Rongalite-mediated sequential homologative fluorination of oxindoles *en route* to 3-(fluoromethyl)-3-methylindolin-2-ones

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1. **General Information:** All chemicals were purchased from Aldrich, Alfa Aesar, TCI, Finar, and used as received. All solvents were purchased from commercial sources, then distilled by the standard protocol, and stored over molecular sieves under nitrogen atmosphere prior to use. Thin layer chromatography was performed on 200 μm aluminium-foilbacked silica gel plates, and the column chromatography were performed using 100-200 mesh silica gel (Merck). ^{1}H NMR spectra were recorded on Bruker's AVANCE 400 MHz spectrometer, $CDCl_3$, and DMSO-d_6 as a solvent and TMS as an internal standard. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, br = broad Coupling constants, *J* were reported in Hertz unit (Hz). ^{13}C NMR spectrum and ^{19}F NMR spectra were recorded on Bruker's AVANCE 100 MHz spectrometer, and 376 MHz spectrometer respectively, and they were fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center line of a triplet at 77.16 ppm of chloroform-*d* (a multiplet at 39.52 ppm of DMSO-d_6). Melting points were determined with a Stuart SMP30 apparatus, and are uncorrected. Indolin-2-ones **1b-1z** were synthesized according to the previous reports.[1] *N*-protected indolin-2-ones **1n-1z** were prepared by the following reported procedure.[2, 3]

2. **General Procedure**

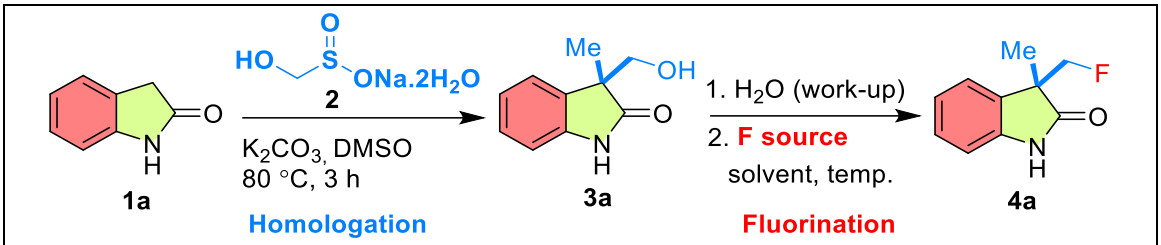
General Procedure for Synthesis of 3-(fluoromethyl)-3-methylindolin-2-one(4a-4z): An oven-dried 10 mL round-bottom flask equipped with a magnetic stir bar was charged with the appropriate indolin-2-one derivative **1a** (1.0 mmol), rongalite **2** (3.0 mmol), K_2CO_3 (2.5 mmol), and DMSO (2 mL). The reaction mixture was stirred at 80 °C and progress was monitored by TLC. After completion, the reaction mixture was washed with water, extracted with diethyl ether and evaporated to afford the crude 3-(hydroxymethyl)-3-methylindolin-2-one (**3a**),[4] which was used directly in the next step.

The crude residue (**3a**) was re-dissolved in CH_2Cl_2 (2 mL), cooled to 0 °C, and treated dropwise with DAST (4.0 mmol). The mixture was stirred at 0 °C for 5-10 min and monitored

by TLC. The reaction was quenched with saturated aqueous $NaHCO_3$, stirred for 10 min, and extracted with CH_2Cl_2 (3 × 10 mL). The combined organic extracts were dried over Na_2SO_4, filtered, and concentrated. Purification by column chromatography afforded the desired 3-(fluoromethyl)-3-methylindolin-2-one derivatives (**4a-4z**).

3. Optimization Studies

Optimization studies for fluorinating reagents [a]



Entry	Fluorinating reagent (mmol)	Base (mmol)	Solvent	Temp. (°C)	Time	Yield[b] (%)
1.	PyFluor (1.0)	-	CH_2Cl_2	0-rt	24 h	n.r.
2.	PyFluor (1.0)	DBU (1.0)	CH_2Cl_2	0-rt	24 h	n.r.
3.	PyFluor (2.0)	DBU (2.0)	Toluene	rt	24 h	n.r.
4.	PyFluor (2.0)	DBU (2.0)	Toluene	80	24 h	n.r.
5.	PyFluor (1.0)	DBU (1.0)	DMSO	rt	24 h	n.r.
6.	PyFluor (1.0)	DBU (2.0)	DMSO	80	24 h	n.r.
7.	AlkylFluor (2.0)	CsF (4.0)	1,4-dioxane	rt	24 h	n.r.
8.	AlkylFluor (2.0)	CsF (4.0)	DMSO	rt	24 h	n.r.

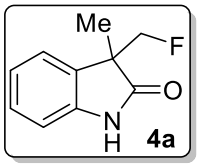
[a]Reaction conditions: indolin-2-one **1a** (1 mmol), rongalite **2** (3 mmol) and K_2CO_3 (2.5 mmol) in 2 mL of DMSO at 80 °C, after completing the C1 homologation, the reaction mixture **3a** was washed with water and extracted with Et_2O, evaporated, re-dissolved in solvent (2 mL), and added fluorinating reagents. [b]Isolated yield from homologation-fluorination sequence, n.r. = no reaction, rt = room temperature.

References

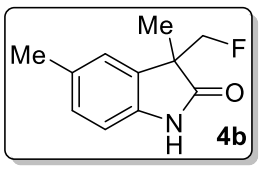
1. C.-Y. Lai, M.-J. Wang, L.-J. Huang, J.-P. Wang, C.-M. Teng, C.-Y. Chang and C.-N. Lin, *Bioorg. Med. Chem. Lett.*, 2010, **20**, 2220–2224.
2. Z. Wu, X. Fang, Y. Leng, H. Yao and A. Lin, *Adv. Synth. Catal.*, 2018, **360**, 1289–1295.
3. Y. Zhang, L. Luo, J. Ge, S.-Q. Yan, Y.-X. Peng, Y.-R. Liu, J.-X. Liu, C. Liu, T. Ma and H.-Q. Luo, *J. Org. Chem.*, 2019, **84**, 4000–4008.
4. S. Golla, S. Jalagam, S. Poshala and H. P. Kokatla, *Org. Biomol. Chem.*, 2022, **20**, 4926–4932.

Characterization Data

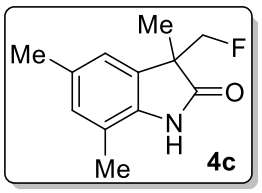
3-(fluoromethyl)-3-methylindolin-2-one (4a). Pale yellow liquid; Yield (127 mg, 85%); The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 9.47 (s, 1H), 7.28 – 7.22 (m, 2H), 7.07 (td, J = 7.6, 0.8 Hz, 1H), 6.97 (dt, J = 7.6, 0.8 Hz, 1H), 4.68 – 4.61 (m, 1H), 4.56 – 4.49 (m, 1H), 1.42 (d, J = 1.6 Hz, 3H); ^{13}C {^{1}H} NMR(100 MHz, $CDCl_3$) δ (ppm): 180.7 (d, $^{3}J_{C\text{-}F}$ = 5.4 Hz), 140.8, 131.5, 128.6, 123.4, 122.8, 110.4, 87.0, (d, $^{1}J_{C\text{-}F}$ = 176.8 Hz), 50.1, (d, $^{2}J_{C\text{-}F}$ = 19.2 Hz), 18.4, (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.32; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{10}H_{11}FNO$ 180.0825; found 180.0813.



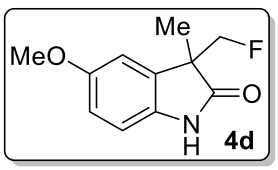
3-(fluoromethyl)-3,5-dimethylindolin-2-one (4b). Pale yellow solid; Yield (108 mg, 72%); mp: 182-183 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.59 (s, 1H), 7.09 (s, 1H), 7.05 (d, J = 7.6 Hz, 1H), 6.84 (d, J = 7.6 Hz, 1H), 4.67 – 4.60 (m, 1H), 4.55 – 4.48 (m, 1H), 2.34 (s, 3H), 1.41 (d, J = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 180.0, (d, $^{3}J_{C\text{-}F}$ = 5.8 Hz), 138.0, 132.3, 131.5, 128.9, 124.3, 109.8, 87.1, (d, $^{1}J_{C\text{-}F}$ = 176.4 Hz), 49.9, (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 21.1, 18.5, (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.41; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{11}H_{13}FNO$ 194.0981; found 194.0982.



3-(fluoromethyl)-3,5,7-trimethylindolin-2-one (4c). Pale yellow solid; Yield (107 mg, 71%); mp: 196-197 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 9.00 (s, 1H), 6.94 (d, J = 9.9 Hz, 2H), 4.69 – 4.61 (m, 1H), 4.57 – 4.49 (m, 1H), 2.34 (s, 3H), 2.29 (s, 3H), 1.42 (d, J = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 179.0, 135.7, 131.2, 130.1, 129.4, 120.6, 118.0, 86.1 (d, $^{1}J_{C\text{-}F}$ = 176.4 Hz), 49.2 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 20.0, 17.5 , (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz), 15.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.37; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{12}H_{15}FNO$ 208.1138; found 208.1135.

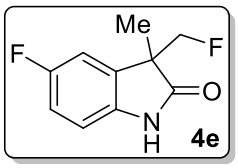


3-(fluoromethyl)-5-methoxy-3-methylindolin-2-one (4d). Light brown solid; Yield (113 mg, 75%); mp: 139-140 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.89 (s, 1H), 6.82 – 6.78 (m, 2H), 6.71 (dd, J = 8.4, 2.4 Hz, 1H), 4.56 (m, 1H), 4.45 (m, 1H), 3.72 (s, 3H), 1.35 (d, J = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 180.1 (d, $^{3}J_{C\text{-}F}$ = 5.8 Hz), 156.1, 133.9, 132.8, 113.0, 110.8, 110.6, 87.1 (d, $^{1}J_{C\text{-}F}$ = 176.4 Hz), 55.8, 50.4 (d, $^{2}J_{C\text{-}}$

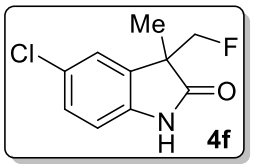


$_F$ = 19.3 Hz), 18.5 (d, $^3J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.861; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{11}H_{13}FNO_2$ 210.0930; found 210.0929.

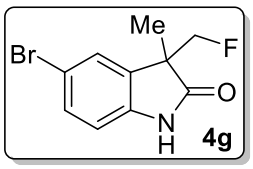
5-fluoro-3-(fluoromethyl)-3-methylindolin-2-one (4e). White crystalline solid; Yield (123 mg, 82%); mp: 138-139 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.78 (s, 1H), 7.05 (dd, *J* = 8.0, 2.6 Hz, 1H), 6.99 (td, *J* = 8.8, 2.4 Hz, 1H), 6.91 (dd, *J* = 8.4, 4.4 Hz, 1H), 4.70 – 4.63 (m, 1H), 4.58 – 4.51 (m, 1H), 1.45 (d, *J* = 2.0 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 179.8 (d, $^3J_{C\text{-}F}$ = 5.9 Hz), 160.5 (d, $^1J_{C\text{-}F}$ = 239.8 Hz), 136.4 (d, $^4J_{C\text{-}F}$ = 2.3 Hz), 133.1 (d, $^3J_{C\text{-}F}$ = 8.5 Hz), 115.1 (d, $^3J_{C\text{-}F}$ = 23.4 Hz), 111.8 (d, $^3J_{C\text{-}F}$ = 8.0 Hz), 110.8 (d, $^3J_{C\text{-}F}$ = 8.0 Hz), 86.8 (d, $^1J_{C\text{-}F}$ = 177.2 Hz), 50.5 (d, $^2J_{C\text{-}F}$ = 19.1 Hz)., 18.4 (d, $^3J_{C\text{-}F}$ = 6.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): δ -120.09, -223.86; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{10}H_{10}F_2NO$ 198.0730; found 198.0727.



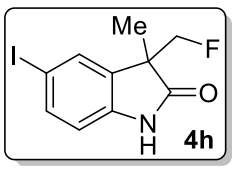
5-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4f). Off-White solid; Yield (126 mg, 84%); mp: 139-140 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 9.13 (s, 1H), 7.28 – 7.20 (m, 2H), 6.90 (d, *J* = 8.0 Hz, 1H), 4.68 – 4.60 (m, 1H), 4.56 – 4.48 (m, 1H), 1.42 (d, *J* = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 179.8, 139.2, 133.1, 128.6, 128.2, 124.1, 111.2, 86.7 (d, $^1J_{C\text{-}F}$ = 177.2 Hz), 50.3 (d, $^2J_{C\text{-}F}$ = 19.3 Hz), 18.4(d, $^3J_{C\text{-}F}$ = 5.8 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.46; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{10}H_{10}ClFNO$ 214.0435; found 214.0440.



5-bromo-3-(fluoromethyl)-3-methylindolin-2-one (4g). Yellow solid; Yield (123 mg, 82%); mp: 94-95 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.75 (s, 1H), 7.32 (d, *J* = 7.6 Hz, 2H), 6.80 – 6.75 (m, 1H), 4.61 – 4.52 (m, 1H), 4.49 – 4.40 (m, 1H), 1.35 (d, *J* = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 178.4, 138.6, 132.5, 130.5, 125.9, 114.5, 110.6, 85.7 (d, $^1J_{C\text{-}F}$ = 177.2 Hz), 49.2 (d, $^2J_{C\text{-}F}$ = 19.7 Hz), 17.4 (d, $^3J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.41; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{10}H_{10}BrFNO$ 257.9930; found 257.9929.

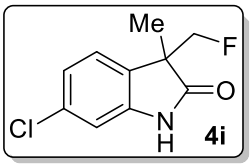


3-(fluoromethyl)-5-iodo-3-methylindolin-2-one (4h). Brown solid; Yield (114 mg, 76%); mp: 215-216 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.61 (s, 1H), 7.65 – 7.58 (m, 2H), 6.78 (d, *J* = 8.0 Hz, 1H), 4.69 – 4.61 (m, 1H), 4.57 – 4.49 (m, 1H), 1.43 (d, *J* = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 179.1, 140.3, 137.5, 133.8,

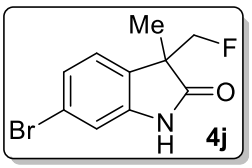


132.5, 112.1, 86.7 (d, $^{1}J_{C\text{-}F}$ = 177.2 Hz), 85.3, 50.0 (d, $^{2}J_{C\text{-}F}$ = 19.7 Hz), 18.4 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.27; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{10}H_{10}IFNO$ 305.9791; found 305.9804.

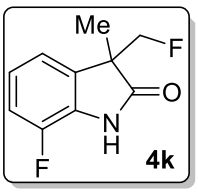
6-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4i). White crystalline solid; Yield (120 mg, 80%); mp: 149-150 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.47 (s, 1H), 7.13 (d, *J* = 8.0 Hz, 1H), 6.99 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.90 (d, *J* = 2.0 Hz, 1H), 4.60 – 4.52 (m, 1H), 4.48 – 4.40 (m, 1H), 1.34 (d, *J* = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 179.6 (d, $^{3}J_{C\text{-}F}$ = 5.5 Hz), 141.6, 134.3, 129.8, 124.5, 122.8, 110.8, 86.8 (d, $^{1}J_{C\text{-}F}$ = 177.2 Hz), 49.7 (d, $^{2}J_{C\text{-}F}$ = 19.6 Hz), 18.4 (d, $^{3}J_{C\text{-}F}$ = 5.8 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.56; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{10}H_{10}ClFNO$ 214.0435; found 214.0433.



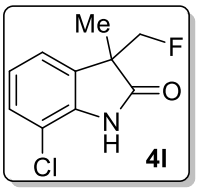
6-bromo-3-(fluoromethyl)-3-methylindolin-2-one (4j). Pale yellow crystalline solid; Yield (119 mg, 79%); mp: 129-130 °C; The title compound is prepared according to the general procedure described as above**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.96 (s, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.17 (d, *J* = 5.6 Hz, 2H), 4.68 – 4.61 (m, 1H), 4.57 – 4.50 (m, 1H), 1.43 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 179.6, 141.8, 130.3, 125.7, 124.9, 122.1, 113.6, 86.7 (d, $^{1}J_{C\text{-}F}$ = 177.1 Hz), 49.8 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 18.3 (d, $^{3}J_{C\text{-}F}$ = 5.8 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.40; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{10}H_{10}BrFNO$ 257.9930; found 257.9917.



7-fluoro-3-(fluoromethyl)-3-methylindolin-2-one (4k). White crystalline solid; Yield (113 mg, 75%); mp: 135-136 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.57 (s, 1H), 7.10 – 7.02 (m, 3H), 4.70 – 4.62 (m, 1H), 4.58 – 4.50 (m, 1H), 1.43 (d, *J* = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 178.9 (d, $^{3}J_{C\text{-}F}$ = 5.5 Hz), 148.4 (d, $^{1}J_{C\text{-}F}$ = 242.8 Hz), 134.2 (d, $^{3}J_{C\text{-}F}$ = 4.4 Hz), 127.9 (d, $^{2}J_{C\text{-}F}$ = 12.4 Hz), 123.5 (d, $^{3}J_{C\text{-}F}$ = 5.9 Hz), 119.2 (d, $^{4}J_{C\text{-}F}$ = 3.7 Hz), 115.8 (d, $^{2}J_{C\text{-}F}$ = 17.1 Hz), 86.9 (d, $^{1}J_{C\text{-}F}$ = 176.8 Hz), 50.4 (dd, $^{2,4}J_{C\text{-}F}$ = 19.4, 2.2 Hz), 18.51 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -58.31, -223.72; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{10}H_{10}F_2NO$ 198.0730; found 198.0727.

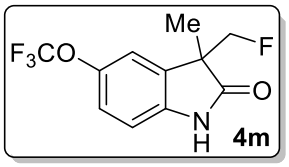


7-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4l). Yellow solid; Yield (116 mg, 77%); mp: 140-141 °C; The title compound is prepared according to the general procedure described as above**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.24 (s, 1H), 7.27 – 7.23 (m, 1H), 7.18 (d, *J* = 7.2 Hz, 1H), 7.03 (t, *J* = 7.6 Hz, 1H), 4.69 – 4.61 (m, 1H), 4.57 – 4.49 (m, 1H), 1.43 (d, *J* = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ



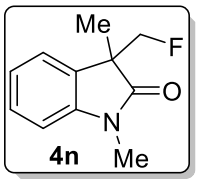
(ppm): 178.4 (d, $^{3}J_{C\text{-}F}$ = 6.0 Hz), 138.3, 132.8, 128.6, 123.7, 121.9, 115.3, 86.8 (d, $^{1}J_{C\text{-}F}$ = 177.2 Hz), 51.0 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 18.5 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.48; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{10}H_{10}ClFNO$ 214.0435; found 214.0433.

3-(fluoromethyl)-3-methyl-5-(trifluoromethoxy)indolin-2-one (4m). White crystalline solid; Yield



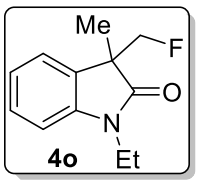
(120 mg, 80%); mp: 139-140 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 9.04 (s, 1H), 7.19 – 7.10 (m, 2H), 6.96 (d, *J* = 8.8 Hz, 1H), 4.68 – 4.61 (m, 1H), 4.56 - 4.49 (m, 1H), 1.44 (d, *J* = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 180.0 (d, $^{3}J_{C\text{-}F}$ = 5.8 Hz), 144.9, 144.9, 139.3, 121.8, 119.3, 117.6, 110.7, 86.7 (d, $^{1}J_{C\text{-}F}$ = 177.6 Hz), 50.4 (d, $^{2}J_{C\text{-}F}$ = 19.7 Hz), 18.4 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -58.31, -223.73; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{11}H_{10}F_4NO_2$ 264.0648; found 264.0646.

3-(fluoromethyl)-1,3-dimethylindolin-2-one (4n). Pale yellow liquid; Yield (140 mg, 93%); The



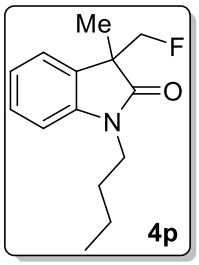
title compound is prepared according to the general procedure described as above**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.35 – 7.29 (m, 2H), 7.10 (td, *J* = 7.6, 0.8 Hz, 1H), 6.88 (dt, *J* = 8.0, 0.8 Hz, 1H), 4.63 (s, 1H), 4.51 (s, 1H), 3.23 (s, 3H), 1.40 (d, *J* = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 177.4, 143.4, 131.0, 128.6, 123.2, 122.8, 108.3, 87.2 (d, $^{1}J_{C\text{-}F}$ = 176.0 Hz), 49.4 (d, $^{2}J_{C\text{-}F}$ = 19.7 Hz), 26.4, 18.5 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.76; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{11}H_{13}FNO$ 194.0981; found 194.0981.

1-ethyl-3-(fluoromethyl)-3-methylindolin-2-one (4o). Pale yellow liquid; Yield (137 mg, 91%);



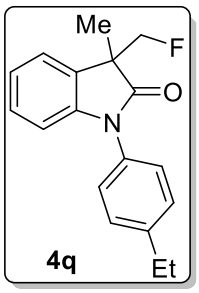
The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.23 – 7.17 (m, 2H), 6.98 (td, *J* = 7.6, 0.8 Hz, 1H), 6.79 (dd, *J* = 8.0, 1.2 Hz, 1H), 4.53 – 4.49 (m, 1H), 4.42 – 4.37 (m, 1H), 3.71 – 3.63 (m, 2H), 1.28 (d, *J* = 2.0 Hz, 3H), 1.16 (t, *J* = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 176.0 (d, $^{3}J_{C\text{-}F}$ = 5.9 Hz), 141.5, 130.2, 127.5, 122.3, 121.5, 107.4, 86.1 (d, $^{1}J_{C\text{-}F}$ = 176.1 Hz), 48.3 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 33.7, 17.4 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz), 11.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.79; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{12}H_{15}FNO$ 208.1138; found 208.1138.

1-butyl-3-(fluoromethyl)-3-methylindolin-2-one (4p). Pale yellow liquid; Yield (140 mg, 93%);



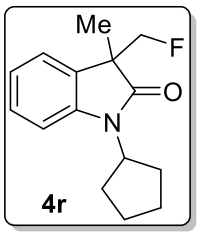
The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.22 – 7.17 (m, 2H), 6.98 (td, J = 7.6, 1.2 Hz, 1H), 6.80 (dd, J = 8.4, 1.2 Hz, 1H), 4.55 – 4.50 (m, 1H), 4.43 – 4.38 (m, 1H), 3.70 – 3.56 (m, 2H), 1.62 – 1.53 (m, 2H), 1.33 – 1.23 (m, 5H), 0.85 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 177.4 (d, $^{3}J_{C\text{-}F}$ = 5.9 Hz), 142.9, 131.2, 128.5, 123.3, 122.5, 108.6, 87.2 (d, $^{1}J_{C\text{-}F}$ = 176.4 Hz), 49.31 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 39.8, 29.4, 20.0, 18.5 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz), 13.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.63; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{14}H_{19}FNO$ 236.1451; found 236.1450.

1-(4-ethylphenyl)-3-(fluoromethyl)-3-methylindolin-2-one (4q). White semi-liquid; Yield (139



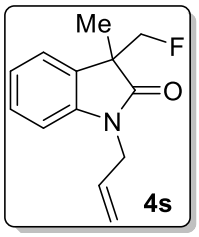
mg, 93%); The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.40 – 7.32 (m, 5H), 7.28 – 7.24 (m, 1H), 7.15 (td, J = 7.6, 0.8 Hz, 1H), 6.87 (dt, J = 7.6, 0.8 Hz, 1H), 4.79 – 4.71 (m, 1H), 4.68 – 4.59 (m, 1H), 2.74 (q, J = 7.6 Hz, 2H), 1.53 (d, J = 1.6 Hz, 3H), 1.31 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, CDCl3) δ (ppm): 177.0 (d, $^{3}J_{C\text{-}F}$ = 5.8 Hz), 144.4, 143.7, 131.8, 130.9, 129.1, 128.4, 126.5, 123.5, 123.1, 109.7, 87.4 (d, $^{1}J_{C\text{-}F}$ = 176.4 Hz), 49.5 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 28.6, 18.8 (d, $^{3}J_{C\text{-}F}$ = 5.8 Hz) 15.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.55; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{18}H_{19}FNO$ 284.1451; found 284.1451.

1-cyclopentyl-3-(fluoromethyl)-3-methylindolin-2-one (4r). Pale yellow semi-liquid; Yield (115



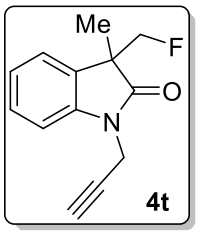
mg, 76%); The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.25 – 7.18 (m, 2H), 7.00 (td, J = 7.6, 1.2 Hz, 1H), 6.89 (dt, J = 8.0, 0.8 Hz, 1H), 4.71 (p, J = 8.8 Hz, 1H), 4.53 (s, 1H), 4.41 (s, 1H), 2.06 – 1.97 (m, 2H), 1.90 – 1.81 (m, 4H), 1.69 – 1.60 (m, 2H), 1.31 (d, J = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 176.3, 141.0, 130.6, 127.1, 122.5, 121.2, 108.9, 86.4 (d, $^{1}J_{C\text{-}F}$ = 176.4 Hz), 51.4, 48.1 (d, $^{2}J_{C\text{-}F}$ = 6.2 Hz), 26.7, 26.7, 24.2, 17.6 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -224.19; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{15}H_{19}FNO$ 248.1451; found 248.1451.

1-allyl-3-(fluoromethyl)-3-methylindolin-2-one (4s). Brown gummy; Yield (118 mg, 78%); The



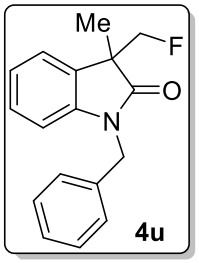
title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.22 – 7.15 (m, 2H), 6.99 (td, J = 7.6, 1.2 Hz, 1H), 6.76 (dt, J = 8.0, 0.8 Hz, 1H), 5.78 – 5.68 (m, 1H), 5.12 – 5.05 (m, 2H), 4.59 – 4.52 (m, 1H), 4.47 – 4.41 (m, 1H), 4.32 – 4.20 (m, 2H), 1.31 (d, J = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 177.3 (d, $^{3}J_{C\text{-}F}$ = 5.5 Hz), 142.7, 131.1, 131.0, 128.5, 123.2, 122.7, 117.3, 109.2, 87.2 (d, $^{1}J_{C\text{-}F}$ = 176.1 Hz), 49.4 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 42.2, 18.6 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.24; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{13}H_{15}FNO$ 220.1138; found 220.1139.

3-(fluoromethyl)-3-methyl-1-(prop-2-yn-1-yl)indolin-2-one (4t). Brown gummy; Yield (122 mg,



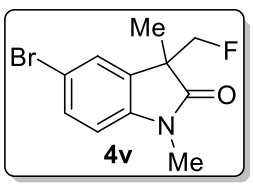
81%); The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, CDCl3) δ (ppm): 7.30 – 7.23 (m, 2H), 7.09 – 7.01 (m, 2H), 4.57 – 4.37 (m, 4H), 2.17 (t, J = 2.4 Hz, 1H), 1.34 (d, J = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 175.5 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz), 140.5, 129.8, 127.5, 122.3, 122.2, 108.3, 86.0 (d, $^{1}J_{C\text{-}F}$ = 176.8 Hz), 71.4, 48.4 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 28.7, 28.3, 17.5 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.81; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{13}H_{13}FNO$ 218.0981; found 218.0975.

1-benzyl-3-(fluoromethyl)-3-methylindolin-2-one (4u). White solid; Yield (134 mg, 89%); mp: 75-



76 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.24 – 7.16 (m, 6H), 7.12 – 7.08 (m, 1H), 6.99 – 6.96 (m, 1H), 6.64 (d, J = 8.0 Hz, 1H), 4.95 – 4.76 (m, 2H), 4.66 – 4.59 (m, 1H), 4.54 – 4.46 (m, 1H), 1.36 (d, J = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 176.6 (d, $^{3}J_{C\text{-}F}$ = 5.4 Hz), 141.5, 134.6, 129.9, 127.8, 127.4, 126.6, 126.0, 122.1, 121.8, 108.3, 86.2 (d, $^{1}J_{C\text{-}F}$ = 176.4 Hz), 48.4 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 42.7, 17.6 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -222.70; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{17}H_{17}FNO$ 270.1294; found 270.1292.

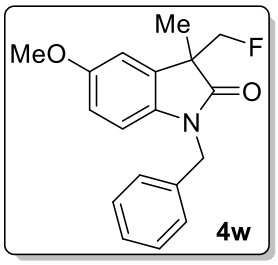
5-bromo-3-(fluoromethyl)-1,3-dimethylindolin-2-one (4v). Off-white solid; Yield (135 mg, 90%);



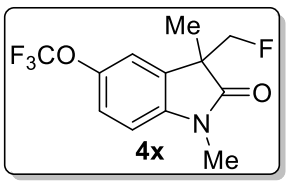
mp: 95-96 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.39 – 7.34 (m, 2H), 6.68 (d, J = 8.0 Hz, 1H), 4.56 – 4.51 (m, 1H), 4.43 – 4.39 (m, 1H), 3.14 (s, 3H), 1.32 (d, J = 1.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm): 176.8 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz), 142.5, 133.1, 131.4, 126.6, 115.5, 109.7, 86.9 (d, $^{1}J_{C\text{-}F}$ = 176.8 Hz),

49.6 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 26.5, 18.4 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.57; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{11}H_{12}BrFNO$ 272.0086; found 272.0085.

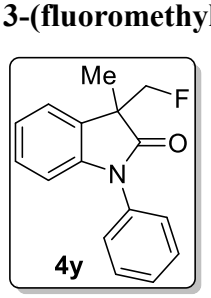
1-benzyl-3-(fluoromethyl)-5-methoxy-3-methylindolin-2-one (4w). White solid; Yield (137 mg, 91%); mp: 64-65 °C; The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.22 – 7.13 (m, 5H), 6.86 – 6.81 (m, 1H), 6.62 – 6.50 (m, 2H), 4.92 – 4.73 (m, 2H), 4.64 – 4.46 (m, 2H), 3.66 (d, *J* = 5.6 Hz, 3H), 1.35 (d, *J* = 4.0 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ (ppm): 177.3 (d, $^{3}J_{C\text{-}F}$ = 5.9 Hz), 156.2, 135.9, 135.7, 132.4, 128.8, 127.6, 127.1, 112.7, 110.9, 109.8, 87.3 (d, $^{1}J_{C\text{-}F}$ = 176 Hz), 55.8, 49.9 (d, $^{2}J_{C\text{-}F}$ = 19.4 Hz), 43.8, 18.7 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -223.06; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{18}H_{19}FNO_2$ 300.1400; found 300.1400.



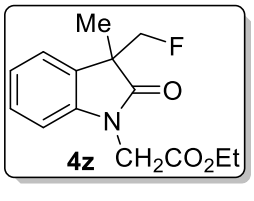
3-(fluoromethyl)-1,3-dimethyl-5-(trifluoromethoxy)indolin-2-one (4x). Pale yellow semi-liquid; Yield (143 mg, 95%); The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.13 (d, *J* = 8.0 Hz, 2H), 6.78 (d, *J* = 8.8 Hz, 1H), 4.55 (s, 1H), 4.43 (s, 1H), 3.16 (s, 3H), 1.34 (d, *J* = 1.6 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ (ppm): 176.1, 143.9, 141.1, 131.5, 120.6, 116.4, 107.7, 85.8 (d, $^{1}J_{C\text{-}F}$ = 177.2 Hz), 48.8 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 25.5, 17.4 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -58.32, -223.95; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{12}H_{12}F_4NO$ 278.0804; found 278.0804.



3-(fluoromethyl)-3-methyl-1-phenylindolin-2-one (4y). Pale yellow liquid; Yield (125 mg, 83%); The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.46 – 7.42 (m, 2H), 7.35 – 7.27 (m, 4H), 7.18 – 7.14 (m, 1H), 7.05 (td, *J* = 7.4, 0.8 Hz, 1H), 6.77 (dt, *J* = 7.6, 1.2 Hz, 1H), 4.69 – 4.61 (m, 1H), 4.57 – 4.49 (m, 1H), 1.42 (d, *J* = 1.6 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ (ppm): 177.0 (d, $^{3}J_{C\text{-}F}$ = 5.8 Hz), 143.5, 134.3, 130.8, 129.6, 128.5, 128.2, 126.6, 123.5, 123.2, 109.6, 87.4 (d, $^{1}J_{C\text{-}F}$ = 176.5 Hz), 49.6 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz), 18.8 (d, $^{3}J_{C\text{-}F}$ = 6.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -222.74; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{16}H_{15}FNO$ 256.1138; found 256.1139.

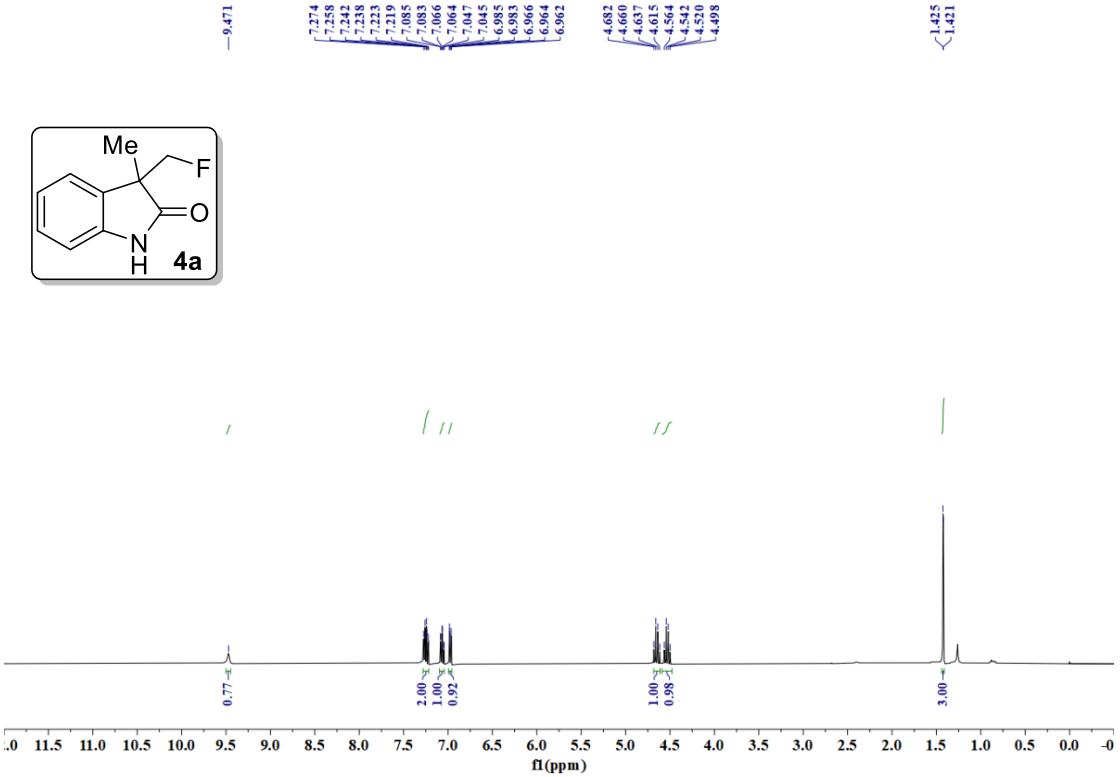


ethyl 2-(3-(fluoromethyl)-3-methyl-2-oxoindolin-1-yl)acetate (4z). Pale yellow semi-liquid; Yield (122 mg, 81%); The title compound is prepared according to the general procedure described as above; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.26 – 7.19 (m, 2H), 7.07 – 7.02 (m, 1H), 6.69 (d, *J* = 7.6 Hz, 1H), 4.58 – 4.32 (m, 4H), 4.13 (q, *J* = 7.2 Hz, 2H), 1.38 (d, *J* = 1.6 Hz, 3H), 1.19 – 1.15 (m, 3H);

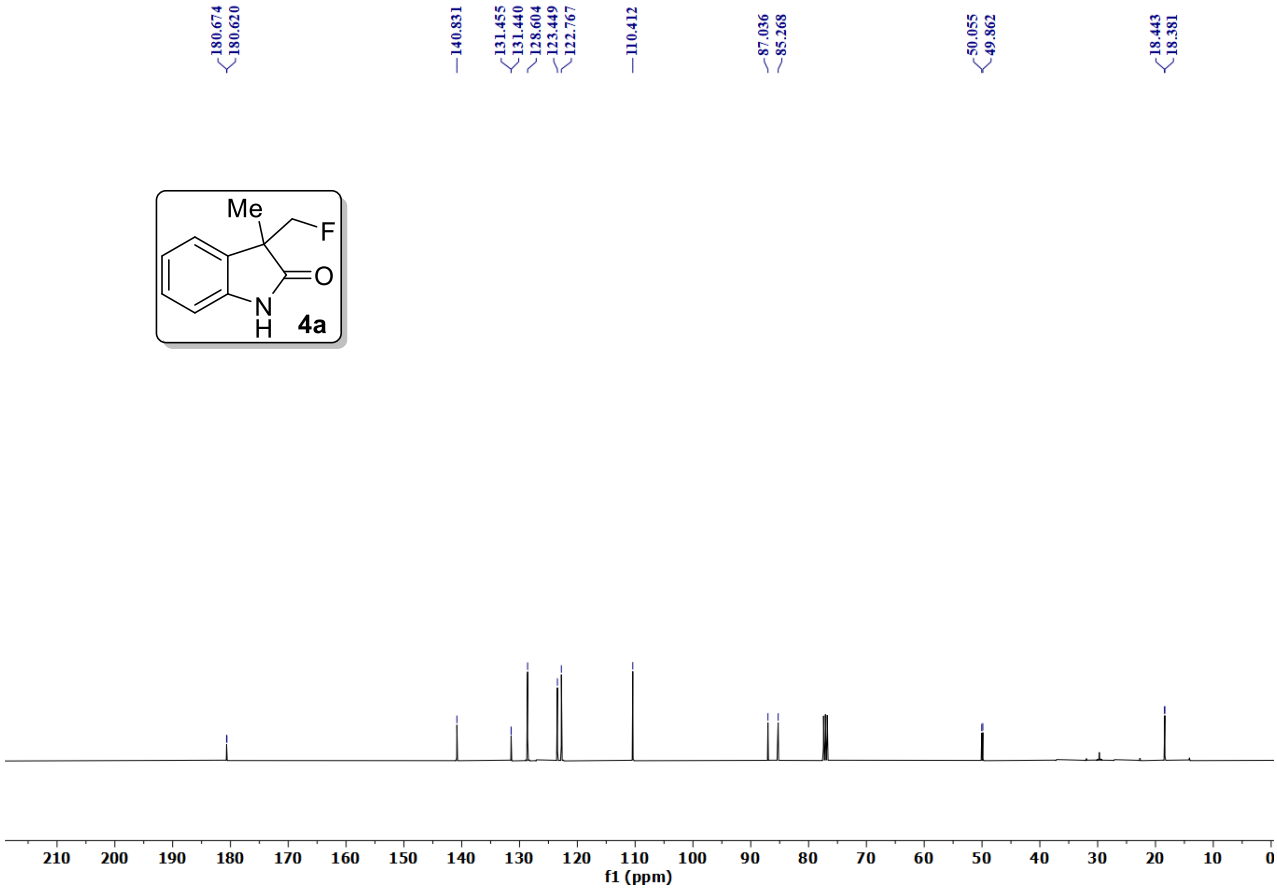


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ (ppm): 177.5, 167.4, 142.1, 130.8, 128.6, 123.5, 123.1, 108.3, 87.0 (d, $^{1}J_{C\text{-}F}$ = 176.8 Hz), 61.8, 49.4 (d, $^{2}J_{C\text{-}F}$ = 19.3 Hz) 41.4, 18.7 (d, $^{3}J_{C\text{-}F}$ = 5.9 Hz), 14.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -224.01; HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{14}H_{17}FNO_3$ 266.1192; found 266.1191.

