = 7.7 Hz, 2H), 7.67 (t, *J* = 7.3 Hz, 1H), 7.55 (t, *J* = 7.7 Hz, 2H), 7.43-7.28 (m, 5H), 6.50 (d, *J* = 7.7 Hz, 1H), 5.09 (s, 2H), 4.14 (dd, *J* = 13.4, 8.3 Hz, 1H), 3.17 (t, *J* = 6.9 Hz, 2H), 1.95-1.52 (m, 6H), 1.46 (s, 9H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 172.4, 166.9, 157.0, 138.3, 134.1, 129.9, 129.6, 129.2, 128.7, 128.6, 81.5, 66.7, 55.6, 52.7, 32.6, 28.2, 27.7, 24.0; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{25}H_{33}N_2O_6$ 457.2333; Found 457.2311.

To a solution of the intermediate **7** (0.46g, 1.0mmol) and K_2CO_3 (0.14g, 1.0mmol) in acetone (5 mL) was added palmitoyl chloride (305 μL, 1.0mmol) dropwise at 0 ºC. Then the mixture was stirred for another 1 h and filtrated. The filtrate was evaporated in vacuo and the residue was purified by silica gel column chromatography eluting with petroleum ether-ethyl acetate (12:1, v/v) to get the intermediate **8**. Yield 93% (0.65g); Colorless oil; $[a]_D^{25}$ = -10.57 (C=1.5, MeOH); ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.14 (d, *J* = 7.7 Hz, 2H), 7.78 (t, *J* = 7.3 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 2H), 7.42-7.27 (m, 5H), 6.46 (d, *J* = 7.8 Hz, 1H), 5.09 (s, 2H), 4.12 (dd, *J* = 13.1, 7.8 Hz, 1H), 3.85 (t, *J* = 6.6 Hz, 2H), 2.34 (s, 2H), 1.94-1.49 (m, 8H), 1.46 (s, 9H), 1.38-1.21 (m, 24H), 0.90 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 171.4, 164.4, 156.1, 137.4, 134.4, 129.8, 129.0, 128.3, 127.7, 65.8, 54.6, 31.9, 31.7, 31.4, 29.50, 29.47, 29.43, 29.20, 29.18, 27.3, 26.6, 24.3, 22.7, 22.4, 13.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{41}H_{63}N_2O_7$ 695.4630; Found 695.4623.

Synthesis of (*S*)-3-(((benzyloxy)carbonyl)amino)-2-oxoazepan-1-yl benzoate 10

To a solution of the intermediate **7** (3.04g, 6.7mmol) in dichlomethane (20 mL) was added trifluoroacetic acid (10 mL) dropwise at ice-bath water. Then the solution was stirred at r.t. for 3.5 hs and evaporated in vacuo. The residue was dissolved in ethyl acetate (30 mL) and the sodium bicarbonate solution (1 mol/L) was added to pH=6. The organic layer was washed with saturated NaCl solution, dried over anhydrous Na_2SO_4 and evaporated in vacuo. Colorless oil; The intermediate 9 was used directly in the next step. To a solution of EDCI (3.42g, 18.0mmol), DMAP (2.20g, 18.0mmol) and DMAP. HCl (2.86g, 18.0mmol) in chloroform (150 mL) was added the intermediate 9 (1.8g, 4.5mmol) solution (in 50 mL chloroform) for 10 hs at 80 ºC. Then the mixture was stirred for another 11 hs and quenched with HCl water solution (1 mol/L). The

organic layer was washed with saturated NaCl solution and evaporated in vacuo. Finally, the residue was purified by silica gel column chromatography eluting with petroleum ether-ethyl acetate (5:1, v/v) to get the intermediate **10**. Yield 62% (two steps, 1.58g); Colorless oil; $[a]_D^{25}$ = -36.15 (C=1.5, MeOH); ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.09-8.04 (d, J = 7.5 Hz, 2H), 7.73 (t, J = 7.5 Hz, 1H), 7.58 (t, J = 7.8 Hz, 2H), 7.42-7.27 (m, 5H), 6.40 (s, 1H), 5.09 (s, 2H), 4.53-4.45 (m, 1H), 4.30-4.15 (m, 1H), 3.90-3.83 (m, 1H), 1.94-1.82 (m, 3H), 1.82-1.68 (m, 1H), 1.35-1.26 (m, 2H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 168.5, 163.5, 155.3, 137.3, 134.1, 129.7, 128.8, 128.3, 127.74, 127.72, 127.4, 65.8, 53.4, 52.8, 31.4, 27.6, 26.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{21}H_{23}N_2O_5$ 383.1602; Found 383.1598.

Synthesis of (*S*)-3-((*S*)-3-(((benzyloxy)carbonyl)amino)-2-((*tert*-butoxycarbonyl) amino)propanamido)-2-oxoazepan-1-yl benzoate 17

To a solution of the intermediate **10** (3.82g, 10.0mmol) in methanol (40 mL) and trifluoroacetic acid (10 mL) was added 5% Pd/C (0.76g, w/w, 20%) at r.t. The mixture was stirred under H_2 (gas) at for 5 hs. Then the solution was filtrated and evaporated in vacuo. The residue was dissolved in ethyl acetate (15 mL) and the saturated sodium bicarbonate solution (2 mL) was added. The organic layer was washed with saturated NaCl solution, dried over anhydrous Na_2SO_4 and evaporated in vacuo. Yield 99% (2.48g); White solid; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{13}H_{17}N_2O_3$ 249.1234; Found 249.1232. The intermediate 11 was used directly in the next step without purification. To a solution of the intermediate 11 (2.48g, 10.0mmol) and 3-(*N*-Cbz)-2-(*N*-Boc)-2,3-diaminobutyric acid **14** (3.38g, 10.0mmol) in dichlomethane (30 mL) was added HOBT (2.03g, 15.0mmol), EDCI (2.87g, 15.0mmol) at r.t. Then the mixture was stirred at for another 4 hs. The reaction was quenched with ice water (50.0 mL). The organic layers were evaporated in vacuo. The intermediate **17** was obtained as white powder after purification by silica gel column chromatography eluting with petroleum ether-ethyl acetate (5:1, v/v). Yield 83% (4.72g); White solid; mp 85-88 °C; $[a]_D^{25}$ = -33.18 (C=1.0, MeOH); ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.08 (d, J = 7.2 Hz, 2H), 7.75 (t, J = 7.4 Hz, 1H), 7.70-7.63 (m, 1H), 7.60 (t, J = 7.8 Hz, 2H), 7.36-7.28 (m, 5H), 6.55 (s, 1H), 6.29 (s, 1H), 5.07 (s, 2H), 4.69-4.61 (m, 1H), 4.26 (s, 2H), 3.85-3.42 (m,

1H), 3.61-3.45 (m, 2H), 1.94-1.82 (m, 3H), 1.82-1.68 (m, 1H), 1.41 (s, 9H), 1.35-1.26 (m, 2H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 169.4, 168.4, 163.5, 156.9, 155.4, 137.3, 134.1, 129.7, 128.9, 128.3, 127.7, 127.6, 127.3, 78.8, 65.8, 55.2, 52.8, 52.0, 42.7, 30.9, 27.7, 27.5, 26.2; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{29}H_{37}N_4O_8$ 569.2606; Found 569.2606.

Synthesis of (*S*)-6-(*N*-(benzoyloxy)palmitamido)-2-((*S*)-2-(2-hydroxyphenyl)-4,5-dihydrooxazole-4-carboxamido)hexanoic acid 16

The intermediate 13 was prepared from intermediate **8** in a similar manner to the synthesis of intermediate 11 as colorless oil. And it was used directly in the next step. Then the intermediate **15** was prepared from intermediate 13 and **A** in a similar manner to the synthesis of intermediate **17** as colorless oil. Yield 79% (2.96g); $[a]_D^{25}$ = +6.37 (C=1.8, MeOH); ^{1}H NMR (400 MHz, Acetone-d_6) δ 11.62 (s, 1H), 8.09 (d, J = 7.5 Hz, 2H), 7.74 (t, J = 7.5 Hz, 1H), 7.65 (dd, J = 7.8, 1.3 Hz, 2H), 7.58 (t, J = 7.7 Hz, 2H), 7.43 (dd, J = 7.6 , 1.6 Hz, 1H), 6.97-6.88 (m, 2H), 5.05 (t, J = 9.2 Hz, 1H), 4.73-4.63 (m, 2H), 4.41-4.34 (m, 1H), 3.85-3.73 (m, 2H), 2.29 (t, J = 6.7 Hz, 2H), 1.95-1.82 (m, 1H), 1.82-1.63 (m, 3H), 1.62-1.41 (m, 12H), 1.35-1.19 (m, 25H), 0.88 (t, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 134.9, 130.8, 130.0, 129.3, 119.8, 117.7, 70.5, 69.1, 53.9, 32.9, 32.8, 32.3, 30.4-30.7 (m), 30.3, 30.2, 28.3, 23.7, 23.5, 14.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{43}H_{64}N_3O_8$ 750.4688; Found 750.4668.

