

Supplementary Material

One-pot synthesis of 2,4,5-trisubstituted 1, 2, 3-triazoles through cascade reaction of acid chlorides, terminal acetylenes, sodium azide and aryl halides

Xiang, Liu^{a,b} Jihui, Li^{a,b} Baohua, Chen^{*a,b}

State Key Laboratory of Applied Organic Chemistry and Key Laboratory of
Nonferrous Metal Chemistry and Resources Utilization of Gansu Province, Lanzhou
University, Gansu Lanzhou 730000, P. R. China

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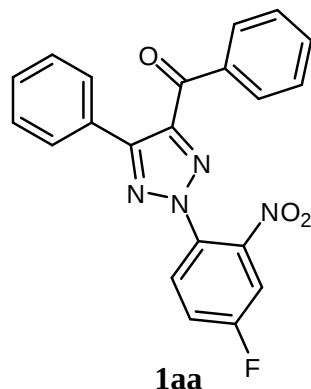
1. General remarks:

Column chromatography was carried out on silica gel. ^1H NMR spectra were recorded on 300 or 400 MHz in CDCl_3 and ^{13}C NMR spectra were recorded on 75 or 100 MHz in CDCl_3 or Dimethyl Sulfoxide- D_6 using TMS as internal standard. IR spectra were recorded on a FT-IR spectrometer and only major peaks are reported in cm^{-1} . Melting points were determined on a microscopic apparatus and were uncorrected. All desired products were further characterized by ESI HRMS, EI MS or element analysis; copies of their ^1H NMR and ^{13}C NMR spectra are provided. Commercially available reagents and solvents were used without further purification.

The general procedure of the reaction between acid chlorides, terminal acetylenes, sodium azide and alkyl halides: regioselective synthesis of (2-(4-fluoro-2-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone **1aa:**

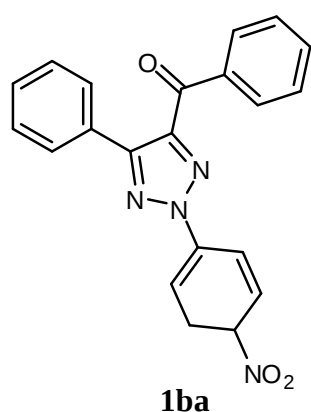
All reactions were performed on a 0.25 mmol scale relative to acid chlorides. A round-bottom sidearm flask (10 mL) containing $\text{PdCl}_2(\text{PPh}_3)_2$ (0.0025 mmol), CuI (0.005 mmol) was subjected to the Schlenk-line procedures of evacuation and purging of N_2 for three cycles. Phenyl acetylene (0.25 mmol), benzoyl chloride (0.25 mmol) and 3.0 equiv Et_3N (0.75 mmol) was successively added, and the flask was put into ultrasonic (32KHz, 160 W) to react at room temperature for 1h, the flask was took out, then NaN_3 (0.25 mmol), K_2CO_3 (0.125 mmol), 2,5-diF- $\text{C}_6\text{H}_3\text{NO}_2$ (0.375 mmol) and 3 mL DMSO were added to the mixture and the reaction continued at 100 °C for three hours. Following, to the reaction mixture was added water (2 mL), 20% HCl solution (1 mL) and extracted with ester (3×10 mL). The combined organic phases were washed with brine (2×5 mL), dried over anhydrous MgSO_4 and concentrated in vacuo. The residue was subjected to flash column chromatography with hexanes/ EtOAc (15/1) as eluent to obtain the desired **1aa** (84 mg, 87% yield).

2. Spectral data of the compounds:



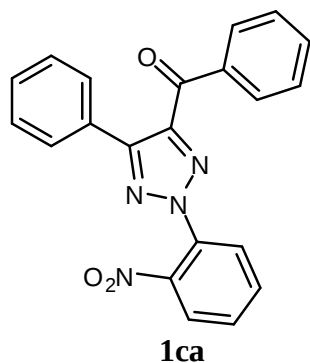
(2-(4-fluoro-2-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone

1aa^b: **1aa** was purified by flash chromatography (Hexane-EtOAc, v/v=15/1) as light yellow solid (yield: 87%), mp: 128-130 °C. IR (cm⁻¹): 3071, 1656, 1549. ¹H NMR (400 MHz, CDCl₃): δ 8.14-8.27 (m, 5H), 7.87-7.89 (m, 2H), 7.64 (t, *J*=7.4 Hz, 1H), 7.51 (t, *J*=7.6 Hz, 2H), 7.43-7.45 (m, 3H). ¹³C NMR (100 MHz, CDCl₃): δ 187.4, 162.8, 160.3, 151.3, 144.2, 136.7, 133.8, 130.4, 129.7, 128.8, 128.6, 128.5, 128.48, 127.8, 127.7, 120.4, 120.1, 113.0, 112.8. ESI HRMS: calcd. for C₂₁H₁₄FN₄O₃ [M+H]⁺: 389.1044, found: 389.1050.

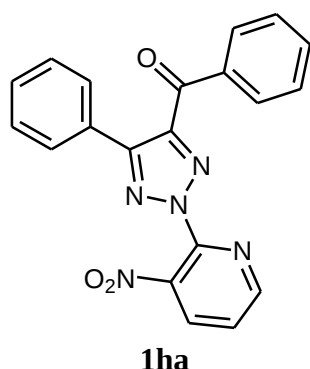


(2-(4-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone (1ba)^b: **1ba** was purified by flash chromatography (Hexane-EtOAc, v/v=20/1) as green-yellow solid, mp: 145-147 °C. IR (cm⁻¹): 3075, 2918, 1653, 1594 ¹H NMR (400 MHz, CDCl₃): δ 8.33-8.35 (m, 4H), 8.11-8.13 (m, 2H), 7.87-7.90 (m, 2H), 7.64-7.67 (m, 1H),

7.44-7.54 (m, 5H). ^{13}C NMR (100 MHz, CDCl_3): δ 187.5, 151.3, 146.9, 144.4, 143.1, 136.6, 133.9, 130.4, 129.8, 128.7, 128.6, 128.56, 128.52, 125.2, 119.5. EI-MS: m/z = 370 $[\text{M}]^+$.
Anal. Calcd. For $\text{C}_{21}\text{H}_{14}\text{N}_4\text{O}_3$: C, 68.10; H, 3.81; N, 15.13. Found: C, 68.14; H, 3.79; N, 15.15.

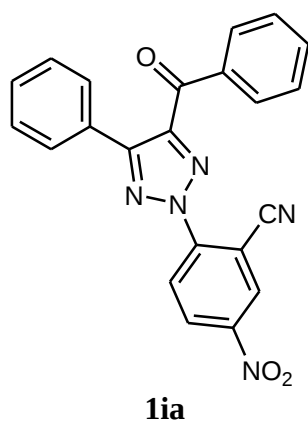


(2-(2-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone 1ca^b: **1ca** was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as green-yellow solid, mp: 102-104 °C. IR (cm^{-1}): 3067, 1664, 1602. ^1H NMR (300 MHz, CDCl_3): δ 8.07-8.10 (m, 2H), 8.0 (dd, J =8.1, 0.9 Hz, 1H), 7.87-7.91 (m, 3H), 7.69-7.74 (m, 1H), 7.42-7.64 (m, 7H). ^{13}C NMR (75 MHz, CDCl_3): δ 187.5, 151.3, 144.1, 143.8, 136.8, 133.9, 133.1, 131.9, 130.5, 129.8, 129.7, 128.9, 128.7, 128.5, 125.8, 125.1. ESI HRMS: calcd. for $\text{C}_{21}\text{H}_{18}\text{N}_5\text{O}_3$ $[\text{M}+\text{NH}_4]^+$: 388.1404, found: 388.1411.

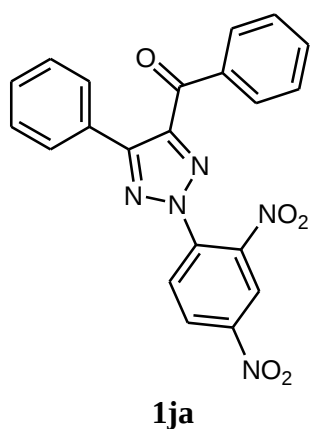


(2-(3-nitropyridin-2-yl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone 1ha^b: **1ha** was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as green-yellow solid (yield: 80%), mp: 144-146 °C. IR (cm^{-1}): 3068, 1663, 1592. ^1H NMR (300 MHz, CDCl_3): δ 8.81-8.83 (m, 1H), 8.27 (dd, J =8.1, 0.9 Hz, 1H), 8.09 (d, J =7.5 Hz, 2H), 7.89-7.92 (m, 2H),

7.59-7.66 (m, 2H), 7.43-7.5 (m, 5H). ^{13}C NMR (75 MHz, CDCl_3): δ 187.3, 151.7, 151.6, 144.7, 142.0, 139.9, 136.4, 134.2, 133.9, 130.4, 129.9, 128.9, 128.5, 128.47, 128.3, 124.7. ESI HRMS: calcd. for $\text{C}_{20}\text{H}_{14}\text{N}_5\text{O}_3$ $[\text{M}+\text{H}]^+$: 372.1091, found: 372.1097.

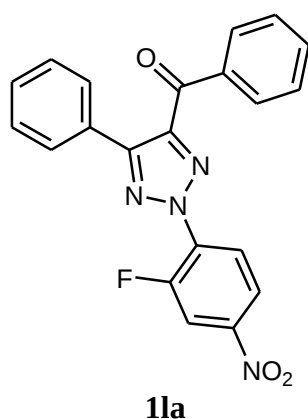


2-(4-benzoyl-5-phenyl-2H-1,2,3-triazol-2-yl)-5-nitrobenzonitrile 1ia^b: **1ia** was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as green-yellow solid (yield: 90%), mp: 134-136 °C. IR (cm^{-1}): 3086, 1664, 1583. ^1H NMR (400 MHz, CDCl_3): δ 8.72 (t, J =2.6 Hz, 1H), 8.52-8.55 (m, 1H), 8.43 (dd, J =9.0, 2.2 Hz, 1H), 8.20 (d, J =7.6 Hz, 2H), 7.90-7.91 (m, 2H), 7.66 (t, J =7.4 Hz, 1H), 7.53 (t, J =7.6 Hz, 2H), 7.44-7.46 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ 186.8, 152.2, 146.2, 145.2, 142.9, 136.1, 134.3, 131.0, 130.6, 130.3, 128.8, 128.7, 128.6, 127.9, 123.1, 114.8, 105.2. ESI HRMS: calcd. for $\text{C}_{22}\text{H}_{14}\text{N}_5\text{O}_3$ $[\text{M}+\text{H}]^+$: 396.1091, found: 396.1100.

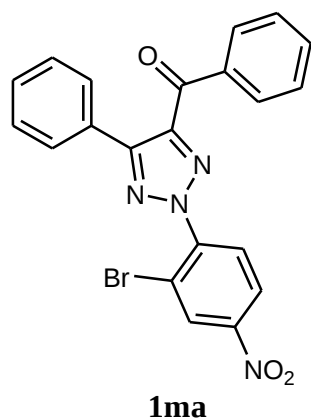


(2-(2,4-dinitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone 1ja^b: **1ja** was purified by flash chromatography (Hexane-EtOAc, v/v=15/1) as yellow solid (yield: 95%),

mp: 156-158 °C . IR (cm⁻¹): 3089, 1665, 1602. ¹H NMR (400 MHz, CDCl₃): δ 8.67 (d, *J*=2.4 Hz, 1H), 8.55 (dd, *J*=9.0, 2.2 Hz, 1H), 8.35 (d, *J*=8.8 Hz, 1H), 8.06 (d, *J*=7.6 Hz, 1H), 7.84 (t, *J*=3.8 Hz, 2H), 7.66 (t, *J*=7.4 Hz, 2H), 7.53 (t, *J*=7.6 Hz, 2H), 7.44-7.46 (m, 3H). ¹³C NMR (100 MHz, CDCl₃): δ 186.9, 152.3, 146.5, 145.3, 142.5, 136.2, 135.0, 134.2, 130.5, 130.2, 128.8, 128.6, 127.9, 127.2, 125.3, 120.8. HRMS: calcd. for C₂₁H₁₄N₅O₅ [M+H]⁺: 416.09916, Found: 416.09895.^a

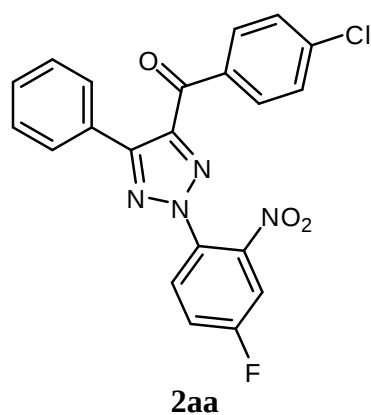


(2-(2-fluoro-4-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone 1la^b: **1la** was purified by flash chromatography (Hexane-EtOAc, v/v=15/1) as light yellow solid (yield: 87%), mp: 135-137 °C. IR (cm⁻¹): 3092, 1664, 1536. ¹H NMR (400 MHz, CDCl₃): δ 8.14-8.27 (m, 5H), 7.87-7.89 (m, 2H), 7.64 (t, *J*=7.4 Hz, 1H), 7.51 (t, *J*=7.8 Hz, 2H), 7.44 (dd, *J*=6.4, 3.6 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃): δ 187.2, 154.7, 152.0, 151.4, 147.4, 147.3, 144.6, 136.6, 134.0, 132.3, 132.2, 130.5, 129.9, 128.8, 128.6, 128.5, 128.4, 124.8, 120.0, 119.96, 114.2, 114.0. ESI HRMS: calcd. for C₂₁H₁₄FN₄O₃ [M+H]⁺: 389.1044, found: 389.1048.



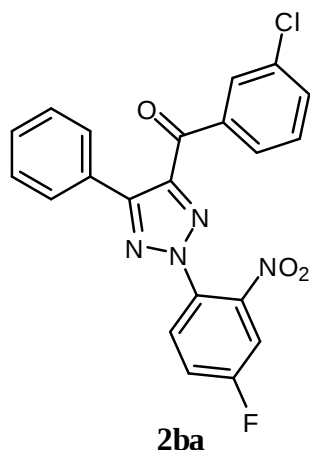
(2-(2-bromo-4-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone 1ma^b:

1ma was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as light yellow solid (yield: 55%), mp: 140-142 °C. IR (cm⁻¹): 3069, 1661, 1541. ¹H NMR (400 MHz, CDCl₃): δ 8.01-8.07 (m, 3H), 7.92 (d, *J*=8.2 Hz, 1H), 7.83-7.88 (m, 3H), 7.61-7.64 (m, 1H), 7.49-7.53 (m, 2H), 7.42-7.44 (m, 3H). ¹³C NMR (100 MHz, CDCl₃): δ 187.2, 151.5, 144.3, 143.7, 136.6, 135.9, 133.9, 130.7, 130.5, 129.8, 128.8, 128.52, 128.5, 128.4, 127.9, 126.5, 122.7. ESI HRMS: calcd. for C₂₁H₁₄BrN₄O₃ [M+H]⁺: 449.0244, found: 449.0240.



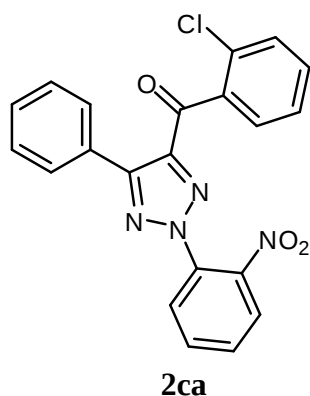
(4-chlorophenyl)(2-(4-fluoro-2-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)methanone

2aa^b: **2aa** was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as white solid (yield: 89%), mp: 162-164 °C. IR (cm⁻¹): 3086, 1660, 1581. ¹H NMR (400 MHz, CDCl₃): δ 8.00-8.04 (m, 3H), 7.87-7.89 (m, 2H), 7.67 (dd, *J*= 7.4, 2.6 Hz, 1H), 7.45-7.50 (m, 6H). ¹³C NMR (100 MHz, CDCl₃): δ 185.9, 162.9, 160.3, 151.6, 144.2, 143.7, 140.4, 135.0, 131.8, 129.9, 128.9, 128.8, 128.5, 128.4, 128.3, 128.29, 127.7, 127.6, 120.4, 120.2, 113.2, 112.8. ESI HRMS: calcd. for C₂₁H₁₃ClFN₄O₃ [M+H]⁺: 423.0655, found: 423.0652.



(3-chlorophenyl)(2-(4-fluoro-2-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)methanone

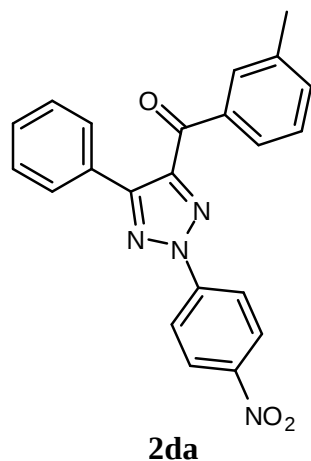
2ba^b: **2ba** was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as white solid (yield: 87%), mp: 122-124 °C. IR (cm⁻¹): 3081, 1668, 1548. ¹H NMR (400 MHz, CDCl₃): δ 8.08 (d, *J*=1.6 Hz, 1H), 8.03 (dd, *J*=9.2, 4.8 Hz, 1H), 7.95-7.97 (m, 1H), 7.88-7.90 (m, 2H), 7.68 (dd, *J*=7.2, 2.8 Hz, 1H), 7.59-7.62 (m, 1H), 7.44-7.51 (m, 5H). ¹³C NMR (100 MHz, CDCl₃): δ 185.8, 162.9, 160.4, 151.7, 144.2, 143.6, 138.2, 134.8, 133.6, 130.2, 129.9, 129.8, 128.9, 128.7, 128.5, 128.4, 128.3, 128.28, 127.7, 127.6, 120.4, 120.2, 113.1, 112.8. ESI HRMS: calcd. for C₂₁H₁₃ClFN₄O₃ [M+H]⁺: 423.0655, found: 423.0650.



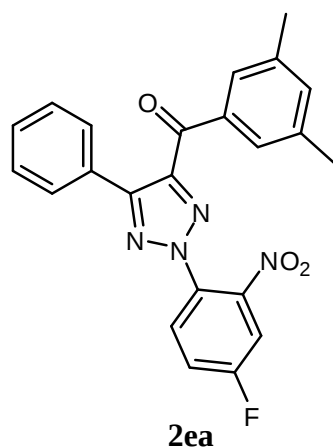
(2-chlorophenyl)(2-(2-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)methanone 2ca^c:

2ca was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as light yellow solid (yield: 82%), mp: 126-128 °C. IR (cm⁻¹): 3085, 1655, 1526. ¹H NMR (300 MHz, CDCl₃): δ 7.98-8.01 (m, 2H), 7.85-7.93 (m, 2H), 7.66-7.72 (m, 1H), 7.54-7.59 (m, 2H), 7.34-7.47 (m, 6H). ¹³C NMR (75 MHz, CDCl₃): δ 187.6, 151.4, 144.4, 143.8, 138.0, 133.0, 132.2, 131.8,

130.4, 130.3, 130.0, 129.98, 129.2, 128.5, 128.4, 126.6, 126.0, 125.1. ESI HRMS: calcd. for $C_{21}H_{14}ClN_4O_3$ $[M+H]^+$: 405.0749, found: 405.0742.

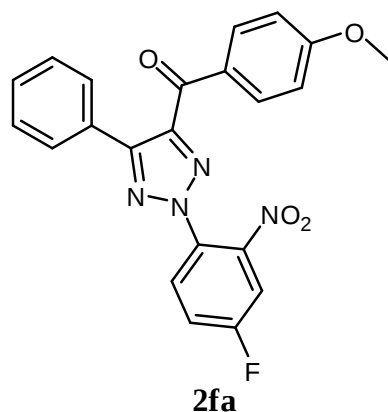


(2-(4-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(m-tolyl)methanone 2da^d: **2da** was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as slight yellow solid (yield: 82%), mp: 136-138 °C. IR (cm⁻¹): 3064, 1663, 1597. ¹H NMR (300 MHz, CDCl₃): δ 8.34-8.38 (m, 4H), 7.86-7.91 (m, 4H), 7.37-7.48 (m, 5H), 2.43 (s, 3H). ¹³C NMR (75 MHz, CDCl₃): δ 187.8, 151.2, 146.9, 144.7, 143.2, 138.5, 136.6, 134.8, 130.7, 129.8, 128.6, 128.58, 128.4, 127.9, 125.2, 119.5, 21.3. EI-MS: m/z = 384 $[M]^+$. Anal. Calcd. For C₂₂H₁₆N₄O₃: C, 68.74; H, 4.20; N, 14.58. Found: C, 68.66; H, 4.25; N, 14.50.



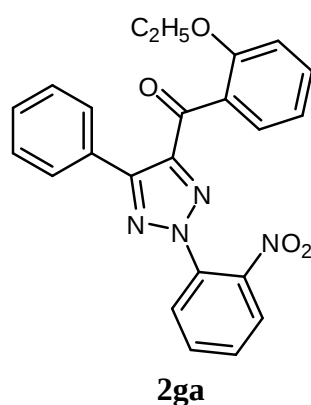
(3,5-dimethylphenyl)(2-(4-fluoro-2-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)methanone 2ea^b: **2ea** was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as white solid (yield: 89%), mp: 127-129 °C. IR (cm⁻¹): 3080, 1663, 1601. ¹H NMR (400 MHz, CDCl₃): δ 8.02 (dd, *J*=9.2, 4.8 Hz, 1H), 7.86-7.88 (m, 2H), 7.63-7.66 (m, 3H), 7.42-7.48 (m, 4H), 7.25

(s, 1H), 2.40 (s, 6H). ^{13}C NMR (100 MHz, CDCl_3): δ 187.8, 162.7, 160.2, 151.1, 144.4, 144.3, 138.2, 136.6, 135.7, 129.7, 128.7, 128.6, 128.5, 128.2, 127.7, 127.6, 120.3, 120.1, 113.0, 112.7, 21.1. ESI HRMS: calcd. for $\text{C}_{23}\text{H}_{18}\text{FN}_4\text{O}_3$ $[\text{M}+\text{H}]^+$: 417.1357, found: 417.1347.



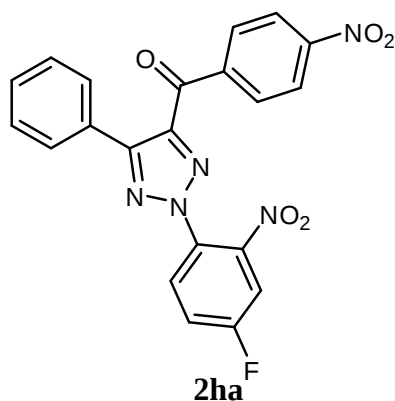
(2-(4-fluoro-2-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(4-methoxyphenyl)methanone

2fa^b: **2fa** was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as light yellow solid (yield: 88%), mp: 150-152 °C. IR (cm^{-1}): 3080, 1653, 1598. ^1H NMR (400 MHz, CDCl_3): δ 8.07 (d, J =8.8 Hz, 2H), 8.02 (dd, J =9.2, 4.8 Hz, 1H), 7.85-7.87 (m, 2H), 7.66 (dd, J =7.2, 2.8 Hz, 1H), 7.42-7.49 (m, 4H), 6.99 (d, J =8.8 Hz, 2H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ 185.9, 164.4, 162.7, 160.2, 150.9, 144.5, 144.2, 144.1, 133.0, 129.6, 129.5, 128.7, 128.5, 127.7, 127.6, 120.4, 120.1, 113.9, 113.0, 112.8, 55.5. ESI HRMS: calcd. for $\text{C}_{22}\text{H}_{16}\text{FN}_4\text{O}_4$ $[\text{M}+\text{H}]^+$: 419.1150, found: 419.1148.