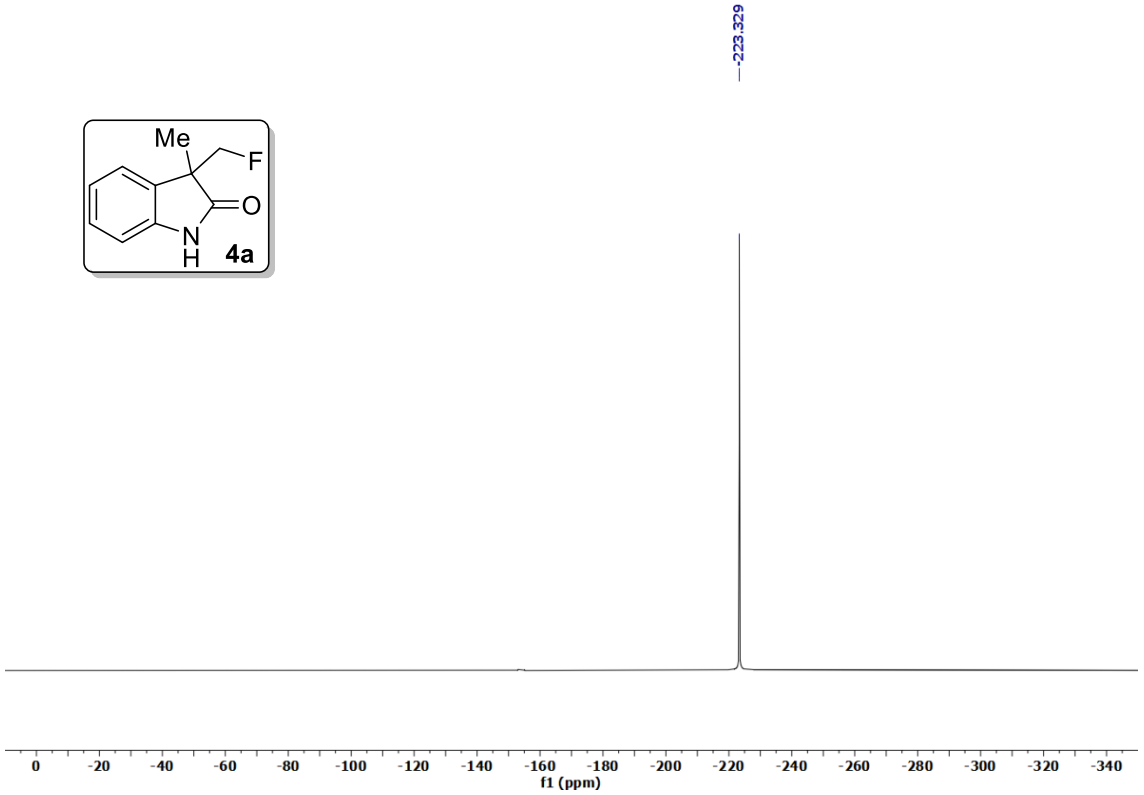
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methylindolin-2-one (4a)



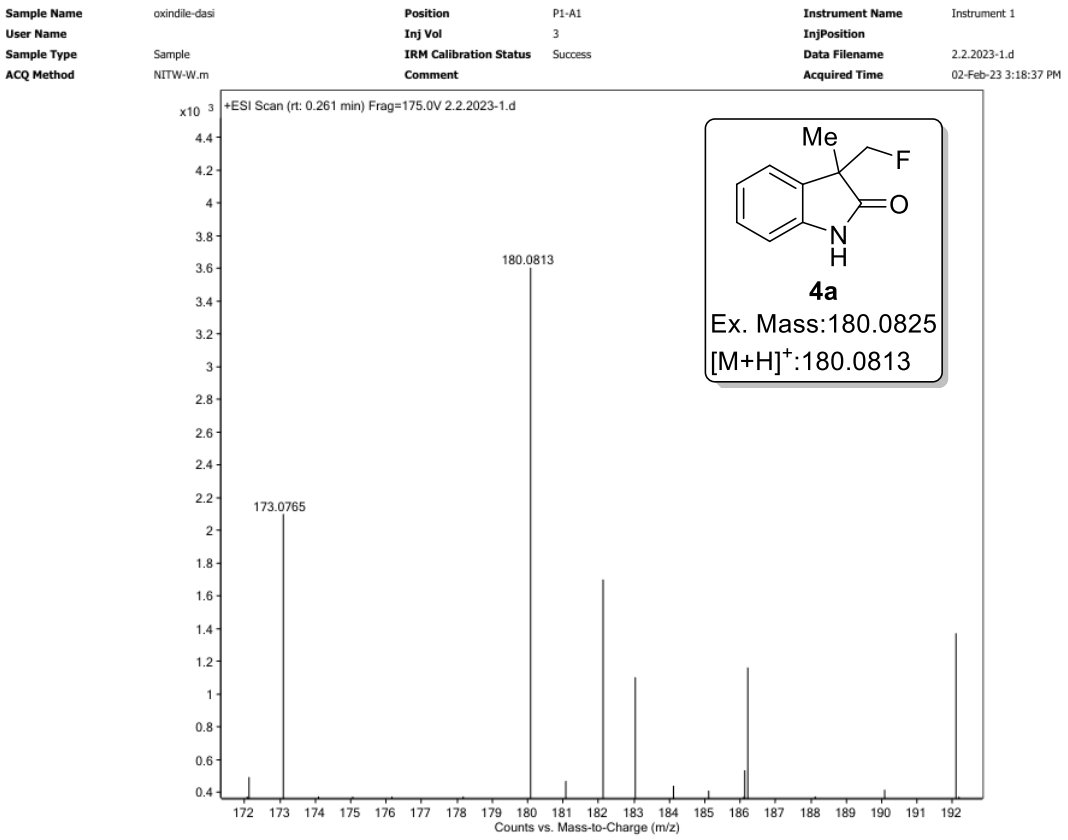
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methylindolin-2-one (4a)



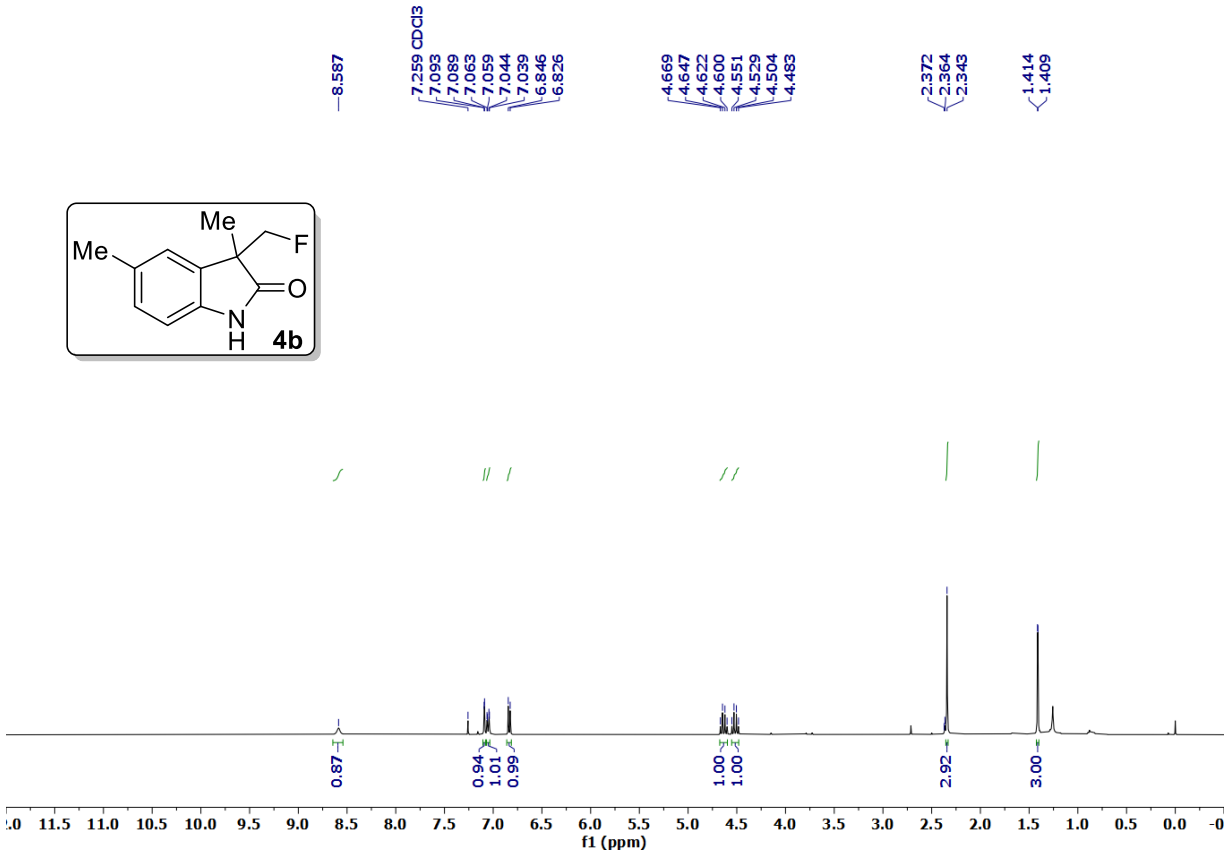
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methylindolin-2-one (4a)



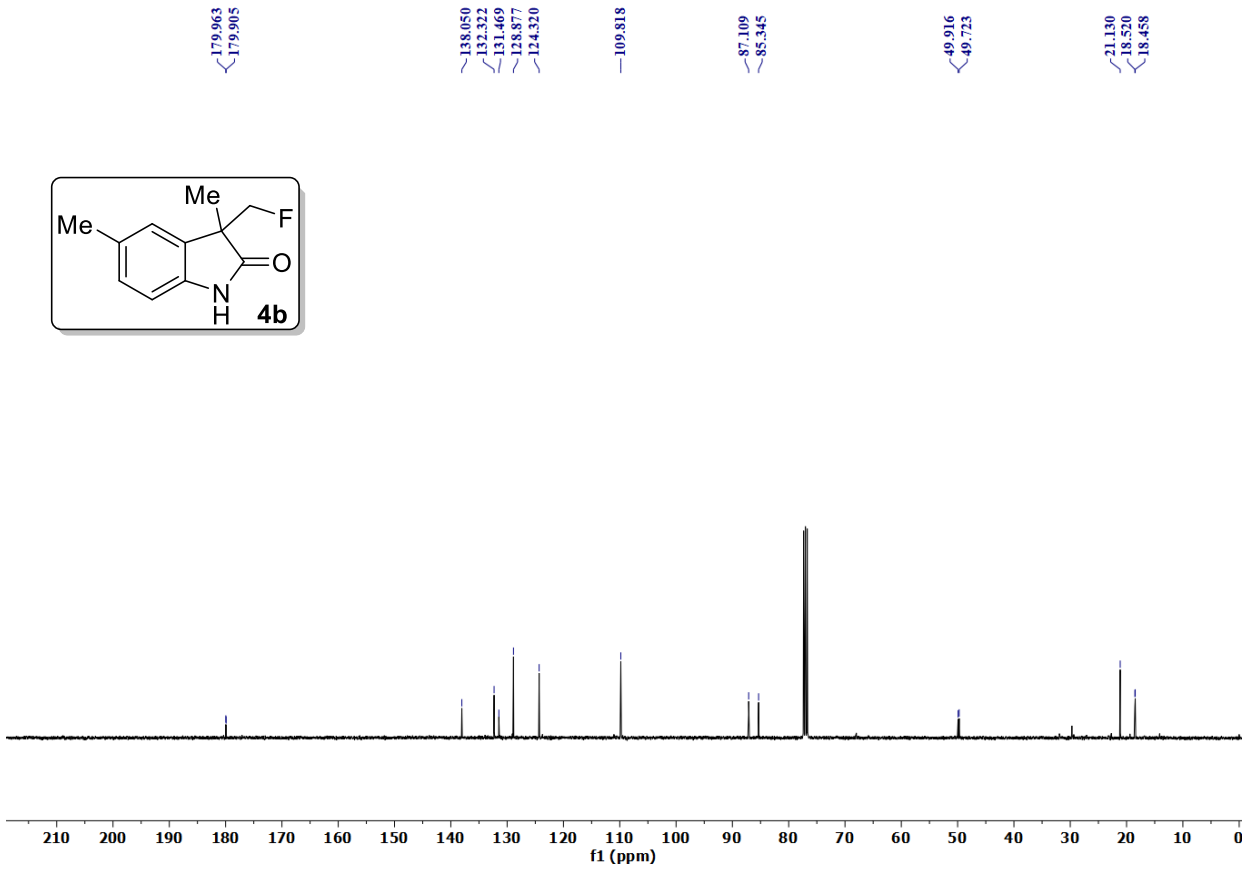
HRMS of 3-(fluoromethyl)-3-methylindolin-2-one (4a)



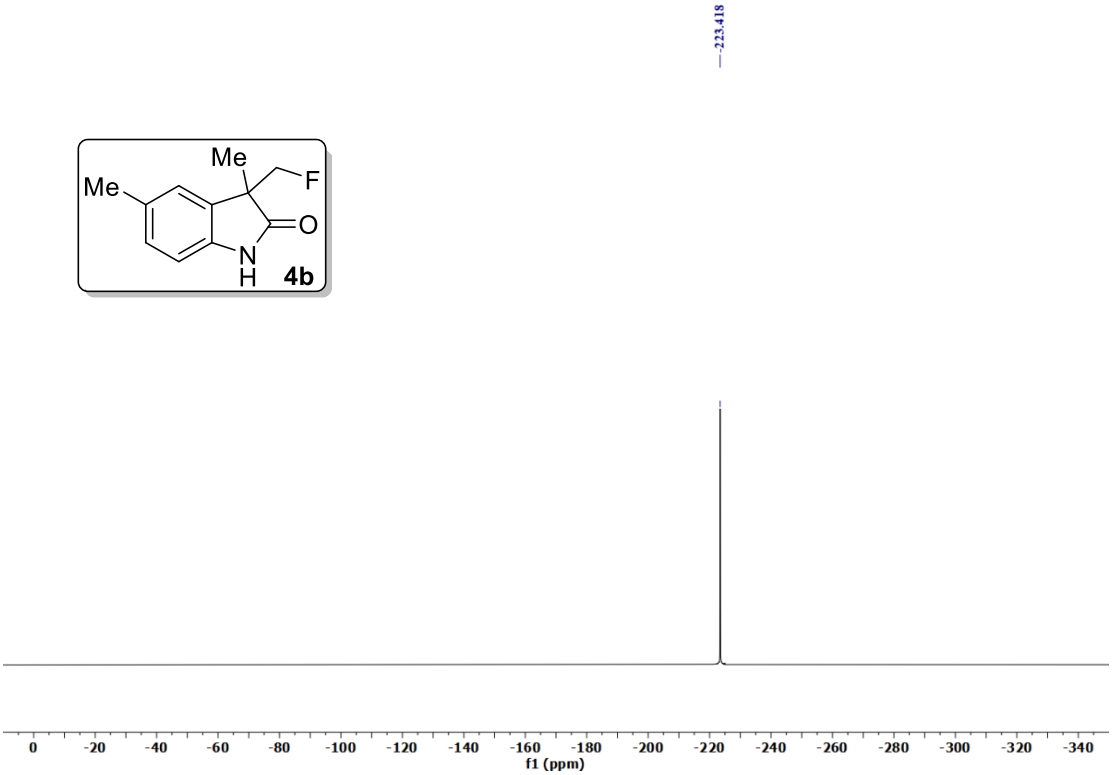
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3,5-dimethylindolin-2-one (4b)



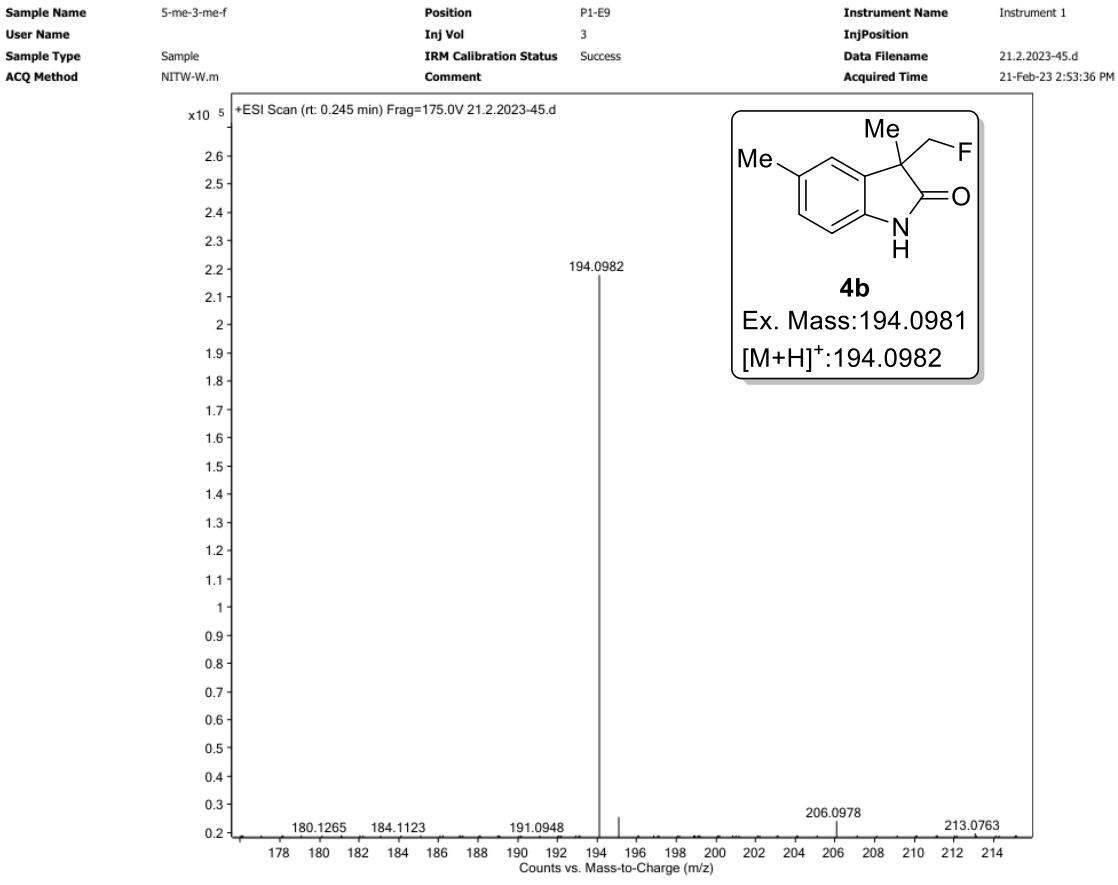
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3,5-dimethylindolin-2-one (4b)



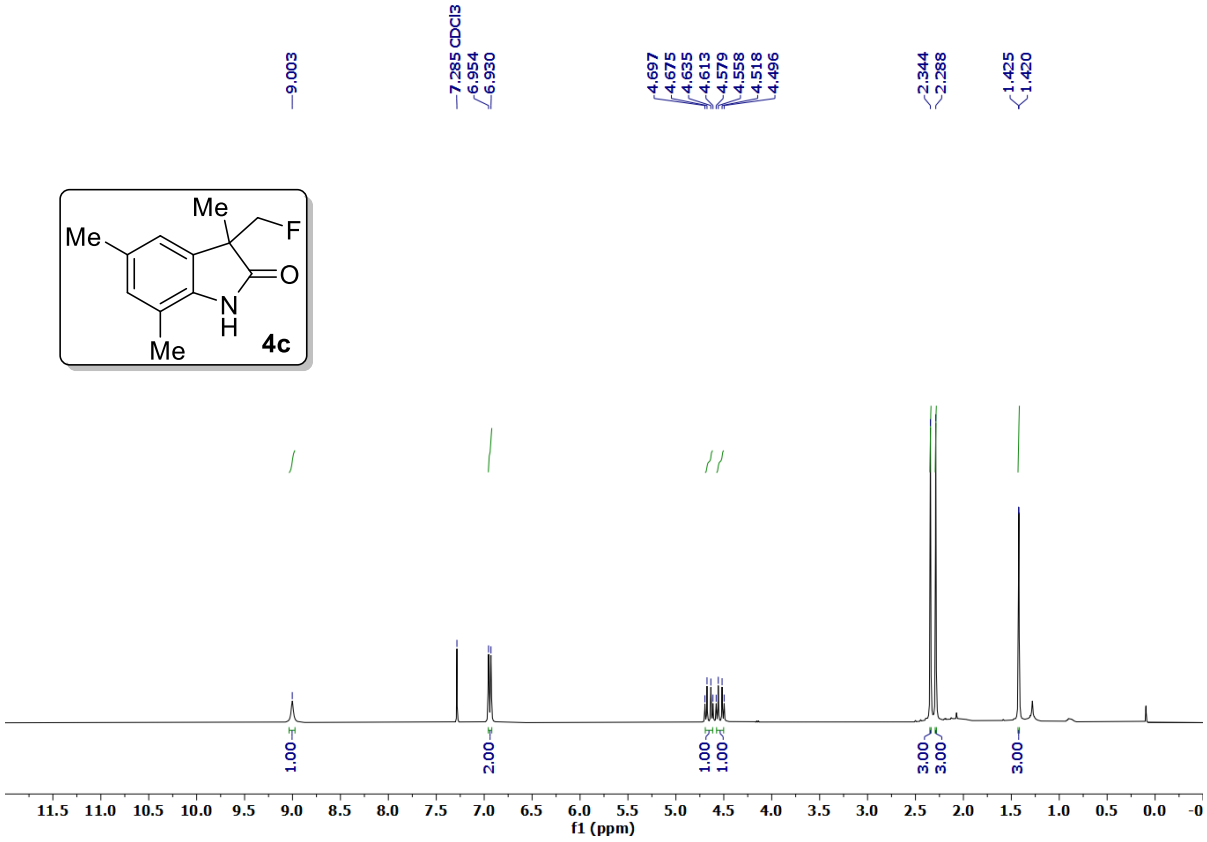
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3,5-dimethylindolin-2-one (4b)



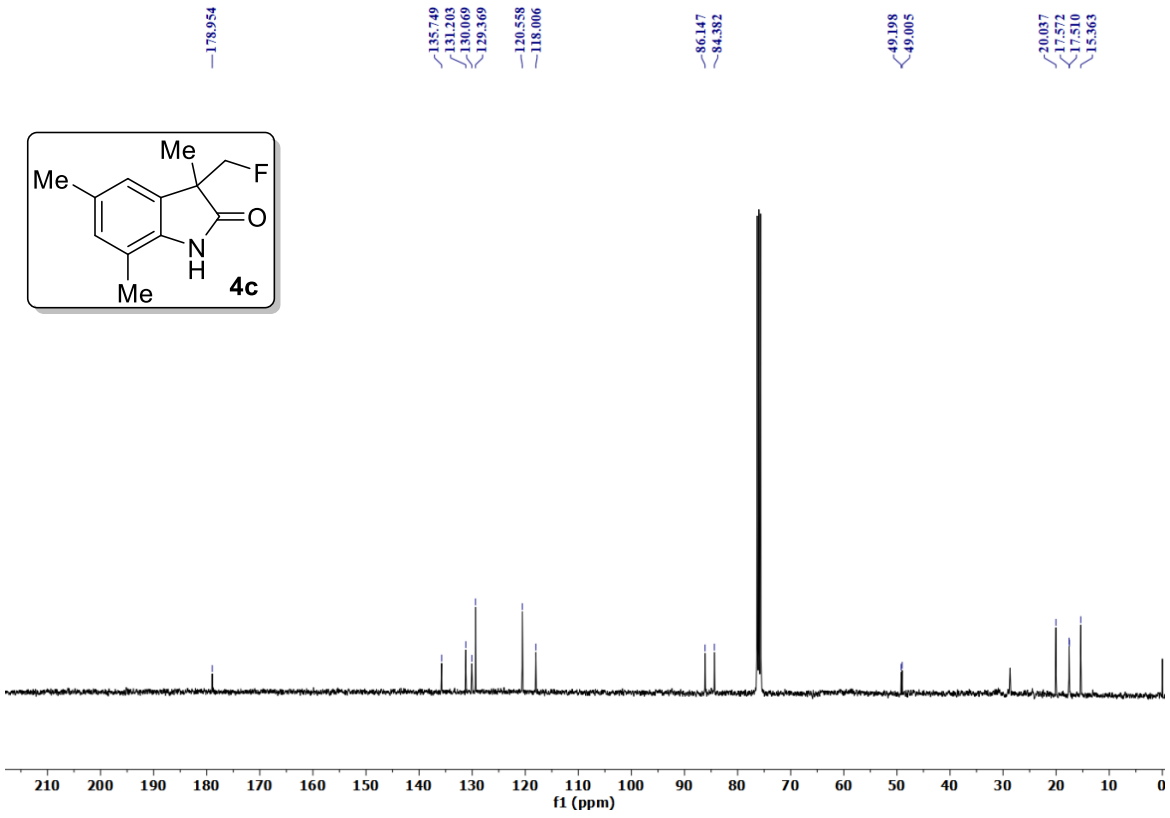
HRMS of 3-(fluoromethyl)-3,5-dimethylindolin-2-one (4b)



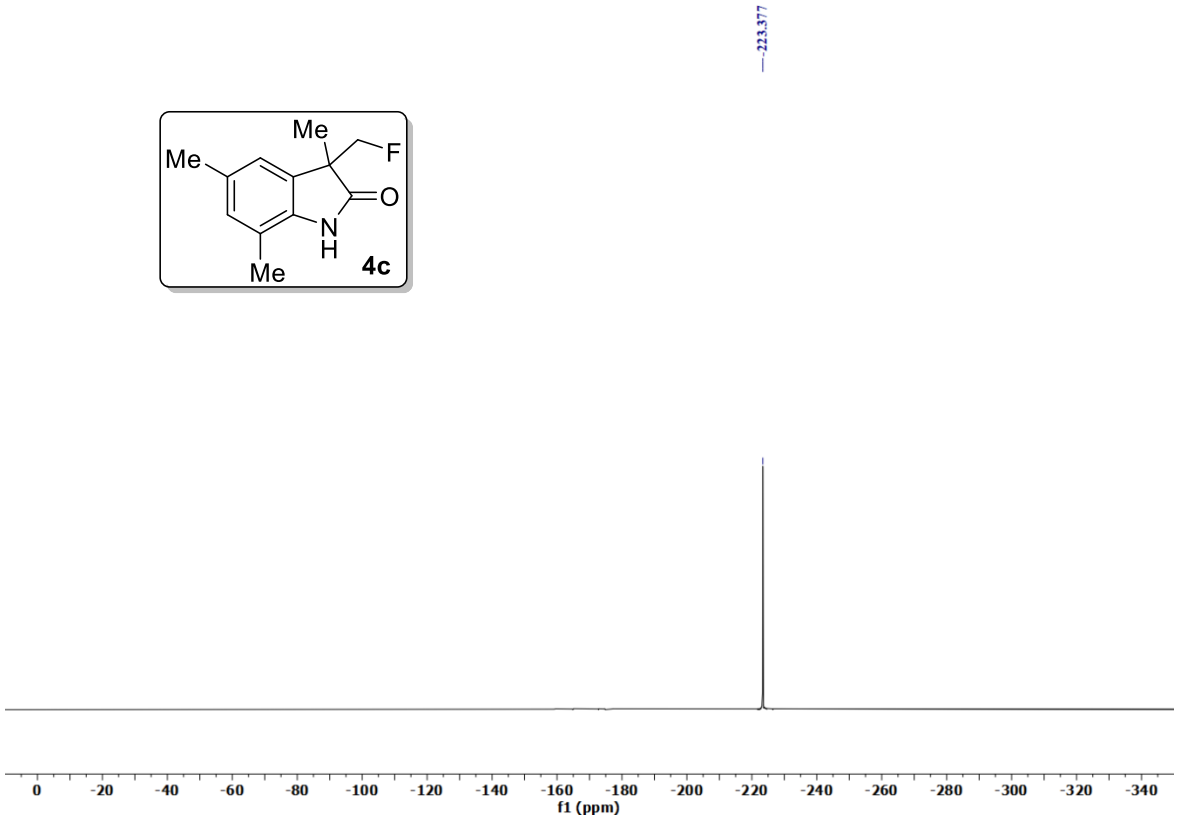
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3,5,7-trimethylindolin-2-one (4c)



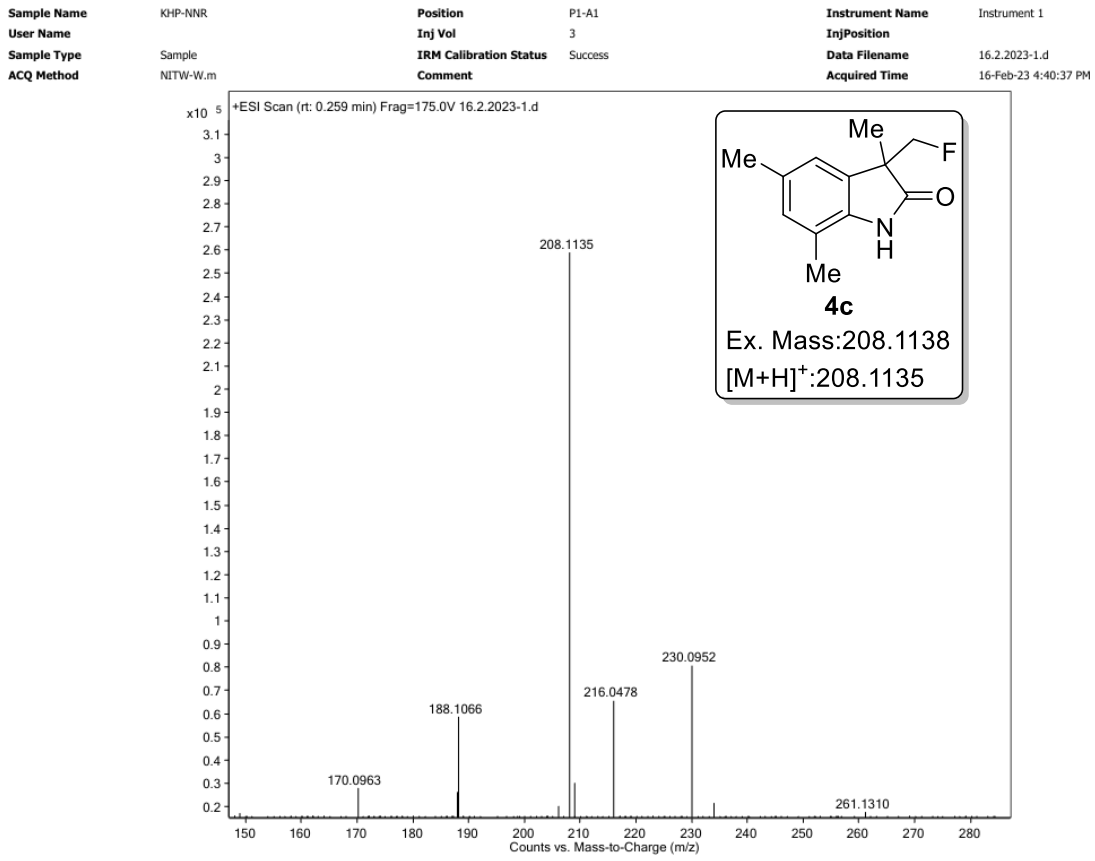
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3,5,7-trimethylindolin-2-one (4c)



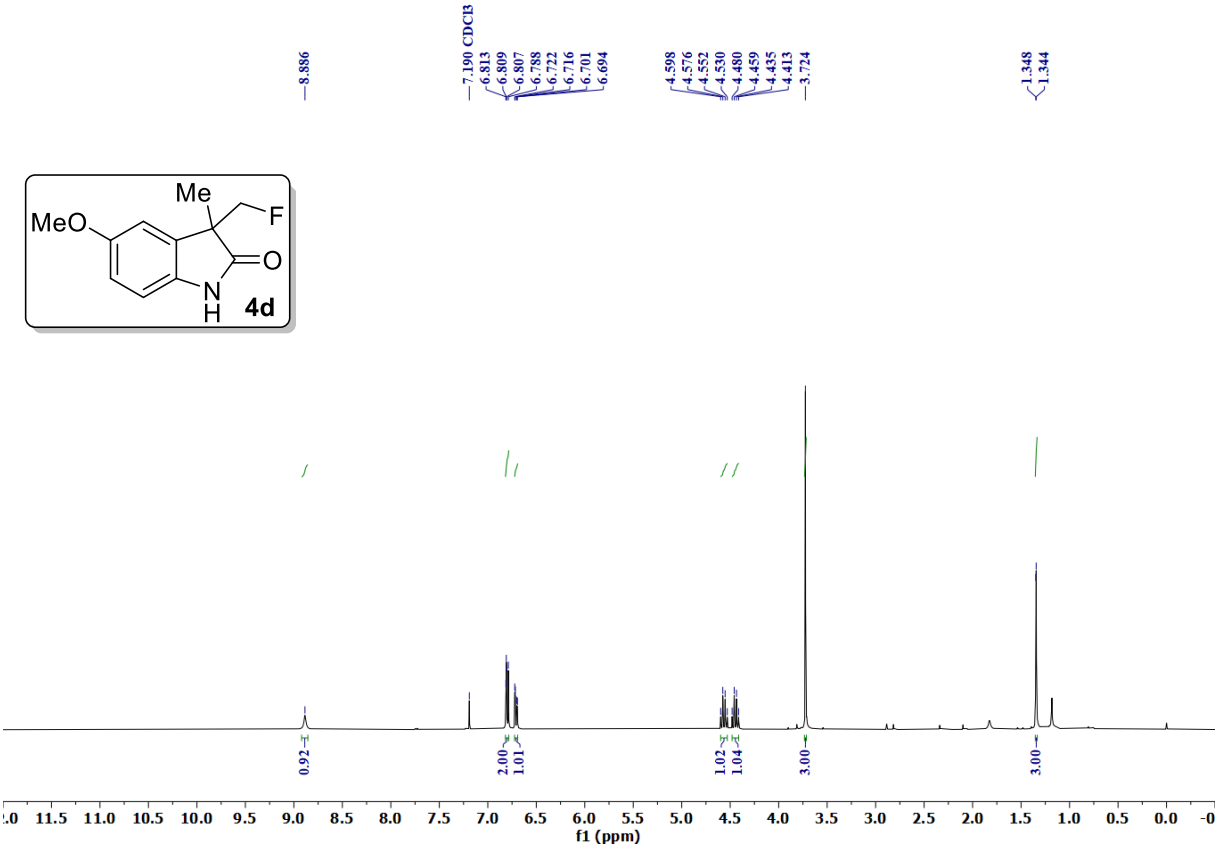
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3,5,7-trimethylindolin-2-one (4c)



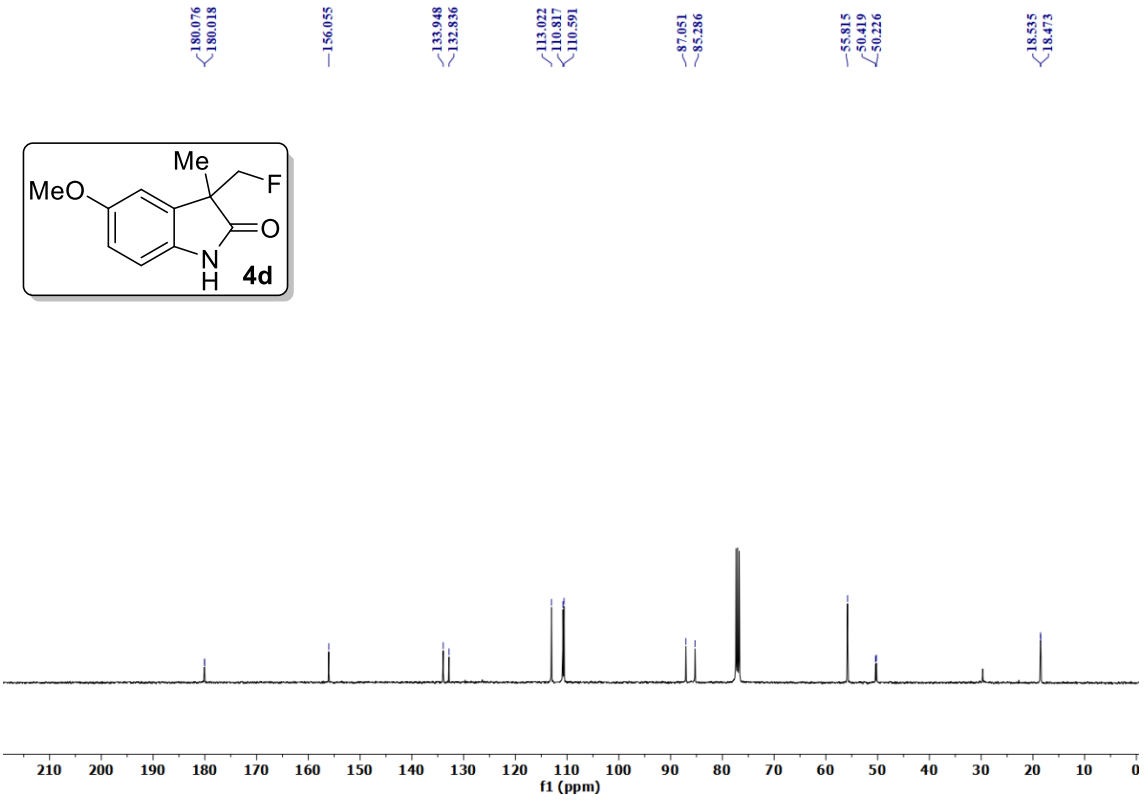
HRMS of 3-(fluoromethyl)-3,5,7-trimethylindolin-2-one (4c)



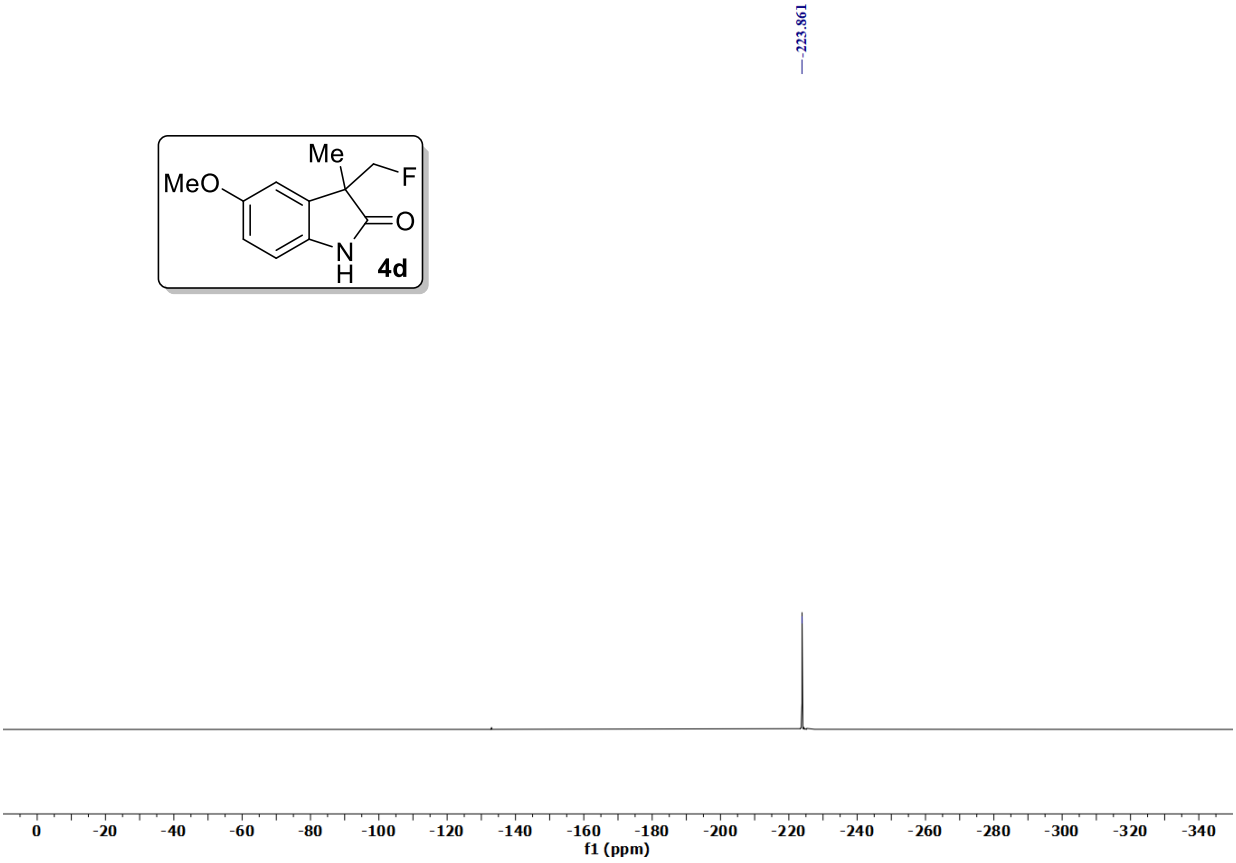
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-5-methoxy-3-methylindolin-2-one (4d)



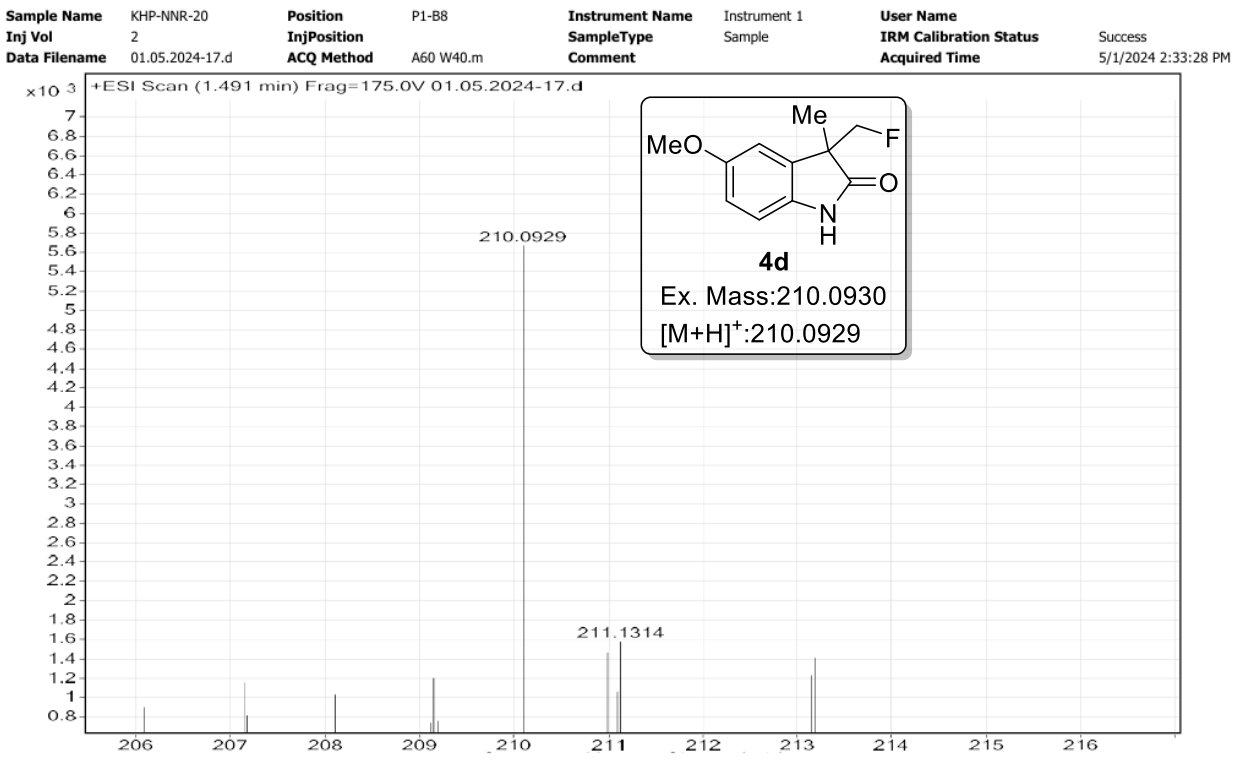
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-5-methoxy-3-methylindolin-2-one (4d)



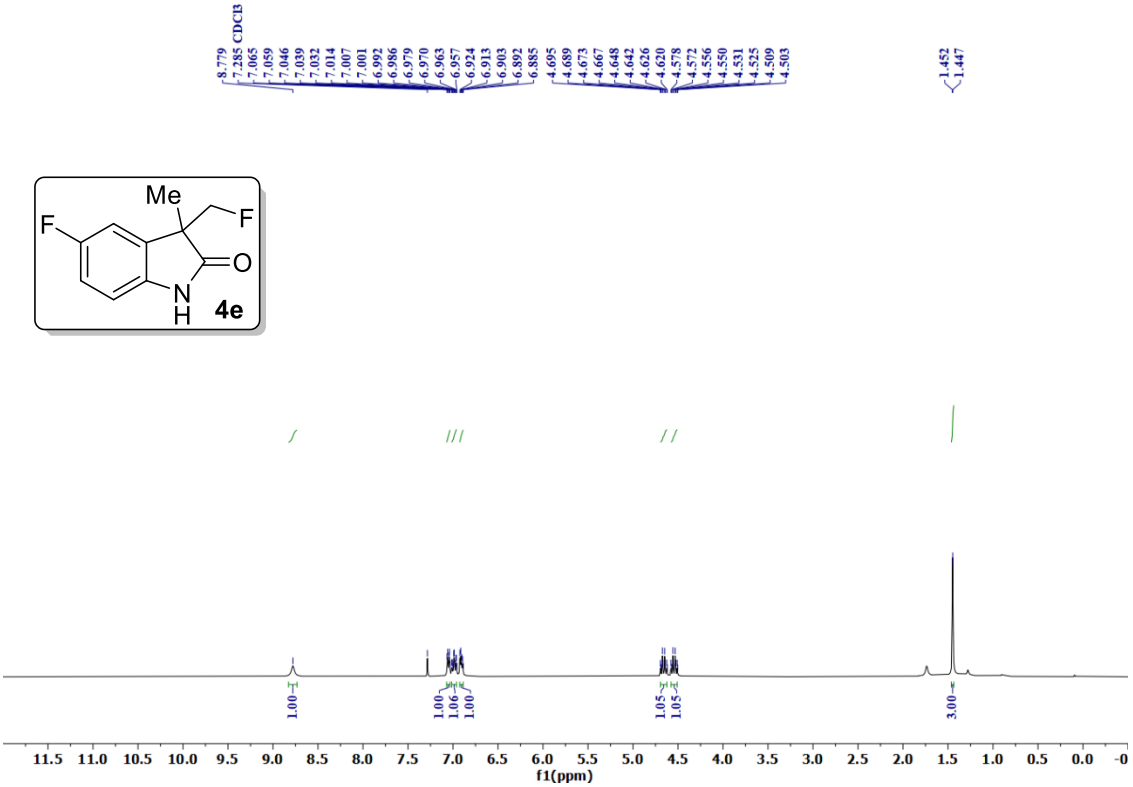
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-5-methoxy-3-methylindolin-2-one (4d)



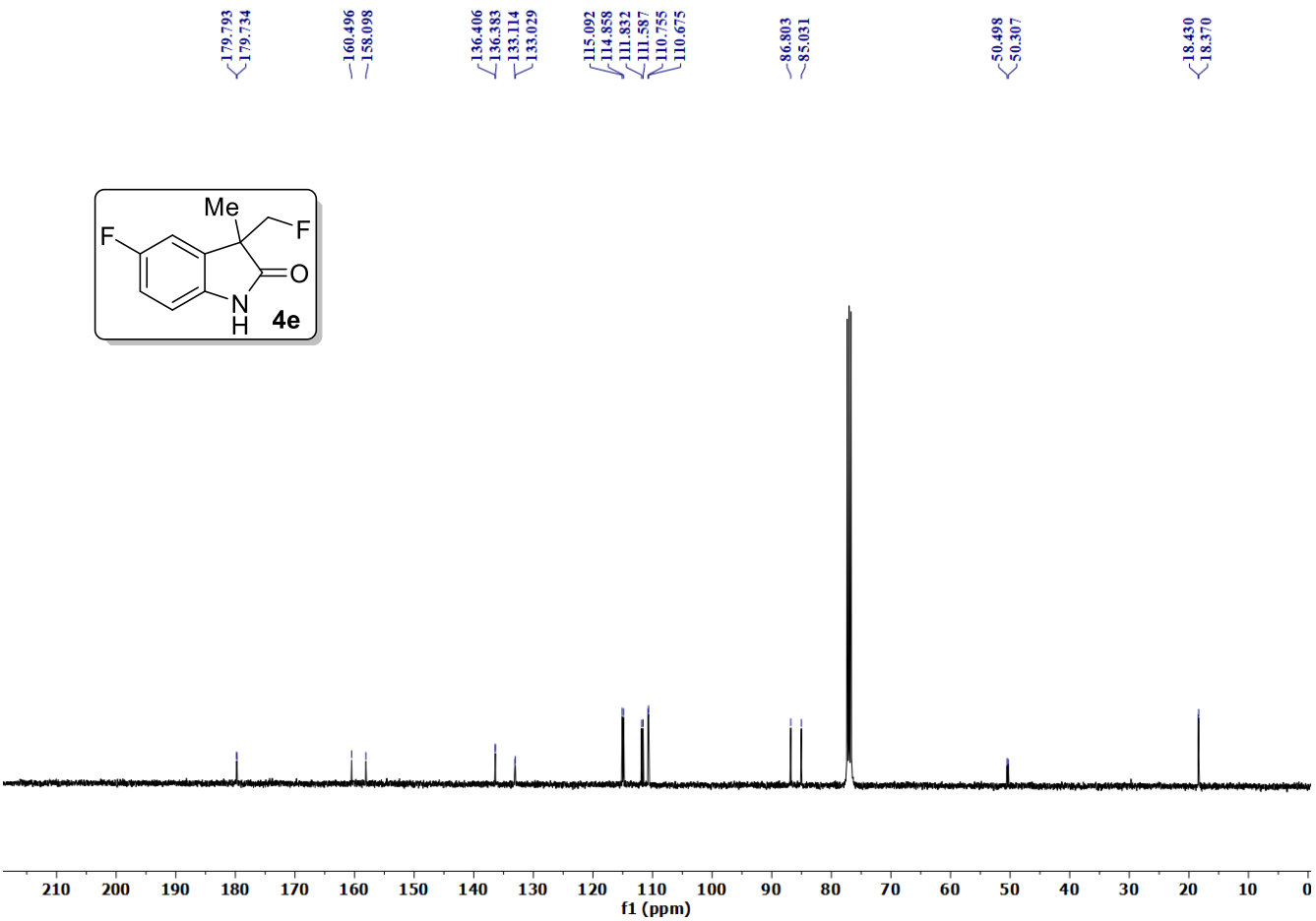
HRMS of 3-(fluoromethyl)-5-methoxy-3-methylindolin-2-one (4d)