Finally，the intermediate **16** was prepared from intermediate **15** in a similar manner to the synthesis of intermediate 9 as white solid. Yield 98% (2.69g); mp 57-59 °C; $[a]_D^{25}$ = +10.26 (C=1.0, MeOH); ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.82 (br, 1H), 8.43 (s, 1H), 8.01 (d, J = 7.5 Hz, 2H), 7.73 (t, J = 7.2 Hz, 1H), 7.62-7.56 (m, 3H), 7.42 (t, J = 7.8 Hz, 1H), 6.95-6.85 (m, 2H), 5.03 (t, J = 8.7 Hz, 1H), 4.62 (t, J = 9.2 Hz, 1H), 4.53 (t, J = 7.8 Hz, 1H), 4.22-4.18 (m, 1H), 3.75-3.65 (m, 2H), 2.22 (s, 2H), 1.85-1.75 (m, 1H), 1.71-1.53 (m, 3H), 1.50-1.43 (s, 2H), 1.40-1.30 (s, 2H), 1.25-1.10 (m, 24H), 0.83 (t, J = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 174.6, 173.2, 169.8, 166.2, 164.5, 159.6, 135.0, 134.3, 130.0, 129.5, 128.6, 128.4, 127.8, 126.9, 119.3, 116.9, 110.3, 70.2, 69.7, 67.8, 53.0, 31.9, 31.8, 31.5, 29.5, 29.44, 29.33, 29.2, 28.9, 26.8, 24.5, 23.1, 22.6,

14.3. HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{39}H_{56}N_3O_8$ 694.4062; Found 694.4056.

Synthesis of (*S*)-3-((*S*)-3-((*S*)-6-(*N*-(benzoyloxy)palmitamido)-2-((*S*)-2-(2-hydroxy phenyl)-4,5-dihydrooxazole-4-carboxamido)hexanamido)-2-((*tert*-butoxycarbonyl)amino)propanamido)-2-oxoazepan-1-yl benzoate 19

The intermediate 18 was prepared from intermediate **17** in a similar manner to the synthesis of intermediate 11 as yellow solid. HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{60}H_{84}N_7O_{13}$ 435.2238; Found 435.2235. It was used directly in the next step without purification. The intermediate **19** was prepared from intermediate **16** and 18 in a similar manner to the synthesis of intermediate **17** as white solid. Yield 88% (2.44g); mp 79-81 °C; $[a]_D^{25}$ = +4.51 (C=1.0, MeOH); ^{1}H NMR (400 MHz, Acetone-d_6) δ 11.61 (s, 1H), 8.07 (d, *J* = 7.5 Hz, 2H), 8.02 (d, *J* = 7.3 Hz, 2H), 7.91 (d, *J* = 5.4 Hz, 2H), 7.80 (d, *J* = 7.0 Hz, 1H), 7.73 (t, *J* = 7.4 Hz, 1H), 7.65-7.54 (m, 4H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 1H), 6.96-6.86 (m, 2H), 6.21 (d, *J* = 7.5 Hz, 1H), 5.03 (dd, *J* = 10.3, 7.7 Hz, 1H), 4.76-4.63 (m, 2H), 4.57 (t, *J* = 9.4 Hz, 1H), 4.33-4.17 (m, 3H), 3.89-3.81 (m, 1H), 3.80-3.59 (m, 3H), 3.31-3.20 (m, 1H), 2.26 (t, *J* = 6.5 Hz, 2H), 2.03-1.95 (m, 2H), 1.93-1.75 (m, 5H), 1.73-1.64 (m, 1H), 1.62-1.51 (m, 4H), 1.40 (s, 9H), 1.33-1.20 (m, 26H), 0.87 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 172.7, 171.1, 170.9, 170.2, 167.5, 165.3, 164.3, 160.7, 156.0, 135.2, 135.0, 134.7, 130.7, 130.6, 129.8, 129.7, 129.1, 128.1, 128.0, 119.6, 117.5, 111.2, 79.5, 70.0, 68.9, 55.2, 54.8, 53.8, 53.1, 41.8, 32.7, 32.6, 32.2, 30.9, 30.42, 30.38, 30.35, 30.32, 30.1, 28.6, 28.4, ,27.4, 27.0, 25.2, 23.6, 23.3, 14.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{60}H_{84}N_7O_{13}$ 1110.6122; Found 1110.6115.

Synthesis of (*S*)-*N*-((*S*)-1-(((*S*)-2-amino-3-(((*S*)-1-hydroxy-2-oxoazepan-3-yl) amino)-3-oxopropyl)amino)-6-(*N*-hydroxypalmitamido)-1-oxohexan-2-yl)-2-(2-hydroxyphenyl)-4,5-dihydrooxazole-4-carboxamide hydrochloride (MbT-1)

To a solution of the intermediate **19** (0.08g, 0.1mmol) in methanol (0.5 mL) was added NH_3/CH_3OH (1.5 mL, 7mol/L) at r.t. The mixture solution was stirred for another 2 hs and evaporated in vacuo. Then the residue was dissolved in ethyl acetate (EA) (1 mL) and HCL/EA (4 mL, 1.8 mol/L) was added at r.t. The solution was stirred for another 20 hs and filtrated to get the **MbT-1** as white solid. Yield 85% (two steps, 0.07g);

mp 136-139 °C; $[a]_D^{25}$ = +6.21 (C=0.8, H_2O); ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.18 (br, 1H), 9.65 (s, 1H), 9.16 (d, *J* = 7.6 Hz, 0.4H), 8.80 (d, *J* = 6.8 Hz, 0.6H), 8.71 (d, *J* = 6.9 Hz, 1H), 8.50 (d, *J* = 6.8 Hz, 1H), 8.46-8.30 (m, 3H), 7.95 (d, *J* = 7.9 Hz, 0.4H), 7.68 (d, *J* = 7.4 Hz, 0.6H), 7.55-7.38 (m, 1H), 7.09-7.00 (m, 1H), 7.08-6.89 (m, 1H), 5.19-5.07 (m, 0.6H), 4.97-4.93 (m, 1H), 4.79-4.66 (m, 1H), 4.53-4.49 (m, 1H), 4.22-4.10 (m, 1H), 4.04 (d, *J* = 5.3 Hz, 1H), 3.95-3.88 (m, 2H), 3.78-3.59 (m, 1H), 3.53 (d, *J* = 14.3 Hz, 1H), 3.53-3.45 (m, 1H), 3.33-3.28 (m, 1H), 2.35-2.29 (m, 2H), 2.04-1.57 (m, 6H), 1.55-1.40 (m, 6H), 1.35-1.00 (m, 25H), 0.86 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.2, 172.2, 168.9, 168.7, 167.5, 166.8, 158.7, 134.0, 130.0, 119.4, 117.6, 116.9, 54.6, 54.1, 54.0, 52.9, 52.1, 52.0, 47.4, 45.5, 32.2, 31.8, 31.5, 30.0, 29.9, 29.5, 29.47, 29.43, 29.4, 29.2, 27.3, 26.5, 26.0, 24.7, 22.9, 22.8, 22.6, 14.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd for $C_{41}H_{68}N_7O_9$ 802.5079; Found 802.5078.

2. ^{1}H and ^{13}C-NMR spectra

Figure S1: ^{1}H-NMR and ^{13}C-NMR spectra of **MbT-1**

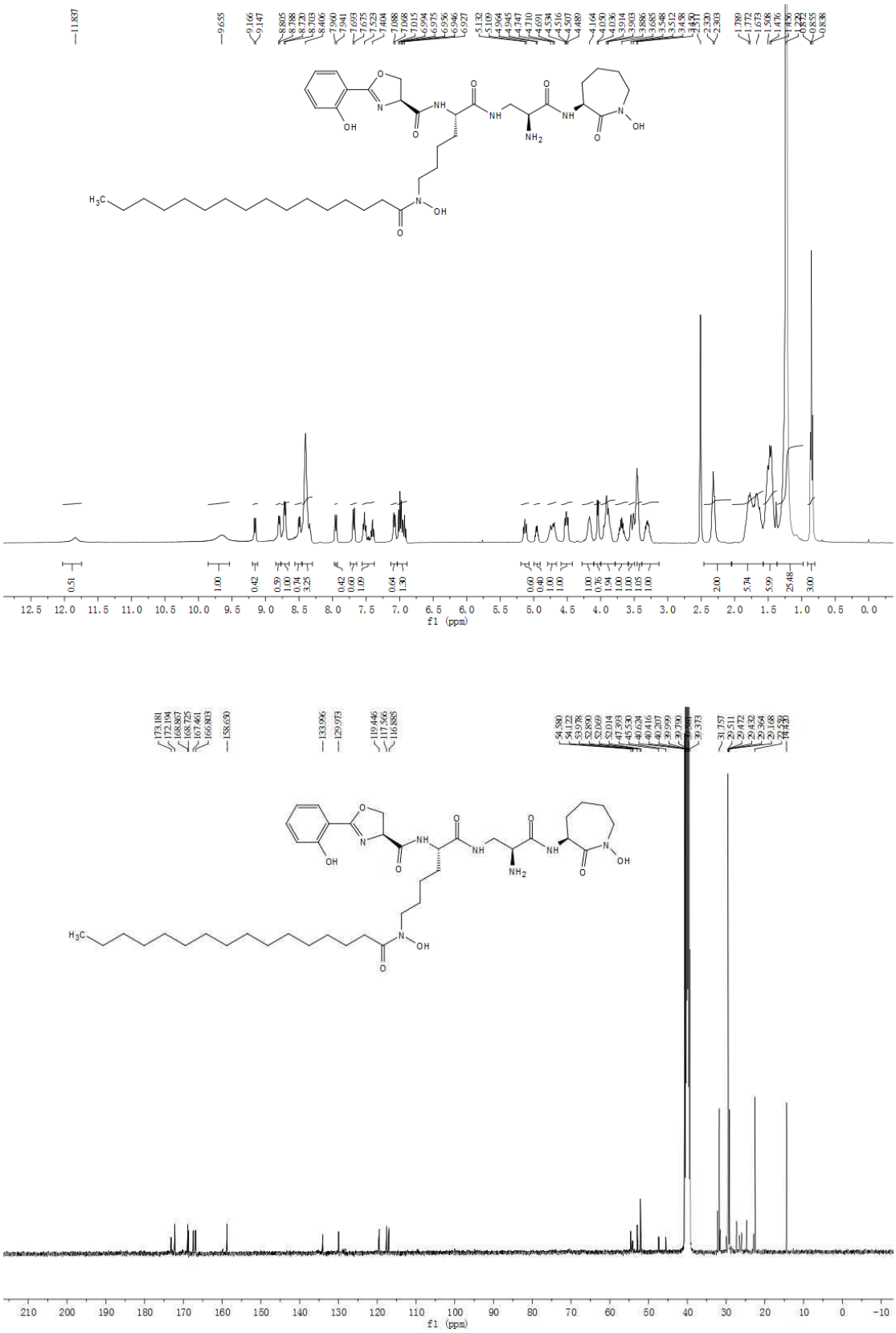
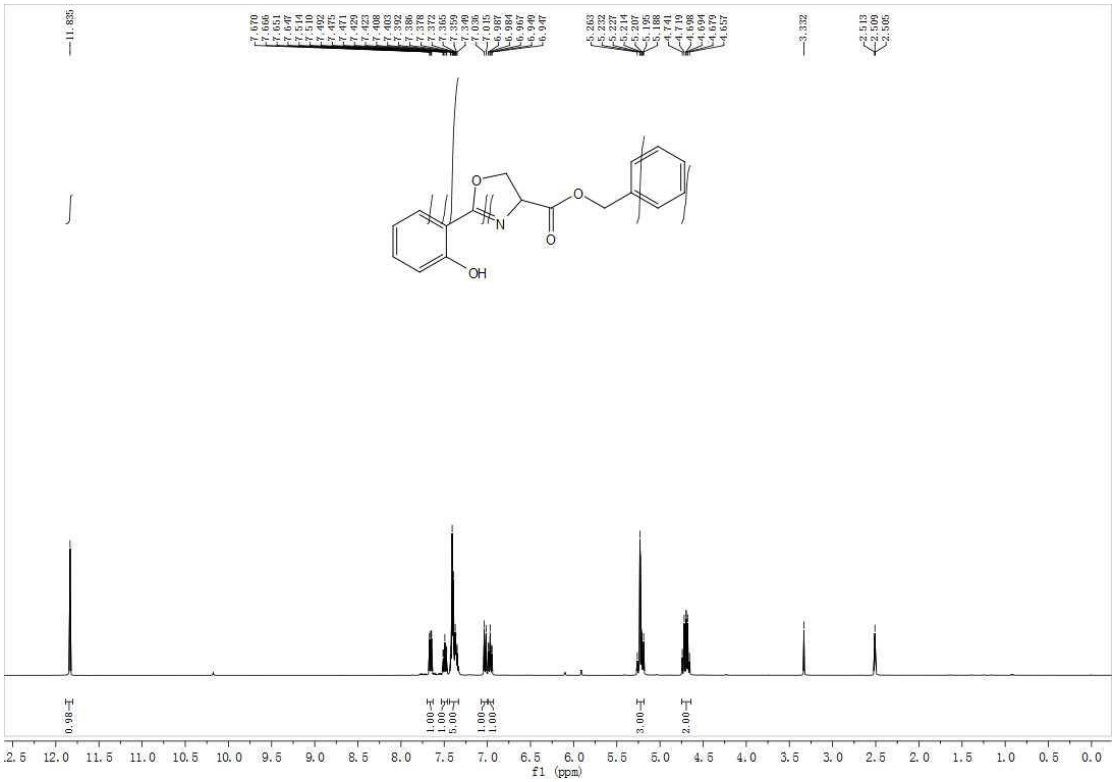


