Supporting Information

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A: General Information and Starting Materials

General Information. Proton nuclear magnetic resonance (^{1}H NMR) spectra and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker ACF300 spectrometer (500 MHz and 125 MHz). Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent ($CDCl_3$: δ 7.26). Chemical shifts for carbon are reported in parts per million downfield from tetramethylsilane and are referenced to the carbon resonances of the solvent ($CDCl_3$: δ 77.16). Data are represented as follows: chemical shift, integration, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz). All high resolution mass spectra were obtained on a Finnigan/MAT 95XL-T mass spectrometer. For thin layer chromatography (TLC), Merck pre-coated TLC plates (Merck 60 F254) were used, and compounds were visualized with a UV light at 254 nm. Flash chromatography separations were performed on Merck 60 (0.040-0.063 mm) mesh silica gel.

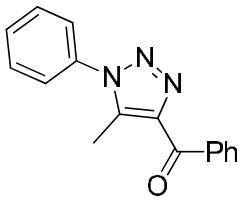
Starting Materials. All solvents and inorganic reagents were from commercial sources and used without purification unless otherwise noted. The allyl ketones and azides were prepared following the literature procedures.[1-2]

B: General Procedure for Cascade Reactions

To a solution of CH_3CN (0.2 mL) were added allyl ketones **1** (0.10 mmol), azides **2** (0.20 mmol) and catalyst **II** (0.02 mmol). The reaction mixture was stirred at 80^{o}C for 72h in the air and then the solvent was removed under vacuum to give a residue, which was purified by silica gel chromatography to yield the desired product.

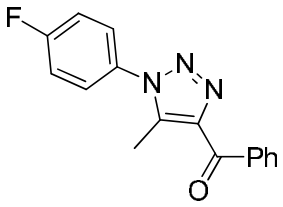
C: Characterization Data

(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3aa)



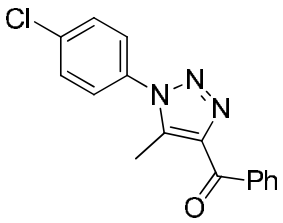
Yellow oil, 72% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.39-8.38 (m, 2H), 7.61-7.49 (m, 8H), 2.68 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.6, 143.5, 139.9, 137.4, 135.4, 132.9, 130.6, 130.1, 129.7, 128.3, 125.4, 10.6. HRMS (EI): exact mass calculated for M ($C_{16}H_{13}N_3O$) requires m/z 263.1059, found m/z 263.1057.

(1-(4-Fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ab)



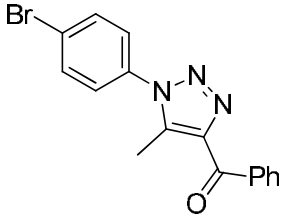
Yellow solid, 62% yield. mp = 87-88°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.38-8.36 (m, 2H), 7.62-7.60 (m, 1H), 7.54-7.48 (m, 4H), 7.31-7.27 (m, 2H), 2.66 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.5, 163.2 (d, J = 1000.0 Hz), 143.5, 140.0, 137.3, 133.0, 131.5 (d, J = 10.0 Hz), 130.6, 128.3, 127.4 (d, J = 30.0 Hz), 116.8 (d, J = 95.0 Hz), 10.6. HRMS (EI): exact mass calculated for M ($C_{16}H_{12}FN_3O$) requires m/z 281.0964, found m/z 281.0953.

(1-(4-Chlorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ac)



Yellow solid, 63% yield. mp = 93-94°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.38-8.36 (m, 2H), 7.61-7.45 (m, 7H), 2.67 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.4, 143.6, 139.9, 137.3, 136.3, 133.9, 130.6, 130.0 128.3, 126.6, 10.6. HRMS (EI): exact mass calculated for M ($C_{16}H_{12}ClN_3O$) requires m/z 297.0669, found m/z 297.0675.

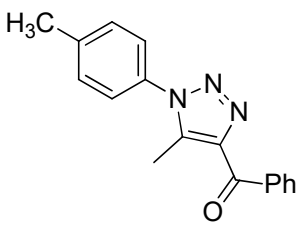
(1-(4-Bromophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ad)



Yellow solid, 67% yield. mp = 109-110°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.38-8.36 (m, 2H), 7.75-7.74 (m, 2H), 7.62-7.60 (m, 1H), 7.54-7.51 (m, 2H), 7.40-7.38 (m, 2H), 2.67 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.4, 143.6, 139.8, 137.3, 134.4, 133.0, 132.9, 130.6 128.3, 126.8, 124.3, 10.6. HRMS (EI): exact mass calculated for M ($C_{16}H_{12}BrN_3O$) requires m/z 341.0164, found m/z 341.0156.

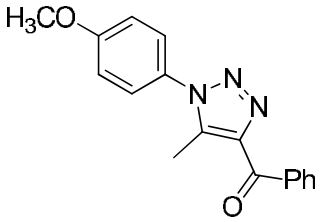
(5-Methyl-1-(*p*-tolyl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ae)

Yellow solid, 61% yield. mp = 97-98°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm)



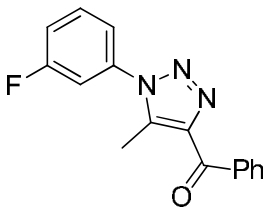
8.39-8.37 (m, 2H), 7.62-7.59 (m, 1H), 7.53-7.50 (m, 2H), 7.40 (d, *J* = 10.0 Hz, 2H), 7.07 (d, *J* = 10.0 Hz, 2H), 3.89 (s, 3H), 2.64 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.6, 143.4, 140.4, 139.9, 137.4, 132.9, 132.8, 130.6, 130.2, 128.2, 125.2, 21.3, 10.6. HRMS (EI): exact mass calculated for M ($C_{17}H_{15}N_3O$) requires m/z 277.1215, found m/z 277.1219.

(1-(4-Methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3af)



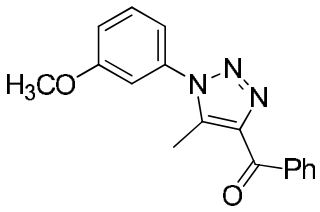
Yellow solid, 66% yield. mp = 101-102°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.39-8.37 (m, 2H), 7.62-7.59 (m, 1H), 7.53-7.50 (m, 2H), 7.40 (d, *J* = 10.0 Hz, 2H), 7.07 (d, *J* = 10.0 Hz, 2H), 3.89 (s, 3H), 2.64 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.6, 160.7, 143.3, 140.0, 137.4, 132.9, 130.6, 128.3, 128.2, 126.8, 114.8, 55.7, 10.6. HRMS (EI): exact mass calculated for M ($C_{17}H_{15}N_3O_2$) requires m/z 293.1164, found m/z 293.1162.

(1-(3-Fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ag)



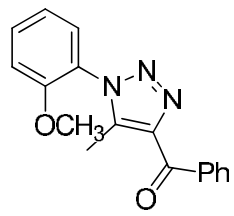
Yellow oil, 61% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.38-8.36 (m, 2H), 7.63-7.51 (m, 4H), 7.33-7.28 (m, 3H), 2.70 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.4, 162.8 (d, *J* = 1000.0 Hz), 143.6, 139.9, 137.3, 136.5, 133.0, 131.1 (d, *J* = 35.0 Hz), 130.6, 128.3, 121.0 (d, *J* = 15.0 Hz), 117.2 (d, *J* = 85.0 Hz), 113.2 (d, *J* = 100.0 Hz), 10.7. HRMS (EI): exact mass calculated for M ($C_{16}H_{12}FN_3O$) requires m/z 281.0964, found m/z 281.0958.

1-(3-Methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ah)



Yellow oil, 74% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.38-8.37 (m, 2H), 7.62-7.59 (m, 1H), 7.54-7.46 (m, 3H), 7.10-7.04 (m, 3H), 3.87 (s, 3H), 2.68 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.6, 160.4, 143.5, 139.9, 137.4, 136.4, 132.9, 130.6, 130.4, 128.3, 117.4, 115.9, 111.2, 55.7, 10.7. HRMS (EI): exact mass calculated for M ($C_{17}H_{15}N_3O_2$) requires m/z 293.1164, found m/z 293.1159.

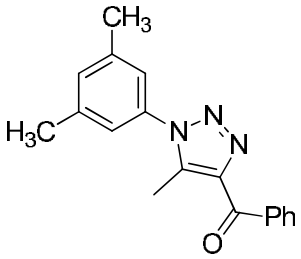
(1-(2-Methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ai)



Yellow solid, 51% yield. mp = 96-97°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.41-8.40 (m, 2H), 7.61-7.51 (m, 4H), 7.41-7.39 (m, 1H), 7.15-7.10 (m, 2H), 3.82 (s, 3H), 2.51 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.7, 154.0, 142.8, 142.1, 137.5,

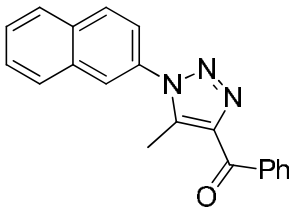
132.8, 132.0, 130.6, 128.5, 128.2, 124.1, 121.1, 112.2, 55.8, 10.1. HRMS (EI): exact mass calculated for M^+ ($C_{17}H_{15}N_3O_2$) requires m/z 293.1164, found m/z 293.1160.

(1-(3,5-Dimethylphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3aj)



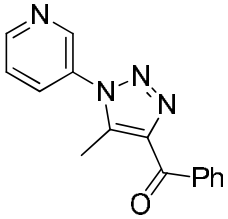
Yellow oil, 66% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.38-8.37 (m, 2H), 7.62-7.59 (m, 1H), 7.54-7.51 (m, 2H), 7.18 (s, 1H), 7.09 (s, 2H), 2.65 (s, 3H), 2.42 (s, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.6, 143.3, 139.9, 139.7, 137.4, 135.2, 132.9, 131.7, 130.6, 128.3, 123.1, 21.2, 10.6. HRMS (EI): exact mass calculated for M ($C_{18}H_{17}N_3O$) requires m/z 291.1372, found m/z 291.1370.

(5-Methyl-1-(naphthalen-2-ylmethyl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ak)



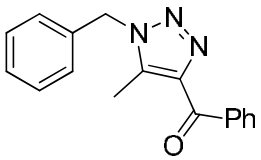
Yellow oil, 54% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.49-8.47 (m, 2H), 8.11-8.10 (m, 1H), 8.01-7.99 (m, 1H), 7.67-7.53 (m, 7H), 7.22-7.20 (m, 1H), 2.49 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.6, 143.1 142.0, 137.4, 134.2, 133.0, 131.5, 131.2, 130.7, 129.4, 128.5, 128.3, 128.2, 127.3, 125.3, 125.1, 121.9, 10.2. HRMS (EI): exact mass calculated for M ($C_{20}H_{15}N_3O$) requires m/z 313.1215, found m/z 313.1210.

(5-Methyl-1-(pyridin-3-yl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3al)



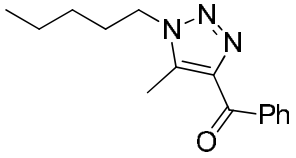
Yellow solid, 64% yield. mp = 89-90°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.83-8.82 (m, 2H), 8.37-8.36 (m, 2H), 7.91-7.89 (m, 1H), 7.63-7.51 (m, 4H), 2.71 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.3, 151.2, 146.0, 143.8, 140.1, 137.2, 133.1, 132.8, 132.3, 130.6, 128.3, 124.2, 10.5. HRMS (EI): exact mass calculated for M ($C_{15}H_{12}N_4O$) requires m/z 264.1011, found m/z 264.1008.

(1-Benzyl-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3am)



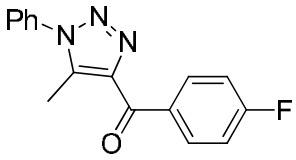
Yellow oil, 64% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.34-8.33 (m, 2H), 7.60-7.57 (m, 1H), 7.51-7.48 (m, 2H), 7.38-7.33 (m, 3H), 7.22-7.21 (m, 2H), 5.57 (s, 2H), 2.55 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.6, 143.8, 139.3, 137.4, 134.0, 132.8, 130.6, 129.1, 128.6, 128.2, 127.3, 51.8, 9.6. HRMS (EI): exact mass calculated for M ($C_{17}H_{15}N_3O$) requires m/z 277.1215, found m/z 277.1210.

(5-Methyl-1-pentyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3an)



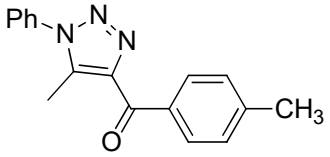
Yellow oil, 61% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.33-8.32 (m, 2H), 7.59-7.56 (m, 1H), 7.50-7.47 (m, 2H), 4.32 (t, *J* = 10.0 Hz, 2H), 2.65 (s, 3H), 1.94-1.88 (m, 2H), 1.40-1.33 (m, 4H), 0.91 (t, *J* = 10.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.7, 143.4, 138.8, 137.5, 132.7, 130.6, 128.2, 47.8, 29.4, 28.6, 22.1, 13.8, 9.5. HRMS (EI): exact mass calculated for M ($C_{15}H_{19}N_3O$) requires m/z 257.1528, found m/z 257.1524.

(4-Fluorophenyl)(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)methanone (3ba)



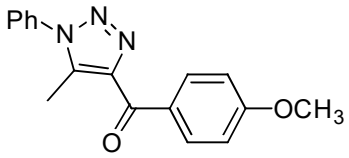
Yellow solid, 71% yield. mp = 88-89°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.50-8.47 (m, 2H), 7.61-7.58 (m, 3H), 7.50-7.49 (m, 2H), 7.21-7.18 (m, 2H), 2.67 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 185.8, 165.7 (d, *J* = 1000.0 Hz), 143.4, 140.1, 135.4, 133.7 (d, *J* = 10.0 Hz), 133.4 (d, *J* = 35.0 Hz), 130.1, 129.7, 125.4, 115.4 (d, *J* = 85.0 Hz), 10.7. HRMS (EI): exact mass calculated for M ($C_{16}H_{12}FN_3O$) requires m/z 281.0964, found m/z 281.0957.

(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(p-tolyl)methanone (3ca)



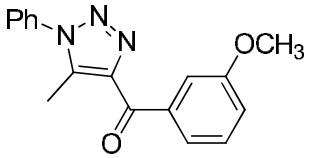
Yellow solid, 63% yield. mp = 99-100°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.32-8.30 (m, 2H), 7.59-7.56 (m, 3H), 7.50-7.49 (m, 2H), 7.33-7.32 (m, 2H), 2.66 (s, 3H), 2.44 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.2, 143.8, 143.7, 139.7, 135.5, 134.8, 130.8, 130.0, 129.7, 129.0, 125.4, 21.7, 10.6. HRMS (EI): exact mass calculated for M ($C_{17}H_{15}N_3O$) requires m/z 277.1215, found m/z 277.1214.

(4-Methoxyphenyl)(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)methanone (3da)



Yellow solid, 57% yield. mp = 102-103°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.47-8.45 (m, 2H), 7.60-7.56 (m, 3H), 7.49 (d, *J* = 10.0 Hz, 2H), 7.01 (d, *J* = 10.0 Hz, 2H), 3.90 (s, 3H), 2.65 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 185.9, 163.5, 143.8, 139.6, 135.5, 133.1, 130.3, 130.0, 129.7, 125.4, 113.6, 55.5, 10.6. HRMS (EI): exact mass calculated for M ($C_{17}H_{15}N_3O_2$) requires m/z 293.1164, found m/z 293.1155.

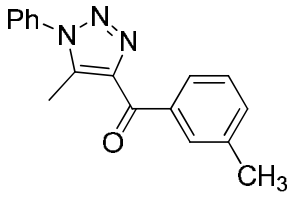
(3-Methoxyphenyl)(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)methanone (3ea)



Yellow oil, 63% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.05-8.04 (m, 1H), 7.89 (s, 1H), 7.60-7.57 (m, 3H), 7.50-7.49 (m, 2H), 7.45-7.42 (m, 1H), 7.17-7.15 (m, 1H), 3.89 (s, 3H), 2.67 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ

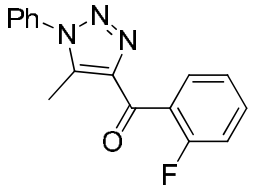
(ppm) 187.3, 159.5, 143.5, 140.0, 138.6, 135.4, 130.1, 129.7, 129.3, 125.4, 123.6, 119.8, 114.5, 55.5, 10.7. HRMS (EI): exact mass calculated for M ($C_{17}H_{15}N_3O_2$) requires m/z 293.1164, found m/z 293.1158.

(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(*m*-tolyl)methanone (3fa)



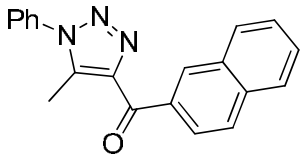
Yellow solid, 65% yield. mp = 104-105°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.19-8.15 (m, 2H), 7.60-7.57 (m, 3H), 7.51-7.49 (m, 2H), 7.42-7.41 (m, 2H), 2.67 (s, 3H), 2.46 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.9, 143.6, 139.8, 138.0, 137.4, 135.4, 133.7, 131.0, 130.1, 129.7, 128.2, 127.9, 125.4, 21.5, 10.6. HRMS (EI): exact mass calculated for M ($C_{17}H_{15}N_3O$) requires m/z 277.1215, found m/z 277.1203.

(2-Fluorophenyl)(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)methanone (3ga)



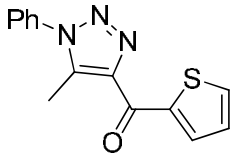
Yellow solid, 45% yield. mp = 92-93°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 7.83-7.80 (m, 1H), 7.61-7.49 (m, 6H), 7.30-7.27 (m, 1H), 7.21-7.18 (m, 1H), 2.69 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 186.7, 160.6 (d, *J* = 1000.0 Hz), 143.6, 139.3, 135.3, 133.4 (d, *J* = 35.0 Hz), 131.1 (d, *J* = 10.0 Hz), 130.1, 129.7, 127.1 (d, *J* = 50.0 Hz), 125.3, 123.9 (d, *J* = 15.0 Hz), 116.4 (d, *J* = 85.0 Hz), 10.4. HRMS (EI): exact mass calculated for M ($C_{16}H_{12}FN_3O$) requires m/z 281.0964, found m/z 281.0959.

(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(naphthalen-2-yl)methanone (3ha)



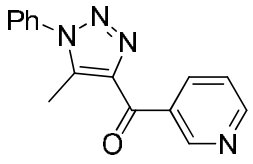
Yellow solid, 54% yield. mp =109-110°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 9.16 (s, 1H), 8.35-8.33 (m, 1H), 8.06-8.04 (m, 1H), 7.97-7.95 (m, 1H), 7.91-7.89 (m, 1H), 7.62-7.52 (m, 7H), 2.71 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 187.3, 143.7 140.0, 135.6, 135.5, 134.6, 133.4, 132.5, 130.1, 130.0, 129.7, 128.4, 128.1, 127.7, 126.5, 125.7, 125.4, 10.7. HRMS (EI): exact mass calculated for M ($C_{20}H_{15}N_3O$) requires m/z 313.1215, found m/z 313.1212.

