Supporting Information

Efficient copper-catalyzed Michael addition of acrylic derivatives with primary alcohols in the presence of base

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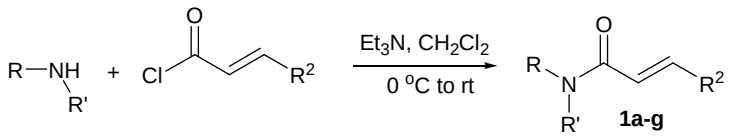
General experimental procedures

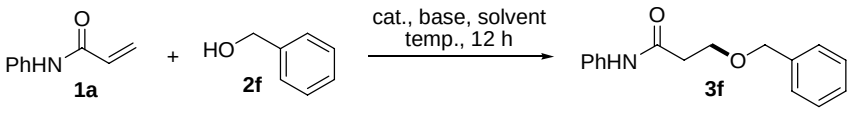
All reactions were carried out in air except special statement. Commercially available reagents and solvents were purchased and used as received. Proton and carbon magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded on a JEOL-300 or JEOL-600 spectrometers using tetramethylsilane (TMS) in the solvent of $CDCl_3$ as the internal standard (^{1}H NMR: TMS at 0.00 ppm, $CHCl_3$ at 7.26 ppm; ^{13}C NMR: $CHCl_3$ at 77.36 ppm). Low resolution Mass spectra (LRMS) were recorded on a Bruker Esquire-2000 mass spectrometer (ESI). Melting points were measured on an uncorrected X-4 digital melting point Apparatus.

General procedure for synthesis of compounds 1a-g[1-5]



Amine (10 mmol) and triethylamine (11 mmol) were dissolved in dichloromethane (20 mL), the solution was cooled to 0 ℃, and acyl chloride (11 mmol) in 5 mL dichloromethane was added dropwise to the solution over 15 min. After stirring for another 15 min, the mixture was warmed to room temperature and stirred until the amine was consumed completely (monitored by TLC). The resulting solution was concentrated, and the residue was dissolved in 20 mL of EtOAc and filtered. The organic layer was washed with 5% HCl solution (3 × 20 mL), saturated $NaHCO_3$ solution (20 mL) and brine (20 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated *in vacuo*. After purification by flash chromatography on silica gel (EtOAc in petroleum) or recrystallization, pure compounds (**1a-g**) were obtained. Compounds (**1g-j**) were purchased from Alfa Aesar Company.

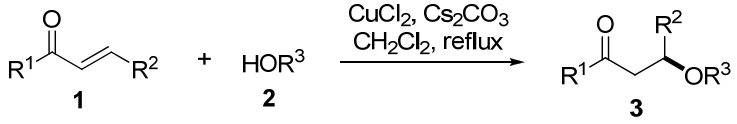
General procedure for Michael reaction conditions screening



N-Phenylacrylamide (**1a**) (74 mg, 0.5 mmol), phenylmethanol (**2f**) (54 mg, 0.5 mmol),

base, catalyst, and 1 mL of solvent were added to a 5 mL round-bottom flask with a magnetic stir bar, and the mixture was refluxed overnight (about 12 h). The resulting solution was cooled to room temperature and flushed through a short column of silica gel with dichloromethane. The solution was concentrated by rotary evaporation, and the residue was purified by flash chromatography on silica gel (petroleum ether/acetyl acetate, 5:1) to give 3-benzoxyl-*N*-phenyl propanamide (**3f**).

General procedure for synthesis of compounds 3a-w

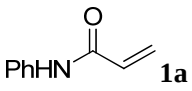


Acrylic derivative (**1**) (2.0 mmol), alcohol (**2**) (4.0 mmol), CH_3ONa (216 mg, 4.0 mmol) for entry 18 in Table 2, Cs_2CO_3 (652 mg, 2.0 mmol) for other entries in Table 2, $CuCl_2$ (27 mg, 0.2 mmol), and CH_3OH (4.0 mL) for entry 18 in Table 2, dichloromethane (4.0 mL) for other entries in Table 2 were added to a 10 mL round-bottom flask with a magnetic stir bar, and the mixture was refluxed under air overnight (about 12 h) (For entry 17 in Table 2, the reaction was performed under nitrogen atmosphere). After **1** was completely consumed (monitored by TLC), the resulting solution was cooled to room temperature. For products **3a-t**, the solution was flushed through a short column of silica gel with dichloromethane and concentrated by rotary evaporation, and the residue was purified by flash chromatography on silica gel (petroleum ether/acetyl acetate) to give **3a-t**. For products **3u-w**, the solvent and other materials with low boiling point were removed by rotary evaporation, and 4 mL of 5% HCl aqueous solution was added to the residue. The aqueous solution was extracted with EtOAc (2 × 5 mL), and the combined organic layer was washed with saturated brine (2 × 5 mL) and dried over anhydrous Na_2SO_4. After concentrated *in vacuo*, the residue was purified by flash chromatography on silica gel (petroleum ether/acetyl acetate) to provide **3u-w**.

General procedure for synthesis of compound 3x

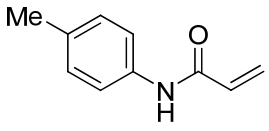
Compound **3x** was synthesized using the same procedure as **3a-t**.

Characterization data of compounds 1a-g



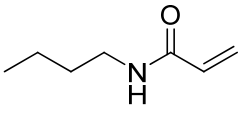
1a

***N*-Phenylacrylamide (1a).**[1,2] Eluent: petroleum ether/ethyl acetate (4:1). Yield: 1.21 g (82%). White solid, mp 106-107 °C (lit.[1] 102-104 °C). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.20 (bs, 1H), 7.60-7.58 (m, 2H), 7.32-7.26 (m, 2H), 7.13-7.08 (m, 1H), 6.44-6.26 (m, 2H), 5.70 (dd, *J* = 9.6, 1.7 Hz, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 164.3, 138.1, 131.6, 129.3, 127.9, 124.8, 120.6. ESIMS: $[M+H]^+$ m/z 148.3, $[M+Na]^+$ m/z 170.2.



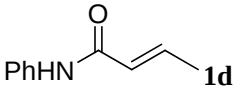
1b

***N*-*p*-Tolylacrylamide (1b).**[1] Eluent: petroleum ether/ethyl acetate (2:1). Yield: 1.19 g (74%). White solid, mp 145-146 °C (lit.[1] 138-139 °C). ^{1}H NMR ($CDCl_3$, 600 MHz): δ 7.94 (bs, 1H), 7.46 (d, *J* = 8.3 Hz, 2H), 7.10 (d, *J* = 6.9 Hz, 2H), 6.40-6.37 (m, 1H), 6.30-6.25 (m, 1H), 5.69 (d, *J* = 8.9 Hz, 1H), 2.30 (s, 3H),. ^{13}C NMR ($CDCl_3$, 150 MHz): δ 164.0, 135.6, 134.5, 131.7, 129.8, 127.6, 120.6, 21.2. ESIMS: $[M+H]^+$ m/z 162.3, $[M+Na]^+$ m/z 184.2.



1c

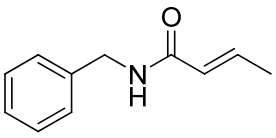
***N*-Butylacrylamide (1c).**[1] Eluent: petroleum ether/ethyl acetate (3:1). Yield: 1.11 g (87%). Oil. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 6.27-6.13 (m, 3H), 5.70 (d, *J* = 10.3 Hz, 1H), 3.32 (t, *J* = 6.9 Hz, 2H), 1.52-1.50 (m, 2H), 1.37-1.36 (m, 2H), 0.93 (t, *J* = 5.6 Hz, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz): δ 166.0, 131.4, 126.1, 39.6, 31.9, 20.4, 14.0. ESIMS: $[M+H]^+$ m/z 128.4, $[M+Na]^+$ m/z 150.2.



1d

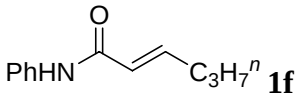
(*E*)-*N*-Phenylbut-2-enamide (1d).[3,4] Eluent: petroleum ether/ethyl acetate (5:1). Yield: 1.45 g (90%). White solid, mp 113-114 °C (lit.[3] 113-115 °C). ^{1}H NMR ($CDCl_3$, 600 MHz): δ 7.94 (bs, 1H), 7.59-7.57 (m, 2H), 7.31-7.26 (m, 2H), 7.10-7.08 (m, 1H), 7.02-6.90 (m, 1H), 6.00 (d, *J* = 15.1 Hz, 1H), 1.84 (dd, *J* = 6.9, 1.4 Hz, 3H). ^{13}C NMR

($CDCl_3$, 150 MHz): δ 164.7, 141.7, 138.4, 129.2, 125.9, 124.5, 120.5, 18.1. ESIMS: $[M+H]^+$ m/z 162.3, $[M+Na]^+$ m/z 184.2.



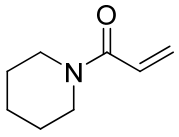
1e

(*E*)-*N*-Benzylbut-2-enamide (1e).[5] Recrystallization: petroleum ether/ethyl acetate (8:1). Yield: 1.33 mg (76%). White solid, mp 118-119 °C. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 7.31-7.26 (m, 5H), 6.88-6.80 (m, 1H), 6.03 (bs, 1H), 5.82 (d, *J* = 15.1 Hz, 3H), 4.47-4.46 (m, 2H), 1.83 (d, *J* = 6.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz): δ 166.2, 140.5, 138.7, 129.0, 128.1, 127.7, 125.2, 43.8, 18.0. ESIMS: $[M+H]^+$ m/z 176.3, $[M+Na]^+$ m/z 198.2.



1f

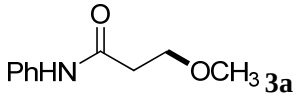
(*E*)-*N*-Phenylhex-2-enamide (1f). Eluent: petroleum ether/ethyl acetate (5:1). Yield: 0.86 g (45%). White solid, mp 106-107 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.23 (bs, 1H), 7.61-7.53 (m, 2H), 7.30-7.24 (m, 2H), 7.09-7.03 (m, 1H), 7.00-6.87 (m, 1H), 6.00 (dt, *J* = 15.1, 1.4 Hz, 1H), 2.17-2.09 (m, 2H), 1.50-1.37 (m, 2H), 0.90 (t, *J* = 7.6 Hz, 3H),. ^{13}C NMR ($CDCl_3$, 75 MHz): δ 165.0, 146.4, 138.5, 129.2, 124.4, 120.5, 34.4, 21.7, 14.0. ESIMS: $[M+H]^+$ m/z 190.3, $[M+Na]^+$ m/z 212.2.



1g

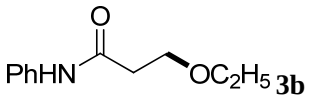
***N*-Acrylpiperidine (1g).**[1] Eluent: petroleum ether/ethyl acetate (2:1). Yield: 0.72 g (52%). Pale yellow oil. ^{1}H NMR($CDCl_3$, 300 MHz): δ 6.59 (dd, *J* = 16.9, 10.7 Hz, 1H), 6.24 (dd, *J* = 16.9, 2.1 Hz, 1H), 5.65 (dd, *J* = 10.7, 2.1 Hz, 1H), 3.61-3.49 (m, 4H), 1.67-1.58 (m, 6H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 165.4, 128.2, 127.0, 46.9, 43.1, 26.7, 25.6, 24.6. ESIMS: $[M+H]^+$ m/z 140.4, $[M+Na]^+$ m/z 162.3.

Characterization data of compounds 3a-w



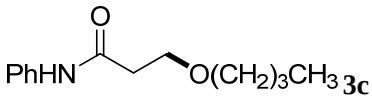
3a

3-Methoxy-*N*-phenylpropanamide (3a). Eluent: petroleum ether/ethyl acetate (5:1). Yield: 319 mg (89%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.41 (bs, 1H), 7.53-7.50 (m, 2H), 7.31-7.26 (m, 2H), 7.10-7.07 (m, 1H), 3.71 (t, J = 5.7 Hz, 2H), 3.41 (s, 3H), 2.61 (t, J = 5.5 Hz, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 170.2, 138.3, 129.2, 124.4, 120.2, 68.9, 59.1, 38.2. ESIMS: $[M+H]^+$ m/z 180.3, $[M+Na]^+$ m/z 202.2.



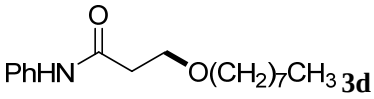
3b

3-Ethoxy-*N*-phenylpropanamide (3b). Eluent: petroleum ether/ethyl acetate (5:1). Yield: 340 mg (88%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.51 (bs, 1H), 7.52-7.49 (m, 2H), 7.33-7.26 (m, 2H), 7.11-7.06 (m, 1H), 3.76 (t, J = 5.5 Hz, 2H), 3.60 (q, J = 6.7 Hz, 2H), 2.63 (t, J = 5.5 Hz, 2H), 1.28 (t, J = 6.7 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 170.3, 138.5, 129.3, 124.3, 120.0, 67.0, 66.8, 38.3, 15.5. ESIMS: $[M+Na]^+$ m/z 216.2.



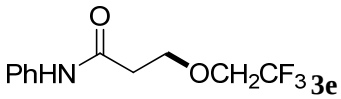
3c

3-Butoxy-*N*-phenylpropanamide (3c). Eluent: petroleum ether/ethyl acetate (5:1). Yield: 256 mg (58%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.53 (bs, 1H), 7.52-7.49 (m, 2H), 7.33-7.26 (m, 2H), 7.11-7.06 (m, 1H), 3.75 (t, J = 5.5 Hz, 2H), 3.53 (t, J = 6.5 Hz, 2H), 2.63 (t, J = 5.5 Hz, 2H), 1.68-1.59 (m, 2H), 1.49-1.39 (m, 2H), 0.95 (t, J = 7.4 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 170.4, 138.5, 129.3, 124.3, 120.1, 76.9, 67.0, 38.3, 32.0, 19.7, 14.2. ESIMS: $[M+H]^+$ m/z 222.2.



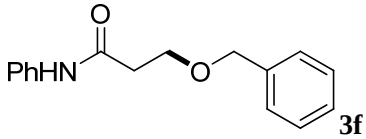
3d

3-(Octyloxy)-*N*-phenylpropanamide (3d). Eluent: petroleum ether/ethyl acetate (5:1). Yield: 205 mg (37%). White solid, mp 37-38 °C. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 8.52 (bs, 1H), 7.51-7.50 (m, 2H), 7.31-7.29 (m, 2H), 7.09-7.06 (m, 1H), 3.75 (t, J = 5.5 Hz, 2H), 3.52 (t, J = 6.5 Hz, 2H), 2.63 (t, J = 5.5 Hz, 2H), 1.65-1.62 (m, 2H), 1.40-1.37 (m, 2H), 1.31-1.26 (m, 8H), 0.88 (t, J = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz): δ 170.4, 138.5, 129.2, 124.3, 120.1, 71.8, 67.0, 38.4, 32.1, 30.0, 29.7, 29.6, 26.6, 23.0, 14.4. ESIMS: $[M+H]^+$ m/z 278.2, $[M+Na]^+$ m/z 300.2.



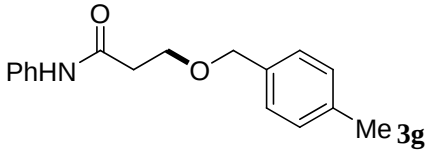
3e

***N*-Phenyl-3-(2,2,2-trifluoroethoxy)propanamide (3e).** Eluent: petroleum ether/ethyl acetate (3:1). Yield: 425 mg (86%). White solid, mp 74-75 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.86 (bs, 1H), 7.54-7.49 (m, 2H), 7.34-7.26 (m, 2H), 7.13-7.08 (m, 1H), 3.99-3.86 (m, 4H), 2.67 (t, *J* = 5.7 Hz, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 169.2, 138.1, 129.3, 124.7, 124.1 (q, *J* = 279.6 Hz), 120.3, 69.0, 68.9 (q, *J* = 34.7 Hz), 38.3. ESIMS: $[M+H]^+$ m/z 248.3, $[M+Na]^+$ m/z 270.1.



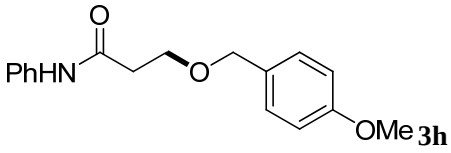
3f

3-(Benzyloxy)-*N*-phenylpropanamide (3f). Eluent: petroleum ether/ethyl acetate (4:1). Yield: 418 mg (82%). Oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.32 (bs, 1H), 7.45-7.42 (m, 2H), 7.35-7.25 (m, 7H), 7.10-7.05 (m, 1H), 4.59 (s, 2H), 3.83 (t, *J* = 5.5 Hz, 2H), 2.66 (t, *J* = 5.5 Hz, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 170.1, 138.4, 137.7, 129.2, 129.0, 128.4, 128.2, 124.4, 120.1, 73.9, 66.7, 38.4. ESIMS: $[M+H]^+$ m/z 256.3, $[M+Na]^+$ m/z 278.2.



3g

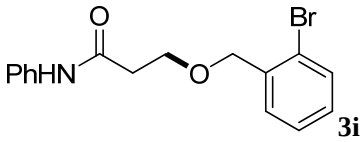
3-(4-Methylbenzyloxy)-*N*-phenylpropanamide (3g). Eluent: petroleum ether/ethyl acetate (3:1). Yield: 409 mg (76%). White solid, mp 86-87 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.33 (bs, 1H), 7.45-7.42 (m, 2H), 7.31-7.16 (m, 6H), 7.09-7.05 (m, 1H), 4.56 (s, 2H), 3.82 (t, *J* = 5.7 Hz, 2H), 2.65 (t, *J* = 5.7 Hz, 2H), 2.36 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 170.1, 138.4, 138.3, 134.6, 129.7, 129.2, 128.4, 124.3, 120.0, 73.8, 66.5, 38.5, 21.5. ESIMS: $[M+H]^+$ m/z 270.4, $[M+Na]^+$ m/z 292.2.



3h

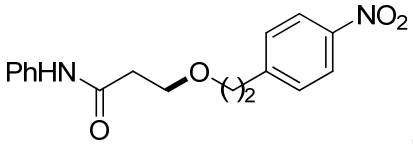
3-(4-Methoxybenzyloxy)-*N*-phenylpropanamide (3h). Eluent: petroleum ether/ethyl acetate (3:1). Yield: 353 mg (62%). White solid, mp 81-82 °C. ^{1}H NMR ($CDCl_3$, 300

MHz): δ 8.37 (bs, 1H), 7.45-7.42 (m, 2H), 7.31-7.25 (m, 4H), 7.09-7.05 (m, 1H), 6.89 (d, *J* = 8.6 Hz, 2H), 4.52 (s, 2H), 3.82-3.78 (m, 5H), 2.64 (t, *J* = 5.7 Hz, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 170.1, 159.8, 138.4, 129.9, 129.2, 128.9, 124.3, 120.0, 114.3, 73.5, 66.4, 55.6, 38.4. ESIMS: $[M+Na]^+$ m/z 308.2.



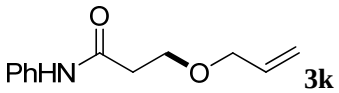
3i

3-(2-Bromobenzyloxy)-*N*-phenylpropanamide (3i). Eluent: petroleum ether/ethyl acetate (3:1). Yield: 400 mg (60%). White solid, mp 68-69 °C. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 8.36 (bs, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.47-7.43 (m, 3H), 7.30-7.25 (m, 3H), 7.08-7.05 (m, 1H), 4.64 (s, 2H), 3.88 (t, *J* = 5.2 Hz, 2H), 2.68 (t, *J* = 5.7 Hz, 2H). ^{13}C NMR ($CDCl_3$, 150 MHz): δ 170.0, 138.4, 137.1, 133.1, 129.9, 129.8, 129.2, 127.9, 124.4, 123.5, 120.4, 73.1, 67.1, 38.5. ESIMS: $[M+H]^+$ m/z 334.3, 336.2, $[M+Na]^+$ m/z 356.2, 358.0.



3j

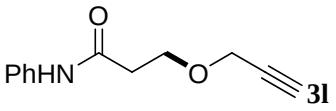
3-(4-Nitrophenethoxy)-*N*-phenylpropanamide (3j). Gradient eluent: petroleum ether/ethyl acetate (4:1 to 1:1). Yield: 427 mg (68%). Pale yellow solid, mp 134-135 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.06 (dd, *J* = 2.0 Hz, 8.6 Hz, 2H), 7.87 (bs, 1H), 7.37 (d, *J* = 8.6 Hz, 2H), 3.82-3.77 (m, 4H), 3.02 (t, *J* = 6.3 Hz, 2H), 2.59 (t, *J* = 5.7 Hz, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 169.8, 147.0, 138.1, 129.9, 129.2, 124.7, 124.0, 120.1, 71.2, 67.3, 38.4, 36.3. ESIMS: $[M+H]^+$ m/z 315.3, $[M+Na]^+$ m/z 337.0.



3k

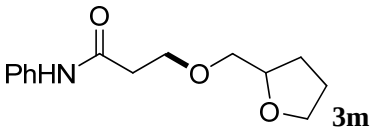
3-(Allyloxy)-N-phenylpropanamide (3k). Eluent: petroleum ether/ethyl acetate (4:1). Yield: 320 mg (78%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.40 (bs, 1H), 7.52-7.49 (m, 2H), 7.33-7.26 (m, 2H), 7.11-7.06 (m, 1H), 6.01-5.89 (m, 1H), 5.36-5.23 (m, 2H), 4.07 (d, *J* = 5.5 Hz, 2H), 3.78 (t, *J* = 5.7 Hz, 2H), 2.65 (t, *J* = 5.7 Hz, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 170.1, 138.4, 134.2, 129.2, 124.4, 120.1,

118.0, 72.4, 66.5, 38.3. ESIMS: $[M+H]^+$ m/z 206.3, $[M+Na]^+$ m/z 228.1.



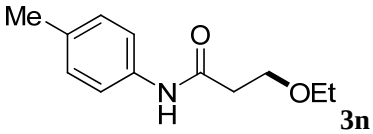
3l

***N*-Phenyl-3-(prop-2-ynyloxy)propanamide (3l).** Eluent: petroleum ether/ethyl acetate (4:1). Yield: 284 mg (70%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.13 (bs, 1H), 7.54-7.51 (m, 2H), 7.33-7.26 (m, 2H), 7.11-7.07 (m, 1H), 4.23 (d, *J* = 2.4 Hz, 2H), 3.88 (t, *J* = 5.7 Hz, 2H), 2.66 (t, *J* = 5.7 Hz, 2H), 2.49 (t, *J* = 2.4 Hz, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 169.7, 138.3, 129.2, 124.5, 120.2, 79.3, 75.6, 66.3, 58.8, 38.2. ESIMS: $[M+H]^+$ m/z 204.3, $[M+Na]^+$ m/z 226.1.



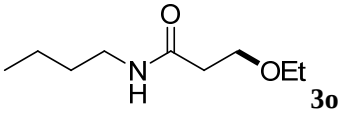
3m

***N*-Phenyl-3-((tetrahydrofuran-2-yl)methoxy)propanamide (3m).** Eluent: petroleum ether/ethyl acetate (2:1). Yield: 364 mg (73%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.73 (bs, 1H), 7.59-7.57 (m, 2H), 7.32-7.27 (m, 2H), 7.09-7.04 (m, 1H), 4.16-4.09 (m, 1H), 3.93-3.74 (m, 4H), 3.64-3.59 (m, 1H), 3.49-3.43 (m, 1H), 2.65 (t, *J* = 5.7 Hz, 2H), 2.04-1.86 (m, 3H), 1.64-1.55 (m, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 170.4, 138.7, 129.1, 124.1, 120.2, 77.9, 74.0, 68.5, 67.5, 38.2, 28.1, 26.0. ESIMS: $[M+H]^+$ m/z 250.3, $[M+Na]^+$ m/z 272.2.



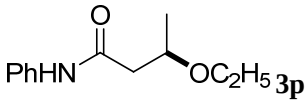
3n

3-Ethoxy-*N*-*p*-tolylpropanamide (3n). Eluent: petroleum ether/ethyl acetate (5:1). Yield: 248 mg (60%). White solid, mp 65-67 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.41 (bs, 1H), 7.39 (d, *J* = 8.6 Hz, 2H), 7.10 (d, *J* = 8.3 Hz, 2H), 3.75 (t, *J* = 5.7 Hz, 2H), 3.59 (q, *J* = 6.8 Hz, 2H), 2.61 (t, *J* = 5.5 Hz, 2H), 2.30 (s, 3H), 1.27 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 170.1, 135.9, 133.9, 129.7, 120.1, 66.9, 66.8, 38.3, 21.1, 15.5. ESIMS: $[M+H]^+$ m/z 208.3, $[M+Na]^+$ m/z 230.2.



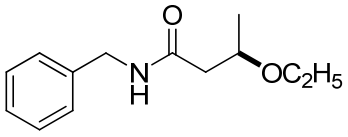
3o

***N*-Butyl-3-ethoxypropanamide (3o).** Eluent: petroleum ether/ethyl acetate (5:1). Yield: 291 mg (84%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 6.38 (bs, 1H), 3.67 (t, *J* = 5.7 Hz, 2H), 3.52 (q, *J* = 7.2 Hz, 2H), 3.25 (q, *J* = 5.9 Hz, 2H), 2.45 (t, *J* = 5.7 Hz, 2H), 1.54-1.41 (m, 2H), 1.39-1.29 (m, 2H), 1.21 (t, *J* = 6.9 Hz, 3H), 0.93 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 171.6, 66.7, 66.5, 39.1, 37.2, 31.7, 20.1, 15.1, 13.8. ESIMS: $[M+H]^+$ m/z 174.3, $[M+Na]^+$ m/z 196.2.



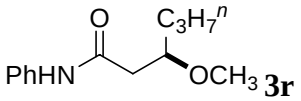
3p

3-Ethoxy-*N*-phenylbutanamide (3p). Eluent: petroleum ether/ethyl acetate (5:1). Yield: 344 mg (83%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.64 (bs, 1H), 7.52-7.50 (m, 2H), 7.33-7.26 (m, 2H), 7.09-7.05 (m, 1H), 3.91-3.85 (m, 1H), 3.73-3.63 (m, 1H), 3.53-3.43 (m, 1H), 2.52 (d, *J* = 5.5 Hz, 2H), 1.31-1.19 (m, 6H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 169.9, 138.5, 129.2, 124.2, 119.9, 72.7, 64.3, 44.9, 19.8, 15.9. ESIMS: $[M+Na]^+$ m/z 230.2.



3q

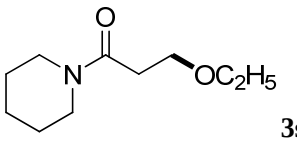
***N*-Benzyl-3-ethoxybutanamide (3q).** Eluent: petroleum ether/ethyl acetate (5:1). Yield: 309 mg (70%, under nitrogen atmosphere). Colorless oil. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 7.34-7.31 (m, 2H), 7.29-7.25 (m, 3H), 6.69 (bs, 1H), 4.49 (dd, *J* = 14.8, 5.5 Hz, 1H), 4.40 (dd, *J* = 14.8, 5.5 Hz, 1H), 3.84-3.80 (m, 1H), 3.61-3.56 (m, 1H), 3.39-3.34 (m, 1H), 2.39 (d, *J* = 5.5 Hz, 2H), 1.20 (d, *J* = 6.2 Hz, 3H), 1.09 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz): δ 171.4, 138.8, 128.9, 128.0, 127.7, 72.7, 64.2, 44.2, 43.7, 19.9, 15.7. ESIMS: $[M+H]^+$ m/z 222.2.



3r

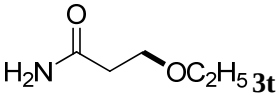
3-Methoxy-*N*-phenylhexanamide (3r). Eluent: petroleum ether/ethyl acetate (8:1). Yield: 341 mg (77%). Oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.39 (bs, 1H), 7.53-7.50 (m, 2H), 7.33-7.27 (m, 2H), 7.10-7.05 (m, 1H), 3.65-3.60 (m, 1H), 3.43 (s, 3H), 2.62-2.44 (m, 2H), 1.65-1.32 (m, 4H), 0.93 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ

169.9, 138.4, 129.2, 124.3, 120.1, 78.5, 57.1, 42.1, 35.7, 18.6, 14.4. ESIMS: $[M+H]^+$ m/z 222.3, $[M+Na]^+$ m/z 244.2.



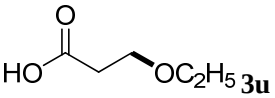
3s

3-Ethoxy-1-(piperidin-1-yl)propan-1-one (3s). Eluent: petroleum ether/ethyl acetate (4:1). Yield: 178 mg (48%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 3.74 (t, *J* = 6.9 Hz, 2H), 3.57-3.48 (m, 4H), 3.42 (t, *J* = 5.3 Hz, 2H), 2.62 (t, *J* = 6.9 Hz, 2H), 1.64-1.49 (m, 6H), 1.19 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 169.5, 67.1, 66.7, 47.0, 42.9, 34.0, 26.7, 25.8, 24.8, 15.5. ESIMS: $[M+H]^+$ m/z 186.2, $[M+Na]^+$ m/z 208.2.



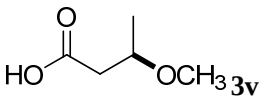
3t

3-Ethoxypropanamide (3t). Eluent: petroleum ether/ethyl acetate (1:4). Yield: 220 mg (94%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 6.43 (bs, 1H), 5.97 (bs, 1H), 3.68 (t, *J* = 5.8 Hz, 2H), 3.54 (q, *J* = 6.9 Hz, 2H), 2.49 (t, *J* = 5.8 Hz, 2H), 1.22 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 174.7, 66.8, 66.6, 36.9, 15.3. ESIMS: $[M+H]^+$ m/z 118.4, $[M+Na]^+$ m/z 140.3.



3u

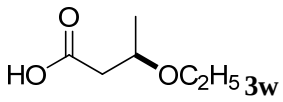
3-Ethoxypropanoic acid (3u). Eluent: petroleum ether/ethyl acetate (1:1). Yield: 201 mg (85%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 10.46 (bs, 1H), 3.71 (t, *J* = 5.8 Hz, 2H), 3.54 (q, *J* = 6.9 Hz, 2H), 2.63 (t, *J* = 5.8 Hz, 2H), 1.21 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 177.5, 66.6, 65.5, 35.0, 15.0. ESIMS: $[M+Na]^+$ m/z 141.3.



3v

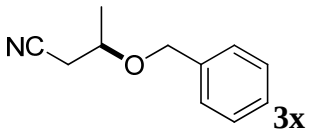
3-Methoxybutanoic acid (3v). Eluent: petroleum ether/ethyl acetate (3:1). Yield: 177 mg (75%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 10.22 (bs, 1H), 3.80-3.76 (m, 1H), 3.37 (s, 3H), 1.61 (dd, *J* = 15.5, 7.2 Hz, 1H), 1.61 (dd, *J* = 15.5, 5.5 Hz, 1H),

1.24 (d, J = 5.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 300 MHz): δ 177.0, 73.5, 56.4, 41.5, 19.1. ESIMS: $[M+H]^+$ m/z 119.6, $[M+Na]^+$ m/z 141.4.



3w

3-Ethoxybutanoic acid (3w). Eluent: petroleum ether/ethyl acetate (3:1). Yield: 193 mg (73%). Colorless oil. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 8.37 (bs, 1H), 3.90-3.87 (m, 1H), 3.61-3.58 (m, 1H), 3.51-3.46 (m, 1H), 2.61 (dd, J = 15.5, 6.9 Hz, 1H), 2.46 (dd, J = 15.8, 5.5 Hz, 1H), 1.24 (d, J = 6.2 Hz, 3H), 1.20 (t, J = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz): δ 176.7, 72.0, 64.5, 42.0, 20.1, 15.7. ESIMS: $[M+H]^+$ m/z 133.3, $[M+Na]^+$ m/z 155.2.



3x

3-(Benzyloxy)butanenitrile (3x).[6] Eluent: petroleum ether/ethyl acetate (25:1). Yield: 336 mg (96%). Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.36-7.24 (m, 5H), 4.62-4.51 (m, 2H), 3.87-3.77 (m, 1H), 2.52 (d, J = 5.9 Hz, 2H), 1.34 (d, J = 6.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 137.9, 128.8, 128.2, 127.9, 117.8, 71.3, 70.7, 25.3, 19.9. ESIMS: $[M+Na]^+$ m/z 198.3.

