Supplementary Information

for

Tandem Grinding Reactions for Synthesis of 3,4,5-Trisubstituted Isoxazoles by aldol Condensation-Michael Addition Consequence

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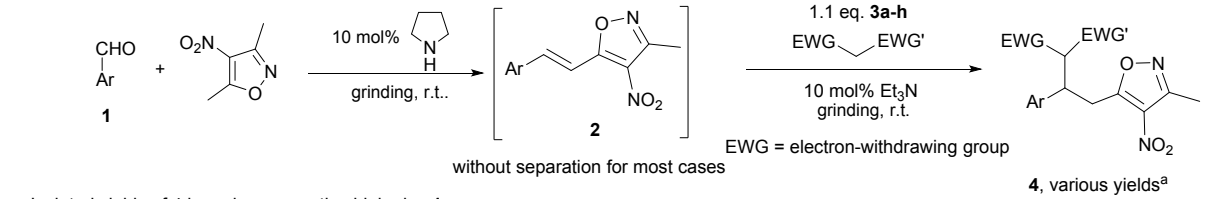
Contents

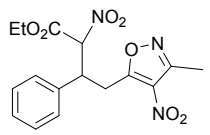
General

^{1}H NMR and ^{13}C NMR spectra were measured in $CDCl_3$, solution on a Bruker AV-400 spectrometer using TMS as an internal reference. Coupling constant (*J*) values are given in Hz. Multiplicities are designated by the following abbreviations: s, singlet; d, doublet; t, triplet; q, quartet; br, broad; m, multiplet. High-resolution mass spectra were performed on a *Bruker* microTOF-Q II Mass Spectrometer with ES ionization (ESI). All commercially available reagents were used as received. Thin-layer chromatography on silica (with GF_{254}) was used to monitor all reactions. Products were purified by flash column chromatography on silica gel purchased from Qingdao Haiyang Chemical Co., Ltd.

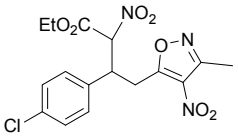
Typical procedures for the synthesis of 3,4,5-trisubstituted isoxazoles



a. Isolated yields of 4 based on aromatic aldehydes **1**.



4aa, 89%



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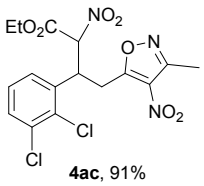

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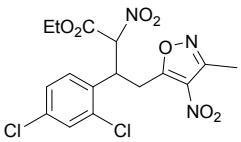

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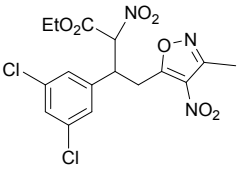

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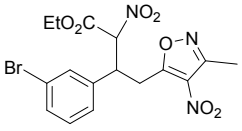

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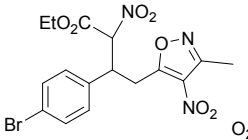

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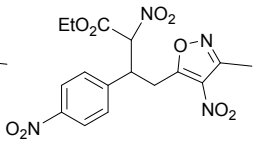

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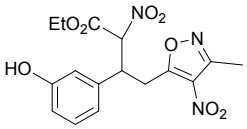

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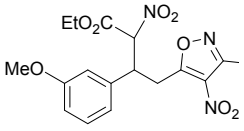

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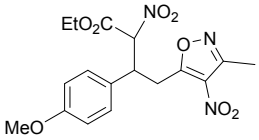

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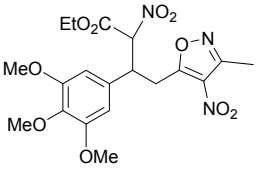

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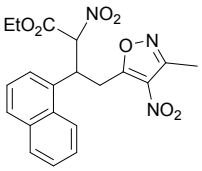

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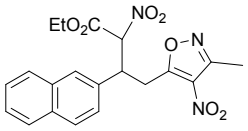

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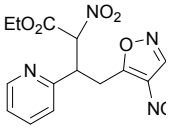

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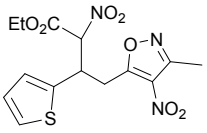

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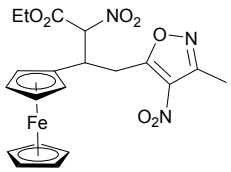

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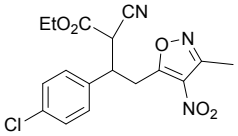

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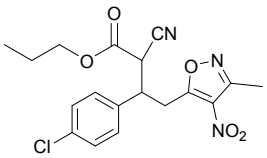

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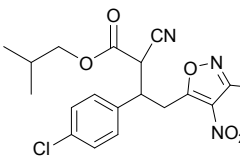

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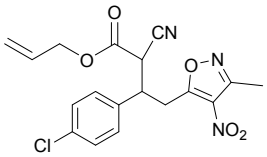

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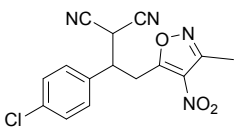

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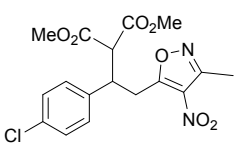

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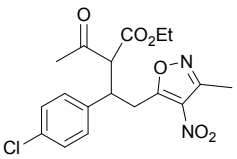

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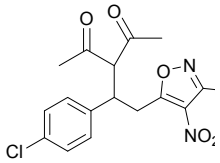


4bh, 0%

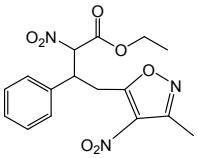
To a dried agate mortar, aromatic aldehyde **1** (1 mmol), 3,5-dimethyl-4-nitroisoxazole (white crystal, 0.15 g, 1.1 mmol) and pyrrolidine (liquid, 8 μL, 0.1 mmol) were added successively. The mixture is grinding at room temperature for 3~5 min, and the reaction was monitored by TLC (for most cases, the color of the reaction mixture was changed obviously during the grinding process), when TLC indicates that aromatic aldehyde **1** was consumed (aldehydes **1i**, **1j**, **1k**, **1l** and **1q** are not used up under standard conditions, the corresponding aldol condensation products **2i**, **2j**, **2k**, **2l** and **2q** are separated from a flash column chromatography, respectively), the activated methylene compound **3** (liquid, 1.2 mmol) and Et_3N (liquid, 12 μL, 0.1 mmol) were added, keep on grinding for another 3~5 min. TLC checked the reaction process. The crude product was diluted with DCM (20 mL) and the resulted solution successively was washed with H_2O (5 mL) and brine (5 mL). The organic layers were dried over Na_2SO_4, filtered, and concentrated. The pure product **4** was obtained by a flash column chromatography (eluted by petroleum ether/ethyl acetate = 10/1 to 5/1, v/v).

Table S1 The physical appearance (PA) and R_f of all products.

aldehyde **1**	PA	**2**	PA	R_f[a]	**4**	PA	R_f[b]
1a, Ph-	colorless liquid	**2a**	light yellow solid	0.55	**4aa**	Pale oil	0.43
1b, 4-Cl-C_6H_4	light yellow crystal	**2b**	yellow soild	0.42	**4ab**	light yellow oil	0.38
1c, 2,3-Cl_2-C_6H_3	white crystal	**2c**	light yellow solid	0.40	**4ac**	light yellow oil	0.27
1d, 2,4-Cl_2-C_6H_3	white crystal	**2d**	yellow soild	0.53	**4ad**	dark yellow oil	0.35
1e, 3,5-Cl_2-C_6H_3	white crystal	**2e**	light yellow solid	0.49	**4ae**	off-white solid	0.30
1f, 3-Br-C_6H_4	white liquid	**2f**	yellow solid	0.42	**4af**	off-white solid	0.42
1g, 4-Br-C_6H_4	white needle	**2g**	light yellow solid	0.47	**4ag**	yellow oil	0.42
1h, 4-NO_2-C_6H_4	white crystal	**2h**	light yellow solid	0.26	**4ah**	brown oil	0.14
1i, 3-OH-C_6H_4	white crystal	**2i**	light yellow solid	0.06	**4ai**	light yellow oil	0.14
1j, 3-OMe-C_6H_4	light yellow liquid	**2j**	light yellow solid	0.68	**4aj**	light yellow oil	0.39
1k, 4-OMe-C_6H_4	colorless oil	**2k**	yellow solid	0.56	**4ak**	yellow oil	0.38
1l, 3,4,5-$(OMe)_3$-C_6H_2	white needle	**2l**	orange solid	0.12	**4al**	light yellow solid	0.15
1m, 1-naphtyl	light yellow crystal	**2m**	yellow solid	0.47	**4am**	yellow oil	0.36
1n, 2-naphtyl	light yellow crystal	**2n**	yellow solid	0.42	**4an**	light yellow oil	0.38
1o, 2-pyridinyl	light yellow liquid	**2o**	yellow solid	0.07	**4ao**	brown oil	0.21
1p, 2-thiophenyl	light yellow liquid	**2p**	yellow solid	0.41	**4ap**	brown oil	0.33
1q, ferrocenyl-	orange solid	**2q**	purple solid	0.42	**4aq**	brown oil	0.38
1b, 4-Cl-C_6H_4	white crystal	**2b**	yellow solid	0.42	**4ba**	pale oil	0.35
1b, 4-Cl-C_6H_4	white crystal	**2b**	yellow solid	0.42	**4bb**	pale oil	0.35
1b, 4-Cl-C_6H_4	white crystal	**2b**	yellow solid	0.42	**4bc**	pale oil	0.36
1b, 4-Cl-C_6H_4	white crystal	**2b**	yellow solid	0.42	**4bd**	pale oil	0.33
1b, 4-Cl-C_6H_4	white crystal	**2b**	yellow solid	0.42	**4be**	pale oil	0.30

a. eluent system: petroleum ether/ethyl acetate = 15/1 (v/v); b. eluent system: petroleum ether/ethyl acetate = 5/1 (v/v).

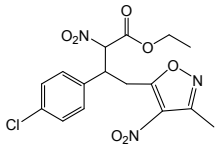
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-phenylbutanoate (4aa)



Pale oil; 89% yield; R_f = 0.43 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.24-7.19 (m, 3H, Ar-H), 7.13 (m, 2H, Ar-H), 5.41 (dd, *J* = 18.9, 9.7 Hz, 1H), 4.31-4.23 (m, 2H, CH_2), 4.03-3.75 (m, 2H, CH_2), 3.57 (m, 1H), 2.38 (d, *J* = 3.6 Hz, 3H, CH_3 in isoxazole ring), 1.28 (t, *J* = 7.1 Hz, 1.5H, CH_3), 0.98 (t, *J* = 7.1 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.95, 163.10, 162.57, 155.64, 135.34, 134.54, 129.35, 128.25, 127.84, 91.52, 63.92, 63.45, 43.98, 30.27, 13.99, 11.66; HRMS (ESI) *m/z* Calcd. for $C_{16}H_{17}N_3O_7Na^+$ $[M+Na]^+$: 386.0959,

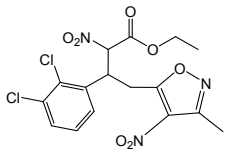
Found:386.0962.

ethyl 3-(4-chlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ab)



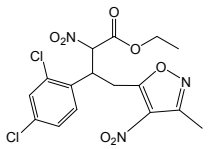
Light yellow oil; 93% yield; R_f = 0.38 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.22-7.16 (m, 2H, Ar-H), 7.10 (m, 2H, Ar-H), 5.38 (dd, *J* = 14.9, 9.6 Hz, 1H), 4.27 (dd, *J* = 10.3, 5.4 Hz, 2H, CH_2), 4.03 (m, 1H, CH_2), 3.84 (m, 1H, CH_2), 3.56 (m, 1H), 2.39 (d, *J* = 3.4 Hz, 3H, CH_3 in isoxazole ring), 1.27 (t, *J* = 7.1 Hz, 1.5H, CH_3), 1.03 (t, *J* = 7.1 Hz, 1.5H, CH_3); ^{13}C NMR (101 MHz, Chloroform-*d*) δ: 170.56, 162.83, 162.37, 155.72, 135.04, 133.84, 133.12, 129.56, 129.30, 91.19, 64.02, 63.62, 43.23, 30.07, 13.94, 11.63; HRMS (ESI) *m/z* Calcd. for $C_{16}H_{15}ClN_3O_7^-$ [M-H]$^-$: 396.0599, Found: 396.0600.

ethyl 3-(2,3-dichlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ac)



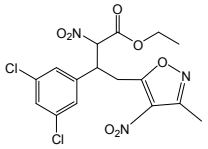
Light yellow oil; 91% yield; R_f = 0.27 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.34 (m, 1H, Ar-H), 7.14 (m, 2H, Ar-H), 4.36-4.23 (m, 1H), 4.16 (d, *J* = 5.2 Hz, 2H), 4.09-3.61 (m, 3H), 2.42 (dd, *J* = 3.5, 1.3 Hz, 3H, CH_3 in isoxazole ring), 1.28 (t, *J* = 7.0 Hz, 1.5H, CH_3), 1.14 (t, *J* = 7.0 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.47, 162.78, 162.43, 155.81, 134.91, 134.55, 131.10, 128.05, 127.96, 89.75, 64.07, 63.93, 29.84, 28.43, 13.98, 11.69; HRMS (ESI) *m/z* Calcd. for $C_{16}H_{14}Cl_2N_3O_7^-$ [M-H]$^-$: 430.0209, Found: 430.0209.

ethyl 3-(2,4-dichlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ad)



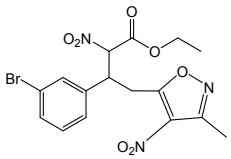
Dark yellow oil; 90% yield; R_f = 0.35 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.37-7.32 (m, 1H, Ar-H), 7.13 (m, 2H, Ar-H), 4.29 (m, 1H), 4.20-4.13 (m, 2H), 4.07-3.66 (m, 3H), 2.42 (d, *J* = 3.5 Hz, 3H, CH_3 in isoxazole ring), 1.28 (t, *J* = 7.1 Hz, 1.5H, CH_3), 1.14 (t, *J* = 6.7 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.34, 162.30, 155.68, 135.21, 134.78, 134.42, 132.62, 130.97, 127.92, 88.79, 63.93, 54.19, 29.71, 28.29, 13.67, 11.56; HRMS (ESI) *m/z* Calcd. for $C_{16}H_{14}Cl_2N_3O_7^-$ [M-H]$^-$: 430.0209, Found: 430.0207.

ethyl 3-(3,5-dichlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ae)



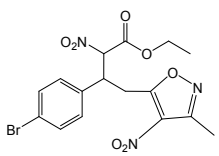
Off-white solid; 91% yield; R_f = 0.30 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.22 (m, 1H, Ar-H), 7.07 (m, 2H, Ar-H), 5.35 (dd, *J* = 11.5, 9.2 Hz, 1H), 4.32-4.20 (m, 2H), 4.10 (m, 1H), 3.87-3.53 (m, 2H), 2.44 (d, *J* = 2.7 Hz, 3H, CH_3 in isoxazole ring), 1.28 (t, *J* = 7.1 Hz, 1.5H, CH_3), 1.09 (t, *J* = 7.1 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.05, 162.55, 162.16, 155.87, 138.86, 138.20, 135.97, 129.45, 126.93, 90.74, 64.23, 63.90, 43.15, 29.98, 13.96, 11.66; HRMS (ESI) *m/z* Calcd. for $C_{16}H_{14}Cl_2N_3O_7^-$ [M-H]$^-$: 430.0209, Found: 430.0205.

ethyl 3-(3-bromophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4af)



Off-white solid; 88% yield; R_f = 0.42 (petroleum ether: ethyl acetate = 1: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.37-7.29 (m, 2H, Ar-H), 7.11 (m, 2H, Ar-H), 5.38 (dd, *J* = 15.4, 9.5 Hz, 1H), 4.32-4.22 (m, 2H), 4.04 (m, 1H), 3.92-3.71 (m, 1H), 3.58 (m, 1H), 2.41 (d, *J* = 3.0 Hz, 3H, CH_3 in isoxazole ring), 1.28 (t, *J* = 7.1 Hz, 1.5H, CH_3), 1.03 (t, *J* = 7.1 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.46, 162.79, 155.74, 137.69, 132.25, 130.84, 126.87, 123.24, 91.08, 64.06, 63.67, 43.42, 30.08, 13.95, 11.63; HRMS (ESI) *m/z* Calcd. for $C_{16}H_{15}BrN_3O_7^-$ [M-H]$^-$: 440.0088, Found: 440.0098.

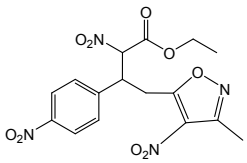
ethyl 3-(4-bromophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ag)



Yellow oil; 89% yield; R_f = 0.42 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.43-7.31 (m, 2H, Ar-H), 7.05 (dd, *J* = 8.5, 2.2 Hz, 2H, Ar-H), 5.38

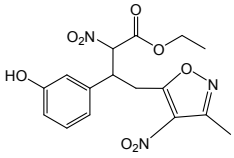
(dd, *J* = 15.1, 9.5 Hz, 1H), 4.33-4.25 (m, 2H), 4.11-4.02 (m, 1H), 3.86 (m, 1H), 3.57 (m, 1H), 2.42 (d, *J* = 3.5 Hz, 3H, CH_3 in isoxazole ring), 1.29 (t, *J* = 7.1 Hz, 1.5H, CH_3), 1.06 (t, *J* = 7.1 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.53, 162.82, 162.36, 155.75, 134.37, 132.55, 129.94, 129.60, 123.22, 91.14, 64.04, 63.66, 43.31, 30.06, 13.96, 11.67; HRMS (ESI) *m/z* Calcd. for $C_{16}H_{15}BrN_3O_7^-$ [M-H]$^-$: 440.0088, Found: 440.0090.

ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(4-nitrophenyl)butanoate (4ah)



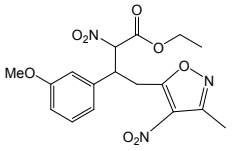
Brown oil; 88% yield; R_f = 0.14 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 8.10 (dd, *J* = 8.6, 3.3 Hz, 2H, Ar-H), 7.45-7.35 (m, 2H, Ar-H), 5.45 (dd, *J* = 14.1, 9.4 Hz, 1H), 4.45-4.27 (m, 2H), 4.12-4.03 (m, 1H), 3.98-3.79 (m, 1H), 3.66 (m, 1H), 2.40 (d, *J* = 4.2 Hz, 3H, CH_3 in isoxazole ring), 1.28 (t, *J* = 7.1 Hz, 1.5H, CH_3), 1.06 (t, *J* = 7.1 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 169.92, 162.51, 162.09, 155.83, 148.17, 142.68, 129.53, 129.19, 124.44, 90.64, 64.29, 63.90, 43.44, 30.02, 13.92, 11.56; HRMS (ESI) *m/z* Calcd. for $C_{16}H_{15}N_4O_9^-$ [M-H]$^-$: 407.0845, Found: 407.0848.

ethyl 3-(3-hydroxyphenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ai)



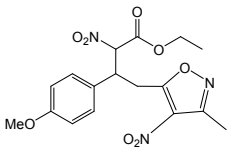
Light yellow oil; 82% yield; R_f = 0.14 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.74 (dd, *J* = 5.7, 3.3 Hz, 2H, Ar-H), 7.56 (dd, *J* = 5.7, 3.3 Hz, 2H, Ar-H), 7.17 (m, 1H), 5.47 (dd, *J* = 16.1, 9.6 Hz, 1H), 4.32 (d, *J* = 6.7 Hz, 2H), 4.13 (dd, *J* = 7.1, 3.5 Hz, 1H), 4.00 (dd, *J* = 15.2, 10.7 Hz, 1H), 3.70-3.58 (m, 1H), 2.49 (d, *J* = 3.2 Hz, 3H, CH_3 in isoxazole ring), 1.37 (t, *J* = 7.2 Hz, 1.5H, CH_3), 1.11 (d, *J* = 7.2 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.77, 167.79, 162.94, 156.04, 137.00, 130.94, 128.86, 120.25, 115.13, 91.30, 65.62, 43.58, 30.58, 19.20, 13.73, 11.55; HRMS (ESI) *m/z* Calcd. for $C_{16}H_{16}N_3O_8^-$ [M-H]$^-$: 378.0943, Found: 378.0949.

ethyl 3-(3-methoxyphenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4aj)



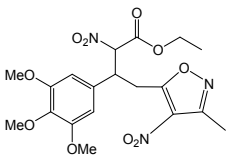
Light yellow oil; 81% yield; R_f = 0.39 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.12 (m, 2H, Ar-H), 6.75-6.65 (m, 2H, Ar-H), 5.47-5.37 (m, 1H), 4.32-4.21 (m, 2H), 4.03 (m, 1H), 3.87 (m, 1H), 3.69 (d, *J* = 2.8 Hz, 3H, OCH_3), 3.55 (m, 1H), 2.39 (d, *J* = 3.2 Hz, 3H, CH_3 in isoxazole ring), 1.28 (t, *J* = 7.1 Hz, 1.5H, CH_3), 1.02 (t, *J* = 7.1 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.94, 163.09, 160.09, 155.64, 136.84, 130.39, 120.29, 114.48, 113.91, 91.52, 63.48, 55.42, 43.92, 30.15, 29.84, 13.72, 11.67; HRMS (ESI) *m/z* Calcd. for $C_{17}H_{18}N_3O_8^-$ [M-H]$^-$: 392.1099, Found: 392.1103.

ethyl 3-(4-methoxyphenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ak)



Yellow oil; 85% yield; R_f = 0.38 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.04 (d, *J* = 8.5 Hz, 2H, Ar-H), 6.74-6.68 (m, 2H, Ar-H), 5.36 (dd, *J* = 14.5, 9.7 Hz, 1H), 4.25 (dt, *J* = 13.1, 6.4 Hz, 2H), 4.05-3.98 (m, 1H), 3.92-3.74 (m, 1H), 3.67 (d, *J* = 2.6 Hz, 3H, OCH_3), 3.60-3.46 (m, 1H), 2.38 (d, *J* = 3.1 Hz, 3H, CH_3 in isoxazole ring), 1.27 (t, *J* = 7.1 Hz, 1.5H, CH_3), 1.01 (t, *J* = 7.1 Hz, 1H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 171.12, 163.11, 159.84, 155.58, 129.38, 129.00, 126.99, 126.17, 114.57, 91.63, 63.78, 63.35, 55.31, 43.20, 30.28, 13.69, 11.60; HRMS (ESI) *m/z* Calcd. for $C_{17}H_{18}N_3O_8^-$ [M-H]$^-$: 392.1099, Found: 392.1109.

ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(3,4,5-trimethoxyphenyl)butanoate (4al)

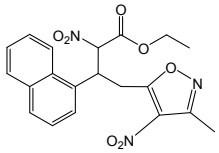


Pale oil; 81% yield; R_f = 0.15 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 6.40 (d, *J* = 2.6 Hz, 2H, Ar-H), 5.48 (dd, *J* = 17.9, 9.5 Hz, 1H), 4.36 (dd, *J* = 7.1, 1.9 Hz, 2H), 4.13 (d, *J* = 7.0 Hz, 1H), 4.09 (d, *J* = 7.2 Hz, 1H), 3.81-3.77 (m, 9H, $3OCH_3$), 3.63-3.49 (m, 1H), 2.46 (s, 3H, CH_3 in isoxazole ring), 1.36 (t, *J* = 7.1 Hz, 1.5H, CH_3), 1.11 (t, *J* = 7.1 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.82, 162.62, 155.63,

153.59, 138.26, 130.56, 129.75, 105.15, 104.84, 91.48, 63.87, 63.44, 60.89, 56.28, 44.21, 29.71, 13.94, 13.74, 11.61;

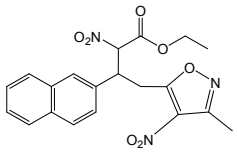
HRMS (ESI) *m/z* Calcd. for $C_{19}H_{22}N_3O_{10}^-$ [M-H]$^-$: 452.1311, Found: 452.1317.

ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-3-(naphthalen-1-yl)-2-nitrobutanoate (4am)



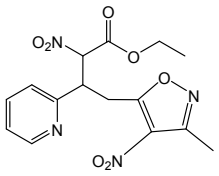
Brown oil; 88% yield; R_f = 0.36 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 8.03-7.98 (m, 1H, Ar-H), 7.78-7.69 (m, 2H, Ar-H), 7.54-7.48 (m, 1H, Ar-H), 7.45-7.32 (m, 3H, Ar-H), 5.59 (dd, *J* = 13.7, 8.6 Hz, 1H), 5.35-5.26 (m, 1H), 4.28 (dd, *J* = 7.1, 1.7 Hz, 1H), 4.15-3.98 (m, 1H), 3.93-3.85 (m, 1H), 3.80-3.64 (m, 1H), 2.27 (s, 3H, CH_3 in isoxazole ring), 1.26 (t, *J* = 7.1 Hz, 1.5H, CH_3), 0.84 (t, *J* = 7.0 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.93, 163.20, 162.64, 155.54, 134.14, 131.04, 130.71, 129.58 (d, *J* = 5.1 Hz), 129.37, 127.36, 126.40, 125.31, 124.35, 121.96, 90.35, 63.82, 37.52, 30.12, 29.90, 13.98, 11.54; HRMS (ESI) *m/z* Calcd. for $C_{20}H_{18}N_3O_7^-$ [M-H]$^-$: 412.1150, Found: 412.1160.

ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-3-(naphthalen-2-yl)-2-nitrobutanoate (4an)



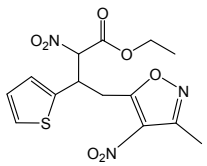
Light yellow oil; 88% yield; R_f = 0.38 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.80 (m, 3H, Ar-H), 7.72-7.68 (m, 1H, Ar-H), 7.51 (m, 2H, Ar-H), 7.36 (m, 1H, Ar-H), 5.61 (dd, *J* = 16.9, 9.6 Hz, 1H), 4.57 (m, 1H), 4.39 (m, 1H), 4.20-3.98 (m, 2H), 3.73 (m, 1H), 2.42 (d, *J* = 4.6 Hz, 3H, CH_3 in isoxazole ring), 1.37 (t, *J* = 7.1 Hz, 1.5H, CH_3), 0.98 (t, *J* = 7.1 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.86, 163.09, 162.57, 155.65, 133.25, 132.65, 131.89, 129.38, 128.06, 127.96, 127.82, 126.89, 125.15, 91.57, 63.92, 63.46, 43.99, 30.18, 13.98, 11.62; HRMS (ESI) *m/z* Calcd. for $C_{20}H_{18}N_3O_7^-$ [M-H]$^-$: 412.1150, Found: 412.1158.

ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(pyridin-2-yl)butanoate (4ao)



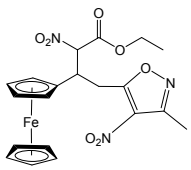
Brown oil; 89% yield; R_f = 0.21 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 8.43 (s, 1H, pyridinyl-H), 7.52 (d, *J* = 6.8 Hz, 1H, pyridinyl-H), 7.14-7.00 (m, 2H, pyridinyl-H), 5.85 (d, *J* = 10.4 Hz, 1H), 4.31 (q, *J* = 7.5 Hz, 2H), 4.10-3.95 (m, 1H), 3.93-3.72 (m, 1H), 3.58 (m, 1H), 2.41 (d, *J* = 4.0 Hz, 3H, CH_3 in isoxazole ring), 1.30 (t, *J* = 7.0 Hz, 1.5H, CH_3), 1.04 (t, *J* = 7.0 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 171.16, 163.67, 162.87, 155.71, 150.03, 137.28, 124.19, 123.41, 90.01, 63.85, 63.30, 44.82, 29.83, 13.99, 11.64; HRMS (ESI) *m/z* Calcd. for $C_{15}H_{15}N_4O_7^-$ [M-H]$^-$: 363.0946, Found: 363.0946.

ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(thiophen-2-yl)butanoate (4ap)



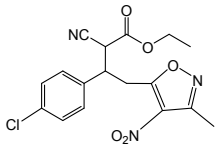
Brown oil; 87% yield; R_f = 0.33 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.15 (dd, *J* = 6.2, 2.3 Hz, 1H, thiophenyl-H), 6.90-6.79 (m, 2H, thiophenyl-H), 5.39 (dd, *J* = 8.6, 2.4 Hz, 1H), 4.60 (m, 1H), 4.32-4.21 (m, 1H), 4.16-4.08 (m, 1H), 3.89 (m, 1H), 3.63 (m, 1H), 2.42 (d, *J* = 2.2 Hz, 3H, CH_3 in isoxazole ring), 1.27 (t, *J* = 7.1 Hz, 1.5H, CH_3), 1.10 (t, *J* = 7.1 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.43, 162.56, 162.29, 155.60, 137.26, 127.33, 126.26, 91.18, 63.83, 63.60, 39.18, 31.13, 13.65, 11.54; HRMS (ESI) *m/z* Calcd. for $C_{14}H_{14}N_3O_7S^-$ [M-H]$^-$: 368.0558, Found: 368.0558.

ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(ferrocene-2-yl)butanoate (4aq)



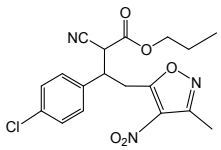
Brown oil; 72% yield; R_f = 0.38 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 5.48 (dd, *J* = 21.1, 4.3 Hz, 1H), 4.27 (d, *J* = 7.2 Hz, 1H), 4.22 (s, 9H, ferrocenyl-H), 4.07 (d, *J* = 10.3 Hz, 2H), 3.91-3.74 (m, 1H), 2.60 (d, *J* = 1.2 Hz, 3H, CH_3 in isoxazole ring), 1.28 (m, 3H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 172.02, 171.85, 163.22, 163.08, 156.02, 130.86, 91.19, 69.57, 63.66, 63.54, 38.71, 38.60, 30.39, 30.33, 13.95, 11.79; HRMS (ESI) *m/z* Calcd. for $C_{20}H_{20}FeN_3O_7^-$ [M-H]$^-$: 470.0656, Found: 470.0642.

ethyl 3-(4-chlorophenyl)-2-cyano-4-(3-methyl-4-nitroisoxazol-5-yl)butanoate (4ba)



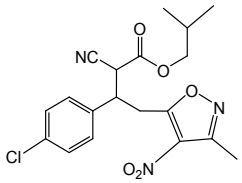
Pale oil; 88% yield; R_f = 0.35 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.37-7.30 (m, 3H, Ar-H), 7.27 (d, *J* = 8.3 Hz, 1H, Ar-H), 4.24 (q, *J* = 7.1 Hz, 1H), 4.17 (t, *J* = 7.1 Hz, 1H), 4.04 (m, 1H), 3.99-3.80 (m, 2H), 3.78-3.67 (m, 1H), 2.52 (d, *J* = 10.9 Hz, 3H, CH_3 in isoxazole ring), 1.28 (t, *J* = 7.1 Hz, 1.5H, CH_3), 1.20 (t, *J* = 7.1 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.58, 163.97, 155.78, 135.14, 135.03, 134.89, 134.32, 129.50, 129.36, 128.86, 114.33, 63.41, 43.80, 42.11, 31.35, 13.85, 11.56 .

propyl 3-(4-chlorophenyl)-2-cyano-4-(3-methyl-4-nitroisoxazol-5-yl)butanoate (4bb)



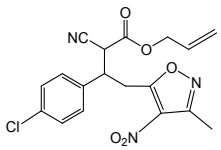
Pale oil; 85% yield; R_f = 0.36 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.32 (d, *J* = 3.5 Hz, 3H, Ar-H), 7.26 (s, 1H, Ar-H), 4.13 (t, *J* = 6.3 Hz, 1H), 4.09-4.01 (m, 2H), 3.99-3.78 (m, 2H), 3.78-3.66 (m, 1H), 2.52 (d, *J* = 10.8 Hz, 3H, CH_3 in isoxazole ring), 1.67 (d, *J* = 7.2 Hz, 1H), 1.60-1.53 (m, 1H), 0.93 (t, *J* = 7.5 Hz, 1.5H, CH_3), 0.85 (t, *J* = 7.4 Hz, 1.5H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.59, 164.06, 155.78, 135.03, 134.88, 134.33, 129.50, 129.36, 128.85, 114.32, 68.84, 43.81, 42.13, 31.32, 30.18, 21.62, 11.56, 10.04 .

isobutyl 3-(4-chlorophenyl)-2-cyano-4-(3-methyl-4-nitroisoxazol-5-yl)butanoate (4bc)



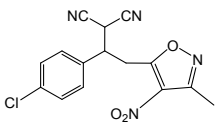
Pale oil; 82% yield; R_f = 0.35 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.36-7.29 (m, 3H, Ar-H), 7.27 (d, *J* = 9.0 Hz, 1H, Ar-H), 4.07-4.01 (m, 1H), 3.98-3.93 (m, 2H), 3.92-3.82 (m, 2H), 3.80-3.67 (m, 1H), 2.52 (d, *J* = 10.9 Hz, 3H, CH_3 in isoxazole ring), 1.90 (m, 1H), 0.92 (d, *J* = 6.7 Hz, 3H, CH_3), 0.84 (dd, *J* = 6.7, 5.6 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.58, 164.04, 155.79, 135.05, 134.89, 134.31, 129.51, 129.37, 128.83, 114.51, 73.17, 43.82, 42.15, 31.31, 30.19, 27.48, 18.80, 18.67, 11.56 .

allyl 3-(4-chlorophenyl)-2-cyano-4-(3-methyl-4-nitroisoxazol-5-yl)butanoate (4bd)



Pale oil; 88% yield; R_f = 0.33 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-*d*) δ: 7.33 (dd, *J* = 8.9, 3.7 Hz, 3H, Ar-H), 7.27 (d, *J* = 8.9 Hz, 1H, Ar-H), 5.92-5.72 (m, 1H), 5.39-5.24 (m, 2H), 4.70-4.58 (m, 2H), 4.12-4.01 (m, 1H), 3.99-3.80 (m, 2H), 3.79-3.66 (m, 1H), 2.52 (d, *J* = 11.0 Hz, 3H, CH_3 in isoxazole ring); ^{13}C NMR (100 MHz, Chloroform-*d*) δ: 170.53, 163.70, 155.69, 135.03, 134.94, 134.21, 130.16, 129.53, 129.39, 128.86, 120.25, 114.17, 67.63, 43.80, 42.11, 31.32, 30.13, 11.56 .

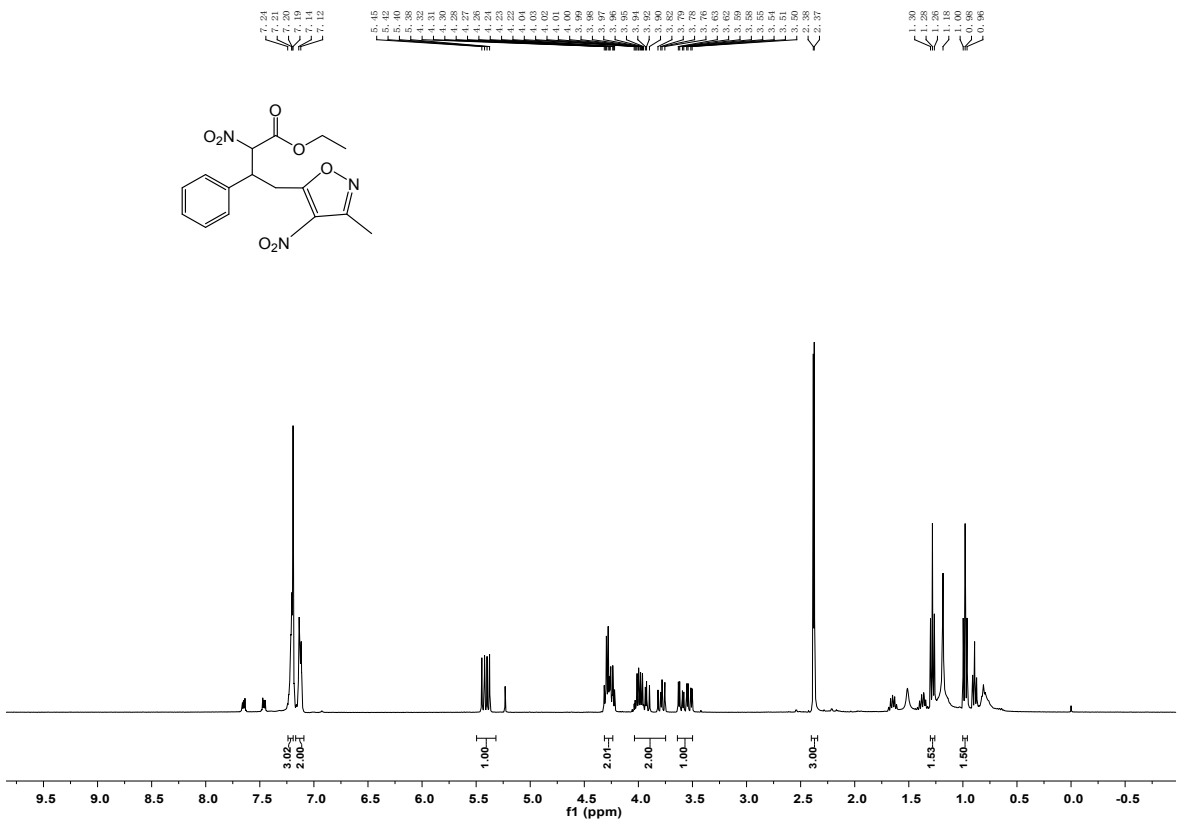
2-(1-(4-chlorophenyl)-2-(3-methyl-4-nitroisoxazol-5-yl)ethyl)malononitrile (4be)

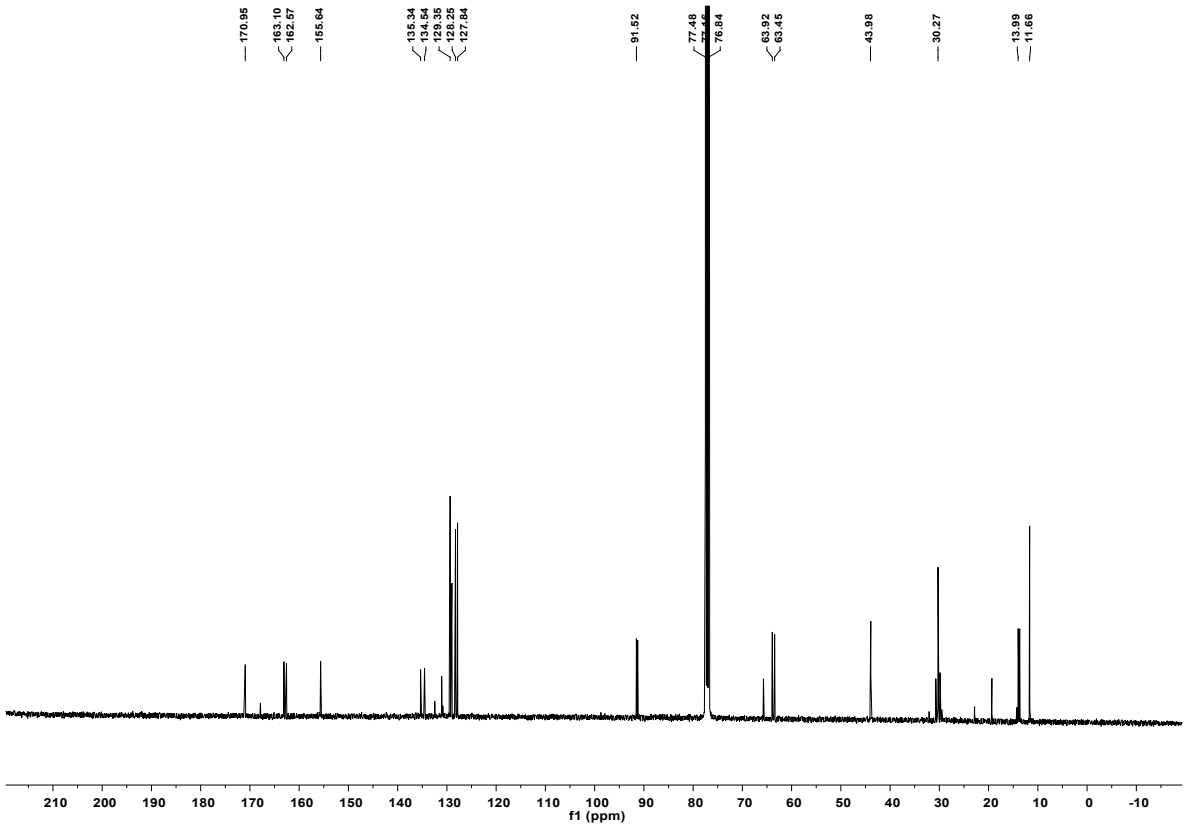


Pale oil; 85% yield; R_f = 0.30 (petroleum ether: ethyl acetate = 5: 1, v/v); ^{1}H NMR (400 MHz, Chloroform-d) δ: 7.42 (d, *J* = 8.5 Hz, 2H, Ar-H), 7.34 (d, *J* = 8.5 Hz, 2H, Ar-H), 4.14-4.10 (m, 1H), 4.05-3.95 (m, 2H), 3.90-3.82 (m,1H), 2.54 (s, 3H, CH_3 in isoxazole ring); ^{13}C NMR (100 MHz, Chloroform-d) δ: 169.21, 155.93, 136.15, 132.49, 131.03, 129.98, 128.96, 110.61, 110.54,60.41, 43.10, 30.18, 29.70, 14.21, 11.52 .

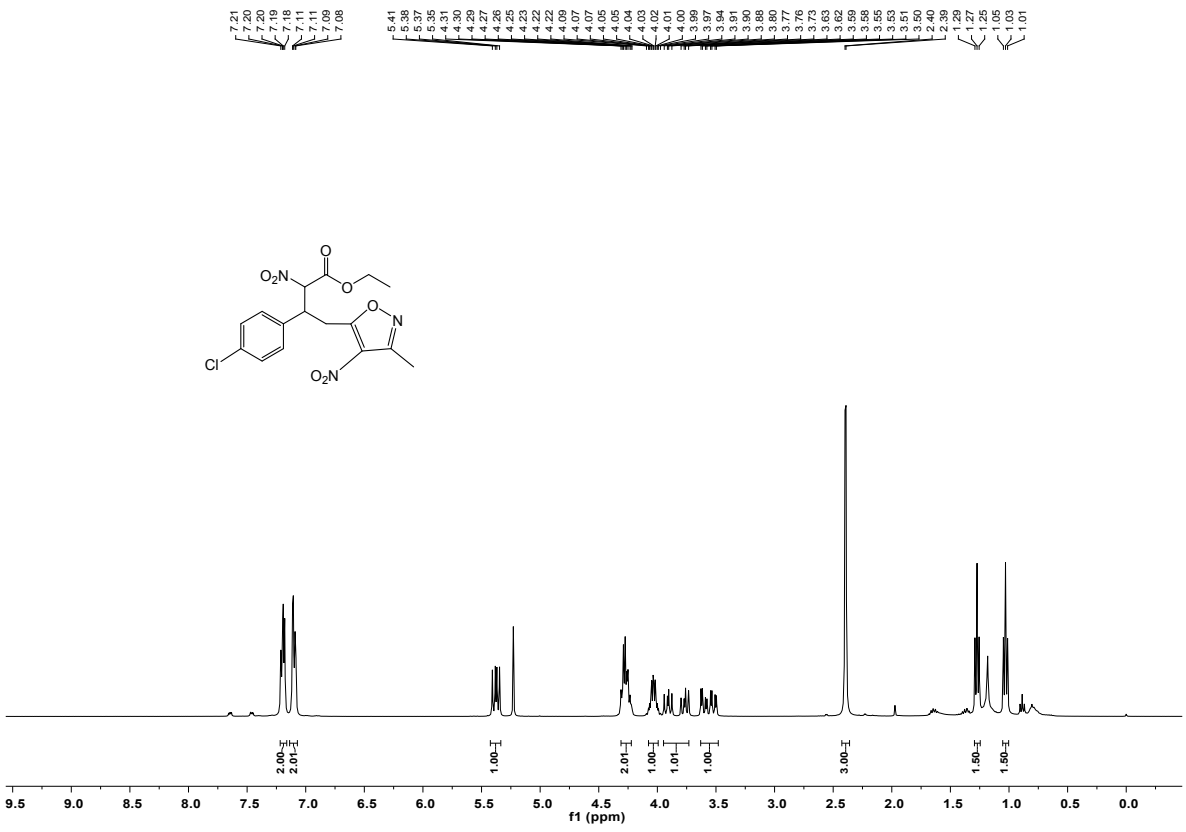
^{1}H and ^{13}C NMR Spectra of 3,4,5-trisubstituted isoxazoles

