Electronic Supplementary Material (ESI) for ChemComm.

Supporting information for

Guanidinium Iodide-Catalyzed Oxidative α-Nitroalkylation of β-Ketoamides

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Table of Contents:

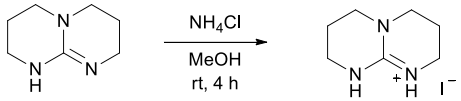
1. General Information

Flash chromatography was performed using silica gel 60 (spherical, particle size 0.040-0.100 mm; Kanto Co., Inc., Japan). ^{1}H and ^{13}C NMR spectra were recorded on JEOL EX300, ECA/ECX400 instruments. Chemical shifts in chloroform-d was reported in the scale relative to chloroform-d (^{1}H NMR; δ = 7.26 ppm, ^{13}C NMR; δ = 77.0 ppm) as an internal reference. Data for ^{1}H NMR were recorded as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constant (Hz), integration. Data for ^{13}C NMR are reported in terms of chemical shift (δ ppm). Mass spectra were recorded on JEOL JMS-T100X spectrometer.

2. Experimental Section

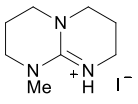
Preparation of onium iodides

n-Bu_4PI and Py·HI were prepared according to the previous reports.[1,2]



TBD TBD·HI

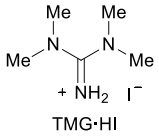
TBD·HI: To a mixture of 1,5,7-Triazabicyclo[4.4.0]dec-5-ene (TBD) (1.0 g, 7.2 mmol) in MeOH (20 ml) was added NH_4Cl (423 mg, 7.9 mmol) and the reaction mixture was stirred for 4 h under N_2 atmosphere. The reaction mixture was evaporated *in vacuo* to give a white solid. This white solid was diluted with CH_2Cl_2 and filtered. The filtrates were evaporated *in vacuo* to give TBD·HCl. Then TBD·HCl (955 mg, 5.4 mmol) was dissolved in dry CH_2Cl_2 and added NaI (815 mg, 5.4 mmol) under N_2 atmosphere. After 24 h, the reaction mixture was filtered through a pad of Celite, and concentrated *in vacuo* to give TBDHI (1.4 g, 56% 2 steps). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 (s, 2H), 3.36-3.30 (m, 8 H), 2.05-1.97 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.1, 46.4, 37.6, 20.2; HRMS (ESI, M+Na) calcd for $C_7H_{14}Na_3$ 140.1188, found 140.1146.



MeTBD·HI

MeTBD·HI: Prepared from 7-Methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (MeTBD) according to the procedure for TBD·HI; (67%, 2 steps). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (s, 1H), 3.55-3.50 (m, 2H), 3.43-3.35 (m, 6H), 3.27 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.7, 48.1, 47.8, 47.0, 39.7,

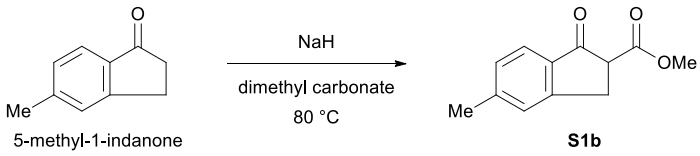
38.4,20.8, 20.4; HRMS (ESI, M+Na) calcd for $C_8H_{16}Na_3$ 154.1344, found 154.1362.



TMG·HI

TMG·HI: Prepared from 1,1,3,3-Tetramethylguanidine (TMG) according to the procedure for TBD·HI; (70%, 2 steps): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 (s, 2H), 3.11 (s, 12H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.5, 40.9; HRMS (ESI, M+Na) calcd for $C_5H_{14}Na_3$ 116.1188, found 116.1164.

Synthesis of β-ketoester S1b

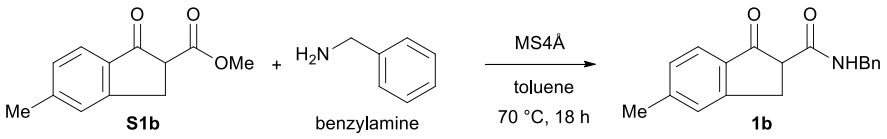


5-methyl-1-indanone **S1b**

5-Methyl-1-oso-2-indanecarboxylate (S1b).

To a suspension of NaH (80% in mineral oil, 84 mg, 2.11 mmol) in dimethyl carbonate (2 mL) was added a solution of 5-methyl-1-indanone (140 mg, 0.56 mmol) in dimethyl carbonate (2 mL) dropwise. The resulting mixture was heated at 80 °C for 1 h. After cooling to 0 °C, to the reaction mixture was added 1N HCl (3 mL). The organic layer was extracted with dichloromethane (×3). The extracts were washed with brine, dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (*n*-hexane/ethyl acetate, 9:1 as eluent) to give methyl ester **S1b (**165 mg, 90%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.5 Hz, 1H), 7.30 (s, 1H), 7.20 (d, *J* = 7.5 Hz, 1H), 3.79 (s, 3H), 3.73 (dd, *J* = 7.8, 4.2 Hz, 1H), 3.52 (dd, *J* = 17.4, 4.2 Hz, 1H), 3.32 (dd, *J* = 17.4, 7.8 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.9, 169.7, 154.1, 146.9, 132.9, 129.1, 126.8, 124.5, 53.3, 52.8, 30.1, 22.1; HRMS (ESI, M+Na) calcd for $C_{12}H_{12}Na_1O_3$ 227.0684, found 227.0711.

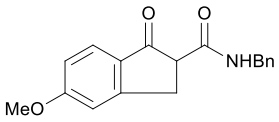
General procedure for amidation of methyl esters



S1b benzylamine **1b**

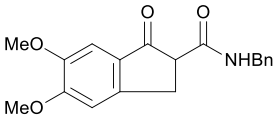
***N*-Benzyl-5-methyl-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (1b).**

To a suspension of activated MS4A (386 mg) in toluene (4.5 mL) was added β-ketomethyl ester **S1b** (134 mg, 0.66 mmol) and benzylamine (108 μL, 0.99 mmol) under N_2 atmosphere. The resulting mixture was heated at 70 °C, for 18 h. The reaction mixture was then cooled to an ambient temperature, and filtered through a pad of Celite, and the filtrates were concentrated *in vacuo.* The residue was purified by column chromatography on silica gel (*n*-hexane/ethyl acetate, 5:1 as eluent) to give β-ketoamide **1b (**165 mg, 90%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.8 Hz, 1H), 7.54 (br, 1H), 7.38-7.24 (m, 6H), 7.17 (d, *J* = 7.8 Hz, 1H), 4.57 (dd, *J* = 14.7, 6.0 Hz, 1H), 4.45 (dd, *J* = 14.7, 5.4 Hz, 1H), 3.77 (dd, *J* = 17.7, 3.9 Hz, 1H), 3.59 (dd, *J* = 8.4, 4.2 Hz, 1H), 3.33 (dd, *J* = 17.7, 8.4 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.7, 166.6, 154.7, 147.2, 138.1, 133.0, 128.9, 128.6, 127.6, 127.3, 127.0, 124.1, 52.9, 43.7, 28.5, 22.2; HRMS (ESI, M+Na) calcd for $C_{18}H_{17}N_1Na_1O_2$ 302.1157, found 302.1162.



***N*-Benzyl-5-methoxy-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (1c).**

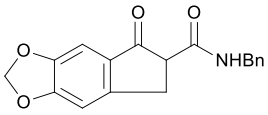
Prepared from corresponding β-ketomethyl ester[3] according to the general procedure for amidation of methyl esters (50% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.8 Hz, 1H), 7.57 (br, 1H), 7.38-7.20 (m, 5H), 6.93-6.90 (m, 2H), 4.56 (dd, *J* = 14.8, 6.0 Hz, 1H), 4.45 (dd, *J* = 14.8, 5.6 Hz, 1H), 3.90 (s, 3H), 3.78 (dd, *J* = 18.0, 3.6 Hz, 1H), 3.58 (dd, *J* = 8.4, 3.6 Hz, 1H), 3.31 (dd, *J* = 18.0, 8.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.1, 166.7, 166.2, 157.4, 138.1, 128.6, 128.4, 127.6, 127.3, 126.1, 116.0, 109.5, 55.7, 52.9, 43.7, 28.7; HRMS (ESI, M+Na) calcd for $C_{18}H_{17}N_1Na_1O_3$ 318.1106, found 318.1146.



***N*-Benzyl-5,6-dimethoxy-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (1d)**.

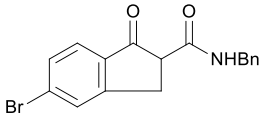
Prepared from corresponding β-ketomethyl ester[4] according to the general procedure for amidation of methyl esters (51% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (br, 1H), 7.37-7.23 (m, 5H), 7.14 (s, 1H), 6.92 (s, 1H), 4.56 (dd, *J* = 15.2, 6.0 Hz, 1H), 4.46 (dd, *J* = 15.2, 5.6 Hz, 1H), 3.98 (s, 3H). 3.90 (s, 3H), 3.73 (dd, *J* = 17.6, 3.6 Hz, 1H), 3.59 (dd, *J* = 7.6, 3.6 Hz, 1H), 3.28 (dd, *J* = 17.6, 7.6 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.6, 166.8, 156.4, 150.1, 149.6, 138.1, 128.6, 127.9, 127.6,

127.4, 107.4, 104.4, 56.4, 56.1, 53.0, 43.7, 28.4; HRMS (ESI, M+Na) calcd for $C_{19}H_{19}N_1Na_1O_4$ 348.1212, found 348.1254.



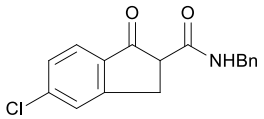
***N*-Benzyl-5-oxo-6,7-dihydro-5*H*-indeno[5,6-*d*][1,3]dioxole-6-carboxamide (1e).**

Prepared from corresponding β-ketomethyl ester[4] according to the general procedure for amidation of methyl esters (70% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (br, 1H), 7.40-7.24 (m, 5H), 7.07 (s, 1H), 6.87 (s, 1H), 4.56 (dd, *J* = 15.0, 6.0 Hz, 1H), 4.44 (dd, *J* = 15.0, 6.0 Hz, 1H), 3.70 (dd, *J* = 17.4, 3.6 Hz, 1H), 3.58 (dd, *J* = 7.8, 3.6 Hz, 1H), 3.24 (dd, *J* = 17.4, 7.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.9, 166.6, 155.2, 152.4, 148.5, 138.1, 129.7, 128.7, 127.4, 105.8, 102.6, 102.4, 53.2, 43.8, 31.1, 28.6; HRMS (ESI, M+Na) calcd for $C_{18}H_{15}N_1Na_1O_4$ 332.0899, found 332.0891.



***N*-Benzyl-5-bromo-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (1f).**

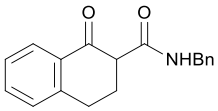
Prepared from corresponding β-ketomethyl ester according to the general procedure for amidation of methyl esters (85% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.71 (s, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.43-7.24 (m, 6H), 3.83 (dd, *J* = 18.0, 4.2 Hz, 1H), 3.60 (dd, *J* = 8.4, 4.2 Hz, 1H), 3.35 (dd, *J* = 18.0, 8.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.8, 165.9, 155.7, 137.9, 134.1, 131.3, 130.0, 128.6, 127,6, 127.4, 125.5, 52.9, 43.8, 28.4; HRMS (ESI, M+Na) calcd for $C_{17}H_{14}{}^{81}Br_1N_1Na_1O_2$ 368.0085 and $C_{17}H_{14}{}^{79}Br_1N_1Na_1O_2$ 366.0106, found 368.0132 and 366.0080.



***N*-Benzyl-5-chloro-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (1g).**

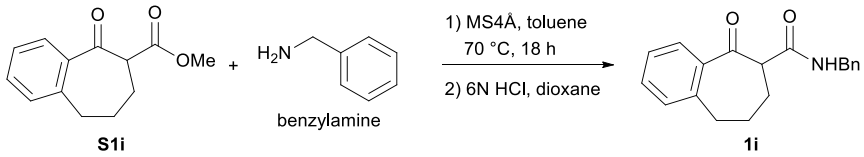
Prepared from corresponding β-ketomethyl ester[3] according to the general procedure for amidation of methyl esters; (68% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.4 Hz, 1H), 7.50 (s, 1H), 7.41 (s, 1H), 7.68-7.24 (m, 6H), 4.54 (dd, *J* = 15.2, 6.0 Hz, 1H), 4.44 (dd, *J* = 15.2, 6.0 Hz, 1H), 3.80 (dd, *J* = 18.0, 4.0 Hz, 1H), 3.60 (dd, *J* = 8.4, 4.0 Hz, 1H), 3.32 (dd, *J* = 18.0, 8.4 Hz, 1H); ^{13}C NMR

(75 MHz, $CDCl_3$) δ 201.7, 165.9, 155.7, 142.4, 137.9, 133.7, 128.7, 128.5, 127.7, 127.5, 126.9, 125.4, 53.0, 43.8, 28.4; HRMS (ESI, M+Na) calcd for $C_{17}H_{14}Cl_1N_1Na_1O_2$ 322.0611, found 322.0620.



***N*-Benzyl-5-chloro-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (1h).**

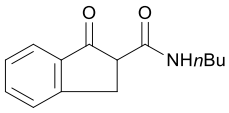
Prepared from corresponding β-ketomethyl ester[5] according to the general procedure for amidation of methyl esters; (71% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.46 (br, 1H), 7.38-7.20 (m, 7H), 4.56 (dd, *J* = 15.2, 6.0 Hz, 1H), 4.44 (dd, *J* = 15.2, 5.6 Hz, 1H), 3.42 (dd, *J* = 8.8, 5.2 Hz, 1H), 3.17 (ddd, *J* = 16.8, 6.4, 4.4 Hz, 1H), 2.96 (ddd, *J* = 16.8, 8.4, 4.4 Hz, 1H), 2.58-2.43 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.6, 167.6, 144.8, 138.1, 134.3, 131.9, 128.8, 128.6, 127.8, 127.6, 127.3, 126.8, 52.6, 43.7, 27.9, 25.4; HRMS (ESI, M+Na) calcd for $C_{18}H_{17}N_1Na_1O_2$ 302.1157, found 302.1121.



S1i **1i**

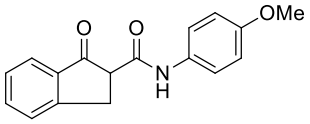
***N*-Benzyl-5-oxo-6,7,8,9-tetrahydro-5*H*-benzo[7]annulene-6-carboxamide (1i)**.

To a suspension of activated MS4A (973 mg) in toluene (10 mL) was added β-ketomethyl ester **S1i**[5] (638 mg, 2.92 mmol) and benzylamine (1.1 ml, 10.2 mmol) under N_2 atmosphere. The resulting mixture was heated to 70 °C for 24 h. The reaction mixture was cooled to an ambient temperature, filtered through a pad of Celite, and the filtrates were concentrated *in vacuo*. To the residue was added dioxane (5 mL) and 6N HCl (1 mL), and the mixture was stirred at room temperature for 24 h. The resulting mixture was extracted with ethyl acetate (×2), and the combined extracts were washed with sat. $NaHCO_3$, brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (*n*-hexane/ethyl acetate, 5:1 as eluent) to give β-ketoamide **1i (**282 mg, 33% 2 steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (br, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.38-7.20 (m, 7H), 4.60-4.44 (m, 2H), 3.72 (dd, *J* = 10.0, 4.8 Hz, 1H), 3.00-2.86 (m, 2H), 2.34-2.22 (m, 1H), 2.18-2.00 (m, 2H), 2.00-1.82 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 205.1, 168.7, 141.5, 138.8, 138.2, 132.4, 129.7, 128.6, 128.5, 127.6, 127.3, 126.6, 55.4, 43.5, 32.5, 27.3, 24.4; HRMS (ESI, M+Na) calcd for $C_{19}H_{19}N_1Na_1O_2$ 316.1314, found 316.1362.



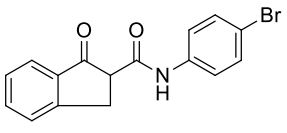
***N*-Butyl-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (1j).**

Prepared from corresponding β-ketomethyl ester[6] and *n*-butylamine according to the general procedure for amidation of methyl esters (59% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 7.5, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.14 (br, 1H), 3.79 (dd, *J* = 17.7, 3.9 Hz, 1H), 3.54 (dd, *J* = 8.4, 3.9 Hz, 1H), 3.35 (dd, *J* = 17.7, 8.4 Hz, 1H), 3.36-3.27 (m, 2H), 1.58-1.49 (m, 2H), 1.43-1.31 (m, 2H), 0.93 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.5, 166.2, 154.3, 135.6, 135.3, 127.5, 126.6, 124.2, 52.8, 39.5, 31.5, 28.7, 20.0, 13.7; HRMS (ESI, M+Na) calcd for $C_{14}H_{17}N_1Na_1O_2$ 254.1157, found 254.1117.



***N*-(4-methoxyphenyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (1l).**

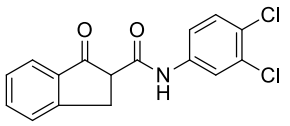
According to the general procedure for amidation of methyl esters, the title compound was prepared from corresponding β-ketomethyl ester and 4-methoxyaniline (87% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.05 (s, 1H), 7.79 (d, *J* = 7.5 Hz, 1H), 7.66 (td, *J* = 7.5, 0.9 Hz, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.50 (d, *J* = 9.0 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 2H), 6.87 (d, *J* = 9.0 Hz, 2H), 3.86 (dd, *J* = 18.0, 3.9 Hz, 1H), 3.73 (dd, *J* = 8.4, 3.9 Hz, 1H), 3.44 (dd, *J* = 18.0, 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.6, 164.1, 156.4, 154.2, 136.0, 135.3, 130.9, 127.7, 126.7, 124.4, 121.7, 114.1, 55.4, 53.2, 28.6; HRMS (ESI, M+Na) calcd for $C_{17}H_{15}N_1Na_1O_3$ 304.0950, found 304.0921.



***N*-(4-bromophenyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (1m).**

According to the general procedure for amidation of methyl esters, the title compound was prepared from corresponding β-ketomethyl ester and 4-bromoaniline (85% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.23 (s, 1H), 7.80 (d, *J* = 7.5 Hz, 1H), 7.68 (td, *J* = 7.5, 0.9 Hz, 1H), 7.55 (d, *J* = 7.5 Hz,

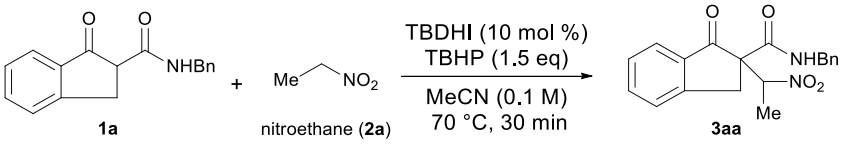
1H), 7.51 (d, *J* = 9.0 Hz, 2H), 7.44 (d, *J* = 9.0 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 1H), 3.85 (dd, *J* = 17.4, 4.2 Hz, 1H), 3.74 (dd, *J* = 8.1, 4.2 Hz, 1H), 3.45 (dd, *J* = 17.4, 8.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.4, 164.4, 154.1, 136.8, 136.1, 135.1, 131.9, 127.8, 126.7, 124.5, 121.4, 116.8, 53.3, 28.4; HRMS (ESI, M+Na) calcd for $C_{16}H_{12}{}^{81}Br_1N_1Na_1O_2$ 353.9929 and $C_{16}H_{12}{}^{79}Br_1N_1Na_1O_2$ 351.9949, found 353.9946 and 351.9953.



***N*-(3,4-dichlorophenyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (1n).**

According to the general procedure for amidation of methyl esters, the title compound was prepared from corresponding β-ketomethyl ester and 3,4-dichroloaniline (88% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.30 (s, 1H), 7.86 (d, *J* = 2.1 Hz, 1H), 7.80 (d, *J* = 7.5 Hz, 1H), 7.69 (td, *J* = 7.5, 0.9 Hz, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.42 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.38 (d, *J* = 8.1 Hz, 1H), 3.84 (dd, *J* = 17.7, 4.2 Hz, 1H), 3.74 (dd, *J* = 8.4, 4.2 Hz, 1H), 3.45 (dd, *J* = 17.7, 8.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.3, 164.5, 154.1, 137.2, 136.3, 135.0, 132.7, 130.4, 127.9, 127.4, 126.7, 124.6, 121.5, 119.1, 53.3, 28.4; HRMS (ESI, M+Na) calcd for $C_{16}H_{11}Cl_2N_1Na_1O_2$ 342.0065, found 342.0079.

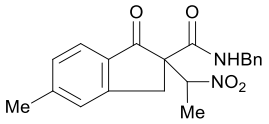
General procedure for oxidative α-nitroalkylation of β-ketoamides.



***N*-Benzyl-2-(1-nitroethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (3aa).**

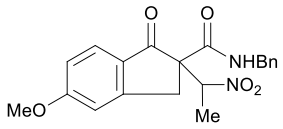
To a mixture of β-ketoamide **1a**[7] (26.5 mg, 0.1 mmol) and nitroethane (**2a**) (214 μL, 3.0 mmol) in acetonitrile (1 mL) was added TBD·HI (2.7 mg, 0.01 mmol) under Ar atmosphere at room temperature, and the resulting mixture was heated at 70 °C. To the resulting mixture was added TBHP (70% in H_2O, 21.2 μL, 0.15 mmol) dropwise at this temperature, and the mixture was stirred for 30 min. Then the reaction mixture was cool to room temperature, and was added 10% $Na_2S_2O_3$. The reaction mixture was extracted with ethyl acetate (×3), and the extracts were washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel (*n*-hexane/ethyl acetate = 9:1 as eluent) to give **3aa** as a 1:1 mixture of

separable diastereomers (32 mg, 94% combined yield) with a trace amount of **4a**.[7] **3aa** (less polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.1 Hz, 1H), 7.65 (dt, *J* = 1.5, 7.5 Hz, 1H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.46-7.26 (m, 5H), 7.21 (dd, *J* = 8.1, 1.8 Hz, 2H), 5.26 (q, *J* = 6.9 Hz, 1H), 4.52 (dd, *J* = 14.7, 6.0 Hz, 1H), 4.27 (dd, *J* = 14.7, 5.4 Hz, 1H), 4.21 (d, *J* = 18.0 Hz, 1H), 3.16 (d, *J* = 18.0 Hz, 1H), 1.63 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.2, 164.6, 153.3, 137.2, 136.2, 134.4, 128.8, 128.0, 127.8, 127.6, 126.6, 124.8, 85.2, 63.7, 44.5, 30.9, 15.2; HRMS (ESI, M+Na) calcd for $C_{19}H_{18}N_2Na_1O_4$ 361.1164, found 361.1184. **3aa** (polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.5 Hz, 1H), 7.69 (dt, *J* = 0.9, 7.5 Hz, 1H), 7.54 (d, *J* = 7.5 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.38-7.24 (m, 5H), 7.14 (brs, 1H), 5.29 (q, *J* = 6.9 Hz, 1H), 4.56 (dd, *J* = 14.7, 6.0 Hz, 1H), 4.33 (dd, *J* = 14.7, 5.1 Hz, 1H), 4.07 (d, *J* = 18.9 Hz, 1H), 3.52 (d, *J* = 18.9 Hz, 1H), 1.48 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.4, 165.7, 153.8, 137.3, 136.8, 134.7, 128.8, 128.2, 127.8, 127.7, 126.6, 124.9, 86.9, 63.1, 44.4, 32.5, 15.0; HRMS (ESI, M+Na) calcd for $C_{19}H_{18}N_2Na_1O_4$ 361.11643, found 361.11421.



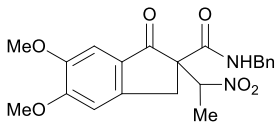
***N*-Benzyl-5-methyl-2-(1-nitroethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (3ba).**

According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 1:1 mixture of inseparable diastereomers (88% combined yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.2 Hz, 0.5H), 7.65 (d, *J* = 6.9 Hz, 0.5H), 7.46-7.12 (m, 9H), 5.27 (q, *J* = 6.9 Hz, 0.5H), 5.24 (q, *J* = 6.9 Hz, 0.5H), 4.56 (dd, *J* = 14.7, 5.7 Hz, 0.5H), 4.52 (dd, *J* = 14.7, 6.0 Hz, 0.5H), 4.33 (dd, *J* = 14.7, 5.1 Hz, 0.5H), 4.27 (dd, *J* = 14.7, 5.4 Hz, 0.5H), 4.14 (d, *J* = 18.0 Hz, 0.5H), 4.01 (d, *J* = 18.6 Hz, 0.5H), 3.47 (d, *J* = 18.6 Hz, 0.5H), 3.11 (d, *J* = 18.0 Hz, 0.5H), 2.47 (s, 1.5H), 2.45 (s, 1.5H), 1.62 (d, *J* = 6.9 Hz, 1.5H), 1.47 (d, *J* = 6.9 Hz, 1.5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.4, 201.5, 165.9, 164.8, 154.3, 153.7, 148.6, 147.9, 137.3, 137.3, 132.3, 132.1, 129.5, 129.3, 128.8, 128.7, 127.8, 127.7, 127.6, 126.9, 124.7, 124.7, 86.8, 85.2, 63.7, 63.2, 44.4, 44.3, 32.1, 30.7, 22.3, 22.2, 15.1, 14.9; HRMS (ESI, M+Na) calcd for $C_{20}H_{20}N_2Na_1O_4$ 375.1321, found 375.1285.



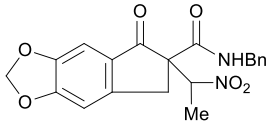
***N*-Benzyl-5-methoxy-2-(1-nitroethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (3ca).**

According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 1:1 mixture of inseparable diastereomers (73% combined yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.71-7.64 (m, 2H), 7.50 (t, *J* = 5.1 Hz, 1H), 7.36-7.20 (m, 11H), 6.97-6.91 (m, 4H), 5.26 (q, *J* = 6.9 Hz, 1H), 5.24 (q, *J* = 6.9 Hz, 1H), 4.56 (dd, *J* = 14.1, 6.0 Hz, 1H), 4.52 (dd, *J* = 14.1, 6.0 Hz, 1H), 4.32 (dd, *J* = 14.7, 5.1 Hz, 1H), 4.28 (dd, *J* = 14.7, 5.1 Hz, 1H), 4.14 (d, *J* = 17.7 Hz, 1H), 4.02 (d, *J* = 18.9 Hz, 1H), 3.91 (s, 3H), 3.89 (s, 3H), 3.48 (d, *J* = 18.9 Hz, 1H), 3.14 (d, *J* = 17.7 Hz, 1H), 1.61 (d, *J* = 6.9 Hz, 3H), 1.45 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.8, 199.9, 167.0 , 166.6, 166.1, 165.1, 157.3, 156.6, 137.4, 137.3, 128.8, 128.7, 127.8, 127.7, 127.6, 127.4, 116.9, 116.5, 109.4, 109.2, 86.8, 85.1, 63.7, 63.3, 55.9, 55.8, 44.4, 44.3, 31.9, 30.8, 15.2, 14.8; HRMS (ESI, M+Na) calcd for $C_{20}H_{20}N_2Na_1O_5$ 391.1270, found 391.1256.



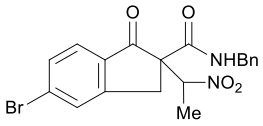
***N*-Benzyl-5,6-dimethoxy-2-(1-nitroethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide(3da).**

According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 1:1 mixture of separable diastereomers (84% combined yield). **3da** (less polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50 (brt, *J* = 5.7 Hz, 1H), 7.36-7.28 (m, 3H), 7.23-7.21 (m, 3H), 7.16 (s, 1H), 6.89 (s, 1H), 5.24 (q, *J* = 6.9, 1H), 4.52 (dd, *J* = 14.7, 6.0 Hz, 1H), 4.28 (dd, *J* = 14.7, 5.4 Hz, 1H), 4.08 (d, *J* = 17.7 Hz, 1H), 3.10 (d, *J* = 17.7 Hz, 1H), 1.61 (d, *J* = 6.9 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.1, 165.1, 156.9, 149.9, 149.4, 137.3, 128.8, 127.7, 127.7 127.0 107.4, 104.8, 85.1, 63.9, 56.4, 56.1, 44.4, 30.5, 15.2; HRMS (ESI, M+Na) calcd for $C_{21}H_{22}N_2Na_1O_6$ 421.1376, found 421.1333. **3da** (polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36-7.21 (m, 6H), 7.12 (s, 1H), 6.93 (s, 1H), 5.27 (q, *J* = 6.9 Hz, 1H), 4.56 (dd, *J* = 14.7, 6.0 Hz, 1H), 4.34 (dd, *J* = 14.7, 5.1 Hz, 1H), 4.00 (s, 3H), 3.95 (d, *J* = 18.3 Hz, 1H), 3.90 (s, 3H), 3.43 (d, *J* = 18.3 Hz, 1H), 1.45 (d, *J* = 6.9 Hz, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.2, 166.2, 157.3, 150.1, 137.4, 128.7, 127.8, 127.6, 127.2, 107.2, 104.6, 86.8, 63.3, 56.5, 56.1, 44.3, 31.8, 14.8; HRMS (ESI, M+Na) calcd for $C_{21}H_{22}N_2Na_1O_6$ 421.1376, found 421.1358.



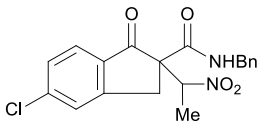
***N*-Benzyl-6-(1-nitroethyl)-5-oxo-6,7-dihydro-5*H*-indeno[5,6-*d*][1,3]dioxole-6-carboxamide (3ea).**

According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 1:1 mixture of separable diastereomers (93% combined yield). **3ea** (less polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46 (br, 1H), 7.36-7.20 (m, 5H), 7.10 (s, 1H), 6.85 (s, 1H), 6.09 (s, 1H), 6.09 (s, 1H), 5.21 (q, *J* = 6.9 Hz, 1H), 4.52 (dd, *J* = 14.7, 6.0 Hz, 1H), 4.28 (dd, *J* = 14.7, 5.1 Hz, 1H), 4.05 (d, *J* = 18.0 Hz, 1H), 3.06 (d, *J* = 18.0 Hz, 1H), 1.61 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.6, 164.9, 155.7, 151.7, 148.8, 137.3, 128.8, 128.8, 127.7, 127.6, 105.8, 103.0, 102.6, 85.1, 64.0, 44.4, 30.7, 15.1; HRMS (ESI, M+Na) calcd for $C_{20}H_{18}N_2Na_1O_6$ 405.1063, found 405.1062. **3ea** (polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37-7.23 (m, 5H), 7.22 (br, 1H), 7.06 (s, 1H), 6.89 (s, 1H), 6.11 (s, 2H), 5.23 (q, *J* = 6.9 Hz, 1H), 4.57 (dd, *J* = 15.0, 6.3 Hz, 1H), 4.33 (dd, *J* = 15.0, 5.4 Hz, 1H), 3.92 (d, *J* = 18.9 Hz, 1H), 3.40 (d, *J* = 18.9 Hz, 1H), 1.24 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.7, 165.9, 156.2, 152.4, 149.0, 137.4, 129.0, 128.7, 127.8, 127.6, 105.7, 102.8, 102.8, 86.8, 63.5, 44.3, 32.0, 14.8; HRMS (ESI, M+Na) calcd for $C_{20}H_{18}N_2Na_1O_6$ 405.10626, found 405.10437.



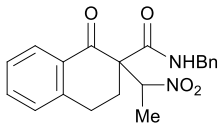
***N*-Benzyl-5-bromo-2-(1-nitroethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (3fa)**.

According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 7:3 mixture of inseparable diastereomers (85% combined yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.73-7.53 (m, 3H), 7.38-7.23 (m, 5.7H), 7.23-7.18 (m, 1H), 7.12 (brs, 0.3H), 5.26 (q, *J* = 6.9 Hz, 0.3H), 5.23 (q, *J* = 6.9 Hz, 0.7H), 4.54 (dd, *J* = 14.7, 6.0 Hz, 0.3H), 4.52 (dd, *J* = 14.7, 6.3 Hz, 0.7H), 4.33 (dd, *J* = 14.7, 5.4 Hz, 0.3H), 4.27 (dd, *J* = 14.7, 5.4 Hz, 0.7H), 4.20 (d, *J* = 18.0 Hz, 0.7H), 4.06 (d, *J* = 18.6 Hz, 0.3H), 3.48 (d, *J* = 18.6 Hz, 0.3H), 3.13 (d, *J* = 18.0 Hz, 0.7H), 1.62 (d, *J* = 6.9 Hz, 2.7H), 1.50 (d, *J* = 6.9 Hz, 0.9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.1, 201.3, 165.2, 164.2, 155.0, 154.6, 137.1, 137.1, 133.5, 133.3, 132.6, 132.0, 131.7, 129.9, 128.9, 128.8, 127.8, 127.7, 127.6, 125.9, 86.8, 85.1, 63.8, 63.1, 44.6, 44.5, 32.3, 30.6, 15.1, 15.1; HRMS (ESI, M+Na) calcd for $C_{19}H_{17}{}^{81}Br_1N_2Na_1O_4$ 441.0249 and $C_{19}H_{17}{}^{79}Br_1N_2Na_1O_4$ 439.0269, found 441.0222 and 439.0240.



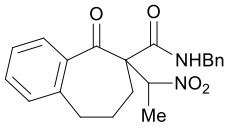
***N*-Benzyl-5-chloro-2-(1-nitroethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (3ga).**

According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 1:1 mixture of inseparable diastereomers (85% combined yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.01 (brt, *J* = 6.3 Hz, 1H), 7.51 (d, *J* = 9.9 Hz, 1H), 7.42-7.10 (m, 9H), 5.26 (q, *J* = 6.9, 0.5H), 5.23 (q, *J* = 6.9, 0.5H), 4.56 (dd, *J* = 14.7, 6.0 Hz, 0.5H), 4.52 (dd, *J* = 14.7, 6.3 Hz, 0.5H), 4.33 (dd, *J* = 14.7, 5.4 Hz, 0.5H), 4.28 (dd, *J* = 14.7, 5.4 Hz, 0.5H), 4.20 (d, *J* = 17.4 Hz, 0.5H), 4.06 (d, *J* = 18.6 Hz, 0.5H), 3.48 (d, *J* = 18.6 Hz, 0.5H), 3.13 (d, *J* = 17.4 Hz, 0.5H), 1.63 (d, *J* = 6.9 Hz, 1.5H), 1.50 (d, *J* = 6.9 Hz, 1.5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.8, 201.1, 165.3, 164.2, 155.0, 154.6, 143.6, 143.0, 137.1, 133.1, 132.9, 129.2, 128.9, 128.8, 127.8, 127.8, 127.7, 126.8, 126.0, 125.9, 86.9, 85.2, 63.9, 63.2, 44.6, 44.5, 32.4, 30.7, 15.1, 15.1; HRMS (ESI, M+Na) calcd for $C_{19}H_{17}Cl_1N_2Na_1O_4$ 395.0775, found 395.0744.



***N*-Benzyl-2-(1-nitroethyl)-1-oxo-1,2,3,4-tetrahydronaphthalene-2-carboxamide (3ha).**

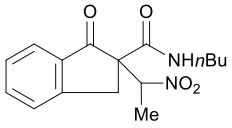
According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 7:3 mixture of inseparable diastereomers (88% combined yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 7.5, 1.2 Hz, 0.7H), 8.02 (dd, *J* = 7.5, 0.9 Hz, 0.3H), 7.56 (td, *J* = 7.5, 1.2 Hz, 0.3H), 7.55 (td, *J* = 7.5, 1.5 Hz, 0.7H), 7.38-7.24 (m, 5H), 7.20-7.12 (m, 2H), 7.02 (br, 0.7H), 6.62 (br, 0.3H), 5.48 (q, *J* = 6.9 Hz, 0.7H), 5.35 (q, *J* = 6.9 Hz, 0.3H), 4.53 (dd, *J* = 14.7, 6.3 Hz, 0.3H), 4.51 (dd, *J* = 14.7, 6.6 Hz, 0.7H), 4.29 (dd, *J* = 14.7, 5.1 Hz, 0.3H), 4.22 (dd, *J* = 14.7, 5.1 Hz, 0.7H), 3.24-3.12 (m, 1H), 2.98-2.78 (m, 2H), 2.35-2.16 (m, 1H), 1.61 (d, *J* = 6.9 Hz, 0.3H), 1.56 (d, *J* = 6.9 Hz, 0.7H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.5, 196.8, 164.7, 164.0, 144.3, 143.9, 137.2, 137.2, 135.1, 134.9, 131.3, 128.8, 128.8, 128.7, 128.7, 128.4, 127.7, 127.7, 127.6, 127.5, 127.4, 127.0, 127.0, 87.5, 85.5, 61.0, 60.8, 44.4, 44.3, 26.3, 25.9, 25.8, 24.3, 15.7, 14.0; HRMS (ESI, M+Na) calcd for $C_{20}H_{20}N_2Na_1O_4$ 375.1321, found 375.1342.



***N*-Benzyl-6-(1-nitroethyl)-5-oxo-6,7,8,9-tetrahydro-5*H*-benzo[7]annulene-6-carboxamide (3ia).**

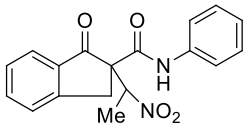
According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 3:2 mixture of inseparable diastereomers (84% combined yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.5, 0.4H), 7.58 (d, *J* = 7.5, 0.6H), 7.52 (br, 0.6H), 7.51-7.38

(m, 2H), 7.37-7.22 (m, 6.4H), 7.12 (d, J = 7.5, 0.6H), 7.08 (d, J = 7.5, 0.4H), 5.43 (q, J = 6.9 Hz, 0.6H), 5.06 (q, J = 6.9 Hz, 0.4H), 4.57-4.37 (m, 2H), 2.78-2.38 (m, 3H), 3.36-3.26 (m, 0.6H), 2.24-2.10 (m, 0.4H), 1.91-1.50 (m, 2H), 1.65 (d, J = 6.9 Hz, 1.2H), 1.52 (d, J = 6.9 Hz, 1.8H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 210.8, 210.1, 165.0, 164.2, 140.1, 139.2, 138.3, 137.4, 137.3, 137.2, 133.0, 132.4, 129.5, 128.8, 128.8, 128.5, 128.2, 127.9, 127.8, 127.1, 91.3, 88.5, 62.4, 62.0, 44.3, 44.2, 31.2, 30.8, 28.3, 22.9, 22.4, 22.1, 16.5, 14.0; HRMS (ESI, M+Na) calcd for $C_{21}H_{22}N_2Na_1O_4$ 389.1477, found 389.1513.



***N*-Butyl-2-(1-nitroethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (3ja).**

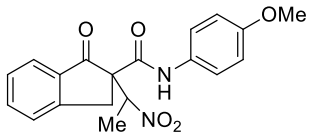
According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 1:1 mixture of separable diastereomers (80% combined yield). **3ja** (less polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 (d, J = 8.1 Hz, 1H), 7.64 (td, J = 7.2, 1.2 Hz, 1H), 7.49 (d, J = 8.1 Hz, 1H), 7.40 (td, J = 7.2, 1.2 Hz, 1H), 7.00 (bs, 1H), 5.26 (q, J = 6.9 Hz, 1H), 4.19 (d, J = 17.4 Hz, 1H), 3.34-3.23 (m, 1H), 3.20-3.09 (m, 1H) 3.13 (d, J = 17.4 Hz, 1H), 1.67 (d, J = 6.9 Hz, 1H), 1.54-1.42 (m, 2H), 1.36-1.24 (m, 2H), 0.90 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.5, 164.5, 153.3, 136.2, 134.5, 127.9, 126.6, 124.8, 85.4, 63.7, 40.3, 31.2, 30.9, 20.0, 15.2, 13.7; HRMS (ESI, M+Na) calcd for $C_{16}H_{20}N_2Na_1O_4$ 327.1321, found 327.1296. **3ja** (polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.77 (d, J = 7.5 Hz, 1H), 7.68 (bt, J = 7.5 Hz, 1H), 7.53 (d, J = 7.5 Hz, 1H), 7.42 (t, J = 7.5 Hz, 1H), 6.87 (bs, 1H), 5.25 (q, J = 6.9 Hz, 1H), 4.03 (d, J = 18.6 Hz, 1H), 3.48 (d, J = 18.6 Hz, 1H), 3.40-3.28 (m, 1H), 3.21-3.10 (m, 1H), 1.52 (d, J = 6.9 Hz, 3H), 1.57-1.43 (m, 2H), 1.39-1.25 (m, 2H), 0.91 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.8, 165.5, 153.7, 136.7, 134.8, 128.1, 126.6, 124.8, 87.2, 62.9, 40.1, 32.7, 31.1, 20.0, 15.1, 13.7; HRMS (ESI, M+Na) calcd for $C_{16}H_{20}N_2Na_1O_4$ 327.1321, found 327.1295.



2-(1-nitroethyl)-1-oxo-*N*-phenyl-2,3-dihydro-1*H*-indene-2-carboxamide (5ka).

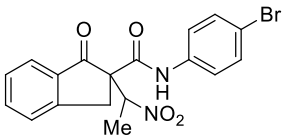
According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 10:7 mixture of separable diastereomers (92% combined yield). **5ka** (less polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.92 (s, 1H), 7.83 (d, J = 7.8 Hz, 1H), 7.67 (td, J = 7.8,

0.9 Hz, 1H), 7.54-7.49 (m, 3H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.14 (t, *J* = 7.5 Hz, 1H), 5.39 (q, *J* = 6.9 Hz, 1H), 4.26 (d, *J* = 18.0 Hz, 1H), 3.21 (d, *J* = 18.0 Hz, 1H), 1.74 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.6, 162.4, 153.3, 137.0, 136.5, 134.4, 129.1, 128.1, 126.6, 125.1, 125.0, 119.9, 85.3, 64.2, 30.7, 15.3; HRMS (ESI, M+Na) calcd for $C_{18}H_{16}N_2Na_1O_4$ 347.1008, found 347.0987. **5ka** (polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.85 (s, 1H), 7.82 (d, *J* = 7.5 Hz, 1H), 7.72 (td, *J* = 7.5, 0.9 Hz, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 7.5 Hz, 2H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.14 (t, *J* = 7.5 Hz, 1H), 5.34 (q, *J* = 6.9 Hz, 1H), 4.12 (d, *J* = 18.9 Hz, 1H), 3.55 (d, *J* = 18.9 Hz, 1H), 1.57 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.0, 163.6, 153.7, 137.0, 136.9, 134.7, 129.0, 128.3, 126.6, 125.1, 125.0, 120.4, 87.3, 63.5, 32.3, 15.0; HRMS (ESI, M+Na) calcd for $C_{18}H_{16}N_2Na_1O_4$ 347.1008, found 347.0985.



***N*-(4-methoxyphenyl)-2-(1-nitroethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (5la).**

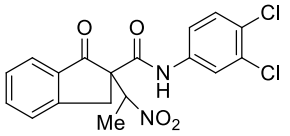
According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 10:7 mixture of separable diastereomers (97% combined yield). **5la** (less polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.79 (s, 1H), 7.83 (d, *J* = 7.5 Hz, 1H), 7.67 (td, *J* = 7.5, 1.2 Hz, 1H), 7.52 (d, *J* = 7.5 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.41 (bd, *J* = 9.0 Hz, 2H), 6.86 (bd, *J* = 9.0 Hz, 1H), 5.39 (q, *J* = 6.9 Hz, 1H), 4.25 (d, *J* = 18.0 Hz, 1H), 3.20 (d, *J* = 18.0 Hz, 1H), 1.73 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.7, 162.2, 156.9, 153.3, 136.5, 134.5, 130.1, 128.0, 126.6, 125.0, 121.6, 114.2, 85.3, 64.1, 55.5, 30.8, 15.3; HRMS (ESI, M+Na) calcd for $C_{19}H_{18}N_2Na_1O_5$ 377.1113, found 377.1132. **5la** (polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.72 (s, 1H), 7.82 (d, *J* = 7.5 Hz, 1H), 7.71 (d, *J* = 7.5 Hz, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.40 (d, *J* = 9.0 Hz, 1H), 6.86 (d, *J* = 9.0 Hz, 1H), 5.33 (q, *J* = 6.9 Hz, 1H), 4.11 (d, *J* = 18.6 Hz, 1H), 3.79 (s, 3H), 4.55 (d, *J* = 18.6 Hz, 1H), 1.56 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.1, 163.5, 156.9, 153.7, 137.0, 134.7, 130.0, 128.3, 126.6, 125.0, 122.2, 114.1, 87.3, 63.3, 55.5, 32.4, 15.0; HRMS (ESI, M+Na) calcd for $C_{19}H_{18}N_2Na_1O_5$ 377.1113, found 377.1104.



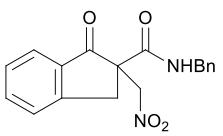
***N*-(4-bromophenyl)-2-(1-nitroethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (5ma).**

According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title

compound was obtained as a 10:7 mixture of separable diastereomers (95% combined yield). **5ma** (less polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.95 (s, 1H), 7.83 (d, *J* = 7.5 Hz, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 7.5 Hz, 1H), 7.46-7.36 (m, 5H), 5.34 (q, *J* = 6.9 Hz, 1H), 4.23 (d, *J* = 17.7 Hz, 1H), 3.21 (d, *J* = 17.7 Hz, 1H), 1.72 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.6, 162.5, 153.3, 136.6, 136.1, 134.3, 132.1, 128.2, 126.6, 125.0, 121.4, 117.8, 85.2, 64.1, 30.7, 15.3; HRMS (ESI, M+Na) calcd for $C_{18}H_{15}{}^{81}Br_1N_2Na_1O_4$ 427.0092 and $C_{18}H_{15}{}^{79}Br_1N_2Na_1O_4$ 425.0113, found 427.0076 and 425.0159. **5ma** (polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.92 (s, 1H), 7.82 (d, *J* = 7.5 Hz, 1H), 7.73 (td, *J* = 7.5, 0.9 Hz, 1H), 7.57 (d, *J* = 7.5 Hz, 1H), 7.49-7.39 (m, 5H), 5.30 (q, *J* = 6.9 Hz, 1H), 4.10 (d, *J* = 18.6 Hz, 1H), 3.55 (d, *J* = 18.6 Hz, 1H), 1.53 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.9, 163.7, 153.8, 137.2, 136.0, 134.5, 132.0, 128.4, 126.6, 125.1, 121.9, 117.7, 87.1, 63.5, 31.9, 30.1, 14.8; HRMS (ESI, M+Na) calcd for $C_{18}H_{15}{}^{81}Br_1N_2Na_1O_4$ 427.0092 and $C_{18}H_{15}{}^{79}Br_1N_2Na_1O_4$ 425.0113, found 427.0070 and 425.0068.

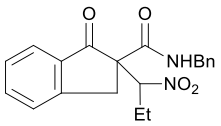


***N*-(3,4-dichlorophenyl)-2-(1-nitroethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (5na).**
According to the general procedure for oxidative α-nitroalkylation of β-ketoamides, the title compound was obtained as a 10:7 mixture of separable diastereomers (63% combined yield). **5na** (less polar):^{1}H NMR (300 MHz, $CDCl_3$) δ 8.98 (s, 1H), 7.83 (d, *J* = 7.8 Hz, 1H), 7.78 (d, *J* = 2.4 Hz, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.52 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 9.0 Hz, 1H), 7.32 (dd, *J* = 9.0, 2.4 Hz, 1H), 5.34 (q, *J* = 7.2 Hz, 1H), 4.21 (d, *J* = 17.7 Hz, 1H), 3.25 (d, *J* = 17.7 Hz, 1H), 1.72 (d, *J* = 17.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.4, 162.9, 153.3, 136.7, 136.6, 134.4, 133.1, 130.7, 128.6, 128.2, 126.6, 125.1, 121.8, 119.2, 85.3, 64.3, 30.9, 15.3; HRMS (ESI, M+Na) calcd for $C_{18}H_{14}Cl_2N_2Na_1O_4$ 415.0228, found 415.0201. **5na** (polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.88 (s, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.75-7.70 (m, 2H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.41-7.32 (m, 2H), 5.27 (q, *J* = 6.9 Hz, 1H), 4.97 (d, *J* = 18.9 Hz, 1H), 3.54 (d, *J* = 18.9 Hz, 1H), 1.53 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.8, 163.9, 153.8, 137.3, 136.6, 134.6, 133.0, 130.6, 128.5, 126.7, 125.2, 122.2, 119.7, 87.1, 63.7, 32.1, 14.9; HRMS (ESI, M+Na) calcd for $C_{18}H_{14}Cl_2N_2Na_1O_4$ 415.0228, found 415.0276.



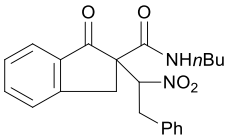
***N*-Benzyl-2-(nitromethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (3ab).**

According to the general procedure for oxidative α-nitroalkylation of β-ketoamides using $CHCl_3$ as a solvent, the title compound was obtained as a 1:1 mixture of separable diastereomers (90% combined yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.8 Hz, 1H), 7.68 (brt, *J* = 7.8 Hz, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.36-7.24 (m, 3H), 7.21 (brd, *J* = 6.3 Hz, 2H), 7.03 (brs, 1H), 5.00 (d, *J* = 13.5 Hz, 1H), 4.92 (d, *J* = 13.5 Hz, 1H), 4.49 (dd, *J* = 14.7, 6.0 Hz, 1H), 4.32 (dd, *J* = 14.7, 5.4 Hz, 1H), 4.18 (d, *J* = 18.0 Hz, 1H), 3.25 (d, *J* = 18.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.0, 164.9, 152.9, 137.1, 136.5, 134.2, 128.7, 128.2, 127.6, 127.4, 126.6, 124.9, 78.6, 59.3, 44.2, 34.3; HRMS (ESI, M+Na) calcd for $C_{18}H_{16}N_2Na_1O_4$ 347.1008, found 347.0994.



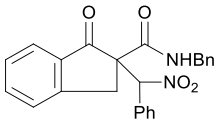
***N*-Benzyl-2-(1-nitropropyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (3ac).**

According to the general procedure for oxidative α-nitroalkylation of β-ketoamides using $CHCl_3$ as a solvent, the title compound was obtained as a 1:1 mixture of separable diastereomers (82% combined yield). **3ac** (less polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.1 Hz, 1H), 7.66 (td, *J* = 7.5, 2.1 Hz, 1H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.44-7.18 (m, 7H), 5.07 (dd, *J* = 10.2, 2.7 Hz, 1H), 4.54 (dd, *J* = 14.7, 6.3 Hz, 1H), 4.28 (dd, *J* = 14.7, 5.4 Hz, 1H), 4.17 (d, *J* = 17.7 Hz, 1H), 3.49 (d, *J* = 17.7 Hz, 1H), 2.16-2.05 (m, 1H), 1.96-1.82 (m, 1H), 1.00 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.0, 164.8, 153.8, 137.3, 136.5, 133.9, 128.8, 128.0, 127.7, 127.6, 126.6, 124.9, 92.1, 63.7, 44.4, 31.1, 23.2, 10.9; HRMS (ESI, M+Na) calcd for $C_{20}H_{20}N_2Na_1O_4$ 375.1321, found 375.1278. **3ac** (polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.1 Hz, 1H), 7.69 (td, *J* = 7.5, 2.1 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.38-7.21 (m, 6H), 5.03 (dd, *J* = 11.4, 3.0 Hz, 1H), 4.56 (dd, *J* = 14.7, 6.3 Hz, 1H), 4.33 (dd, *J* = 14.7, 5.1 Hz, 1H), 4.05 (d, *J* = 18.9 Hz, 1H), 3.62 (d, *J* = 18.9 Hz, 1H), 2.18-2.02 (m, 1H), 1.60-1.40 (m, 1H), 0.92 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.7, 165.6, 153.9, 137.2, 136.8, 134.6, 128.7, 128.1, 127.9, 127.7, 126.6, 124.9, 94.2, 63.1, 44.4, 32.7, 22.7, 10.5; HRMS (ESI, M+Na) calcd for $C_{20}H_{20}N_2Na_1O_4$ 375.1321, found 375.1279.



***N*-Benzyl-2-(1-nitro-2-phenylethyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (3ad).**

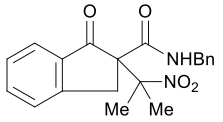
According to the general procedure for oxidative α-nitroalkylation of β-ketoamides using $CHCl_3$ as a solvent, the title compound was obtained as a 1:1 mixture of separable diastereomers (81% combined yield). **3ad** (less polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.5 Hz, 1H), 7.67 (dt, *J* = 0.9, 7.5 Hz, 1H), 7.59-7.48 (m, 2H), 7.44-7.20 (m, 9H), 7.02-6.95 (m, 2H), 5.36 (dd, *J* = 10.5, 3.0 Hz, 1H), 4.59 (dd, *J* = 14.4, 6.6 Hz, 1H), 4.24 (d, *J* = 18.0 Hz, 1H), 4.24 (dd, *J* = 14.4, 5.0 Hz, 1H), 3.57 (d, *J* = 18.0 Hz, 1H), 3.35 (dd, *J* = 15.0, 10.5 Hz, 1H), 3.13 (dd, *J* = 15.0, 3.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.5, 164.6, 153.7, 137.3, 136.7, 135.1, 133.9, 128.9, 128.8, 128.8, 128.8, 128.0, 128.0, 127.9, 127.5, 126.6, 125.1, 92.1, 63.5, 44.5, 35.5, 30.9; HRMS (ESI, M+Na) calcd for $C_{25}H_{22}N_2Na_1O_4$ 437.14773, found 437.15143. **3ad** (polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.8 Hz, 1H), 7.71 (td, *J* = 7.5, 0.9 Hz, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.37-7.21 (m, 9H), 7.10-7.04 (m, 2H), 5.34 (dd, *J* = 11.4, 2.7 Hz, 1H), 4.55 (dd, *J* = 14.7, 5.7 Hz, 1H), 4.35 (dd, *J* = 14.7, 5.1 Hz, 1H), 4.11 (d, *J* = 18.9 Hz, 1H), 3.71 (d, *J* = 18.9 Hz, 1H), 3.32 (dd, *J* = 14.4, 11.4 Hz, 1H), 2.84 (dd, *J* = 14.4, 2.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.7, 165.4, 153.7, 137.1, 136.9, 134.7, 134.4, 128.8, 128.8, 128.8, 128.3, 127.9, 127.7, 126.7, 125.0, 94.1, 63.0, 44.5, 35.4, 32.9; HRMS (ESI, M+Na) calcd for $C_{25}H_{22}N_2Na_1O_4$ 437.1477, found 437.1483.



