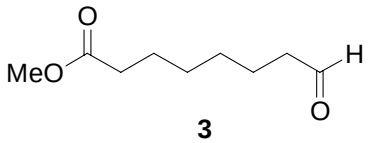
Supporting Information for Regio- and Stereospecific Syntheses and Nitric Oxide Donor Properties of (*E*)-9- and (*E*)-10-Nitrooctadec-9-enoic Acids

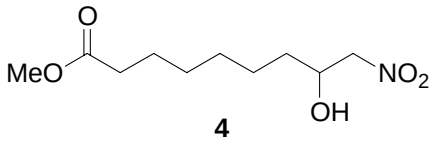
Michael J. Gorczynski, Jinming Huang, and S. Bruce King
Department of Chemistry, Wake Forest University, Winston-Salem, NC 27109

General. Melting points (mp) were determined on a Mel-Temp capillary melting point apparatus and are uncorrected. Analytical TLC was performed on silica gel plates with QF-254 indicator. Visualization was accomplished with UV light, iodine, $KMnO_4$, bromocresol green, and/or dinitrophenylhydrazine. Solvents for extraction and purification were technical grade and were used as received. All reactions were performed in flame-dried glassware under an inert atmosphere of dry argon. ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ using a Bruker Avance 300 MHz NMR spectrometer. Chemical shifts are given in ppm (δ); multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and br (broadened). Mass spectra were performed by HT Laboratories (San Diego, CA). Data are reported in the form *m/z*. Elemental combustion analyses were performed by Atlantic Microlab, Inc. (Atlanta, GA).



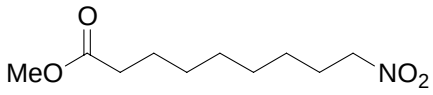
3

Methyl 8-oxooctanoate (3). Ozone was bubbled into a mixture of *cis*-cyclooctene (3.31 g, 3.90 mL, 30.00 mmol) and anhydrous Na_2CO_3 (0.82 g, 7.74 mmol) in CH_2Cl_2 (90 mL) and methanol (18 mL) at -78 ºC until a faint blue color appeared. Argon was then bubbled into the mixture until the blue color was discharged. The cooling bath was removed and the mixture slowly warmed to room temperature. After filtration, benzene (30 mL) was added and the mixture concentrated to ~20 mL with the resulting viscous liquid being diluted with CH_2Cl_2 (80 mL). After cooling to 0 ºC, anhydrous Et_3N (4.50 g, 6.2 mL, 44.48 mmol) and anhydrous Ac_2O (8.53 g, 7.90 mL, 83.57 mmol) were sequentially added dropwise and the mixture was stirred at 0 ºC for 0.5 h and then at room temperature overnight. The organic phase was washed with 0.1 M aqueous HCl (2 x 60 mL), 10% aqueous NaOH (2 x 60 mL), water (60 mL), and dried over $MgSO_4$. The solution was filtered and concentrated in vacuo to give **3** as a crude oil, which was purified by column chromatography (silica gel, 20% EtOAc: 80% hexanes, R_f = 0.25) to give a colorless oil (4.85 g, 94%): ^{1}H NMR 9.75 (t, *J* = 1.8 Hz, 1H), 3.65 (s, 3H), 2.41 (td, *J* = 7.2, 1.8 Hz, 2H), 2.27 (t, *J* = 7.5 Hz, 2H), 1.68 – 1.58 (m, 4H), 1.38 – 1.30 (m, 4H).



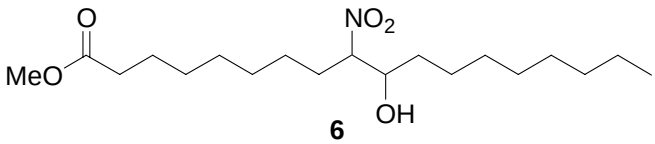
4

Methyl 8-hydroxy-9-nitrononanoate (4). Powdered *t*-BuOK (81 mg, 0.73 mmol) was added to a solution of **3** (2.50 g, 14.50 mmol) and nitromethane (1.77 g, 1.57 mL, 29.00 mmol) in *t*-BuOH:THF (1:1, 10 mL) at 0 ºC. After stirring at room temperature for 15 h, the solution was diluted with Et_2O (50 mL) and water (50 mL). The organic layer was washed with saturated aqueous $NaHCO_3$ (50 mL) and brine (50 mL). The combined aqueous layers were back-extracted with Et_2O (2 × 100 mL) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated in vacuo. The crude residue was purified by column chromatography (silica gel, 20% EtOAc: 80% hexanes, R_f = 0.25) to give **4** as a white solid (3.17 g, 94%): mp 34 - 36 ºC; ^{1}H NMR 4.43 – 4.28 (m, 3H), 3.65 (s, 3H), 2.29 (t, *J* = 7.5 Hz, 2H), 1.68 – 1.28 (m, 10H); ^{13}C NMR 174.7, 81.1, 69.0, 51.9, 34.3, 34.0, 29.3, 29.3, 25.3, 25.1.



5

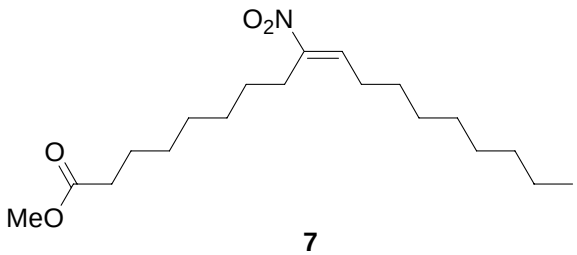
Methyl 9-nitrononanoate (5). A solution of **4** (2.31 g, 9.91 mmol), DMAP (61 mg, 0.50 mmol), Ac_2O (1.11 g, 1.03 mL, 10.91 mmol), and Et_2O (25 mL) was stirred for 4 h at room temperature and concentrated. A solution of $NaBH_4$ (0.75 g, 19.82 mmol) in EtOH (20 mL) was added dropwise to the crude nitroacetates at 0 ºC and the solution was stirred for 2 h at room temperature, and then acidified with 1 M aq. HCl. The mixture was extracted with Et_2O (3 × 50 mL), dried over $MgSO_4$, filtered, and concentrated in vacuo to give a crude residue that was purified by column chromatography (silica gel, 30% EtOAc: 70% hexanes, R_f = 0.49) to give **5** as a pale yellow oil (1.79 g, 83%): ^{1}H NMR 4.36 (t, *J* = 7.2 Hz, 2H), 3.65 (s, 3H), 2.28 (t, *J* = 7.5 Hz, 2H), 2.02 – 1.96 (m, 2H), 1.63 – 1.56 (m, 2H), 1.40 – 1.27 (m, 8H); ^{13}C NMR 174.6, 76.1, 51.9, 34.4, 29.28, 29.26, 29.01, 27.7, 26.5, 25.2.



6

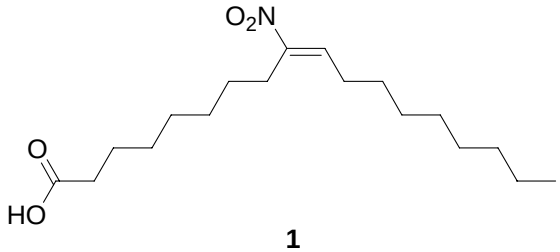
Methyl 10-hydroxy-9-nitrooctadecanoate (6). Powdered *t*-BuOK (41 mg, 0.36 mmol) was added to a solution of **5** (1.57 g, 7.23 mmol) and nonanal (1.02 g, 1.24 mL, 7.23 mmol) in *t*-BuOH:THF (1:1, 10 mL) at 0 ºC. After stirring at room temperature for 22 h, the solution was diluted with Et_2O (25 mL) and water (25 mL). The organic layer was washed with saturated aqueous $NaHCO_3$ (25 mL) and brine (25 mL). The combined aqueous layers were back-extracted with Et_2O (2 × 50 mL) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated in vacuo. The crude residue was purified by column chromatography (silica gel, 20% EtOAc: 80% hexanes, R_f = 0.12) to give **6** as a mixture of diastereomers (2.33 g, 90%): ^{1}H NMR 4.47 – 4.34 (m, 1H), 4.08 – 3.80 (m, 1H), 3.66 (s, 3H), 2.30 (t, *J* = 7.5 Hz, 2H), 1.80 – 1.20 (m, 26H), 0.87 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR 174.6, 93.2, 92.7, 72.77, 72.46, 51.9,

34.39, 34.02, 33.6, 32.2, 30.8, 29.80, 29.75, 29.70, 29.58, 29.27, 29.23, 29.18, 29.13, 26.28, 26.01, 25.68, 25.19, 23.0, 14.6; ESI MS *m/z* 358 ($M-H^-$).



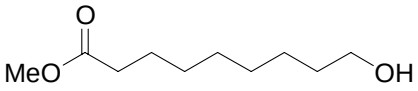
7

(*E*)-Methyl 9-nitrooctadec-9-enoate (7). A solution of **6** (0.36 g, 1.00 mmol), DMAP (12 mg, 0.10 mmol), and Ac_2O (0.11 g, 0.10 mL, 1.10 mmol) in Et_2O (2 mL) was stirred for 5 h at room temperature and concentrated. DMAP (0.15 g, 1.20 mmol) was added to a solution of the crude nitroacetates in CH_2Cl_2 (2 mL) and the solution was stirred at room temperature for 2 h, diluted with CH_2Cl_2 (50 mL) and washed with water (50 mL), 0.1 N aqueous HCl (50 mL), and brine (50 mL). The combined aqueous layers were back-extracted with CH_2Cl_2 (2 × 50 mL) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated in vacuo. The crude residue was purified by column chromatography (silica gel, 20% EtOAc: 80% hexanes, R_f = 0.55) to give **7** as a yellow oil (0.23 g, 68%): ^{1}H NMR 7.07 (t, *J* = 7.8 Hz, 1H), 3.66 (s, 3H), 2.56 (t, *J* = 7.2 Hz, 2H), 2.30 (t, *J* = 7.2 Hz, 2H), 2.20 (q, *J* = 7.5 Hz, 2H), 1.67 – 1.55 (m, 2H), 1.55 – 1.40 (m, 4H), 1.37 – 1.22 (m, 16H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR 174.6, 152.2, 136.9, 51.8, 34.4, 32.2, 29.72, 29.69, 29.54, 29.43, 29.37, 29.30, 28.91, 28.40, 28.24, 26.7, 25.3, 23.0, 14.5; ESI MS *m/z* 340 ($M-H^-$).



