Supporting Information for:

tert-Butyl Nitrite-mediated Radical Cyclization of Tetrazole Amines and Alkynes toward Tetrazolo[1,5-a]quinolines

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1. General Information

Solvents and reagents were reagent grade and used without purification unless otherwise noted. The alkynes were commercially available. Anhydrous solvents were obtained as follows: THF, 1,4-dioxane and toluene were dried by distillation from sodium and benzophenone; $CHCl_3$, DMF were redistilled over CaH_2. Column chromatography was performed using silica gel (300-400 mesh). ^1H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ operating at 400 and 100 MHz in the presence of tetramethylsilane (TMS) as an internal standard and are reported in ppm (δ). Coupling constants are reported in Hertz (Hz). Spectral splitting patterns are designated as s, singlet; d, doublet; t, triplet; q, quartet; p, pentet; m, multiplet; and br, broad. The crystal (**3da**) was obtained by slowly evaporation of the solvents (cyclohexane/dichloromethane = 1:1) at room temperature. High resolution mass spectroscopic data of the products were collected on a Waters Micromass GCT instrument using ESI (70 eV) or an AB 5600+Triple-TOF.

Caution!!! General caution: *Tetrazolate compounds in this paper are hazardous materials, which might cause severe injury upon explosion. Proper protective measures such as the use of safety glasses, face shield, leather coat and plastic spatulas should be taken.*

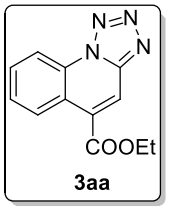
2. General Procedure for Synthesis of *1H*-Tetrazol-5-amines Derivatives (1)

The starting materials, *1H*-tetrazol-5-amines derivatives (**1**), were synthesized according to the reported procedures without modification. Please see: A. N. Vorobiov, P. N. Gaponik, P. T. Petrov and O. A. Ivashkevich, *Synthesis*, **2006**, *8*, 1307-1312.

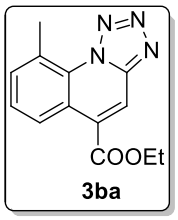
3. General Procedure for Synthesis of Substituted Tetrazolo[1,5-*a*]quinolines

1-phenyl-1*H*-tetrazol-5-amine **1a** (0.15 mmol, 1.0 equiv.) and ethyl propiolate **2a** (1.05 mmol, 7.0 equiv.) were added into a thick-walled pressure pipe with acetone (1.5 mL), followed by the addition of *t*-BuONO (5.0 equiv.) in two portions for 10 minutes. The mixture was stirred for 10 min at room temperature and monitored by TLC until completion. After evaporating all of the volatiles, the residue was purified by flash chromatography (petroleum ether/EtOAc = 3:1) on silica gel to give the desired product **3aa** as a yellow solid (29 mg, 80% yield, m.p.: 140.6-141.4 °C).

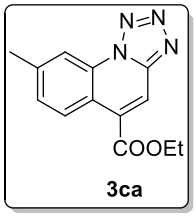
4. Characterization Data of Compounds 3



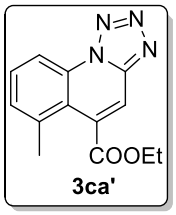
Ethyl tetrazolo[1,5-a]quinoline-5-carboxylate (3aa) Yellow solid (29 mg, 80% yield), m.p.: 140.6-141.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.93 (d, J = 8.4 Hz, 1H), 8.78 (d, J = 8.4 Hz, 1H), 8.55 (s, 1H), 7.94 (t, J = 7.7 Hz, 1H), 7.80 (t, J = 7.8 Hz, 1H), 4.57 (q, J = 7.1 Hz, 2H), 1.52 (t, J = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.4, 146.2, 133.1, 131.6, 130.9, 128.6, 128.0, 121.2, 117.0, 116.5, 62.6, 14.2. **HRMS** (ESI) *m/z* Calcd. for $C_{12}H_{11}N_4O_2$ ($[M+H]^+$): 243.0882, Found: 243.0876. **IR** (film) ν 3053, 1704, 1653, 1608, 1244, 1141 cm^{-1}.



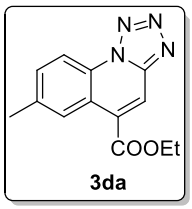
***Ethyl 9-methyltetrazolo[1,5-a]quinoline-5-carboxylate (3ba)*.** Yellow solid (12 mg, 31% yield), m.p.: 198.8−199.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.69 (d, J = 8.3 Hz, 1H), 8.46 (s, 1H), 7.76 (d, J = 7.4 Hz, 1H), 7.67 (t, J = 7.9 Hz, 1H), 4.56 (q, J = 7.1 Hz, 2H), 3.23 (s, 3H), 1.52 (t, J = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.9, 147.0, 134.6, 130.9, 129.8, 127.9, 125.5, 122.4, 115.9, 62.6, 23.9, 14.2. **HRMS** (ESI) *m/z* Calcd. for $C_{13}H_{13}N_4O_2$ ($[M+H]^+$): 257.1039, Found: 257.1032. **IR** (film) ν 2962, 1721, 1408, 1258, 1011, 864, 789 cm^{-1}.



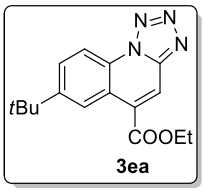
***Ethyl 8-methyltetrazolo[1,5-a]quinoline-5-carboxylate (3ca)*.** Yellow solid, m.p.: 155.8−156.9 °C (13 mg, 34% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.82 (d, J = 8.6 Hz, 1H), 8.60 (s, 1H), 8.49 (s, 1H), 7.61 (dd, J = 8.6, 1.1 Hz, 1H), 4.56 (q, J = 7.1 Hz, 2H), 2.70 (s, 3H), 1.52 (t, J = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.5, 146.4, 143.0, 131.05, 131.03, 130.2, 127.7, 116.8, 115.3, 62.5, 22.0, 14.2. **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{13}H_{13}N_4O_2$: 257.1039, Found: 257.1031. **IR** (film) ν 2920, 1714, 1606, 1374, 1242, 1223, 1157, 1037, 834 cm^{-1}.



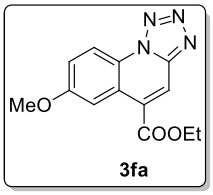
Ethyl 6-methyltetrazolo[1,5-a]quinoline-5-carboxylate (3ca'). Yellow solid, m.p.: 137.8−138.5 °C (8 mg, 20% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.4 Hz, 1H), 7.94 (s, 1H), 7.82 (t, *J* = 7.9 Hz, 1H), 7.59 (d, *J* = 7.5 Hz, 1H), 4.56 (q, *J* = 7.2 Hz, 2H), 2.69 (s, 3H), 1.49 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.9, 137.3, 137.0, 131.8, 131.5, 131.4, 119.6, 115.5, 112.9, 63.0, 21.8, 14.0. **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{13}H_{13}N_4O_2$: 257.1039, Found: 257.1031. **IR** (film) *v* 2986, 1728, 1454, 1255, 1180, 1022, 794, 769 cm^{-1}.



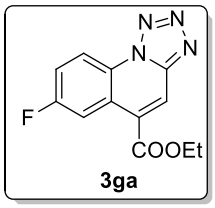
Ethyl 7-methyltetrazolo[1,5-a]quinoline-5-carboxylate (3da). Yellow solid (20 mg, 51% yield), m.p.: 135.5−136.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.72 – 8.62 (m, 2H), 8.51 (s, 1H), 7.75 (d, *J* = 8.5 Hz, 1H), 4.57 (q, *J* = 7.1 Hz, 2H), 2.63 (s, 3H), 1.52 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.5, 146.0, 139.0, 132.9, 132.9, 129.1, 127.4, 121.2, 116.8, 116.3, 62.5, 21.9, 14.2. **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{13}H_{13}N_4O_2$: 257.1039, Found: 257.1030. **IR** (film) *v* 2969, 1718, 1514, 1378, 1235, 1079, 1039, 824 cm^{-1}.



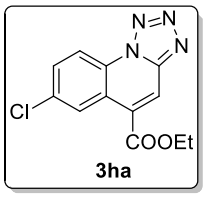
Ethyl 7-(tert-butyl)tetrazolo[1,5-a]quinoline-5-carboxylate (3ea). Yellow solid (29 mg, 65% yield), m.p.:212.6−213.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.96 (s, 1H), 8.70 (d, *J* = 8.8 Hz, 1H), 8.54 (s, 1H), 8.01 (d, *J* = 8.8 Hz, 1H), 4.58 (q, *J* = 7.1 Hz, 2H), 1.54 (t, *J* = 7.1 Hz, 3H), 1.48 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.7, 152.0, 146.1, 133.2, 129.7, 129.0, 124.0, 121.0, 116.6, 116.4, 62.5, 35.5, 31.3, 14.3. **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{16}H_{19}N_4O_2$: 299.1508, Found: 299.1498. **IR** (film) *v* 2957, 1720, 1613, 1560, 1465, 1377, 1262, 1239, 1217, 1037 cm^{-1}.



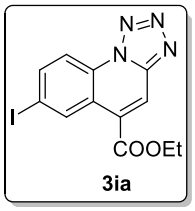
Ethyl 7-methoxytetrazolo[1,5-a]quinoline-5-carboxylate (3fa). Yellow solid (29 mg, 72% yield), m.p.: 169.3−170.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 9.2 Hz, 1H), 8.59 (s, 1H), 8.45 (s, 1H), 7.51 (dd, *J* = 9.1, 2.3 Hz, 1H), 4.56 (q, *J* = 7.1 Hz, 2H), 4.01 (s, 3H), 1.53 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.5, 159.4, 145.6, 131.9, 125.5, 122.8, 121.3, 118.3, 117.2, 108.6, 62.5, 55.9, 14.2. **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{13}H_{13}N_4O_3$: 273.0988, Found: 273.0979. **IR** (film) *v* 2915, 1717, 1566, 1244, 1028, 828 cm^{-1}.



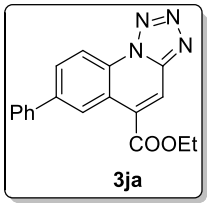
Ethyl 7-fluorotetrazolo[1,5-a]quinoline-5-carboxylate (3ga). Yellow solid (24 mg, 61% yield), mp 161.8−163.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.82 – 8.72 (m, 2H), 8.65 (s, 1H), 7.72 – 7.64 (m, 1H), 4.56 (q, *J* = 7.1 Hz, 2H), 1.52 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.9, 161.7 (d, *J* = 249.3 Hz), 146.0, 131.9 (d, *J* = 3.7 Hz), 127.6, 122.9 (d, *J* = 10.3 Hz), 120.2 (d, *J* = 25.3 Hz), 119.1 (d, *J* = 9.1 Hz), 118.1, 113.9 (d, *J* = 26.5 Hz), 62.8, 14.2. **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{12}H_9FN_4O_2$: 261.0788, Found: 261.0780. **IR** (film) *v* 2920, 1720, 1560, 1244, 1217, 1143, 1036, 827, 784 cm^{-1}.



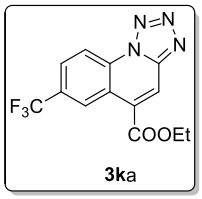
Ethyl 7-chlorotetrazolo[1,5-a]quinoline-5-carboxylate (3ha). Yellow solid (22 mg, 53% yield), m.p.: 176.0−177.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.72 (d, *J* = 8.9 Hz, 1H), 8.63 (s, 1H), 7.89 (d, *J* = 8.9 Hz, 1H), 4.57 (q, *J* = 7.1 Hz, 2H), 1.53 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.8, 146.2 135.0, 132.0, 131.8, 129.4, 127.7, 122.37, 118.4, 117.9, 62.8, 14.2. **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{12}H_{10}ClN_4O_2$: 277.0492, Found: 277.0481. **IR** (film) *v* 2920, 1719, 1494, 1238, 1093, 825 cm^{-1}.



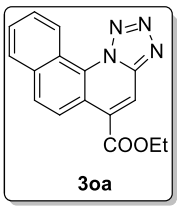
Ethyl 7-iodotetrazolo[1,5-a]quinoline-5-carboxylate (3ia). Yellow solid (23 mg, 58% yield), m.p.: 222.6−223.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.39 (s, 1H), 8.59 (s, 1H), 8.52 (d, *J* = 8.8 Hz, 1H), 8.23 (d, *J* = 8.7 Hz, 1H), 7.97 (d, *J* = 8.7 Hz, 2H), 7.33 (d, *J* = 8.6 Hz, 2H), 4.57 (q, *J* = 7.1 Hz, 2H), 1.53 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.9, 140.3, 139.1, 136.9, 131.7, 130.3, 127.2, 122.7, 118.4, 117.6, 62.8, 14.2. **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{12}H_{10}IN_4O_2$: 368.9848, Found: 368.9837. **IR** (film) *v* 3078, 1715, 1544, 1365, 1239, 1219, 1000, 822 cm^{-1}.



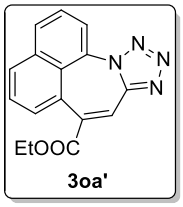
Ethyl 7-phenyltetrazolo[1,5-a]quinoline-5-carboxylate (3ja). Yellow solid (20 mg, 41% yield), m.p.: 165.1−167.0 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 8.83 (d, *J* = 8.7 Hz, 1H), 8.59 (s, 1H), 8.17 (d, *J* = 8.6 Hz, 1H), 7.75 (d, *J* = 7.4 Hz, 2H), 7.55 (t, *J* = 7.4 Hz, 2H), 7.47 (t, *J* = 7.3 Hz, 1H), 4.59 (q, *J* = 7.1 Hz, 2H), 1.54 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.4, 146.2, 141.7, 139.3, 133.0, 130.7, 130.0, 129.2, 128.5, 127.5, 126.1, 121.7, 117.4, 116.9, 62.6, 14.3. **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{18}H_{15}N_4O_2$: 319.1195, Found: 319.1187. **IR** (film) *v* 2961, 1719, 1566, 1237, 1220, 1165, 1039, 764, 691 cm^{-1}.



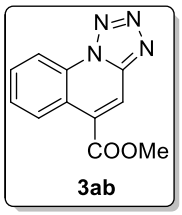
Ethyl 7-(trifluoromethyl)tetrazolo[1,5-a]quinoline-5-carboxylate (3ka). Yellow solid (24 mg, 52% yield), m.p.: 148.7−150.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.39 (s, 1H), 8.91 (d, *J* = 8.7 Hz, 1H), 8.70 (s, 1H), 8.17 (d, *J* = 8.7 Hz, 1H), 4.60 (q, *J* = 7.1 Hz, 2H), 1.54 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.7, 146.6, 132.5, 132.4, 130.8 (q, *J* = 33.2 Hz), 128.0 (q, *J* = 3.3 Hz), 126.1 (q, *J* = 4.2 Hz), 123.3 (q, *J* = 271.2 Hz), 121.2, 118.4, 118.0, 63.0, 14.2. **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{13}H_{10}F_3N_4O_2$: 311.0756, Found: 311.0747. **IR** (film) *v* 2987, 1724, 1616, 1438, 1315, 1122, 842 cm^{-1}.



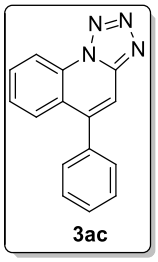
Ethyl benzo[h]tetrazolo[1,5-a]quinoline-5-carboxylate (3oa). Yellow solid (16 mg, 36% yield), m.p.: 178.5−190.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.38 (d, *J* = 8.8 Hz, 1H), 8.75 (d, *J* = 9.1 Hz, 1H), 8.70 (s, 1H), 8.12 (t, *J* = 7.9 Hz, 2H), 7.96 (dd, *J* = 11.5, 4.2 Hz, 1H), 7.87 (t, *J* = 7.1 Hz, 1H), 4.62 (q, *J* = 7.1 Hz, 2H), 1.56 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.1, 147.3, 134.3, 134.2, 129.8, 129.3, 128.9, 128.6, 127.7, 123.3, 122.7, 120.6, 115.9, 62.75 (s), 14.26 (s). **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{16}H_{13}N_4O_2$: 293.1039, Found: 293.1032. **IR** (film) *v* 2982, 1719, 1409, 1227, 1052, 837, 157 cm^{-1}.



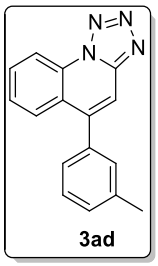
Ethyl naphtho[1,8-ef]tetrazolo[1,5-a]azepine-11-carboxylate (3oa'). Yellow solid (19 mg, 43% yield), m.p.: 213.6−214.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.41 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.89 – 7.81 (m, 2H), 7.58 (t, *J* = 8.0 Hz, 1H), 7.52 – 7.41 (m, 2H), 7.19 (s, 1H), 4.44 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 168.4, 149.5, 144.0, 136.4, 131.8, 131.7, 131.5, 130.5, 127.7, 127.4, 126.5, 126.1, 120.0, 114.3, 62.5, 14.1. **HRMS** (ESI) ($[M+H]^+$) Calcd. for $C_{16}H_{13}N_4O_2$: 293.1039, Found: 293.1028. **IR** (film) *v* 2919, 1709, 1504, 1255, 1092, 827, 761 cm^{-1}.



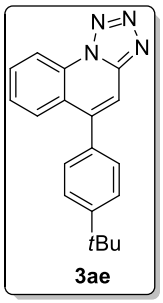
Methyl tetrazolo[1,5-a]quinoline-5-carboxylate (3ab). Yellow solid (18 mg, 52% yield), m.p.: 212.6−213.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.94 (d, *J* = 8.4 Hz, 1H), 8.80 (d, *J* = 8.3 Hz, 1H), 8.56 (s, 1H), 7.95 (dd, *J* = 11.5, 4.1 Hz, 1H), 7.87 – 7.72 (m, 1H), 4.12 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.8, 146.2, 132.8, 131.6, 131.0, 128.6, 128.0, 121.2, 117.1, 116.7, 53.3. **HRMS** (ESI) *m/z* Calcd. for $C_{11}H_9N_4O_2$ ($[M+H]^+$): 229.0726, Found: 229.0718. **IR** (film) *v* 3066, 1721, 1603, 1558, 1447, 1247, 1157 cm^{-1}.



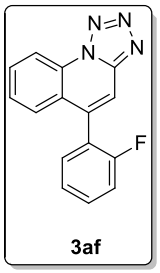
5-phenyltetrazolo[1,5-a]quinoline (3ac). Yellow solid (19 mg, 51% yield), m.p.: 212.6−213.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.86 – 8.78 (m, 1H), 7.98 – 7.88 (m, 2H), 7.82 (s, 1H), 7.71 – 7.64 (m, 1H), 7.60 (dt, *J* = 4.3, 1.8 Hz, 3H), 7.56 – 7.52 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.0, 146.2, 136.8, 131.2, 130.9, 129.4, 129.3, 129.0, 128.2, 127.8, 123.6, 117.1, 112.1. **HRMS** (ESI) *m/z* Calcd. for $C_{15}H_{11}N_4$ ([M+H]$^+$): 247.0984, Found: 247.0977. **IR** (film) *v* 2921, 1607, 1498, 1455, 1014, 821, 759 cm^{-1}.



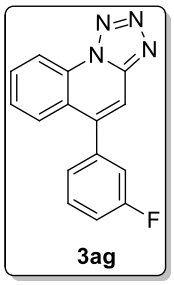
5-(m-tolyl)tetrazolo[1,5-a]quinoline(3ad). Yellow solid (23 mg, 58% yield), m.p.: 212.6−213.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.81 (d, *J* = 8.3 Hz, 1H), 7.98 – 7.88 (m, 2H), 7.80 (s, 1H), 7.68 (t, *J* = 7.7 Hz, 1H), 7.47 (d, *J* = 7.4 Hz, 1H), 7.39 (d, *J* = 7.7 Hz, 1H), 7.33 (d, *J* = 8.7 Hz, 2H), 2.50 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.0, 146.4, 138.8, 136.8, 131.1, 129.97, 129.95, 128.3, 127.8, 126.5, 123.7, 117.1, 111.9, 21.5. **HRMS** (ESI) *m/z*Calcd. for $C_{16}H_{13}N_4$ ([M+H]$^+$): 261.1140, $C_{16}H_{13}N_4$, Found: 261.1124. **IR** (film) *v* 2918, 1606, 1557, 1085, 881, 761 cm^{-1}.



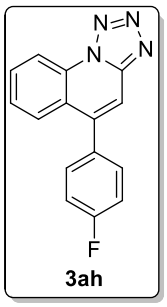
5-(4-(tert-butyl)phenyl)tetrazolo[1,5-a]quinoline(3ae). Yellow solid (29 mg, 64% yield), m.p.: 190.8−191.6°C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 8.3 Hz, 1H), 8.01 (d, *J* = 8.3 Hz, 1H), 7.90 (t, *J* = 7.6 Hz, 1H), 7.80 (s, 1H), 7.68 (t, *J* = 7.9 Hz, 1H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.48 (d, *J* = 8.1 Hz, 2H), 1.44 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.5, 147.1, 146.3, 133.8, 131.1, 131.0, 129.2, 128.4, 127.7, 125.9, 123.7, 117.1, 111.8, 34.9, 31.4. **HRMS** (ESI) *m/z* Calcd. for $C_{19}H_{19}N_4$ ([M+H]$^+$): 303.1610, Found: 303.1599. **IR** (film) *v* 2961, 1605, 1557, 1269, 1109, 836, 767 cm^{-1}.



5-(2-fluorophenyl)tetrazolo[1,5-a]quinoline (3af). Yellow solid (20 mg, 51% yield), m.p.: 212.6−213.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.81 (d, *J* = 8.4 Hz, 1H), 7.91 (dd, *J* = 15.6, 7.6 Hz, 1H), 7.87 (s, 1H), 7.76 – 7.65 (m, 2H), 7.60 (dd, *J* = 13.6, 7.3 Hz, 1H), 7.50 – 7.43 (m, 1H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.32 (t, *J* = 9.1 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.6 (d, *J* = 249.0 Hz), 146.9, 140.5, 131.6, 131.5, 131.4 (d, *J* = 2.7 Hz), 131.3, 130.7, 123.0, 127.9 (d, *J* = 1.3 Hz), 124.9 (d, *J* = 3.7 Hz), 124.3 (d, *J* = 15.8 Hz), 123.4, 117.1, 116.3 (d, *J* = 21.4 Hz), 113.5. **HRMS** (ESI) *m/z* Calcd. for $C_{15}H_{10}FN_4$ ($[M+H]^+$): 265.0889, Found: 265.0883. **IR** (film) *v* 2920, 1611, 1489, 1447, 1087, 156 cm^{-1}.

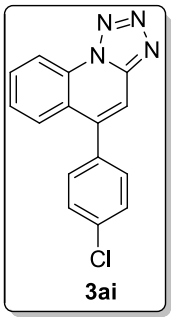


5-(3-fluorophenyl)tetrazolo[1,5-a]quinoline (3ag). Yellow solid (16 mg, 40% yield), m.p.: 212.6−213.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 8.3 Hz, 1H), 7.97 – 7.90 (m, 2H), 7.82 (s, 1H), 7.74 – 7.68 (m, 1H), 7.59 (td, *J* = 7.9, 5.9 Hz, 1H), 7.35 – 7.31 (m, 1H), 7.31 – 7.26 (m, 2H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.8 (d, *J* = 247.0 Hz), 146.9, 144.8 (d, *J* = 2.0 Hz), 138.8 (d, *J* = 7.8 Hz), 131.4, 130.9, 130.8 (d, *J* = 8.4 Hz), 129.7, 127.9 (d, *J* = 12.5 Hz), 125.2 (d, *J* = 3.1 Hz), 123.8, 123.3, 117.3, 116.7, 116.2, 112.3. **HRMS** (ESI) *m/z* Calcd. for $C_{15}H_{10}FN_4$ ($[M+H]^+$): 265.0889, Found: 265.0883. **IR** (film) *v* 2919, 1612, 1584, 1417, 1266, 860, 765 cm^{-1}.

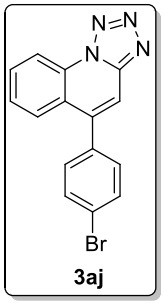


5-(4-fluorophenyl)tetrazolo[1,5-a]quinoline (3ah). Yellow solid (27 mg, 67% yield), m.p.: 212.6−213.9 °C.**^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.82 (d, *J* = 8.3 Hz, 1H), 7.92 (dd, *J* = 15.8, 7.9 Hz, 2H), 7.80 (s, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.58 – 7.49 (m, 2H), 7.33 – 7.28 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$)

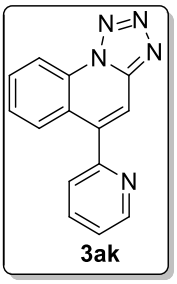
δ 163.29 (d, *J* = 249.7 Hz), 146.9, 145.1, 132.8 (d, *J* = 3.5 Hz), δ 131.26 (d, *J* = 3.4 Hz), 131.6, 130.9, 127.9 (d, *J* = 2.5 Hz), 123.5, 117.2, 116.2, 116.0, 112.3. **HRMS** (ESI) *m/z* Calcd. for $C_{15}H_{10}FN_4$ ($[M+H]^+$): 265.0889, Found: 265.0883. **IR** (film) *v* 2921, 1600, 1506, 1239, 840, 762 cm^{-1}.



5-(4-chlorophenyl)tetrazolo[1,5-a]quinoline (3ai). Yellow solid (32 mg, 75% yield), m.p.: 212.6−213.9 °C.**^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 8.3 Hz, 1H), 7.94 (t, *J* = 7.8 Hz, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.81 (s, 1H), 7.70 (t, *J* = 7.4 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.3 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.9, 145.0, 135.6, 135.2, 131.4, 131.0, 130.7, 129.3, 128.0, 127.9, 123.4, 117.3, 112.2. **HRMS** (ESI) *m/z* Calcd. for $C_{15}H_{10}ClN_4$ ($[M+H]^+$): 281.0594, Found: 281.0589. **IR** (film) *v* 2921, 1611, 1482, 1401, 1091, 1011, 840, 760 cm^{-1}.

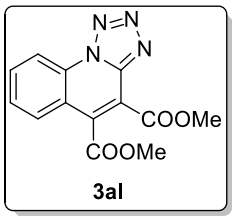


5-(4-bromophenyl)tetrazolo[1,5-a]quinoline (3aj). Yellow solid (30 mg, 62% yield), m.p.: 212.6−213.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 8.3 Hz, 1H), 7.98 – 7.86 (m, 2H), 7.81 (s, 1H), 7.78 – 7.66 (m, 3H), 7.43 (d, *J* = 8.4 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.9, 144.9, 135.7, 132.3, 131.4, 131.0, 128.0, 127.9, 123.8, 123.3, 117.3, 112.2. **HRMS** (ESI) *m/z* Calcd. for $C_{15}H_{10}BrN_4$ ($[M+H]^+$): 325.0089, Found: 325.0081. **IR** (film) *v* 2921, 1610, 1556, 1489, 1396, 1007, 759 cm^{-1}.

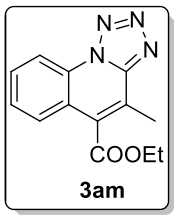


5-(pyridin-2-yl)tetrazolo[1,5-a]quinoline (3ak). Yellow solid (23 mg, 64% yield), m.p.: 212.6−213.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.88 (d, *J* = 4.7 Hz, 1H), 8.82 (d, *J* = 8.4 Hz, 1H), 8.20 (d, *J* = 8.3 Hz, 1H), 8.02

– 7.95 (m, 2H), 7.92 (t, *J* = 7.8 Hz, 1H), 7.71 (t, *J* = 7.7 Hz, 2H), 7.52 (dd, *J* = 7.0, 5.5 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 155.6, 150.0, 146.9, 144.0, 137.5, 131.3, 131.1, 128.2, 128.0, 124.7, 123.9, 122.8, 117.1, 112.9. **HRMS** (ESI) *m/z* Calcd. for $C_{14}H_{10}N_5$ ($[M+H]^+$): 248.0936, Found:248.0931. **IR** (film) *v* 3006, 1612, 1474, 1287, 1157, 889, 771 cm^{-1}.



3al ***Dimethyl tetrazolo[1,5-a]quinoline-4,5-dicarboxylate (3al).*** Yellow solid (20 mg, 46% yield), m.p.: 212.6−213.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.82 (d, *J* = 8.4 Hz, 1H), 8.05 (dd, *J* = 19.1, 7.9 Hz, 2H), 7.84 (t, *J* = 7.8 Hz, 1H), 4.16 (d, *J* = 3.2 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.7, 162.7, 144.9, 140.8, 134.0, 131.6, 129.1, 128.2, 120.4, 117.4, 114.7, 53.9, 53.8. **HRMS** (ESI) *m/z* Calcd. For $C_{13}H_{11}N_4O_4$ ($[M+Na]^+$): 309.0600, Found: 309.0590. **IR** (film) *v* 2919, 1722, 1556, 1431, 1357, 1226, 1000, 776 cm^{-1}.



3am ***Ethyl 4-methyltetrazolo[1,5-a]quinoline-5-carboxylate (3am).*** Yellow solid (17 mg, 45% yield), m.p.: 212.6−213.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.72 (d, *J* = 8.3 Hz, 1H), 7.92 (d, *J* = 8.3 Hz, 1H), 7.87 (t, *J* = 7.6 Hz, 1H), 7.73 (t, *J* = 7.7 Hz, 1H), 4.63 (q, *J* = 7.1 Hz, 2H), 2.83 (s, 3H), 1.52 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.1, 147.9, 134.1, 130.6, 129.5, 128.4, 126.3, 121.9, 121.5, 117.0, 62.6. HRMS (ESI) *m/z* Calcd. for $C_{13}H_{13}N_4O_2$ ($[M+H]^+$): 257.1039, Found: 257.1032. **IR** (film) *v* 2919, 1729, 1524, 1350, 1213, 1038, 763 cm^{-1}.

5. X-Ray Crystallography Data of 3da (CCDC No.1511247)

The ellipsoid contour percent probability level is 30%.