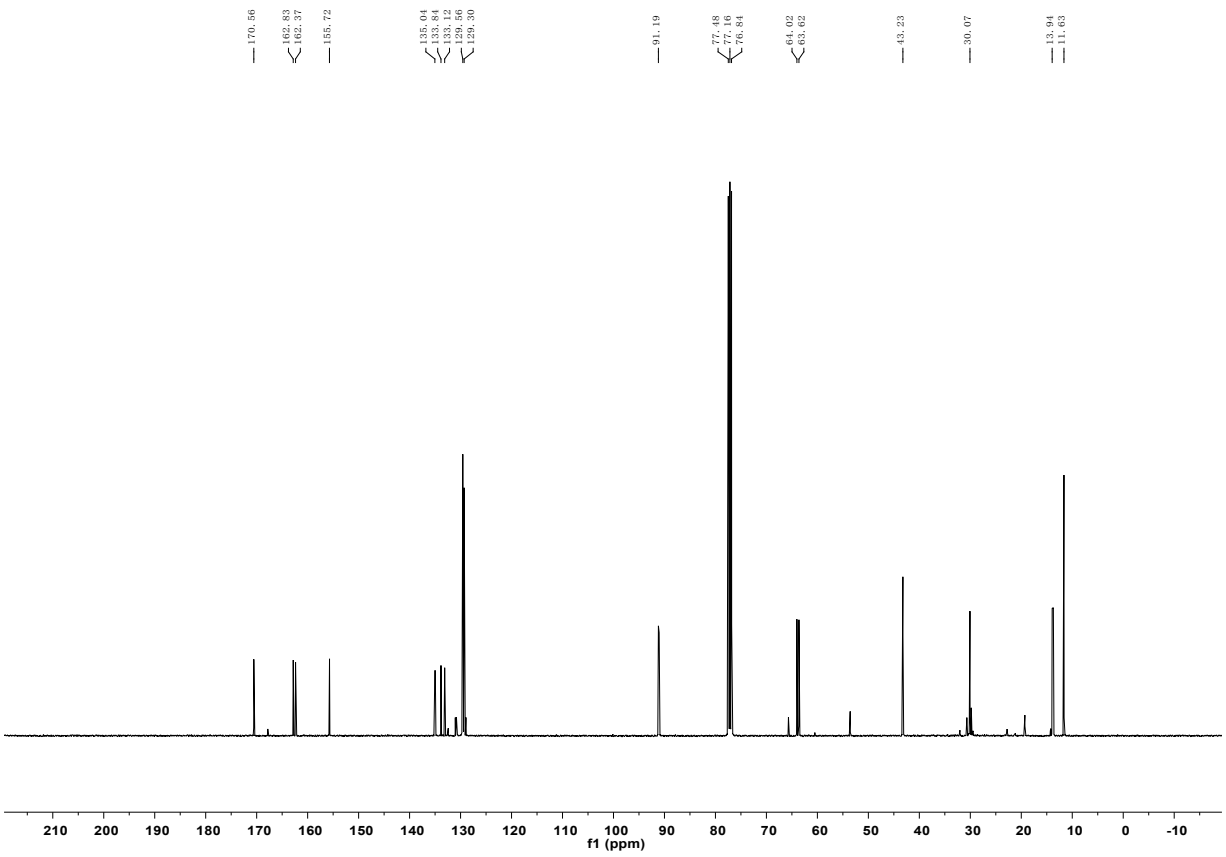
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-phenylbutanoate (4aa)



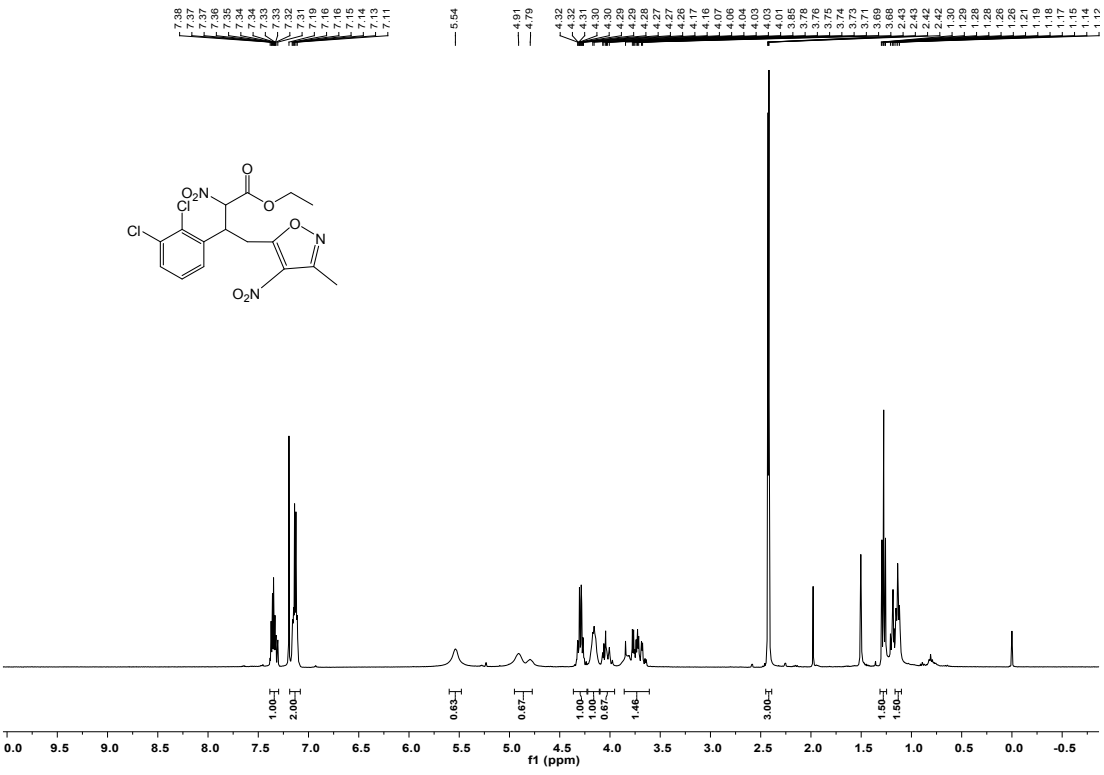


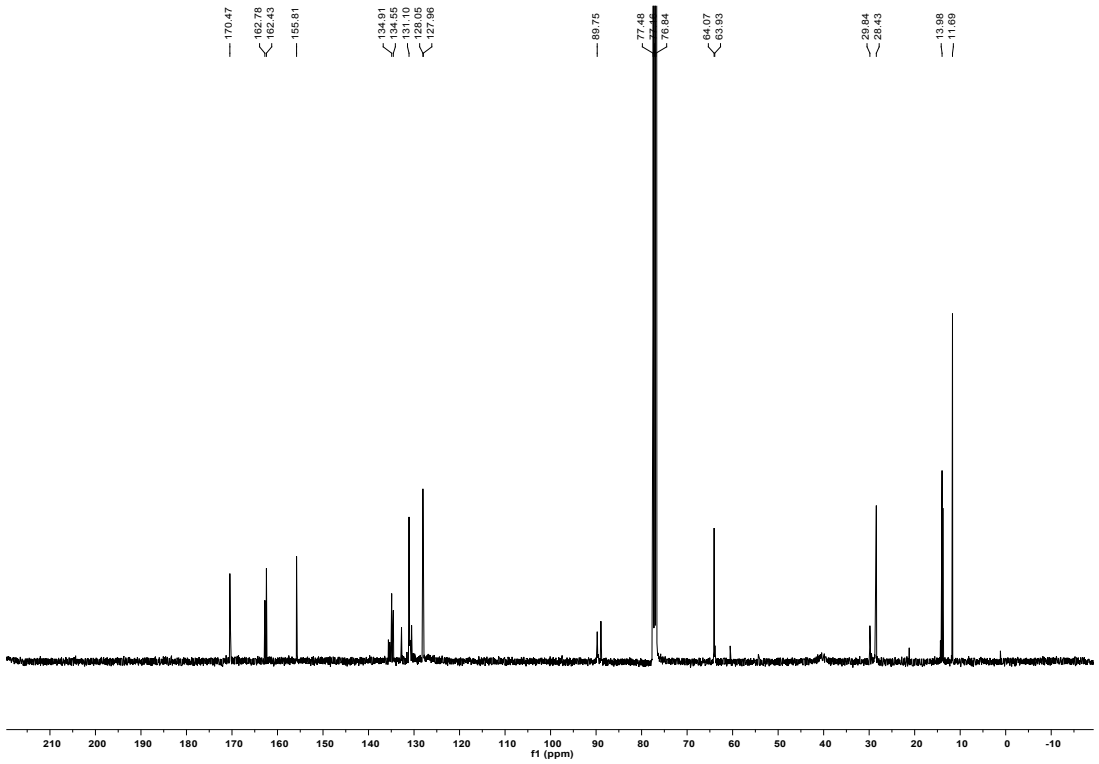
ethyl 3-(4-chlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ab)



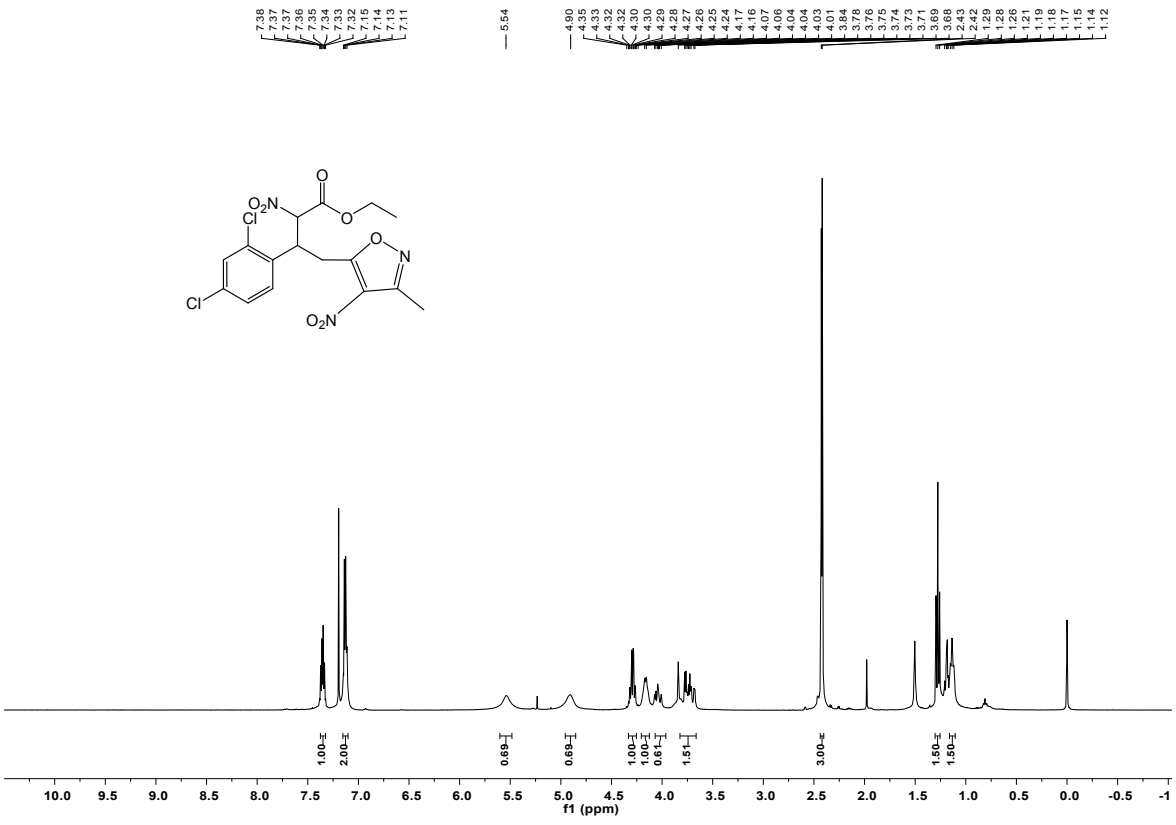


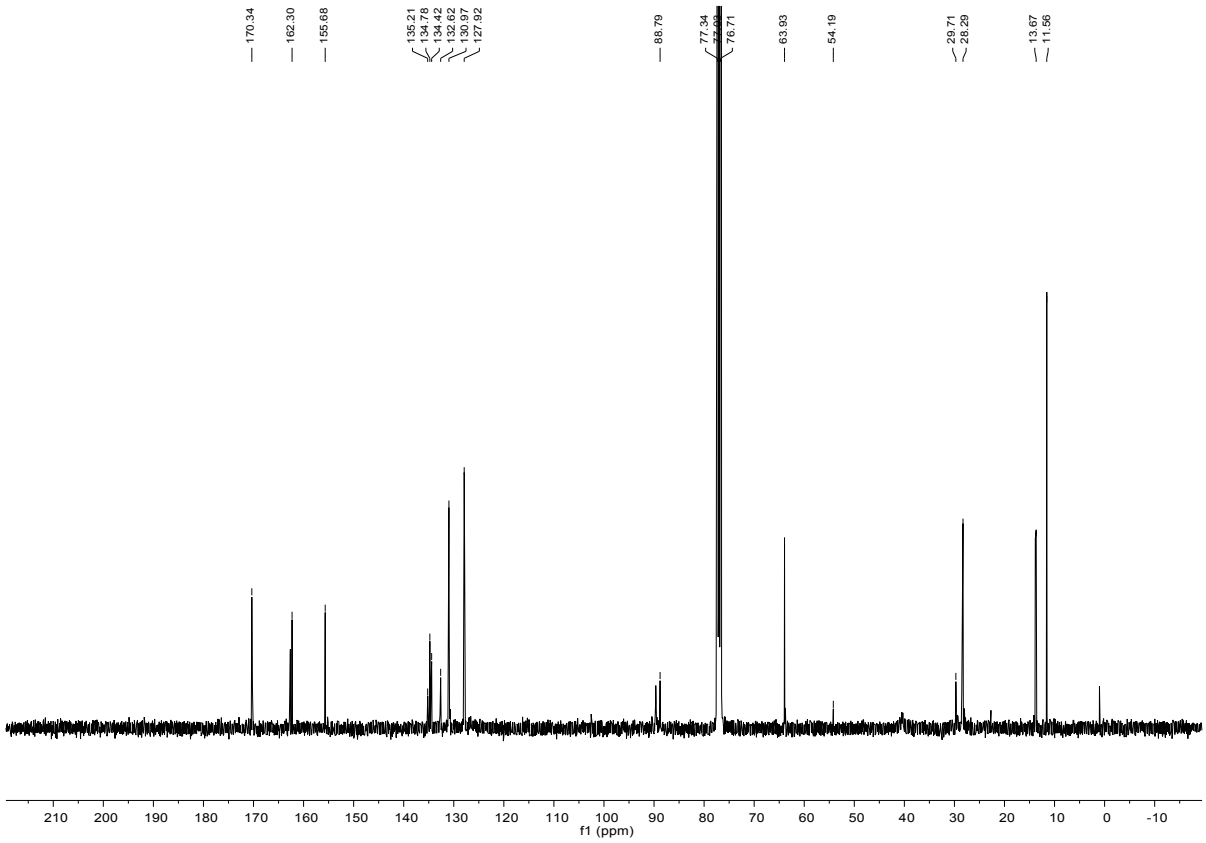
ethyl 3-(2,3-dichlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ac)



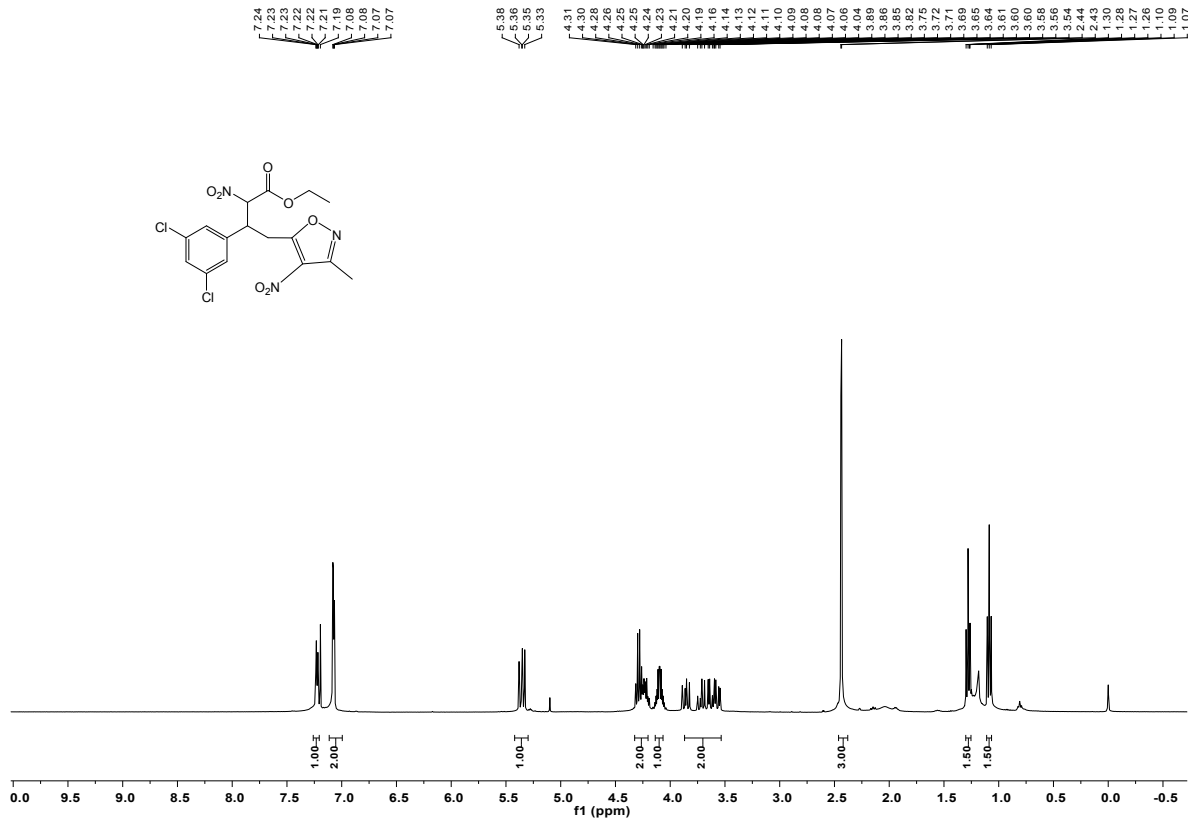


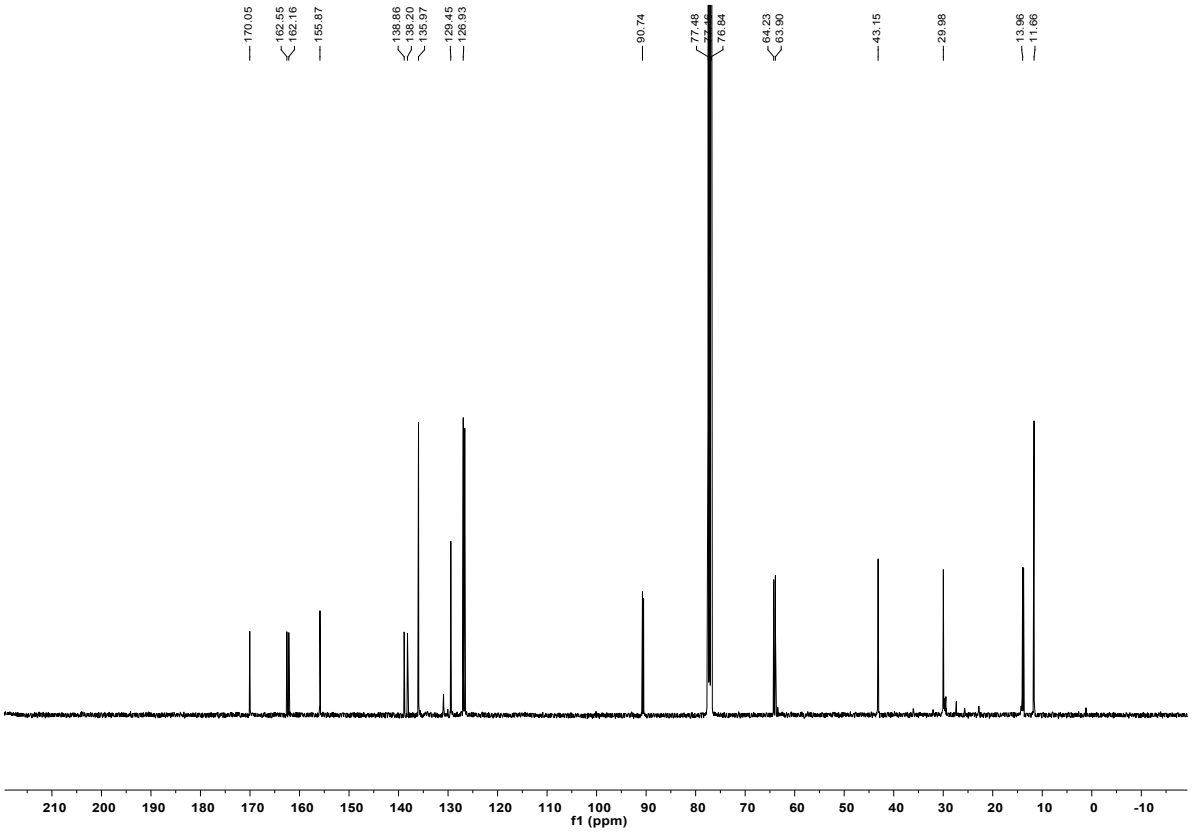
ethyl 3-(2,4-dichlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ad)



