Supporting Information

Rhodium-Catalyzed Homodimerization-Cyclization Reaction of Two Vinyl Isocyanides: A General Route to 2-(Isoquinolin-1-yl)oxazole

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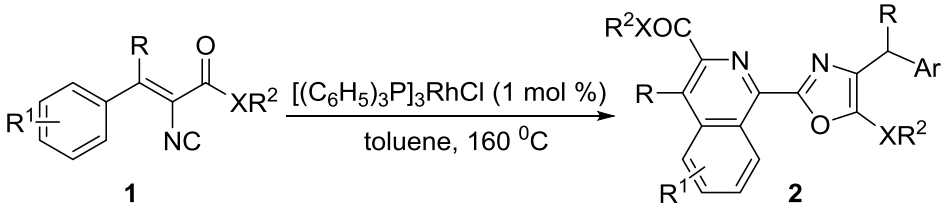
I. General Information:

Unless stated otherwise, all reactions were carried out in glassware under air. All glassware and stirrers were dried in an oven at 85 ℃ overnight. All reagents were commercially available and were used without further purification. The vinyl isocyanides **1** were prepared according to the previous method reported.[1] Elevated temperatures were maintained by an IKA heating block for 1 dram vials. The chromatographic purification of the products was performed on silica gel 300–400 mesh. NMR-spectra were measured in the given solvent at room temperature on a Bruker Avance (600 MHz, ^{1}H; 151 MHz, ^{13}C) instrument. Data for ^{1}H NMR and ^{13}C NMR are reported in terms of chemical shift (δ, ppm). High-resolution mass spectra (HRMS) were obtained using a Bruker microTOF II focus spectrometer (ESI). The compound **2k** was glued on a glass fiber. Data were collected at 293 Kusing graphite-monochromated Mo Kα radiation (λ = 0.71073Å) and IP technique in the range 2.19° < θ < 27.48°. Empirical absorption correction was applied. The structures were solved by the direct method and refined by the full-matrix least-squares method on F^2 using the SHELXS 97 crystallographic software package. Anisotropic thermal parameters were used to refine all non-hydrogen atoms. Hydrogen atoms were located from difference Fourier maps.

1. H. Jiang, Y. Cheng, R. Wang, Y. Zhang, S. Yu, *Chem. Commun.* **2014**, *50*, 6164-6167.

II. General Procedure for the Preparation of 2 (2a as Example):



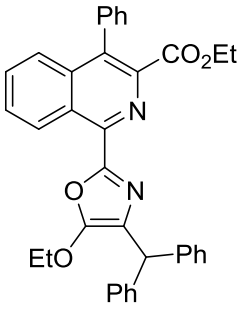
1 2

To a solution of ethyl 2-isocyano-3,3-diphenylacrylate **1a** (0.2 mmol, 55.4 mg) in toluene (2.0 mL) was added the $[(C_6H_5)_3P]_3RhCl$ (1.8 mg, 0.002 mmol). The reaction mixture was stirred for 12 h at 160 ℃ in a 10 mL sealed tube. After the reaction was complete, the reaction mixture was poured into saturated aqueous NaCl (5.0 mL) and extracted with CH_2Cl_2 (2.0 mL × 3). The combined organic extracts were dried over anhydrous Mg_2SO_4, filtered and concentrated under reduced pressure to yield the crude product, which was purified by chromatography (ethyl acetate/petroleum ether = 1/5, V/V) to give **2a** (82.1 mg, 74%) as a yellow solid.

A gram-scale synthesis of compound 2d:

To a solution of ethyl 2-isocyano-3,3-di-p-tolylacrylate **1d** (4.0 mmol, 1.22 g) in toluene (12.0 mL) was added the $[(C_6H_5)_3P]_3RhCl$ (36.0 mg, 0.04 mmol). The reaction mixture was stirred for 12 h at 160 ℃ in a 35 mL sealed tube. After the reaction was complete, the reaction mixture was poured into saturated aqueous NaCl (100.0 mL) and extracted with CH_2Cl_2 (40.0 mL × 3). The combined organic extracts were dried over anhydrous Mg_2SO_4, filtered and concentrated under reduced pressure to yield the crude product, which was purified by chromatography (ethyl acetate/petroleum ether = 1/5, V/V) to give **2d** (1.49 g, 61%) as a yellow solid.

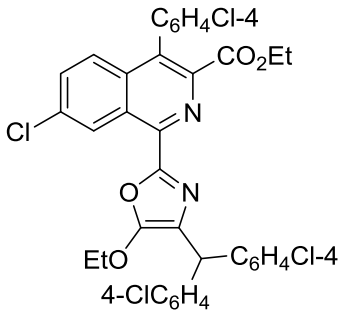
Ethyl 1-(4-benzhydryl-5-ethoxyoxazol-2-yl)-4-phenylisoquinoline-3-carboxylate (2a):



Eluent: ethyl acetate/petroleum ether (1/5). Yellow solid (82.1 mg, 74%), mp. 60–61 ^oC; R_f = 0.45 (ethyl acetate/petroleum ether = 3/10); ^1H NMR (600 MHz, $CDCl_3$) δ: 9.58 (d, *J* = 8.5 Hz, 1H),

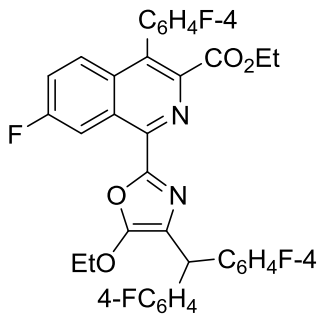
7.72–7.69 (m, 1H), 7.67–7.64 (m, 2H), 7.49 (d, *J* = 7.2 Hz, 3H), 7.41 (d, *J* = 7.8 Hz, 4H), 7.36–7.35 (m, 2H), 7.32 (t, *J* = 7.7 Hz, 4H), 7.23 (t, *J* = 7.3 Hz, 2H), 5.47 (s, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 4.14 (q, *J* = 7.1 Hz, 2H), 1.30 (t, *J* = 7.1 Hz, 3H), 0.99 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 166.95, 155.86, 150.09, 144.27, 142.72, 141.63, 136.64, 136.08, 134.13, 130.73, 129.87, 129.41, 129.00, 128.29, 128.22, 128.09, 127.94, 126.55, 126.46, 126.38, 120.34, 70.29, 61.37, 47.22, 15.02, 13.69; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{36}H_{30}N_2NaO_4^+$: 577.2098, found: 577.2104.

Ethyl 1-(4-(bis(4-chlorophenyl)methyl)-5-ethoxyoxazol-2-yl)-7-chloro-4-(4-chlorophenyl)isoquinoline-3-carboxylate (2b):



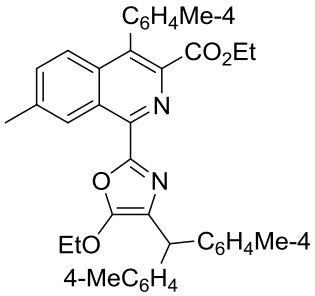
Eluent: ethyl acetate/petroleum ether (1/5). Yellow solid (108.0 mg, 78%), mp. 96–97 °C; R_f = 0.45 (ethyl acetate/petroleum ether = 3/10); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.59 (d, *J* = 1.9 Hz, 1H), 7.62–7.60 (m, 1H), 7.56 (d, *J* = 9.1 Hz, 1H), 7.49 (d, *J* = 8.3 Hz, 2H), 7.34 (s, 1H), 7.32 (d, *J* = 5.3 Hz, 6H), 7.30 (s, 1H), 7.28 (d, *J* = 8.3 Hz, 2H), 5.37 (s, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 4.19 (q, *J* = 7.1 Hz, 2H), 1.36 (t, *J* = 7.1 Hz, 3H), 1.08 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 166.26, 155.78, 149.55, 143.12, 140.70, 136.05, 134.87, 134.61, 133.89, 132.87, 132.62, 131.94, 131.07, 130.13, 128.65, 128.59, 127.96, 127.11, 126.70, 119.12, 70.28, 61.68, 45.60, 15.01, 13.74; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{36}H_{26}Cl_4N_2NaO_4^+$: 713.0539, found: 713.0532.

Ethyl 1-(4-(bis(4-fluorophenyl)methyl)-5-ethoxyoxazol-2-yl)-7-fluoro-4-(4-fluorophenyl)isoquinoline-3-carboxylate (2c):



Eluent: ethyl acetate/petroleum ether (1/5). Yellow solid (96.5 mg, 77%), mp. 112–114 ^{o}C; R_f = 0.50 (ethyl acetate/petroleum ether = 3/10); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.31–9.29 (m, 1H), 7.66–7.64 (m, 1H), 7.46–7.43 (m, 1H), 7.36 (d, *J* = 1.8 Hz, 1H), 7.35 (d, *J* = 3.2 Hz, 2H), 7.34 (t, *J* = 2.0 Hz, 1H), 7.32 (d, *J* = 3.3 Hz, 1H), 7.31 (d, *J* = 2.1 Hz, 1H), 7.23–7.20 (m, 2H), 7.04–7.00 (m, 4H), 5.41 (s, 1H), 4.32 (q, *J* = 7.1 Hz, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 1.34 (t, *J* = 7.1 Hz, 3H), 1.07 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 166.49, 162.44 (d, *J* = 54.0 Hz), 161.95 (d, *J* = 57.8 Hz), 161.57 (d, *J* = 245.2 Hz), 160.81, 155.65, 149.82, 143.35 (d, *J* = 5.6 Hz), 138.16, 138.13 (d, *J* = 3.2 Hz), 133.80, 133.05, 131.50 (d, *J* = 8.1 Hz), 131.44, 130.27 (d, *J* = 7.9 Hz), 130.22, 129.33 (d, *J* = 8.8 Hz), 129.27, 127.39 (d, *J* = 10.3 Hz), 121.44 (d, *J* = 25.4 Hz), 121.27, 119.79 (d, *J* = 24.6 Hz), 115.52 (d, *J* = 21.7 Hz), 115.38, 115.23, 115.08, 112.00, 111.84, 70.24, 61.54, 45.52, 14.96, 13.74; ^{19}F NMR (565 MHz, $CDCl_3$) δ: -106.84–-106.88 (m, 1F), -112.23–-114.49 (m, 1F), -115.46–-119.21 (m, 2F); HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{36}H_{26}F_4N_2NaO_4^+$: 649.1721, found: 649.1729.

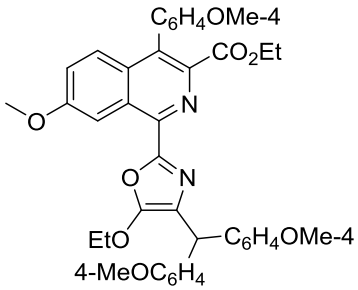
Ethyl 1-(4-(di-*p*-tolylmethyl)-5-ethoxyoxazol-2-yl)-7-methyl-4-(*p*-tolyl)isoquinoline-3-carboxylate (2d):



Eluent: ethyl acetate/petroleum ether (1/5). Yellow solid (83.1 mg, 68%), mp. 84–85 ^{o}C; R_f = 0.45 (ethyl acetate/petroleum ether = 3/10); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.31 (s, 1H), 7.58 (d, *J* = 8.7 Hz, 1H), 7.47–7.45 (m, 1H), 7.32 (d, *J* = 8.0 Hz, 4H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.23 (t, *J* = 6.4

Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 4H), 5.37 (s, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 2.53 (s, 3H), 2.45 (s, 3H), 2.32 (s, 6H), 1.34 (t, *J* = 7.1 Hz, 3H), 1.04 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 167.02, 155.42, 149.99, 140.72, 140.11, 139.53, 137.65, 135.77, 134.99, 134.35, 133.16, 132.7, 129.62, 128.89, 128.81, 128.75, 126.95, 126.62, 126.38, 120.36, 70.27, 61.25, 46.06, 22.10, 21.31, 20.99, 15.03, 13.68; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{40}H_{38}N_2NaO_4^+$: 633.2724, found: 633.2731.

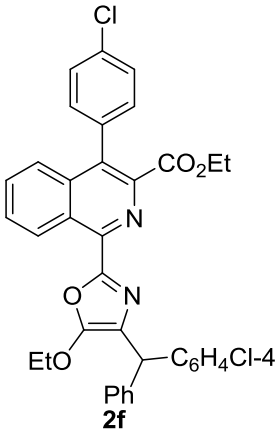
Ethyl 1-(4-(bis(4-methoxyphenyl)methyl)-5-ethoxyoxazol-2-yl)-7-methoxy-4-(4-methoxyphenyl)isoquinoline-3-carboxylate (2e):



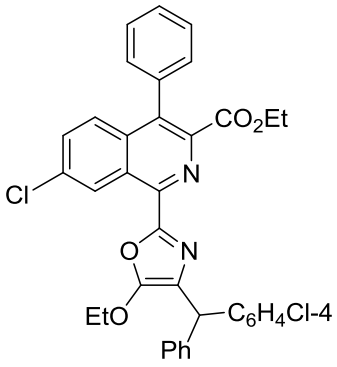
Eluent: ethyl acetate/petroleum ether (1/5). Yellow solid (85.0 mg, 63%), mp. 107–108 °C; R_f = 0.45 (ethyl acetate/petroleum ether = 3/10); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.02 (d, *J* = 2.3 Hz, 1H), 7.59 (d, *J* = 9.3 Hz, 1H), 7.29 (d, *J* = 8.6 Hz, 4H), 7.26–7.24 (m, 3H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 4H), 5.36 (s, 1H), 4.34 (q, *J* = 7.0 Hz, 2H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.88 (s, 3H), 3.78 (s, 9H), 1.36 (t, *J* = 7.1 Hz, 3H), 1.07 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 167.11, 160.13, 159.45, 158.05, 135.38, 134.19, 132.36, 130.91, 129.76, 128.35, 128.14, 128.02, 123.70, 120.54, 113.70, 113.63, 113.53, 105.34, 70.32, 61.20, 55.46, 55.31, 55.19, 45.00, 15.08, 13.81; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{40}H_{38}N_2NaO_8^+$: 697.2520, found: 697.2545.

Ethyl 4-(4-chlorophenyl)-1-(4-((4-chlorophenyl)(phenyl)methyl)-5-ethoxyoxazol-2-yl)isoquinoline-3-carboxylate (2f):

Ethyl 7-chloro-1-(4-((3-chlorophenyl)(phenyl)methyl)-5-ethoxyoxazol-2-yl)-4-phenylisoquinoline-3-carboxylate (2f'):



2f

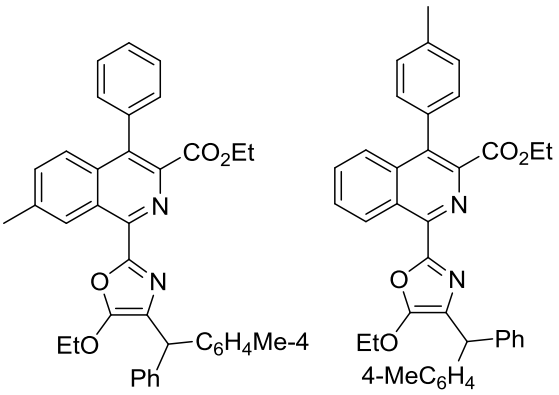


2f'

Eluent: ethyl acetate/petroleum ether (1/5). According to the ^{1}H NMR, the ratio of isomer (**2f**/**2f'**) was approximately 2:1; Red solid (89.8 mg, 72%); R_f = 0.50 (ethyl acetate/petroleum ether = 3/10); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.64 (s, 1H×0.34), 9.55 (d, *J* = 8.5 Hz, 1H×0.66), 7.70 (t, *J* = 7.6 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H×0.66), 7.61–7.59 (m, 1H), 7.57–7.55 (m, 1H×0.34), 7.49–7.47 (m, 2H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.39 (s, 1H), 7.38 (s, 1H), 7.35 (s, 1H), 7.34 (s, 2H), 7.32–7.29 (m, 4H), 7.25–7.22 (m, 1H), 5.44 (s, 1H×0.66), 5.41 (s, 1H×0.34), 4.33 (q, *J* = 7.2 Hz, 2H×0.34), 4.29 (q, *J* = 7.1 Hz, 2H×0.66), 4.18 (q, *J* = 7.1 Hz, 2H×0.66), 4.13 (q, *J* = 7.1 Hz, 2H×0.34), 1.34 (t, *J* = 7.1 Hz, 3H×0.34), 1.31 (t, *J* = 7.0 Hz, 3H×0.66), 1.08 (t, *J* = 7.1 Hz, 3H×0.66), 0.98 (t, *J* = 7.1 Hz, 3H×0.34); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 166.50, 166.44, 155.74, 155.66, 149.90, 149.56, 144.24, 142.91, 142.13, 142.08, 141.87, 141.28, 141.16, 141.10, 136.38, 135.66, 135.34, 134.87, 134.42, 134.18, 133.78, 132.96, 132.26, 132.20, 131.59, 131.10, 130.86, 130.23, 130.18, 129.66, 129.53, 128.73, 128.68, 128.40, 128.39, 128.37, 128.30, 128.28, 128.23, 128.14, 127.78, 126.99, 126.65, 126.62, 126.58, 126.17, 70.21, 70.13, 61.43, 61.36, 46.43, 46.16, 14.94, 14.91, 13.68, 13.56.

Ethyl 1-(5-ethoxy-4-(phenyl(p-tolyl)methyl)oxazol-2-yl)-7-methyl-4-phenylisoquinoline-3-carboxylate (2g):

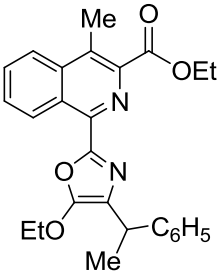
Ethyl 1-(5-ethoxy-4-(phenyl(p-tolyl)methyl)oxazol-2-yl)-4-(p-tolyl)isoquinoline-3-carboxylate (2g'):



2g **2g'**

Eluent: ethyl acetate/petroleum ether (1/5). According to the ^{1}H NMR, the ratio of isomer (**2g**/**2g'**) was approximately 4:1; Red solid (76.9 mg, 66%); R_f = 0.45 (ethyl acetate/petroleum ether = 3/10); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.58 (d, *J* = 8.4 Hz, 1H×0.8), 9.46 (d, *J* = 8.8 Hz, 1H×0.2), 7.69 (d, *J* = 8.0 Hz, 1H), 7.65–7.63 (m, 1H), 7.53–7.47 (m, 1H), 7.41 (d, *J* = 7.8 Hz, 2H), 7.39–7.35 (m, 1H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.27 (s, 1H), 7.24 (d, *J* = 5.5 Hz, 1H), 7.22–7.21 (m, 3H), 7.17–7.14 (m, 2H), 7.05–7.04 (m, 1H), 5.42 (s, 1H×0.8), 5.41 (s, 1H×0.2), 4.27 (q, *J* = 7.0 Hz, 2H), 4.18–4.11 (m, 2H), 2.43 (s, 3H×0.2), 2.42 (3H×0.8), 2.34 (s, 3H), 1.30 (t, *J* = 7.1 Hz, 3H), 1.02–0.97 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 166.96, 155.75, 149.99, 142.79, 142.56, 141.60, 137.76, 136.60, 135.87, 134.19, 130.60, 130.41, 129.84, 129.70, 129.25, 128.91, 128.75, 128.20, 128.15, 128.12, 128.05, 127.89, 127.17, 126.96, 126.57, 126.33, 126.02, 120.33, 70.22, 61.26, 47.06, 21.51, 21.41, 14.97, 13.64.

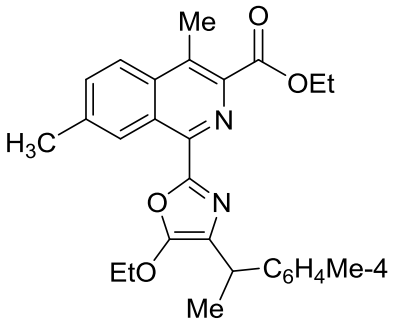
Ethyl 1-(5-ethoxy-4-(1-phenylethyl)oxazol-2-yl)-4-methylisoquinoline-3-carboxylate (2h):



Eluent: ethyl acetate/petroleum ether (1/7). Yellow liquid (64.6 mg, 75%); R_f = 0.50 (ethyl acetate/petroleum ether = 1/4); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.58 (d, *J* = 8.4 Hz, 1H), 8.15 (d, *J* = 8.3 Hz, 1H), 7.81–7.75 (m, 2H), 7.42 (d, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.20 (t, *J* = 7.3 Hz, 1H), 4.52 (q, *J* = 7.1 Hz, 2H), 4.32–4.24 (m, 2H), 4.16 (q, *J* = 7.2 Hz, 1H), 2.87 (s, 3H), 1.72 (d, *J* = 7.2 Hz, 3H), 1.48 (t, *J* = 7.1 Hz, 3H), 1.35 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (151 MHz,

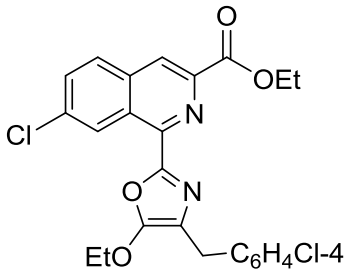
$CDCl_3$) δ: 167.25, 154.58, 145.22, 141.30, 136.86, 130.58, 129.88, 129.22, 128.28, 127.34, 126.19, 126.15, 124.21, 122.21, 70.16, 61.71, 36.08, 20.91, 15.05, 14.65, 14.28; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{26}H_{26}N_2NaO_4^+$: 453.1785, found: 453.1694.