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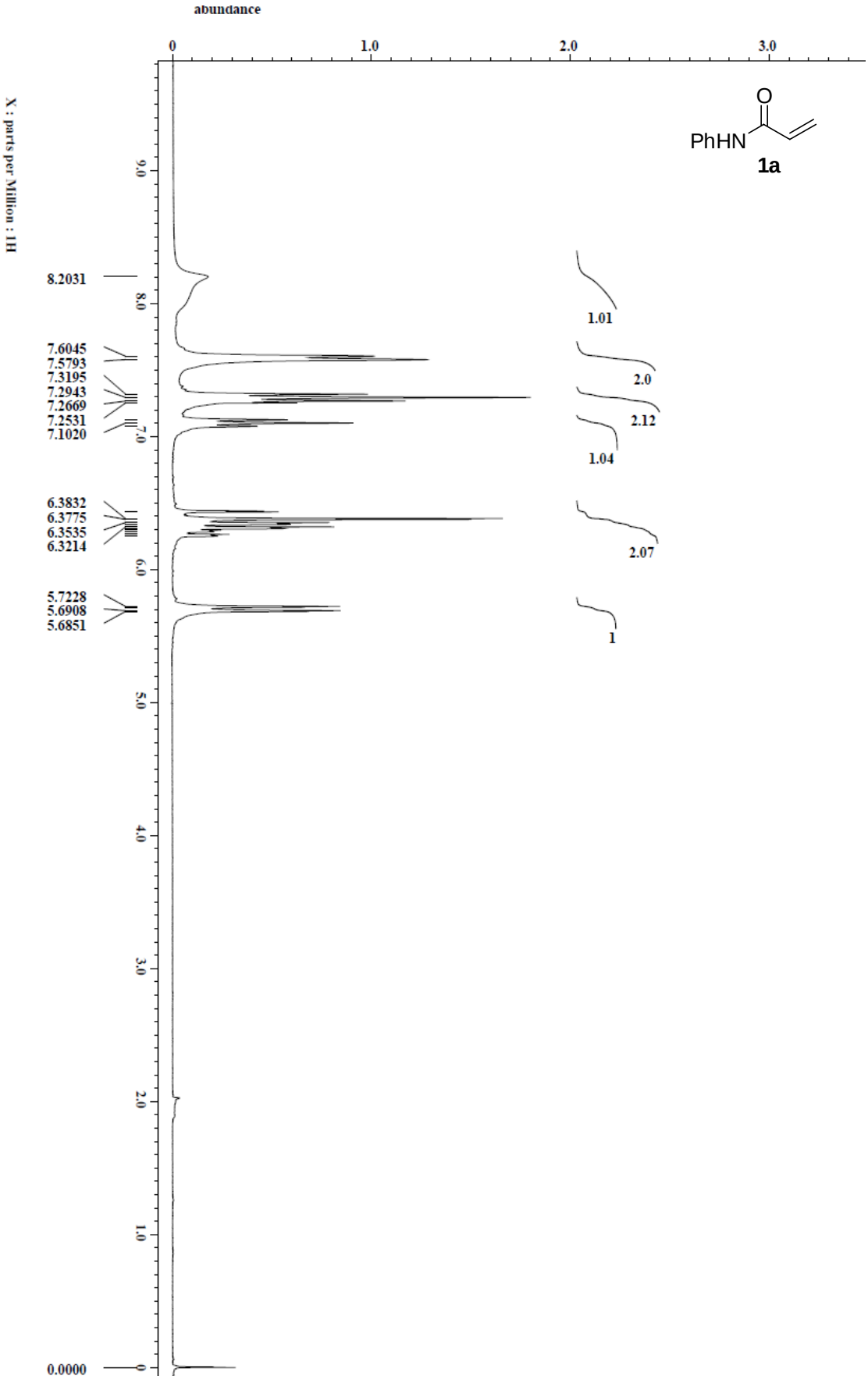
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7.2531
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6.3775
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2.0
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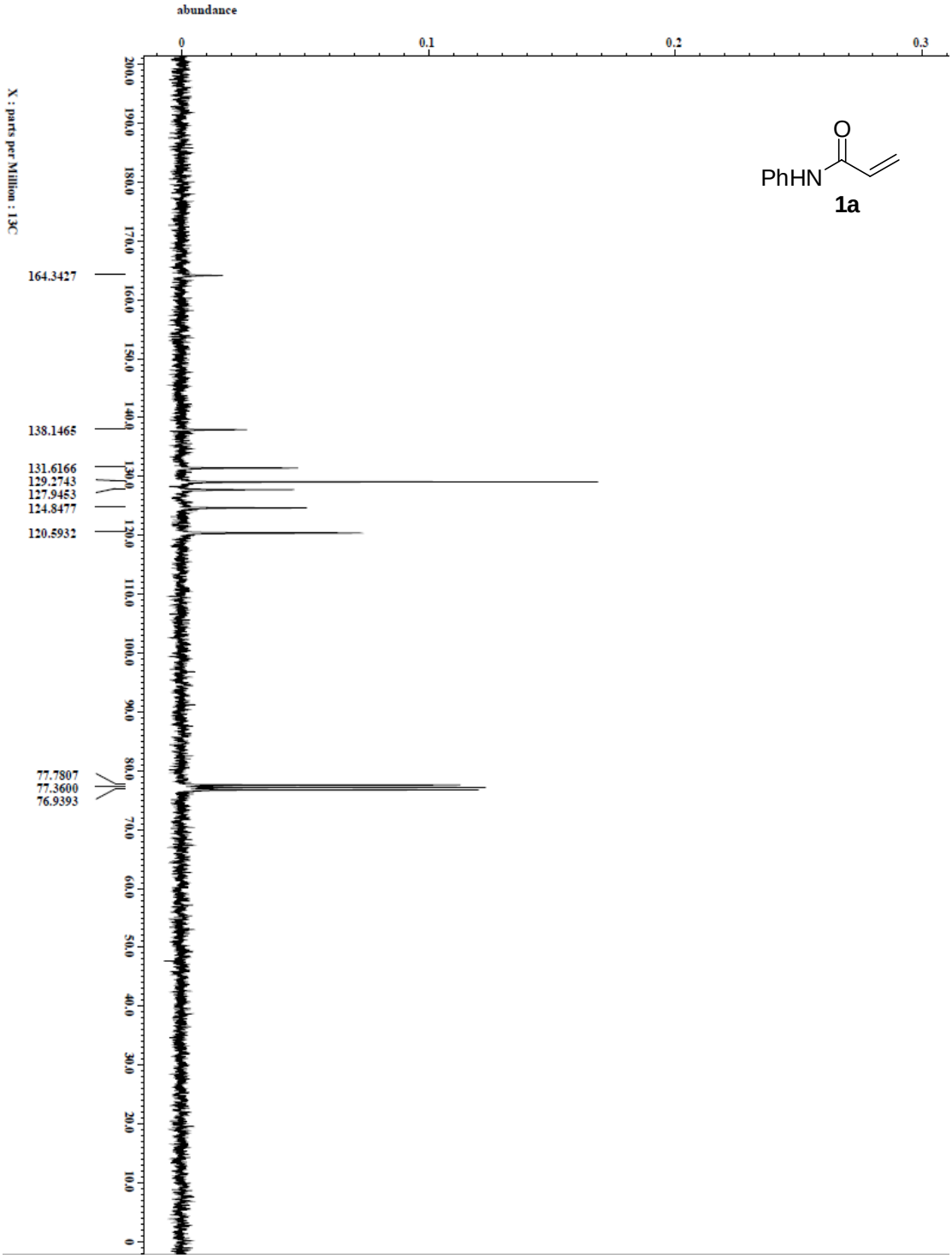
1.04
2.07
1


abundance
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0.2
0.3
X : parts per Million : 13C
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131.6166
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124.8477
120.5932
77.7807
77.3600
76.9393
O
PhHN
1a


abundance
X : parts per Million : 1H
Me
O
N
H
1b
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7.4703
7.4566
7.2539
7.1015
7.0901
6.3995
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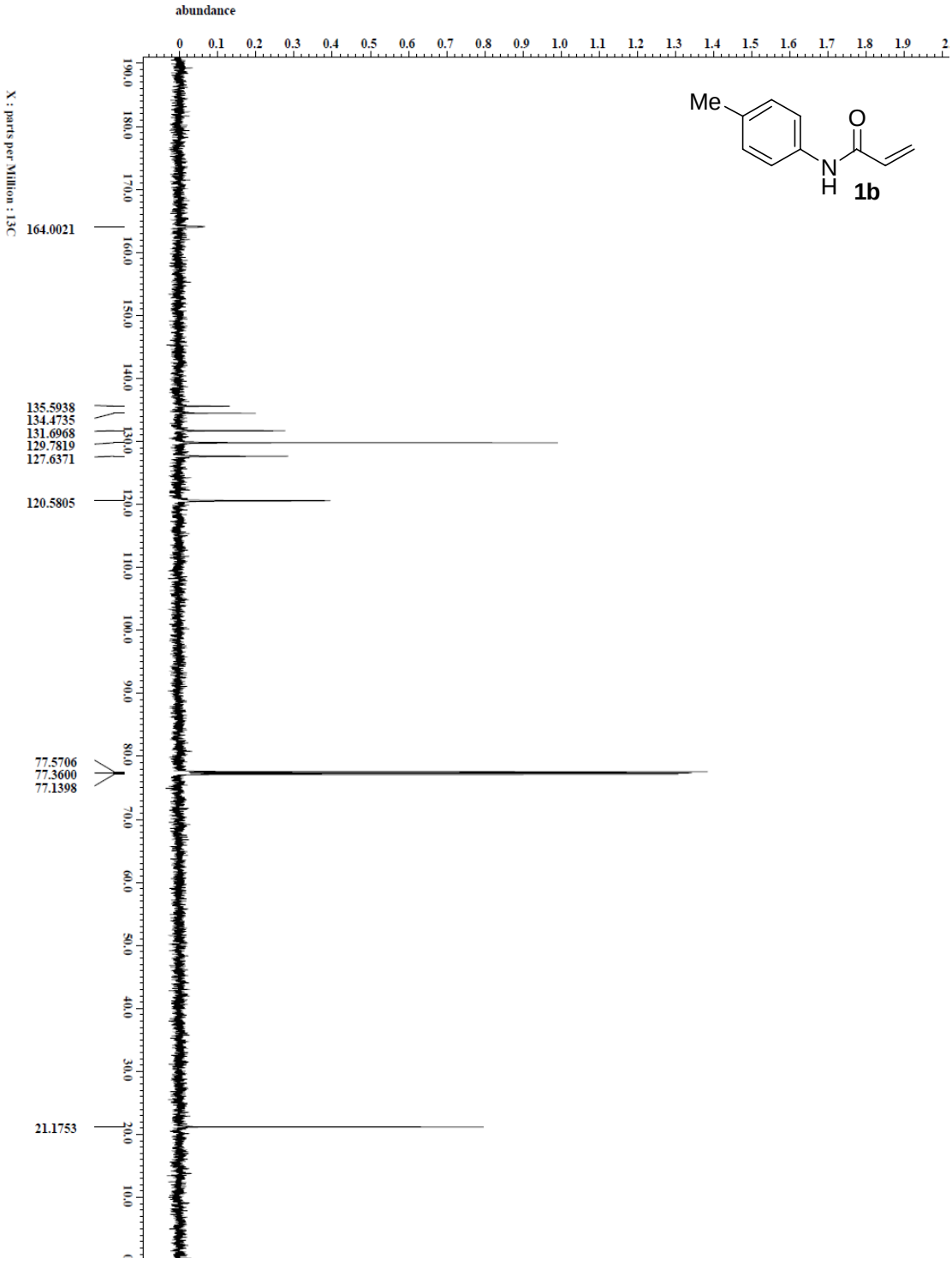
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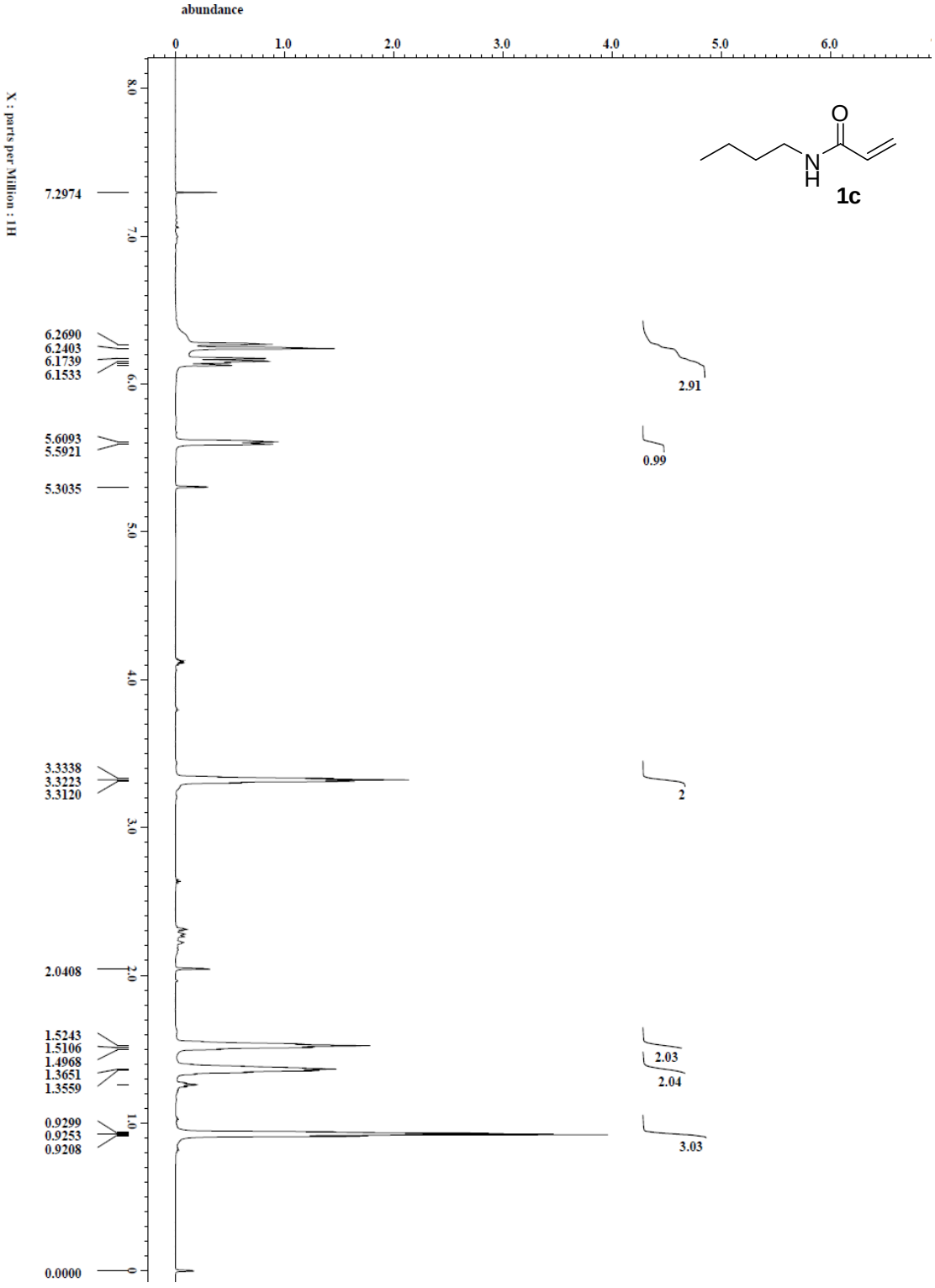
H
1b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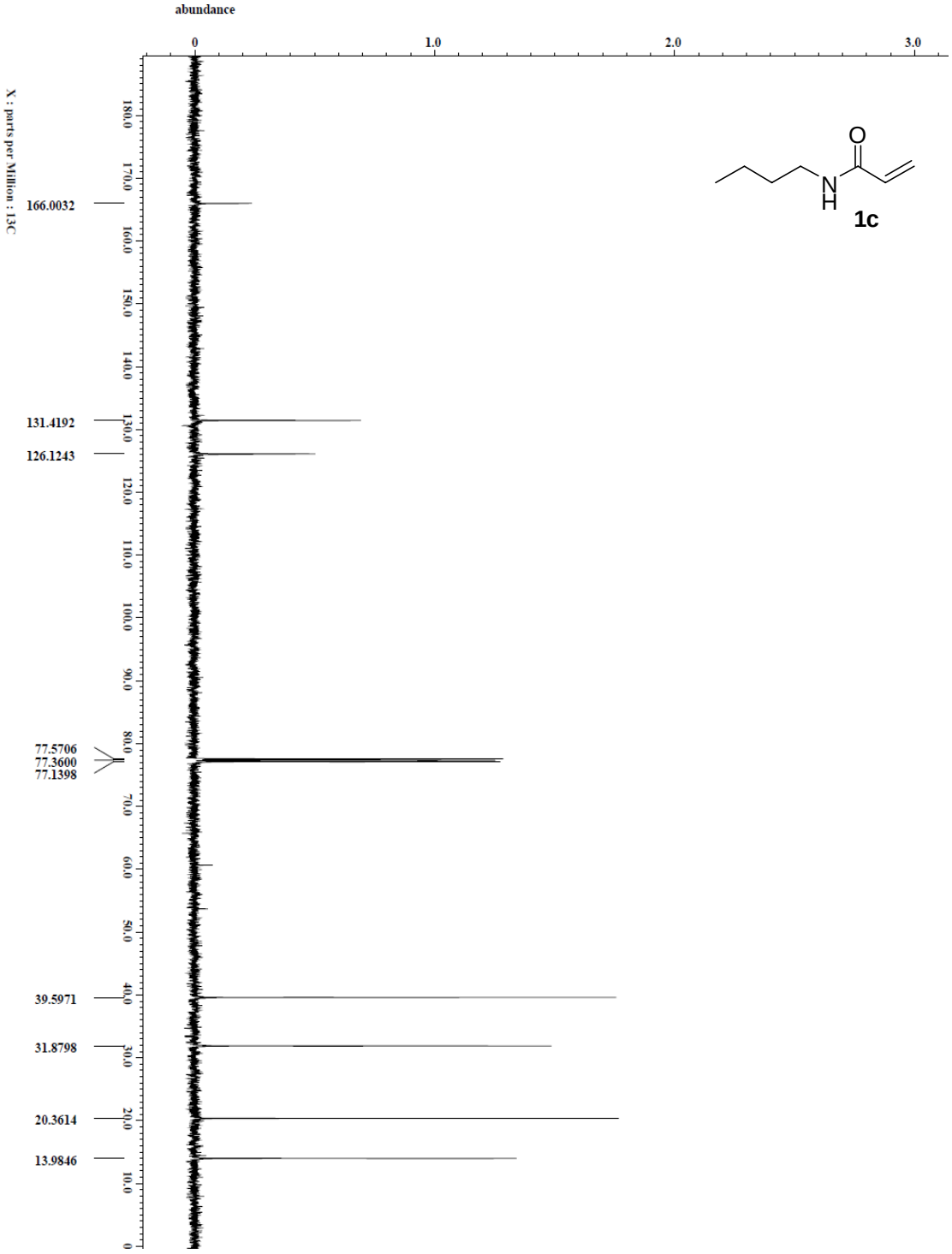
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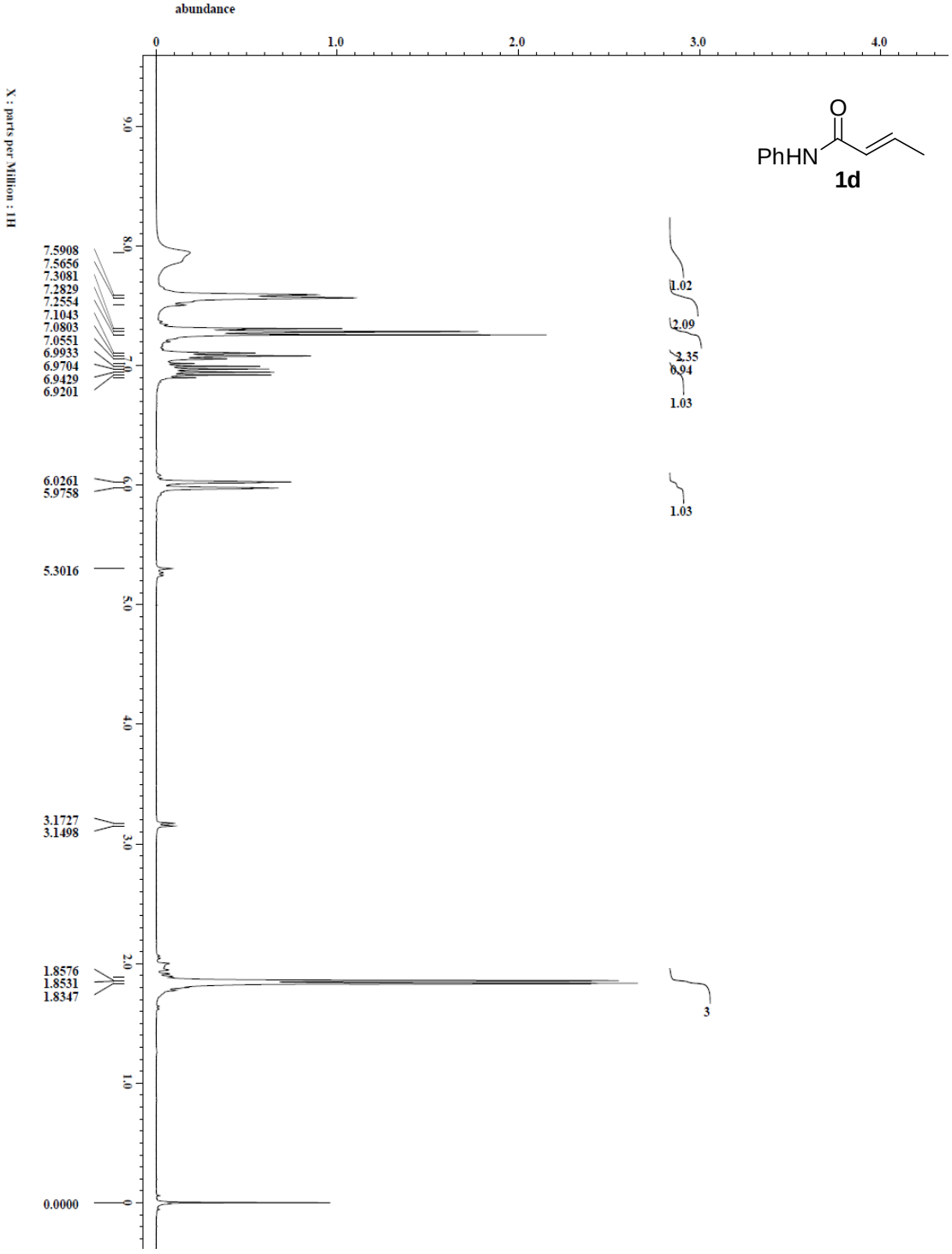
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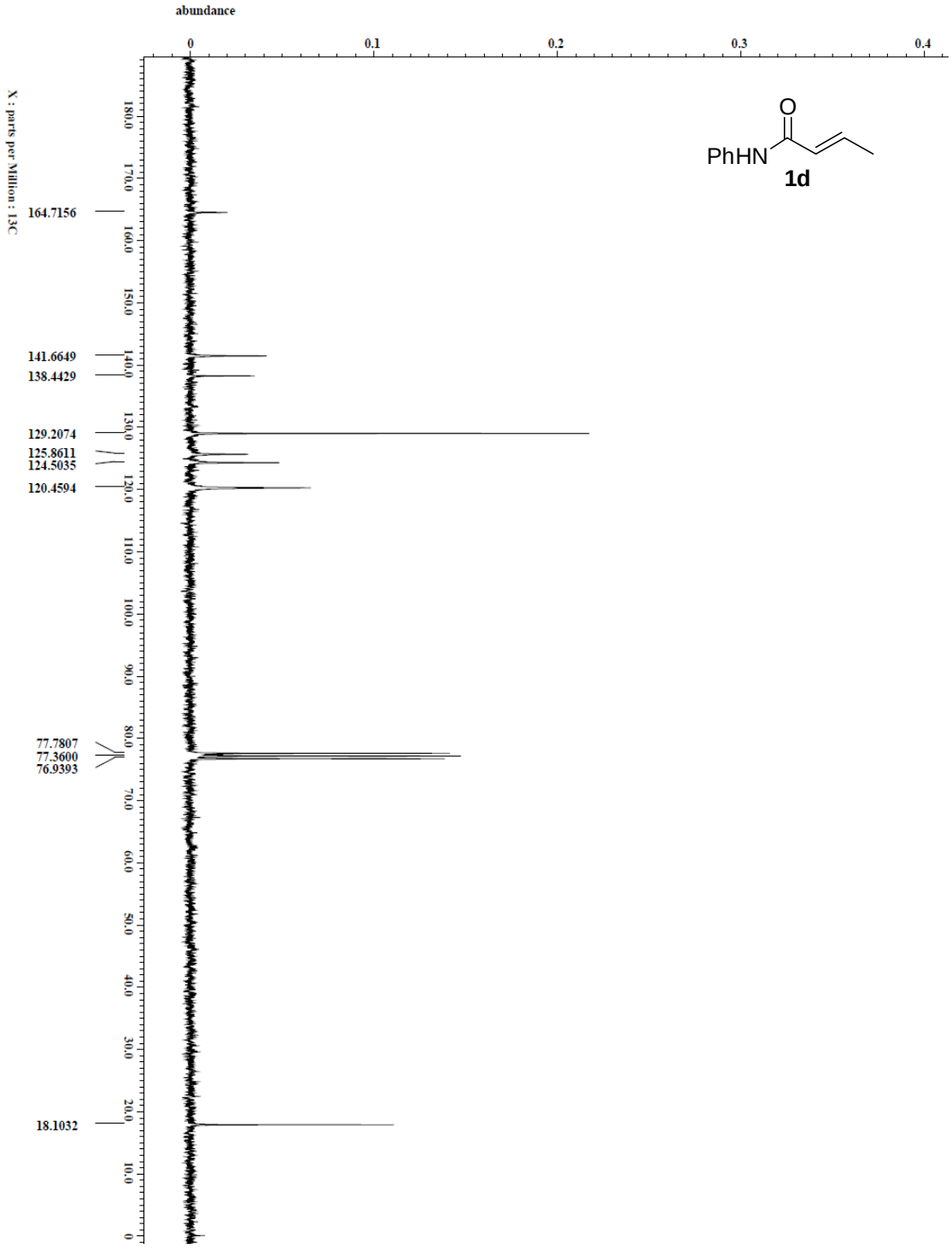
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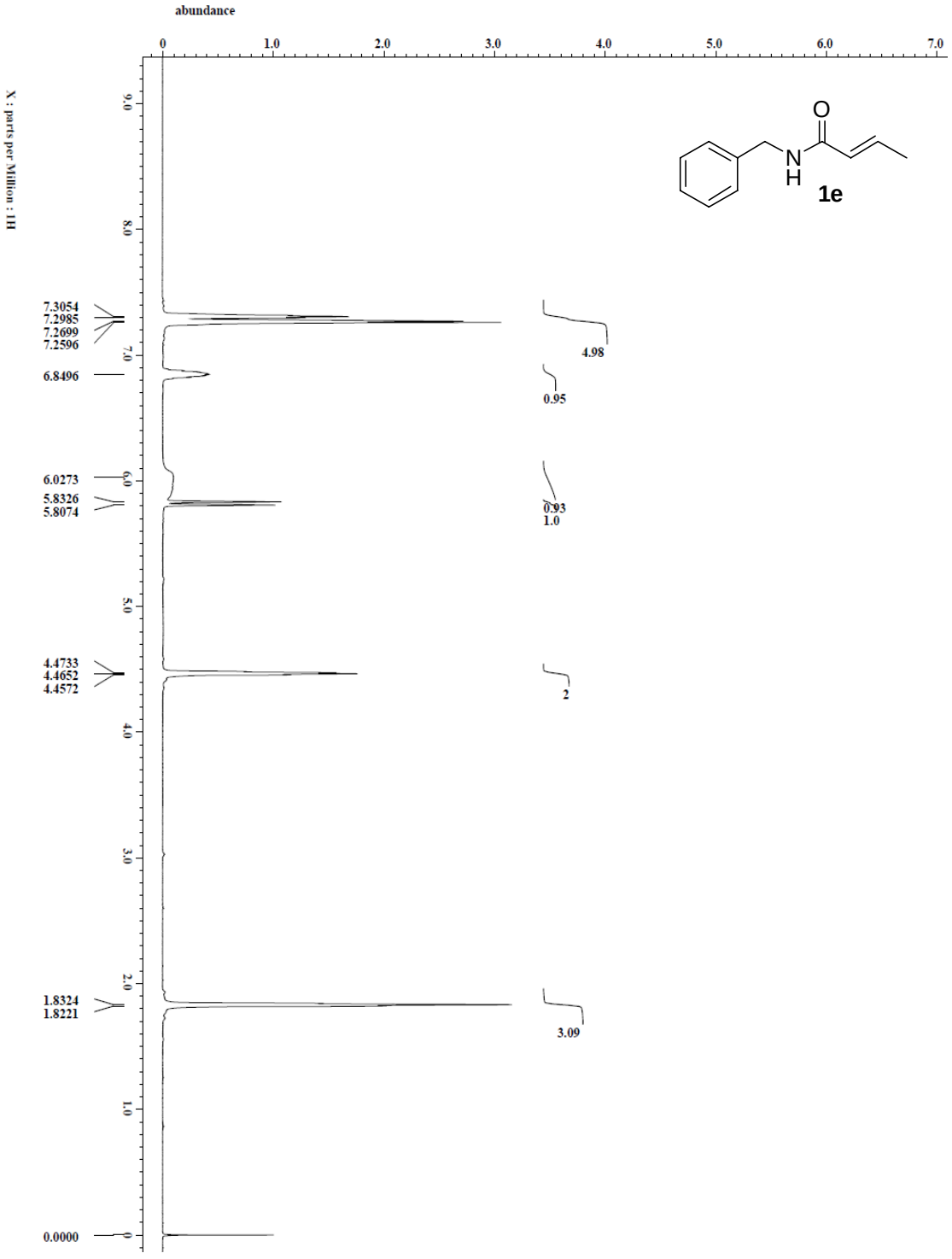
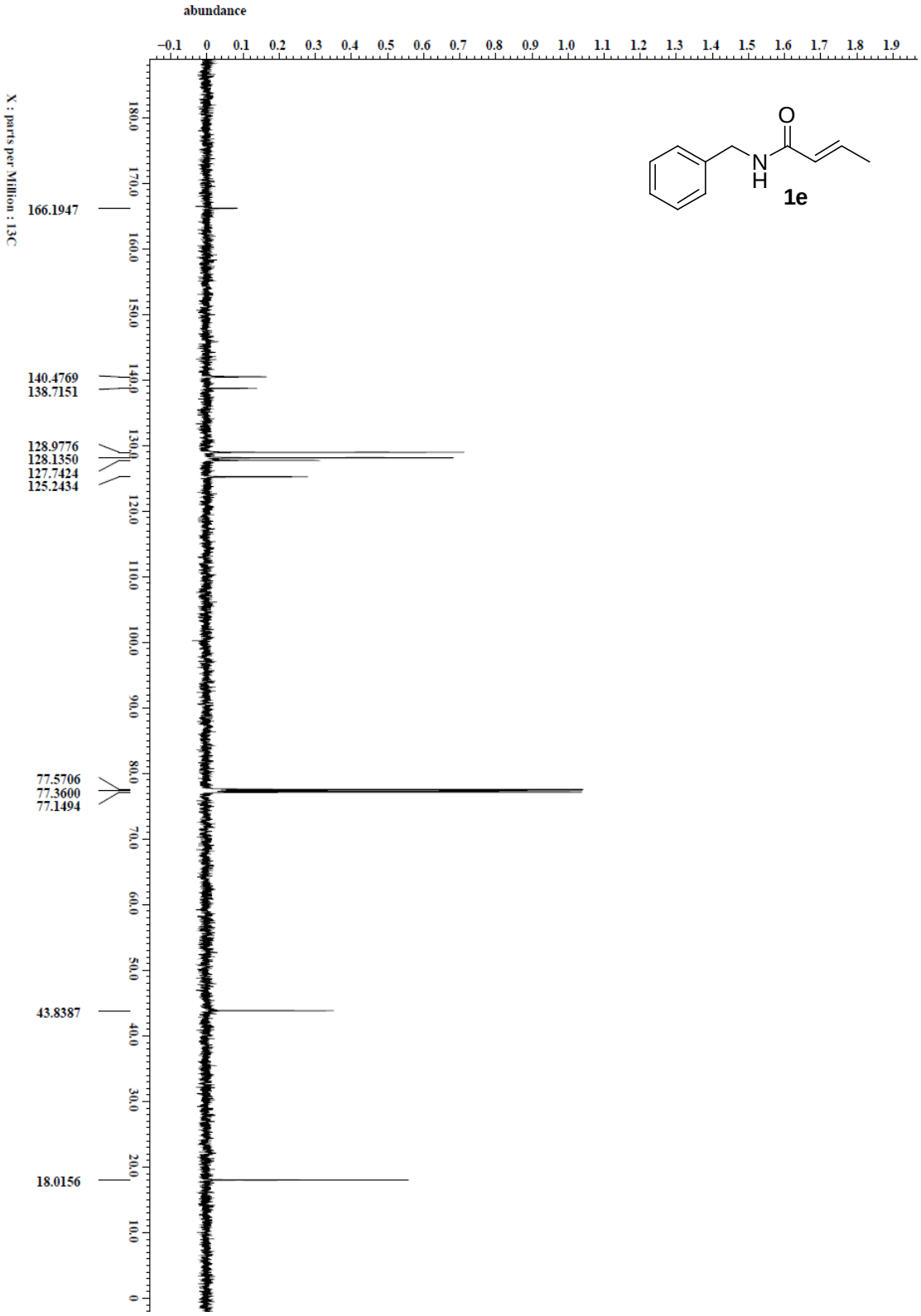
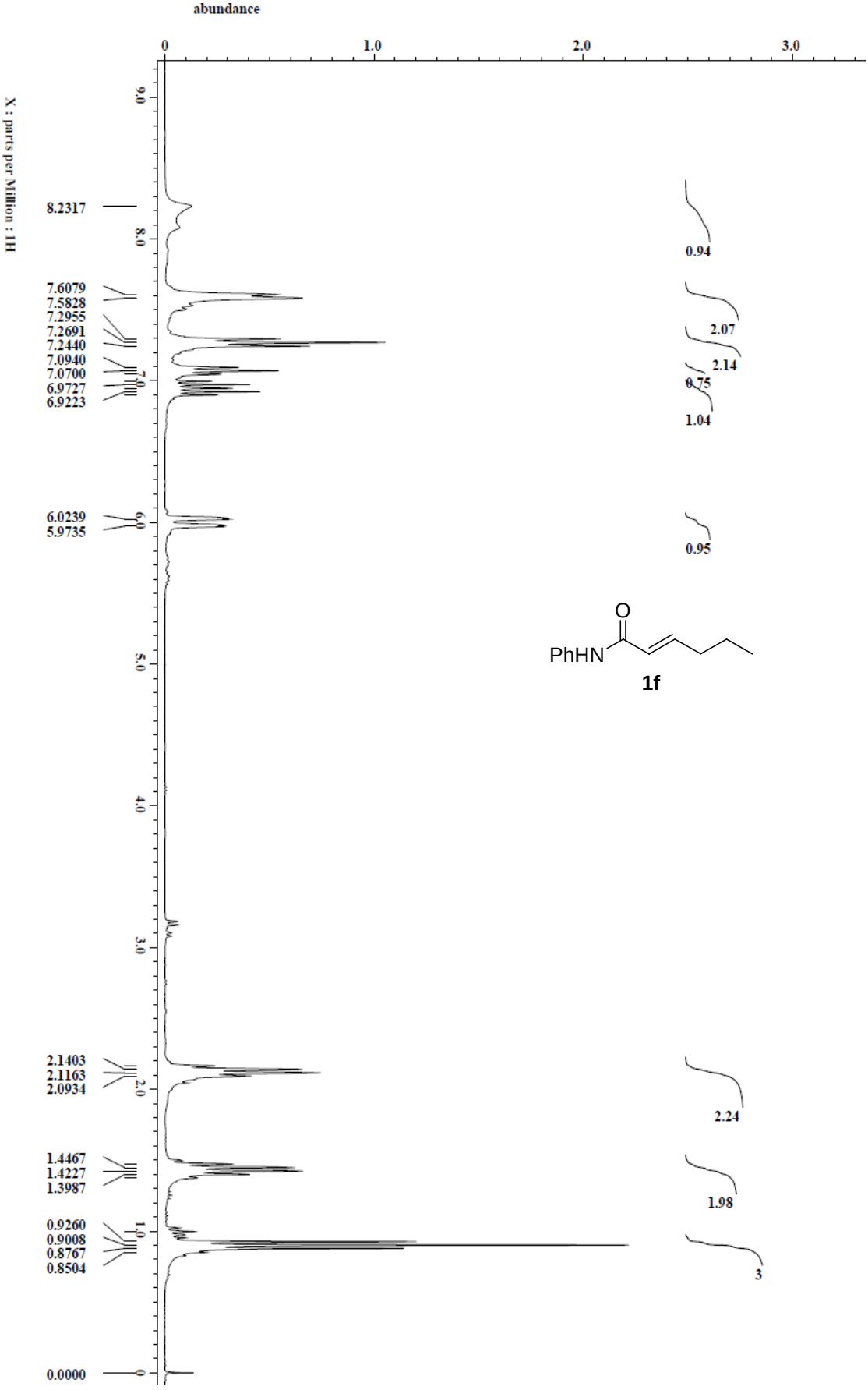
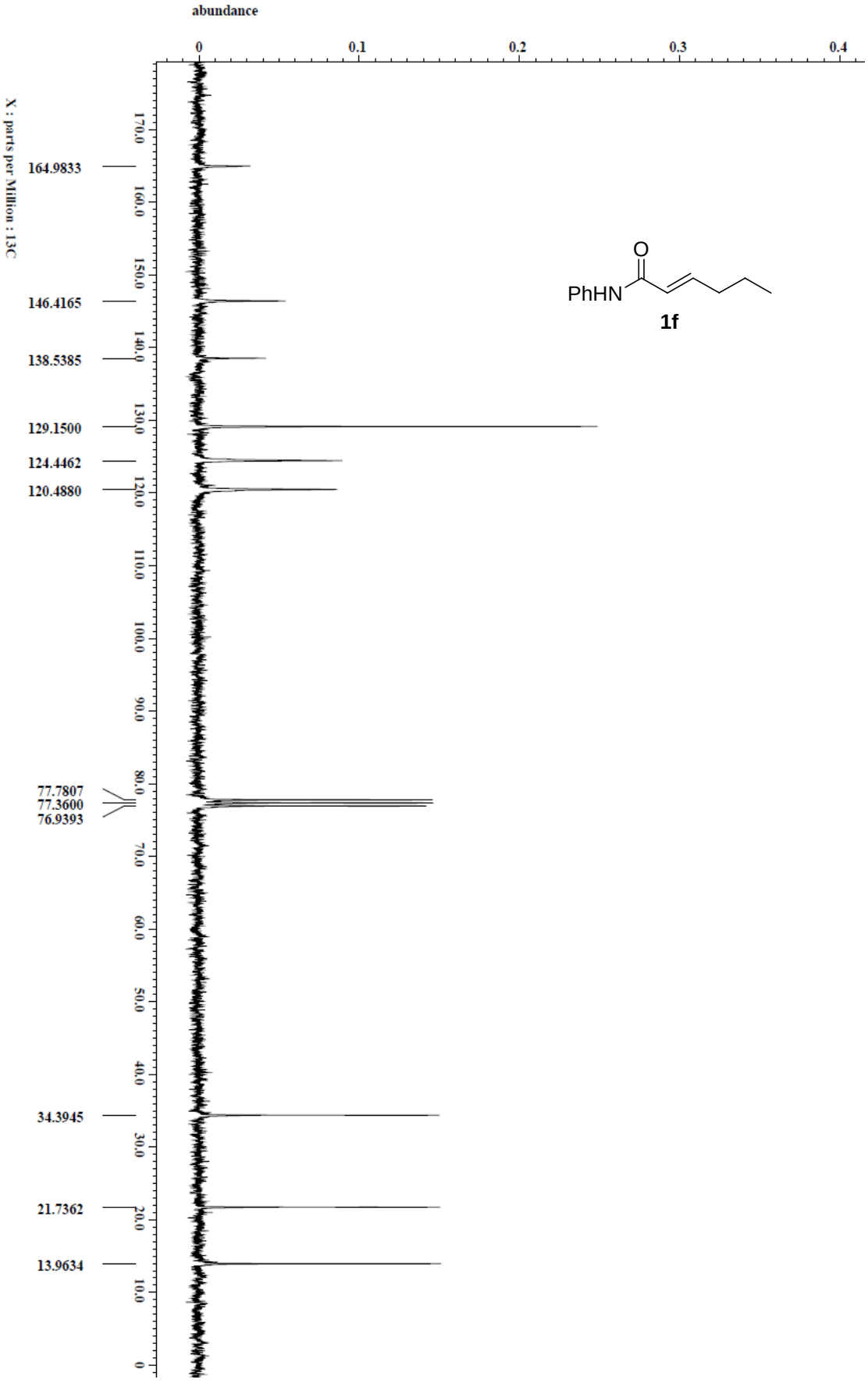
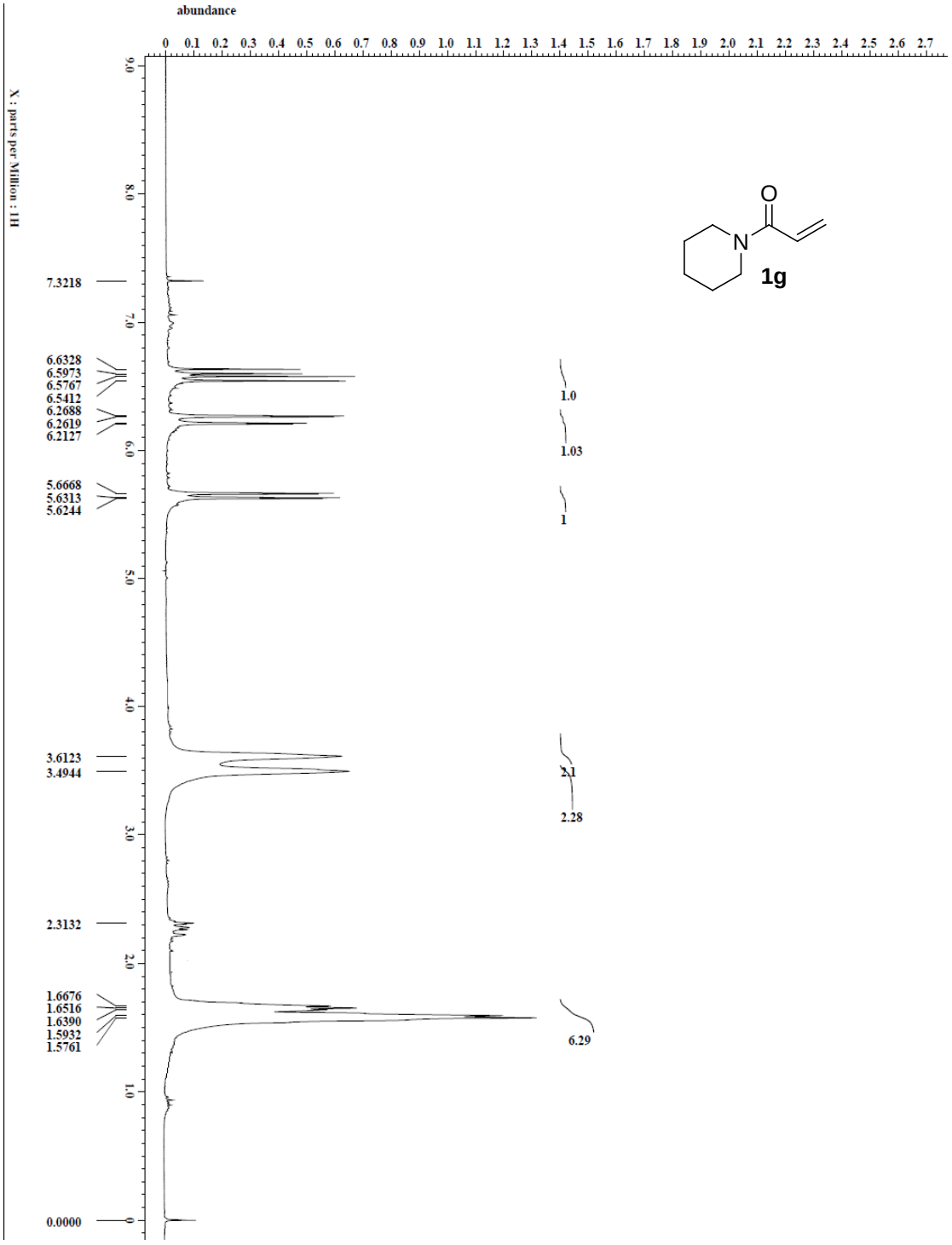
77.7807
77.3600
76.9393
18.1032
O
PhHN
1d