(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(thiophen-2-yl)methanone (3ia)



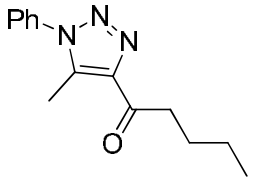
Yellow oil, 61% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 8.72-8.71 (m, 1H), 7.74-7.73 (m, 1H), 7.60-7.57 (m, 3H), 7.50-7.48 (m, 2H), 7.24-7.22 (m, 1H), 2.67 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 178.8, 143.1, 142.8, 139.5, 136.0, 135.4, 134.7, 130.1, 129.7, 128.3, 125.4, 10.5. HRMS (EI): exact mass calculated for M ($C_{14}H_{11}N_3OS$) requires m/z 269.0623, found m/z 269.0622.

(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(pyridin-3-yl)methanone (3ja)



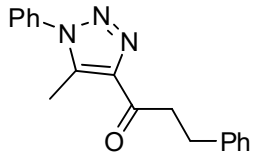
Yellow solid, 50% yield. mp = 91-92°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 9.54 (s, 1H), 8.82-8.81 (m, 1H), 8.74-8.72 (m, 1H), 7.61-7.59 (m, 3H), 7.51-7.46 (m, 3H), 2.70 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 186.0, 153.0, 151.6, 143.1, 140.3, 138.1, 135.2, 133.0, 130.2, 129.8, 125.4, 123.2, 10.6. HRMS (EI): exact mass calculated for M ($C_{15}H_{12}N_4O$) requires m/z 264.1011, found m/z 264.1007.

1-(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)pentan-1-one (3ka)



Yellow oil, 66% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 7.57-7.55 (m, 3H), 7.45-7.43 (m, 2H), 3.20 (t, *J* = 10.0 Hz, 2H), 2.58 (s, 3H), 1.78-1.72 (m, 2H), 1.46-1.42 (m, 2H), 0.96 (t, *J* = 10.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 197.1, 143.4, 137.4, 135.4, 130.0, 129.7, 125.3, 39.7, 26.2, 22.5, 13.9, 10.2. HRMS (EI): exact mass calculated for M ($C_{14}H_{17}N_3O$) requires m/z 243.1372, found m/z 243.1377.

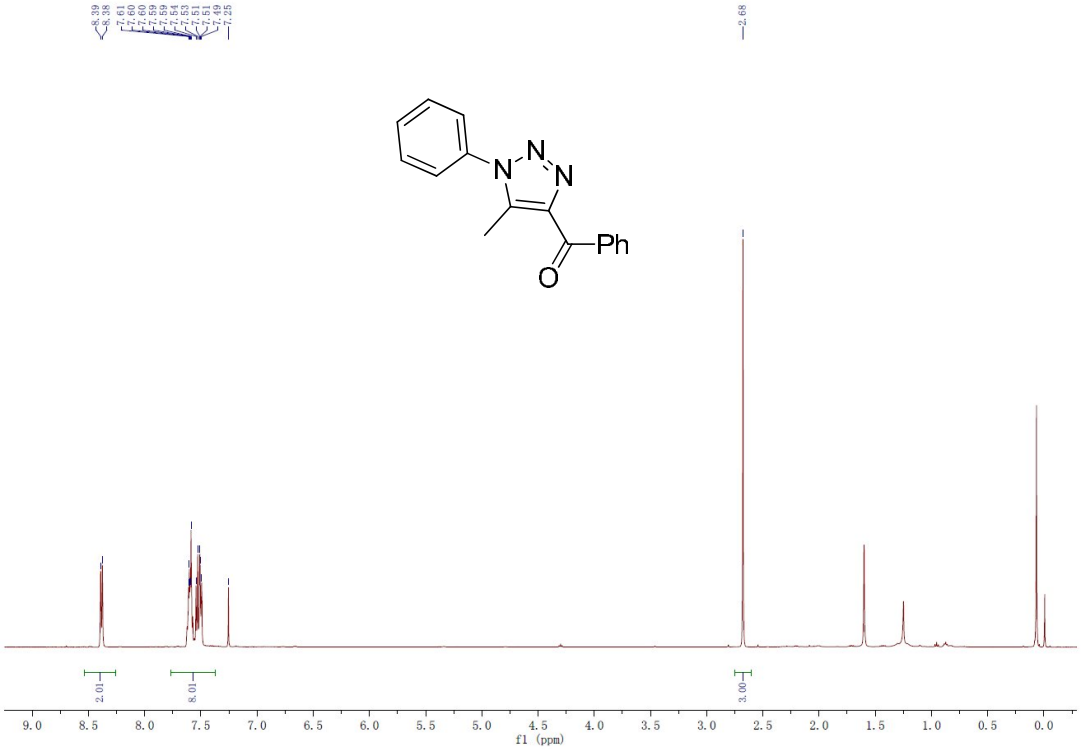
1-(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)-3-phenylpropan-1-one (3la)

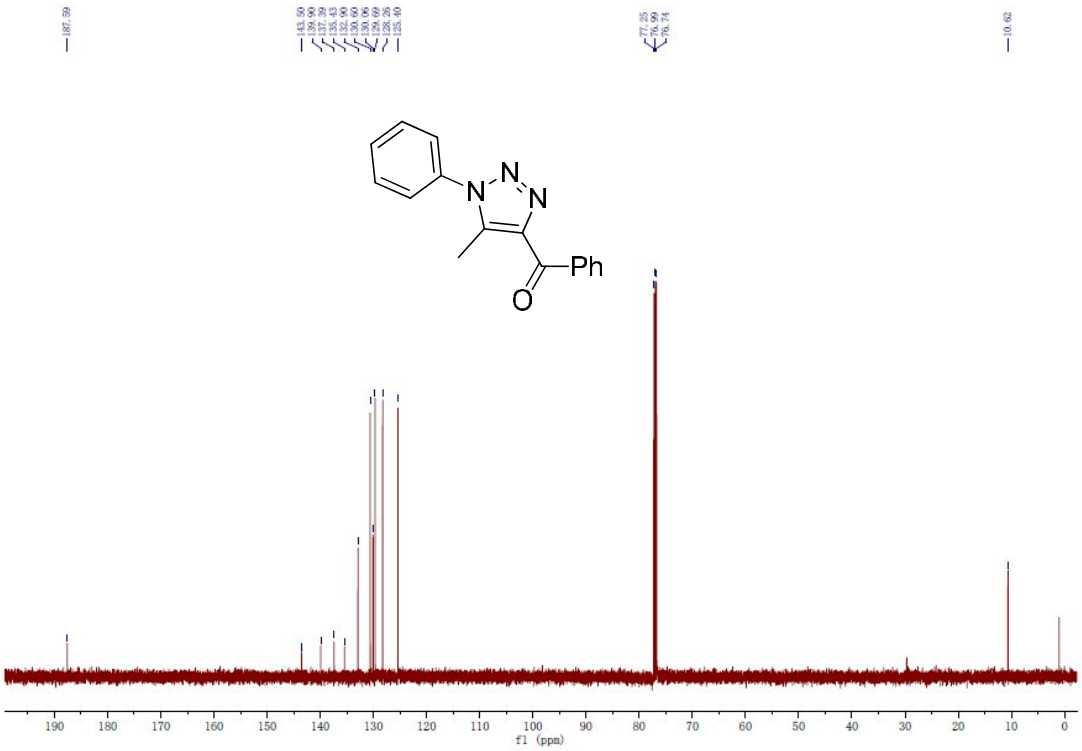


Yellow oil, 73% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) 7.58-7.57 (m, 3H), 7.45-7.44 (m, 2H), 7.30-7.26 (m, 4H), 7.21-7.20 (m, 1H), 3.57 (t, *J* = 10.0 Hz, 2H), 3.12 (t, *J* = 10.0 Hz, 2H), 2.59 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) 195.7, 143.3, 141.2, 137.5, 135.3, 130.1, 129.7, 128.5, 128.4, 126.0, 125.3, 41.3, 29.8, 10.2. HRMS (EI): exact mass calculated for M ($C_{18}H_{17}N_3O$) requires m/z 291.1372, found m/z 291.1368.

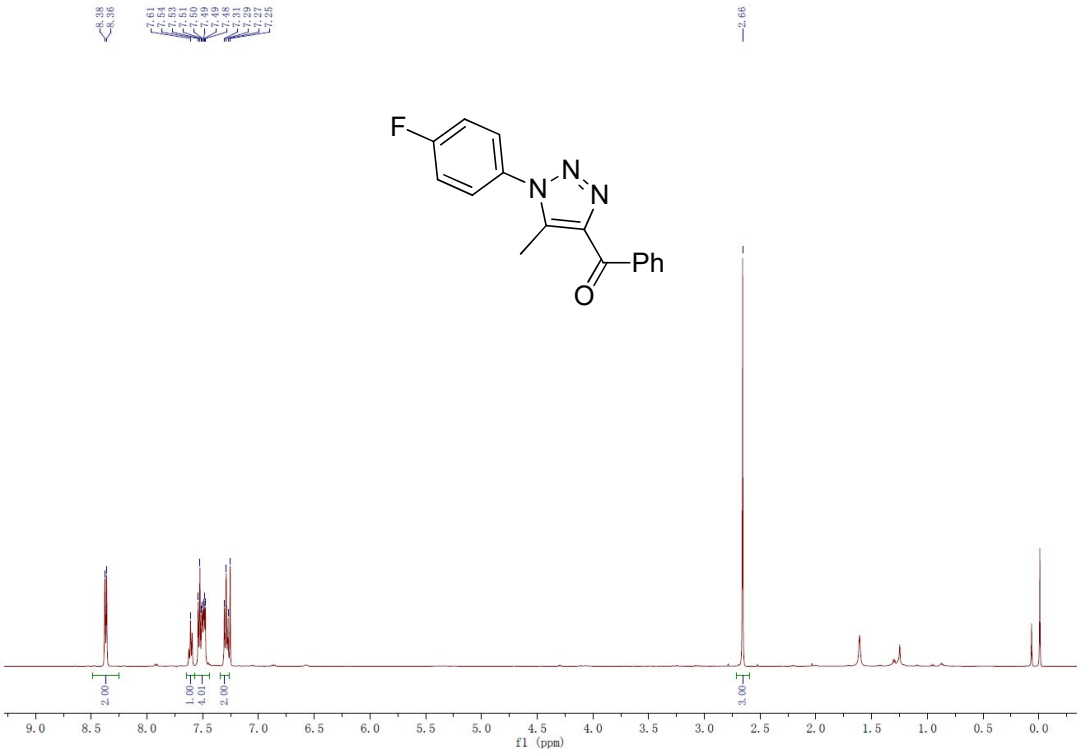
D: NMR Analysis

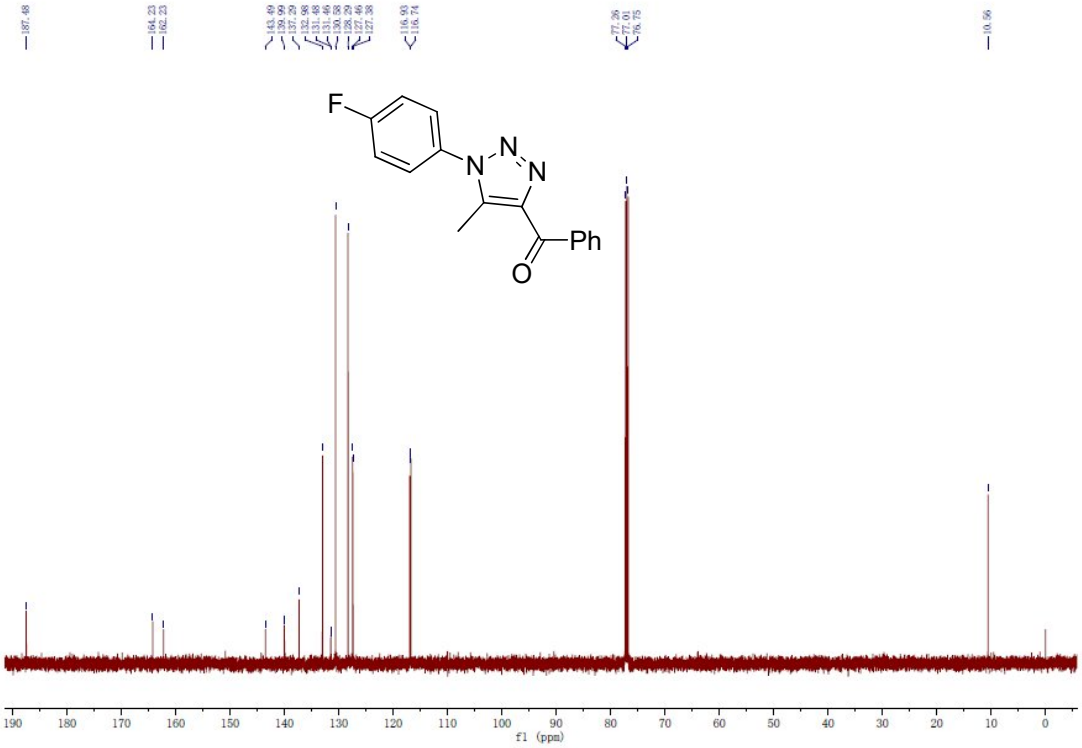
(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3aa)



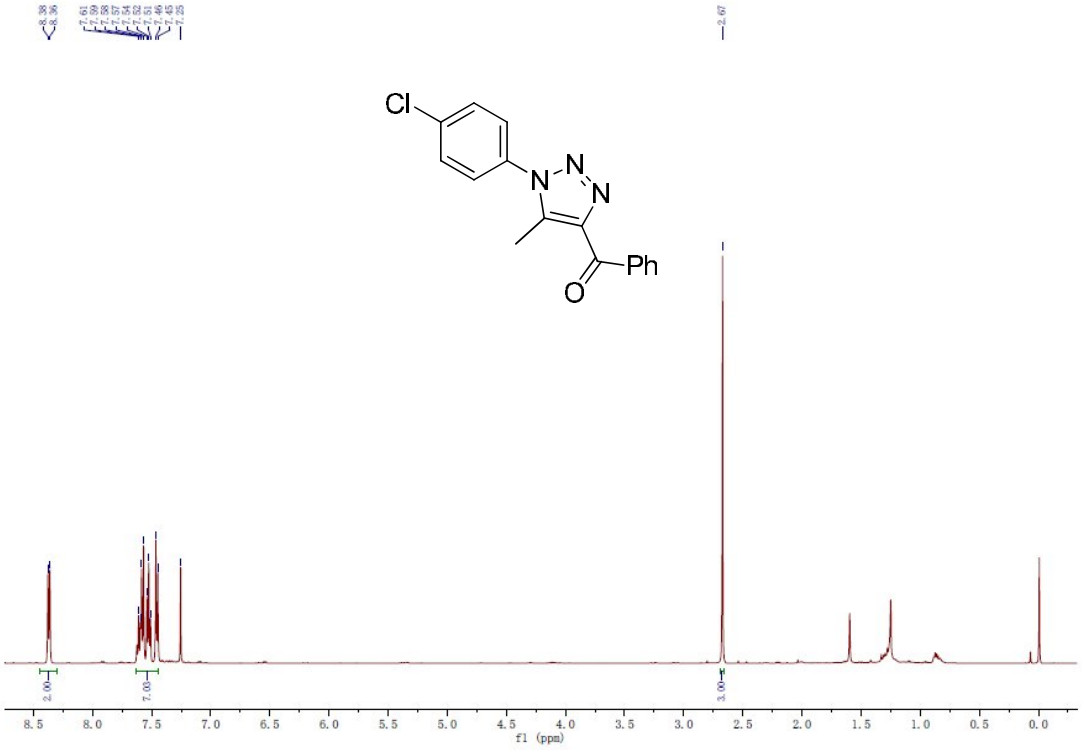


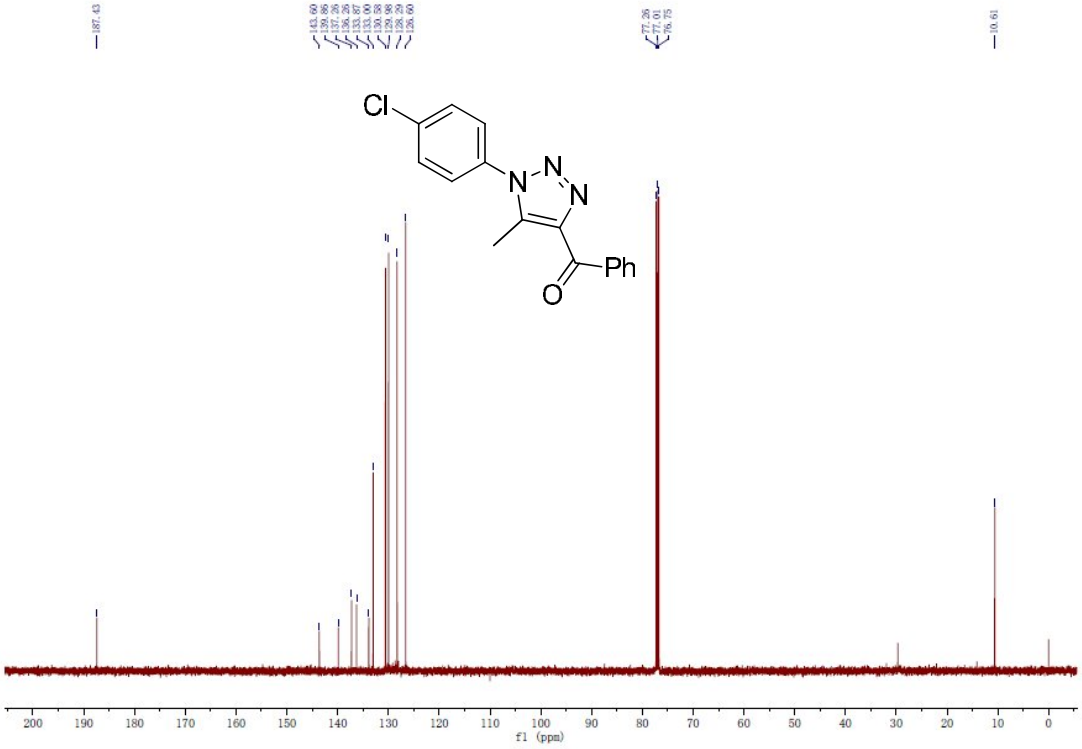
(1-(4-Fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ab)