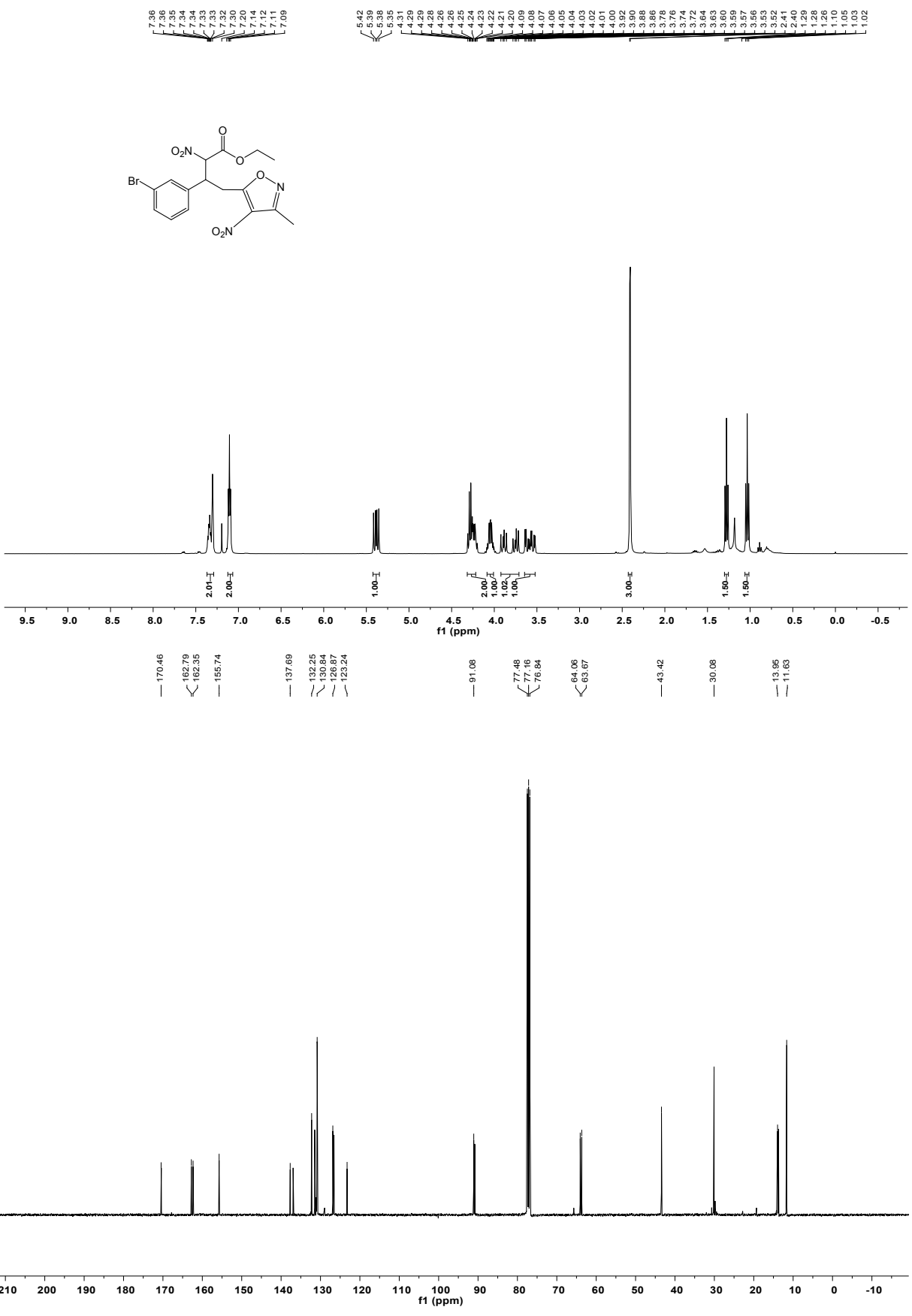


ethyl 3-(3,5-dichlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ae)

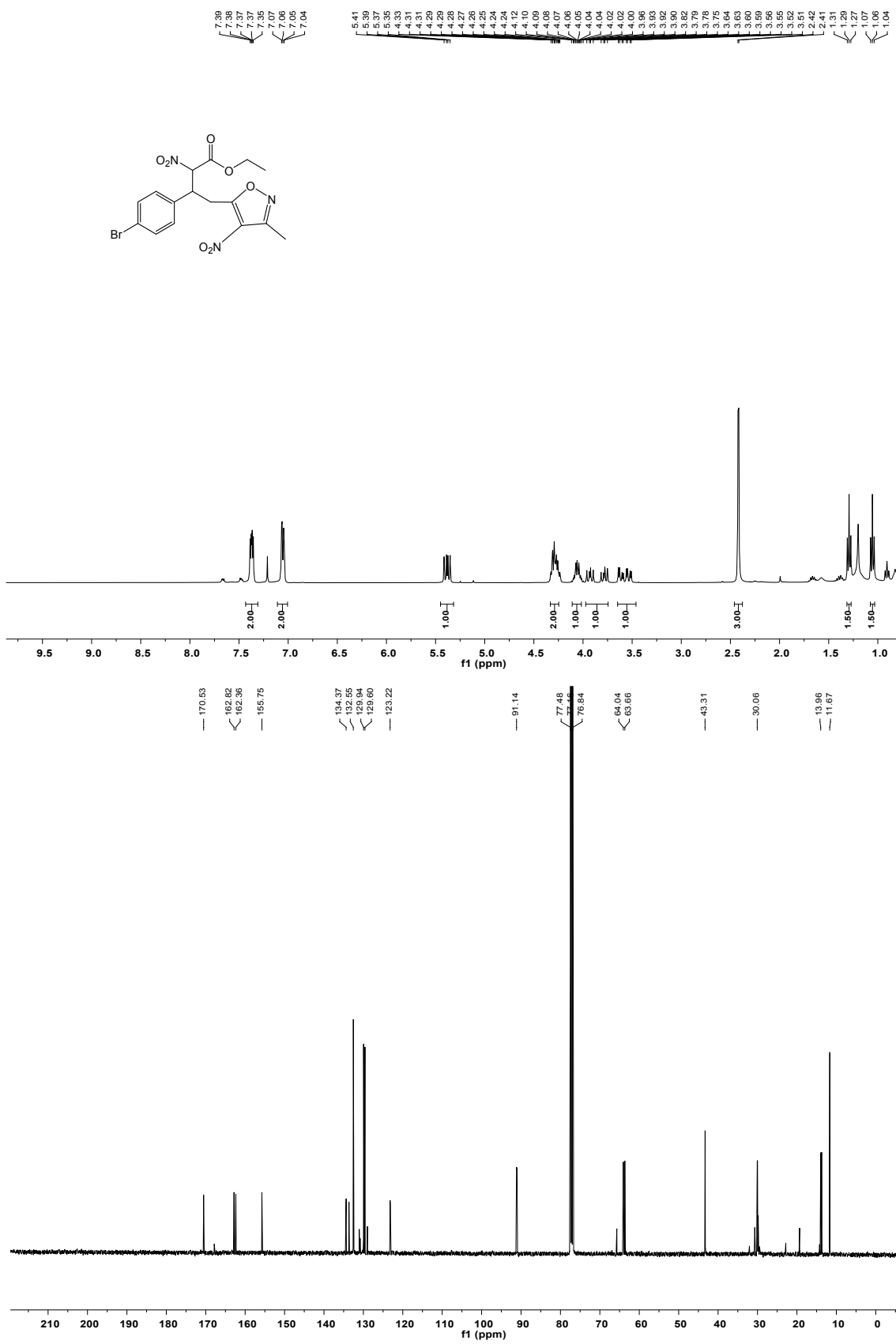




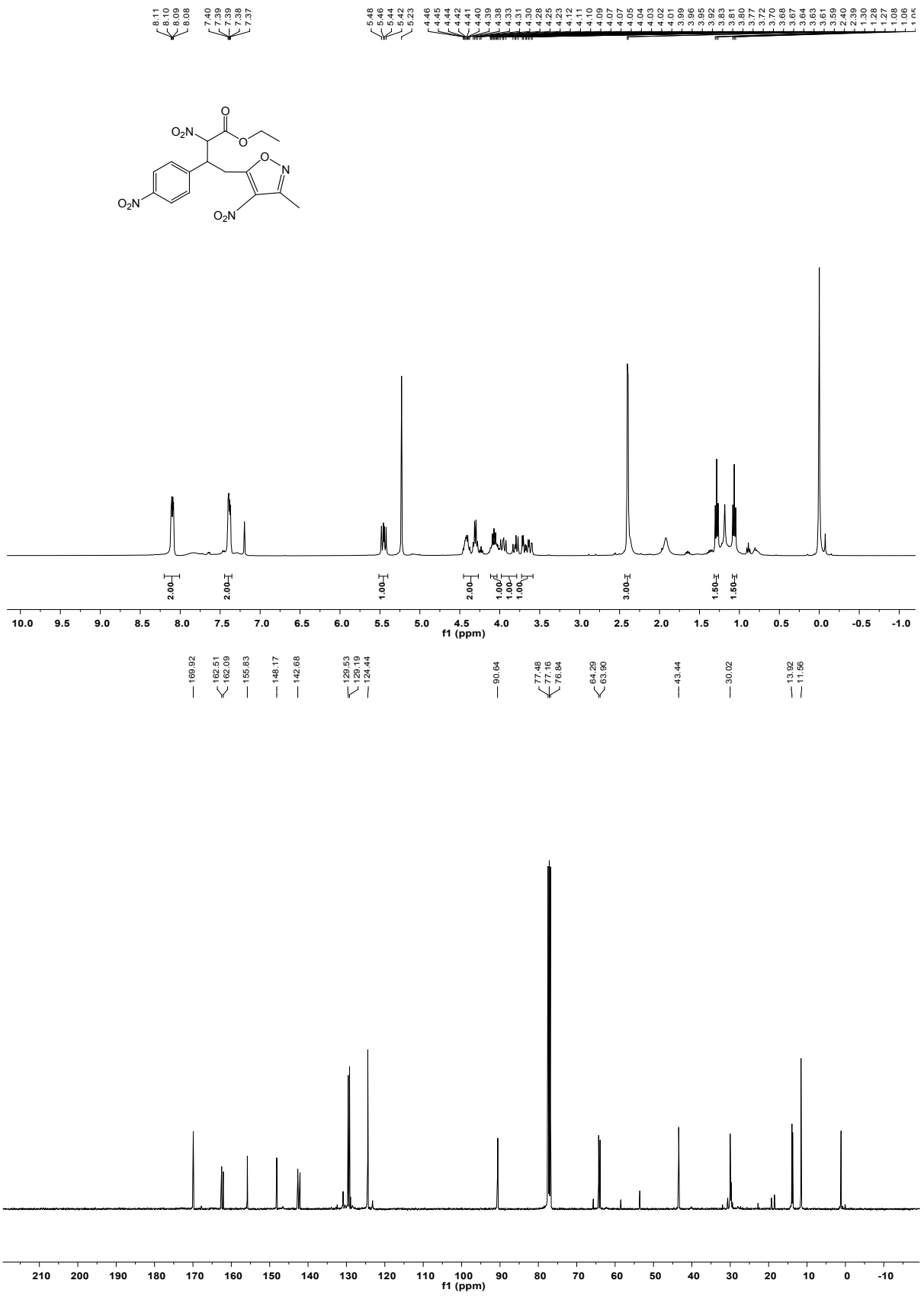
ethyl 3-(3-bromophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4af)



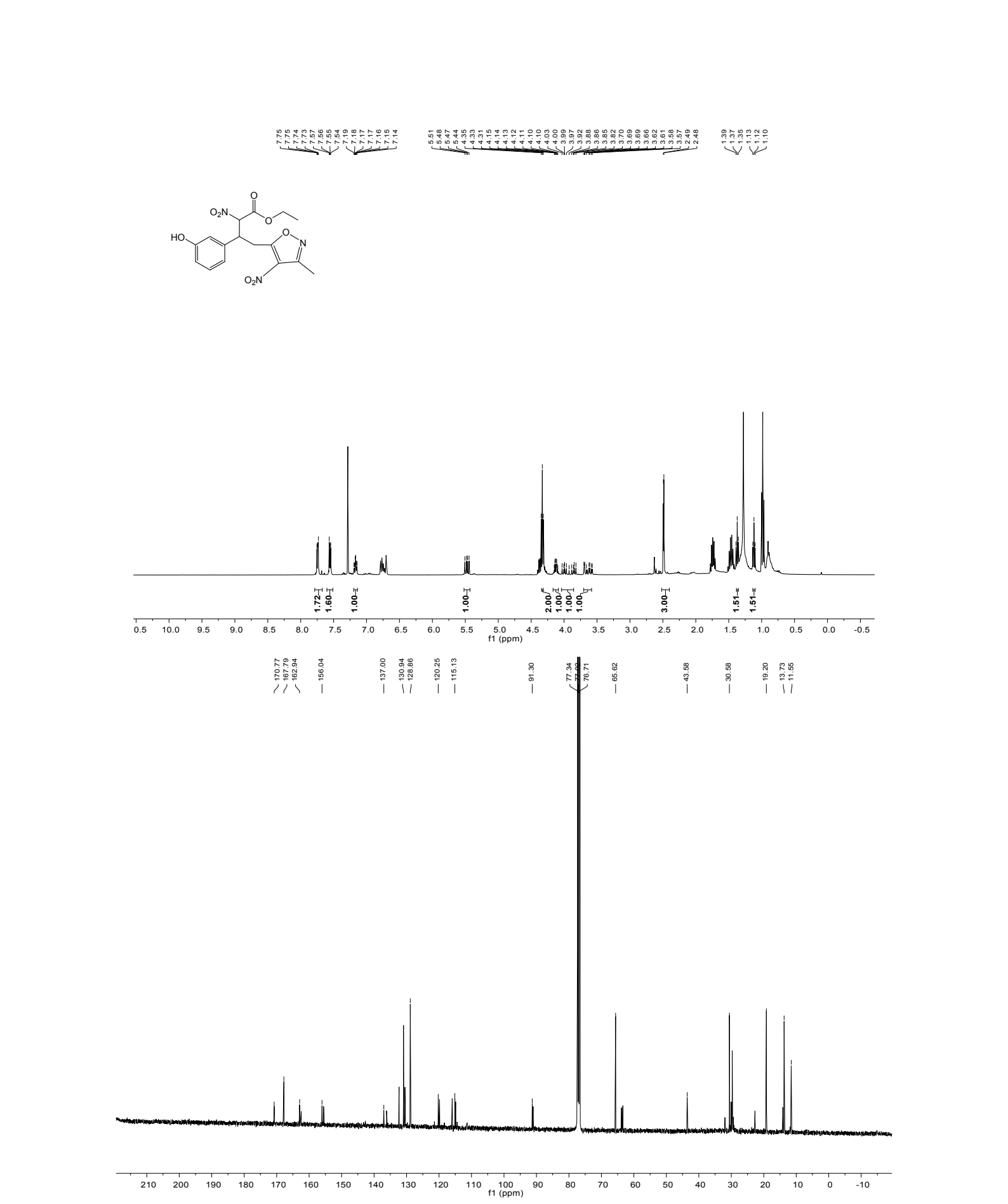
ethyl 3-(4-bromophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ag)



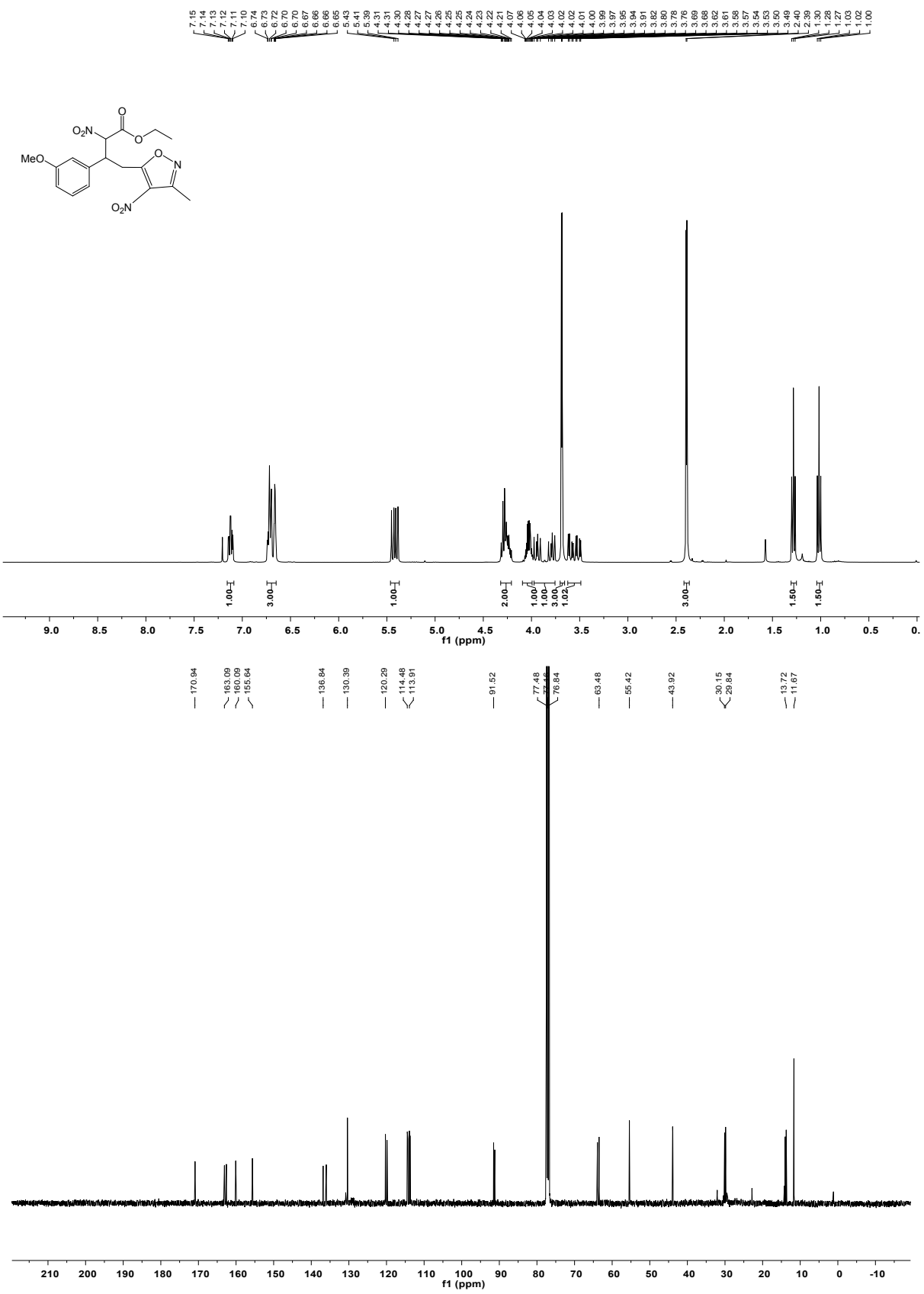
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(4-nitrophenyl)butanoate (4ah)



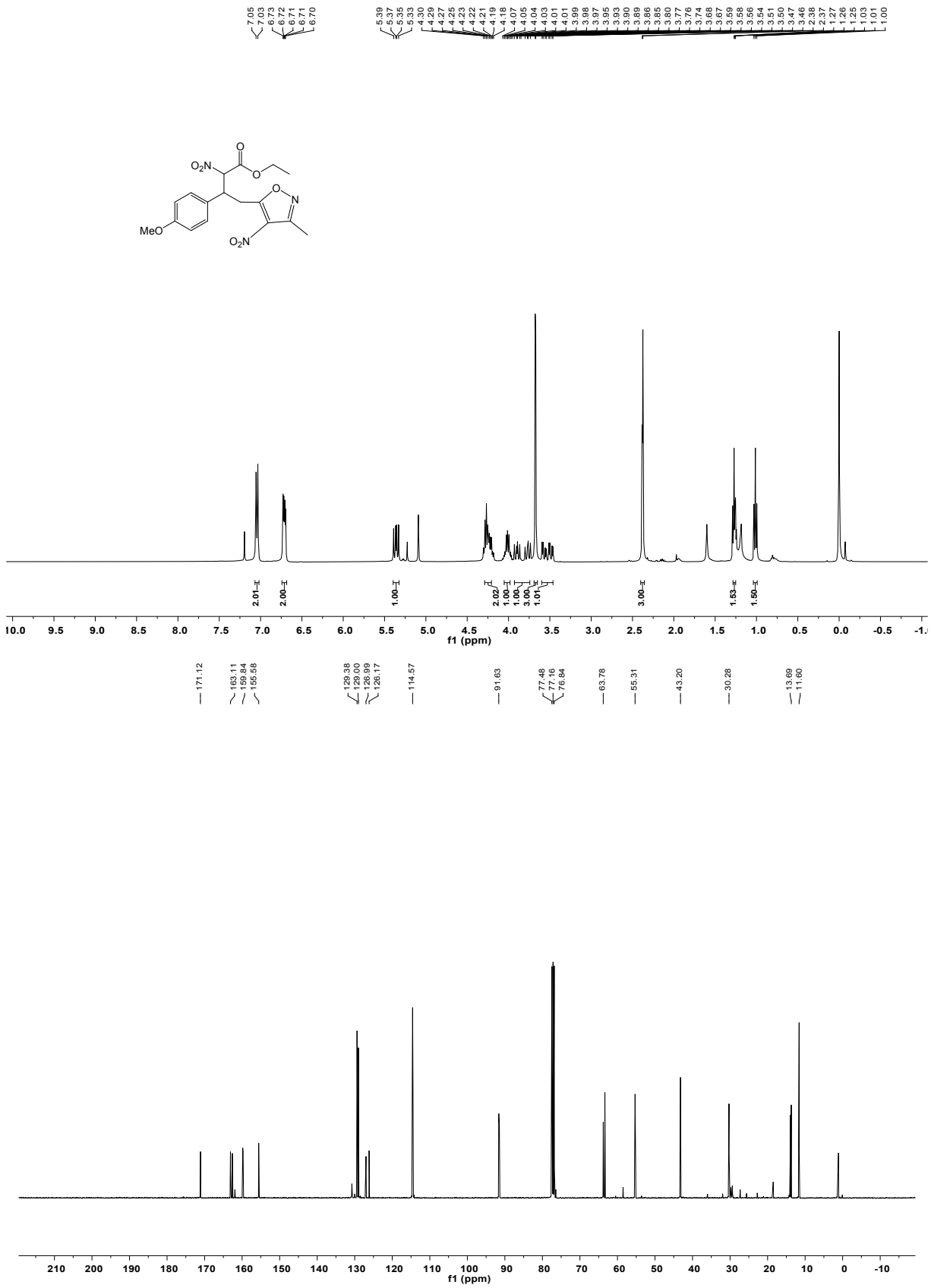
ethyl 3-(3-hydroxyphenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ai)