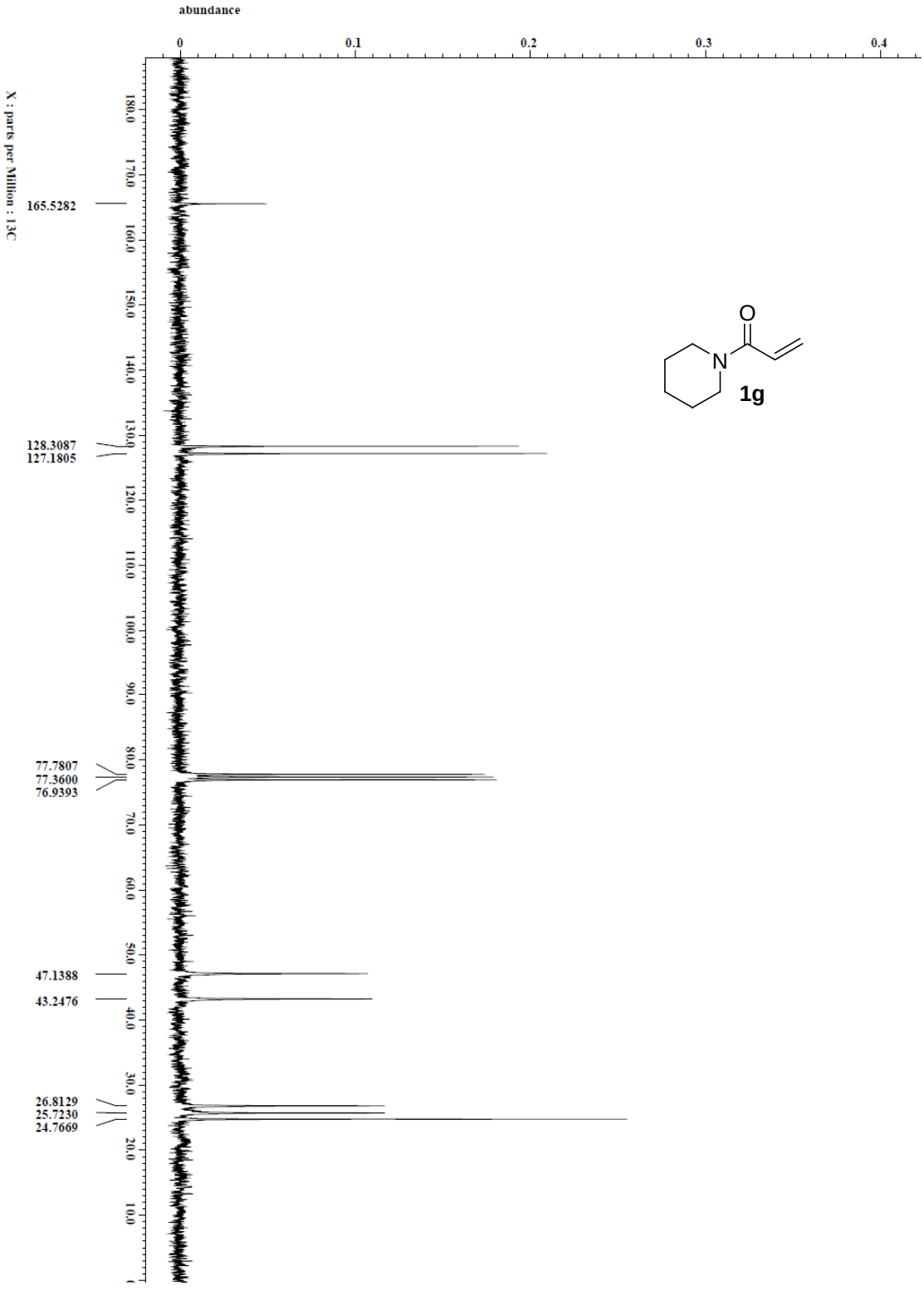

abundance
X : parts per Million : 1H
7.3054
7.2985
7.2699
7.2596
6.8496
6.0273
5.8326
5.8074
4.4733
4.4652
4.4572
1.8324
1.8221
0.0000
4.98
0.95
0.93
1.0
2
3.09
1e

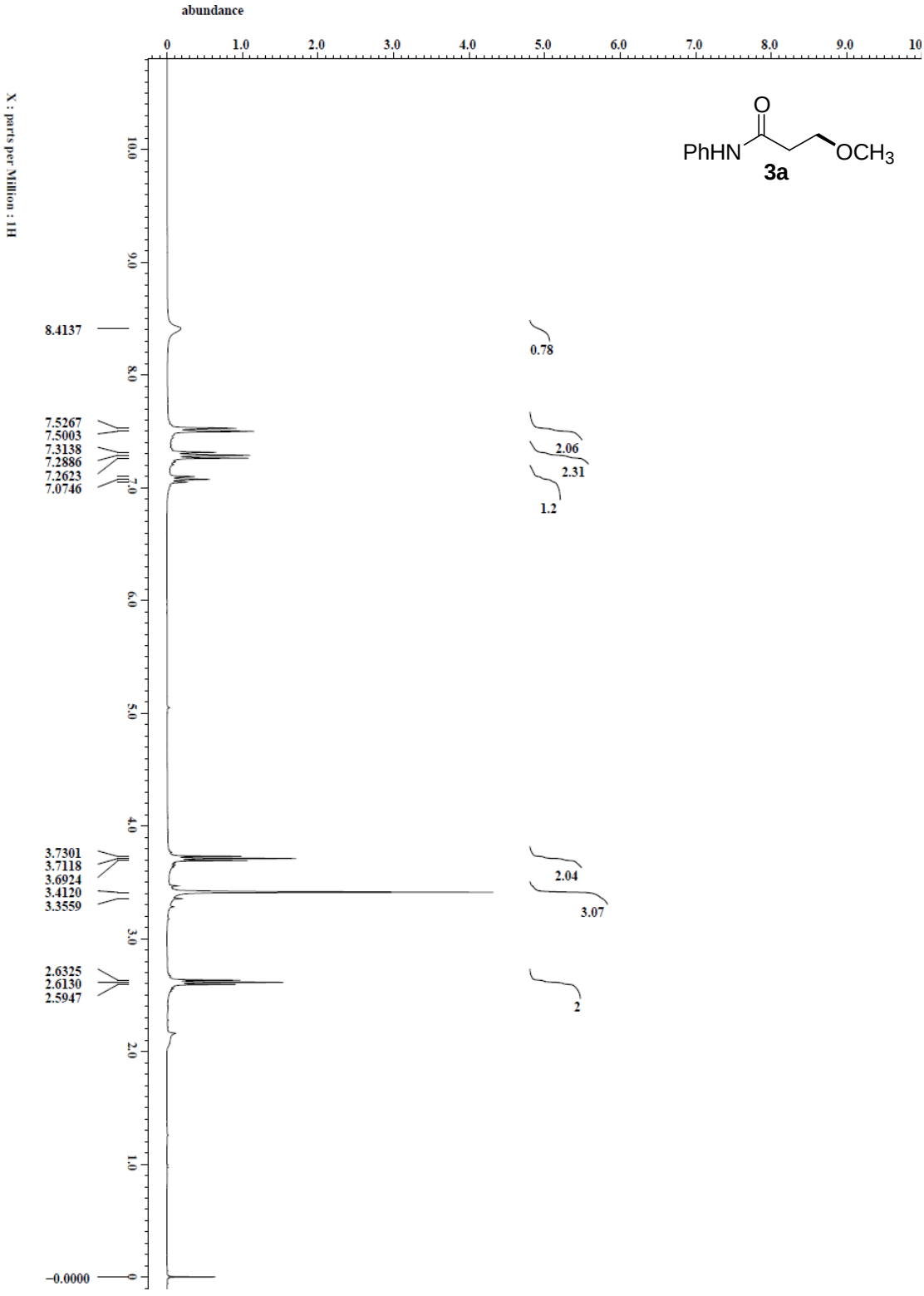

abundance
X : parts per Million : 13C
166.1947
140.4769
138.7151
128.9776
128.1350
127.7424
125.2434
77.5706
77.3600
77.1494
43.8387
18.0156
O
N
H
1e

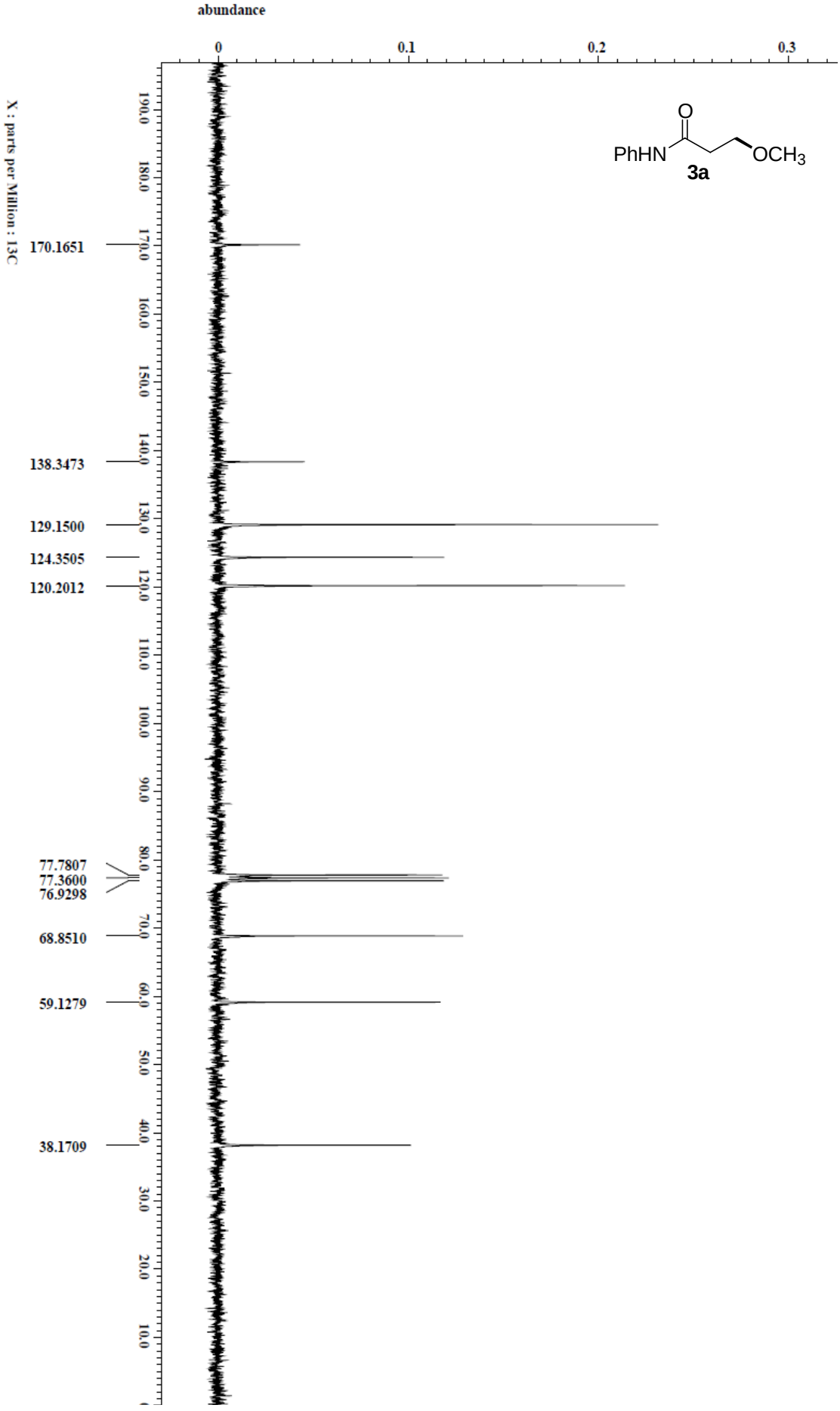

abundance
0
1.0
2.0
3.0
X : parts per Million : 1H
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.2317
7.6079
7.5828
7.2955
7.2691
7.2440
7.0940
7.0700
6.9727
6.9223
6.0239
5.9735
2.1403
2.1163
2.0934
1.4467
1.4227
1.3987
0.9260
0.9008
0.8767
0.8504
0.0000
0.94
2.07
2.14
0.75
1.04
0.95
2.24
1.98
3
O
PhHN
1f

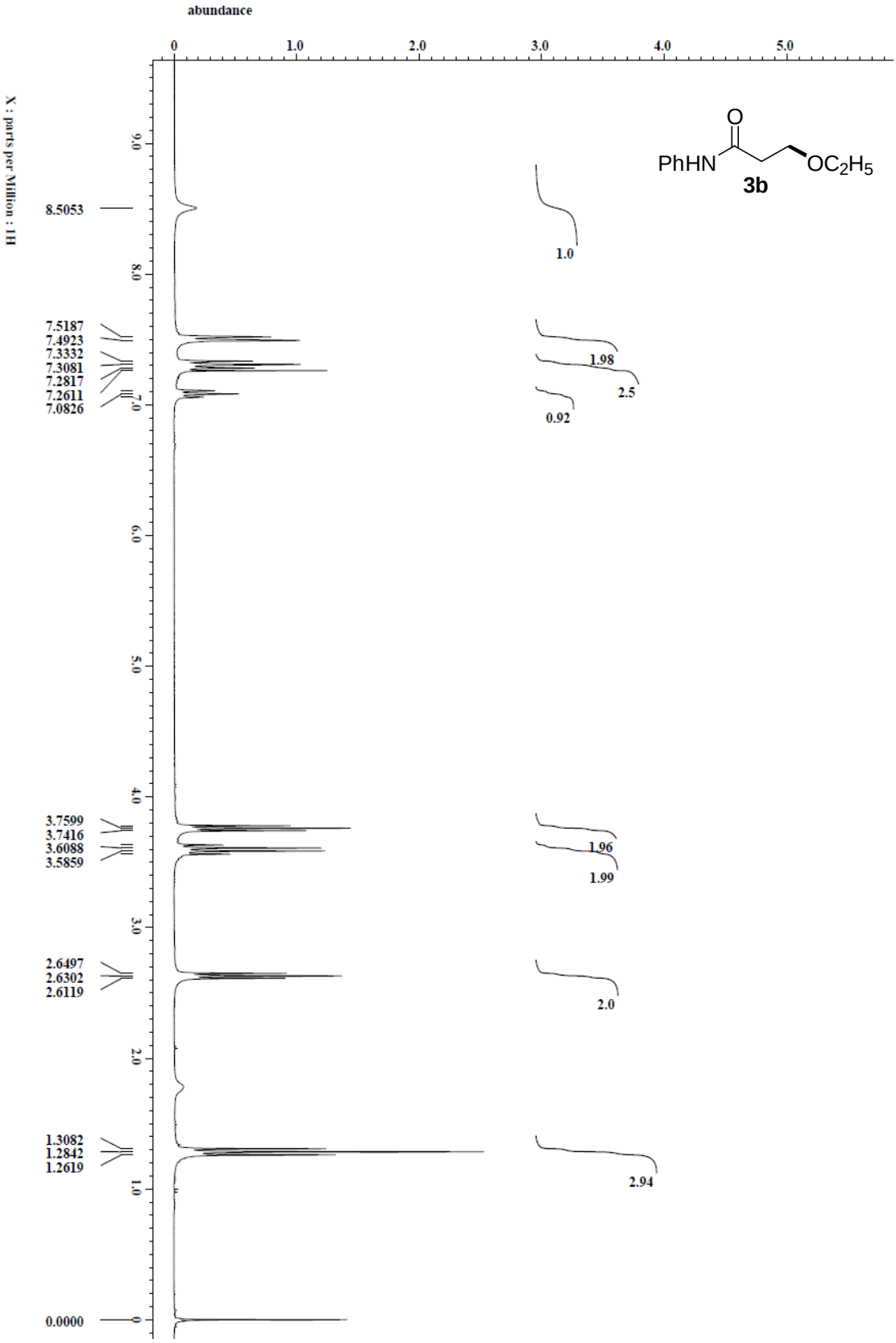

abundance
0
0.1
0.2
0.3
0.4
X : parts per Million : 13C
164.9833
146.4165
138.5385
129.1500
124.4462
120.4880
77.7807
77.3600
76.9393
34.3945
21.7362
13.9634
O
PhHN
1f

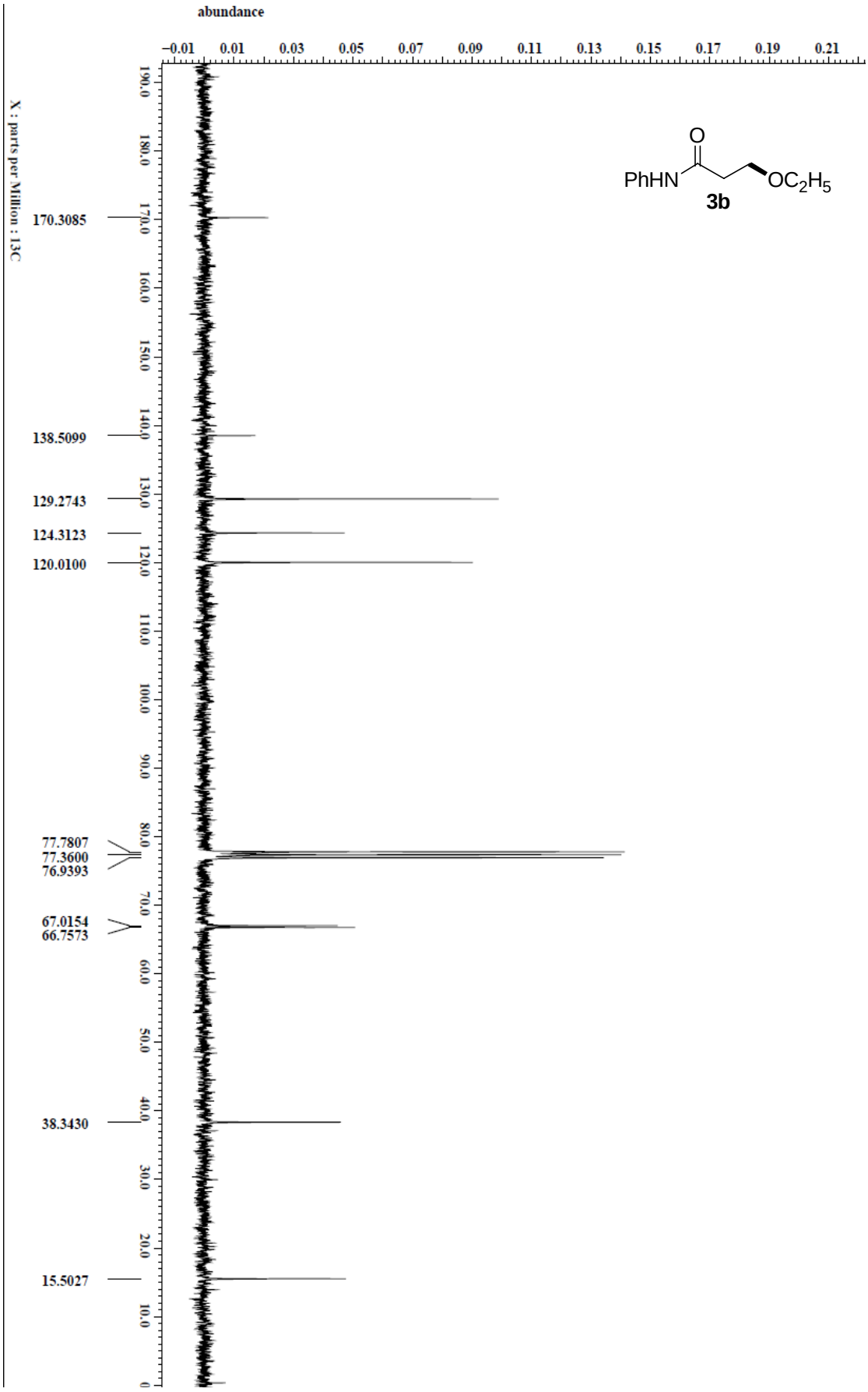

abundance
X : parts per Million : 1H
7.3218
6.6328
6.5973
6.5767
6.5412
6.2688
6.2619
6.2127
5.6668
5.6313
5.6244
3.6123
3.4944
2.3132
1.6676
1.6516
1.6390
1.5932
1.5761
0.0000
1.0
1.03
1
2.1
2.28
6.29
O
N
1g

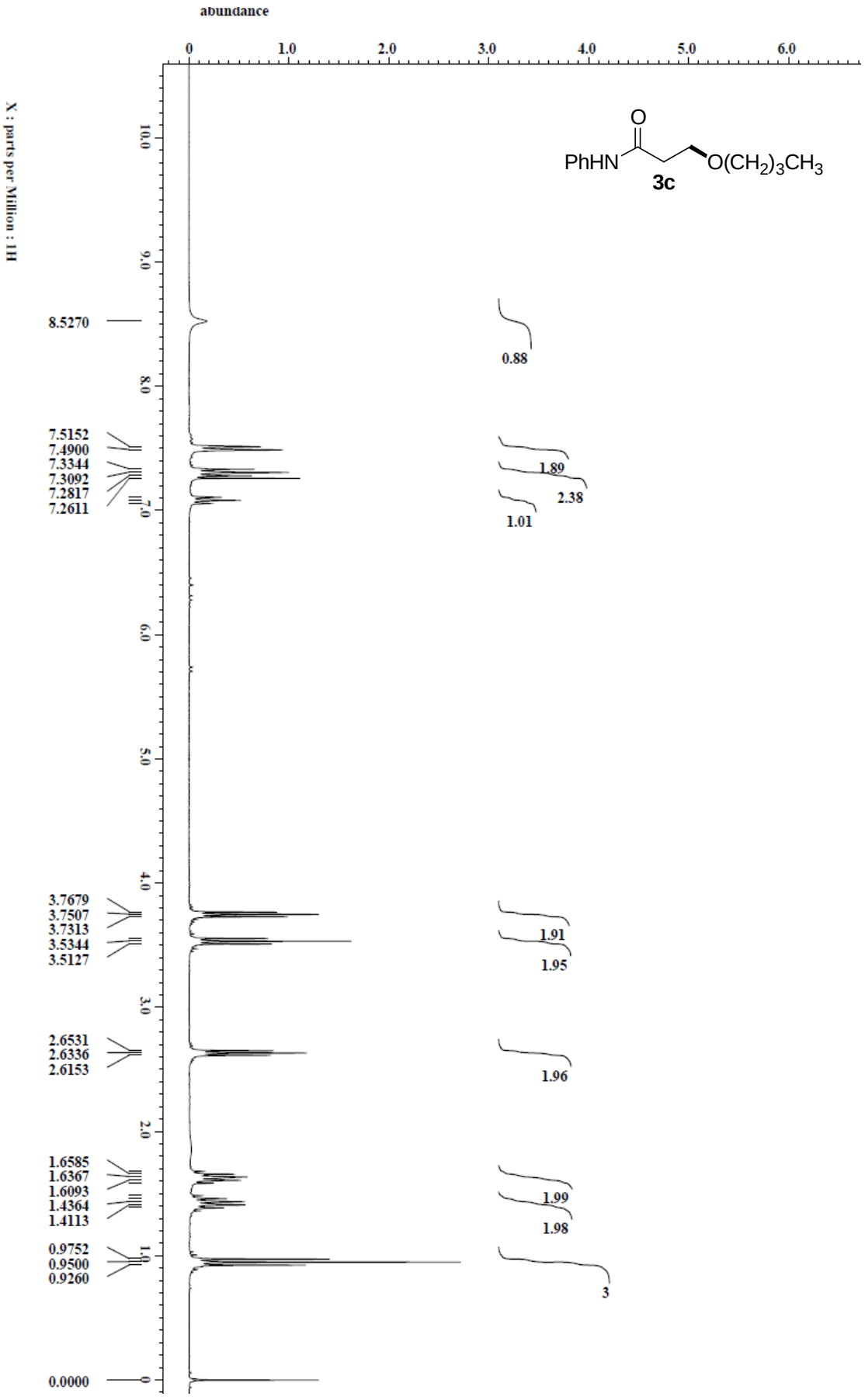

abundance
0
0.1
0.2
0.3
0.4
X : parts per Million : 13C
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
165.5282
128.3087
127.1805
77.7807
77.3600
76.9393
47.1388
43.2476
26.8129
25.7230
24.7669
O
N
1g

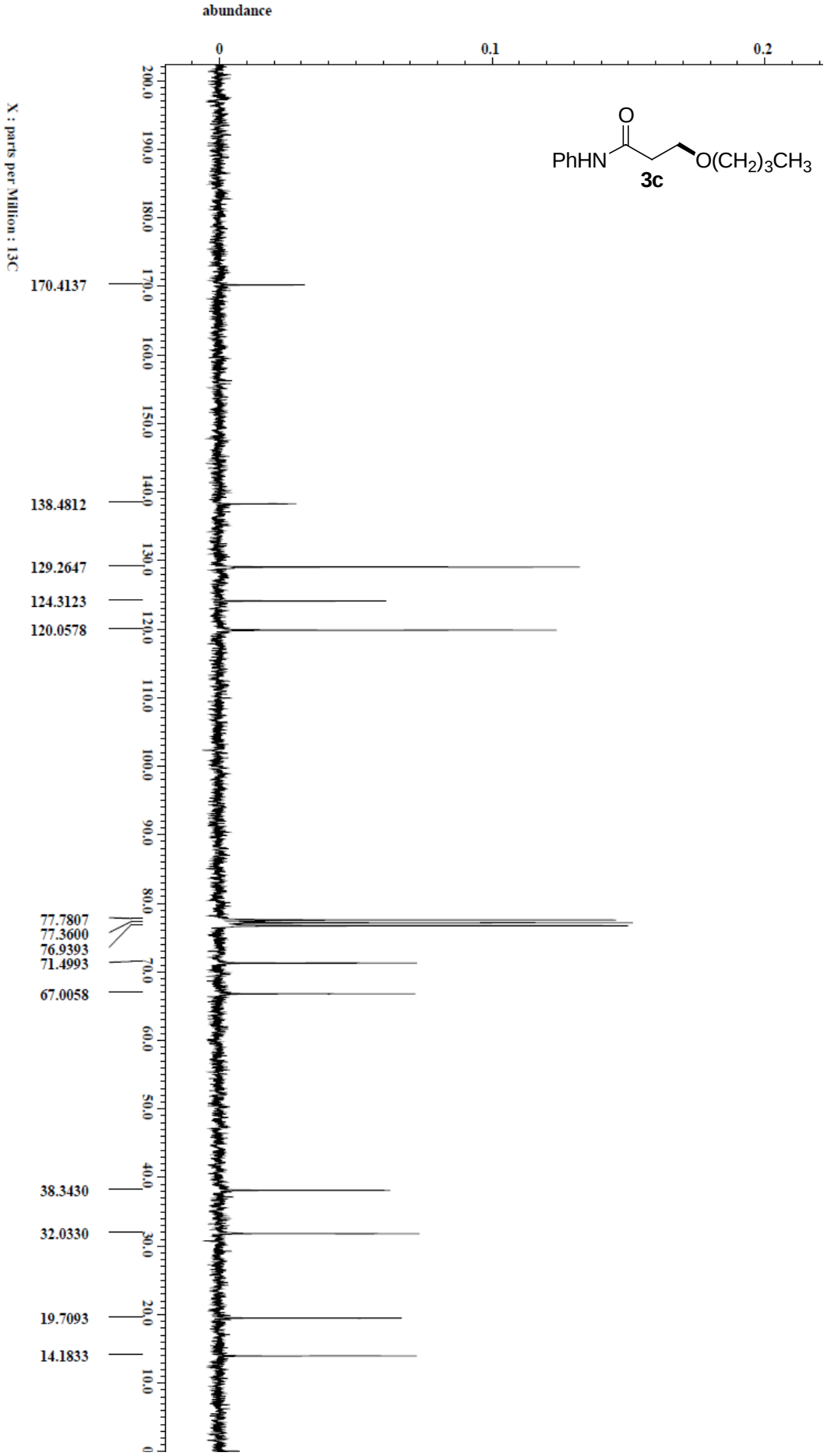

abundance
X : parts per Million : 1H
PhHN
O
OCH3
3a
8.4137
7.5267
7.5003
7.3138
7.2886
7.2623
7.0746
3.7301
3.7118
3.6924
3.4120
3.3559
2.6325
2.6130
2.5947
−0.0000
0.78
2.06
2.31
1.2
2.04
3.07
2