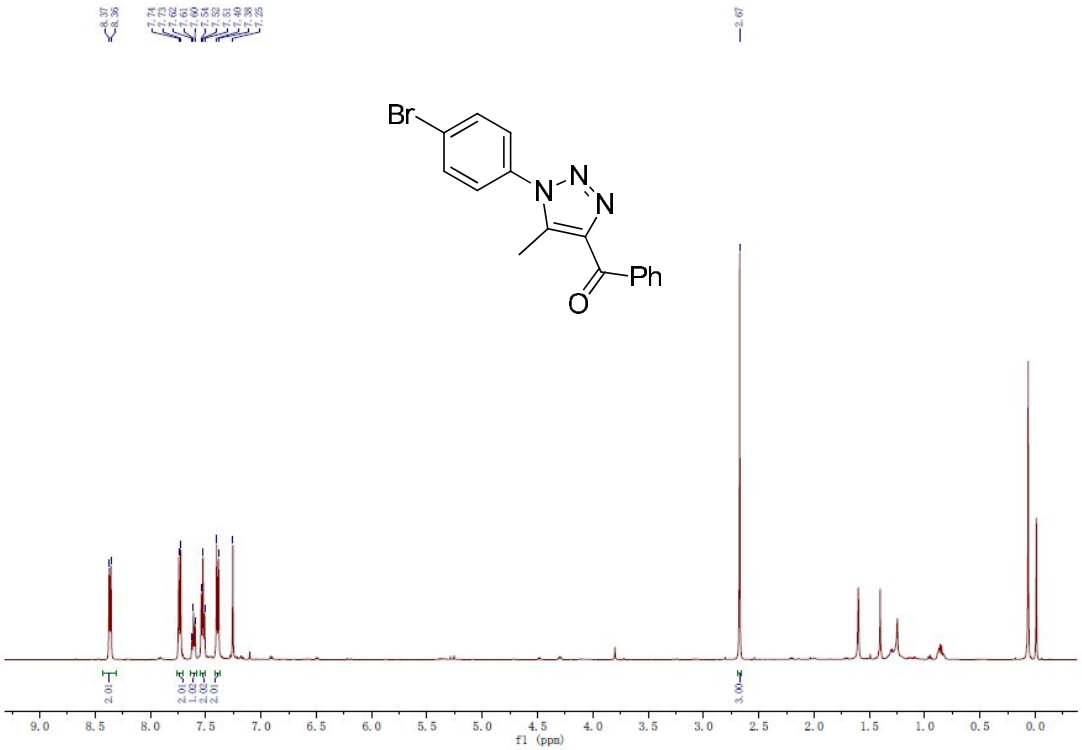


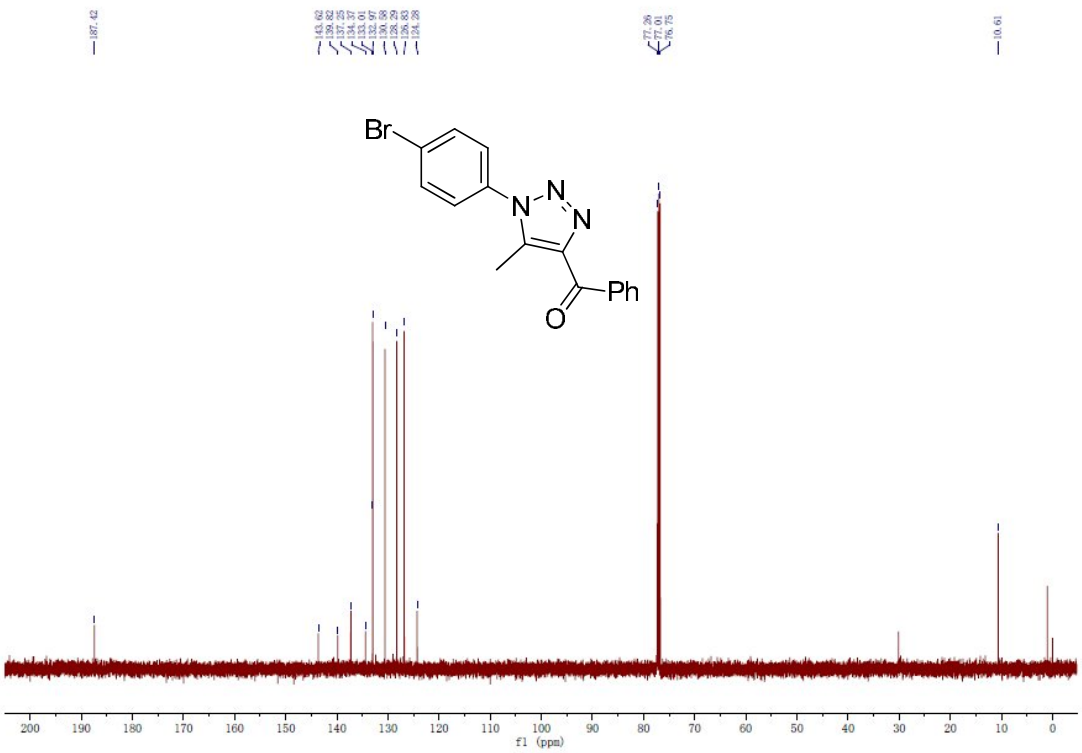
(1-(4-Chlorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ac)



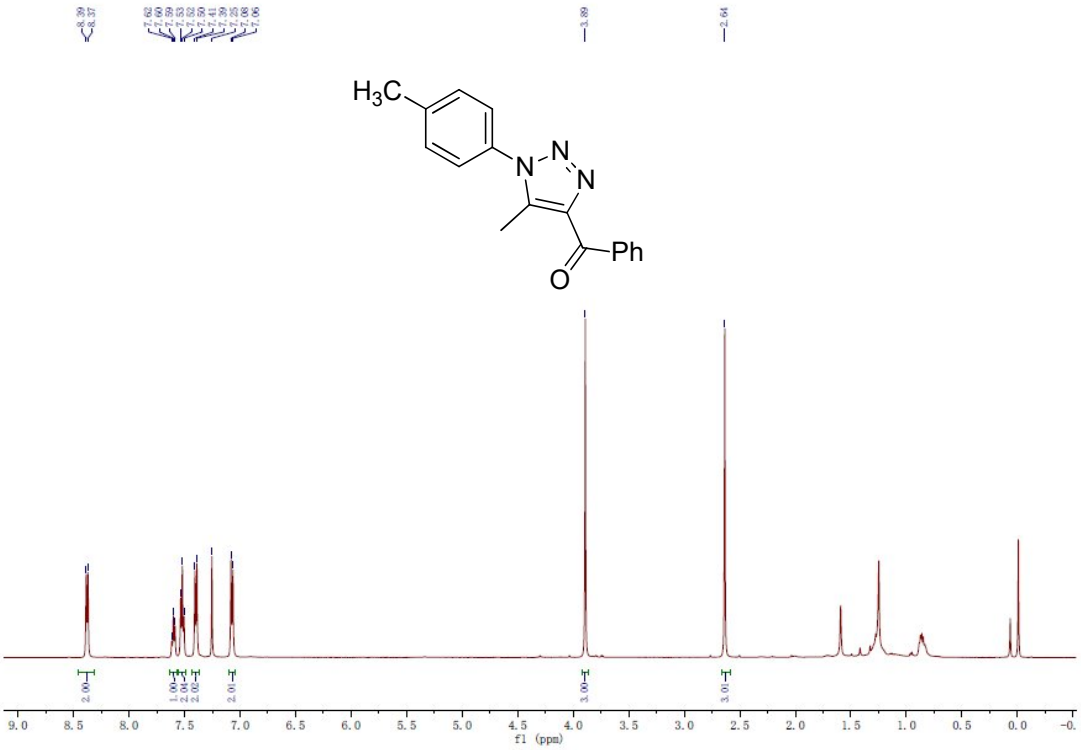


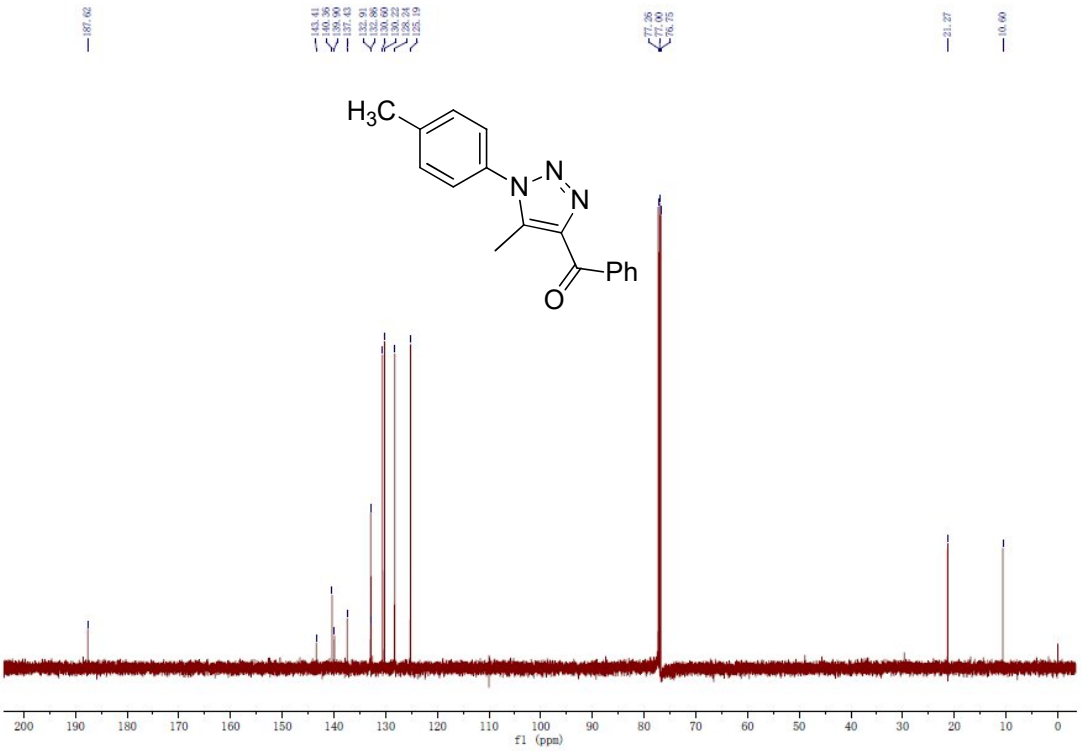
(1-(4-Bromophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ad)



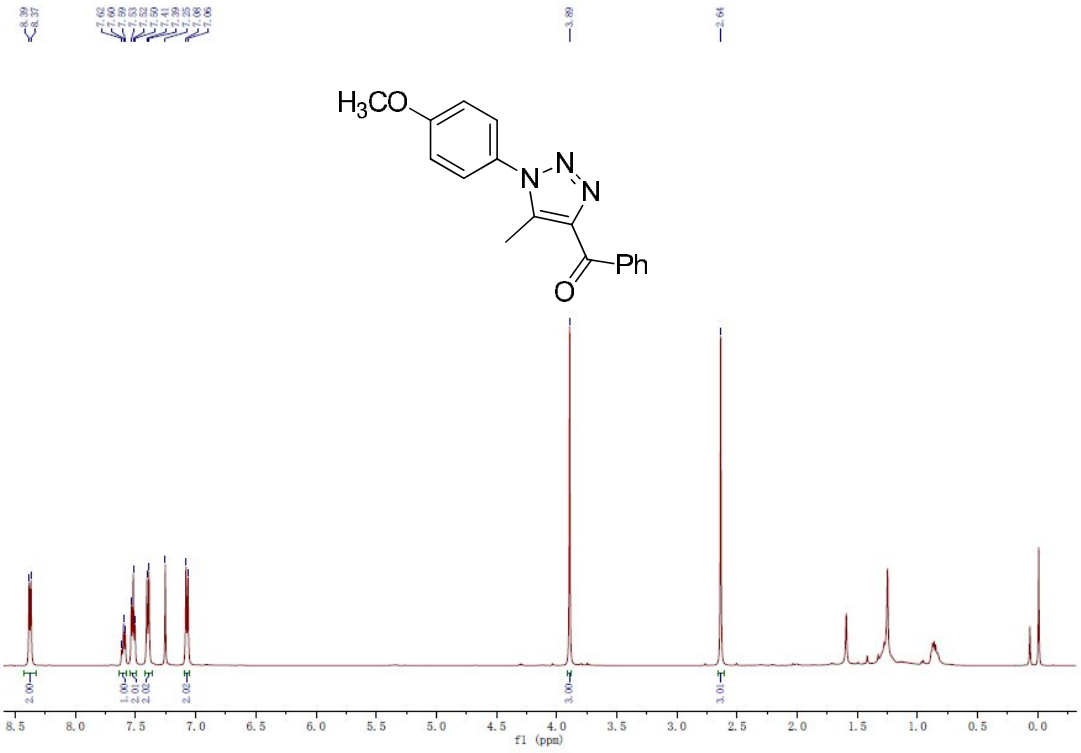


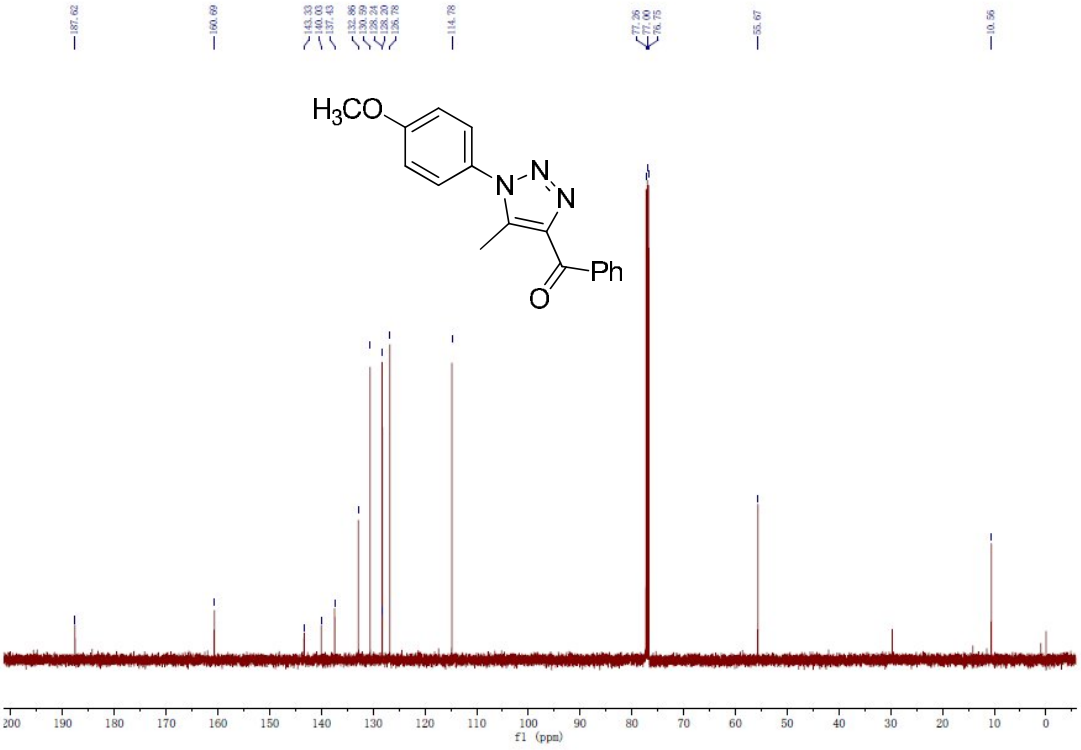
(5-Methyl-1-(*p*-tolyl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ae)



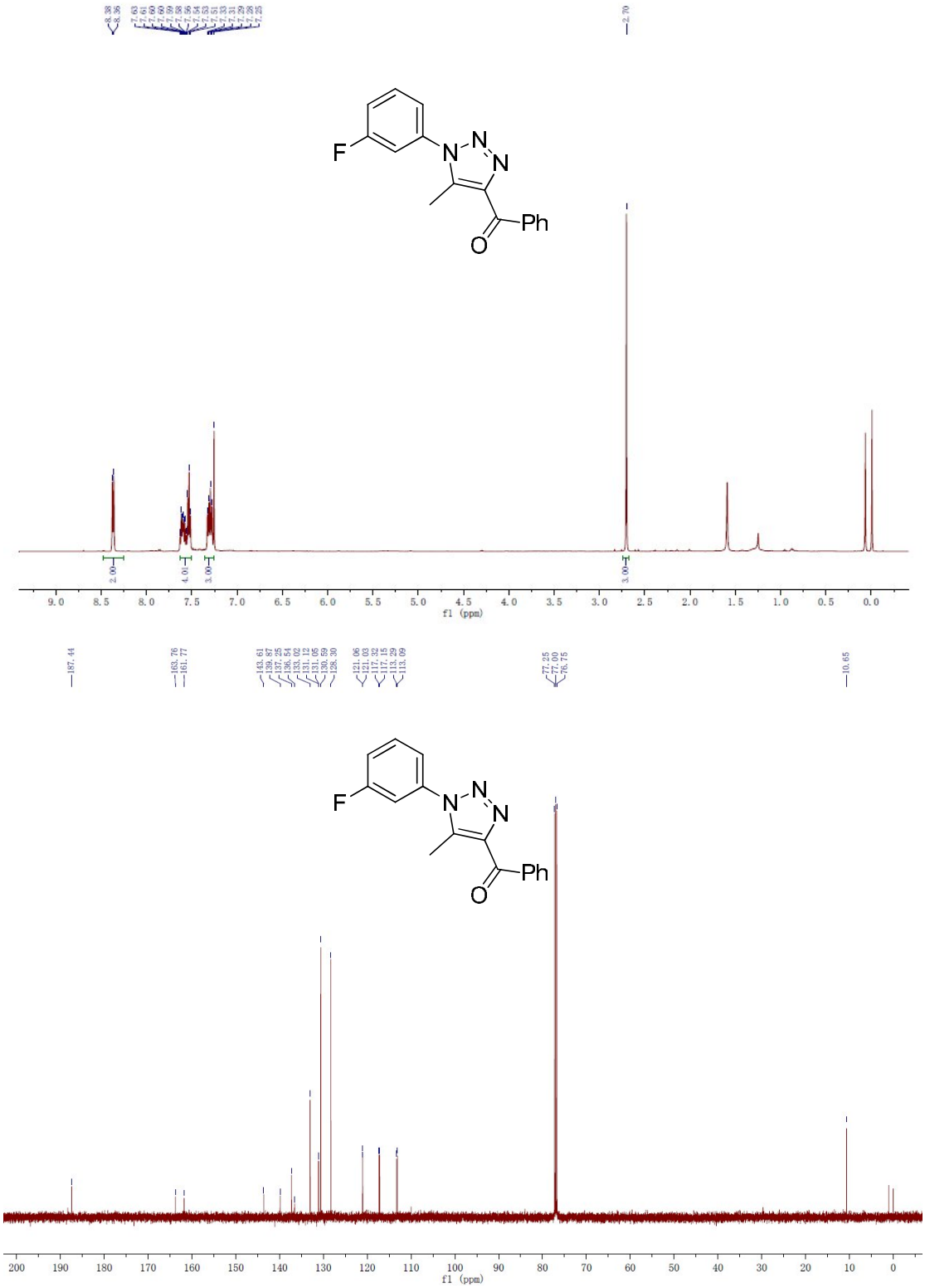


(1-(4-Methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3af)

