Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting information

Preparation of fluoroalkoxy or fluorophenoxy substituted *N*-heterocycles from heterocyclic *N*-oxides and polyfluoroalcohols

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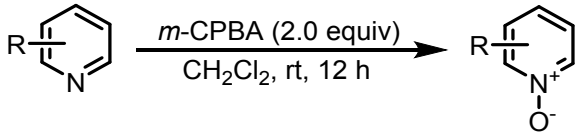
1. General Information

All reactions were carried out with magnetic stirring and in dried glassware. Standard syringe techniques were applied for transfer of dry solvents. All reagents and solvents were commercially available and used without any further purification unless specified. Proton (^{1}H NMR) and carbon(^{13}C NMR) nuclear magnetic resonance spectra were recorded at 400 MHz and 100 MHz respectively. The chemical shifts are given in parts per million (ppm) on the delta (δ) scale. ^{1}H NMR chemical shifts were determined relative to internal TMS at δ 0.0 ppm. ^{13}C NMR chemical shifts were determined relative to $CDCl_3$ at δ 77.16 ppm. The following abbreviations were used to explain multiplicities: s =singlet, d =doublet, dd = doublet of doublet, t = triplet, td = triplet of doublet, q = quartet, m = multiplet, and br = broad. Analytical TLC was performed on precoated silica gel plates. High-resolution mass spectra (HRMS) were obtained on an Agilent mass spectrometer using ESI-TOF (electrospray ionization-time of flight).

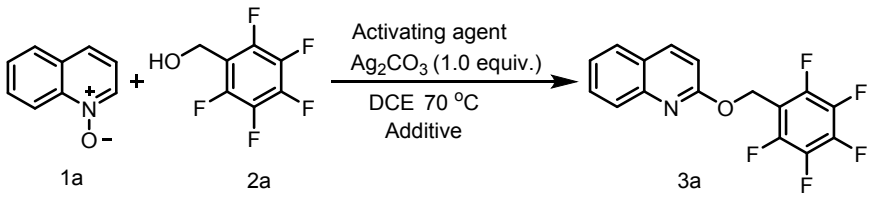
2. Experimental Section

2.1 General Procedure for the synthesis of starting materials



To a solution of the corresponding *N*-heterocycles (10.0 mmol) in CH_2Cl_2 (20 mL), *m*-chloroperoxybenzoic acid (*m*-CPBA, 20.0 mmol, 2.0 equiv) was added at 0 °C. The reaction mixture was allowed to stir at room temperature for 12 h. Then saturated aqueous $NaHCO_3$ (20 mL) was added. The aqueous was extracted with CH_2Cl_2 (10 mL x 3) and the combined organic extracts were dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with EtOAc/*n*-hexene or EtOAc/MeOH to afford desired *N*-oxides.

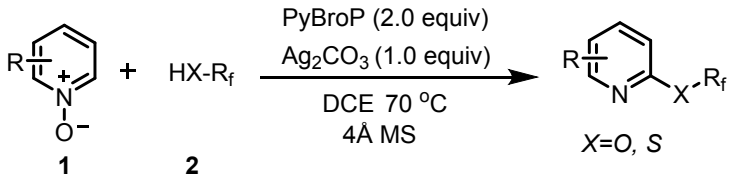
2.2 Optimization of atmosphere and activating agent



Entry	Additive	Activating agent (equiv.)	Yield[b] (%, 3a)
1	--	PyBroP (2.0) [c]	70%
2	4 Å MS	PyBroP (2.0) [c]	83%
3	4 Å MS	PyBroP (1.0)	64%
4	4 Å MS	PyBroP (1.5)	75%
5	4 Å MS	PyBroP (3.0)	83%
6	4 Å MS	PyCloP (2.0)	57%

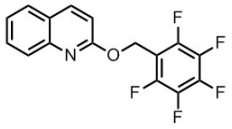
[a] Reaction conditions: **1a** (0.2 mmol, 1.0equiv), **2a**, Base (1.0 equiv), Activating agent and Additive (10% (w/v)), DCE (2.0 mL), stirred under air in a sealed tube at 70 °C for 12 h . [b] Isolated yield. [c] Under an Ar atmosphere.

2.3 Preparation of fluoroalkoxy or fluorophenoxy substituted *N*-heterocycles



1 **2**

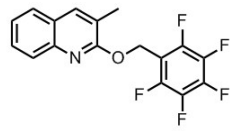
To a 35 mL sealed tube (with a Teflon cap) equipped with a magnetic stir bar were sequentially added heterocyclic *N*-oxide **1** (0.2 mmol, 1.0 equiv), polyfluoroalcohols **2** (0.6mmol, 3.0 equiv), PyBroP (186.4 mg, 0.4 mmol, 2.0 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1.0 equiv), 4 Å molecular sieves (10% (w/v) and 2 mL DCE. The tube was capped and submerged into a pre-heated 70 °C oil bath. The reaction was stirred for 12 h and cooled down to room temperature. Then the reaction mixture was diluted with EtOAc (5 mL) and filtered through a pad of silica gel. The sealed tube and silica gel were washed with an additional of EtOAc (20 mL). The filtrate was concentrated *in vacuo*, and the resulting residue was purified by flash column chromatography using EtOAc/*n*-hexane as the eluent to afford the product.



2-((perfluorophenyl) methoxy) quinoline (**3a**)

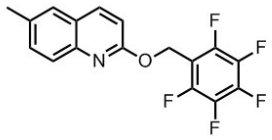
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.8 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 8.4 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 1H), 5.59 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.63 (dd, *J* = 15.04, 7.52 Hz, 2F), -153.70 (t, *J* = 18.8 Hz), -162.30 (td, *J* = 22.56, 8.6 Hz). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.78, 146.15, 145.89 (dm, *J* = 250 Hz), 141.24 (dm, *J* = 253 Hz), 139.15, 137.47 (dm, *J* = 251 Hz), 129.74, 127.46, 127.31, 125.32, 124.47, 112.56 , 110.88

(tm, J = 18 Hz), 55.00. HRMS (ESI-TOF) m/z Calcd for $C_{16}H_8F_5NO$ $[M+H]^+$: 326.0599, found: 326.0591.



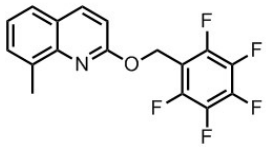
3-methyl-2-((perfluorophenyl) methoxy) quinoline (**3b**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 8.3 Hz, 1H), 7.60 (s, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.44 (t, J = 7.7 Hz, 1H), 7.23 (t, J = 7.5 Hz, 1H), 5.47 (s, 2H), 2.16 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.78 (dd, J = 15.04 , 7.52 Hz, 2F), -154.03 (t, J = 18.8 Hz, 1F), -162.47 (td, J = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.82, 145.91 (dm, J = 257 Hz), 144.88, 142.825 (dm, J = 253 Hz), 137.41 (dm, J = 251 Hz), 137.33, 128.50, 126.83, 126.55, 125.78, 124.24, 122.21, 111.05 (tm, J = 17 Hz), 55.22, 16.19. HRMS (ESI-TOF) m/z Calcd for $C_{17}H_{10}F_5NO$ $[M+H]^+$: 340.0755, found: 340.0752.



6-methyl-2-((perfluorophenyl) methoxy) quinoline (**3c**)

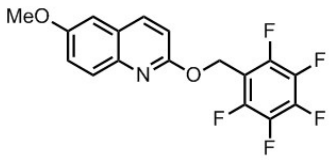
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 8.8 Hz, 1H), 7.64 (d, J = 8.9 Hz, 1H), 7.35 (d, J = 6.9 Hz, 1H), 6.74 (d, J = 8.8 Hz, 1H), 5.46 (s, 2H), 2.38 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.68 (dd, J = 23.1, 7.8 Hz, 2F), -153.83 (t, J = 24.2 Hz, 1F), -162.40 (td, J = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.82, 145.90 (dm, J = 257 Hz), 144.88, 141.33 (dm, J = 253 Hz), 137.40 (dm, J = 251 Hz), 137.33, 128.50, 126.83, 126.55, 125.78, 124.24, 122.21, 111.05 (tm, J = 17 Hz), 55.22, 16.19. HRMS (ESI-TOF) m/z Calcd for $C_{17}H_{10}F_5NO$ $[M+H]^+$: 340.0755, found: 340.0748.



8-methyl-2-((perfluorophenyl) methoxy) quinoline (**3d**)

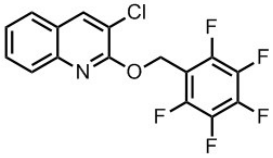
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.8 Hz, 1H), 7.57 (d, J = 8.0 Hz, 1H), 7.50 (d, J = 7.0 Hz, 1H), 7.30 (t, 1H), 6.89 (d, J = 8.8 Hz, 1H), 5.65 (s, 2H), 2.71 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.66 (dd, J = 22.56, 7.52 Hz, 2F), -153.81 (t, J = 22.56 Hz, 1F), -162.23 (td, J = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.84, 145.79 (dm, J = 250 Hz), 144.92, 141.37 (dm, J = 253Hz),

139.51, 137.48 (dm, J = 251 Hz), 135.37, 130.02, 125.29, 125.14, 124.08, 112.07, 111.03 (tm, J = 19 Hz), 54.70, 17.66 . HRMS (ESI-TOF) m/z Calcd for $C_{17}H_{10}F_5NO$ $[M+H]^+$: 340.0755, found: 340.0743.



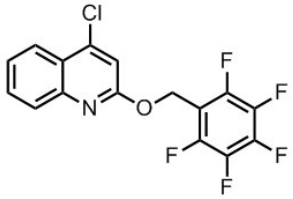
6-methoxy-2-((perfluorophenyl) methoxy) quinoline (**3e**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.8 Hz, 1H), 7.76 (d, J = 9.1 Hz, 1H), 7.29 (dd, J = 9.1, 2.8 Hz, 1H), 7.02 (d, J = 2.8 Hz, 1H), 6.86 (d, J = 8.8 Hz, 1H), 5.55 (s, 2H), 3.88 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.70 (dd, J = 26.32, 11.28 Hz, 2F), -153.85 (t, J = 22.56 Hz, 1F), -162.37 (td, J = 18.8, 7.52 Hz, 2F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.45, 156.35, 145.86 (dm, J = 264 Hz), 141.46, 141.38 (dm, J = 253 Hz), 138.07, 137.38 (dm, J = 246 Hz), 128.53, 125.85, 121.31, 112.58, 110.92 (tm, J = 18 Hz), 106.06, 55.43, 54.82. HRMS (ESI-TOF) m/z Calcd for $C_{17}H_{10}F_5NO_2$ $[M+H]^+$: 356.0704, found: 356.0710.



3-chloro-2-((perfluorophenyl) methoxy) quinoline (**3f**)

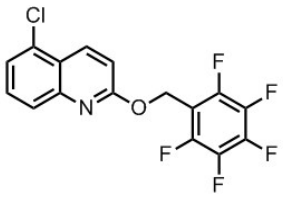
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.85 (d, J = 8.2 Hz, 1H), 7.65 (d, 2H), 7.42 (t, 1H), 5.66 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.27 (dd, J = 22.56, 11.28 Hz, 2F), -153.19 (t, J = 22.56 Hz, 1F), -162.04 (td, J = 18.8, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.76, 145.99 (dm, J = 242 Hz), 144.21, 141.65 (dm, J = 256 Hz), 137.48 (dm, J = 251 Hz), 137.37, 129.83, 127.10, 126.55, 125.81, 125.26, 118.57, 110.30 (tm, J = 17 Hz), 56.02. HRMS (ESI-TOF) m/z Calcd for $C_{16}H_7ClF_5NO$ $[M+H]^+$: 360.0209, found: 360.0213.



4-chloro-2-((perfluorophenyl) methoxy) quinoline (**3g**)

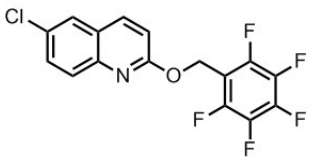
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.3 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.68 (t, 1H), 7.47 (t, 1H), 7.00 (s, 1H), 5.58 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.54 (dd, J = 18.8, 7.52 Hz, 2F), -

153.29 (t, J = 22.56 Hz, 1F), -162.11 (td, J = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.16, 146.45, 145.87 (dm, J = 249 Hz), 144.22, 141.56 (dm, J = 254 Hz), 137.45 (dm, J = 251 Hz), 130.70 , 127.62 , 125.23, 124.04 , 123.50 , 112.32, 110.45 (tm, J = 16 Hz), 55.26. HRMS (ESI-TOF) m/z Calcd for $C_{16}H_7ClF_5NO$ $[M+H]^+$: 360.0209, found: 360.0205.



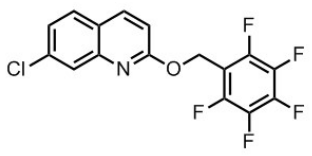
5-chloro-2-((perfluorophenyl) methoxy) quinoline (**3h**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, J = 9.1 Hz, 1H), 7.77 (d, J = 8.3 Hz, 1H), 7.53 (t, J = 8.0 Hz, 1H), 7.45 (d, J = 8.2 Hz, 1H), 6.97 (d, J = 9.1 Hz, 1H), 5.60 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.55 (dd, J = 22.56, 7.52 Hz, 2F), -153.35 (t, J = 22.56 Hz, 1F), -162.12 (td, J = 18.80, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.17, 147.05, 145.93 (dm, J = 241 Hz), 135.98, 141.55 (dm, J = 253 Hz), 137.46 (dm, J = 251 Hz), 131.37, 129.55, 126.44, 124.66, 123.36, 113.45, 110.59 (tm, J = 17 Hz), 55.2 . HRMS (ESI-TOF) m/z Calcd for $C_{16}H_7ClF_5NO$ $[M+H]^+$: 360.0209, found: 360.0212.



6-chloro-2-((perfluorophenyl) methoxy) quinoline (**3i**)

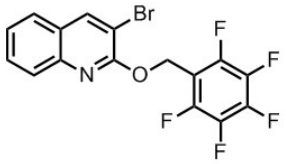
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, J = 8.9 Hz, 1H), 7.76 (d, J = 8.9 Hz, 1H), 7.64 (d, J = 2.3 Hz, 1H), 7.54 (dd, J = 8.9, 2.4 Hz, 1H), 6.89 (d, J = 8.9 Hz, 1H), 5.57 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.64 (dd, J = 22.56, 7.52 Hz, 2F), -153.45 (t, J = 22.56 Hz, 1F), -162.18 (td, J = 18.80, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.90, 145.85 (dm, J = 257 Hz), 144.50, 141.50 (dm, J = 253 Hz), 137.42 (dm, J = 246 Hz), 138.10, 130.30, 129.86, 128.77, 126.16, 125.8, 113.53, 110.58 (tm, J = 17 Hz), 55.0 . HRMS (ESI-TOF) m/z Calcd for $C_{16}H_7ClF_5NO$ $[M+H]^+$: 360.0209, found: 360.0207.



7-chloro-2-((perfluorophenyl) methoxy) quinoline (**3j**)

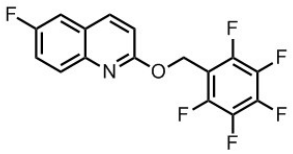
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 8.8 Hz, 1H), 7.81 (d, J = 2.0 Hz, 1H), 7.60 (d, J = 8.6 Hz,

1H), 7.32 (dd, *J* = 8.6, 2.1 Hz, 1H), 6.86 (d, *J* = 8.8 Hz, 1H), 5.57 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.64 (dd, *J* = 22.56, 7.52 Hz, 2F), -153.44 (t, *J* = 18.80 Hz, 1F), -162.13 (td, *J* = 18.80, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.41, 146.67, 145.84 (dm, *J* = 253 Hz), 141.51 (dm, *J* = 254 Hz), 138.75, 137.44 (dm, *J* = 251 Hz), 135.54, 128.47, 126.46, 125.26, 123.59 , 112.72, 110.59 (tm, *J* = 14 Hz), 55.0 . HRMS (ESI-TOF) m/z Calcd for $C_{16}H_7ClF_5NO$ $[M+H]^+$: 360.0209, found: 360.0211.



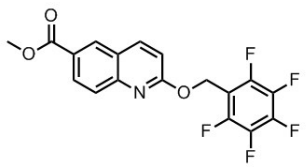
3-bromo-2-((perfluorophenyl) methoxy) quinoline(**3k**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.65 (t, 2H), 7.41 (t, 1H), 5.64 (d, *J* = 1.6 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.20 (dd, *J* = 18.80, 7.52 Hz, 2F), -153.23 (t, *J* = 18.80 Hz, 1F), -162.05 (td, *J* = 18.80, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.12, 145.91 (dm, *J* = 253 Hz), 144.72, 141.60 (dm, *J* = 254 Hz), 141.19, 137.53 (dm, *J* = 240 Hz), 129.99 , 127.14 , 126.49, 126.31, 125.21, 110.33 (tm, *J* = 18 Hz), 107.26, 56.18. HRMS (ESI-TOF) m/z Calcd for $C_{16}H_7BrF_5NO$ $[M+H]^+$: 403.9704, found: 403.9710.



6-fluoro-2-((perfluorophenyl) methoxy) quinoline (**3l**)

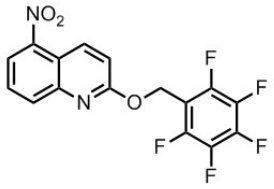
H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.9 Hz, 1H), 7.70 (dd, *J* = 9.1, 5.2 Hz, 1H), 7.27 (t, 1H), 7.21 (d, *J* = 8.8 Hz, 1H), 6.79 (d, *J* = 8.9 Hz, 1H), 5.45 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.02 (s, 1F), δ -141.71 (dd, *J* = 18.80, 7.52 Hz, 2F), -15362 (t, *J* = 22.56 Hz, 1F), -162.30 (td, *J* = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.33 (d, *J* = 2 Hz), 159.25 (d, *J* = 243 Hz), 145.88 (dm, *J* = 249 Hz), 142.90, 141.49 (dm, *J* = 254 Hz), 138.44 (d, *J* = 4 Hz), 137.44 (dm, *J* = 251 Hz), 129.29 (d, *J* = 8 Hz), 125.60 (d, *J* = 10 Hz), 119.14 (d, *J* = 25 Hz), 113.43, 110.99 (d, *J* = 21 Hz), 110.74 (tm, *J* = 17 Hz), 54.98. HRMS (ESI-TOF) m/z Calcd for $C_{16}H_7F_6NO$ $[M+H]^+$: 344.0505, found: 344.0508.



methyl 2-((perfluorophenyl) methoxy) quinoline-6-carboxylate (**3m**)

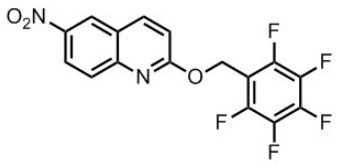
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.12 (d, *J* = 8.7 Hz, 1H), 7.97 (d, *J* = 8.9 Hz, 1H), 7.76 (d,

J = 8.7 Hz, 1H), 6.84 (d, *J* = 8.8 Hz, 1H), 5.51 (s, 2H), 3.87 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.61 (dd, *J* = 22.56, 7.52 Hz, 2F), -153.30 (t, *J* = 18.80 Hz, 1F), -162.11 (td, *J* = 18.80, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.68, 162.20, 148.63, 145.78 (dm, *J* = 249 Hz), 141.61 (dm, *J* = 240 Hz), 140.03, 137.43 (dm, *J* = 251 Hz), 130.32, 129.52, 127.40, 126.05, 124.39, 113.46, 110.42 (tm, *J* = 17 Hz), 55.21, 52.20. HRMS (ESI-TOF) m/z Calcd for $C_{18}H_{10}F_5NO_3$ $[M+H]^+$: 384.0684, found: 384.0649.



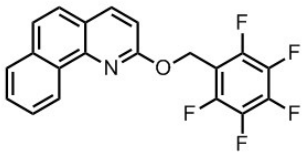
5-nitro-2-((perfluorophenyl) methoxy) quinoline (**3n**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (d, *J* = 9.4 Hz, 1H), 8.18 (dd, *J* = 15.2, 8.6 Hz, 2H), 7.73 (t, *J* = 8.1 Hz, 1H), 7.13 (d, *J* = 9.4 Hz, 1H), 5.64 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.46 (dd, *J* = 22.56, 7.52 Hz, 2F), -152.89 (t, *J* = 22.56 Hz, 1F), -162.11 (td, *J* = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.21, 146.92, 145.80 (dm, *J* = 253 Hz), 145.77, 141.67 (dm, *J* = 254 Hz), 137.50 (dm, *J* = 252 Hz), 134.97, 134.08, 128.04, 122.21, 118.16, 115.84, 110.24 (tm, *J* = 14 Hz), 55.35. HRMS (ESI-TOF) m/z Calcd for $C_{16}H_7F_5N_2O_3$ $[M+H]^+$: 371.0450, found: 371.0448.



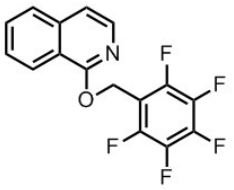
6-nitro-2-((perfluorophenyl) methoxy) quinoline (**3o**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 2.5 Hz, 1H), 8.43 (dd, *J* = 9.2, 2.5 Hz, 1H), 8.18 (d, *J* = 8.9 Hz, 1H), 7.95 (d, *J* = 9.2 Hz, 1H), 7.06 (d, *J* = 8.9 Hz, 1H), 5.66 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.48 (dd, *J* = 22.56, 7.52 Hz, 2F), -152.76 (t, *J* = 22.56 Hz, 1F), -161.81 (td, *J* = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.08, 149.30, 145.86 (dm, *J* = 234 Hz), 144.05, 141.65 (dm, *J* = 259 Hz), 140.34, 137.50 (dm, *J* = 252 Hz), 128.63, 124.07, 124.02, 123.53, 114.92, 110.11 (tm, *J* = 17 Hz), 55.58. HRMS (ESI-TOF) m/z Calcd for $C_{16}H_7F_5N_2O_3$ $[M+H]^+$: 371.0450, found: 371.0453.



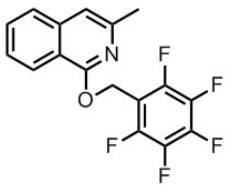
2-((perfluorophenyl) methoxy) benzo quinoline (**3p**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (d, *J* = 8.8 Hz, 1H), 8.08 (d, *J* = 8.6 Hz, 1H), 7.90 (d, *J* = 8.9 Hz, 1H), 7.72 (t, 3H), 7.65 (t, *J* = 8.7 Hz, 1H), 7.01 (d, *J* = 8.6 Hz, 1H), 5.78 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.74 (dd, *J* = 22.56, 7.52 Hz, 2F), -152.52 (t, *J* = 22.56 Hz, 1F), -161.00 (td, *J* = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.63, 145.84 (dm, *J* = 245 Hz), 144.10, 139.25, 137.46 (dm, *J* = 234 Hz), 133.94, 130.64, 129.82 (dm, *J* = 207 Hz), 127.89, 127.73, 126.43, 125.23, 124.91, 124.31, 122.42, 111.77, 110.89 (tm, *J* = 17 Hz), 54.93. HRMS (ESI-TOF) m/z Calcd for $C_{20}H_{10}F_5NO$ $[M+H]^+$: 376.0755, found: 376.0751.



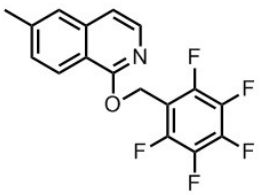
1-((perfluorophenyl) methoxy) isoquinoline (**3q**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.3 Hz, 1H), 8.00 (d, *J* = 5.9 Hz, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.64 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.25 (d, *J* = 6.0 Hz, 1H), 5.64 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.90 (dd, *J* = 22.56, 7.52 Hz, 2F), -153.54 (t, *J* = 18.80 Hz, 1F), -161.09 (td, *J* = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.34, 145.91 (dm, *J* = 242 Hz), 141.46 (dm, *J* = 248 Hz), 139.27, 137.93, 137.46 (dm, *J* = 245 Hz), 130.61, 126.80, 126.09, 123.89, 119.29, 115.74, 110.70 (tm, *J* = 17 Hz), 55.26. HRMS (ESI-TOF) m/z Calcd for $C_{16}H_8F_5NO$ $[M+H]^+$: 326.0599, found: 325.0597.



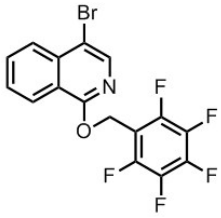
3-methyl-1-((perfluorophenyl) methoxy) isoquinoline (**3r**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.2 Hz, 1H), 7.66 (t, *J* = 8.0 Hz, 2H), 7.46 (t, *J* = 7.2 Hz, 1H), 7.11 (s, 1H), 5.70 (s, 2H), 2.58 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -140.53 (dd, *J* = 26.32, 11.28 Hz, 2F), -152.81 (t, *J* = 26.32 Hz, 1F), -161.30 (td, *J* = 26.32, 11.28 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.51, 149.98 (dm, *J* = 310 Hz), 148.56, 145.93 (dm, *J* = 245 Hz), 138.82, 137.46 (dm, *J* = 249 Hz), 130.49, 125.72, 125.50, 123.83, 117.42, 113.20, 111.04 (tm, *J* = 17 Hz), 55.16, 23.85. HRMS (ESI-TOF) m/z Calcd for $C_{17}H_{10}F_5NO$ $[M+H]^+$: 340.0755, found: 340.0761.



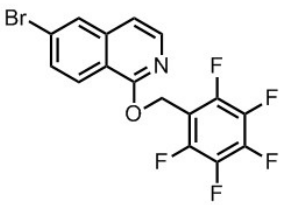
6-methyl-1-((perfluorophenyl) methoxy) isoquinoline (**3s**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.5 Hz, 1H), 7.96 (d, *J* = 5.9 Hz, 1H), 7.49 (s, 1H), 7.32 (d, *J* = 8.5 Hz, 1H), 7.17 (d, *J* = 5.8 Hz, 1H), 5.63 (s, 2H), 2.50 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.74 (dd, *J* = 22.56, 7.52 Hz, 2F), -152.52 (t, *J* = 22.56 Hz, 1F), -161.00 (td, *J* = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.35, 145.87 (dm, *J* = 249 Hz), 141.46 (dm, *J* = 253 Hz), 140.99, 139.35, 138.26, 137.47 (dm, *J* = 250 Hz), 128.87, 125.29, 123.72, 117.43, 115.40, 110.78 (tm, *J* = 18 Hz), 55.18, 21.86. HRMS (ESI-TOF) m/z Calcd for $C_{17}H_{10}F_5NO$ $[M+H]^+$: 340.0755, found: 340.0749.



4-bromo-1-((perfluorophenyl) methoxy) isoquinoline (**3t**)

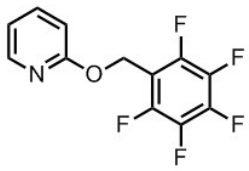
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 8.09 (d, *J* = 8.3 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.71 (t, *J* = 4 Hz,1H), 7.51 (t, *J* = 8.1 Hz, 1H), 5.56 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.745 (dd, *J* = 22.56, 7.52 Hz, 2F), -153.08 (t, *J* = 22.56 Hz, 1F), -161.835 (td, *J* = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.86, 145.865 (dm, *J* = 261 Hz), 141.905 (dm, *J* = 225 Hz), 140.53, 137.775 (dm, *J* = 266 Hz), 136.25, 131.79, 127.78, 125.85, 124.34, 120.44, 112.47, 110.36 (tm, *J* = 12 Hz), 55.60. HRMS (ESI-TOF) m/z Calcd for $C_{16}H_7BrF_5NO$ $[M+H]^+$: 403.9704, found: 403.9713.



6-bromo-1-((perfluorophenyl) methoxy) isoquinoline (**3u**)

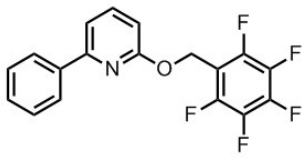
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (t, *J* = 4 Hz 2H), 7.88 (d, *J* = 1.6 Hz, 1H), 7.57 (d, *J* = 10.6 Hz, 1H), 7.16 (d, *J* = 5.9 Hz, 1H), 5.64 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.82 (dd, *J* = 22.56, 7.52 Hz,

2F), -153.17 (t, *J* = 18.80 Hz, 1F), -161.87 (td, *J* = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.39, 145.93 (dm, *J* = 260 Hz), 141.555 (dm, *J* = 249 Hz), 140.64, 139.11, 137.505 (dm, *J* = 261 Hz), 130.27, 128.35, 125.74, 125.53, 117.73, 114.69, 110.48 (tm, *J* = 261 Hz), 55.42. HRMS (ESI-TOF) m/z Calcd for $C_{16}H_7BrF_5NO$ $[M+H]^+$: 403.9704, found: 403.9707.



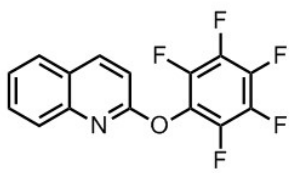
2-((perfluorophenyl) methoxy) pyridine (**3v**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 6.3 Hz, 1H), 7.59 (t, *J* = 12 Hz 1H), 6.96 – 6.88 (m, 1H), 6.74 (d, *J* = 8.4 Hz, 1H), 5.45 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -142.105 (dd, *J* = 18.80, 7.52 Hz, 2F), -153.70 (t, *J* = 18.80 Hz, 1F), -162.215 (td, *J* = 18.80, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.64, 146.71, 145.835 (dm, *J* = 261 Hz), 141.475 (dm, *J* = 253 Hz), 138.82, 137.465 (dm, *J* = 260 Hz), 117.48, 111.03, 110.77 (tm, *J* = 17 Hz), 54.75. HRMS (ESI-TOF) m/z Calcd for $C_{12}H_6F_5NO$ $[M+H]^+$: 276.0442, found: 276.0438.



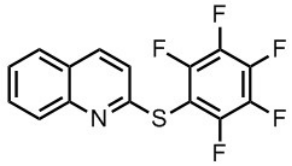
2-((perfluorophenyl) methoxy)-6-phenylpyridine (**3w**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.0 Hz, 2H), 7.57 (t, *J* = 2 Hz, 1H), 7.39 (t, *J* = 7.3 Hz, 2H), 7.32 (dd, *J* = 10.6, 7.3 Hz, 2H), 6.61 (dd, *J* = 8.2, 0.6 Hz, 1H), 5.51 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -141.885 (dd, *J* = 22.56, 7.52 Hz, 2F), -153.68 (t, *J* = 22.56 Hz, 1F), -161.13 (td, *J* = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.28, 154.70, 145.82 (dm, *J* = 246 Hz), 141.445 (dm, *J* = 247 Hz), 139.58, 138.66, 137.555 (dm, *J* = 267 Hz), 129.01, 128.62, 126.69, 113.69, 110.97 (tm, *J* = 21 Hz), 109.41, 54.67. HRMS (ESI-TOF) m/z Calcd for $C_{18}H_{10}F_5NO$ $[M+H]^+$: 352.0755, found: 352.0750.



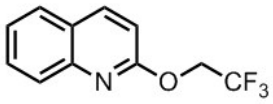
2-(perfluorophenoxy) quinoline (**6a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.8 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.62 (t, *J* = 7.7 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.405 (dd, *J* = 26.32, 3.76 Hz, 2F), -160.03 (t, *J* = 22.56 Hz, 1F), -163.35 (td, *J* = 26.32, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.04, 145.67, 142.07 (dm, *J* = 250 Hz), 140.55, 138.99 (dm, *J* = 250 Hz), 137.995 (dm, *J* = 249 Hz), 131.38 (tm, *J* = 16 Hz), 130.17, 127.71, 127.48, 126.20, 125.46, 111.2. HRMS (ESI-TOF) m/z Calcd for $C_{15}H_6F_5NO$ $[M+H]^+$: 312.0442, found: 312.0439.



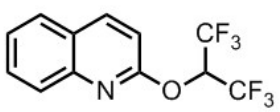
2-((perfluorophenyl) thio) quinoline (**6b**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.6 Hz, 1H), 7.74 (t, *J* = 9.6 Hz, 2H), 7.62 (t, *J* = 7.7 Hz, 1H), 7.45 (t, *J* = 8.1 Hz, 1H), 7.23 (d, *J* = 8.6 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -130.00 (dd, *J* = 26.32, 3.76 Hz, 2F), -150.22 (tt, *J* =18.80, 3.76 Hz, 1F), -16o.865 (td, *J* = 17.80, 3.76 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.04, 145.67, 142.07 (dm, *J* = 250 Hz), 140.55, 138.99 (dm, *J* = 250 Hz), 137.995 (dm, *J* = 249 Hz), 131.38 (tm, *J* = 11 Hz), 130.17, 127.71, 127.48, 126.20, 125.46, 111.21. HRMS (ESI-TOF) m/z Calcd for $C_{15}H_6F_5NS$ $[M+H]^+$: 328.0214, found: 328.0227.



2-(2,2,2-trifluoroethoxy) quinoline (**6c**)

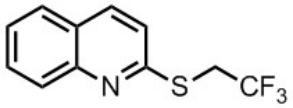
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.8 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.65 (t, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.00 (d, *J* = 8.8 Hz, 1H), 4.93 (q, *J* = 8.6 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.64 (s, 3F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.90, 145.85, 139.58, 129.89, 127.50, 127.33, 125.58, 124.78, 123.595 (q, *J* = 276 Hz), 112.33, 62.13 (q, *J* = 36 Hz). HRMS (ESI-TOF) m/z Calcd for $C_{11}H_8F_3NO$ $[M+H]^+$: 228.0631, found: 228.0627.



2-((1,1,1,3,3,3-hexafluoropropan-2-yl) oxy) quinoline (**6d**)

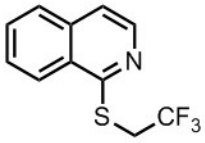
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.8 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.1 Hz,

1H), 7.69 (t, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 8.8 Hz, 1H), 6.90 (p, *J* = 6.4 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.16 (s, 6F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.05, 145.06, 140.64, 130.32, 127.53, 127.48, 126.24, 125.52, 121.19 (qm, *J* = 284 Hz), 111.74, 67.23 (m). HRMS (ESI-TOF) m/z Calcd for $C_{12}H_7F_6NO$ $[M+H]^+$: 296.0505, found: 296.0518.



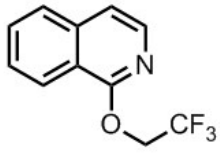
2-((2,2,2-trifluoroethyl) thio) quinoline (**6e**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.5 Hz, 1H), 7.87 (d, *J* = 8.6 Hz, 1H), 7.68 (d, *J* = 8.1 Hz, 1H), 7.64 (t, *J* = 8.0 Hz, 1H), 7.42 (t, *J* = 8.1 Hz, 1H), 7.17 (d, *J* = 8.6 Hz, 1H), 4.23 (q, *J* = 10.1 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.10 (s, 3F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.49, 147.78, 136.18, 129.95, 128.02, 127.59, 126.37, 125.8, 125.46 (q, *J* = 274 Hz), 120.30, 30.535 (q, *J* = 34 Hz). HRMS (ESI-TOF) m/z Calcd for $C_{11}H_8F_3NS$ $[M+H]^+$: 244.0402, found: 244.0411.



1-((2,2,2-trifluoroethyl) thio) isoquinoline (**6f**)

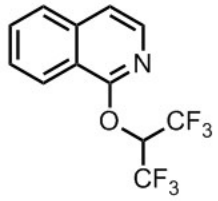
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 5.7 Hz, 1H), 8.10 (d, *J* = 8.9 Hz, 1H), 7.71 (d, *J* = 8.2 Hz, 3H), 7.62 (t, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 8.3 Hz, 1H), 7.34 (d, *J* = 5.7 Hz, 1H), 4.27 (q, *J* = 10.1 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.99 (s, 3F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.76, 141.32, 135.73, 130.57, 127.33, 127.15, 126.62, 125.465 (q, *J* = 275 Hz), 123.99, 118.29, 30.505 (q, *J* = 33 Hz). HRMS (ESI-TOF) m/z Calcd for $C_{11}H_8F_3NS$ $[M+H]^+$: 244.0402, found: 244.0417.



1-(2,2,2-trifluoroethoxy) isoquinoline (**6g**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.3 Hz, 1H), 7.97 (d, *J* = 5.9 Hz, 1H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.70 (t, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 8.2 Hz, 1H), 7.31 (d, *J* = 5.8 Hz, 1H), 4.94 (q, *J* = 8.6 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.63 (s, 3F). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 158.39, 138.93, 138.09, 130.90, 127.15, 126.17, 123.89, 123.81 (q, *J* = 275 Hz), 119.10, 116.48, 62.44 (q, *J* = 36 Hz).

HRMS (ESI-TOF) m/z Calcd for $C_{11}H_8F_3NO$ $[M+H]^+$: 228.0631, found: 228.0637.

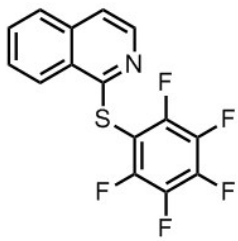


1-((1,1,1,3,3,3-hexafluoropropan-2-yl) oxy) isoquinoline (**6h**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 5.8 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.4 (t, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 5.8 Hz, 1H), 6.87 (q, *J* = 6.3 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.22 (s, 6F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.55, 138.59, 138.25, 131.36, 127.64, 126.33, 123.56, 121.205 (q, *J* = 281 Hz), 118.66, 117.93, 67.611 (m). HRMS (ESI-TOF) m/z Calcd for $C_{12}H_7F_6NO$ $[M+H]^+$: 296.0505, found: 296.0513.