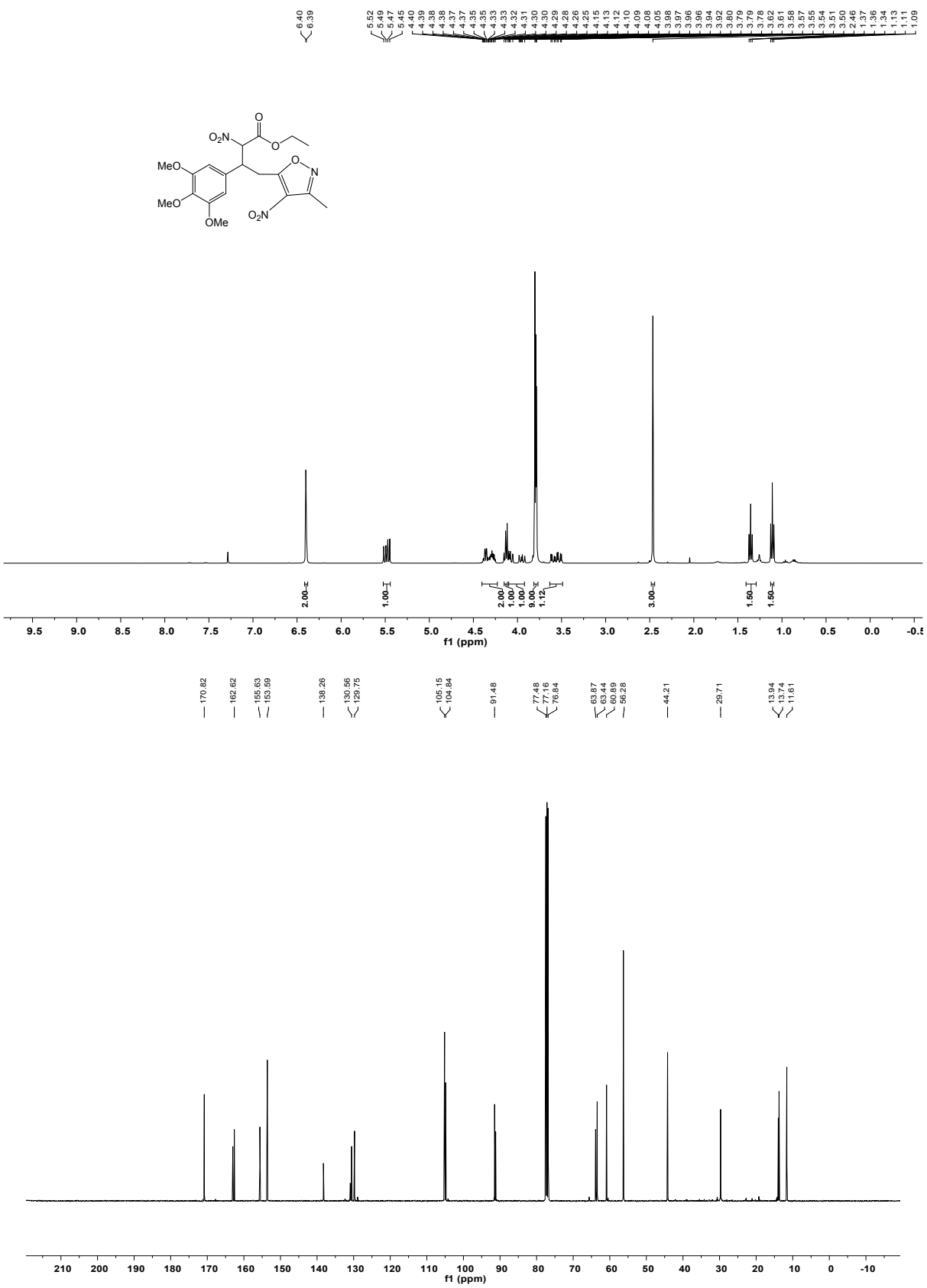
ethyl 3-(3-methoxyphenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4aj)



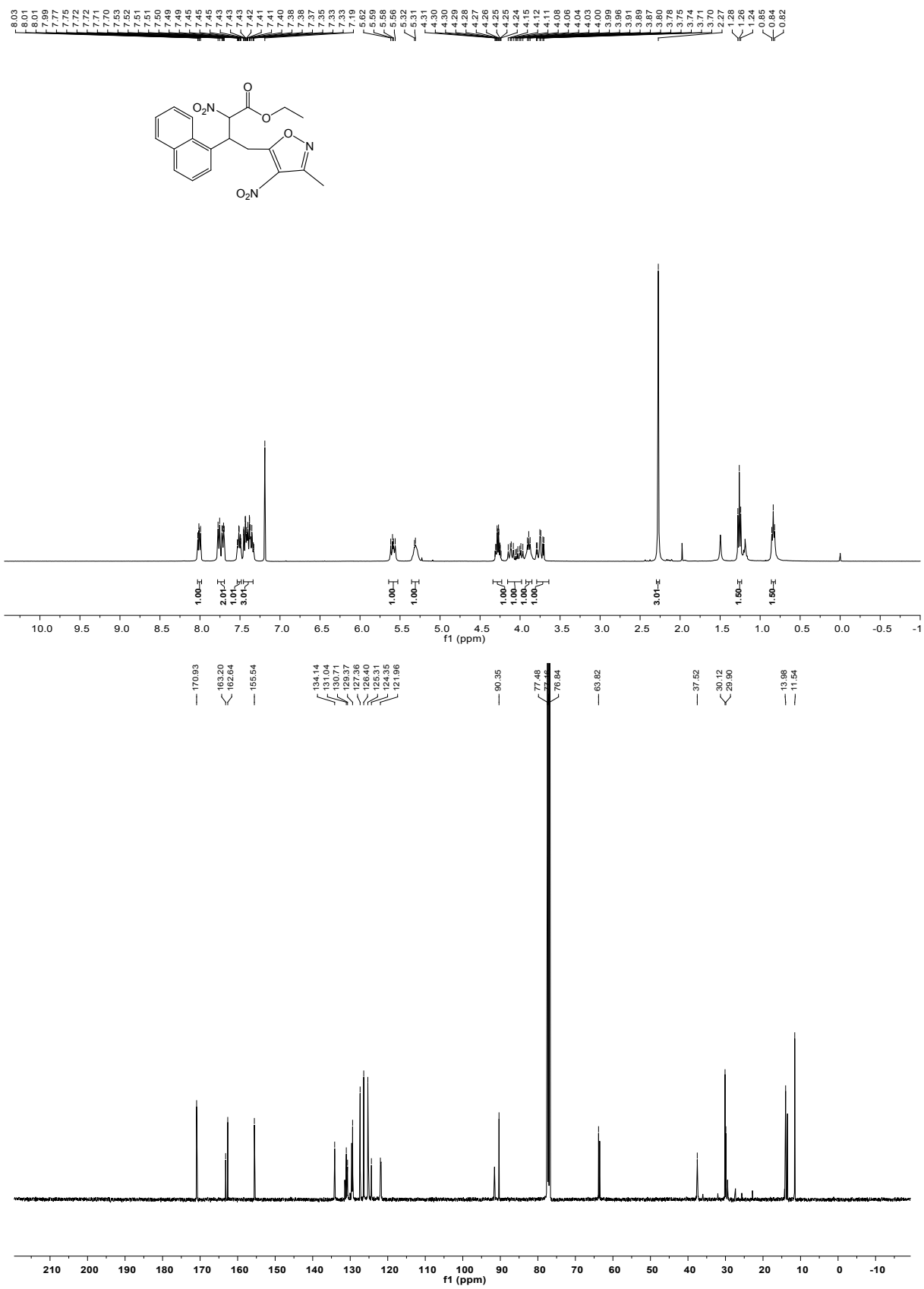
ethyl 3-(4-methoxyphenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ak)



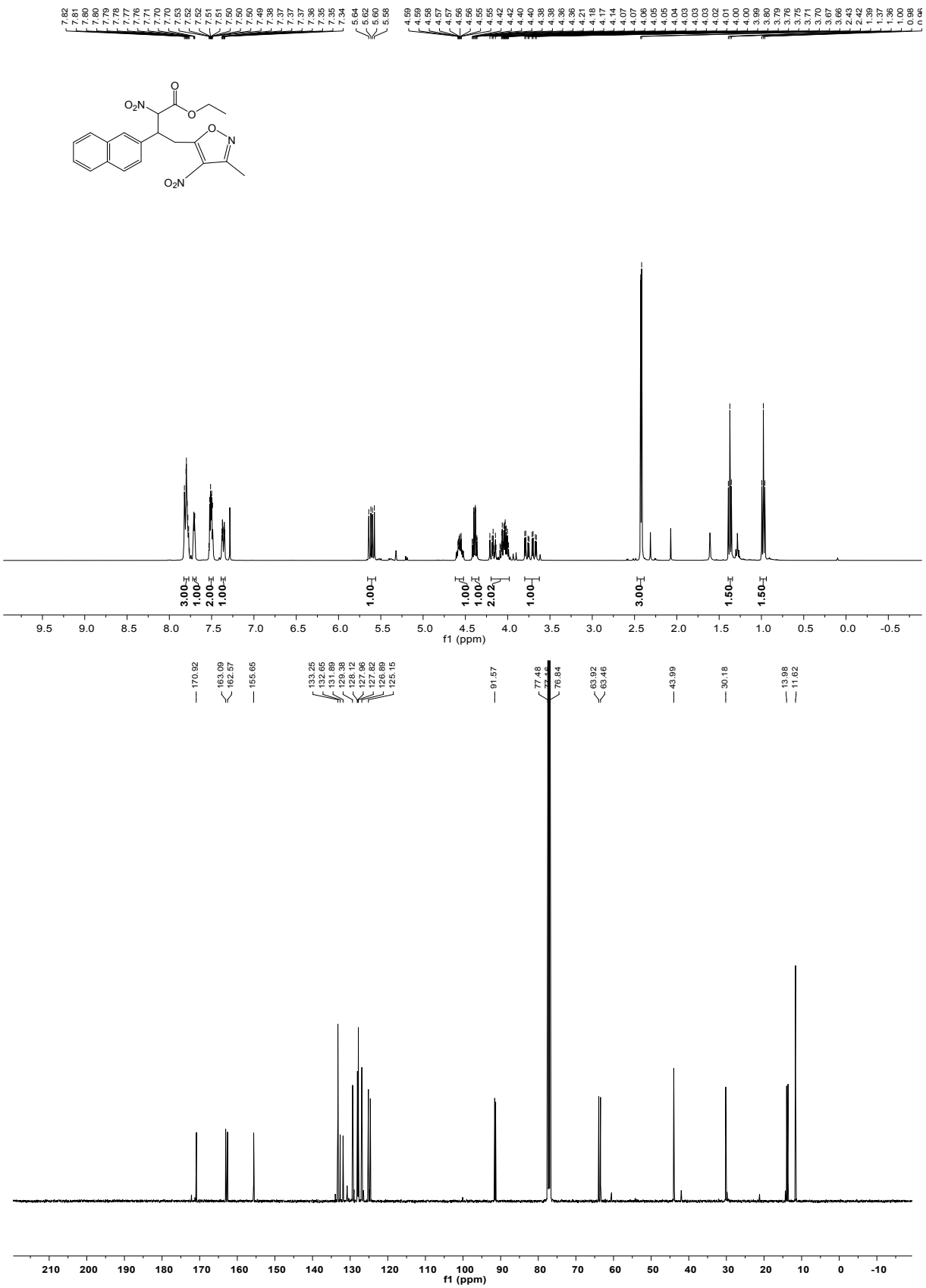
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(3,4,5-trimethoxyphenyl)butanoate (4al)



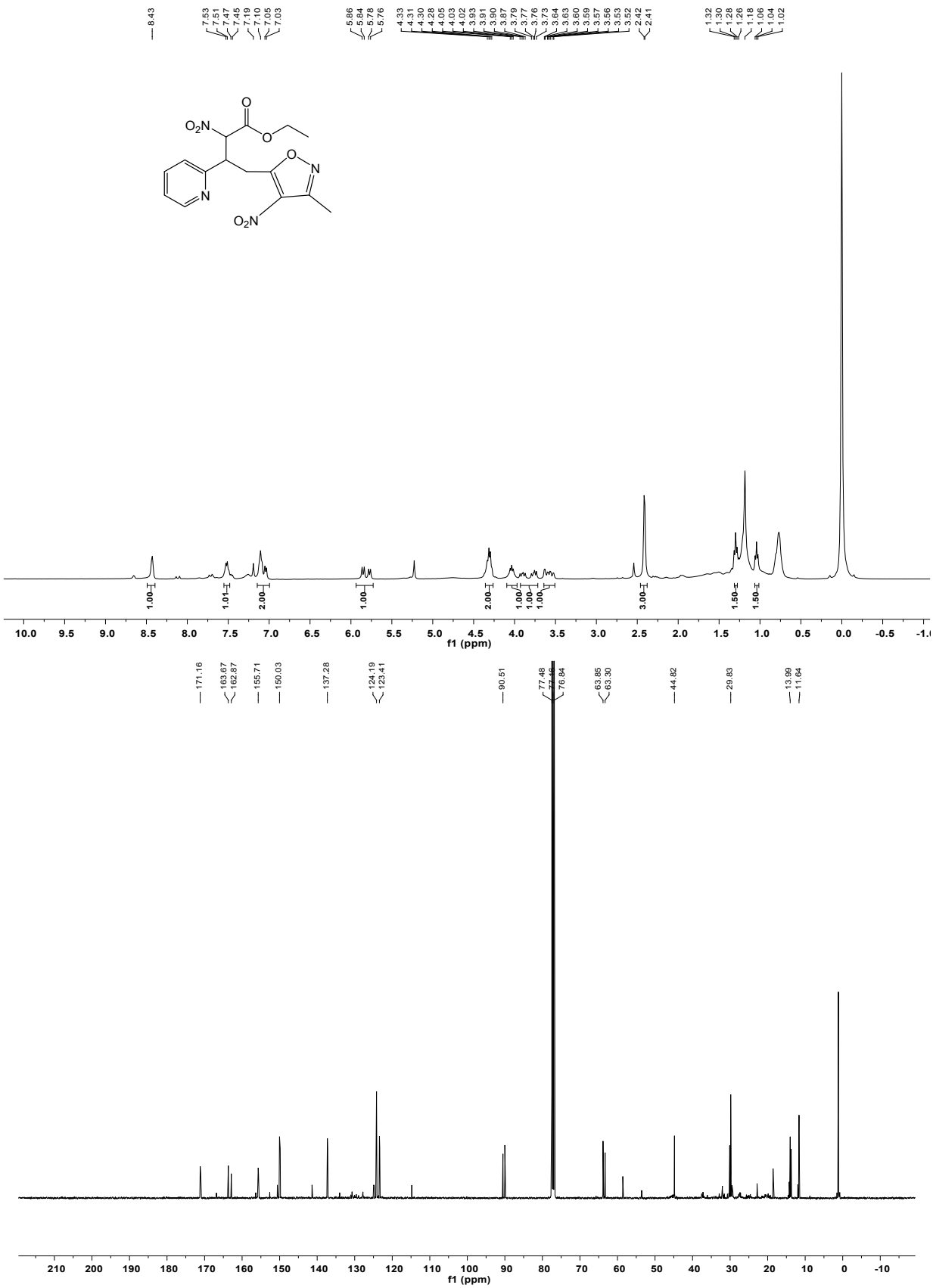
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-3-(naphthalen-1-yl)-2-nitrobutanoate (4am)



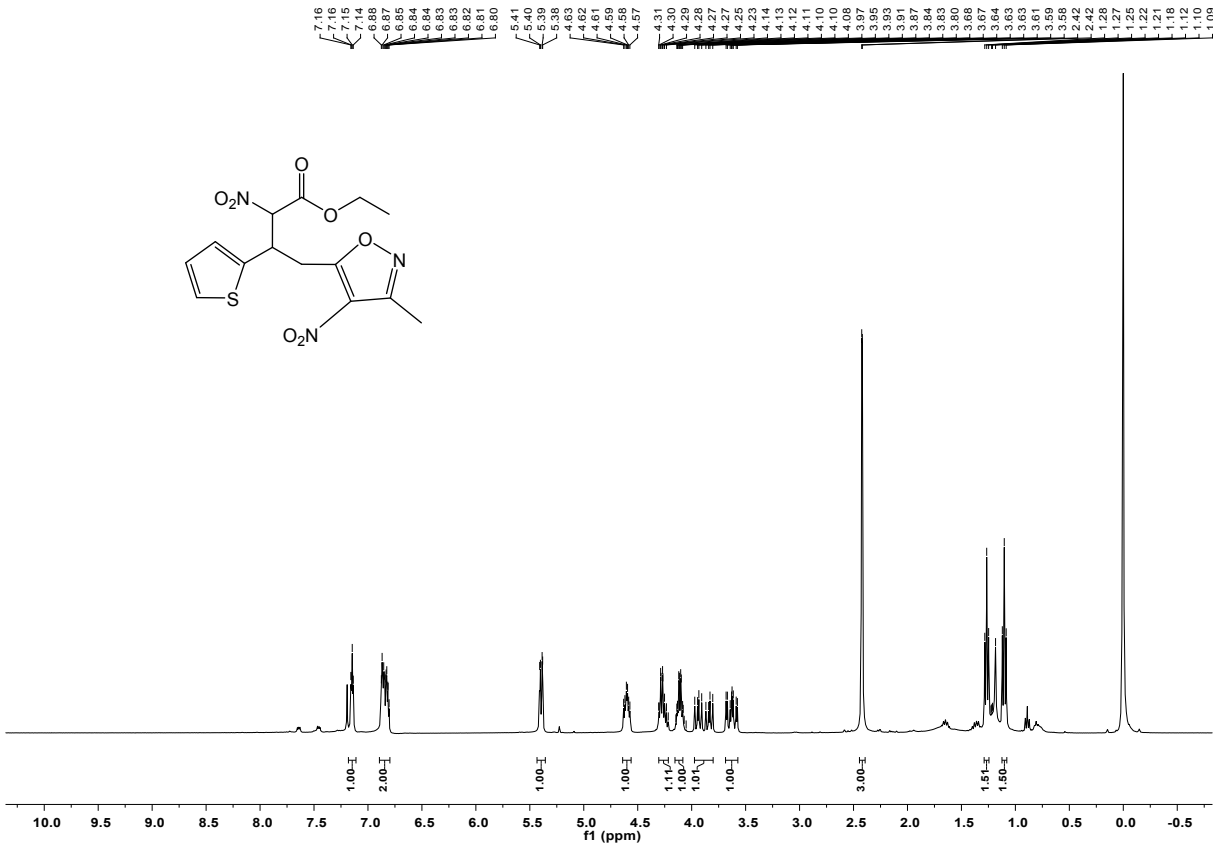
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-3-(naphthalen-2-yl)-2-nitrobutanoate (4an)

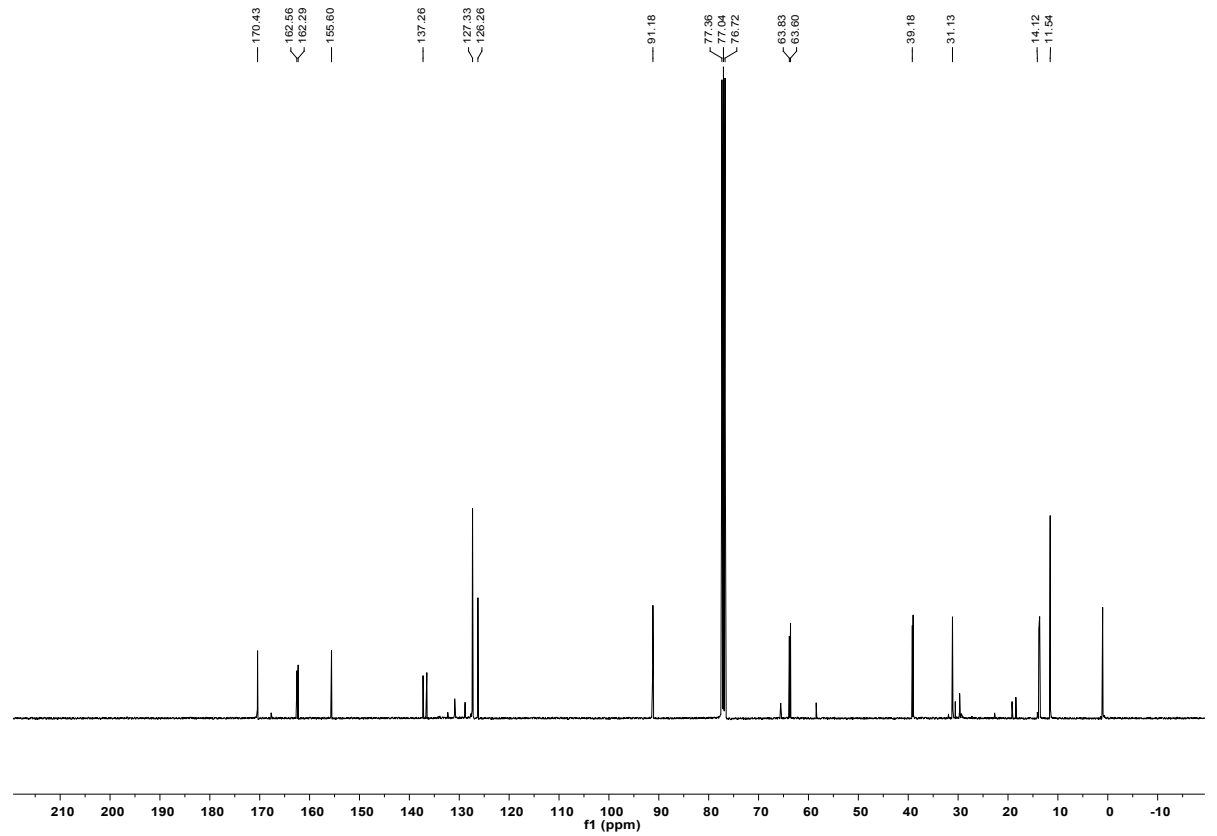


ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(pyridin-2-yl)butanoate (4ao)

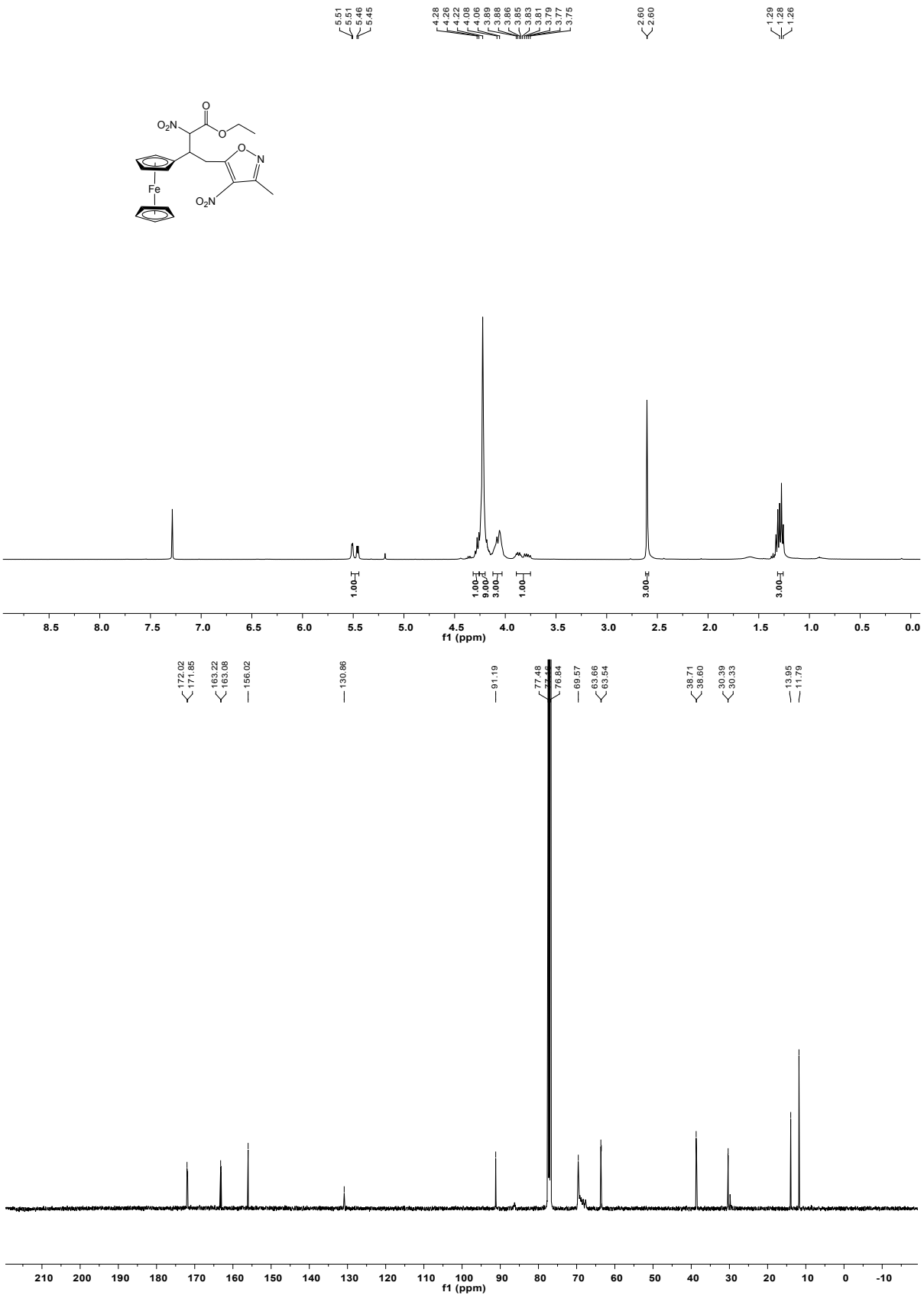


ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(thiophen-2-yl)butanoate (4ap)