***N*-Benzyl-2-(nitro(phenyl)methyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (3ae).**

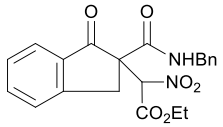
According to the general procedure for oxidative α-nitroalkylation of β-ketoamides using $CHCl_3$ as reaction solvent, the title compound was obtained as a 1:1 mixture of separable diastereomers (90% combined yield). **3ae** (less polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.5 Hz, 1H), 7.68 (td, *J* = 7.5, 0.9 Hz, 1H), 7.54 (d, *J* = 8.1 Hz, 1H), 7.48-7.40 (m, 2H), 7.40-7.32 (m, 2H), 7.30-7.26 (m, 3H), 7.24-7.19 (m, 2H), 7.15 (brt, *J* = 5.4, 1H), 6.33 (s, 1H), 4.40 (dd, *J* = 14.4, 6.6 Hz, 1H), 4.27 (d, *J* = 17.4 Hz, 1H), 4.08 (dd, *J* = 14.4 Hz, 1H), 3.55 (d, *J* = 17.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.8, 163.6, 153.7, 137.0, 136.3, 134.0, 130.6, 130.1, 128.9, 128.8, 128.7, 128.0, 127.7, 126.6, 124.9, 92.5, 64.9, 44.6, 32.3; HRMS (ESI, M+Na) calcd for $C_{24}H_{20}N_2Na_1O_4$ 423.1321, found 423.1329. **3ae** (polar): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.1 Hz, 1H), 7.56 (td, *J* = 7.5, 1.2 Hz, 1H), 7.39 (d, *J* = 7.5 Hz, 1H), 7.37-7.24 (m, 9H), 7.08-7.04 (m, 2H), 6.64 (brt, *J* = 4.8, 1H), 6.51 (s, 1H), 4.34 (dd, *J* = 14.7, 4.8 Hz, 1H), 4.29 (dd, *J* = 14.7, 4.8 Hz, 1H), 4.18 (dd, *J* = 18.6 Hz, 1H), 3.59 (d, *J* = 18.6 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.9, 165.7, 153.1, 137.0, 136.3, 134.7, 130.3, 129.9, 128.8, 128.7, 128.1, 127.9, 127.6, 127.5, 126.4, 124.9, 94.1, 64.4, 44.4, 33.7; HRMS (ESI, M+Na) calcd for $C_{24}H_{20}N_2Na_1O_4$ 423.1321, found 423.1285.

.



***N*-Benzyl-2-(2-nitropropan-2-yl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (3af).**

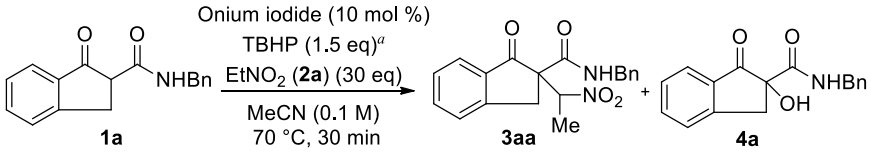
According to the general procedure for oxidative α-nitroalkylation of β-ketoamides using $CHCl_3$ as reaction solvent and neutral silica gel for purification, the titled compound was obtained in 87%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.5 Hz, 1H), 7.63 (t, 1H), 7.44-7.38 (m, 2H), 7.36-7.20 (m, 5H), 4.57 (dd, *J* = 14.7, 6.0 Hz, 1H), 4.27 (dd, *J* = 14.7, 5.4 Hz, 1H), 4.18 (d, *J* = 17.7 Hz, 1H), 3.20 (d, *J* = 17.7 Hz, 1H), 1.89 (s, 3H), 1.74 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.9, 165.2, 151.8, 137.2, 136.0, 135.5, 128.8, 127.8, 127.8, 127.7, 126.1, 124.5, 93.4, 64.5, 44.6, 35.3, 24.5, 24.2; HRMS (ESI, M+Na) calcd for $C_{20}H_{20}N_2Na_1O_4$ 375.1321, found 375.1298.



Ethyl 2-(2-(benzylcarbamoyl)-1-oxo-2,3-dihydro-1*H*-inden-2-yl)-2-nitroacetate (3ag).

According to the general procedure for oxidative α-nitroalkylation of β-ketoamides using $CHCl_3$ as a reaction solvent and neutral silica gel for purification, the titled compound was obtained as a 3:2 mixture of inseparable diastereomers (79% combined yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 (brd, *J* = 7.5 Hz, 1H), 7.69 (brt, *J* = 7.8 Hz, 1H), 7.55 (brd, *J* = 7.8, 1H), 7.45 (brt, *J* = 7.2 Hz, 0.6H), 7.37-7.26 (m, 3.4H), 7.21-7.15 (m, 2H), 6.77 (brt, *J* = 4.8 Hz, 0.4H), 6.46 (brt, *J* = 4.8 Hz, 0.6 H), 6.14 (s, 0.6H), 5.98 (s, 0.4H), 4.50 (dd, *J* = 14.4, 6.3 Hz, 0.4H), 4.45 (dd, *J* = 14.4, 5.7 Hz, 0.6H), 4.37-4.20 (m, 2H), 4.18-4.04 (m, 2H), 3.56 (d, *J* = 18.0 Hz, 0.4H), 3.54 (d, *J* = 18.6 Hz, 0.6H), 1.31 (t, *J* = 7.2 Hz, 1.2H), 1.01 (t, *J* = 7.2 Hz, 1.8H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.7, 198.9, 164.5, 163.4, 162.7, 162.5, 153.4, 153.2, 137.0, 136.3, 134.1, 133.9, 128.7, 128.3, 128.1, 127.6, 127.6, 127.5, 127.5, 126.6, 126.6, 125.1, 125.1, 90.8, 88.7, 63.6, 63.5, 62.3, 62.1, 44.4, 34.0, 32.5, 13.7, 13.3; HRMS (ESI, M+Na) calcd for $C_{21}H_{20}N_2Na_1O_6$ 419.1219, found 419.1224.

Table SI-1 Screening of the onium salts of iodide for oxidative coupling of 2,3-dihydroindanone-derived β-ketoamide **1a** and nitroethane (**2a**) in the presence of TBHP.



Entry	Onium iodide	**3aa** (%)[b]	**4a** (%)[b]
1	TBD·HI	94	2
2	MeTBD·HI	<3	18
3	nBu$_4$NI	<2	<2
4	nBu$_4$PI	<2	31
5	TMG·HI	<2	85

[a] 70% TBHP in H_2O was used. [b] Isolated yield.

^{1}H NMR studies for detecting the complex of TBD with nitronate from 2e.

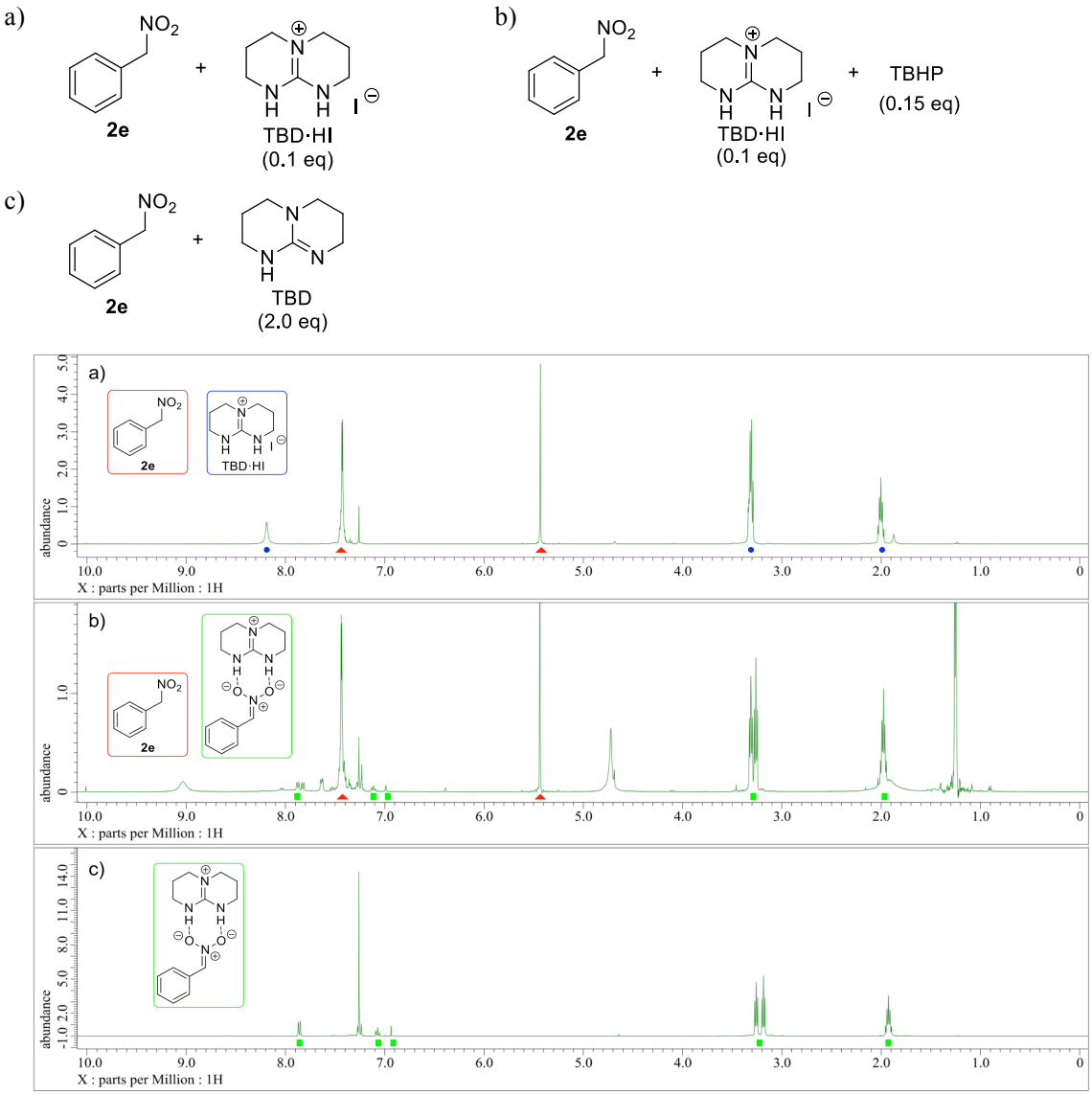


Figure SI-1 ^{1}H NMR spectra: a) α-nitrotolene:TBD·HI, b) α-nitrotolene:TBD·HI in the presence of TBHP, c) α-nitrotolene:TBD.

We performed the following NMR experiments. By mixing α-nitrotoluene **2e** and TBD·HI, we confirmed the spectra for these two species (experiment-(a)). Then, we added TBHP to the mixture of (a). With this experiment, we observed new peaks marked with green (experiment (b)). These peaks are consistent with the NMR peaks obtained by mixing with **2e** and TBD (experiment (c)), which is considered as complexation mixture of nitronate salt with TBD.

References

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6. K. V. Emelen, T. D. Wit, J. Hoornaert and F. Compernolle, *Tetrahedron,* 2002, **58**, 4225.
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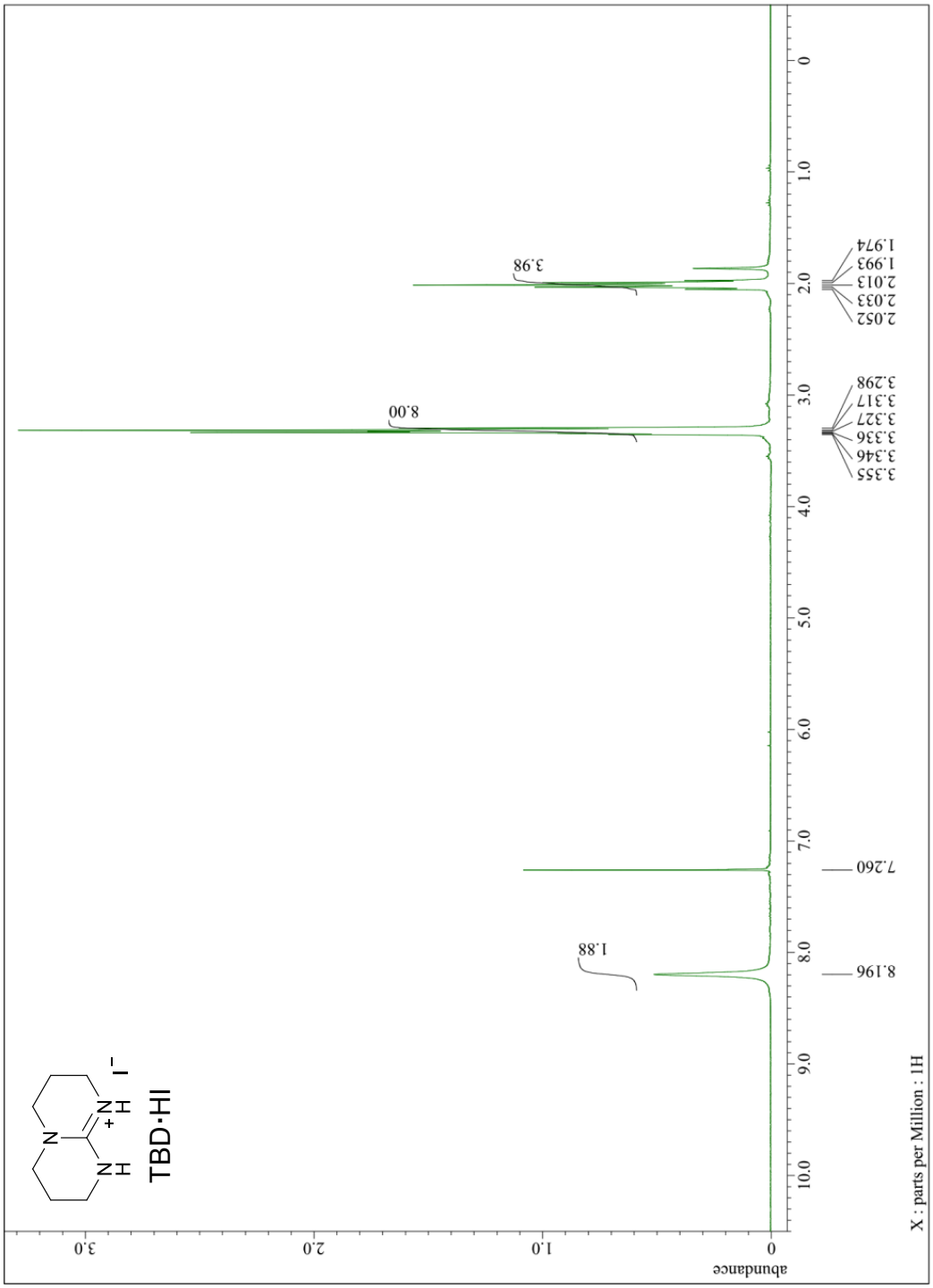
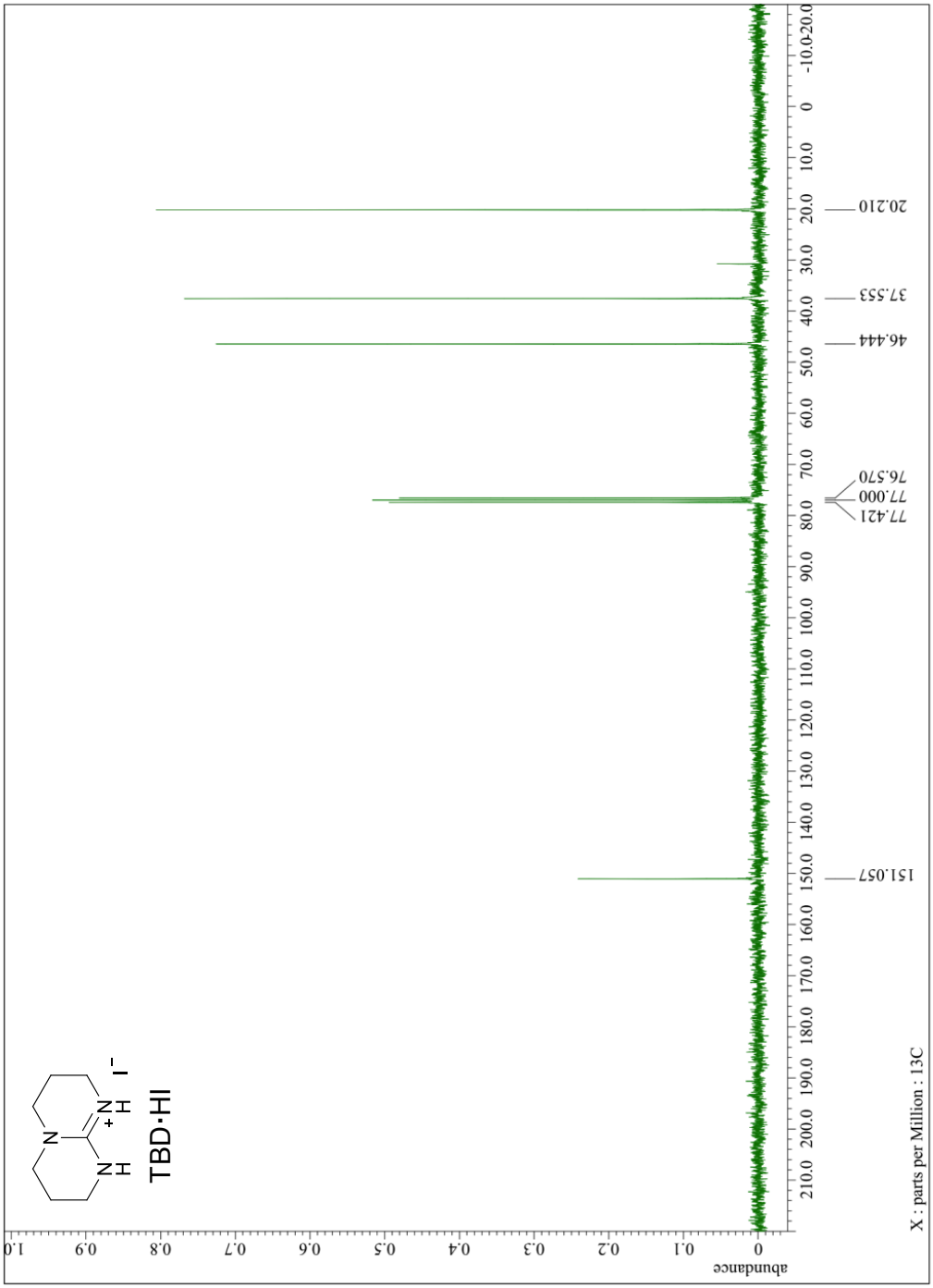
4. Copies of ^{1}H and ^{13}C NMR spectra

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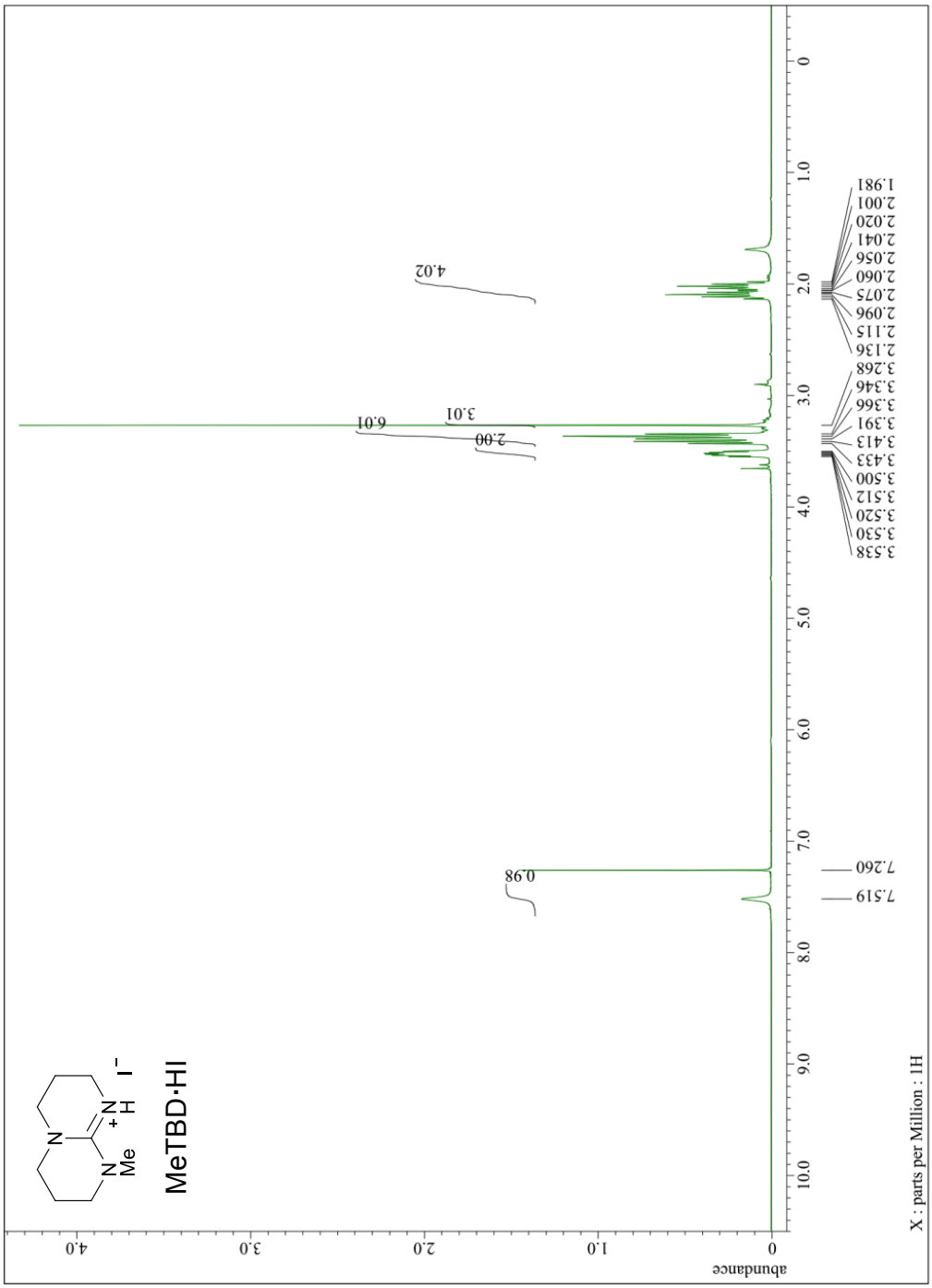
77.421
77.000
76.570
46.444
37.553
20.210


MeTBD·HI
abundance
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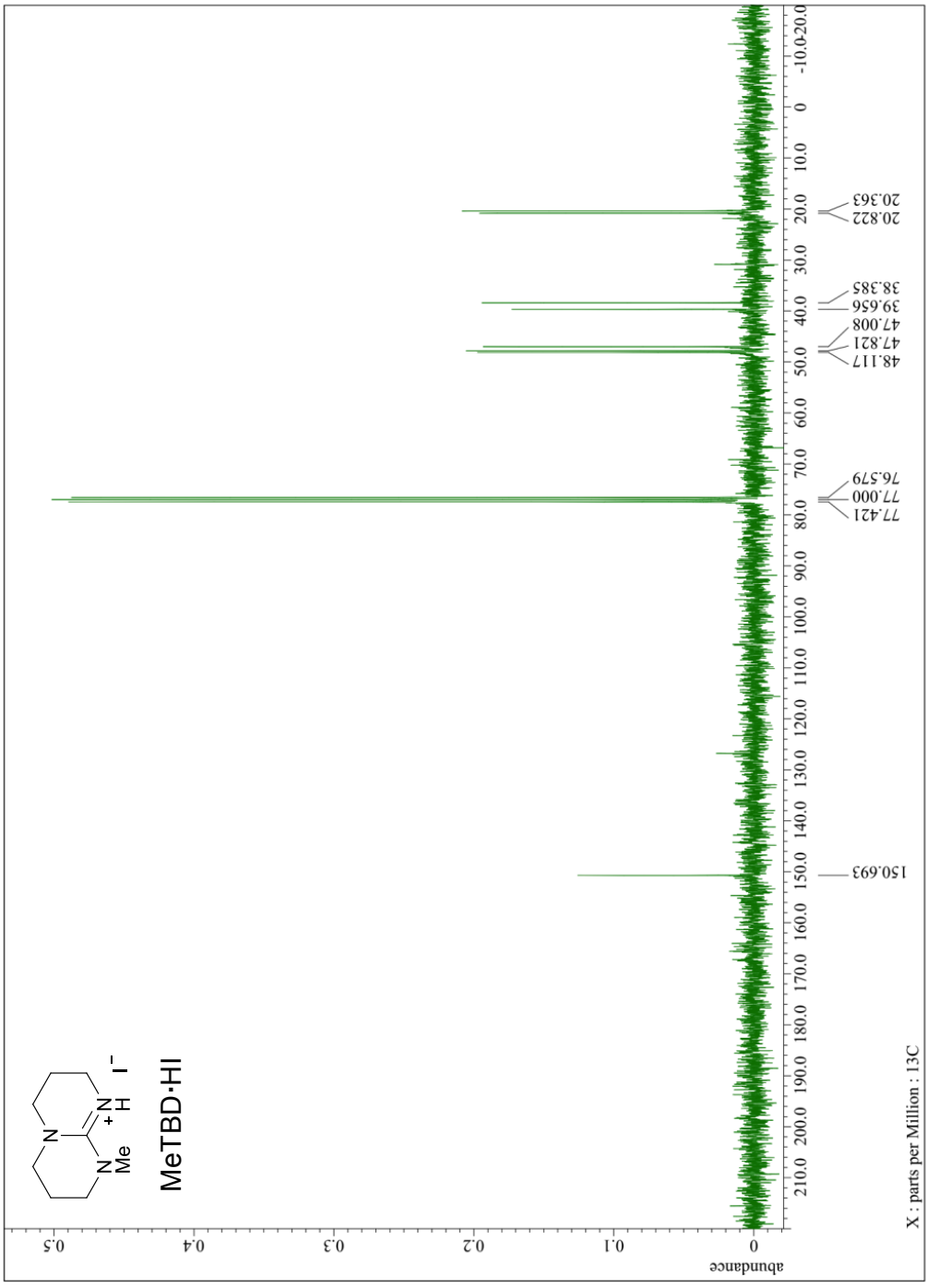
7.260
0.98
4.02
6.01
3.01
2.00
3.538
3.530
3.520
3.512
3.500
3.433
3.413
3.391
3.366
3.346
3.268
2.136
2.115
2.096
2.075
2.060
2.056
2.041
2.020
2.001
1.981


MeTBD·HI
abundance
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39.656
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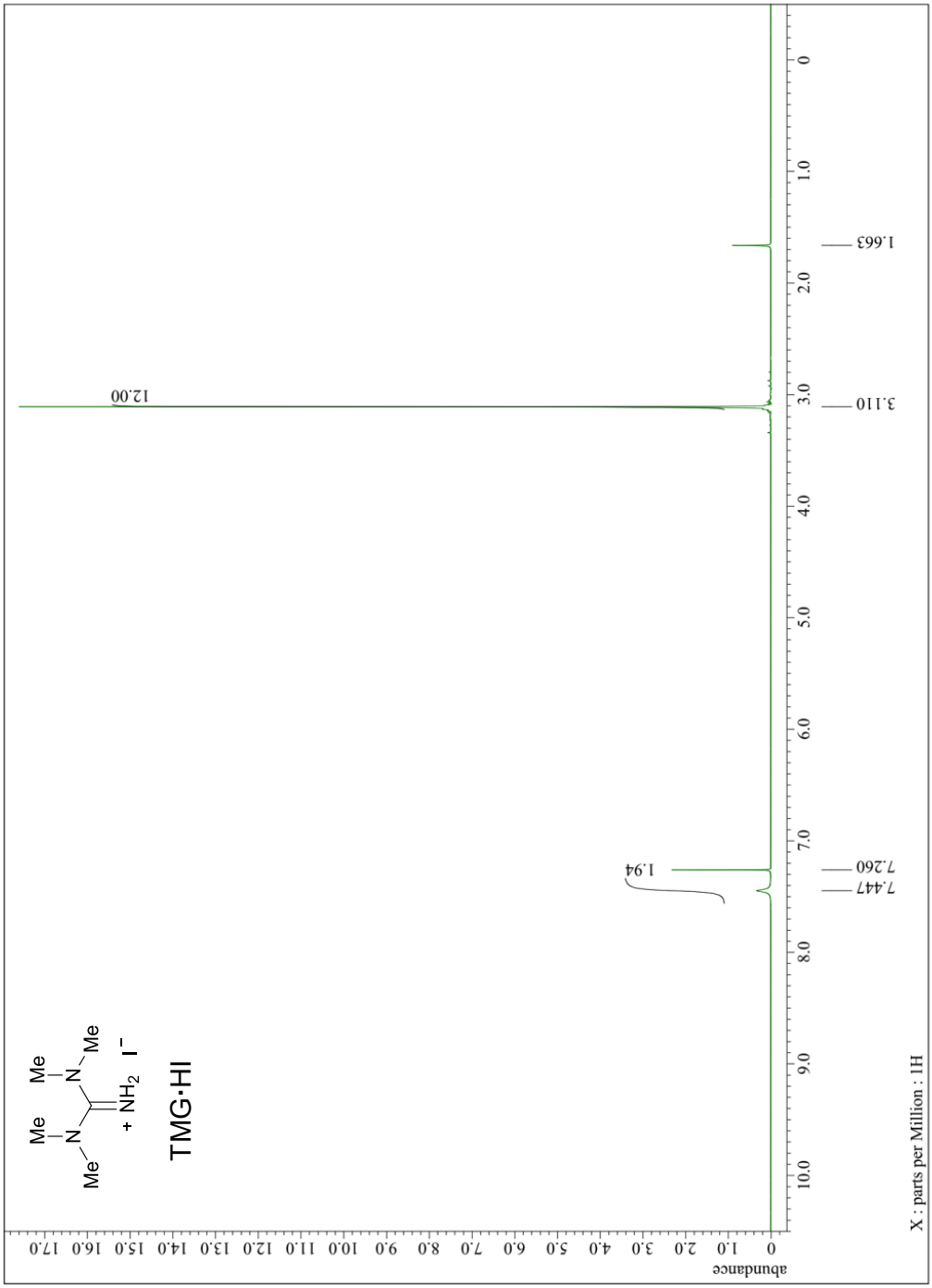
20.822
20.363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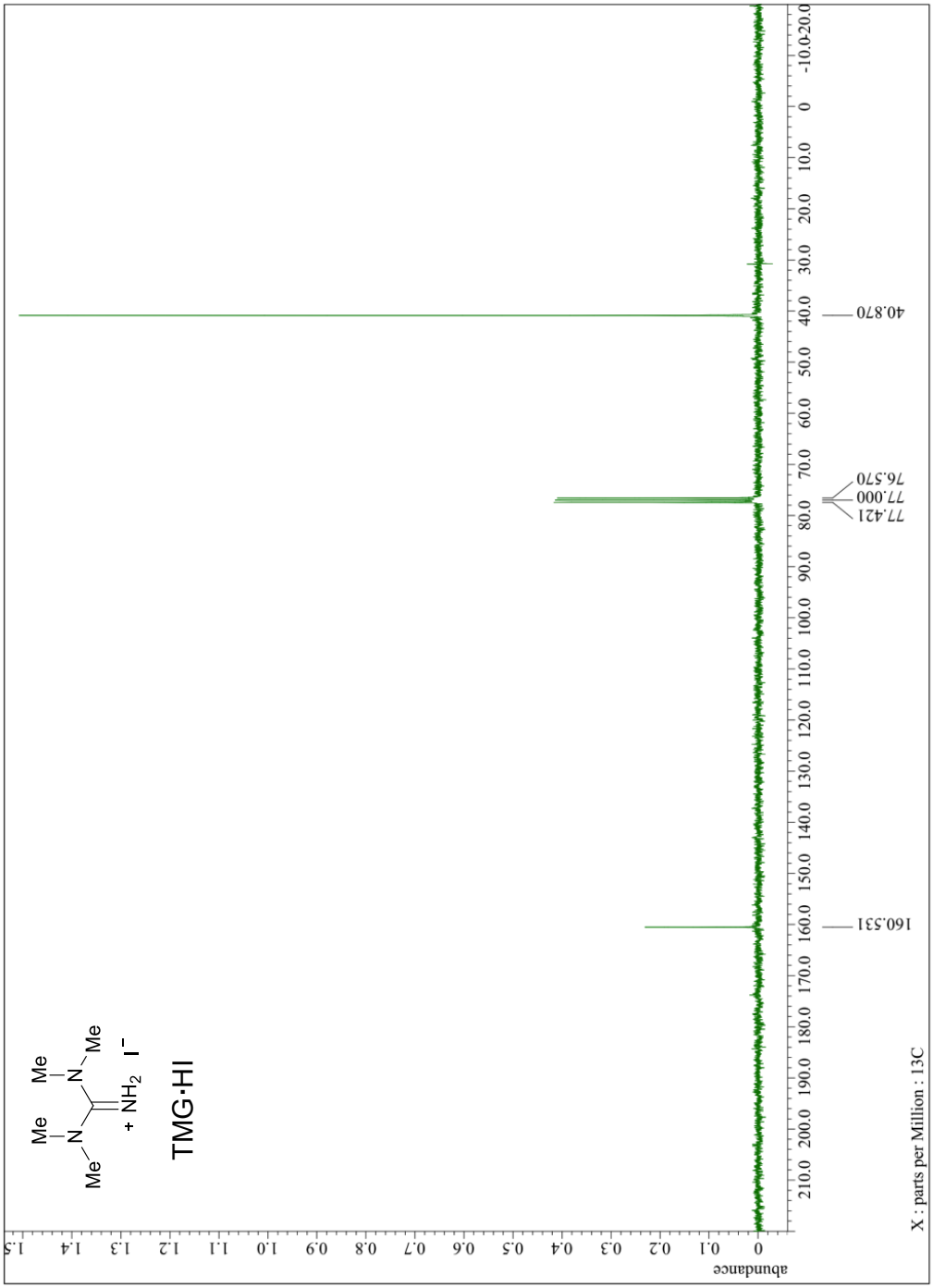
1.94
3.110
1.663
7.447
7.260
abundance
X : parts per Million : 1H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77.000
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40.870
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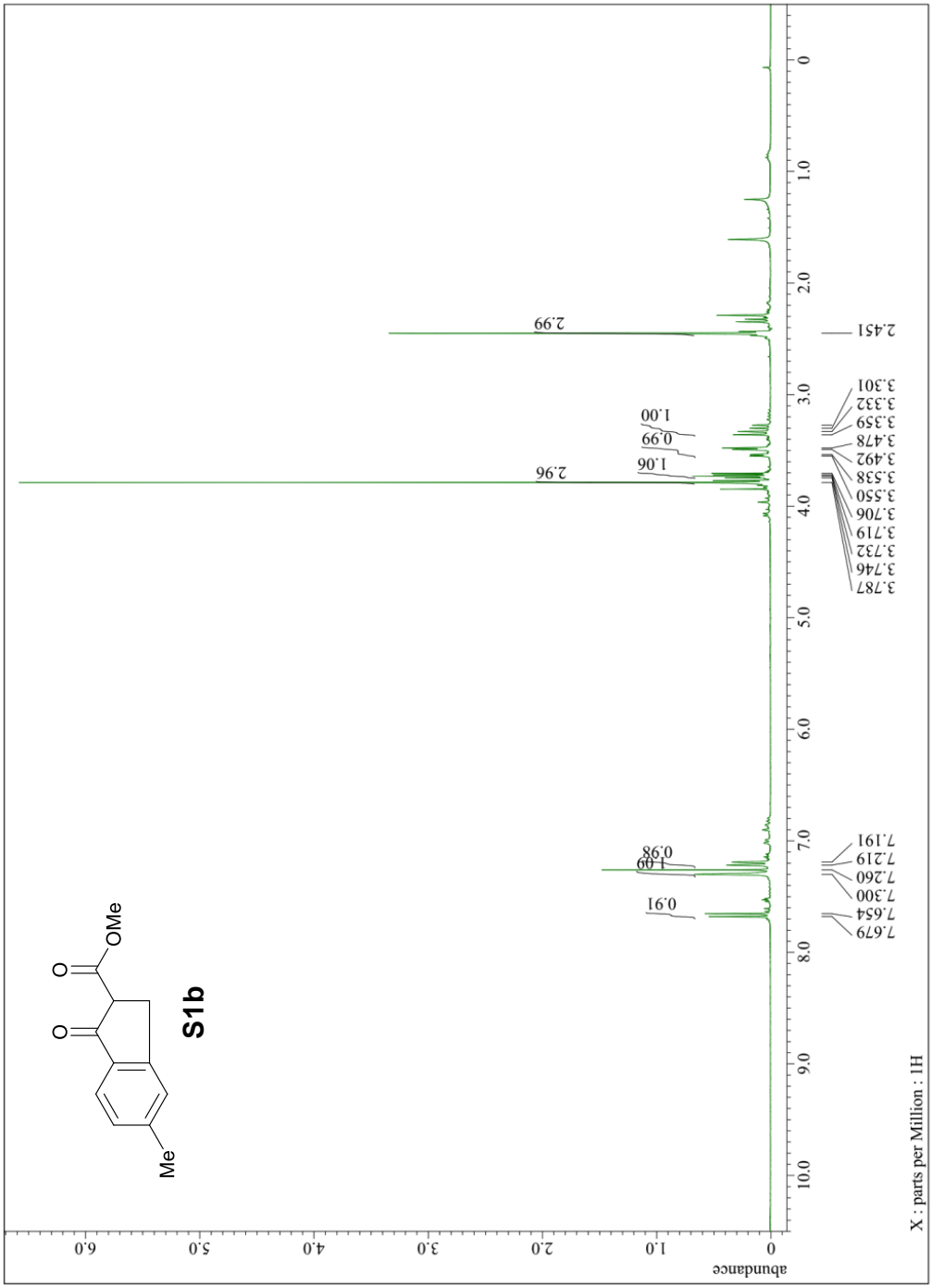
abundance


S1b
OMe
O
O
Me
abundance
X : parts per Million : 1H
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0.98
2.99
2.96
1.06
0.99
1.00
2.451
3.301
3.332
3.359
3.478
3.492
3.538
3.550
3.706
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3.732
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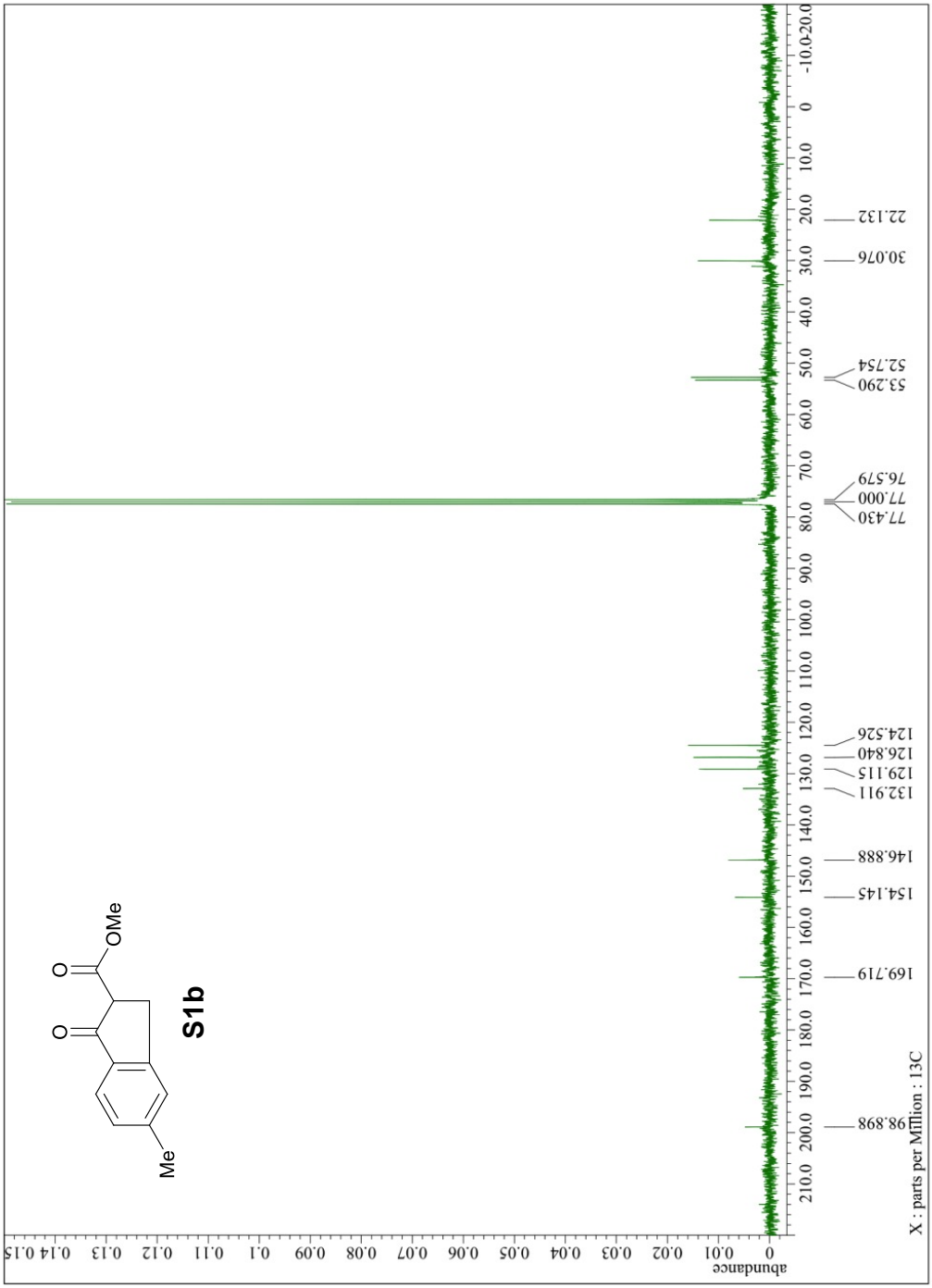
7.191
7.219
7.260
7.300
7.654
7.679