Figure S2: ^{1}H-NMR and ^{13}C-NMR spectra of the intermediate **4**



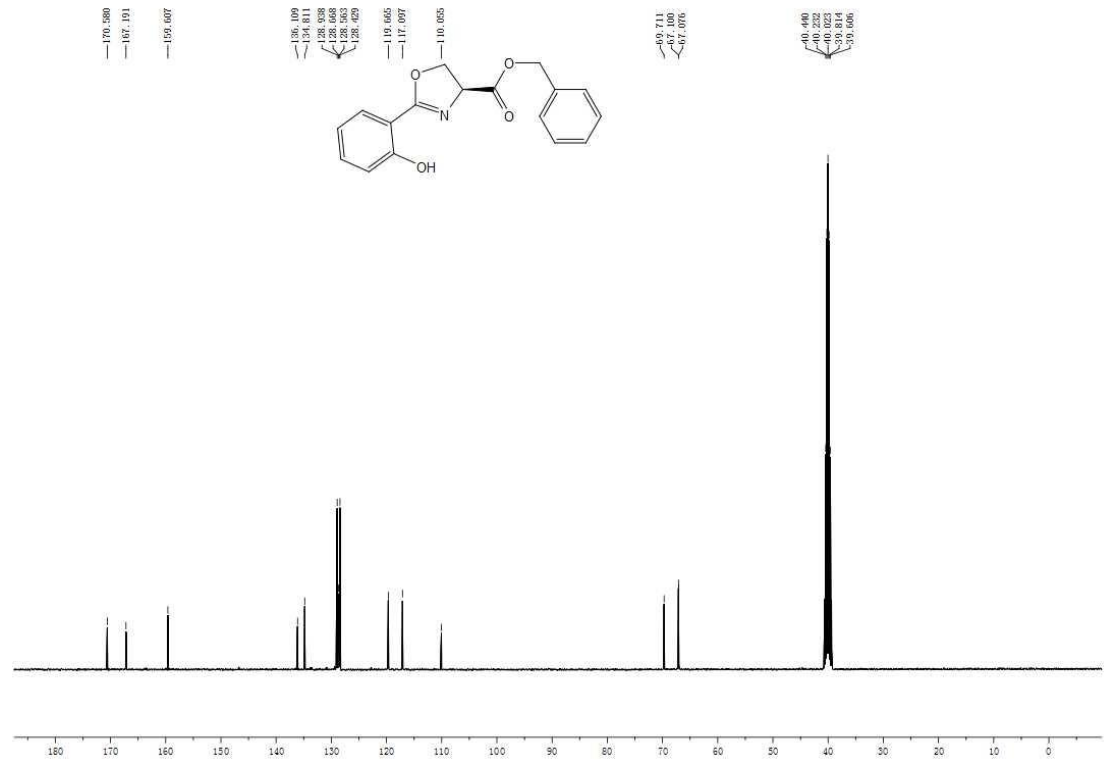


Figure S3: ^{1}H-NMR and ^{13}C-NMR spectra of the intermediate **A**

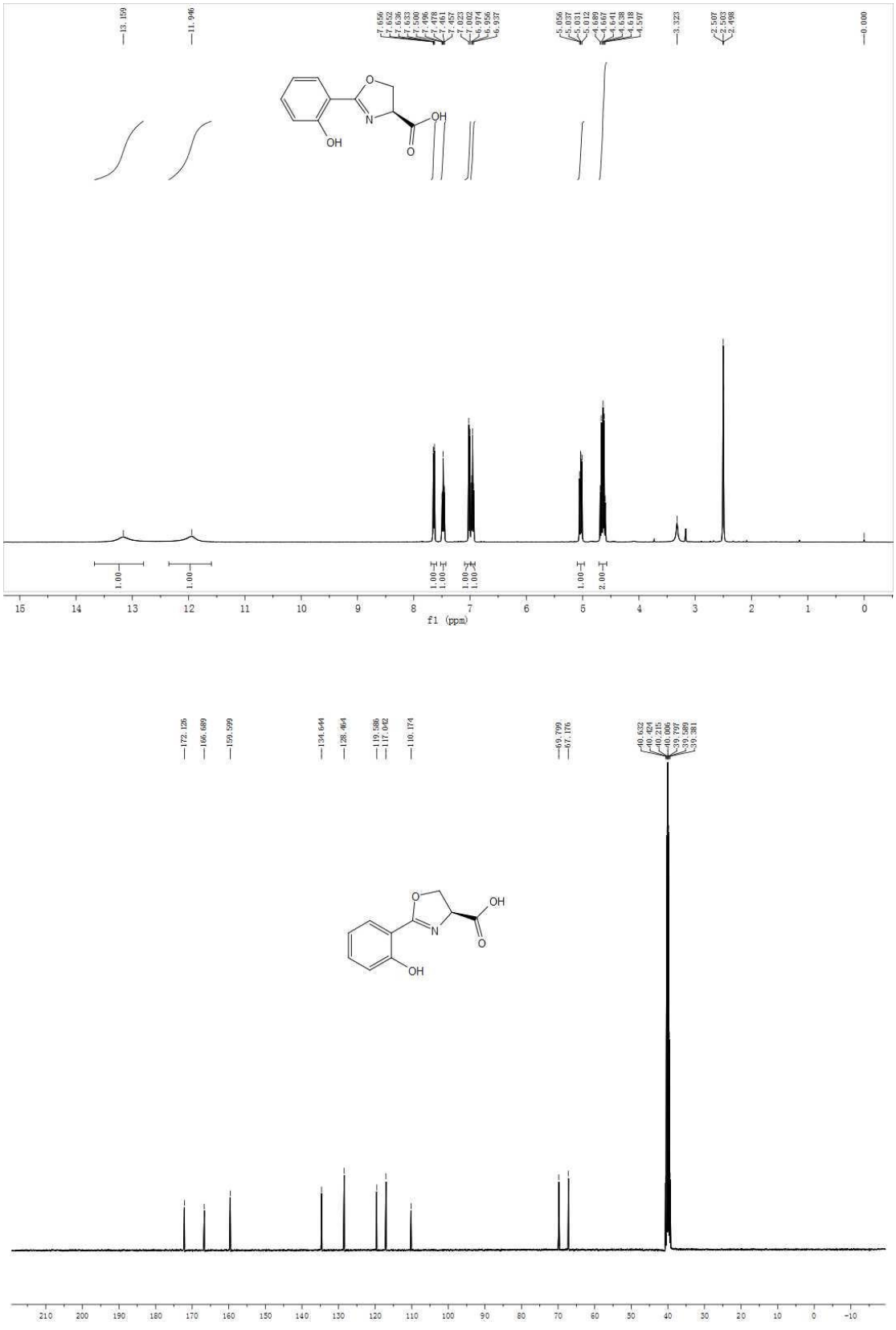


Figure S4: ^{1}H-NMR and ^{13}C-NMR spectra of the intermediate **7**

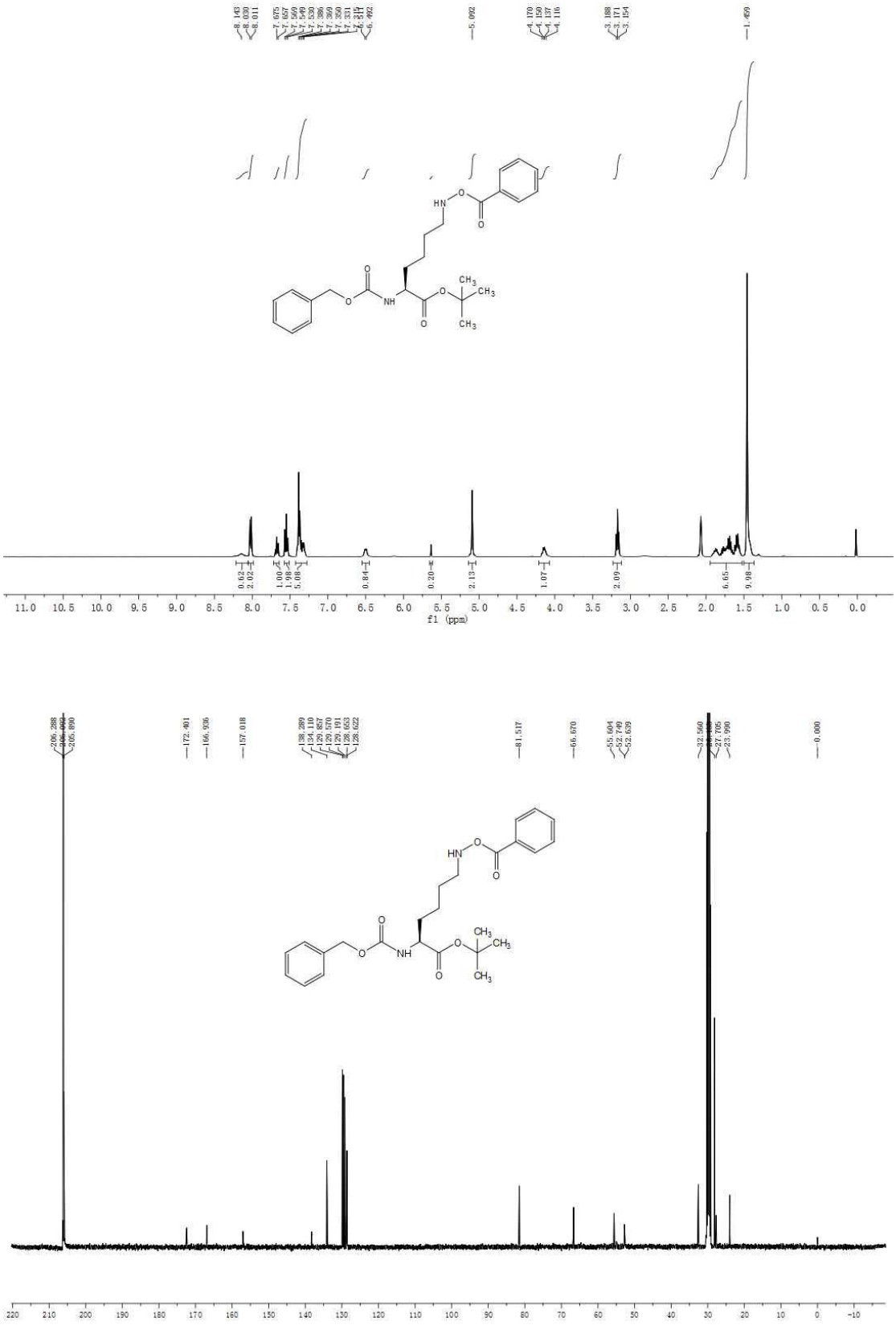