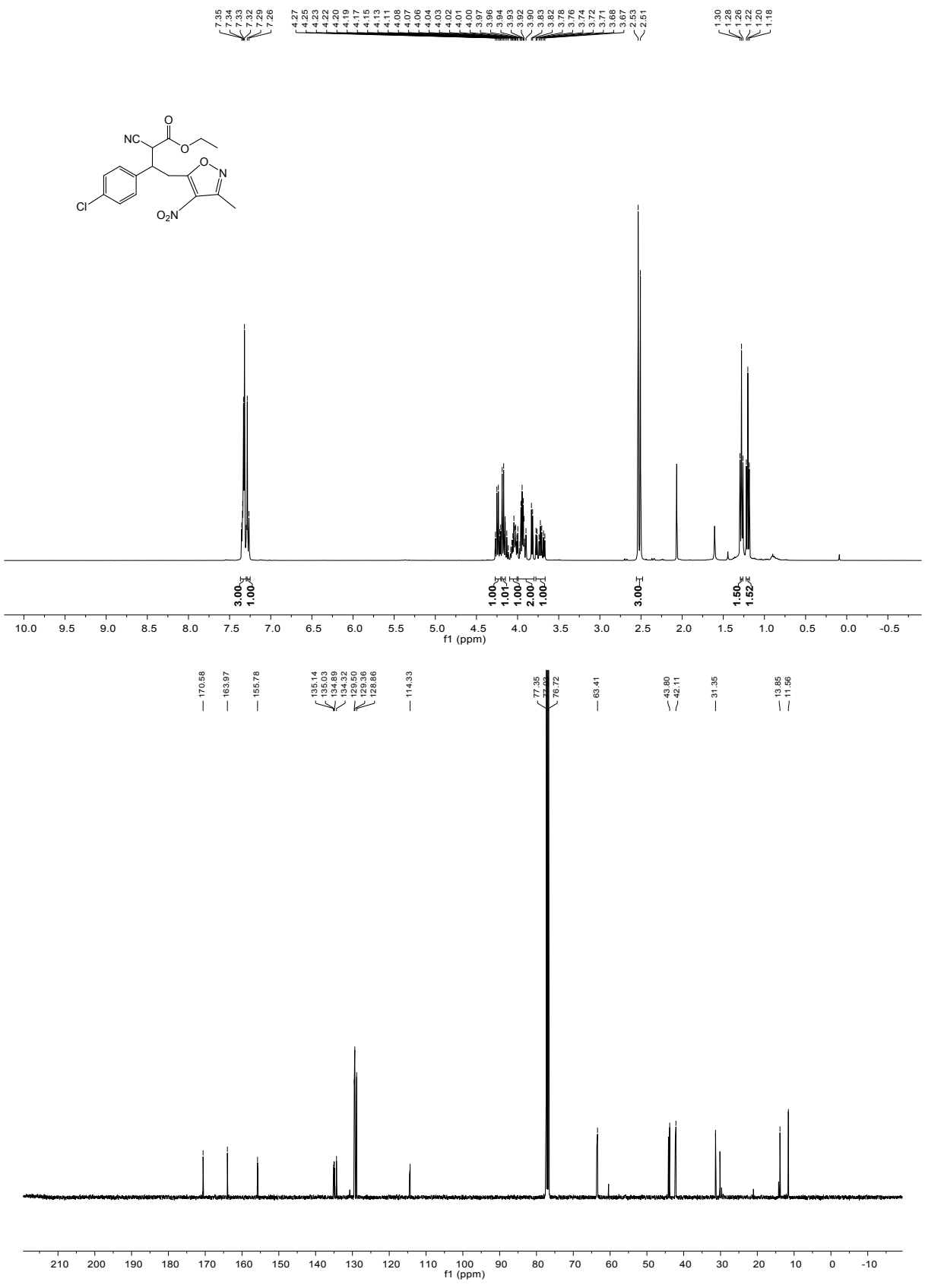




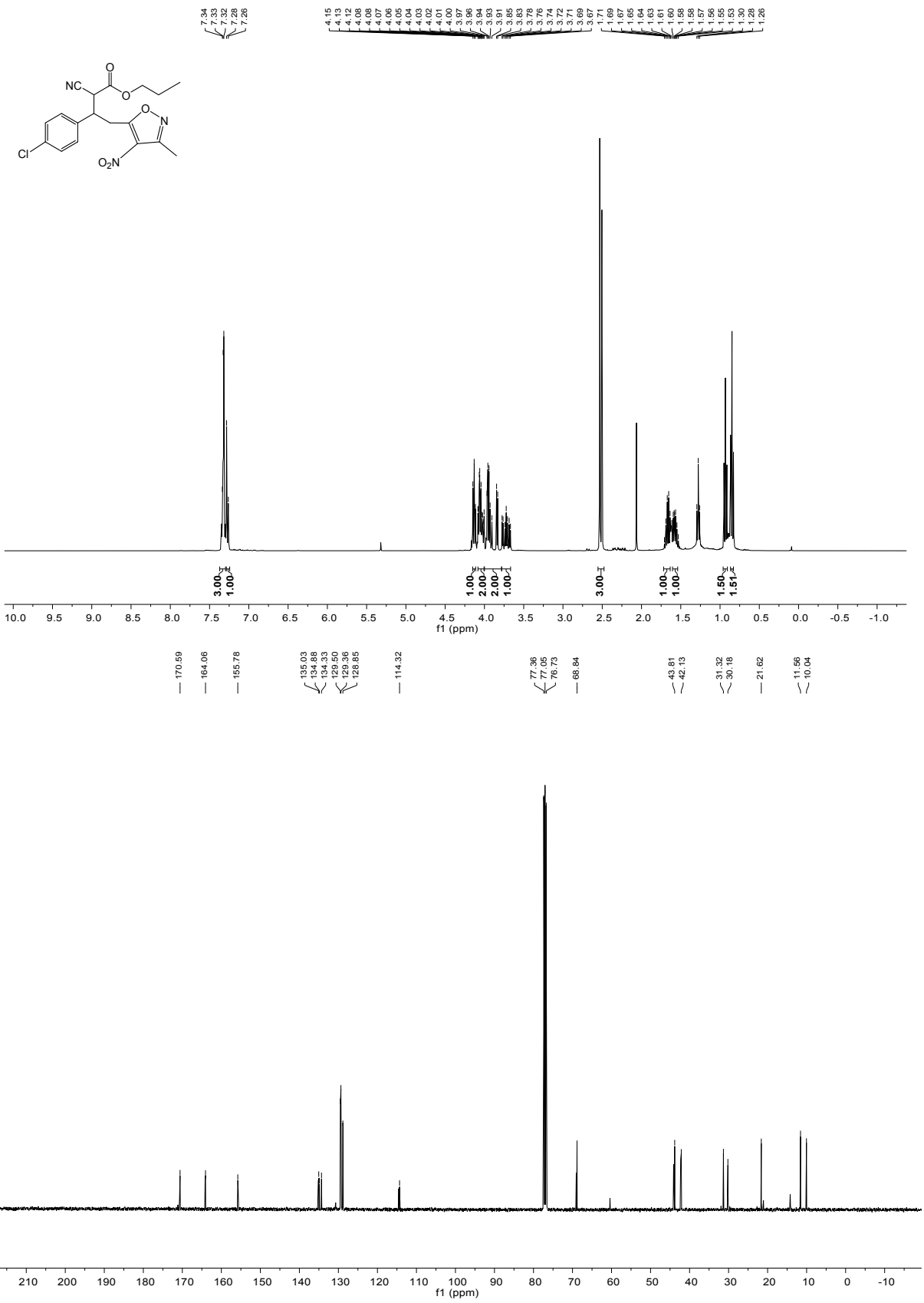
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(ferrocene-2-yl)butanoate (4aq)



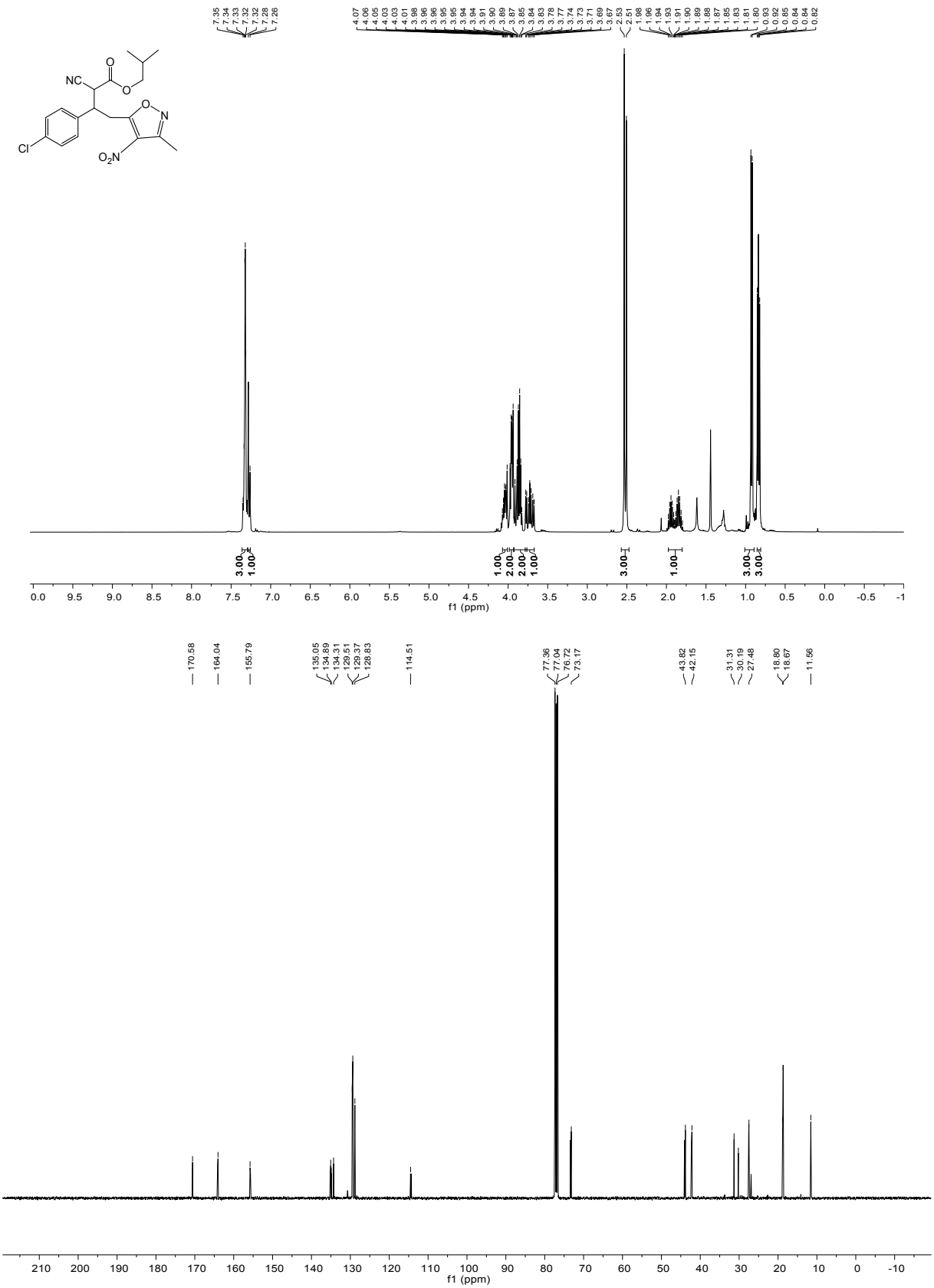
ethyl 3-(4-chlorophenyl)-2-cyano-4-(3-methyl-4-nitroisoxazol-5-yl)butanoate (4ba)



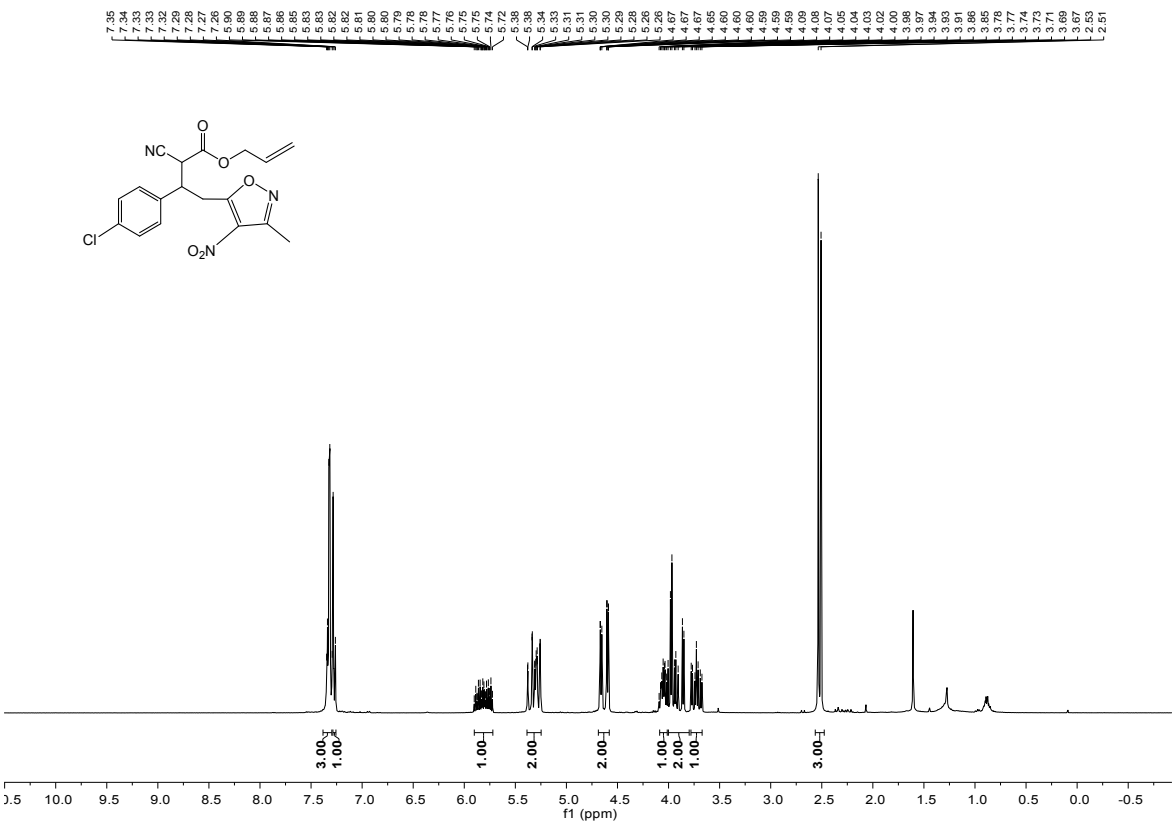
propyl 3-(4-chlorophenyl)-2-cyano-4-(3-methyl-4-nitroisoxazol-5-yl)butanoate (4bb)

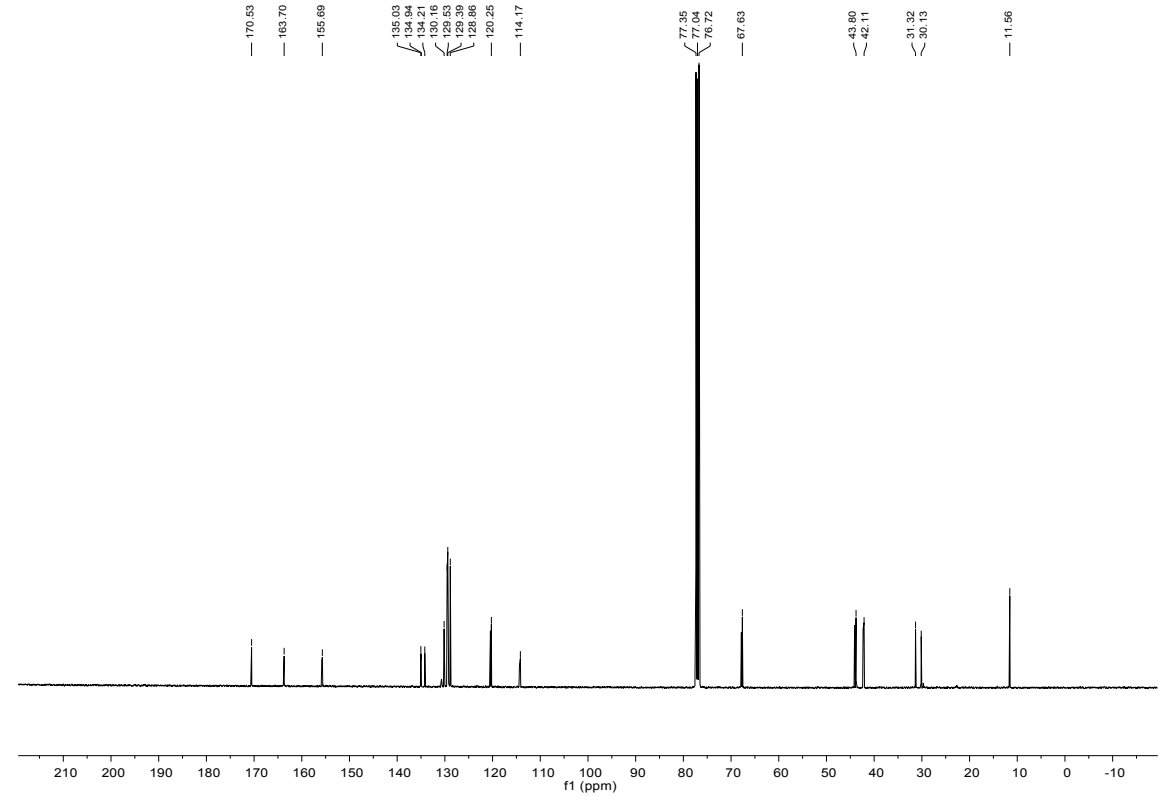


isobutyl 3-(4-chlorophenyl)-2-cyano-4-(3-methyl-4-nitroisoxazol-5-yl)butanoate (4bc)

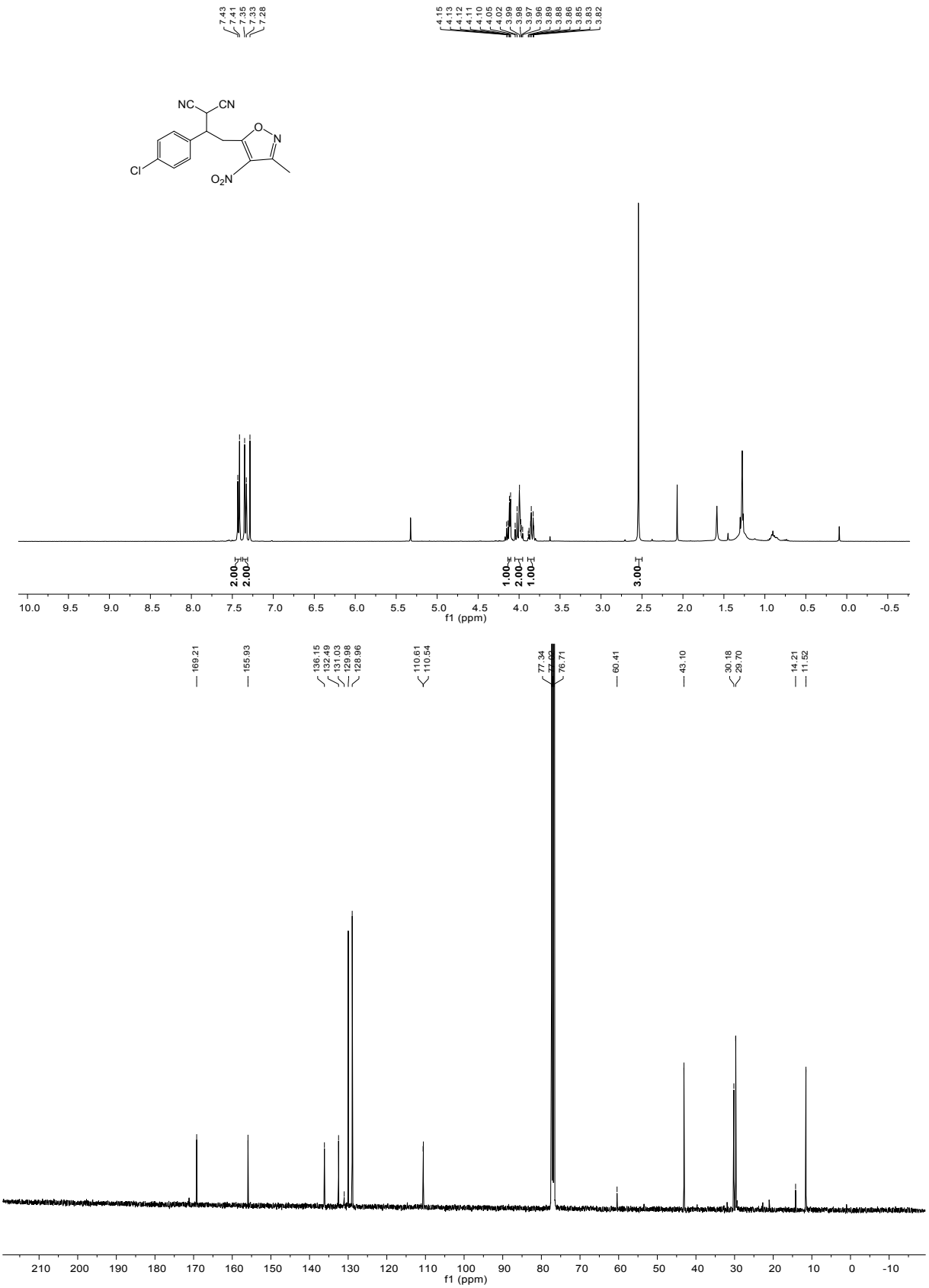


allyl 3-(4-chlorophenyl)-2-cyano-4-(3-methyl-4-nitroisoxazol-5-yl)butanoate (4bd)