S1b
OMe
O
O
Me
X : parts per Million : 13C
abundance
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77.000
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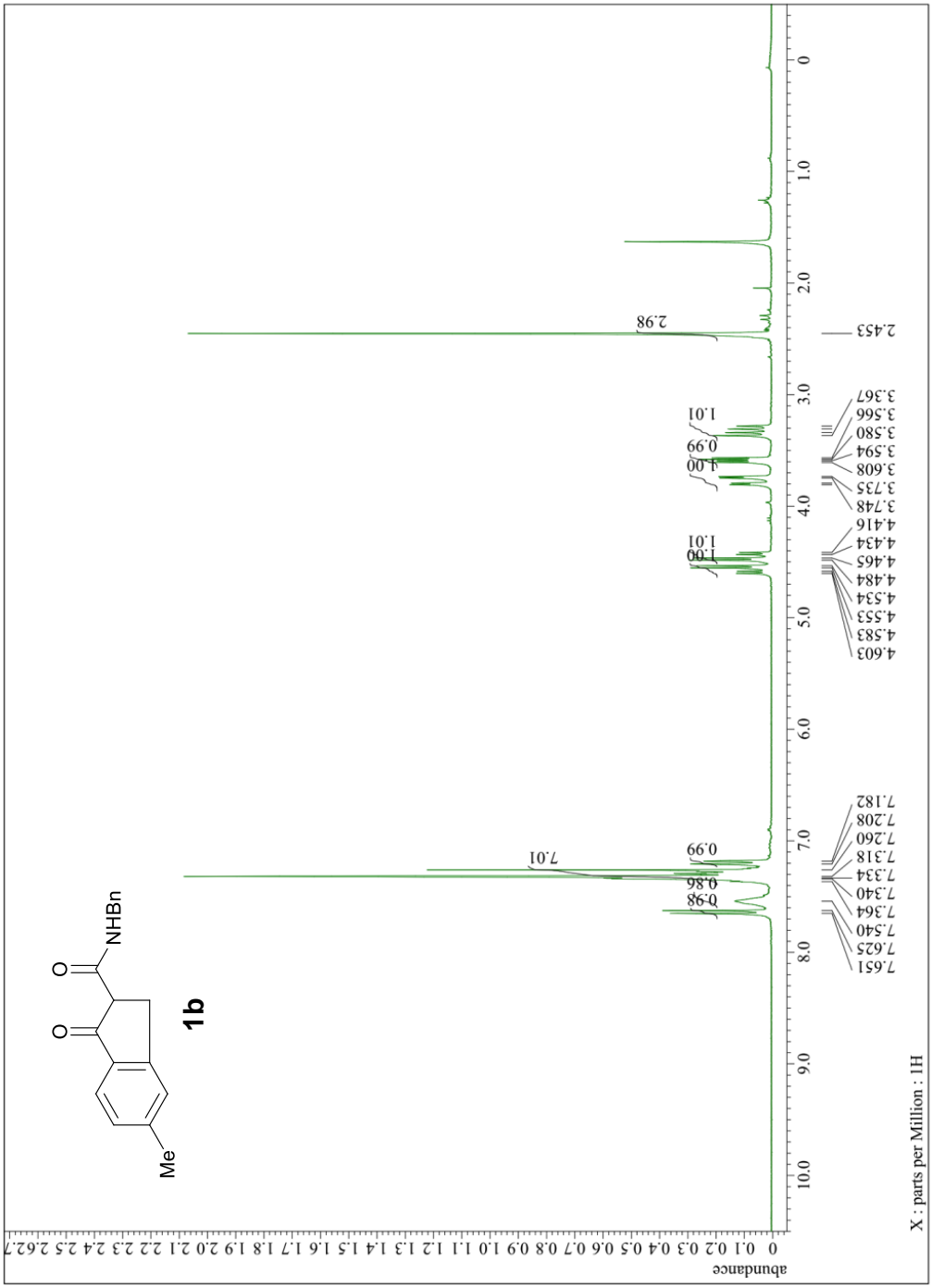
52.754
30.076
22.132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4.583
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4.534
4.484
4.465
4.434
4.416
3.748
3.735
3.608
3.594
3.580
3.566
3.367
2.453
2.98
1.01
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1.01
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0.98
abundance
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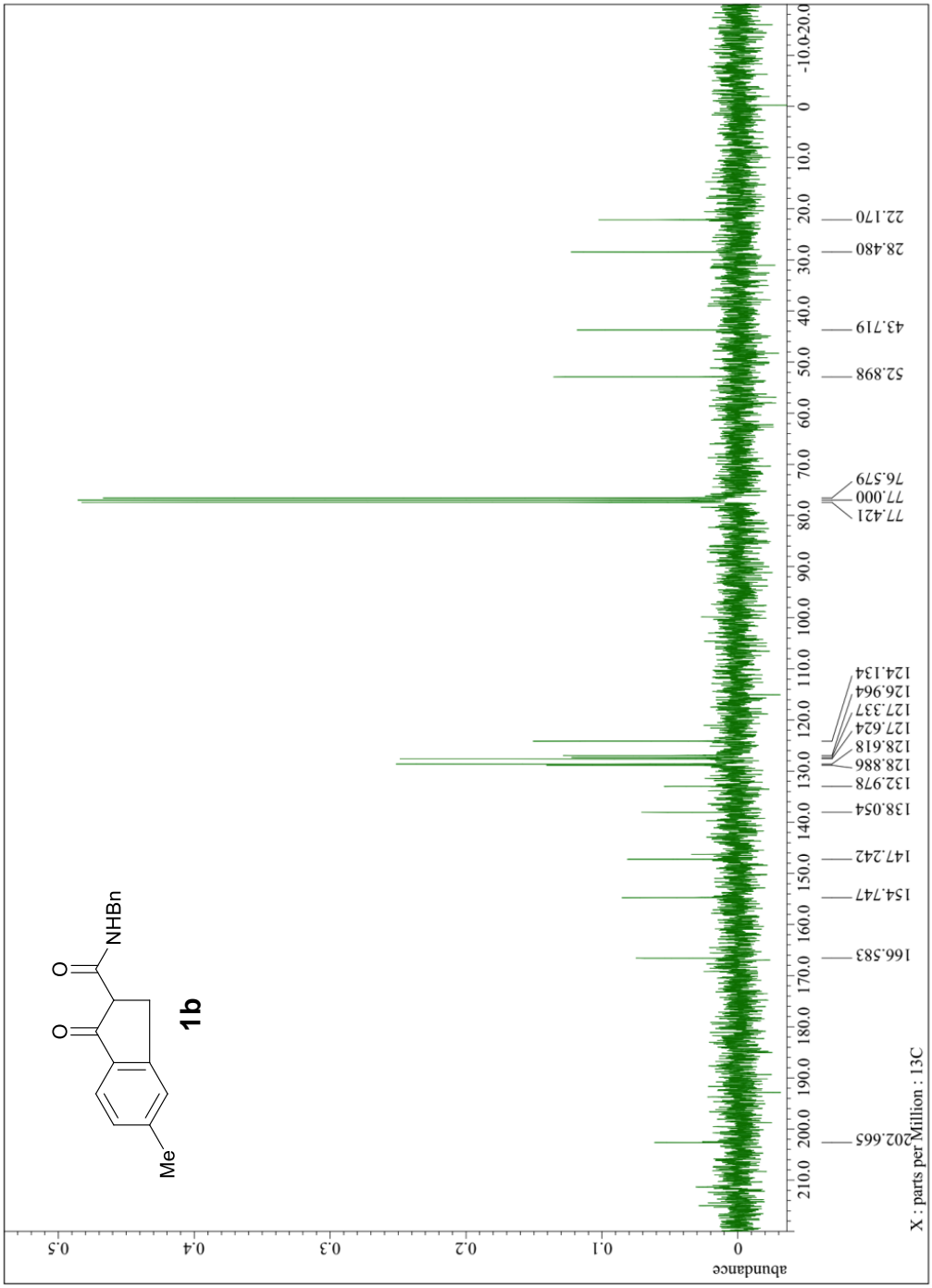
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O
Me
1b
abundance
X : parts per Million : 13C
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132.978
128.886
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77.421
77.000
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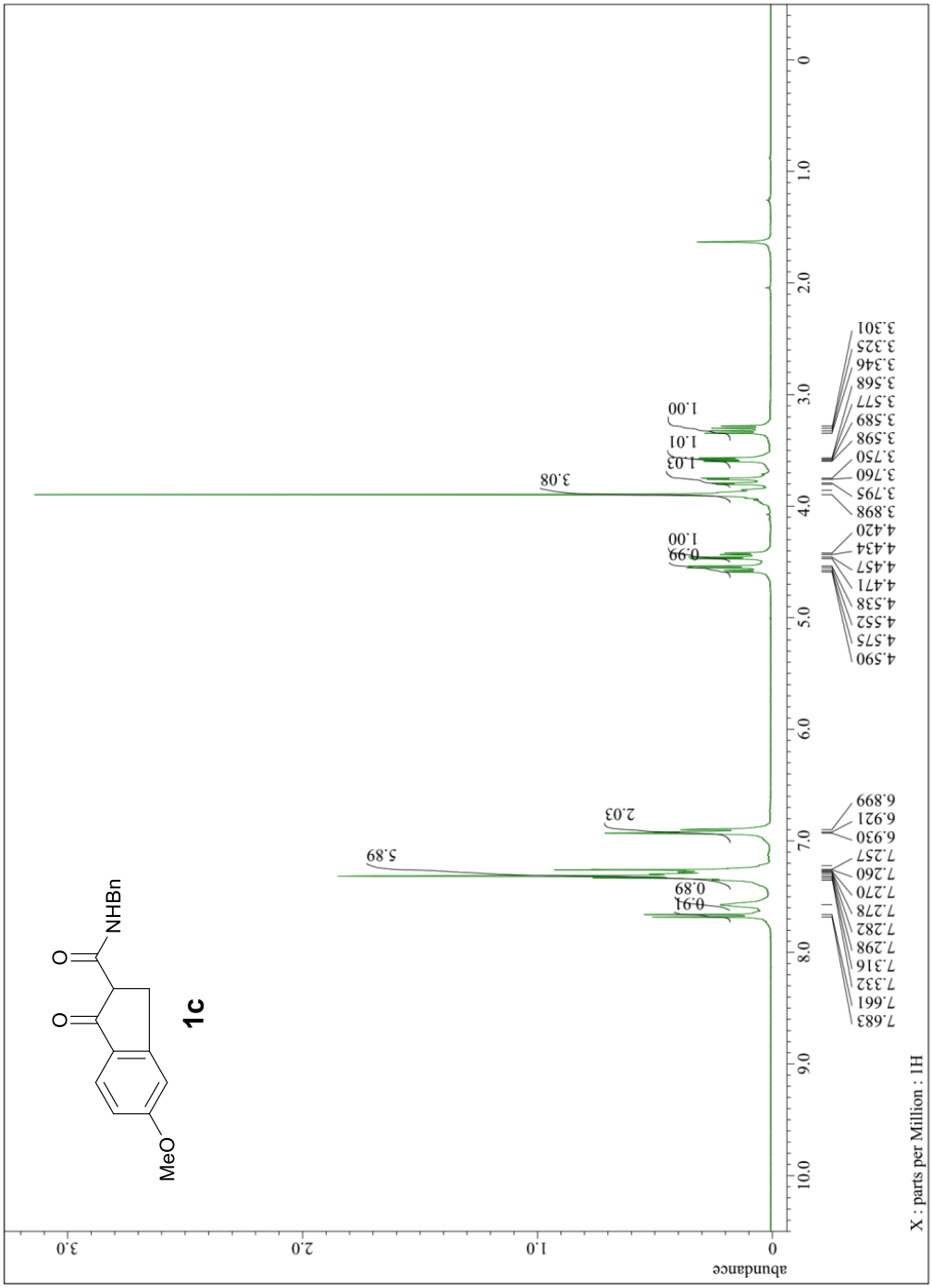
52.898
43.719
28.480
22.170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O
MeO
1c
abundance
X : parts per Million : 1H
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7.278
7.270
7.260
7.257
6.930
6.921
6.899
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4.575
4.552
4.538
4.471
4.457
4.434
4.420
3.898
3.795
3.760
3.750
3.598
3.589
3.577
3.568
3.346
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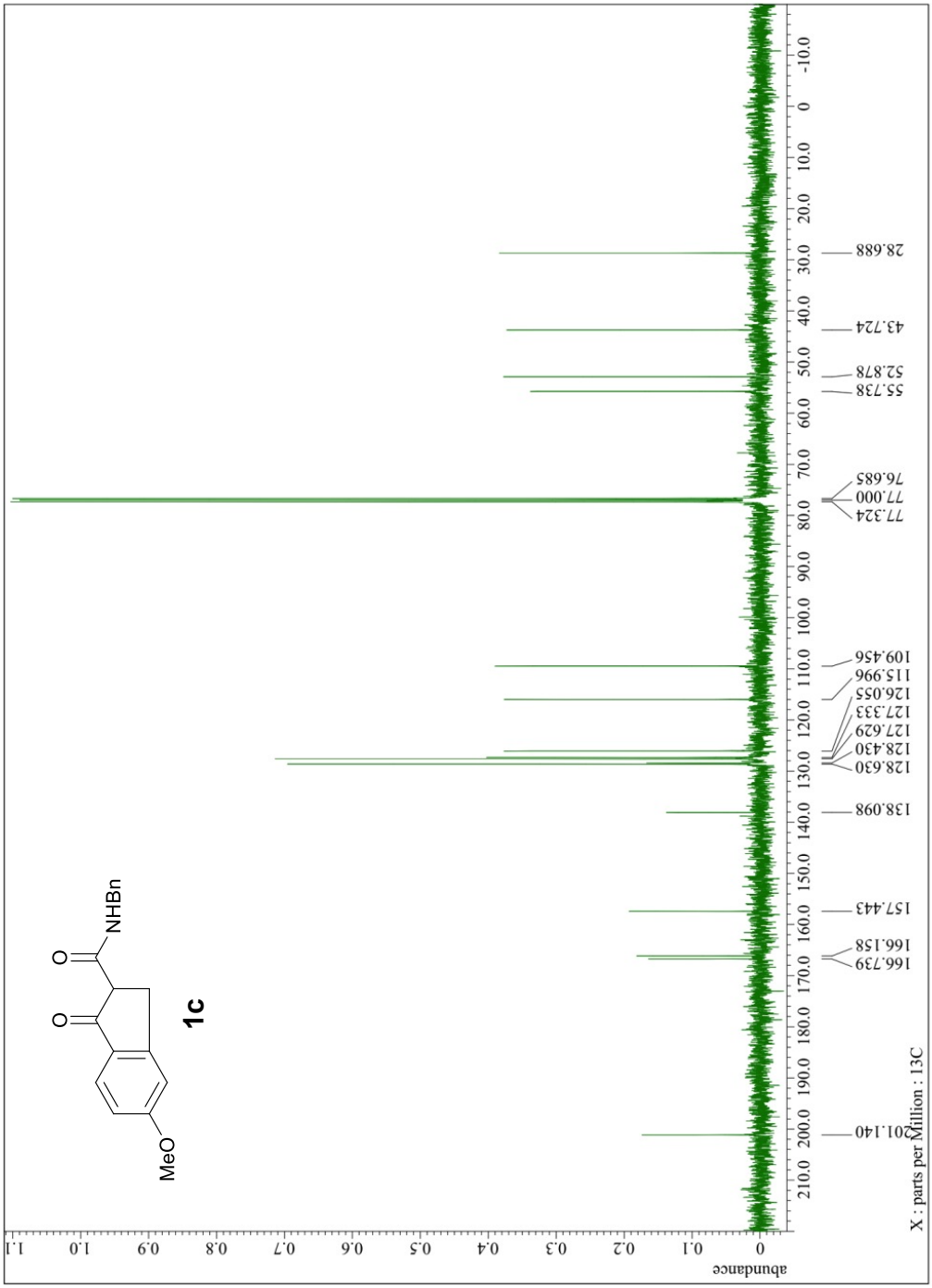
1.03
1.01
1.00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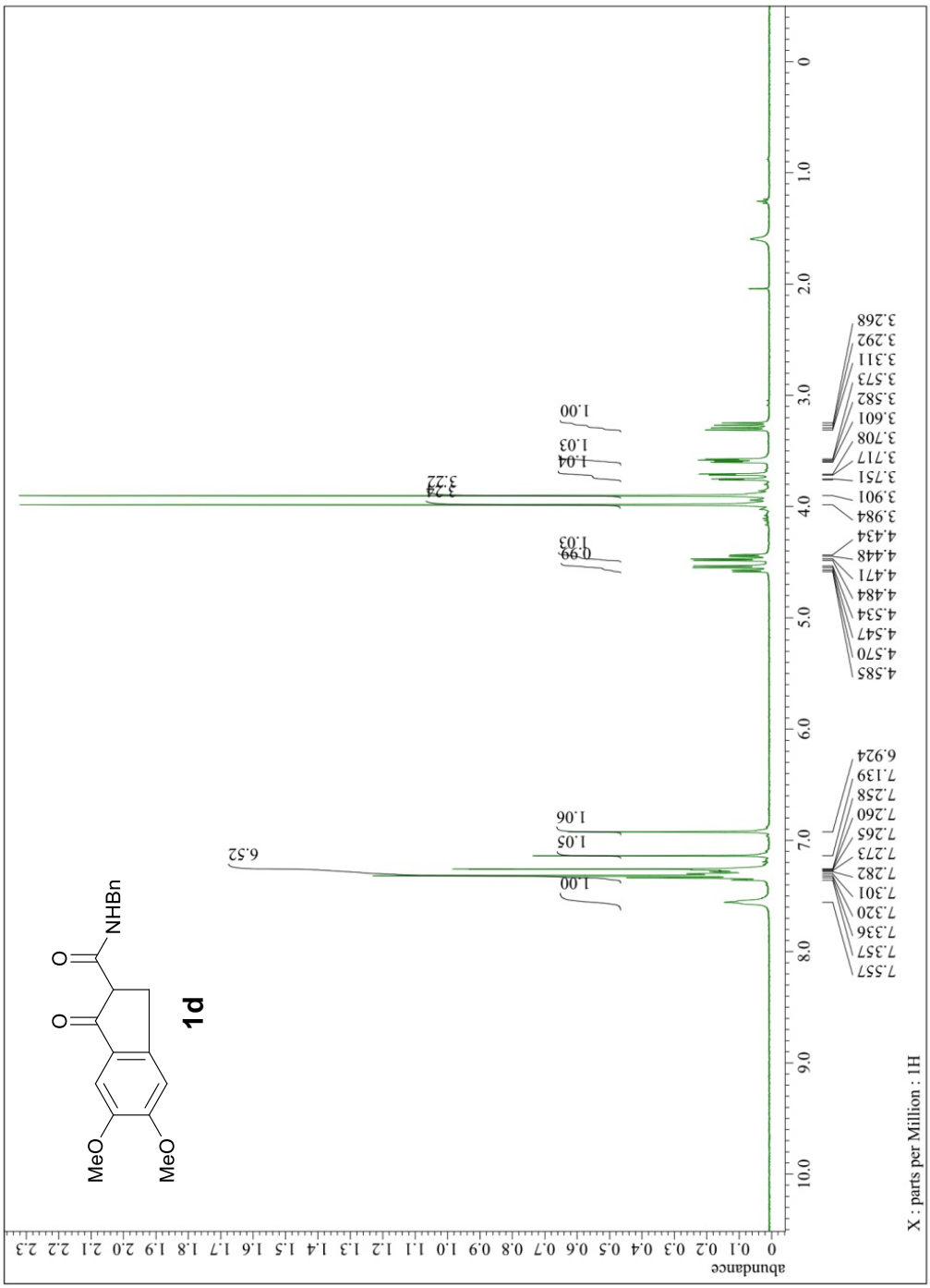
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4.547
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3.984
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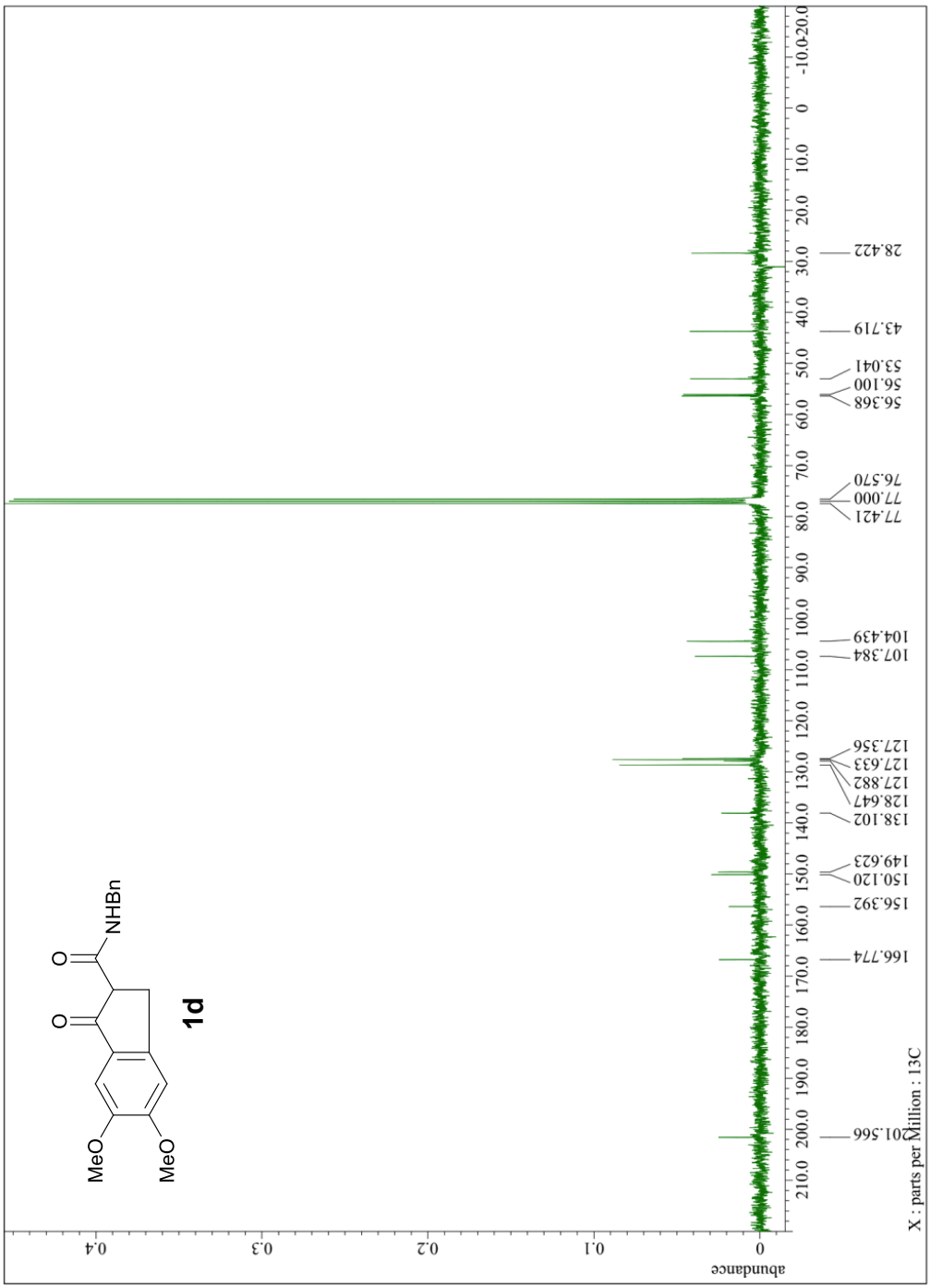
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MeO
1d
abundance
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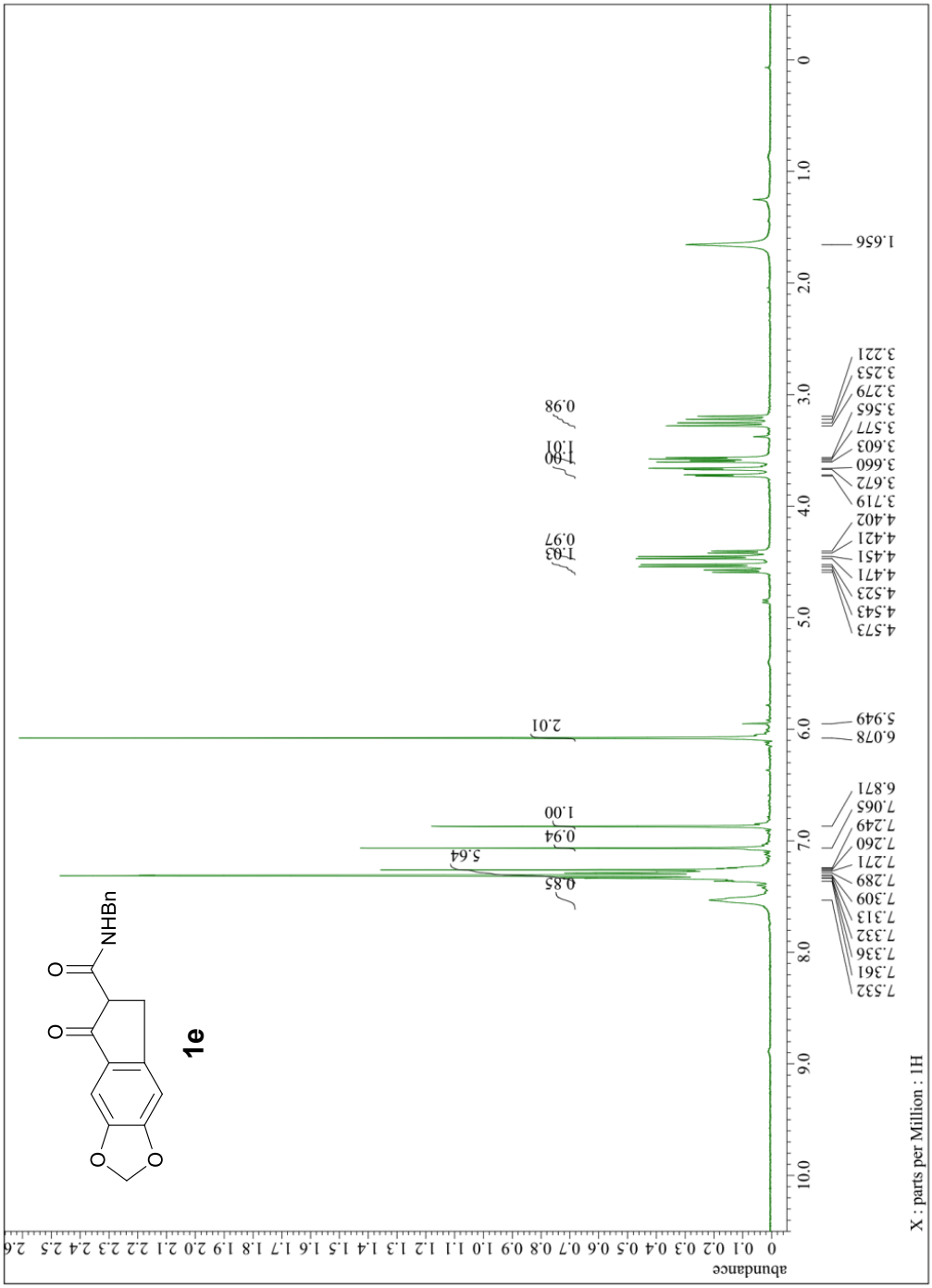
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O
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abundance
X : parts per Million : 1H
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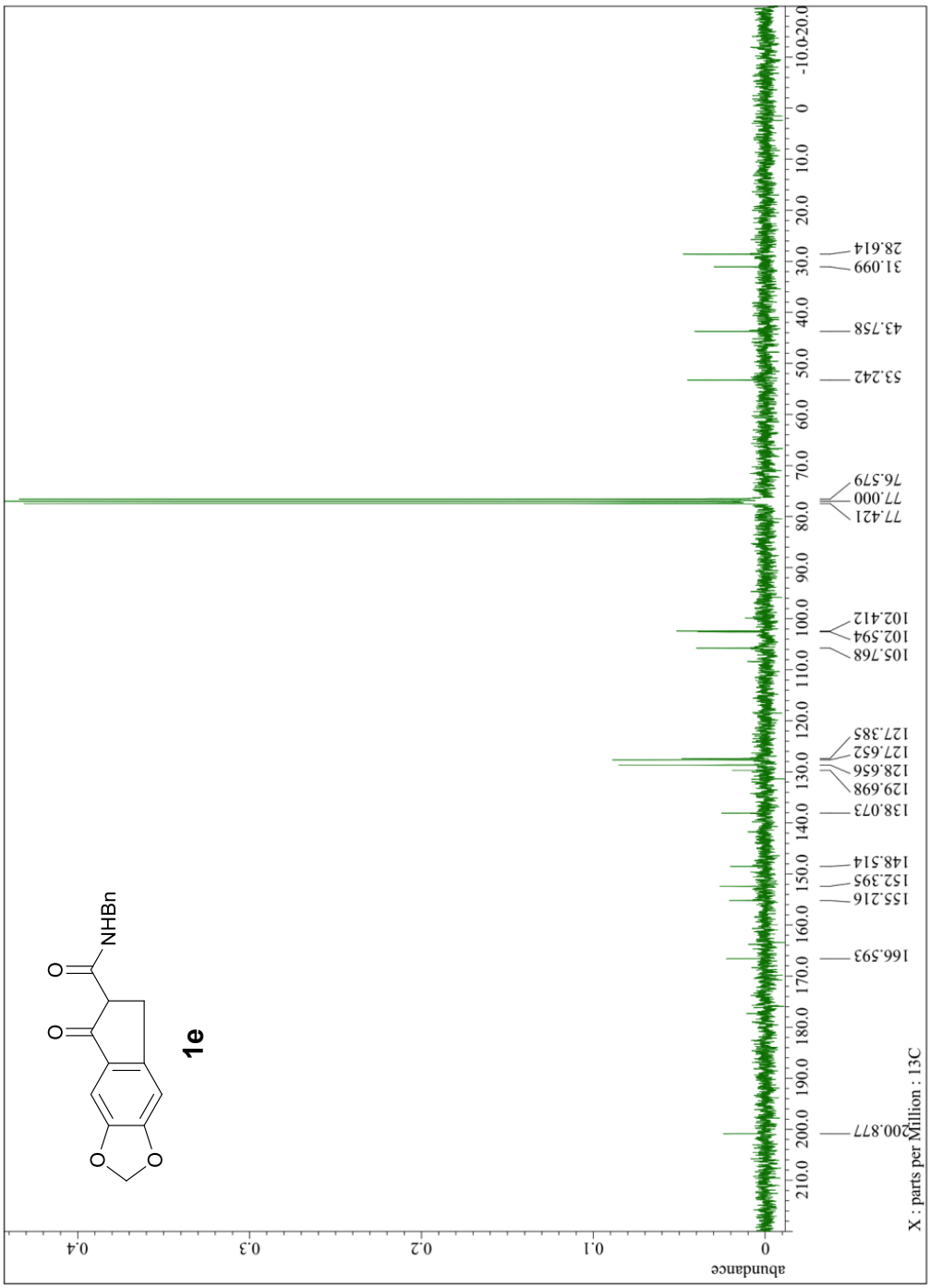
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NHBn
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abundance
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X : parts per Million : 13C
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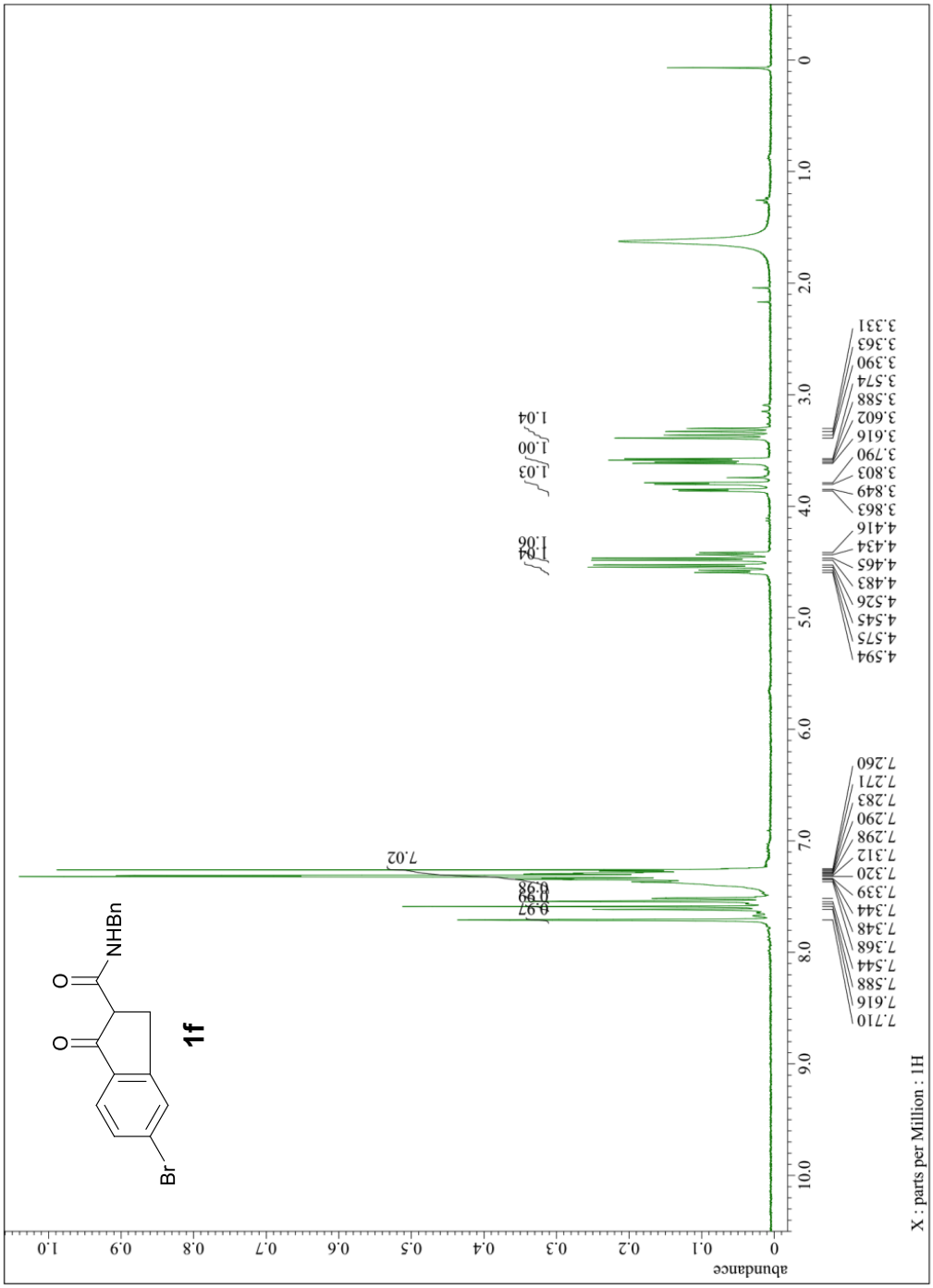
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O
Br
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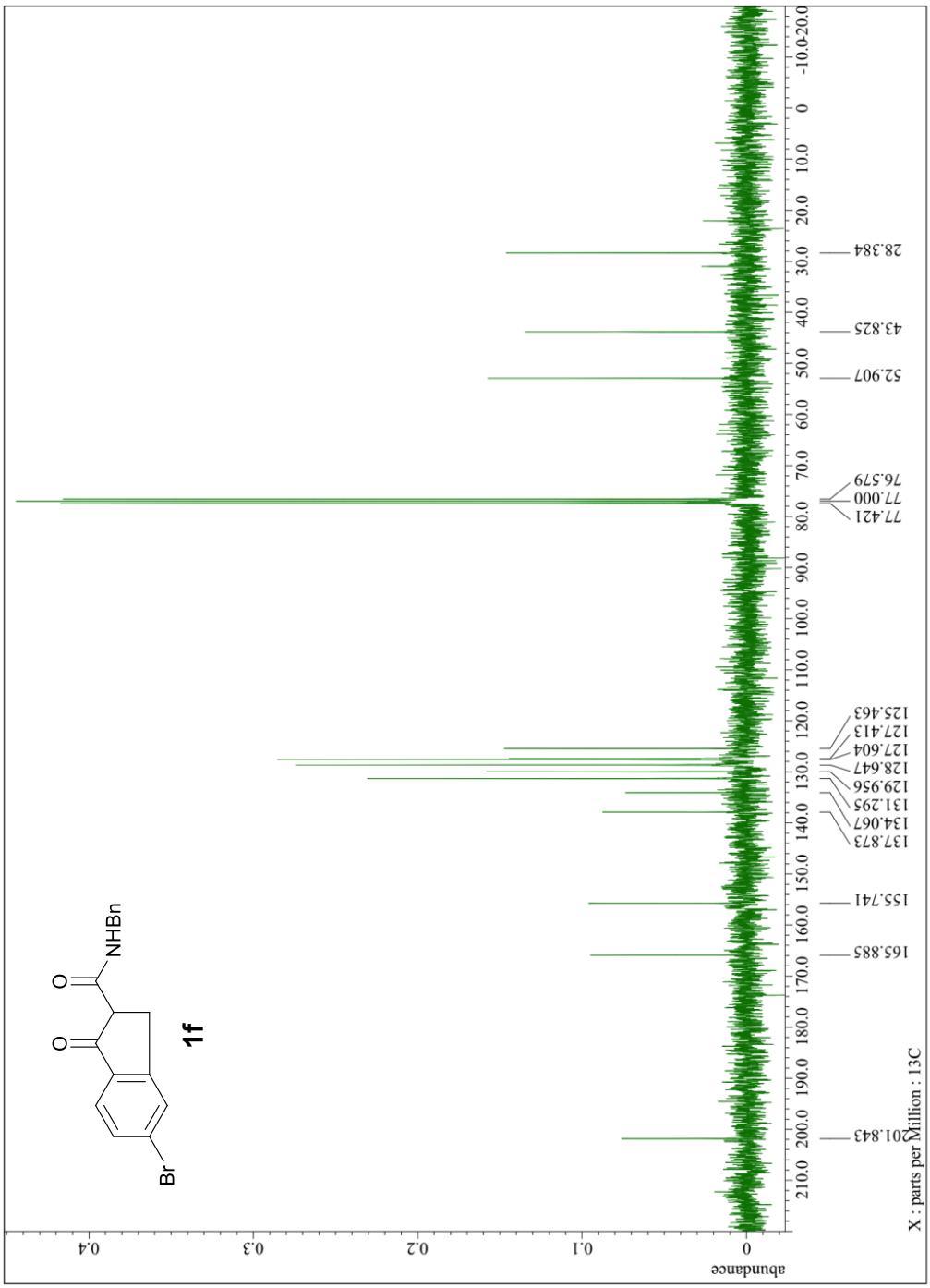
1.06
1.03
1.00
1.04
abundance
X : parts per Million : 1H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NHBn
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O
Br
X : parts per Million : 13C
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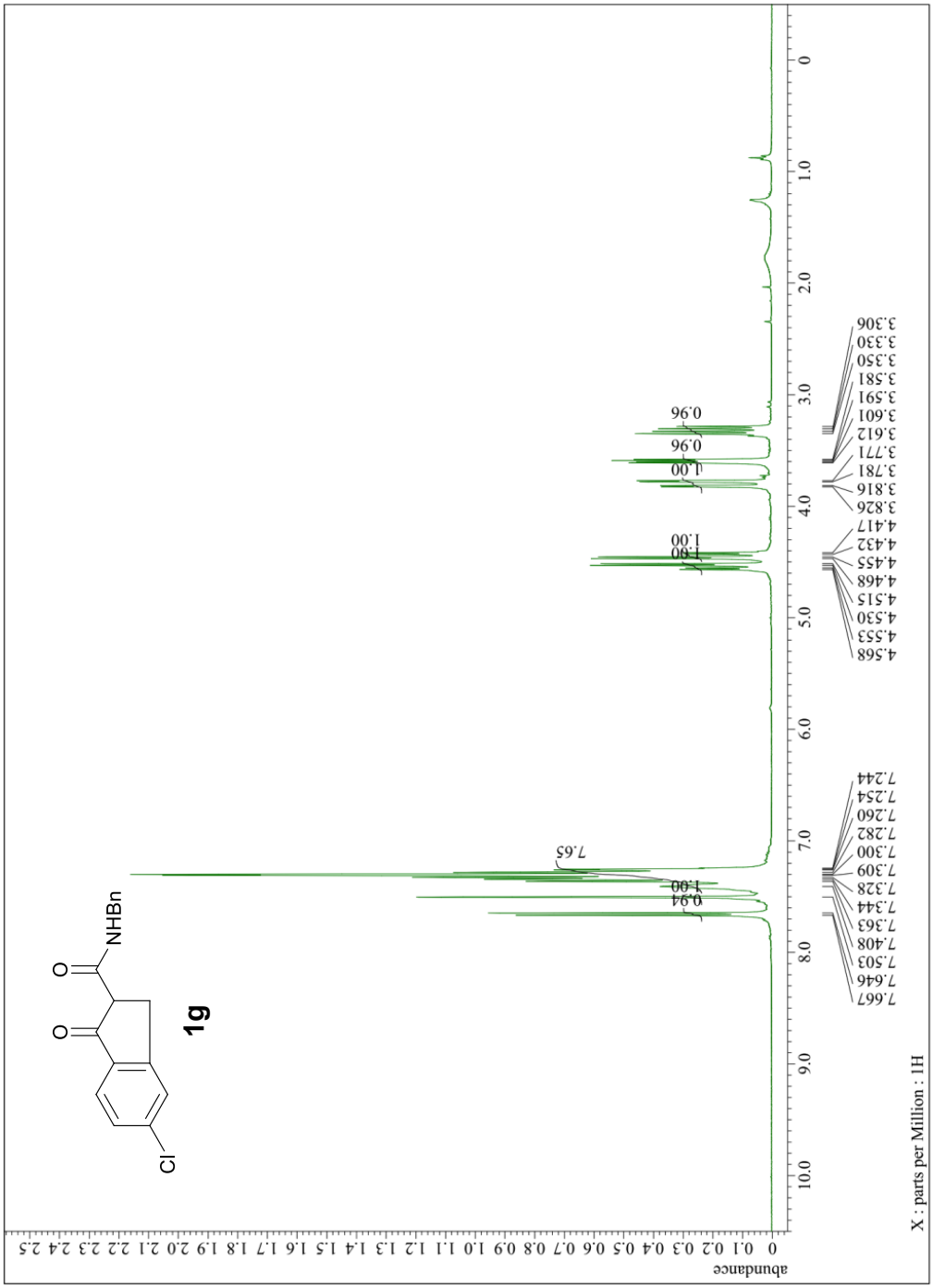
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O
Cl
1g
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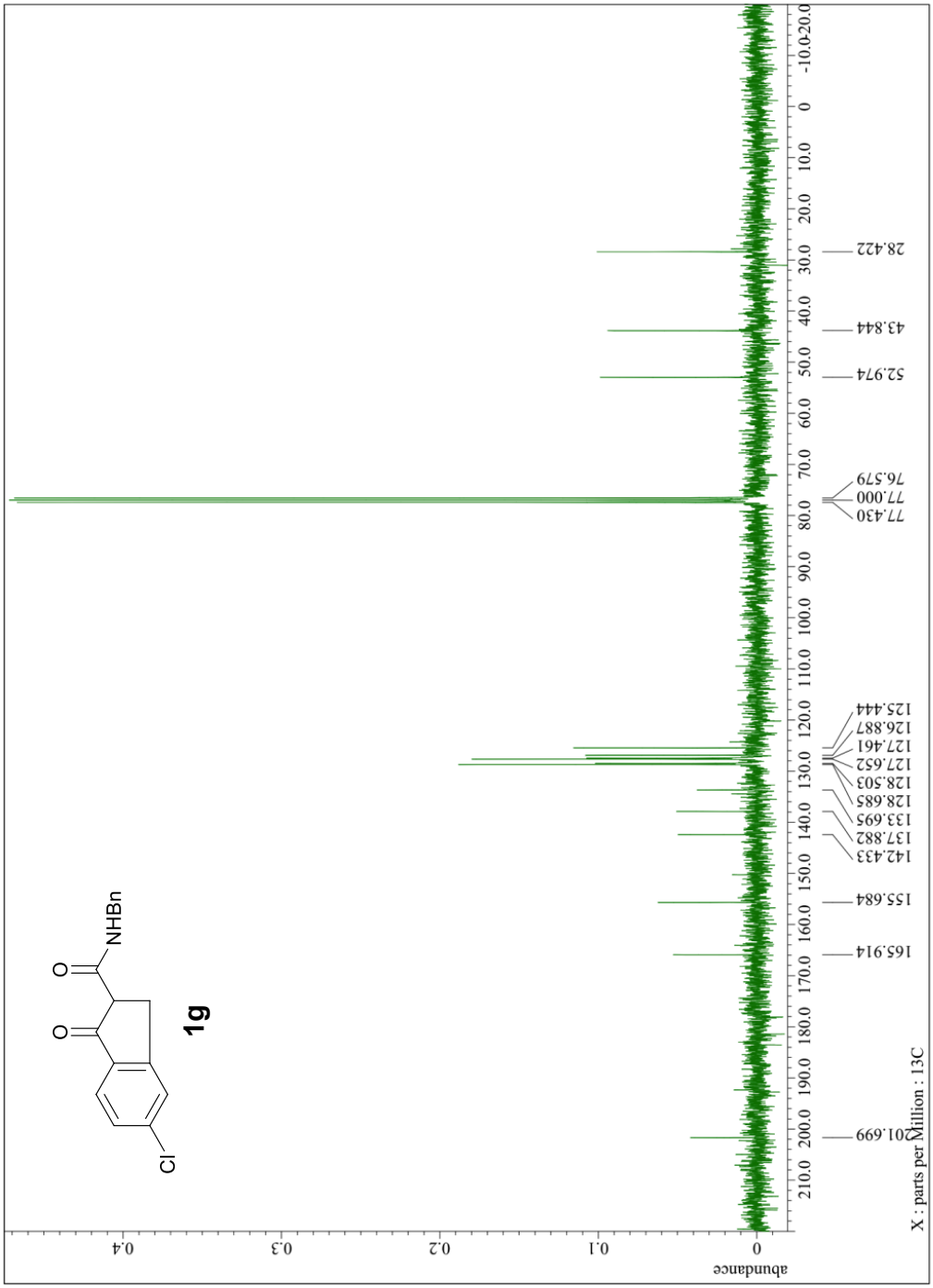
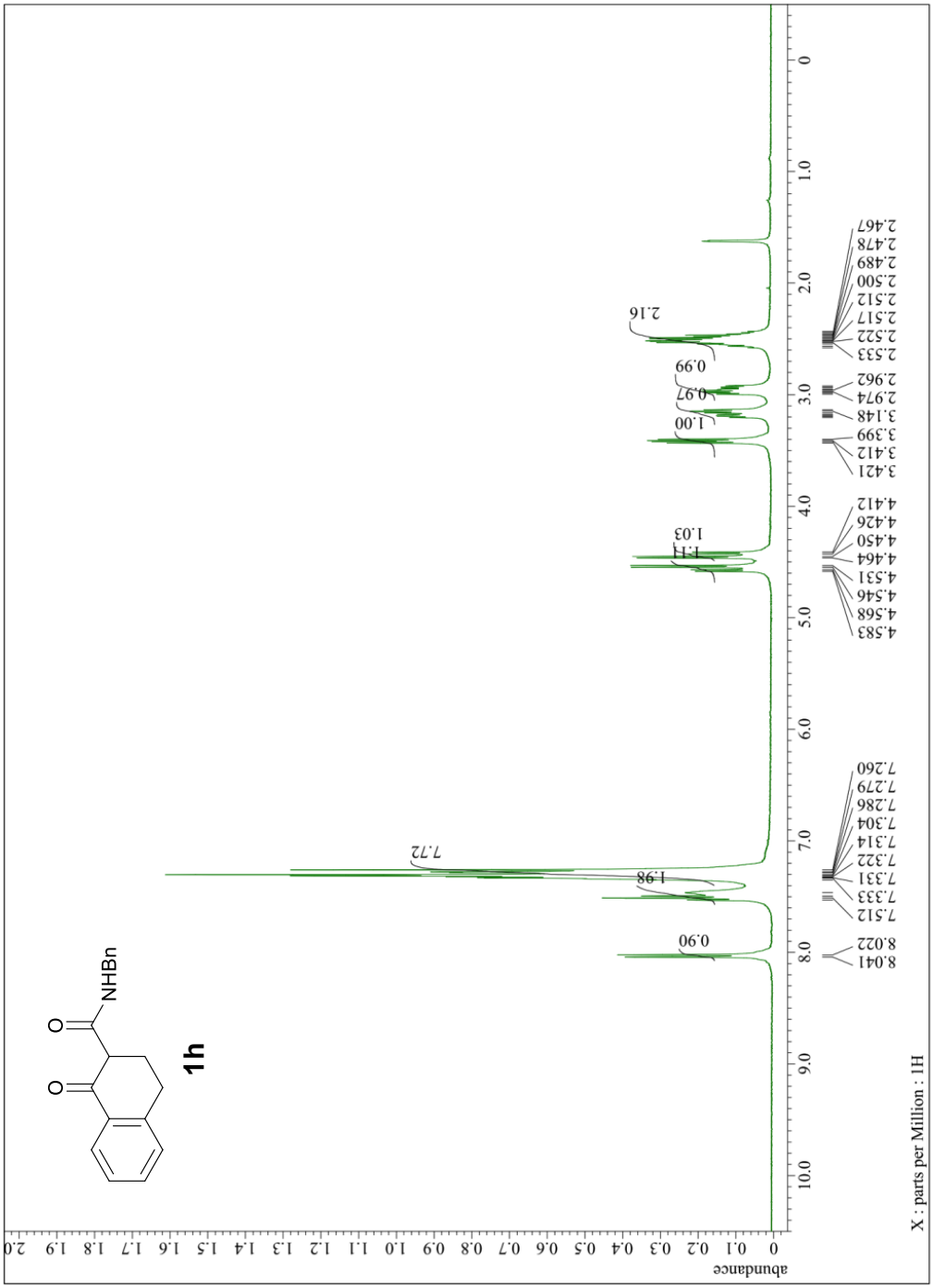
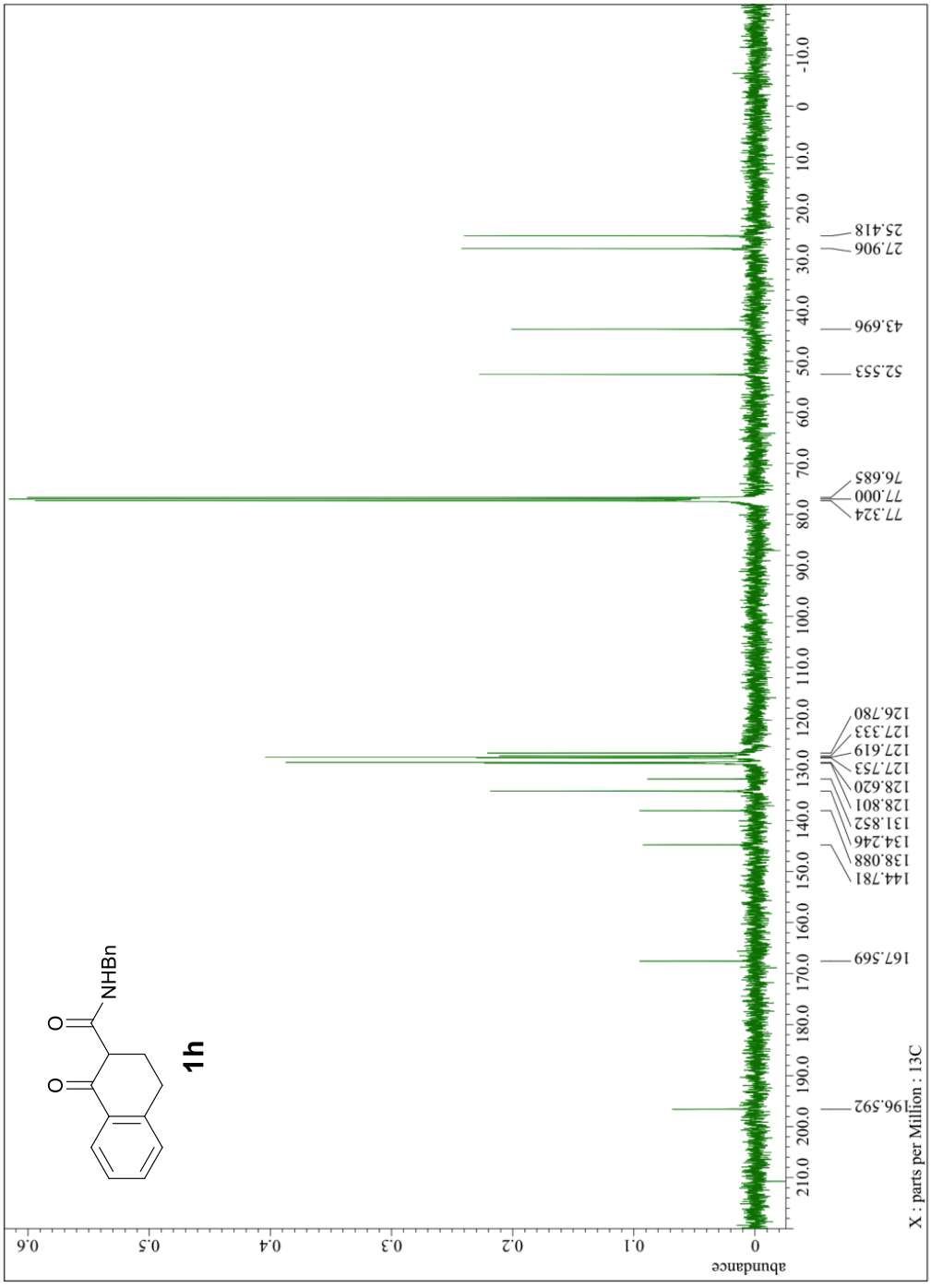
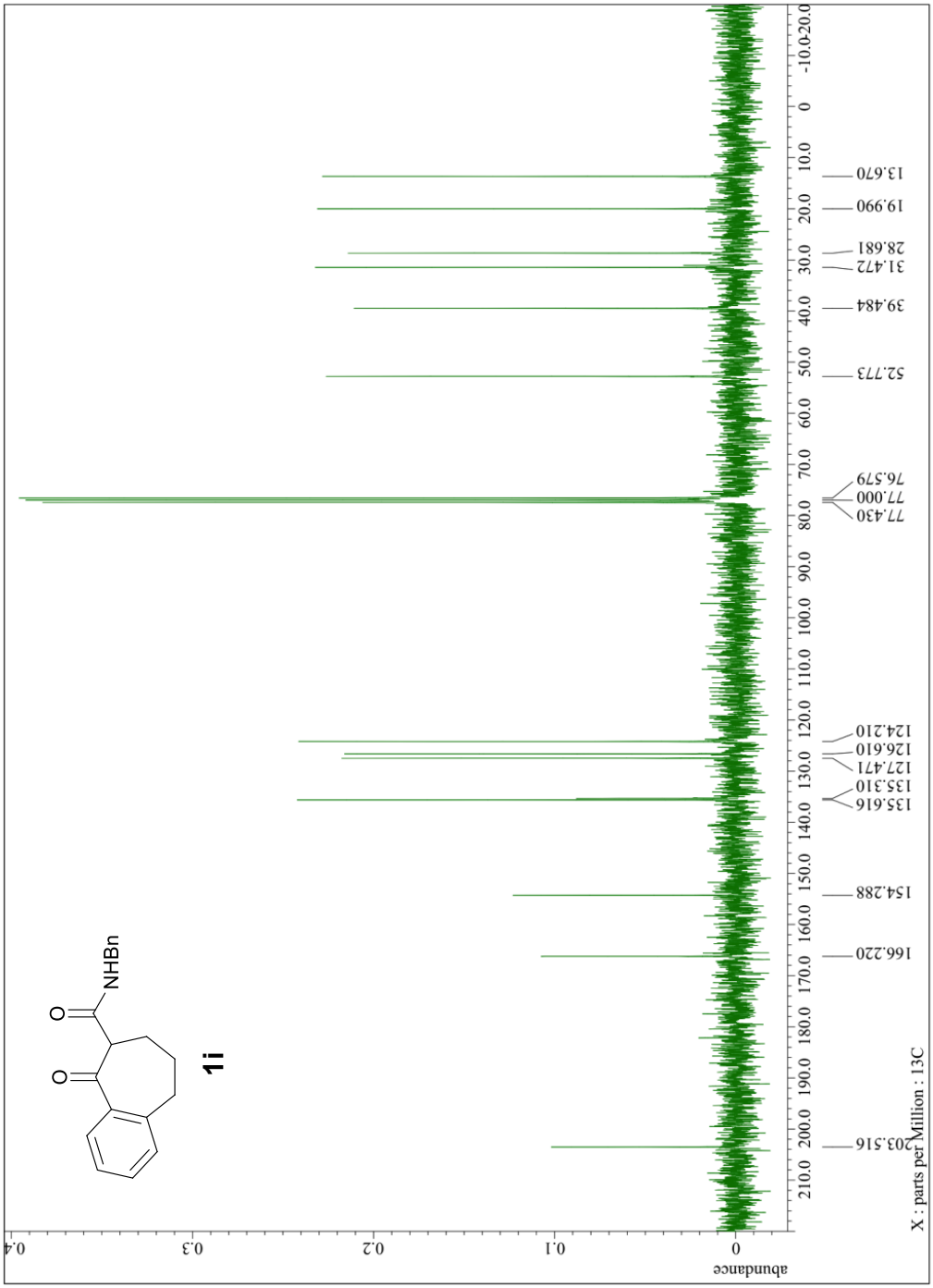
0.94
1.00
1.00
1.00
0.96
0.96
abundance
X : parts per Million : 1H

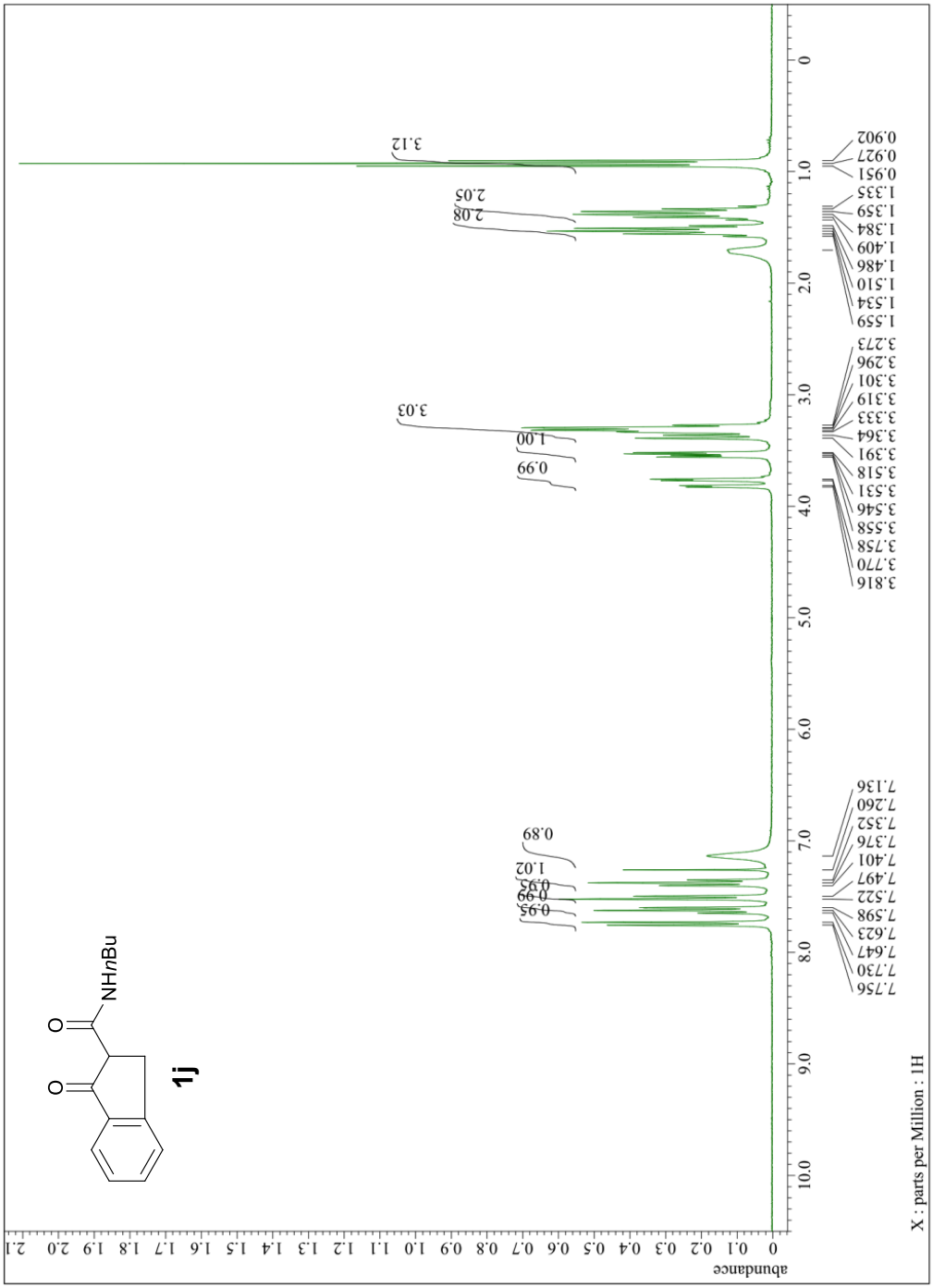

1g
NHBn
O
O
Cl
abundance
X : parts per Million : 13C
201.699
165.914
155.684
142.433
137.882
133.695
128.685
128.503
127.652
127.461
126.887
125.444
77.430
77.000
76.579
52.974
43.844
28.422

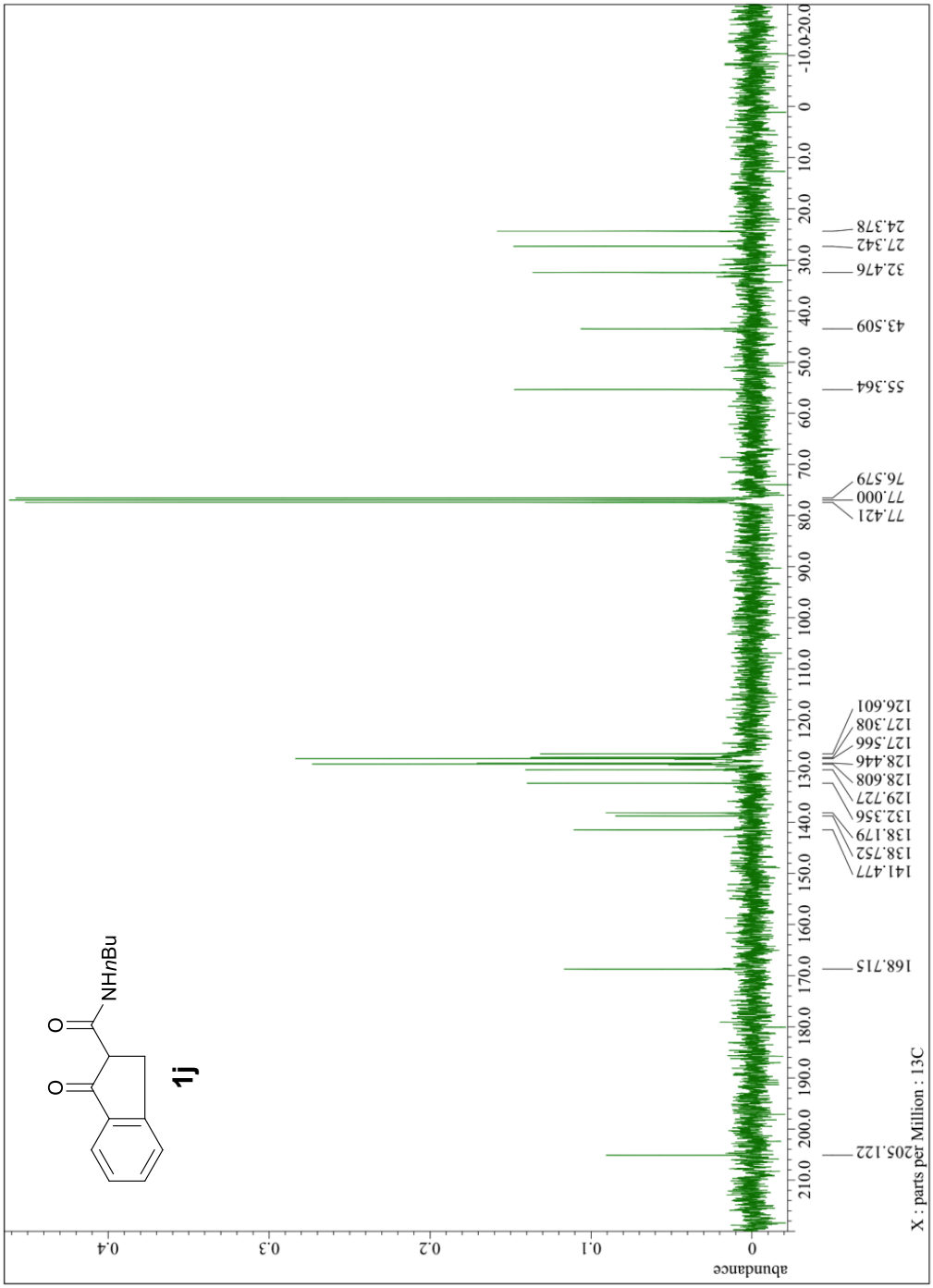

NHBn
O
O
1h
abundance
X : parts per Million : 1H
7.72
1.98
0.90
2.16
0.99
0.97
1.00
1.03
1.11
8.041
8.022
7.512
7.333
7.331
7.322
7.314
7.304
7.286
7.279
7.260
4.583
4.568
4.546
4.531
4.464
4.450
4.426
4.412
3.421
3.412
3.399
3.148
2.974
2.962
2.533
2.522
2.517
2.512
2.500
2.489
2.478
2.467

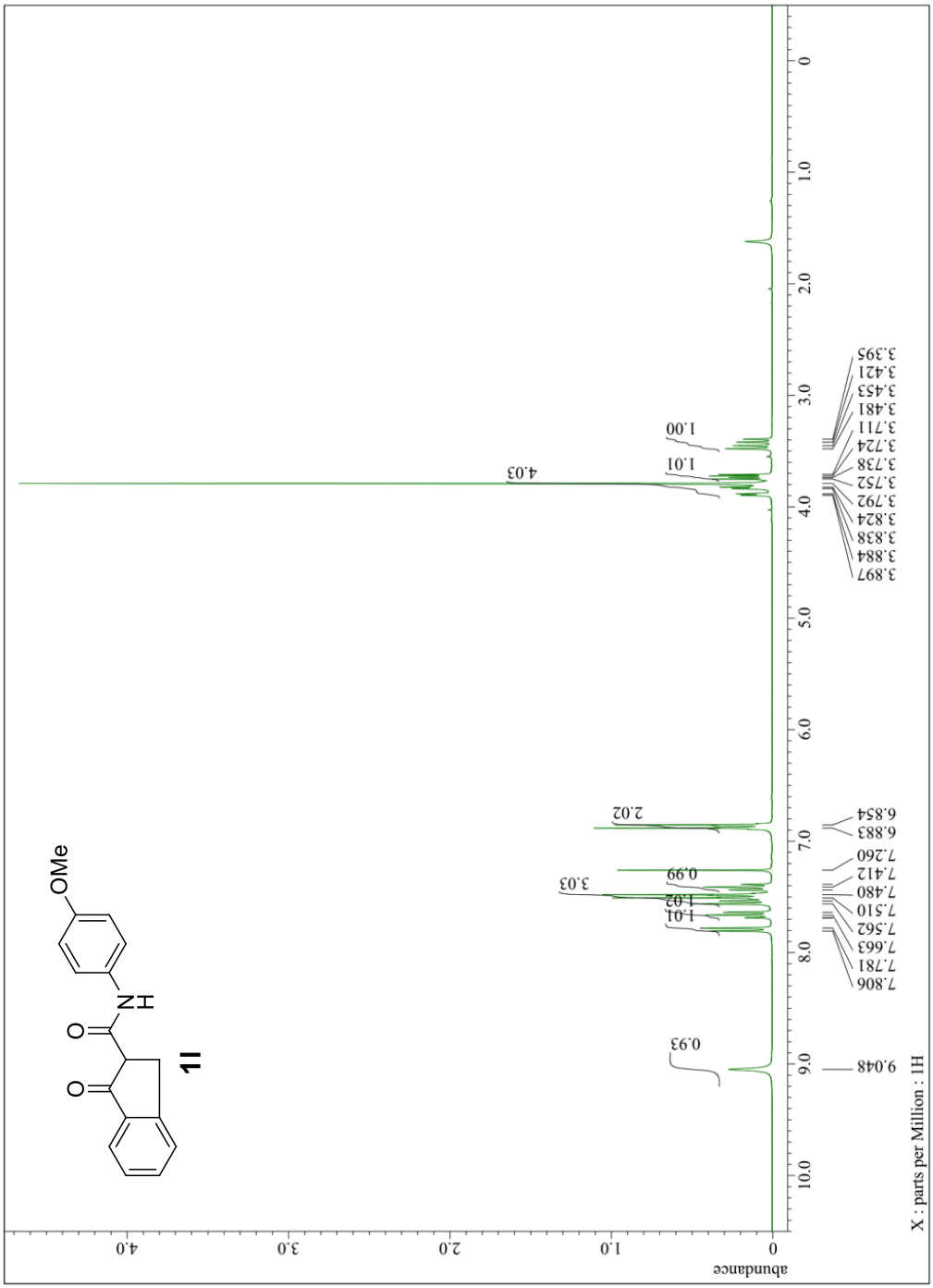

1h
NHBn
O
O
abundance
X : parts per Million : 13C
196.592
167.569
144.781
138.088
134.246
131.852
128.801
128.620
127.753
127.619
127.333
126.780
77.324
77.000
76.685
52.553
43.696
27.906
25.418

