Supporting Information

Synthesis of *o*-(Dimethylamino)aryl Ketones and Acridones by the Reaction of 1,1-Dialkylhydrazones and Arynes

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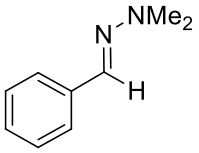
General Information. The ^{1}H and ^{13}C NMR spectra were recorded at 300 and 75.5 MHz or 400 and 100 MHz respectively. Thin layer chromatography was performed using 60 mesh silica gel plates, and visualization was effected by short wavelength UV light (254 nm). All melting points are uncorrected. All high resolution mass spectra were recorded using EI at 70 eV. All reagents were used directly as obtained commercially, unless otherwise noted.

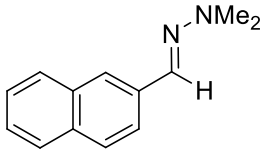
General procedure for synthesis of the starting hydrazones.[1]
A mixture of the aldehyde (1.5 mmol), anhydrous magnesium sulfate (3.0 mmol, 2 equiv), and 1,1-dimethylhydrazone (2.0 mmol, 1.3 equiv) (except for the product **28** where 1-amino-morpholine was used) was stirred for 10 hours at room temperature in dichloromethane (5 mL). The reaction mixture was filtered and the filtrate was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel using hexanes/EtOAc as the eluent to afford the desired hydrazones.

Benzaldehyde dimethylhydrazone (1)



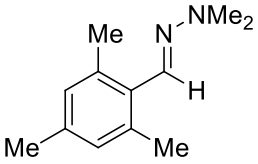
This compound was obtained as a pale yellow liquid in an 89% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.97 (s, 6H), 7.22 (t, J = 7.3 Hz, 1H), 7.25 (s, 1H), 7.32 (t, J = 7.5 Hz, 2H), 7.57 (d, J = 8.2 Hz, 2H). The ^{1}H NMR spectral data are in good agreement with the literature data.[1]

2-Naphthaldehyde dimethylhydrazone (9)



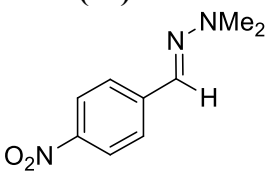
This compound was obtained as a white solid in a 97% yield: mp 69-70 ^{o}C (lit.[2] 67 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.04 (s, 6H), 7.42-7.48 (m, 3H), 7.79-7.82 (m, 4H), 7.93 (d, J = 7.5 Hz, 1H)).

2,4,6-Trimethylbenzaldehyde dimethylhydrazone (11)



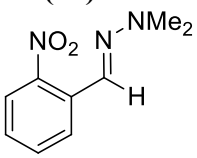
This compound was obtained as a colorless liquid in an 84% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.30 (s, 3H), 2.41 (s, 6H), 2.96 (s, 6H), 6.88 (s, 2H), 7.47 (s, 1H).

4-Nitrobenzaldehyde dimethylhydrazone (13)



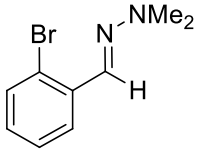
This compound was obtained as bright orange crystals in a 96% yield: mp 113-114 °C (lit.[3] 113-114 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.10 (s, 6H), 7.10 (s, 1H), 7.63 (d, J = 8.8 Hz, 2H), 8.15 (d, J = 8.9 Hz, 2H).

2-Nitrobenzaldehyde dimethylhydrazone (15)



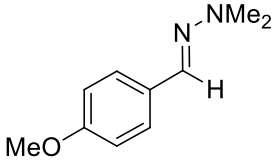
This compound was obtained as a bright red liquid in a 98% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.08 (s, 6H), 7.27 (t, J = 7.7 Hz, 1H), 7.51 (t, J = 7.4 Hz, 1H), 7.68 (s, 1H), 7.91 (d, J = 8.2 Hz, 1H), 8.11 (d, J = 7.3 Hz, 1H).

2-Bromobenzaldehyde dimethylhydrazone (17)



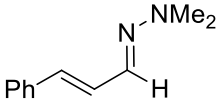
This compound was obtained as a pale yellow liquid in an 86% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.03 (s, 6H), 7.06 (t, J = 7.7 Hz, 1H), 7.25 (t, J = 7.6 Hz, 1H), 7.46 (s, 1H), 7.50 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H).

4-Methoxybenzaldehyde dimethylhydrazone (19)



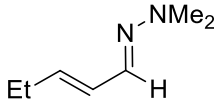
This compound was obtained as a pale yellow liquid in a 98% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.92 (s, 6H), 3.81 (s, 3H), 6.87 (d, J = 8.8 Hz, 2H), 7.26 (s, 1H), 7.51 (d, J = 8.7 Hz, 2H).

Cinnamaldehyde dimethylhydrazone (21)



This compound was obtained as a yellow liquid in a 95% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.93 (s, 6H), 6.61 (d, J = 15.9 Hz, 1H), 6.91-6.97 (m, 1H), 7.14 (d, J = 9.0 Hz, 1H), 7.21 (t, J = 7.3 Hz, 1H), 7.31 (t, J = 7.6 Hz, 2H), 7.41 (d, J = 7.4 Hz, 2H). The ^{1}H NMR spectral data are in good agreement with the literature data.[1]

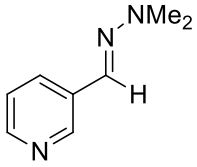
(*E*)-Pent-2-enal dimethylhydrazone (22)



This compound was obtained as a dark yellow liquid in a 60% yield (caution: the compound is volatile under a moderate vacuum): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.00 (t, J = 7.5 Hz, 3H), 2.08-

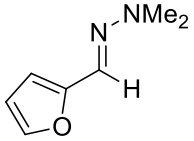
2.18 (m, 2H), 2.78 (s, 6H), 5.84 (dt, J = 15.5, 6.4 Hz, 1H), 6.16 (dd, J = 8.9, 15.6 Hz, 1H), 6.99 (d, J = 8.8 Hz, 1H).

Nicotinaldehyde dimethylhydrazone (24)



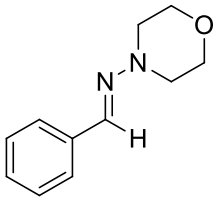
This compound was obtained as a yellow liquid in an 88% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.94 (s, 6H), 7.08 (s, 1H), 7.16 (dd, J = 4.8, 7.8 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 8.36 (d, J = 4.7 Hz, 1H), 8.64 (s, 1H).

Furan-2-carbaldehyde dimethylhydrazone (26)



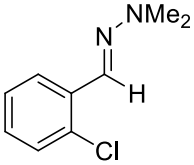
This compound was obtained as a dark brown liquid in a 67% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.95 (s, 6H), 6.37 (d, J = 13.5 Hz, 2H), 7.12 (s, 1H), 7.38 (s, 1H).

(*E*)-*N*-Benzylidenemorpholin-4-amine (28)



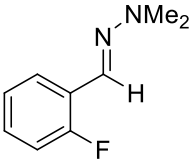
This compound was obtained as white crystals in a 71% yield: mp 90-91 ^{o}C (lit.[4] 89 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.17-3.19 (m, 4H), 3.88-3.90 (m, 4H), 7.29 (d, J = 7.1 Hz, 1H), 7.35 (t, J = 7.3 Hz, 2H), 7.60-7.61 (m, 3H).

2-Chlorobenzaldehyde dimethylhydrazone (31)



This compound was obtained as a pale yellow liquid in a 92% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.03 (s, 6H), 7.13 (t, J = 7.6 Hz, 1H), 7.21 (t, J = 7.6 Hz, 1H), 7.31 (d, J = 8.0 Hz, 1H), 7.51 (s, 1H), 7.93 (d, J = 7.8 Hz, 1H).

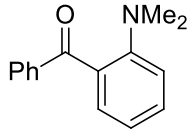
2-Fluorobenzaldehyde dimethylhydrazone (32)



This compound was obtained as a colorless liquid in a 92% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.00 (s, 6H), 6.98-7.03 (m, 1H), 7.09 (t, J = 7.3 Hz, 1H), 7.15-7.19 (m, 1H), 7.39 (s, 1H), 7.86 (t, J = 7.6 Hz, 1H).

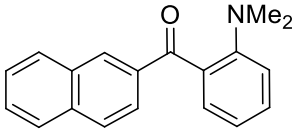
General procedure for synthesis of the *o*-(dimethylamino)aryl ketones.
To a mixture of the appropriate dimethylhydrazone (0.25 mmol), CsF (0.75 mmol, 3 equiv) and 5 mL of acetonitrile in a 10 mL vial, the silylaryl triflate (0.28 mmol, 1.1 equiv) was added. The vial was capped and the reaction mixture was allowed to stir for 10 h at 65 °C. Then 3 mL of 1M HCl was added and the mixture was heated at 65 °C for an additional 2 h. After cooling to room temperature, 25 ml of dichloromethane was added to the residue, and the reaction mixture was poured into 25 ml of water in a separatory funnel. After shaking the layers, the organic fraction was separated and the aqueous layer was extracted with dichloromethane (2 × 10 ml). All organic fractions were combined and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel using hexanes/EtOAc as the eluent to afford the desired *o*-(dimethylamino)aryl ketones.

2-(Dimethylamino)benzophenone (4)



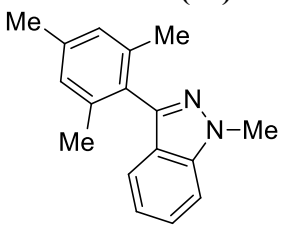
This compound was obtained as a yellow oil in a 93% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.70 (s, 6H), 6.90 (t, J = 7.4 Hz, 1H), 6.99 (d, J = 8.3 Hz, 1H), 7.32 (d, J = 7.5 Hz, 1H), 7.37-7.44 (m, 3H), 7.54 (t, J = 7.4 Hz, 1H), 7.83 (d, J = 7.1 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 43.6, 116.6, 119.0, 128.3, 129.2, 130.1, 130.9, 131.6, 132.8, 137.9, 151.8, 198.4; HRMS (EI) calcd for $C_{15}H_{16}NO$ [M+H] 226.1226, found 226.1230. The ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[5]

(2-(Dimethylamino)phenyl)(naphthalen-2-yl)methanone (10)



This compound was obtained as a yellow oil in a 91% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.72 (s, 6H), 6.95 (t, J = 7.2 Hz, 1H), 7.04 (d, J = 8.2 Hz, 1H), 7.40-7.47 (m, 2H), 7.52 (t, J = 7.3 Hz, 1H), 7.59 (t, J = 7.3 Hz, 1H), 7.87-7.90 (m, 3H), 7.99 (d, J = 8.7 Hz, 1H), 8.34 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 43.6, 116.6, 119.0, 125.7, 126.7, 127.9, 128.0, 128.4, 129.3, 129.7, 131.0, 131.6, 132.0, 132.6, 135.1, 135.6, 151.8, 198.2; HRMS (EI) calcd for $C_{19}H_{18}NO$ [M+H] 276.1383, found 276.1384.

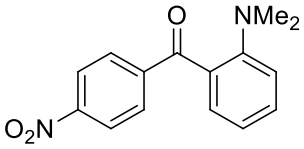
1-Methyl-3-(2,4,6-trimethylphenyl)-*1H*-indazole (12)



This compound was obtained as a light yellow amorphous solid in a 33% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.05 (s, 6H), 2.36 (s, 3H), 4.14 (s, 3H), 6.98 (s, 2H), 7.11 (t, J = 7.2 Hz, 1H), 7.39-7.46 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 20.6, 21.4, 35.7, 109.1, 120.3, 121.3, 123.6,

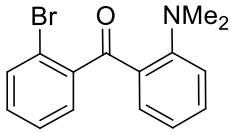
126.3, 128.3, 129.2, 137.9, 138.3, 140.8, 144.0; HRMS (EI) calcd for $C_{17}H_{19}N_2$ [M+H] 251.1543, found 251.1549.

2-(Dimethylamino)-4'-nitrobenzophenone (14)



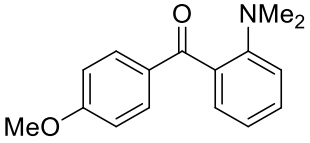
This compound was obtained as a dark red oil in an 88% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (s, 6H), 6.98 (t, J = 7.4 Hz, 1H), 7.03 (d, J = 8.2 Hz, 1H), 7.39 (d, J = 7.6 Hz, 1H), 7.45 (t, J = 7.8 Hz, 1H), 7.90 (d, J = 8.9 Hz, 2H), 8.24 (d, J = 8.9 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 43.8, 117.3, 120.2, 123.4, 128.8, 130.6, 131.1, 132.7, 143.1, 150.1, 152.3, 196.4; HRMS (EI) calcd for $C_{15}H_{15}N_2O_3$ [M+H] 271.1077, found 271.1079.

2'-Bromo-2-(dimethylamino)-benzophenone (18)



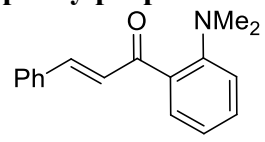
This compound was obtained as a yellow amorphous solid in an 85% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.84 (s, 6H), 6.81 (t, J = 7.4 Hz, 1H), 6.98 (d, J = 8.2 Hz, 1H), 7.26-7.29 (m, 1H), 7.34 (t, J = 7.3 Hz, 1H), 7.38-7.42 (m, 3H), 7.62 (d, J = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 44.0, 116.8, 118.4, 120.7, 126.8, 127.2, 130.9, 131.5, 133.4, 133.6, 133.7, 141.2, 152.9, 195.3; HRMS (EI) calcd for $C_{15}H_{15}BrNO$ [M+H] 304.0332, found 304.0334.