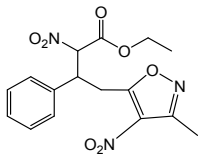


2-(1-(4-chlorophenyl)-2-(3-methyl-4-nitroisoxazol-5-yl)ethyl)malononitrile (4be)

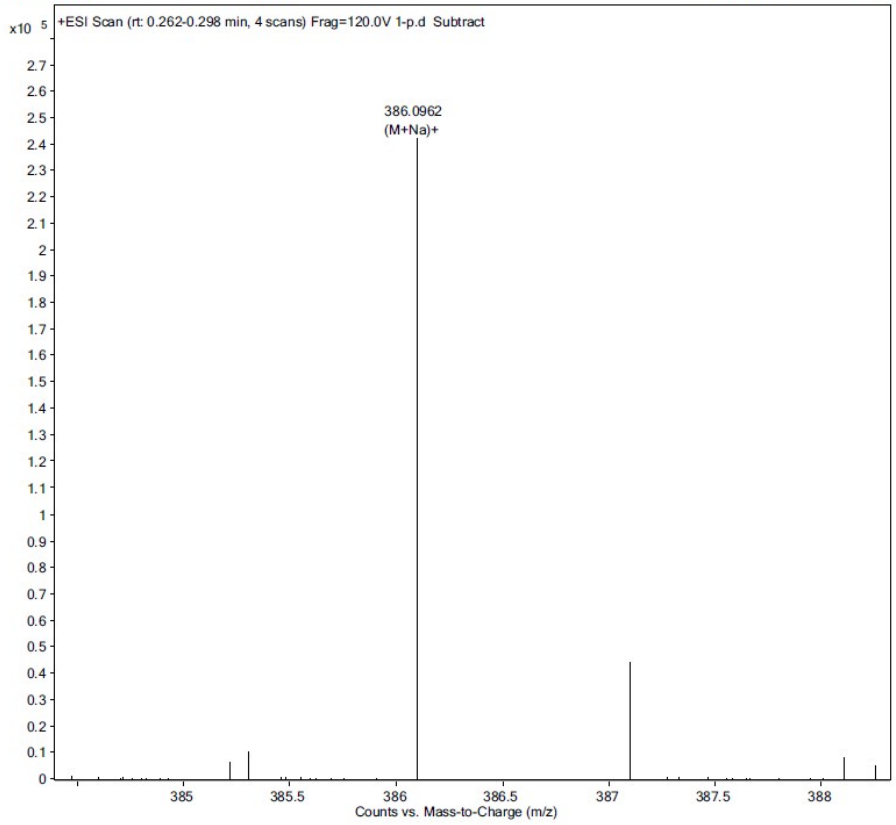


HRMS of 3,4,5-trisubstituted isoxazoles

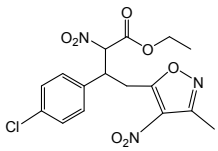
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-phenylbutanoate (4aa)



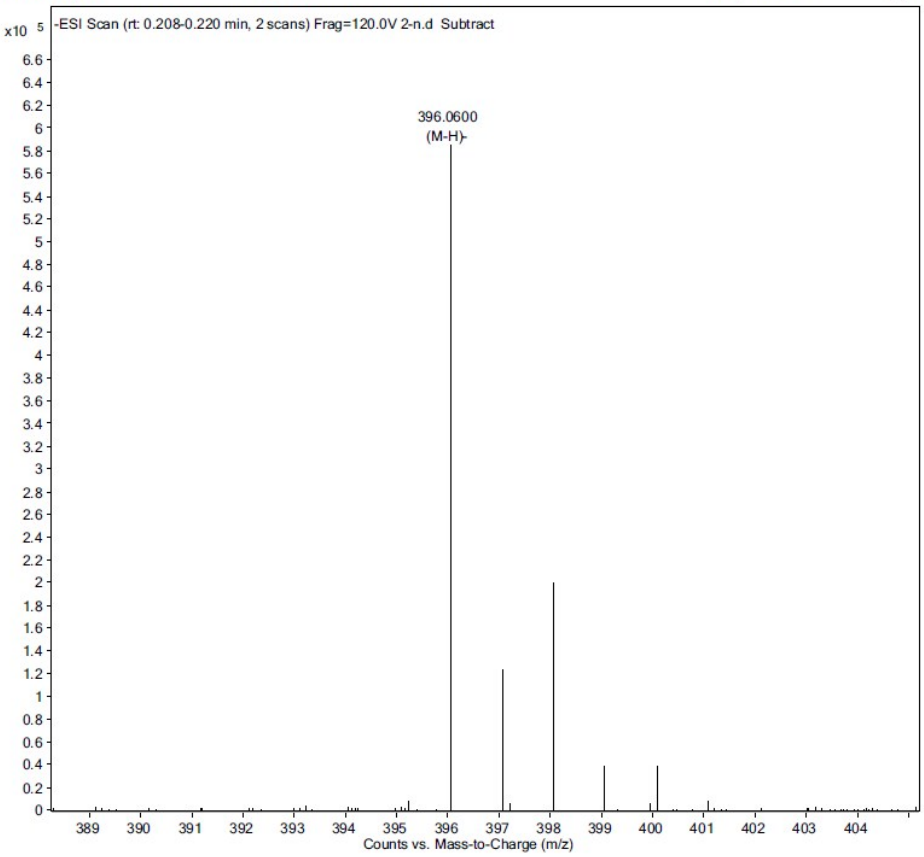
Sample Name		**Position**	P2a1	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	1-p.d
ACQ Method	20110418-MSonly-p.m	**Comment**		**Acquired Time**	3/4/2019 2:16:25 PM



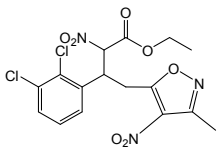
ethyl 3-(4-chlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ab)



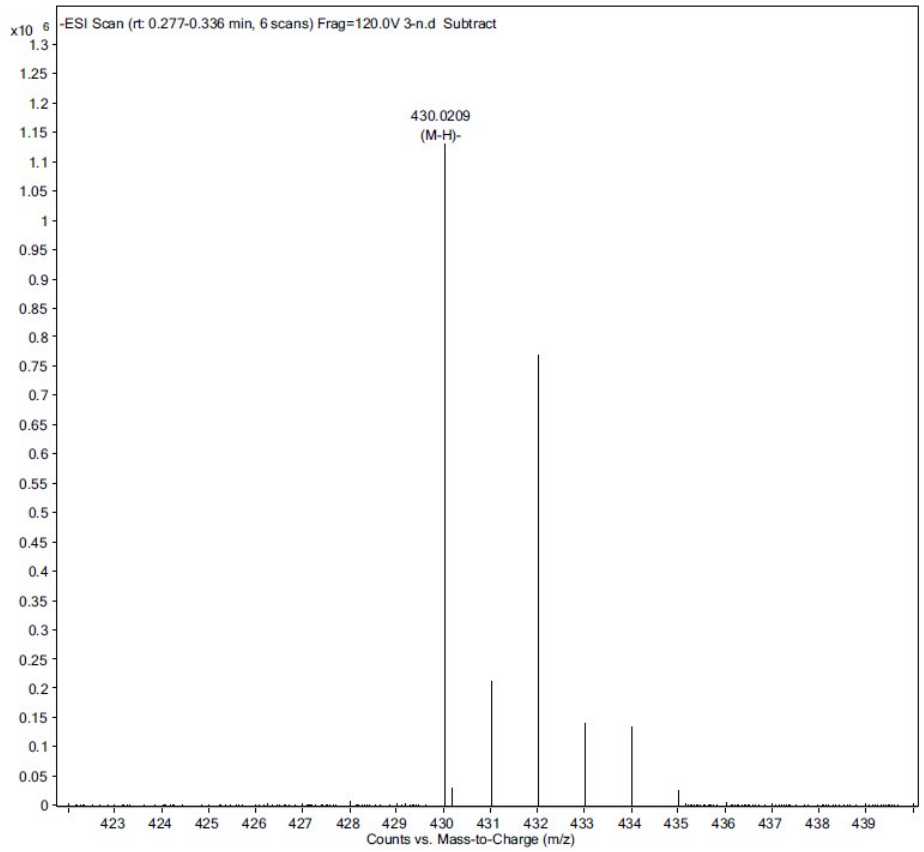
Sample Name		**Position**	P2a2	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 2:40:23 PM



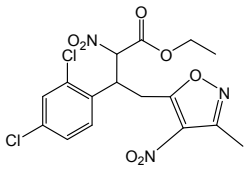
ethyl 3-(2,3-dichlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ac)



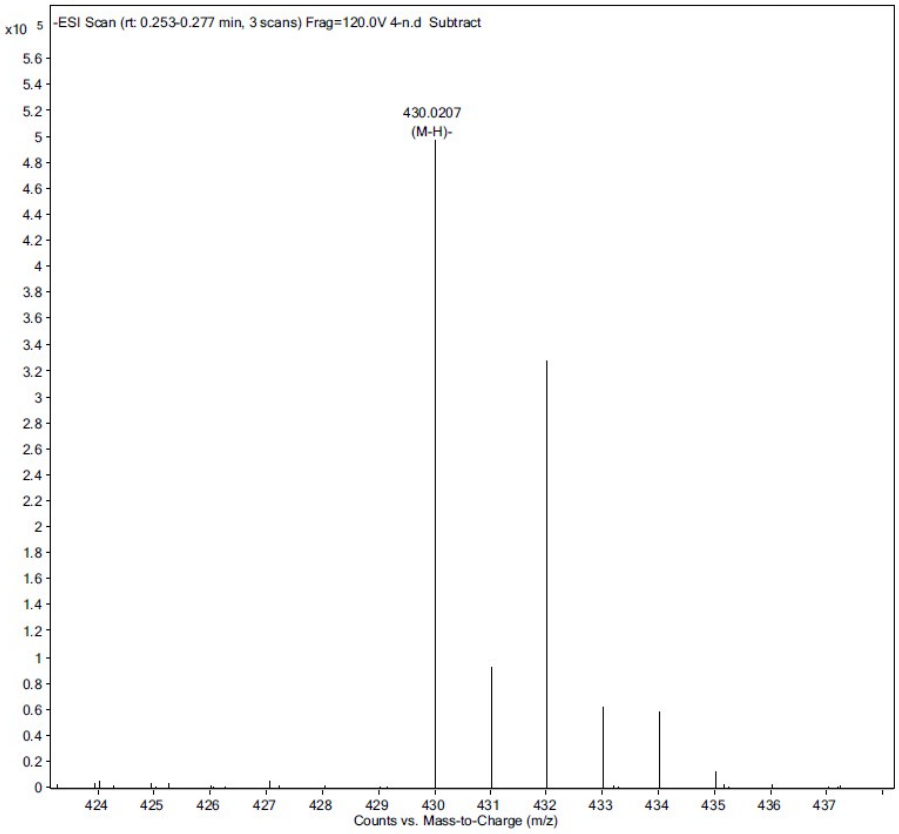
Sample Name		**Position**	P2a3	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	3-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 2:44:26 PM



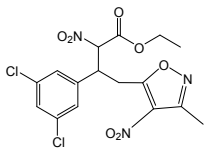
ethyl 3-(2,4-dichlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ad)



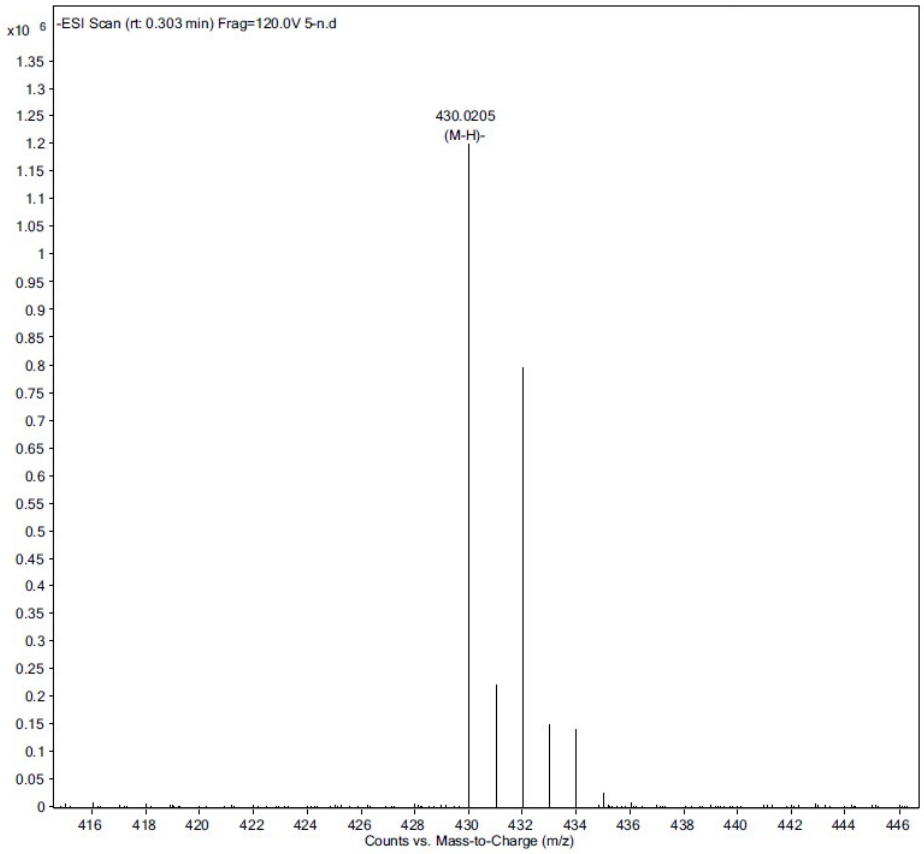
Sample Name		**Position**	P2a4	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 2:46:30 PM



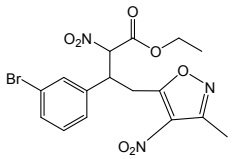
ethyl 3-(3,5-dichlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ae)



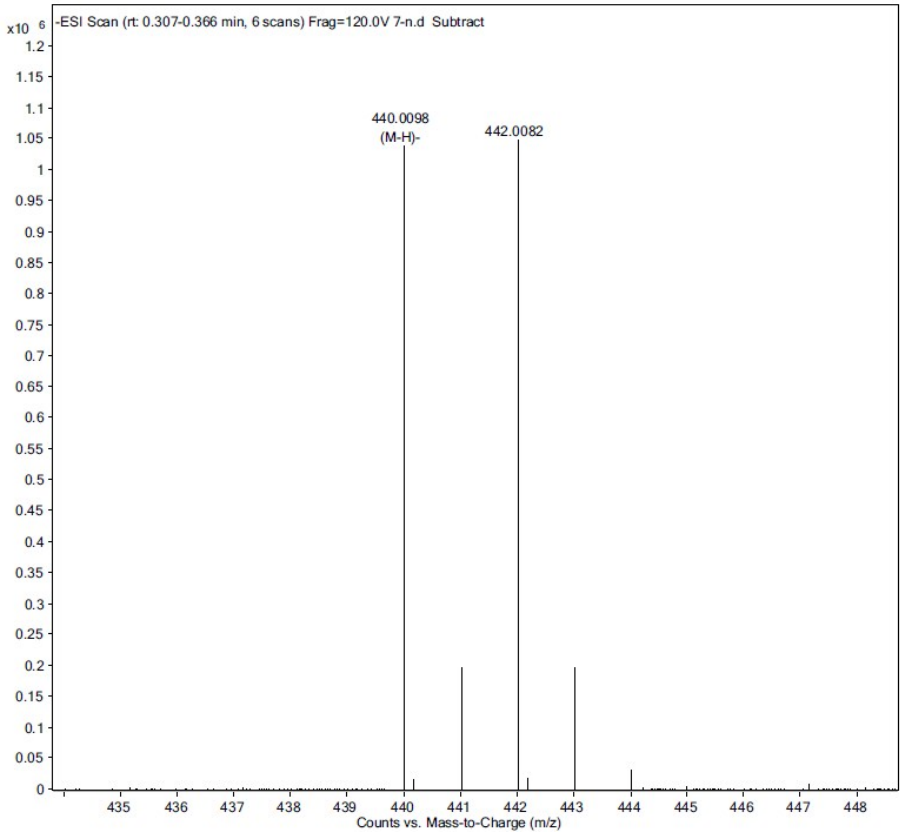
Sample Name		**Position**	P2a5	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	5-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 2:48:52 PM



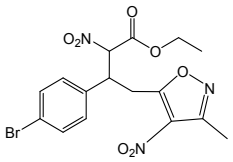
ethyl 3-(3-bromophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4af)



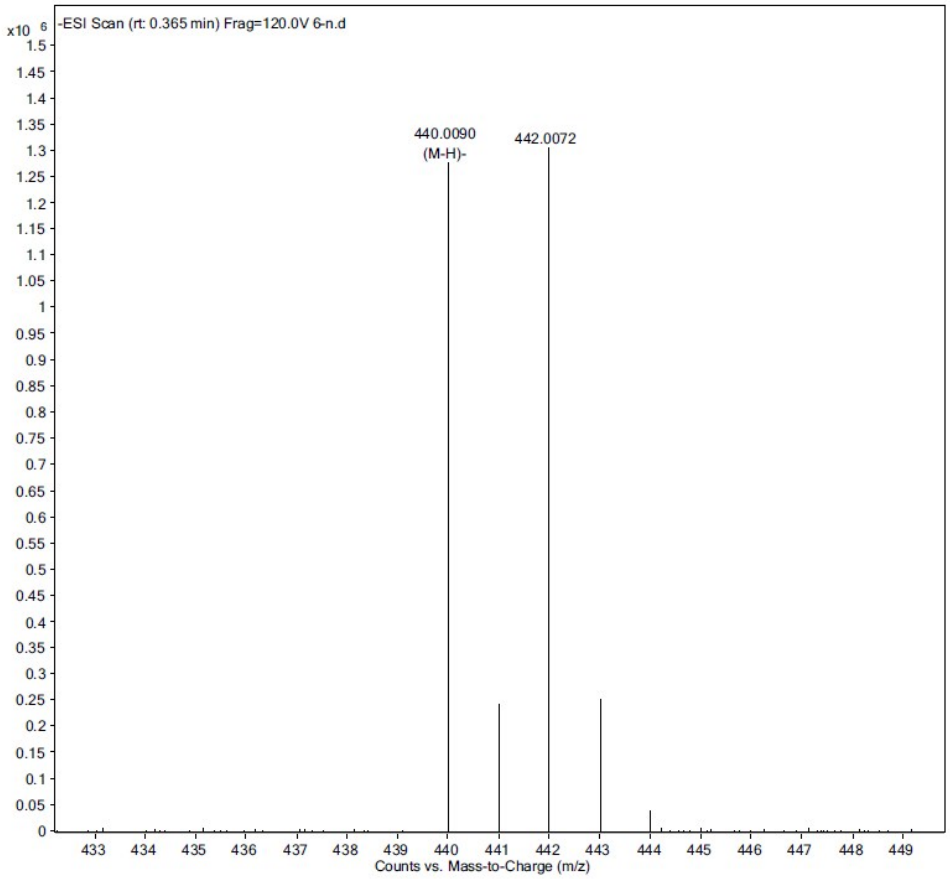
Sample Name		**Position**	P2a7	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	7-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 2:53:07 PM



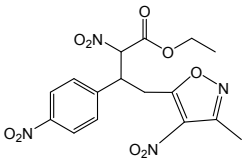
ethyl 3-(4-bromophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ag)



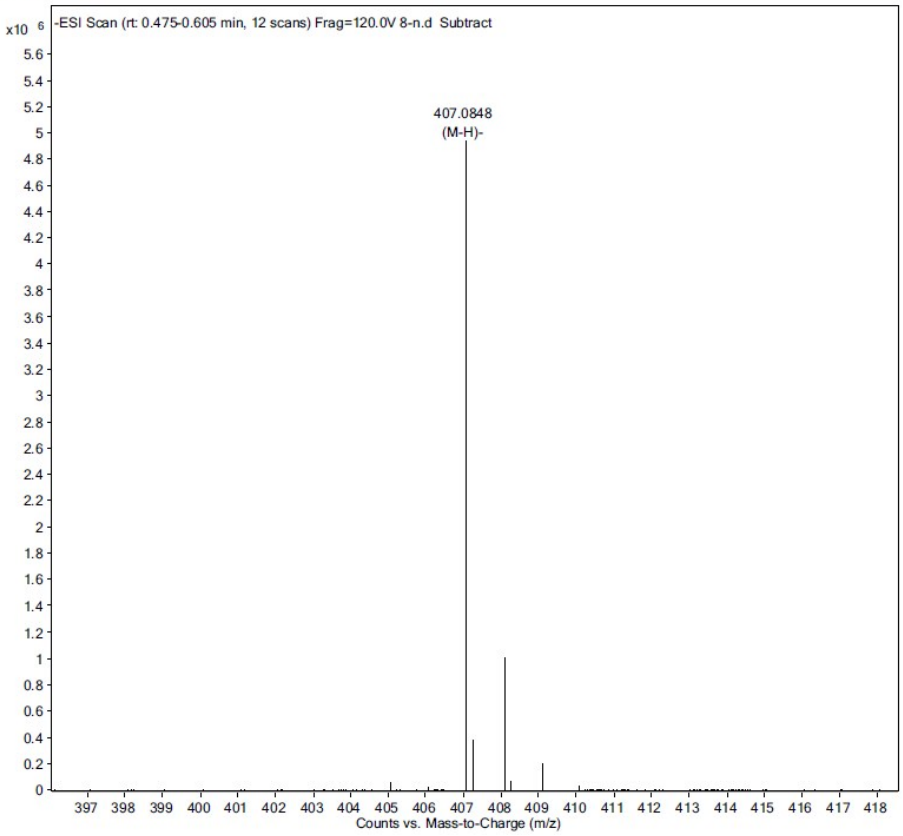
Sample Name		**Position**	P2a6	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	6-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 2:50:51 PM



