Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Solvent-controlled Chemoselective *N*-dealkylation-*N*-Nitrosation or *C*-Nitration of *N*-Alkyl Anilines with *Tert*-butyl Nitrite

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1. General Information

TBN was purchased from commercial source and used without further purification. Anhydrous solvents were obtained using standard drying techniques. Commercial grade reagents were used without further purification unless stated otherwise. Flash chromatography was performed on 200-300 mesh silica gel with the indicated solvent systems. ^{1}H NMR were recorded on a Bruker 400 (400 MHz) spectrometer and chemical shifts are reported in ppm down field from TMS, using TMS (0.00 ppm) or residual chloroform (7.26 ppm) as an internal standard. Data are reported as: (s = singlet, br = broad, d = doublet, t = triplet, q = quartet, quint = quintuplet, hept = heptalet, m = multiplet; *J* = coupling constant in Hz, integration.). ^{13}C NMR spectra were recorded on a Bruker 400 (100 MHz) spectrometer, using proton decoupling unless otherwise noted. Chemical shifts are reported in ppm down field from TMS, using the central resonance of $CDCl_3$ (77.00 ppm) as the internal standard. HRMS were recorded by using Waters Xevo G2-XS QTof Benchtop Mass Spectrometer.

2. General Experimental Procedure

2.1 General Procedure for *N*-dealkylation-*N*-Nitrosation of *N*-Alkyl Anilines in *t*-BuOH

N-Alkyl anilines (1.0 equiv., 1.0 mmol) were dissolved in 2 mL *t*-BuOH and then *t*-BuONO (1.5 equiv., 178 uL) was added. The reaction mixtures were stirred at 60 ℃ in air. After certain time of the reaction, determined by TLC, the solution was concentrated in vacuo. The crude residues were purified by column chromatography using ethyl acetate /hexane mixture to obtain corresponding products (1**b**-21**b**).

2.2 General Procedure for *C*-Nitration of *N*-Alkyl Anilines in H_2O

N-Alkyl anilines (1.0 equiv., 1.0 mmol) were dissolved in 2 mL H_2O and then *t*-BuONO (1.5 equiv., 178 uL) was added. The reaction mixtures were stirred at 30-60 ℃ in air. After certain time of the reaction, determined by TLC, the solution was concentrated in vacuo. The crude residues were purified by column chromatography using ethyl acetate/hexane mixture to obtain corresponding products (1**c**-13**c**).

2.3 General Procedure for *N*-dealkylation-*N*-Nitrosation and *C*-Nitration of *N*-Alkyl Anilines in CH_3CN

N-Alkyl anilines (1.0 equiv., 1.0 mmol) were dissolved in 2 mL CH_3CN and then *t*-BuONO (4.0 equiv., 475 uL) was added. The reaction mixtures were stirred at 30-60 ℃ in air. After certain time of the reaction, determined by TLC, the solution was concentrated in vacuo. The crude residues were purified by column chromatography using ethyl acetate/hexane mixture to obtain corresponding products (1**d**-4**d**).

2.4 General Procedure for the Denitrosation Followed by Reduction of Nitro Group in *N*-Nitroso-*N*-Alkyl Nitroaniline

According to Kandasamy's synthesis method[1]. *N*-Nitrosamine (1 equiv., 1.0 mmol) and zinc dust (4 equiv., 4.0 mmol) was stirred in MeOH (4.5 mL) at 50 ℃ in oil-bath in Ar condition. Then acetic acid (3 mL) was added. The reaction was allowed to stir for 12 h at the same temperature. After completion, the reaction mixture was cooled to room temperature and filtered through Celite. The filtrated (methanol solution) was evaporated, diluted with chloroform (50 mL), and washed with saturated sodium bicarbonate solution. The organic layer was dried over anhydrous sodium sulfate, concentrated, and subjected for column chromatography (SiO_2, eluent: hexane/ethyl acetate) to obtain corresponding pure *N*-substituted-*o*-phenylenediamines (1**f**).

2.5 General Procedure for the Denitrosation of *N*-nitrosamine

According to Kandasamy's synthesis method[2]. *N*-nitrosamine (1.0 equiv., 0.92 mmol) was allowed to stir in CH_2Cl_2 (3 mL) approximately for 2 min at room temperature to which iodine (0.3 equiv., 72 mg) and triethylsilane (1.5 equiv., 223 uL) was added. The reaction was further allowed to stir for 6.5 h and the progress of the reaction was monitored by TLC. After completion, the reaction mixture filtered through Celite. Then the reaction mixture was dried over anhydrous sodium sulfate, concentrated, and subjected for column chromatography (SiO_2, eluent: hexane/ethyl acetate) to obtain corresponding pure substituted secondary amines (1**e**).

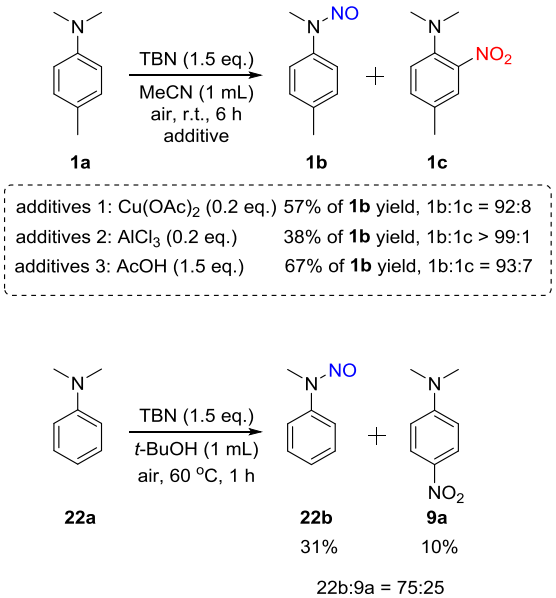
According to Kandasamy's synthesis method[2]. *N*-nitrosamine (1.0 equiv., 0.35 mmol) was allowed to stir in CH_2Cl_2 (3 mL) approximately for 2 min at room temperature to which iodine (0.3 equiv., 126 mg) and triethylsilane (1.5 equiv., 100 uL) was added. The reaction was further allowed to stir for 12 h and the progress of the reaction was monitored by TLC. After completion, the reaction mixture filtered through Celite.

Then the reaction mixture was dried over anhydrous sodium sulfate, concentrated, and subjected for column chromatography (SiO_2, eluent: hexane/ethyl acetate) to obtain corresponding pure substituted secondary amines (6**i**).

2.6 General Procedure for the Reduction of *N*- nitrosamines

According to Kandasamy's synthesis method[3]. *N*-methyl-*N*-(*p*-tolyl) nitrous amide (1.0 equiv., 0.733 mmol) and thiourea dioxide (TDO, 2 equiv., 1.5 mmol) was stired in MeOH (2 mL) approximately for 5 min at 50 ℃ in Ar condition. Then aqueous solution of sodium hydroxide (1 M, 10 equiv.) was added. The reaction was allowed to stir for 12 h and the progress of the reaction was monitored by TLC. After completion, the reaction mixture was diluted with chloroform and washed with water. The organic layer was dried over anhydrous sodium sulphate, concentrated and subjected for column chromatography (SiO_2: ethyl acetate/hexane) to obtain corresponding pure substituted 1-methyl-1-(*p*-tolyl) hydrazine (1**g**).

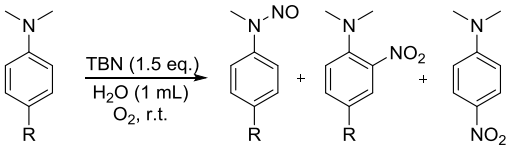
3. Supplementary Data



Scheme S1 Supplementary experiment data of *N*-dealkylation-*N*-nitrosation of *N*-dimethyl anilines

The supplementary experiment data of *N*-dealkylation-*N*-nitrosation of *N*-dimethyl anilines are shown in Scheme S1. Additives such as $Cu(OAc)_2$, $AlCl_3$ or AcOH had a negative effect on the reaction. The yields are less than 70%, even the selectivities are higher than the reaction without additives. Based on the optimized reaction conditions

(*N*-dealkylation-*N*-nitrosation: Table 1, entry 12), the aniline without a substitute on *para* position of the phenyl ring **22a** was surveyed in *t*-BuOH. The reaction provides 31% yield of nitrosation product **22b** and 10% yield of *N*, *N*-dimethyl-4-nitroaniline (**9a)**.



	a	b	c	9a
R =	Br (5a)	11%	47%	24%
	CHO (11a)	11%	54%	34%
	COMe (12a)	22%	32%	44%

Scheme S2 Formation of *N*,*N*-dimethyl-4-nitroaniline **9a**

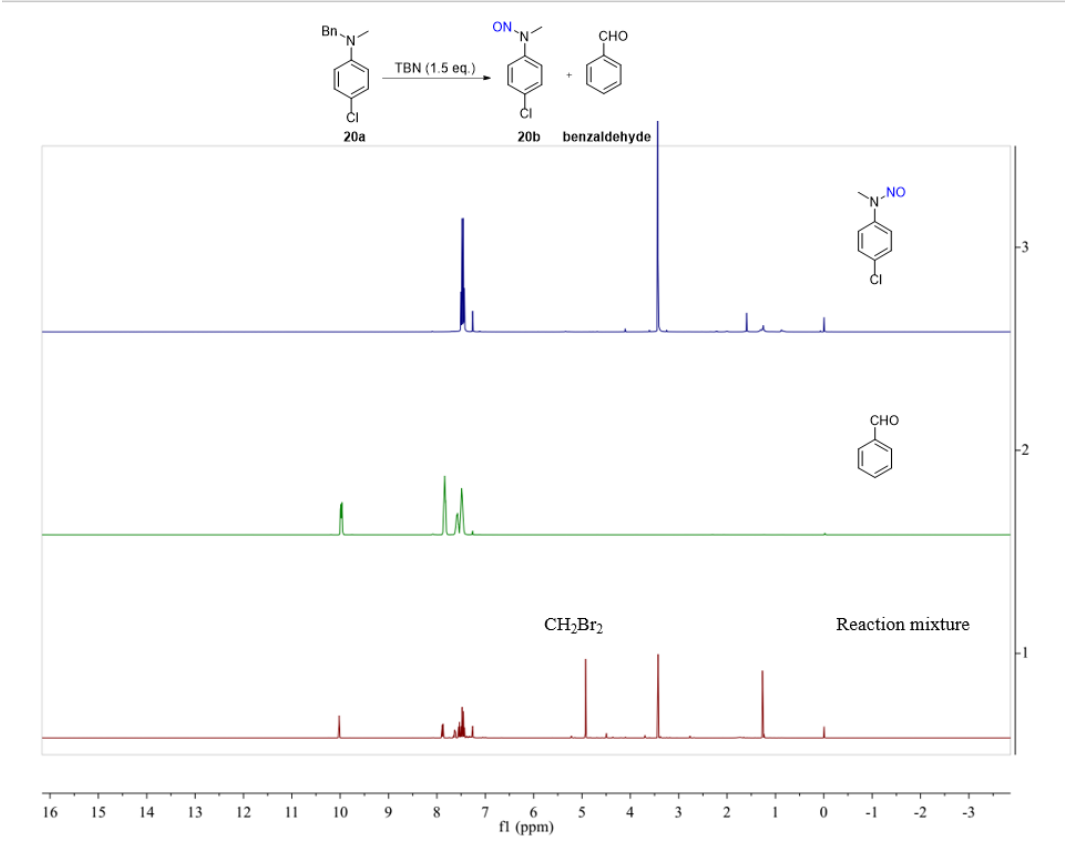
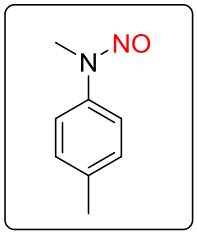


Figure S1 Mechanism experiments detected by ^{1}H NMR

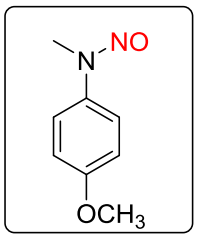
To understand of the reaction mechanism, a control experiments detected by ^{1}HNMR were carried out under the standard conditions (Figure S1). When the *N*-benzyl-*N*-(4-chlorophenyl)nitrous amide **20a** was used as substrate, the benzaldehyde was detected by ^{1}H NMR, which suggests that C–N bond may be cleaved

through the decomposition of the iminium intermediate by affording the corresponding aldehyde.

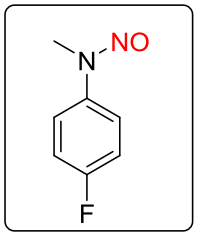
4. Analytical Data for Compounds



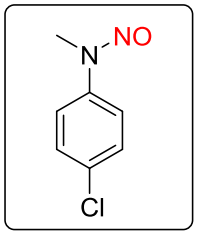
***N*-methyl-*N*-(*p*-tolyl)nitrous amide (1b)**: Prepared according to the general procedure. 126.1 mg, 84% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.41 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 2H), 3.44 (s, 3H), 2.40 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 139.9, 137.3, 130.0, 119.3, 31.7, 20.9. **HRMS** (ESI): calcd for $C_8H_{11}N_2O$ $(M+H)^+$: 151.0871. Found: 151.0867.



***N*-(4-methoxyphenyl)-*N*-methylnitrous amide (2b):** Prepared according to the general procedure. 156.2 mg, 94% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.44 (d, *J* = 9.0 Hz, 2H), 7.00 (d, *J* = 9.0 Hz, 2H), 3.86 (s, 3H), 3.45 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 158.9, 135.7, 121.1, 114.6, 55.6, 32.2. **HRMS** (ESI): calcd for $C_8H_{11}N_2O_2$ $(M+H)^+$: 167.0821. Found: 167.0817.

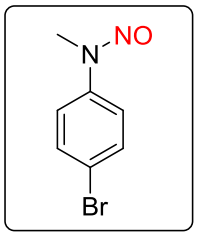


***N*-(4-fluorophenyl)-*N*-methylnitrous amide (3b):** Prepared according to the general procedure. 106.1 mg, 76% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.52 – 7.49 (m, 2H), 7.20 – 7.16 (m, 2H), 3.45 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 162.9, 160.4, 138.61, 138.58, 121.1, 121.0, 116.4, 116.2, 31.8. **HRMS** (ESI): calcd for $C_7H_8FN_2O$ $(M+H)^+$: 155.0621. Found: 155.0616.

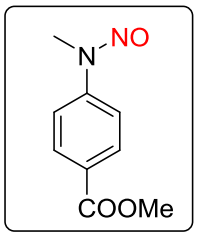


***N*-(4-chlorophenyl)-*N*-methylnitrous amide (4b):** Prepared according to the general procedure. 121.7 mg, 80% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.50 (d, *J* = 9.1 Hz, 2H), 7.45 (d, *J* = 9.1

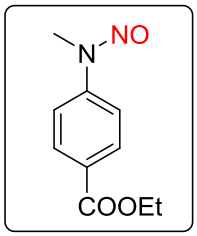
Hz, 2H), 3.44 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 140.8, 132.9, 129.6, 120.1, 31.2. **HRMS** (ESI): calcd for $C_7H_8ClN_2O$ $(M+H)^+$: 171.0325. Found: 171.0322.



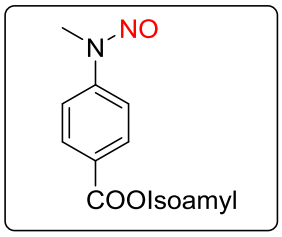
***N*-(4-bromophenyl)-*N*-methylnitrous amide (5b)[4]:** Prepared according to the general procedure. 154.8 mg, 72% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.60 (d, *J* = 9.0 Hz, 2H), 7.44 (d, *J* = 9.0 Hz, 2H), 3.43 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 141.3, 132.5, 120.6, 120.3, 31.1.



methyl 4-(methyl(nitroso)amino)benzoate (6b): Prepared according to the general procedure. 170.7 mg, 88% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.14 (d, *J* = 8.9 Hz, 2H), 7.64 (d, *J* = 8.8 Hz, 2H), 3.94 (s, 3H), 3.45 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 166.2, 145.6, 131.0, 128.5, 117.8, 52.3, 30.5. **HRMS** (ESI): calcd for $C_9H_{11}N_2O_3$ $(M+H)^+$: 195.0770. Found: 195.0765.

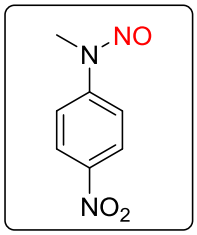


ethyl 4-(methyl(nitroso)amino)benzoate (7b): Prepared according to the general procedure. 166.4 mg, 80% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.15 (d, *J* = 8.9 Hz, 2H), 7.63 (d, *J* = 8.9 Hz, 2H), 4.40 (q, *J* = 7.1 Hz, 2H), 3.45 (s, 3H), 1.41 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 165.7, 145.5, 131.0, 128.9, 117.8, 61.2, 30.5, 14.3. **HRMS** (ESI): calcd for $C_{10}H_{13}N_2O_3$ $(M+H)^+$: 209.0926. Found: 209.0922.

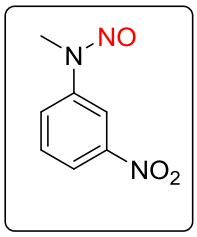


isopentyl 4-(methyl(nitroso)amino)benzoate (8b): Prepared according to the general procedure. 232.6 mg, 93% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.12 (d, *J* = 8.9 Hz, 2H), 7.62 (d, *J* = 8.9 Hz, 2H), 4.36 (t, *J* = 6.8 Hz, 2H), 3.44 (s, 3H), 1.84 – 1.74 (m, 1H), 1.67 (q, *J* = 6.8 Hz, 2H), 0.97 (d, *J* = 6.6 Hz, 6H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 165.7, 145.5,130.9, 128.8, 117.8, 63.9,

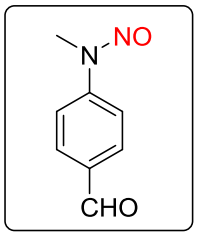
37.4, 30.5, 25.2, 22.5. **HRMS** (ESI): calcd for $C_{13}H_{19}N_2O_3$ $(M+H)^+$: 251.1396. Found: 251.1394.



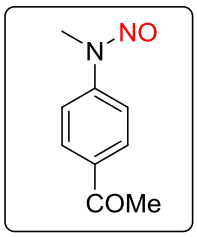
***N*-methyl-*N*-(4-nitrophenyl)nitrous amide (9b):** Prepared according to the general procedure. 152.3 mg, 85% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.34 (d, *J* = 9.2 Hz, 2H), 7.76 (d, *J* = 9.2 Hz, 2H), 3.47 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 147.0, 145.9, 125.2, 117.8, 30.1. **HRMS** (ESI): calcd for $C_7H_8N_3O_3$ $(M+H)^+$: 182.0566. Found: 182.0571.



***N*-methyl-*N*-(3-nitrophenyl)nitrous amide (10b):** Prepared according to the general procedure. 146.6 mg, 81% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.39 (t, *J* = 2.2 Hz, 1H), 8.21 (ddd, *J* = 8.3, 2.3, 0.9 Hz, 1H), 7.99 (ddd, *J* = 8.3, 2.2, 0.9 Hz, 1H), 7.68 (t, *J* = 8.2 Hz, 1H), 3.50 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 148.9, 143.3, 130.5, 123.9, 121.4, 113.1, 30.6. **HRMS** (ESI): calcd for $C_7H_8N_3O_3$ $(M+H)^+$: 182.0566. Found: 182.0570.

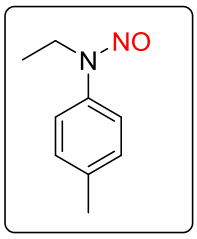


***N*-(4-formylphenyl)-*N*-methylnitrous amide (11b):** Prepared according to the general procedure. 148.3 mg, 91% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 10.01 (s, 1H), 7.97 (d, *J* = 8.6 Hz, 2H), 7.73 (d, *J* = 8.6 Hz, 2H), 3.45 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 190.9, 146.7, 134.5, 131.1, 118.2, 30.3. **HRMS** (ESI): calcd for $C_8H_9N_2O_2$ $(M+H)^+$: 165.0664. Found: 165.0659.

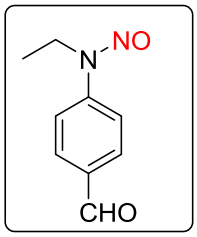


***N*-(4-acetylphenyl)-*N*-methylnitrous amide (12b):** Prepared according to the general procedure. 148.7 mg, 84% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.07 (d, *J* = 8.6 Hz, 2H), 7.67 (d, *J* = 8.6 Hz, 2H), 3.46 (s, 3H), 2.63 (s, 3H). **^{13}C NMR** (100 MHz,

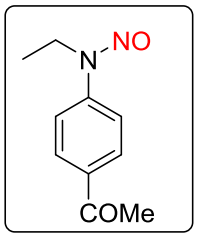
Chloroform-*d*) δ 196.7, 145.7, 135.3, 129.8, 117.9, 30.4, 26.6. **HRMS** (ESI): calcd for $C_9H_{11}N_2O_2$ $(M+H)^+$: 179.0821. Found: 179.0815.



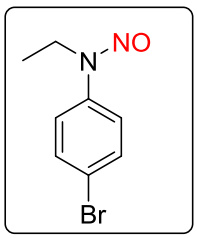
***N*-ethyl-*N*-(*p*-tolyl)nitrous amide (13b):** Prepared according to the general procedure. 121.4 mg, 74% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.41 (d, *J* = 8.5 Hz, 2H), 7.28 (d, *J* = 8.5 Hz, 2H), 4.06 (q, *J* = 7.2 Hz, 2H), 2.40 (s, 3H), 1.16 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 139.0, 137.3, 130.0, 119.7, 39.4, 20.9, 11.7. **HRMS** (ESI): calcd for $C_9H_{13}N_2O$ $(M+H)^+$: 165.1028. Found: 165.1026.



***N*-ethyl-*N*-(4-formylphenyl)nitrous amide (14b):** Prepared according to the general procedure. 154.8 mg, 87% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 10.03 (s, 1H), 7.99 (d, *J* = 8.7 Hz, 2H), 7.75 (d, *J* = 8.7 Hz, 2H), 4.09 (q, *J* = 7.2 Hz, 2H), 1.18 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 190.8, 146.0, 134.5, 131.2, 118.1, 38.2, 11.7. **HRMS** (ESI): calcd for $C_9H_{11}N_2O_2$ $(M+H)^+$: 179.0821. Found: 179.0822.

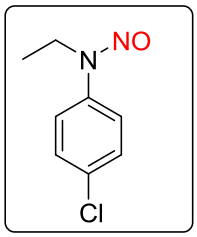


***N*-(4-acetylphenyl)-*N*-ethylnitrous amide (15b):** Prepared according to the general procedure. 171 mg, 89% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.09 – 8.04 (m, 2H), 7.69 – 7.63 (m, 2H), 4.09 (q, *J* = 7.2 Hz, 2H), 2.63 (s, 3H), 1.18 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 196.7, 144.9, 135.3, 129.9, 117.9, 38.2, 26.6, 11.7. **HRMS** (ESI): calcd for $C_{10}H_{13}N_2O_2$ $(M+H)^+$: 193.0977. Found: 193.0987.

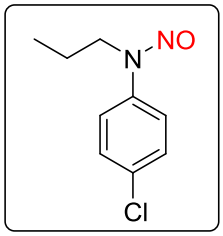


***N*-(4-bromophenyl)-*N*-ethylnitrous amide (16b):** Prepared according to the general procedure. 206 mg, 90% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.66 – 7.54 (m, 2H), 7.50 – 7.37 (m, 2H),

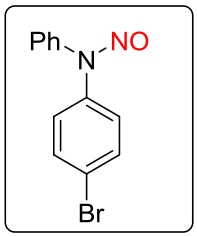
4.06 (q, *J* = 7.2 Hz, 2H), 1.17 (t, *J* = 7.2 Hz, 3H).**^{13}C NMR** (100 MHz, Chloroform-*d*) δ 140.4, 132.6, 120.6, 120.6, 38.8, 11.6. **HRMS** (ESI): calcd for $C_8H_{10}BrN_2O$ $(M+H)^+$: 228.9977, 230.9957. Found: 228.9993, 230.9973.



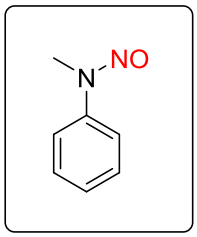
***N*-(4-chlorophenyl)-*N*-ethylnitrous amide (17b):** Prepared according to the general procedure. 126 mg, 68% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.51 – 7.46 (m, 1H), 7.46 – 7.41 (m, 1H), 4.05 (q, *J* = 7.2 Hz, 1H), 1.16 (t, *J* = 7.2 Hz, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 139.9, 132.9, 129.6, 120.4, 38.9, 11.6. **HRMS** (ESI): calcd for $C_8H_{10}ClN_2O$ $(M+H)^+$: 185.0482. Found: 185.0497.



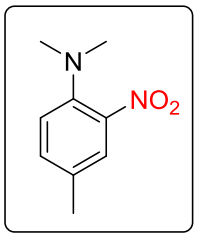
***N*-(4-chlorophenyl)-*N*-propylnitrous amide (18b):** Prepared according to the general procedure. 143.5 mg, 73% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.50 – 7.46 (m, 2H), 7.46 – 7.41 (m, 2H), 4.02 – 3.93 (t, *J* = 8.0 Hz, 2H), 1.56 (qt, *J* = 8.0 Hz, 8.0 Hz, 2H), 0.89 (t, *J* = 8.0 Hz, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 140.2, 132.9, 129.6, 120.6, 45.1, 19.9, 11.4. **HRMS** (ESI): calcd for $C_9H_{12}ClN_2O$ $(M+H)^+$: 199.0638. Found: 199.0646.



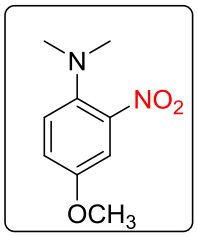
***N*-(4-bromophenyl)-*N*-phenylnitrous amide (21b):** Prepared according to the reaction conditions: 1 mmol of anilines, 1 mL of 1,4-dioxane, 1.5 eq. of TBN, r.t., under air. 201 mg, 73% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.64 (d, *J* = 8.6 Hz, 1H), 7.57 – 7.34 (m, 5H), 7.30 (d, *J* = 8.9 Hz, 1H), 7.06 (d, *J* = 6.9 Hz, 1H), 6.98 (d, *J* = 8.6 Hz, 1H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 142.1, 141.6, 136.2, 135.6, 133.0, 132.4, 129.9, 129.4, 128.9, 127.4, 123.5, 120.8, 120.3, 119.8, 114.7. **HRMS** (ESI): calcd for $C_{12}H_{10}BrN_2O$ $(M+H)^+$: 276.9977, 278.9957. Found: 276.9978, 278.9955.



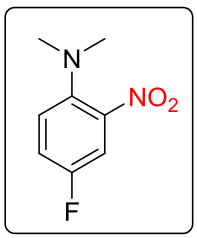
***N*-methyl-*N*-phenylnitrous amide (22b):** Prepared according to the general procedure. 42 mg, 31% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.52 (d, *J* = 8.1 Hz, 2H), 7.46 (t, *J* = 7.9 Hz, 2H), 7.34 (t, *J* = 7.3 Hz, 1H), 3.43 (d, *J* = 1.2 Hz, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 142.3, 129.4, 127.3, 119.2, 31.4. **HRMS** (ESI): calcd for $C_7H_9N_2O$ $(M+H)^+$: 137.0715. Found: 137.0729.



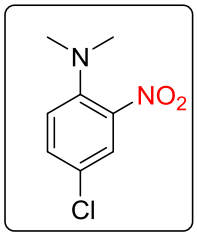
***N*,*N*,4-trimethyl-2-nitroaniline (1c):** Prepared according to the general procedure. 151.2 mg, 84% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.57 (d, *J* = 1.3 Hz, 1H), 7.22 (dd, *J* = 8.5, 1.8 Hz, 1H), 6.95 (d, *J* = 8.5 Hz, 1H), 2.84 (s, 6H), 2.30 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 144.3, 139.9, 134.1, 128.4, 126.4, 118.5, 42.8, 20.0. **HRMS** (ESI): calcd for $C_9H_{13}N_2O_2$ $(M+H)^+$: 181.0977. Found: 181.0980.



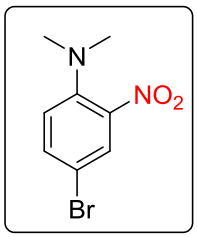
4-methoxy-*N*,*N*-dimethyl-2-nitroaniline (2c): Prepared according to the general procedure. 160.7 mg, 82% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.30 (d, *J* = 3.4 Hz, 1H), 7.08 - 7.05 (m, 2H), 3.80 (s, 3H), 2.81 (s, 6H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 152.8, 141.3, 141.1, 121.0, 120.8, 109.6, 55.9, 43.5. **HRMS** (ESI): calcd for $C_9H_{13}N_2O_3$ $(M+H)^+$: 197.0926. Found: 197.0926.



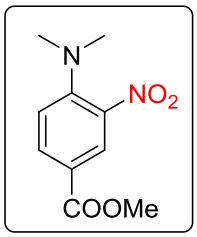
4-fluoro-*N*,*N*-dimethyl-2-nitroaniline (3c): Prepared according to the general procedure. 149.5 mg, 81% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.53 (dd, *J* = 8.2, 3.1 Hz, 1H), 7.19 (ddd, *J* = 10.2, 7.2, 3.1 Hz, 1H), 7.04 (dd, *J* = 9.2, 4.6 Hz, 1H), 2.85 (s, 6H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 155.9, 153.5, 143.41, 143.38, 139.4, 139.3, 121.0, 120.7, 120.10, 120.03, 113.1, 112.9, 43.0. **HRMS** (ESI): calcd for $C_8H_{10}FN_2O_2$ $(M+H)^+$: 185.0726. Found: 185.0724.



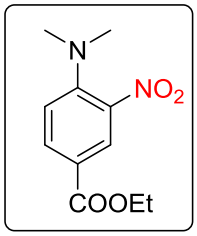
4-chloro-*N*,*N*-dimethyl-2-nitroaniline (4c): Prepared according to the general procedure. 144.4 mg, 72% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.77 (s, 1H), 7.35 (d, *J* = 9.0 Hz, 1H), 6.96 (d, *J* = 9.6 Hz, 1H), 2.89 (s, 6H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 144.9, 138.8, 133.2, 126.2, 122.4, 119.3, 42.4. **HRMS** (ESI): calcd for $C_8H_{10}ClN_2O_2$ $(M+H)^+$: 201.0431. Found: 201.0426.



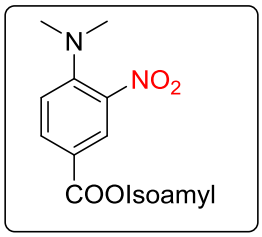
4-bromo-*N*,*N*-dimethyl-2-nitroaniline (5c): Prepared according to the general procedure. 115.2 mg, 47% yield. **1H NMR** (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 2.4 Hz, 1H), 7.47 (dd, *J* = 9.0, 2.4 Hz, 1H), 6.90 (d, *J* = 9.0 Hz, 1H), 2.89 (s, 6H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 145.2, 135.9, 133.9, 129.1, 119.5, 108.8, 42.4. **HRMS** (ESI): calcd for $C_8H_{10}BrN_2O_2$ $(M+H)^+$: 244.9925, 246.9905. Found: 244.9920, 246.9900.



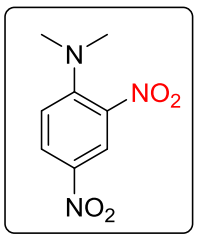
methyl 4-(dimethylamino)-3-nitrobenzoate (6c): Prepared according to the general procedure. 186.0 mg, 83% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.45 (s, 1H), 8.00 (d, *J* = 9.0 Hz, 1H), 6.98 (d, *J* = 9.0 Hz, 1H), 3.89 (s, 3H), 2.99 (s, 6H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 165.6, 148.4, 137.2, 133.7, 129.2, 118.2, 116.7, 52.1, 42.1. **HRMS** (ESI): calcd for $C_{10}H_{13}N_2O_4$ $(M+H)^+$: 225.0875. Found: 225.0869.



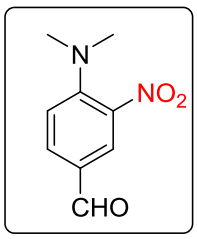
ethyl 4-(dimethylamino)-3-nitrobenzoate (7c): Prepared according to the general procedure. 199.9 mg, 84% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.44 (d, *J* = 2.0 Hz, 1H), 8.00 (dt, *J* = 9.0, 1.9 Hz, 1H), 6.97 (d, *J* = 9.0 Hz, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 2.98 (s, 6H), 1.38 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 165.1, 148.4, 137.2, 133.7, 129.1, 118.6, 116.6, 61.0, 42.1, 14.3. **HRMS** (ESI): calcd for $C_{11}H_{15}N_2O_4$ $(M+H)^+$: 239.1032. Found: 239.1034.



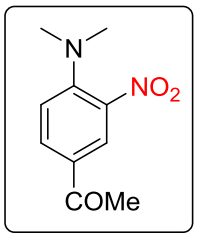
isopentyl 4-(dimethylamino)-3-nitrobenzoate (8c): Prepared according to the general procedure. 174.8 mg, 63% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.42 (d, *J* = 2.1 Hz, 1H), 7.99 (dd, *J* = 9.0, 2.1 Hz, 1H), 6.97 (d, *J* = 9.0 Hz, 1H), 4.32 (t, *J* = 6.8 Hz, 2H), 2.98 (s, 6H), 1.82 – 1.72 (m, 1H), 1.64 (q, *J* = 6.8 Hz, 2H), 0.96 (d, *J* = 6.6 Hz, 6H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 165.2, 148.4, 137.2, 133.7, 129.1, 118.7, 116.6, 63.7, 42.1, 37.4, 25.2, 22.5. **HRMS** (ESI): calcd for $C_{14}H_{21}N_2O_4$ $(M+H)^+$: 281.1501. Found: 281.1495.