2-(Dimethylamino)-4'-methoxybenzophenone (20)



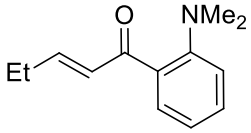
This compound was obtained as a yellow amorphous solid in a 91% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.70 (s, 6H), 3.86 (s, 3H), 6.87-6.91 (m, 3H), 6.97 (d, J = 8.2 Hz, 1H), 7.28 (d, J = 7.6 Hz, 1H), 7.37 (t, J = 7.7 Hz, 1H), 7.82 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 43.6, 55.6, 113.5, 116.5, 119.1, 129.8, 130.5, 130.6, 131.2, 132.5, 151.4, 163.5, 197.2; HRMS (EI) calcd for $C_{16}H_{18}NO_2$ [M+H] 256.1332, found 256.1336.

(*E*)-1-[2-(Dimethylamino)phenyl]-3-phenylprop-2-en-1-one (5)



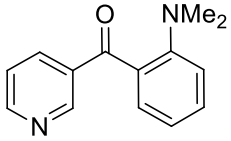
This compound was obtained as a red amorphous solid in a 91% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.83 (s, 6H), 6.97 (t, J = 7.5 Hz, 1H), 7.03 (d, J = 7.8 Hz, 1H), 7.36-7.44 (m, 5H), 7.53-7.60 (m, 3H), 7.73 (d, J = 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 44.5, 117.0, 120.2, 126.3, 128.4, 129.1, 130.3, 130.7, 131.8, 132.1, 135.4, 142.6, 152.4, 195.2; HRMS (EI) calcd for $C_{17}H_{18}NO$ [M+H] 251.1383, found 251.1310. The ^{1}H NMR spectral data are in good agreement with the literature data.[6]

(*E*)-1-[2-(Dimethylamino)phenyl]pent-2-en-1-one (23)



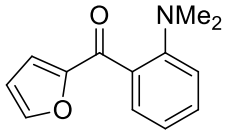
This compound was obtained as a dark orange liquid in a 77% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.08 (t, J = 7.4 Hz, 3H), 2.27 (quintet, J = 6.4 Hz, 2H), 2.78 (s, 6H), 6.66 (d, J = 15.7 Hz, 1H), 6.90 (t, J = 7.4 Hz, 1H), 6.95-7.01 (m, 2H), 7.34 (t, J = 7.7 Hz, 1H), 7.42 (d, J = 7.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 43.8, 117.3, 120.2, 123.4, 128.8, 130.6, 131.1, 132.7, 143.1, 150.1, 152.3, 196.4; HRMS (EI) calcd for $C_{13}H_{18}NO$ [M+H] 204.1383, found 204.1385.

[2-(Dimethylamino)phenyl](pyridin-3-yl)methanone (25)



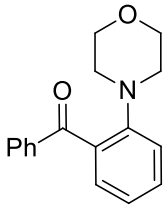
This compound was obtained as a dark yellow oil in a 55% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.63 (s, 6H), 6.96 (t, J = 7.5 Hz, 1H), 7.01 (d, J = 8.3 Hz, 1H), 7.34-7.39 (m, 2H), 7.43 (t, J = 8.6 Hz, 1H), 8.10 (d, J = 8.0 Hz, 1H), 8.72 (d, J = 4.9 Hz, 1H), 8.90 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 43.7, 117.0, 120.0, 123.3, 128.8, 131.0, 132.5, 133.1, 136.9, 151.5, 152.1, 152.9, 196.7; HRMS (EI) calcd for $C_{14}H_{14}N_2O$ [M+H] 227.1179, found 227.1177.

[2-(Dimethylamino)phenyl](furan-2-yl)methanone (27)



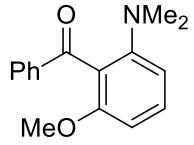
This compound was obtained as a dark yellow amorphous solid in a 90% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.78 (s, 6H), 6.52 (s, 1H), 6.85 (t, J = 7.4 Hz, 1H), 6.96 (d, J = 8.3 Hz, 1H), 7.04 (d, J = 2.8 Hz, 1H), 7.34-7.40 (m, 2H), 7.64 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 43.7, 112.3, 116.7, 118.5, 120.2, 128.0, 130.7, 131.9, 147.2, 151.6, 153.1, 185.2; HRMS (EI) calcd for $C_{13}H_{14}NO_2$ [M+H] 216.1019, found 216.1023.

(2-Morpholinophenyl)(phenyl)methanone (29)



This compound was obtained as a light yellow amorphous solid in an 89% yield: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.86-2.89 (m, 4H), 3.25-3.27 (m, 4H), 7.05 (d, J = 8.1 Hz, 1H), 7.14 (t, J = 7.5 Hz, 1H), 7.38-7.49 (m, 4H), 7.54 (t, J = 7.4 Hz, 1H), 7.74 (t, J = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 52.5, 66.7, 118.7, 123.0, 128.2, 129.9, 130.4, 131.9, 133.0, 133.6, 137.6, 151.1, 198.8; HRMS (EI) calcd for $C_{17}H_{18}NO_2$ [M+H] 268.1332, found 268.1333.

2-(Dimethylamino)-6-methoxybenzophenone (8)

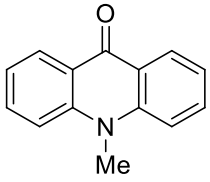


This compound was obtained as a pale yellow solid in an 83% yield starting from the dimethylhydrazone **1** and 3-methoxy-2-(trimethylsilyl)phenyl triflate: mp 112-113 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.63 (s, 6H), 3.66 (s, 3H), 6.60 (d, J = 8.2 Hz, 1H), 6.72 (d, J = 8.2 Hz, 1H), 7.32 (t, J = 8.2 Hz, 1H), 7.39 (t, J = 7.6 Hz, 2H), 7.51 (t, J = 7.4 Hz, 1H), 7.82 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 44.5, 55.9, 104.5, 111.1, 121.9, 128.4, 129.4, 130.7, 133.0, 138.1, 152.9, 157.8, 197.5; HRMS (EI) calcd for $C_{16}H_{18}NO_2$ [M+H] 256.1332, found 256.1334. Note: in the 1D-NOE experiment a correlation of 6.71 (d, 1H) – 2.63 (s, 6H) and of 6.59 (d, 1H) – 3.66 (s, 3H) is observed. This would not be the case if the compound **8** was the other regioisomer.

General procedure for synthesis of the acridones.

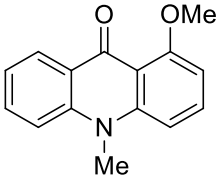
To a mixture of the appropriate dimethylhydrazone (0.25 mmol), CsF (0.75 mmol, 3 equiv) and 5 mL of acetonitrile in a 10 mL vial, the silylaryl triflate (0.28 mmol, 1.1 equiv) was added. The vial was capped and the reaction mixture was allowed to stir for 10 h at 65 °C. Then 3 mL of 1M HCl was added and the mixture was heated at 65 °C for 2 h. Then 5 mL of 1M NaOMe was added and the mixture was heated at 100 °C for an additional 2 h. After cooling to room temperature, 25 ml of dichloromethane was added to the residue, and the reaction mixture was poured into 25 ml of water in a separatory funnel. After shaking the layers, the organic fraction was separated and the aqueous layer was extracted with dichloromethane (2 × 10 ml). All organic fractions were combined and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel using hexanes/EtOAc as the eluent to afford the desired
o-(dimethylamino)aryl ketones.

***N*-Methyl-9-acridone (30)**



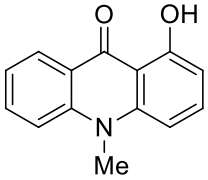
This compound was obtained as light brown crystals in a 95% yield starting from the substrate **17**, a 91% yield starting from the substrate **31**, and a 94% yield starting from the substrate **32**: mp 201-203 °C (lit.[7] 201-202 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, 3H), 7.26 (t, J = 7.5 Hz, 2H), 7.47 (d, J = 8.7 Hz, 2H), 7.68 (t, J = 7.8 Hz, 2H), 8.53 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.8, 114.9, 121.4, 122.6, 127.8, 133.9, 142.7, 178.2; HRMS (EI) calcd for $C_{14}H_{12}NO$ [M+H] 210.0913, found 210.0917. The ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[8]

***N*-Methyl-1-methoxy-9-acridone (33)**



This compound was obtained as a pale brown solid in a 76% yield: mp 164-165 °C (lit.[9] 162-164 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.63 (s, 3H), 3.95 (s, 3H), 6.60 (d, J = 8.2 Hz, 1H), 6.88 (d, J = 8.7 Hz, 1H), 7.14 (t, J = 7.5 Hz, 1H), 7.26 (d, J = 8.6 Hz, 1H), 7.45 (t, J = 8.5 Hz, 1H), 7.51 (t, J = 7.8 Hz, 1H), 8.42 (d, J = 8.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 34.7, 56.3, 102.7, 107.0, 113.2, 114.3, 121.2, 124.4, 127.6, 133.0, 133.8, 141.7, 145.2, 161.5, 177.9; HRMS (EI) calcd for $C_{15}H_{14}NO_2$ [M+H] 240.1019, found 240.1024. The ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[9]

Synthesis of the natural product *N*-methyl-1-hydroxy-9-acridone (34).



A mixture of *N*-methyl-1-methoxy-9-acridone (**33**) (62 mg, 27.5 mmol) and HI (47% aqueous solution, 3 mL) was stirred for 24 h at 100 °C in a closed vial. After cooling to room temperature, 15 ml of dichloromethane was added to the residue, and the reaction mixture was poured into 15 ml of water in a separatory funnel. After shaking the layers, the organic fraction was separated and the aqueous layer was extracted with dichloromethane (2 × 10 ml). All organic fractions were combined and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel using hexanes/EtOAc (3/1) as the eluent to afford the desired *N*-methyl-1-hydroxy-9-acridone as yellow needles in a 94% yield: mp 189-190 °C (lit.[10] 190 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.71 (s, 3H), 6.56 (d, J = 8.1 Hz, 1H), 6.72 (d, J = 8.7 Hz, 1H), 7.18 (t, J = 7.5 Hz, 1H), 7.39 (d, J = 8.8 Hz, 1H), 7.44 (t, J = 8.4 Hz, 1H), 7.64 (d, J = 7.9 Hz, 1H), 8.30 (d, J = 8.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 34.2, 103.8, 107.6, 109.8, 114.8, 120.9, 121.5, 126.6, 134.5, 136.0, 142.2, 143.2, 163.5, 182.1; ^{13}C NMR (100 MHz, DMSO + $CDCl_3$) δ 33.9. 104.2, 106.4, 108.8, 115.4, 119.8, 121.1, 125.4, 134.3, 135.7, 141.7, 142.7, 162.4, 181.0; HRMS (EI) calcd for $C_{14}H_{12}NO_2$ [M+H] 226.0863, found 226.0862.

References

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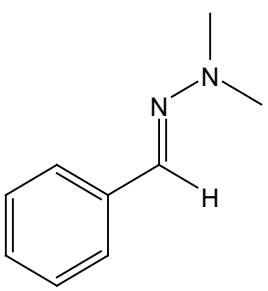
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N
H