Figure S5: ^{1}H-NMR and ^{13}C-NMR spectra of the intermediate **8**

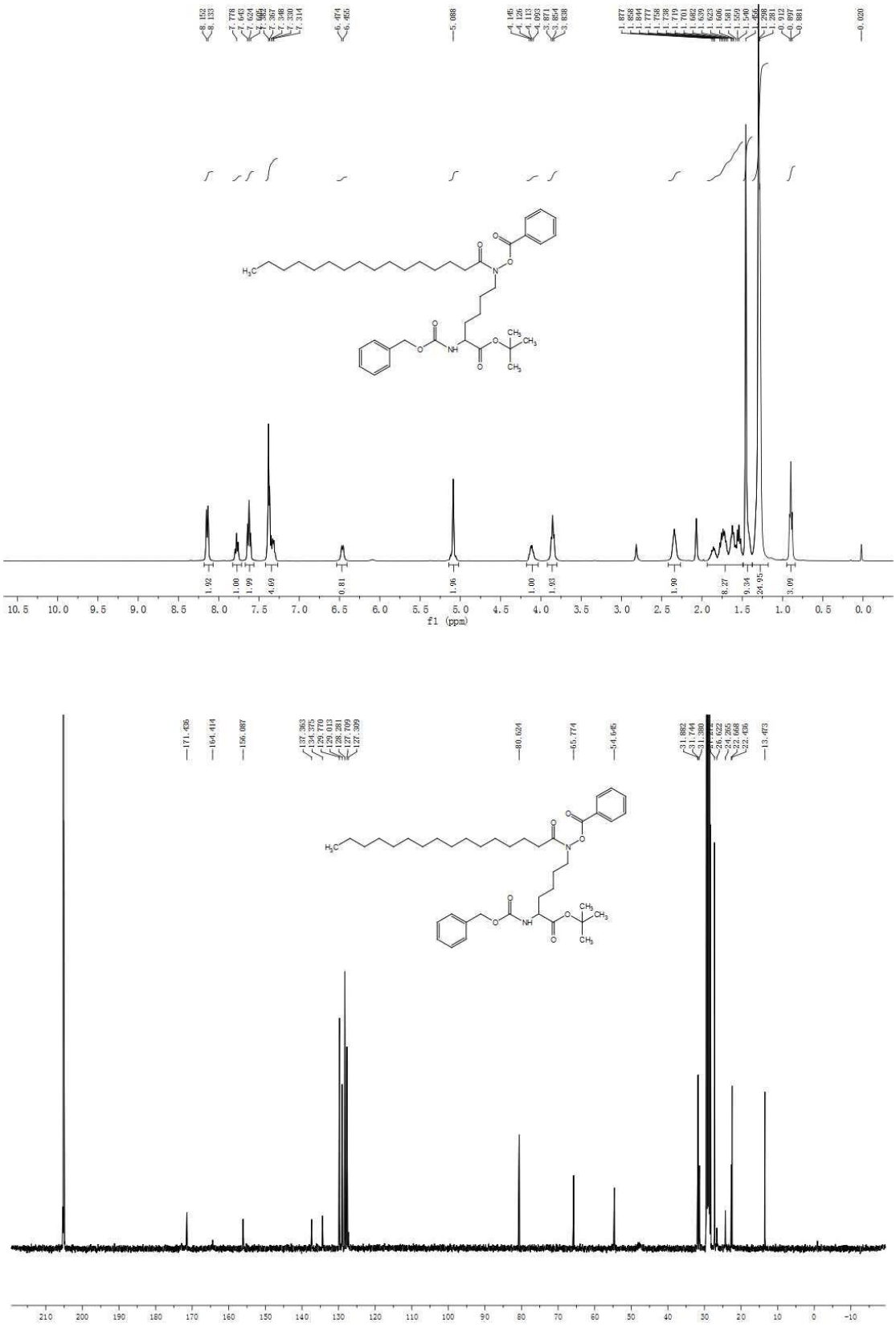


Figure S6: ^{1}H-NMR and ^{13}C-NMR spectra of the intermediate **10**

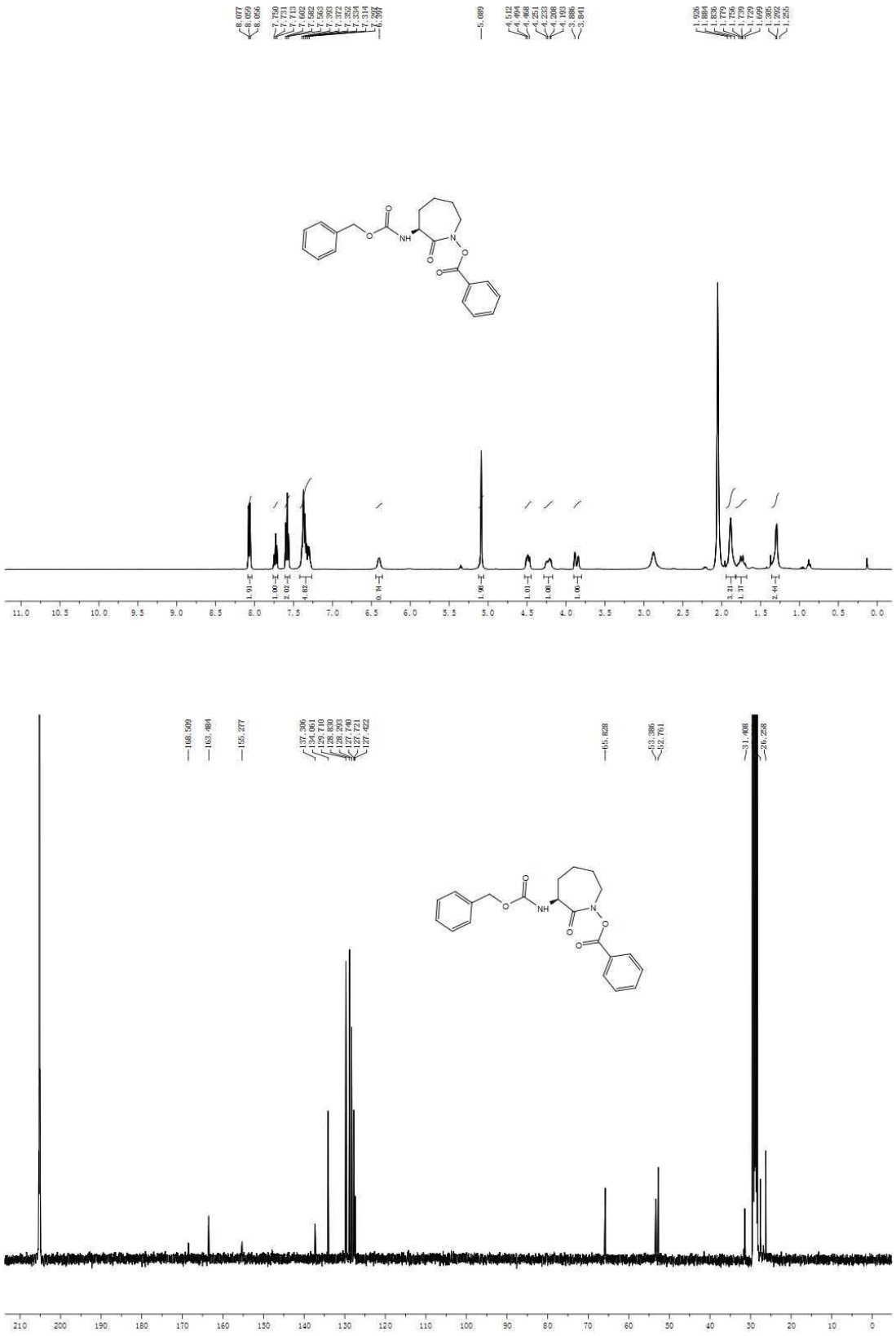


Figure S7: ^{1}H-NMR and ^{13}C-NMR spectra of the intermediate **15**

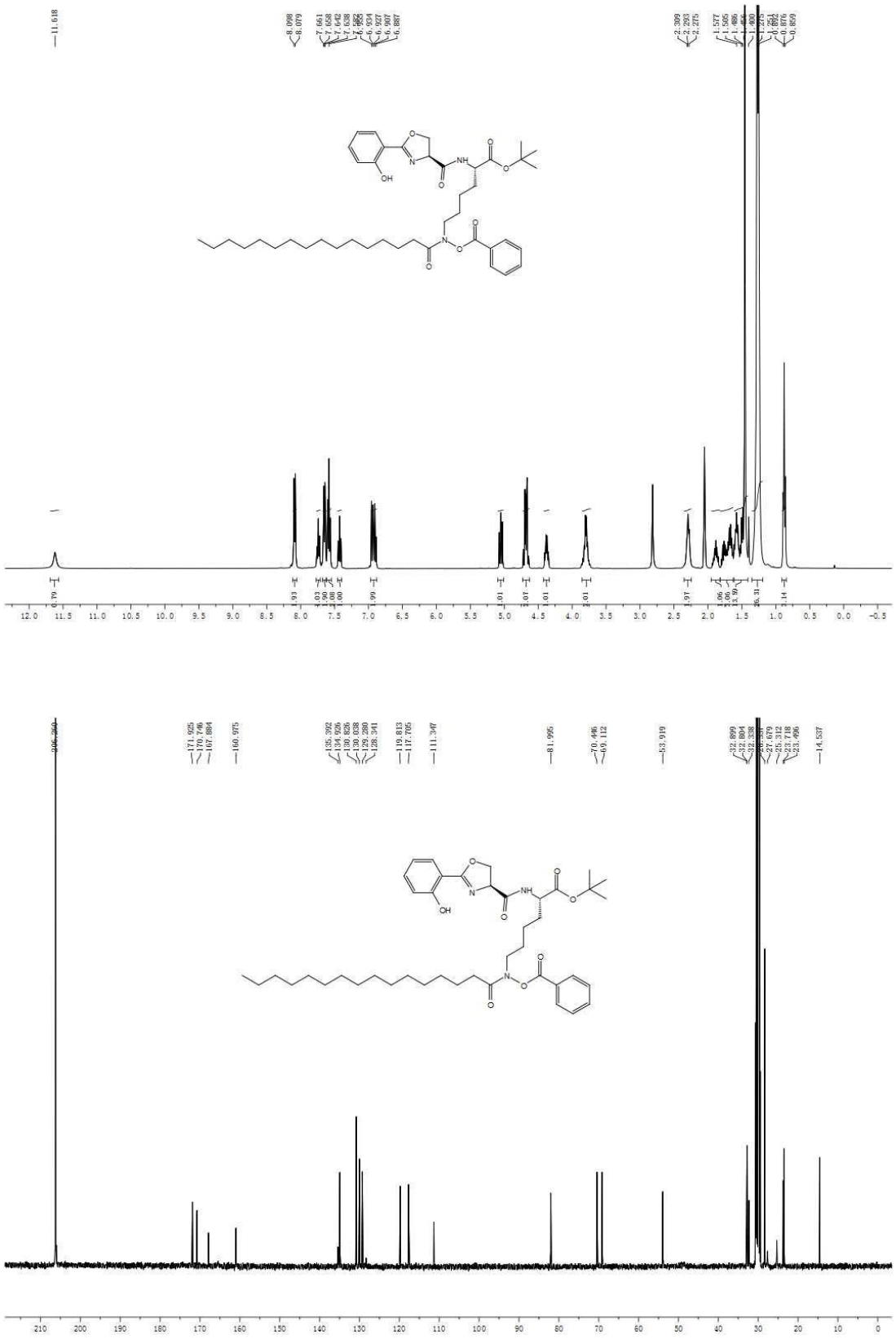