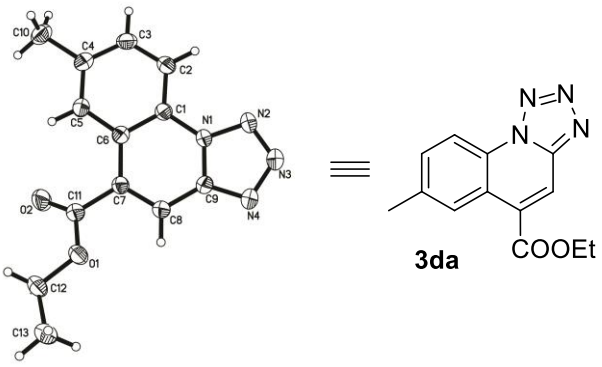


Table S1. Crystal data and structure refinement for **3da**.

Identification code	ZL02	
Empirical formula	C13 H12 N4 O2	
Formula weight	256.27	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5827(7) Å	= 74.850(2)°.
	b = 11.8639(10) Å	= 89.545(2)°.
	c = 12.5606(10) Å	= 88.331(2)°.
Volume	1234.00(18) $Å^3$	
Z	4	
Density (calculated)	1.379 Mg/m^3	
Absorption coefficient	0.097 mm^{-1}	
F(000)	536	
Crystal size	0.23 x 0.21 x 0.18 mm^3	
Theta range for data collection	2.374 to 24.999°.	
Index ranges	-10<=h<=10, -14<=k<=14, -14<=l<=14	
Reflections collected	15051	
Independent reflections	4286 [R(int) = 0.0380]	
Completeness to theta = 24.999°	98.9 %	
Absorption correction	Multi-sacn	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4286 / 0 / 347	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0523, wR2 = 0.1452	

R indices (all data)	R1 = 0.0809, wR2 = 0.1645
Extinction coefficient	n/a
Largest diff. peak and hole	0.421 and -0.231 e.Å^{-3}

Table S2. Bond lengths [Å] and angles [°] for **3da**.

C(1)-C(2)	1.391(3)
C(1)-N(1)	1.396(2)
C(1)-C(6)	1.404(3)
C(2)-C(3)	1.366(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.392(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.377(3)
C(4)-C(10)	1.503(3)
C(5)-C(6)	1.407(3)
C(5)-H(5)	0.9300
C(6)-C(7)	1.460(3)
C(7)-C(8)	1.357(3)
C(7)-C(11)	1.497(3)
C(8)-C(9)	1.415(3)
C(8)-H(8)	0.9300
C(9)-N(4)	1.330(3)
C(9)-N(1)	1.348(3)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-O(2)	1.202(2)
C(11)-O(1)	1.320(2)
C(12)-O(1)	1.452(3)
C(12)-C(13)	1.459(4)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
N(1)-N(2)	1.354(2)
N(2)-N(3)	1.300(3)

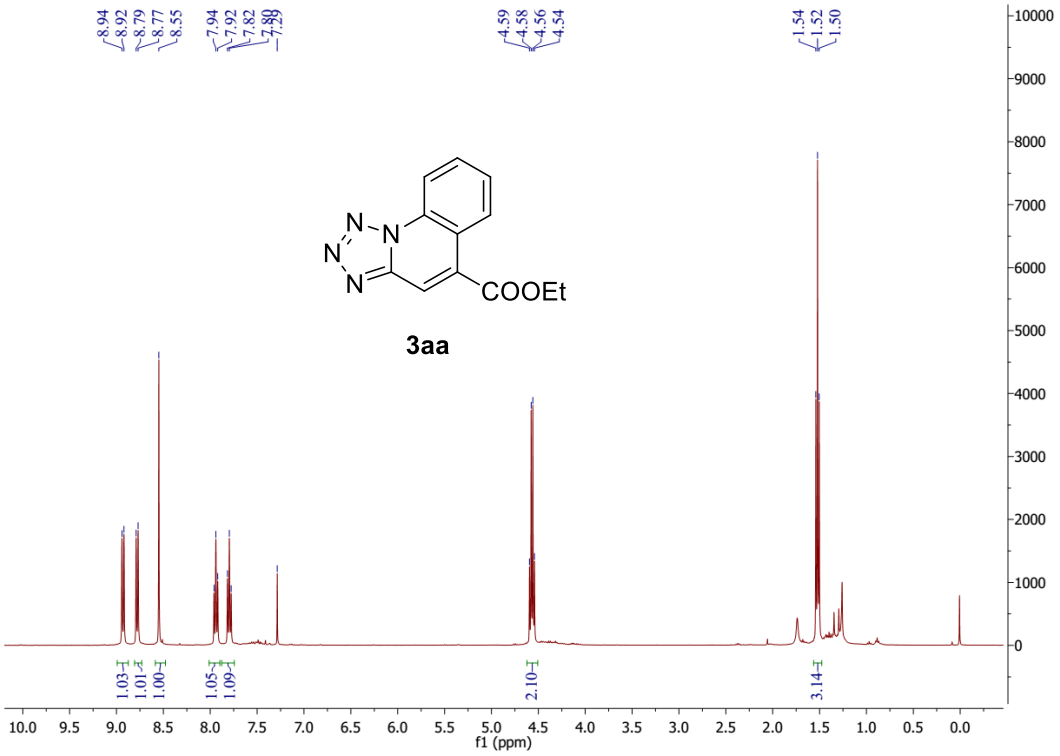
N(3)-N(4)	1.348(3)
C(2)-C(1)-N(1)	121.03(18)
C(2)-C(1)-C(6)	122.15(19)
N(1)-C(1)-C(6)	116.83(17)
C(3)-C(2)-C(1)	119.0(2)
C(3)-C(2)-H(2)	120.5
C(1)-C(2)-H(2)	120.5
C(2)-C(3)-C(4)	121.52(19)
C(2)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2
C(5)-C(4)-C(3)	118.57(19)
C(5)-C(4)-C(10)	121.1(2)
C(3)-C(4)-C(10)	120.29(19)
C(4)-C(5)-C(6)	122.6(2)
C(4)-C(5)-H(5)	118.7
C(6)-C(5)-H(5)	118.7
C(1)-C(6)-C(5)	116.11(18)
C(1)-C(6)-C(7)	118.91(17)
C(5)-C(6)-C(7)	124.98(18)
C(8)-C(7)-C(6)	120.90(18)
C(8)-C(7)-C(11)	118.19(18)
C(6)-C(7)-C(11)	120.82(17)
C(7)-C(8)-C(9)	119.36(18)
C(7)-C(8)-H(8)	120.3
C(9)-C(8)-H(8)	120.3
N(4)-C(9)-N(1)	108.20(18)
N(4)-C(9)-C(8)	132.50(19)
N(1)-C(9)-C(8)	119.30(18)
C(4)-C(10)-H(10A)	109.5
C(4)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(4)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
O(2)-C(11)-O(1)	122.9(2)
O(2)-C(11)-C(7)	125.05(19)
O(1)-C(11)-C(7)	112.01(18)

O(1)-C(12)-C(13)	108.6(2)
O(1)-C(12)-H(12A)	110.0
C(13)-C(12)-H(12A)	110.0
O(1)-C(12)-H(12B)	110.0
C(13)-C(12)-H(12B)	110.0
H(12A)-C(12)-H(12B)	108.4
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(9)-N(1)-N(2)	108.69(16)
C(9)-N(1)-C(1)	124.69(17)
N(2)-N(1)-C(1)	126.61(16)
N(3)-N(2)-N(1)	105.42(17)
N(2)-N(3)-N(4)	112.17(17)

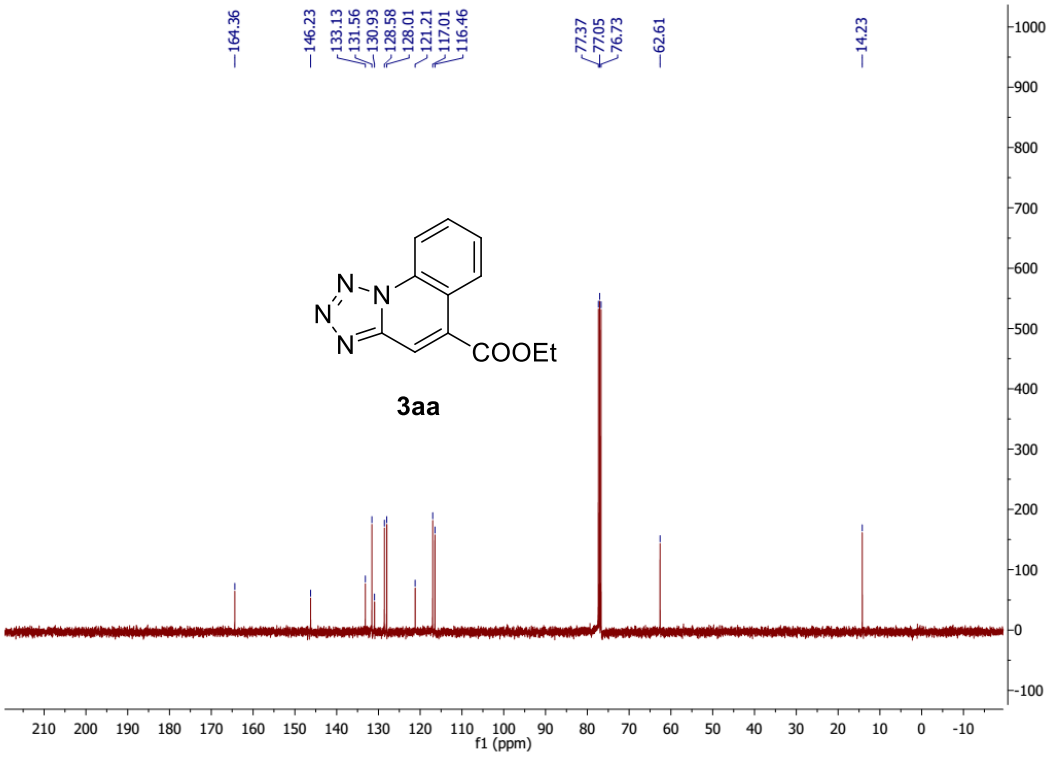
6. ^{1}HNMR and ^{13}CNMR spectra of Products

Ethyl tetrazolo[1,5-a]quinoline-5-carboxylate (3aa)

^{1}H NMR (400 MHz, $CDCl_3$)

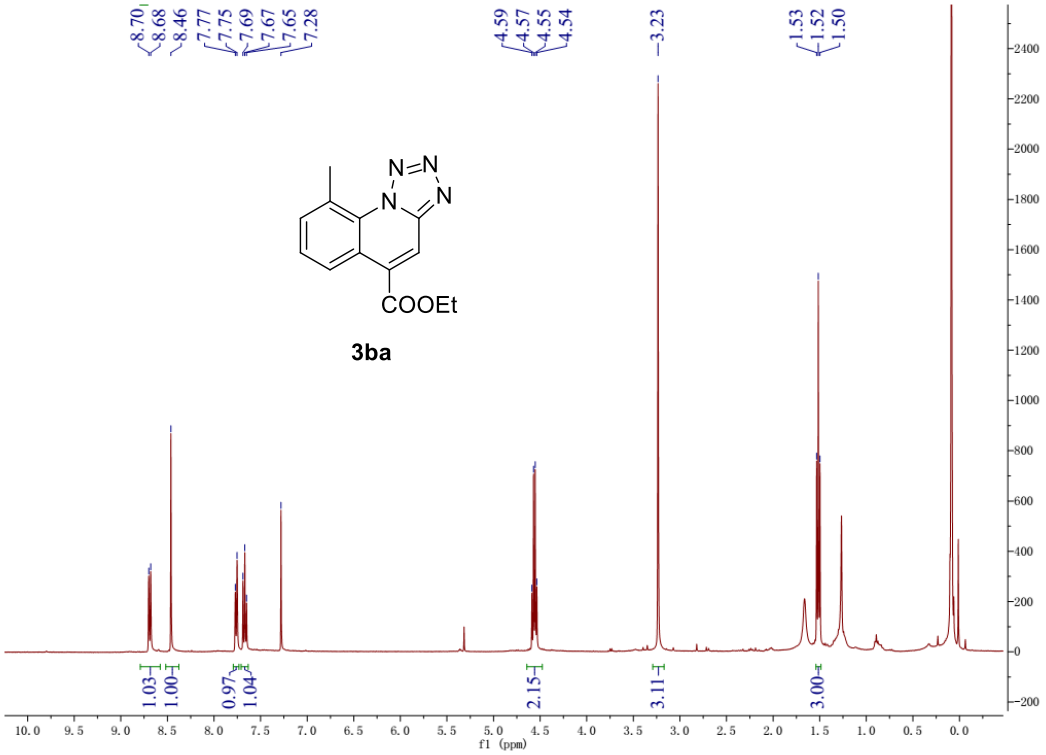


^{13}C NMR (100 MHz, $CDCl_3$)

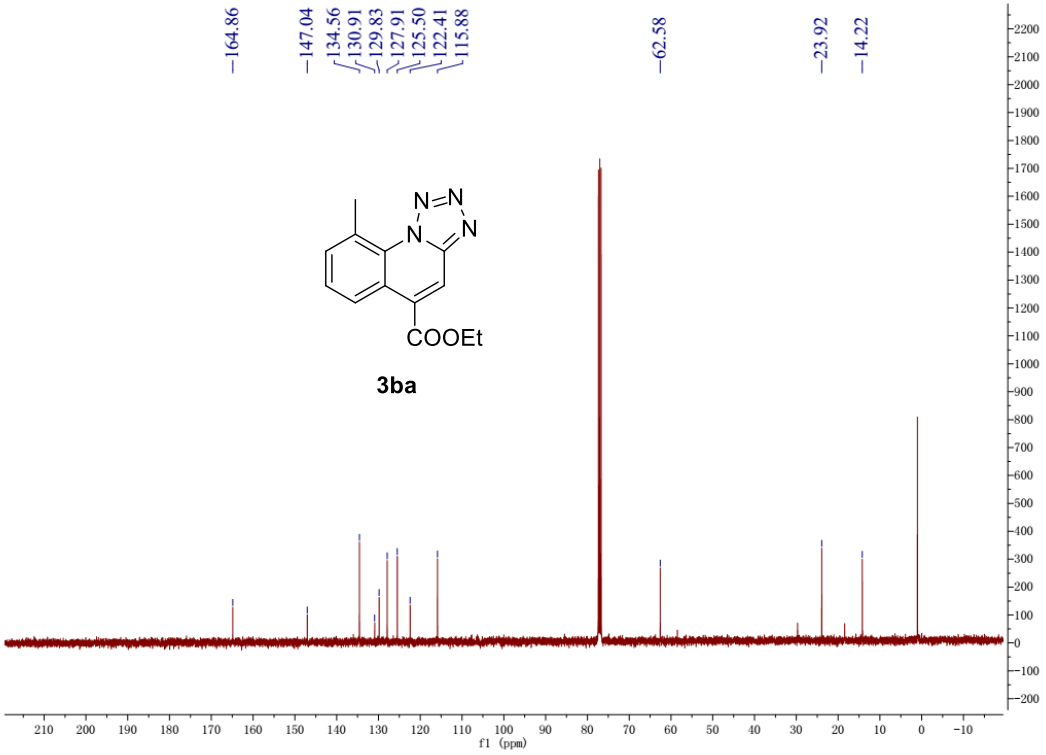


Ethyl 9-methyltetrazolo[1,5-a]quinoline-5-carboxylate (3ba)

^{1}H NMR (400 MHz, $CDCl_3$)

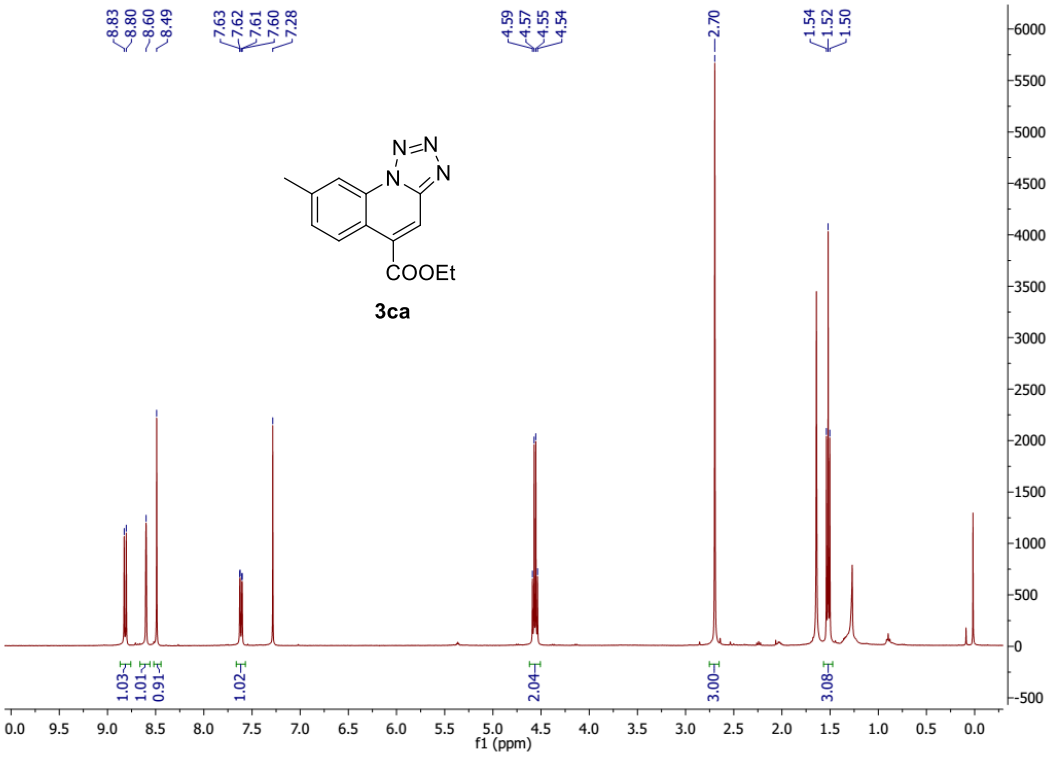


^{13}C NMR (100 MHz, $CDCl_3$)

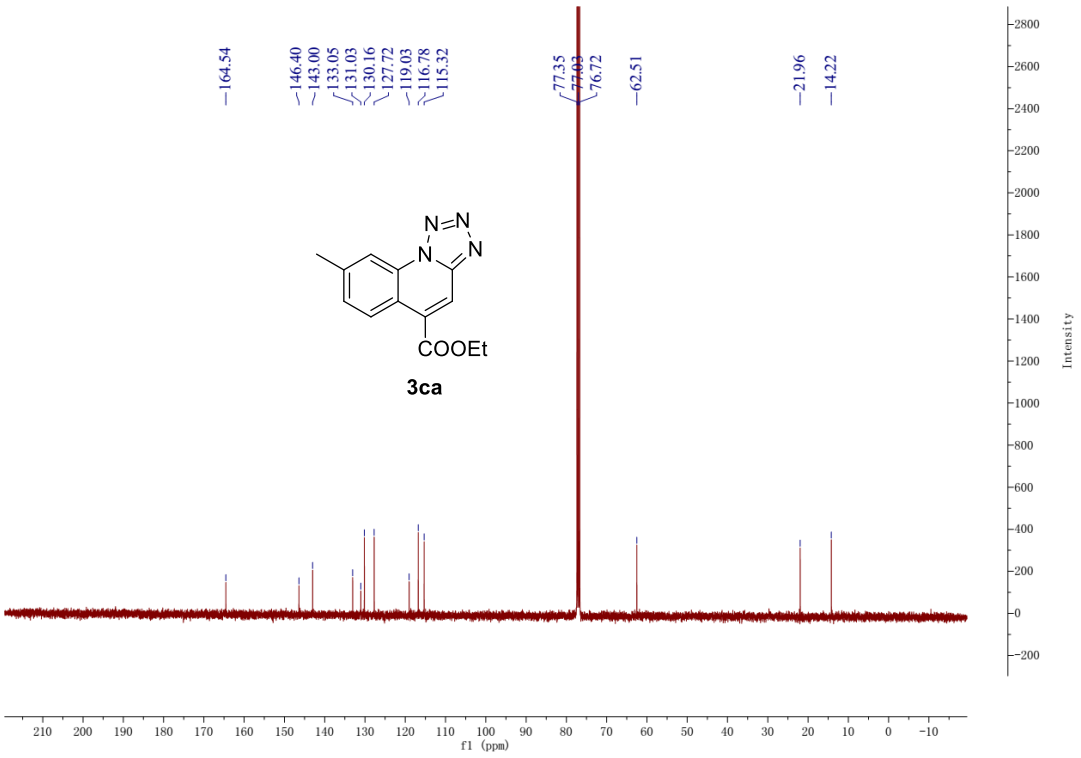


Ethyl 8-methyltetrazolo[1,5-a]quinoline-5-carboxylate (3ca)

^{1}H NMR (400 MHz, $CDCl_3$)

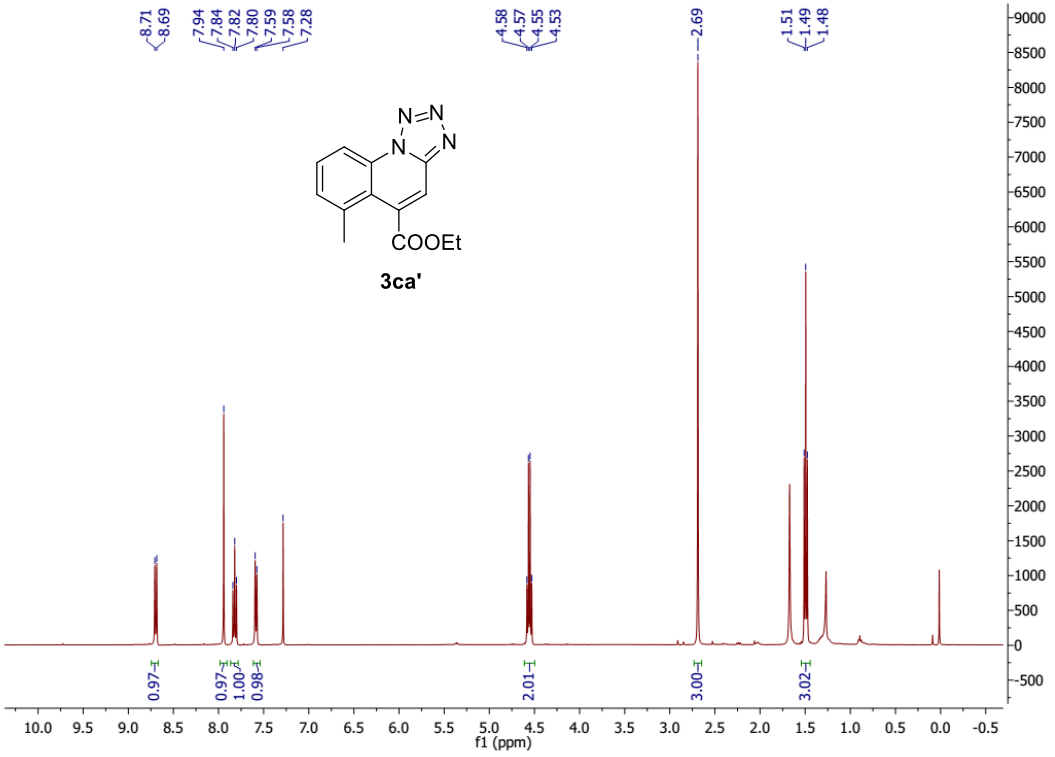


^{13}C NMR (100 MHz, $CDCl_3$)

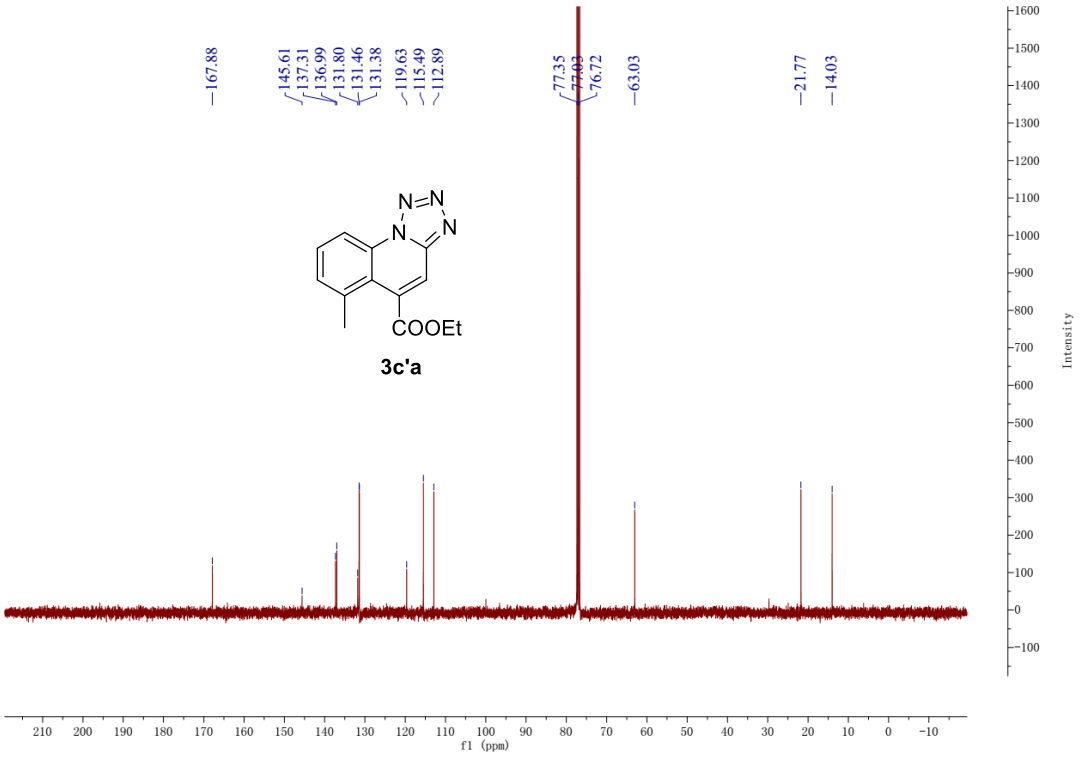


Ethyl 6-methyltetrazolo[1,5-a]quinoline-5-carboxylate (3ca')

^{1}H NMR (400 MHz, $CDCl_3$)

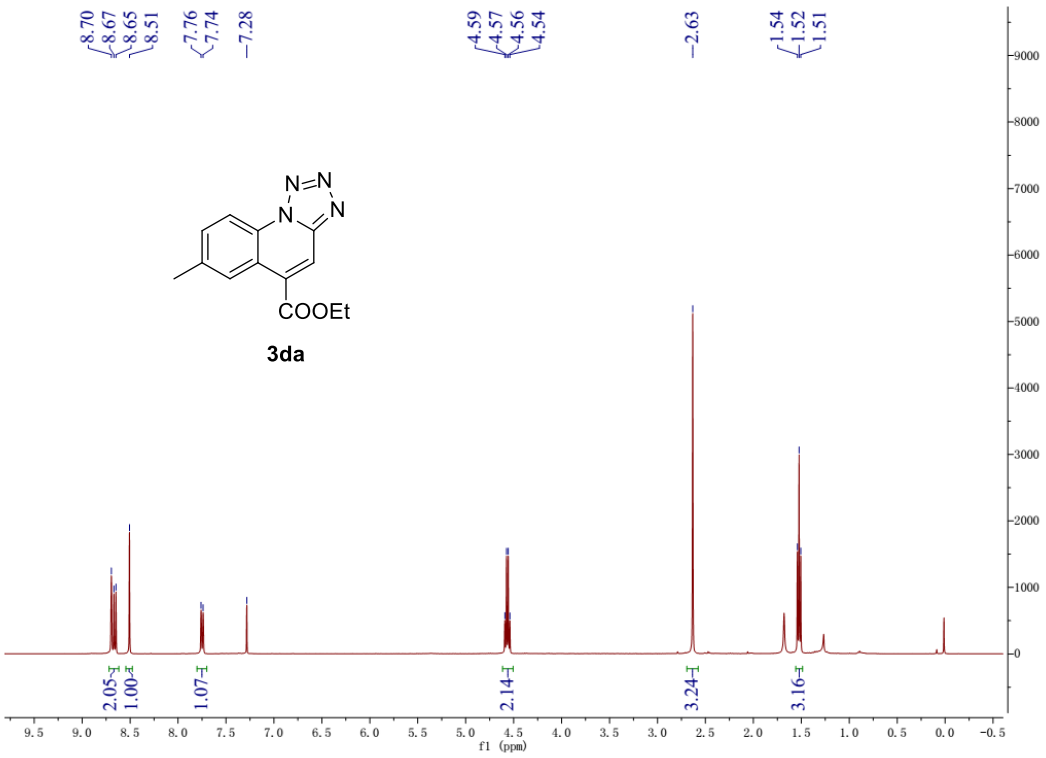


^{13}C NMR (100 MHz, $CDCl_3$)