Ethyl 1-(5-ethoxy-4-(1-(p-tolyl)ethyl)oxazol-2-yl)-4,7-dimethylisoquinoline-3-carboxylate (2i):



Eluent: ethyl acetate/petroleum ether (1/7). Yellow liquid (58.7 mg, 64%); R_f = 0.50 (ethyl acetate/petroleum ether = 1/4); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.29 (s, 1H), 8.00 (d, *J* = 8.7 Hz, 1H), 7.57 (d, *J* = 8.7 Hz, 1H), 7.36 (d, *J* = 7.9 Hz, 2H), 7.13 (d, *J* = 7.8 Hz, 2H), 4.51 (q, *J* = 7.1 Hz, 2H), 4.33–4.25 (m, 2H), 4.13 (q, *J* = 7.2 Hz, 1H), 2.84 (s, 3H), 2.57 (s, 3H), 2.32 (s, 3H), 1.70 (d, *J* = 7.3 Hz, 3H), 1.47 (t, *J* = 7.1 Hz, 3H), 1.37 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 167.29, 142.46, 142.29, 140.41, 139.48, 135.63, 135.14, 132.70, 130.19, 128.96, 127.30, 127.29, 126.50, 124.12, 122.34, 70.23, 61.65, 35.63, 22.17, 21.10, 20.98, 15.08, 14.65, 14.30; HRMS(ESI-TOF): $[M + H]^+$ calculated for $C_{28}H_{31}N_2O_4^+$: 459.2278, found: 459.2289.

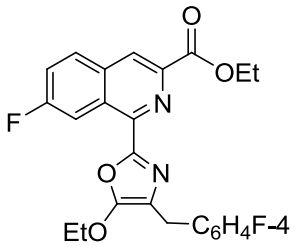
Ethyl 7-chloro-1-(4-(4-chlorobenzyl)-5-ethoxyoxazol-2-yl)isoquinoline-3-carboxylate (2j):



Eluent: ethyl acetate/petroleum ether (1/7). Yellow solid (68.8 mg, 73%), mp. 86–87 °C; R_f = 0.50 (ethyl acetate/petroleum ether = 1/4); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.35–9.33 (m, 1H), 8.55 (s, 1H), 8.02–7.99 (m, 1H), 7.60–7.56 (m, 1H), 7.32–7.28 (m, 2H), 7.00 (t, *J* = 8.7 Hz, 2H), 4.53 (q, *J* = 7.1 Hz, 2H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.90 (s, 2H), 1.50 (t, *J* = 7.1 Hz, 3H), 1.42 (t, *J* = 7.1 Hz,

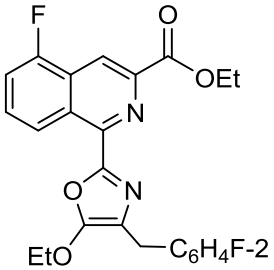
3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 165.09, 145.26, 141.82, 136.67, 134.89, 132.74, 131.06, 130.40, 130.28, 129.36, 128.22, 127.76, 127.12, 126.75, 120.62, 116.15, 70.17, 62.17, 28.91, 15.06, 14.35; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{24}H_{20}Cl_2N_2NaO_4^+$: 493.0692, found: 493.0681.

Ethyl 1-(5-ethoxy-4-(4-fluorobenzyl)oxazol-2-yl)-7-fluoroisoquinoline-3-carboxylate (2k):



Eluent: ethyl acetate/petroleum ether (1/7). Yellow solid (67.5 mg, 77%), mp. 127–129 °C; R_f = 0.50 (ethyl acetate/petroleum ether = 1/4); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.35–9.32 (m, 1H), 8.54 (s, 1H), 8.01–7.99 (m, 1H), 7.59–7.56 (m, 1H), 7.32–7.30 (m, 2H), 7.01–6.98 (m, 2H), 4.53 (q, *J* = 7.1 Hz, 2H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.90 (s, 2H), 1.50 (t, *J* = 7.1 Hz, 3H), 1.42 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 165.20, 162.24 (d, *J* = 237.7 Hz), 161.48 (d, *J* = 229.2 Hz), 155.73, 149.73, 144.19 (d, *J* = 5.8 Hz), 140.49, 134.89 (d, *J* = 3.2 Hz), 134.87, 133.88, 131.06 (d, *J* = 9.1 Hz), 131.00, 129.96 (d, *J* = 7.8 Hz), 129.90, 128.21 (d, *J* = 10.3 Hz), 124.15, 121.74 (d, *J* = 25.9 Hz), 121.56, 117.72, 115.23 (d, *J* = 21.3 Hz), 115.09, 112.38 (d, *J* = 24.5 Hz), 112.22, 70.18, 62.01, 30.34, 15.06, 14.32; ^{19}F NMR (565 MHz, $CDCl_3$) δ: -96.00–-112.05 (m, 1F), -109.37–-121.37 (m, 1F); HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{24}H_{20}F_2N_2NaO_4^+$: 461.1283, found: 461.1299.

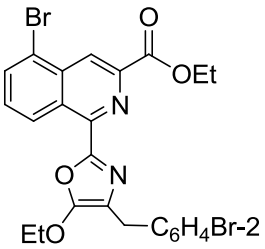
Ethyl 1-(5-ethoxy-4-(2-fluorobenzyl)oxazol-2-yl)-5-fluoroisoquinoline-3-carboxylate (2l):



Eluent: ethyl acetate/petroleum ether (1/7). Yellow solid (50.0 mg, 57%), mp. 91–93 °C; R_f = 0.50 (ethyl acetate/petroleum ether = 1/4); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.38 (d, *J* = 8.6 Hz, 1H),

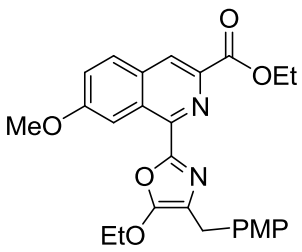
8.79 (s, 1H), 7.75–7.71 (m, 1H), 7.47–7.44 (m, 1H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.21 (q, *J* = 6.2 Hz, 1H), 7.10–7.03 (m, 2H), 4.55 (q, *J* = 7.1 Hz, 2H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.97 (s, 2H), 1.50 (t, *J* = 7.1 Hz, 3H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 164.98, 160.93 (d, *J* = 245.7 Hz), 158.33 (d, *J* = 255.9 Hz), 156.12, 149.70, 144.69, 141.13, 130.64 (d, *J* = 4.5 Hz), 130.61, 130.54, 130.49 (d, *J* = 7.9 Hz), 128.06 (d, *J* = 8.1 Hz), 128.01, 127.75 (d, *J* = 3.4 Hz), 124.02 (d, *J* = 4.4 Hz), 123.98, 123.96, 117.18 (d, *J* = 5.0 Hz), 116.59, 115.22 (d, *J* = 21.9 Hz), 115.07, 114.64, 114.52 (d, *J* = 18.6 Hz), 70.25, 62.11, 24.22, 24.20, 15.03, 14.34; ^{19}F NMR (565 MHz, $CDCl_3$) δ: -118.09–-118.15 (m, 1F), -120.14-120.17 (m, 1F); HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{24}H_{20}F_2N_2NaO_4^+$: 461.1283, found: 461.1298.

Ethyl 5-bromo-1-(4-(2-bromobenzyl)-5-ethoxyoxazol-2-yl)isoquinoline-3-carboxylate (2m):



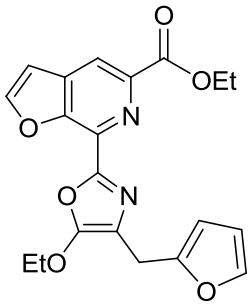
Eluent: ethyl acetate/petroleum ether (1/7). Yellow solid (49.3 mg, 44%), mp. 65–67 °C; R_f = 0.50 (ethyl acetate/petroleum ether = 1/4); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.63 (d, *J* = 8.6 Hz, 1H), 8.92 (s, 1H), 8.06 (d, *J* = 7.5 Hz, 1H), 7.63–7.61 (m, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 7.3 Hz, 1H), 7.24 (d, *J* = 7.5 Hz, 1H), 7.10 (t, *J* = 7.1 Hz, 1H), 4.56 (q, *J* = 7.1 Hz, 2H), 4.38 (q, *J* = 7.0 Hz, 2H), 4.06 (s, 2H), 1.51 (t, *J* = 7.1 Hz, 3H), 1.39 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 156.37, 145.36, 142.05, 138.35, 136.09, 134.88, 132.69, 130.72, 130.44, 128.49, 128.02, 127.82, 127.39, 124.52, 123.29, 123.24, 116.15, 70.16, 62.18, 31.62, 15.07, 14.35; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{24}H_{20}Br_2N_2NaO_4^+$: 580.9682, found: 580.9670.

Ethyl 1-(5-ethoxy-4-(4-methoxybenzyl)oxazol-2-yl)-7-methoxyisoquinoline-3-carboxylate (2n):



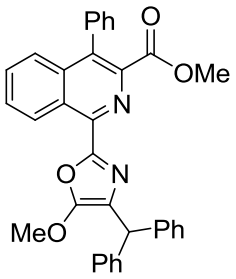
Eluent: ethyl acetate/petroleum ether (1/7). Yellow solid (62.0 mg, 67%), mp. 76–77 °C; R_f = 0.51 (ethyl acetate/petroleum ether = 1/4); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.99 (d, *J* = 2.3 Hz, 1H), 8.49 (s, 1H), 7.85 (d, *J* = 9.0 Hz, 1H), 7.40–7.38 (m, 1H), 7.28 (d, *J* = 8.5 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 4.52 (q, *J* = 7.1 Hz, 2H), 4.42 (q, *J* = 7.1 Hz, 2H), 3.87 (s, 3H), 3.85 (s, 2H), 3.78 (s, 3H), 1.49 (t, *J* = 7.1 Hz, 3H), 1.45 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 165.59, 161.26, 158.10, 155.18, 139.01, 132.34, 131.64, 129.85, 129.72, 128.94, 124.45, 124.16, 118.03, 113.74, 105.80, 70.31, 61.82, 55.48, 55.27, 30.28, 15.16, 14.39; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{26}H_{26}N_2NaO_6^+$: 485.1683, found: 485.1689.

Ethyl 7-(5-ethoxy-4-(furan-2-ylmethyl)oxazol-2-yl)furo[2,3-c]pyridine-5-carboxylate (2o):



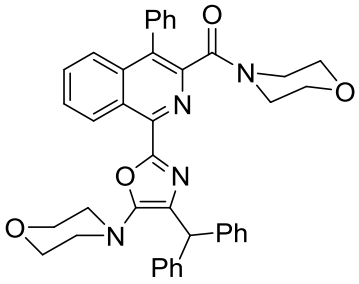
Eluent: ethyl acetate/petroleum ether (1/8). Brown liquid (32.1 mg, 42%); R_f = 0.50 (ethyl acetate/petroleum ether = 1/4); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.30 (s, 1H), 7.87 (d, *J* = 2.0 Hz, 1H), 7.65 (s, 1H), 7.34 (s, 1H), 6.31 (d, *J* = 2.1 Hz, 1H), 6.11 (d, *J* = 2.8 Hz, 1H), 4.52 (q, *J* = 7.1 Hz, 2H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.92 (s, 2H), 1.49 (t, *J* = 7.1 Hz, 3H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 165.11, 160.47, 155.76, 152.52, 148.80, 143.48, 141.33, 139.85, 124.82, 115.81, 110.38, 109.42, 107.68, 106.17, 70.58, 62.18, 24.45, 15.03, 14.33; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{20}H_{18}N_2NaO_6^+$: 405.1057, found: 405.1065.

Methyl 1-(4-benzhydryl-5-methoxyoxazol-2-yl)-4-phenylisoquinoline-3-carboxylate (2p):



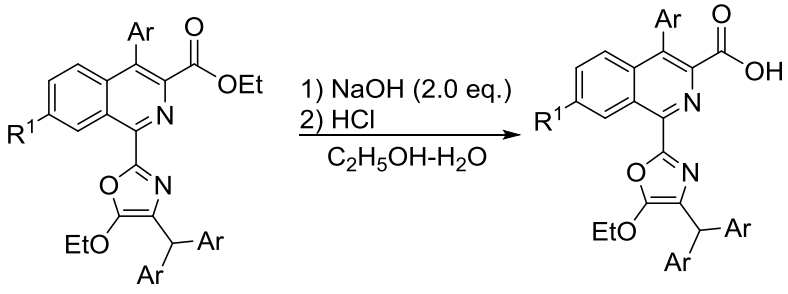
Eluent: ethyl acetate/petroleum ether (1/7). Brown liquid (75.8 mg, 72%); R_f = 0.45 (ethyl acetate/petroleum ether = 1/4); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.56 (d, *J* = 8.6 Hz, 1H), 7.73–7.70 (m, 1H), 7.65 (d, *J* = 3.5 Hz, 2H), 7.53–7.48 (m, 3H), 7.41 (d, *J* = 7.4 Hz, 4H), 7.36–7.30 (m, 6H), 7.25–7.22 (m, 2H), 5.47 (s, 1H), 3.99 (s, 3H), 3.73 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 142.61, 140.69, 136.80, 135.95, 134.99, 130.82, 129.65, 129.63, 128.94, 128.33, 128.26, 128.13, 127.89, 126.76, 126.51, 126.49, 119.59, 60.77, 52.48, 47.15; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{34}H_{26}N_2NaO_4^+$: 549.1785, found: 549.1789.

(1-(4-Benzhydryl-5-morpholinooxazol-2-yl)-4-phenylisoquinolin-3-yl)(morpholino)methanone (2q):



Eluent: acetone/petroleum ether (1/10). Brown liquid (87.9 mg, 69%); R_f = 0.50 (acetone/petroleum ether = 2/5); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.45–9.43 (m, 1H), 7.76–7.74 (m, 1H), 7.69–7.67 (m, 1H), 7.65–7.63 (m, 2H), 7.53–7.50 (m, 3H), 7.49–7.47 (t, *J* = 6.3 Hz, 3H), 7.42 (d, *J* = 7.7 Hz, 3H), 7.33 (t, *J* = 7.6 Hz, 4H), 7.24 (d, *J* = 7.3 Hz, 1H), 5.52 (s, 1H), 3.77–3.75 (m, 4H), 3.62–3.60 (m, 2H), 3.50–3.49 (m, 2H), 3.26–3.24 (m, 2H), 3.17–3.13 (m, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 167.36, 142.90, 136.01, 134.64, 132.08, 130.77, 130.69, 130.55, 129.05, 128.68, 128.62, 128.54, 128.46, 128.34, 127.94, 126.51, 126.11, 125.73, 66.82, 66.50, 50.79, 47.76, 46.90, 41.74; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{40}H_{36}N_4NaO_4^+$: 659.2629, found: 659.2639.

III. General Procedure for the Preparation of 3 (3a as Example):

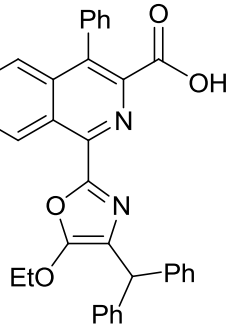


2a, Ar = C_6H_5, R^1 = H
2d, Ar = C_6H_4Me-*p*, R^1 = Me

3a, Ar = C_6H_5, R^1 = H, 99%
3d, Ar = C_6H_4Me-*p*, R^1 = Me, 98%

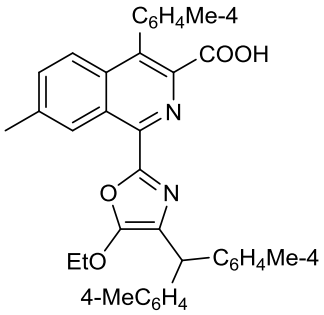
To a suspension solution of **2a** (0.5 mmol, 277.3 mg) in a C_2H_5OH/H_2O (10 mL, v/v = 1/1) was added the NaOH (40.0 mg, 1.0 mmol). The reaction mixture was stirred for 8 h under refluxing until compound **2a** was consumed (monitored by TLC). The reaction mixture was poured into saturated aqueous NaCl (15.0 mL), followed by acidification with HCl solution to adjust the pH value of the solution to 4, and extracted with CH_2Cl_2 (6 mL × 3). The combined organic extracts were dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure to yield the product **3a** (260.7 mg, 99%), which may be used in the next step without purification.

1-(4-Benzhydryl-5-ethoxyoxazol-2-yl)-4-phenylisoquinoline-3-carboxylic acid (3a):



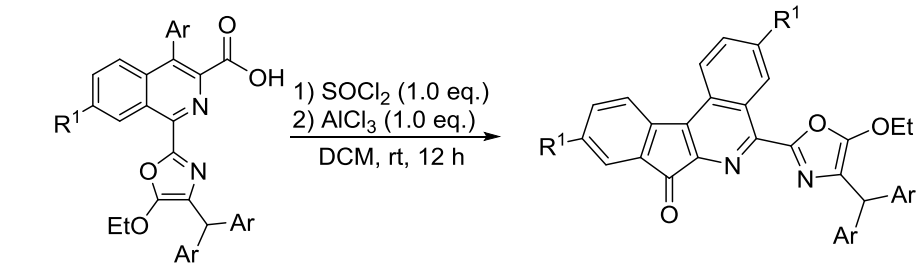
Yellow solid (260.7 mg, 99%); mp. 179–180 °C; R_f = 0.45 (acetone/acetic acid/petroleum ether = 1/1/5); ^{1}H NMR (600 MHz, DMSO-d_6) δ: 13.17 (s, 1H), 9.43 (d, *J* = 7.5 Hz, 1H), 7.85–7.77 (m, 2H), 7.59 (d, *J* = 7.4 Hz, 1H), 7.55–7.50 (m, 3H), 7.44 (d, *J* = 6.3 Hz, 4H), 7.41–7.38 (m, 2H), 7.35 (s, 4H), 7.24 (s, 2H), 5.51 (s, 1H), 4.30–4.22 (m, 2H), 1.24 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 168.33, 155.66, 143.31, 142.99, 136.30, 135.42, 131.95, 131.83, 130.38, 129.89, 129.09, 128.82, 128.78, 128.72, 127.23, 126.94, 126.43, 125.64, 120.66, 71.27, 46.66, 15.23; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{34}H_{26}N_2NaO_4^+$: 549.1785, found: 549.1760.

1-(4-(Di-*p*-tolylmethyl)-5-ethoxyoxazol-2-yl)-7-methyl-4-(*p*-tolyl)isoquinoline-3-carboxylic acid (3d):



Yellow solid (285.5 mg, 98%); mp. 185–186 °C; R_f = 0.45 (acetone/acetic acid/petroleum ether = 1/1/5); ^{1}H NMR (600 MHz, DMSO-d_6) δ: 8.90 (s, 1H), 7.36 (d, *J* = 8.5 Hz, 1H), 7.31 (d, *J* = 8.6 Hz, 1H), 7.17 (d, *J* = 7.5 Hz, 4H), 7.14 (d, *J* = 7.4 Hz, 2H), 7.10 (d, *J* = 7.3 Hz, 2H), 7.00 (d, *J* = 7.5 Hz, 4H), 5.21 (s, 1H), 4.12 (q, *J* = 6.8 Hz, 2H), 2.32 (s, 3H), 2.24 (s, 3H), 2.12 (s, 6H), 1.12 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 171.54, 154.87, 151.10, 140.49, 137.06, 136.74, 135.82, 134.93, 134.19, 132.62, 130.68, 129.27, 128.91, 128.85, 127.54, 125.83, 125.71, 120.44, 71.16, 45.61, 22.03, 21.35, 21.05, 15.26; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{38}H_{34}N_2NaO_4^+$: 605.2411, found: 605.2408.

IV. General Procedure for the Preparation of 4 (4a as Example):

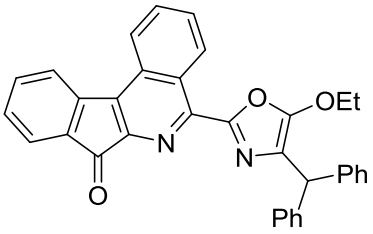


3a, Ar = C_6H_5, R^1 = H
3d, Ar = C_6H_4Me-*p*, R^1 = Me

4a, Ar = C_6H_5, R^1 = H, 57%
4d, Ar = C_6H_4Me-*p*, R^1 = Me, 53%

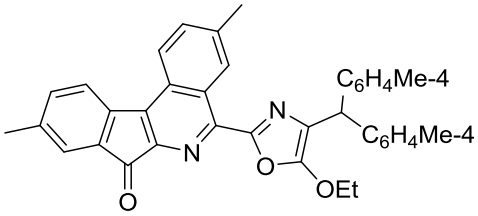
To a solution of thionyl chloride (0.6 mmol) in CH_2Cl_2 (15.0 mL) was slowly added the **3a** (0.5 mmol, 263 mg) under nitrogen atmosphere at room temperature. After the reaction mixture was stirred for 12 h at room temperature, $AlCl_3$ (0.6 mmol, 80.0 mg) was added in one-pot. After the reaction mixture was stirred at room temperature for 1 h, the mixture was poured into saturated aqueous NaCl (15.0 mL), followed by basification with saturated aqueous $NaHCO_3$ solution to adjust the pH value of the solution to 7, and extracted with CH_2Cl_2 (6 mL × 3). The combined organic extracts were dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure to yield the crude product, which was purified by chromatography (acetone/petroleum ether = 3:10, V/V) to give **4a** (144.9 mg, 57%) as a red solid.