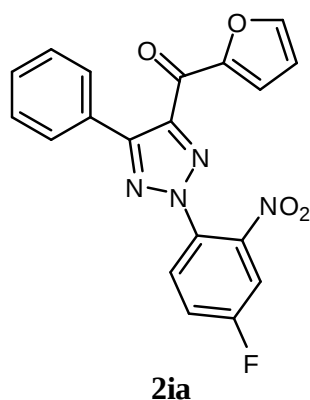
(2-ethoxyphenyl)(2-(2-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)methanone 2ga^c: **2ga** was purified by flash chromatography (Hexane-EtOAc, v/v =10/1) as light yellow solid (yield: 92%), mp: 100-102 °C IR (cm^{-1}): 2982, 1667, 1600. ^1H NMR (400 MHz, CDCl_3): δ 7.93 (d, J =8.0 Hz, 1H), 7.81-7.86 (m, 3H), 7.67-7.72 (m, 2H), 7.54 (t, J =7.6 Hz, 1H), 7.38-7.47 (m, 3H), 7.04 (t, J =7.4 Hz, 1H), 6.83 (d, J =8.4 Hz, 1H), 3.89 (q, J =6.8 Hz, 2H), 1.13(t, J =7.0 Hz,

3H). ^{13}C NMR (100 MHz, CDCl_3): 189.0, 158.3, 149.6, 146.9, 143.5, 134.1, 132.8, 131.9, 130.4, 129.3, 128.8, 128.5, 128.3, 128.1, 125.5, 124.8, 120.2, 112.1, 63.8, 14.1. ESI HRMS: calcd. for $\text{C}_{23}\text{H}_{22}\text{N}_5\text{O}_4$ $[\text{M}+\text{NH}_4]^+$: 432.1666, found: 432.1656.



(2-(4-fluoro-2-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(4-nitrophenyl)methanone

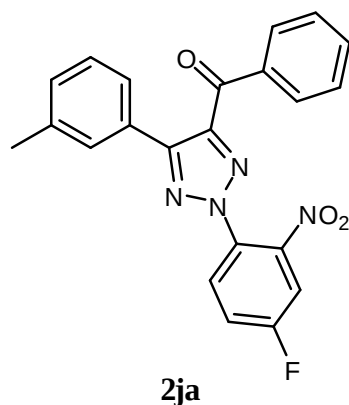
2ha^b: **2ha** was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as yellow solid (yield: 50%), mp: 170-172 °C. IR (cm^{-1}): 3056, 1662, 1548. ^1H NMR (400 MHz, CDCl_3): δ 8.36 (d, $J=8.8$ Hz, 2H), 8.24-8.30 (m, 4H), 7.85-7.92 (m, 3H), 7.52 (t, $J=3.2$ Hz, 3H). ^{13}C NMR (100 MHz, $\text{D}_6\text{-DMSO}$): δ 185.4, 162.7, 160.2, 151.0, 150.1, 143.9, 143.8, 142.9, 141.4, 131.5, 130.0, 128.8, 128.6, 128.4, 128.3, 128.1, 127.3, 127.2, 123.5, 121.4, 121.2, 113.7, 113.4. The molecular signal did not find in ESI HRMS. EI-MS: $m/z = 433$ $[\text{M}]^+$. Anal. Calcd. for $\text{C}_{21}\text{H}_{12}\text{FN}_5\text{O}_5$: C, 58.20; H, 2.79; N, 16.16. Found: C, 58.10; H, 2.84; N, 16.23.



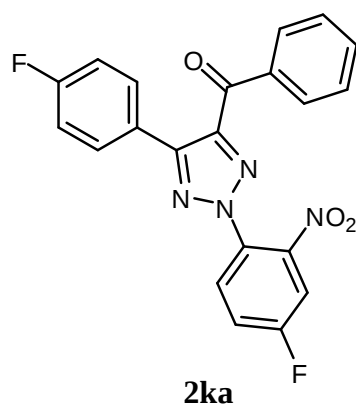
(2-(4-fluoro-2-nitrophenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(furan-2-yl)methanone 2ia^b:

2ia was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as yellow solid (yield: 88%), mp: 130-132 °C. IR (cm^{-1}): 3076, 1649, 1548. ^1H NMR (400 MHz, CDCl_3): δ 8.06 (dd, $J=4.8, 9.2$ Hz, 1H), 7.92-7.94 (m, 2H), 7.74 (d, $J=1.2$ Hz, 1H), 7.66 (dd, $J=7.2, 2.8$ Hz, 1H), 7.56 (d, $J=3.6$ Hz, 1H), 7.44-7.51 (m, 4H), 6.62 (dd, $J=3.6, 1.6$ Hz, 1H). ^{13}C NMR (100 MHz,

CDCl₃): δ 173.0, 162.8, 160.2, 151.4, 151.3, 148.4, 143.9, 143.3, 129.8, 129.1, 128.5, 128.4, 128.3, 128.2, 128.16, 127.5, 127.4, 123.0, 120.4, 120.1, 113.0, 112.8, 112.7. ESI HRMS: calcd. for C₁₉H₁₂FN₄O₄ [M+H]⁺: 379.0837, found: 379.0829.

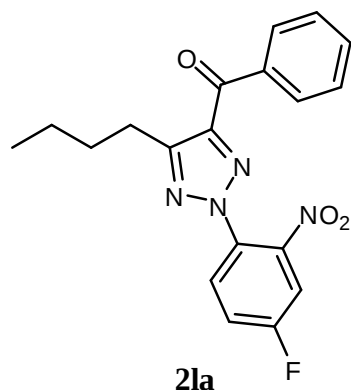


(2-(4-fluoro-2-nitrophenyl)-5-m-tolyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone 2ja^b: **2ja** was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as white solid (yield: 88%), mp: 123-125 °C. IR (cm⁻¹): 3081, 1665, 1546. ¹H NMR (400 MHz, CDCl₃): δ 8.04-8.06 (m, 2H), 8.00 (dd, J=8.8, 4.8 Hz, 1H), 7.60-7.67(m, 4H), 7.42-7.52 (m, 3H), 7.32 (t, J=7.6 Hz, 1H), 7.23-7.25 (m, 1H), 2.39 (s, 3H). ³C NMR (100 MHz, CDCl₃): δ 187.4, 162.8, 160.2, 151.5, 144.2, 144.1, 138.2, 136.7, 133.8, 130.5, 130.4, 129.3, 128.5, 128.4, 128.36, 127.8, 127.7, 125.9, 120.4, 120.1, 113.0, 112.7, 21.4. C₂₂H₁₉FN₅O₃ [M+NH₄]⁺: 420.1466, found: 420.1477.

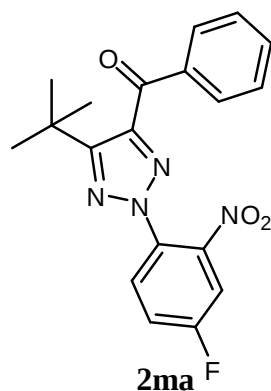


(2-(4-fluoro-2-nitrophenyl)-5-(4-fluorophenyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone 2ka^b: **2ka** was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as white solid

(yield: 95%), mp: 121-123 °C. IR (cm⁻¹): 3084, 1663, 1544. ¹H NMR (400 MHz, CDCl₃): δ 8.06 (d, *J*=7.2 Hz, 2H), 7.98-8.05 (m, 1H), 7.90 (dd, *J*=8.8, 5.6 Hz, 2H), 7.61-7.67 (m, 2H), 7.44-7.52 (m, 3H), 7.12 (t, *J*=8.6 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃): δ 187.2, 164.9, 162.9, 162.4, 160.3, 150.6, 144.3, 144.2, 143.9, 136.6, 133.9, 131.0, 130.9, 130.5, 128.5, 128.4, 128.3, 127.7, 127.6, 124.7, 124.7, 120.4, 120.2, 115.7, 115.5, 113.1, 112.8. ESI HRMS: calcd. for C₂₁H₁₃F₂N₄O₃ [M+H]⁺: 407.0950, found: 407.0954.

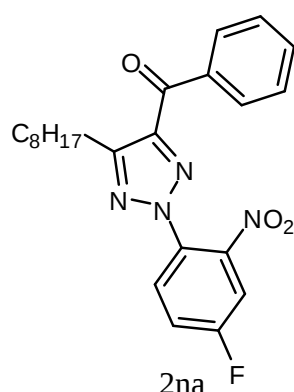


(5-butyl-2-(4-fluoro-2-nitrophenyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone 2la^b: 2la was purified by flash chromatography (Hexane-EtOAc, v/v=10/1) as light yellow oil (yield: 60%). IR (cm⁻¹): 3080, 1657, 1549. ¹H NMR (400 MHz, CDCl₃): δ 8.13-8.15 (m, 2H), 7.97 (dd, *J*=9.2, 4.8 Hz, 1H), 7.59-7.64 (m, 2H), 7.42-7.53 (m, 3H), 3.09 (t, *J*=7.8 Hz, 2H), 1.73-1.81 (m, 2H), 1.41-1.50 (m, 2H), 0.97 (t, *J*=7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃): δ 186.9, 162.6, 160.1, 155.0, 144.5, 136.9, 133.4, 130.3, 128.5, 128.49, 128.4, 127.5, 127.4, 120.2, 120.0, 112.9, 112.6, 30.4, 25.7, 22.4, 13.8. ESI HRMS: calcd. for C₁₉H₁₈FN₄O₃ [M+H]⁺: 369.1357, found: 369.1359.

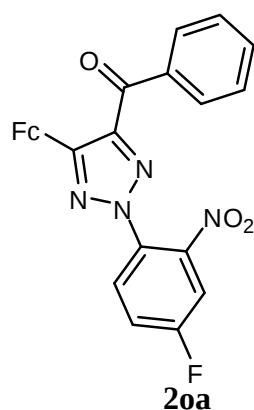


(5-tert-butyl-2-(4-fluoro-2-nitrophenyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone 2ma^b: 2ma

was purified by flash chromatography (Hexane-EtOAc, v/v =80/1) as colorless oil (yield: 72%). IR (cm⁻¹): 2968, 1666, 1548. ¹H NMR (400 MHz, CDCl₃): δ 7.94-8.00 (m, 3H), 7.61-7.65 (m, 2H), 7.50-7.53 (m, 2H), 7.42-7.47 (m, 1H), 1.48 (s, 9H). ¹³C NMR (100 MHz, CDCl₃): 188.8, 162.5, 160.7, 160.0, 144.5, 137.4, 133.6, 130.34, 128.6, 128.5, 128.4, 127.4, 127.3, 120.1, 119.9, 112.9, 112.6, 32.6, 29.3. ESI HRMS: calcd. for C₁₉H₁₈FN₄O₃ [M+H]⁺: 369.1357, found:369.1350.

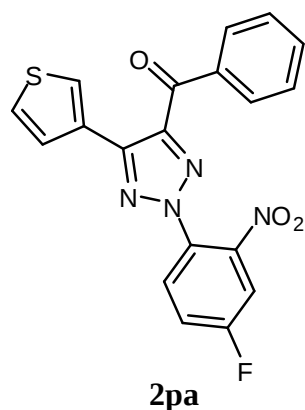


(2-(4-fluoro-2-nitrophenyl)-5-octyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone 2na^b: **2na** was purified by flash chromatography (Hexane-EtOAc, v/v =80/1) as light yellow oil (yield: 68%). IR (cm⁻¹): 2927, 1656, 1548. ¹H NMR (400 MHz, CDCl₃): δ 8.14 (d, J=7.2 Hz, 2H), 7.97 (dd, J=9.2, 4.8 Hz, 1H), 7.59-7.63 (m, 2H), 7.42-7.53 (m, 3H), 3.08 (t, J=7.6 Hz, 2H), 1.74-1.80 (m, 2H), 1.27-1.44 (m, 10H), 0.87 (t, J=6.6 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃): 186.8, 162.6, 160.0, 155.0, 144.5, 144.1, 136.8, 133.3, 130.3, 128.5, 128.45, 128.4, 127.4, 127.3, 120.2, 120.0, 112.9, 112.6, 31.8, 29.3, 29.26, 29.2, 28.3, 26.0, 22.6, 14.1. ESI HRMS: calcd. for C₂₃H₂₉FN₅O₃ [M+NH₄]⁺: 442.2294, found: 442.2298.



(2-(4-fluoro-2-nitrophenyl)-5-ferrocenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone 2oa^b: **2oa**

was purified by flash chromatography (Hexane-EtOAc, v/v =10/1) as brown-red solid (yield: 88%), mp: 113-115 °C. IR (cm⁻¹): 3085, 1663, 1549. ¹H NMR (400 MHz, CDCl₃): δ 8.08 (d, J=7.2 Hz, 2H), 7.93 (dd, J=8.4, 4.8, 1H), 7.61-7.65 (m, 2H), 7.53 (t, J=7.6 Hz, 2H), 7.43 (t, J=6.8 Hz, 1H), 5.07 (s, 2H), 4.40 (s, 2H), 4.10 (s, 5H). ¹³C NMR (100 MHz, CDCl₃): 187.2, 162.6, 160.0, 152.0, 144.2, 144.1, 143.6, 137.1, 133.6, 130.3, 128.5, 128.4, 127.6, 127.5, 120.3, 120.1, 112.9, 112.6, 72.3, 70.1, 69.6. EI-MS: m/z = 496 [M]⁺.

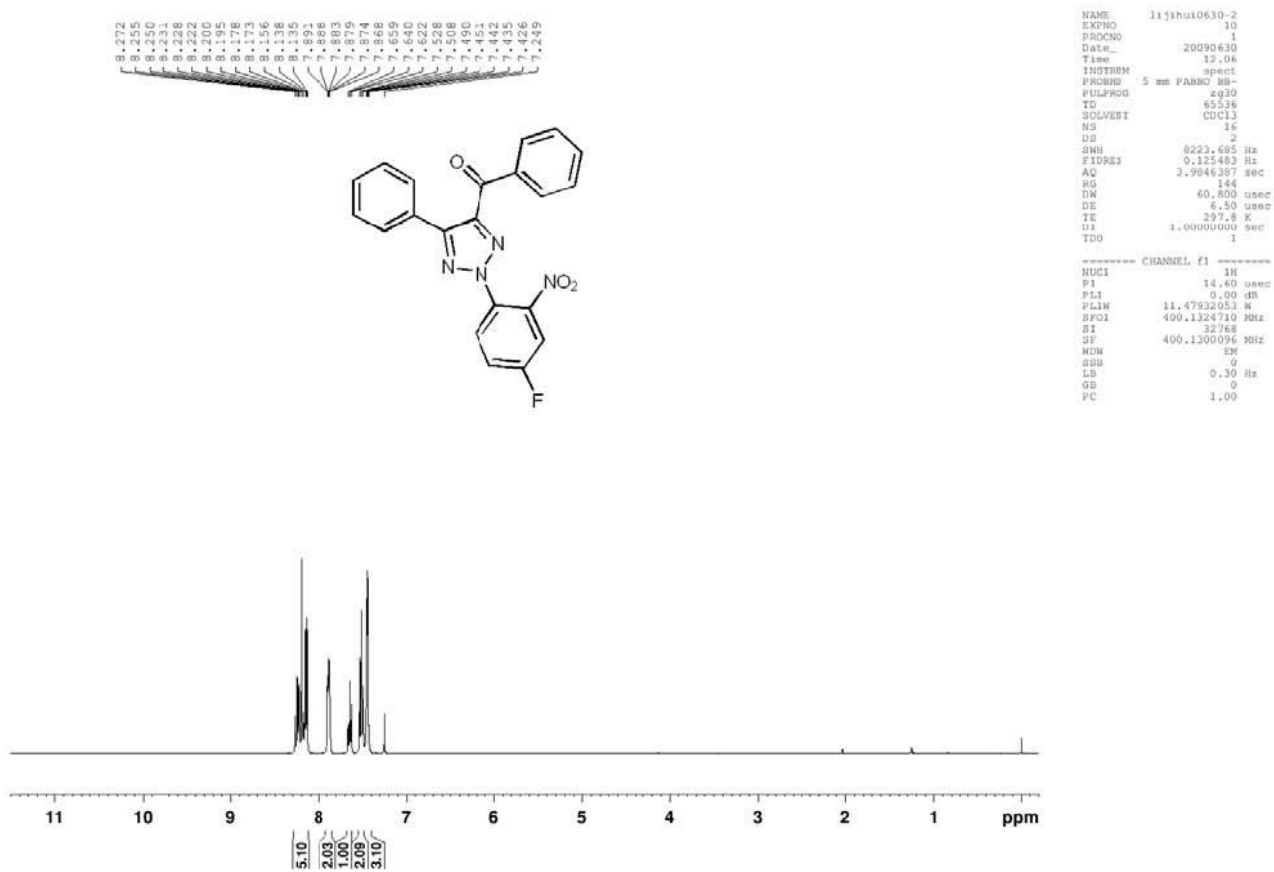


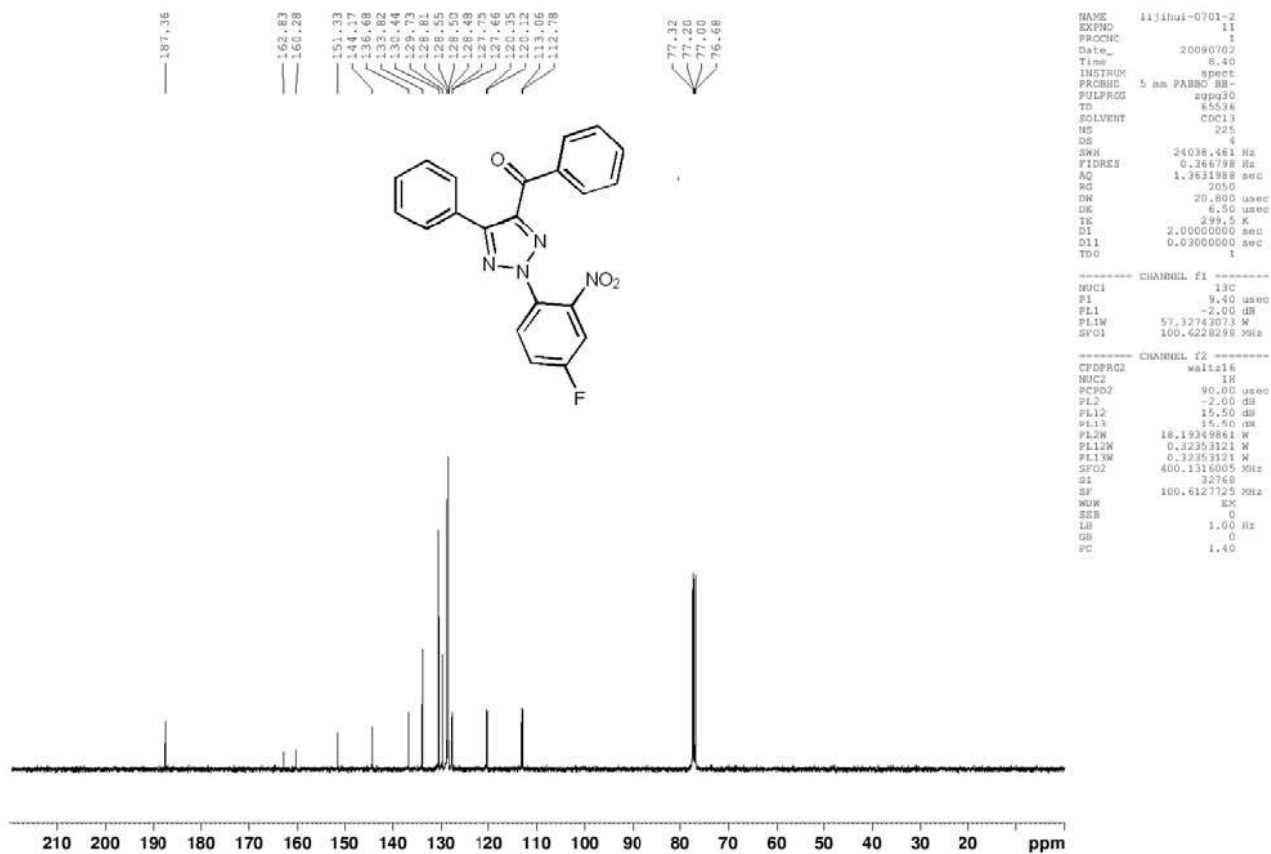
(2-(4-fluoro-2-nitrophenyl)-5-(thiophen-3-yl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone

2pa^b: **2pa** was purified by flash chromatography (Hexane-EtOAc, v/v =10/1) as white solid, mp: 120-122 °C. IR (cm⁻¹): 3083, 1662, 1547. ¹H NMR (400 MHz, CDCl₃): δ 8.35-8.36 (m, 1H), 8.05-8.07 (m, 2H), 7.99 (dd, J=8.8, 4.8 Hz, 1H), 7.60-7.70 (m, 3H), 7.43-7.53 (m, 3H), 7.38 (dd, J=5.0, 3.0 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃): δ 187.3, 162.8, 160.3, 147.2, 143.7, 136.9, 133.7, 130.4, 129.2, 128.4, 128.3, 127.9, 127.7, 127.6, 127.6, 125.7, 120.3, 120.1, 113.0, 112.8. ESI HRMS: calcd. for C₁₉H₁₂FN₄O₃S [M+H]⁺: 395.0609, found: 395.0619.