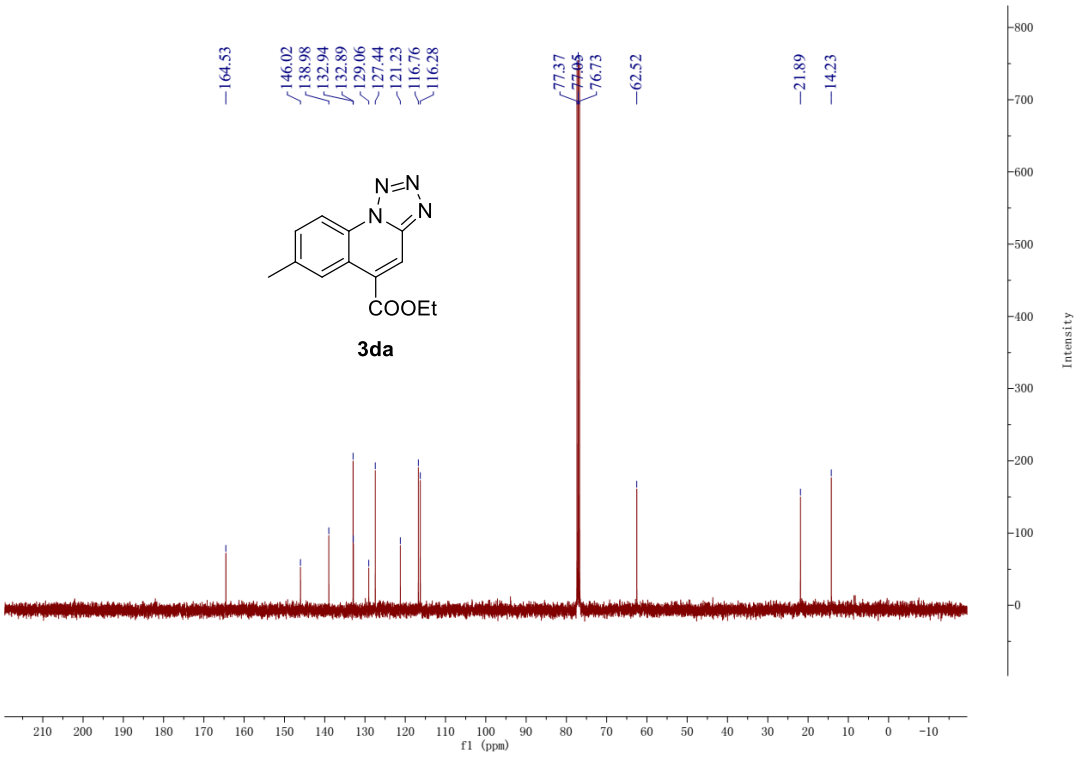


Ethyl 7-methyltetrazolo[1,5-a]quinoline-5-carboxylate (3da)

^{1}H NMR (400 MHz, $CDCl_3$)

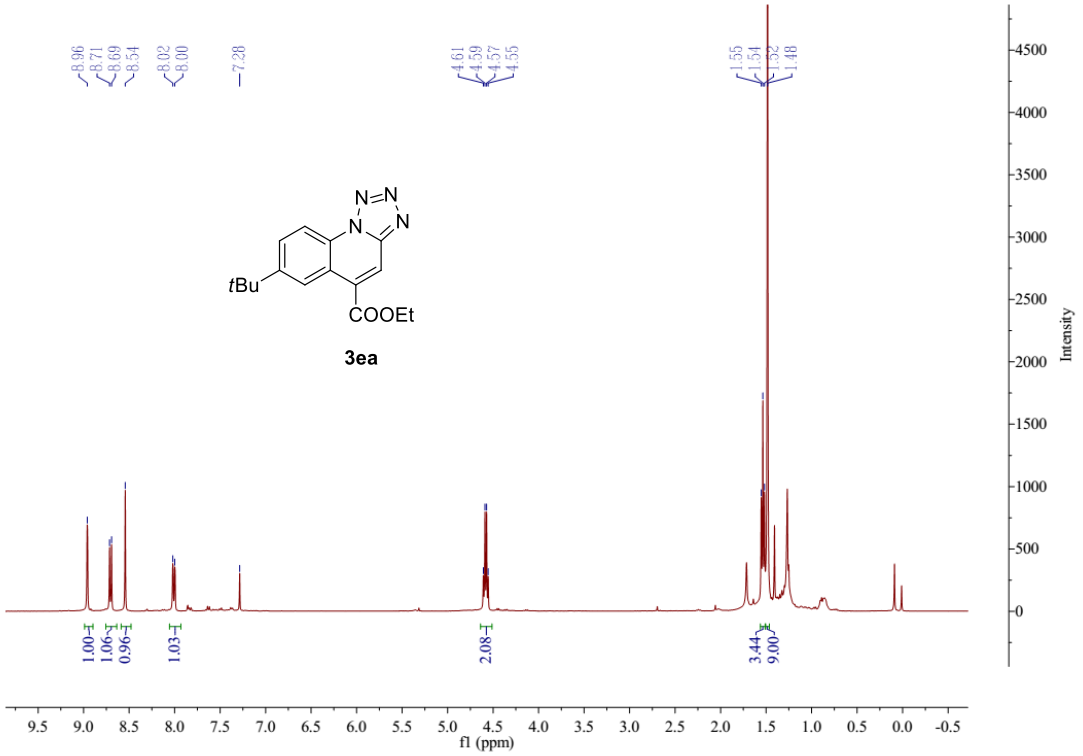


^{13}C NMR (100 MHz, $CDCl_3$)

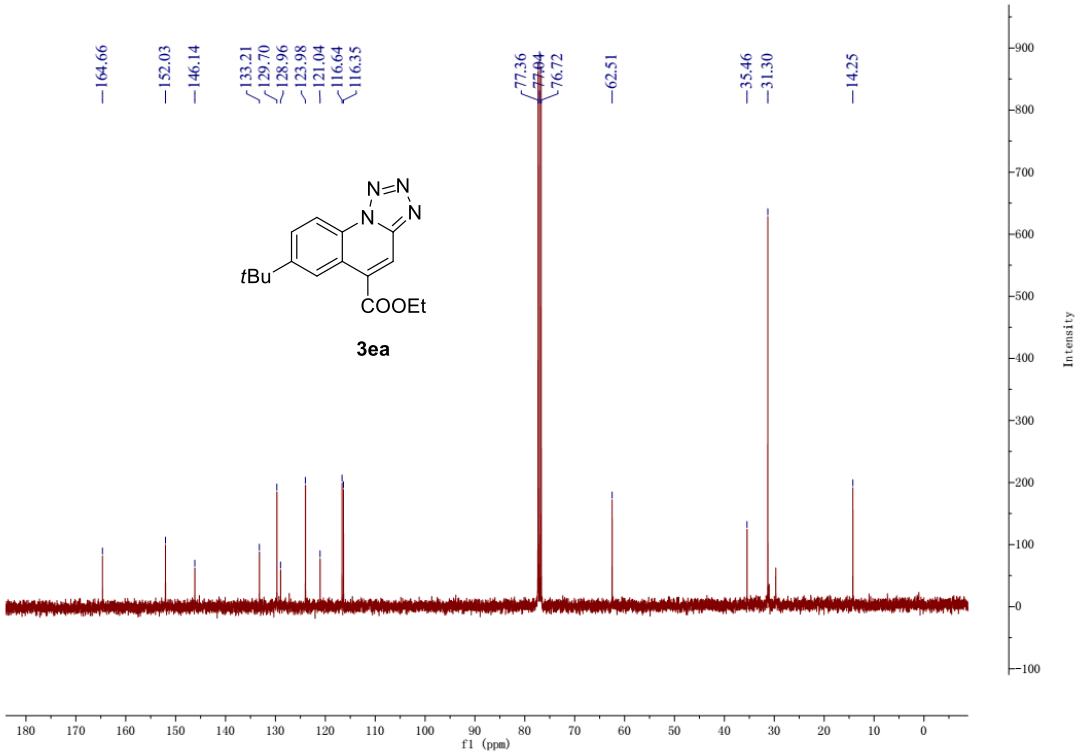


Ethyl 7-(tert-butyl)tetrazolo[1,5-a]quinoline-5-carboxylate (3ea)

^{1}H NMR (400 MHz, $CDCl_3$)

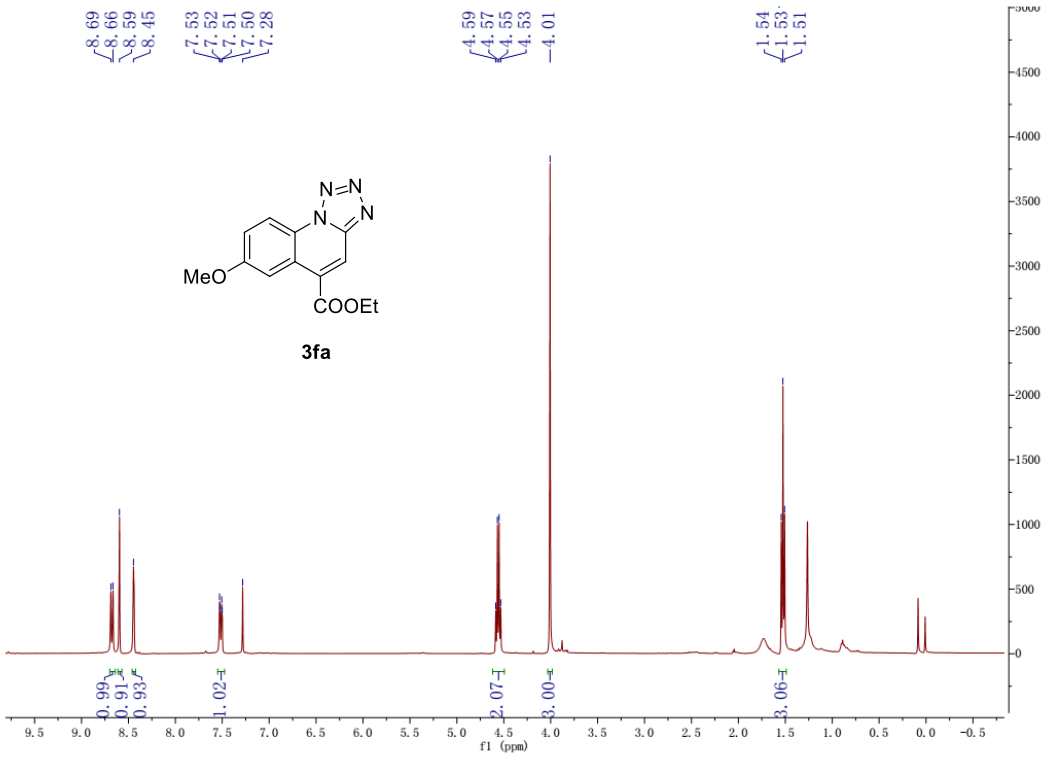


^{13}C NMR (100 MHz, $CDCl_3$)

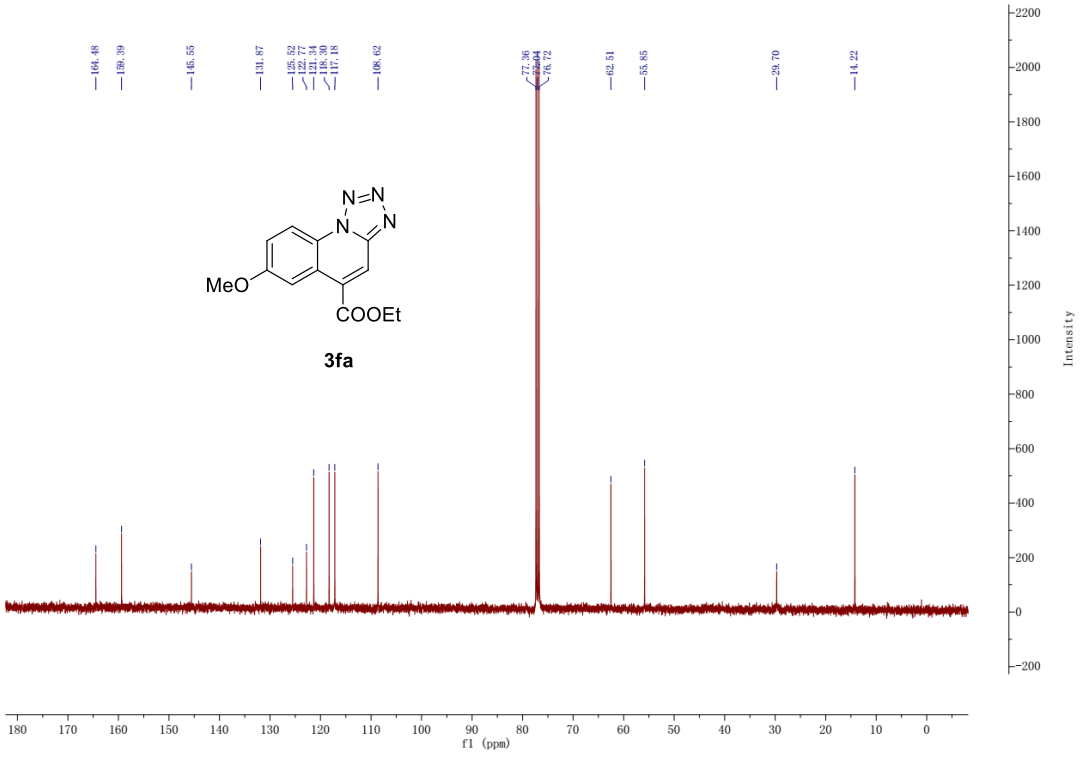


Ethyl 7-methoxytetrazolo[1,5-a]quinoline-5-carboxylate (3fa)

^{1}H NMR (400 MHz, $CDCl_3$)

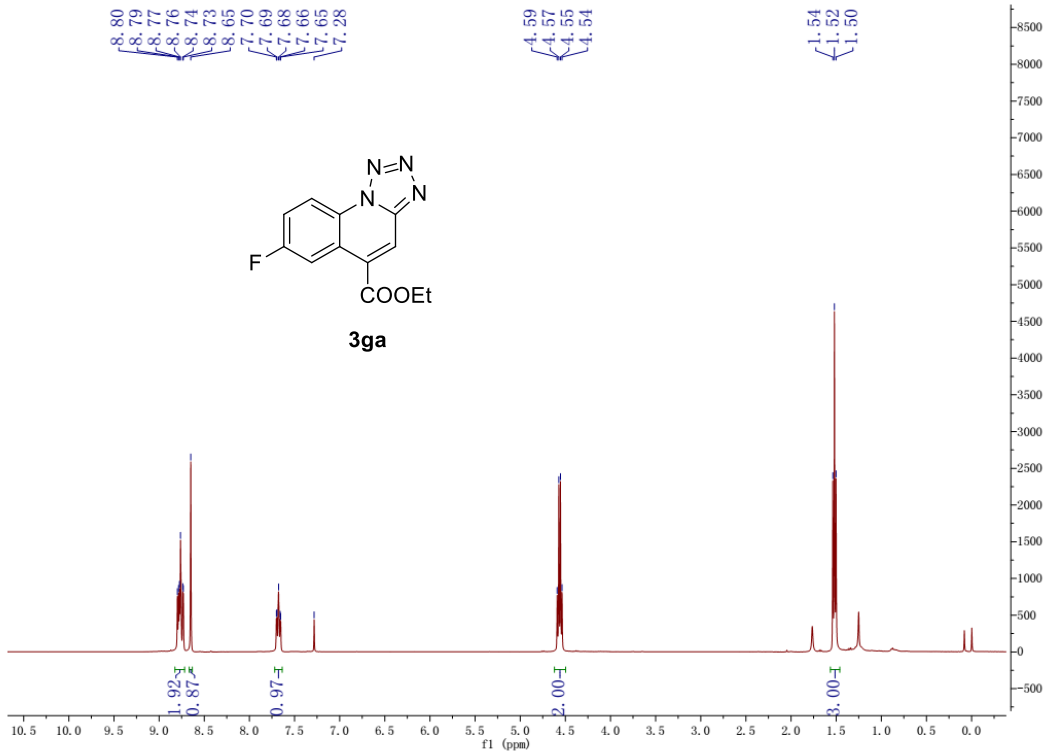


^{13}C NMR (100 MHz, $CDCl_3$)

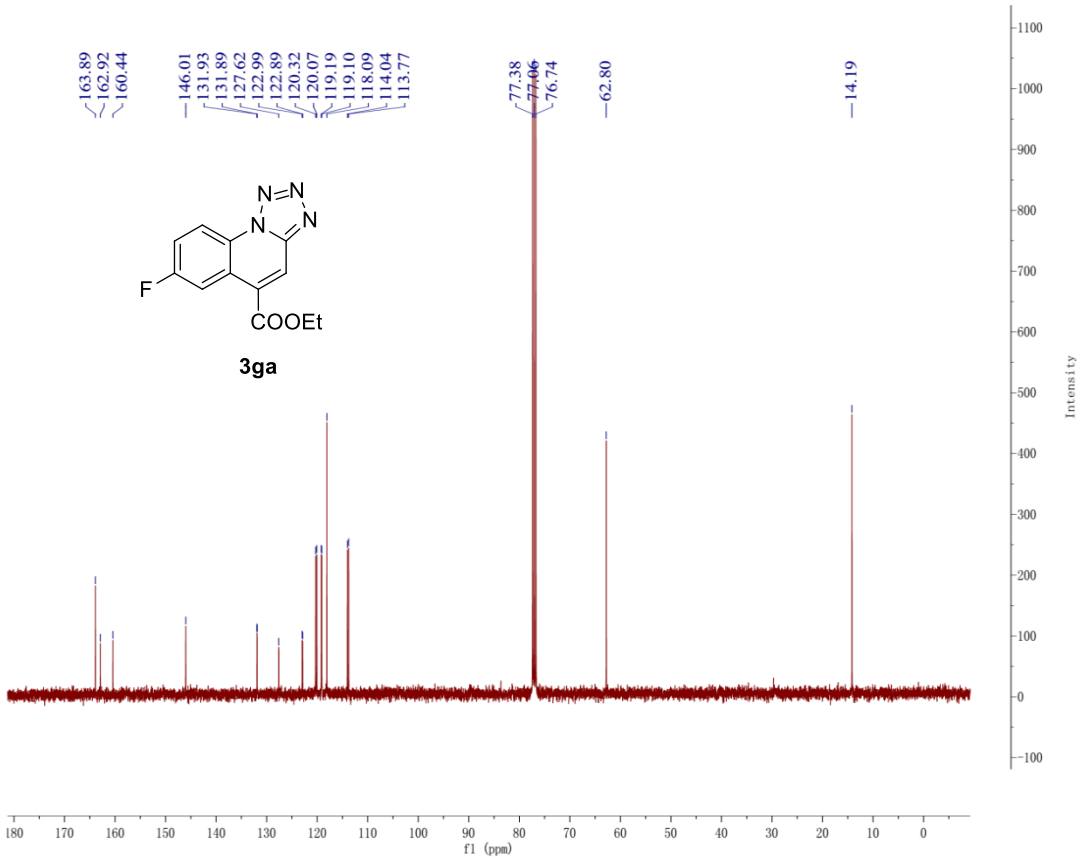


Ethyl 7-fluorotetrazolo[1,5-a]quinoline-5-carboxylate (3ga)

^{1}H NMR (400 MHz, $CDCl_3$)

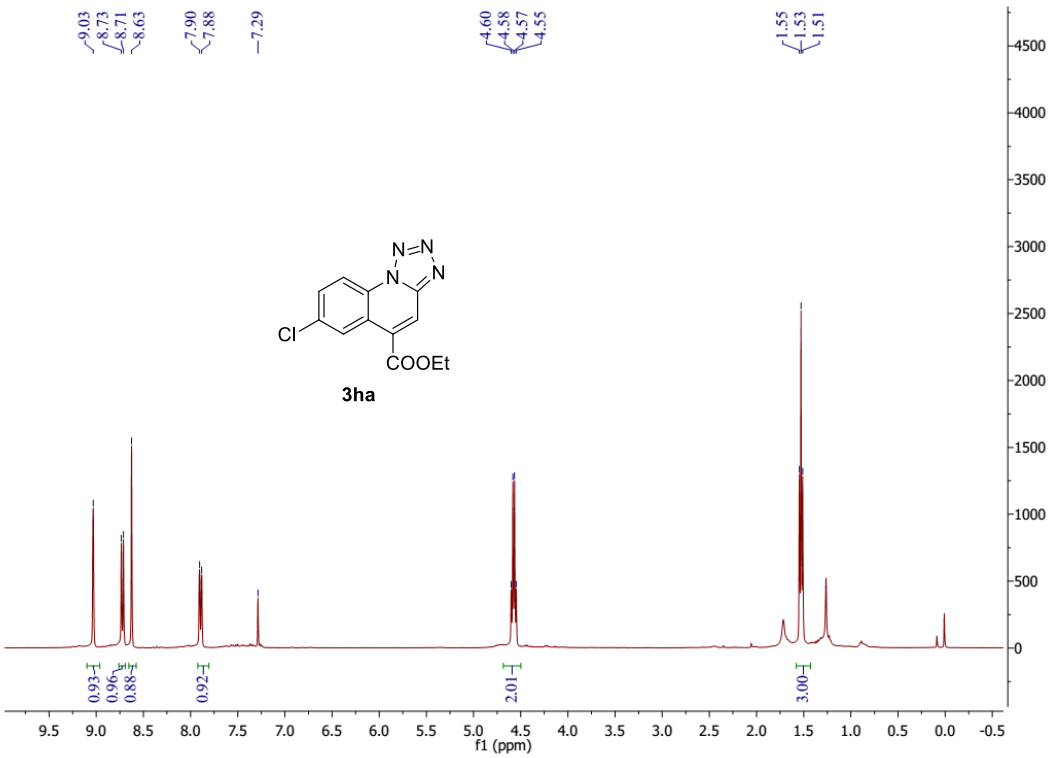


^{13}C NMR (100 MHz, $CDCl_3$)

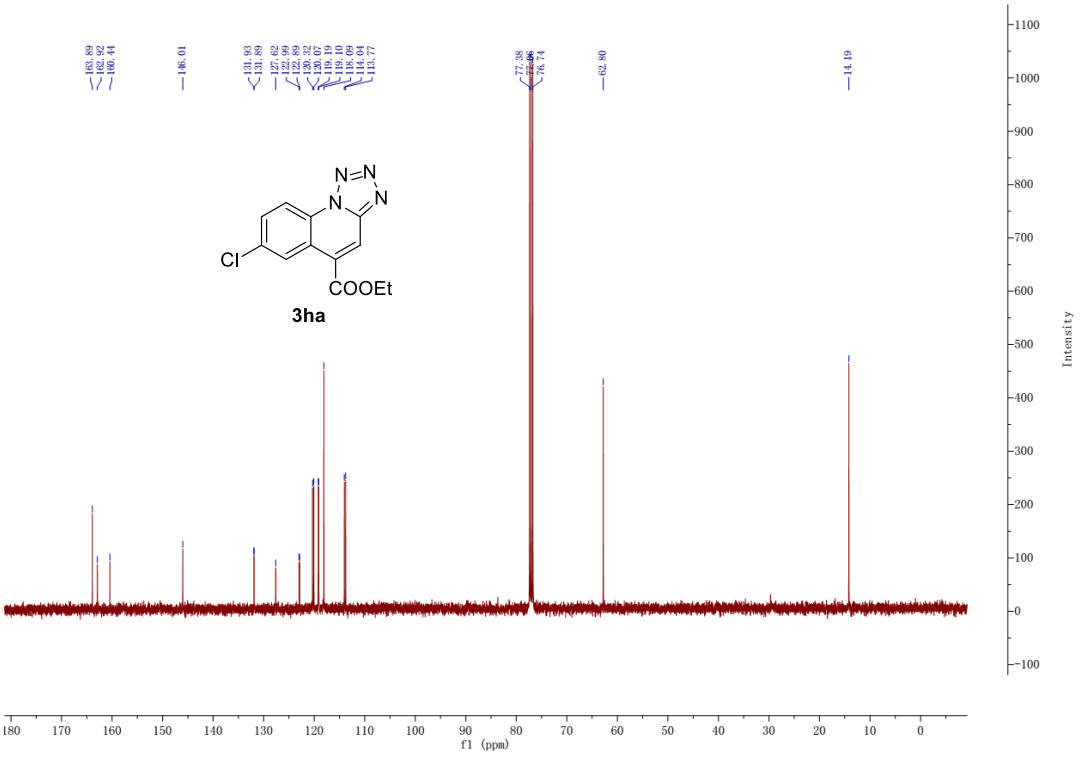


Ethyl 7-chlorotetrazolo[1,5-a]quinoline-5-carboxylate (3ha)

^{1}H NMR (400 MHz, $CDCl_3$)

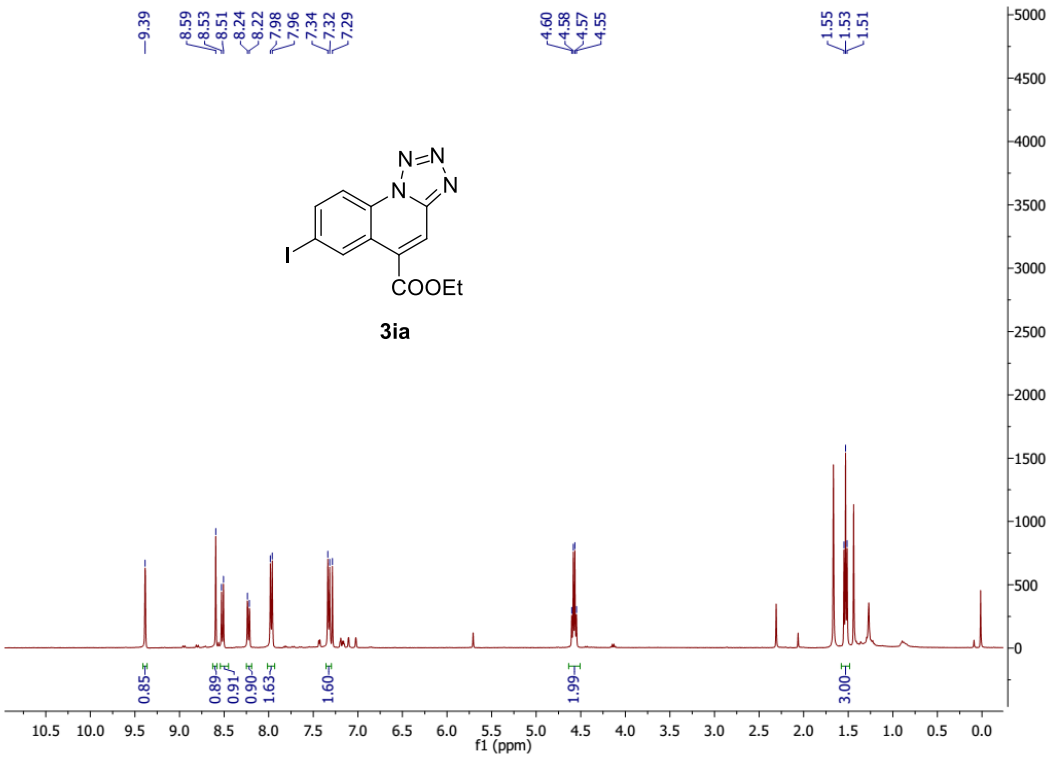


^{13}C NMR (100 MHz, $CDCl_3$)

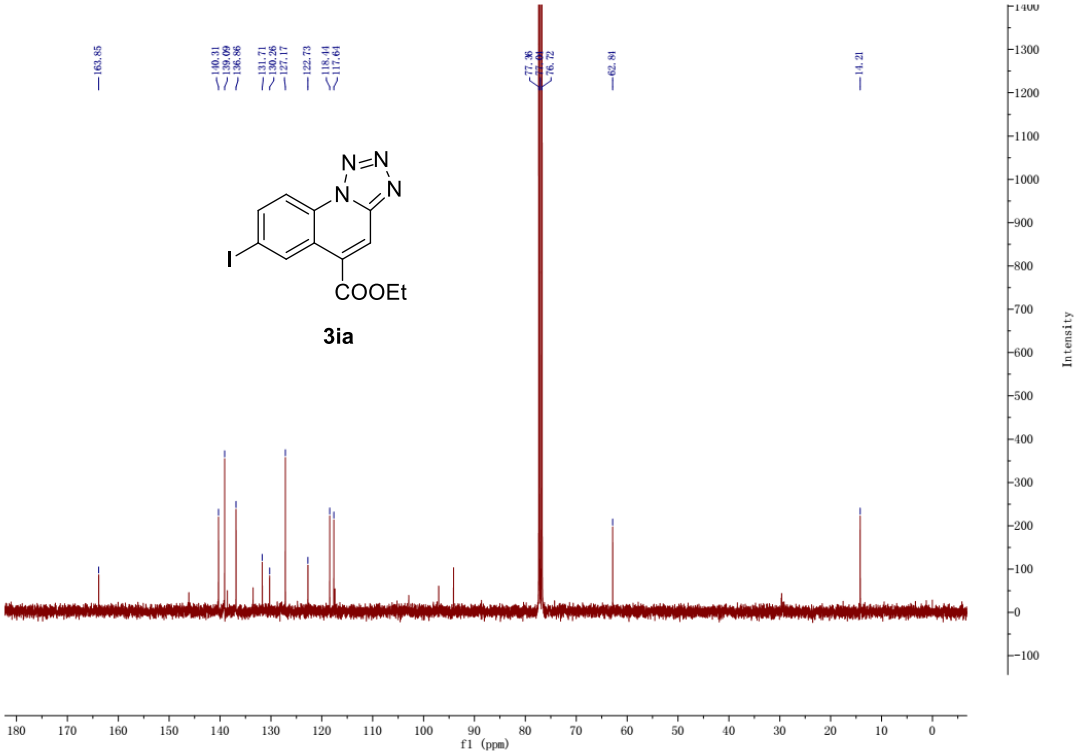


Ethyl 7-iodotetrazolo[1,5-a]quinoline-5-carboxylate (3ia)

^{1}H NMR (400 MHz, $CDCl_3$)