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2.00
1.98
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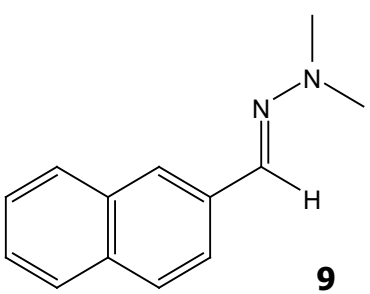
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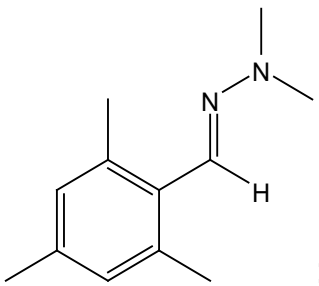
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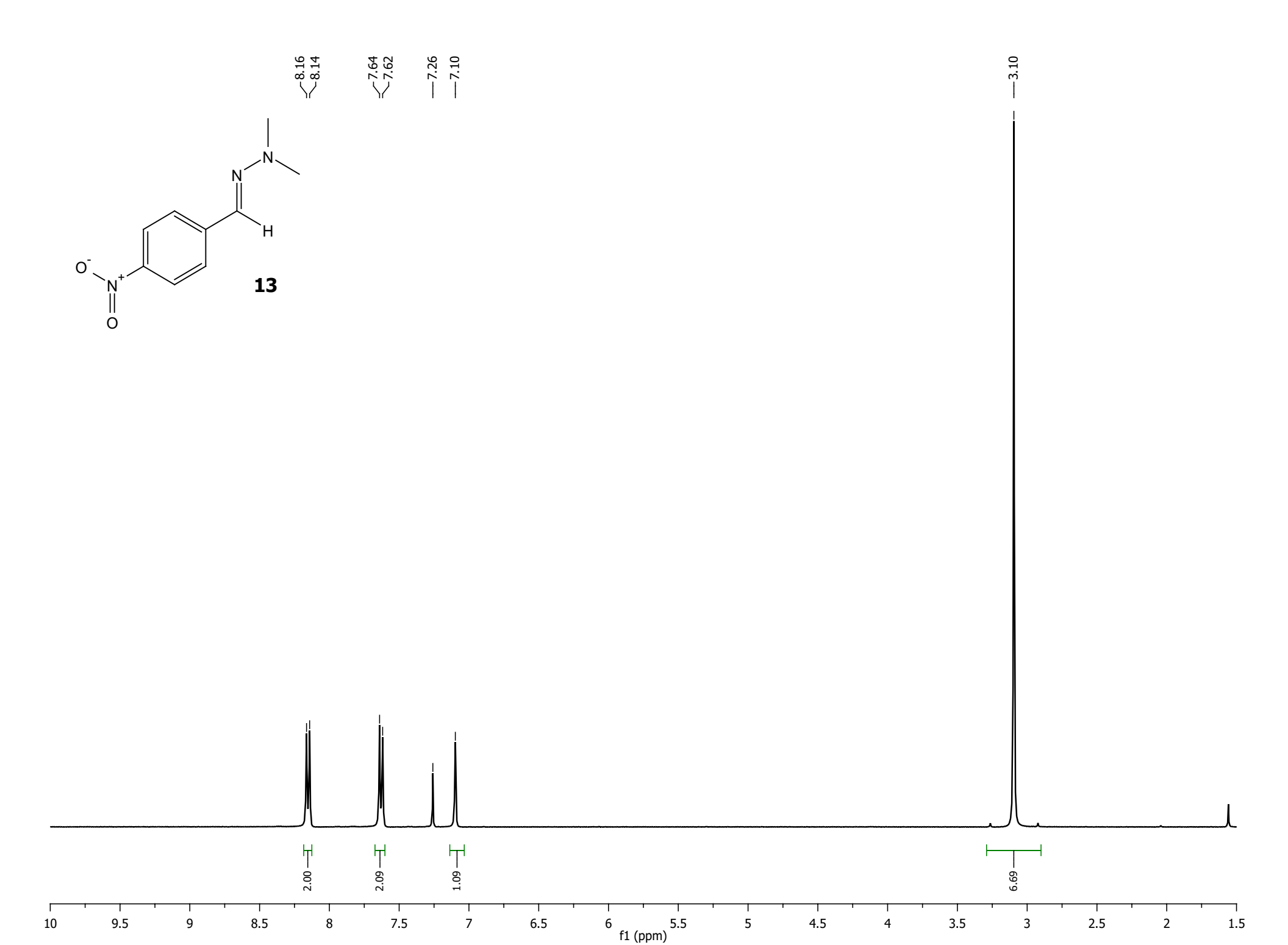
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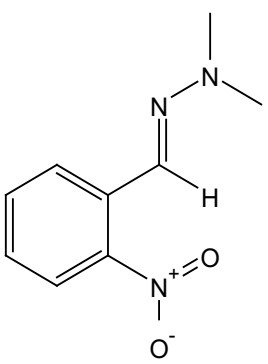
1.5
f1 (ppm)



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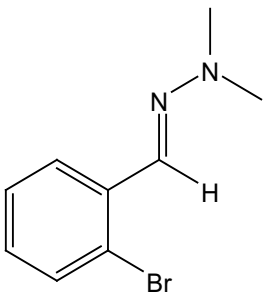
f1 (ppm)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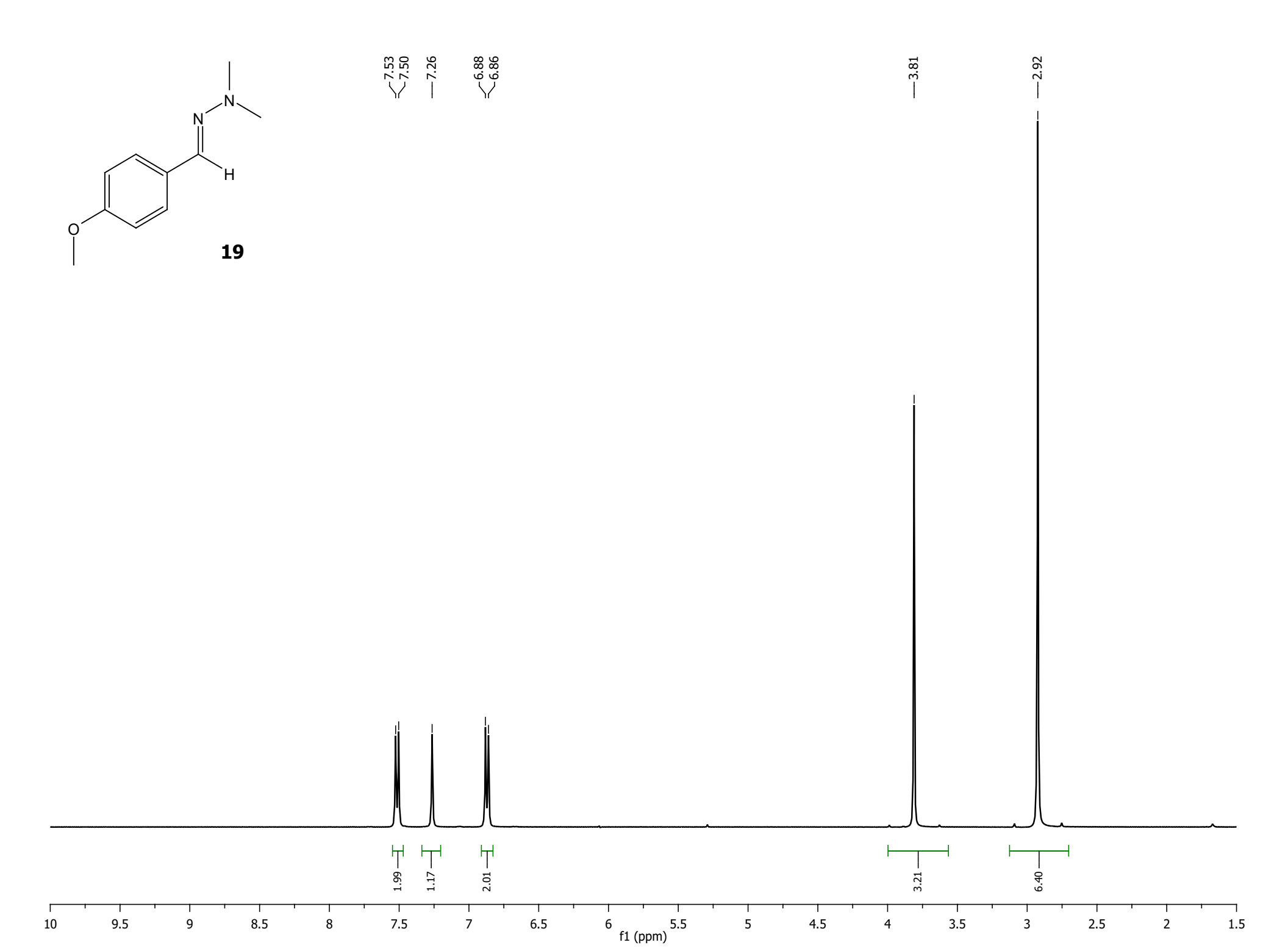
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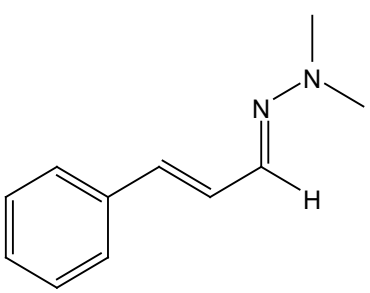
f1 (ppm)

19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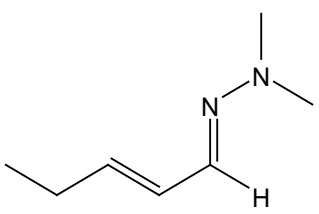

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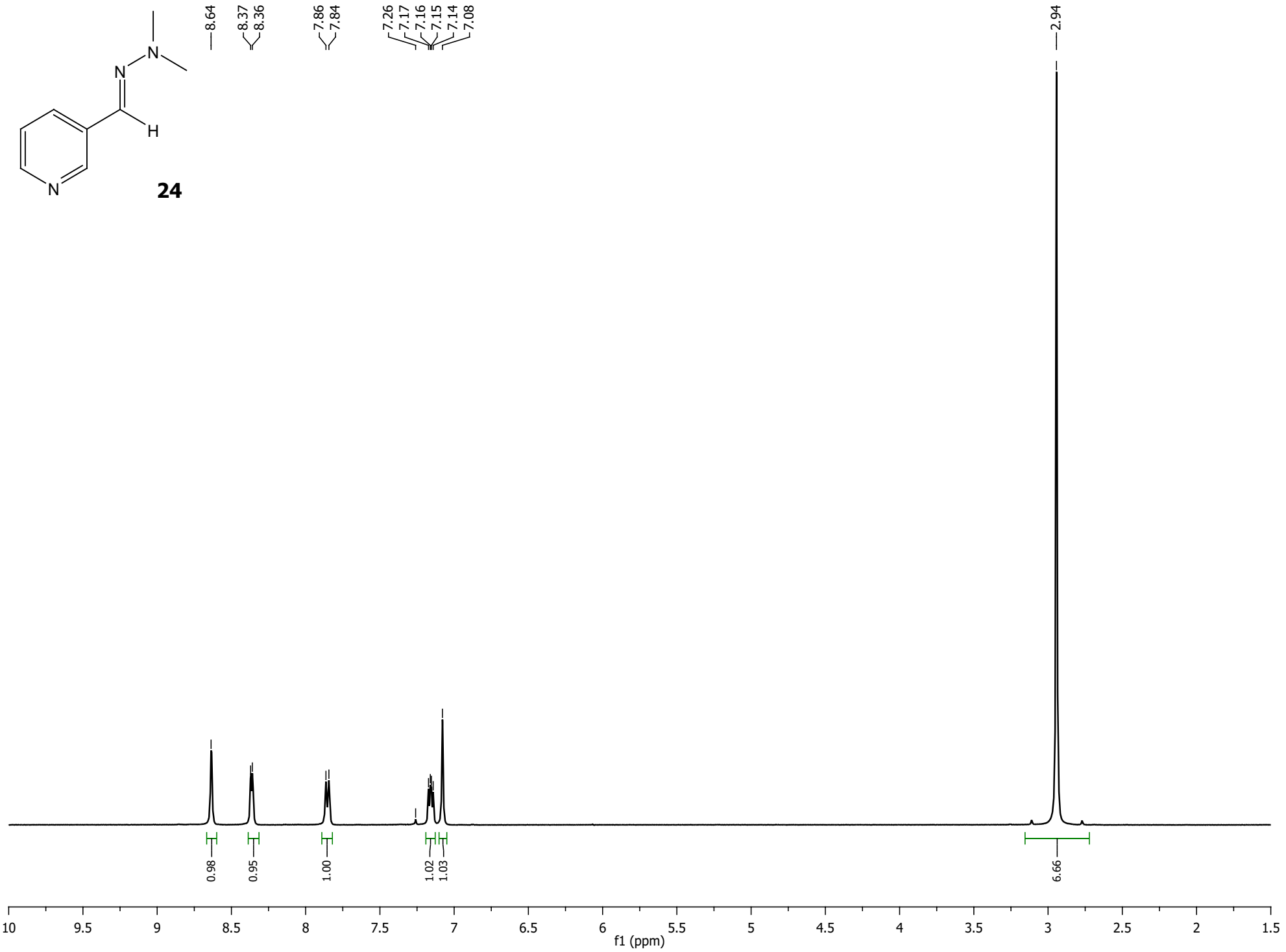
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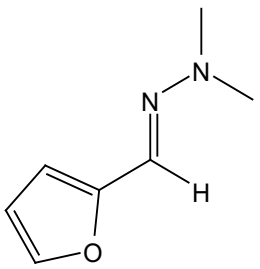
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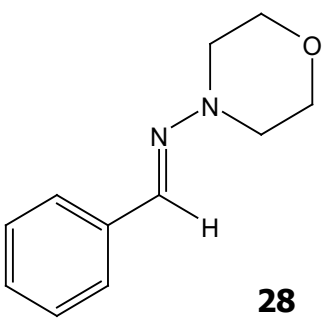
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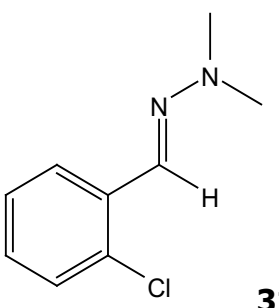
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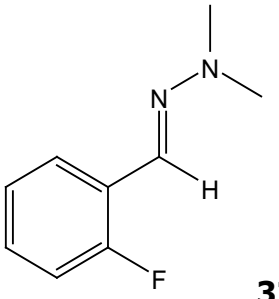
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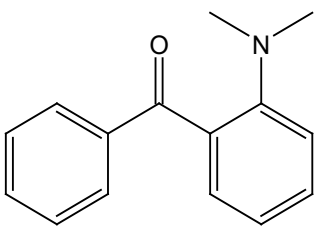
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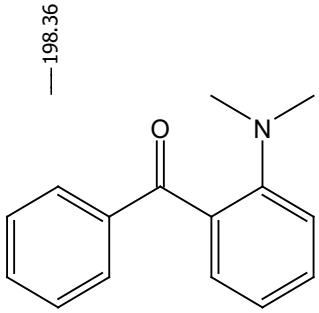