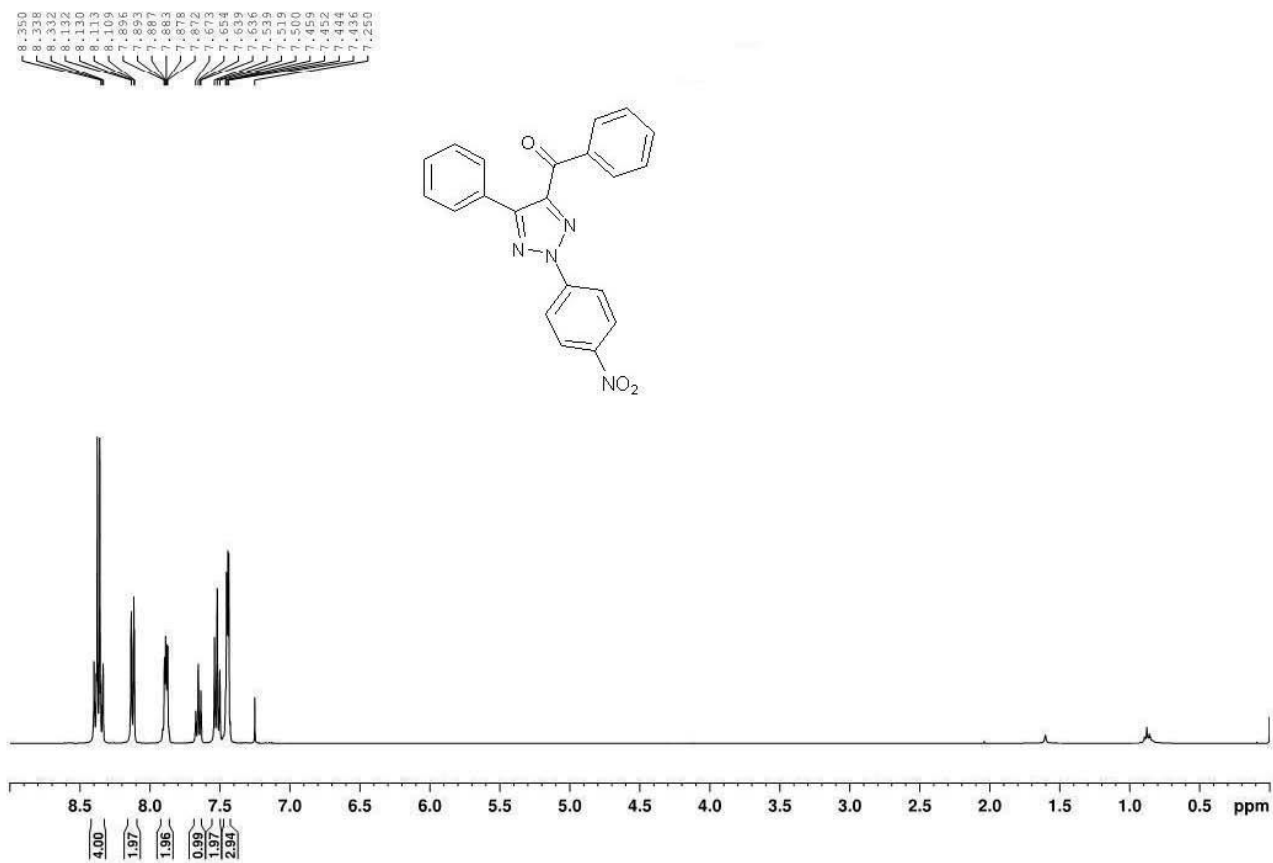
2. ^1H and ^{13}C NMR spectra of the compounds:

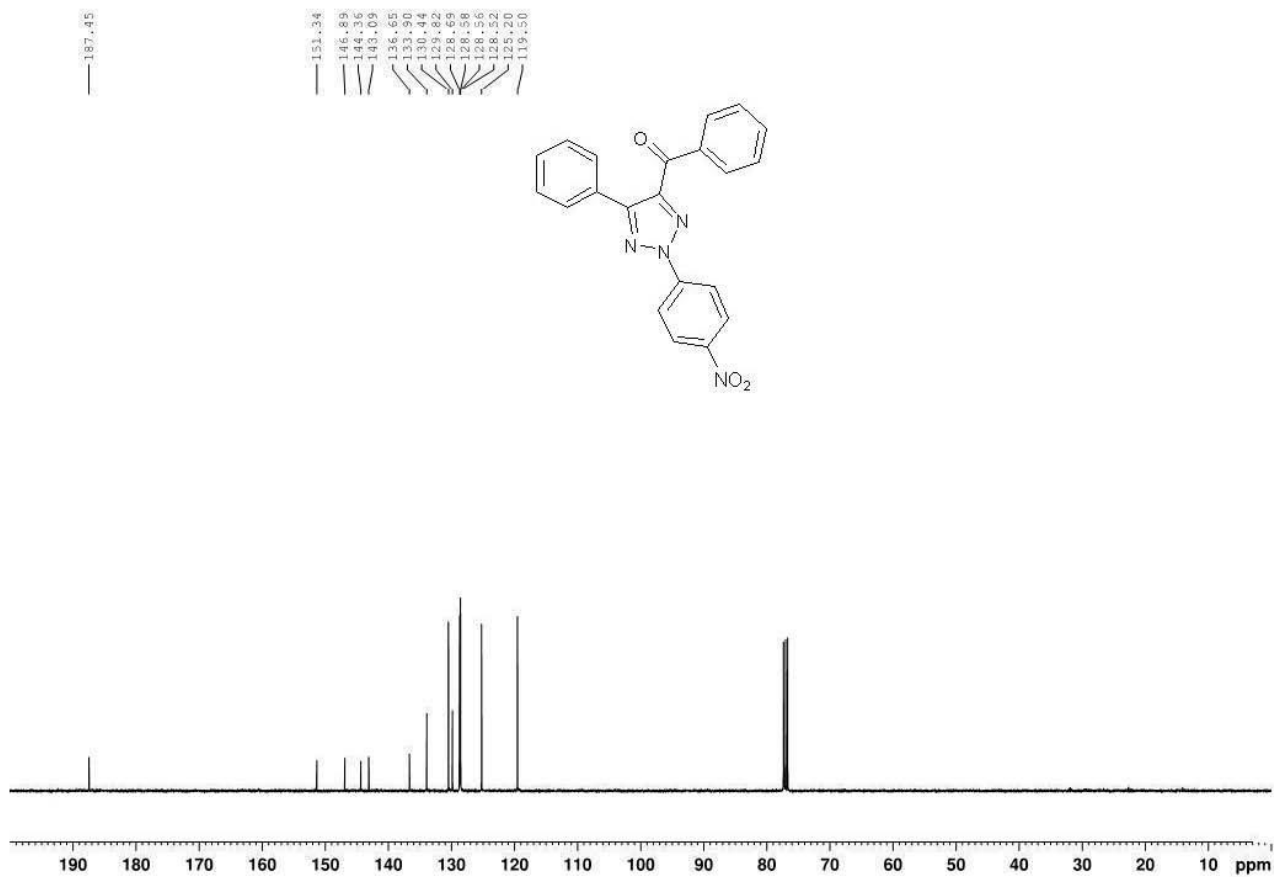
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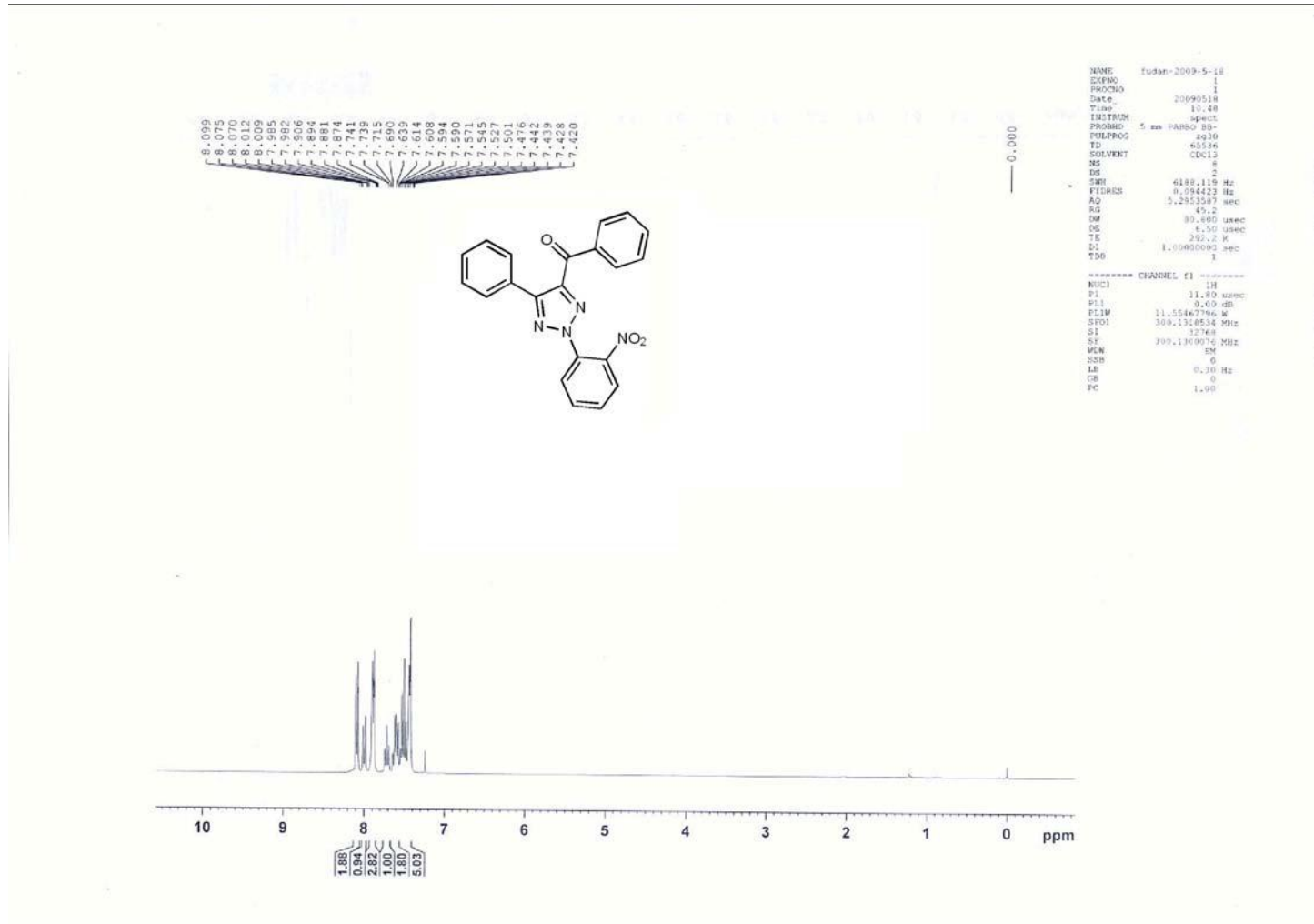


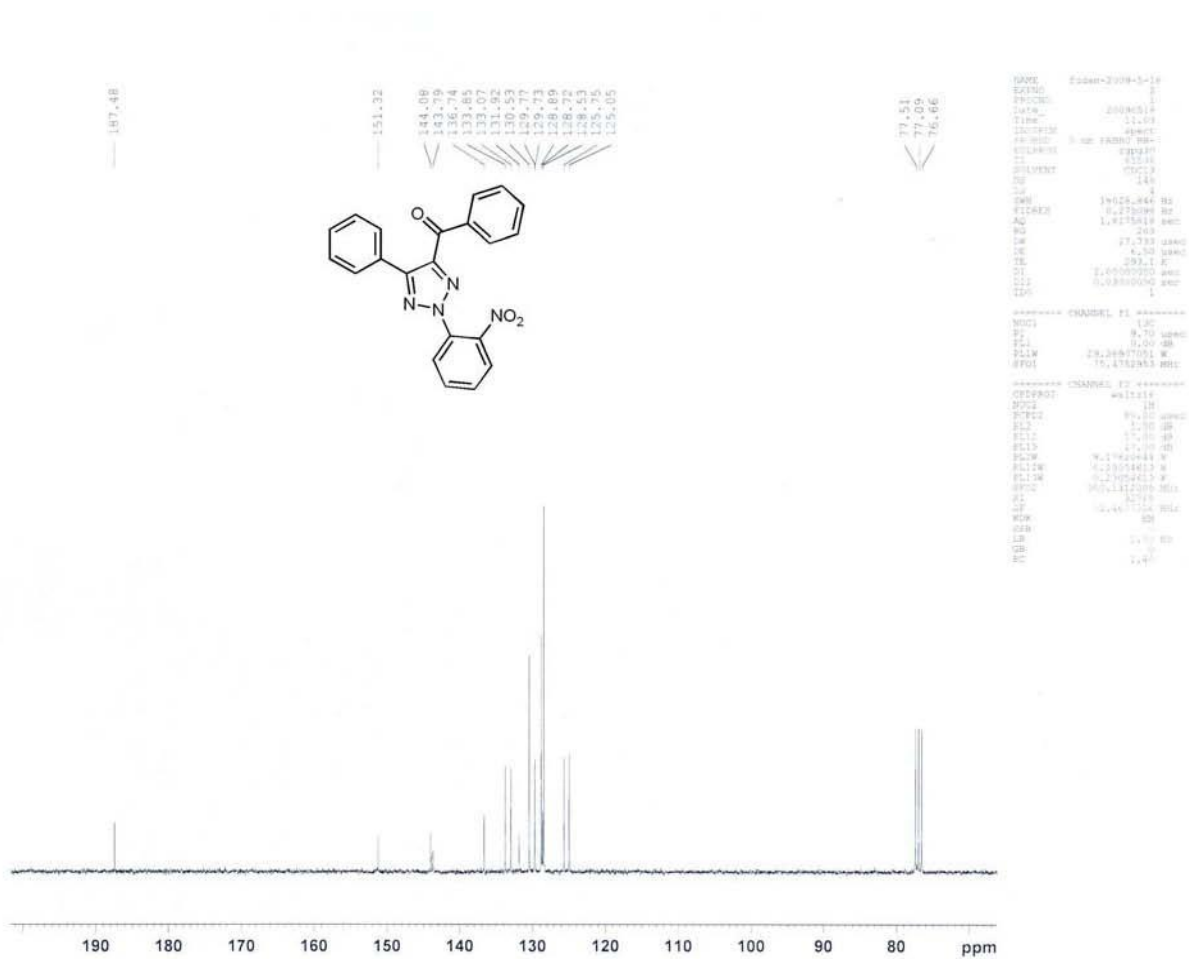
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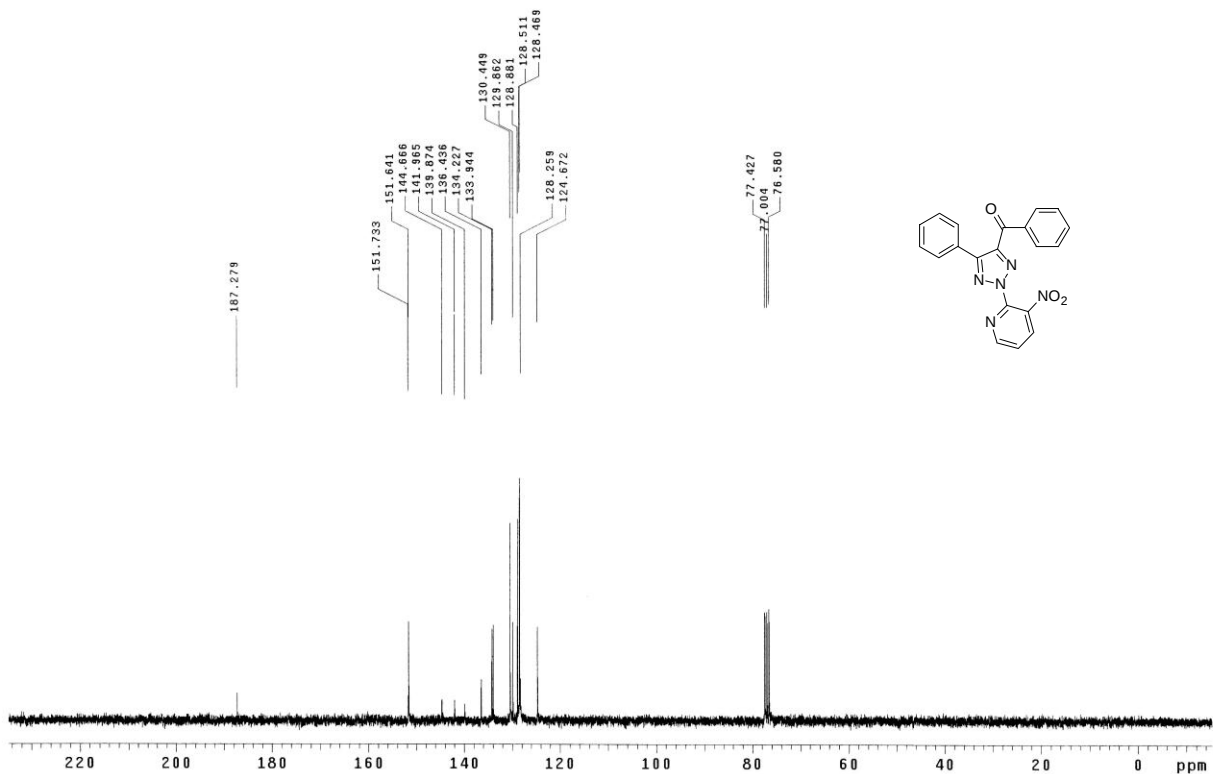
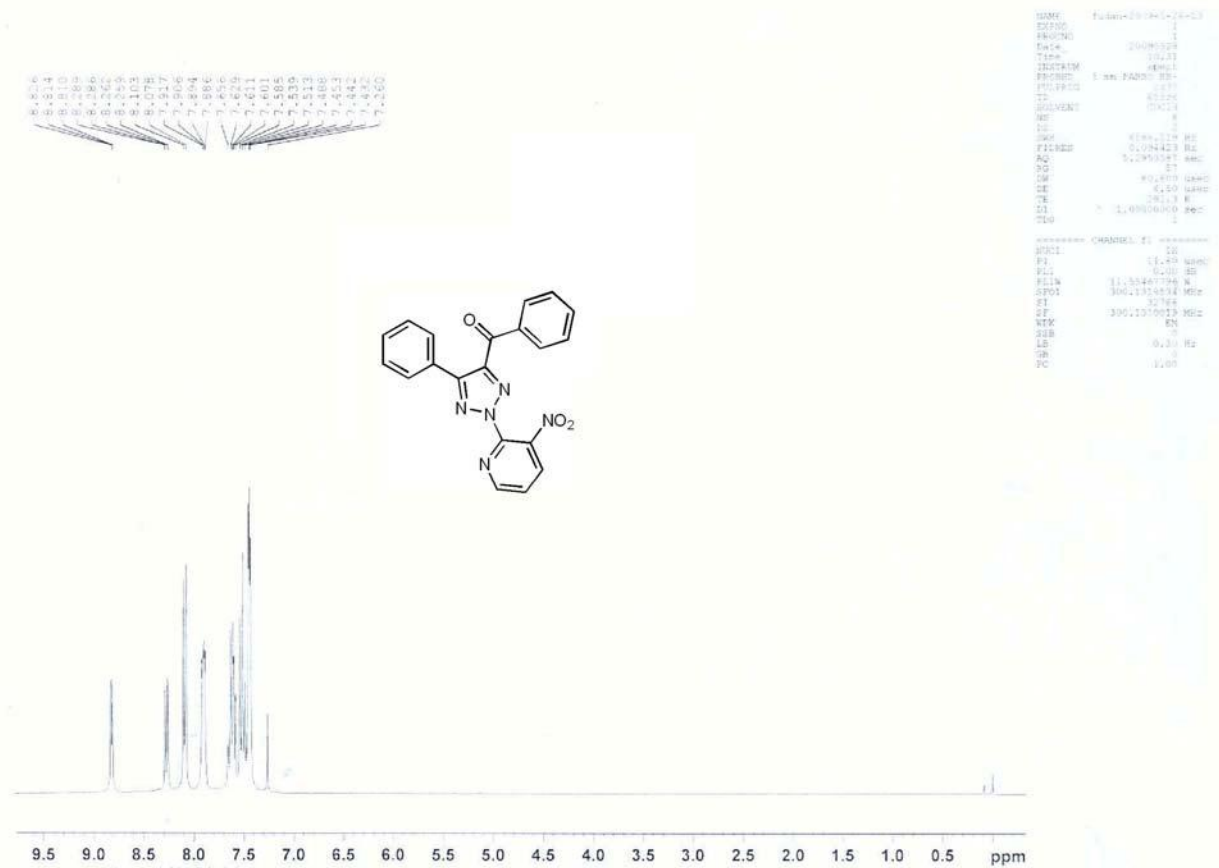




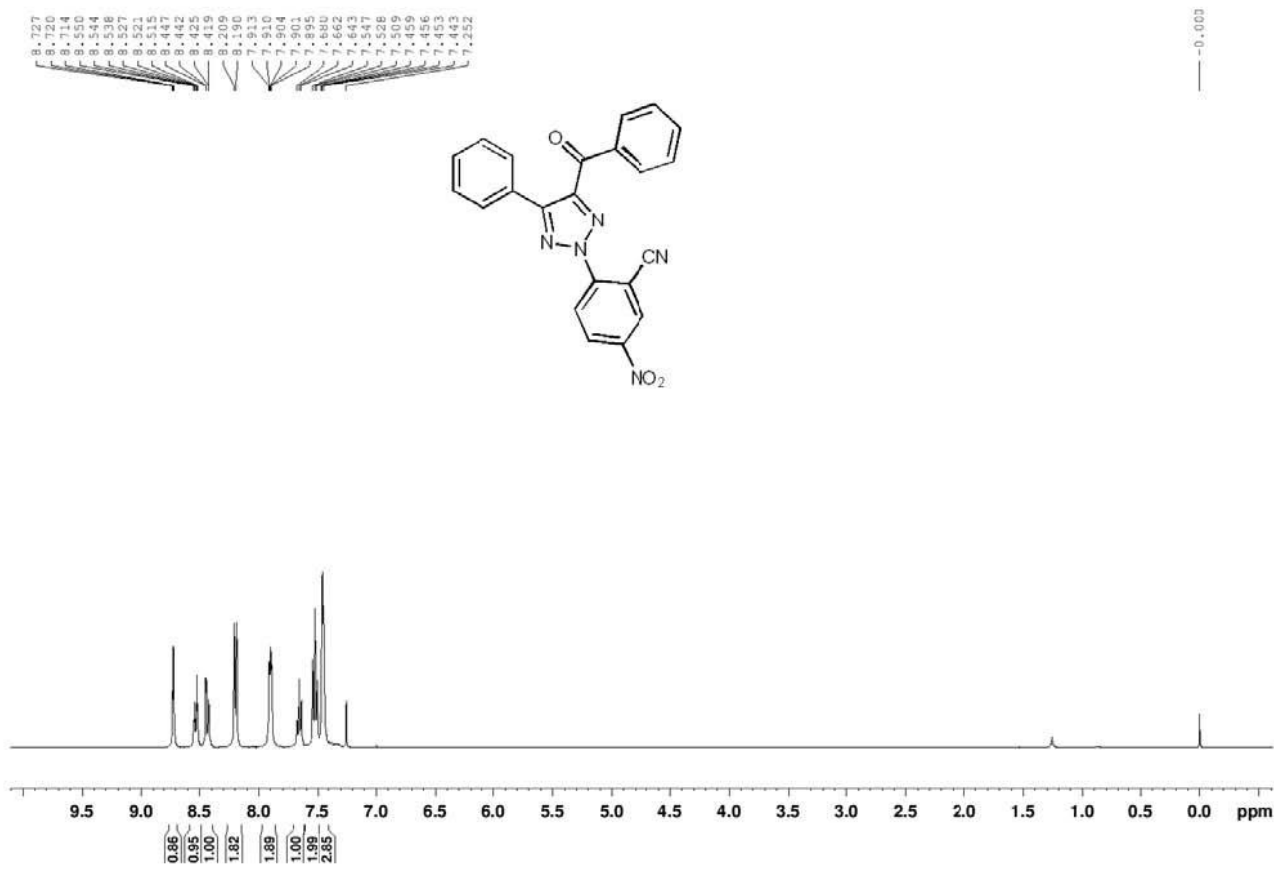
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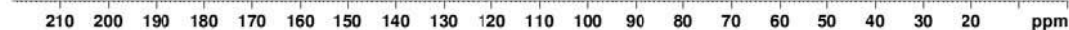