5-(4-Benzhydryl-5-ethoxyoxazol-2-yl)-7*H*-indeno[2,1-*c*]isoquinolin-7-one (4a):



Eluent: acetone/petroleum ether (1/4). Red solid (144.9 mg, 57%), mp. 92–94 ^oC; R_f = 0.45 (acetone/petroleum ether = 2/5); ^1H NMR (600 MHz, $CDCl_3$) δ: 9.60 (d, *J* = 8.6 Hz, 1H), 8.44 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 7.5 Hz, 1H), 7.82 (t, *J* = 7.6 Hz, 1H), 7.76–7.72 (m, 2H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.40 (d, *J* = 7.5 Hz, 4H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 4H), 7.24 (t, *J* = 7.3 Hz, 2H), 5.47 (s, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 1.30 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 192.48, 155.92, 150.13, 145.76, 145.17, 142.64, 142.06, 136.74, 135.00, 133.01, 132.15, 131.69, 130.62, 129.75, 129.71, 128.95, 128.40, 128.27, 126.46, 124.49, 124.02, 123.86, 120.39, 70.29, 47.16, 14.95; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{34}H_{24}N_2NaO_3^+$: 531.1679, found: 531.1668.

5-(4-(Di-*p*-tolylmethyl)-5-ethoxyoxazol-2-yl)-3,9-dimethyl-7*H*-indeno[2,1-*c*]isoquinolin-7-one (4d):



Eluent: acetone/petroleum ether (1/4). Red solid (149.6 mg, 53%), mp. 112–114 °C; R_f = 0.45 (acetone/petroleum ether = 2/5); ^{1}H NMR (600 MHz, $CDCl_3$) δ: 9.27 (s, 1H), 8.21 (d, *J* = 8.6 Hz, 1H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 1H), 7.48 (s, 1H), 7.31 (d, *J* = 8.0 Hz, 4H), 7.27 (d, *J* = 7.7 Hz, 1H), 7.13 (d, *J* = 7.9 Hz, 4H), 5.37 (s, 1H), 4.34 (q, *J* = 7.0 Hz, 2H), 2.51 (s, 3H), 2.36 (s, 3H), 2.32 (s, 6H), 1.34 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ: 192.77, 155.52, 150.16, 144.63, 144.44, 141.05, 140.10, 140.07, 139.16, 137.16, 135.84, 135.02, 133.57, 133.33, 130.03, 128.93, 128.78, 128.69, 125.15, 123.82, 123.54, 120.43, 70.34, 46.02, 22.32, 21.33, 21.00, 15.03; HRMS(ESI-TOF): $[M + Na]^+$ calculated for $C_{38}H_{32}N_2NaO_3^+$: 587.2305, found: 587.2302.

V. ORTEP Drawing of Compound 2k:

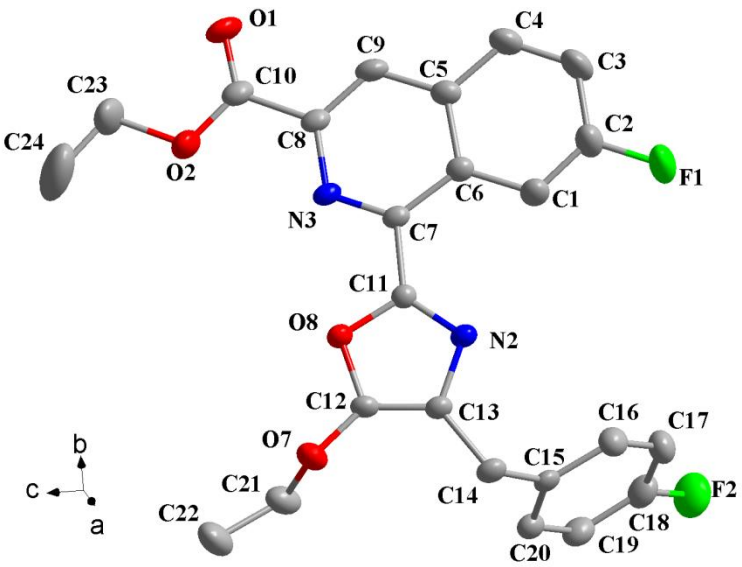


Figure 1. Crystal ORTEP drawing of compound 2k

VI. Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR Spectra of Compounds 2-4:

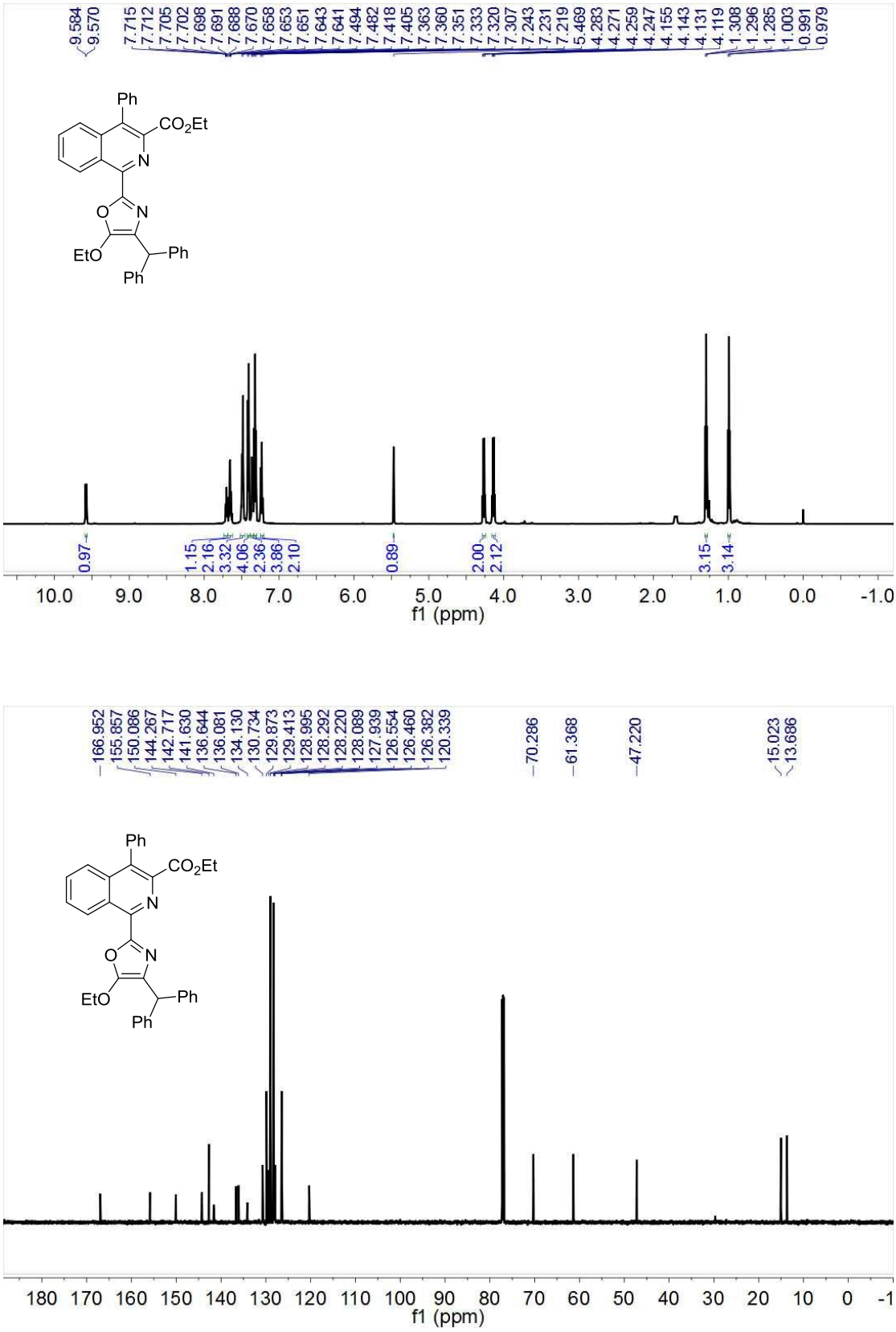


Figure 2. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2a**

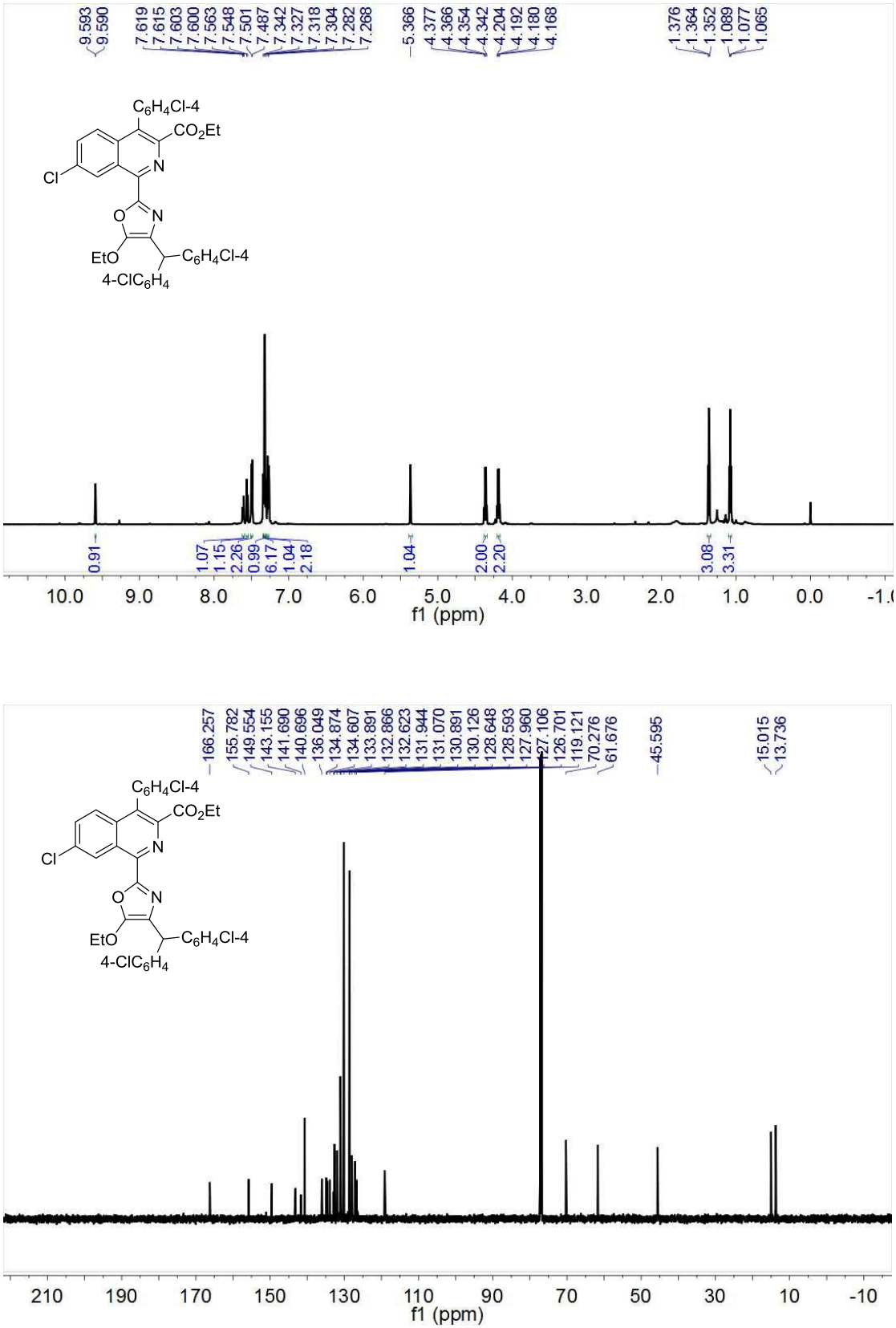
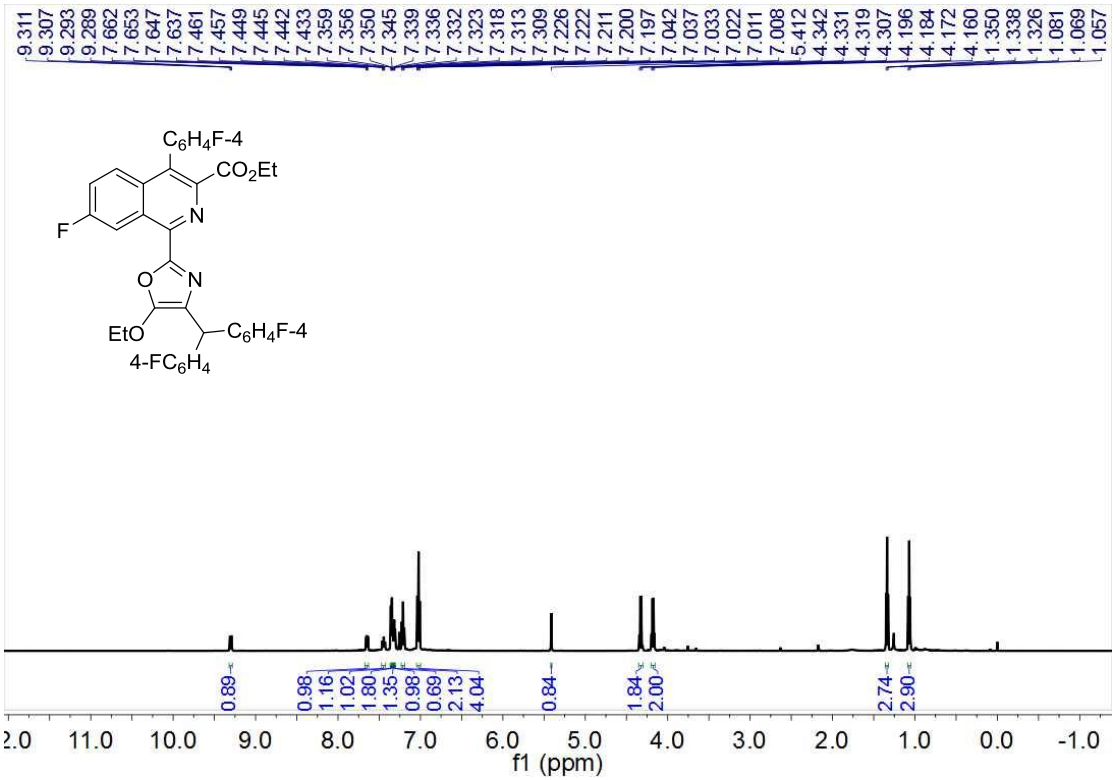
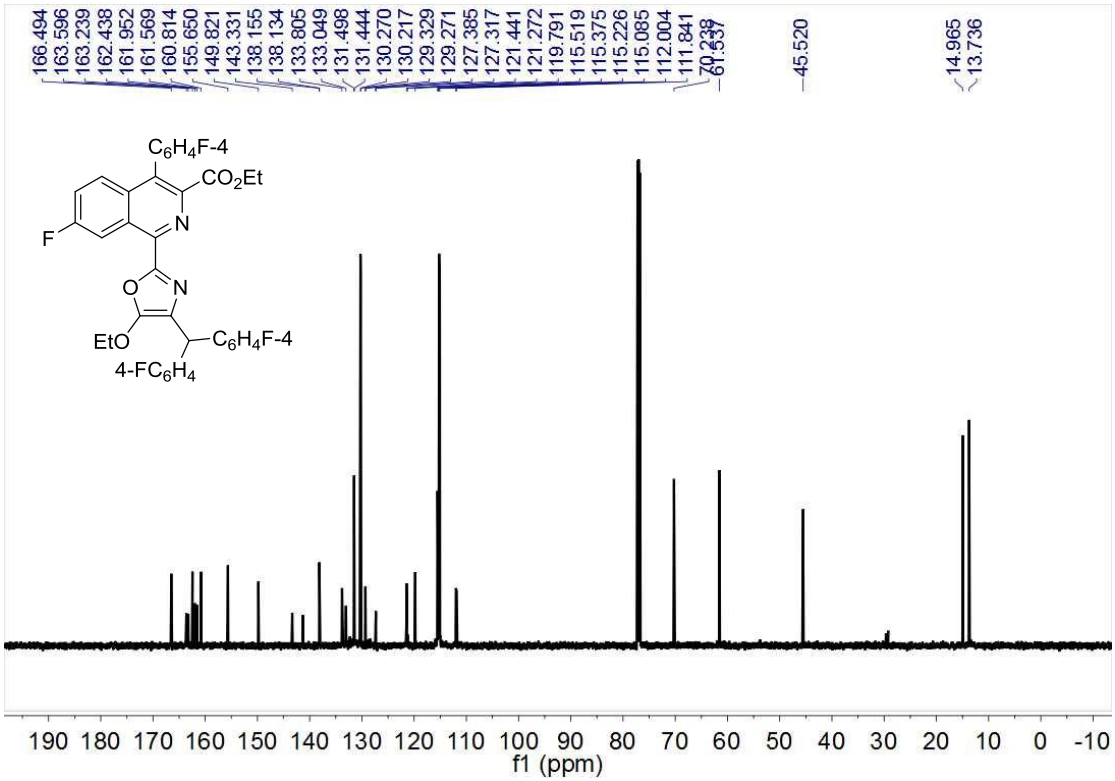


Figure 3. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2b**

.


9.311
9.307
9.293
9.289
7.662
7.653
7.647
7.637
7.461
7.457
7.449
7.445
7.442
7.433
7.359
7.356
7.350
7.345
7.339
7.336
7.332
7.323
7.318
7.313
7.309
7.226
7.222
7.211
7.200
7.197
7.042
7.037
7.033
7.022
7.011
7.008
5.412
4.342
4.331
4.319
4.307
4.196
4.184
4.172
4.160
1.350
1.338
1.326
1.081
1.069
1.057
C6H4F-4
CO2Et
F
N
O
N
EtO
C6H4F-4
4-FC6H4
0.89
0.98
1.16
1.02
1.80
1.35
0.98
0.69
2.13
4.04
0.84
1.84
2.00
2.74
2.90
f1 (ppm)


166.494
163.596
163.239
162.438
161.952
161.569
160.814
155.650
149.821
143.331
138.155
138.134
133.805
133.049
131.498
131.444
130.270
130.217
129.329
129.271
127.385
127.317
121.441
121.272
119.791
115.519
115.375
115.226
115.085
112.004
111.841
70.238
61.537
45.520
14.965
13.736
C6H4F-4
CO2Et
F
N
O
N
EtO
C6H4F-4
4-FC6H4
f1 (ppm)

