Supporting Information for:

Synthesis of 1,3-Diaminated Stereotriads *via* Rearrangement of 1,4-Diazaspiro[2.2]pentanes

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I. General Information.

All glassware was either oven-dried overnight at 130 °C or flame-dried under a stream of dry nitrogen prior to use. Unless otherwise specified, reagents were used as obtained from the vendor without further purification. Tetrahydrofuran and diethyl ether were freshly distilled from purple Na/benzophenone ketyl. Dichloromethane, acetonitrile and toluene were dried over CaH_2 and freshly distilled prior to use. All other solvents were purified in accordance with "Purification of Laboratory Chemicals".[1] Analytical thin layer chromatography (TLC) was performed utilizing pre-coated silica gel 60 F_{254} plates containing a fluorescent indicator, while preparative chromatography was performed using SilicaFlash P60 silica gel (230-400 mesh) via Still's method.[2] Unless otherwise stated, the mobile phases for column chromatography were mixtures of hexanes/ethyl acetate. Columns were typically run using a gradient method, beginning with 100% hexanes and gradually increasing the polarity using ethyl acetate. Various stains were used to visualize reaction products, including *p*-anisaldehyde, $KMnO_4$, ceric ammonium nitrate (CAM) and phosphomolybdic acid (PMA) in ethanol stain.

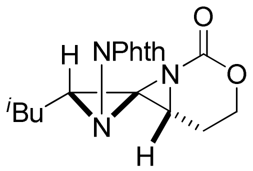
^1H NMR and ^{13}C NMR spectra were obtained using Bruker-300, Varian Inova-500, Varian Unity-500 or Varian Inova-600 NMR spectrometers. For ^1H NMR, chemical shifts are reported relative to residual protiated solvent peaks (δ 7.26, 2.49, 7.15 and 4.80 ppm for $CDCl_3$, $(CD_3)_2SO$, C_6D_6 and CD_3OD respectively). ^{13}C NMR spectra were measured at either 125 MHz or 150 MHz on the same instruments noted above for recording ^1H NMR spectra. Chemical shifts were again reported in accordance to residual protiated solvent peaks (δ 77.0, 39.5, 128.0 and 49.0 ppm for $CDCl_3$, $(CD_3)_2SO$, C_6D_6, and CD_3OD, respectively). IR spectral data were obtained using a Bruker Vector 22 spectrometer using either a thin film or an ATR adapter.

Melting points were obtained with a Mel-Temp II (Laboratory Devices, Inc.) melting point apparatus. High-pressure liquid chromatography (HPLC) analyses were performed at 224 and 254 nm using Shimadzu HPLC, Model LC-20AB. An AD-H column (4.6 µm diameter x 258 mm) at a temperature of 40 ºC was employed, using a flow rate of 1 mL/min and a gradient starting at 10% isopropanol in hexanes for 10 min and increasing to 30% isopropanol in hexanes. The eluant was then held at 30% isopropanol in hexanes until the run was completed. Accurate mass measurements were acquired at the University of Wisconsin, Madison using a Micromass LCT (electrospray ionization, time-of-flight analyzer or electron impact methods). The NMR and Mass Spectrometry facilities are funded by the NSF (CHE-9974839, CHE-9304546, CHE-9208463, CHE-9629688) and the University of Wisconsin, as well as the NIH (RR08389-01).

II. Synthesis of 1,4-Diazaspiro[2.2]pentane Substrates.

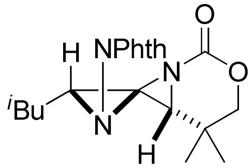
The following 1,4-diazaspiro[2,2]pentanes were prepared according to literature procedures: **7a**, **7b**, **7c**, **7d** and **7e**.[3]

General Procedure. To a mixture of the allenic carbamate (1.0 mmol, 1.0 equiv), $Rh_2(TPA)_4$ or Rh_2esp_2 catalyst (0.025 mmol, 0.025 equiv) and 4Å molecular sieves (500 mg), 10 mL of dry dichloromethane was added. The solution was allowed to stir 10 min to achieve uniformity and PhIO (2.0 mmol, 2.0 equiv) was added in a single portion. The solution was monitored by TLC until complete consumption of the carbamate starting material was indicated, typically 2-4 h. The mixture was then cooled to 0 ºC and treated with *N*-aminophthalimide (1.5 mmol, 1.5 equiv) and dry potassium carbonate (3.5 mmol, 3.5 equiv), followed by PhIO as the oxidant (1.6 mmol, 1.6 equiv). The resulting light yellow slurry was allowed to warm slowly to rt and monitored carefully by TLC. When reaction was complete, the dichloromethane was removed under reduced pressure on a vacuum line, the residue diluted with EtOAc and the organics decanted. The residual salts were washed two more times with EtOAc and the volatiles removed under reduced pressure on a vacuum line. A silica gel column was packed using 99.5:0.5 hexanes/triethylamine, followed by flushing with four column volumes of hexanes prior to loading the sample onto the column to improve the separation and prevent the decomposition of sensitive DASPs. The residue was loaded onto the column and eluted using a hexanes/ethyl acetate gradient. Phenyl iodide eluted first from the column, followed by unreacted MA (if present), then the desired 1,4-diazaspiro[2.2]pentane(s) and finally, *N*-aminophthalimide/hydrolysis products and/or products arising from DASP ring-opening. The DASPs were stored in a freezer at -20 ºC. It was best to run NMRs in deuterated benzene if the sample was to be recovered, as any residual acid in the $CDCl_3$ caused decomposition of the product.



Compound 7g. The product was isolated in 20% overall yield as an off-white solid from the corresponding allenic carbamate. The crude reaction mixture included C-H amination products and unreacted *Z* methylene aziridine. ^{1}H-NMR: (499.9 MHz, $CDCl_3$) δ 7.78 (dd, J = 5.7, 3.1 Hz, 2H), 7.69 (dd, J = 5.7, 3.1 Hz, 1H), 4.59 (ddd, J = 13.4, 11.1, 1.6 Hz, 1H), 4.40 (ddd, J = 10.5, 3.8, 1.6 Hz, 1H), 4.02 (ddd, J = 8.6, 4.8, 0.6 Hz, 1H), 3.88 (dd, J = 9.1, 6.8 Hz, 1H), 2.45 (ddt, J = 14.7, 6.7, 2.2 Hz, 1H), 2.13 (sep, J = 6.8 Hz, 1H), 1.74-1.62 (overlapping signals, 3H), 1.13 (d, J = 6.5 Hz, 3H), 1.05 (d, J = 6.5 Hz, 3H). ^{13}C-NMR: (125.7 MHz, acetone-d_6) δ 164.58, 157.22,

134.35, 130.48, 122.84, 68.96, 66.73, 43.76, 42.34, 38.19, 26.19, 22.44, 22.17, 21.79. HRMS (ESI) *m/z* calculated for $C_{18}H_{19}N_3O_4$ $[M + H]^+$ 342.1449, found 342.1455.

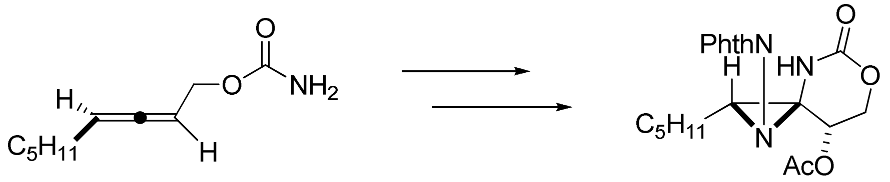


Compound 7h. The product was obtained in 31% overall yield as an off-white solid from the corresponding allenic carbamate. Much of the remaining mass was unreacted *Z* methylene aziridine. ^{1}H-NMR: (499.9 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.69 (dd, *J* = 5.5, 3.0 Hz, 2H), 4.37 (d, *J* = 10.6 Hz, 1H), 4.26 (dd, *J*= 10.6, 3.2 Hz, 1H), 3.82 (d, *J*= 10.6 Hz, 1H), 3.70 (s, 1H), 2.27 (sep of t, *J*= 6.7, 2.1 Hz, 1H), 1.68 (ddd, *J*= 14.2, 8.6, 2.9 Hz, 1H), 1.50 (ddd, *J*= 14.5, 10.5, 4.3 Hz, 1H), 1.32 (s, 3H), 1.19 (d, *J*= 6.6 Hz, 3H), 1.06 (d, *J*= 6.6 Hz, 3H), 0.97 (s, 3H); ^{13}C-NMR: (125.7 MHz, $CDCl_3$) δ 167.97, 160.11, 136.97, 133.14, 126.25, 125.87, 80.68, 79.95, 67.67, 53.91, 47.32, 43.44, 32.29, 28.57, 26.76, 26.11, 24.72, 23.86; HRMS (ESI) *m/z* calculated for $C_{20}H_{23}N_3O_4Na$ $[M + Na]^+$ 392.1581, found 392.1589.

III. Synthesis of Ring-Opened DASPs.

The following acetate-opened DASPs were synthesized according to literature procedures: **5** and the ring-opened **7d**.[3]

General Procedure for Acetic Acid DASP Ring Openings: The DASP was dissolved in enough THF to prepare a 0.1 M solution and cooled to 0 °C. Glacial acetic acid (20.0-25.0 equivalents) was added dropwise to the reaction mixture over 2 min, ensuring that the reaction temperature remained at 0 °C. The reaction was warmed to room temperature and monitored by TLC until complete (24-36 h). After complete consumption of the starting material was indicated by TLC, the reaction mixture was concentrated under reduced pressure and purified *via* column chromatography (hexanes/ethyl acetate gradient) to afford the desired ring-opened DASP as white solids.



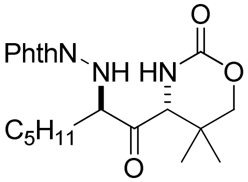
Compound 7f. To a mixture of the allenic carbamate (1.0 mmol, 1.0 equiv), Rh_2esp_2 catalyst (0.025 mmol, 0.025 equiv) and 4Å molecular sieves (500 mg), 10 mL of dry dichloromethane was added. The solution was allowed to stir 10 min to achieve uniformity and PhIO (2.0 mmol, 2.0 equiv) was added in a single portion. The mixture was allowed to stir four hours to ensure complete the methylene aziridine formation, then cooled to 0 °C. $PhthNNH_2$ was added, followed by $PhI(OAc)_2$ and K_2CO_3. The mixture was stirred for 19 h and then was concentrated under reduced pressure. The mixture was redissolved in EtOAc and decanted. The residual salts were washed two more times with EtOAc, and the volatiles were removed under reduced pressure. The residue was loaded onto a silica gel column and eluted using a hexanes/ethyl acetate gradient. The *N, N*–aminal **7f** was obtained in 15% overall yield as a white solid from the corresponding allenic carbamate (estimated 38% yield methylene aziridine formation, 39% diaziridine formation and ring-opening). ^{1}H-NMR: (500.2 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 5.4, 3.2 Hz, 2H), 7.75 (dd, *J* = 5.4, 3.2 Hz, 2H), 6.47 (s, 1H), 4.63 (dd, *J* = 9.2, 3.0 Hz, 1H), 4.44 (t, *J* = 8.6 Hz, 1H), 3.88 (dd, *J* = 8.4, 3.0 Hz, 1H), 3.66 (t, *J* = 6.5 Hz, 1H), 1.99 (s, 3H), 1.78-1.59 (m, 4H), 1.44-1.34 (m, 4H), 0.93 (t, *J* = 6.8 Hz, 3H). ^{13}C-NMR: (125.7 MHz, $CDCl_3$) δ 170.33, 165.69, 159.73, 134.70, 130.21, 123.67, 74.74, 65.66, 56.25, 31.64, 28.93, 26.22, 22.59, 20.84, 14.17. HRMS (ESI) *m/z* calculated for $C_{20}H_{23}N_3O_6$ $[M + Na]^+$ 424.1480, found 424.1495.

IV. Rearrangements of Ring-Opened DASPs to 1,3-Diaminated Ketones.

General Procedure for Rearrangements of Ring-Opened DASPs to 1,3-Diaminated Ketones: The ring-opened DASP was dissolved in enough THF to prepare a 0.1 M solution and 0.05 equivalents of $Bi(OTf)_3$ were added. The reaction was monitored by TLC and was generally completed in 3-4 h. The reaction was quenched with deionized H_2O and the mixture was extracted with EtOAc, dried over Na_2SO_4, concentrated under reduced pressure and immediately purified via column chromatography to afford the desired 1,3-diaminated ketones as white solids.

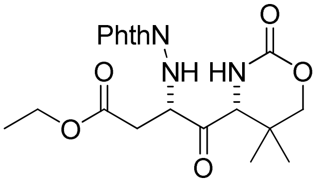
General Procedure for One-pot Ring-Opening/Rearrangements of DASPs to 1,3-Diaminated Ketones. Procedure A: The DASP was dissolved in enough THF to prepare a 0.1 M solution and cooled to 0 °C. Glacial acetic acid (20.0-25.0 equiv) was added dropwise to the reaction mixture over 2 min, ensuring that the reaction temperature remained at 0 °C. The reaction was warmed to room temperature and brought to reflux at 35 ^{o}C. For some substrates, a DASP decomposition product was formed upon heating and reactions were conducted at room temperature. Reactions were monitored by TLC and, upon completion, the reaction was cooled to room temperature and 0.05 equiv $Bi(OTf)_3$ was added to the mixture. The reaction was monitored by TLC and was generally completed in 3-4 h. The reaction was quenched with deionized H_2O and the mixture was extracted with EtOAc, dried over Na_2SO_4, concentrated under reduced pressure and immediately purified via column chromatography to afford the desired 1,3-diaminated ketones as white solids.

Procedure B: For some substrates, a mixture of diastereomers was observed when rearrangements were conducted in the presence of acetic acid. The DASP was dissolved in enough THF to prepare a 0.1 M solution and cooled to 0 °C. Glacial acetic acid (20.0-25.0 equiv) was added dropwise to the reaction mixture over 2 min, ensuring that the reaction temperature remained at 0 °C. The reaction was warmed to room temperature and brought to reflux at 35 ^{o}C. For some substrates, a DASP decomposition product was formed upon heating and reactions were conducted at room temperature. Reactions were monitored by TLC and, upon completion, were cooled to room temperature and quenched with $NaHCO_3$. The resulting mixture was extracted with EtOAc, washed with H_2O, dried over Na_2SO_4 and concentrated under reduced pressure. The resulting mixture was redissolved in enough THF to form a 0.1 M solution, and 0.05 equivalents $Bi(OTf)_3$ were added. The reaction was monitored by TLC and was generally completed in 3-4 h. The reaction was quenched with deionized H_2O and the reaction mixture was extracted with EtOAc, dried over Na_2SO_4, concentrated under reduced pressure and immediately purified *via* column chromatography to afford the desired 1,3-diaminated ketones as white solids.

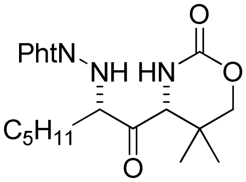


Compound 6. The product was obtained in 96% yield as a white solid from the ring-opened DASP **5**. ^{1}H-NMR: (300.1 MHz, acetone-d_6) δ 7.89-7.83 (m, 4H), 6.71 (br s, 1H), 5.72 (d, J = 4.8 Hz, 1H), 4.43 (d, J = 2.4 Hz, 1H), 4.20 (q, J = 5.4 Hz, 1H), 4.04 (d, J = 11.4 Hz, 1H), 3.89 (d, J = 11.4 Hz, 1H), 1.86-1.71 (m, 1H), 1.68-1.54 (m, 1H), 1.54-1.42 (m, 1H), 1.38-1.24 (overlapping multiplet and singlet, 8H), 1.04 (s, 3H), 0.92-0.85 (m, 3H). ^{13}C-NMR: (125.7 MHz, $CDCl_3$) δ 206.15, 166.68, 152.97, 134.60, 129.88, 123.71, 76.80, 75.22, 66.37, 65.63,

31.71, 29.55, 26.48, 25.34, 23.43, 22.38, 19.29, 13.95. HRMS (ESI) *m/z* calculated for [$C_{21}H_{27}N_3O_5$ + Na^+] 424.1843, found 424.1843.

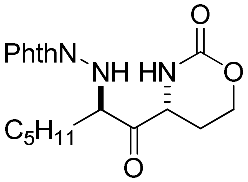


Compound 8b. The product was obtained in 65% yield as a yellow solid from ring opened DASP **7b**. ^{1}H-NMR: (299.9 MHz, acetone-d_6) δ 7.89 (s, 4H), 6.13 (d, *J* = 6.2 Hz, 1H), 6.04 (br s, 1H), 5.22 (dd, *J* = 2.2, 0.7 Hz, 1H), 4.38 (ddd, *J* = 11.1, 6.2, 4.9 Hz, 1H), 4.08 (q, *J* = 7.1 Hz, 2H), 4.01 (d, *J* = 11.0 Hz, 1H), 3.90 (d, *J* = 11.0 Hz, 1H), 3.00-2.82 (m, 2H), 1.38 (s, 3H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.05 (s, 3H). ^{13}C-NMR (75.4 MHz, acetone-d_6) δ 206.83, 171.19, 167.35, 152.19, 134.88, 130.50, 123.49, 73.79, 64.29, 62.76, 60.47, 33.21, 31.05, 23.74, 19.30, 13.75. HRMS (ESI) *m/z* calculated for $C_{20}H_{23}N_3O_7$ [M+Na^+] 440.1429, found 440.1440.

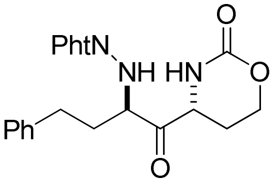


Compound 8c. The product was obtained in 90% yield (average of two runs) from DASP **7c**. ^{1}H-NMR: (499.9 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.4, 3.0 Hz, 2H), 7.76 (dd, *J* = 5.4, 3.0 Hz, 2H), 6.17 (br s, 1H), 5.06 (br s, 1H), 4.66 (d, *J* = 1.7 Hz, 1H), 4.00 (d, *J* = 10.9 Hz, 1H), 3.90 (d, *J* = 10.9 Hz, 1H), 3.65 (td, *J* = 6.7, 5.0 Hz, 1H), 1.80-1.57 (m, 2H), 1.40-1.24 (overlapping singlet and multiplets, 9H), 0.99 (s, 3H), 0.89 (t, *J* = 6.9 Hz, 3H). ^{13}C-NMR: (125.7 MHz, $CDCl_3$) δ 206.10, 166.92, 134.93, 129.96, 124.05, 74.39, 68.28, 65.26, 31.88, 31.59, 28.25, 26.06, 24.73,

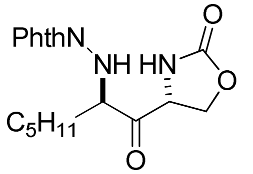
22.61, 20.39, 14.15. HRMS (ESI) *m/z* calculated for [$C_{21}H_{27}N_3O_5$ + Na^+] 402.2024, found 402.2030.



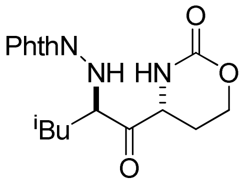
Compound 8d. The product was obtained in 89% yield from the ring-opened DASP **7d** and in 81% from the DASP **7d** itself as a white solid. ^{1}H-NMR (300 MHz, $CDCl_3$), δ 7.86 (m, 4H), 6.39 (br s, 1H), 4.90 (d, *J*= 4.7 Hz, 1H), 4.76 (ddd, *J* =7.5, 5.5, 1.8 Hz, 1H), 4.33 (dd, *J* = 5.5, 5.5 Hz, 2H), 3.90 (m, 1H), 2.39 (m, 1H), 2.05 (m, 1H), 1.74 (m, 2H), 1.33 (m, 6H), 0.90 (m, 3H). ^{13}C-NMR (75.4 MHz, $CDCl_3$) δ 206.55, 166.77, 153.46, 134.86, 129.99, 123.95, 66.88, 65.00, 56.14, 31.73, 30.69, 25.65, 23.72, 22.54, 14.12. HRMS (ESI) *m/z* calculated for $C_{19}H_{23}N_3O_5$ [M+H$^+$] 374.1711, found 374.1711.



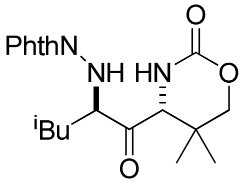
Compound 8e. Obtained in 60% yield from DASP **7e** as an off-white solid. ^{1}H-NMR: (499.9 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.77 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.31-7.27 (m, 2H), 7.22-7.18 (m, 3H), 6.25 (br s, 1H), 5.06 (d, *J* = 6.2 Hz, 1H), 4.56 (ddd, *J* = 7.5, 6.0, 1.9 Hz, 1H), 4.26 (ddd, *J* = 7.1, 3.9, 2.6 Hz, 2H), 3.97 (q, *J* = 6.2 Hz, 1H), 2.82 (t, *J* = 7.7 Hz, 2H), 2.25 (m, 1H) 2.16-1.99 (m, 3H), ^{13}C-NMR: (125.7 MHz, $CDCl_3$) δ 206.43, 166.77, 134.97, 130.01, 128.94, 128.78, 126.77, 124.07, 77.49, 65.64, 64.96, 56.61, 32.41, 31.98, 30.54, 23.73. HRMS (ESI) *m/z* calculated for $C_{22}H_{21}N_3O_5$ [M+H$^+$] 408.1554, found 408.1554.



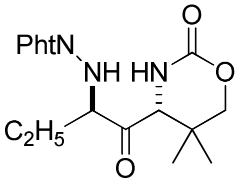
Compound 8f. The product was obtained in 78% yield from ring-opened DASP **7f** as a white solid. ^{1}H-NMR: (500 MHz, CDCl$_3$) δ 7.85 (dd, *J* = 5.6, 3.1 Hz, 2H), 7.77 (dd, *J* = 5.6, 3.1 Hz, 2H), 7.05 (s, 1H), 5.01 (dd, *J* = 9.5, 5.6 Hz, 1H), 4.95 (d, *J* = 5.6 Hz, 1H), 4.62 (t, *J* = 9.5 Hz, 1H), 4.47 (dd, *J* = 9.5, 5.6 Hz, 1H), 3.83 (q, *J* = 6.4 Hz, 1H), 1.80-1.70 (m, 2H), 1.42-1.28 (m, 6H), 0.91-0.86 (m, 3H). ^{13}C-NMR: (125 MHz, CDCl$_3$) δ 208.93, 169.35, 161.58, 137.48, 132.39, 126.55, 69.99, 68.89, 59.71, 34.23, 32.07, 27.92, 25.00, 16.57. HRMS (ESI) *m/z* calculated for $C_{18}H_{21}N_3O_5$ [M+H$^+$] 360.1554, found 360.1549.



Compound 8g. The product was obtained in 57% yield from DASP **7g** as a white solid. ^{1}H-0NMR: (500 MHz, CDCl$_3$) δ 7.85 (dd, *J* = 5.5, 3.4 Hz, 2H), 7.78 (dd, *J* = 5.5, 3.4 Hz, 2H), 6.27 (br s, 1H), 4.87 (d, *J* = 3.9 Hz, 1H), 4.83 (ddd, *J* = 7.7, 5.6, 1.8 Hz, 1H), 4.38-4.29 (m, 2H), 3.96 (td, *J* = 7.5, 3.1 Hz, 1H), 2.42 (dtd, *J* = 13.9, 5.6, 4.5 Hz, 1H), 2.07-1.99 (m, 1H), 1.85 (sep, *J*= 6.9 Hz, 1H), 1.66-1.55 (m, 2H), 0.99 (d, *J* = 6.7 Hz, 3H), 0.98 (d, *J* = 6.7 Hz, 3H). ^{13}C-NMR: (125.7 MHz, CDCl$_3$) δ 206.62, 166.46, 153.00, 134.75, 129.74, 123.84, 65.61, 64.73, 55.62, 39.63, 25.00, 23.92, 22.75, 22.16. HRMS (ESI) *m/z* calculated for $C_{18}H_{21}N_3O_5$ [M+Na$^+$] 382.1374, found 382.1374.



Compound 8h. The product was obtained in 77% yield from DASP **7h** as a white solid. ^{1}H-NMR: (500 MHz, CDCl$_3$) δ 7.84 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.76 (dd, *J* = 5.5, 3.0 Hz, 2H), 6.91 (br s, 1H), 5.11 (d, *J* = 4.9 Hz, 1H), 4.24 (d, *J* = 1.3 Hz, 1H), 4.10 (ddd, *J* = 10.8, 6.0, 5.1 Hz, 1H), 3.98 (s, 2H), 1.87 (sep, *J* = 6.6 Hz, 1H), 1.55 (ddd, *J* = 14.1, 7.0, 6.3 Hz, 1H), 1.50 (ddd, *J* = 14.1, 7.0, 6.3 Hz, 1H), 1.21 (s, 3H), 1.00 (s, 3H), 0.96 (d, *J* = 6.6 Hz, 6H). ^{13}C-NMR: (125.7 MHz, CDCl$_3$) δ 206.38, 166.88, 153.00, 134.89, 130.04, 124.02, 70.84, 65.98, 64.66, 38.54, 31.98, 24.64, 23.52, 23.07, 22.52, 19,49. HRMS (ESI) *m/z* calculated for $C_{20}H_{25}N_3O_5$ [M+H$^+$] 390.2024, found 390.2032.