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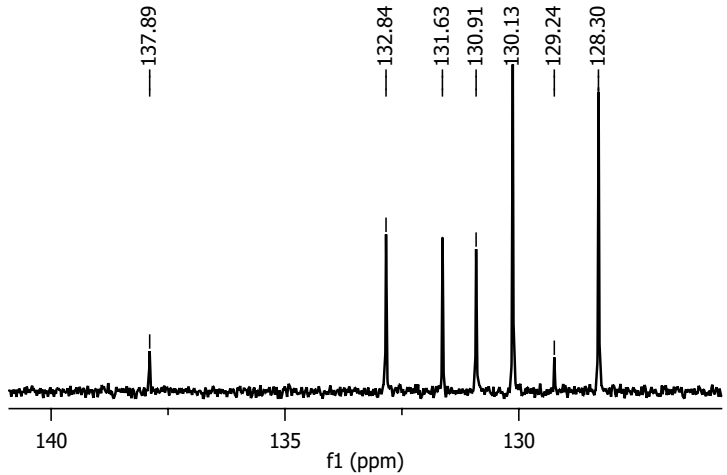

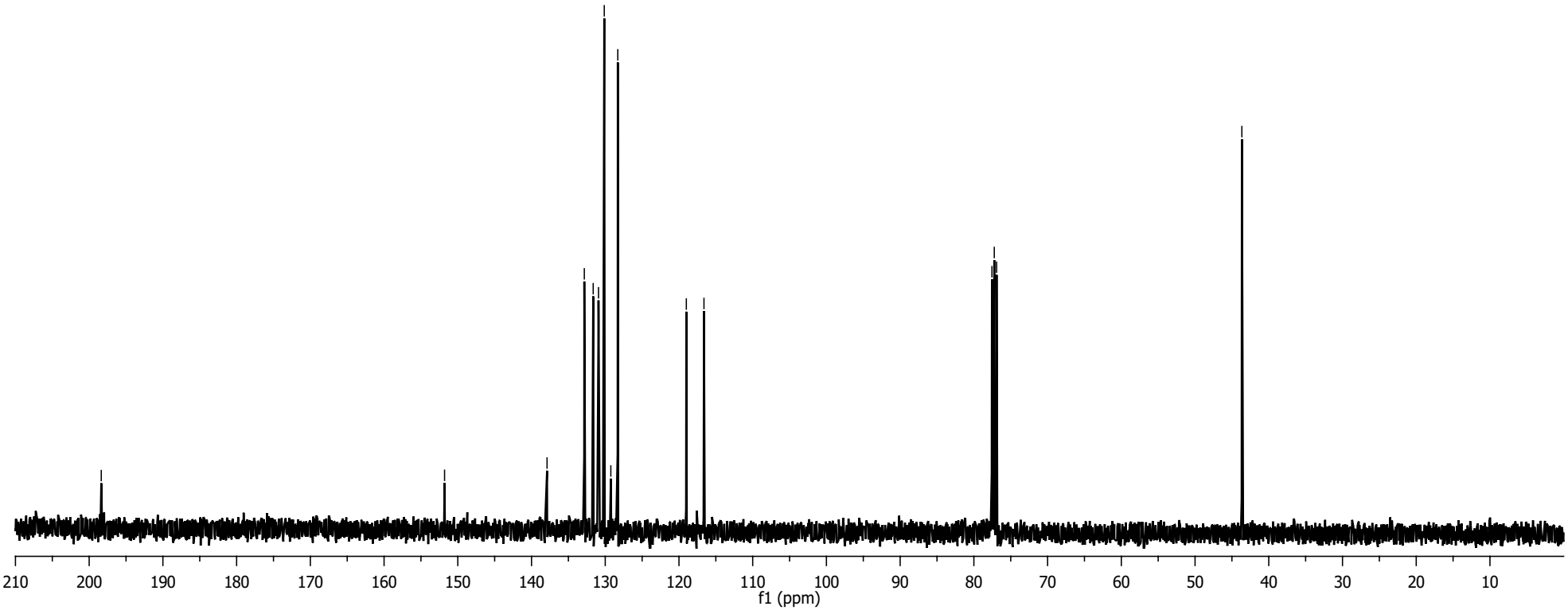

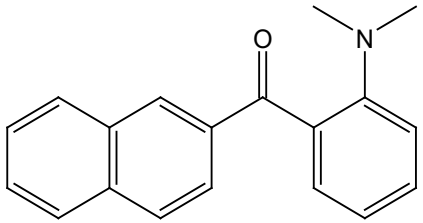
O
N

10

8.34
7.90
7.89
7.87
7.50
7.45
7.40
7.26
7.05
7.03
6.97
6.95
6.93
2.72
1.00
0.99
3.14
1.03
1.02
2.12
0.98
1.02
6.55
10
9.5
9
8.5
8
7.5
7
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5.5
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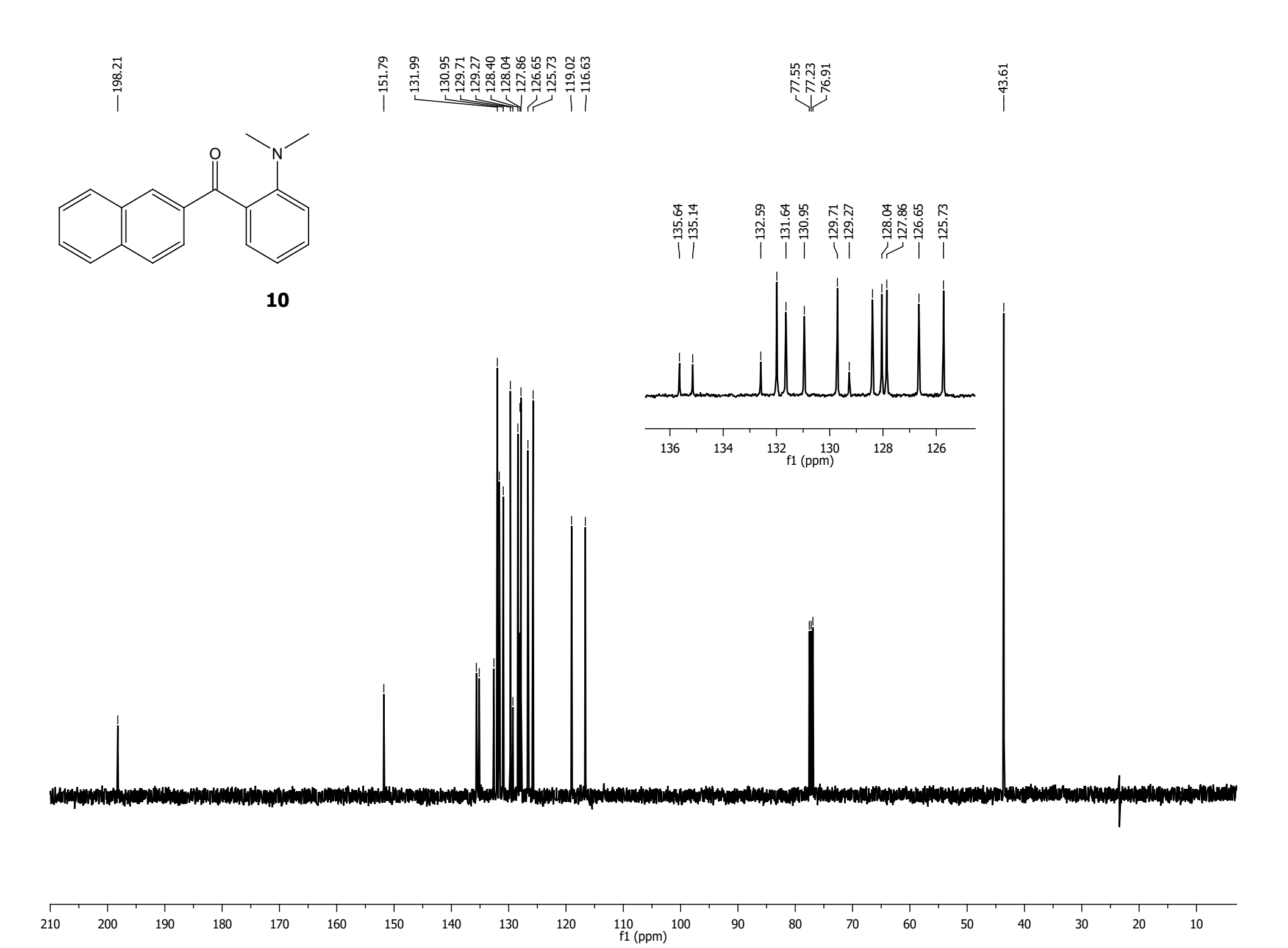
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)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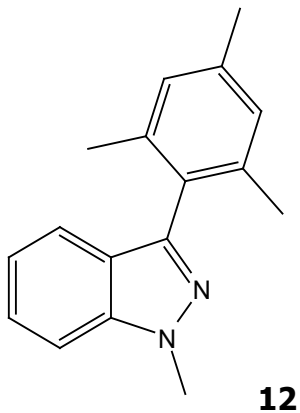
151.79
131.99
130.95
129.71
129.27
128.40
128.04
127.86
126.65
125.73
119.02
116.63
77.55
77.23
76.91
43.61
O
N
10
135.64
135.14
132.59
131.64
130.95
129.71
129.27
128.04
127.86
126.65
125.73
136
134
132
130
128
126
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


N
N

12

7.46
7.43
7.43
7.42
7.41
7.39
7.26
7.09
6.98
4.14
2.36
2.05
3.00
1.06
2.01
3.20
3.11
6.15
10
9.5
9
8.5
8
7.5
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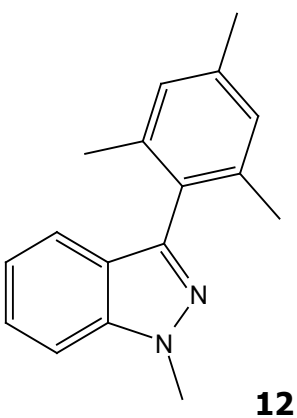
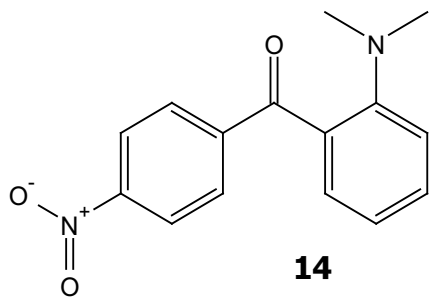
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)


N
N

12

143.97
140.81
138.34
137.93
129.18
128.34
126.28
123.59
121.35
120.35
109.14
77.65
77.23
76.81
35.68
21.39
20.57
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


O
N
O
N
O

14

8.25
8.22
7.91
7.89
7.45
7.40
7.38
7.26
7.04
7.02
6.99
6.98
6.96
2.62
1.99
2.00
1.02
1.01
1.03
1.04
6.40
10
9.5
9
8.5
8
7.5
7
6.5
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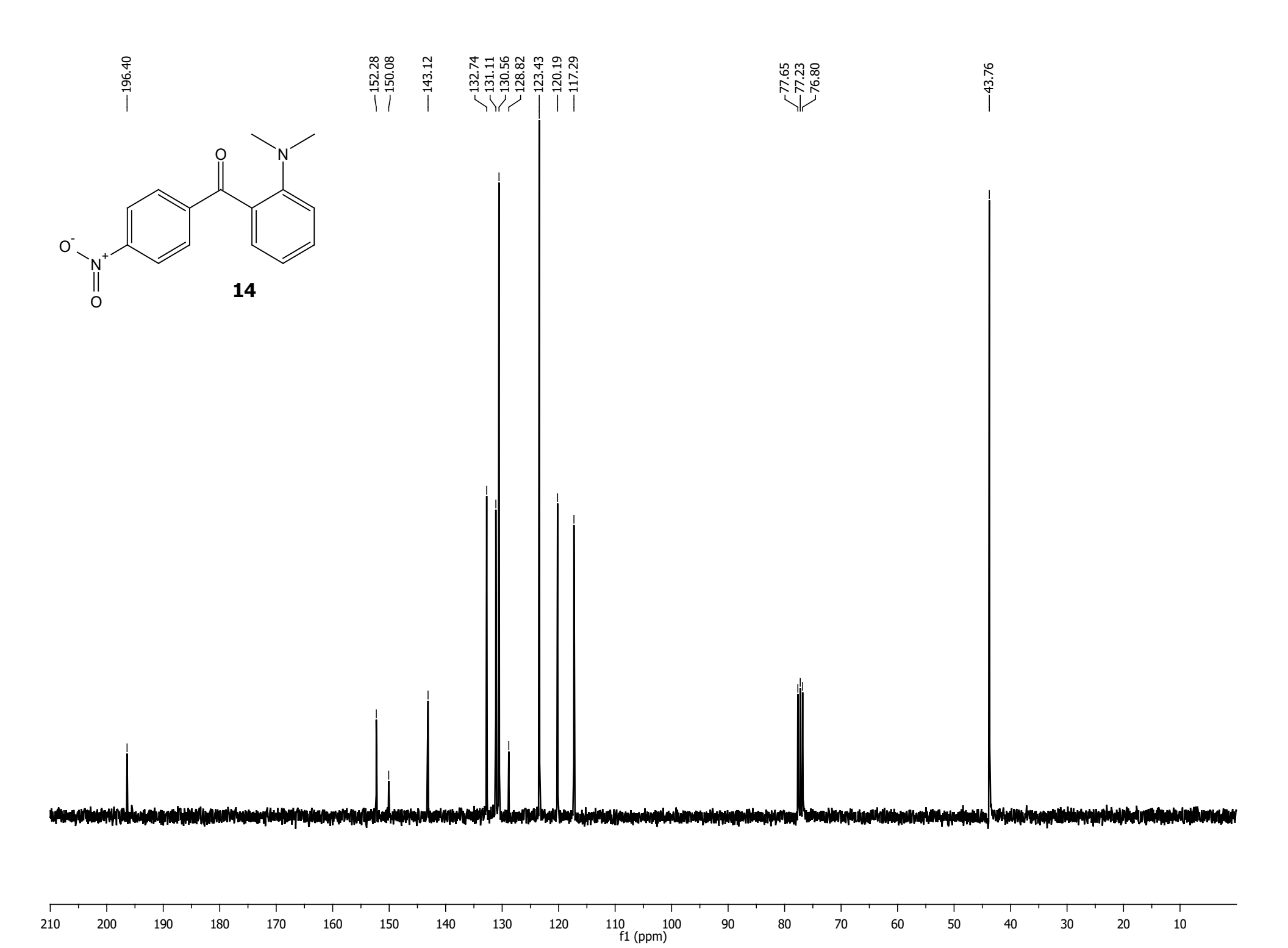
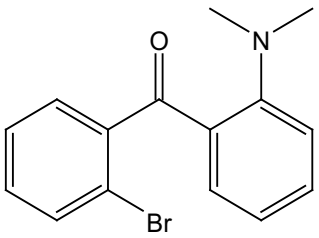
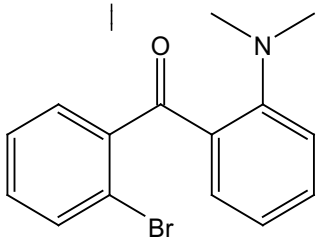
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)