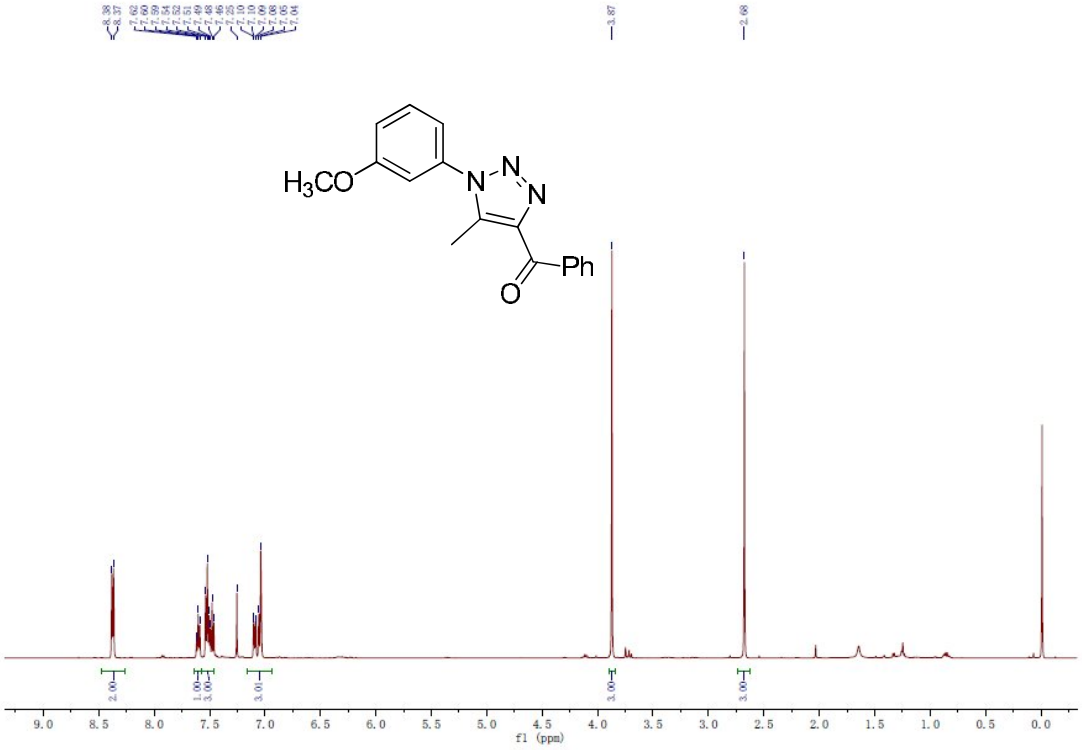


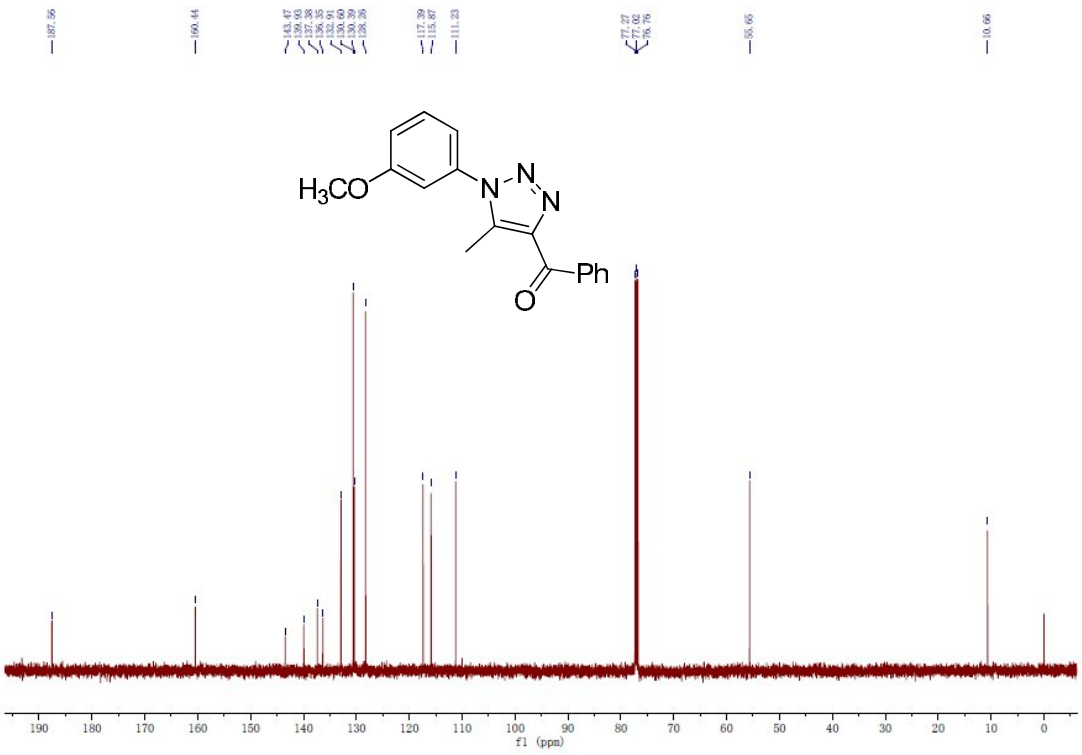


(1-(3-Fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ag)

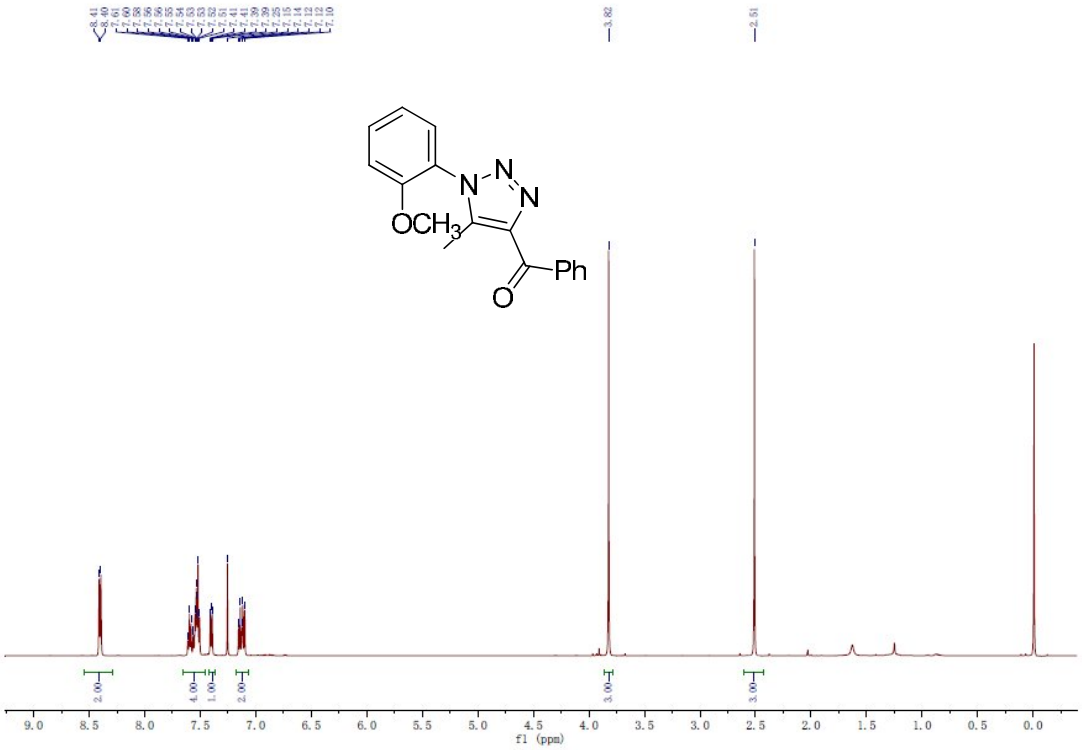


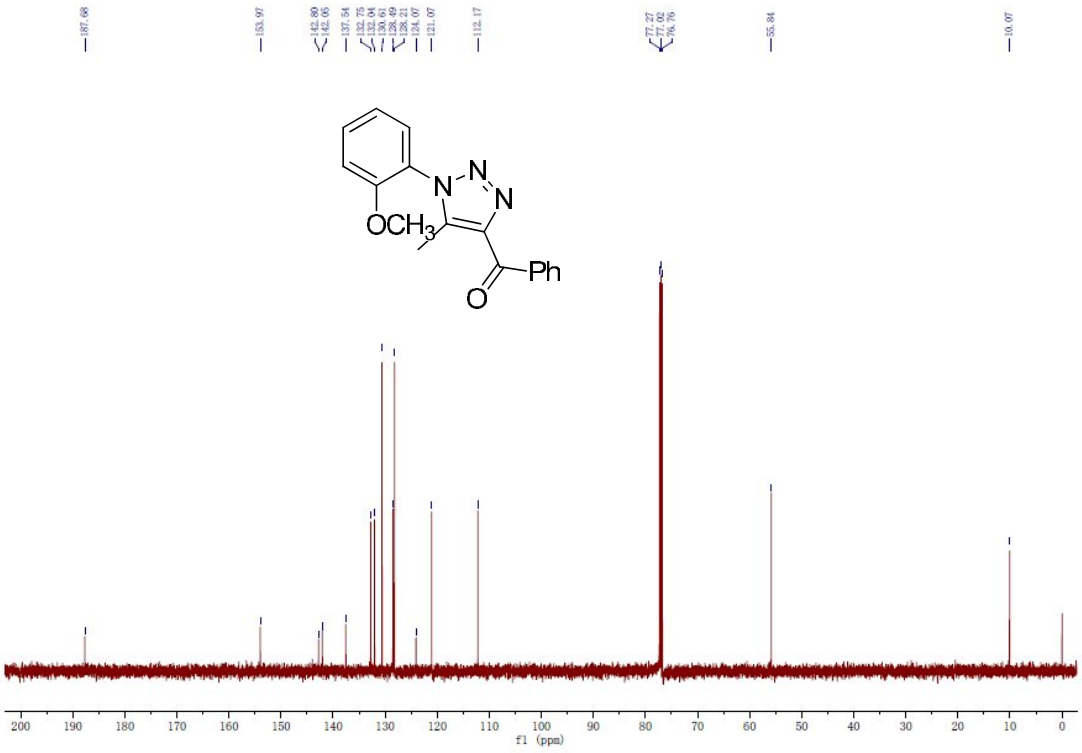
1-(3-Methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ah)



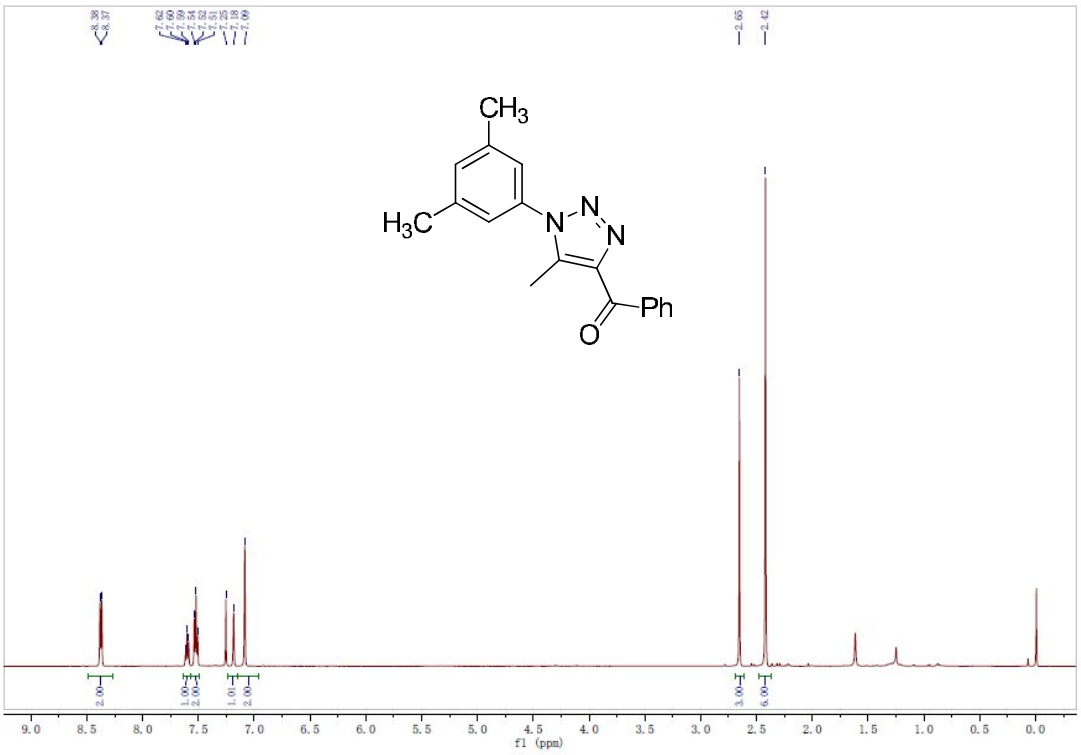


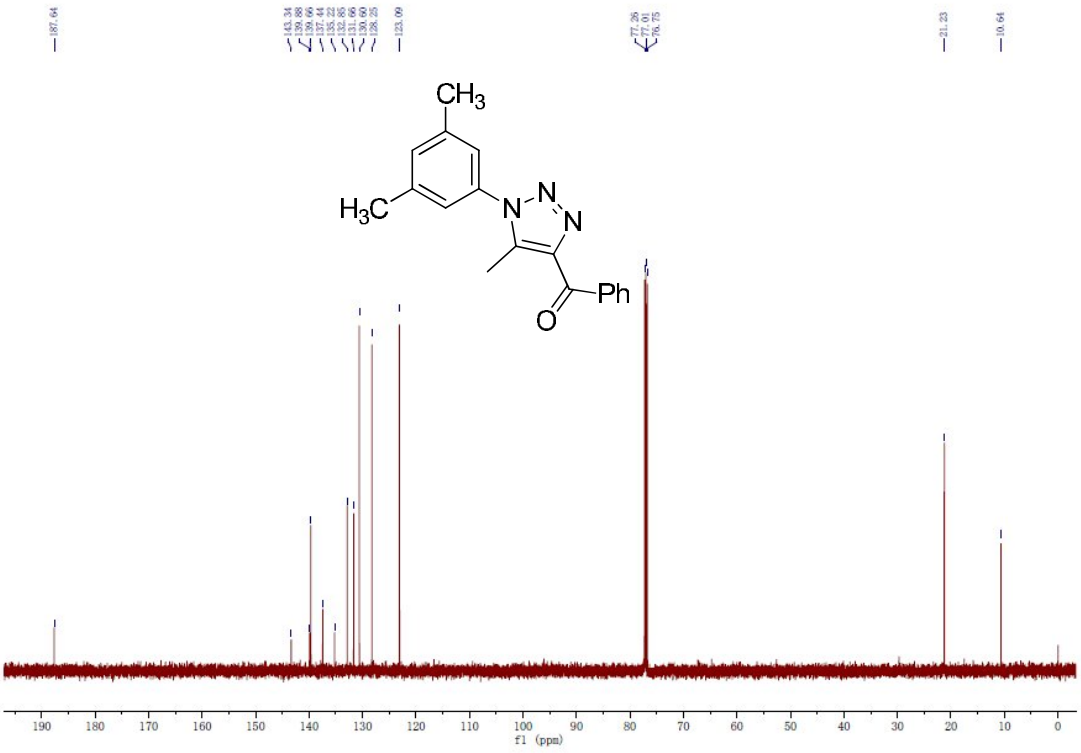
(1-(2-Methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ai)



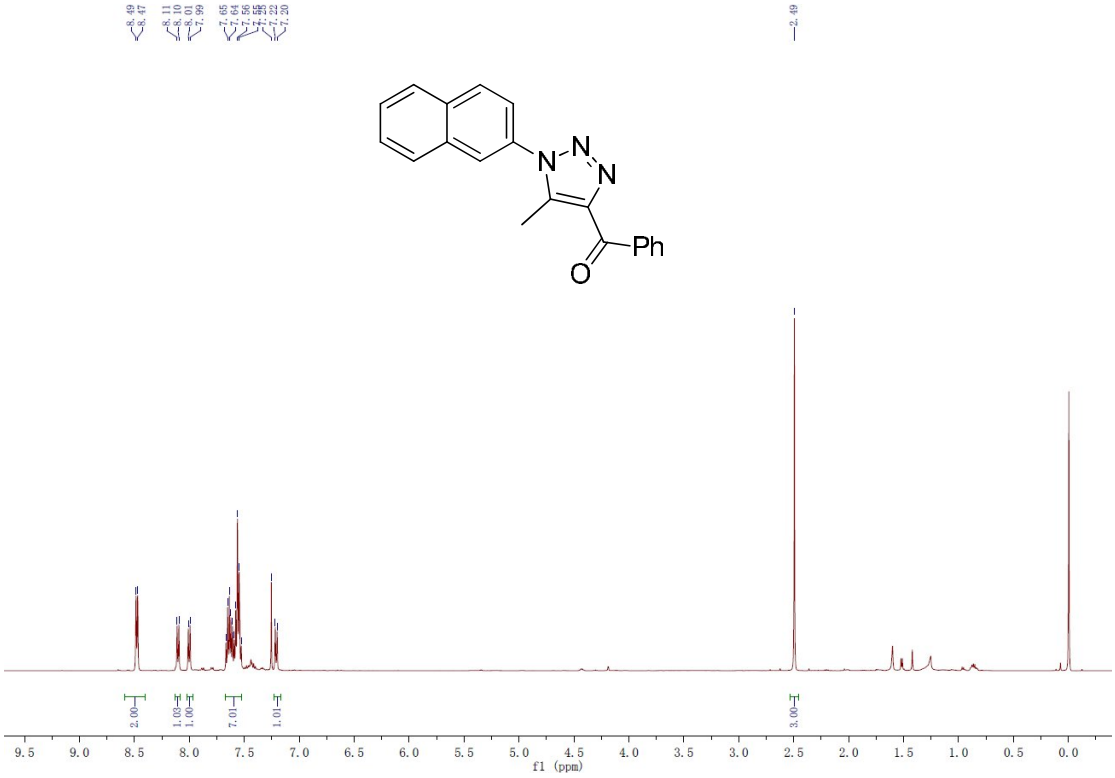


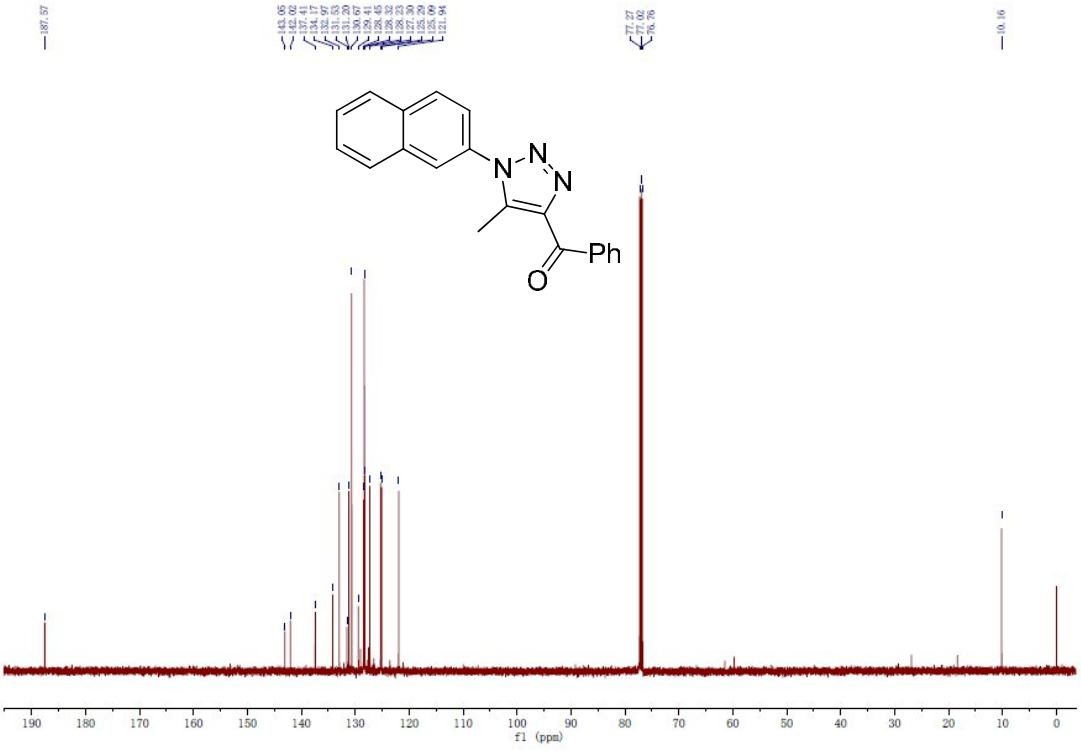
(1-(3,5-Dimethylphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3aj)



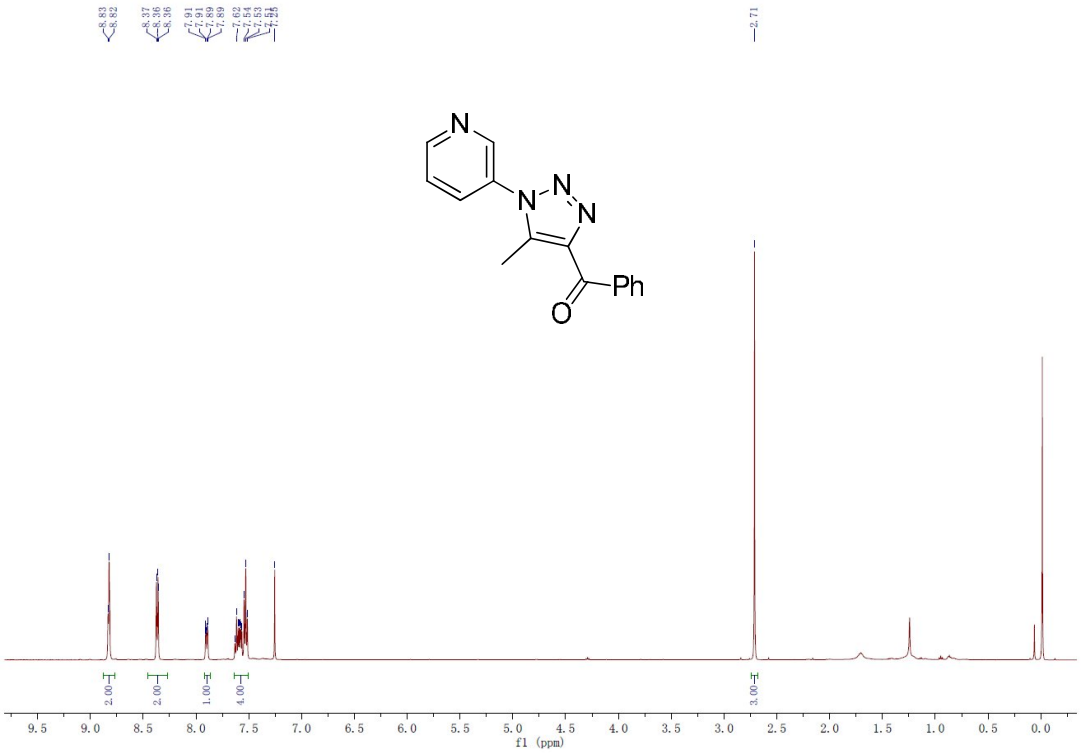


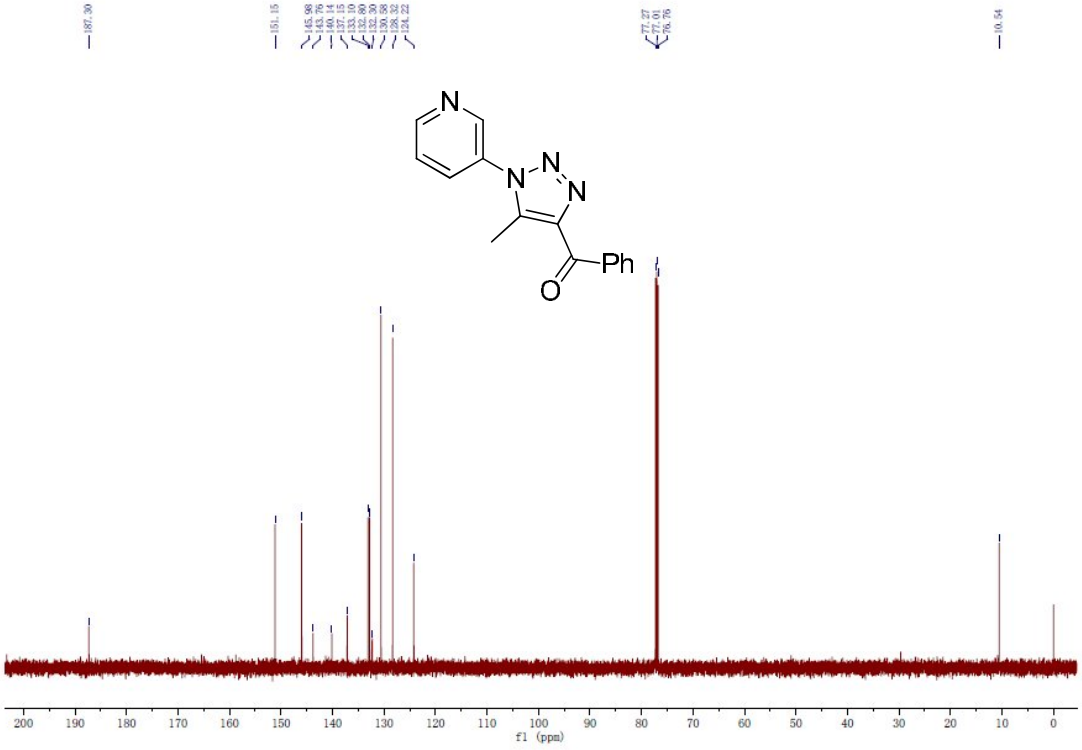
(5-Methyl-1-(naphthalen-2-ylmethyl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ak)



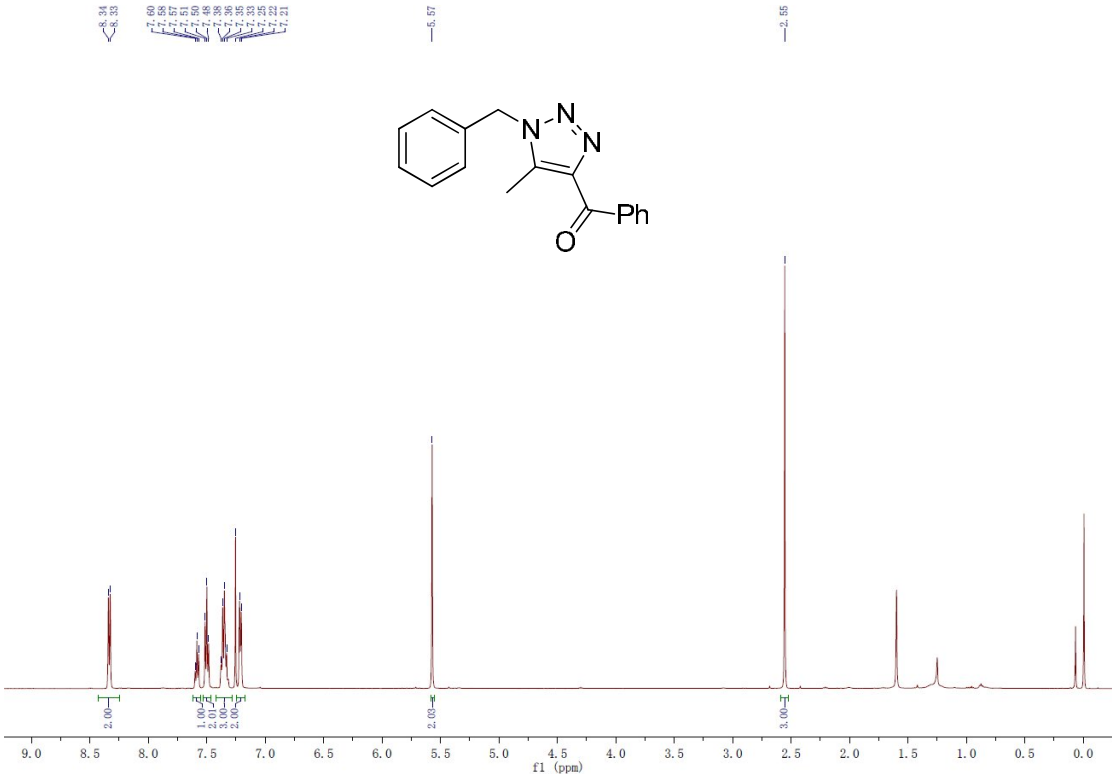


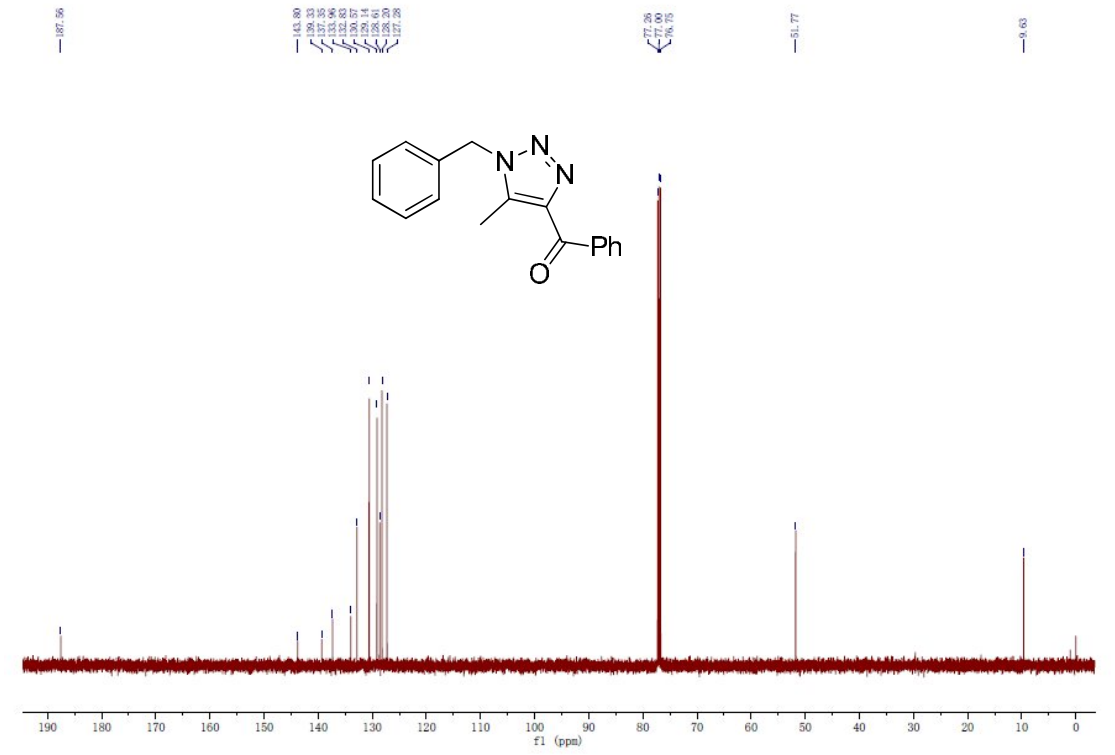
(5-Methyl-1-(pyridin-3-yl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3al)



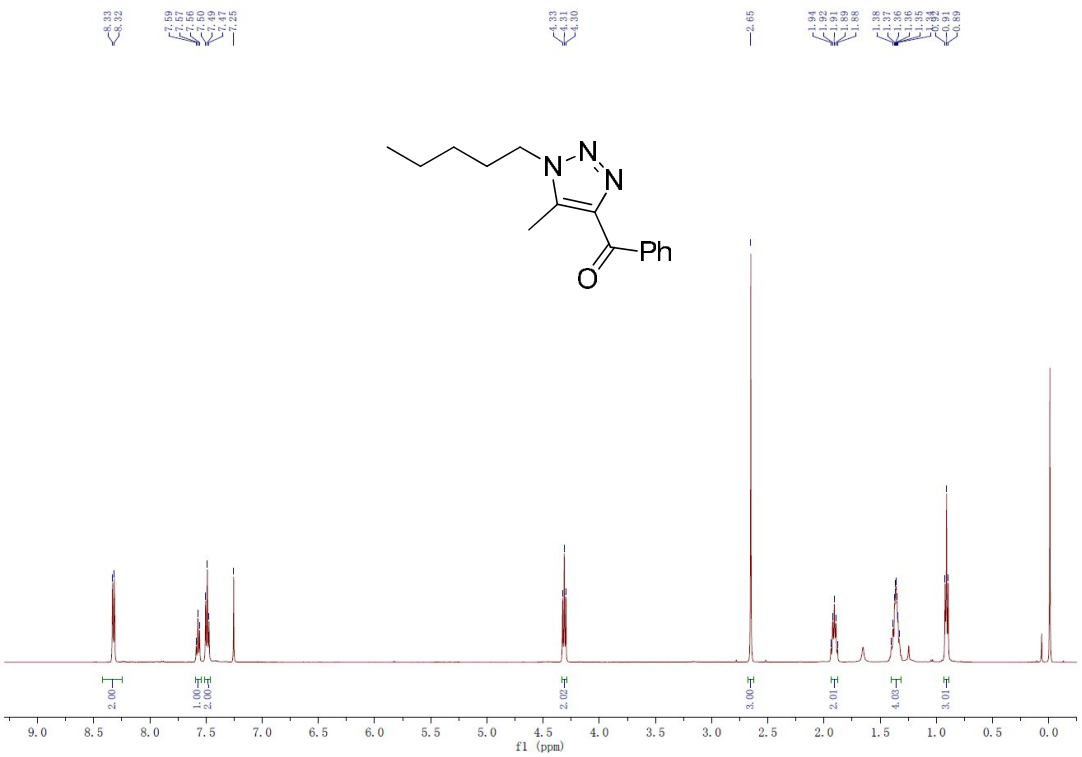


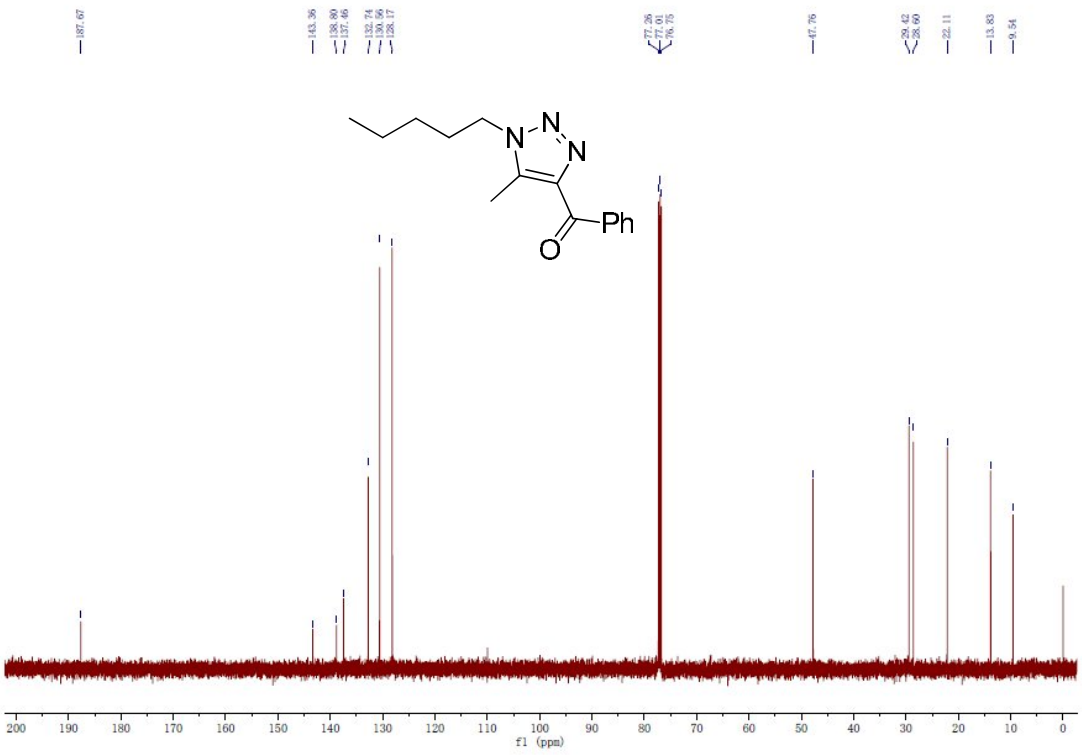
(1-Benzyl-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3am)



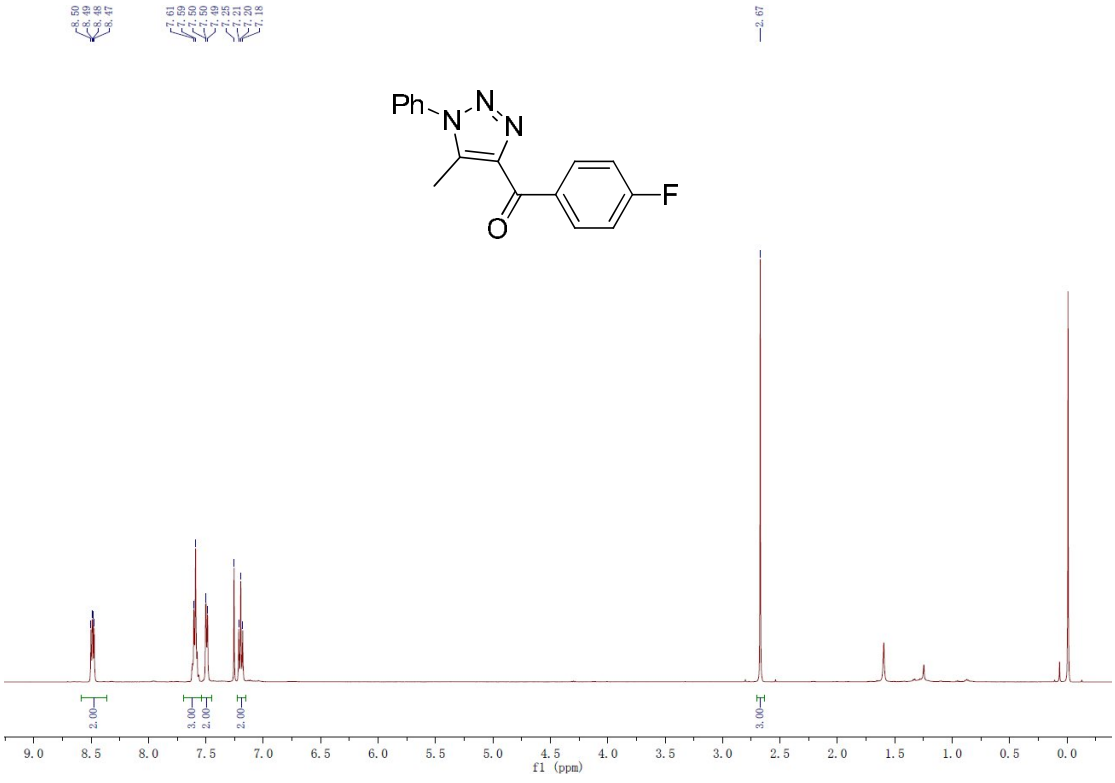


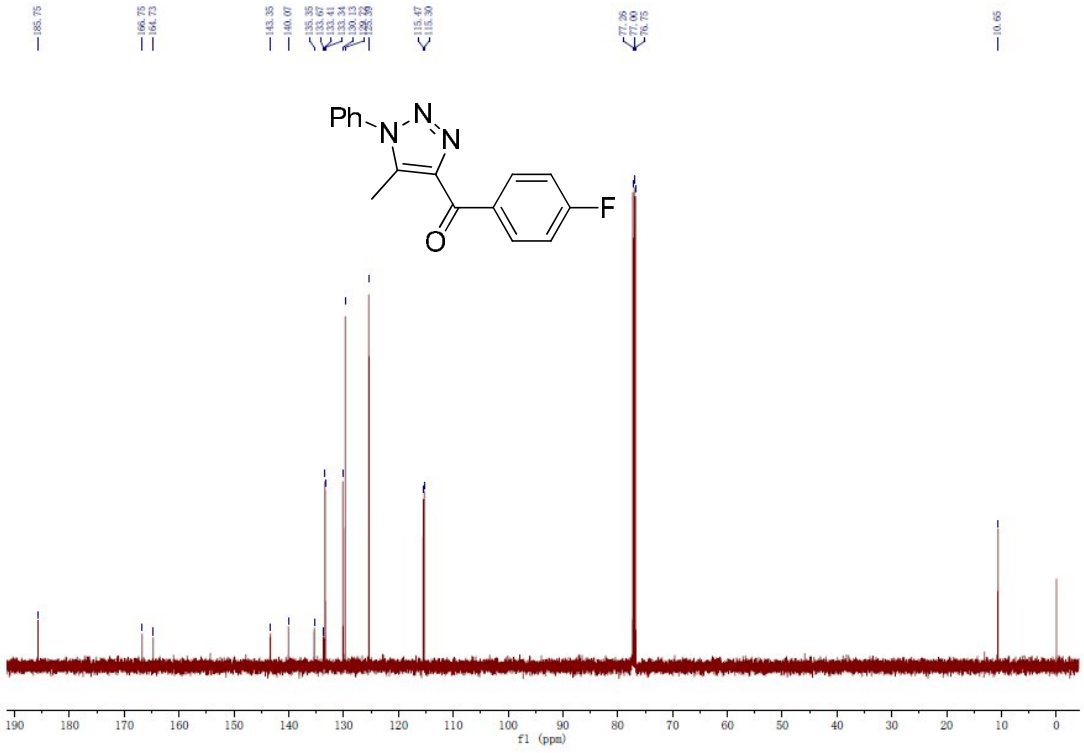
(5-Methyl-1-pentyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3an)



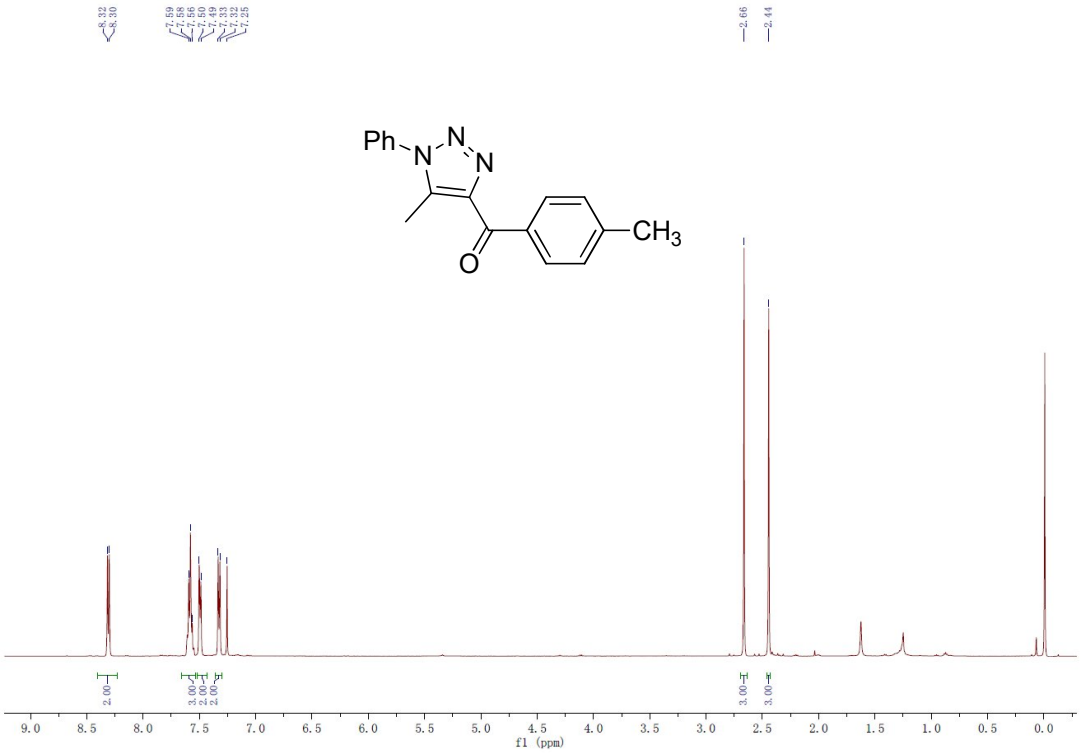


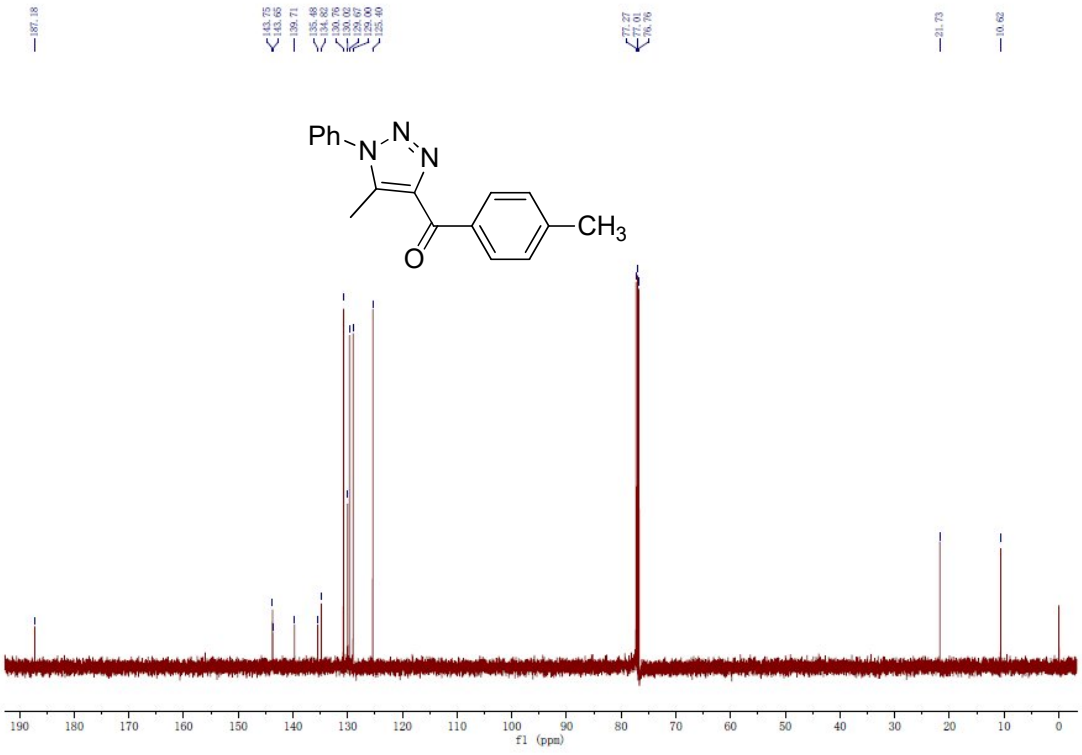
(4-Fluorophenyl)(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)methanone (3ba)



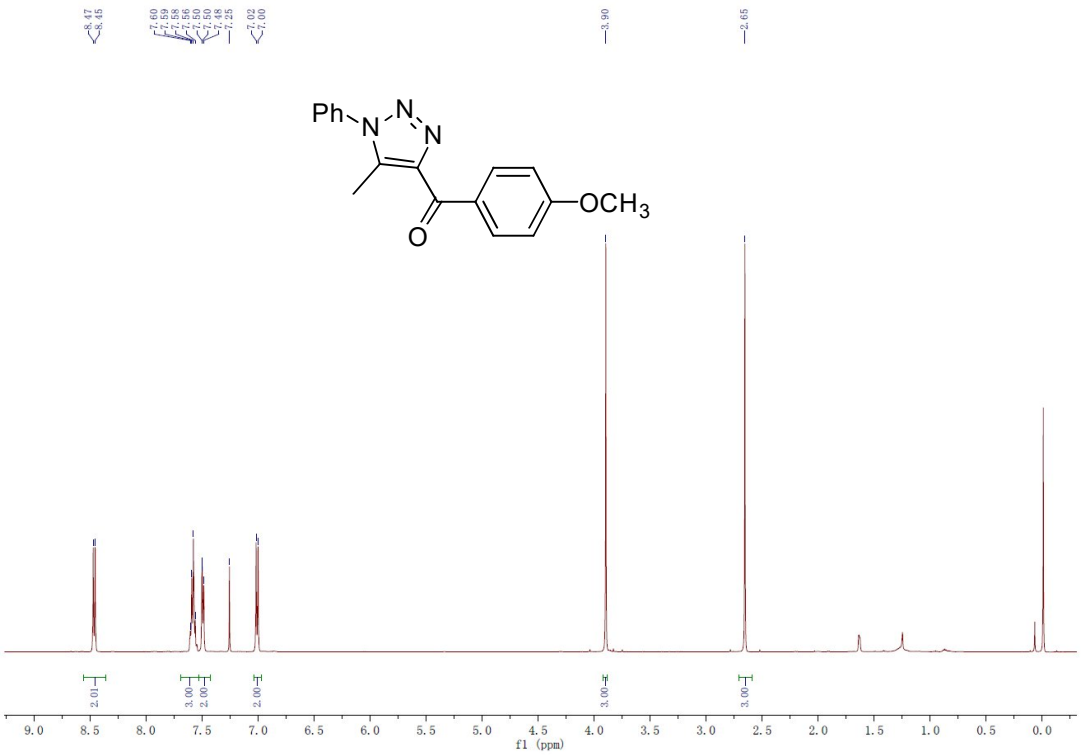


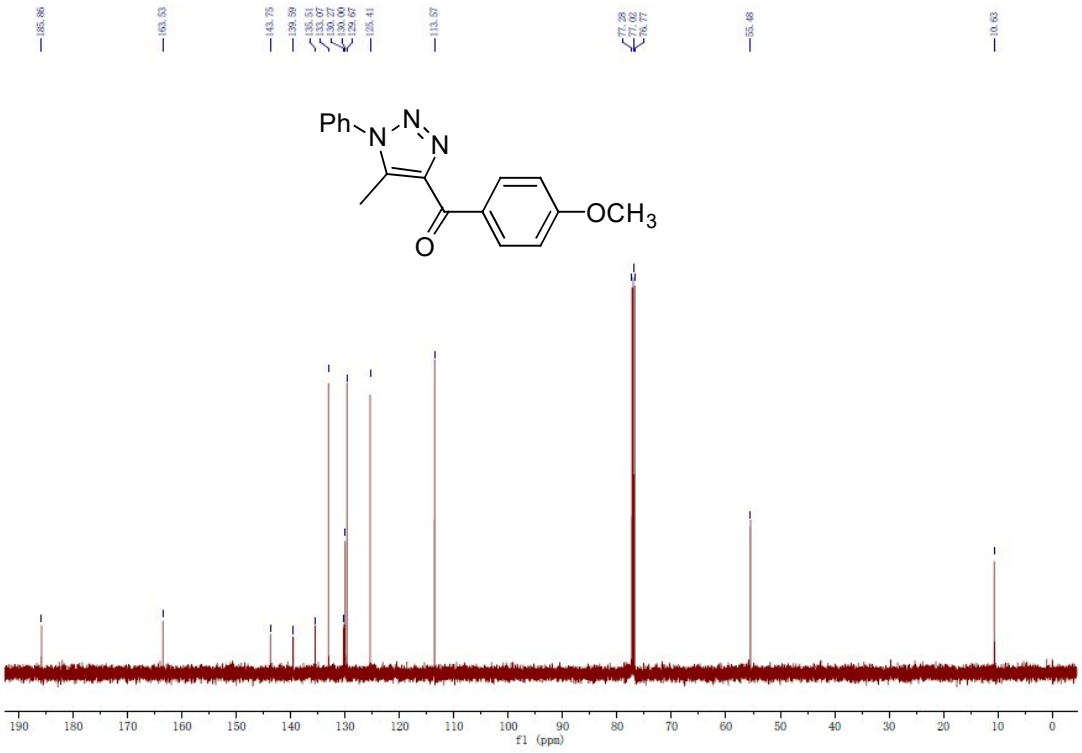
(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(p-tolyl)methanone (3ca)



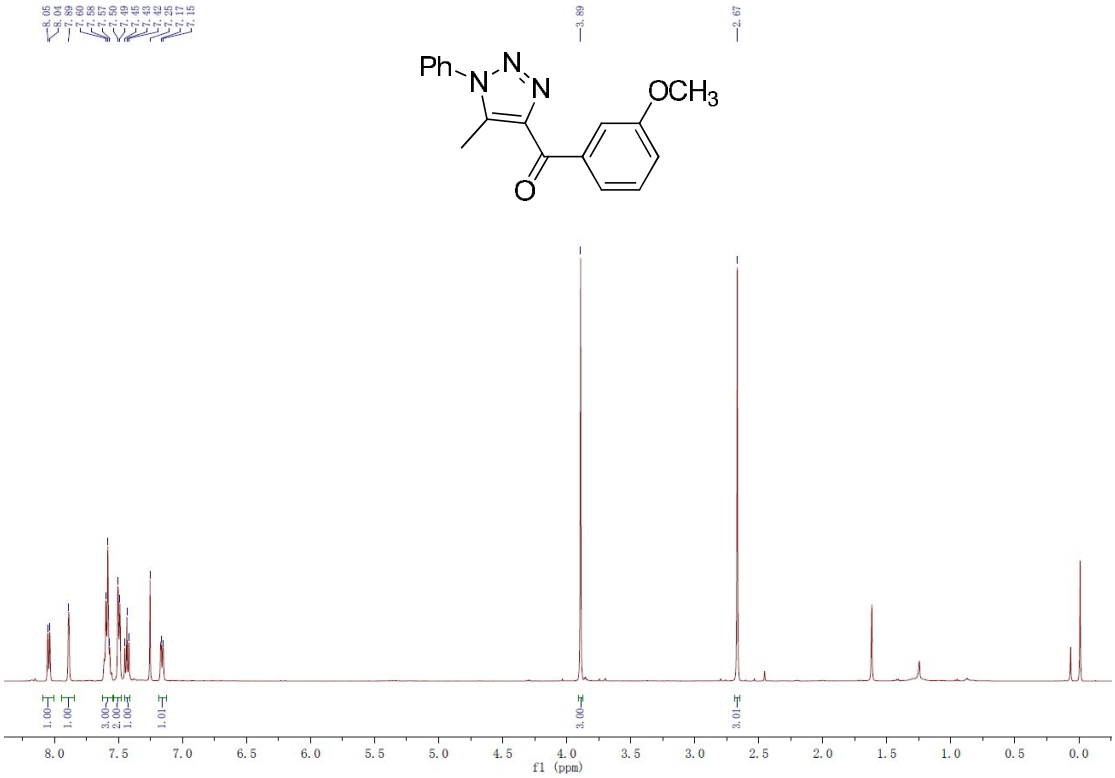


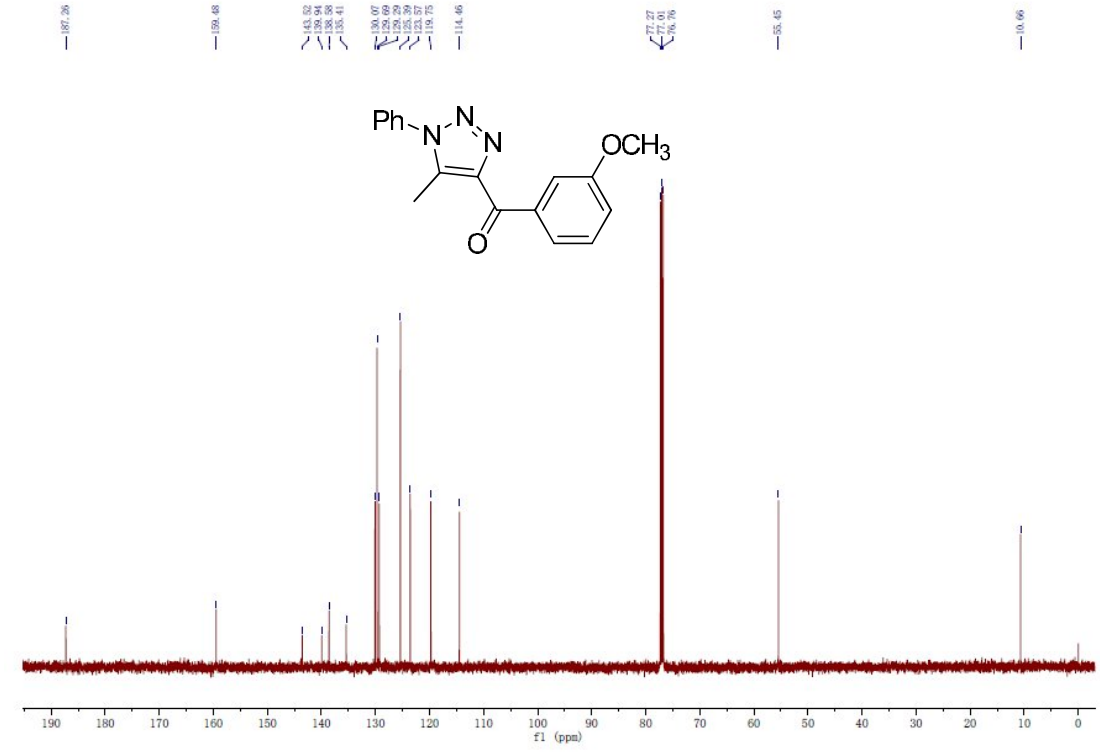
(4-Methoxyphenyl)(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)methanone (3da)



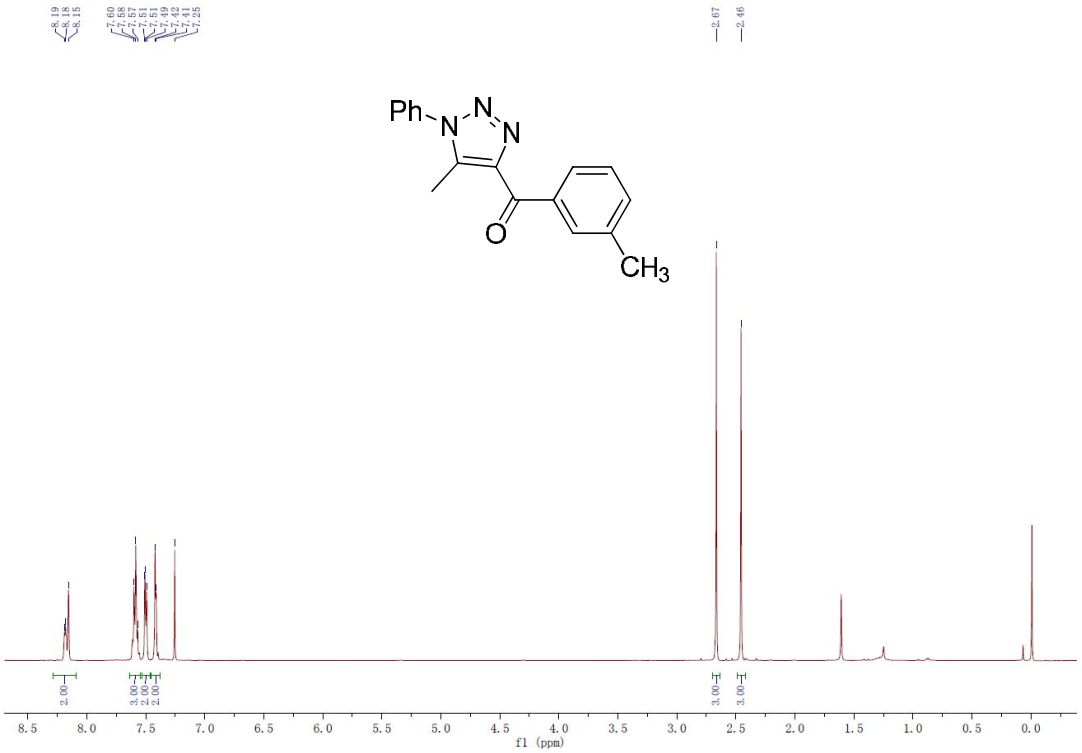


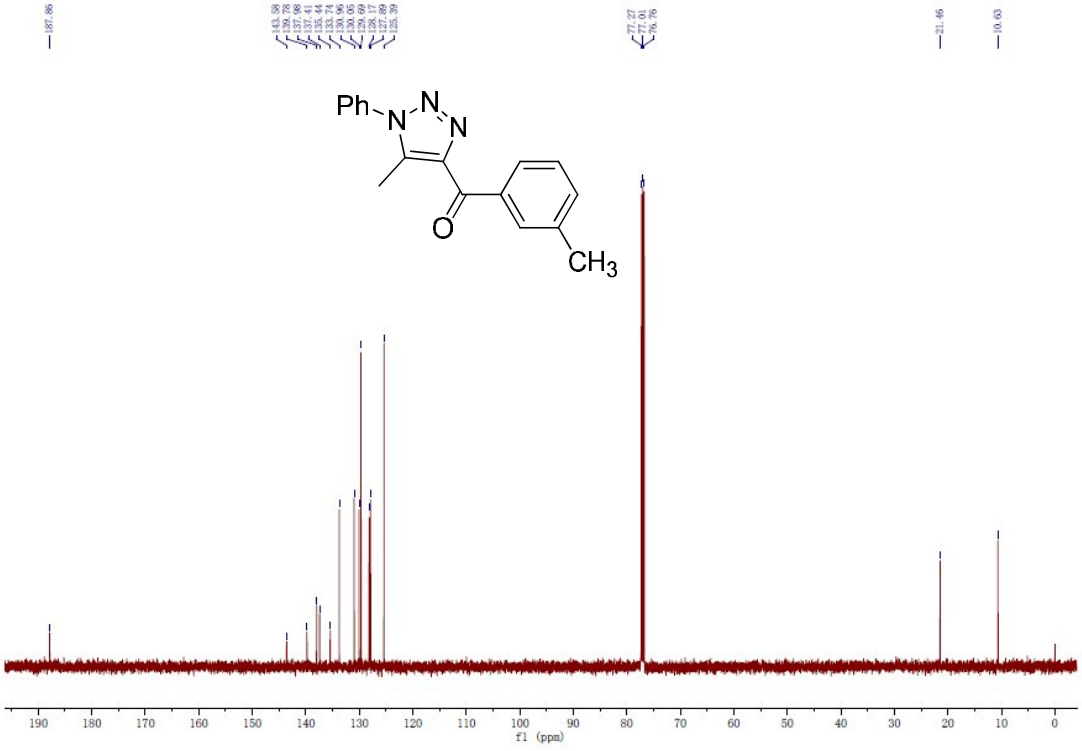
(3-Methoxyphenyl)(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)methanone (3ea)



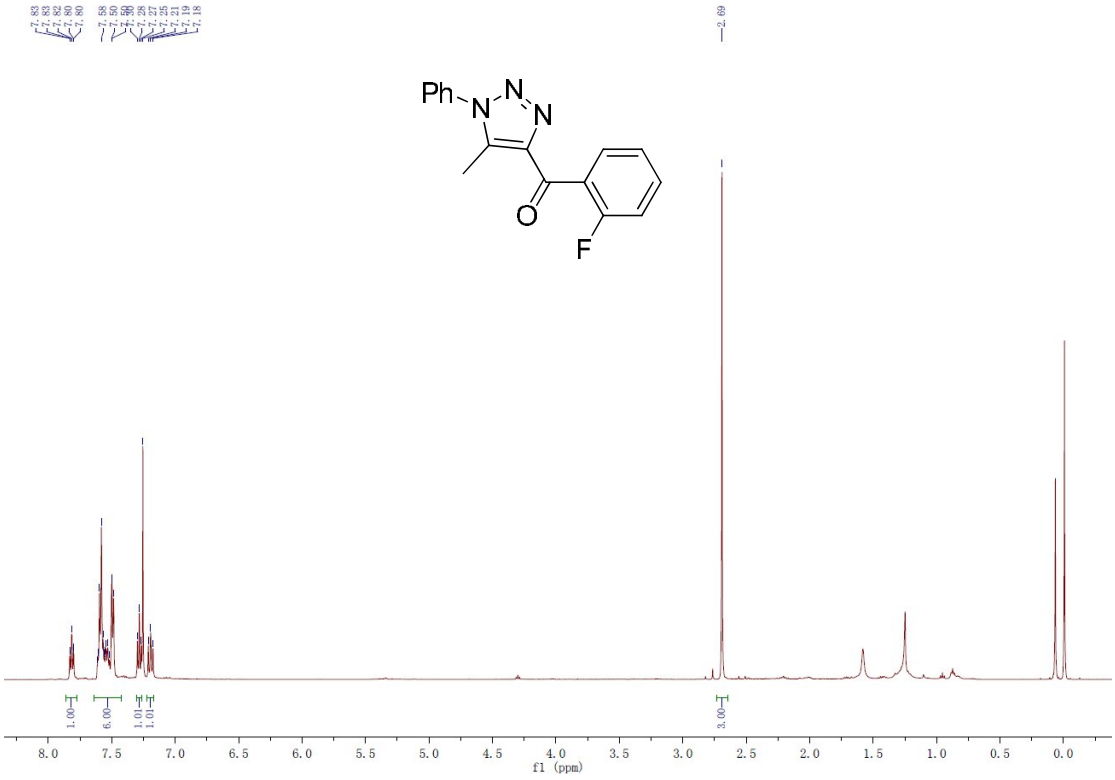


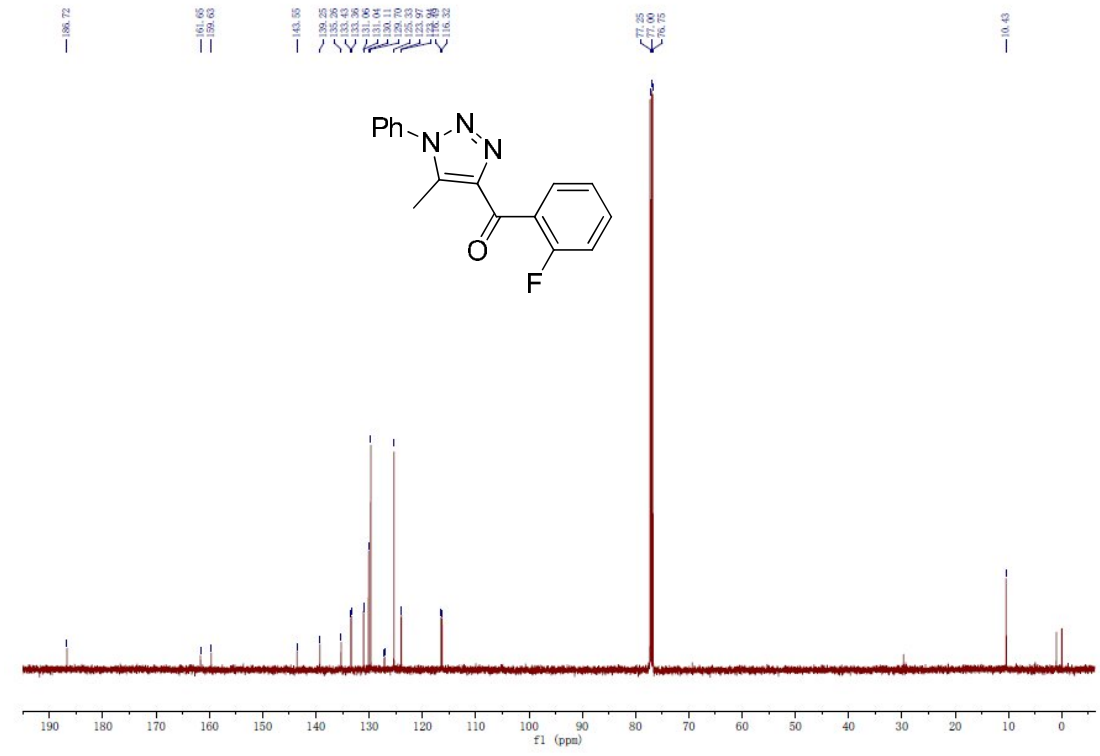
(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(*m*-tolyl)methanone (3fa)



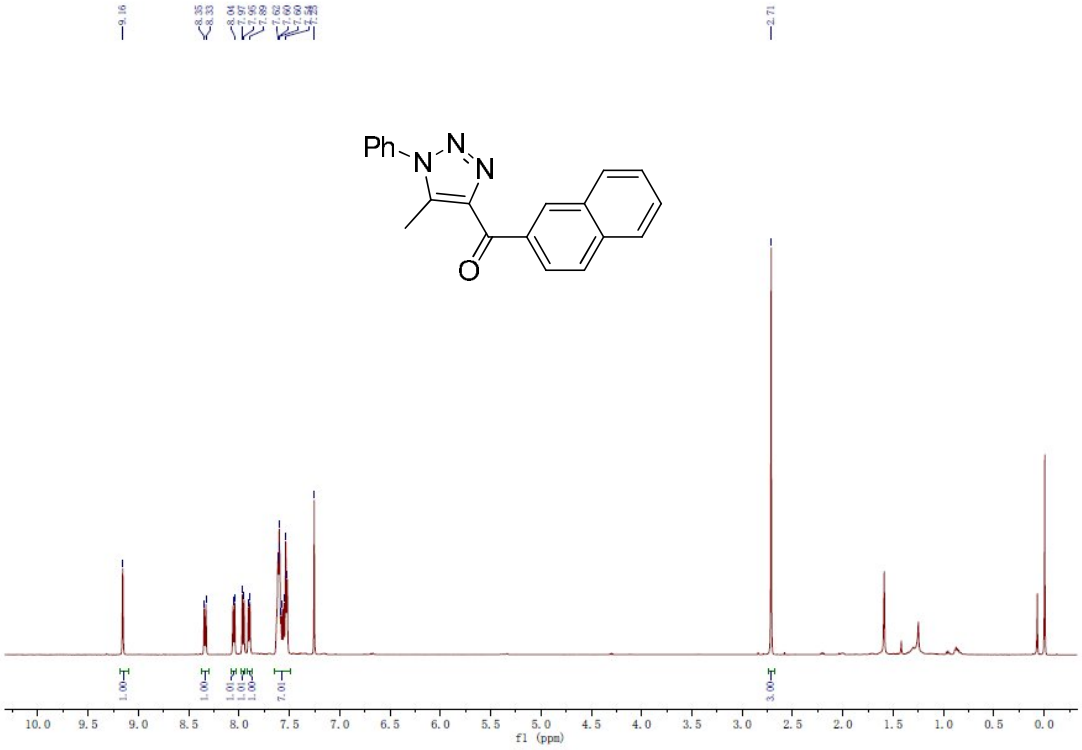


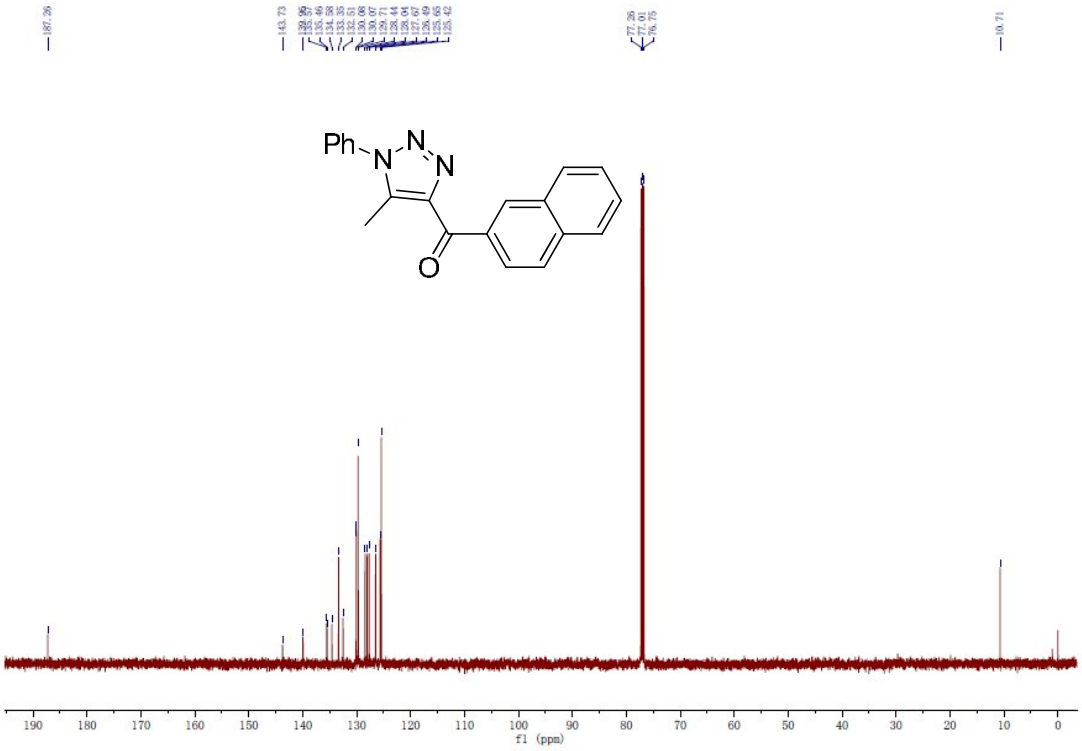
(2-Fluorophenyl)(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)methanone (3ga)



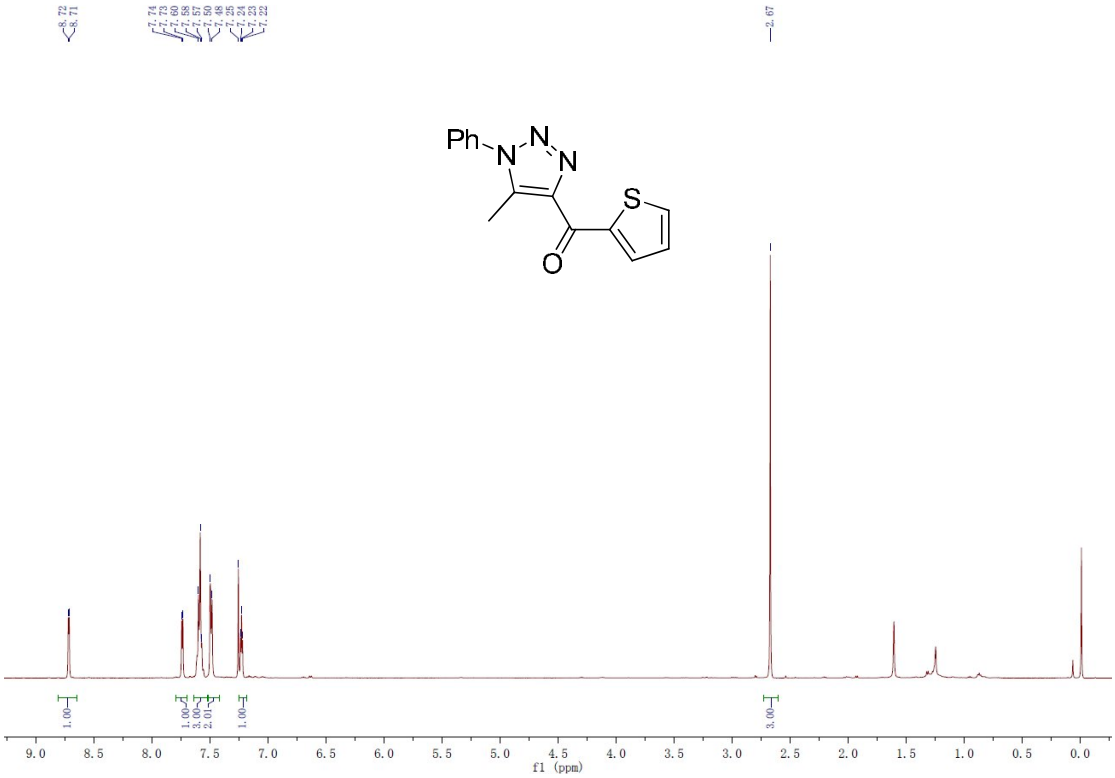


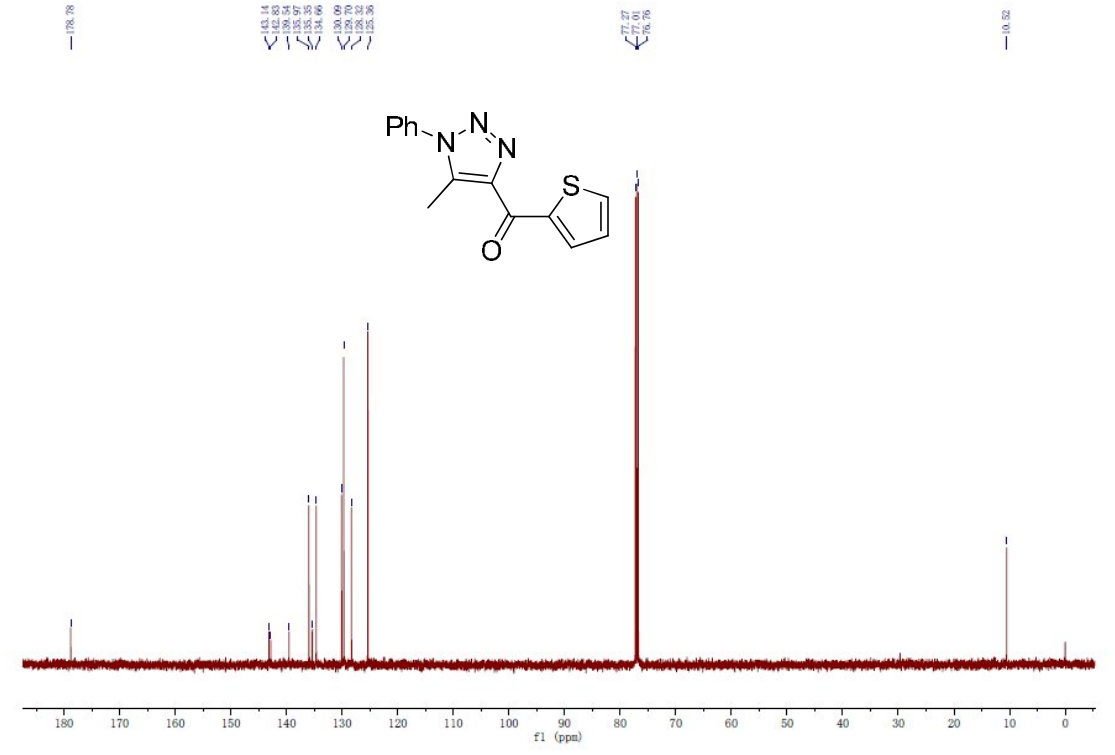
(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(naphthalen-2-yl)methanone (3ha)



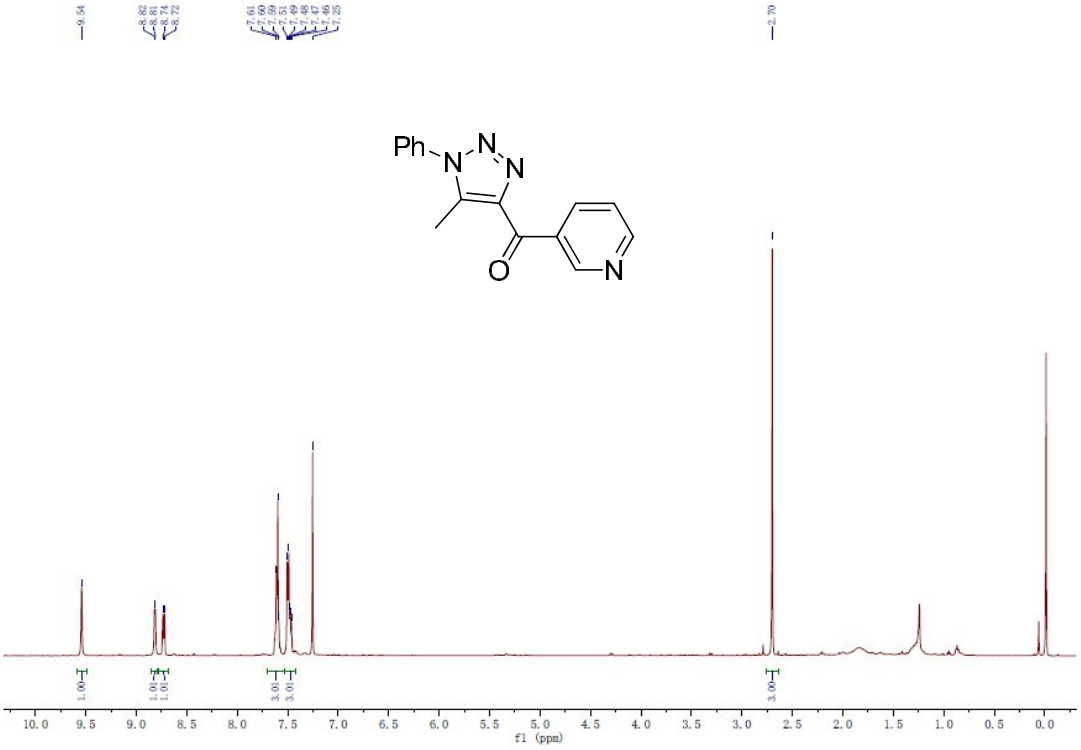


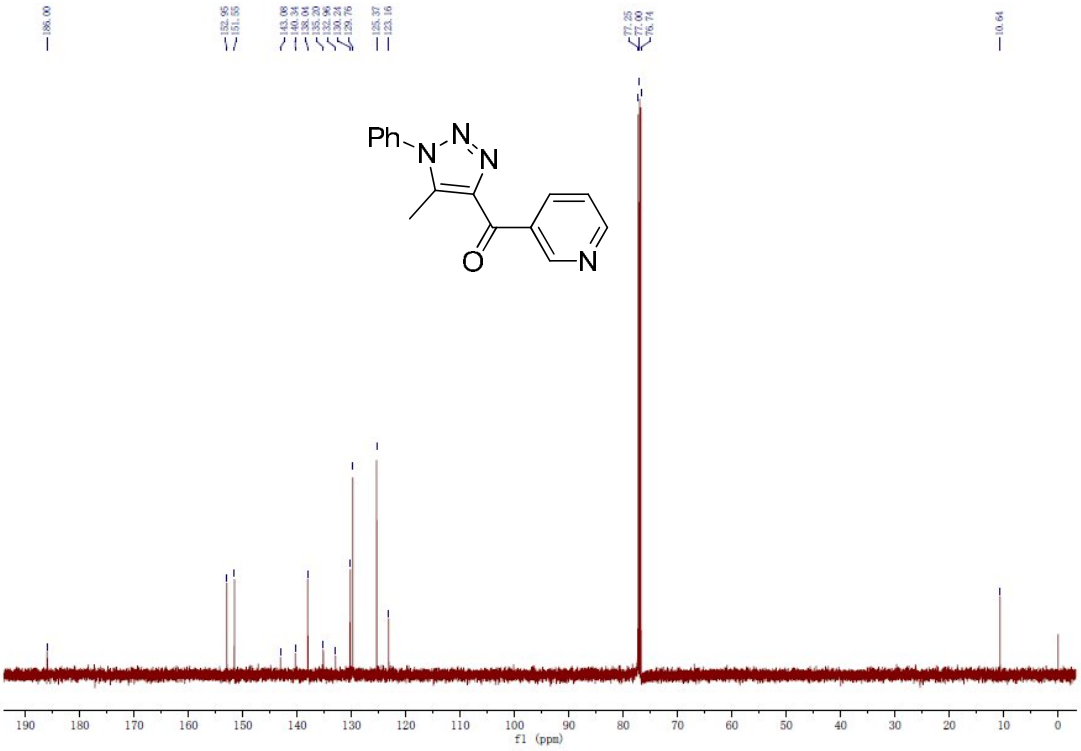
(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(thiophen-2-yl)methanone (3ia)



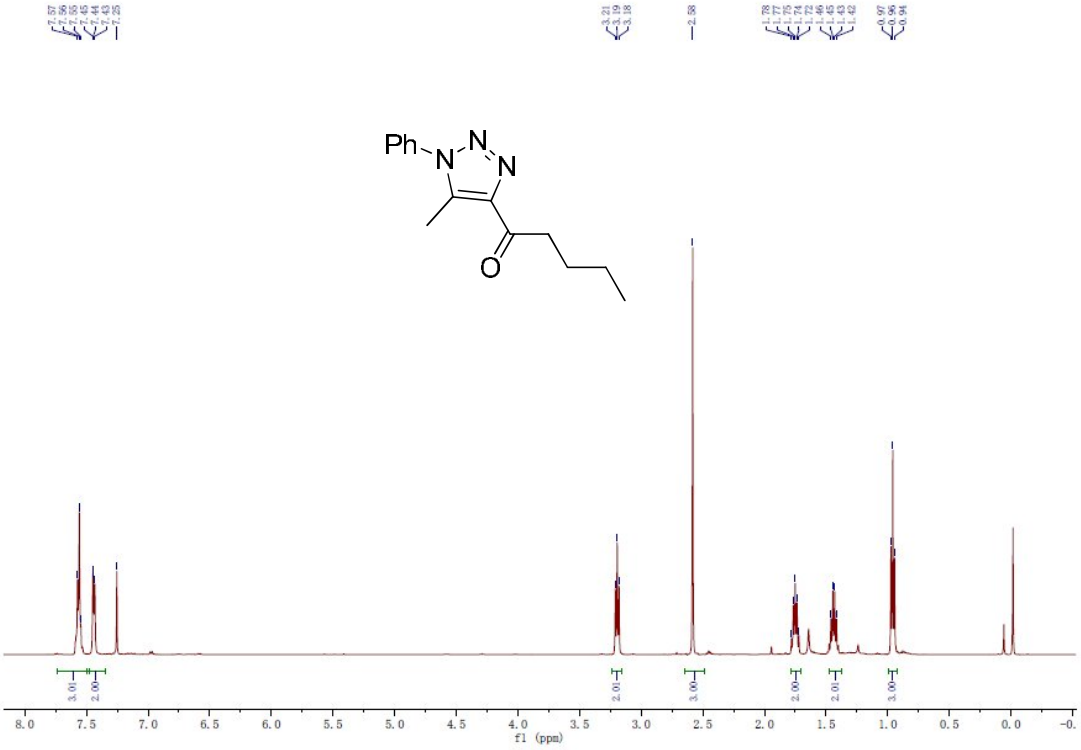


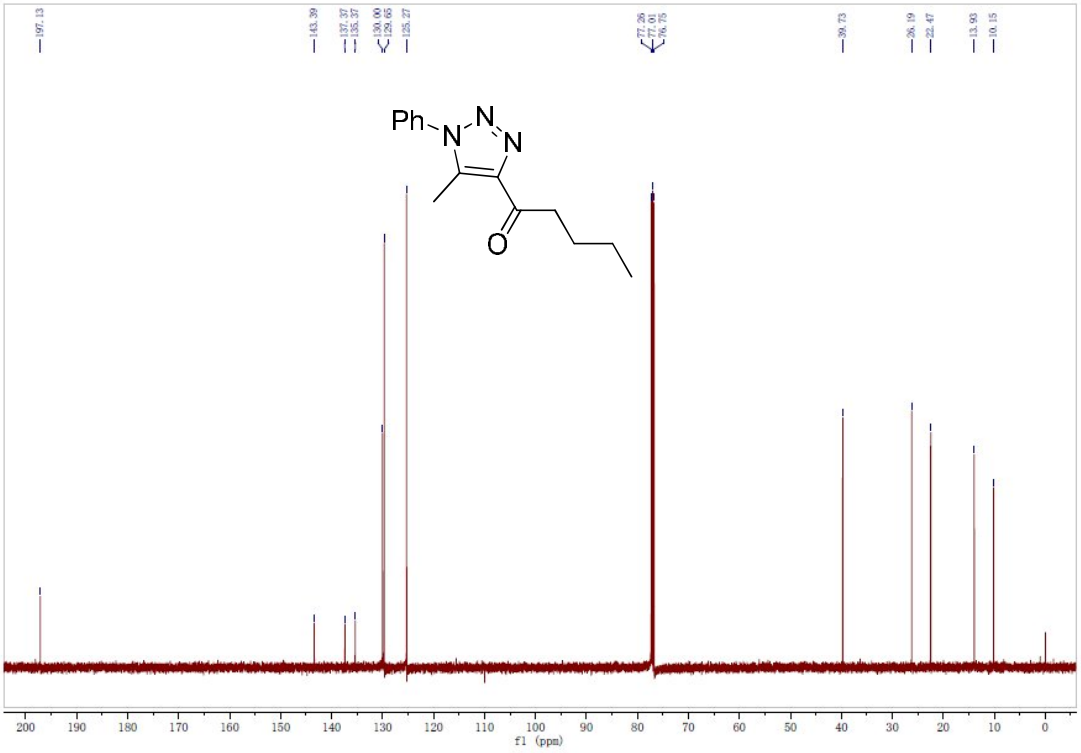
(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)(pyridin-3-yl)methanone (3ja)



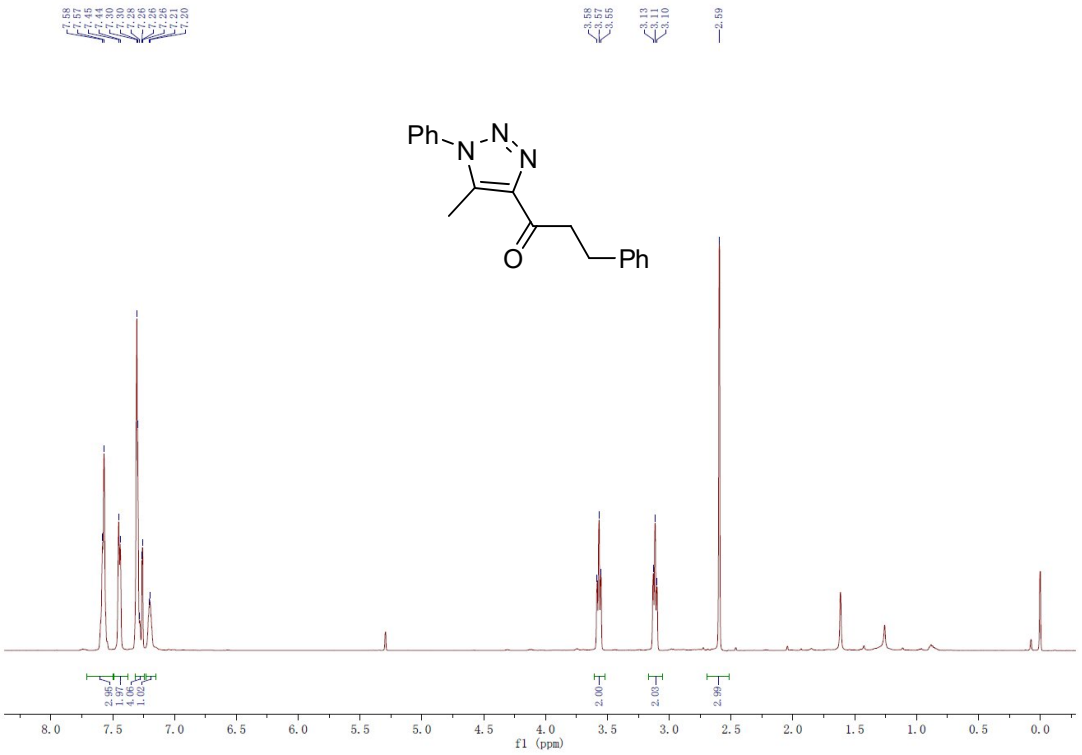


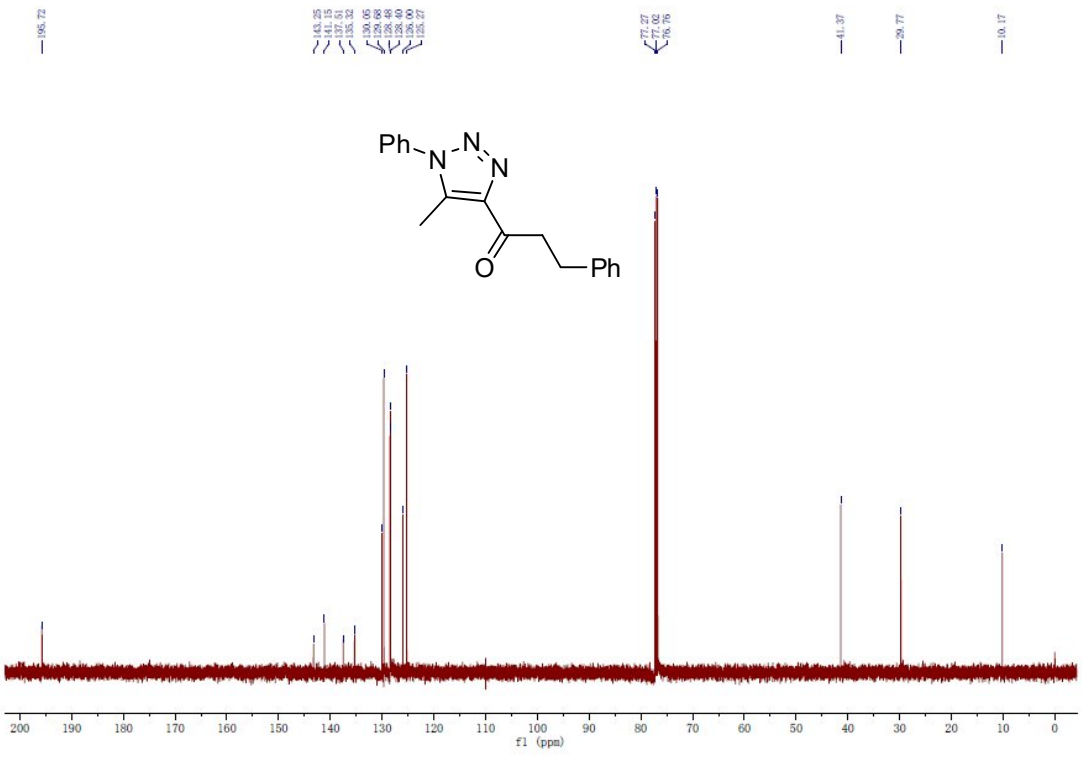
1-(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)pentan-1-one (3ka)



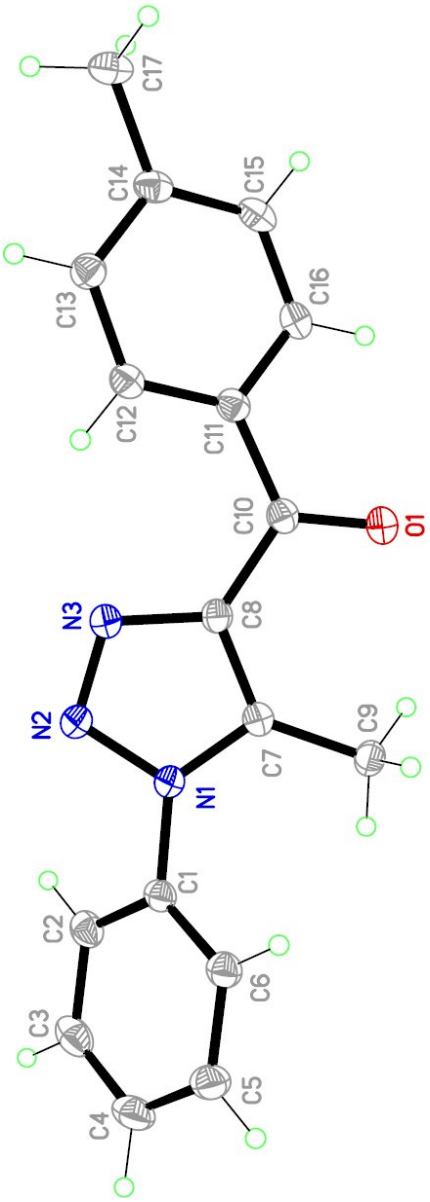


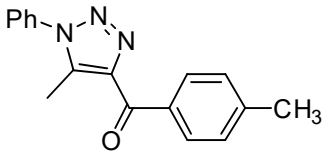
1-(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)-3-phenylpropan-1-one (3la)





E: X-ray Analysis





3ca

Table 1. Crystal data and structure refinement for **3ca**.

Identification code	**3ca**	
Empirical formula	C17 H15 N3 O	
Formula weight	277.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 14.9957(12) Å	α= 90°.
	b = 7.6225(6) Å	β= 91.022(3)°.
	c = 11.9828(10) Å	γ = 90°.
Volume	1369.47(19) $Å^3$	
Z	4	
Density (calculated)	1.345 Mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	584	
Crystal size	0.400 x 0.300 x 0.300 mm^3	
Theta range for data collection	2.717 to 27.499°.	
Index ranges	-19<=h<=19, -9<=k<=9, -15<=l<=15	
Reflections collected	49120	
Independent reflections	3141 [R(int) = 0.0335]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.7083	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3141 / 0 / 192	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0381, wR2 = 0.0883	
R indices (all data)	R1 = 0.0472, wR2 = 0.0941	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.291 and -0.171 $e.Å^{-3}$	

F: References

1. O. Berger, A. Kanthi, C. Tran van Ba, H. Vial, S. A. Ward, G. A. Biagini, P. G. Gray, P. M. O'Neil, *ChemMedChem* **2011**, 6, 2094-2108.
2. A. S. Lee, L. Lin, *Tetrahedron Lett.* **2000**, 41, 8803-8806.