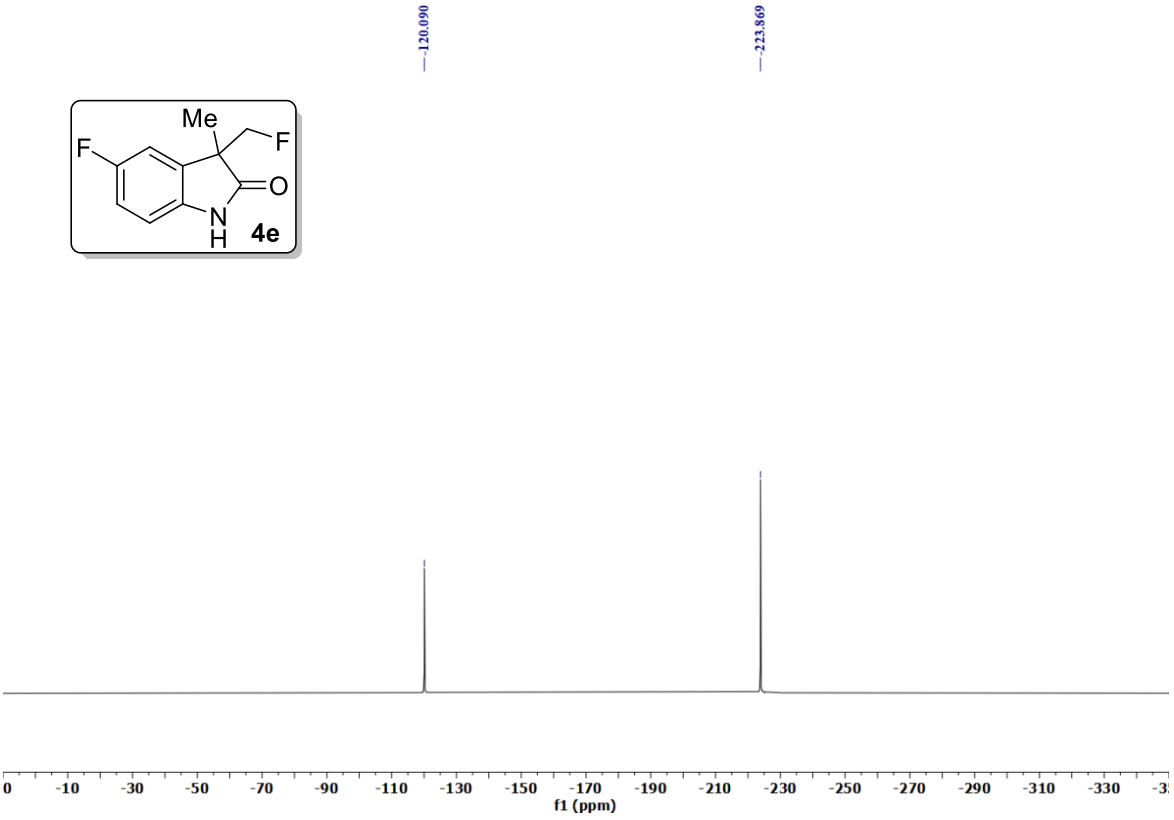
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5-fluoro-3-(fluoromethyl)-3-methylindolin-2-one (4e)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 5-fluoro-3-(fluoromethyl)-3-methylindolin-2-one (4e)

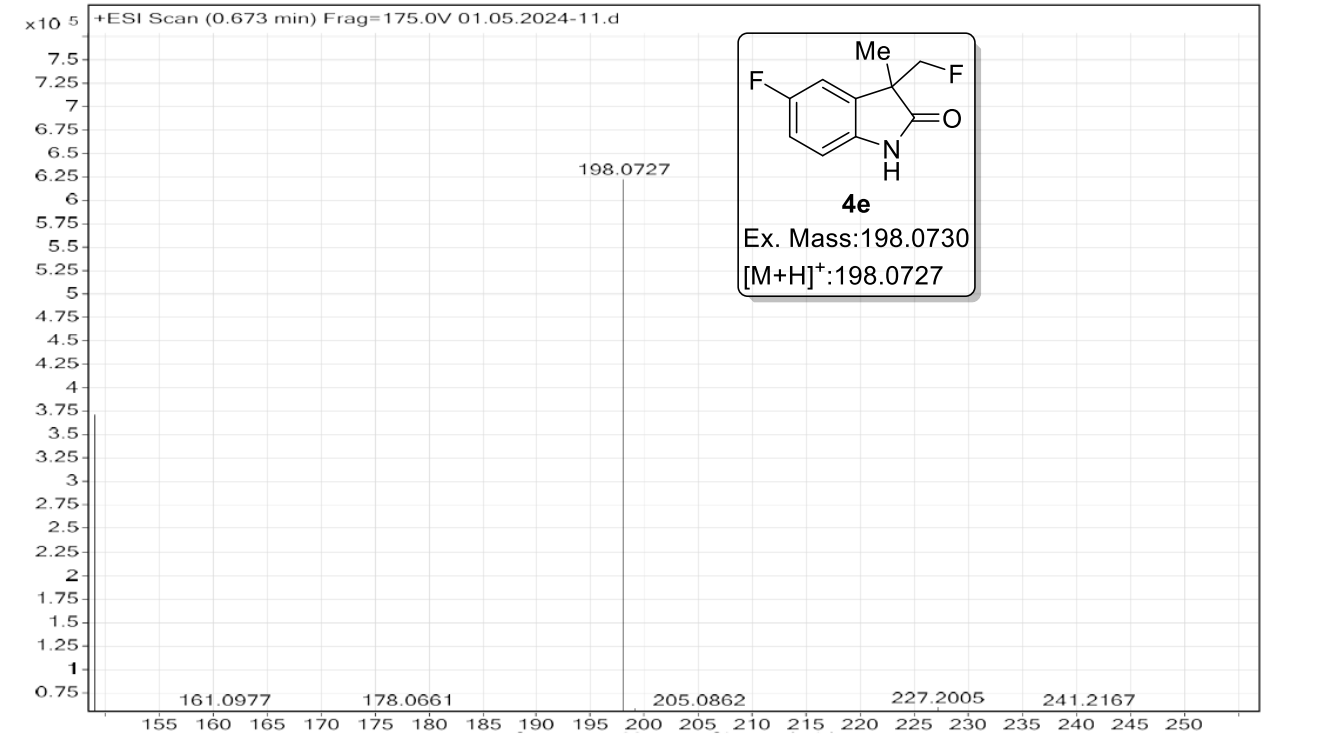


^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 5-fluoro-3-(fluoromethyl)-3-methylindolin-2-one (4e)

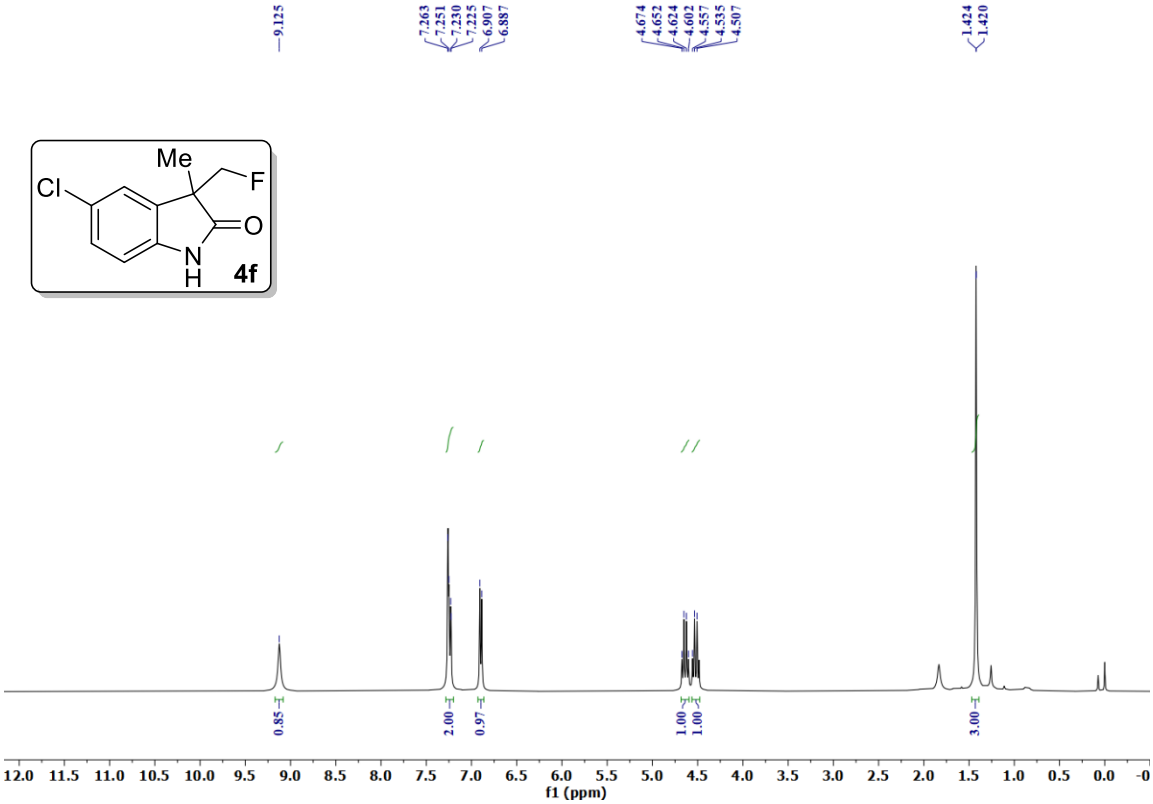


HRMS of 5-fluoro-3-(fluoromethyl)-3-methylindolin-2-one (4e)

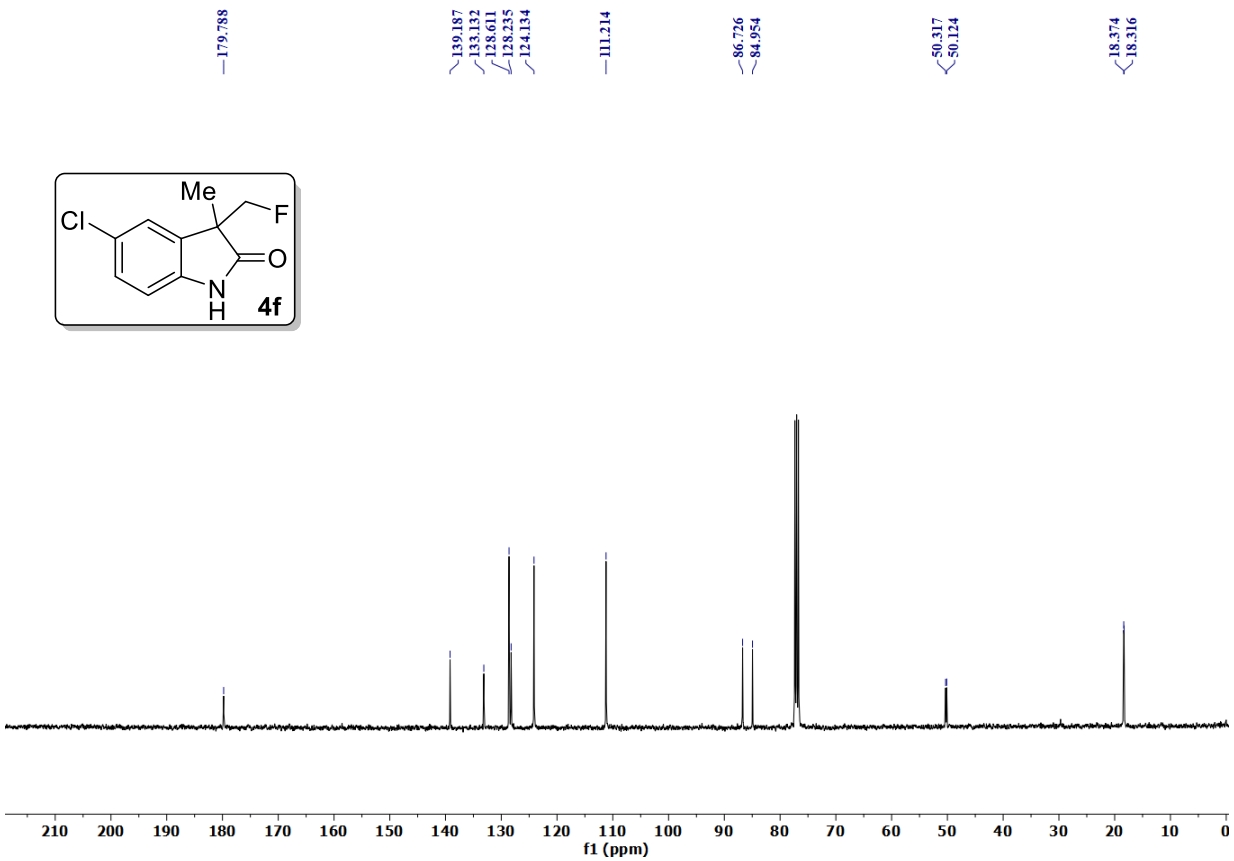
Sample Name	KHP-NNR-13	**Position**	P1-B2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	01.05.2024-11.d	**ACQ Method**	A60 W40.m	**Comment**		**Acquired Time**	5/1/2024 2:09:19 PM



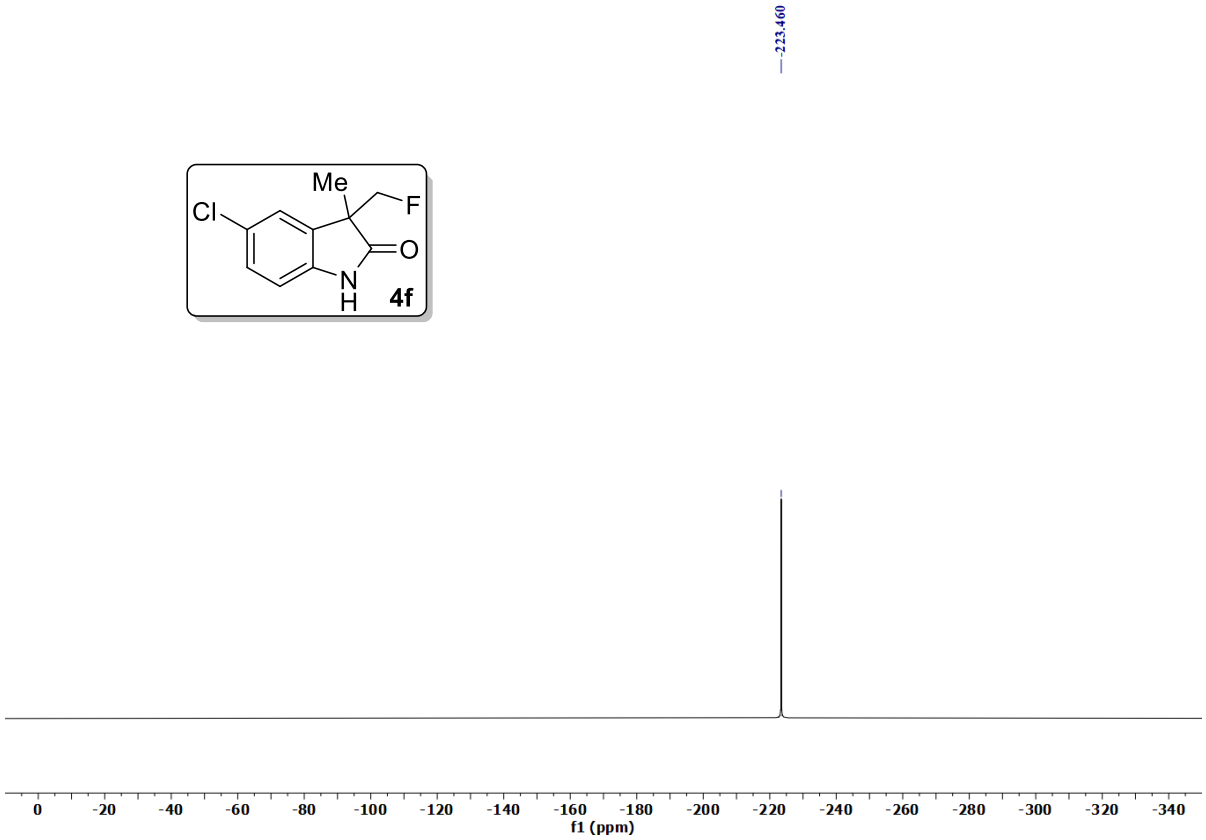
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4f)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 5-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4f)

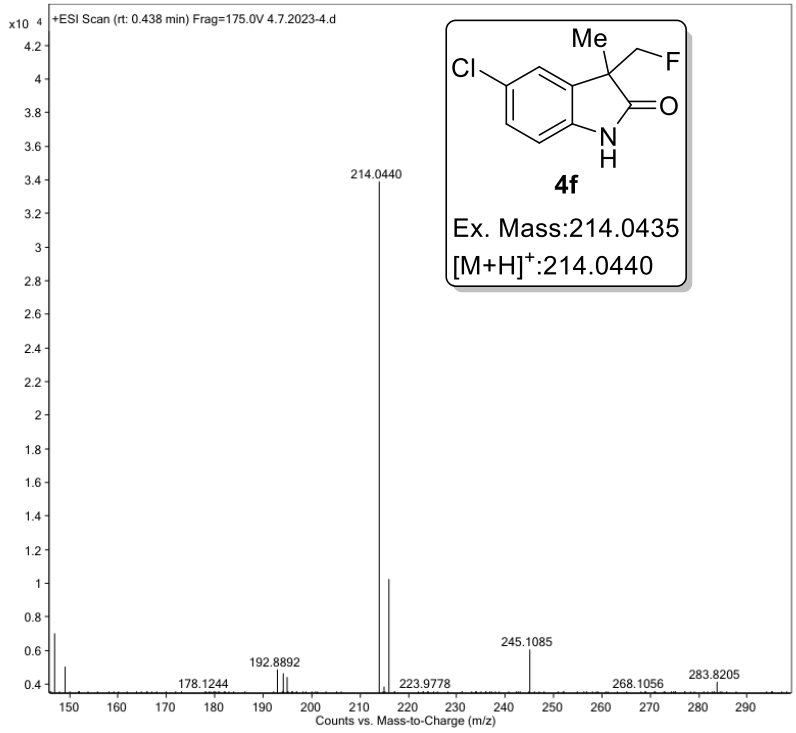


^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 5-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4f)

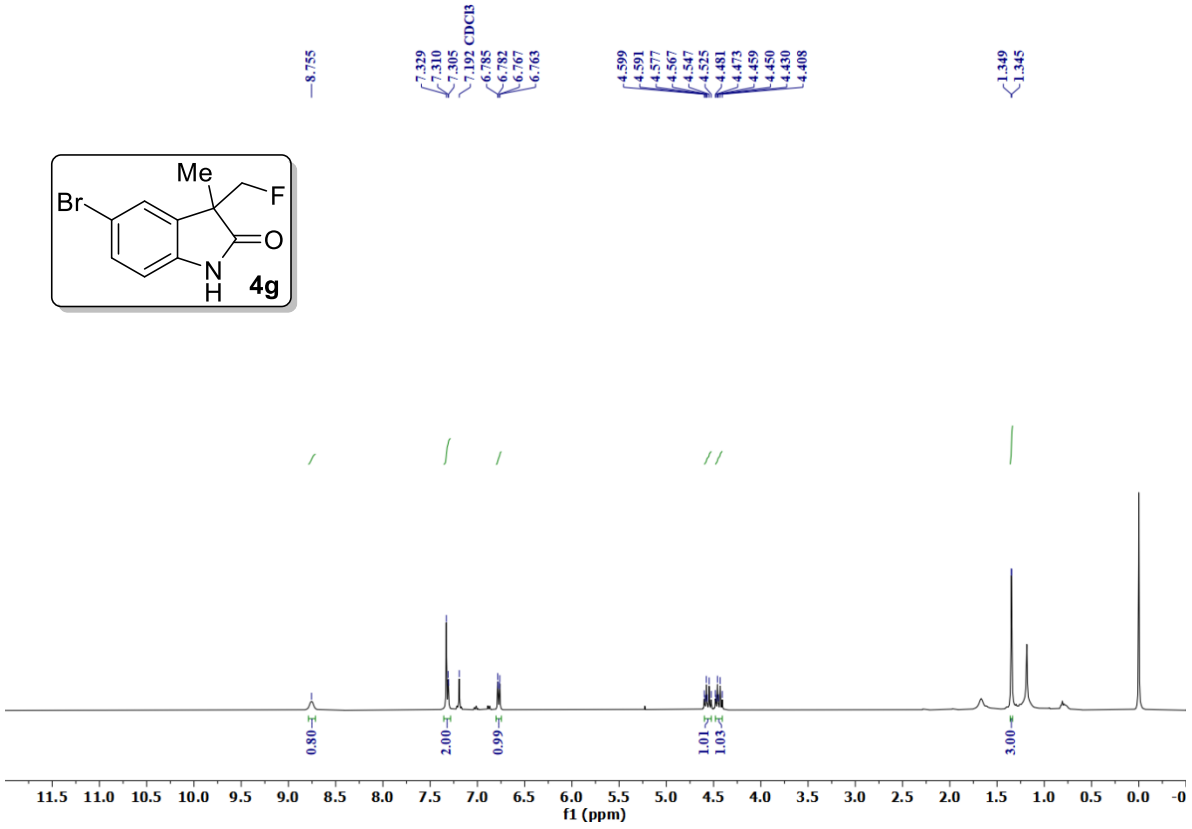


HRMS of 5-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4f)

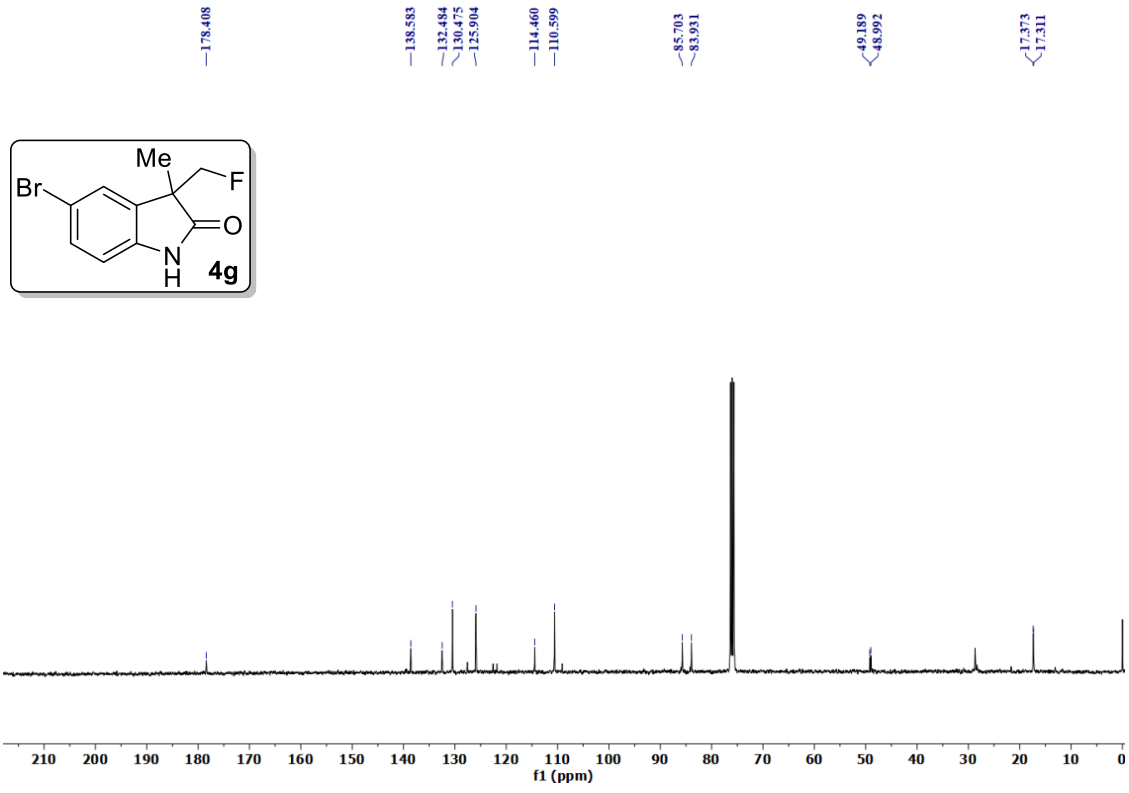
Sample Name	khp-nnr-- I-OXI0F-08	**Position**	P1-A4	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	4.7.2023-4.d
ACQ Method	HRMS-NITW.m	**Comment**		**Acquired Time**	04-Jul-23 4:20:38 PM



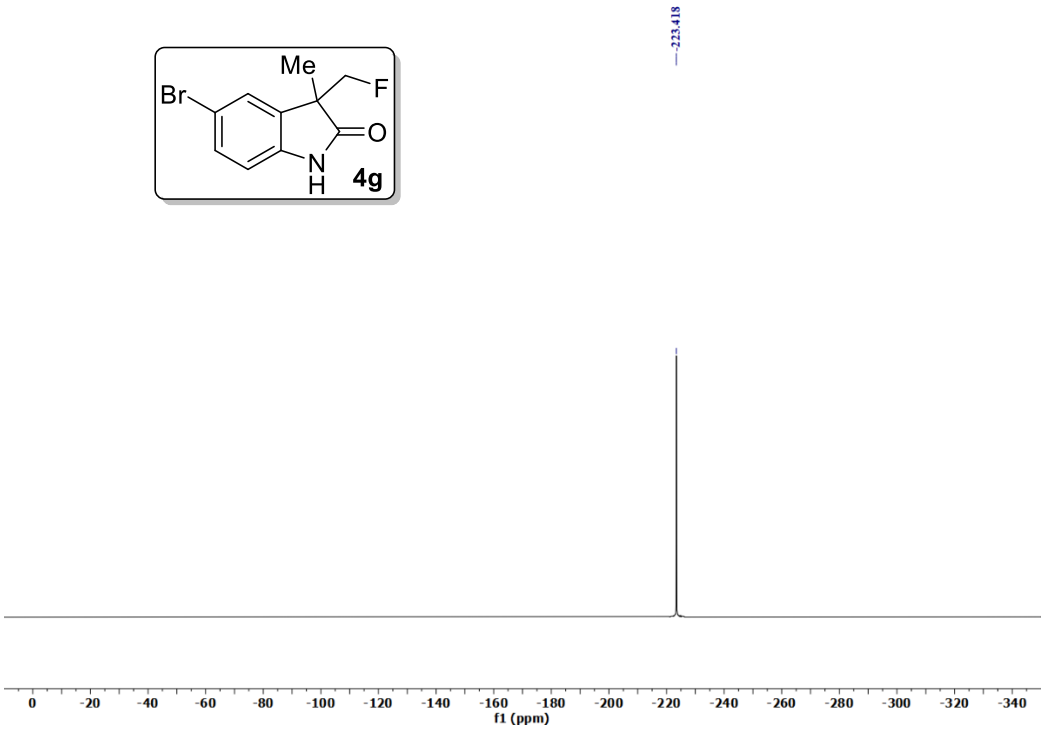
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5-bromo-3-(fluoromethyl)-3-methylindolin-2-one (4g)



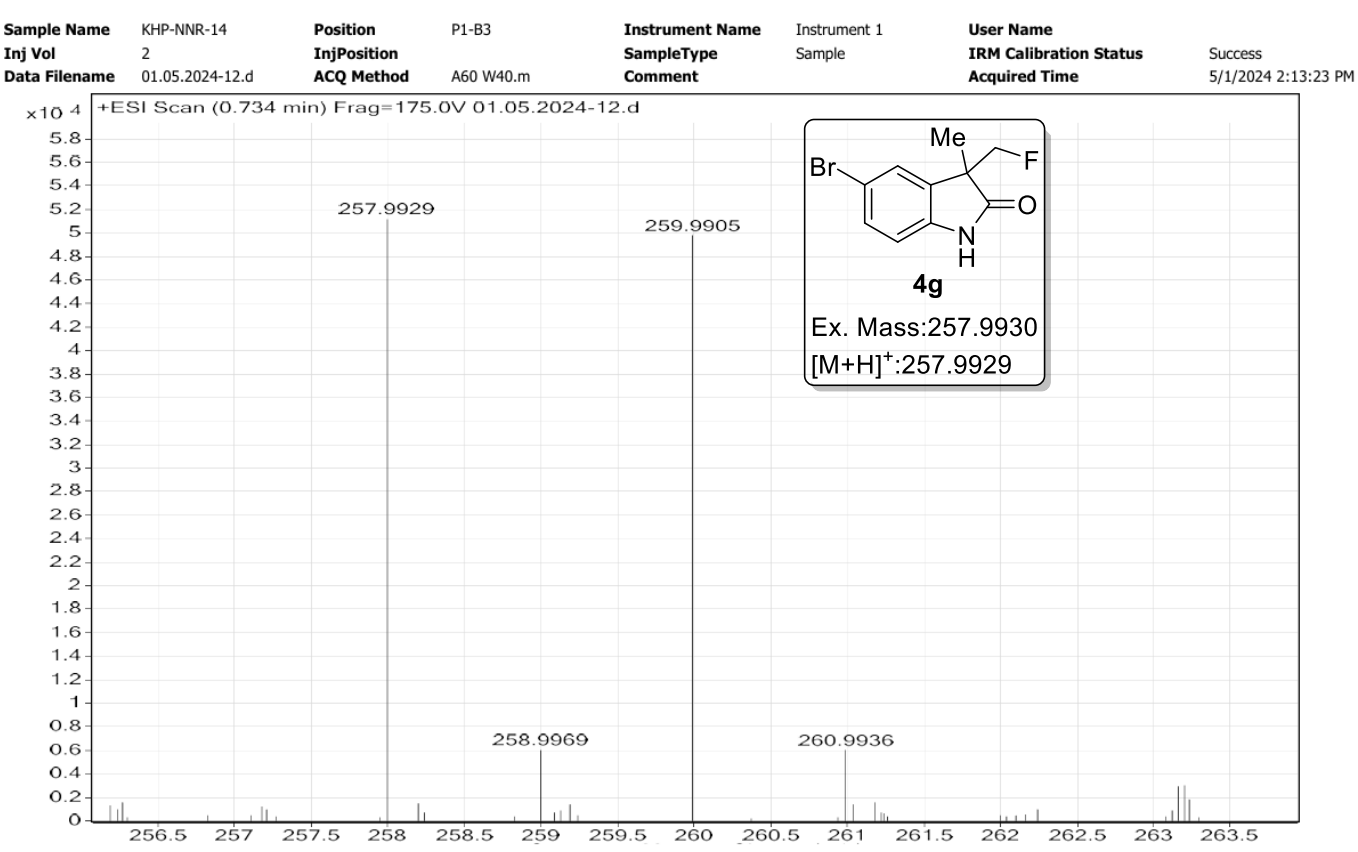
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 5-bromo-3-(fluoromethyl)-3-methylindolin-2-one (4g)



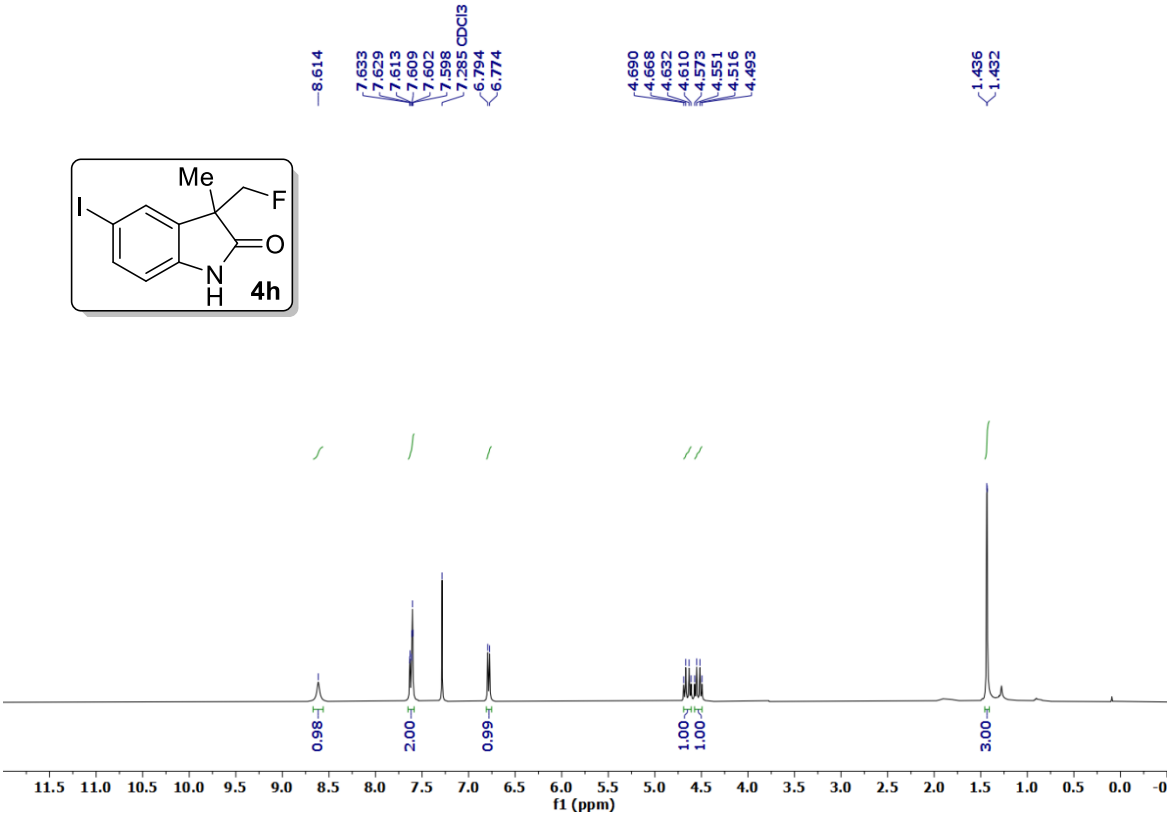
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 5-bromo-3-(fluoromethyl)-3-methylindolin-2-one (4g)



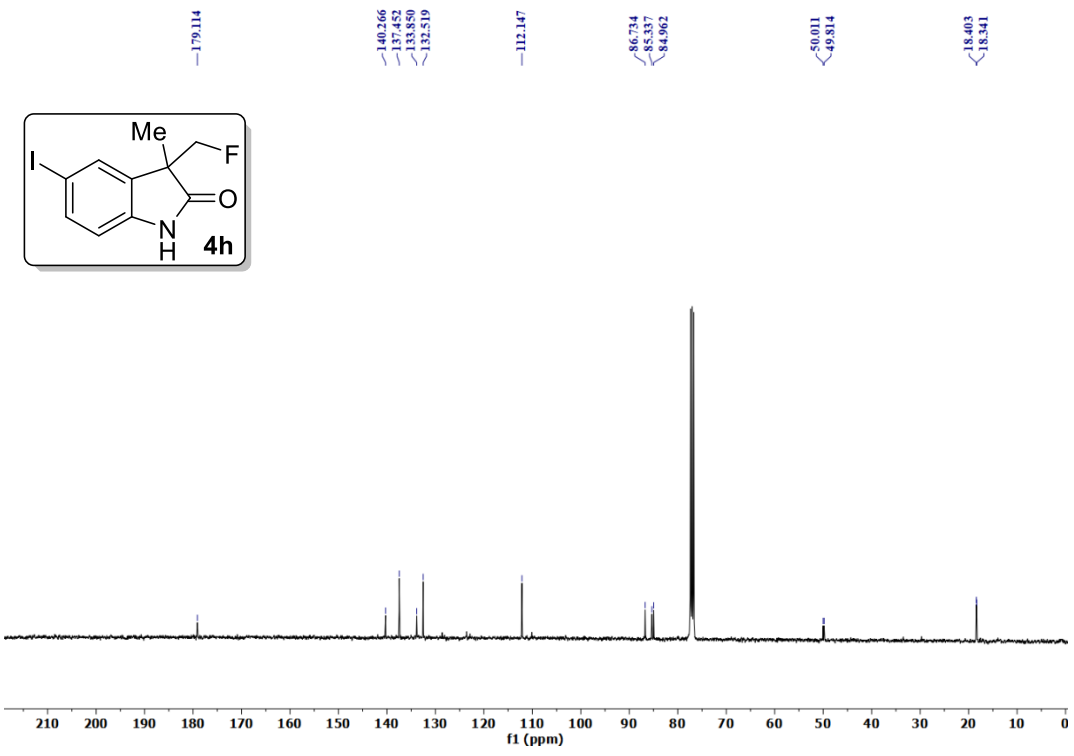
HRMS of 5-bromo-3-(fluoromethyl)-3-methylindolin-2-one (4g)



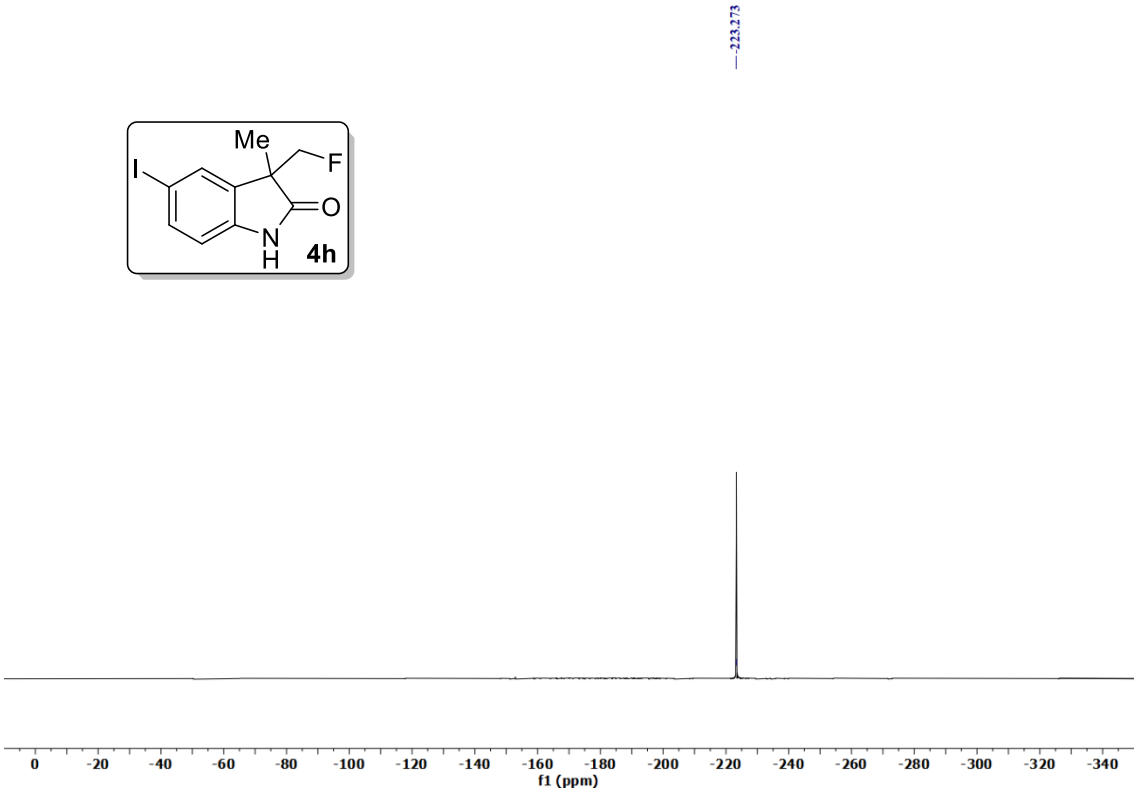
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-5-iodo-3-methylindolin-2-one (4h)



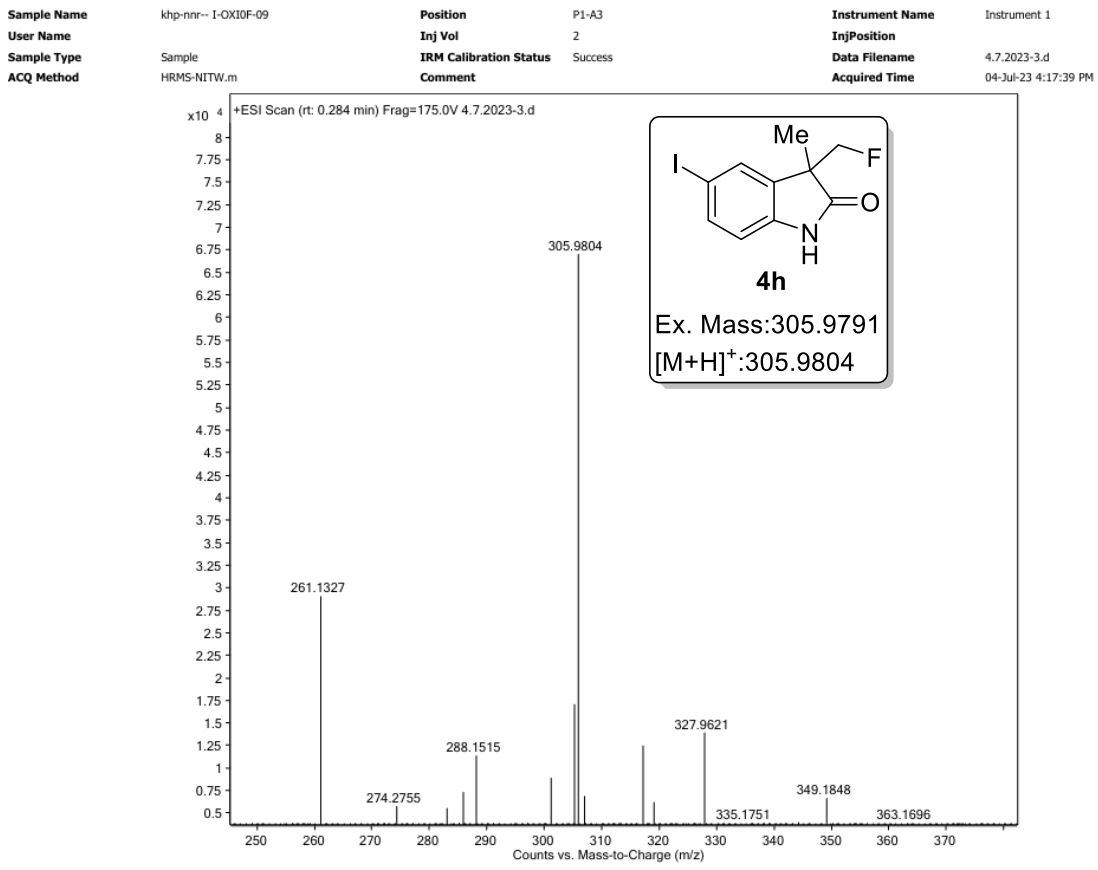
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-5-iodo-3-methylindolin-2-one (4h)