196.40
152.28
150.08
143.12
132.74
131.11
130.56
128.82
123.43
120.19
117.29
77.65
77.23
76.80
43.76
O
N
O-
N+
O
14
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


O
N
Br

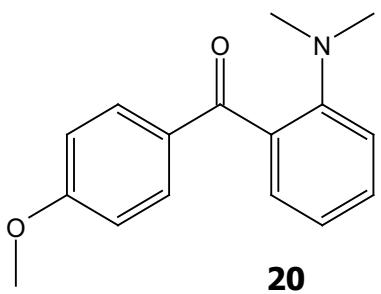
18

7.63
7.61
7.34
7.26
6.99
6.97
6.83
6.81
6.79
2.84
1.00
3.01
1.12
1.08
1.01
1.01
6.61
10
9.5
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)


O
N
Br

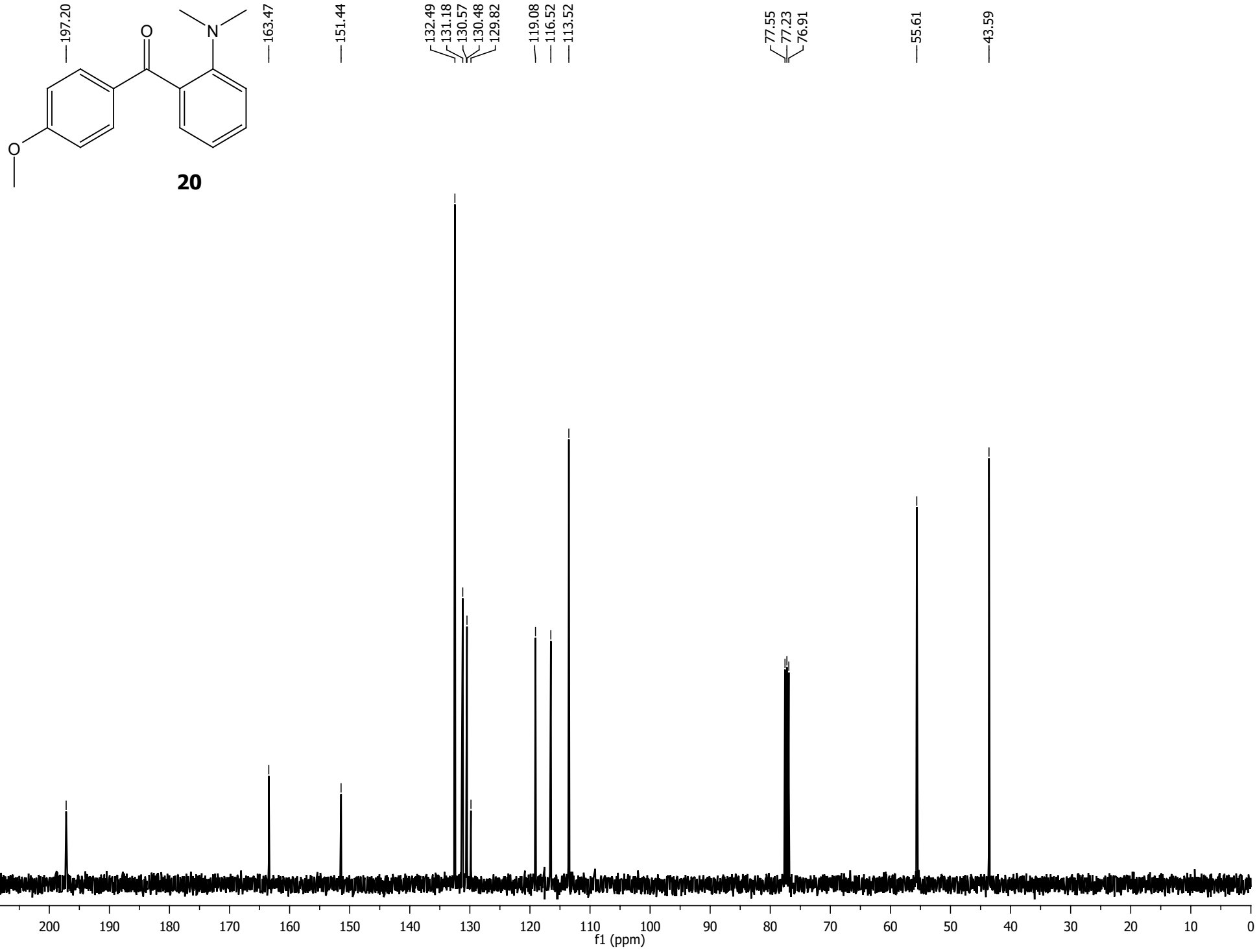
18

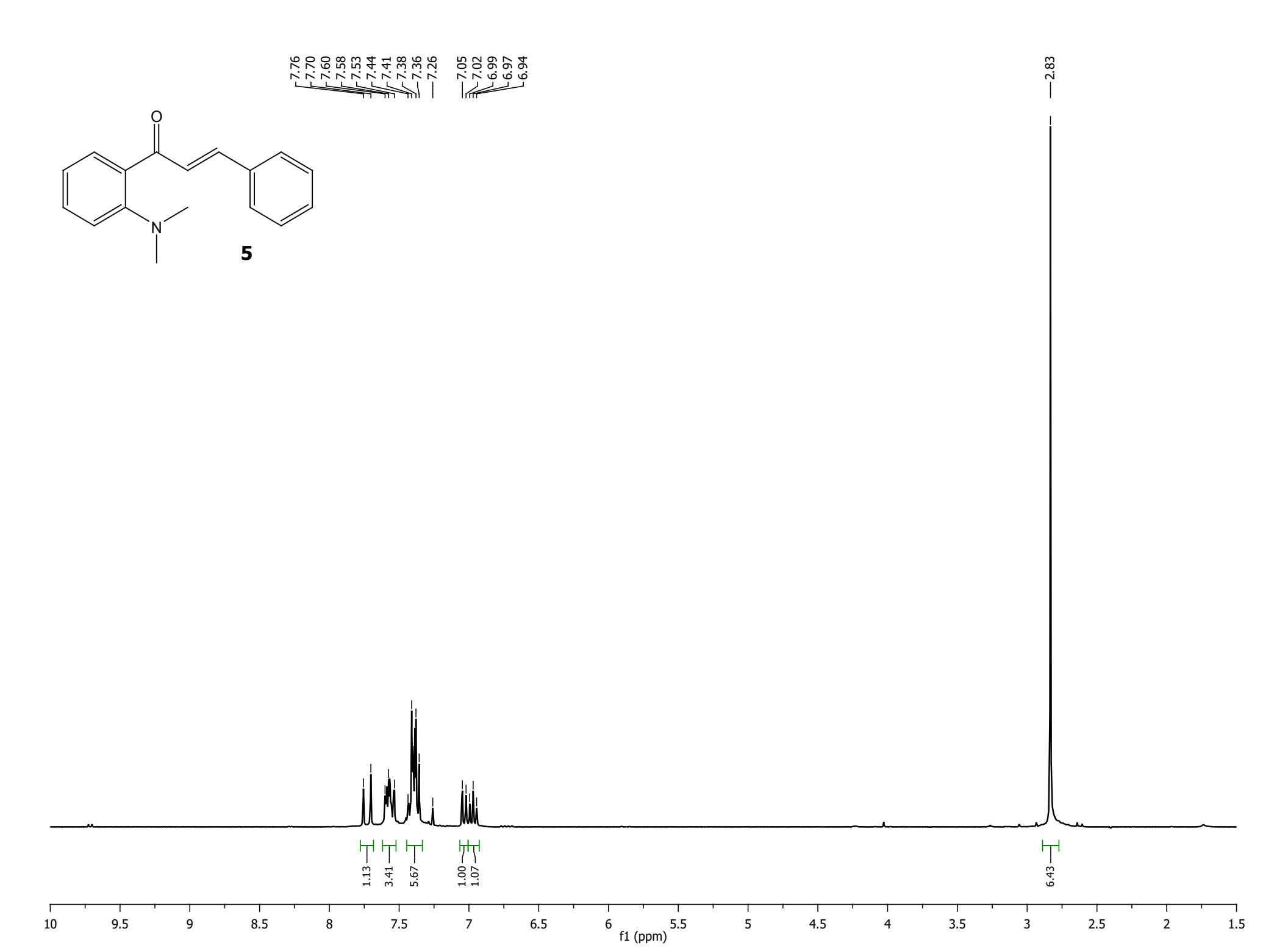
195.30
152.85
141.19
133.73
131.50
130.90
127.19
126.76
120.68
118.39
116.78
77.55
77.23
76.91
43.98
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

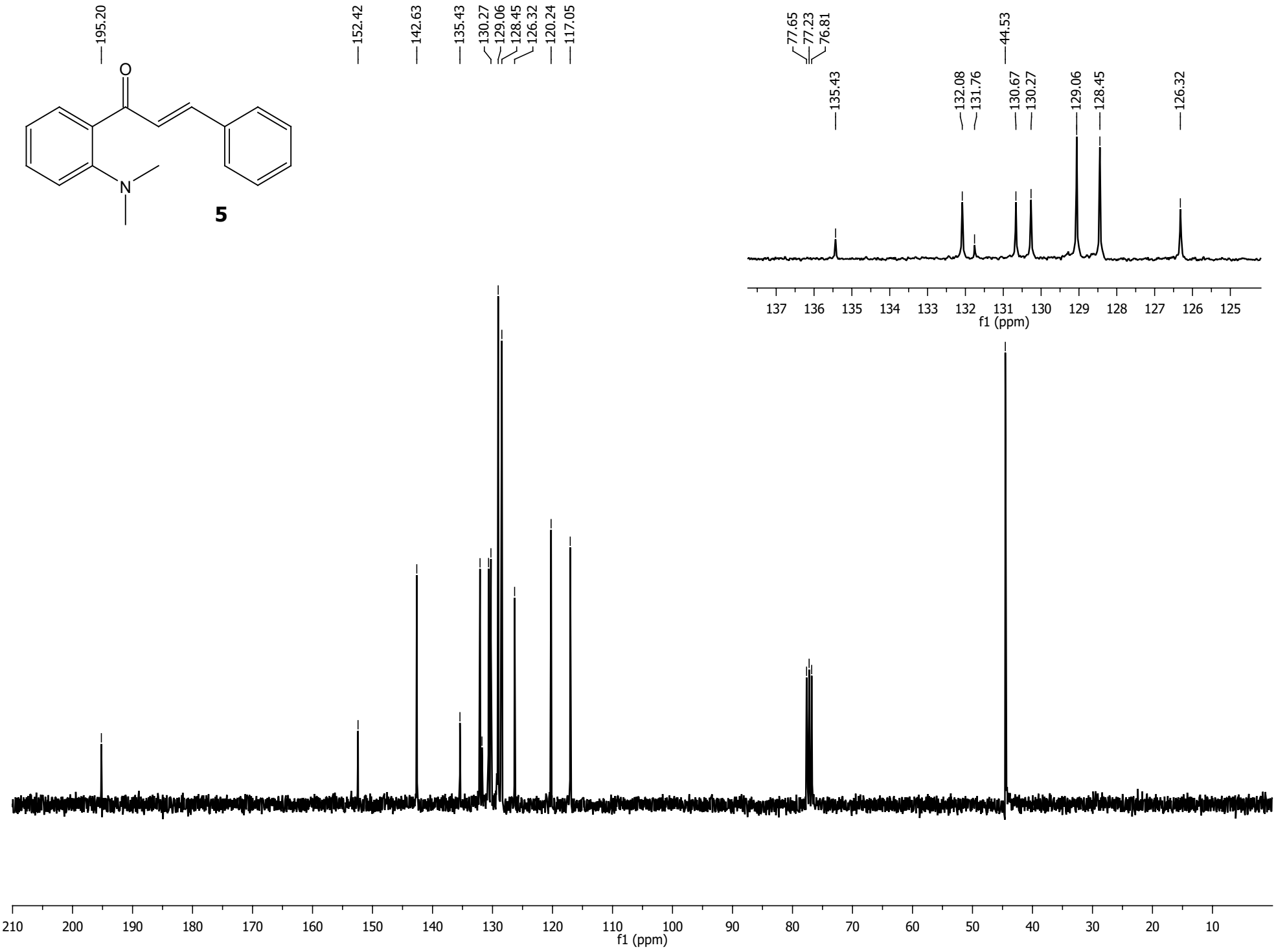

O
N
O

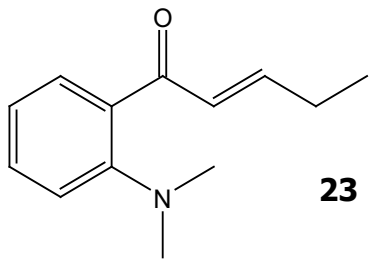
20

7.83
7.81
7.36
7.29
7.27
7.26
6.98
6.96
6.91
6.88
6.87
3.86
2.70
1.97
0.97
1.03
1.03
3.00
3.19
6.17
10
9.5
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)