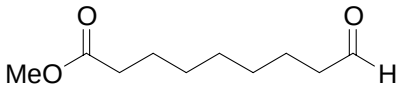
1

(*E*)-9-Nitrooctadec-9-enoic acid (1). A solution of **7** (0.34 g, 1 mmol) in 6 M aq. HCl (10 mL) was refluxed for 12 h. The solution was cooled to room temperature and extracted with EtOAc (3 × 20 mL). The combined organic layers were washed with water (30 mL) and brine (30 mL), dried over $MgSO_4$, filtered, and concentrated. The crude residue was purified by column chromatography (silica gel, 20% EtOAc: 80% hexanes, R_f = 0.23) to give **1** as a yellow oil (0.19 g, 58%): ^{1}H NMR 11.48 (bs, 1H), 7.07 (t, *J* = 8.1 Hz, 1H), 2.56 (t, *J* = 7.5 Hz, 2H), 2.34 (t, *J* = 7.2 Hz, 2H), 2.20 (q, *J* = 7.2, 7.5 Hz, 2H), 1.66 – 1.58 (m, 2H), 1.55 – 1.40 (m, 4H), 1.38 – 1.21 (m, 16H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR 180.5, 152.2, 136.9, 34.4, 32.2, 30.1, 29.72, 29.69, 29.53, 29.41, 29.28, 28.91, 28.40, 28.24, 26.7, 25.0, 23.0, 14.5; ESI MS *m/z* 326 ($M-H^-$). Anal. calcd. for $C_{18}H_{33}NO_4$: C, 66.02; H, 10.16; N, 4.28. Found: C, 66.13; H, 10.26; N, 4.10.



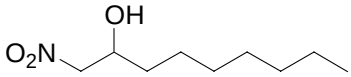
8

Methyl 9-hydroxynonanoate (8). BH_3·THF complex (50 mL, 50.00 mmol, 1.0 M solution in THF) was added dropwise over 20 minutes to a solution of *mono*-methyl azelate (11.89 g, 11.38 mL, 50.00 mmol, 85% tech) in anhydrous THF (25 mL) at -18 ºC. The solution was stirred for 10 minutes, allowed to warm to room temperature, stirred for 4 h, and quenched with water (100 mL) at 0 ºC. Solid K_2CO_3 (11.8 g, 85.38 mmol) and Et_2O (200 mL) were added to the mixture and the organic phase was separated. The aqueous phase was extracted with Et_2O (3 x 100 mL), and the combined organic layers were washed with brine (150 mL), dried over $MgSO_4$, filtered, and concentrated in vacuo to give **8** as an oil. TLC (30% EtOAc: 70% hexanes, R_f = 0.30) and ^{1}H NMR indicated **8** was pure and as such was used without further purification (8.97 g, 95%): ^{1}H NMR 3.54 (s, 3H), 3.47 (t, *J* = 6.6 Hz, 2H), 2.18 (t, *J* = 7.5 Hz, 2H), 1.53 – 1.38 (m, 4H), 1.28 – 1.12 (m, 8H).



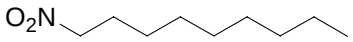
9

Methyl 9-oxononanoate (9). A solution of **8** (8.97 g, 47.70 mmol) in anhydrous CH_2Cl_2 (15 mL) was added dropwise to a stirring suspension of PCC (15.42 g, 71.60 mmol) and Celite (15.42 g, weight equivalent of PCC) in CH_2Cl_2 (80 mL). The mixture was stirred at room temperature for 4 h and diluted with Et_2O (150 mL). The suspension was filtered through Florisil and the filter cake was washed with Et_2O (2 x 100 mL). The solvent was removed and the crude product was purified by column chromatography (silica gel, 20% EtOAc: 80% hexanes, R_f = 0.44) to give **9** as a yellow oil (7.37 g, 83%): ^{1}H NMR 9.73 (t, *J* = 1.8 Hz, 1H), 3.64 (s, 3H), 2.39 (dt, *J* = 7.2, 1.8 Hz, 2H), 2.27 (t, *J* = 7.5 Hz, 2H), 1.67 – 1.52 (m, 4H), 1.38 – 1.23 (m, 6H).



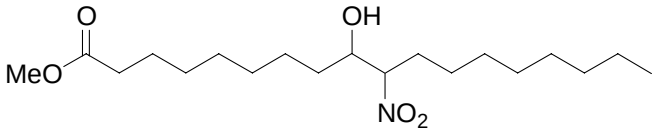
10

2-Hydroxy-1-nitrononane (10). Powdered *t*-BuOK (0.11 g, 1.00 mmol) was added to a solution of nitromethane (2.40 g, 2.13 mL, 39.40 mmol) and octanal (2.52 g, 3.07 mL, 19.70 mmol) in *t*-BuOH:THF (1:1, 10 mL) at 0 ºC. After stirring at room temperature for 18.5 h, the mixture was diluted with Et_2O (100 mL) and water (100 mL). The organic layer was washed with saturated aqueous $NaHCO_3$ (100 mL) and brine (100 mL). The combined aqueous layers were back-extracted with Et_2O (2 x 100 mL) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated in vacuo. The crude residue was purified by column chromatography (silica gel, 20% EtOAc: 80% hexanes, R_f = 0.30) to give **10** as an oil (3.50 g, 94%): ^{1}H NMR 4.46 – 4.29 (m, 3H), 1.60 – 1.24 (m, 12H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR 81.3, 69.4, 34.4, 32.4, 29.94, 29.76, 25.8, 23.3, 14.7.



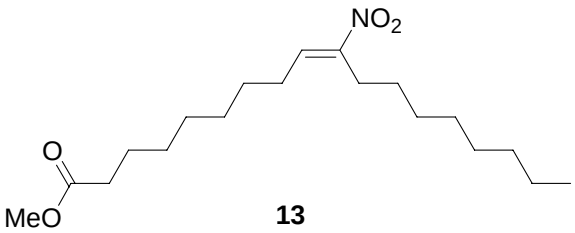
11

1-Nitrononane (11). A solution of **10** (3.72 g, 19.70 mmol), DMAP (0.12 g, 0.99 mmol), Ac_2O (2.51 g, 2.32 mL, 24.63 mmol), and Et_2O (40 mL) was stirred for 4 h at room temperature and concentrated. A solution of $NaBH_4$ (1.49 g, 39.40 mmol) in EtOH (40 mL) was added dropwise to the crude nitroacetates at 0 ºC and the solution was stirred for 2 h at room temperature, and then acidified with 1 M aq. HCl. The mixture was extracted with Et_2O (3 × 100 mL), dried over $MgSO_4$, filtered, and concentrated in vacuo to give a crude residue that was purified by column chromatography (silica gel, 20% EtOAc: 80% hexanes, R_f = 0.79) to give **11** as a pale yellow oil (2.19 g, 64%): ^{1}H NMR 4.36 (t, *J* = 6.9 Hz, 2H), 2.05 – 1.94 (m, 2H), 1.40 – 1.17 (m, 12H), 0.87 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR 76.1, 32.2, 29.60, 29.49, 29.22, 27.8, 26.6, 23.0, 14.4.



12

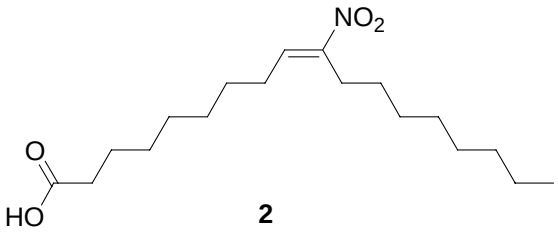
Methyl 9-hydroxy-10-nitrooctadecanoate (12). Powdered *t*-BuOK (22 mg, 0.20 mmol) was added to a solution of **9** (0.74 g, 4.00 mmol) and **11** (0.69 g, 4 mmol) in *t*-BuOH:THF (1:1, 4 mL) at 0 ºC. After stirring at room temperature for 21 h, the solution was diluted with Et_2O (25 mL) and water (25 mL). The organic layer was washed with saturated aqueous $NaHCO_3$ (25 mL) and brine (25 mL). The combined aqueous layers were back-extracted with Et_2O (2 × 50 mL) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated in vacuo. The crude residue was purified by column chromatography (silica gel, 20% EtOAc: 80% hexanes, R_f = 0.12) to give **12** as a mixture of diastereomers (0.95 g, 66%): ^{1}H NMR 4.47 – 4.38 (m, 1H), 4.04 – 3.86 (m, 1H), 3.65 (s, 3H), 2.29 (t, *J* = 7.2 Hz, 2H), 1.83 – 1.17 (m, 26H), 0.86 (t, *J* = 6.9 Hz); ^{13}C NMR 174.4, 93.1, 92.5, 72.46, 72.14, 51.6, 34.1, 33.60, 33.27, 31.9, 30.6, 29.31, 29.22, 29.14, 29.06, 28.2, 26.1, 25.8, 25.63, 25.30, 24.9, 22.7, 14.2; ESI MS *m/z* 358 ($M-H^-$).