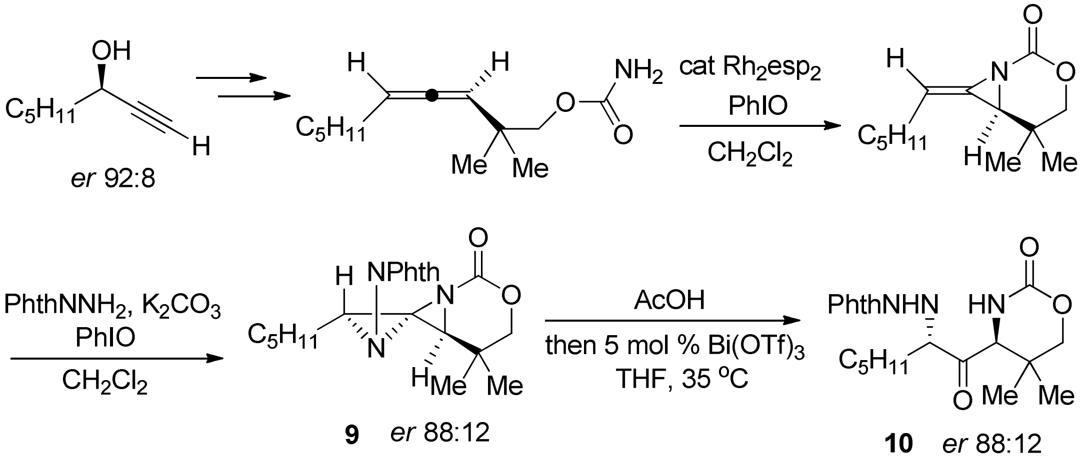


Compound 14a. Obtained as a white powder from the corresponding ring-opened DASP in 66% yield. ^{1}H-NMR: (299.9 MHz, CDCl$_3$) δ 7.85 (m, 2H), 7.76 (m, 2H), 6.81 (br s, 1H), 5.08 (d, 1H), 4.21 (d, 1H), 4.03 – 3.94 (overlapping multiplets, 3H), 1.89-1.65 (overlapping multiplets, 2H), 1.23 (s, 3H), 1.04 (s, 3H), 1.02 (t, 3H); ^{13}C NMR: (125.8 MHz, CDCl$_3$) δ 205.79, 166.85, 152.90, 134.89, 130.06, 124.01, 75.68, 67.81, 66.29, 32.12, 26.73, 23.51, 22.94, 19.39; HRMS (ESI) *m/z* calculated for $C_{18}H_{21}N_3O_5$ [M+Na$^+$] 382.1374, found 382.1371.

General Procedure for the One-Pot Oxidation of Allenes to 1,3-Diaminated Ketones: To a mixture of the allenic carbamate (1.0 mmol, 1.0 equiv), Rh$_2$(TPA)$_4$ or Rh$_2$esp$_2$ catalyst (0.025

mmol, 0.025 equiv) and 4Å molecular sieves (500 mg), 10 mL of dry dichloromethane was added. The solution was allowed to stir 10 min to achieve uniformity and PhIO (2.0 mmol, 2.0 equiv) was added in a single portion. The solution was monitored by TLC until consumption of the carbamate starting material, typically 2-4 h. The mixture was then cooled to 0 ºC and treated with *N*-aminophthalimide (1.5 mmol, 1.5 equiv) and dry potassium carbonate (3.5 mmol, 3.5 equiv), followed by PhIO as the oxidant (1.6 mmol, 1.6 equiv). The resulting light yellow slurry was allowed to warm slowly to rt and monitored carefully by TLC. When reaction was complete, the dichloromethane was removed under reduced pressure on a vacuum line, the residue diluted with EtOAc and the organics decanted. The residual salts were washed two more times with EtOAc and the volatiles removed under reduced pressure on a vacuum line. The mixture was dissolved in enough THF to prepare a 0.1 M solution and cooled to 0 °C. Glacial acetic acid (20.0-25.0 equivalents) was added dropwise to the reaction mixture over 2 min, ensuring that the reaction temperature remained at 0 °C. The reaction was warmed to room temperature. The reaction was monitored by TLC and, upon completion, was quenched with $NaHCO_3$. The resulting mixture was extracted with EtOAc, washed with H_2O dried over Na_2SO_4, and concentrated under reduced pressure. The resulting mixture was redissolved in enough THF to form a 0.1 M solution, and 0.05 equivalents $Bi(OTf)_3$ were added. The reaction was monitored by TLC and was generally completed in 3-4 h. The reaction was quenched with deionized H_2O and the reaction mixture was extracted with EtOAc, dried over Na_2SO_4, concentrated under reduced pressure and immediately purified via column chromatography (hexanes/ethyl acetate gradient) to afford the desired 1,3-diaminated ketones as white solids.

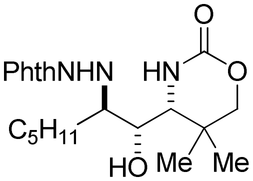
V. Verification of the Transfer of Axial Chirality from the DASP 9 to the 1,3-Diaminated Ketone 10. The enantioenriched DASP **9** was prepared according to literature procedure.[3]



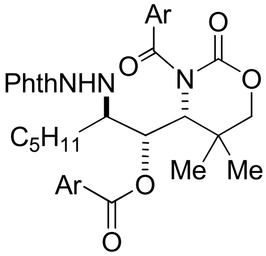
The enantioenriched propargyl alcohol was prepared according to literature procedure.[4] The same procedure previously reported for the synthesis of racemic DASPs was used to prepare the enantioenriched sample. High-pressure liquid chromatography (HPLC) analyses were performed at 224 and 254 nm using Shimadzu HPLC, Model LC-20AB. An AD-H column (4.6 μm diameter x 258 mm) at a temperature of 40 ºC was employed, using a flow rate of 1 mL/min and a gradient starting at 10% isopropanol in hexanes for 10 min and increasing to 30% isopropanol in hexanes. The eluant was then held at 30% isopropanol in hexanes until the run was completed. The reaction for the conversion of **9** to **10** followed the general procedure and the HPLC was run in the same manner as described above.

VI. Reductions of 1,3-Diaminated Ketones.

General Procedure: The 1,3-diaminated ketone was dissolved in enough dichloromethane to make a 0.01 M solution. Glacial acetic acid (5.0 equiv) was added and the mixture was allowed to stir for 30 min. Portions of $Na(OAc)_3BH$ (3.0 equiv) were added at hourly intervals, and the reaction was sonicated for 30 min after each addition. Typically, 6-7 portions were required to bring the reaction near completion, while further additions had little effect on yield. The reaction mixture was quenched with saturated $NaHCO_3$, extracted with dichloromethane, and purified via column chromatography (hexanes/ethyl acetate gradient) to yield the desired 1,3-diaminated alcohol.

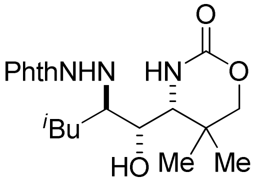


Compound 11. Obtained as a white powder from diaminoketone **6** in 70% yield as a 9:1 mixture of diastereomers. ^{1}H-NMR: (499.9 MHz, acetone-d$_6$) δ 7.88 (s, 4H), 7.09 (s, 1H), 5.13 (d, *J* = 8.5 Hz, 1H), 4.31 (d, *J* = 6.9 Hz, 1H), 3.91 (d, *J* = 11.4 Hz, 1H), 3.88 (ddd, *J* = 8.7, 6.8, 2.0 Hz, 1H), 3.81 (d, *J* = 11.4 Hz, 1H), 3.46 (dd, *J* = 9.0, 2.1 Hz, 1H), 3.25 (tdd, *J* = 8.4, 5.5, 2.0 Hz, 1H), 1.84-1.75 (m, 1H), 1.61 (m, 1H), 1.51-1.42 (m, 1H), 1.38-1.22 (m, 5H), 1.20 (s, 3H), 1.15 (s, 3H), 0.85-0.81 (t, 3H). ^{13}C-NMR: (125.7 MHz, acetone-d$_6$) δ 208.06, 207.90, 207.75, 169.35, 154.87, 137.11, 133.15, 125.77, 76.74, 72.67, 64.56, 63.37, 34.61, 33.48, 28.34, 26.91, 25.00, 21.80, 16.04. HRMS (ESI) *m/z* calculated for $C_{21}H_{29}N_3O_5$ [M+H$^+$] 404.2180, found 404.2175.

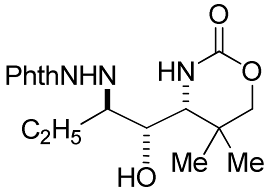


Compound 12. The alcohol **11** (10.0 mg, 0.025 mmol, 1 equiv) was dissolved in 0.5 mL of dichloromethane and treated with *p*-nitrobenzoyl chloride (91.6 mg, 0.50 mmol, 20 equiv) and triethylamine (0.50 mmol, 20 equiv). The reaction mixture was stirred at rt for 48 h, then

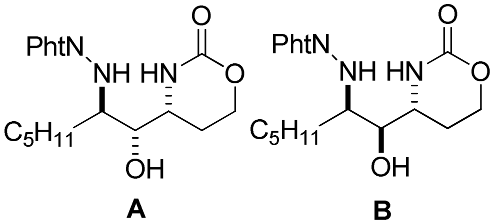
quenched with 15% NaOH solution. The mixture was extracted with portions of dichloromethane, the combined organics washed with brine, dried over Na_2SO_4 and the volatiles removed under reduced pressure. The residue was purified twice by column chromatography (hexanes/ethyl acetate gradient). The resulting solid was dissolved in a minimum amount of ethyl acetate in a vial. The vial was placed inside a larger vial containing pentane; vapor diffusion provided X-ray quality crystals of **11**. The structure was verified by X-ray crystallography (see Section VIII).



Compound 13. The product was obtained as a white powder from the 1,3-diamino-2-one **8h** in 66% yield as a 9:1 mixture of diastereomers. ^{1}H-NMR: (499.9 MHz, $CDCl_3$) δ 7.88 (dd, J = 5.5, 3.1 Hz, 2H), 7.76 (dd, J = 5.5, 3.1 Hz, 2H), 7.17 (br s, 1H), 4.70 (d, J = 8.8 Hz, 1H), 3.90 (d, J = 11.0 Hz, 1H), 3.83 (d, J = 11.0 Hz, 1H), 3.71 (ddd, J = 8.3, 5.9, 1.7 Hz, 1H), 3.41 (dd, J = 8.9, 2.4 Hz, 1H), 3.33-3.26 (m, 1H), 1.95 (d, J = 6.0 Hz, 1H), 1.71-1.58 (m, 2H), 1.46-1.38 (m, 1H), 1.25 (s, 3H), 1.15 (s, 3H), 0.95 (d, J = 6.5 Hz, 3H), 0.83 (dd, J = 6.5 Hz, 3H). ^{13}C-NMR: (125.7 MHz, $CDCl_3$) δ 169.51, 137.23, 132.68, 126.52, 79.93, 79.67, 79.42, 79.06, 78.97, 78.86, 78.05, 76.97, 73.99, 63.42, 61.75, 41.47, 33.64, 27.70, 27.54, 26.12, 24.72, 22.67. HRMS (ESI) *m/z* calculated for $[C_{21}H_{27}N_3O_5+H^+]$ 404.2180, found 404.2175.



Compound 14. The product was obtained as a 9:1 mixture of diastereomers in 57% yield as a white powder. 1H NMR: (500.2 MHz, $CDCl_3$) δ 7.89-7.82 (m, 2H), 7.78-7.72 (m, 2H), 4.78 (d, J = 9.8 Hz, 1H), 3.93 (d, J = 11.2 Hz, 1H), 3.82 (dd, J = 11.2, 1.1 Hz, 1H), 3.77 (ddd, J = 8.0, 6.6, 1.3 Hz, 1H), 3.43 (ddd, J = 8.6, 3.2, 0.8 Hz, 1H), 3.14 (tdd, J = 9.6, 5.2, 1.7 Hz, 1H), 2.06 (d, J = 5.9 Hz, 1H), 1.77-1.64 (m, 2H), 1.27 (s, 3H), 1.15 (s, 3H), 0.92 (t, J = 7.6 Hz, 3H); ^{13}C-NMR: (125.7 MHz, $CDCl_3$) δ 167.08, 153.76, 134.73, 130.27, 124.00, 74.22, 70.71, 62.50, 60.91, 31.15, 29.91, 25.27, 22.84, 20.50, 10.72. HRMS (ESI) *m/z* calculated for [$C_{18}H_{23}N_3O_5+H^+$] 362.1711, found 362.1719.



Compound 15. The general procedure was followed using only 2.5 equivalents of $Na(OAc)_3BH$, and the reaction was completed within two hours. The compound was obtained as a white solid in 65% yield as a 1.7:1 mixture of diastereomers. The diastereomers were not separated. ^{1}H-MR: (500.2 MHz, $CDCl_3$) δ 7.90-7.86 (m, 2H, **B**), 7.85-7.81 (m, 2H, **A**), 7.81-7.77 (m, 2H, **B**), 7.76-7.71 (m, 2H, **A**), 6.97 (d, *J* = 2.7 Hz, 1H, **A**), 6.04 (br s, 1H, **B**), 4.95 (d, *J* = 8.4 Hz, 1H, **A**), 4.57 (d, *J* = 3.2 Hz, 1H, **B**), 4.36-4.25 (m, 2H **A**, 2H **B**), 4.18 (td, *J* = 12.1, 1.9 Hz, 1H, **A**), 3.99 (d, *J* = 1.9 Hz, 1H, **B**), 3.89-3.84 (m, 1H, **A**), 3.65-3.54 (m, 1H, **A**, 1H, **B**), 3.29 (d, *J* = 8.3 Hz, 1H, **B**), 3.19 (tdd, *J* = 3.0, 5.1, 8.1 Hz, 1H, **A**), 3.10 (dq, J = 3.0, 8.3 Hz, 1H, **B**), 2.19-2.13 (m, 1H **A**, 1H

B), 1.87-1.17 (m, 9H, **A**, 9H, **B**), 0.93 (t, *J* = 7.4 Hz, 3H, **B**), 0.83 (t, *J* = 5.9 Hz, 3H, **A**); ^{13}C NMR: (125.8 MHz, $CDCl_3$) δ 167.69, 167.22, 154.90, 153.92, 135.01, 134.65, 130.27, 130.01, 124.11, 123.85, 73.42, 72.49, 65.26, 64.51, 60.94, 60.37, 52.07, 51.85, 32.16, 31.99, 30.09, 26.52, 25.91, 25.86, 23.87, 23.30, 22.72, 14.21, 14.17; HRMS (ESI) *m/z* calculated for $C_{19}H_{25}N_3O_5$ [M+H$^+$] 376.1867, found 376.1874.

VII. References.

1) Armarego, W.L.F.; Chai, C.L.L. *Purification of Laboratory Chemicals* 6th ed., Elsevier: Burlington, MA, 2009.

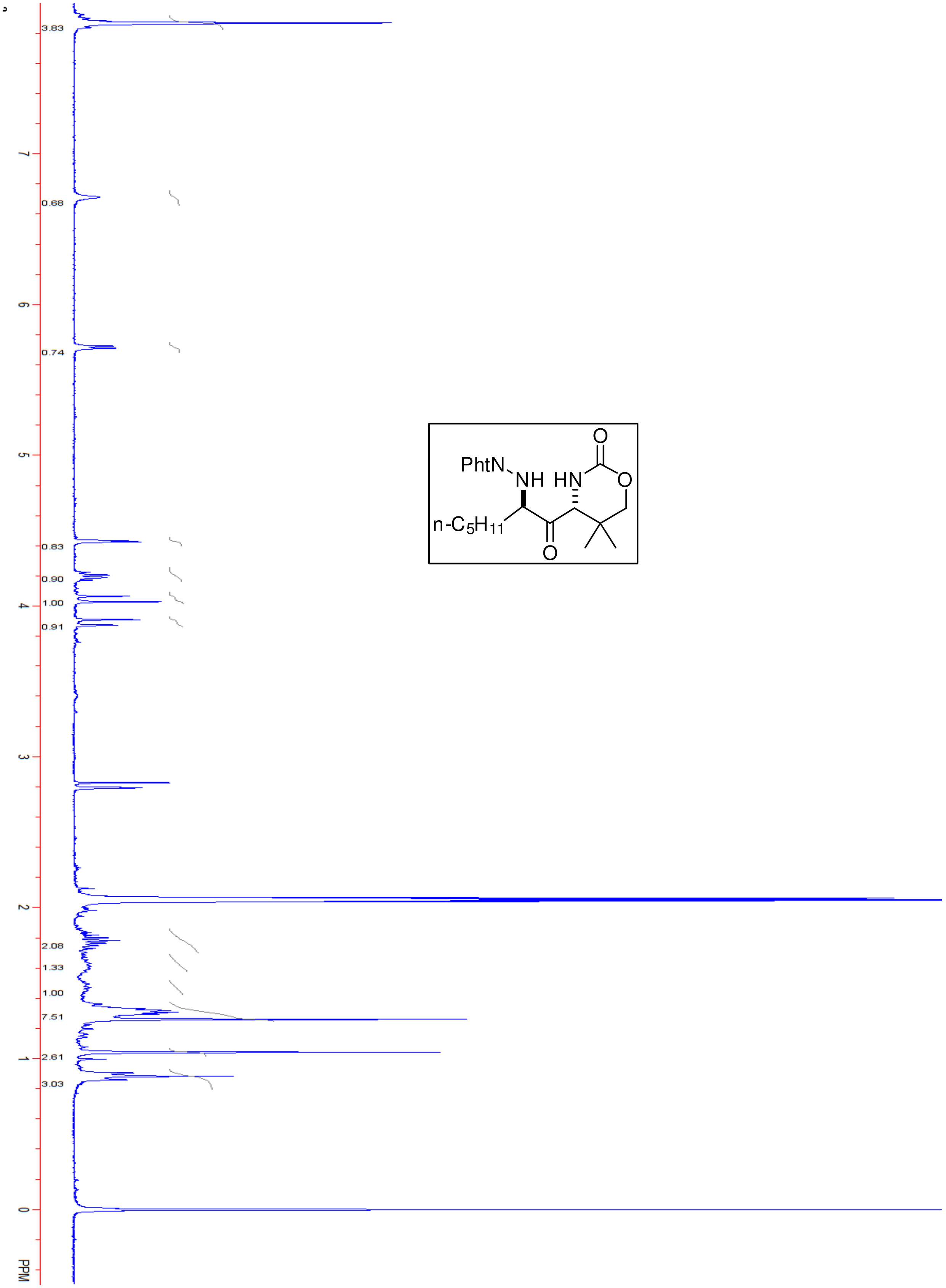
2) Still, W. C.; Kahn, M.; Mitra, A. *J. Org. Chem.* **1978**, *43*, 2923.

3) Rigoli, J.W. ; Boralsky, L.A. ; Hershberger, J.C. ; Meis, A.R. ; Marston, D. ; Fry, C.G. ; Guzei, I.A. ; Schomaker, J.M. *submitted.*

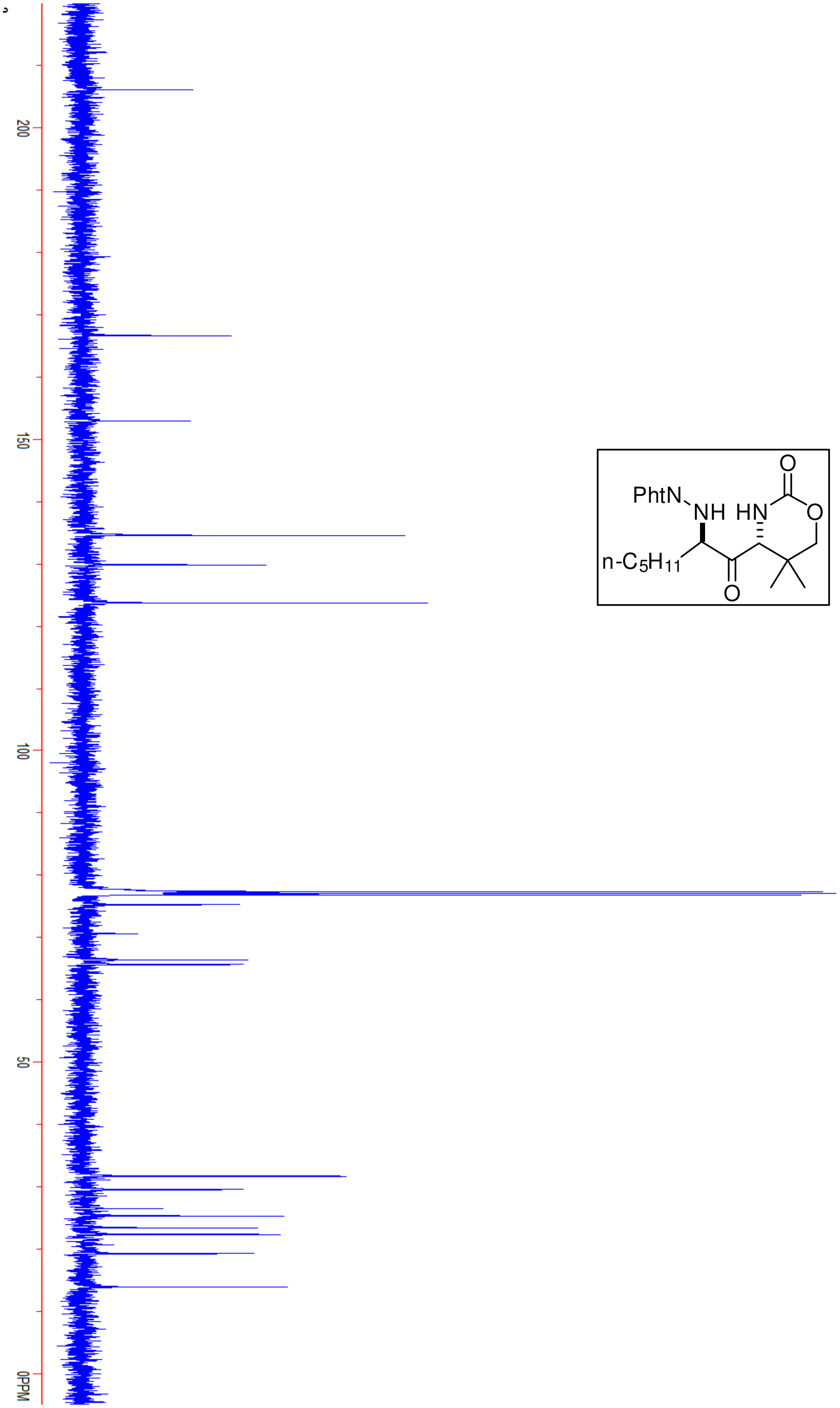
4) Larock, R.C.; Babu, S. *Tetrahedron* **1987**, *43*, 2013.

VIII. NMR Spectra.

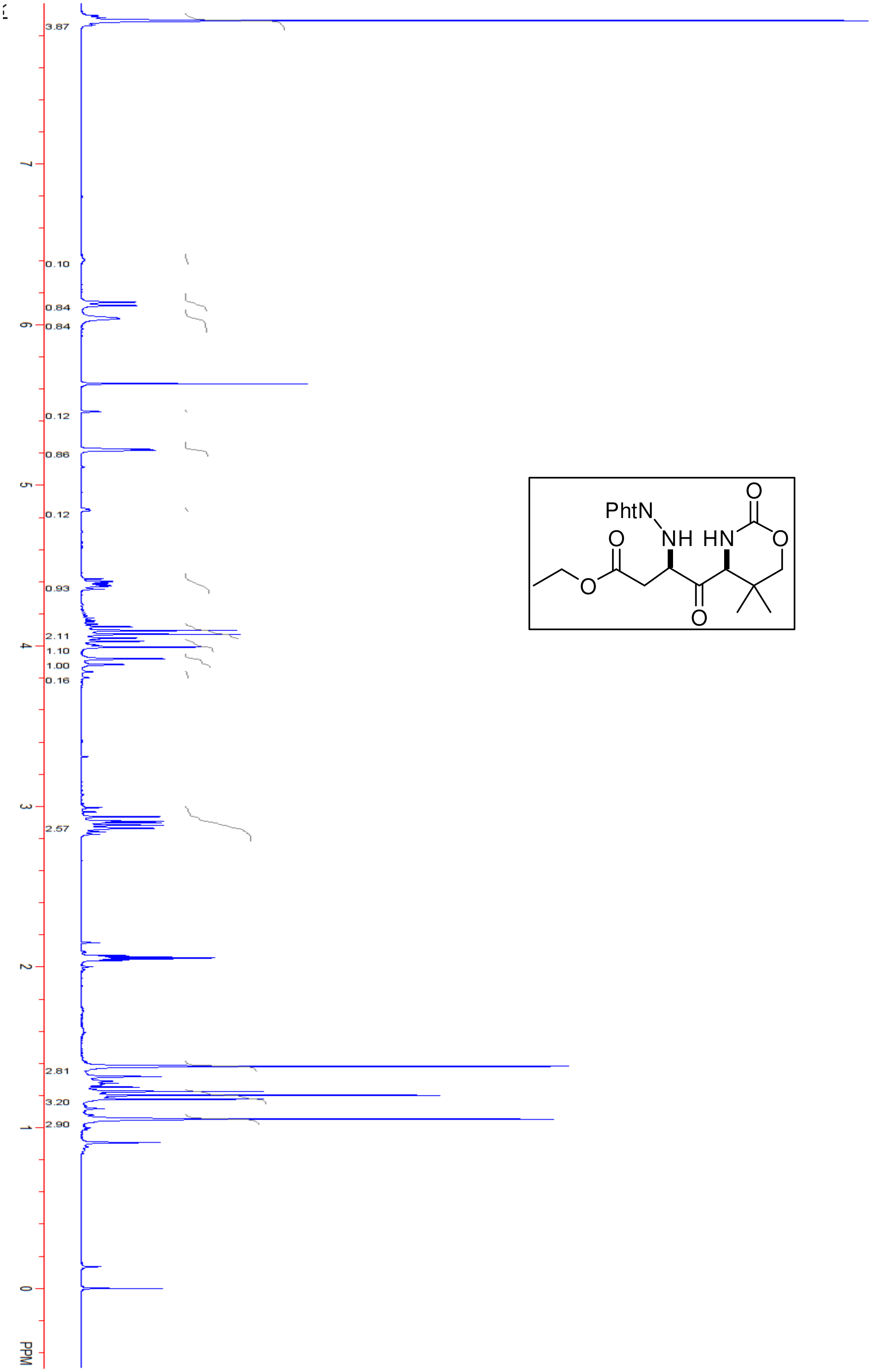
Compound 6.