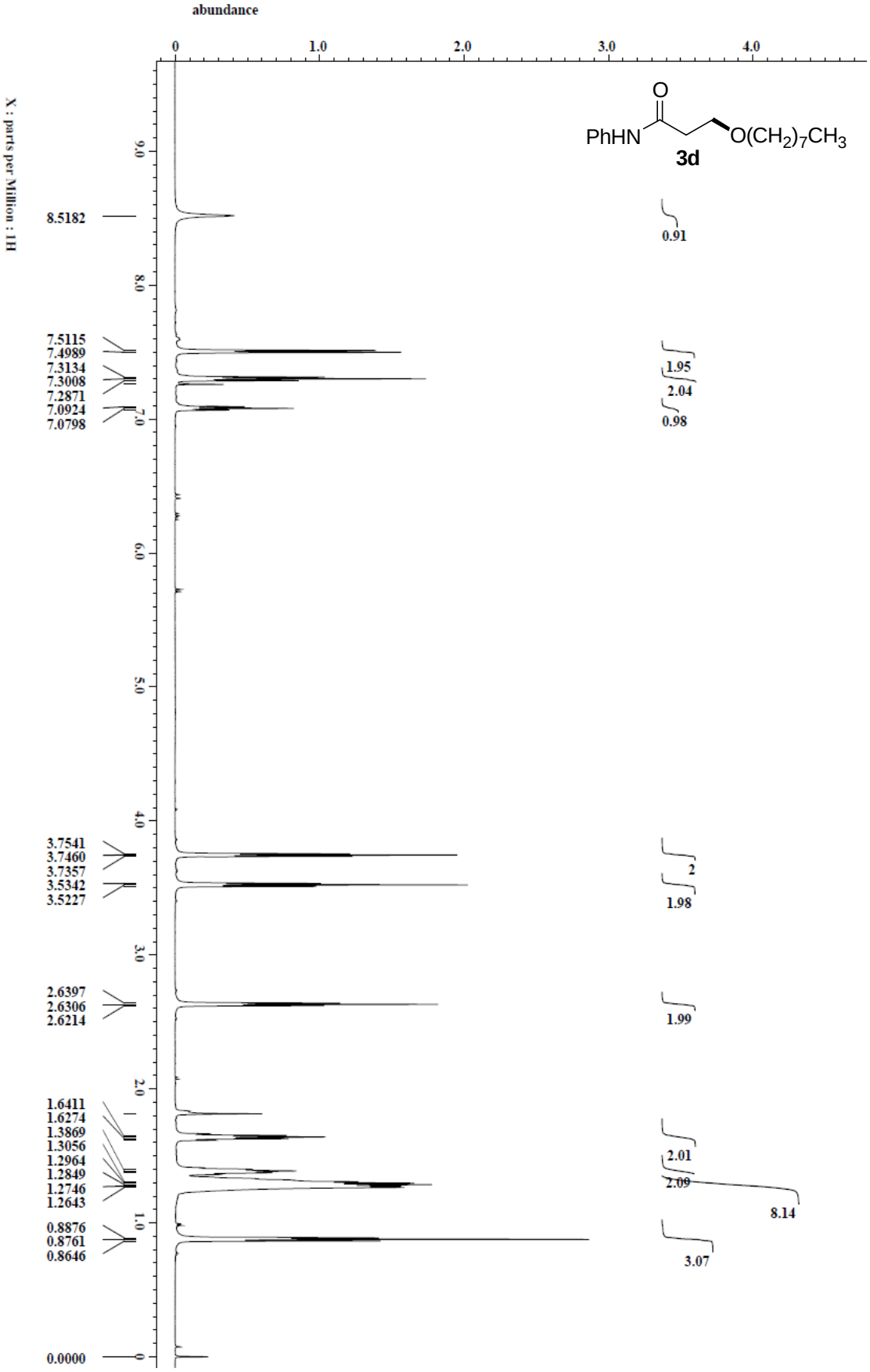

abundance
0
0.1
0.2
0.3
X : parts per Million : 13C
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.1651
138.3473
129.1500
124.3505
120.2012
77.7807
77.3600
76.9298
68.8510
59.1279
38.1709
O
PhHN
OCH3
3a

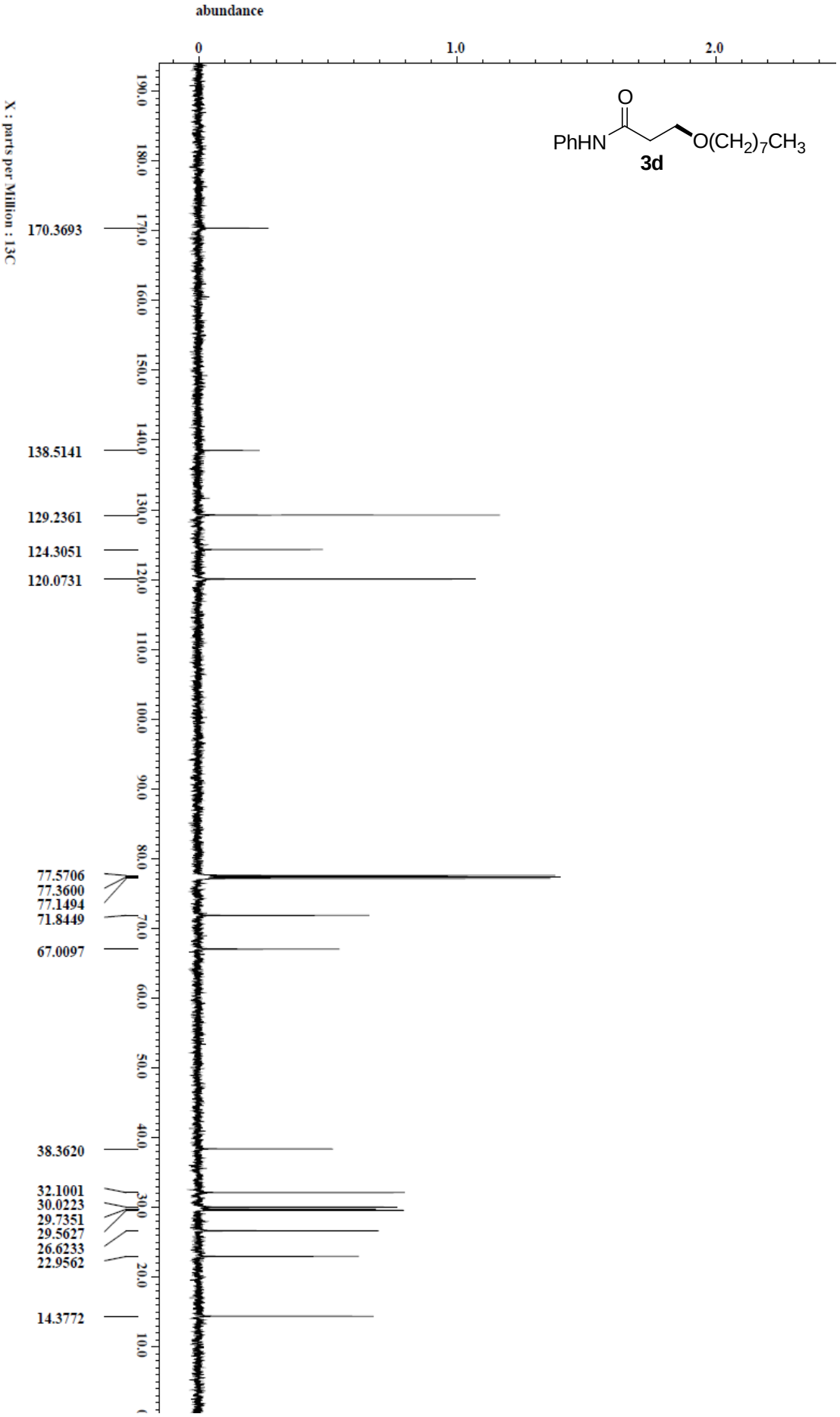

abundance
X : parts per Million : 1H
PhHN
O
OC2H5
3b
8.5053
7.5187
7.4923
7.3332
7.3081
7.2817
7.2611
7.0826
3.7599
3.7416
3.6088
3.5859
2.6497
2.6302
2.6119
1.3082
1.2842
1.2619
0.0000
1.0
1.98
2.5
0.92
1.96
1.99
2.0
2.94

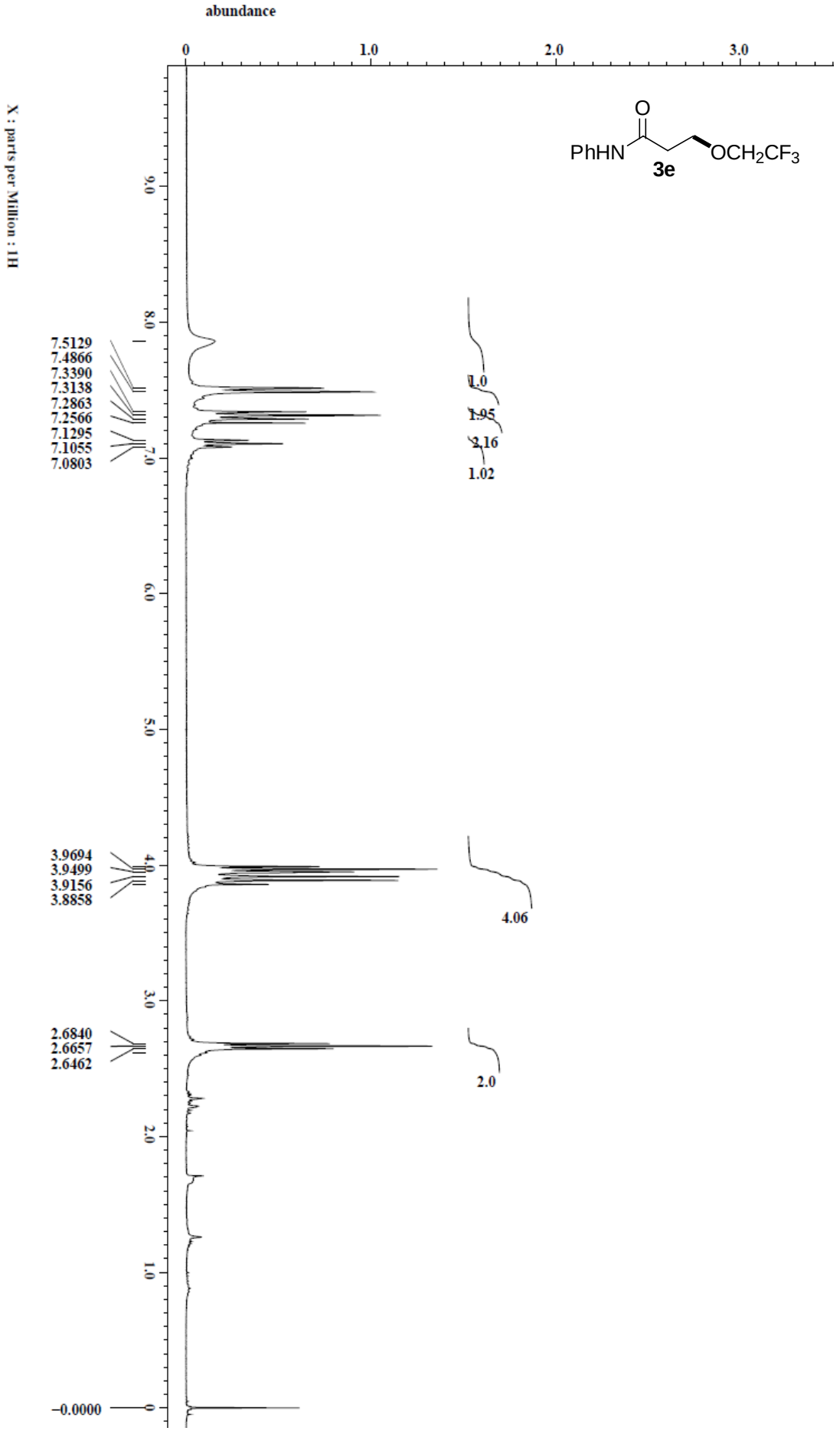

abundance
X : parts per Million : 13C
170.3085
138.5099
129.2743
124.3123
120.0100
77.7807
77.3600
76.9393
67.0154
66.7573
38.3430
15.5027
PhHN
O
OC2H5
3b

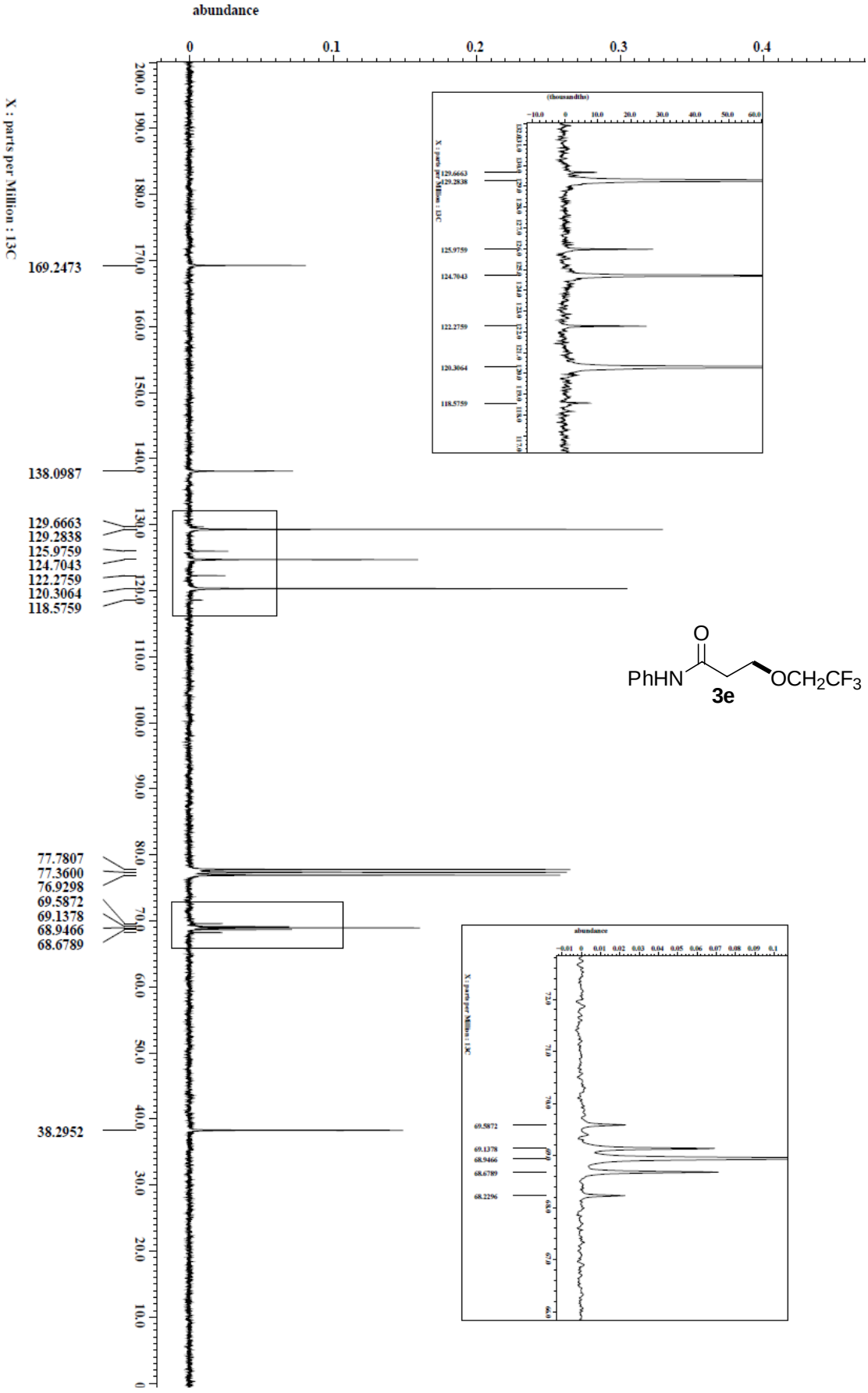

abundance
X : parts per Million : 1H
PhHN
O
O(CH2)3CH3
3c
8.5270
7.5152
7.4900
7.3344
7.3092
7.2817
7.2611
3.7679
3.7507
3.7313
3.5344
3.5127
2.6531
2.6336
2.6153
1.6585
1.6367
1.6093
1.4364
1.4113
0.9752
0.9500
0.9260
0.0000
0.88
1.89
2.38
1.01
1.91
1.95
1.96
1.99
1.98
3

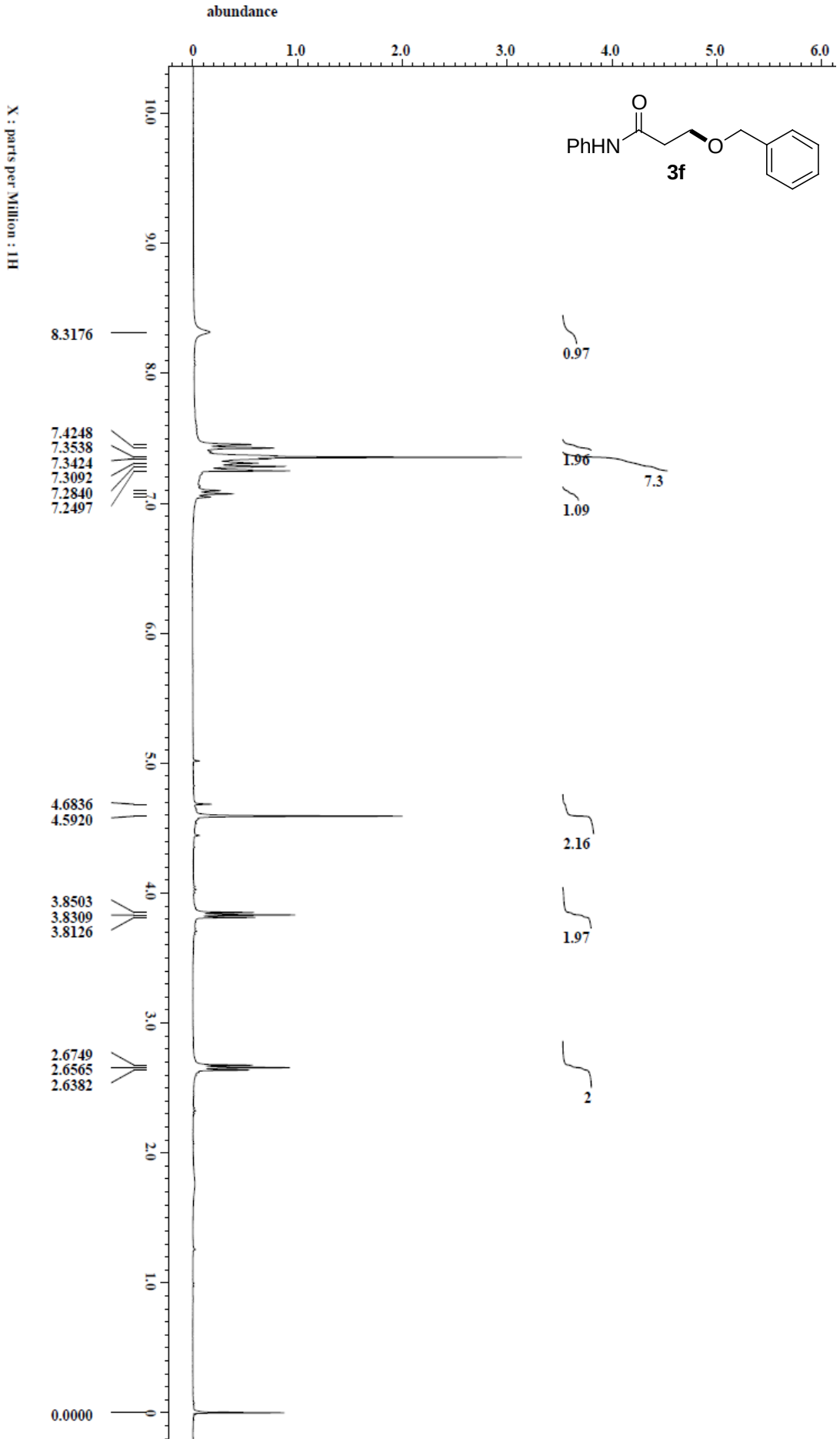

abundance
0
0.1
0.2
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.4137
138.4812
129.2647
124.3123
120.0578
77.7807
77.3600
76.9393
71.4993
67.0058
38.3430
32.0330
19.7093
14.1833
O
PhHN
O(CH2)3CH3
3c

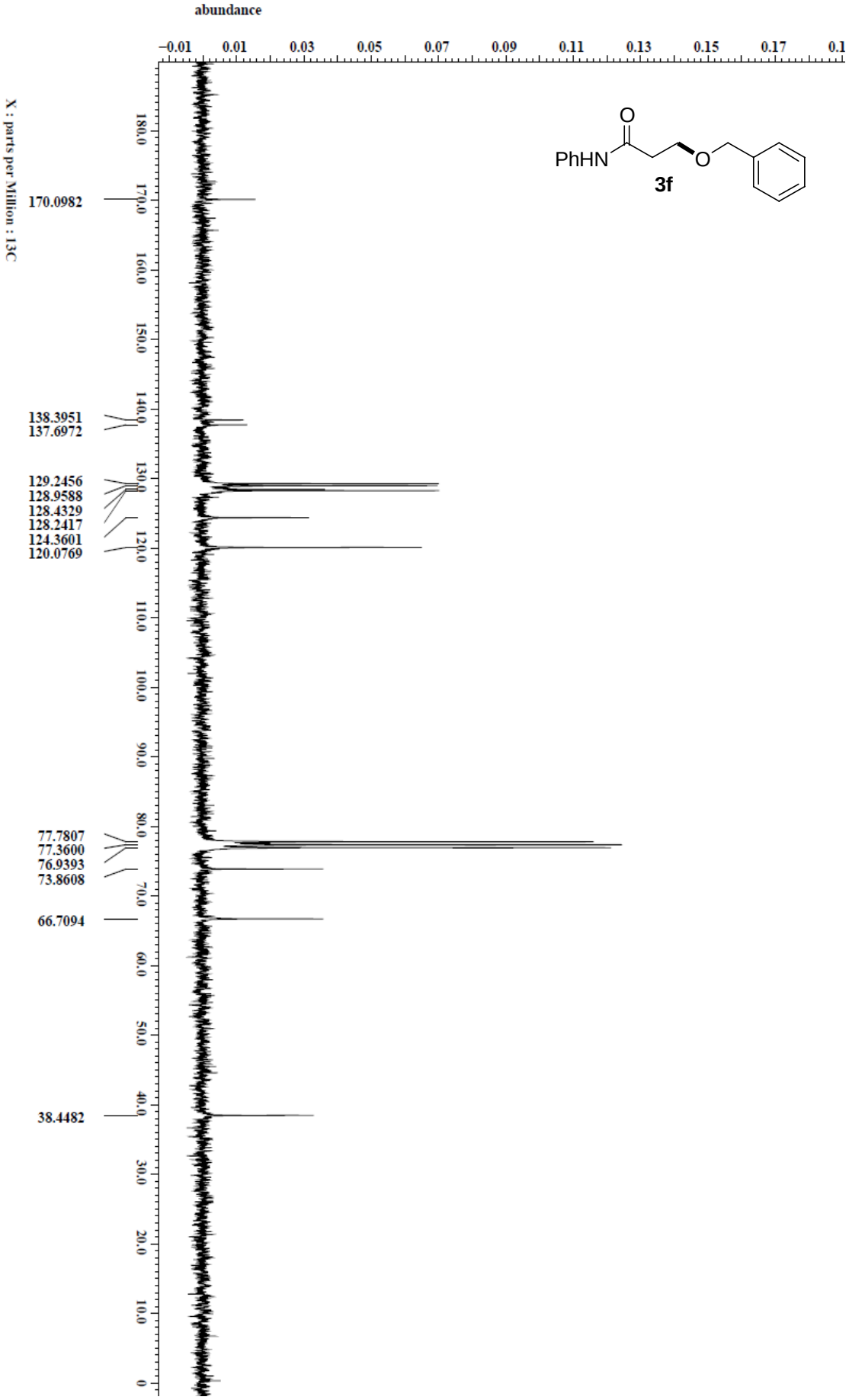

abundance
X : parts per Million : 1H
PhHN
O(CH2)7CH3
3d
8.5182
7.5115
7.4989
7.3134
7.3008
7.2871
7.0924
7.0798
3.7541
3.7460
3.7357
3.5342
3.5227
2.6397
2.6306
2.6214
1.6411
1.6274
1.3869
1.3056
1.2964
1.2849
1.2746
1.2643
0.8876
0.8761
0.8646
0.0000
0.91
1.95
2.04
0.98
2
1.98
1.99
2.01
2.09
8.14
3.07

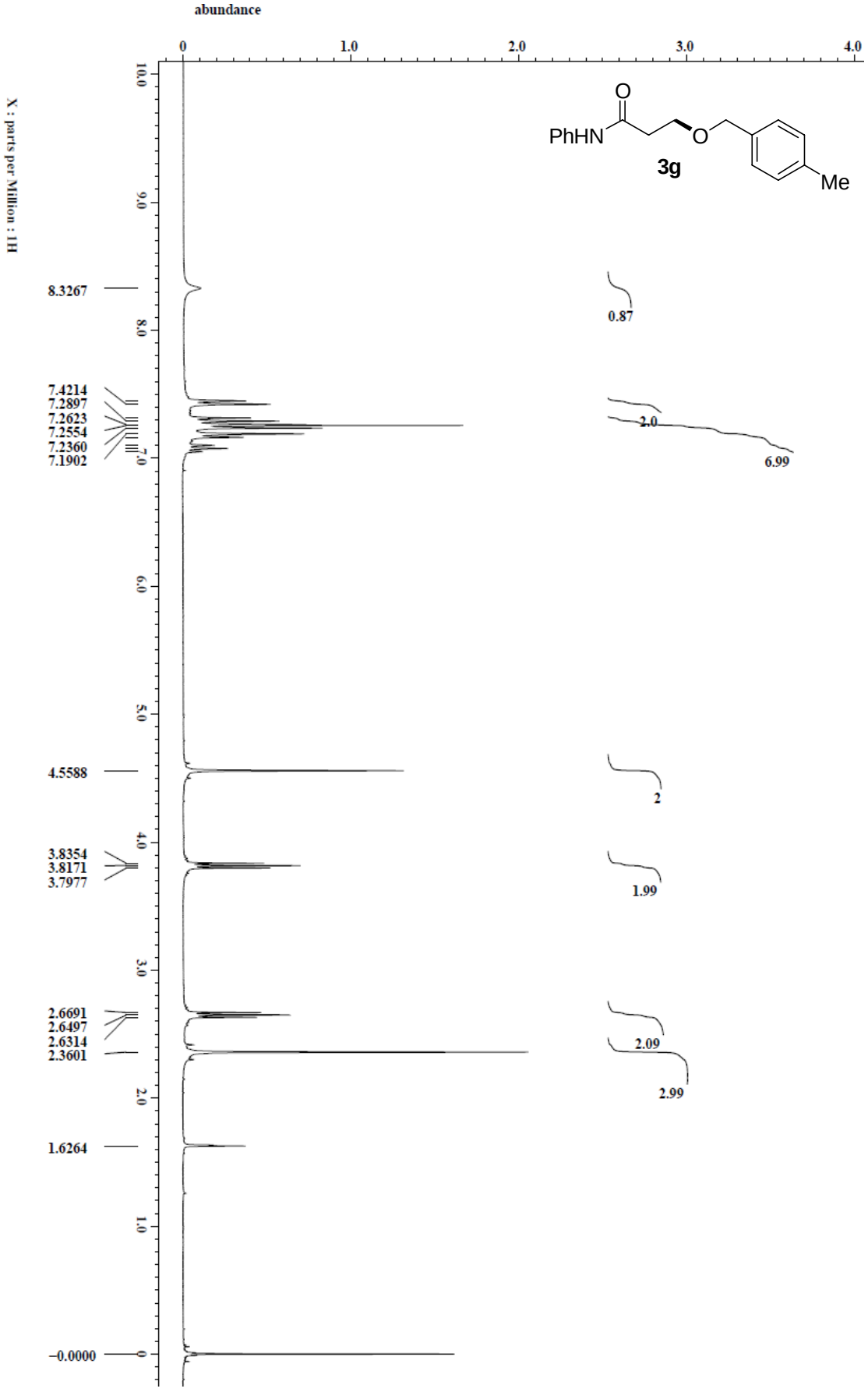

abundance
0
1.0
2.0
X : parts per Million : 13C
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.3693
138.5141
129.2361
124.3051
120.0731
77.5706
77.3600
77.1494
71.8449
67.0097
38.3620
32.1001
30.0223
29.7351
29.5627
26.6233
22.9562
14.3772
O
PhHN
O(CH2)7CH3
3d

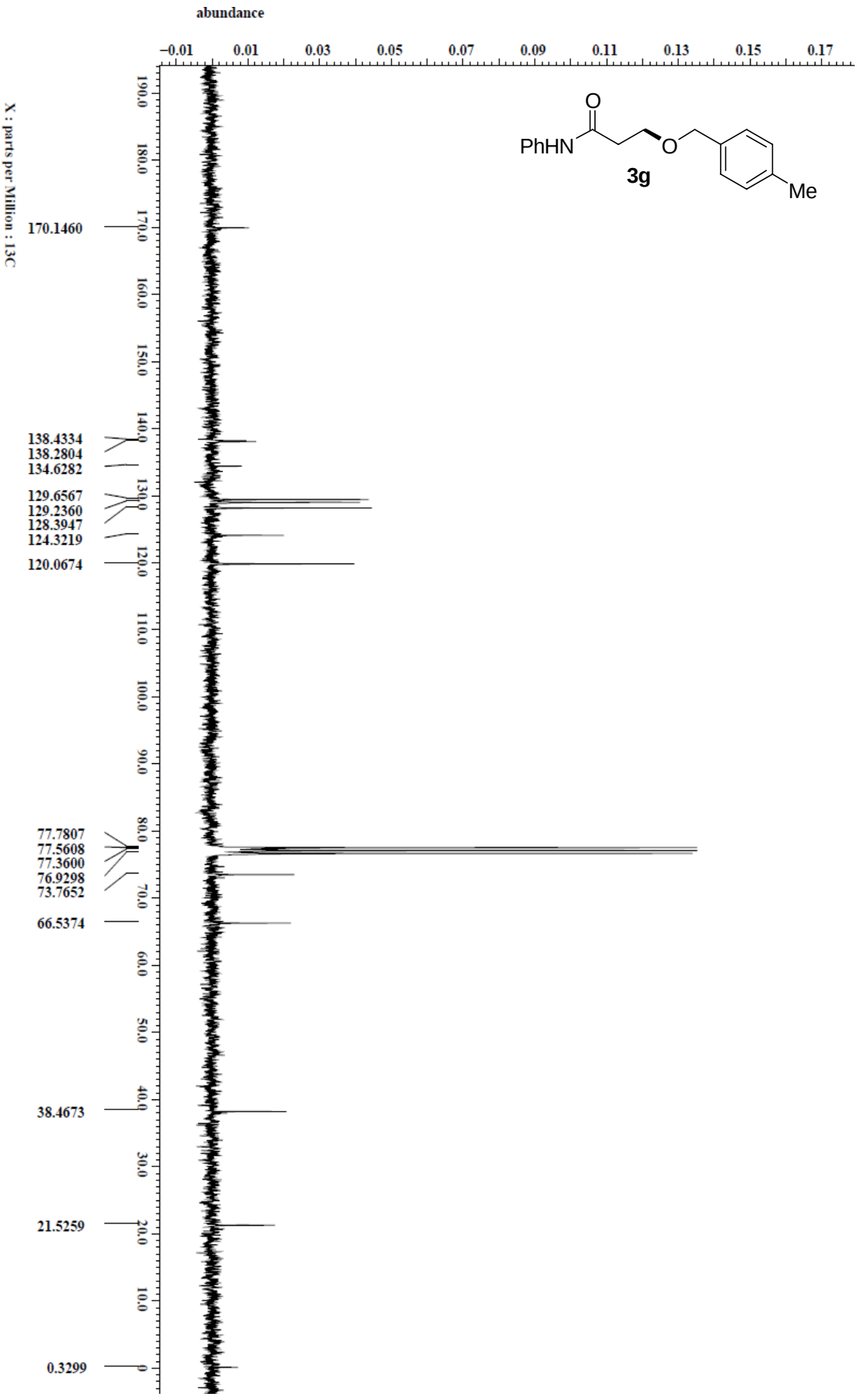

abundance
X : parts per Million : 1H
PhHN
O
OCH2CF3
3e
7.5129
7.4866
7.3390
7.3138
7.2863
7.2566
7.1295
7.1055
7.0803
3.9694
3.9499
3.9156
3.8858
2.6840
2.6657
2.6462
−0.0000
1.0
1.95
2.16
1.02
4.06
2.0