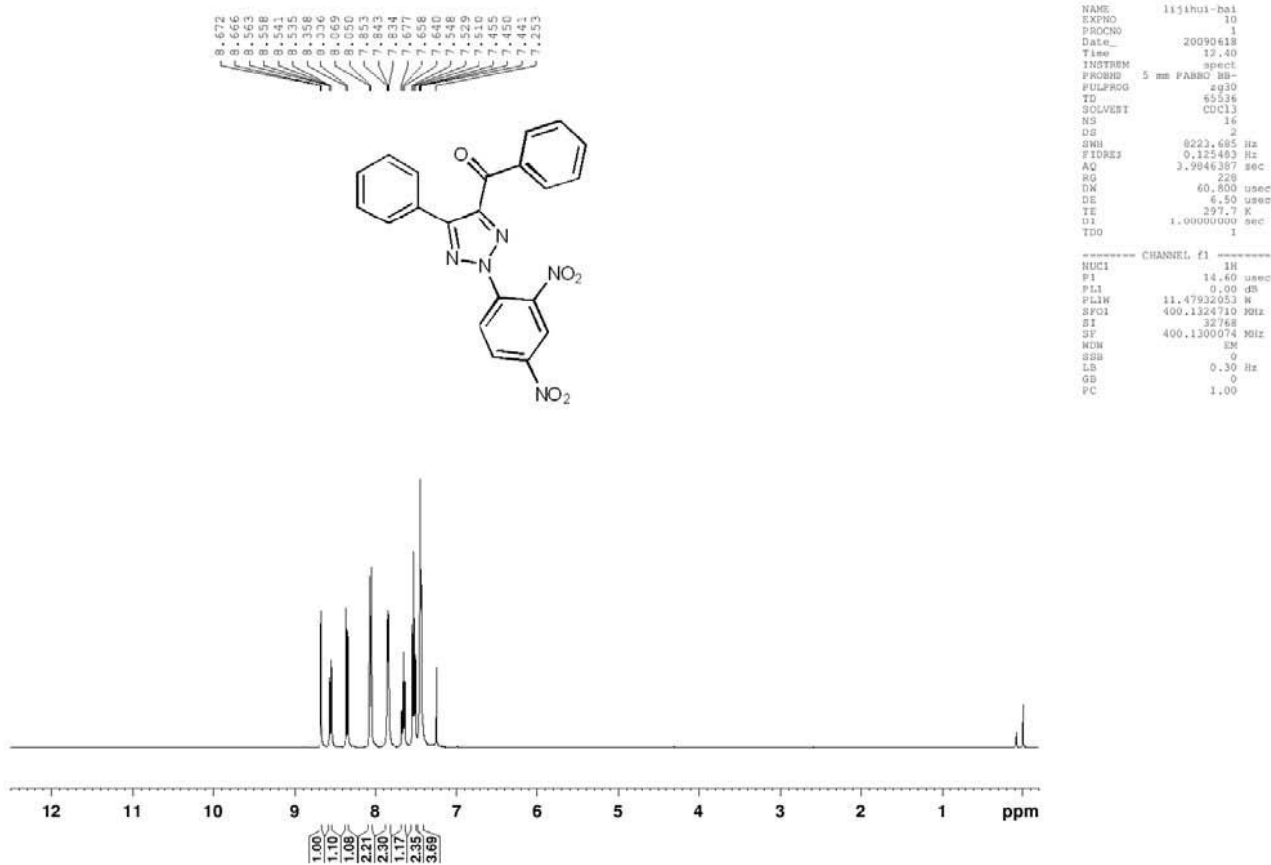


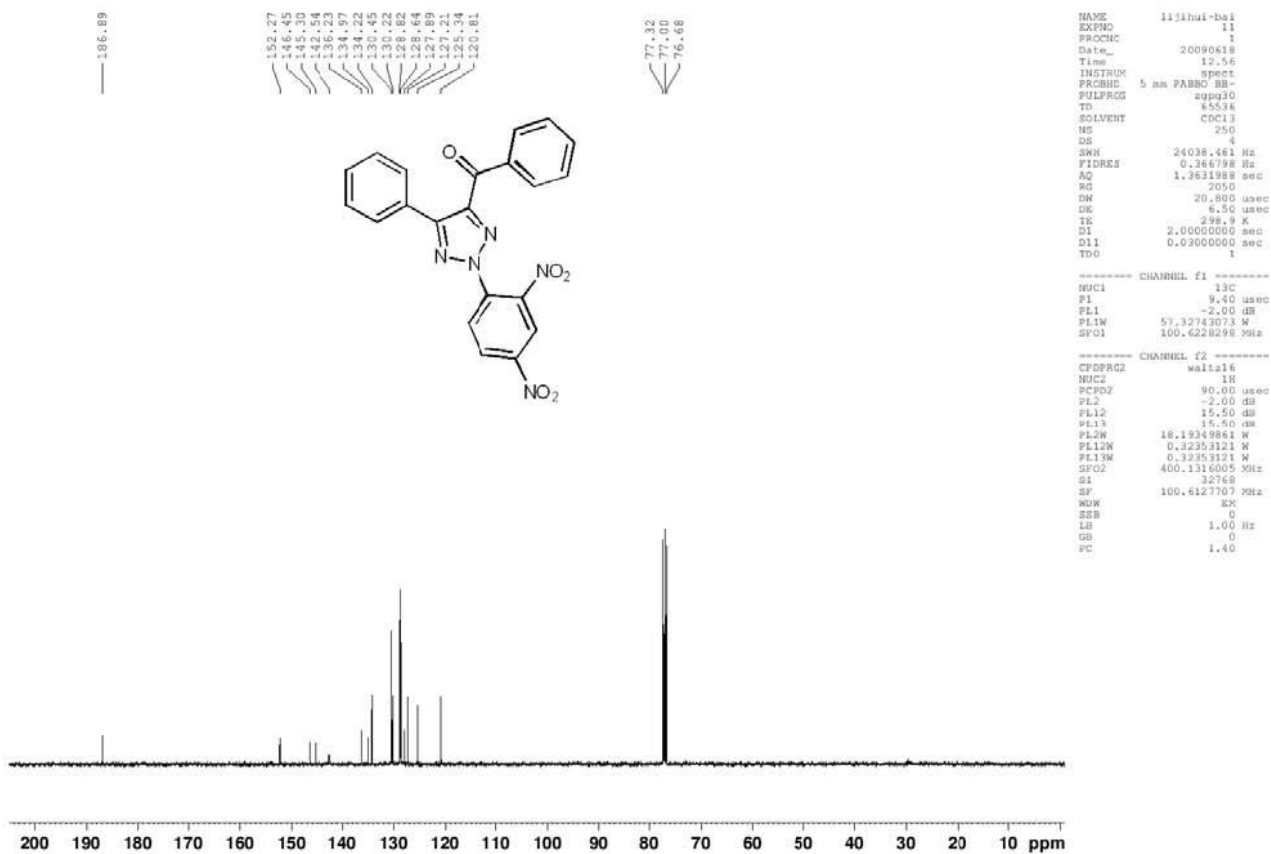
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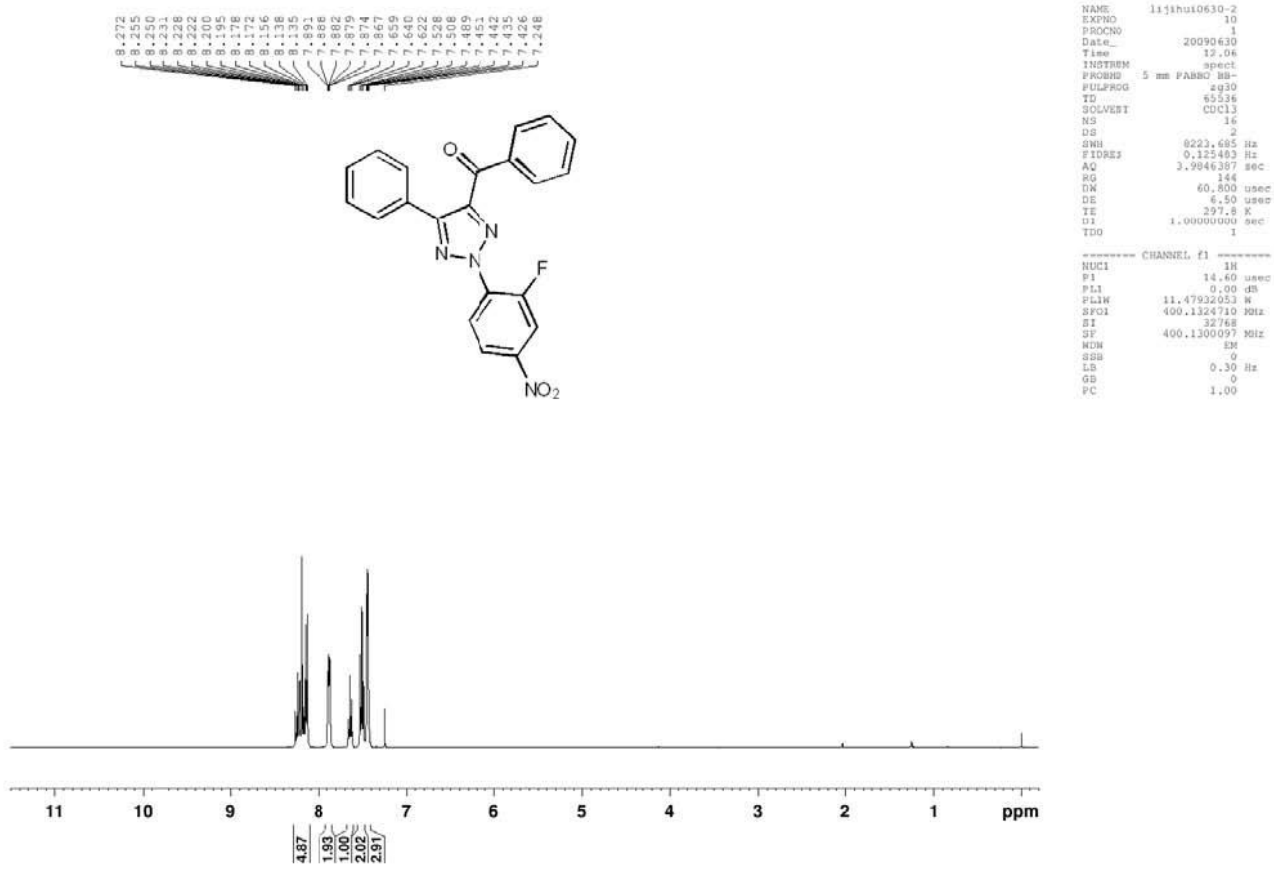


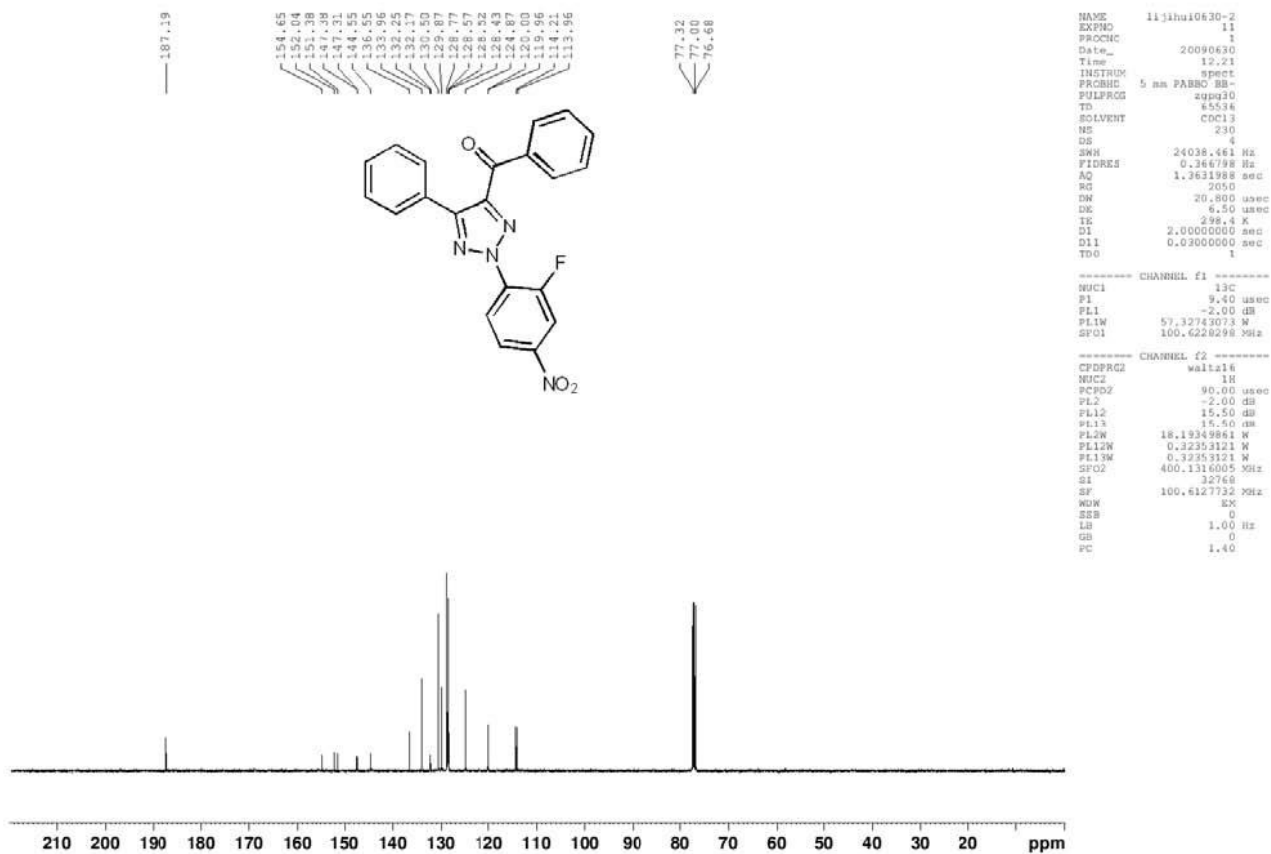
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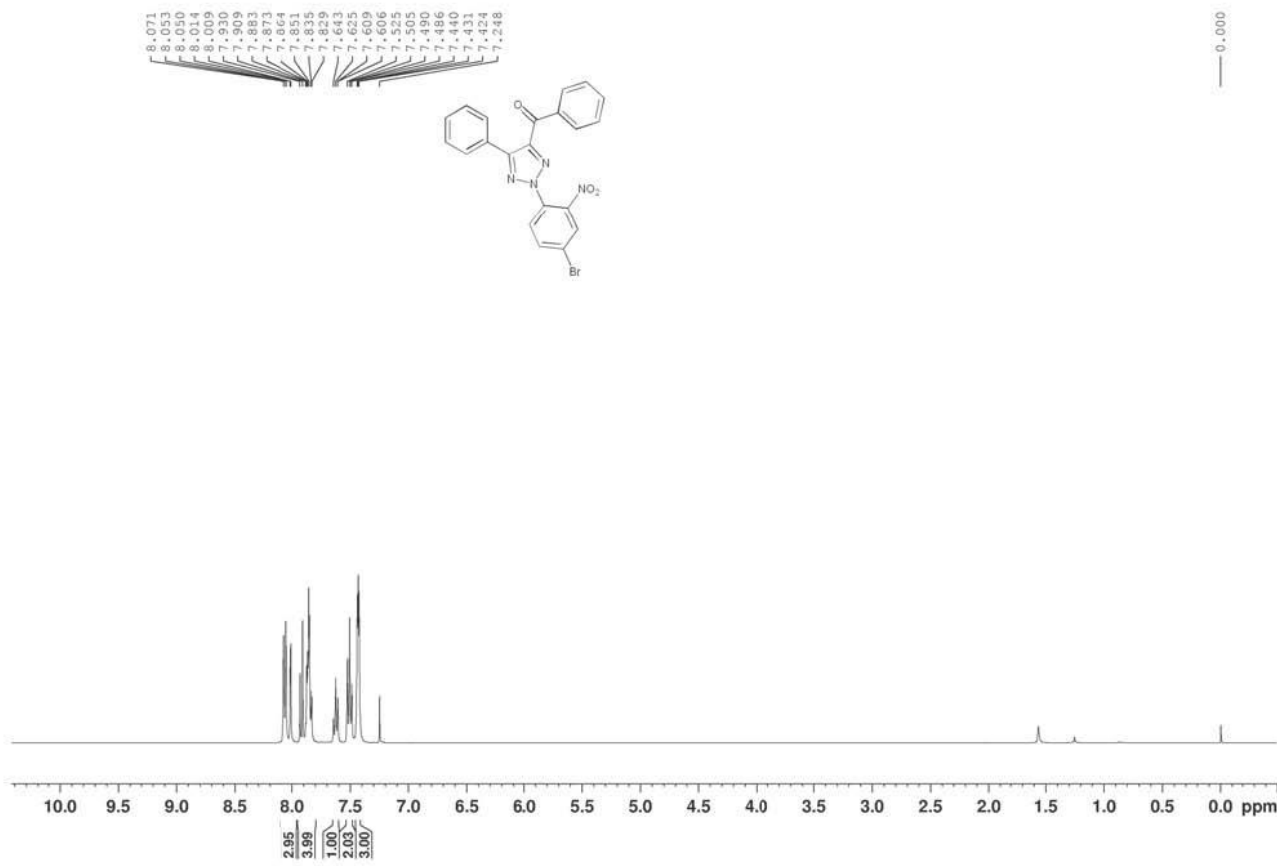


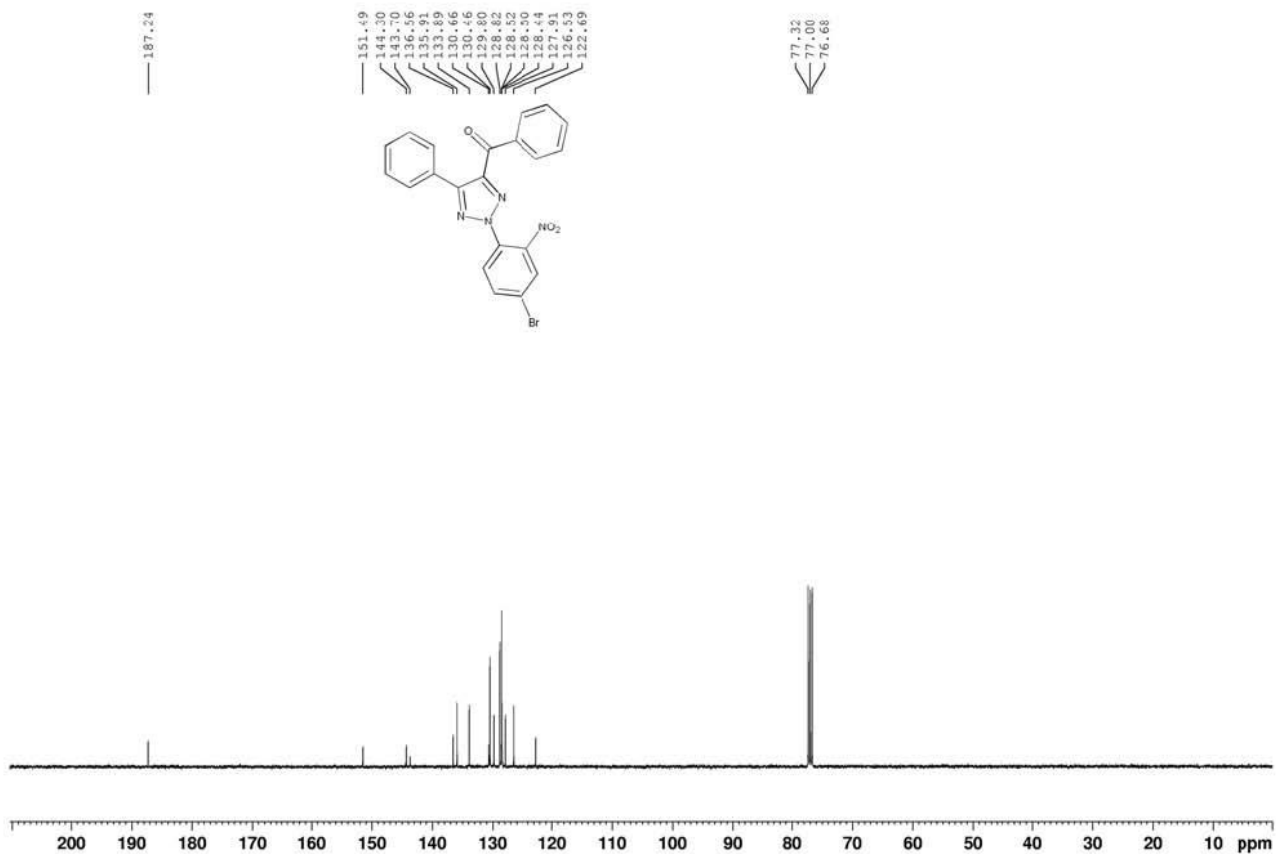
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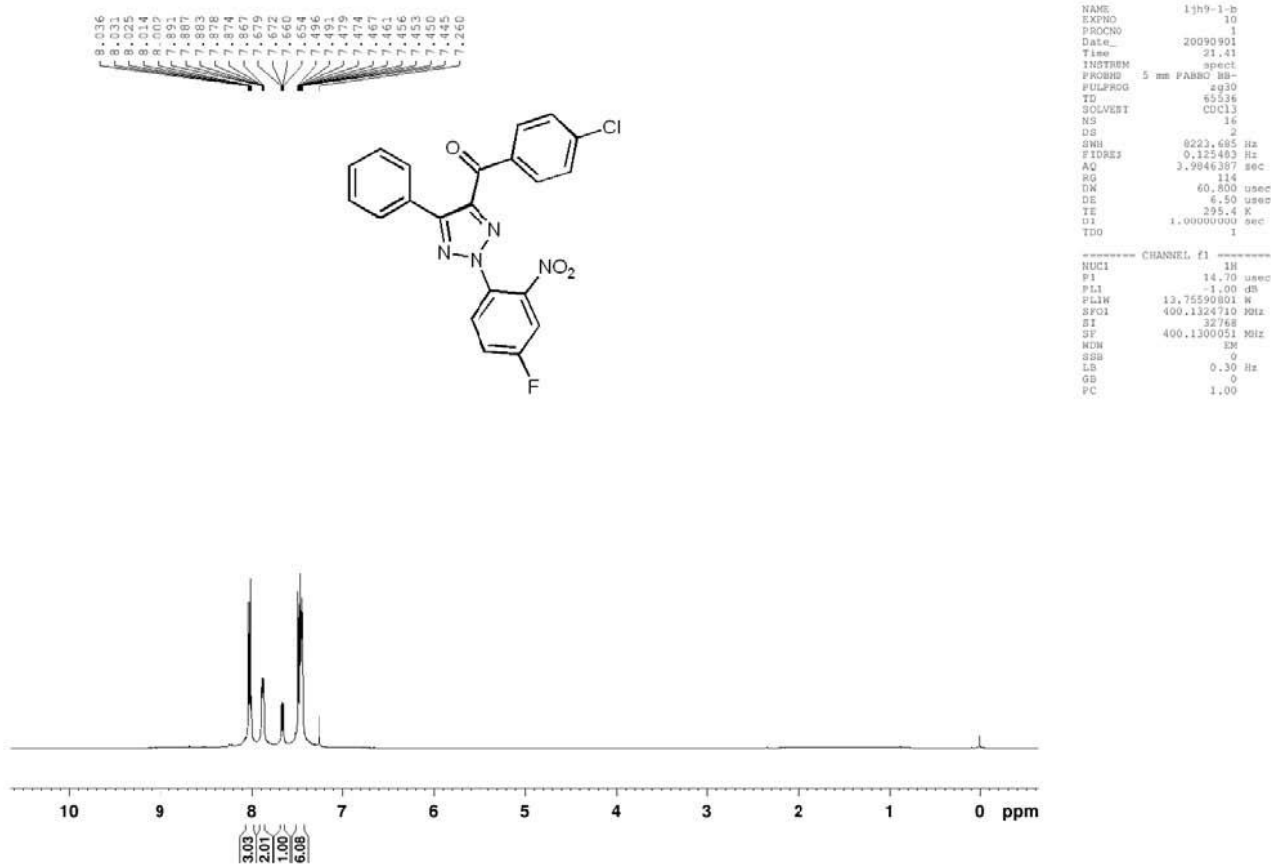