13

(*E*)-Methyl 10-nitrooctadec-9-enoate (13). A solution of **12** (0.42 g, 1.17 mmol), DMAP (10 mg, 0.06 mmol), and Ac_2O (0.13 g, 0.12 mL, 1.29 mmol) in Et_2O (2 mL) was stirred for 2 h at room temperature and concentrated. DMAP (0.17 g, 1.40 mmol) was added to a solution of the crude nitroacetates in CH_2Cl_2 (2 mL) and the solution was stirred at room temperature for 3 h, diluted with CH_2Cl_2 (50 mL) and washed with water (50 mL), 0.1 N aqueous HCl (50 mL), and brine (50 mL). The combined aqueous layers were back-extracted with CH_2Cl_2 (2 × 50 mL) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated in vacuo. The crude residue was purified by column chromatography (silica gel, 20% EtOAc: 80% hexanes, R_f

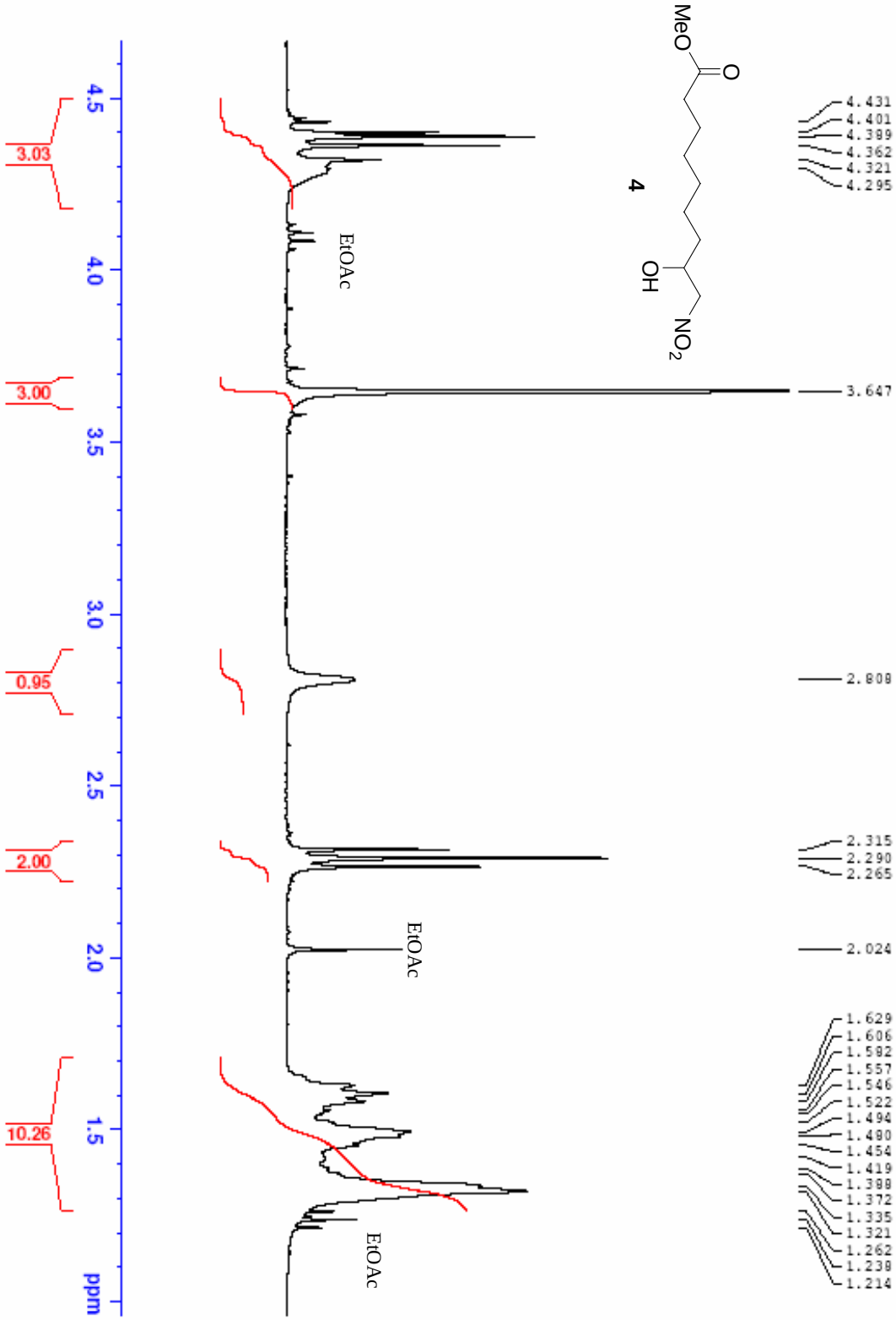
= 0.53) to give **13** as a yellow oil (0.14 g, 36%): ^{1}H NMR 7.05 (t, *J* = 7.8 Hz, 1H), 3.65 (s, 3H), 2.55 (t, *J* = 7.2 Hz, 2H), 2.29 (t, *J* = 7.5 Hz, 2H), 2.20 (q, *J* = 7.5 Hz, 2H), 1.69 – 1.58 (m, 2H), 1.56 – 1.42 (m, 4H), 1.38 – 1.23 (m, 16H), 0.87 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR 174.6, 152.4, 136.6, 51.9, 34.4, 32.2, 29.63, 29.56, 29.54, 29.53, 29.38, 29.35, 28.86, 28.36, 28.30, 26.8, 25.2, 23.0, 14.5 ESI MS *m/z* 340 (M-H$^-$).



2

(*E*)-10-Nitrooctadec-9-enoic acid (2). A solution of **13** (0.34 g, 1 mmol) in 6 M aq. HCl (10 mL) was refluxed for 12 h. The solution was cooled to room temperature and extracted with EtOAc (3 × 20 mL). The combined organic layers were washed with water (30 mL) and brine (30 mL), dried over $MgSO_4$, filtered, and concentrated. The crude residue was purified by column chromatography (silica gel, 20% EtOAc: 80% hexanes, R_f = 0.17) to give **2** as a yellow oil (0.17 g, 53%): ^{1}H NMR 11.46 (bs, 1H), 7.06 (t, *J* = 7.8 Hz, 1H), 2.56 (t, *J* = 7.5 Hz, 2H), 2.35 (t, *J* = 7.2 Hz, 2H), 2.20 (q, *J* = 7.2, 7.5 Hz, 2H), 1.66 – 1.57 (m, 2H), 1.55 – 1.39 (m, 4H), 1.38 – 1.18 (m, 16H), 0.87 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR 180.6, 152.4, 136.6, 34.4, 32.2, 29.62, 29.55, 29.51, 29.36, 29.25, 29.12, 28.85, 28.35, 28.30, 26.7, 25.0, 23.0, 14.5; ESI MS *m/z* 326 (M-H$^-$). Anal. calcd. for $C_{18}H_{33}NO_4$: C, 66.02; H, 10.16; N, 4.28. Found: C, 66.25; H, 10.10; N, 4.08.