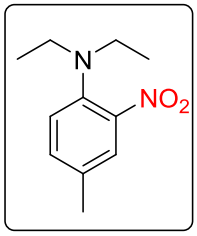
***N,N*-dimethyl-2,4-dinitroaniline (9c):** Prepared according to the general procedure. 133.0 mg, 63% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.71 (d, *J* = 2.7 Hz, 1H), 8.22 (dd, *J* = 9.5, 2.7 Hz, 1H), 7.01 (d, *J* = 9.5 Hz, 1H), 3.06 (s, 6H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 149.1, 136.5, 135.8, 127.8, 124.2, 116.5, 42.4. **HRMS** (ESI): calcd for $C_8H_{10}N_3O_4$ $(M+H)^+$: 212.0671. Found: 212.0667.



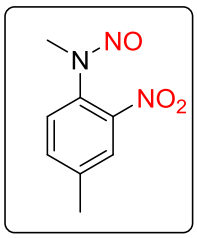
4-(dimethylamino)-3-nitrobenzaldehyde (11c): Prepared according to the general procedure. 114.1 mg, 54% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 9.80 (s, 1H), 8.25 (d, *J* = 2.1 Hz, 1H), 7.88 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.06 (d, *J* = 8.9 Hz, 1H), 3.03 (s, 6H).**^{13}C NMR** (100 MHz, Chloroform-*d*) δ 188.6, 149.3, 137.0, 132.3, 131.0, 125.4, 117.3, 42.3. **HRMS** (ESI): calcd for $C_9H_{11}N_2O_3$ $(M+H)^+$: 195.0770. Found: 195.0768.



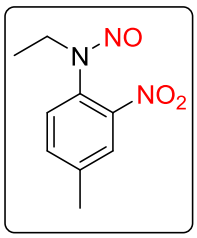
1-(4-(dimethylamino)-3-nitrophenyl)ethan-1-one (12c): Prepared according to the general procedure. 66.6 mg, 32% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.37 (d, *J* = 2.2 Hz, 1H), 7.99 (dd, *J* = 9.0, 2.2 Hz, 1H), 7.00 (d, *J* = 9.0 Hz, 1H), 3.01 (s, 6H), 2.55 (s, 3H).**^{13}C NMR** (100 MHz, Chloroform-*d*) δ 194.89, 136.81, 132.48, 129.89, 128.62, 125.88, 116.84, 42.20, 26.09. **HRMS** (ESI): calcd for $C_{10}H_{13}N_2O_3$ $(M+H)^+$: 209.0926. Found: 209.0925.



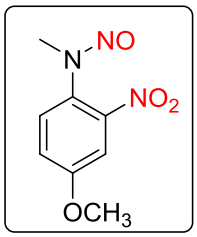
***N*,*N*-diethyl-4-methyl-2-nitroaniline (13c):** Prepared according to the general procedure. 208 mg, 99.8% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.44 (d, *J* = 1.1 Hz, 1H), 7.23 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 1H), 3.08 (q, *J* = 7.1 Hz, 4H), 2.32 (s, 3H), 1.04 (t, *J* = 7.1 Hz, 6H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 145.4, 142.0, 133.1, 131.7, 125.0, 123.3, 47.3, 20.3, 12.6. **HRMS** (ESI): calcd for $C_{11}H_{17}N_2O_2$ $(M+H)^+$: 209.1290. Found: 209.1287.



***N*-methyl-*N*-(4-methyl-2-nitrophenyl)nitrous amide (1d):** Prepared according to the general procedure. 203.0 mg, 92% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 2.0 Hz, 1H), 7.56 (dd, *J* = 8.1, 2.0 Hz, 0.8H), 7.53 (dd, *J* = 8.1, 2.0 Hz, 0.2H), 7.39 (d, *J* = 8.1 Hz, 0.8H), 7.04 (d, *J* = 8.0 Hz, 0.2H), 4.20 (s, 0.5H), 3.39 (s, 2.5H), 2.52 (s, 2.5H), 2.48 (s, 0.5H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 144.1, 141.5, 140.6, 135.2, 134.6, 133.4, 127.3, 127.1, 126.0, 125.7, 40.6, 35.1, 21.0, 14.1. **HRMS** (ESI): calcd for $C_8H_{10}N_3O_3$ $(M+H)^+$: 196.0722. Found: 196.0724.

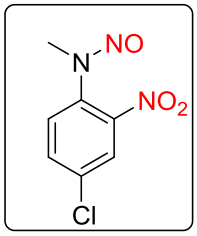


***N*-ethyl-*N*-(4-methyl-2-nitrophenyl)nitrous amide (2d):** Prepared according to the general procedure. 154.7 mg, 74% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.88 (s, 0.4H), 7.85 (s, 0.6H), 7.55 (d, *J* = 8.0 Hz, 0.6H), 7.52 (d, *J* = 8.0 Hz, 0.4H), 7.34 (d, *J* = 8.1 Hz, 0.6H), 7.01 (d, *J* = 8.1 Hz, 0.4H), 4.63 (q, *J* = 7.3 Hz, 0.8H), 3.99 (q, *J* = 7.3 Hz, 1.2H), 2.49 (s, 1.9H), 7.45 (s, 1.1H), 1.49 (t, *J* = 7.3 Hz, 1H), 1.15 (t, *J* = 7.3 Hz, 2H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 145.7, 145.0, 141.5, 140.7, 135.1, 134.4, 131.9, 127.6, 126.0, 125.7, 49.0, 42.0, 21.0, 13.9, 11.3. **HRMS** (ESI): calcd for $C_9H_{12}N_3O_3$ $(M+H)^+$: 210.0879. Found: 210.0883.

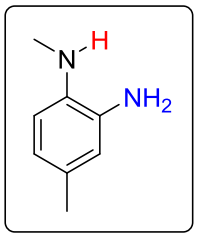


***N*-(4-methoxy-2-nitrophenyl)-*N*-methylnitrous amide (3d):** Prepared according to the general procedure. 202.7 mg, 97% yield.

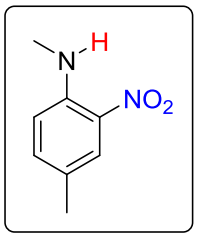
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 (s, 0.5H), 7.59 (s, 0.5H), 7.42 (s, 0.4H), 7.40 (s, 0.4H), 7.28 (d, *J* = 2.9 Hz, 0.4H), 7.25 (d, *J* = 2.9 Hz, 0.4H), 7.24 (d, *J* = 2.9 Hz, 0.1H), 7.22 (d, *J* = 2.9 Hz, 0.1H), 7.06 (s, 0.1H), 7.04 (s, 0.1H), 4.19 (s, 0.5H), 3.94 (s, 2.5H), 3.90 (s, 0.5H), 3.38 (s, 2.5H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 160.5, 160.1, 145.2, 129.0, 128.77, 128.70, 124.5, 120.4, 120.0, 110.5, 110.4, 56.32, 56.24, 40.7,35.4. **HRMS** (ESI): calcd for $C_8H_{10}N_3O_4$ $(M+H)^+$: 212.0671. Found: 212.0675.



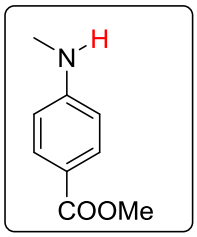
***N*-(4-chloro-2-nitrophenyl)-*N*-methylnitrous amide (4d):** Prepared according to the general procedure. 187.0 mg, 87% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.07 (d, *J* = 2.4 Hz, 0.2H), 8.06 (d, *J* = 2.4 Hz, 0.8H), 7.74 (dd, *J* = 8.6, 2.4 Hz, 0.8H), 7.72 (dd, *J* = 8.6, 2.4 Hz, 0.2H), 7.48 (d, *J* = 8.6 Hz, 0.8H), 7.13 (d, *J* = 8.6 Hz, 0.2H), 4.21 (s, 0.5H), 3.38 (s, 2.5H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 144.4, 135.2, 134.7, 134.3, 134.0, 130.3, 128.6, 127.9, 126.0, 125.6, 40.4, 34.7. **HRMS** (ESI): calcd for $C_7H_7ClN_3O_3$ $(M+H)^+$: 216.0176. Found: 216.0176.



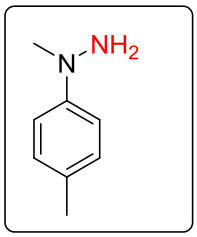
***N*^{1},4-dimethylbenzene-1,2-diamine (1f):** Prepared according to the general procedure. 93.4 mg, 69% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 6.66 (d, *J* = 7.8 Hz, 1H), 6.62 – 6.52 (m, 2H), 3.27 (br, 3H), 2.85 (s, 3H), 2.24 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 136.4, 134.4, 128.1, 120.8, 117.1, 111.3, 31.3, 20.6. **HRMS** (ESI): calcd for $C_8H_{13}N_2$ $(M+H)^+$: 137.1079. Found: 137.1079.



***N*,4-dimethyl-2-nitroaniline (1e):** Prepared according to the general procedure. 84.7 mg, 55% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.98 (s, 1H), 7.93 (s, 1H), 7.30 (d, *J* = 8.7 Hz, 1H), 6.76 (d, *J* = 8.7 Hz, 1H), 3.01 (d, *J* = 5.1 Hz, 3H), 2.27 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 144.6, 137.8,131.5, 126.0, 124.7, 113.3, 29.8, 19.9. **HRMS** (ESI): calcd for $C_8H_{11}N_2O_2$ $(M+H)^+$: 167.0821. Found: 167.0824.



methyl 4-(methylamino)benzoate (5i): Prepared according to the general procedure. 47.5 mg, 83% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 8.9 Hz, 2H), 6.55 (d, *J* = 8.8 Hz, 2H), 4.18 (s, 1H), 3.85 (s, 3H), 2.89 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 167.3, 152.8, 131.5, 118.2, 111.1, 51.5, 30.1. **HRMS** (ESI): calcd for $C_9H_{12}NO_2$ $(M+H)^+$: 166.0868. Found: 166.0868.



1-methyl-1-(*p*-tolyl)hydrazine (1g): Prepared according to the general procedure. 114.3 mg, 84% yield. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.08 (d, *J* = 8.2 Hz, 2H), 6.93 (d, *J* = 8.5 Hz, 2H), 3.68 (br, 2H), 3.07 (s, 3H), 2.28 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 150.8, 129.4, 114.0, 114.0, 45.1, 45.1, 20.3. **HRMS** (ESI): calcd for $C_8H_{13}N_2$ $(M+H)^+$: 137.1079. Found: 137.1079.

4. References

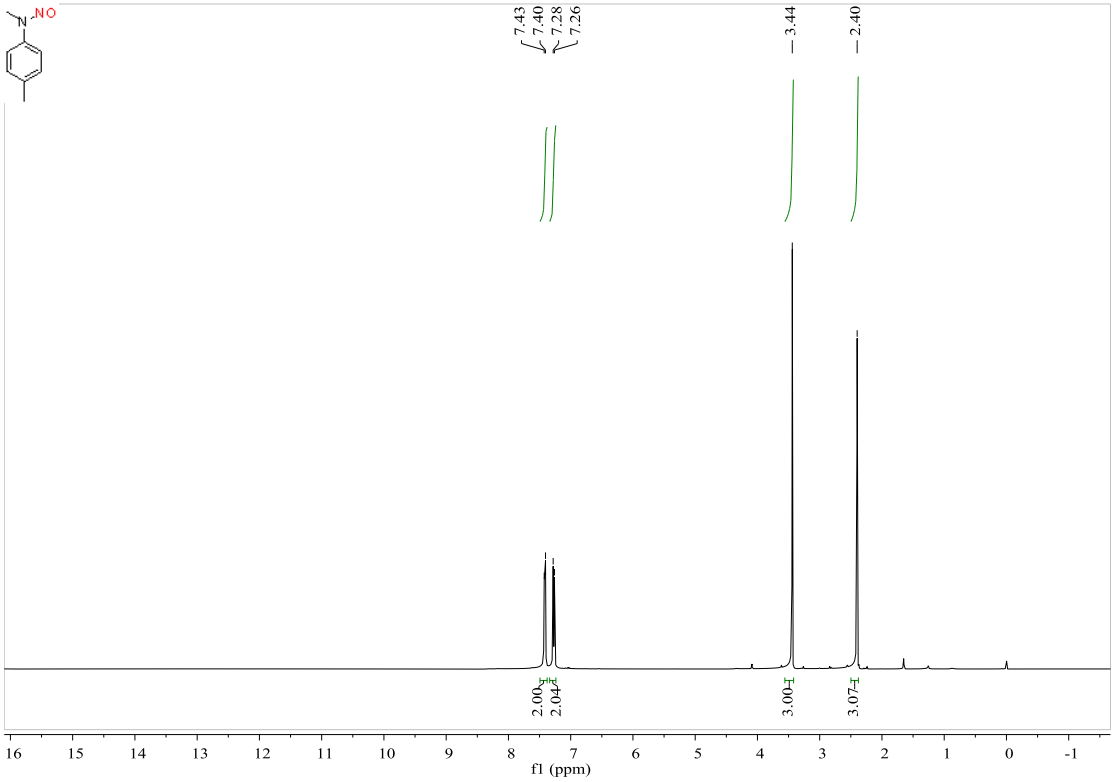
1. Chaudhary, P.; Gupta, S.; Muniyappan, N.; Sabiah, S.; Kandasamy, J. *J. Org. Chem.* **2019,** *84* (1), 104-119.

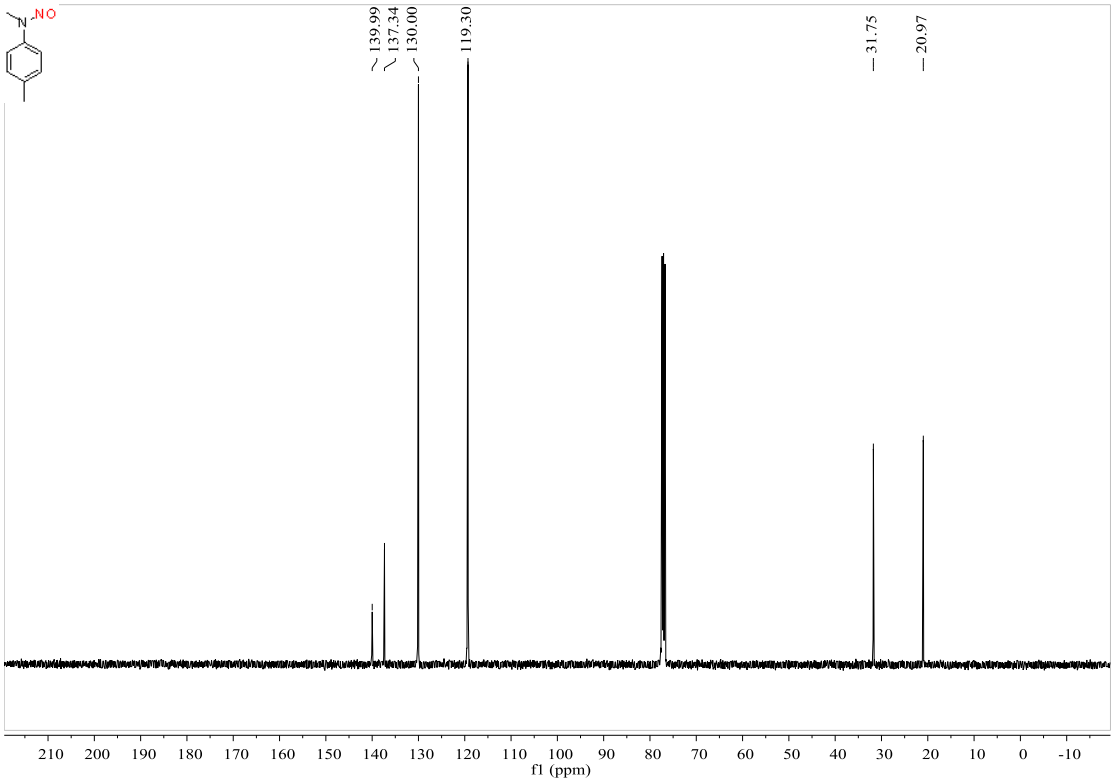
2. Chaudhary, P.; Korde, R.; Gupta, S.; Sureshbabu, P.; Sabiah, S.; Kandasamy, J. *Adv. Synth. Catal.* **2018,** *360* (3), 556-561.

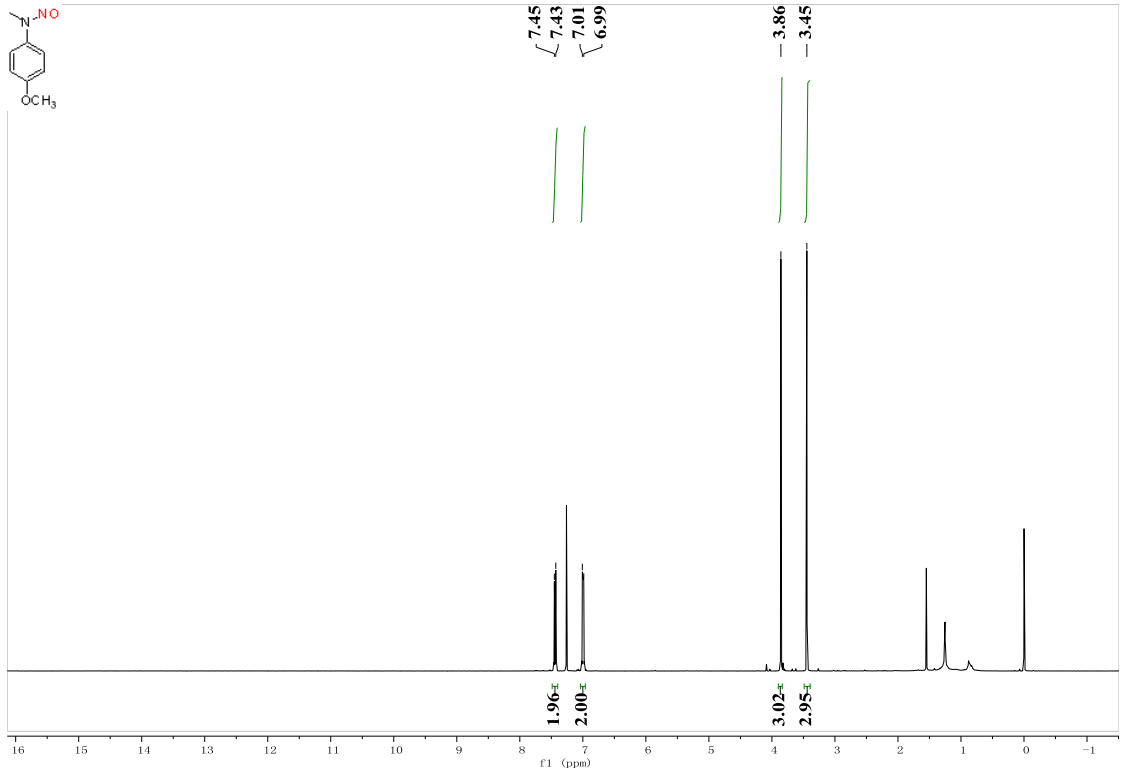
3. Chaudhary, P.; Gupta, S.; Sureshbabu, P.; Sabiah, S.; Kandasamy, J. *Green Chem.* **2016,** *18* (23), 6215-6221.

4. Jia, X.; Li, P.; Shao, Y.; Yuan, Y.; Ji, H.; Hou, W.; Liu, X.; Zhang, X. *Green Chem.* **2017**, *19* (23), 5568-5574.