197.20
163.47
151.44
132.49
131.18
130.57
130.48
129.82
119.08
116.52
113.52
77.55
77.23
76.91
55.61
43.59
O
N
O
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

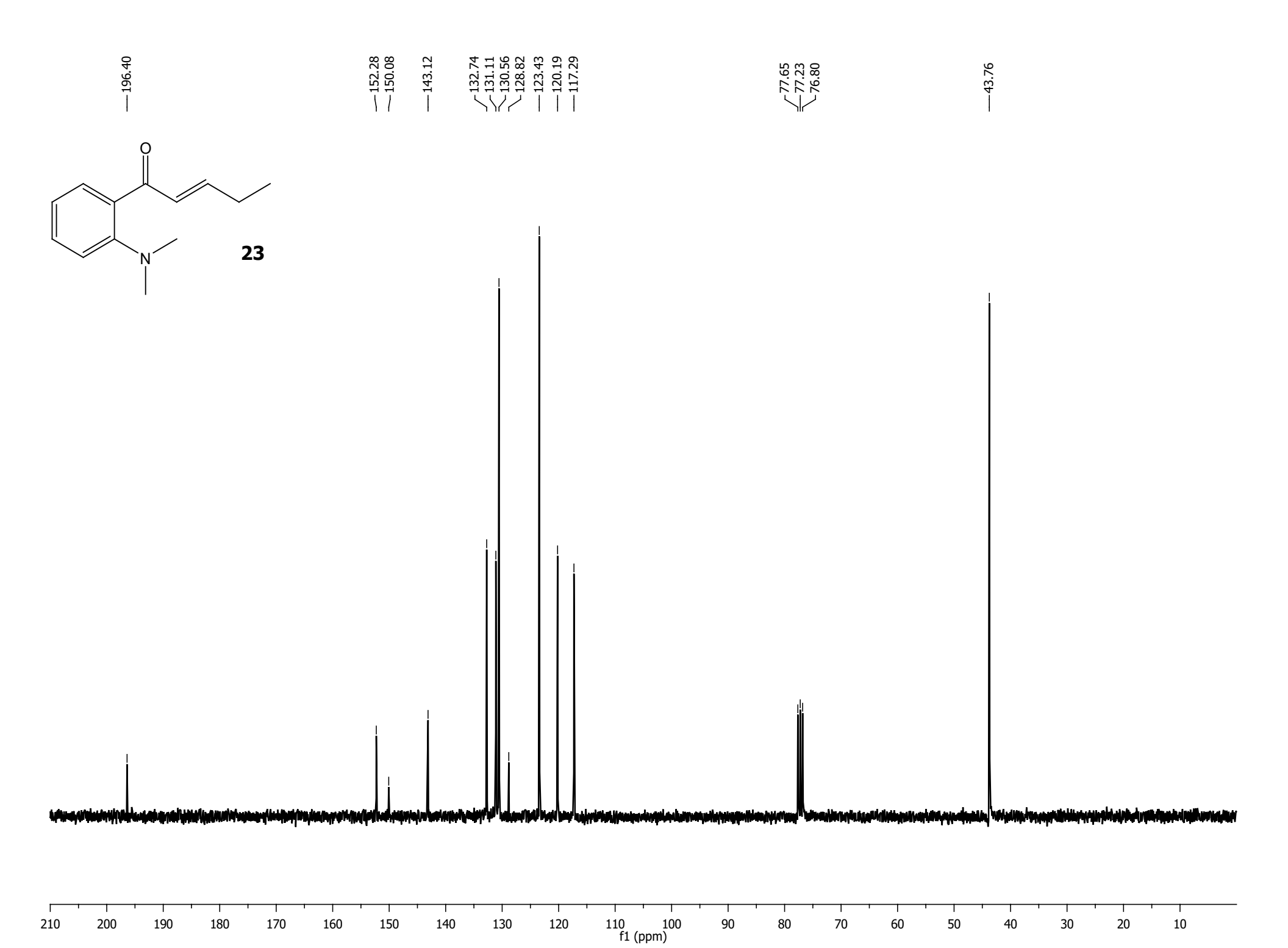

7.76
7.70
7.60
7.58
7.53
7.44
7.41
7.38
7.36
7.26
7.05
7.02
6.99
6.97
6.94
2.83
O
N
5
1.13
3.41
5.67
1.00
1.07
6.43
10
9.5
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)

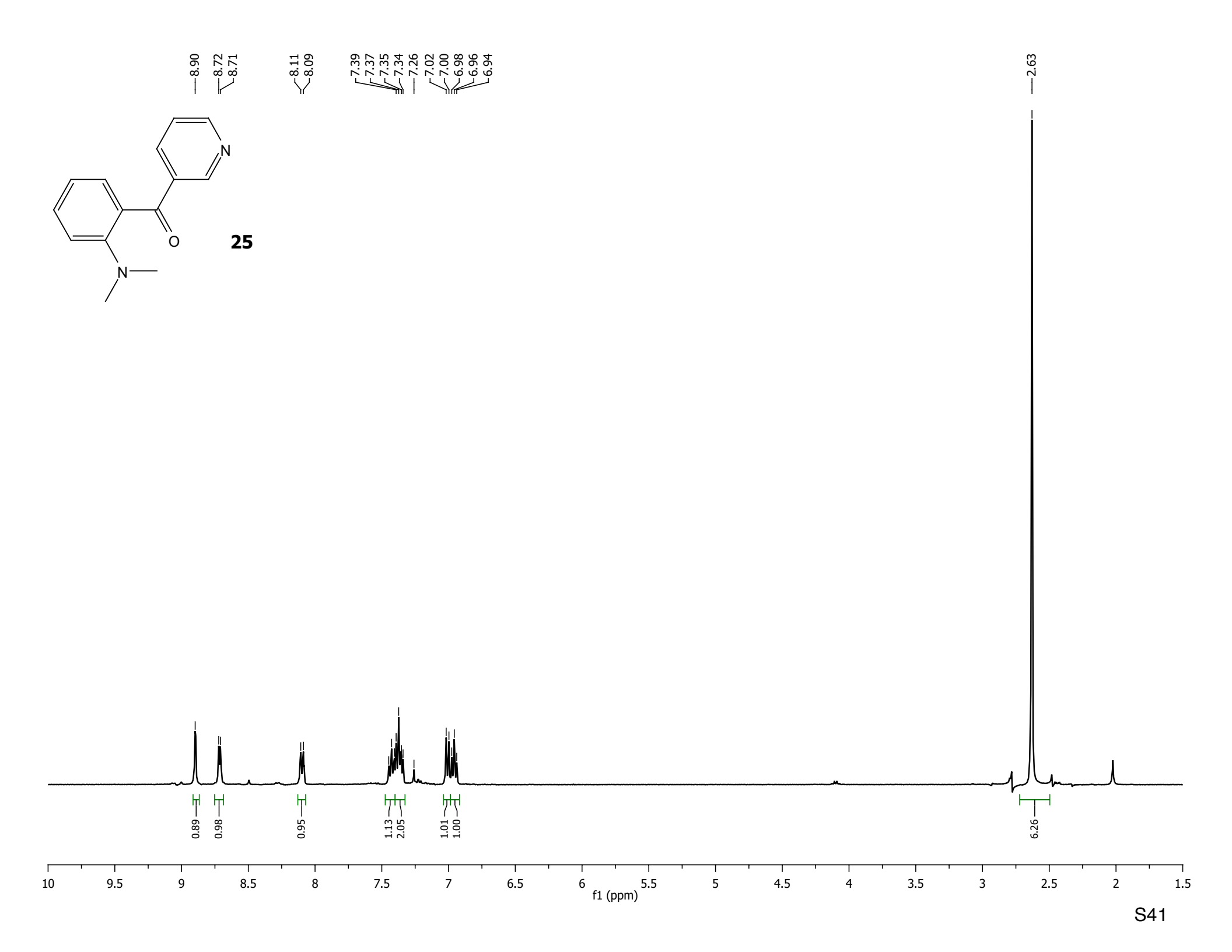

195.20
152.42
142.63
135.43
130.27
129.06
128.45
126.32
120.24
117.05
77.65
77.23
76.81
44.53
135.43
132.08
131.76
130.67
130.27
129.06
128.45
126.32
O
N
5
f1 (ppm)
f1 (ppm)

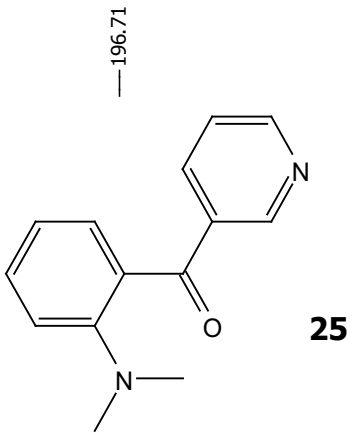

O
N

23

7.42
7.41
7.36
7.34
7.33
6.92
6.88
6.68
6.65
2.78
2.29
2.27
2.25
1.10
1.08
1.07
1.05
1.19
3.34
1.04
6.73
2.07
3.00
10
9.5
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
f1 (ppm)

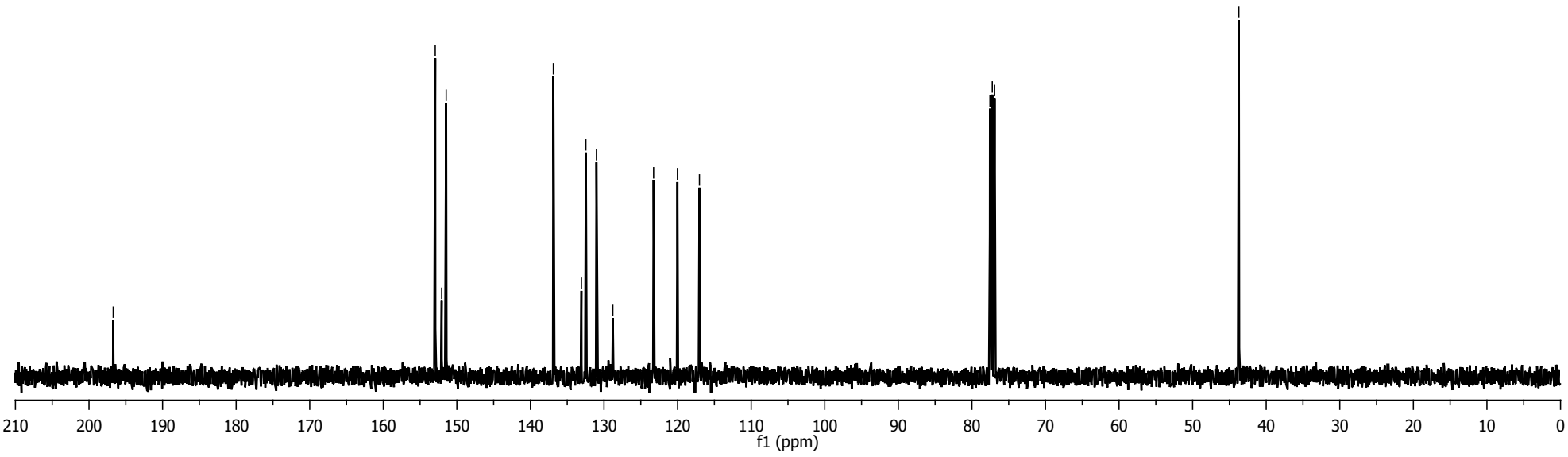

196.40
152.28
150.08
143.12
132.74
131.11
130.56
128.82
123.43
120.19
117.29
77.65
77.23
76.80
43.76
O
N
23
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

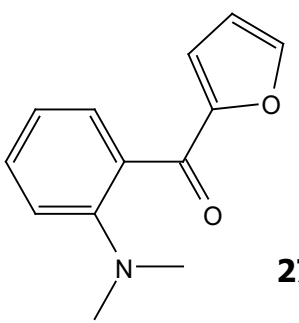

8.90
8.72
8.71
8.11
8.09
7.39
7.37
7.35
7.34
7.26
7.02
7.00
6.98
6.96
6.94
2.63
N
O
N
25
0.89
0.98
0.95
1.13
2.05
1.01
1.00
6.26
10
9.5
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)