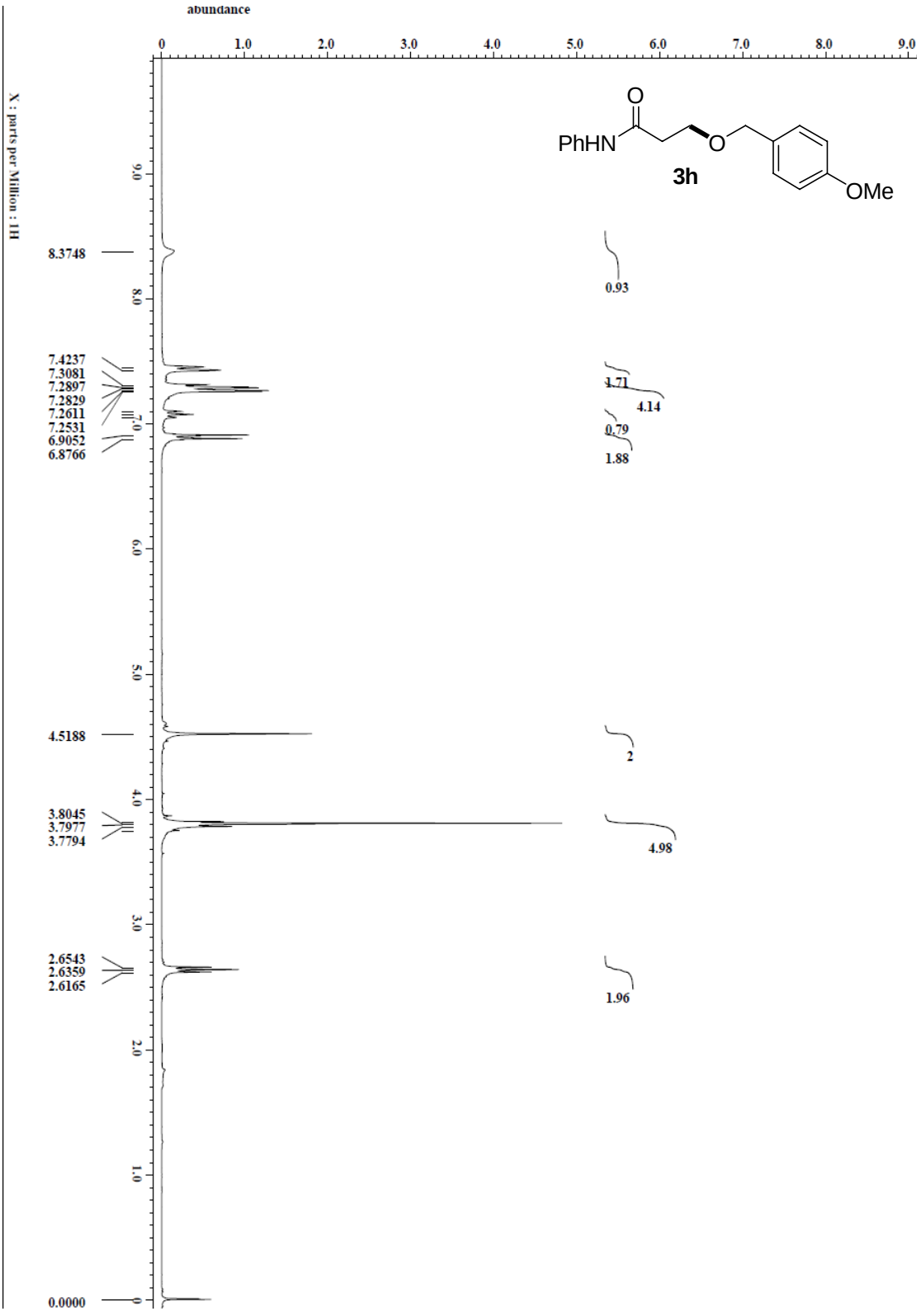

abundance
X : parts per Million : 13C
169.2473
138.0987
129.6663
129.2838
125.9759
124.7043
122.2759
120.3064
118.5759
77.7807
77.3600
76.9298
69.5872
69.1378
68.9466
68.6789
38.2952
PhHN
O
OCH2CF3
3e

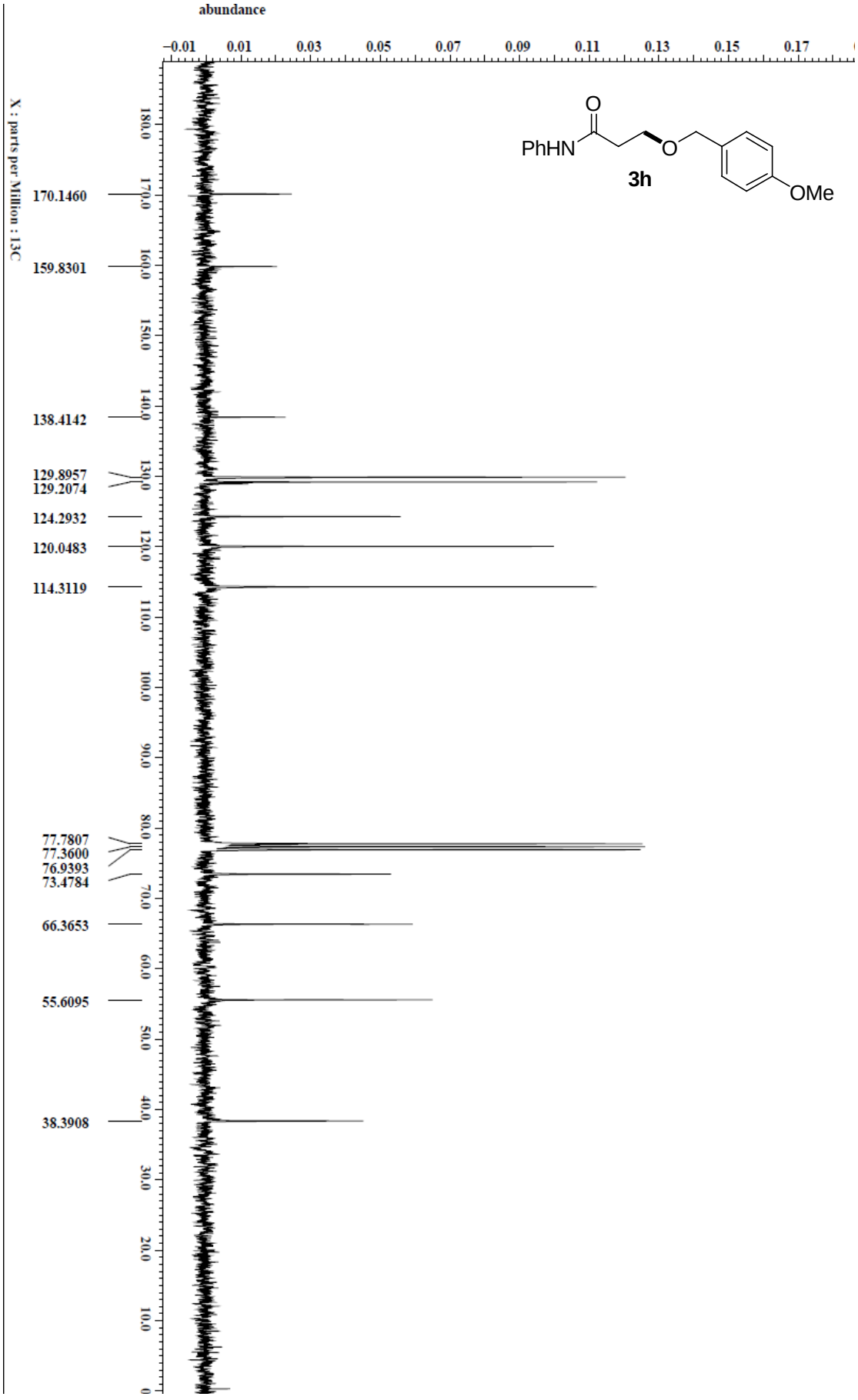

abundance
X : parts per Million : 1H
PhHN
O
O
3f
8.3176
7.4248
7.3538
7.3424
7.3092
7.2840
7.2497
4.6836
4.5920
3.8503
3.8309
3.8126
2.6749
2.6565
2.6382
0.0000
0.97
1.96
7.3
1.09
2.16
1.97
2

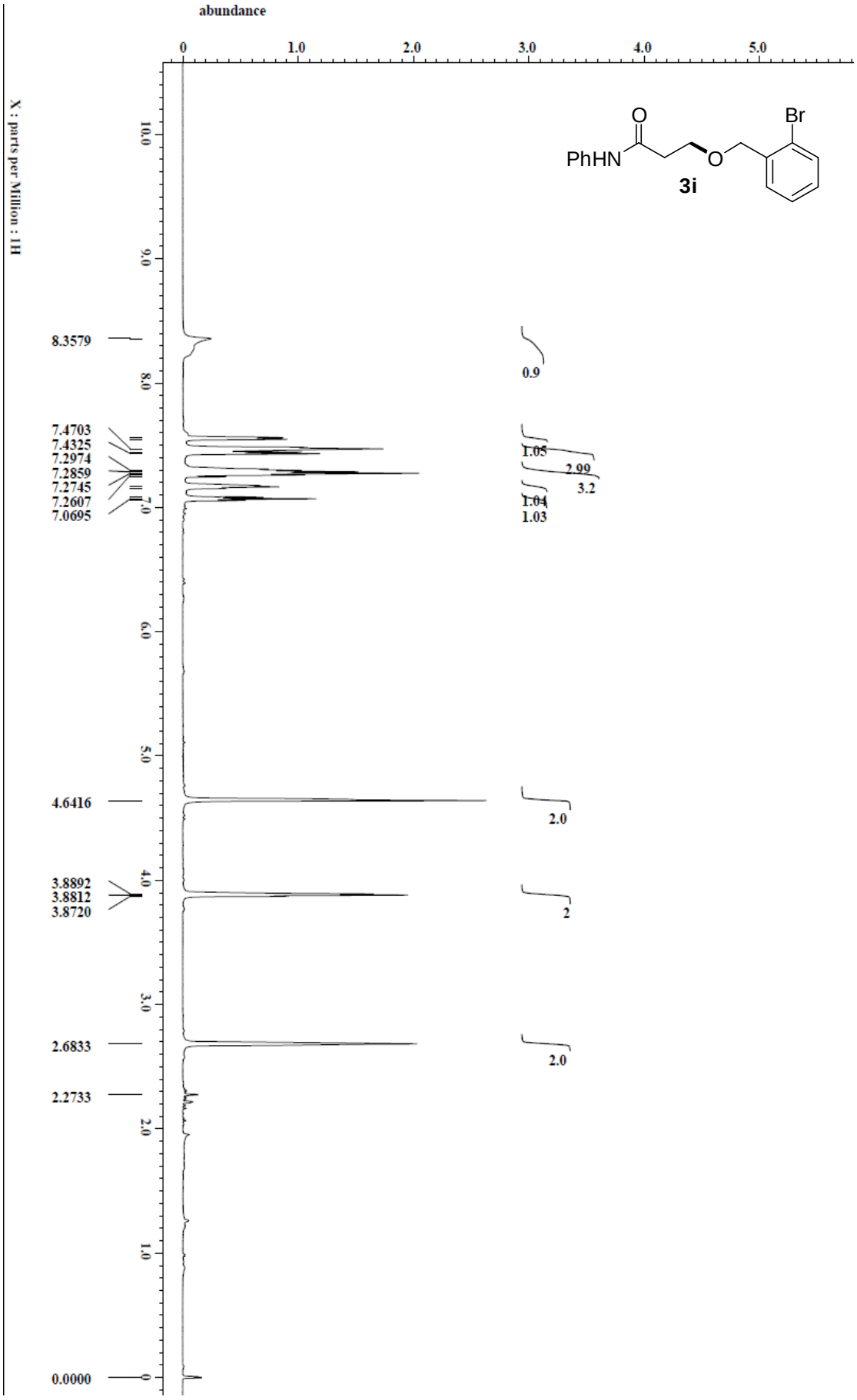

abundance
−0.01
0.01
0.03
0.05
0.07
0.09
0.11
0.13
0.15
0.17
0.1
X : parts per Million : 13C
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.0982
138.3951
137.6972
129.2456
128.9588
128.4329
128.2417
124.3601
120.0769
77.7807
77.3600
76.9393
73.8608
66.7094
38.4482
O
PhHN
O
3f

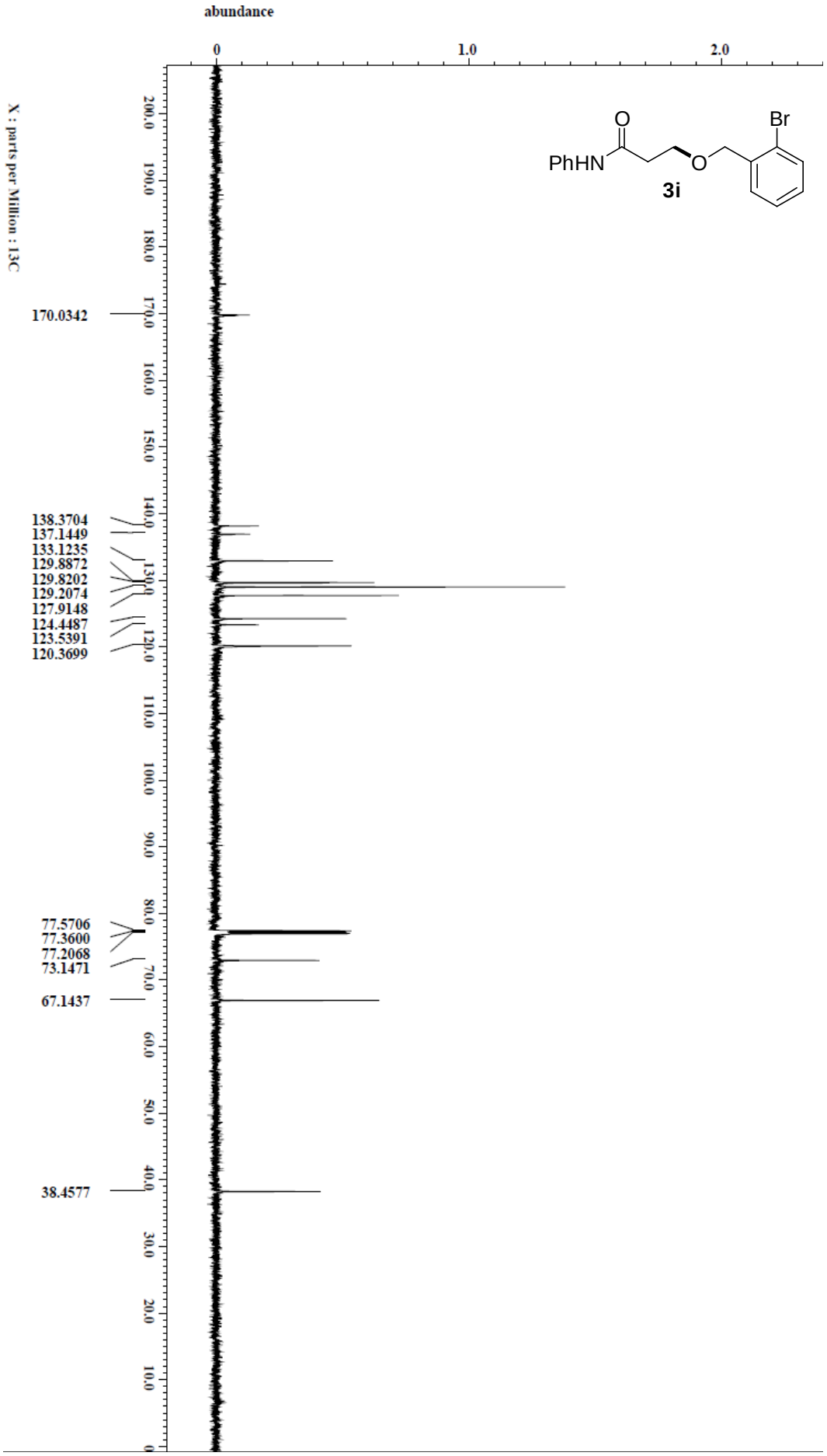

abundance
X : parts per Million : 1H
PhHN
O
O
Me
3g
8.3267
7.4214
7.2897
7.2623
7.2554
7.2360
7.1902
4.5588
3.8354
3.8171
3.7977
2.6691
2.6497
2.6314
2.3601
1.6264
-0.0000
0.87
2.0
6.99
2
1.99
2.09
2.99

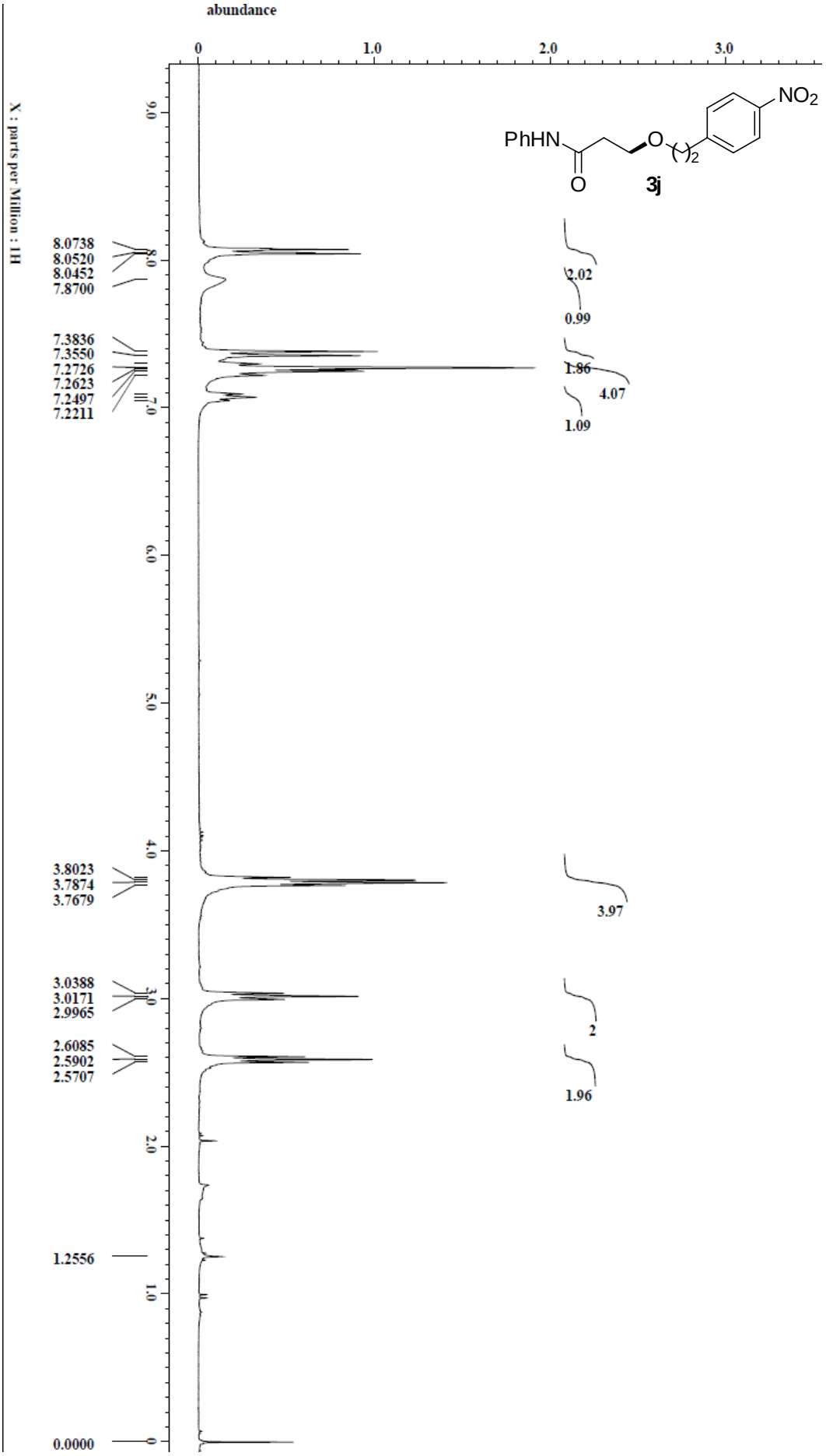

abundance
X : parts per Million : 13C
PhHN
O
O
Me
3g
170.1460
138.4334
138.2804
134.6282
129.6567
129.2360
128.3947
124.3219
120.0674
77.7807
77.5608
77.3600
76.9298
73.7652
66.5374
38.4673
21.5259
0.3299

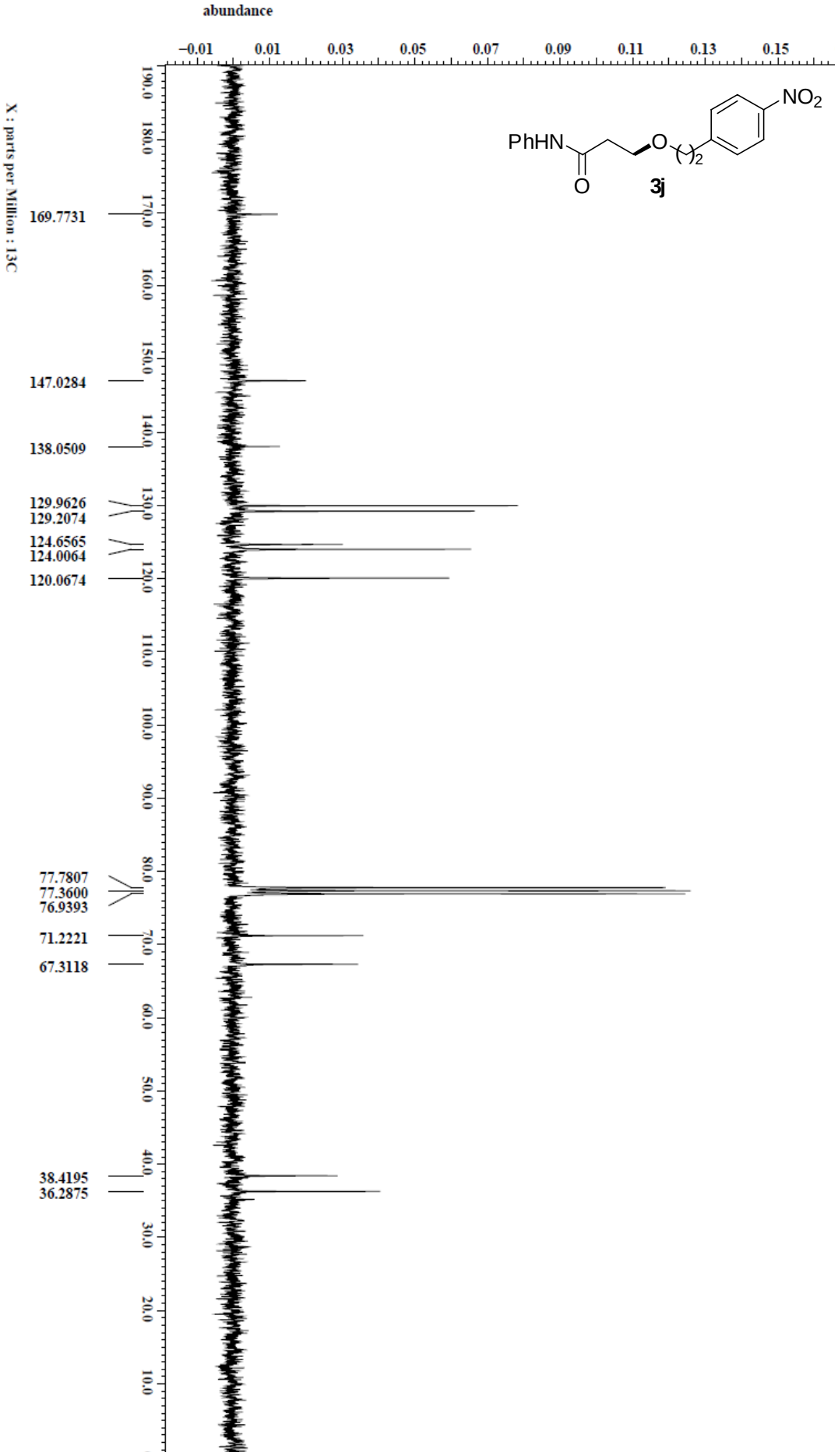

abundance
X : parts per Million : 1H
PhHN
O
O
OMe
3h
8.3748
7.4237
7.3081
7.2897
7.2829
7.2611
7.2531
6.9052
6.8766
4.5188
3.8045
3.7977
3.7794
2.6543
2.6359
2.6165
0.0000
0.93
1.71
4.14
0.79
1.88
2
4.98
1.96

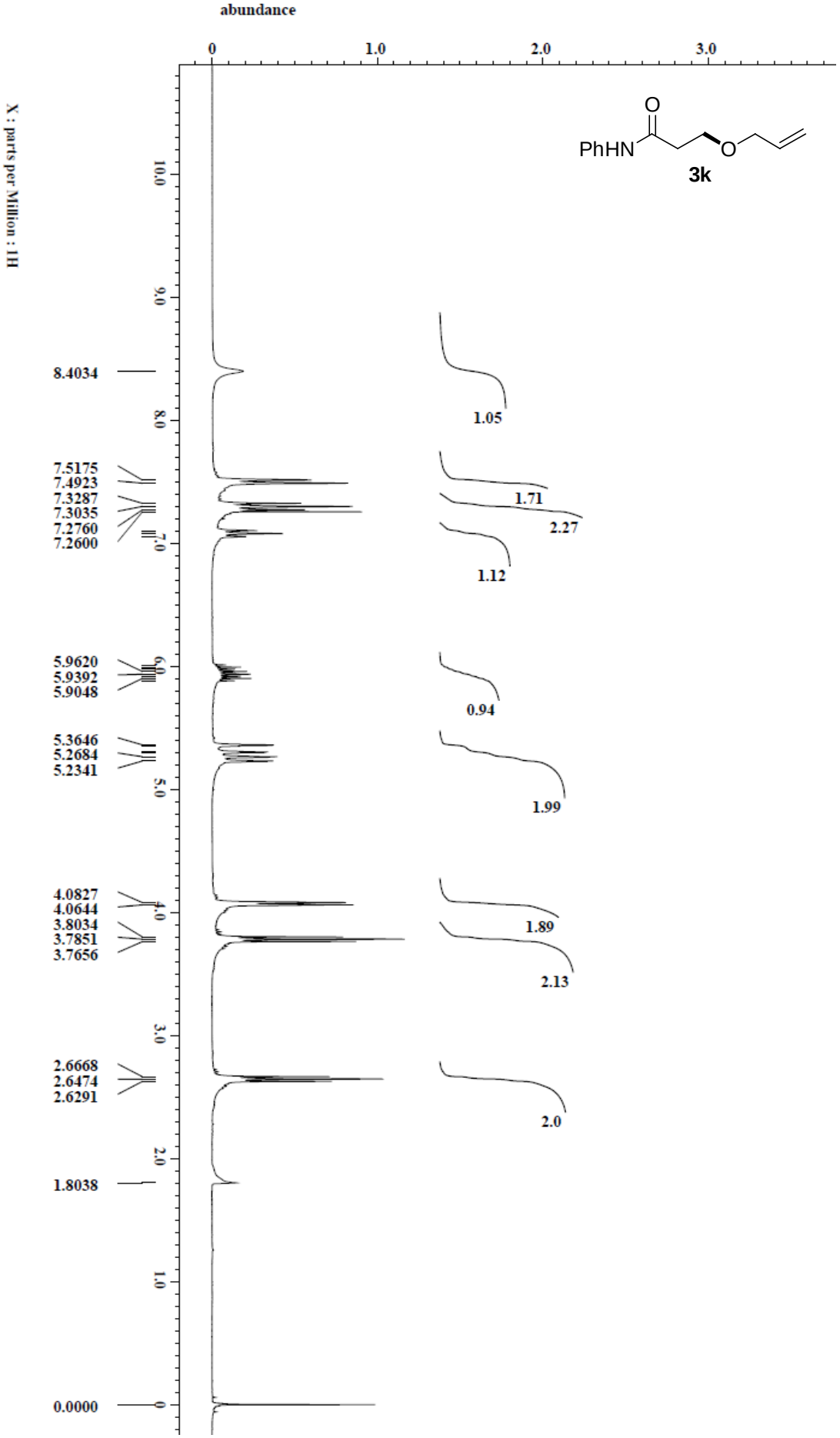

abundance
−0.01
0.01
0.03
0.05
0.07
0.09
0.11
0.13
0.15
0.17
X : parts per Million : 13C
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.1460
159.8301
138.4142
129.8957
129.2074
124.2932
120.0483
114.3119
77.7807
77.3600
76.9393
73.4784
66.3653
55.6095
38.3908
O
PhHN
O
OMe
3h




abundance
0
1.0
2.0
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.0342
138.3704
137.1449
133.1235
129.8872
129.8202
129.2074
127.9148
124.4487
123.5391
120.3699
77.5706
77.3600
77.2068
73.1471
67.1437
38.4577
O
Br
PhHN
O
3i


abundance
X : parts per Million : 1H
PhHN
O
O
NO_2
3j
8.0738
8.0520
8.0452
7.8700
7.3836
7.3550
7.2726
7.2623
7.2497
7.2211
3.8023
3.7874
3.7679
3.0388
3.0171
2.9965
2.6085
2.5902
2.5707
1.2556
0.0000
2.02
0.99
1.86
4.07
1.09
3.97
2
1.96


abundance
−0.01
0.01
0.03
0.05
0.07
0.09
0.11
0.13
0.15
X : parts per Million : 13C
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
169.7731
147.0284
138.0509
129.9626
129.2074
124.6565
124.0064
120.0674
77.7807
77.3600
76.9393
71.2221
67.3118
38.4195
36.2875
PhHN
O
O
2
NO2
3j


