Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Radical Cascade Cyanomethylation of Activated Alkenes to Construct Cyano Substituted Oxindoles

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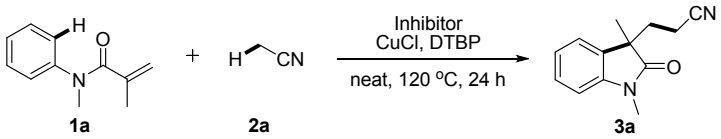
I. General remarks

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. CH_3CN was dried over CaH_2 and stored under N_2 over activated 4Å molecular sieves. Unless otherwise indicated, all reactions were carried out under N_2 atmosphere. All starting materials were prepared according to the literatures and were identified by comparison of their spectral data with those reported in the literatures.[1]

NMR spectra were obtained on a Bruker AV II-400 MHz spectrometer (^{1}H NMR at 400 MHz and ^{13}C NMR at 100 MHz). The ^{1}H NMR chemical shifts were measured relative to $CDCl_3$ or DMSO-d_6 as the internal reference ($CDCl_3$: δ = 7.26 ppm; DMSO-d_6: δ = 2.50 ppm). The ^{13}C NMR chemical shifts were given using $CDCl_3$ or DMSO-d_6 as the internal standard ($CDCl_3$: δ = 77.16 ppm; DMSO-d_6: δ = 39.52 ppm). High-resolution mass spectra (HRMS) were obtained with a Waters-Q-TOF-Premier (ESI). Melting points were determined with XRC-1 and are uncorrected.

II. Radical trapping experiment



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

Entry	Inhibitor	Equivalent	Yield (%)[a,b]
1	TEMPO	1.0 eq.	63
2	TEMPO	2.0 eq.	15
3	TEMPO	3.0 eq.	N. R.
4	BHT	0.3 eq.	73
5	BHT	0.5 eq.	19
6	BHT	1.0 eq.	N. R.

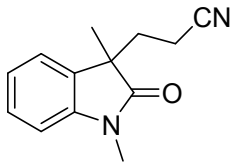
[a] Reactions conditions: **1a** (0.25 mmol), CuCl (10 mol%), DTBP (3.0 equiv), inhibitors and CH_3CN (2.0 mL) at 120 °C under nitrogen atmosphere for 24 h. [b] Isolated yield. N. R. = no reaction.

III. General procedure for the reaction

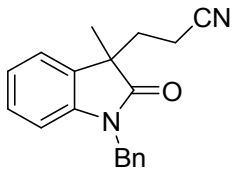
To a Schlenk tube were added *N*-arylacrylamide **1** (0.25 mmol), CuCl (10 mol%), DTBP (3.0 equiv) and dry CH_3CN (2.0 mL). The reaction was stirred at 120 °C under

nitrogen for 24 h. After the reaction was cooled down to ambient temperature, the solvent was removed using rotarvapor and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5/1, v/v) to provide the desired product.

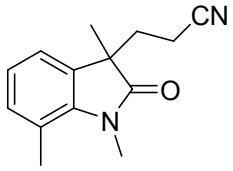
IV. Characterization data for products



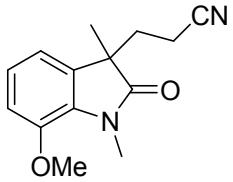
3-(1,3-Dimethyl-2-oxoindolin-3-yl) propanenitrile (3a): A white solid (44 mg, 82% yield). M.p.: 70-71 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.38 (s, 3H), 1.96-2.10 (m, 3H), 2.26-2.32 (m, 1H), 3.21 (s, 3H), 6.87 (d, J = 7.6 Hz, 1H), 7.10 (td, J = 7.6 Hz, 0.8 Hz, 1H), 7.18 (dd, J = 7.6 Hz, 0.8 Hz, 1H), 7.30 (td, J = 7.6 Hz, 1.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 23.6, 26.4, 33.6, 47.5, 108.6, 118.9, 122.7, 123.2, 128.8, 131.8, 143.3, 179.0 ppm. HRMS (ESI$^+$): calcd for $C_{13}H_{14}N_2ONa$ $[M+Na]^+$ 237.1004, found 237.1007.



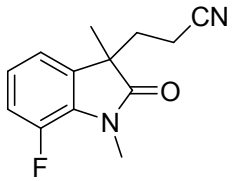
3-(1-Benzyl-3-methyl-2-oxoindolin-3-yl)propanenitrile (3c): Colorless oil (58 mg, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.46 (s, 3H), 1.95-2.16 (m, 3H), 2.34-2.42 (m, 1H), 4.91 (dd, J = 22.4 Hz, 15.6 Hz, 2H), 6.79 (d, J = 7.6 Hz, 1H), 7.08 (td, J = 7.6 Hz, 0.8 Hz, 1H), 7.19-7.23 (m, 2H), 7.27-7.35 (m, 5H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 23.9, 33.6, 43.9, 47.4, 109.6, 119.0, 122.8, 123.2, 127.4, 127.9, 128.7, 129.0, 131.8, 135.8, 142.3, 179.1 ppm. HRMS (ESI$^+$): calcd for $C_{19}H_{18}N_2ONa$ $[M+Na]^+$ 313.1317, found 313.1321.