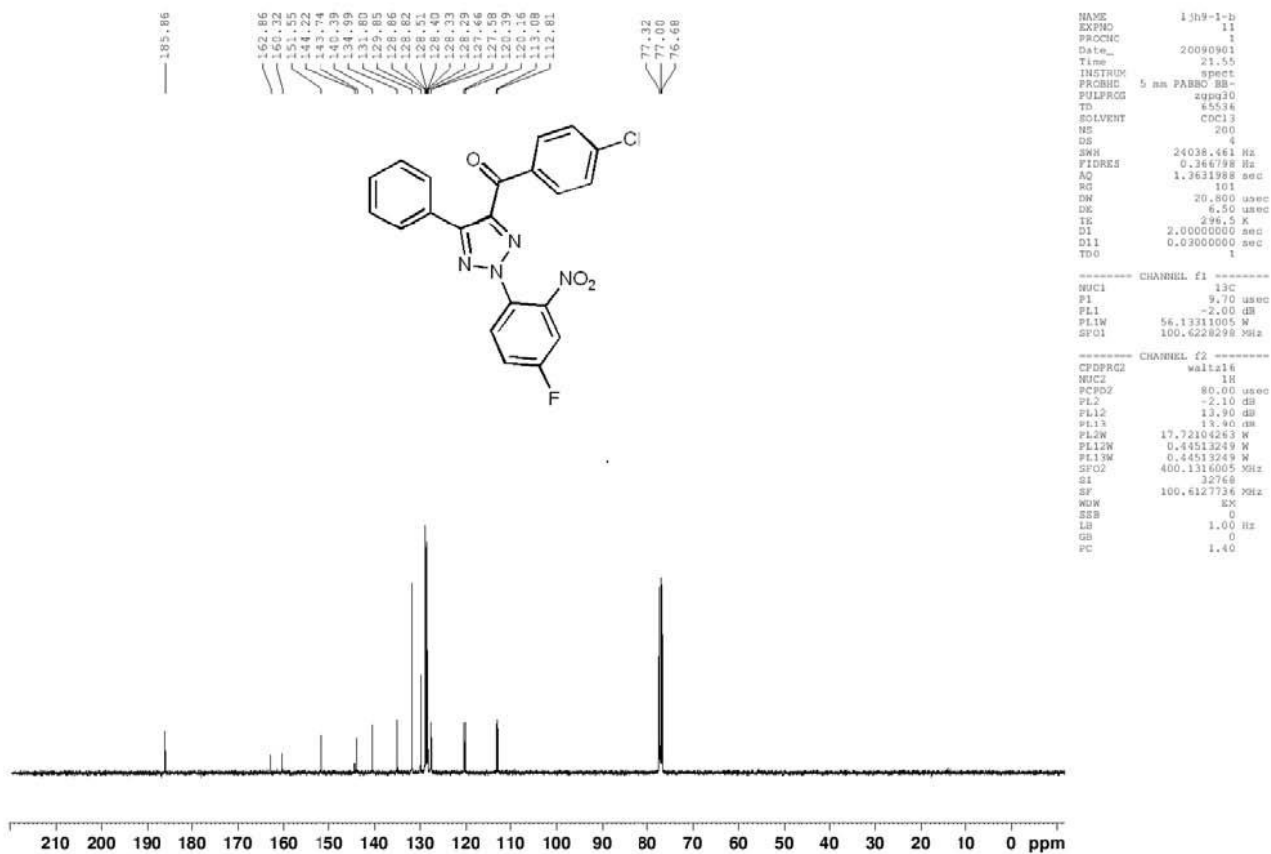
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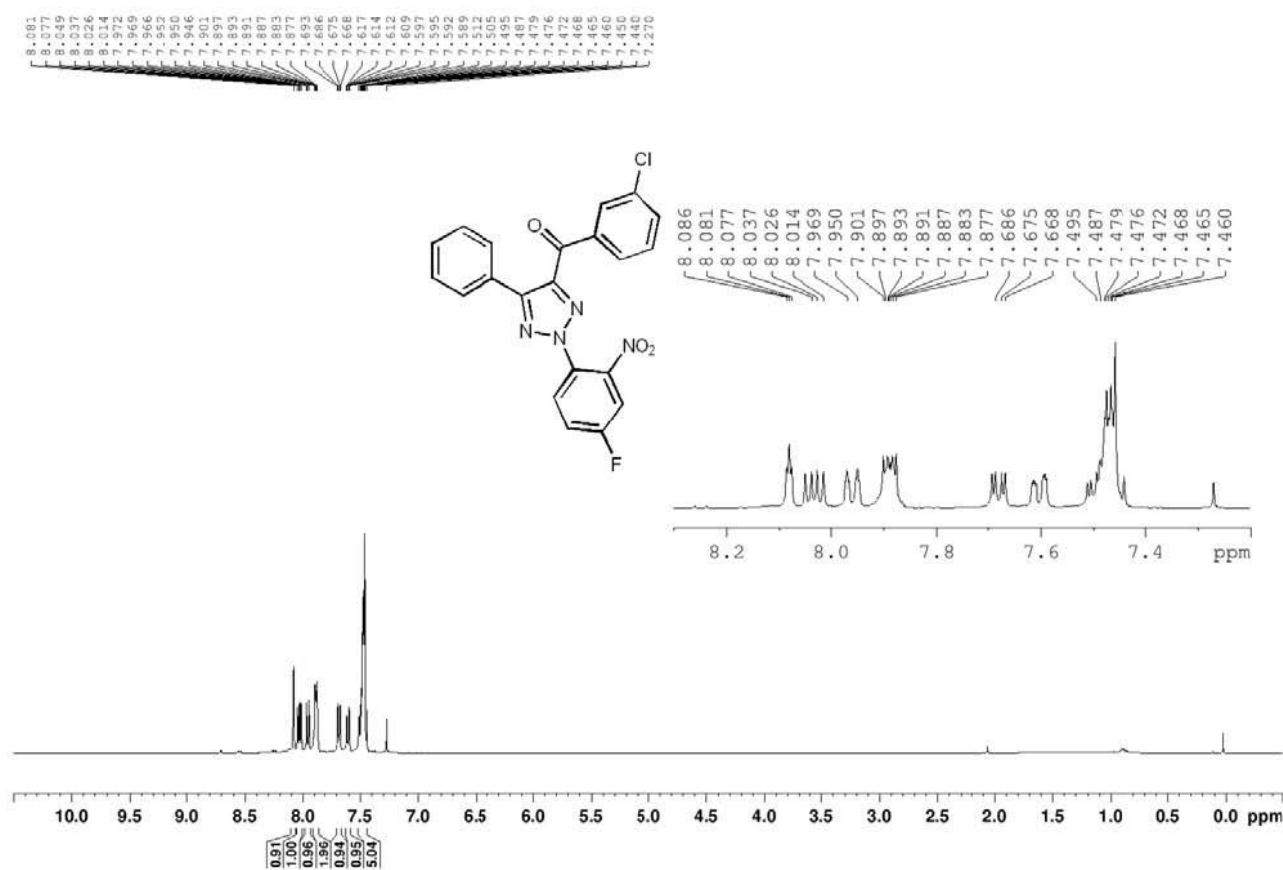


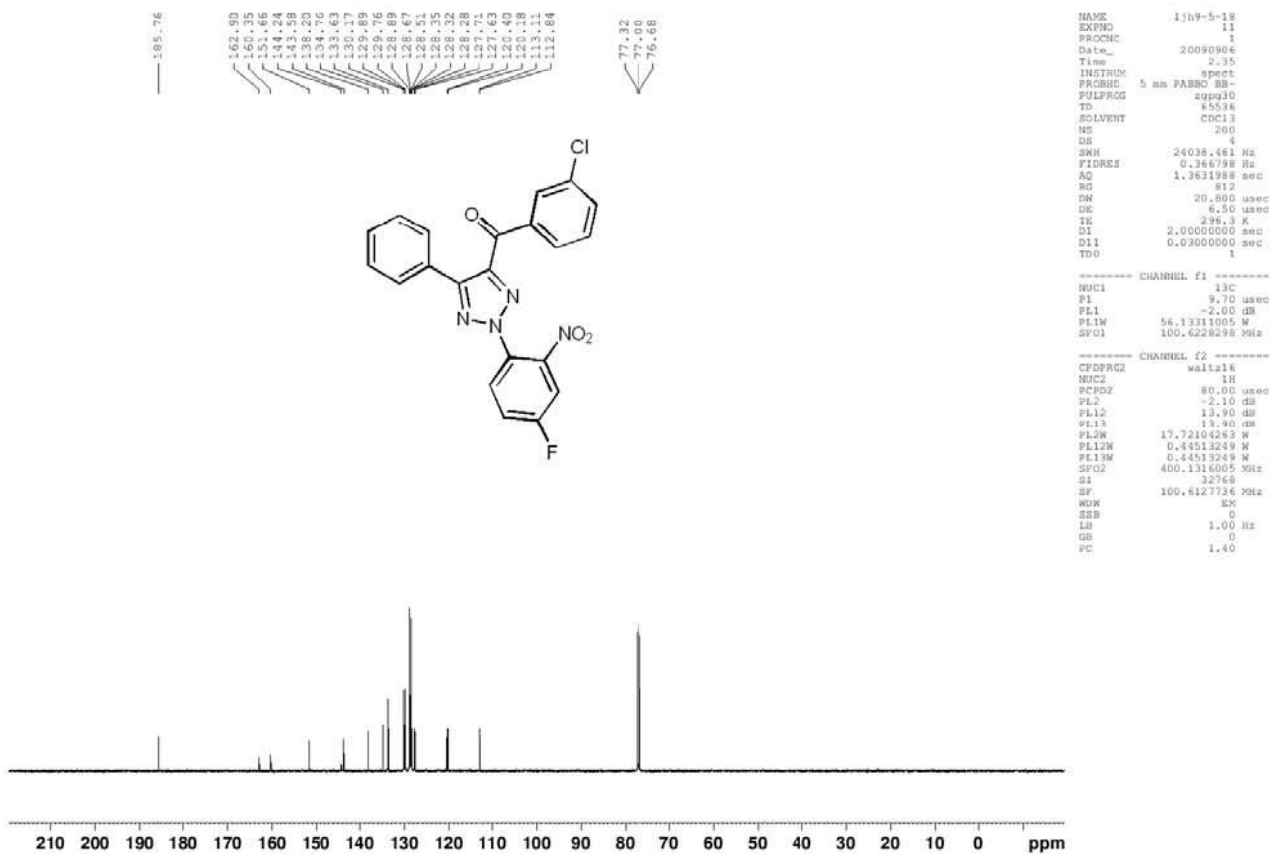
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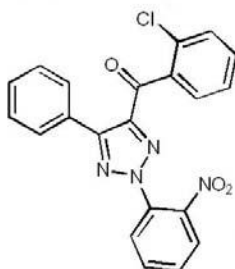


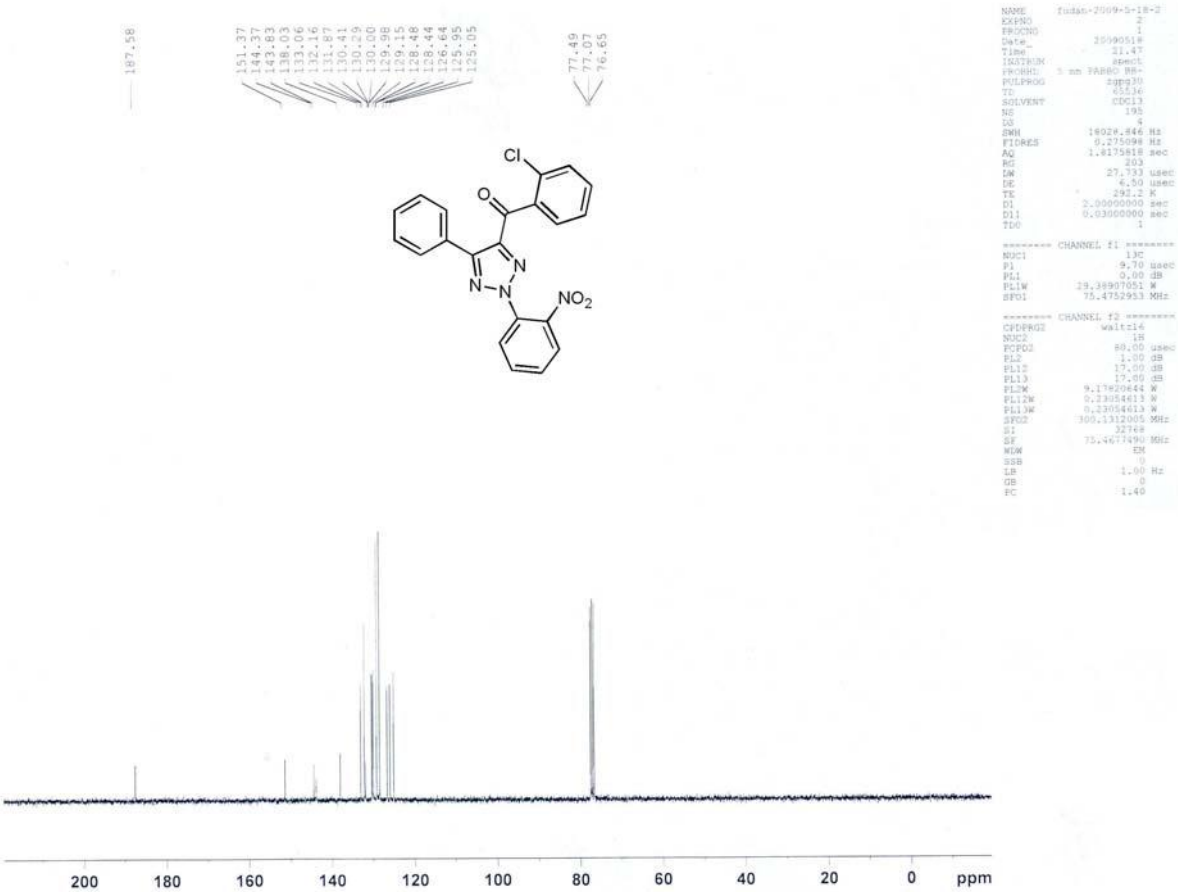


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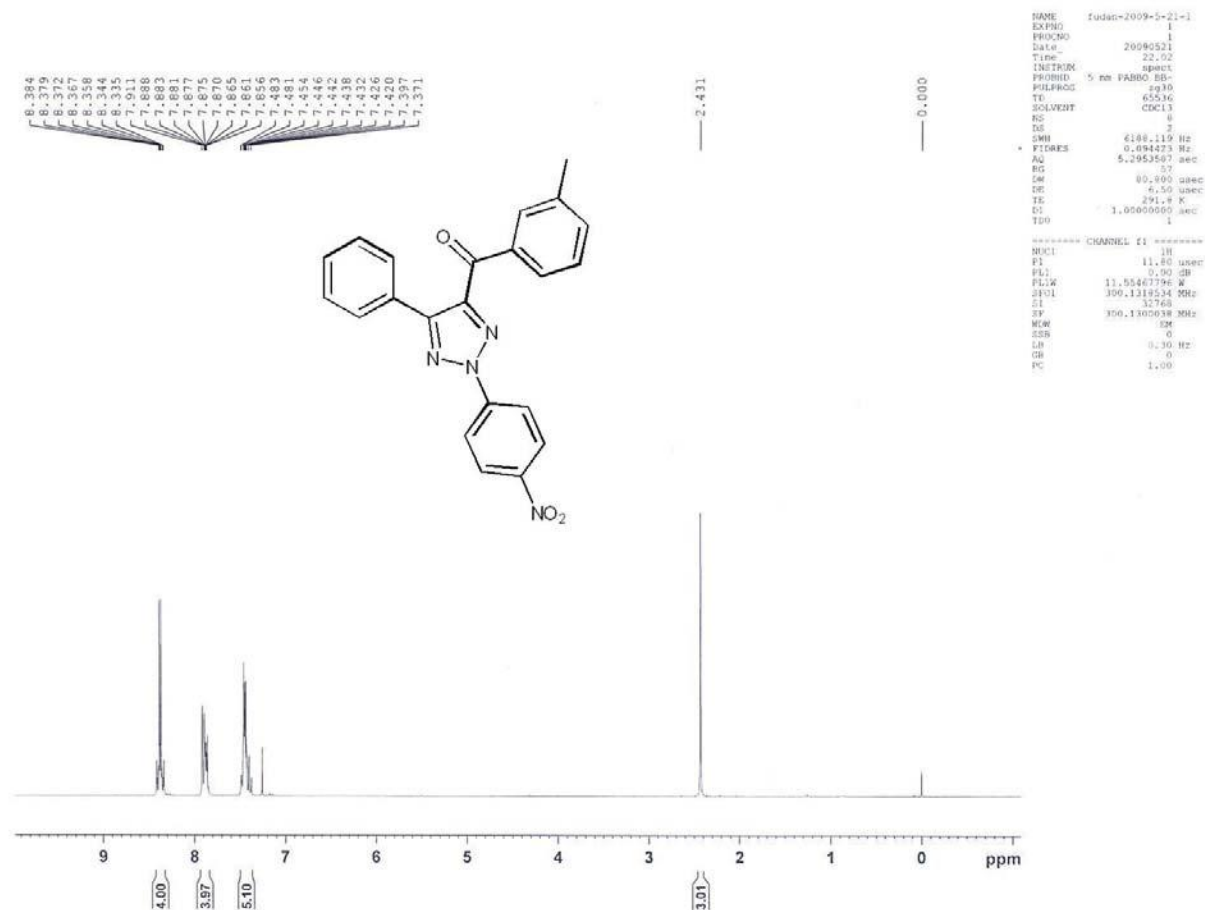


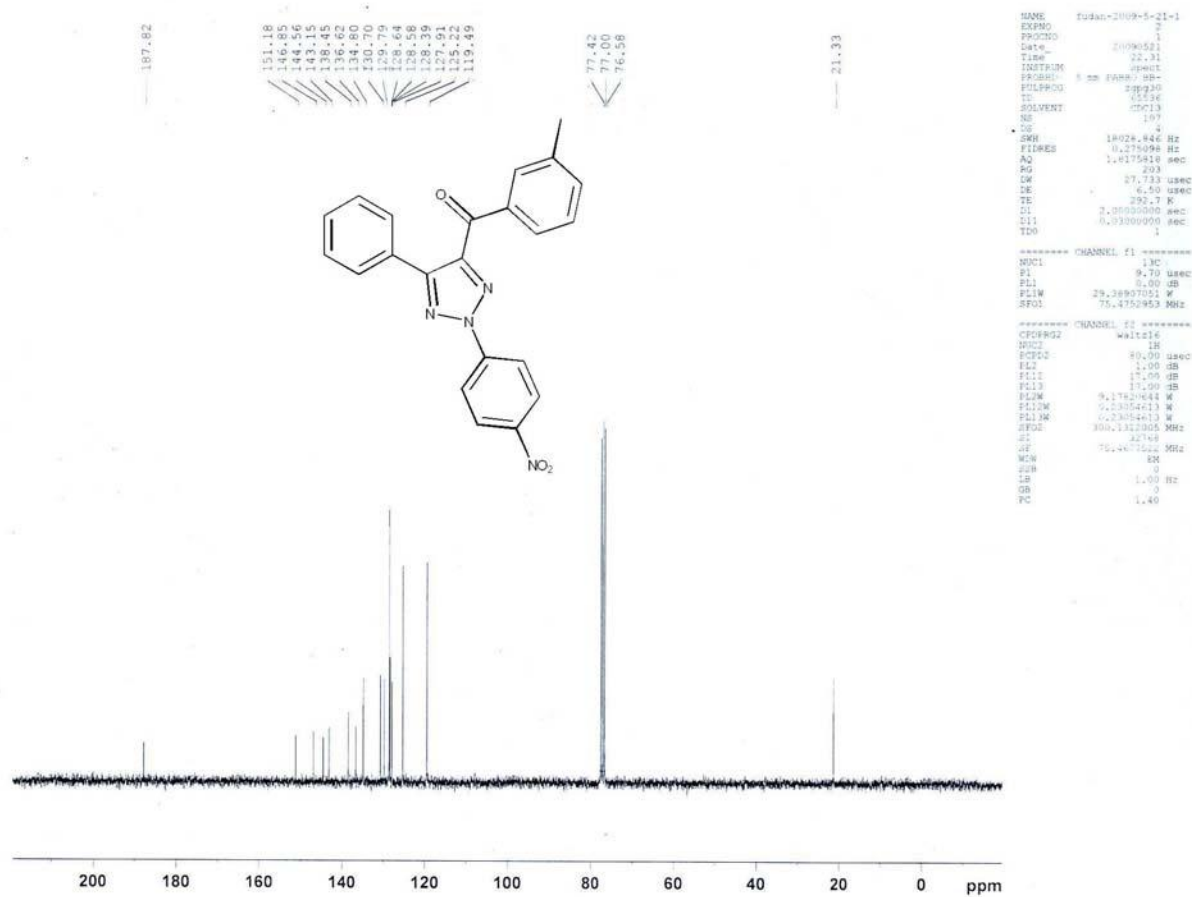


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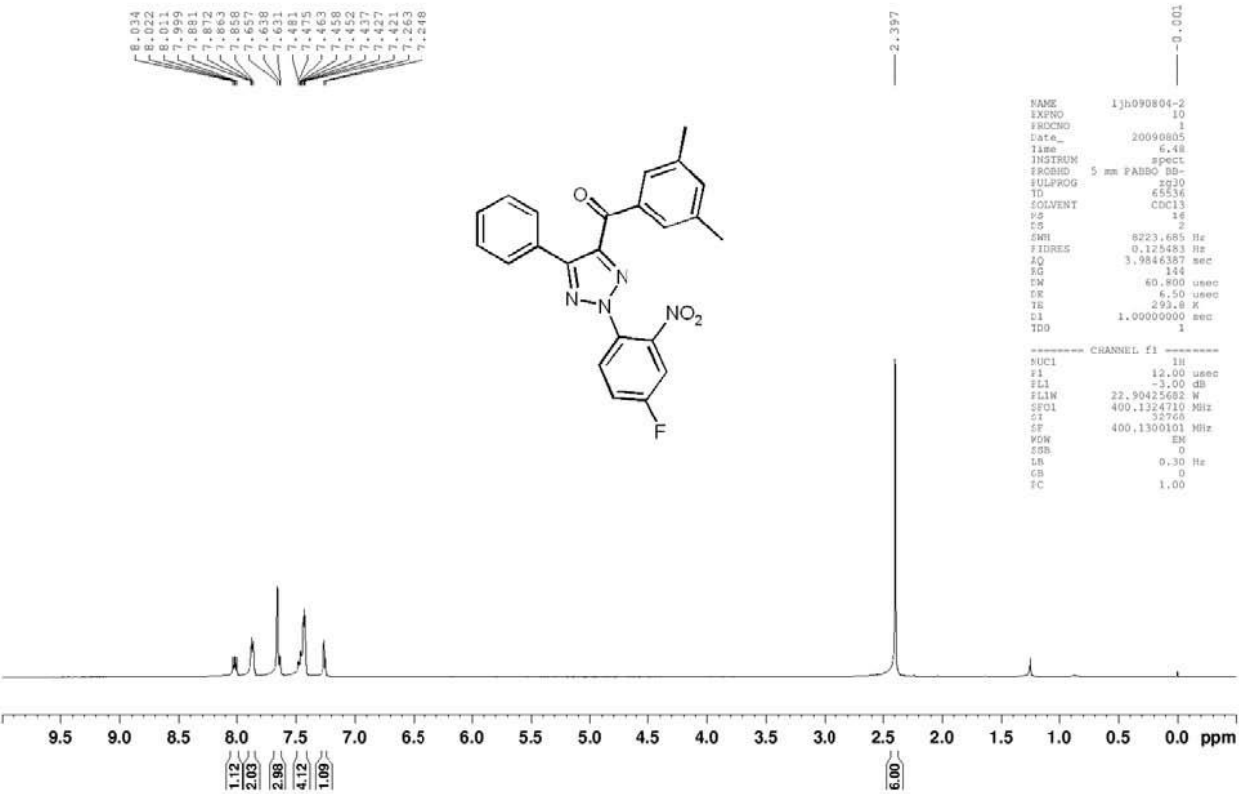