5. Spectral Data



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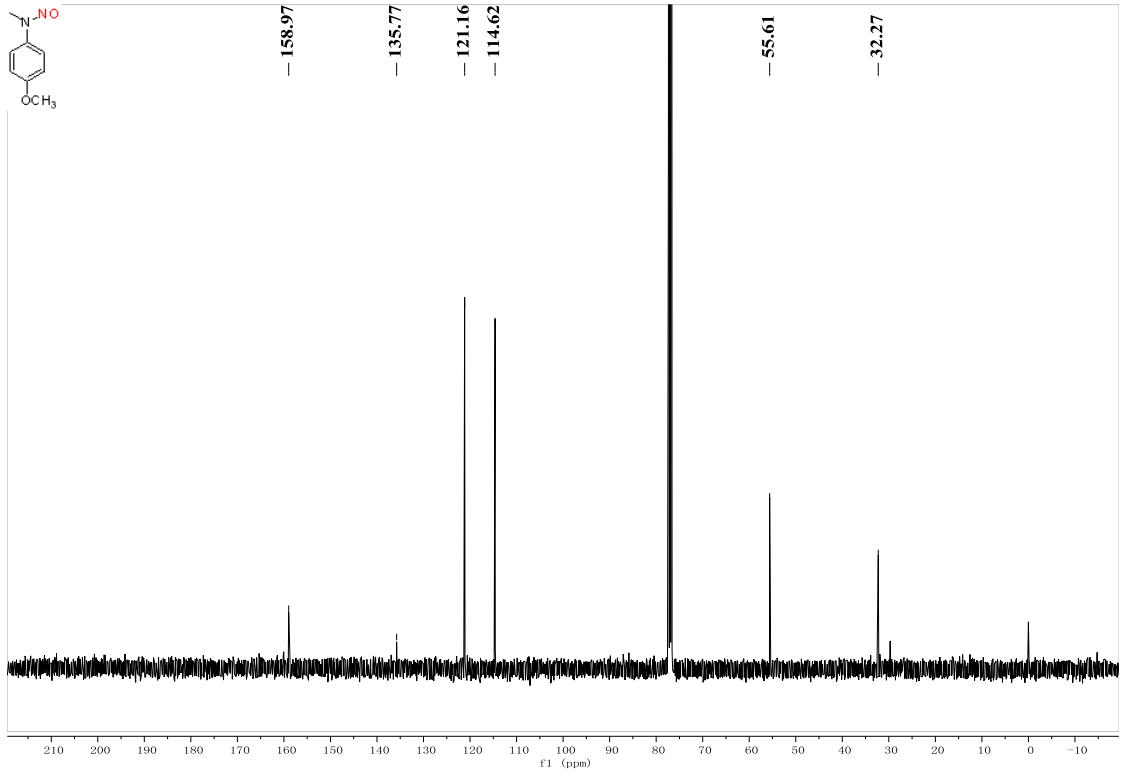
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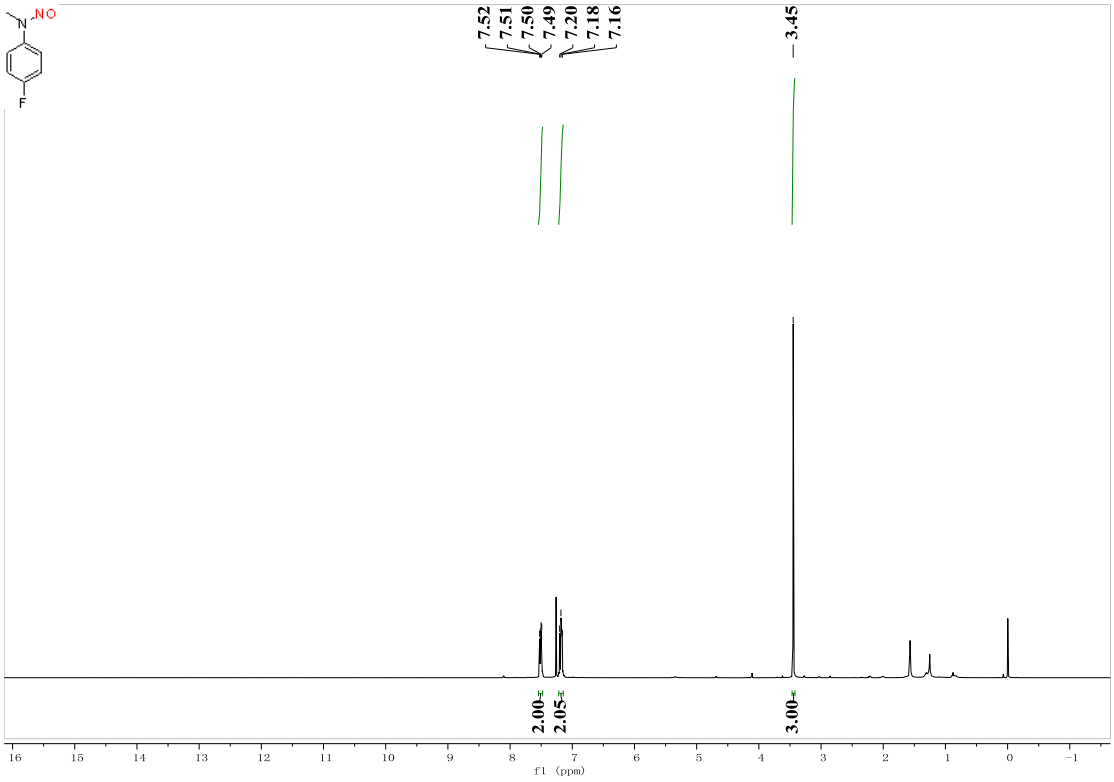
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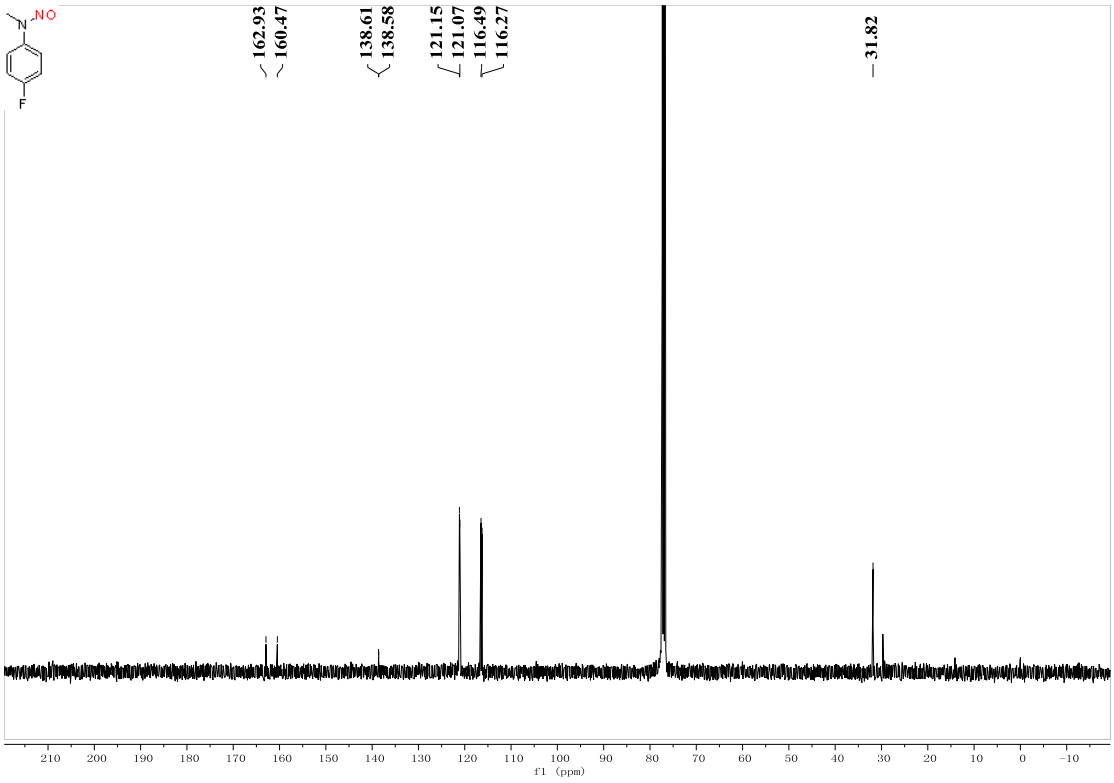
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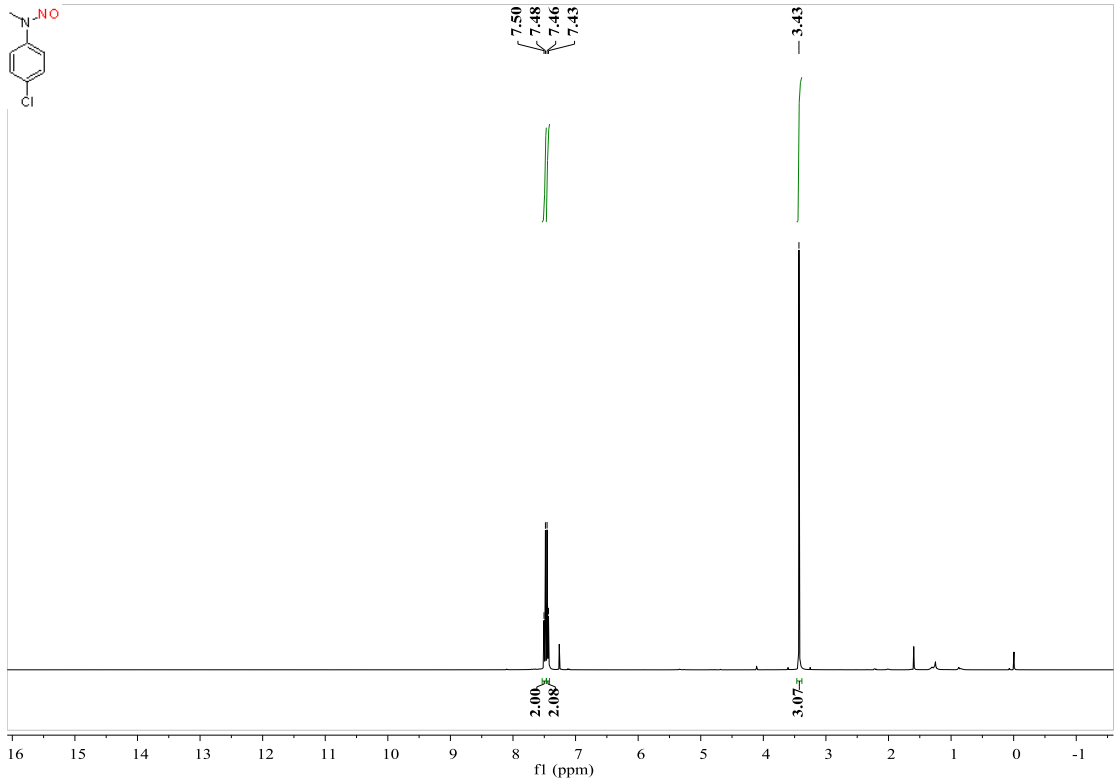
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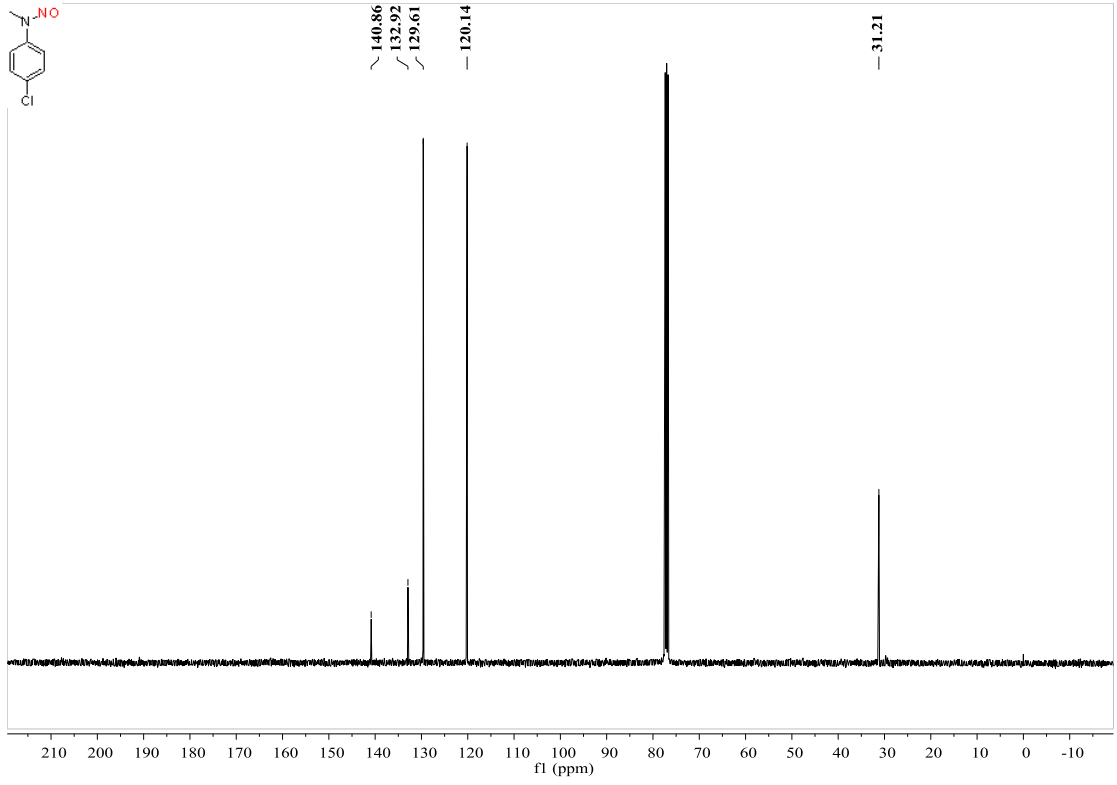
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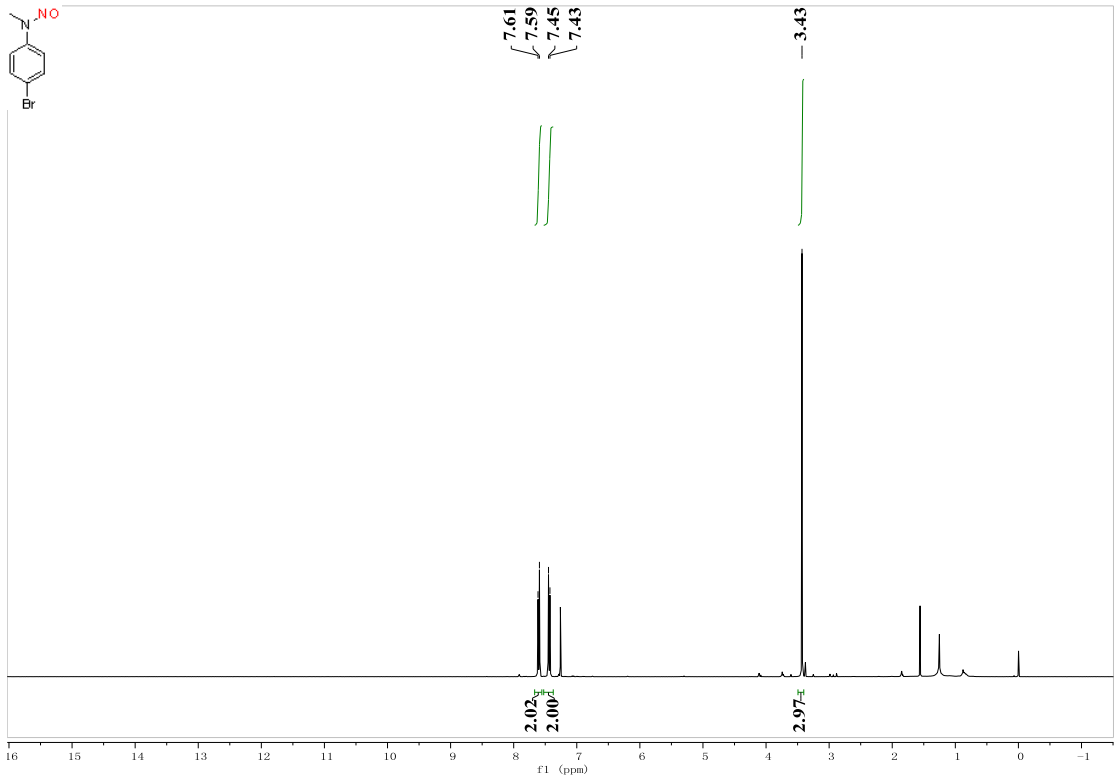
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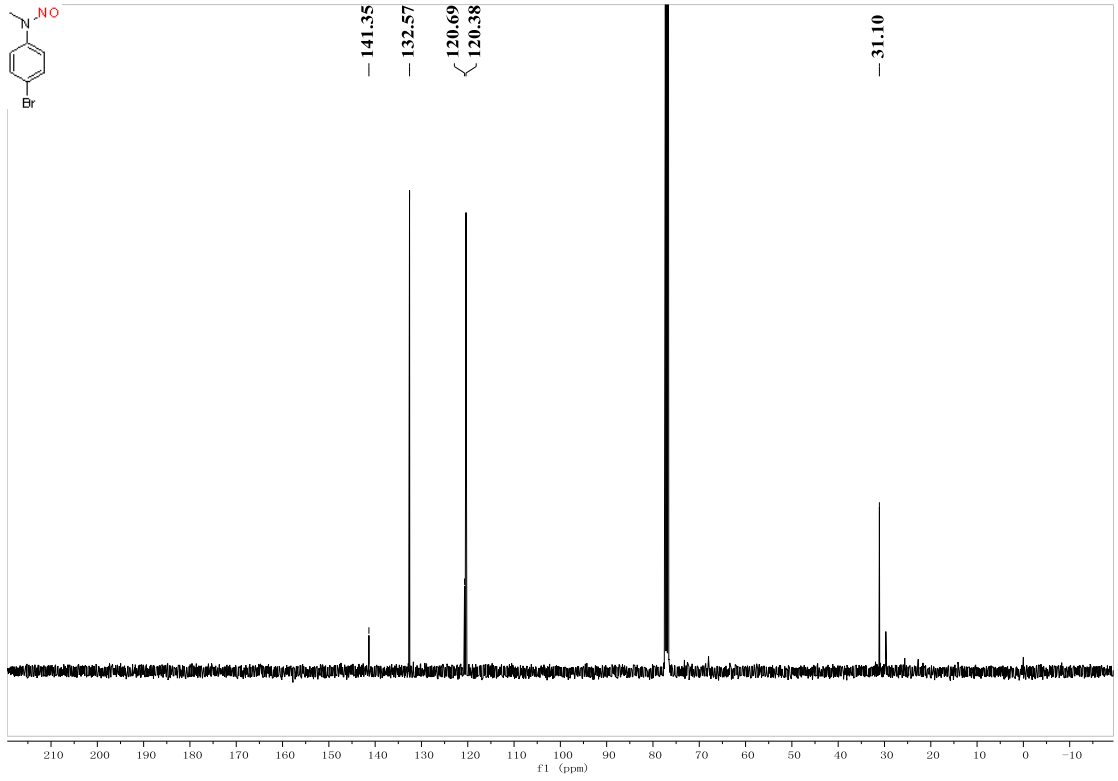
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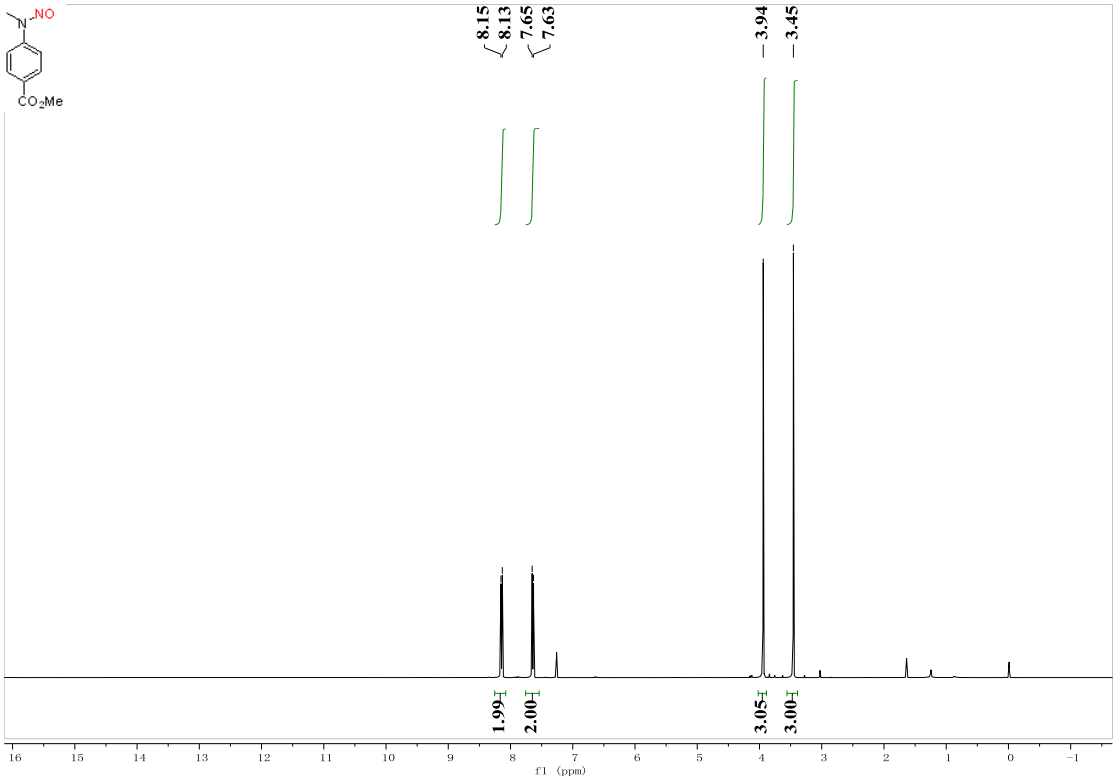
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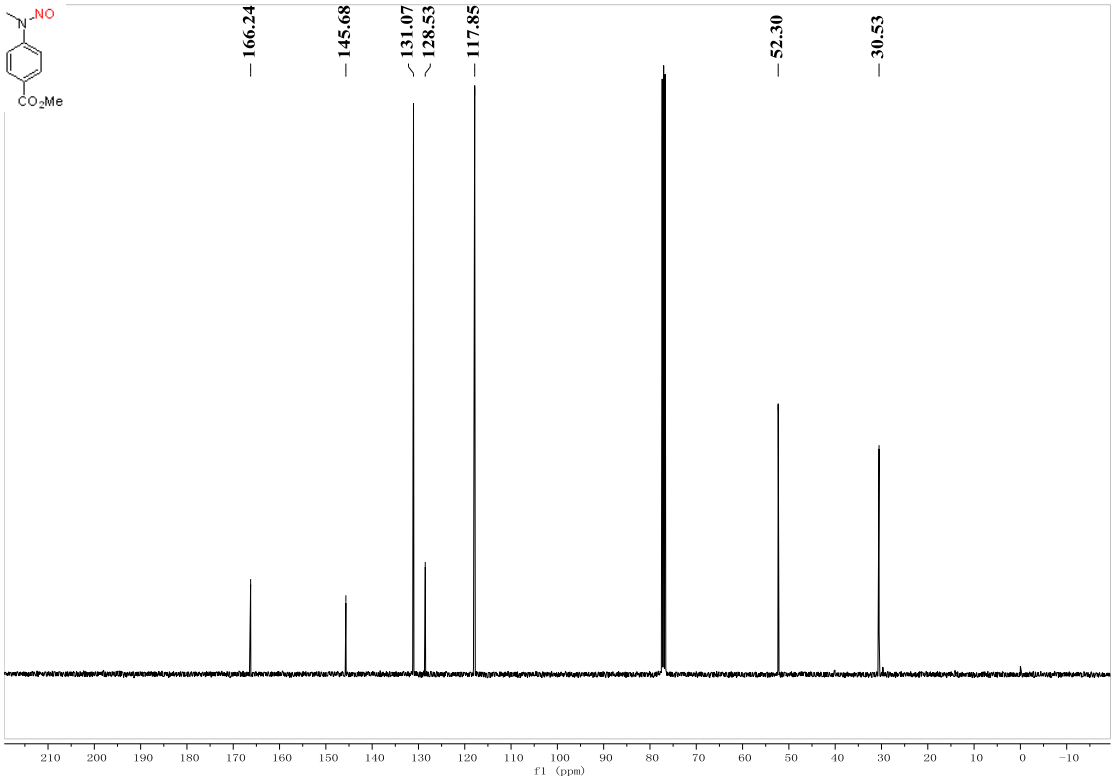
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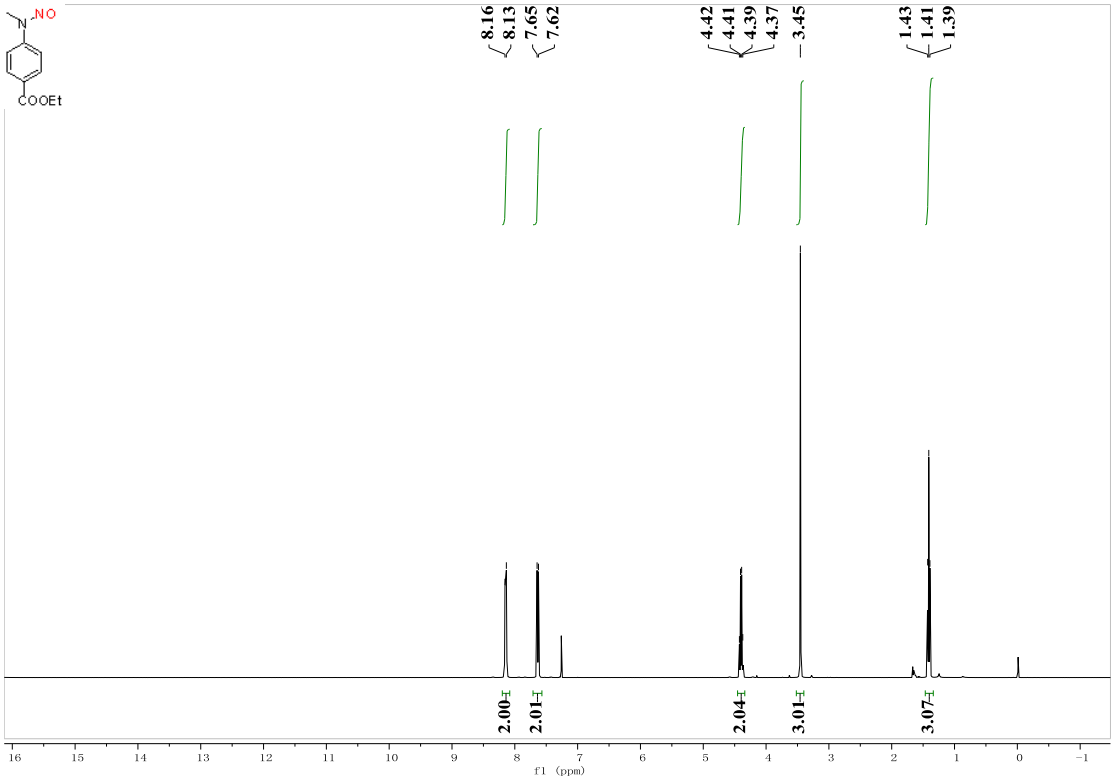
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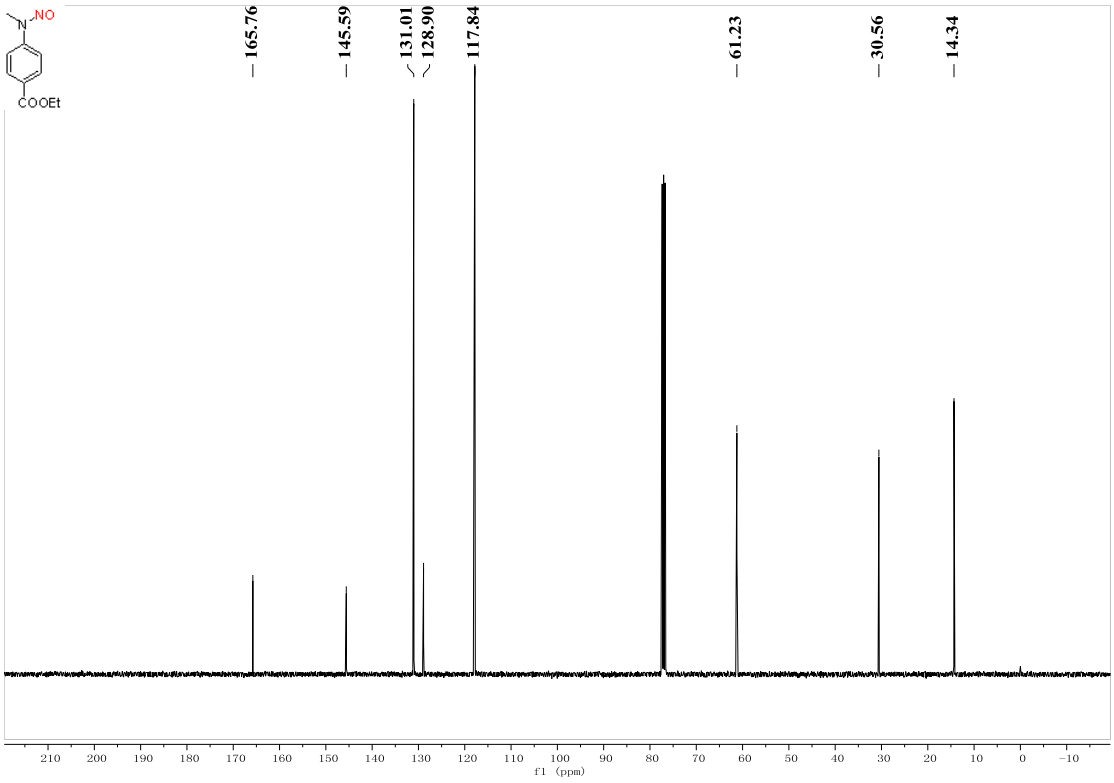
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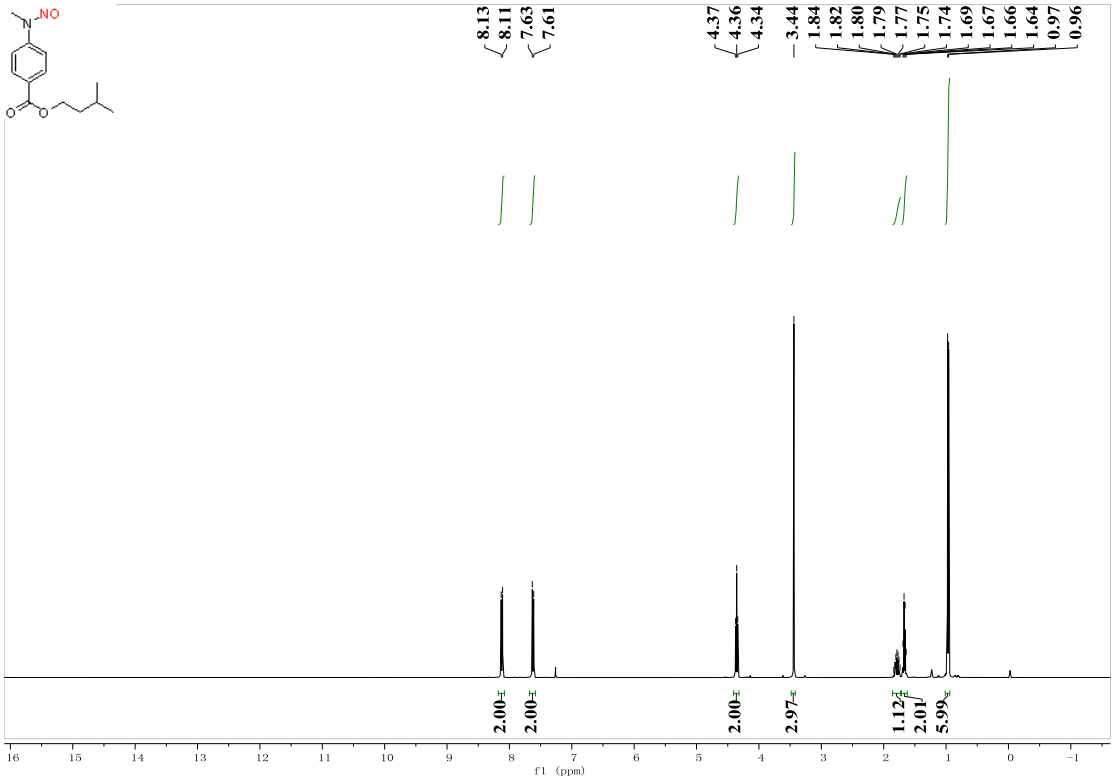
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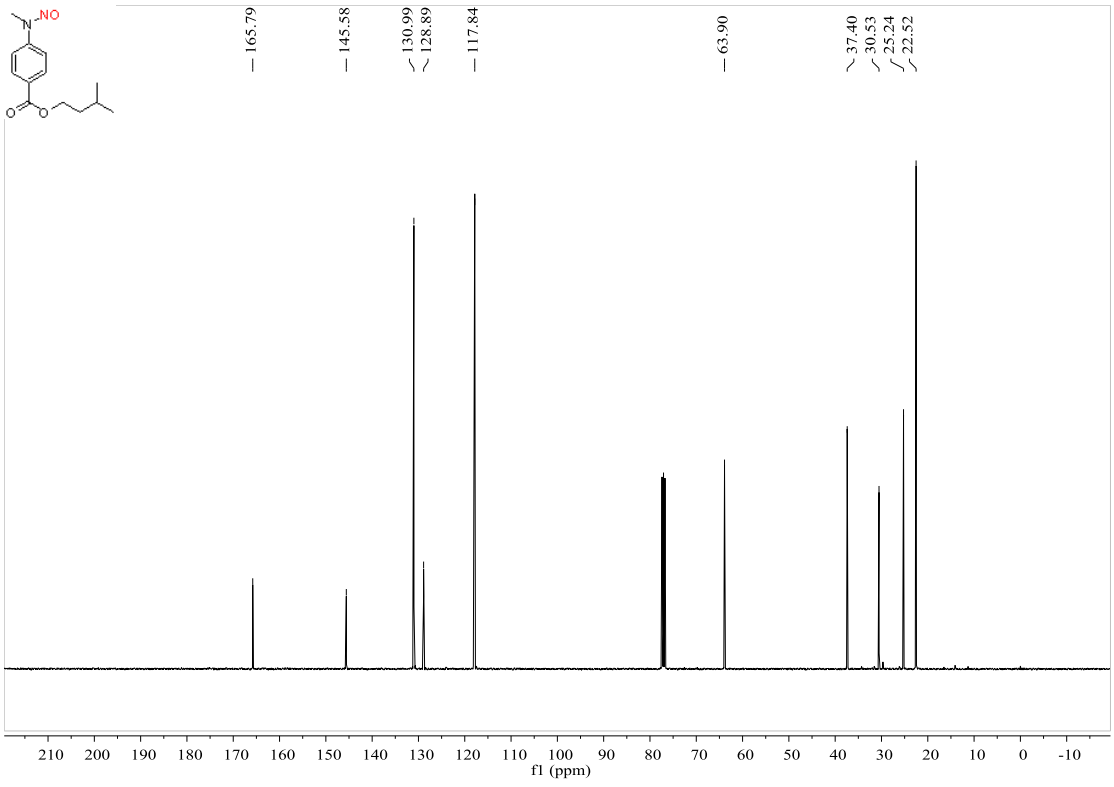
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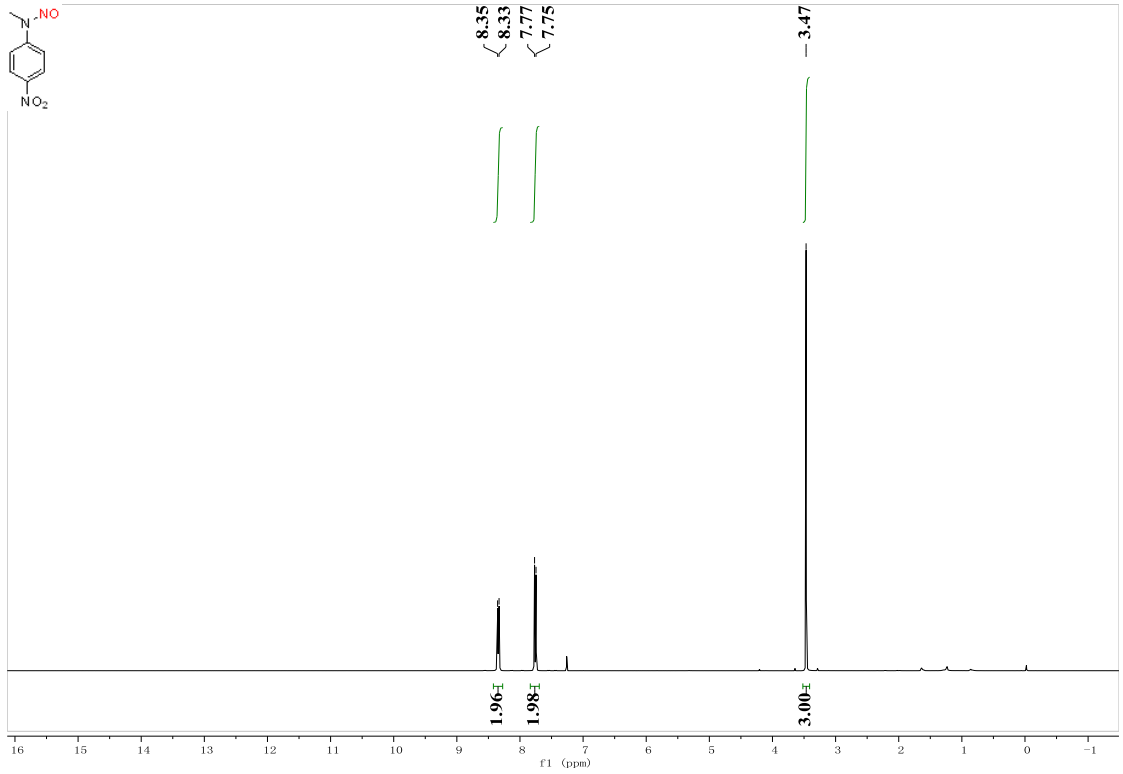
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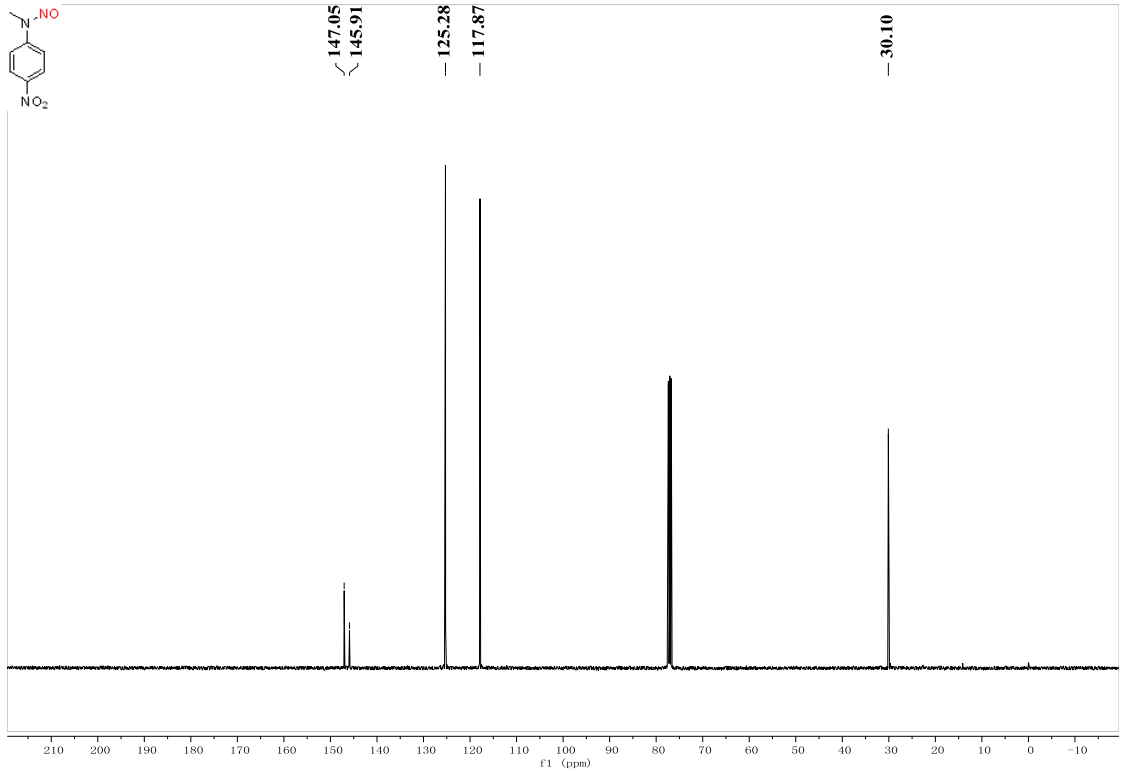
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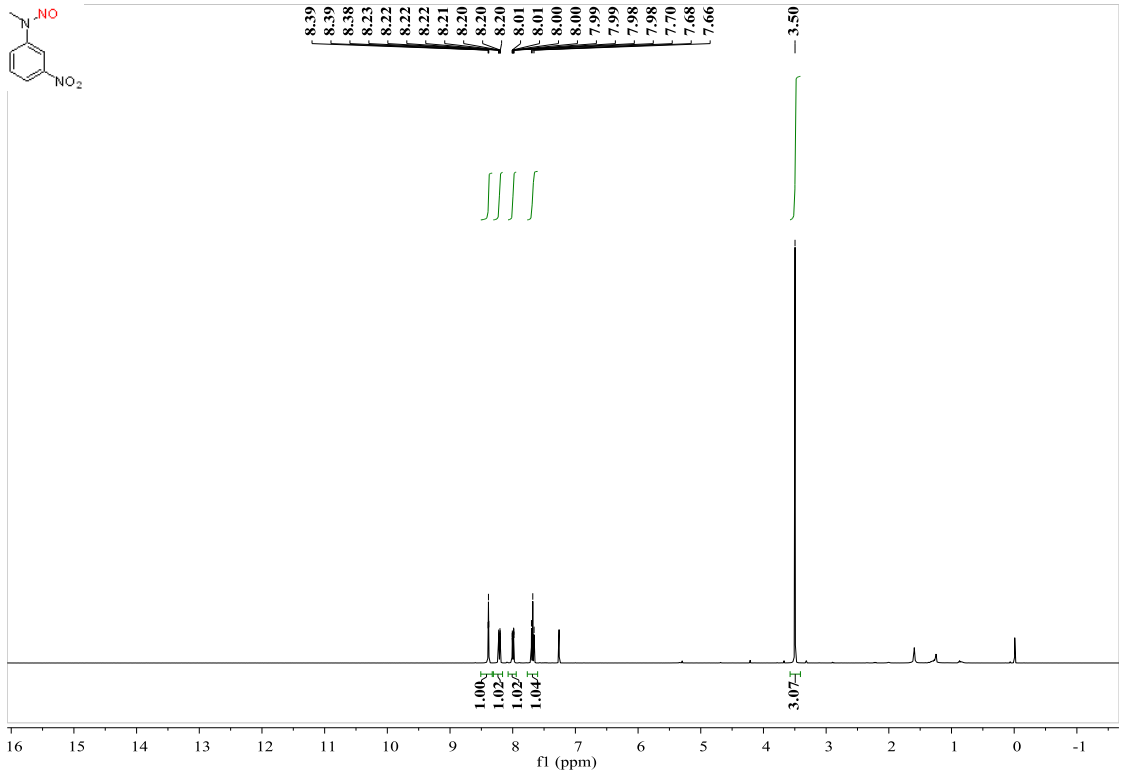
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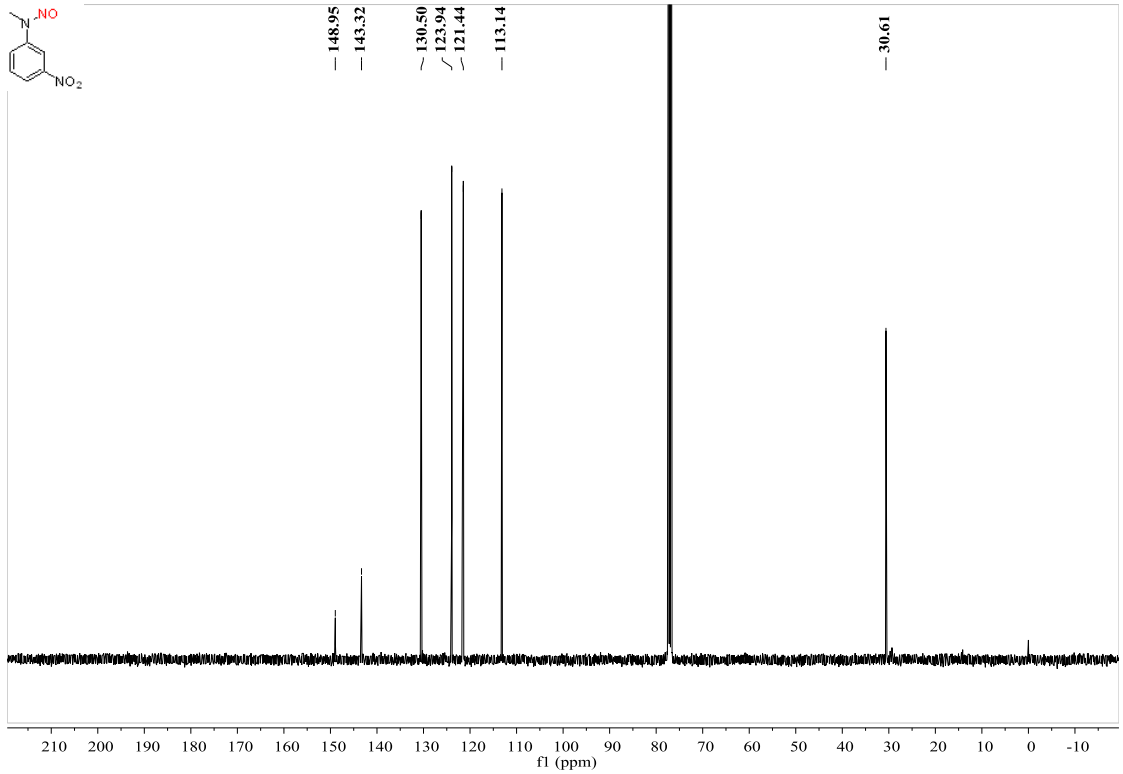
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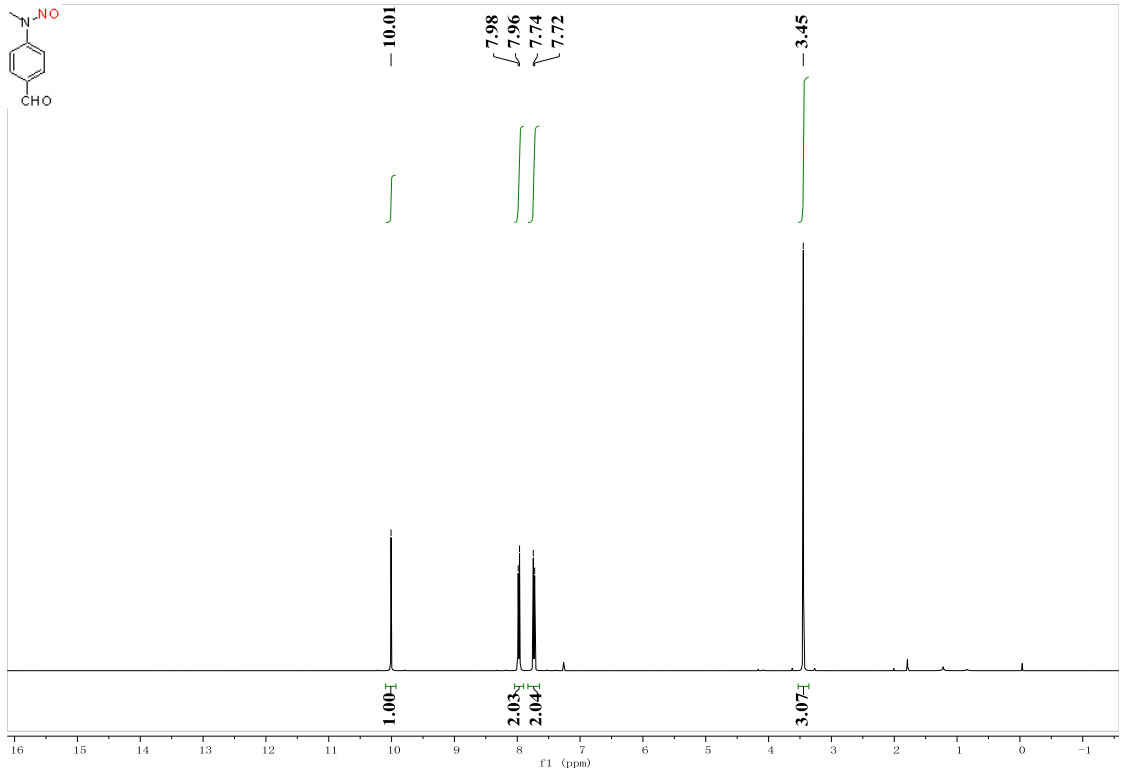
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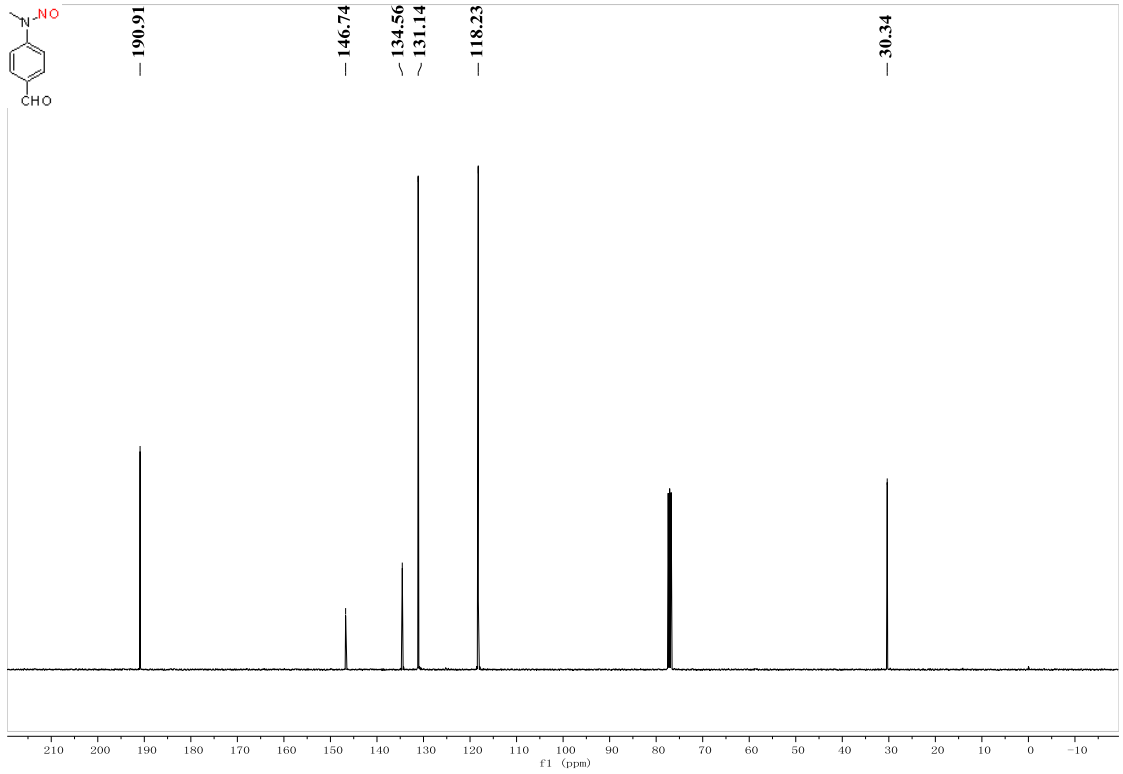
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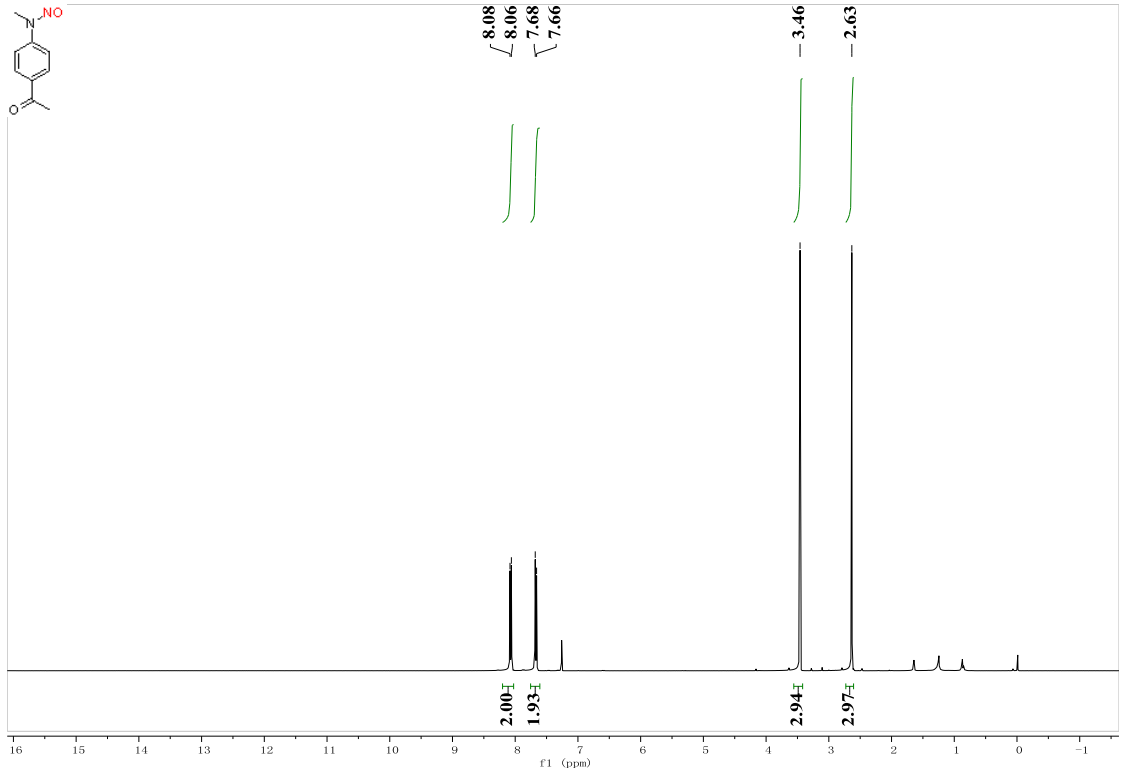
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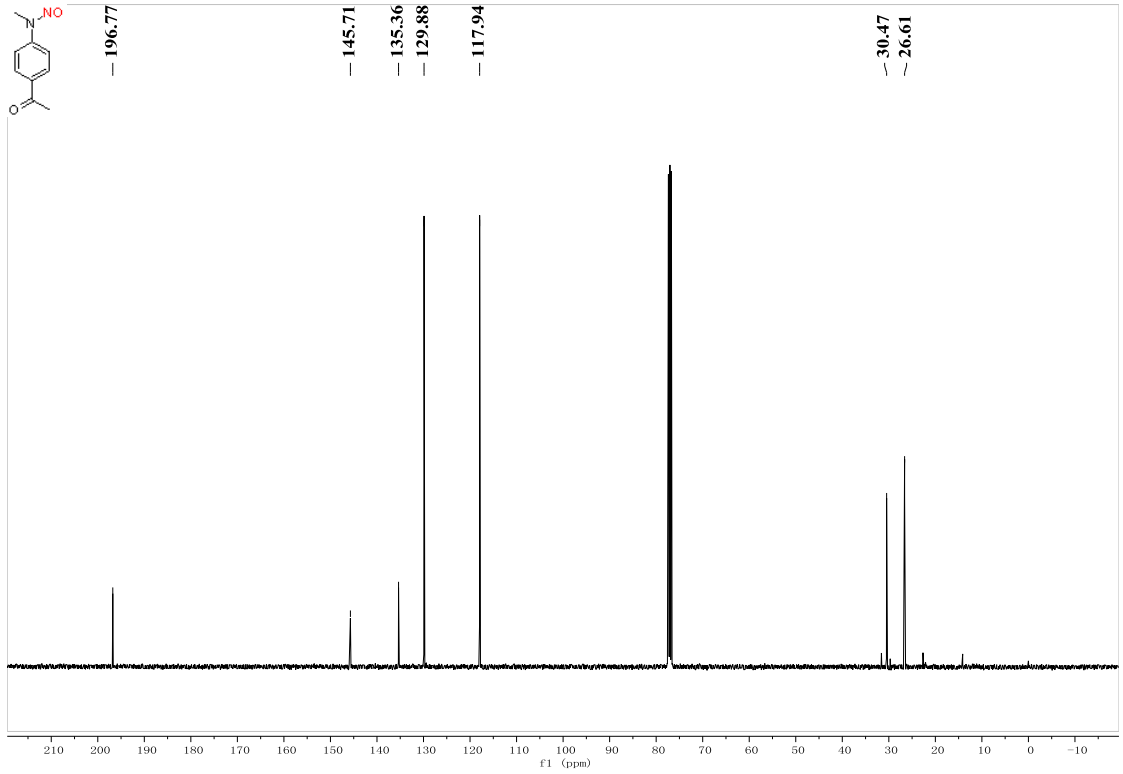
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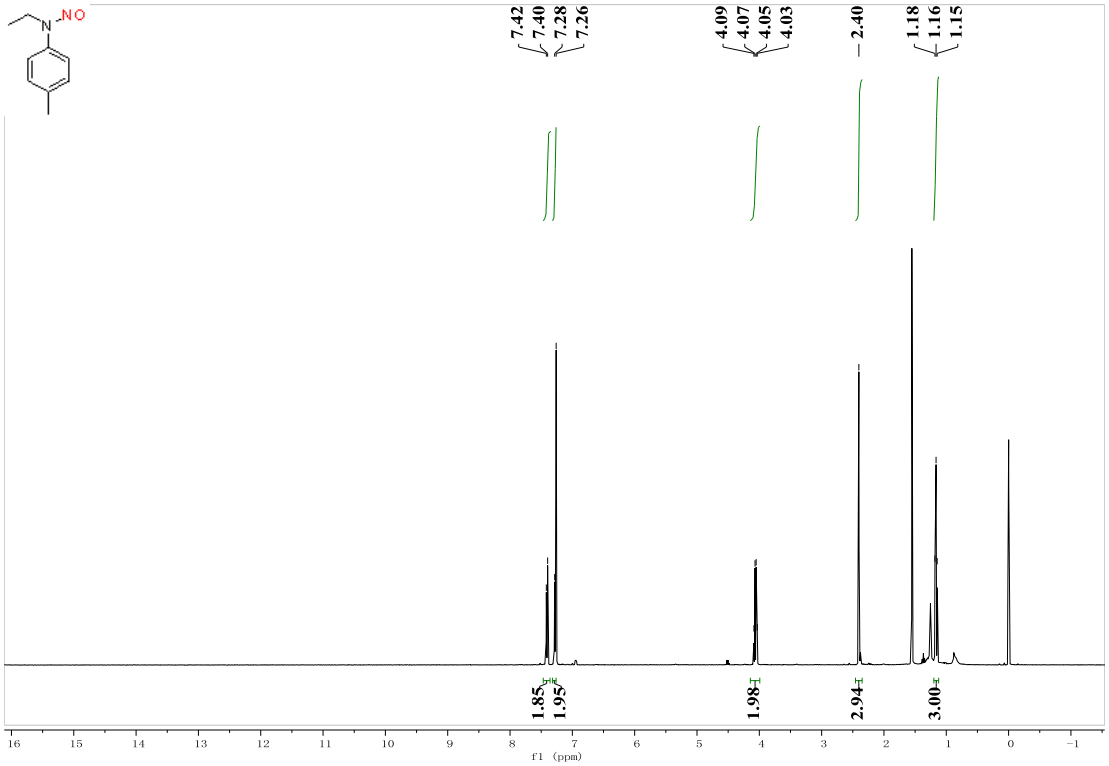
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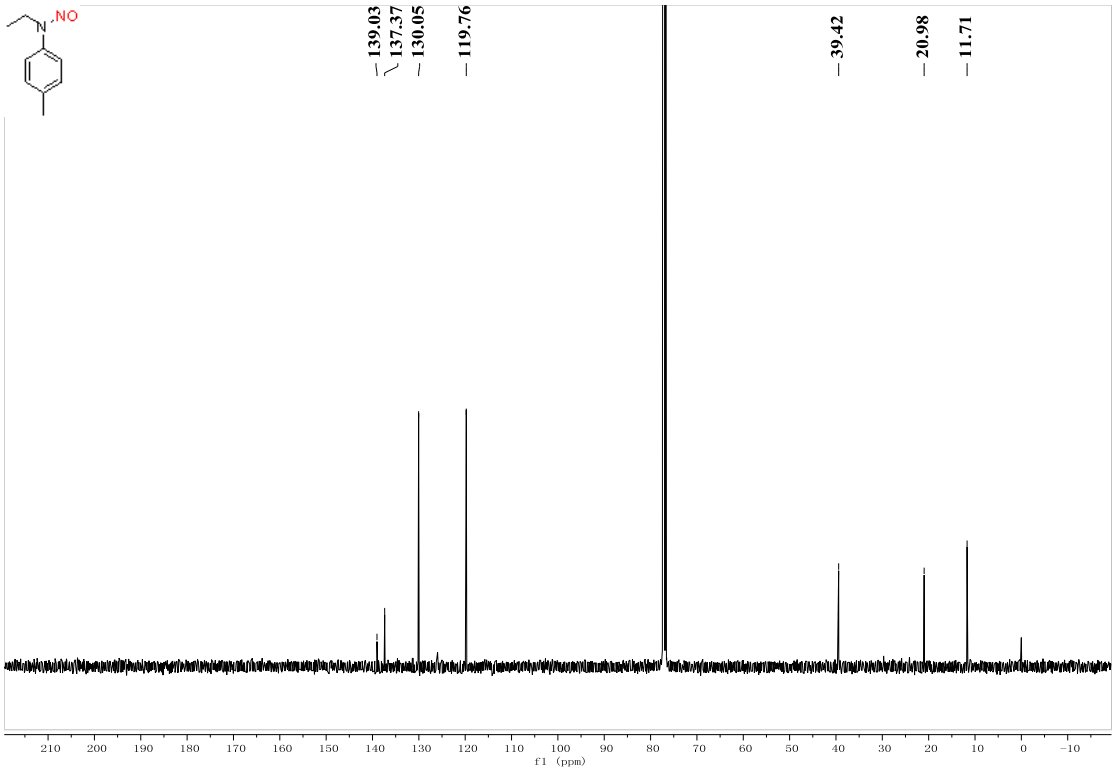
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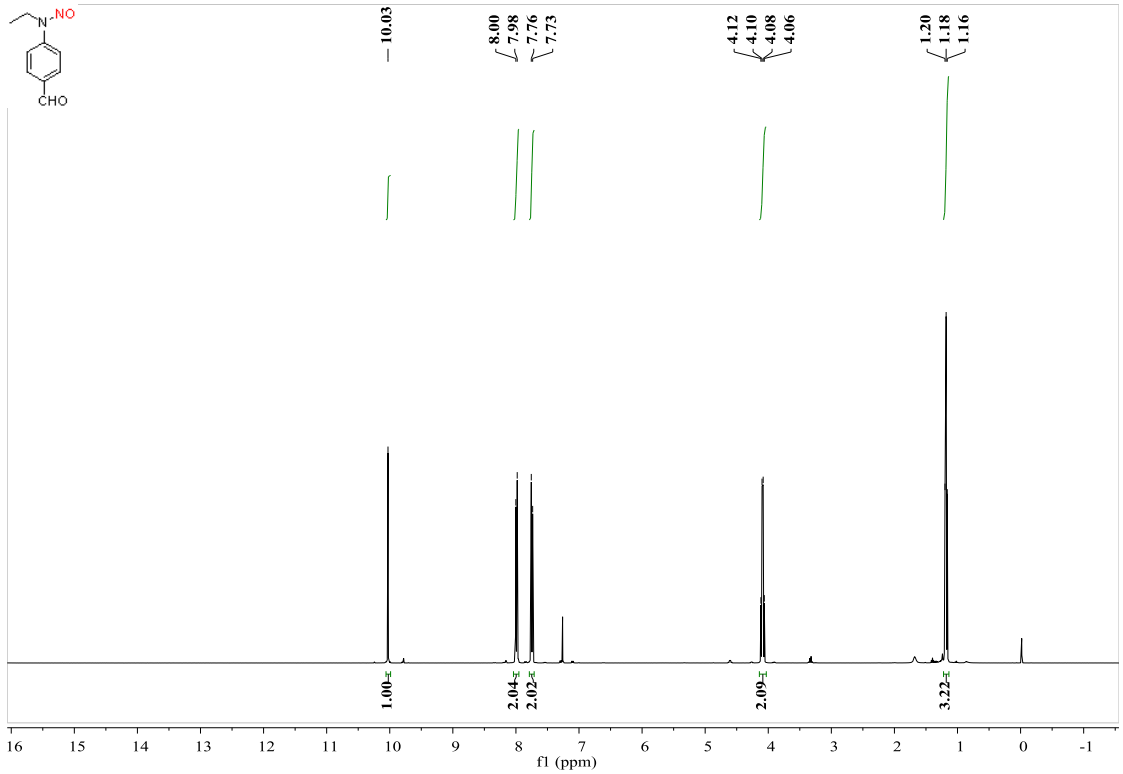
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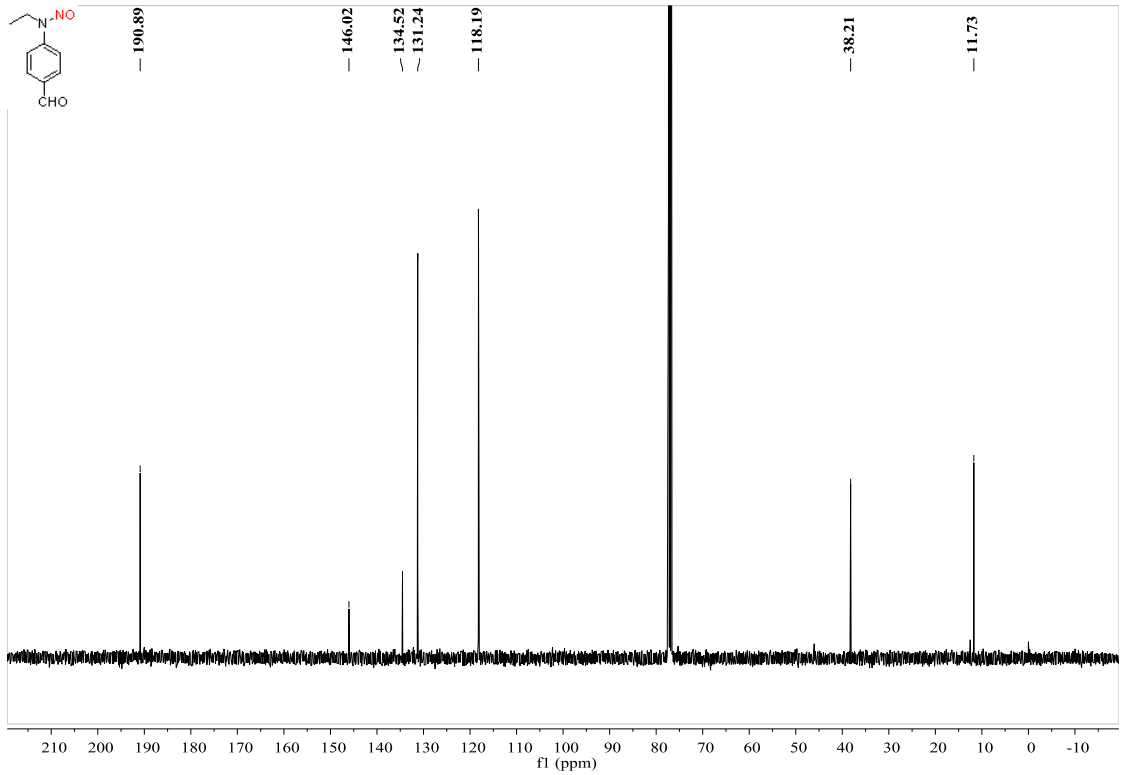
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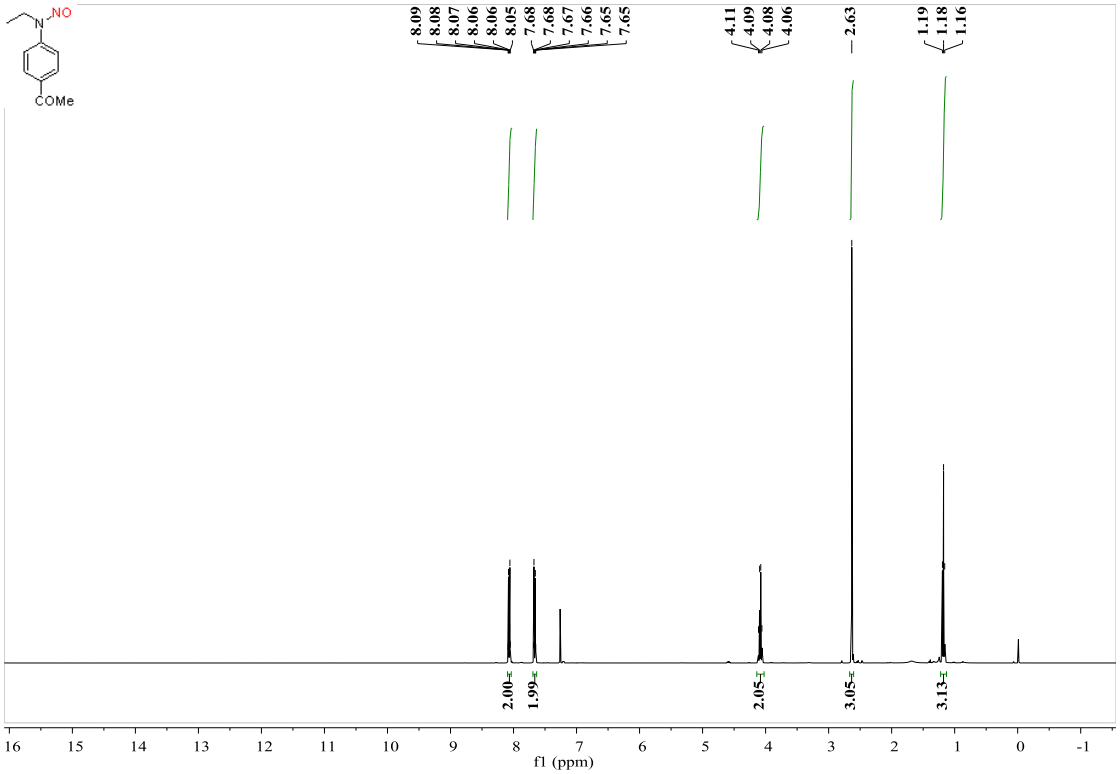
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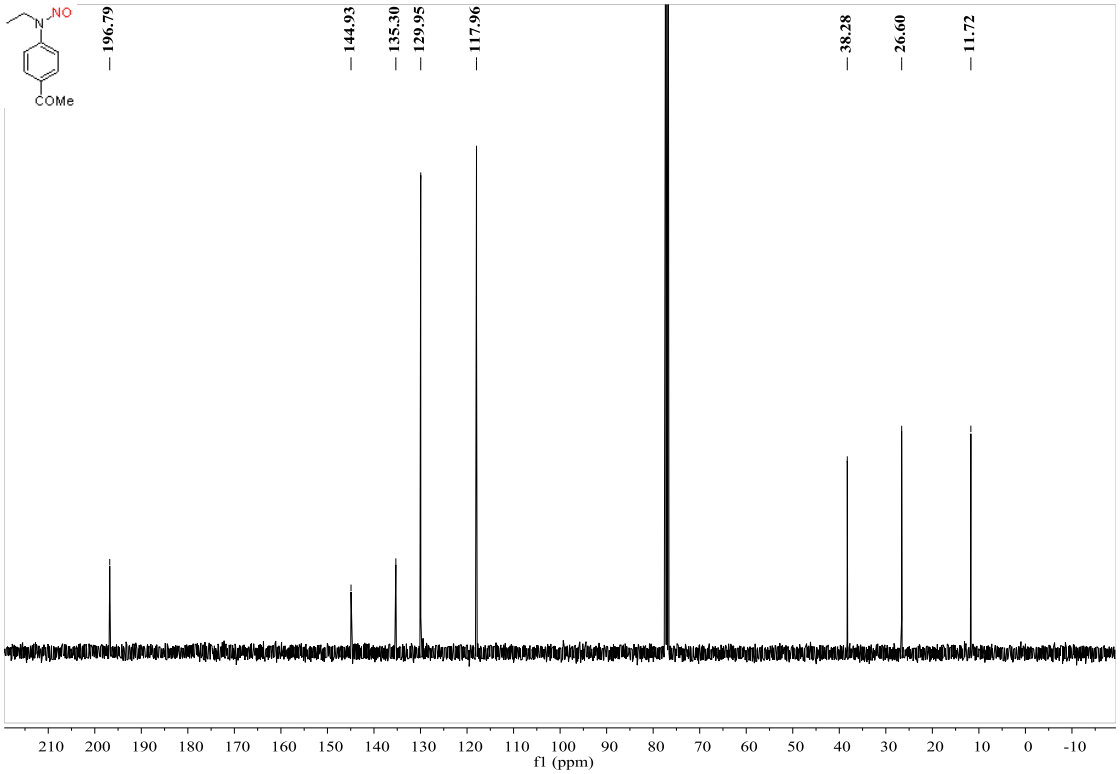
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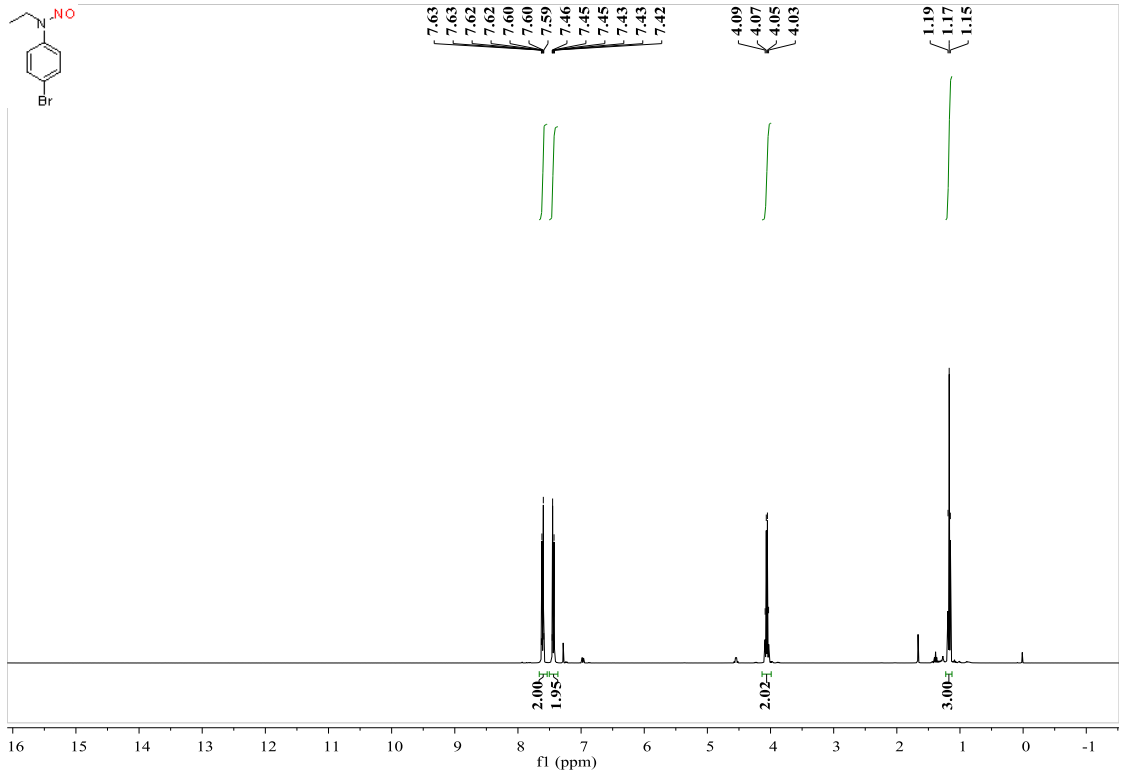
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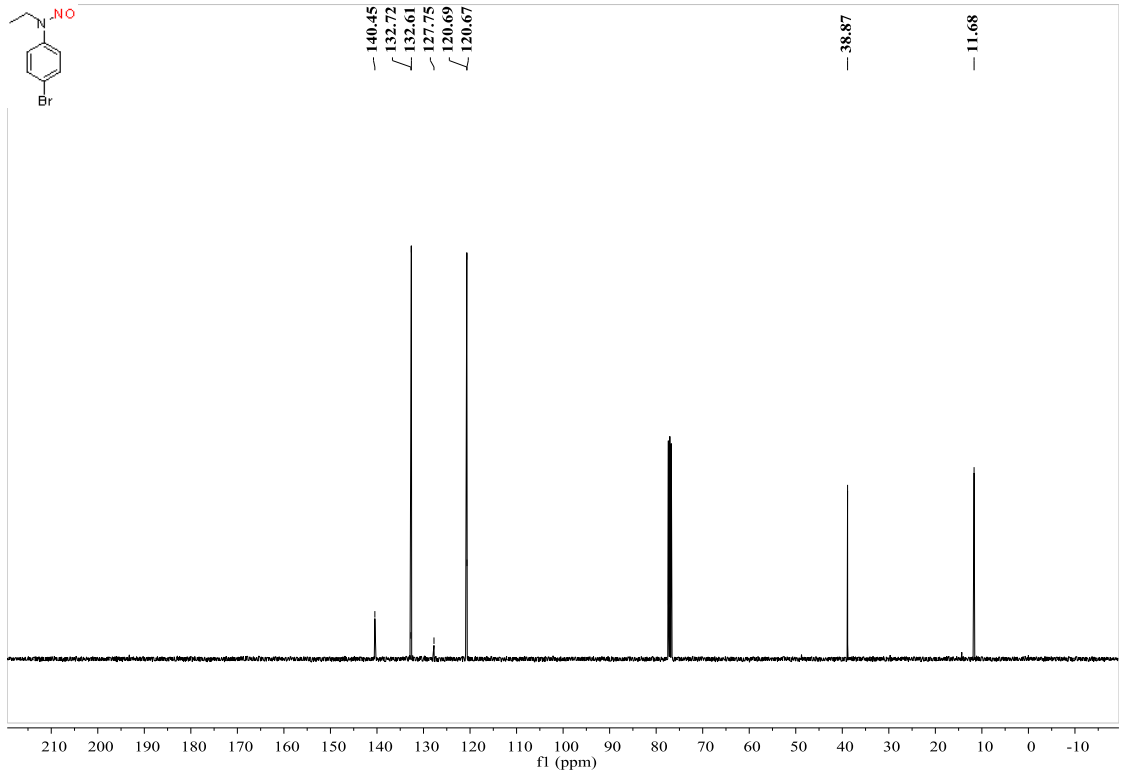
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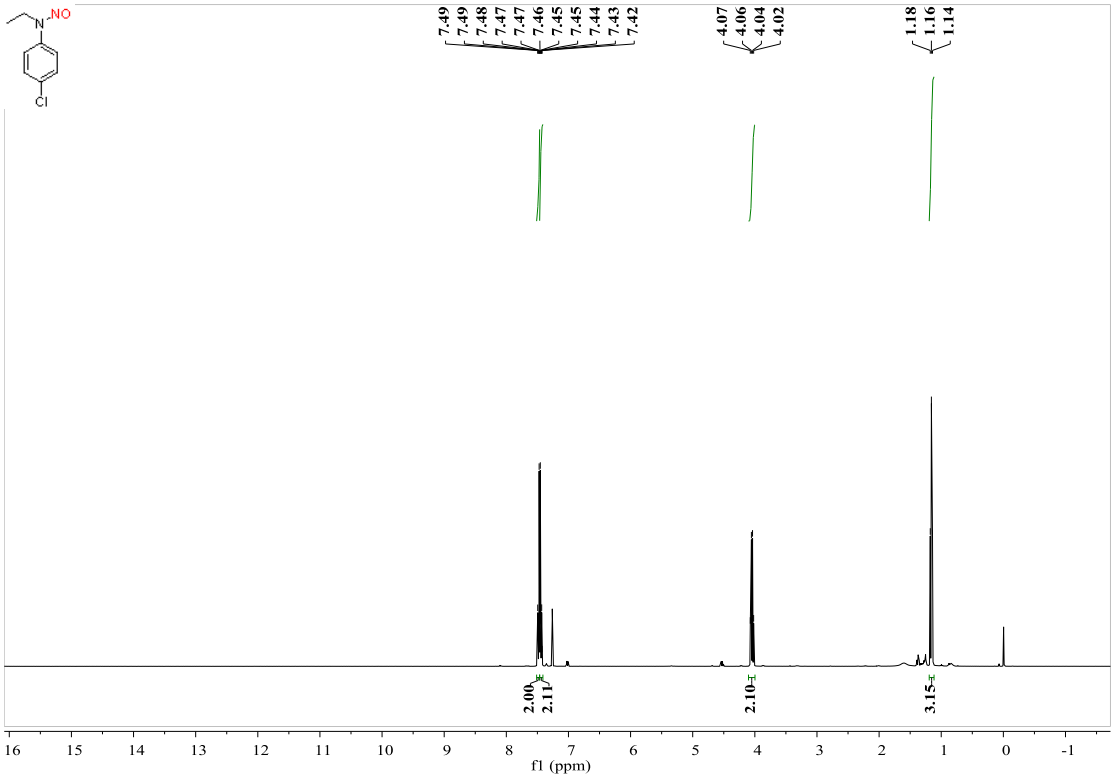
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7.49
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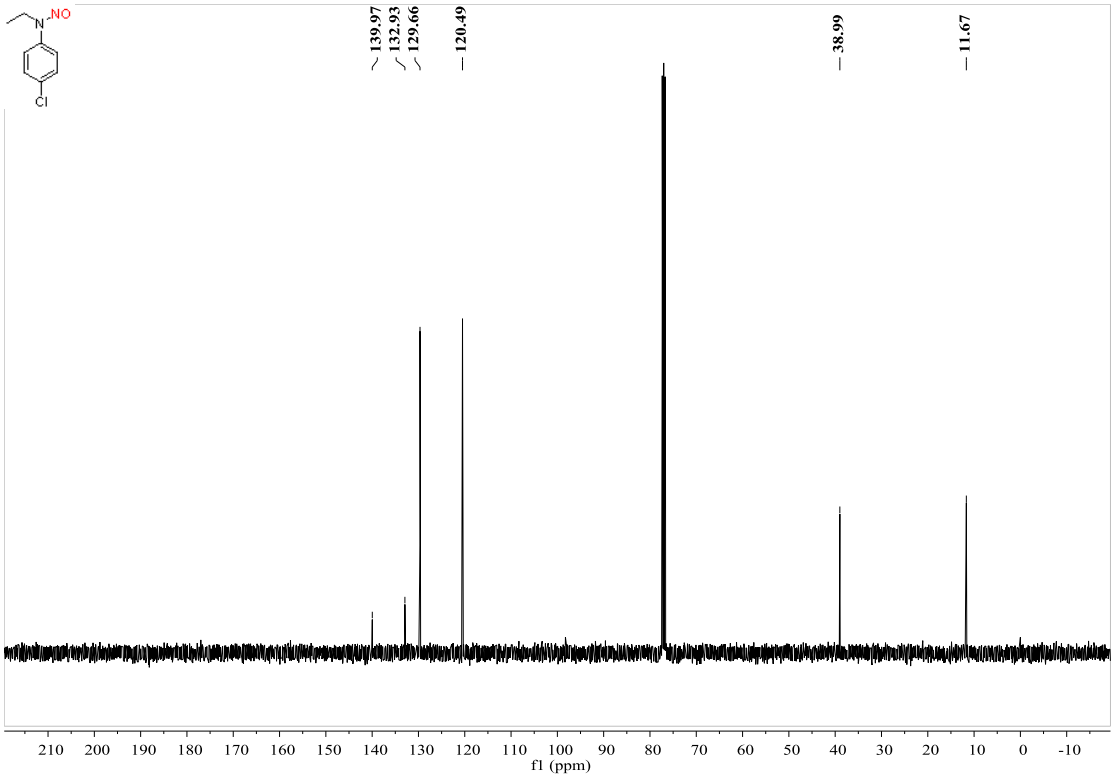
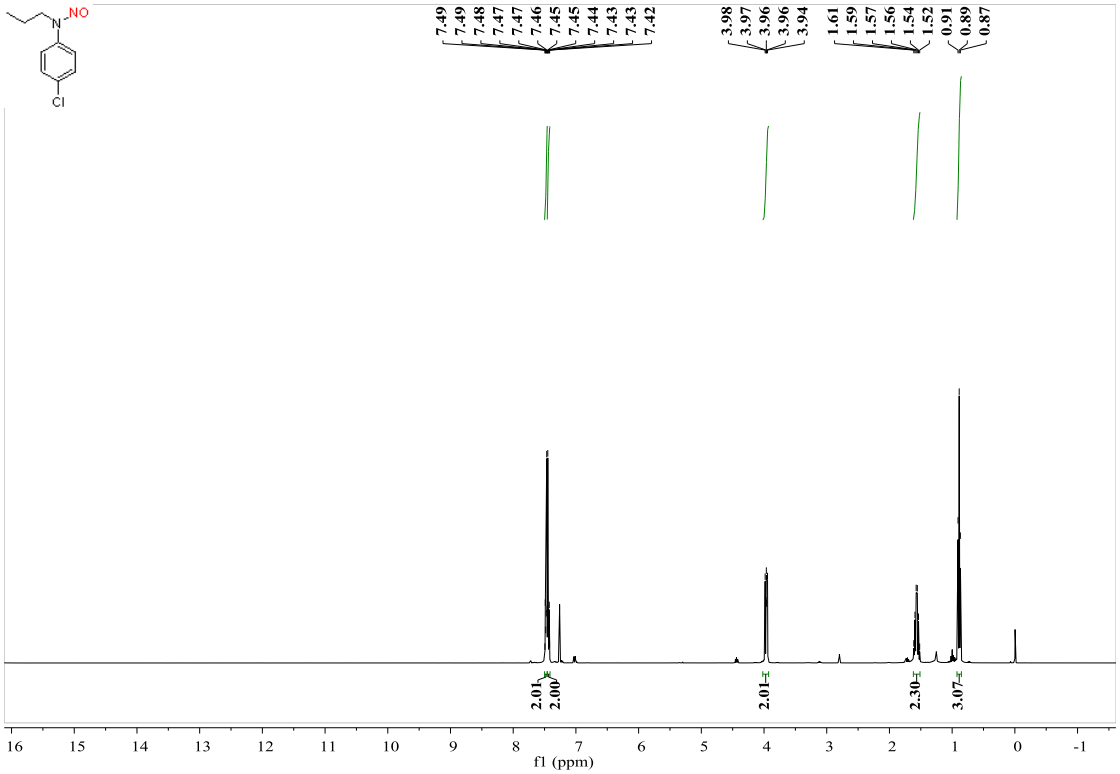
7.47
7.47
7.46
7.45
7.45
7.44
7.43
7.42
4.07
4.06
4.04
4.02
1.18
1.16
1.14
2.00
2.11
2.10
3.15
f1 (ppm)