abundance
X : parts per Million : 1H
PhHN
O
O
3k
8.4034
7.5175
7.4923
7.3287
7.3035
7.2760
7.2600
5.9620
5.9392
5.9048
5.3646
5.2684
5.2341
4.0827
4.0644
3.8034
3.7851
3.7656
2.6668
2.6474
2.6291
1.8038
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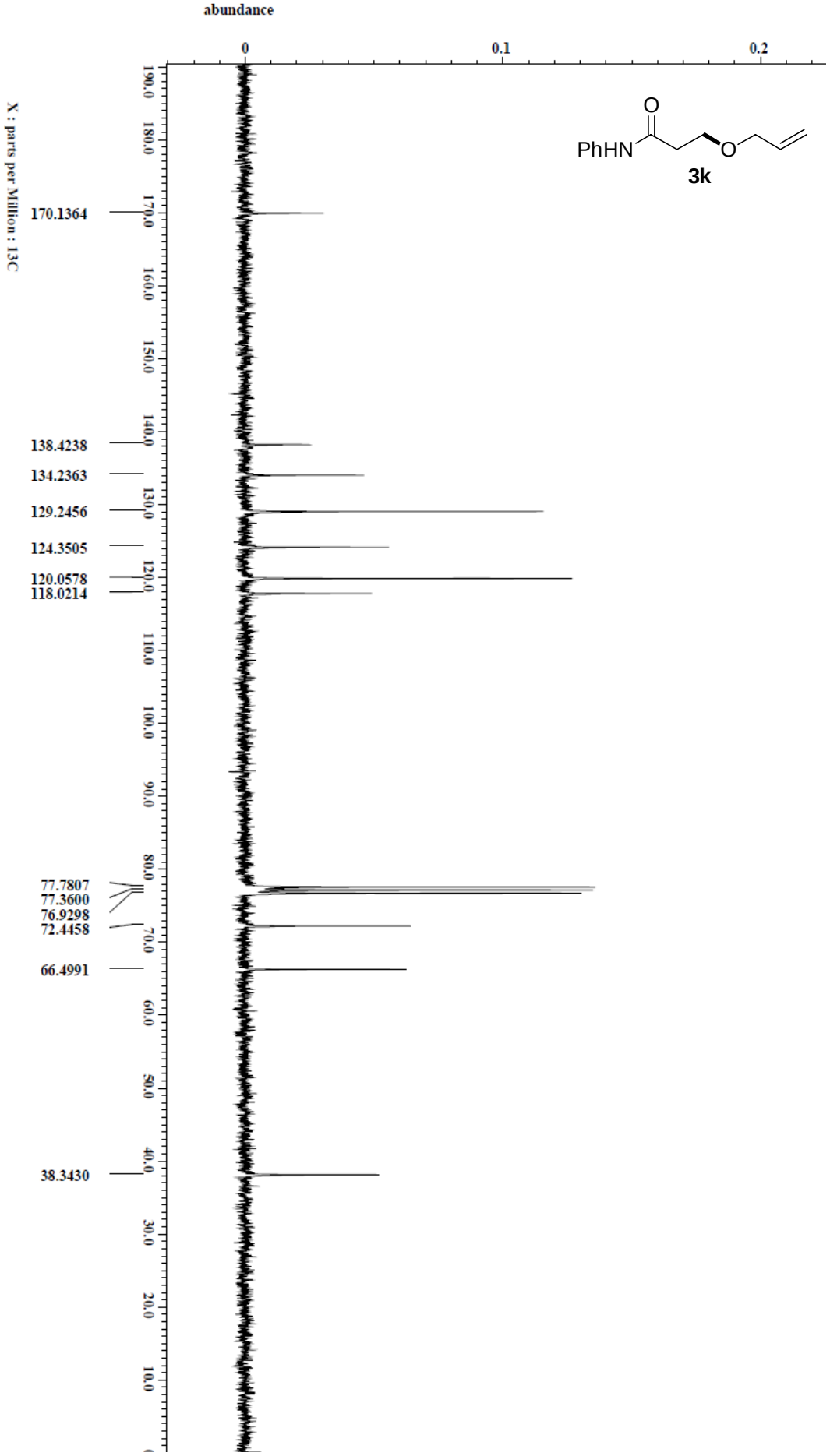
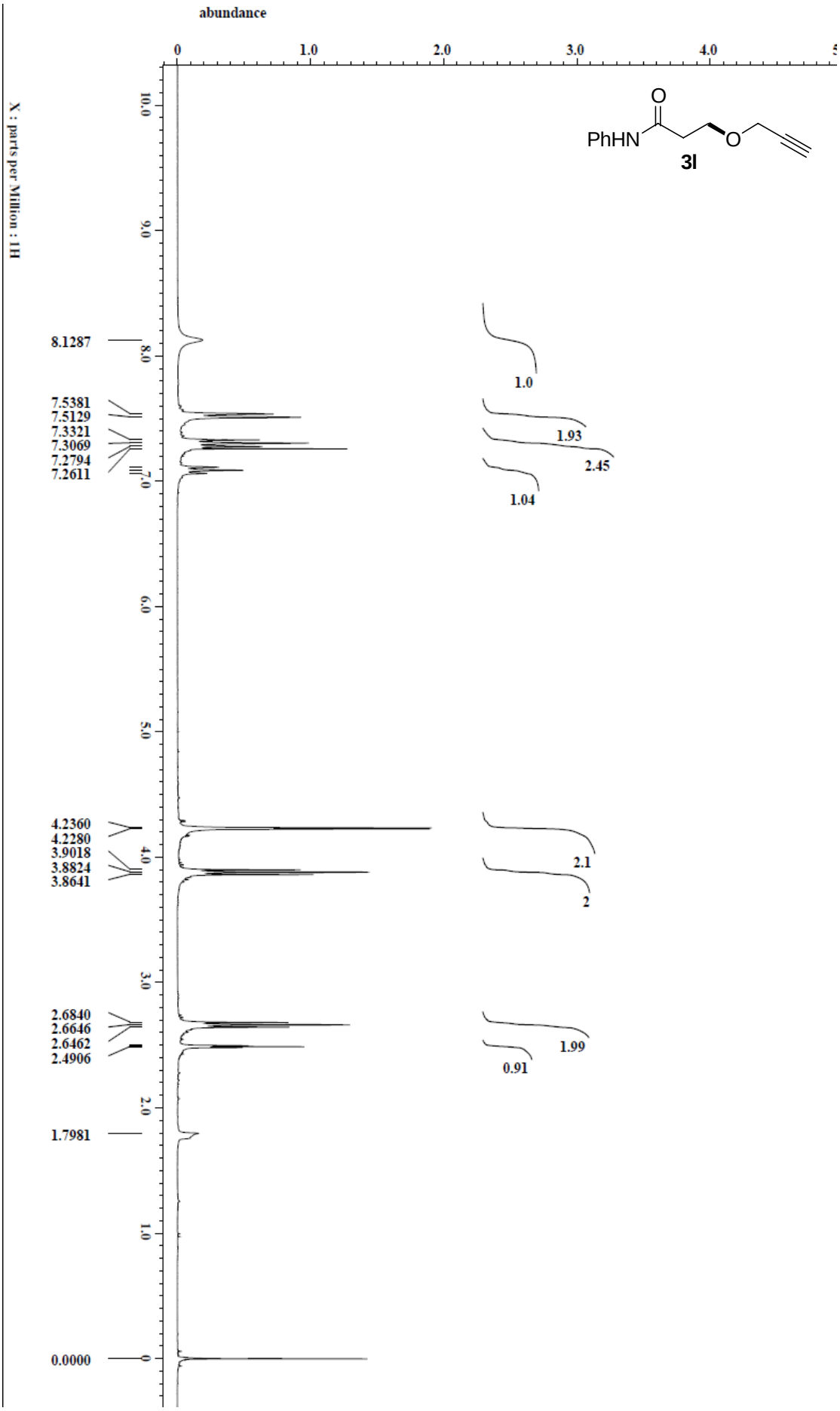
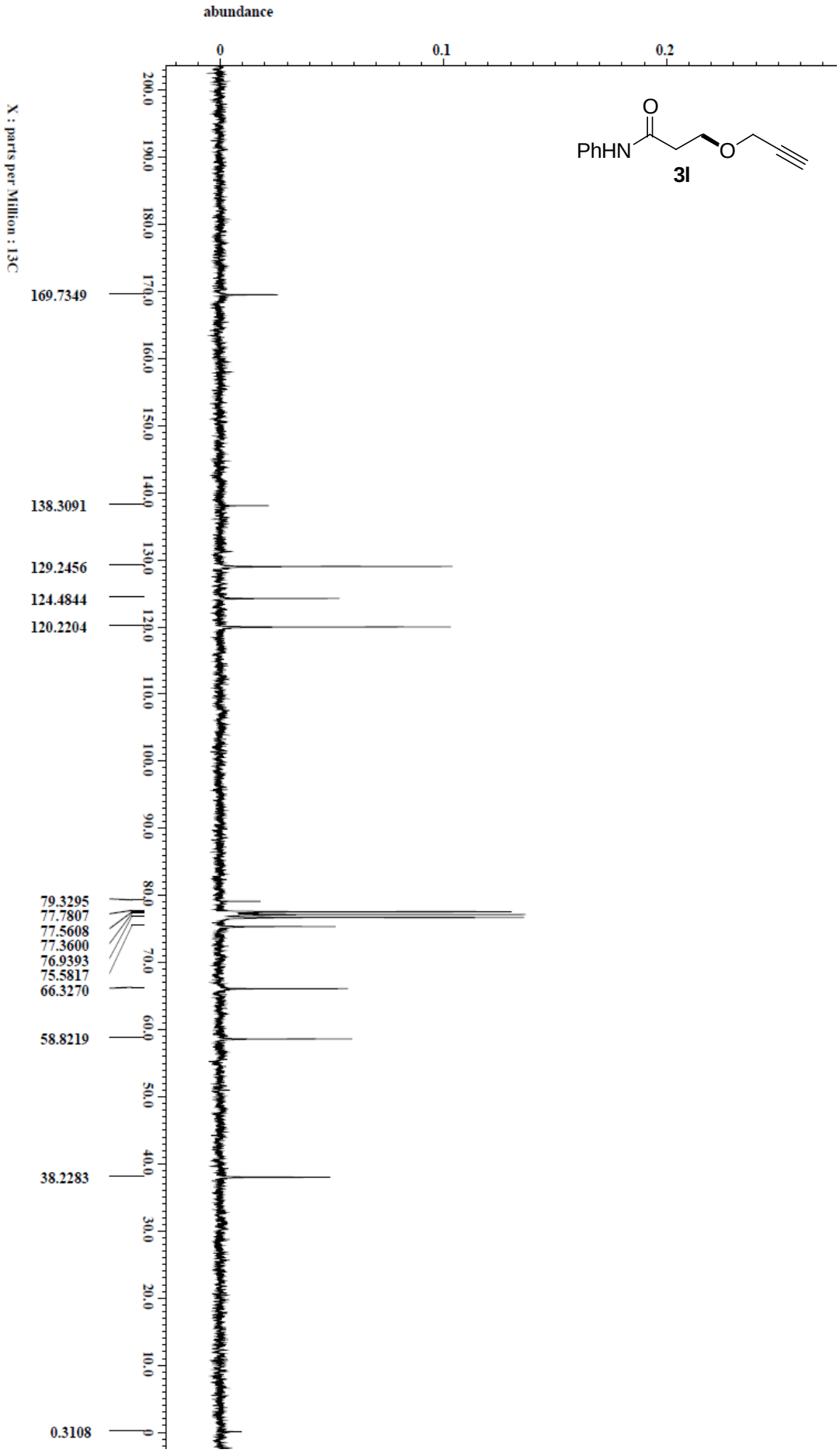
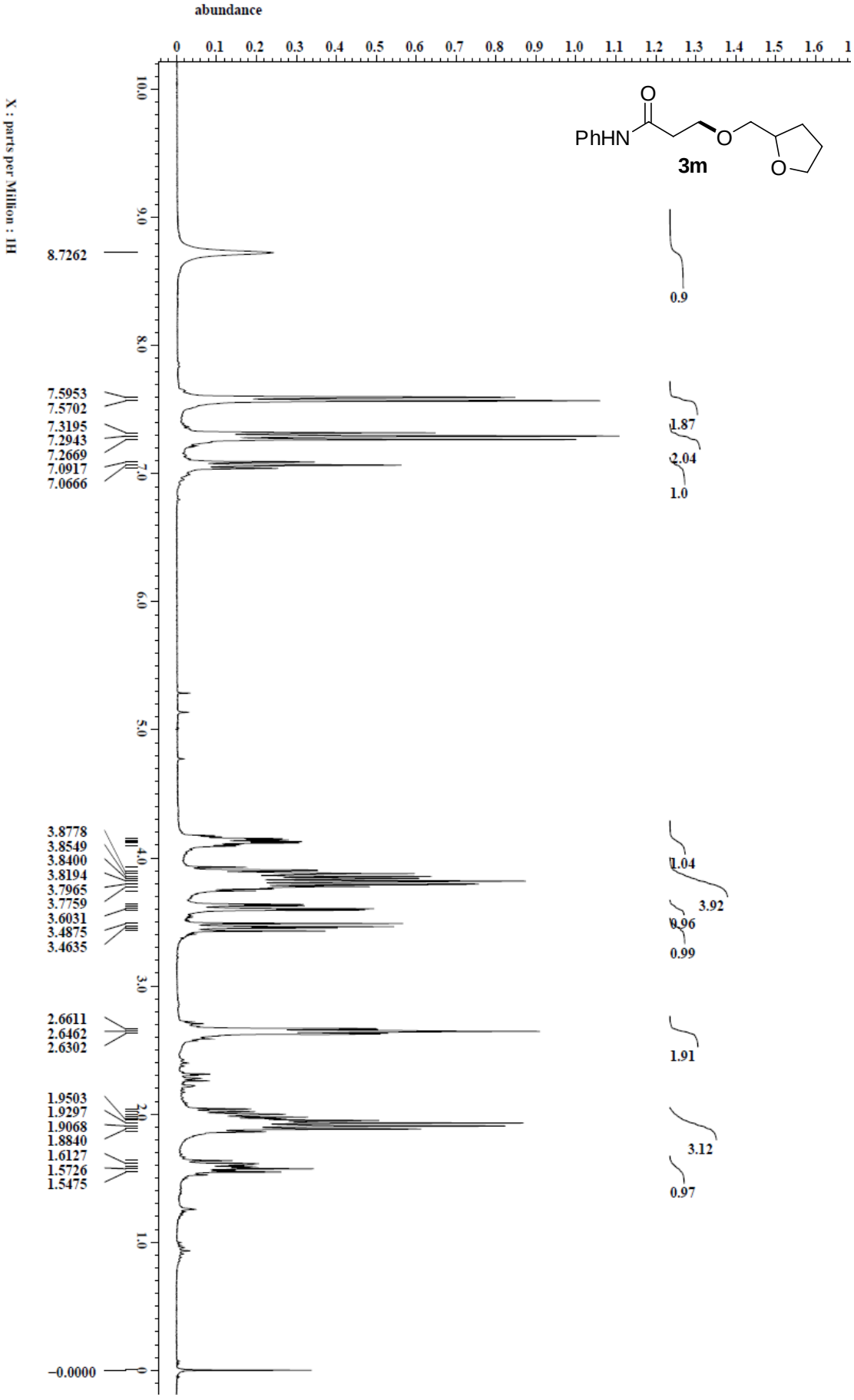
1.05
1.71
2.27
1.12
0.94
1.99
1.89
2.13
2.0

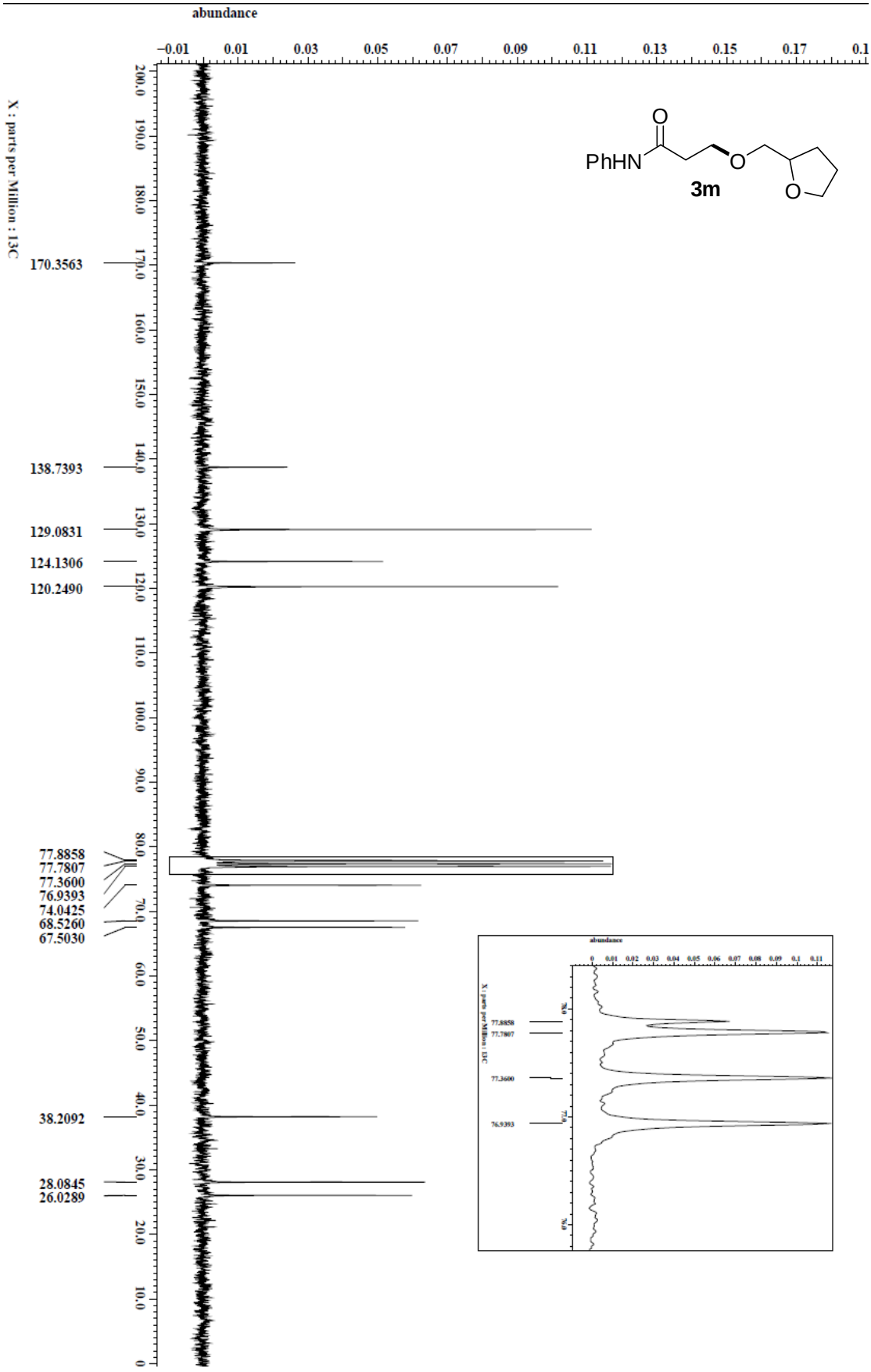

abundance
0
0.1
0.2
X : parts per Million : 13C
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.1364
138.4238
134.2363
129.2456
124.3505
120.0578
118.0214
77.7807
77.3600
76.9298
72.4458
66.4991
38.3430
O
PhHN
O
3k


abundance
X : parts per Million : 1H
PhHN
O
O
3l
8.1287
7.5381
7.5129
7.3321
7.3069
7.2794
7.2611
4.2360
4.2280
3.9018
3.8824
3.8641
2.6840
2.6646
2.6462
2.4906
1.7981
0.0000
1.0
1.93
2.45
1.04
2.1
2
1.99
0.91


abundance
0
0.1
0.2
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
169.7349
138.3091
129.2456
124.4844
120.2204
79.3295
77.7807
77.5608
77.3600
76.9393
75.5817
66.3270
58.8219
38.2283
0.3108
O
PhHN
O

3l


abundance
X : parts per Million : 1H
PhHN
O
O
O
3m
8.7262
7.5953
7.5702
7.3195
7.2943
7.2669
7.0917
7.0666
3.8778
3.8549
3.8400
3.8194
3.7965
3.7759
3.6031
3.4875
3.4635
2.6611
2.6462
2.6302
1.9503
1.9297
1.9068
1.8840
1.6127
1.5726
1.5475
−0.0000
0.9
1.87
2.04
1.0
1.04
3.92
0.96
0.99
1.91
3.12
0.97


abundance
X : parts per Million : 13C
PhHN
O
O
O
3m
170.3563
138.7393
129.0831
124.1306
120.2490
77.8858
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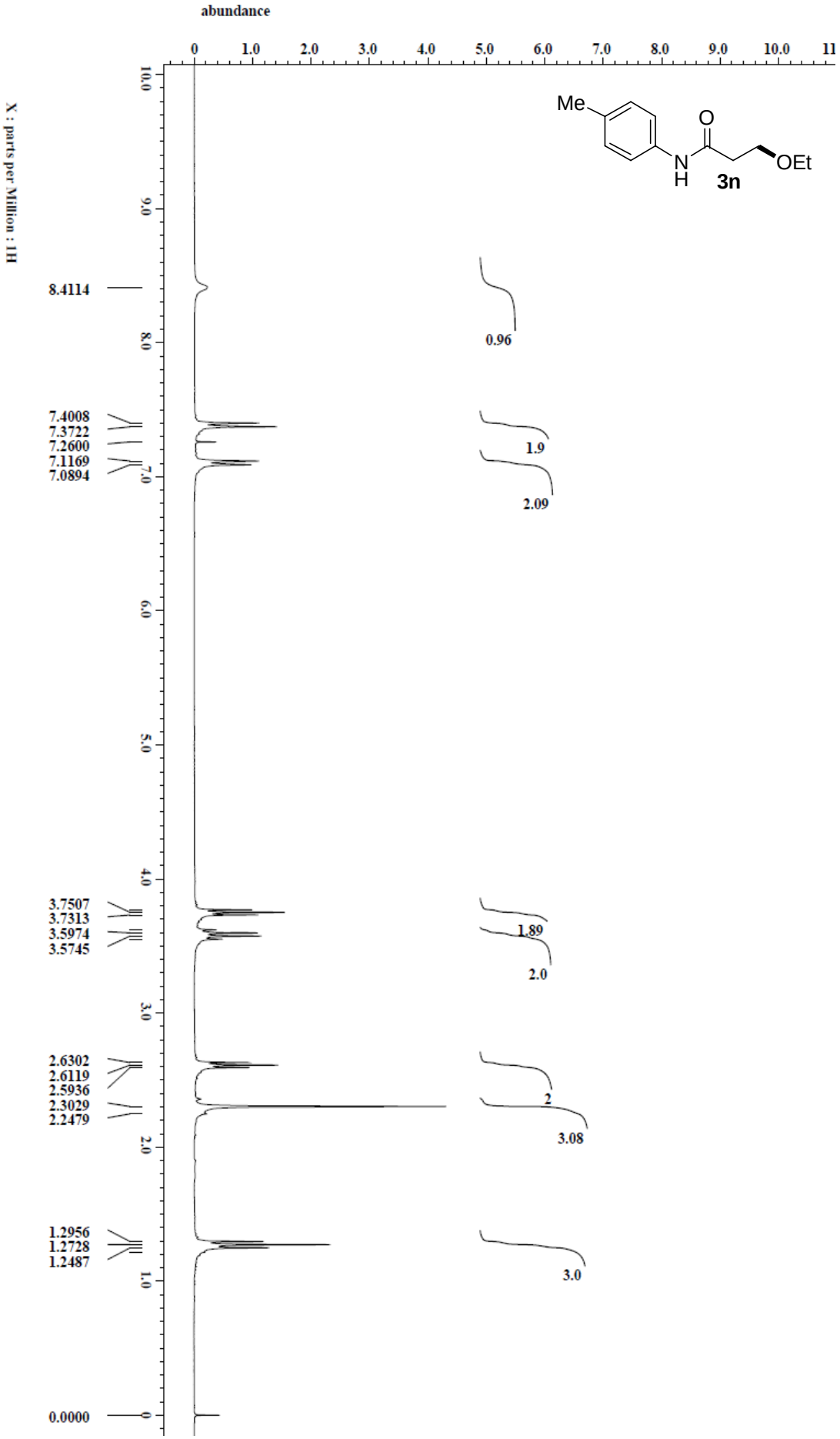
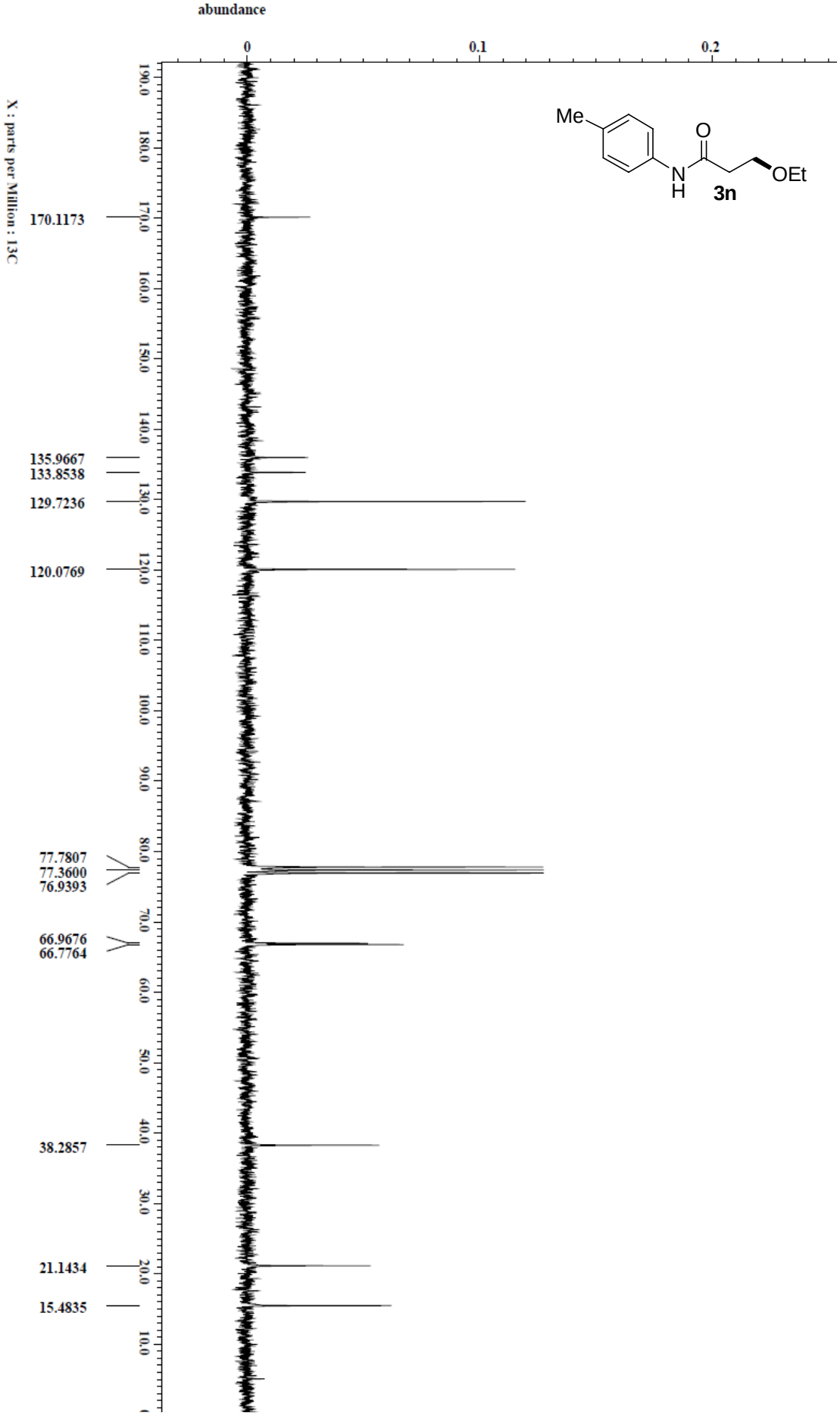
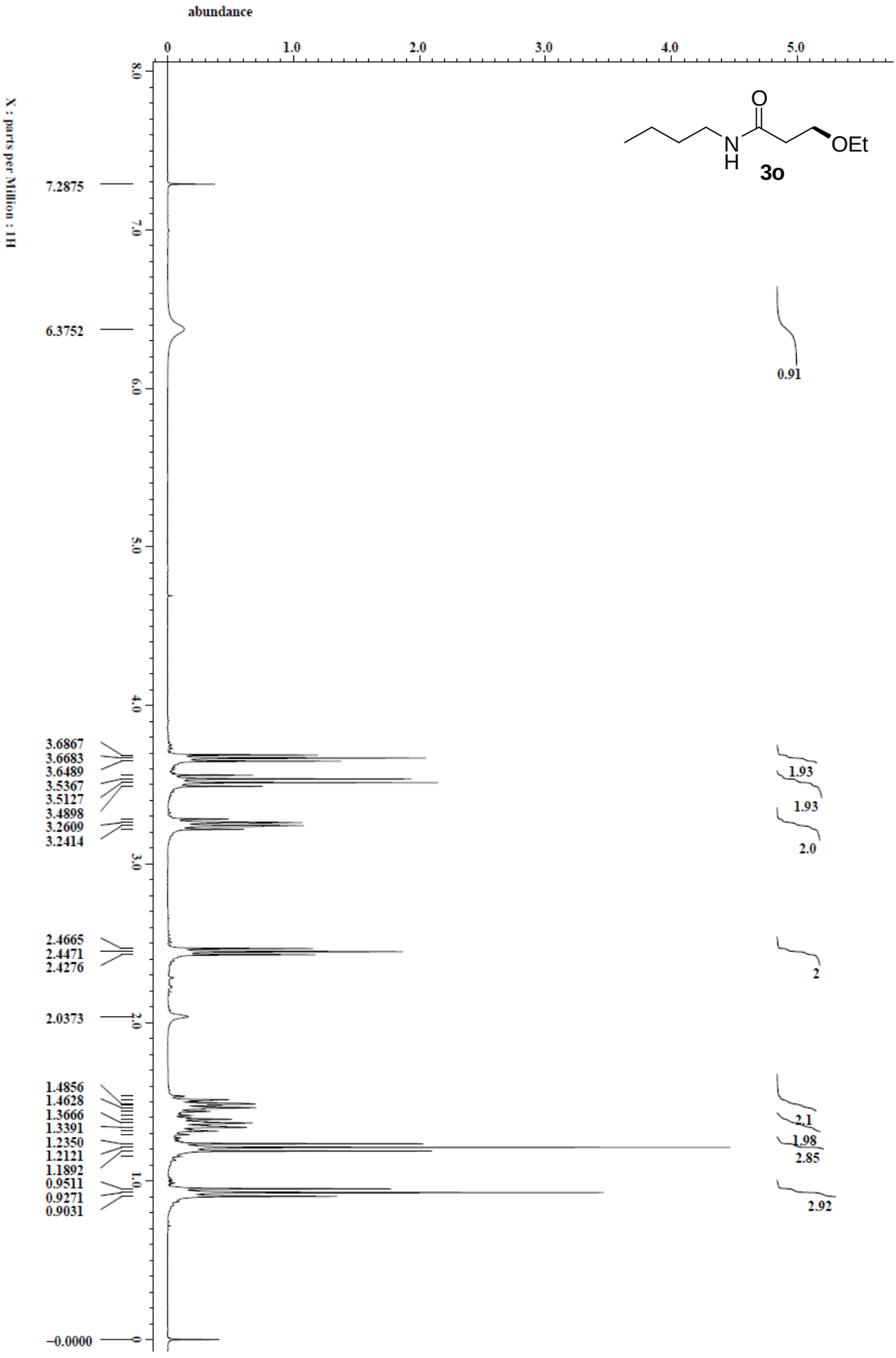
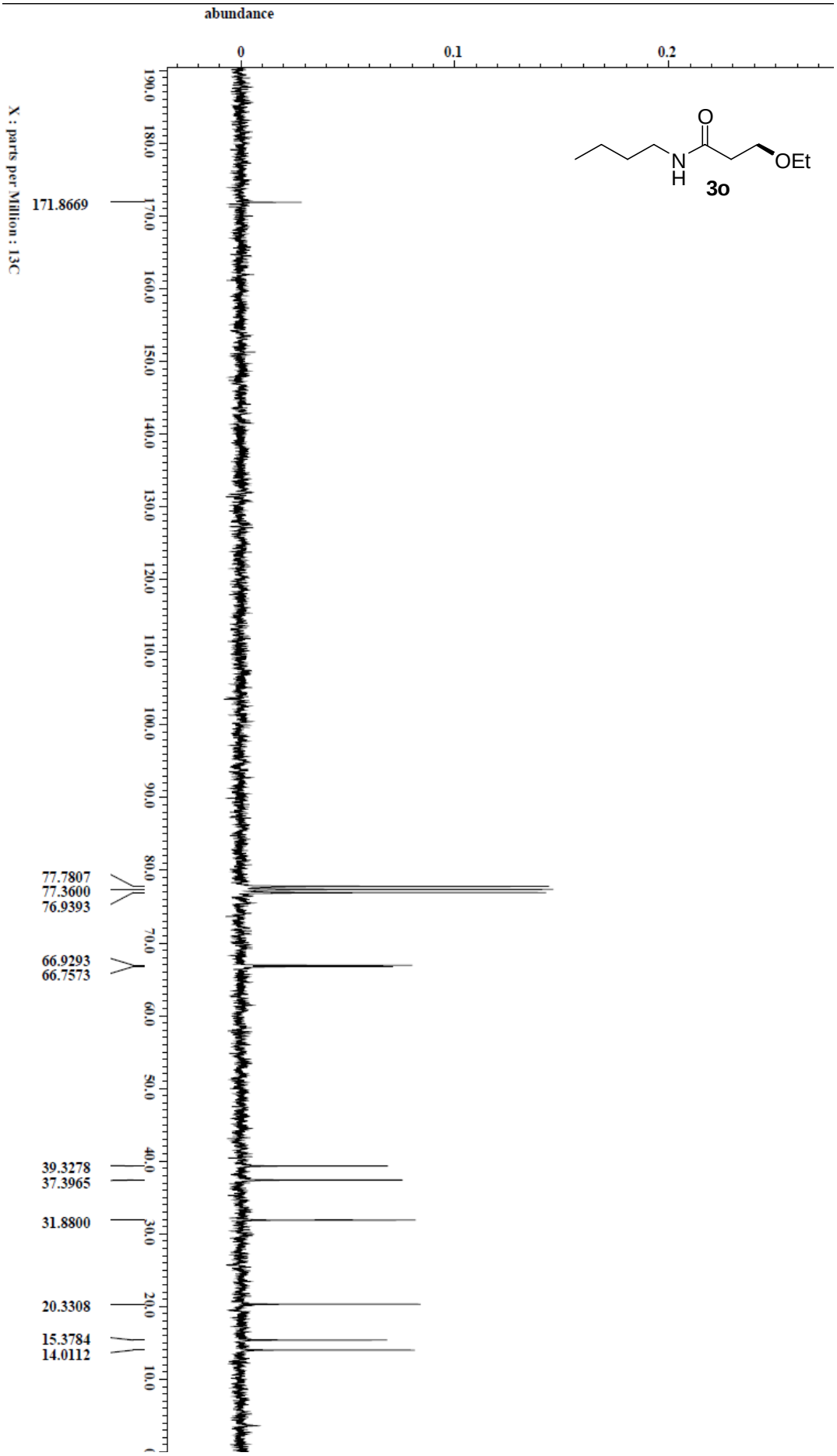
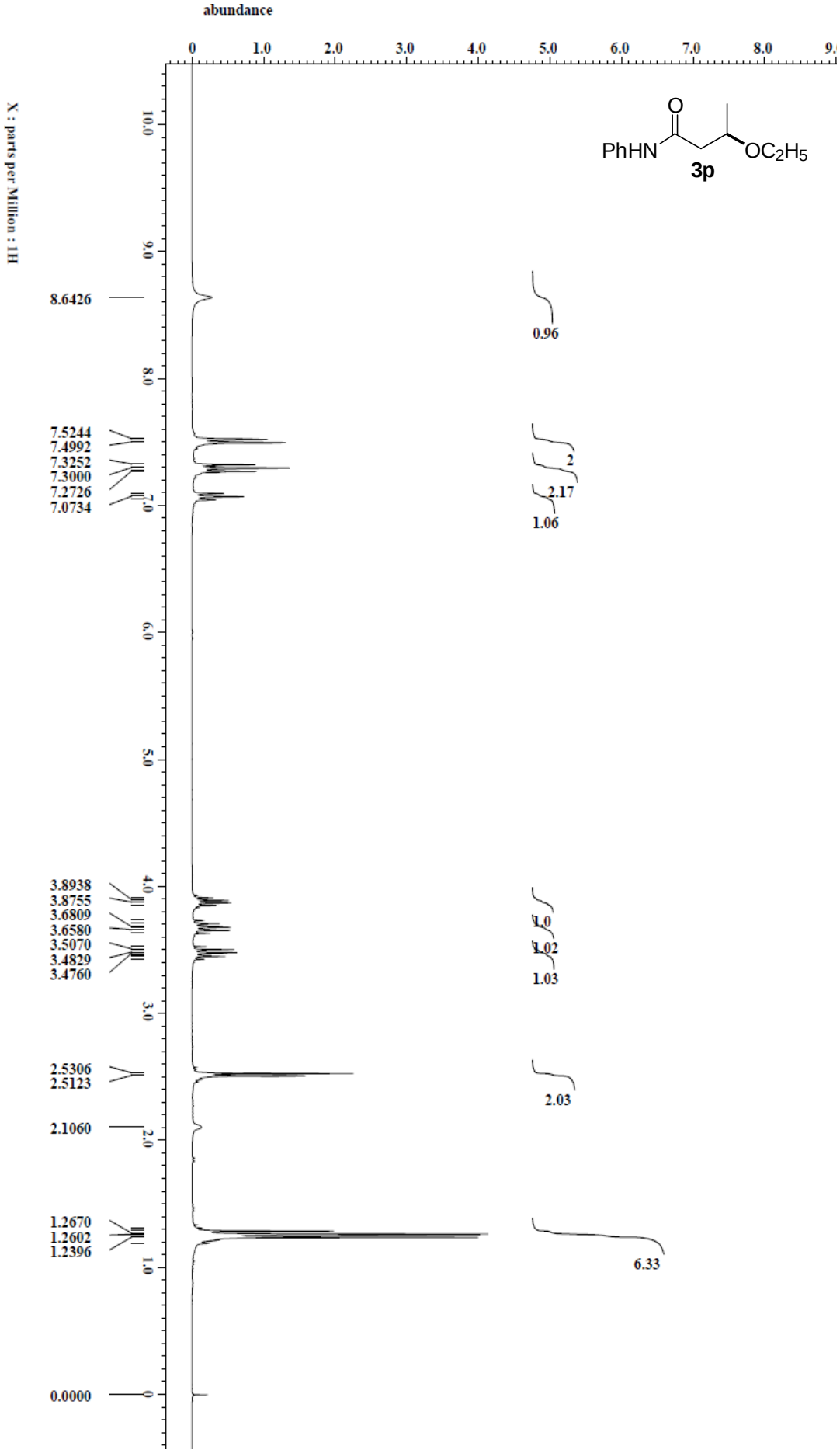
77.3600
76.9393
74.0425
68.5260
67.5030
38.2092
28.0845
26.0289