Compound 6.



Compound 8b.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6
0.84
0.12
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0.12
0.93
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1.00
0.16
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2
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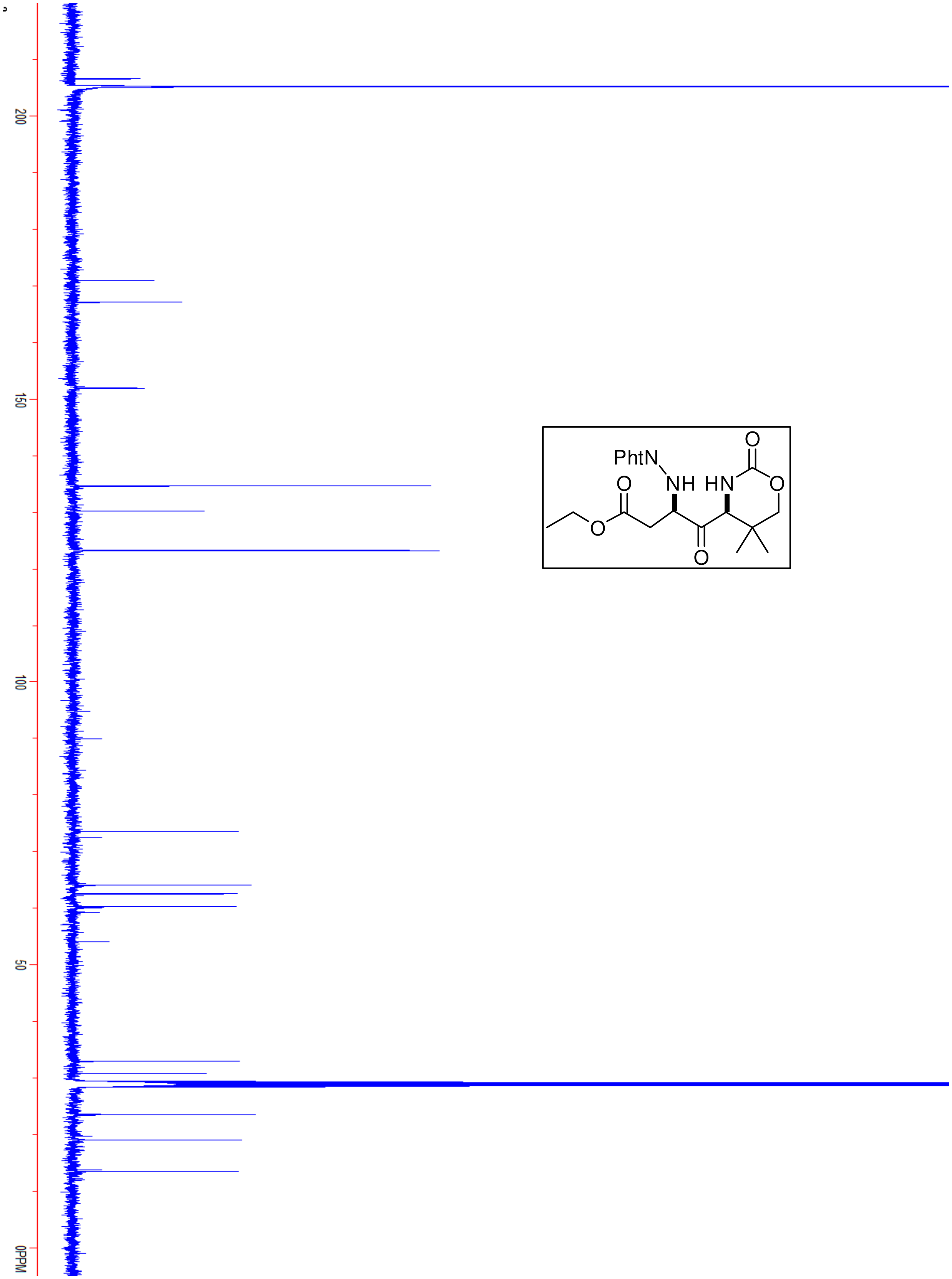
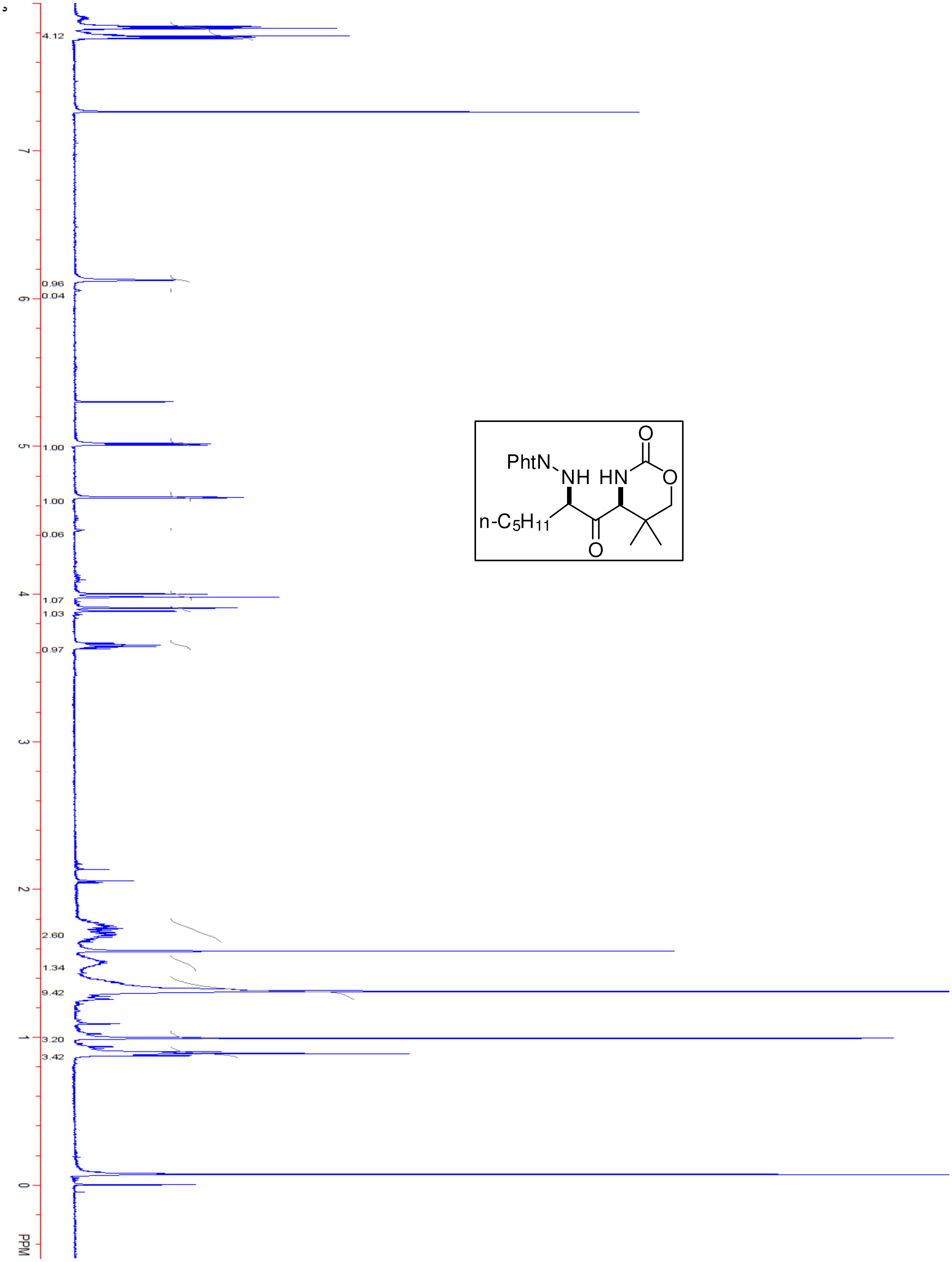
NH
HN
O

Compound 8b.



Compound 8c.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2.60
1.34
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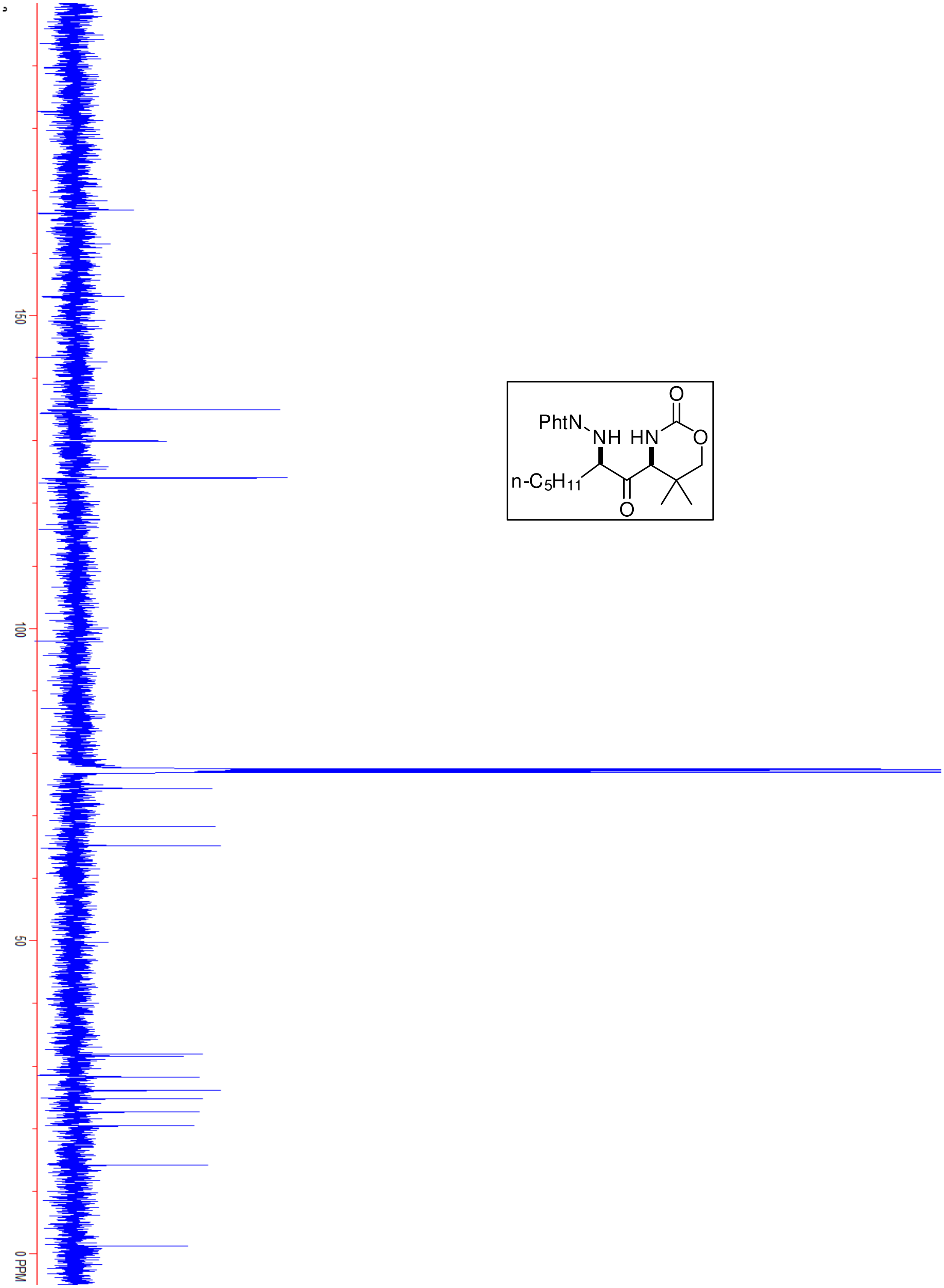
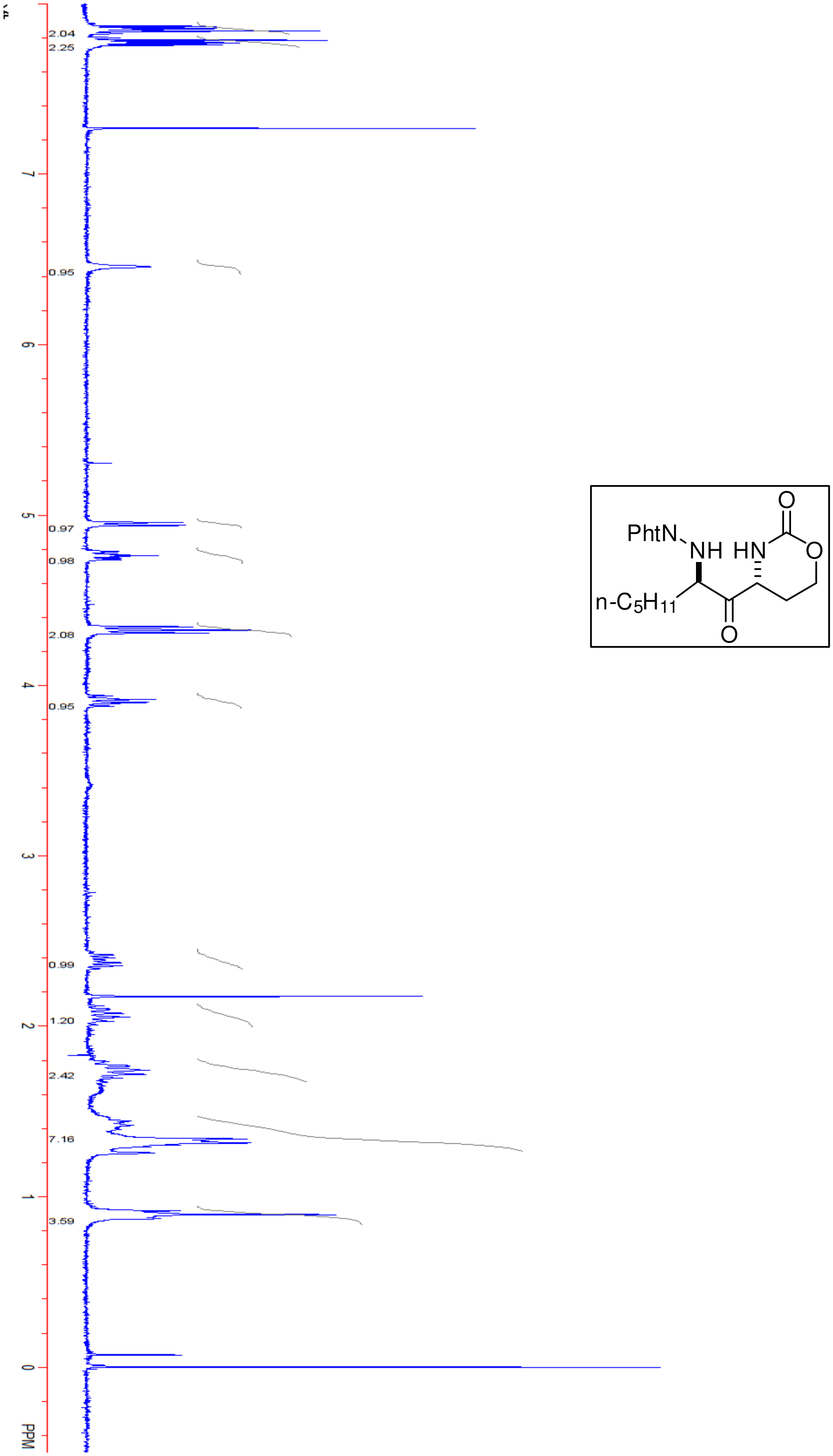
n-C5H11

Compound 8c.



Compound 8d.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6
5
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NH
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O
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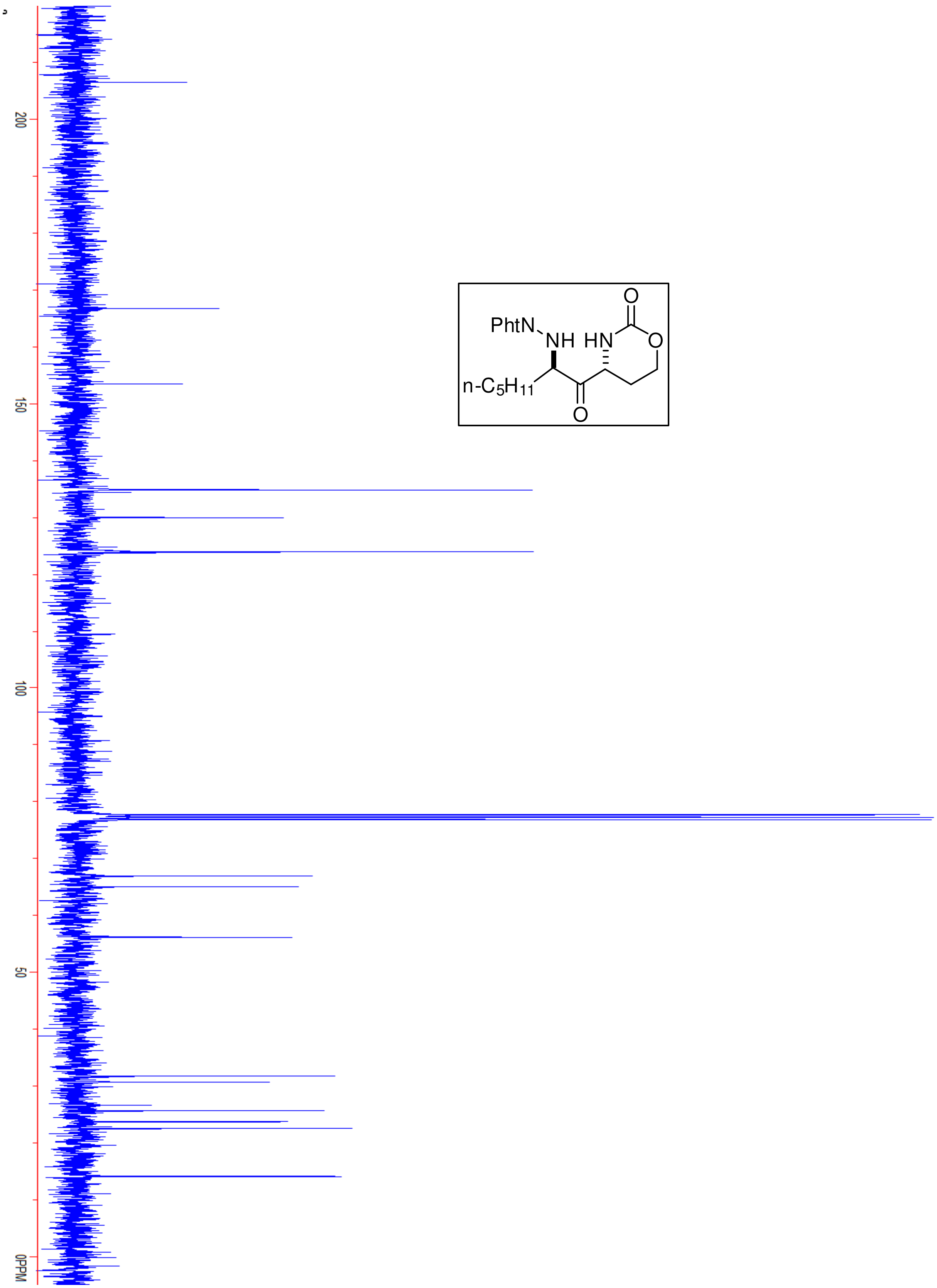
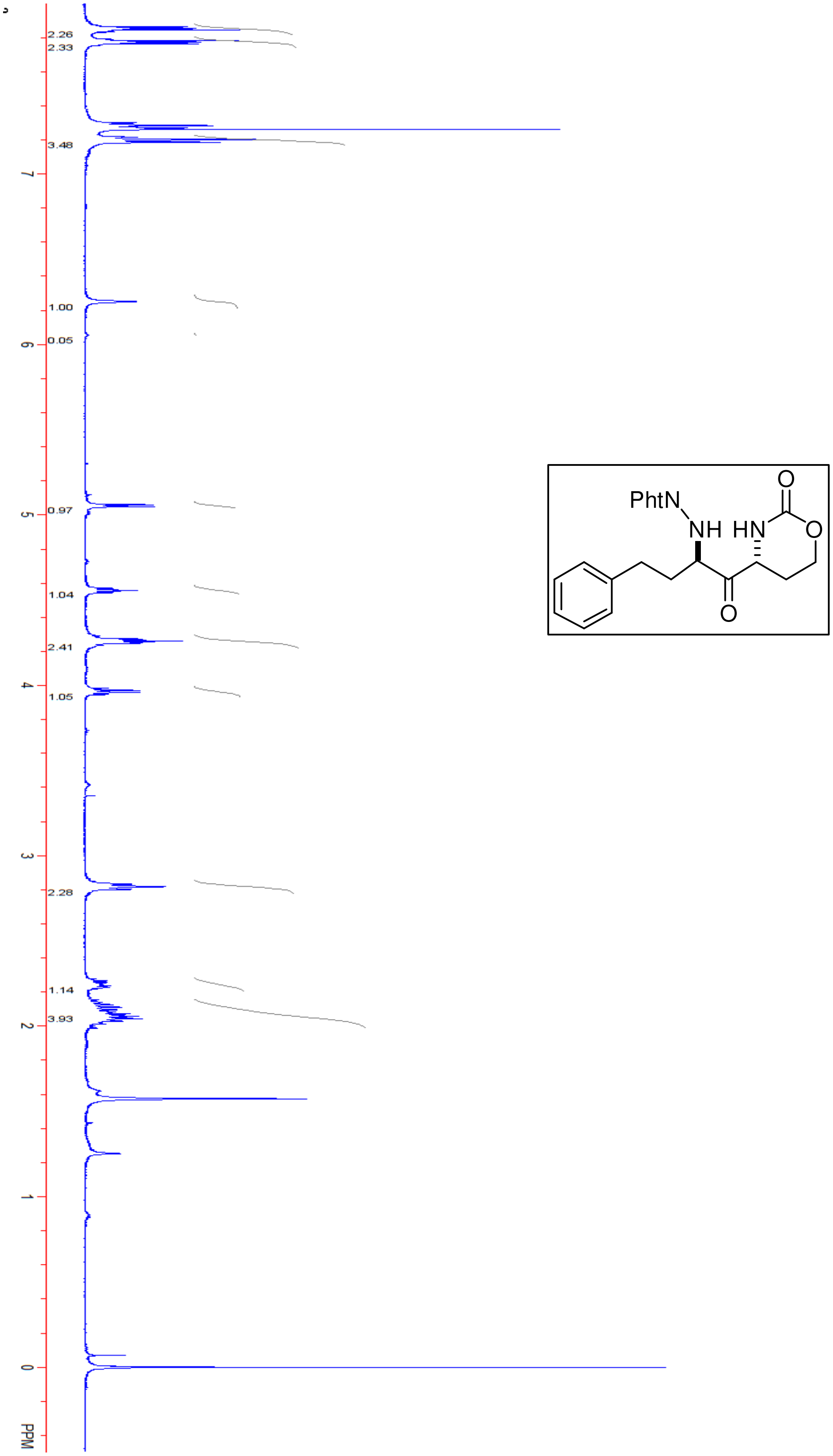
Compound 8d.