139.97
132.93
129.66
120.49
38.99
11.67
f1 (ppm)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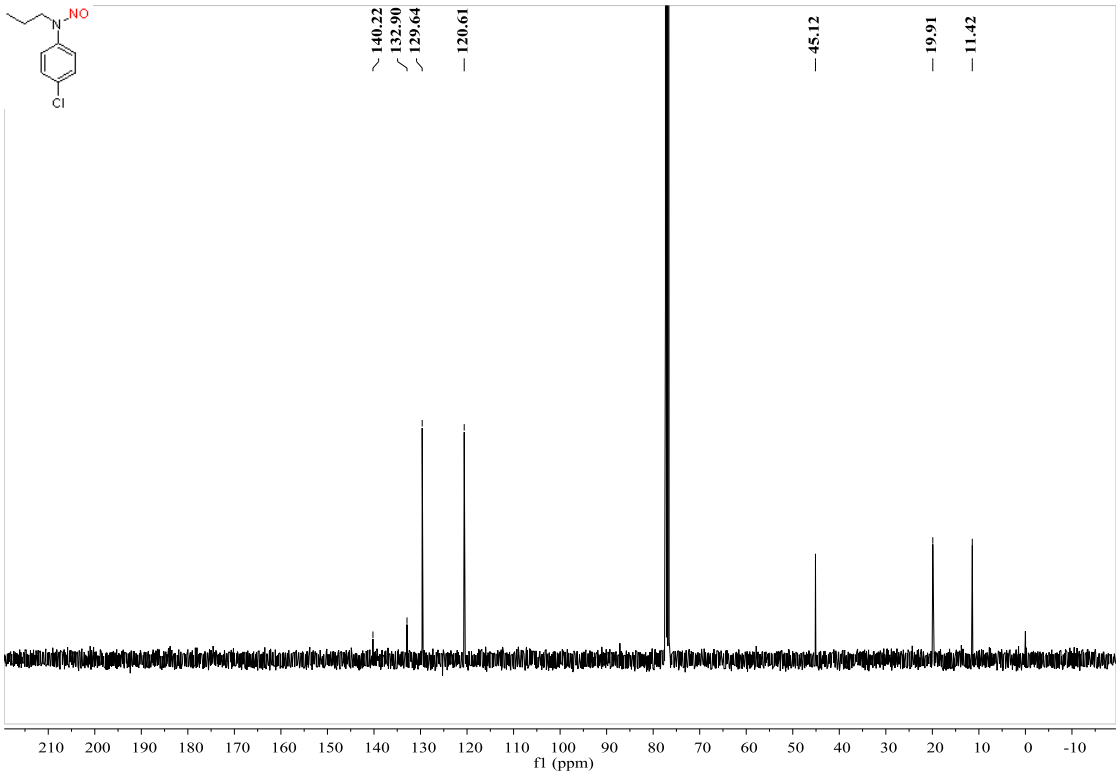
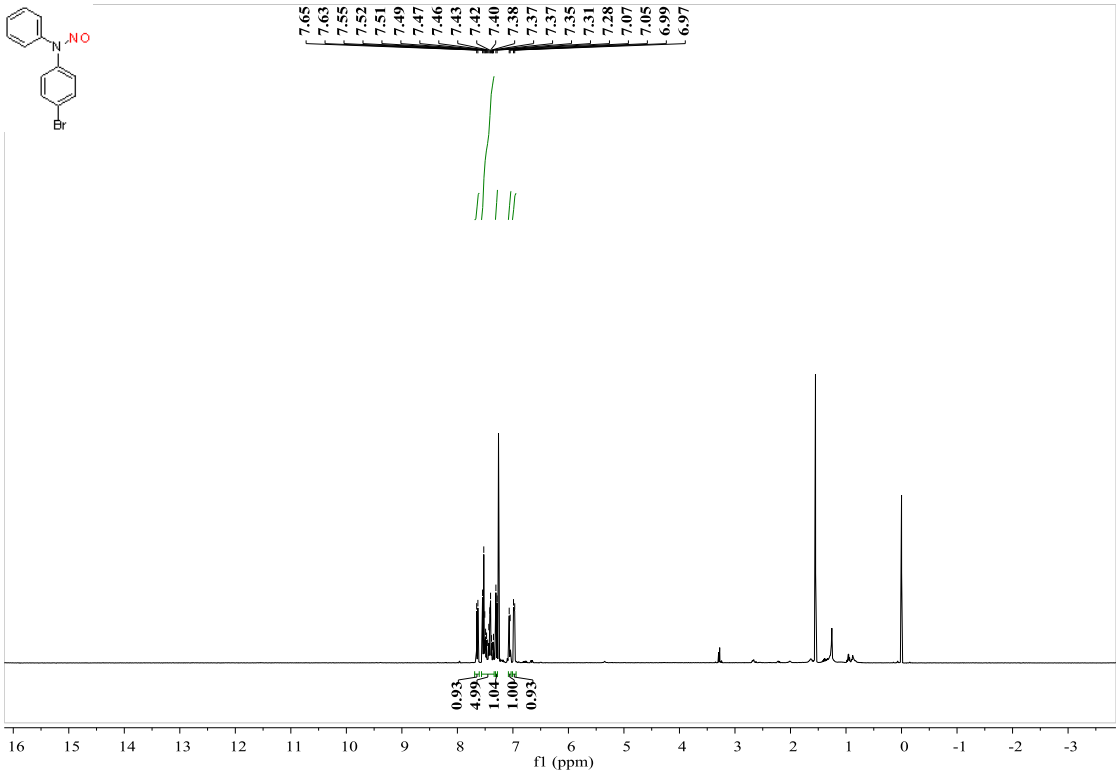
Cl
7.49
7.49
7.48
7.47
7.47
7.46
7.45
7.45
7.44
7.43
7.43
7.42
3.98
3.97
3.96
3.96
3.94
1.61
1.59
1.57
1.56
1.54
1.52
0.91
0.89
0.87
2.01
2.00
2.01
2.30
3.07
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