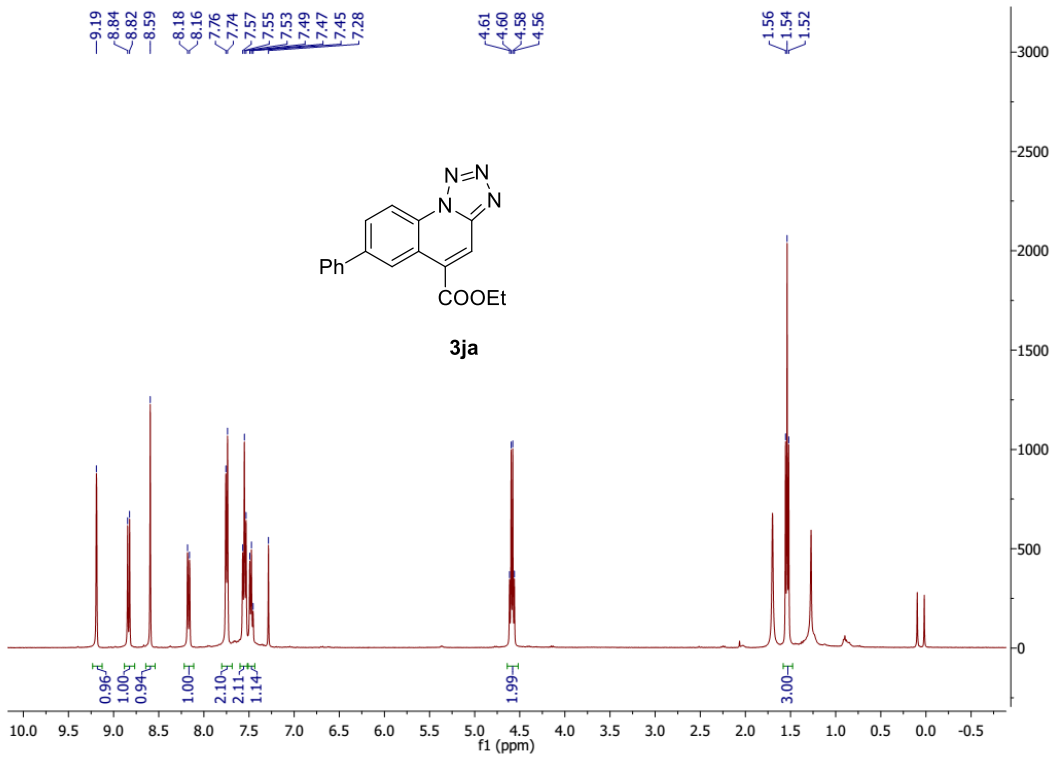


^{13}C NMR (100 MHz, $CDCl_3$)

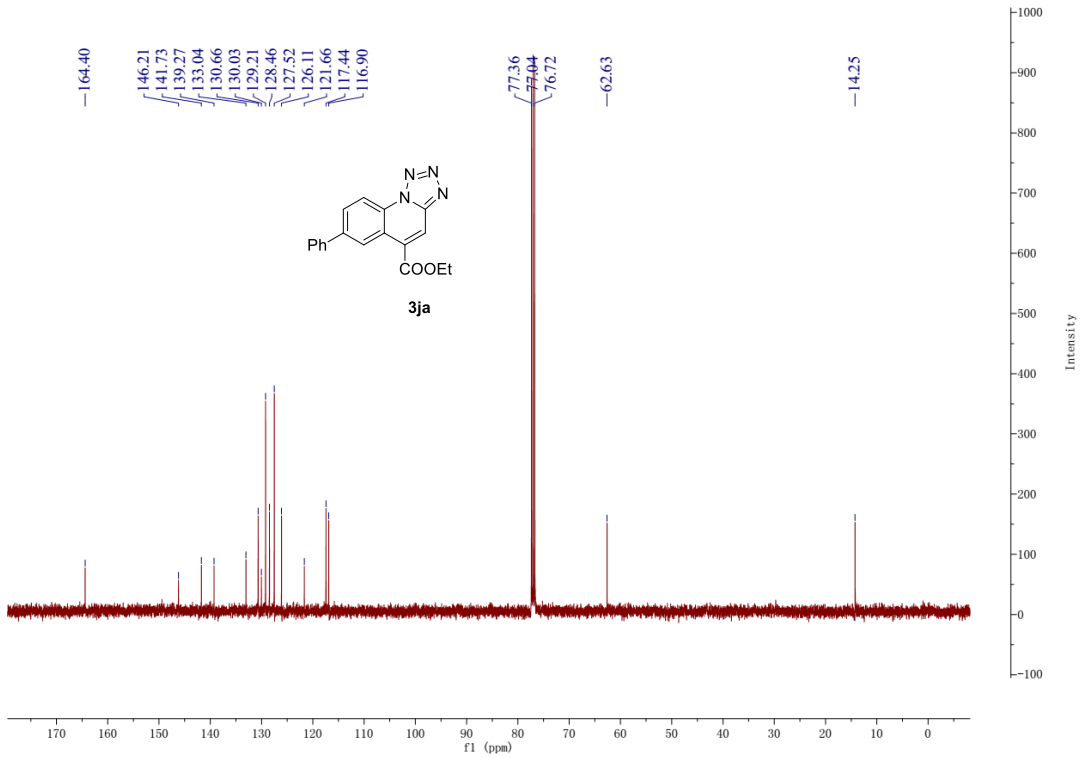


Ethyl 7-phenyltetrazolo[1,5-a]quinoline-5-carboxylate (3ja)

^{1}H NMR (400 MHz, $CDCl_3$)

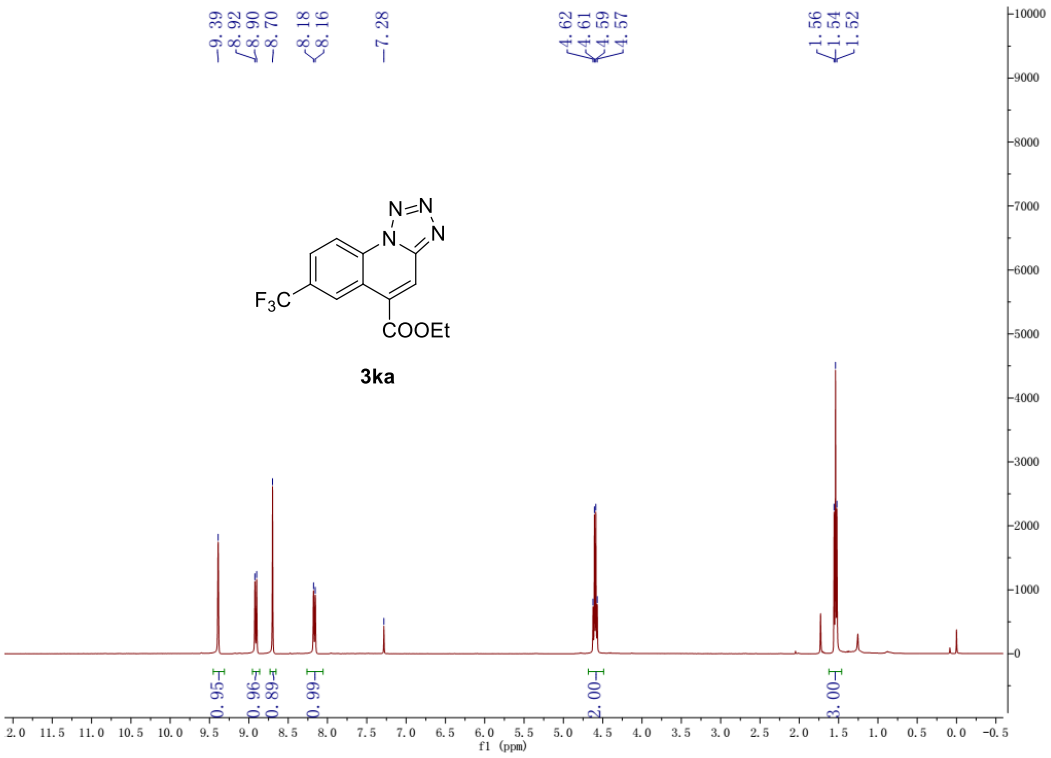


^{13}C NMR (100 MHz, $CDCl_3$)

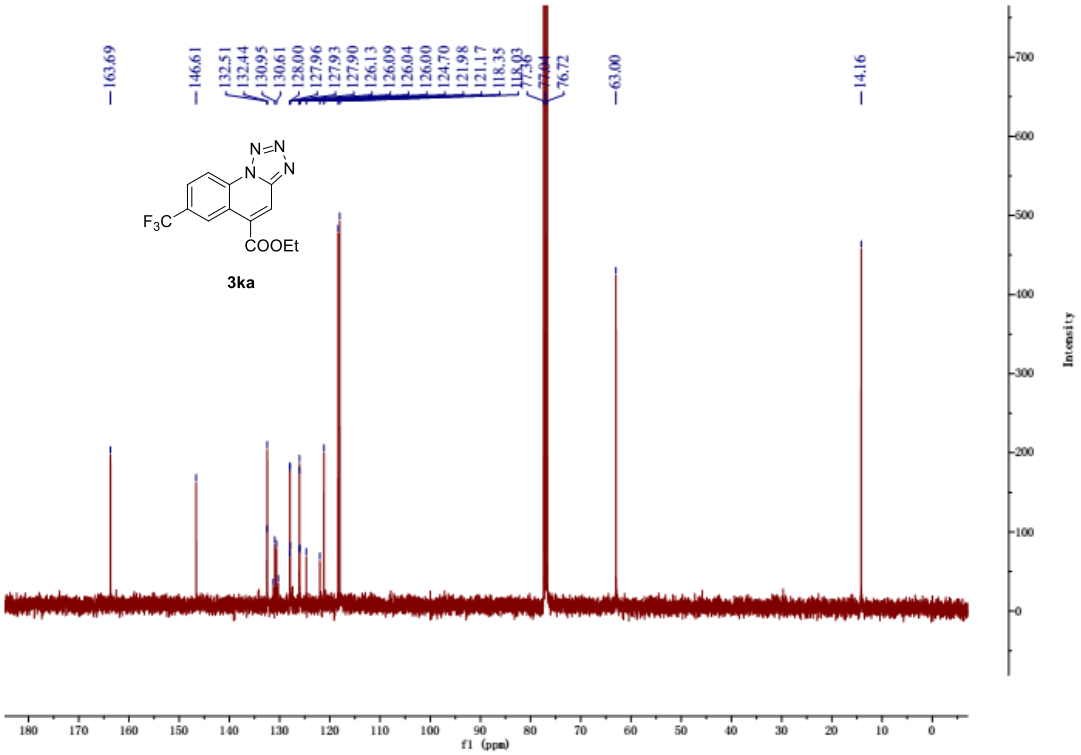


Ethyl 7-(trifluoromethyl)tetrazolo[1,5-a]quinoline-5-carboxylate (3ka)

^{1}H NMR (400 MHz, $CDCl_3$)

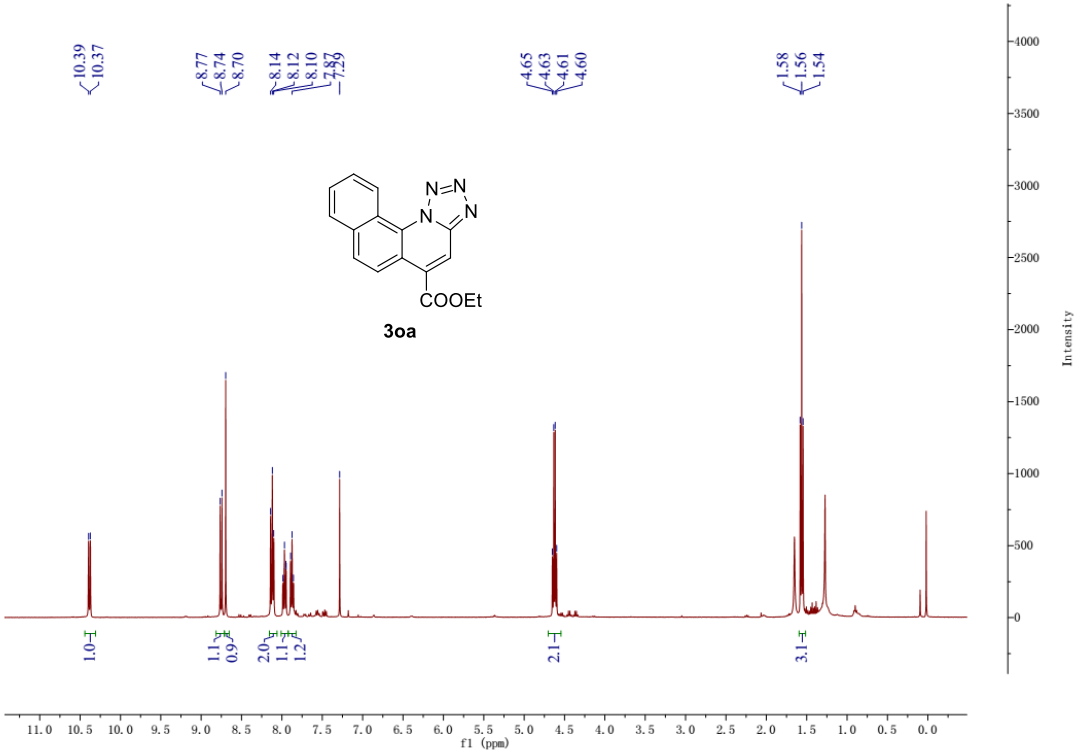


^{13}C NMR (100 MHz, $CDCl_3$)

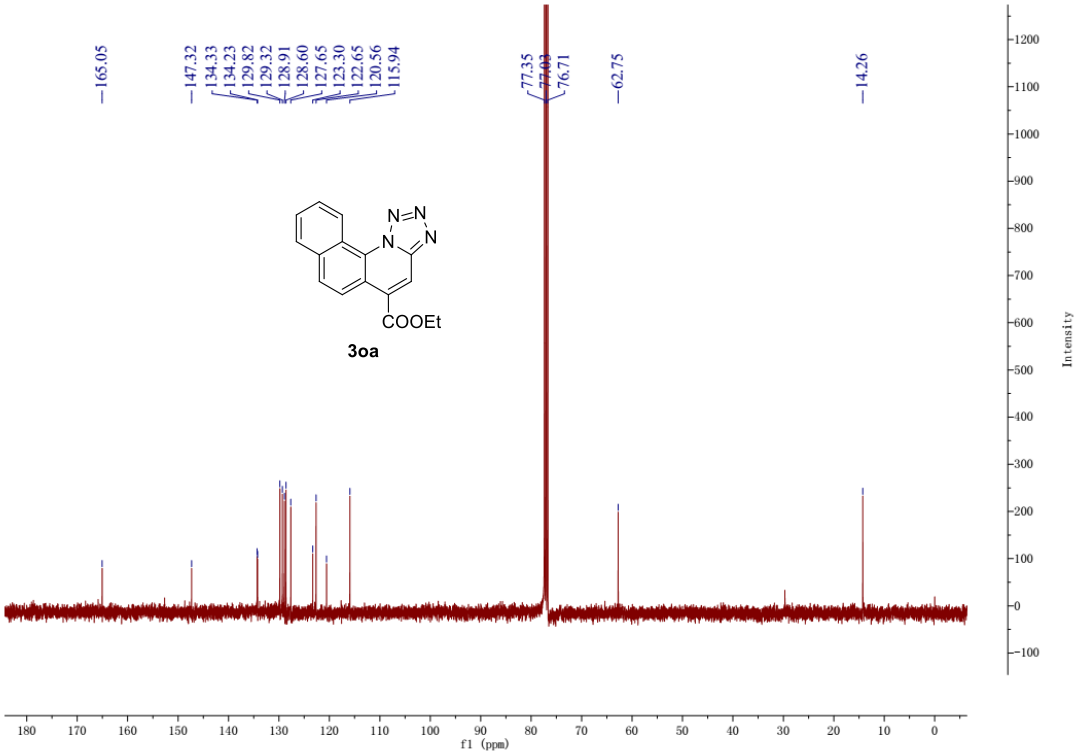


Ethyl benzo[h]tetrazolo[1,5-a]quinoline-5-carboxylate (3oa)

^{1}H NMR (400 MHz, $CDCl_3$)

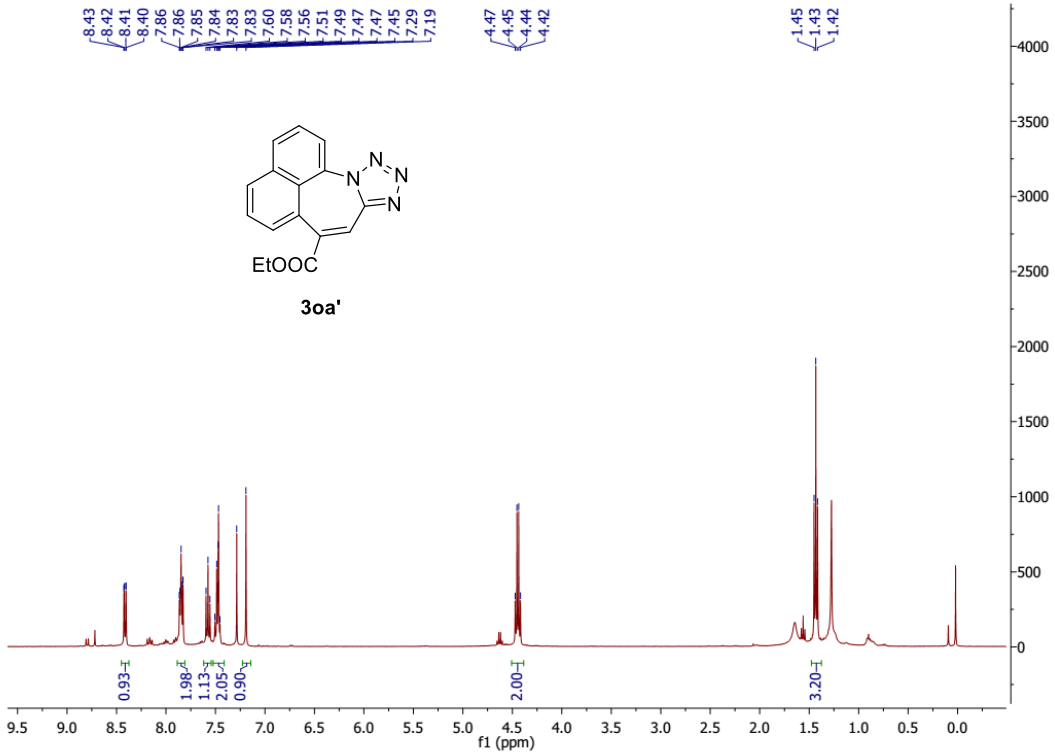


^{13}C NMR (100 MHz, $CDCl_3$)

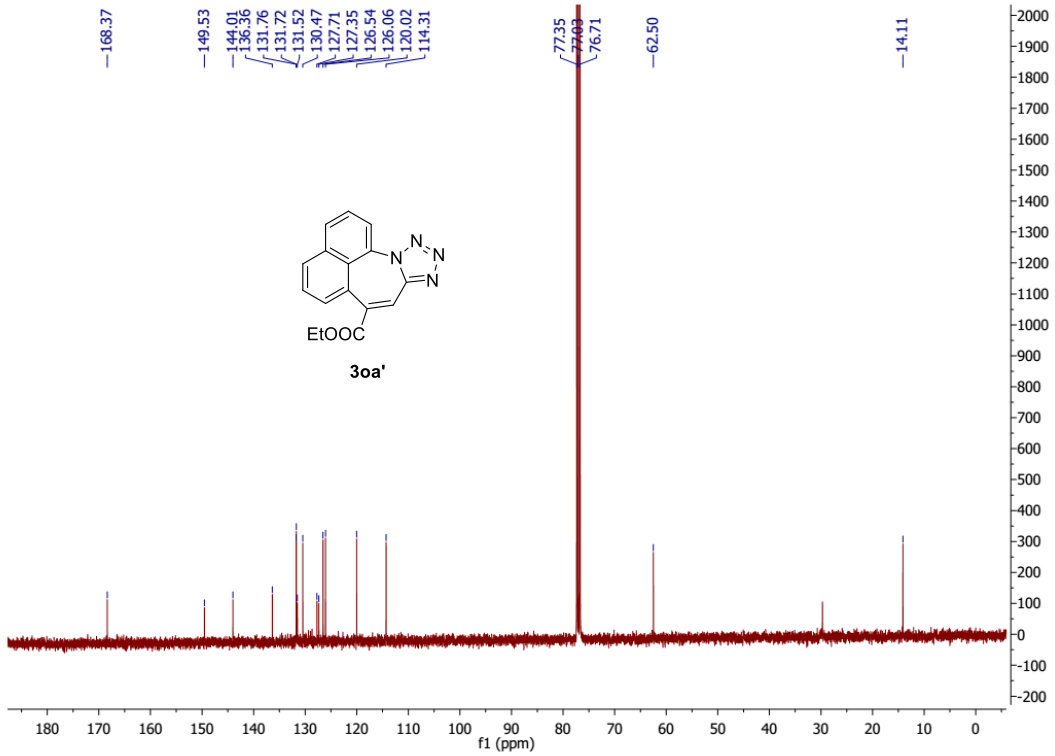


Ethyl naphtho[1,8-ef]tetrazolo[1,5-a]azepine-11-carboxylate (3oa')

^{1}H NMR (400 MHz, $CDCl_3$)

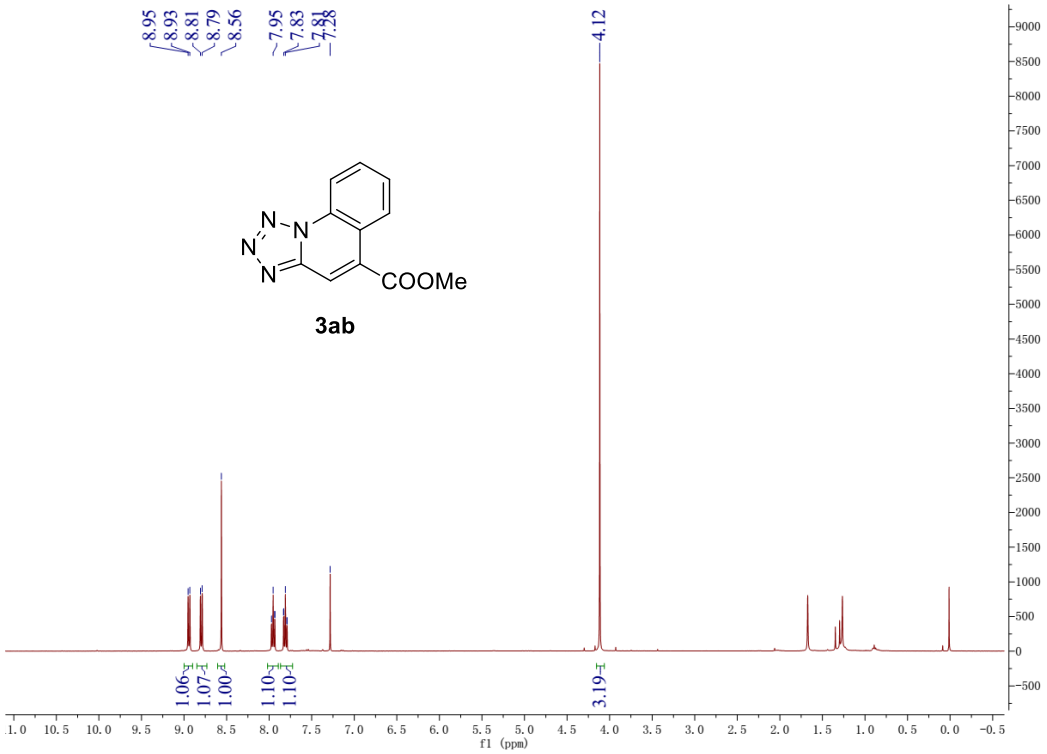


^{13}C NMR (100 MHz, $CDCl_3$)

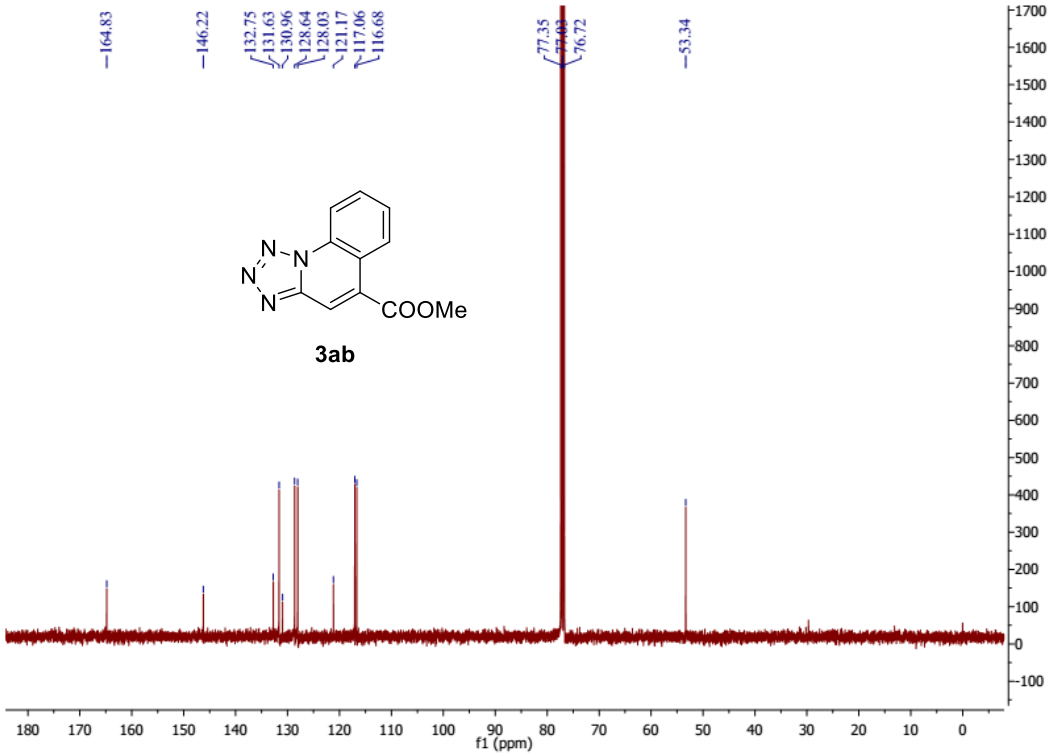


Methyl tetrazolo[1,5-a]quinoline-5-carboxylate (3ab)

^{1}H NMR (400 MHz, $CDCl_3$)

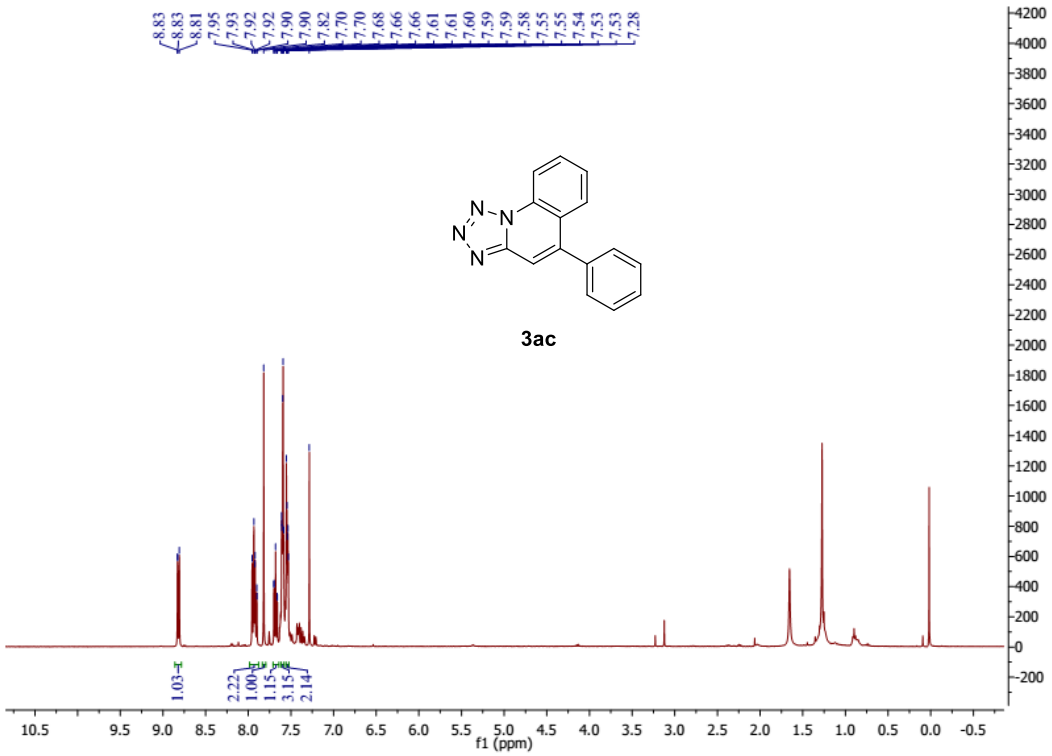


^{13}C NMR (100 MHz, $CDCl_3$)

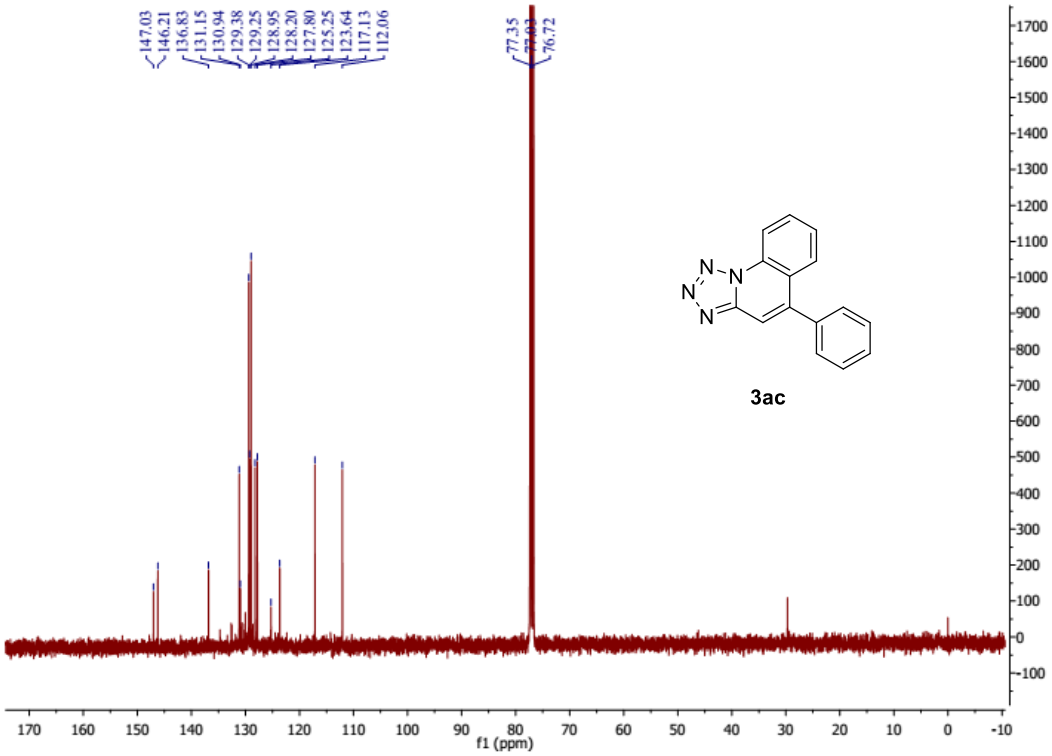


5-phenyltetrazolo[1,5-a]quinoline (3ac)