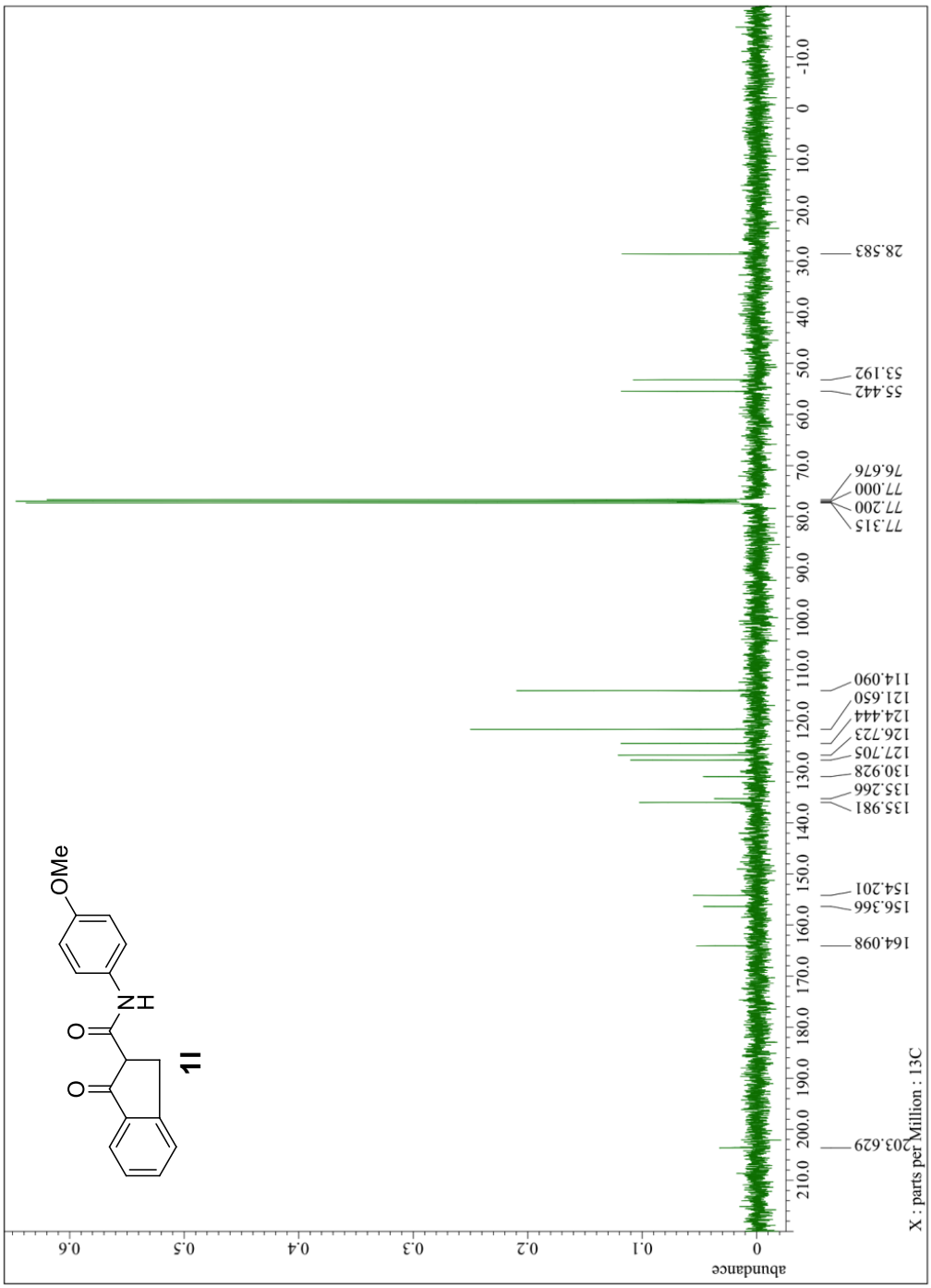
NHBn
O
O
1i
abundance
X : parts per Million : 1H
7.641
7.622
7.436
7.418
7.367
7.346
7.329
7.321
7.302
7.284
7.275
7.260
7.257
7.235
7.216
4.585
4.573
4.558
4.536
4.520
4.504
4.482
4.467
3.736
3.724
3.711
3.699
2.966
2.956
2.945
2.285
2.145
2.136
2.128
2.119
2.111
2.093
2.076
2.065
2.057
2.048

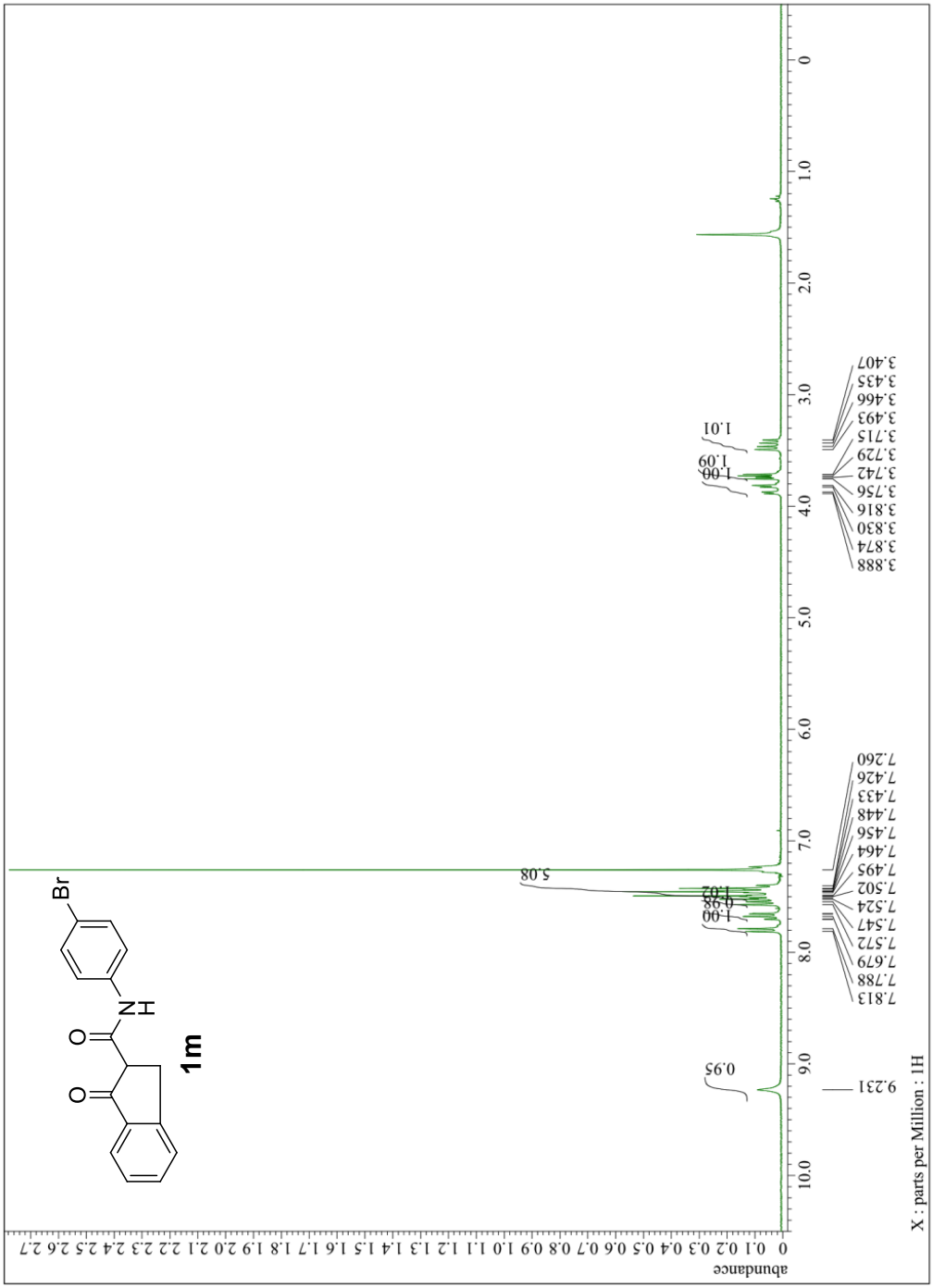

1i
NHBn
O
O
abundance
0.4
0.3
0.2
0.1
0
X : parts per Million : 13C
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
203.516
166.220
154.288
135.616
135.310
127.471
126.610
124.210
77.430
77.000
76.579
52.773
39.484
31.472
28.681
19.990
13.670

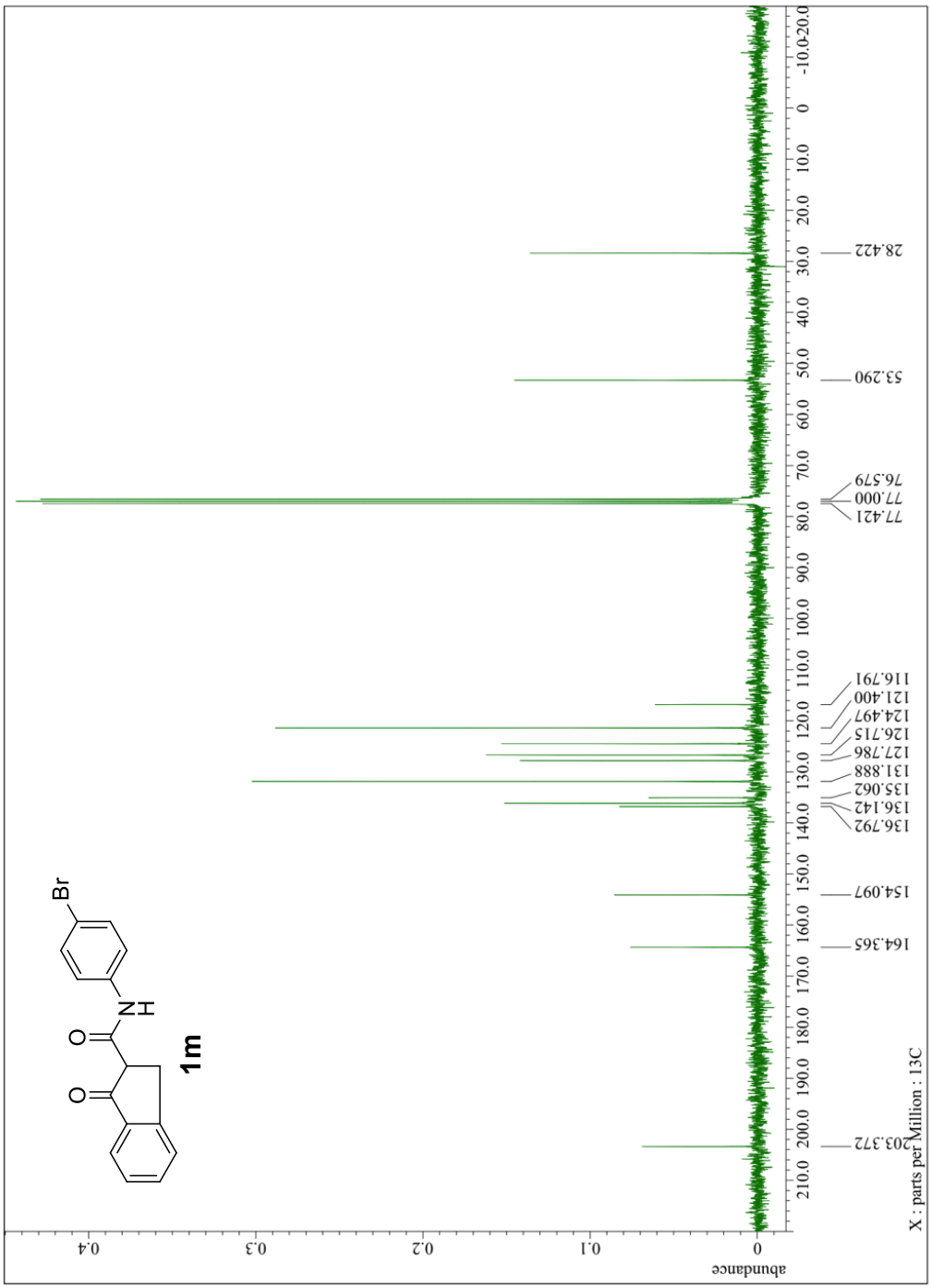

NHnBu
O
O
1j
X : parts per Million : 1H
abundance
7.756
7.730
7.647
7.623
7.598
7.522
7.497
7.401
7.376
7.352
7.260
7.136
3.816
3.770
3.758
3.558
3.546
3.531
3.518
3.391
3.364
3.333
3.319
3.301
3.296
3.273
1.559
1.534
1.510
1.486
1.409
1.384
1.359
1.335
0.951
0.927
0.902
3.12
2.08
2.05
3.03
1.00
0.99
0.89
1.02
0.95
0.99
0.95

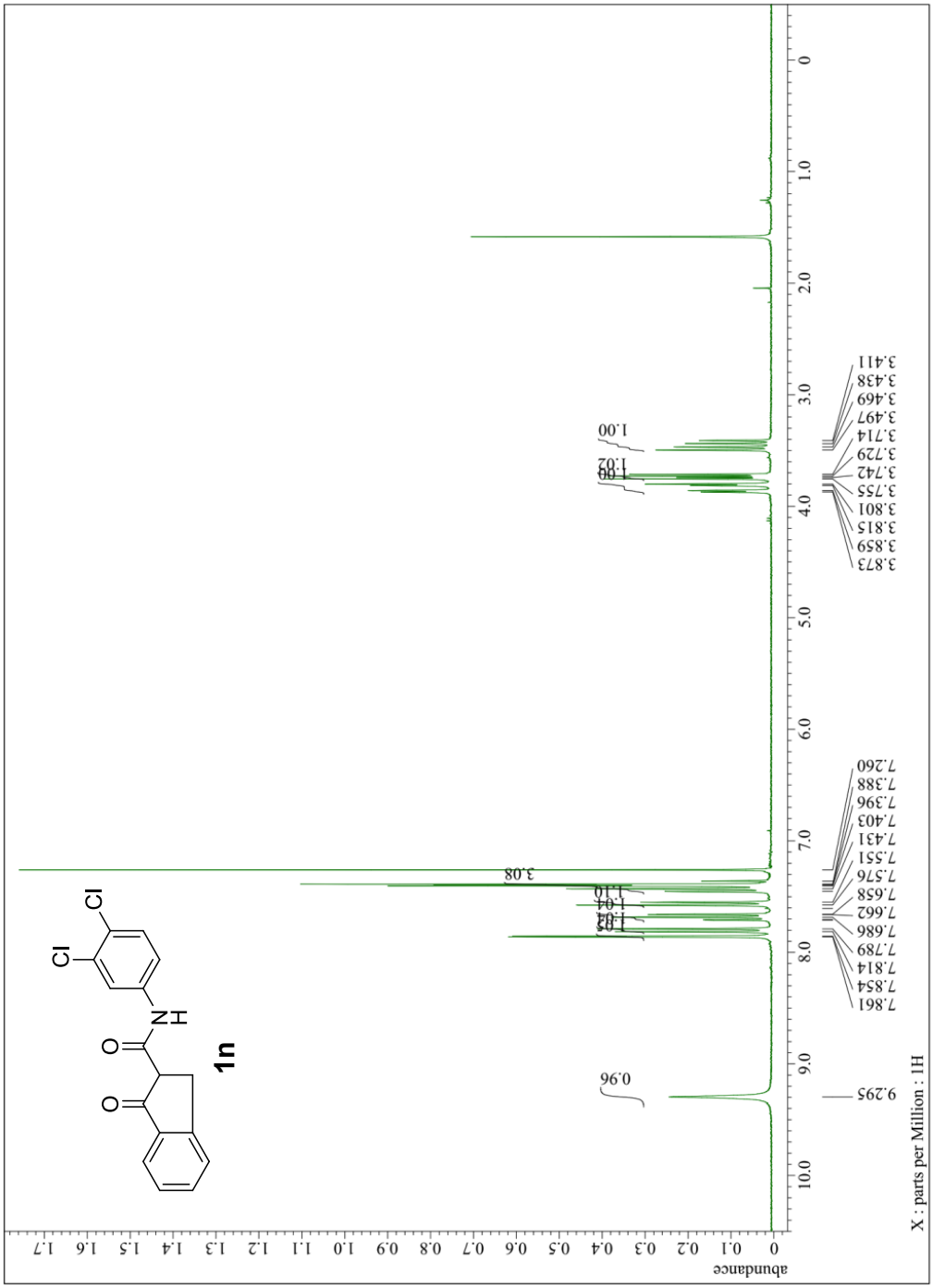

NHnBu
O
O
1j
205.122
168.715
141.477
138.752
138.179
132.356
129.727
128.608
128.446
127.566
127.308
126.601
77.421
77.000
76.579
55.364
43.509
32.476
27.342
24.378
X : parts per Million : 13C
abundance

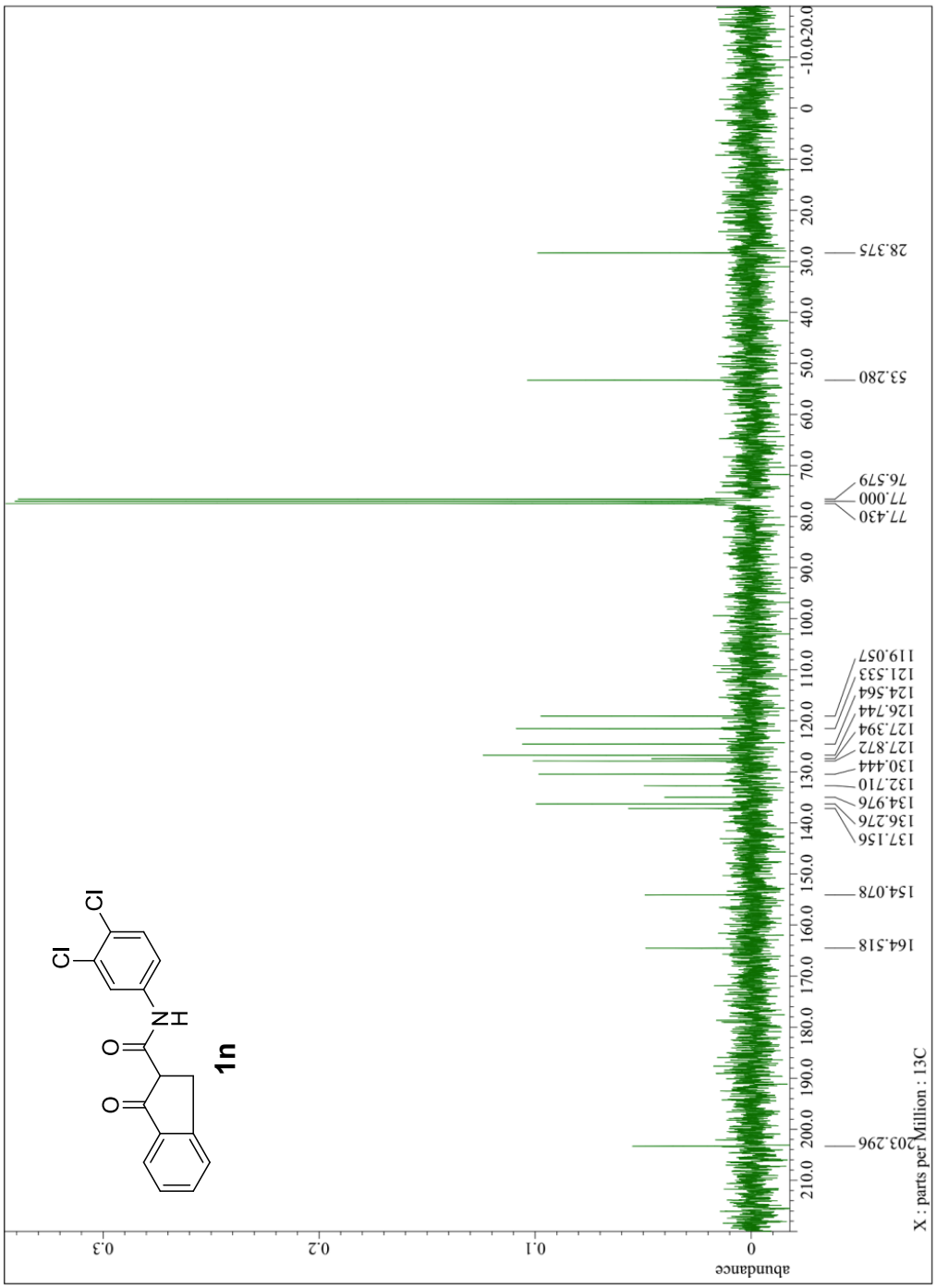

OMe
HN
O
O
1l
X : parts per Million : 1H
abundance
9.048
7.806
7.781
7.663
7.562
7.510
7.480
7.412
7.260
6.883
6.854
4.03
3.03
2.02
1.01
1.00
0.99
0.93
3.897
3.884
3.838
3.824
3.792
3.752
3.738
3.724
3.711
3.481
3.453
3.421
3.395

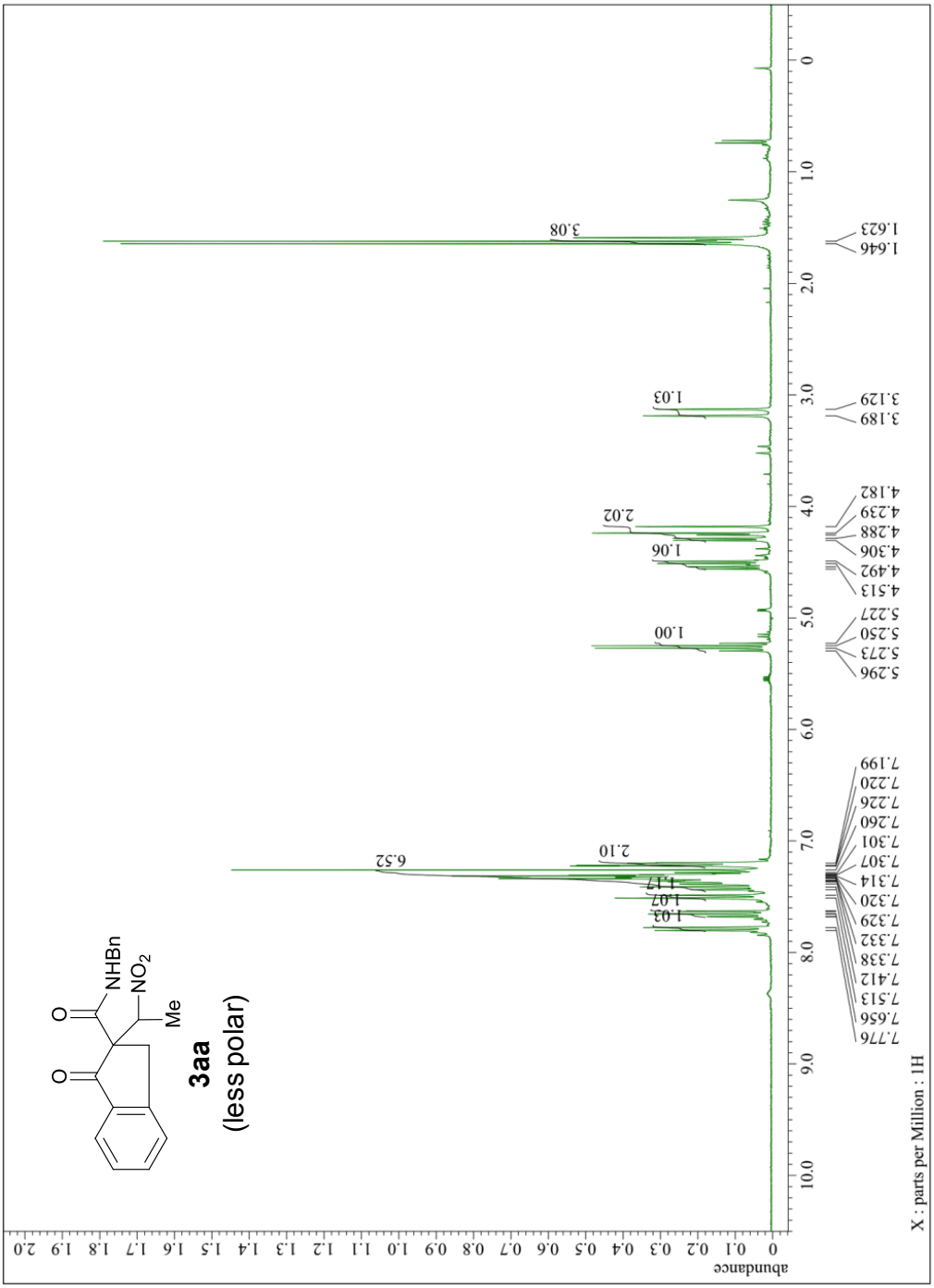

OMe
H
N
O
O
1l
abundance
0.6
0.5
0.4
0.3
0.2
0.1
0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
203.629
164.098
156.366
154.201
135.981
135.266
130.928
127.705
126.723
124.444
121.650
114.090
77.315
77.200
77.000
76.676
55.442
53.192
28.583
X : parts per Million : 13C

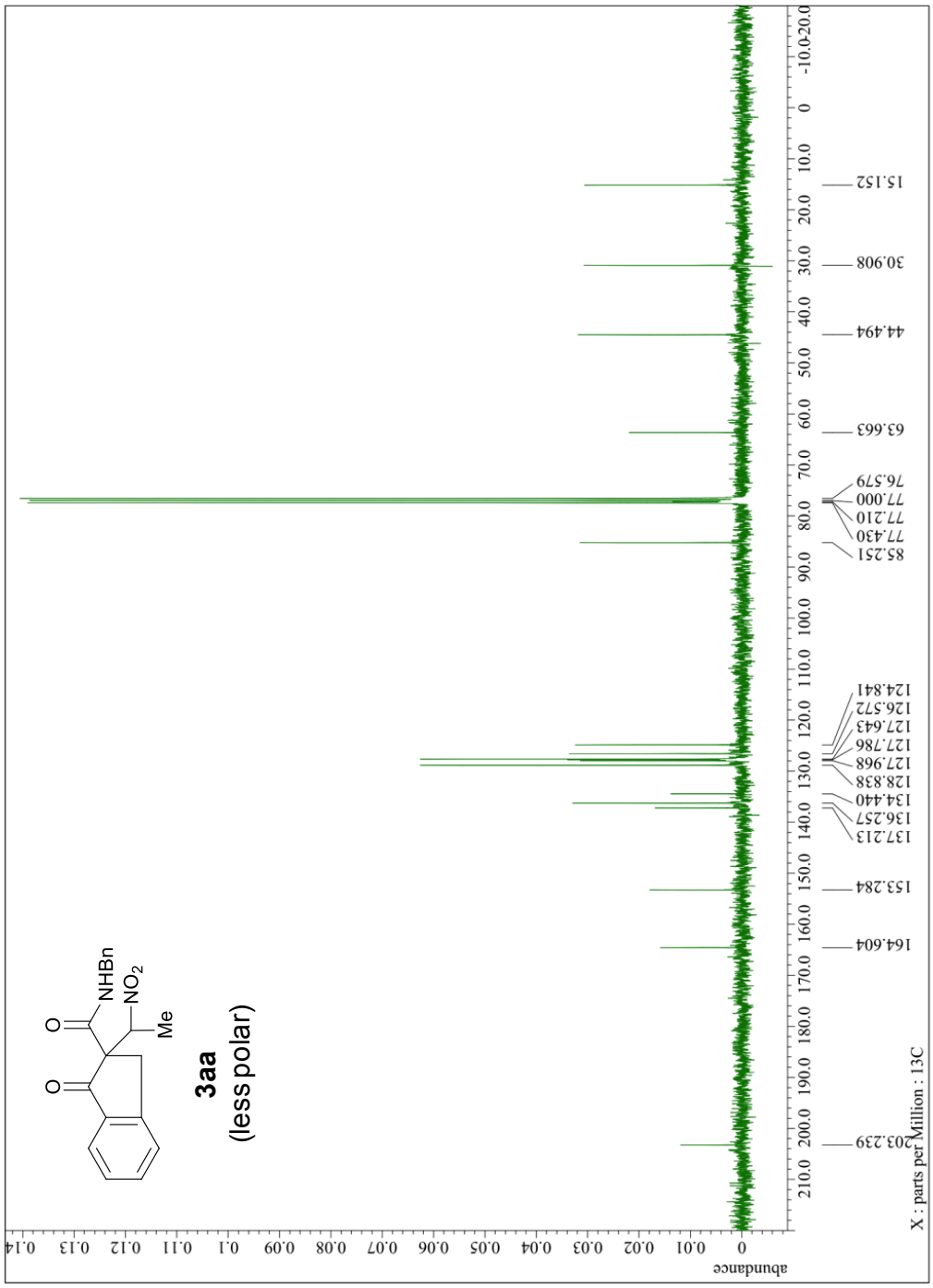

1m
Br
N
H
O
O
9.231
0.95
7.813
7.788
7.679
7.572
7.547
7.524
7.502
7.495
7.464
7.456
7.448
7.433
7.426
7.260
5.08
1.00
0.98
1.02
1.01
1.09
1.00
3.888
3.874
3.830
3.816
3.756
3.742
3.729
3.715
3.493
3.466
3.435
3.407
abundance
X : parts per Million : 1H

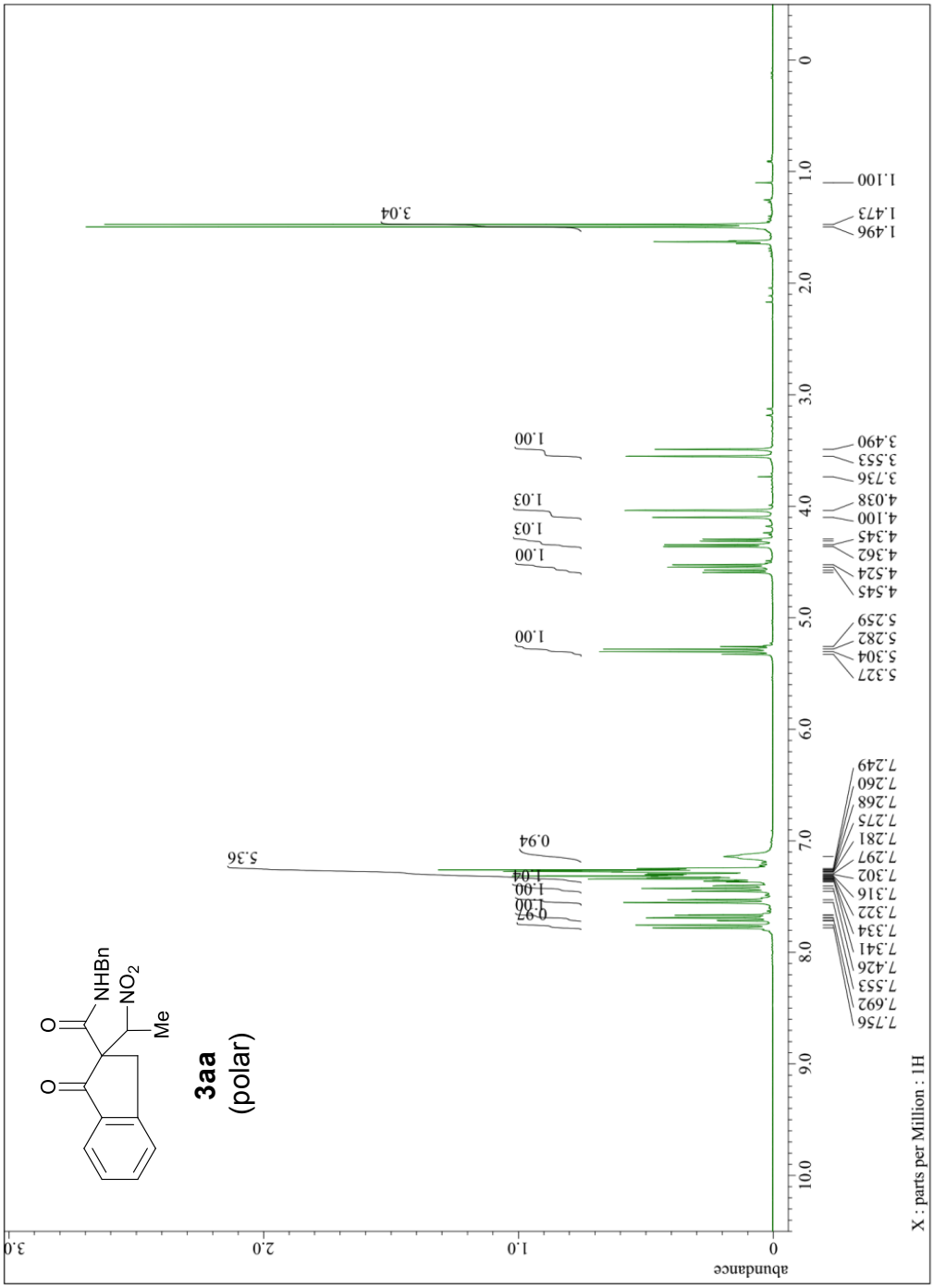

Br
N
H
O
O
1m
abundance
0.4
0.3
0.2
0.1
0
X : parts per Million : 13C
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
203.372
164.365
154.097
136.792
136.142
135.062
131.888
127.786
126.715
124.497
121.400
116.791
77.421
77.000
76.579
53.290
28.422

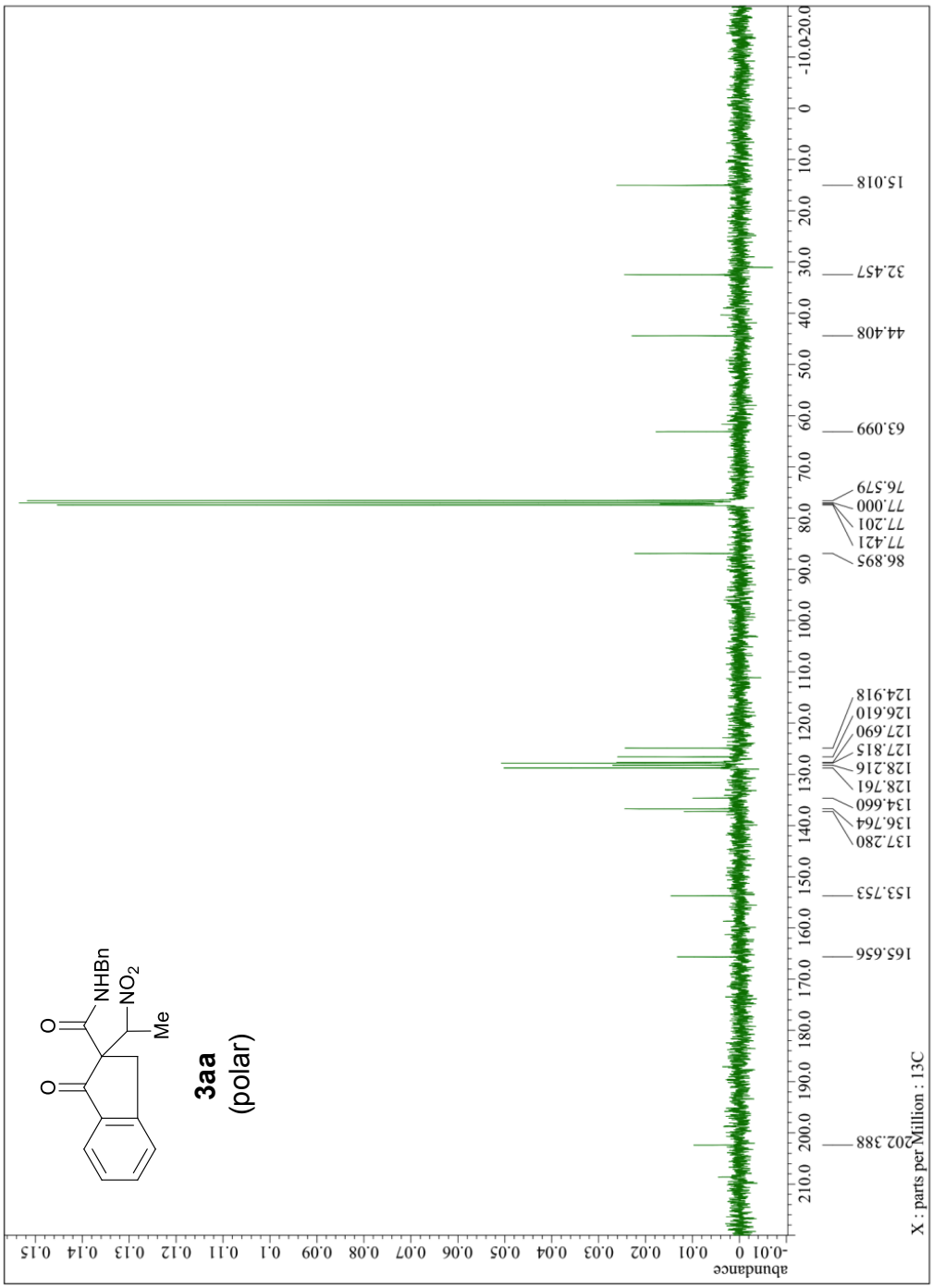

1n
Cl
Cl
O
O
NH
abundance
X : parts per Million : 1H
9.295
7.861
7.854
7.814
7.789
7.686
7.662
7.658
7.576
7.551
7.431
7.403
7.396
7.388
7.260
3.873
3.859
3.815
3.801
3.755
3.742
3.729
3.714
3.497
3.469
3.438
3.411
0.96
3.08
1.00
1.02

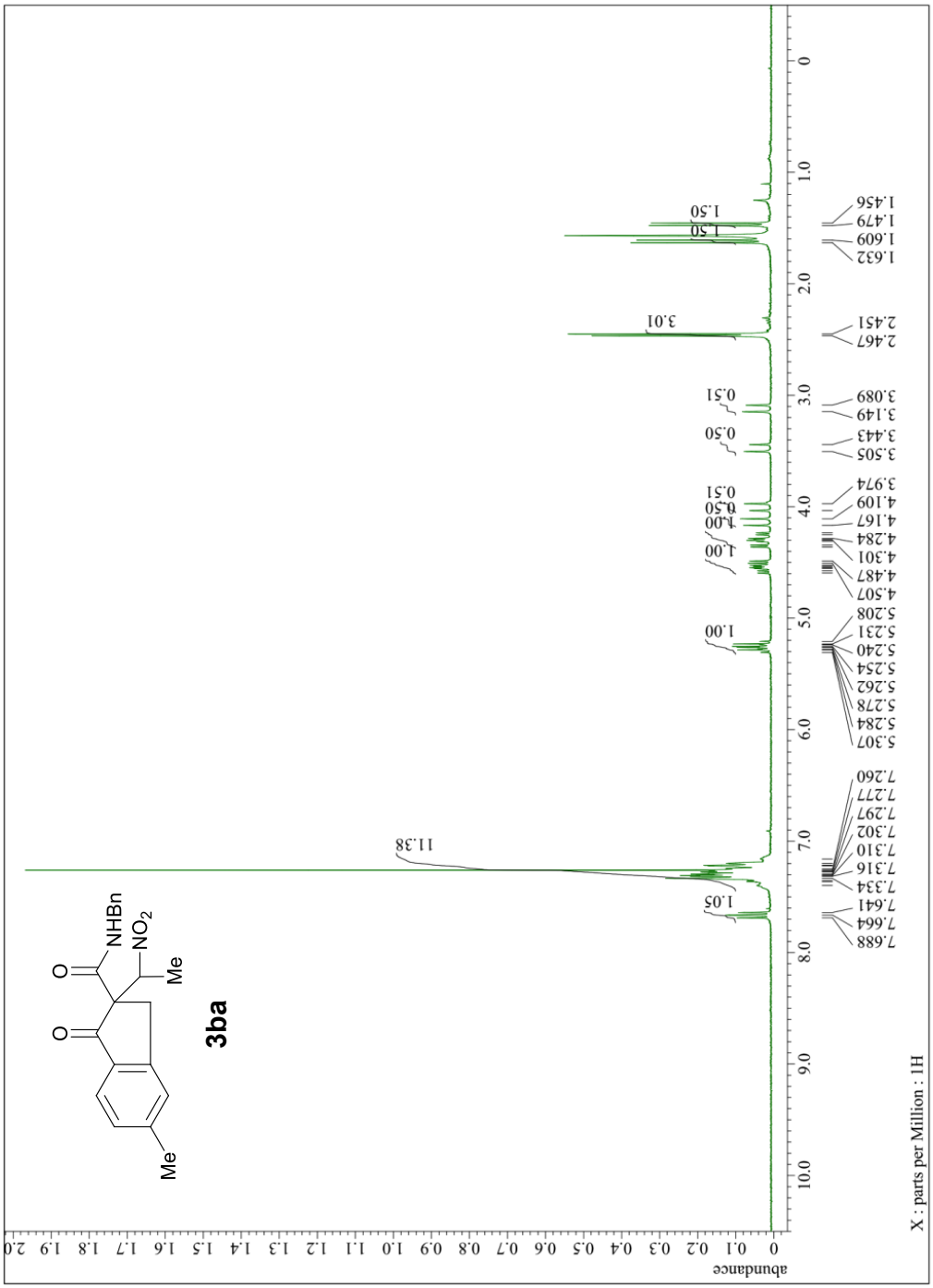

1n
Cl
Cl
NH
O
O
abundance
0
0.1
0.2
0.3
X : parts per Million : 13C
203.296
164.518
154.078
137.156
136.276
134.976
132.710
130.444
127.872
127.394
126.744
124.564
121.533
119.057
77.430
77.000
76.579
53.280
28.375

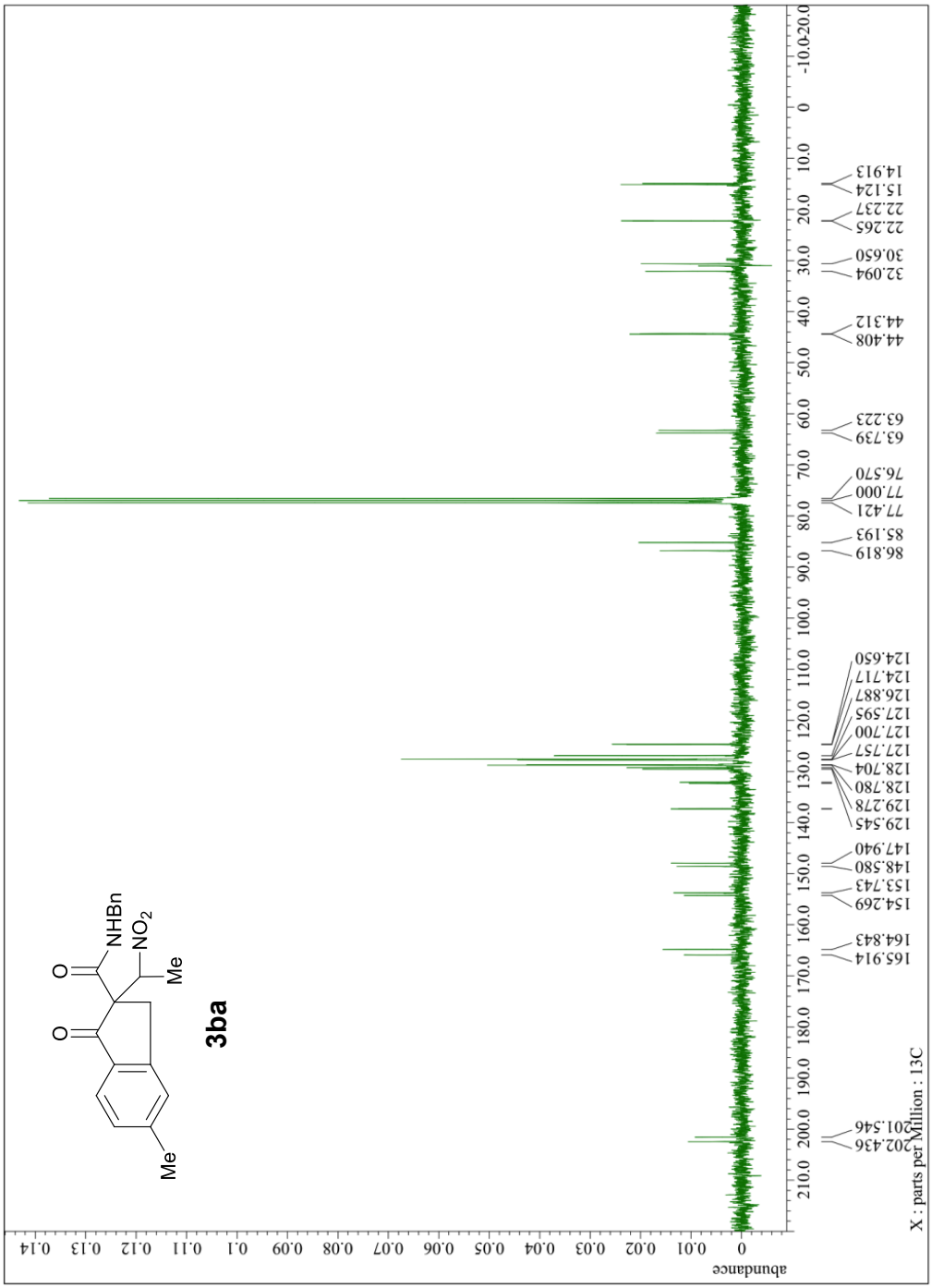

NHBn
NO2
Me
O
O
3aa
(less polar)
abundance
X : parts per Million : 1H
6.52
2.10
1.03
1.07
1.17
1.00
1.06
2.02
1.03
3.08
7.776
7.656
7.513
7.412
7.338
7.332
7.329
7.320
7.314
7.307
7.301
7.260
7.226
7.220
7.199
5.296
5.273
5.250
5.227
4.513
4.492
4.306
4.288
4.239
4.182
3.189
3.129
1.646
1.623

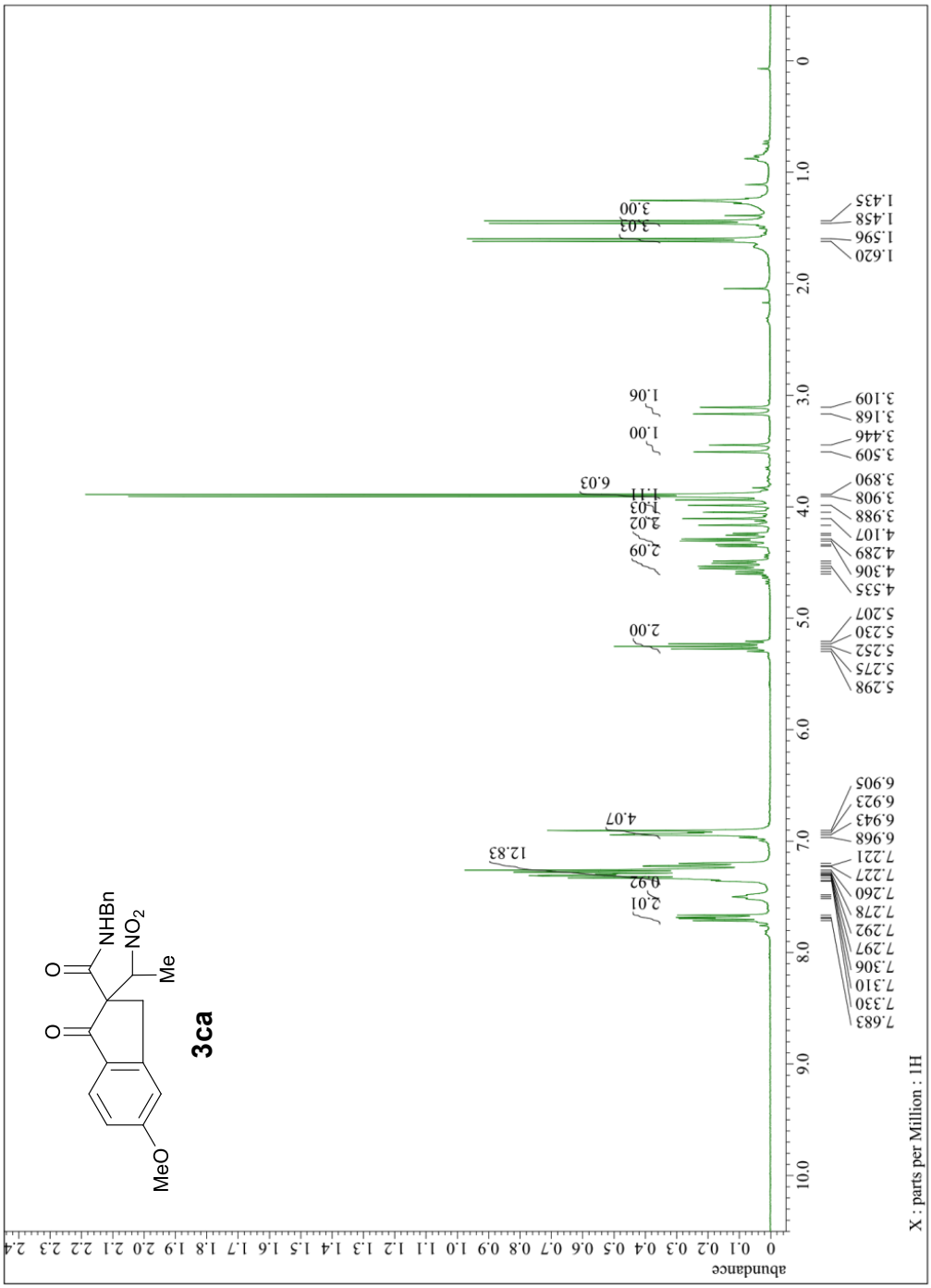

NHBn
NO2
Me
O
O
3aa
(less polar)
abundance
X : parts per Million : 13C
203.239
164.604
153.284
137.213
136.257
134.440
128.838
127.968
127.786
127.643
126.572
124.841
85.251
77.430
77.210
77.000
76.579
63.663
44.494
30.908
15.152

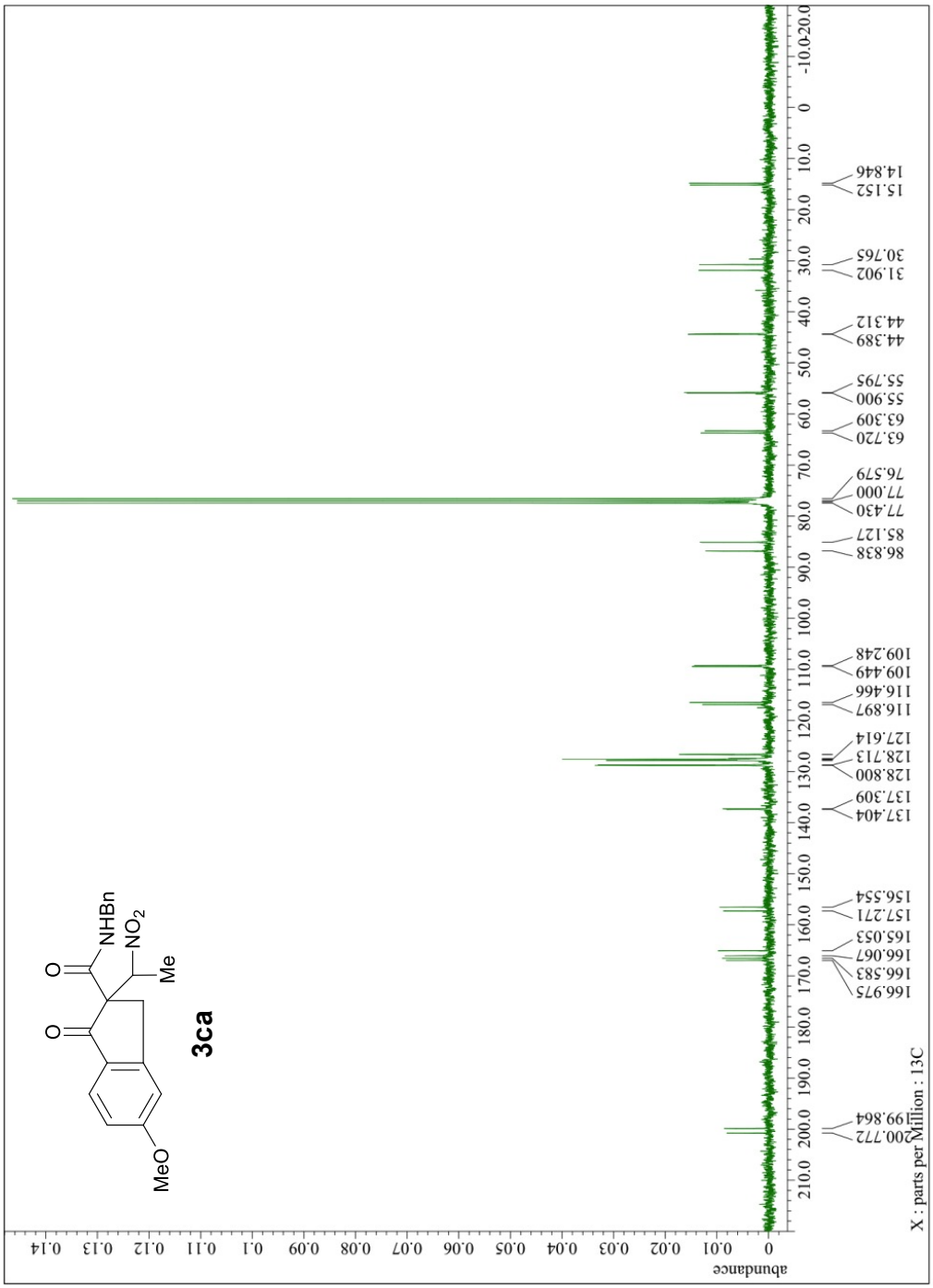

3aa
(polar)
NHBn
NO2
Me
O
O
abundance
X : parts per Million : 1H
5.36
3.04
0.94
1.00
1.03
1.03
1.00
1.00
1.00
1.100
1.473
1.496
3.490
3.553
3.736
4.038
4.100
4.345
4.362
4.524
4.545
5.259
5.282
5.304
5.327
7.249
7.260
7.268
7.275
7.281
7.297
7.302
7.316
7.322
7.334
7.341
7.426
7.553
7.692
7.756