Compound 8e.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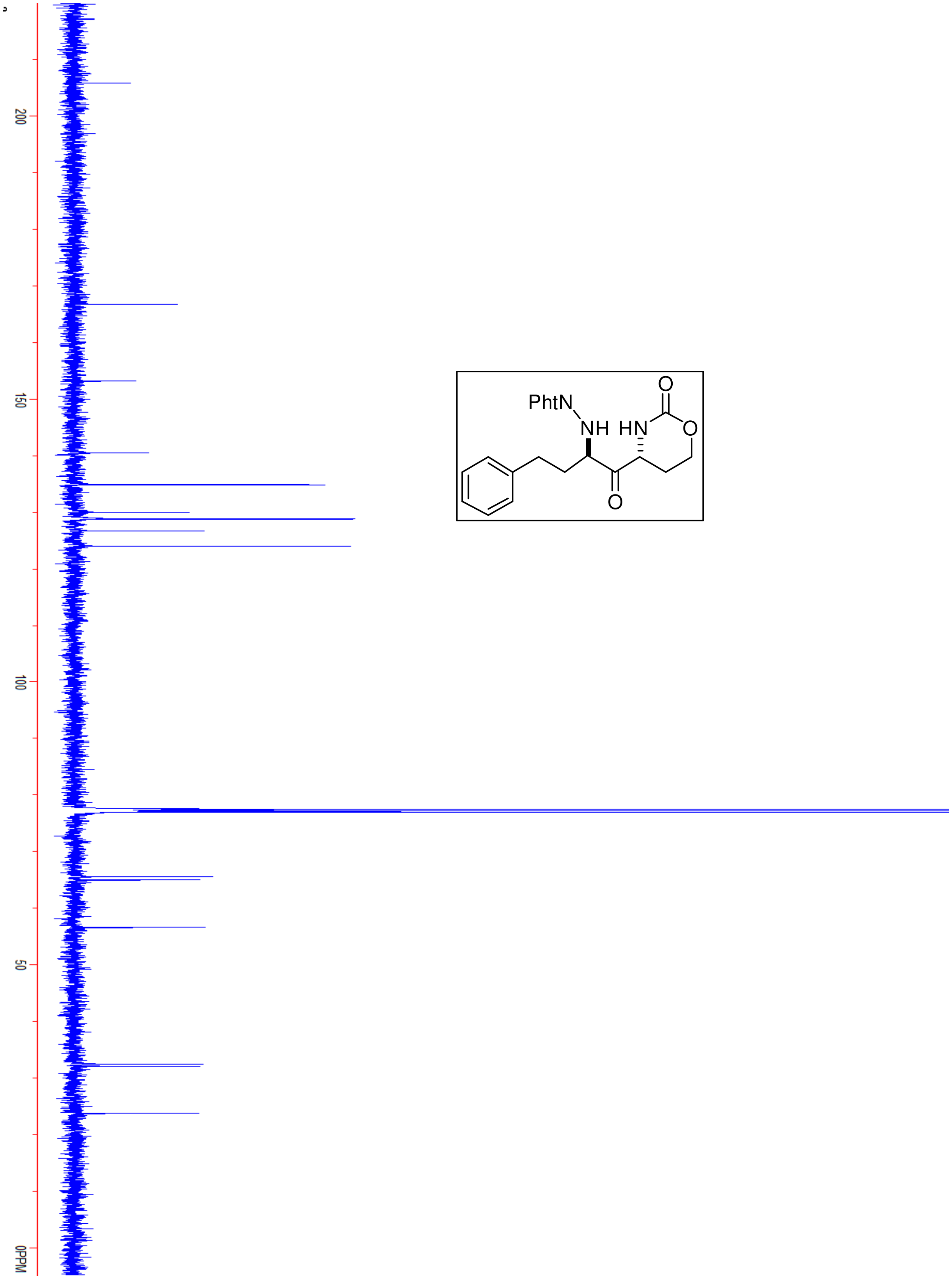
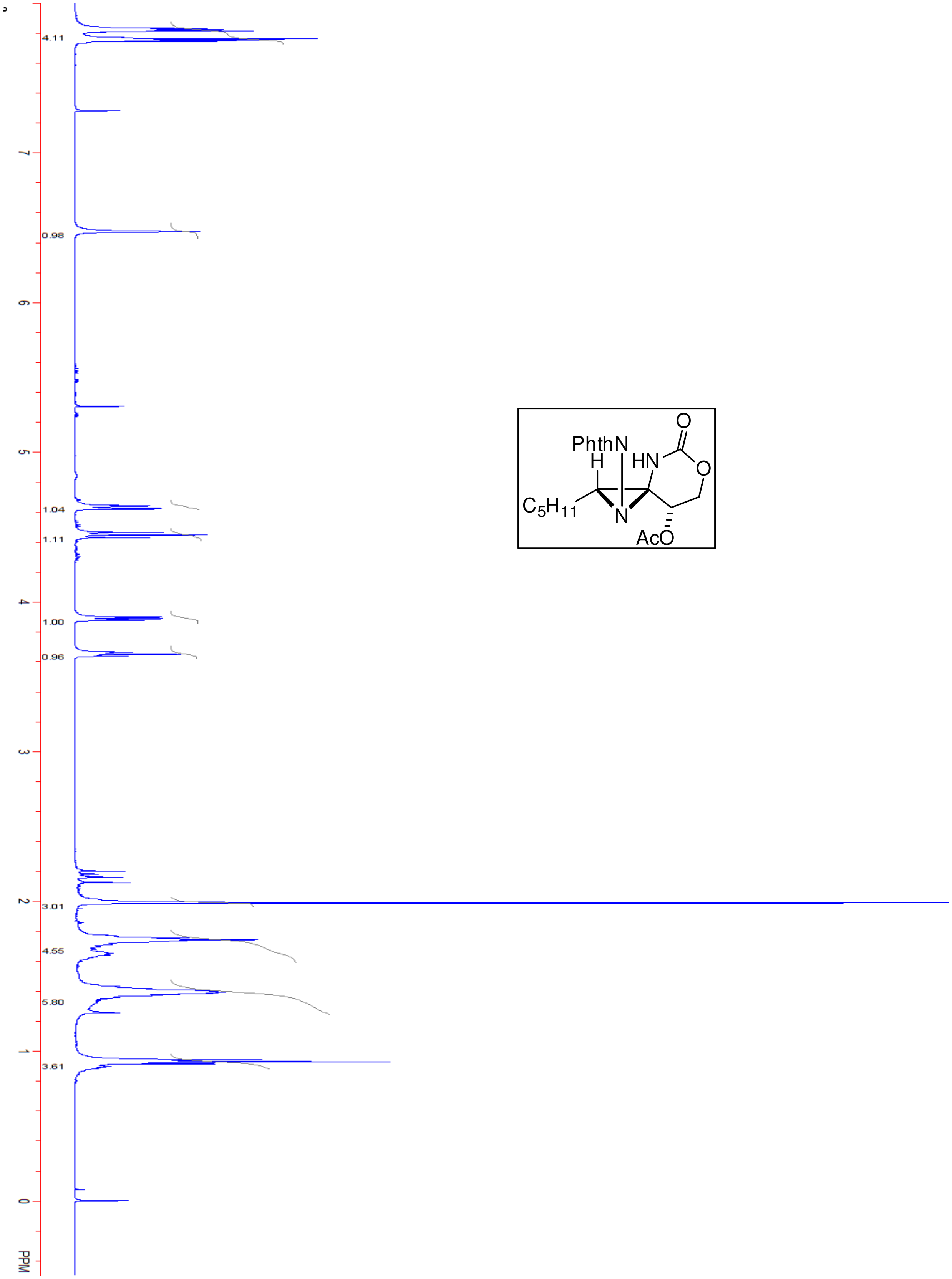
O
O

Compound 8e.



Compound 7f.



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1.11
4
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C_5H_{11}
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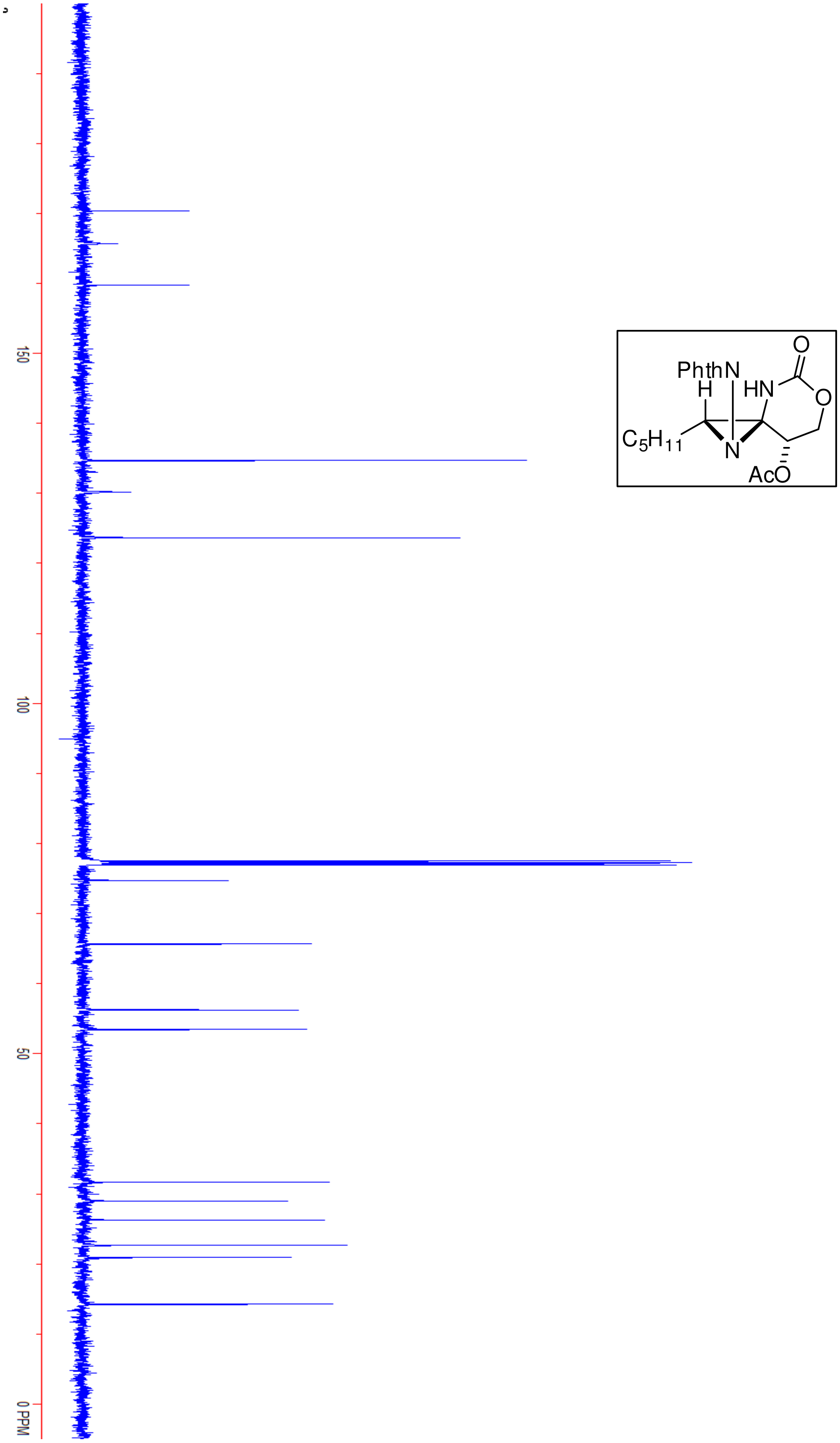
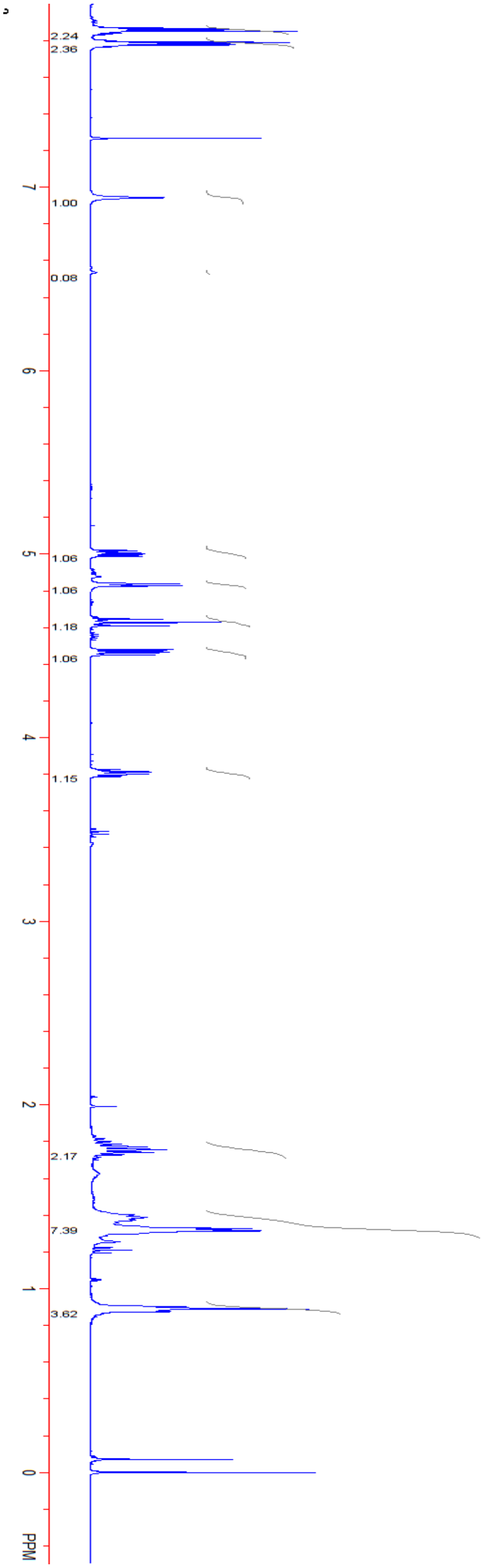
Compound 7f.



Compound 8f.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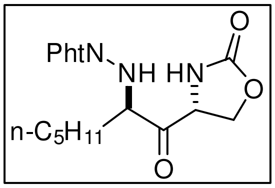
1
3.62
0
PPM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n-C5H11
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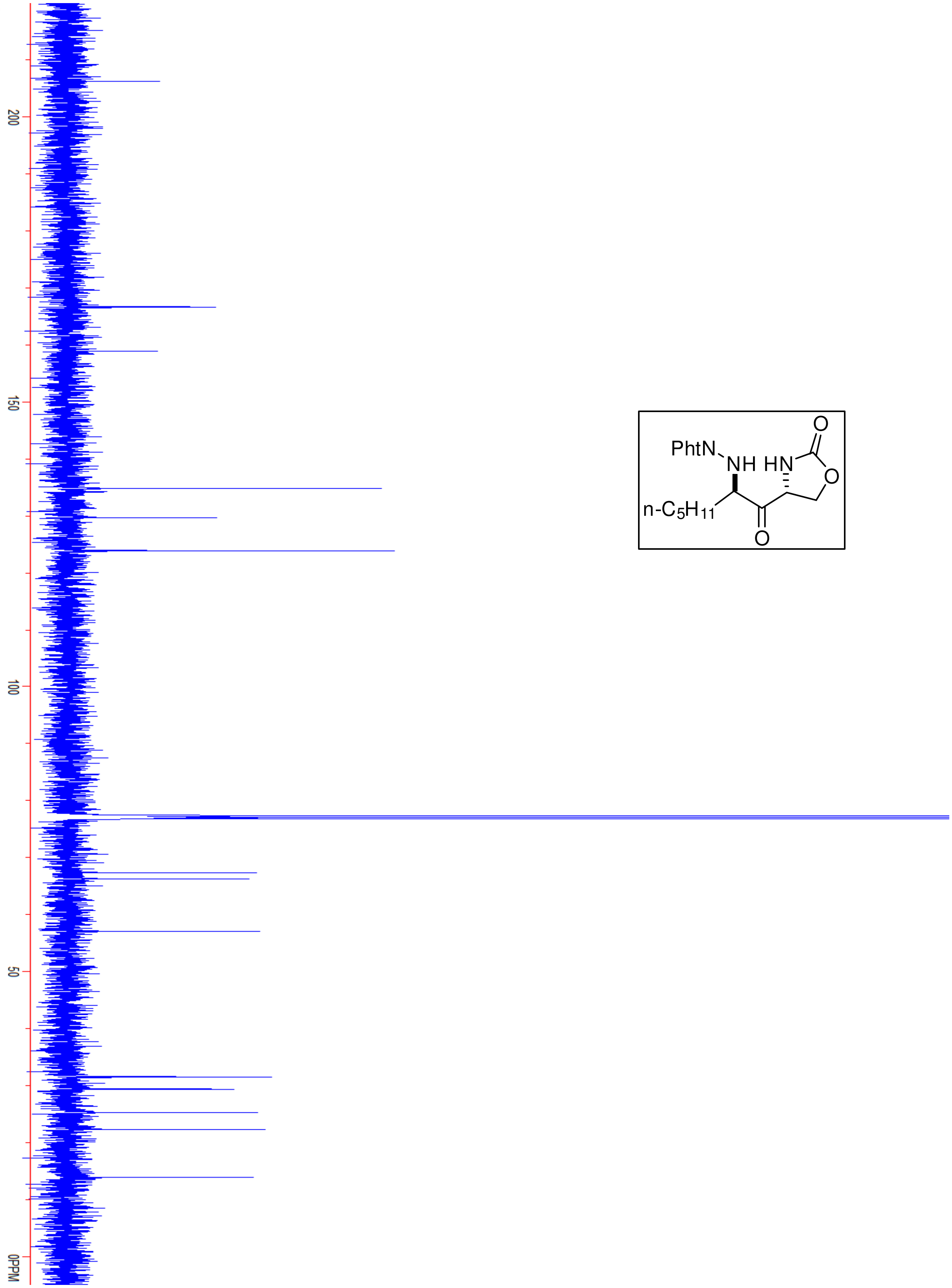
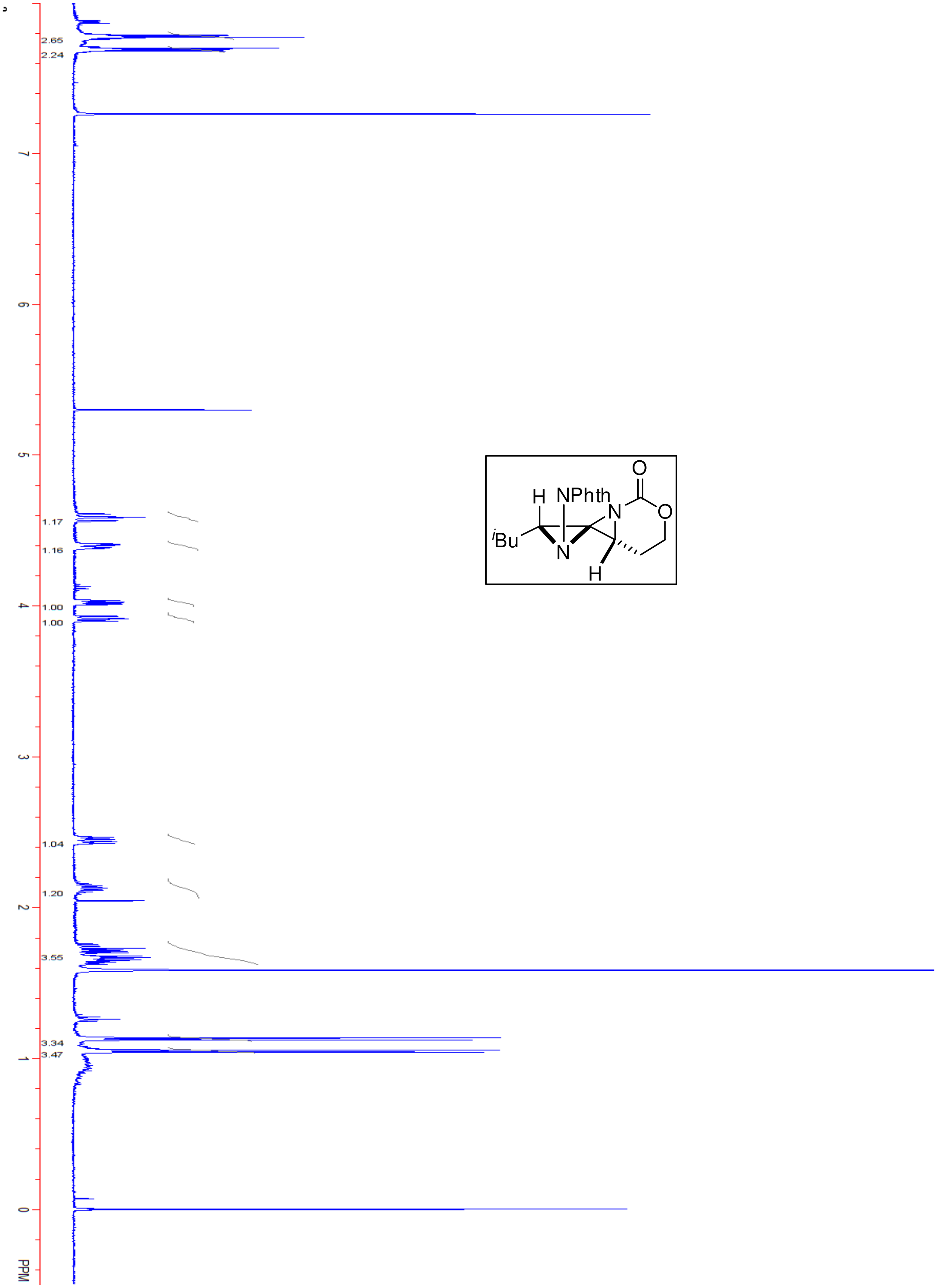
Compound 8f.



Compound 7g.



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6
5
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1.16
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NPhth
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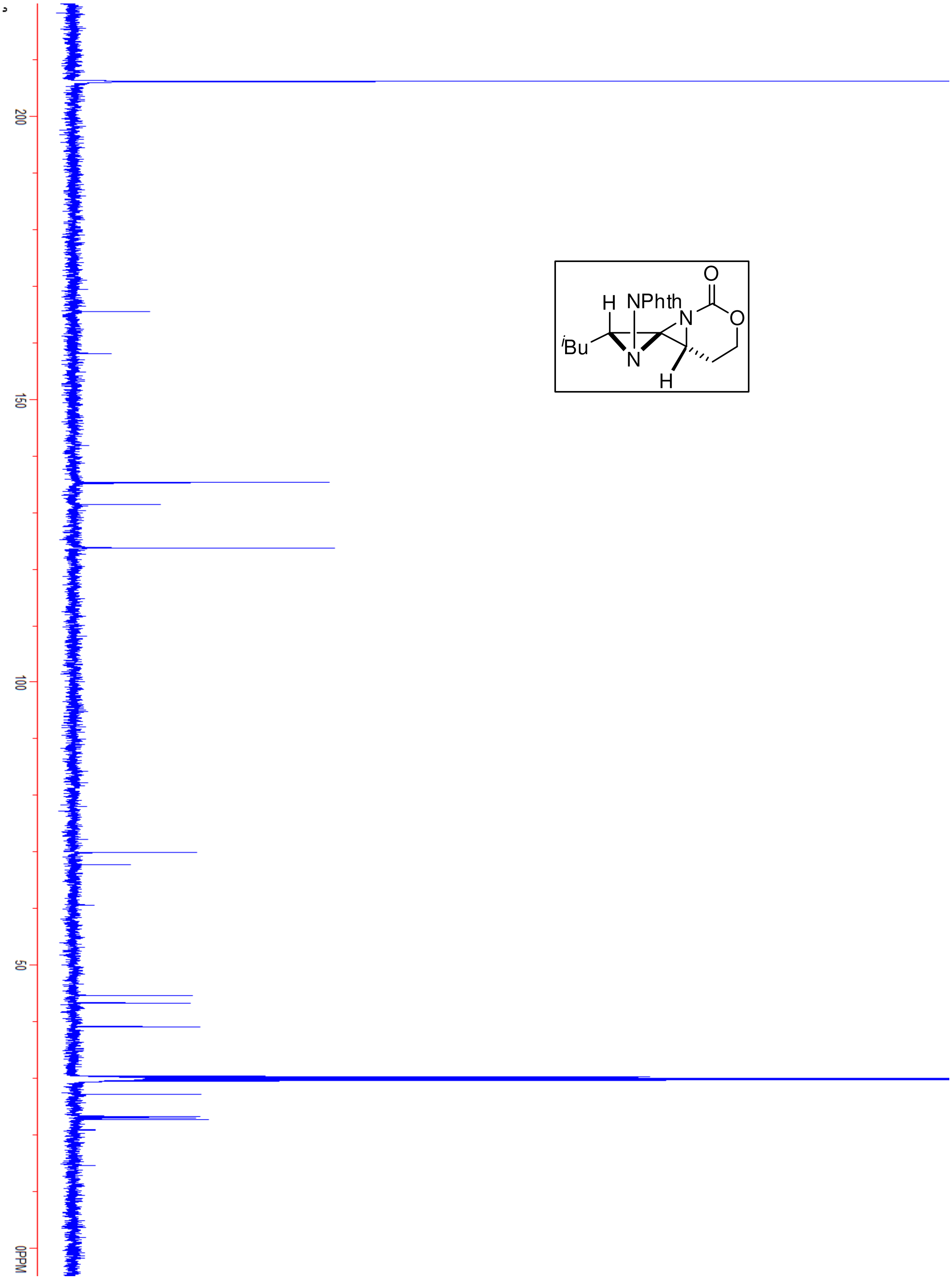
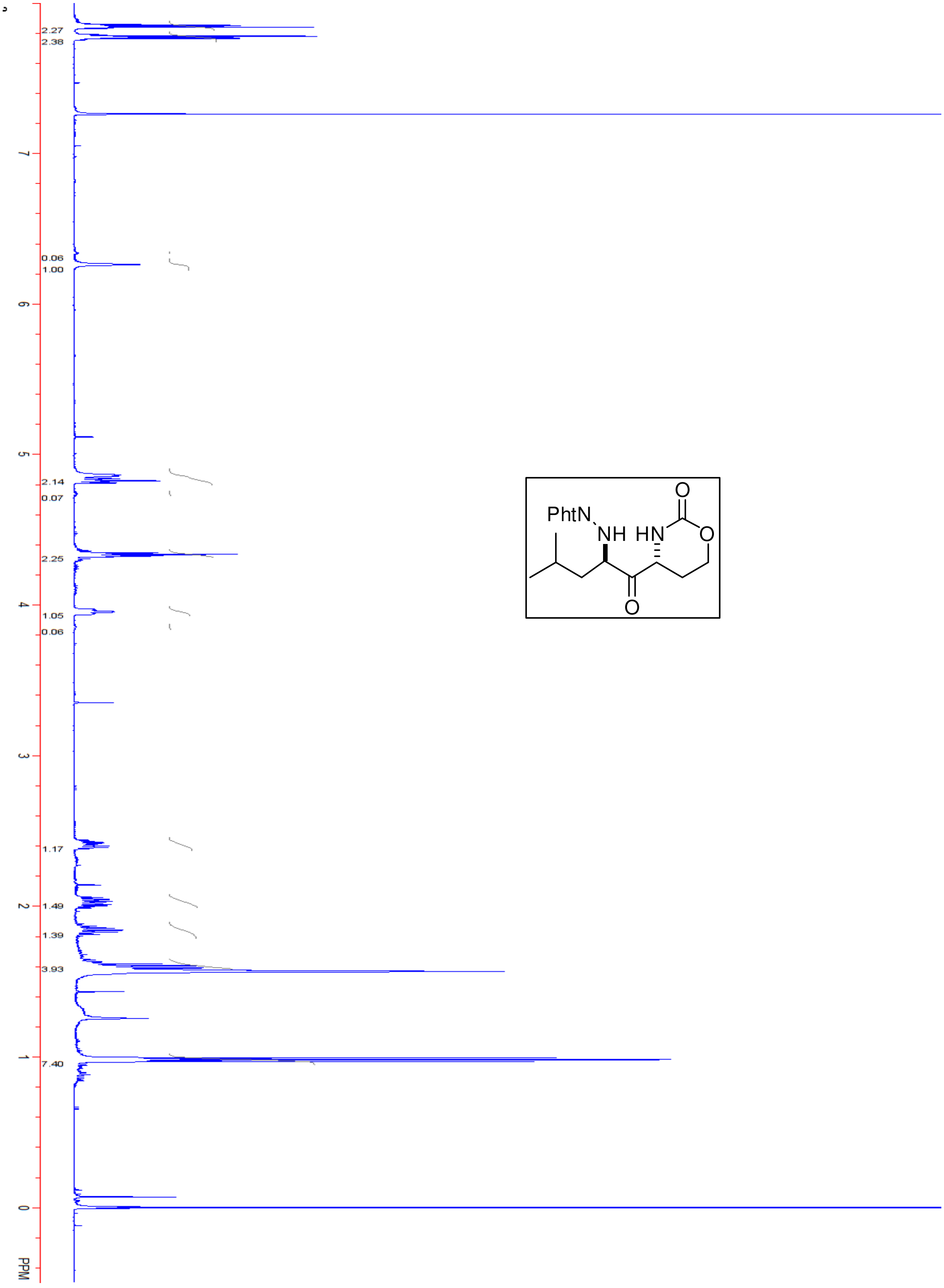
O
^{i}Bu
N
H

Compound 7g.