1-(perfluorophenoxy) isoquinoline (**6i**)

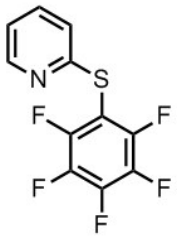
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.3 Hz, 1H), 7.78 (d, *J* = 5.8 Hz, 1H), 7.70 (d, *J* = 8.2 Hz, 1H), 7.63 (t, *J* = 8.2 Hz, 1H), 7.54 (t, *J* = 8.1 Hz, 1H), 7.28 (d, *J* = 5.8 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.705 (dd, *J* = 22.56, 7.52 Hz, 2F), -159.72 (t, *J* = 22.56 Hz, 1F), -163.07 (td, *J* = 22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.84, 142.03 (dm, *J* = 250 Hz), 139.09 (dm, *J* = 250 Hz), 138.94, 138.68, 138.06 (dm, *J* = 250 Hz), 131.30, 127.86 (tm, *J* = 15 Hz), 127.70, 126.39, 123.77, 118.38, 118.09. HRMS (ESI-TOF) m/z Calcd for $C_{15}H_6F_5NO$ $[M+H]^+$: 312.0442, found: 312.0447.



1-((perfluorophenyl) thio) isoquinoline (**6j**)

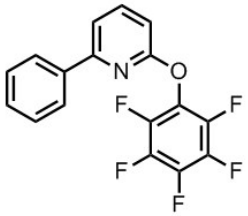
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 5.7 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.72 (t, *J* = 7.0 Hz, 1H), 7.66 (d, *J* = 8.3 Hz, 1H), 7.41 (d, *J* = 5.6 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -130.30 (dd, *J* = 18.80, 7.52 Hz, 2F), -150.39 (td, *J* = 18.80, 3.76 Hz, 1F), -161.03 (td, *J* =

22.56, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.99, 148.125 (dm, *J* = 243 Hz), 142.495 (dm, *J* = 255 Hz), 142.05, 137.83 (dm, *J* = 252 Hz), 136.03, 130.77, 127.73, 127.31, 126.41, 124.29, 118.91, 104.50 (tm, *J* = 20 Hz). HRMS (ESI-TOF) m/z Calcd for $C_{15}H_6F_5NS$ $[M+H]^+$: 328.0214, found: 328.0231.



2-((perfluorophenyl) thio) pyridine (**6k**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 4.8 Hz, 1H), 7.59 (td, *J* = 8.0, 4.0 Hz 1H), 7.22 (d, *J* = 8.1 Hz, 1H), 7.12 – 7.05 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -130.485 (dd, *J* = 18.80, 3.76 Hz, 2F), -150.46 (td, *J* = 18.80, 1F), -160.755 (td, *J* = 18.80, 7.52 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.25 , 150.01 , 147.72 (dm, *J* = 246 Hz), 142.445 (dm, *J* = 255 Hz), 137.83 (dm, *J* = 254 Hz), 136.93 , 121.47 , 121.02, 105.21 (tm, *J* = 21 Hz). HRMS (ESI-TOF) m/z Calcd for $C_{11}H_4F_5NS$ $[M+H]^+$: 278.0057, found: 278.0049.

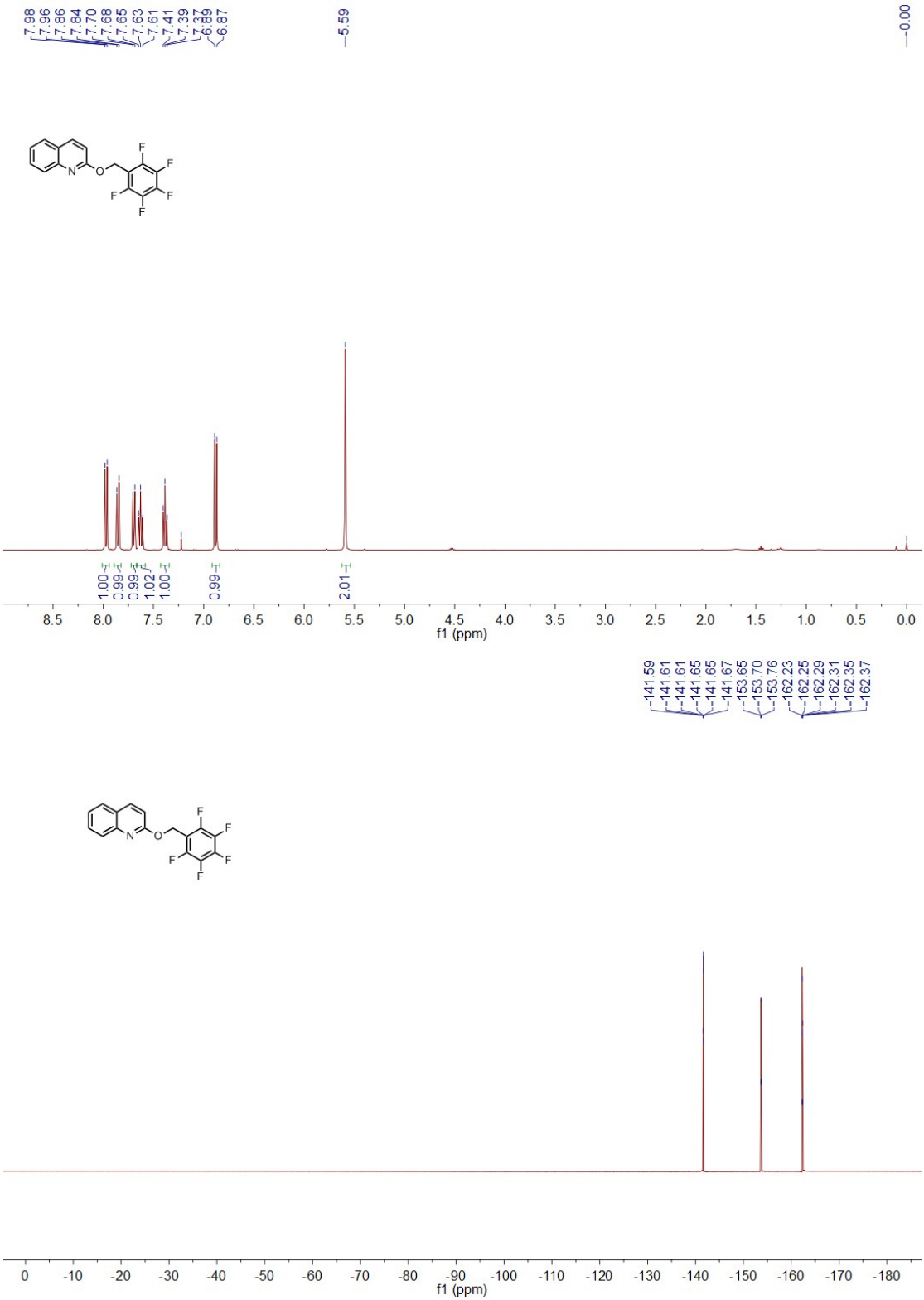


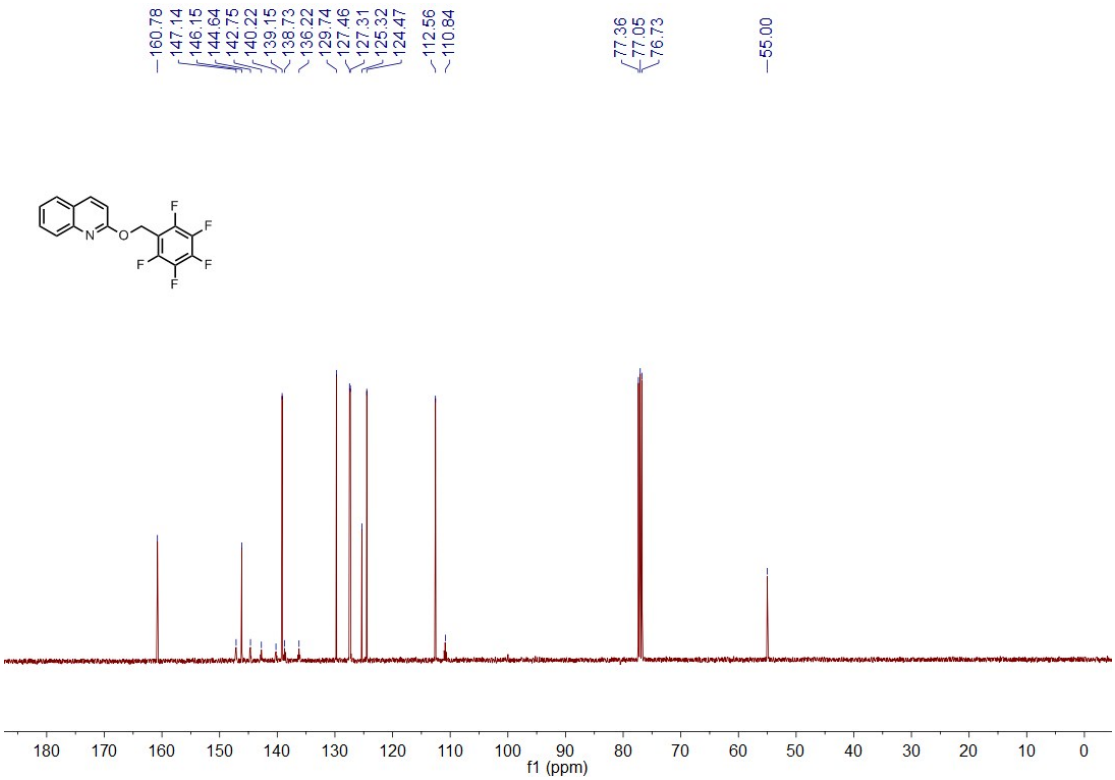
2-(perfluorophenoxy)-6-phenylpyridine (**6l**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (t, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.53 (d, *J* = 7.5 Hz, 1H), 7.39 (d, *J* = 7.2 Hz, 3H), 7.04 (d, *J* = 8.1 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.50 (dd, *J* = 22.56, 3.76 Hz, 2F), -160.09 (td, *J* = 18.80, 1F), -163.465 (td, *J* = 22.56, 3.76 Hz, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.65, 155.16, 142.09 (dm, *J* = 260 Hz), 140.66, 138.80 (dm, *J* = 246 Hz), 137.905 (dm, *J* = 251 Hz), 137.69, 129.36, 128.70, 127.91 (tm, *J* = 15 Hz), 126.57, 115.89, 108.69. HRMS (ESI-TOF) m/z Calcd for $C_{17}H_8F_5NO$ $[M+H]^+$: 338.0599, found: 338.0563.

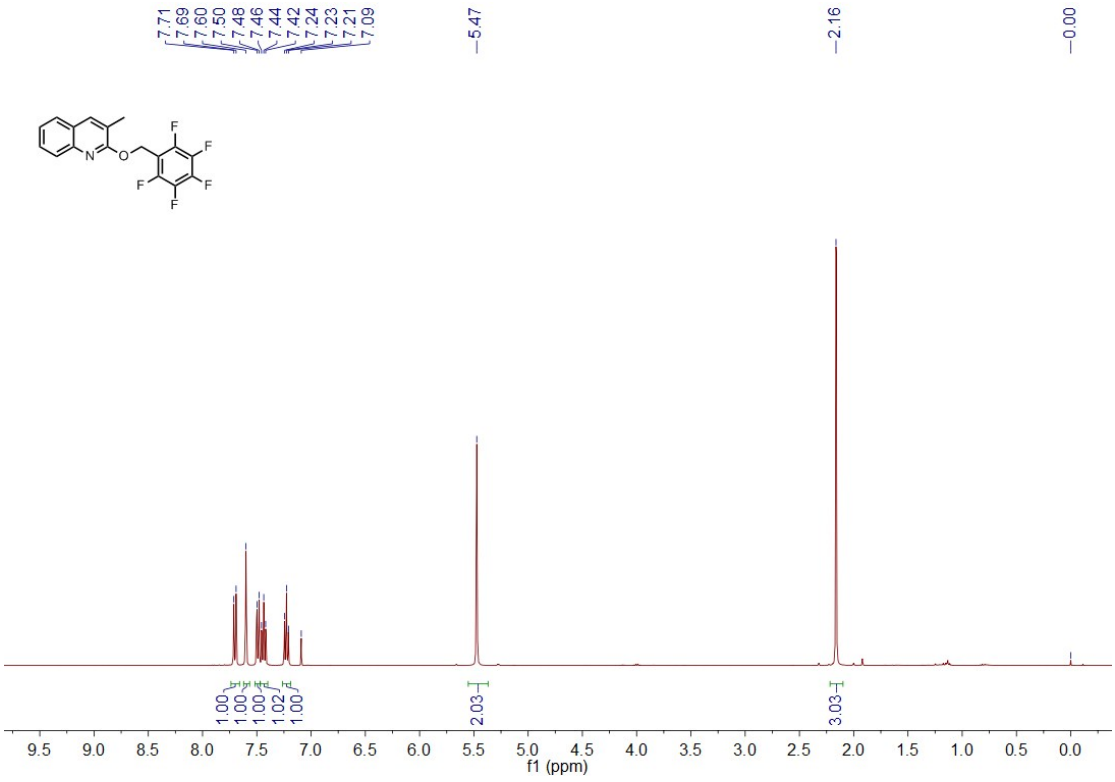
3. ^{1}H NMR and ^{13}C NMR spectra

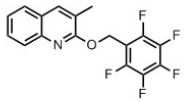
2-((perfluorophenyl) methoxy) quinoline (**3a**)





3-methyl-2-((perfluorophenyl) methoxy) quinoline (**3b**)





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-141.82
-153.98
-154.03
-154.09
-162.40
-162.42
-162.46
-162.48
-162.51
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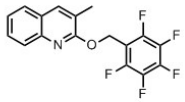
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)



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144.88
144.62
142.59
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138.66
137.33
136.15
128.50
126.83
126.55
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124.24
122.21
111.05
77.32
77.00
76.68
55.22
16.19
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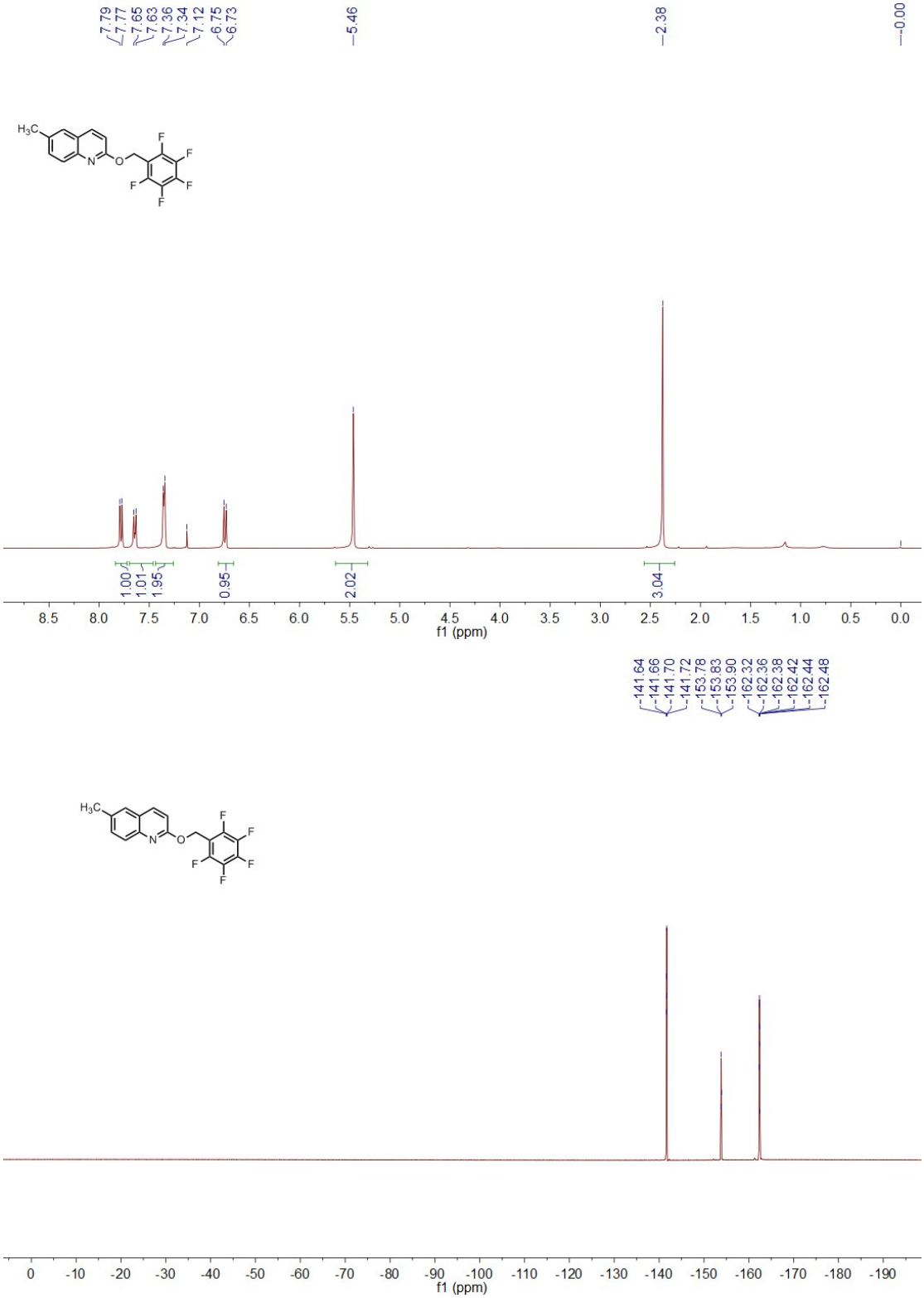
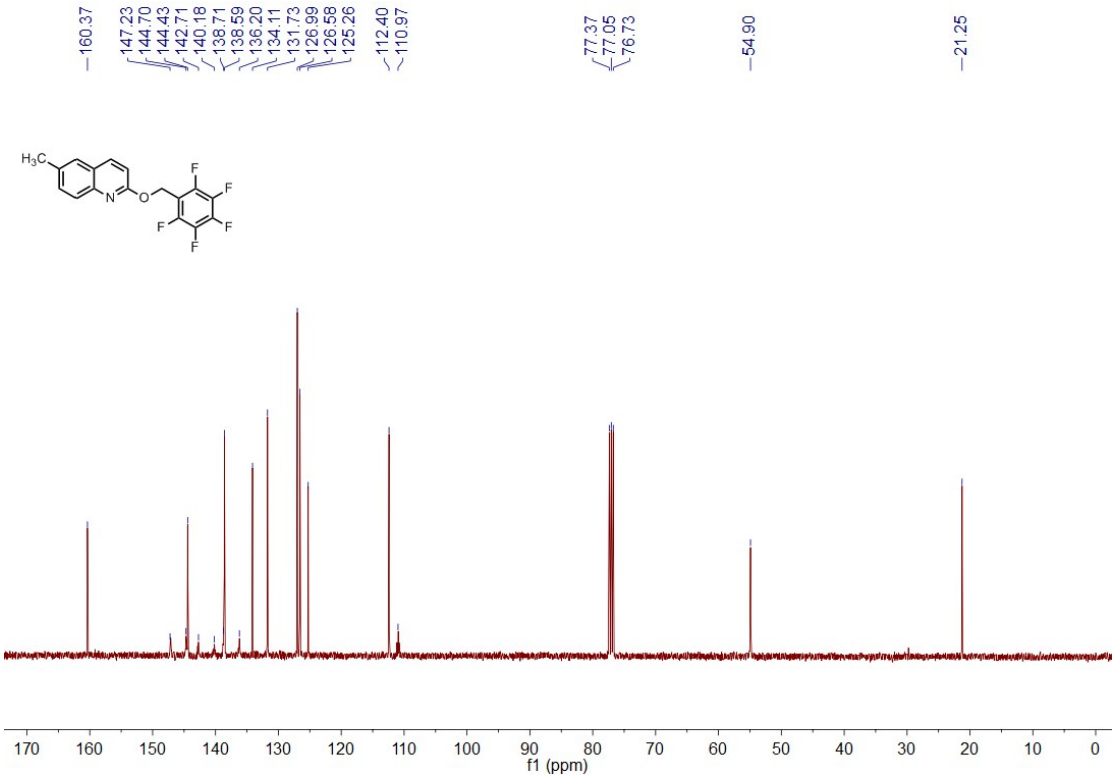
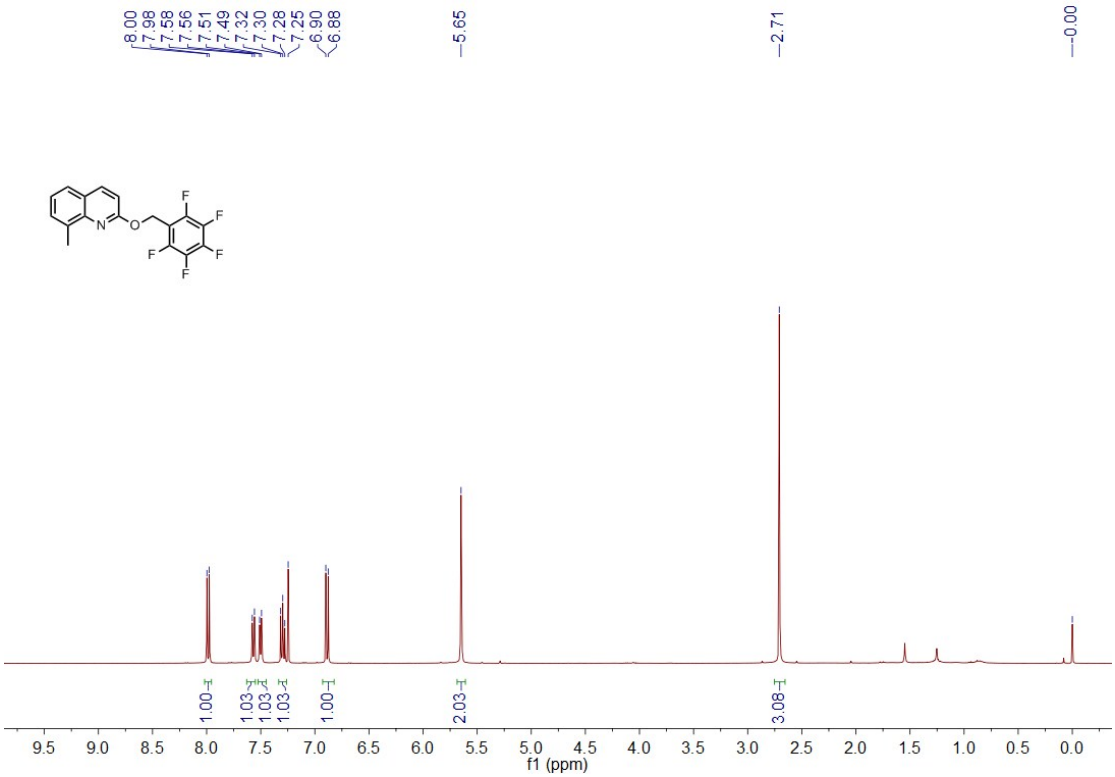
f1 (ppm)

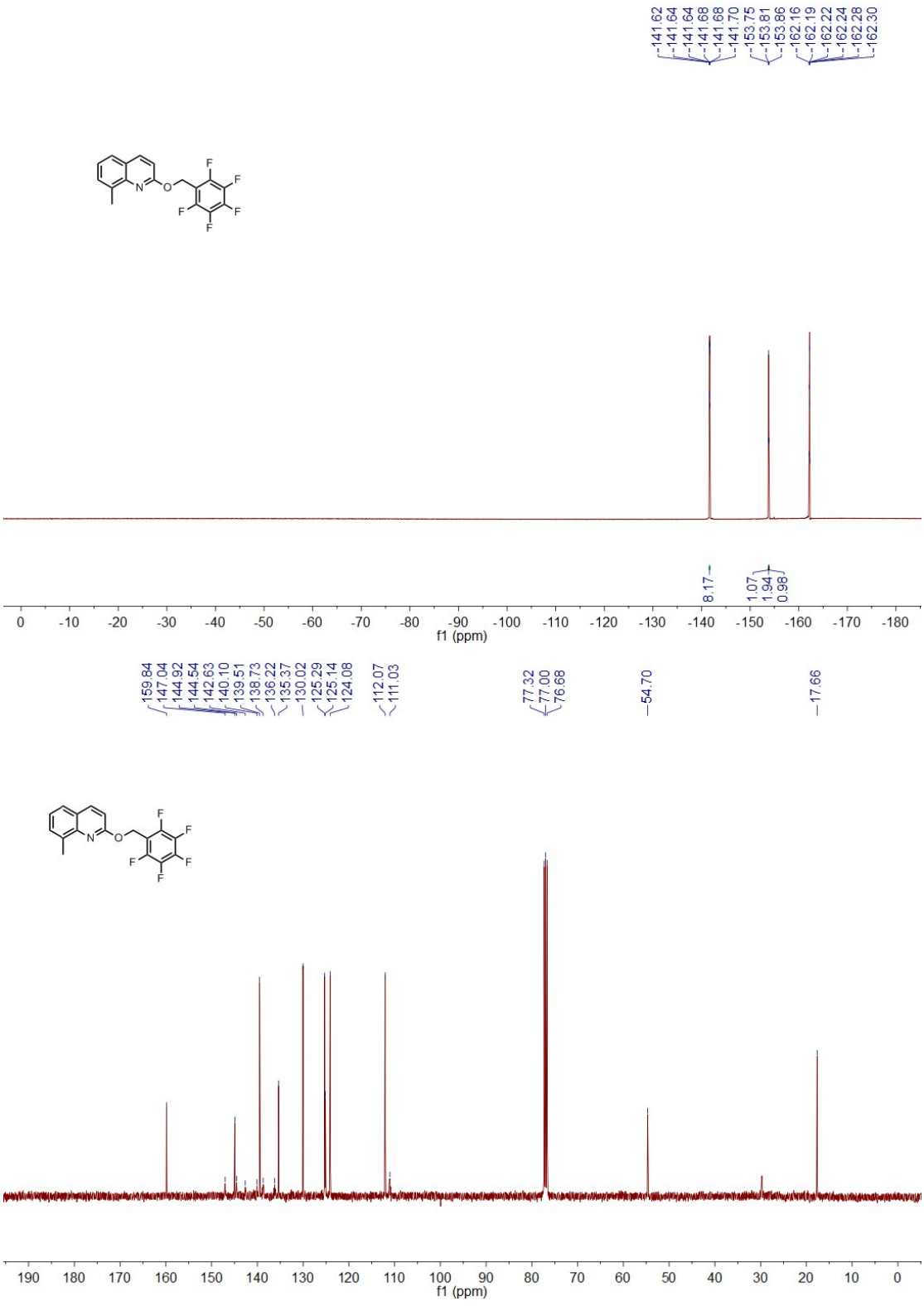
6-methyl-2-((perfluorophenyl) methoxy) quinoline (**3c**)





8-methyl-2-((perfluorophenyl) methoxy) quinoline (**3d**)

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-162.22
-162.24
-162.28
-162.30
F
F
F
F
F
N
O
8.17
1.07
1.94
0.98
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)
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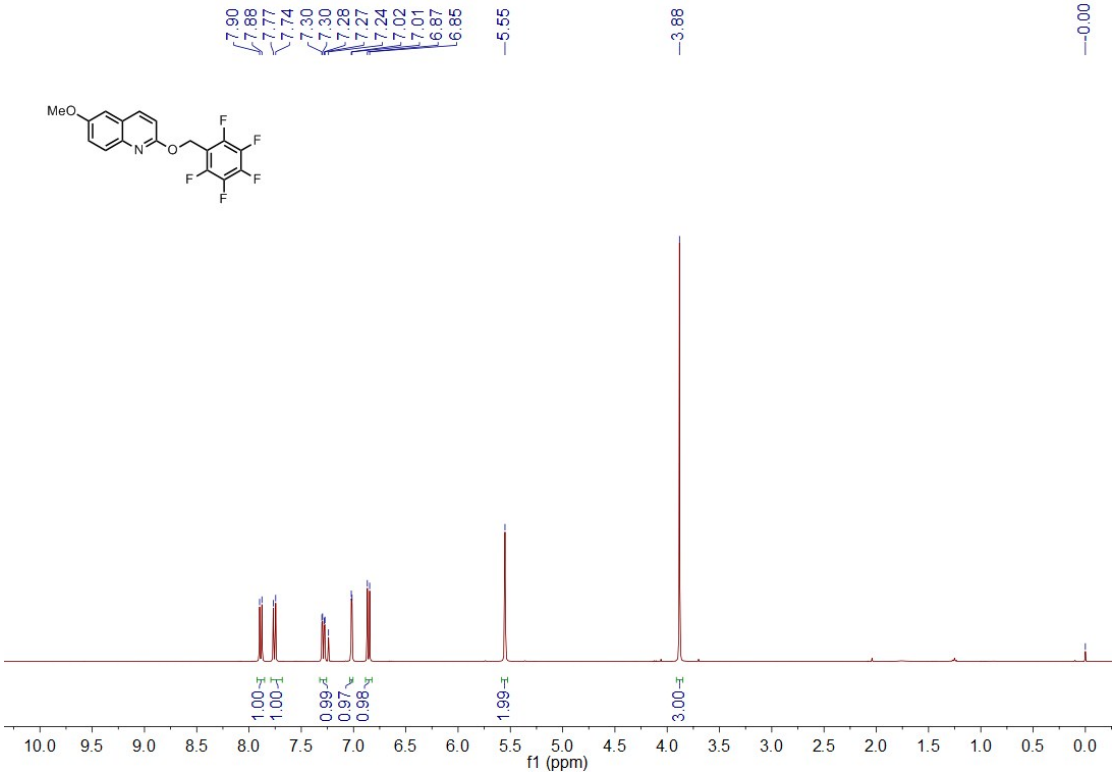
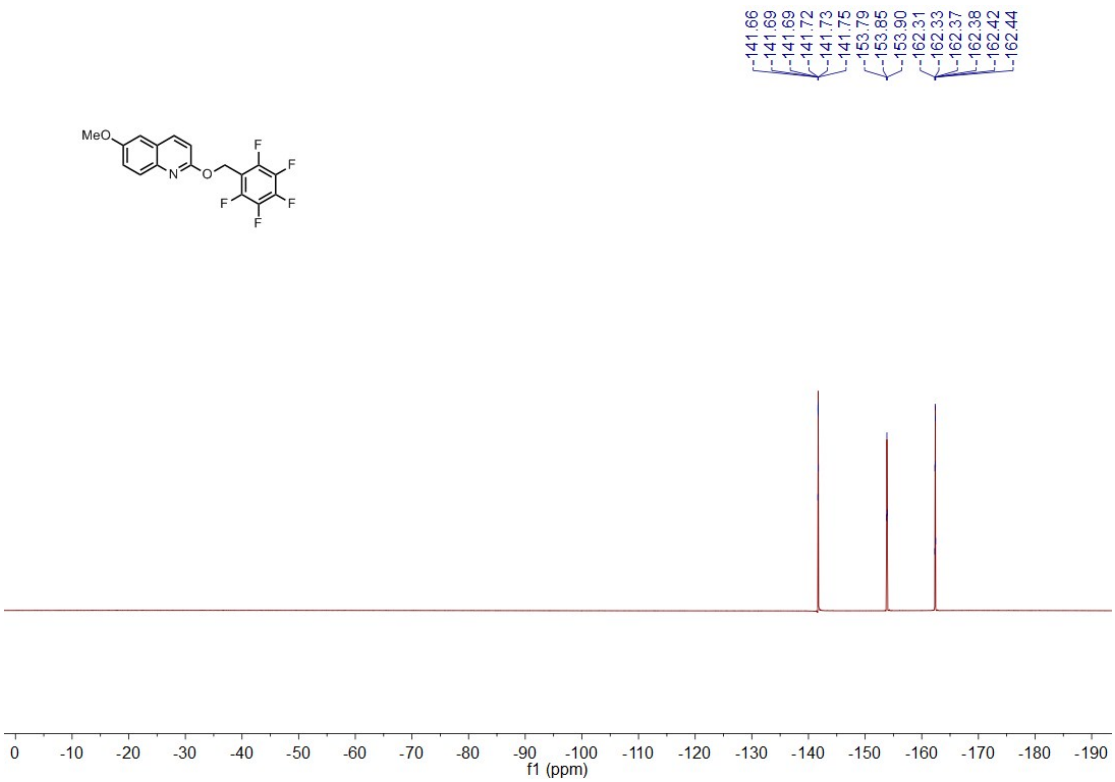
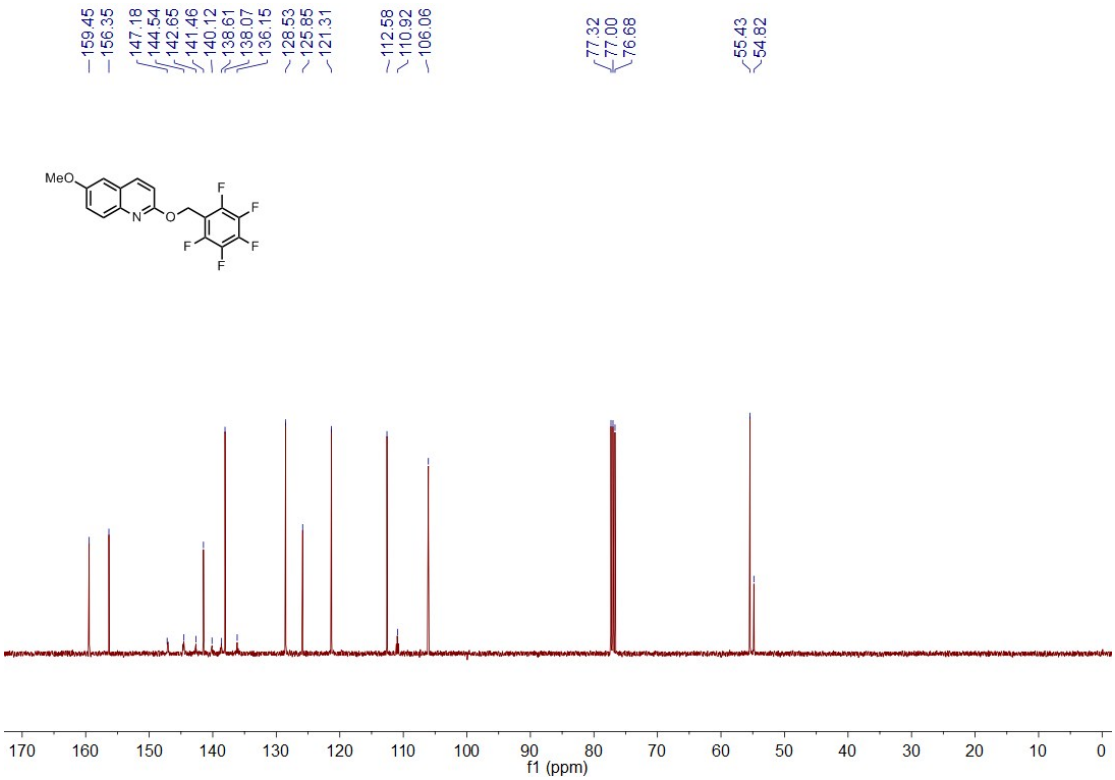
147.04
144.92
144.54
142.63
140.10
139.51
138.73
136.22
135.37
130.02
125.29
125.14
124.08
112.07
111.03
77.32
77.00
76.68
54.70
17.66
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

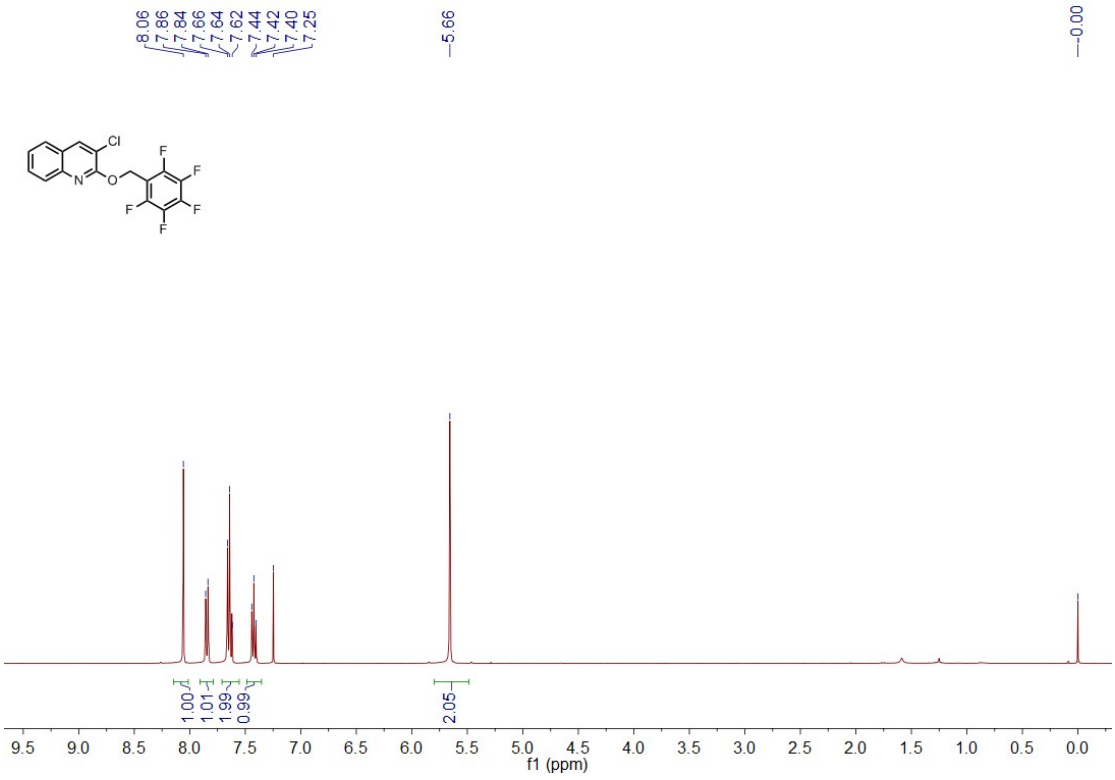
6-methoxy-2-((perfluorophenyl) methoxy) quinoline (**3e**)

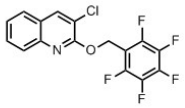


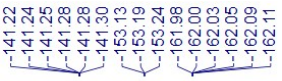




3-chloro-2-((perfluorophenyl) methoxy) quinoline (**3f**)