NO
N
Cl
140.22
132.90
129.64
120.61
45.12
19.91
11.42
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.52
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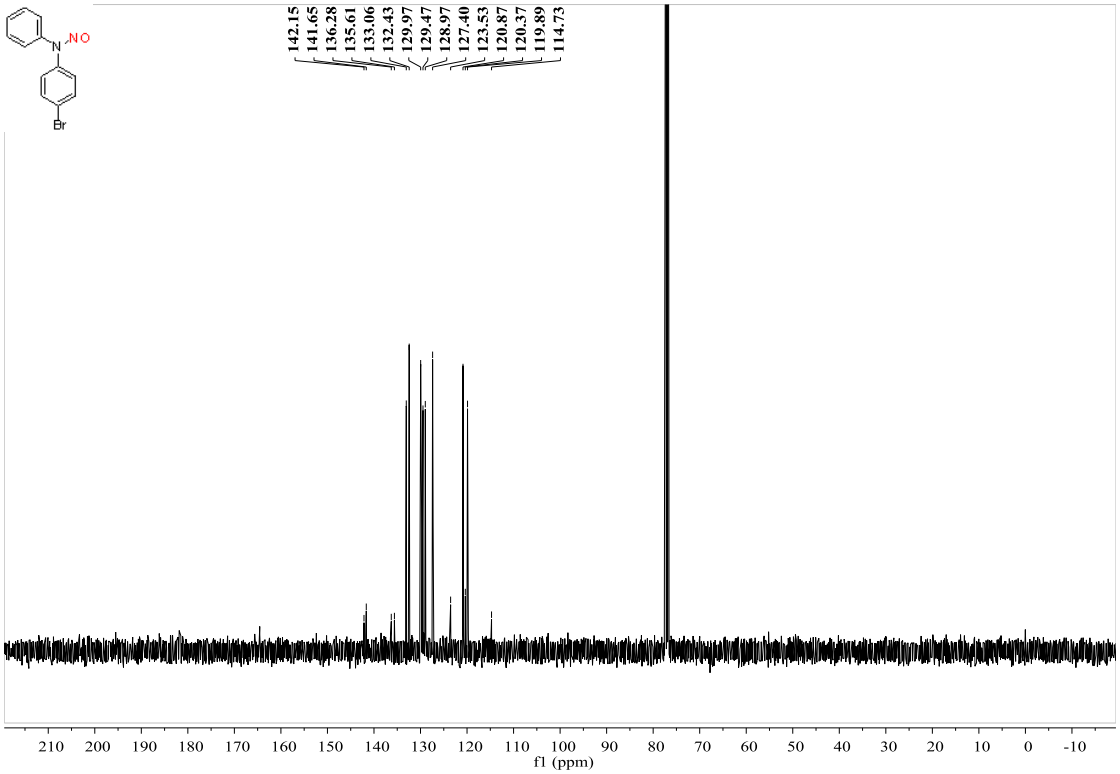
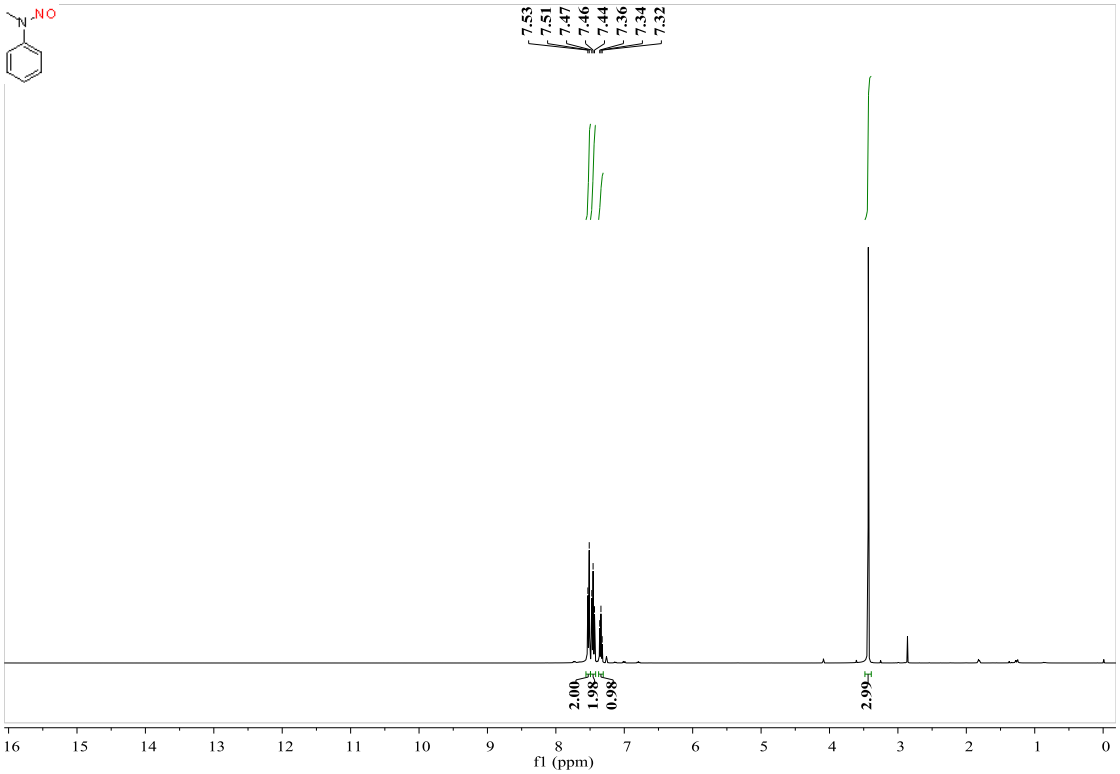
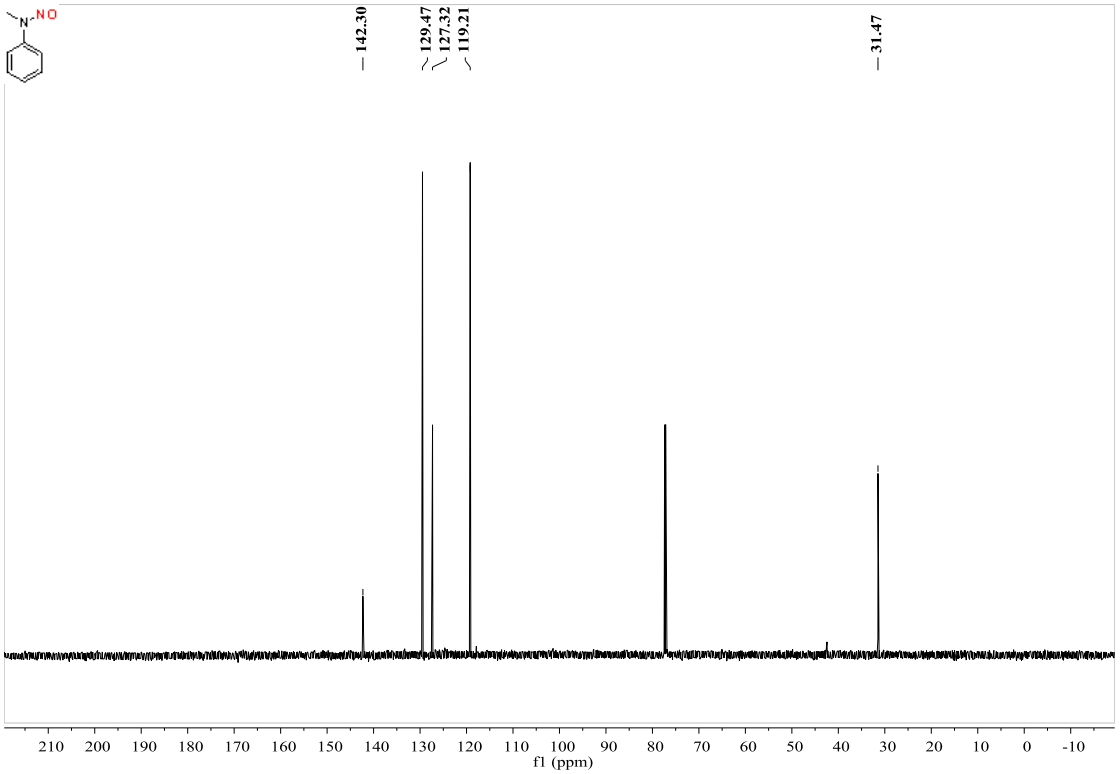
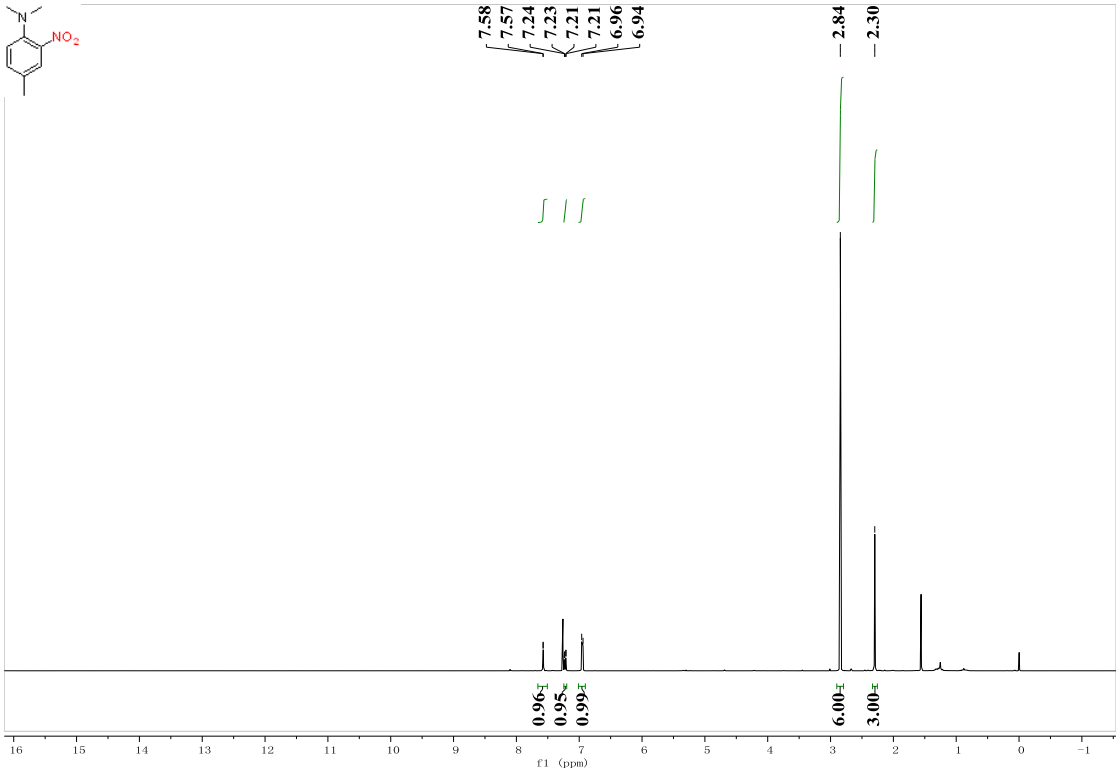
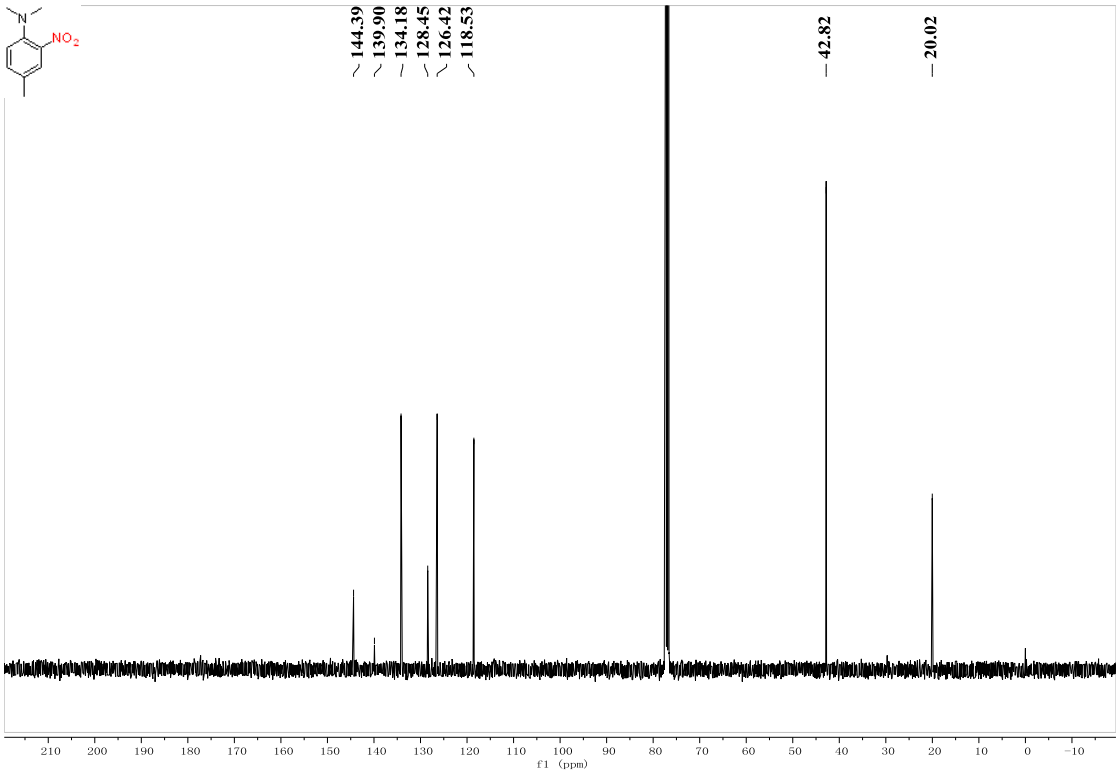
7.47
7.46
7.43
7.42
7.40
7.38
7.37
7.37
7.35
7.31
7.28
7.07
7.05
6.99
6.97
0.93
4.99
1.04
1.00
0.93
f1 (ppm)

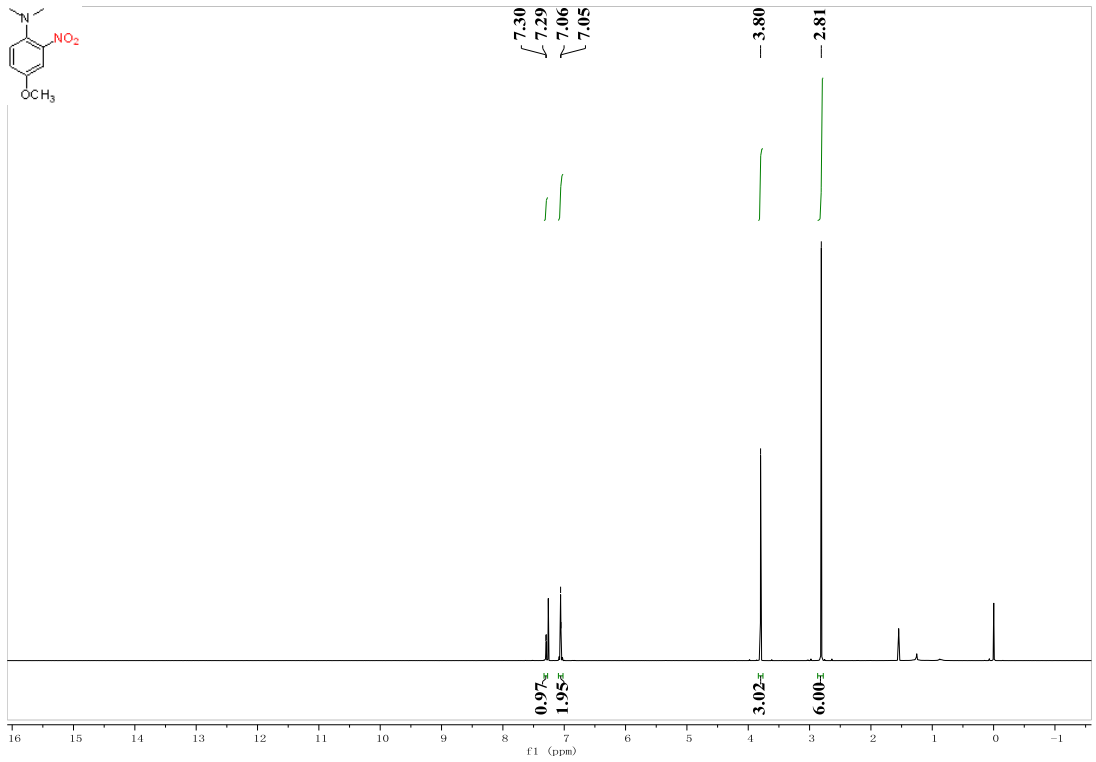

142.15
141.65
136.28
135.61
133.06
132.43
129.97
129.47
128.97
127.40
123.53
120.87
120.37
119.89
114.73
f1 (ppm)

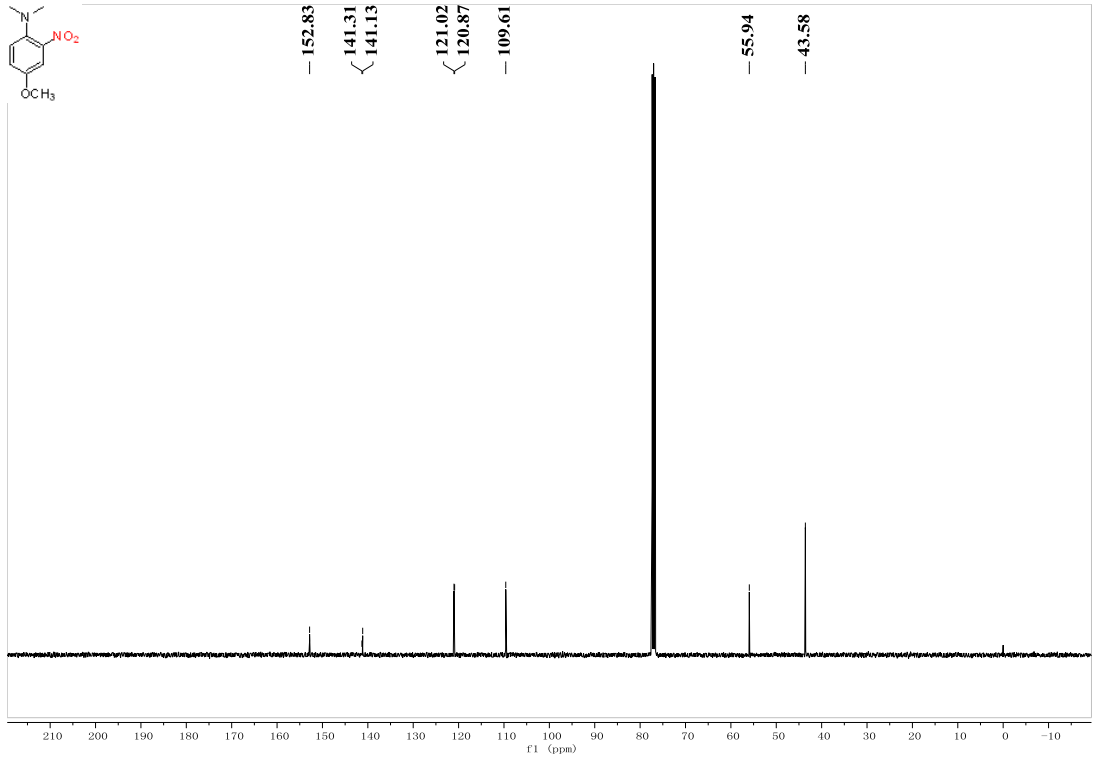

7.53
7.51
7.47
7.46
7.44
7.36
7.34
7.32
2.00
1.98
0.98
2.99
f1 (ppm)

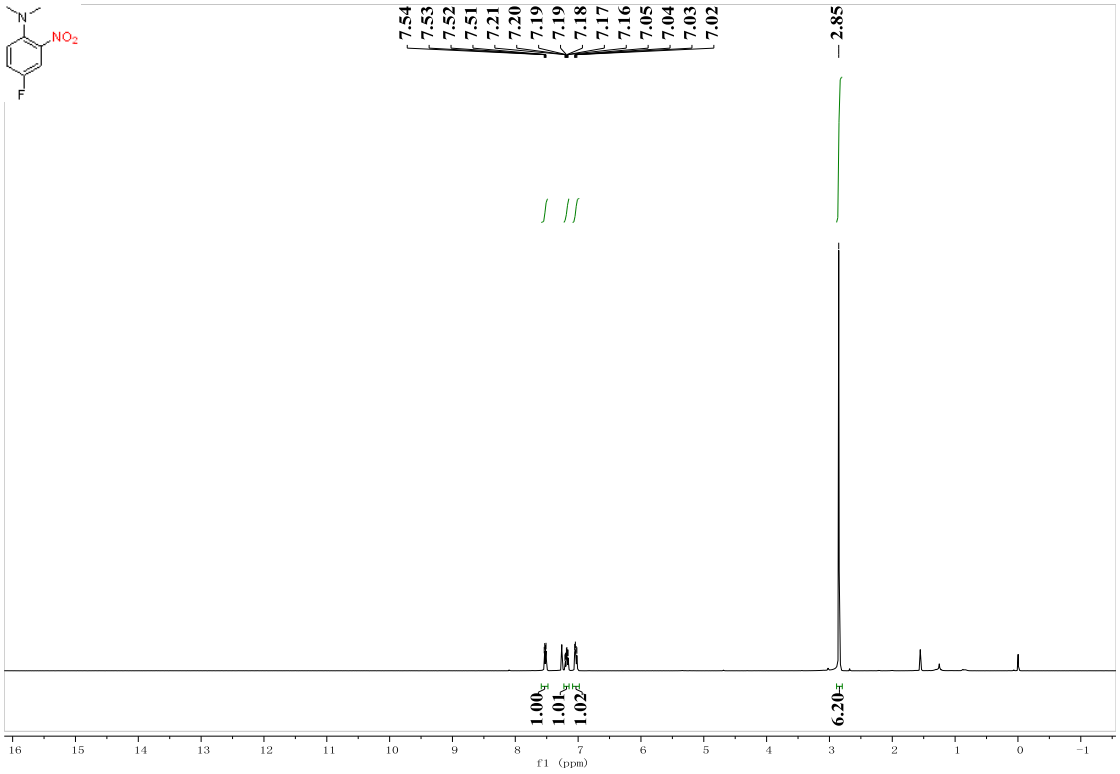

142.30
129.47
127.32
119.21
31.47
f1 (ppm)