^{1}H NMR (400 MHz, $CDCl_3$)

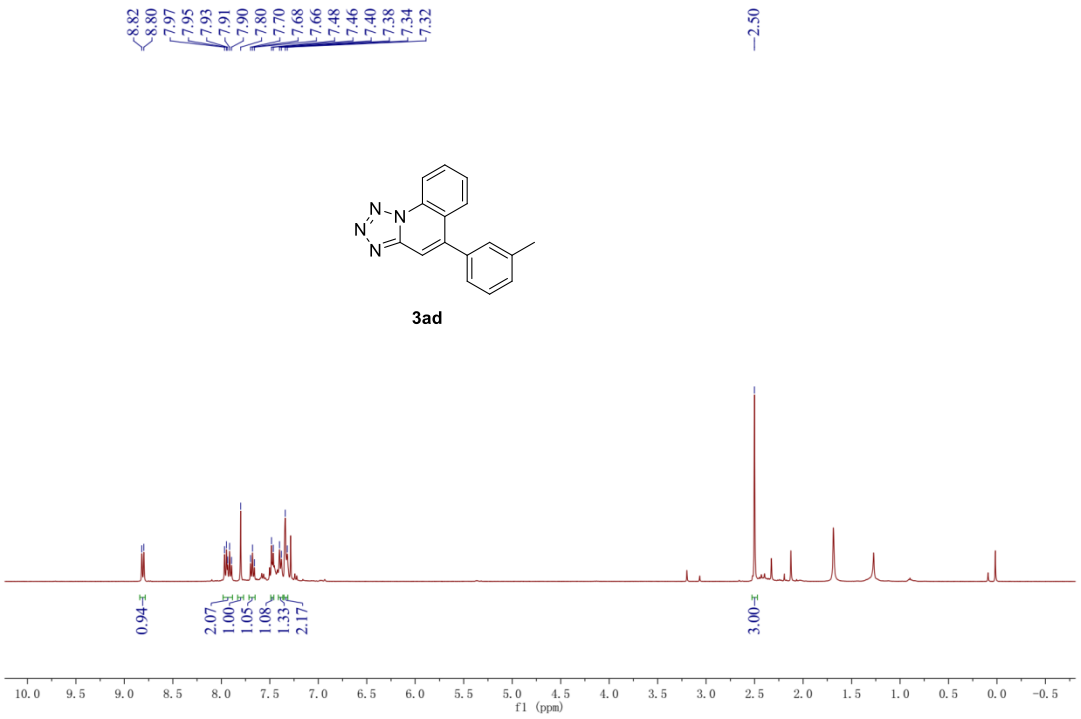


^{13}C NMR (100 MHz, $CDCl_3$)

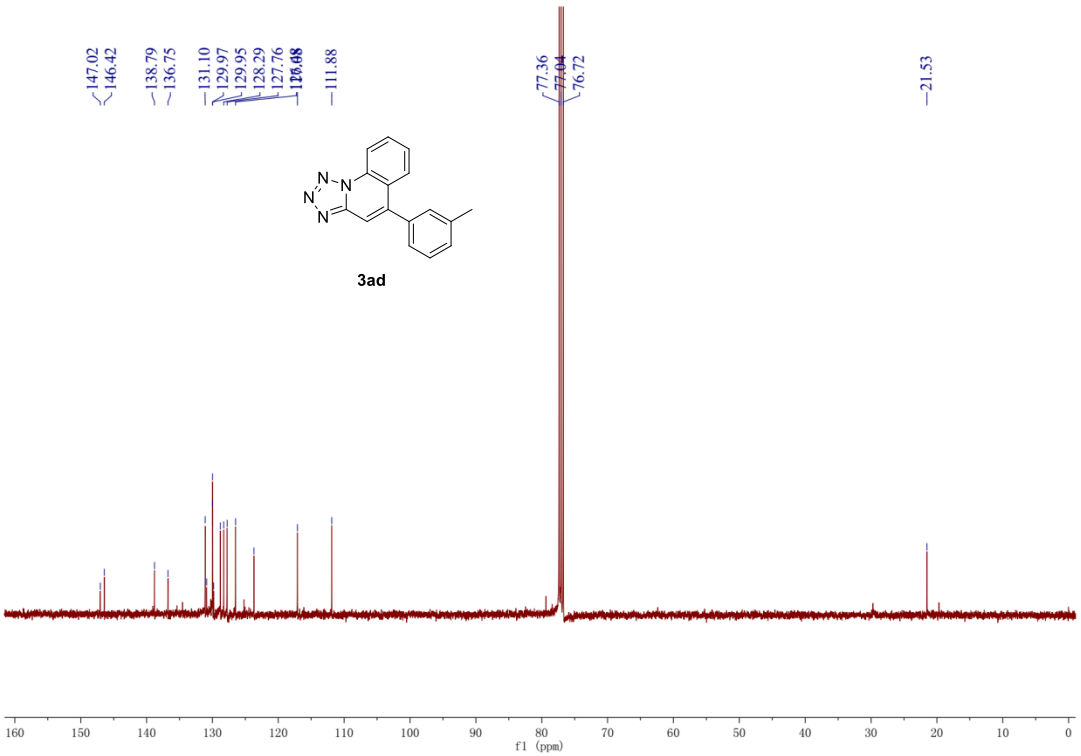


5-(m-tolyl)tetrazolo[1,5-a]quinoline(3ad)

^{1}H NMR (400 MHz, $CDCl_3$)

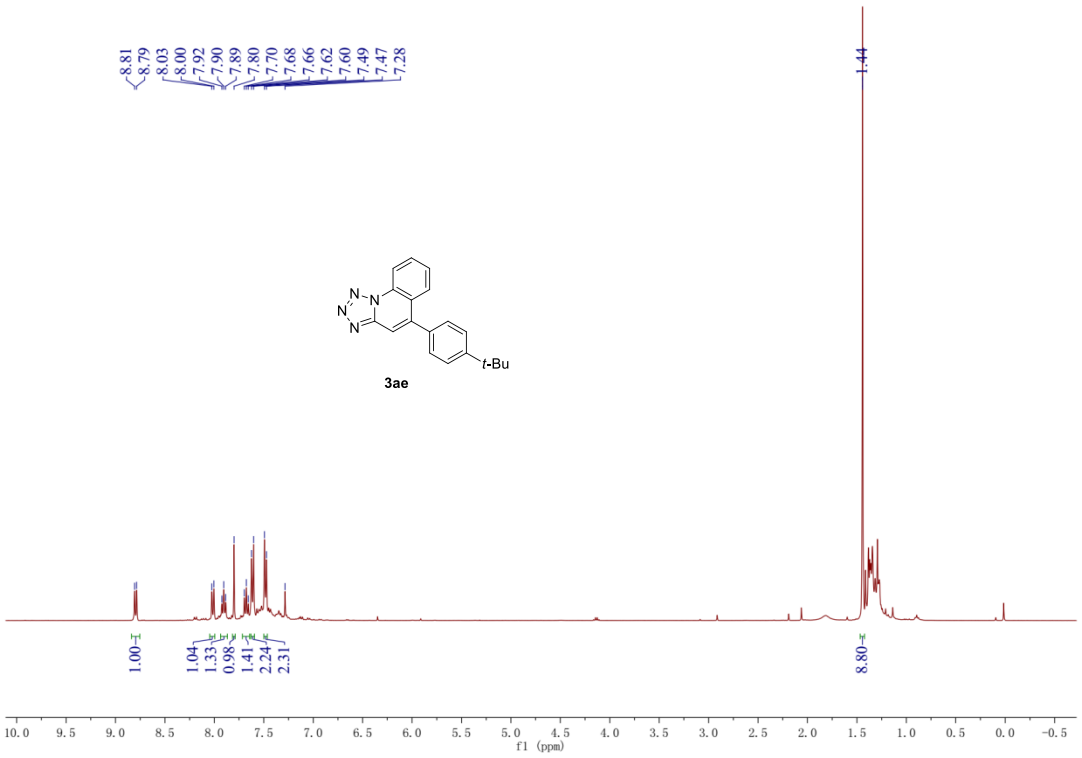


^{13}C NMR (100 MHz, $CDCl_3$)

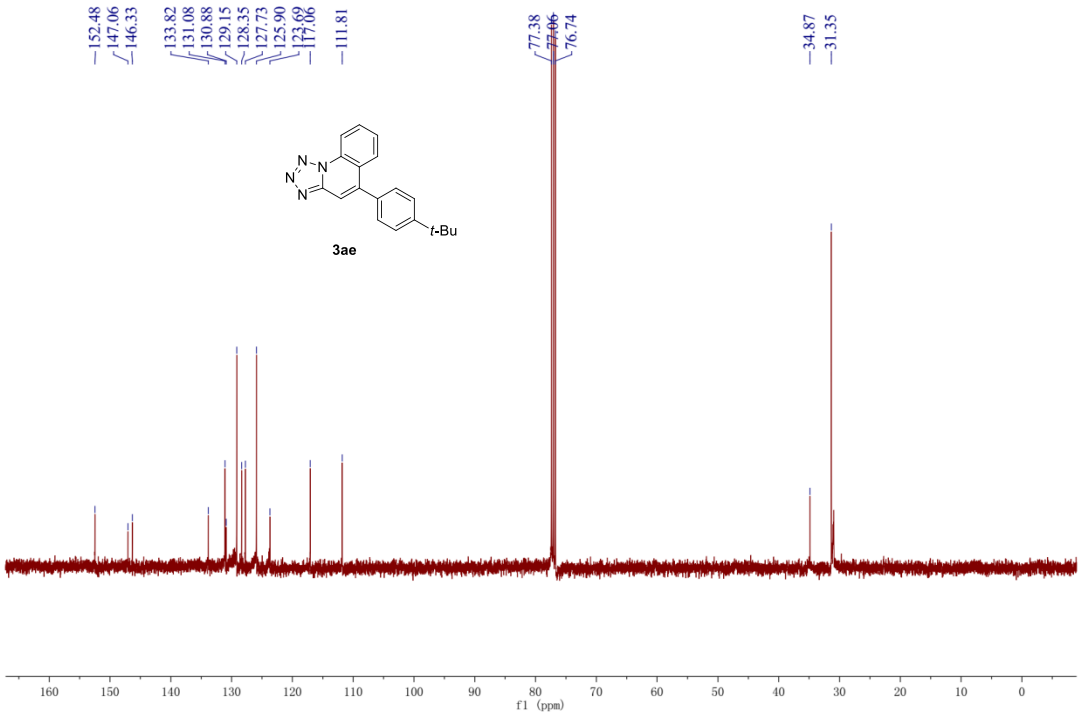


5-(4-(tert-butyl)phenyl)tetrazolo[1,5-a]quinoline(3ae)

^{1}H NMR (400 MHz, $CDCl_3$)

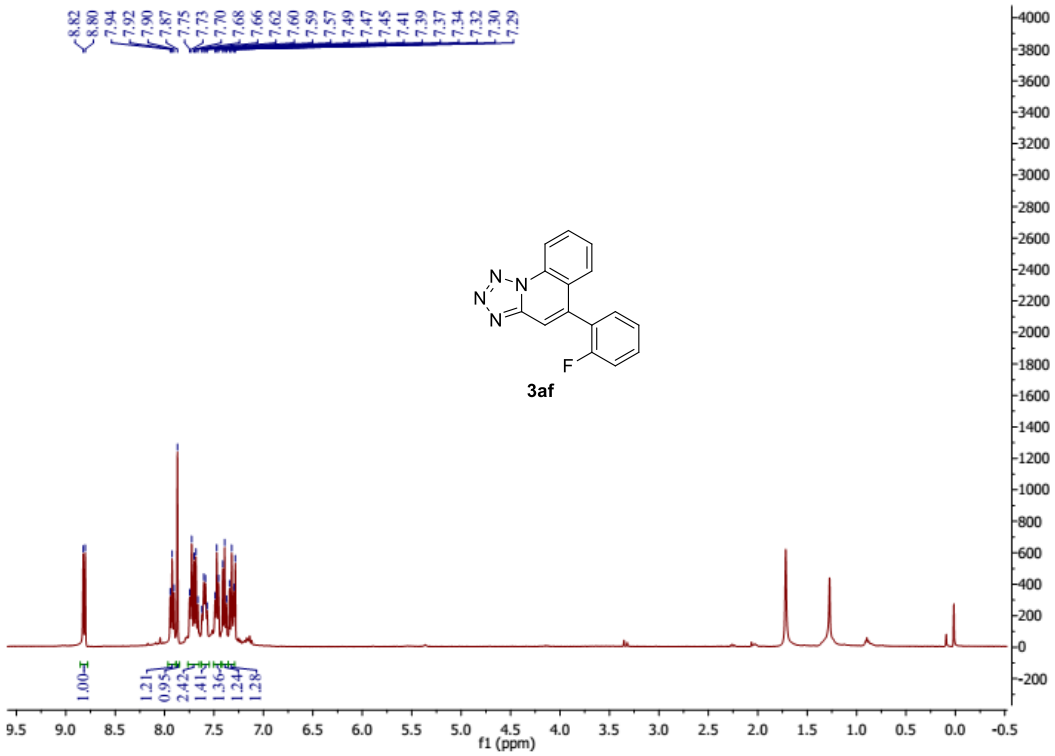


^{13}C NMR (100 MHz, $CDCl_3$)

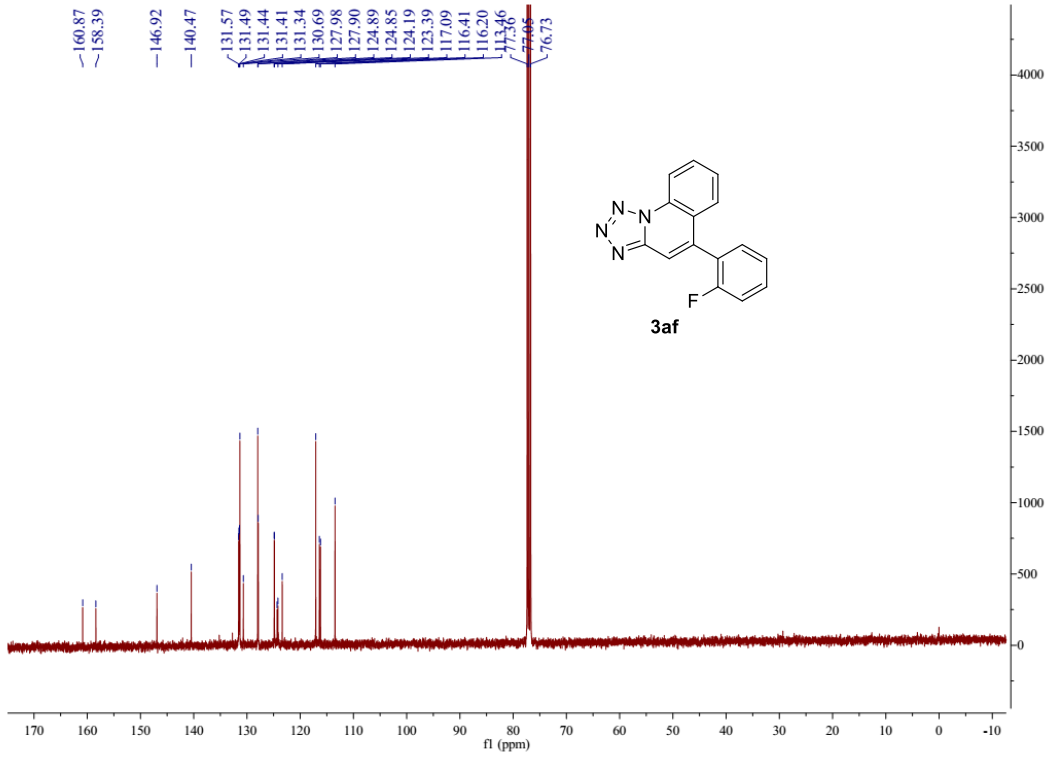


5-(2-fluorophenyl)tetrazolo[1,5-a]quinoline (3af)

^{1}H NMR (400 MHz, $CDCl_3$)

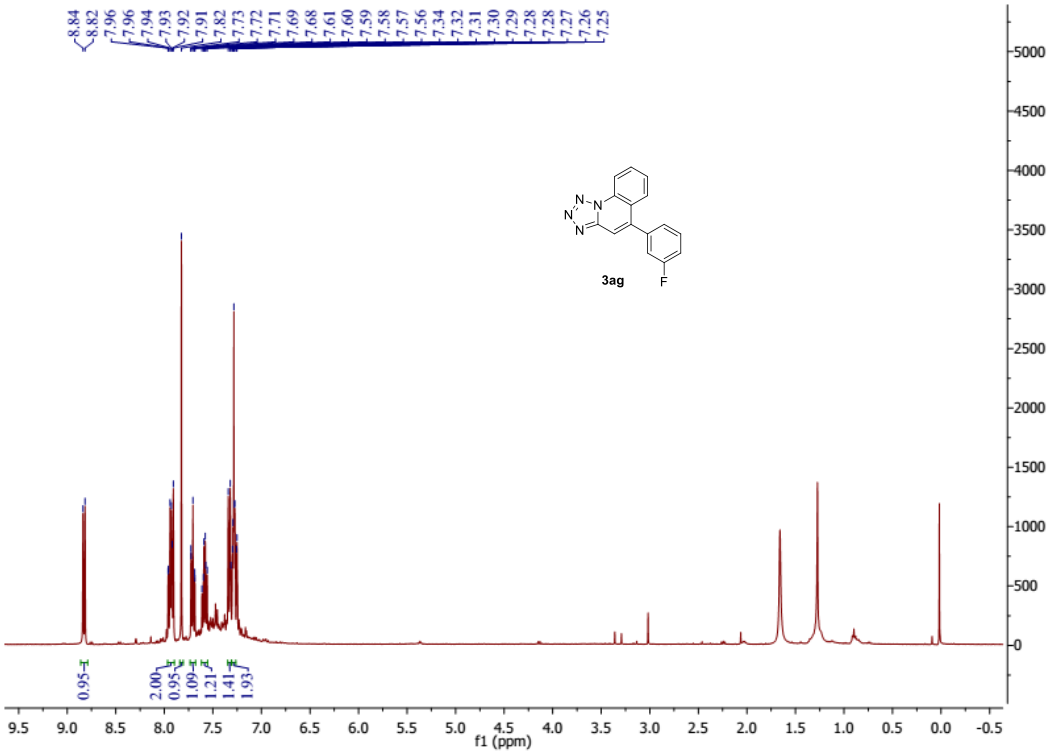


^{13}C NMR (100 MHz, $CDCl_3$)

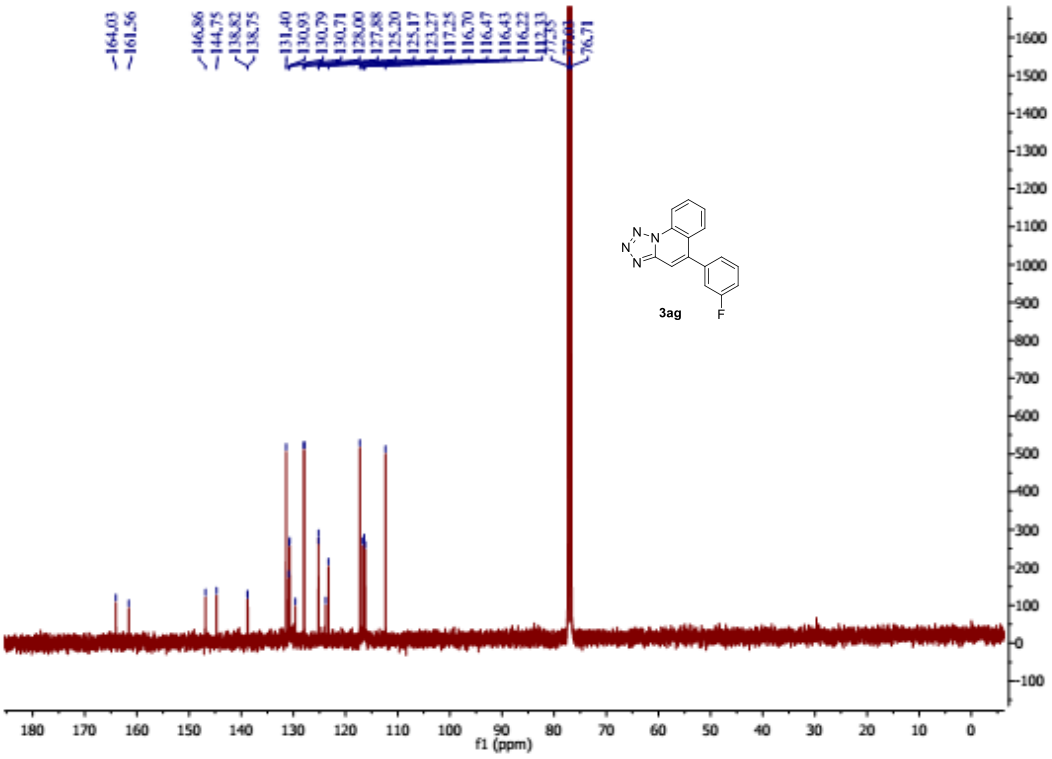


5-(3-fluorophenyl)tetrazolo[1,5-a]quinoline (3ag)

^{1}H NMR (400 MHz, $CDCl_3$)

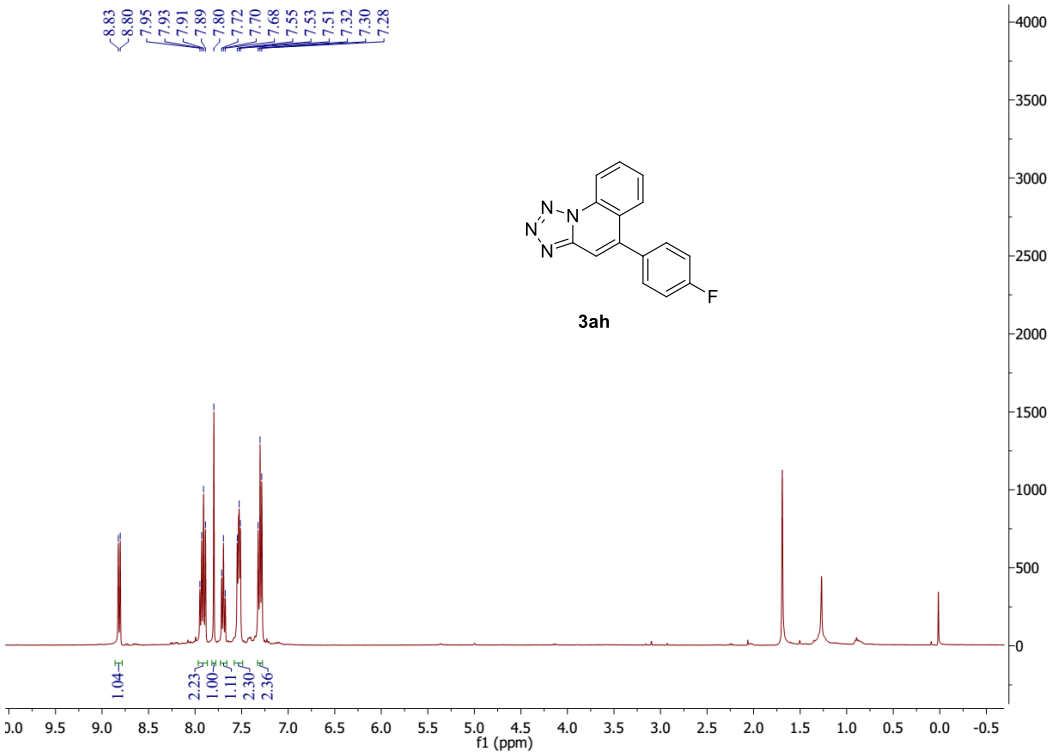


^{13}C NMR (100 MHz, $CDCl_3$)

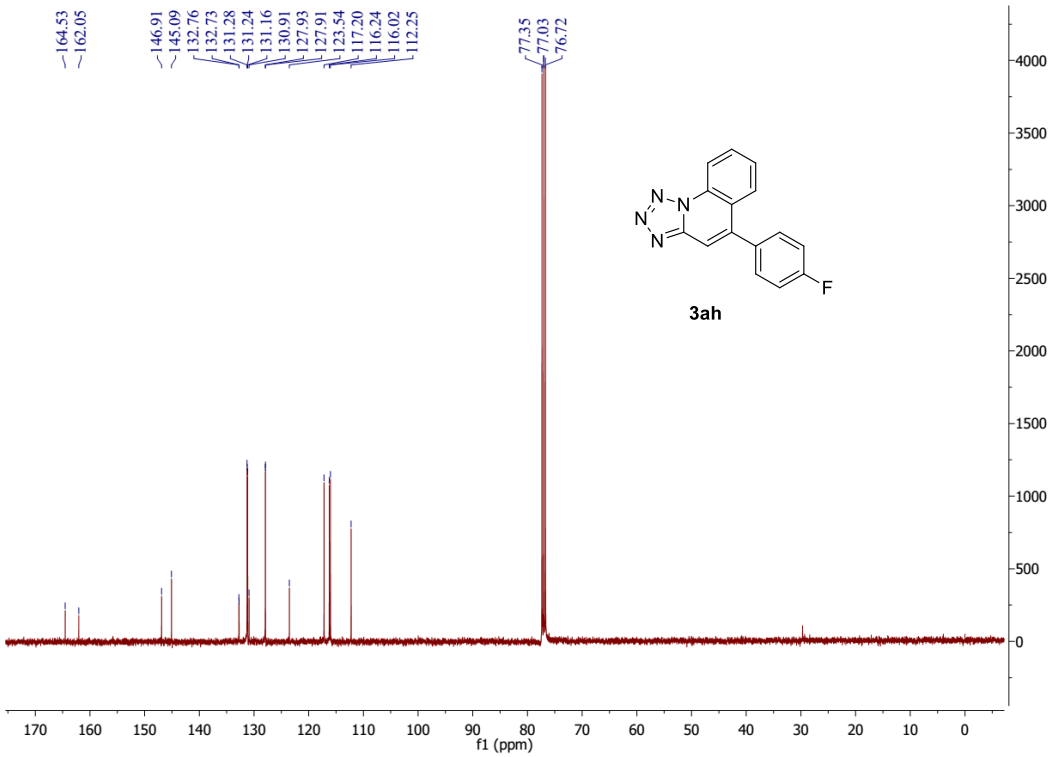


5-(4-fluorophenyl)tetrazolo[1,5-a]quinoline (3ah)

^{1}H NMR (400 MHz, $CDCl_3$)

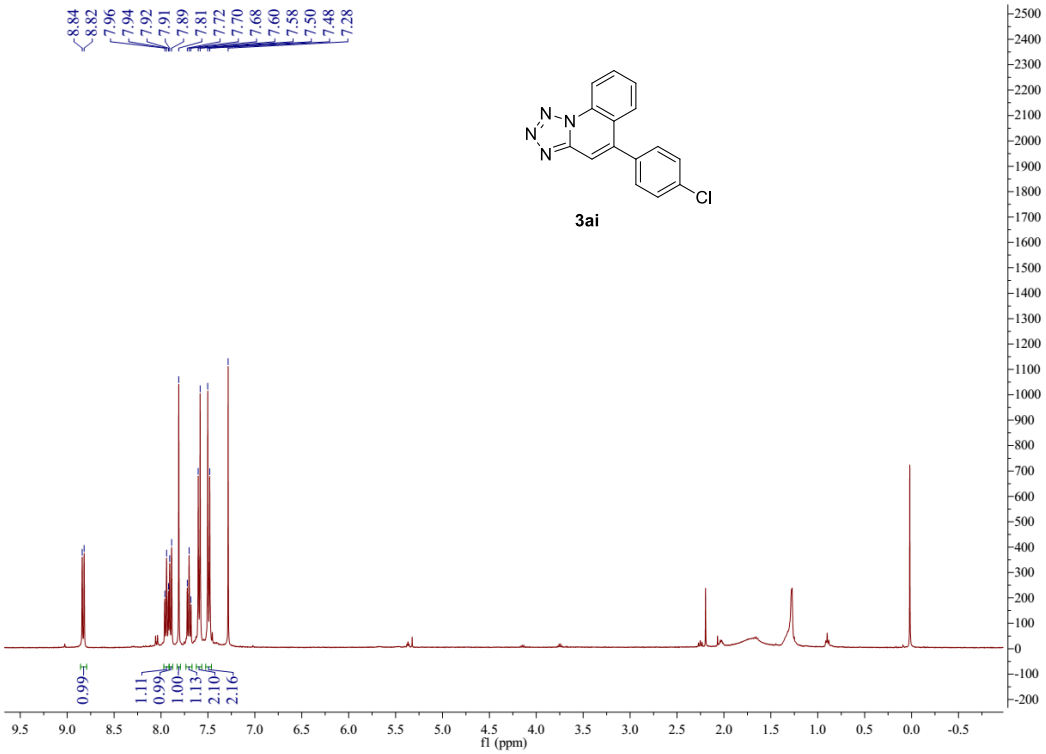


^{13}C NMR (100 MHz, $CDCl_3$)