Figure S8: ^{1}H-NMR and ^{13}C-NMR spectra of the intermediate **16**

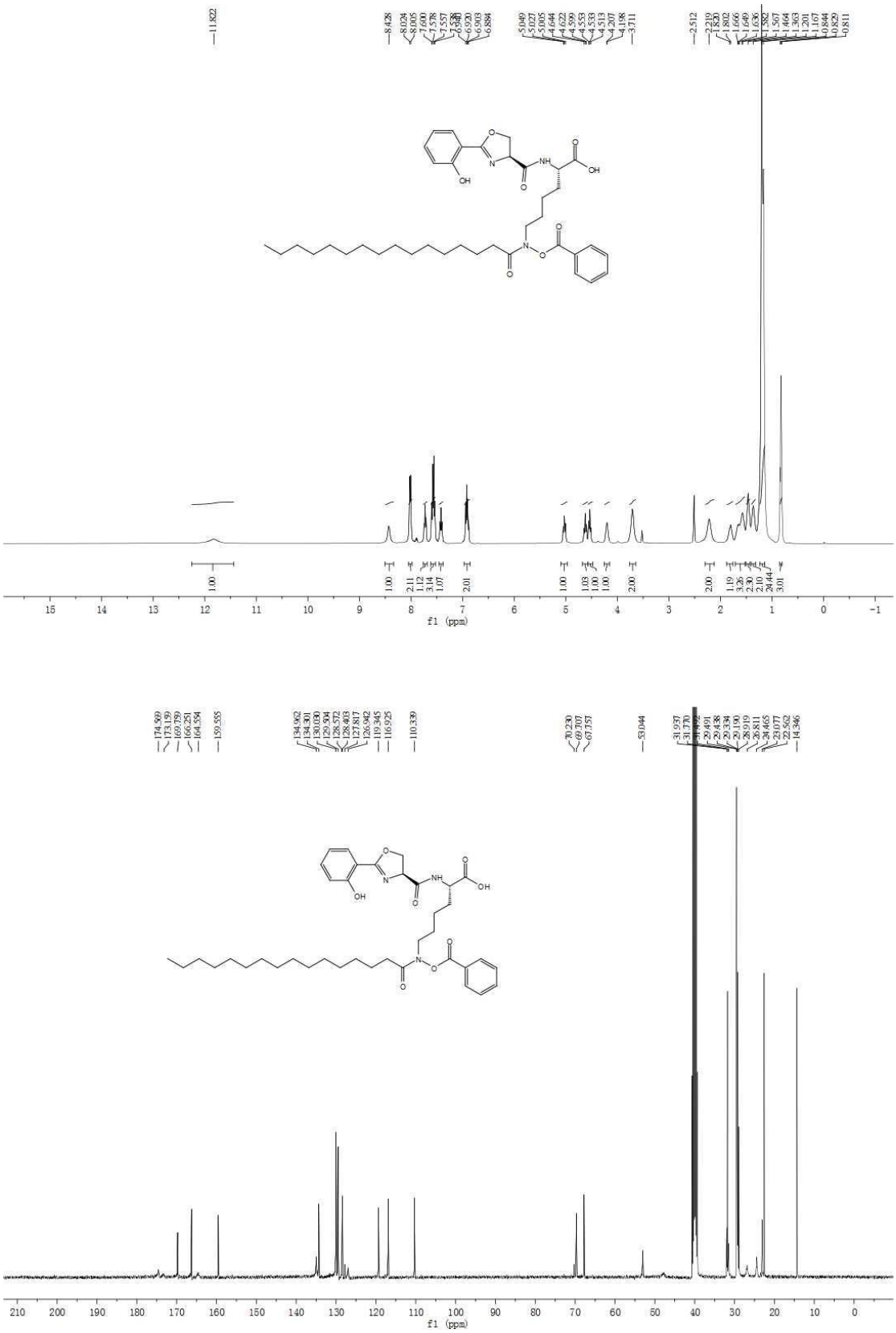


Figure S9: ^{1}H-NMR and ^{13}C-NMR spectra of the intermediate **17**

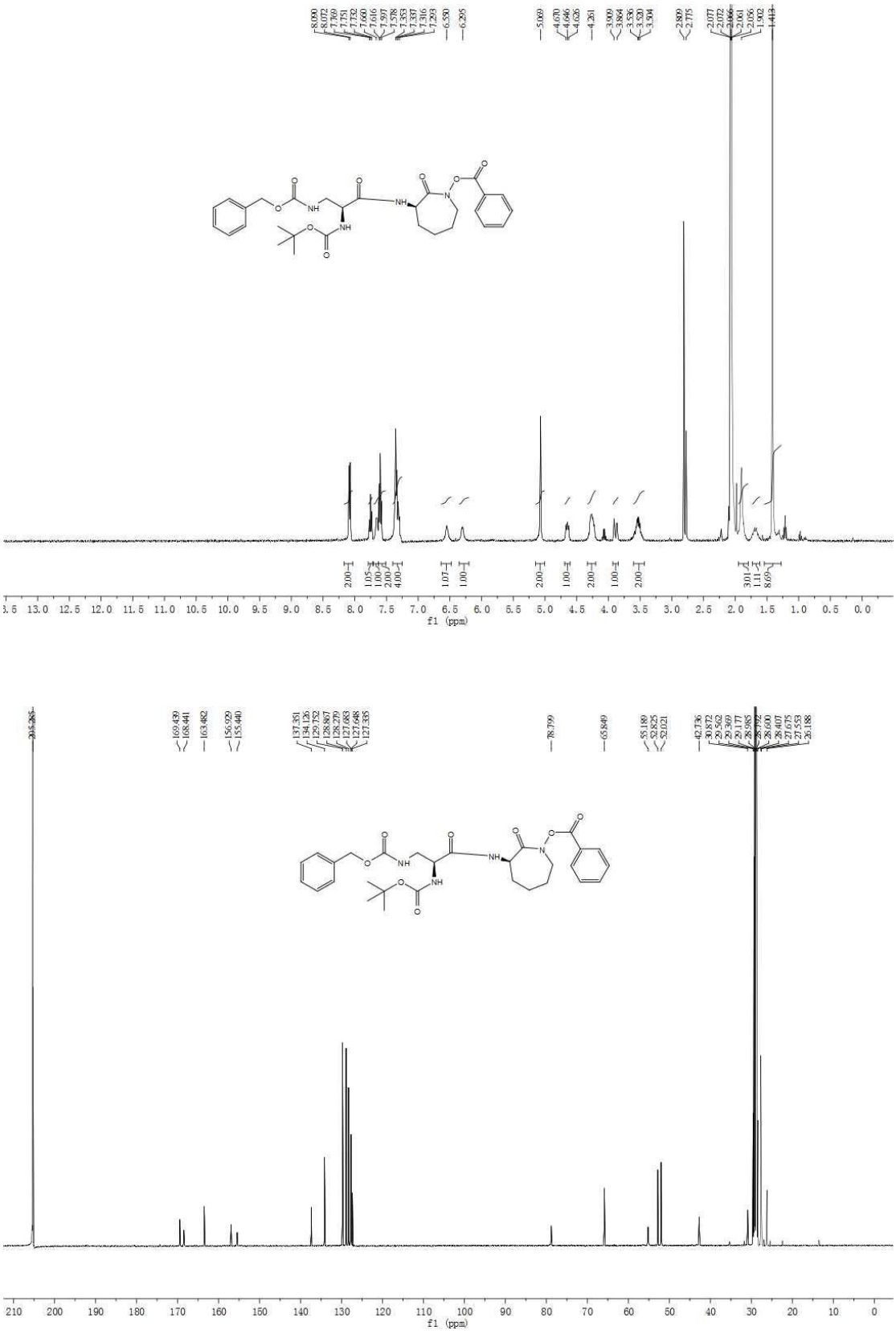
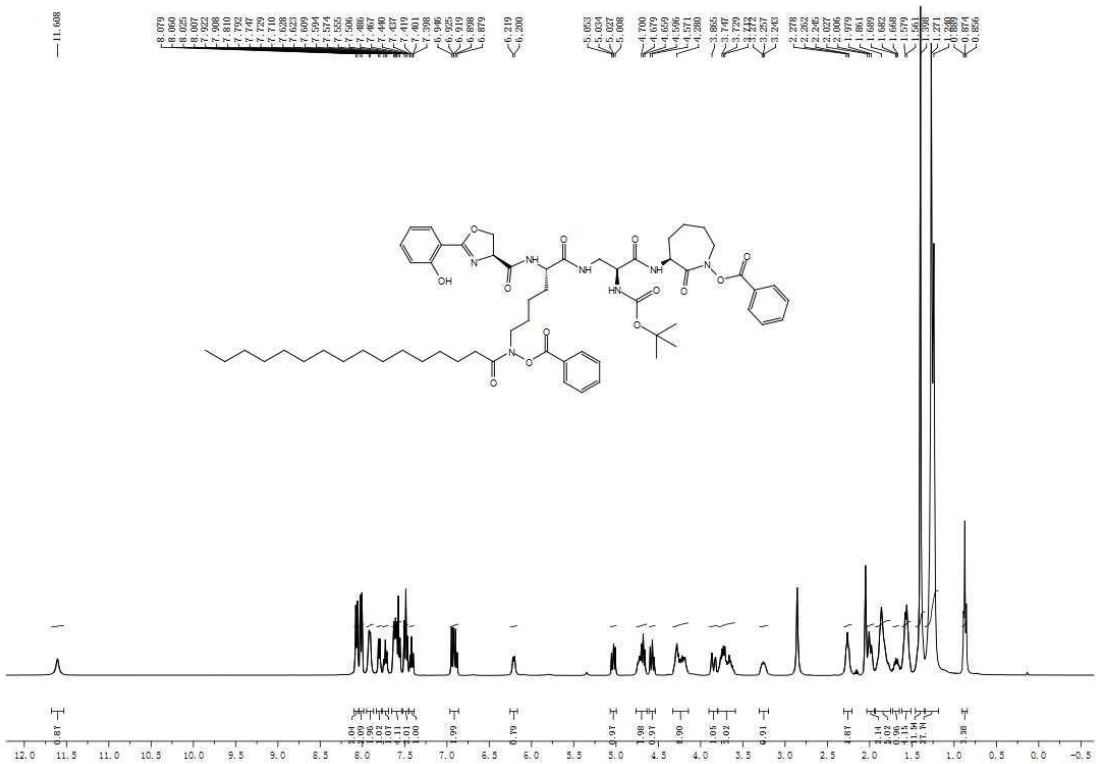
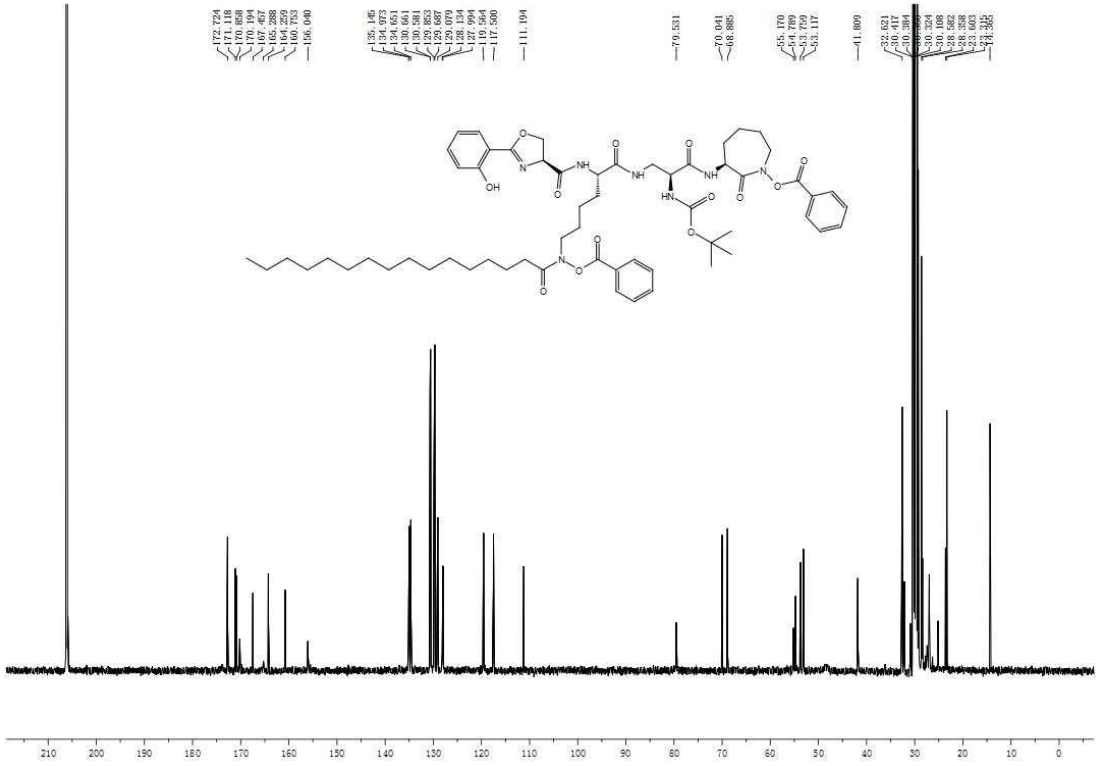


Figure S10: ^{1}H-NMR and ^{13}C-NMR spectra of the intermediate **19**