7.58
7.57
7.24
7.23
7.21
7.21
6.96
6.94
2.84
2.30
0.96
0.95
0.99
6.00
3.00
f1 (ppm)


144.39
139.90
134.18
128.45
126.42
118.53
42.82
20.02
f1 (ppm)


7.30
7.29
7.06
7.05
3.80
2.81
0.97
1.95
3.02
6.00
f1 (ppm)


152.83
141.31
141.13
121.02
120.87
109.61
55.94
43.58
f1 (ppm)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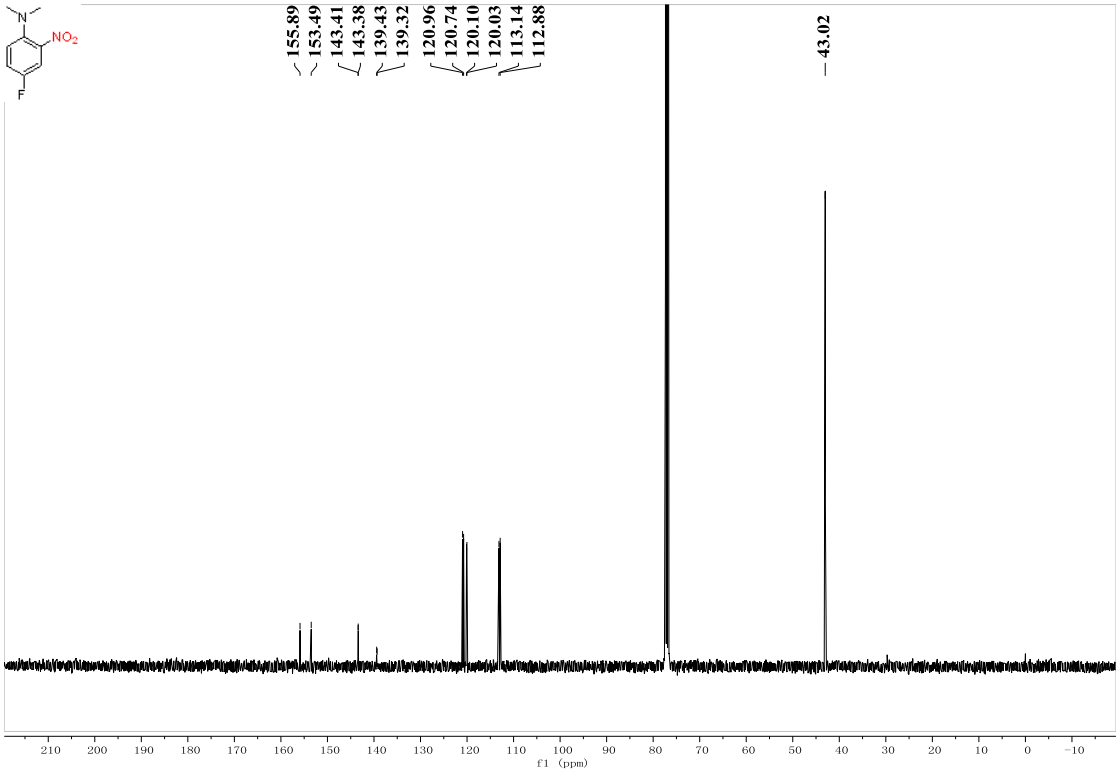
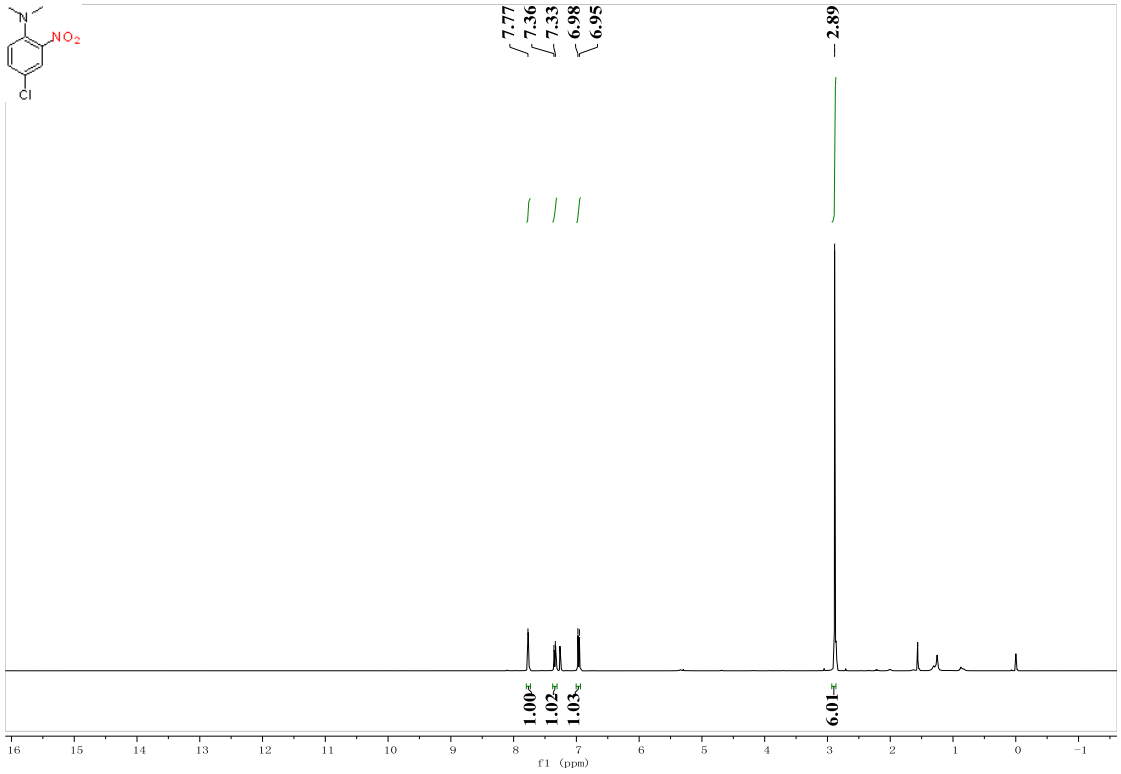
7.53
7.52
7.51
7.21
7.20
7.19
7.19
7.18
7.17
7.16
7.05
7.04
7.03
7.02
2.85
1.00
1.01
1.02
6.20
f1 (ppm)


155.89
153.49
143.41
143.38
139.43
139.32
120.96
120.74
120.10
120.03
113.14
112.88
43.02
f1 (ppm)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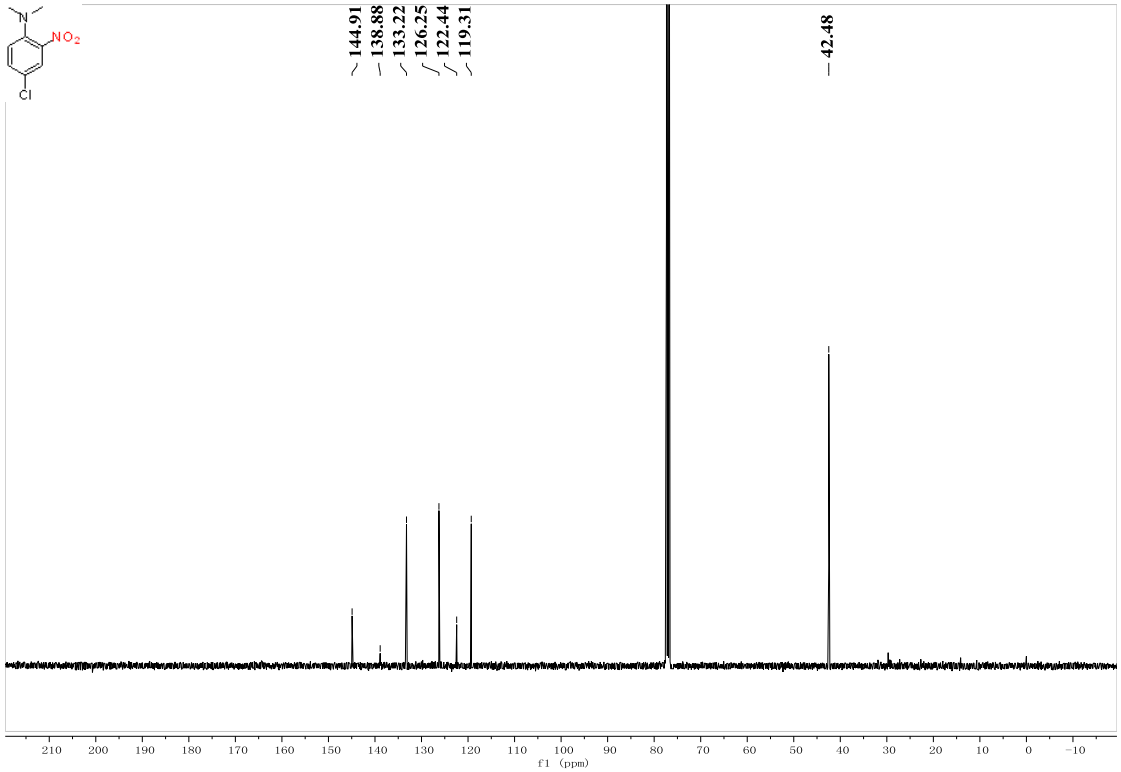
7.36
7.33
6.98
6.95
2.89
1.00
1.02
1.03
6.01
f1 (ppm)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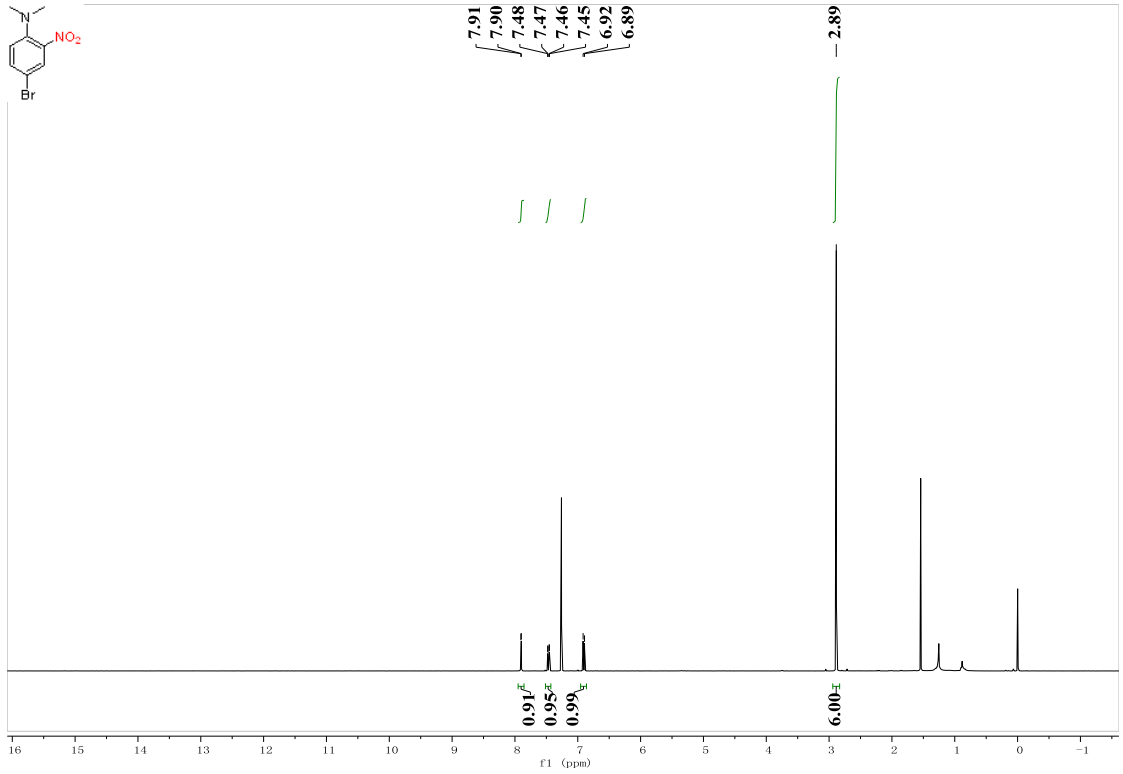
126.25
122.44
119.31
42.48
f1 (ppm)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7.90
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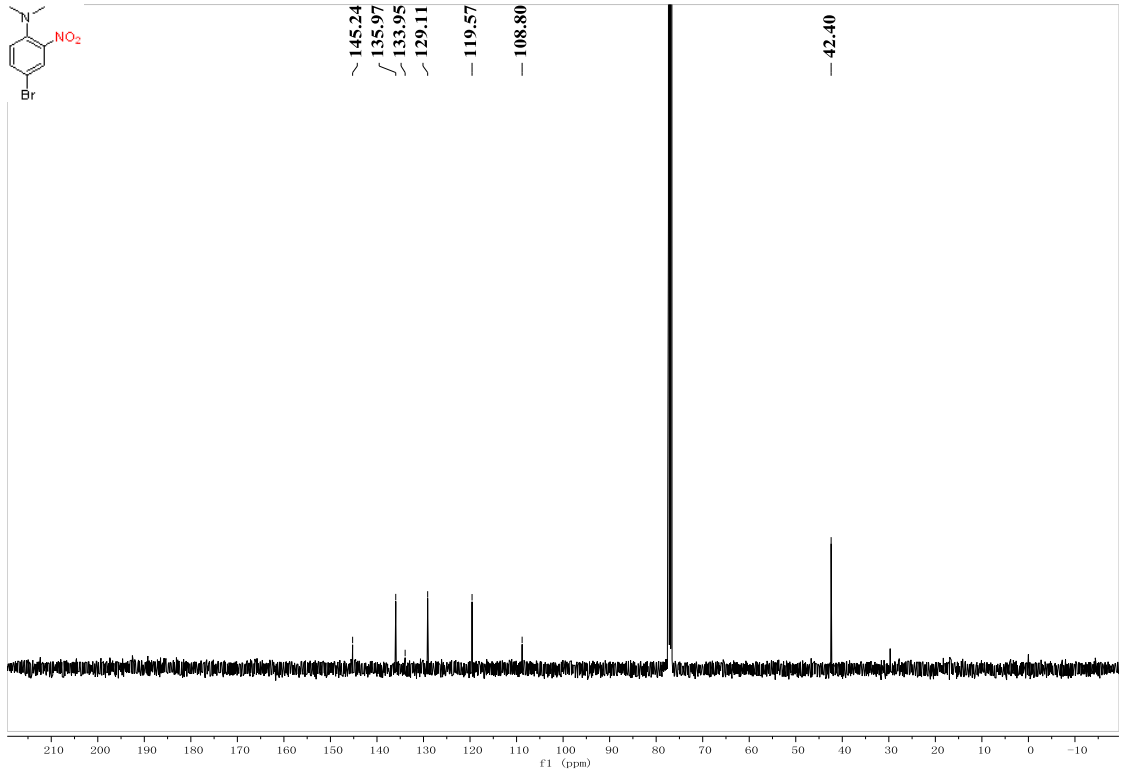
7.47
7.46
7.45
6.92
6.89
2.89
0.91
0.95
0.99
6.00
f1 (ppm)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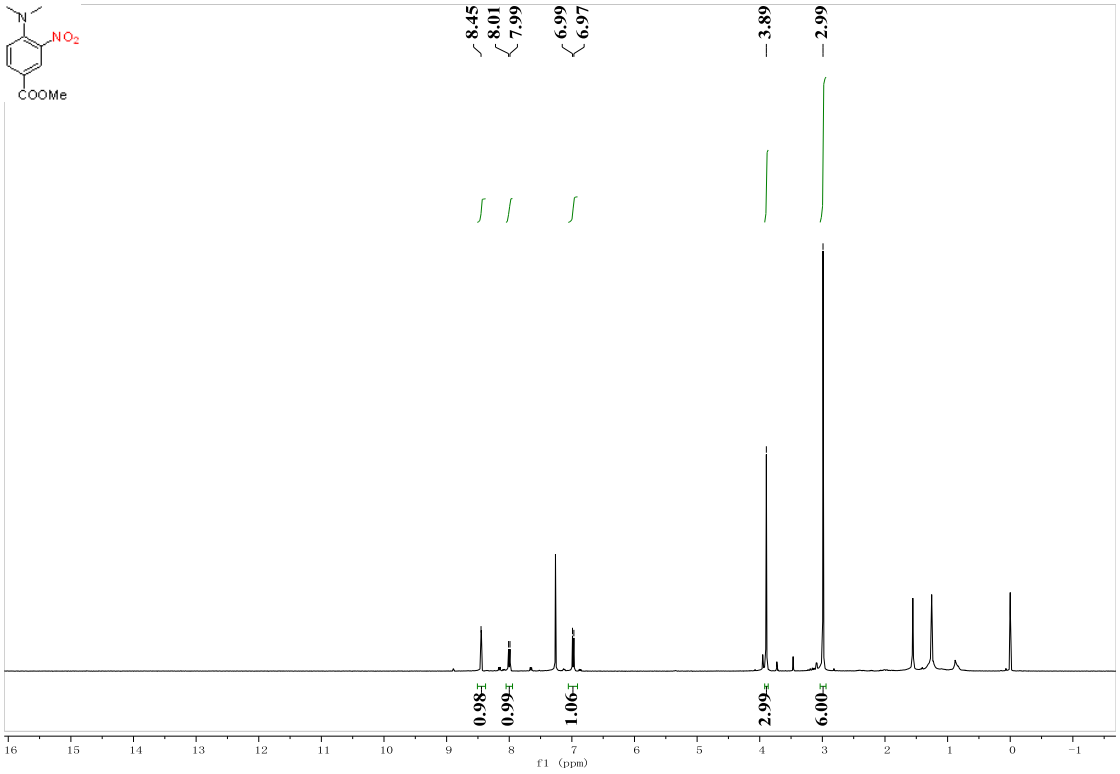
119.57
108.80
42.40
f1 (ppm)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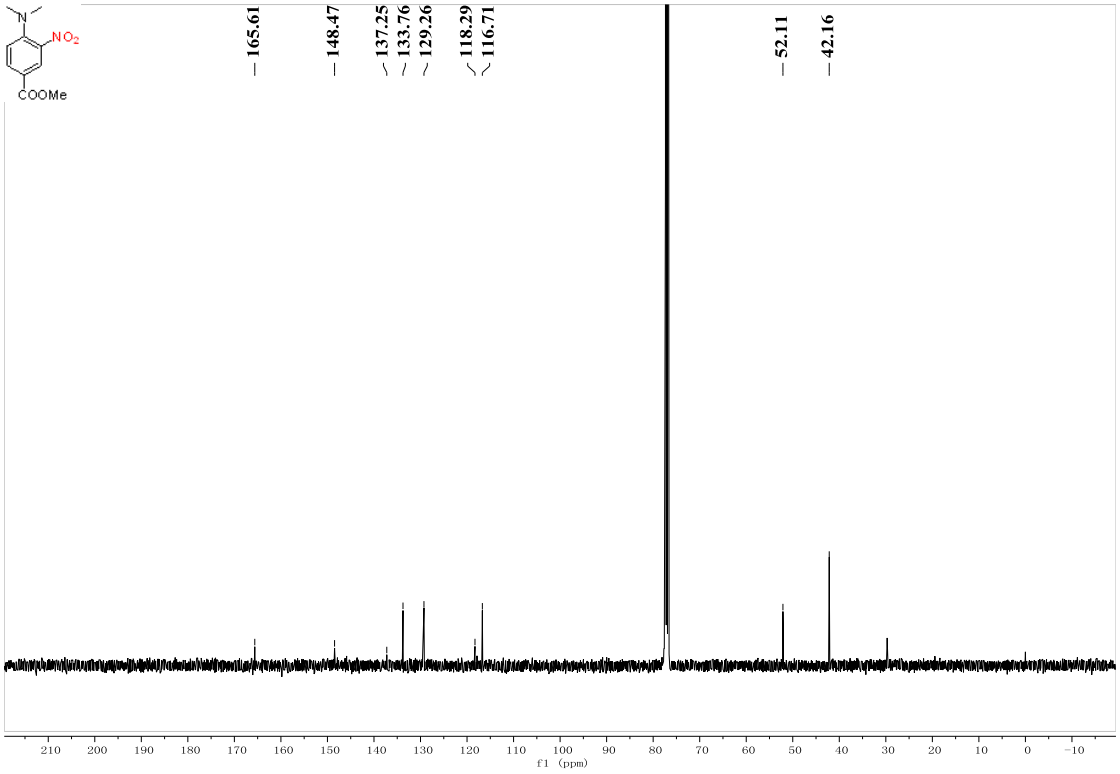
7.99
6.99
6.97
3.89
2.99
0.98
0.99
1.06
2.99
6.00
f1 (ppm)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129.26
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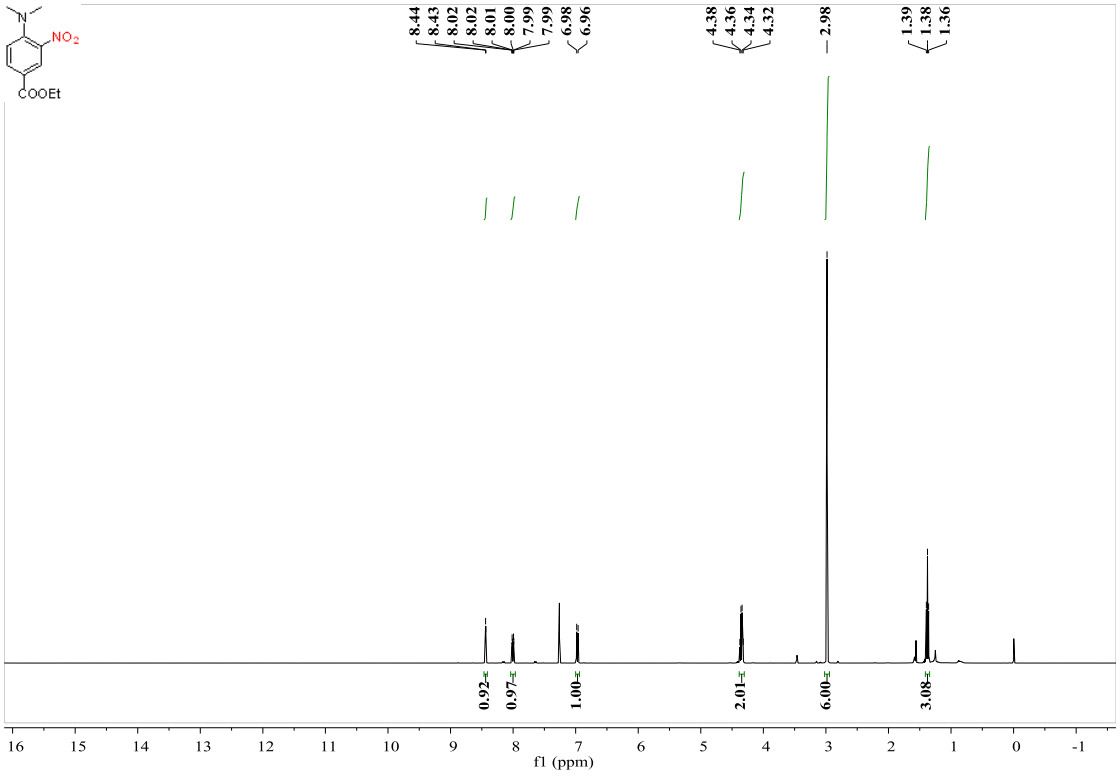
116.71
52.11
42.16
f1 (ppm)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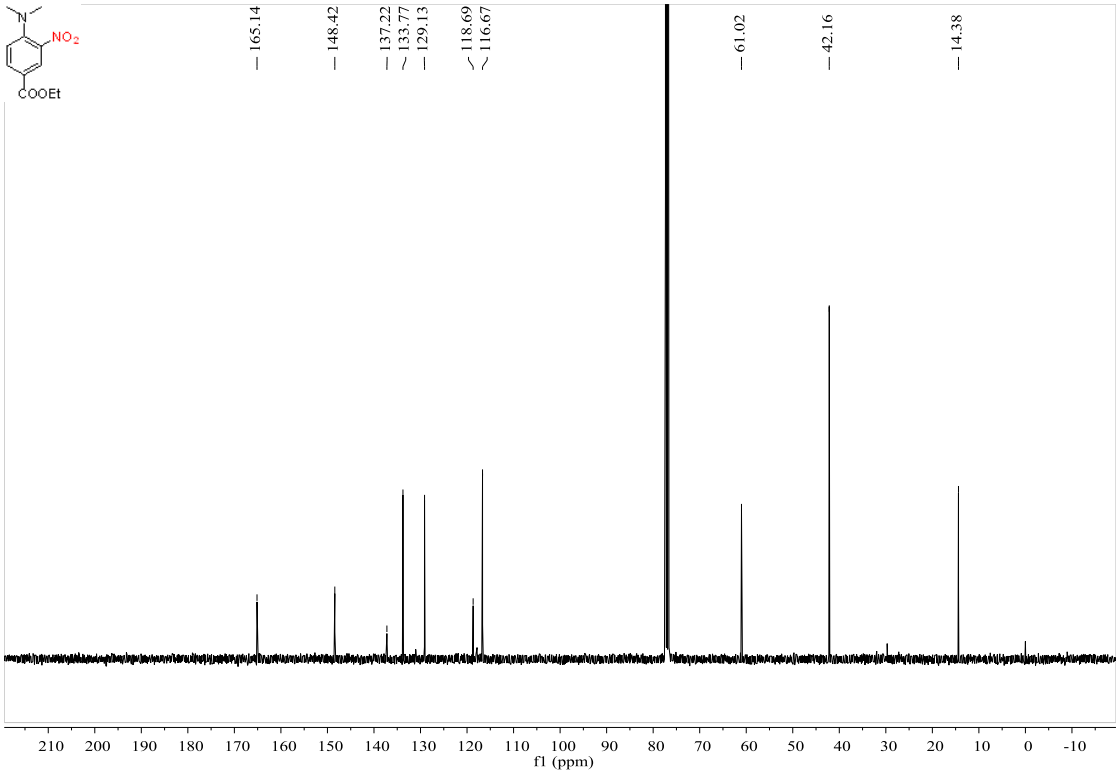
8.43
8.02
8.02
8.01
8.00
7.99
7.99
6.98
6.96
4.38
4.36
4.34
4.32
2.98
1.39
1.38
1.36
0.92
0.97
1.00
2.01
6.00
3.08
f1 (ppm)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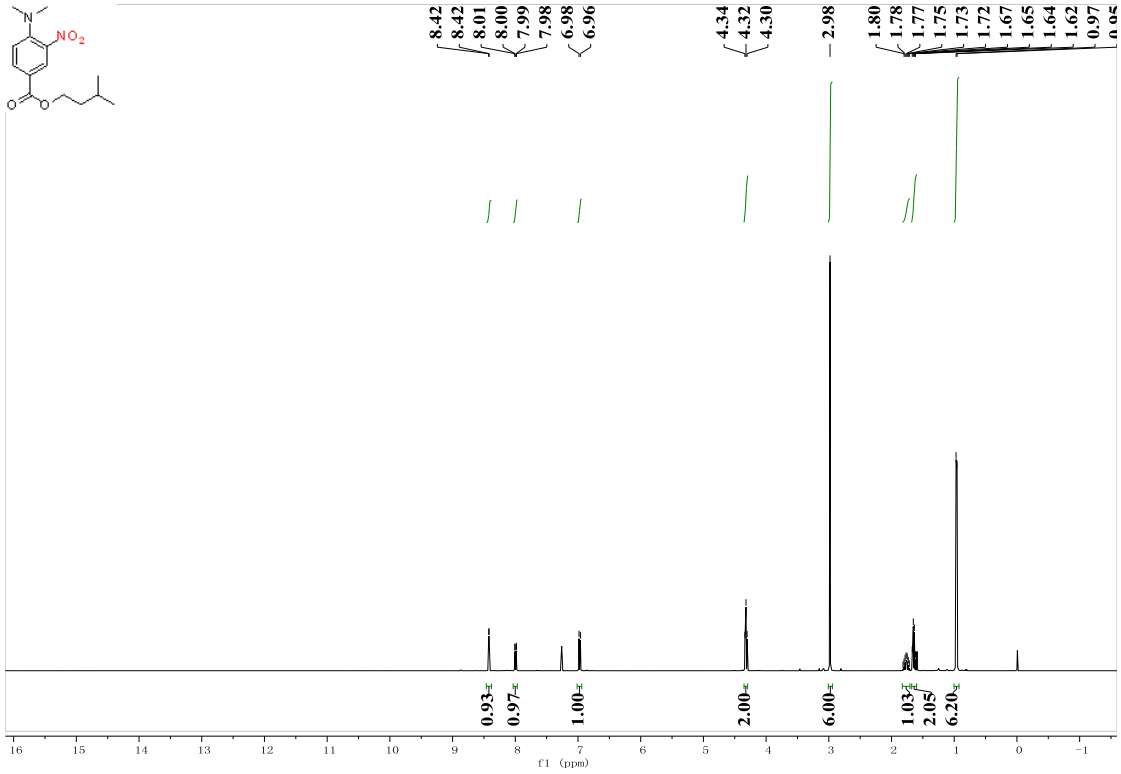
129.13
118.69
116.67
61.02
42.16
14.38
f1 (ppm)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8.42
8.01
8.00
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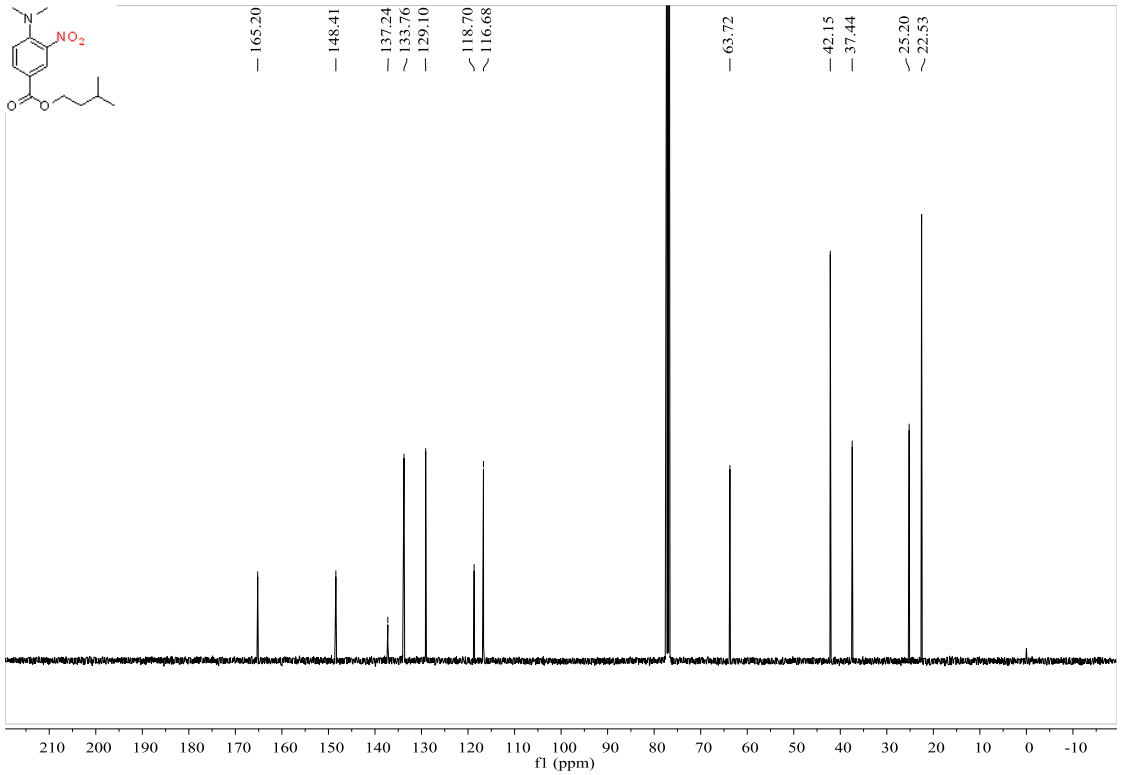
7.98
6.98
6.96
4.34
4.32
4.30
2.98
1.80
1.78
1.77
1.75
1.73
1.72
1.67
1.65
1.64
1.62
0.97
0.93
0.97
1.00
2.00
6.00
1.03
2.05
6.20
f1 (ppm)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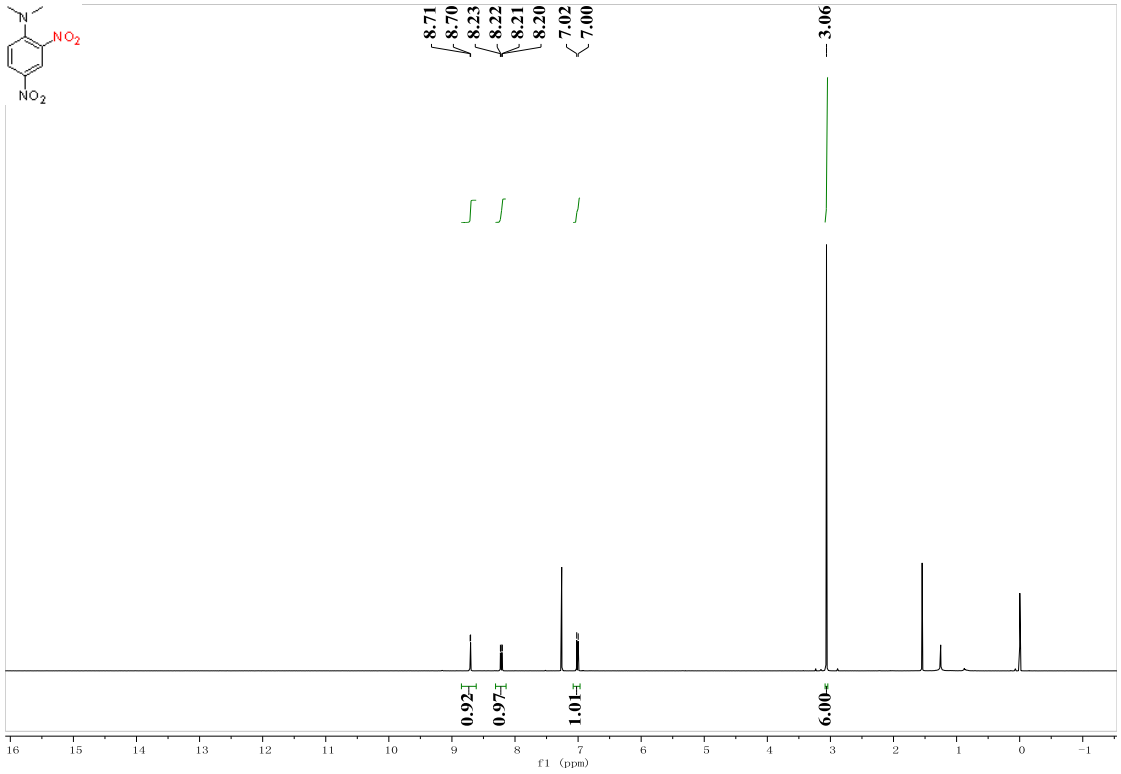
129.10
118.70
116.68
63.72
42.15
37.44
25.20
22.53
f1 (ppm)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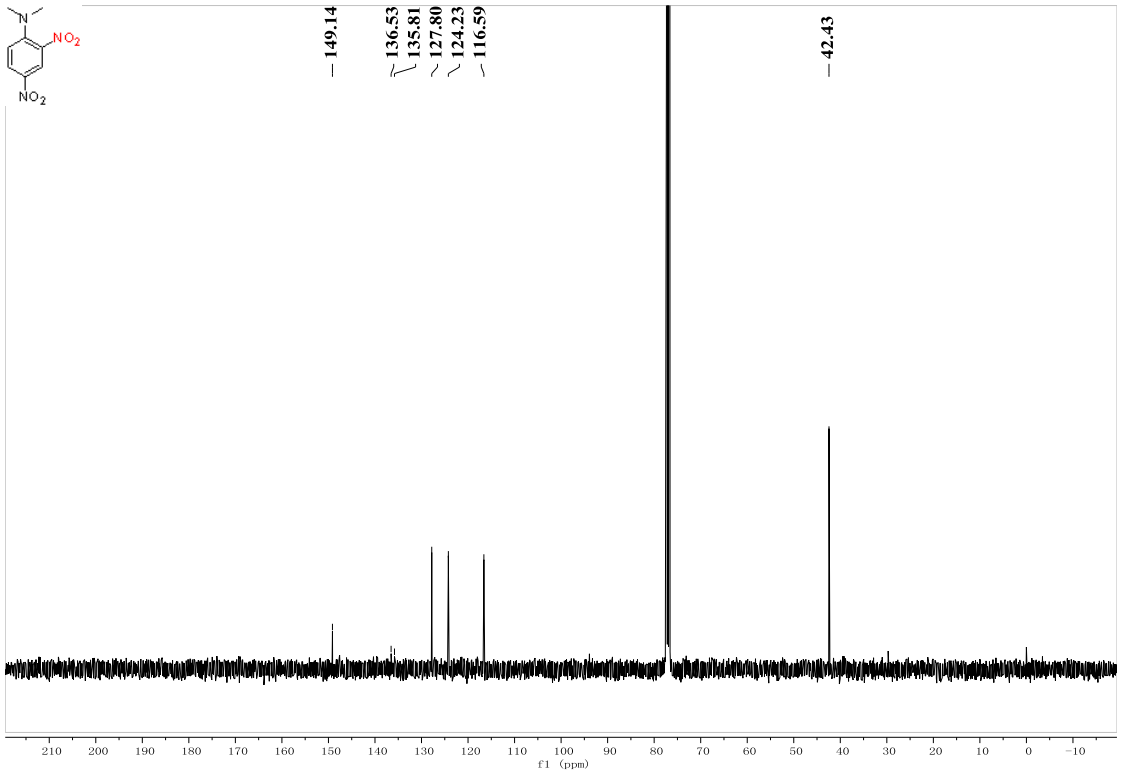
8.22
8.21
8.20
7.02
7.00
3.06
0.92
0.97
1.01
6.00
f1 (ppm)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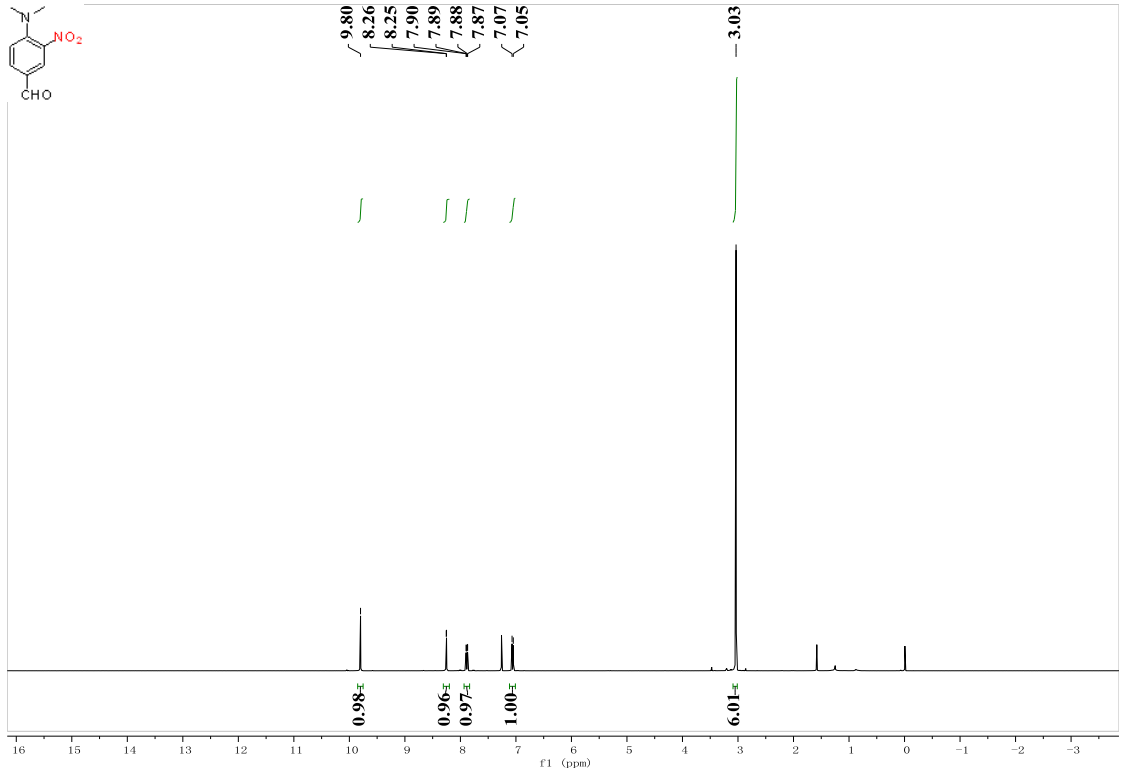
124.23
116.59
42.43
f1 (ppm)