Chemiluminescence Detection of Nitric Oxide and Nitrite. Test compounds were weighed into vials, sealed with rubber septa and deoxygenated with argon for 20 minutes. Deoxygenated phosphate buffer (25 mM, pH 7.4) or other solvents (1:1 EtOH:phosphate buffer or 1:1 EtOH:deionized water) were injected through the septa to give final concentrations of test compounds of 50 mM. After incubation of these solutions at room temperature for various times, aliquots of the reaction headspace or the solution were injected into the reaction chamber of a Sievers 280 Nitric Oxide Analyzer (NOA). For NO detection, aliquots (100 of 500 μL) of the headspace were injected into the reaction chamber containing only deionized water. For nitrite analysis, aliquots (5 μL) of the reaction solution were injected into the reaction chamber containing 1% w/v potassium iodide in glacial acetic acid to reduce nitrite to NO. The concentrations of nitrite and nitric oxide were calculated using standard curves.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OH
NO2
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1.389
1.372
1.335
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1.262
1.239
1.214
EtOAc
EtOAc
EtOAc
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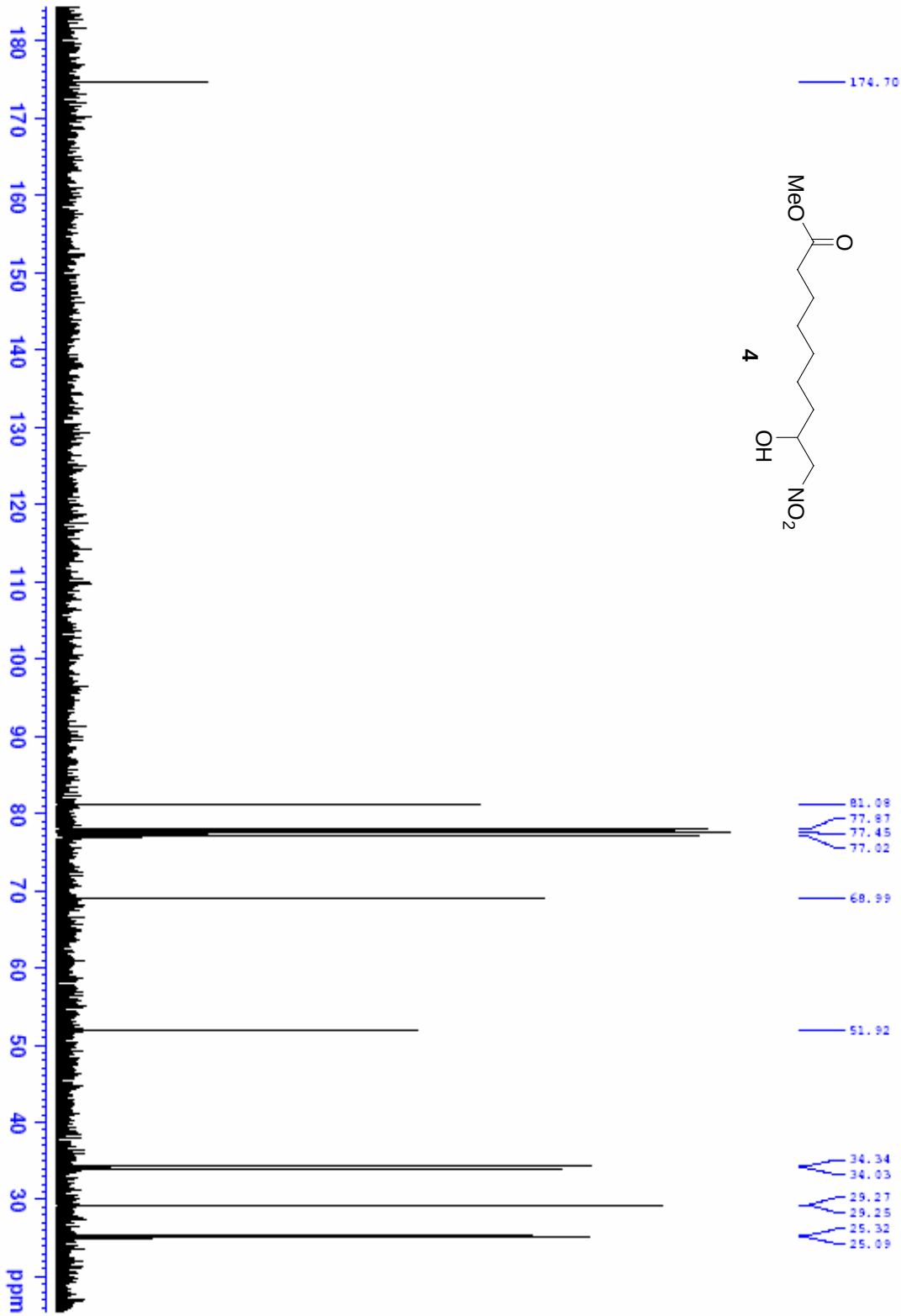
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81.08
77.87
77.45
77.02
68.99
51.92
34.34