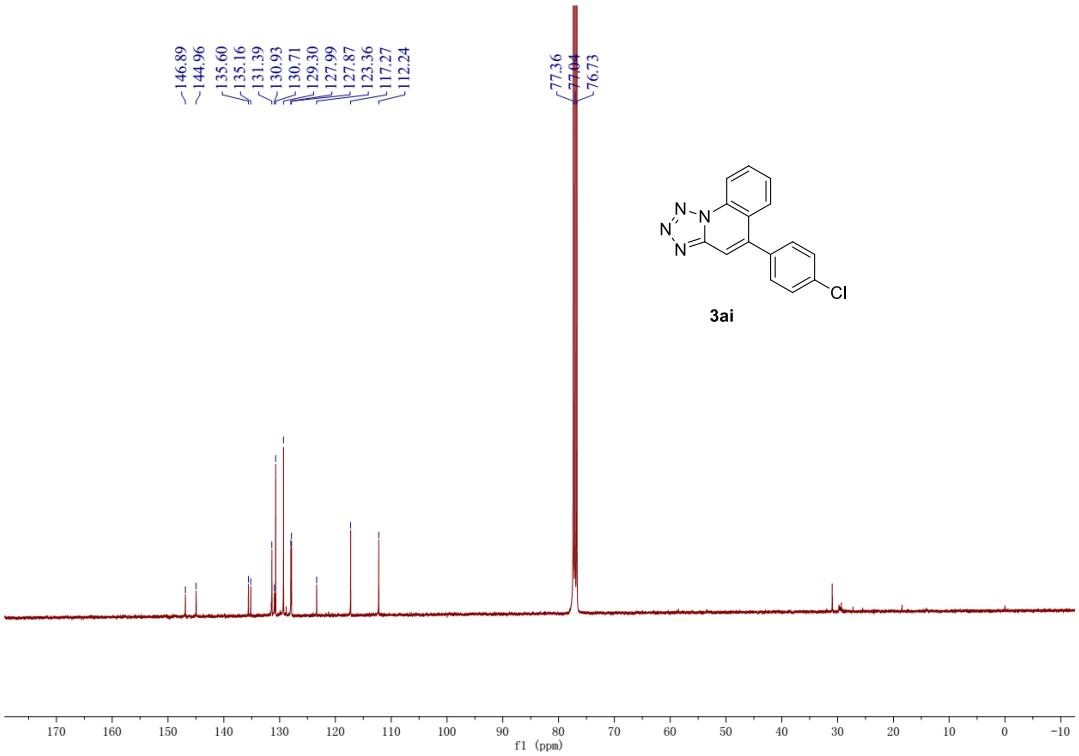


5-(4-chlorophenyl)tetrazolo[1,5-a]quinoline (3ai)

^{1}H NMR (400 MHz, $CDCl_3$)

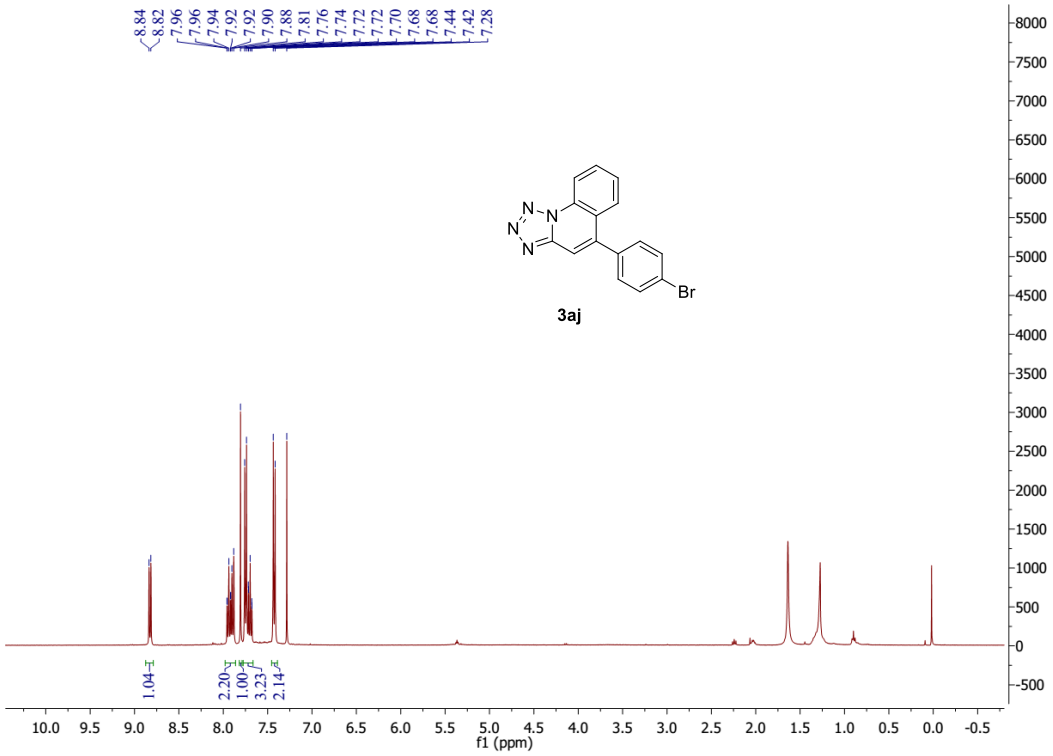


^{13}C NMR (100 MHz, $CDCl_3$)

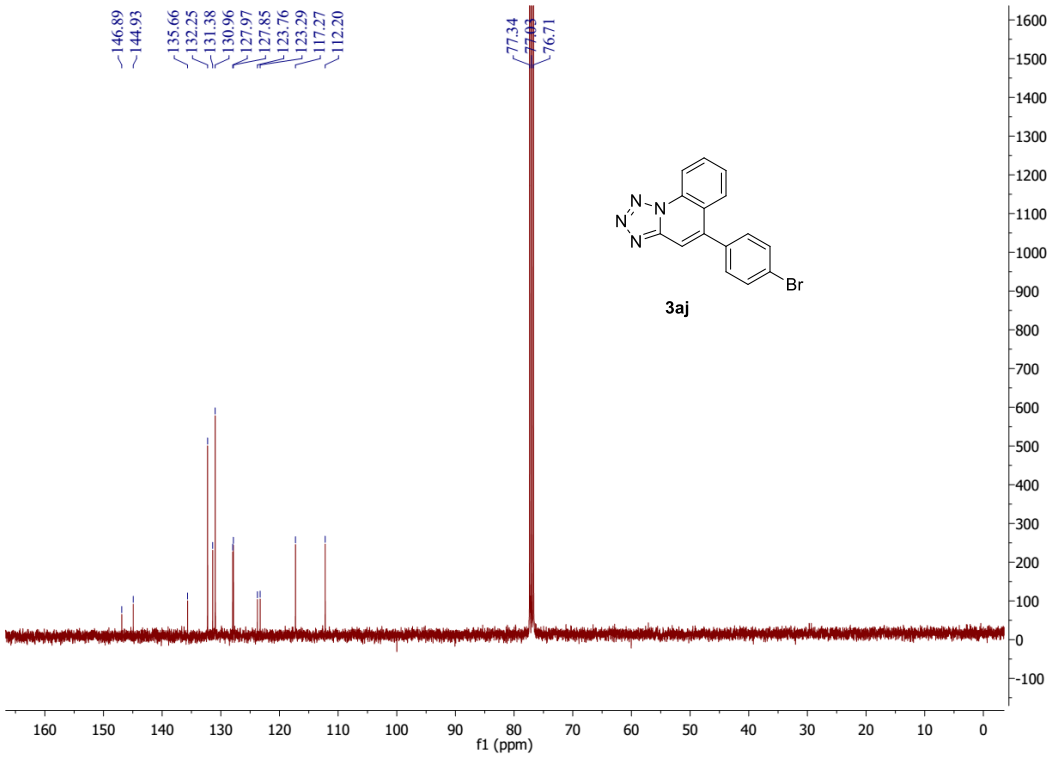


5-(4-bromophenyl)tetrazolo[1,5-a]quinoline (3aj)

^{1}H NMR (400 MHz, $CDCl_3$)

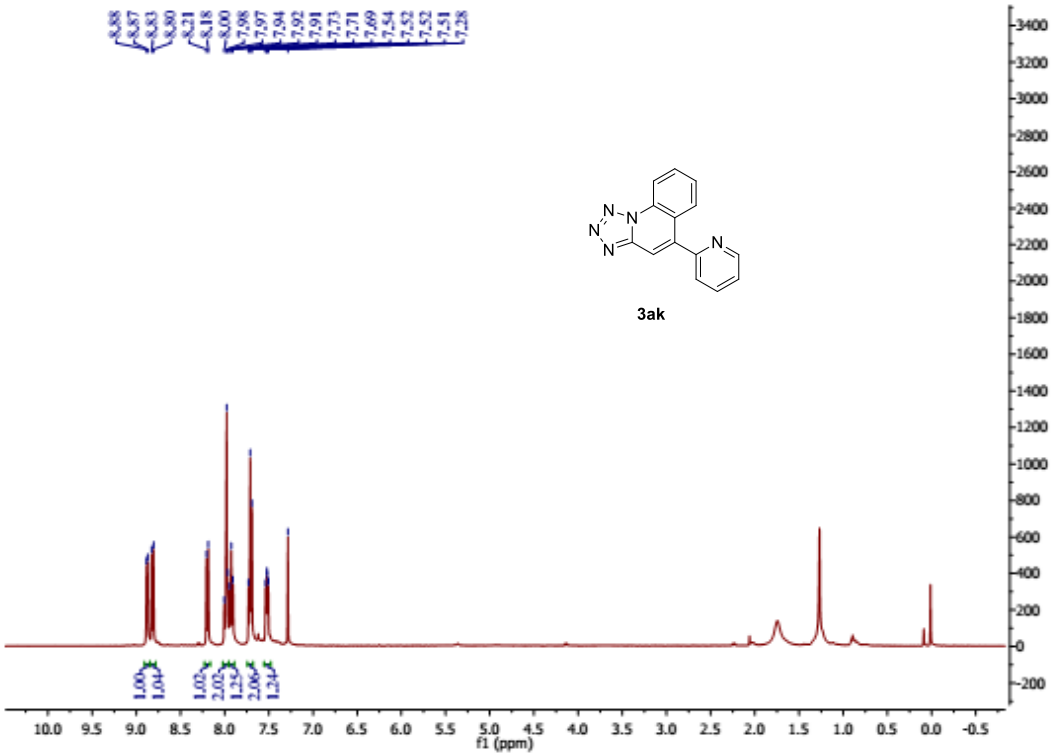


^{13}C NMR (100 MHz, $CDCl_3$)

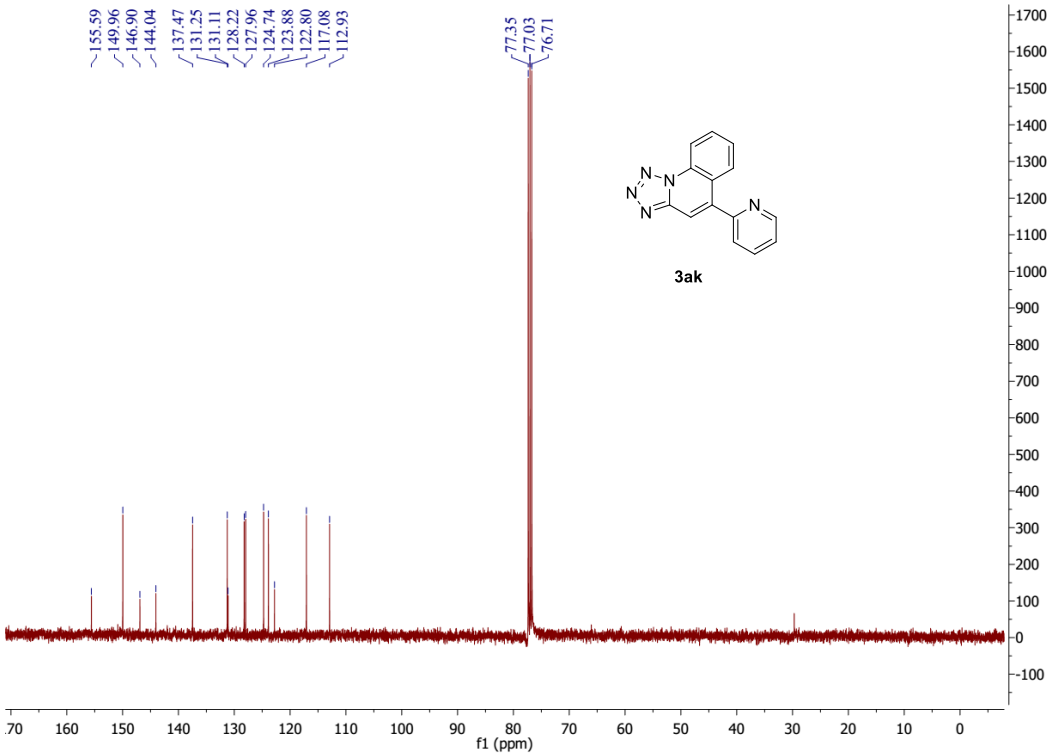


5-(pyridin-2-yl)tetrazolo[1,5-a]quinoline (3ak)

^{1}H NMR (400 MHz, $CDCl_3$)

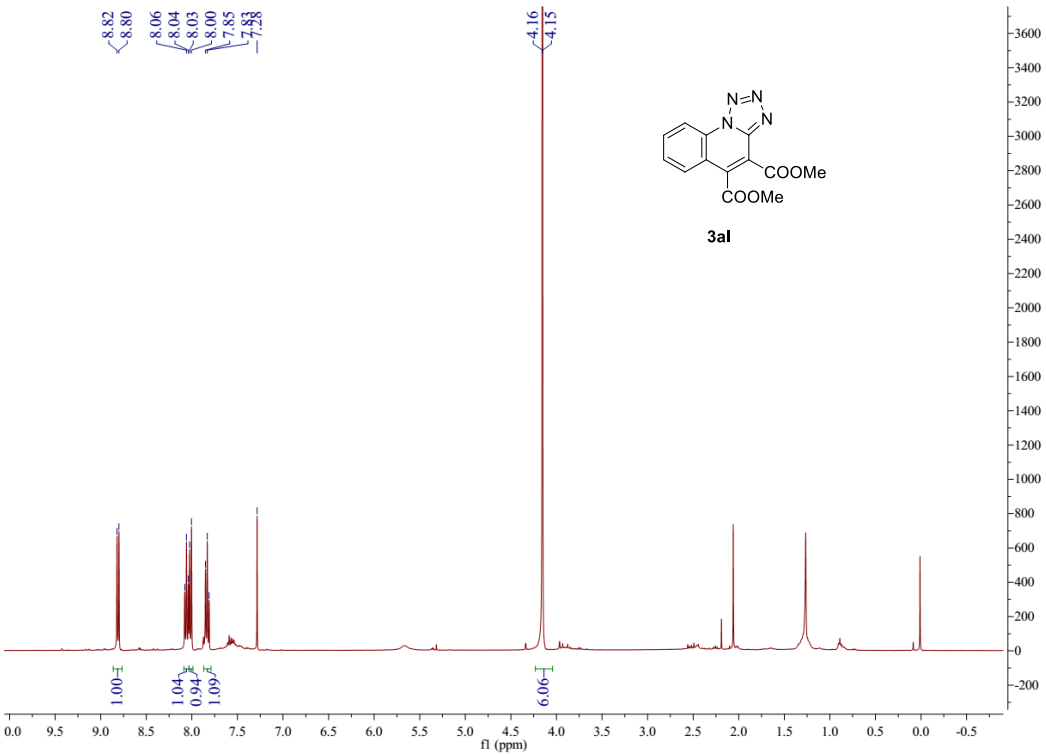


^{13}C NMR (100 MHz, $CDCl_3$)

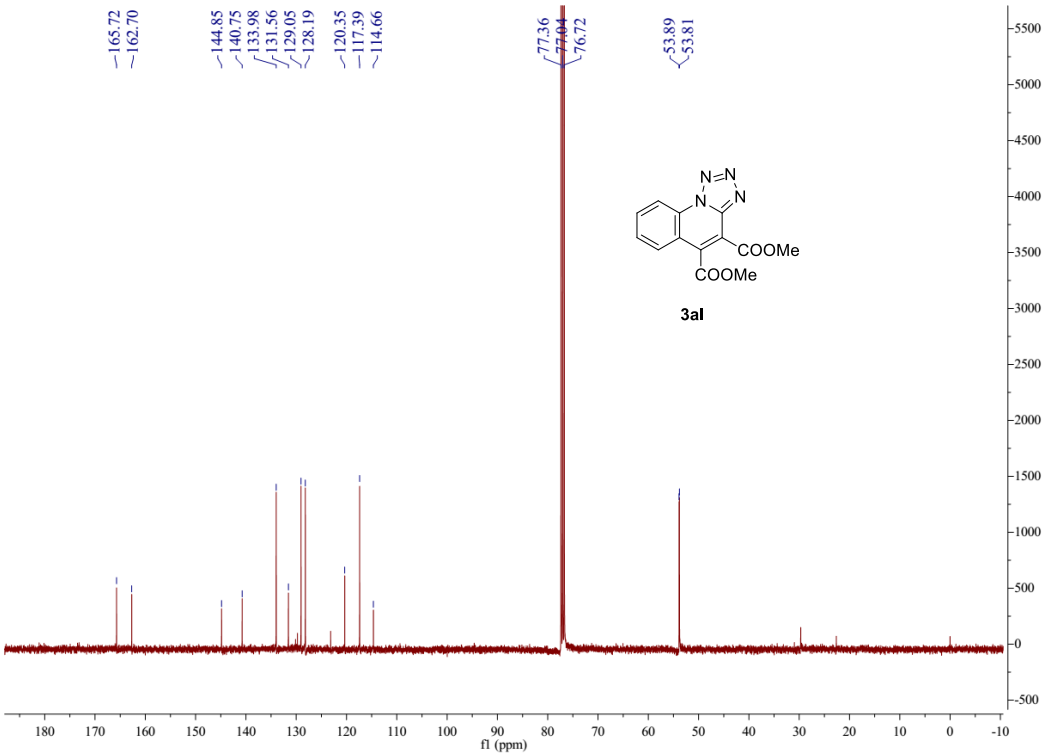


dimethyltetrazolo[1,5-a]quinoline-4,5-dicarboxylate (3al)

^{1}H NMR (400 MHz, $CDCl_3$)

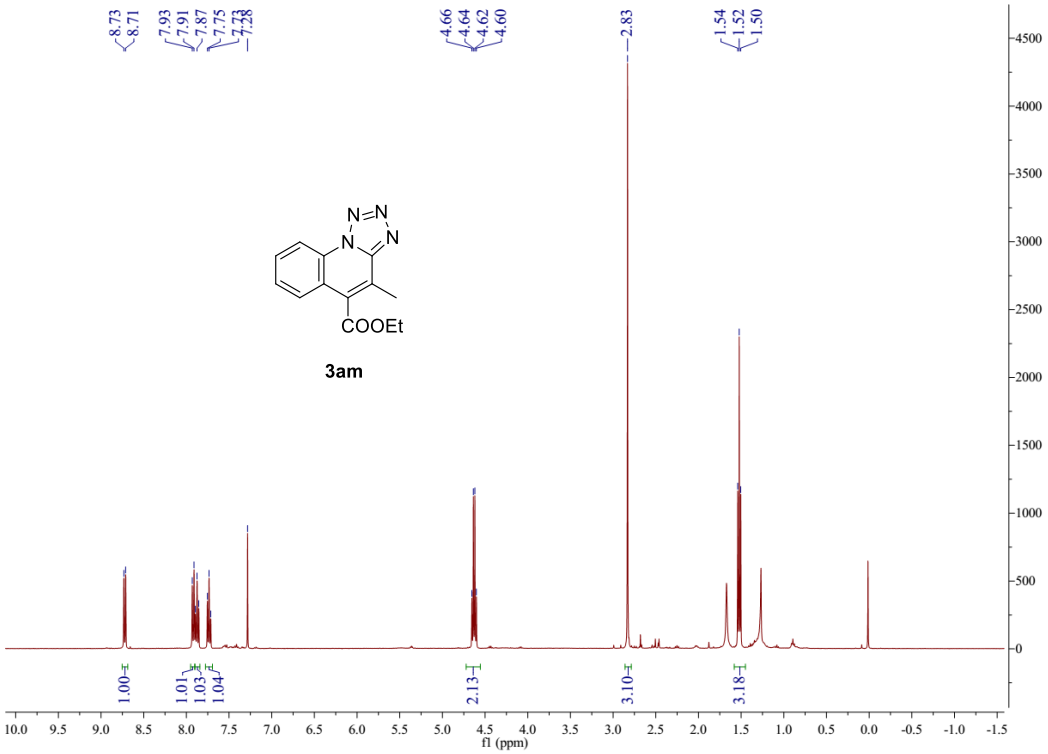


^{13}C NMR (100 MHz, $CDCl_3$)

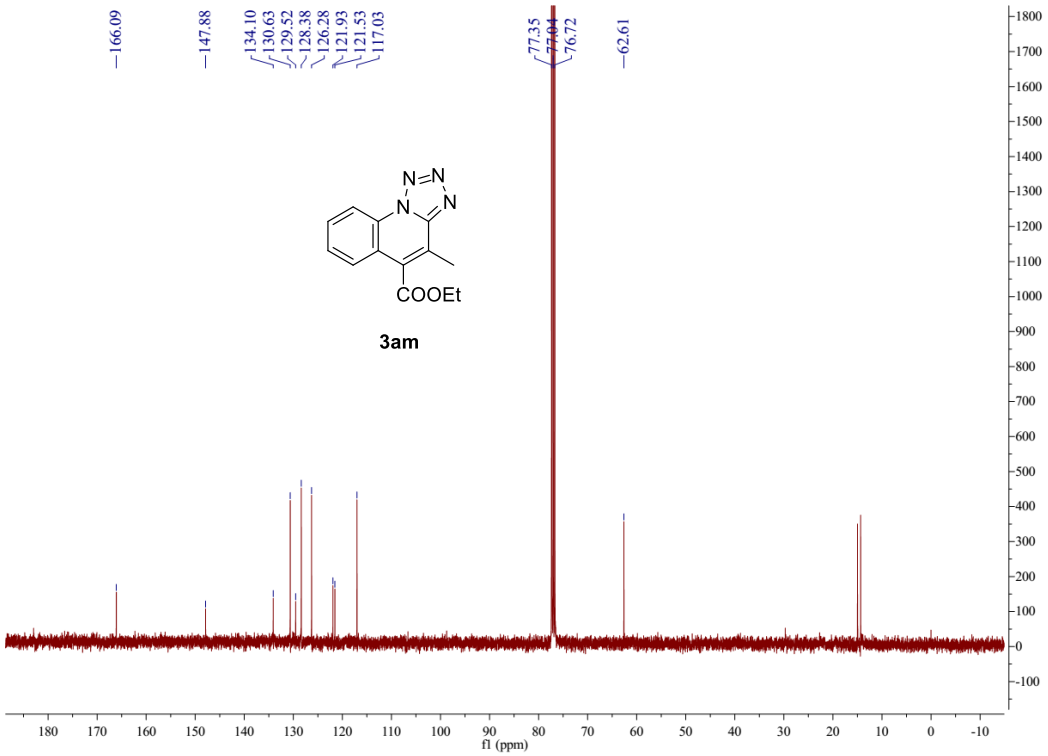


Ethyl 4-methyltetrazolo[1,5-a]quinoline-5-carboxylate (3am)

^{1}H NMR (400 MHz, $CDCl_3$)

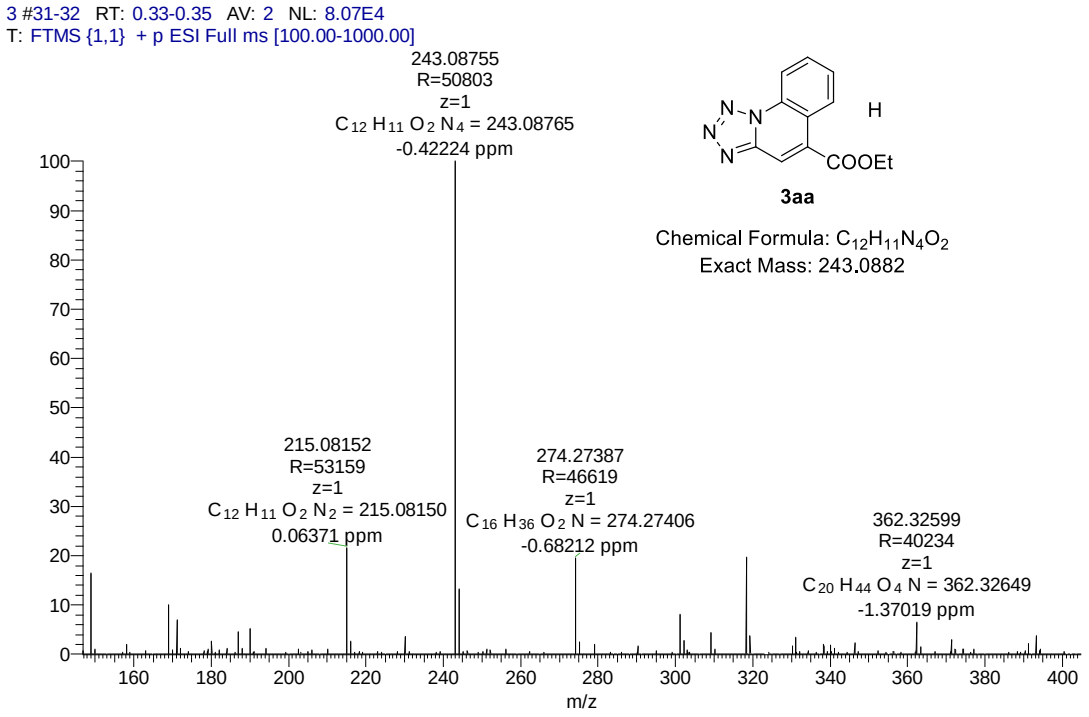


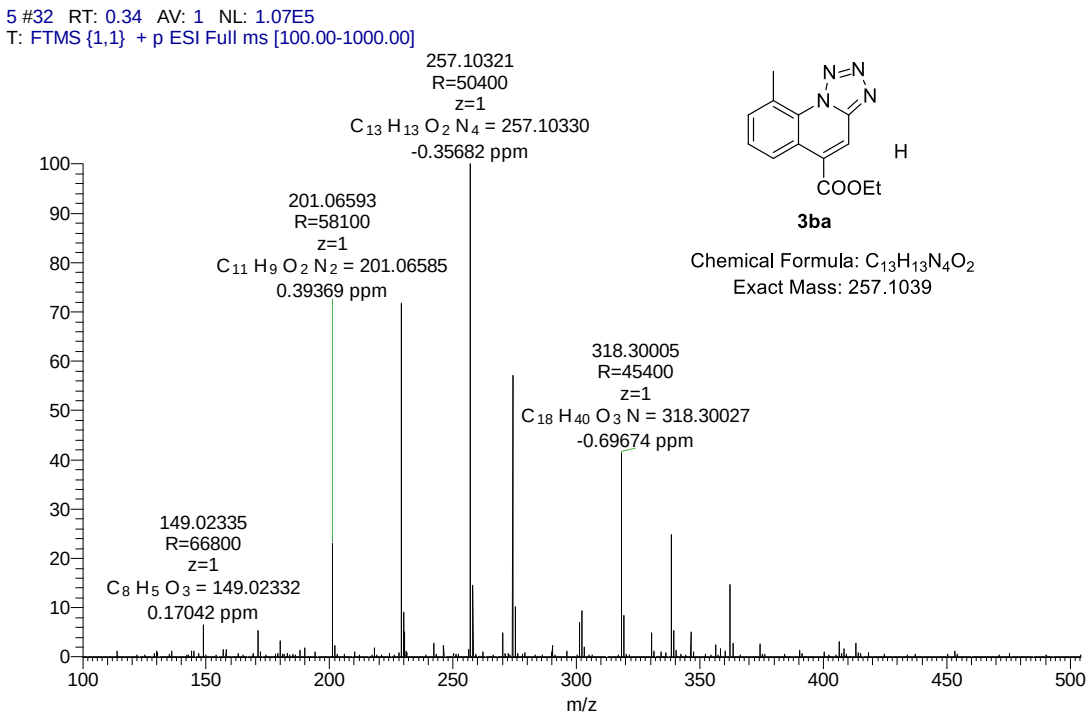
^{13}C NMR (100 MHz, $CDCl_3$)



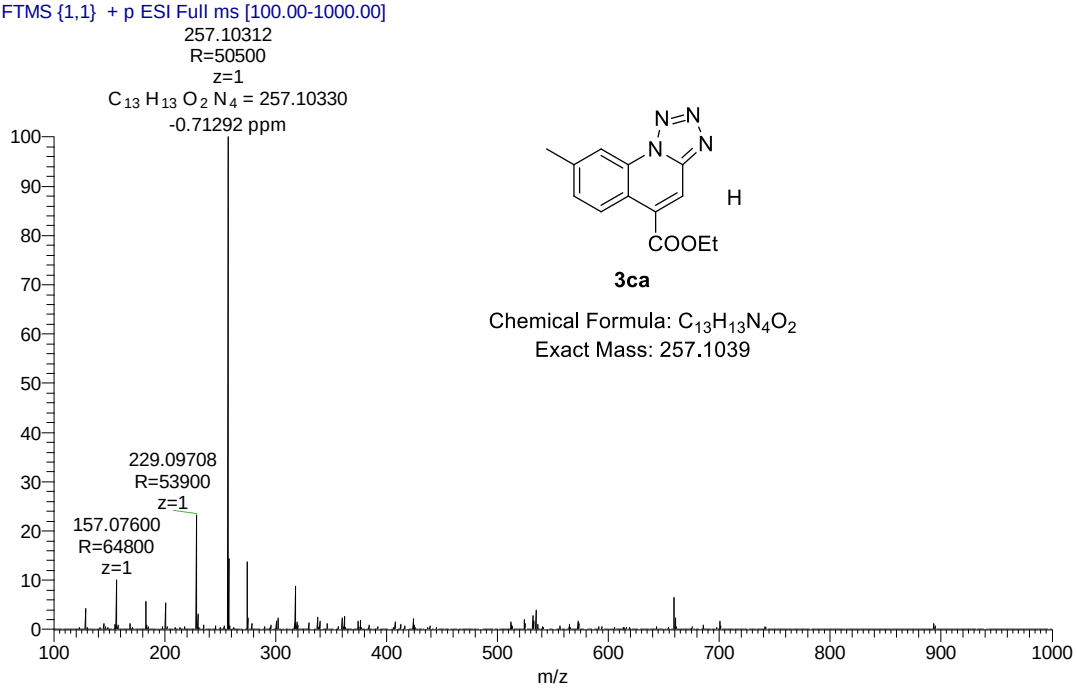
7. HR-MS Spectra of New Compounds

NOTE: High resolution mass spectroscopic data of the products were collected on a Waters Micromass GCT instrument [the blue-colored spectra (**3ad**, **3ae**) were recorded with an AB 5600+Triple-TOF using ESI].