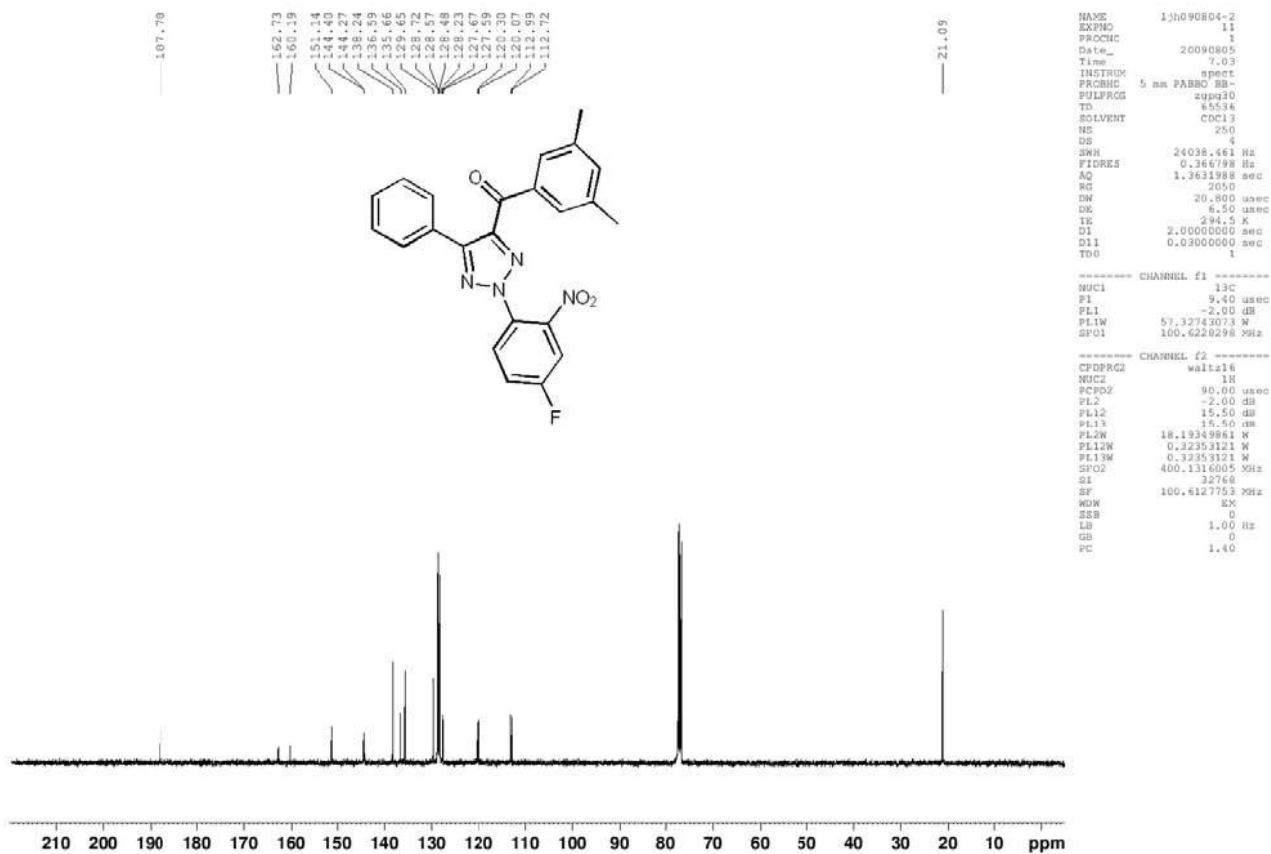
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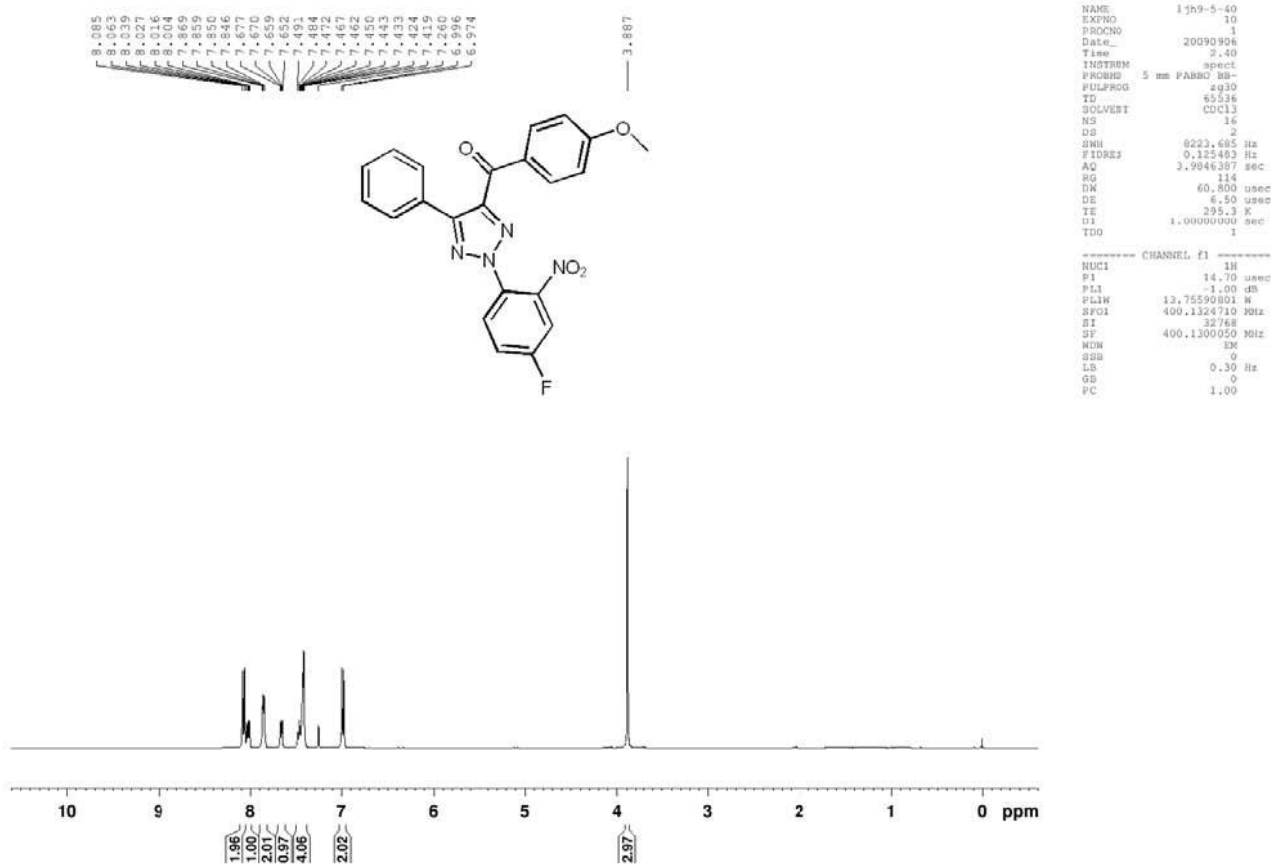


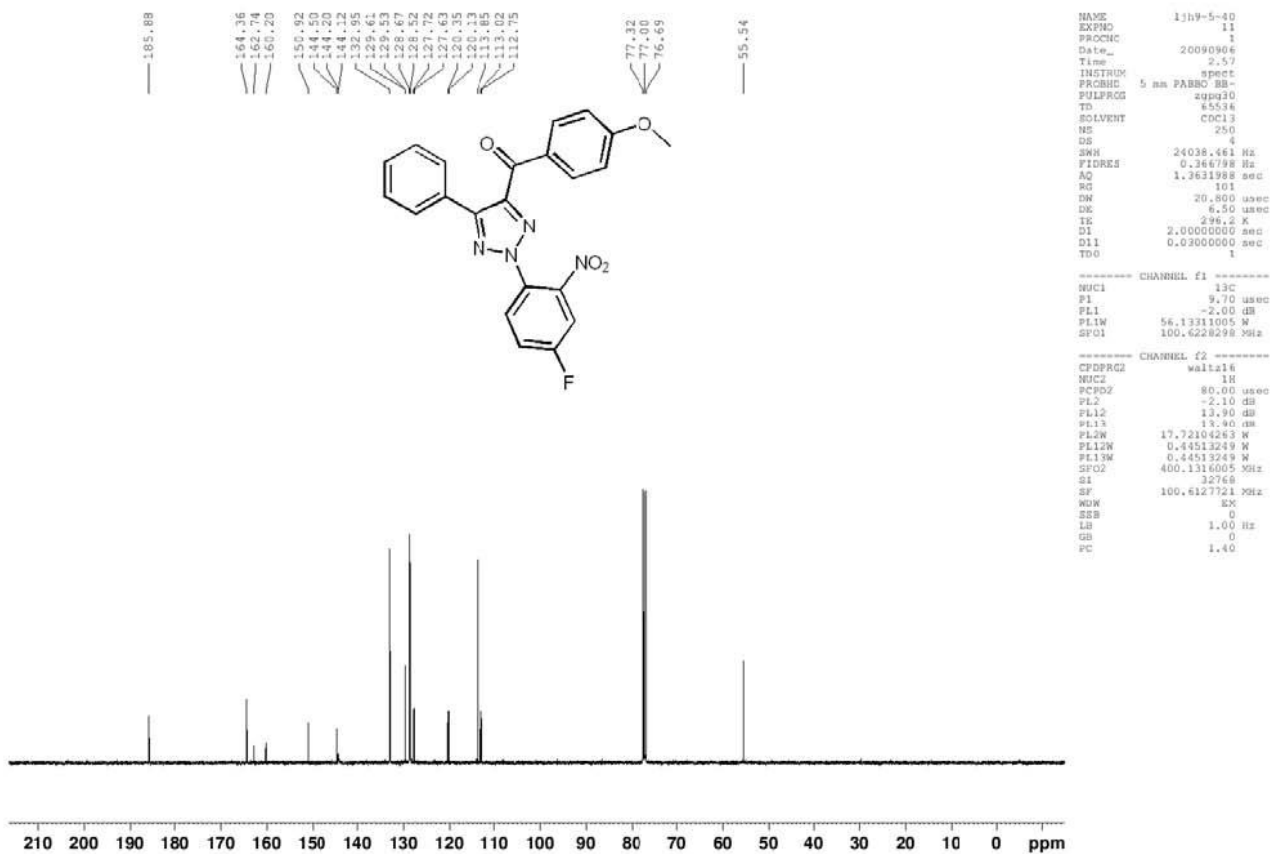
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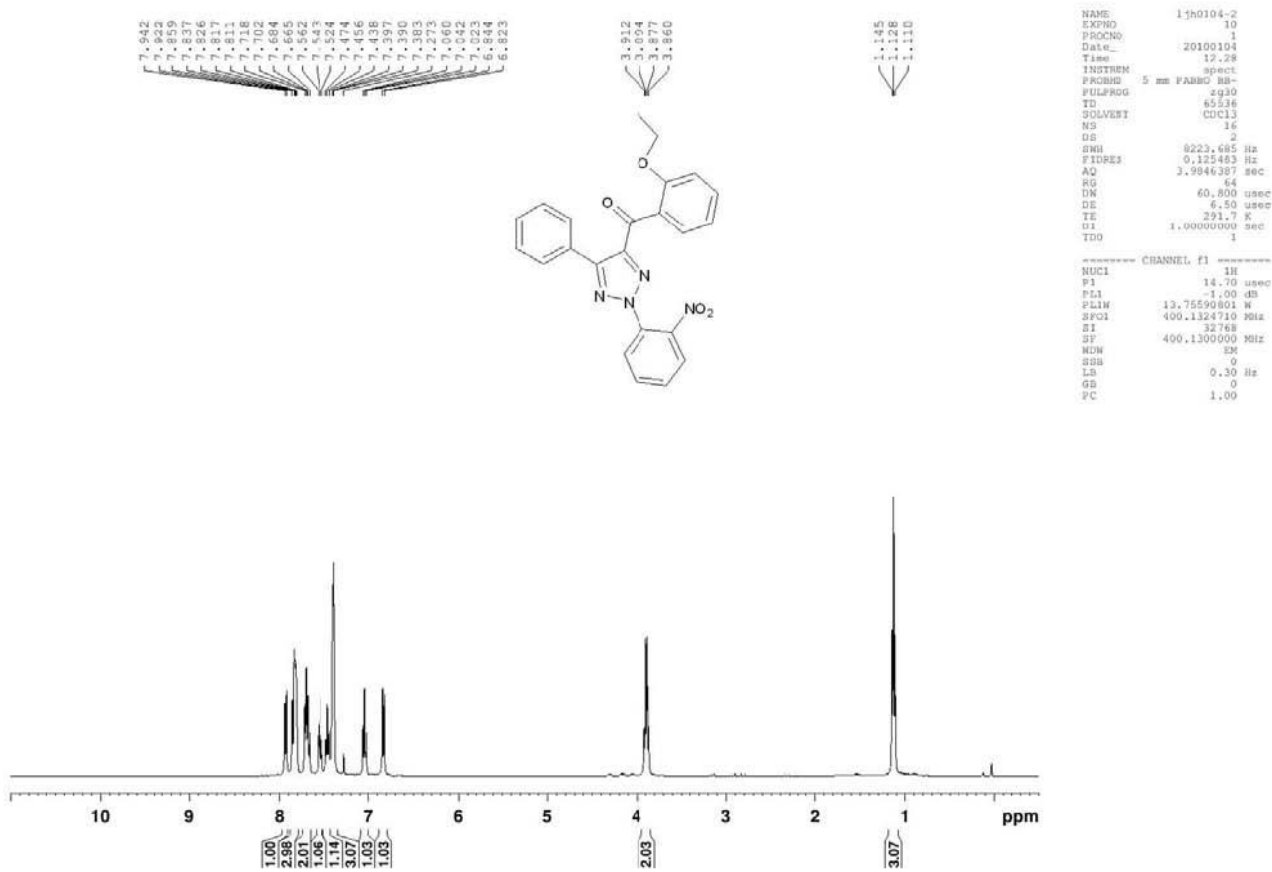


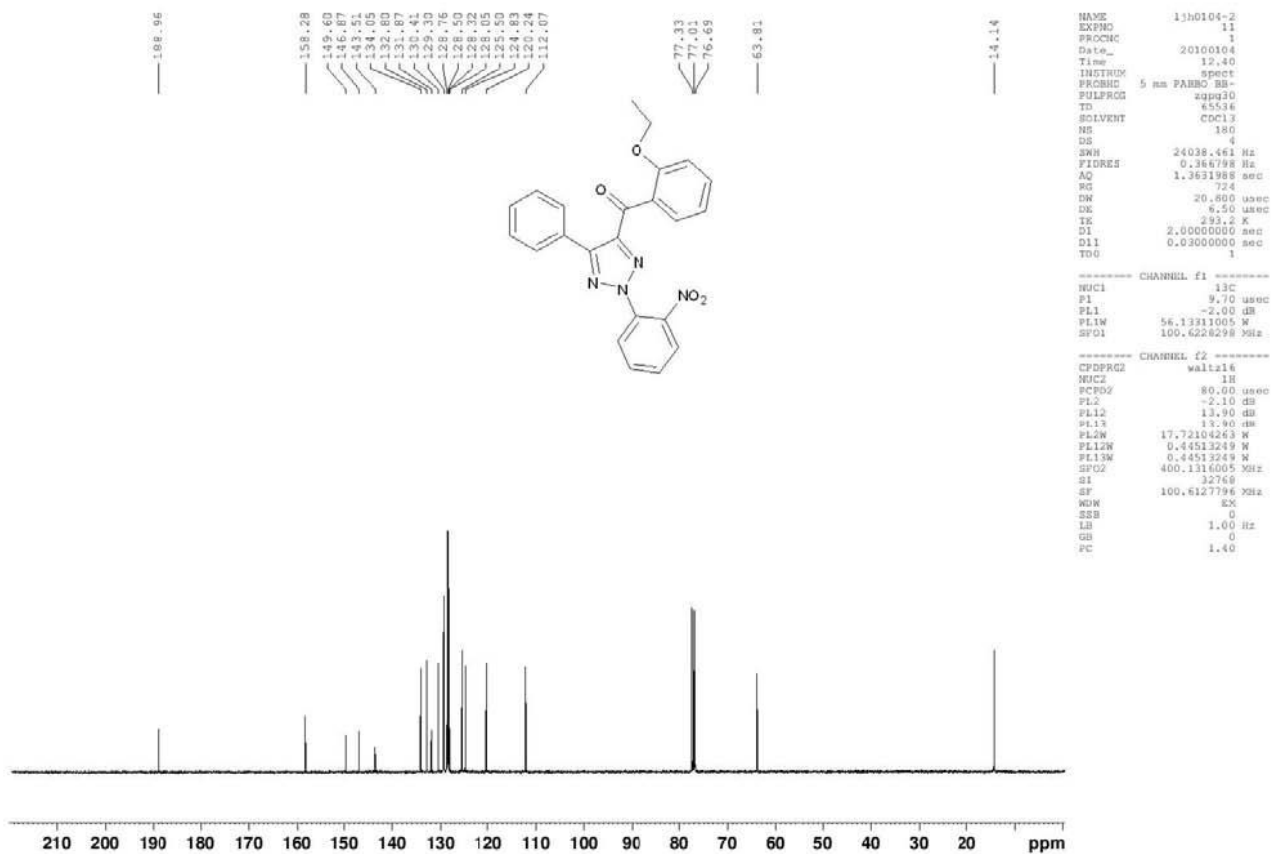
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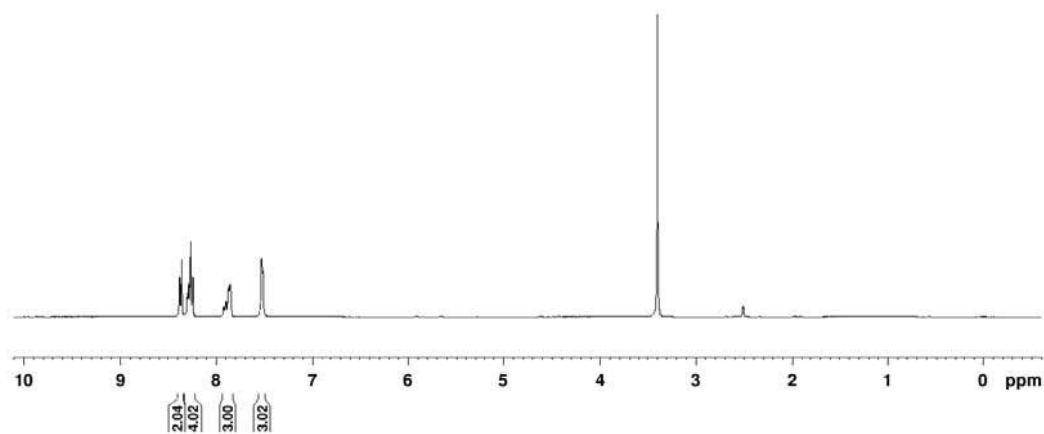
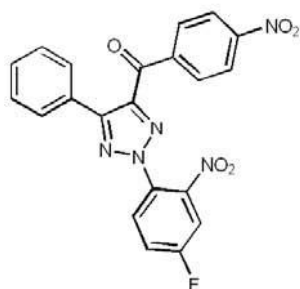


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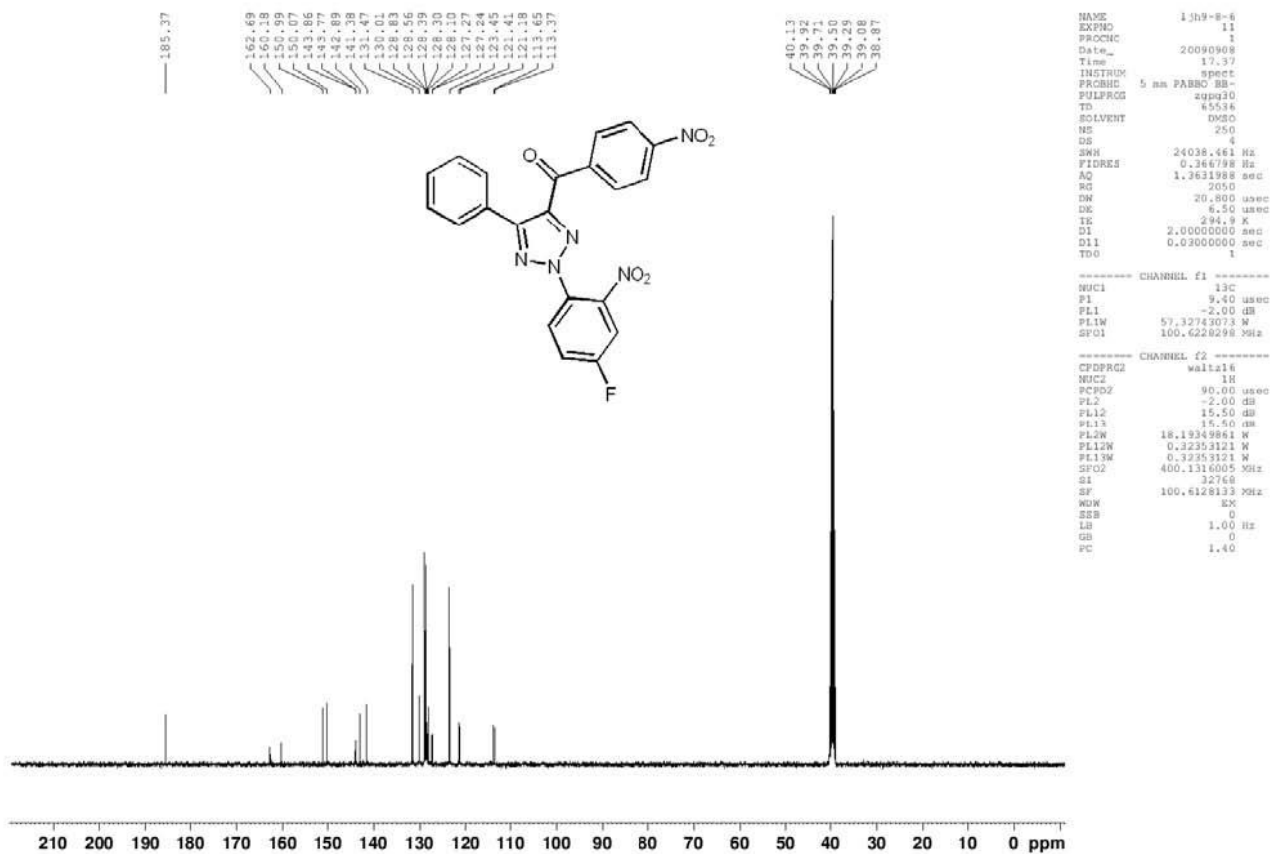