34.03
29.27
29.25
25.32
25.09
MeO
O
OH
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110
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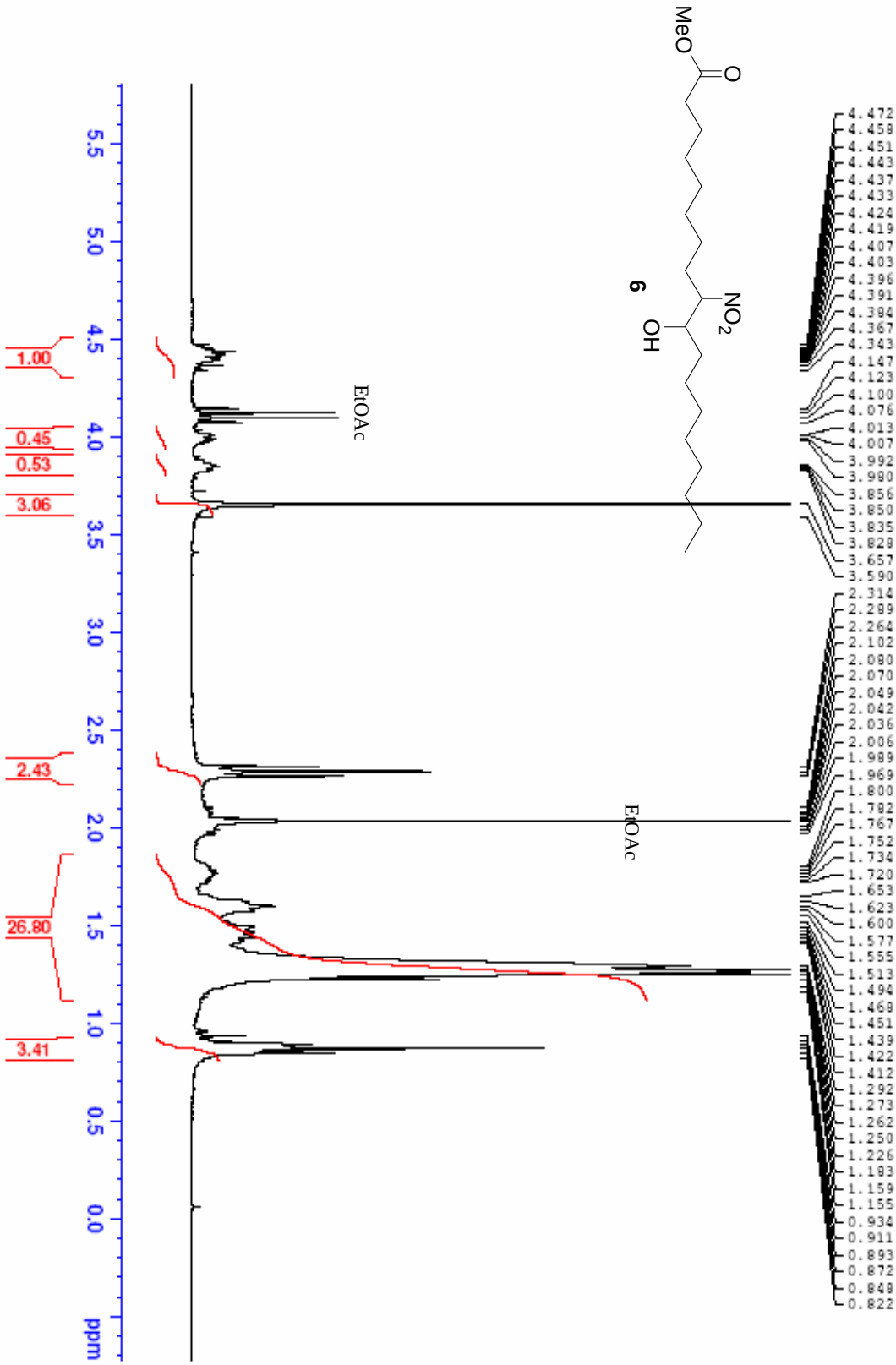
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O
NO2
OH
6
EtOAc
EtOAc
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4.451
4.443
4.437
4.433
4.424
4.419
4.407
4.403
4.396
4.391
4.384
4.367
4.343
4.147
4.123
4.100
4.076
4.013
4.007
3.992
3.980
3.856
3.850
3.835
3.828
3.657
3.590
2.314
2.289
2.264
2.102
2.090
2.070
2.049
2.042
2.036
2.006
1.989
1.969
1.800
1.782
1.767
1.752
1.734
1.720
1.653
1.623
1.600
1.577
1.555
1.513
1.494
1.469
1.451
1.439
1.422
1.412
1.292
1.273
1.262
1.250
1.226
1.193
1.159
1.155
0.934
0.911
0.893
0.872
0.848
0.822
1.00
0.45
0.53
3.06
2.43
26.80
3.41
5.5
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
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0.0
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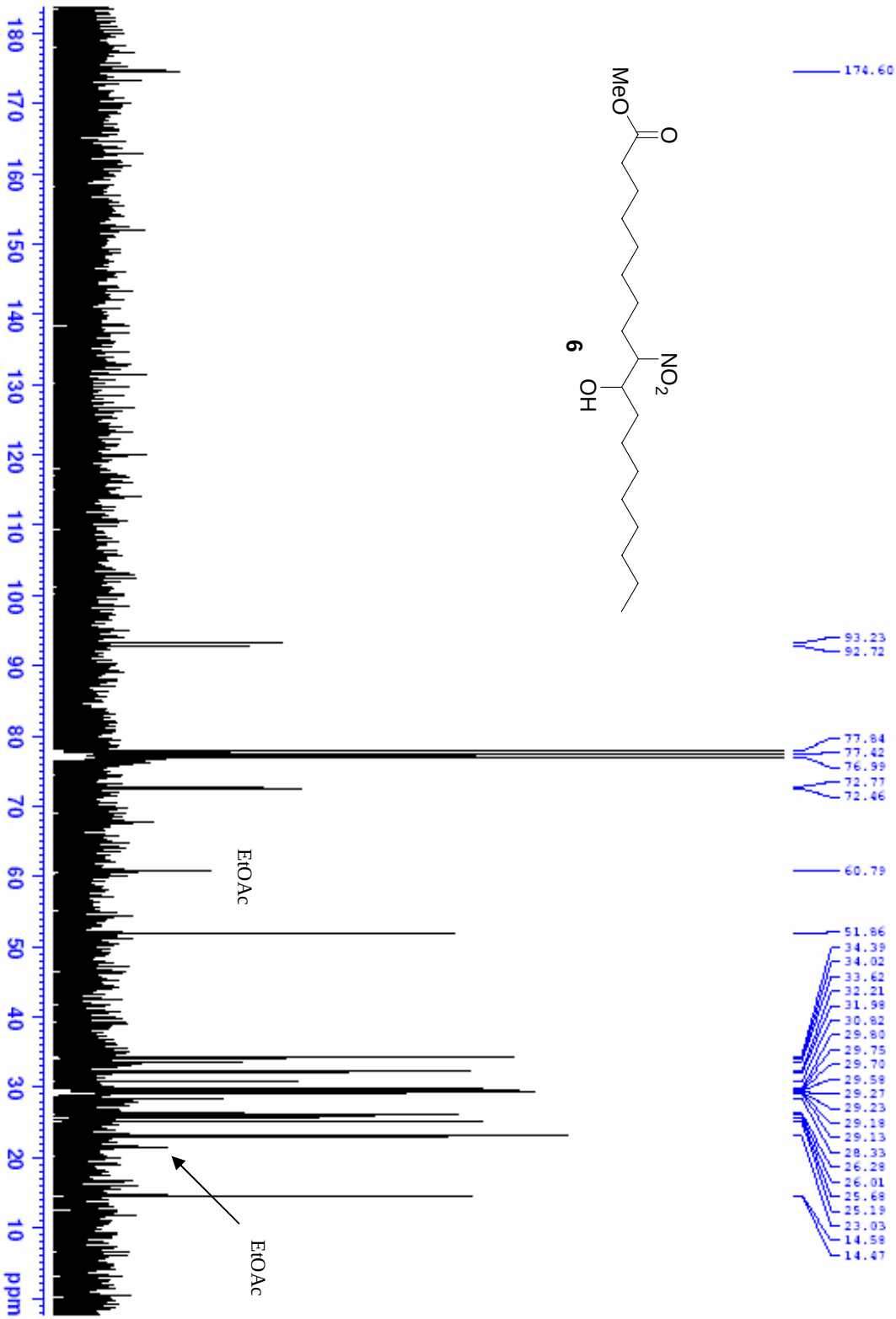
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O
NO2
OH
6
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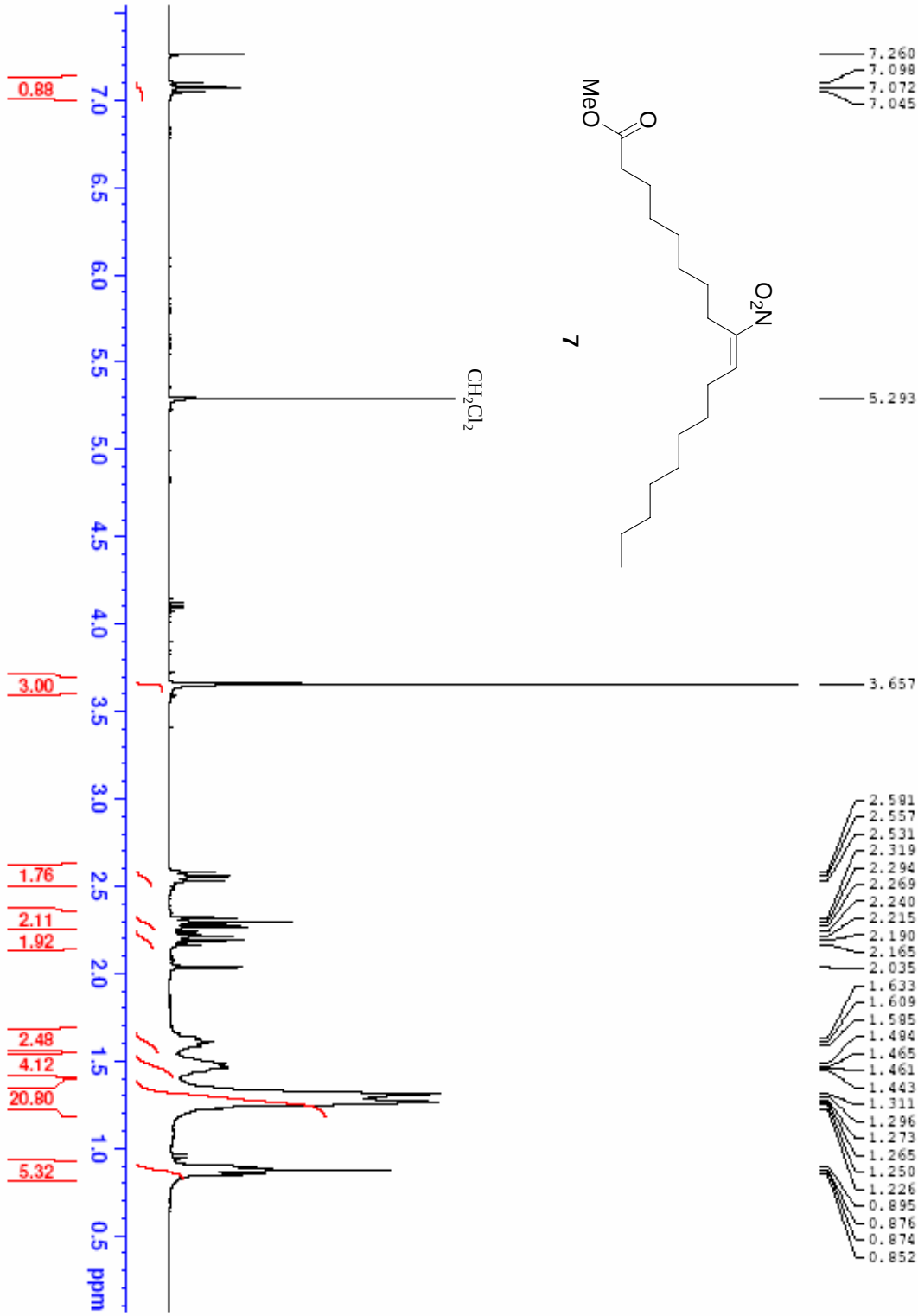
92.72
77.84
77.42
76.99
72.77
72.46
60.79
51.86
34.39
34.02
33.62
32.21
31.98
30.82
29.80
29.75
29.70
29.58
29.27
29.23
29.18
29.13
28.33
26.28
26.01
25.68
25.19
23.03
14.58
14.47
EtOAc
EtOAc
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