Compound 8g.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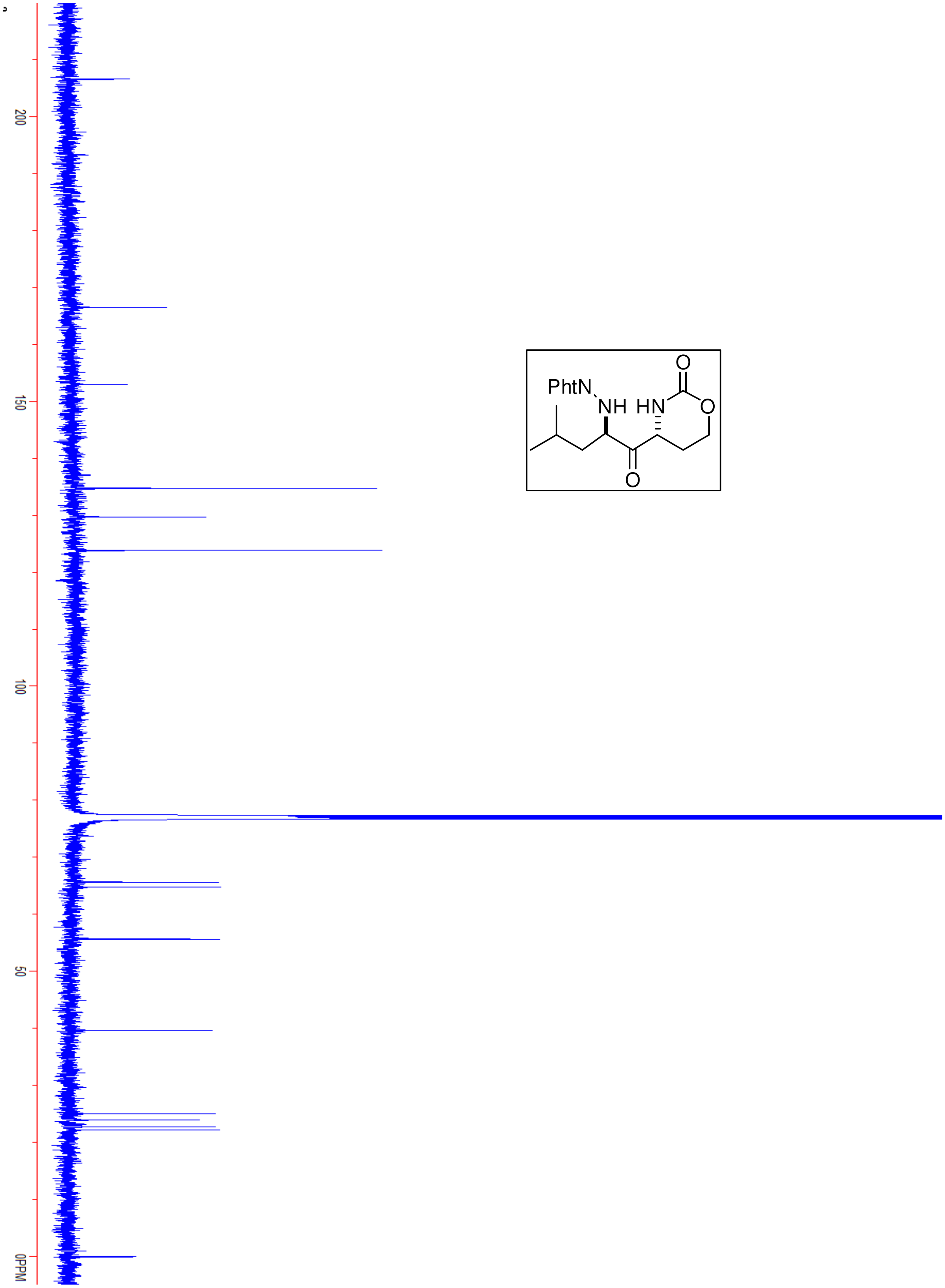
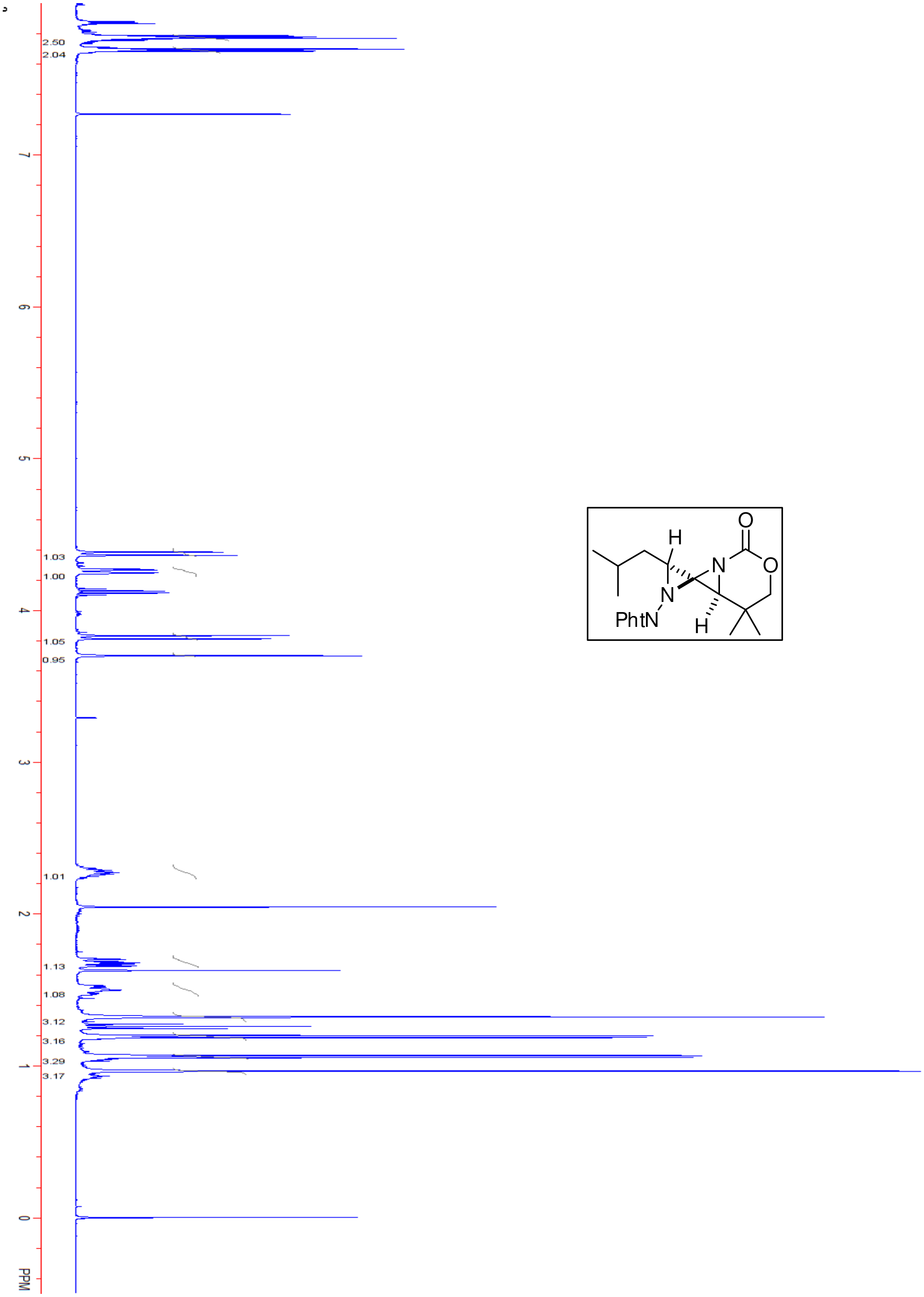
3.93
7.40
7
6
5
4
3
2
1
0
PPM
PhtN
NH
HN
O
O
O

Compound 8g.



Compound 7h.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1.08
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0
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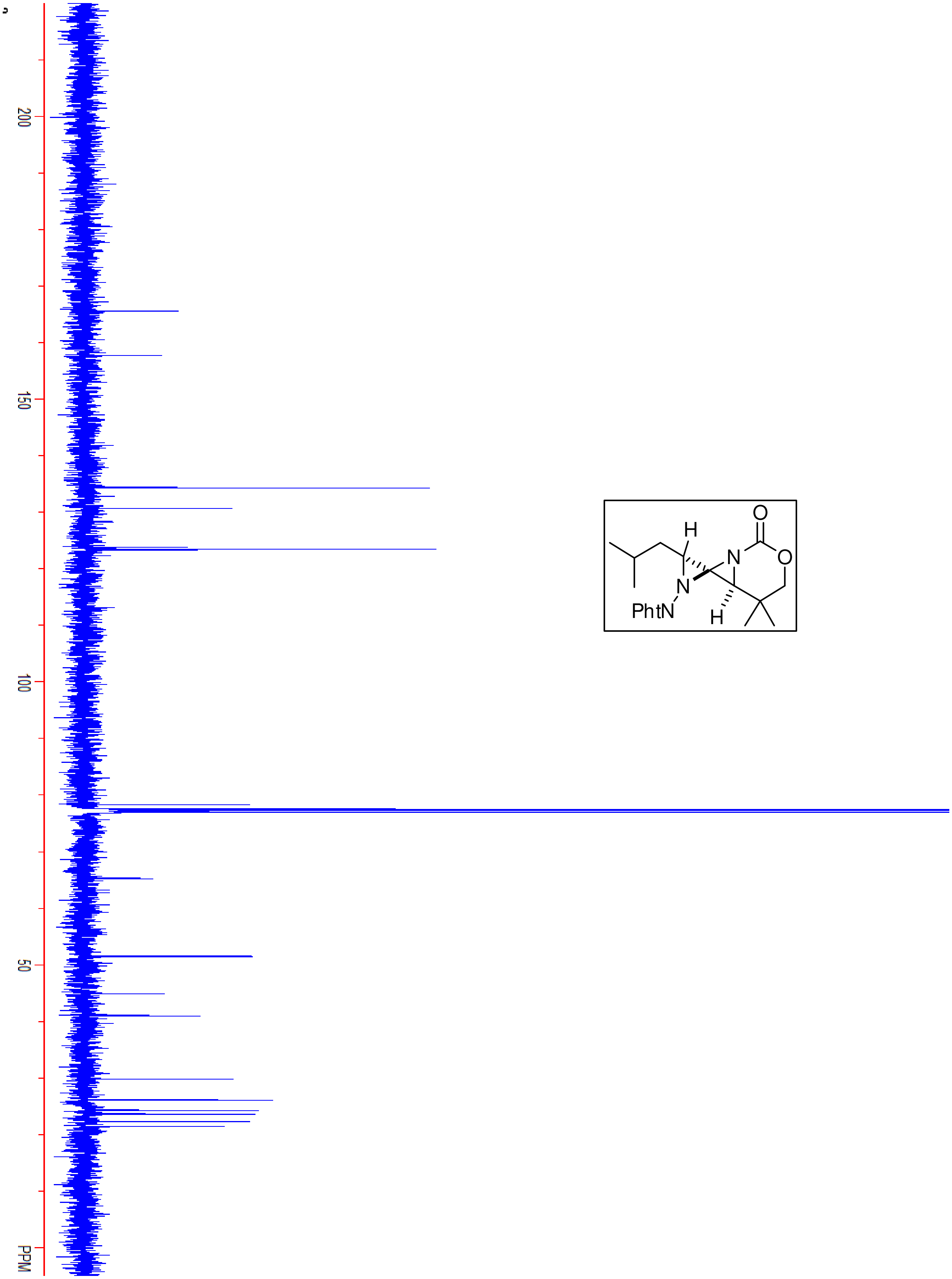
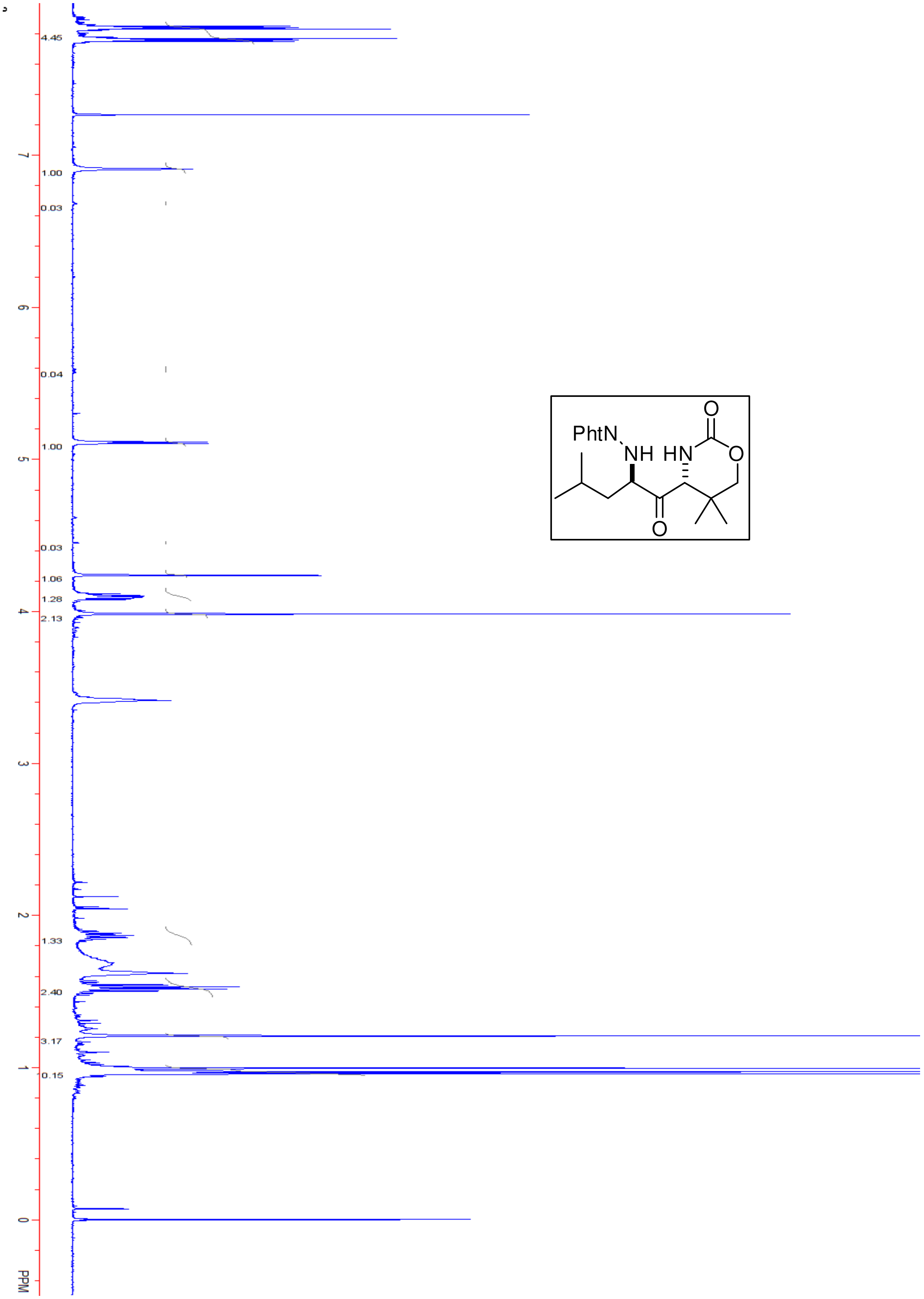
O
H
N
O
N
PhtN
H

Compound 7h.



Compound 8h.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7
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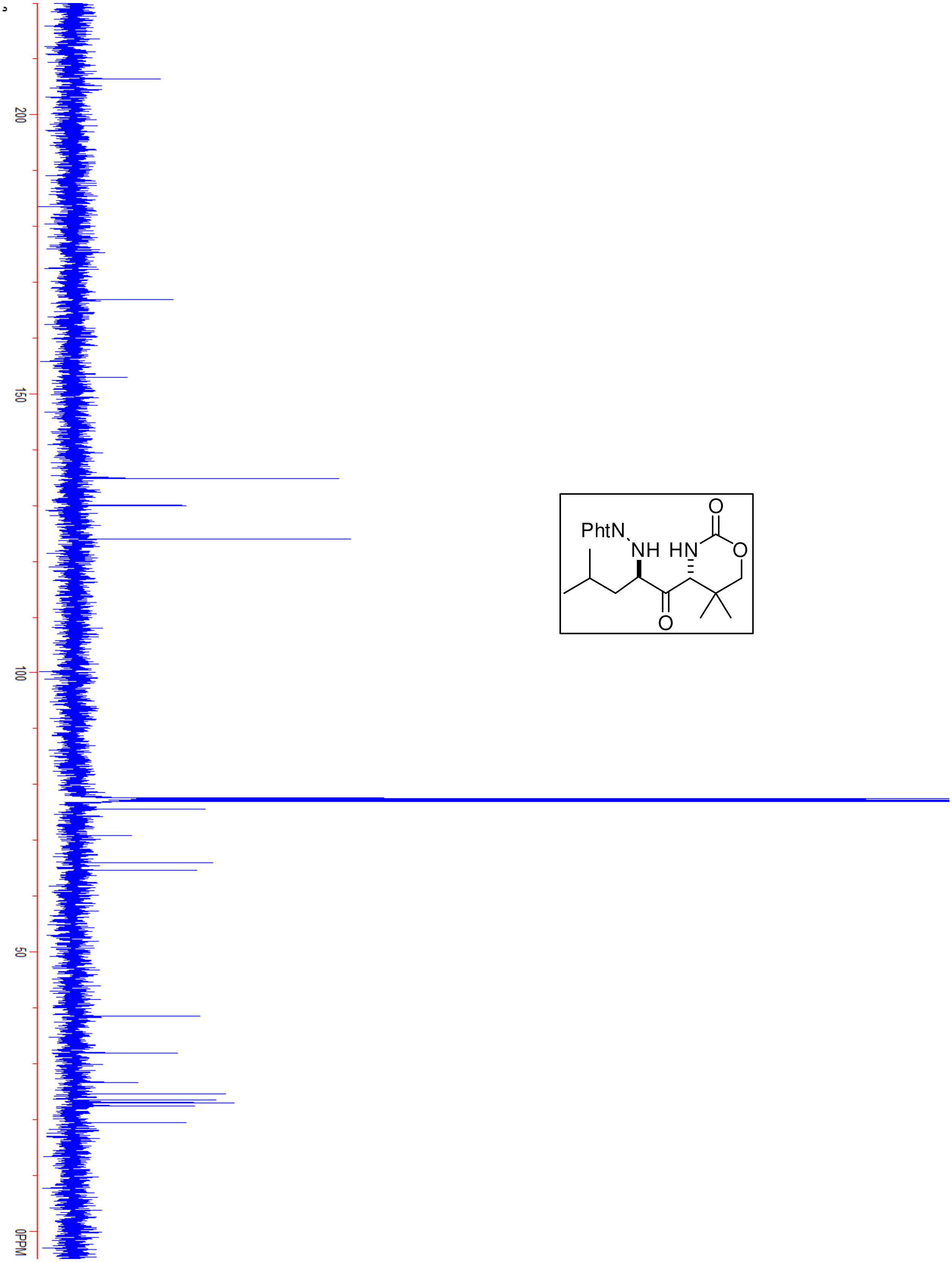
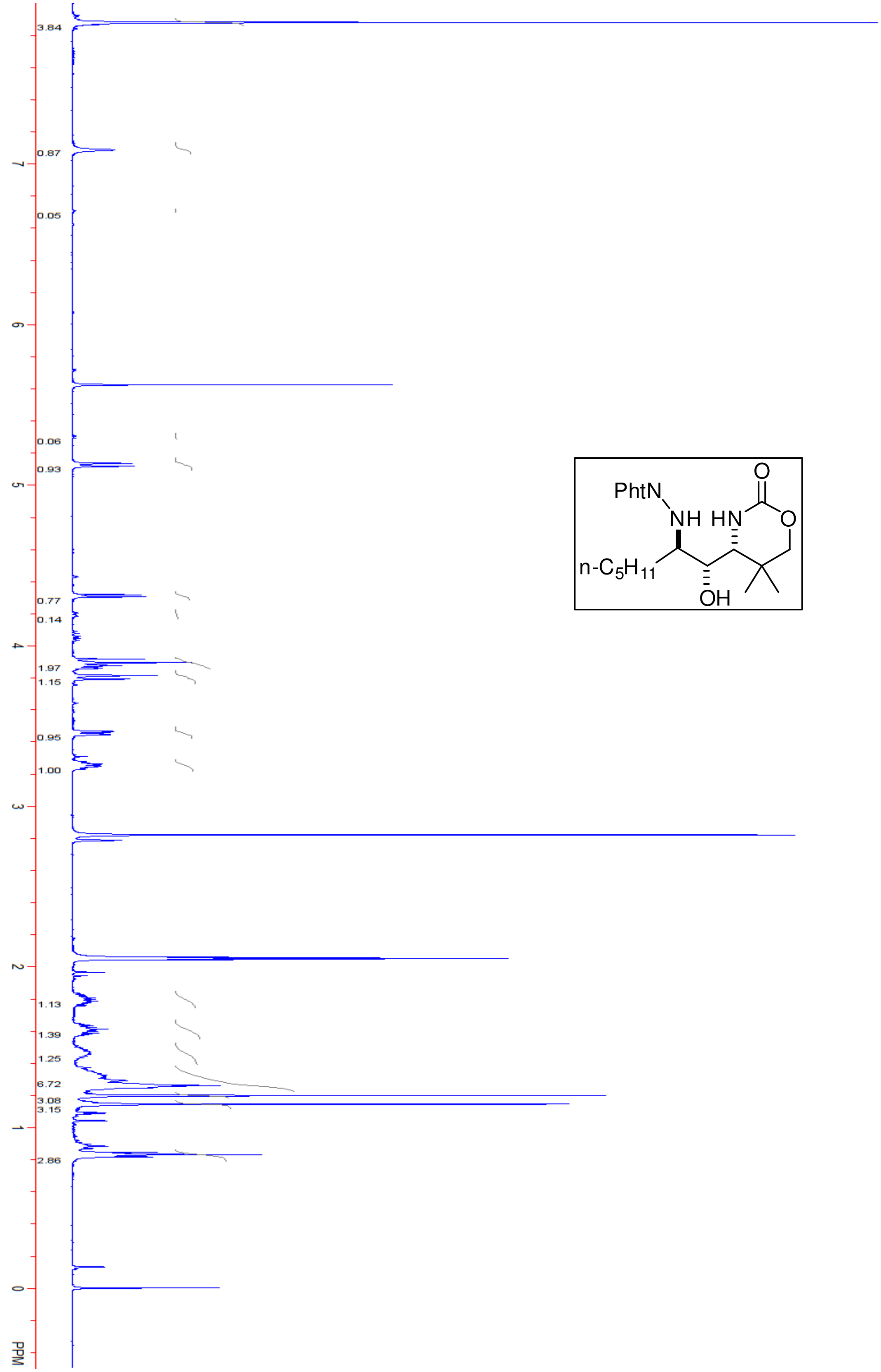
0.03
6
0.04
1.00
5
0.03
1.06
1.28
4
2.13
3
2
1.33
2.40
3.17
1
0.15
0
PPM
PhtN
NH
HN
O
O
O