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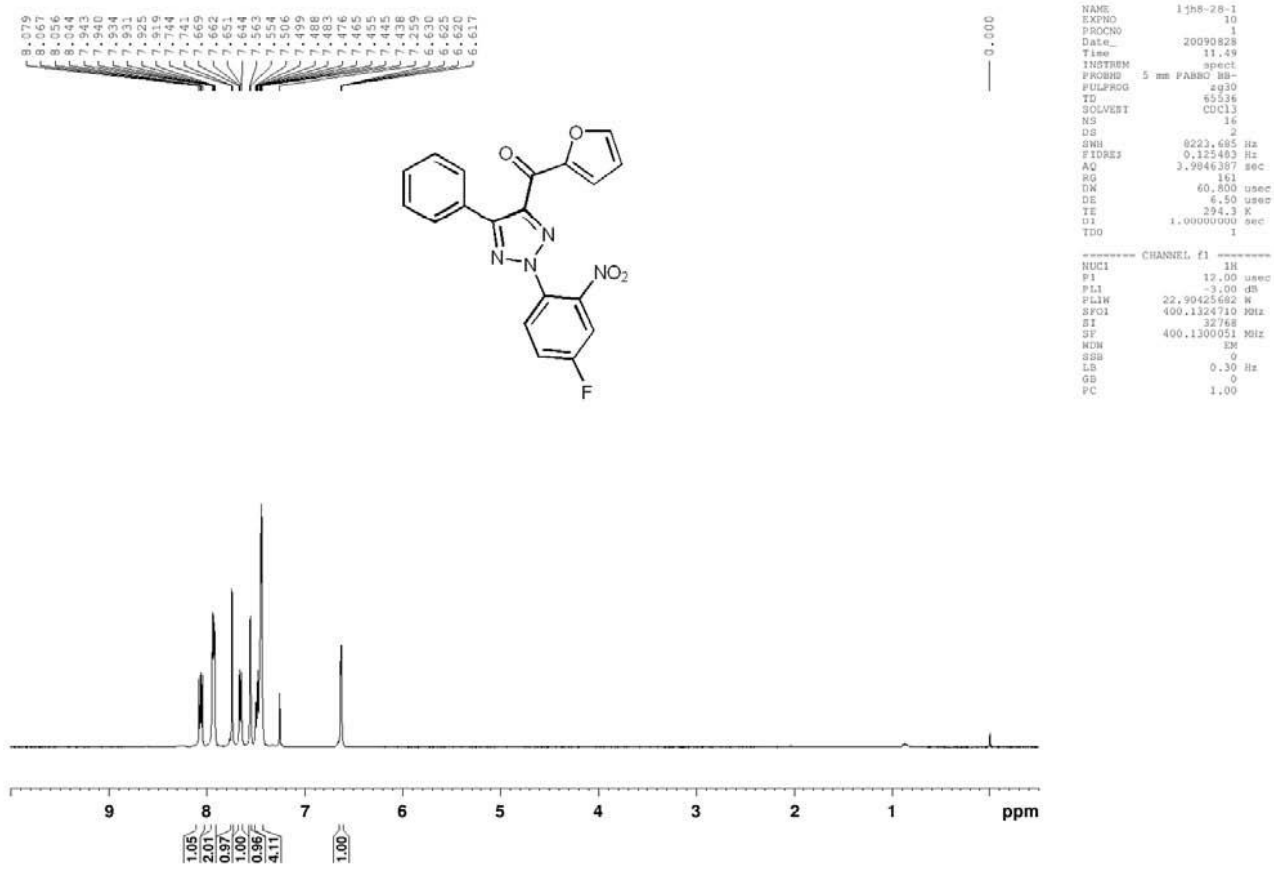
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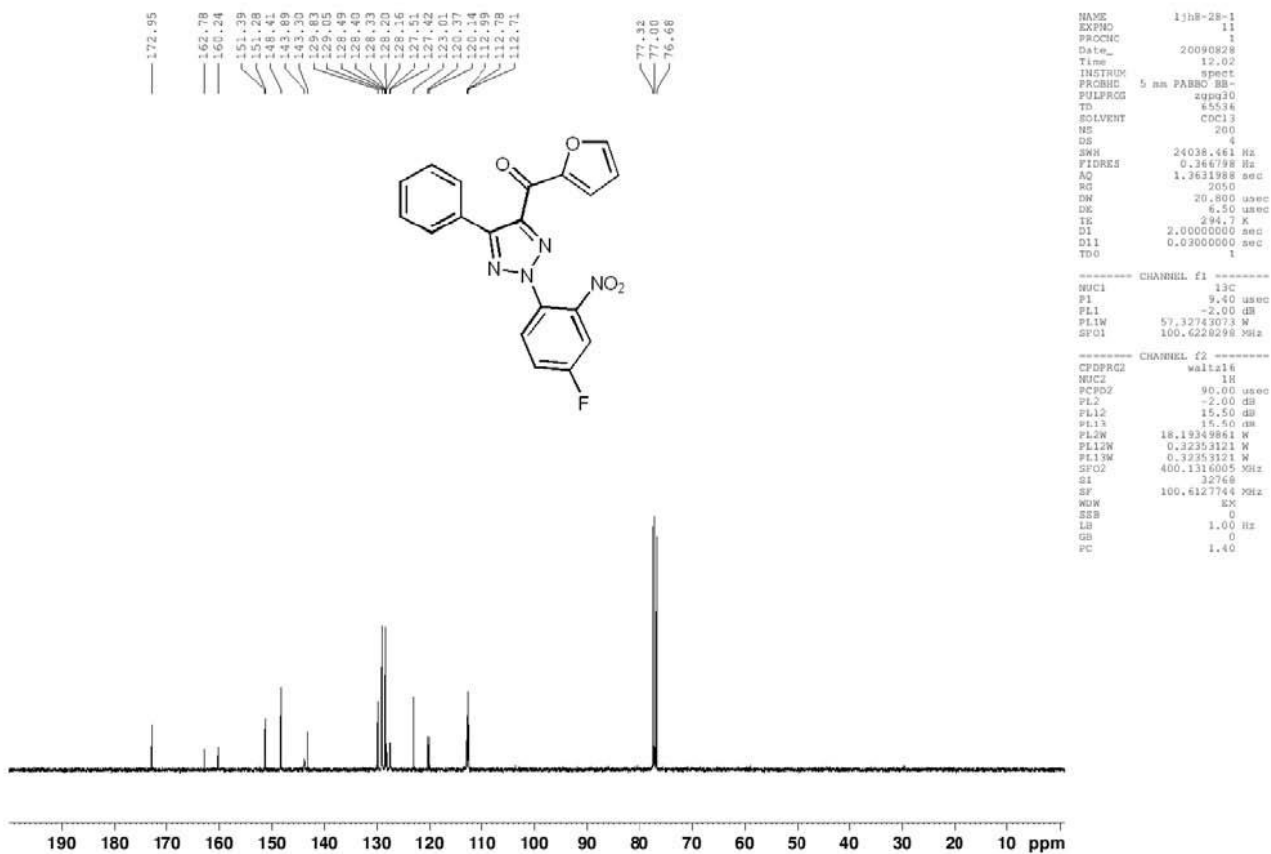
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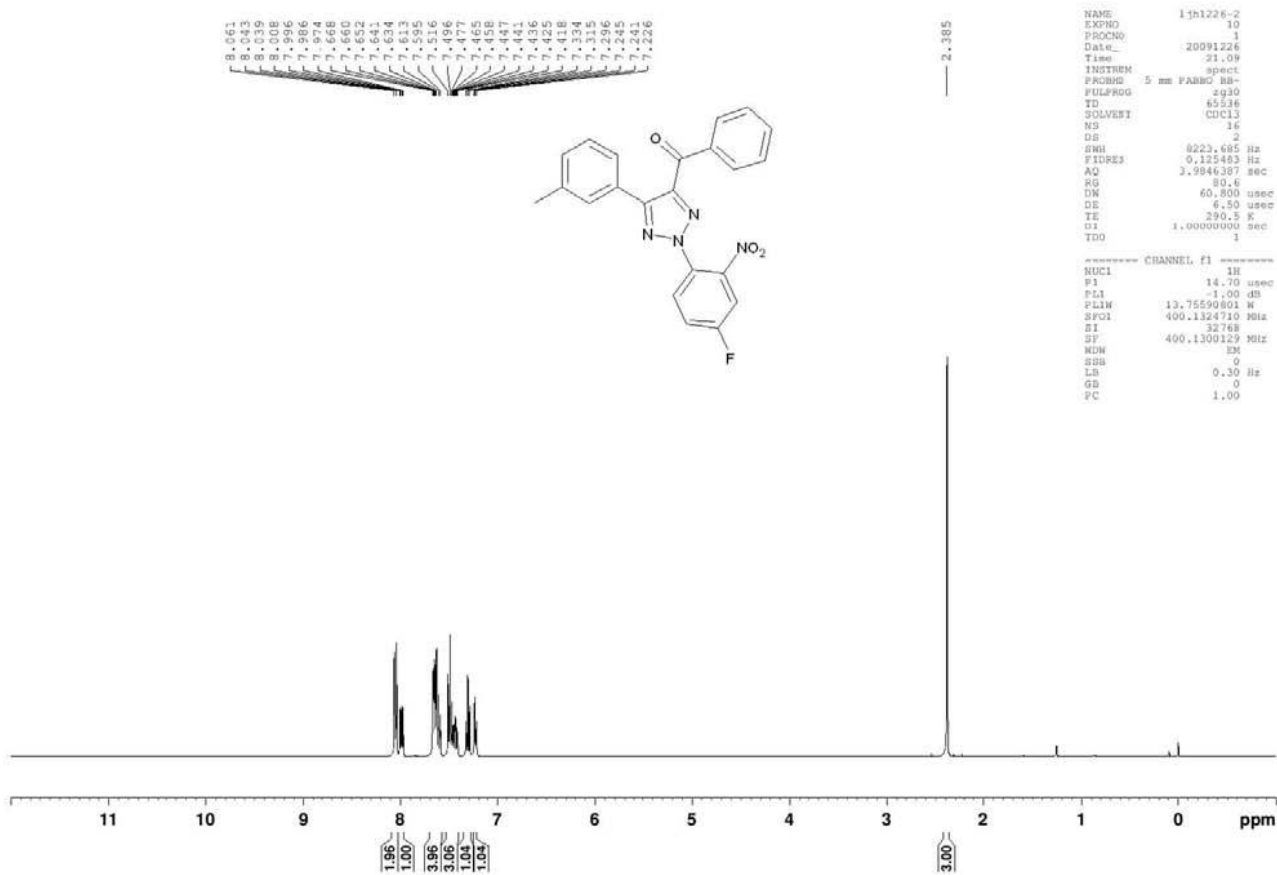


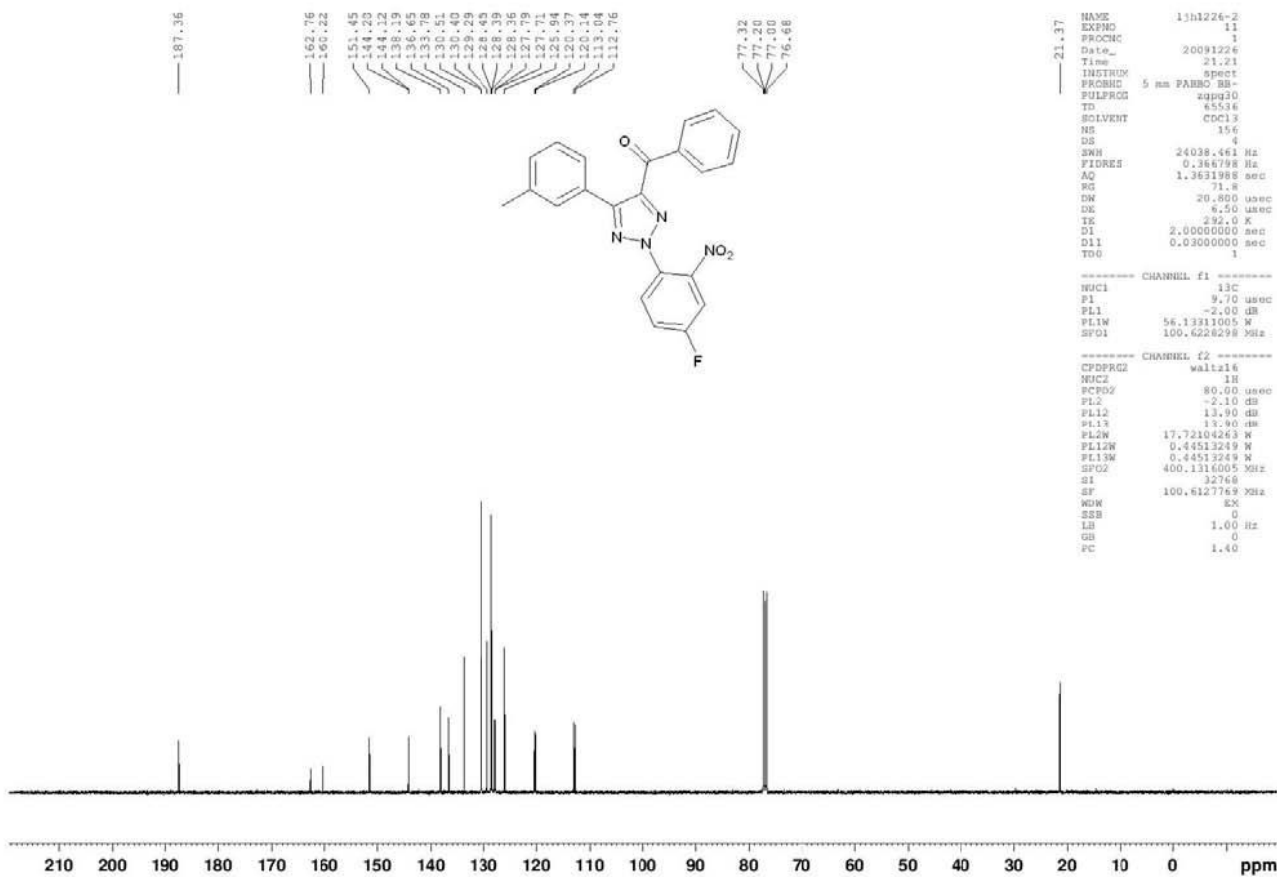
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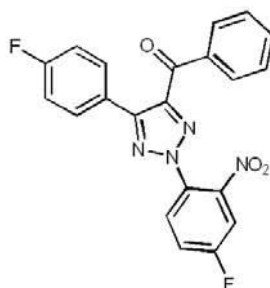




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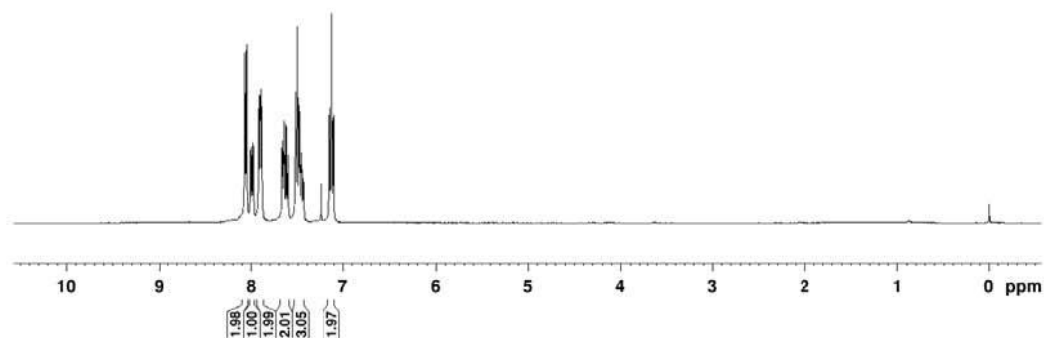


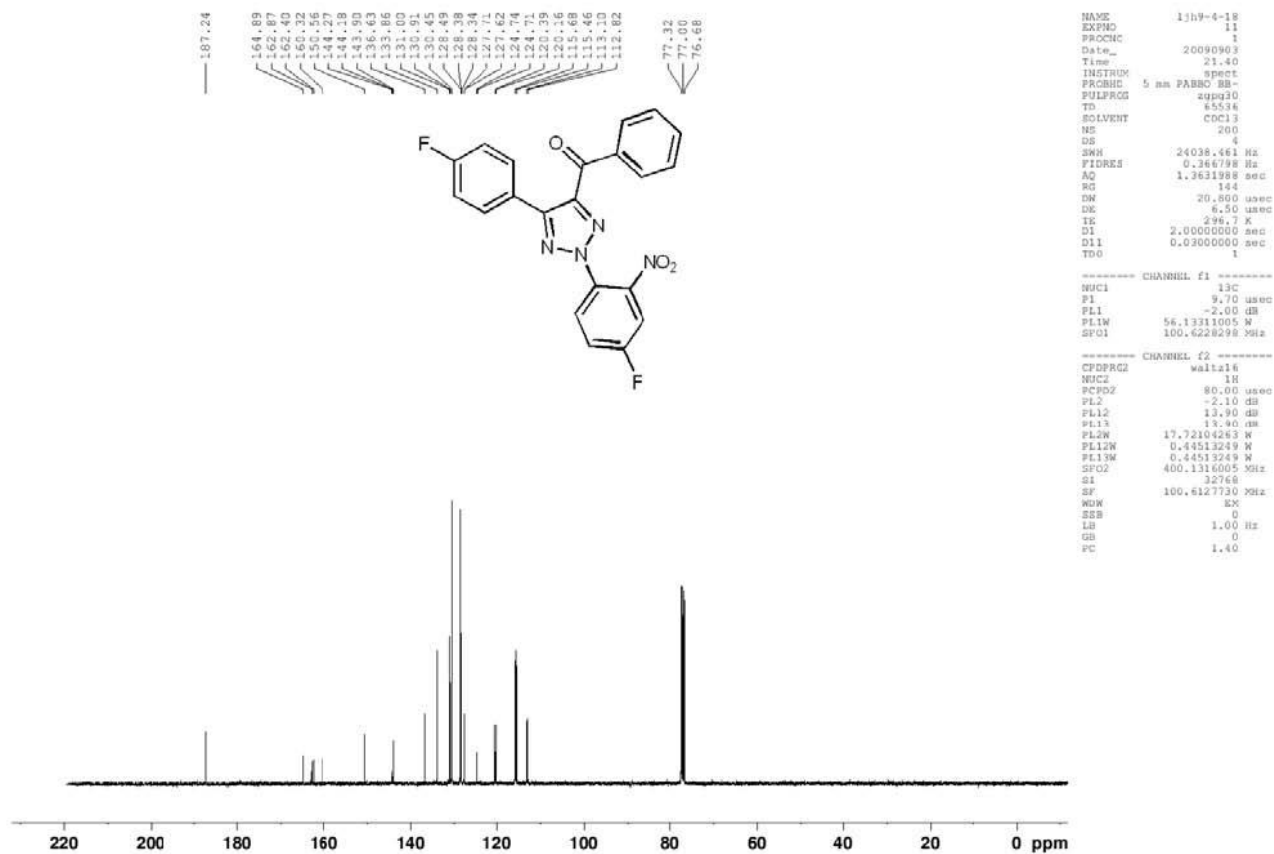
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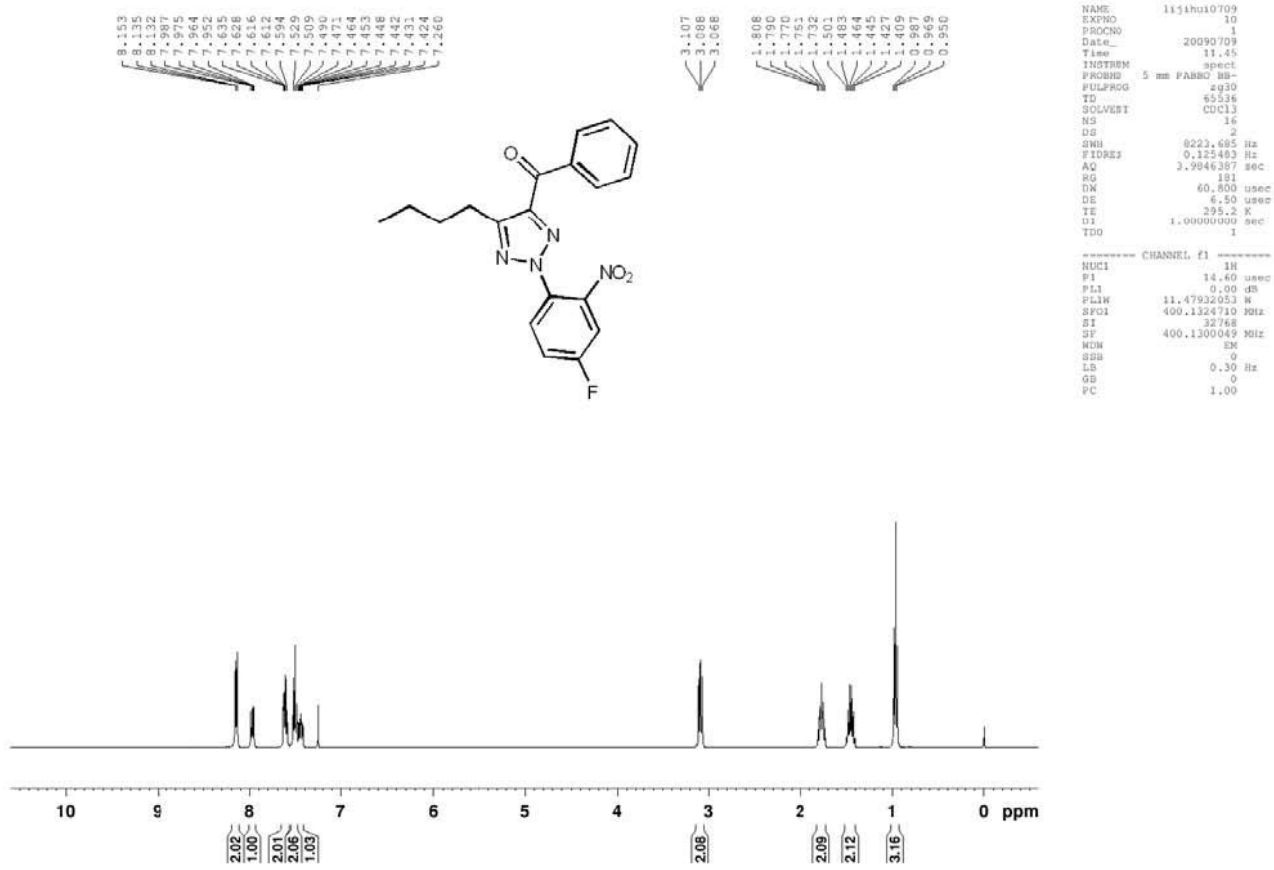
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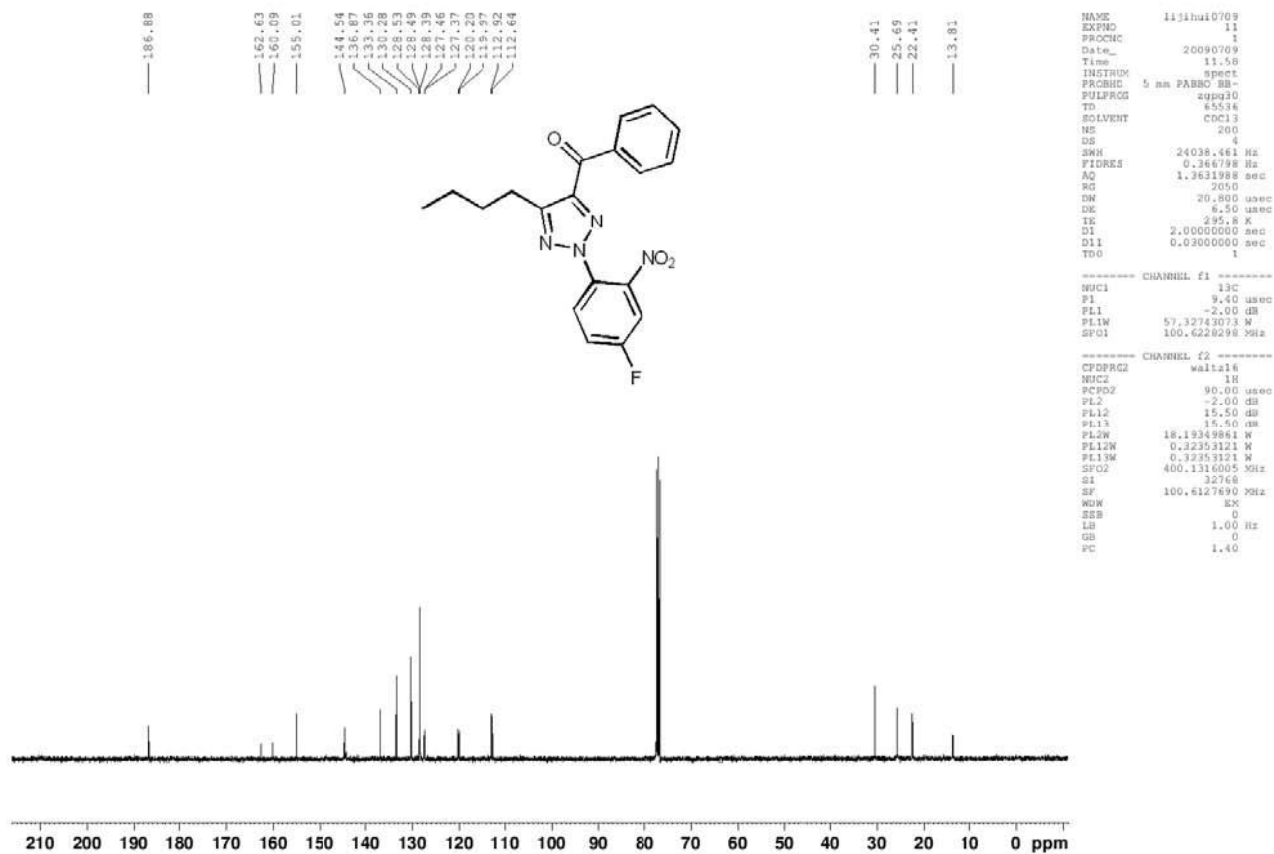
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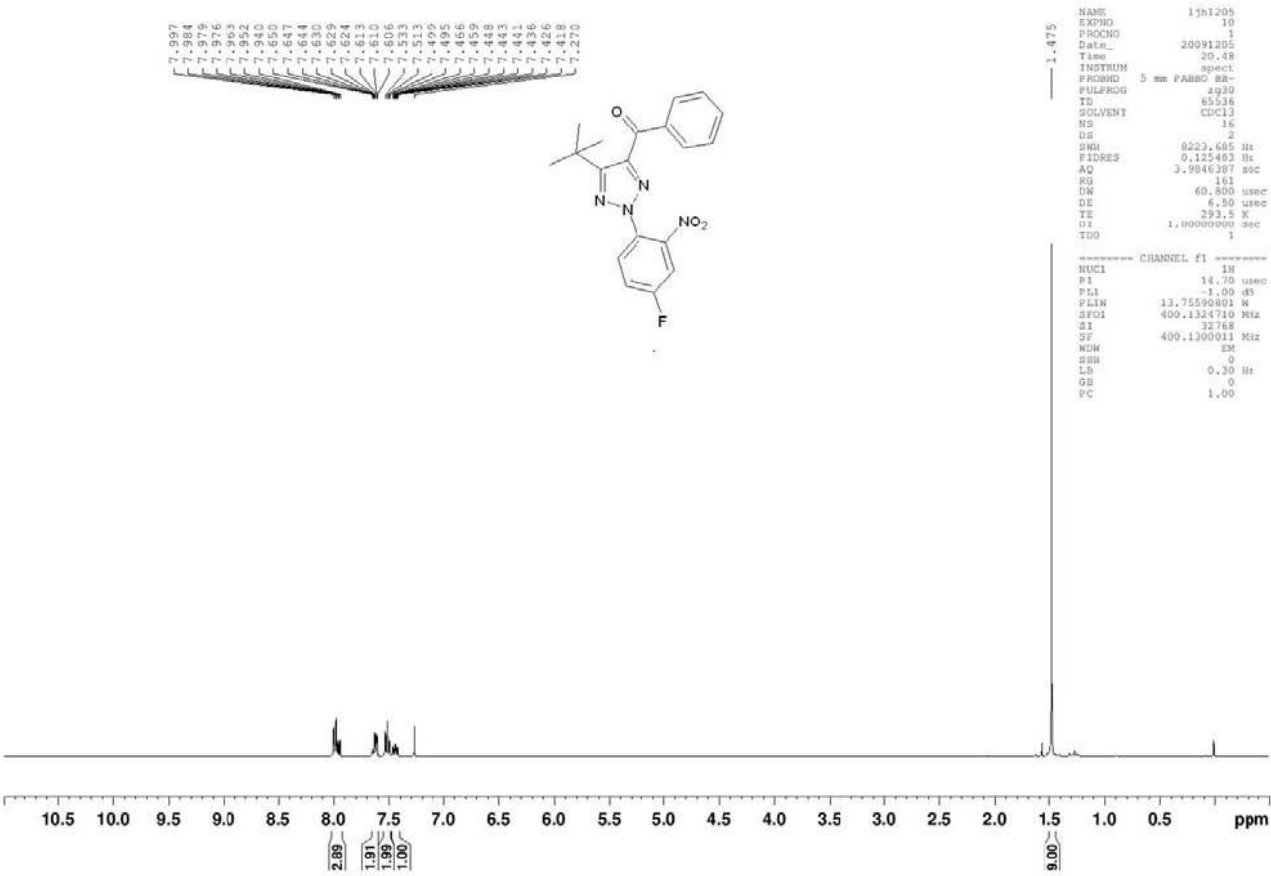