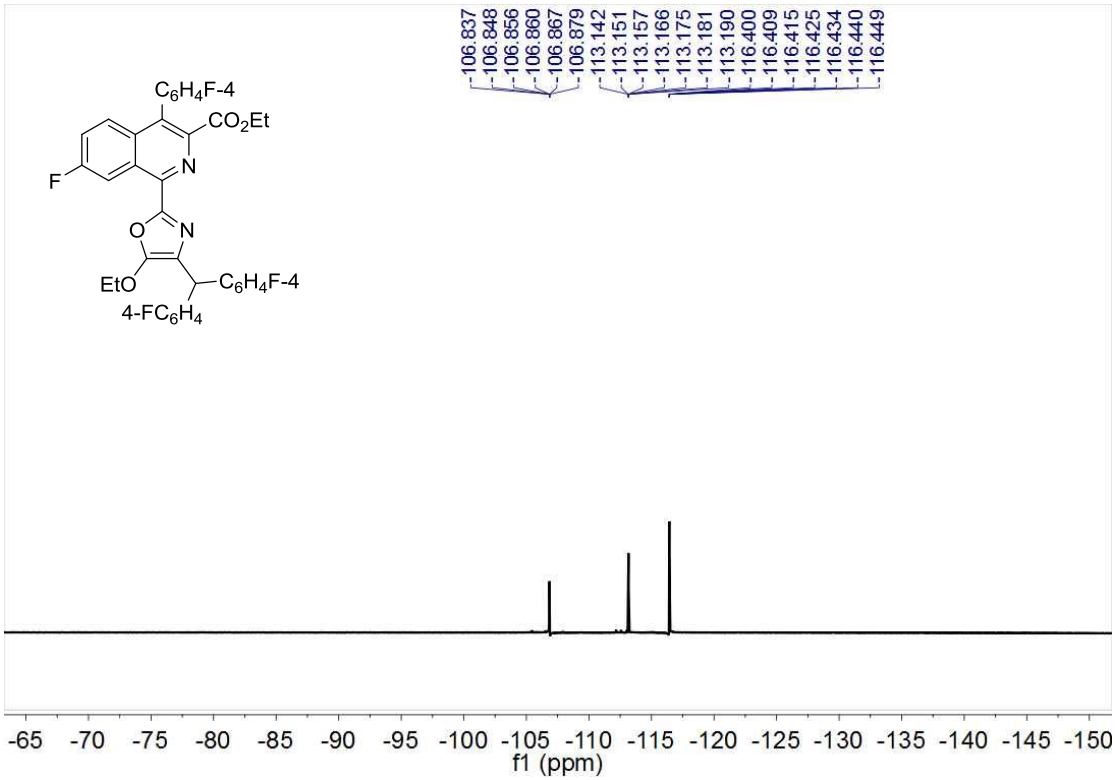
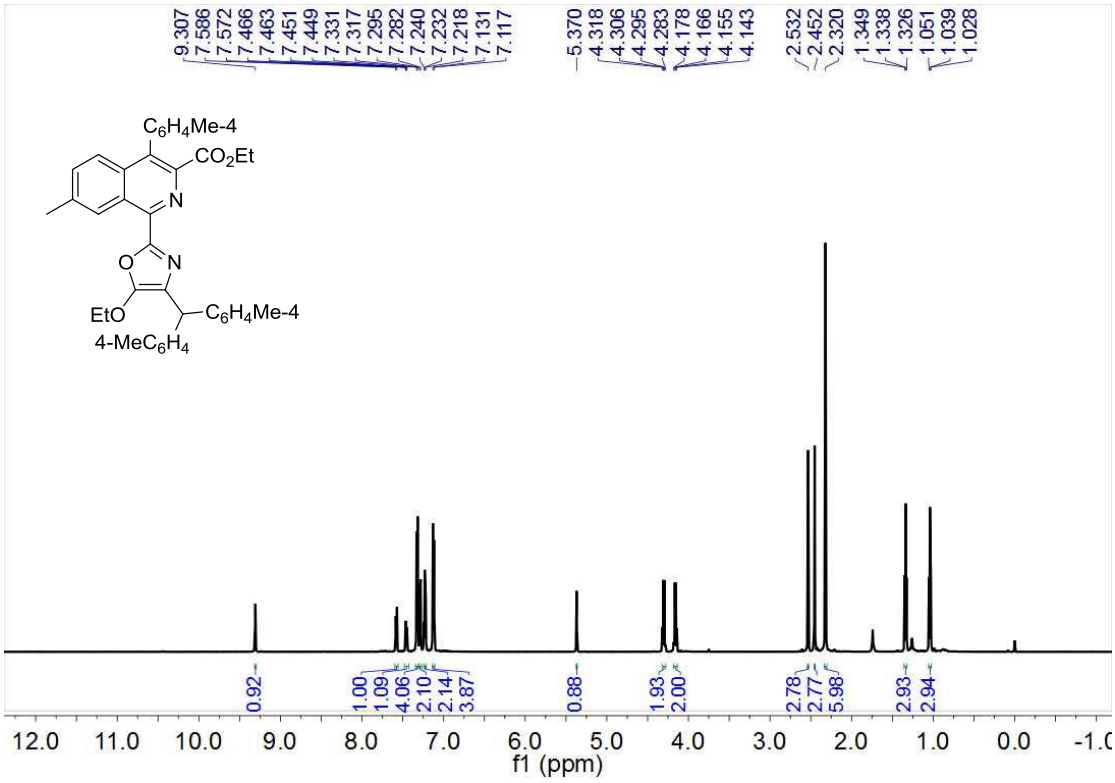


Figure 4. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra of compound **2c**

.



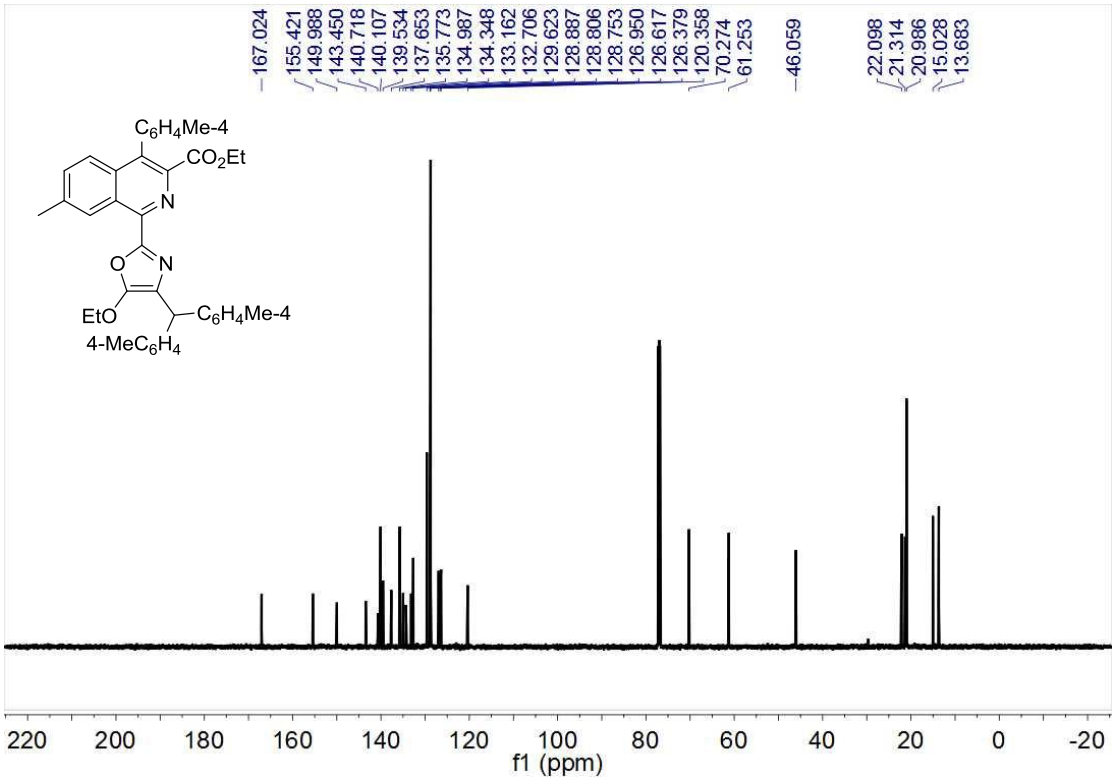
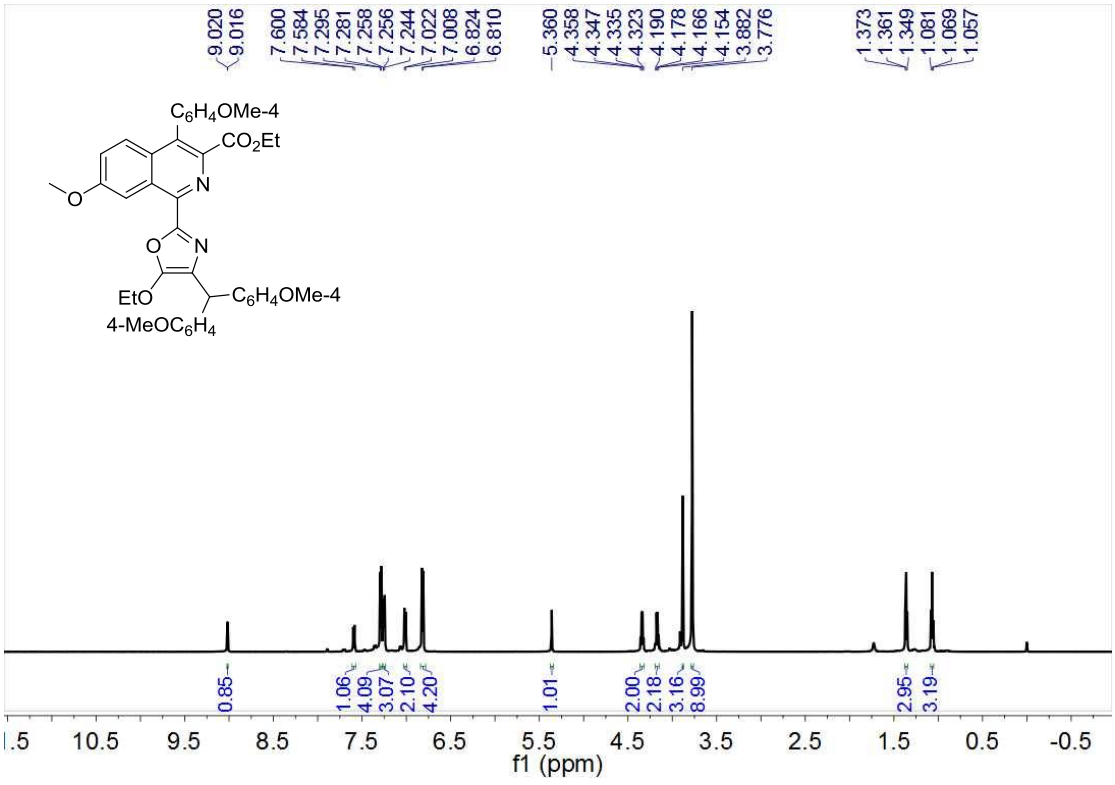


Figure 5. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2d**



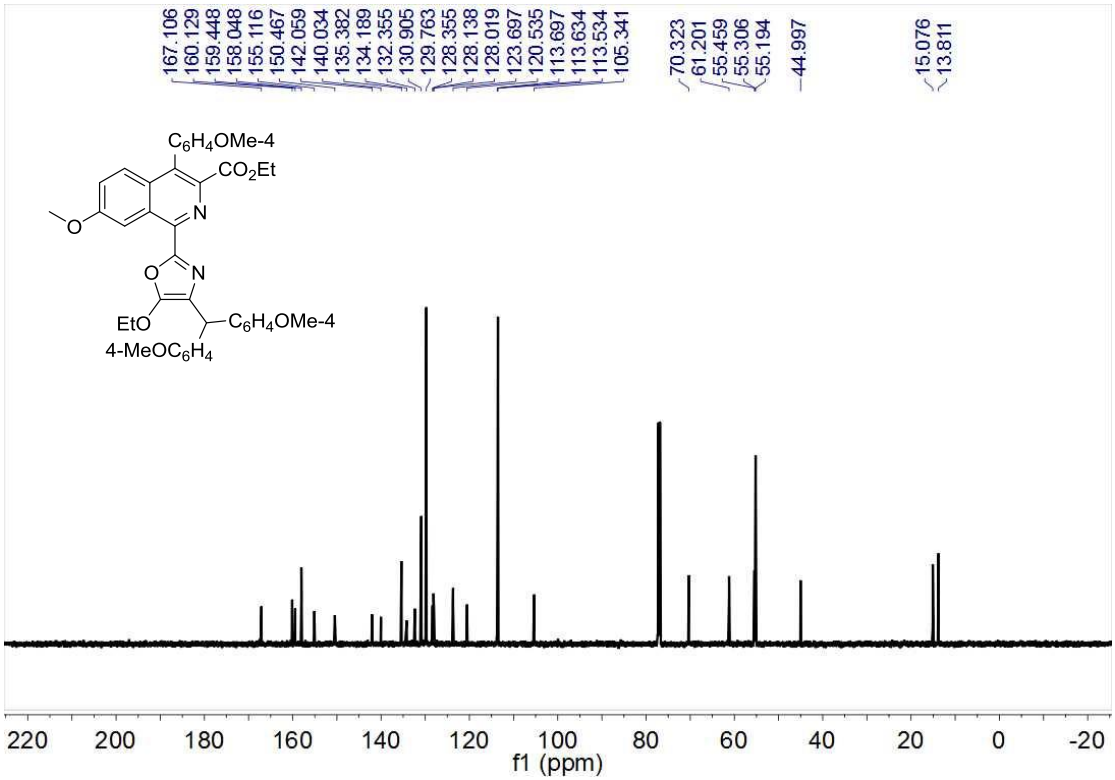
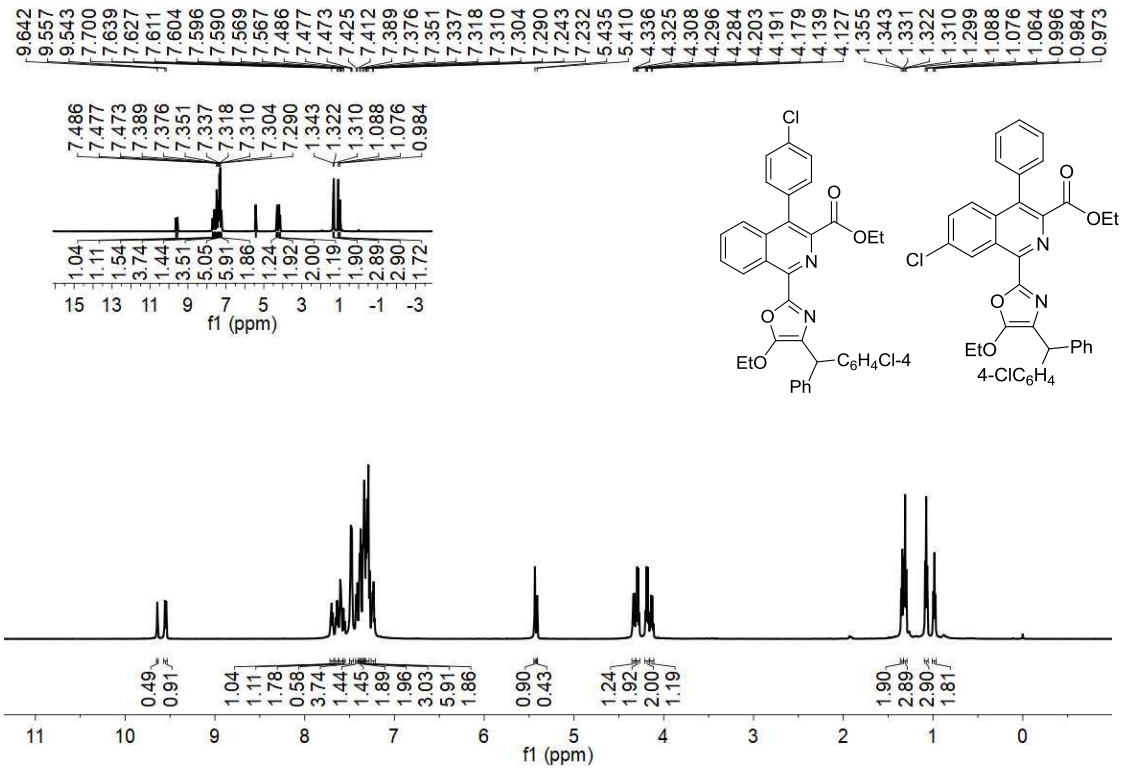


Figure 6. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2e**



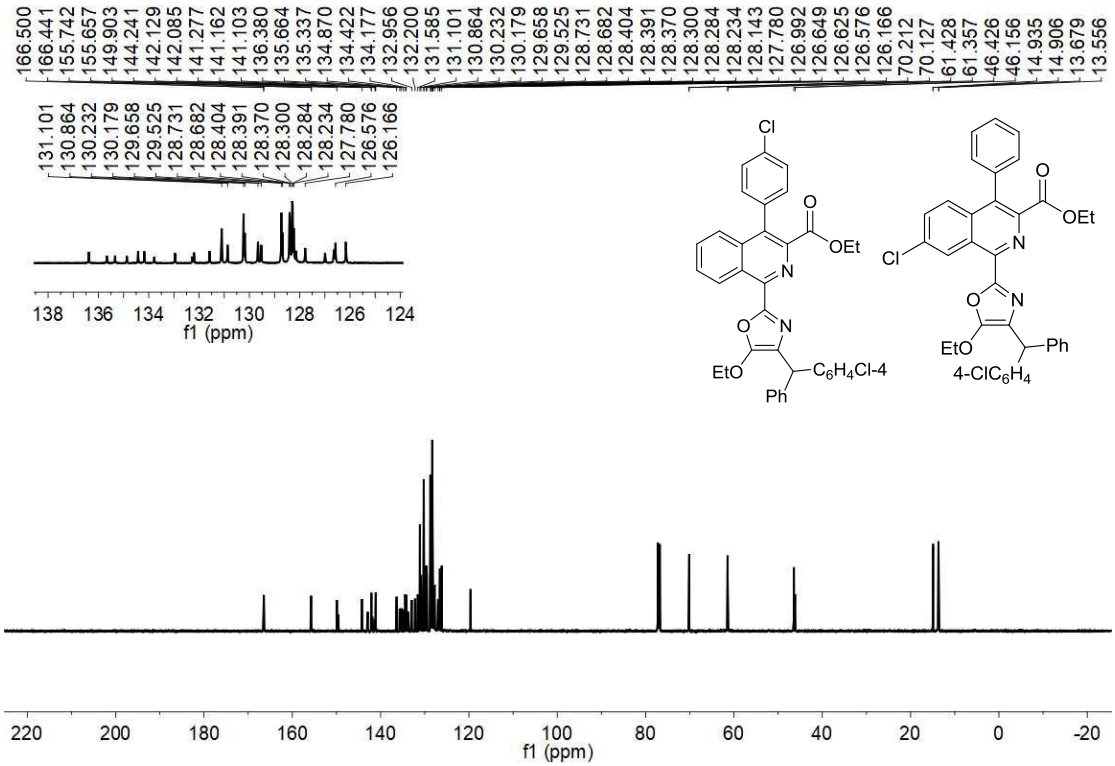
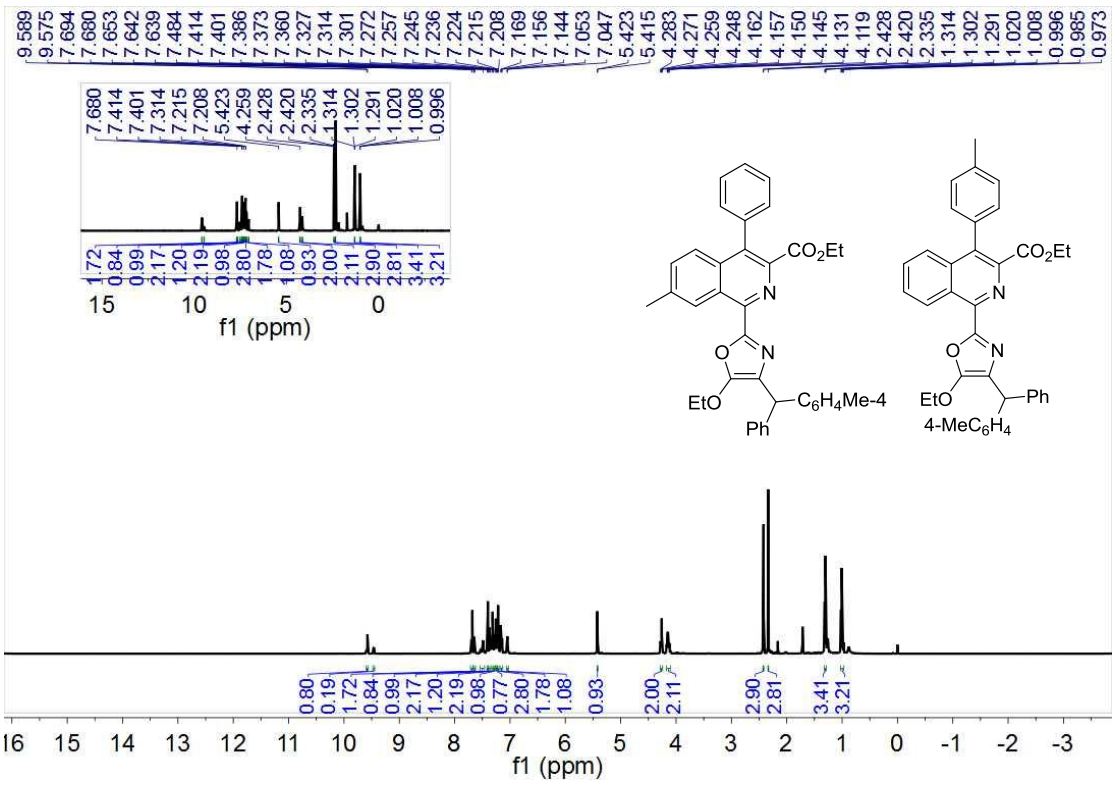


Figure 7. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2f** and **2f'**



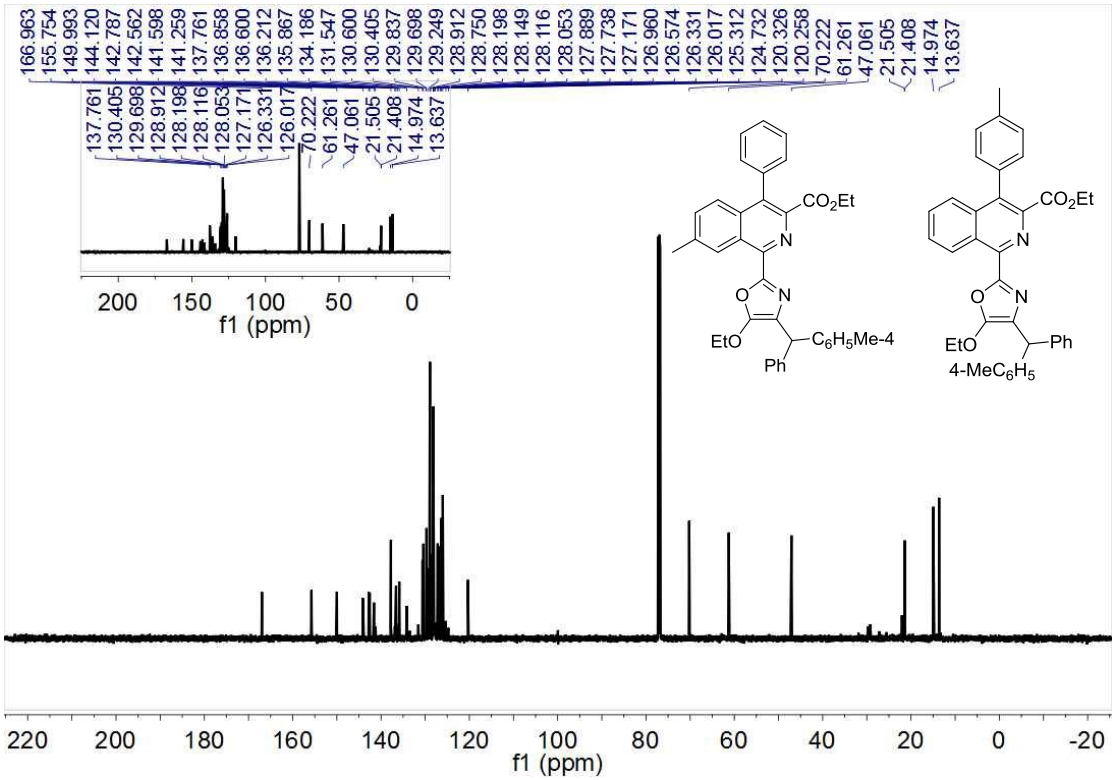
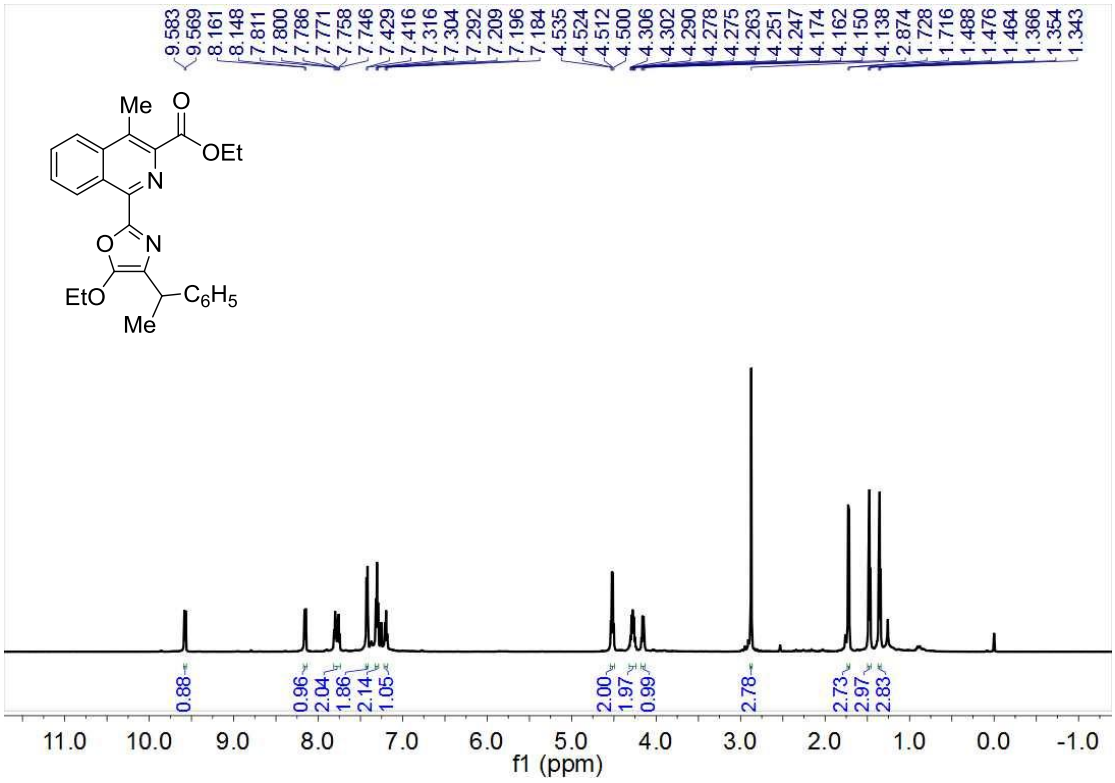


Figure 8. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2g** and **2g'**



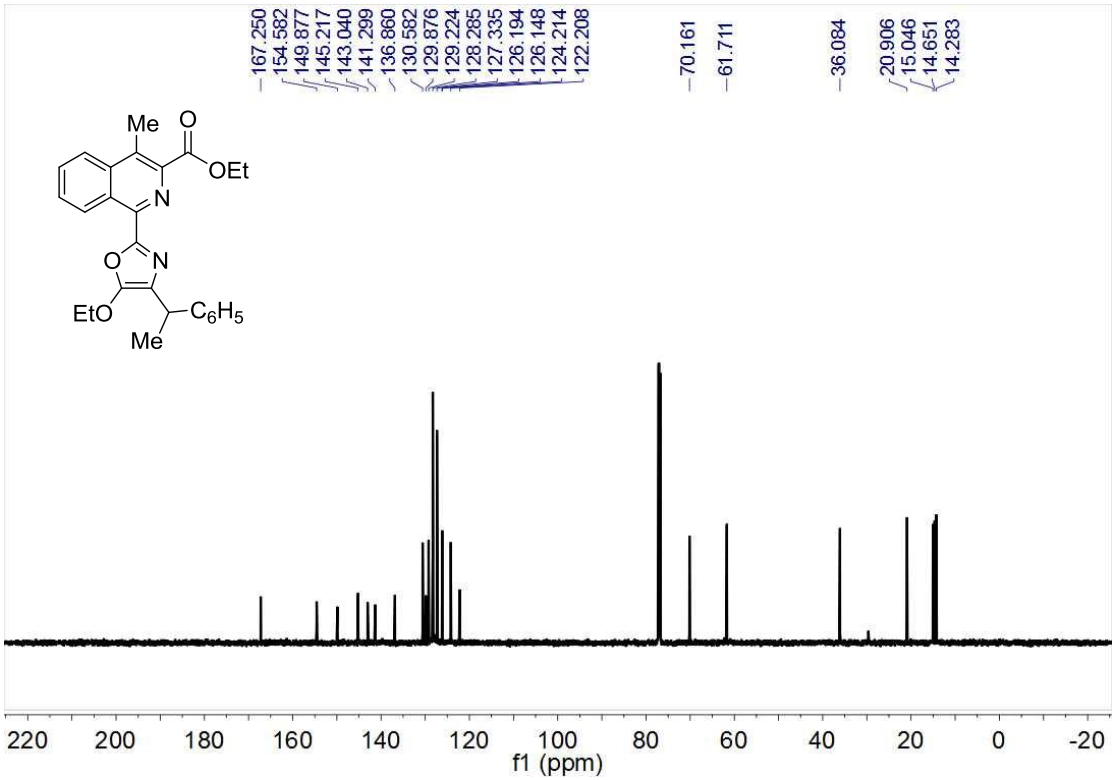
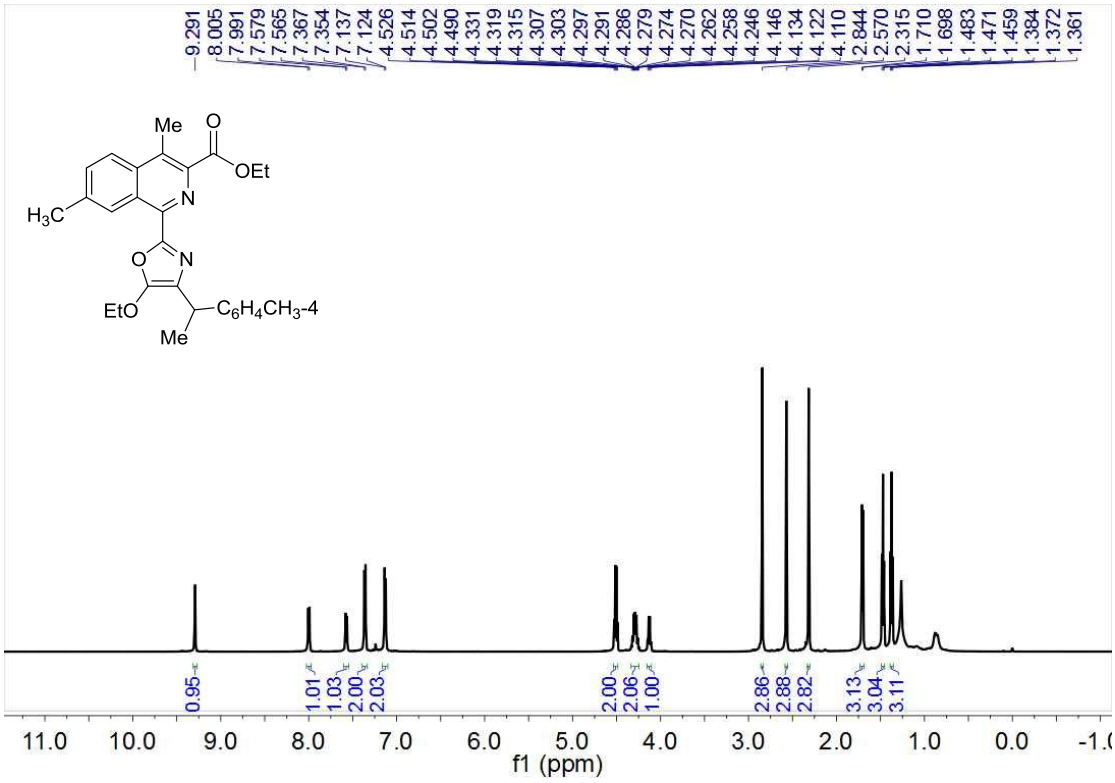


Figure 9. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2h**



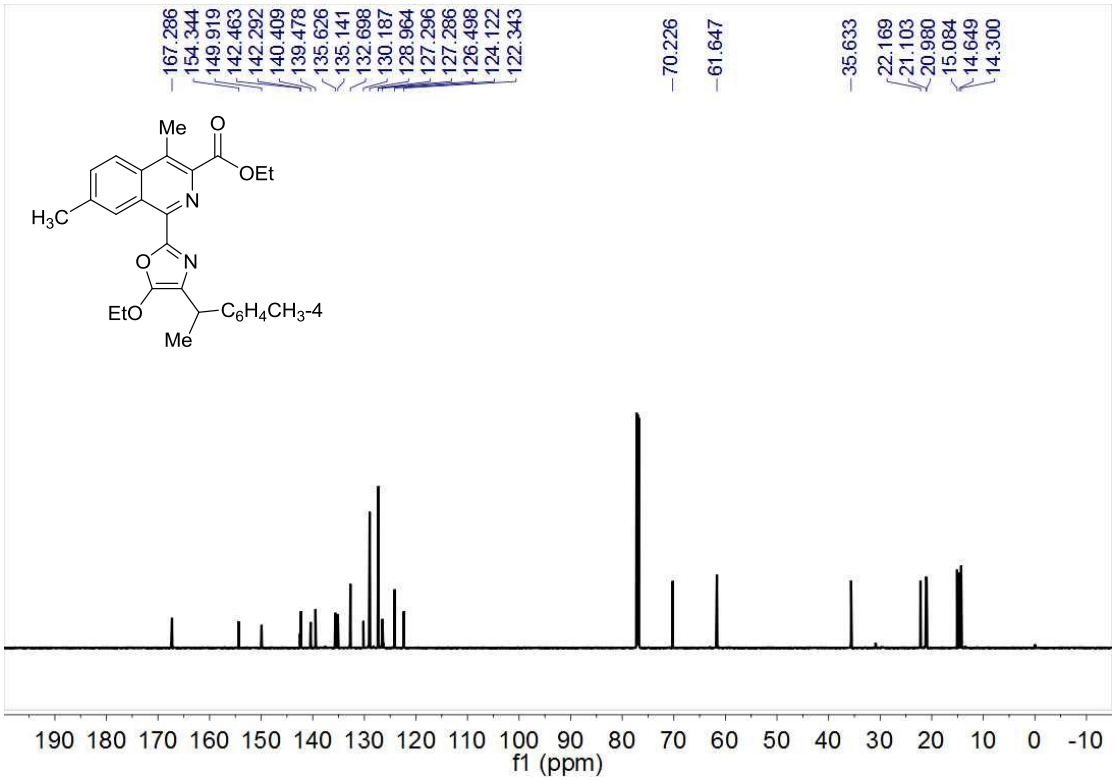
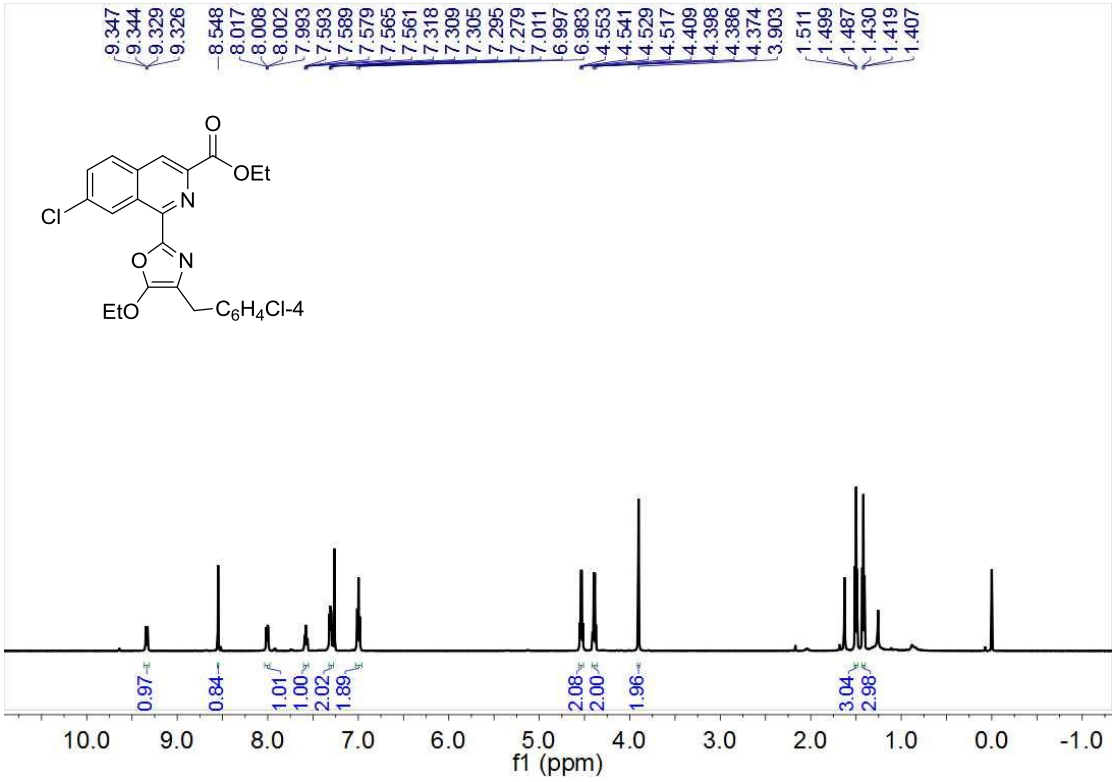


Figure 10. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2i**



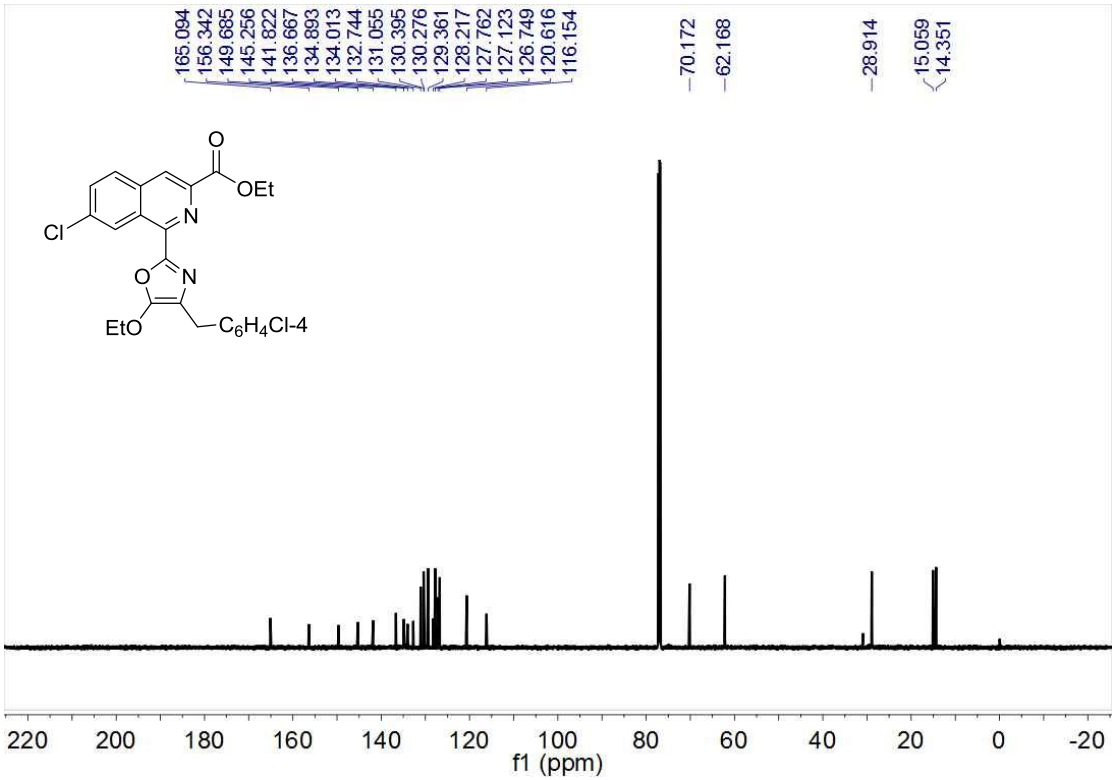
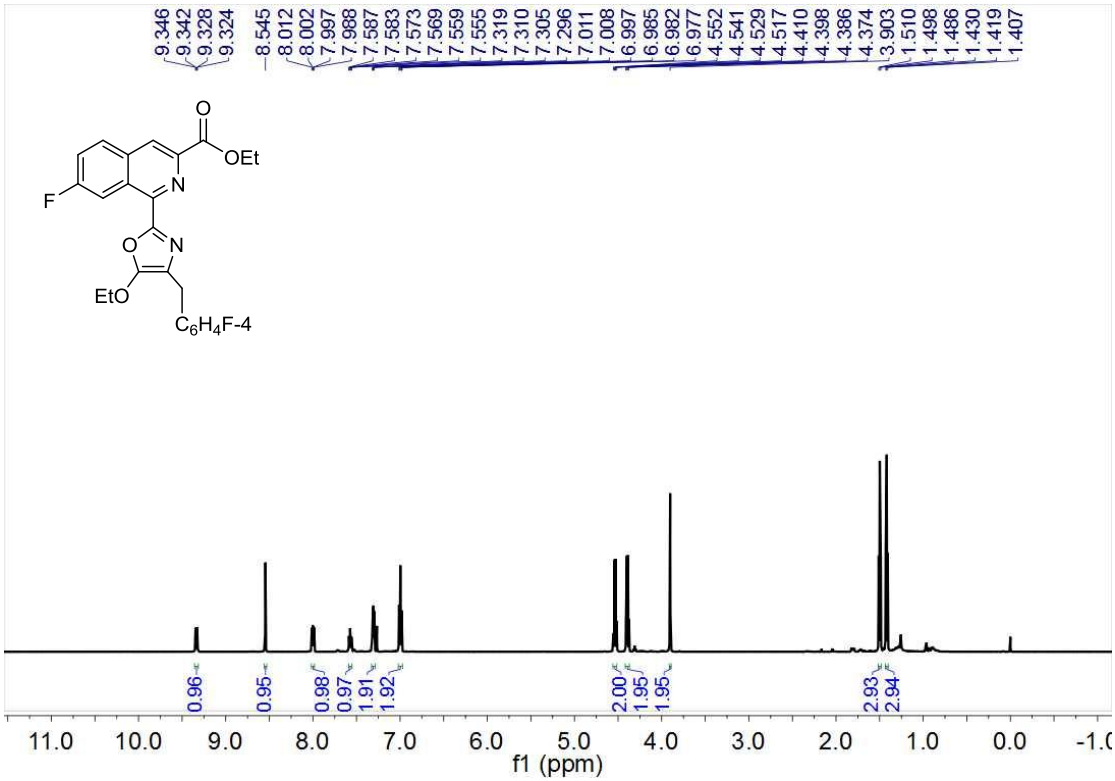
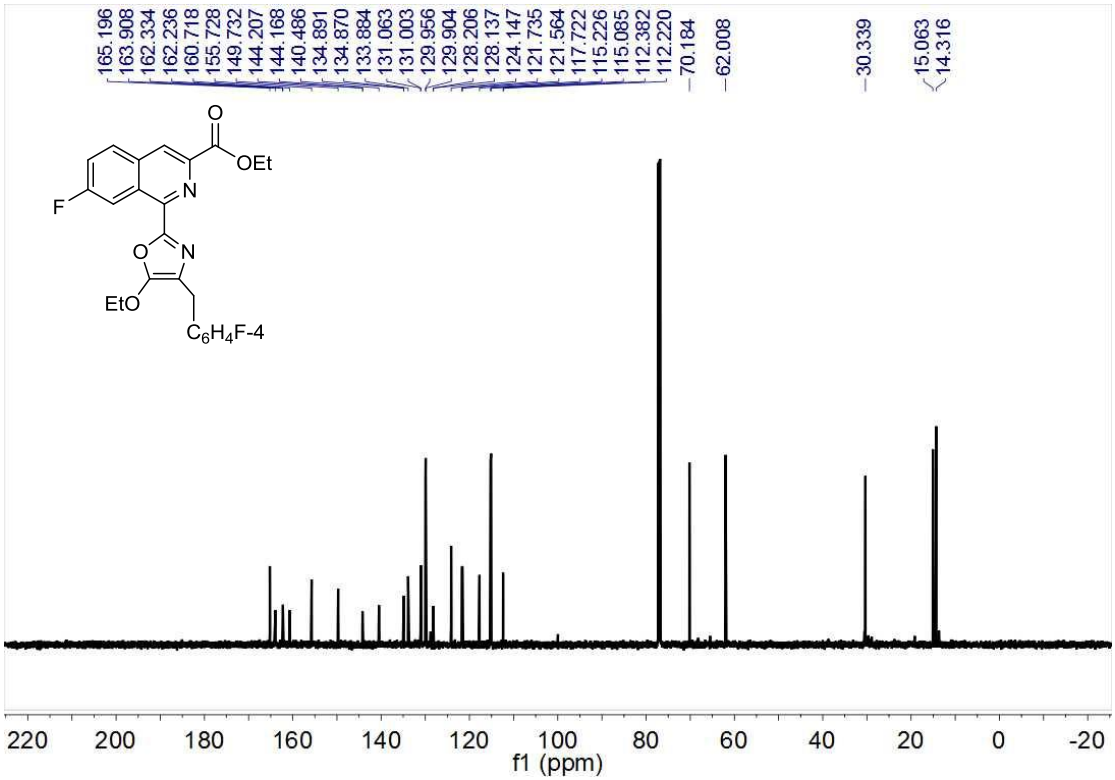


Figure 11. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2j**





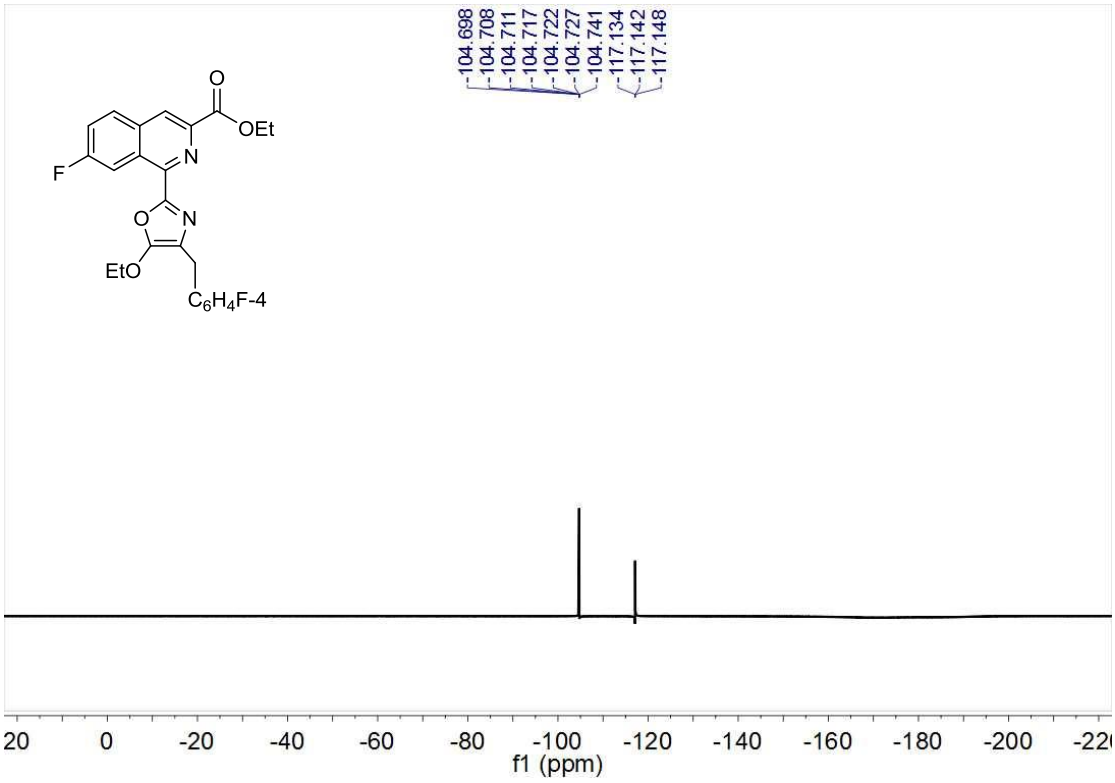
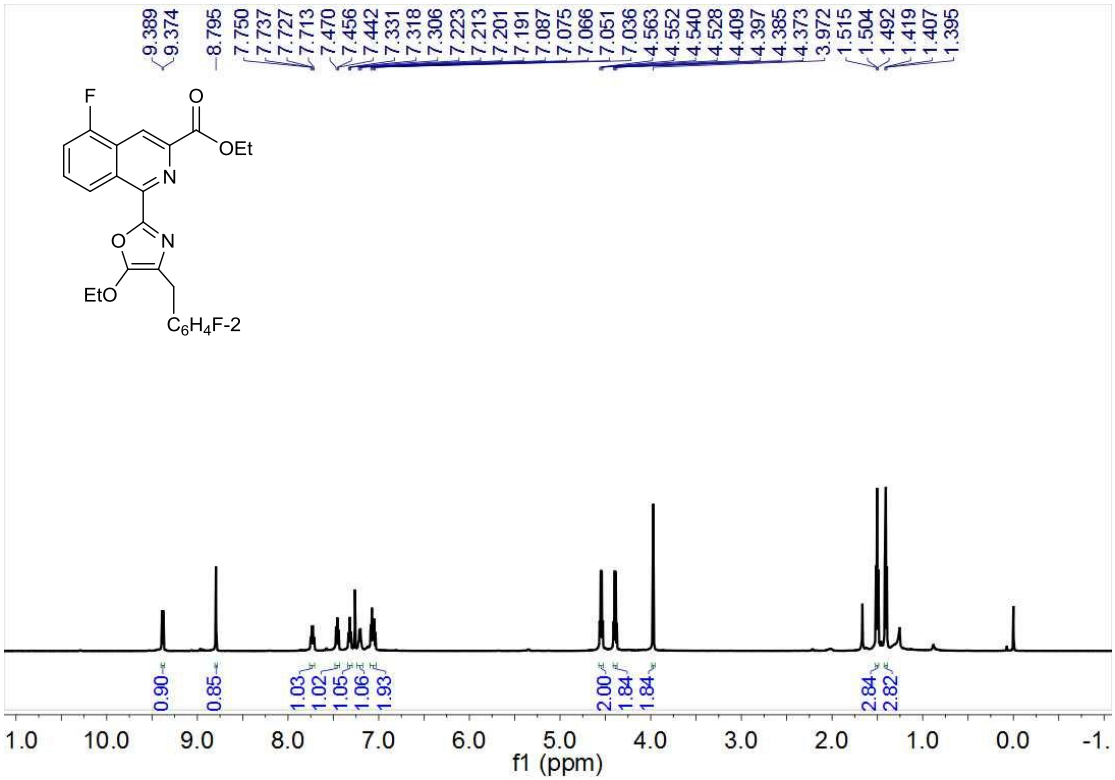
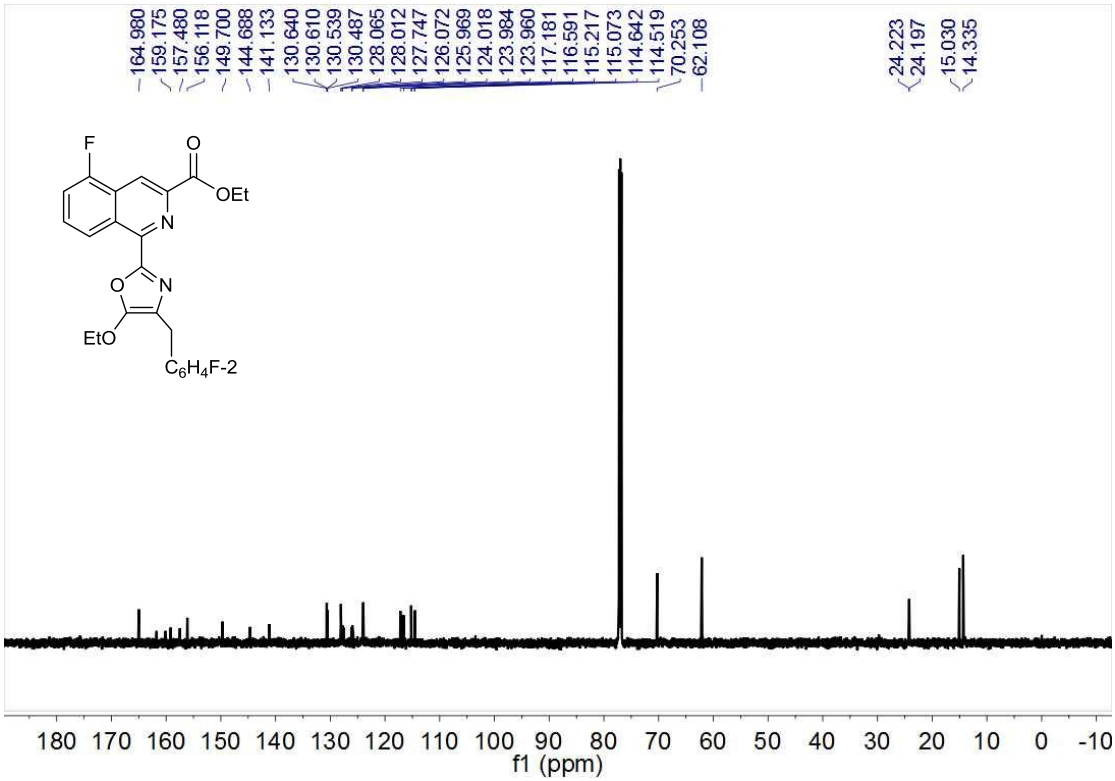


Figure 12. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra of compound **2k**


9.389
9.374
8.795
7.750
7.737
7.727
7.713
7.470
7.456
7.442
7.331
7.318
7.306
7.223
7.213
7.201
7.191
7.087
7.075
7.066
7.051
7.036
4.563
4.552
4.540
4.528
4.409
4.397
4.385
4.373
3.972
1.515
1.504
1.492
1.419
1.407
1.395
F
O
OEt
N
O
N
EtO
C6H4F-2
0.90
0.85
1.03
1.02
1.05
1.06
1.93
2.00
1.84
1.84
2.84
2.82
1.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.
f1 (ppm)


164.980
159.175
157.480
156.118
149.700
144.688
141.133
130.640
130.610
130.539
130.487
128.065
128.012
127.747
126.072
125.969
124.018
123.984
123.960
117.181
116.591
115.217
115.073
114.642
114.519
70.253
62.108
24.223
24.197
15.030
14.335
F
O
OEt
N
O
N
EtO
C6H4F-2
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

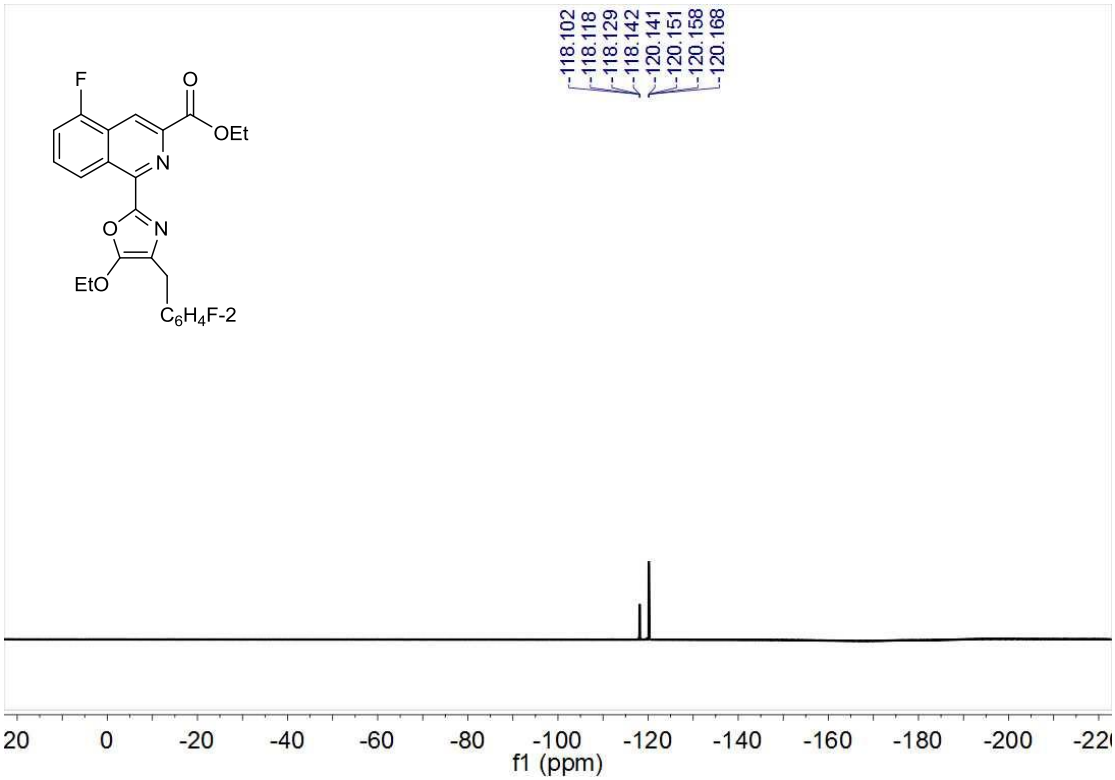
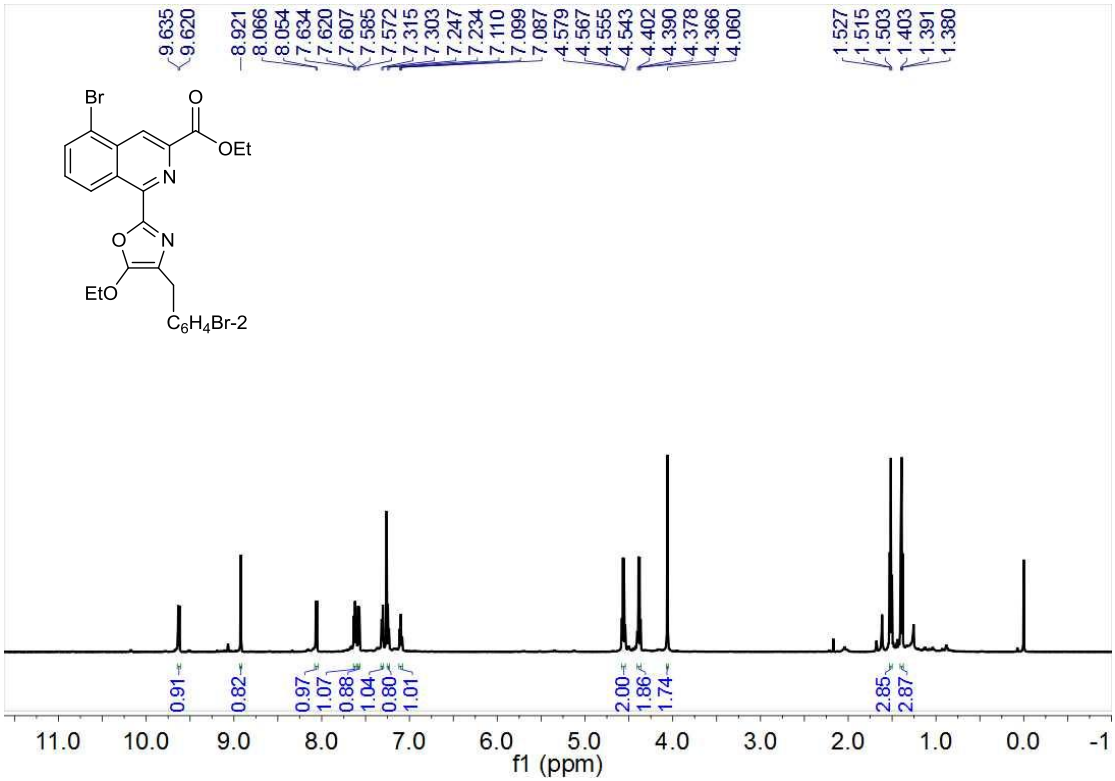


Figure 13. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra of compound **2l**



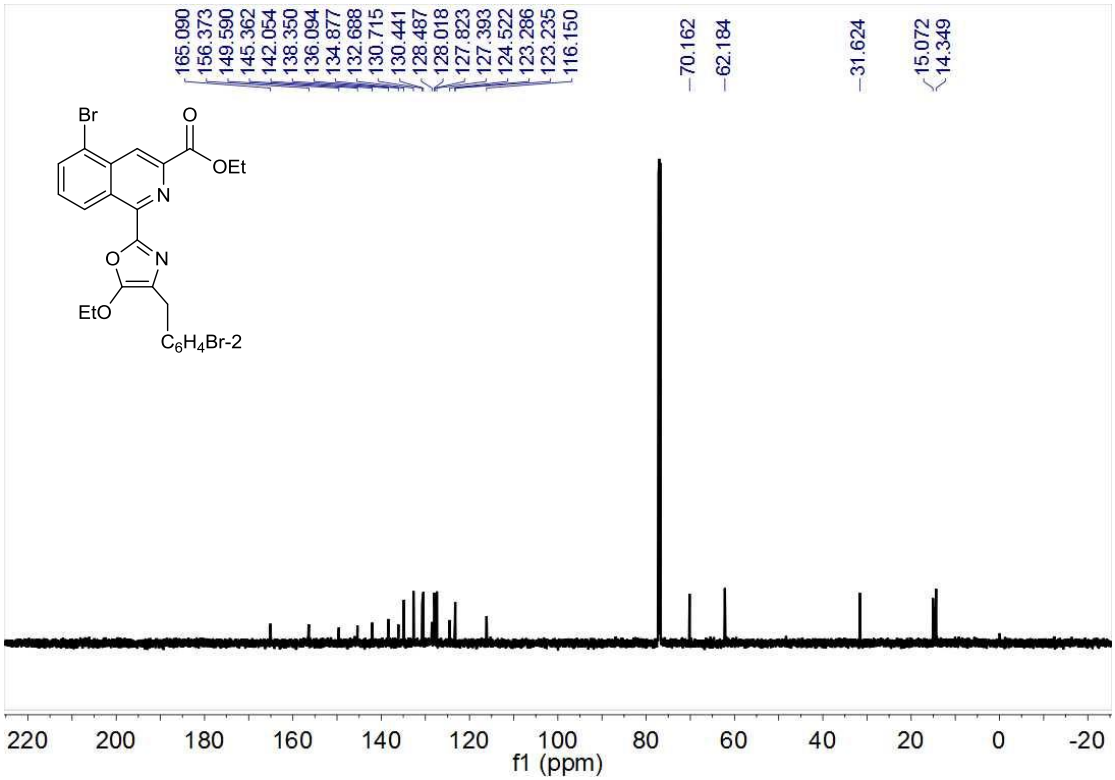
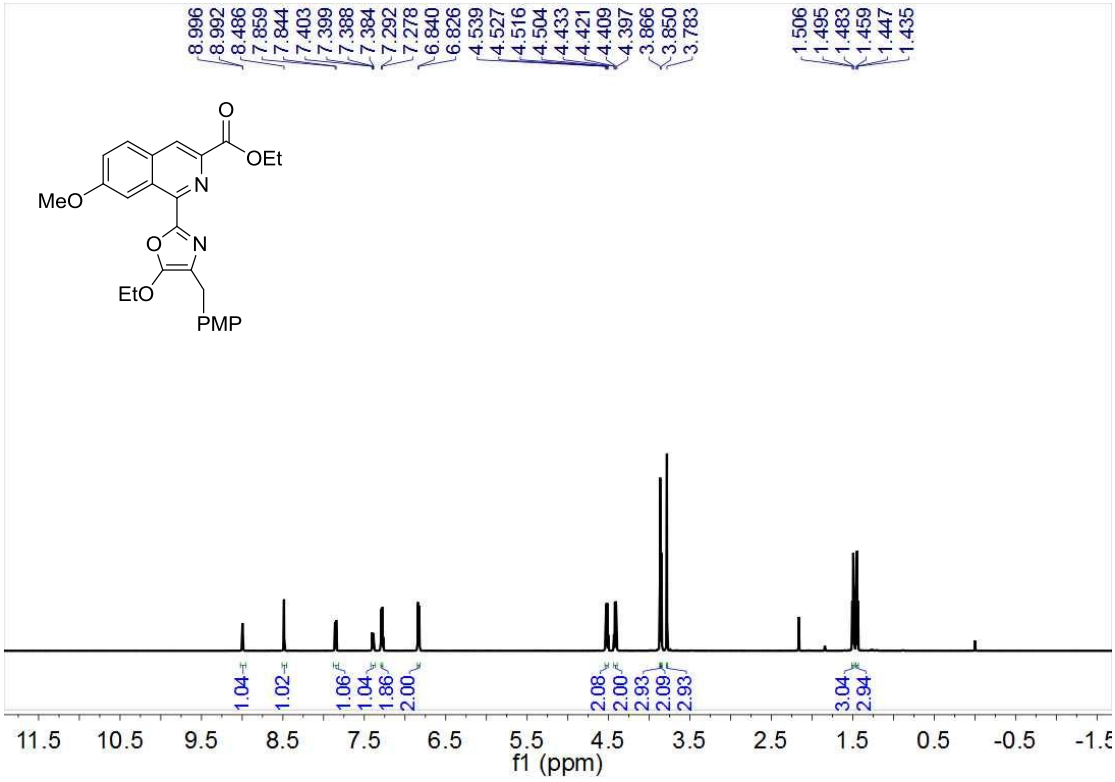


Figure 14. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2m**



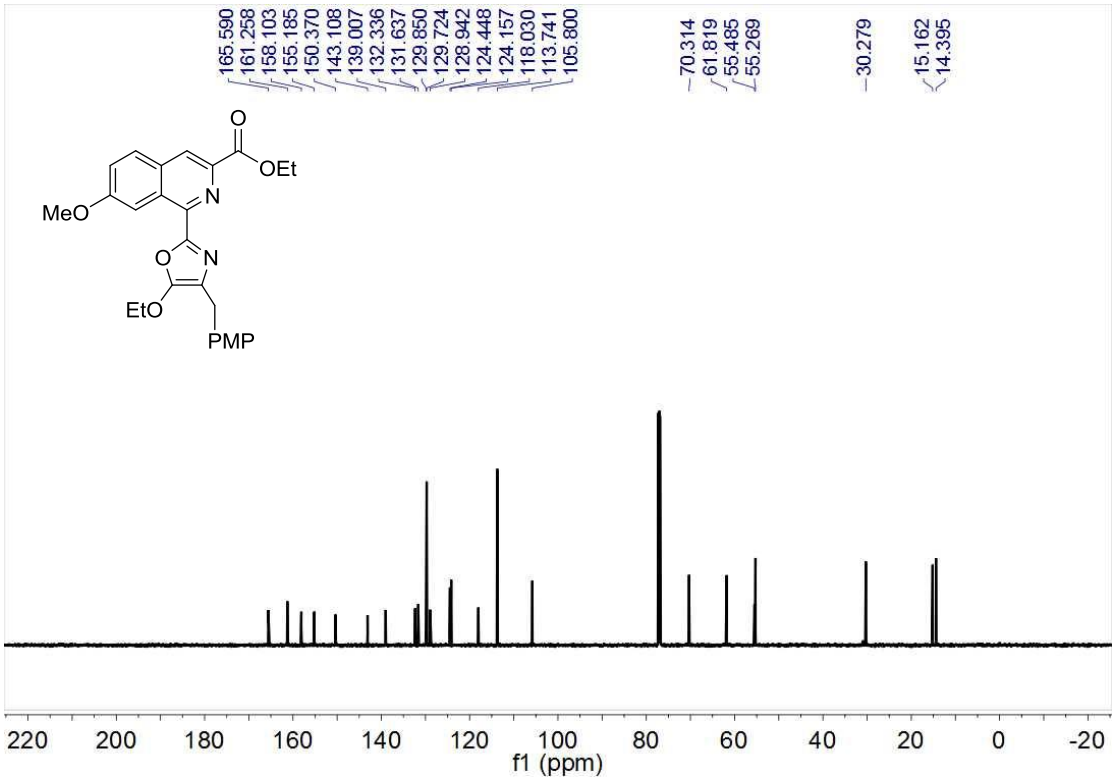
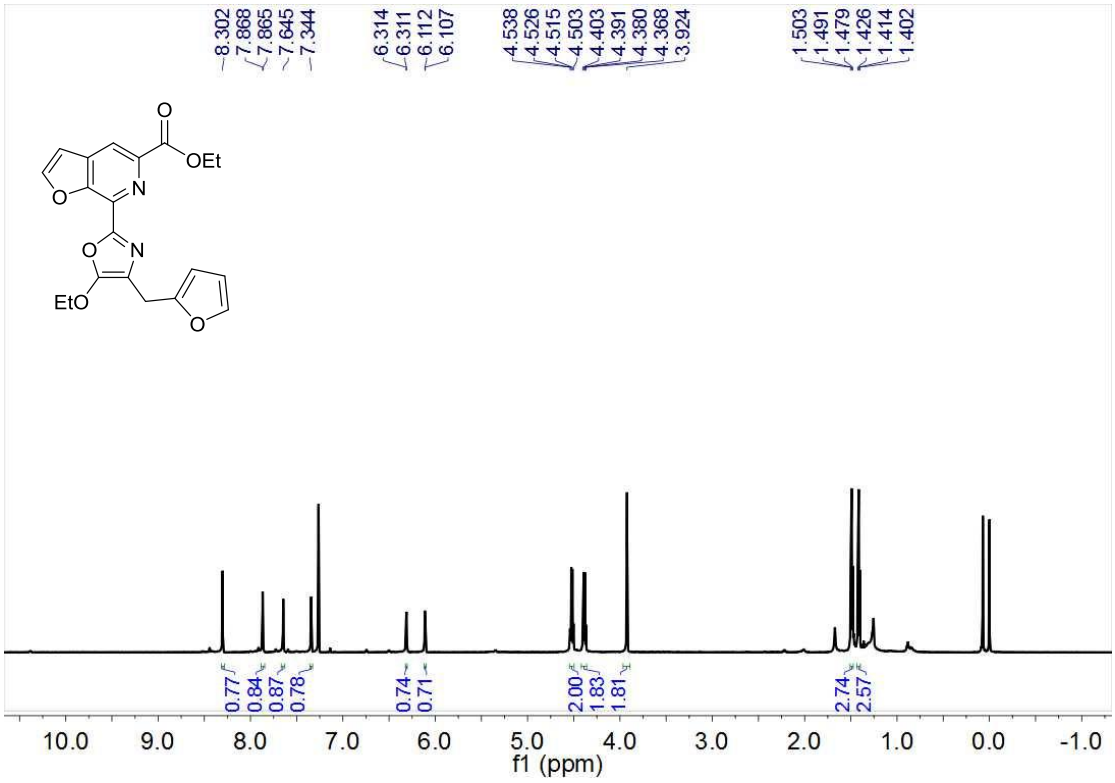


Figure 15. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2n**



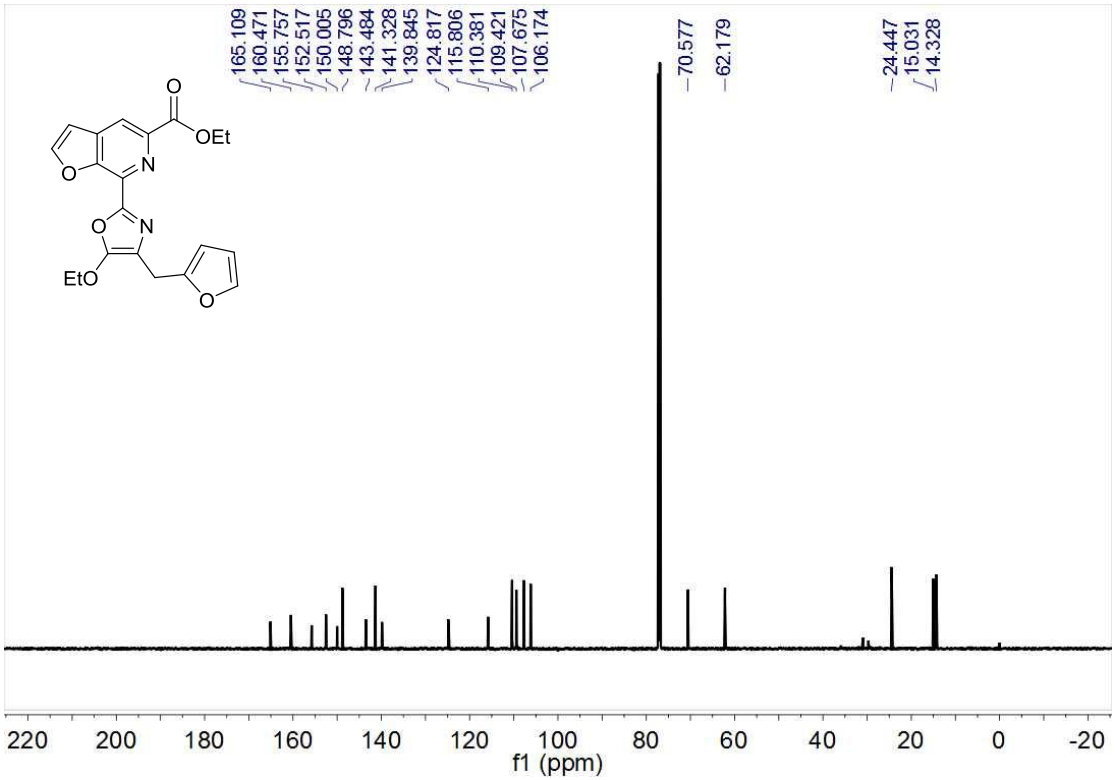
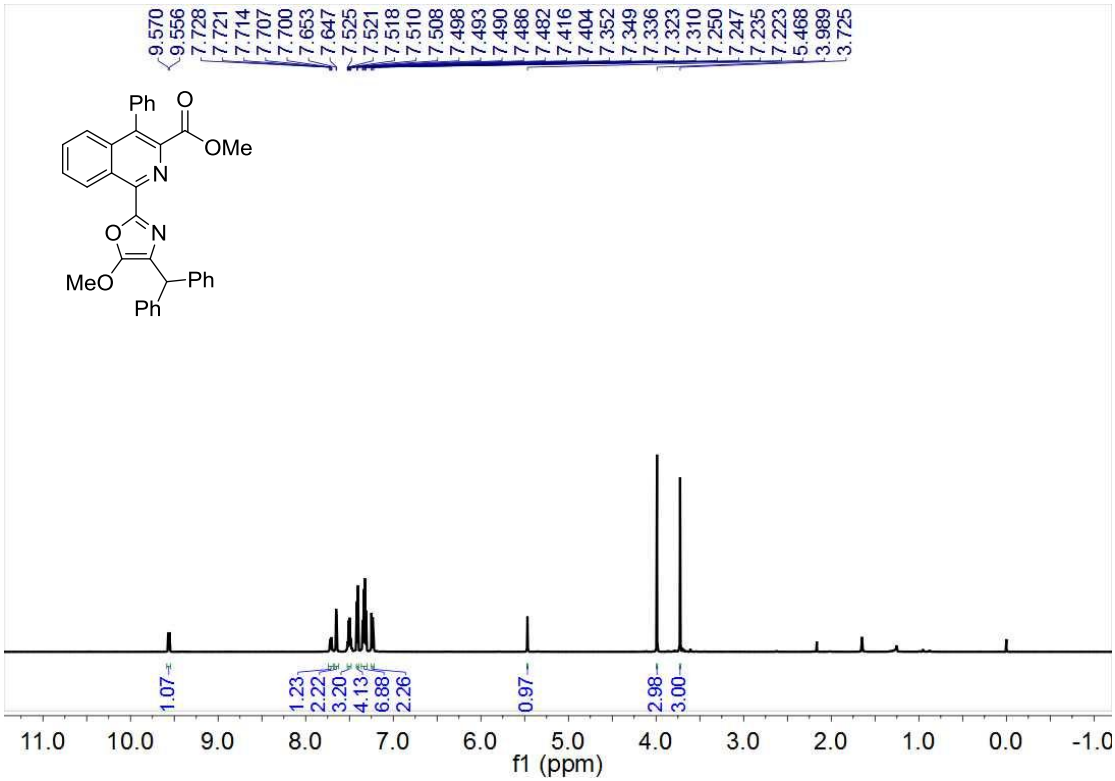


Figure 16. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2o**



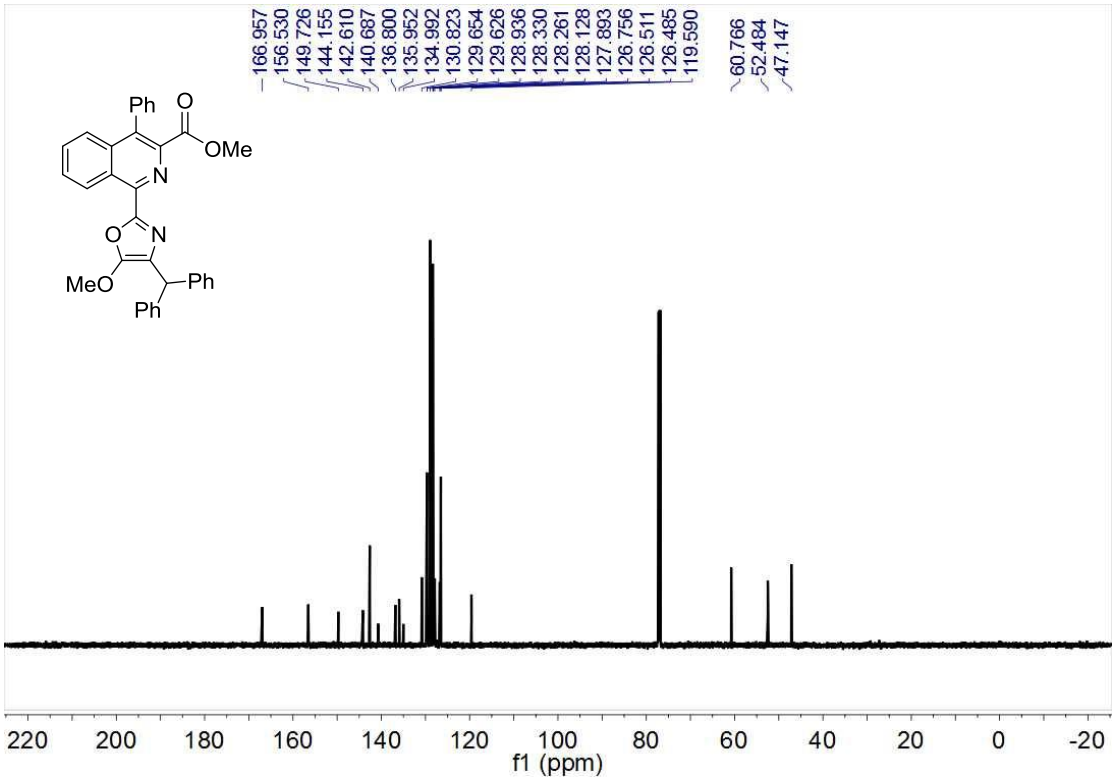
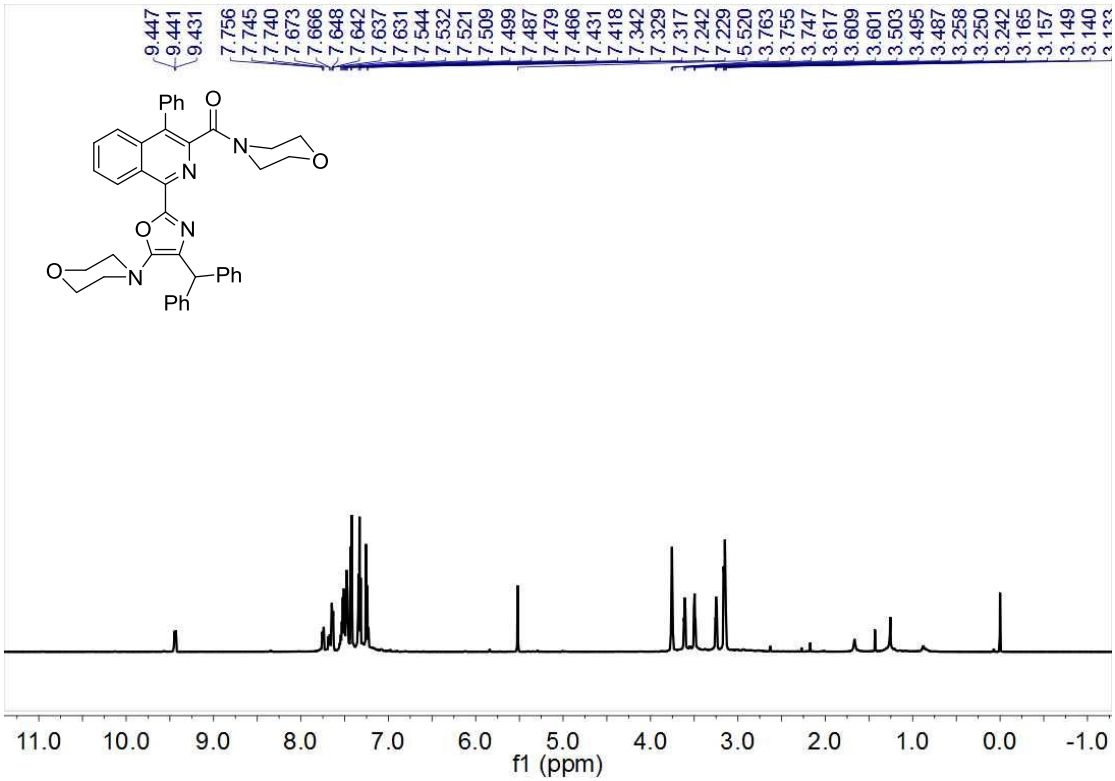


Figure 17. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2p**



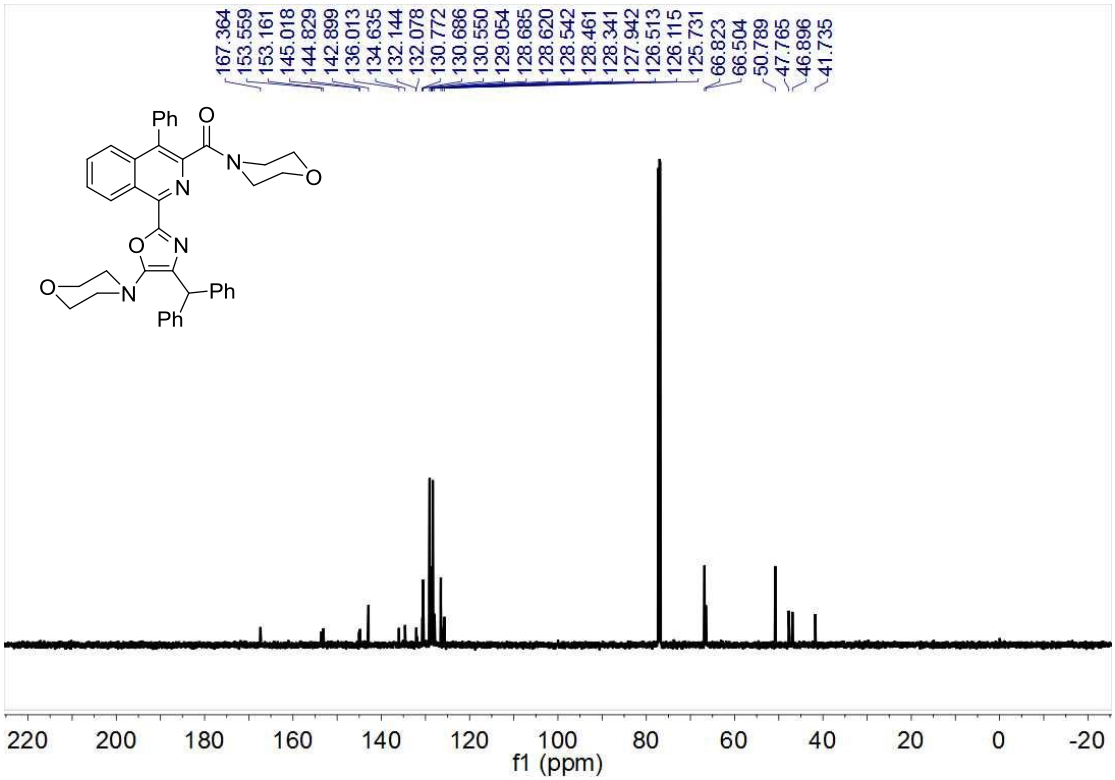
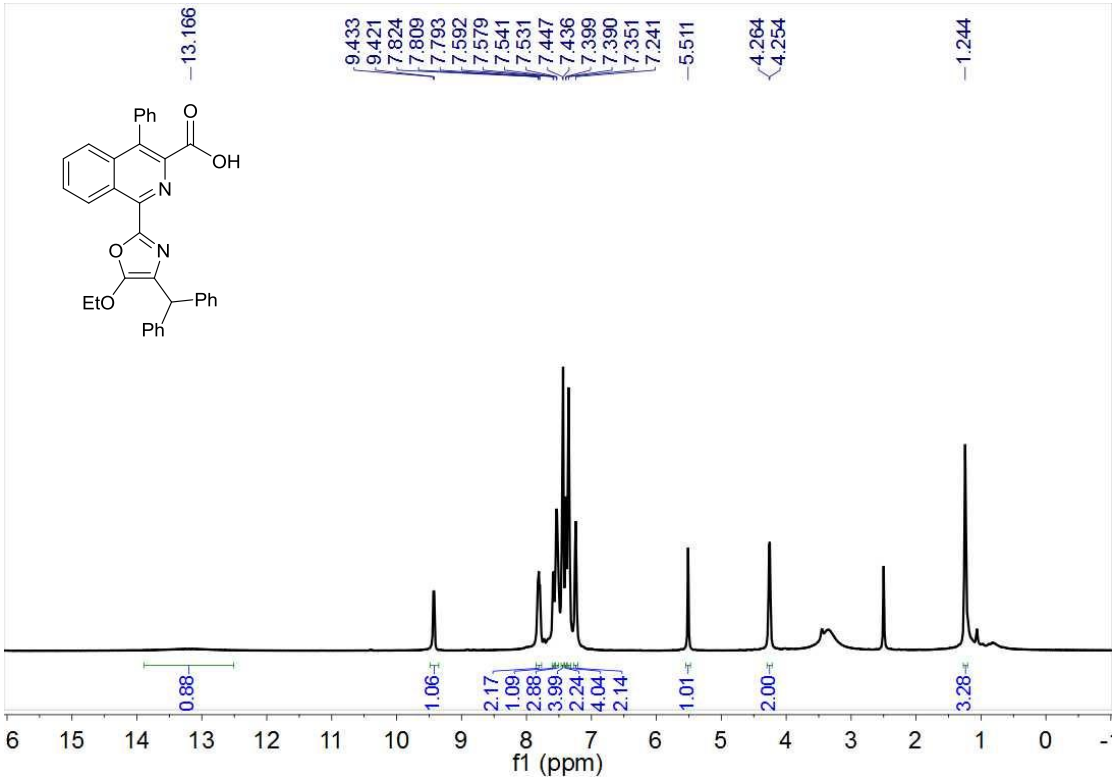


Figure 18. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **2q**



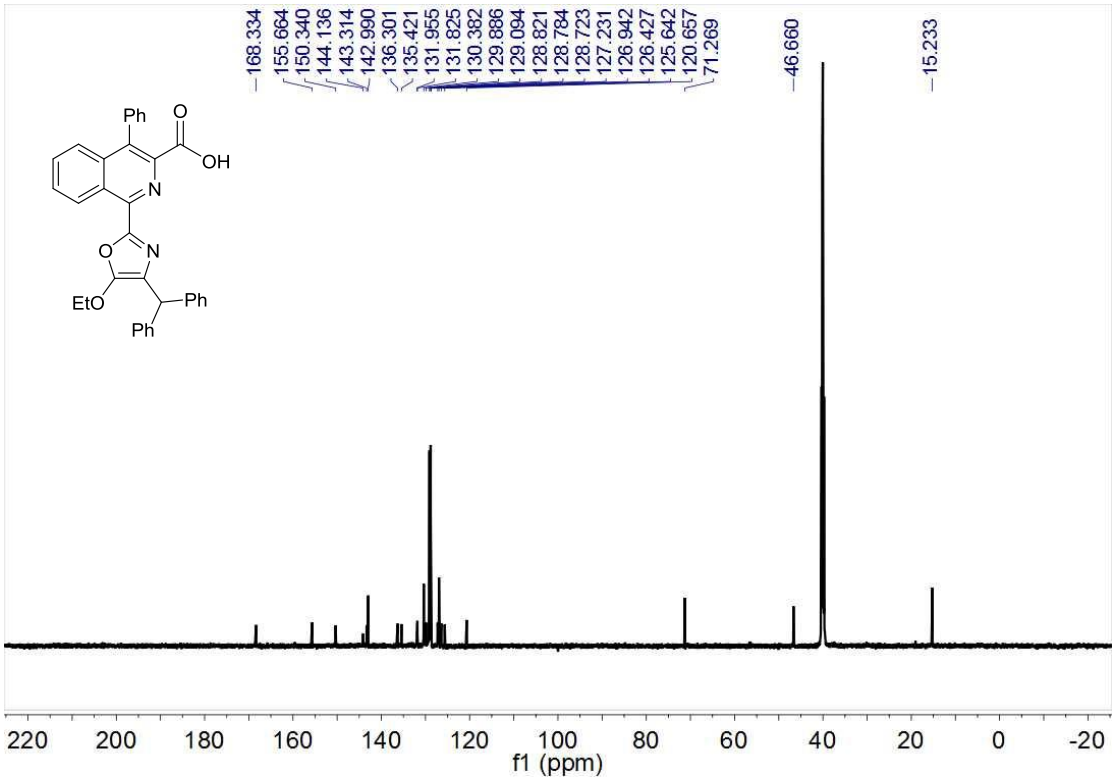
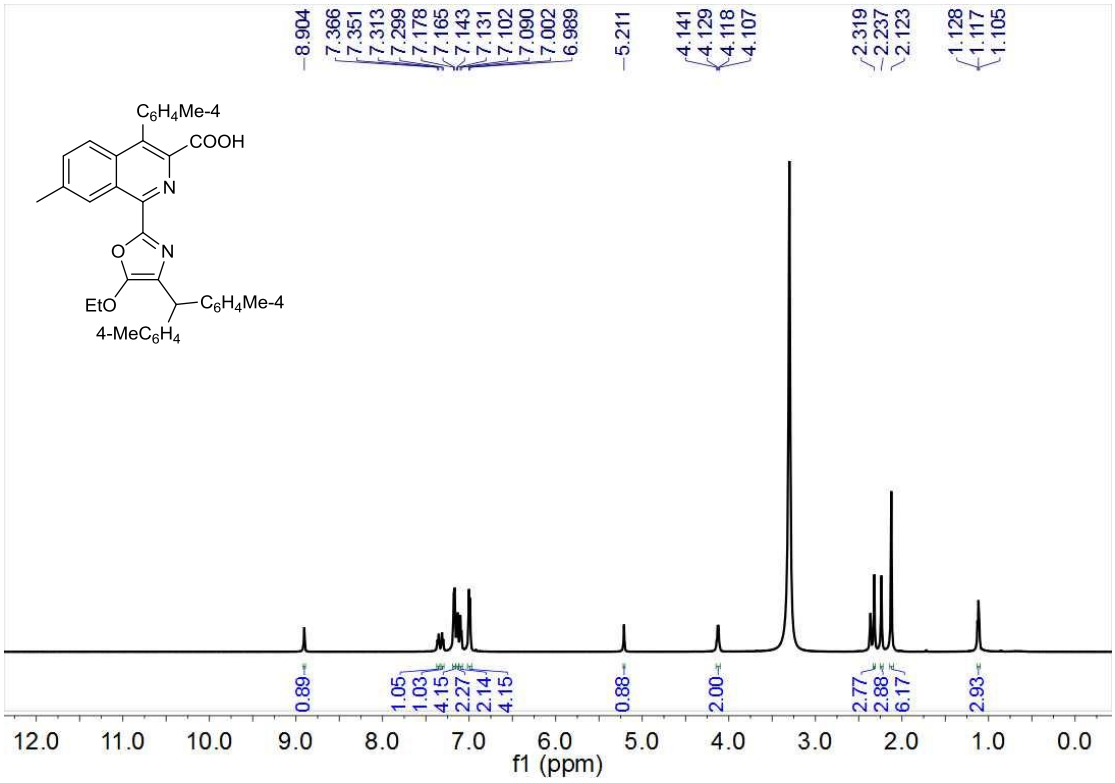


Figure 19. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **3a**



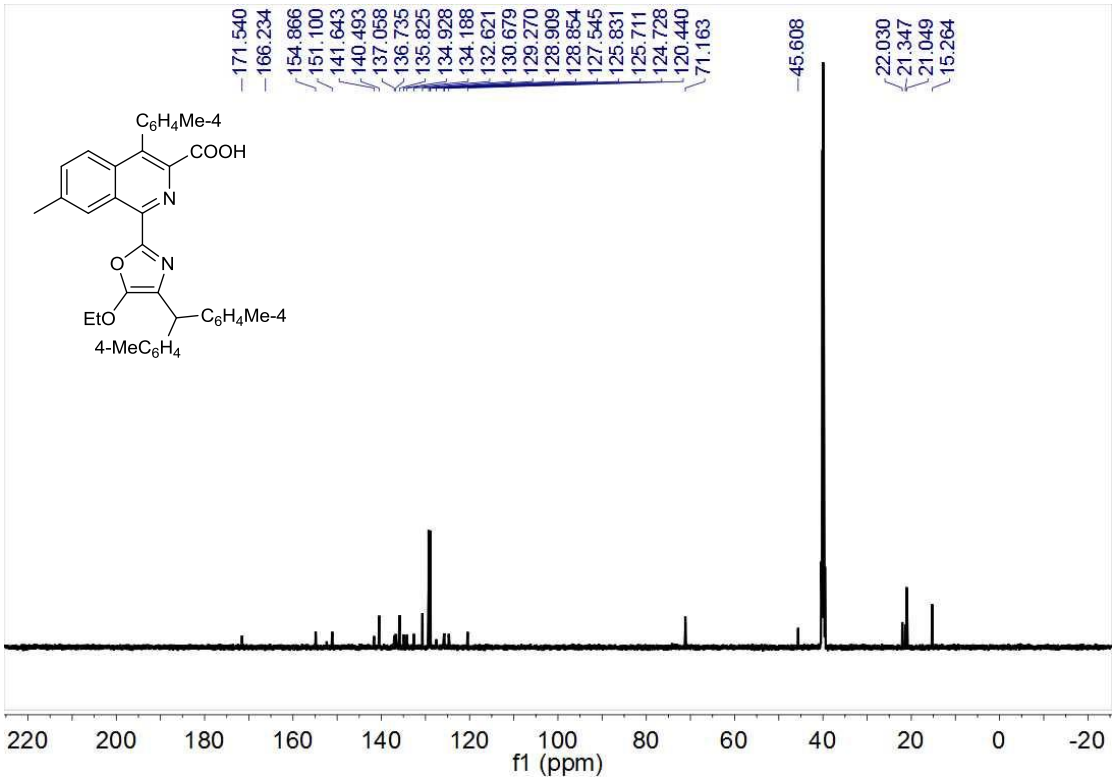
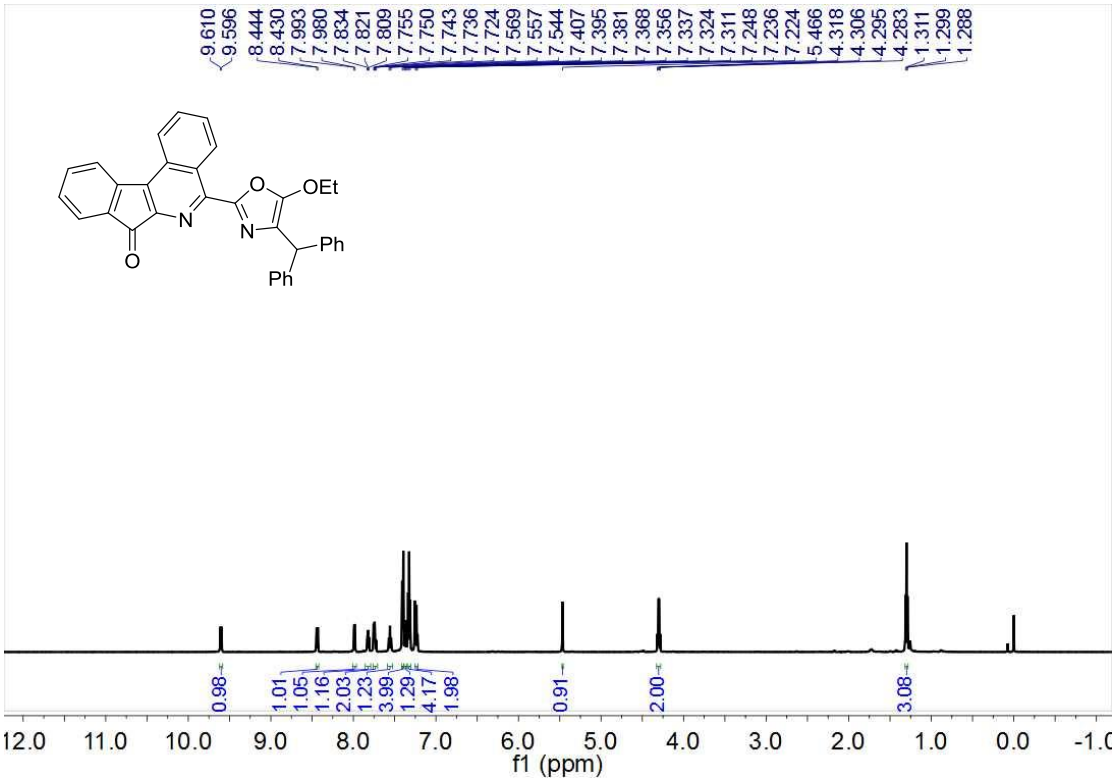


Figure 20. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **3d**



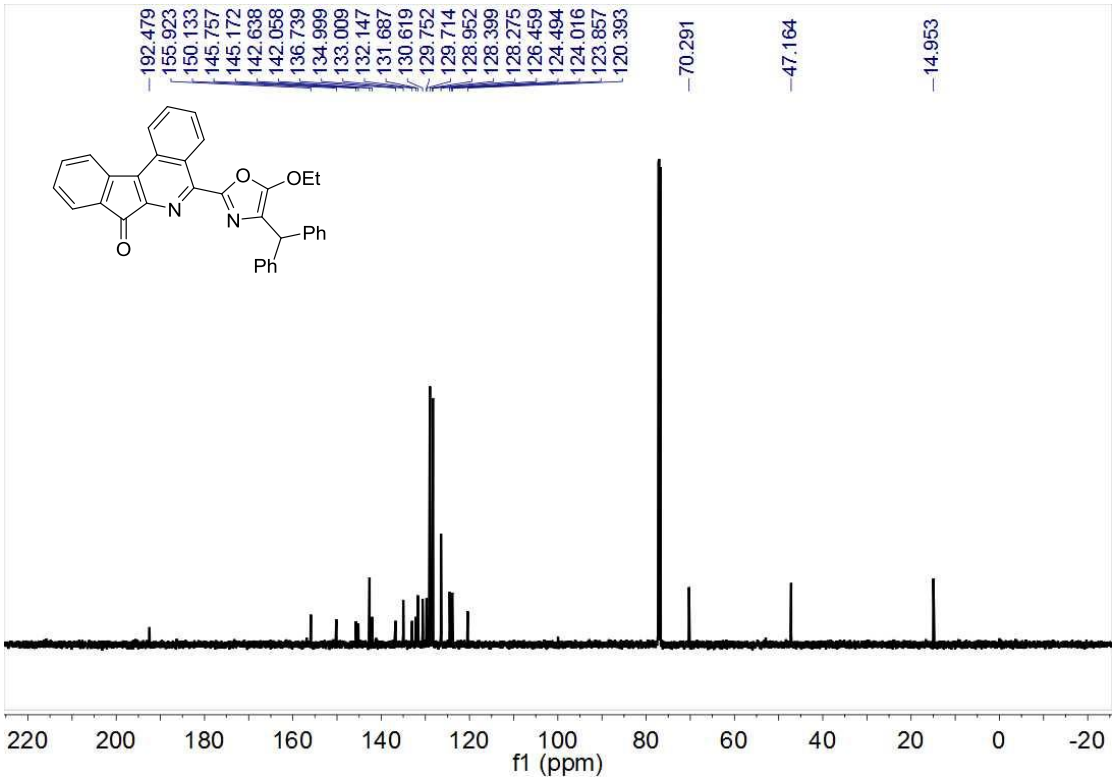
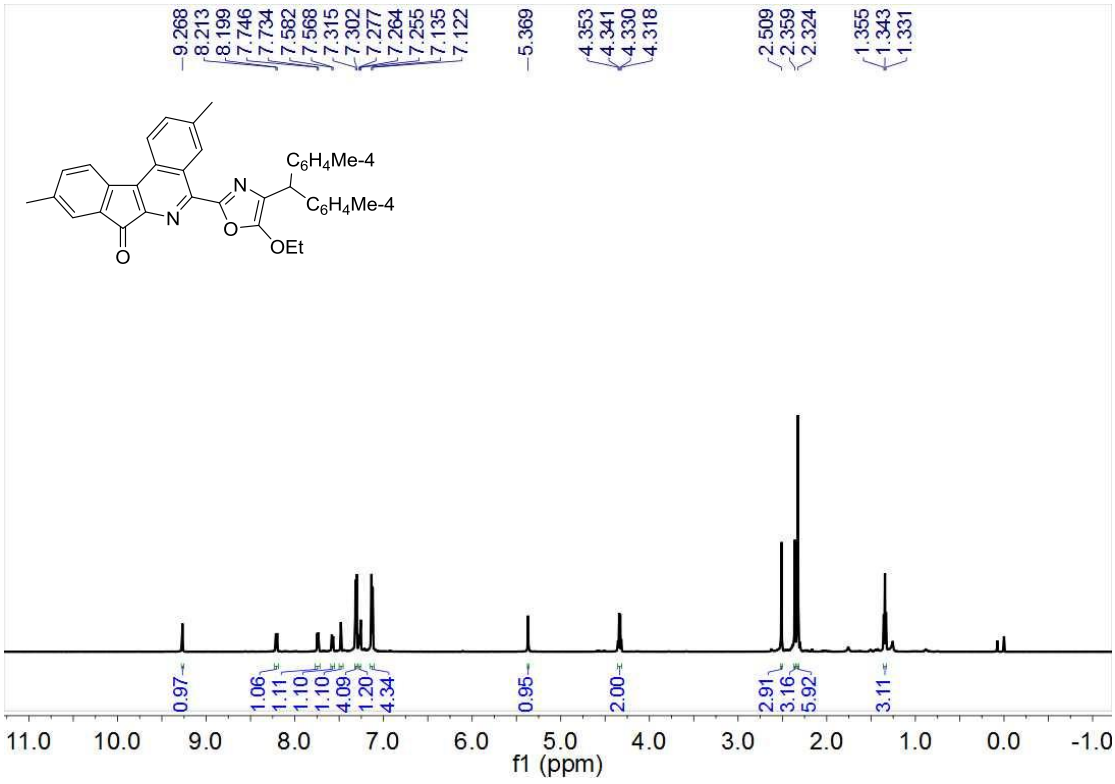


Figure 21. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **4a**



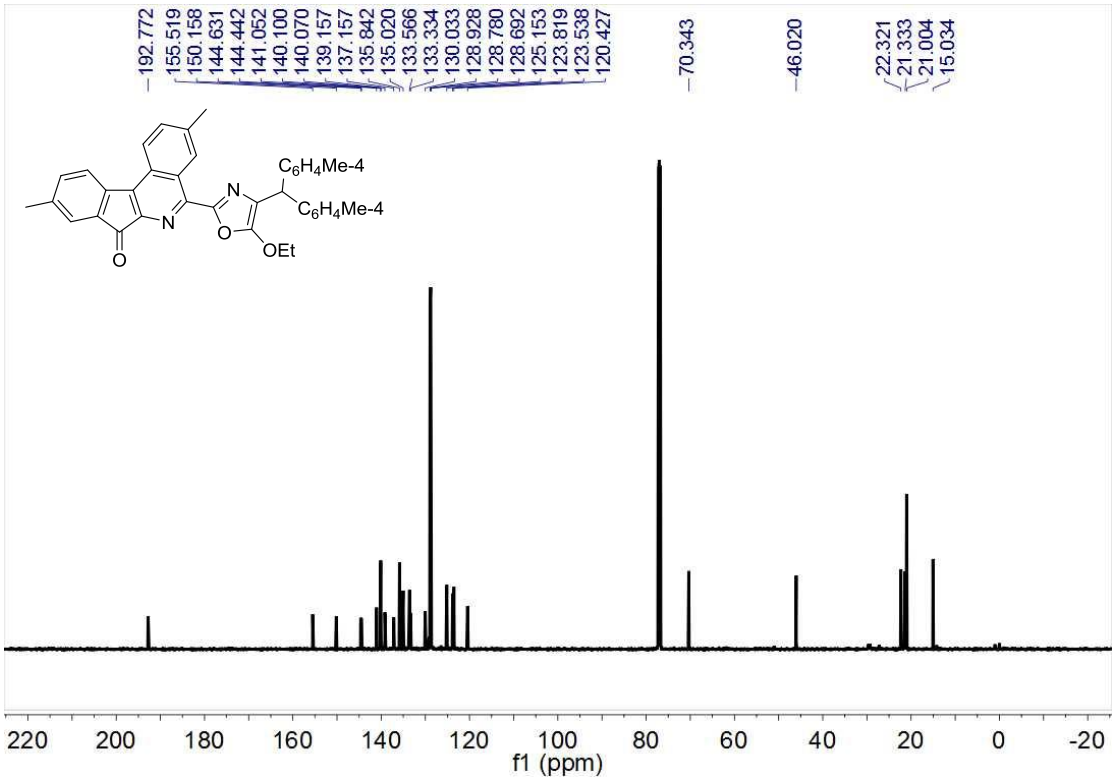


Figure 22. ^{1}H- (upper) and ^{13}C-NMR (lower) spectra of compound **4d**