25

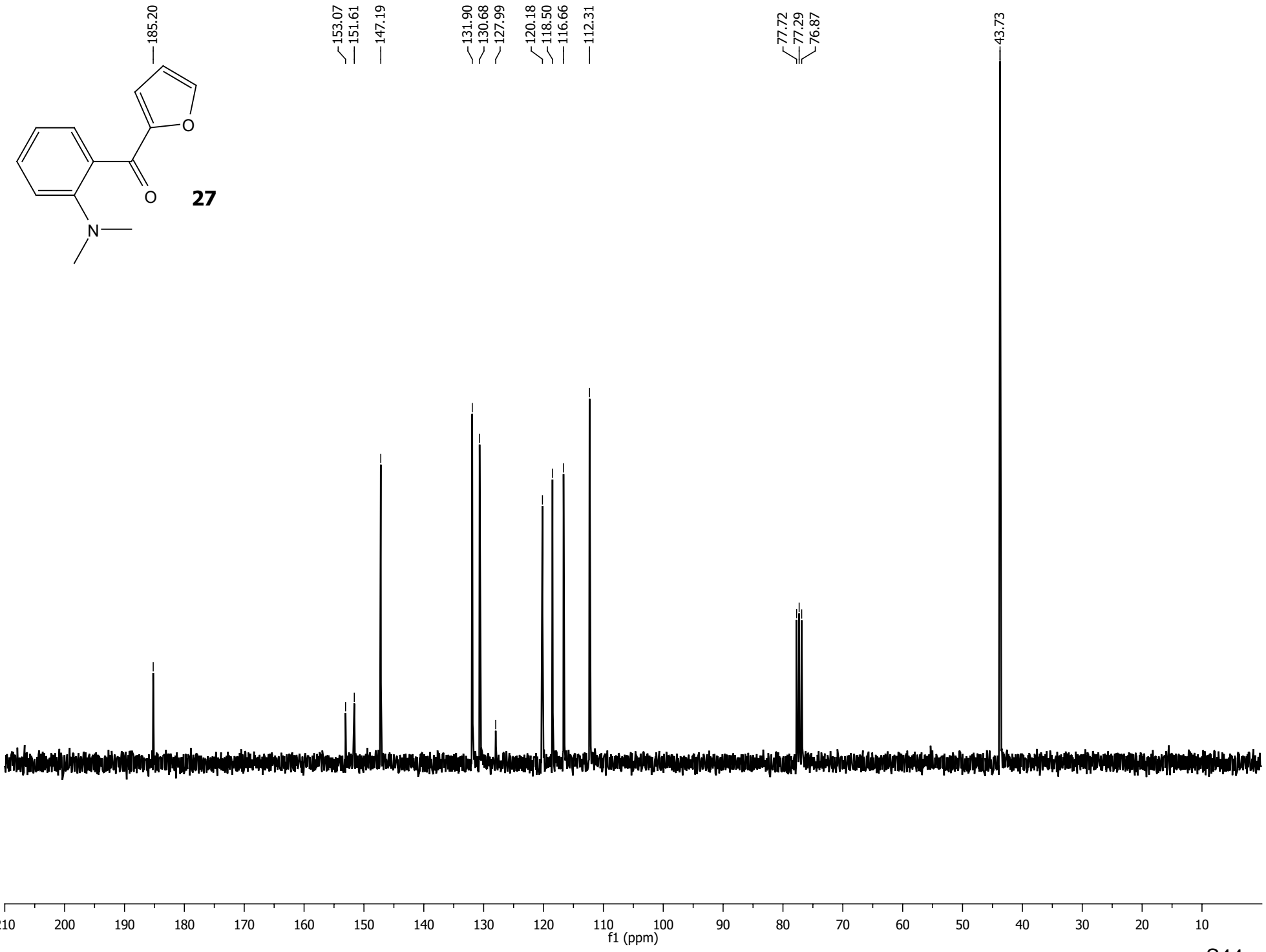
196.71
152.94
152.07
151.45
136.89
132.47
131.03
128.80
123.26
120.02
117.03
77.55
77.23
76.91
43.71

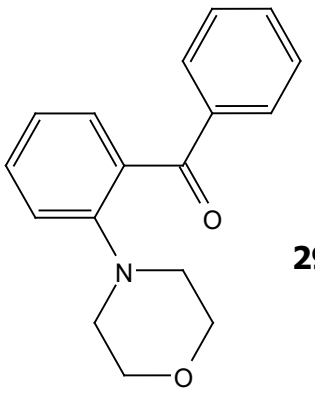




27

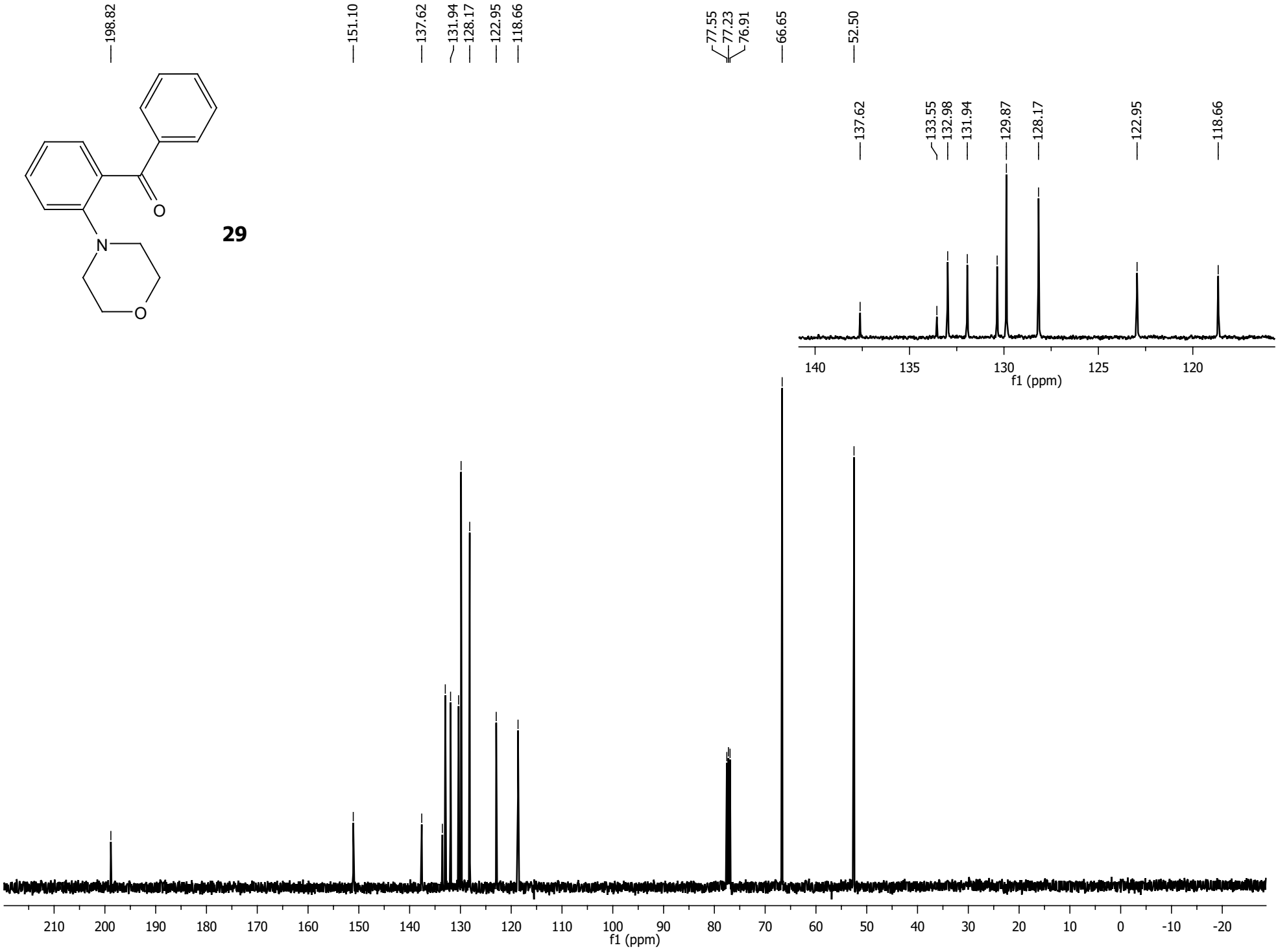
7.64
7.38
7.34
7.26
7.04
6.97
6.87
6.83
6.52
2.78
1.00
2.11
1.03
1.09
1.08
1.03
6.47
10
9.5
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)

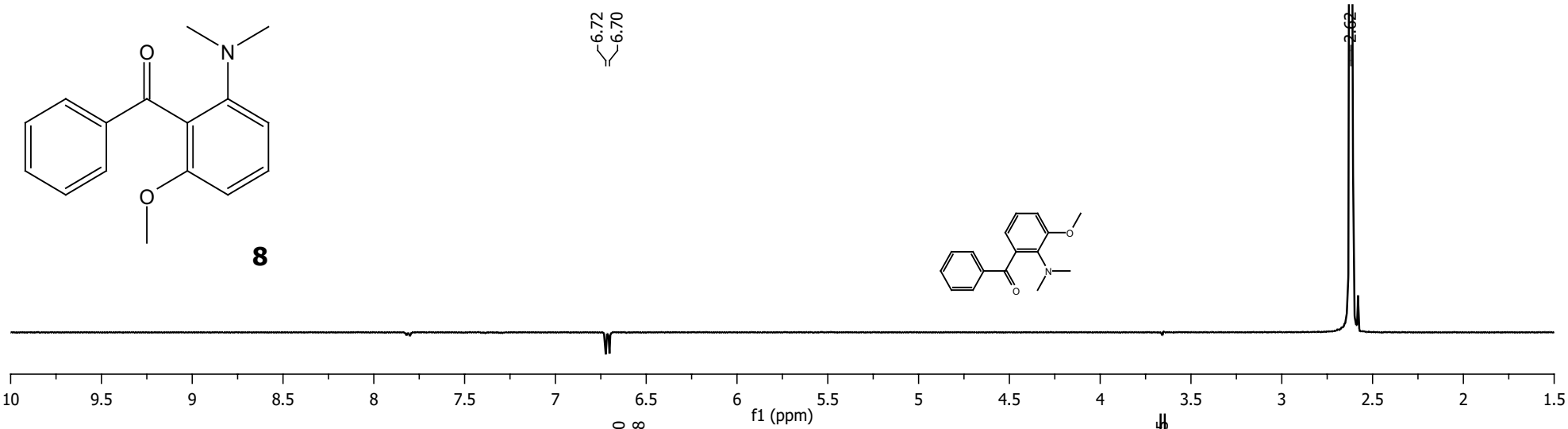

185.20
153.07
151.61
147.19
131.90
130.68
127.99
120.18
118.50
116.66
112.31
77.72
77.29
76.87
43.73
O
O
N
27
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

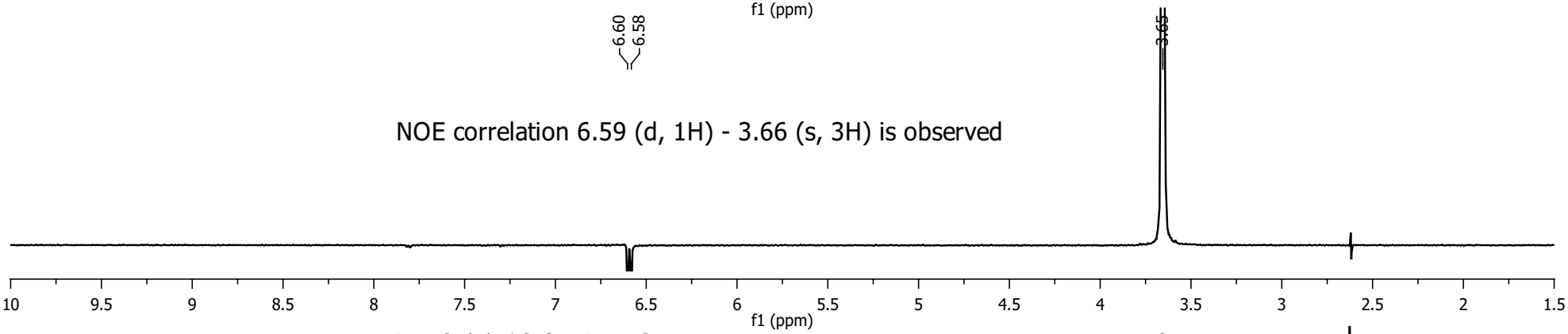

O
N
O

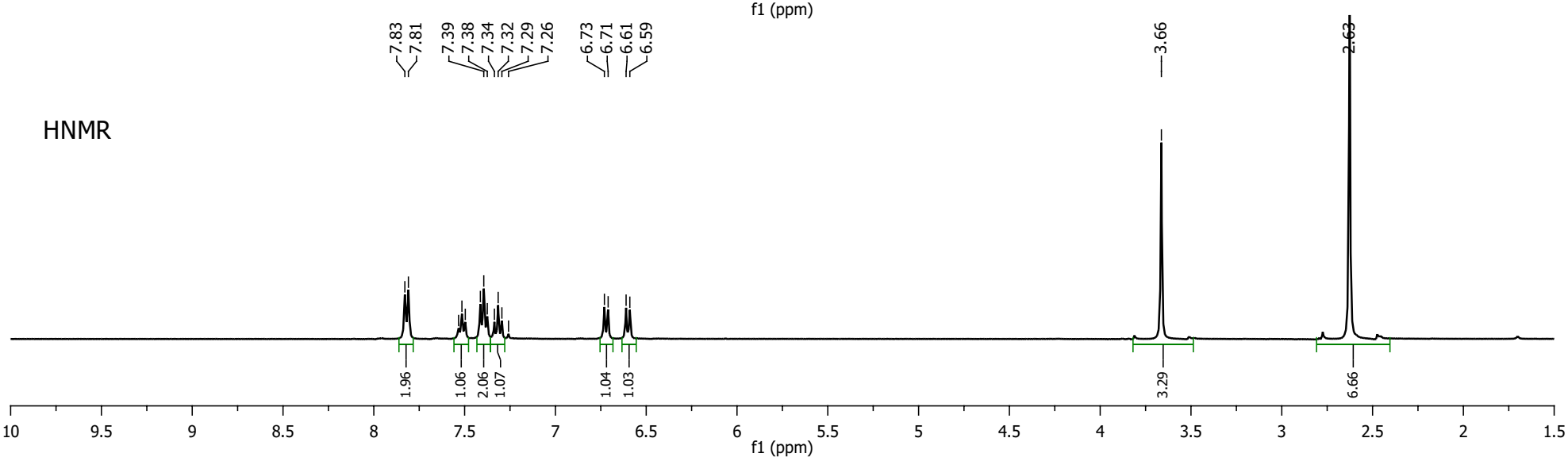
29

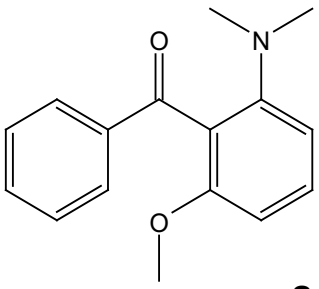
7.75
7.73
7.45
7.38
7.26
7.16
7.14
7.12
7.06
7.04
3.27
3.26
3.25
2.89
2.87
2.86
2.12
1.00
4.28
1.00
1.05
4.41
4.45
10
9.5
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)