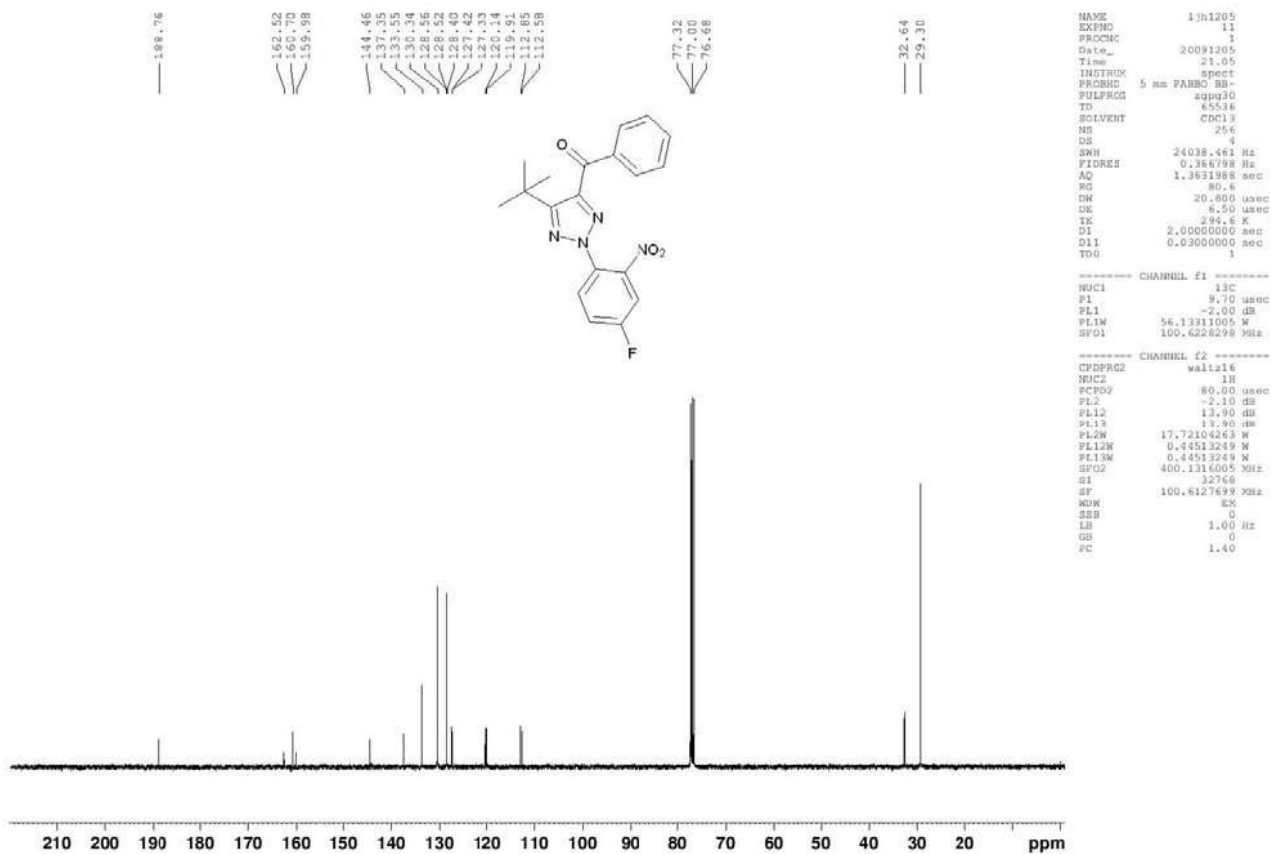
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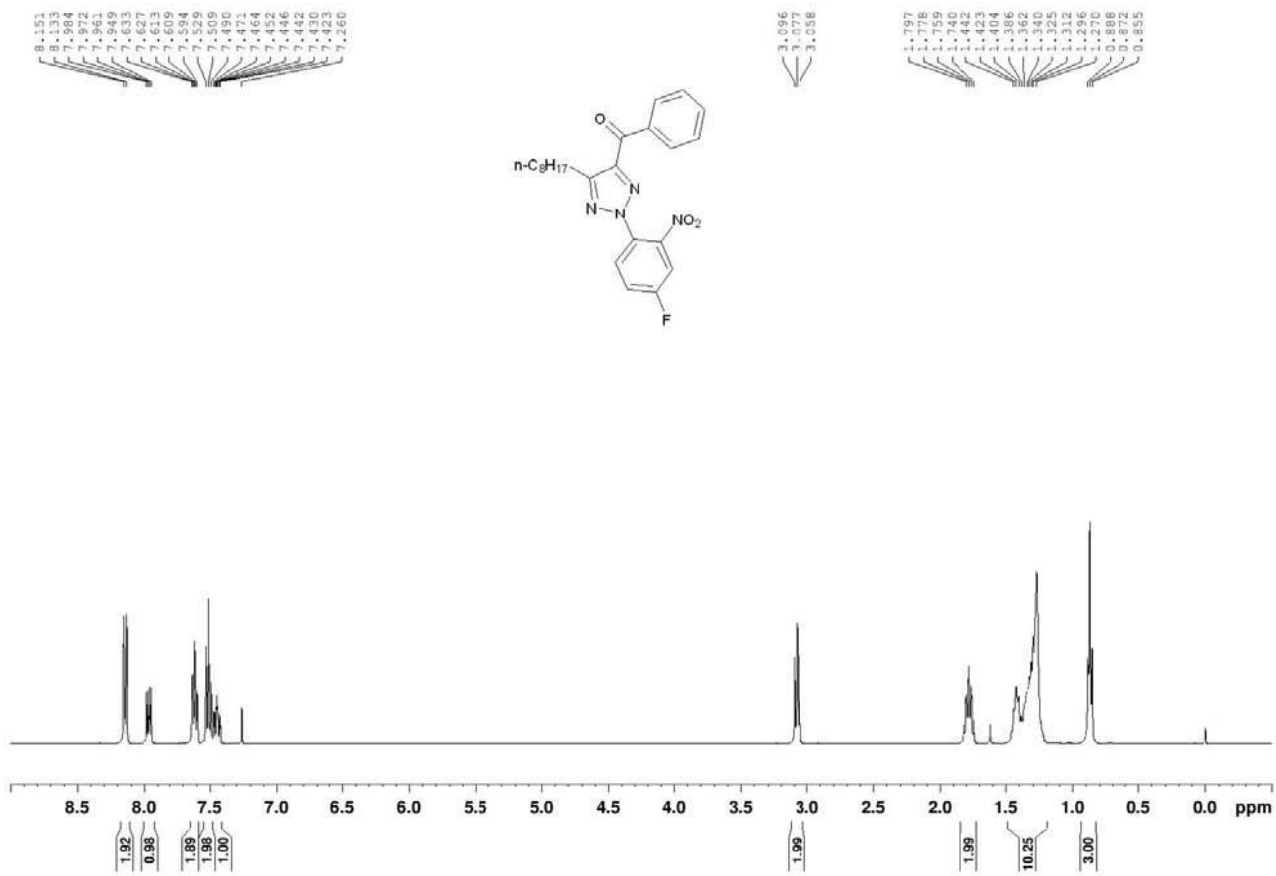


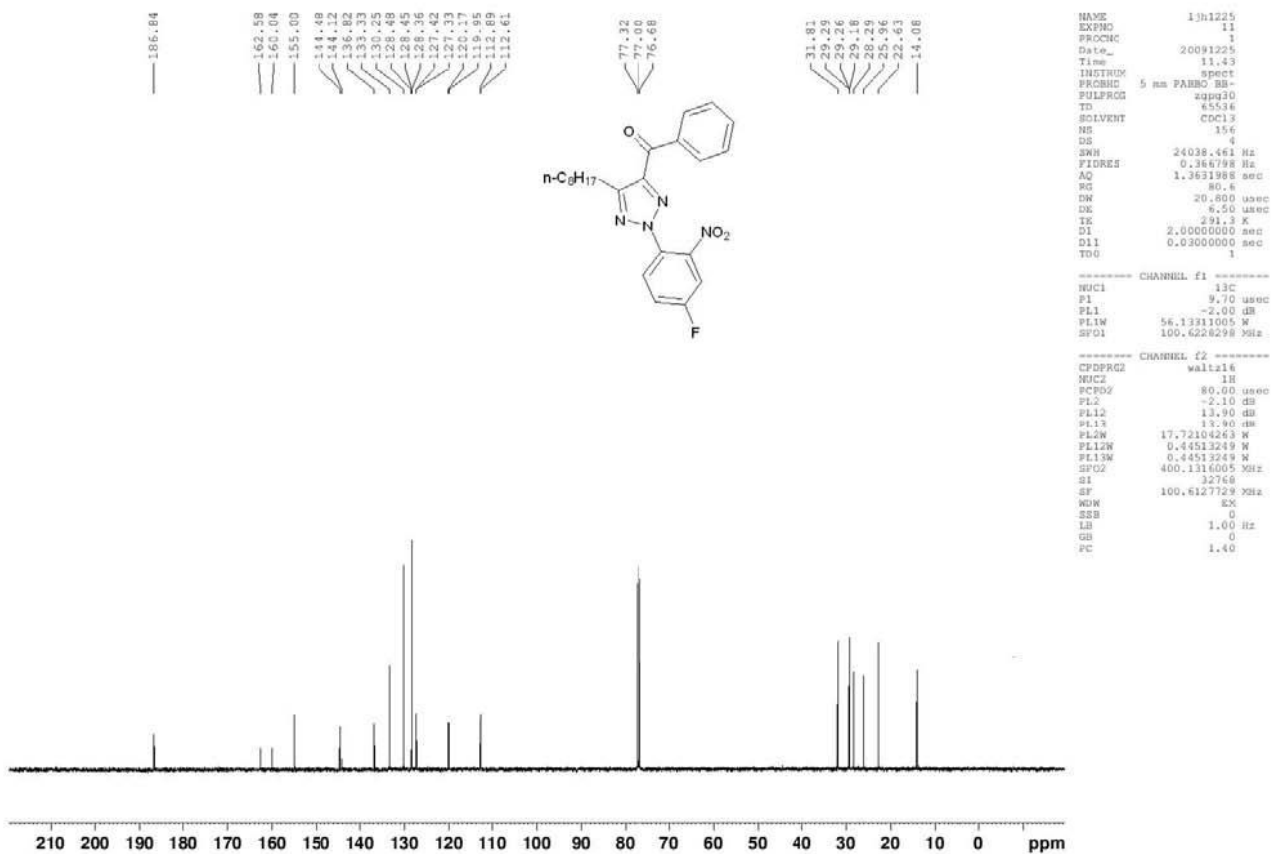
2ma:



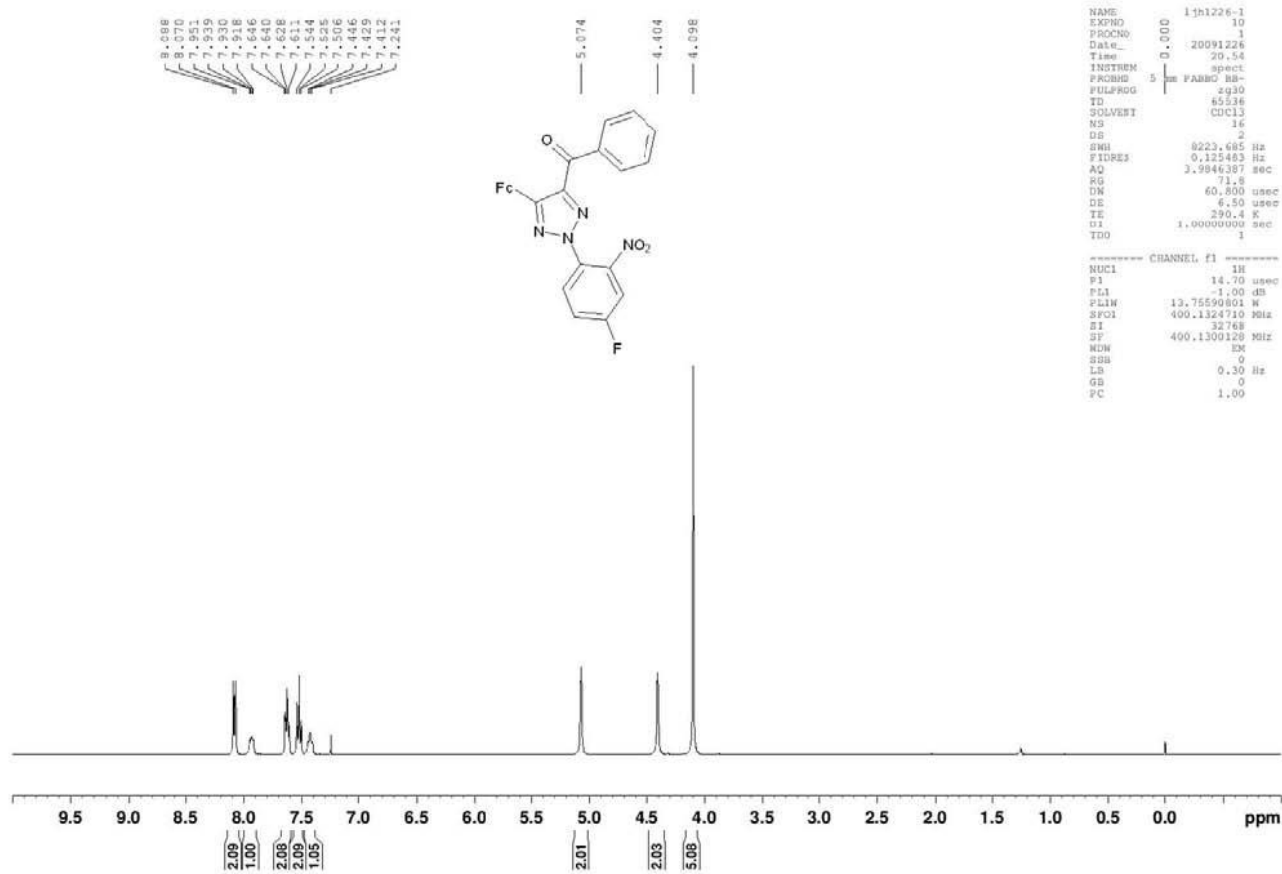


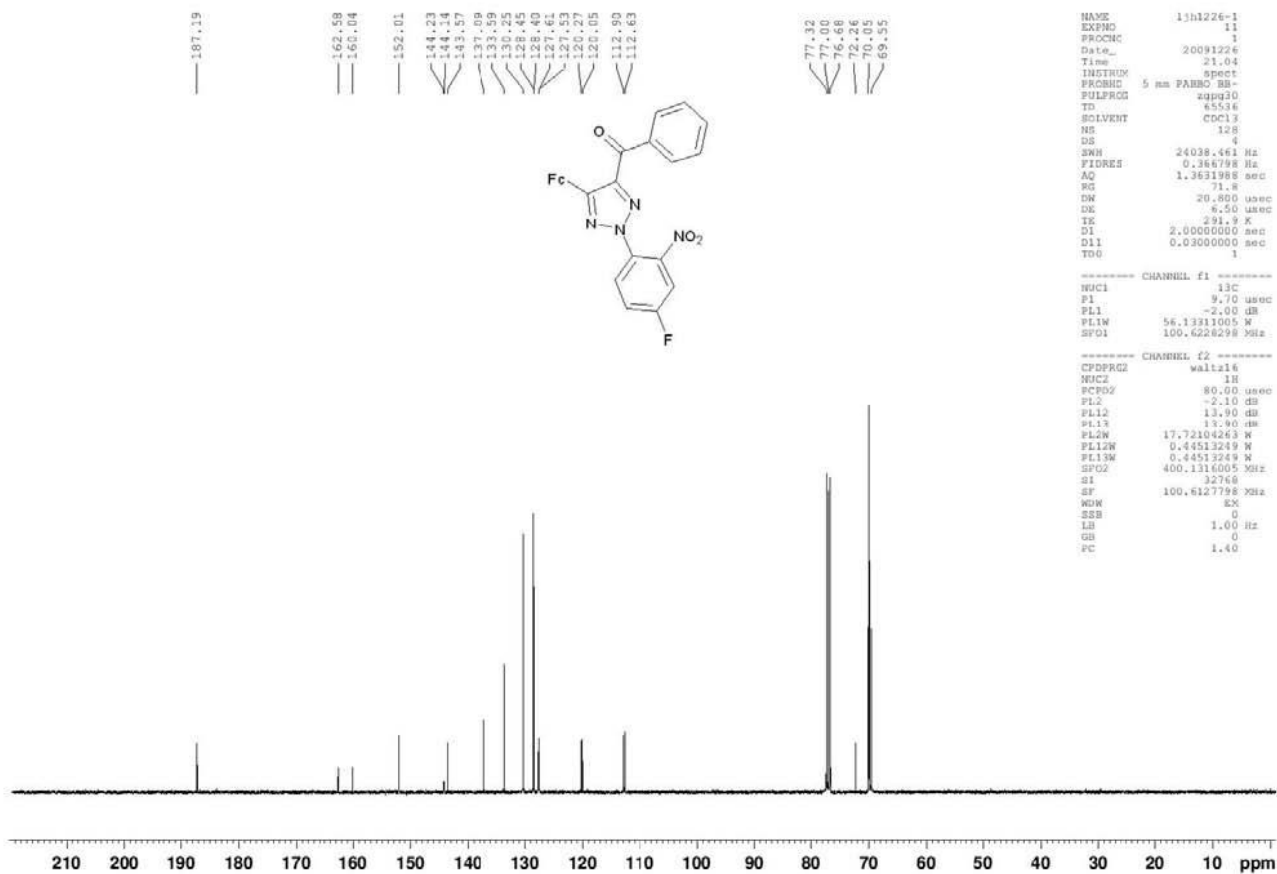
2na:

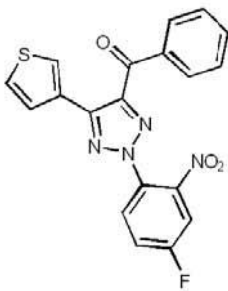




20a:







NAME	1788-29.4
EXPO	10
PROGNO	1
DATE	20090826
Time	9.24
INSTRUM	spect
PROB	5 mm FARB0 30
FILTRF	2430
TD	55356
SCALVEST	CUC13
NS	16
FILES	8222.685 Hz
DIDRES	0.125403 Hz
DM	3.9846387 sec
AC	90.144
QW	60.800 used
DE	6.50 used
Q	295.1 K
Q1	1.0000000 sec
TDO	1
CHANNEL f1	
MU1	M
PL1	14.70 used
PL1	1.00 dB
PLIN	13.75590010 MHz
PLIF	490.133110 MHz
PLF	32768
SF	406.1300091 MHz
MUW	EW
SC	0.30 Hz
LB	5 mm
FC	1.00 Hz