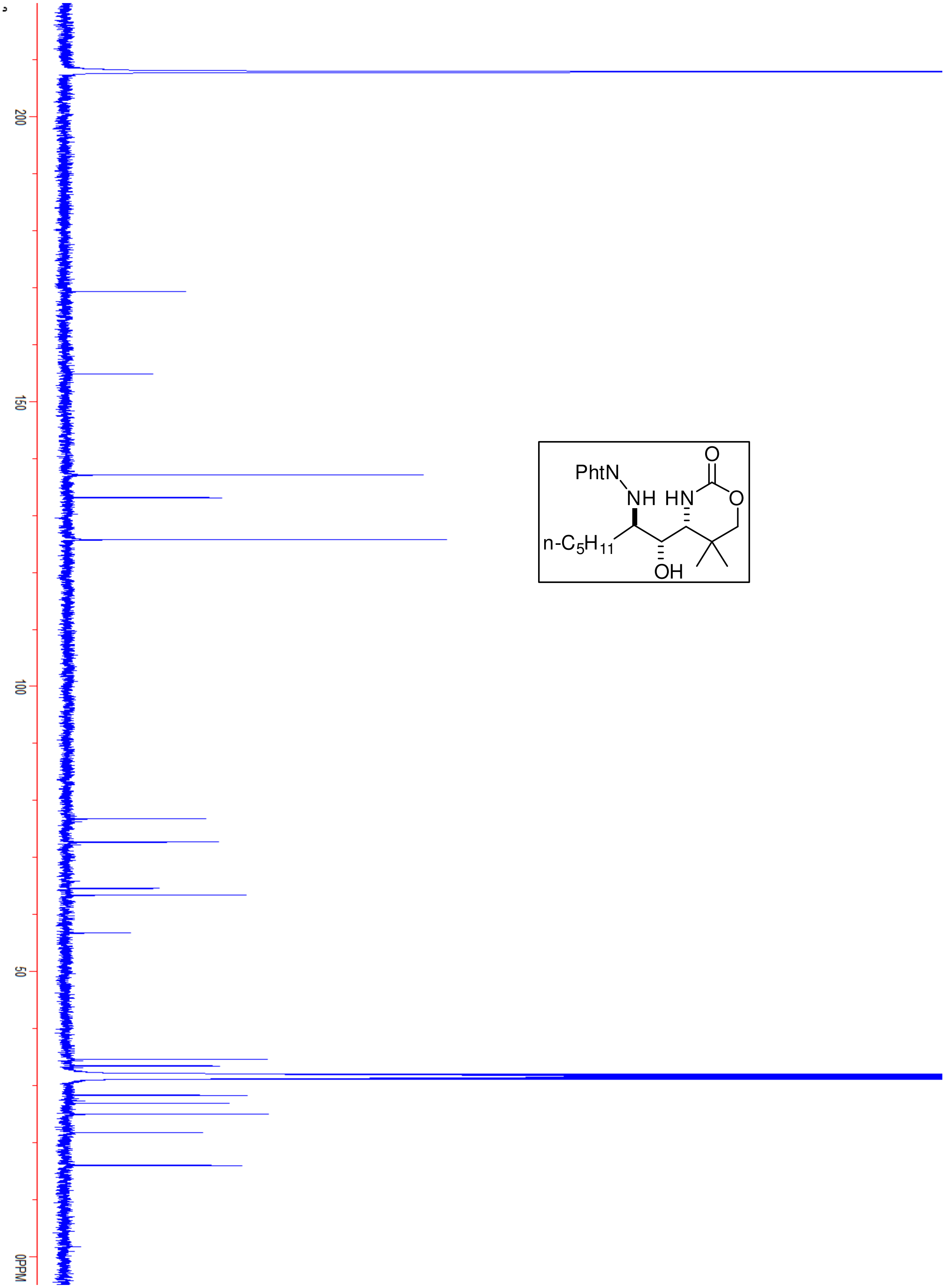
Compound 8h.



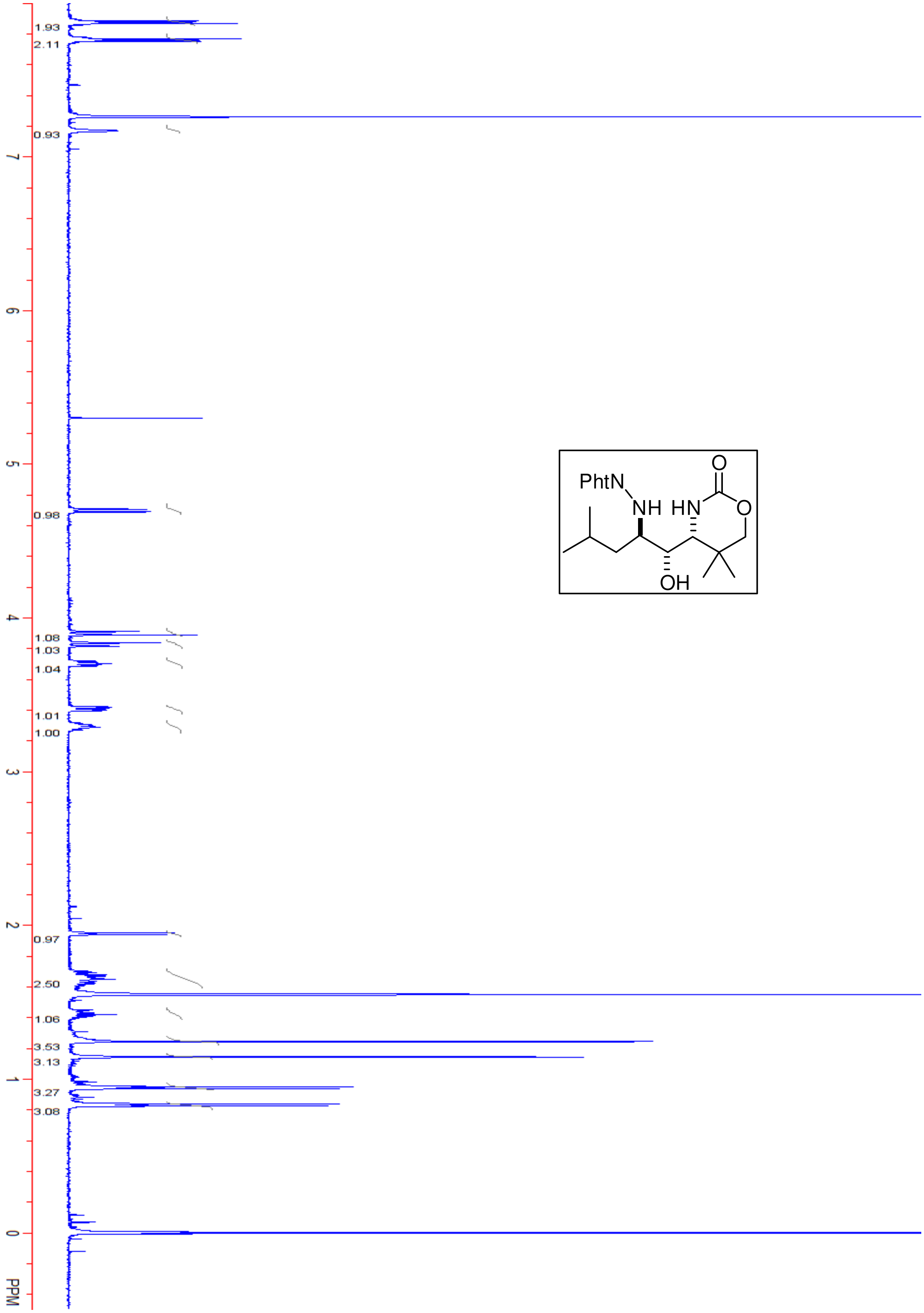
Compound 11.


3.84
0.87
7
0.05
6
0.06
0.93
5
0.77
0.14
4
1.97
1.15
0.95
1.00
3
2
1.13
1.39
1.25
6.72
3.08
3.15
1
2.86
0
PPM
O
PhtN
NH
HN
O
n-C5H11
OH

Compound 11.



Compound 13.


1.93
2.11
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6
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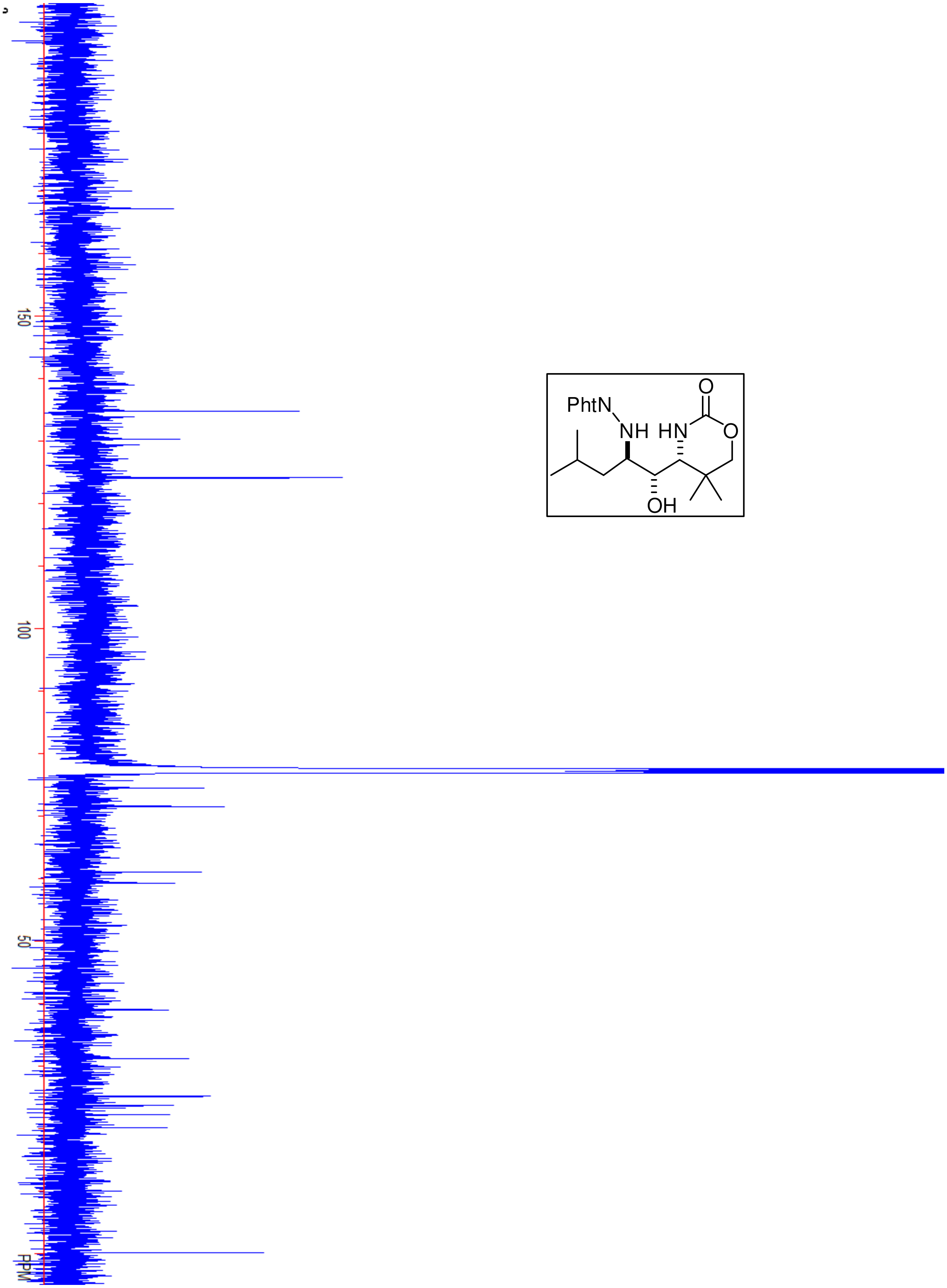
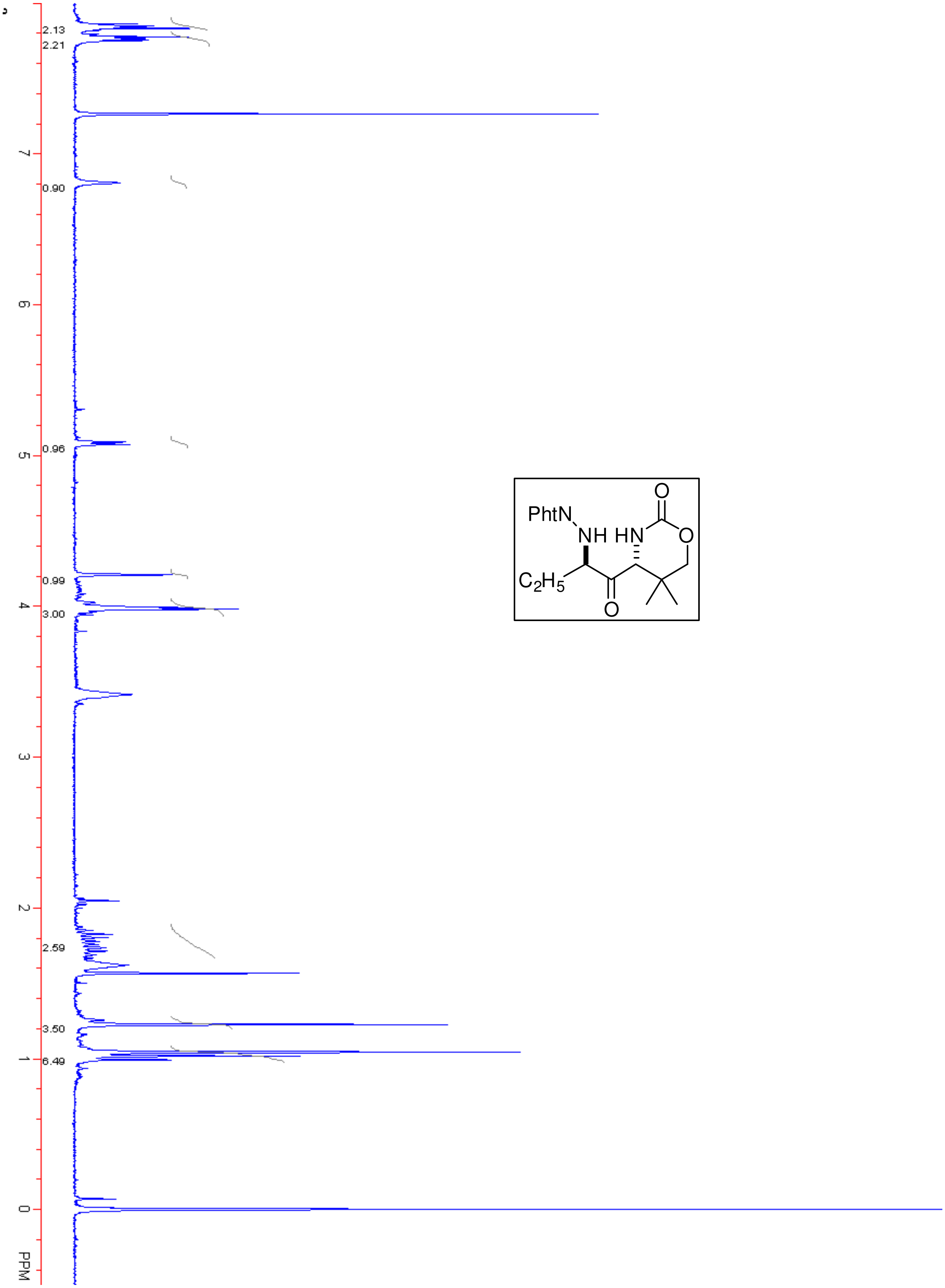
4
1.08
1.03
1.04
1.01
1.00
3
2
0.97
2.50
1.06
3.53
3.13
1
3.27
3.08
0
PPM
PhtN
NH
HN
O
O
OH

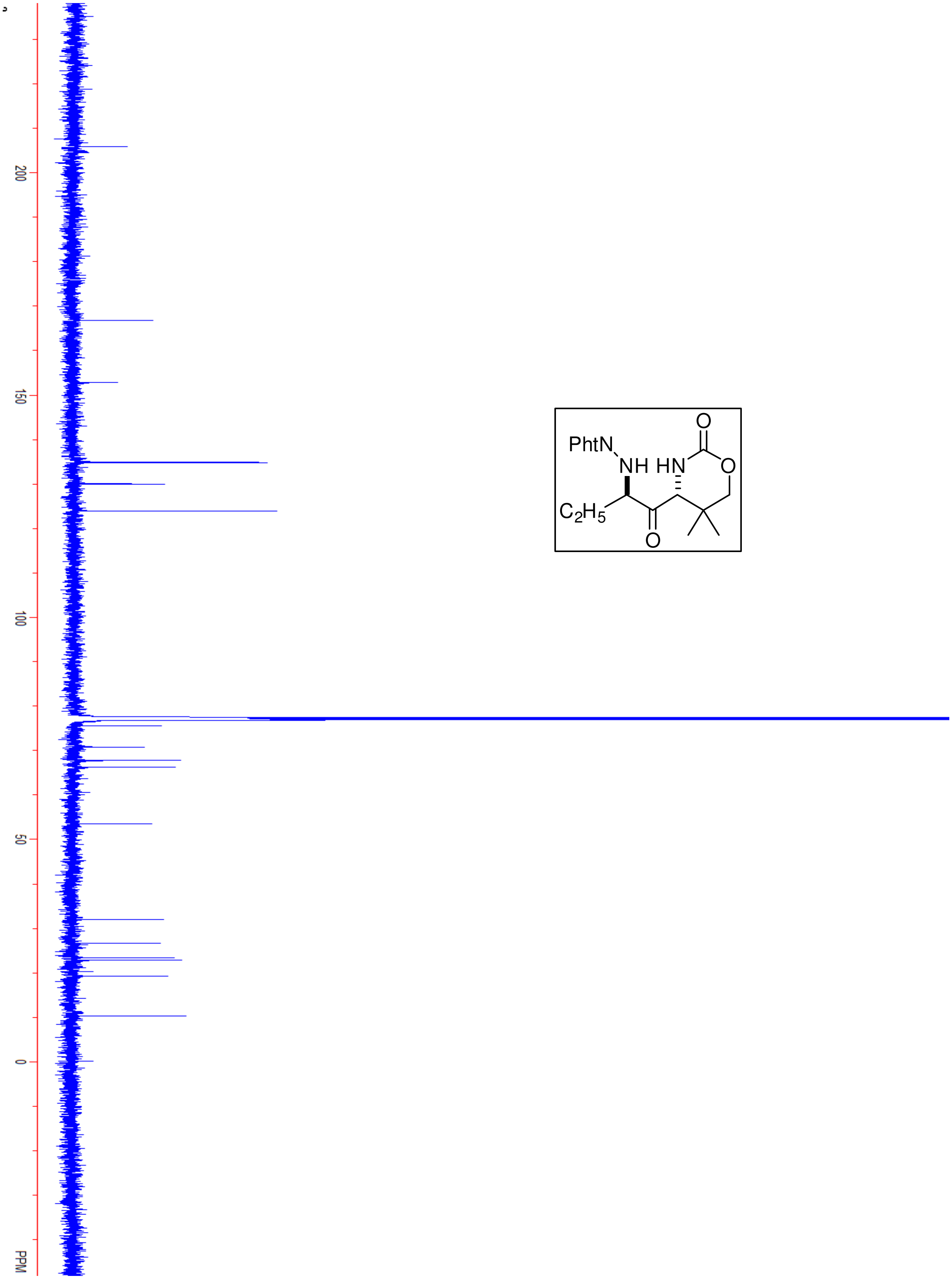
Compound 13.



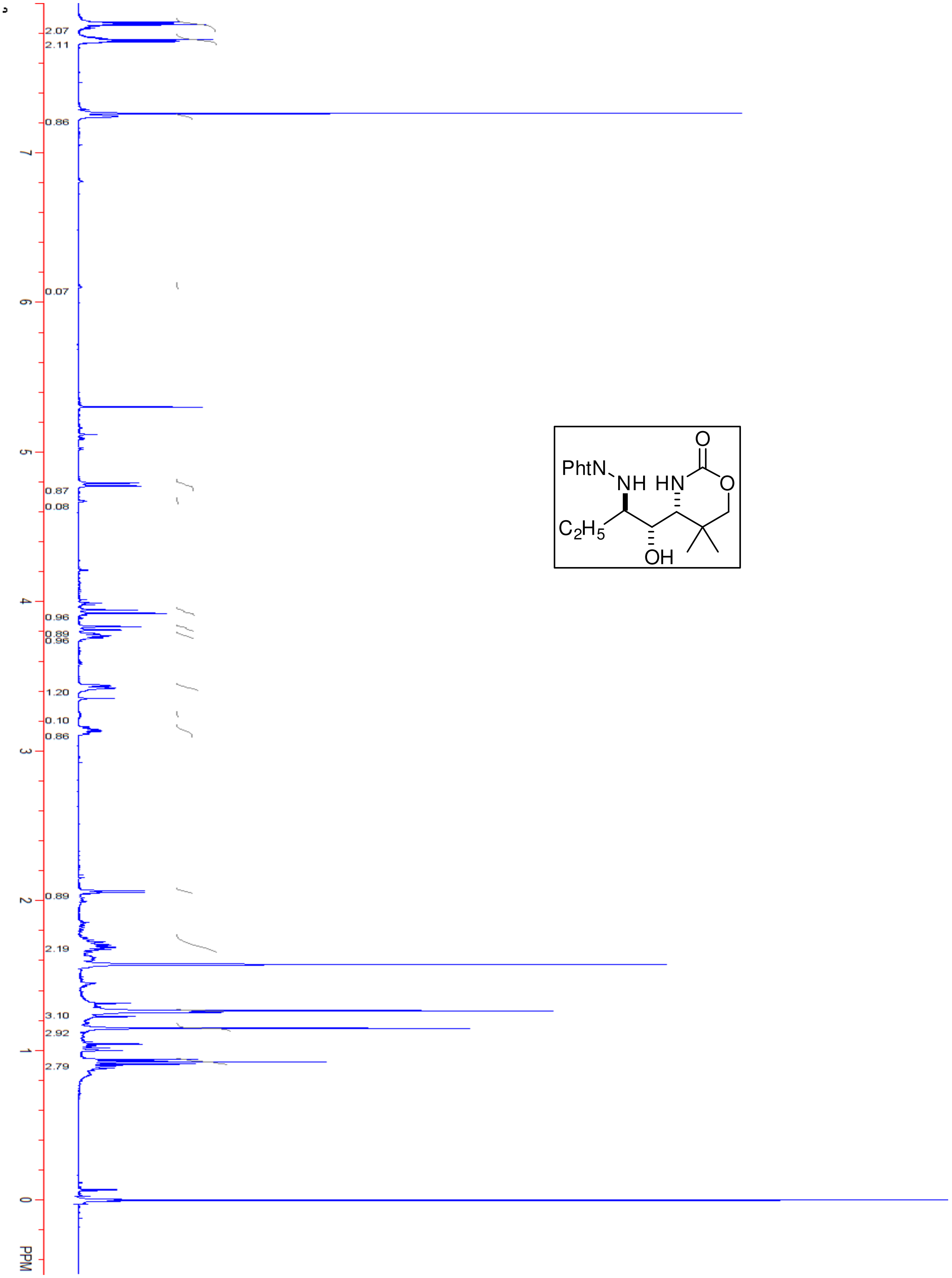
Compound 14a.