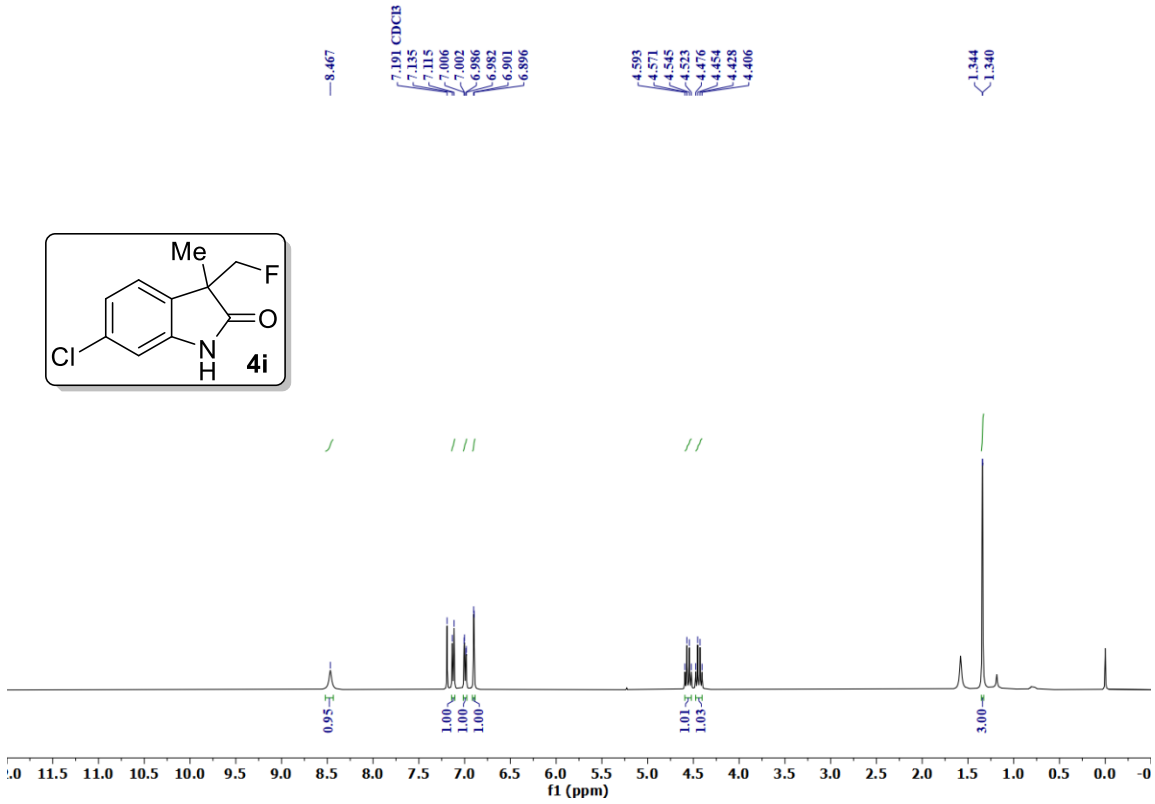
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-5-iodo-3-methylindolin-2-one (4h)



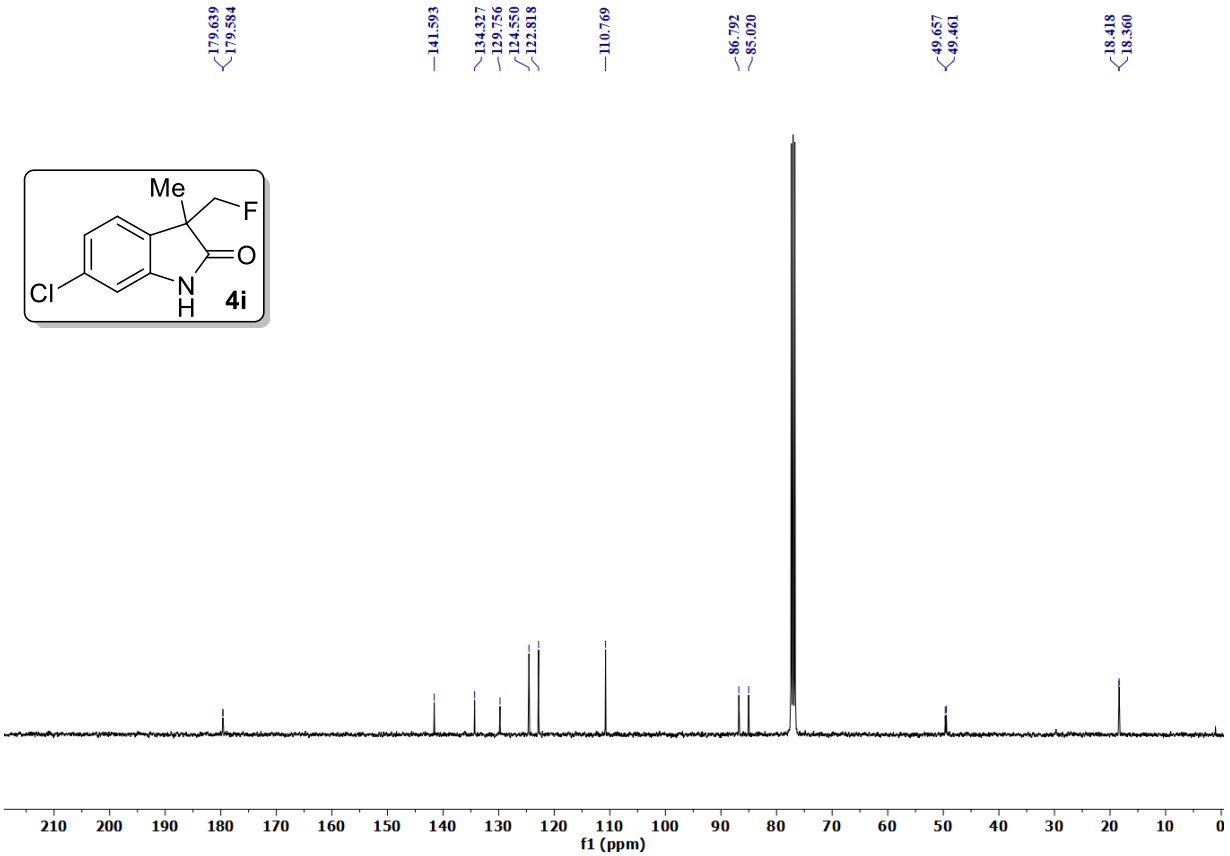
HRMS of 3-(fluoromethyl)-5-iodo-3-methylindolin-2-one (4h)



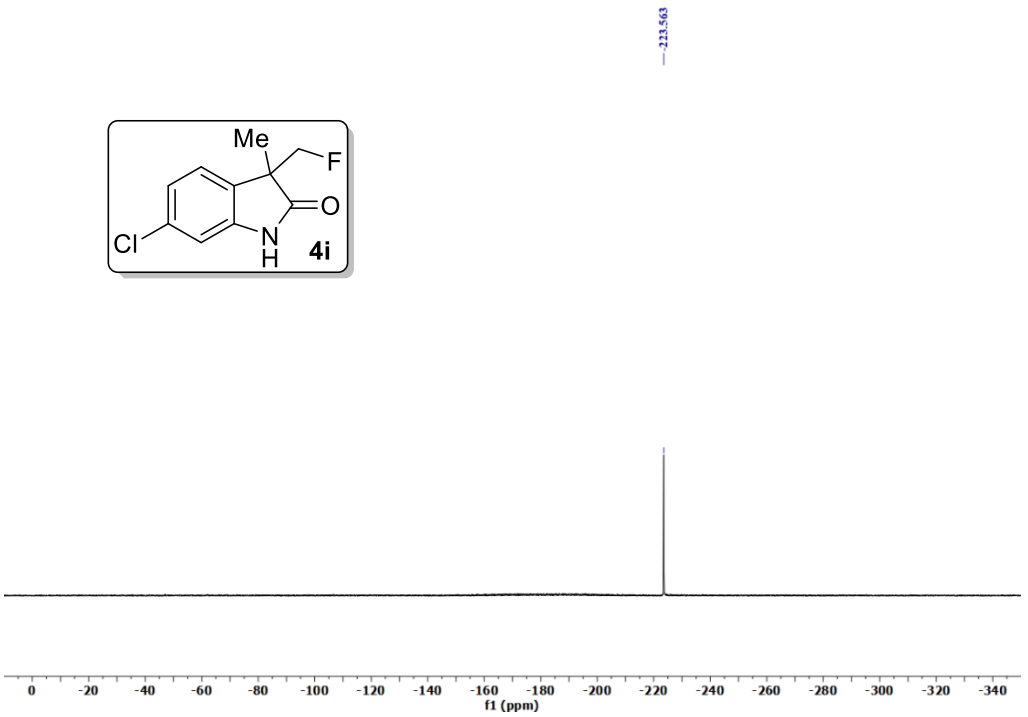
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 6-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4i)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 6-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4i)

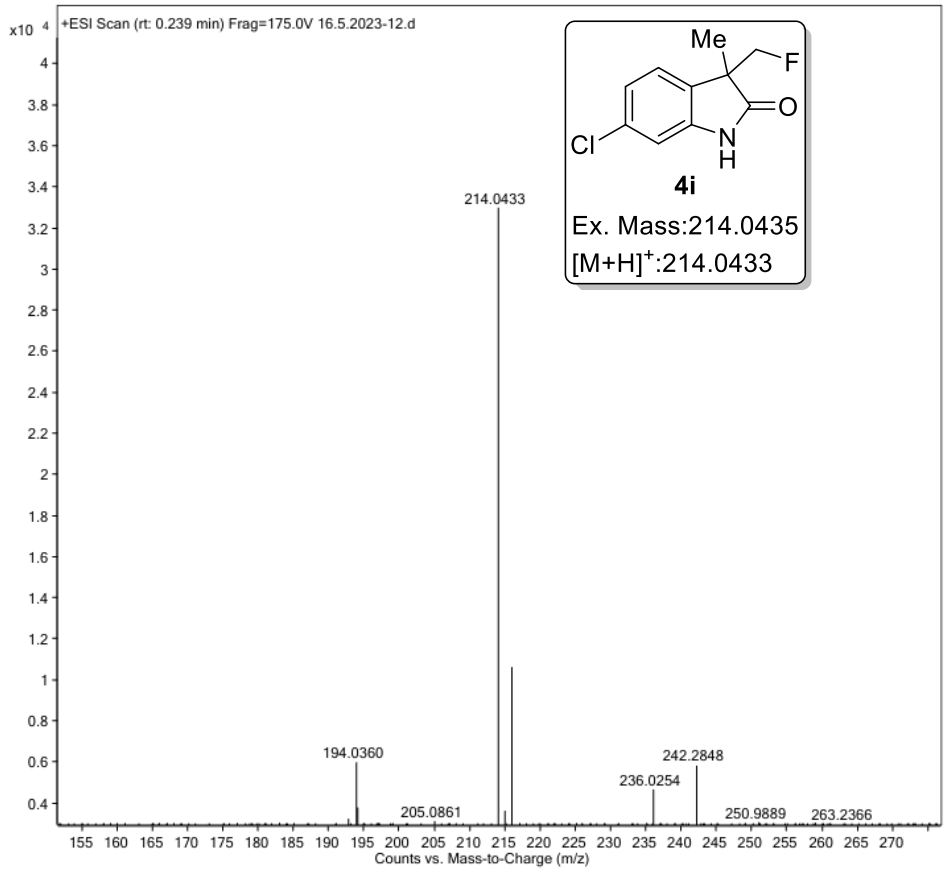


^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 6-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4i)

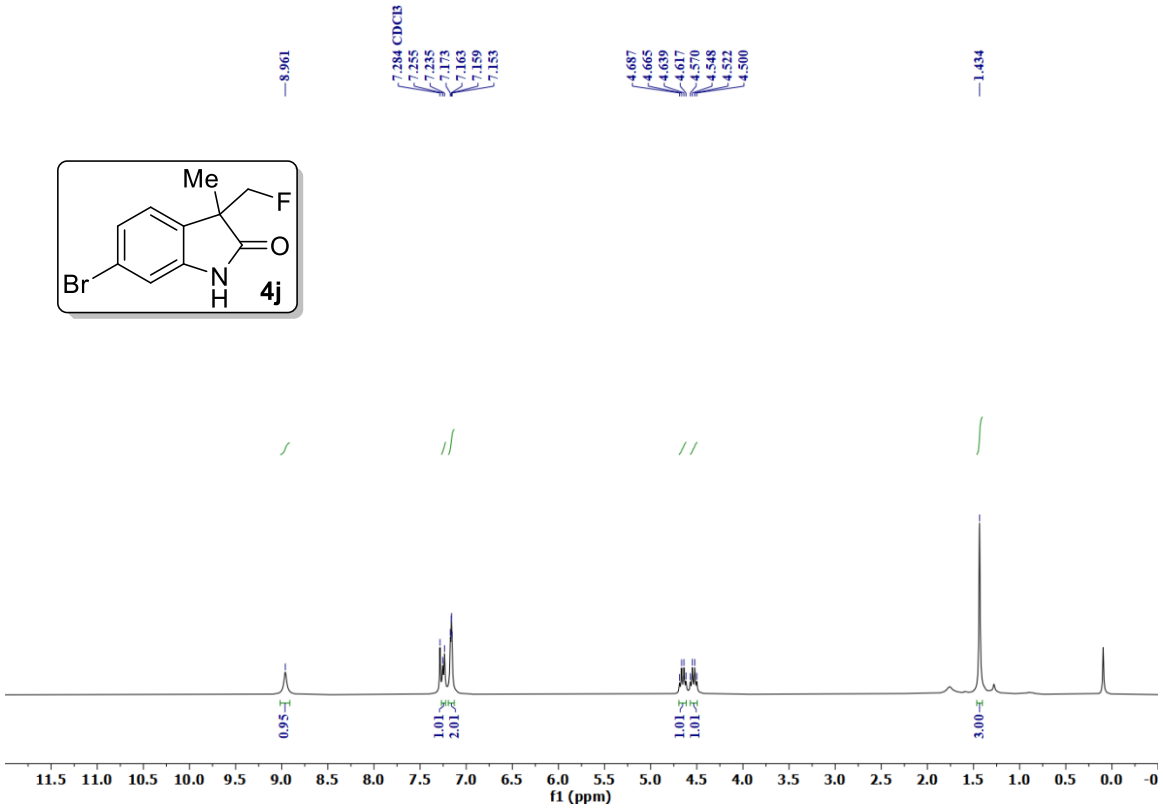


HRMS of 6-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4i)

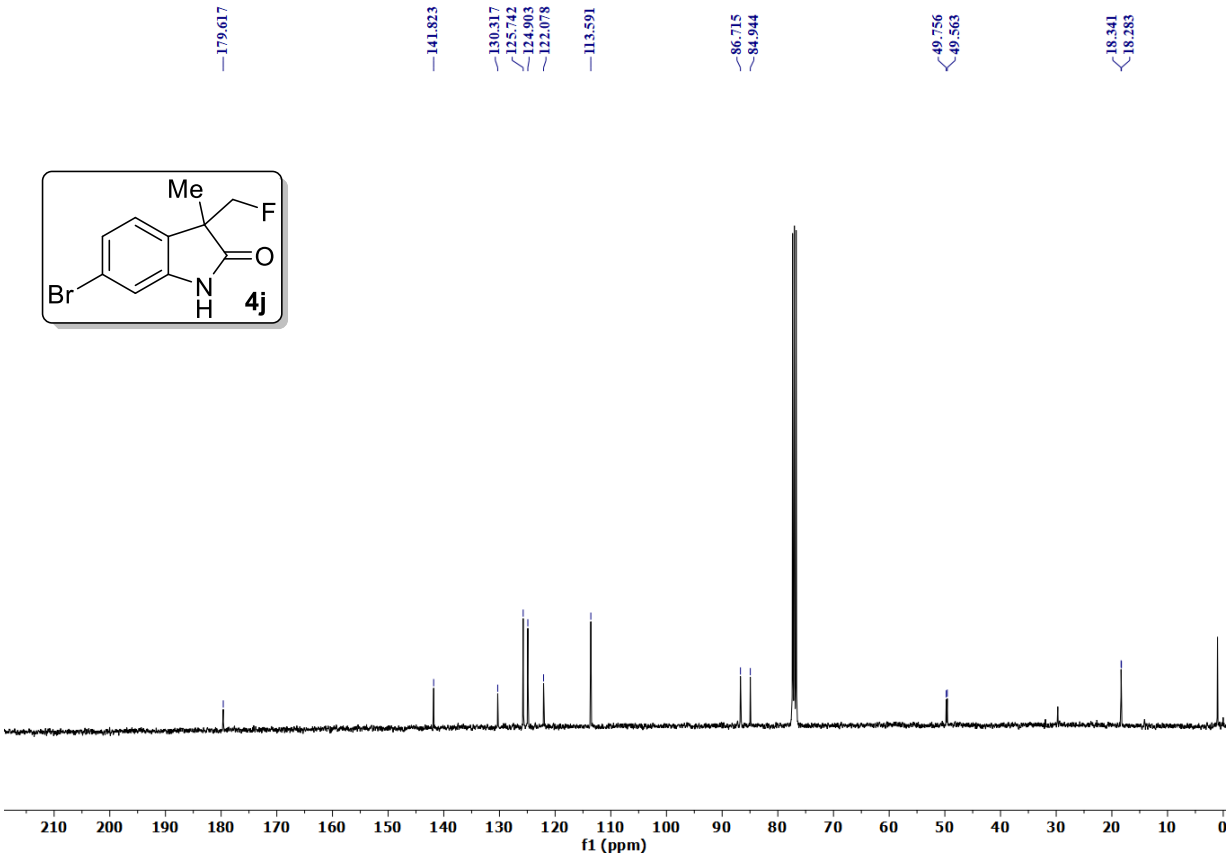
Sample Name	i-oxi-f-07	**Position**	P1-B3	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	3	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	16.5.2023-12.d
ACQ Method	HRMS-NITW.m	**Comment**		**Acquired Time**	16-Jun-23 4:31:24 PM



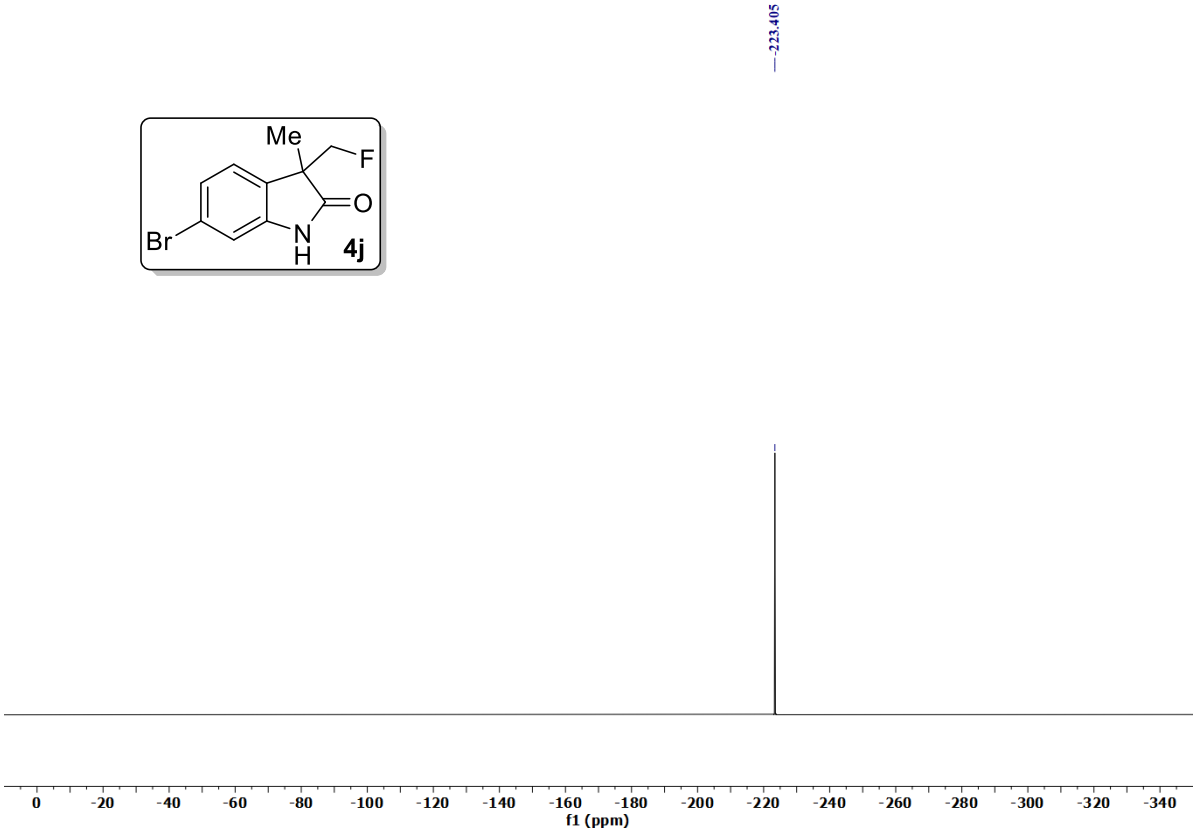
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 6-bromo-3-(fluoromethyl)-3-methylindolin-2-one (4j)



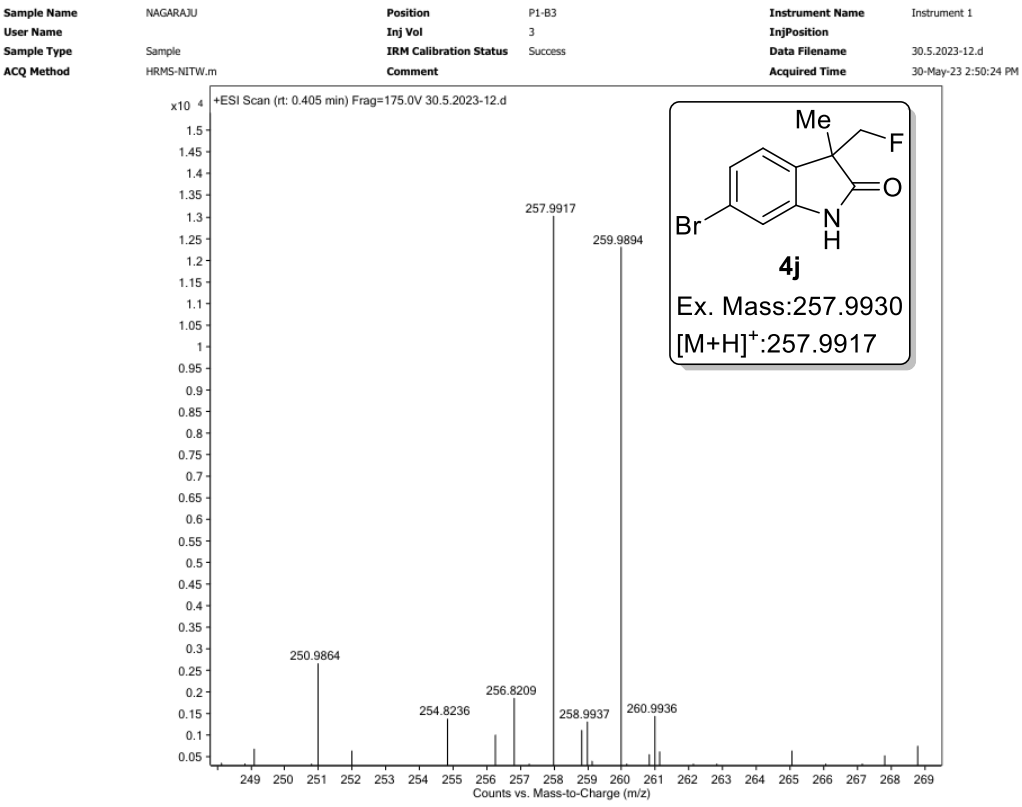
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 6-bromo-3-(fluoromethyl)-3-methylindolin-2-one (4j)



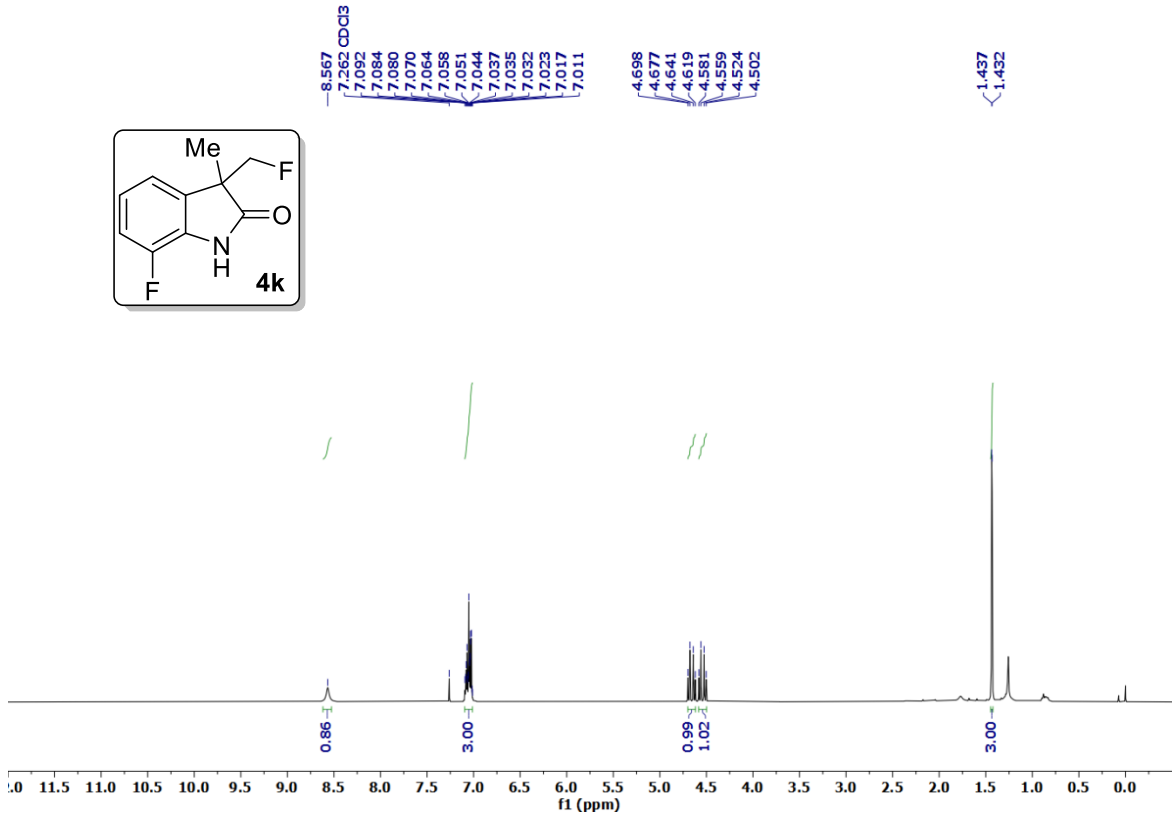
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 6-bromo-3-(fluoromethyl)-3-methylindolin-2-one (4j)



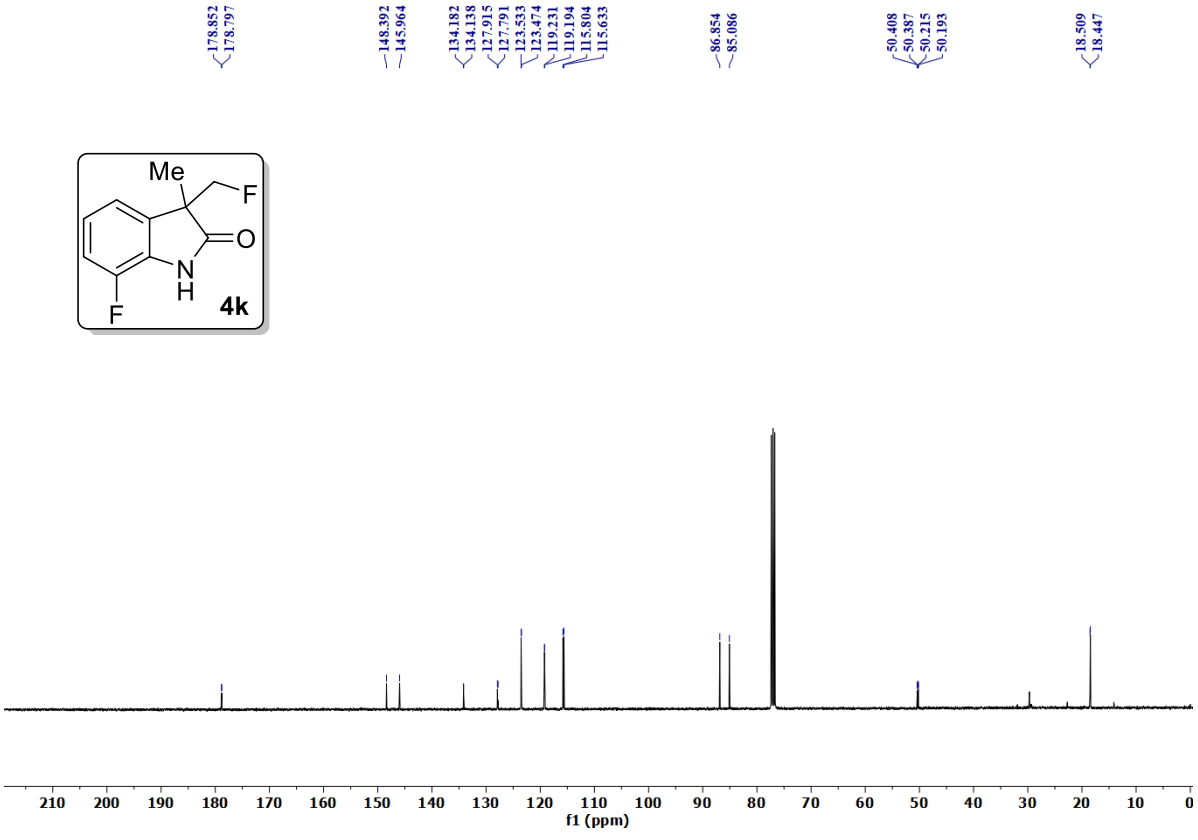
HRMS of 6-bromo-3-(fluoromethyl)-3-methylindolin-2-one (4j)



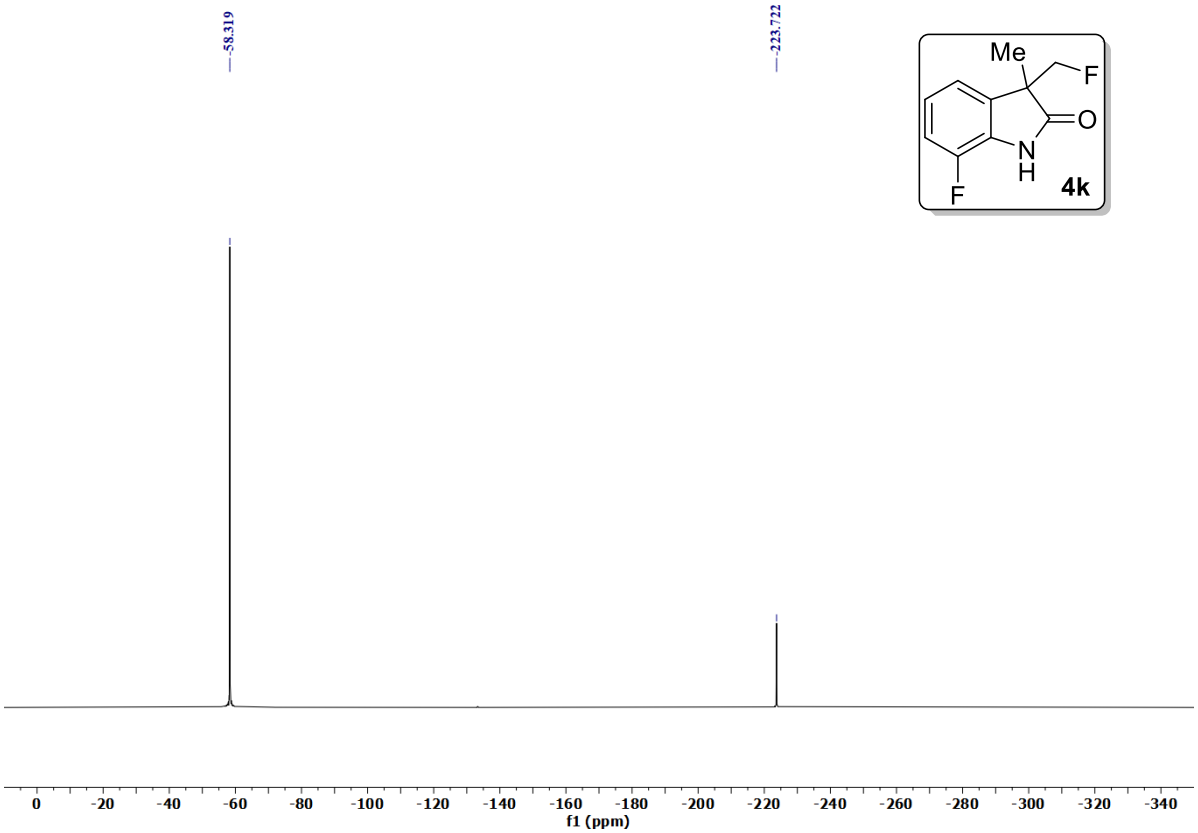
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 7-fluoro-3-(fluoromethyl)-3-methylindolin-2-one (4k)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 7-fluoro-3-(fluoromethyl)-3-methylindolin-2-one (4k)

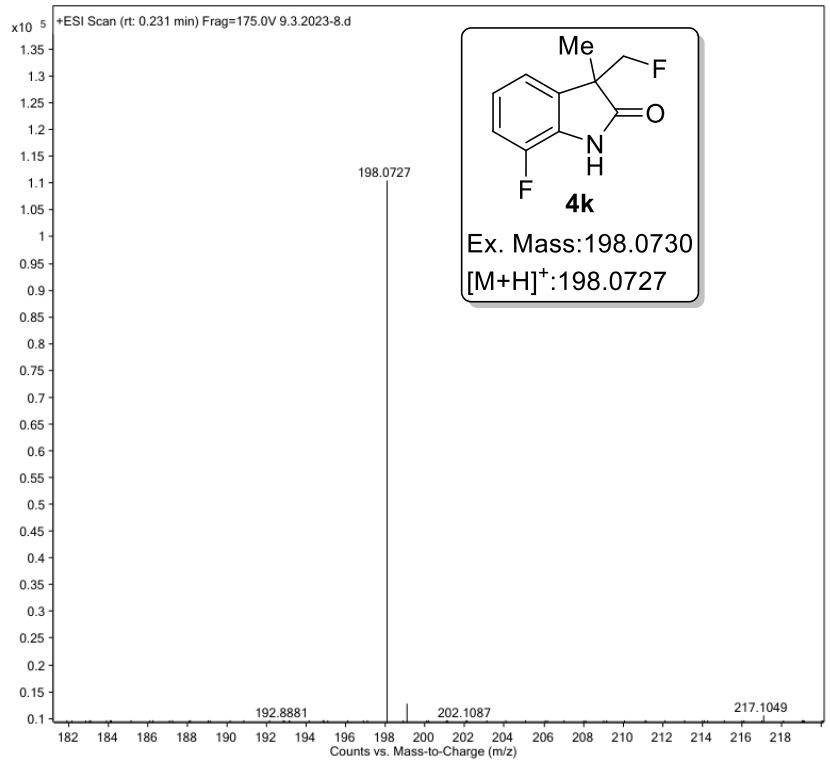


^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 7-fluoro-3-(fluoromethyl)-3-methylindolin-2-one (4k)

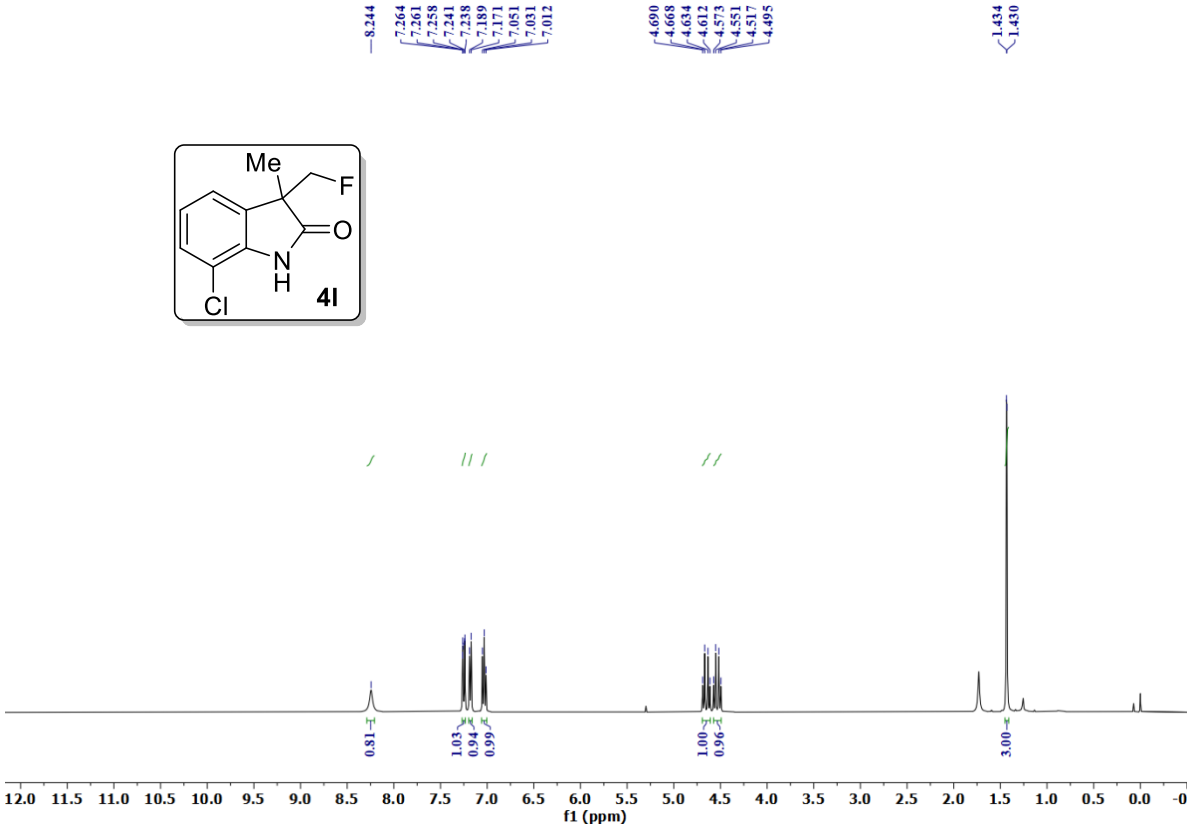


HRMS of 7-fluoro-3-(fluoromethyl)-3-methylindolin-2-one (4k)

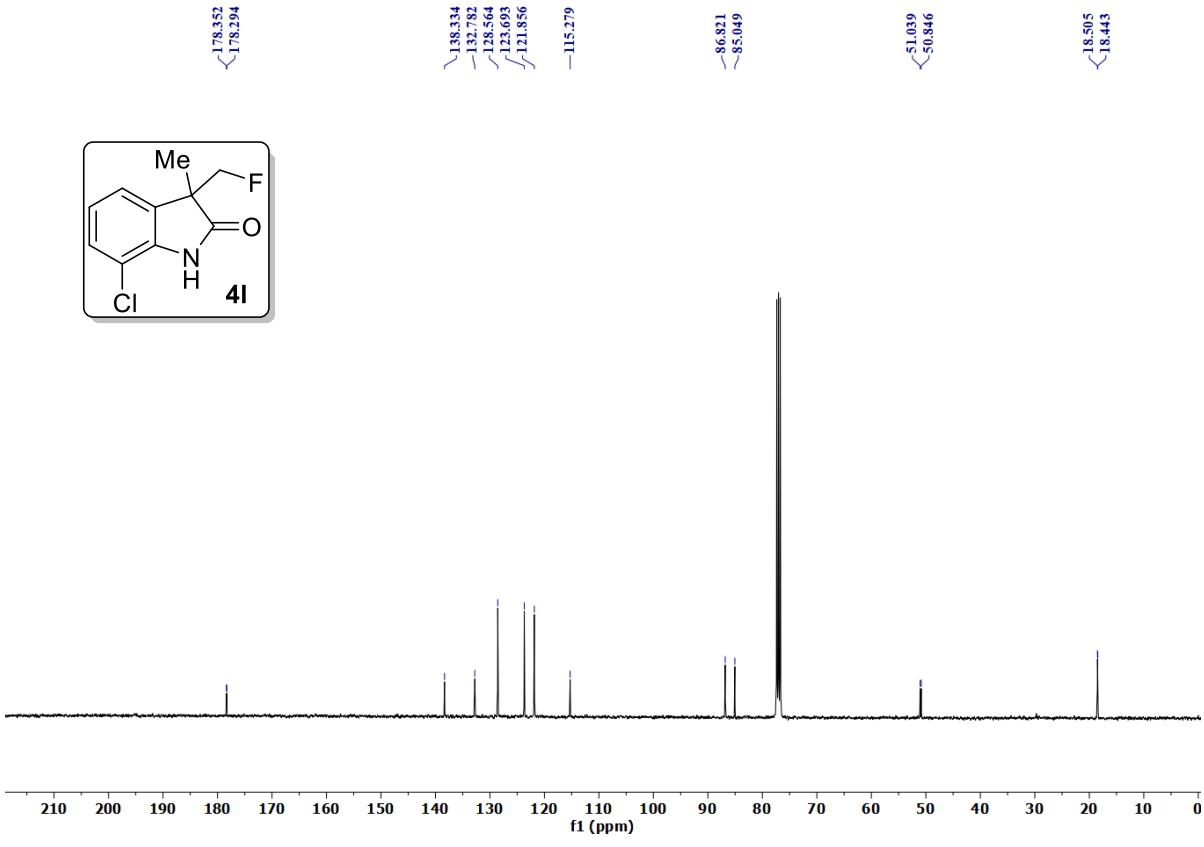
Sample Name	7-f-3-me-f	**Position**	P1-A8	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	3	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	9.3.2023-8.d
ACQ Method	NITW-W.m	**Comment**		**Acquired Time**	09-Mar-23 5:42:45 PM



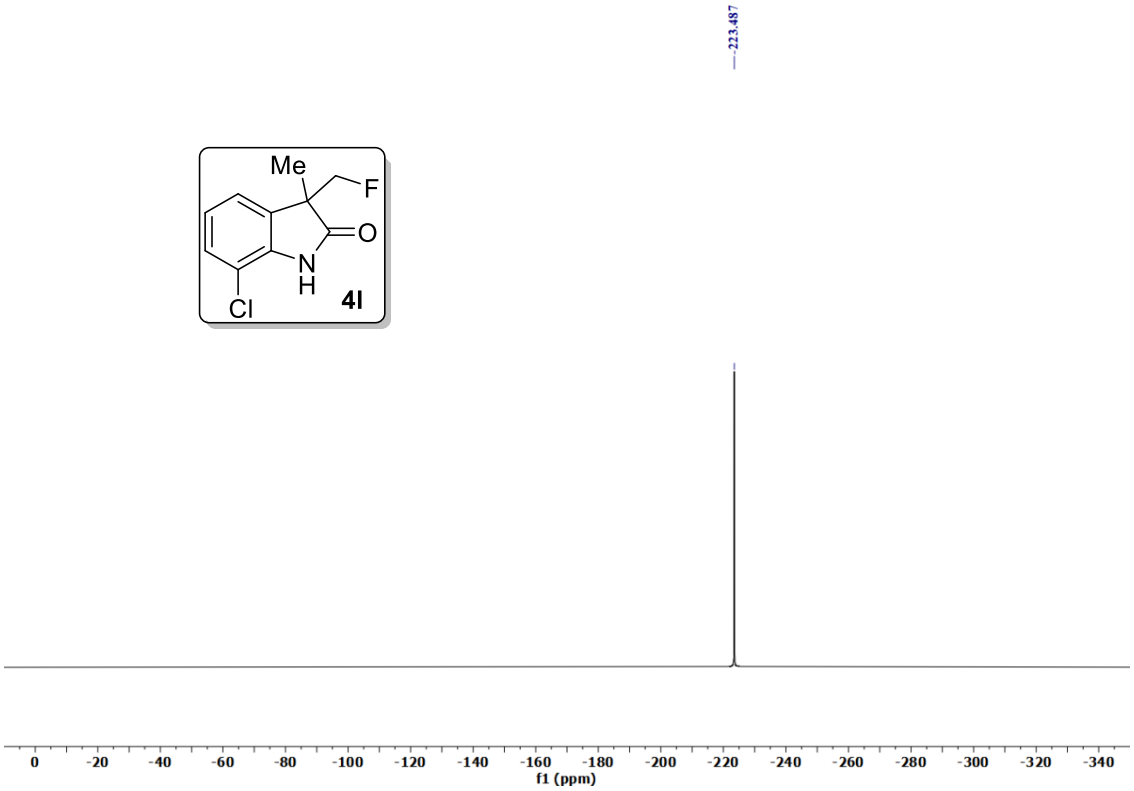
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 7-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4l)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 7-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4l)