MeO
O
O2N
7
CH2Cl2
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7.098
7.072
7.045
5.293
3.657
2.591
2.557
2.531
2.319
2.294
2.269
2.240
2.215
2.190
2.165
2.035
1.633
1.609
1.585
1.494
1.465
1.461
1.443
1.311
1.296
1.273
1.265
1.250
1.226
0.895
0.876
0.874
0.852
0.88
3.00
1.76
2.11
1.92
2.48
4.12
20.80
5.32
7.0
6.5
6.0
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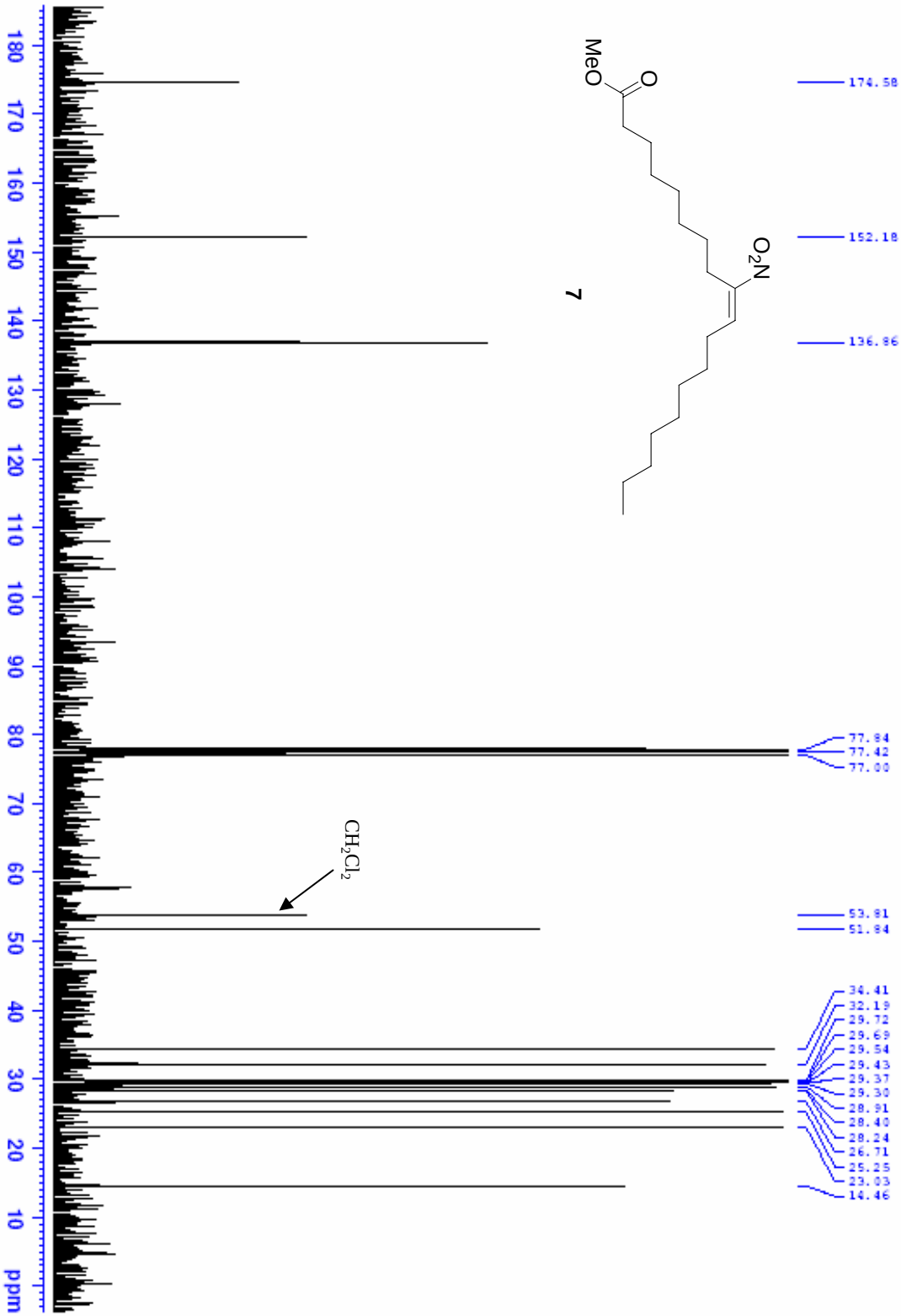
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm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O
O2N
7
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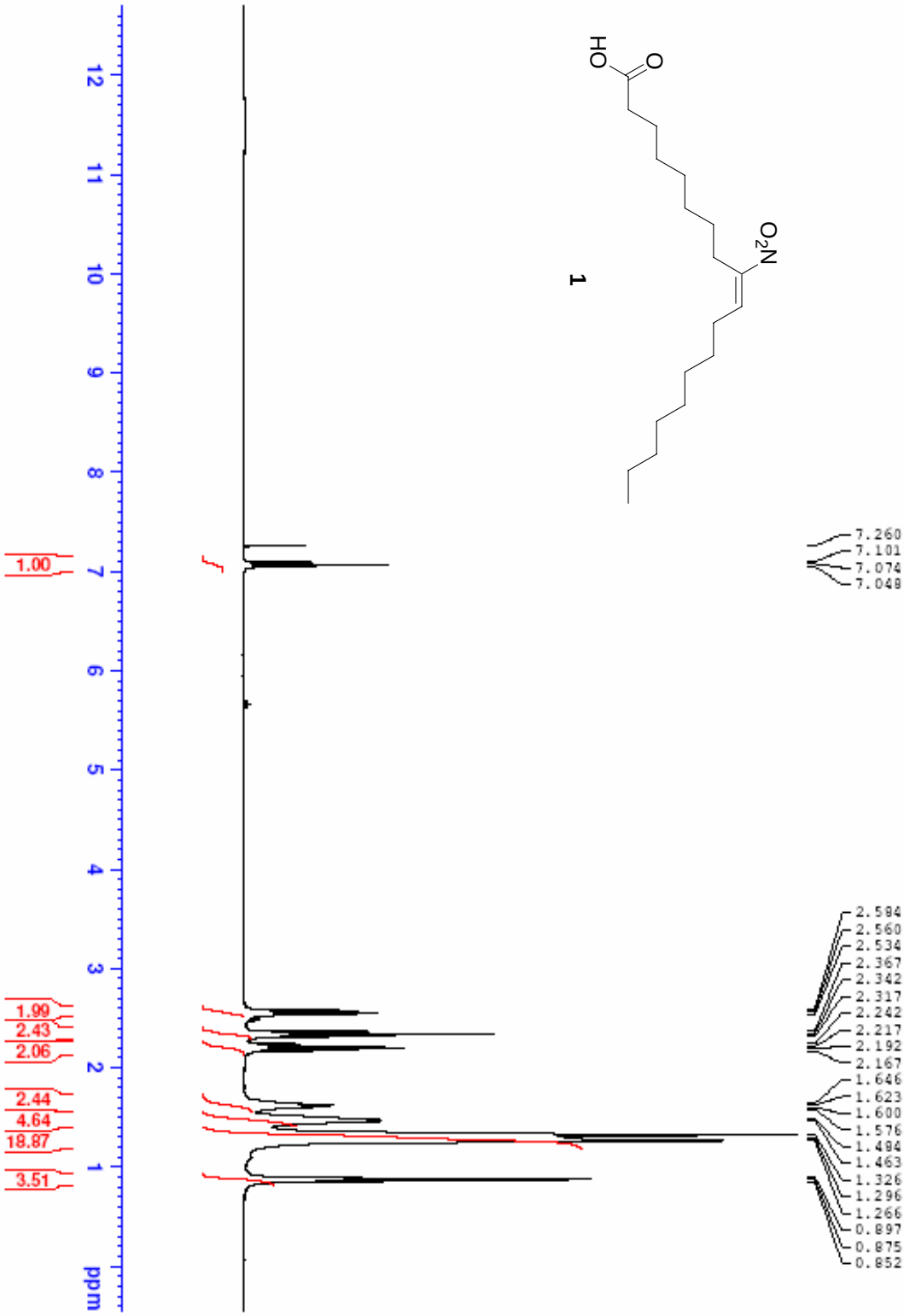
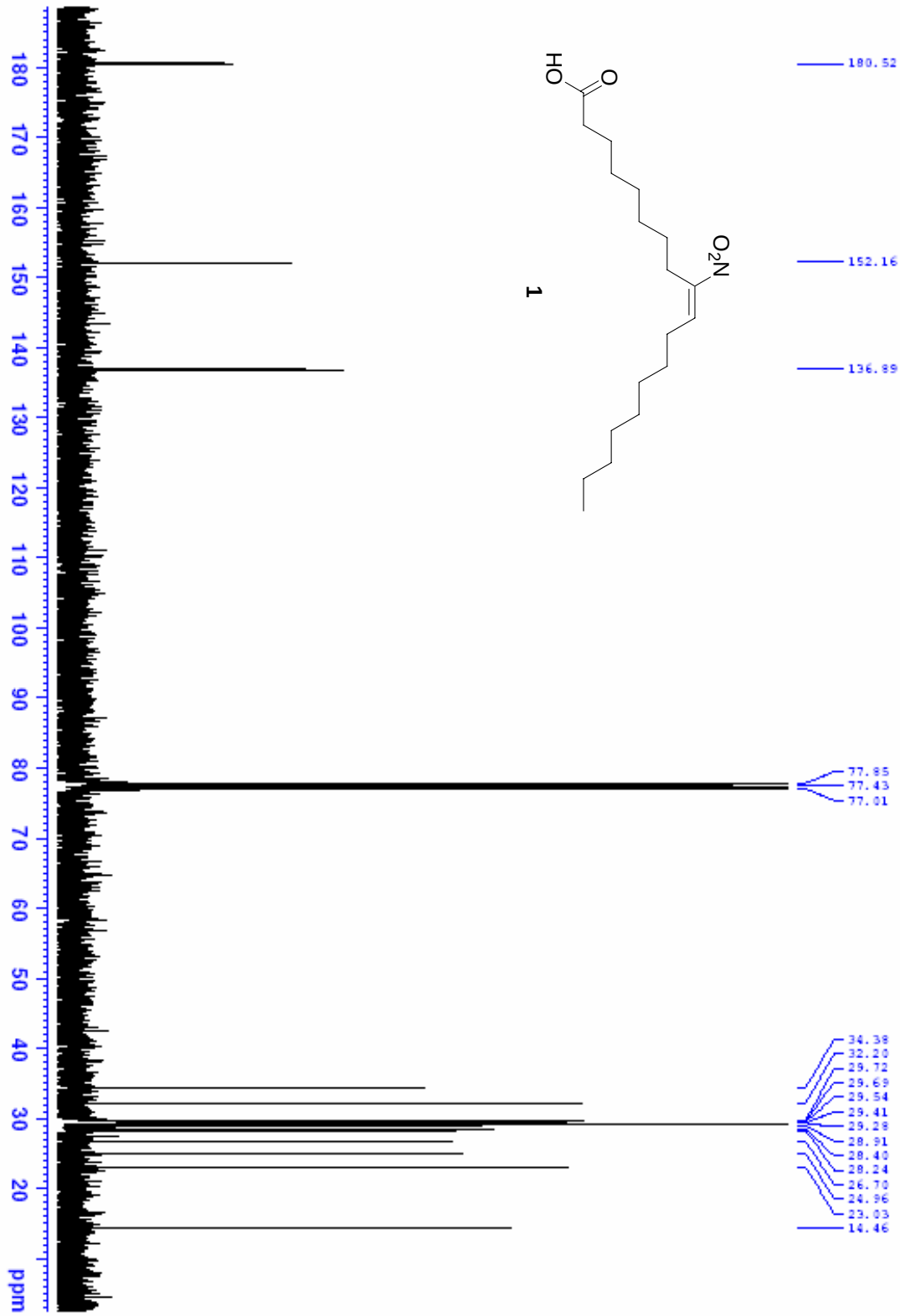
152.18
136.86
77.84
77.42
77.00
CH2Cl2
53.81
51.84
34.41
32.19
29.72
29.69
29.54
29.43
29.37
29.30
28.91
28.40
28.24
26.71
25.25
23.03
14.46
ppm