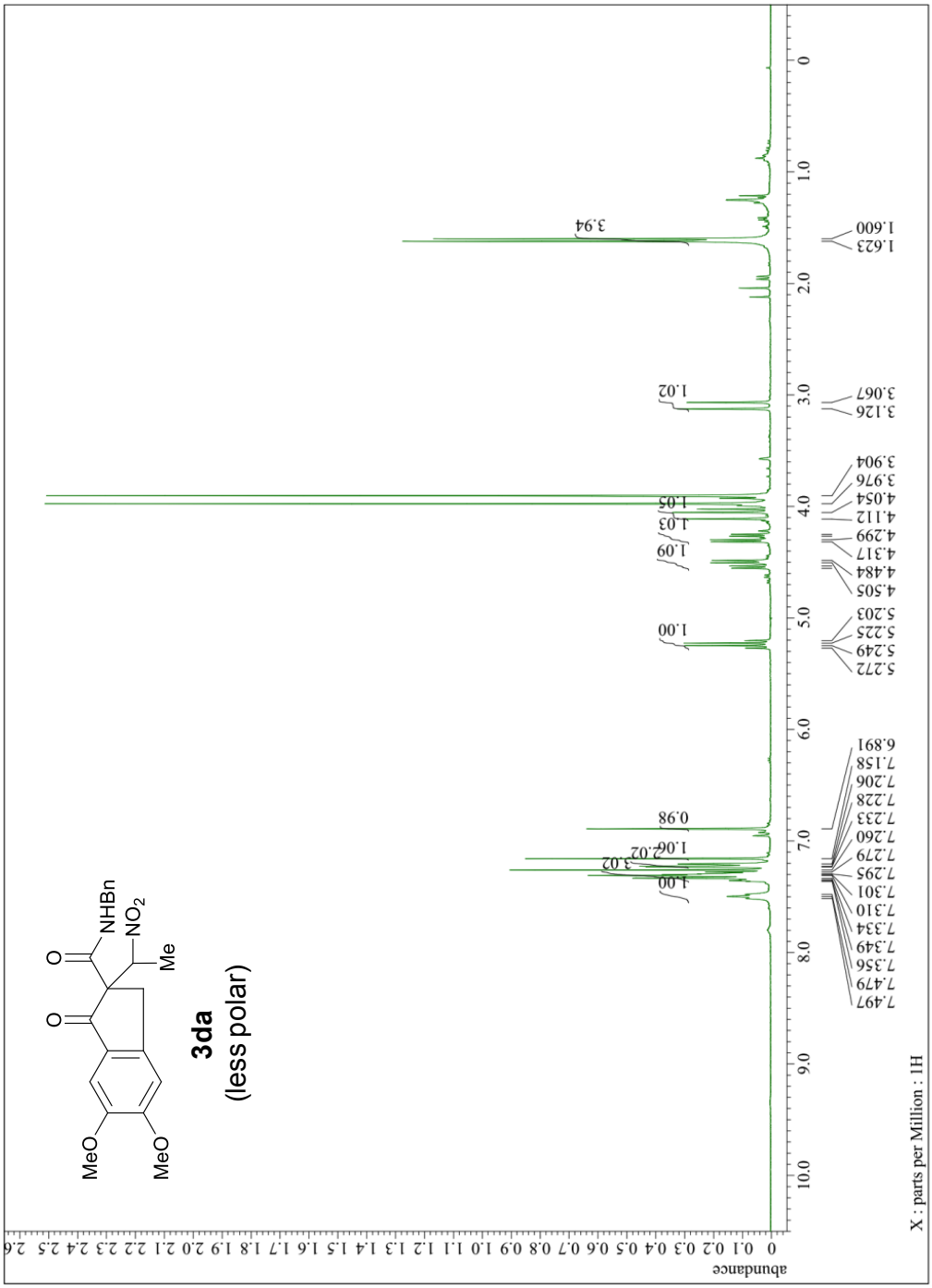

3aa
(polar)
NHBn
NO2
Me
O
O
abundance
X : parts per Million : 13C
202.388
165.656
153.753
137.280
136.764
134.660
128.761
128.216
127.815
127.690
126.610
124.918
86.895
77.421
77.201
77.000
76.579
63.099
44.408
32.457
15.018

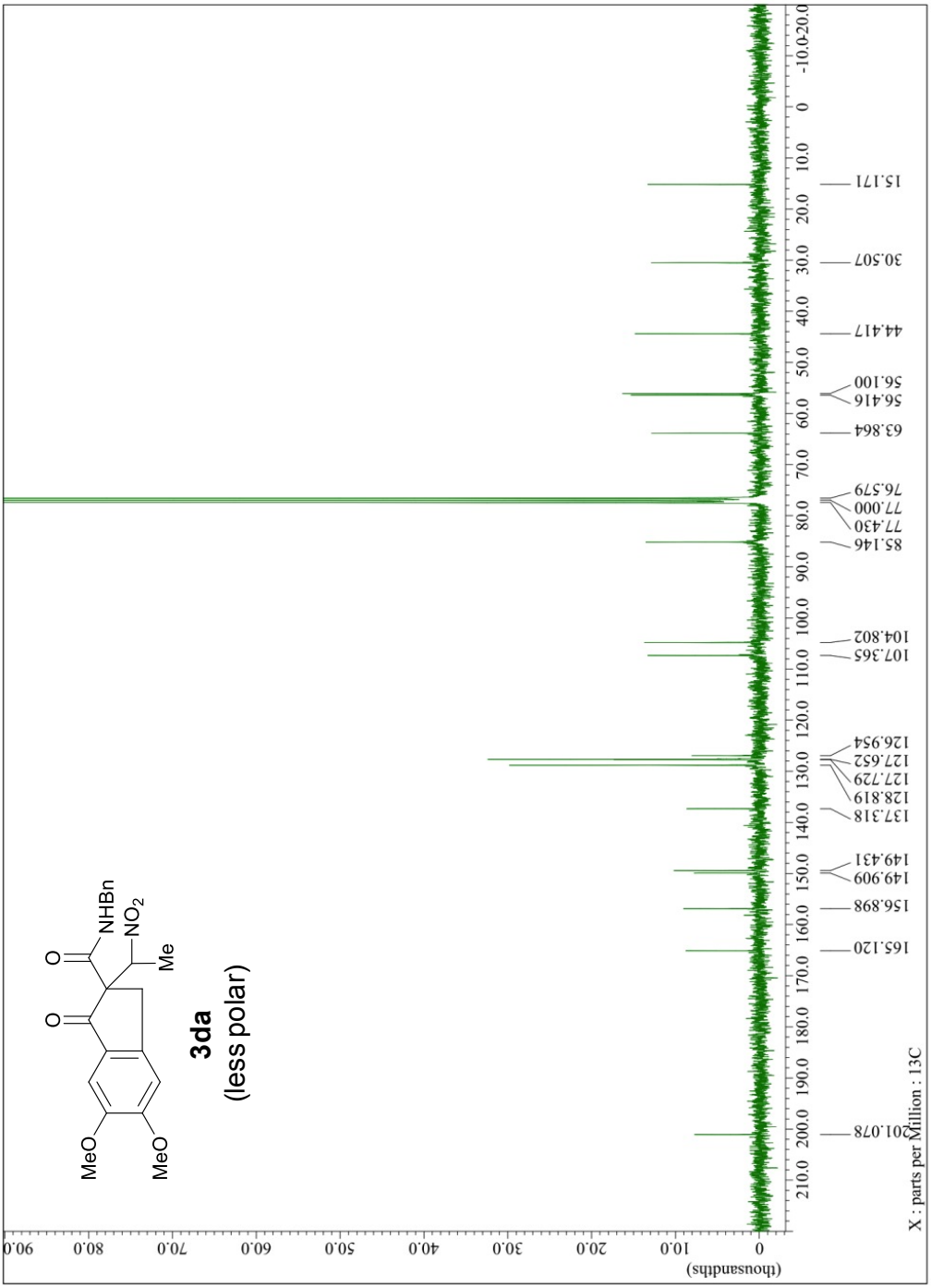

3ba
NHBn
NO2
Me
O
O
Me
11.38
3.01
1.50
1.50
1.05
1.00
1.00
1.00
0.51
0.50
0.51
0.50
abundance
X : parts per Million : 1H

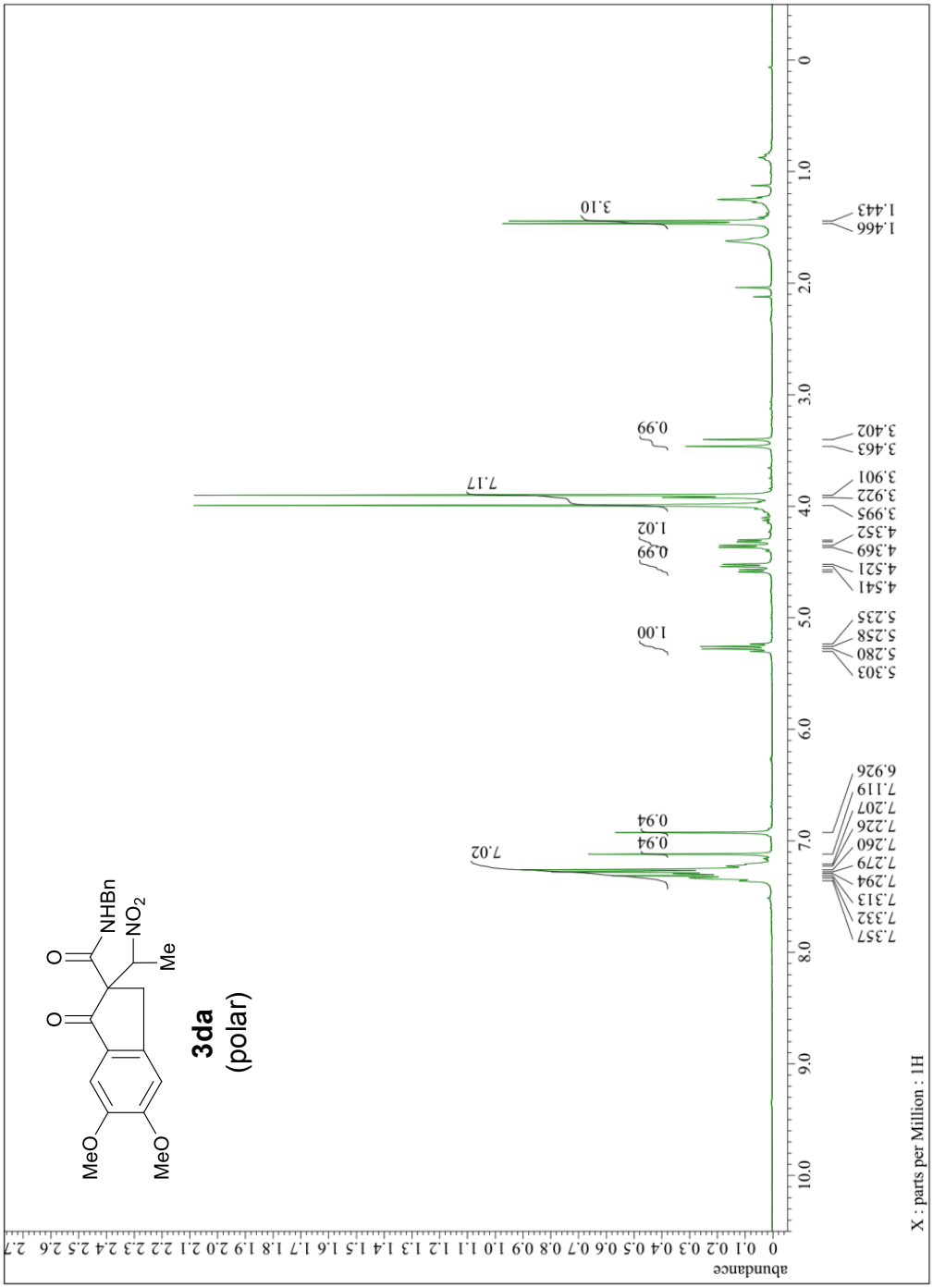

3ba
NHBn
NO2
Me
Me
O
O
X : parts per Million : 13C
abundance
202.436
201.546
165.914
164.843
154.269
153.743
148.580
147.940
129.545
129.278
128.780
128.704
127.757
127.700
127.595
126.887
124.717
124.650
86.819
85.193
77.421
77.000
76.570
63.739
63.223
44.408
44.312
32.094
30.650
22.265
22.237
15.124
14.913

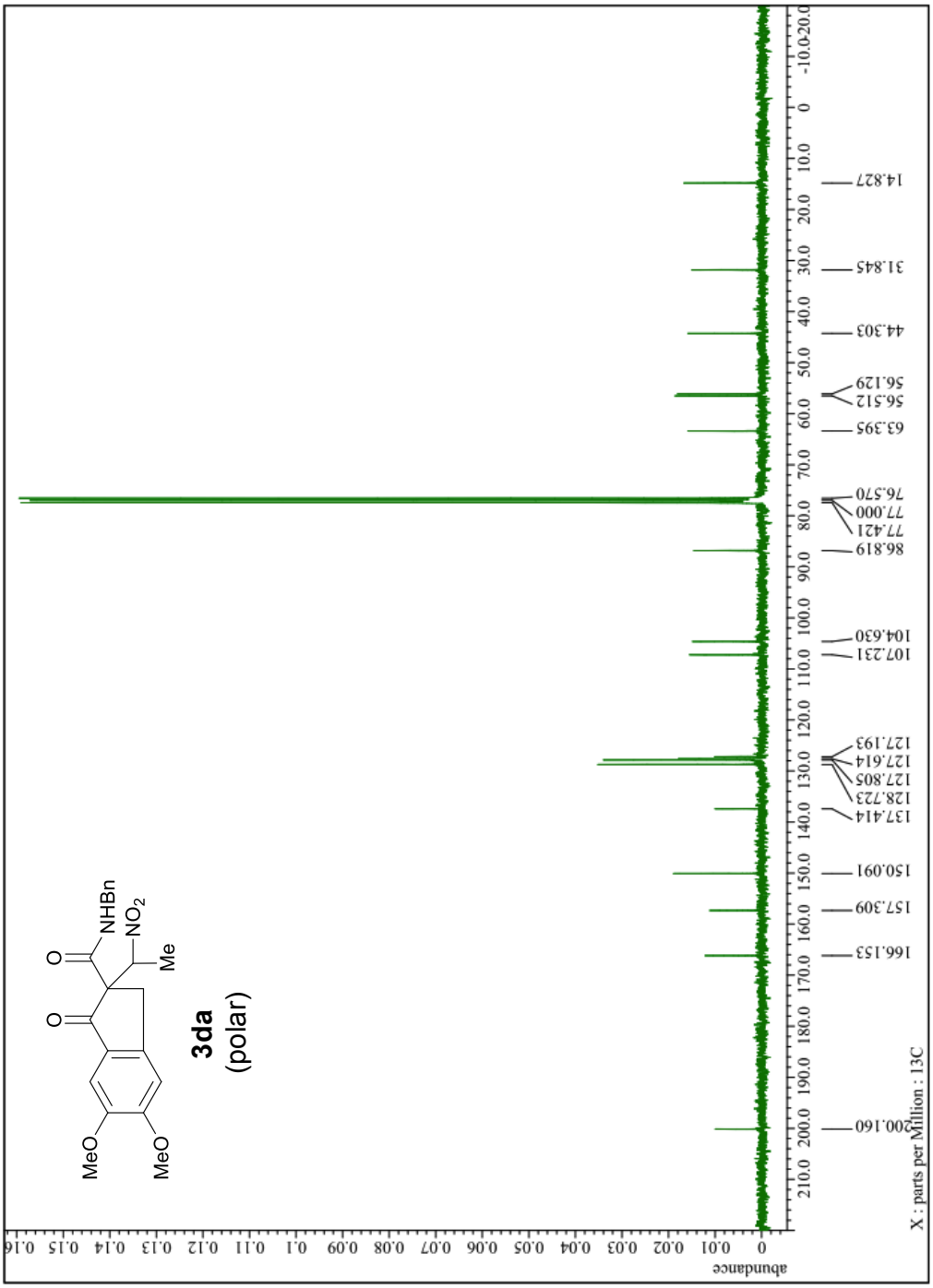

3ca
NHBn
NO2
Me
O
O
MeO
abundance
X : parts per Million : 1H

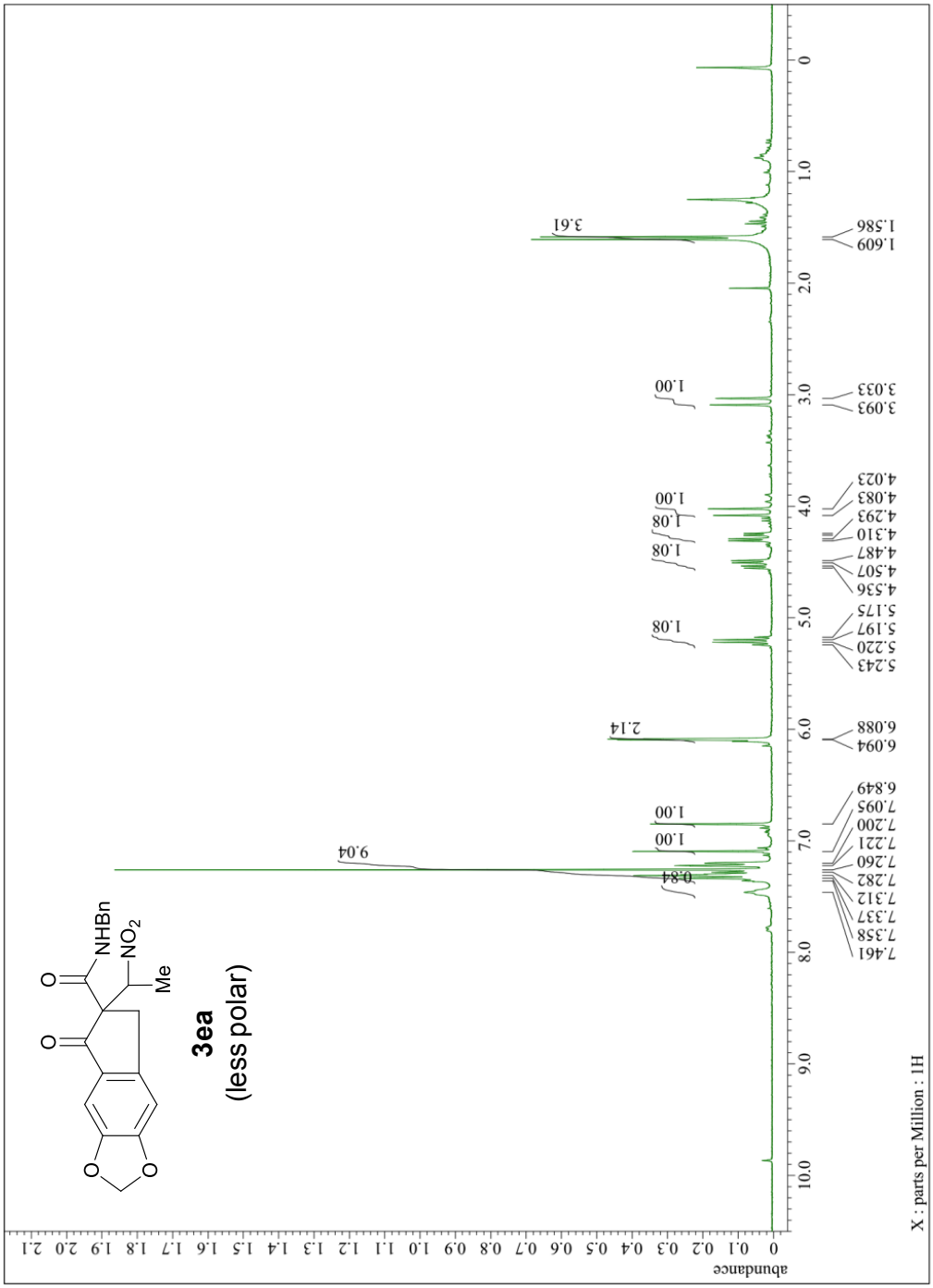

3ca
NHBn
NO2
Me
O
O
MeO
X : parts per Million : 13C
abundance
199.864
200.772
166.975
166.583
166.067
165.053
157.271
156.554
137.404
137.309
128.800
128.713
127.614
116.897
116.466
109.449
109.248
86.838
85.127
77.430
77.000
76.579
63.720
63.309
55.900
55.795
44.389
44.312
31.902
30.765
15.152
14.846

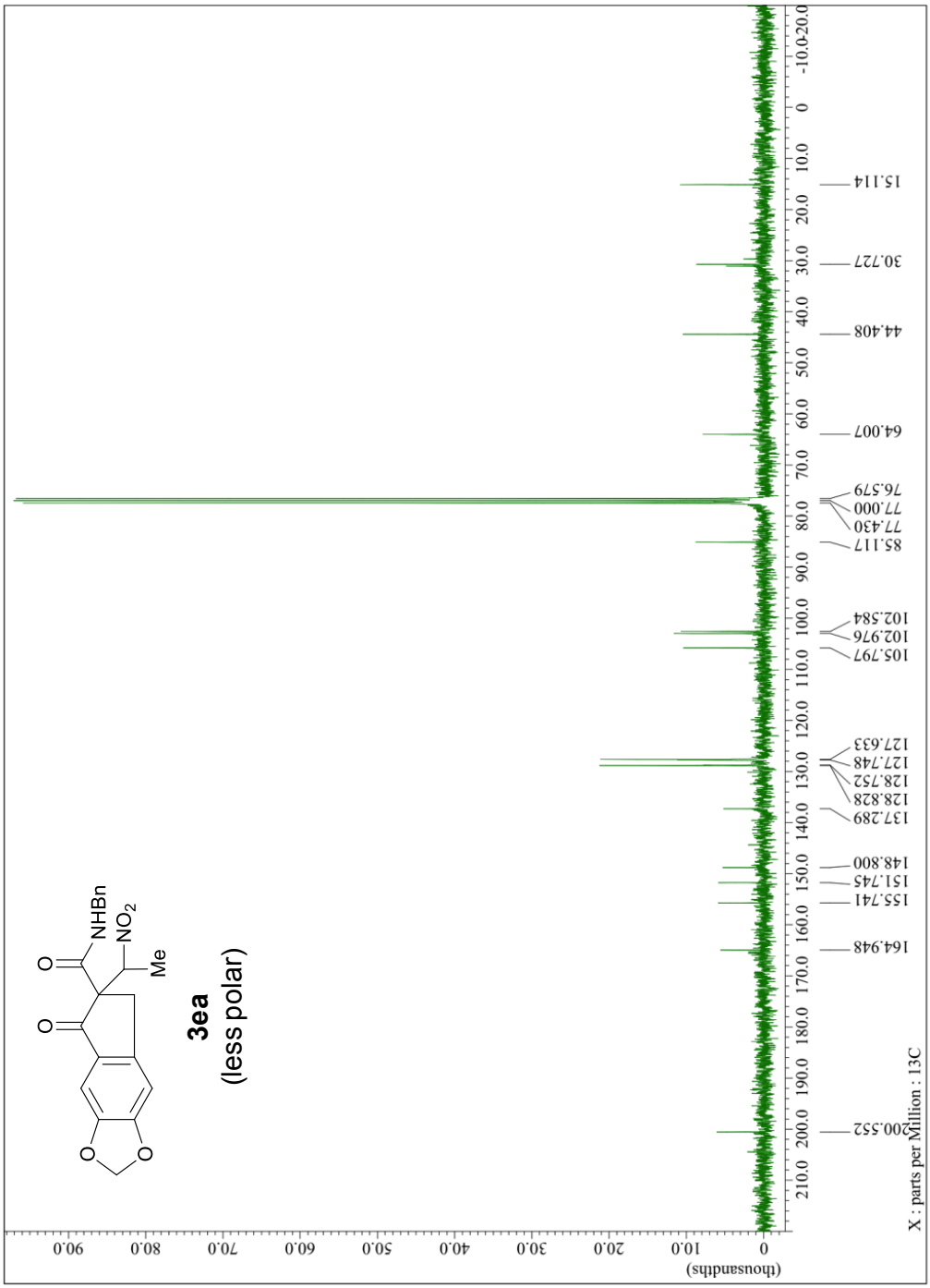

3da
(less polar)
NHBn
NO2
Me
O
O
MeO
MeO
X : parts per Million : 1H
abundance

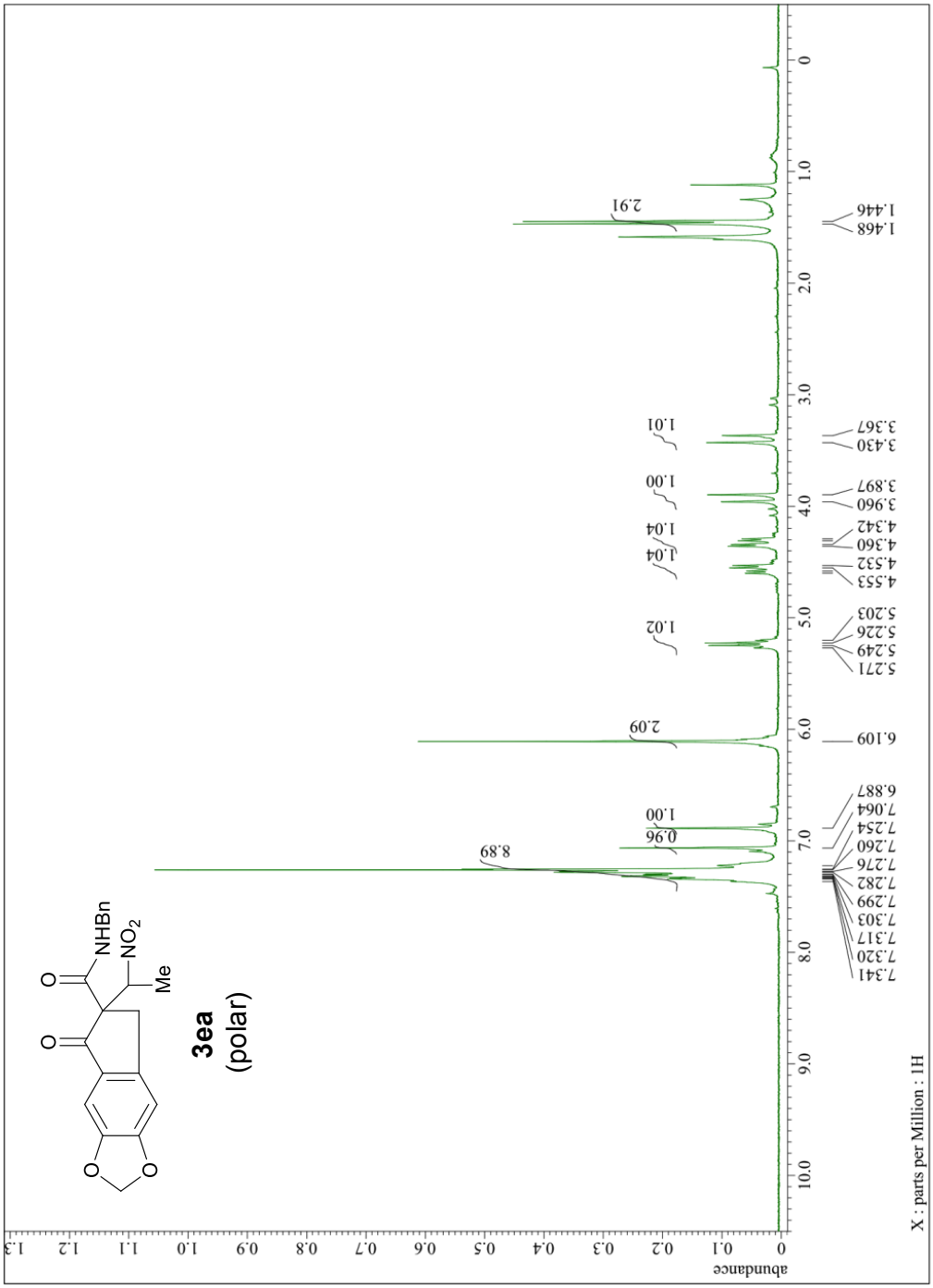

3da
(less polar)
NHBn
NO2
Me
O
O
MeO
MeO
201.078
165.120
156.898
149.909
149.431
137.318
128.819
127.729
127.652
126.954
107.365
104.802
85.146
77.430
77.000
76.579
63.864
56.416
56.100
44.417
30.507
15.171
X : parts per Million : 13C
(thousandths)

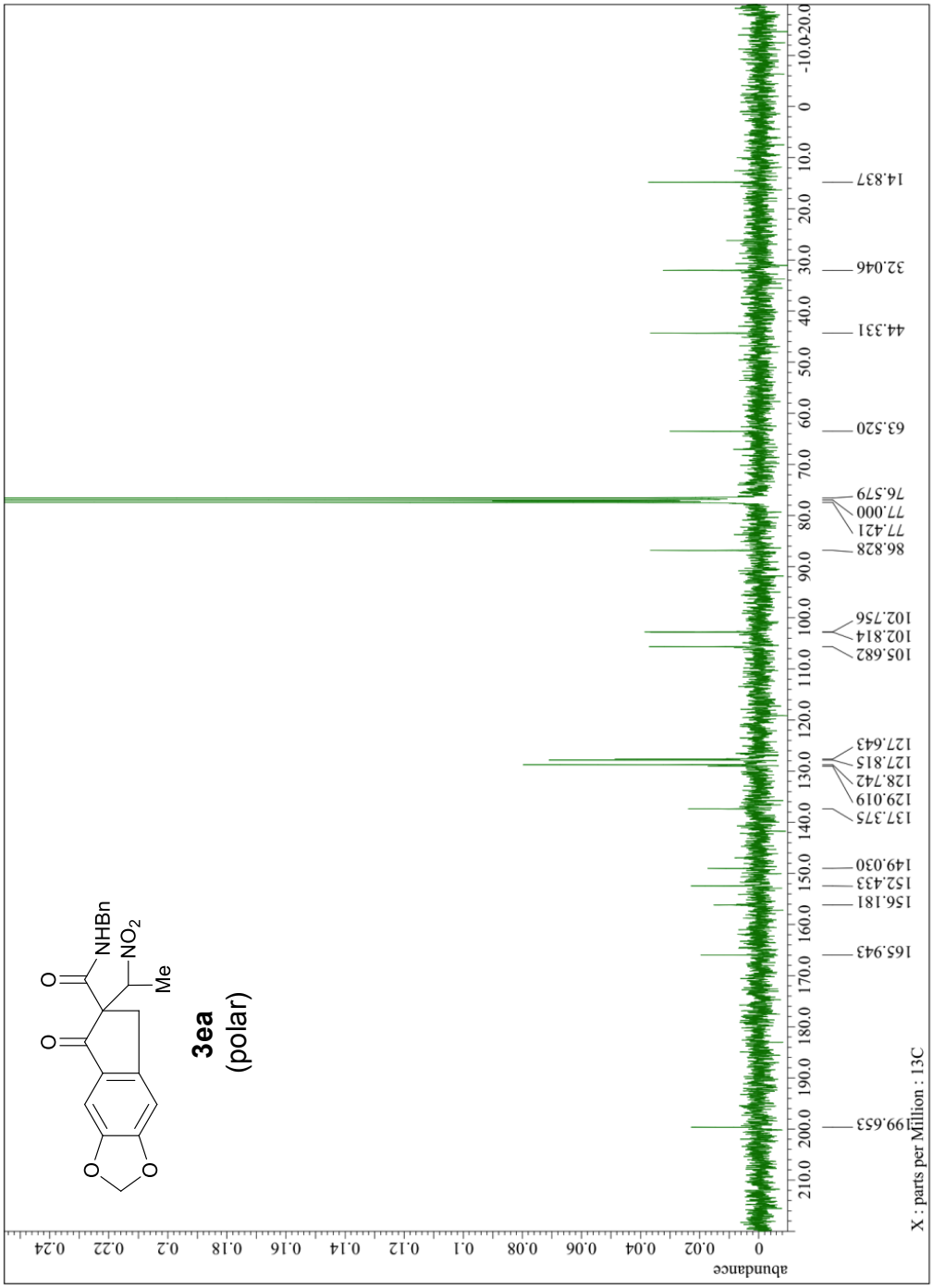

O
O
NHBn
NO2
Me
MeO
MeO
3da
(polar)
X : parts per Million : 1H
abundance
7.357
7.332
7.313
7.294
7.279
7.260
7.226
7.207
7.119
6.926
7.02
0.94
0.94
5.303
5.280
5.258
5.235
1.00
4.541
4.521
4.369
4.352
0.99
1.02
3.995
3.922
3.901
7.17
3.463
3.402
0.99
3.10
1.466
1.443

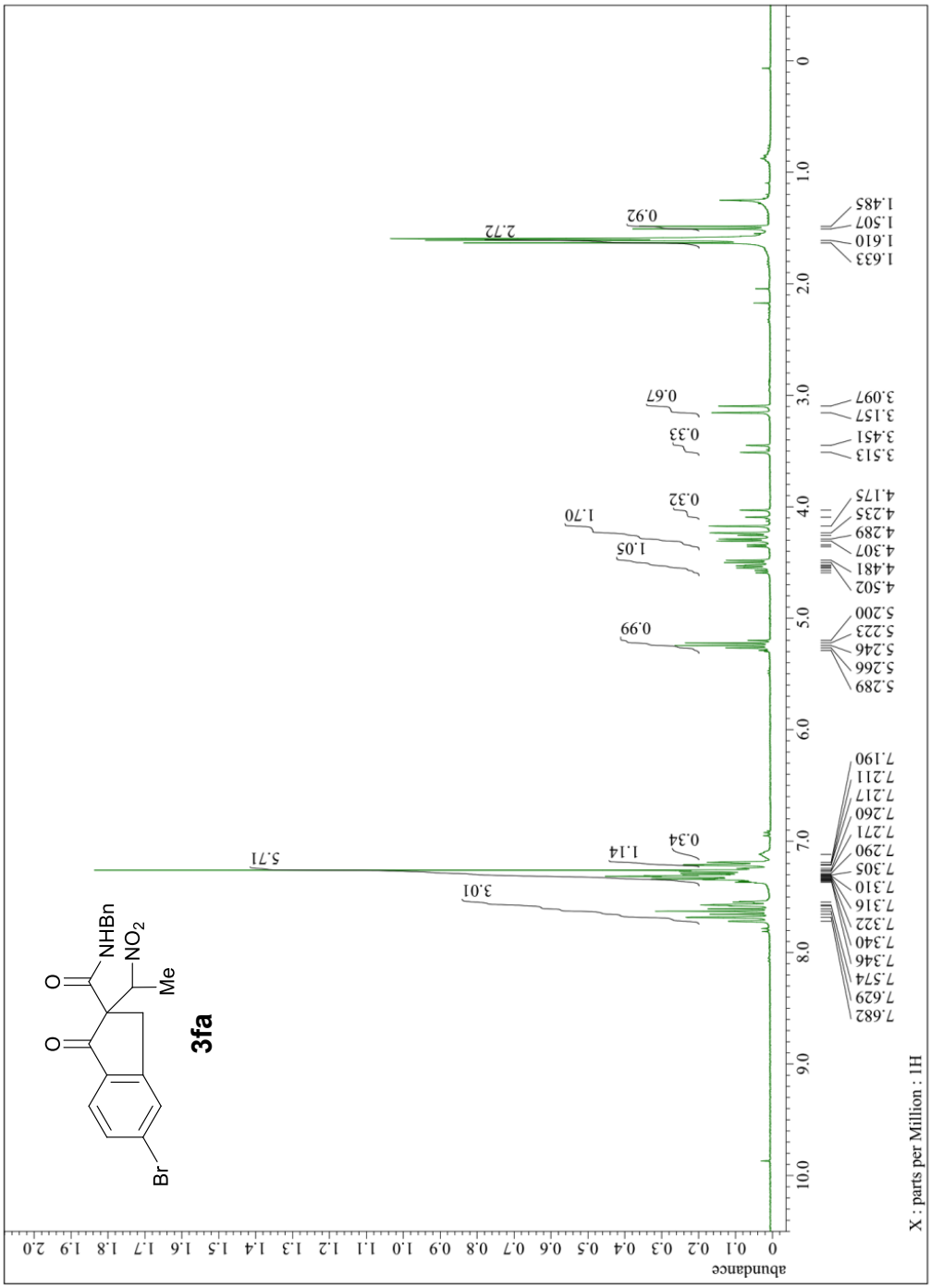

3da
(polar)
NHBn
NO2
Me
O
O
MeO
MeO
200.160
166.153
157.309
150.091
137.414
128.723
127.805
127.614
127.193
107.231
104.630
86.819
77.421
77.000
76.570
63.395
56.512
56.129
44.303
31.845
14.827
X : parts per Million : 13C
abundance

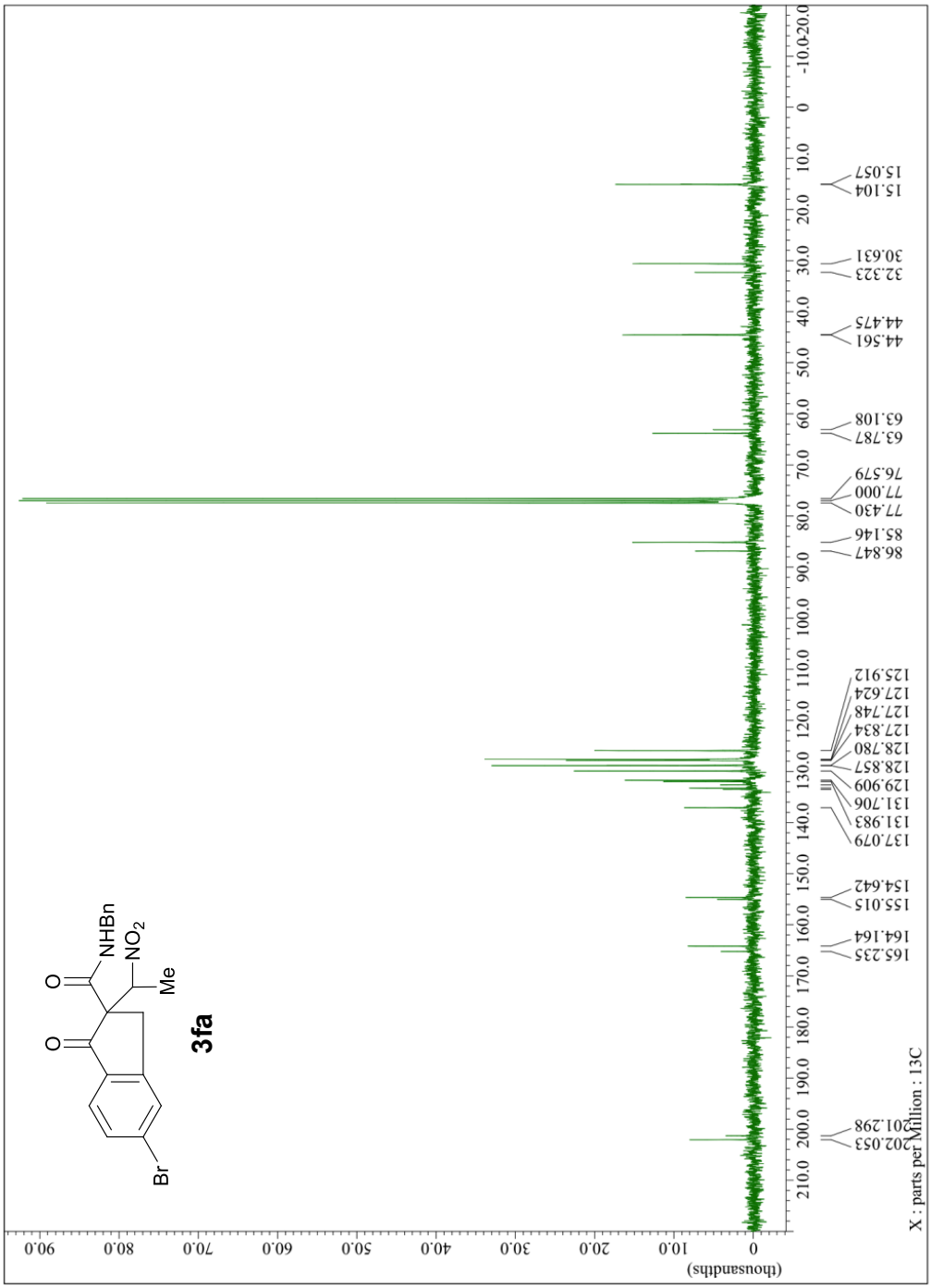

3ea
(less polar)
NHBn
NO2
Me
O
O
O
O
abundance
X : parts per Million : 1H
9.04
2.14
1.08
1.08
1.08
1.00
1.00
1.00
1.00
3.61
0.84
7.461
7.358
7.337
7.312
7.282
7.260
7.221
7.200
7.095
6.849
6.094
6.088
5.243
5.220
5.197
5.175
4.536
4.507
4.487
4.310
4.293
4.083
4.023
3.093
3.033
1.609
1.586

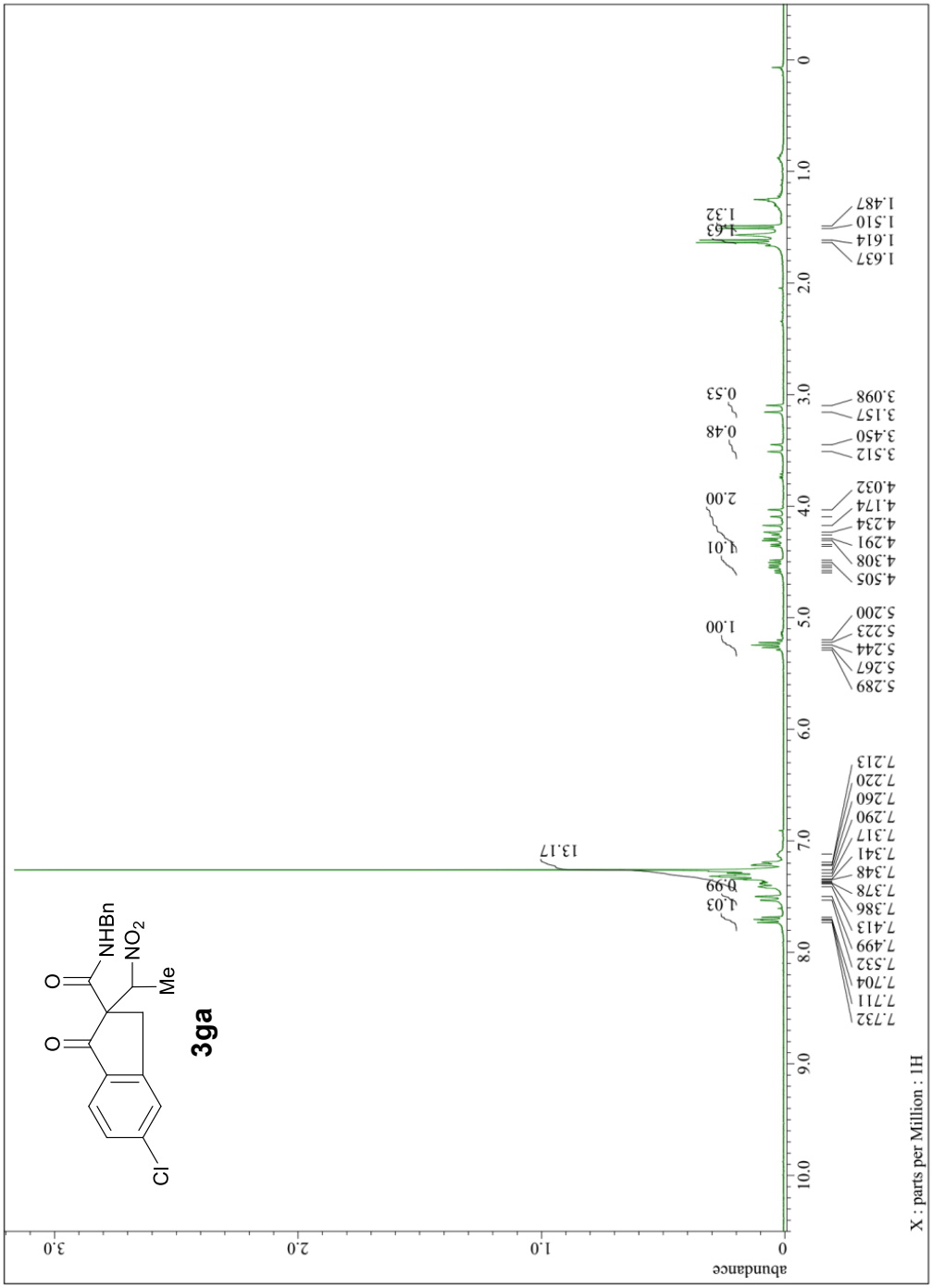

NHBn
NO2
Me
O
O
O
O
3ea
(less polar)
(thousandths)
X : parts per Million : 13C
200.552
164.948
155.741
151.745
148.800
137.289
128.828
128.752
127.748
127.633
105.797
102.976
102.584
85.117
77.430
77.000
76.579
64.007
44.408
30.727
15.114

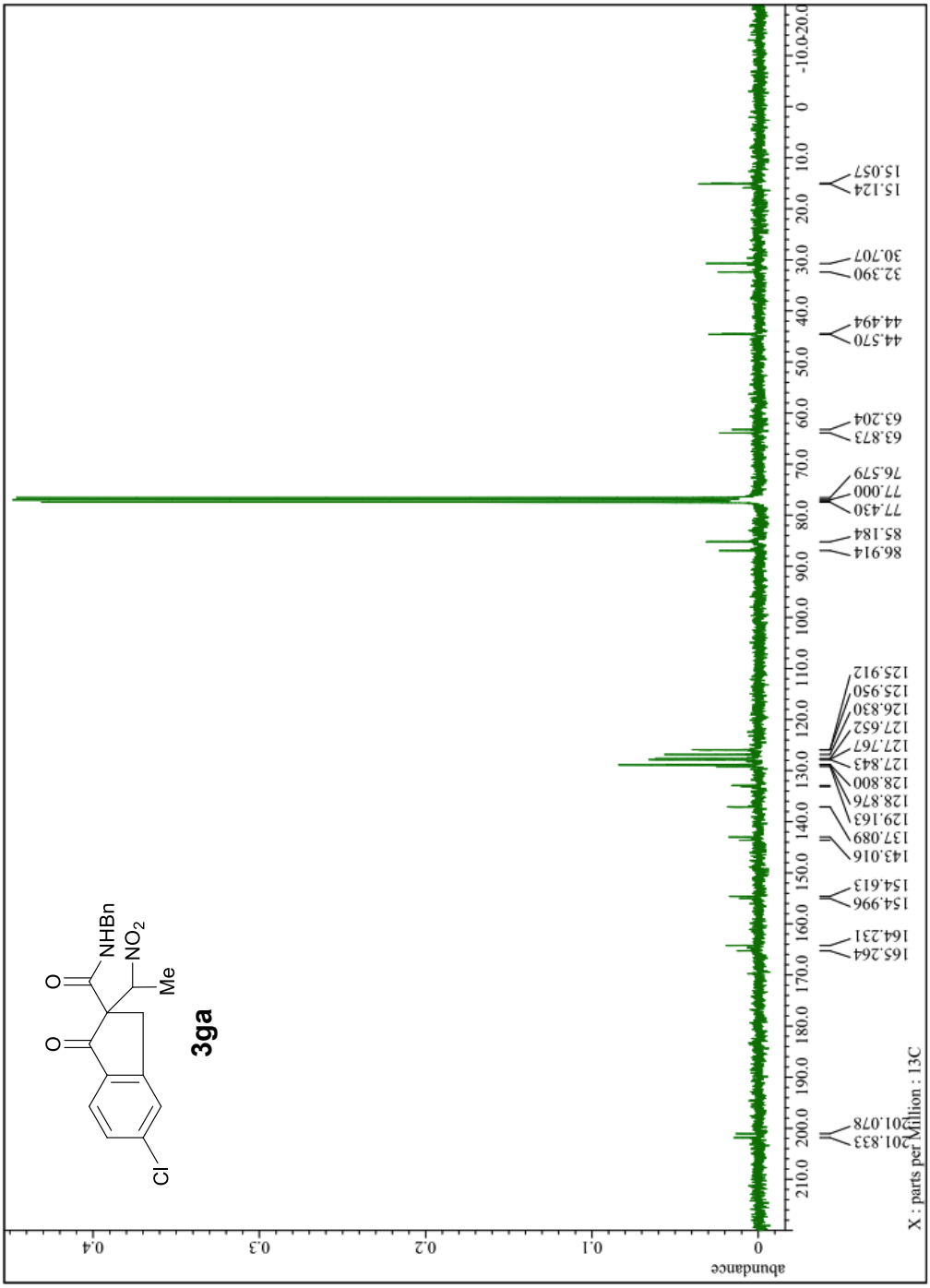

3ea
(polar)
NHBn
NO2
Me
O
O
O
O
8.89
0.96
1.00
2.09
1.02
1.04
1.04
1.00
1.01
2.91
7.341
7.320
7.317
7.303
7.299
7.282
7.276
7.260
7.254
7.064
6.887
6.109
5.271
5.249
5.226
5.203
4.553
4.532
4.360
4.342
3.960
3.897
3.430
3.367
1.468
1.446
abundance
X : parts per Million : 1H

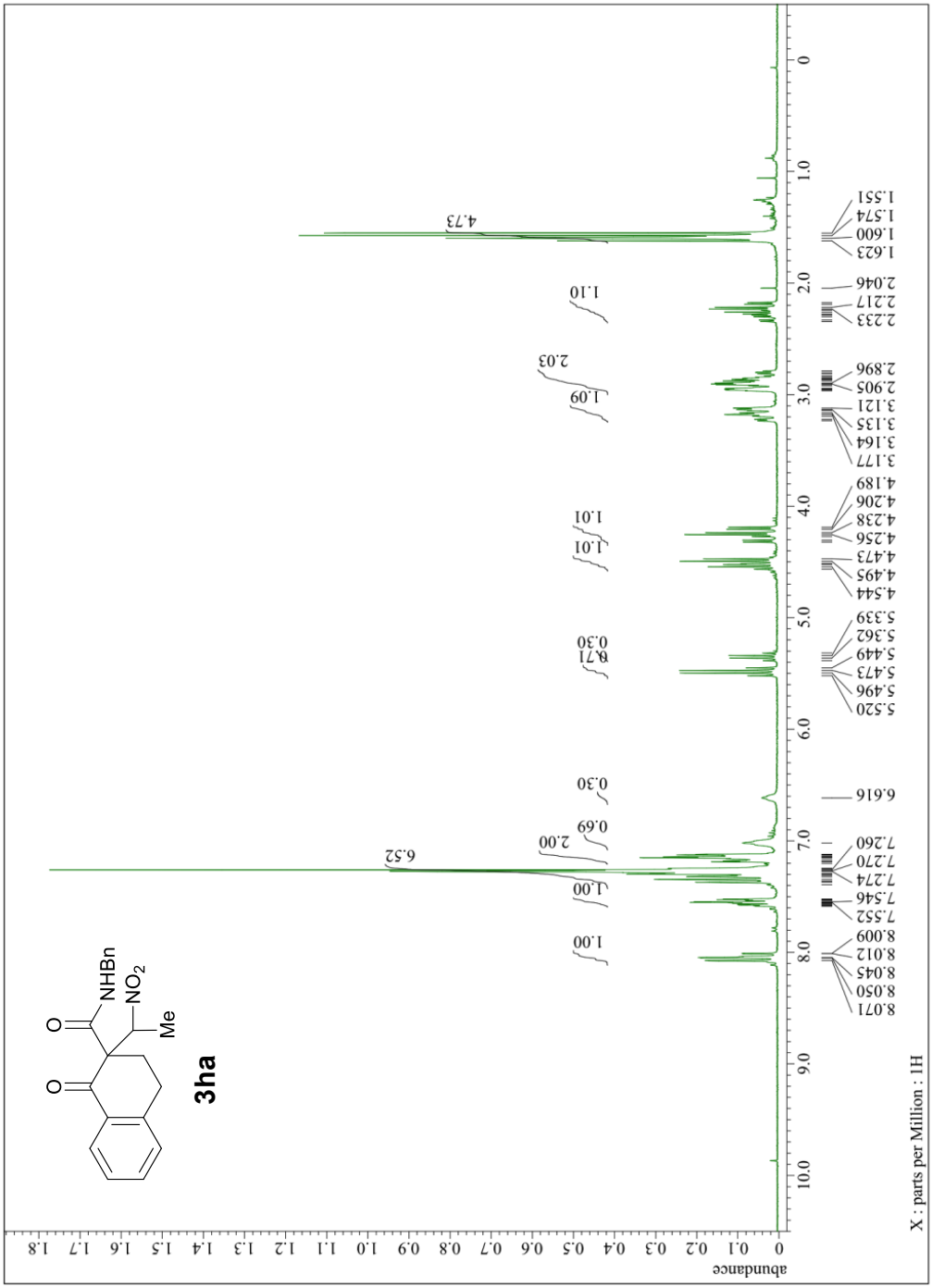

3ea
(polar)
NHBn
NO2
Me
O
O
O
O
abundance
X : parts per Million : 13C
199.653
165.943
156.181
152.433
149.030
137.375
129.019
128.742
127.815
127.643
105.682
102.814
102.756
86.828
77.421
77.000
76.579
63.520
44.331
32.046
14.837

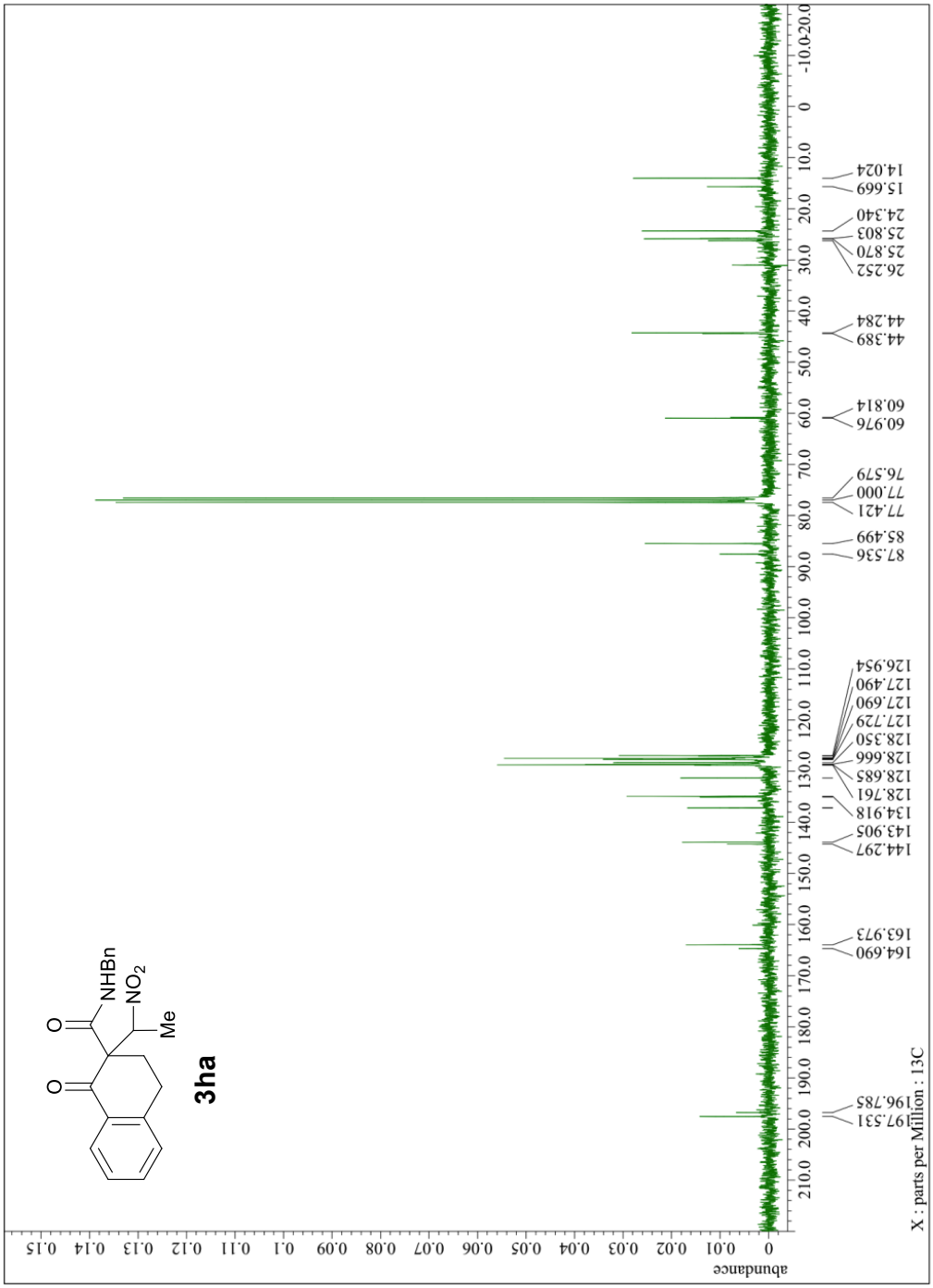

3fa
NHBn
NO2
Me
O
O
Br
abundance
X : parts per Million : 1H
7.682
7.629
7.574
7.346
7.340
7.322
7.316
7.310
7.305
7.290
7.271
7.260
7.217
7.211
7.190
5.289
5.266
5.246
5.223
5.200
4.502
4.481
4.307
4.289
4.235
4.175
3.513
3.451
3.157
3.097
1.633
1.610
1.507
1.485
5.71
3.01
2.72
1.70
1.14
1.05
0.99
0.92
0.67
0.34
0.33
0.32