3. HRMS spectra

Figure S11: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of **MbT-1**

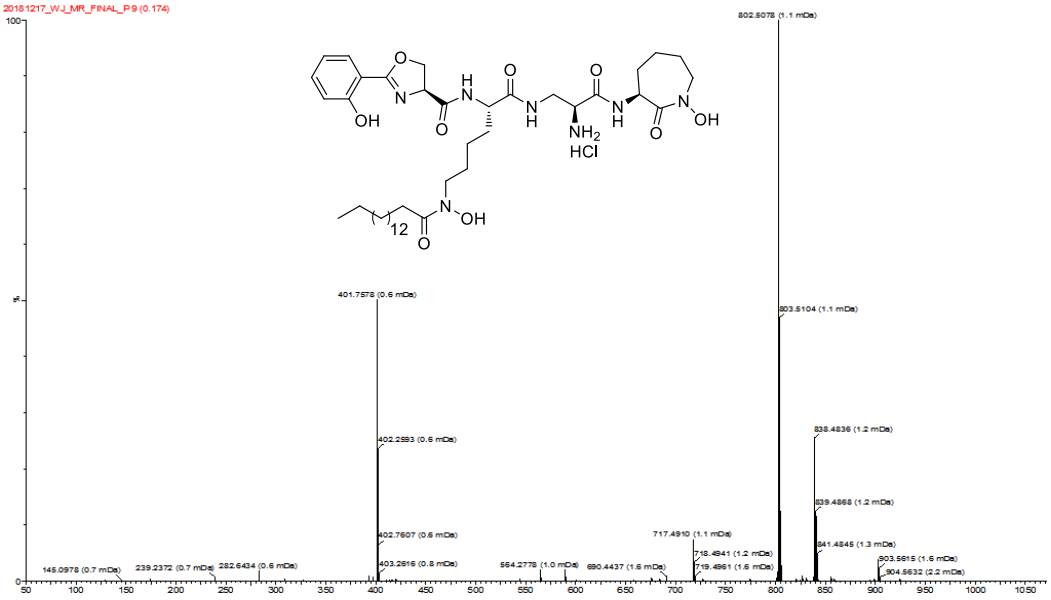


Figure S12: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of the intermediate **4**

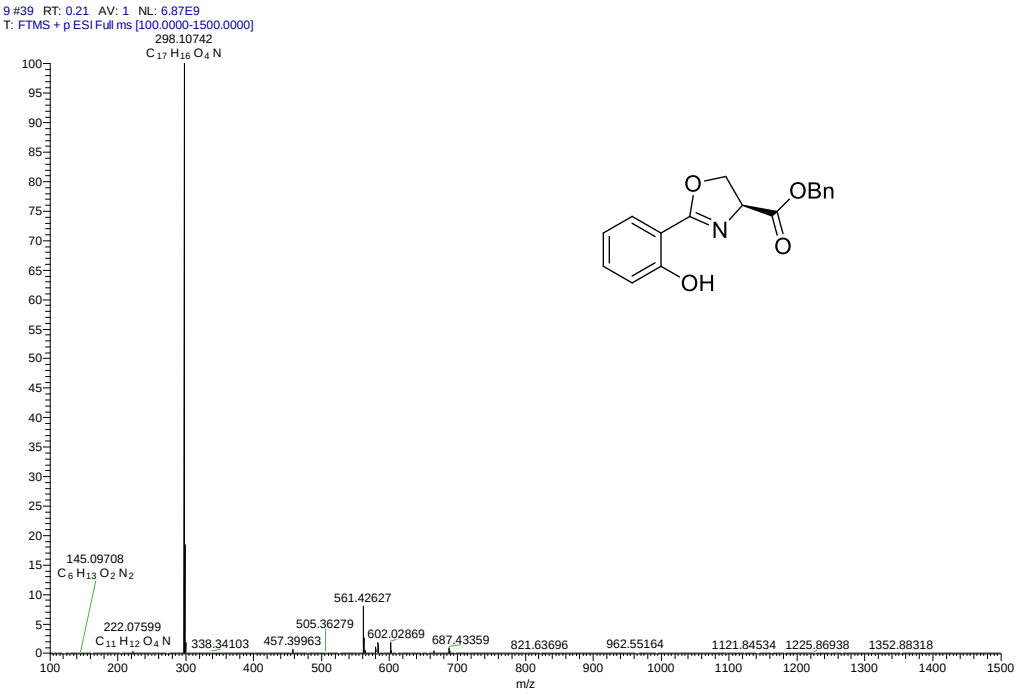


Figure S13: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of the intermediate **A**