Cl
N
O
F
F
F
F
F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141.24
141.25
141.28
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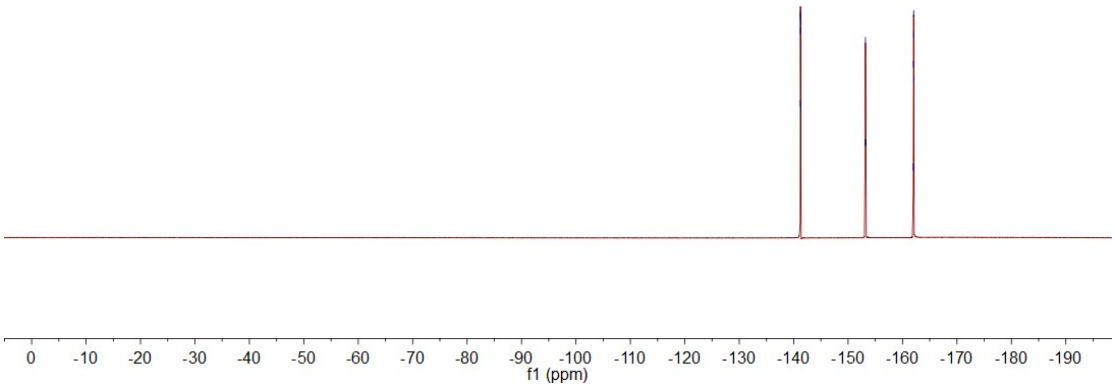
141.30
153.13
153.19
153.24
161.98
162.00
162.03
162.05
162.09
162.11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f1 (ppm)


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144.21
142.93
140.37
138.74
137.37
136.23
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127.10
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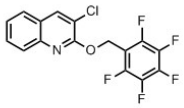
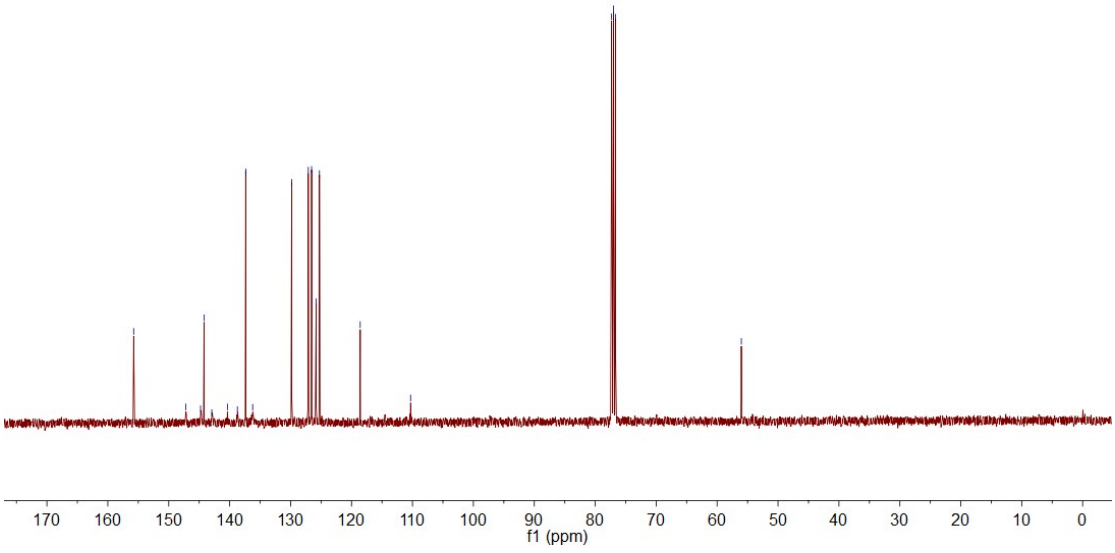
125.26
118.57
110.30
77.32
77.00
76.68
56.02


Cl
N
O
F
F
F
F
F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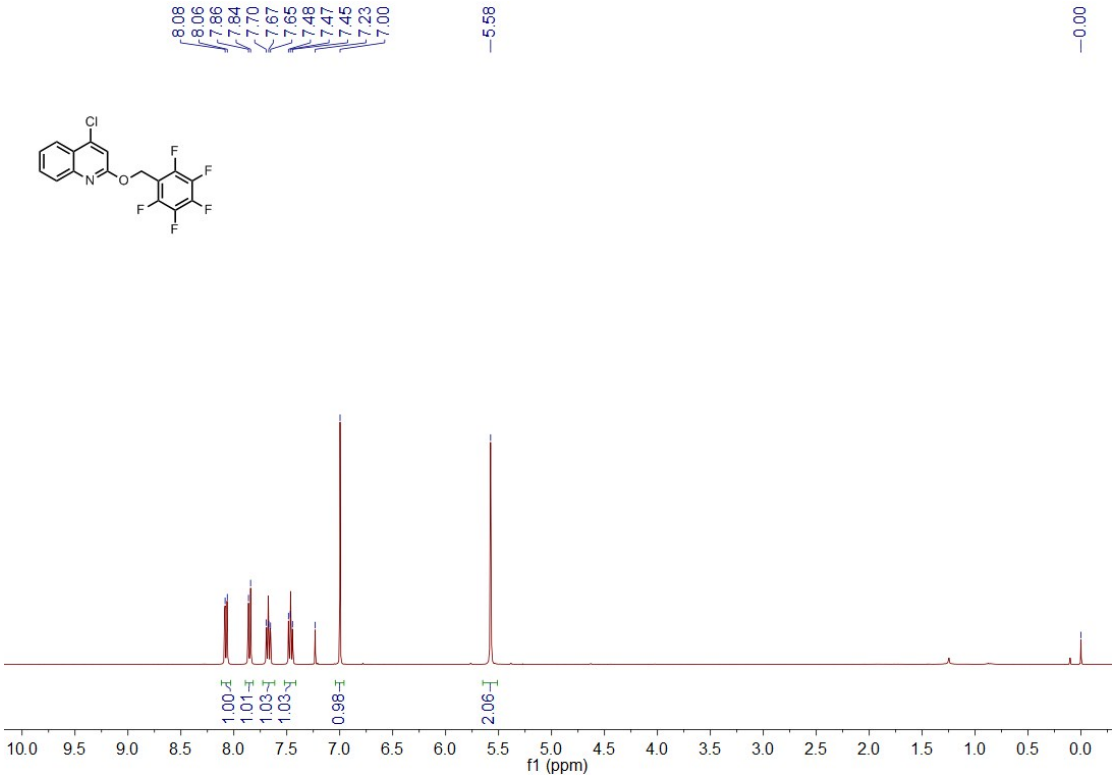
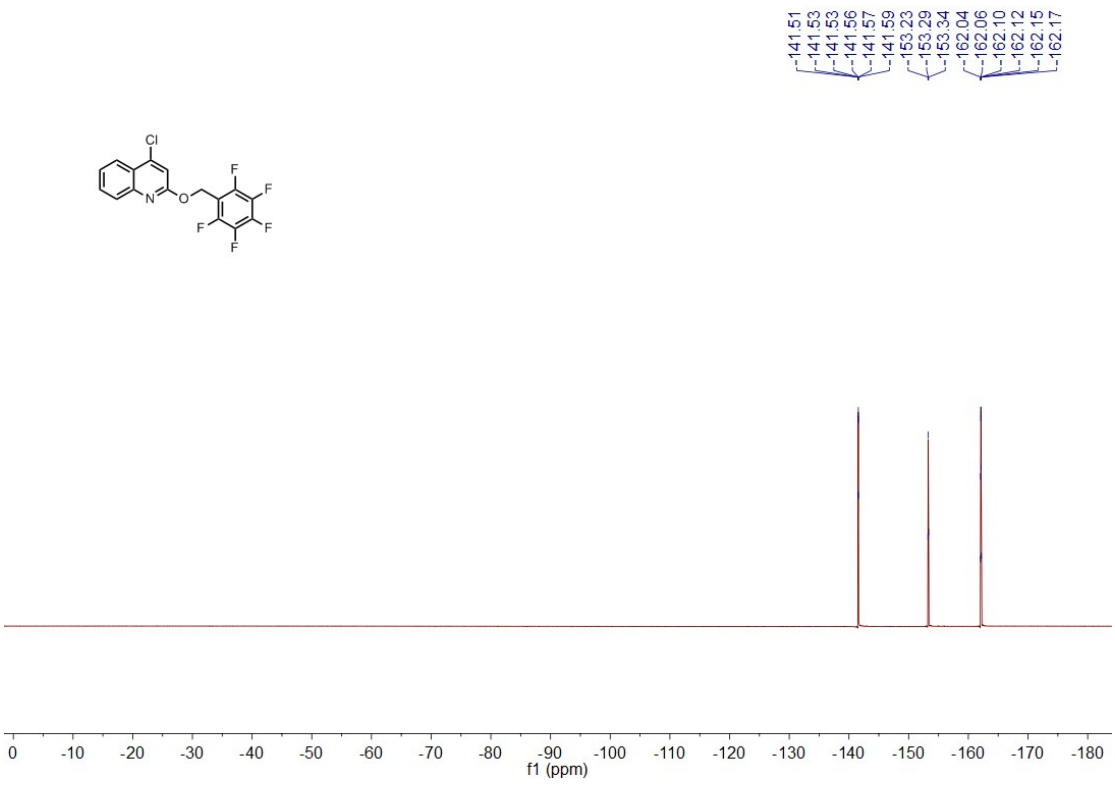
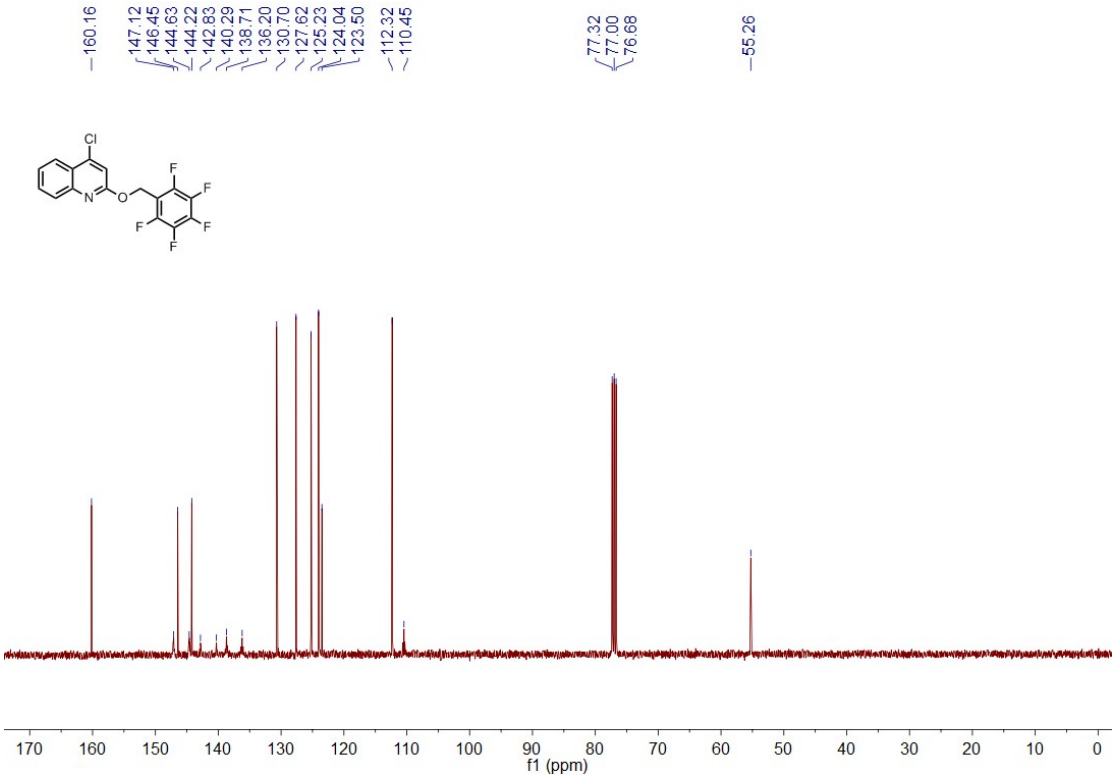
f1 (ppm)

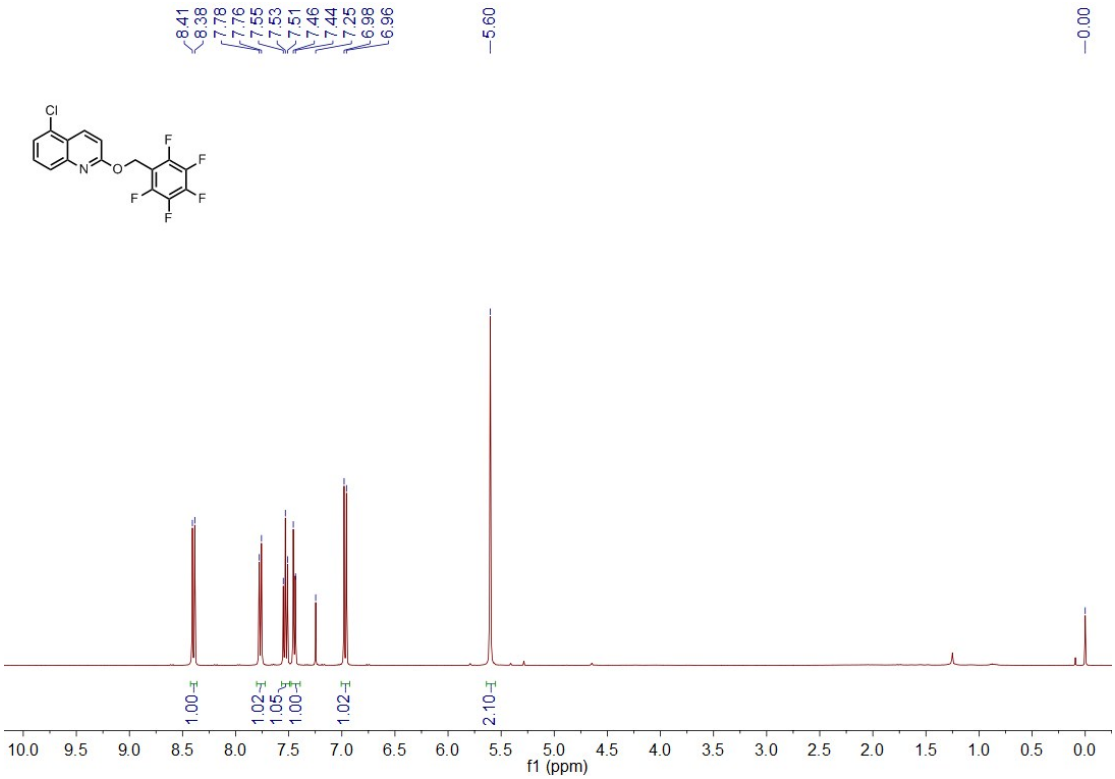
4-chloro-2-((perfluorophenyl) methoxy) quinoline (**3g**)

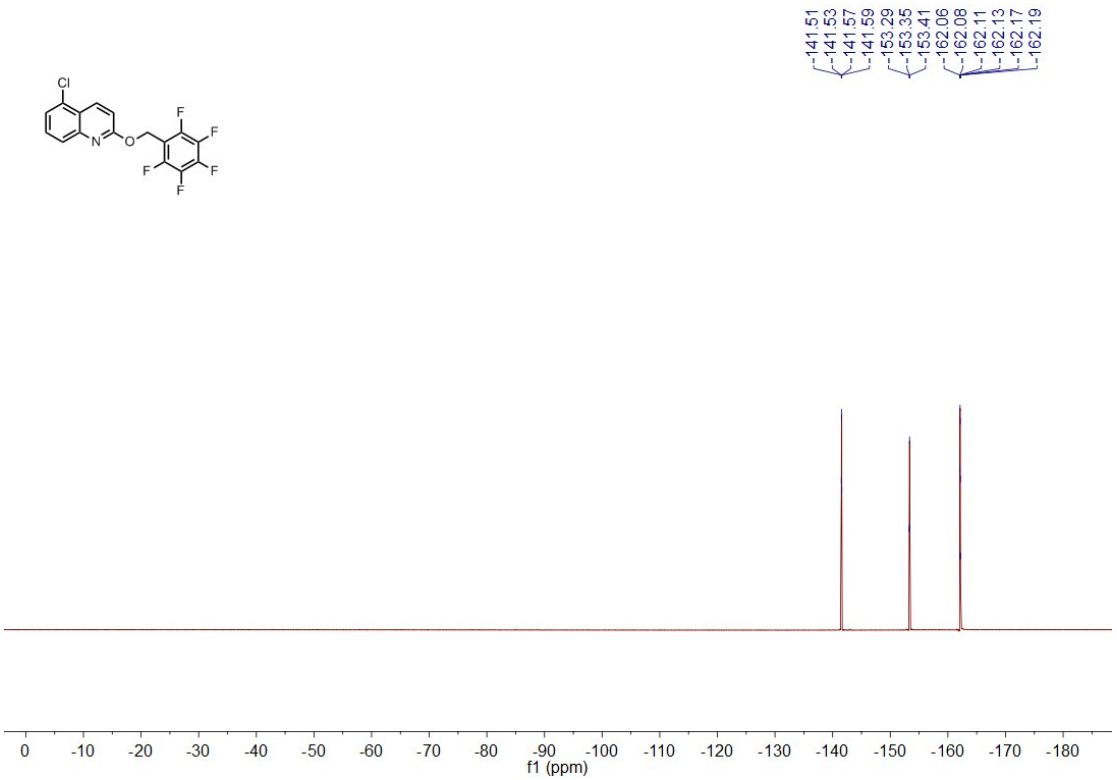






5-chloro-2-((perfluorophenyl) methoxy) quinoline (**3h**)




141.51
141.53
141.57
141.59
153.29
153.35
153.41
162.06
162.08
162.11
162.13
162.17
162.19
Cl
N
O
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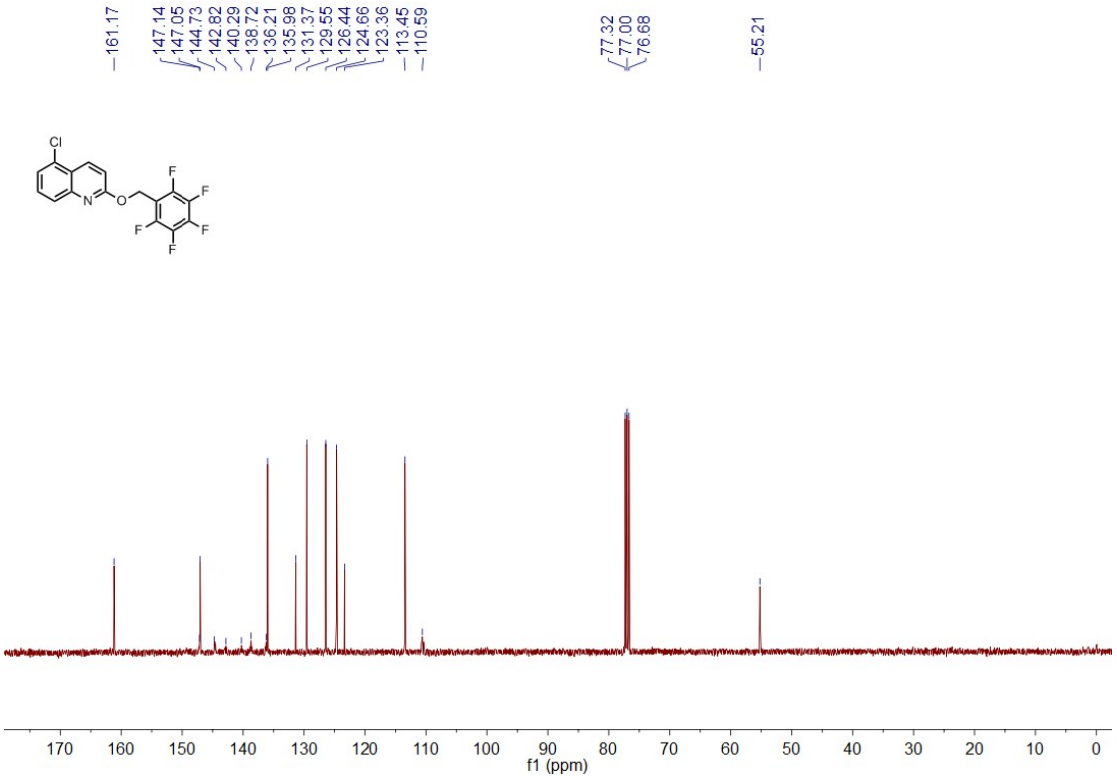
f1 (ppm)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140.29
138.72
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135.98
131.37
129.55
126.44
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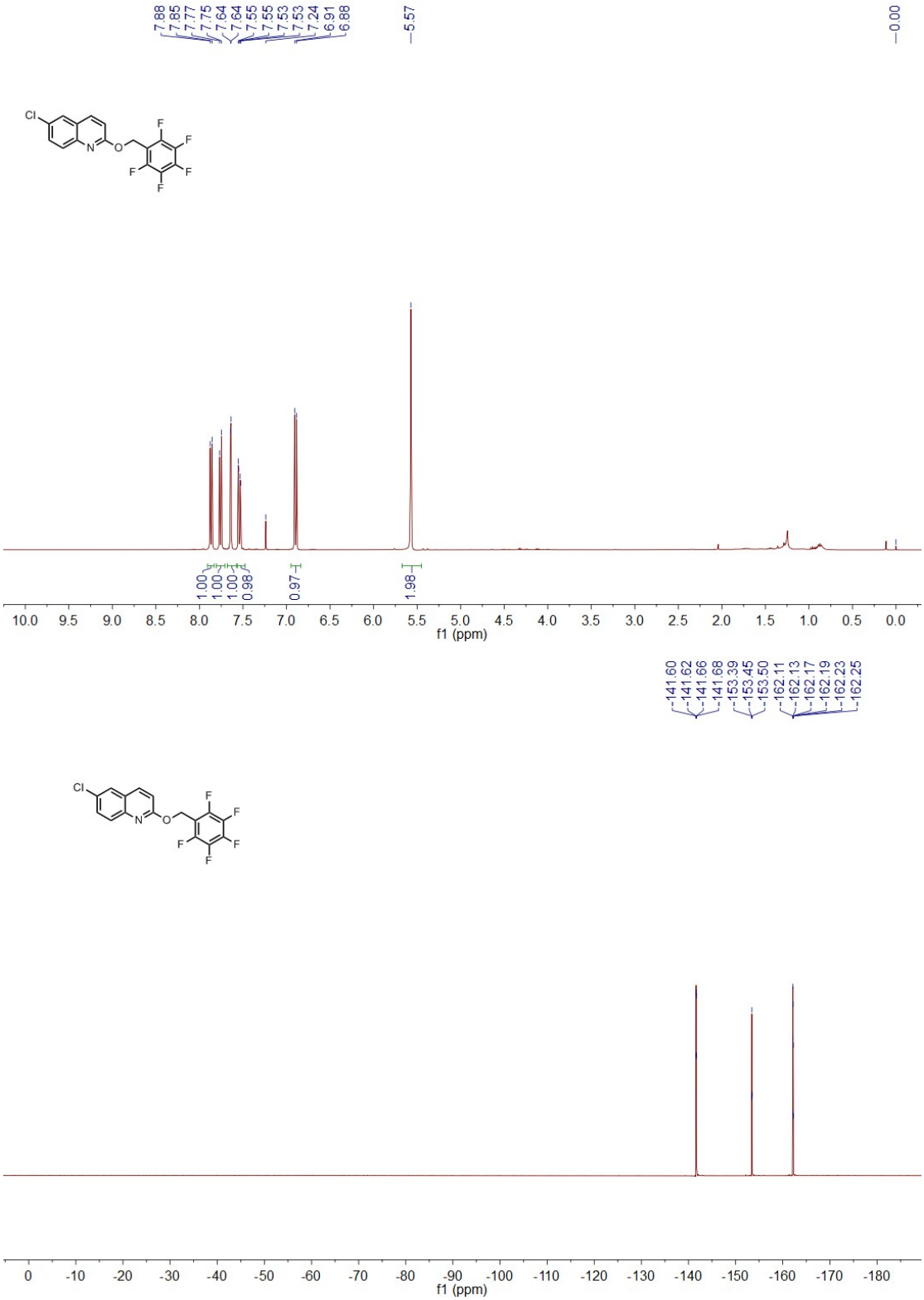
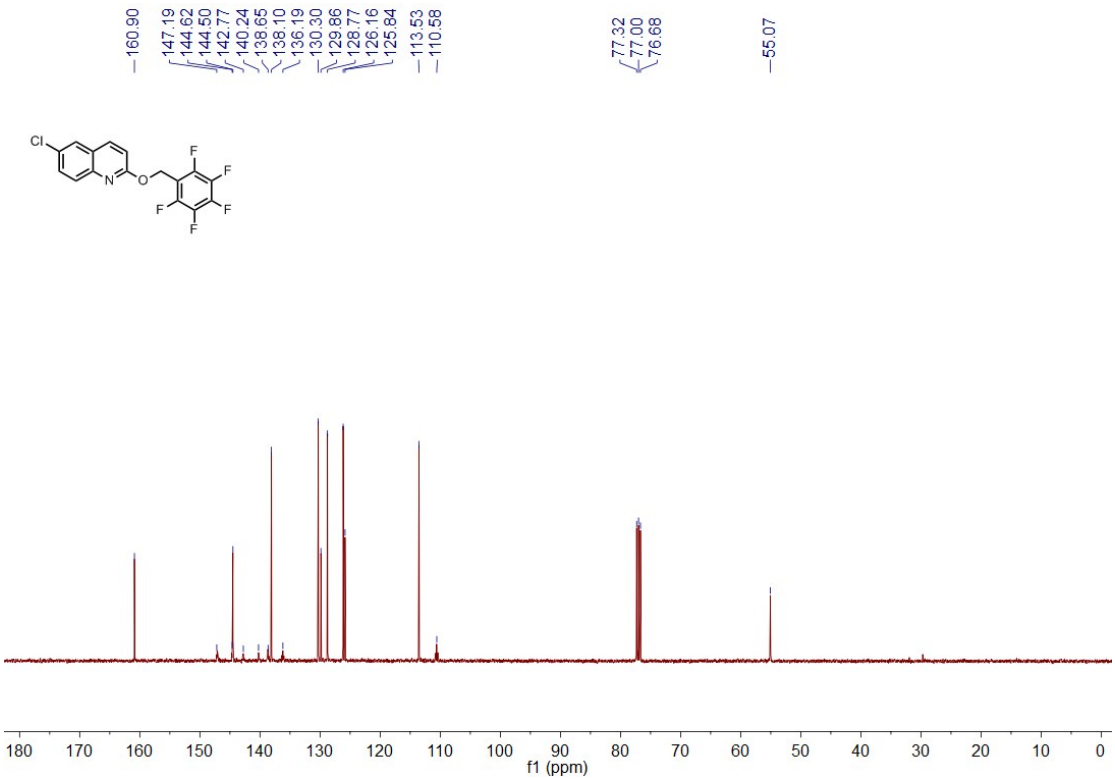
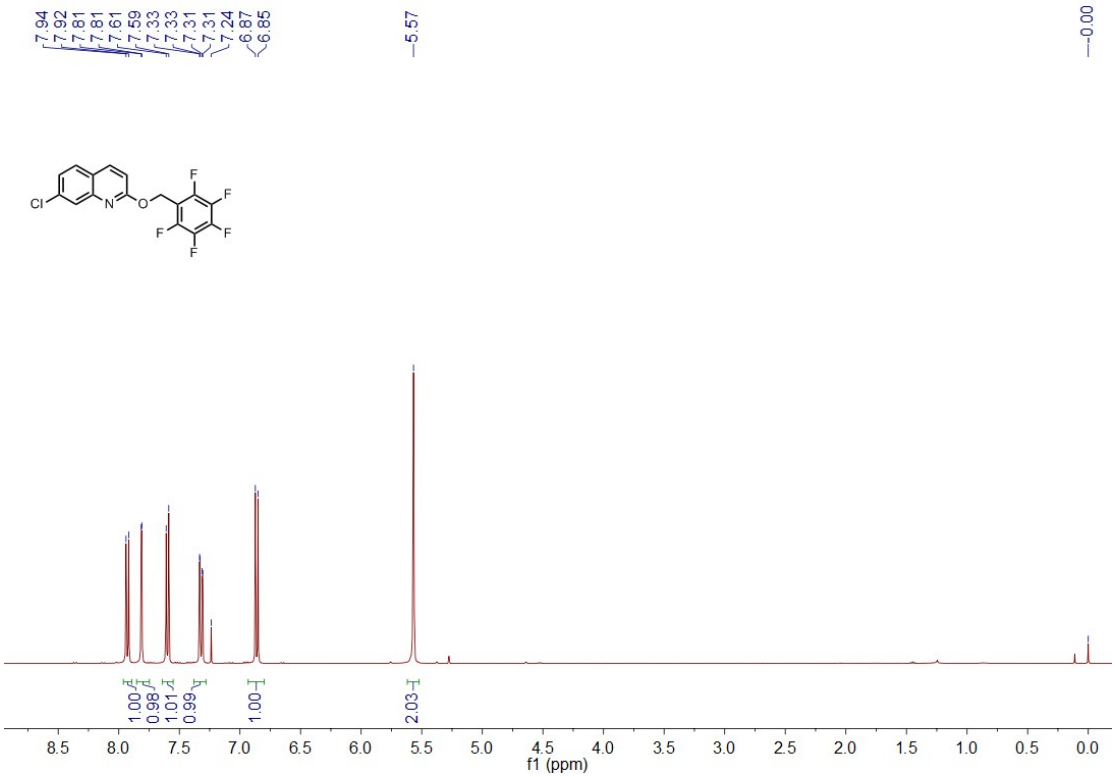
123.36
113.45
110.59
77.32
77.00
76.68
55.21
Cl
N
O
F
F
F
F
F
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

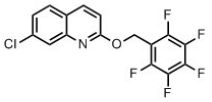
6-chloro-2-((perfluorophenyl) methoxy) quinoline (**3i**)

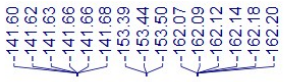




7-chloro-2-((perfluorophenyl) methoxy) quinoline (**3j**)




Cl
N
O
F
F
F
F
F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-141.66
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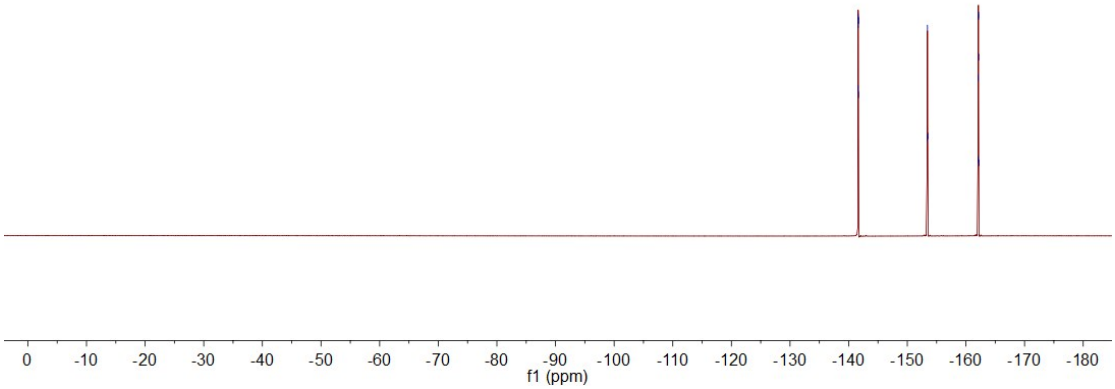
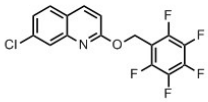
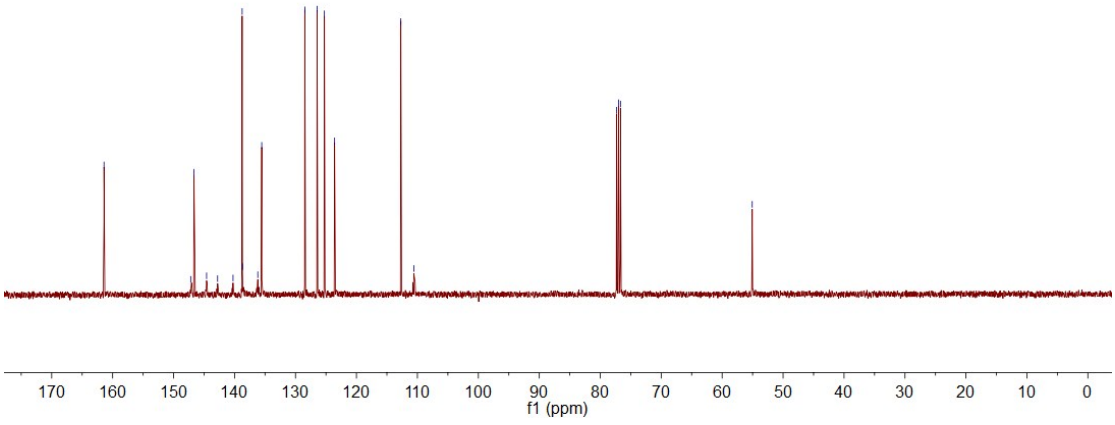
-162.09
-162.12
-162.14
-162.18
-162.20

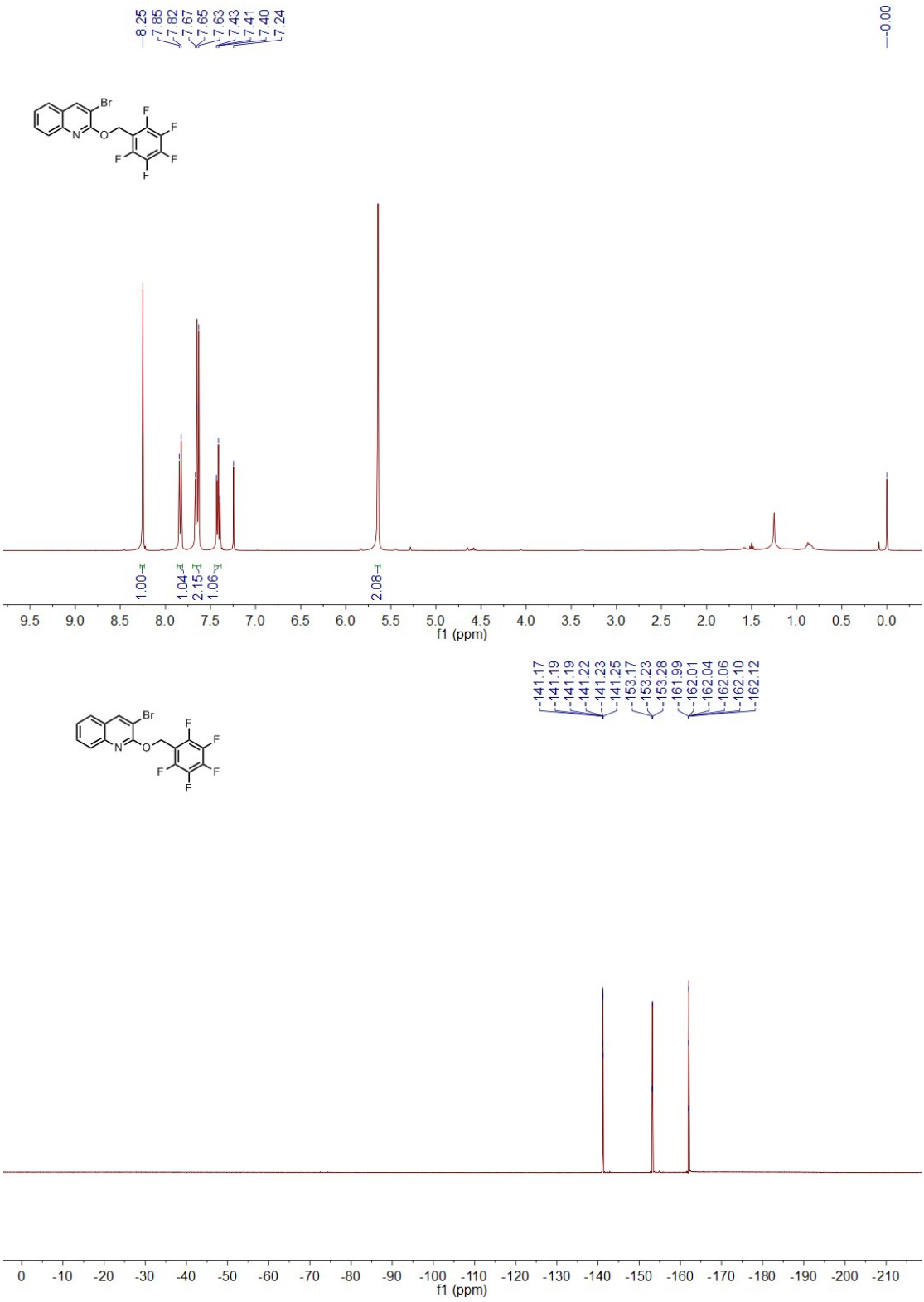

0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
f1 (ppm)