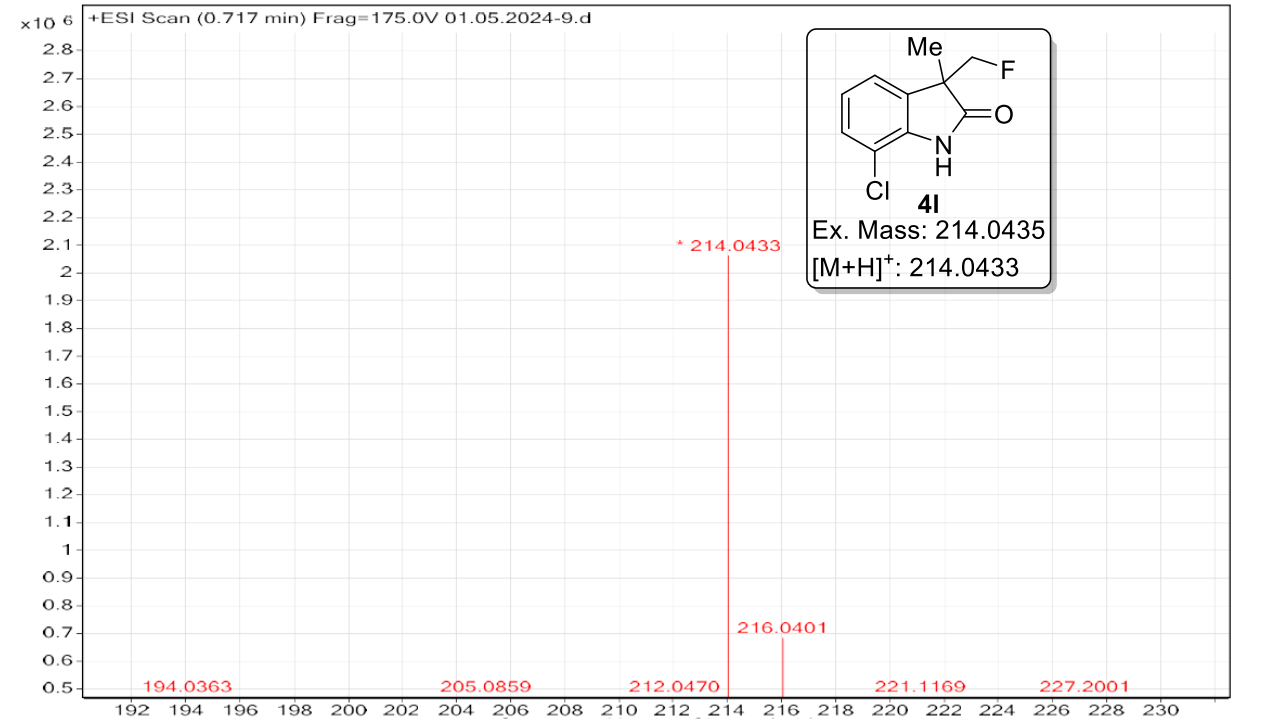


^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 7-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4l)

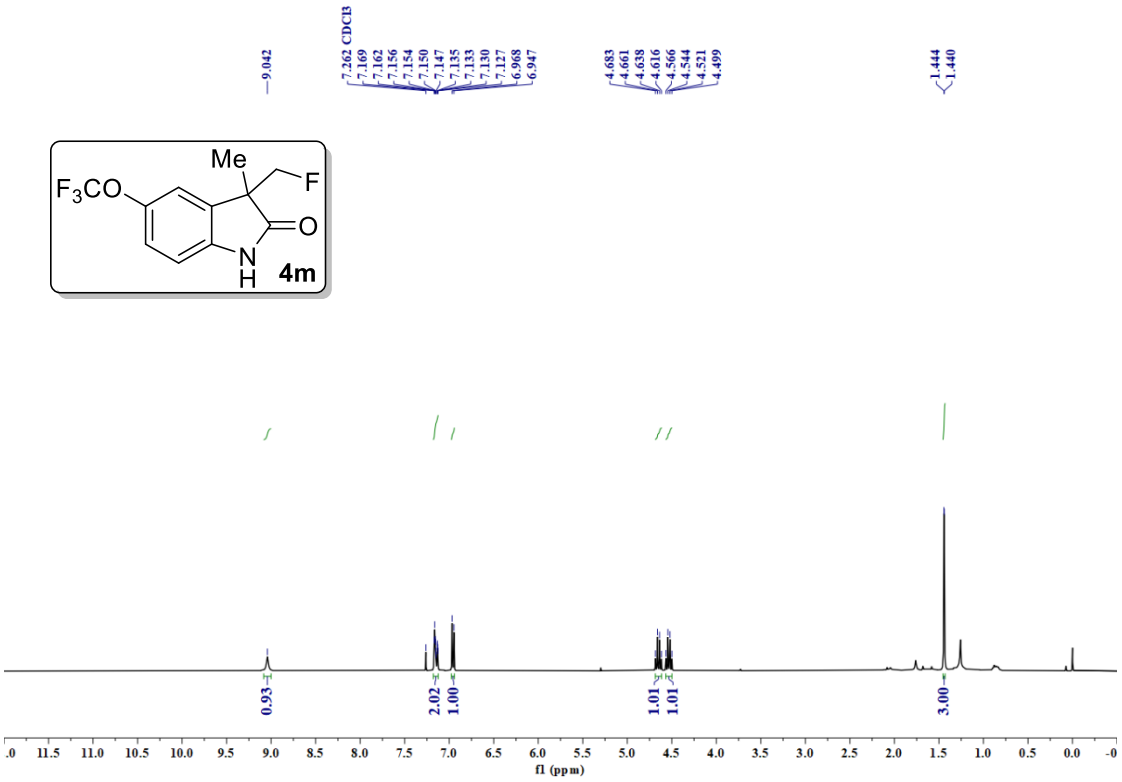


HRMS of 7-chloro-3-(fluoromethyl)-3-methylindolin-2-one (4l)

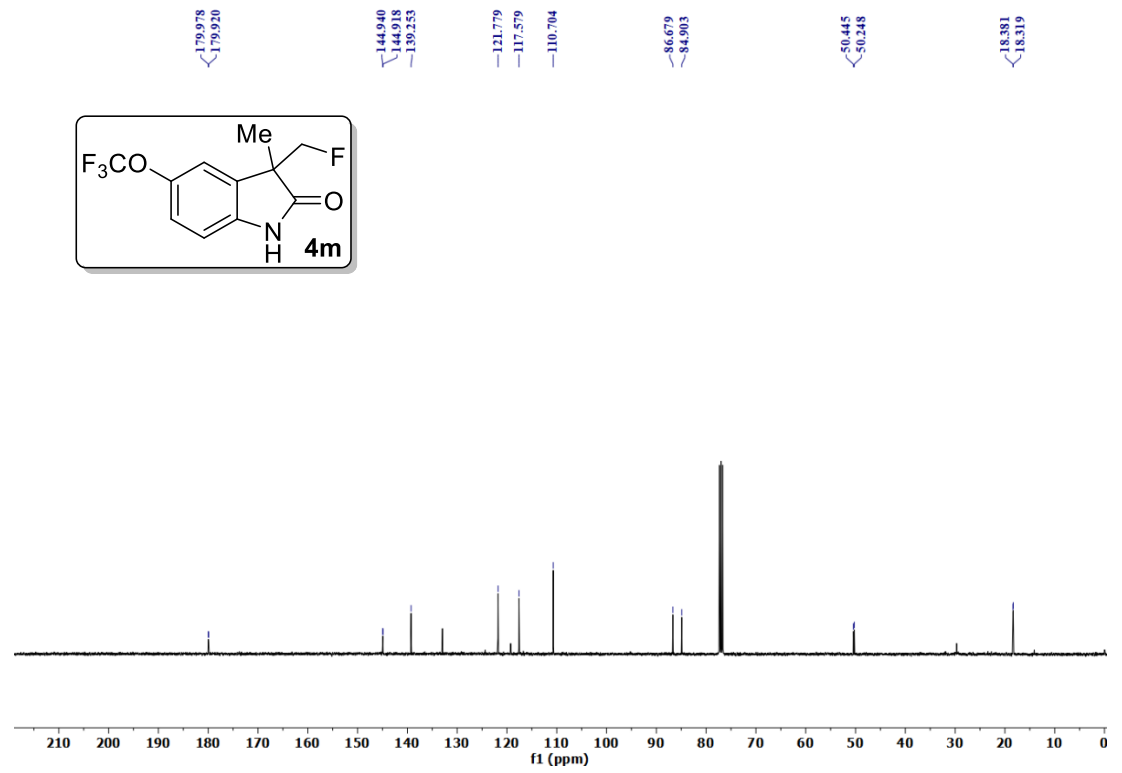
Sample Name	KHP-NNR-11	**Position**	P1-A9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	01.05.2024-9.d	**ACQ Method**	A60 W40.m	**Comment**		**Acquired Time**	5/1/2024 2:01:22 PM



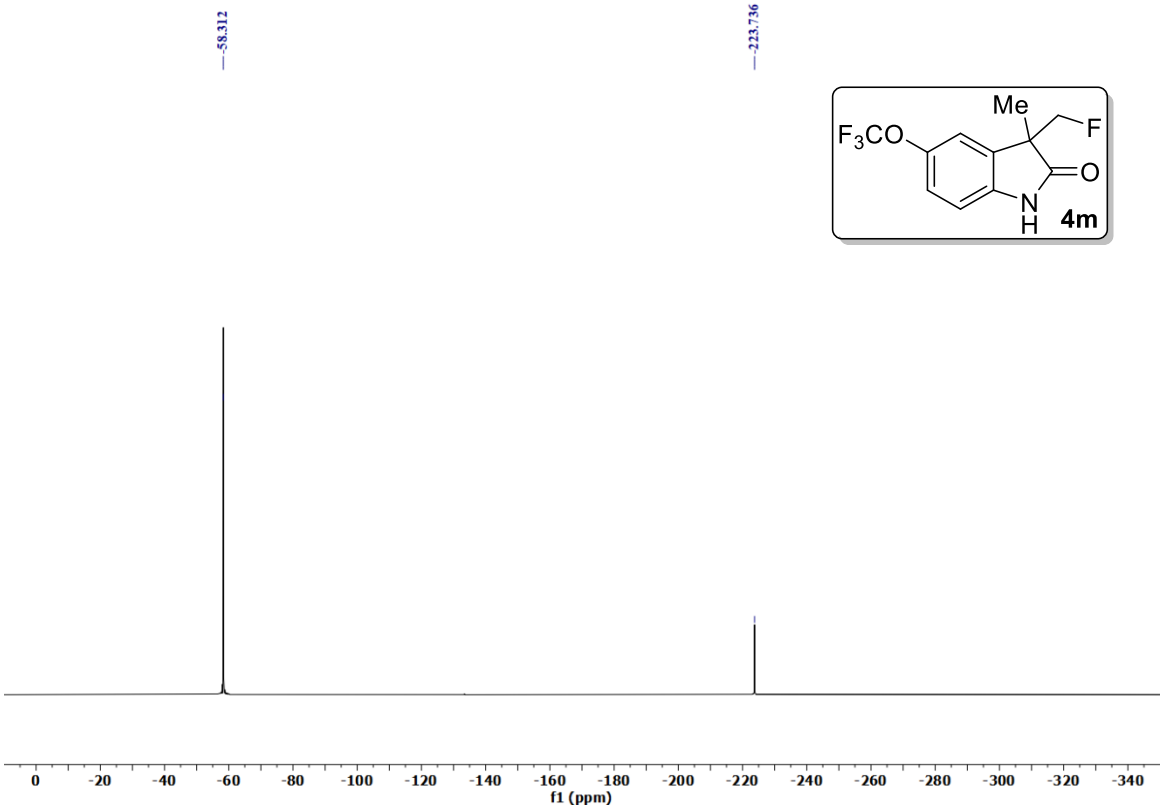
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methyl-5-(trifluoromethoxy)indolin-2-one (4m)



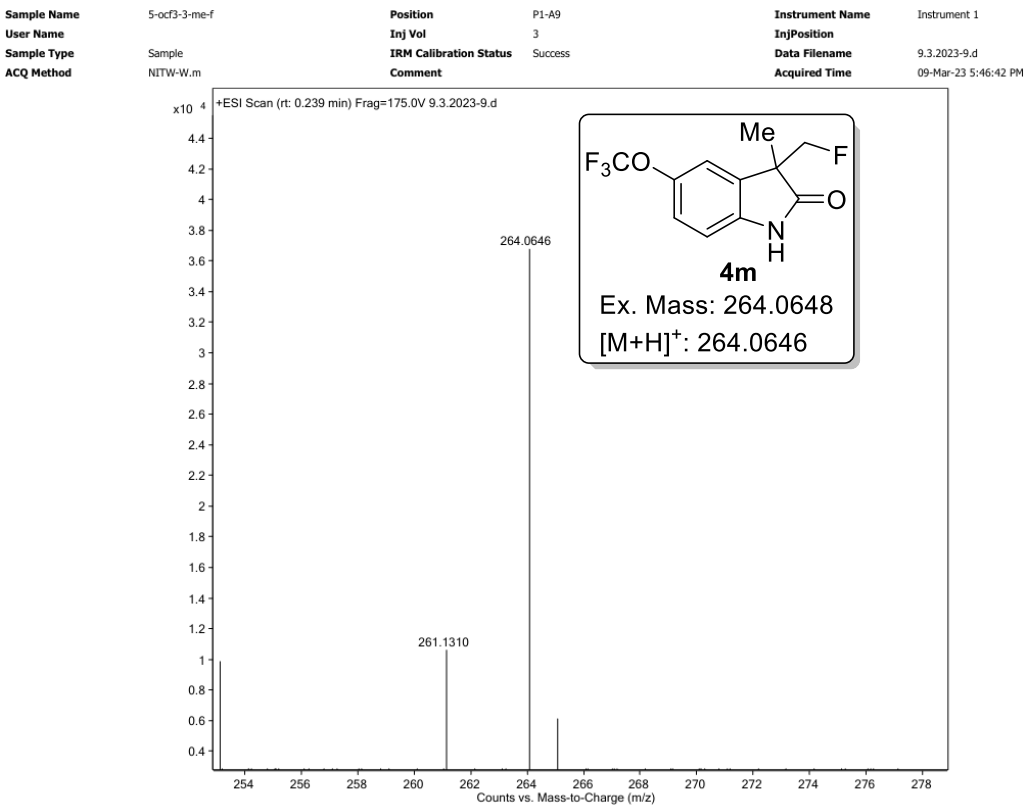
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methyl-5-(trifluoromethoxy)indolin-2-one (4m)



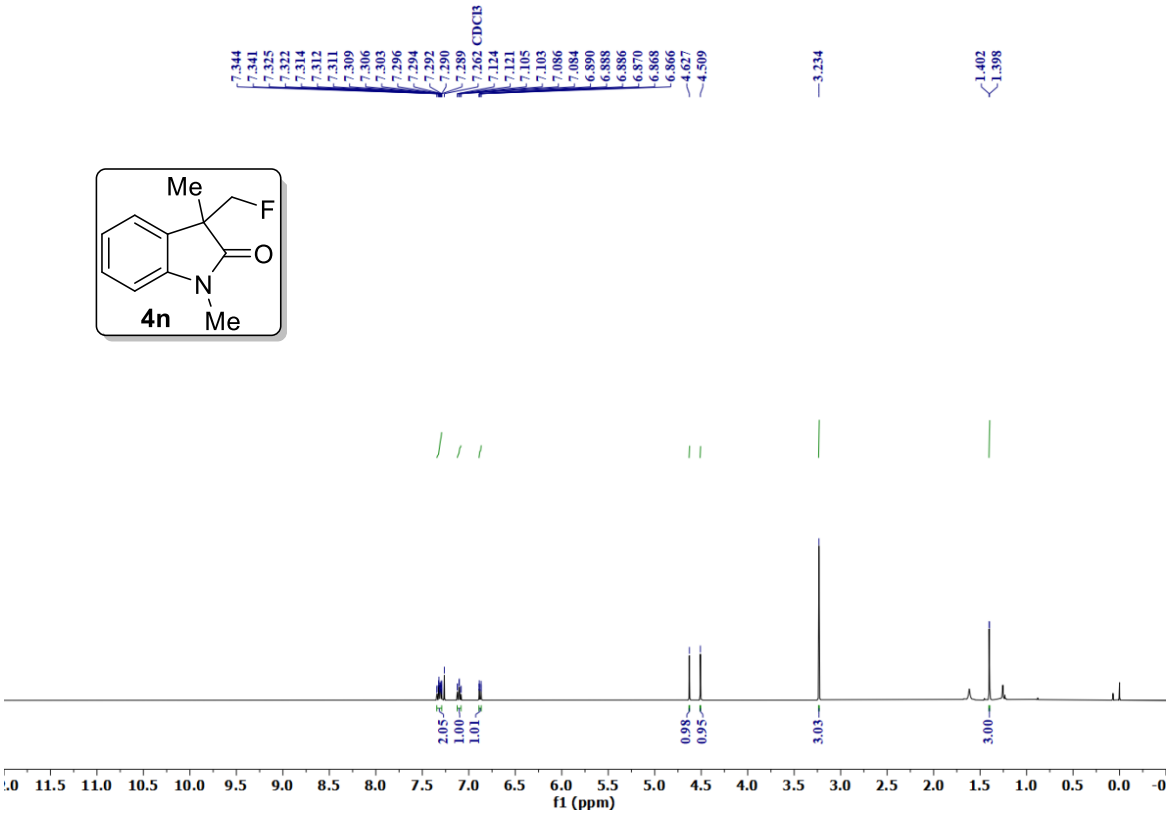
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methyl-5-(trifluoromethoxy)indolin-2-one (4m)



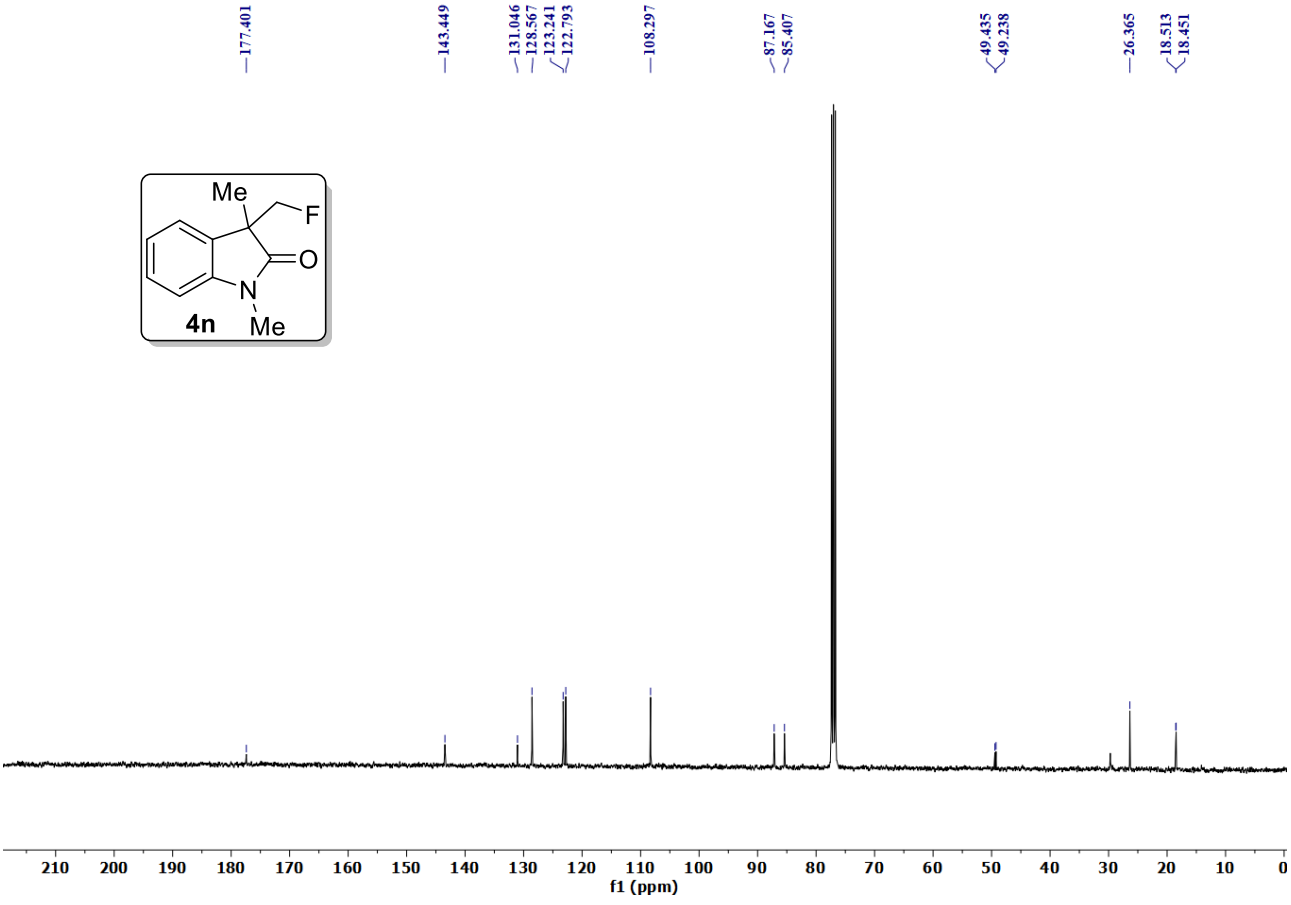
HRMS of 3-(fluoromethyl)-3-methyl-5-(trifluoromethoxy)indolin-2-one (4m)



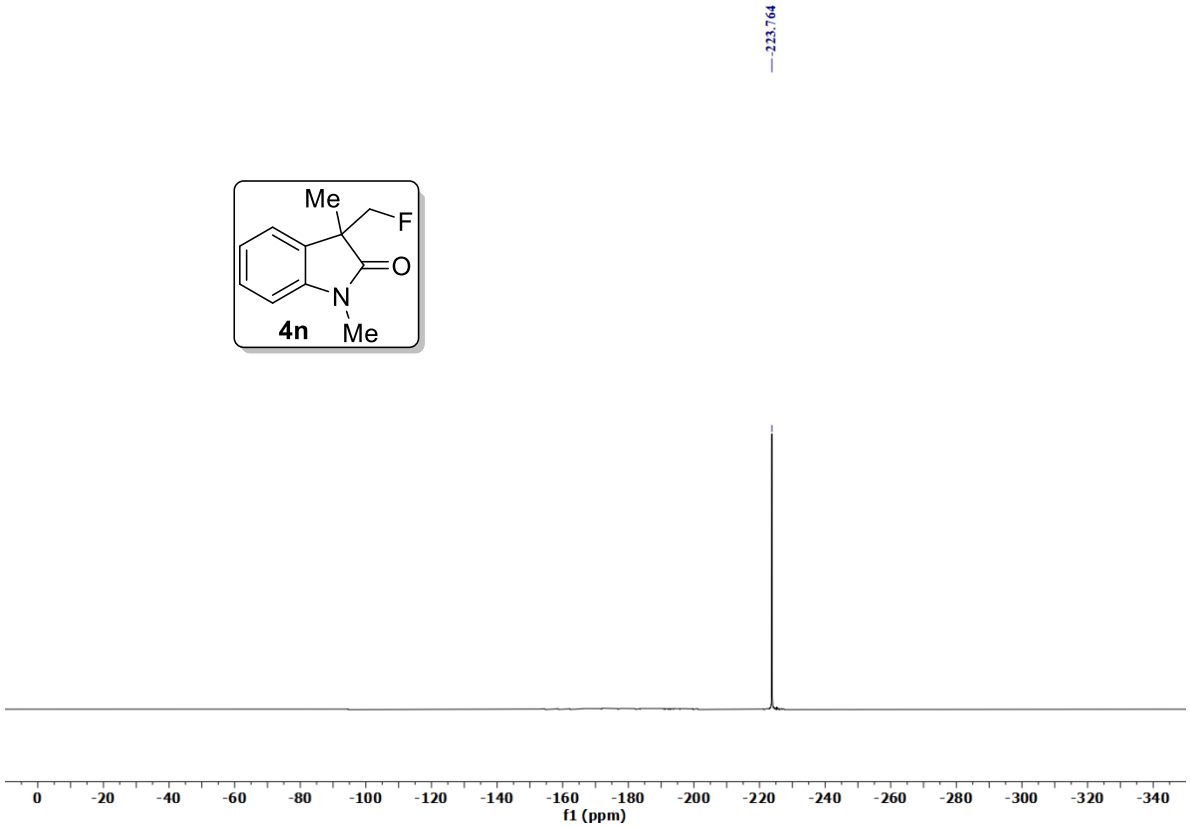
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-1,3-dimethylindolin-2-one (4n)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-1,3-dimethylindolin-2-one (4n)

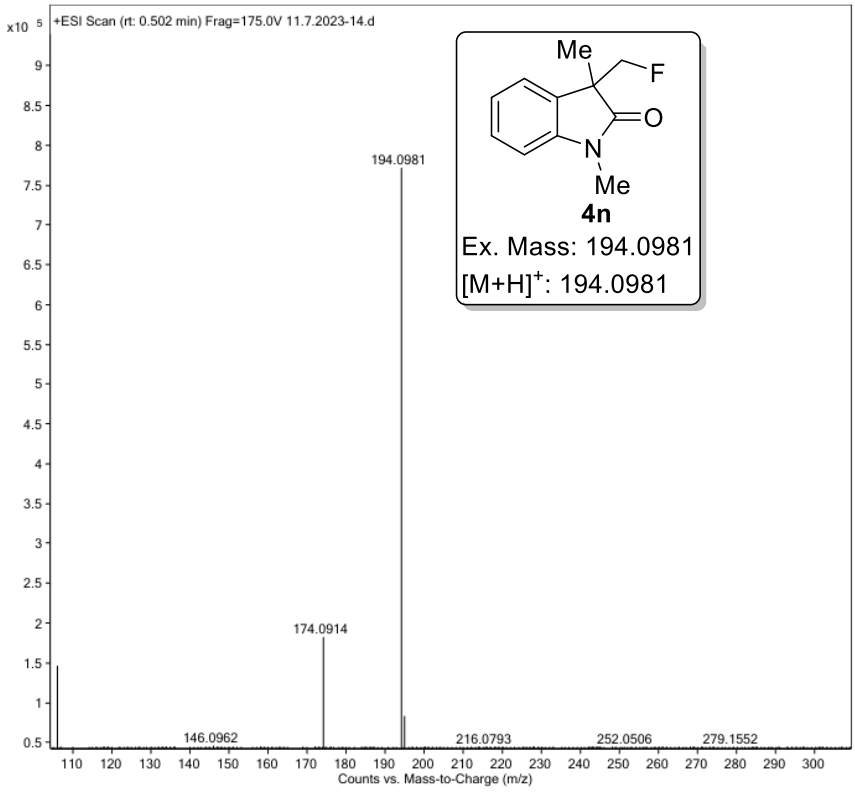


^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-1,3-dimethylindolin-2-one (4n)

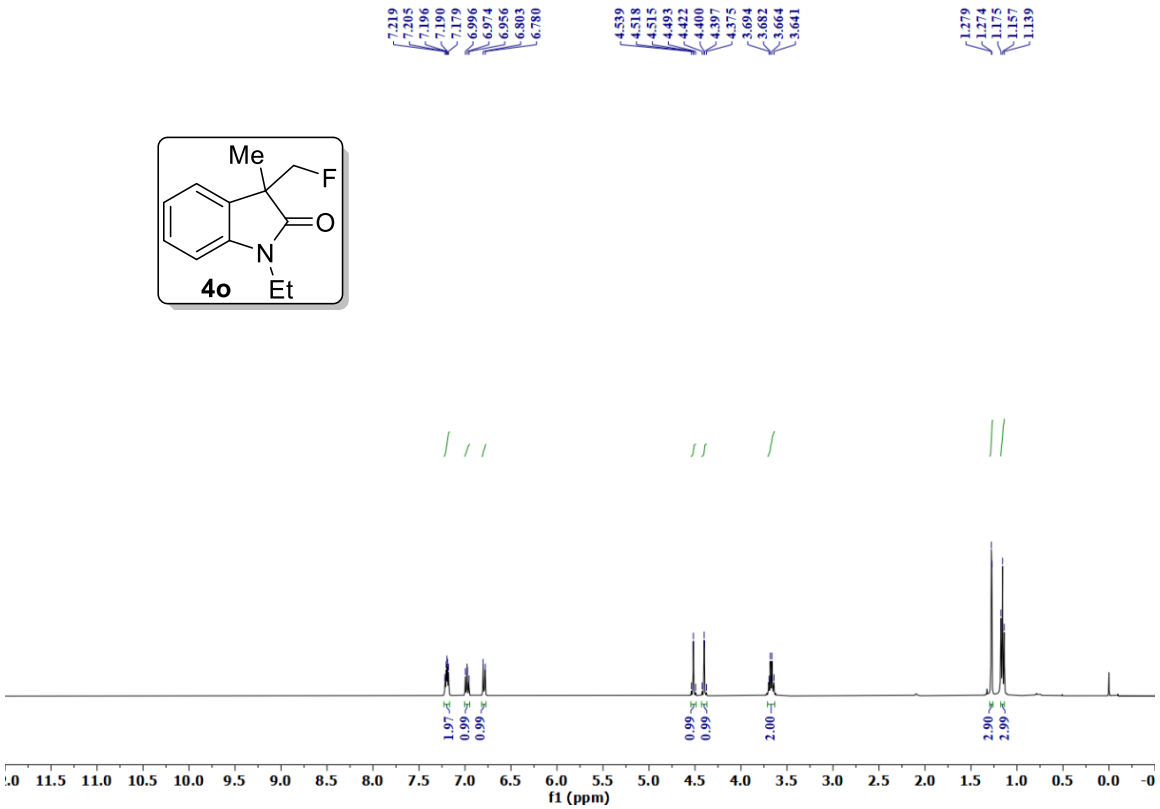


HRMS of 3-(fluoromethyl)-1,3-dimethylindolin-2-one (4n)

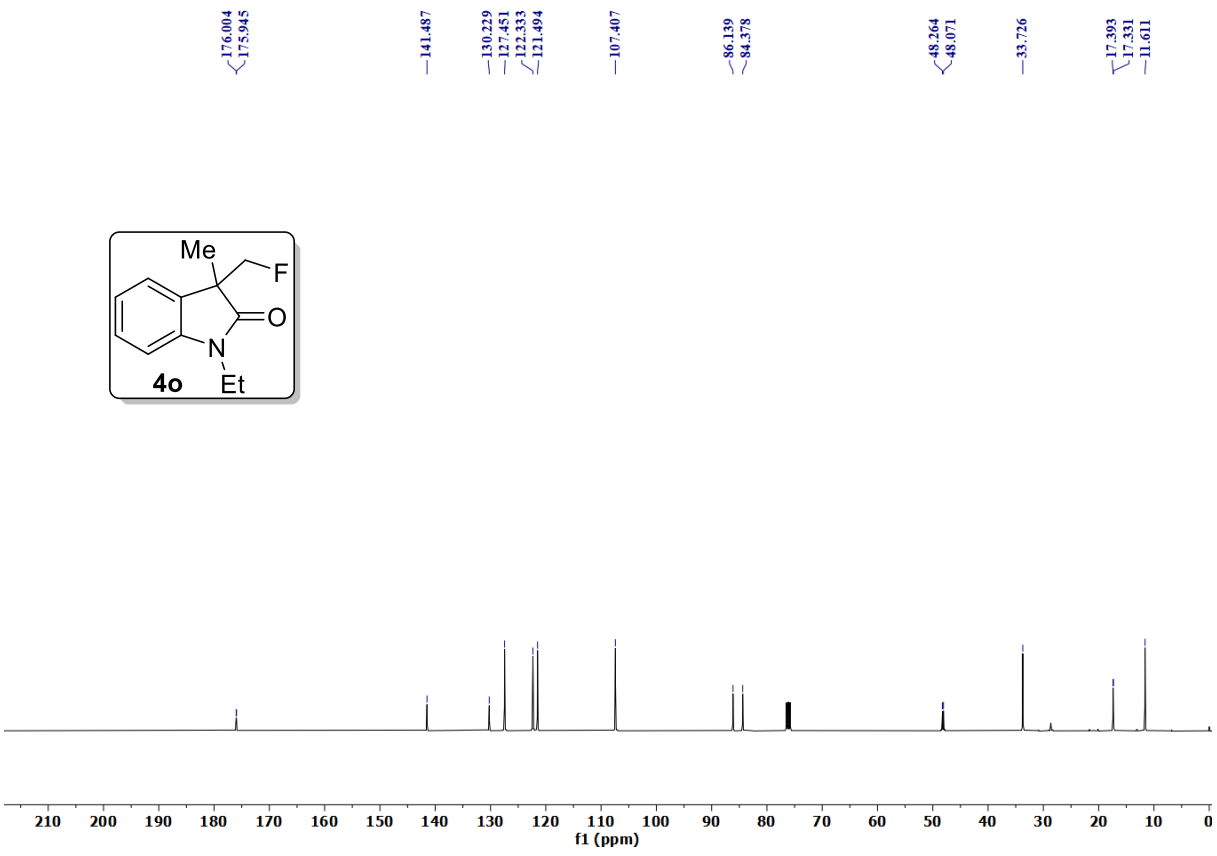
Sample Name	KHP-NNR	**Position**	P1-B5	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	11.7.2023-14.d
ACQ Method	HRMS-NITW.m	**Comment**		**Acquired Time**	11-Jul-23 5:47:01 PM



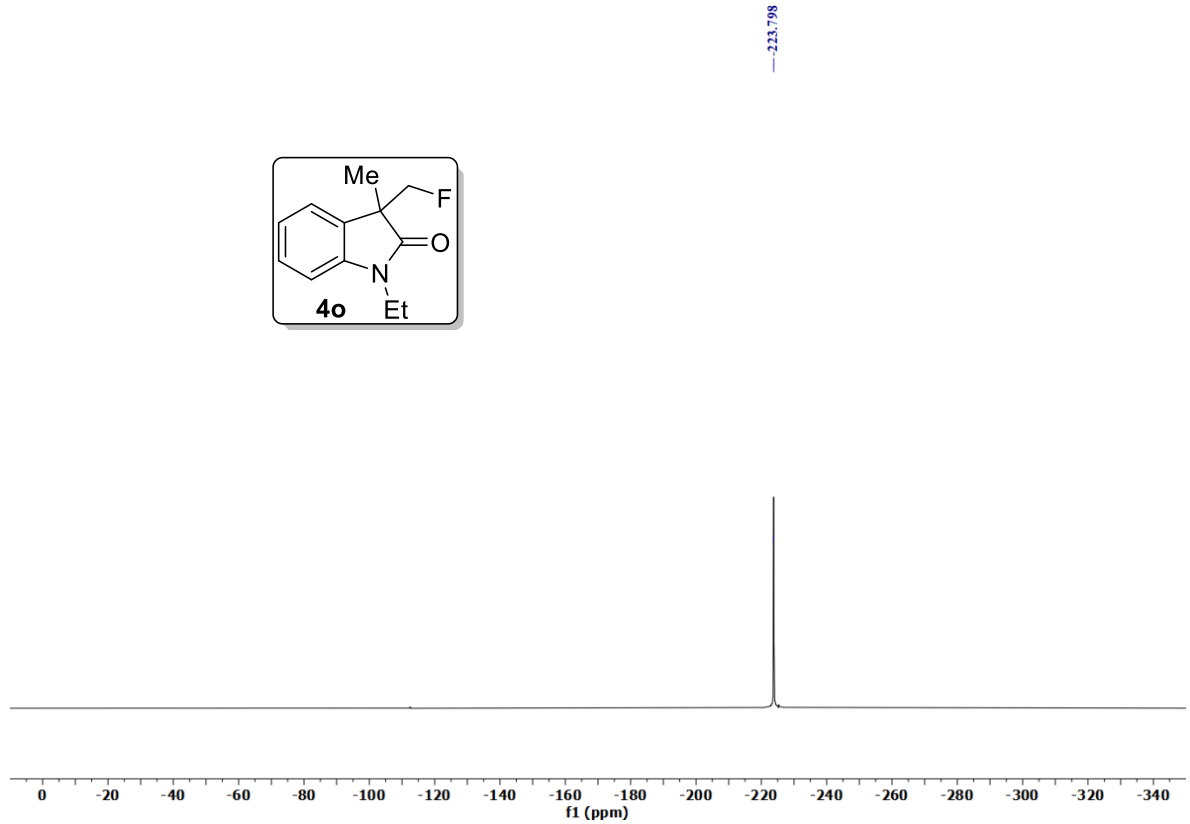
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 1-ethyl-3-(fluoromethyl)-3-methylindolin-2-one (4o)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 1-ethyl-3-(fluoromethyl)-3-methylindolin-2-one (4o)

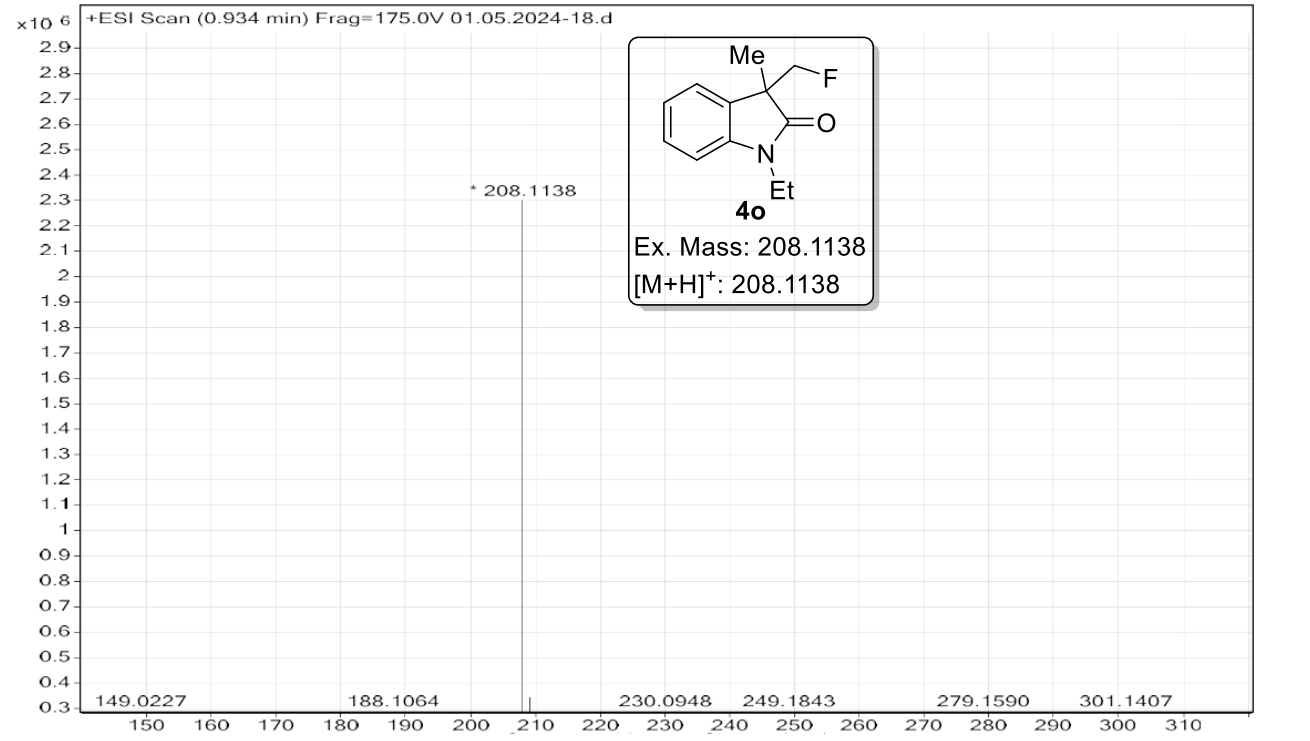


^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 1-ethyl-3-(fluoromethyl)-3-methylindolin-2-one (4o)

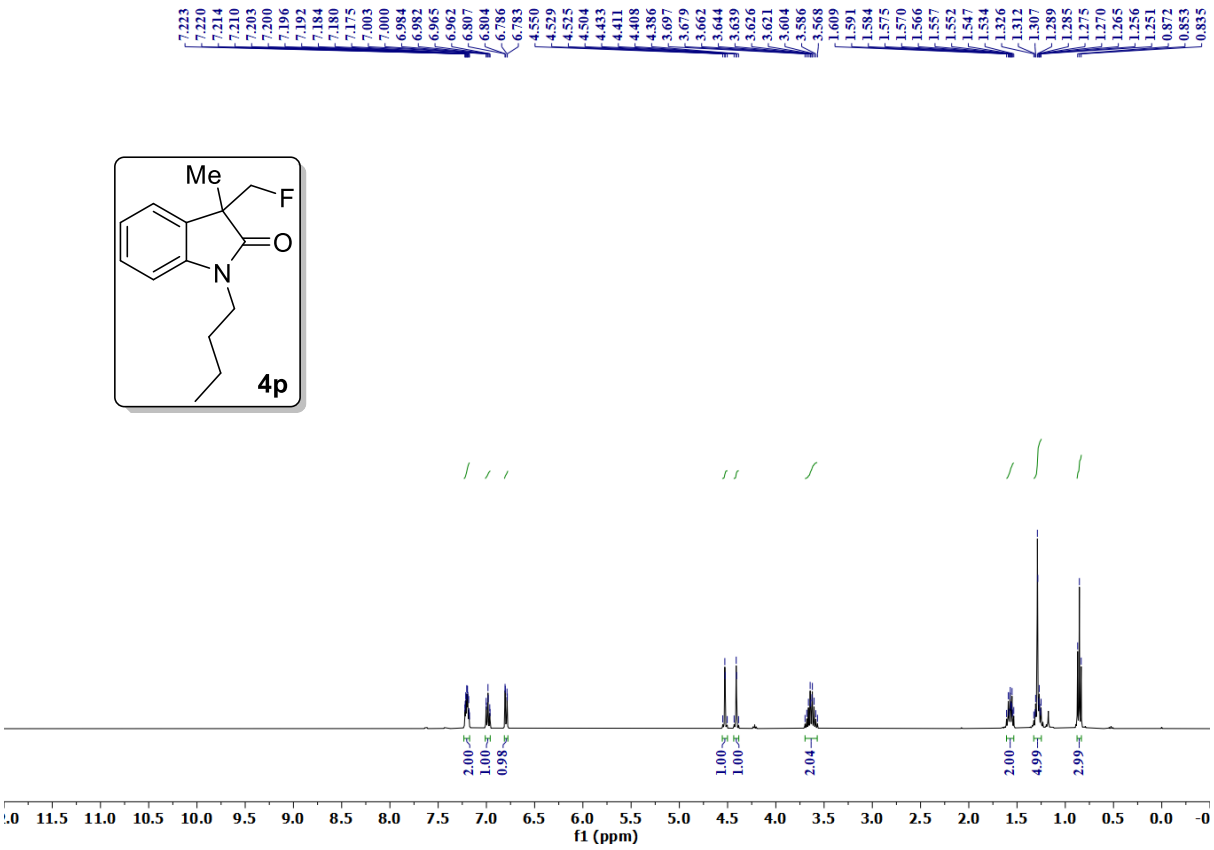


HRMS of 1-ethyl-3-(fluoromethyl)-3-methylindolin-2-one (4o)