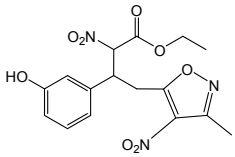
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(4-nitrophenyl)butanoate (4ah)



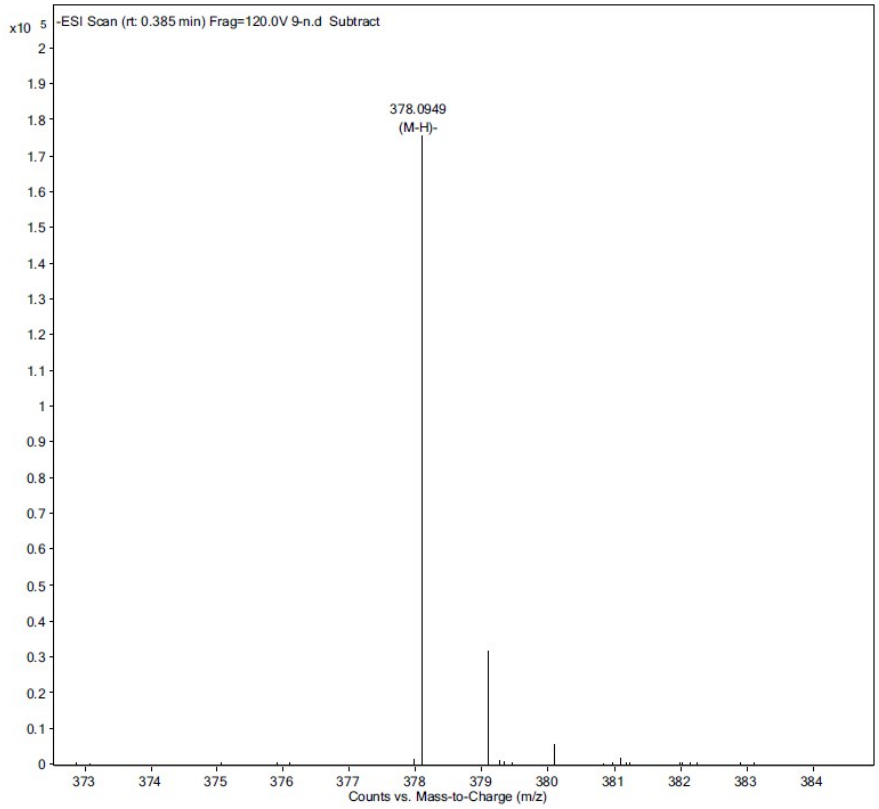
Sample Name		**Position**	P2a8	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	8-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 2:55:12 PM



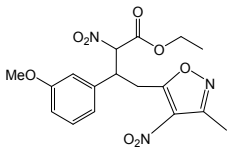
ethyl 3-(3-hydroxyphenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ai)



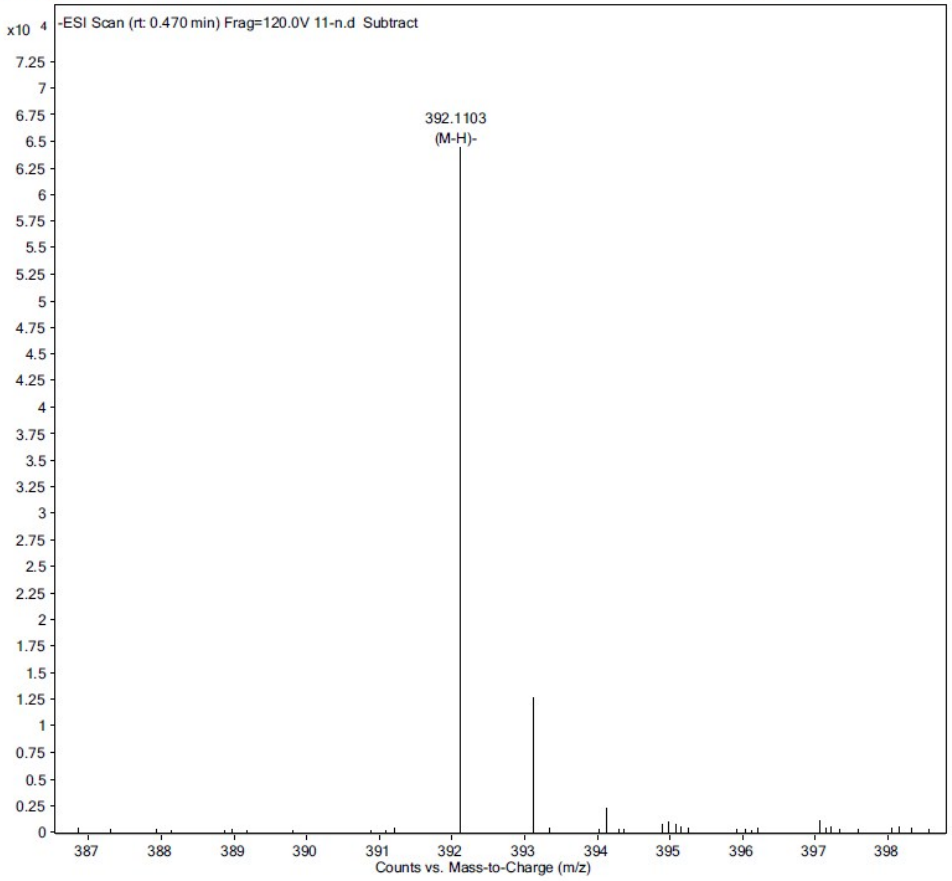
Sample Name		**Position**	P2a9	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	9-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 2:57:55 PM



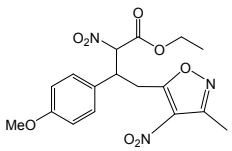
ethyl 3-(3-methoxyphenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4aj)



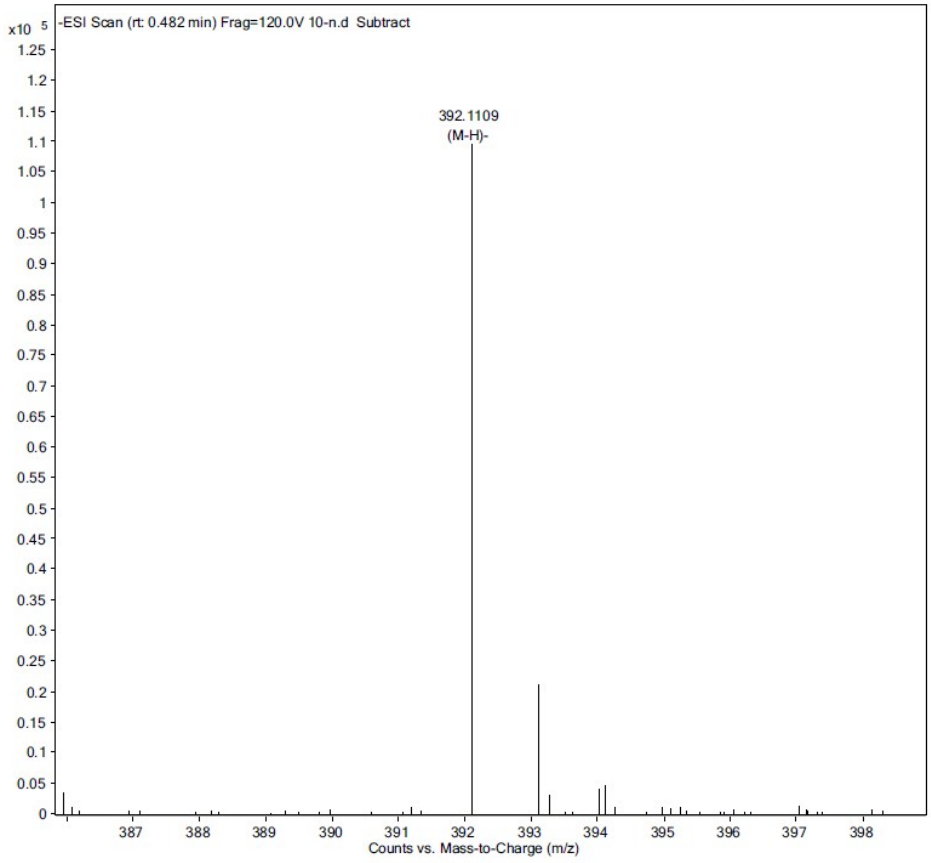
Sample Name		**Position**	P2b2	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	11-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 3:01:44 PM



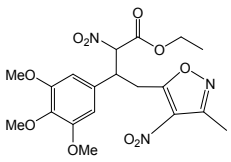
ethyl 3-(4-methoxyphenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitrobutanoate (4ak)



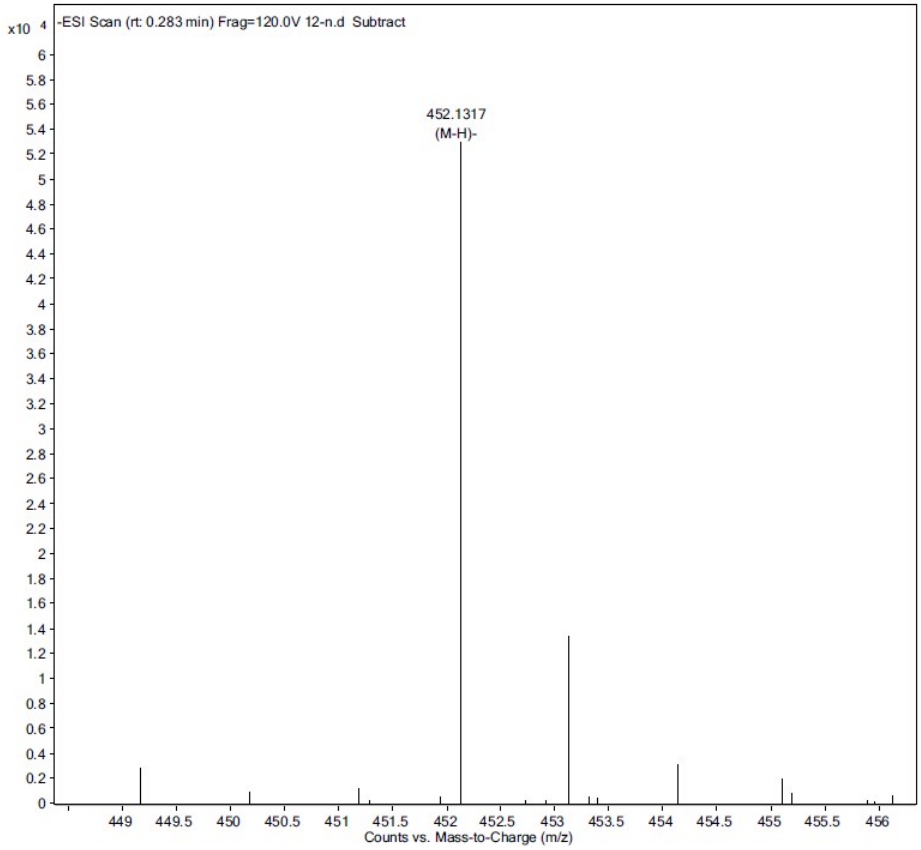
Sample Name		**Position**	P2b1	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	10-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 2:59:44 PM



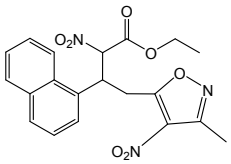
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(3,4,5-trimethoxyphenyl)butanoate (4al)



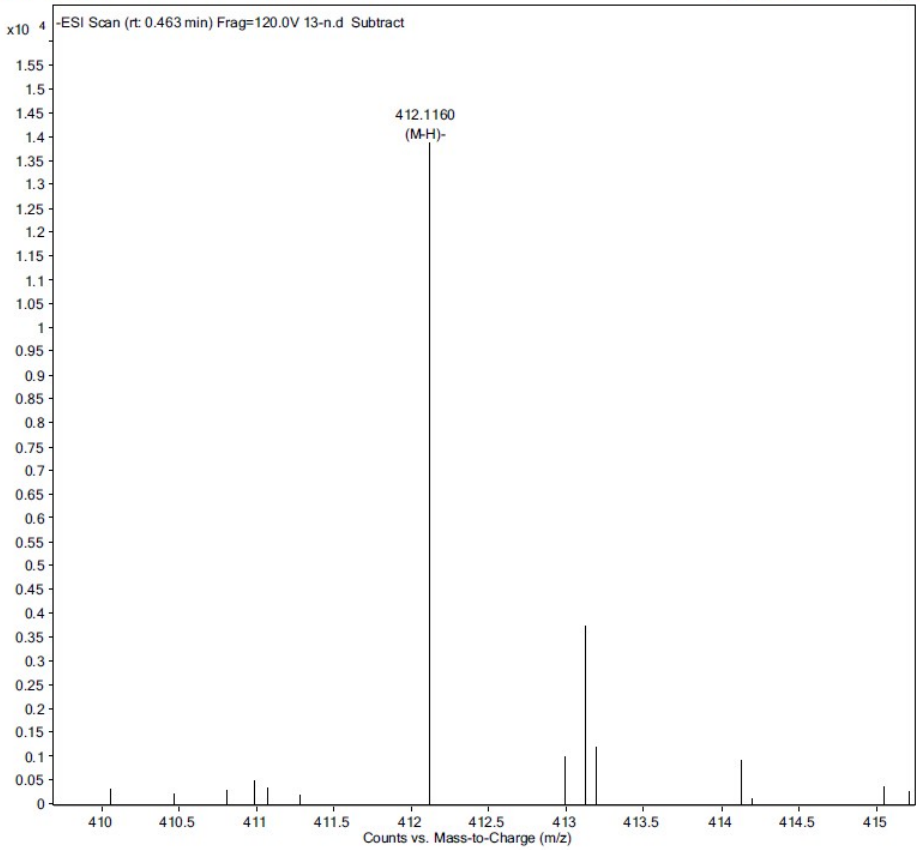
Sample Name		**Position**	P2b3	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	12-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 3:03:25 PM



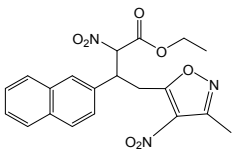
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-3-(naphthalen-1-yl)-2-nitrobutanoate (4am)



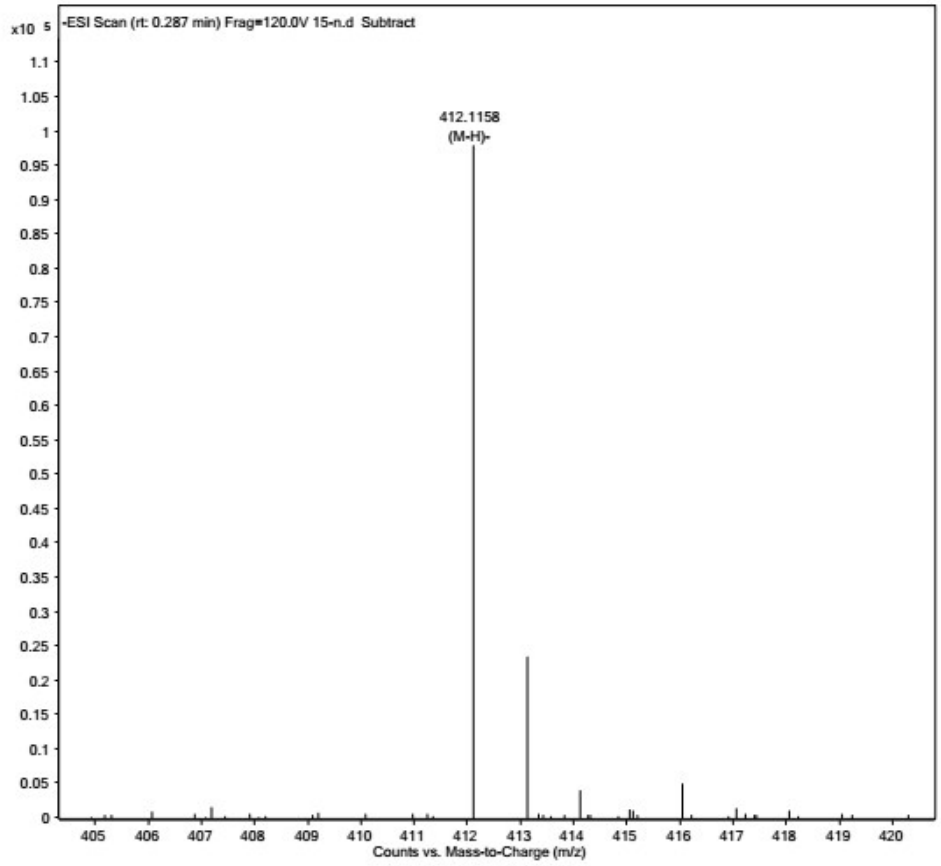
Sample Name		**Position**	P2b4	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	13-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 3:05:42 PM



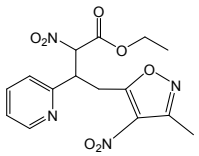
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-3-(naphthalen-2-yl)-2-nitrobutanoate (4an)



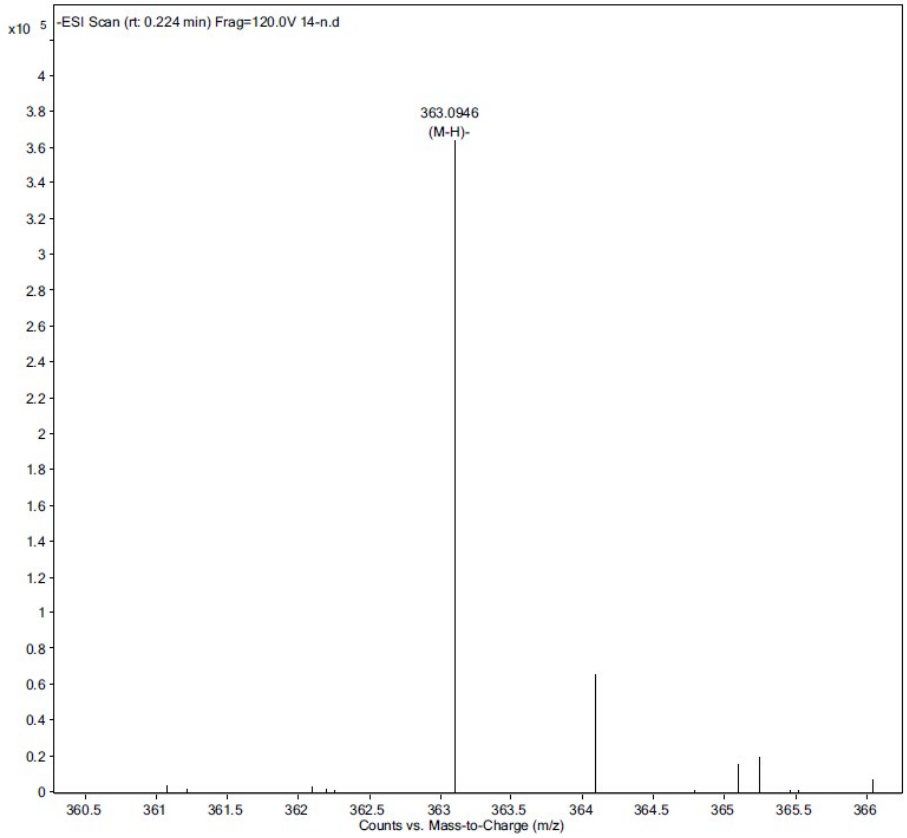
Sample Name		**Position**	P2b6	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	15-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 3:11:40 PM



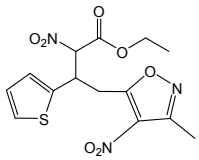
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(pyridin-2-yl)butanoate (4ao)



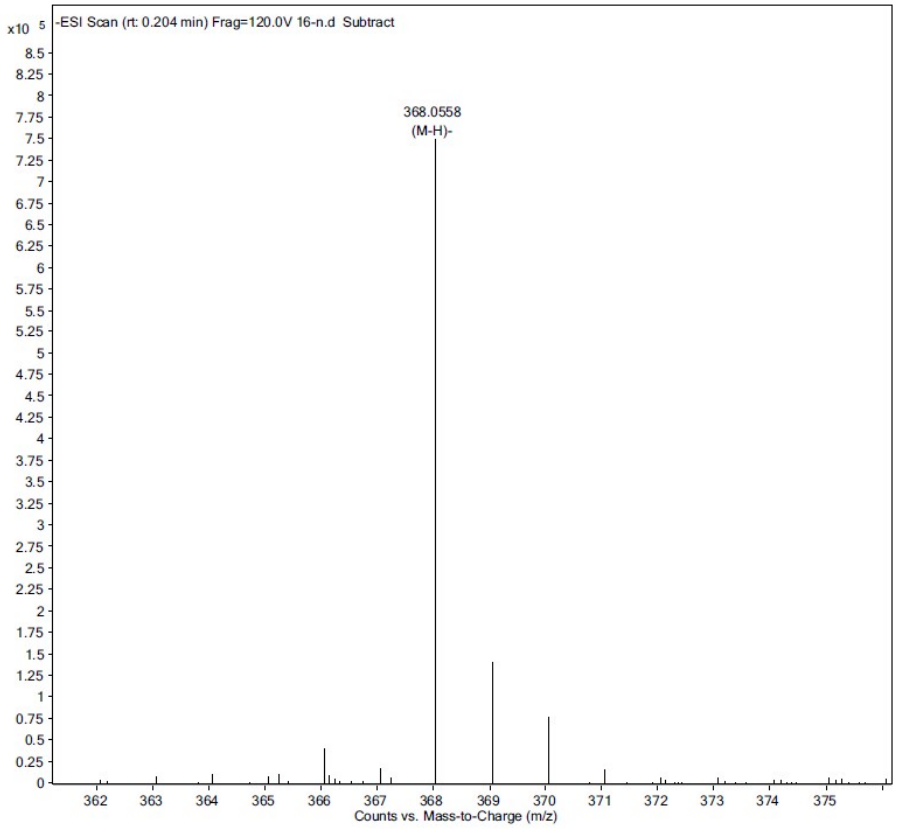
Sample Name		**Position**	P2b5	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	14-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 3:17:59 PM



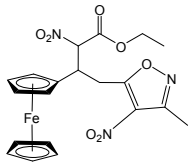
ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(thiophen-2-yl)butanoate (4ap)



Sample Name		**Position**	P2b7	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	16-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 3:19:54 PM



ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-nitro-3-(ferrocene-2-yl)butanoate (4aq)



Sample Name		**Position**	P2b8	**Instrument Name**	Instrument 1
User Name	QTOF-PC\QTOF	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	17-n.d
ACQ Method	20110418-MSonly-n.m	**Comment**		**Acquired Time**	3/4/2019 3:21:42 PM