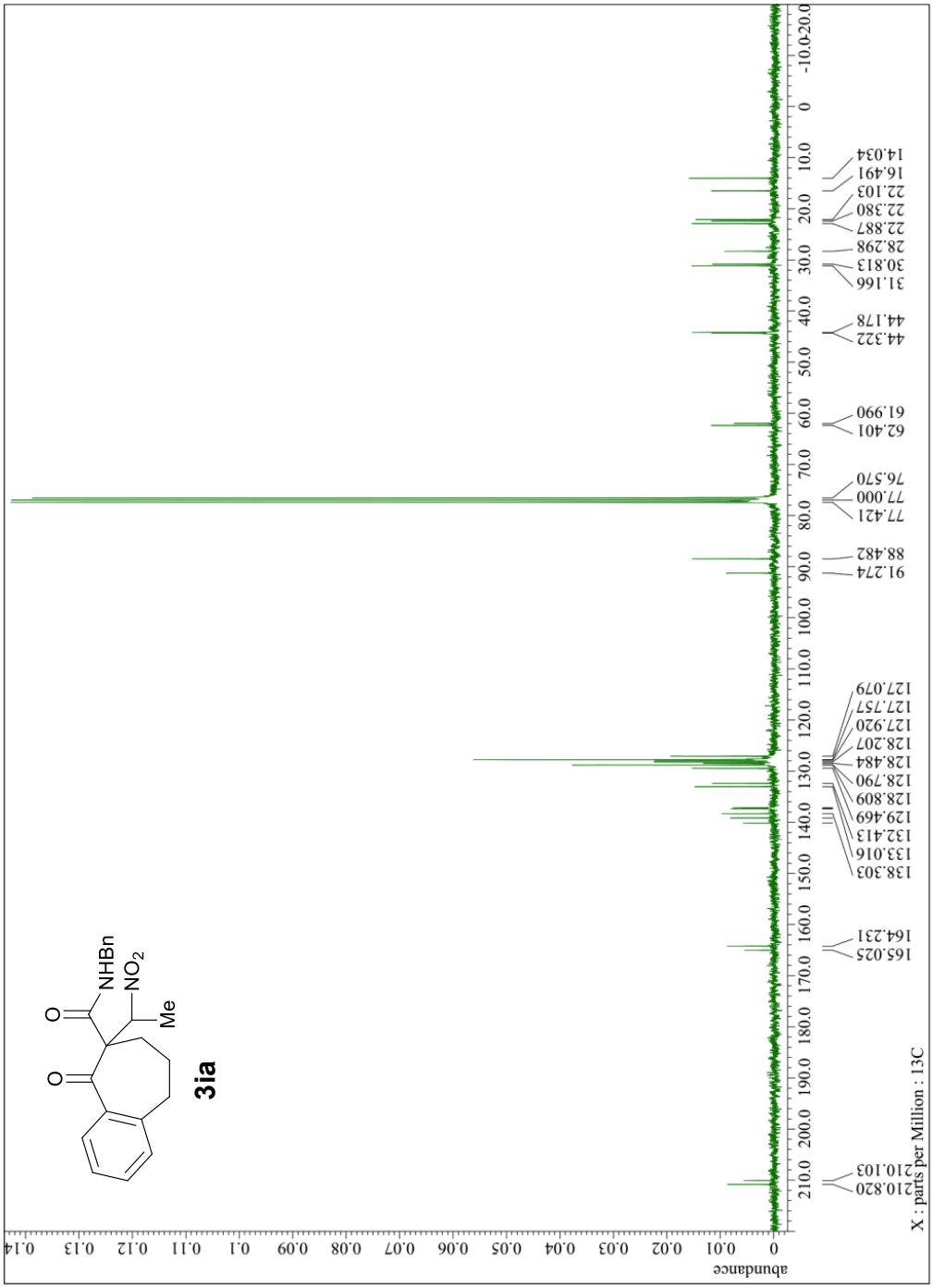

3fa
NHBn
NO2
Me
O
O
Br
(thousandths)
X : parts per Million : 13C
201.298
202.053
165.235
164.164
155.015
154.642
137.079
131.983
131.706
129.909
128.857
128.780
127.834
127.748
127.624
125.912
86.847
85.146
77.430
77.000
76.579
63.787
63.108
44.561
44.475
32.323
30.631
15.104
15.057

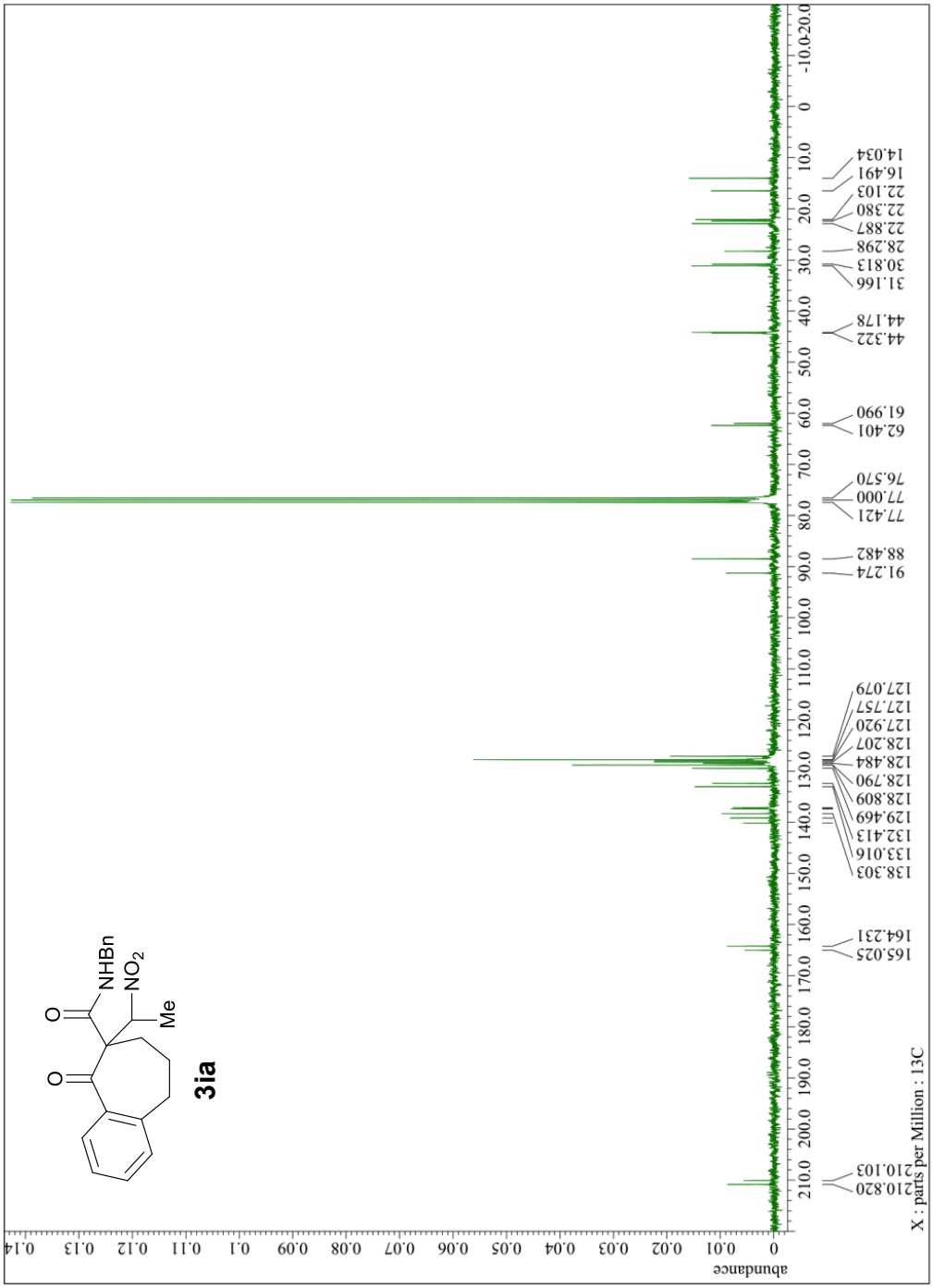

3ga
NHBn
NO2
Me
O
O
Cl
13.17
1.03
0.99
1.00
1.01
2.00
0.48
0.53
1.63
1.32
7.732
7.711
7.704
7.532
7.499
7.413
7.386
7.378
7.348
7.341
7.317
7.290
7.260
7.220
7.213
5.289
5.267
5.244
5.223
5.200
4.505
4.308
4.291
4.234
4.174
4.032
3.512
3.450
3.157
3.098
1.637
1.614
1.510
1.487
abundance
X : parts per Million : 1H

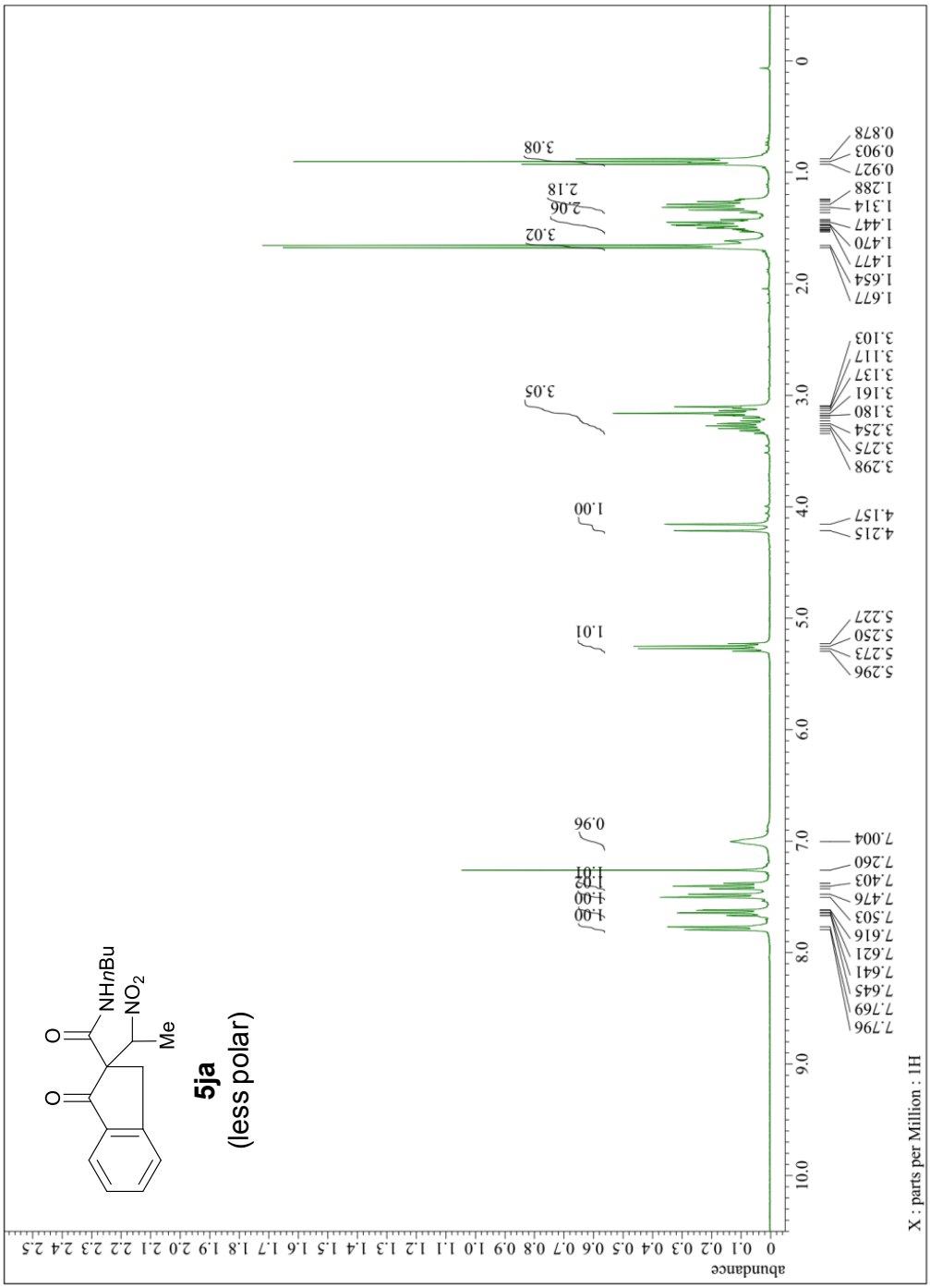

3ga
NHBn
NO2
Me
O
O
Cl
abundance
X : parts per Million : 13C
201.833
201.078
165.264
164.231
154.996
154.613
143.016
137.089
129.163
128.876
128.800
127.843
127.767
127.652
126.830
125.950
125.912
86.914
85.184
77.430
77.000
76.579
63.873
63.204
44.570
44.494
32.390
30.707
15.124
15.057

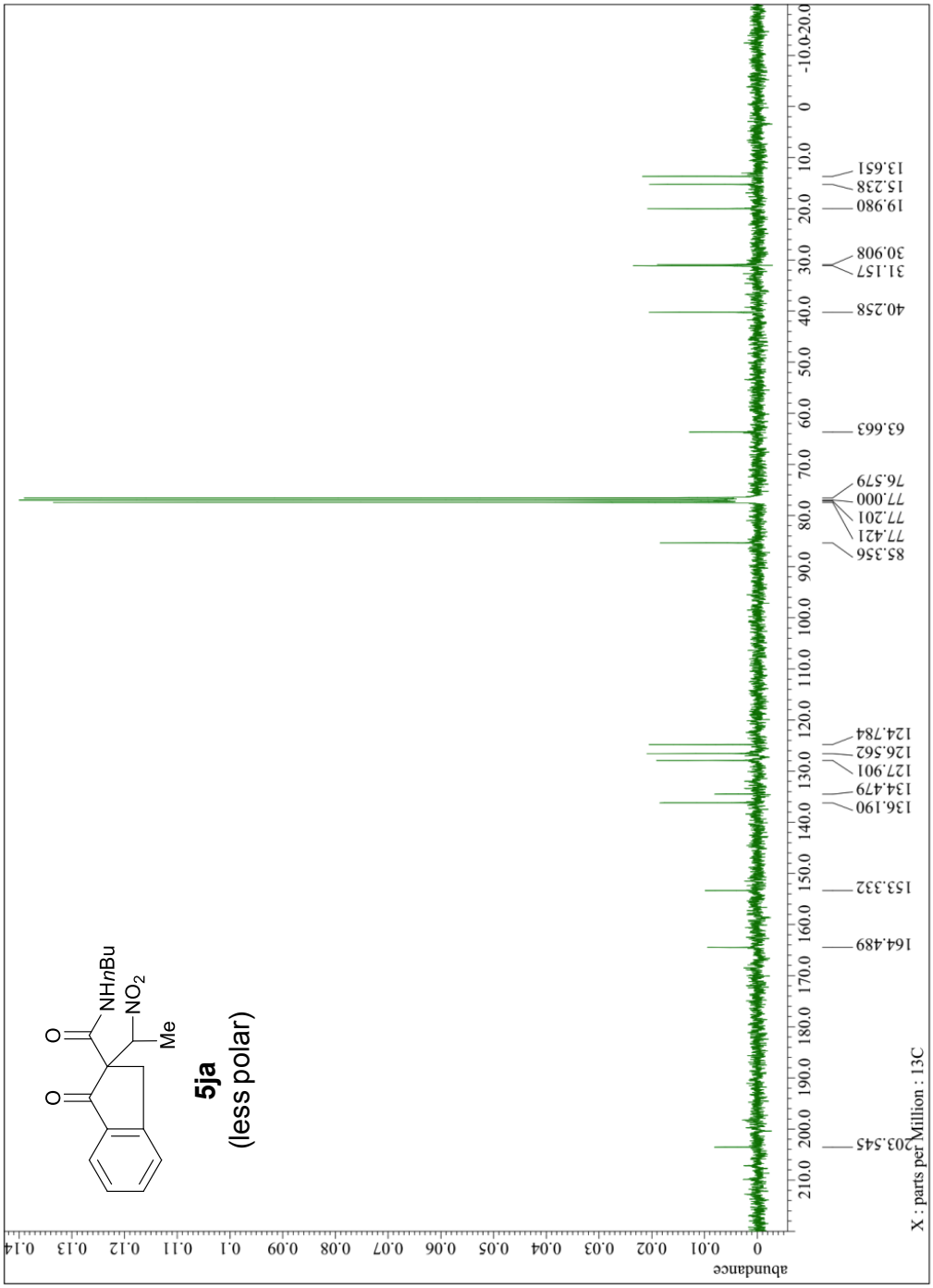

3ha
NHBn
NO2
Me
O
O
X : parts per Million : 1H
abundance

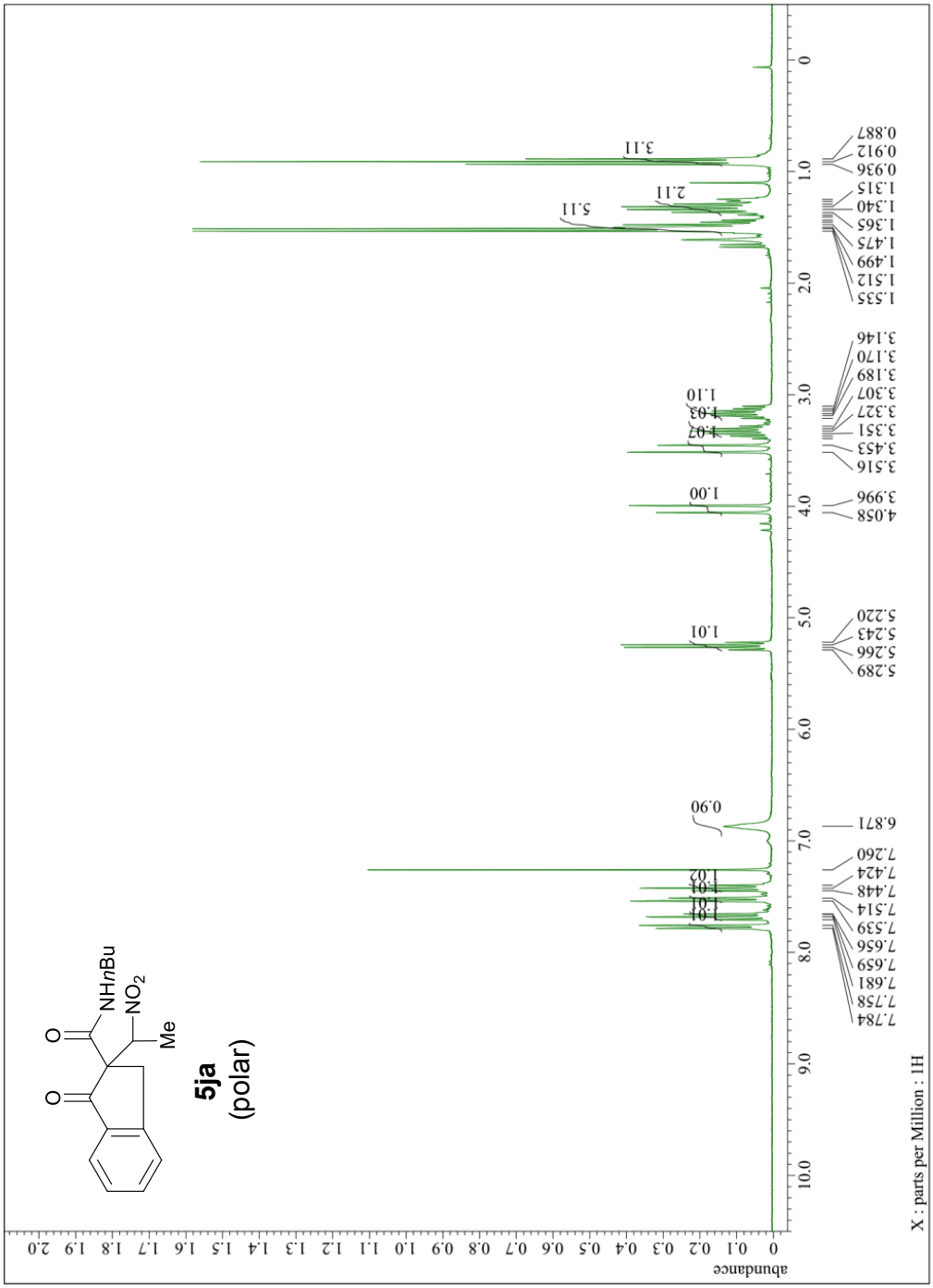

3ha
NHBn
NO2
Me
O
O
X : parts per Million : 13C
abundance
197.531
196.785
164.690
163.973
144.297
143.905
134.918
128.761
128.685
128.666
128.350
127.729
127.690
127.490
126.954
87.536
85.499
77.421
77.000
76.579
60.976
60.814
44.389
44.284
26.252
25.870
25.803
24.340
15.669
14.024

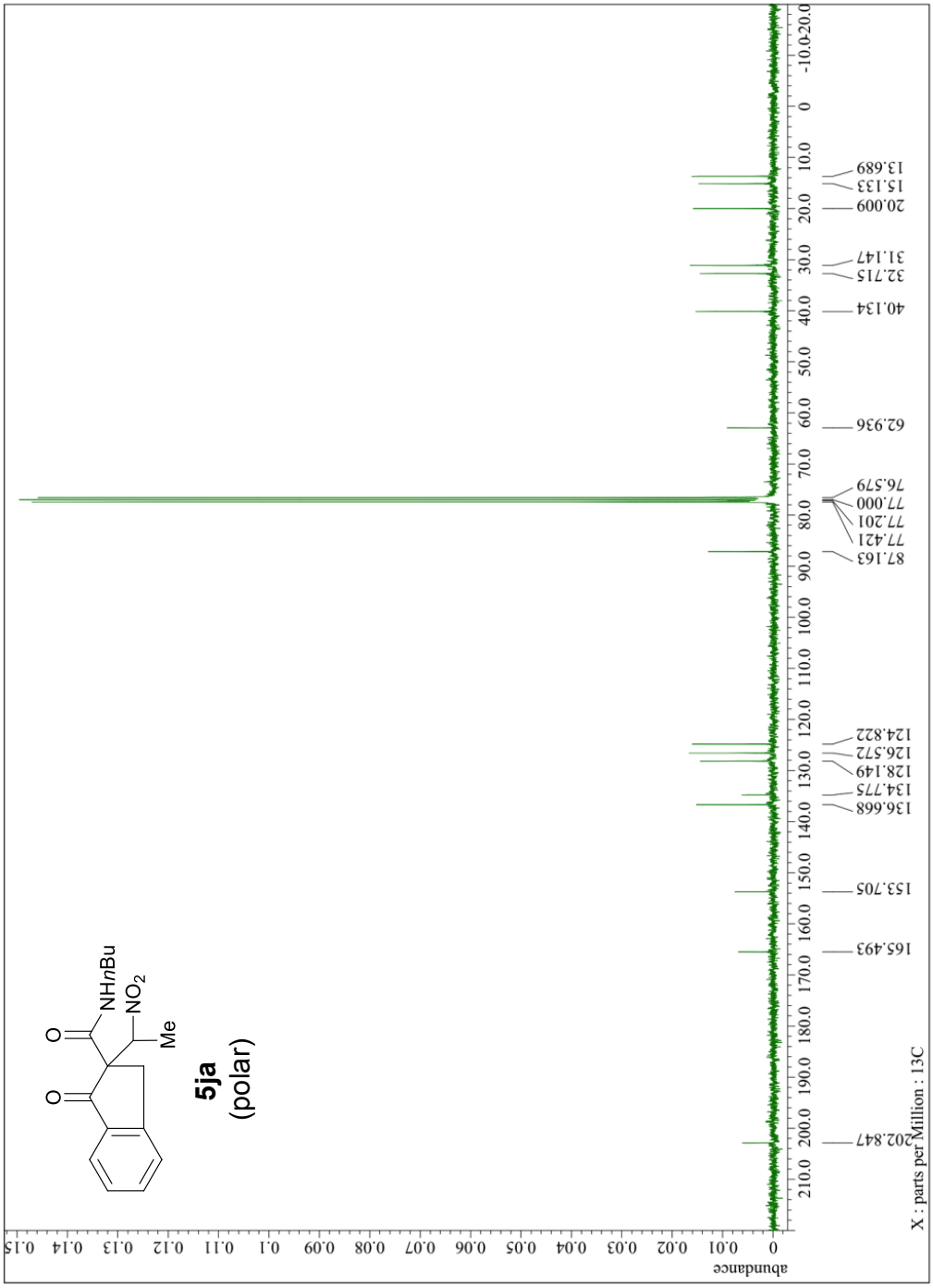

NHBn
NO2
Me
O
O
3ia
abundance
X : parts per Million : 13C
210.820
210.103
165.025
164.231
138.303
133.016
132.413
129.469
128.809
128.790
128.484
128.207
127.920
127.757
127.079
91.274
88.482
77.421
77.000
76.570
62.401
61.990
44.322
44.178
31.166
30.813
28.298
22.887
22.380
22.103
16.491
14.034

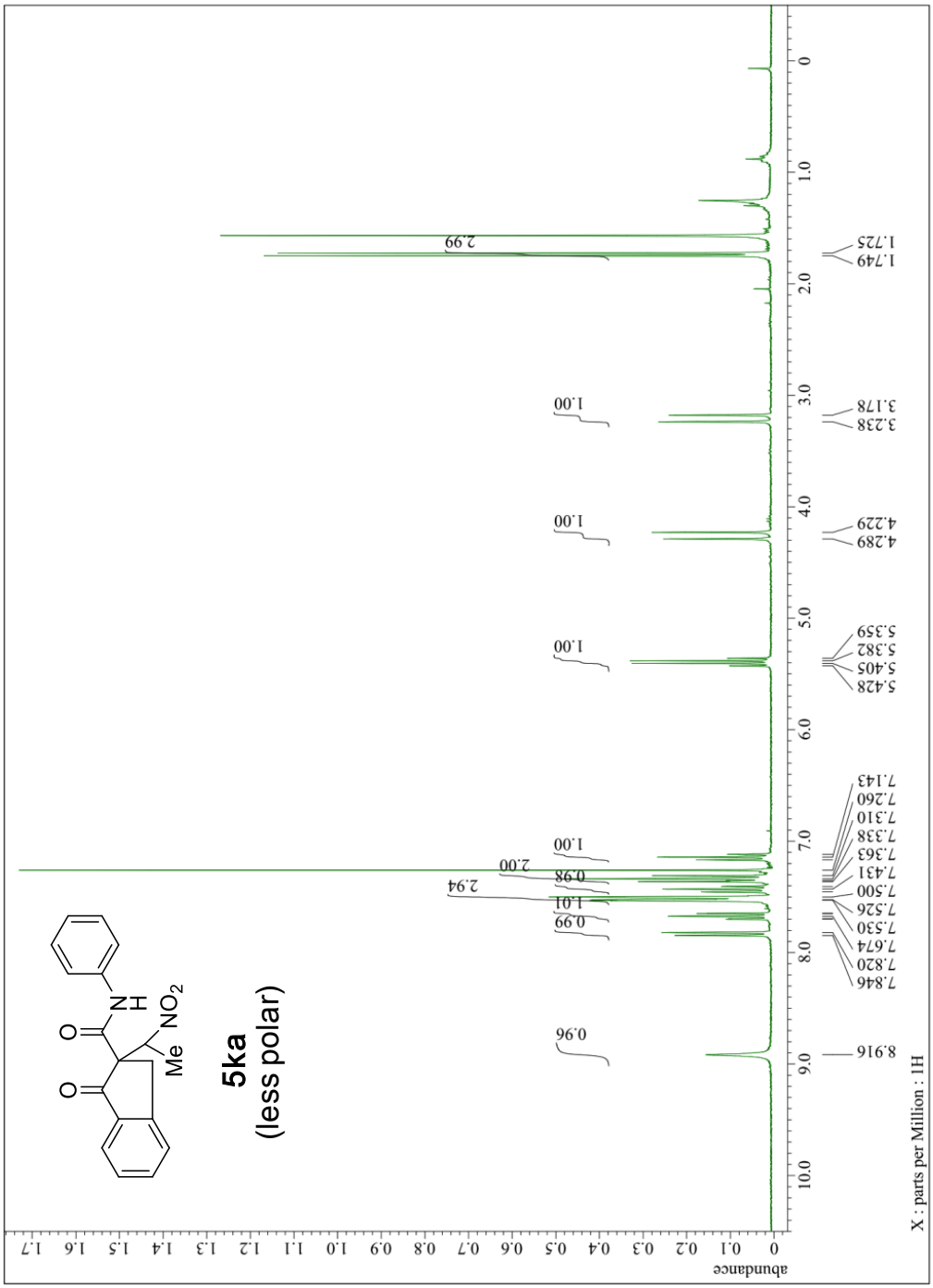

3ia
NHBn
NO2
Me
O
O
abundance
X : parts per Million : 13C
210.820
210.103
165.025
164.231
138.303
133.016
132.413
129.469
128.809
128.790
128.484
128.207
127.920
127.757
127.079
91.274
88.482
77.421
77.000
76.570
62.401
61.990
44.322
44.178
31.166
30.813
28.298
22.887
22.380
22.103
16.491
14.034

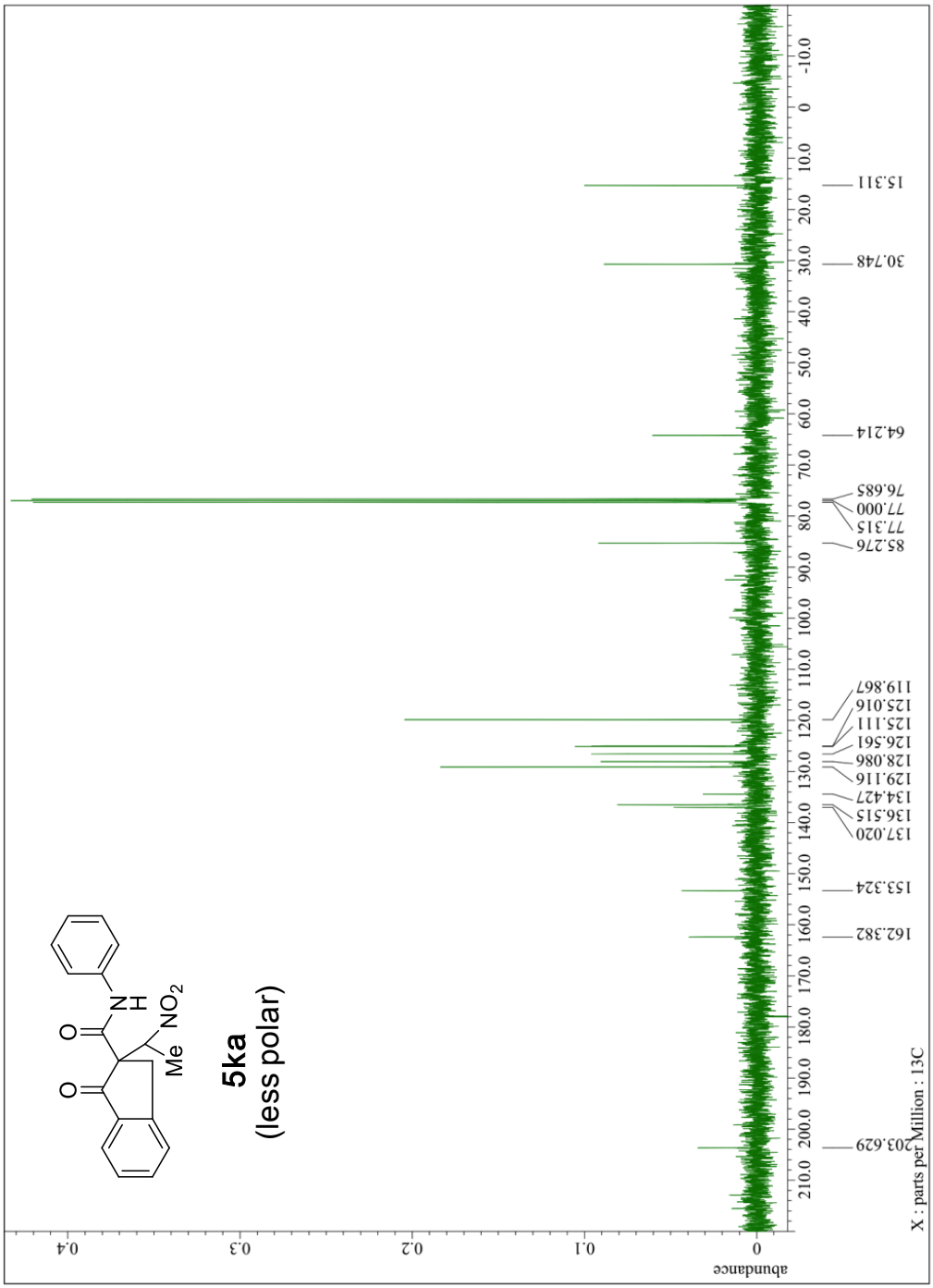

5ja
(less polar)
NHnBu
NO2
Me
O
O
abundance
X : parts per Million : 1H

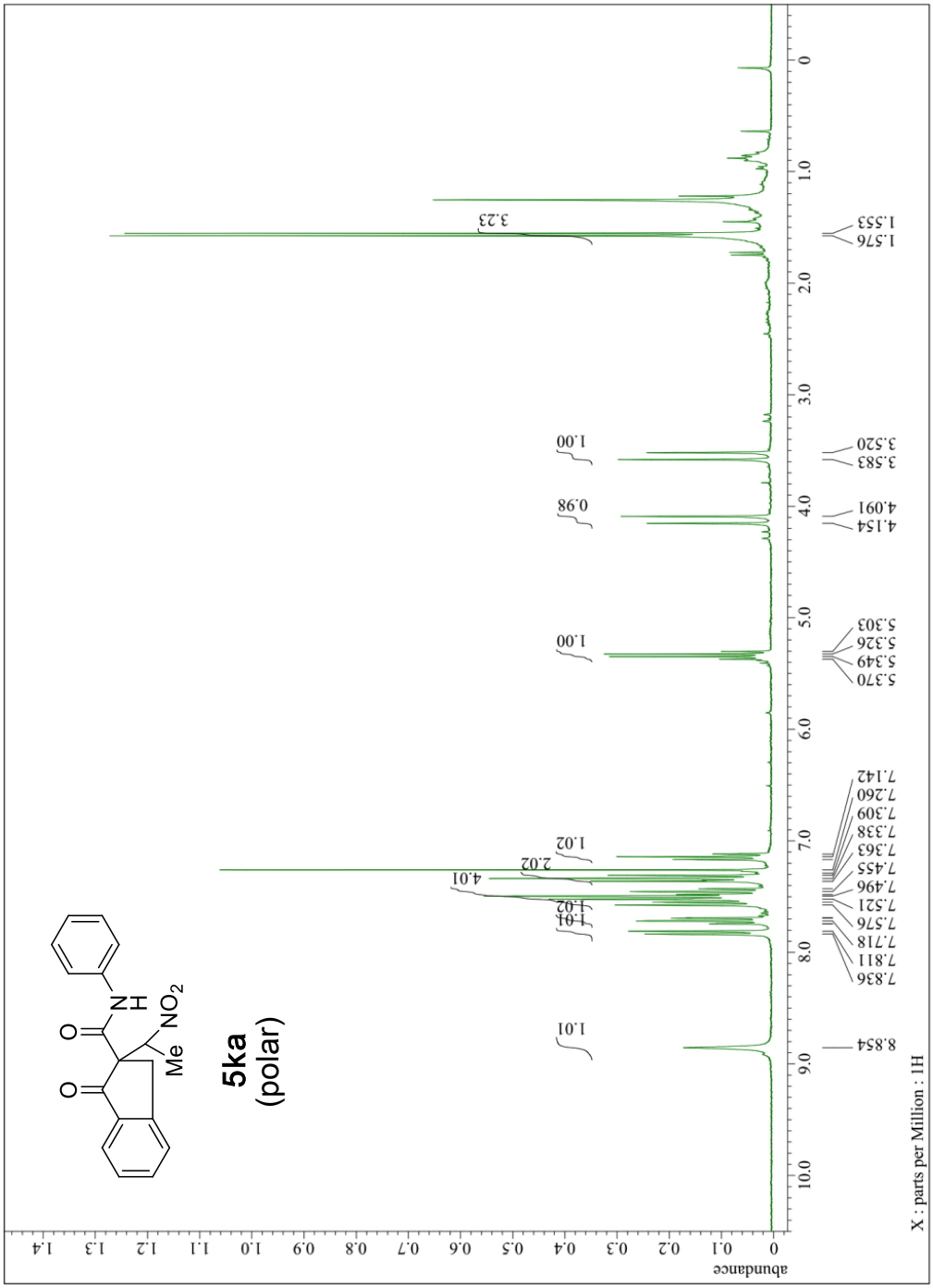

5ja
(less polar)
NHnBu
NO2
Me
O
O
abundance
X : parts per Million : 13C
203.545
164.489
153.332
136.190
134.479
127.901
126.562
124.784
85.356
77.421
77.201
77.000
76.579
63.663
40.258
31.157
30.908
19.980
15.238
13.651

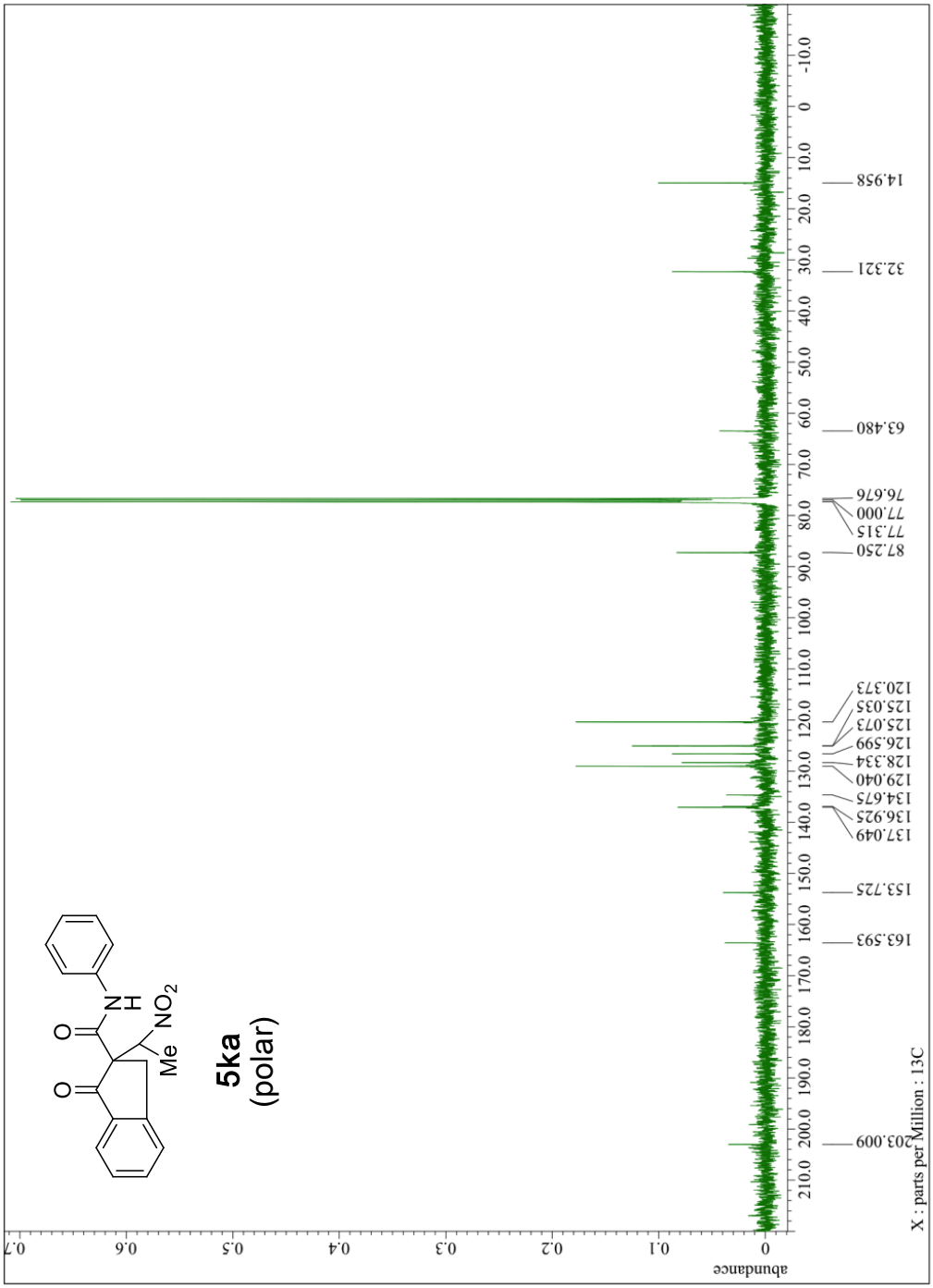

5ja
(polar)
NHnBu
NO2
Me
O
O
abundance
X : parts per Million : 1H
7.784
7.758
7.681
7.659
7.656
7.539
7.514
7.448
7.424
7.260
6.871
5.289
5.266
5.243
5.220
4.058
3.996
3.516
3.453
3.351
3.327
3.307
3.189
3.170
3.146
1.535
1.512
1.499
1.475
1.365
1.340
1.315
0.936
0.912
0.887
0.90
1.01
1.00
1.07
1.03
1.10
2.11
5.11
3.11

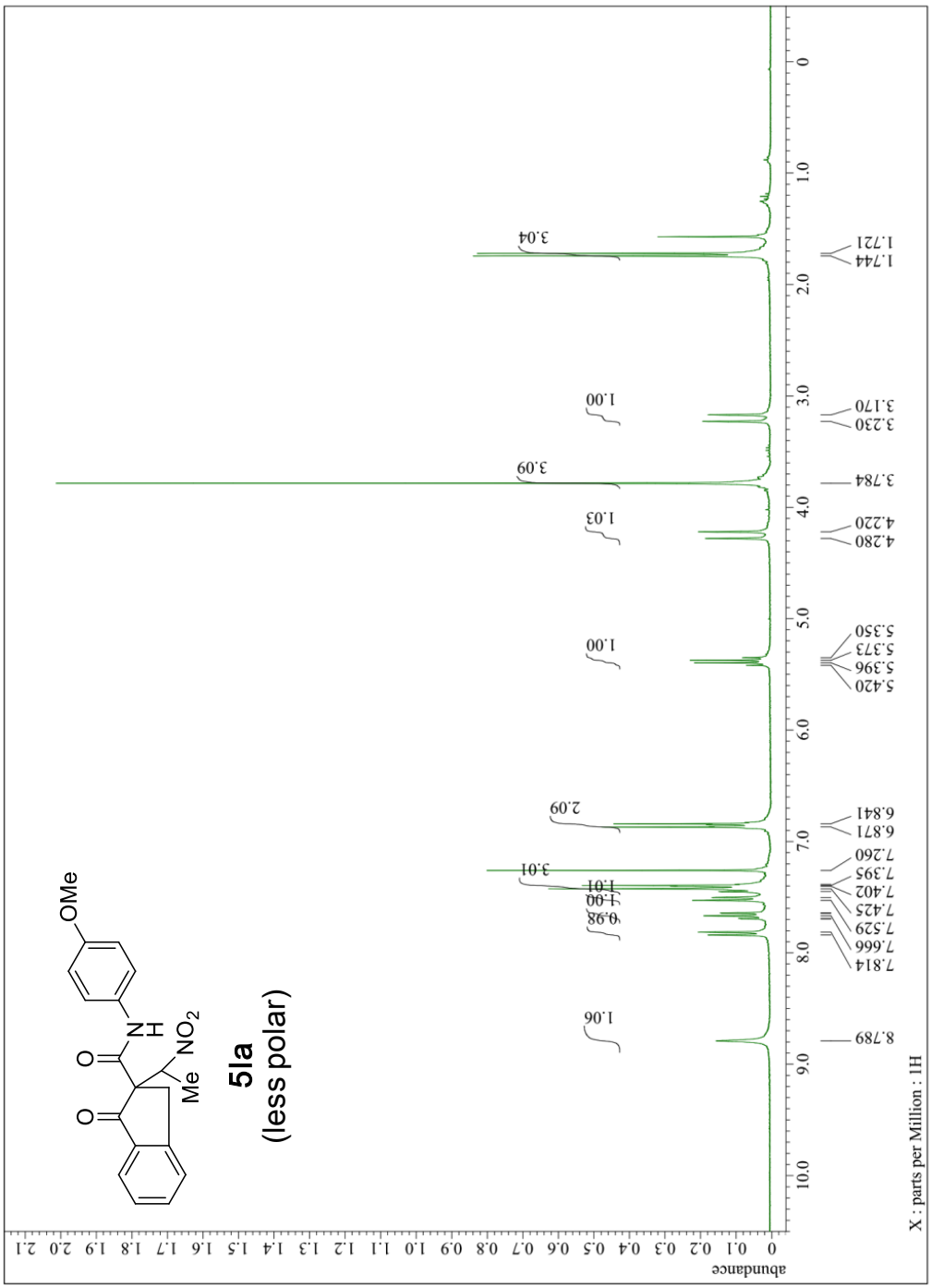

5ja
(polar)
NHnBu
NO2
Me
O
O
202.847
165.493
153.705
136.668
134.775
128.149
126.572
124.822
87.163
77.421
77.201
77.000
76.579
62.936
40.134
32.715
31.147
20.009
15.133
13.689
X : parts per Million : 13C
abundance

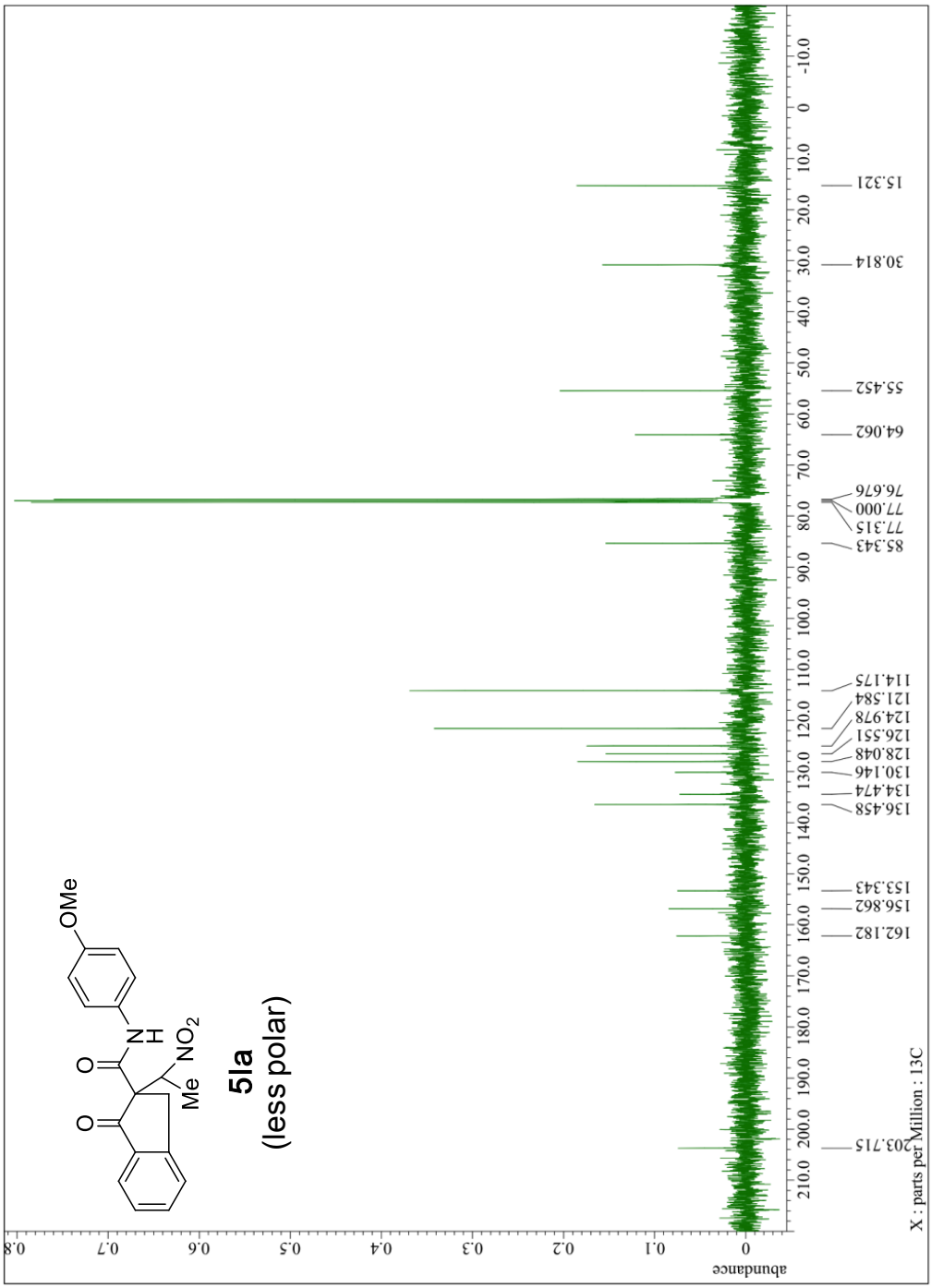

5ka
(less polar)
X : parts per Million : 1H
abundance
8.916
7.846
7.820
7.674
7.530
7.526
7.500
7.431
7.363
7.338
7.310
7.260
7.143
5.428
5.405
5.382
5.359
4.289
4.229
3.238
3.178
1.749
1.725
2.99
2.94
0.96
0.99
1.01
0.98
2.00
1.00

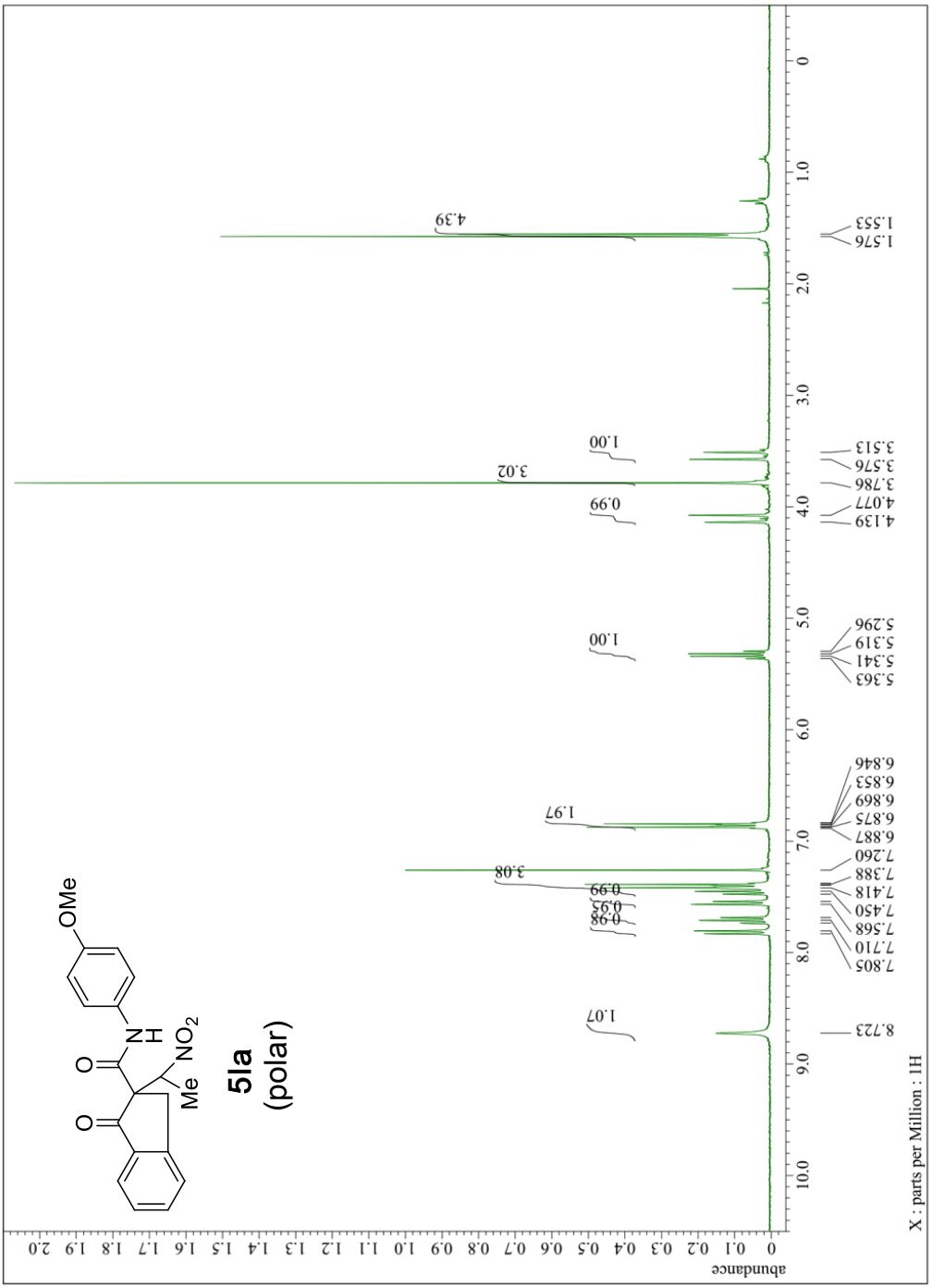

5ka
(less polar)
Me
NO2
H
N
O
O
abundance
X : parts per Million : 13C
203.629
162.382
153.324
137.020
136.515
134.427
129.116
128.086
126.561
125.111
125.016
119.867
85.276
77.315
77.000
76.685
64.214
30.748
15.311