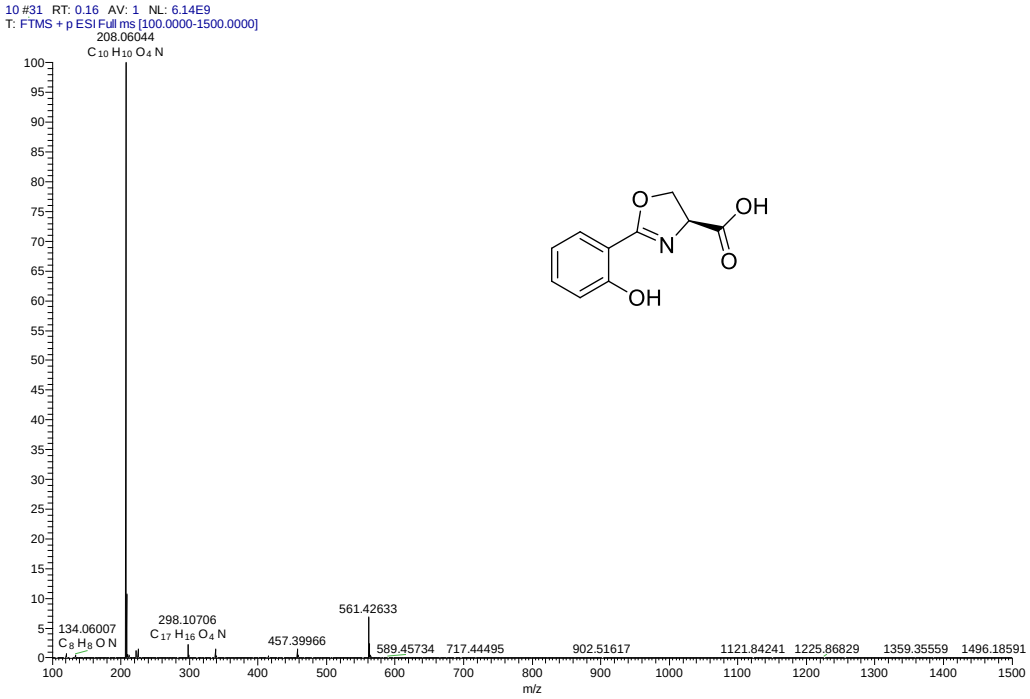


Figure S14: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of the intermediate **7**

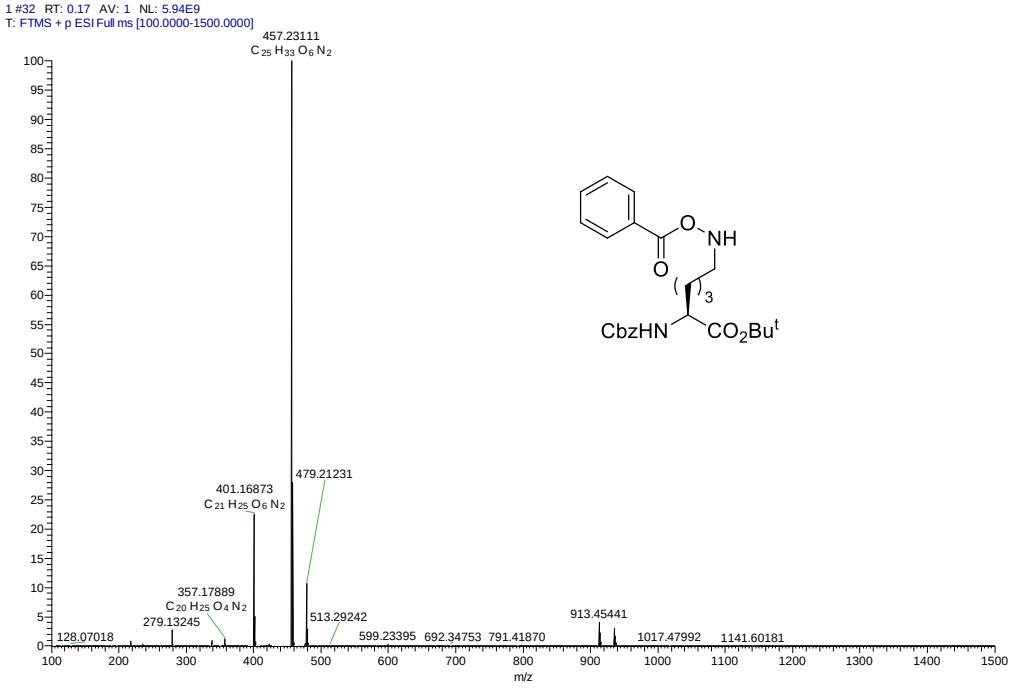


Figure S15: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of the intermediate **8**

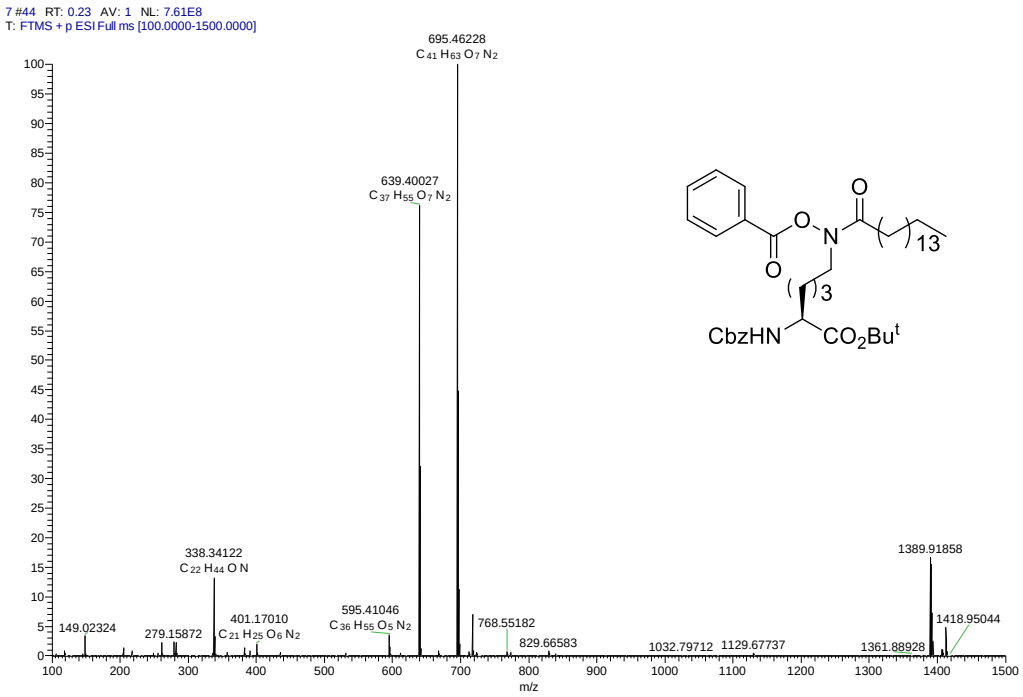


Figure S16: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of the intermediate **10**

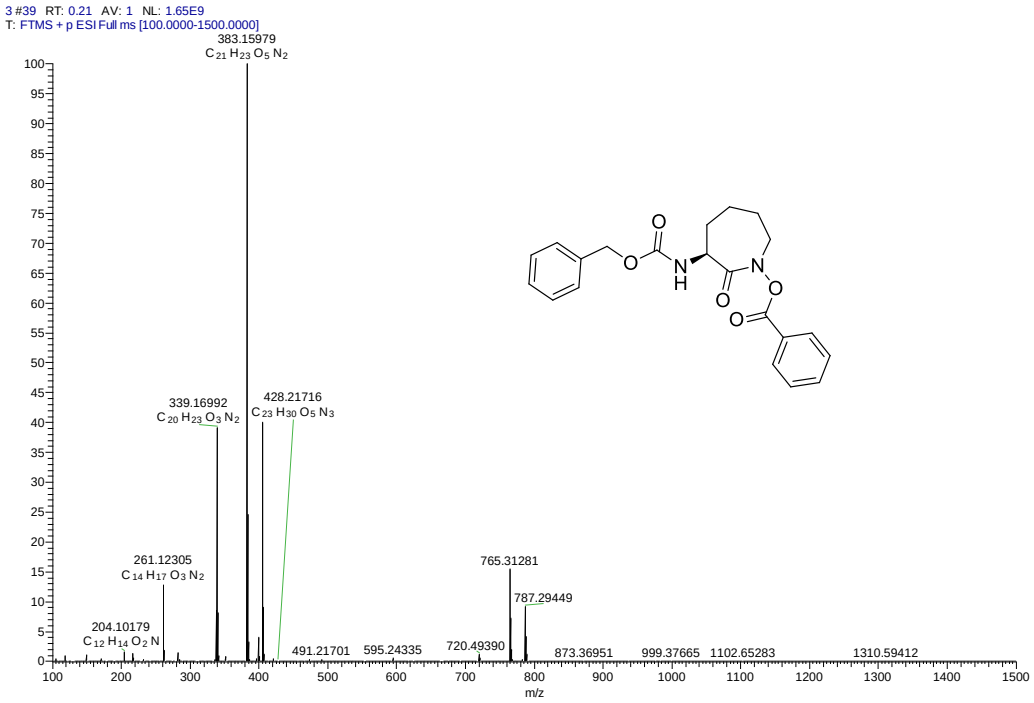


Figure S17: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of the intermediate **11**

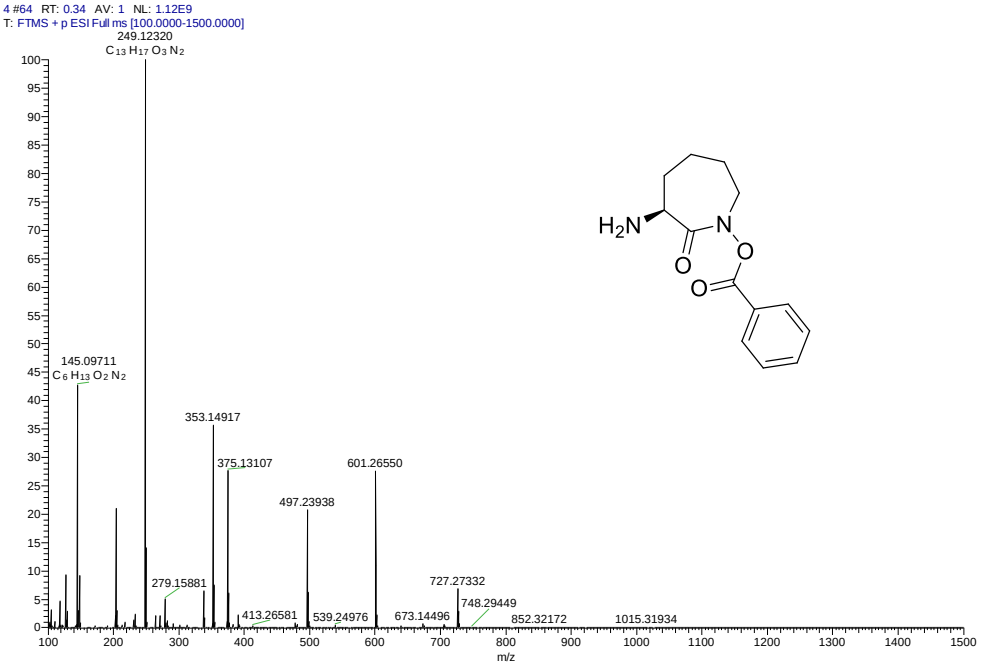


Figure S18: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of the intermediate **15**