9.80
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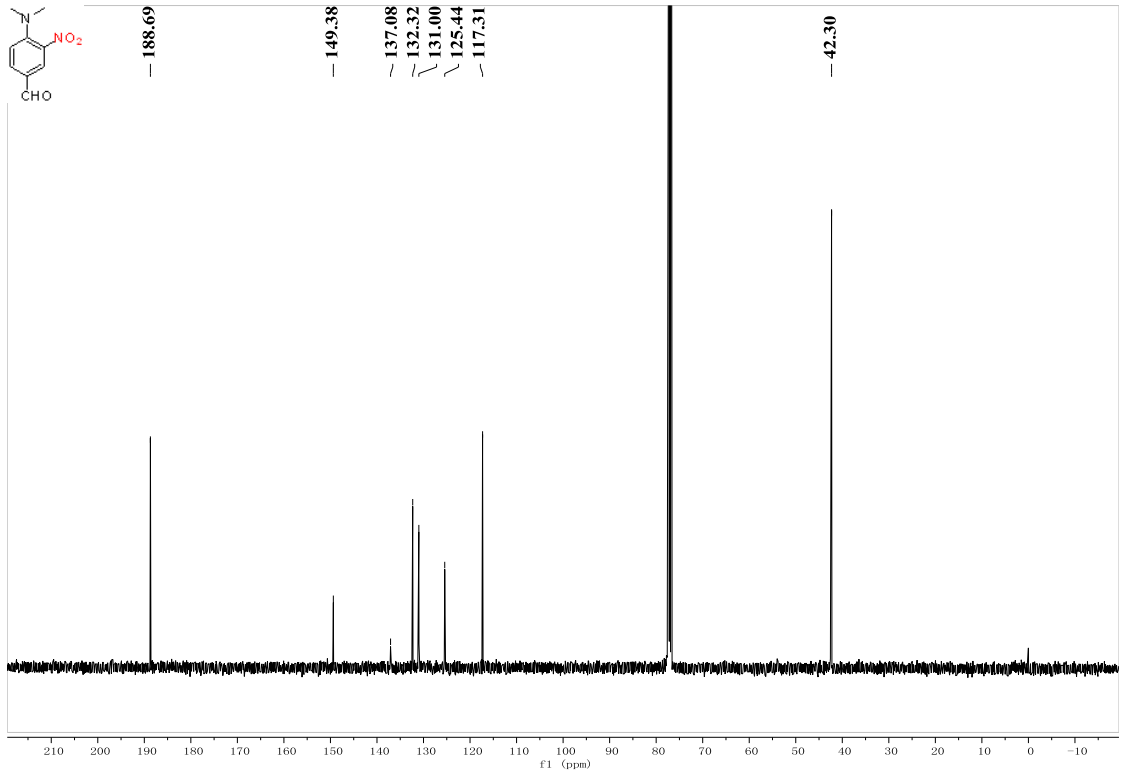
8.25
7.90
7.89
7.88
7.87
7.07
7.05
3.03
0.98
0.96
0.97
1.00
6.01
f1 (ppm)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131.00
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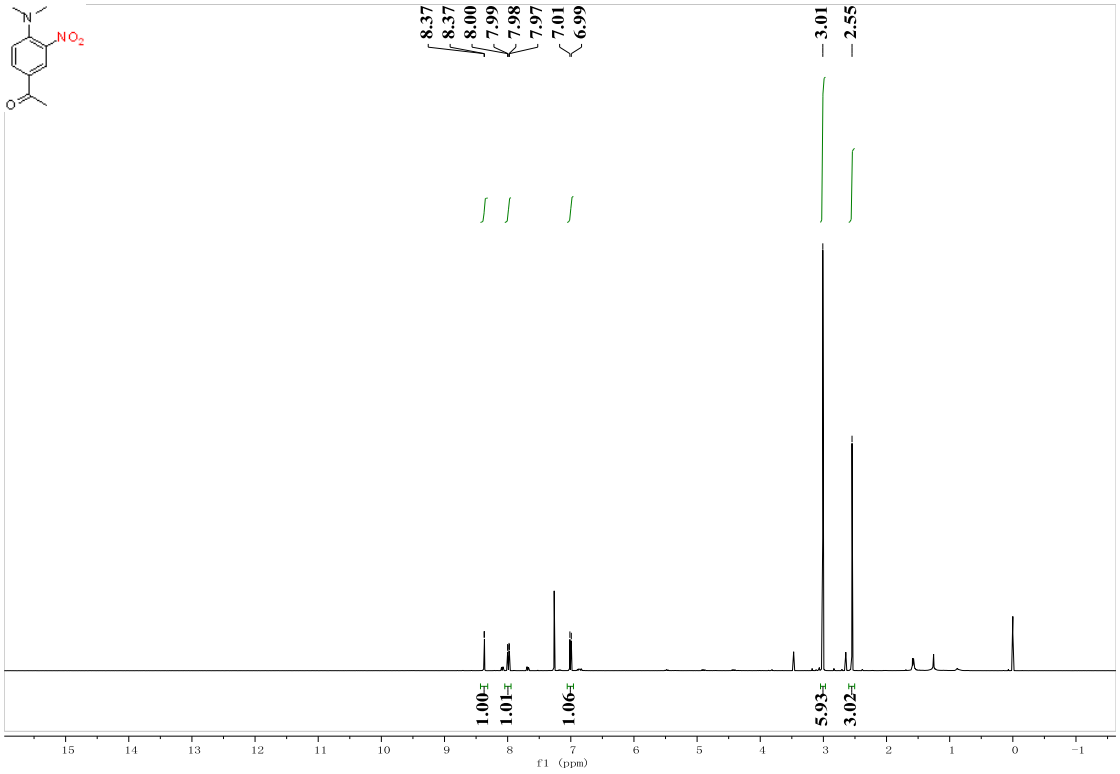
117.31
42.30
f1 (ppm)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7.97
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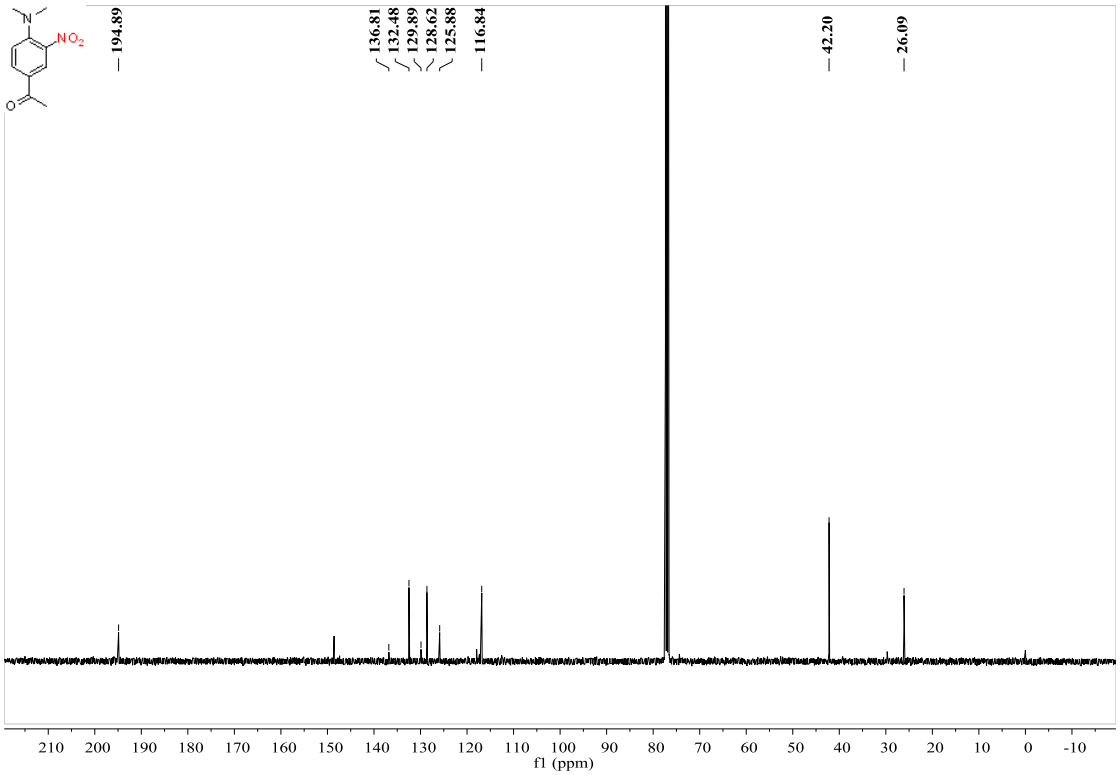
2.55
1.00
1.01
1.06
5.93
3.02
f1 (ppm)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116.84
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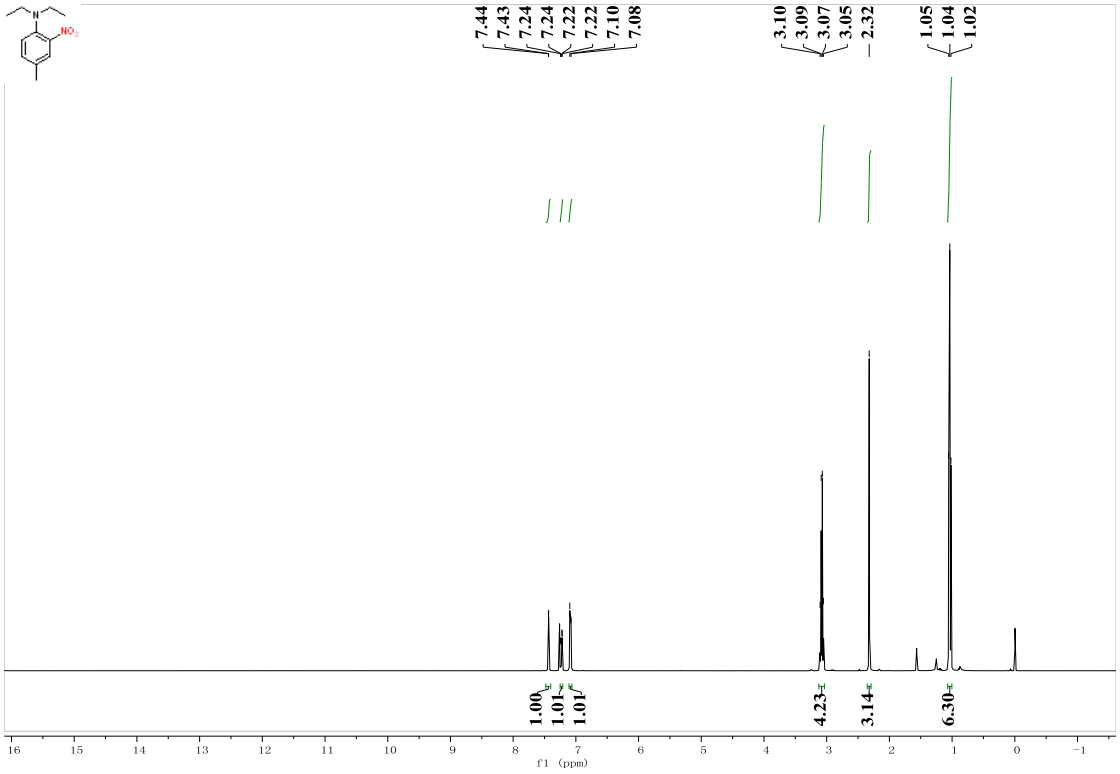
26.09
f1 (ppm)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7.43
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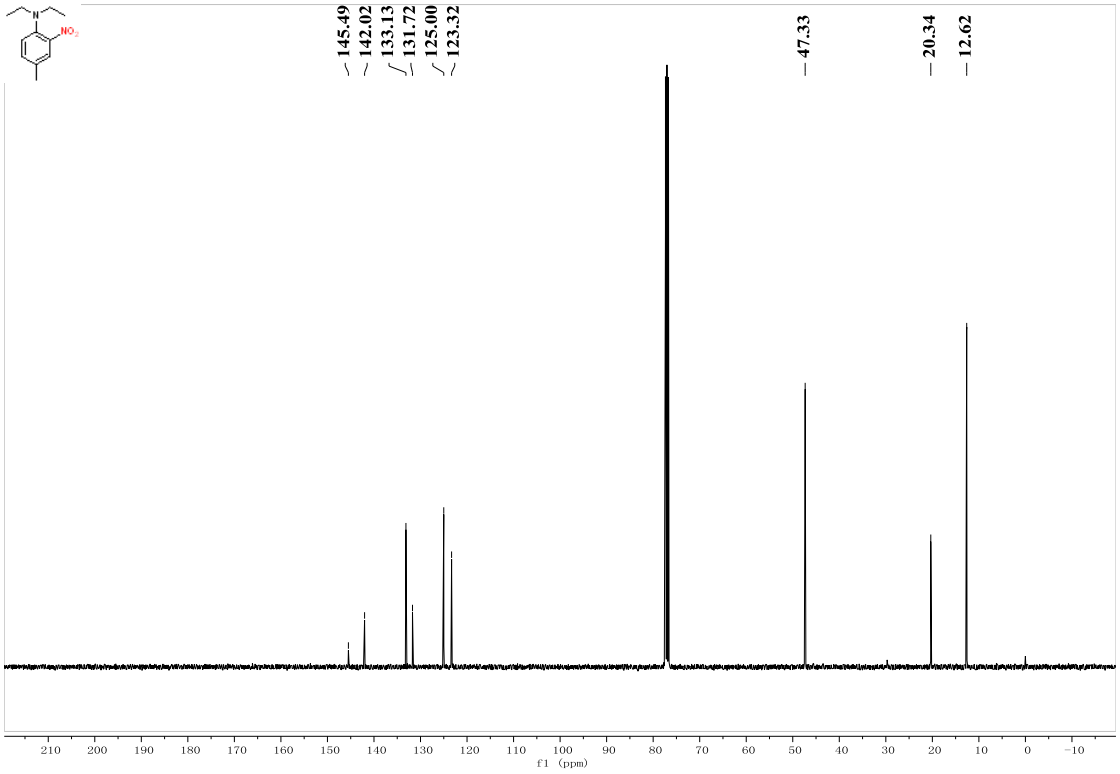
7.24
7.22
7.22
7.10
7.08
3.10
3.09
3.07
3.05
2.32
1.05
1.04
1.02
1.00
1.01
1.01
4.23
3.14
6.30
f1 (ppm)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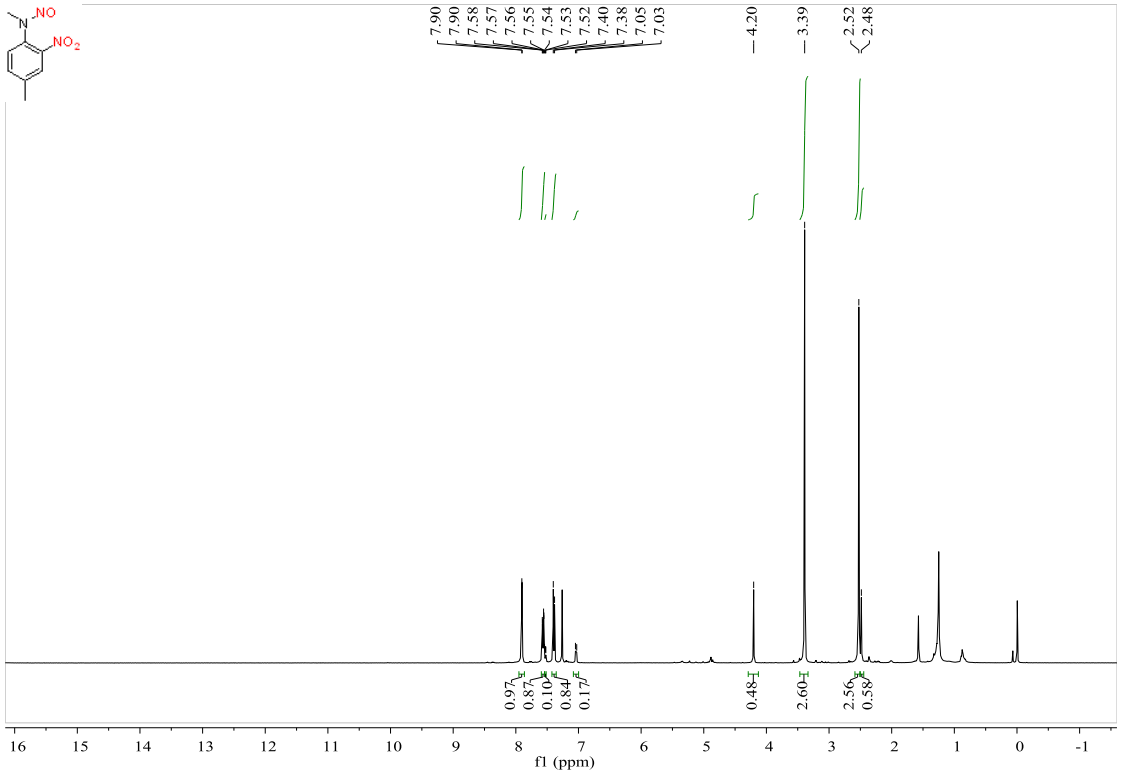
131.72
125.00
123.32
47.33
20.34
12.62
f1 (ppm)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7.90
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7.56
7.55
7.54
7.53
7.52
7.40
7.38
7.05
7.03
4.20
3.39
2.52
2.48
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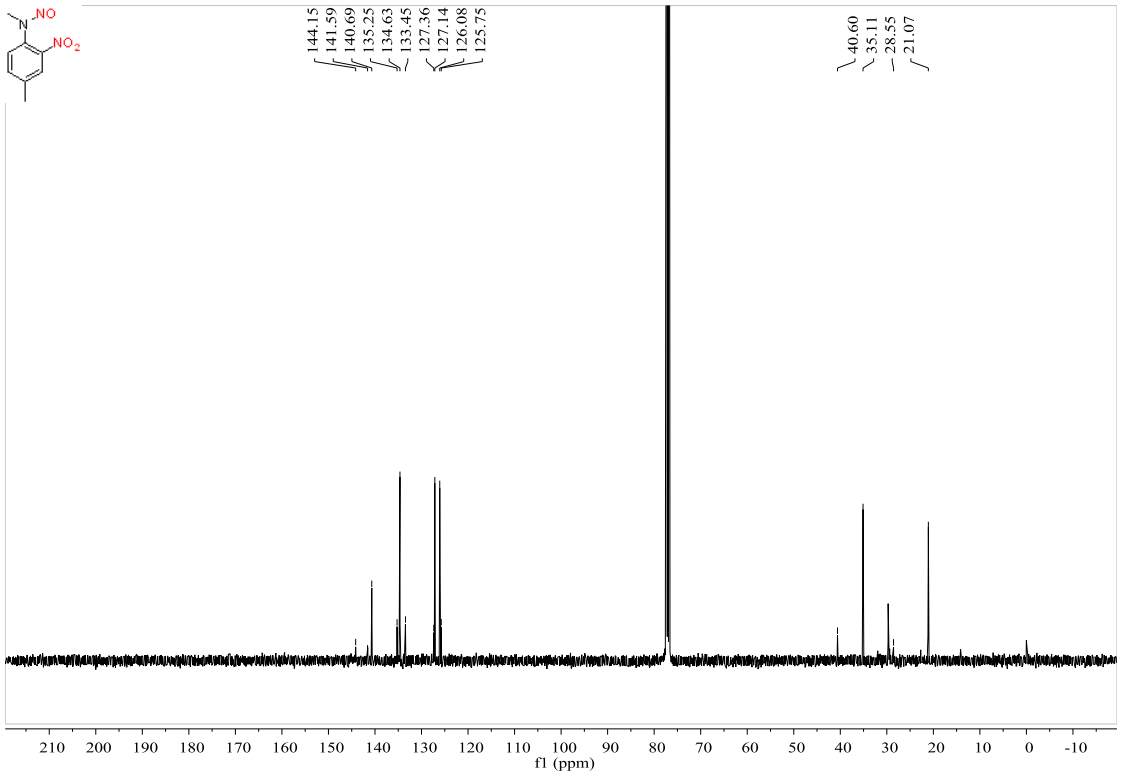
0.87
0.10
0.84
0.17
0.48
2.60
2.56
0.58
f1 (ppm)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140.69
135.25
134.63
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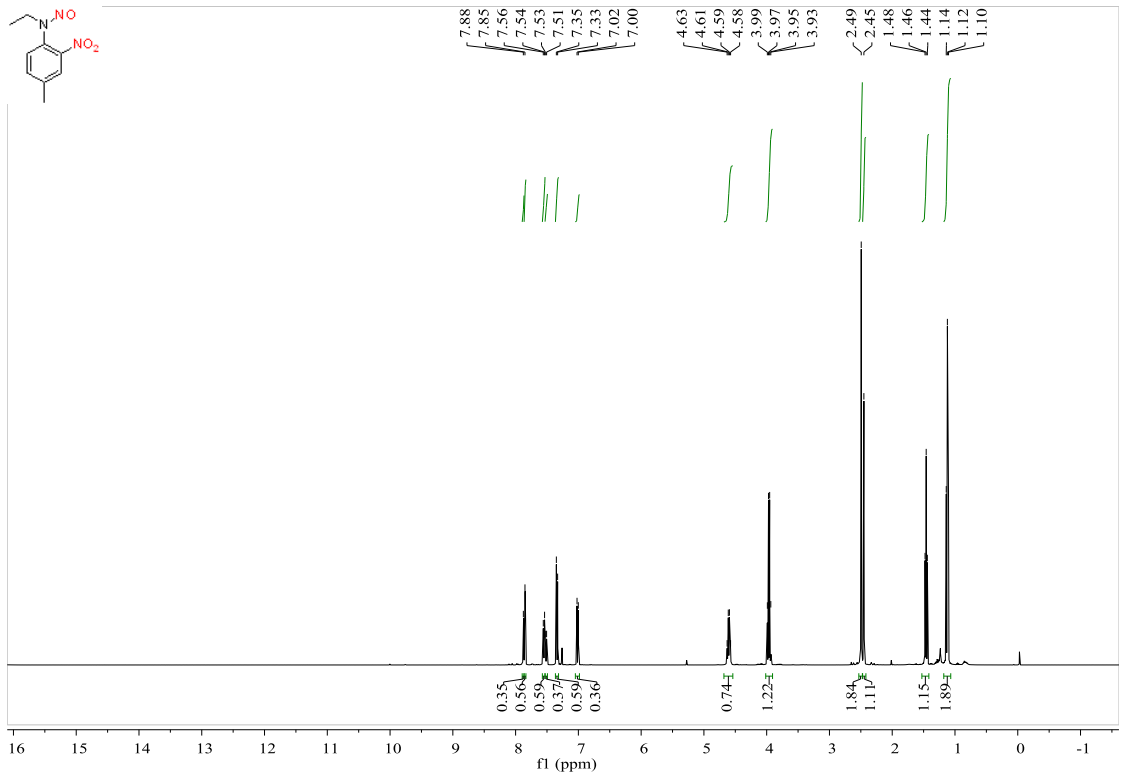
127.36
127.14
126.08
125.75
40.60
35.11
28.55
21.07
f1 (ppm)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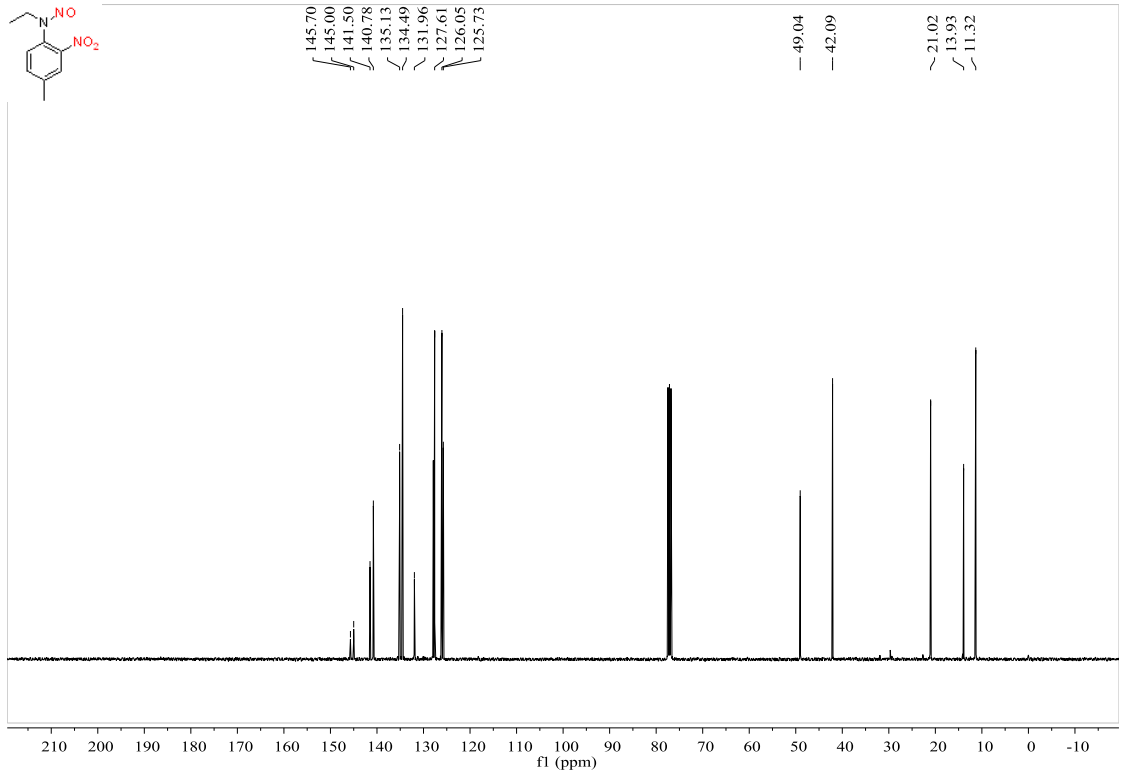
7.54
7.53
7.51
7.35
7.33
7.02
7.00
4.63
4.61
4.59
4.58
3.99
3.97
3.95
3.93
2.49
2.45
1.48
1.46
1.44
1.14
1.12
1.10
0.35
0.56
0.59
0.37
0.59
0.36
0.74
1.22
1.84
1.11
1.15
1.89
f1 (ppm)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145.00
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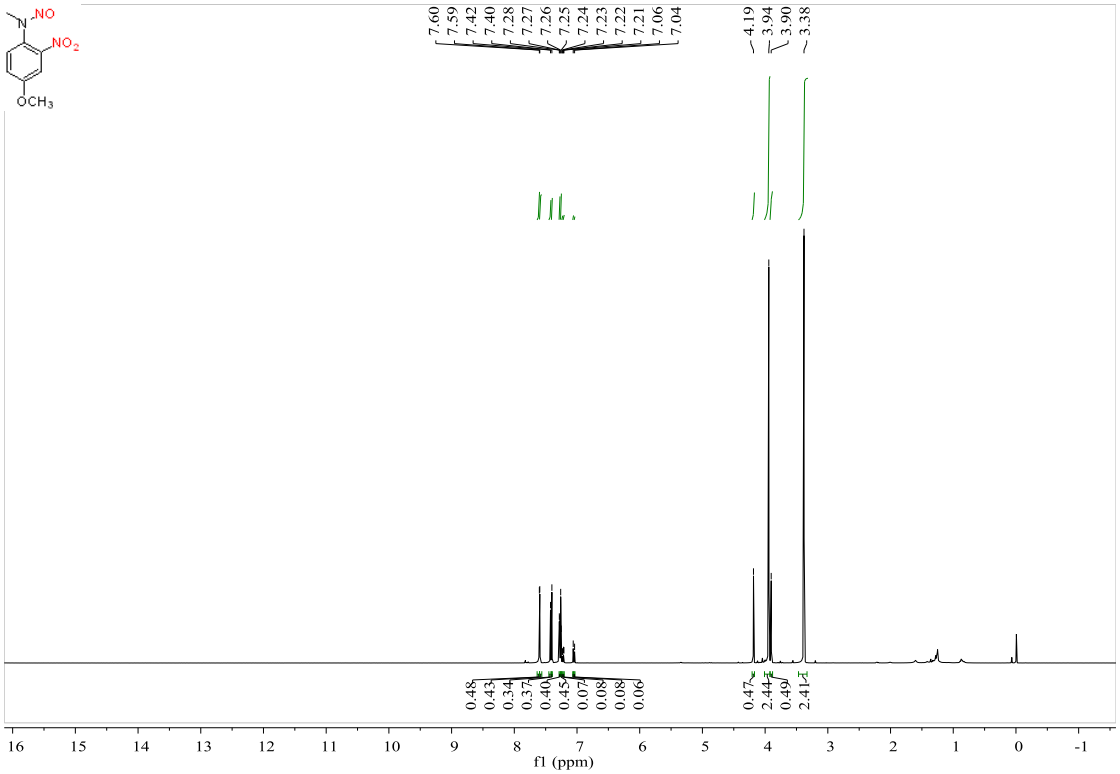
135.13
134.49
131.96
127.61
126.05
125.73
49.04
42.09
21.02
13.93
11.32
f1 (ppm)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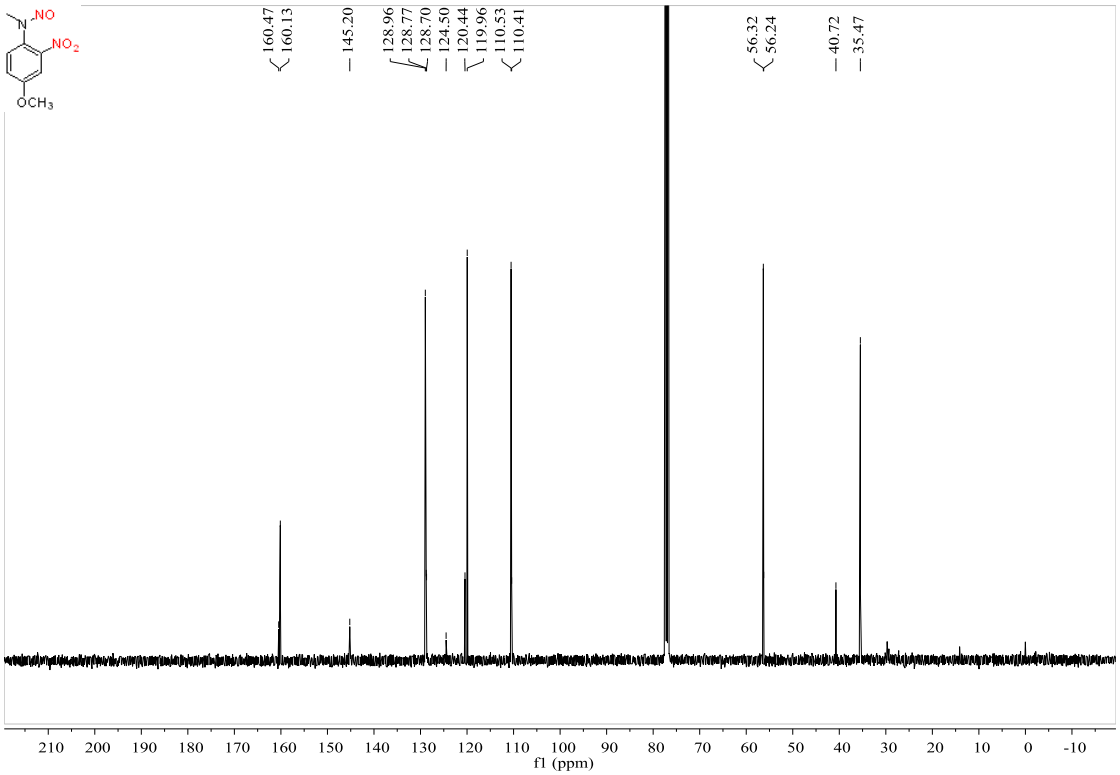
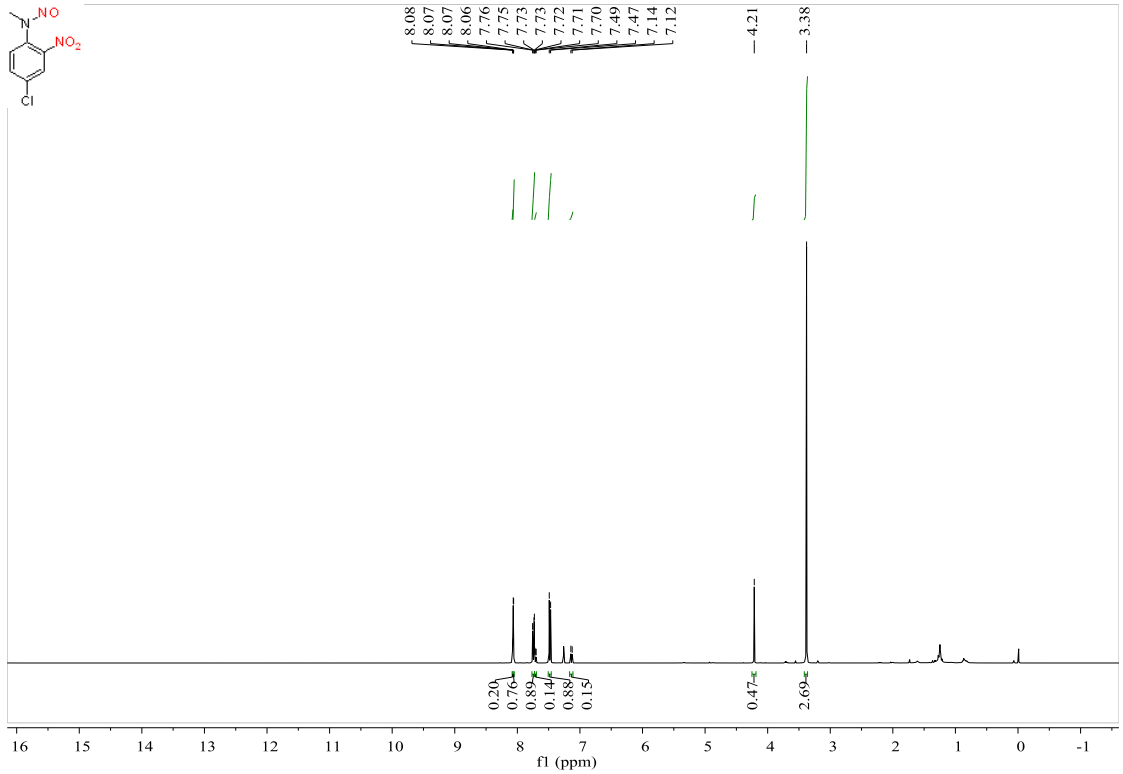
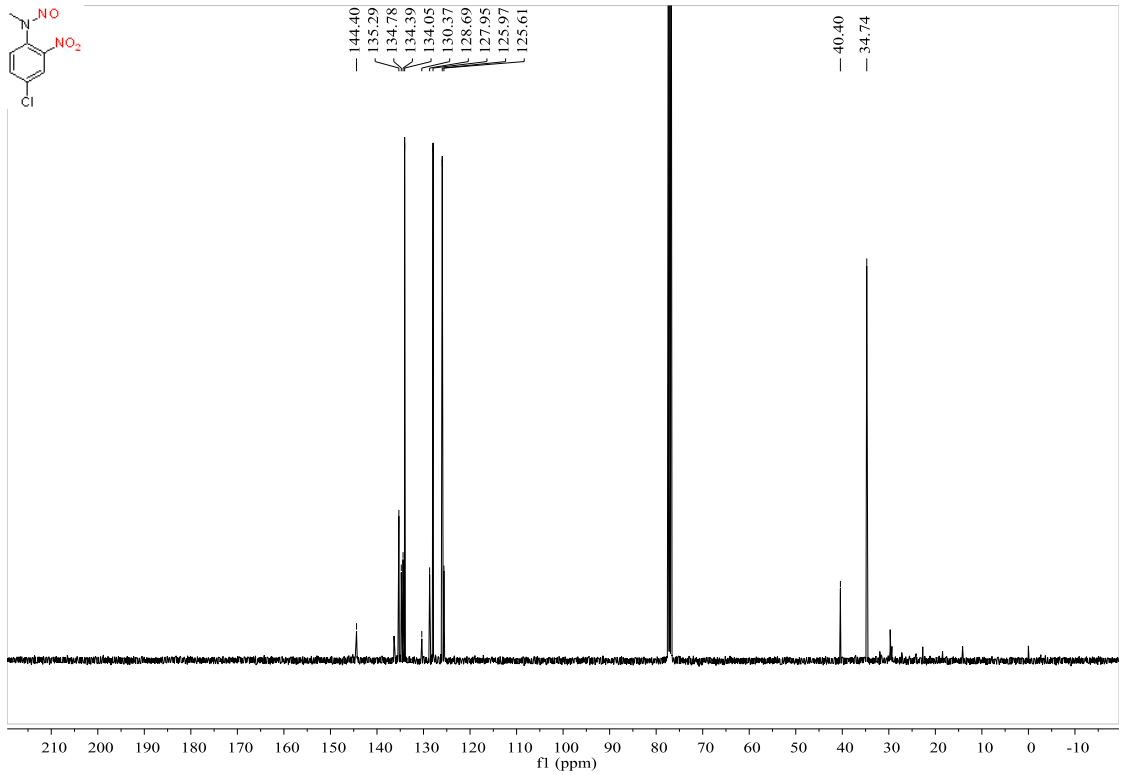
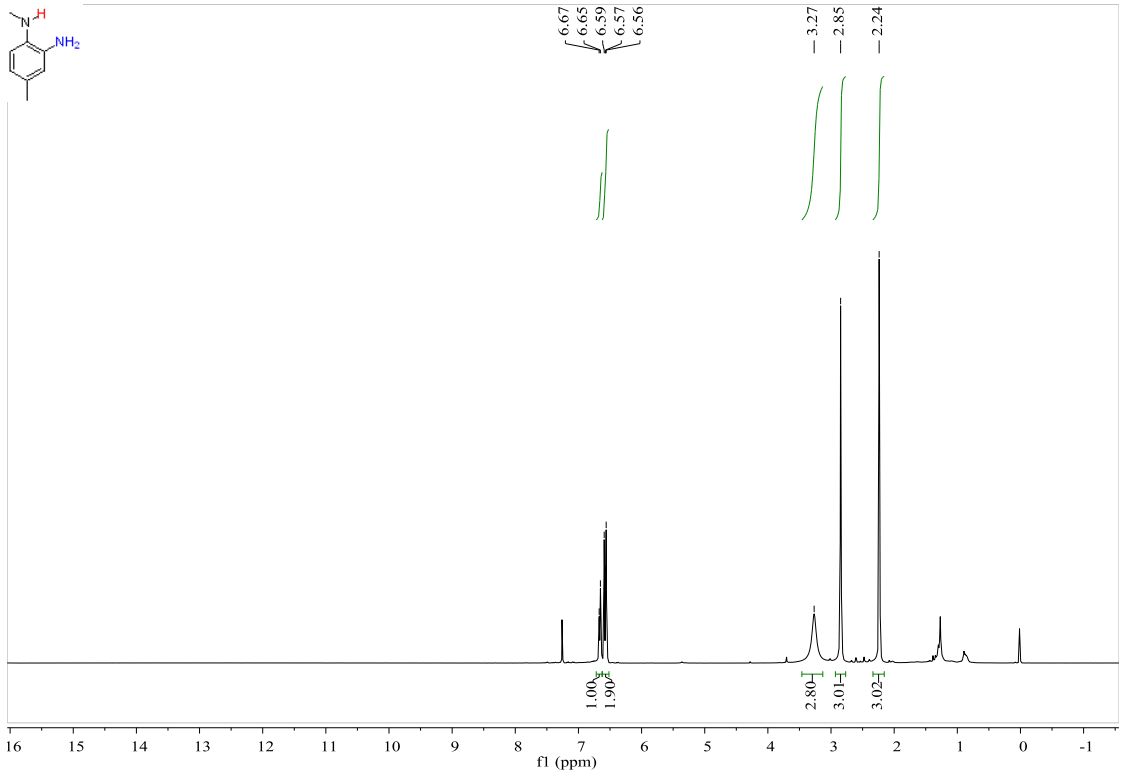
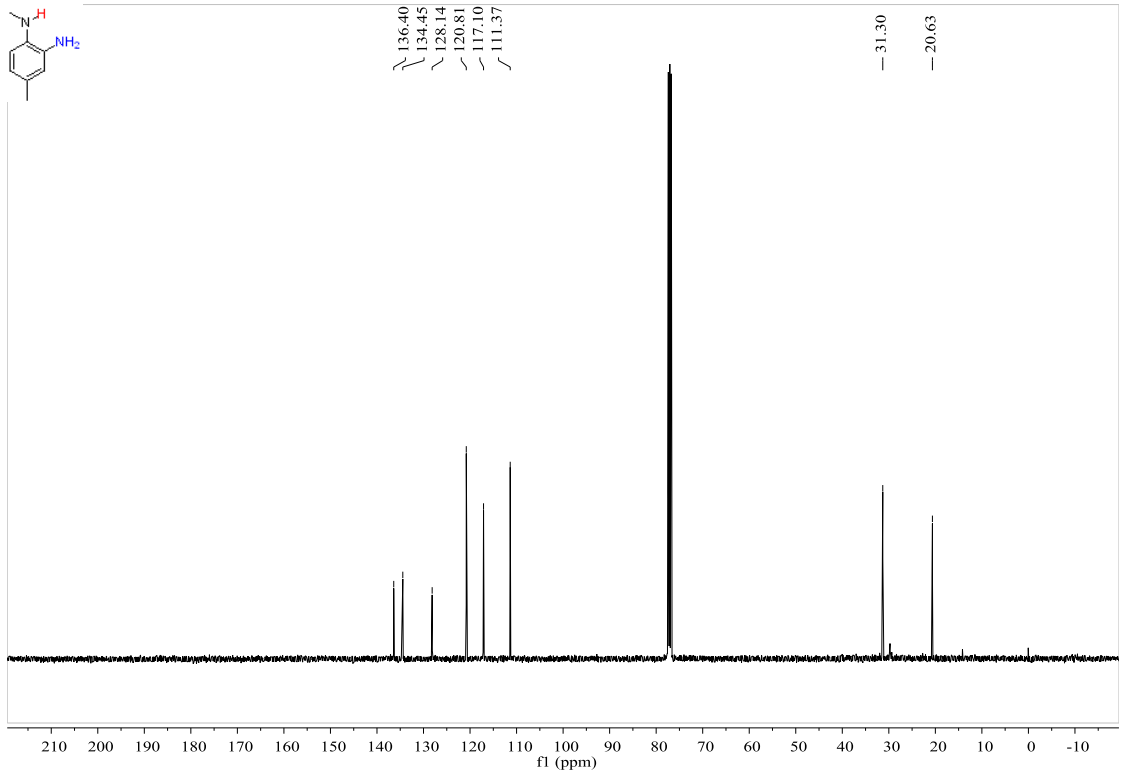
NO2
OCH3
7.60
7.59
7.42
7.40
7.28
7.27
7.26
7.25
7.24
7.23
7.22
7.21
7.06
7.04
4.19
3.94
3.90
3.38
0.48
0.43
0.34
0.37
0.40
0.45
0.07
0.08
0.08
0.06
0.47
2.44
0.49
2.41
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