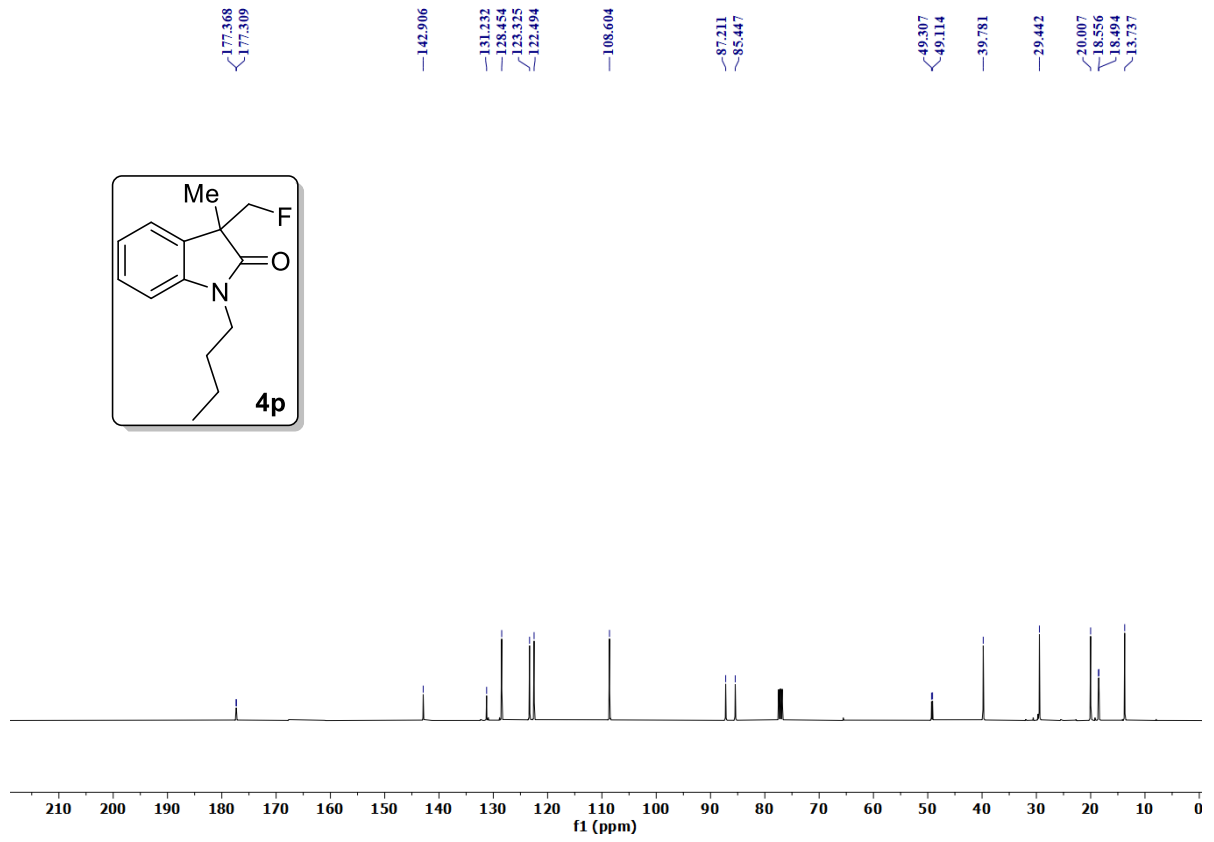
Sample Name	KHP-NNR-21	**Position**	P1-B9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	01.05.2024-18.d	**ACQ Method**	A60 W40.m	**Comment**		**Acquired Time**	5/1/2024 2:37:25 PM



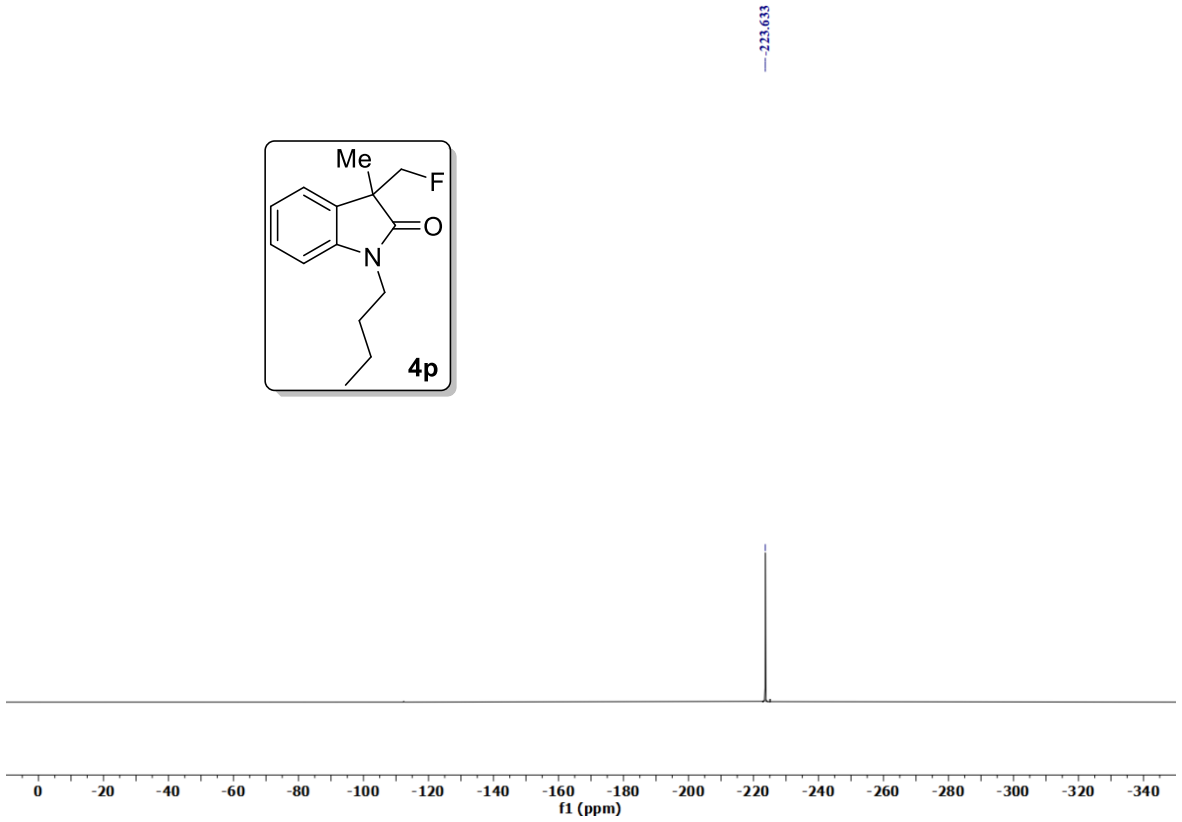
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 1-butyl-3-(fluoromethyl)-3-methylindolin-2-one (4p)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 1-butyl-3-(fluoromethyl)-3-methylindolin-2-one (4p)

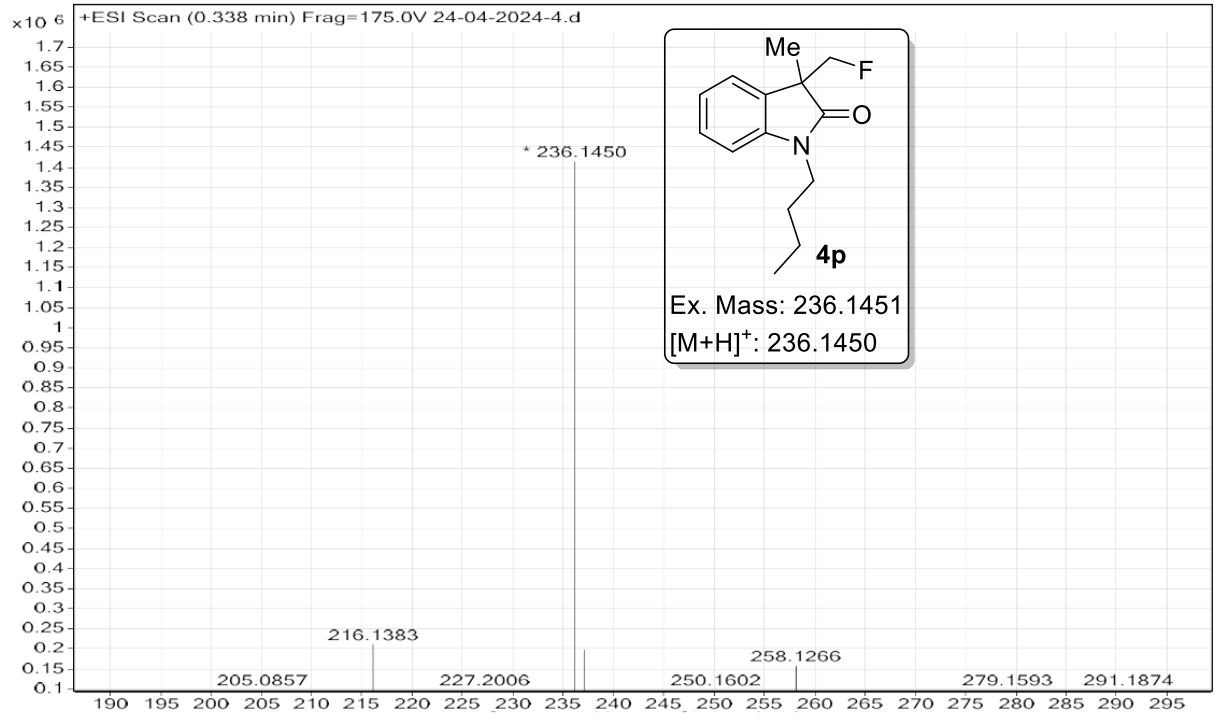


^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 1-butyl-3-(fluoromethyl)-3-methylindolin-2-one (4p)

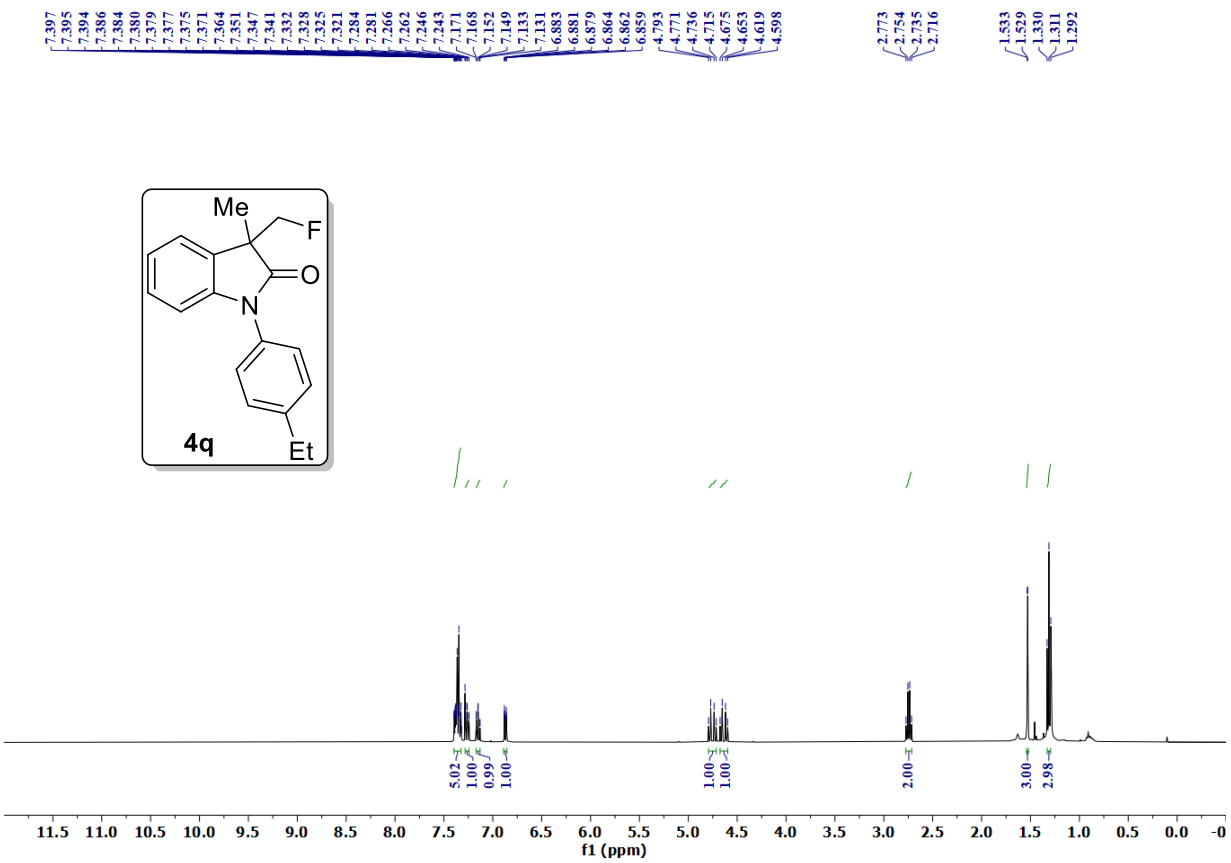


HRMS of 1-butyl-3-(fluoromethyl)-3-methylindolin-2-one (4p)

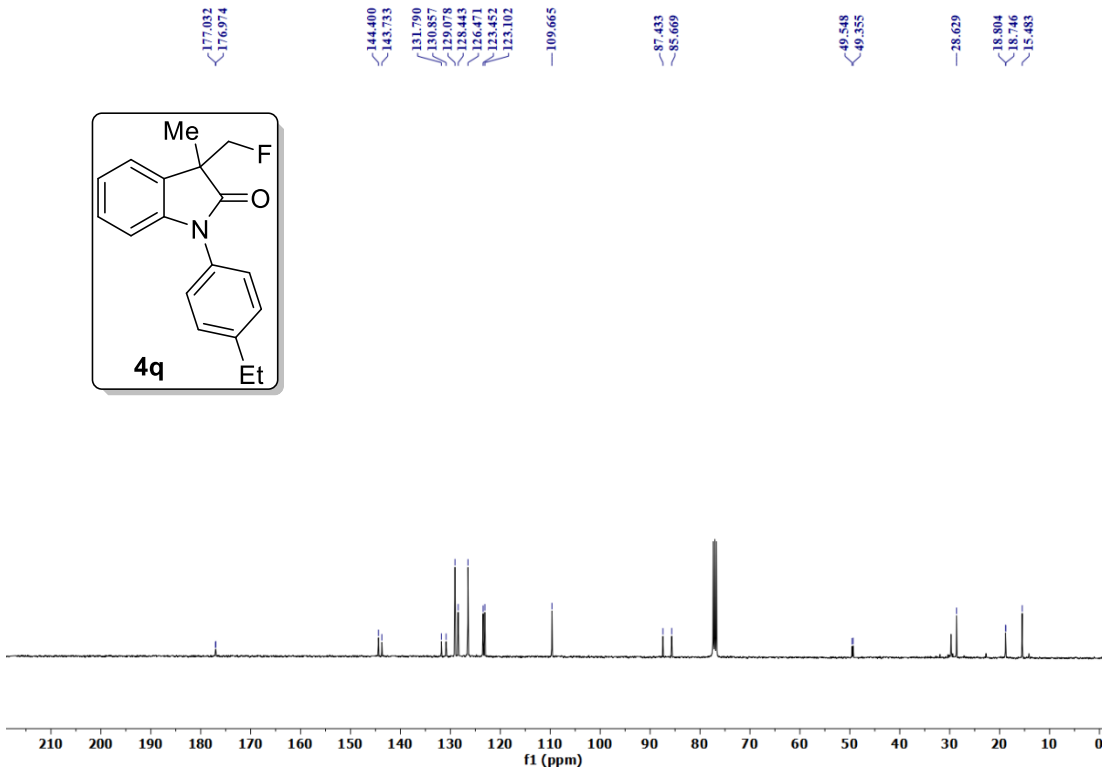
Sample Name	khp-nnr-f-23	**Position**	P1-A4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	24-04-2024-4.d	**ACQ Method**	A60 W40.m	**Comment**		**Acquired Time**	4/24/2024 3:19:35 PM



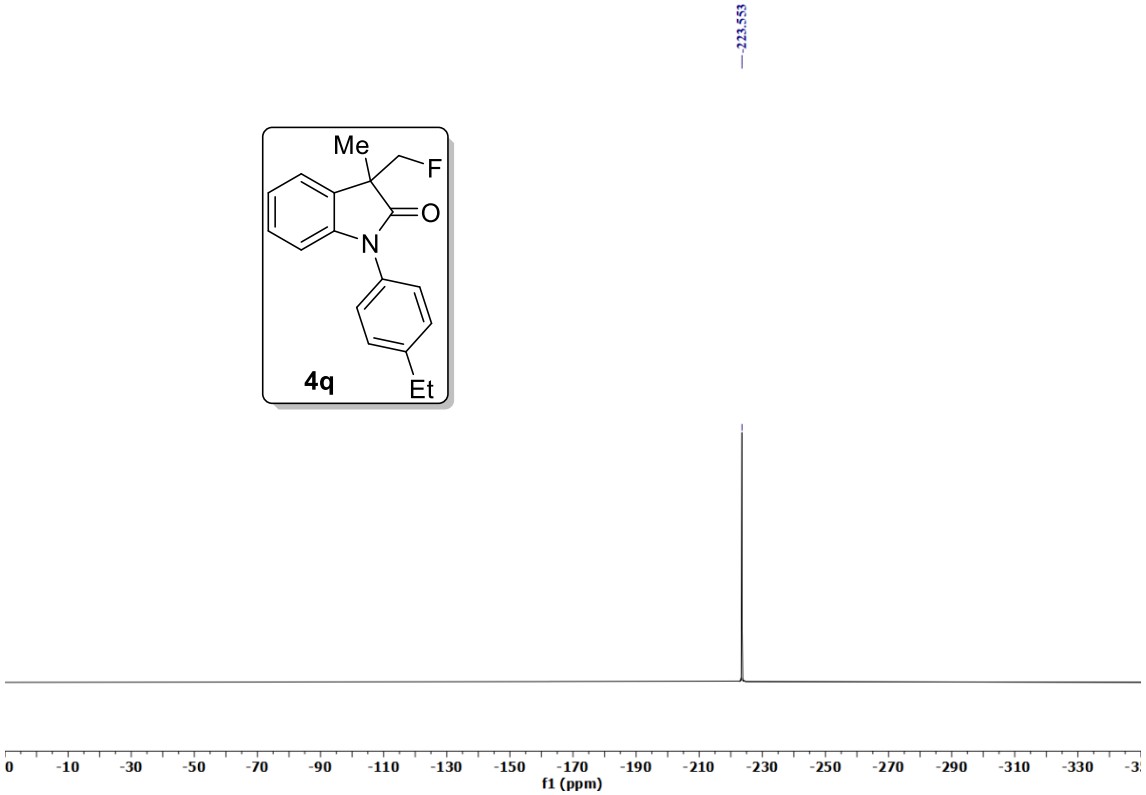
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 1-(4-ethylphenyl)-3-(fluoromethyl)-3-methylindolin-2-one (4q)



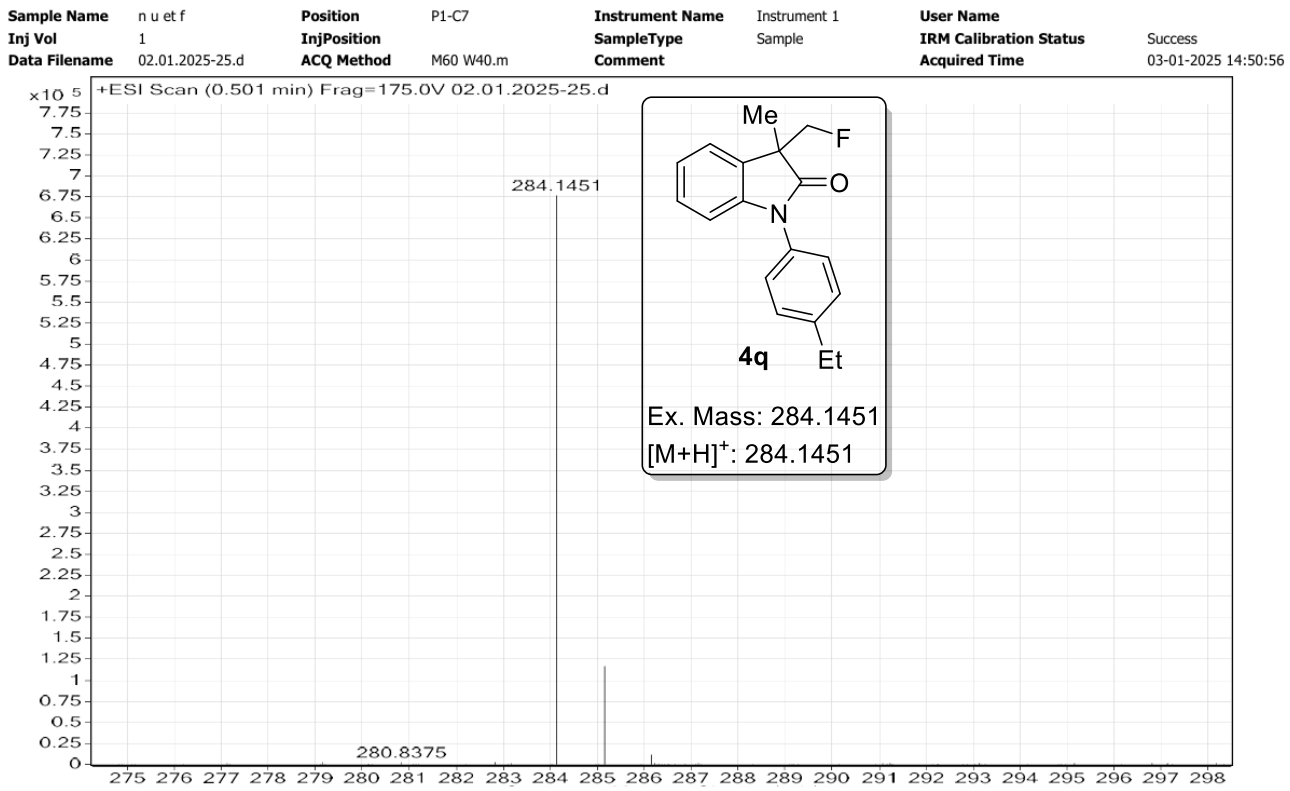
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 1-(4-ethylphenyl)-3-(fluoromethyl)-3-methylindolin-2-one (4q)



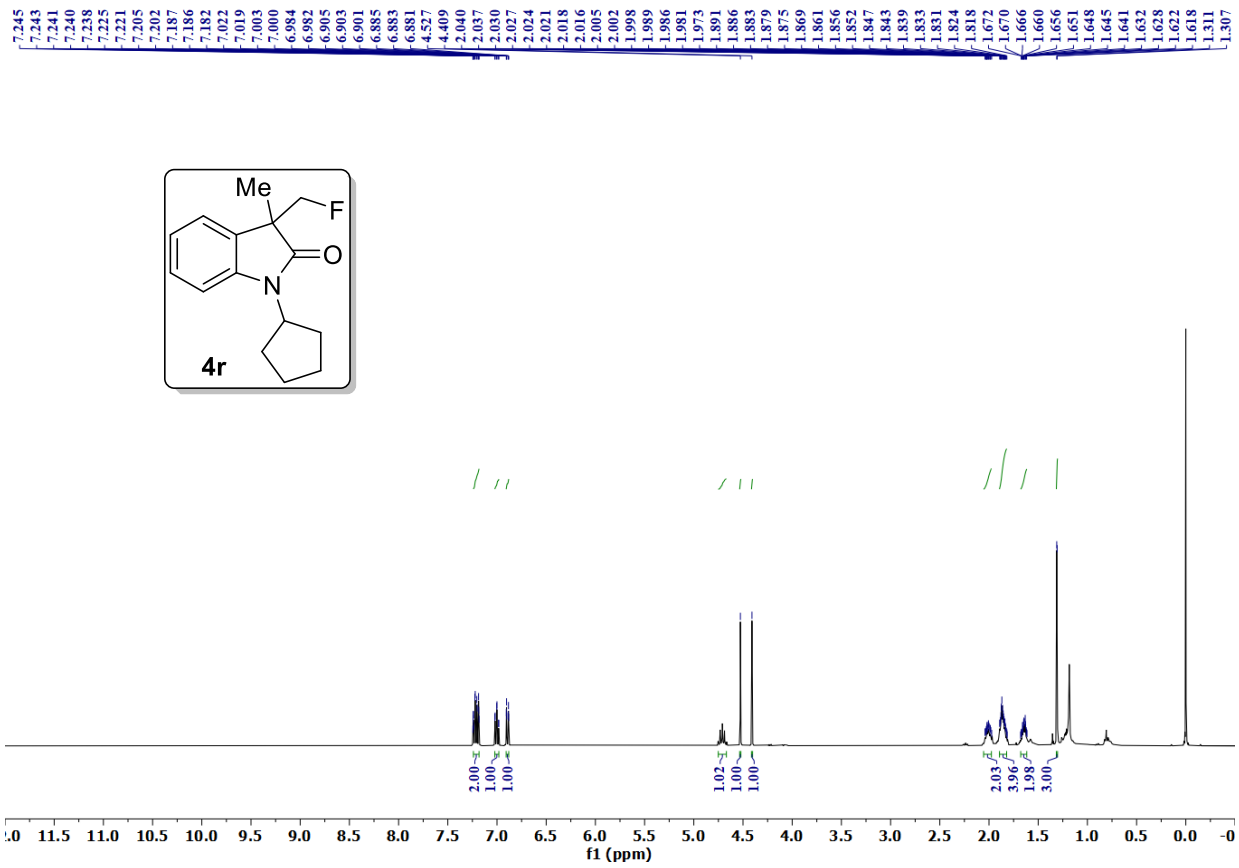
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 1-(4-ethylphenyl)-3-(fluoromethyl)-3-methylindolin-2-one (4q)



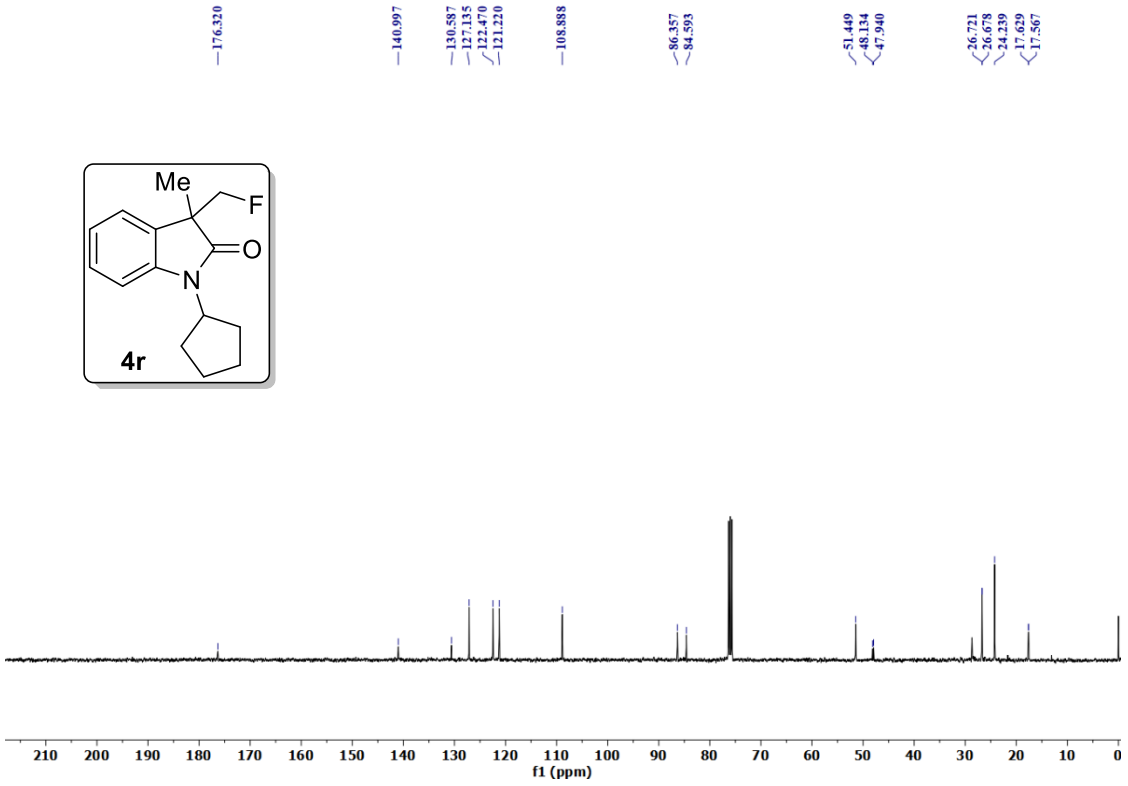
HRMS of 1-(4-ethylphenyl)-3-(fluoromethyl)-3-methylindolin-2-one (4q)



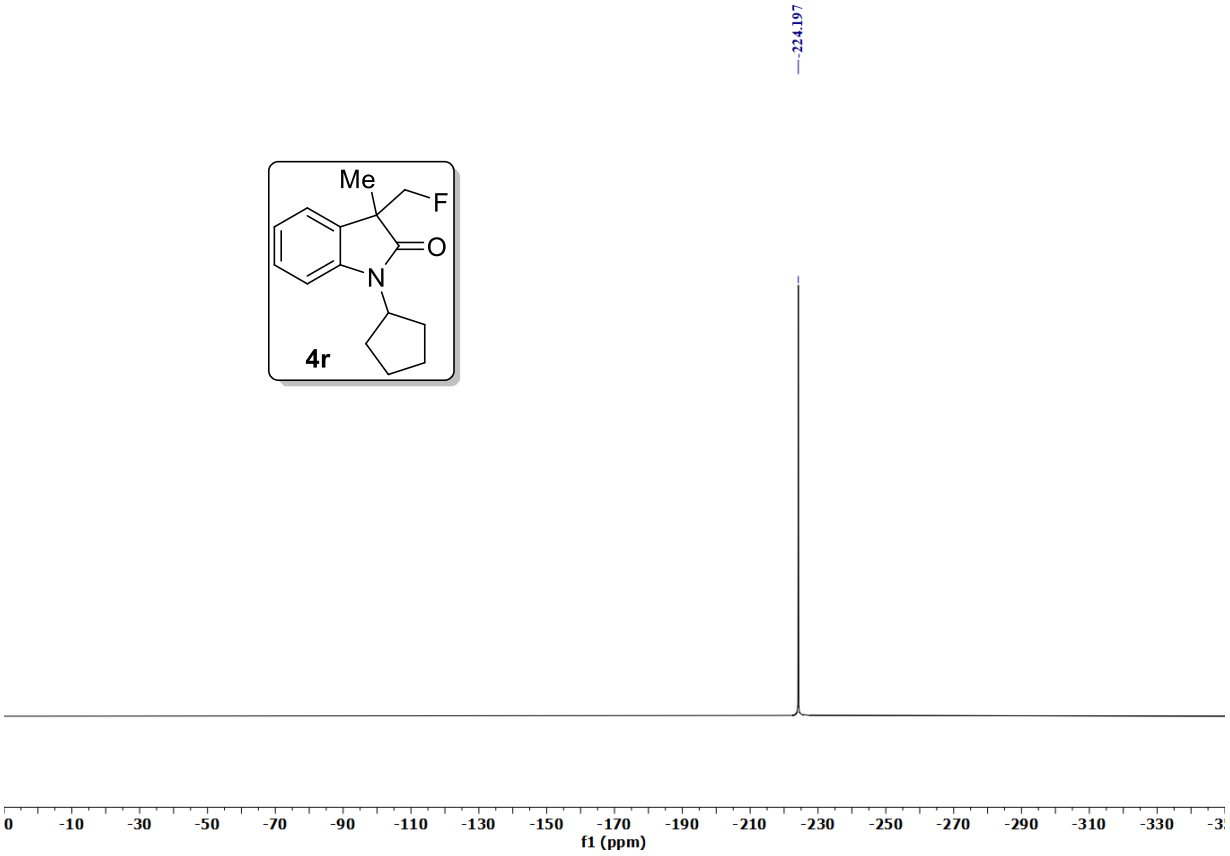
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 1-cyclopentyl-3-(fluoromethyl)-3-methylindolin-2-one (4r)



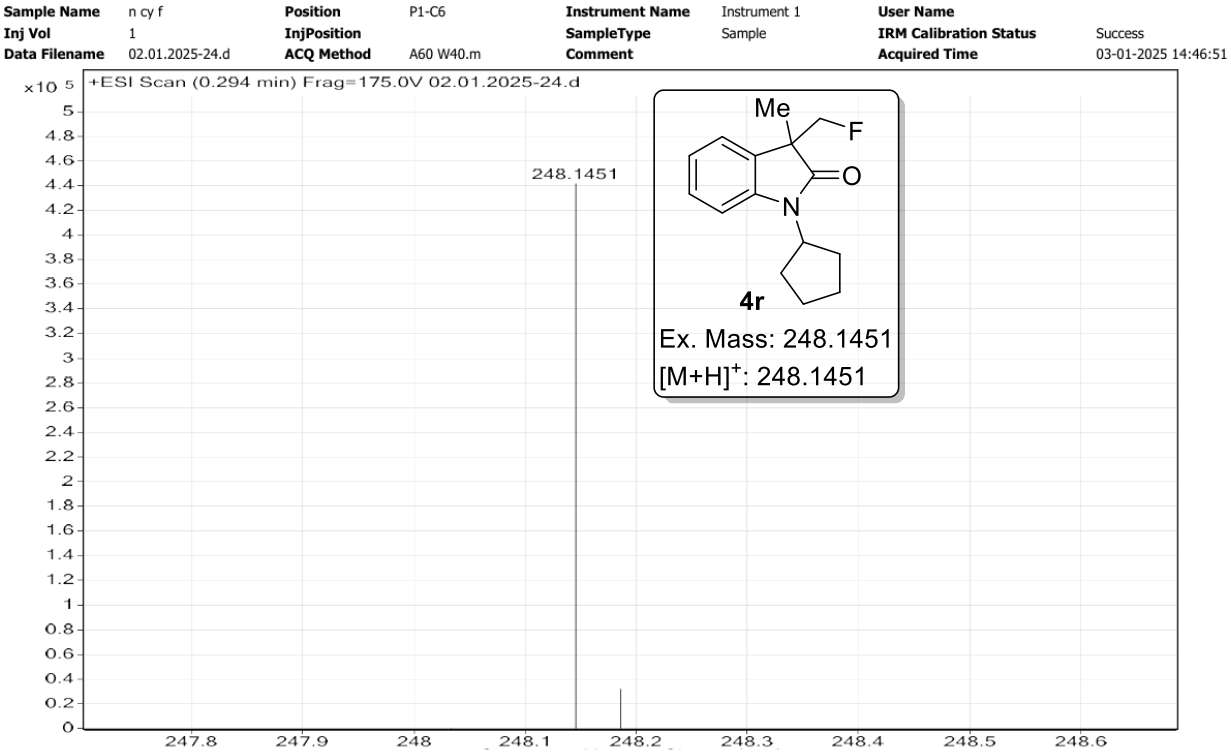
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 1-cyclopentyl-3-(fluoromethyl)-3-methylindolin-2-one (4r)



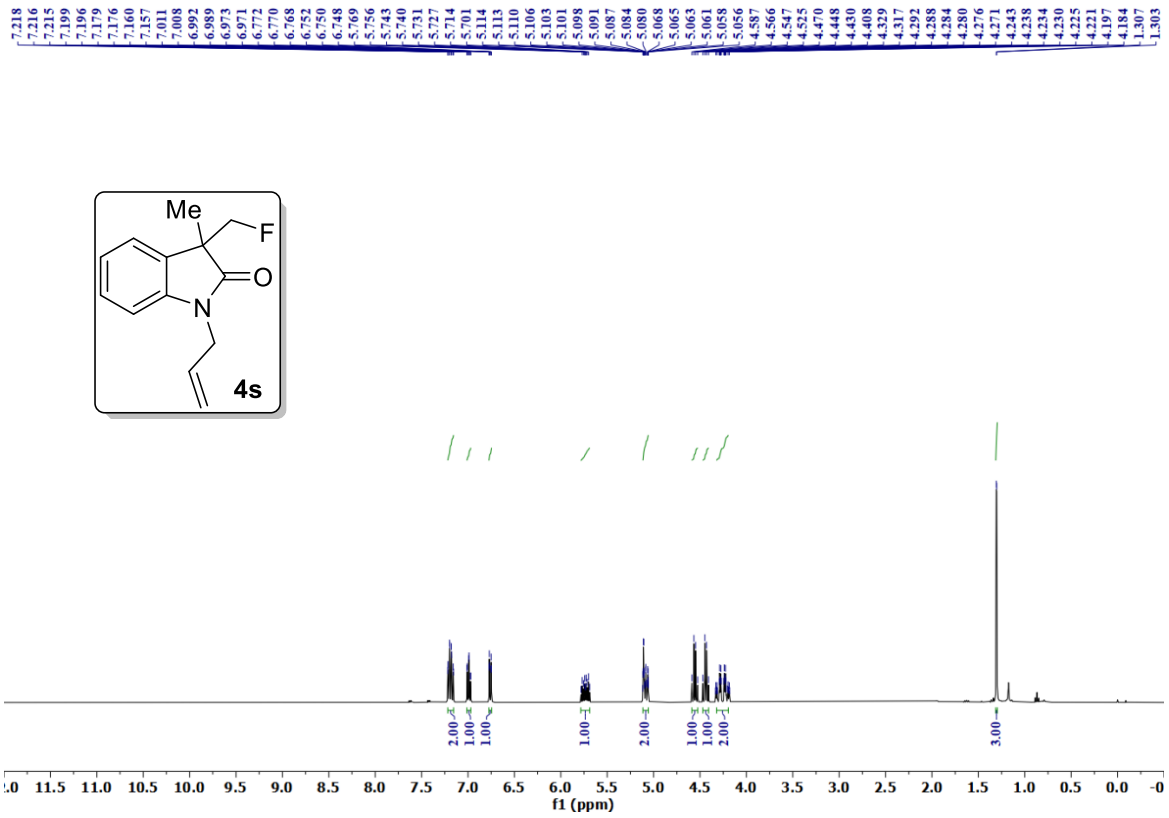
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 1-cyclopentyl-3-(fluoromethyl)-3-methylindolin-2-one (4r)



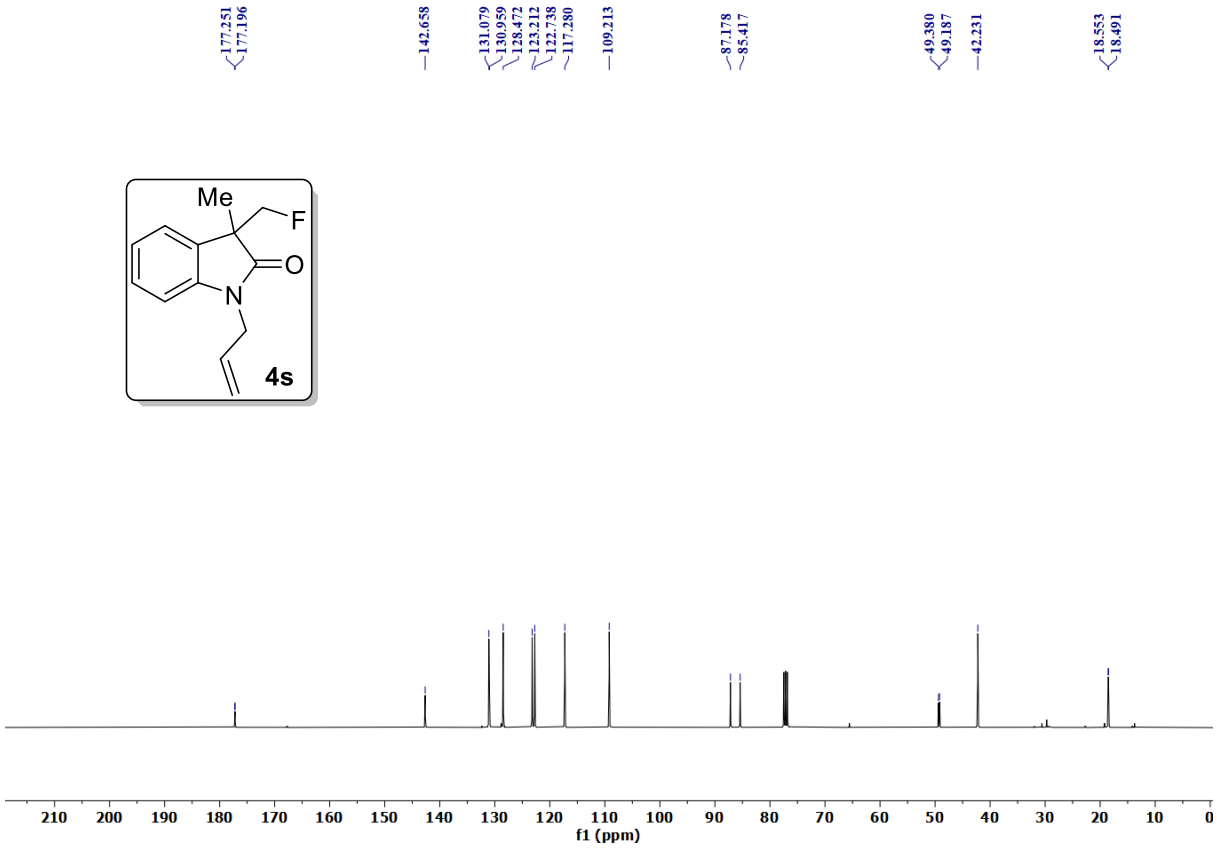
HRMS of 1-cyclopentyl-3-(fluoromethyl)-3-methylindolin-2-one (4r)



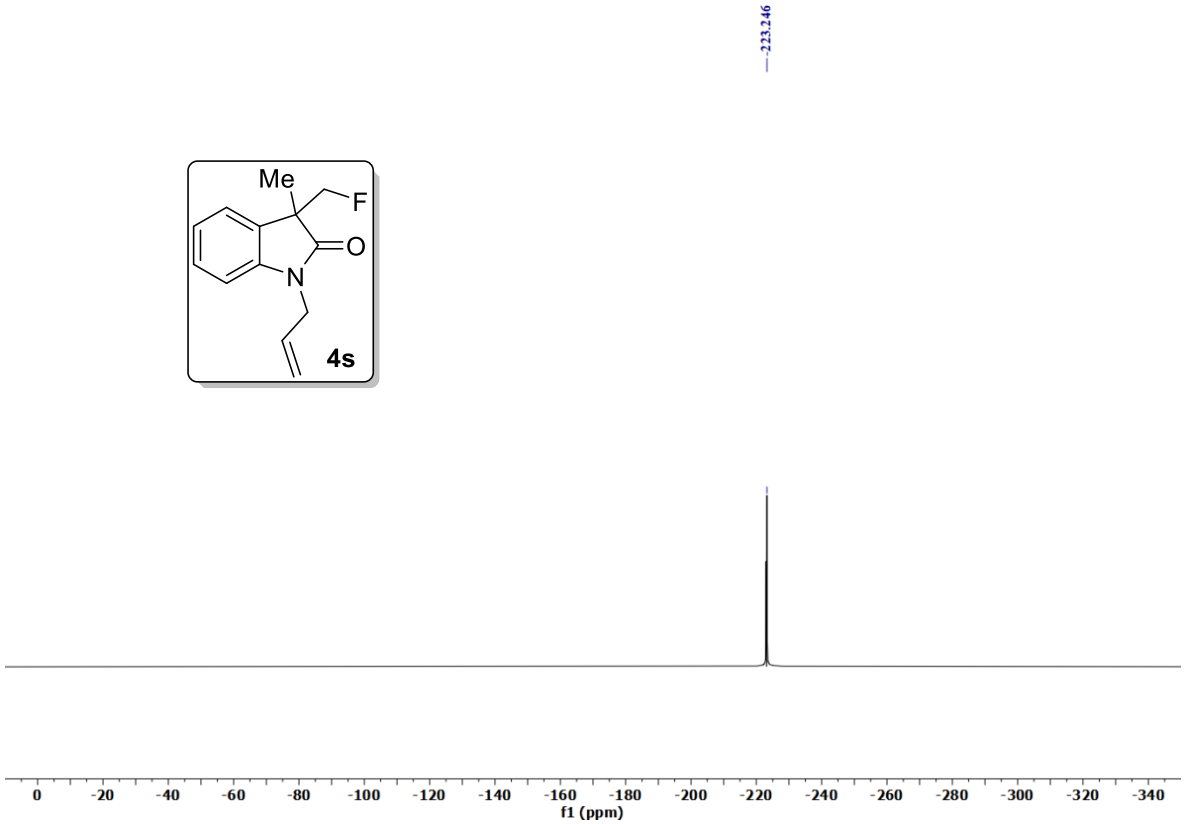
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 1-allyl-3-(fluoromethyl)-3-methylindolin-2-one (4s)



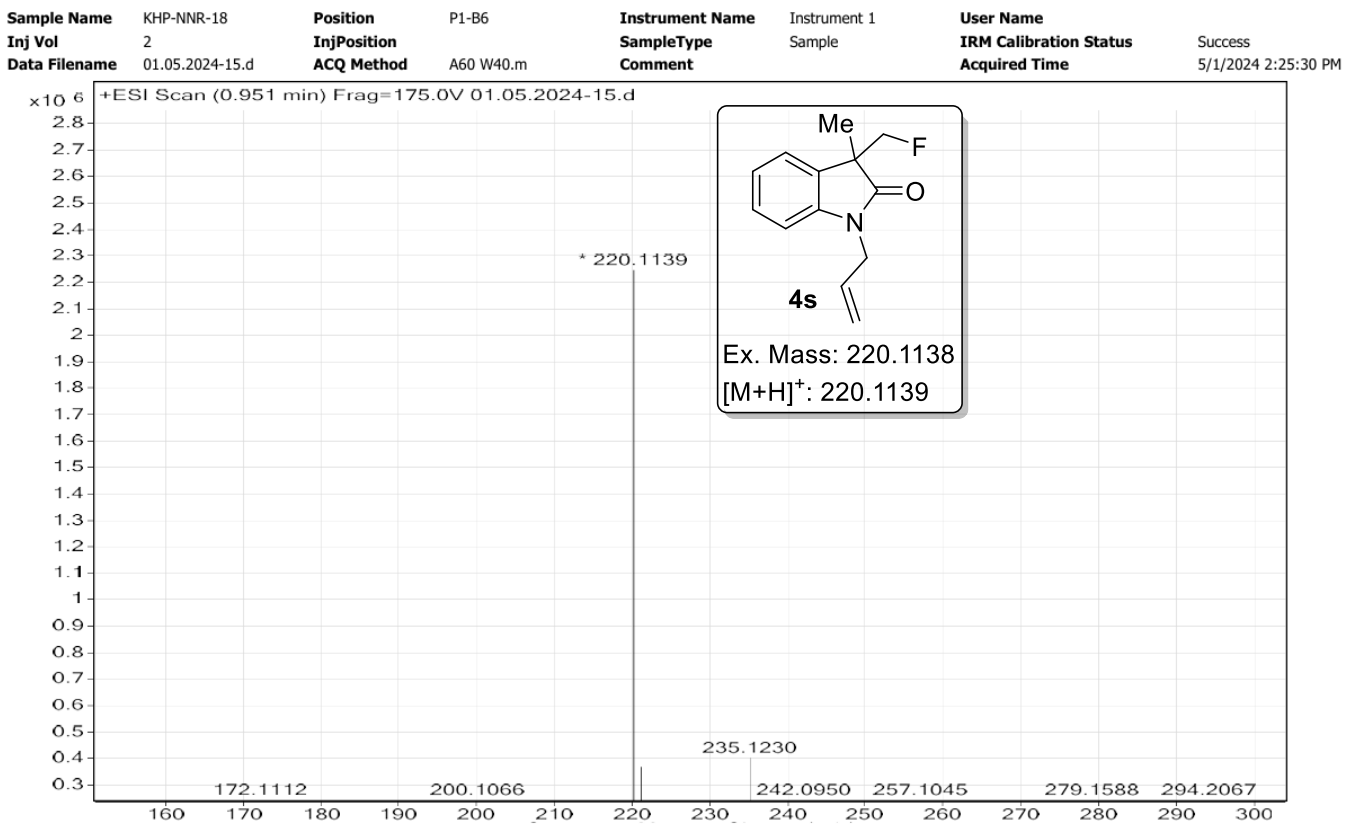
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 1-allyl-3-(fluoromethyl)-3-methylindolin-2-one (4s)



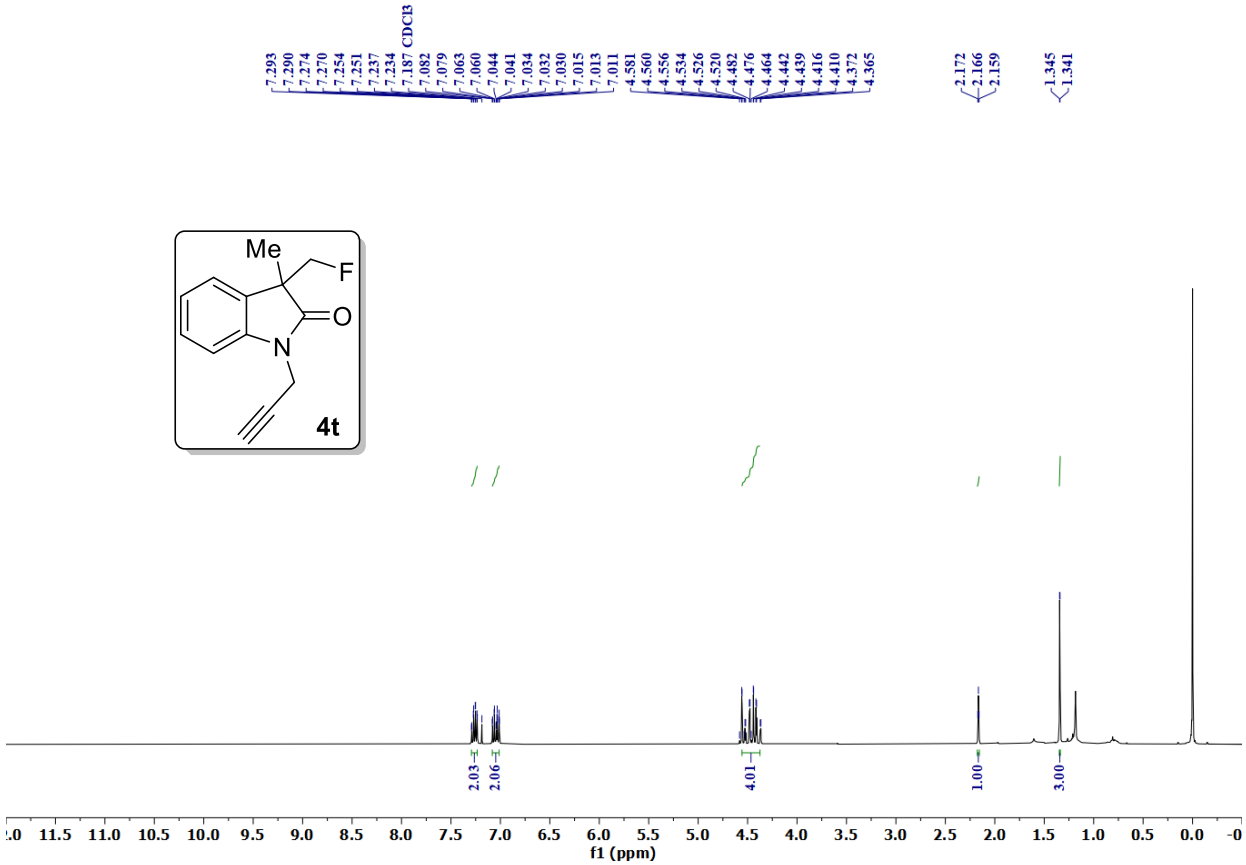
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 1-allyl-3-(fluoromethyl)-3-methylindolin-2-one (4s)



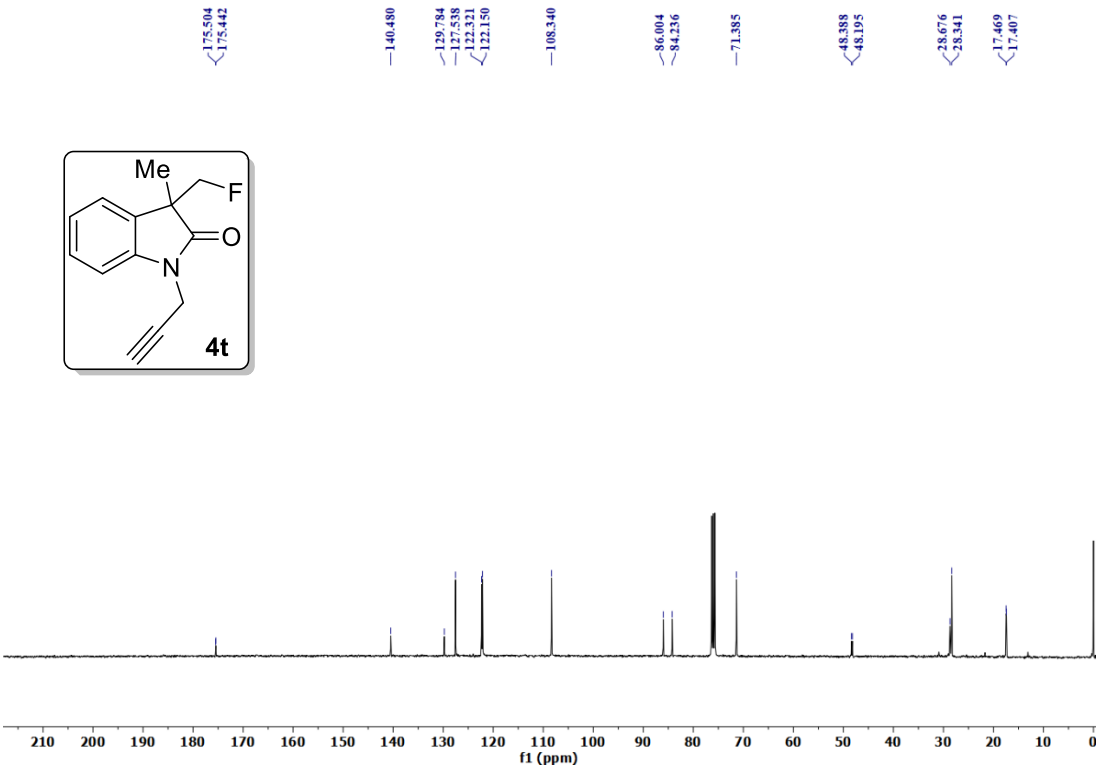
HRMS of 1-allyl-3-(fluoromethyl)-3-methylindolin-2-one (4s)



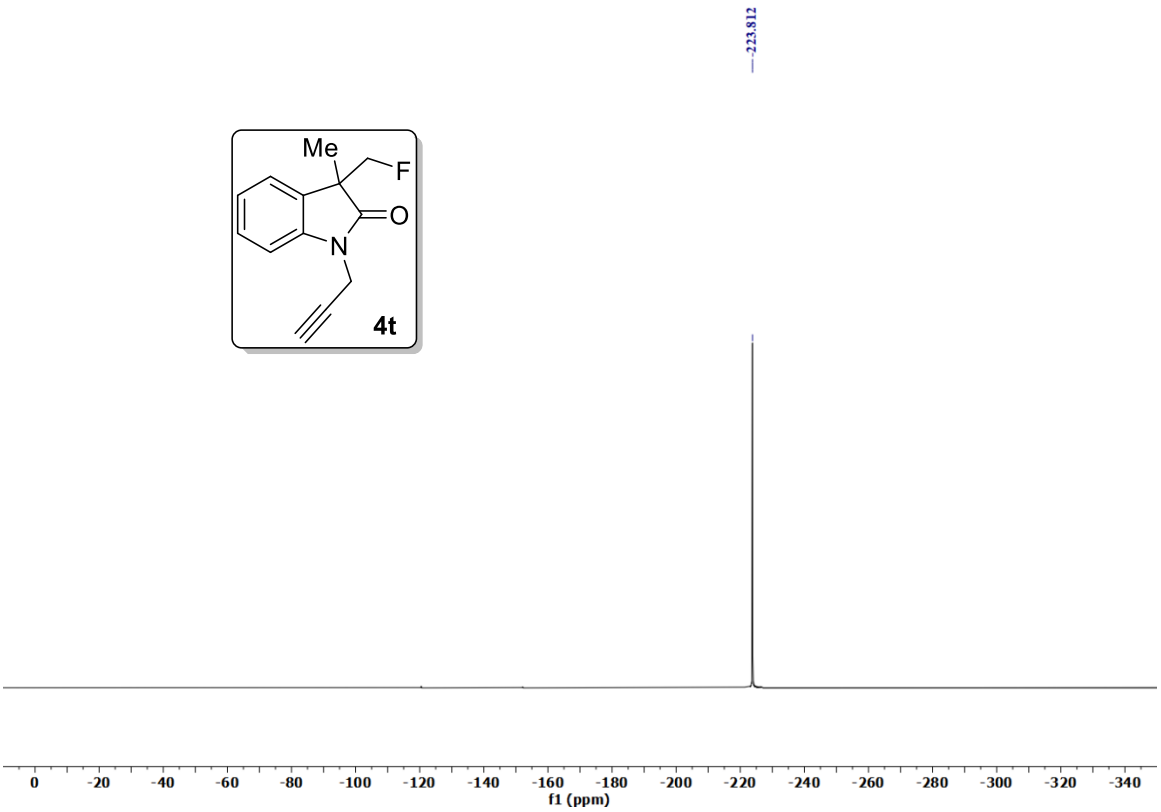
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methyl-1-(prop-2-yn-1-yl)indolin-2-one (4t)



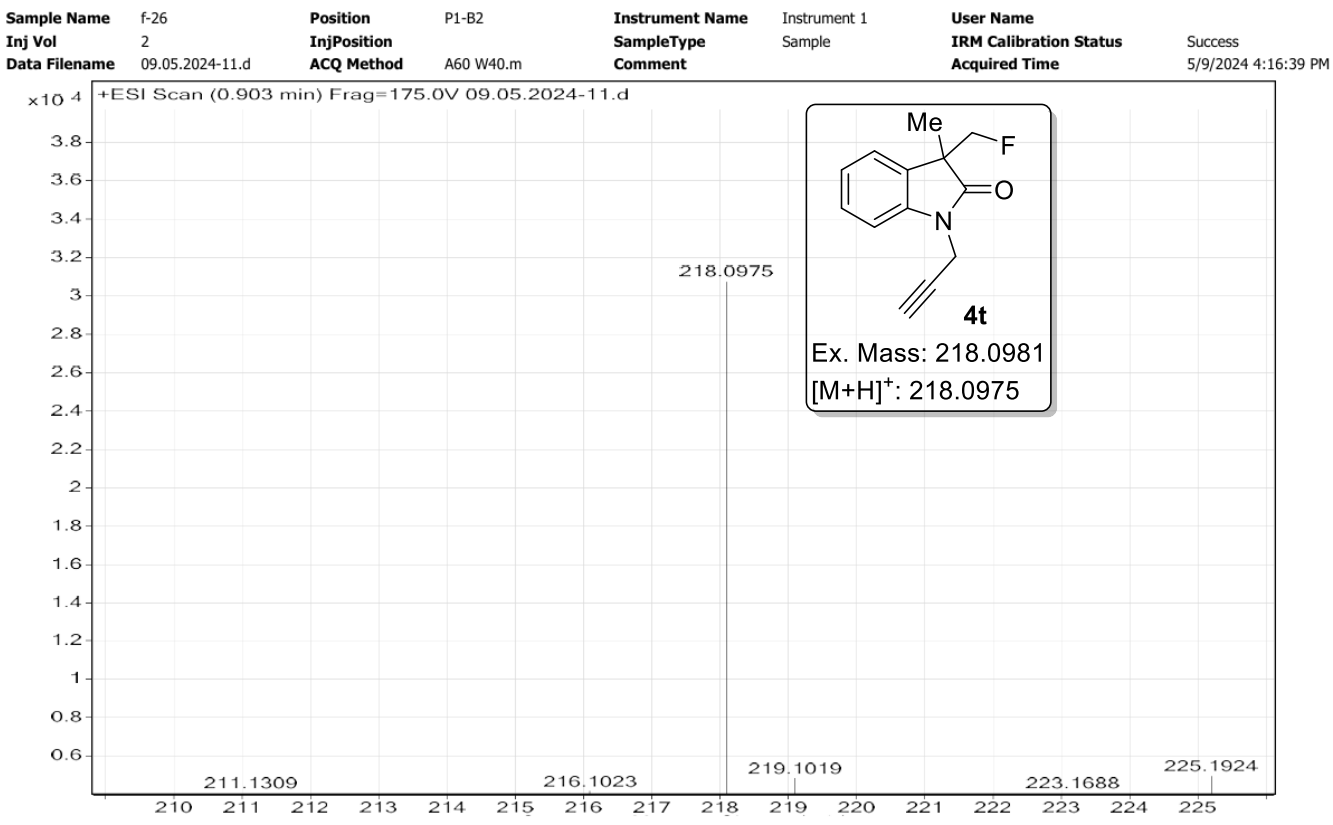
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methyl-1-(prop-2-yn-1-yl)indolin-2-one (4t)



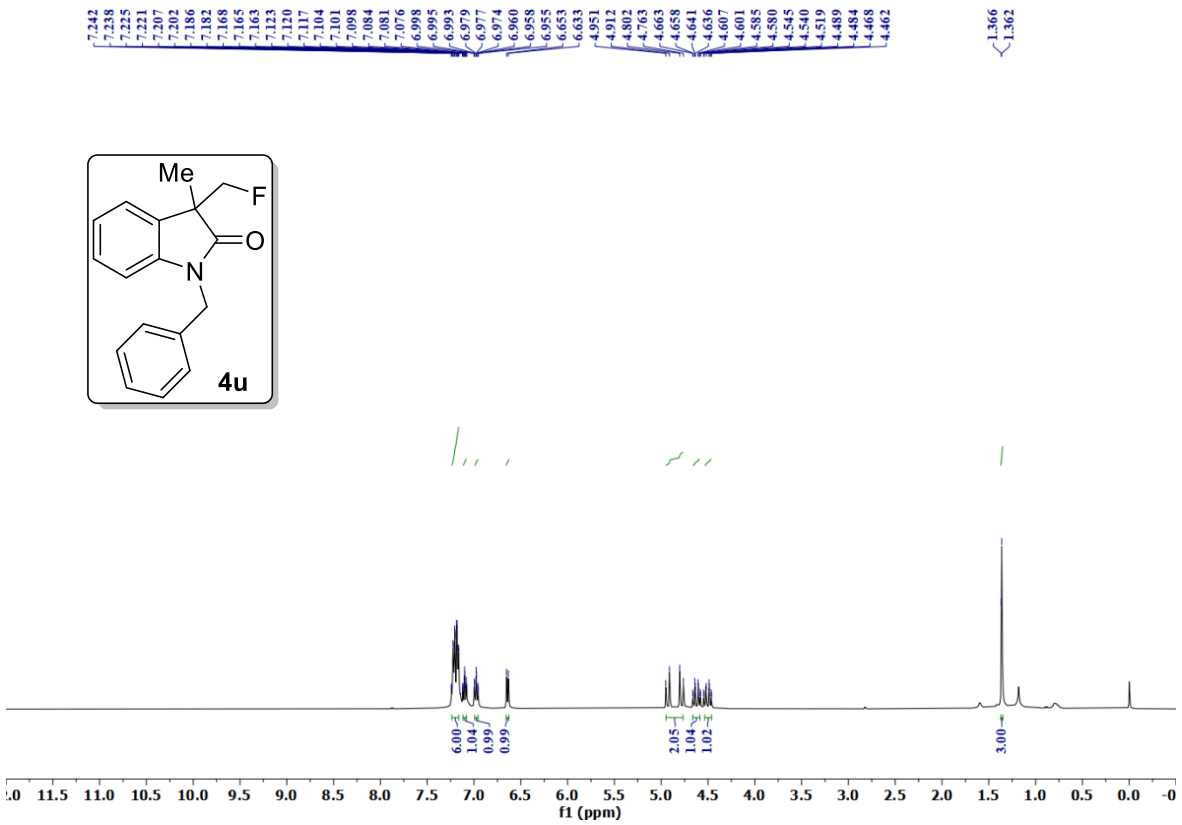
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methyl-1-(prop-2-yn-1-yl)indolin-2-one (4t)



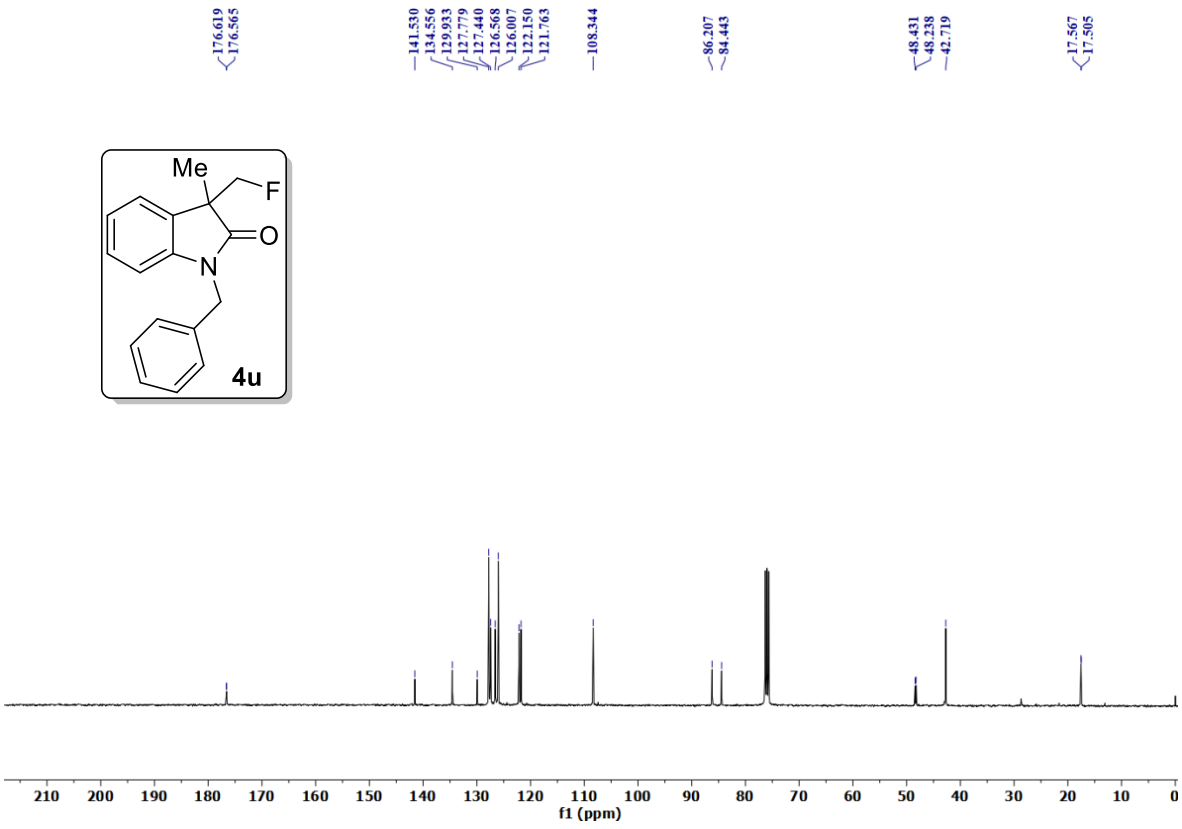
HRMS of 3-(fluoromethyl)-3-methyl-1-(prop-2-yn-1-yl)indolin-2-one (4t)



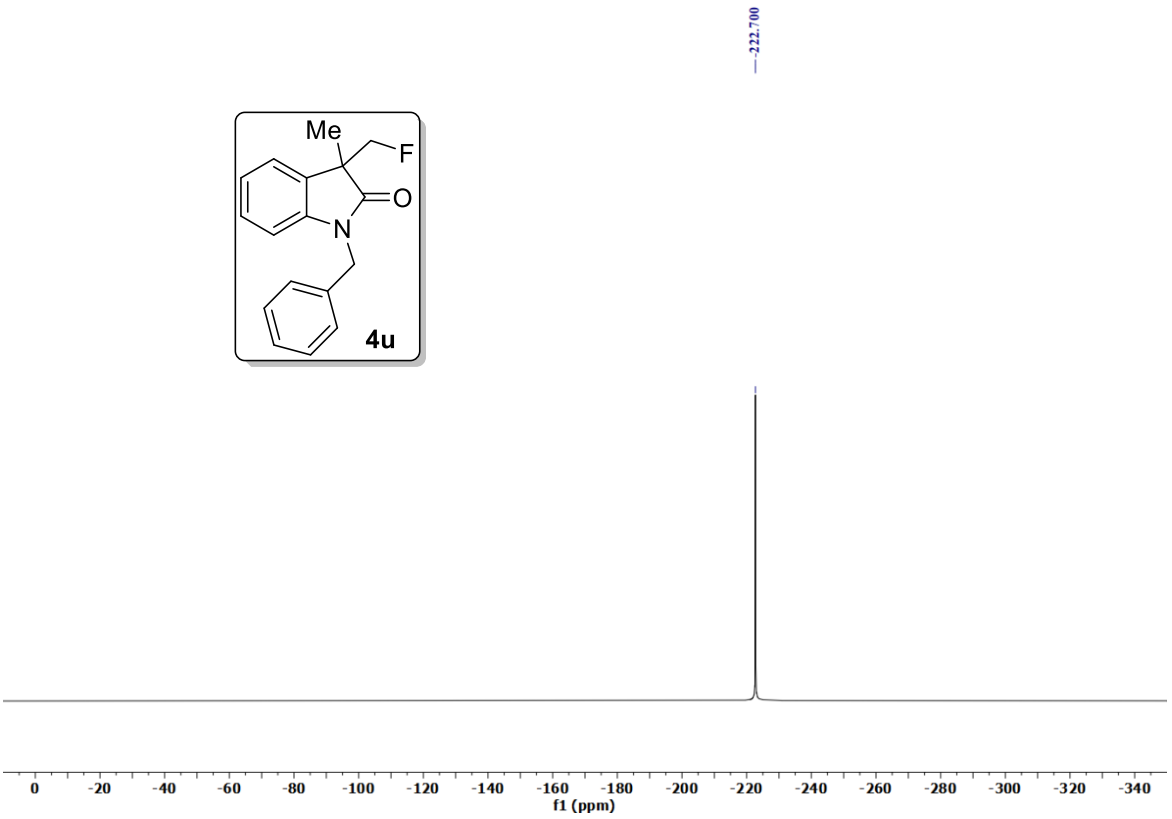
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 1-benzyl-3-(fluoromethyl)-3-methylindolin-2-one (4u)



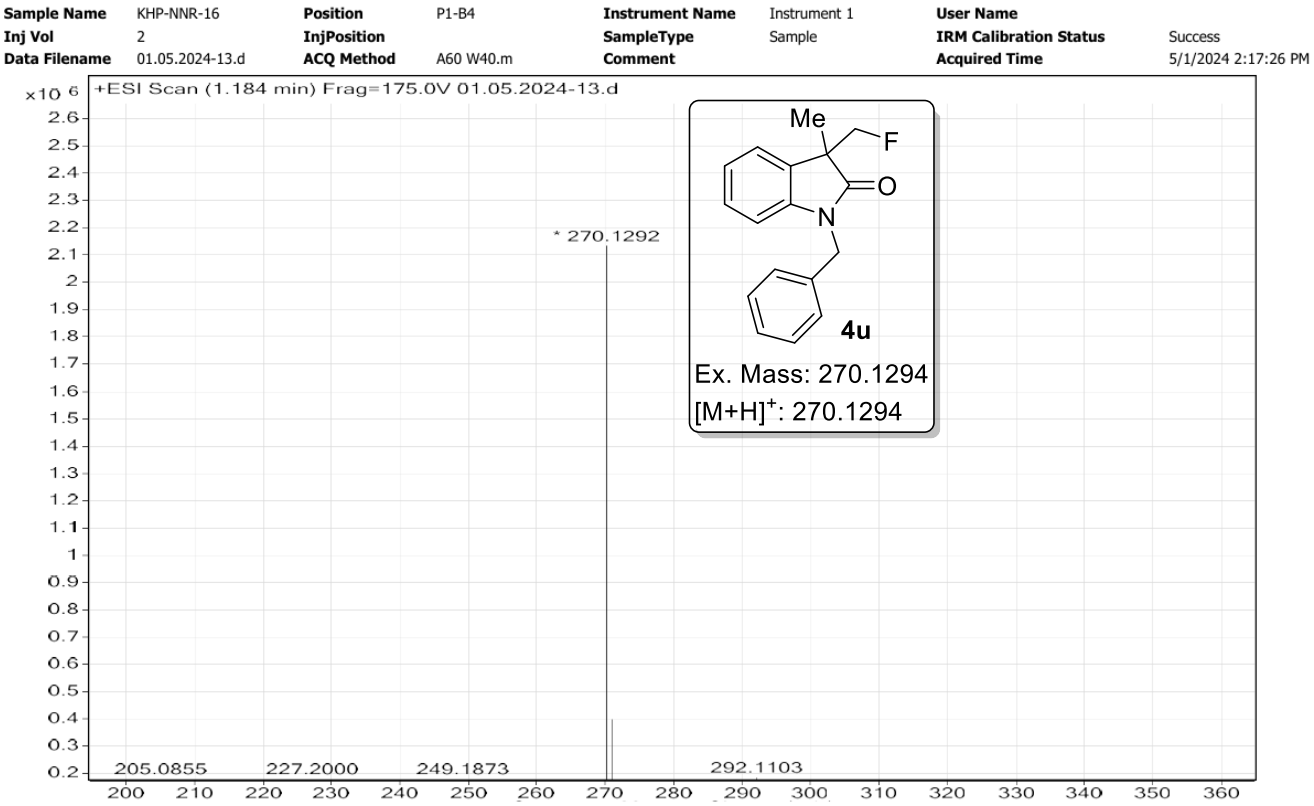
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 1-benzyl-3-(fluoromethyl)-3-methylindolin-2-one (4u)



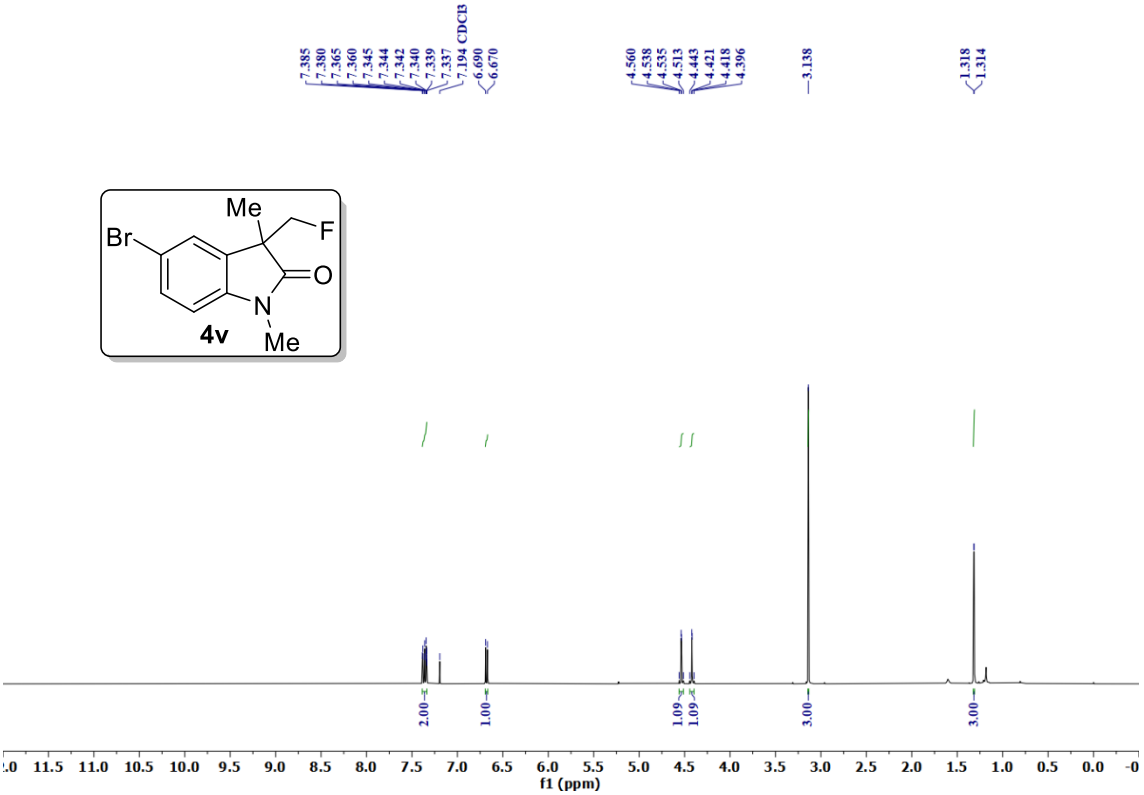
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 1-benzyl-3-(fluoromethyl)-3-methylindolin-2-one (4u)



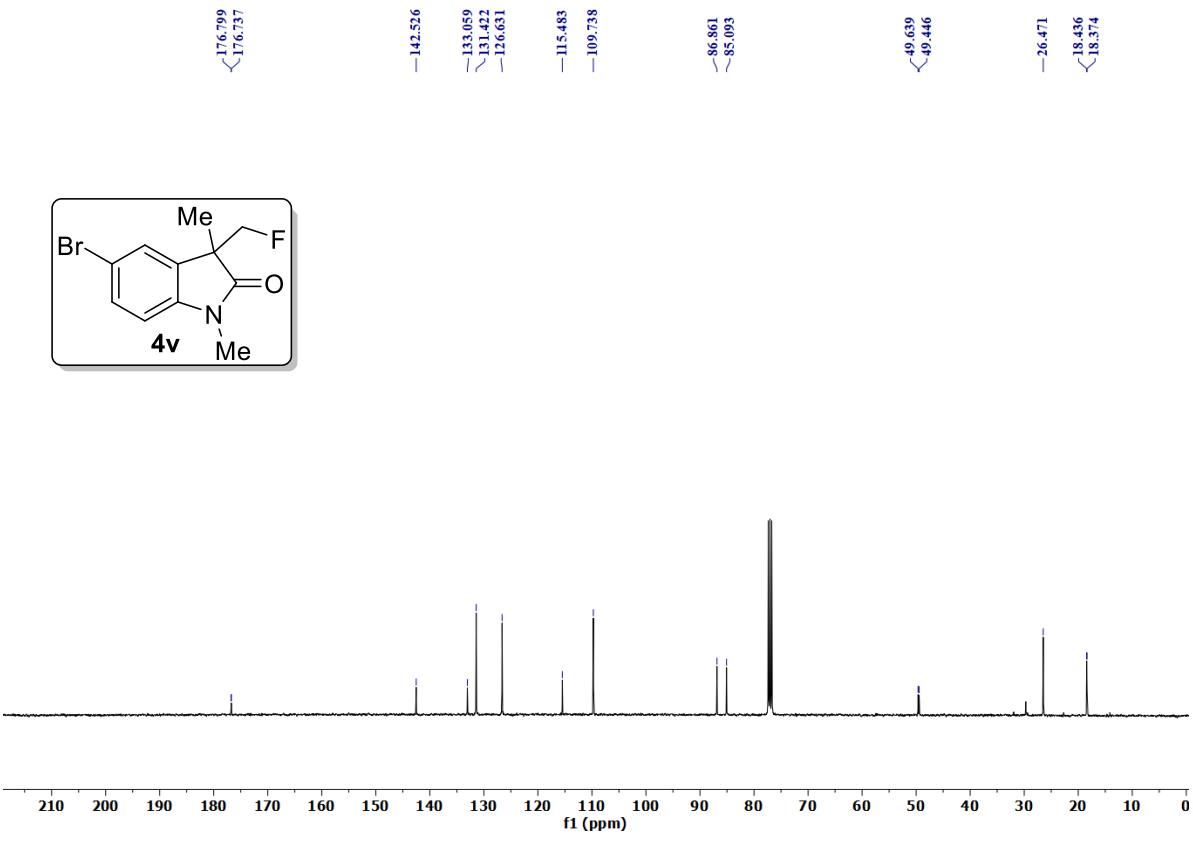
HRMS of 1-benzyl-3-(fluoromethyl)-3-methylindolin-2-one (4u)



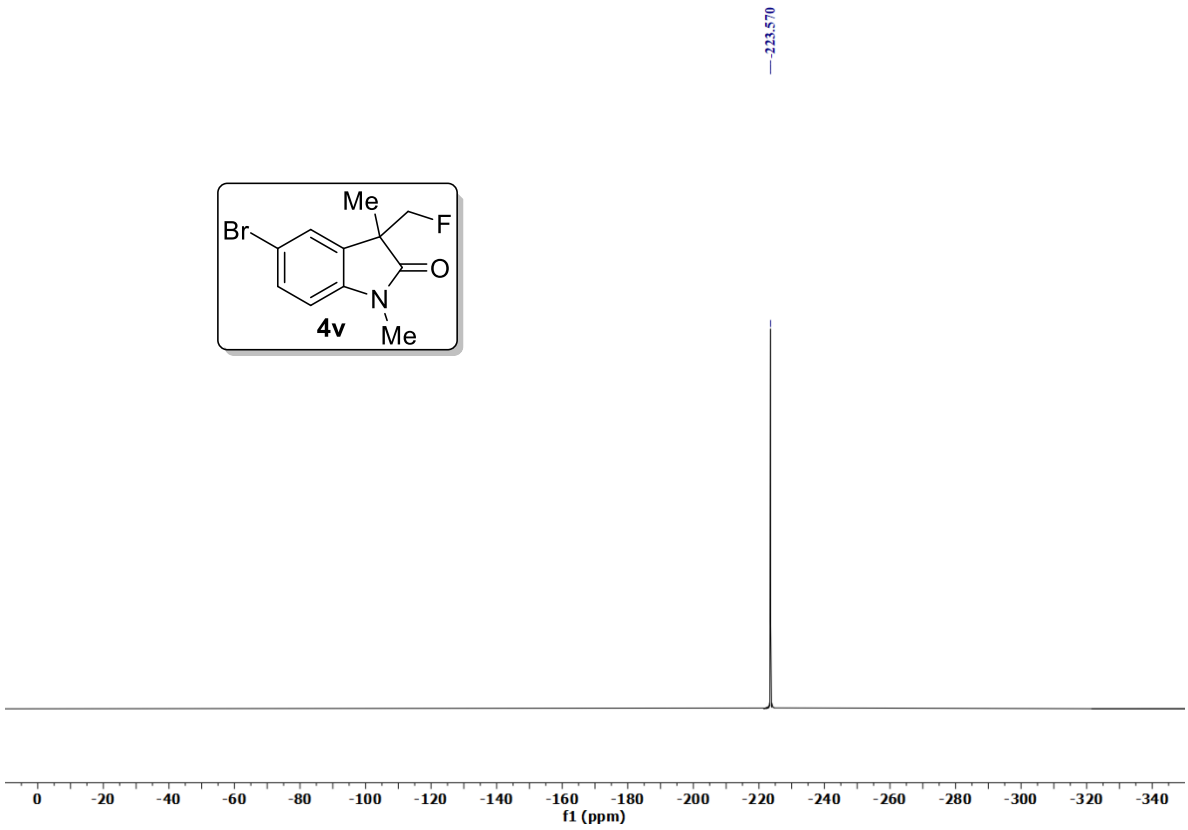
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5-bromo-3-(fluoromethyl)-1,3-dimethylindolin-2-one (4v)



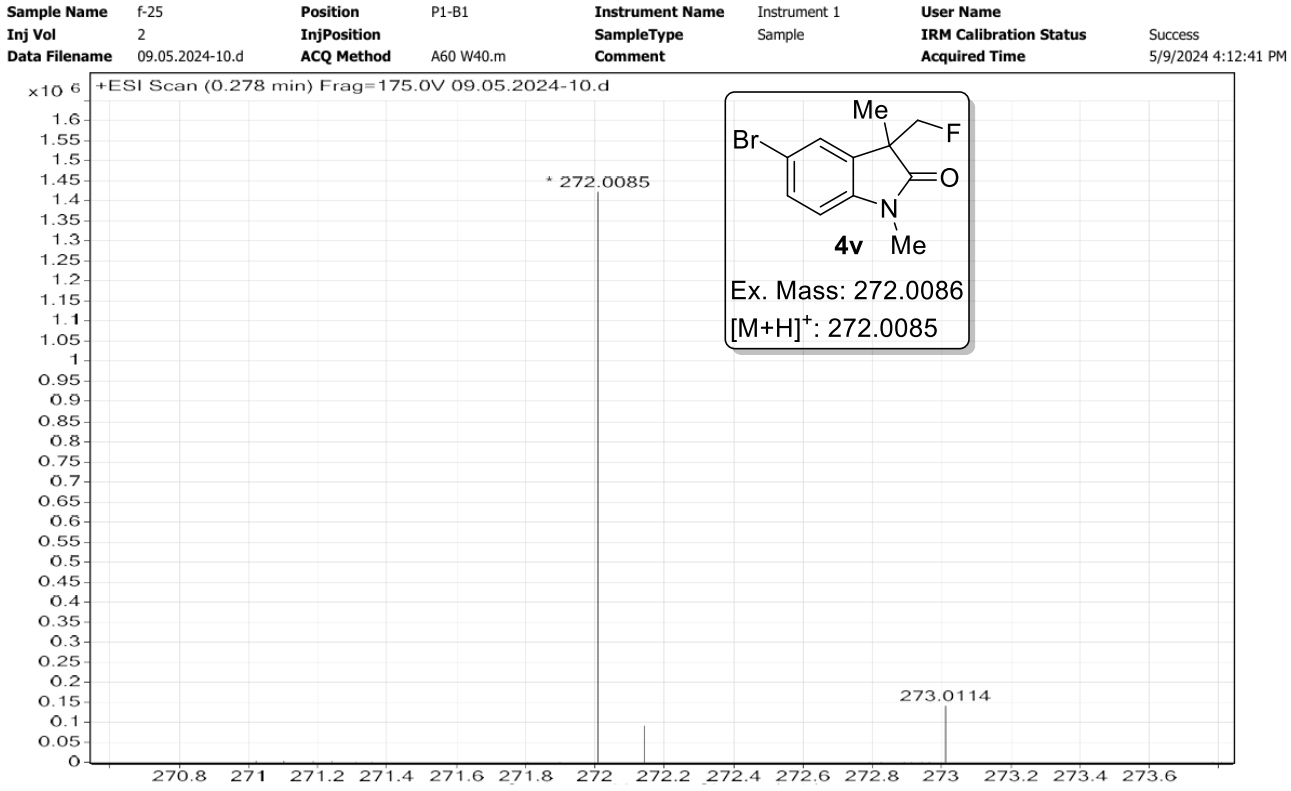
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 5-bromo-3-(fluoromethyl)-1,3-dimethylindolin-2-one (4v)



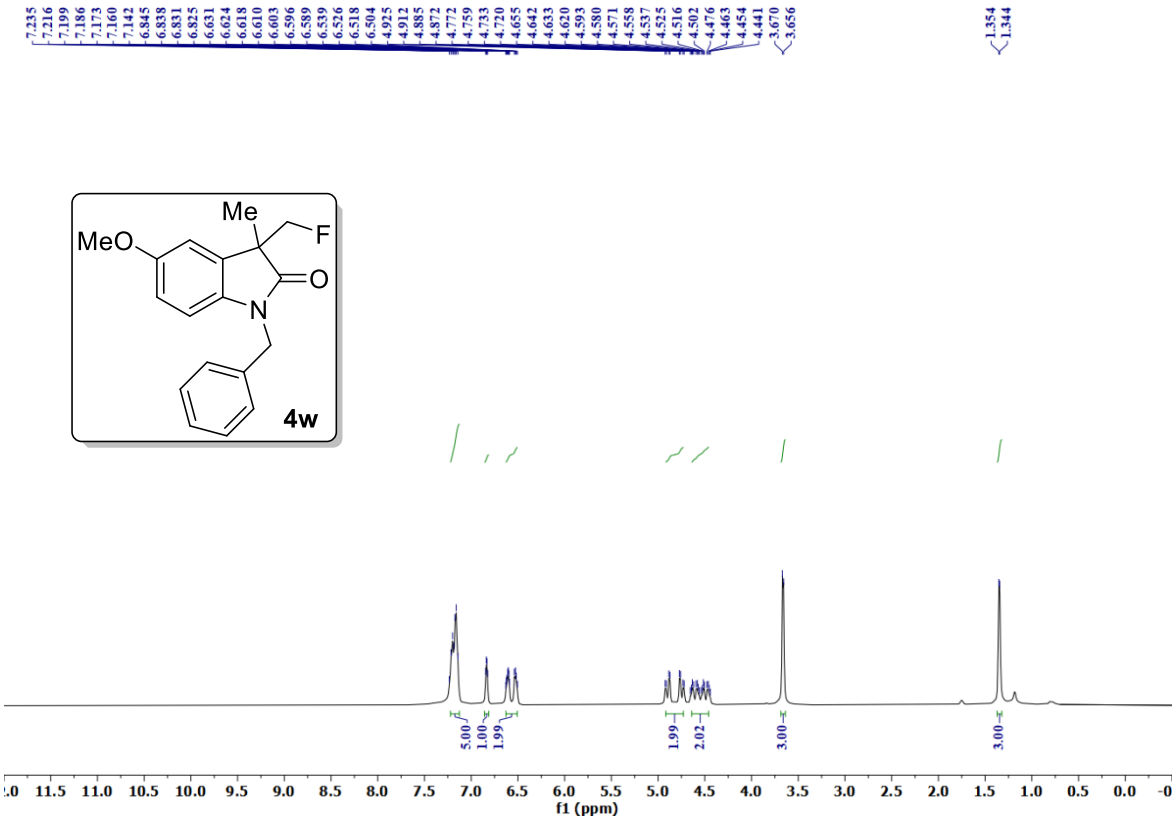
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 5-bromo-3-(fluoromethyl)-1,3-dimethylindolin-2-one (4v)