198.82
151.10
137.62
131.94
128.17
122.95
118.66
77.55
77.23
76.91
66.65
52.50
O
N
O
29
137.62
133.55
132.98
131.94
129.87
128.17
122.95
118.66
140
135
130
125
120
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


O
N
O
8
6.72
6.70
2.62
10
9.5
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)

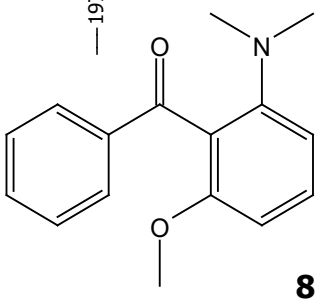

6.60
6.58
3.66
NOE correlation 6.59 (d, 1H) - 3.66 (s, 3H) is observed
10
9.5
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)


7.83
7.81
7.39
7.38
7.34
7.32
7.29
7.26
6.73
6.71
6.61
6.59
3.66
2.63
HNMR
1.96
1.06
2.06
1.07
1.04
1.03
3.29
6.66
10
9.5
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)


O
N
O

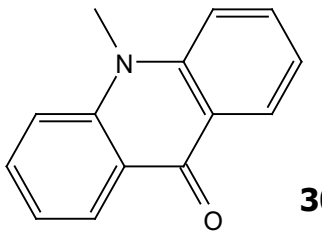
8

7.83
7.81
7.39
7.38
7.34
7.32
7.29
7.26
6.73
6.71
6.61
6.59
3.66
2.63
1.96
1.06
2.06
1.07
1.04
1.03
3.29
6.66
10
9.5
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
f1 (ppm)



8

197.53
157.76
152.93
138.12
132.97
129.40
128.38
121.93
111.12
104.52
77.55
77.23
76.91
55.92
44.53
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


N
O

30

8.54
8.52
7.70
7.68
7.66
7.46
7.27
7.26
7.24
3.83
2.00
2.13
2.17
2.31
3.26
10
9.5
9
8.5
8
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1.5
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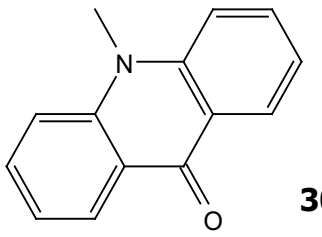
N
O

30

178.22
142.66
133.91
127.85
122.62
121.36
114.90
77.55
77.23
76.91
33.77
210
200
190
180
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120
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90
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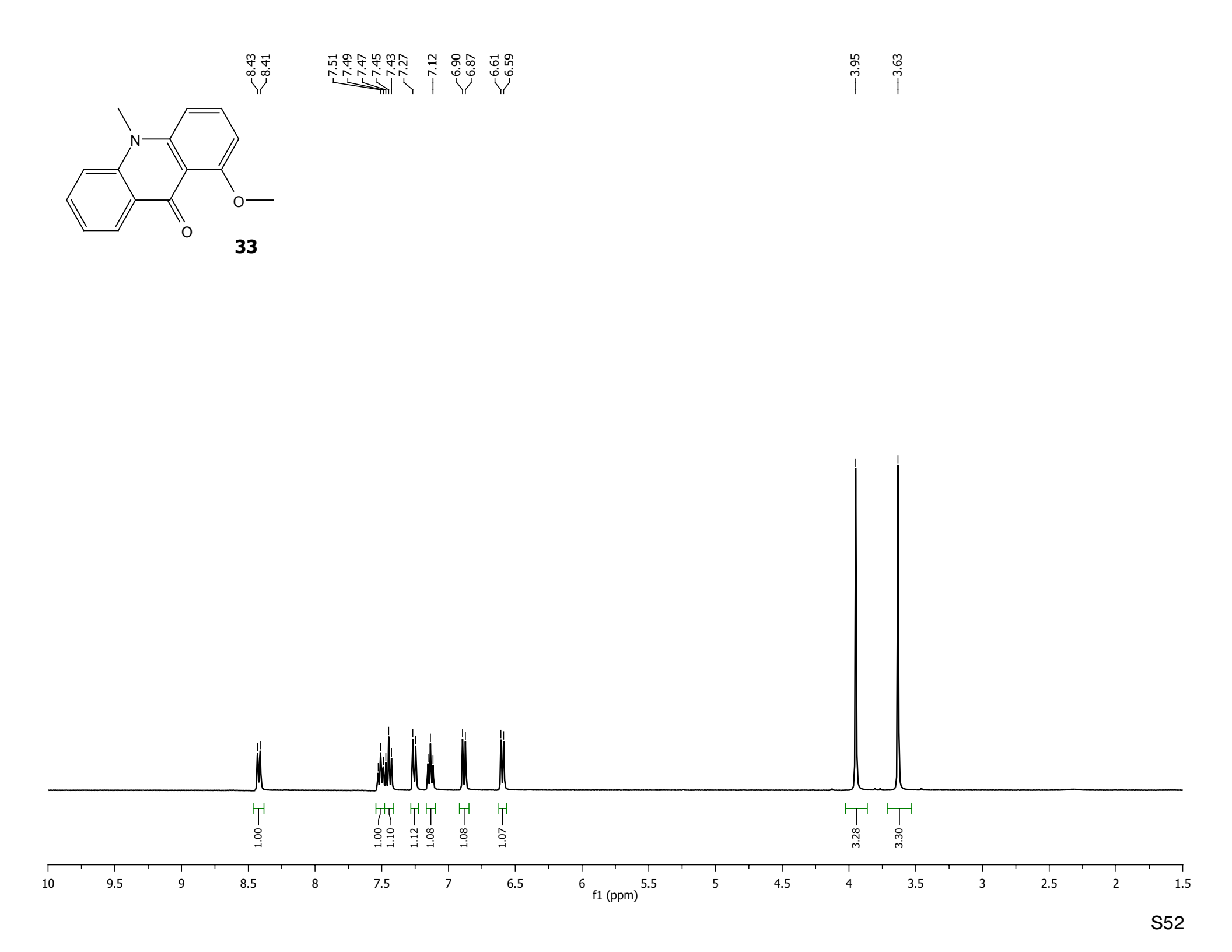
f1 (ppm)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7.49
7.47
7.45
7.43
7.27
7.12
6.90
6.87
6.61
6.59
3.95
3.63
N
O
O
33
1.00
1.00
1.10
1.12
1.08
1.08
1.07
3.28
3.30
10
9.5
9
8.5
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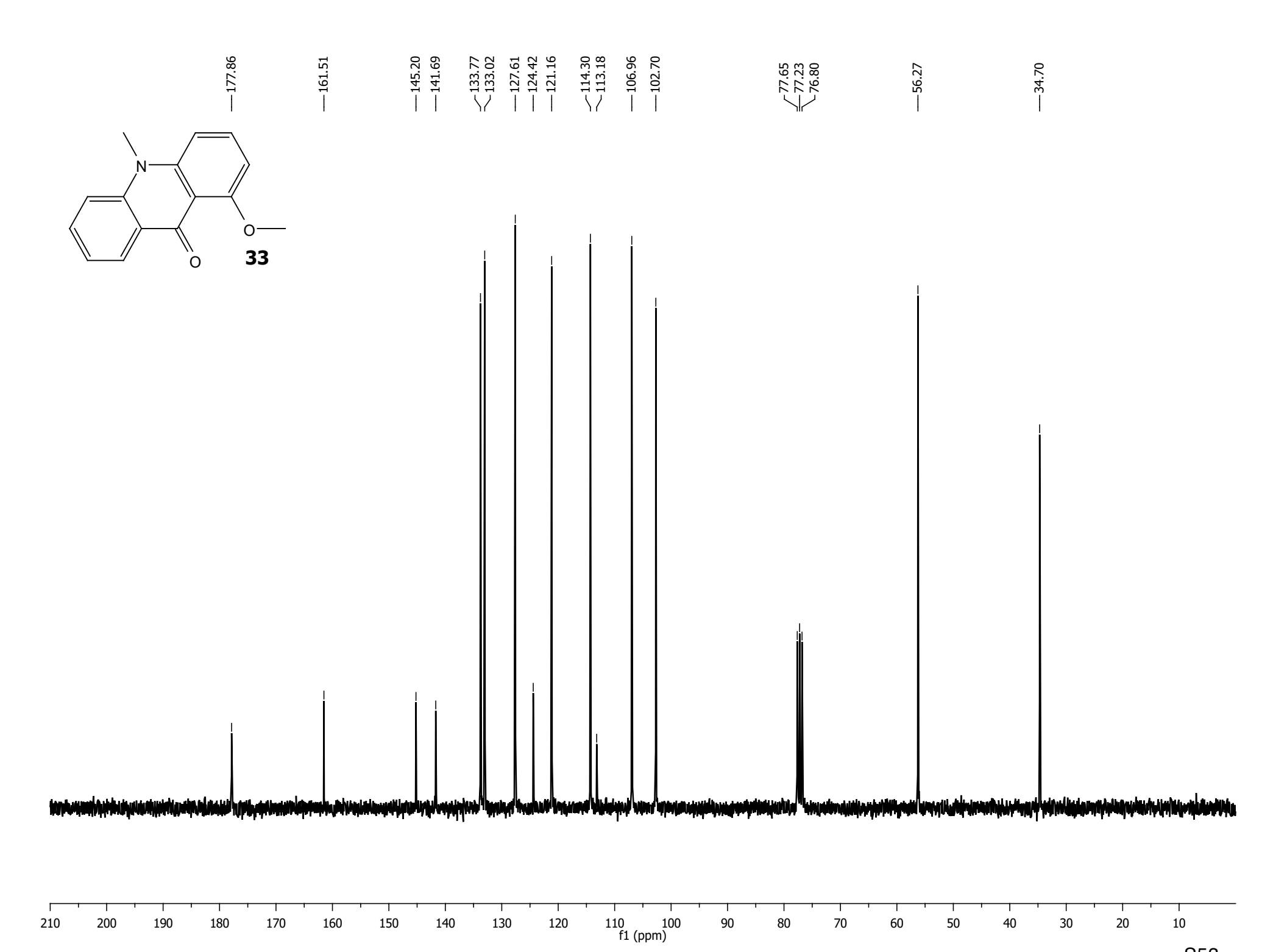
2.5
2
1.5
f1 (ppm)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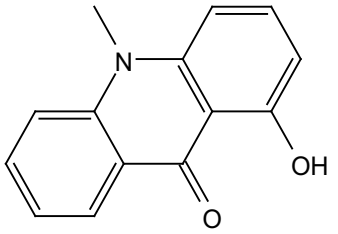
161.51
145.20
141.69
133.77
133.02
127.61
124.42
121.16
114.30
113.18
106.96
102.70
77.65
77.23
76.80
56.27
34.70
N
O
O
33
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


N
OH
O

34

8.31
8.29
7.66
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7.62
7.37
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7.18
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6.71
6.57
6.55
3.71
1.00
1.07
1.09
1.06
1.06
1.06
1.01
3.29
10
9.5
9
8.5
8
7.5
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6
5.5
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4.5
4
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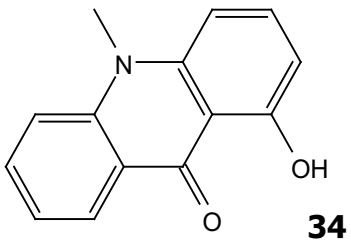
3
2.5
2
1.5
f1 (ppm)


N
OH
O

34

182.05
163.53
143.24
142.22
136.00
134.51
126.64
121.52
120.86
114.80
107.60
103.79
77.55
77.23
76.91
34.20
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)