HO
O
O2N
1
7.260
7.101
7.074
7.048
2.584
2.560
2.534
2.367
2.342
2.317
2.242
2.217
2.192
2.167
1.646
1.623
1.600
1.576
1.484
1.463
1.326
1.296
1.266
0.897
0.875
0.852
1.00
1.99
2.43
2.06
2.44
4.64
18.87
3.51
ppm


HO
O
O2N
1
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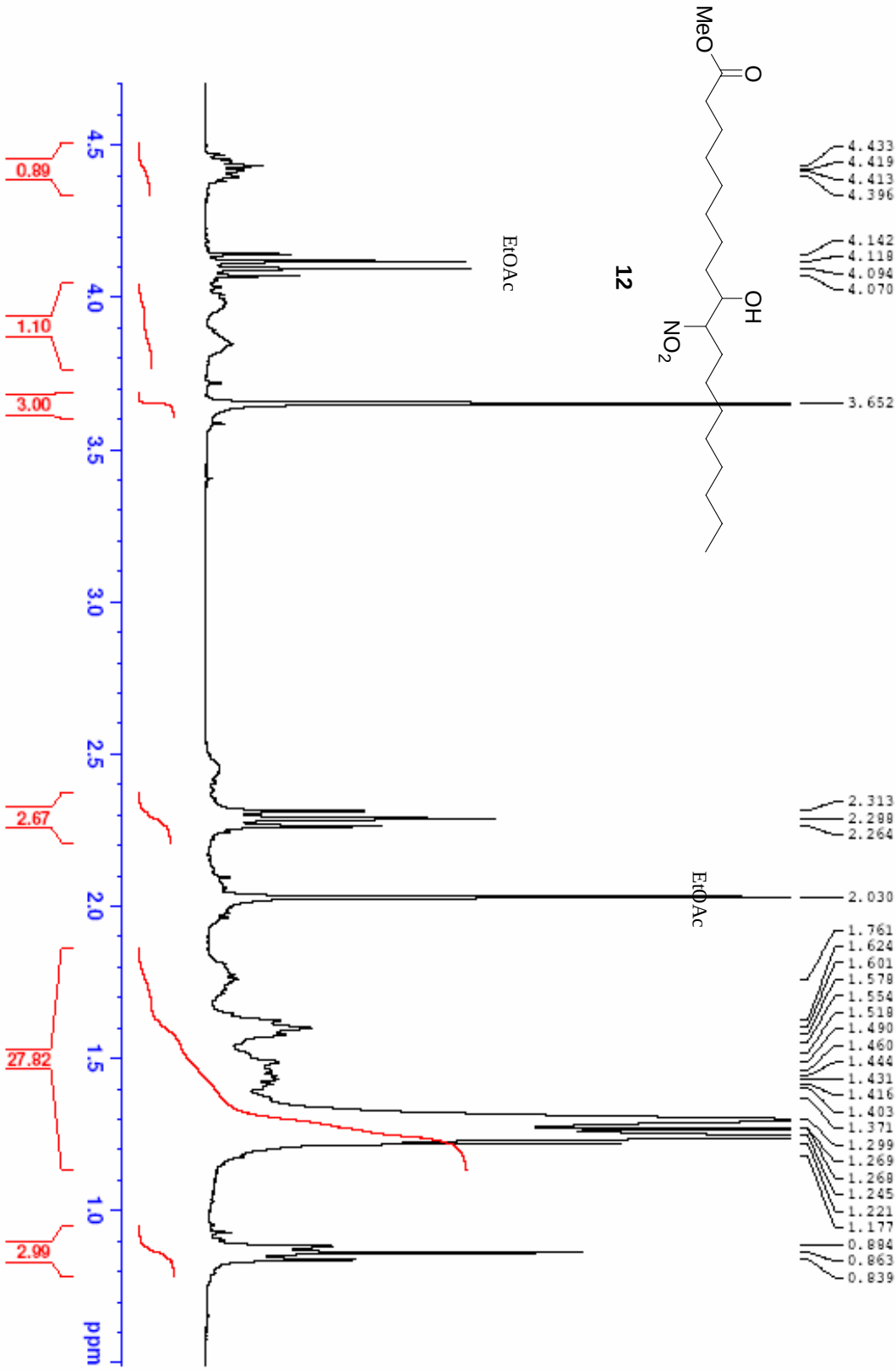
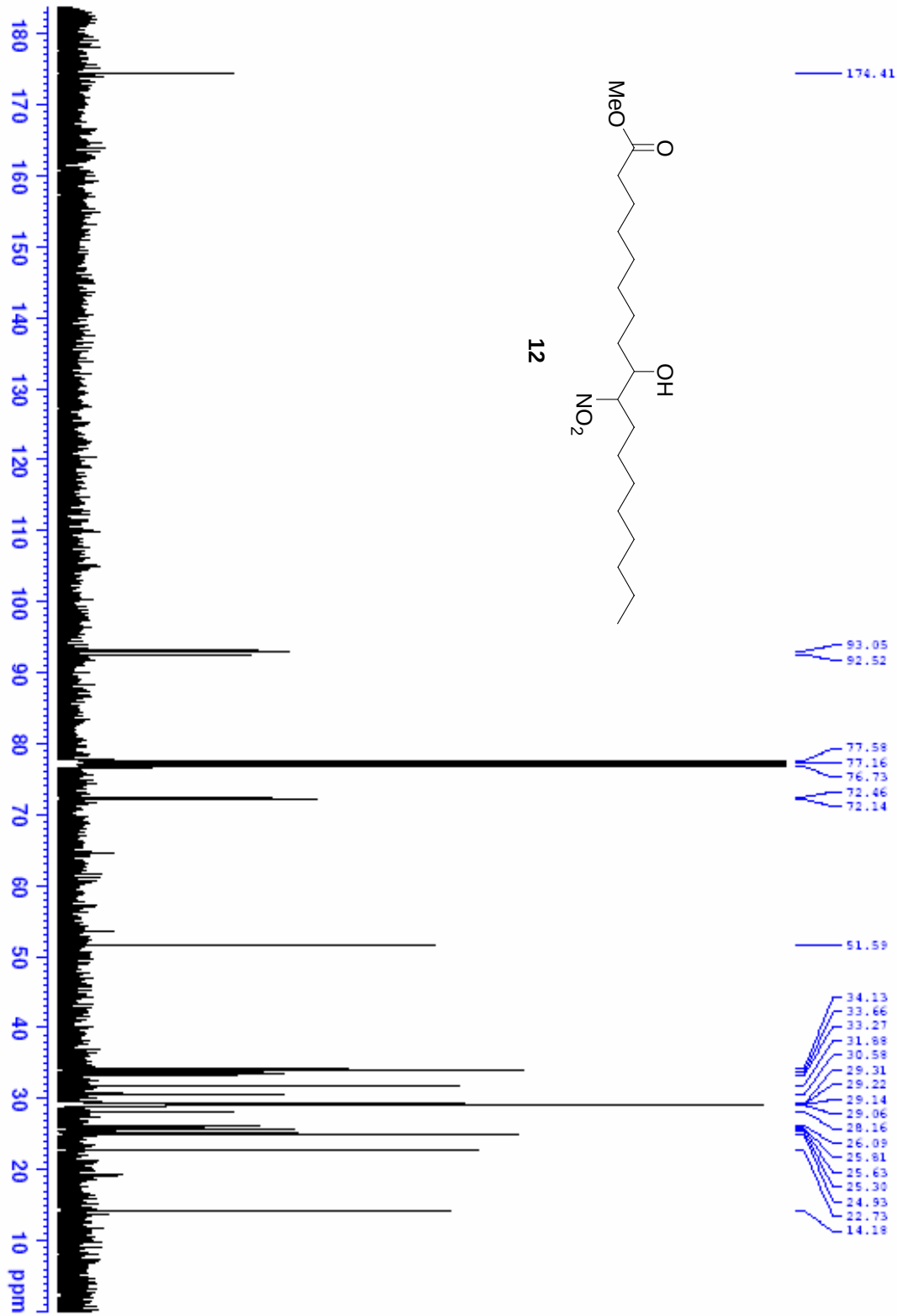
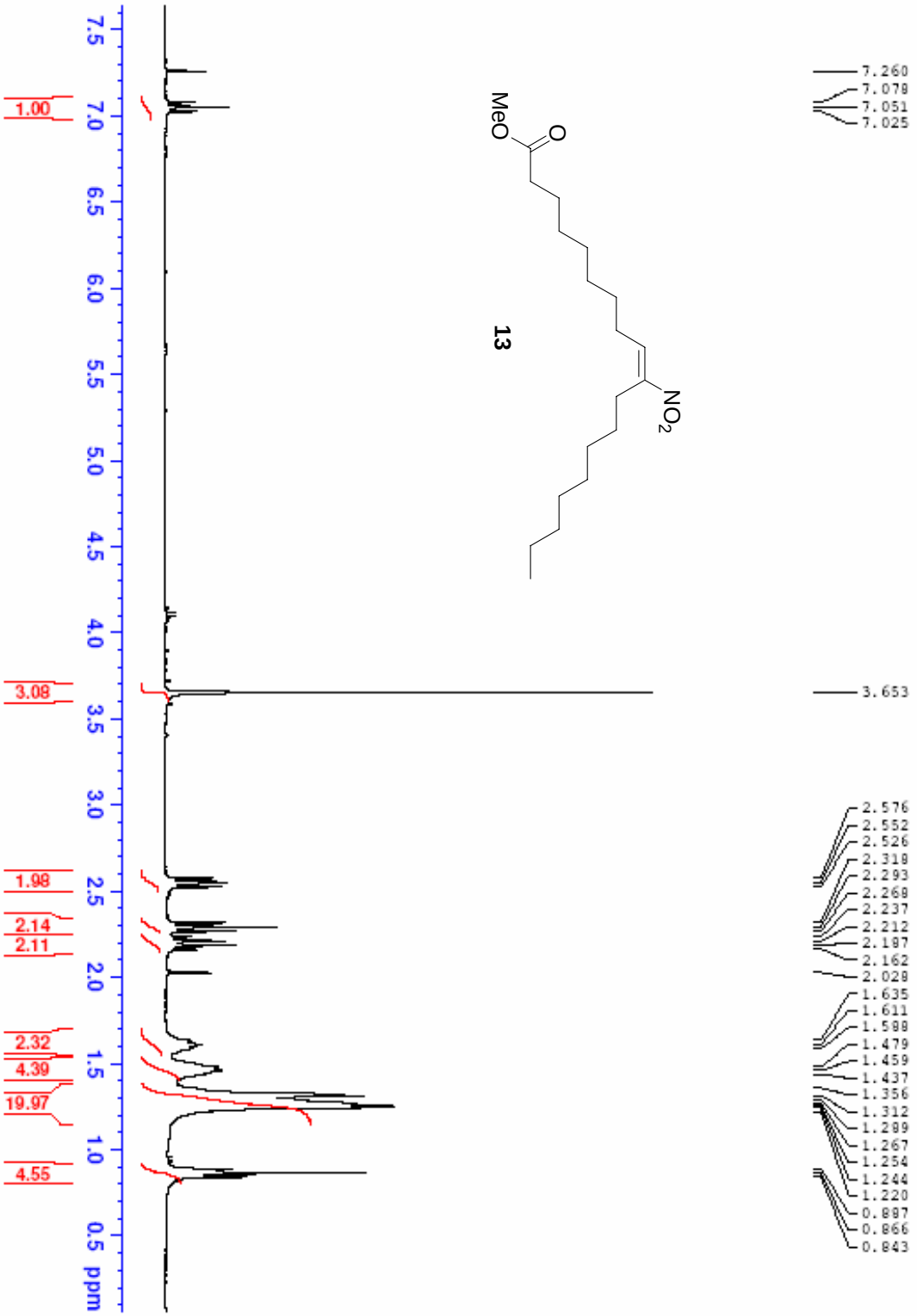
136.89
77.85
77.43
77.01
34.38
32.20
29.72
29.69
29.54
29.41
29.28
28.91
28.40
28.24
26.70
24.96
23.03
14.46
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


MeO
O
OH
NO2
12
EtOAc
EtOAc
4.433
4.419
4.413
4.396
4.142
4.118
4.094
4.070
3.652
2.313
2.288
2.264
2.030
1.761
1.624
1.601
1.578
1.554
1.518
1.490
1.460
1.444
1.431
1.416
1.403
1.371
1.299
1.269
1.260
1.245
1.221
1.177
0.884
0.863
0.839
0.89
1.10
3.00
2.67
27.82
2.99
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm


MeO
O
OH
NO2
12
174.41
93.05
92.52
77.58
77.16
76.73
72.46
72.14
51.59
34.13
33.66
33.27
31.88
30.58
29.31
29.22
29.14
29.06
28.16
26.09
25.81
25.63
25.30
24.93
22.73
14.18
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.078
7.051
7.025
MeO
O
13
NO2
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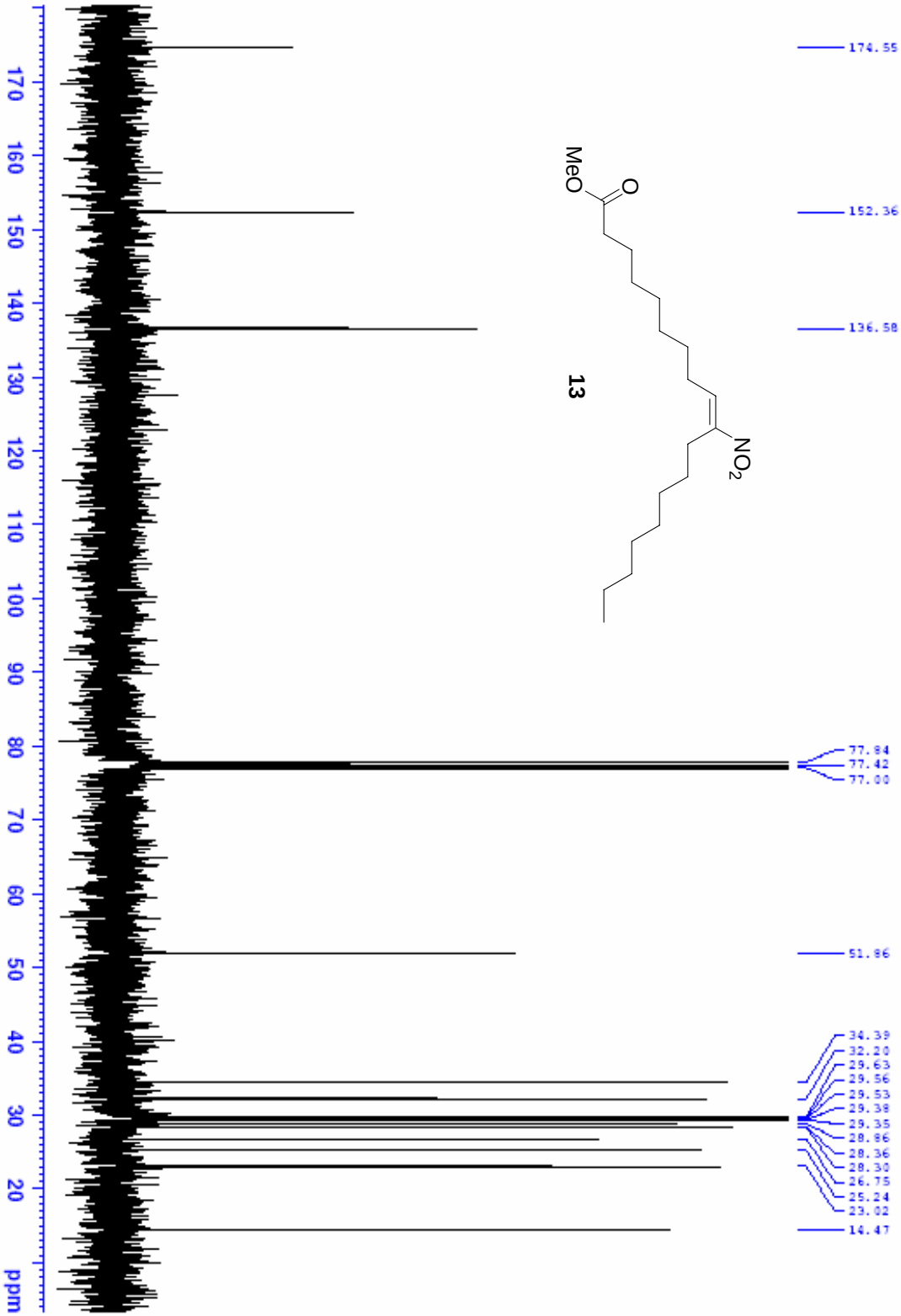
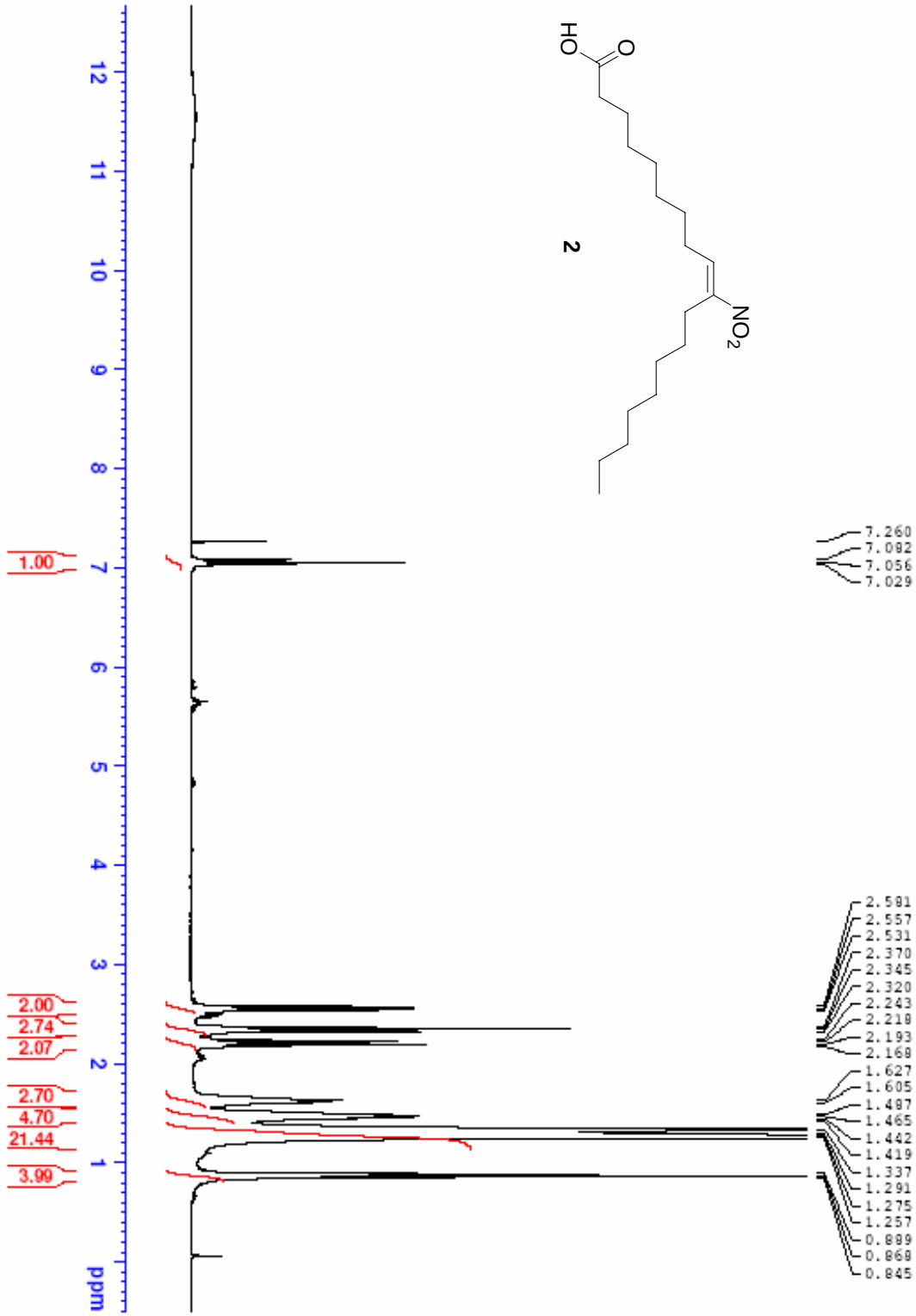
2.552
2.526
2.310
2.293
2.268
2.237
2.212
2.187
2.162
2.028
1.635
1.611
1.598
1.479
1.459
1.437
1.356
1.312
1.289
1.267
1.254
1.244
1.220
0.887
0.866
0.843
1.00
3.08
1.98
2.14
2.11
2.32
4.39
19.97
4.55
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


174.55
152.36
136.58
77.84
77.42
77.00
51.86
34.39
32.20
29.63
29.56
29.53
29.38
29.35
28.86
28.36
28.30
26.75
25.24
23.02
14.47
MeO
O
NO2
13
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


HO
O
NO2
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2.00
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4.70
21.44
3.99
7.260
7.092
7.056
7.029
2.591
2.557
2.531
2.370
2.345
2.320
2.243
2.218
2.193
2.169
1.627
1.605
1.497
1.465
1.442
1.419
1.337
1.291
1.275
1.257
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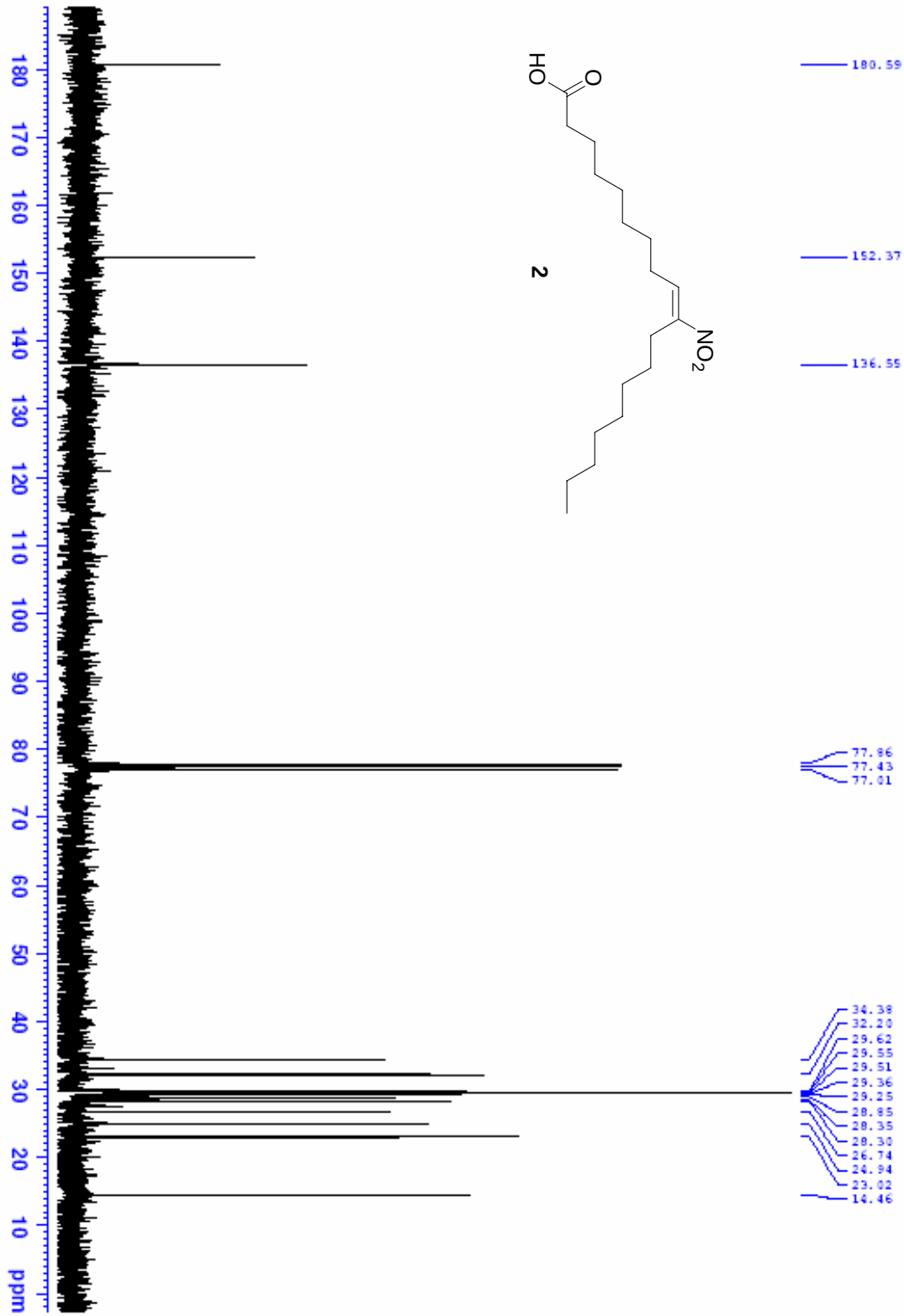
0.845
ppm


HO
O
NO2
2
180.59
152.37
136.55
77.86
77.43
77.01
34.38
32.20
29.62
29.55
29.51
29.36
29.25
28.85
28.35
28.30
26.74
24.94
23.02
14.46
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm