Supporting Information

The Electrochemically Enabled α-C(sp^3)–H Azolation of Ketones

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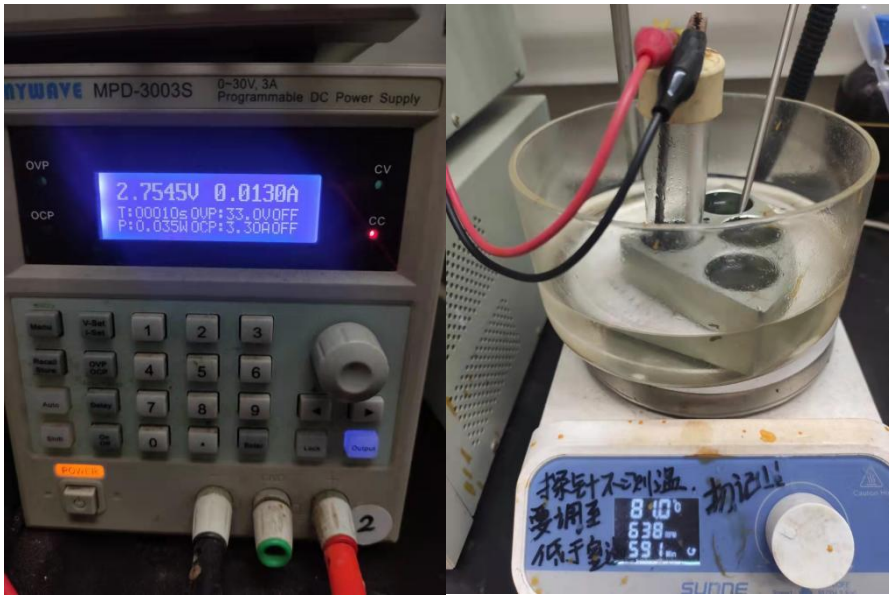
General Remarks

Electrochemical reactions were conducted using an MYWAVE MPD-3003S potentiostat in a constant current mode using undivided cell equipped with graphite plate (1.0 cm × 1.0 cm × 0.2 cm) as the anode and platinum plate (1.0 cm × 1.0 cm × 0.01 cm) as the cathode under air. Acetonitrile(MeCN), tetrabutylammonium iodide(TBAI), graphite plates, platinum(Pt) electrodes, chemicals were obtained from commercial sources and were used without further purification.Graphite plates are from Bei Jing Jinglong Special Carbon Technology Co., Ltd, platinum electrodes are from Tian Jin Aida (China).Yields refer to isolated compounds, estimated to be >95% pure as determined by ^{1}H-NMR. TLC: Macherey-Nagel, TLC plates Alugram®Sil G/UV254. Detection under UV light at 254 nm.Chromatography separations were carried out on silica gel 60H (300-400 mesh) manufactured by Qingdao Haiyang Chemical Group Co. (China). High resolution mass spectrometry (HRMS) was measured on Agilent 6210 LC/MSD TOF mass spectrometer. NMR spectra were recorded on Bruker, AVANCE Ⅲ HD 400 MHz (^{1}H 400 MHz; ^{13}C 100 MHz) in $CDCl_3$. If not otherwise specified, chemical shifts (δ) are given in ppm. Melting point were recorded on JHX-5Plus.

(a)



(b)

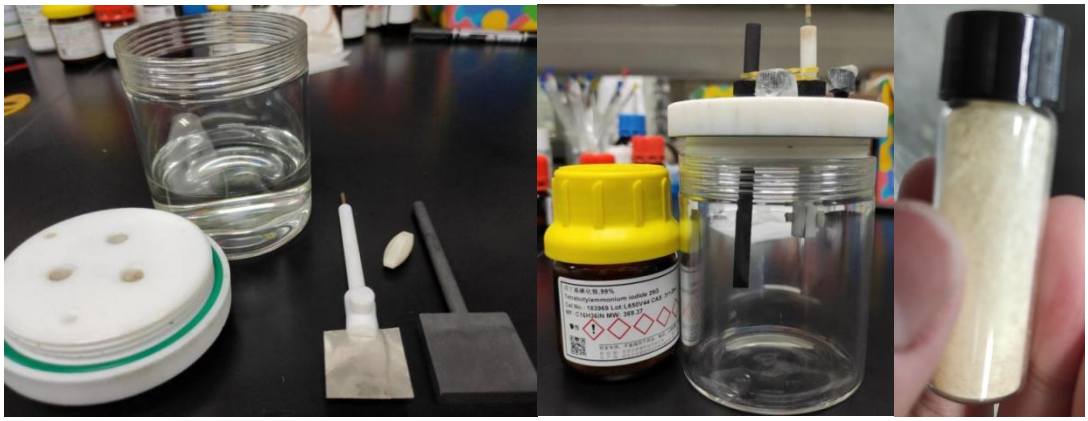
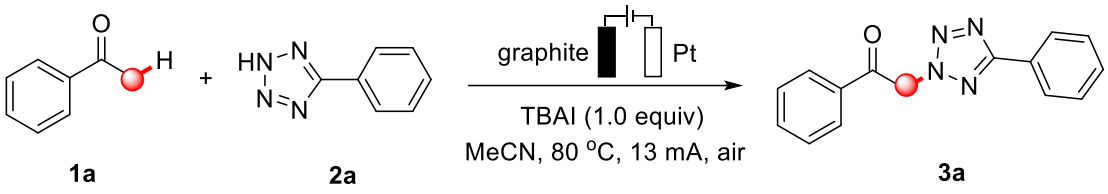


Figure S1. The set up of electrochemical reaction. (a) Equipment of standard reaction; (b) Equipment of gram-scale reaction.

Optimization Studies

Table S1. Optimization of Electrochemical Reaction Conditions[a]



1a **2a** **3a**

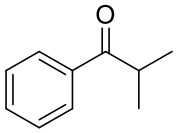
entry	deviation from standard conditions	yield (%) [b]
1	**None**	**85**
2	No TBAI	0
3	NH_4I instead of TBAI	trace
4	*n*-Bu_4NHSO_4 instead of TBAI	0
5	*n*-Bu_4NBF_4 instead of TBAI	0
6	*n*-Bu_4NPF_6 instead of TBAI	0
7	0.5 equiv TBAI instead of 1.0 equiv TBAI	66
8	0.1 equiv TBAI instead of 1.0 equiv TBAI	24
9	r.t. instead of 80 °C	trace
10	DCE as solvent	0
11	MeOH as solvent	0
12	12 h	72
13	16 mA	81
14	No current	0

[a] Reaction conditions: Undivided cell, graphite anode (1 cm × 1 cm × 0.2 cm), Pt cathode (1 cm × 1 cm × 0.01 cm), **1a** (1.5 mmol), **2a** (0.50 mmol), TBAI (0.50 mmol), MeCN (8.0 mL), constant current = 13.0 mA, 16 h (15.5 *F*), 80 °C, under air. [b] Yields of isolated product.

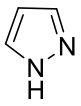
General Procedure for Electrochemical Reactions

General Procedure: In an undivided cell (15 mL) equipped with a stirring bar, a mixture of substrates **1a** (1.5 mmol), **2a** (0.50 mmol), *n*-Bu_4NI (0.50 mmol) and MeCN (8.0 ml) were added. The cell was equipped with graphite plate (1 cm × 1 cm × 0.2 cm) as the anode and platinum plate (1 cm × 1 cm × 0.01 cm) as the cathode connected to an MYWAVE MPD-3003S DC regulated power supply. The reaction mixture was stirred and electrolyzed at a constant current of 13 mA at 80 °C by heating mantle for 16 h. Upon completion, the solvent was removed directly under reduced pressure to afford the crude product, which was further purified by flash column chromatography to afford the desired products **3a-3z**、**3aa-3va** and **3ab-3aj.**

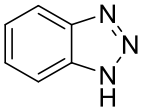
Unsuccessful examples



2-methyl-1-phenylpropan-1-one

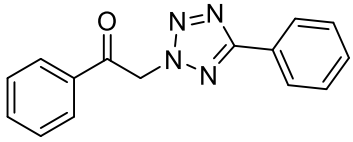


1*H*-pyrazole

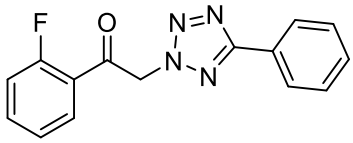


1*H*-benzo[*d*][1,2,3]triazole

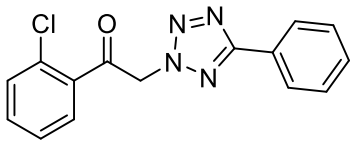
Characterization Data of Products 3a-3z、3aa-3va and 3ab-3aj.



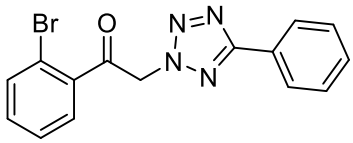
1-Phenyl-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3a): The general procedure was followed using substrate acetophenone **1a** (1.50 mmol, 180 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 20/1→10/1) yielded **3a** (112 mg, 85%) as a white solid. R_f = 0.33 (10:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.17 (d, *J* = 4.8 Hz, 2H), 8.01 (d, *J* = 7.5 Hz, 2H), 7.68 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.55 (dd, *J* = 7.4, 7.4 Hz, 2H), 7.49 (d, *J* = 4.9 Hz, 3H), 6.14 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 188.9, 165.7, 134.7, 133.8, 130.4, 129.2, 128.9, 128.2, 127.2, 127.0, 58.2. HR-MS (ESI) *m/z* calcd for $C_{15}H_{13}N_4O$ $[M+H]^+$ 265.1084, found 265.1082. Analytical data for compound **3a** is consistent with literature report.[1]



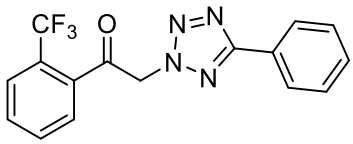
1-(2-Fluorophenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3b): The general procedure was followed using substrate 1-(2-fluorophenyl)ethan-1-one **1a** (1.5 mmol, 207 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→8/1) yielded **3b** (96 mg, 68%) as a white solid. m.p: 115.0-116.8℃. R_f = 0.30 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 3.5 Hz, 2H), 8.03 (dd, *J* = 7.4, 7.4 Hz, 1H), 7.72 – 7.62 (m, 1H), 7.49 (s, 3H), 7.38 – 7.27 (m, 2H), 6.09 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.2, 165.6, 162.6 (d, $^1J_{C\text{-}F}$= 254.3 Hz), 136.6 (d, $^3J_{C\text{-}F}$ = 9.3 Hz), 131.2, 131.2, 130.4, 128.9, 127.3, 125.3, 125.3, 122.0 (d, $^3J_{C\text{-}F}$ = 13.4 Hz), 116.8 (d, $^2J_{C\text{-}F}$ = 23.5 Hz), 61.6. HR-MS (ESI) *m/z* calcd for $C_{15}H_{12}FN_4O$ $[M+H]^+$ 283.0990, found 283.0981. IR (KBr): 3062, 3008, 2963, 1837, 1699, 1606, 1450, 1342, 1277, 1515, 1041, 849, 782, 698, 626 cm^{-1}.



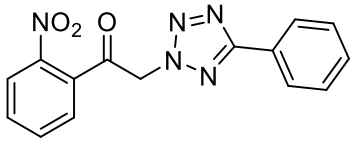
1-(2-Chlorophenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3c): The general procedure was followed using substrate 1-(2-chlorophenyl)ethan-1-one **1a** (1.5 mmol, 231 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→8/1) yielded **3c** (121 mg, 81%) as a white solid. m.p: 133.9-135.2℃. R_f = 0.30 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 5.5 Hz, 2H), 7.76 (d, *J* = 7.5 Hz, 1H), 7.50 (d, *J* = 12.0 Hz, 5H), 7.42 (s, 1H), 6.15 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.1, 165.6, 134.9, 133.8, 132.1, 131.1, 130.7, 130.5, 128.9, 127.5, 127.2, 127.0, 60.9. HR-MS (ESI) *m/z* calcd for $C_{15}H_{12}ClN_4O$ $[M+H]^+$ 299.0694, found 299.0688. IR (KBr): 3081, 2956, 1719, 1588, 1448, 1329, 1211, 1039, 838, 759, 658 cm^{-1}.



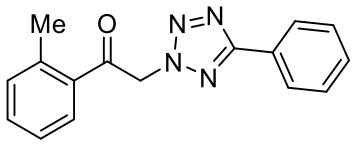
1-(2-Bromophenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3d): The general procedure was followed using substrate 1-(2-bromophenyl)ethan-1-one **1a** (1.5 mmol, 298 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 13/1→6/1) yielded **3d** (141 mg, 82%) as a white solid. m.p: 130.7-132.8℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 6.4, 2.8 Hz, 2H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.62 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.49 (dd, *J* = 5.1, 1.7 Hz, 3H), 7.46 – 7.38 (m, 2H), 6.11 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.2, 165.6, 137.3, 134.3, 133.4, 130.5, 129.9, 128.9, 127.9, 127.2, 127.0, 119.6, 60.2. HR-MS (ESI) *m/z* calcd for $C_{15}H_{12}BrN_4O$ $[M+H]^+$ 343.0189, found 343.0181. IR (KBr): 3082, 2954, 1714, 1583, 1469, 1331, 1206, 1041, 983, 836, 737, 696 cm^{-1}.



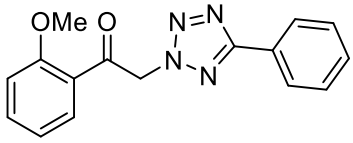
2-(5-Phenyl-2*H*-tetrazol-2-yl)-1-[2-(trifluoromethyl)phenyl]ethan-1-one (3e): The general procedure was followed using substrate 1-(2-(trifluoromethyl)phenyl)-ethan-1-one **1a** (1.5 mmol, 282 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 12/1→4/1) yielded **3e** (114 mg, 68%) as a white solid. m.p: 87.5-89.3℃. R_f = 0.30 (4:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 – 8.13 (m, 2H), 7.80 (d, *J* = 6.8 Hz, 1H), 7.68 (s, 2H), 7.62 (s, 1H), 7.49 (d, *J* = 5.1 Hz, 3H), 5.91 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.0, 165.8, 135.5 (q, $^4J_{C\text{-}F}$ = 3.6 Hz), 132.2, 131.7, 130.5, 128.9,127.9 (dd, $^2J_{C\text{-}F}$ = 32.8, 4.2 Hz), 127.5, 127.2 (q, $^4J_{C\text{-}F}$ = 4.9 Hz), 127.0, 127.0, 123.3 (d, $^1J_{C\text{-}F}$ = 273.9 Hz), 60.4. HR-MS (ESI) *m/z* calcd for $C_{16}H_{12}F_3N_4O$ $[M+H]^+$ 333.0958, found 333.0954. IR (KBr): 3082, 2990, 2882, 1711, 1592, 1520, 1496, 1483, 1308, 1243, 1178, 1113, 1089, 987, 813, 757 cm^{-1}.



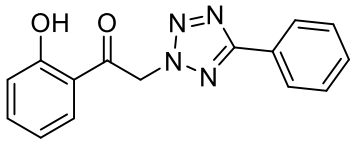
1-(2-Nitrophenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3f): The general procedure was followed using substrate 1-(2-nitrophenyl)ethan-1-one **1a** (1.5 mmol, 247 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 12/1→4/1) yielded **3f** (97 mg, 63%) as a pink solid. m.p:140.7-142.7℃. R_f = 0.30 (4:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.2 Hz, 1H), 8.10 – 8.05 (m, 2H), 7.73 (dd, *J* = 7.5, 7.5 Hz, 1H), 7.62 (dd, *J* = 7.8, 7.8 Hz, 1H), 7.50 – 7.42 (m, 4H), 5.89 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.1, 165.7, 145.5, 134.8, 133.8, 131.7, 130.6, 128.9, 128.0, 126.9, 126.8, 124.4, 60.1. HR-MS (ESI) *m/z* calcd for $C_{15}H_{12}N_5O_3$ $[M+H]^+$ 310.0935, found 310.0929. IR (KBr): 2948, 1729, 1533, 1451, 1344, 1256, 1005, 996, 710, 692 cm^{-1}.



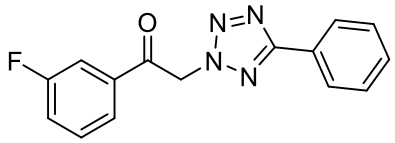
2-(5-Phenyl-2*H*-tetrazol-2-yl)-1-(*o*-tolyl)ethan-1-one (3g): The general procedure was followed using substrate 1-(*o*-tolyl)ethan-1-one **1a** (1.5 mmol, 201 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 13/1 → 10/1) yielded **3g** (65 mg, 47%) as a white solid. m.p: 166.5-168.4℃. R_f = 0.30 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 – 8.13 (m, 2H), 7.79 (d, *J* = 7.6 Hz, 1H), 7.55 – 7.44 (m, 4H), 7.40 – 7.31 (m, 2H), 6.06 (s, 2H), 2.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.3, 165.6, 140.5, 133.2, 132.8, 130.4, 128.9, 128.7, 127.3, 127.0, 127.0, 126.2, 59.5, 21.7. HR-MS (ESI) *m/z* calcd for $C_{16}H_{15}N_4O$ $[M+H]^+$ 279.1240, found 279.1242.



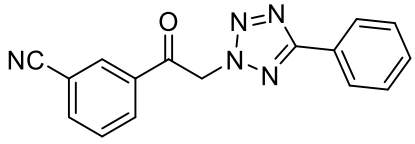
1-(2-Methoxyphenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3h): The general procedure was followed using substrate 1-(2-methoxyphenyl)ethan-1-one **1a** (1.5 mmol, 225 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column ch- romatography (PE/EtOAc: 13/1→6/1) yielded **3h** (68 mg, 51%) as a white solid. m.p:153.0-155.0℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (s, 2H), 7.98 (d, *J* = 9.4 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.48 (s, 3H), 7.14 – 7.01 (m, 2H), 6.11 (s, 2H), 4.05 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 165.3, 159.7, 135.8, 131.5, 130.3, 128.8, 127.5, 127.0, 123.8, 121.4, 111.7, 62.5, 55.8. HR-MS (ESI) *m/z* calcd for $C_{16}H_{15}N_4O_2$ $[M+H]^+$ 295.1190, found 295.1183. IR (KBr): 3074, 2952, 1679, 1595, 1486, 1287, 1204, 1023, 772, 634 cm^{-1}.



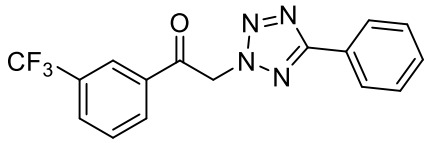
1-(2-Hydroxyphenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3i): The general procedure was followed using substrate 1-(2-hydroxyphenyl)ethan-1-one **1a** (1.5 mmol, 208 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 13/1→8/1) yielded **3i** (41 mg, 29%) as a white solid. m.p: 205.4-207.0℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.34 (s, 1H), 8.26 – 8.13 (m, 2H), 7.79 – 7.71 (m, 1H), 7.64 – 7.45 (m, 4H), 7.05 (dd, *J* = 15.0, 8.0 Hz, 2H), 6.19 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.9, 165.8, 162.7, 137.9, 130.6, 128.9, 128.5, 127.1, 127.0, 119.8, 119.3, 117.1, 57.4. HR-MS (ESI) *m/z* calcd for $C_{15}H_{13}N_4O_2$ $[M+H]^+$ 281.1033, found 281.1025. IR (KBr): 3139, 2992, 2952, 1665, 1450, 1346, 1280, 1204, 1043, 842, 790, 698 cm^{-1}.



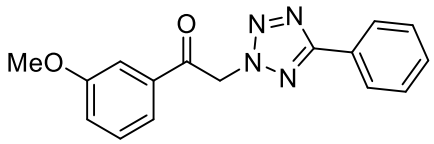
1-(3-Fluorophenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3j): The general procedure was followed using substrate 1-(3-fluorophenyl)ethan-1-one **1a** (1.5 mmol, 207 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→10/1) yielded **3j** (97 mg, 68%) as a white solid. m.p: 149.3-151.5℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 4.8 Hz, 2H), 7.79 (d, *J* = 7.7 Hz, 1H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.56 (dd, *J* = 6.8, 6.8 Hz, 1H), 7.49 (s, 3H), 7.40 (dd, *J* = 7.8, 7.8 Hz, 1H), 6.12 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.0, 165.7, 163.0 (d, $^1J_{C\text{-}F}$ = 250.1 Hz), 135.7, 131.0 (d, $^4J_{C\text{-}F}$ = 7.7 Hz), 130.5, 128.9, 127.1, 127.0, 123.9, 121.8 (d, $^3J_{C\text{-}F}$= 21.5 Hz), 115.0 (d, $^2J_{C\text{-}F}$ = 22.7 Hz), 58.2. HR-MS (ESI) *m/z* calcd for $C_{15}H_{12}FN_4O$ $[M+H]^+$ 283.0990, found 283.0986. IR (KBr): 3072, 2983, 2939, 2853, 1696, 1593, 1452, 1351, 1252, 1048, 876, 791, 730 cm^{-1}.



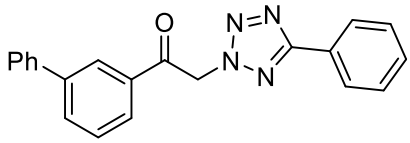
3-[2-(5-Phenyl-2*H*-tetrazol-2-yl)acetyl]benzonitrile (3k): The general procedure was followed using substrate 3-acetylbenzonitrile **1a** (1.5 mmol, 218 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 11/1→6/1) yielded **3k** (138 mg, 95%) as a yellow solid. m.p: 168.5-170.6℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) 8.30 (s, 1H), 8.22 (d, *J* = 8.0 Hz, 1H), 8.18 – 8.13 (m, 2H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.71 (dd, *J* = 7.9, 7.9 Hz, 1H), 7.53 – 7.46 (m, 3H), 6.14 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.4, 165.9, 137.4, 134.6, 132.0, 131.8, 130.6, 130.3, 129.0, 127.0, 126.9, 117.3, 114.0, 58.1. HR-MS (ESI) *m/z* calcd for $C_{16}H_{12}N_5O$ $[M+H]^+$ 290.1036, found 290.1033. IR (KBr): 3073, 2970, 2933, 1708, 1656, 1249, 1188, 1037, 822, 732 cm^{-1}.



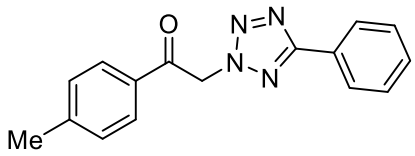
2-(5-Phenyl-2*H*-tetrazol-2-yl)-1-(3-(trifluoromethyl)phenyl)ethan-1-one (3l): The general procedure was followed using substrate 1-(3-(trifluoromethyl)phenyl)-ethan-1-one **1a** (1.5 mmol, 282 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→8/1) yielded **3l** (128 mg, 77%) as a white solid. m.p: 134.5-136.3℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (s, 1H), 8.22 – 8.15 (m, 3H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.72 (dd, *J* = 7.8, 7.8 Hz, 1H), 7.50 (dd, *J* = 5.1, 1.9 Hz, 3H), 6.17 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.0, 165.8, 134.3, 131.9 (d, $^2J_{C\text{-}F}$ = 33.4 Hz), 131.3,131.1 (q, $^4J_{C\text{-}F}$ = 3.5 Hz), 130.6, 130.0, 128.9, 127.1, 127.0, 125.1 (q, $^4J_{C\text{-}F}$ = 3.4 Hz),123.3 (d, $^1J_{C\text{-}F}$ = 272.8 Hz), 58.1. HR-MS (ESI) *m/z* calcd for $C_{16}H_{12}F_3N_4O$ $[M+H]^+$ 333.0958, found 333.0955. IR (KBr): 3081, 2979, 2941, 1710, 1615, 1455, 1329, 1218, 1073, 908, 804, 732, 662 cm^{-1}.



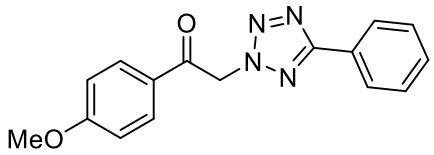
1-(3-Methoxyphenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3m): The general procedure was followed using substrate 1-(3-methoxyphenyl)ethan-1-one **1a** (1.5 mmol, 225 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→6/1) yielded **3m** (120 mg, 81%) as a white solid. m.p: 109.8-111.6℃. R_f = 0.32 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 – 8.14 (m, 2H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.53 – 7.42 (m, 5H), 7.22 (d, *J* = 8.2 Hz, 1H), 6.12 (s, 2H), 3.87 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.9, 165.6, 160.2, 135.1, 130.4, 130.2, 128.9, 127.3, 127.0, 121.2, 120.5, 112.5, 58.3, 55.6. HR-MS (ESI) *m/z* calcd for $C_{16}H_{15}N_4O_2$ $[M+H]^+$ 295.1190, found 295.1185. IR (KBr): 3079, 2988, 2947, 1702, 1597, 1450, 1344, 1263, 1204, 1039, 793, 733 cm^{-1}.



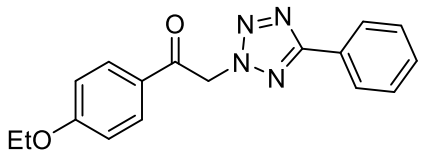
1-([1,1'-Biphenyl]-3-yl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3n): The general procedure was followed using substrate 1-([1,1'-biphenyl]-3-yl)ethan-1-one **1a** (1.5 mmol, 294 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 30/1→10/1) yielded **3n** (129 mg, 76%) as a white solid. m.p: 123.1-124.7℃. R_f = 0.32 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.16 (m, 3H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.89 (s, 1H), 7.63 (dd, *J* = 10.0, 7.8 Hz, 3H), 7.52 – 7.46 (m, 5H), 7.42 (dd, *J* = 7.3, 7.3 Hz, 1H), 6.19 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.0, 165.7, 142.5, 139.6, 134.4, 133.3, 130.5, 129.7, 129.1, 128.9, 128.2, 127.2, 127.0, 126.9, 58.3. HR-MS (ESI) *m/z* calcd for $C_{21}H_{17}N_4O$ $[M+H]^+$ 341.1397, found 341.1392. IR (KBr): 3084, 2961, 2912, 1808, 1452, 1347, 1214, 1128, 1113, 1004, 827, 793, 695 cm^{-1}.



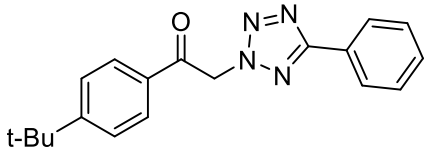
2-(5-Phenyl-2*H*-tetrazol-2-yl)-1-(*p*-tolyl)ethan-1-one (3o): The general procedure was followed using substrate 1-(*p*-tolyl)ethan-1-one **1a** (1.5 mmol, 201 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1 → 10/1) yielded **3o** (118 mg, 85%) as a white solid. m.p: 119.6-121.4℃. R_f = 0.32 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 5.2 Hz, 2H), 7.89 (d, *J* = 6.8 Hz, 2H), 7.47 (s, 3H), 7.34 (d, *J* = 6.9 Hz, 2H), 6.11 (s, 2H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.5, 145.9, 130.4, 129.9, 129.2, 128.9, 128.4, 128.3, 127.3, 127.0, 58.1, 21.9. HR-MS (ESI) *m/z* calcd for $C_{16}H_{15}N_4O$ $[M+H]^+$ 279.1240, found 279.1236. IR (KBr): 3058, 2981, 2947, 1694, 1604, 1530, 1451, 1348, 1233, 1039, 810, 726, 695 cm^{-1}.



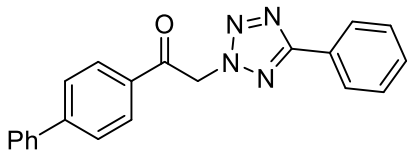
1-(4-Methoxyphenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3p): The general procedure was followed using substrate 1-(4-methoxyphenyl)ethan-1-one **1a** (1.5 mmol, 225 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→8/1) yielded **3p** (145 mg, 98%) as a white solid. R_f = 0.33 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (m, 2H), 7.98 (dd, *J* = 9.0, 2.4 Hz, 2H), 7.48 (dd, *J* = 4.5, 2.8 Hz, 3H), 7.01 (dd, *J* = 9.0, 2.4 Hz, 2H), 6.08 (s, 2H), 3.91 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.3, 165.6, 164.7, 130.6, 130.4, 128.9, 127.3, 127.0, 126.8, 114.4, 57.9, 55.7. HR-MS (ESI) *m/z* calcd for $C_{16}H_{15}N_4O_2$ $[M+H]^+$ 295.1190, found 295.1180. Analytical data for compound **3p** is consistent with literature report.[2]



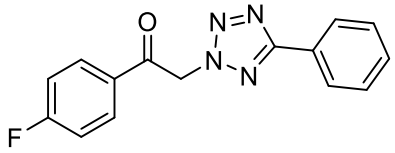
1-(4-Ethoxyphenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3q): The general procedure was followed using substrate 1-(4-ethoxyphenyl)ethan-1-one **1a** (1.5 mmol, 246 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→8/1) yielded **3q** (97 mg, 63%) as a white solid. m.p: 133.0-134.8℃. R_f = 0.33 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.14 (m, 2H), 7.97 (d, *J* = 7.0 Hz, 2H), 7.58 – 7.44 (m, 3H), 7.04 – 6.94 (m, 2H), 6.08 (s, 2H), 4.18 – 4.10 (m, 2H), 1.47 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.3, 165.6, 164.1, 130.6, 130.4, 128.9, 127.3, 127.0, 126.6, 114.8, 64.0, 57.9, 14.6. HR-MS (ESI) *m/z* calcd for $C_{17}H_{17}N_4O_2$ $[M+H]^+$ 309.1346, found 309.1341. IR (KBr): 3053, 2992, 2949, 1675, 1601, 1448, 1346, 1249, 1186, 921, 842, 729, 669 cm^{-1}.



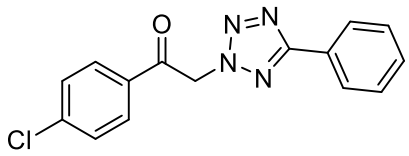
1-[4-(*tert*-Butyl)phenyl]-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3r): The general procedure was followed using substrate 1-[4-(tert-butyl)phenyl]ethan-1-one **1a** (1.5 mmol, 264 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 13/1→8/1) yielded **3r** (146 mg, 91%) as a white solid. m.p: 147.2-149.1℃. R_f = 0.30 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 – 8.15 (m, 2H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.49 (dd, *J* = 5.1, 2.2 Hz, 3H), 6.12 (s, 2H), 1.37 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.5, 165.6, 158.8, 131.3, 130.4, 128.9, 128.2, 127.3, 127.0, 126.2, 58.1, 35.4, 31.0. HR-MS (ESI) *m/z* calcd for $C_{19}H_{21}N_4O$ $[M+H]^+$ 321.1710, found 321.1707. IR (KBr): 3433, 3076, 2966, 1689, 1604, 1448, 1344, 1235, 1107, 996, 831, 729, 691 cm^{-1}.



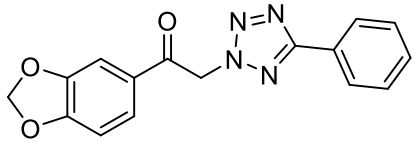
1-([1,1'-Biphenyl]-4-yl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3s): The general procedure was followed using substrate 1-([1,1'-biphenyl]-4-yl)ethan-1-one **1a** (1.5 mmol, 294 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 30/1→10/1) yielded **3s** (84 mg, 50%) as a white solid. m.p: 130.1-131.8℃. R_f = 0.30 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.14 (m, 2H), 8.07 (d, *J* = 5.8 Hz, 2H), 7.81 – 7.72 (m, 2H), 7.65 (d, *J* = 6.3 Hz, 3H), 7.54 – 7.46 (m, 5H), 6.17 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.5, 165.7, 147.4, 139.3, 132.5, 130.4, 129.1, 128.9, 128.8, 128.7, 127.8, 127.3, 127.3, 127.0, 58.2. HR-MS (ESI) *m/z* calcd for $C_{21}H_{17}N_4O$ $[M+H]^+$ 341.1397, found 341.1393. IR (KBr): 3000, 2950, 1699, 1602, 1450, 1339, 1231, 994, 730, 693 cm^{-1}.



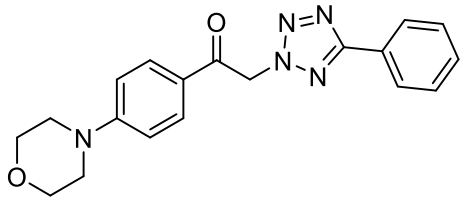
1-(4-Fluorophenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3t): The general procedure was followed using substrate 1-(4-fluorophenyl)ethan-1-one **1a** (1.5 mmol, 207 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→10/1) yielded **3t** (98 mg, 69%) as a white solid. m.p: 141.0-142.4℃. R_f = 0.30 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 6.2, 3.3 Hz, 2H), 8.03 (dd, *J* = 8.7, 5.0 Hz, 2H), 7.48 (d, *J* = 4.9 Hz, 3H), 7.25 – 7.17 (m, 2H), 6.10 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.5, 166.8 (d, $^1J_{C\text{-}F}$ = 258.6 Hz), 165.7,131.0 (d, $^3J_{C\text{-}F}$ = 9.7 Hz), 130.5, 130.3 (d, $^4J_{C\text{-}F}$= 2.9 Hz), 128.9, 127.1, 127.0, 116.5 (d, $^2J_{C\text{-}F}$ = 22.2 Hz), 58.0. HR-MS (ESI) *m/z* calcd for $C_{15}H_{12}FN_4O$ $[M+H]^+$ 283.0990, found 283.0986. IR (KBr): 3072, 2980, 2933, 1694, 1596, 1454, 1353, 1235, 1156, 997, 830, 729, 591 cm^{-1}.



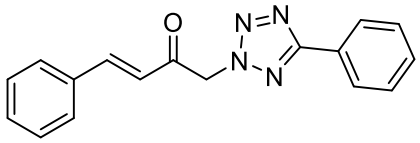
1-(4-Chlorophenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3u): The general procedure was followed using substrate 1-(4-chlorophenyl)ethan-1-one **1a** (1.5 mmol, 232 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 20/1→10/1) yielded **3u** (109 mg, 73%) as a white solid. R_f = 0.30 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 4.5, 3.3 Hz, 2H), 7.94 (d, *J* = 8.6 Hz, 2H), 7.56 – 7.43 (m, 5H), 6.10 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.9, 165.7, 141.4, 132.1, 130.5, 129.6, 129.6, 128.9, 127.1, 127.0, 58.1. HR-MS (ESI) *m/z* calcd for $C_{15}H_{12}ClN_4O$ $[M+H]^+$ 299.0694, found 299.0684. Analytical data for compound **3u** is consistent with literature report.[2]



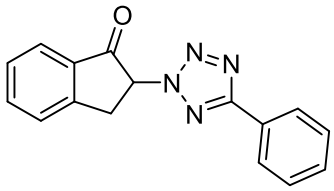
1-(Benzo[d][1,3]dioxol-5-yl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3v): The general procedure was followed using substrate 1-(benzo[d][1,3]dioxol-5-yl)-ethan-1-one **1a** (1.5 mmol, 246 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 20/1→8/1) yielded **3v** (76 mg, 49%) as a white solid. m.p: 122.9-124.7℃. R_f = 0.32 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 2H), 7.59 (d, *J* = 8.1 Hz, 1H), 7.46 (d, *J* = 9.7 Hz, 4H), 6.93 (d, *J* = 8.1 Hz, 1H), 6.10 (s, 2H), 6.06 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.9, 165.6, 153.2, 148.8, 130.4, 128.9, 128.5, 127.3, 127.0, 124.7, 108.4, 107.8, 102.3, 57.9. HR-MS (ESI) *m/z* calcd for $C_{16}H_{13}N_4O_3$ $[M+H]^+$ 309.0982, found 309.0977. IR (KBr): 3072, 2986, 2945, 2900, 1679, 1602, 1504, 1450, 1344, 1256, 1106, 1041, 937, 892, 811, 734 cm^{-1}.



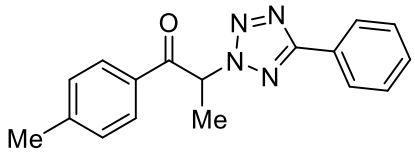
1-(4-Morpholinophenyl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3w): The general procedure was followed using substrate 1-(4-morpholinophenyl)ethan-1-one **1a** (1.0 mmol, 205 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 13/1→6/1) yielded **3w** (33 mg, 20%) as a light yellow solid. m.p: 176.4-179.0℃. R_f = 0.32 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 2H), 7.91 (d, *J* = 7.9 Hz, 2H), 7.47 (s, 3H), 6.91 (d, *J* = 7.9 Hz, 2H), 6.06 (s, 2H), 3.86 (s, 4H), 3.37 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.7, 165.5, 155.0, 130.4, 130.3, 128.9, 127.3, 127.0, 124.0, 113.3, 66.5, 57.8, 47.1. HR-MS (ESI) *m/z* calcd for $C_{19}H_{20}N_5O_2$ $[M+H]^+$ 350.1612, found 350.1608. IR (KBr): 3080, 2911, 2863, 1662, 1599, 1430, 1235, 1103, 1022, 979, 876, 751, 667 cm^{-1}.



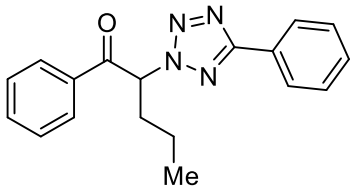
***(E)*-4-Phenyl-1-(5-phenyl-2*H*-tetrazol-2-yl)but-3-en-2-one (3x):** The general procedure was followed using substrate *(E)*-4-phenylbut-3-en-2-one **1a** (1.5 mmol, 150 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 22/1→10/1) yielded **3x** (36 mg, 36%) as a light yellow solid. m.p: 139.2-140.9℃. R_f = 0.32 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 4.7 Hz, 2H), 7.77 (d, *J* = 16.1 Hz, 1H), 7.60 – 7.37 (m, 8H), 6.76 (d, *J* = 16.1 Hz, 1H), 5.74 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.7, 165.7, 146.2, 133.6, 131.6, 130.5, 129.2, 128.9, 128.8, 127.2, 127.0, 121.1, 59.6. HR-MS (ESI) *m/z* calcd for $C_{17}H_{15}N_4O$ $[M+H]^+$ 291.1240, found 291.1230. IR (KBr): 3060, 2954, 1689, 1610, 1452, 1342, 1192, 1039, 978, 741, 698 cm^{-1}.



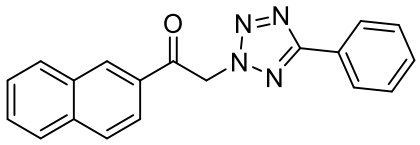
2-(5-Phenyl-2*H*-tetrazol-2-yl)-2,3-dihydro-1*H*-inden-1-one (3y): The general procedure was followed using substrate 2,3-dihydro-1*H*-inden-1-one **1a** (1.5 mmol, 198 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 16/1→8/1) yielded **3y** (68 mg, 49%) as a yellow liquid. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (dd, *J* = 6.5, 2.8 Hz, 2H), 7.90 (d, *J* = 7.7 Hz, 1H), 7.76 (dd, *J* = 7.5, 7.5 Hz, 1H), 7.59 (d, *J* = 7.7 Hz, 1H), 7.52 (dd, *J* = 7.5, 7.5 Hz, 1H), 7.49 – 7.44 (m, 3H), 5.89 (dd, *J* = 8.5, 5.5 Hz, 1H), 3.95 (dd, *J* = 17.1, 8.6 Hz, 1H), 3.82 (dd, *J* = 17.1, 5.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.3, 165.7, 150.8, 136.6, 133.7, 130.4, 128.8, 128.8, 127.2, 127.0, 126.7, 125.3, 65.7, 33.5. HR-MS (ESI) *m/z* calcd for $C_{16}H_{13}N_4O$ $[M+H]^+$ 277.1084, found 277.1082. IR (KBr): 2961, 2917, 2848, 1723, 1608, 1461, 1267, 1208, 1016, 790, 736, 698 cm^{-1}.



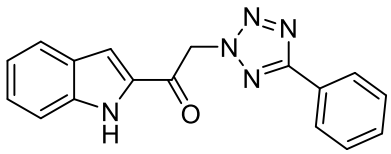
2-(5-Phenyl-2*H*-tetrazol-2-yl)-1-(*p*-tolyl)propan-1-one (3z): The general procedure was followed using substrate 1-(p-tolyl)propan-1-one **1a** (1.5 mmol, 222 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 30/1 → 10/1) yielded **3z** (101 mg, 69%) as a white solid. m.p: 121.3-123.1℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 – 8.09 (m, 2H), 7.87 (d, *J* = 7.8 Hz, 2H), 7.45 (s, 3H), 7.28 (s, 2H), 6.53 (q, *J* = 7.0 Hz, 1H), 2.41 (s, 3H), 2.04 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.8, 165.2, 145.3, 131.3, 131.2, 130.3, 129.8, 128.8, 127.32, 127.0, 63.0, 21.7, 17.0. HR-MS (ESI) *m/z* calcd for $C_{17}H_{17}N_4O$ $[M+H]^+$ 293.1397, found 293.1395. IR (KBr): 3090, 2991, 1802, 1604, 1445, 1256, 1143, 1055, 989, 977, 856, 752, 647 cm^{-1}.



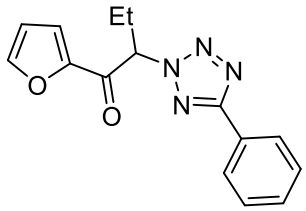
1-Phenyl-2-(5-phenyl-2*H*-tetrazol-2-yl)pentan-1-one (3aa): The general procedure was followed using substrate 1-phenylpentan-1-one **1a** (1.5 mmol, 243 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 20/1→10/1) yielded **3aa** (130 mg, 85%) as a yellow liquid. R_f = 0.32 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 2H), 7.98 (d, *J* = 7.6 Hz, 2H), 7.60 (dd, *J* = 7.2, 7.2 Hz, 1H), 7.52 – 7.41 (m, 5H), 6.46 (dd, *J* = 9.9, 3.0 Hz, 1H), 2.69 – 2.19 (m, 2H), 1.48 – 1.33 (m, 2H), 1.01 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.0, 165.3, 134.3, 134.2, 130.4, 129.1, 128.8, 128.6, 127.3, 127.0, 67.3, 32.8, 19.3, 13.5. HR-MS (ESI) *m/z* calcd for $C_{18}H_{19}N_4O$ $[M+H]^+$ 307.1553, found 307.1553. Analytical data for compound **3aa** is consistent with literature report.[3]



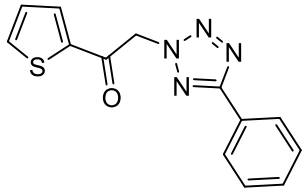
1-(Naphthalen-2-yl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3ba): The general procedure was followed using substrate 1-(naphthalen-2-yl)ethan-1-one **1a** (1.5 mmol, 255 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→10/1) yielded **3ba** (139 mg, 88%) as a white solid. m.p: 203.1-205.1℃. R_f = 0.33 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (s, 1H), 8.19 (d, *J* = 7.0 Hz, 2H), 8.08 – 7.89 (m, 4H), 7.66 (dd, *J* = 16.3, 7.4 Hz, 2H), 7.49 (d, *J* = 2.3 Hz, 3H), 6.28 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.9, 165.7, 136.2, 132.4, 131.2, 130.4, 130.2, 129.7, 129.4, 129.3, 128.9, 128.0, 127.4, 127.3, 127.0, 123.3, 58.2. HR-MS (ESI) *m/z* calcd for $C_{19}H_{15}N_4O$ $[M+H]^+$ 315.1240, found 315.1235. IR (KBr): 3036, 2956, 1696, 1627, 1450, 1353, 1277, 1193, 1043, 861, 818, 737 cm^{-1}.



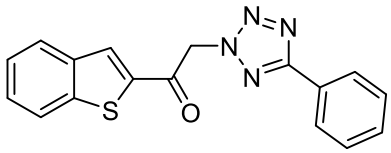
1-(1*H*-indol-2-yl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3ca): The general procedure was followed using substrate 1-(1*H*-indol-2-yl)ethan-1-one **1a** (1.5 mmol, 234 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→8/1) yielded **3ca** (39 mg, 25%) as a white solid. R_f = 0.33 (4:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.18 (d, *J* = 4.6 Hz, 2H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.57 – 7.32 (m, 6H), 7.20 (dd, *J* = 8.0, 8.0 Hz, 1H), 6.10 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 183.5, 164.8, 138.8, 132.8, 131.2, 129.8, 127.2, 126.9, 126.9, 123.5, 121.2, 113.4, 111.8, 100.0, 58.4. HR-MS (ESI) *m/z* calcd for $C_{17}H_{14}N_5O$ $[M+H]^+$ 304.1193, found 304.1187. IR (KBr): 3324, 2962, 2928, 2849, 1667, 1525, 1383, 1262, 1093, 807, 738, 688 cm^{-1}.



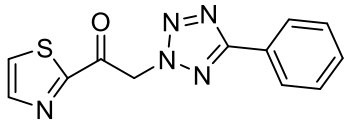
1-(Furan-2-yl)-2-(5-phenyl-2*H*-tetrazol-2-yl)butan-1-one (3da): The general procedure was followed using substrate 1-(furan-2-yl)butan-1-one **1a** (1.5 mmol, 207 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 22/1→10/1) yielded **3da** (105 mg, 74%) as a white liquid. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.10 (m, 2H), 7.62 (s, 1H), 7.46 (s, 3H), 7.31 (s, 1H), 6.57 (s, 1H), 6.13 (dd, *J* = 8.7, 5.2 Hz, 1H), 2.53 (dq, *J* = 22.5, 7.1 Hz, 2H), 1.05 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.5, 165.3, 150.4, 147.6, 130.4, 128.8, 127.3, 127.0, 119.7, 113.0, 69.1, 24.1, 10.6. HR-MS (ESI) *m/z* calcd for $C_{15}H_{15}N_4O_2$ $[M+H]^+$ 283.1190, found 283.1189. IR (KBr): 3107, 2974, 2880, 1667, 1563, 1469, 1465, 1317, 1240, 1160, 1054, 998, 926, 797, 689 cm^{-1}.



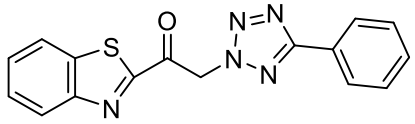
2-(5-Phenyl-2*H*-tetrazol-2-yl)-1-(thiophen-2-yl)ethan-1-one (3ea): The general procedure was followed using substrate 1-(thiophen-2-yl)ethan-1-one **1a** (1.5 mmol, 189 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 18/1→10/1) yielded **3ea** (54 mg, 59%) as a white solid. m.p: 120.9-122.5℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 5.2 Hz, 2H), 7.82 (dd, *J* = 14.1, 4.3 Hz, 2H), 7.49 (d, *J* = 5.0 Hz, 3H), 7.25 – 7.20 (m, 1H), 6.04 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 181.7, 165.7, 140.1, 135.8, 133.0, 130.5, 128.9, 128.7, 127.1, 127.0, 58.0. HR-MS (ESI) *m/z* calcd for $C_{13}H_{11}N_4OS$ $[M+H]^+$ 271.0648, found 271.0640. IR (KBr): 3079, 2954, 1692, 1516, 1469, 1405, 1240, 1043, 937, 797, 742 cm^{-1}.



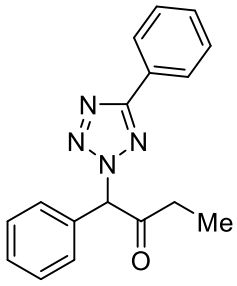
1-(Benzo[b]thiophen-2-yl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3fa): The general procedure was followed using substrate 1-(benzo[b]thiophen-2-yl)ethan-1-one **1a** (1.5 mmol, 264 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 18/1→10/1) yielded **3fa** (150 mg, 93%) as a yellow solid. m.p: 171.8-173.7℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 – 8.15 (m, 2H), 8.11 (s, 1H), 7.94 (dd, *J* = 19.3, 8.1 Hz, 2H), 7.58 – 7.44 (m, 5H), 6.15 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.2, 165.8, 142.9, 139.4, 138.7, 130.5, 130.4, 128.9, 128.5, 127.1, 127.0, 126.4, 125.6, 123.1, 58.0. HR-MS (ESI) *m/z* calcd for $C_{17}H_{13}N_4OS$ $[M+H]^+$ 321.0805, found 321.0798. IR (KBr): 2973, 2891, 1683, 1593, 1513, 1469, 1450, 1341, 1233, 1176, 1041, 839, 738, 700 cm^{-1}.



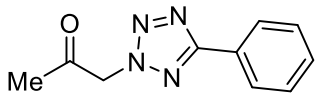
2-(5-Phenyl-2*H*-tetrazol-2-yl)-1-(thiazol-2-yl)ethan-1-one (3ga): The general procedure was followed using substrate 1-(thiazol-2-yl)ethan-1-one **1a** (1.5 mmol, 191 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 12/1→8/1) yielded **3ga** (93 mg, 68%) as a light yellow solid. m.p: 97.2-99.4℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 – 8.10 (m, 3H), 7.90 – 7.83 (m, 1H), 7.55 – 7.45 (m, 3H), 6.34 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.9, 165.7, 162.9, 145.5, 130.5, 128.9, 127.9, 127.2, 127.0, 58.0. HR-MS (ESI) *m/z* calcd for $C_{12}H_{10}N_5OS$ $[M+H]^+$ 272.0601, found 272.0595. IR (KBr): 3041, 3122, 3090, 2985, 2954, 1702, 1527, 1248, 1154, 1047, 950, 834, 734, 695 cm^{-1}.



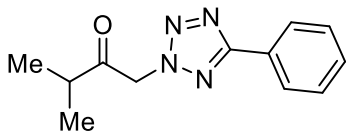
1-(Benzo[d]thiazol-2-yl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3ha): The general procedure was followed using substrate 1-(benzo[d]thiazol-2-yl)ethan-1-one **1a** (1.5 mmol, 265 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 20/1→8/1) yielded **3ha** (78 mg, 40%) as a light yellow solid. m.p: 186.8-188.9℃. R_f = 0.32 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.6 Hz, 1H), 8.19 (s, 2H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.70 – 7.56 (m, 2H), 7.49 (s, 3H), 6.46 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.5, 165.8, 162.3, 153.3, 137.39, 130.5, 128.9, 128.7, 127.6, 127.2, 127.0, 125.8, 122.6, 58.1. HR-MS (ESI) *m/z* calcd for $C_{16}H_{12}N_5OS$ $[M+H]^+$ 322.0757, found 322.0750. IR (KBr): 3081, 3001, 2959, 1718, 1450, 1346, 1043, 949, 836, 734, 689 cm^{-1}.



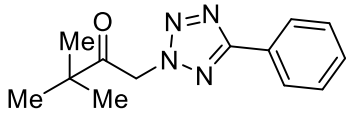
1-Phenyl-1-(5-phenyl-2*H*-tetrazol-2-yl)butan-2-one (3ia): The general procedure was followed using substrate 1-phenylbutan-2-one **1a** (1.5 mmol, 222 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 20/1→10/1) yielded **3ia** (143 mg, 91%) as a yellow liquid. R_f = 0.32 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 2H), 7.53 (d, *J* = 51.7 Hz, 8H), 6.66 (s, 1H), 2.60 – 2.44 (m, 2H), 1.10 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.4, 165.2, 131.3, 130.4, 130.0, 129.9, 129.3, 128.8, 127.3, 127.0, 75.2, 33.4, 7.7. HR-MS (ESI) *m/z* calcd for $C_{17}H_{17}N_4O$ $[M+H]^+$ 293.1397, found 293.1397. IR (KBr): 3060, 2954, 1734, 1450, 1355, 1204, 1102, 1050, 928, 815 733, 693 cm^{-1}.



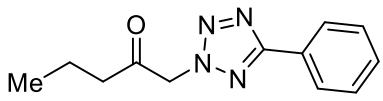
1-(5-Phenyl-2*H*-tetrazol-2-yl)propan-2-one (3ja): The general procedure was followed using substrate propan-2-one **1a** (1.5 mmol, 87 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→10/1) yielded **3ja** (47 mg, 48%) as a white solid. R_f = 0.33 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.53 – 7.47 (m, 3H), 5.48 (s, 2H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.8, 165.8, 130.6, 128.9, 127.0, 127.0, 61.0, 27.1. HR-MS (ESI) *m/z* calcd for $C_{10}H_{11}N_4O$ $[M+H]^+$ 203.0927, found 203.0925. Analytical data for compound **3ja** is consistent with literature report.[3]



3-Methyl-1-(5-phenyl-2*H*-tetrazol-2-yl)butan-2-one (3ka): The general procedure was followed using substrate 3-methylbutan-2-one **1a** (1.5 mmol, 129 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1 → 10/1) yielded **3ka** (39 mg, 34%) as a white solid. m.p: 99.6-100.9℃. R_f = 0.33 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 6.9 Hz, 2H), 7.49 (d, *J* = 4.7 Hz, 3H), 5.56 (s, 2H), 2.75 (p, *J* = 6.8 Hz, 1H), 1.23 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.4, 165.6, 130.5, 128.9, 127.1, 127.0, 58.8, 38.7, 17.9. HR-MS (ESI) *m/z* calcd for $C_{12}H_{15}N_4O$ $[M+H]^+$ 231.1240, found 231.1242. IR (KBr): 2997, 2979, 2877, 1721, 1529, 1469, 1346, 1200, 1050, 829, 730, 693 cm^{-1}.

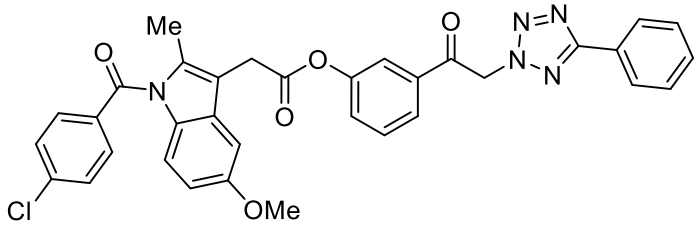


3,3-Dimethyl-1-(5-phenyl-2*H*-tetrazol-2-yl)butan-2-one (3la): The general procedure was followed using substrate 3,3-dimethylbutan-2-one **1a** (1.5 mmol, 150 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 15/1→10/1) yielded **3la** (32 mg, 25%) as a white solid. R_f = 0.33 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 2H), 7.47 (s, 3H), 5.67 (s, 2H), 1.32 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.4, 165.5, 130.4, 128.9, 127.3, 127.0, 56.4, 43.7, 26.2. HR-MS (ESI) *m/z* calcd for $C_{13}H_{17}N_4O$ $[M+H]^+$ 245.1397, found 245.1394. Analytical data for compound **3la** is consistent with literature report.[4]

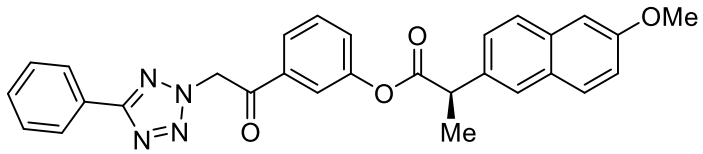


1-(5-Phenyl-2*H*-tetrazol-2-yl)pentan-2-one (3ma): The general procedure was followed using substrate pentan-2-one **1a** (1.5 mmol,129 mg) and 5-phenyltetrazole

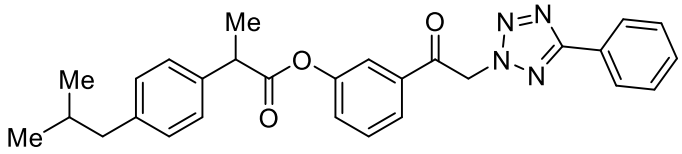
2a (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 30/1→10/1) yielded **3ma** (26 mg, 24%) as a white solid. m.p: 86.6-88.5℃. R_f = 0.33 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 – 8.13 (m, 2H), 7.49 (s, 3H), 5.46 (s, 2H), 2.46 (t, *J* = 7.2 Hz, 2H), 1.69 (q, *J* = 7.3 Hz, 2H), 0.95 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.2, 165.7, 130.5, 128.9, 127.1, 127.0, 60.5, 41.7, 16.6, 13.5. HR-MS (ESI) *m/z* calcd for $C_{12}H_{15}N_4O$ $[M+H]^+$ 231.1240, found 231.1232. IR (KBr): 3074, 2963, 2877, 1728, 1529, 1464, 1407, 1265, 1127, 1048, 923, 791 cm^{-1}.



3-(2-(5-Phenyl-2*H*-tetrazol-2-yl)acetyl)phenyl-2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)acetate (3na): The general procedure was followed using substrate 3-acetylphenyl-2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)-acetate **1a** (0.4 mmol, 190 mg) and 5-phenyltetrazole **2a** (1.2 mmol, 175 mg). Isolation by column chromatography (PE/EtOAc: 7/1→5/1) yielded **3na** (120 mg, 48%) as a light yellow solid. m.p: 128.3-130.1℃. R_f = 0.30 (3:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 – 8.09 (m, 2H), 7.86 (d, *J* = 7.7 Hz, 1H), 7.75 – 7.64 (m, 3H), 7.61 – 7.44 (m, 6H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.05 (s, 1H), 6.88 (d, *J* = 9.0 Hz, 1H), 6.70 (d, *J* = 10.6 Hz, 1H), 6.09 (s, 2H), 3.95 (s, 2H), 3.84 (s, 3H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.0, 169.0, 168.3, 165.7, 156.2, 151.3, 139.5, 136.4, 135.1, 133.7, 131.2, 130.9, 130.5, 130.4, 129.2, 128.9, 127.9, 127.1, 127.0, 125.6, 121.3, 115.1, 111.7, 111.5, 101.3, 58.2, 55.8, 30.5, 13.5. HR-MS (ESI) *m/z* calcd for $C_{34}H_{27}ClN_5O_5$ $[M+H]^+$ 620.1695, found 620.1695. IR (KBr): 2932, 1758, 1671, 1608, 1362, 1241, 1166, 1068, 734, 693 cm^{-1}.

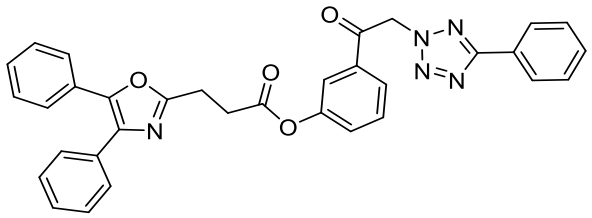


3-[2-(5-Phenyl-2*H*-tetrazol-2-yl)acetyl]phenyl(*R*)-2-(6-methoxynaphthalen-2-yl)-propanoate (3oa): The general procedure was followed using substrate 3-acetylphenyl-(*R*)-2-(6-methoxynaphthalen-2-yl)propanoate **1a** (0.4 mmol, 139 mg) and 5-phenyltetrazole **2a** (1.2 mmol, 175 mg). Isolation by column chromatography (PE/EtOAc: 11/1 → 5/1) yielded **3oa** (66 mg, 33%) as a white solid. m.p: 130.2-132.7℃. R_f = 0.33 (3:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.82 (d, *J* = 7.7 Hz, 1H), 7.79 – 7.72 (m, 3H), 7.66 – 7.59 (m, 1H), 7.56 – 7.43 (m, 5H), 7.35 – 7.28 (m, 1H), 7.21 – 7.08 (m, 2H), 6.06 (s, 2H), 4.13 (q, *J* = 7.1 Hz, 1H), 3.92 (s, 3H), 1.72 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.1, 172.9, 165.7, 157.9, 151.4, 135.0, 134.6, 133.9, 130.5, 130.3, 129.3, 129.0, 128.9, 127.9, 127.6, 127.2, 127.0, 126.3, 125.9, 125.4, 121.3, 119.3, 105.7, 58.1, 55.4, 45.6, 18.4. HR-MS (ESI) *m/z* calcd for $C_{29}H_{25}N_4O_4$ $[M+H]^+$ 493.1870, found 493.1870. IR (KBr): 3060, 2990, 2945, 2830, 1755, 1604, 1445, 1256, 1143, 1055, 989, 977, 856, 752, 647 cm^{-1}.

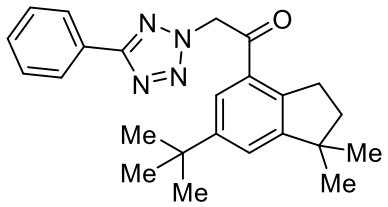


3-[2-(5-Phenyl-2*H*-tetrazol-2-yl)acetyl]phenyl-2-(4-isobutylphenyl)propanoate (3pa): The general procedure was followed using substrate 3-acetylphenyl 2-(4-iso-butylphenyl)propanoate **1a** (0.4 mmol, 160 mg) and 5-phenyltetrazole **2a** (1.2 mmol, 175 mg). Isolation by column chromatography (PE/EtOAc: 7/1→5/1) yielded **3pa** (67 mg, 28%) as a white solid. m.p: 107.7-110.0℃. R_f = 0.31 (3:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 – 8.12 (m, 2H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.68 – 7.60 (m, 1H), 7.57 – 7.44 (m, 4H), 7.37 – 7.27 (m, 3H), 7.16 (d, *J* = 8.0 Hz, 2H), 6.08 (s, 2H), 3.97 (q, *J* = 7.1 Hz, 1H), 2.48 (d, *J* = 7.2 Hz, 2H), 1.92 – 1.82 (m, 1H), 1.63 (d, *J* = 7.1 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$)

δ 188.1, 173.0, 165.7, 151.5, 141.1, 136.8, 135.0, 130.5, 130.2, 129.7, 129.4, 128.9, 128.0, 127.2, 127.0, 125.4, 121.3, 58.2, 45.3, 45.1, 30.2, 22.4, 18.5. HR-MS (ESI) *m/z* calcd for $C_{28}H_{29}N_4O_3$ $[M+H]^+$ 469.2234, found 469.2234. IR (KBr): 2990, 2952, 2869, 1753, 1698, 1448, 1244, 1159, 1068, 920, 734, 673 cm^{-1}.

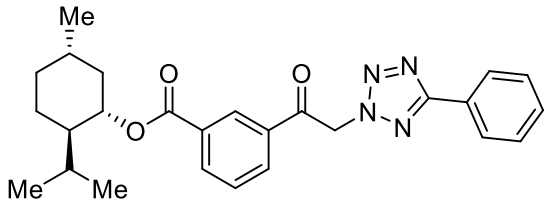


3-[2-(5-Phenyl-2*H*-tetrazol-2-yl)acetyl]phenyl-3-(4,5-diphenyloxazol-2-yl)propanoate (3qa): The general procedure was followed using substrate 3-acetylphenyl 3-(4,5-diphenyloxazol-2-yl)propanoate **1a** (0.4 mmol, 160 mg) and 5-phenyltetrazole **2a** (1.2 mmol, 175 mg). Isolation by column chromatography (PE/EtOAc: 7/1→5/1) yielded **3qa** (111 mg, 49%) as a white solid. m.p: 108.6-110.0℃. R_f = 0.30 (3:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 4.9 Hz, 2H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.72 – 7.62 (m, 3H), 7.61 – 7.39 (m, 8H), 7.34 (q, *J* = 7.1 Hz, 5H), 5.85 (s, 2H), 3.34 (t, *J* = 6.8 Hz, 2H), 3.20 (t, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.1, 170.5, 165.6, 161.3, 151.2, 145.8, 135.1, 135.1, 132.3, 130.5, 130.4, 128.9, 128.8, 128.7, 128.7, 128.3, 128.0, 127.9, 127.2, 127.0, 126.5, 125.8, 125.6, 121.5, 57.9, 31.2, 23.6. HR-MS (ESI) *m/z* calcd for $C_{33}H_{26}N_5O_4$ $[M+H]^+$ 556.1979, found 556.1980. IR (KBr): 3056, 2992, 1764, 1698, 1606, 1447, 1346, 1136, 1028, 957, 732, 691 cm^{-1}.

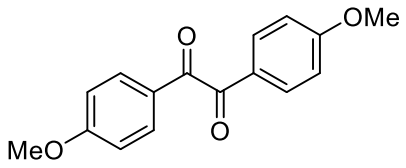


1-[6-(*tert*-Butyl)-1,1-dimethyl-2,3-dihydro-1*H*-inden-4-yl]-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3ra): The general procedure was followed using substrate 1-(6-(*tert*-butyl)-1,1-dimethyl-2,3-dihydro-1*H*-inden-4-yl)ethan-1-one **1a** (1.5 mmol,

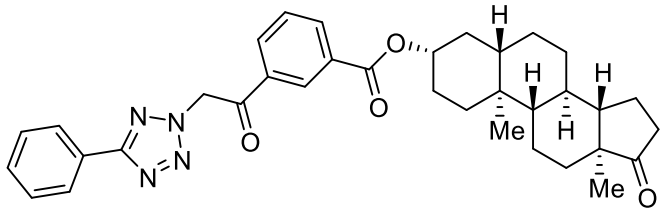
366 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 12/1→8/1) yielded **3ra** (93 mg, 48%) as a white solid. m.p: 160.4-162.6℃. R_f = 0.33 (4:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (dd, *J* = 7.4, 2.2 Hz, 2H), 7.72 (d, *J* = 1.5 Hz, 1H), 7.53 – 7.46 (m, 3H), 7.44 (d, *J* = 1.4 Hz, 1H), 6.12 (s, 2H), 3.18 (t, *J* = 7.3 Hz, 2H), 1.96 (t, *J* = 7.3 Hz, 2H), 1.39 (s, 9H), 1.27 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.2, 165.6, 155.3, 150.6, 142.6, 130.3, 129.9, 128.9, 127.3, 127.0, 125.0, 123.5, 59.2, 43.6, 41.3, 34.9, 31.5, 30.8, 28.7. HR-MS (ESI) *m/z* calcd for $C_{24}H_{29}N_4O$ $[M+H]^+$ 389.2336, found 389.2333. IR (KBr): 3062, 2955, 2864, 1578, 1464, 1346, 1220, 1046, 834, 731, 669 cm^{-1}.



(*1S,2R,5S*)-2-Isopropyl-5-methylcyclohexyl-3-[2-(5-phenyl-2*H*-tetrazol-2-yl)acetyl]benzoate (3sa): The general procedure was followed using substrate (*1S,2R,5S*)-2-isopropyl-5-methylcyclohexyl 3-acetylbenzoate **1a** (0.50 mmol, 150 mg) and 5-phenyltetrazole **2a** (1.5 mmol, 220 mg). Isolation by column chromatography (PE/EtOAc: 12/1 → 8/1) yielded **3sa** (115 mg, 51%) as a white solid. m.p: 110.1-111.8℃. R_f = 0.33 (4:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (s, 1H), 8.35 (d, *J* = 7.8 Hz, 1H), 8.24 – 8.14 (m, 3H), 7.66 (dd, *J* = 7.8, 7.8 Hz, 1H), 7.49 (dd, *J* = 5.3, 1.7 Hz, 3H), 6.19 (s, 2H), 5.00 (td, *J* = 10.9, 4.4 Hz, 1H), 2.13 (d, *J* = 12.0 Hz, 1H), 1.97 – 1.90 (m, 1H), 1.79 – 1.69 (m, 2H), 1.42 (s, 2H), 1.15 (q, *J* = 11.7 Hz, 2H), 0.96 – 0.92 (m, 6H), 0.87 (dd, *J* = 6.4, 4.8 Hz, 1H), 0.81 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.5, 165.7, 164.8, 135.4, 134.0, 132.1, 132.0, 130.5, 129.5, 129.1, 128.9, 127.2, 127.0, 75.8, 58.2, 47.2, 40.9, 34.2, 31.5, 26.6, 23.6, 22.0, 20.8, 16.6. HR-MS (ESI) *m/z* calcd for $C_{26}H_{31}N_4O_3$ $[M+H]^+$ 447.2391, found 447.2391. IR (KBr): 3069, 2957, 2871, 1718, 1604, 1451, 1346, 1213, 1122, 960, 738, 696, 641 cm^{-1}.

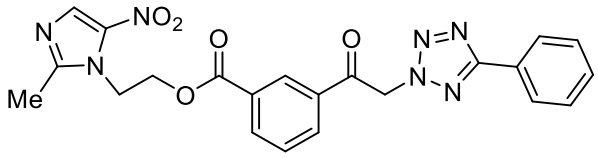


1,2-Bis(4-methoxyphenyl)ethane-1,2-dione (3ta): The general procedure was followed using substrate 1,2-bis(4-methoxyphenyl)ethan-1-one **1a** (1.2 mmol, 308 mg) and 5-phenyltetrazole **2a** (0.4 mmol, 58 mg). Isolation by column chromatography (PE/EtOAc: 10/1→7/1) yielded **3ta** (101 mg, 31%) as a yellow solid. R_f = 0.33 (4:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.90 (m, 4H), 6.99 – 6.93 (m, 4H), 3.87 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.5, 164.9, 132.4, 126.3, 114.3, 55.6. Analytical data for compound **3ta** is consistent with literature report.[5]

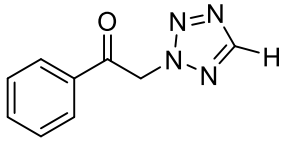


(*3S,5S,8R,9S,10S,13S,14S*)-10,13-Dimethyl-17-oxohexadecahydro-1*H*-cyclopenta[a]phenanthren-3-yl-3-[2-(5-phenyl-2*H*-tetrazol-2-yl)acetyl]benzoate (3ua): The general procedure was followed using substrate (*3S,5S,9S,10S,13S,14S*)-10,13-dimethyl-17-oxohexadecahydro-1*H*-cyclopenta[a]phenanthren-3-yl-3-acetylbenzoate **1a** (1.0 mmol, 400 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg). Isolation by column chromatography (PE/EtOAc: 8/1→5/1) yielded **3ua** (44 mg, 20%) as a white solid. m.p: 196.4-198.5℃. R_f = 0.31 (4:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (s, 1H), 8.34 (d, *J* = 7.5 Hz, 1H), 8.18 (dd, *J* = 6.7, 6.7 Hz, 3H), 7.65 (dd, *J* = 7.7, 7.7 Hz, 1H), 7.49 (s, 3H), 6.19 (s, 2H), 5.00 (m, 1H), 2.44 (dd, *J* = 19.2, 8.8 Hz, 1H), 2.14 – 2.03 (m, 1H), 2.02 – 1.89 (m, 2H), 1.80 (t, *J* = 13.4 Hz, 4H), 1.69 (d, *J* = 12.9 Hz, 2H), 1.52 – 1.47 (m, 1H), 1.31 (dd, *J* = 30.9, 18.0 Hz, 8H), 1.17 – 1.00 (m, 2H), 0.92 (s, 3H), 0.87 (s, 3H), 0.76 (t, *J* = 11.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.5, 165.7, 164.7, 135.4, 134.0, 132.1, 132.0, 130.5, 129.5,

129.1, 128.91, 127.2, 127.0, 75.1, 58.3, 54.3, 51.4, 47.8, 44.7, 36.7, 35.9, 35.7, 35.1, 34.0, 31.5, 30.8, 28.3, 27.5, 21.8, 20.5, 13.8, 12.3. HR-MS (ESI) *m/z* calcd for $C_{35}H_{41}N_4O_4$ $[M+H]^+$ 581.3122, found 581.3123. IR (KBr): 3069, 2939, 2844, 1737, 1713, 1604, 1449, 1287, 1216, 1129, 1008, 824, 734, 693 cm^{-1}.

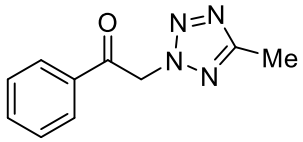


2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl-3-[2-(5-phenyl-2*H*-tetrazol-2-yl)acetyl]benzoate (3va): The general procedure was followed using substrate 2-(2-methyl-5-nitro-1*H*-imidazol-1-yl)ethyl 3-acetylbenzoate **1a** (0.4 mmol, 127 mg) and 5-phenyltetrazole **2a** (1.2 mmol, 175 mg). Isolation by column chromatography (PE/EtOAc: 4/1→1/1) yielded **3va** (55 mg, 30%) as a colorless oil. R_f = 0.30 (2:1 petroleum ether: ethyl acetate). ^1H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1H), 8.26 – 8.19 (m, 2H), 8.16 (dd, *J* = 6.5, 2.8 Hz, 2H), 7.97 (s, 1H), 7.66 (dd, *J* = 7.8, 7.8 Hz, 1H), 7.52 – 7.48 (m, 3H), 6.21 (s, 2H), 4.78 (t, *J* = 5.1 Hz, 2H), 4.71 (t, *J* = 5.0 Hz, 2H), 2.52 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.3, 165.7, 164.7, 150.6, 135.2, 134.3, 133.3, 132.9, 130.5, 130.2, 129.9, 129.0, 128.9, 127.1, 127.0, 63.5, 58.3, 44.9, 14.4. HR-MS (ESI) *m/z* calcd for $C_{22}H_{19}N_7O_5Na$ $[M+Na]^+$ 484.1340, found 484.1330. IR (KBr): 3134, 2996, 2952, 2855, 1716, 1601, 1536, 1472, 1362, 1211, 1100, 827, 729, 675 cm^{-1}.

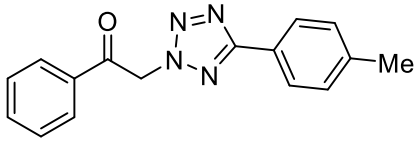


1-Phenyl-2-(2*H*-tetrazol-2-yl)ethan-1-one (3ab): The general procedure was followed using substrate acetophenone **1a** (1.5 mmol, 180 mg) and 2*H*-tetrazole **2a** (0.50 mmol, 35 mg). Isolation by column chromatography (PE/EtOAc: 15/1→10/1) yielded **3ab** (54 mg, 56%) as a white solid. m.p: 100.4-102.3℃. R_f = 0.33 (8:1 petroleum ether: ethyl acetate). ^1H NMR (400 MHz, $CDCl_3$) δ 8.63 (s, 1H), 7.99 (d, *J* = 7.9 Hz, 2H), 7.69 (dd, *J* = 7.4, 7.4 Hz, 1H), 7.56 (dd, *J* = 7.7, 7.7 Hz, 2H), 6.15 (s,

2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.8, 153.4, 134.8, 133.7, 129.2, 128.1, 58.1. HR-MS (ESI) *m/z* calcd for $C_9H_9N_4O$ $[M+H]^+$ 189.0771, found 189.0768. IR (KBr): 3062, 2967, 1709, 1599, 1455, 1342, 1231, 1129, 1034, 869, 756, 686 cm^{-1}.

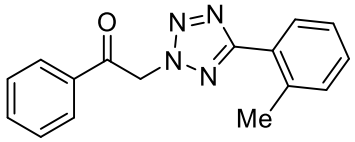


2-(5-Methyl-2*H*-tetrazol-2-yl)-1-phenylethan-1-one (3ac): The general procedure was followed using substrate acetophenone **1a** (1.5 mmol, 180 mg) and 5-methyl-2*H*-tetrazole **2a** (0.8 mmol, 67 mg). Isolation by column chromatography (PE/EtOAc: 14/1 → 10/1) yielded **3ac** (117 mg, 71%) as a white solid. m.p: 82.9-83.9 ℃. R_f = 0.33 (8:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.7 Hz, 2H), 7.68 (dd, *J* = 7.4, 7.4 Hz, 1H), 7.54 (dd, *J* = 7.6, 7.6 Hz, 2H), 6.04 (s, 2H), 2.59 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.2, 163.5, 134.7, 133.8, 129.2, 128.1, 57.9, 11.0. HR-MS (ESI) *m/z* calcd for $C_{10}H_{11}N_4O$ $[M+H]^+$ 203.0927, found 203.0925. IR (KBr): 3062, 2992, 2945, 1700, 1594, 1450, 1348, 1231, 1138, 1034, 996, 757, 686 cm^{-1}.

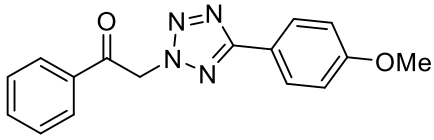


1-Phenyl-2-(5-(*p*-tolyl)-2*H*-tetrazol-2-yl)ethan-1-one (3ad): The general procedure was followed using substrate acetophenone **1a** (1.5 mmol, 180 mg) and 5-(p-tolyl)-2*H*-tetrazole **2a** (0.50 mmol, 80 mg). Isolation by column chromatography (PE/EtOAc: 20/1 → 10/1) yielded **3ad** (57 mg, 41%) as a white solid. m.p: 139.8-141.7℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 20.2, 8.2 Hz, 4H), 7.69 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.56 (m, *J* = 7.6, 7.6 Hz, 2H), 7.30 (d, *J* = 7.8 Hz, 2H), 6.13 (s, 2H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.0, 165.8, 140.6, 134.7, 133.9, 129.6, 129.2, 128.2, 126.9, 124.4,

58.1, 21.5. HR-MS (ESI) *m/z* calcd for $C_{16}H_{15}N_4O$ $[M+H]^+$ 279.1240, found 279.1230. IR (KBr): 2959, 1706, 1463, 1346, 1226, 1047, 834, 755, 683 cm^{-1}.

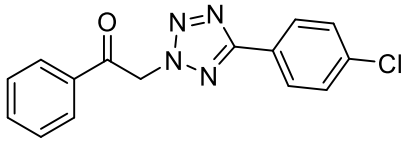


1-Phenyl-2-(5-(*o*-tolyl)-2*H*-tetrazol-2-yl)ethan-1-one (3ae): The general procedure was followed using substrate acetophenone **1a** (1.5 mmol, 180 mg) and 5-(*o*-tolyl)-2*H*-tetrazole **2a** (0.50 mmol, 80 mg). Isolation by column chromatography (PE/EtOAc: 30/1→10/1) yielded **3ae** (125 mg, 90%) as a white solid. m.p: 107.9-109.6℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 – 7.97 (m, 3H), 7.68 (d, *J* = 4.0 Hz, 1H), 7.55 (d, *J* = 4.1 Hz, 2H), 7.34 (dd, *J* = 17.0, 6.5 Hz, 3H), 6.16 (s, 2H), 2.63 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.0, 166.0, 137.6, 134.7, 133.8, 131.3, 130.0, 129.6, 129.2, 128.2, 126.4, 126.0, 58.2, 21.7. HR-MS (ESI) *m/z* calcd for $C_{16}H_{15}N_4O$ $[M+H]^+$ 279.1240, found 279.1236. IR (KBr): 2986, 1706, 1581, 1477, 1448, 1339, 1225, 1035, 748, 682, 637 cm^{-1}.

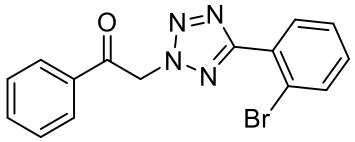


2-(5-(4-Methoxyphenyl)-2*H*-tetrazol-2-yl)-1-phenylethan-1-one (3af): The general procedure was followed using substrate acetophenone **1a** (1.5 mmol, 180 mg) and 5-(4-methoxyphenyl)-2*H*-tetrazole **2a** (0.50 mmol, 88 mg). Isolation by column chromatography (PE/EtOAc: 12/1→8/1) yielded **3af** (141 mg, 95%) as a white solid. m.p: 155.3-156.5℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.9 Hz, 2H), 8.01 (d, *J* = 8.5 Hz, 2H), 7.69 (dd, *J* = 7.4, 7.4 Hz, 1H), 7.56 (dd, *J* = 7.7, 7.7 Hz, 2H), 7.01 (d, *J* = 8.9 Hz, 2H), 6.12 (s, 2H), 3.87 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.0, 165.6, 161.3, 134.7, 133.9, 129.2, 128.5, 128.2, 119.8, 114.3, 58.1, 55.4. HR-MS (ESI) *m/z* calcd for $C_{16}H_{15}N_4O_2$

$[M+H]^+$ 295.1190, found 295.1184. IR (KBr): 3019, 2942, 2841, 1702, 1613, 1458, 1342, 1256, 1027, 837, 763, 684 cm^{-1}.

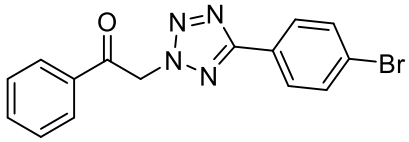


2-[5-(4-Chlorophenyl)-2*H*-tetrazol-2-yl]-1-phenylethan-1-one (3ag): The general procedure was followed using substrate acetophenone **1a** (1.5 mmol, 180 mg) and 5-(4-chlorophenyl)-2*H*-tetrazole **2a** (0.50 mmol, 90 mg). Isolation by column chromatography (PE/EtOAc: 14/1→10/1) yielded **3ag** (98 mg, 66%) as a white solid. m.p: 151.9-153.6℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 – 8.07 (m, 2H), 8.01 (d, *J* = 7.1 Hz, 2H), 7.69 (d, *J* = 7.4 Hz, 1H), 7.58 (d, *J* = 7.9 Hz, 2H), 7.51 – 7.43 (m, 2H), 6.14 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.8, 164.8, 136.5, 134.8, 133.7, 129.3, 129.2, 128.3, 128.2, 125.8, 58.2. HR-MS (ESI) *m/z* calcd for $C_{15}H_{12}ClN_4O$ $[M+H]^+$ 299.0694, found 299.0691. IR (KBr): 3079, 2948, 2848, 1696, 1597, 1452, 1337, 1227, 1087, 849, 755, 685 cm^{-1}.

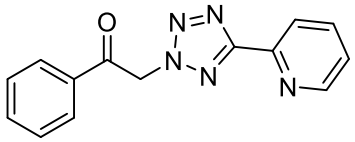


2-(5-(2-Bromophenyl)-2*H*-tetrazol-2-yl)-1-phenylethan-1-one (3ah): The general procedure was followed using substrate acetophenone **1a** (1.5 mmol, 180 mg) and 5-(2-bromophenyl)-2H-tetrazole **2a** (0.50 mmol, 112 mg). Isolation by column chromatography (PE/EtOAc: 15/1→10/1) yielded **3ah** (106 mg, 62%) as a white solid. m.p: 118.3-120.1℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.97 (m, 2H), 7.92 (d, *J* = 7.7 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.69 (dd, *J* = 7.2, 7.2 Hz, 1H), 7.56 (dd, *J* = 7.5, 7.5 Hz, 2H), 7.45 (dd, *J* = 7.5, 7.5 Hz, 1H), 7.34 (dd, *J* = 7.7, 7.7 Hz, 1H), 6.20 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.8, 164.6, 134.7, 134.1, 133.8, 131.9, 131.4, 129.2, 128.4, 128.2, 127.5, 122.2,

58.4. HR-MS (ESI) *m/z* calcd for $C_{15}H_{12}BrN_4O$ $[M+H]^+$ 343.0189, found 343.0185. IR (KBr): 3088, 2994, 2946, 1701, 1588, 1463, 1451, 1411, 1265, 998, 815, 716 cm^{-1}.



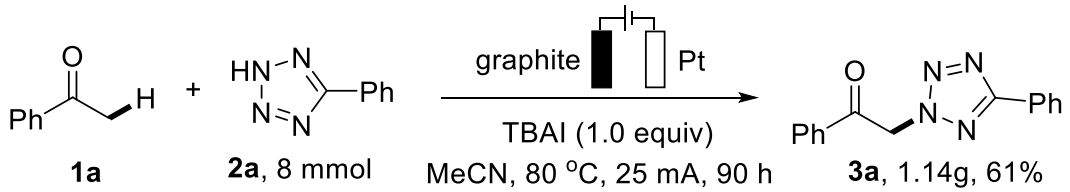
2-[5-(4-Bromophenyl)-2*H*-tetrazol-2-yl]-1-phenylethan-1-one (3ai): The general procedure was followed using substrate acetophenone **1a** (1.5 mmol, 180 mg) and 5-(4-bromophenyl)-2H-tetrazole **2a** (0.50 mmol, 112 mg). Isolation by column chromatography (PE/EtOAc: 15/1→10/1) yielded **3ai** (118 mg, 69%) as a white solid. m.p: 162.4-164.4℃. R_f = 0.30 (6:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (dd, *J* = 14.9, 8.1 Hz, 4H), 7.69 (dd, *J* = 7.2, 7.2 Hz,1H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.56 (dd, *J* = 7.5, 7.5 Hz, 2H), 6.14 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.8, 164.9, 134.7, 133.8, 132.2, 129.2, 128.5, 128.2, 126.2, 124.8, 58.2. HR-MS (ESI) *m/z* calcd for $C_{15}H_{12}BrN_4O$ $[M+H]^+$ 343.0189, found 343.0186. IR (KBr): 3079, 2996, 1706, 1598, 1454, 1343, 1228, 1066, 758, 684 cm^{-1}.



1-Phenyl-2-(5-(pyridin-2-yl)-2*H*-tetrazol-2-yl)ethan-1-one (3aj): The general procedure was followed using substrate acetophenone **1a** (1.5 mmol, 180 mg) and 2-(2H-tetrazol-5-yl)pyridine **2a** (0.50 mmol, 74 mg). Isolation by column chromatography (PE/EtOAc: 15/1→8/1) yielded **3aj** (38 mg, 28%) as a yellow liquid. R_f = 0.33 (4:1 petroleum ether: ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.32 (m, 2H), 7.99 (d, *J* = 6.8 Hz, 2H), 7.85 (dd, *J* = 7.6, 7.6 Hz, 1H), 7.66 (d, *J* = 7.0 Hz, 1H), 7.55 (dd, *J* = 6.9, 6.9 Hz, 2H), 7.31 (s, 1H), 6.46 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 152.4, 149.1, 144.5, 137.6, 134.3, 134.3, 129.1, 128.1, 125.4, 124.1, 55.7. HR-MS (ESI) *m/z* calcd for $C_{14}H_{12}N_5O$ $[M+H]^+$ 266.1036, found 266.1031.

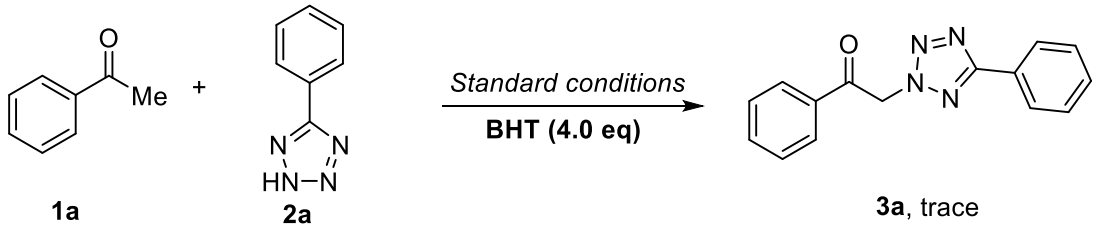
Gram-scale Synthesis and Control Experiments for the Mechanism Studies

(a) Gram-scale Synthesis



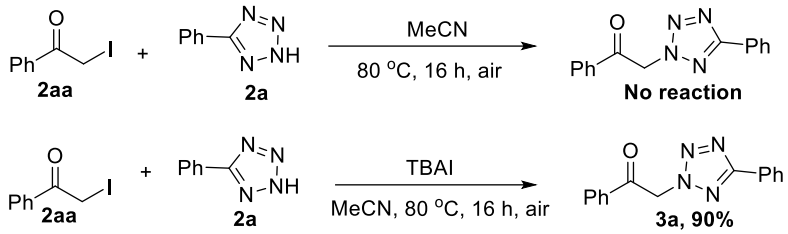
In an undivided cell (250 mL) equipped with a stirring bar, a mixture of substrates **1a** (24.0 mmol, 2.88 g), **2a** (8.0 mmol, 1.17 g), TBAI (8.0 mmol, 2.95 g) and MeCN (100 mL) were added. The cell was equipped with graphite (3 cm × 3 cm × 0.6 cm) as the anode and platinum plate (3 cm × 3 cm × 0.01 cm) as the cathode and connected to a DC regulated power supply. The reaction mixture was stirred and electrolyzed at a constant current of 25 mA at 80°C in oil bath for 90 h. Upon completion, the solvent was further removed directly under reduced pressure to afford the crude product, which was purified by flash column chromatography (PE/EtOAc: 25/1→15/1) yielded **3a** (1.14 g, 61%) as a white solid.

(b) Radical Scavenger Experiments with BHT



In an undivided cell (15 mL) equipped with a stirring bar, a mixture of substrates **1a** (1.5 mmol, 180 mg), BHT (2.0 mmol, 440 mg), **2a** (0.50 mmol, 73 mg), *n*-Bu_4NI (0.50 mmol, 185 mg) and MeCN (8.0 mL) were added. The cell was equipped with graphite as the anode and platinum plate as the cathode connected to an AXIOMET AX-3003P DC regulated power supply. The reaction mixture was stirred and electrolyzed at a constant current of 13 mA at 80℃ by heating mantle for 16 h. Upon completion, the reaction does not give the expected product.

(c) The reaction of **2aa** with **2a** without current



In a round bottom flask (25 mL) equipped with a stirring bar, a mixture of substrates **2aa** (1.0 mmol, 245 mg) and 5-phenyltetrazole **2a** (0.50 mmol, 73 mg), and MeCN (8 mL) were added. The reaction mixture was stirred and refluxed at 80°C by oil bath for 16 h without electricity under air. Upon completion, the reaction does not give the expected product.

Then, in a round bottom flask (25 mL) equipped with a stirring bar, a mixture of substrates **2aa** (1.0 mmol, 245 mg), **2a** (0.50 mmol, 73 mg), TBAI (0.50 mmol, 185 mg) and MeCN (8.0 mL) were added. The reaction mixture was stirred at 80℃ time for 16 h under air. Upon completion, the solvent was removed directly under reduced pressure to afford the crude product, which was further purified by flash column chromatography on silica gel (PE/EtOAc: 20/1→10/1) to give a white solid **3a** (119 mg, 90%).

Crystallographic description of 3a and 3n

(i) Crystallographic description of 1-phenyl-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (3a).

The compound (**3a**) was crystallized from a supersaturated solution of dichloromethane by the slow evaporation method. Suitable single crystal was picked from the mother liquor and covered with perfluorinated polyether oil on a microscope slide. Compound **3a** was collected at 180.00 K on a Rigaku Oxford Diffraction Supernova Dual Source, Cu at Zero equipped with an AtlasS2 CCD using Cu Kα radiation. Data reduction was carried out with the diffractometer's software[6] . The structure was solved by direct methods using Olex2 software[7] , and the non-hydrogen atoms were located from the trial structure and then refined anisotropically with SHELXL-2018[8] using a full-matrix least squares procedure based on F^2. The weighted *R* factor, *wR* and goodness-of-fit *S* values were obtained based on F^2. The

hydrogen atom positions were fixed geometrically at the calculated distances and allowed to ride on their parent atoms. Crystallographic data has been deposited with the Cambridge Crystallographic Centre and allocated with the deposition numbers: CCDC 2180990. Copies of the data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Crystal structure determination of 3a

Crystal Data for $C_{15}H_{12}N_4O$ (M =264.29 g/mol): monoclinic, space group P21/c (no. 14), a = 12.6720(9) Å, b = 11.9871(7) Å, c = 9.0695(8) Å, β = 110.184(9)°, V = 1293.07(18) $Å^3$, Z = 4, T = 180.00(10) K, μ(MoKα) = 0.090 mm^{-1}, D_{calc} = 1.358 g/cm^3, 9622 reflections measured (4.824° ≤ 2Θ ≤ 58.84°), 3185 unique (Rint = 0.0275, Rsigma = 0.0332) which were used in all calculations. The final R_1 was 0.0433 (I > 2σ(I)) and wR_2 was 0.1030 (all data).

Table 1 Crystal data and structure refinement for 3a.

Identification code	**3a**
Empirical formula	$C_{15}H_{12}N_4O$
Formula weight	264.29
Temperature/K	180.00(10)
Crystal system	monoclinic
Space group	P21/c
a/Å	12.6720(9)
b/Å	11.9871(7)
c/Å	9.0695(8)
α/°	90
β/°	110.184(9)
γ/°	90
Volume/$Å^3$	1293.07(18)
Z	4
$\rho_{calc}g/cm^3$	1.358

μ/mm^{-1}	0.090
F(000)	552.0
Crystal size/mm^3	0.15 × 0.13 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.824 to 58.84
Index ranges	-16 ≤ h ≤ 17, -16 ≤ k ≤ 16, -8 ≤ l ≤ 11
Reflections collected	9622
Independent reflections	3185 [Rint = 0.0275, Rsigma = 0.0332]
Data/restraints/parameters	3185/0/182
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0433, wR_2 = 0.0925
Final R indexes [all data]	R_1 = 0.0608, wR_2 = 0.1030
Largest diff. peak/hole / e $Å^{-3}$	0.20/-0.18

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters(Å2×10^3) for 3a. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

Atom	x	y	z	U(eq)
O1	3356.2(8)	514.5(9)	5004.4(12)	42.0(3)
N1	648.5(9)	759.9(9)	3906.3(13)	28.5(3)
C7	3193.9(10)	255.3(11)	6200.6(16)	28.5(3)
N2	1422.5(8)	1267.0(9)	5099.9(13)	29.7(3)
C9	-562.6(10)	1463.0(11)	1322.3(16)	27.8(3)
C6	3980.1(10)	-465.6(10)	7424.2(15)	26.5(3)
C15	315.3(10)	1585.4(10)	2868.5(16)	27.2(3)
N3	1584.1(9)	2328.4(9)	4838.0(15)	37.0(3)
C5	3756.9(10)	-817.3(11)	8749.1(16)	29.9(3)
N4	876.4(10)	2547.6(9)	3415.6(15)	35.4(3)
C8	2132.9(11)	673.0(11)	6469.6(16)	31.2(3)
C1	4963.8(11)	-824.7(11)	7197.2(17)	32.5(3)

C10	-916.3(10)	406.1(11)	710.0(17)	30.6(3)
C4	4486.0(11)	-1537.3(12)	9813.4(17)	35.2(3)
C2	5692.8(11)	-1533.6(12)	8273.6(18)	36.7(3)
C14	-1047.6(11)	2403.0(11)	442.1(17)	35.3(3)
C11	-1730.4(11)	291.6(13)	-762.1(18)	37.8(3)
C3	5453.0(11)	-1901.6(12)	9567.1(18)	37.1(3)
C12	-2201.9(12)	1221.9(14)	-1630.9(18)	43.2(4)
C13	-1857.6(13)	2273.6(14)	-1026.0(19)	43.4(4)

Table 3 Anisotropic Displacement Parameters (Å2×10^3) for 3a. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Atom	U11	U22	U33	U23	U13	U12
O1	42.2(6)	53.0(6)	38.3(6)	11.8(5)	23.4(5)	8.6(5)
N1	28.7(5)	26.5(5)	31.9(6)	2.2(5)	12.7(5)	0.7(4)
C7	28.5(6)	29.2(7)	29.6(7)	-2.6(6)	12.4(5)	-3.6(5)
N2	28.2(6)	28.0(6)	34.1(7)	0.8(5)	12.5(5)	1.0(4)
C9	25.4(6)	29.9(6)	32.2(7)	3.4(5)	15.3(5)	2.3(5)
C6	24.9(6)	26.3(6)	28.5(7)	-5.3(5)	9.3(5)	-2.8(5)
C15	27.0(6)	23.1(6)	35.8(8)	2.4(5)	16.4(5)	2.3(5)
N3	35.3(6)	29.0(6)	44.3(8)	1.7(5)	10.5(5)	-2.0(5)
C5	25.5(6)	34.4(7)	31.1(7)	-4.3(6)	11.5(5)	-1.5(5)
N4	35.4(6)	27.4(6)	41.3(7)	3.1(5)	10.4(5)	-2.4(5)
C8	31.0(7)	34.4(7)	29.3(7)	3.7(6)	12.0(5)	5.0(6)
C1	30.4(6)	36.7(7)	33.3(8)	-4.2(6)	14.7(6)	-0.3(6)
C10	28.1(6)	30.2(7)	38.9(8)	2.4(6)	18.4(6)	2.7(5)
C4	35.4(7)	40.4(8)	28.7(8)	1.0(6)	9.4(6)	-1.1(6)
C2	27.7(7)	40.8(8)	41.6(9)	-6.4(7)	11.8(6)	5.1(6)
C14	36.9(7)	29.8(7)	40.4(9)	5.8(6)	14.9(6)	3.5(6)
C11	31.3(7)	43.9(8)	41.7(9)	-9.2(7)	17.1(6)	-3.5(6)
C3	34.0(7)	35.6(7)	35.7(8)	-1.7(6)	4.3(6)	4.5(6)

C12	31.8(7)	61.9(10)	34.8(9)	-1.8(7)	10.3(6)	3.5(7)
C13	41.1(8)	47.6(9)	40.7(9)	12.8(7)	13.1(7)	11.7(7)

Table 4 Bond Lengths for 3a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C7	1.2124(16)	C6	C1	1.3997(18)
N1	N2	1.3307(15)	C15	N4	1.3559(16)
N1	C15	1.3302(16)	N3	N4	1.3188(16)
C7	C6	1.4859(18)	C5	C4	1.3838(19)
C7	C8	1.5311(18)	C1	C2	1.3806(19)
N2	N3	1.3232(15)	C10	C11	1.384(2)
N2	C8	1.4453(16)	C4	C3	1.390(2)
C9	C15	1.4660(19)	C2	C3	1.382(2)
C9	C10	1.3937(18)	C14	C13	1.381(2)
C9	C14	1.3950(18)	C11	C12	1.377(2)
C6	C5	1.3914(18)	C12	C13	1.384(2)

Table 5 Bond Angles for 3a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C15	N1	N2	101.58(10)	N4	C15	C9	124.35(11)
O1	C7	C6	122.71(12)	N4	N3	N2	105.79(10)
O1	C7	C8	119.23(12)	C4	C5	C6	120.37(12)
C6	C7	C8	118.07(11)	N3	N4	C15	106.39(11)
N1	N2	C8	122.68(11)	N2	C8	C7	110.18(11)
N3	N2	N1	114.18(11)	C2	C1	C6	119.86(13)
N3	N2	C8	122.61(11)	C11	C10	C9	120.31(13)
C10	C9	C15	120.38(12)	C5	C4	C3	119.83(14)
C10	C9	C14	119.25(13)	C1	C2	C3	120.49(12)
C14	C9	C15	120.37(12)	C13	C14	C9	119.68(13)
C5	C6	C7	122.52(11)	C12	C11	C10	120.24(14)

C5	C6	C1	119.38(12)	C2	C3	C4	120.04(13)
C1	C6	C7	118.08(12)	C11	C12	C13	119.71(14)
N1	C15	C9	123.59(11)	C14	C13	C12	120.81(14)
N1	C15	N4	112.06(12)				

Table 6 Torsion Angles for 3a.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
O1	C7	C6	C5	-175.95(13)	C15	C9	C10	C11	-178.81(12)
O1	C7	C6	C1	2.16(19)	C15	C9	C14	C13	178.69(12)
O1	C7	C8	N2	4.94(17)	N3	N2	C8	C7	-82.82(15)
N1	N2	N3	N4	0.92(15)	C5	C6	C1	C2	0.89(19)
N1	N2	C8	C7	88.26(14)	C5	C4	C3	C2	0.9(2)
N1	C15	N4	N3	-0.02(15)	C8	C7	C6	C5	3.46(18)
C7	C6	C5	C4	176.49(12)	C8	C7	C6	C1	-178.43(11)
C7	C6	C1	C2	-177.28(12)	C8	N2	N3	N4	172.70(11)
N2	N1	C15	C9	-179.01(11)	C1	C6	C5	C4	-1.59(19)
N2	N1	C15	N4	0.53(13)	C1	C2	C3	C4	-1.6(2)
N2	N3	N4	C15	-0.51(14)	C10	C9	C15	N1	-15.01(19)
C9	C15	N4	N3	179.52(11)	C10	C9	C15	N4	165.51(12)
C9	C10	C11	C12	-0.3(2)	C10	C9	C14	C13	-0.8(2)
C9	C14	C13	C12	0.6(2)	C10	C11	C12	C13	0.0(2)
C6	C7	C8	N2	-174.50(10)	C14	C9	C15	N1	165.48(12)
C6	C5	C4	C3	0.7(2)	C14	C9	C15	N4	-14.0(2)
C6	C1	C2	C3	0.7(2)	C14	C9	C10	C11	0.71(19)
C15	N1	N2	N3	-0.90(13)	C11	C12	C13	C14	-0.2(2)
C15	N1	N2	C8	-172.66(11)					

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å2×10^3) for 3a.

Atom	**x**	**y**	**z**	**U(eq)**

H5	3114.14	-567	8920.38	36
H8A	1724.2	44.76	6681.3	37
H8B	2341.33	1163.92	7375.17	37
H1	5126.17	-586.34	6323.15	39
H10	-603.65	-225.2	1293.45	37
H4	4329.28	-1776.84	10691.28	42
H2	6350.06	-1765.11	8126.99	44
H14	-826.6	3113.3	842.03	42
H11	-1959.95	-416.03	-1166.05	45
H3	5939.1	-2393.46	10273.21	44
H12	-2749.18	1143.75	-2619.71	52
H13	-2175.53	2900.91	-1615.37	52

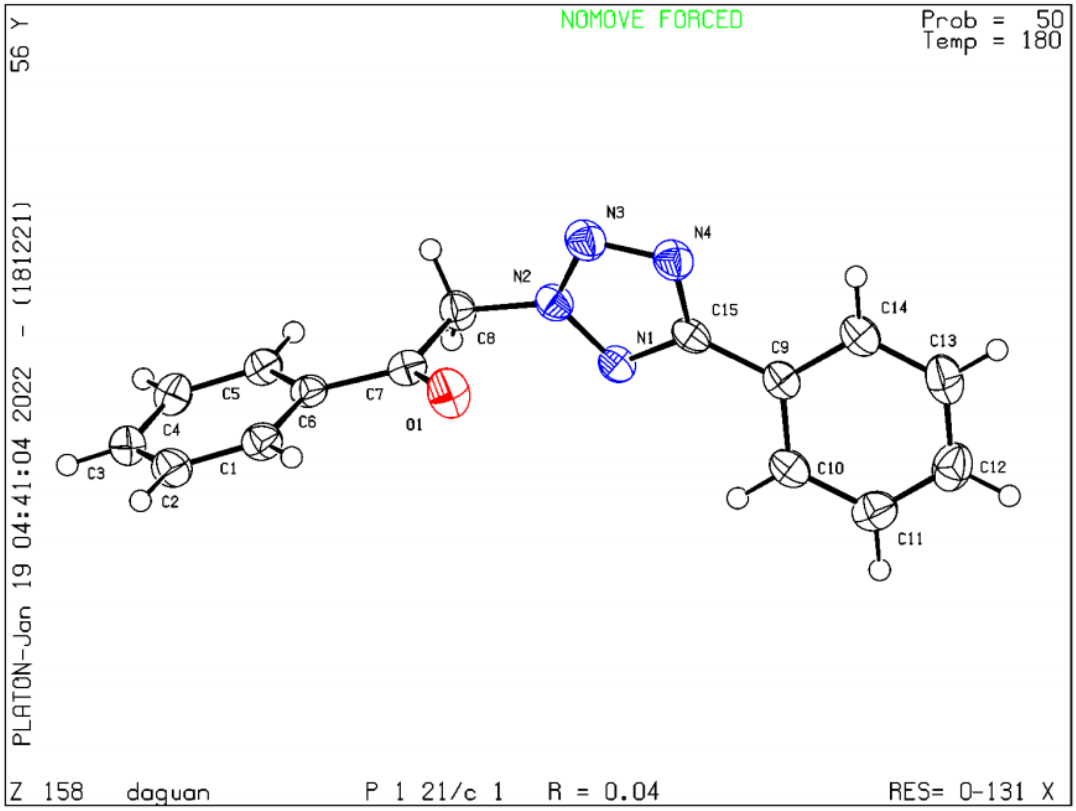


Figure S2. ORTEP view of 1-phenyl-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (**3a**) with ellipsoids at 50% probability.

(ii) Crystallographic description of 1-([1,1'-biphenyl]-3-yl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one(3n).

The compound (**3n**) was crystallized from a supersaturated solution of dichloromethane by the slow evaporation method. Suitable single crystal was picked from the mother liquor and covered with perfluorinated polyether oil on a microscope slide. Compound **3n** was collected at 179.99 K on a Rigaku Oxford Diffraction Supernova Dual Source, Cu at Zero equipped with an AtlasS2 CCD using Cu Kα radiation. Data reduction was carried out with the diffractometer's software[5] . The structure was solved by direct methods using Olex2 software[6] , and the non-hydrogen atoms were located from the trial structure and then refined anisotropically with SHELXL-2018[7] using a full-matrix least squares procedure based on F^2. The weighted *R* factor, *wR* and goodness-of-fit *S* values were obtained based on F^2. The hydrogen atom positions were fixed geometrically at the calculated distances and allowed to ride on their parent atoms. Crystallographic data has been deposited with the Cambridge Crystallographic Centre and allocated with the deposition numbers: CCDC 2180989. Copies of the data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Crystal structure determination of 3n

Crystal Data for $C_{21}H_{16}N_4O$ (M =340.38 g/mol): monoclinic, space group C2/c (no. 15), a = 32.257(5) Å, b = 6.2874(5) Å, c = 17.439(2) Å, β = 103.904(14)°, V = 3433.2(8) $Å^3$, Z = 8, T = 179.99(10) K, μ(CuKα) = 0.674 mm^{-1}, D_{calc} = 1.317 g/cm3, 11406 reflections measured (5.644° ≤ 2Θ ≤ 148.14°), 3400 unique (Rint = 0.0600, Rsigma = 0.0622) which were used in all calculations. The final R_1 was 0.0555 (I > 2σ(I)) and wR_2 was 0.1543 (all data).

Table 8 Crystal data and structure refinement for 3n.

Identification code	**3n**
Empirical formula	$C_{21}H_{16}N_4O$
Formula weight	340.38
Temperature/K	179.99(10)
Crystal system	monoclinic
Space group	C2/c
a/Å	32.257(5)
b/Å	6.2874(5)

c/Å	17.439(2)
α/°	90
β/°	103.904(14)
γ/°	90
Volume/Å^3	3433.2(8)
Z	8
ρ_{calc}g/cm^3	1.317
μ/mm^{-1}	0.674
F(000)	1424.0
Crystal size/mm^3	0.14 × 0.12 × 0.09
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.644 to 148.14
Index ranges	-39 ≤ h ≤ 39, -7 ≤ k ≤ 6, -20 ≤ l ≤ 21
Reflections collected	11406
Independent reflections	3400 [Rint = 0.0600, Rsigma = 0.0622]
Data/restraints/parameters	3400/0/236
Goodness-of-fit on F^2	1.105
Final R indexes [I>=2σ (I)]	R1 = 0.0555, wR2 = 0.1351
Final R indexes [all data]	R1 = 0.0947, wR2 = 0.1543
Largest diff. peak/hole / e Å^{-3}	0.32/-0.20

Table 9 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å2×10^3) for 3n. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

Atom	x	y	z	U(eq)
O1	1066.8(6)	1583(3)	298.7(11)	56.5(5)
N2	1795.5(6)	2320(3)	-128.5(11)	39.7(5)
N1	2095.4(6)	2154(3)	538.8(11)	40.0(5)
C7	598.9(7)	-4263(4)	-1459.7(13)	40.9(6)
N4	1987.4(7)	5495(3)	117.9(12)	48.2(5)
C12	899.1(7)	-2729(3)	-1120.4(13)	39.8(5)
C13	1129.7(7)	383(4)	-207.2(14)	40.3(5)
C21	2213.3(7)	4180(3)	677.9(13)	37.0(5)
C19	3036.5(7)	7585(4)	2006.7(15)	45.4(6)
C8	215.9(8)	-4346(4)	-1223.7(14)	46.9(6)
N3	1722.2(7)	4287(3)	-392.8(12)	49.9(5)
C20	2708.5(7)	6959(4)	1379.1(14)	41.4(6)
C9	134.5(8)	-2941(4)	-669.3(15)	52.0(7)
C6	680.5(8)	-5725(4)	-2079.4(14)	44.6(6)
C15	2554.8(7)	4879(4)	1347.8(13)	38.3(5)
C10	430.2(8)	-1415(4)	-341.7(15)	47.8(6)
C11	818.9(7)	-1306(4)	-563.6(13)	39.5(5)
C16	2728.3(7)	3476(4)	1957.4(15)	45.3(6)
C14	1537.4(7)	545(4)	-499.5(14)	42.1(6)

C1	890.7(8)	-5017(5)	-2636.7(15)	51.6(7)
C17	3050.2(8)	4147(4)	2583.5(15)	50.2(7)
C5	528.7(8)	-7792(4)	-2128.0(16)	52.5(7)
C18	3205.5(8)	6200(4)	2607.4(15)	49.1(6)
C2	947.4(9)	-6346(5)	-3237.1(17)	63.3(8)
C4	589.9(10)	-9129(4)	-2725.7(18)	63.5(8)
C3	798.6(10)	-8406(5)	-3274.5(19)	67.6(9)

Table 10 Anisotropic Displacement Parameters (Å2×103) for 3n. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Atom	U11	U22	U33	U23	U13	U12
O1	56.8(11)	56.4(11)	62.0(12)	-19.0(9)	25.5(9)	-11.7(9)
N2	37.8(11)	35.9(11)	44.6(11)	0.8(9)	8.5(9)	-1.4(8)
N1	38.4(11)	36.2(11)	44.1(11)	1.4(9)	7.4(8)	-1.2(8)
C7	37.9(13)	40.8(13)	40.2(13)	-0.2(10)	2.0(10)	1.6(10)
N4	47.9(12)	38.4(11)	53.8(13)	4.6(10)	3.4(10)	-2.7(9)
C12	35.0(12)	40.8(13)	42.6(13)	0.3(10)	7.4(10)	-0.7(10)
C13	40.1(13)	40.0(13)	40.7(13)	-1.2(10)	9.7(10)	0.1(10)
C21	37.2(12)	35.5(12)	40.8(13)	2.2(10)	14.4(10)	1.2(9)
C19	39.0(13)	37.3(13)	60.2(16)	-5.9(11)	12.9(11)	-3.2(10)
C8	37.7(13)	51.7(15)	48.2(14)	-2.8(12)	4.5(11)	-6.5(11)
N3	51.6(13)	38.8(12)	53.8(13)	6.0(10)	1.8(10)	-3.2(9)
C20	38.2(12)	39.1(13)	47.8(14)	-0.3(11)	11.8(10)	-1.5(10)
C9	39.6(14)	65.3(17)	52.4(16)	-4.4(13)	13.5(11)	-7.5(12)
C6	35.6(12)	47.0(15)	44.9(14)	-6.3(11)	-3.1(10)	3.0(10)
C15	34.9(12)	37.7(12)	44.3(13)	0.3(10)	13.6(10)	-0.2(9)
C10	41.5(14)	55.5(16)	47.5(14)	-7.6(12)	12.9(11)	-2.5(11)
C11	36.9(12)	41.0(13)	39.7(13)	-1.9(10)	7.4(10)	-0.5(10)
C16	38.7(13)	39.3(13)	57.9(16)	6.9(11)	11.3(12)	-1.3(10)
C14	38.4(13)	38.2(13)	48.8(14)	-5.6(11)	8.6(10)	-2.7(10)
C1	38.8(13)	58.1(16)	56.2(16)	-10.5(13)	8.2(12)	4.8(12)
C17	36.5(13)	56.6(16)	54.6(15)	12.2(13)	5.4(11)	-0.8(11)
C5	50.3(16)	43.6(15)	53.6(16)	-1.4(12)	-7.3(12)	5.5(11)
C18	36.1(13)	57.4(16)	52.0(15)	-3.5(12)	7.3(11)	-1.3(11)
C2	48.3(16)	78(2)	61.5(18)	-16.4(16)	9.6(14)	12.6(14)
C4	61.9(19)	47.1(16)	67(2)	-13.3(14)	-12.2(15)	11.0(13)
C3	54.3(18)	74(2)	64.3(19)	-24.7(16)	-5.5(15)	24.9(15)

Table 11 Bond Lengths for 3n.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C13	1.214(3)	C19	C18	1.370(3)
N2	N1	1.327(3)	C8	C9	1.381(3)
N2	N3	1.321(2)	C20	C15	1.395(3)
N2	C14	1.449(3)	C9	C10	1.376(3)

N1	C21	1.335(3)	C6	C1	1.385(4)
C7	C12	1.393(3)	C6	C5	1.384(3)
C7	C8	1.394(3)	C15	C16	1.391(3)
C7	C6	1.490(3)	C10	C11	1.400(3)
N4	C21	1.351(3)	C16	C17	1.380(3)
N4	N3	1.318(3)	C1	C2	1.386(3)
C12	C11	1.390(3)	C17	C18	1.382(3)
C13	C11	1.490(3)	C5	C4	1.389(4)
C13	C14	1.524(3)	C2	C3	1.377(4)
C21	C15	1.467(3)	C4	C3	1.373(4)
C19	C20	1.384(3)			

Table 12 Bond Angles for 3n.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	N2	C14	123.44(18)	C1	C6	C7	120.8(2)
N3	N2	N1	114.28(18)	C5	C6	C7	120.2(2)
N3	N2	C14	122.00(19)	C5	C6	C1	119.0(2)
N2	N1	C21	101.56(17)	C20	C15	C21	120.3(2)
C12	C7	C6	120.6(2)	C16	C15	C21	120.4(2)
C8	C7	C12	118.4(2)	C16	C15	C20	119.4(2)
C8	C7	C6	121.0(2)	C9	C10	C11	119.8(2)
N3	N4	C21	106.60(18)	C12	C11	C13	122.1(2)
C11	C12	C7	121.0(2)	C12	C11	C10	119.4(2)
O1	C13	C11	122.2(2)	C10	C11	C13	118.5(2)
O1	C13	C14	120.7(2)	C17	C16	C15	119.9(2)
C11	C13	C14	117.15(19)	N2	C14	C13	110.58(18)
N1	C21	N4	111.8(2)	C6	C1	C2	120.8(3)
N1	C21	C15	123.9(2)	C16	C17	C18	120.5(2)
N4	C21	C15	124.3(2)	C6	C5	C4	120.1(3)
C18	C19	C20	120.8(2)	C19	C18	C17	119.7(2)
C9	C8	C7	120.9(2)	C3	C2	C1	119.7(3)
N4	N3	N2	105.72(19)	C3	C4	C5	120.3(3)
C19	C20	C15	119.6(2)	C4	C3	C2	120.1(3)
C10	C9	C8	120.5(2)				

Table 13 Torsion Angles for 3n.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C13	C11	C12	-177.5(2)	C8	C9	C10	C11	-0.9(4)
O1	C13	C11	C10	4.2(4)	N3	N2	N1	C21	-0.7(2)
O1	C13	C14	N2	-3.3(3)	N3	N2	C14	C13	-82.5(3)
N2	N1	C21	N4	0.7(2)	N3	N4	C21	N1	-0.5(3)
N2	N1	C21	C15	-177.8(2)	N3	N4	C21	C15	178.0(2)
N1	N2	N3	N4	0.5(3)	C20	C19	C18	C17	0.7(4)
N1	N2	C14	C13	91.0(2)	C20	C15	C16	C17	-0.2(3)

N1	C21	C15	C20	169.0(2)	C9	C10	C11	C12	0.7(4)
N1	C21	C15	C16	-11.0(3)	C9	C10	C11	C13	179.1(2)
C7	C12	C11	C13	-178.4(2)	C6	C7	C12	C11	177.6(2)
C7	C12	C11	C10	-0.1(3)	C6	C7	C8	C9	-177.7(2)
C7	C8	C9	C10	0.4(4)	C6	C1	C2	C3	-0.9(4)
C7	C6	C1	C2	-176.7(2)	C6	C5	C4	C3	-0.4(4)
C7	C6	C5	C4	177.4(2)	C15	C16	C17	C18	-0.6(4)
N4	C21	C15	C20	-9.4(3)	C11	C13	C14	N2	177.12(19)
N4	C21	C15	C16	170.6(2)	C16	C17	C18	C19	0.4(4)
C12	C7	C8	C9	0.2(4)	C14	N2	N1	C21	-174.7(2)
C12	C7	C6	C1	-36.7(3)	C14	N2	N3	N4	174.5(2)
C12	C7	C6	C5	146.3(2)	C14	C13	C11	C12	2.1(3)
C21	N4	N3	N2	0.0(3)	C14	C13	C11	C10	-176.3(2)
C21	C15	C16	C17	179.8(2)	C1	C6	C5	C4	0.4(3)
C19	C20	C15	C21	-178.7(2)	C1	C2	C3	C4	0.9(4)
C19	C20	C15	C16	1.3(3)	C5	C6	C1	C2	0.3(4)
C8	C7	C12	C11	-0.4(3)	C5	C4	C3	C2	-0.2(4)
C8	C7	C6	C1	141.2(2)	C18	C19	C20	C15	-1.5(4)
C8	C7	C6	C5	-35.8(3)					

Table 14 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å2×10^3) for 3n.

Atom	x	y	z	U(eq)
H12	1157.05	-2657.42	-1268.83	48
H19	3143.43	8961.34	2021.05	54
H8	12.38	-5361.98	-1442.73	56
H20	2591.21	7919.48	980.4	50
H9	-122.02	-3025.63	-516.06	62
H10	371.91	-459.75	25.85	57
H16	2627.36	2087.67	1942.92	54
H14A	1699.51	-763.26	-378.83	50
H14B	1464.82	732.91	-1068.27	50
H1	995	-3632.87	-2607.59	62
H17	3163.65	3209.21	2992.64	60
H5	385.48	-8287.02	-1759.93	63
H18	3423.75	6640.12	3029.39	59
H2	1085.31	-5850.02	-3613	76
H4	489.12	-10519.17	-2754.13	76
H3	839.5	-9309.06	-3672.25	81

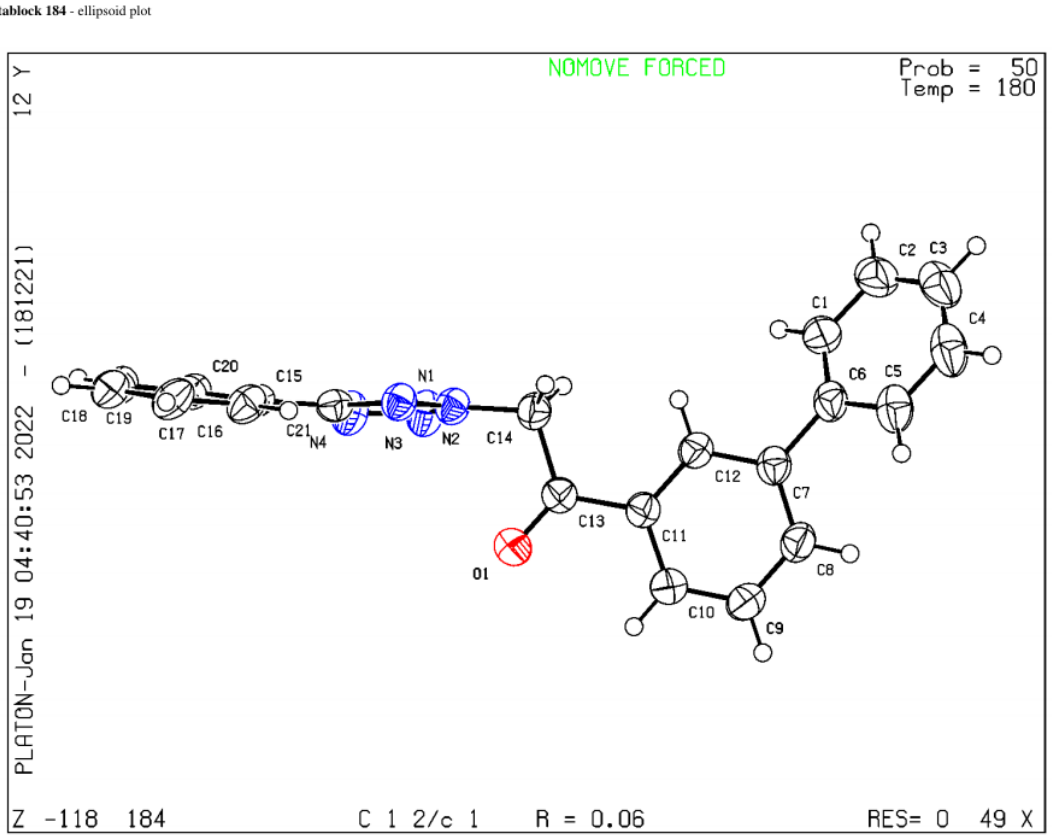


Figure S3. ORTEP view of 1-([1,1'-biphenyl]-3-yl)-2-(5-phenyl-2*H*-tetrazol-2-yl)ethan-1-one (**3n**) with ellipsoids at 50% probability.

References

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[2] Kanakaraju, S.; Suresh, L. *RSC Adv.*, **2015**, *5*, 29325–29334.

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[5] Shinichi K.; Higashikawa G. *RSC Adv.*, **2021**, *11*, 32837–32840.

[6] Dolomanov, O. V.; Bourhis, L. J. *J. Appl. Cryst.*, **2009**, *42*, 339-341.

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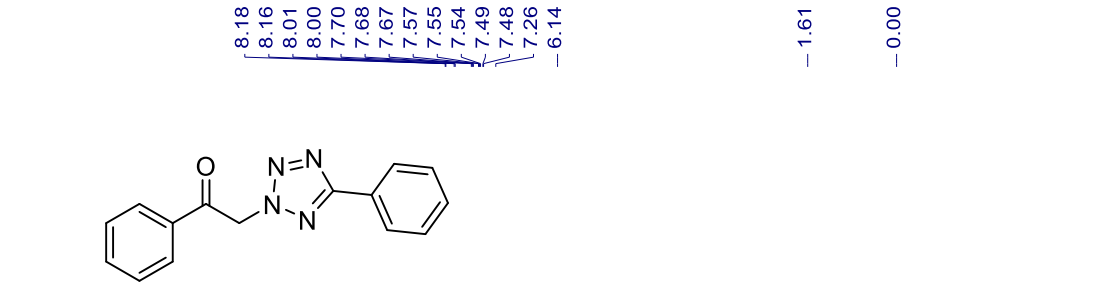
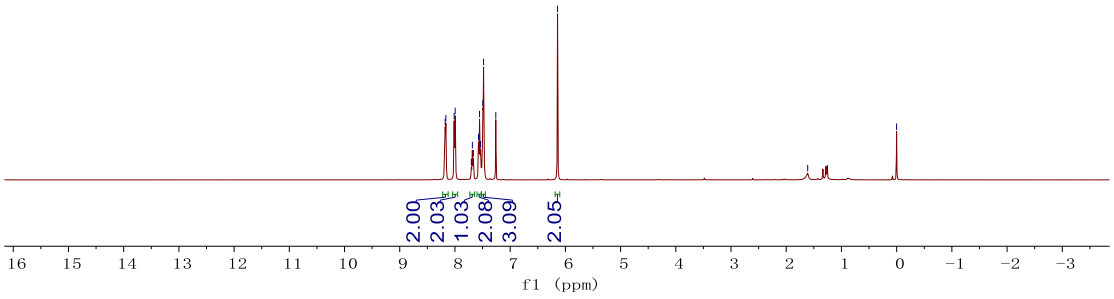
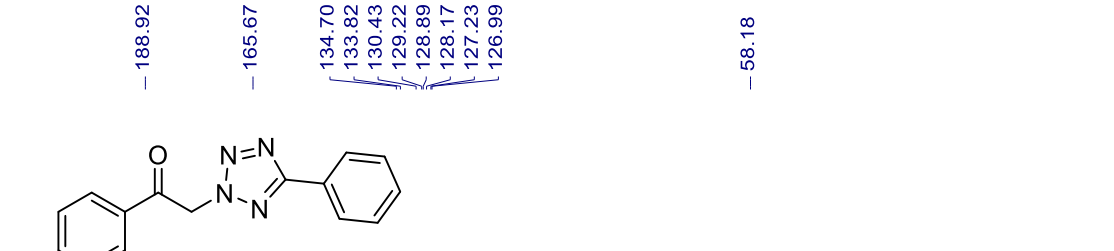
[8] Sheldrick, G.M.; *Acta Cryst.*, **2015**, *C71*, 3-8.

NMR Spectra

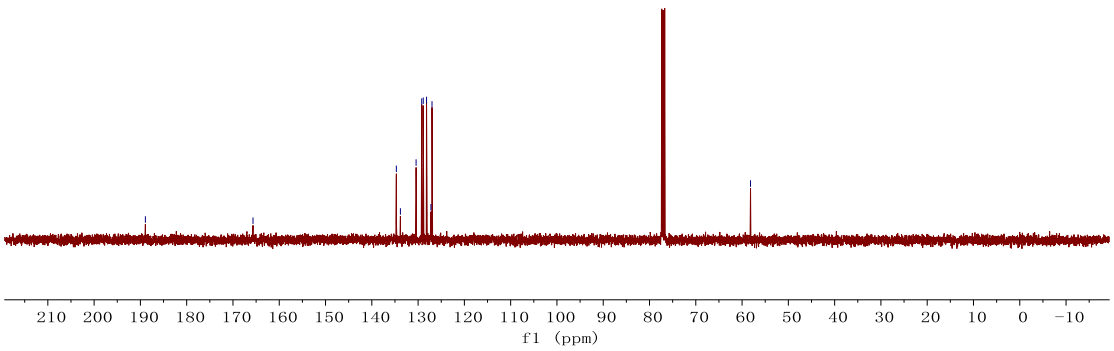


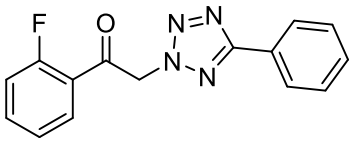
3a, ^{1}H NMR
$CDCl_3$, 400MHz





3a, ^{13}C NMR
$CDCl_3$, 100MHz





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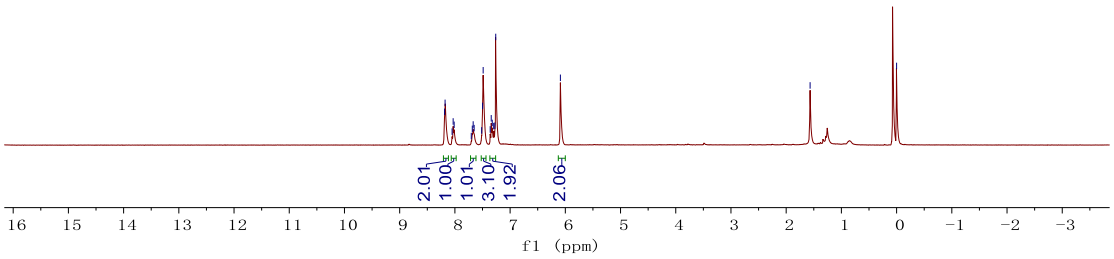
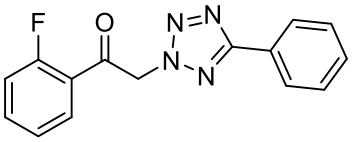
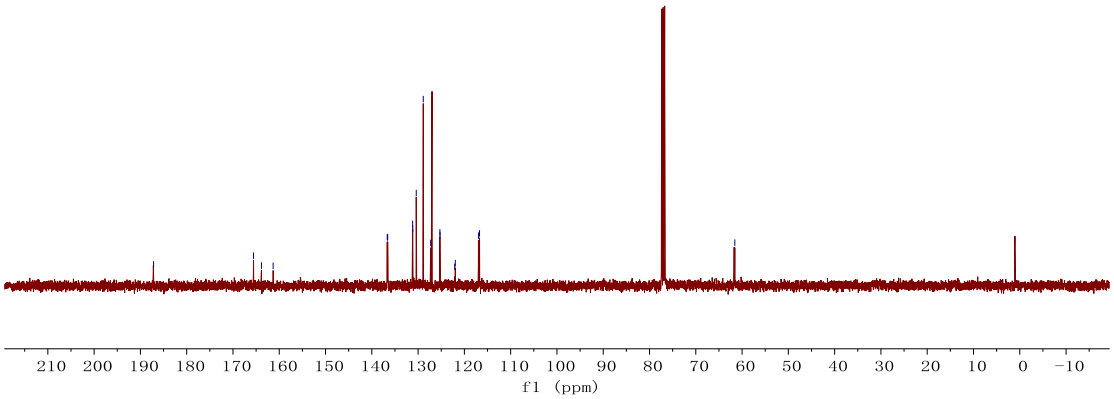
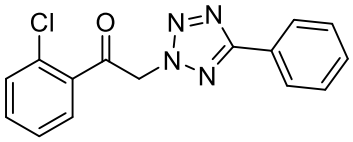




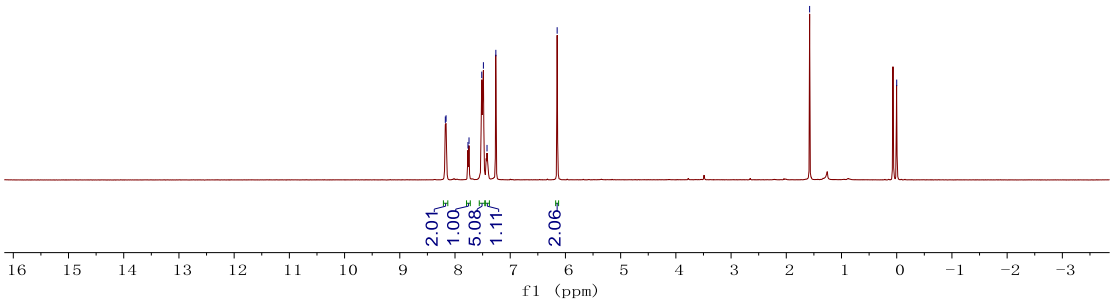
3b, ^{13}C NMR
$CDCl_3$, 100MHz

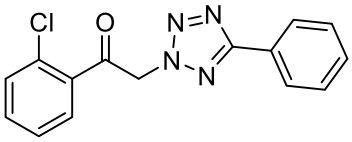




3c, ^{1}H NMR

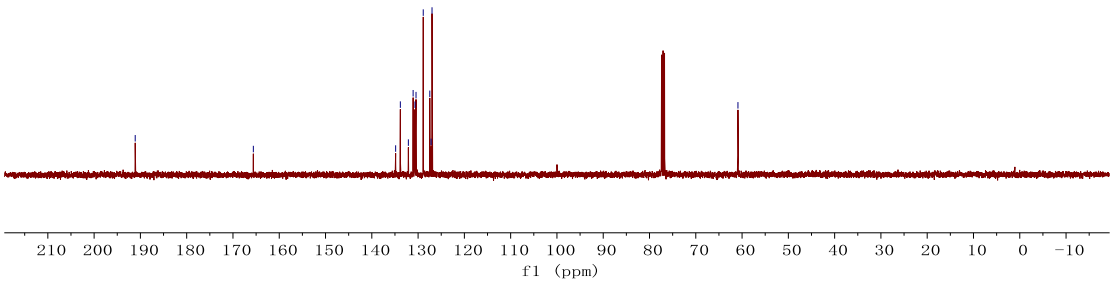
$CDCl_3$, 400MHz

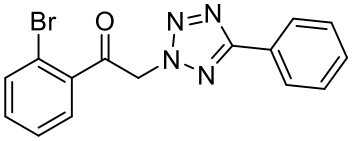




3c, ^{13}C NMR

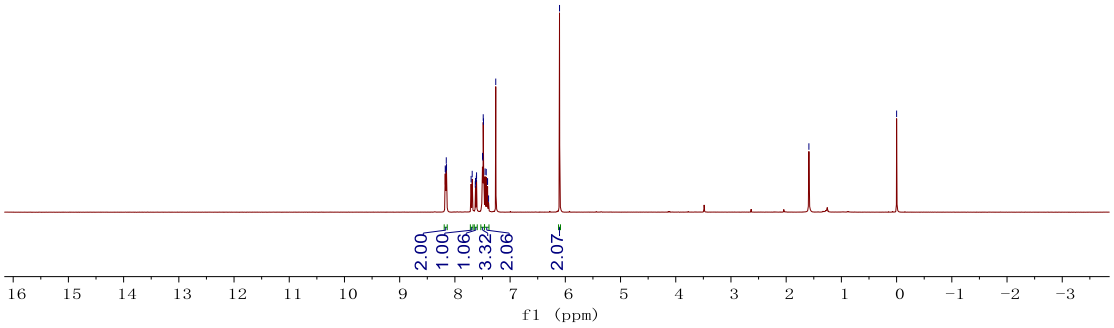
$CDCl_3$, 100MHz

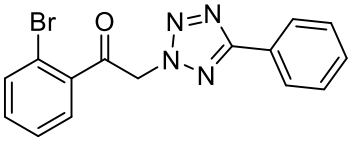




3d, ^{1}H NMR

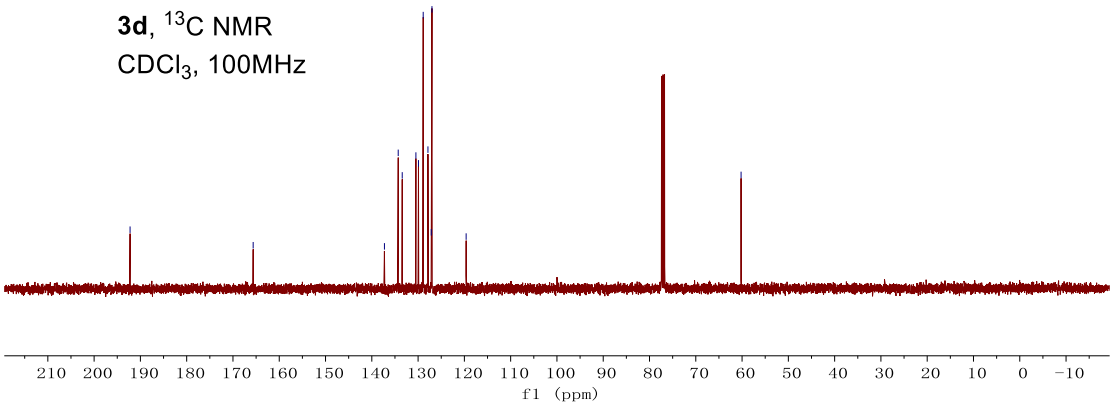
$CDCl_3$, 400MHz

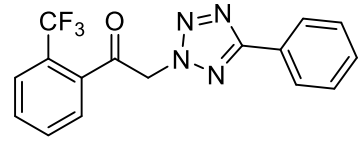




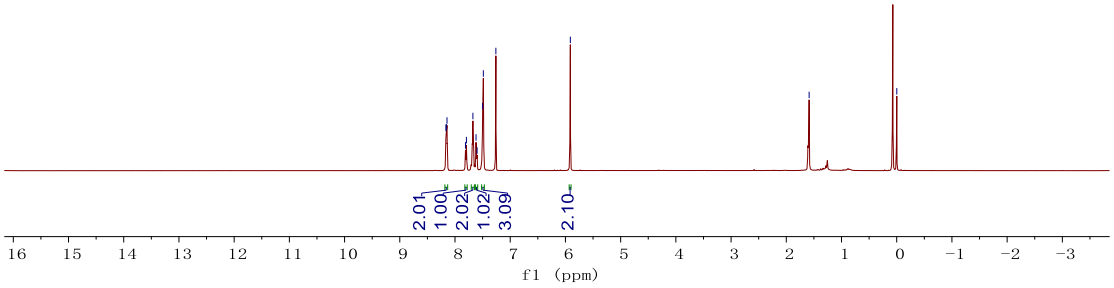
3d, ^{13}C NMR

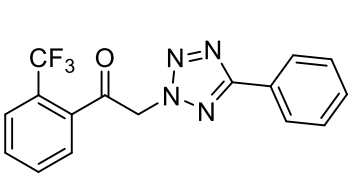
$CDCl_3$, 100MHz





3e, ^{1}H NMR
$CDCl_3$, 400MHz





3e, ^{13}C NMR
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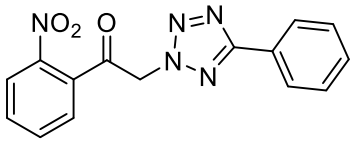
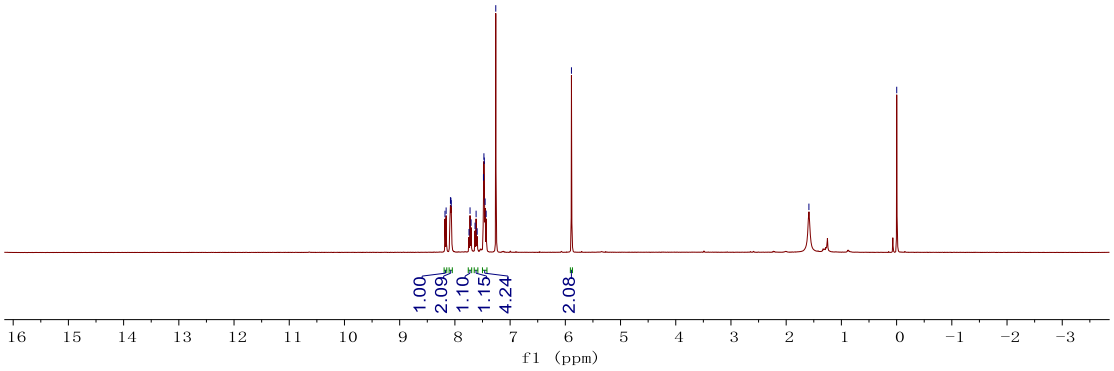
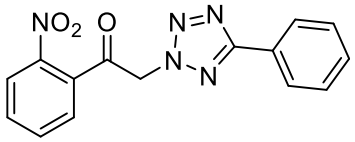


3f, ^{1}H NMR

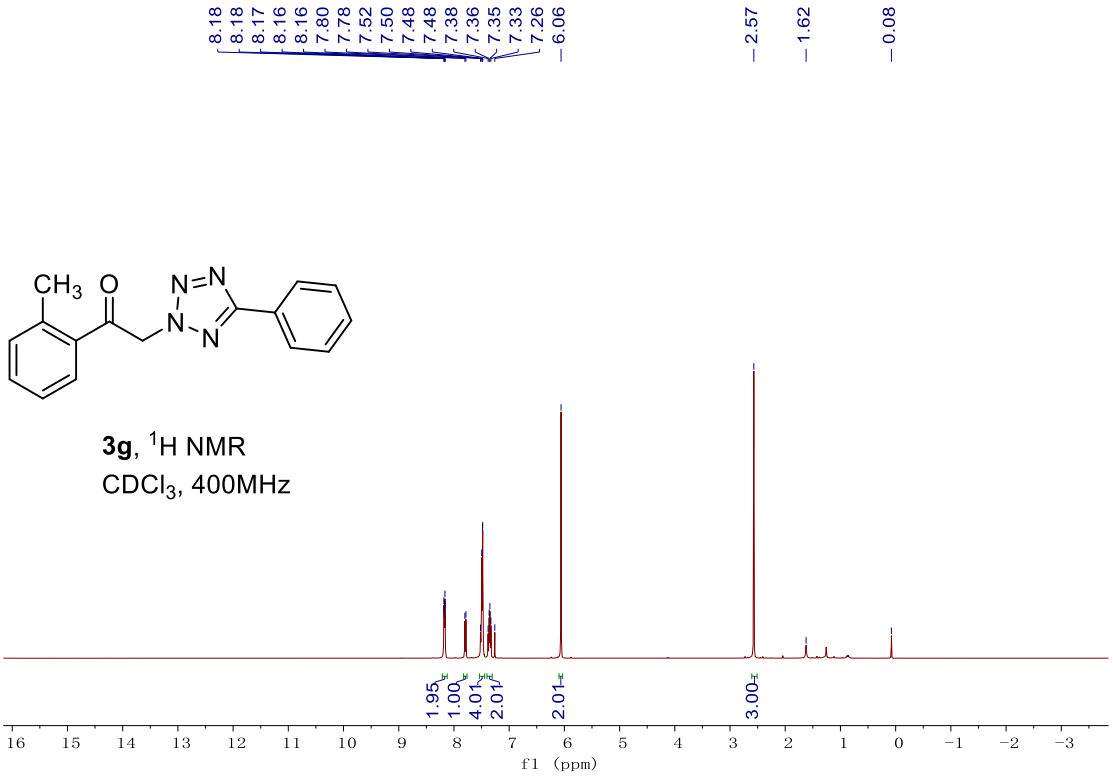
$CDCl_3$, 400MHz





3f, ^{13}C NMR

$CDCl_3$, 100MHz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8.17
8.16
8.16
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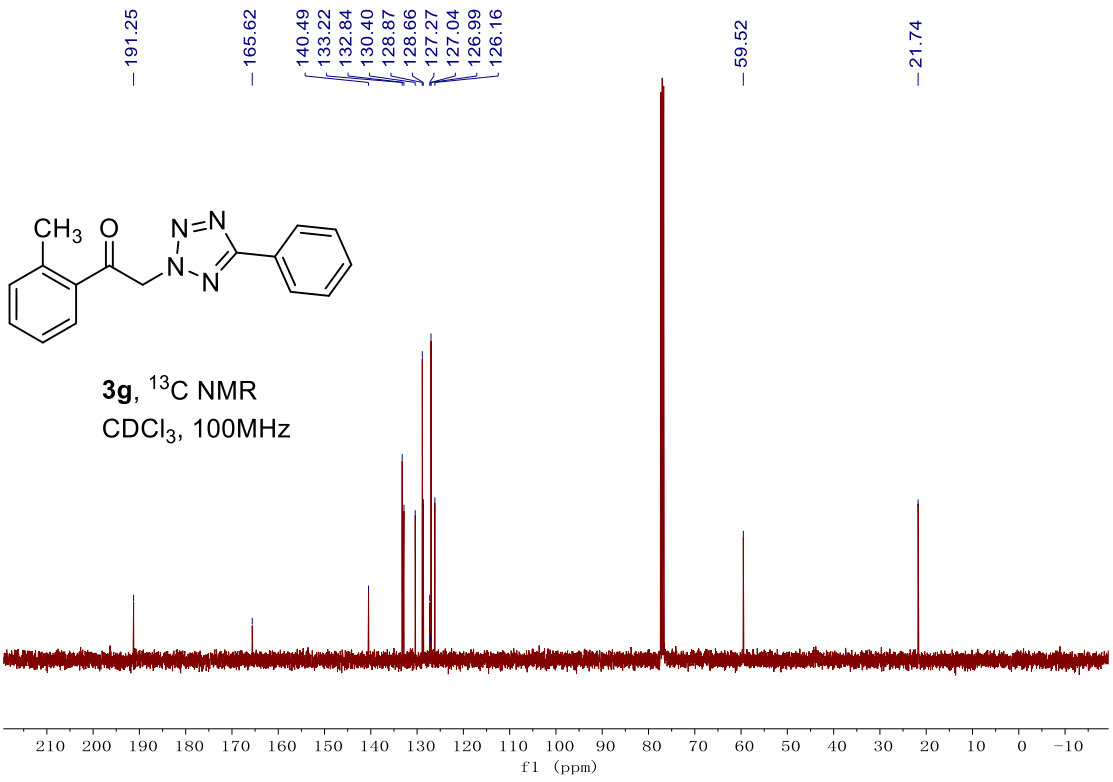
7.52
7.50
7.48
7.48
7.38
7.36
7.35
7.33
7.26
6.06
2.57
1.62
0.08
CH3
O
N=N
N
N
N
3g, 1H NMR
CDCl3, 400MHz
1.95
1.00
4.01
2.01
2.01
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)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140.49
133.22
132.84
130.40
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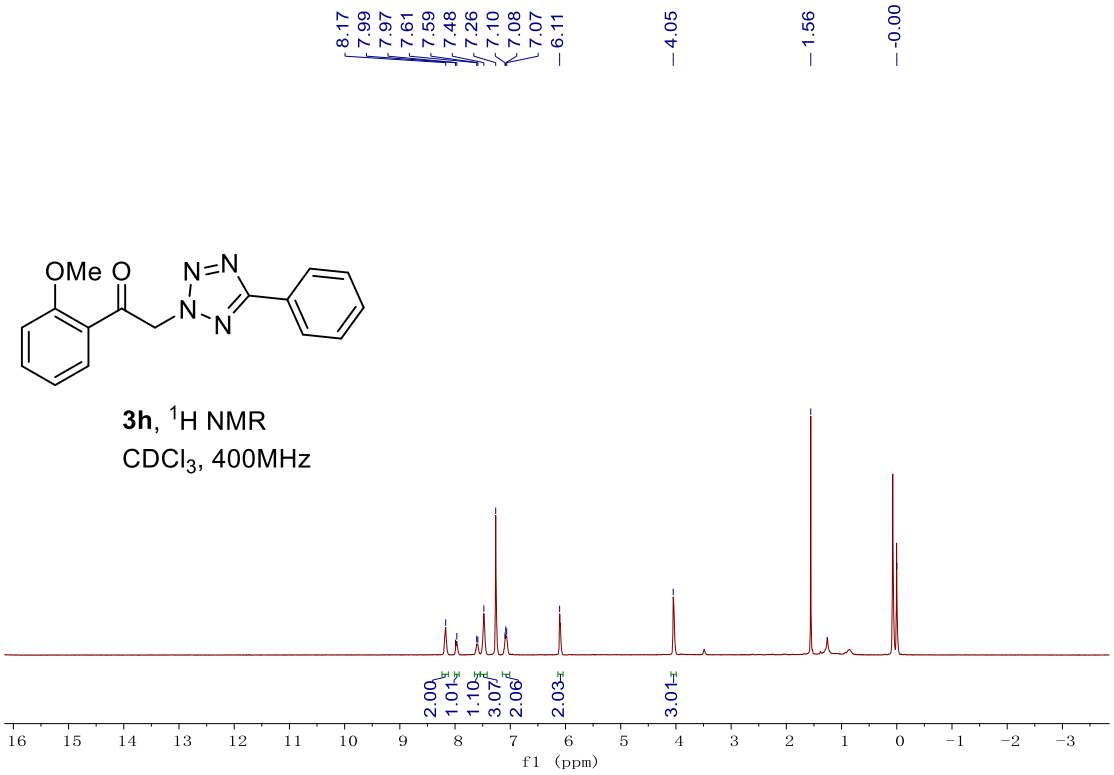
128.66
127.27
127.04
126.99
126.16
59.52
21.74
CH3
O
N=N
N
N
N
3g, 13C NMR
CDCl3, 100MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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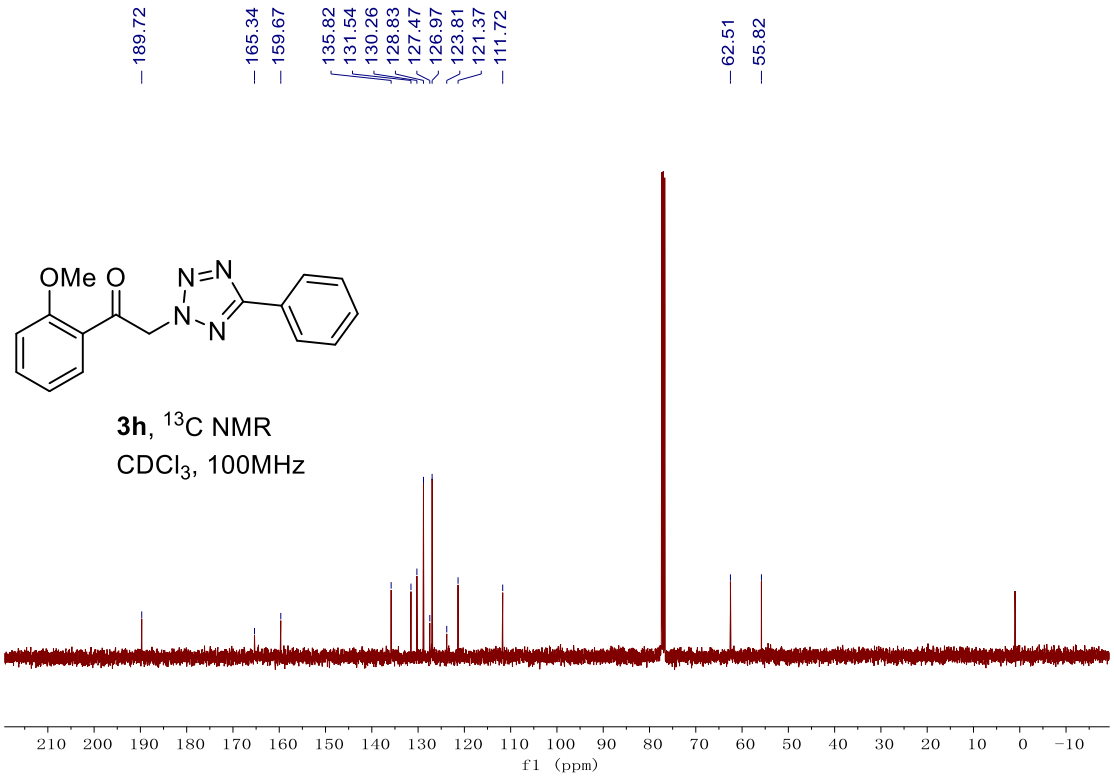
7.61
7.59
7.48
7.26
7.10
7.08
7.07
6.11
4.05
1.56
-0.00
OMe O
N=N
N
N
3h, 1H NMR
CDCl3, 400MHz
2.00
1.01
1.10
3.07
2.06
2.03
3.01
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)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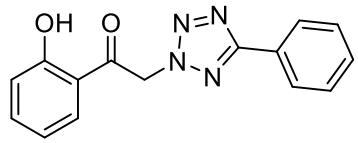
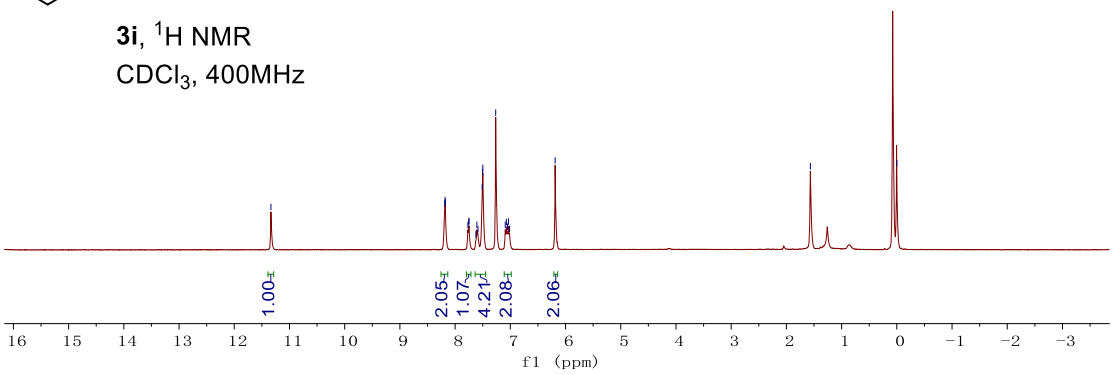
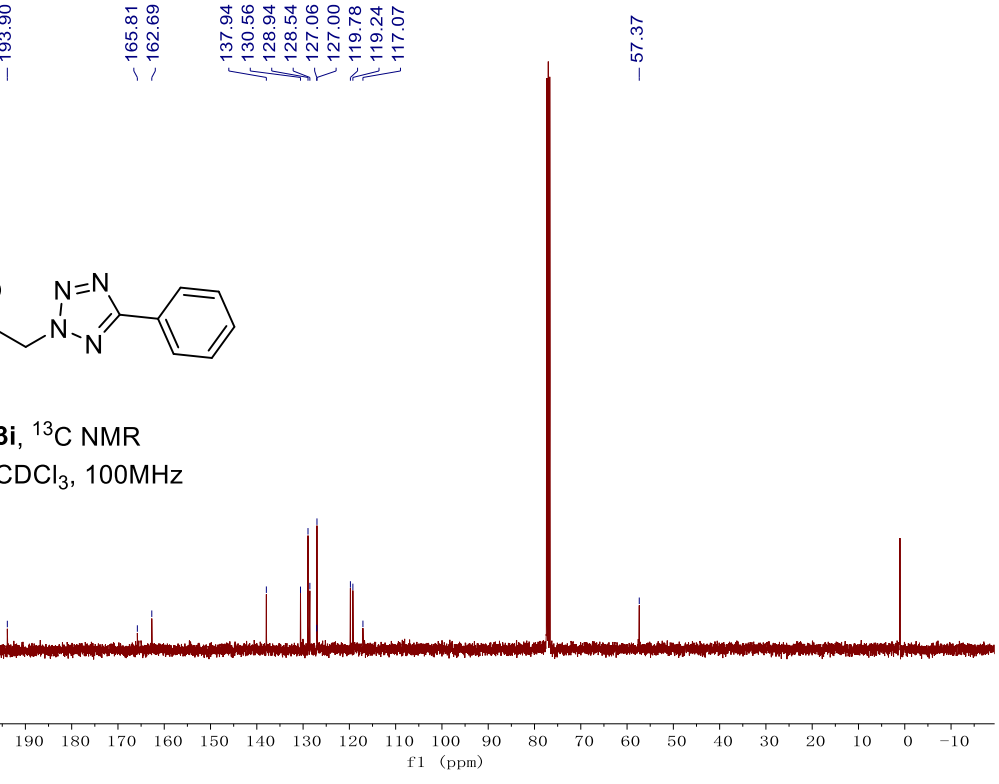
130.26
128.83
127.47
126.97
123.81
121.37
111.72
62.51
55.82
OMe O
N=N
N
N
3h, 13C NMR
CDCl3, 100MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



3i, ^{1}H NMR

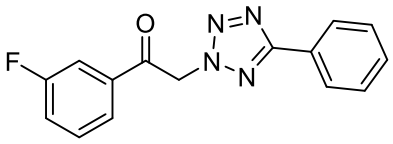
$CDCl_3$, 400MHz





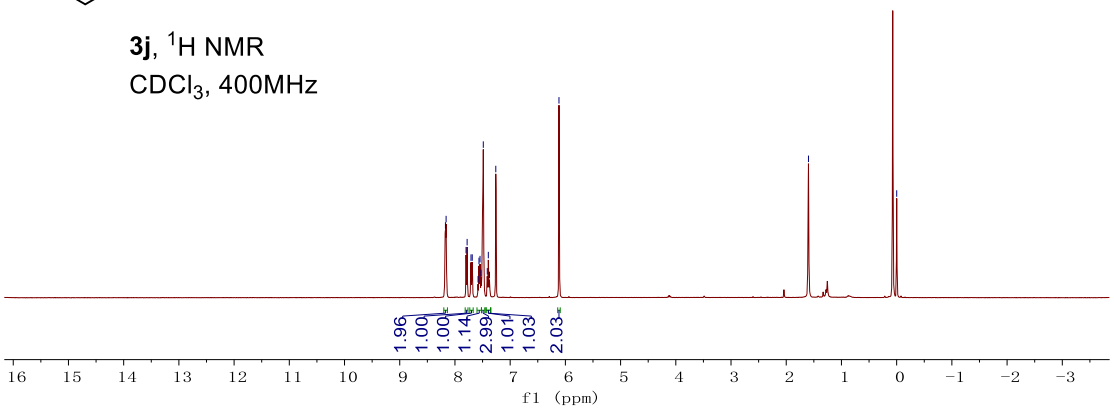
3i, ^{13}C NMR

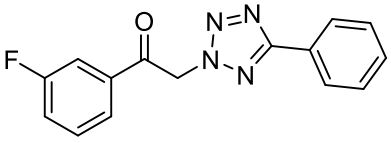
$CDCl_3$, 100MHz



3j, ^{1}H NMR

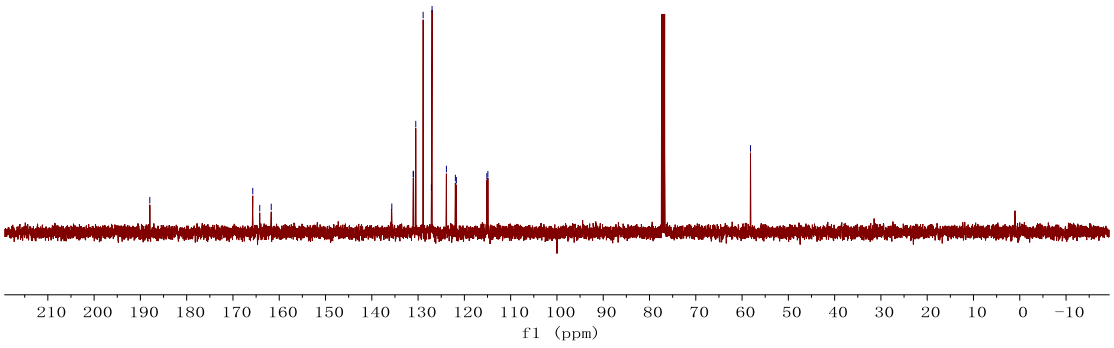
$CDCl_3$, 400MHz

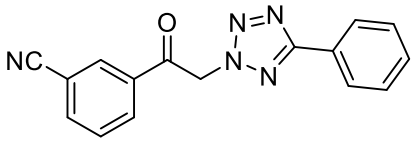




3j, ^{13}C NMR

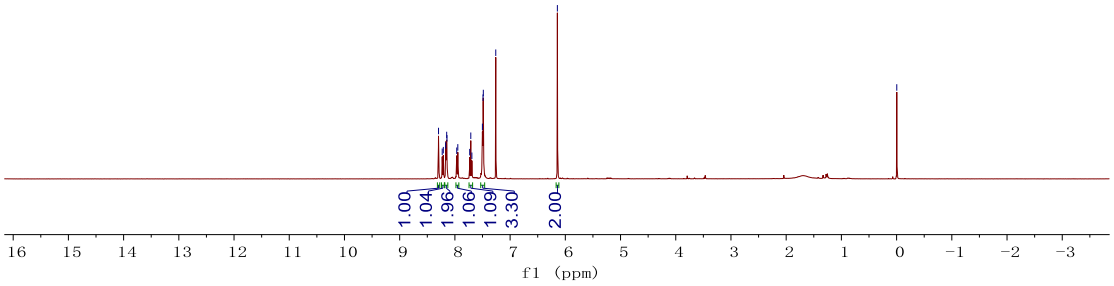
$CDCl_3$, 100MHz

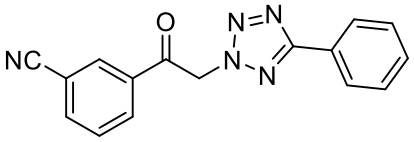




3k, ^{1}H NMR

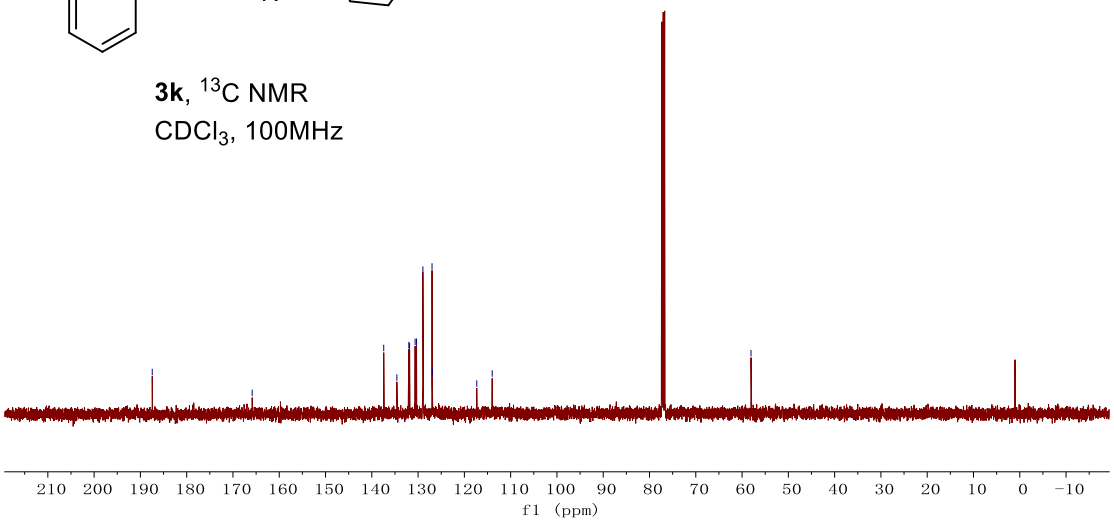
$CDCl_3$, 400MHz

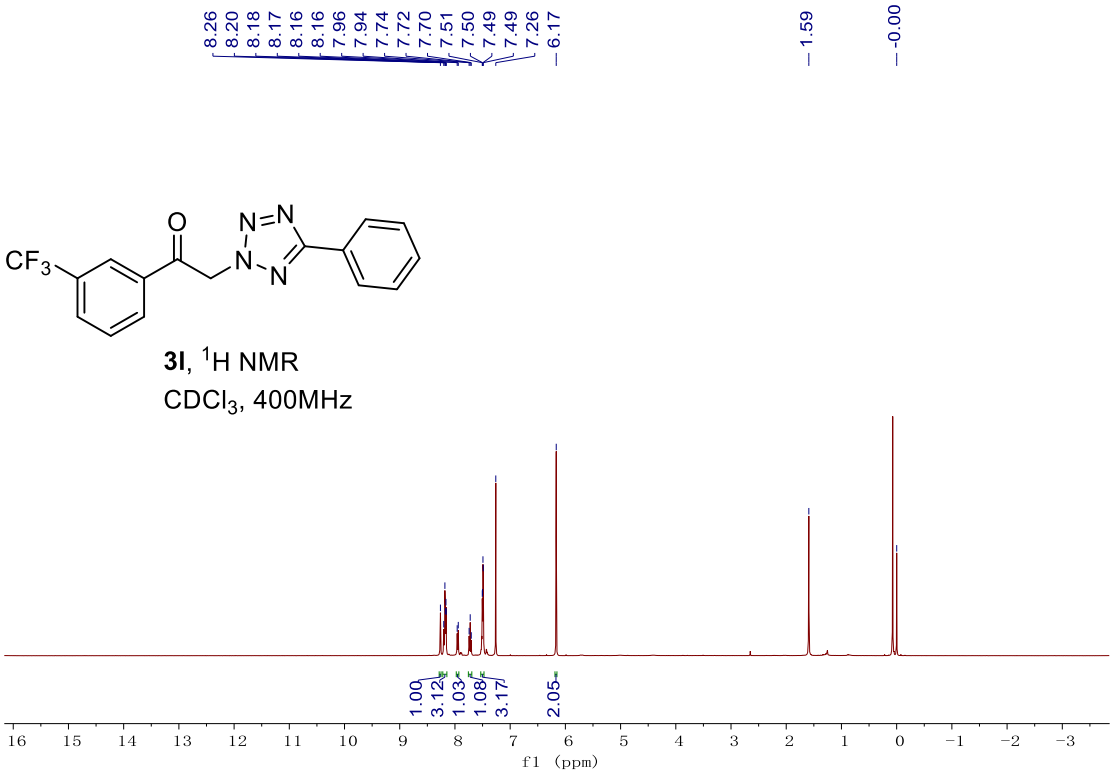




3k, ^{13}C NMR

$CDCl_3$, 100MHz

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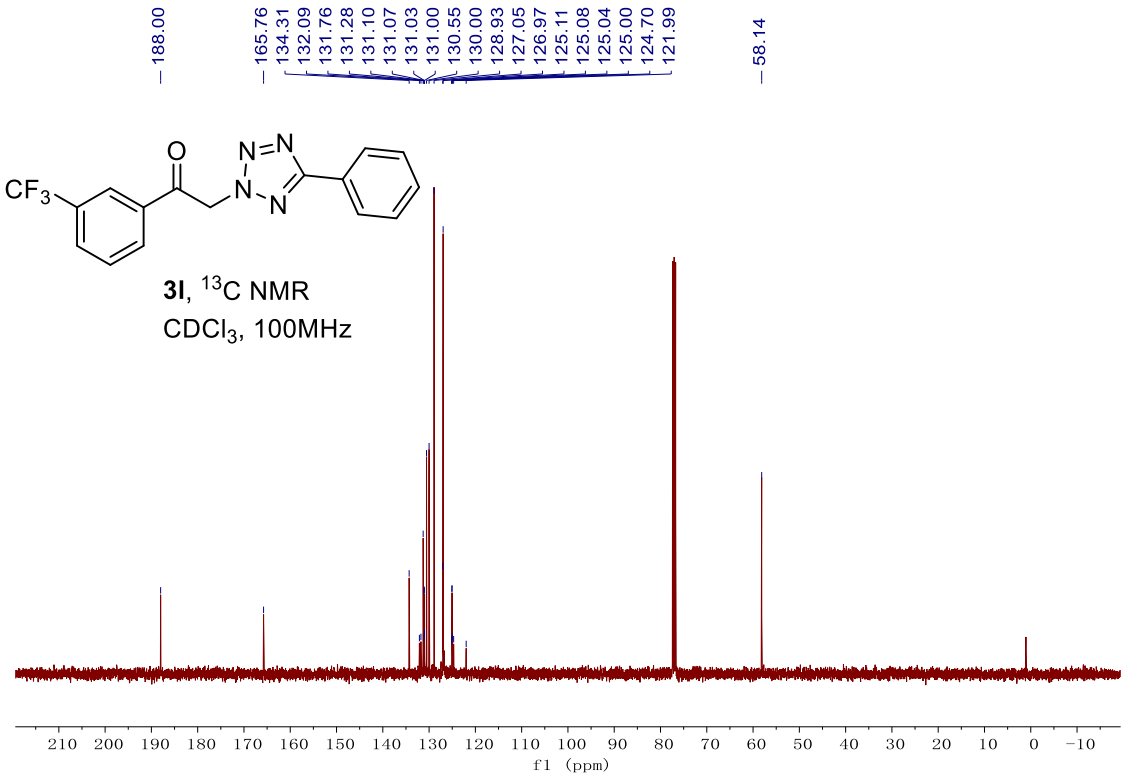
8.20
8.18
8.17
8.16
8.16
7.96
7.94
7.74
7.72
7.70
7.51
7.50
7.49
7.49
7.26
6.17
1.59
-0.00
O
N=N
N
N
CF3
3I, 1H NMR
CDCl3, 400MHz
1.00
3.12
1.03
1.08
3.17
2.05
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)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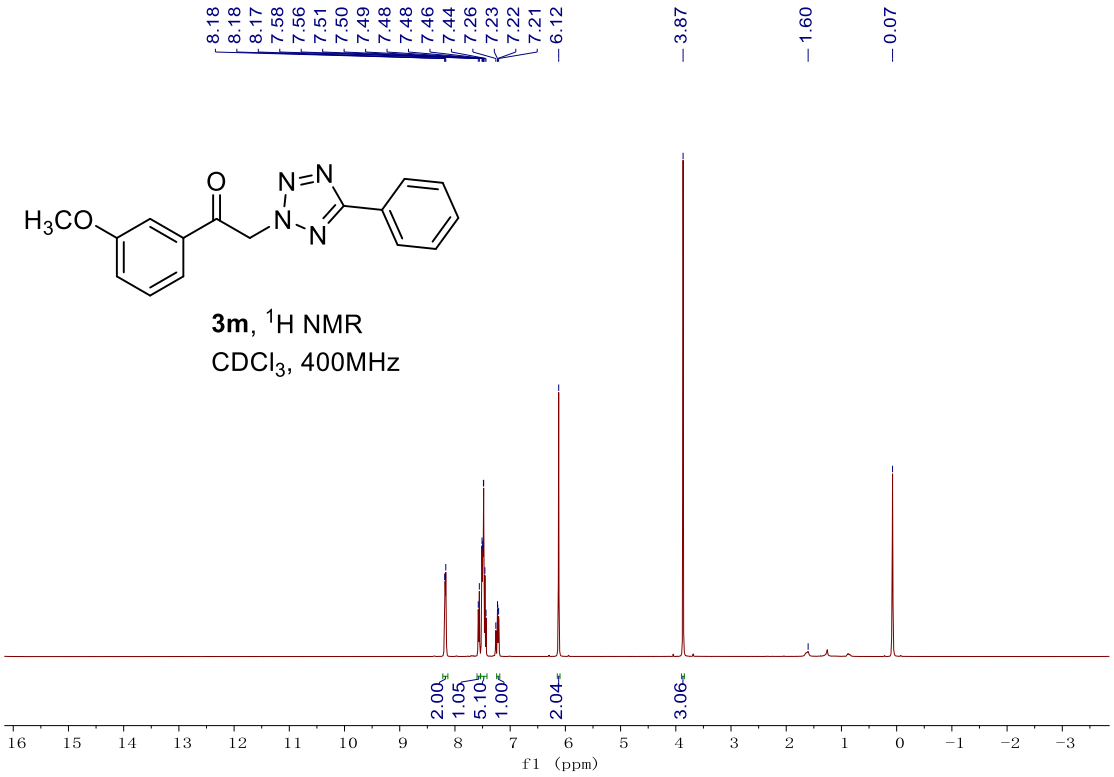
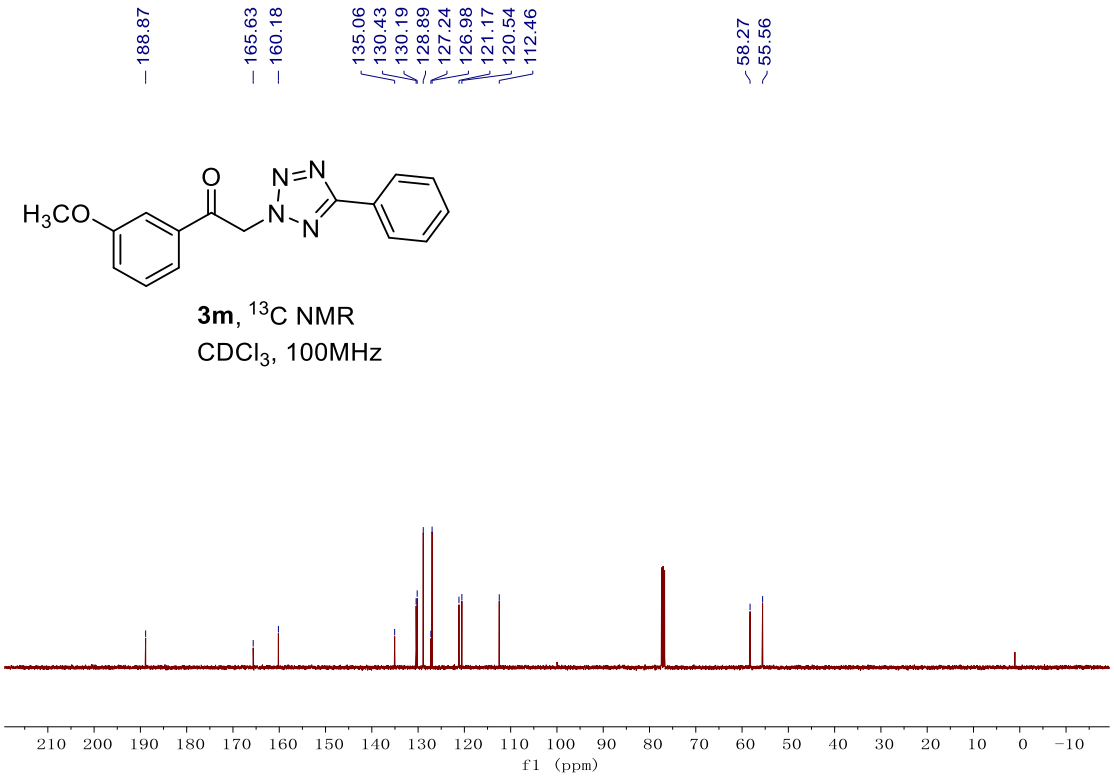
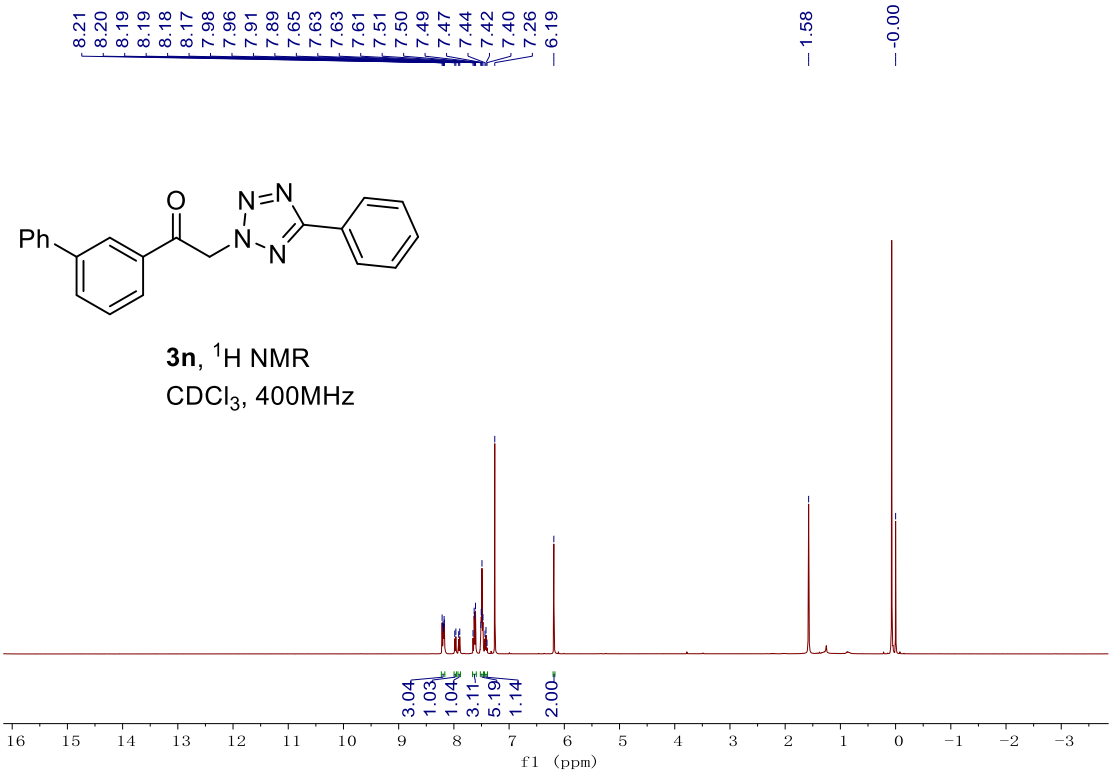
134.31
132.09
131.76
131.28
131.10
131.07
131.03
131.00
130.55
130.00
128.93
127.05
126.97
125.11
125.08
125.04
125.00
124.70
121.99
58.14
O
N=N
N
N
CF3
3I, 13C NMR
CDCl3, 100MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


8.18
8.18
8.17
7.58
7.56
7.51
7.50
7.49
7.48
7.48
7.46
7.44
7.26
7.23
7.22
7.21
6.12
3.87
1.60
0.07
O
N=N
N
N
H3CO
3m, 1H NMR
CDCl3, 400MHz
2.00
1.05
5.10
1.00
2.04
3.06
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)


188.87
165.63
160.18
135.06
130.43
130.19
128.89
127.24
126.98
121.17
120.54
112.46
58.27
55.56
O
N=N
N
N
H3CO
3m, 13C NMR
CDCl3, 100MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


8.21
8.20
8.19
8.19
8.18
8.17
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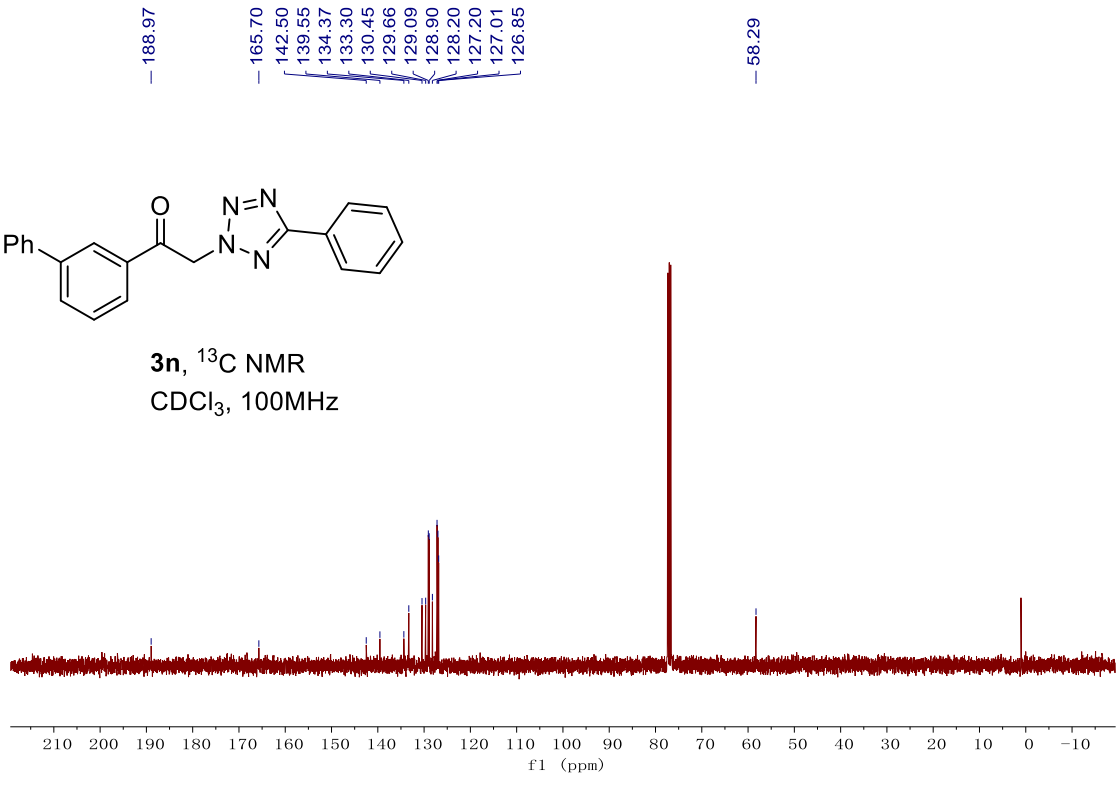
7.96
7.91
7.89
7.65
7.63
7.63
7.61
7.51
7.50
7.49
7.47
7.44
7.42
7.40
7.26
6.19
1.58
-0.00
Ph
O
N
N
N
3n, 1H NMR
CDCl3, 400MHz
3.04
1.03
1.04
3.11
5.19
1.14
2.00
f1 (ppm)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133.30
130.45
129.66
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128.90
128.20
127.20
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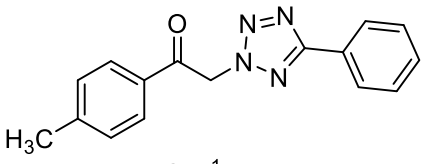
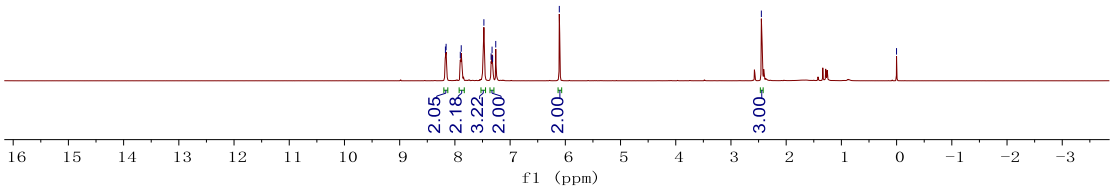
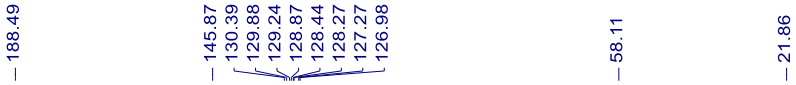
126.85
58.29
Ph
O
N
N
N
3n, 13C NMR
CDCl3, 100MHz
f1 (ppm)

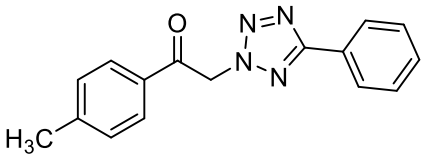


3o, ^{1}H NMR

$CDCl_3$, 400MHz

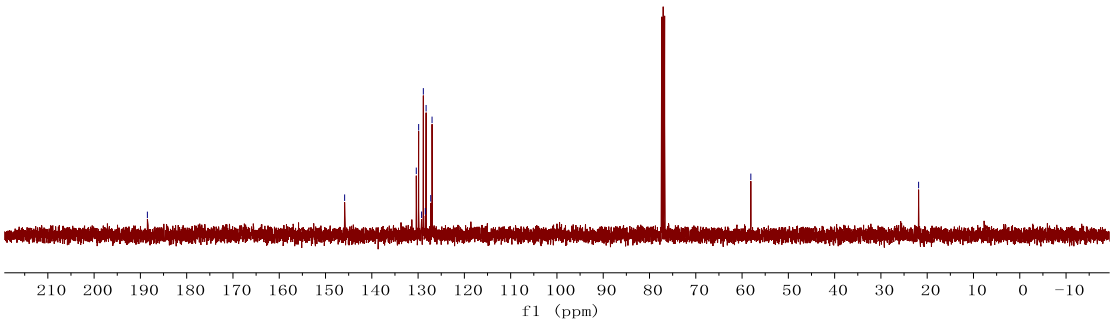


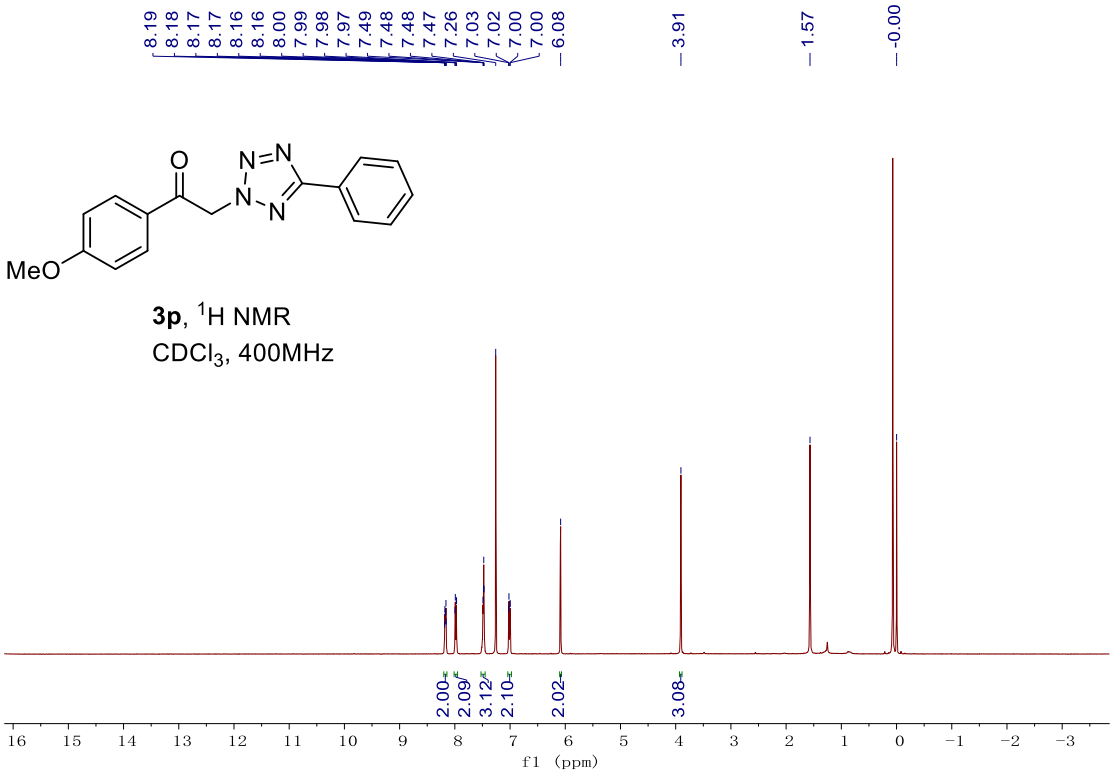


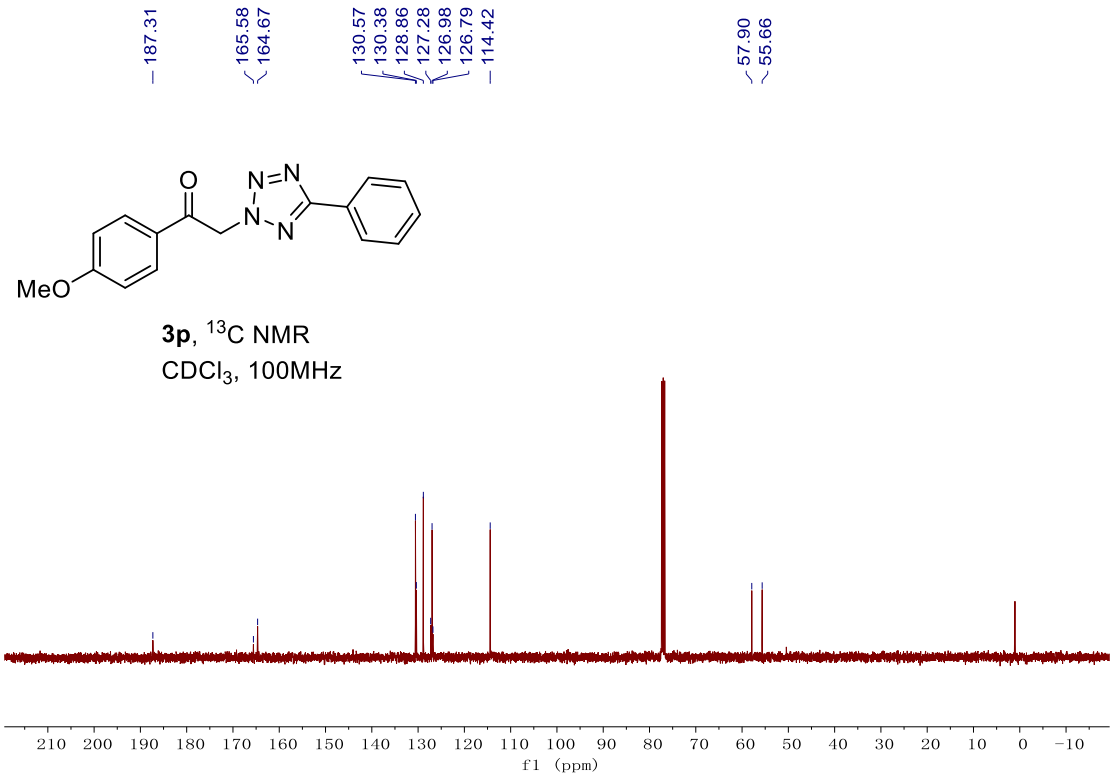


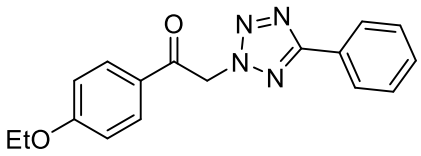
3o, ^{13}C NMR

$CDCl_3$, 100MHz



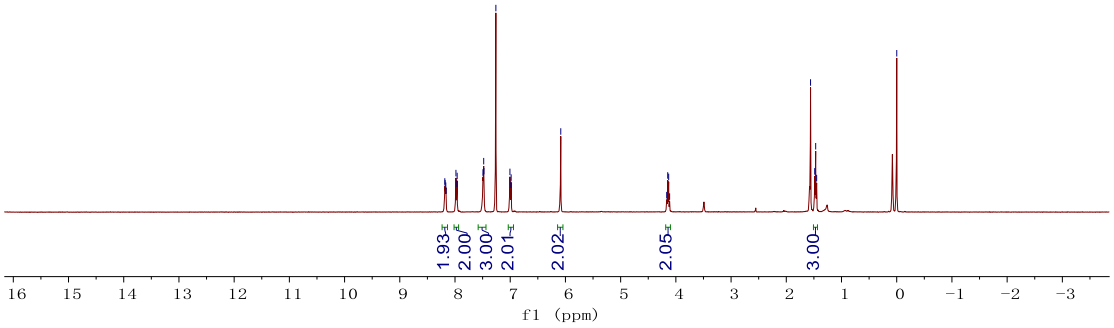

8.19
8.18
8.17
8.17
8.16
8.16
8.00
7.99
7.98
7.97
7.49
7.48
7.48
7.47
7.26
7.03
7.02
7.00
7.00
6.08
3.91
1.57
-0.00
MeO
3p, 1H NMR
CDCl3, 400MHz
2.00
2.09
3.12
2.10
2.02
3.08
f1 (ppm)

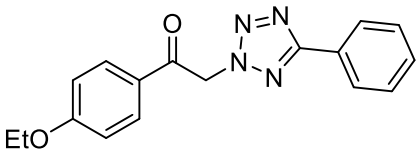

187.31
165.58
164.67
130.57
130.38
128.86
127.28
126.98
126.79
114.42
57.90
55.66
MeO
3p, 13C NMR
CDCl3, 100MHz
f1 (ppm)



3q, ^{1}H NMR

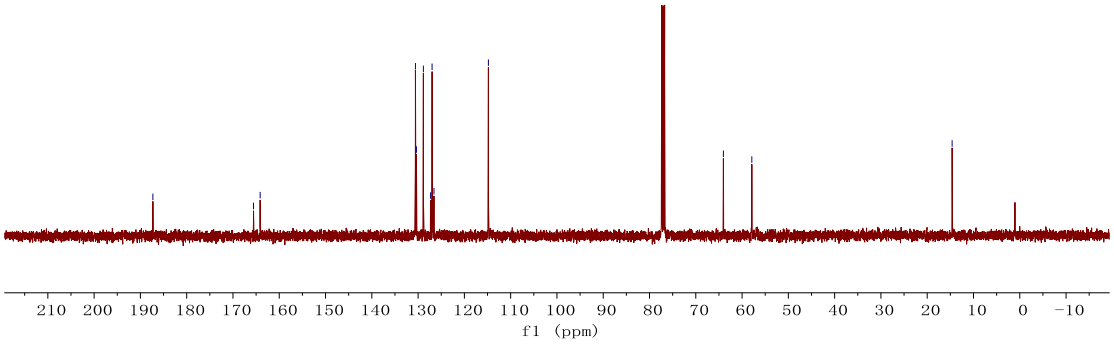
$CDCl_3$, 400MHz

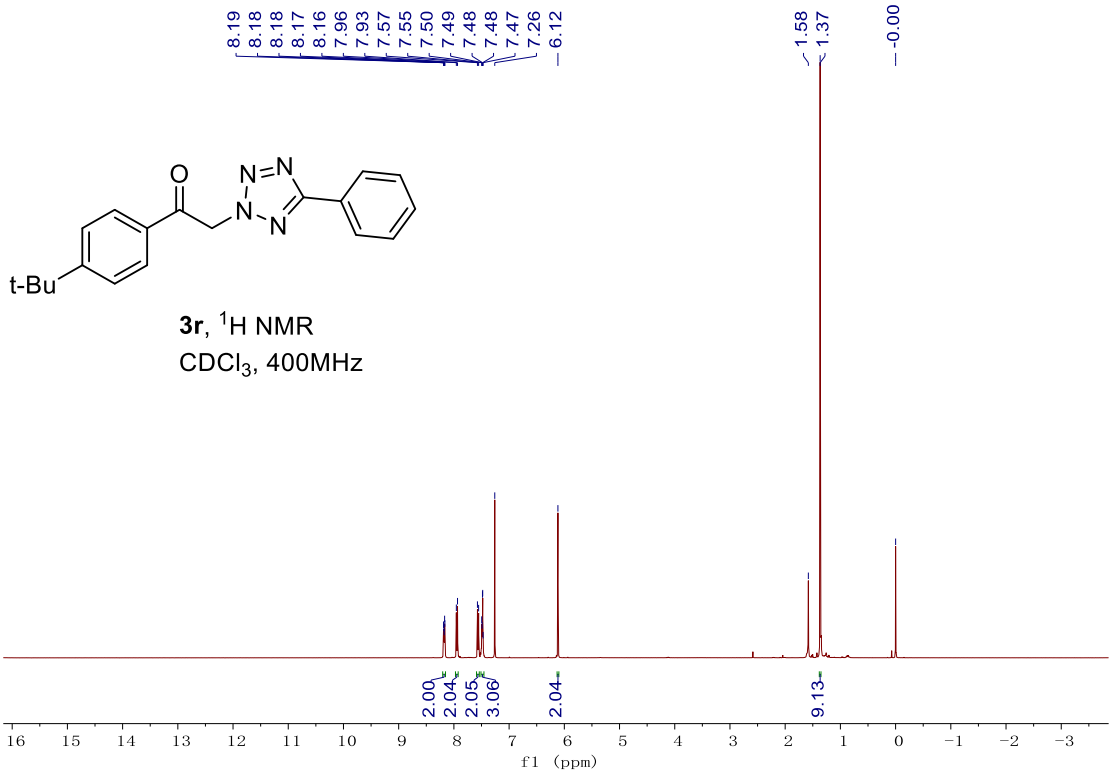




3q, ^{13}C NMR

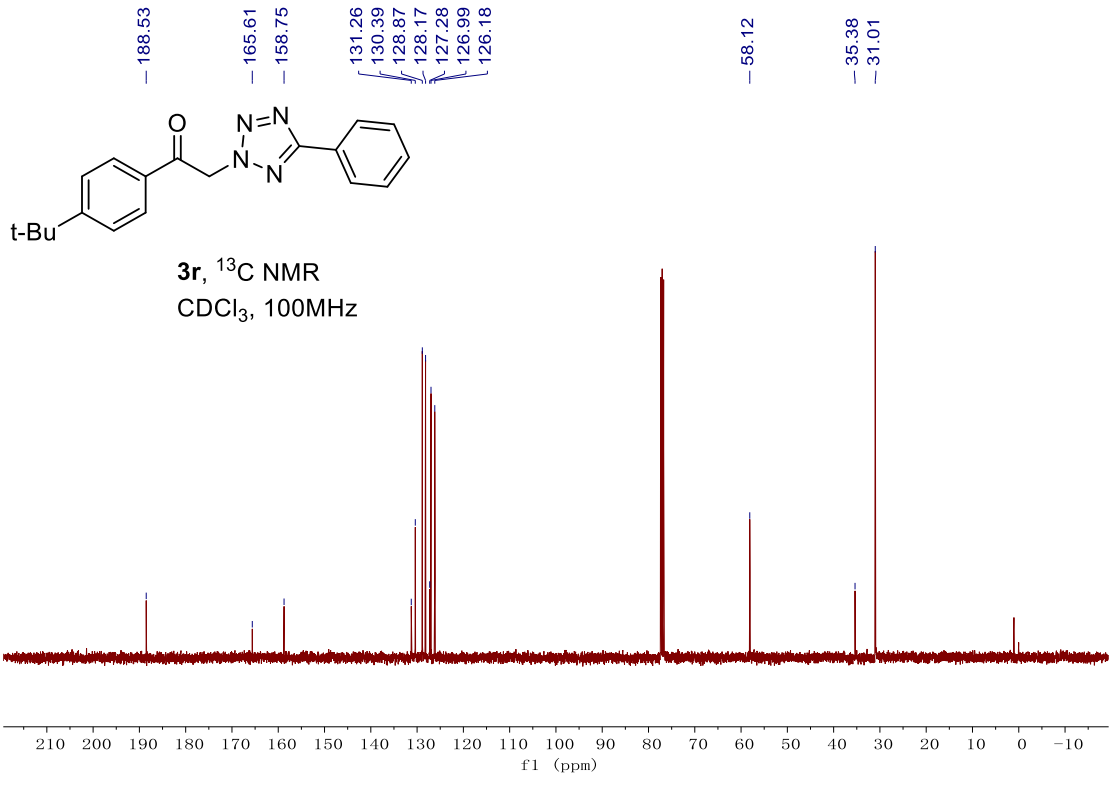
$CDCl_3$, 100MHz





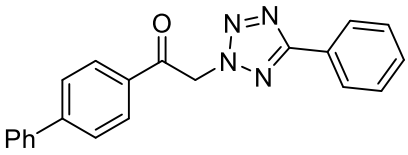
3r, ^{1}H NMR

$CDCl_3$, 400MHz



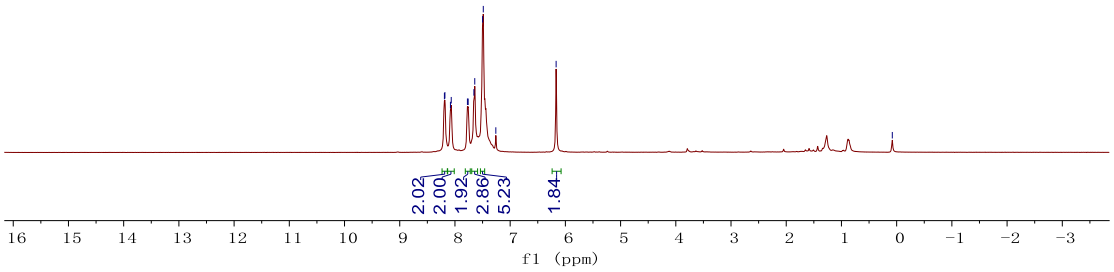
3r, ^{13}C NMR

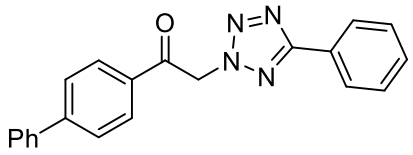
$CDCl_3$, 100MHz



3s, ^{1}H NMR

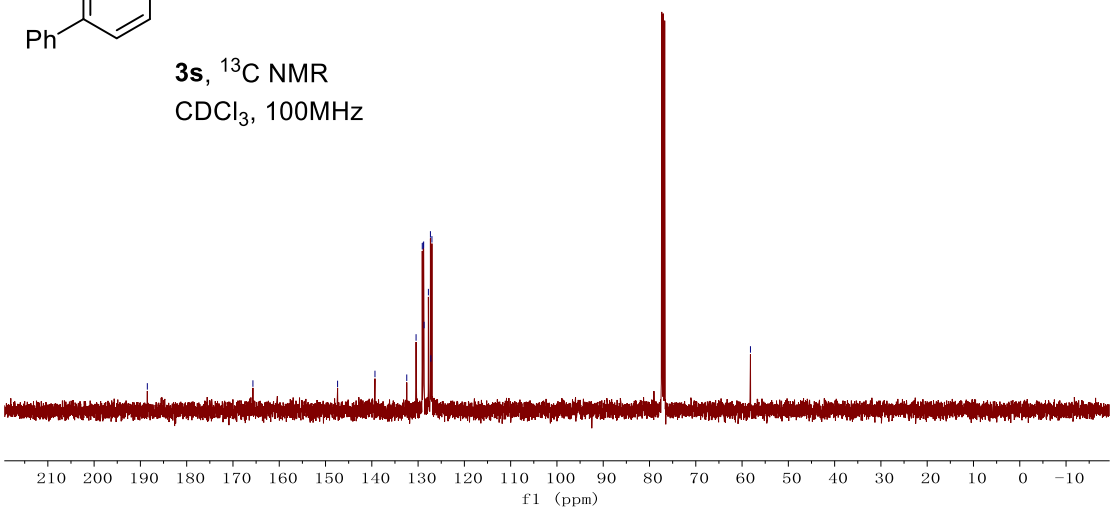
$CDCl_3$, 400MHz

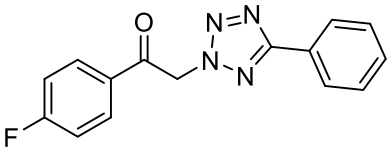




3s, ^{13}C NMR

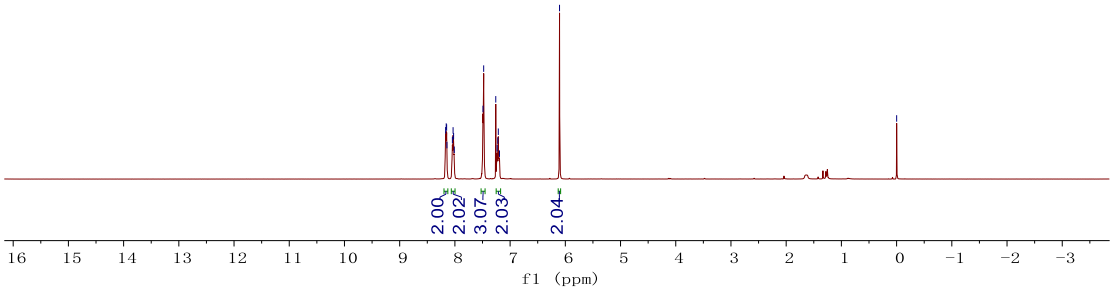
$CDCl_3$, 100MHz

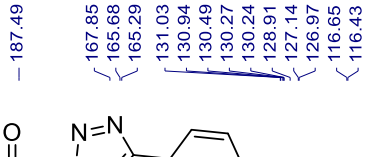


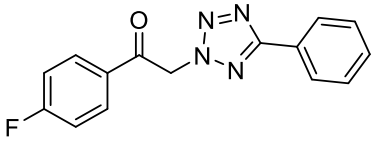


3t, ^{1}H NMR

$CDCl_3$, 400MHz

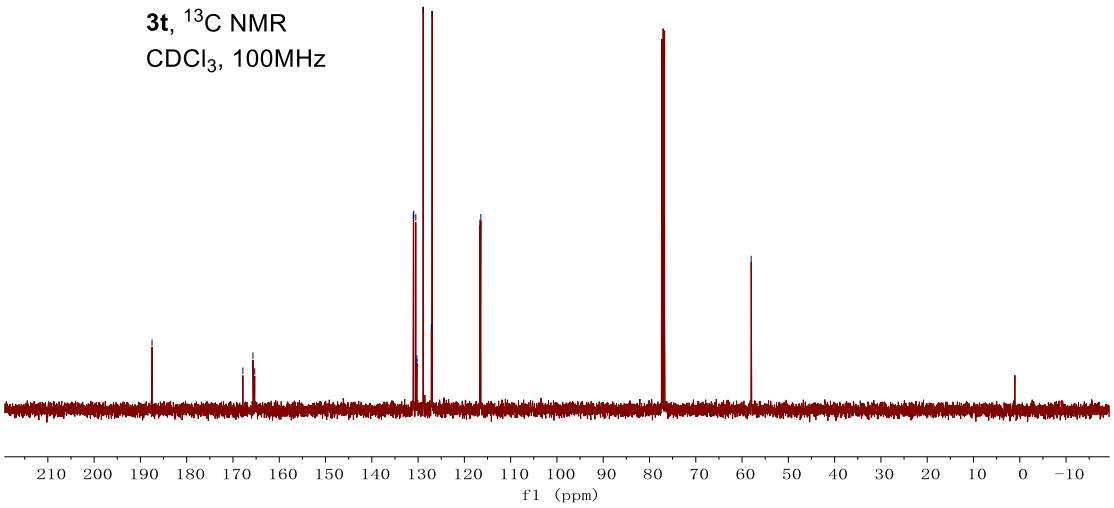


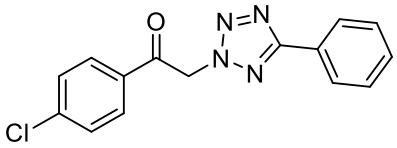




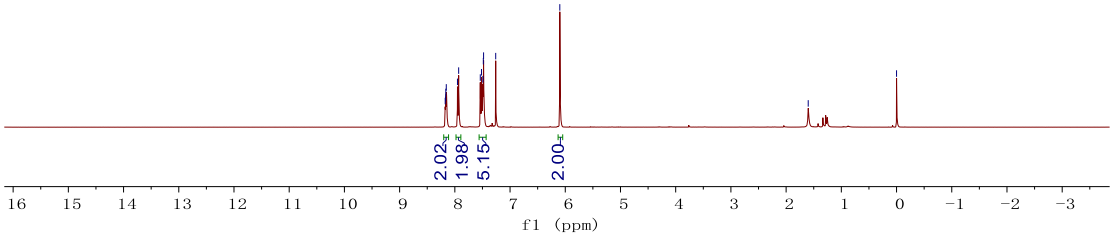
3t, ^{13}C NMR

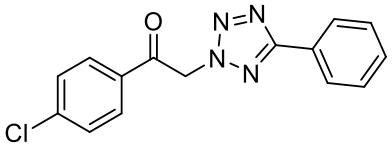
$CDCl_3$, 100MHz



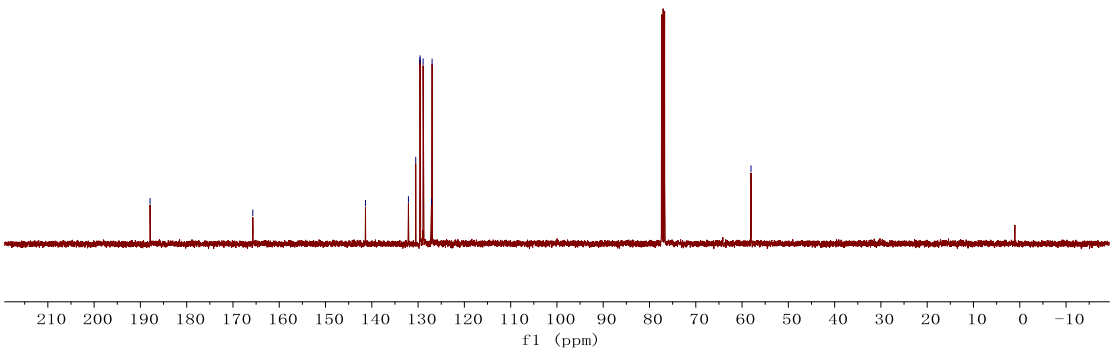


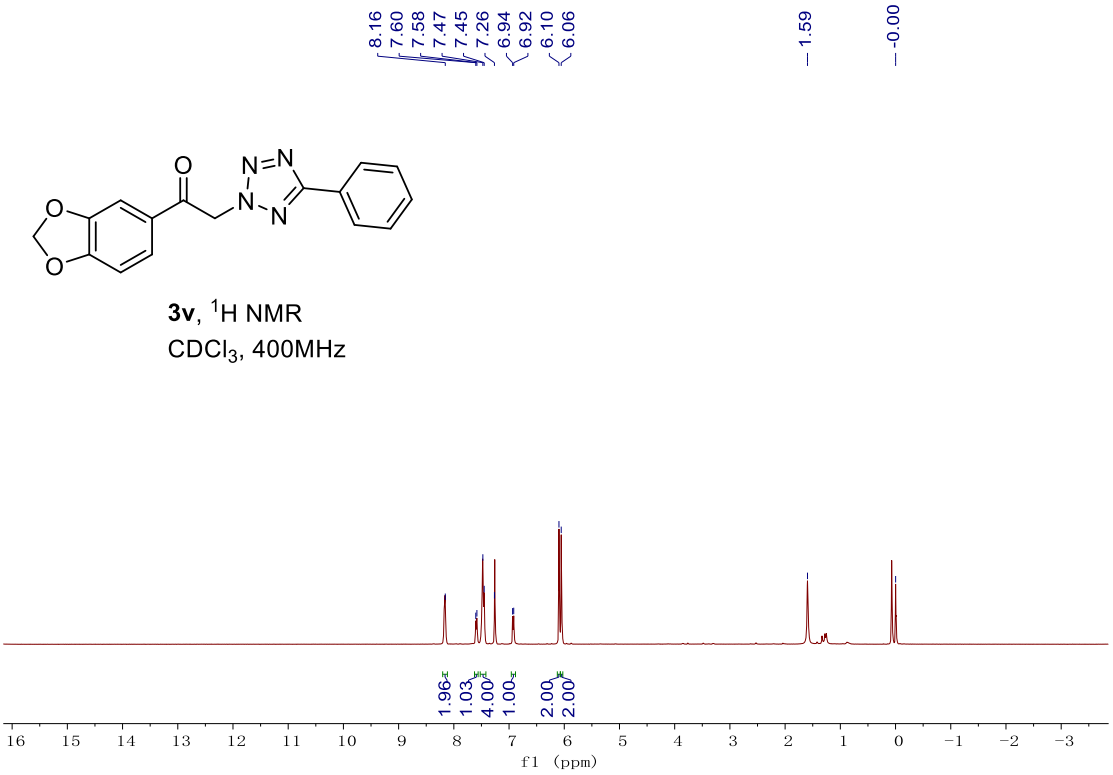
3u, ^{1}H NMR
$CDCl_3$, 400MHz





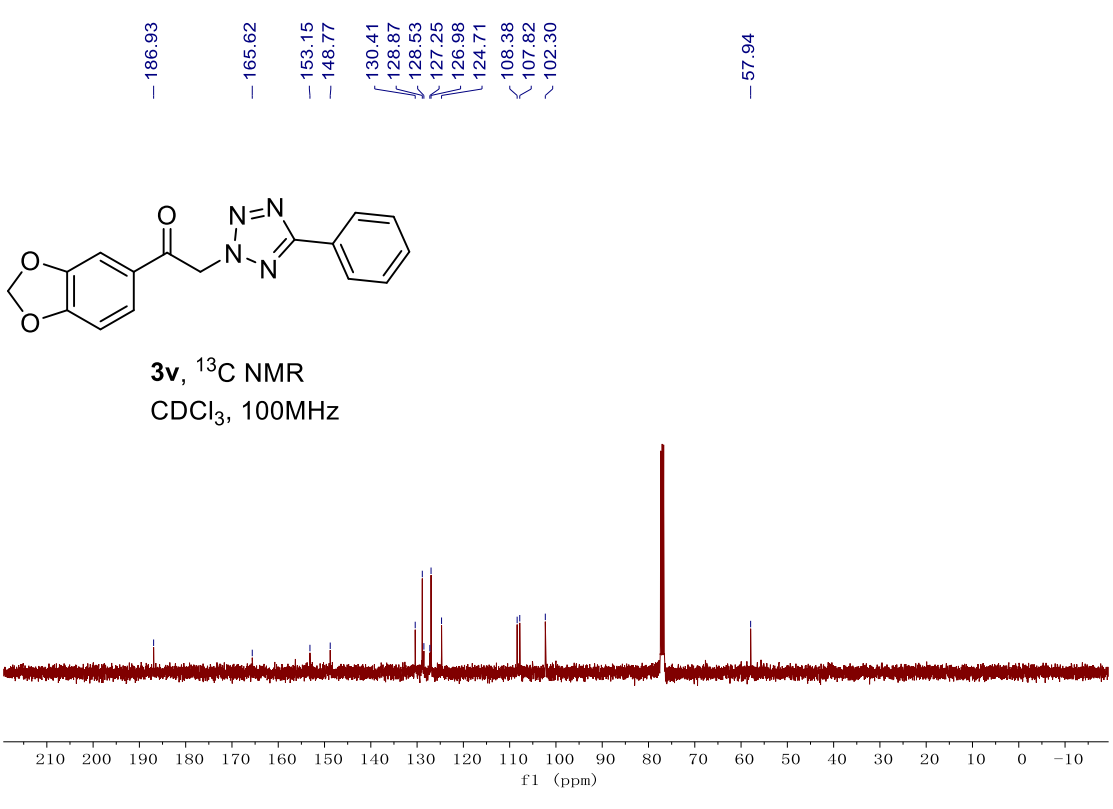
3u, ^{13}C NMR
$CDCl_3$, 100MHz





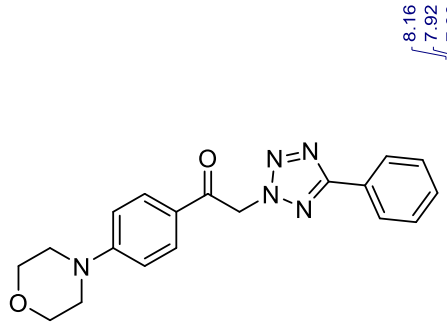
3v, ^{1}H NMR

$CDCl_3$, 400MHz

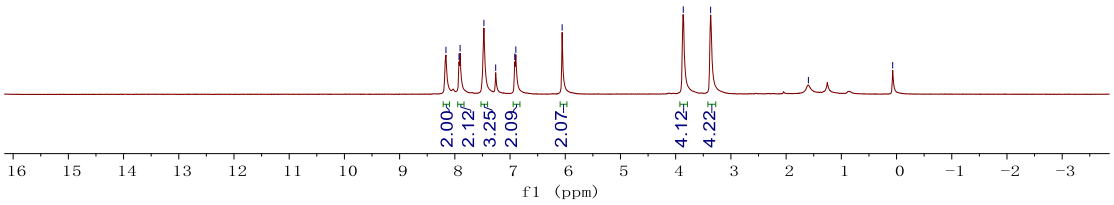


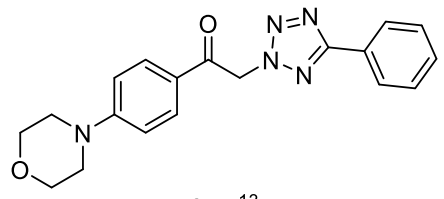
3v, ^{13}C NMR

$CDCl_3$, 100MHz

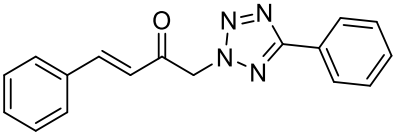


3w, ^{1}H NMR
$CDCl_3$, 400MHz



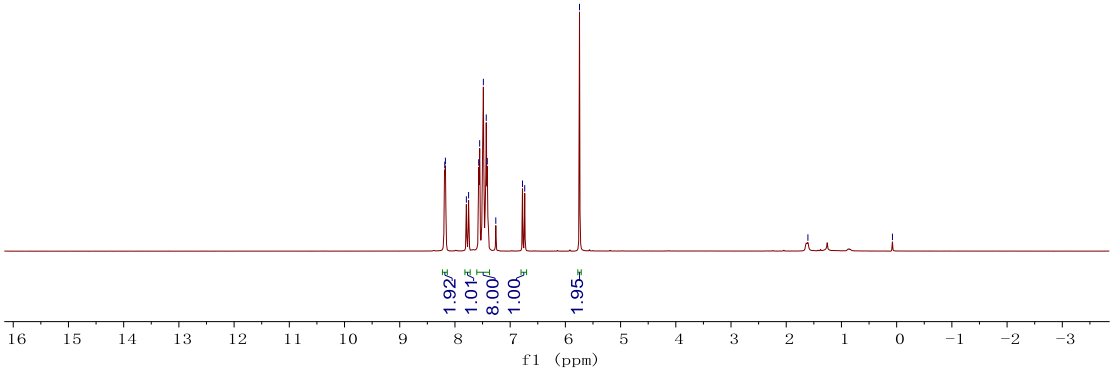


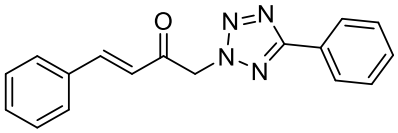
3w, ^{13}C NMR
$CDCl_3$, 100MHz



3x, ^{1}H NMR

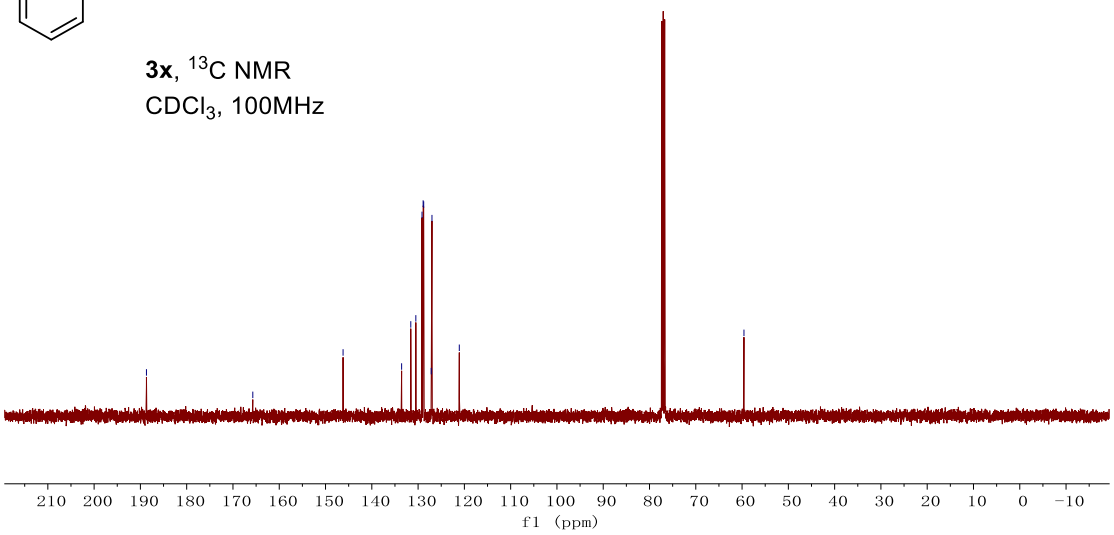
$CDCl_3$, 400MHz

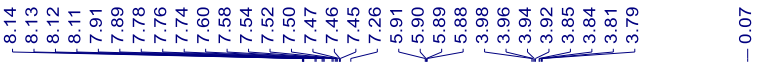


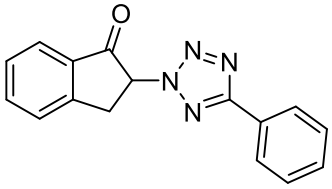


3x, ^{13}C NMR

$CDCl_3$, 100MHz

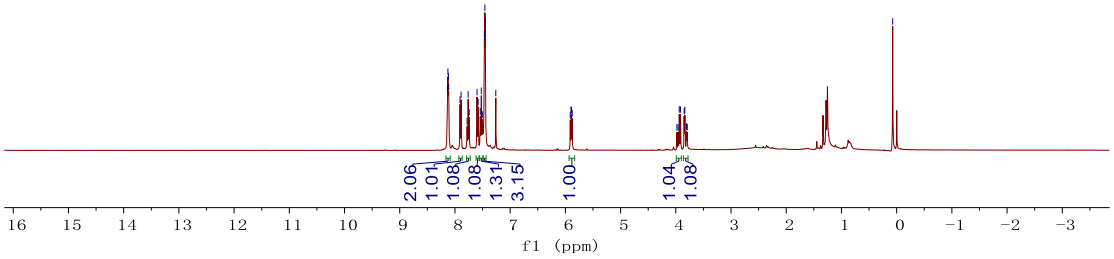


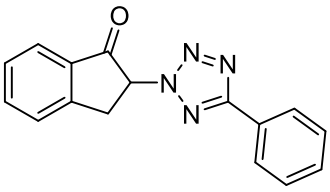




3y, ^{1}H NMR

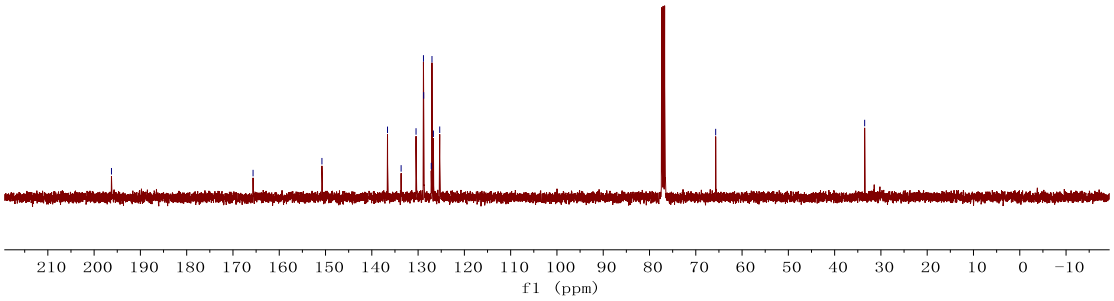
$CDCl_3$, 400MHz

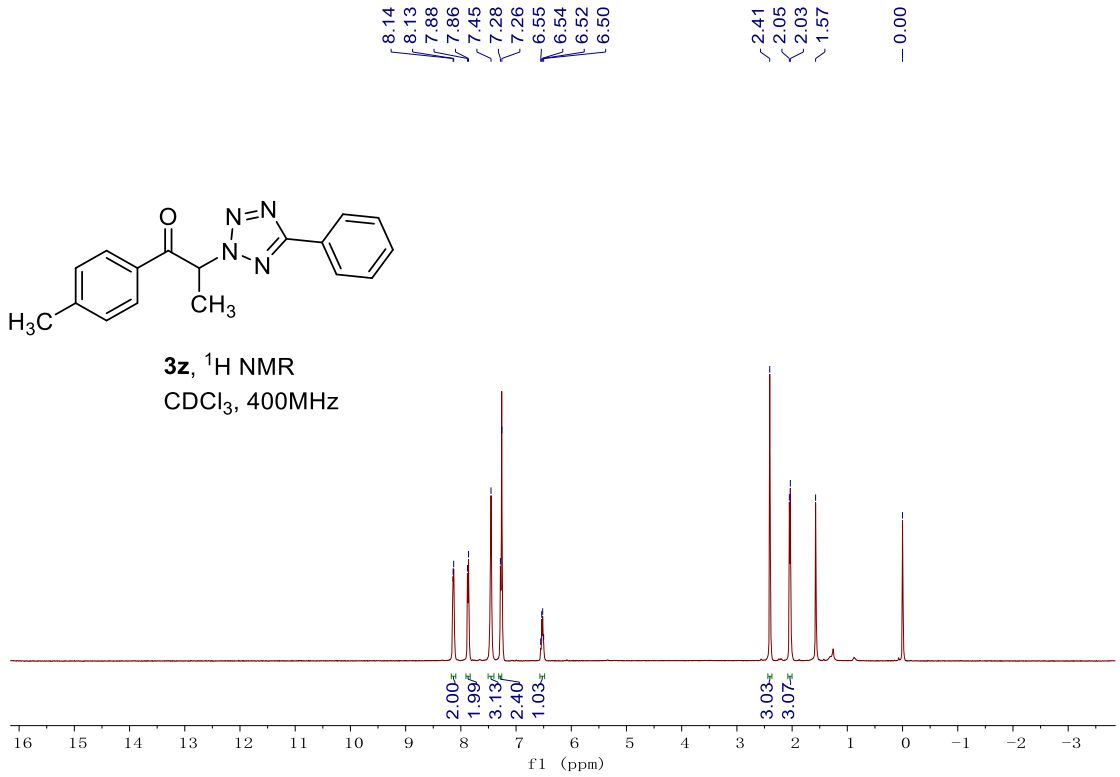




3y, ^{13}C NMR

$CDCl_3$, 100MHz

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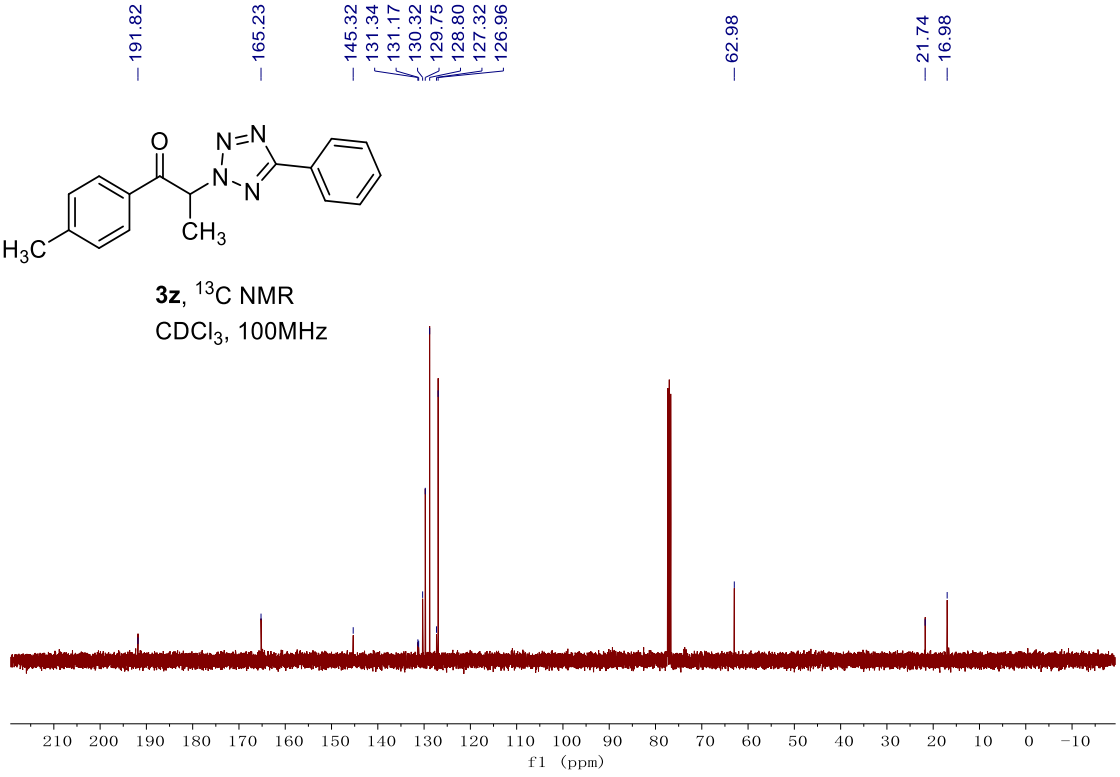
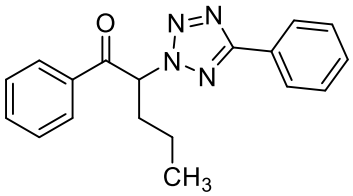
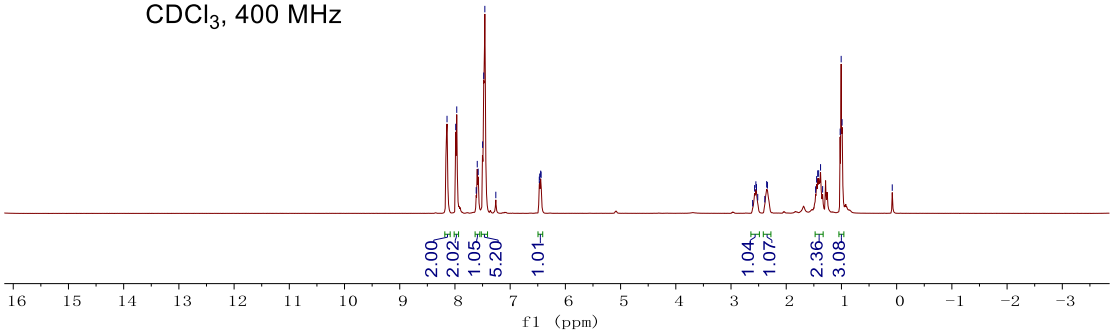
7.45
7.28
7.26
6.55
6.54
6.52
6.50
2.41
2.05
2.03
1.57
0.00
O
N=N
N
N
CH3
H3C
3z, 1H NMR
CDCl3, 400MHz
2.00
1.99
3.13
2.40
1.03
3.03
3.07
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

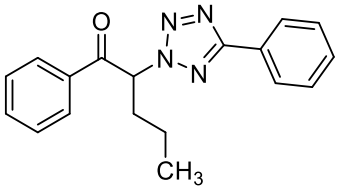

191.82
165.23
145.32
131.34
131.17
130.32
129.75
128.80
127.32
126.96
62.98
21.74
16.98
O
N=N
N
N
CH3
H3C
3z, 13C NMR
CDCl3, 100MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



3aa, ^{1}H NMR

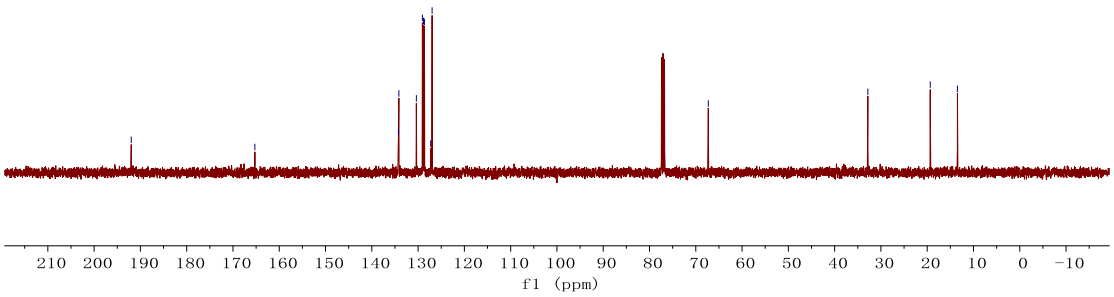
$CDCl_3$, 400 MHz

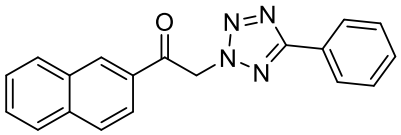




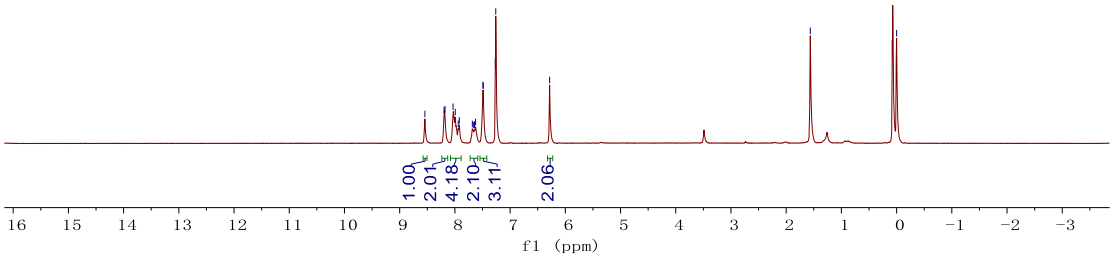
3aa, ^{13}C NMR

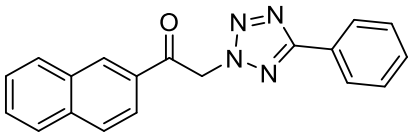
$CDCl_3$, 100 MHz



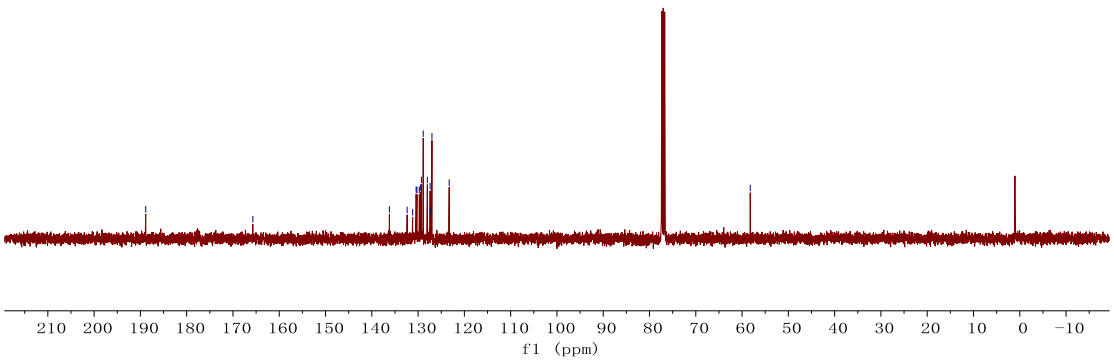


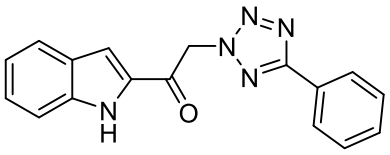
3ba, ^{1}H NMR
$CDCl_3$, 400 MHz



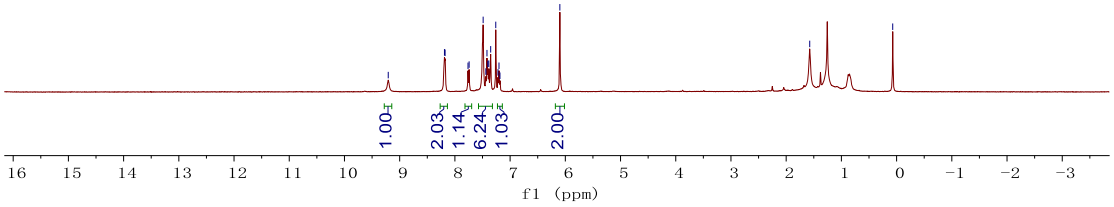


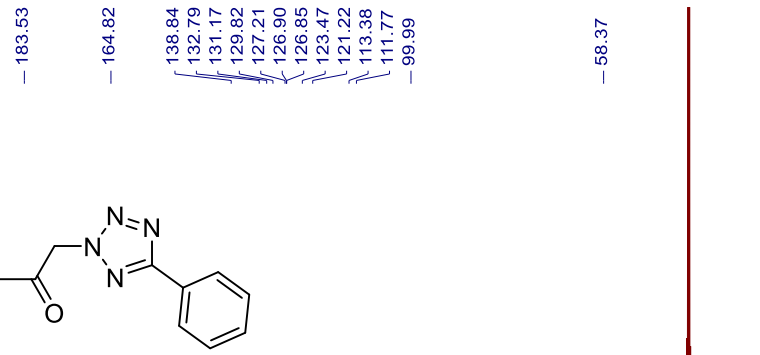
3ba, ^{13}C NMR
$CDCl_3$, 100 MHz



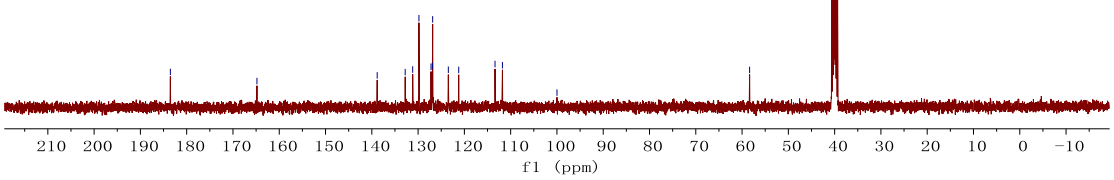


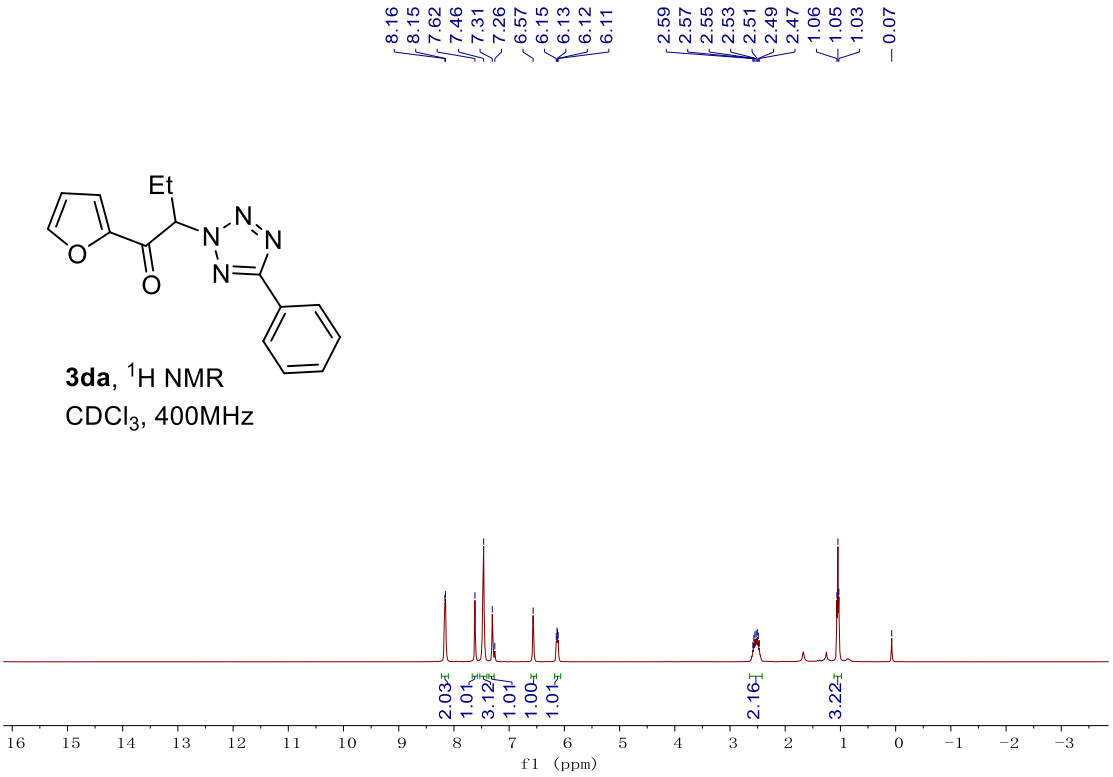
3ca, ^{1}H NMR
$CDCl_3$, 400MHz

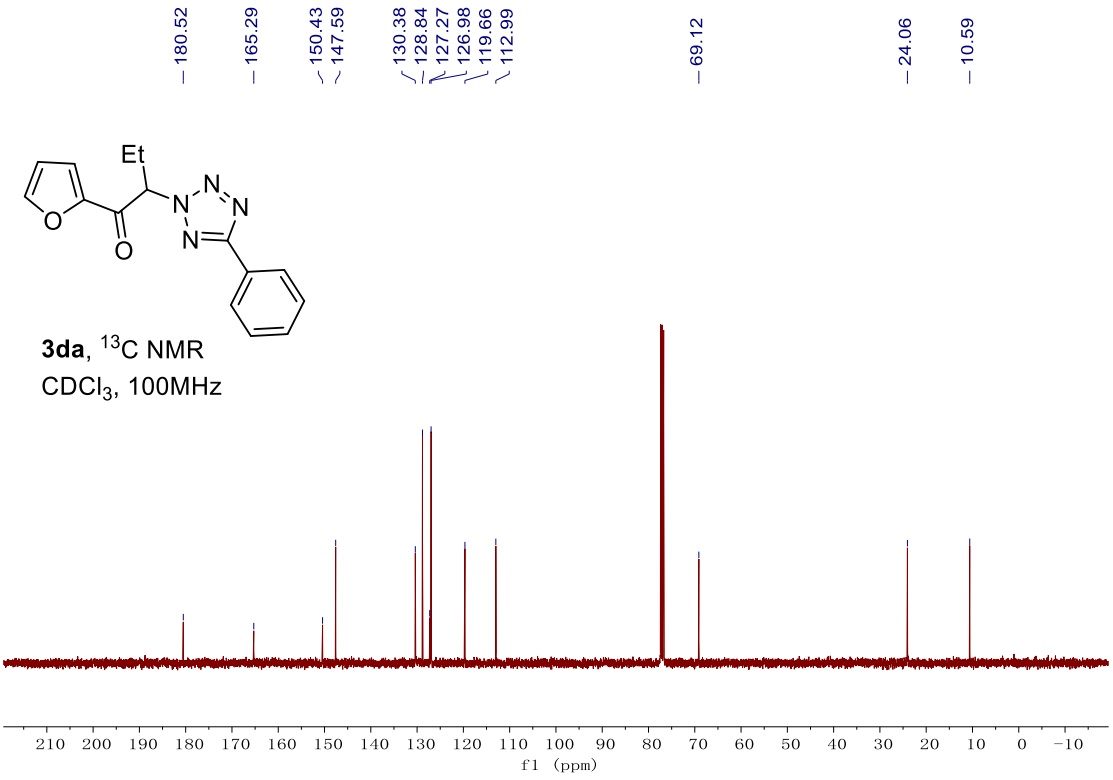


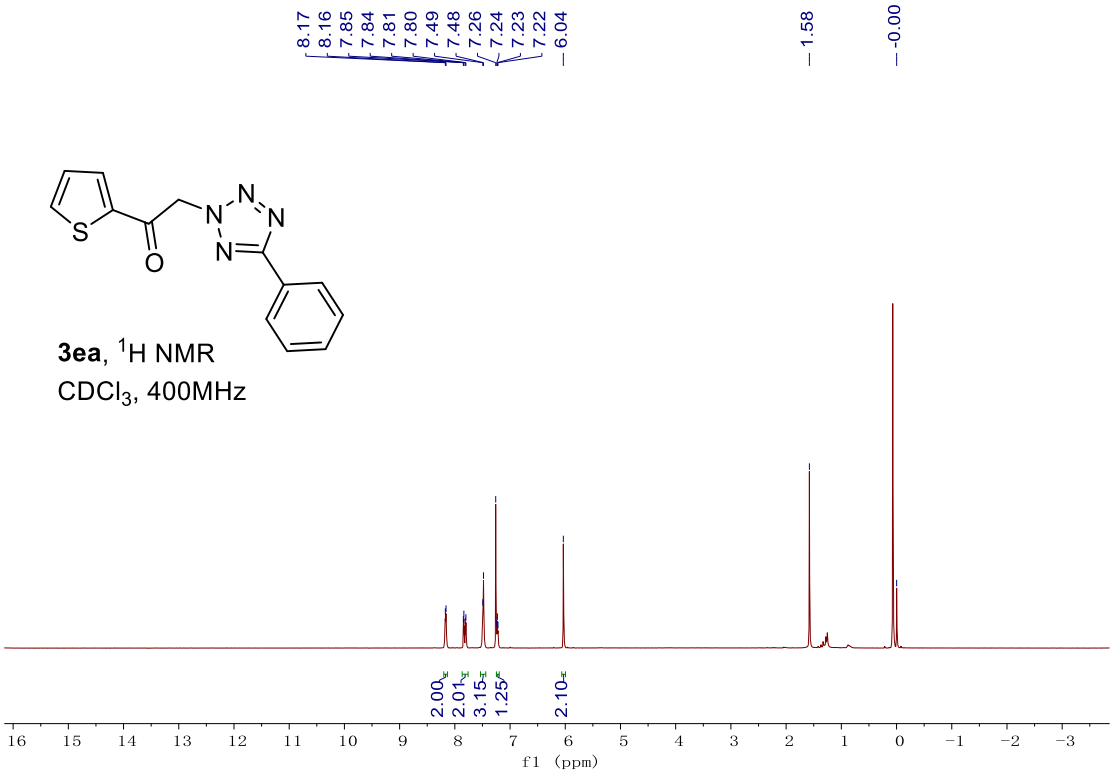


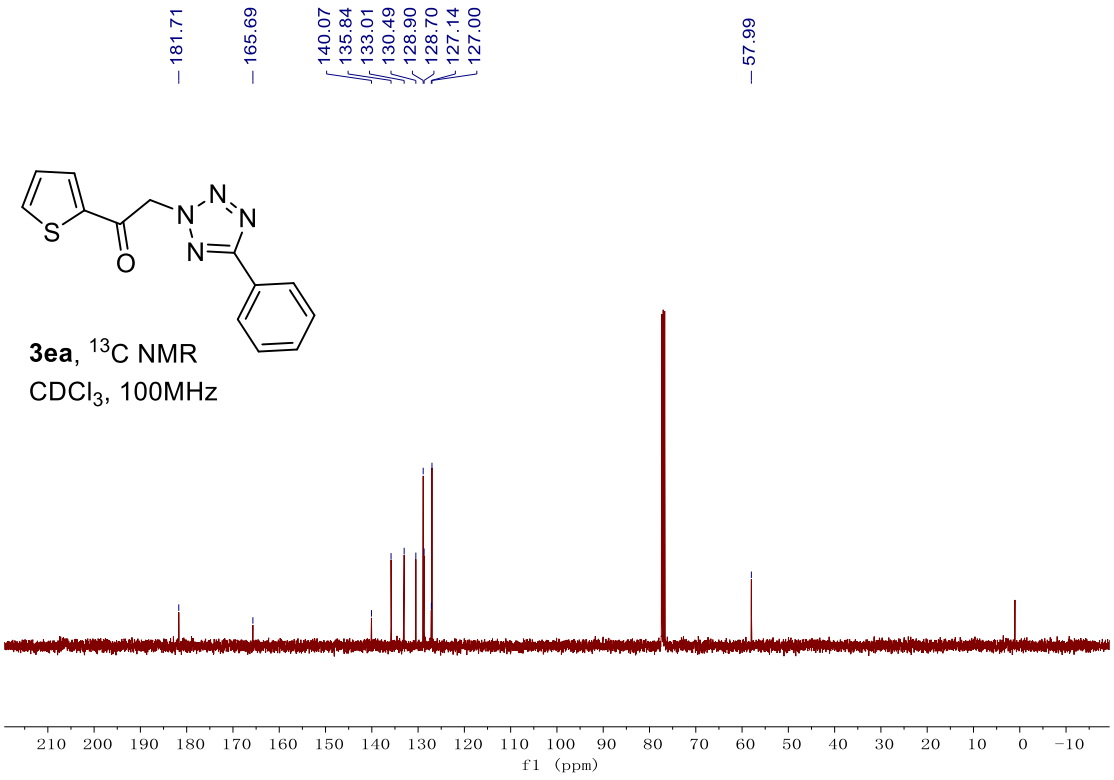
3ca, ^{13}C NMR
DMSO-d_6, 100MHz

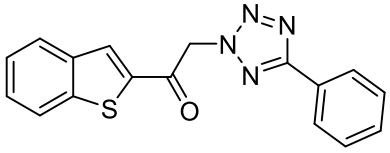



8.16
8.15
7.62
7.46
7.31
7.26
6.57
6.15
6.13
6.12
6.11
2.59
2.57
2.55
2.53
2.51
2.49
2.47
1.06
1.05
1.03
0.07
Et
O
O
N
N
N
N
3da, 1H NMR
CDCl3, 400MHz
2.03
1.01
3.12
1.01
1.00
1.01
2.16
3.22
f1 (ppm)


180.52
165.29
150.43
147.59
130.38
128.84
127.27
126.98
119.66
112.99
69.12
24.06
10.59
Et
O
O
N
N
N
N
3da, 13C NMR
CDCl3, 100MHz
f1 (ppm)

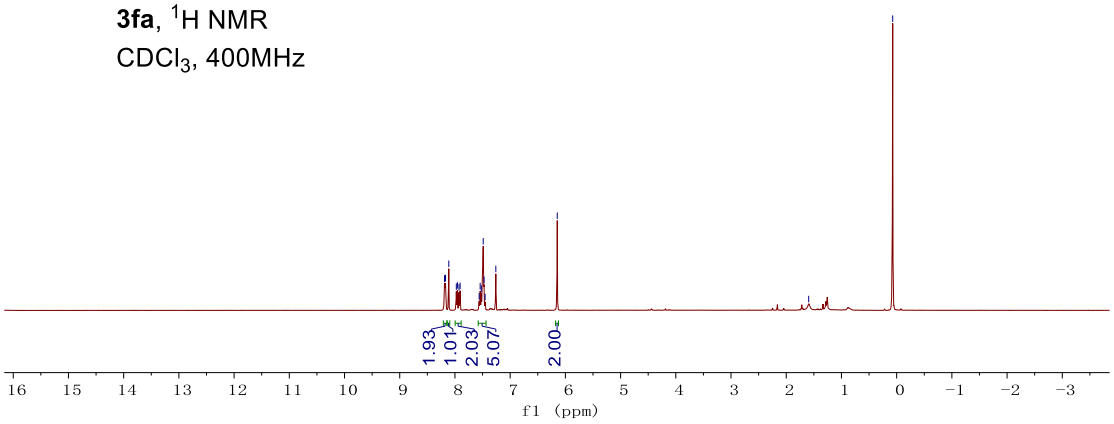

8.17
8.16
7.85
7.84
7.81
7.80
7.49
7.48
7.26
7.24
7.23
7.22
6.04
1.58
-0.00
3ea, 1H NMR
CDCl3, 400MHz
2.00
2.01
3.15
1.25
2.10
f1 (ppm)

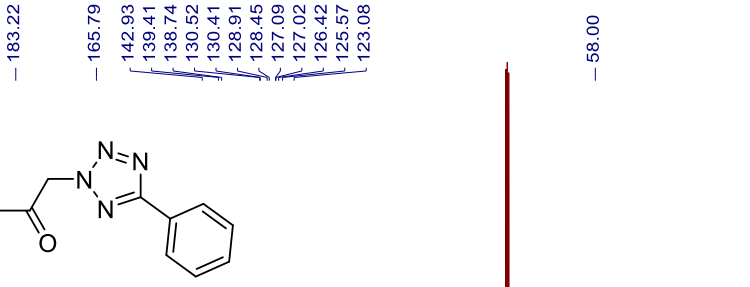

181.71
165.69
140.07
135.84
133.01
130.49
128.90
128.70
127.14
127.00
57.99
3ea, 13C NMR
CDCl3, 100MHz
f1 (ppm)



3fa, ^{1}H NMR

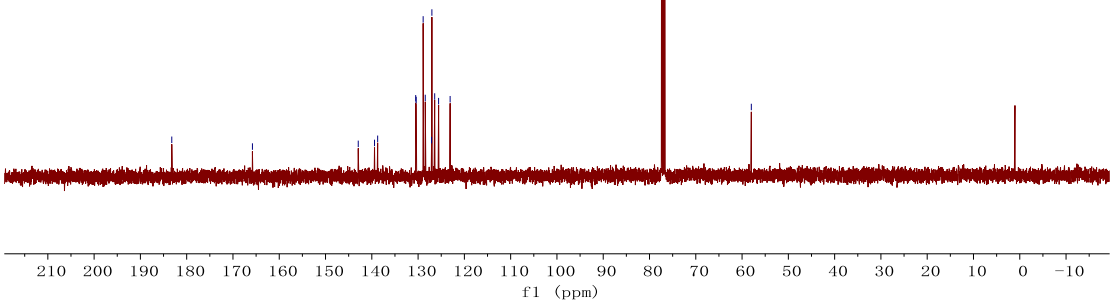
$CDCl_3$, 400MHz

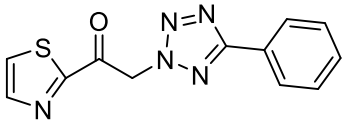




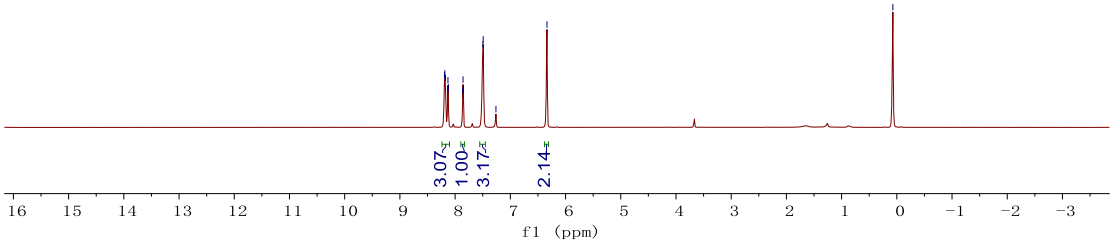
3fa, ^{13}C NMR

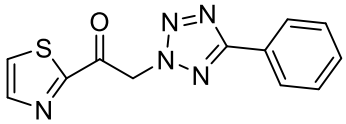
$CDCl_3$, 100MHz



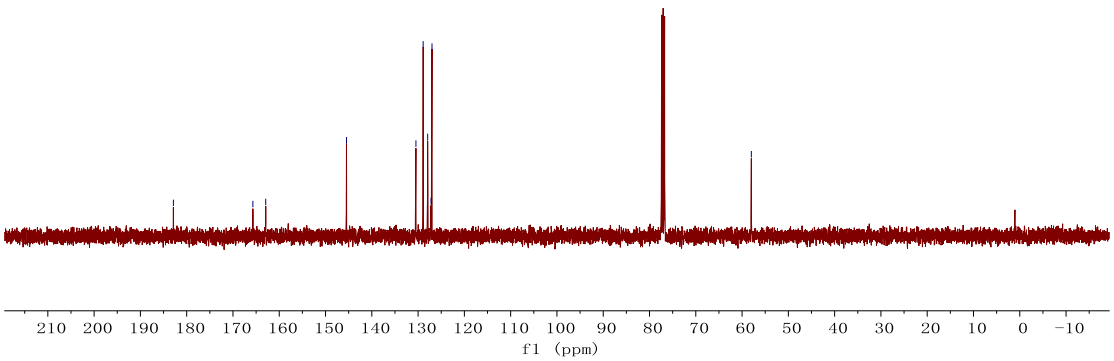


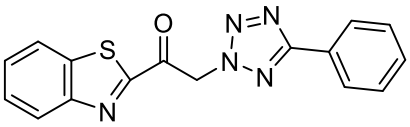
3ga, ^{1}H NMR
$CDCl_3$, 400MHz



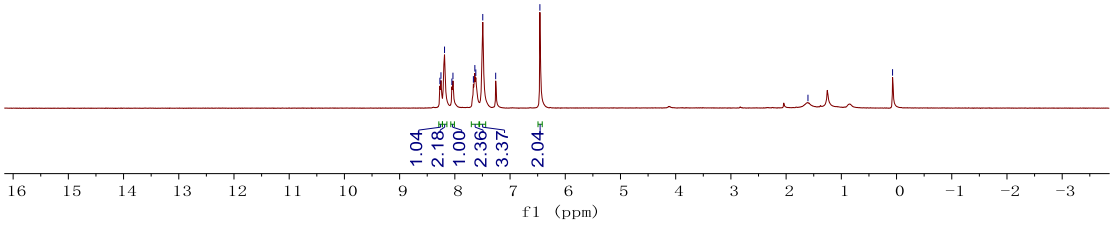


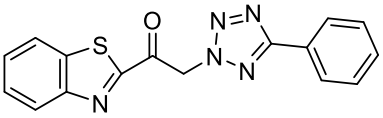
3ga, ^{13}C NMR
$CDCl_3$, 100MHz



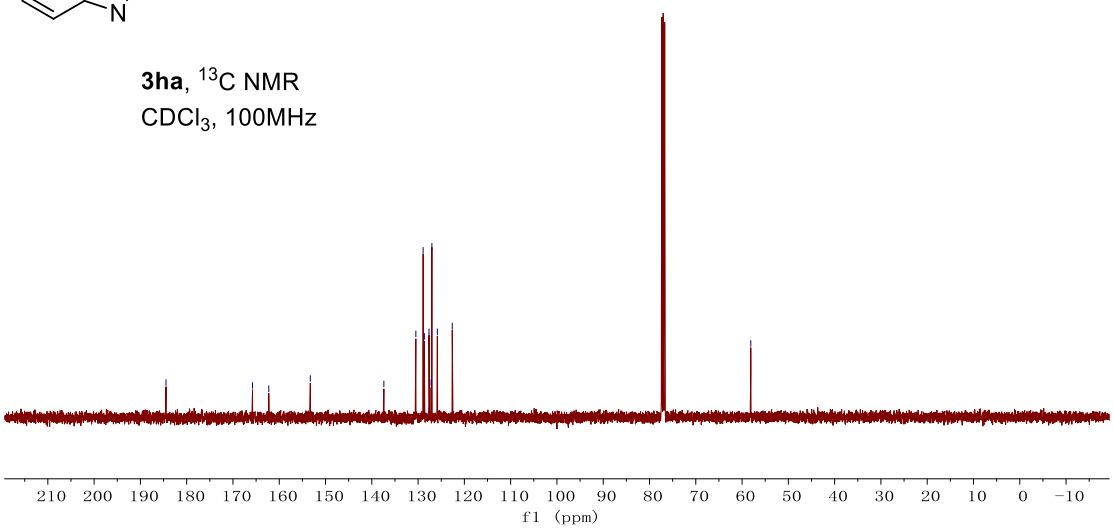


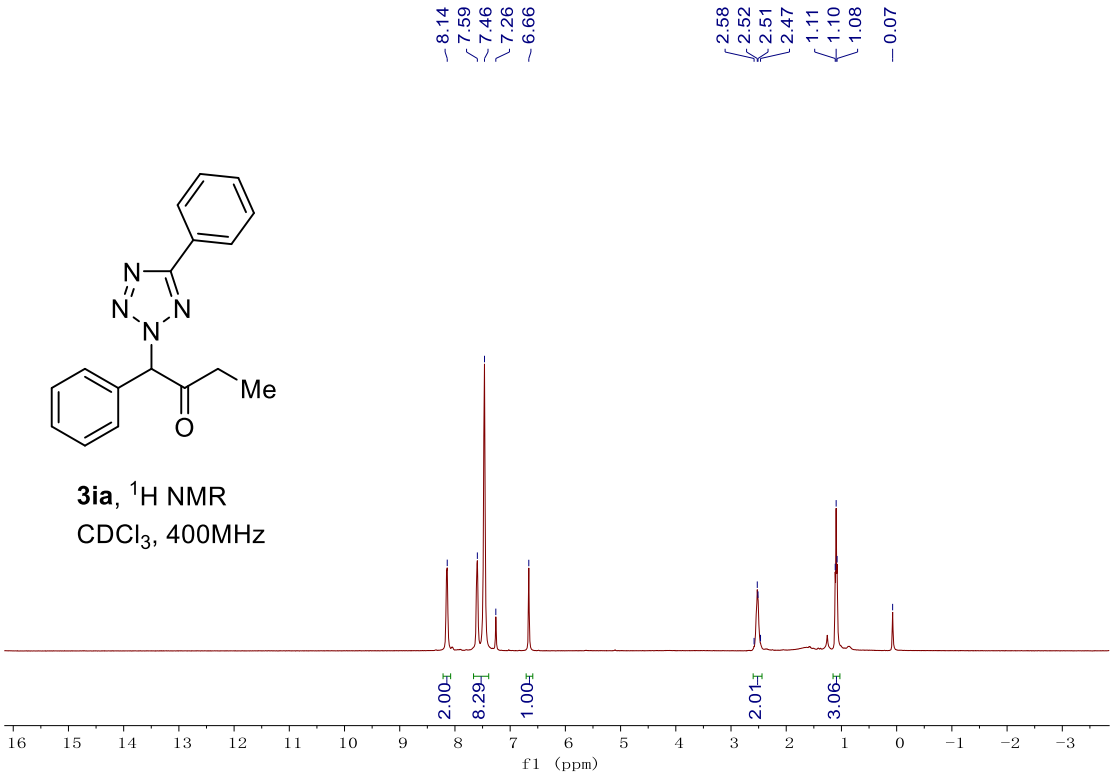
3ha, ^{1}H NMR
$CDCl_3$, 400MHz

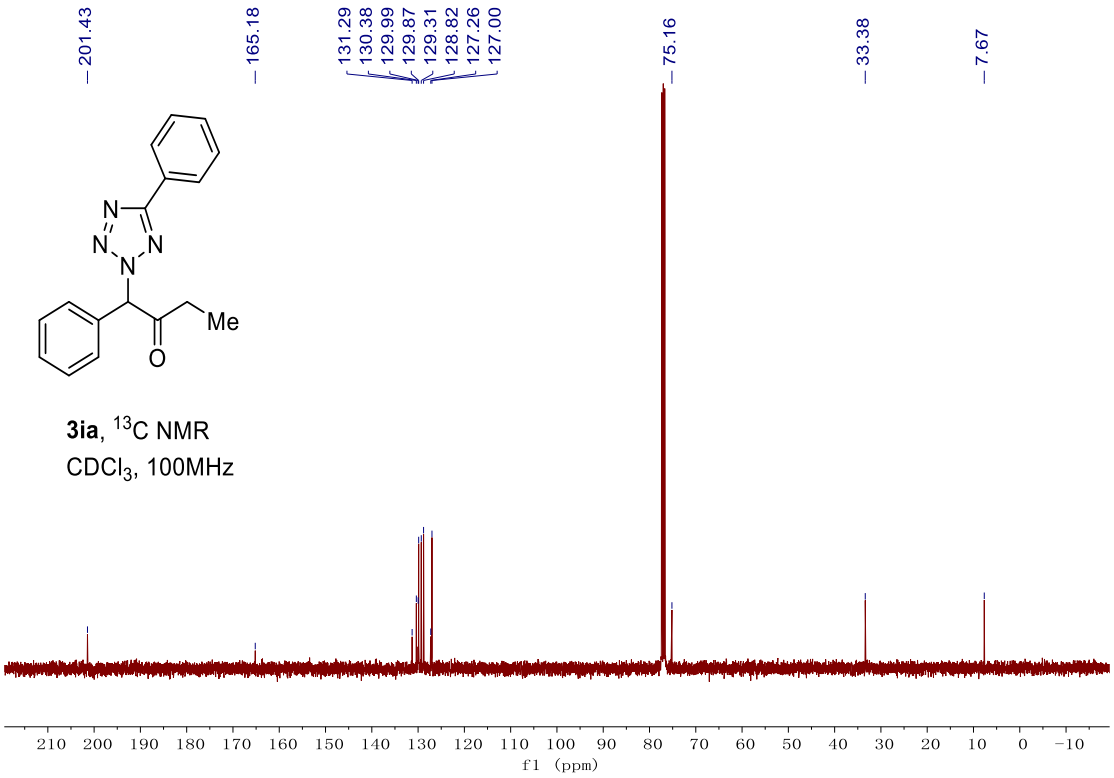


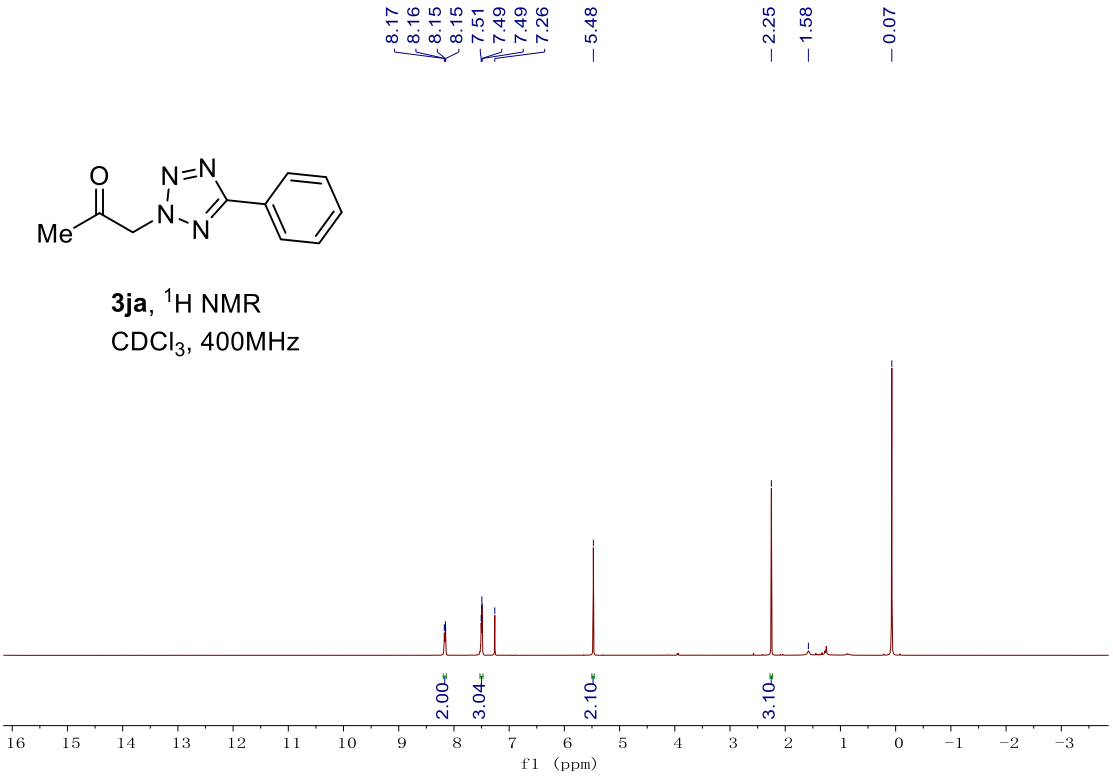


3ha, ^{13}C NMR
$CDCl_3$, 100MHz

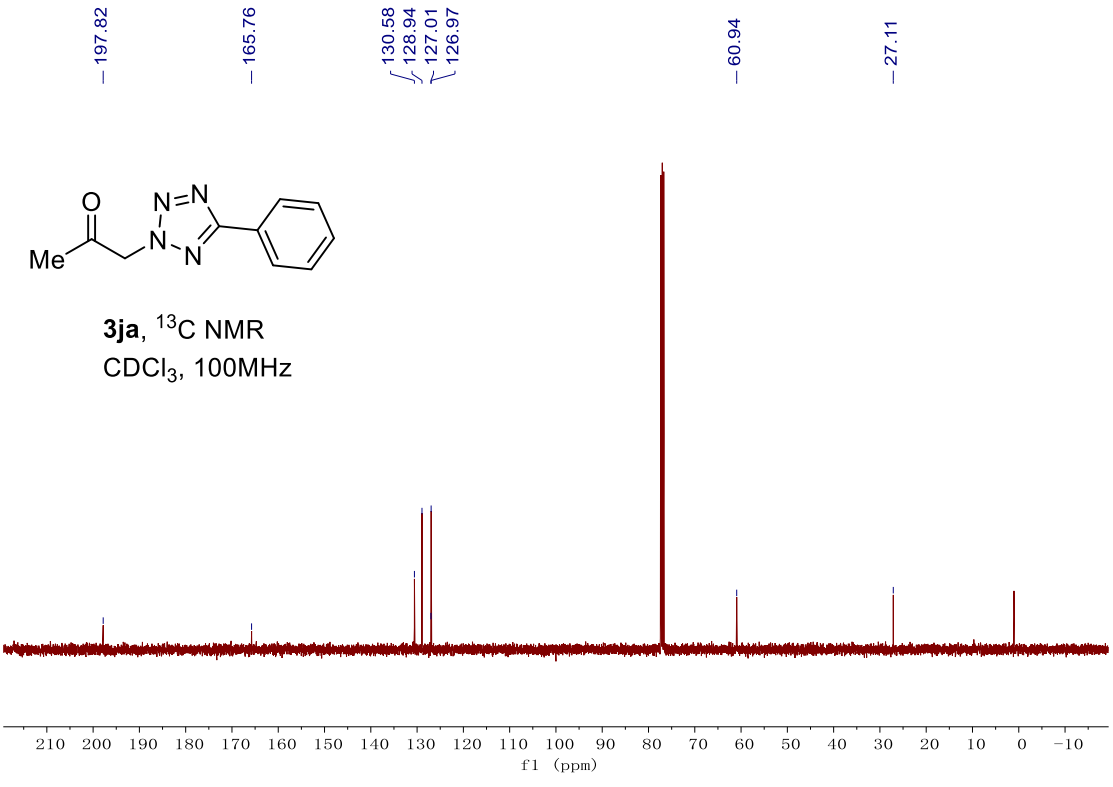



8.14
7.59
7.46
7.26
6.66
2.58
2.52
2.51
2.47
1.11
1.10
1.08
0.07
Me
O
3ia, 1H NMR
CDCl3, 400MHz
2.00
8.29
1.00
2.01
3.06
f1 (ppm)

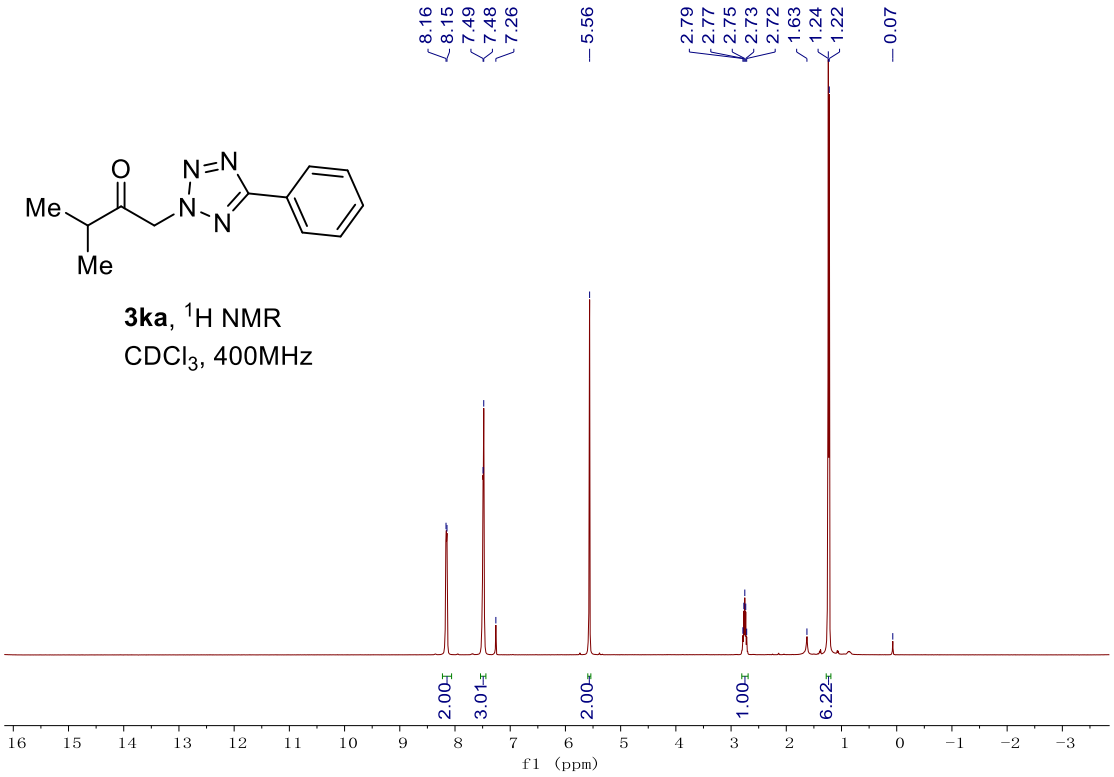

201.43
165.18
131.29
130.38
129.99
129.87
129.31
128.82
127.26
127.00
75.16
33.38
7.67
Me
O
3ia, 13C NMR
CDCl3, 100MHz
f1 (ppm)



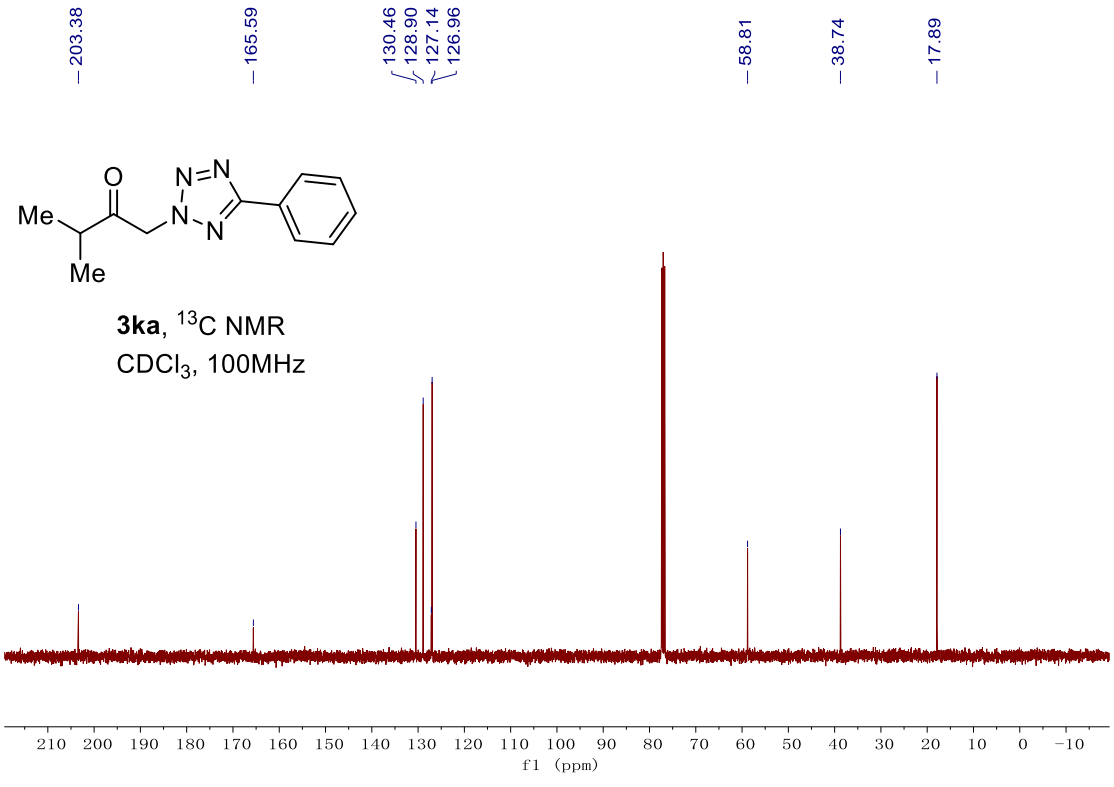
3ja, ^{1}H NMR
$CDCl_3$, 400MHz



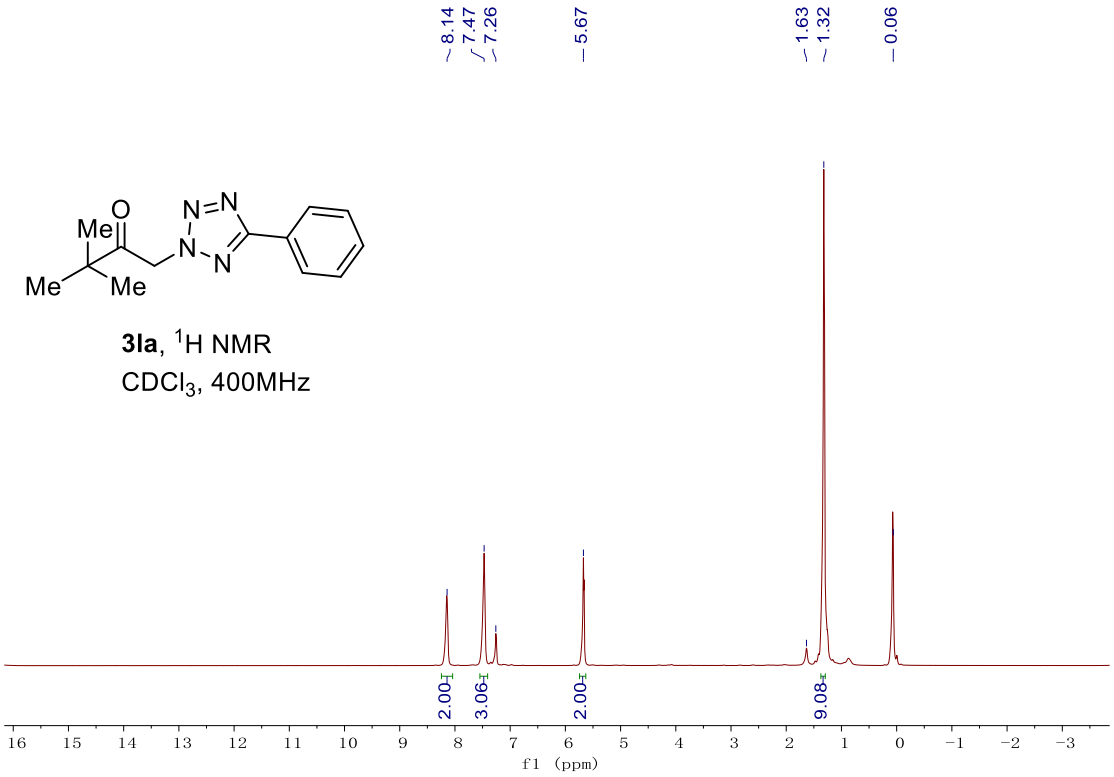
3ja, ^{13}C NMR
$CDCl_3$, 100MHz



3ka, ^{1}H NMR
$CDCl_3$, 400MHz

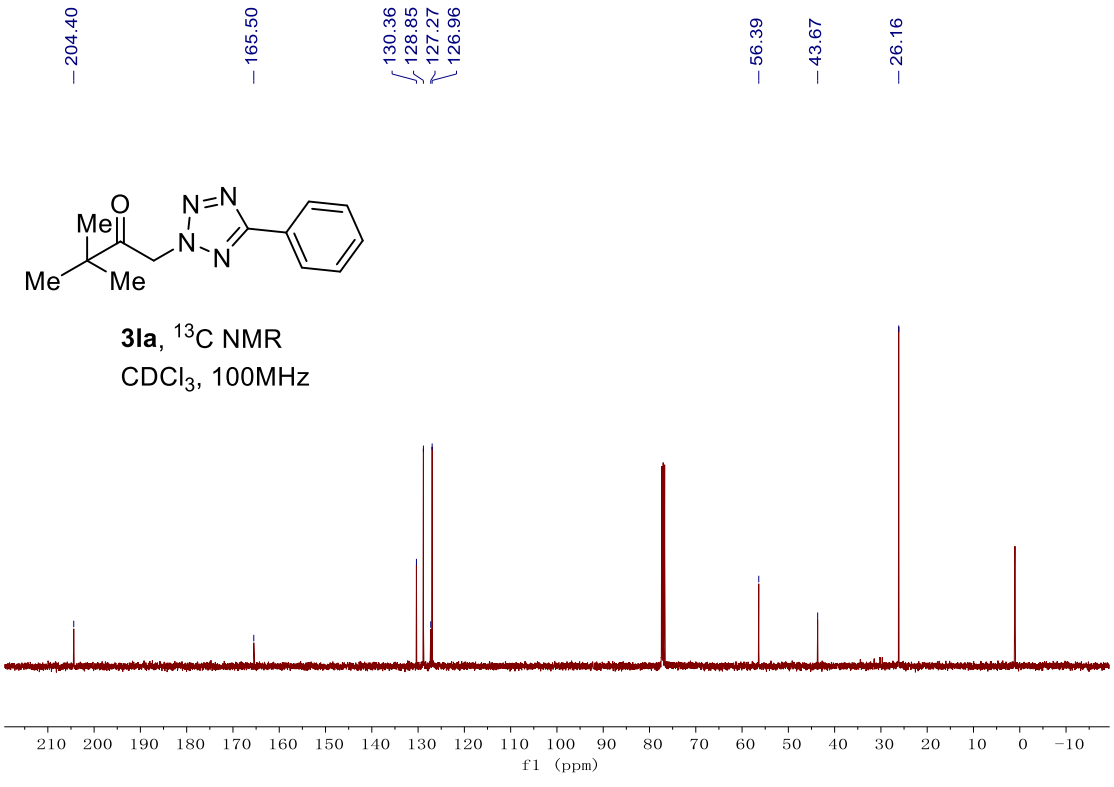


3ka, ^{13}C NMR
$CDCl_3$, 100MHz



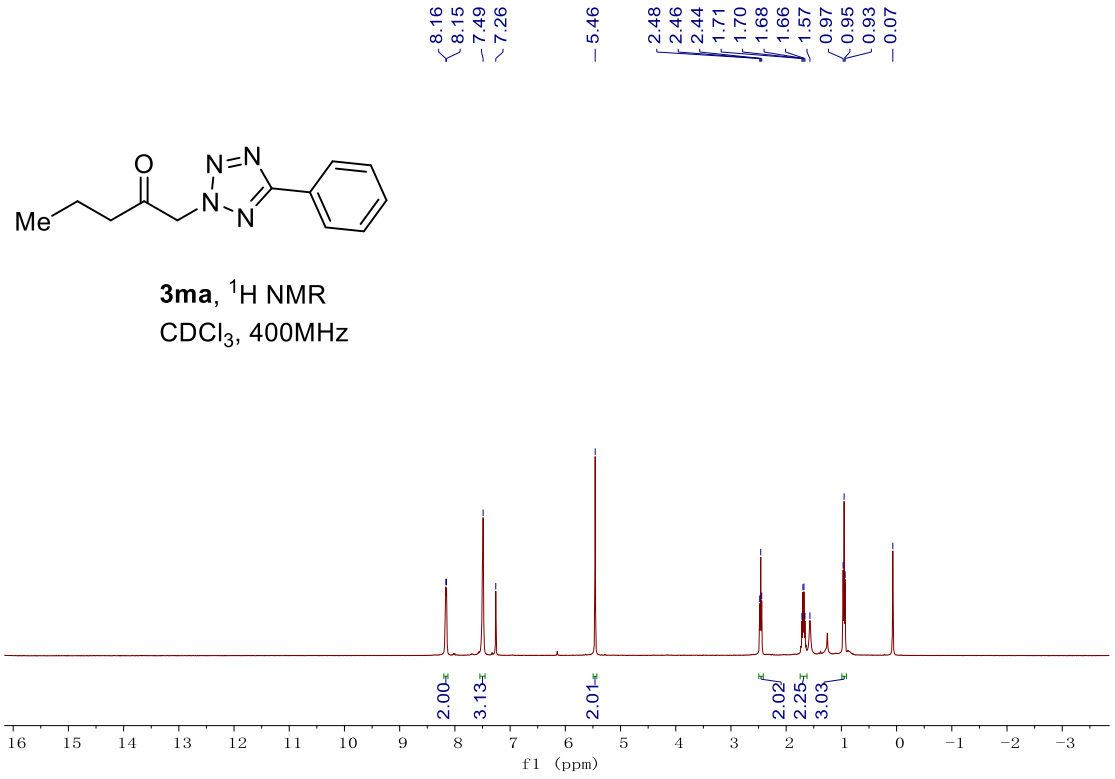
3la, ^{1}H NMR

$CDCl_3$, 400MHz

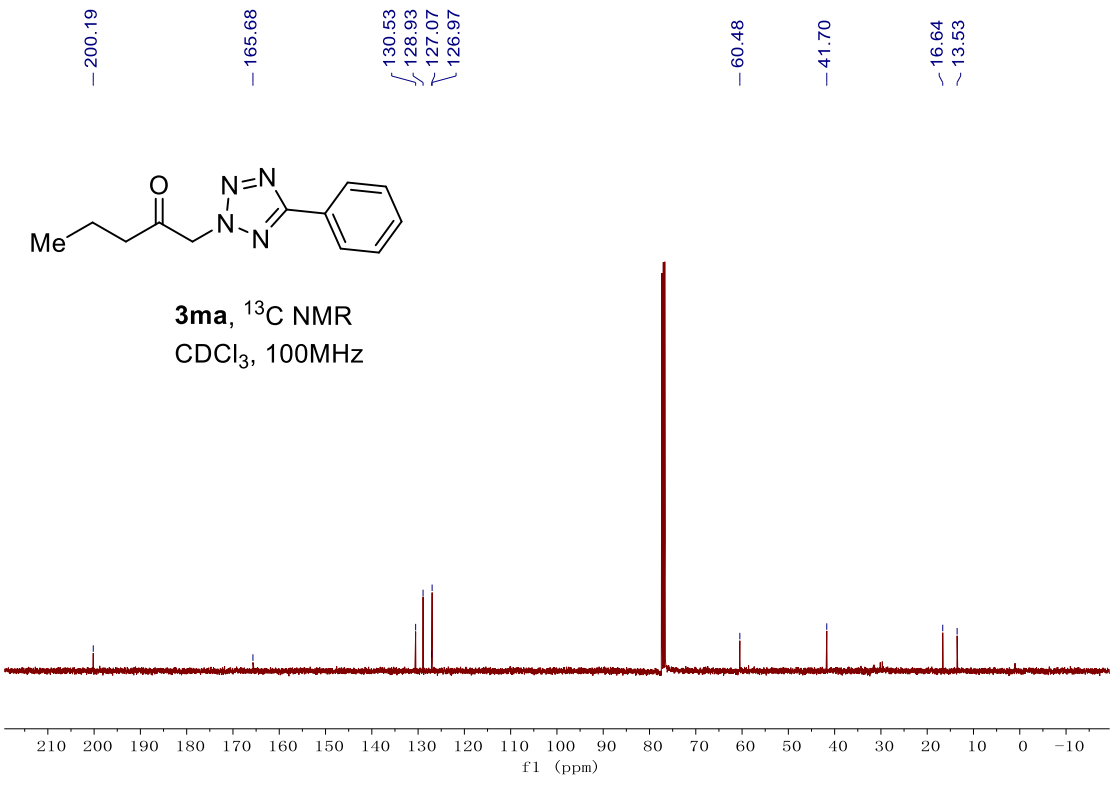


3la, ^{13}C NMR

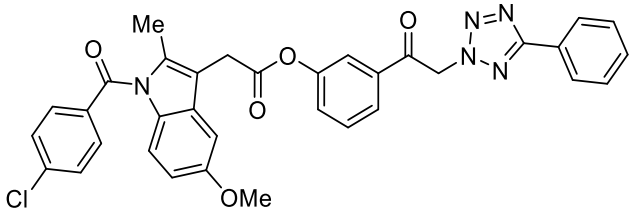
$CDCl_3$, 100MHz



3ma, ^{1}H NMR
$CDCl_3$, 400MHz

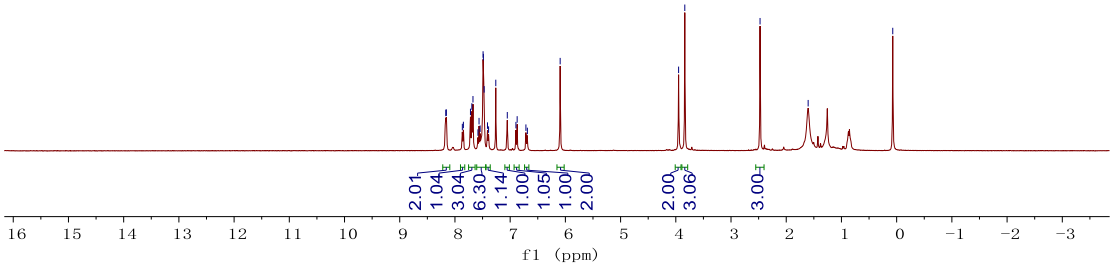


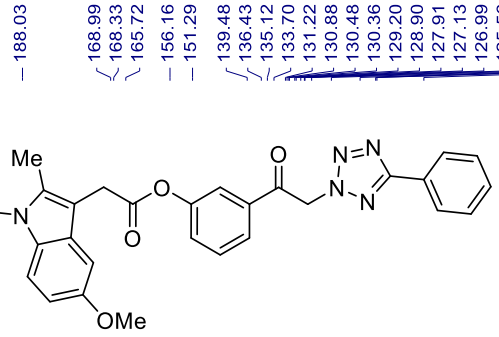
3ma, ^{13}C NMR
$CDCl_3$, 100MHz



3na, ^{1}H NMR

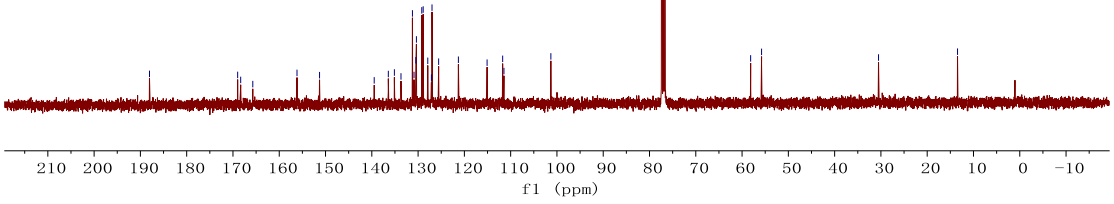
$CDCl_3$, 400MHz

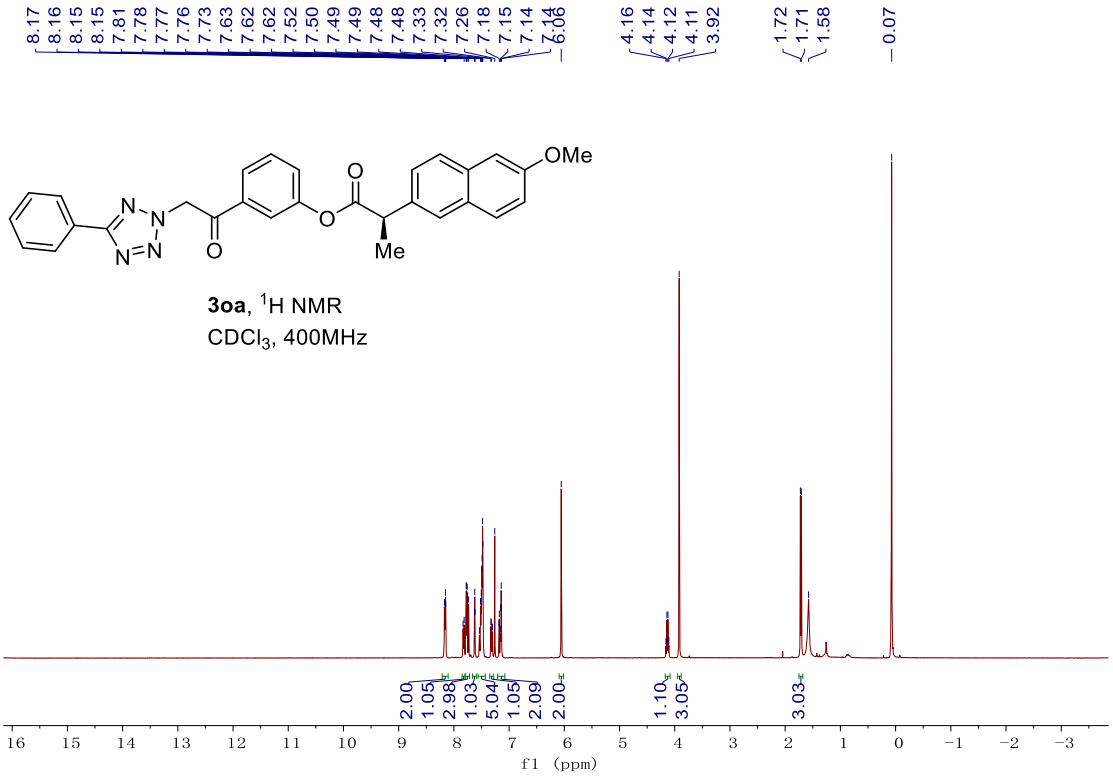




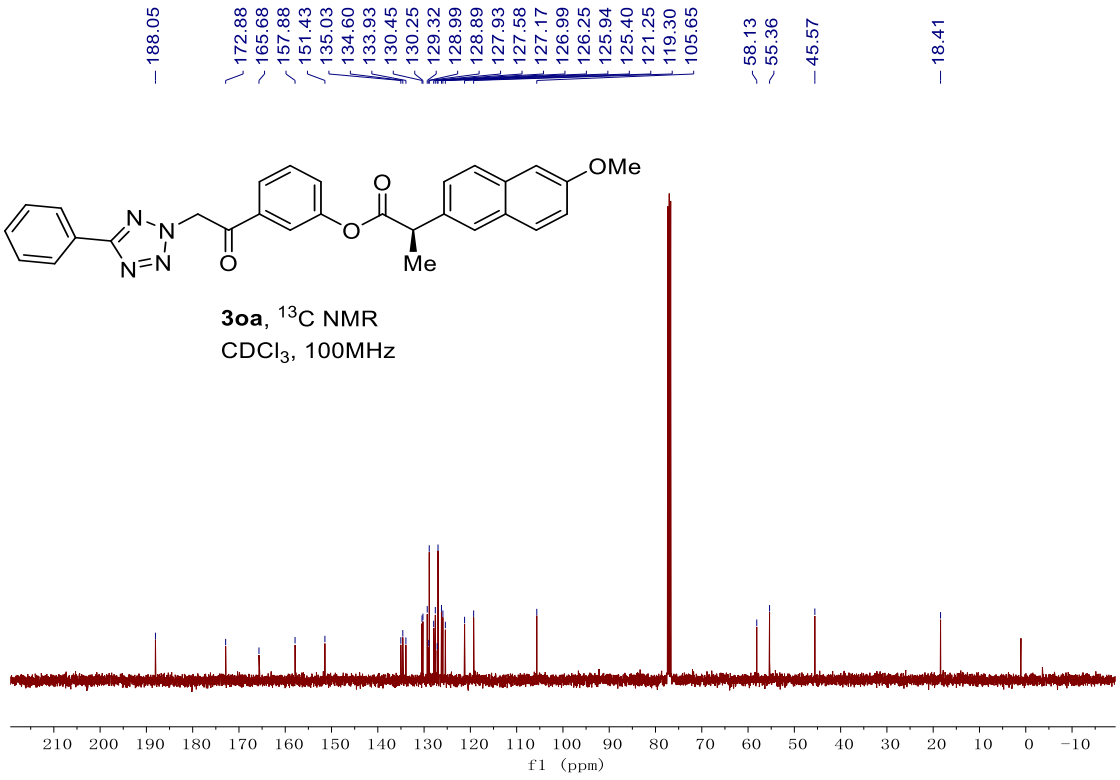
3na, ^{13}C NMR

$CDCl_3$, 100MHz

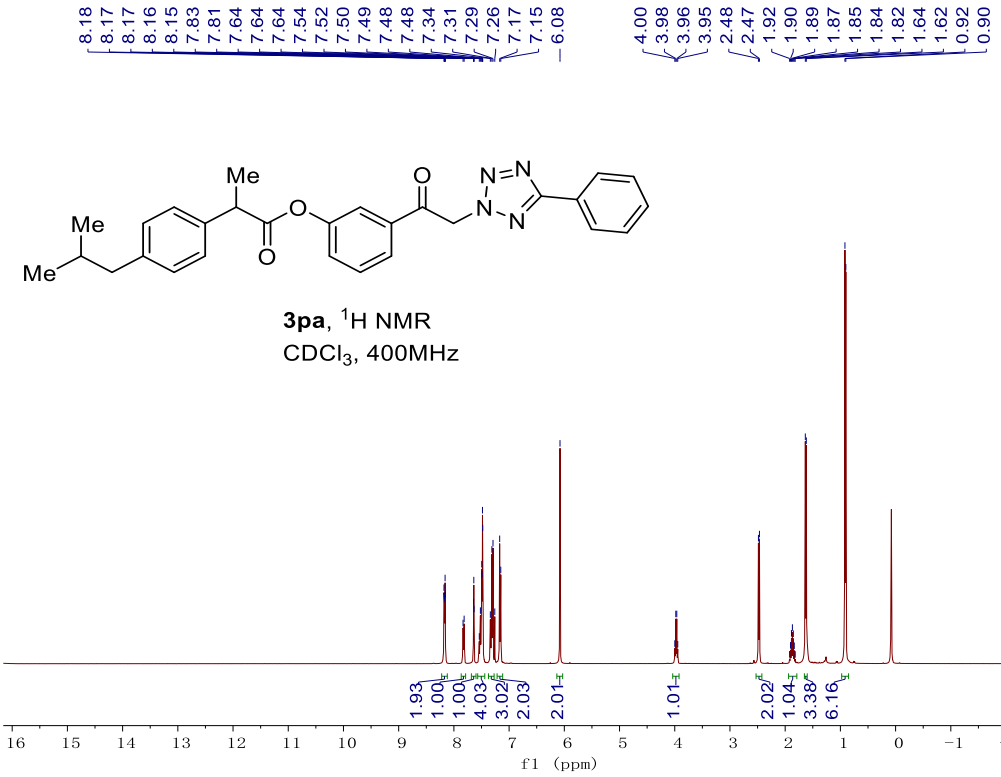




3oa, ^{1}H NMR
$CDCl_3$, 400MHz



3oa, ^{13}C NMR
$CDCl_3$, 100MHz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8.17
8.17
8.16
8.15
7.83
7.81
7.64
7.64
7.64
7.54
7.52
7.50
7.49
7.48
7.48
7.34
7.31
7.29
7.26
7.17
7.15
6.08
4.00
3.98
3.96
3.95
2.48
2.47
1.92
1.90
1.89
1.87
1.85
1.84
1.82
1.64
1.62
0.92
0.90
Me
O
N=N
Me
O
N
N
Me
O
3pa, 1H NMR
CDCl3, 400MHz
1.93
1.00
1.00
4.03
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2.03
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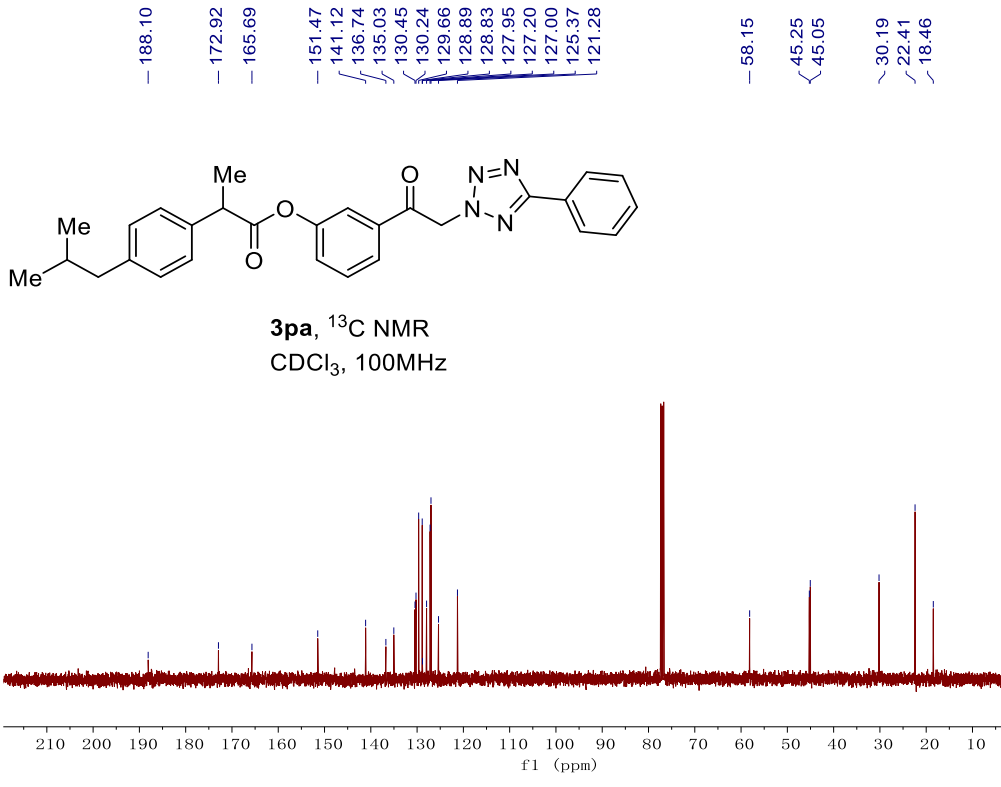
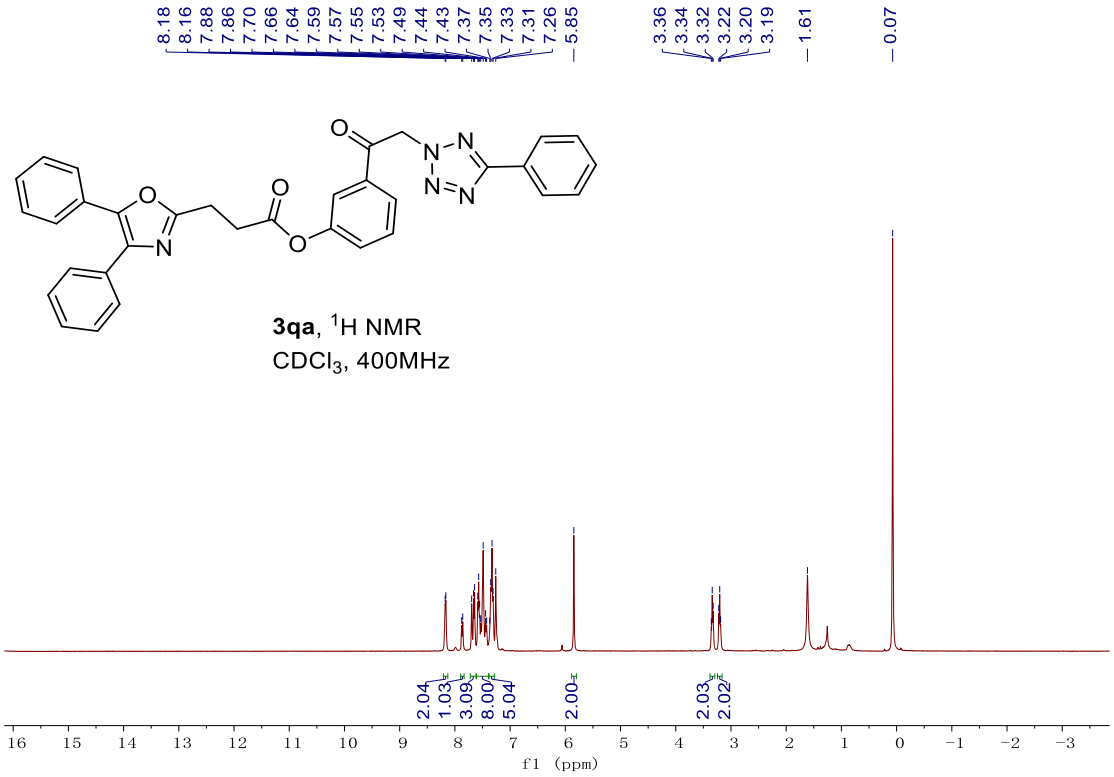
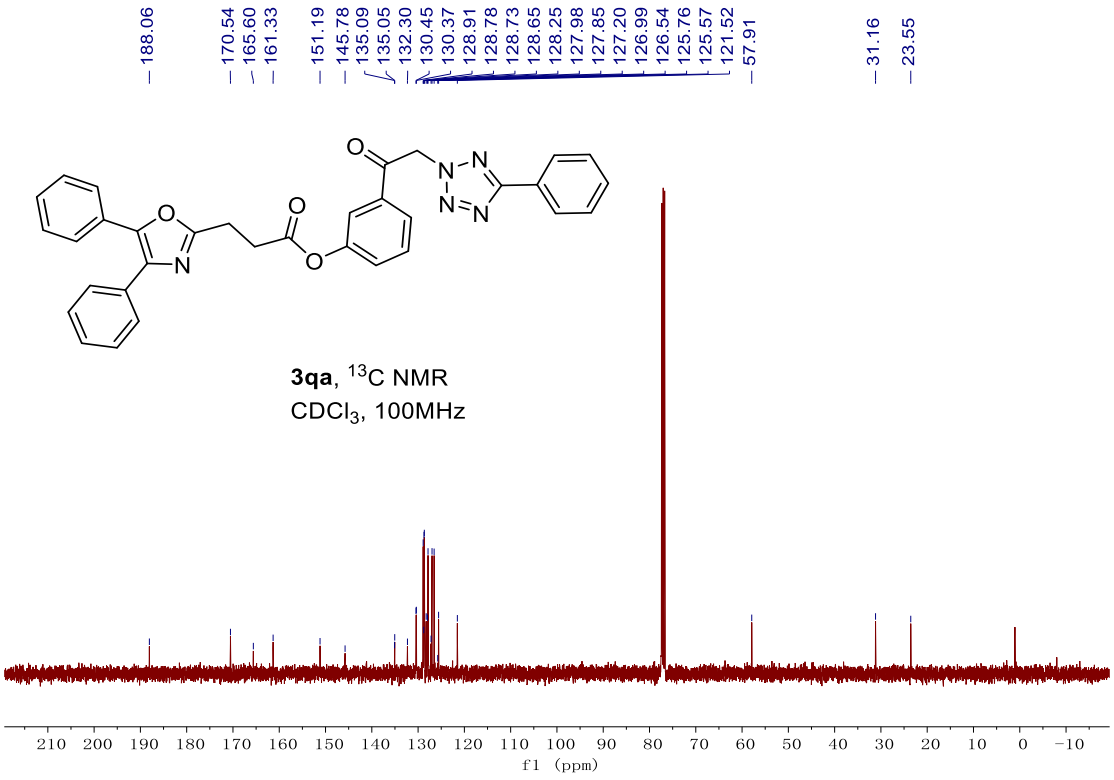
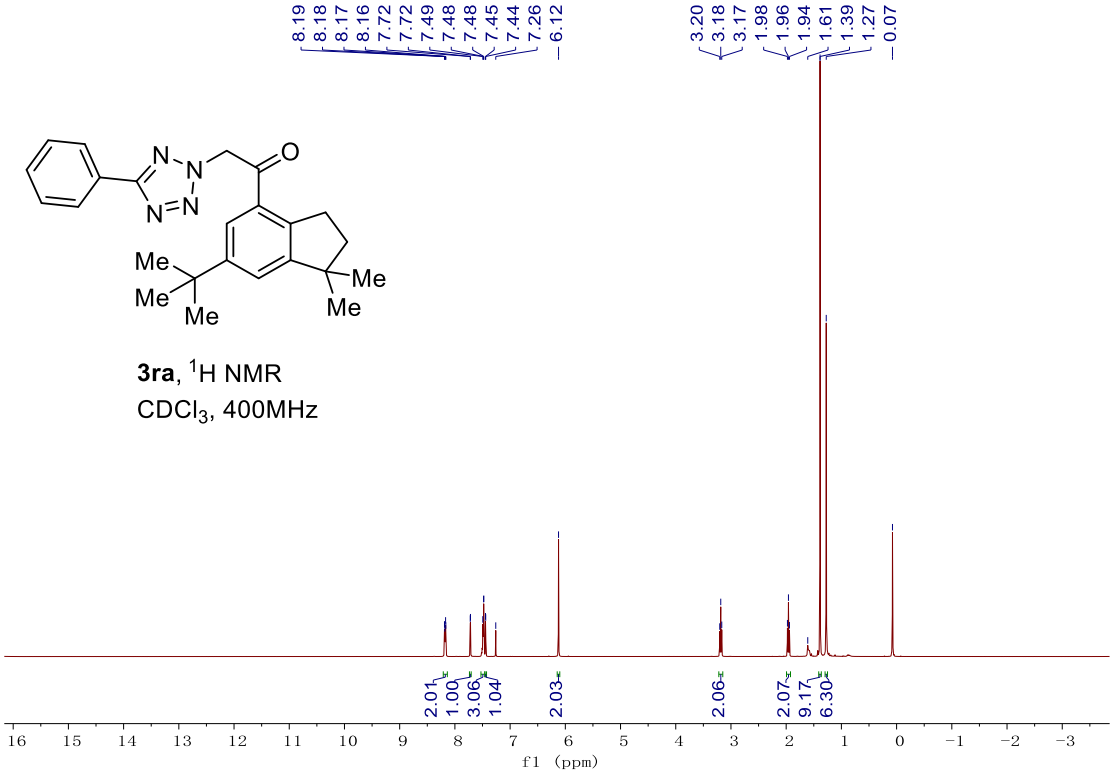
1.01
2.02
1.04
3.38
6.16
f1 (ppm)

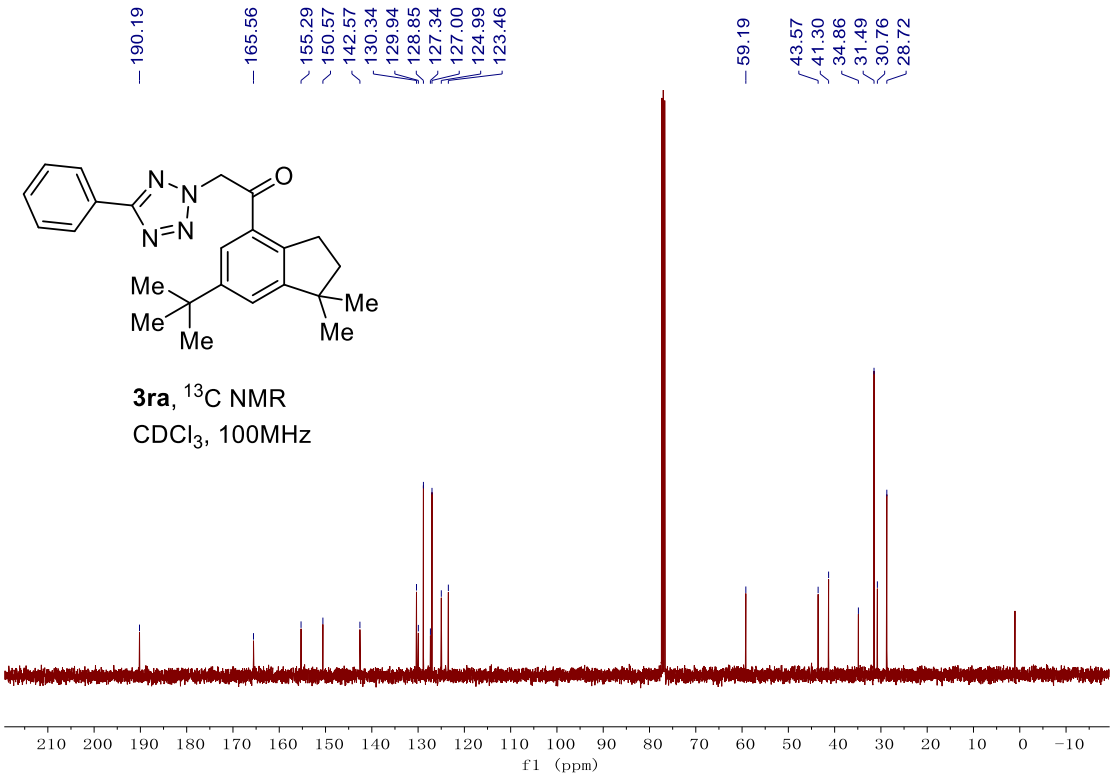

188.10
172.92
165.69
151.47
141.12
136.74
135.03
130.45
130.24
129.66
128.89
128.83
127.95
127.20
127.00
125.37
121.28
58.15
45.25
45.05
30.19
22.41
18.46
Me
O
N=N
Me
O
N
N
Me
O
3pa, 13C NMR
CDCl3, 100MHz
f1 (ppm)


8.18
8.16
7.88
7.86
7.70
7.66
7.64
7.59
7.57
7.55
7.53
7.49
7.44
7.43
7.37
7.35
7.33
7.31
7.26
5.85
3.36
3.34
3.32
3.22
3.20
3.19
1.61
0.07
O
N
N
N
O
O
O
N
3qa, 1H NMR
CDCl3, 400MHz
2.04
1.03
3.09
8.00
5.04
2.00
2.03
2.02
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

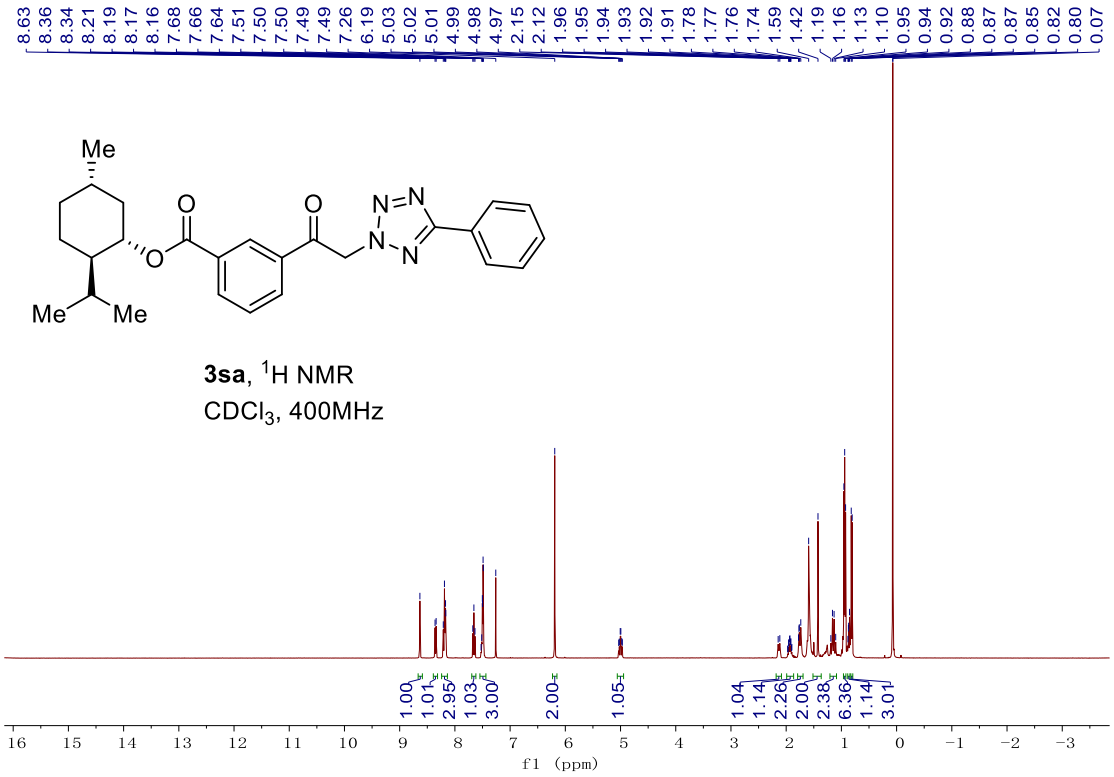

188.06
170.54
165.60
161.33
151.19
145.78
135.09
135.05
132.30
130.45
130.37
128.91
128.78
128.73
128.65
128.25
127.98
127.85
127.20
126.99
126.54
125.76
125.57
121.52
57.91
31.16
23.55
O
N
N
N
O
O
O
N
3qa, 13C NMR
CDCl3, 100MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



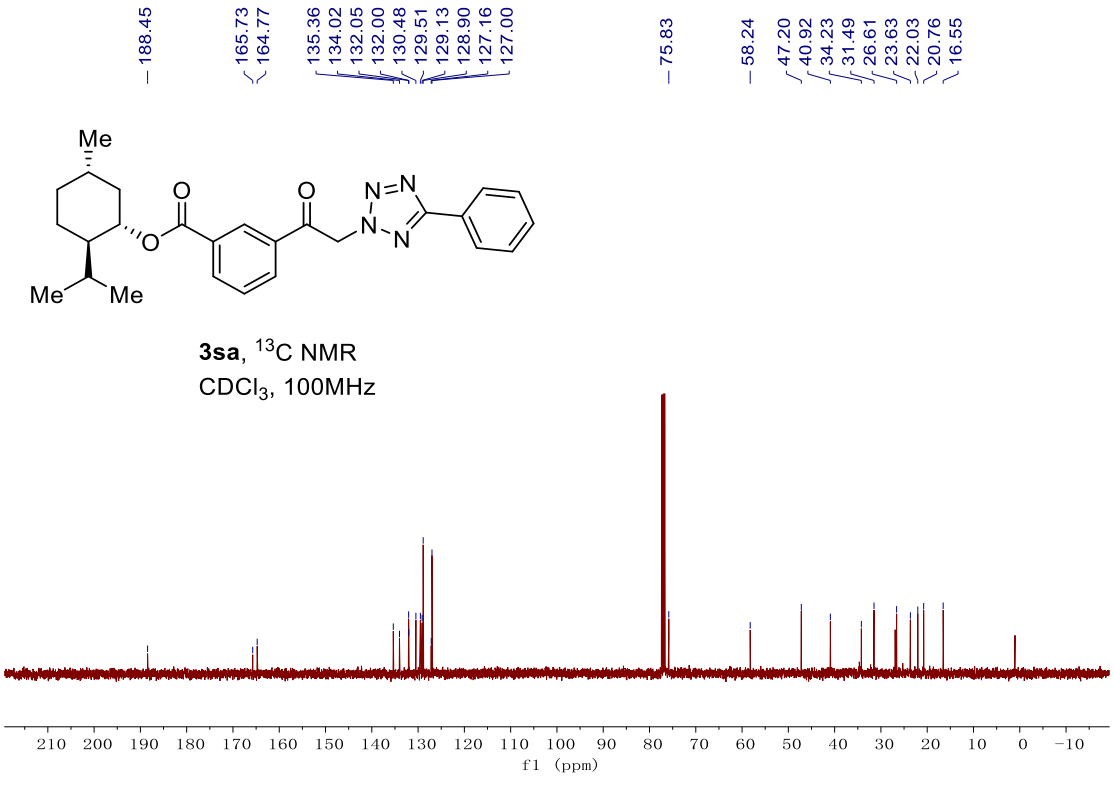
3ra, ^{1}H NMR
$CDCl_3$, 400MHz



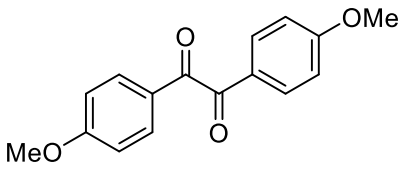
3ra, ^{13}C NMR
$CDCl_3$, 100MHz



3sa, ^{1}H NMR
$CDCl_3$, 400MHz

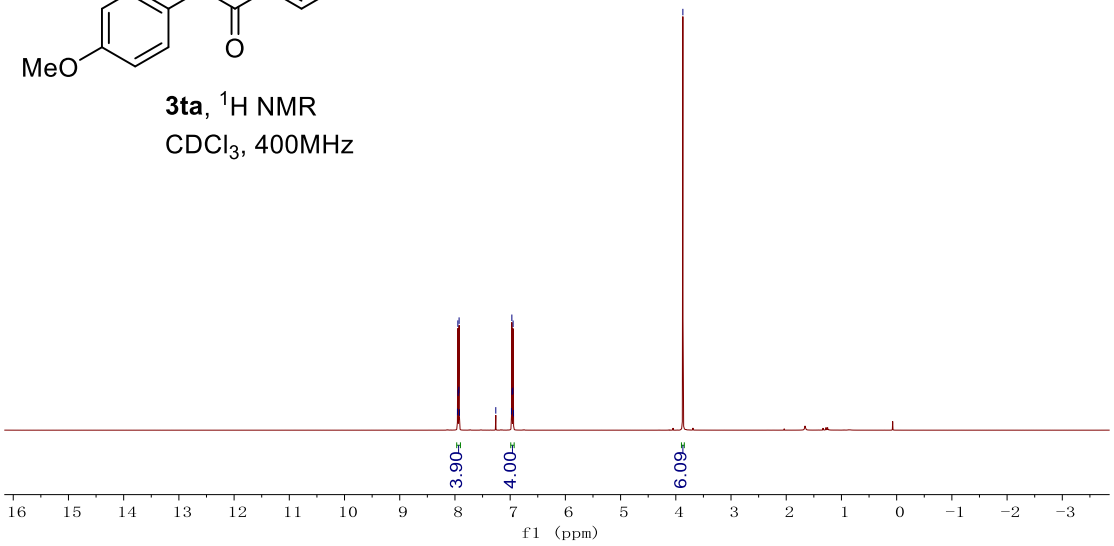


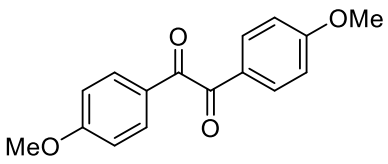
3sa, ^{13}C NMR
$CDCl_3$, 100MHz



3ta, ^{1}H NMR

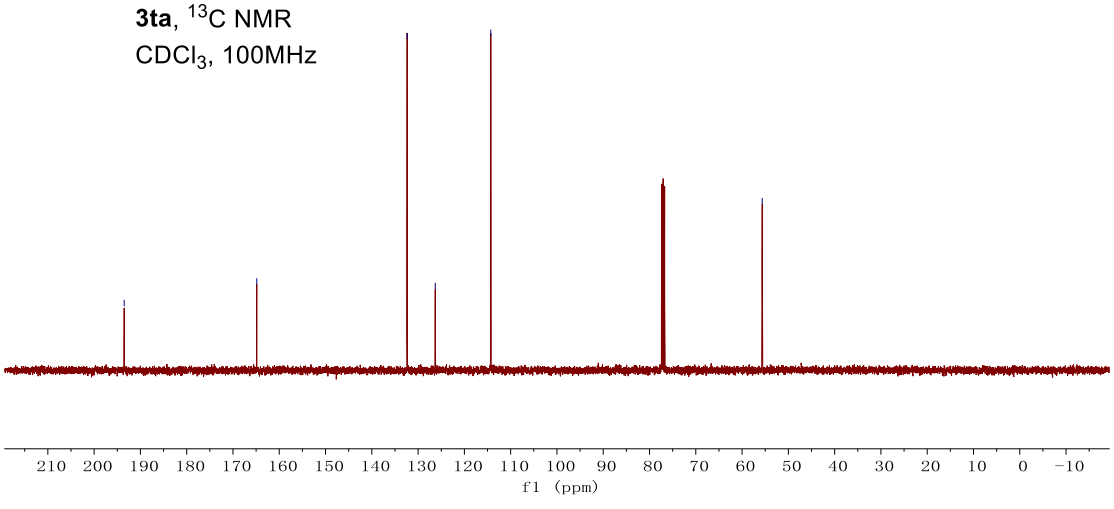
$CDCl_3$, 400MHz

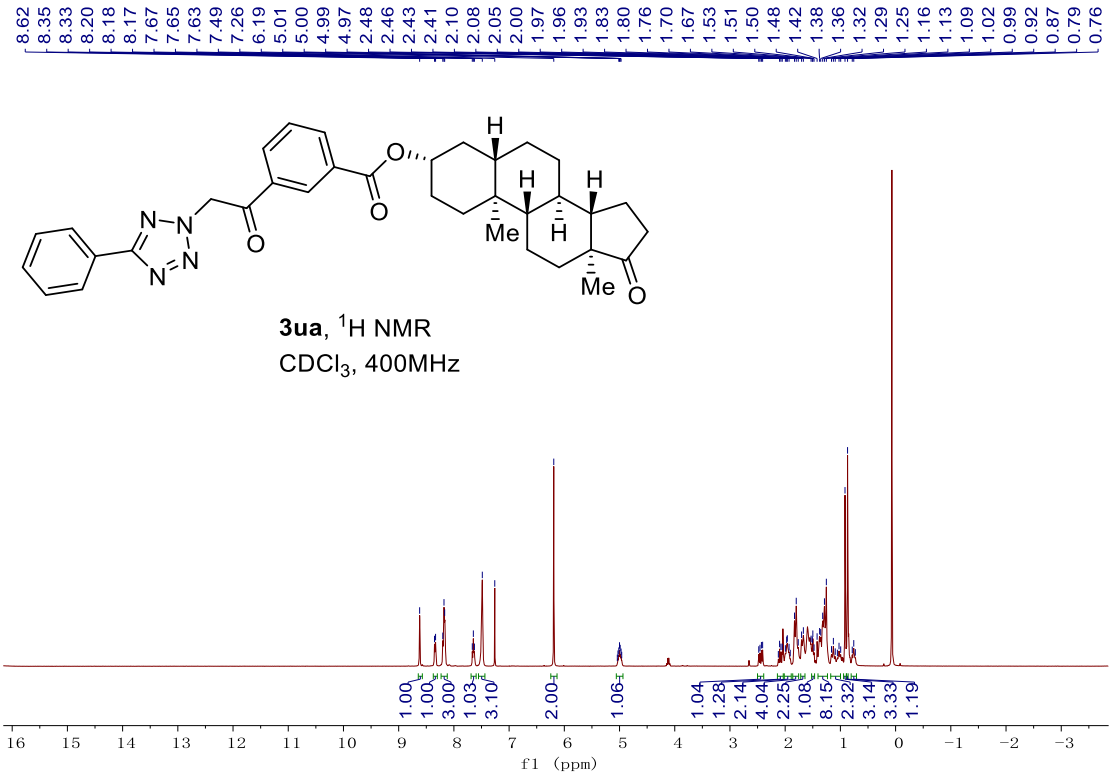




3ta, ^{13}C NMR

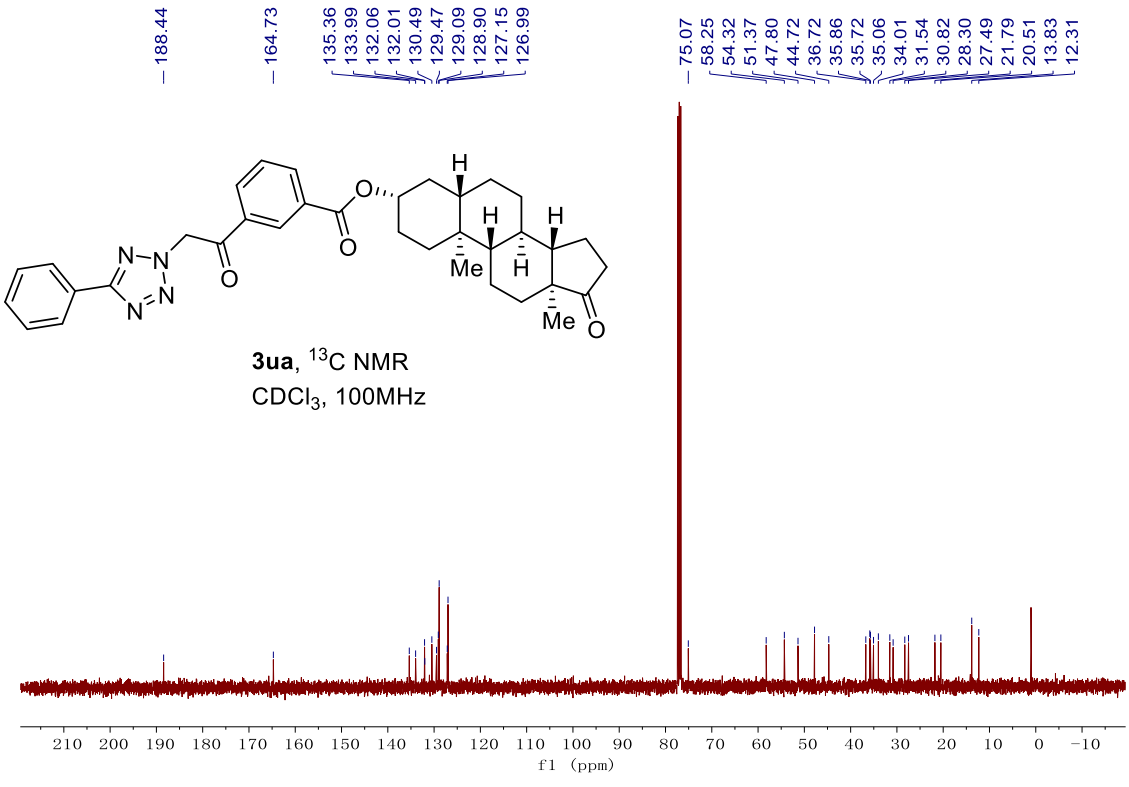
$CDCl_3$, 100MHz





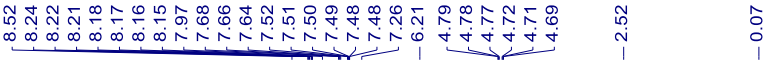
3ua, ^{1}H NMR

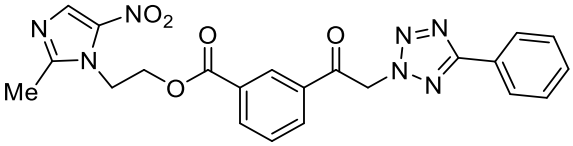
$CDCl_3$, 400MHz



3ua, ^{13}C NMR

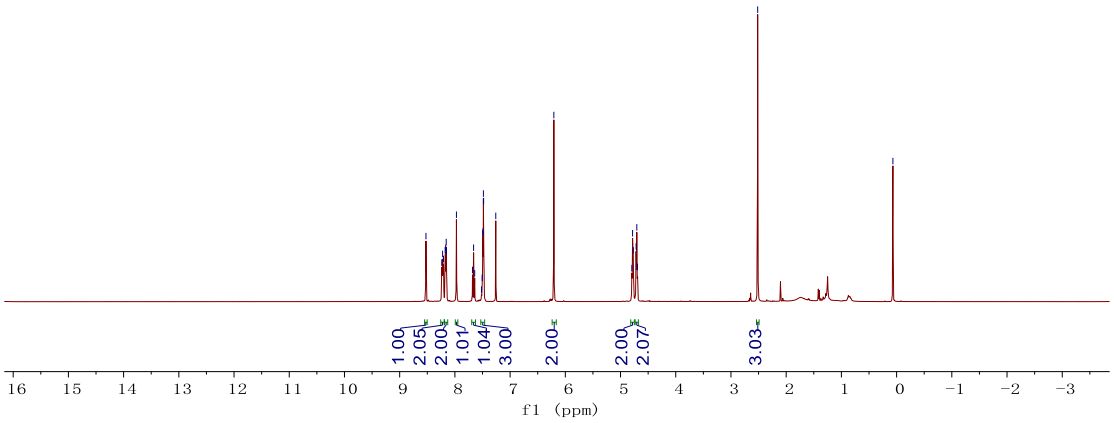
$CDCl_3$, 100MHz

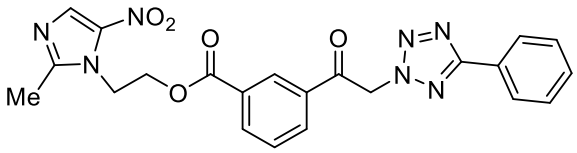




3va, ^{1}H NMR

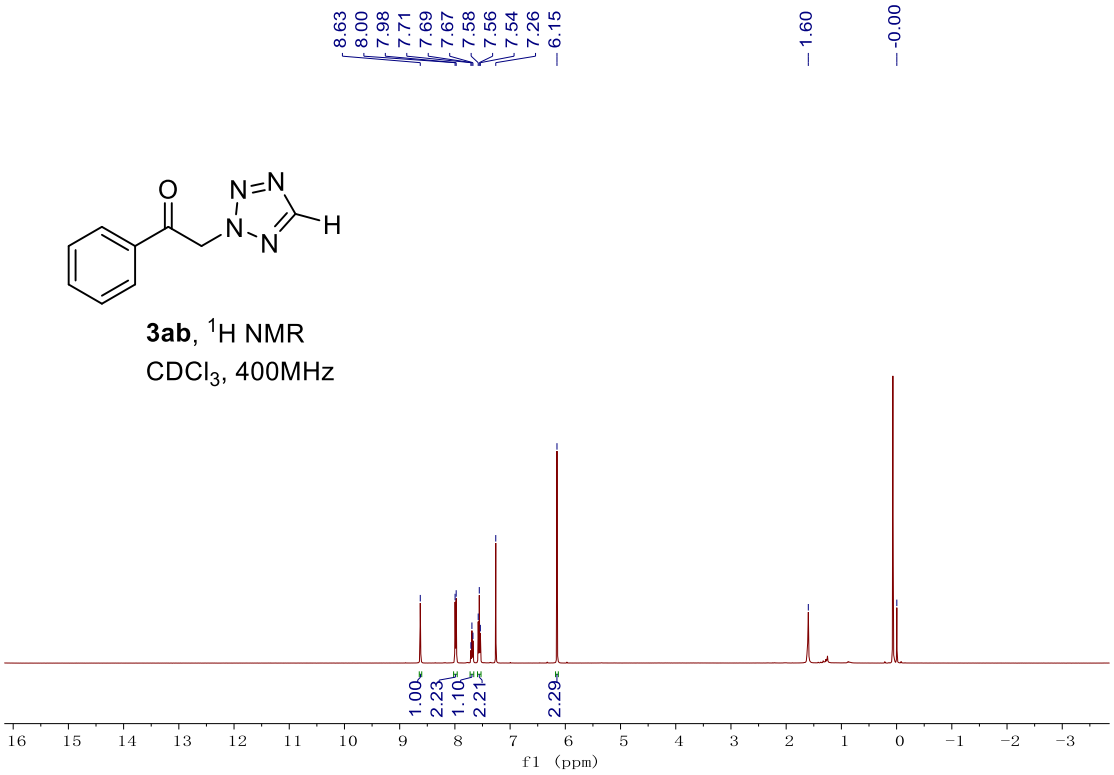
$CDCl_3$, 400MHz

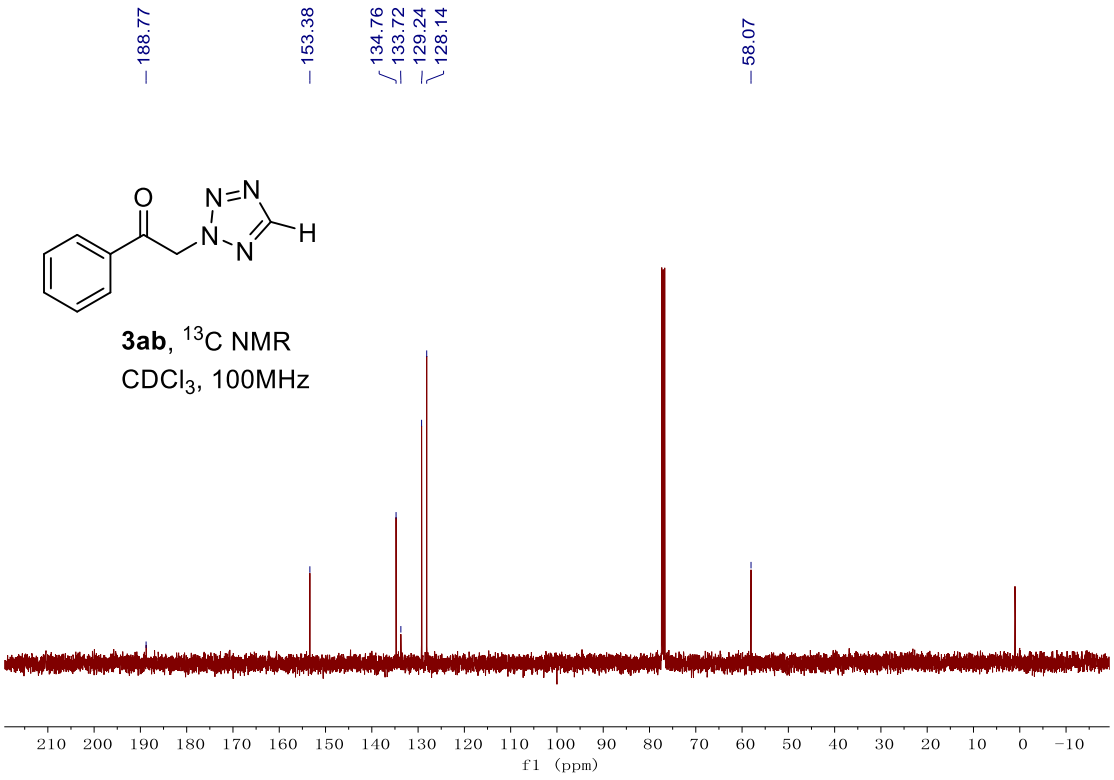


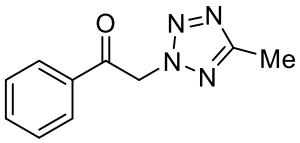


3va, ^{13}C NMR

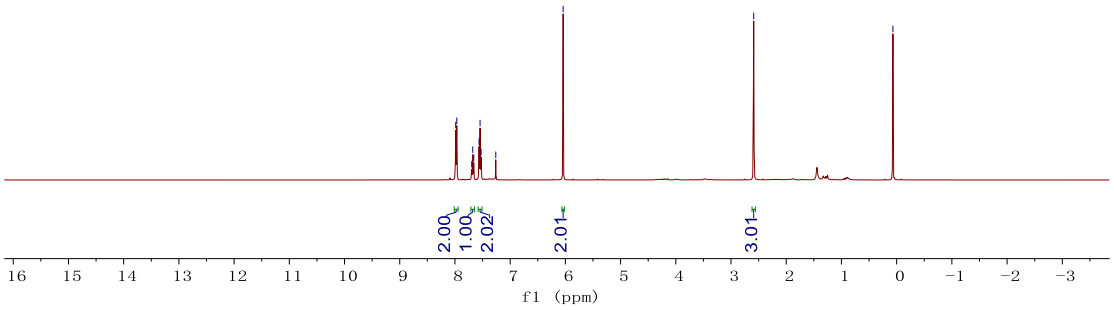
$CDCl_3$, 100MHz

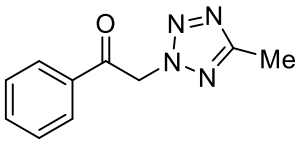

8.63
8.00
7.98
7.71
7.69
7.67
7.58
7.56
7.54
7.26
6.15
1.60
-0.00
O
N=N
N
N
H
3ab, 1H NMR
CDCl3, 400MHz
1.00
2.23
1.10
2.21
2.29
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)


188.77
153.38
134.76
133.72
129.24
128.14
58.07
O
N=N
N
N
H
3ab, 13C NMR
CDCl3, 100MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

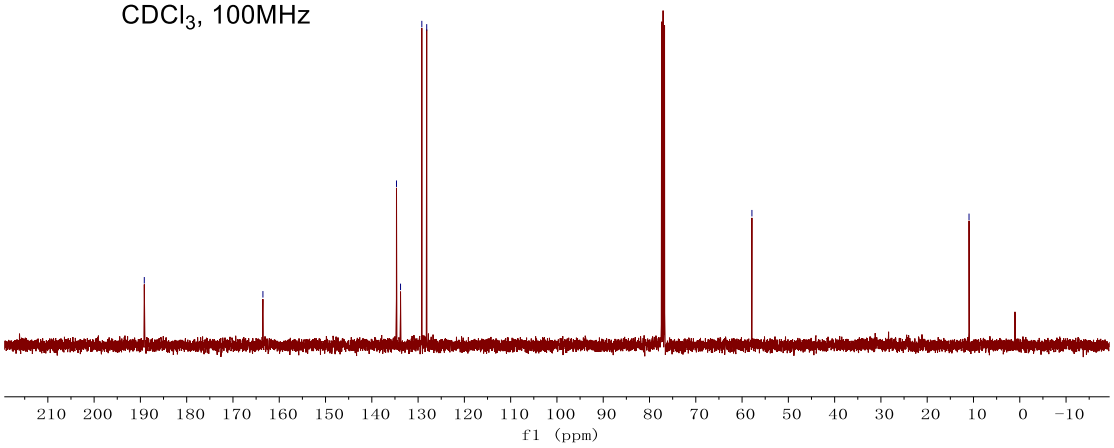


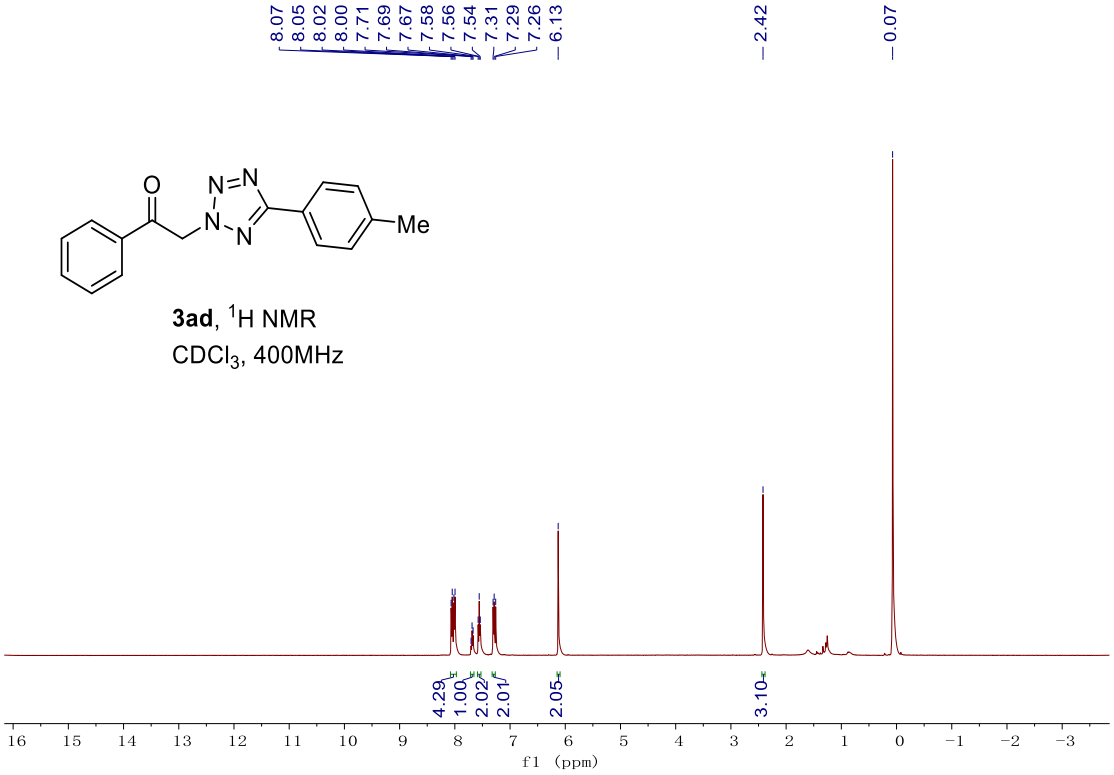
3ac, ^{1}H NMR
$CDCl_3$, 400MHz



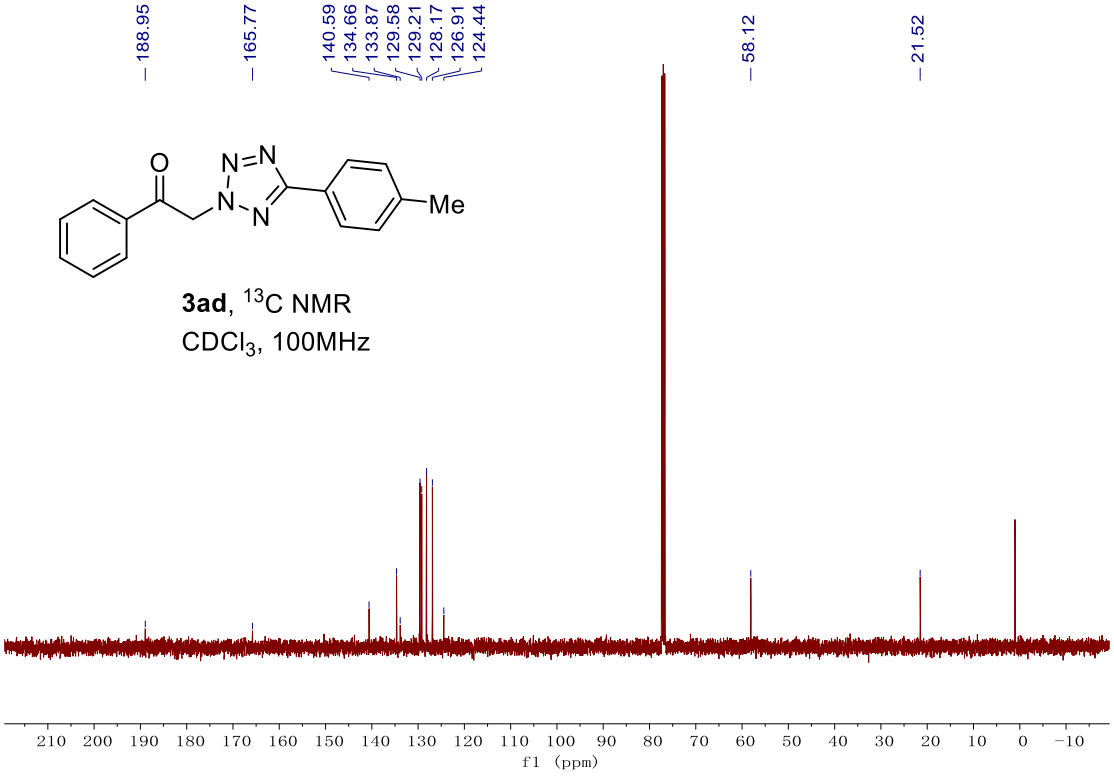


3ac, ^{13}C NMR
$CDCl_3$, 100MHz

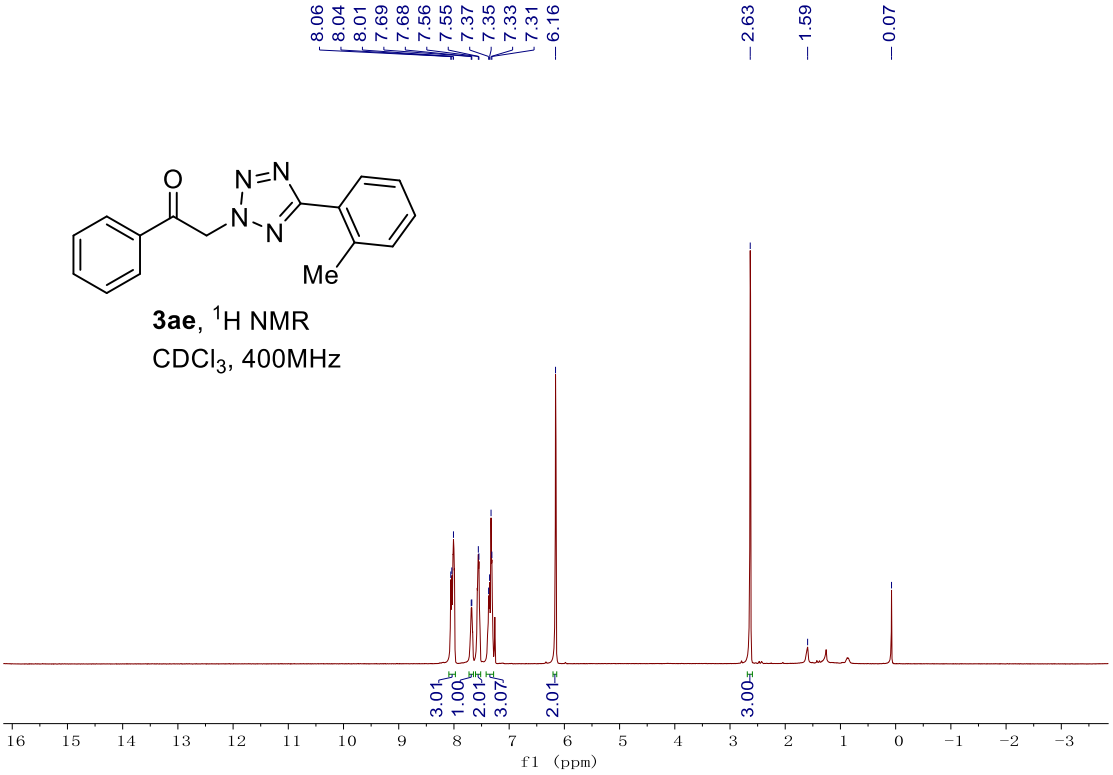


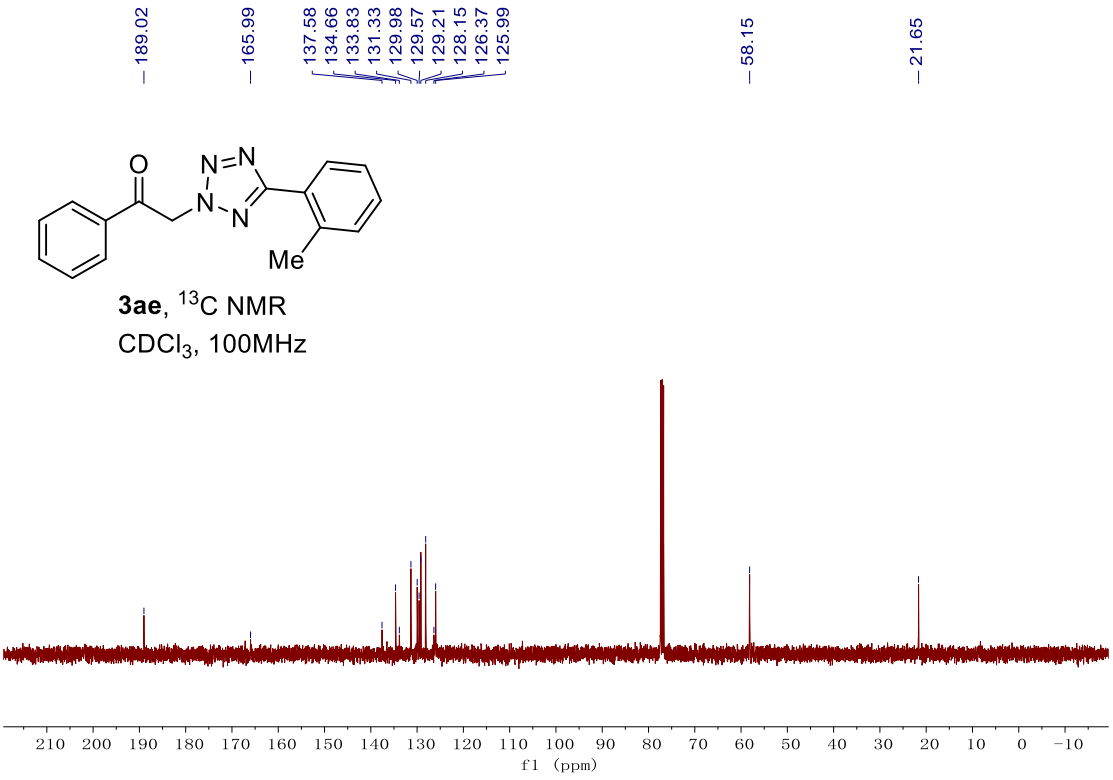


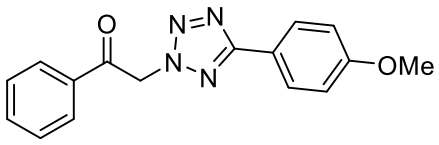
3ad, ^{1}H NMR
$CDCl_3$, 400MHz



3ad, ^{13}C NMR
$CDCl_3$, 100MHz

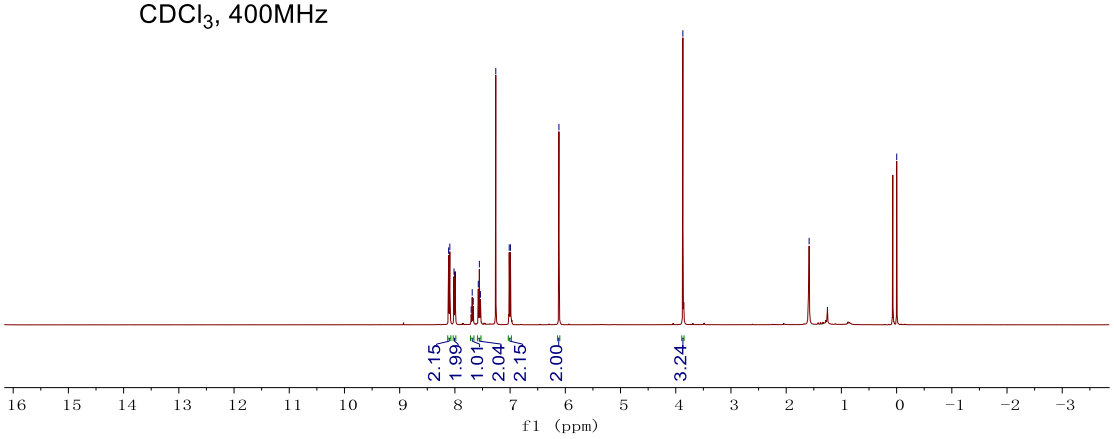

8.06
8.04
8.01
7.69
7.68
7.56
7.55
7.37
7.35
7.33
7.31
6.16
2.63
1.59
0.07
O
N=N
N
N
Me
3ae, 1H NMR
CDCl3, 400MHz
3.01
1.00
2.01
3.07
2.01
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

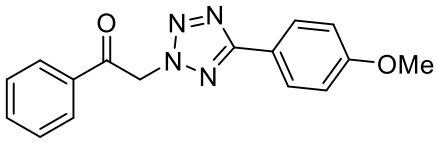

189.02
165.99
137.58
134.66
133.83
131.33
129.98
129.57
129.21
128.15
126.37
125.99
58.15
21.65
O
N=N
N
N
Me
3ae, 13C NMR
CDCl3, 100MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



3af, ^{1}H NMR

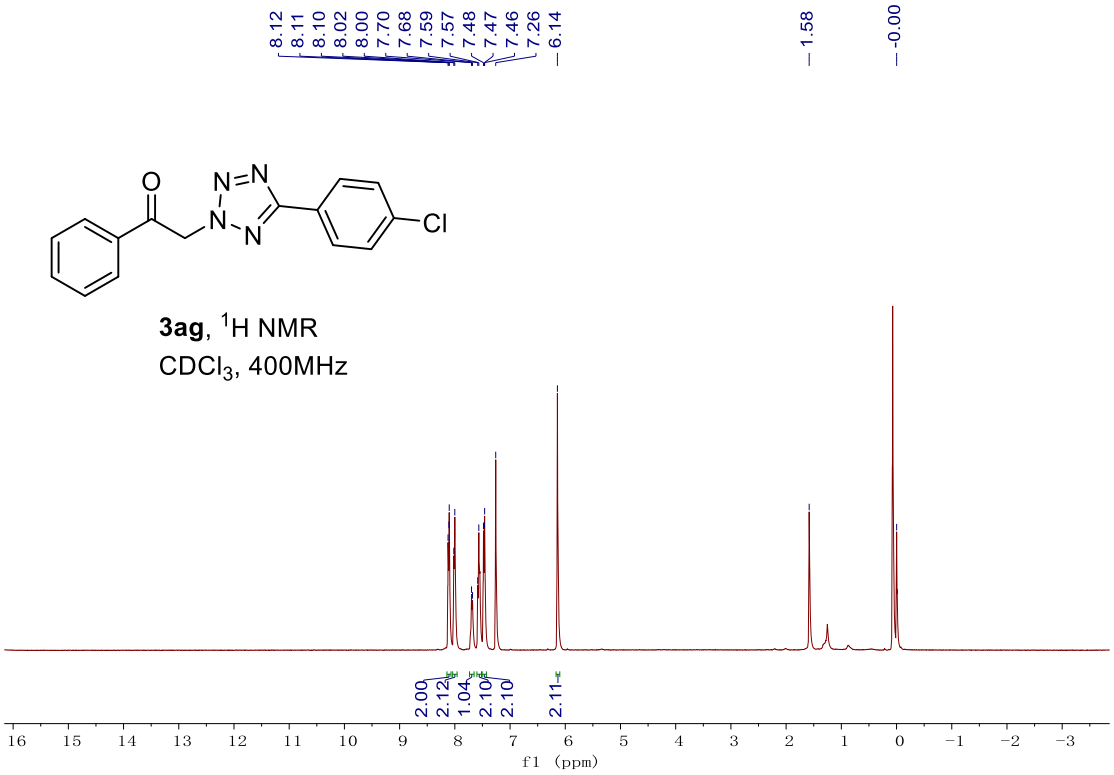
$CDCl_3$, 400MHz

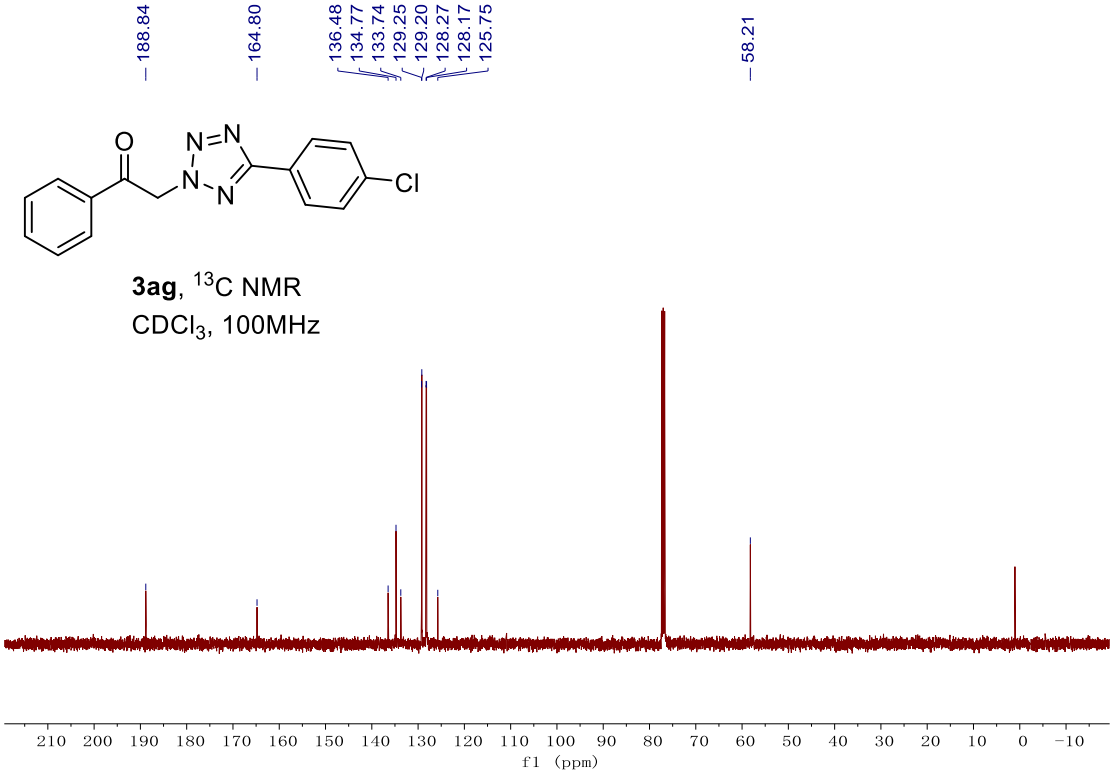


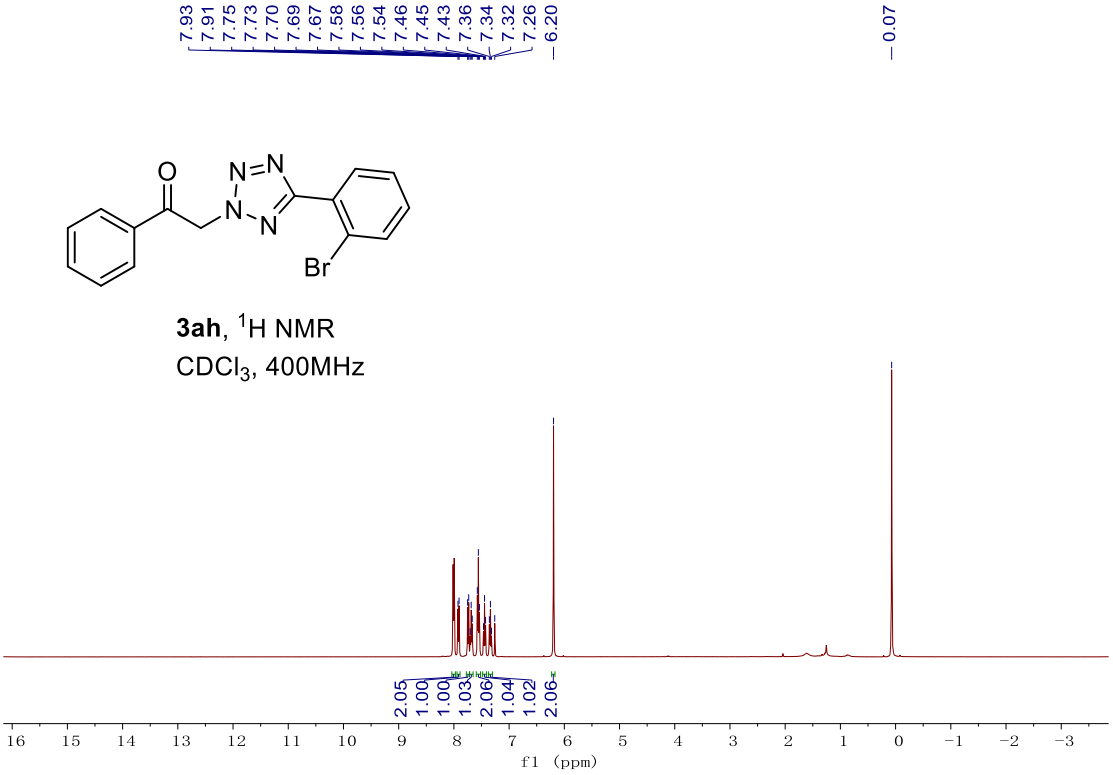


3af, ^{13}C NMR

$CDCl_3$, 100MHz

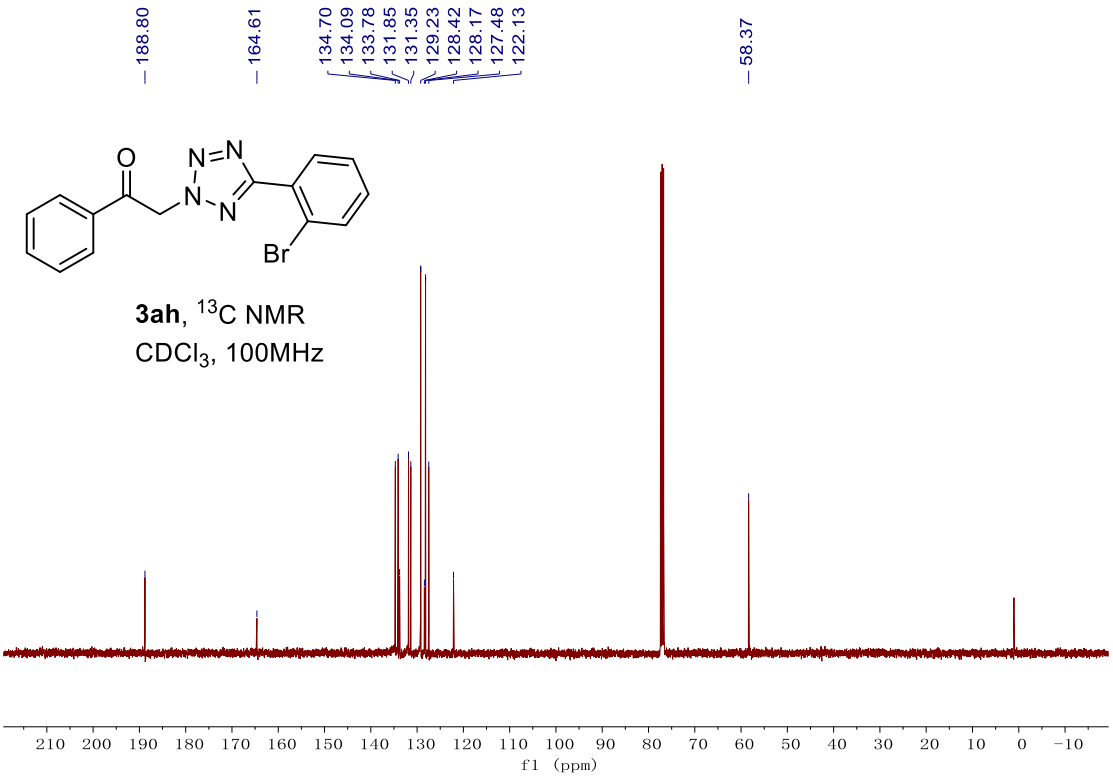

8.12
8.11
8.10
8.02
8.00
7.70
7.68
7.59
7.57
7.48
7.47
7.46
7.26
6.14
1.58
-0.00
O
N
N
N
Cl
3ag, 1H NMR
CDCl3, 400MHz
2.00
2.12
1.04
2.10
2.10
2.11
f1 (ppm)


188.84
164.80
136.48
134.77
133.74
129.25
129.20
128.27
128.17
125.75
58.21
O
N
N
N
Cl
3ag, 13C NMR
CDCl3, 100MHz
f1 (ppm)



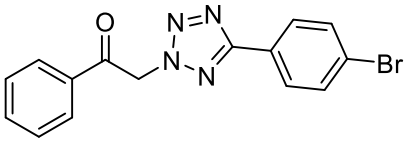
3ah, ^{1}H NMR

$CDCl_3$, 400MHz



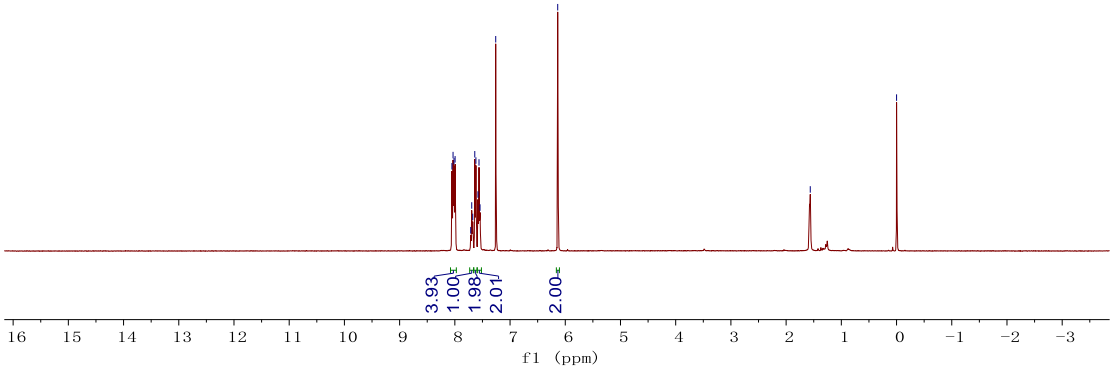
3ah, ^{13}C NMR

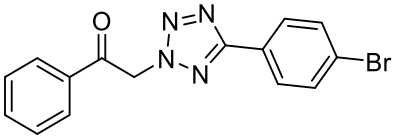
$CDCl_3$, 100MHz



3ai, ^{1}H NMR

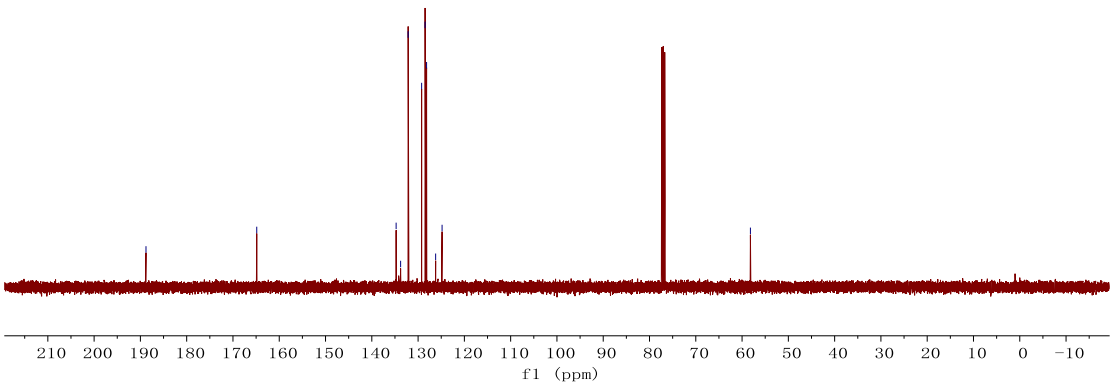
$CDCl_3$, 400MHz

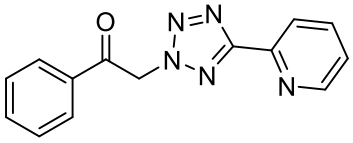




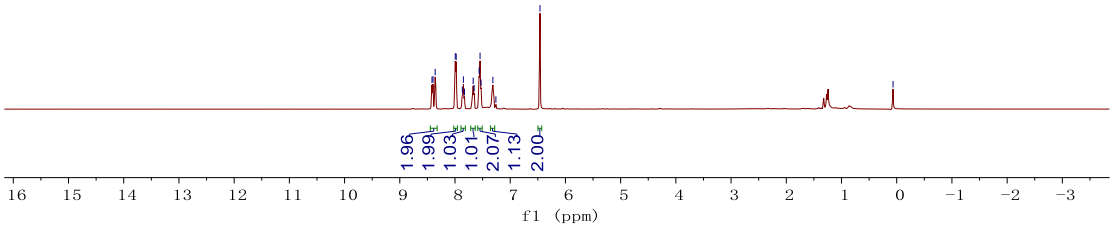
3ai, ^{13}C NMR

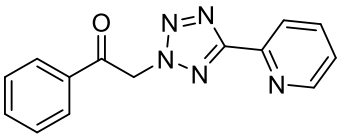
$CDCl_3$, 100MHz





3aj, ^{1}H NMR
$CDCl_3$, 400MHz





3aj, ^{13}C NMR
$CDCl_3$, 100MHz