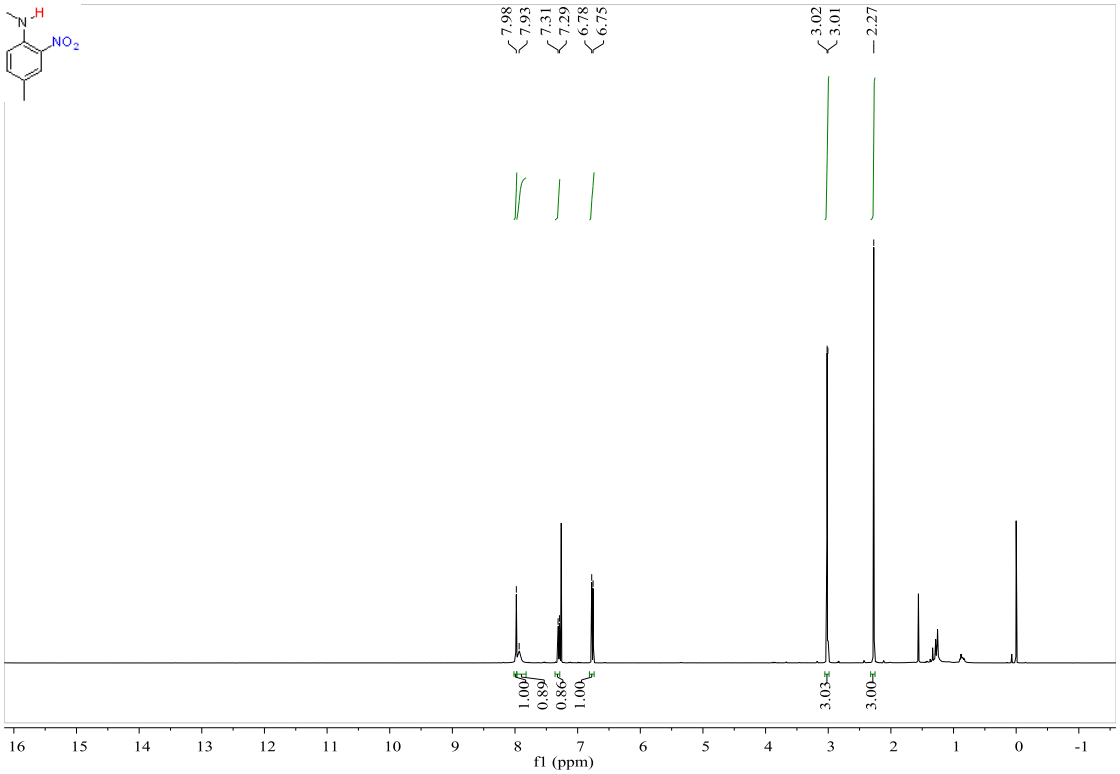

NO
NO2
OCH3
160.47
160.13
145.20
128.96
128.77
128.70
124.50
120.44
119.96
110.53
110.41
56.32
56.24
40.72
35.47
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

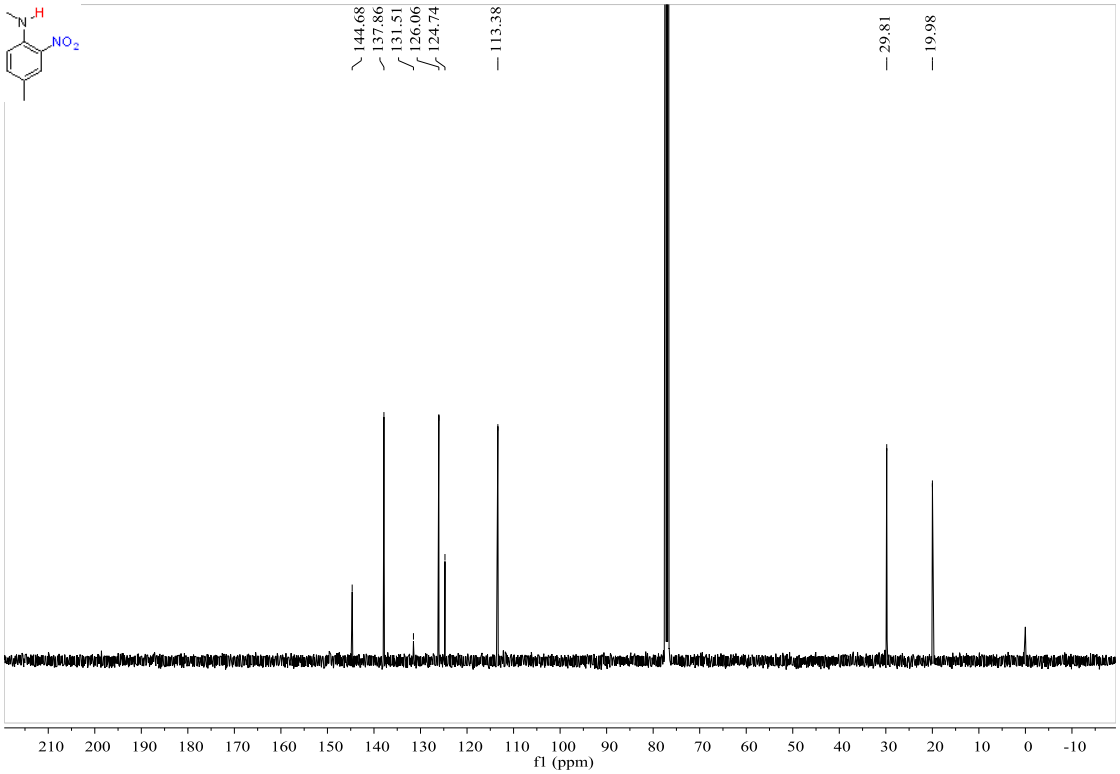

8.08
8.07
8.07
8.06
7.76
7.75
7.73
7.73
7.72
7.71
7.70
7.49
7.47
7.14
7.12
4.21
3.38
0.20
0.76
0.89
0.14
0.88
0.15
0.47
2.69
fl (ppm)

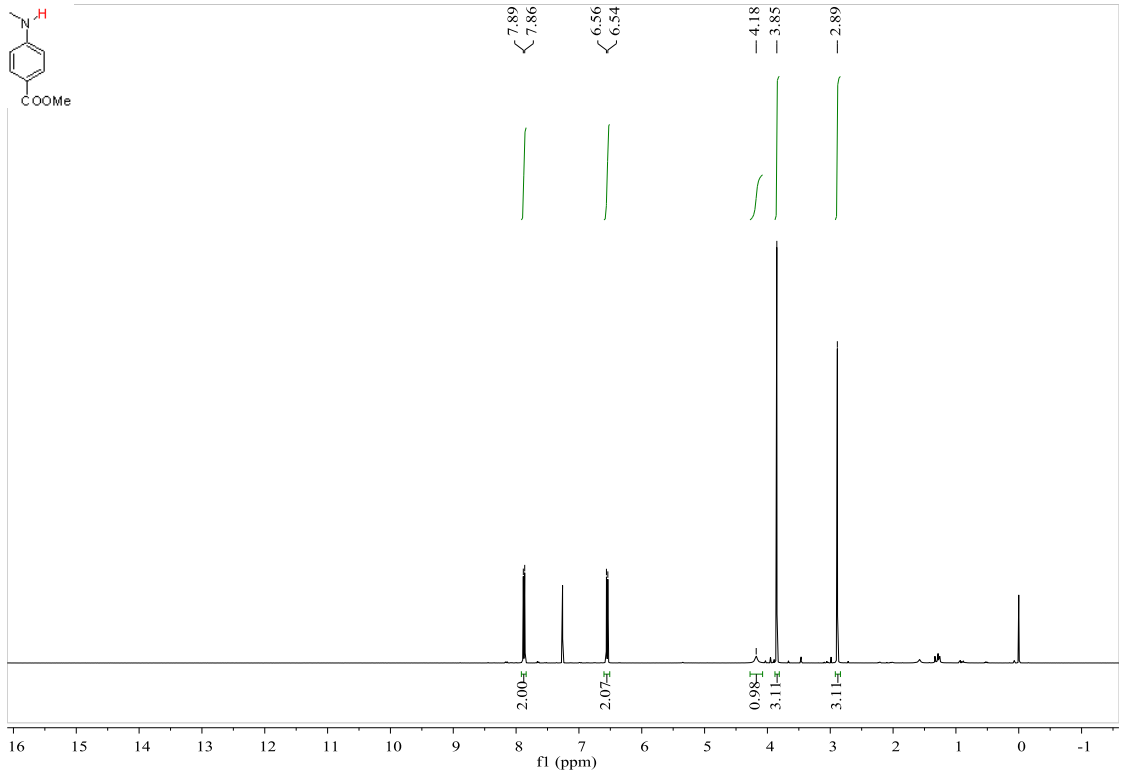

144.40
135.29
134.78
134.39
134.05
130.37
128.69
127.95
125.97
125.61
40.40
34.74
fl (ppm)

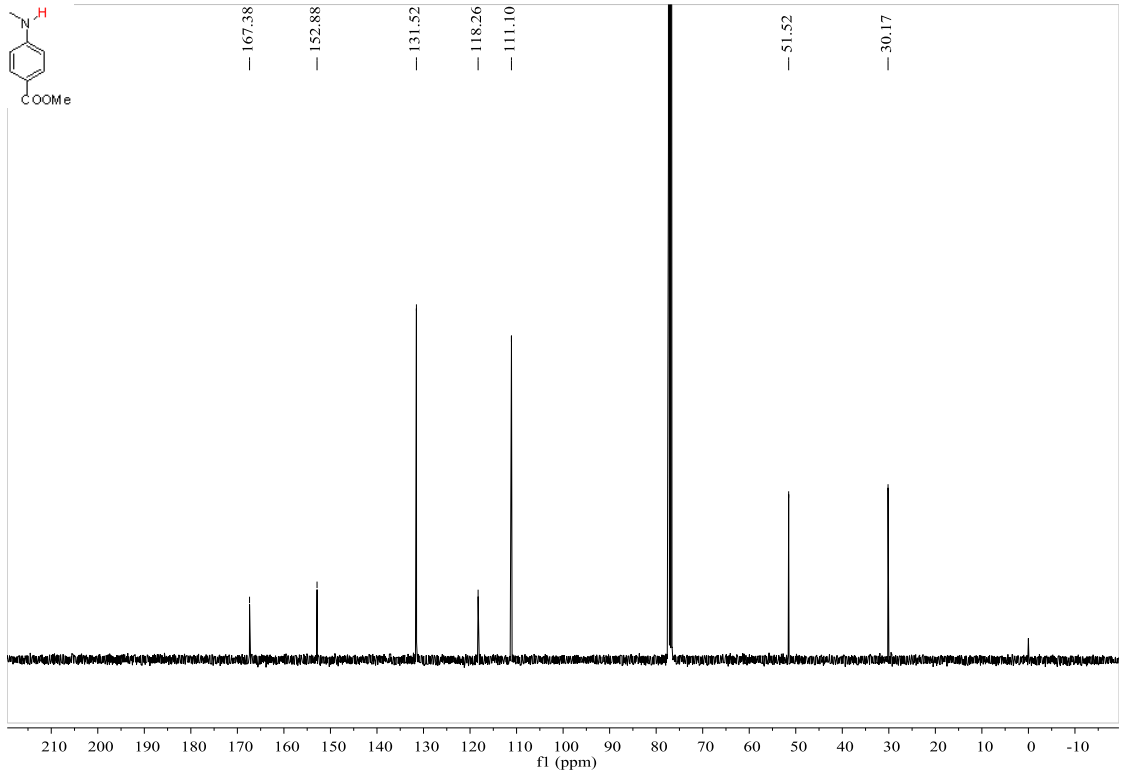

6.67
6.65
6.59
6.57
6.56
3.27
2.85
2.24
1.00
1.90
2.80
3.01
3.02
f1 (ppm)

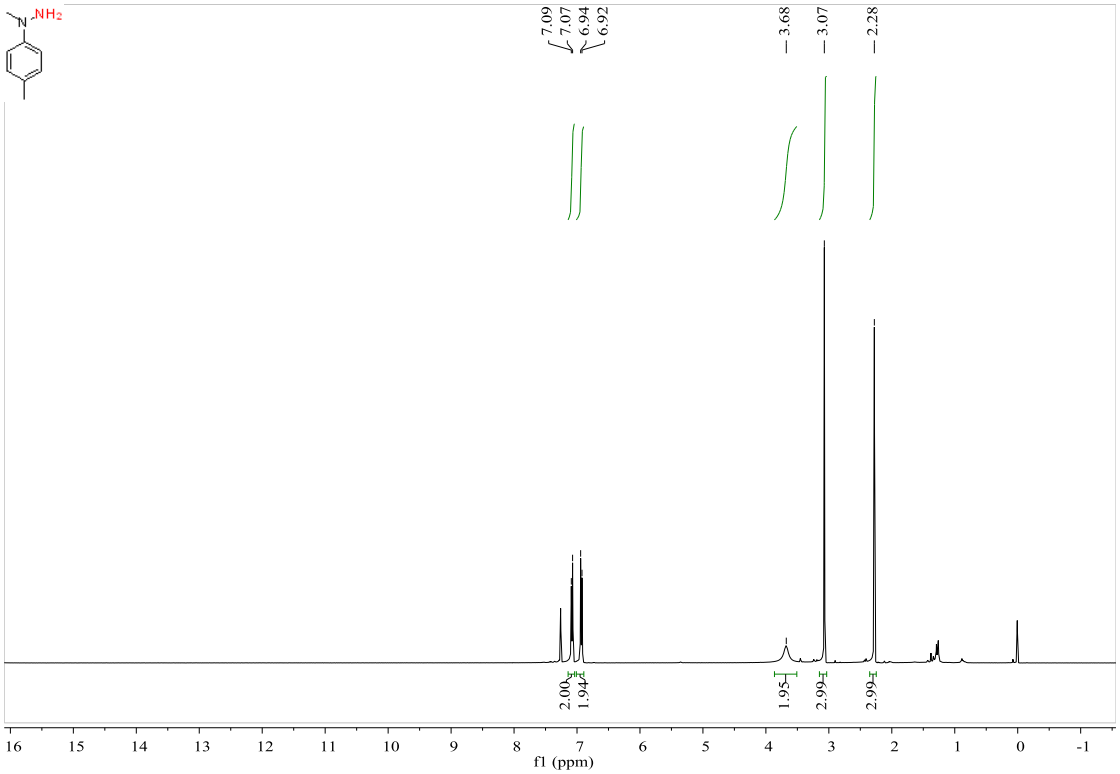

136.40
134.45
128.14
120.81
117.10
111.37
31.30
20.63
f1 (ppm)

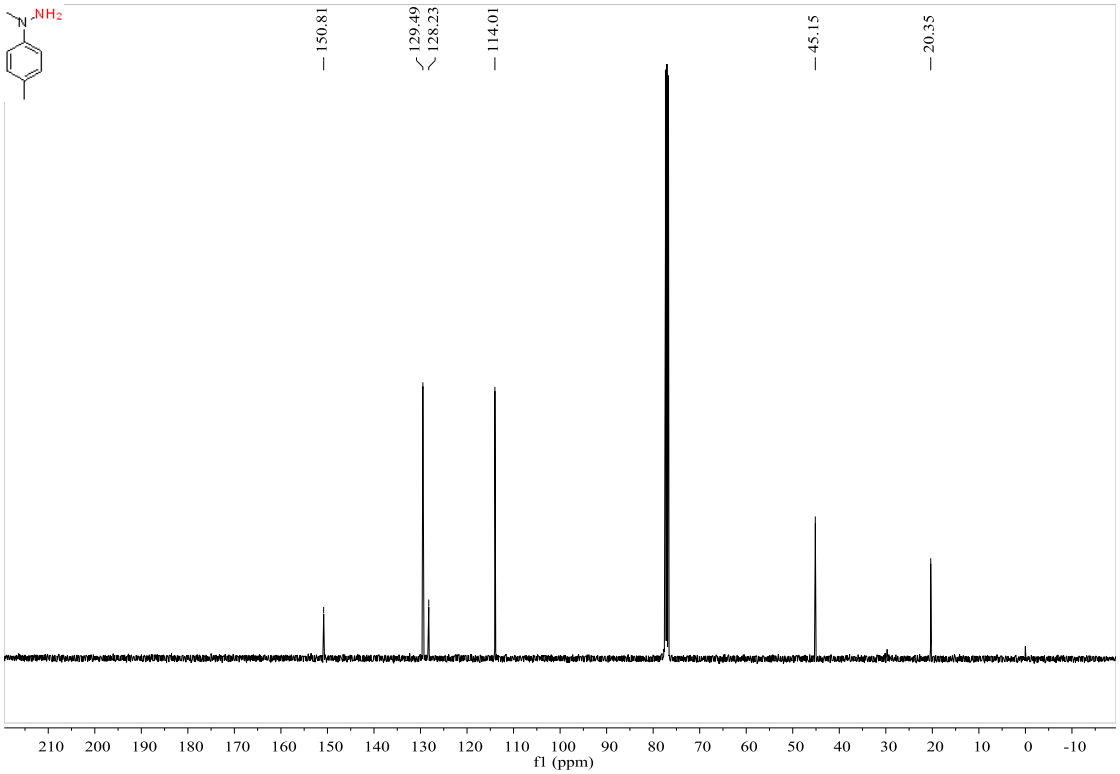

7.98
7.93
7.31
7.29
6.78
6.75
3.02
3.01
2.27
1.00
0.89
0.86
1.00
3.03
3.00
f1 (ppm)


144.68
137.86
131.51
126.06
124.74
113.38
29.81
19.98
f1 (ppm)


7.89
7.86
6.56
6.54
4.18
3.85
2.89
2.00
2.07
0.98
3.11
3.11
f1 (ppm)


167.38
152.88
131.52
118.26
111.10
51.52
30.17
f1 (ppm)


NH2
7.09
7.07
6.94
6.92
3.68
3.07
2.28
2.00
1.94
1.95
2.99
2.99
f1 (ppm)


NH2
150.81
129.49
128.23
114.01
45.15
20.35
f1 (ppm)