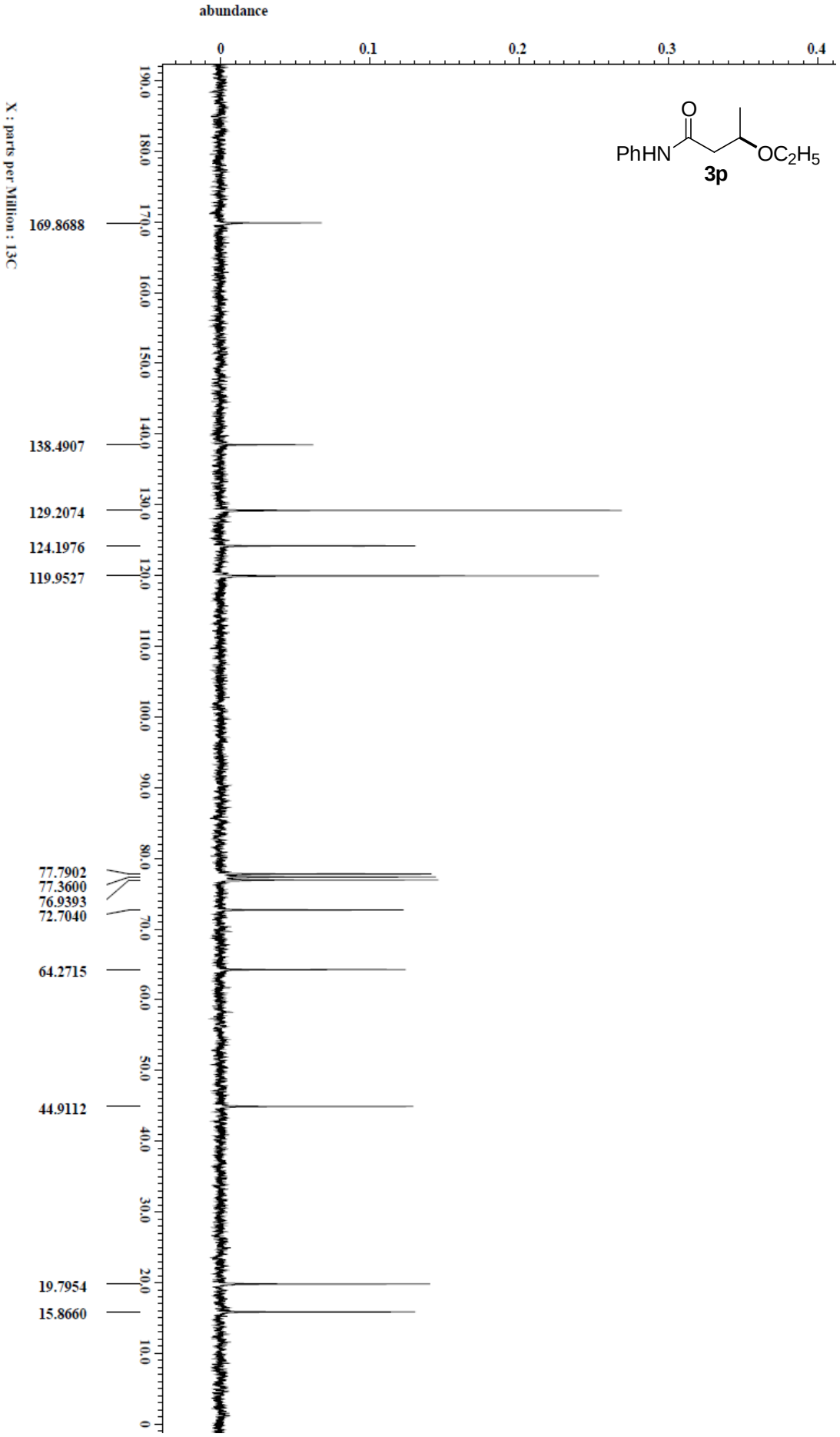

abundance
X : parts per Million : 1H
Me
O
N
H
OEt
3n
8.4114
7.4008
7.3722
7.2600
7.1169
7.0894
3.7507
3.7313
3.5974
3.5745
2.6302
2.6119
2.5936
2.3029
2.2479
1.2956
1.2728
1.2487
0.0000
0.96
1.9
2.09
1.89
2.0
2
3.08
3.0

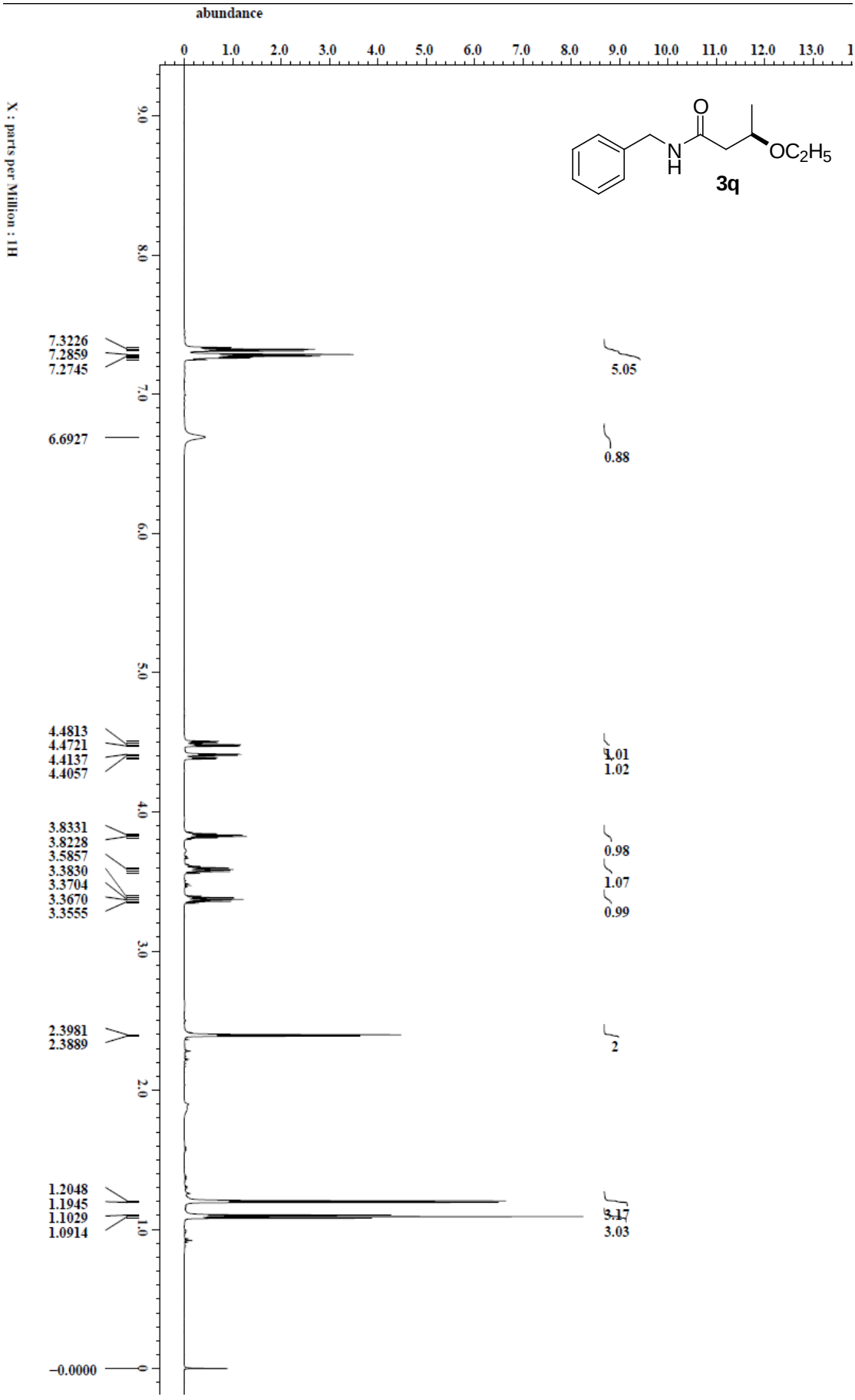

abundance
0
0.1
0.2
X : parts per Million : 13C
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.1173
135.9667
133.8538
129.7236
120.0769
77.7807
77.3600
76.9393
66.9676
66.7764
38.2857
21.1434
15.4835
Me
O
N
H
OEt
3n

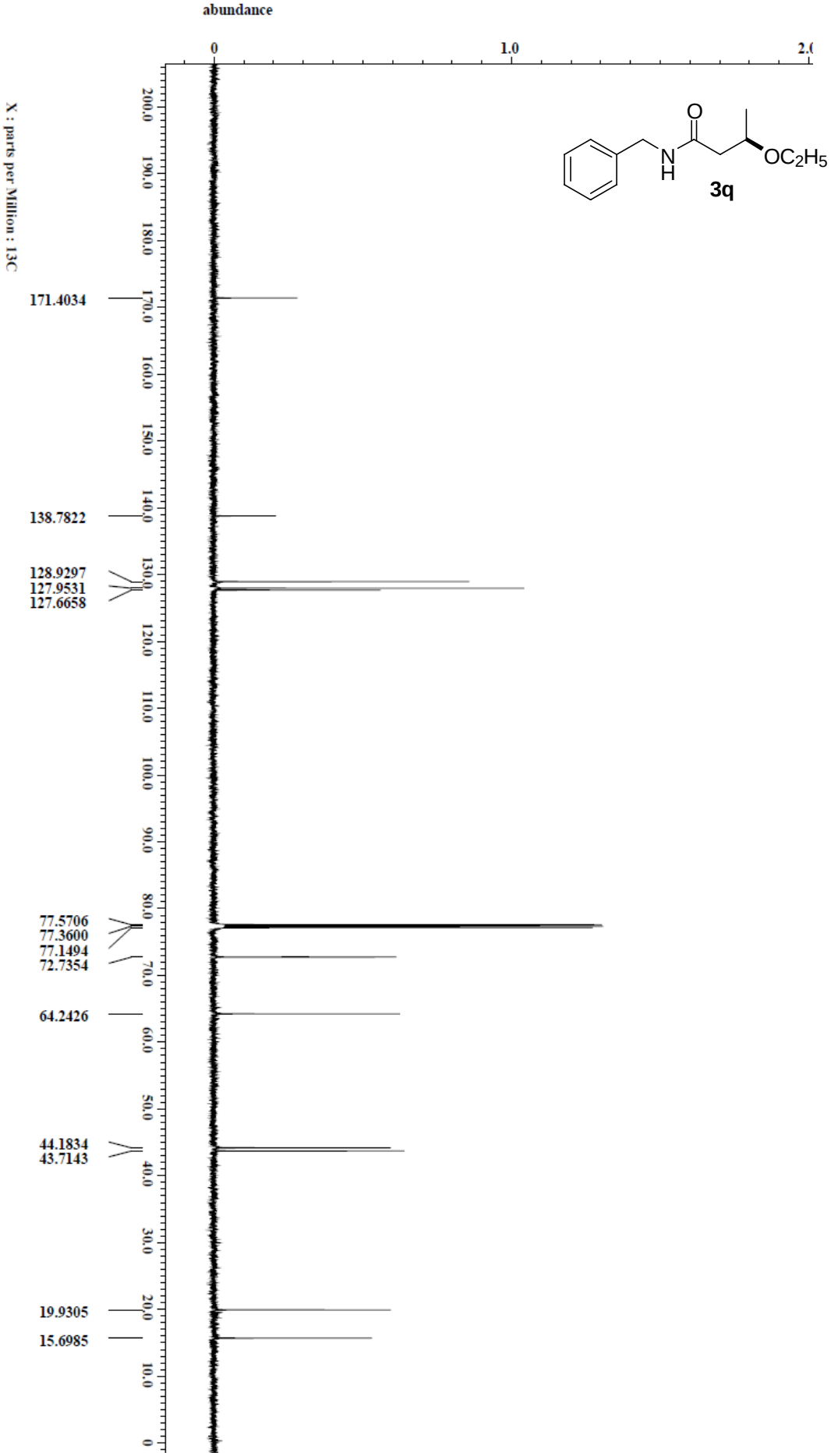

abundance
X : parts per Million : 1H
3o
7.2875
6.3752
3.6867
3.6683
3.6489
3.5367
3.5127
3.4898
3.2609
3.2414
2.4665
2.4471
2.4276
2.0373
1.4856
1.4628
1.3666
1.3391
1.2350
1.2121
1.1892
0.9511
0.9271
0.9031
−0.0000
0.91
1.93
1.93
2.0
2
2.1
1.98
2.85
2.92

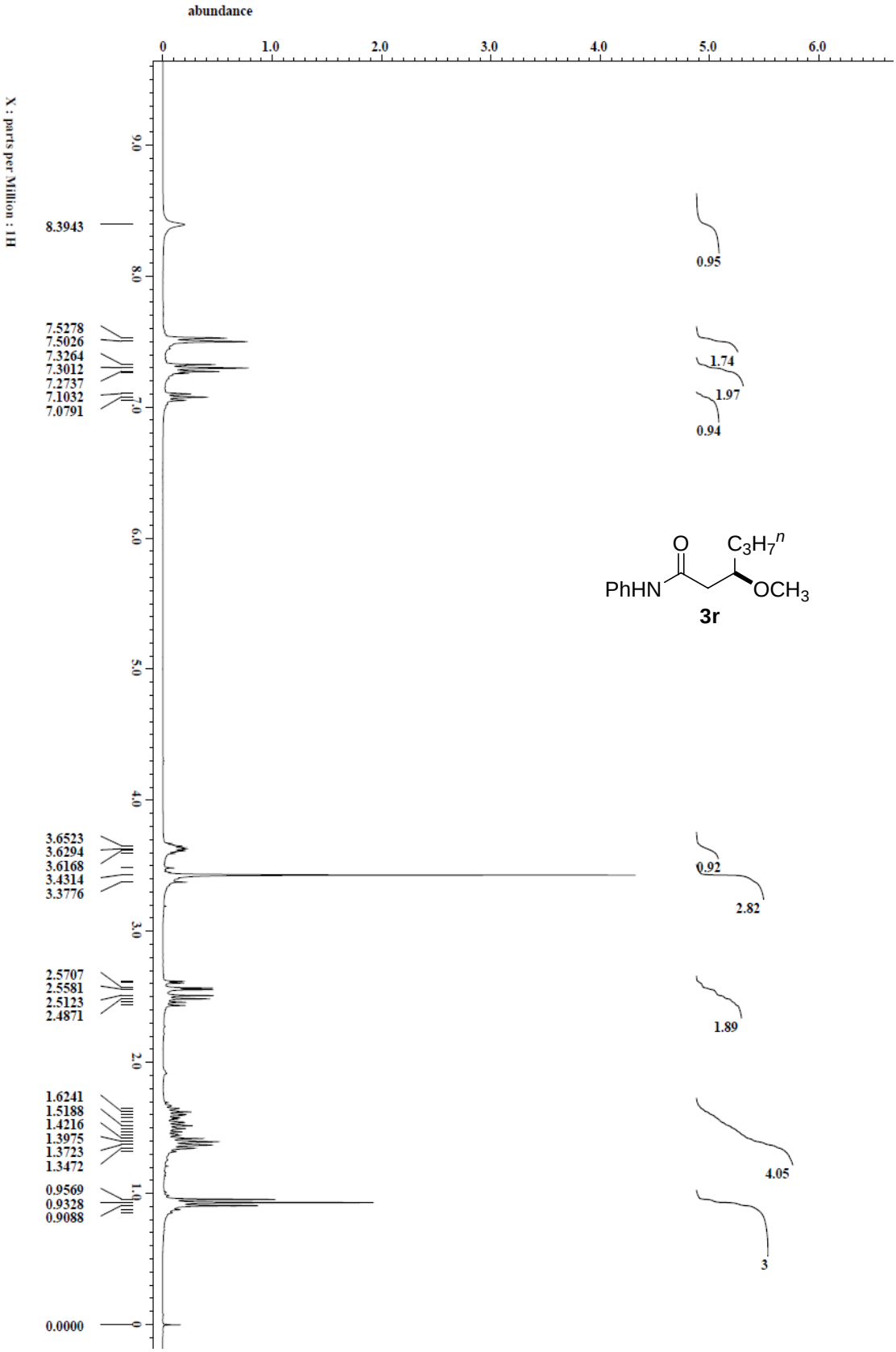

abundance
0
0.1
0.2
X : parts per Million : 13C
171.8669
77.7807
77.3600
76.9393
66.9293
66.7573
39.3278
37.3965
31.8800
20.3308
15.3784
14.0112
O
N
H
OEt
3o

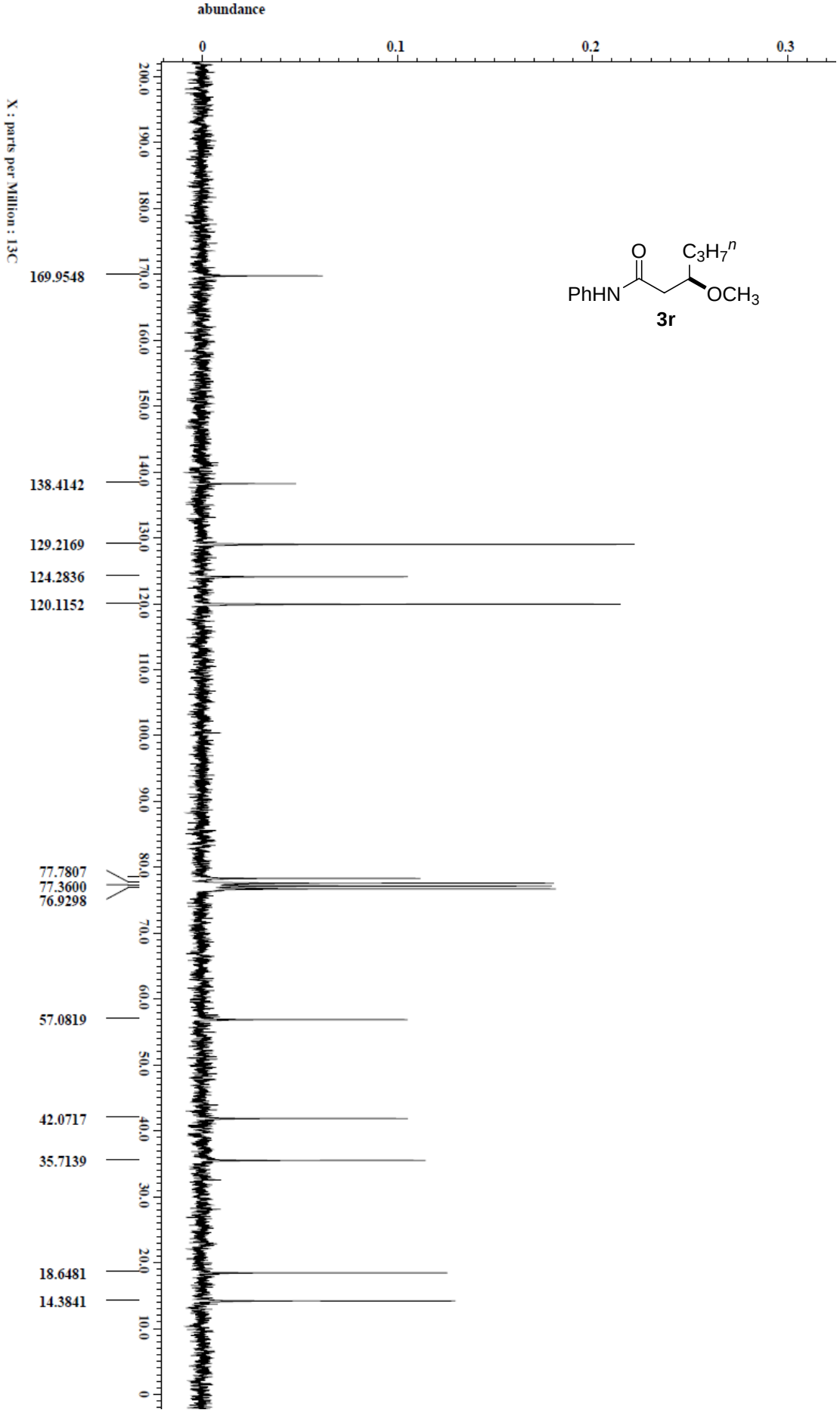

abundance
X : parts per Million : 1H
PhHN
O
OC2H5
3p
8.6426
7.5244
7.4992
7.3252
7.3000
7.2726
7.0734
3.8938
3.8755
3.6809
3.6580
3.5070
3.4829
3.4760
2.5306
2.5123
2.1060
1.2670
1.2602
1.2396
0.0000
0.96
2
2.17
1.06
1.0
1.02
1.03
2.03
6.33

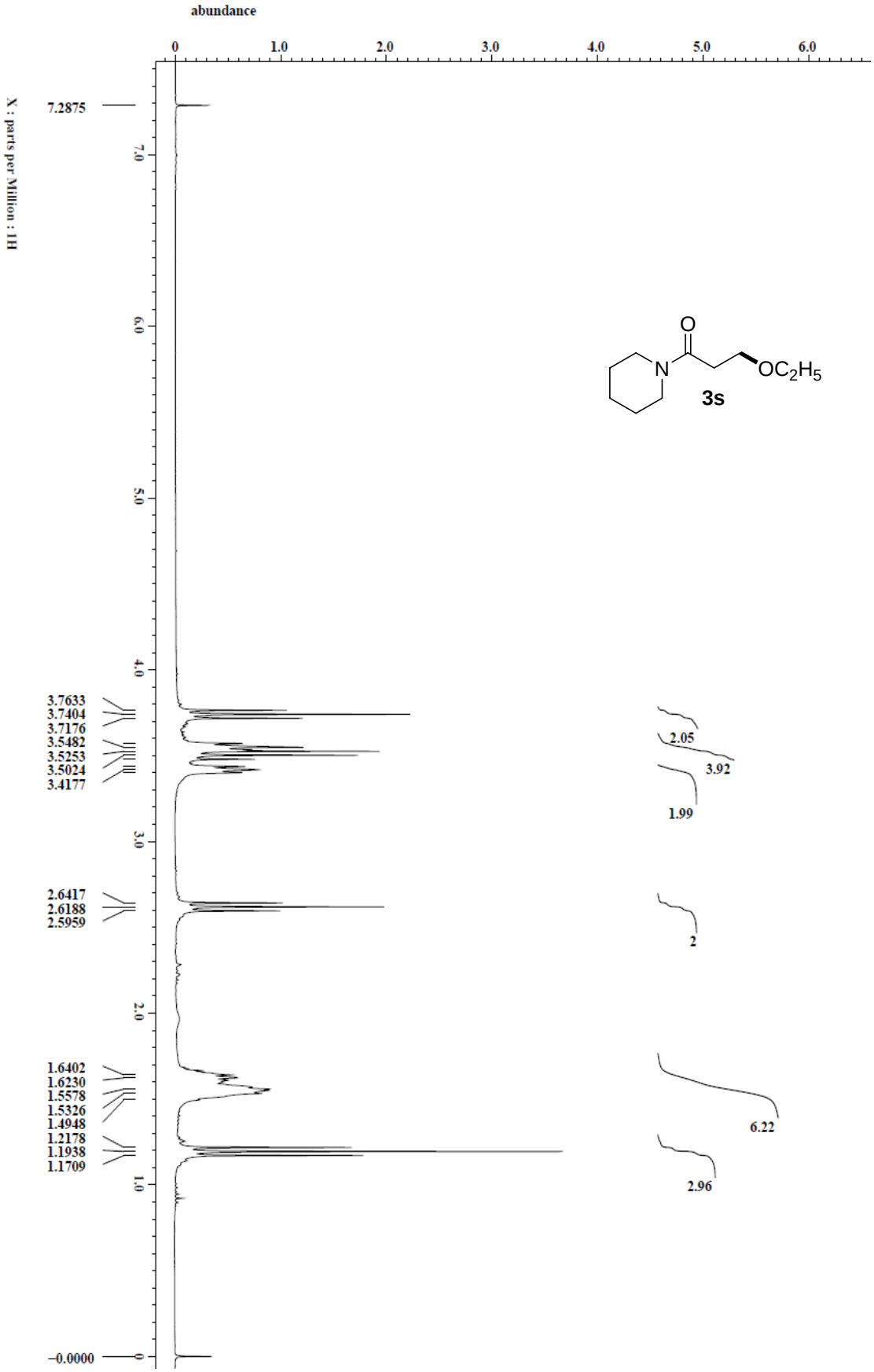

abundance
0
0.1
0.2
0.3
0.4
X : parts per Million : 13C
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
169.8688
138.4907
129.2074
124.1976
119.9527
77.7902
77.3600
76.9393
72.7040
64.2715
44.9112
19.7954
15.8660
O
PhHN
OC2H5
3p

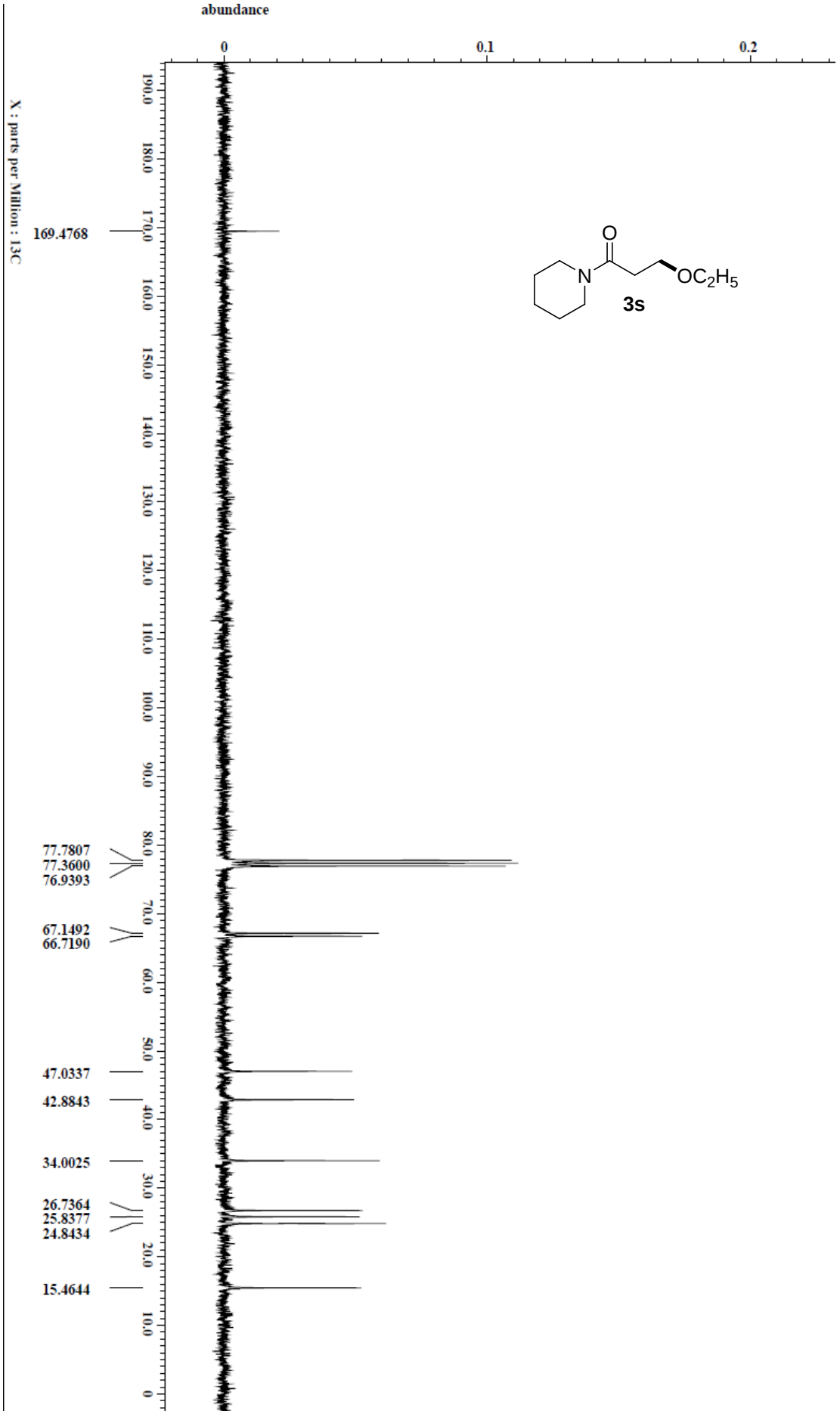

abundance
X : parts per Million : 1H
7.3226
7.2859
7.2745
6.6927
4.4813
4.4721
4.4137
4.4057
3.8331
3.8228
3.5857
3.3830
3.3704
3.3670
3.3555
2.3981
2.3889
1.2048
1.1945
1.1029
1.0914
-0.0000
5.05
0.88
1.01
1.02
0.98
1.07
0.99
2
3.17
3.03
O
N
H
OC2H5
3q

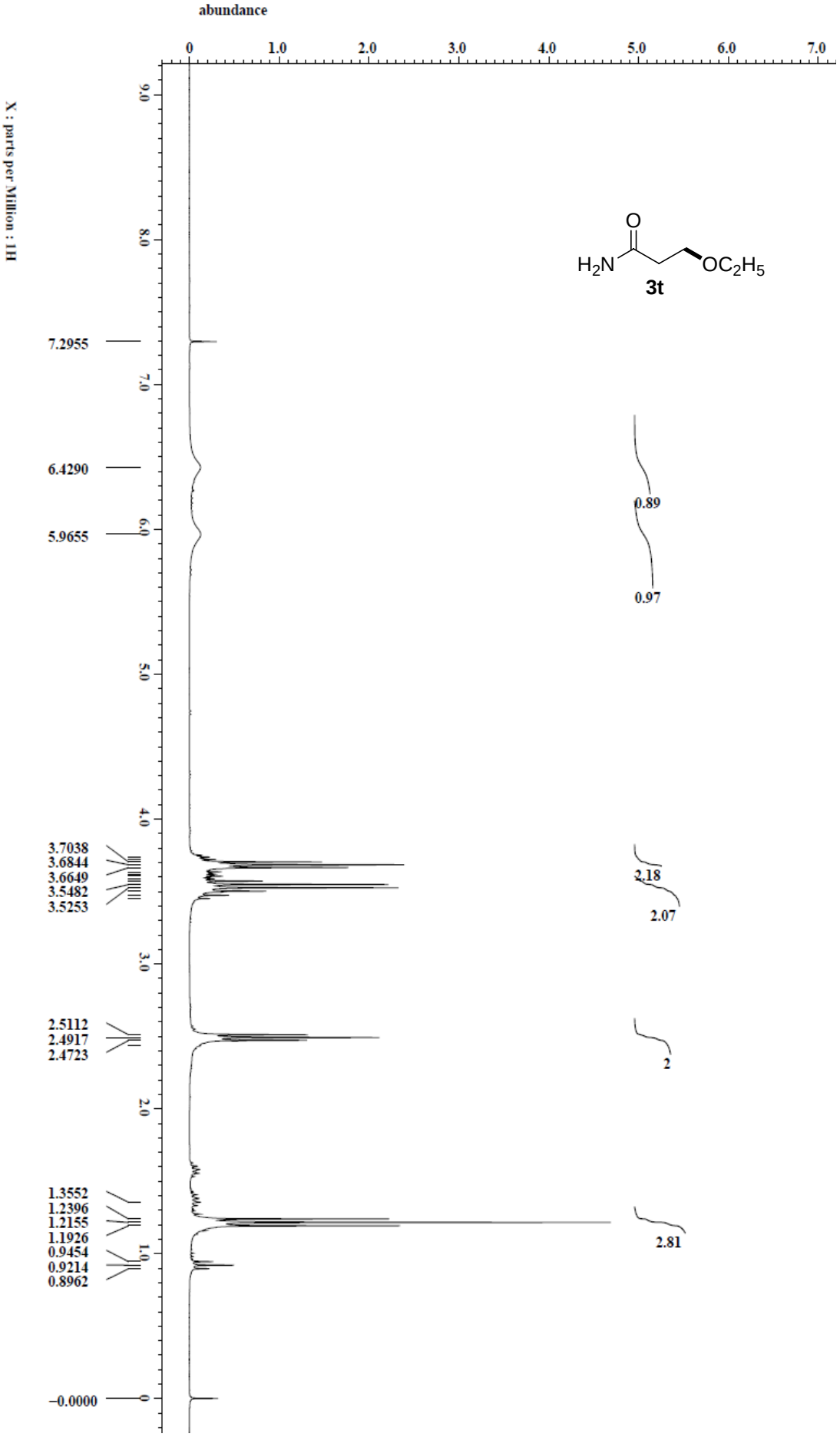

abundance
0
1.0
X : parts per Million : 13C
171.4034
138.7822
128.9297
127.9531
127.6658
77.5706
77.3600
77.1494
72.7354
64.2426
44.1834
43.7143
19.9305
15.6985
O
N
H
OC2H5
3q


abundance
X : parts per Million : 1H
8.3943
7.5278
7.5026
7.3264
7.3012
7.2737
7.1032
7.0791
3.6523
3.6294
3.6168
3.4314
3.3776
2.5707
2.5581
2.5123
2.4871
1.6241
1.5188
1.4216
1.3975
1.3723
1.3472
0.9569
0.9328
0.9088
0.0000
0.95
1.74
1.97
0.94
0.92
2.82
1.89
4.05
3
O
C3H7n
PhHN
OCH3
3r


abundance
0
0.1
0.2
0.3
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
169.9548
138.4142
129.2169
124.2836
120.1152
77.7807
77.3600
76.9298
57.0819
42.0717
35.7139
18.6481
14.3841
O
C3H7n
PhHN
OCH3
3r


abundance
X : parts per Million : 1H
7.2875
3.7633
3.7404
3.7176
3.5482
3.5253
3.5024
3.4177
2.6417
2.6188
2.5959
1.6402
1.6230
1.5578
1.5326
1.4948
1.2178
1.1938
1.1709
−0.0000
2.05
3.92
1.99
2
6.22
2.96
O
N
OC2H5
3s


abundance
0
0.1
0.2
X : parts per Million : 13C
169.4768
77.7807
77.3600
76.9393
67.1492
66.7190
47.0337
42.8843
34.0025
26.7364
25.8377
24.8434
15.4644
O
N
OC2H5
3s