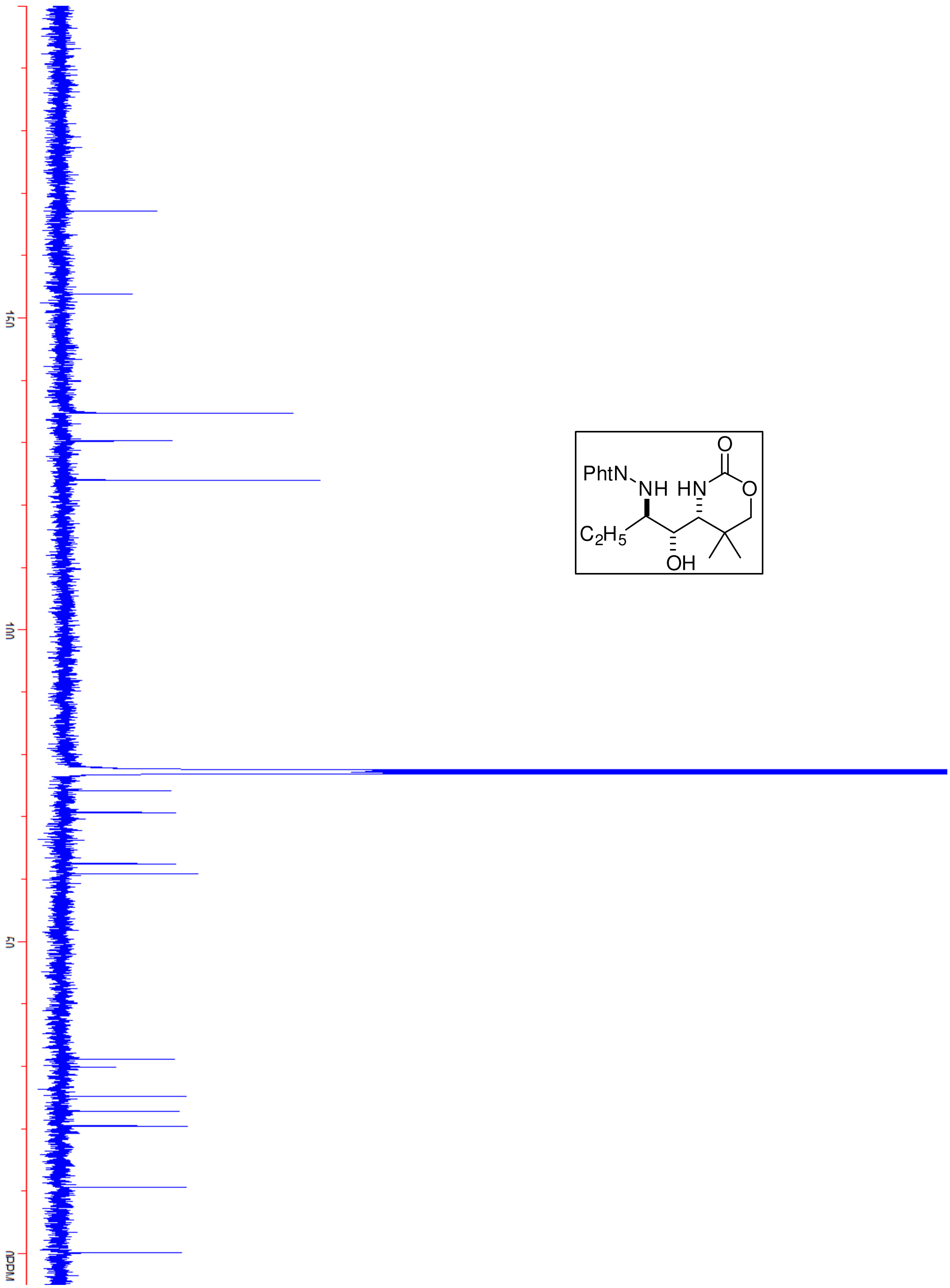
Compound 14a.



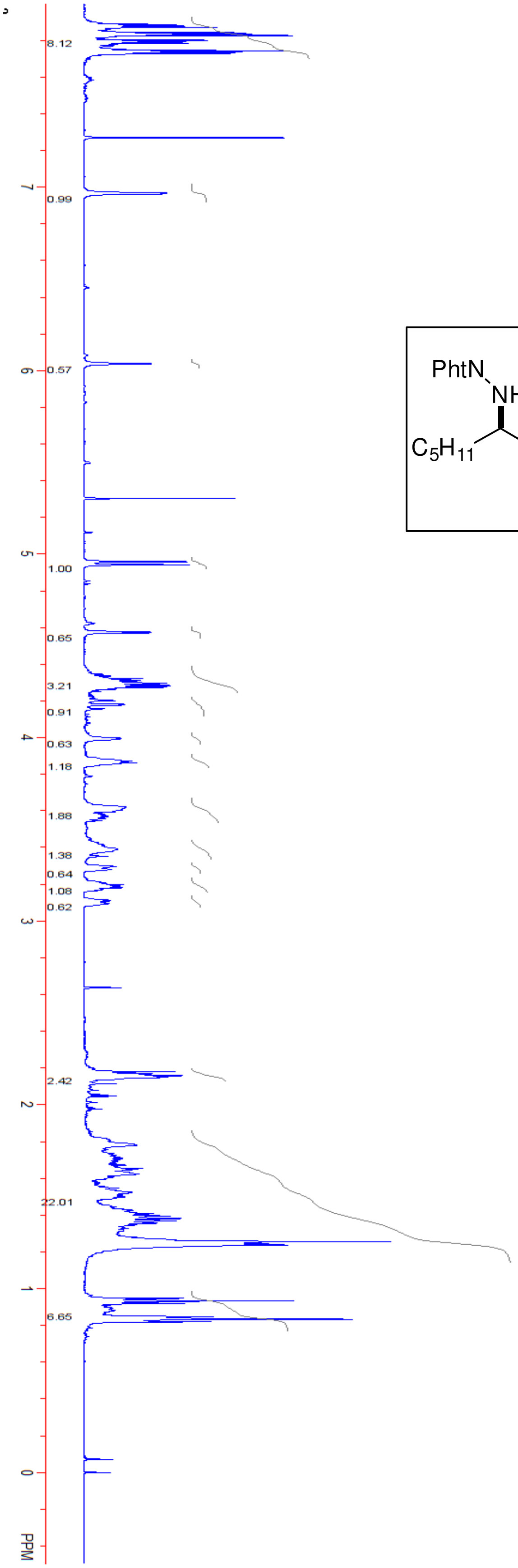
Compound 14.

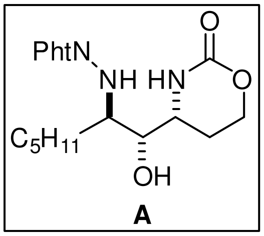

2.07
2.11
0.86
0.07
0.87
0.08
0.96
0.89
0.96
1.20
0.10
0.86
0.89
2.19
3.10
2.92
2.79
7
6
5
4
3
2
1
0
PPM
O
PhtN
NH
HN
O
C_2H_5
OH

Compound 14.

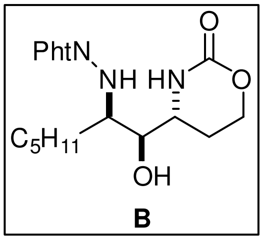


Compound 15.





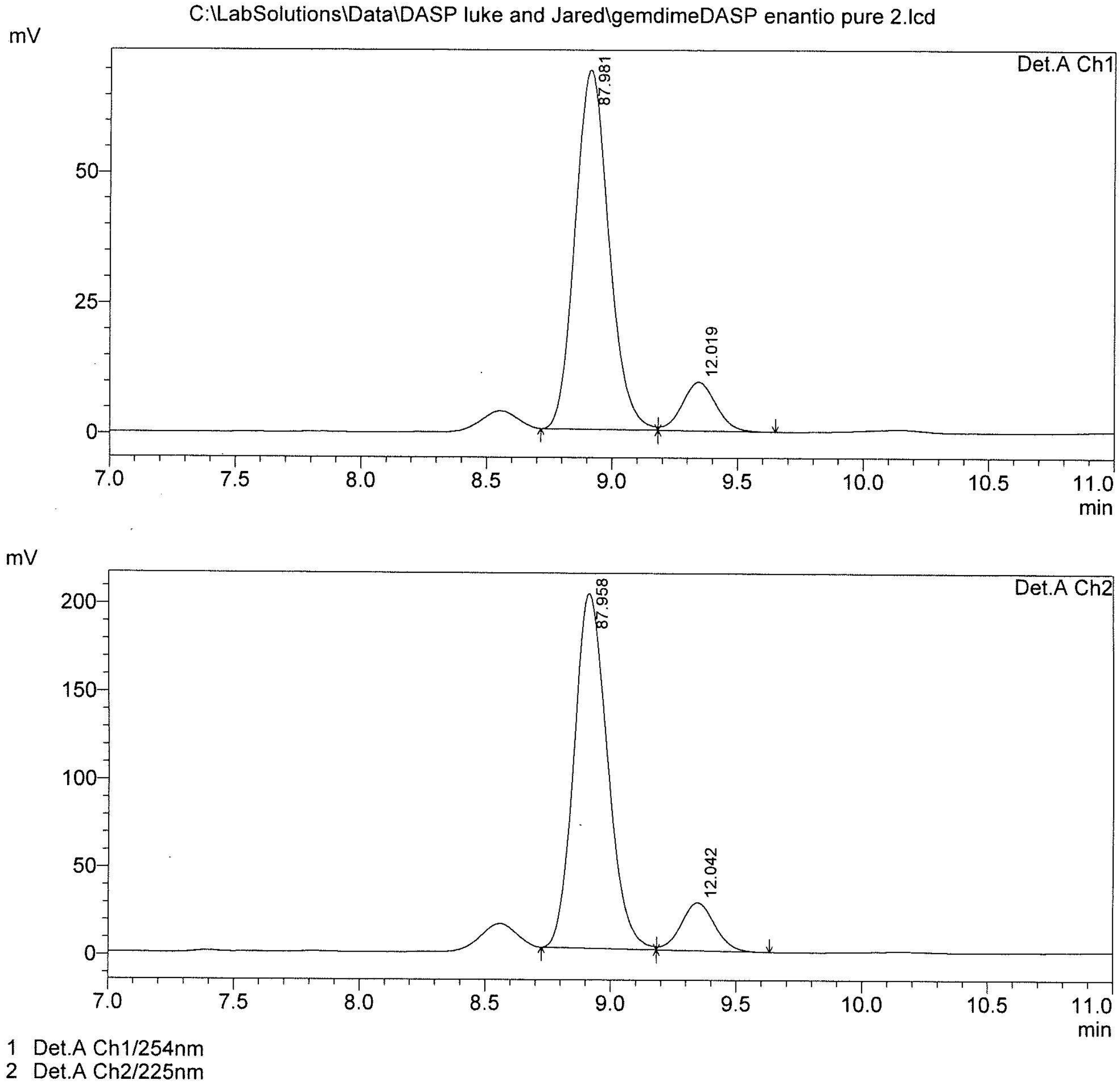
A



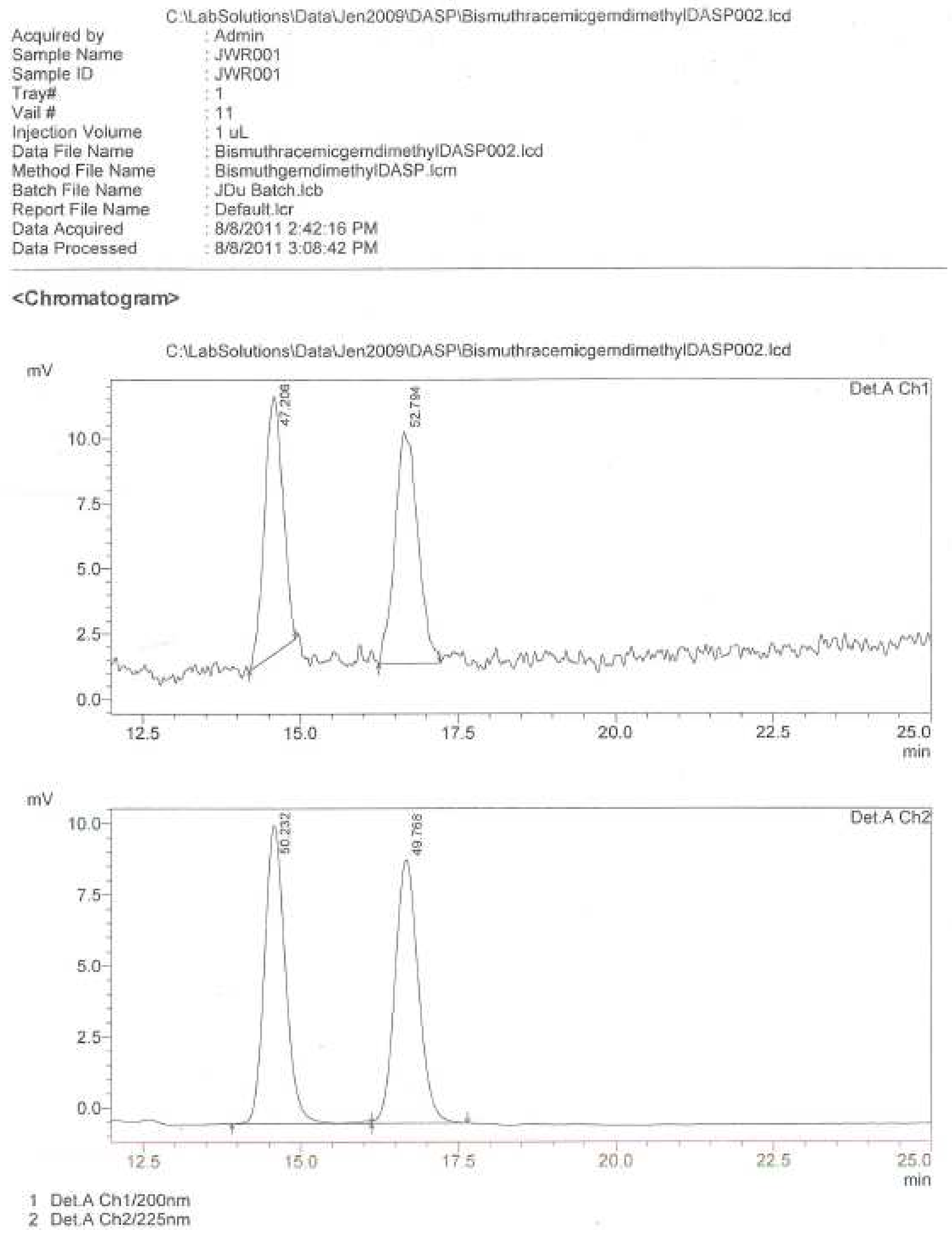
B

Compound 15.

Compound 9 (enantioenriched).



Compound 9 (racemic).



C:\LabSolutions\Data\Jen2009\DASP\BismuthracemicgemdimethylDASP002.lcd

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Sample ID	: JWR001
Tray#	: 1
Vail #	: 11
Injection Volume	: 1 uL
Data File Name	: BismuthracemicgemdimethylDASP002.lcd
Method File Name	: BismuthgemdimethylDASP.lcm
Batch File Name	: JDu Batch.lcb
Report File Name	: Default.lcr
Data Acquired	: 8/8/2011 2:42:16 PM
Data Processed	: 8/8/2011 3:08:42 PM

<Chromatogram>

C:\LabSolutions\Data\Jen2009\DASP\BismuthracemicgemdimethylDASP002.lcd

1 Det.A Ch1/200nm
2 Det.A Ch2/225nm

Compound 10 (enantioenriched).

C:\LabSolutions\Data\Jen2009\DASP\BismuthgemdimethylDASP003 enantioenriched.lcd

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Sample ID : JWR001
Tray# : 1
Vail # : 12
Injection Volume : 1 uL
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Method File Name : BismuthgemdimethylDASP.lcm
Batch File Name : JDu Batch.lcb
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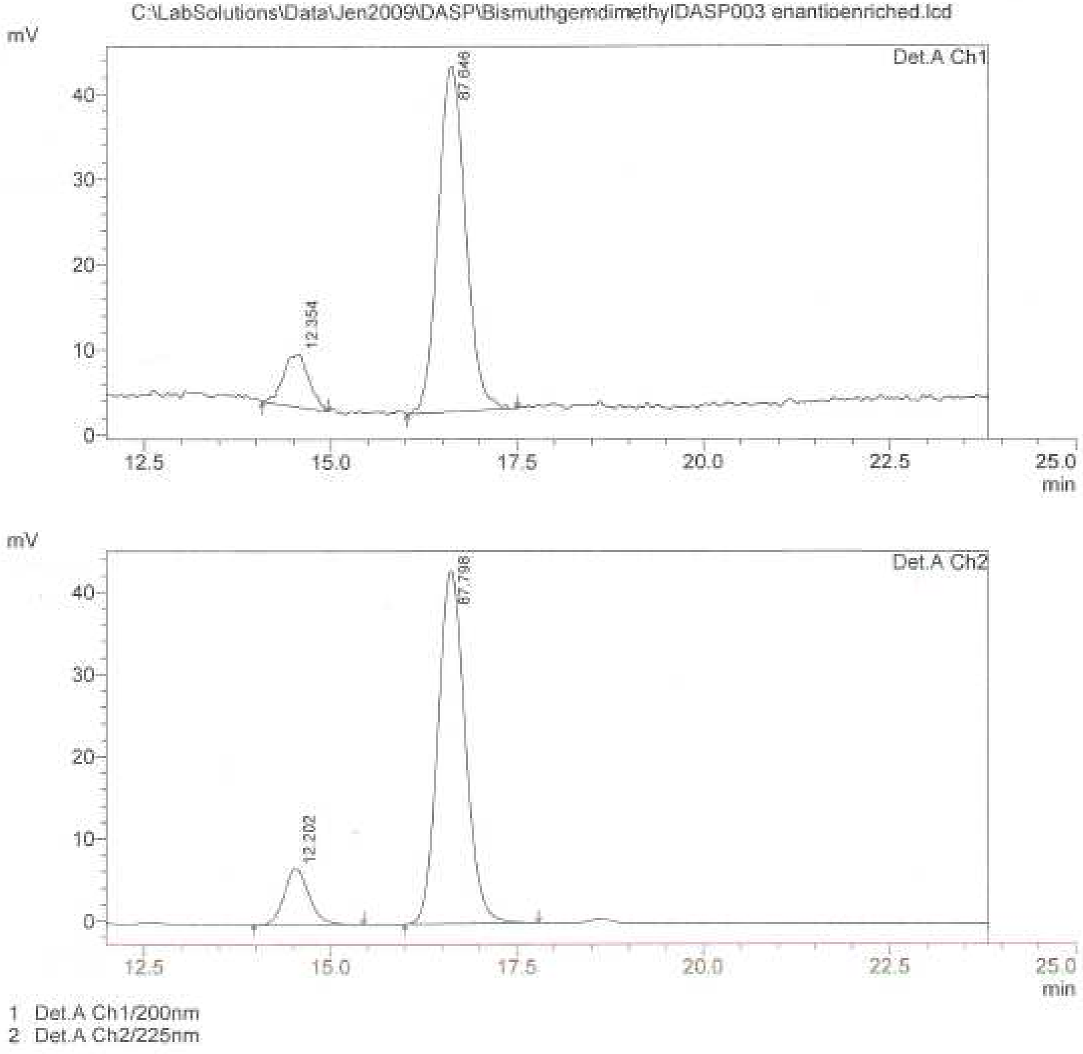

IX. Crystallographic Experimental Section

Data Collection

A pale yellow crystal with approximate dimensions 0.38 x 0.33 x 0.18 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker SMART APEXII diffractometer with Cu K_α (λ = 1.54178 Å) radiation and the diffractometer to crystal distance of 4.03 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 41 frames collected at intervals of 0.6° in a 25° range about ω with the exposure time of 5 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEXII program. The final cell constants were calculated from a set of 9922 strong reflections from the actual data collection.

The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.82 Å. A total of 24547 data were harvested by collecting 19 sets of frames with 0.5° scans in ω with an exposure time 15/40 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

Structure Solution and Refinement

The systematic absences in the diffraction data were consistent for the space groups $P\bar{1}$ and $P1$. The *E*-statistics strongly suggested the centrosymmetric space group $P\bar{1}$ that yielded chemically reasonable and computationally stable results of refinement [2-4].

A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

The crystal selected for the single-crystal X-ray diffraction experiment proved to be a non-merohedral twin with a 18.7(2)% second component contribution. The twin components are related by a 180.0° rotation about reciprocal axis [001].

The crystal contains a racemate. The relative configuration of the three chiral centers (in the arbitrary selected molecule depicted in Figure 1) is SSS.

The final least-squares refinement of 468 parameters against 24547 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0441 and 0.1488, respectively. The final difference Fourier map was featureless.

The molecular diagram is drawn with 30% probability ellipsoids.

References.

[1] Bruker-AXS. (2007-2011) APEX2, SADABS, and SAINT Software Reference Manuals. Bruker-AXS, Madison, Wisconsin, USA.

[2] Sheldrick, G. M. (2008) SHELXL. *Acta Cryst.* **A64**, 112-122.

[3] Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. "OLEX2: a complete structure solution, refinement and analysis program". *J. Appl. Cryst.* (2009) **42**, *339-341*.

[4] Guzei, I.A. (2006-2011). Internal laboratory computer programs "G1", "ResIns", "FCF_filter", "Modicifer".

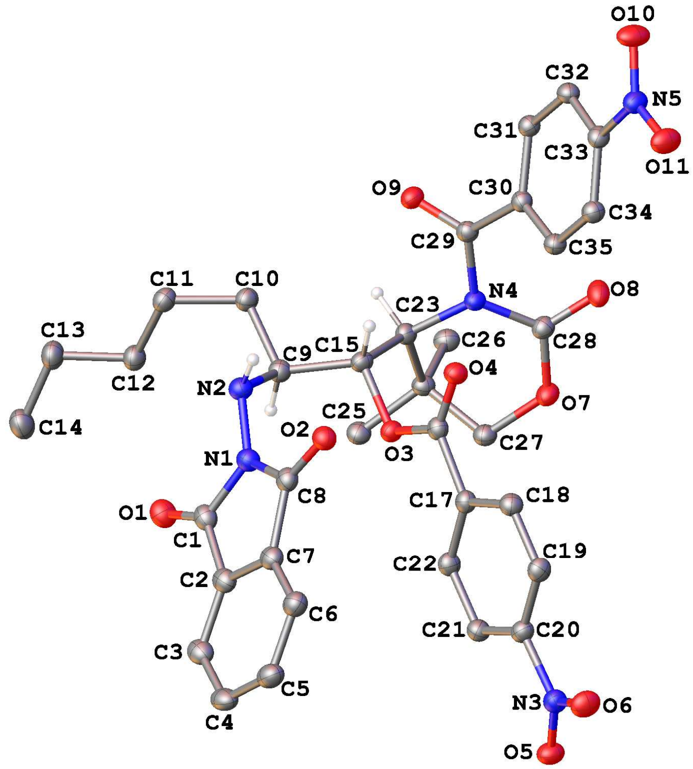

Figure 1. A molecular drawing of Schomaker11. All H atoms except on atom N2 and chiral C atoms are omitted.

Table 1. Crystal data and structure refinement for schomaker11.

Identification code	schomaker11	
Empirical formula	$C_{35}H_{35}N_5O_{11}$	
Formula weight	701.68	
Temperature	100(1) K	
Wavelength	1.54178 Å	
Crystal system	triclinic	
Space group	P$\bar{1}$	
Unit cell dimensions	a = 11.5843(11) Å	α= 73.125(7)°.
	b = 12.0276(13) Å	β= 78.428(9)°.
	c = 12.9101(15) Å	γ = 73.353(5)°.
Volume	1635.6(3) Å^3	
Z	2	
Density (calculated)	1.425 Mg/m^3	
Absorption coefficient	0.902 mm^{-1}	
F(000)	736	
Crystal size	0.38 x 0.33 x 0.18 mm^3	
Theta range for data collection	3.61 to 70.05°.	
Index ranges	-14<=h<=14, -14<=k<=14, -15<=l<=15	
Reflections collected	24547	
Independent reflections	24547 [R(int) = 0.0495]	
Completeness to theta = 67.00°	97.1 %	

Absorption correction	Numerical with SADABS
Max. and min. transmission	0.8545 and 0.7255
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	24547 / 0 / 468
Goodness-of-fit on F^2	0.979
Final R indices [I>2sigma(I)]	R1 = 0.0441, wR2 = 0.1349
R indices (all data)	R1 = 0.0517, wR2 = 0.1488
Largest diff. peak and hole	0.202 and -0.203 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for schomaker11. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5892(2)	5748(2)	3385(1)	45(1)
O(2)	5062(1)	3716(1)	1236(1)	36(1)
O(3)	2813(1)	5702(1)	1780(1)	30(1)
O(4)	2658(1)	4907(1)	440(1)	34(1)
O(5)	1008(2)	988(2)	5617(1)	42(1)
O(6)	1388(2)	-5(2)	4379(1)	45(1)
O(7)	-314(1)	7120(2)	1540(1)	36(1)
O(8)	-630(2)	7410(2)	-154(1)	42(1)
O(9)	2394(1)	8386(1)	-1365(1)	35(1)
O(10)	1339(2)	6101(2)	-5160(1)	51(1)
O(11)	1087(2)	4519(2)	-3909(1)	47(1)
N(1)	5342(2)	5005(2)	2130(2)	34(1)
N(2)	5318(2)	6018(2)	1250(2)	34(1)
N(3)	1341(2)	893(2)	4671(2)	35(1)
N(4)	1203(2)	7567(2)	106(1)	29(1)
N(5)	1204(2)	5546(2)	-4200(2)	36(1)
C(1)	5687(2)	4935(2)	3136(2)	37(1)
C(2)	5725(2)	3690(2)	3788(2)	36(1)
C(3)	5974(2)	3136(2)	4849(2)	42(1)
C(4)	6021(2)	1921(2)	5226(2)	45(1)
C(5)	5827(2)	1286(2)	4559(2)	45(1)
C(6)	5564(2)	1848(2)	3494(2)	41(1)
C(7)	5509(2)	3057(2)	3132(2)	36(1)
C(8)	5269(2)	3900(2)	2050(2)	34(1)
C(9)	4211(2)	6997(2)	1262(2)	32(1)
C(10)	4526(2)	8120(2)	439(2)	35(1)
C(11)	5687(2)	8374(2)	589(2)	37(1)
C(12)	5647(2)	8593(2)	1701(2)	38(1)
C(13)	6773(2)	8920(2)	1825(2)	45(1)
C(14)	6876(3)	8805(3)	3008(2)	52(1)
C(15)	3106(2)	6750(2)	959(2)	30(1)
C(16)	2612(2)	4851(2)	1397(2)	30(1)
C(17)	2302(2)	3830(2)	2293(2)	30(1)
C(18)	2140(2)	2876(2)	1972(2)	33(1)
C(19)	1848(2)	1905(2)	2753(2)	34(1)
C(20)	1705(2)	1909(2)	3841(2)	32(1)
C(21)	1842(2)	2845(2)	4185(2)	34(1)
C(22)	2157(2)	3810(2)	3395(2)	33(1)
C(23)	1945(2)	7794(2)	816(2)	30(1)
C(24)	1114(2)	8132(2)	1828(2)	31(1)
C(25)	1824(2)	8145(2)	2707(2)	35(1)
C(26)	273(2)	9389(2)	1475(2)	36(1)
C(27)	349(2)	7232(2)	2333(2)	33(1)
C(28)	50(2)	7368(2)	463(2)	33(1)
C(29)	1650(2)	7793(2)	-1020(2)	30(1)
C(30)	1323(2)	7232(2)	-1787(2)	29(1)
C(31)	1312(2)	7878(2)	-2877(2)	30(1)
C(32)	1233(2)	7344(2)	-3670(2)	32(1)
C(33)	1186(2)	6152(2)	-3351(2)	31(1)
C(34)	1177(2)	5492(2)	-2272(2)	33(1)
C(35)	1233(2)	6045(2)	-1486(2)	31(1)

Table 3. Bond lengths [Å] and angles [°] for schomaker11.