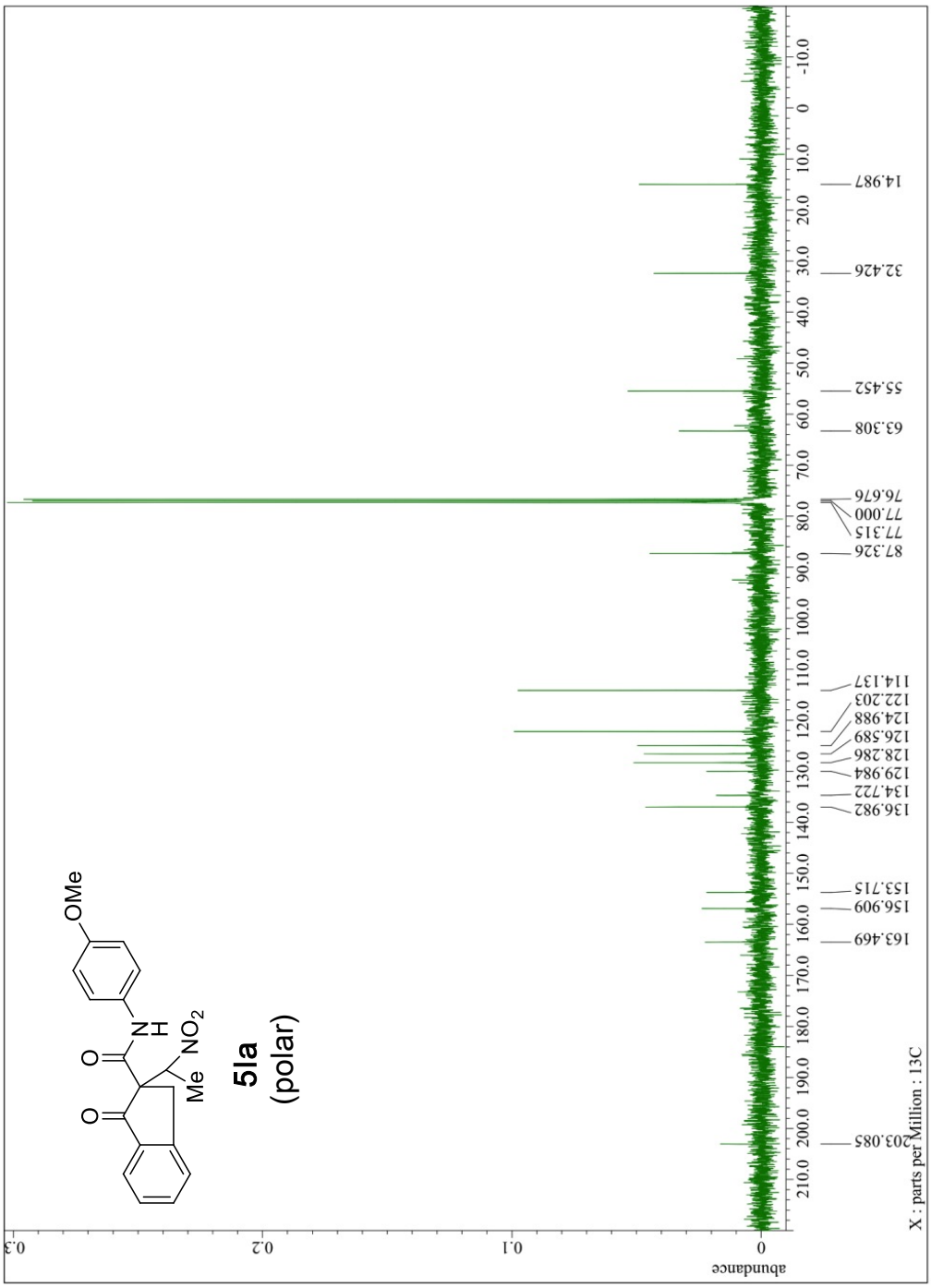

5ka
(polar)
X : parts per Million : 1H
abundance
8.854
7.836
7.811
7.718
7.576
7.521
7.496
7.455
7.363
7.338
7.309
7.260
7.142
5.370
5.349
5.326
5.303
4.154
4.091
3.583
3.520
1.576
1.553
1.01
1.02
2.02
4.01
1.00
0.98
1.00
3.23

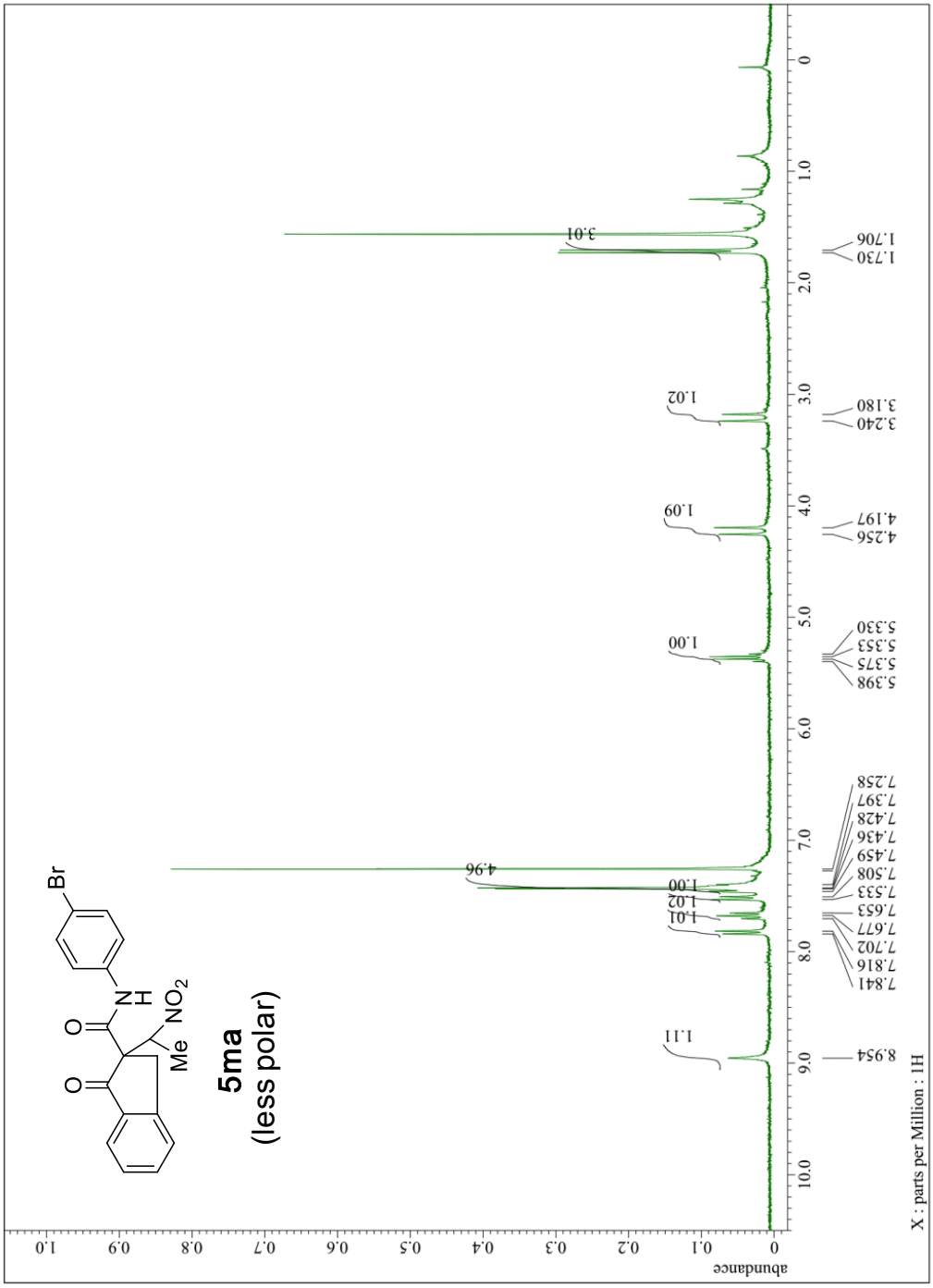

5ka
(polar)
Me
NO2
H
N
O
O
abundance
X : parts per Million : 13C
203.009
163.593
153.725
137.049
136.925
134.675
129.040
128.334
126.599
125.073
125.035
120.373
87.250
77.315
77.000
76.676
63.480
32.321
14.958

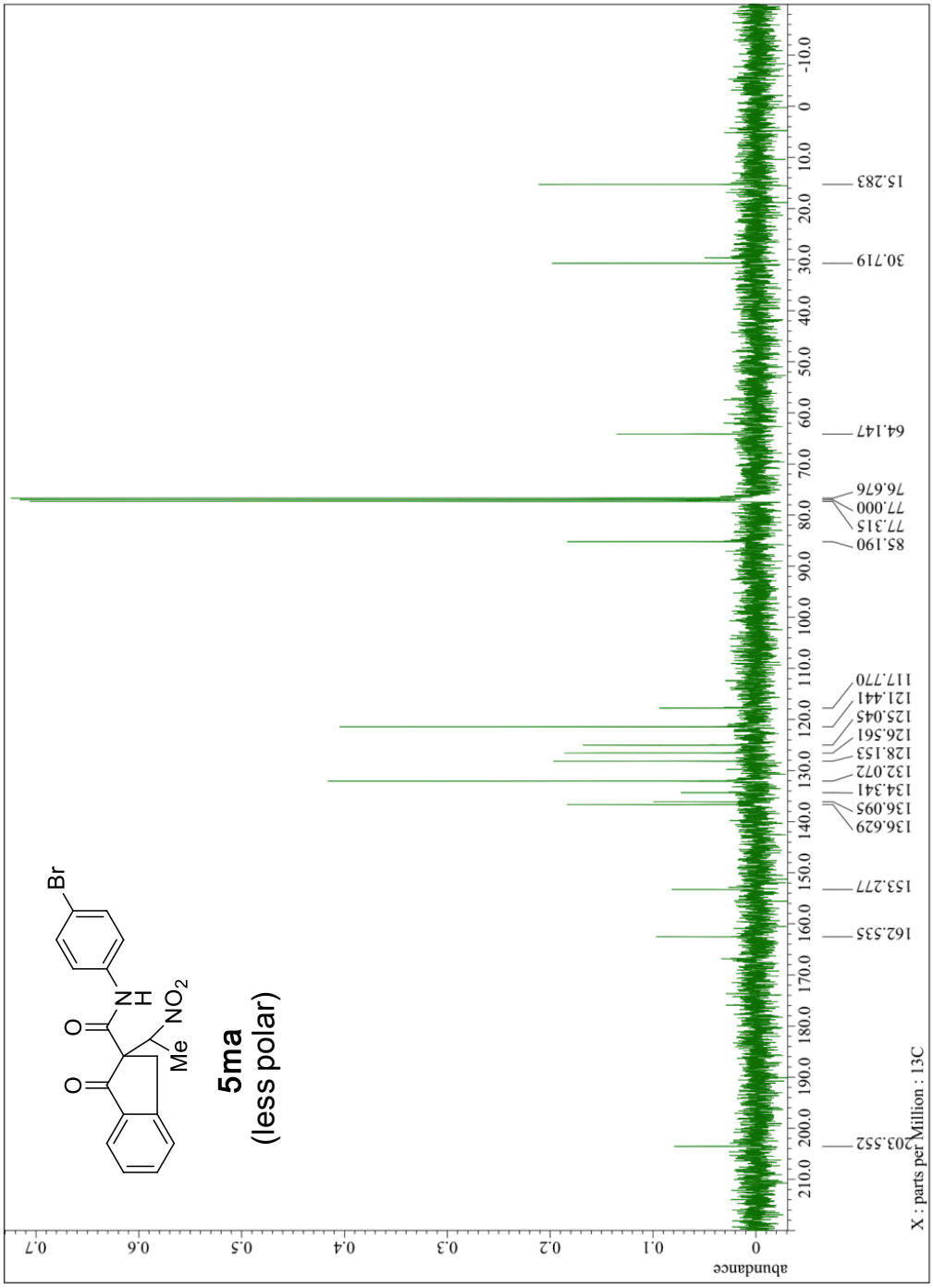

5la
(less polar)
OMe
NH
O
O
Me
NO2
abundance
X : parts per Million : 1H
8.789
7.814
7.666
7.529
7.425
7.402
7.395
7.260
6.871
6.841
5.420
5.396
5.373
5.350
4.280
4.220
3.784
3.230
3.170
1.744
1.721
1.06
0.98
1.00
1.01
2.09
1.00
1.03
3.09
1.00
3.04

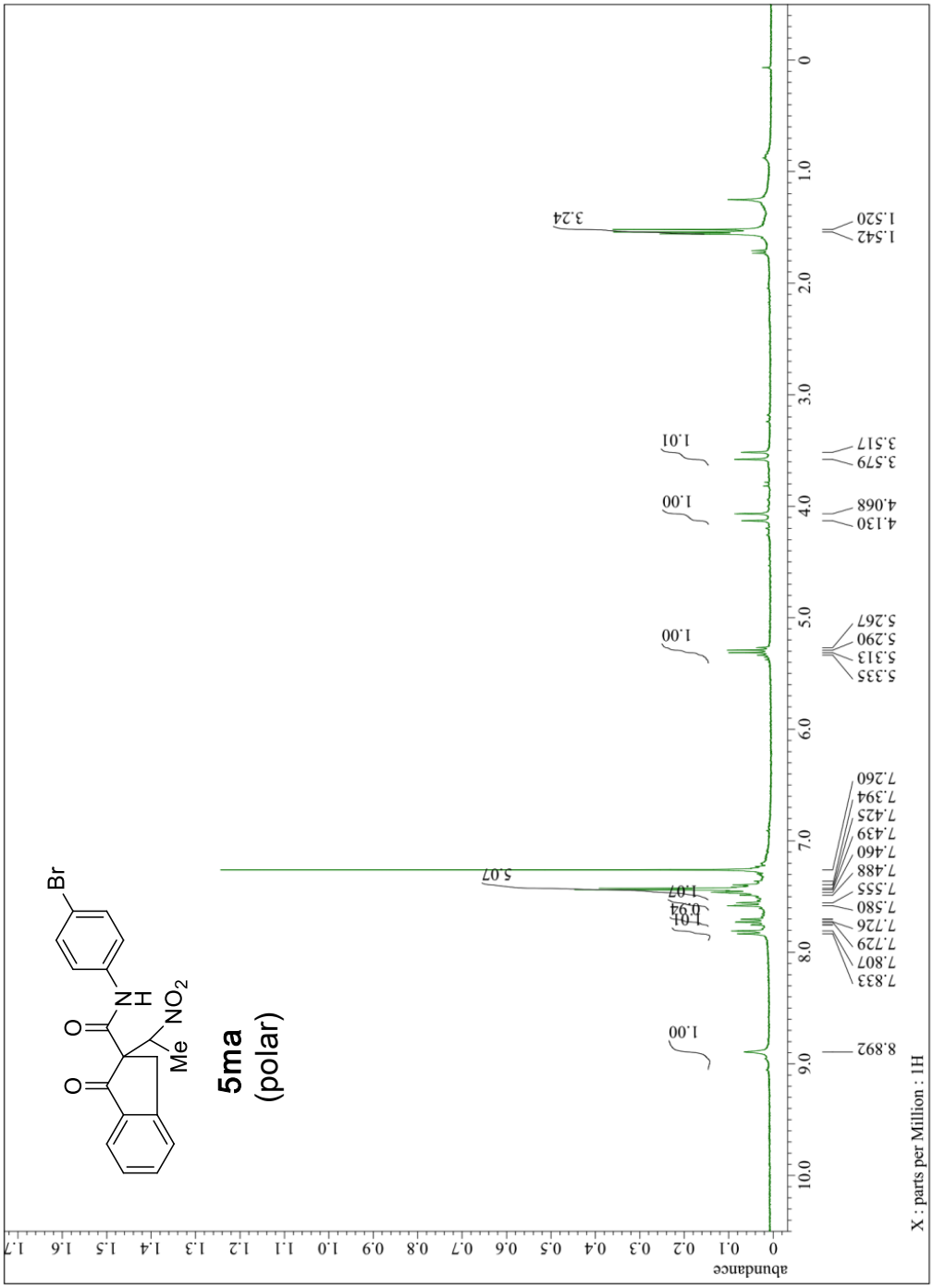

5la
(less polar)
OMe
NH
O
O
Me
NO2
abundance
X : parts per Million : 13C
203.715
162.182
156.862
153.343
136.458
134.474
130.146
128.048
126.551
124.978
121.584
114.175
85.343
77.315
77.000
76.676
64.062
55.452
30.814
15.321

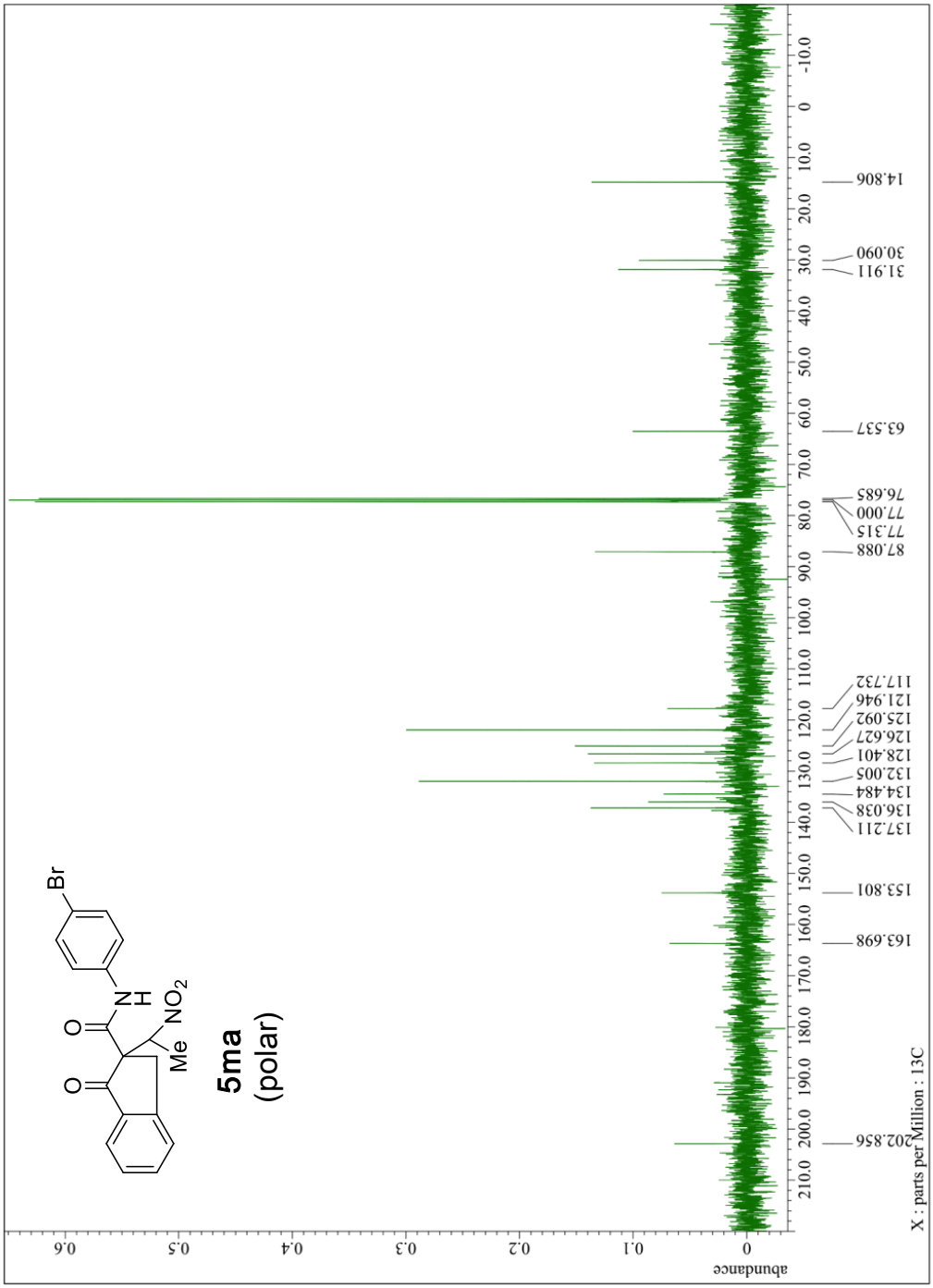

5la
(polar)
OMe
NH
O
O
Me
NO2
X : parts per Million : 1H
abundance
8.723
7.805
7.710
7.568
7.450
7.418
7.388
7.260
6.887
6.875
6.869
6.853
6.846
5.363
5.341
5.319
5.296
4.139
4.077
3.786
3.576
3.513
1.576
1.553
4.39
3.02
3.08
1.97
1.07
1.00
0.99
0.98
0.95
0.99
1.00
1.00

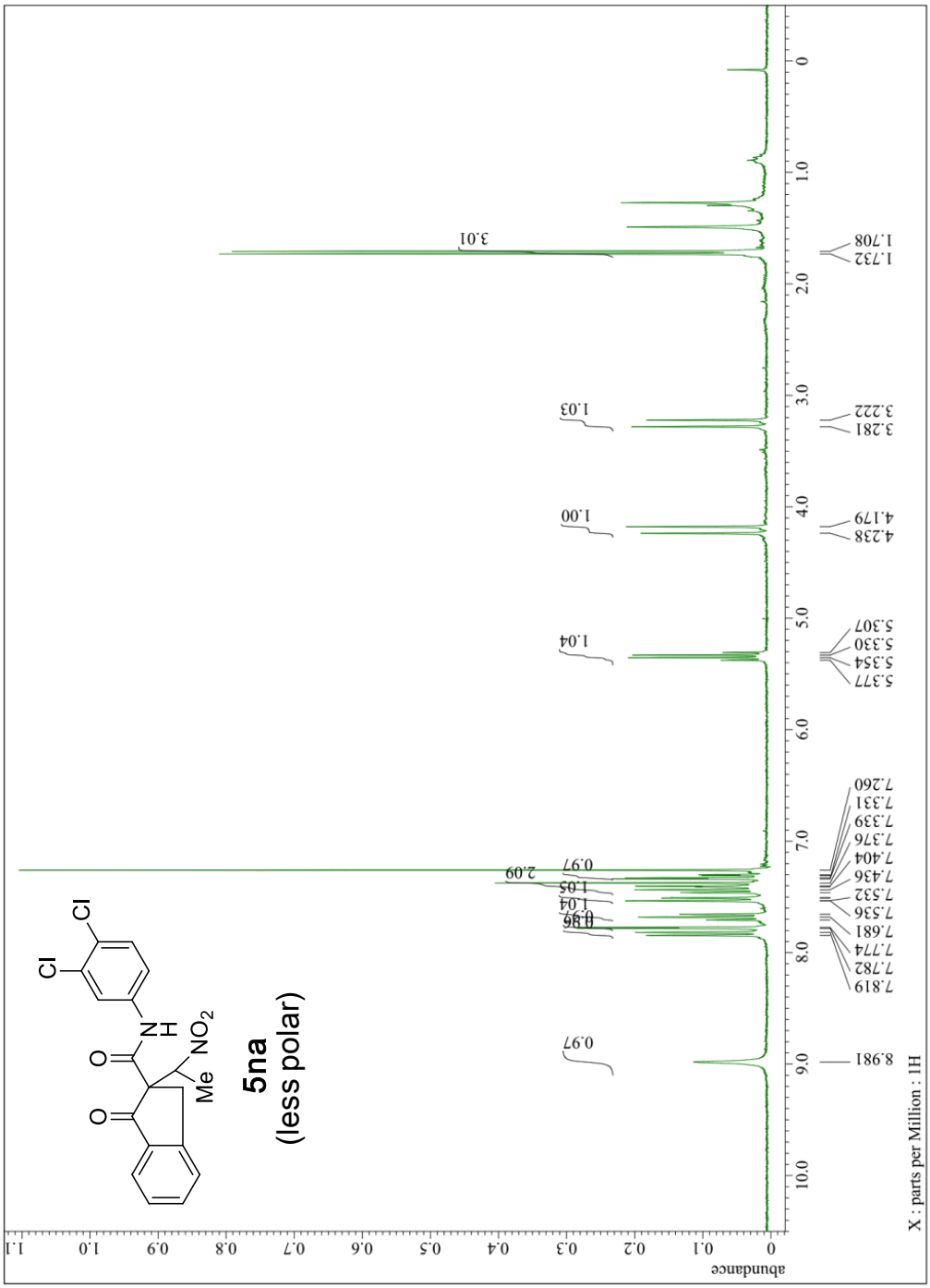

OMe
O
N
H
O
Me
NO2
5la
(polar)
abundance
0
0.1
0.2
0.3
X : parts per Million : 13C
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
203.085
163.469
156.909
153.715
136.982
134.722
129.984
128.286
126.589
124.988
122.203
114.137
87.326
77.315
77.000
76.676
63.308
55.452
32.426
14.987

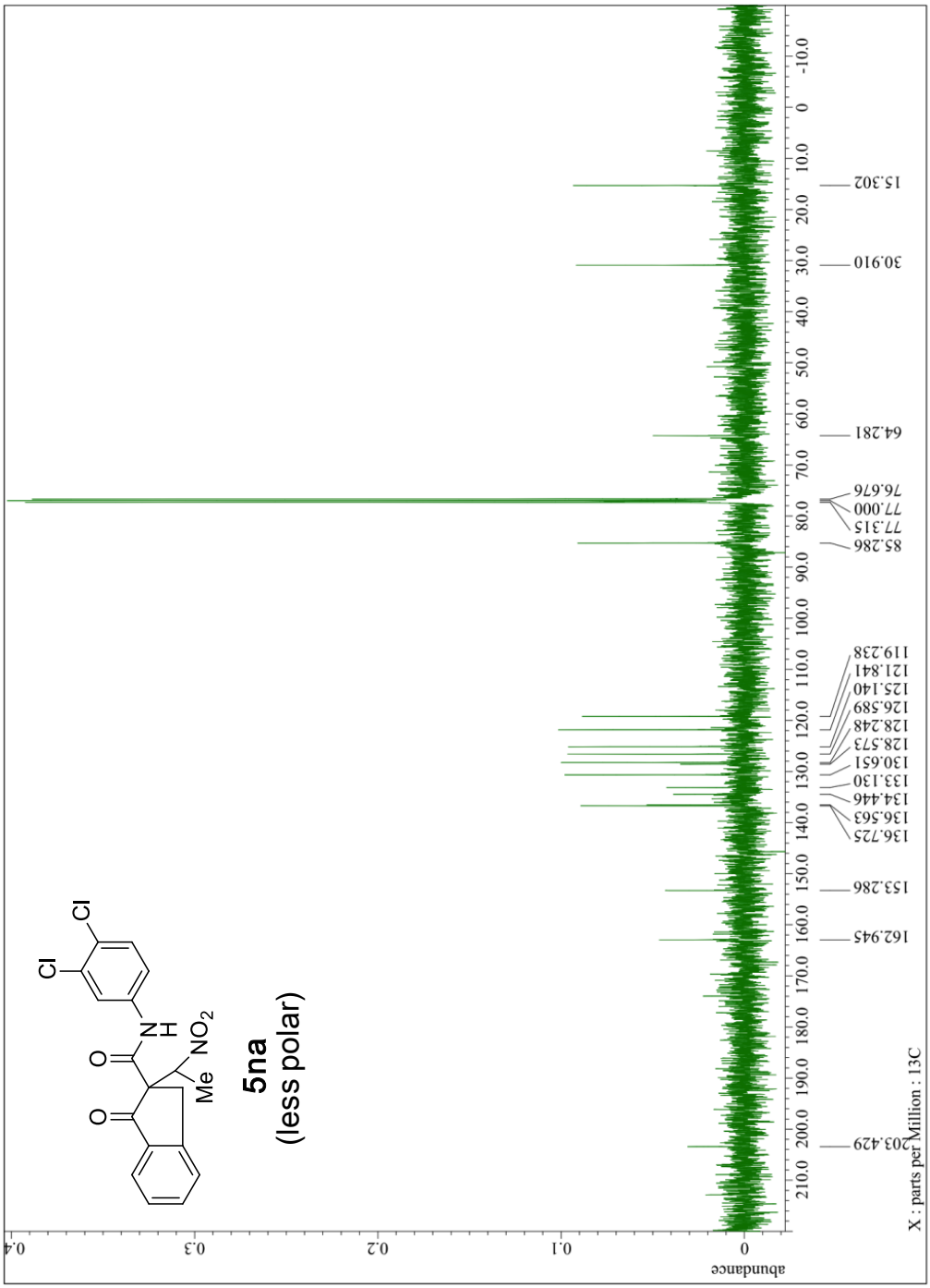

5ma
(less polar)
Br
NH
O
O
Me
NO2
X : parts per Million : 1H
abundance
8.954
7.841
7.816
7.702
7.677
7.653
7.533
7.508
7.459
7.436
7.428
7.397
7.258
5.398
5.375
5.353
5.330
4.256
4.197
3.240
3.180
1.730
1.706
4.96
3.01
1.11
1.01
1.02
1.00
1.09
1.02
1.00

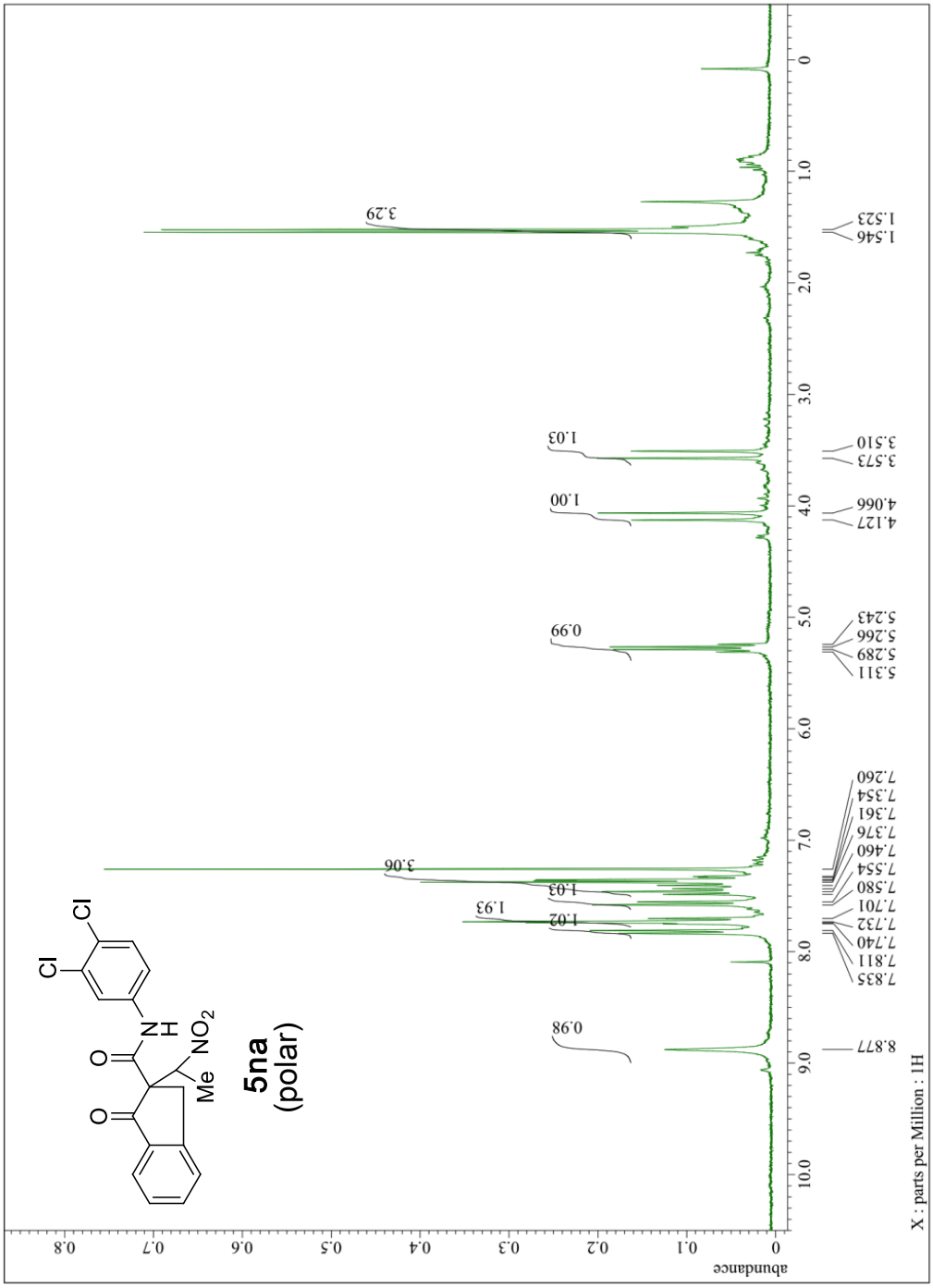

5ma
(less polar)
Br
O
N
H
O
Me
NO2
abundance
X : parts per Million : 13C
203.552
162.535
153.277
136.629
136.095
134.341
132.072
128.153
126.561
125.045
121.441
117.770
85.190
77.315
77.000
76.676
64.147
30.719
15.283

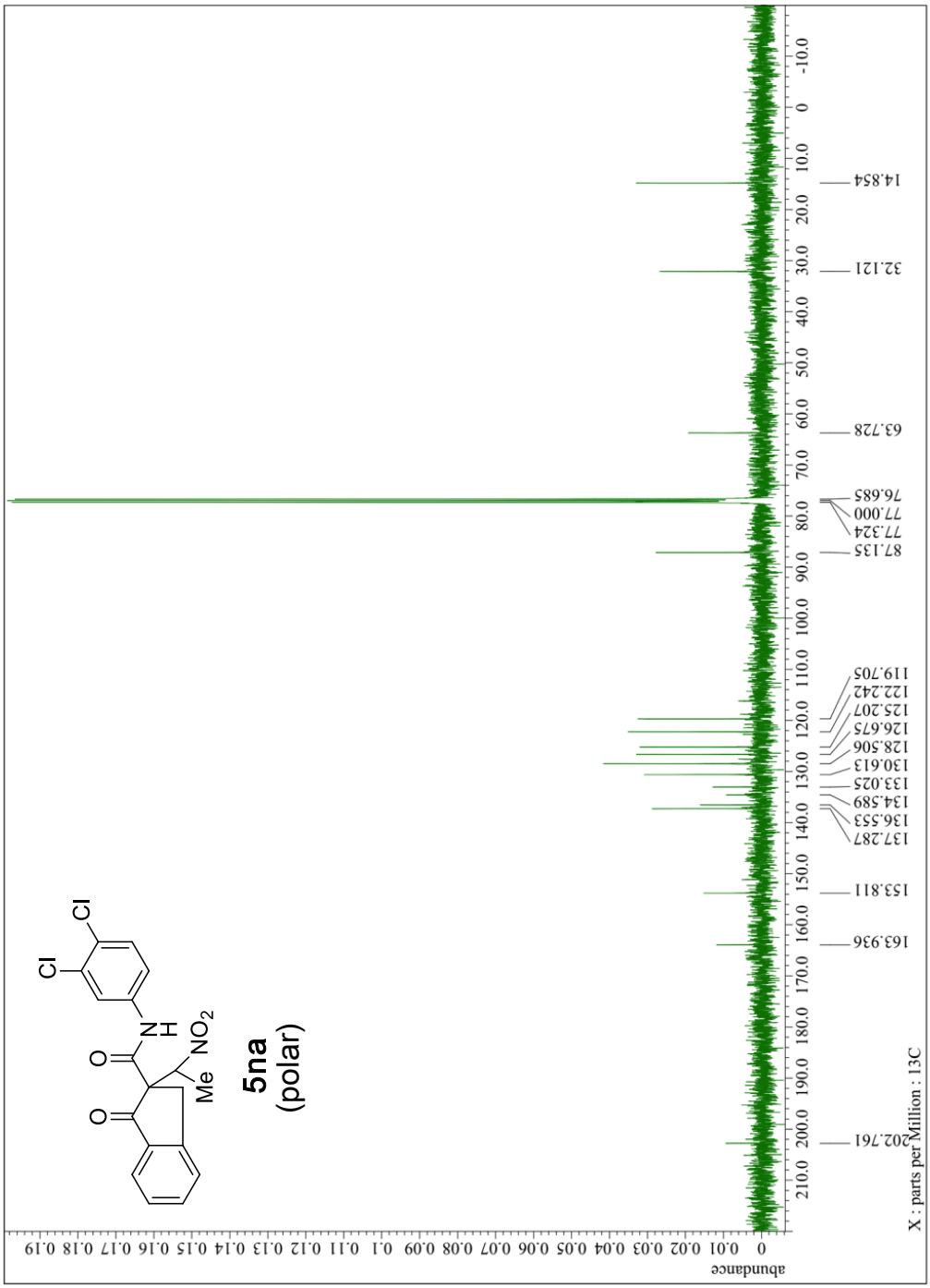

5ma
(polar)
Br
NH
O
O
Me
NO2
X : parts per Million : 1H
abundance
8.892
7.833
7.807
7.729
7.726
7.580
7.555
7.488
7.460
7.439
7.425
7.394
7.260
5.335
5.313
5.290
5.267
4.130
4.068
3.579
3.517
3.24
1.542
1.520
1.00
0.94
1.01
1.07
5.07
1.00
1.00
1.01
1.00

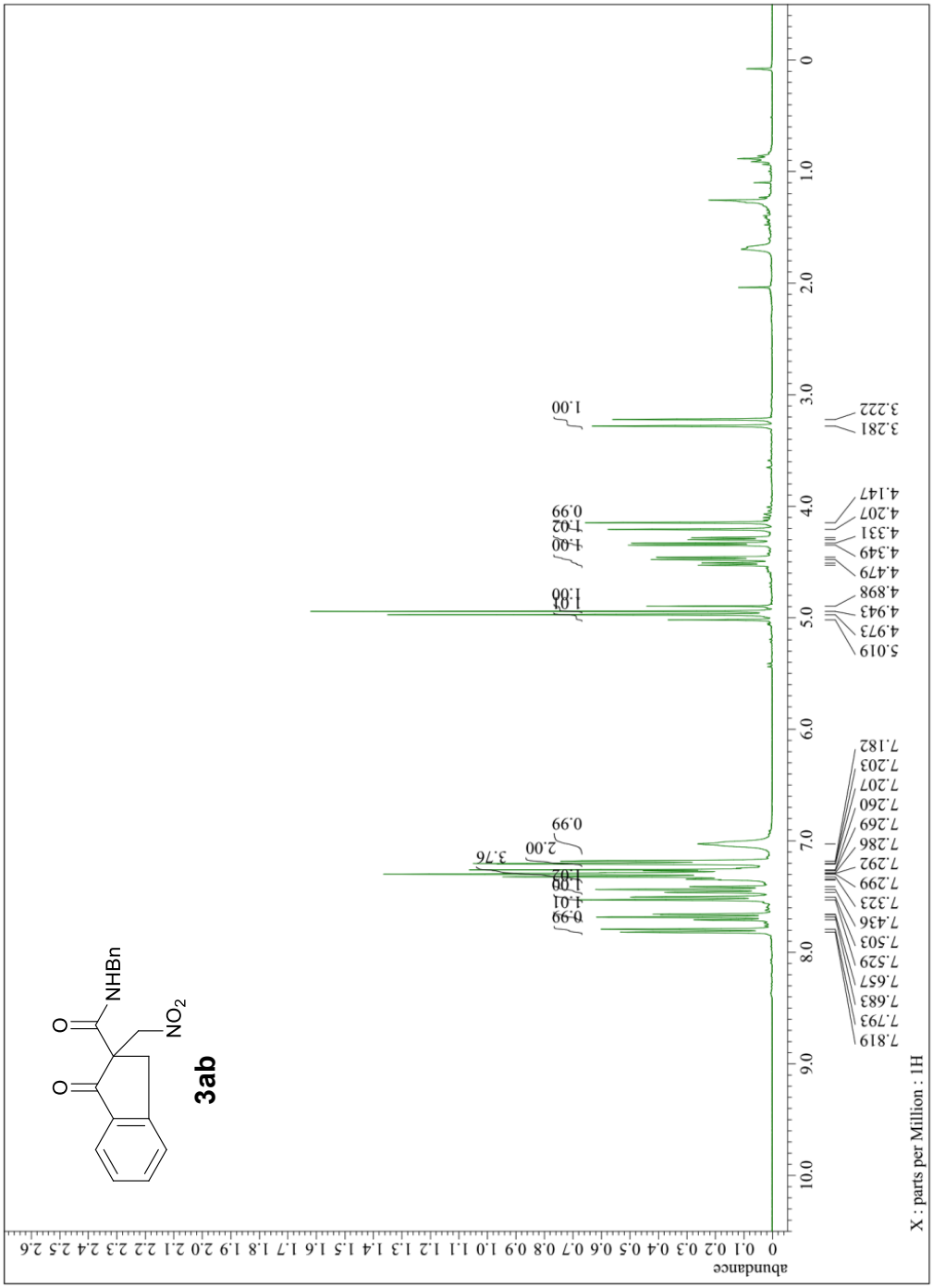

5ma
(polar)
Br
O
N
H
O
Me
NO2
abundance
X : parts per Million : 13C
202.856
163.698
153.801
137.211
136.038
134.484
132.005
128.401
126.627
125.092
121.946
117.732
87.088
77.315
77.000
76.685
63.537
31.911
30.090
14.806

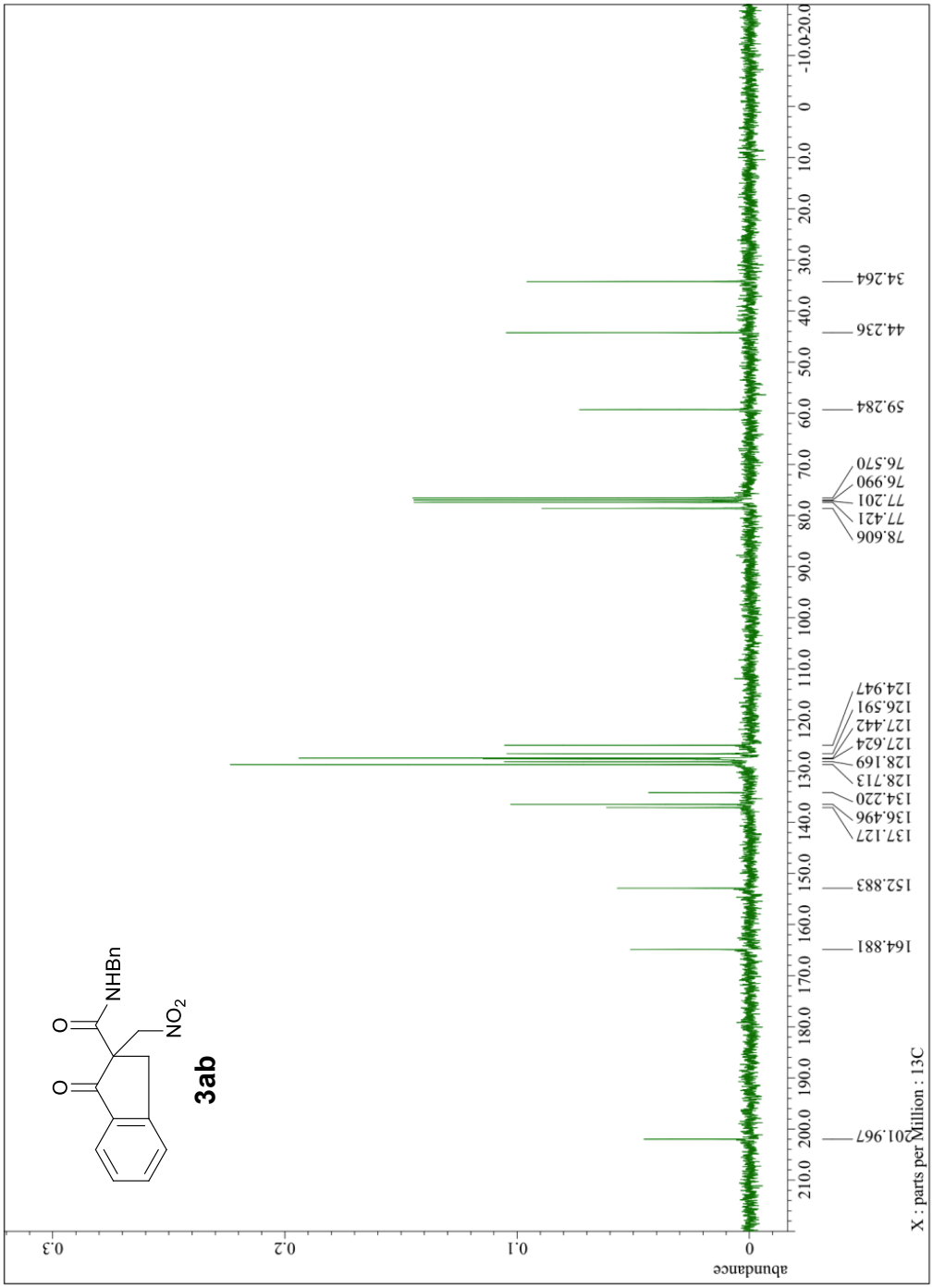

5na
(less polar)
X : parts per Million : 1H
abundance
8.981
7.819
7.782
7.774
7.681
7.536
7.532
7.436
7.404
7.376
7.339
7.331
7.260
5.377
5.354
5.330
5.307
4.238
4.179
3.281
3.222
1.732
1.708
0.97
3.01
1.03
1.00
1.04
2.09
0.97
1.05
1.04
0.96
0.95

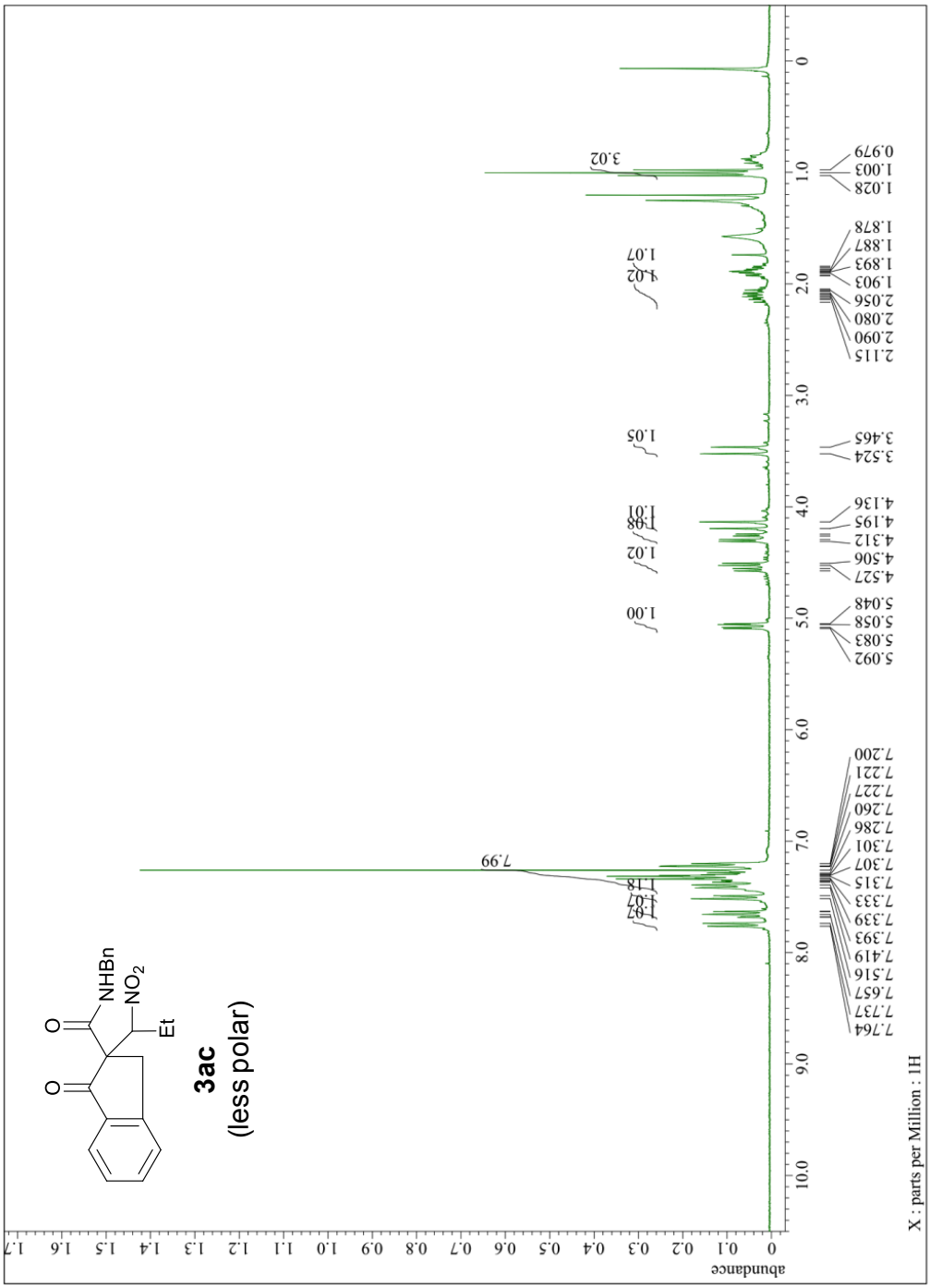

5na
(less polar)
Cl
Cl
O
N
H
O
Me
NO2
abundance
0
0.1
0.2
0.3
0.4
X : parts per Million : 13C
203.429
162.945
153.286
136.725
136.563
134.446
133.130
130.651
128.573
128.248
126.589
125.140
121.841
119.238
85.286
77.315
77.000
76.676
64.281
30.910
15.302

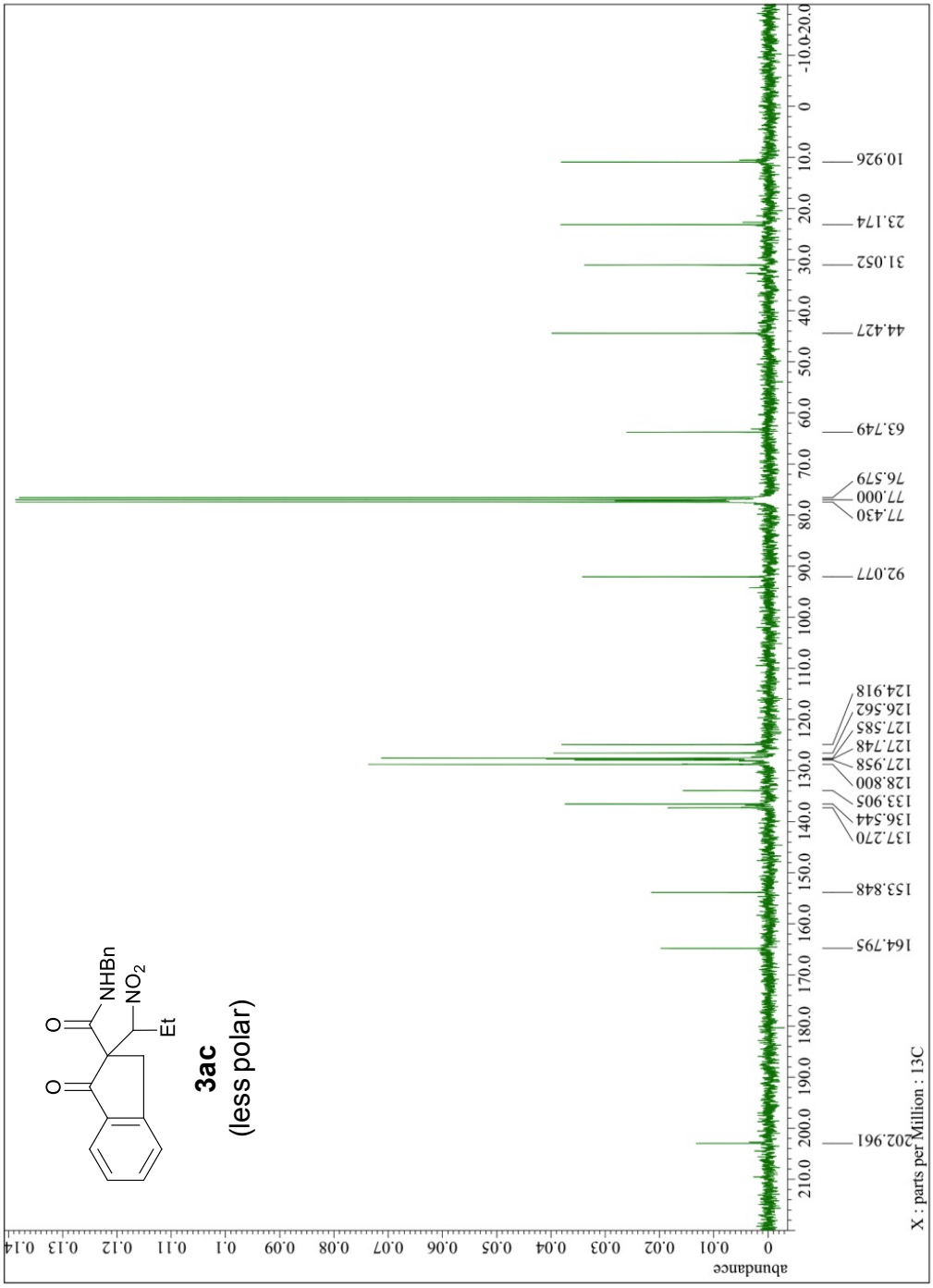

5na
(polar)
Cl
Cl
NH
O
O
Me
NO2
X : parts per Million : 1H
abundance
8.877
7.835
7.811
7.740
7.732
7.701
7.580
7.554
7.460
7.376
7.361
7.354
7.260
5.311
5.289
5.266
5.243
4.127
4.066
3.573
3.510
1.546
1.523
0.98
1.93
1.02
1.03
3.06
0.99
1.00
1.03
3.29

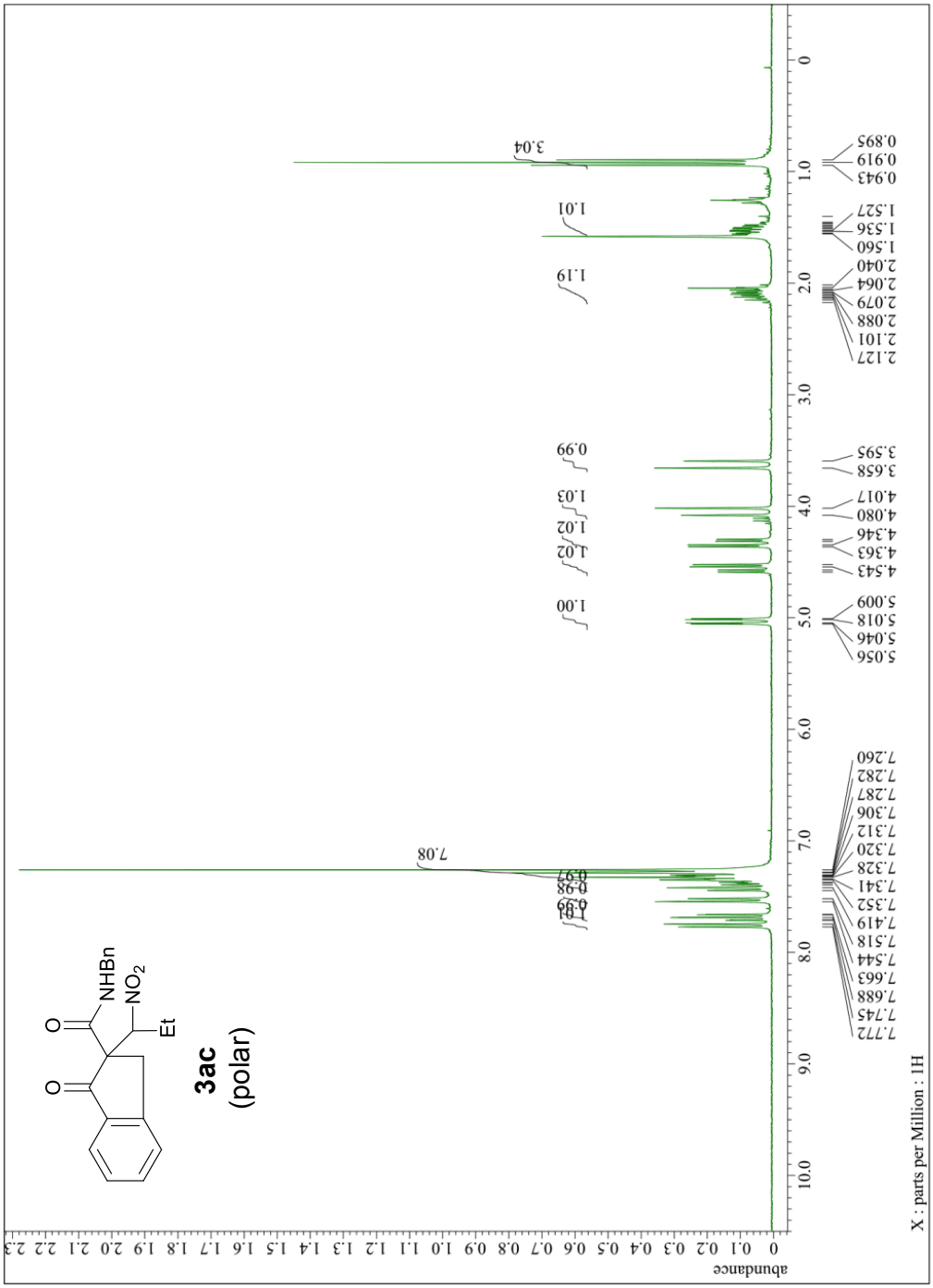

5na
(polar)
Cl
Cl
NH
O
O
Me
NO2
abundance
X : parts per Million : 13C
202.761
163.936
153.811
137.287
136.553
134.589
133.025
130.613
128.506
126.675
125.207
122.242
119.705
87.135
77.324
77.000
76.685
63.728
32.121
14.854