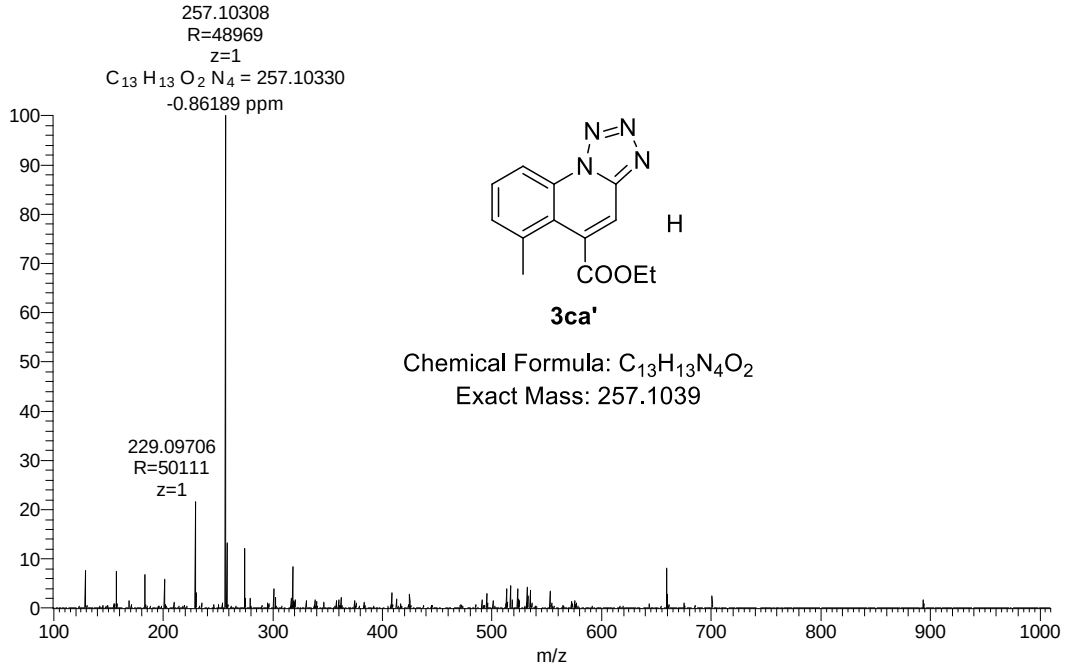
20160913-1 #32 RT: 0.36 AV: 1 NL: 3.68E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



3ca

Chemical Formula: $C_{13}H_{13}N_4O_2$
Exact Mass: 257.1039

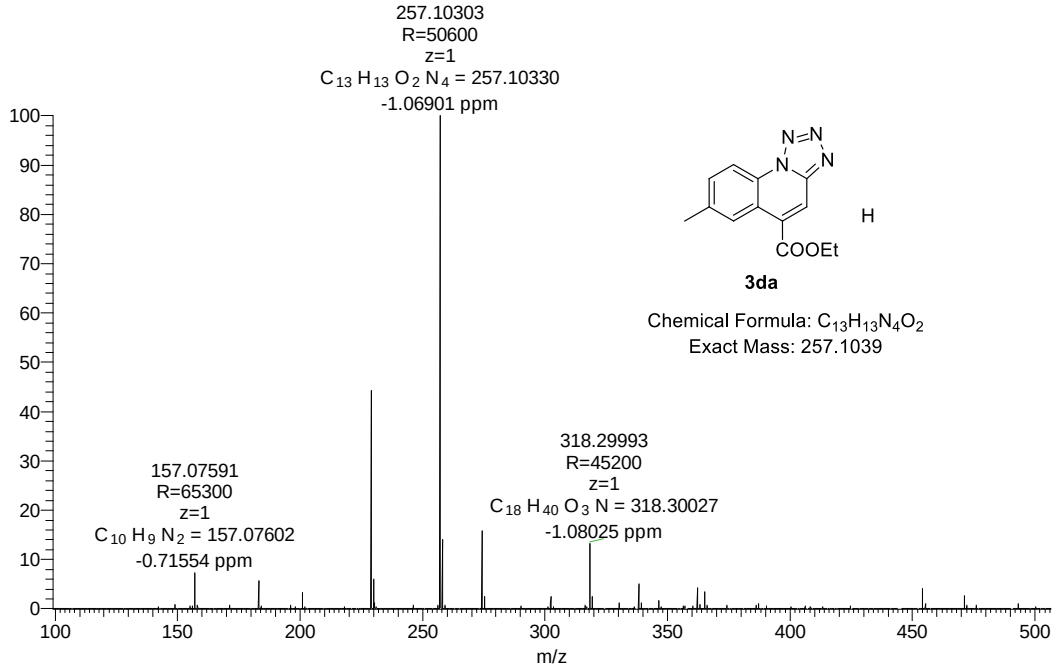
20160913-2 #34-35 RT: 0.35-0.36 AV: 2 NL: 2.43E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



3ca'

Chemical Formula: $C_{13}H_{13}N_4O_2$
Exact Mass: 257.1039

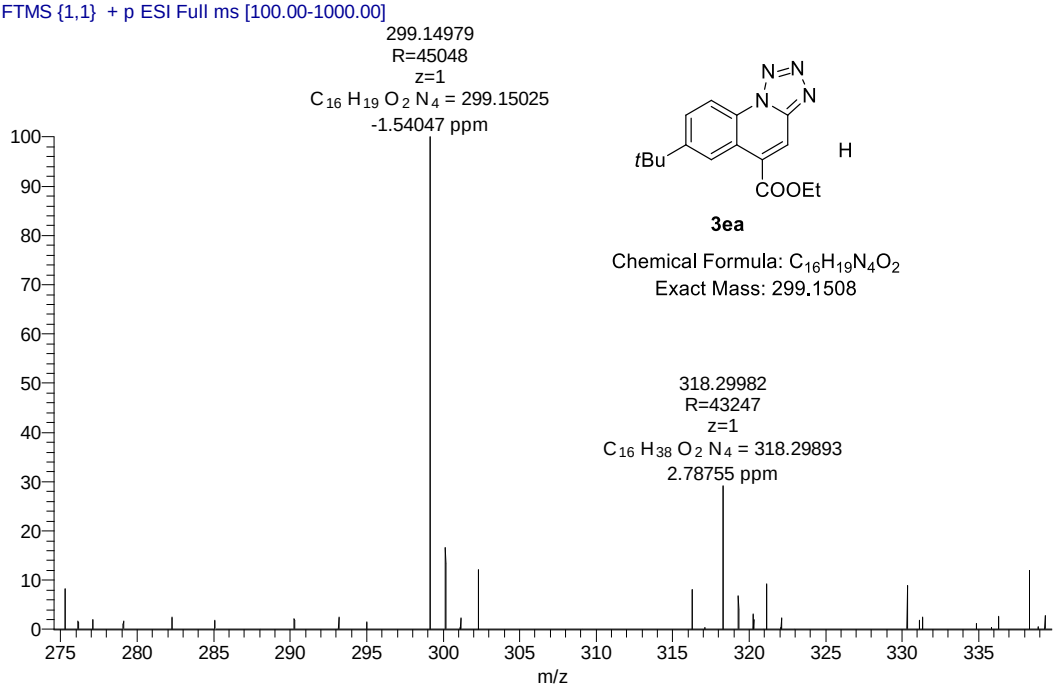
6 #33 RT: 0.34 AV: 1 NL: 8.29E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



3da

Chemical Formula: $C_{13}H_{13}N_4O_2$
Exact Mass: 257.1039

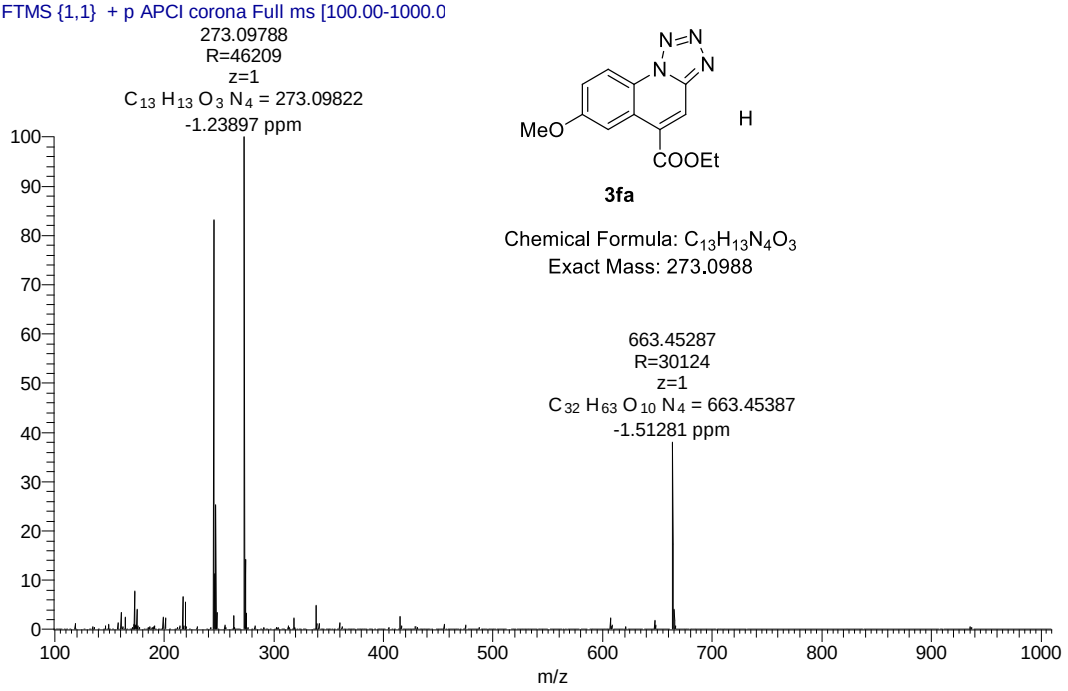
20160715-31 #46 RT: 0.52 AV: 1 SB: 32 0.02-0.06 , 0.70-0.99 NL: 5.00E3
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



3ea

Chemical Formula: $C_{16}H_{19}N_4O_2$
Exact Mass: 299.1508

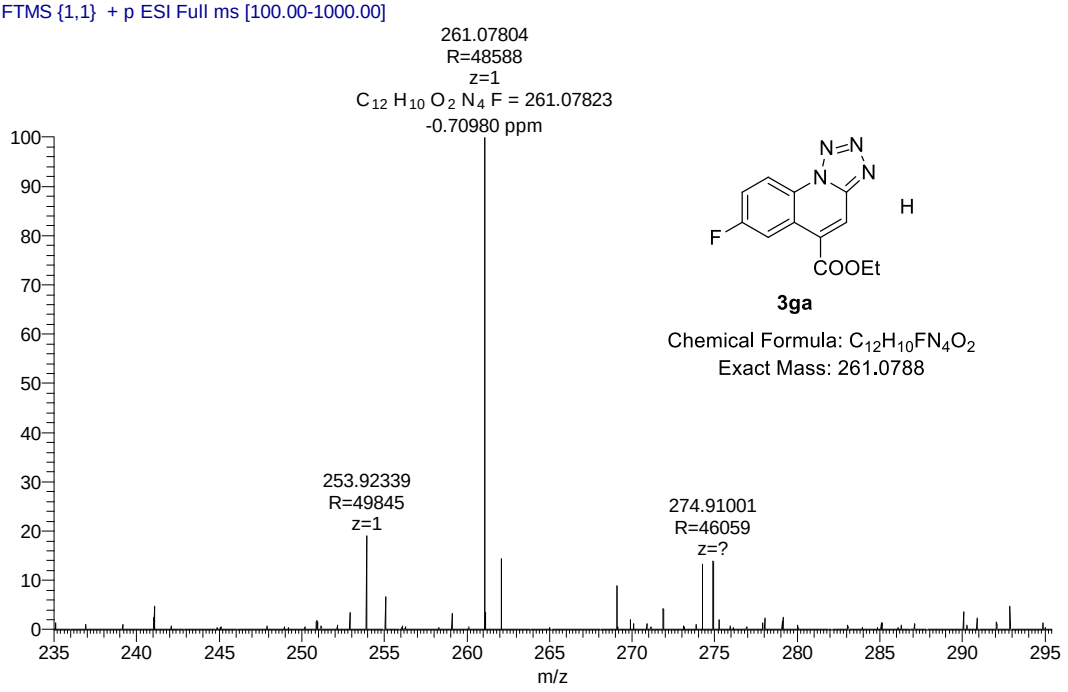
20160704-23_160705093630 #34-37 RT: 0.25-0.27 AV: 4 NL: 8.60E7
T: FTMS {1,1} + p APCI corona Full ms [100.00-1000.0



3fa

Chemical Formula: $C_{13}H_{13}N_4O_3$
Exact Mass: 273.0988

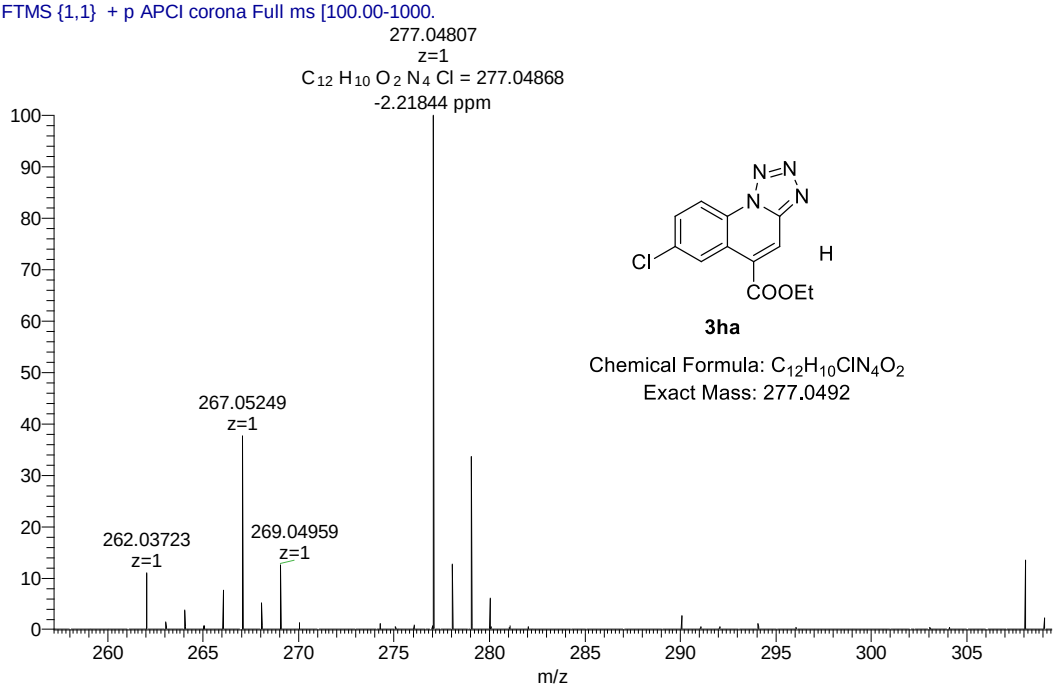
20160715-33 #84-87 RT: 0.94-0.98 AV: 4 NL: 1.91E4
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



3ga

Chemical Formula: $C_{12}H_{10}FN_4O_2$
Exact Mass: 261.0788

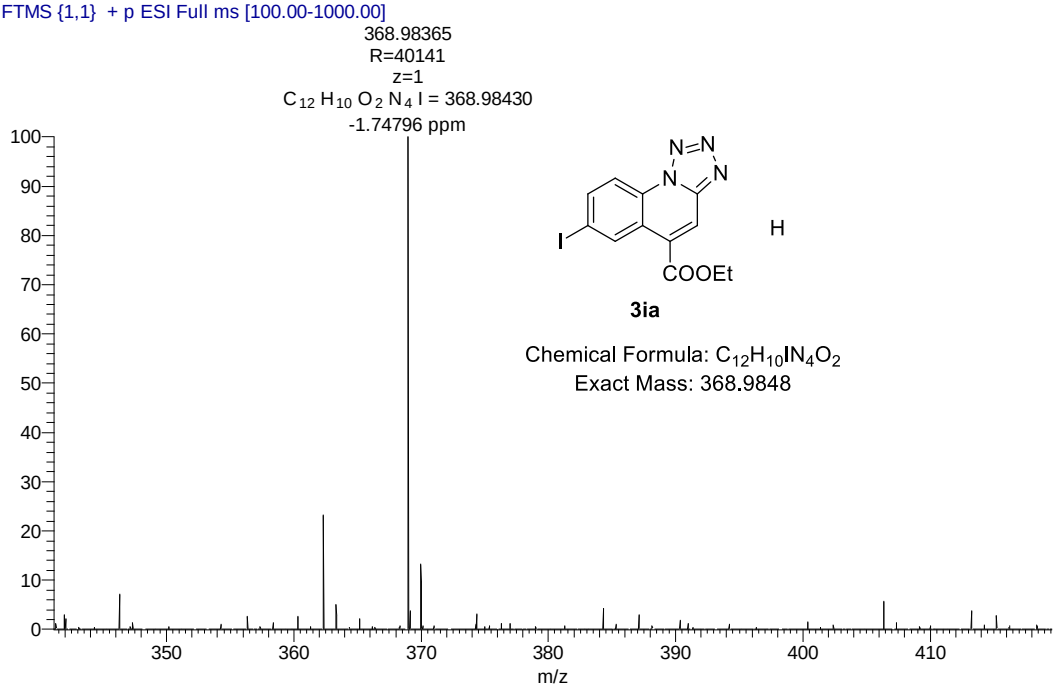
20160930-46_161006123559 #28 RT: 0.21 AV: 1 NL: 1.19E7
T: FTMS {1,1} + p APCI corona Full ms [100.00-1000.



3ha

Chemical Formula: $C_{12}H_{10}ClN_4O_2$
Exact Mass: 277.0492

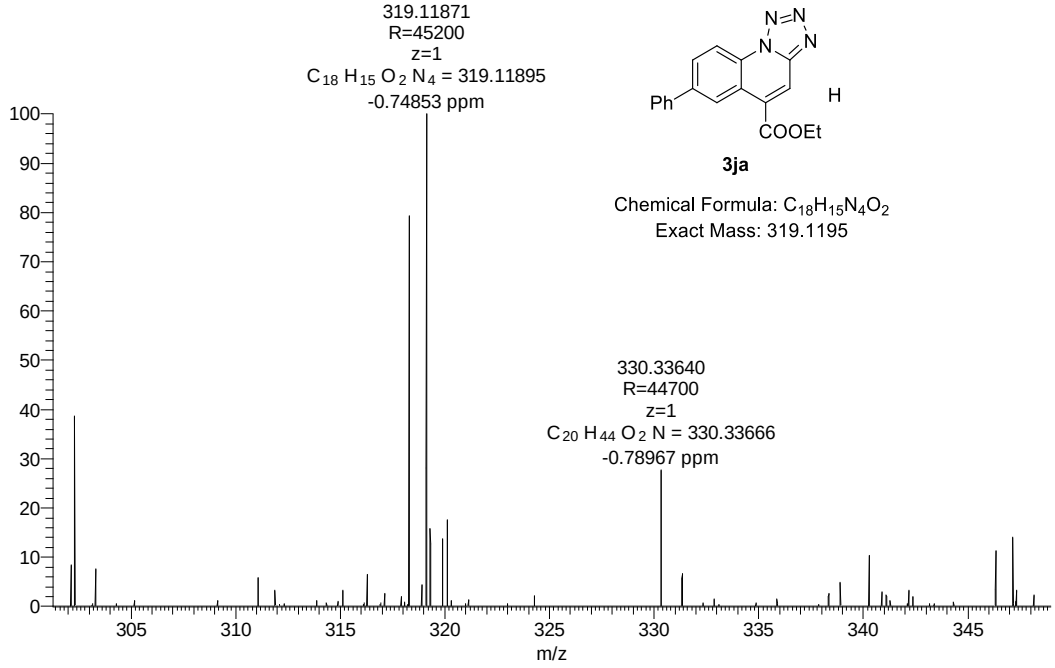
20160715-35 #26-27 RT: 0.29-0.30 AV: 2 NL: 1.71E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



3ia

Chemical Formula: $C_{12}H_{10}IN_4O_2$
Exact Mass: 368.9848

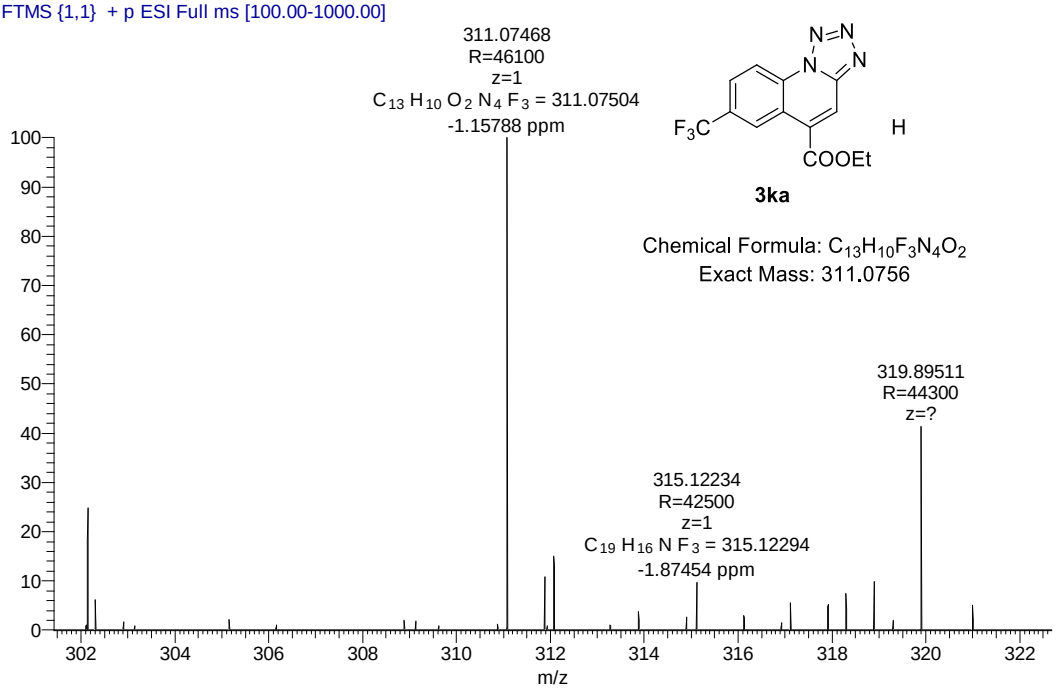
20160715-34 #48 RT: 0.51 AV: 1 NL: 2.22E4
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



3ja

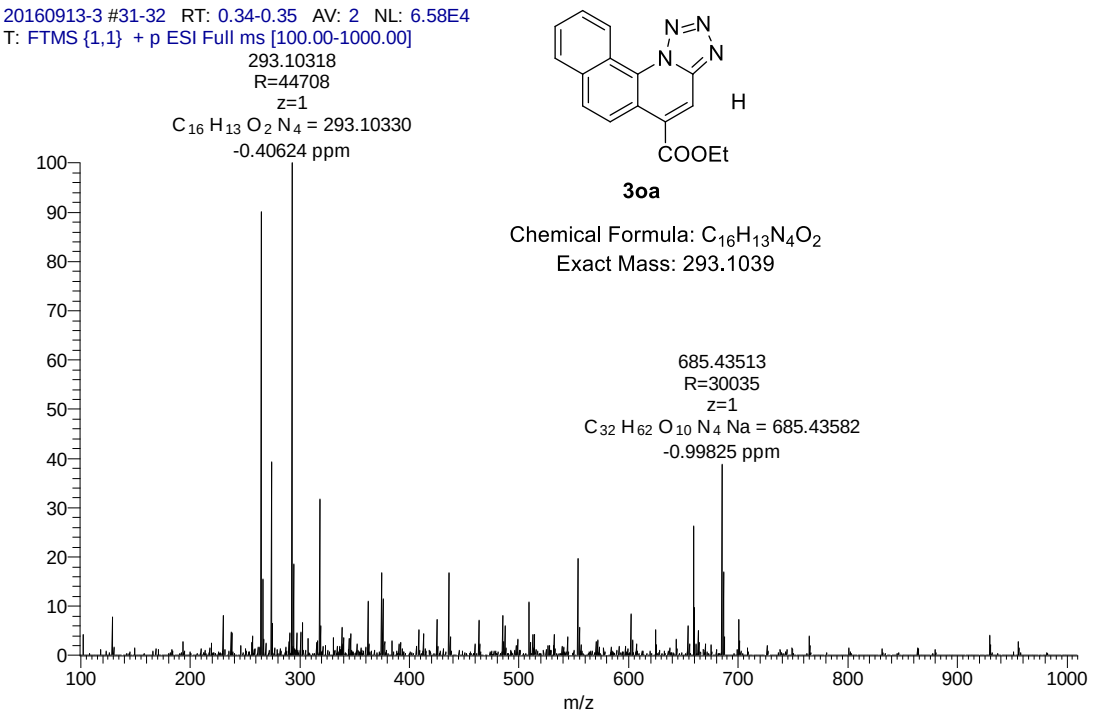
Chemical Formula: $C_{18}H_{15}N_4O_2$
Exact Mass: 319.1195

20160715-32 #83 RT: 0.94 AV: 1 NL: 8.63E3
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



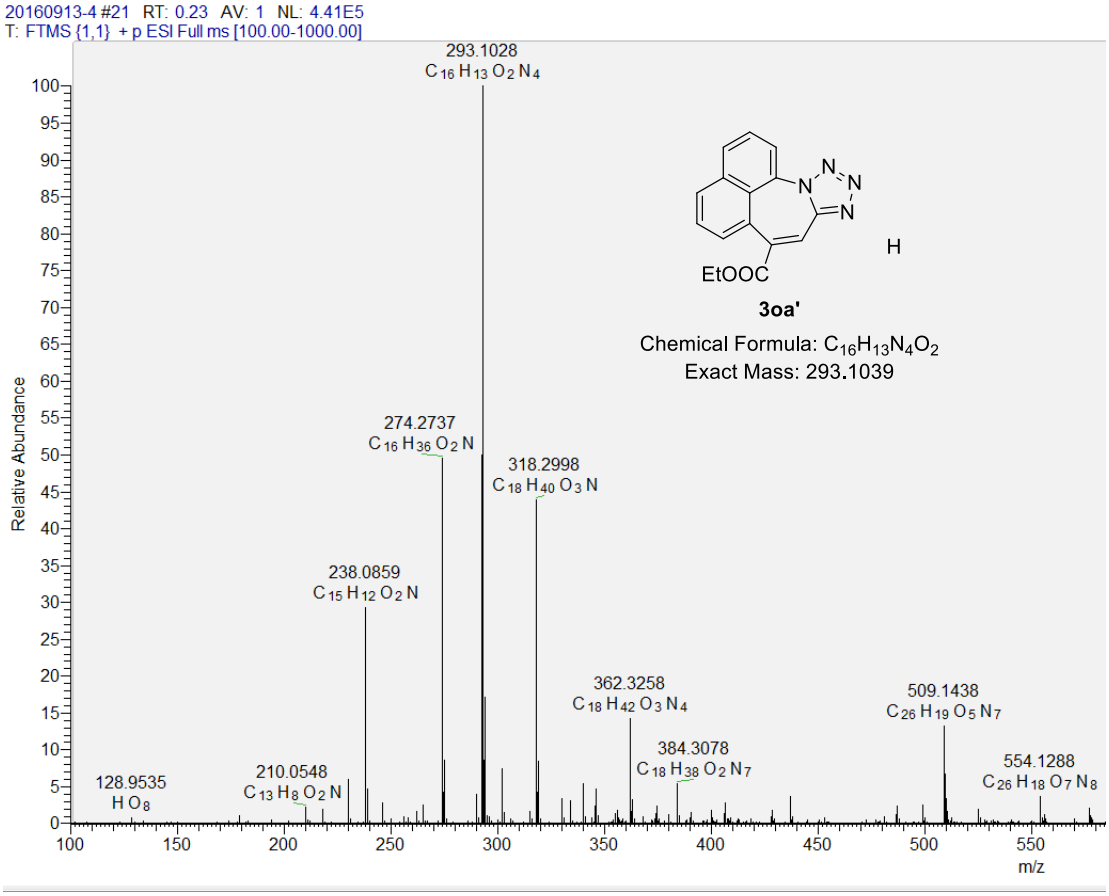
3ka

Chemical Formula: $C_{13}H_{10}F_3N_4O_2$
Exact Mass: 311.0756



3oa

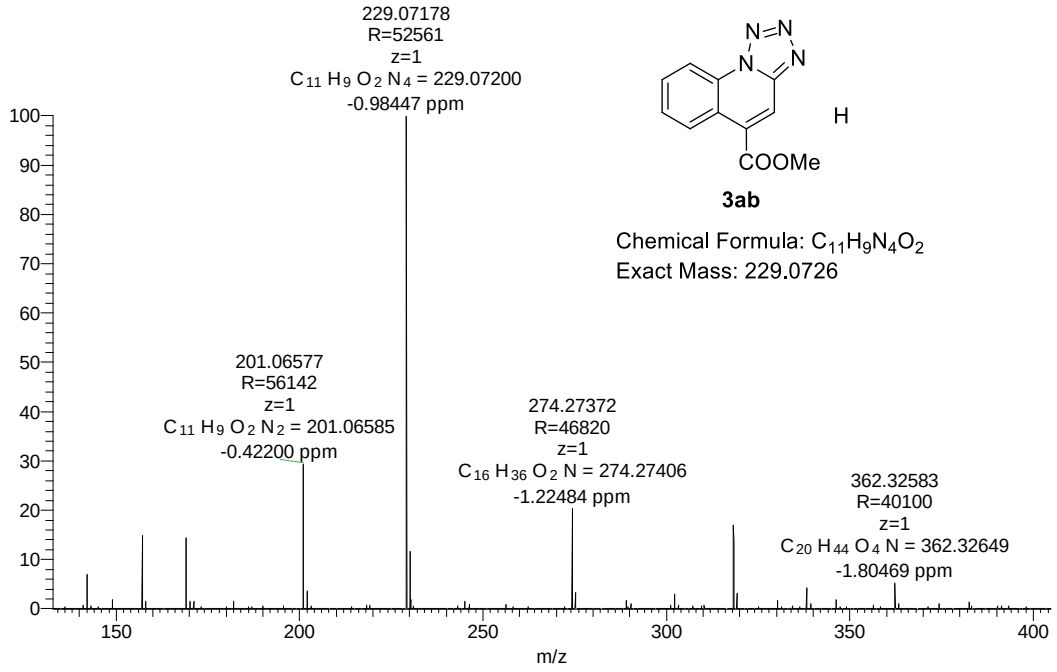
Chemical Formula: $C_{16}H_{13}N_4O_2$
Exact Mass: 293.1039