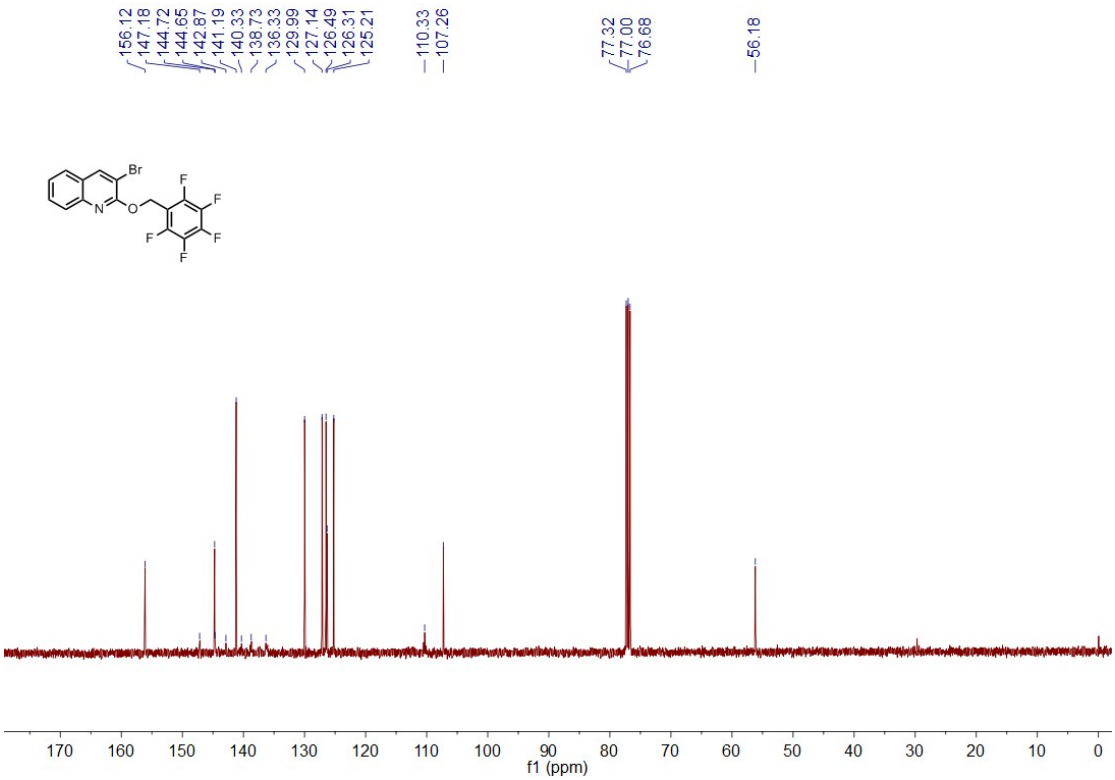

Cl
N
O
F
F
F
F
F


161.41
147.19
146.67
144.58
142.78
140.24
138.75
138.70
136.19
135.54
128.47
126.46
125.26
123.59
112.72
110.59
77.32
77.00
76.68
55.07

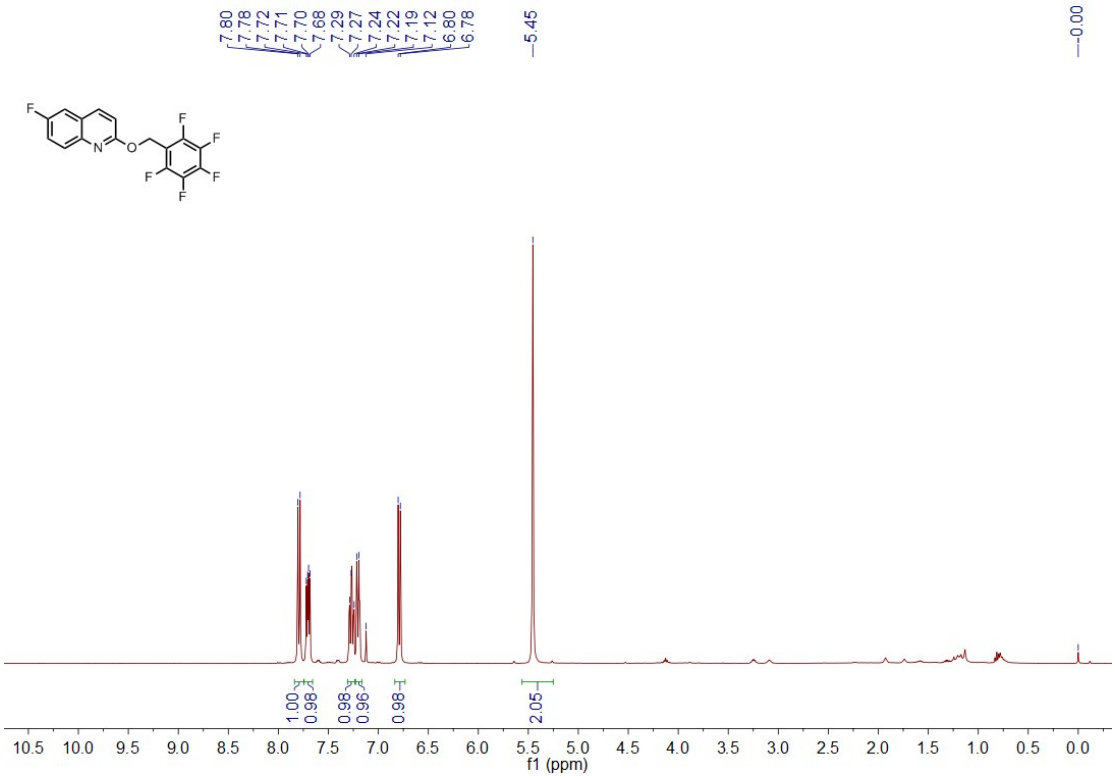

170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

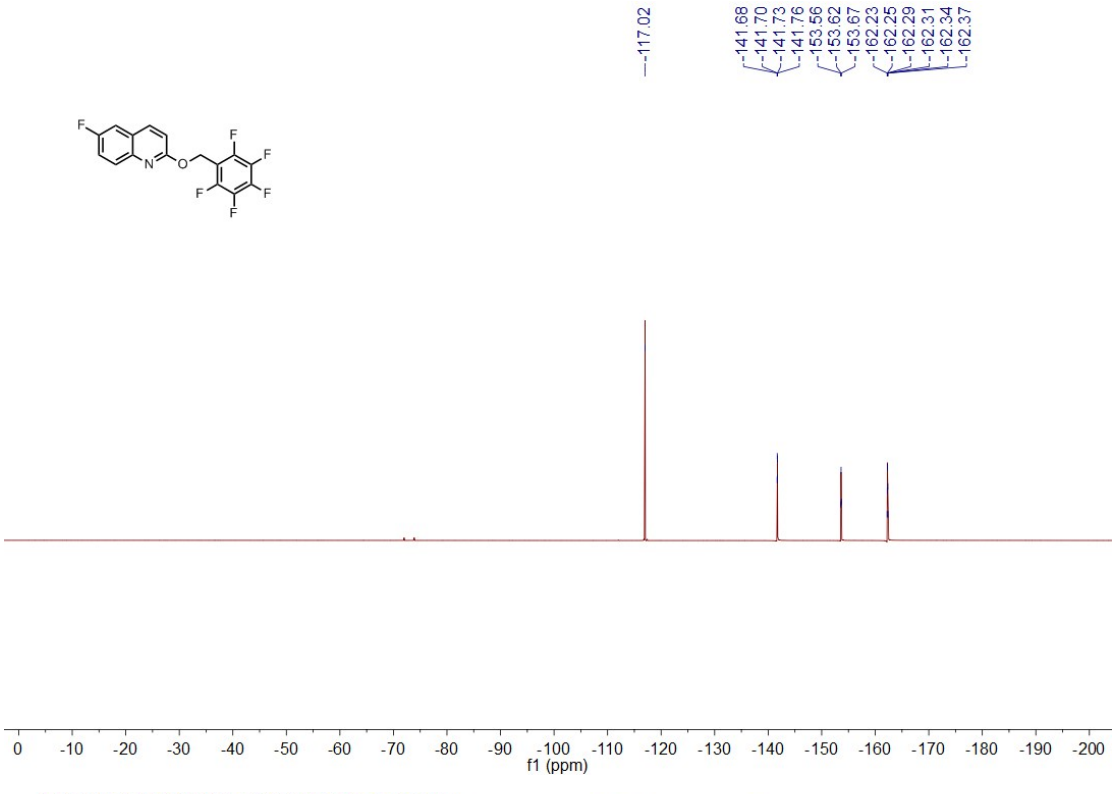
3-bromo-2-((perfluorophenyl) methoxy) quinoline(**3k**)

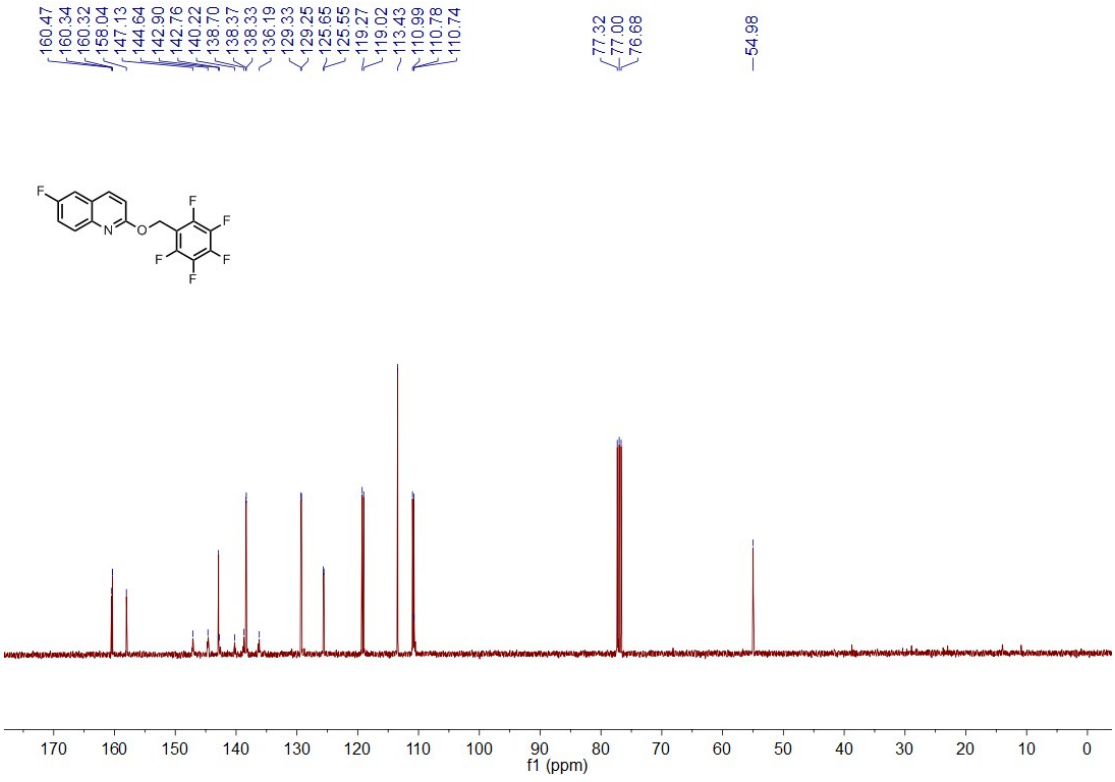




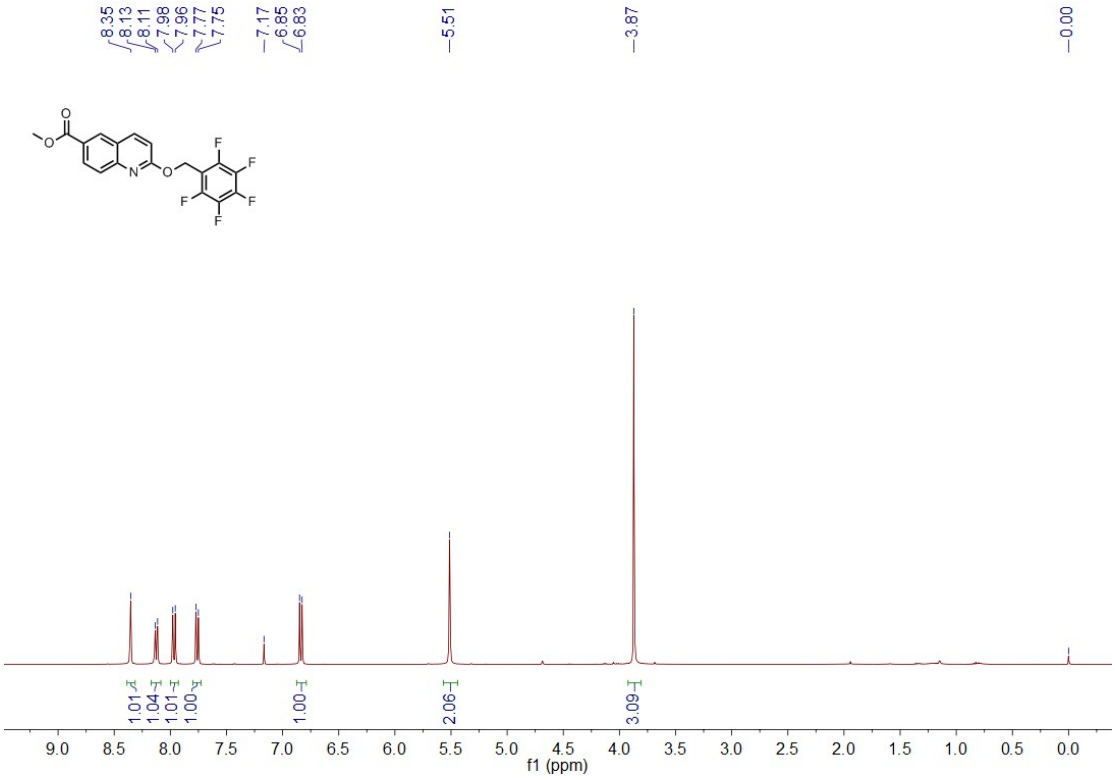
6-fluoro-2-((perfluorophenyl) methoxy) quinoline (**3l**)

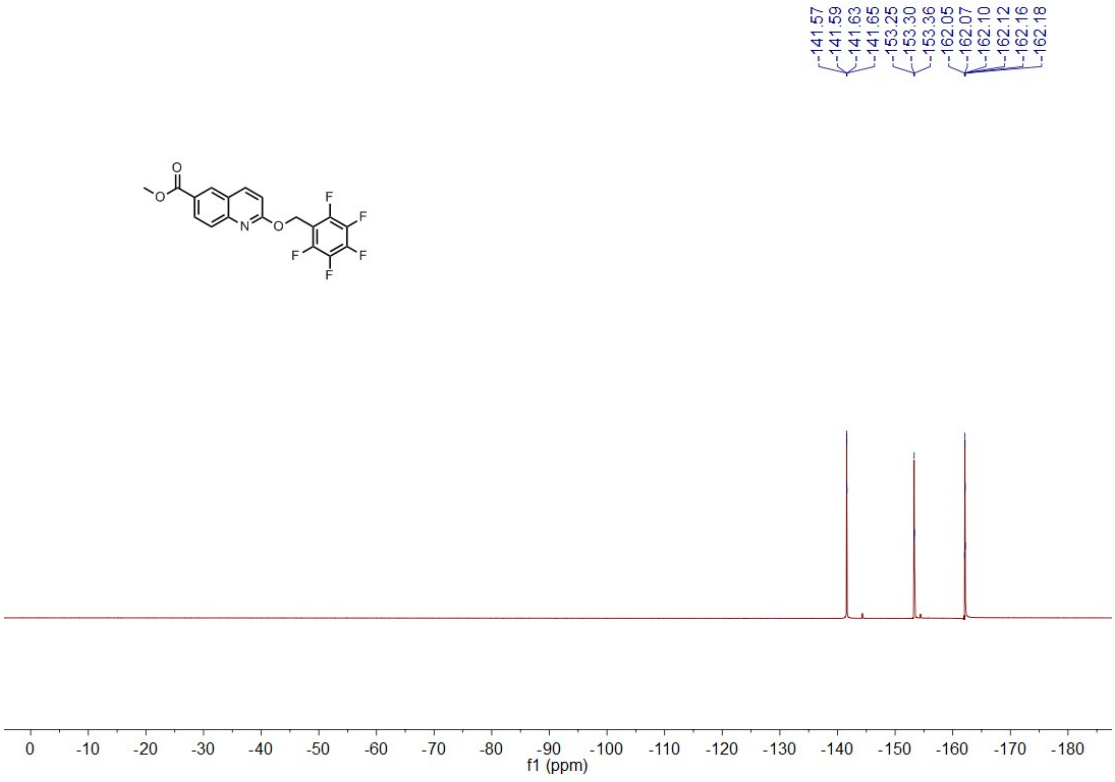


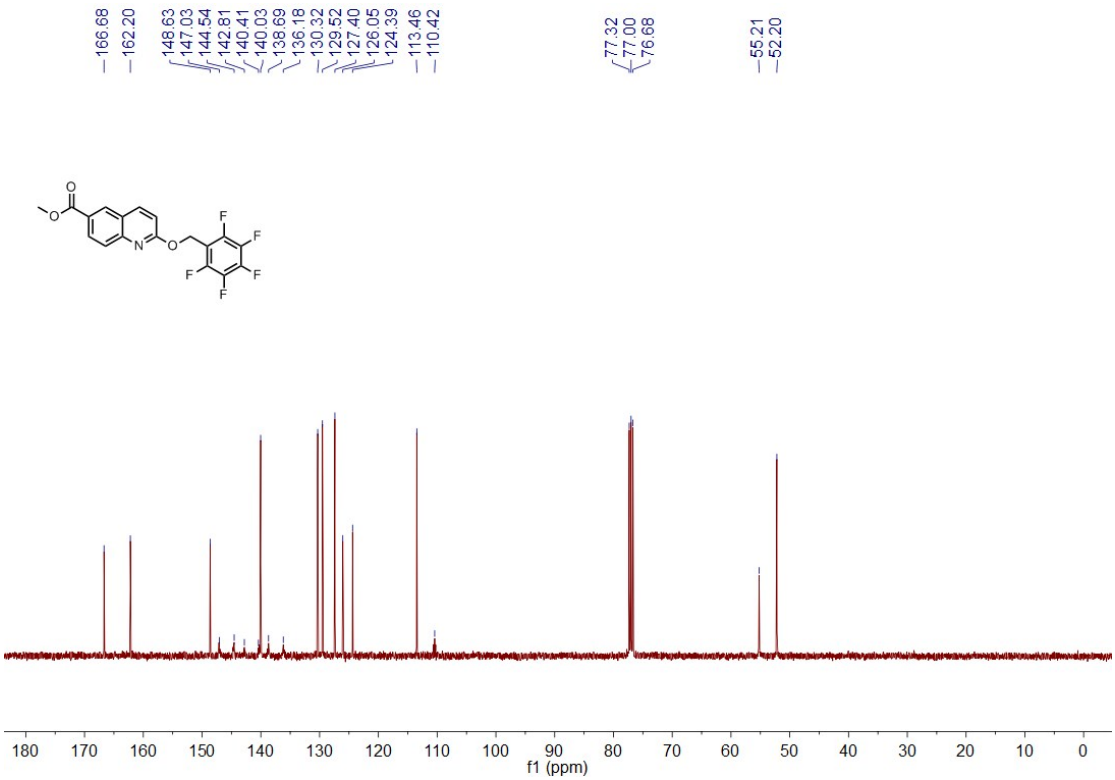

-117.02
-141.68
-141.70
-141.73
-141.76
-153.56
-153.62
-153.67
-162.23
-162.25
-162.29
-162.31
-162.34
-162.37
f1 (ppm)


160.47
160.34
160.32
158.04
147.13
144.64
142.90
142.76
140.22
138.70
138.37
138.33
136.19
129.33
129.25
125.65
125.55
119.27
119.02
113.43
110.99
110.78
110.74
77.32
77.00
76.68
54.98
f1 (ppm)

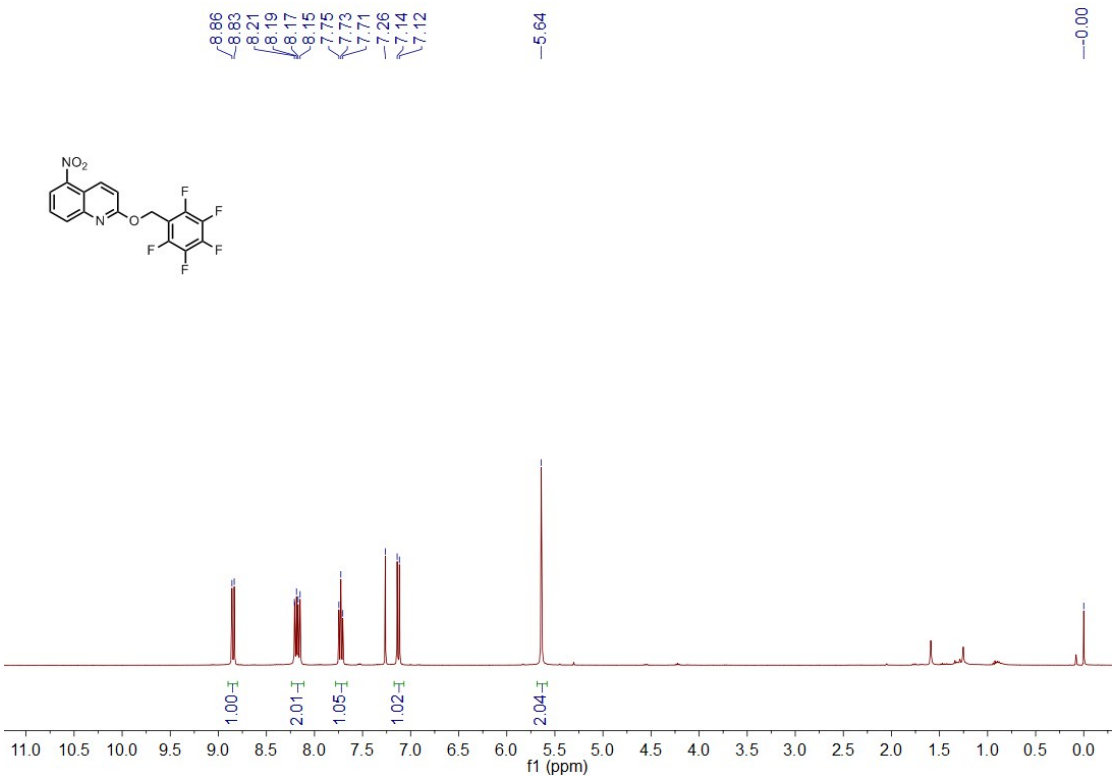
methyl 2-((perfluorophenyl)methoxy) quinoline-6-carboxylate (**3m**)

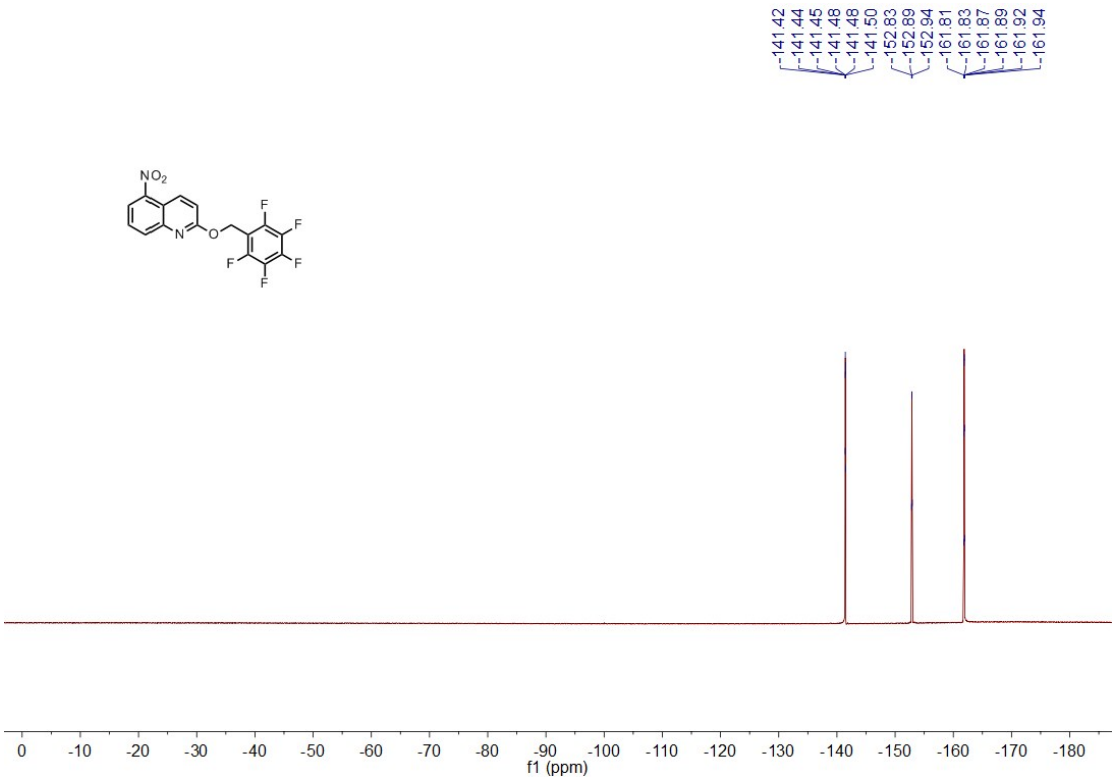


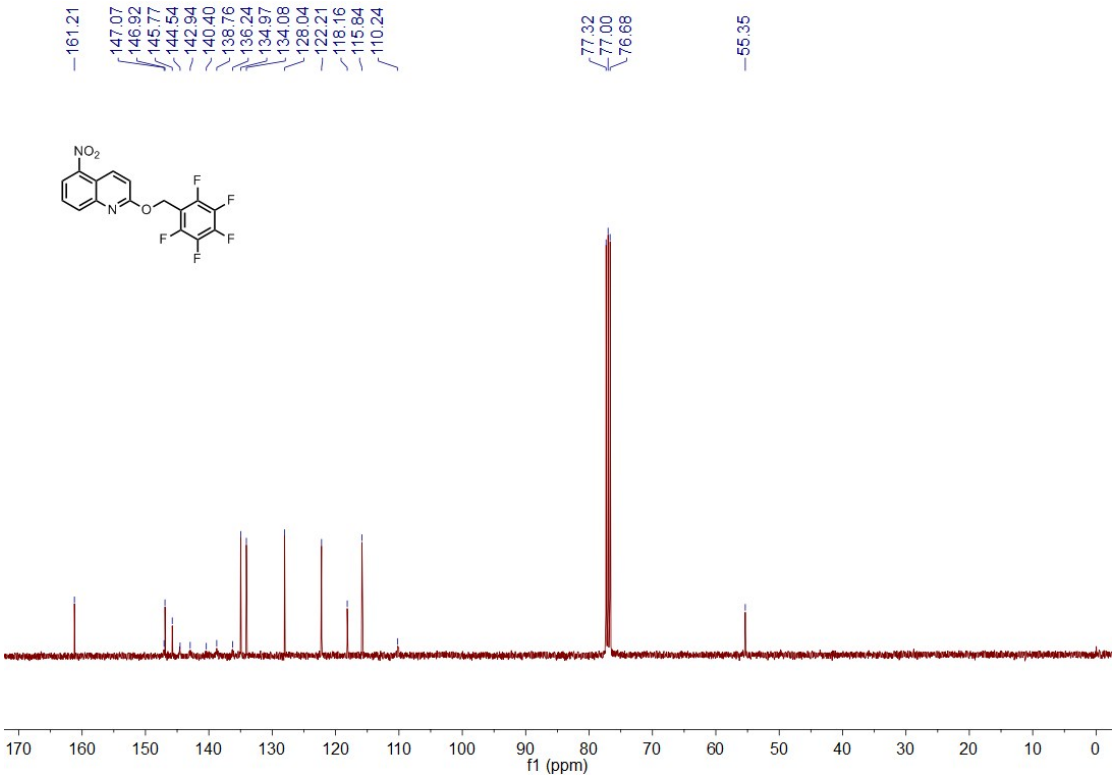




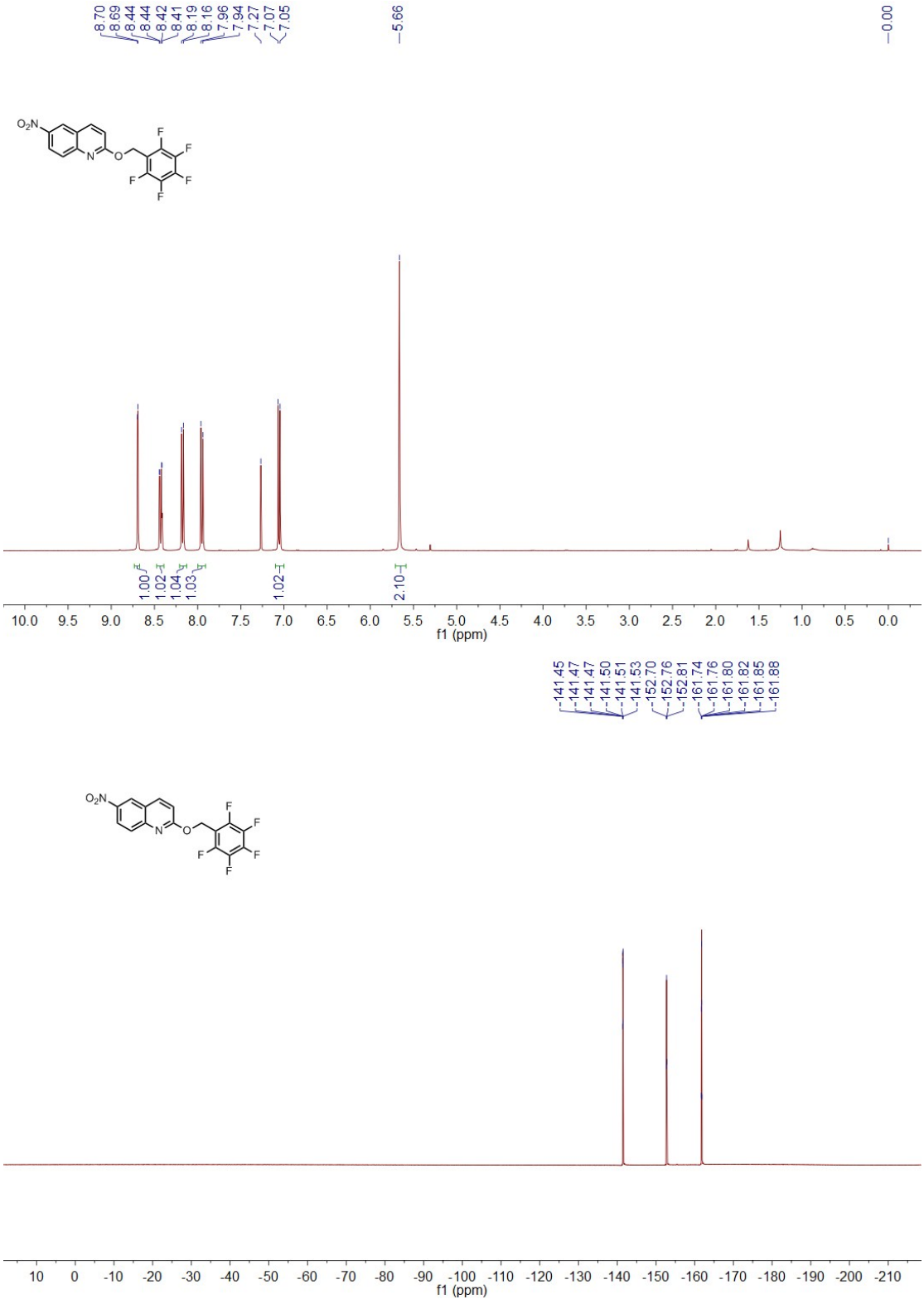
5-nitro-2-((perfluorophenyl) methoxy) quinoline (**3n**)

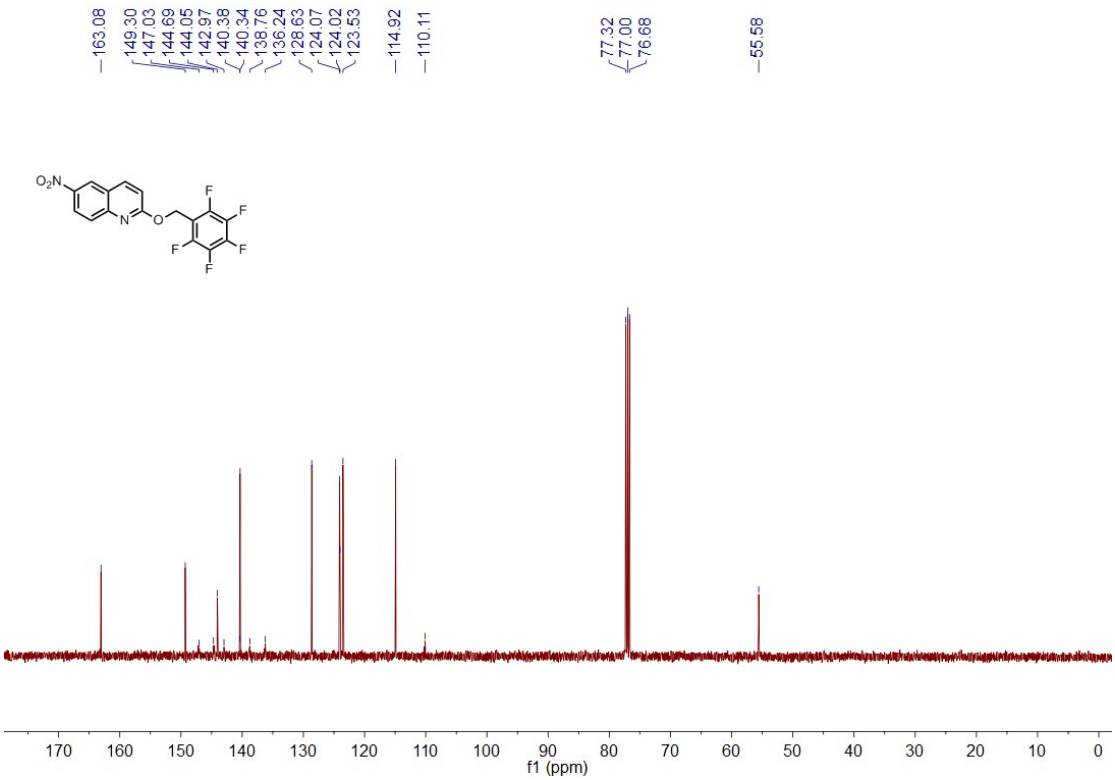



-141.42
-141.44
-141.45
-141.48
-141.48
-141.50
-152.83
-152.89
-152.94
-161.81
-161.83
-161.87
-161.89
-161.92
-161.94
NO2
F
F
F
F
F
N
O
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)

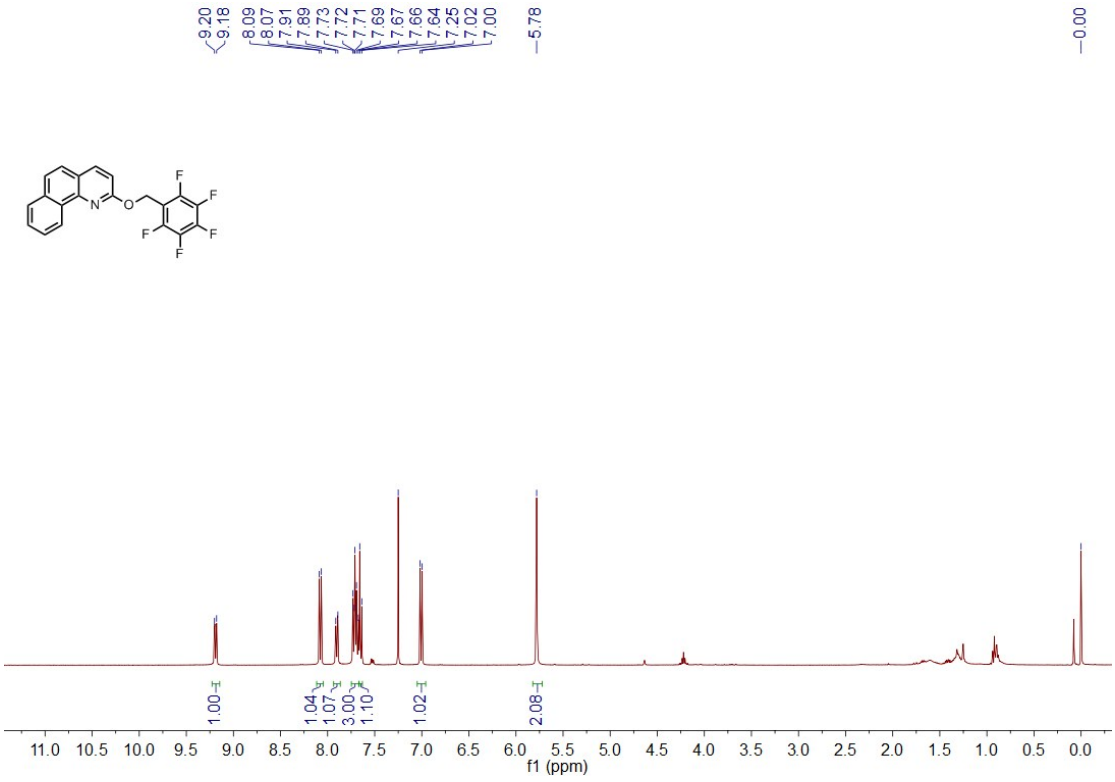

161.21
147.07
146.92
145.77
144.54
142.94
140.40
138.76
136.24
134.97
134.08
128.04
122.21
118.16
115.84
110.24
77.32
77.00
76.68
55.35
NO2
F
F
F
F
F
N
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

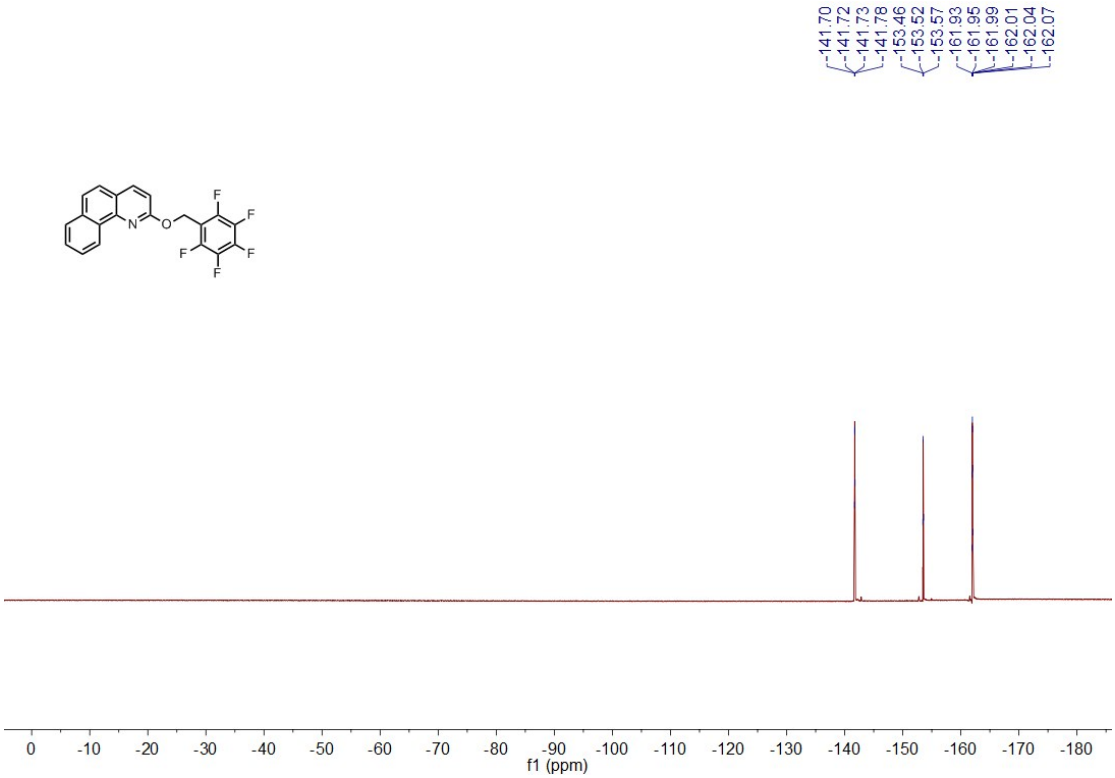
6-nitro-2-((perfluorophenyl) methoxy) quinoline (**3o**)