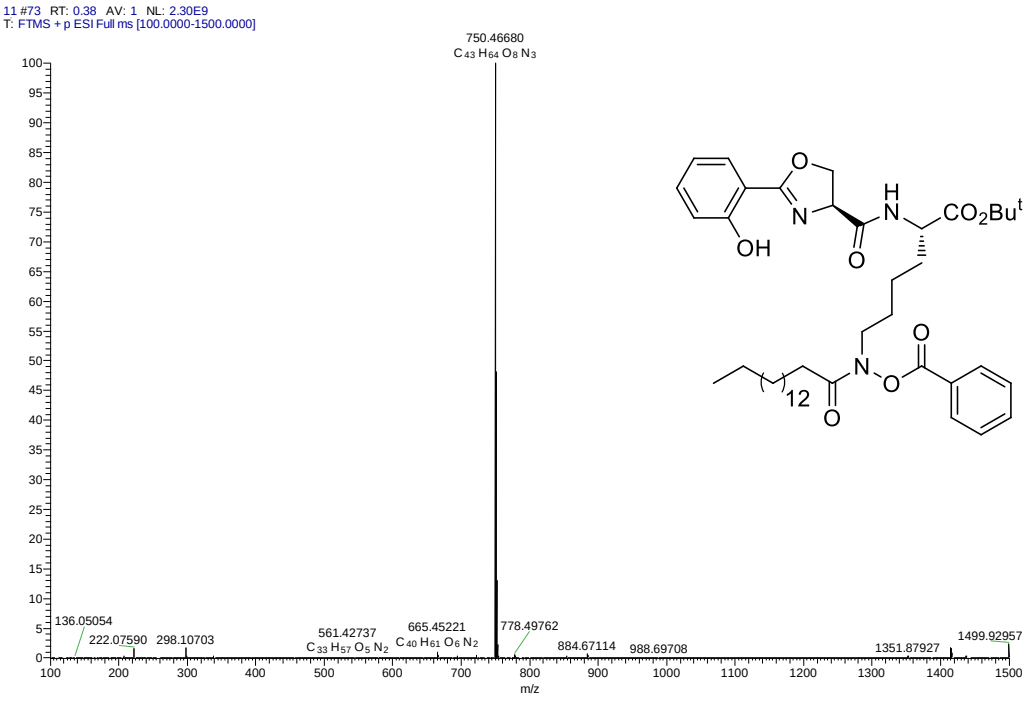


Figure S19: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of the intermediate **16**

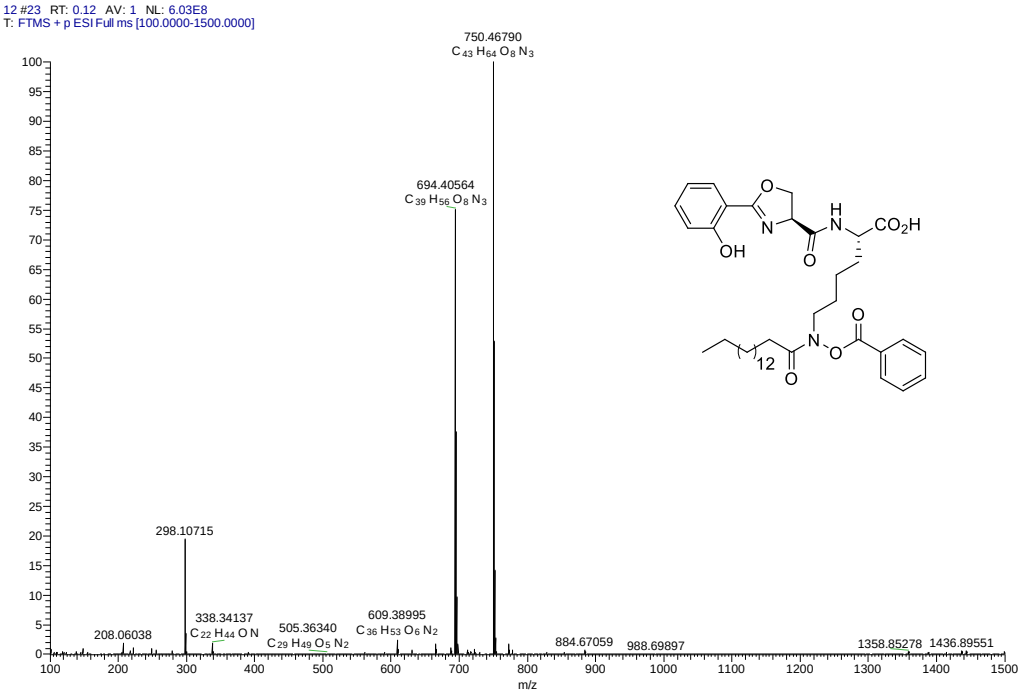


Figure S20: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of the intermediate **17**

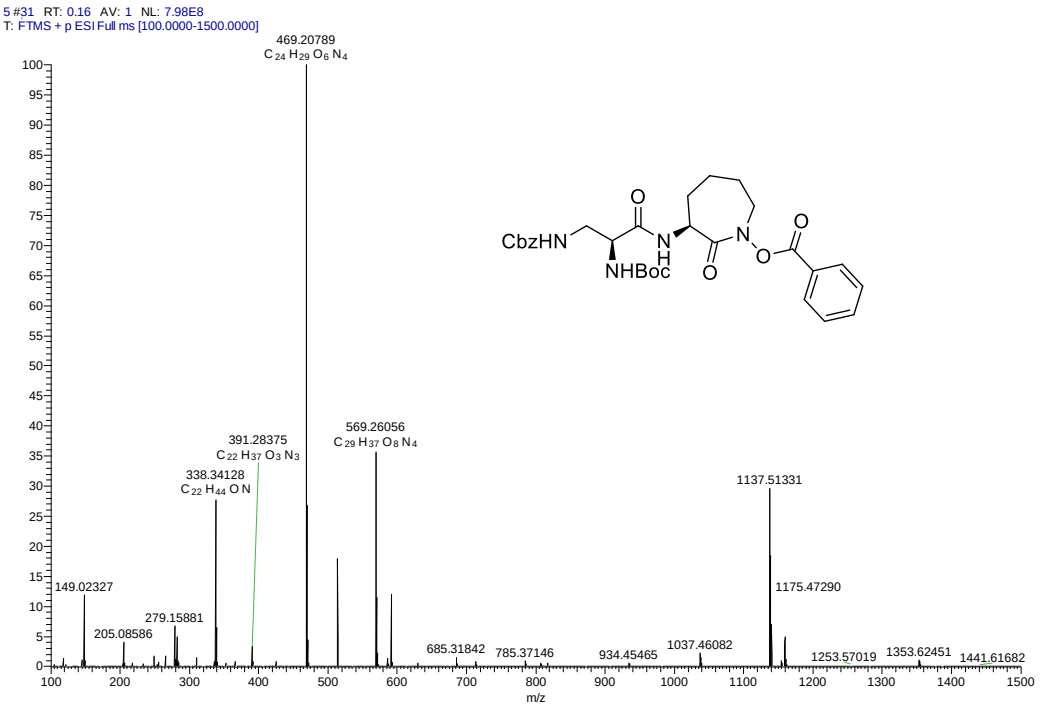


Figure S21: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of the intermediate **18**

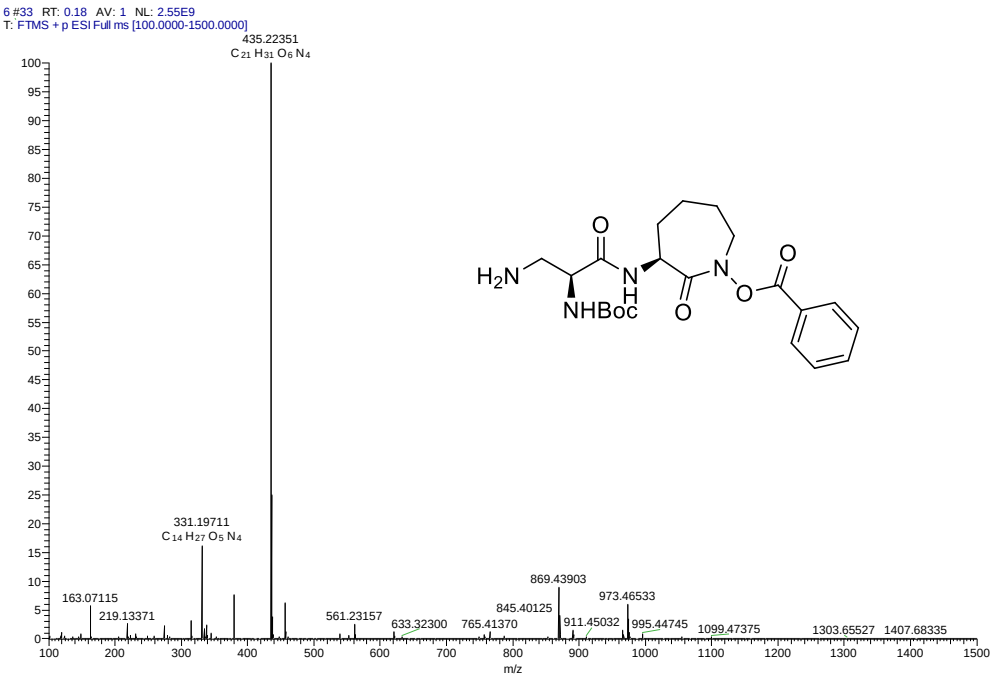


Figure S22: HRMS (ESI-TOF) *m/z*: $[M+H]^+$ spectra of the intermediate **19**