abundance
X : parts per Million : 1H
O
H2N
OC2H5
3t
7.2955
6.4290
5.9655
3.7038
3.6844
3.6649
3.5482
3.5253
2.5112
2.4917
2.4723
1.3552
1.2396
1.2155
1.1926
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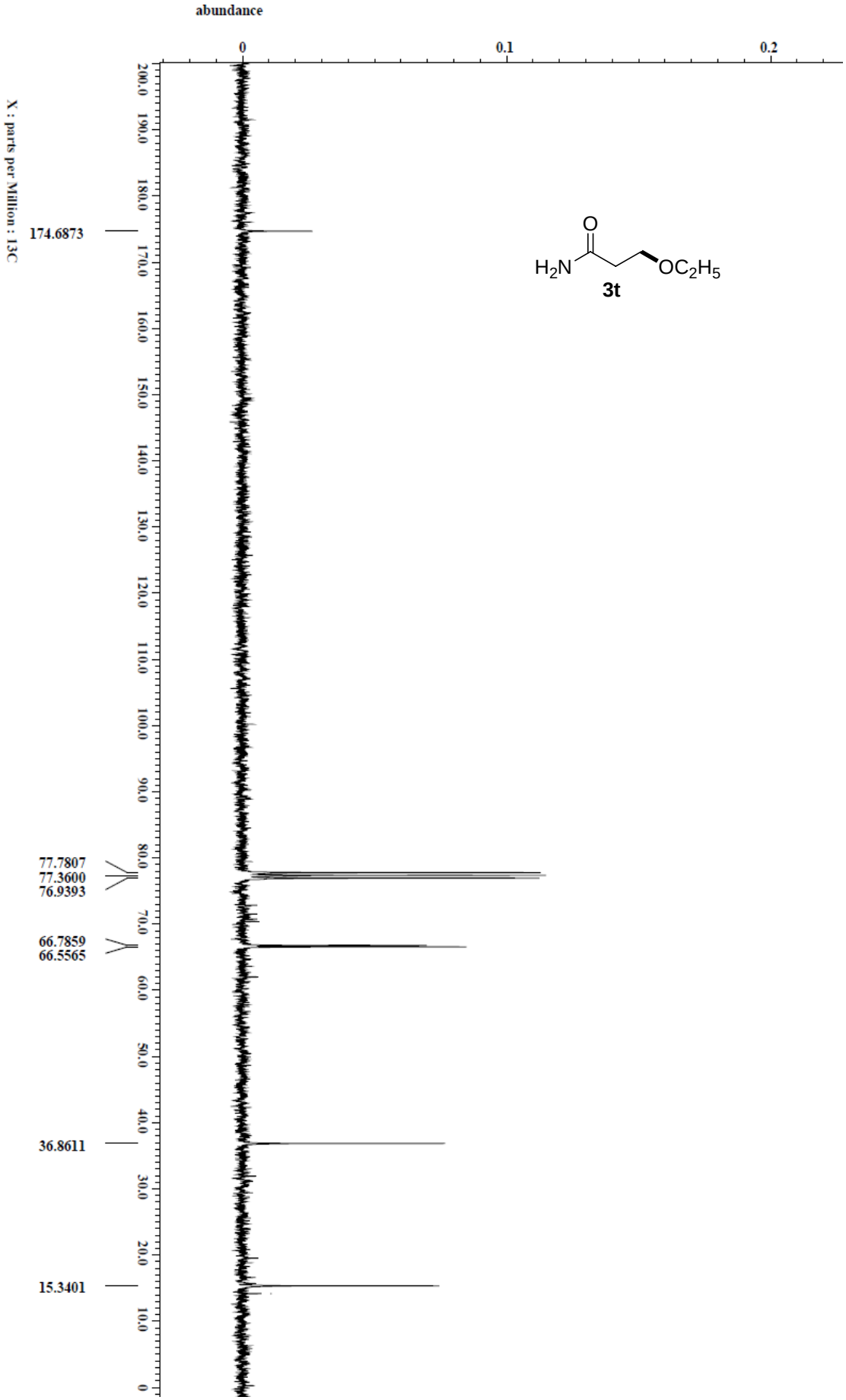
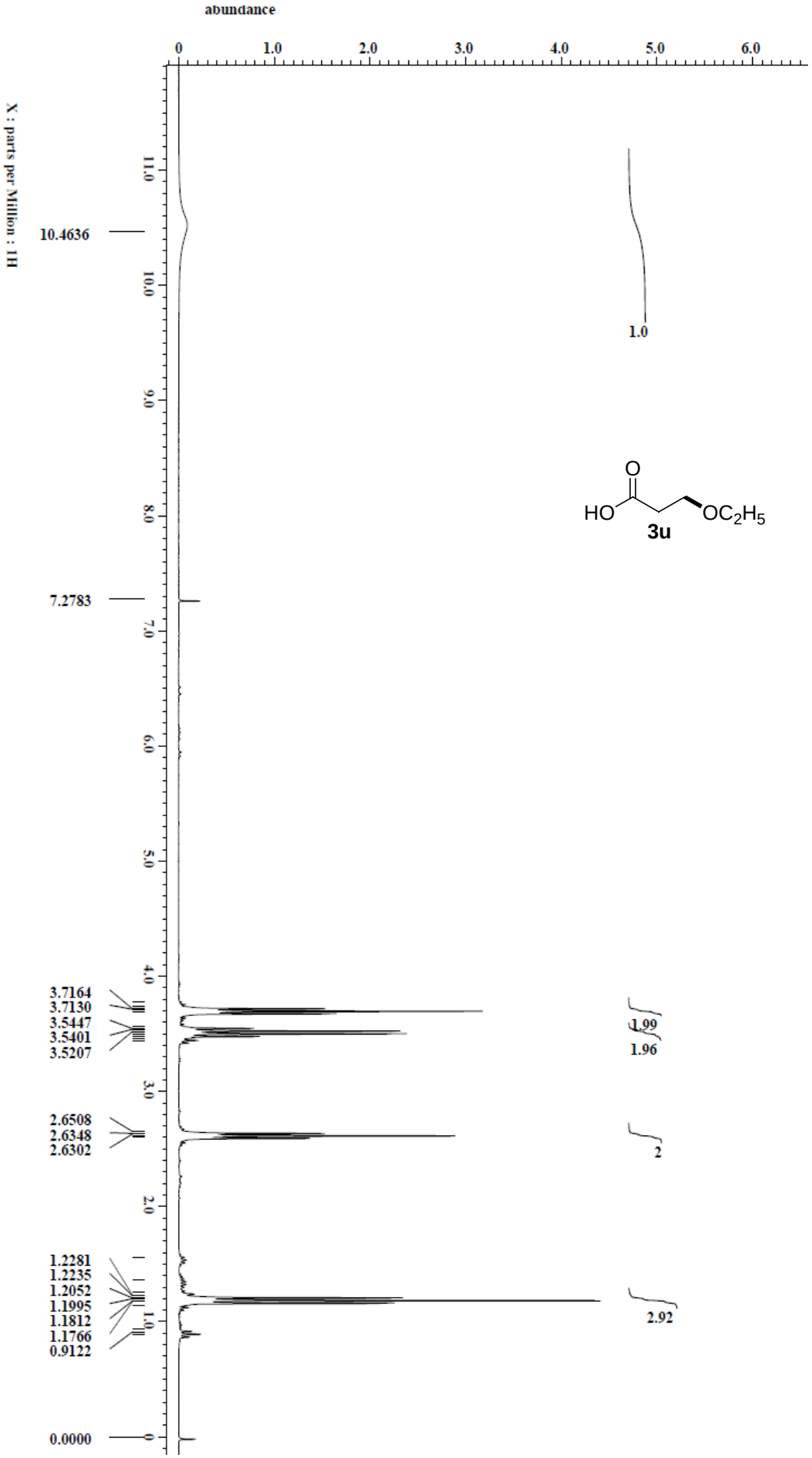
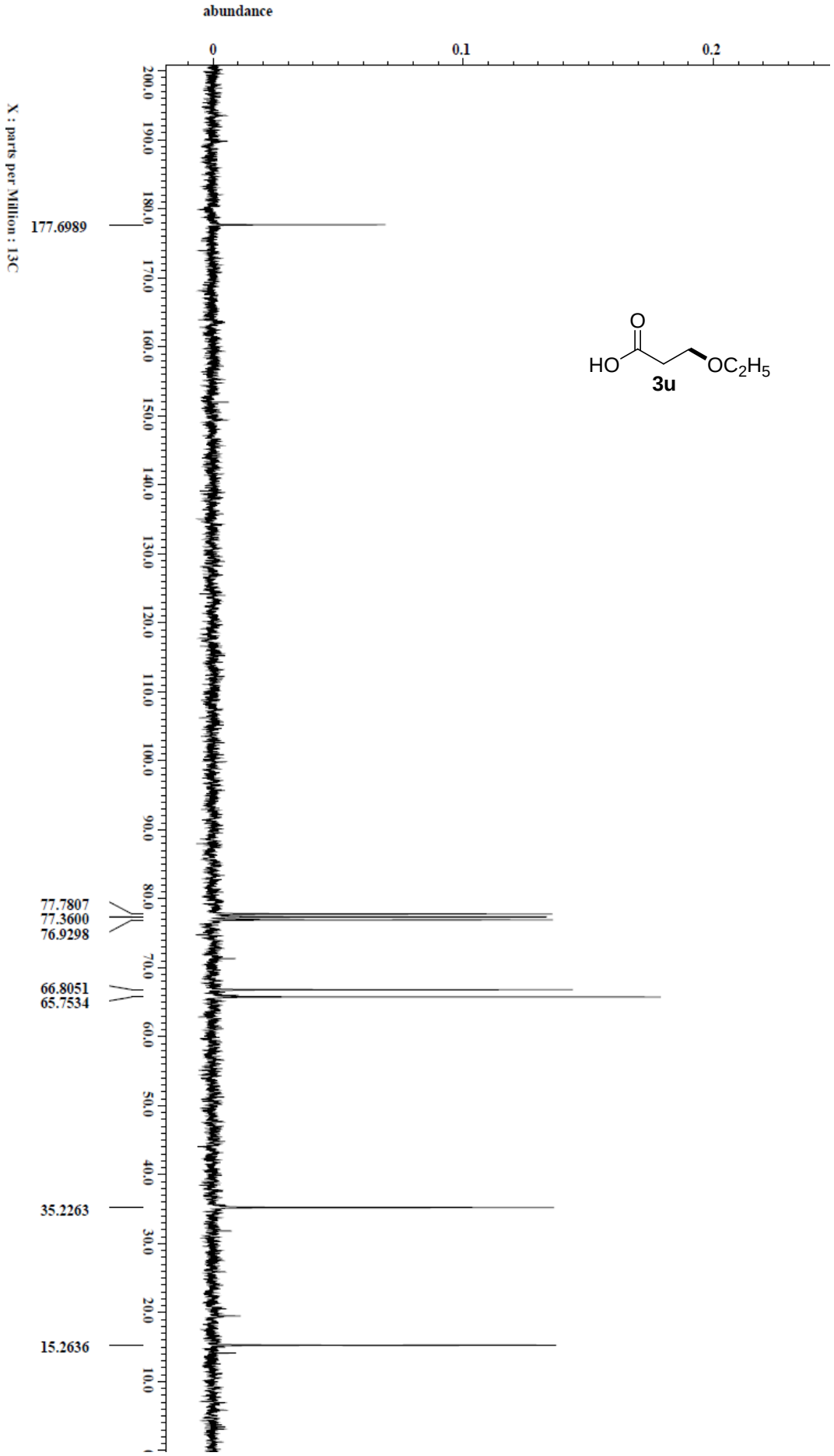
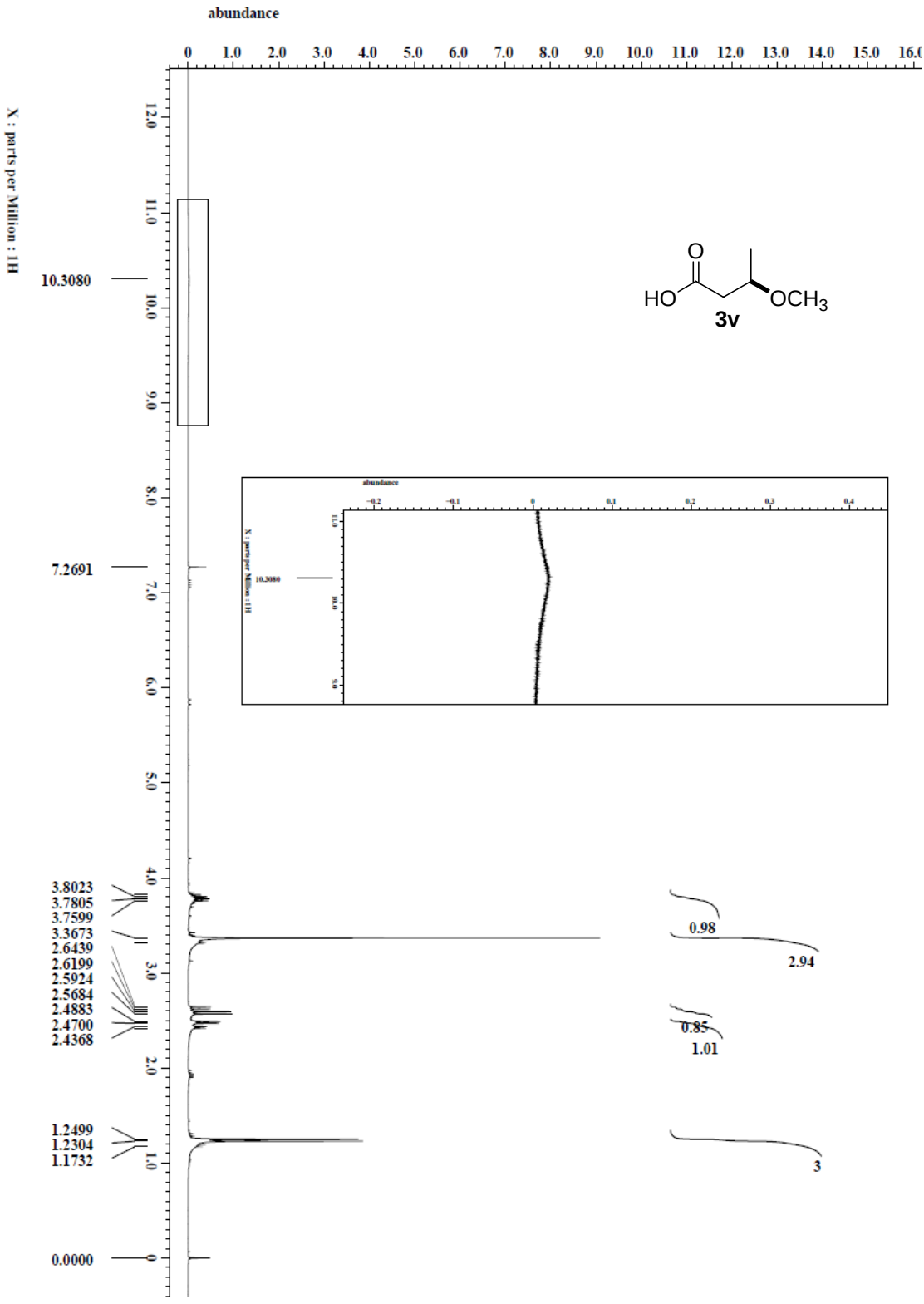
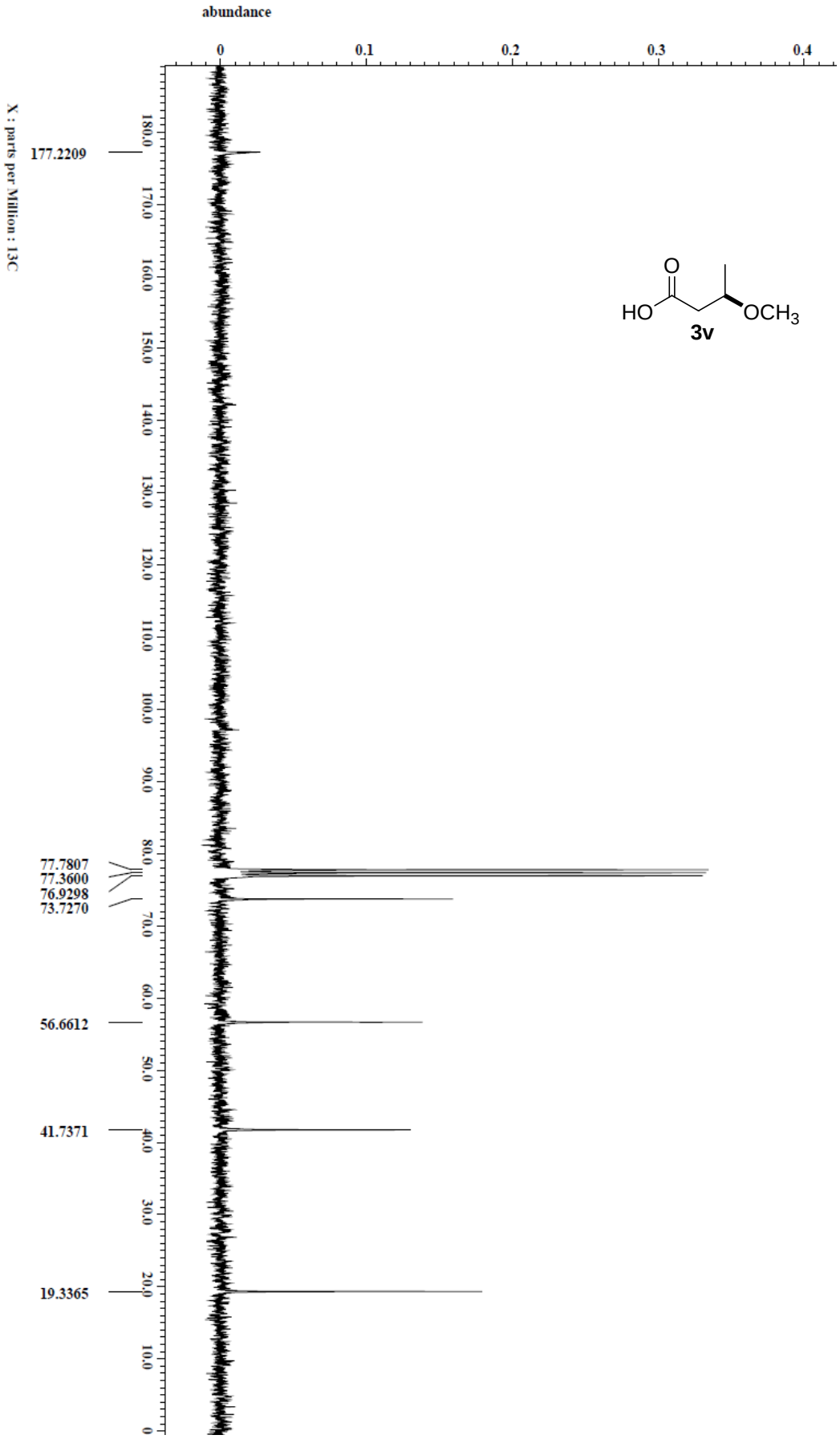
0.9214
0.8962
-0.0000
0.89
0.97
2.18
2.07
2
2.81

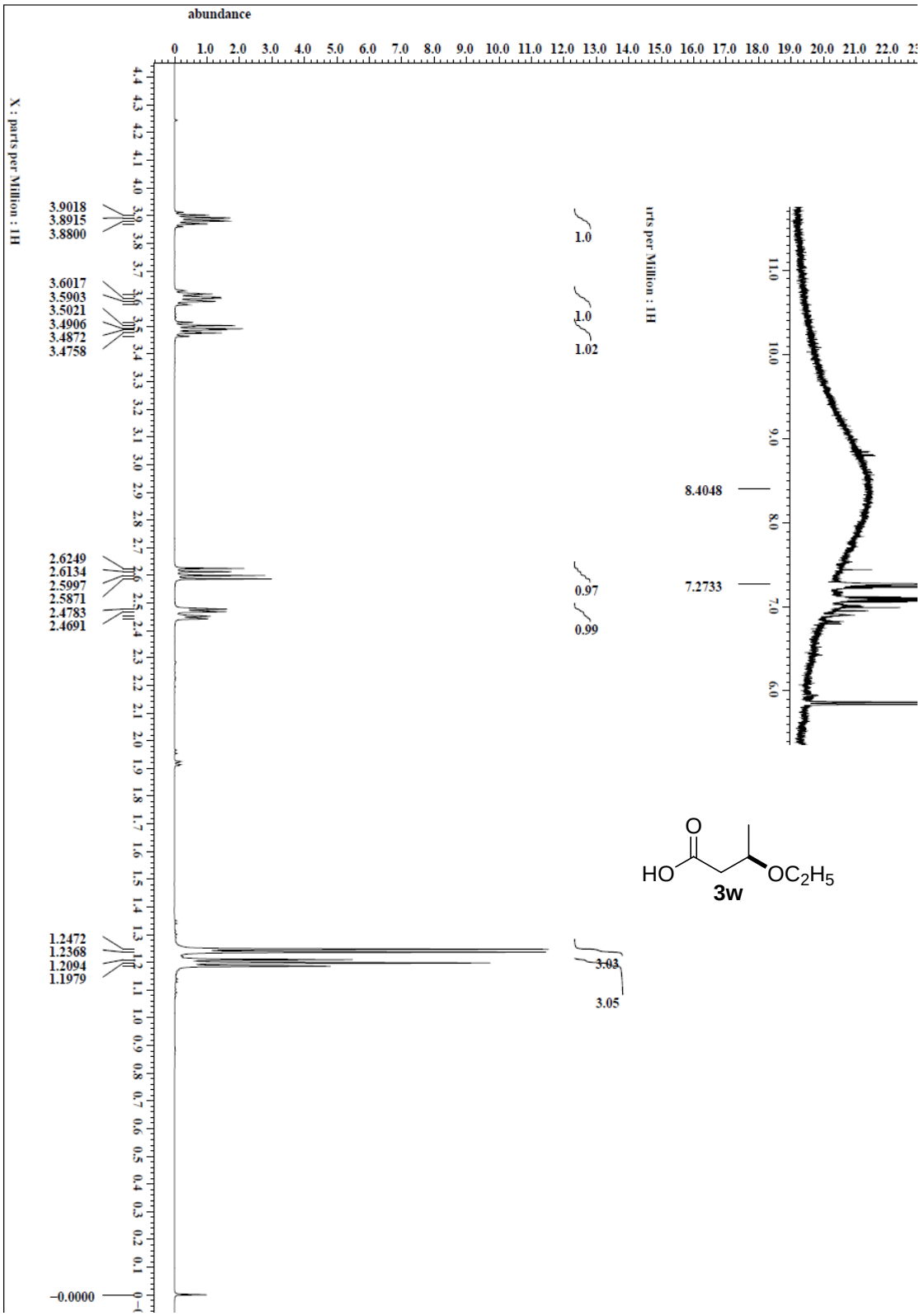

abundance
0
0.1
0.2
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
174.6873
77.7807
77.3600
76.9393
66.7859
66.5565
36.8611
15.3401
O
H2N
OC2H5
3t

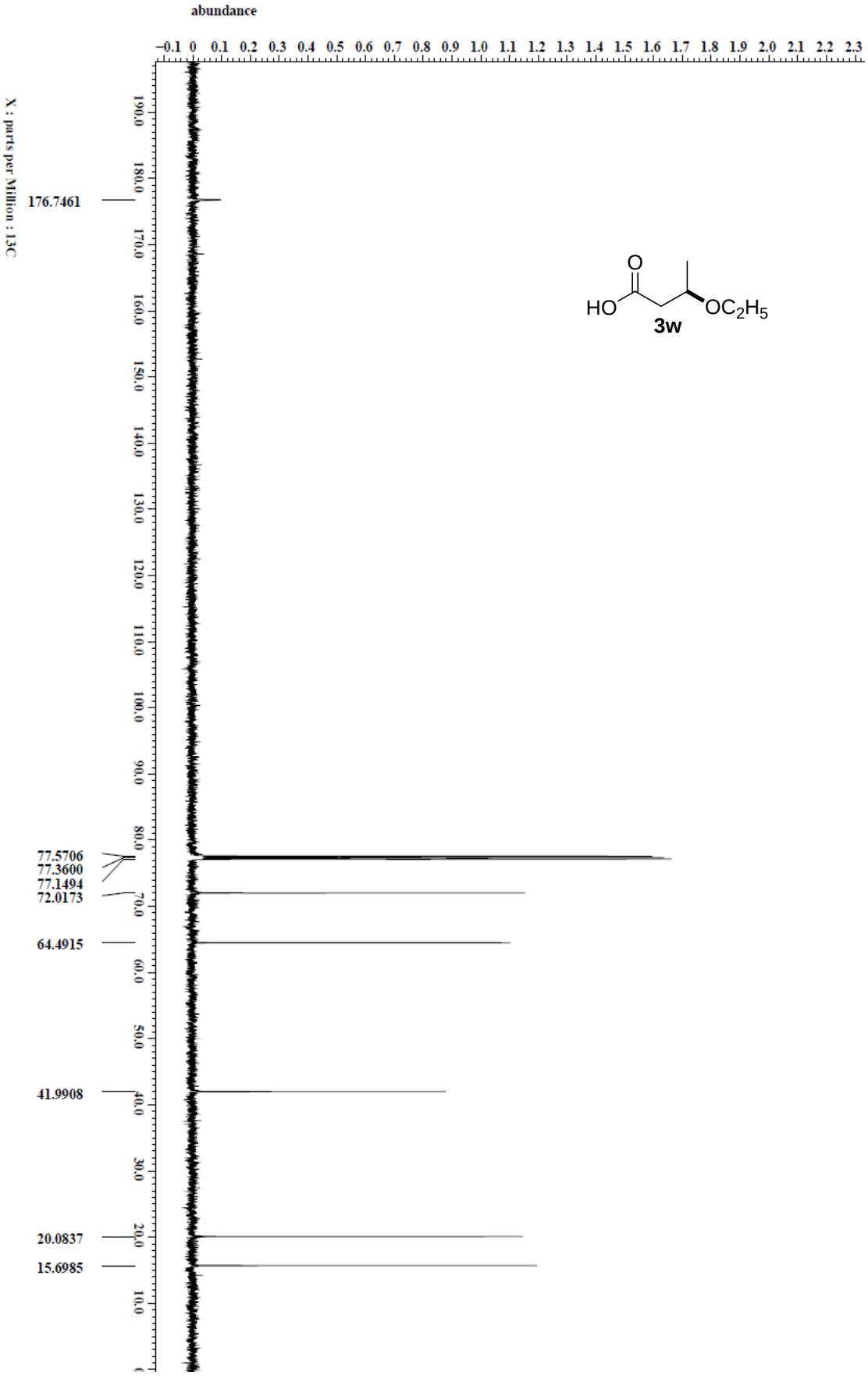

abundance
X : parts per Million : 1H
10.4636
7.2783
3.7164
3.7130
3.5447
3.5401
3.5207
2.6508
2.6348
2.6302
1.2281
1.2235
1.2052
1.1995
1.1812
1.1766
0.9122
0.0000
1.0
1.99
1.96
2
2.92
HO
O
OC2H5
3u

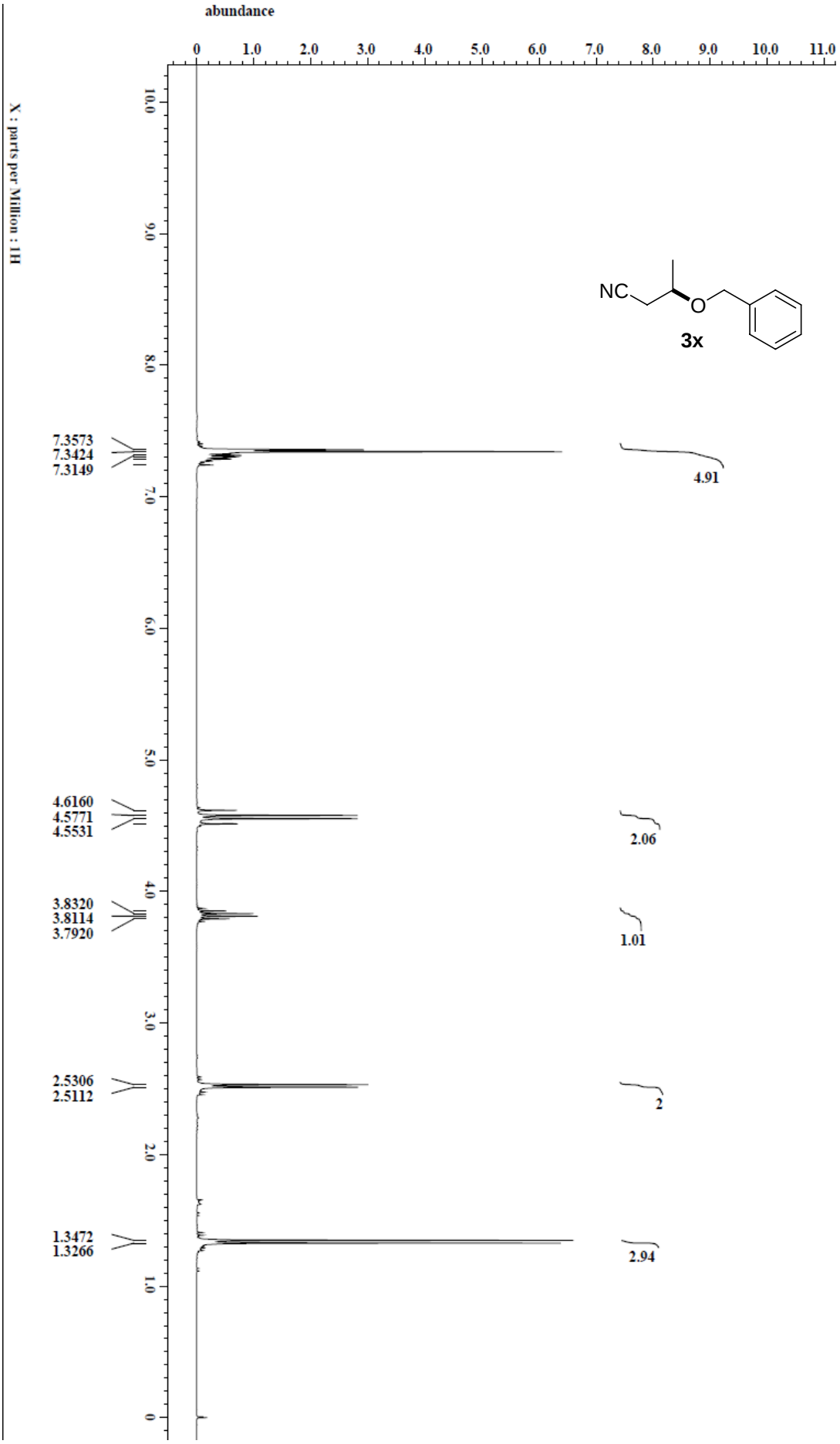

abundance
0
0.1
0.2
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
177.6989
77.7807
77.3600
76.9298
66.8051
65.7534
35.2263
15.2636
O
HO
OC2H5
3u

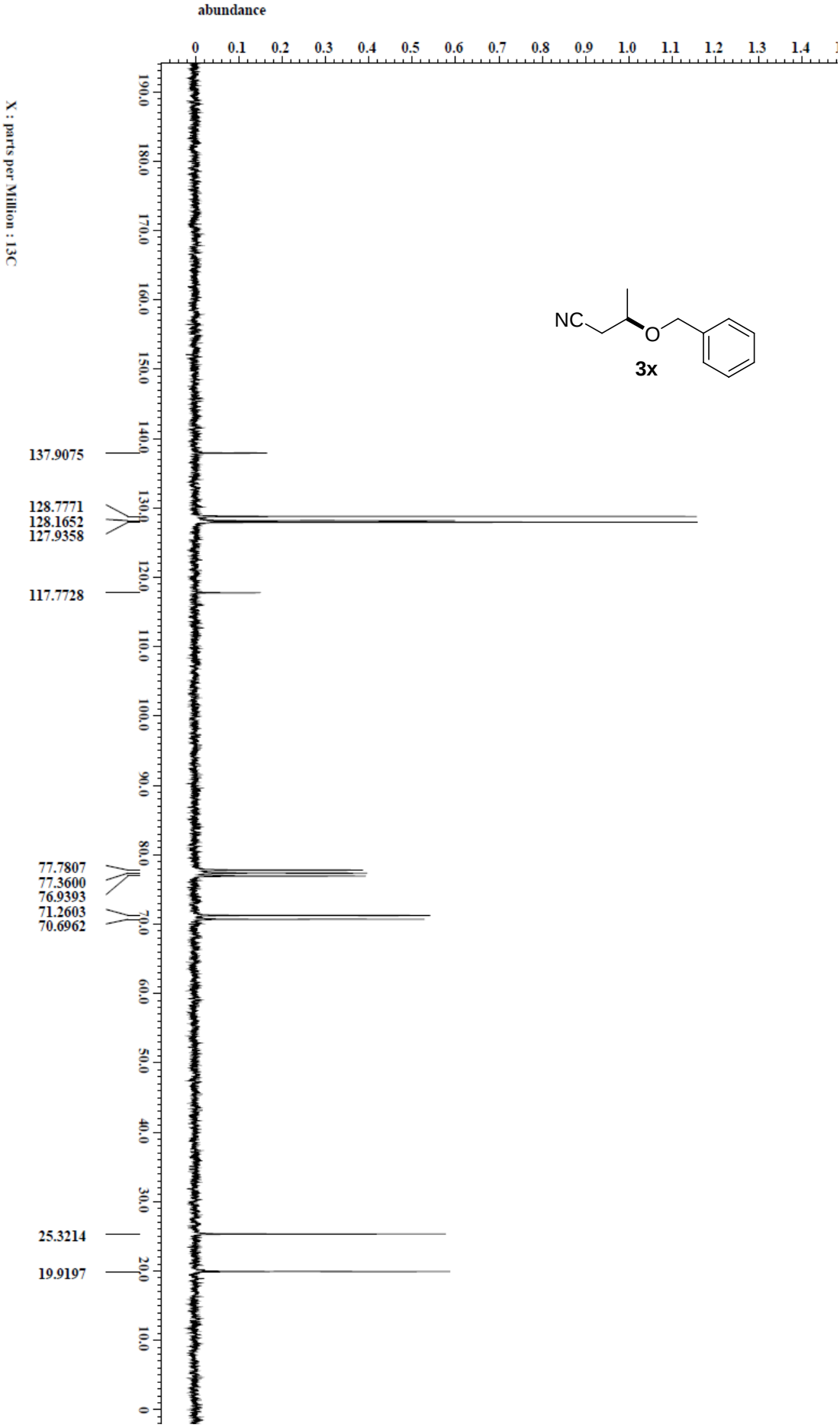

abundance
X : parts per Million : 1H
10.3080
7.2691
3.8023
3.7805
3.7599
3.3673
2.6439
2.6199
2.5924
2.5684
2.4883
2.4700
2.4368
1.2499
1.2304
1.1732
0.0000
0.98
2.94
0.85
1.01
3
HO
O
OCH3
3v


abundance
0
0.1
0.2
0.3
0.4
X : parts per Million : 13C
177.2209
77.7807
77.3600
76.9298
73.7270
56.6612
41.7371
19.3365
HO
O
OCH3
3v


abundance
X : parts per Million : 1H
3.9018
3.8915
3.8800
3.6017
3.5903
3.5021
3.4906
3.4872
3.4758
2.6249
2.6134
2.5997
2.5871
2.4783
2.4691
1.2472
1.2368
1.2094
1.1979
−0.0000
1.0
1.0
1.02
0.97
0.99
3.03
3.05
8.4048
7.2733
HO
O
OC2H5
3w


abundance
X : parts per Million : 13C
176.7461
77.5706
77.3600
77.1494
72.0173
64.4915
41.9908
20.0837
15.6985
HO
O
OC2H5
3w


abundance
X : parts per Million : 1H
NC
O
3x
7.3573
7.3424
7.3149
4.91
4.6160
4.5771
4.5531
2.06
3.8320
3.8114
3.7920
1.01
2.5306
2.5112
2
1.3472
1.3266
2.94


abundance
X : parts per Million : 13C
NC
O
3x
137.9075
128.7771
128.1652
127.9358
117.7728
77.7807
77.3600
76.9393
71.2603
70.6962
25.3214
19.9197