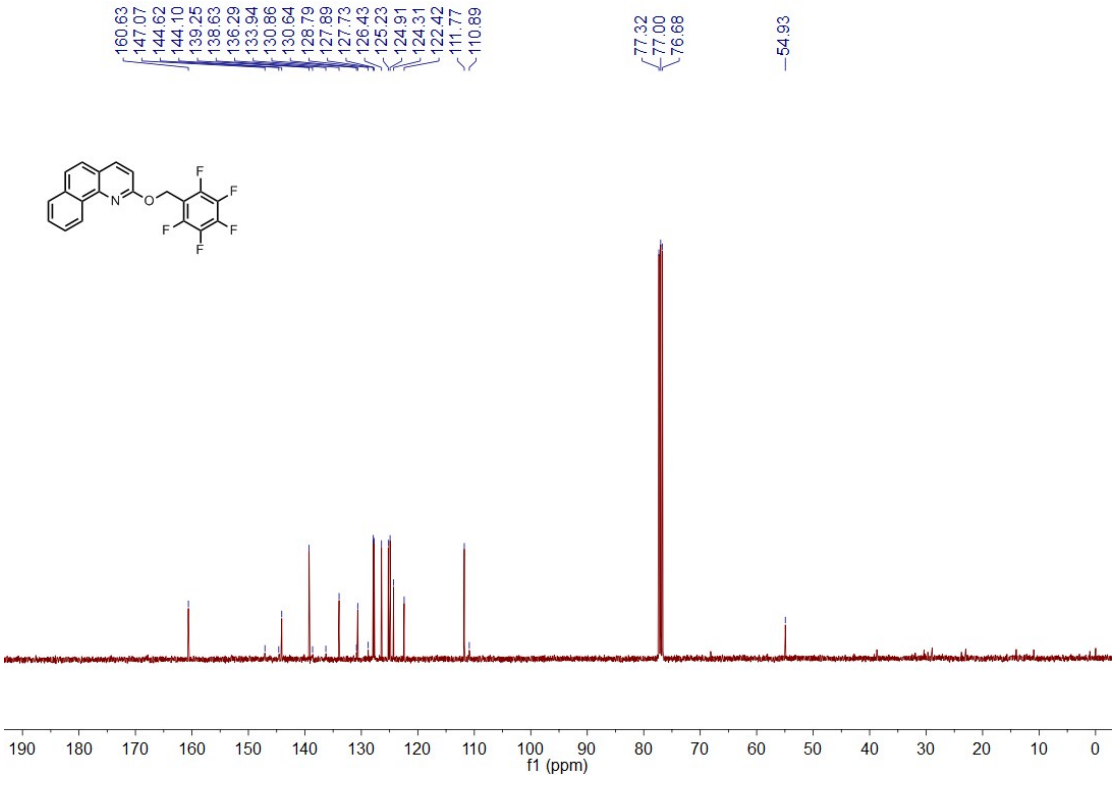




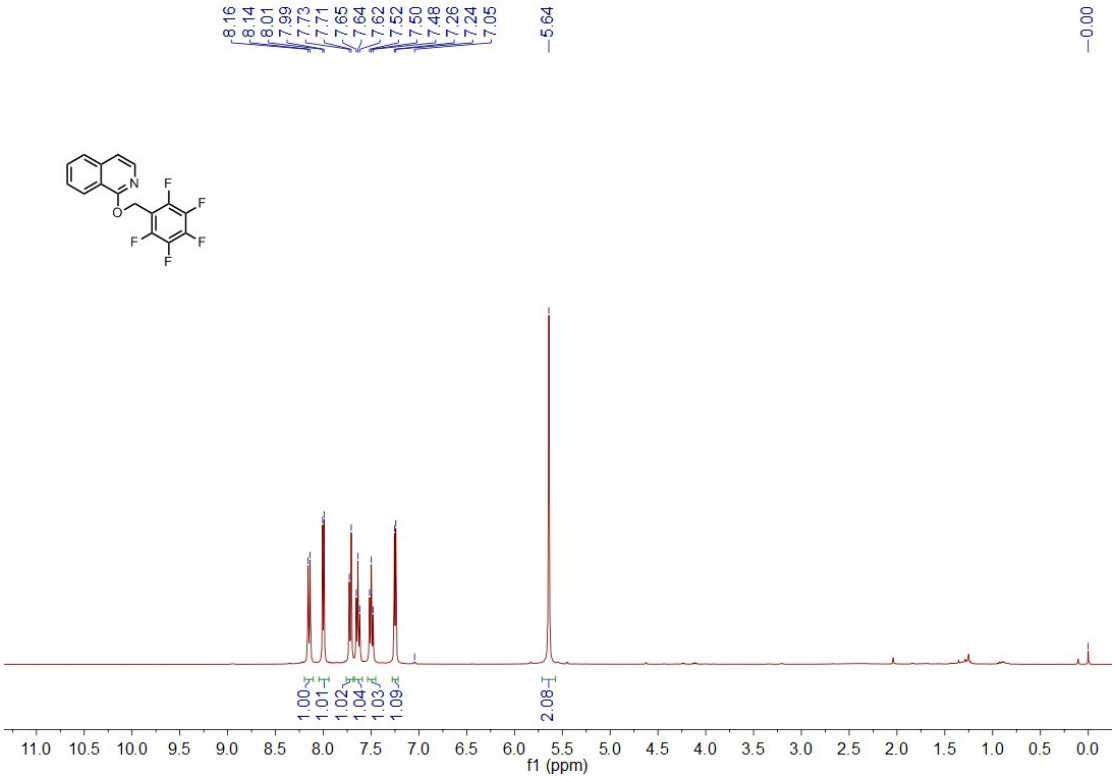
2-((perfluorophenyl)methoxy) benzo quinoline (**3p**)

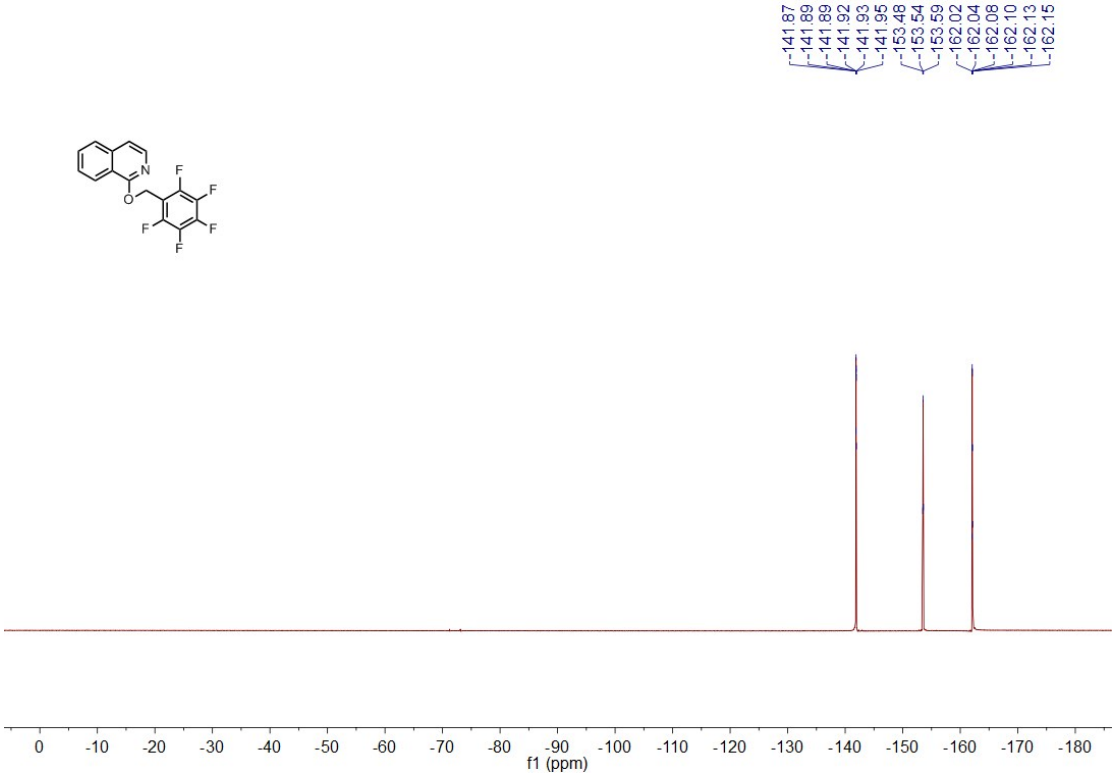


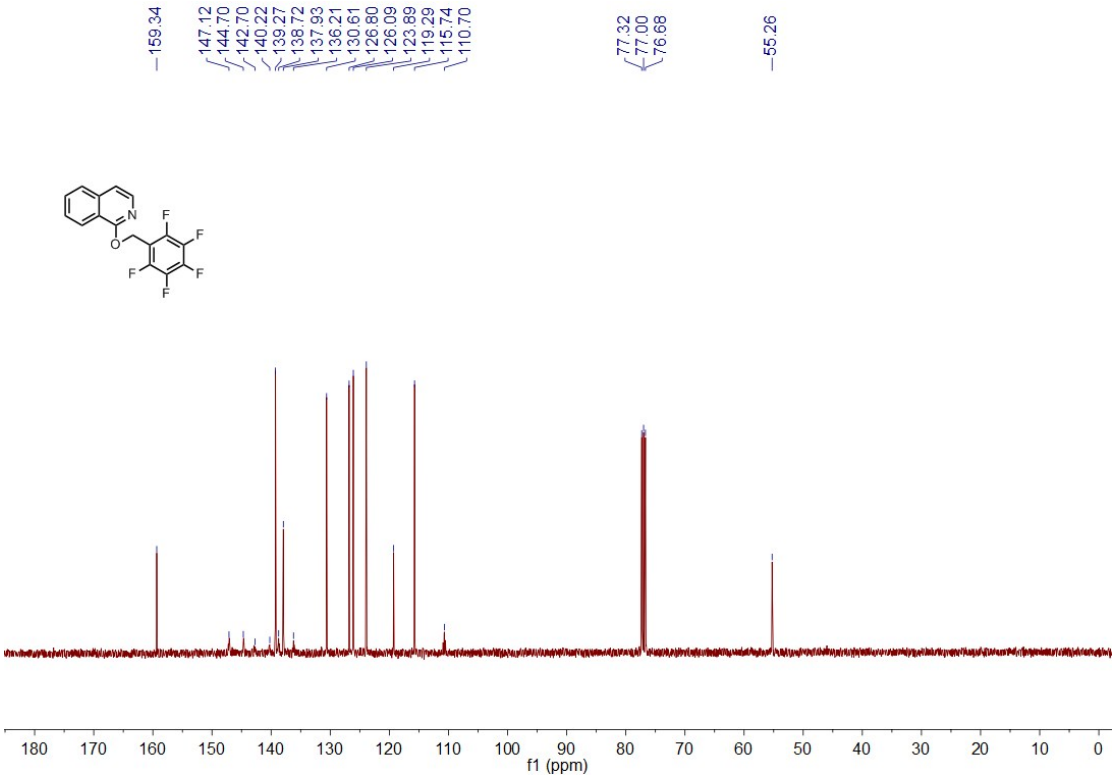

-141.70
-141.72
-141.73
-141.78
-153.46
-153.52
-153.57
-161.93
-161.95
-161.99
-162.01
-162.04
-162.07
F
F
F
F
F
N
O
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)


160.63
147.07
144.62
144.10
139.25
138.63
136.29
133.94
130.86
130.64
128.79
127.89
127.73
126.43
125.23
124.91
124.31
122.42
111.77
110.89
77.32
77.00
76.68
54.93
F
F
F
F
F
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

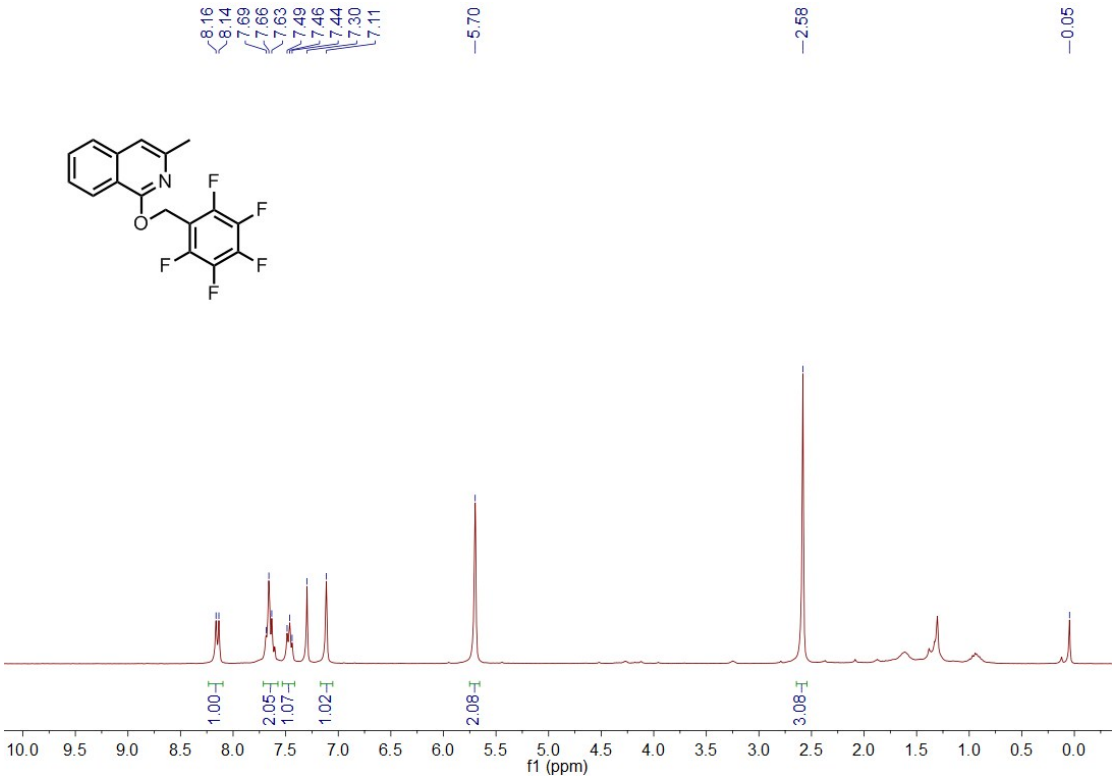
1-((perfluorophenyl)methoxy) isoquinoline (**3q**)

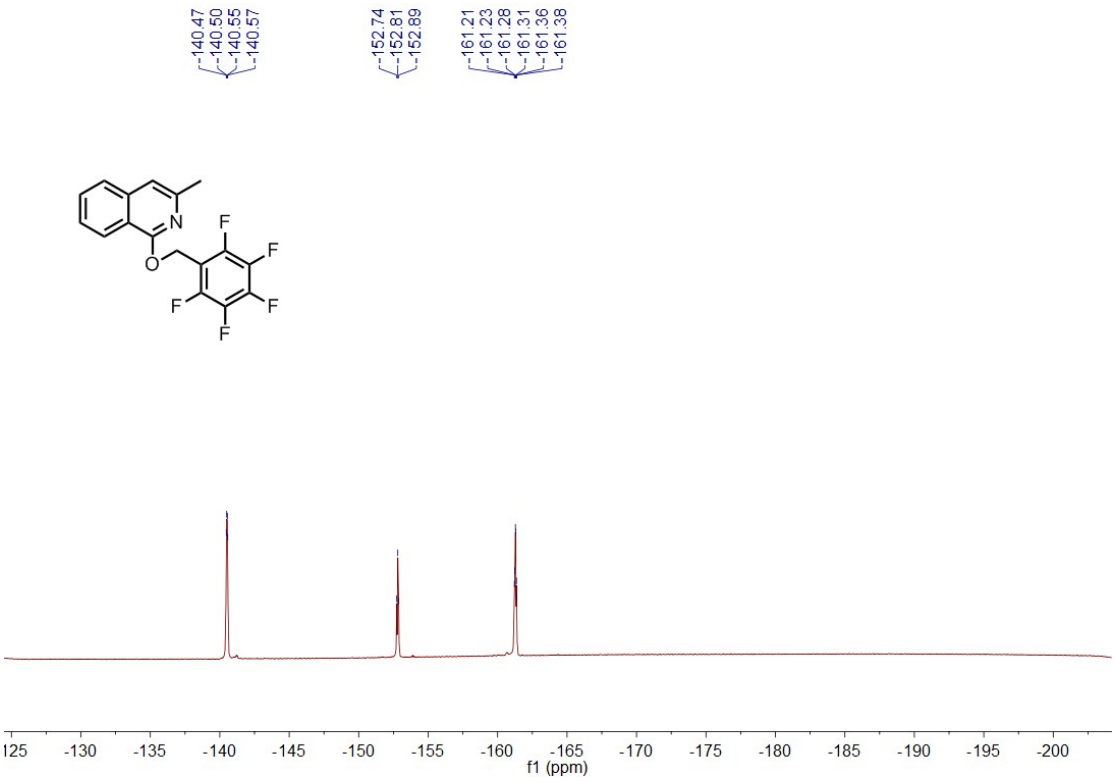


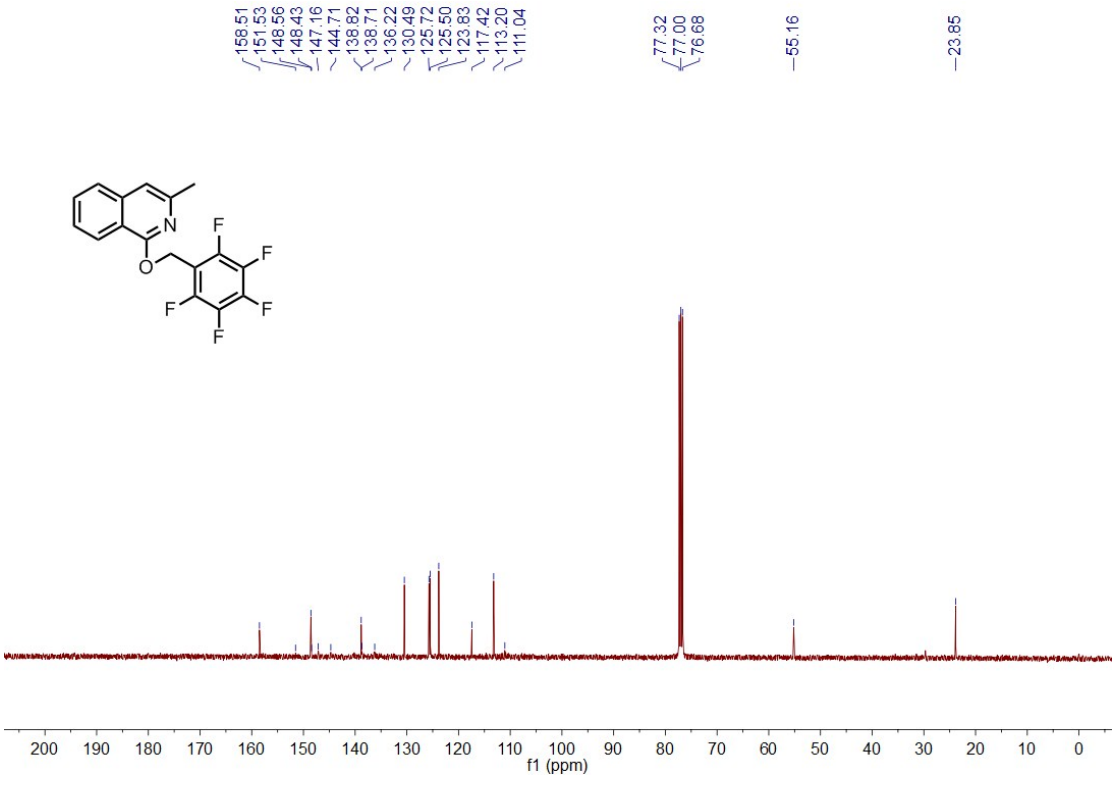




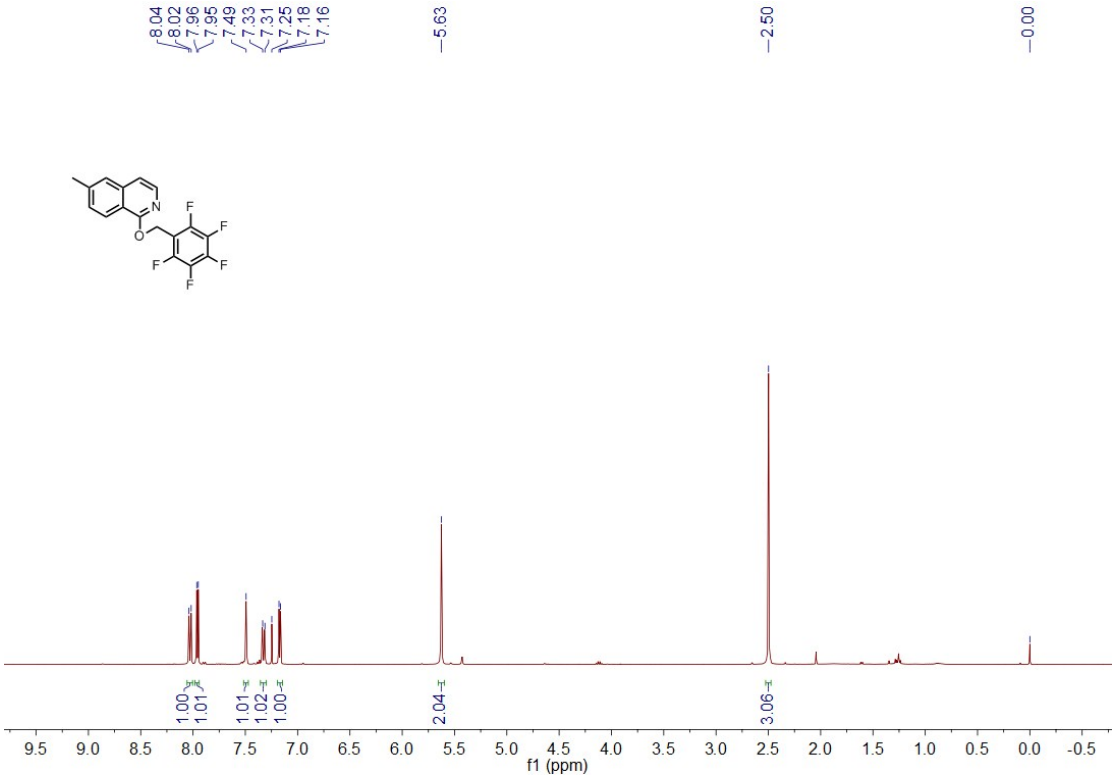
3-methyl-1-((perfluorophenyl) methoxy) isoquinoline (**3r**)

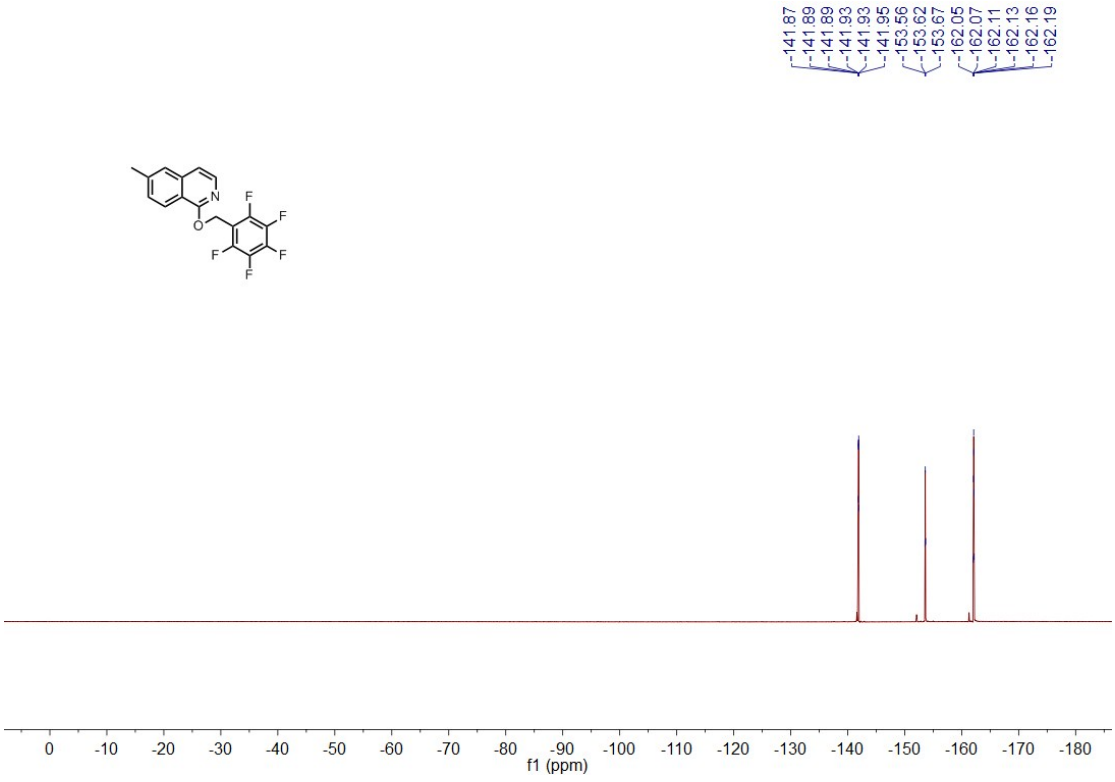


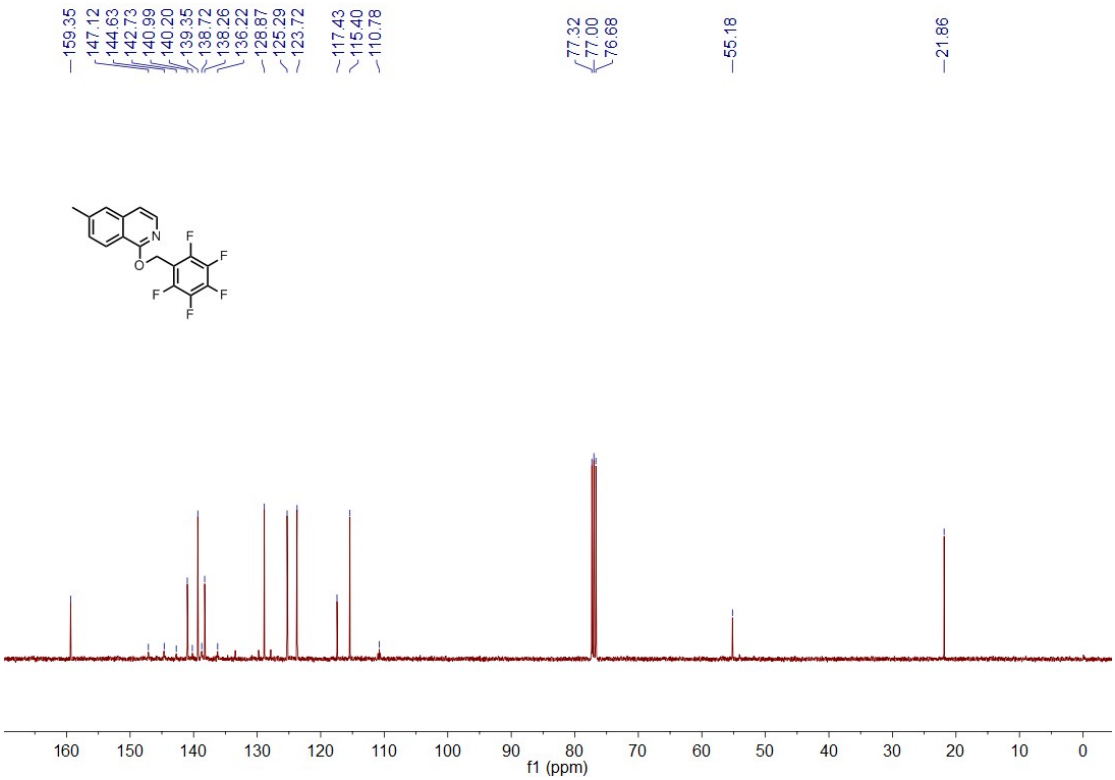

-140.47
-140.50
-140.55
-140.57
-152.74
-152.81
-152.89
-161.21
-161.23
-161.28
-161.31
-161.36
-161.38
N
O
F
F
F
F
F
125 -130 -135 -140 -145 -150 -155 -160 -165 -170 -175 -180 -185 -190 -195 -200
f1 (ppm)


158.51
151.53
148.56
148.43
147.16
144.71
138.82
138.71
136.22
130.49
125.72
125.50
123.83
117.42
113.20
111.04
77.32
77.00
76.68
55.16
23.85
N
O
F
F
F
F
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

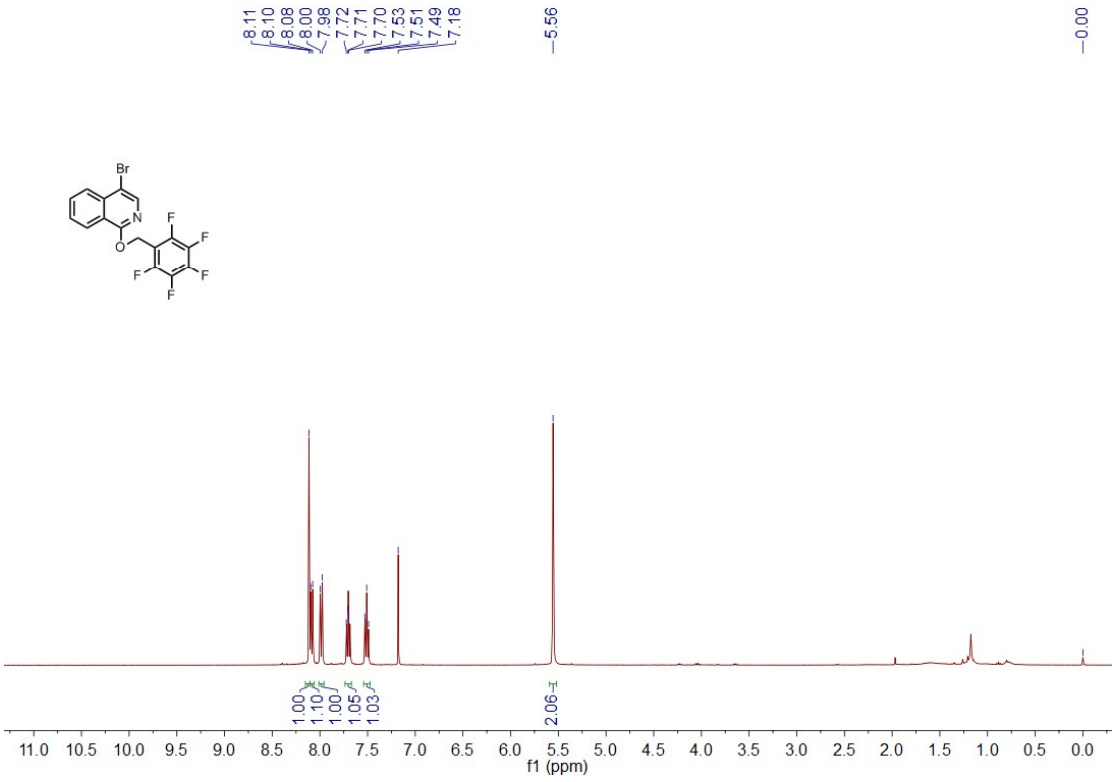
6-methyl-1-((perfluorophenyl) methoxy) isoquinoline (**3s**)

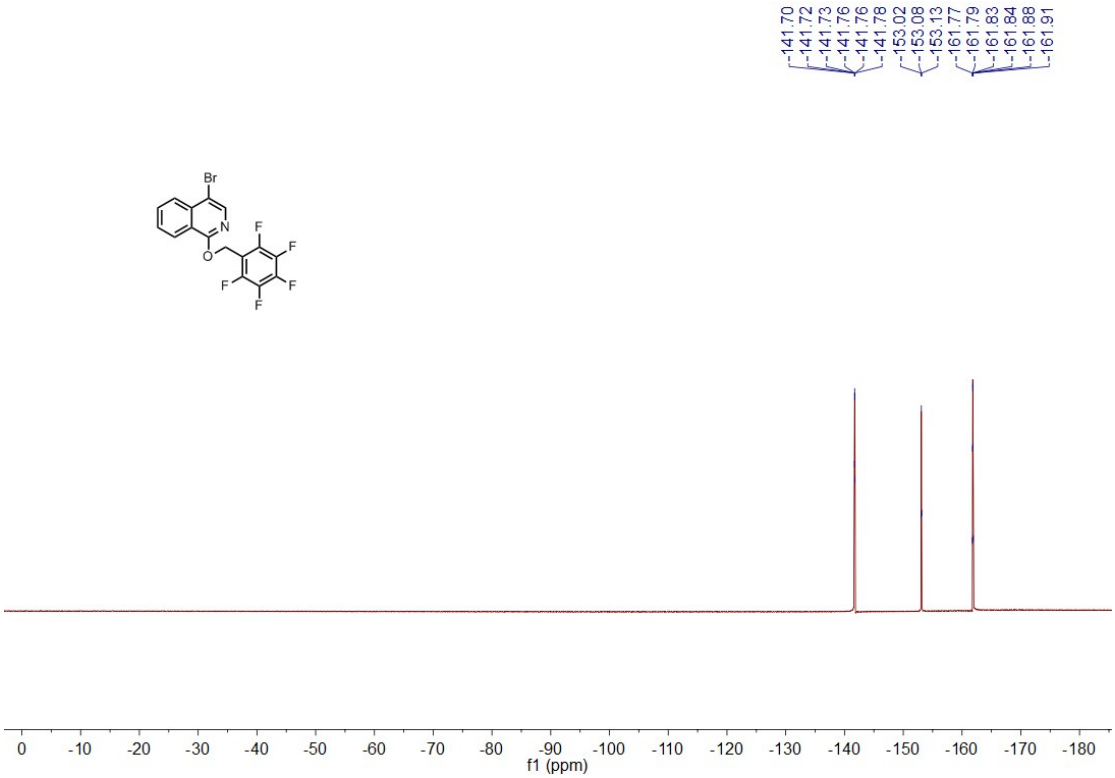


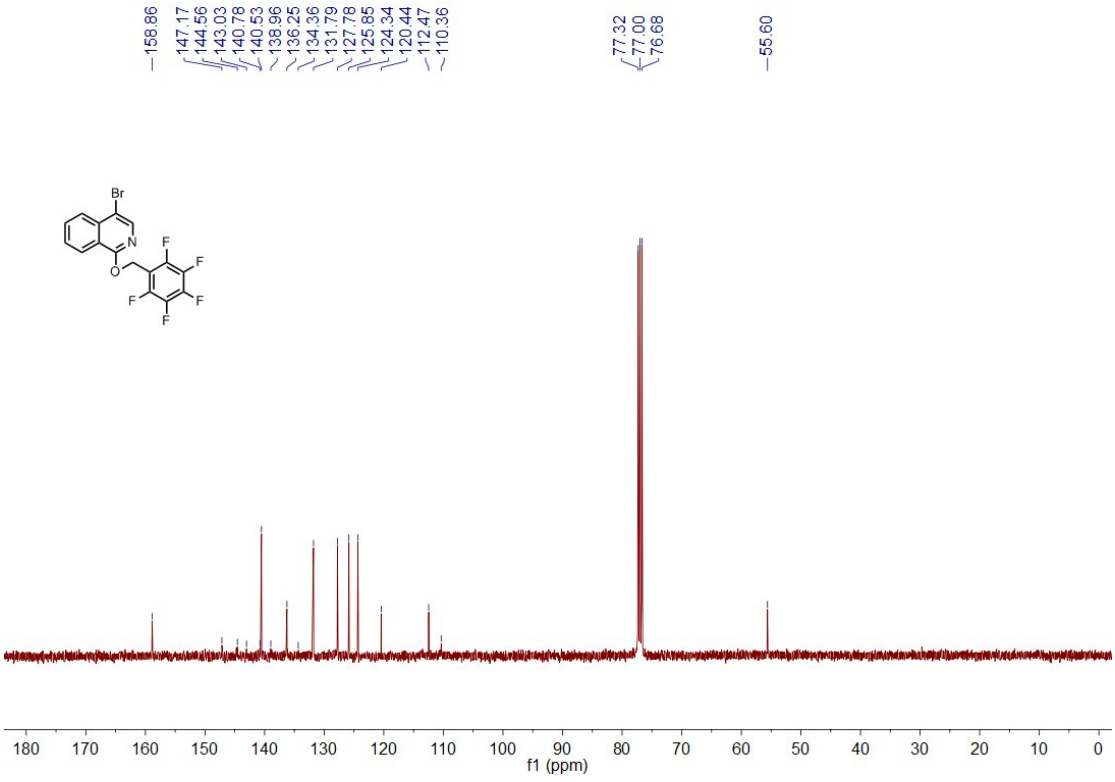




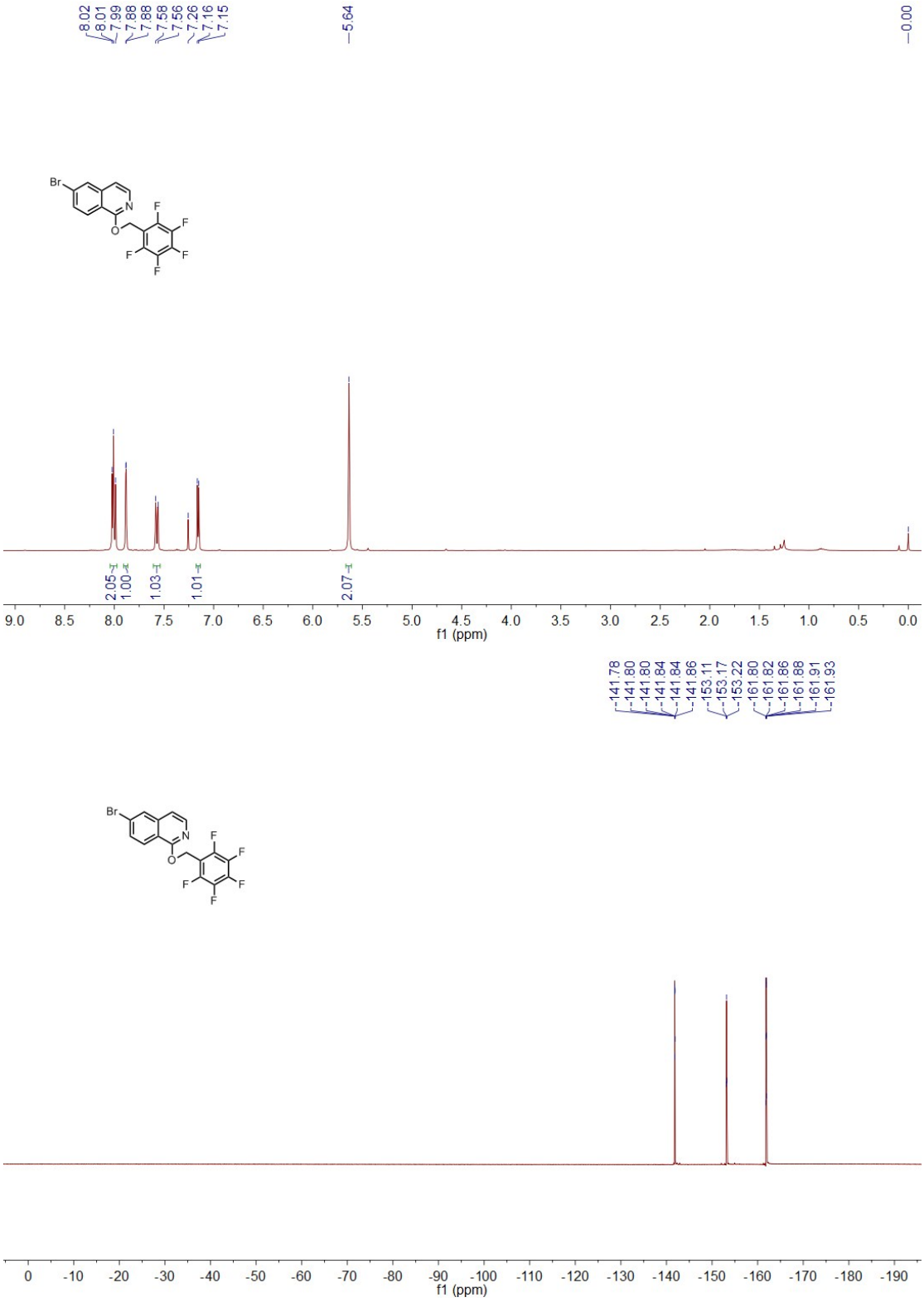
4-bromo-1-((perfluorophenyl) methoxy) isoquinoline (**3t**)