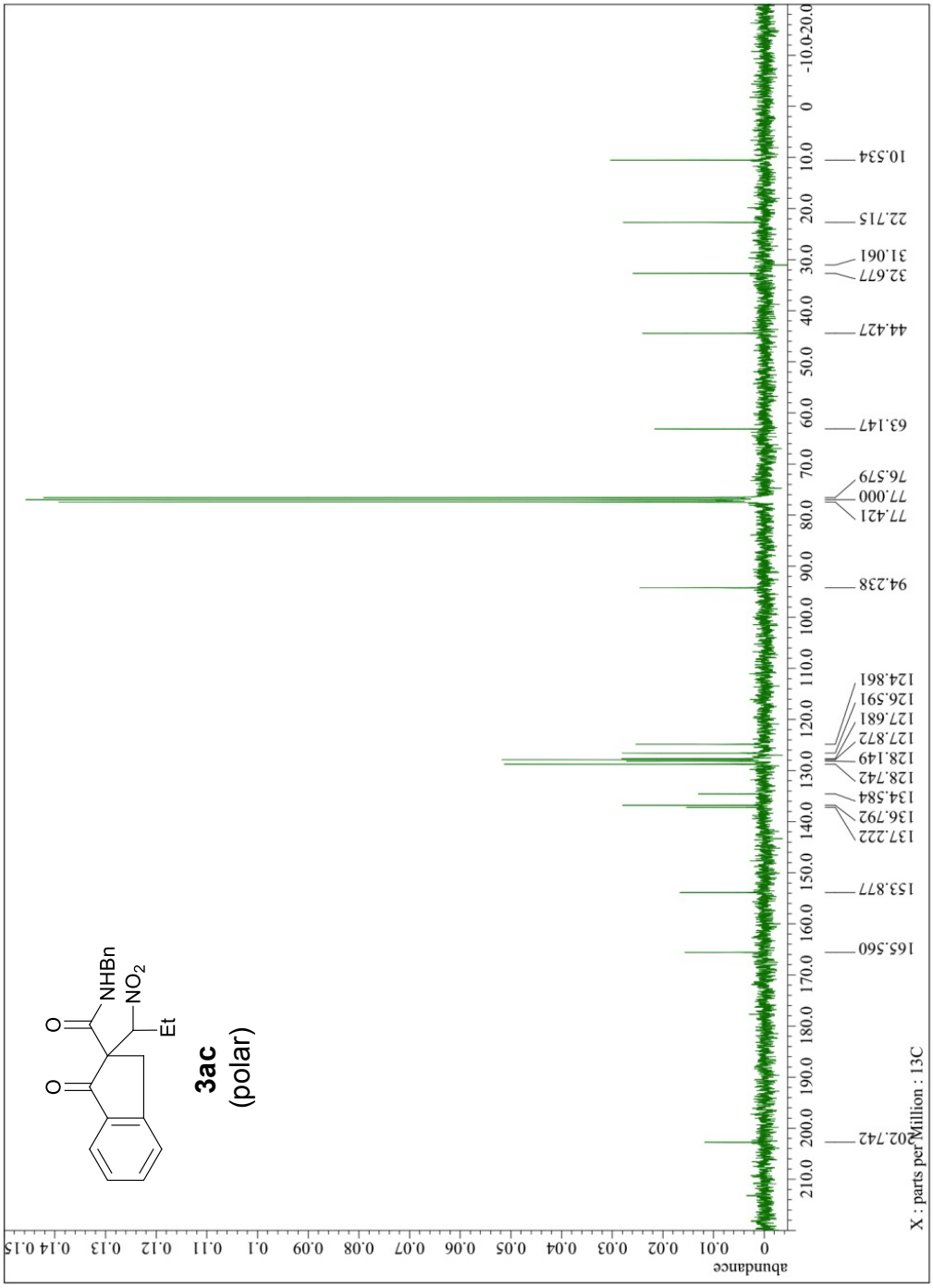

3ab
NHBn
NO2
O
O
X : parts per Million : 1H
abundance

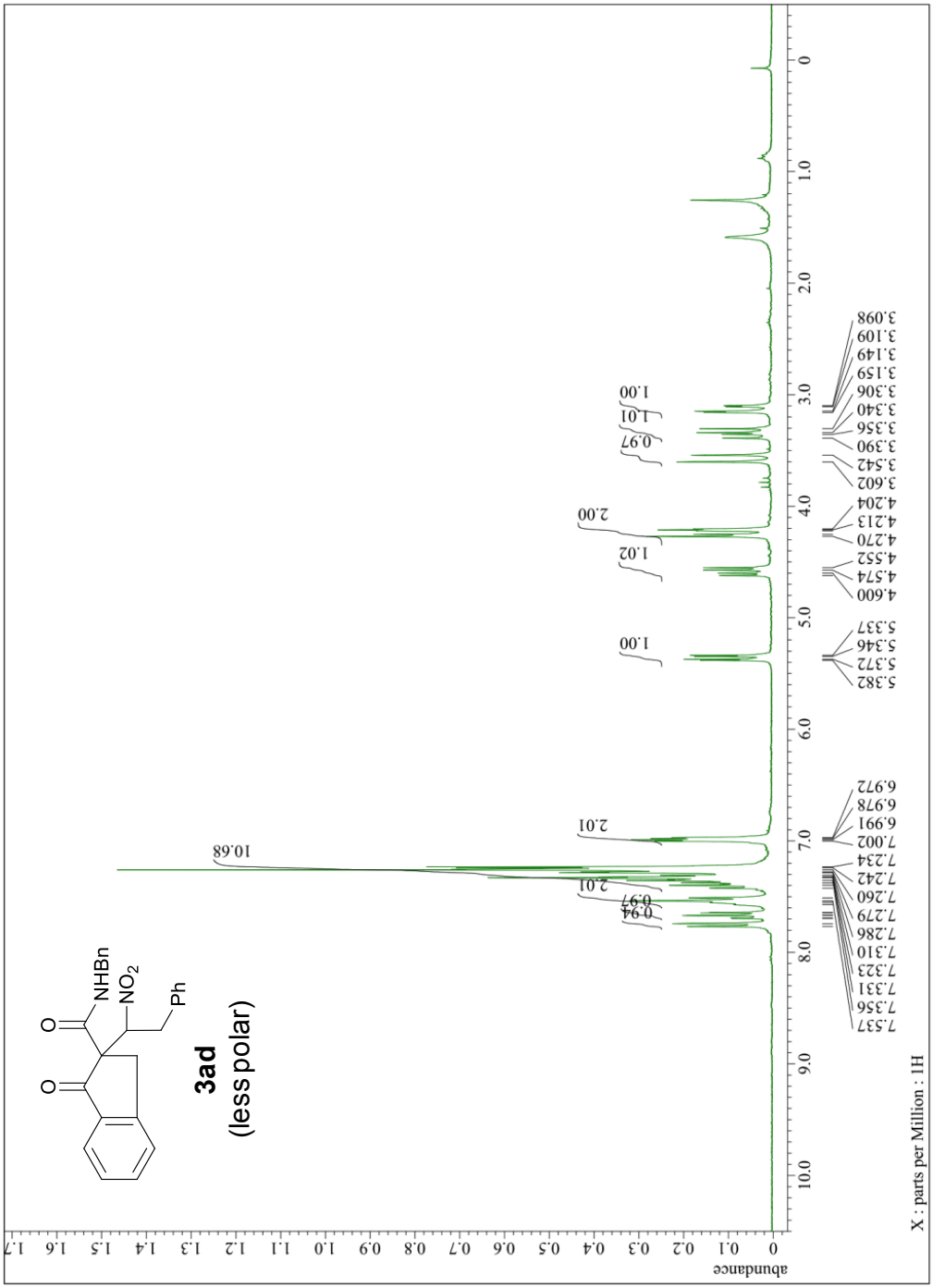

3ab
NHBn
NO2
O
O
abundance
0.3
0.2
0.1
0
X : parts per Million : 13C
201.967
164.881
152.883
137.127
136.496
134.220
128.713
128.169
127.624
127.442
126.591
124.947
78.606
77.421
77.201
76.990
76.570
59.284
44.236
34.264

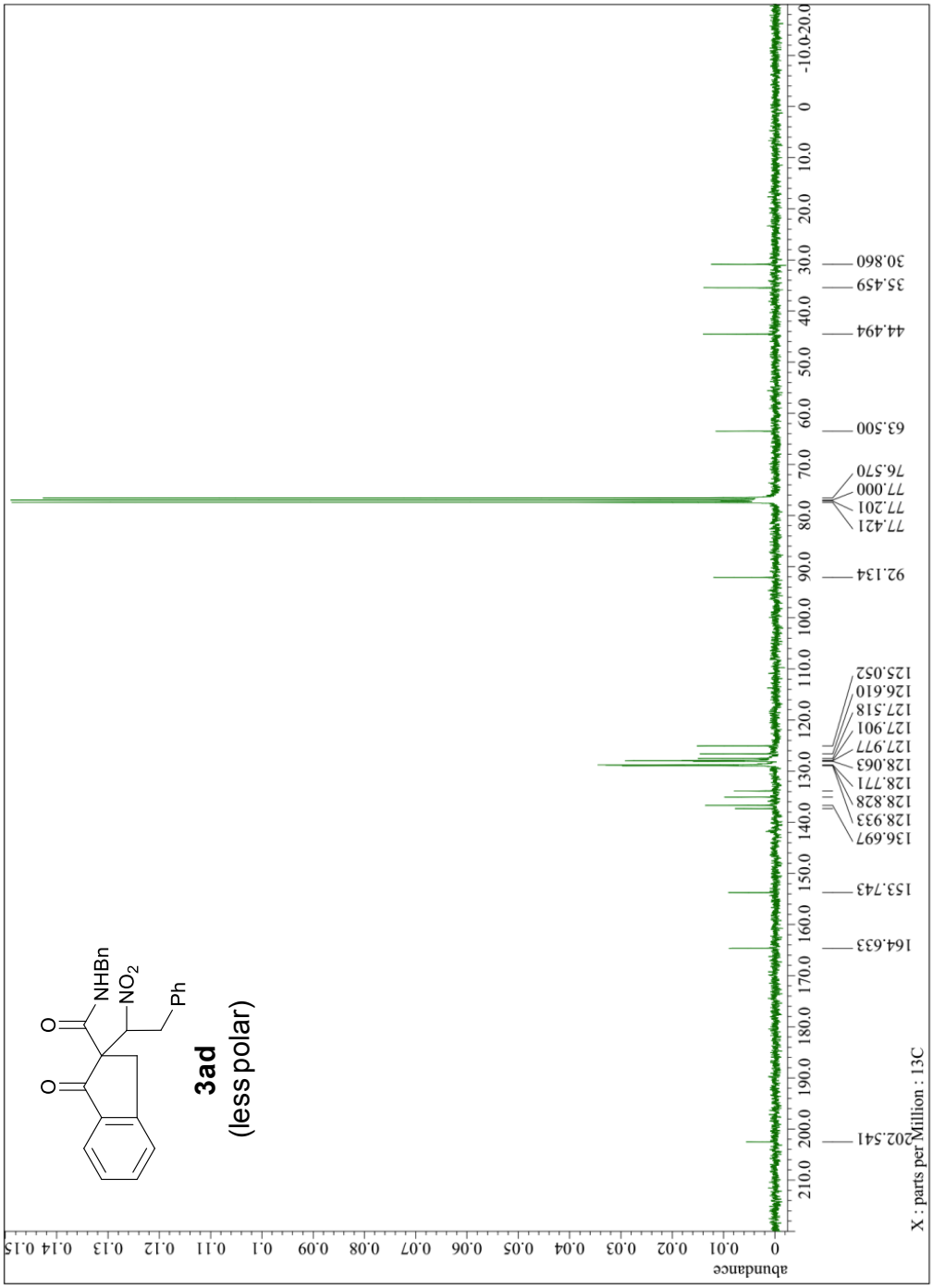

3ac
(less polar)
NHBn
NO2
Et
O
O
X : parts per Million : 1H
abundance

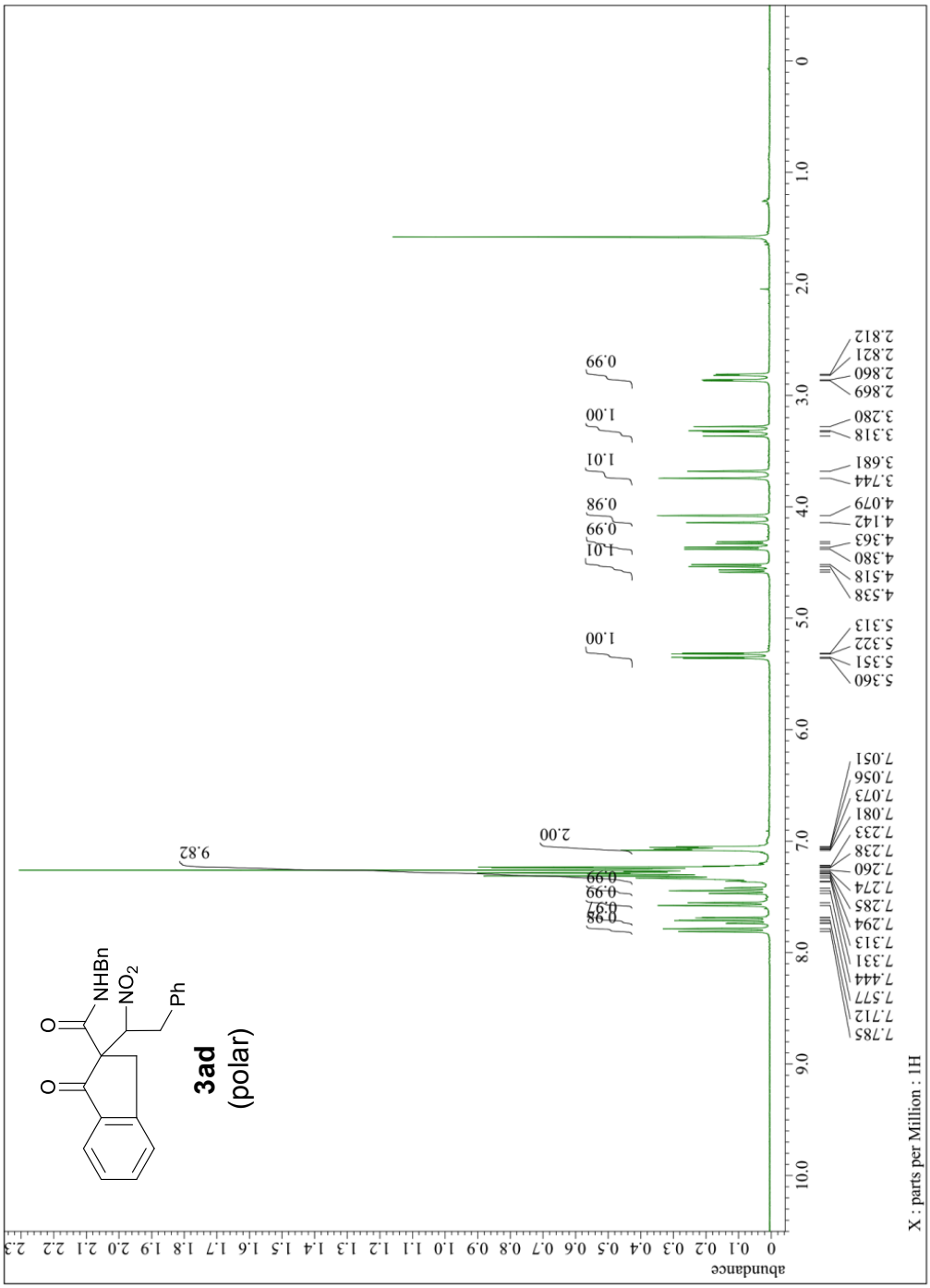

NHBn
NO2
Et
O
O
3ac
(less polar)
abundance
X : parts per Million : 13C
202.961
164.795
153.848
137.270
136.544
133.905
128.800
127.958
127.748
127.585
126.562
124.918
92.077
77.430
77.000
76.579
63.749
44.427
31.052
23.174
10.926

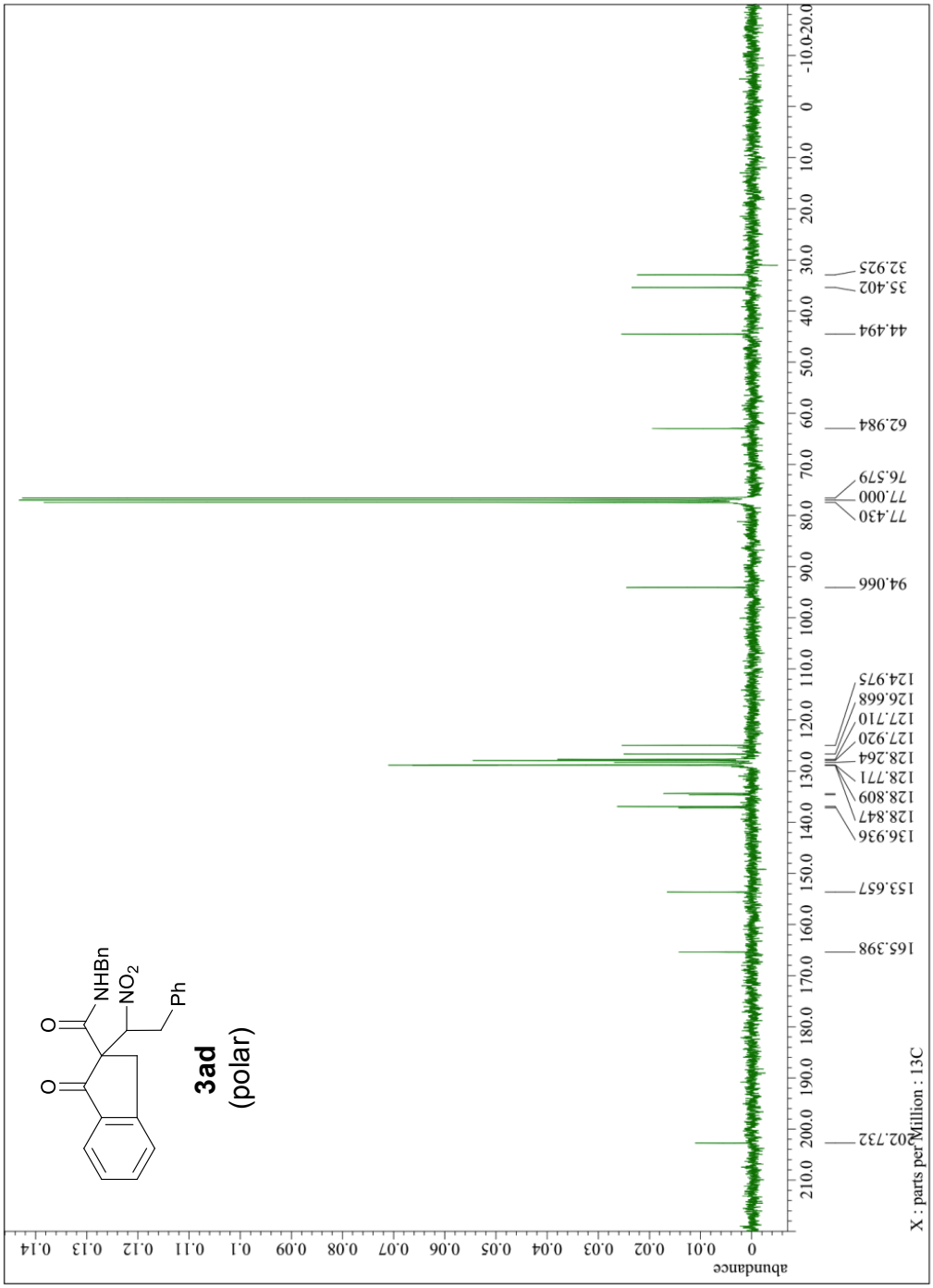

3ac
(polar)
NHBn
NO2
Et
O
O
X : parts per Million : 1H
abundance

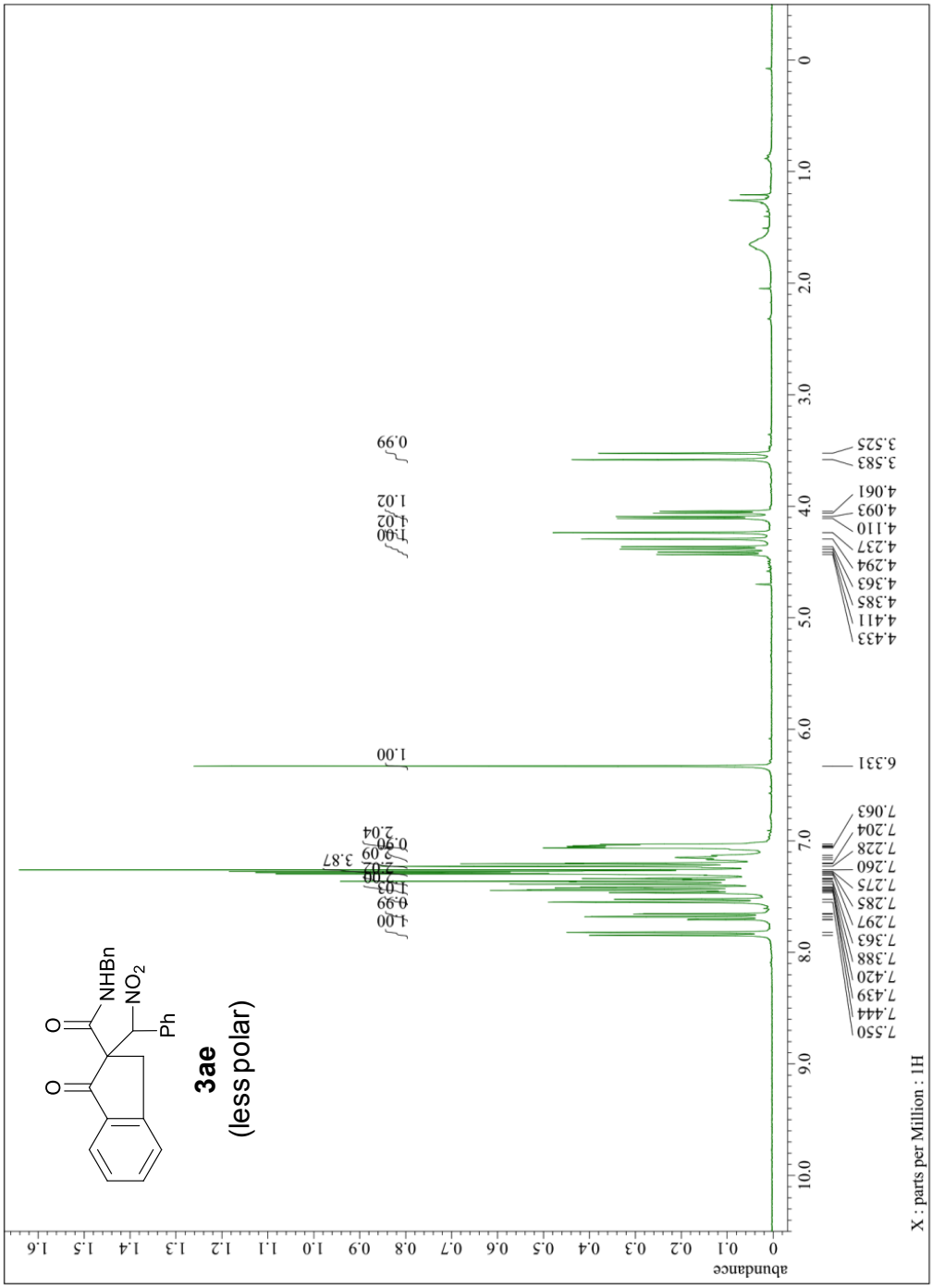

NHBn
NO2
Et
O
O
3ac
(polar)
10.534
22.715
31.061
32.677
44.427
63.147
76.579
77.000
77.421
94.238
124.861
126.591
127.681
127.872
128.149
128.742
134.584
136.792
137.222
153.877
165.560
202.742
X : parts per Million : 13C
abundance

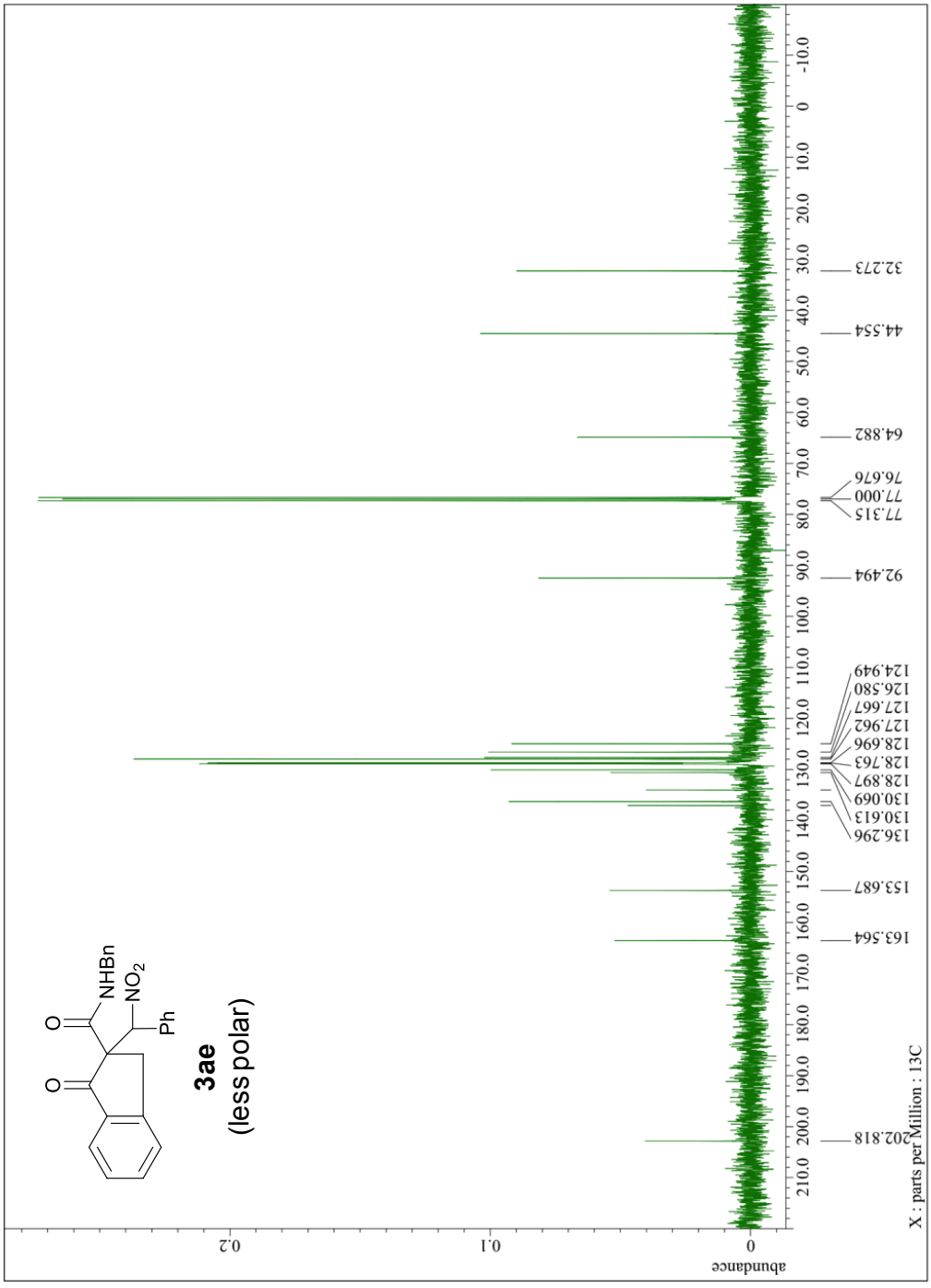

O
O
NHBn
NO2
Ph
3ad
(less polar)
10.68
2.01
0.94
0.97
2.01
1.00
1.02
2.00
0.97
1.01
1.00
7.537
7.356
7.331
7.323
7.310
7.286
7.279
7.260
7.242
7.234
7.002
6.991
6.978
6.972
5.382
5.372
5.346
5.337
4.600
4.574
4.552
4.270
4.213
4.204
3.602
3.542
3.390
3.356
3.340
3.306
3.159
3.149
3.109
3.098
abundance
X : parts per Million : 1H

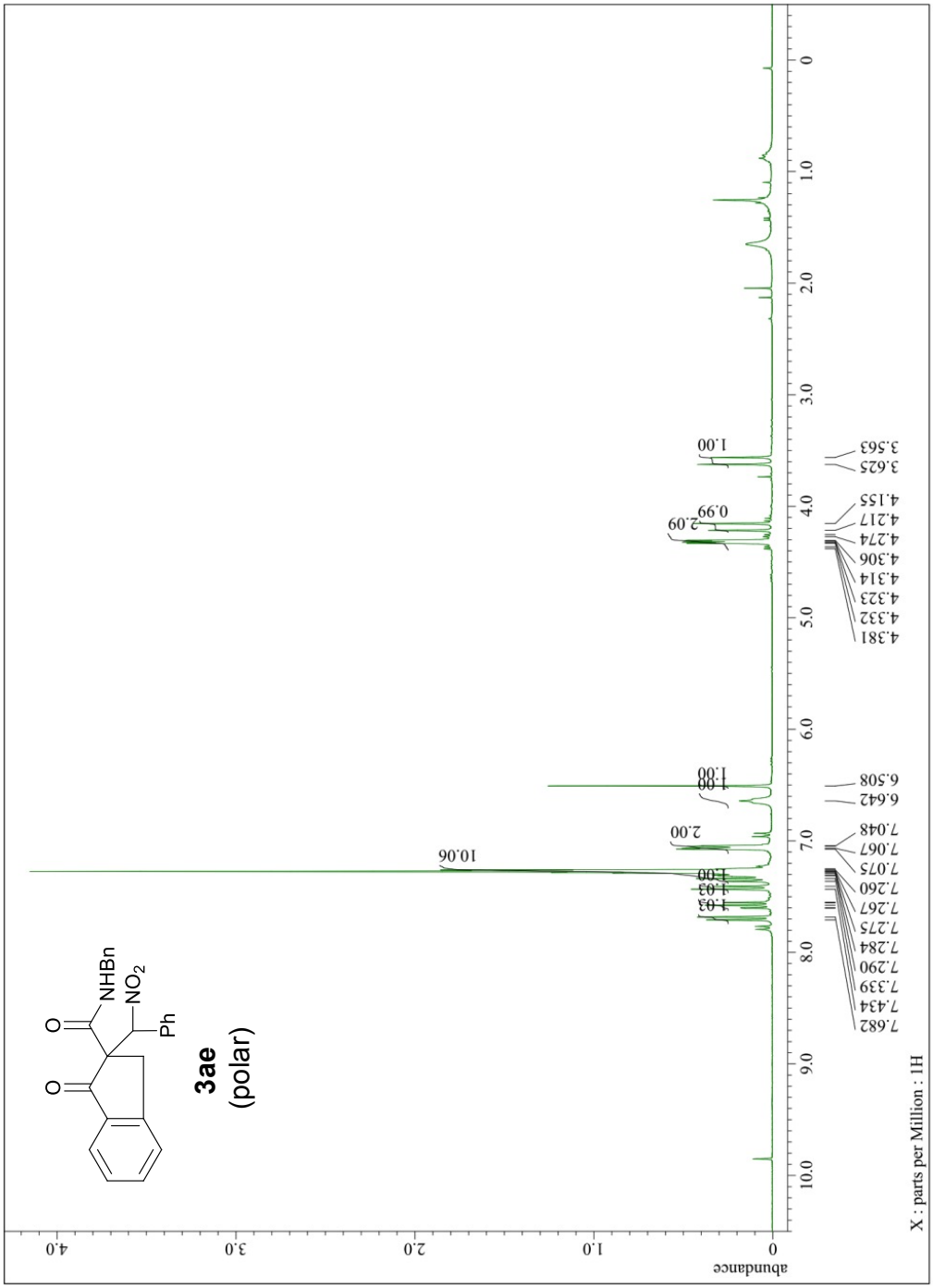

3ad
(less polar)
NHBn
NO2
Ph
O
O
X : parts per Million : 13C
abundance
202.541
164.633
153.743
136.697
128.933
128.828
128.771
128.063
127.977
127.901
127.518
126.610
125.052
92.134
77.421
77.201
77.000
76.570
63.500
44.494
35.459
30.860

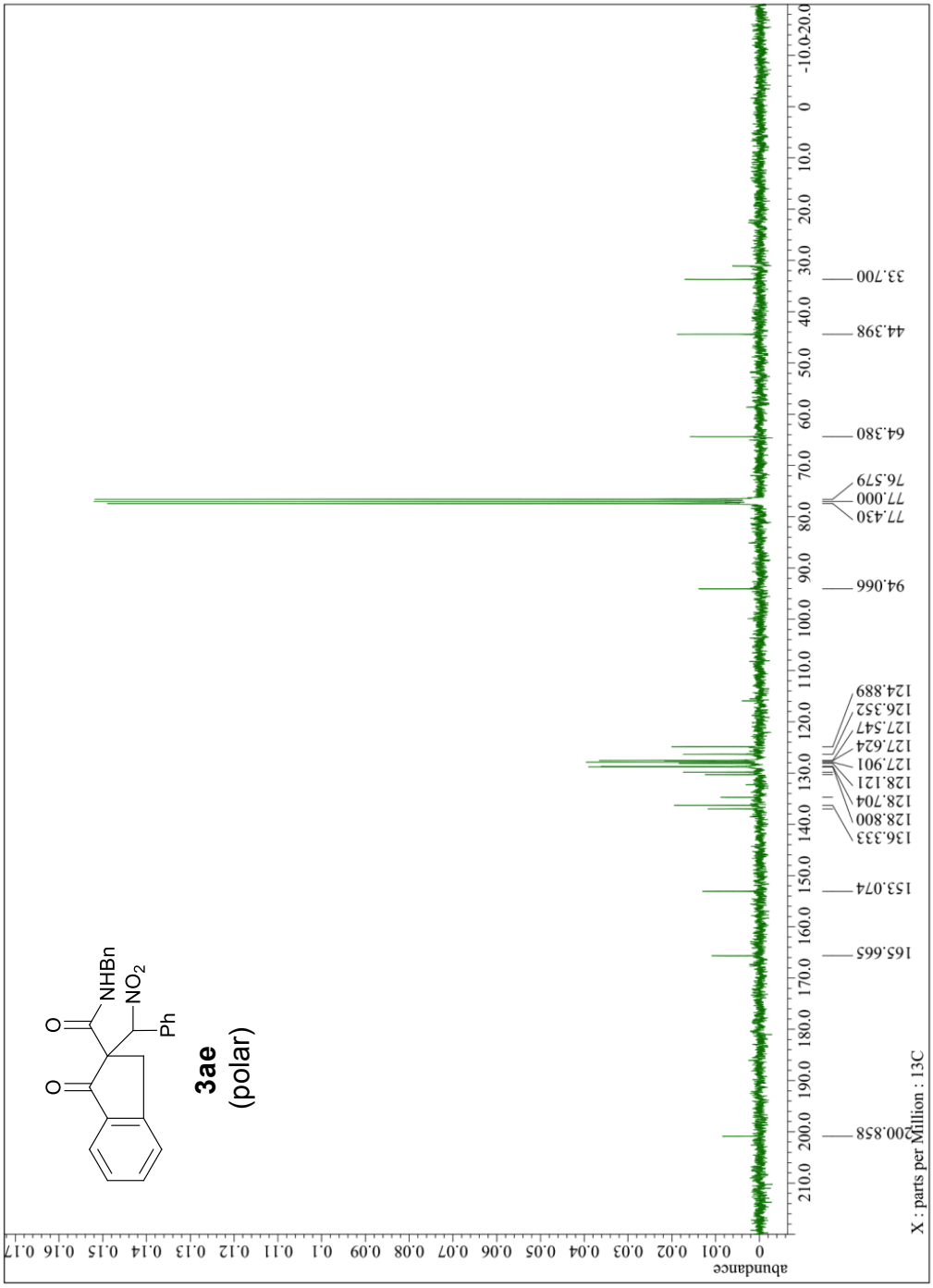

3ad
(polar)
NHBn
NO2
Ph
O
O
X : parts per Million : 1H
abundance

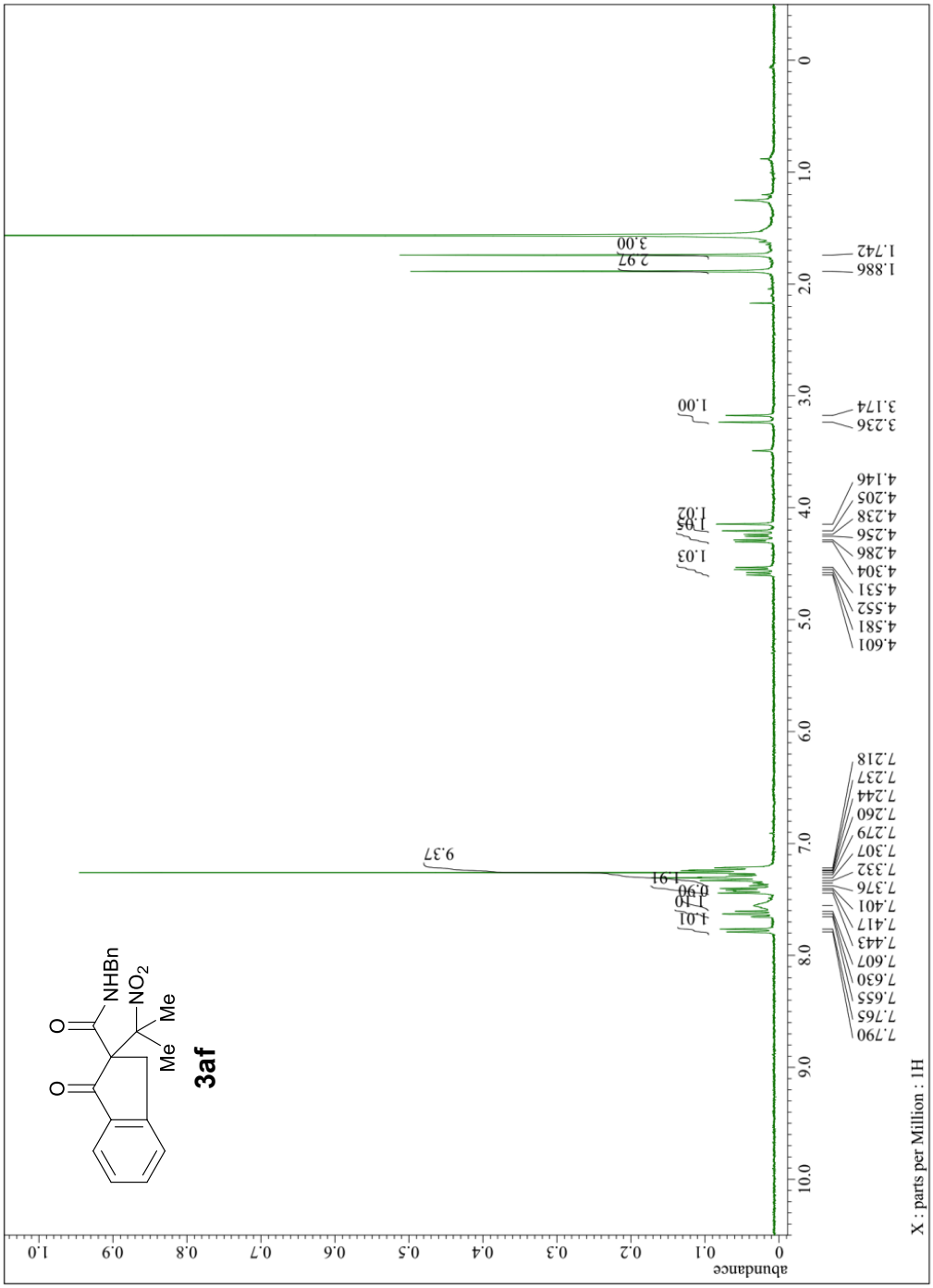

3ad
(polar)
NHBn
NO2
Ph
O
O
202.732
165.398
153.657
136.936
128.847
128.809
128.771
128.264
127.920
127.710
126.668
124.975
94.066
77.430
77.000
76.579
62.984
44.494
35.402
32.925
X : parts per Million : 13C
abundance

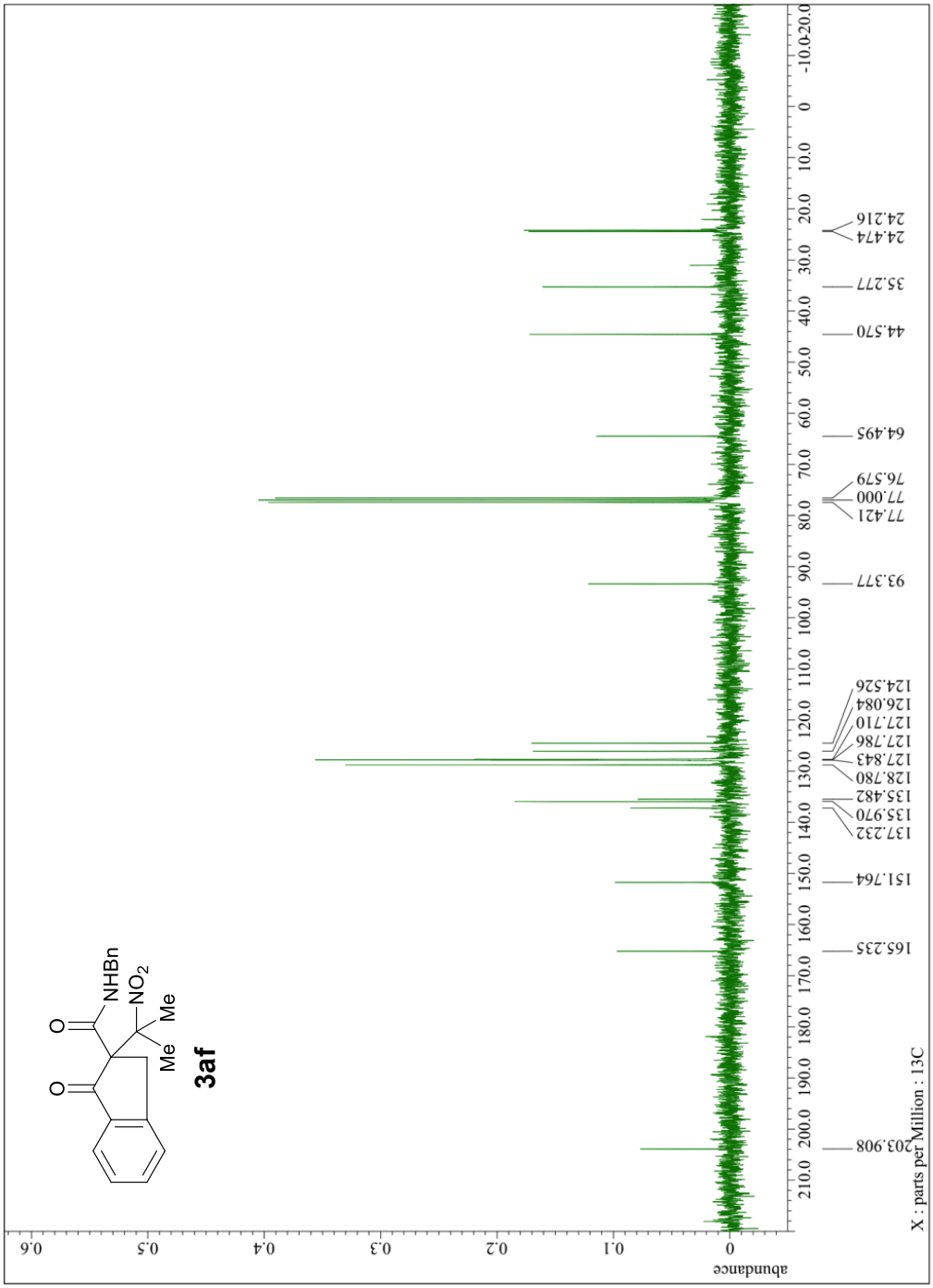

3ae
(less polar)
NHBn
NO2
Ph
O
O
X : parts per Million : 1H
abundance

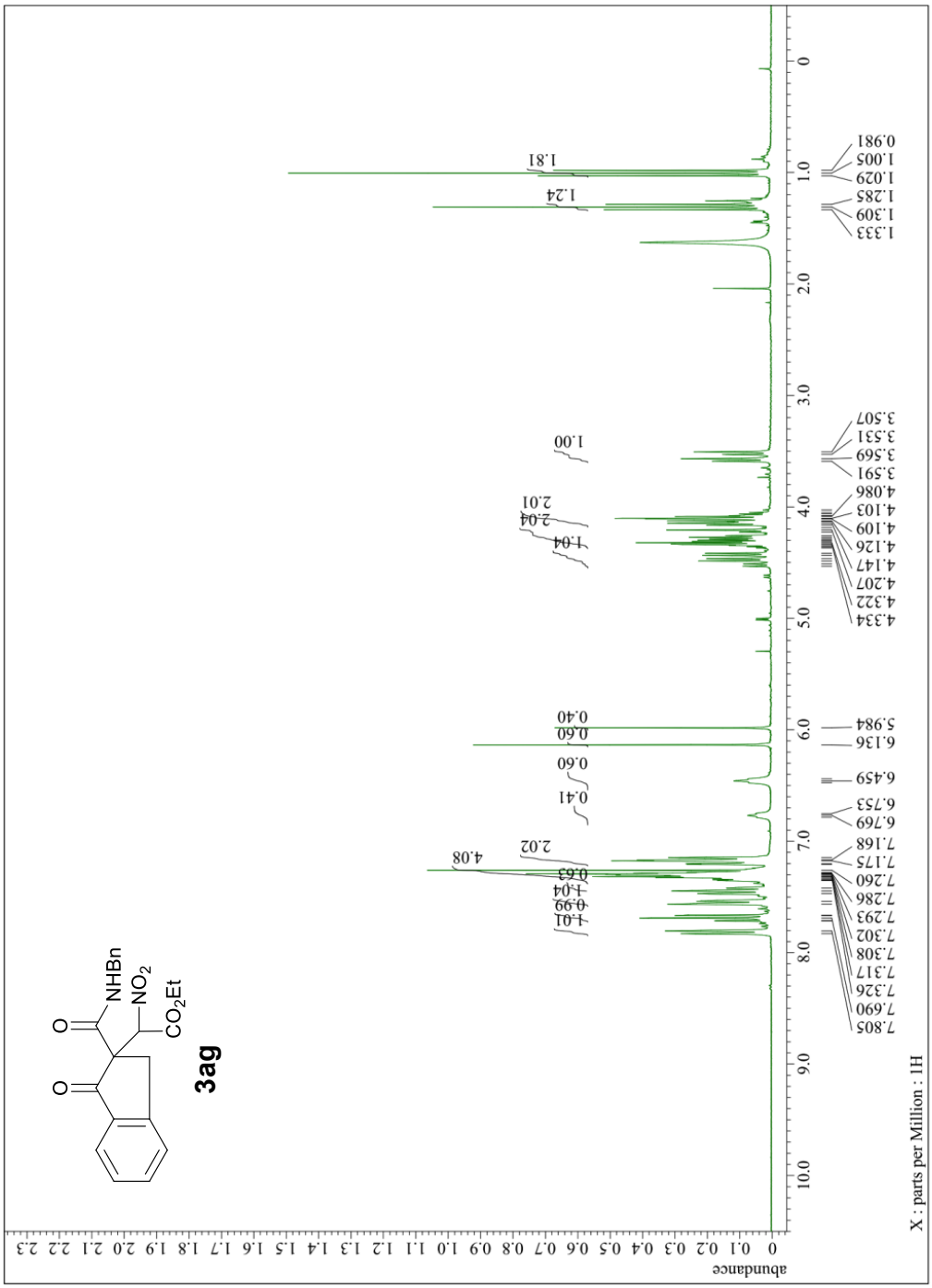

3ae
(less polar)
NHBn
NO2
Ph
O
O
abundance
X : parts per Million : 13C
202.818
163.564
153.687
136.296
130.613
130.069
128.897
128.763
128.696
127.962
127.667
126.580
124.949
92.494
77.315
77.000
76.676
64.882
44.554
32.273

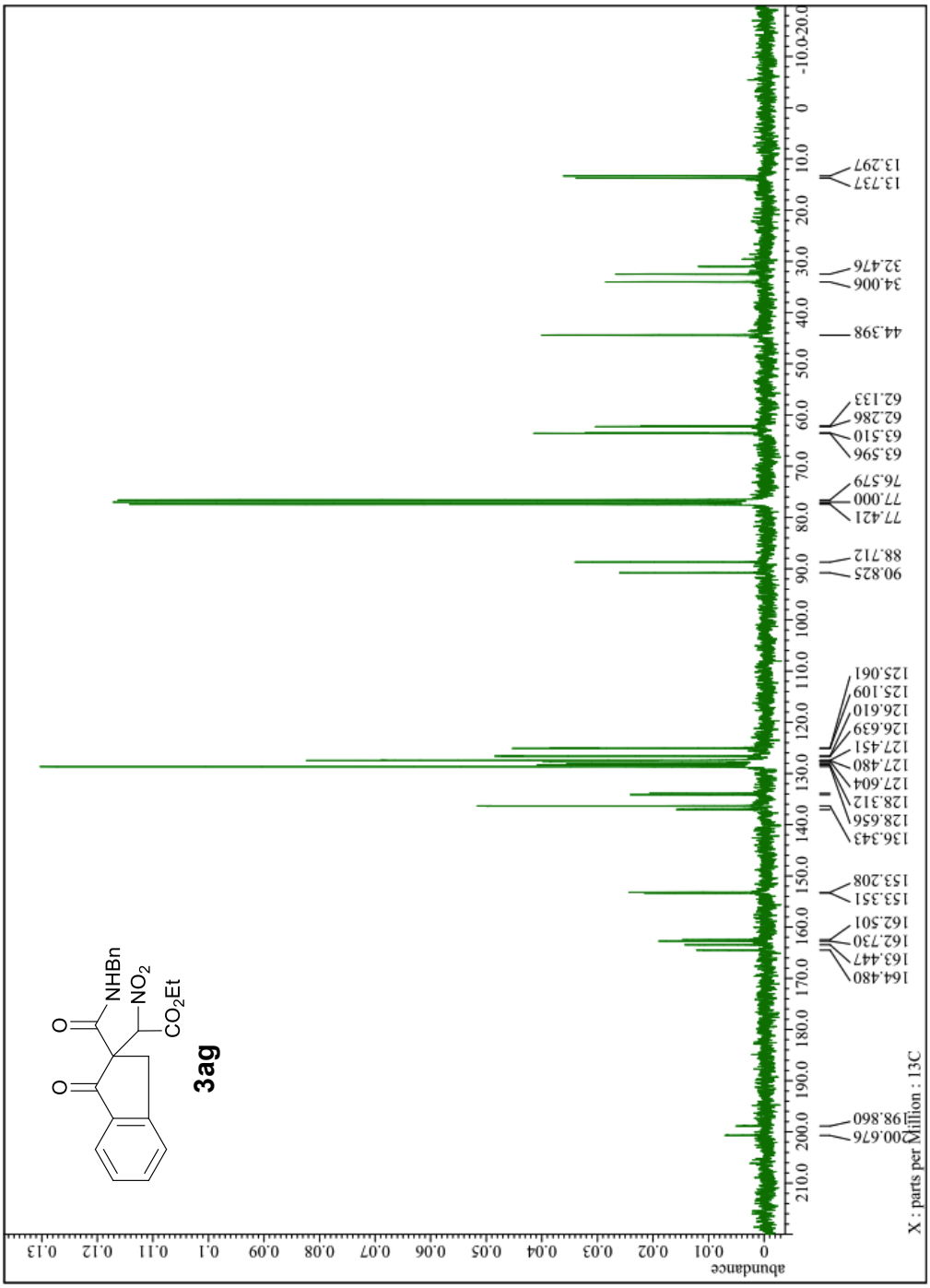

3ae
(polar)
NHBn
NO2
Ph
O
O
10.06
2.09
2.00
1.00
0.99
1.00
1.00
1.03
1.03
1.00
1.00
1.00
7.682
7.434
7.339
7.290
7.284
7.275
7.267
7.260
7.075
7.067
7.048
6.642
6.508
4.381
4.332
4.323
4.314
4.306
4.274
4.217
4.155
3.625
3.563
abundance
X : parts per Million : 1H


3ae
(polar)
NHBn
NO2
Ph
O
O
200.858
165.665
153.074
136.333
128.800
128.704
128.121
127.901
127.624
127.547
126.352
124.889
94.066
77.430
77.000
76.579
64.380
44.398
33.700
X : parts per Million : 13C
abundance


NHBn
NO2
Me
Me
O
O
3af
9.37
1.91
0.90
1.40
1.01
1.03
1.05
1.02
1.00
3.00
2.97
1.886
1.742
3.236
3.174
4.601
4.581
4.552
4.531
4.304
4.286
4.256
4.238
4.205
4.146
7.790
7.765
7.655
7.630
7.607
7.443
7.417
7.401
7.376
7.332
7.307
7.279
7.260
7.244
7.237
7.218
abundance
X : parts per Million : 1H


NHBn
NO2
Me
Me
O
O
3af
abundance
X : parts per Million : 13C
203.908
165.235
151.764
137.232
135.970
135.482
128.780
127.843
127.786
127.710
126.084
124.526
93.377
77.421
77.000
76.579
64.495
44.570
35.277
24.474
24.216


NHBn
NO2
CO2Et
O
O
3ag
X : parts per Million : 1H
abundance


NHBn
NO2
CO2Et
O
O
3ag
13.737
13.297
34.006
32.476
44.398
62.133
62.286
63.510
63.596
76.579
77.000
77.421
88.712
90.825
125.061
125.109
126.610
126.639
127.451
127.480
127.604
128.312
128.656
136.343
153.208
153.351
162.501
162.730
163.447
164.480
198.860
200.676
X : parts per Million : 13C
abundance