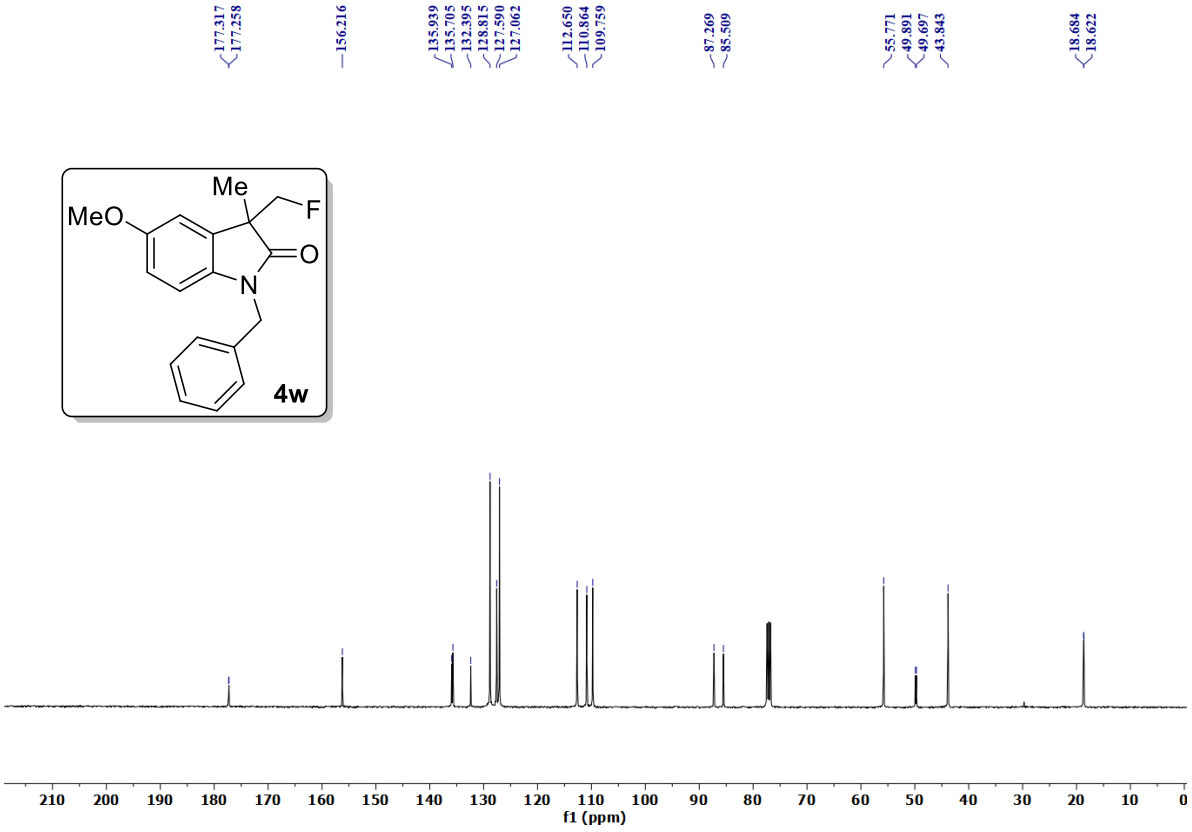
HRMS of 5-bromo-3-(fluoromethyl)-1,3-dimethylindolin-2-one (4v)



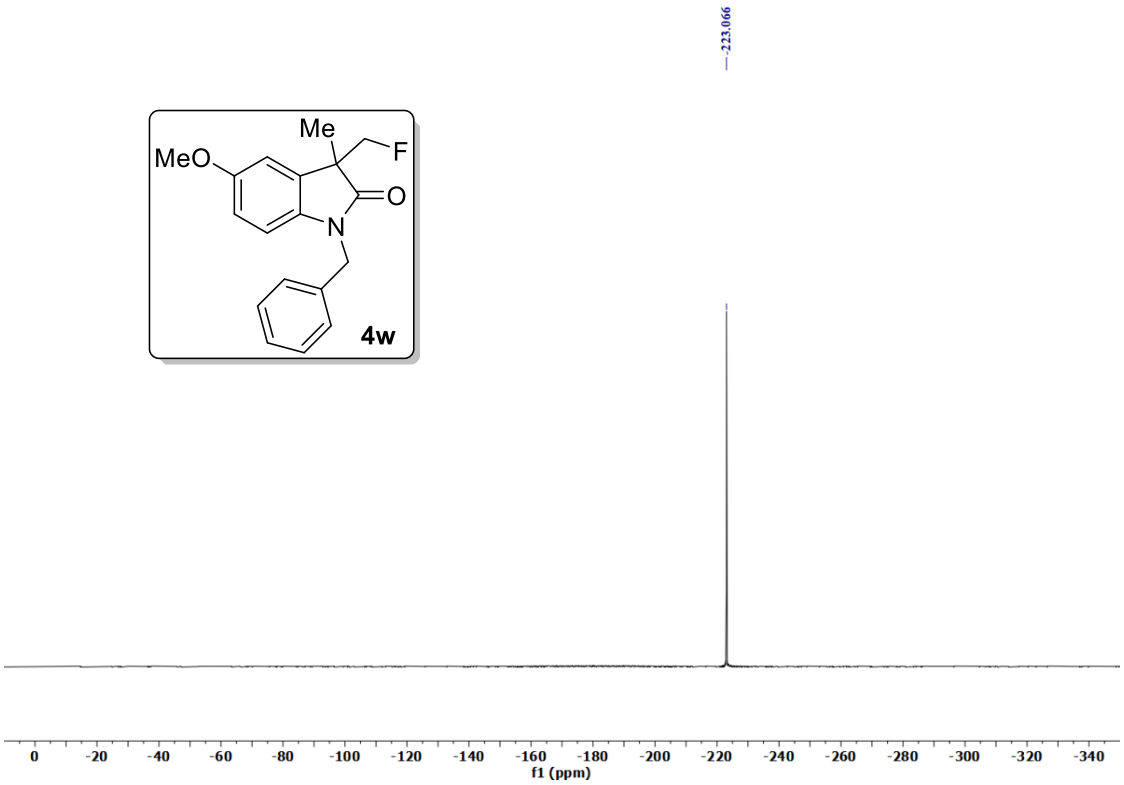
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 1-benzyl-3-(fluoromethyl)-5-methoxy-3-methylindolin-2-one (4w)



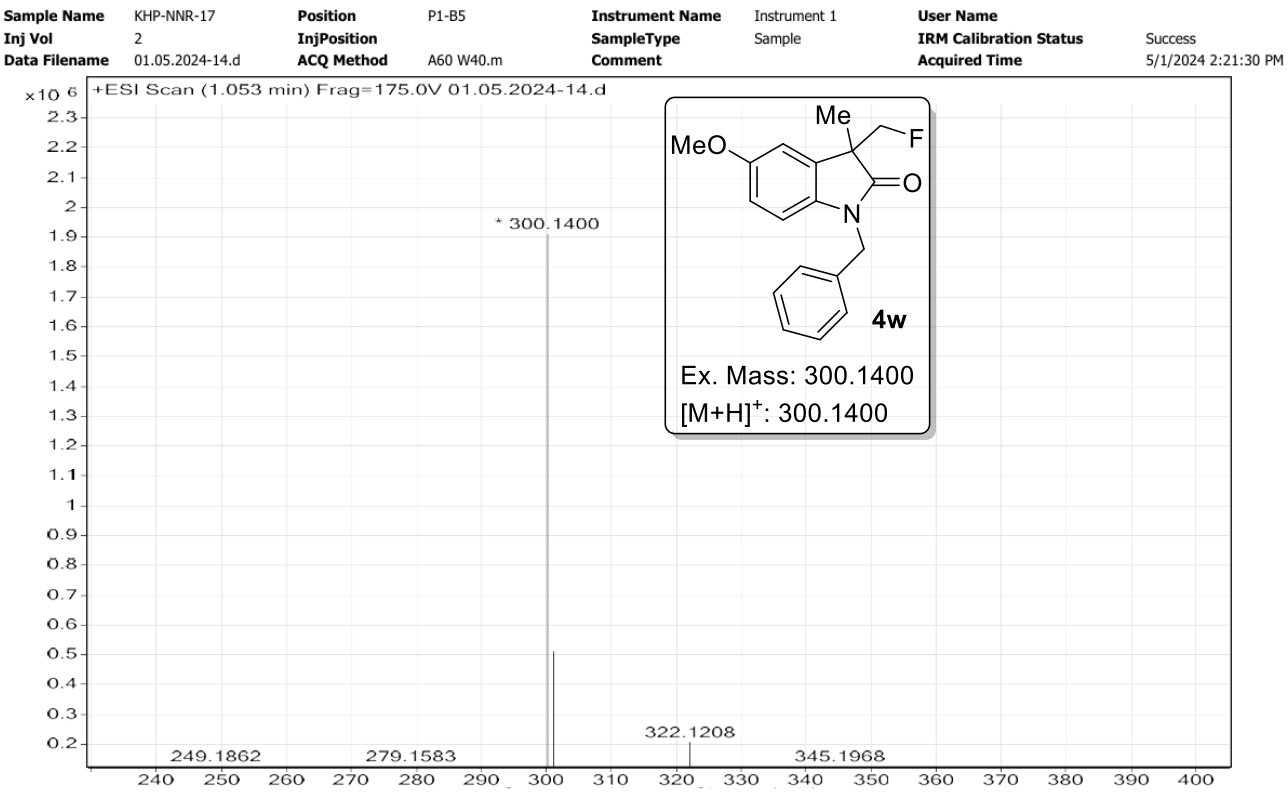
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 1-benzyl-3-(fluoromethyl)-5-methoxy-3-methylindolin-2-one (4w)



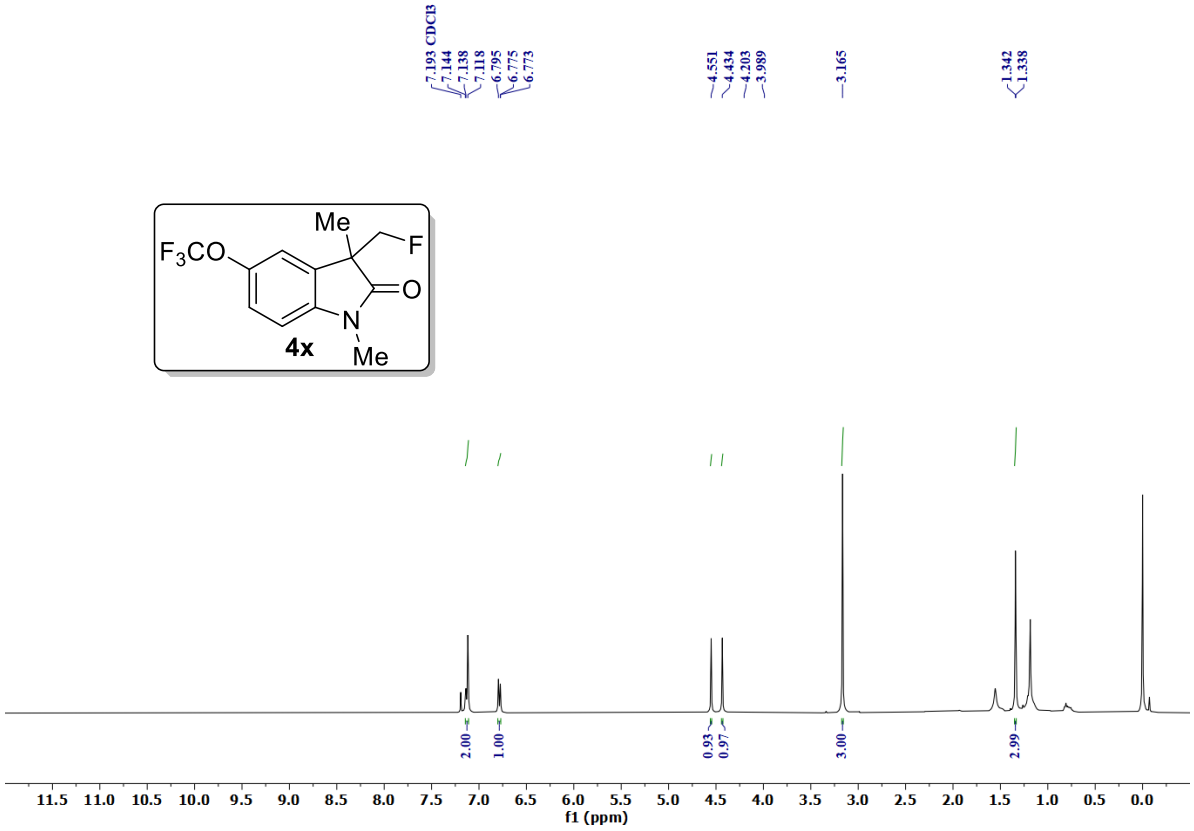
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 1-benzyl-3-(fluoromethyl)-5-methoxy-3-methylindolin-2-one (4w)



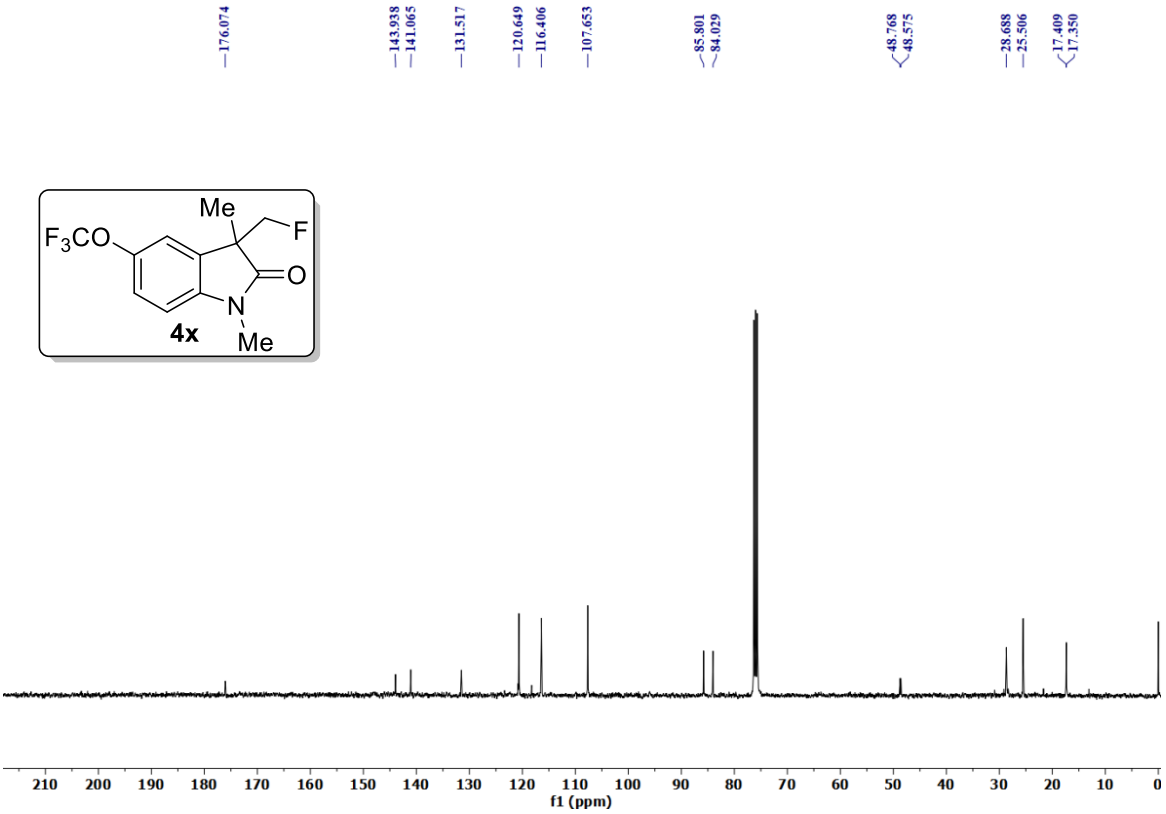
HRMS of 1-benzyl-3-(fluoromethyl)-5-methoxy-3-methylindolin-2-one (4w)



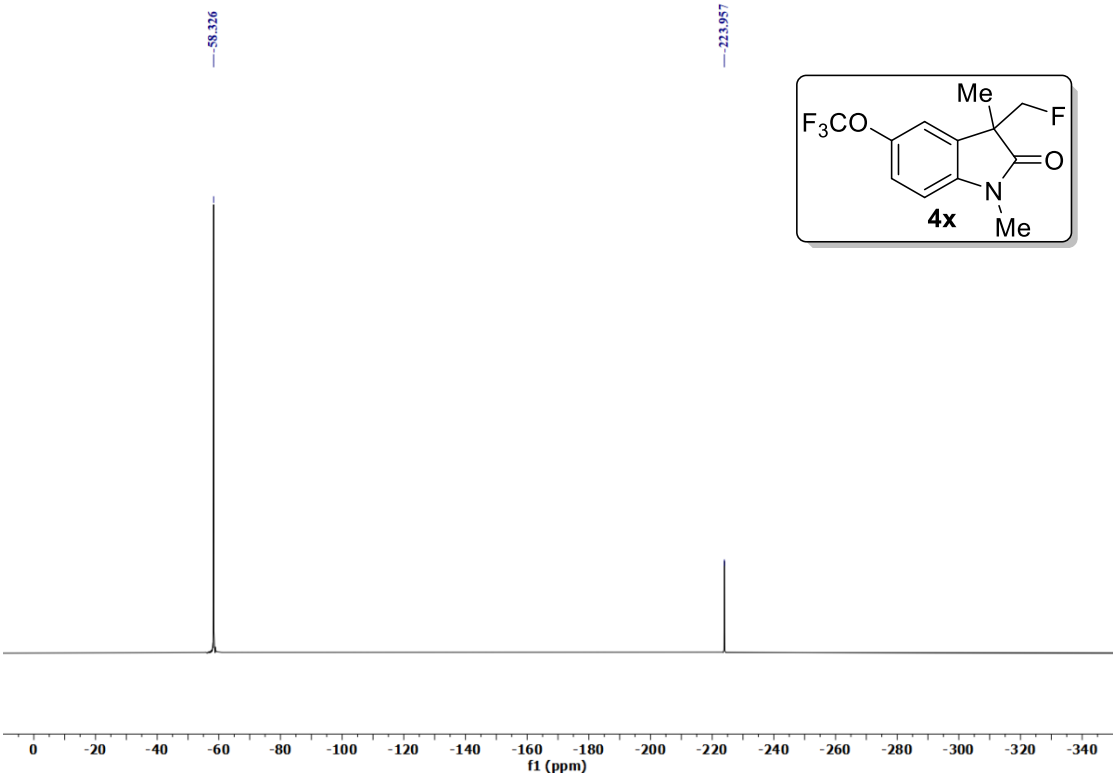
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-1,3-dimethyl-5-(trifluoromethoxy)indolin-2-one (4x)



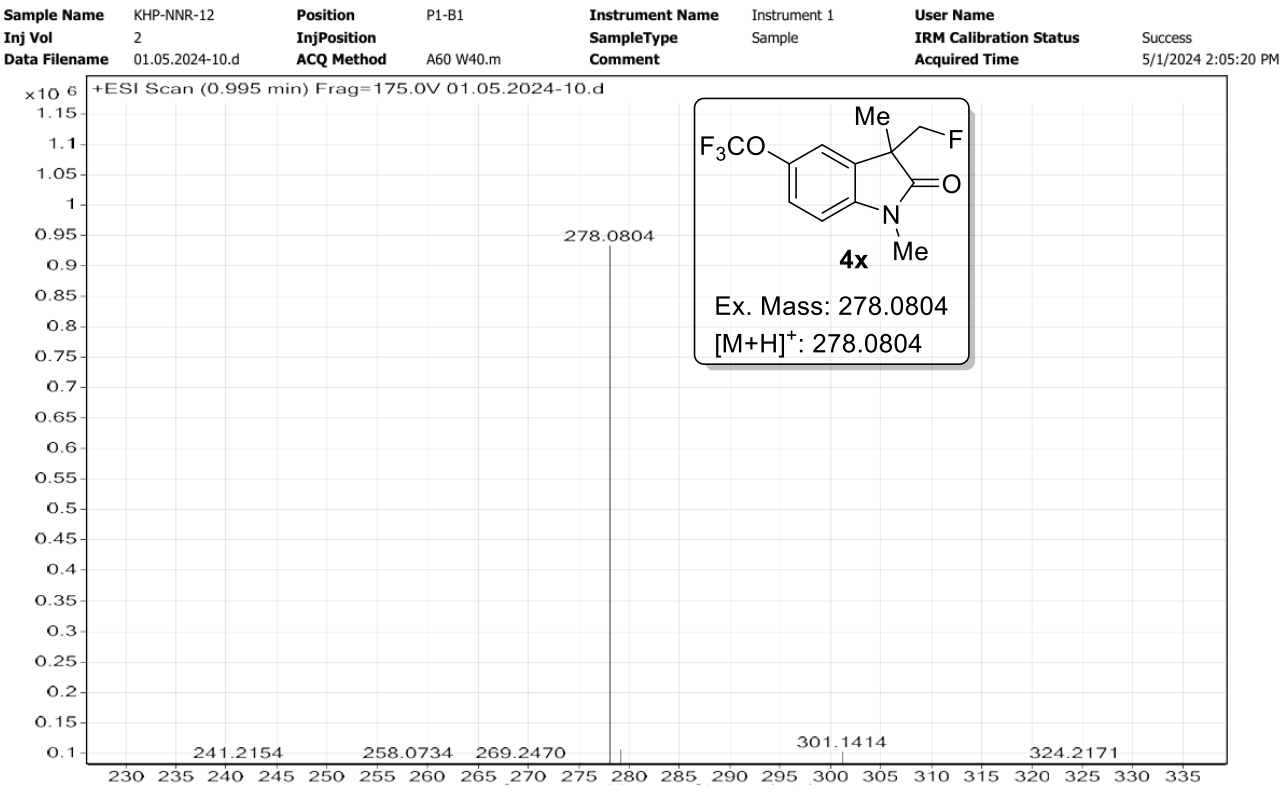
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-1,3-dimethyl-5-(trifluoromethoxy)indolin-2-one (4x)



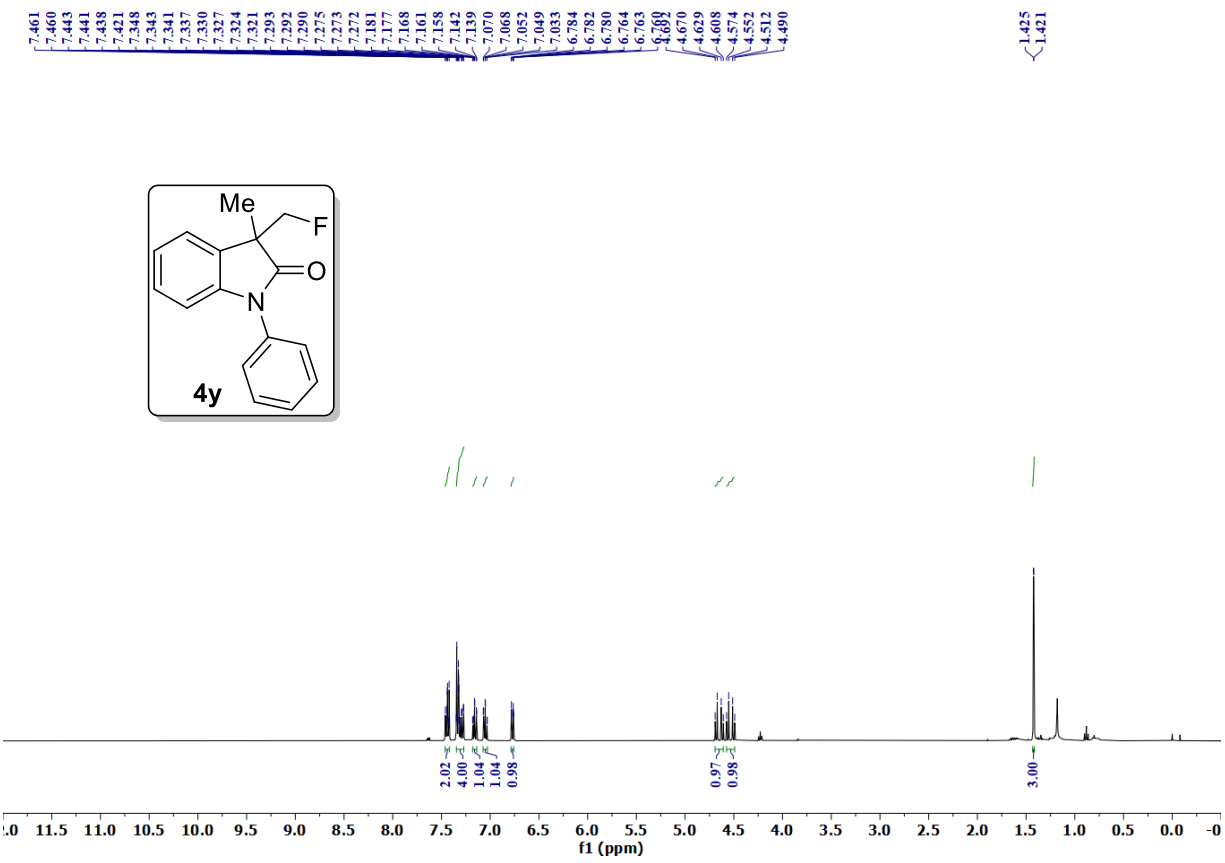
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-1,3-dimethyl-5-(trifluoromethoxy)indolin-2-one (4x)



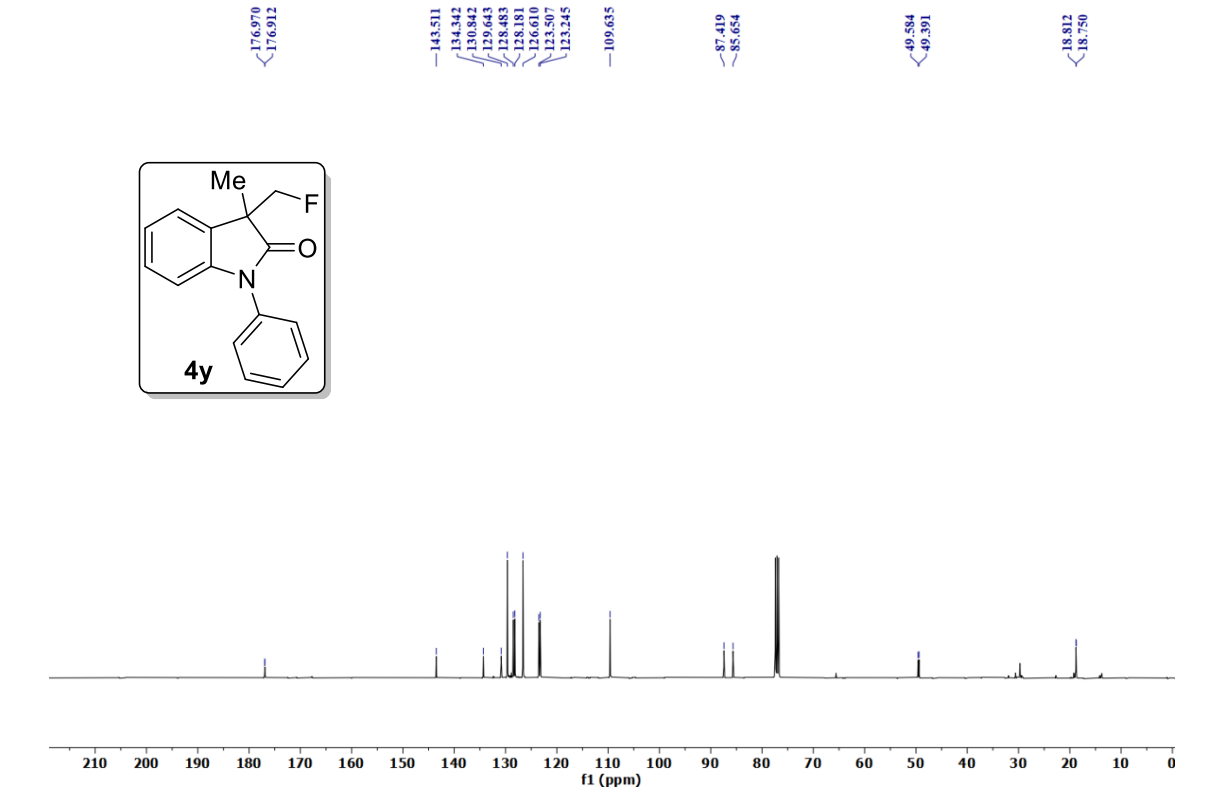
HRMS of 3-(fluoromethyl)-1,3-dimethyl-5-(trifluoromethoxy)indolin-2-one (4x)



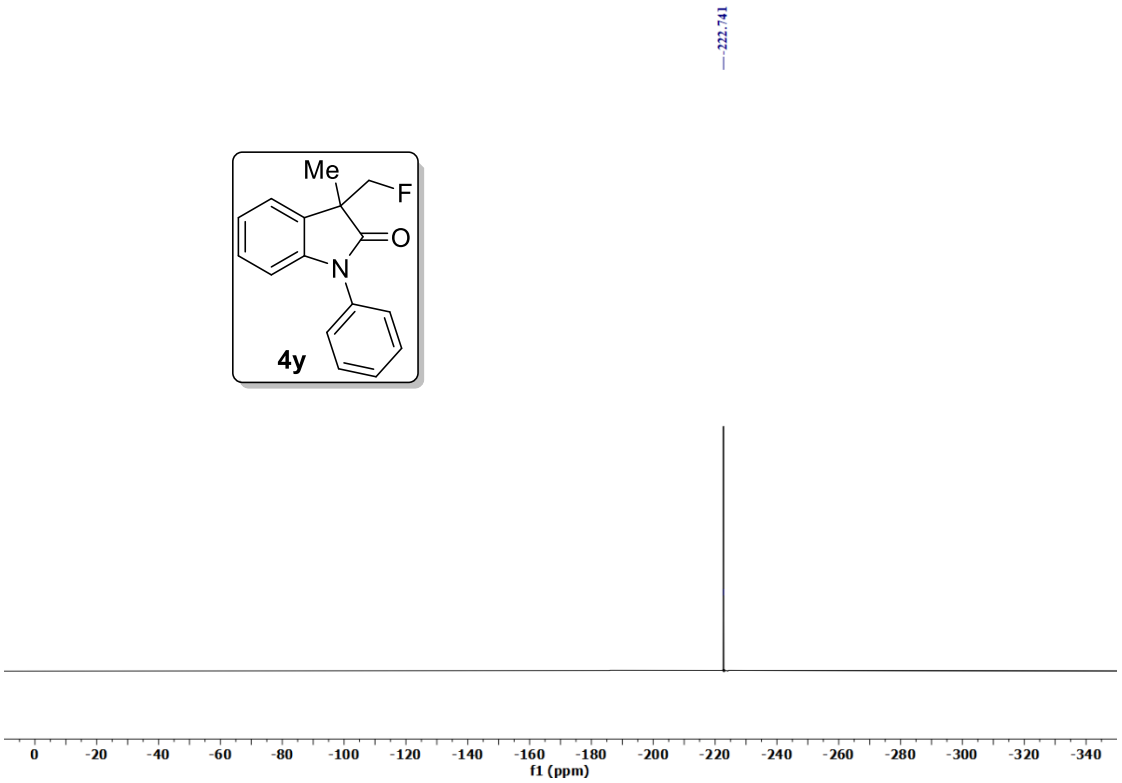
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methyl-1-phenylindolin-2-one (4y)



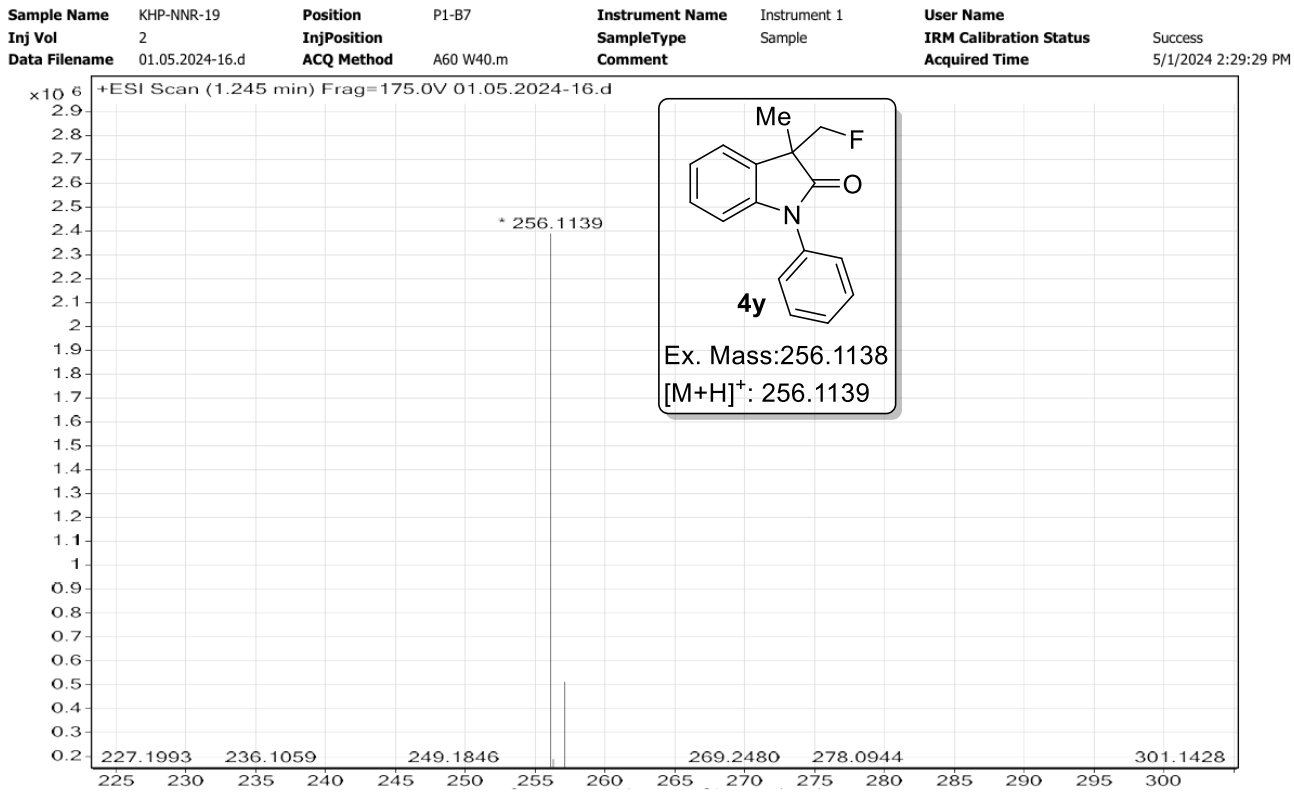
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methyl-1-phenylindolin-2-one (4y)



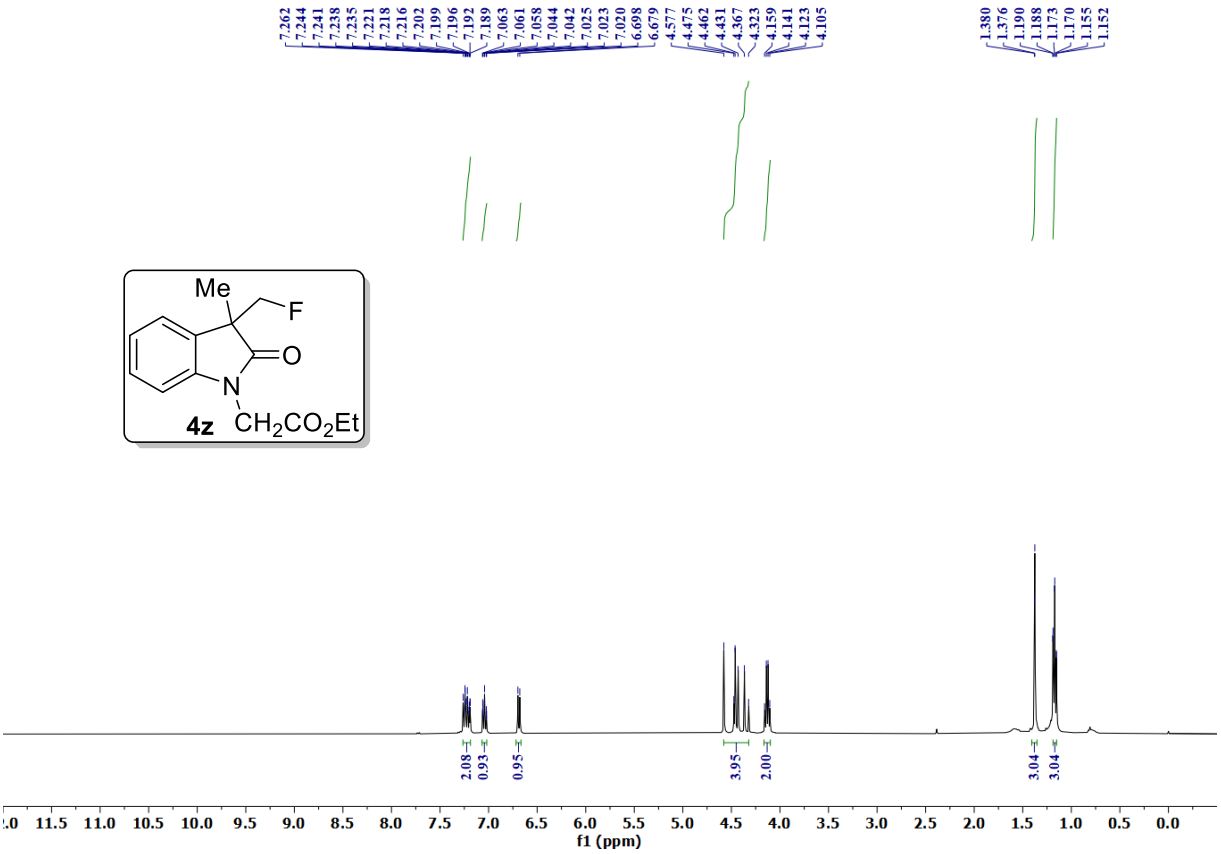
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3-(fluoromethyl)-3-methyl-1-phenylindolin-2-one (4y)



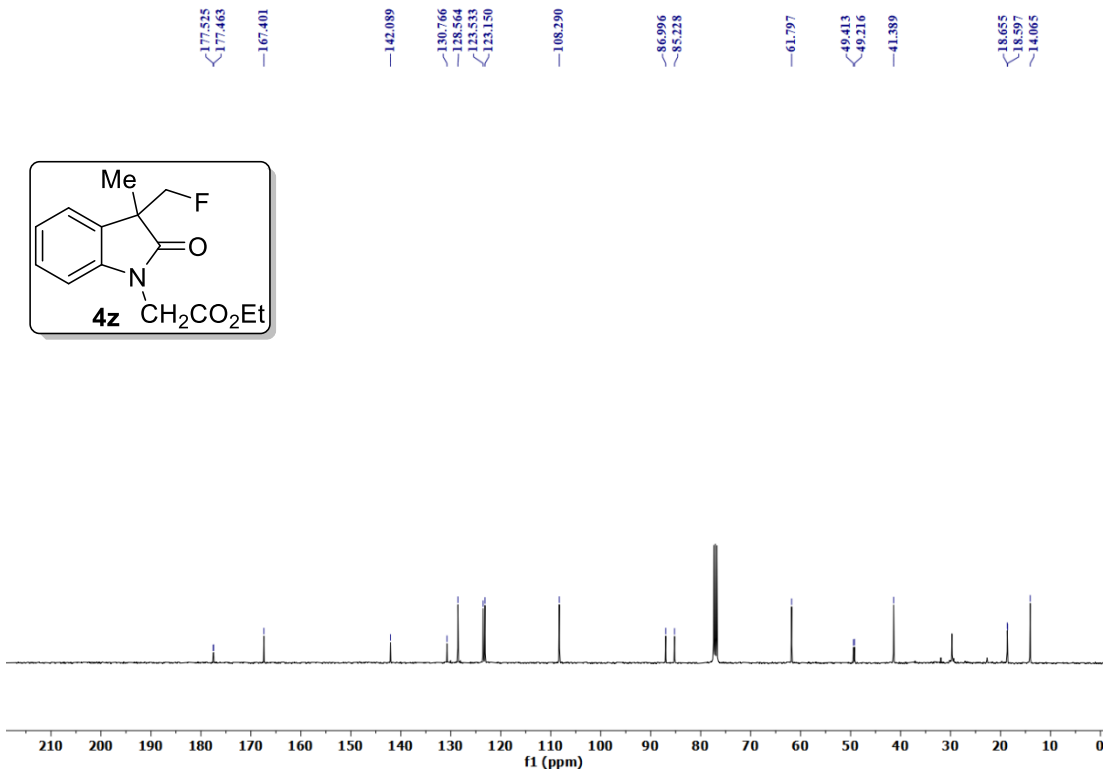
HRMS of 3-(fluoromethyl)-3-methyl-1-phenylindolin-2-one (4y)



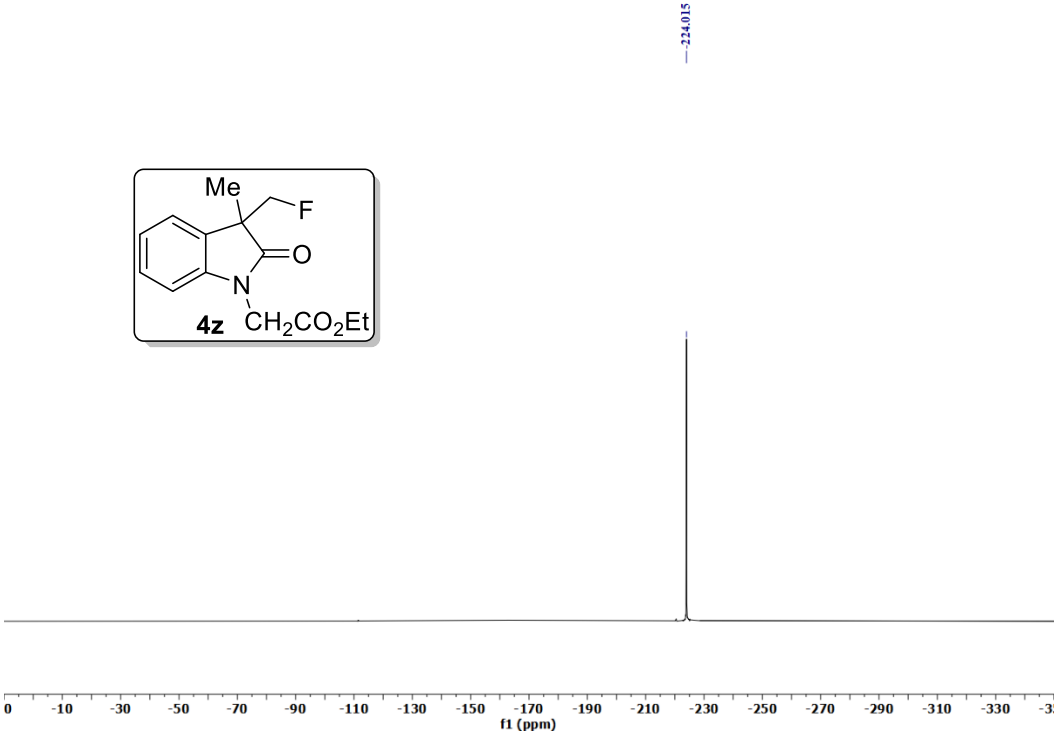
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of ethyl 2-(3-(fluoromethyl)-3-methyl-2-oxoindolin-1-yl)acetate (4z)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of ethyl 2-(3-(fluoromethyl)-3-methyl-2-oxoindolin-1-yl)acetate (4z)



^{19}F NMR (376 MHz, $CDCl_3$) spectrum of ethyl 2-(3-(fluoromethyl)-3-methyl-2-oxoindolin-1-yl)acetate (4z)



HRMS of ethyl 2-(3-(fluoromethyl)-3-methyl-2-oxoindolin-1-yl)acetate (4z)

Sample Name	KHP-NNR-22	**Position**	P1-C1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	01.05.2024-19.d	**ACQ Method**	A60 W40.m	**Comment**		**Acquired Time**	5/1/2024 2:41:24 PM