O(1)-C(1)	1.209(3)
O(2)-C(8)	1.215(3)
O(3)-C(16)	1.351(3)
O(3)-C(15)	1.467(3)
O(4)-C(16)	1.209(3)
O(5)-N(3)	1.233(2)
O(6)-N(3)	1.227(2)
O(7)-C(28)	1.341(3)
O(7)-C(27)	1.453(3)
O(8)-C(28)	1.209(3)
O(9)-C(29)	1.209(3)
O(10)-N(5)	1.228(2)
O(11)-N(5)	1.222(2)
N(1)-C(8)	1.391(3)
N(1)-N(2)	1.402(3)
N(1)-C(1)	1.407(3)
N(2)-C(9)	1.473(3)
N(2)-H(2)	0.90(3)
N(3)-C(20)	1.473(3)
N(4)-C(28)	1.388(3)
N(4)-C(29)	1.415(3)
N(4)-C(23)	1.500(3)
N(5)-C(33)	1.476(3)
C(1)-C(2)	1.483(3)
C(2)-C(3)	1.387(3)
C(2)-C(7)	1.389(3)
C(3)-C(4)	1.388(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.390(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.397(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.378(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.493(3)
C(9)-C(15)	1.538(3)
C(9)-C(10)	1.543(3)
C(9)-H(9)	1.0000
C(10)-C(11)	1.521(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.522(3)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.515(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.519(4)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(23)	1.555(3)
C(15)-H(15)	1.0000
C(16)-C(17)	1.495(3)
C(17)-C(22)	1.392(3)
C(17)-C(18)	1.398(3)
C(18)-C(19)	1.379(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.382(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.383(3)
C(21)-C(22)	1.389(3)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
C(23)-C(24)	1.543(3)
C(23)-H(23)	1.0000
C(24)-C(27)	1.513(3)
C(24)-C(25)	1.535(3)
C(24)-C(26)	1.541(3)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(29)-C(30)	1.505(3)
C(30)-C(35)	1.394(3)
C(30)-C(31)	1.397(3)
C(31)-C(32)	1.386(3)
C(31)-H(31)	0.9500
C(32)-C(33)	1.385(3)
C(32)-H(32)	0.9500
C(33)-C(34)	1.388(3)
C(34)-C(35)	1.386(3)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500

C(16)-O(3)-C(15)	116.36(17)
C(28)-O(7)-C(27)	123.39(17)
C(8)-N(1)-N(2)	124.19(19)
C(8)-N(1)-C(1)	112.10(19)
N(2)-N(1)-C(1)	122.57(19)
N(1)-N(2)-C(9)	116.00(18)
N(1)-N(2)-H(2)	106.6(18)
C(9)-N(2)-H(2)	112.7(17)
O(6)-N(3)-O(5)	123.58(19)
O(6)-N(3)-C(20)	117.9(2)
O(5)-N(3)-C(20)	118.55(19)
C(28)-N(4)-C(29)	120.31(18)
C(28)-N(4)-C(23)	123.46(18)
C(29)-N(4)-C(23)	115.19(17)
O(11)-N(5)-O(10)	123.6(2)
O(11)-N(5)-C(33)	118.19(19)

O(10)-N(5)-C(33)	118.18(19)
O(1)-C(1)-N(1)	125.4(2)
O(1)-C(1)-C(2)	129.1(2)
N(1)-C(1)-C(2)	105.5(2)
C(3)-C(2)-C(7)	121.2(2)
C(3)-C(2)-C(1)	130.4(2)
C(7)-C(2)-C(1)	108.3(2)
C(2)-C(3)-C(4)	117.6(2)
C(2)-C(3)-H(3)	121.2
C(4)-C(3)-H(3)	121.2
C(5)-C(4)-C(3)	121.0(2)
C(5)-C(4)-H(4)	119.5
C(3)-C(4)-H(4)	119.5
C(4)-C(5)-C(6)	121.3(2)
C(4)-C(5)-H(5)	119.4
C(6)-C(5)-H(5)	119.4
C(7)-C(6)-C(5)	117.2(2)
C(7)-C(6)-H(6)	121.4
C(5)-C(6)-H(6)	121.4
C(6)-C(7)-C(2)	121.6(2)
C(6)-C(7)-C(8)	130.2(2)
C(2)-C(7)-C(8)	108.1(2)
O(2)-C(8)-N(1)	124.4(2)
O(2)-C(8)-C(7)	129.9(2)
N(1)-C(8)-C(7)	105.65(19)
N(2)-C(9)-C(15)	114.09(18)
N(2)-C(9)-C(10)	106.66(18)
C(15)-C(9)-C(10)	109.64(18)
N(2)-C(9)-H(9)	108.8
C(15)-C(9)-H(9)	108.8
C(10)-C(9)-H(9)	108.8
C(11)-C(10)-C(9)	114.14(19)
C(11)-C(10)-H(10A)	108.7
C(9)-C(10)-H(10A)	108.7
C(11)-C(10)-H(10B)	108.7
C(9)-C(10)-H(10B)	108.7
H(10A)-C(10)-H(10B)	107.6
C(10)-C(11)-C(12)	113.4(2)
C(10)-C(11)-H(11A)	108.9
C(12)-C(11)-H(11A)	108.9
C(10)-C(11)-H(11B)	108.9
C(12)-C(11)-H(11B)	108.9
H(11A)-C(11)-H(11B)	107.7
C(13)-C(12)-C(11)	113.4(2)
C(13)-C(12)-H(12A)	108.9
C(11)-C(12)-H(12A)	108.9
C(13)-C(12)-H(12B)	108.9
C(11)-C(12)-H(12B)	108.9
H(12A)-C(12)-H(12B)	107.7
C(12)-C(13)-C(14)	112.5(2)
C(12)-C(13)-H(13A)	109.1
C(14)-C(13)-H(13A)	109.1
C(12)-C(13)-H(13B)	109.1
C(14)-C(13)-H(13B)	109.1
H(13A)-C(13)-H(13B)	107.8
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(3)-C(15)-C(9)	107.84(17)
O(3)-C(15)-C(23)	109.91(17)
C(9)-C(15)-C(23)	117.44(18)
O(3)-C(15)-H(15)	107.1
C(9)-C(15)-H(15)	107.1
C(23)-C(15)-H(15)	107.1
O(4)-C(16)-O(3)	124.2(2)
O(4)-C(16)-C(17)	123.3(2)
O(3)-C(16)-C(17)	112.44(19)
C(22)-C(17)-C(18)	120.4(2)
C(22)-C(17)-C(16)	123.2(2)
C(18)-C(17)-C(16)	116.4(2)
C(19)-C(18)-C(17)	119.7(2)
C(19)-C(18)-H(18)	120.2
C(17)-C(18)-H(18)	120.2
C(18)-C(19)-C(20)	118.8(2)
C(18)-C(19)-H(19)	120.6
C(20)-C(19)-H(19)	120.6
C(21)-C(20)-C(19)	122.9(2)
C(21)-C(20)-N(3)	118.4(2)
C(19)-C(20)-N(3)	118.6(2)
C(20)-C(21)-C(22)	117.9(2)
C(20)-C(21)-H(21)	121.0
C(22)-C(21)-H(21)	121.0
C(21)-C(22)-C(17)	120.2(2)
C(21)-C(22)-H(22)	119.9
C(17)-C(22)-H(22)	119.9
N(4)-C(23)-C(24)	109.36(17)
N(4)-C(23)-C(15)	108.46(17)
C(24)-C(23)-C(15)	120.02(18)
N(4)-C(23)-H(23)	106.0
C(24)-C(23)-H(23)	106.0
C(15)-C(23)-H(23)	106.0
C(27)-C(24)-C(25)	107.84(18)
C(27)-C(24)-C(26)	109.24(19)
C(25)-C(24)-C(26)	108.35(18)
C(27)-C(24)-C(23)	109.19(18)
C(25)-C(24)-C(23)	113.00(18)
C(26)-C(24)-C(23)	109.16(18)
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

O(7)-C(27)-C(24)	111.59(18)	C(32)-C(31)-C(30)	120.6(2)
O(7)-C(27)-H(27A)	109.3	C(32)-C(31)-H(31)	119.7
C(24)-C(27)-H(27A)	109.3	C(30)-C(31)-H(31)	119.7
O(7)-C(27)-H(27B)	109.3	C(31)-C(32)-C(33)	118.1(2)
C(24)-C(27)-H(27B)	109.3	C(31)-C(32)-H(32)	121.0
H(27A)-C(27)-H(27B)	108.0	C(33)-C(32)-H(32)	121.0
O(8)-C(28)-O(7)	119.3(2)	C(32)-C(33)-C(34)	122.7(2)
O(8)-C(28)-N(4)	122.9(2)	C(32)-C(33)-N(5)	118.5(2)
O(7)-C(28)-N(4)	117.85(19)	C(34)-C(33)-N(5)	118.7(2)
O(9)-C(29)-N(4)	118.9(2)	C(33)-C(34)-C(35)	118.5(2)
O(9)-C(29)-C(30)	118.4(2)	C(33)-C(34)-H(34)	120.7
N(4)-C(29)-C(30)	122.44(18)	C(35)-C(34)-H(34)	120.7
C(35)-C(30)-C(31)	119.9(2)	C(34)-C(35)-C(30)	120.1(2)
C(35)-C(30)-C(29)	122.2(2)	C(34)-C(35)-H(35)	119.9
C(31)-C(30)-C(29)	116.99(19)	C(30)-C(35)-H(35)	119.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for schomaker11. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	46(1)	46(1)	46(1)	-18(1)	-8(1)	-9(1)
O(2)	36(1)	40(1)	34(1)	-11(1)	-4(1)	-9(1)
O(3)	33(1)	30(1)	29(1)	-7(1)	-3(1)	-11(1)
O(4)	39(1)	36(1)	29(1)	-8(1)	-5(1)	-12(1)
O(5)	53(1)	45(1)	30(1)	-7(1)	-2(1)	-19(1)
O(6)	58(1)	33(1)	45(1)	-11(1)	-2(1)	-16(1)
O(7)	37(1)	46(1)	30(1)	-11(1)	2(1)	-18(1)
O(8)	33(1)	62(1)	37(1)	-20(1)	0(1)	-17(1)
O(9)	38(1)	39(1)	30(1)	-8(1)	-1(1)	-17(1)
O(10)	83(1)	51(1)	26(1)	-8(1)	-3(1)	-30(1)
O(11)	70(1)	40(1)	38(1)	-12(1)	-2(1)	-26(1)
N(1)	34(1)	35(1)	32(1)	-8(1)	-5(1)	-7(1)
N(2)	35(1)	35(1)	32(1)	-8(1)	-2(1)	-9(1)
N(3)	36(1)	35(1)	35(1)	-7(1)	-6(1)	-10(1)
N(4)	32(1)	32(1)	24(1)	-8(1)	-2(1)	-10(1)
N(5)	43(1)	39(1)	30(1)	-10(1)	-2(1)	-16(1)
C(1)	30(1)	44(1)	37(1)	-16(1)	-4(1)	-4(1)
C(2)	28(1)	44(1)	34(1)	-11(1)	-2(1)	-4(1)
C(3)	35(1)	55(2)	34(2)	-14(1)	-1(1)	-6(1)
C(4)	39(1)	58(2)	31(2)	-3(1)	-1(1)	-9(1)
C(5)	41(1)	45(2)	42(2)	-1(1)	-2(1)	-11(1)
C(6)	36(1)	44(1)	41(2)	-8(1)	-3(1)	-11(1)
C(7)	29(1)	43(1)	34(1)	-10(1)	0(1)	-7(1)
C(8)	28(1)	39(1)	35(1)	-12(1)	-1(1)	-7(1)
C(9)	33(1)	35(1)	31(1)	-10(1)	-3(1)	-9(1)
C(10)	37(1)	36(1)	34(1)	-9(1)	-4(1)	-13(1)
C(11)	37(1)	38(1)	38(2)	-10(1)	0(1)	-14(1)
C(12)	36(1)	40(1)	41(2)	-11(1)	-5(1)	-14(1)
C(13)	41(1)	52(2)	51(2)	-15(1)	-7(1)	-19(1)
C(14)	51(2)	56(2)	56(2)	-14(1)	-17(1)	-17(1)
C(15)	35(1)	29(1)	28(1)	-6(1)	-2(1)	-12(1)
C(16)	26(1)	32(1)	33(1)	-10(1)	-4(1)	-5(1)
C(17)	27(1)	31(1)	33(1)	-9(1)	-4(1)	-7(1)
C(18)	35(1)	37(1)	30(1)	-11(1)	-2(1)	-9(1)
C(19)	36(1)	32(1)	37(1)	-11(1)	-3(1)	-10(1)
C(20)	31(1)	31(1)	33(1)	-5(1)	-3(1)	-8(1)
C(21)	35(1)	37(1)	29(1)	-8(1)	-5(1)	-10(1)
C(22)	34(1)	32(1)	36(1)	-10(1)	-6(1)	-9(1)
C(23)	32(1)	31(1)	28(1)	-8(1)	-5(1)	-10(1)
C(24)	36(1)	32(1)	26(1)	-7(1)	-3(1)	-9(1)
C(25)	39(1)	41(1)	29(1)	-12(1)	-2(1)	-12(1)
C(26)	40(1)	33(1)	33(1)	-9(1)	-2(1)	-7(1)
C(27)	35(1)	36(1)	27(1)	-8(1)	-2(1)	-9(1)
C(28)	33(1)	35(1)	32(1)	-11(1)	0(1)	-10(1)
C(29)	30(1)	29(1)	29(1)	-6(1)	-4(1)	-5(1)
C(30)	27(1)	32(1)	28(1)	-9(1)	-3(1)	-7(1)
C(31)	31(1)	31(1)	30(1)	-7(1)	-2(1)	-8(1)
C(32)	32(1)	36(1)	26(1)	-6(1)	-3(1)	-9(1)
C(33)	33(1)	36(1)	28(1)	-12(1)	-1(1)	-11(1)
C(34)	35(1)	32(1)	31(1)	-8(1)	-3(1)	-9(1)
C(35)	33(1)	34(1)	27(1)	-7(1)	-3(1)	-10(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10 ^{3}) for schomaker11.

	x	y	z	U(eq)
H(2)	5480(20)	5750(20)	640(20)	45(8)
H(3)	6108	3572	5302	51
H(4)	6187	1518	5950	54
H(5)	5876	453	4833	55
H(6)	5428	1416	3039	49
H(9)	4001	7148	2007	39
H(10A)	4608	8021	-309	42
H(10B)	3843	8823	509	42
H(11A)	5838	9087	15	44
H(11B)	6377	7686	492	44
H(12A)	4927	9248	1818	46
H(12B)	5548	7861	2274	46
H(13A)	6752	9755	1403	54
H(13B)	7501	8391	1516	54
H(14A)	7574	9094	3042	78
H(14B)	6989	7963	3413	78
H(14C)	6132	9283	3333	78
H(15)	3369	6518	248	37
H(18)	2230	2897	1219	40
H(19)	1747	1245	2547	41
H(21)	1725	2828	4939	40
H(22)	2275	4459	3607	40
H(23)	2230	8525	387	36
H(25A)	2294	7331	3001	53
H(25B)	1254	8439	3296	53
H(25C)	2377	8673	2384	53
H(26A)	765	9974	1145	54
H(26B)	-262	9605	2115	54
H(26C)	-220	9385	942	54
H(27A)	882	6442	2633	39
H(27B)	-234	7486	2944	39
H(31)	1359	8690	-3077	37
H(32)	1211	7782	-4411	38
H(34)	1133	4679	-2077	39
H(35)	1211	5616	-741	38

Table 6. Torsion angles [°] for schomaker11.

C(8)-N(1)-N(2)-C(9)	109.5(2)
C(1)-N(1)-N(2)-C(9)	-83.6(2)
C(8)-N(1)-C(1)-O(1)	175.0(2)
N(2)-N(1)-C(1)-O(1)	6.8(4)
C(8)-N(1)-C(1)-C(2)	-5.5(2)
N(2)-N(1)-C(1)-C(2)	-173.75(19)
O(1)-C(1)-C(2)-C(3)	1.6(4)
N(1)-C(1)-C(2)-C(3)	-177.8(2)
O(1)-C(1)-C(2)-C(7)	-175.7(2)
N(1)-C(1)-C(2)-C(7)	4.8(3)
C(7)-C(2)-C(3)-C(4)	1.1(4)
C(1)-C(2)-C(3)-C(4)	-175.9(2)
C(2)-C(3)-C(4)-C(5)	0.2(4)
C(3)-C(4)-C(5)-C(6)	-0.9(4)
C(4)-C(5)-C(6)-C(7)	0.3(4)
C(5)-C(6)-C(7)-C(2)	1.0(3)
C(5)-C(6)-C(7)-C(8)	179.0(2)
C(3)-C(2)-C(7)-C(6)	-1.8(4)
C(1)-C(2)-C(7)-C(6)	175.9(2)
C(3)-C(2)-C(7)-C(8)	179.8(2)
C(1)-C(2)-C(7)-C(8)	-2.5(3)
N(2)-N(1)-C(8)-O(2)	-7.2(3)
C(1)-N(1)-C(8)-O(2)	-175.3(2)
N(2)-N(1)-C(8)-C(7)	172.05(19)
C(1)-N(1)-C(8)-C(7)	4.0(2)
C(6)-C(7)-C(8)-O(2)	0.3(4)
C(2)-C(7)-C(8)-O(2)	178.4(2)
C(6)-C(7)-C(8)-N(1)	-178.9(2)
C(2)-C(7)-C(8)-N(1)	-0.8(2)
N(1)-N(2)-C(9)-C(15)	-75.0(3)
N(1)-N(2)-C(9)-C(10)	163.78(18)
N(2)-C(9)-C(10)-C(11)	-49.9(3)
C(15)-C(9)-C(10)-C(11)	-173.90(19)
C(9)-C(10)-C(11)-C(12)	-60.8(3)
C(10)-C(11)-C(12)-C(13)	-176.5(2)
C(11)-C(12)-C(13)-C(14)	-164.5(2)
C(16)-O(3)-C(15)-C(9)	-133.21(18)
C(16)-O(3)-C(15)-C(23)	97.6(2)
N(2)-C(9)-C(15)-O(3)	62.3(2)
C(10)-C(9)-C(15)-O(3)	-178.11(17)
N(2)-C(9)-C(15)-C(23)	-172.89(19)
C(10)-C(9)-C(15)-C(23)	-53.3(3)
C(15)-O(3)-C(16)-O(4)	0.0(3)
C(15)-O(3)-C(16)-C(17)	-179.11(17)
O(4)-C(16)-C(17)-C(22)	-174.9(2)
O(3)-C(16)-C(17)-C(22)	4.2(3)
O(4)-C(16)-C(17)-C(18)	4.1(3)
O(3)-C(16)-C(17)-C(18)	-176.79(18)
C(22)-C(17)-C(18)-C(19)	-0.7(3)
C(16)-C(17)-C(18)-C(19)	-179.8(2)
C(17)-C(18)-C(19)-C(20)	1.0(3)
C(18)-C(19)-C(20)-C(21)	-0.1(3)
C(18)-C(19)-C(20)-N(3)	177.4(2)
O(6)-N(3)-C(20)-C(21)	-169.9(2)
O(5)-N(3)-C(20)-C(21)	10.1(3)
O(6)-N(3)-C(20)-C(19)	12.6(3)
O(5)-N(3)-C(20)-C(19)	-167.5(2)
C(19)-C(20)-C(21)-C(22)	-1.0(3)
N(3)-C(20)-C(21)-C(22)	-178.52(19)
C(20)-C(21)-C(22)-C(17)	1.3(3)
C(18)-C(17)-C(22)-C(21)	-0.5(3)
C(16)-C(17)-C(22)-C(21)	178.5(2)
C(28)-N(4)-C(23)-C(24)	-16.4(3)
C(29)-N(4)-C(23)-C(24)	151.95(18)
C(28)-N(4)-C(23)-C(15)	116.2(2)
C(29)-N(4)-C(23)-C(15)	-75.5(2)
O(3)-C(15)-C(23)-N(4)	-79.2(2)
C(9)-C(15)-C(23)-N(4)	157.10(19)
O(3)-C(15)-C(23)-C(24)	47.5(2)
C(9)-C(15)-C(23)-C(24)	-76.3(3)
N(4)-C(23)-C(24)-C(27)	48.9(2)
C(15)-C(23)-C(24)-C(27)	-77.3(2)
N(4)-C(23)-C(24)-C(25)	168.95(17)
C(15)-C(23)-C(24)-C(25)	42.7(3)
N(4)-C(23)-C(24)-C(26)	-70.4(2)
C(15)-C(23)-C(24)-C(26)	163.37(18)
C(28)-O(7)-C(27)-C(24)	25.2(3)
C(25)-C(24)-C(27)-O(7)	-177.30(18)
C(26)-C(24)-C(27)-O(7)	65.1(2)
C(23)-C(24)-C(27)-O(7)	-54.2(2)
C(27)-O(7)-C(28)-O(8)	-170.0(2)
C(27)-O(7)-C(28)-N(4)	10.0(3)
C(29)-N(4)-C(28)-O(8)	-2.1(3)
C(23)-N(4)-C(28)-O(8)	165.7(2)
C(29)-N(4)-C(28)-O(7)	177.89(18)
C(23)-N(4)-C(28)-O(7)	-14.3(3)
C(28)-N(4)-C(29)-O(9)	152.4(2)
C(23)-N(4)-C(29)-O(9)	-16.4(3)
C(28)-N(4)-C(29)-C(30)	-33.4(3)
C(23)-N(4)-C(29)-C(30)	157.87(18)
O(9)-C(29)-C(30)-C(35)	134.8(2)
N(4)-C(29)-C(30)-C(35)	-39.5(3)
O(9)-C(29)-C(30)-C(31)	-34.6(3)
N(4)-C(29)-C(30)-C(31)	151.1(2)
C(35)-C(30)-C(31)-C(32)	-1.1(3)
C(29)-C(30)-C(31)-C(32)	168.56(19)
C(30)-C(31)-C(32)-C(33)	-1.0(3)
C(31)-C(32)-C(33)-C(34)	2.1(3)
C(31)-C(32)-C(33)-N(5)	-175.01(19)
O(11)-N(5)-C(33)-C(32)	-175.5(2)
O(10)-N(5)-C(33)-C(32)	4.6(3)
O(11)-N(5)-C(33)-C(34)	7.3(3)
O(10)-N(5)-C(33)-C(34)	-172.6(2)
C(32)-C(33)-C(34)-C(35)	-0.9(3)
N(5)-C(33)-C(34)-C(35)	176.2(2)
C(33)-C(34)-C(35)-C(30)	-1.3(3)
C(31)-C(30)-C(35)-C(34)	2.3(3)

Table 7. Hydrogen bonds for schomaker11 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(2)#1	0.90(3)	2.48(3)	3.238(3)	142(2)
N(2)-H(2)...O(4)#1	0.90(3)	2.39(3)	3.059(3)	132(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z

C(29)-C(30)-C(35)-C(34)	-166.8(2)