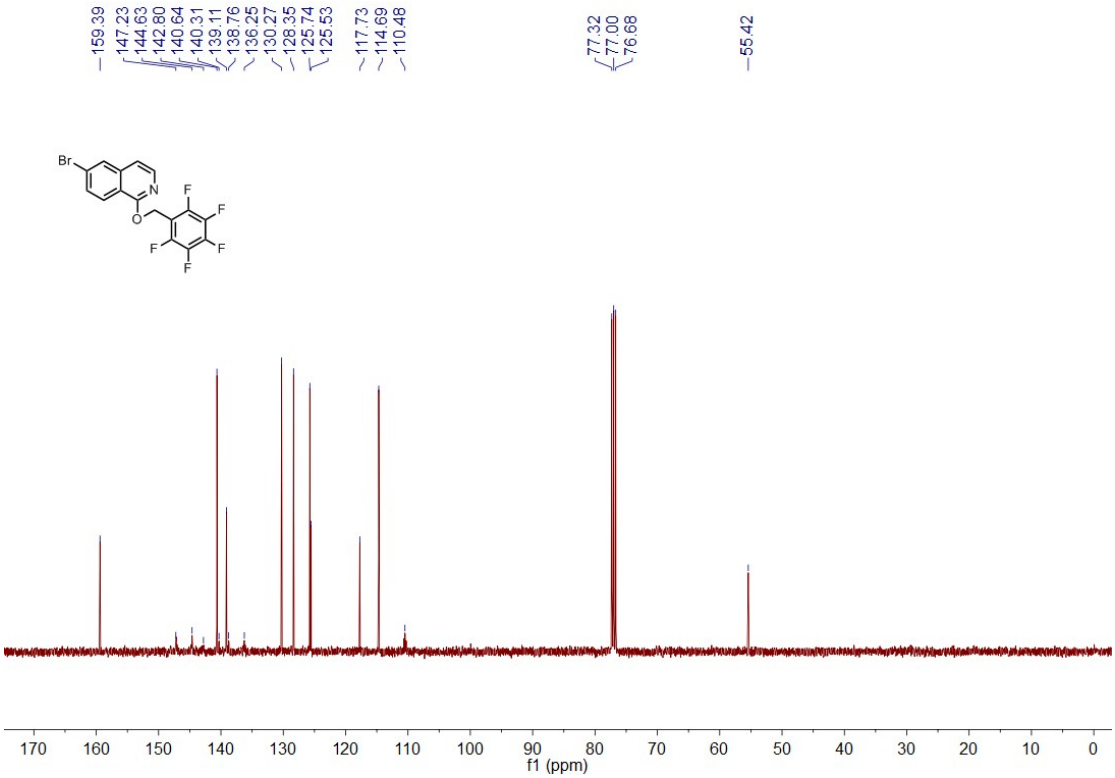



141.70
141.72
141.73
141.76
141.76
141.78
153.02
153.08
153.13
161.77
161.79
161.83
161.84
161.88
161.91
Br
N
O
F
F
F
F
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)

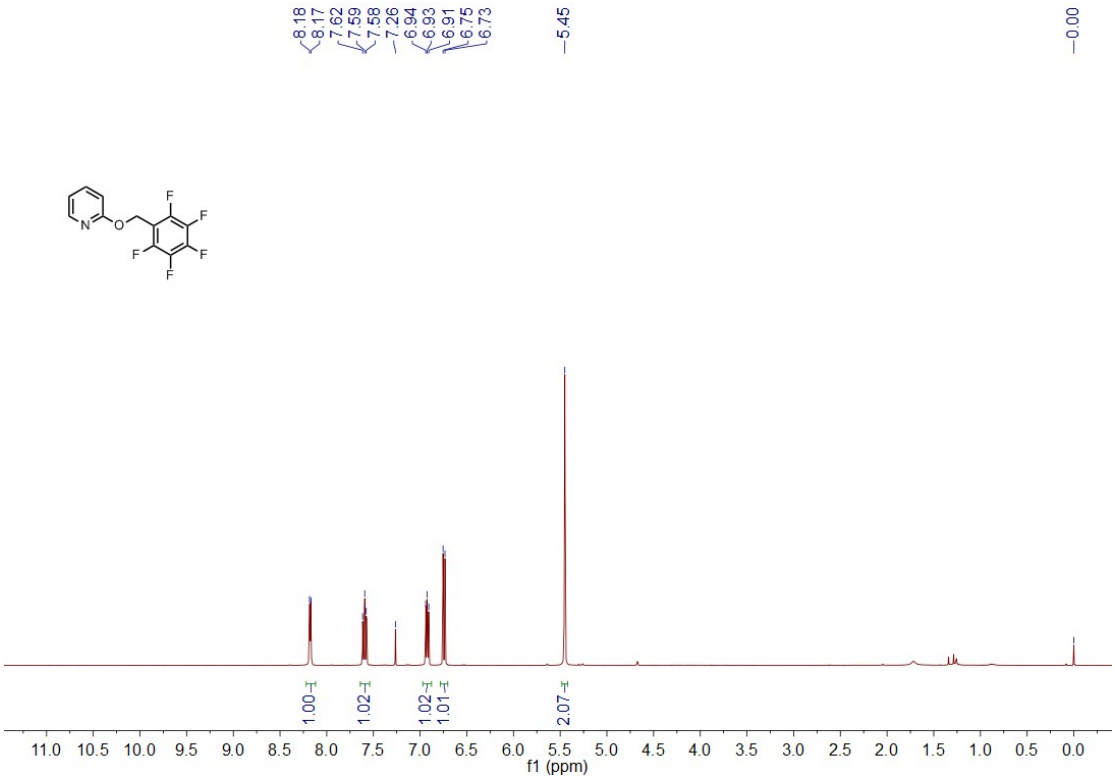

158.86
147.17
144.56
143.03
140.78
140.53
138.96
136.25
134.36
131.79
127.78
125.85
124.34
120.44
112.47
110.36
77.32
77.00
76.68
55.60
Br
N
O
F
F
F
F
F
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

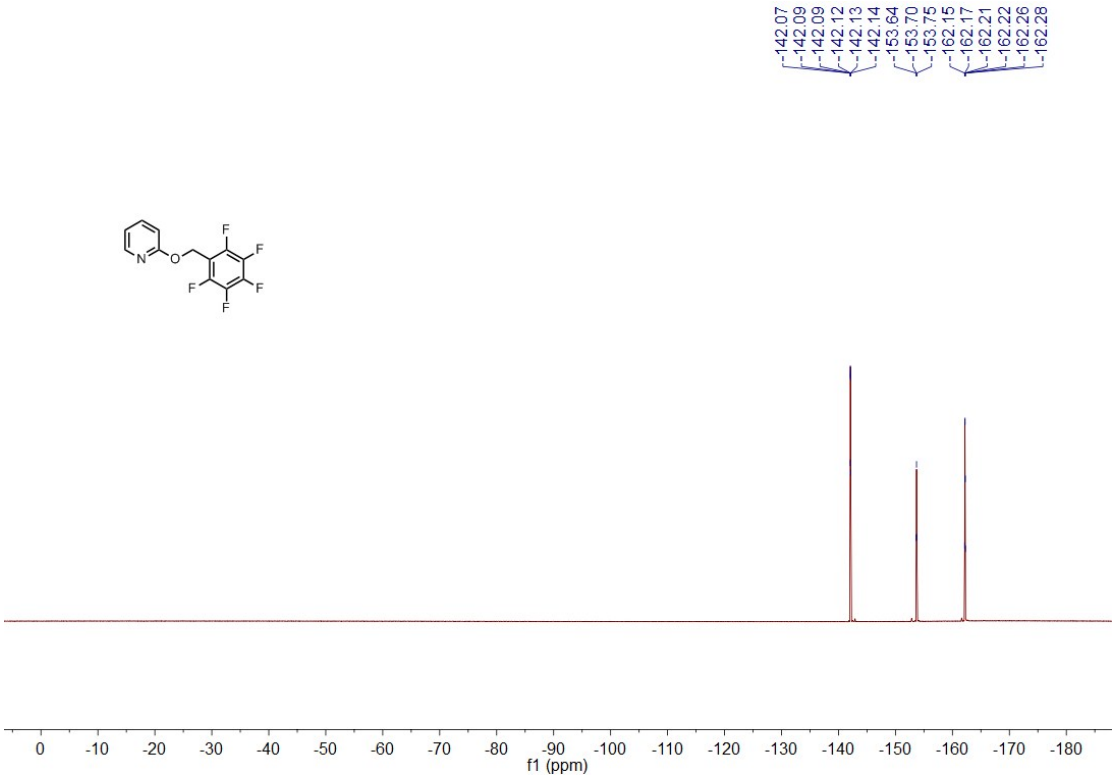
6-bromo-1-((perfluorophenyl) methoxy) isoquinoline (**3u**)

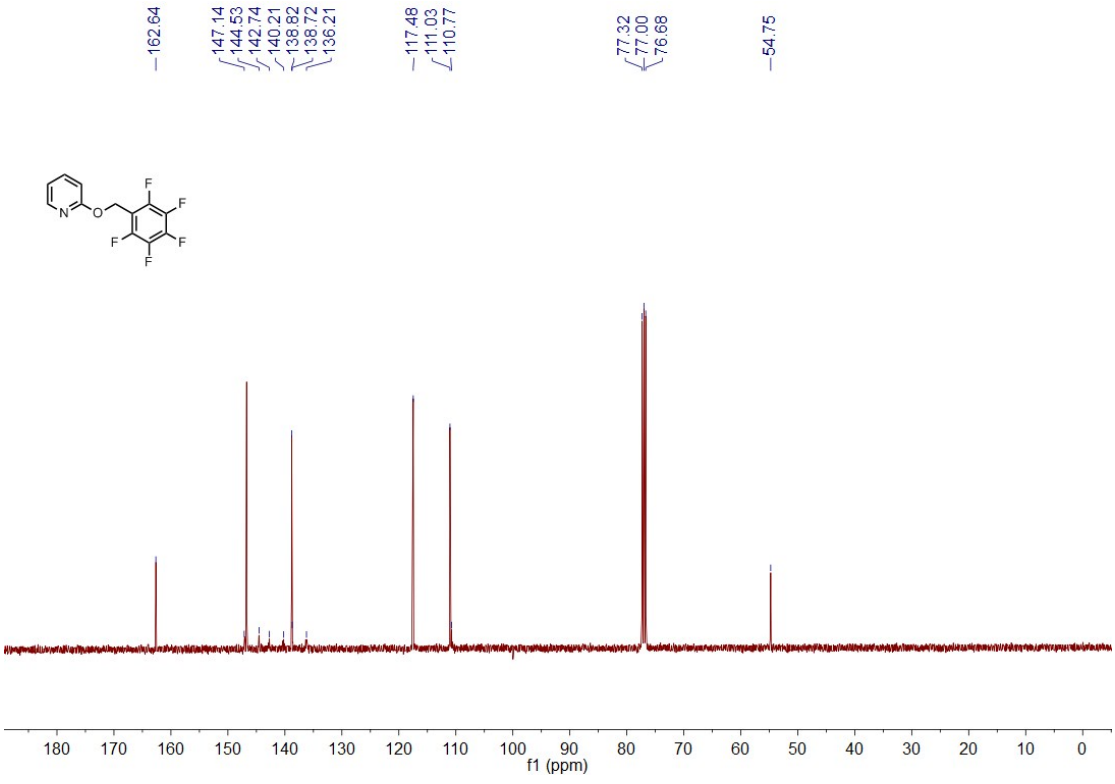




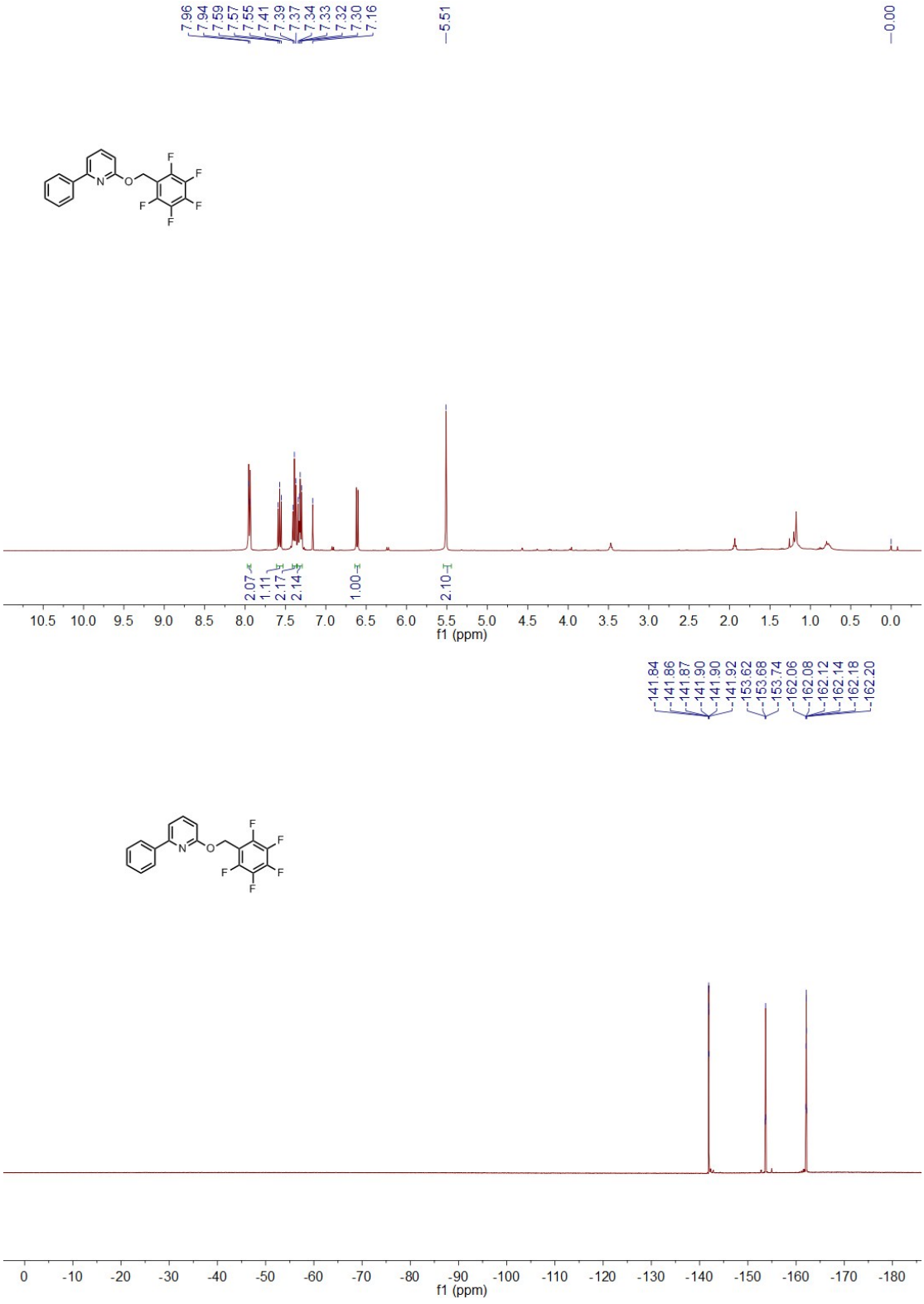
2-((perfluorophenyl)methoxy) pyridine (**3v**)

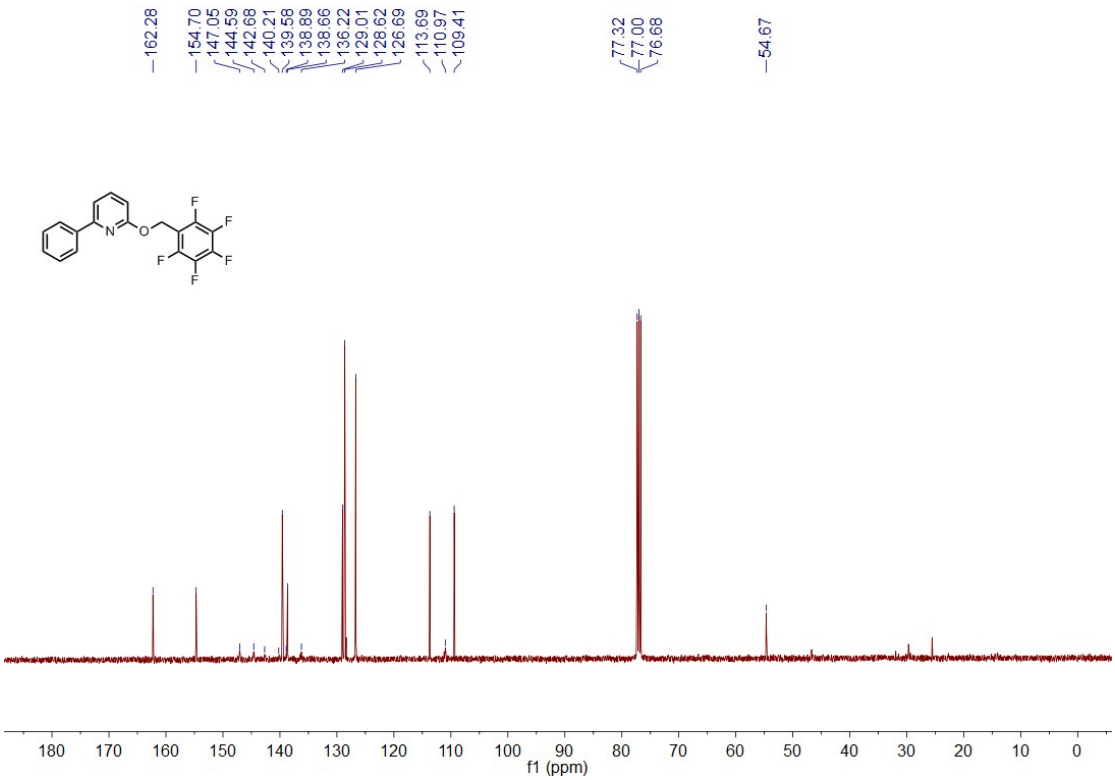



-142.07
-142.09
-142.09
-142.12
-142.13
-142.14
-153.64
-153.70
-153.75
-162.15
-162.17
-162.21
-162.22
-162.26
-162.28
F
F
F
F
F
N
O
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
f1 (ppm)

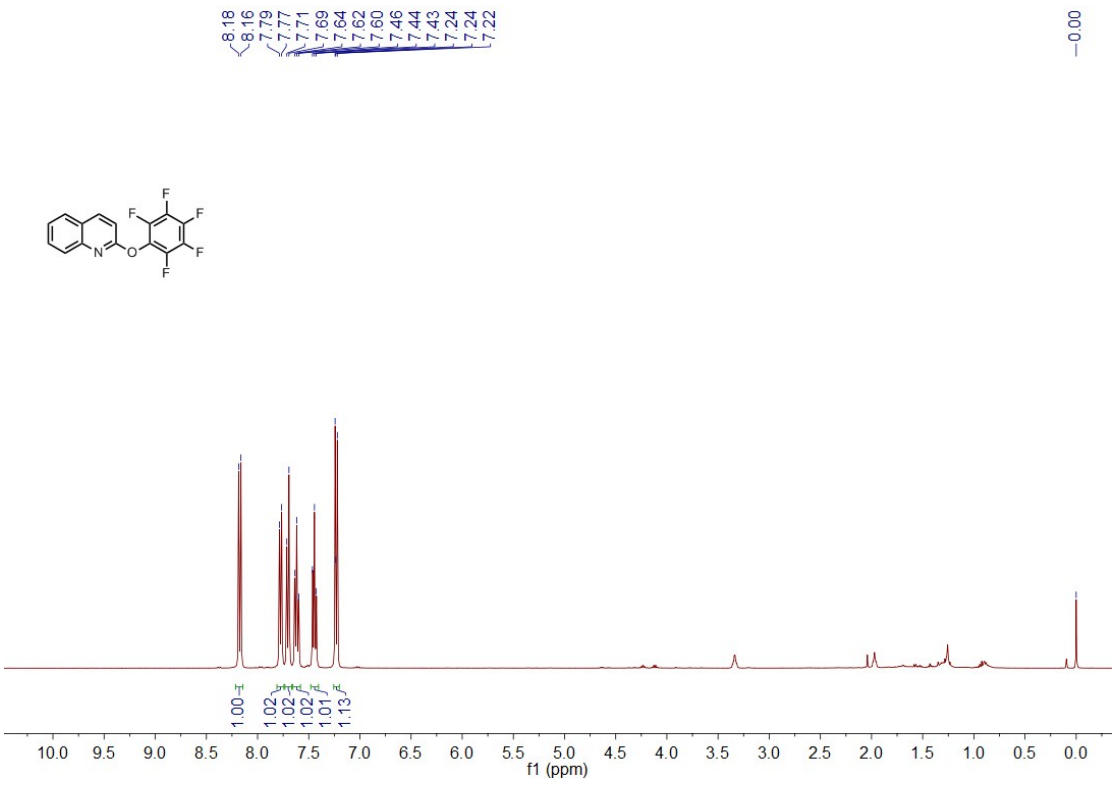

-162.64
147.14
144.53
142.74
140.21
138.82
138.72
136.21
-117.48
111.03
110.77
77.32
77.00
76.68
-54.75
F
F
F
F
F
N
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

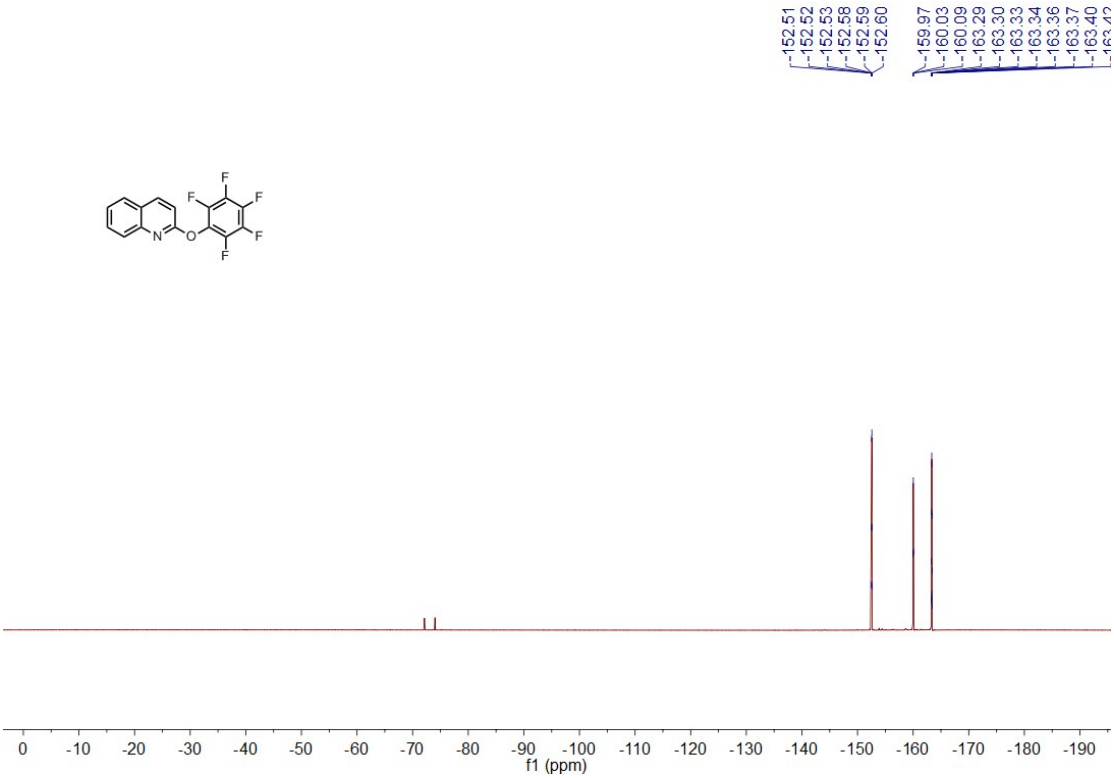
2-((perfluorophenyl) methoxy)-6-phenylpyridine (**3w**)

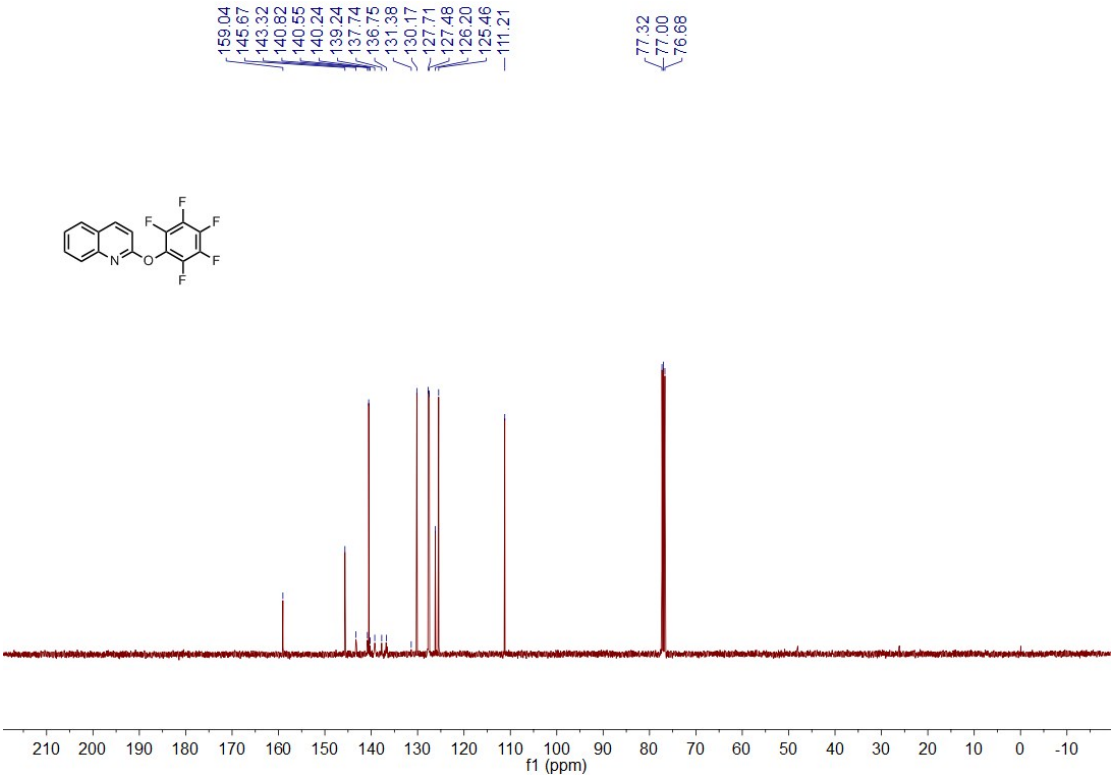




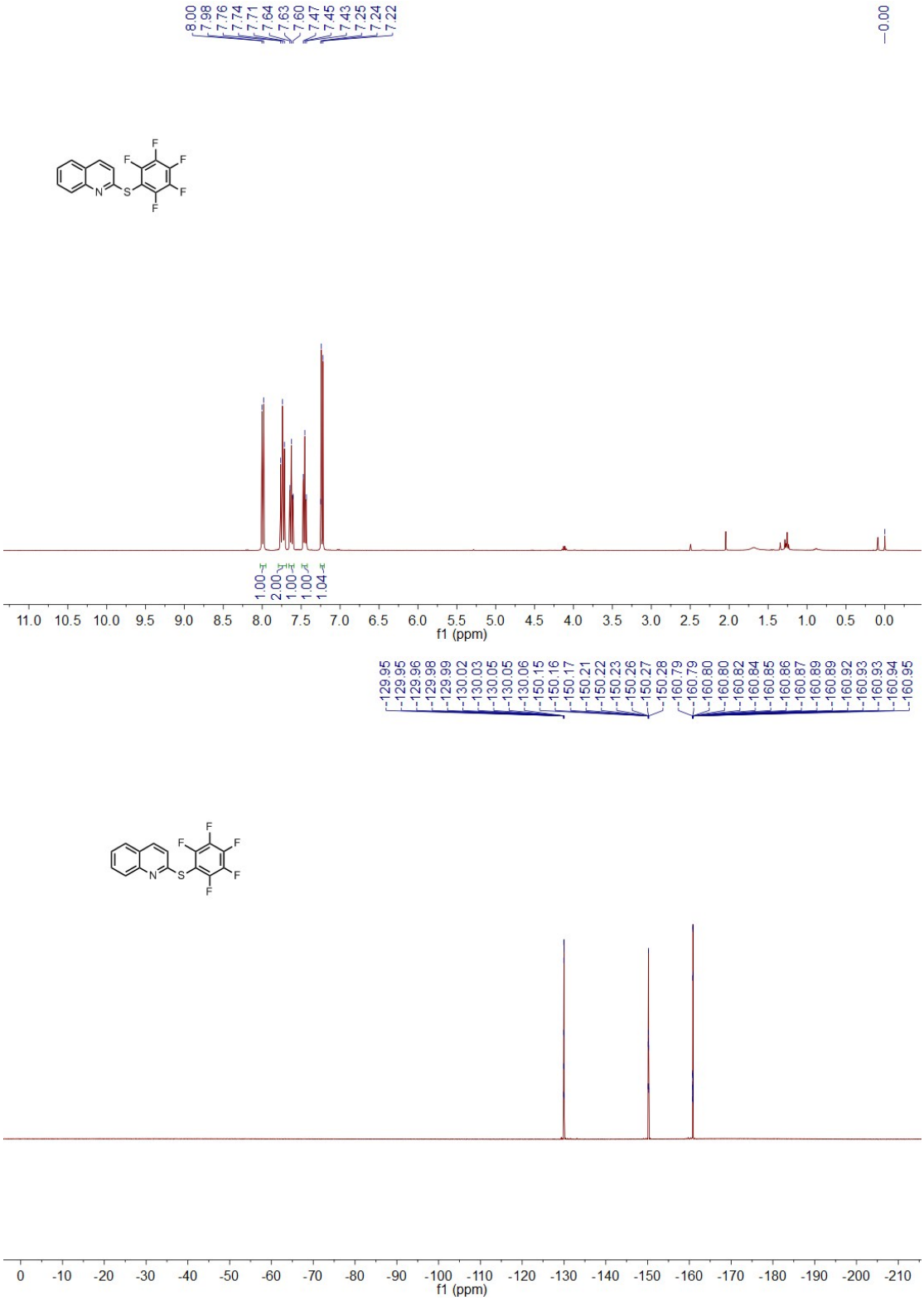
2-(perfluorophenoxy) quinoline (**6a**)

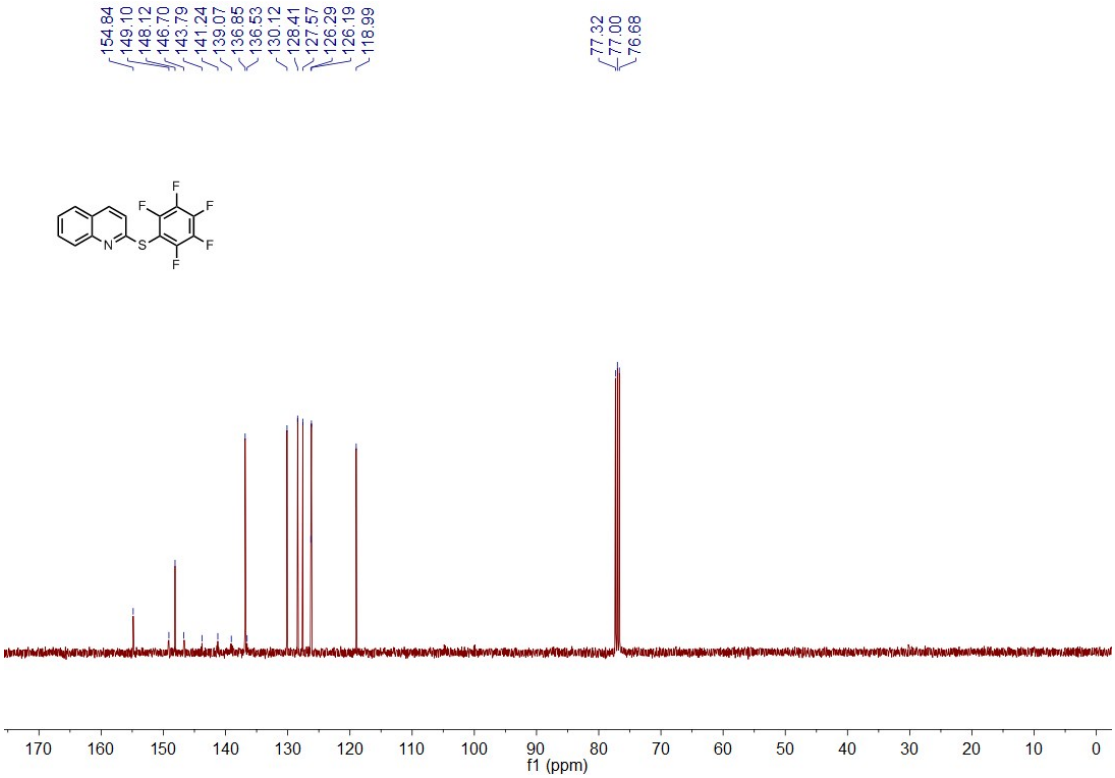



-152.51
-152.52
-152.53
-152.58
-152.59
-152.60
-159.97
-160.03
-160.09
-163.29
-163.30
-163.33
-163.34
-163.36
-163.37
-163.40
F
F
F
F
F
N
O
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

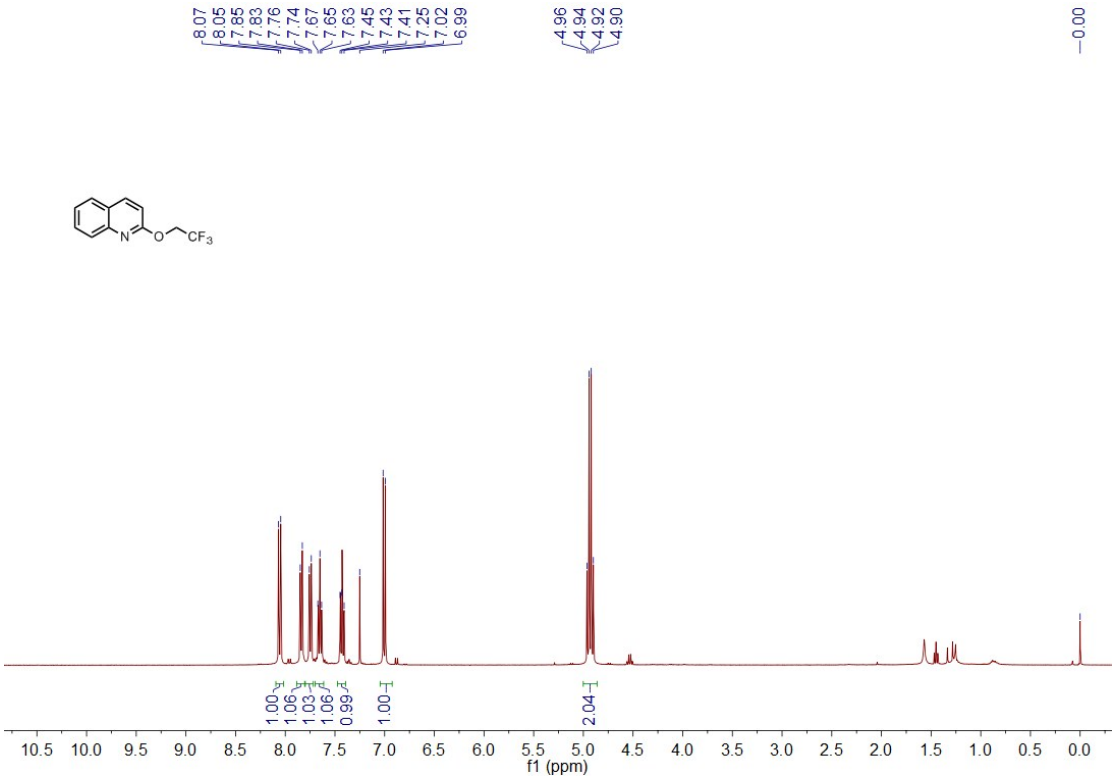

159.04
145.67
143.32
140.82
140.55
140.24
139.24
137.74
136.75
131.38
130.17
127.71
127.48
126.20
125.46
111.21
77.32
77.00
76.68
F
F
F
F
F
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

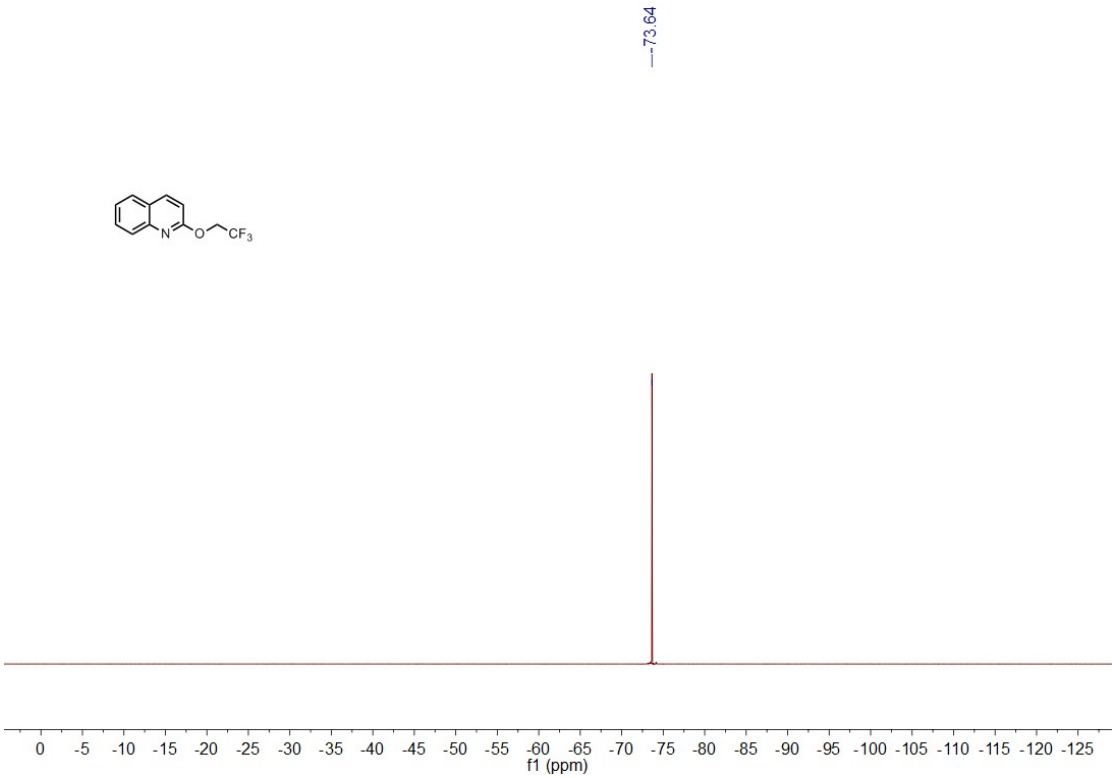
2-((perfluorophenyl) thio) quinoline (**6b**)

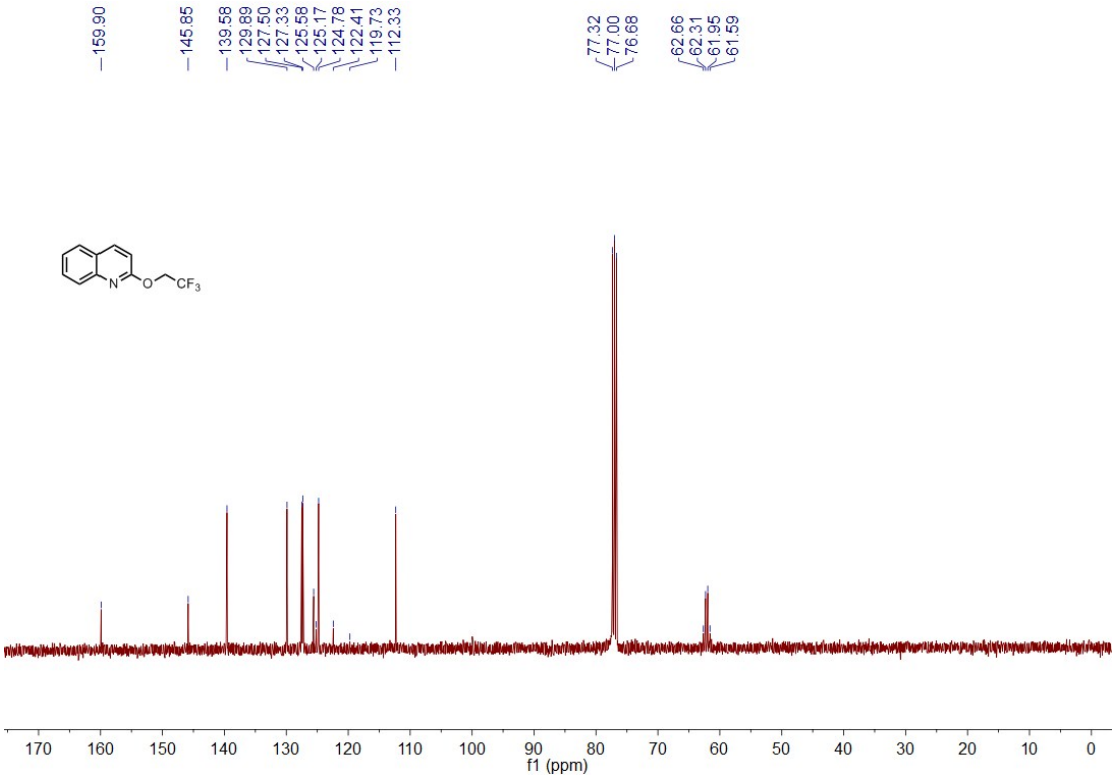




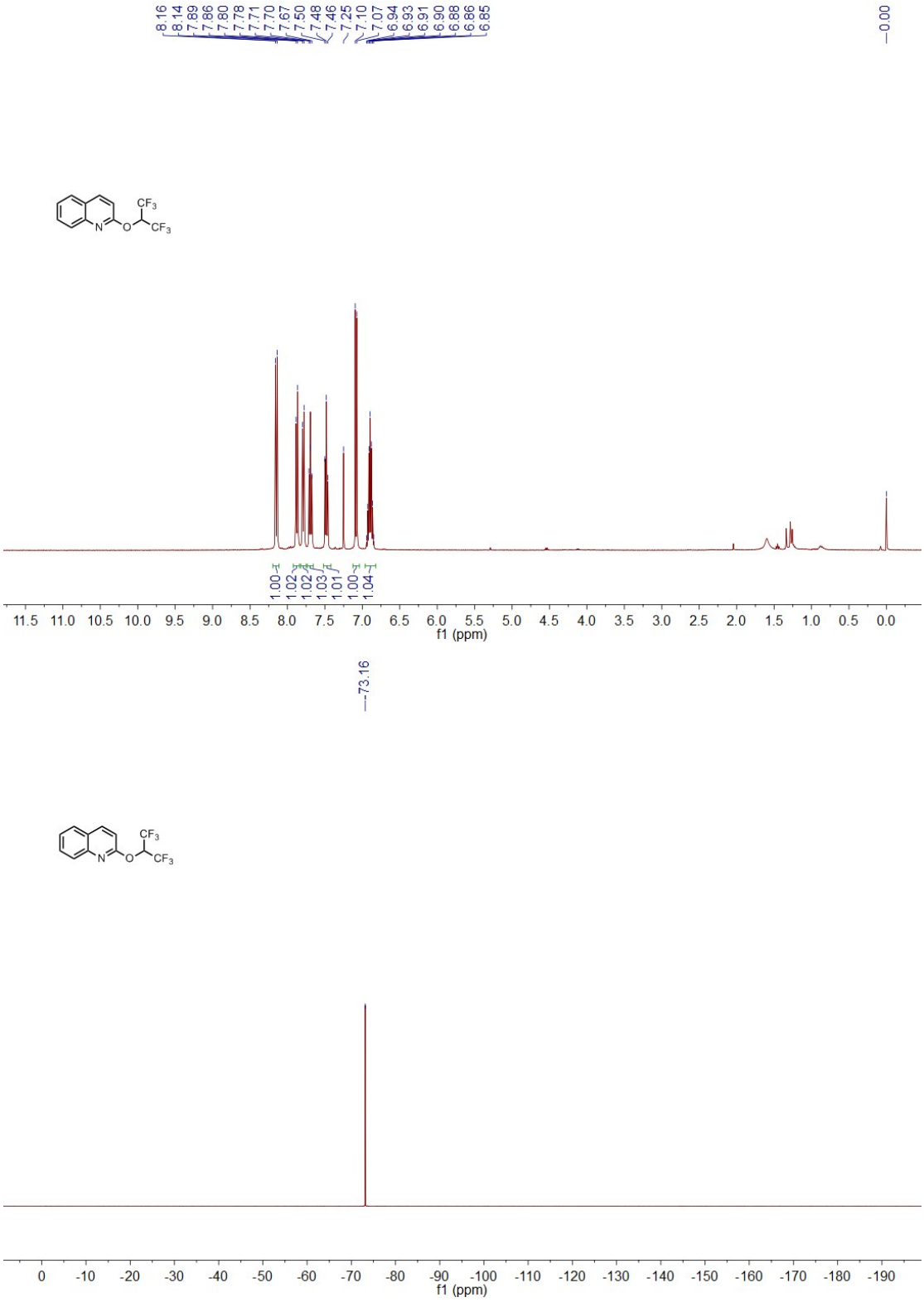
2-(2,2,2-trifluoroethoxy) quinoline (**6c**)

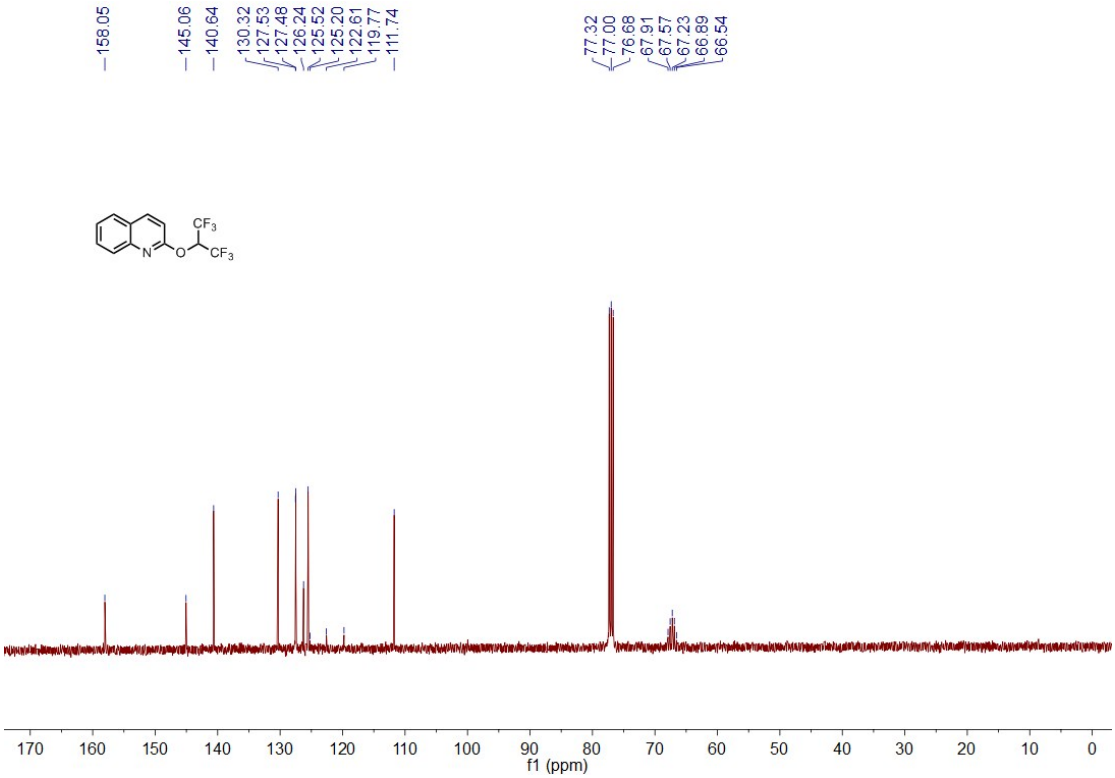



-73.64
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125
f1 (ppm)

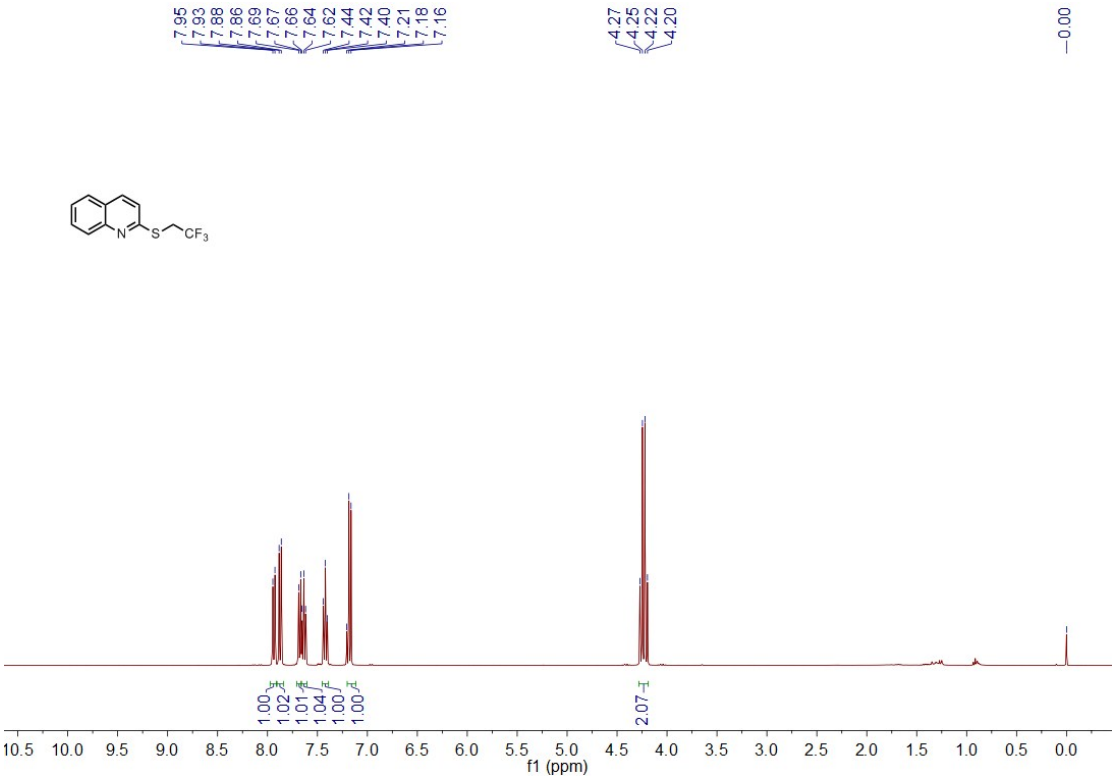

159.90
145.85
139.58
129.89
127.50
127.33
125.58
125.17
124.78
122.41
119.73
112.33
77.32
77.00
76.68
62.66
62.31
61.95
61.59
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

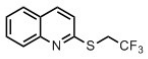
2-((1,1,1,3,3,3-hexafluoropropan-2-yl) oxy) quinoline (**6d**)



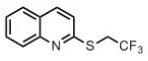


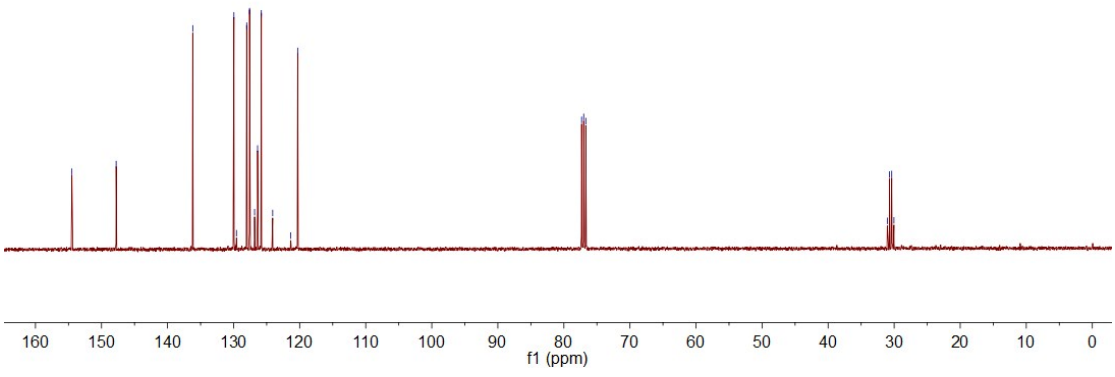
2-((2,2,2-trifluoroethyl)thio) quinoline (**6e**)



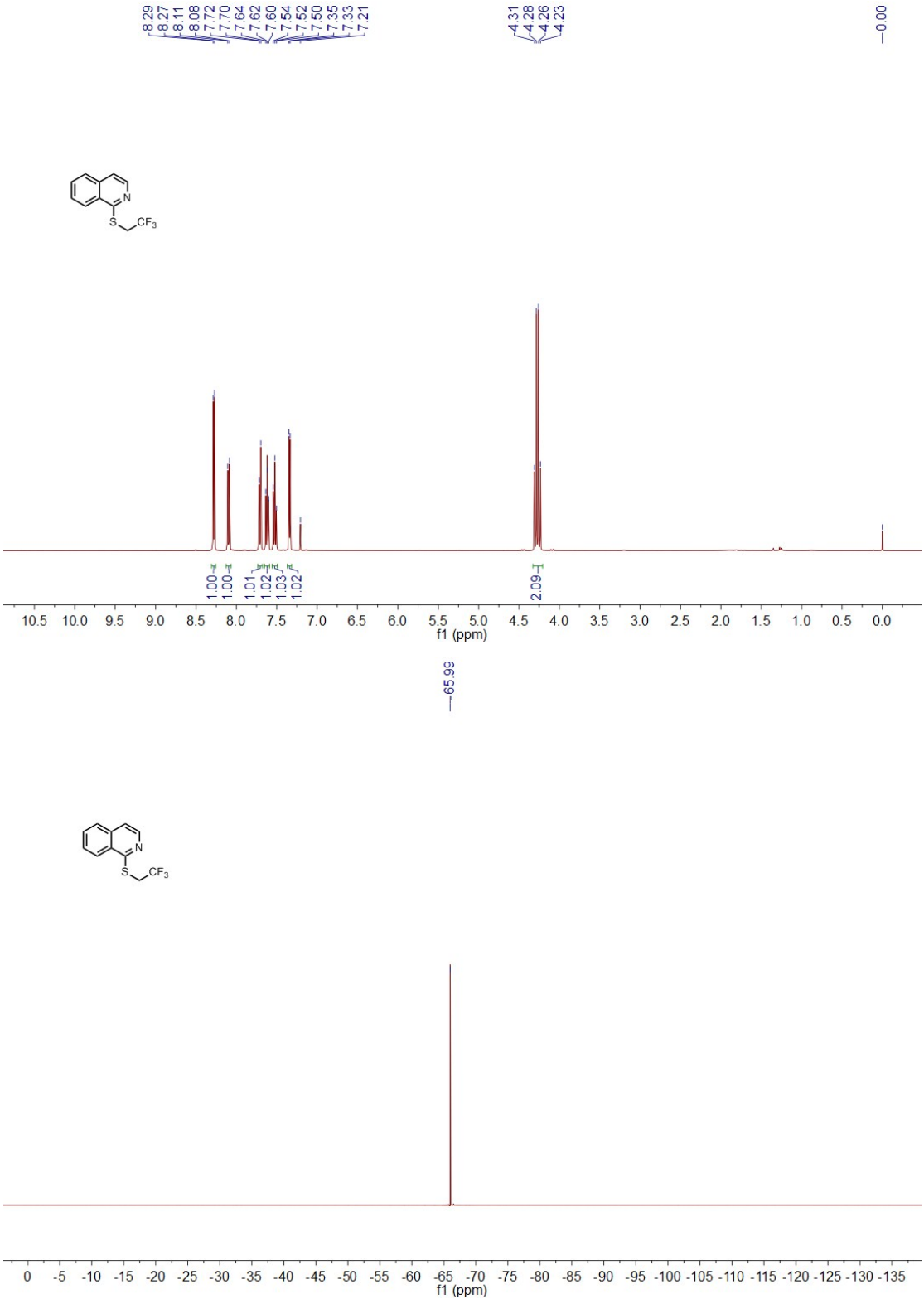


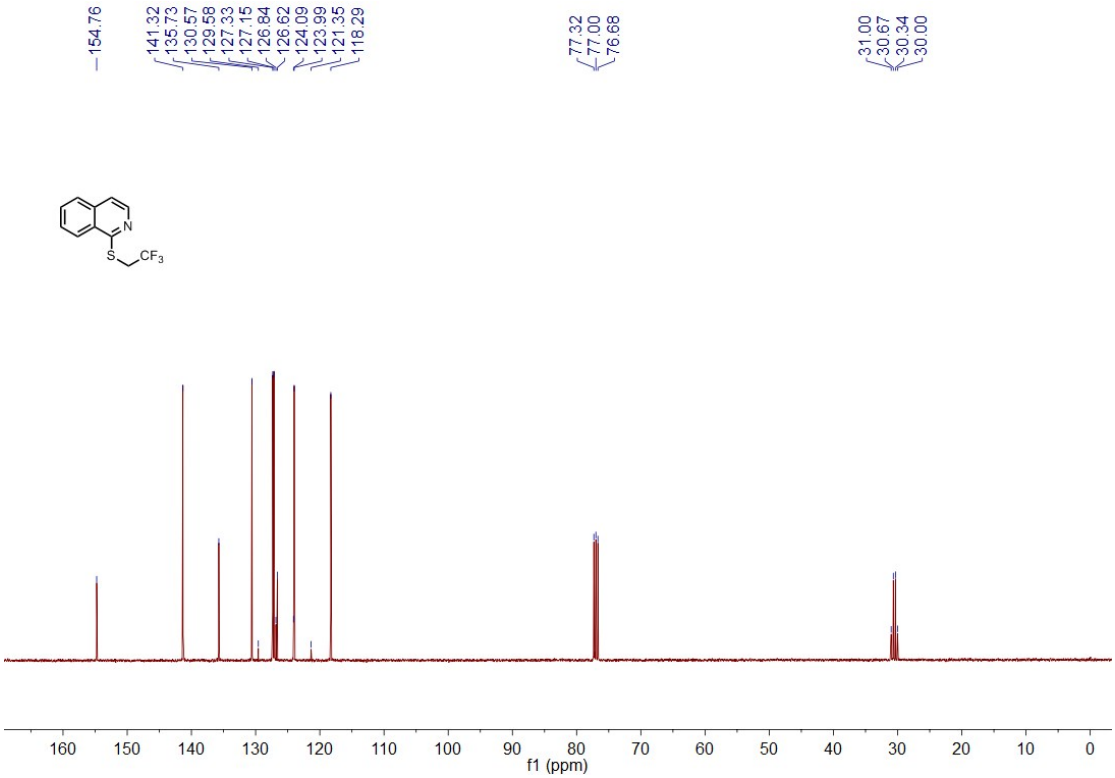
66.10
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125
f1 (ppm)
154.49
147.78
136.18
129.95
129.57
128.02
127.59
126.83
126.37
125.81
124.09
121.35
120.30
77.32
77.00
76.68
31.04
30.70
30.37
30.04



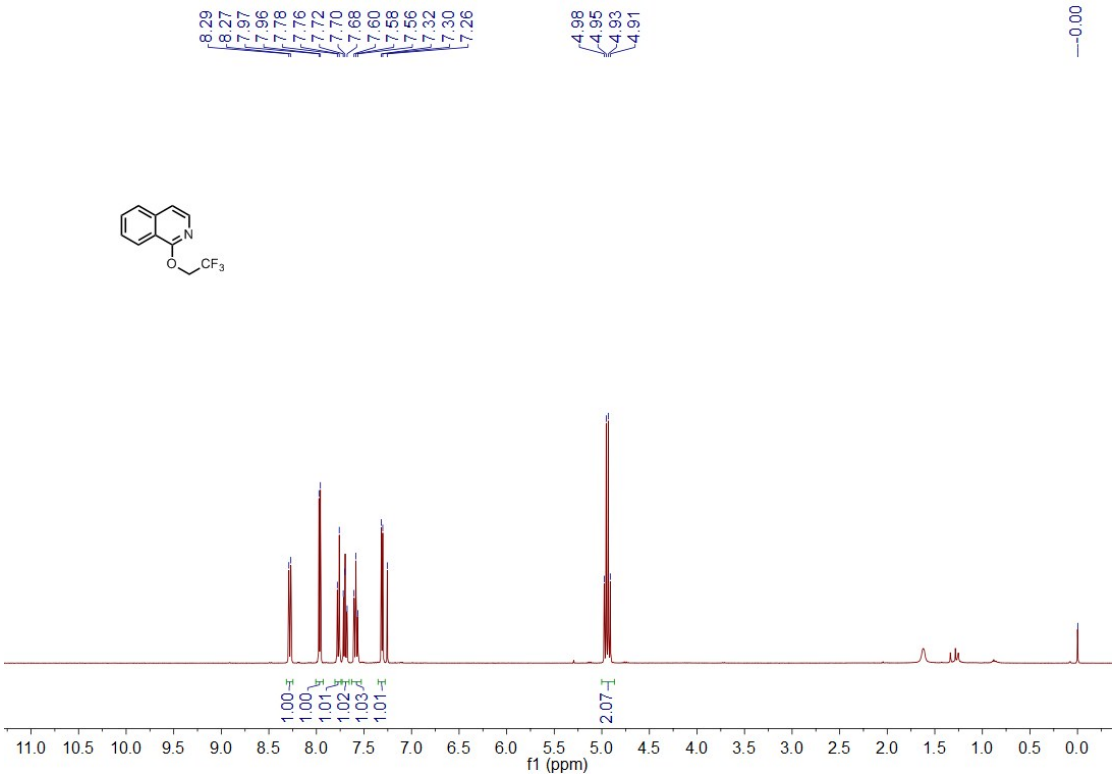

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

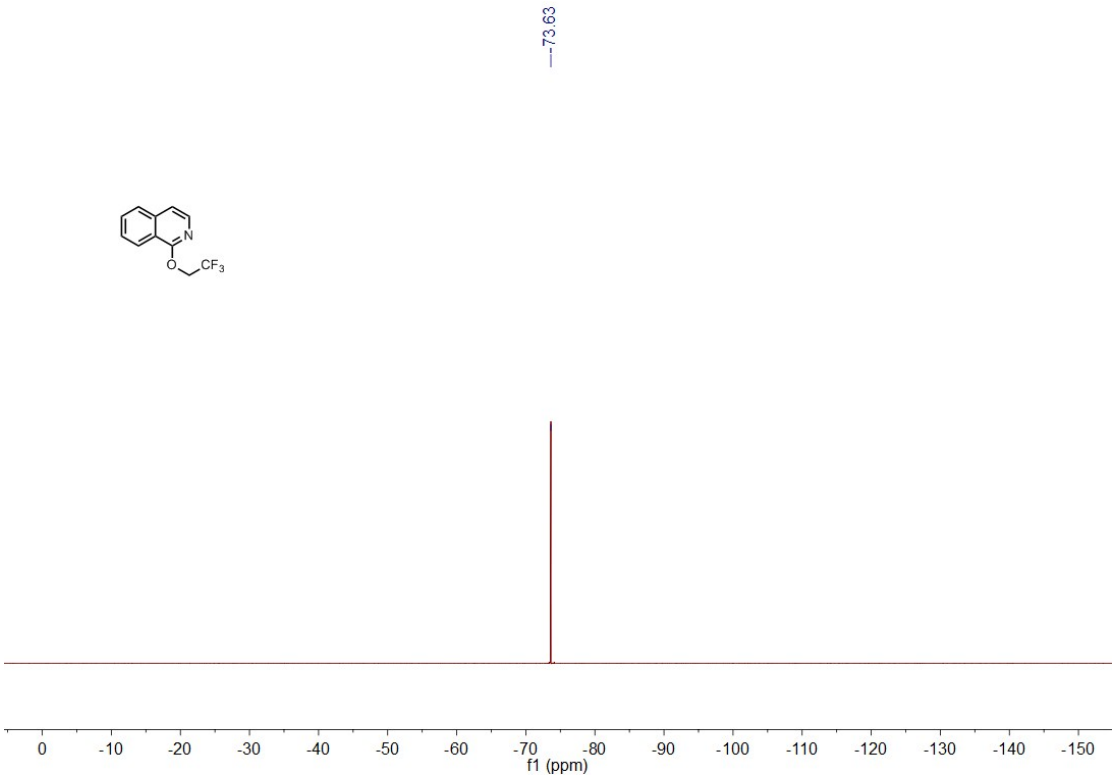
1-((2,2,2-trifluoroethyl)thio) isoquinoline (**6f**)

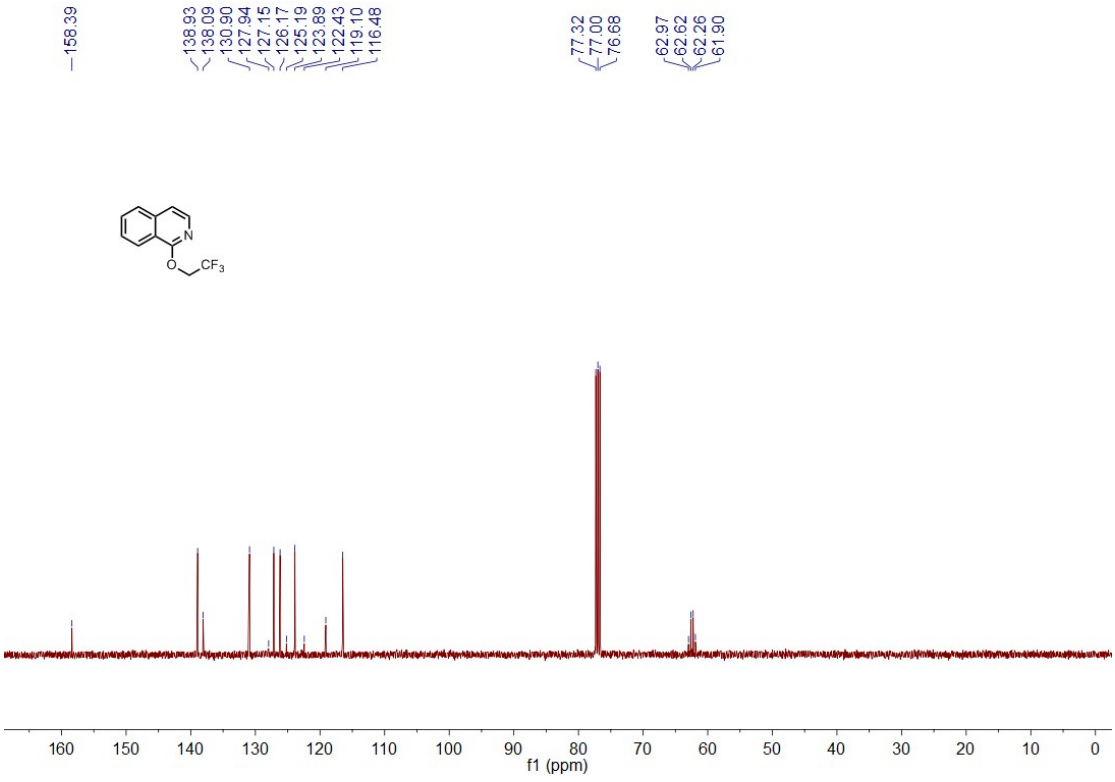




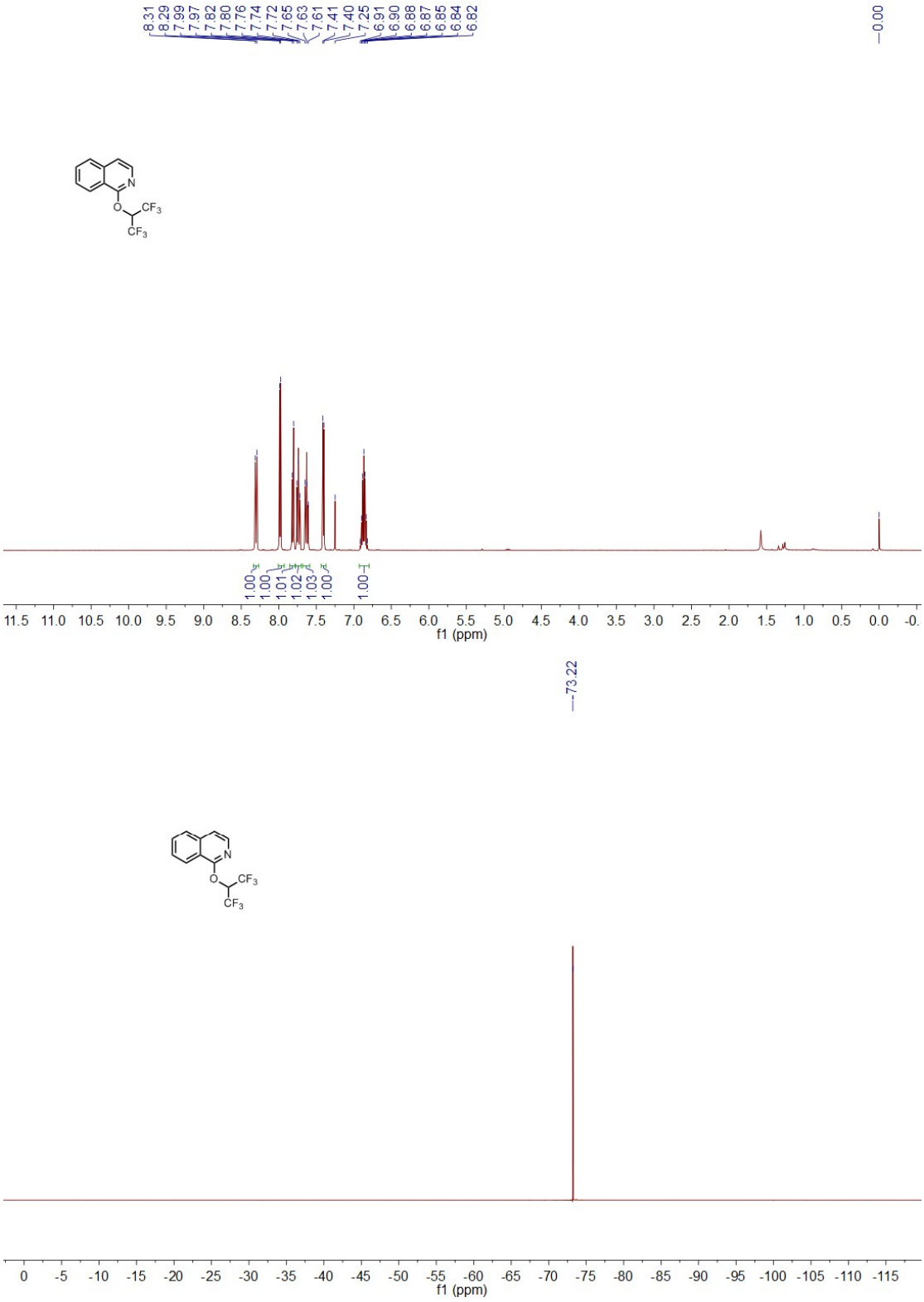
1-(2,2,2-trifluoroethoxy) isoquinoline (**6g**)

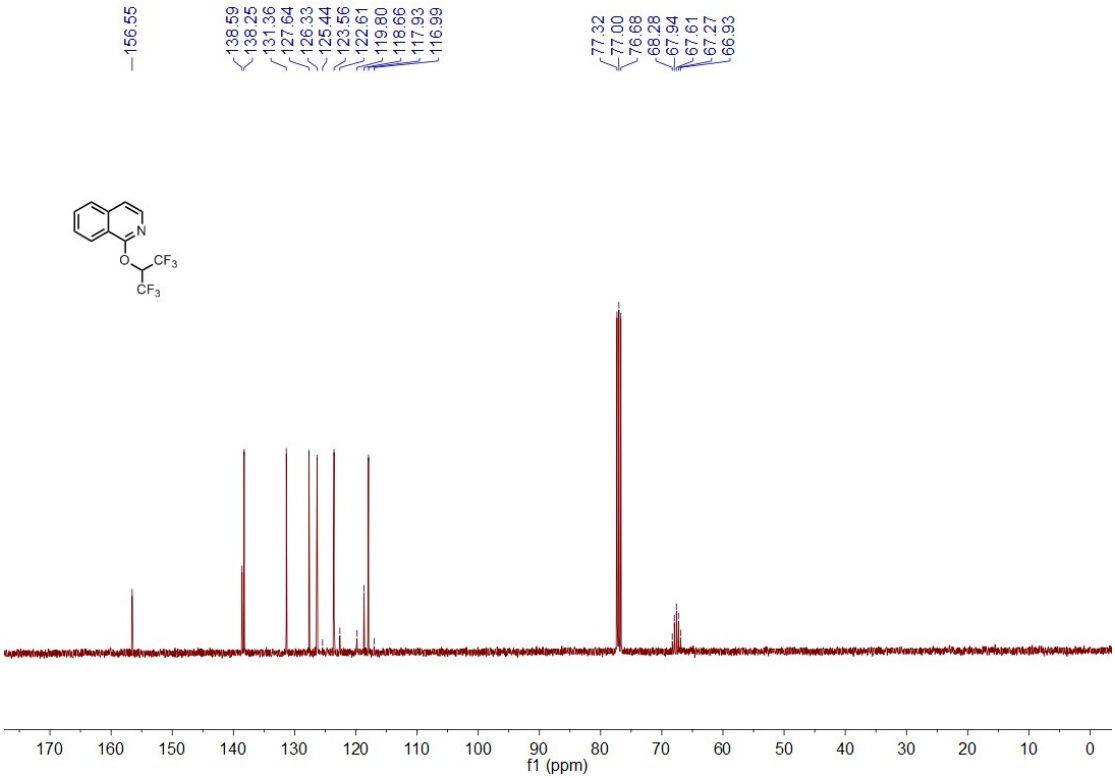



-73.63
N
O
CF3
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

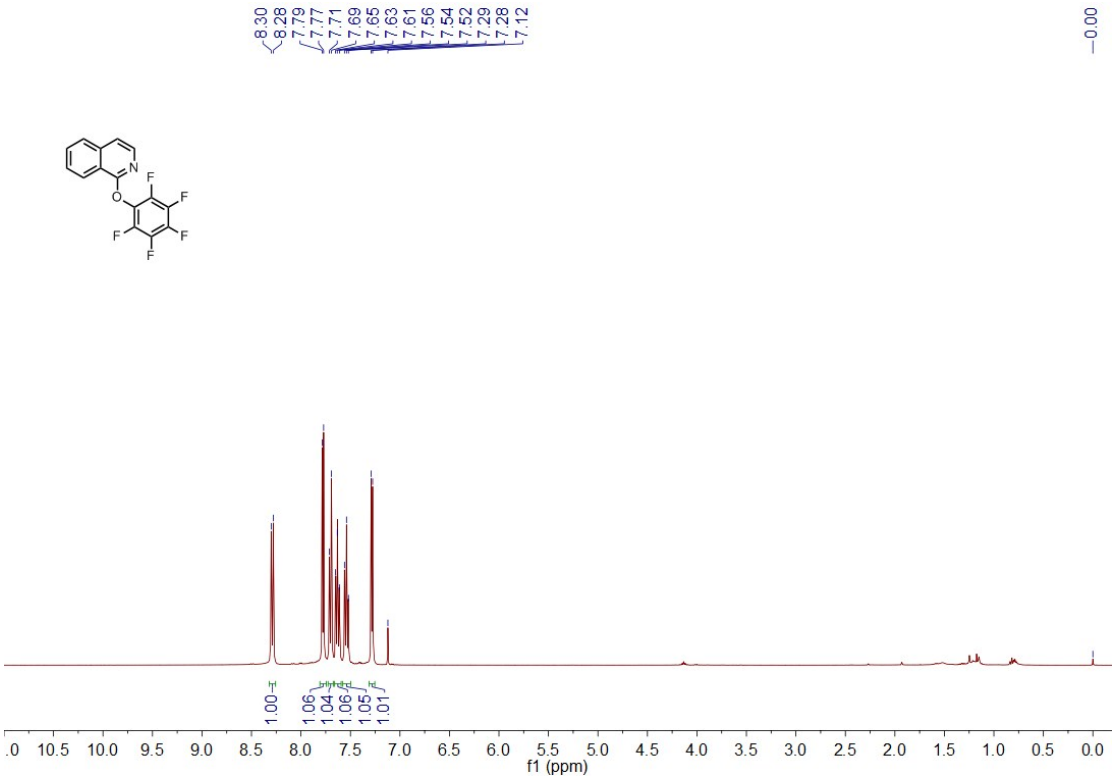

158.39
138.93
138.09
130.90
127.94
127.15
126.17
125.19
123.89
122.43
119.10
116.48
77.32
77.00
76.68
62.97
62.62
62.26
61.90
N
O
CF3
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

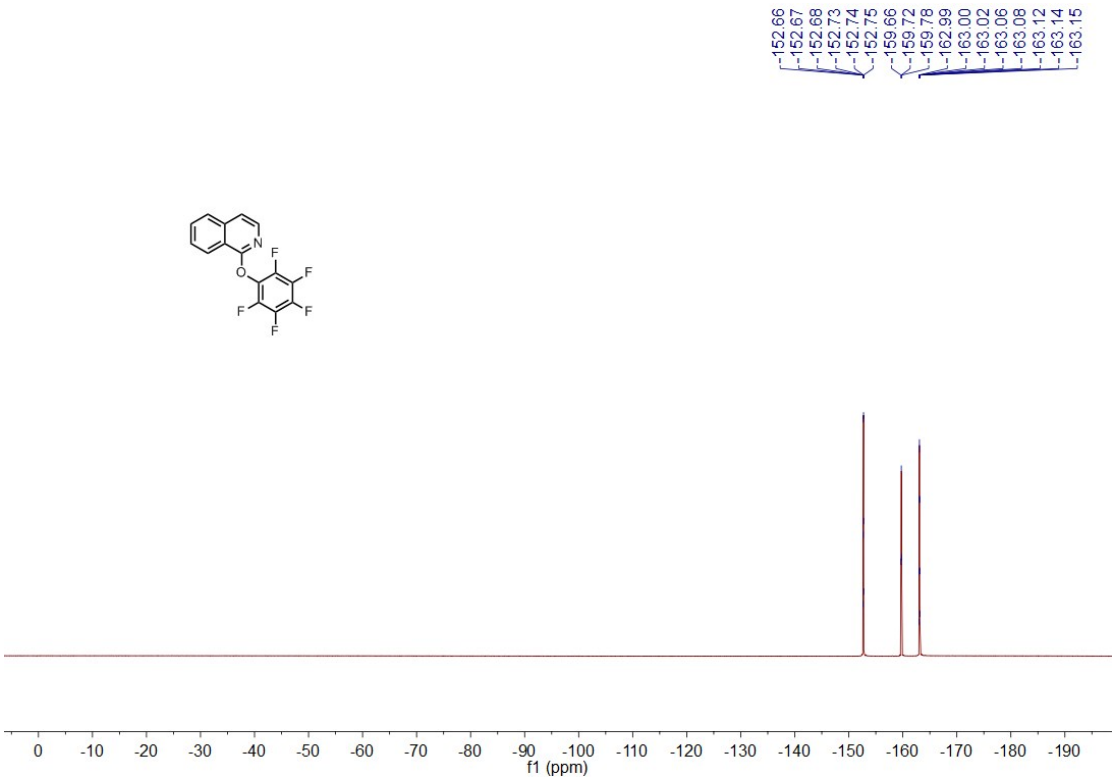
1-((1,1,1,3,3,3-hexafluoropropan-2-yl)oxy) isoquinoline (**6h**)

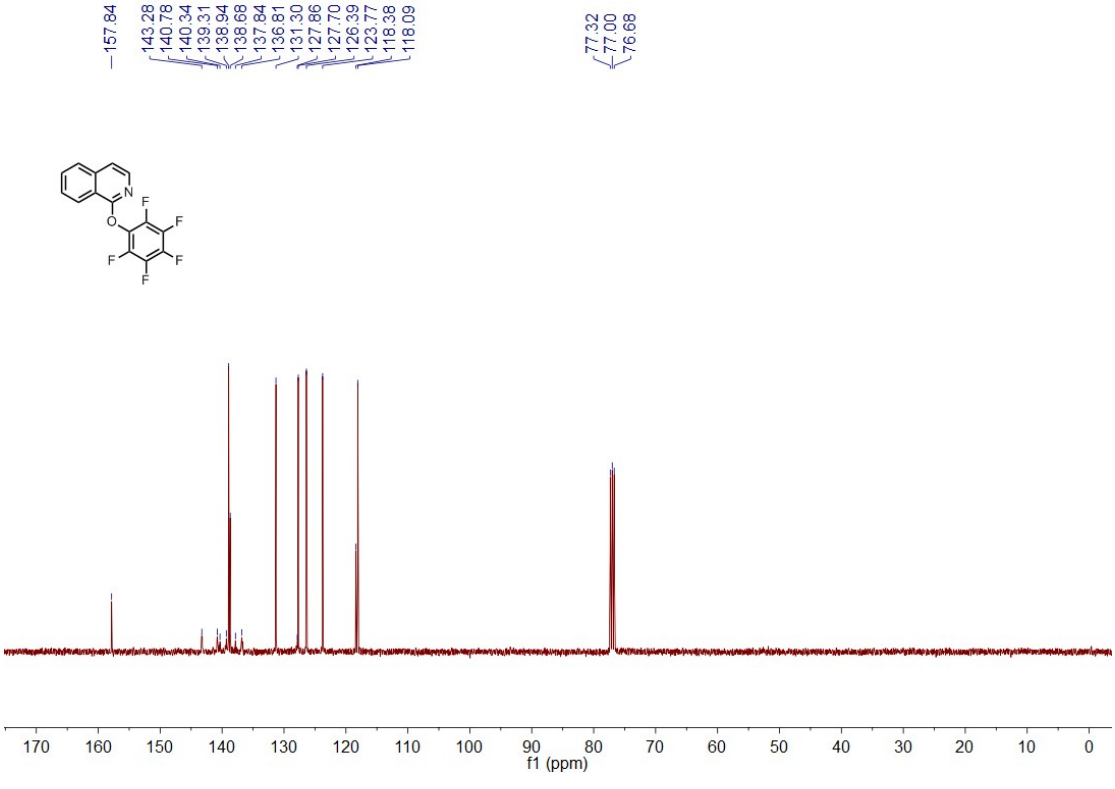




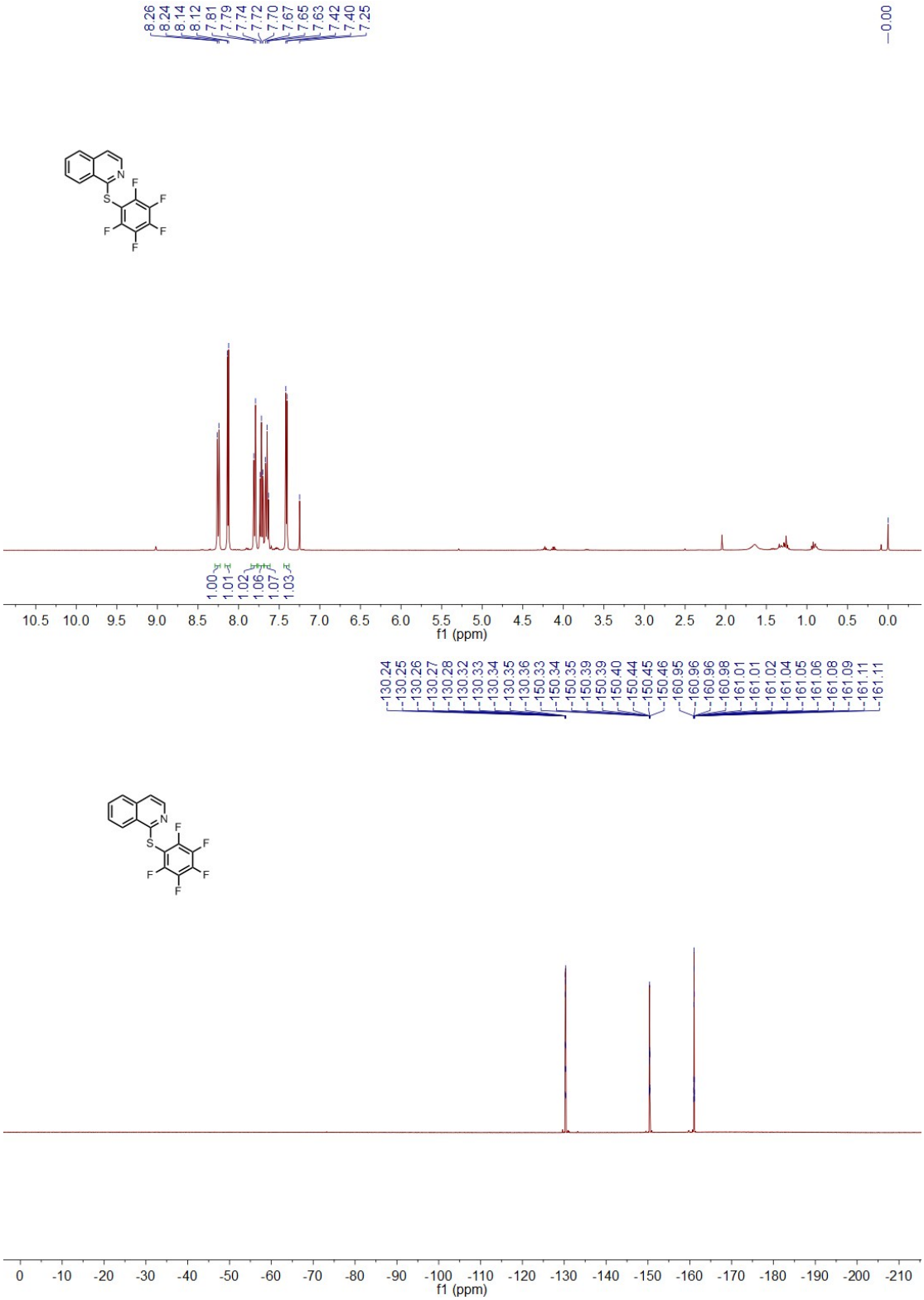
1-(perfluorophenoxy) isoquinoline (**6i**)

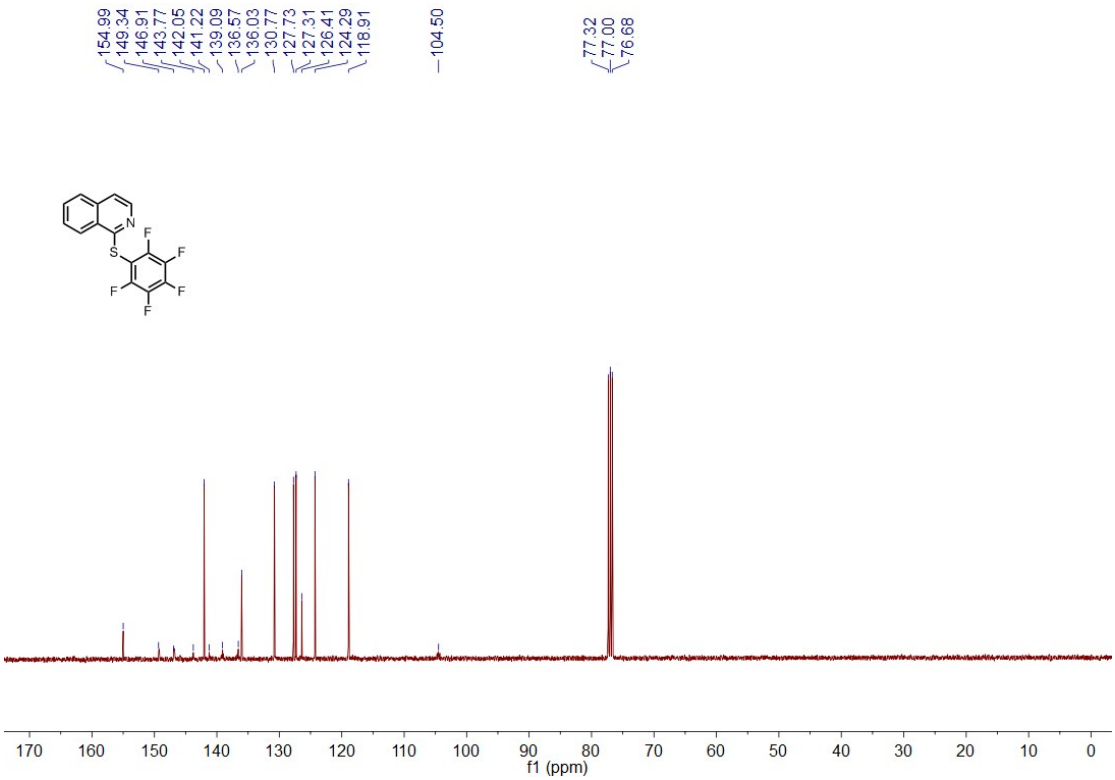



-152.66
-152.67
-152.68
-152.73
-152.74
-152.75
-159.66
-159.72
-159.78
-162.99
-163.00
-163.02
-163.06
-163.08
-163.12
-163.14
-163.15
F
F
F
F
F
O
N
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

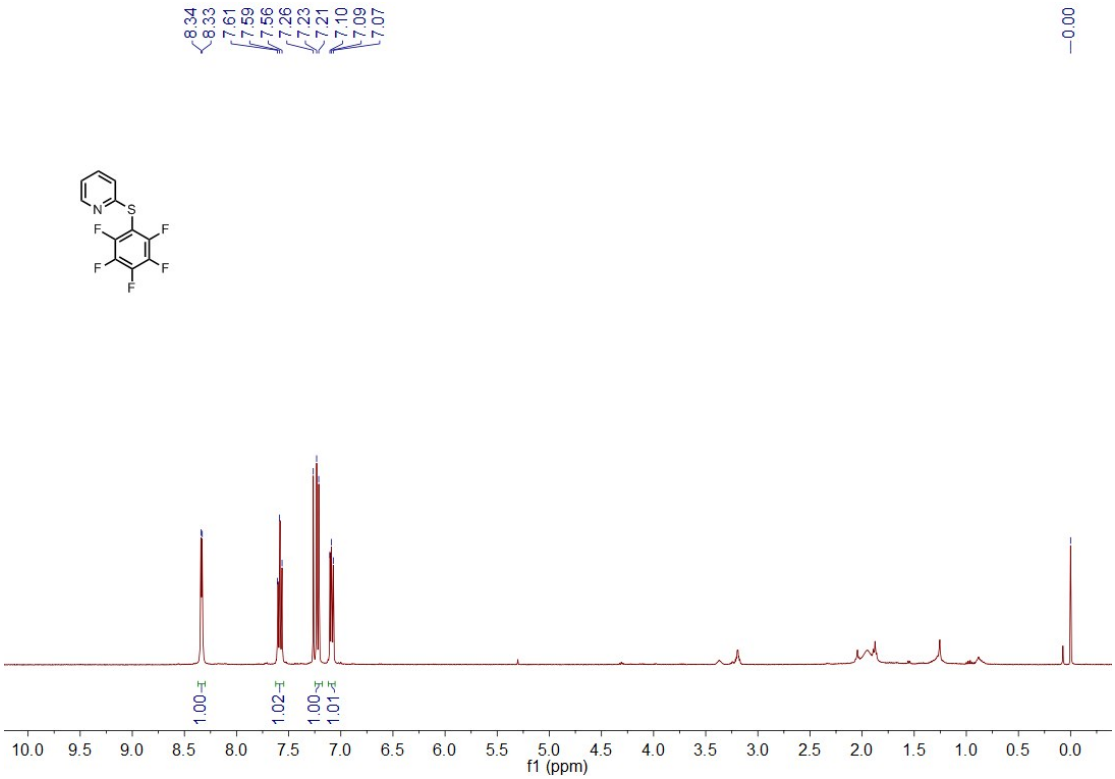

-157.84
-143.28
-140.78
-140.34
-139.31
-138.94
-138.68
-137.84
-136.81
-131.30
-127.86
-127.70
-126.39
-123.77
-118.38
-118.09
-77.32
-77.00
-76.68
F
F
F
F
F
O
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

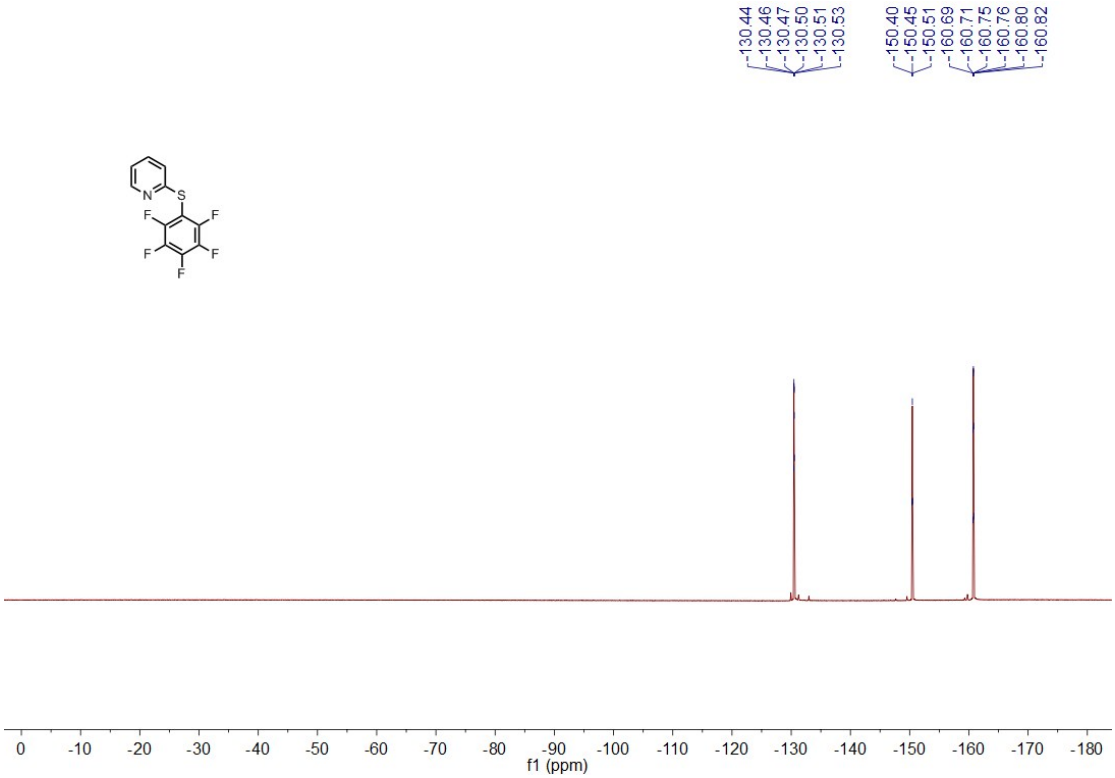
1-((perfluorophenyl)thio) isoquinoline (**6j**)

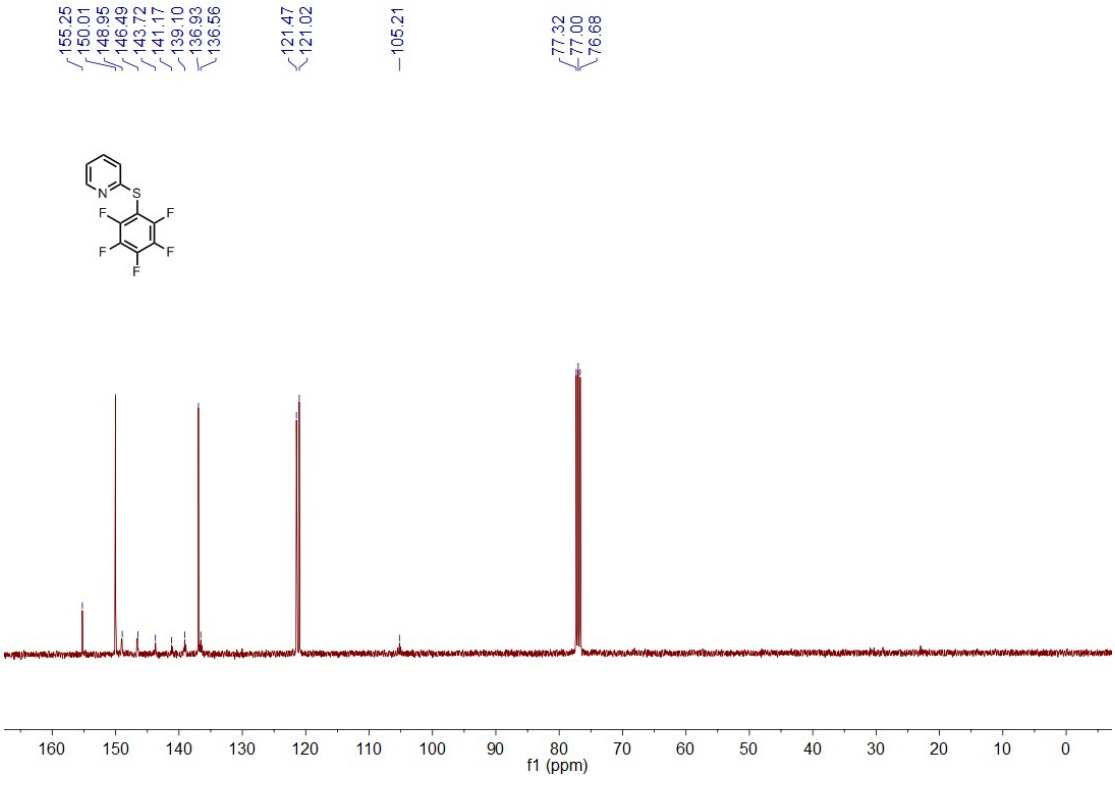




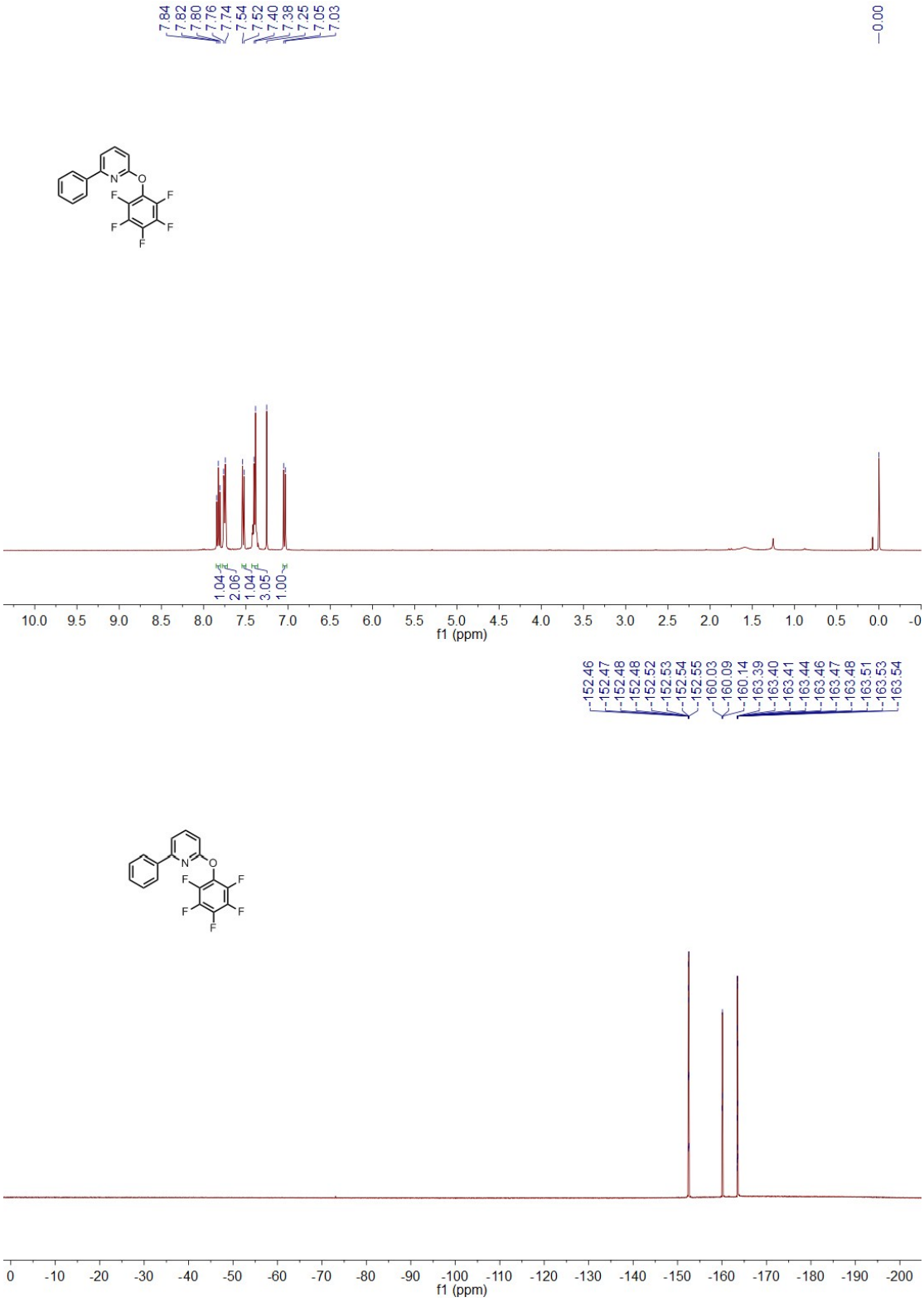
2-((perfluorophenyl)thio) pyridine (**6k**)

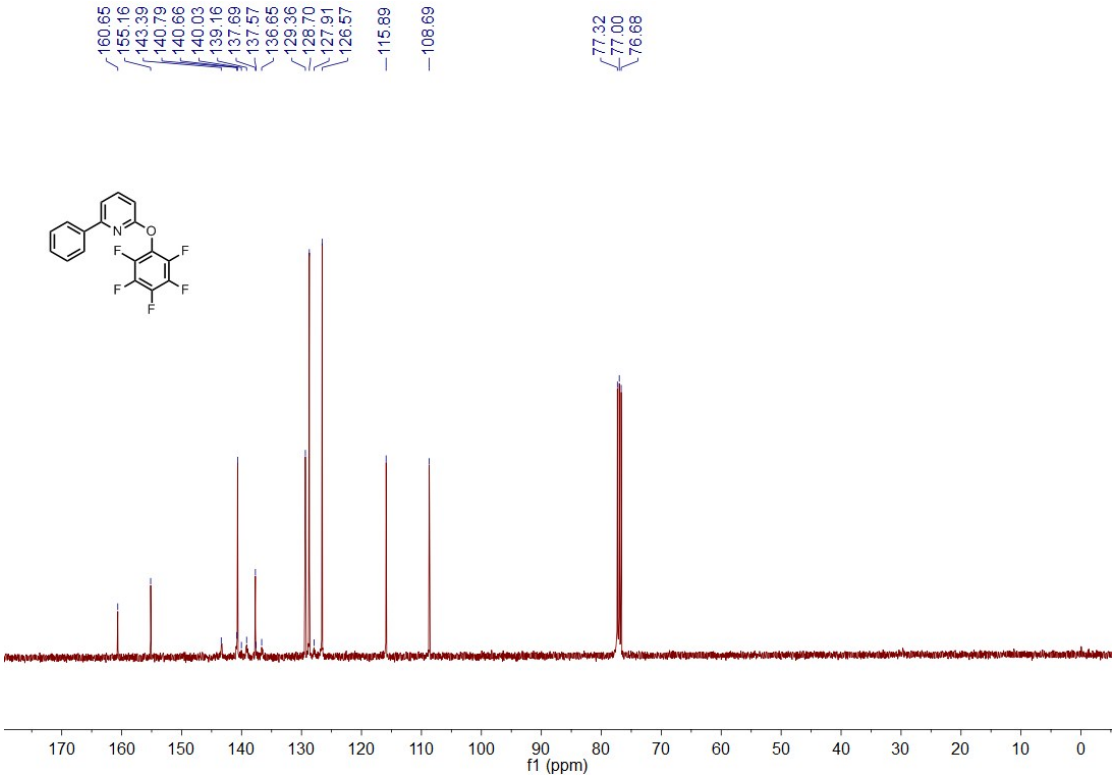



130.44
130.46
130.47
130.50
130.51
130.53
150.40
150.45
150.51
160.69
160.71
160.75
160.76
160.80
160.82
F
F
F
F
F
S
N
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
f1 (ppm)

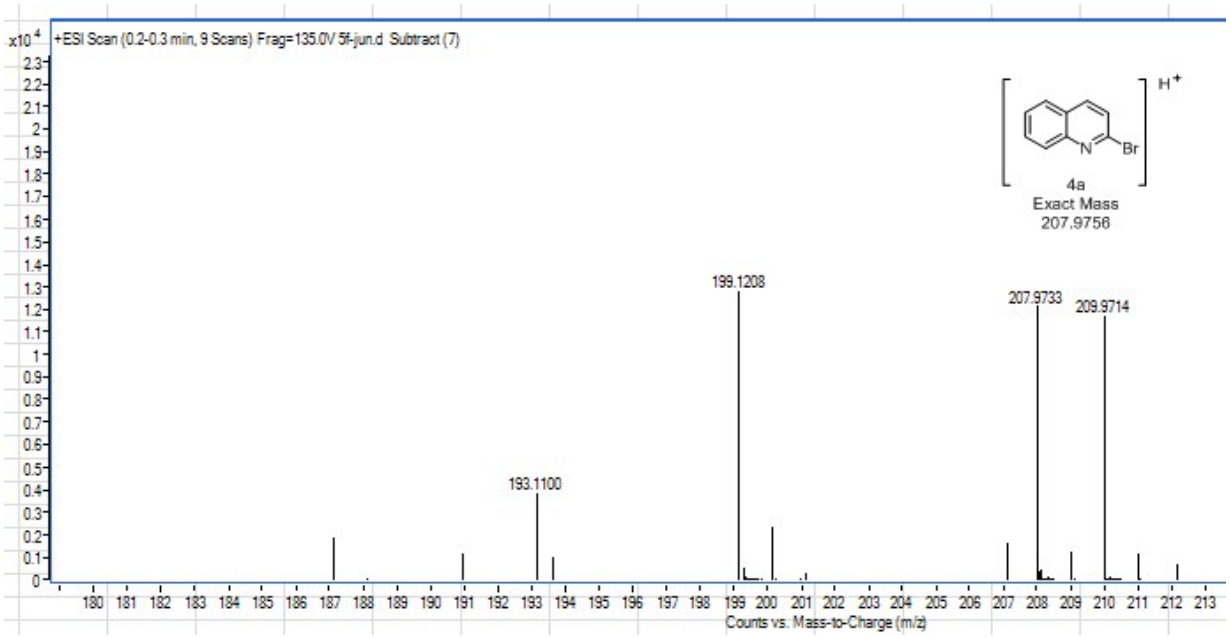

155.25
150.01
148.95
146.49
143.72
141.17
139.10
136.93
136.56
121.47
121.02
105.21
77.32
77.00
76.68
F
F
F
F
F
S
N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

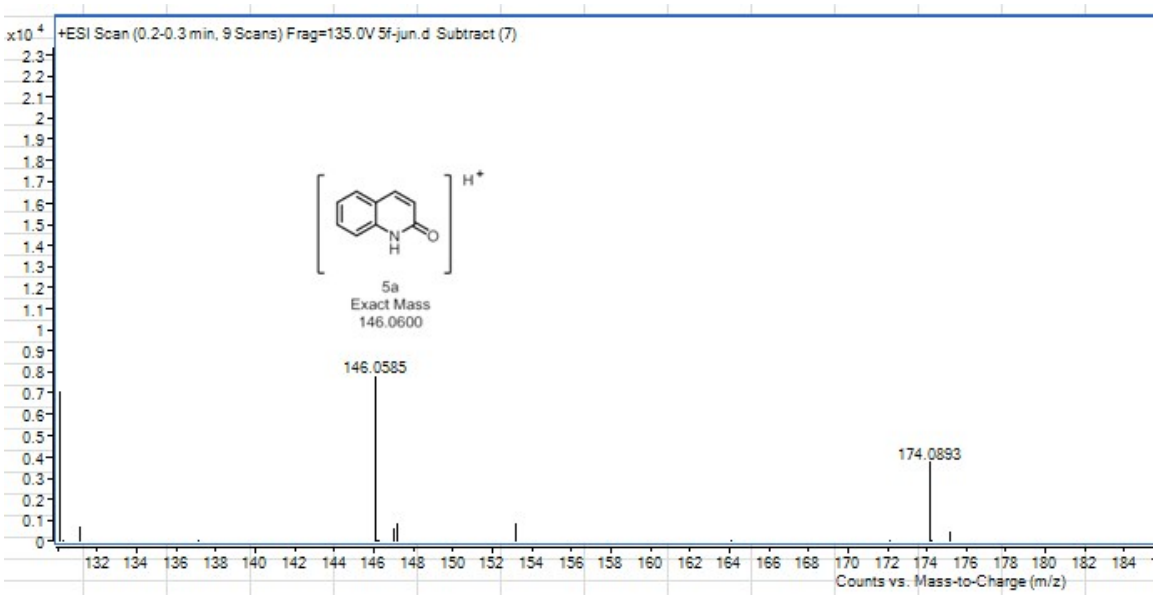
2-(perfluorophenoxy)-6-phenylpyridine (**6l**)





Electrospray Ionization-Time-of-Flight-Mass Spectrometry (ESI-TOF-MS) of compound 4a and 5a.




x10 4
+ESI Scan (0.2-0.3 min, 9 Scans) Frag=135.0V 5f-jun.d Subtract (7)
H+
N
H
O
5a
Exact Mass
146.0600
146.0585
174.0893
Counts vs. Mass-to-Charge (m/z)