3oa'

Chemical Formula: $C_{16}H_{13}N_4O_2$
Exact Mass: 293.1039

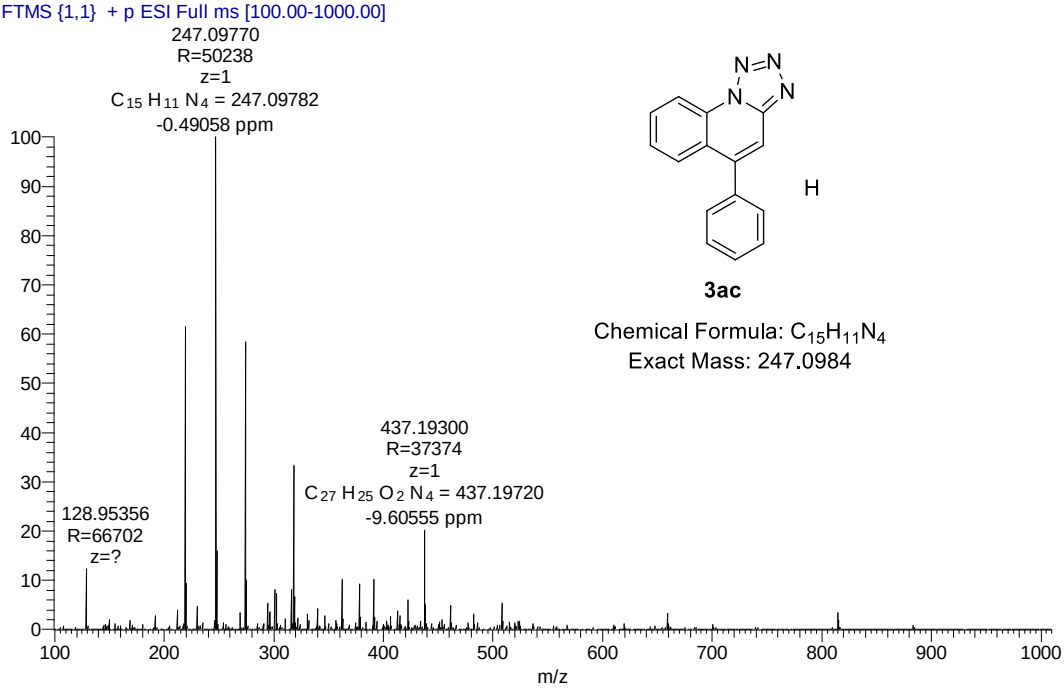
4 #32-33 RT: 0.33-0.34 AV: 2 NL: 3.15E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



3ab

Chemical Formula: $C_{11}H_9N_4O_2$
Exact Mass: 229.0726

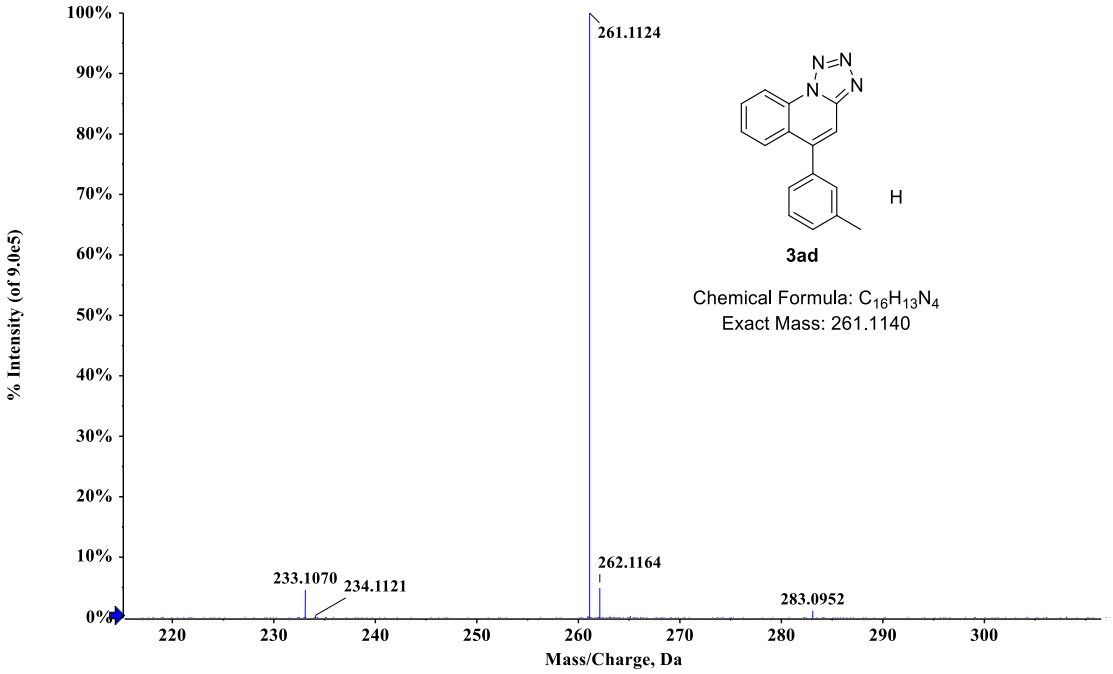
20160704-22 #29-31 RT: 0.32-0.34 AV: 3 NL: 9.47E4
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



3ac

Chemical Formula: $C_{15}H_{11}N_4$
Exact Mass: 247.0984

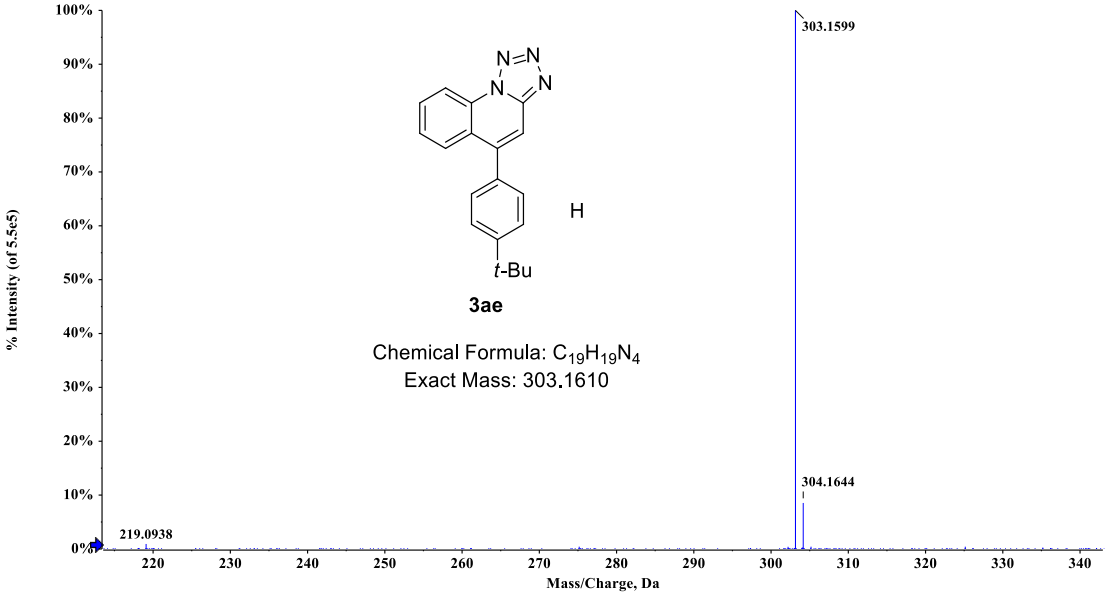
Spectrum from 1.wiff (sample 1) - 1, +TOF MS (100 - 800) from 0.133 min



3ad

Chemical Formula: $C_{16}H_{13}N_4$
Exact Mass: 261.1140

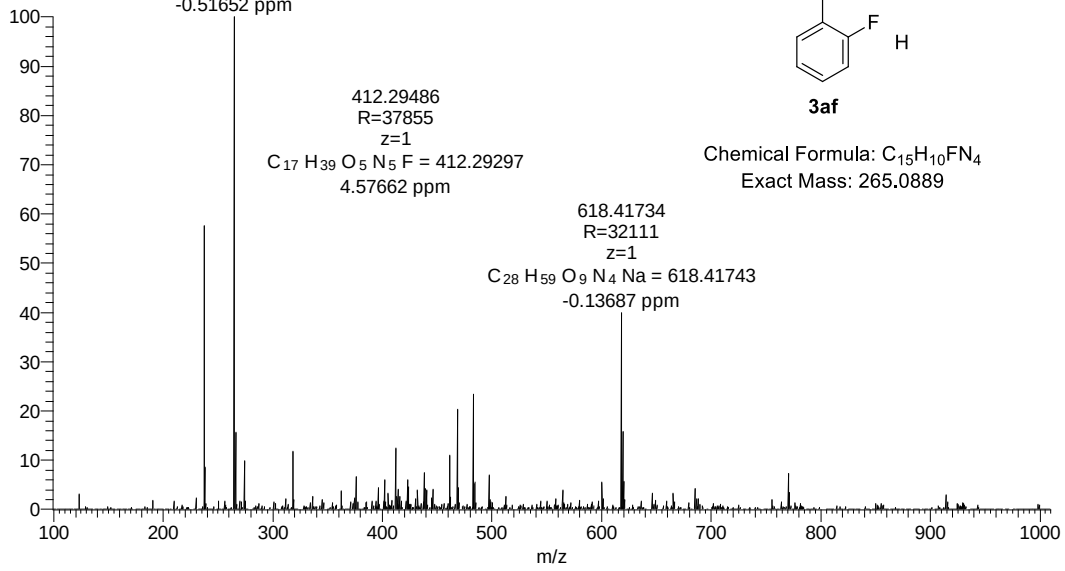
Spectrum from 2.wiff (sample 1) - 2, +TOF MS (100 - 800) from 0.155 min

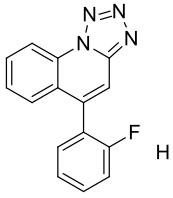


3ae

Chemical Formula: $C_{19}H_{19}N_4$
Exact Mass: 303.1610

20160913-13 #36-37 RT: 0.35-0.36 AV: 2 NL: 2.37E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]

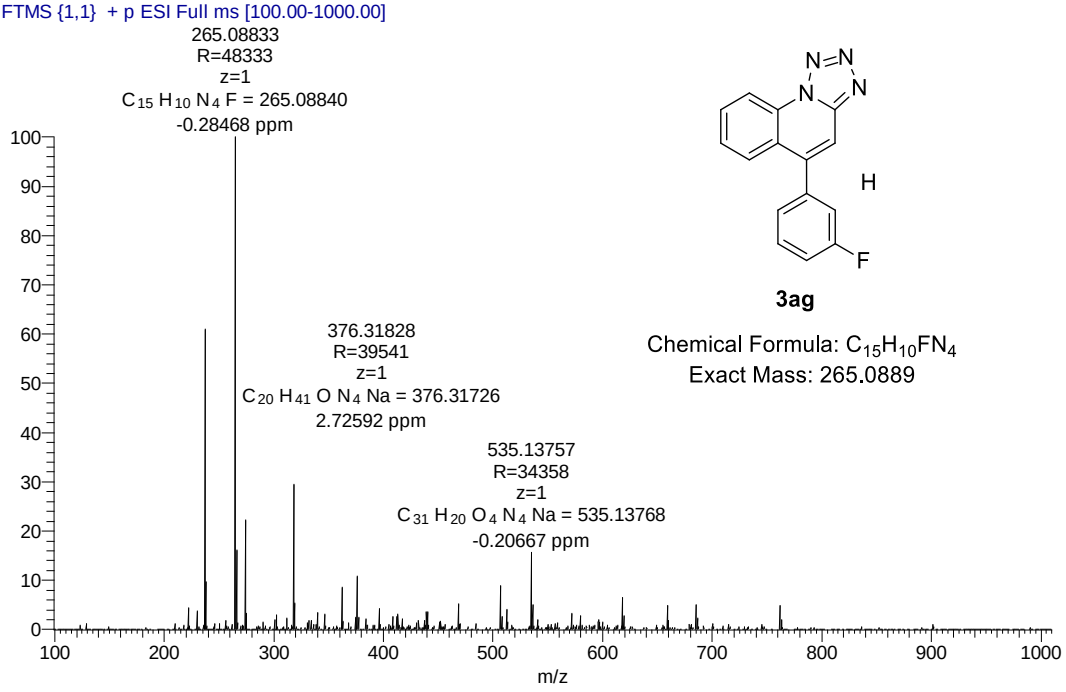




3af

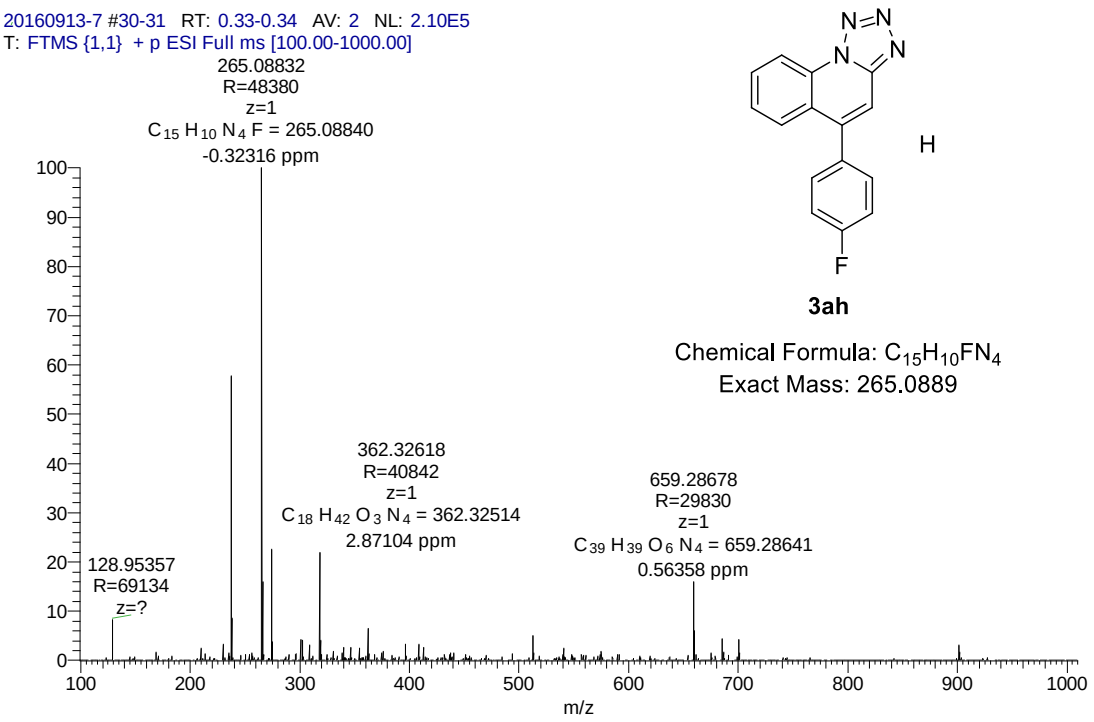
Chemical Formula: $C_{15}H_{10}FN_4$
Exact Mass: 265.0889

20160913-14 #29-31 RT: 0.30-0.32 AV: 3 NL: 2.29E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



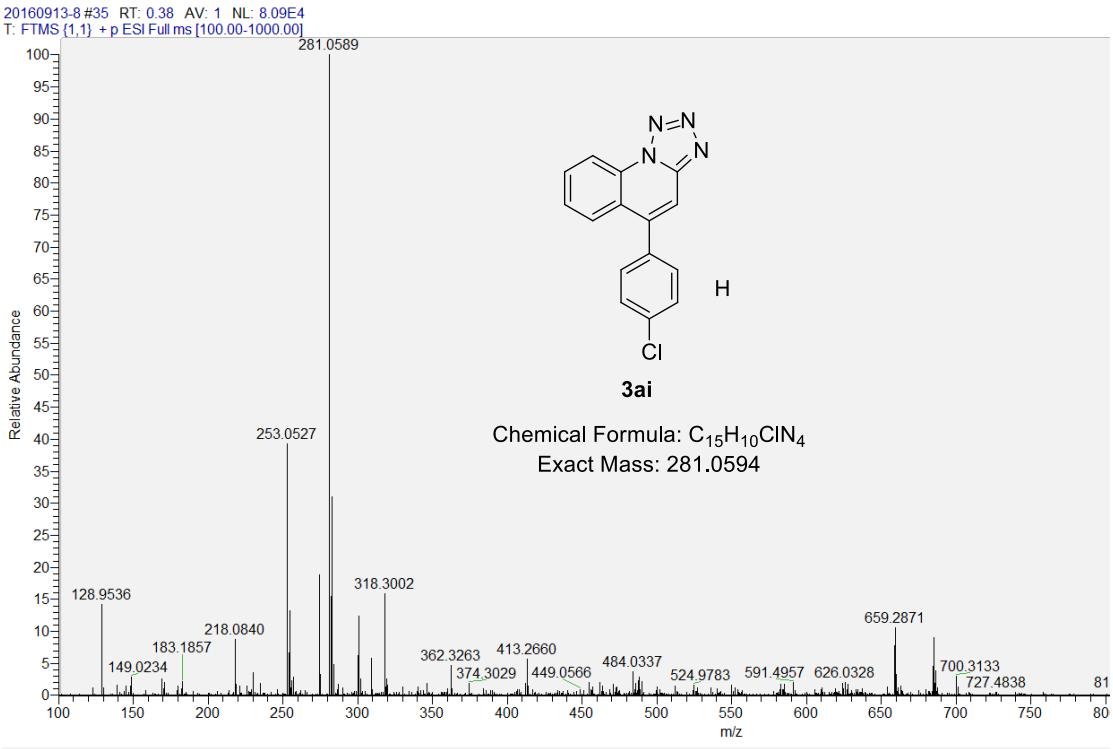
3ag

Chemical Formula: $C_{15}H_{10}FN_4$
Exact Mass: 265.0889



3ah

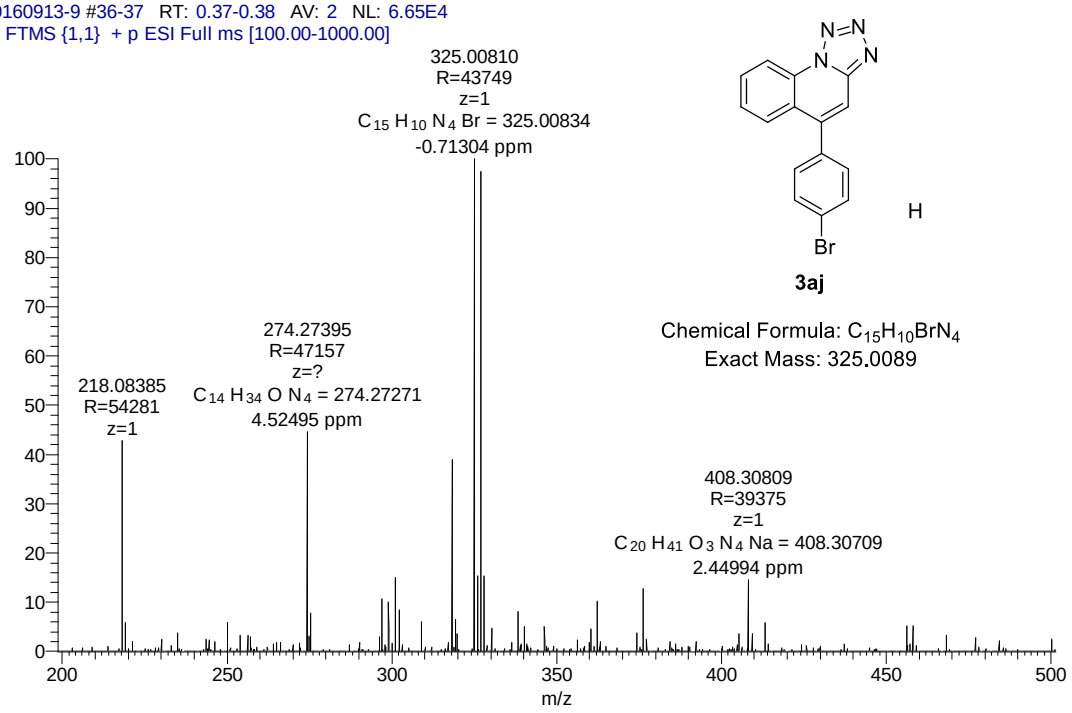
Chemical Formula: $C_{15}H_{10}FN_4$
Exact Mass: 265.0889



3ai

Chemical Formula: $C_{15}H_{10}ClN_4$
Exact Mass: 281.0594

20160913-9 #36-37 RT: 0.37-0.38 AV: 2 NL: 6.65E4
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]

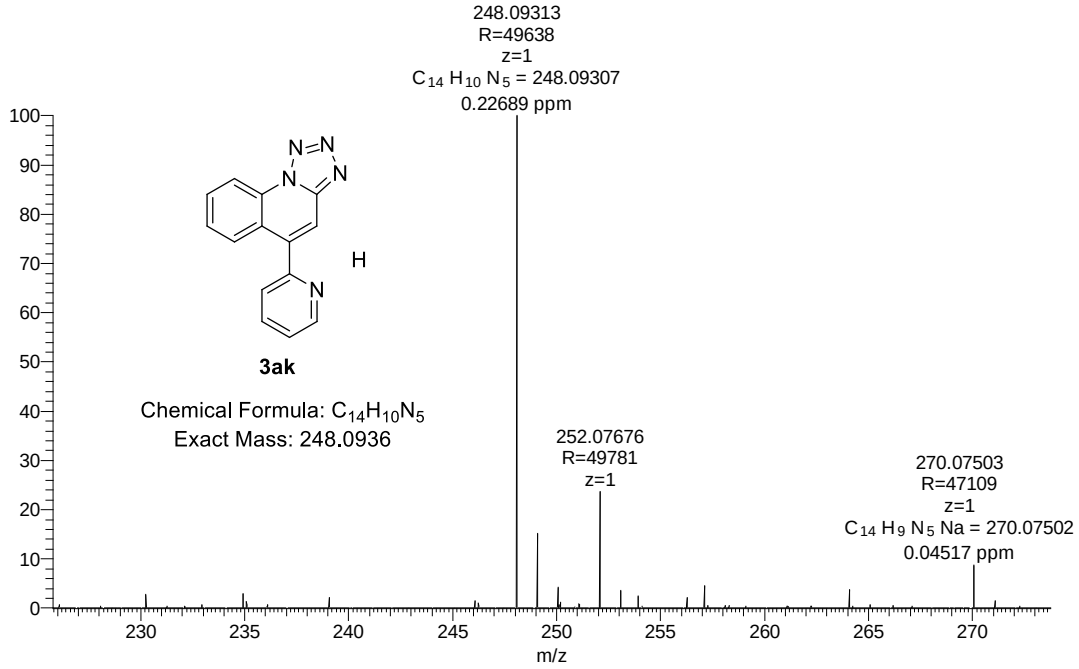


H

3aj

Chemical Formula: $C_{15}H_{10}BrN_4$
Exact Mass: 325.0089

20160913-12 #33-35 RT: 0.37-0.39 AV: 3 NL: 6.44E4
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]

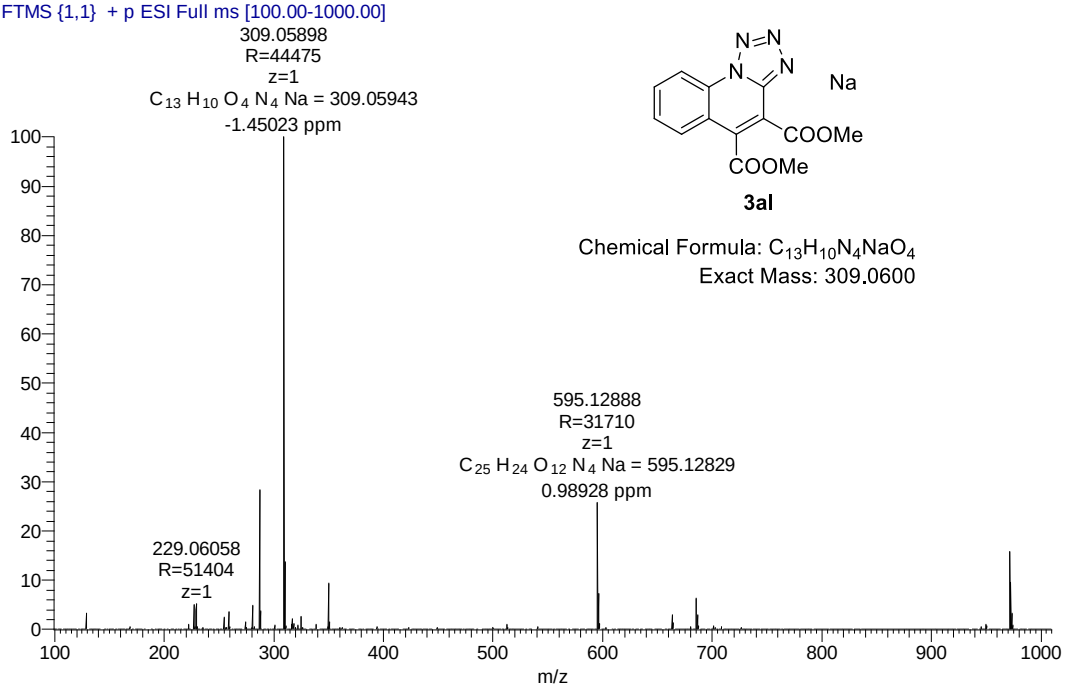


H

3ak

Chemical Formula: $C_{14}H_{10}N_5$
Exact Mass: 248.0936

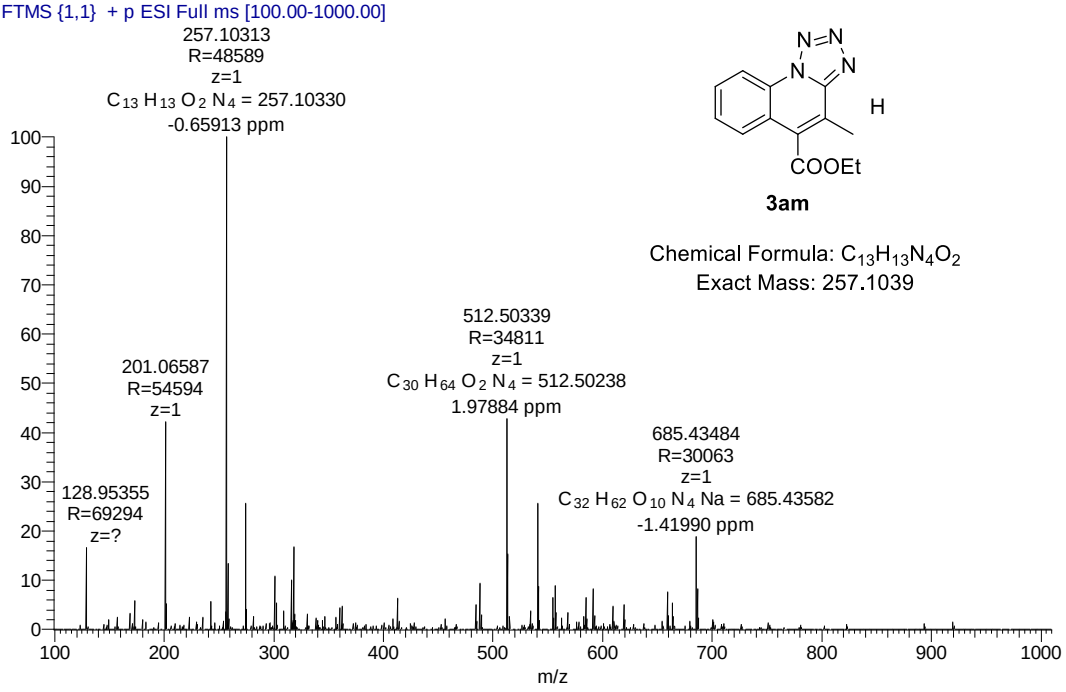
20160913-5 #39-40 RT: 0.39-0.41 AV: 2 NL: 6.58E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



3al

Chemical Formula: $C_{13}H_{10}N_4NaO_4$
Exact Mass: 309.0600

20160913-10 #41-42 RT: 0.43-0.44 AV: 2 NL: 1.34E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



3am

Chemical Formula: $C_{13}H_{13}N_4O_2$
Exact Mass: 257.1039