3-(1,3,7-Trimethyl-2-oxoindolin-3-yl)propanenitrile (3e): A white solid (51 mg, 89% yield). M.p.: 72-73 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.37 (s, 3H), 1.95-2.12 (m, 3H), 2.28-2.34 (m, 1H), 2.58 (s, 3H), 3.50 (s, 3H), 6.97-7.05 (m, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 19.2, 24.0, 29.8, 33.8, 46.8, 119.0, 120.3, 120.6, 123.1, 132.4, 132.5, 141.0, 179.7 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{16}N_2ONa$ $[M+Na]^+$ 251.1160, found 251.1161.

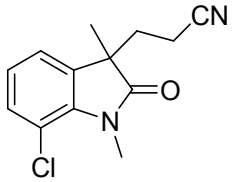


3-(7-Methoxy-1,3-dimethyl-2-oxoindolin-3-yl)propanenitrile (3f): Pale yellow oil (47 mg, 77% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.37 (s, 3H), 1.93-2.12 (m, 3H), 2.26-2.34 (m, 1H), 3.48 (s, 3H), 3.86 (s, 3H), 6.79 (d, J = 7.2 Hz, 1H), 6.87 (d, J = 8.0 Hz, 1H), 7.05 (t, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 12.9, 23.8, 29.7, 33.8, 47.5, 56.0, 112.4, 115.2, 119.0, 123.8, 131.0, 133.4, 145.7, 179.2 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{16}N_2O_2Na$ $[M+Na]^+$ 267.1109, found 267.1110.

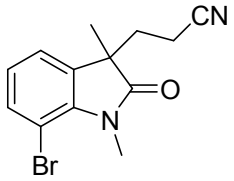


3-(7-Fluoro-1,3-dimethyl-2-oxoindolin-3-yl)propanenitrile (3g): A white solid (30 mg, 52% yield). M.p.: 59-61 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.40 (s, 3H), 1.99-2.15 (m, 3H), 2.28-2.36 (m, 1H), 3.43 (d, J = 2.4 Hz, 3H), 6.96-7.00 (m, 1H), 7.01-7.06 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 23.9, 28.9 (d, J = 5.0 Hz), 33.6, 47.8 (d, J = 2.0 Hz), 116.8 (d, J = 19.0 Hz), 118.6 (d, J = 4.0 Hz), 118.7, 123.8 (d, J = 6.0 Hz), 129.9 (d, J = 8.0 Hz), 134.8 (d, J = 3.0 Hz), 148.0 (d, J = 243.0 Hz),

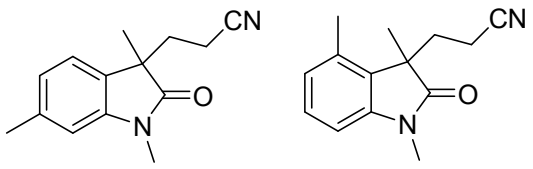
178.6 ppm. HRMS (ESI$^+$): calcd for $C_{13}H_{13}FN_2ONa$ $[M+Na]^+$ 255.0910, found 255.0906.



3-(7-Chloro-1,3-dimethyl-2-oxoindolin-3-yl)propanenitrile (3h): Pale yellow oil (50 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.39 (s, 3H), 1.97-2.14 (m, 3H), 2.29-2.36 (m, 1H), 3.59 (s, 3H), 7.00-7.08 (m, 2H), 7.24 (dd, J = 8.0 Hz, 1.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 24.0, 29.8, 33.7, 47.2, 116.2, 118.7, 121.2, 124.0, 131.2, 134.6, 139.2, 179.2 ppm. HRMS (ESI$^+$): calcd for $C_{13}H_{13}ClN_2ONa$ $[M+Na]^+$ 271.0614, found 271.0619.



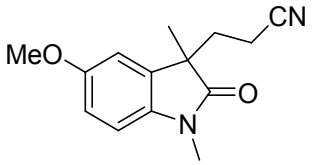
3-(7-Bromo-1,3-dimethyl-2-oxoindolin-3-yl)propanenitrile (3i): A pale yellow solid (47 mg, 64% yield). M.p.: 63-66 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.39 (s, 3H), 1.97-2.17 (m, 3H), 2.29-2.36 (m, 1H), 3.60 (s, 3H), 6.96 (t, J = 8.0 Hz, 1H), 7.11 (dd, J = 7.2 Hz, 1.2 Hz, 1H), 7.42 (dd, J = 8.0 Hz, 0.8 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 24.0, 30.0, 33.8, 47.2, 103.1, 118.7, 121.8, 124.4, 134.5, 135.0, 140.7, 179.4 ppm. HRMS (ESI$^+$): calcd for $C_{13}H_{13}BrN_2ONa$ $[M+Na]^+$ 315.0109, found 315.0107.



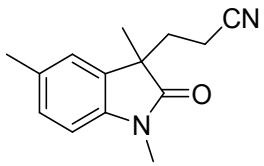
3j : 3j' = 1:4

3-(1,3,6-Trimethyl-2-oxoindolin-3-yl)propanenitrile (3j) and 3-(1,3,4-Trimethyl-

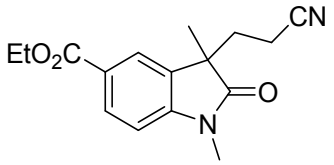
2-oxoindolin-3-yl)propanenitrile (3j'): A mixture of **3j** and **3j'** as colorless oil (47 mg, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.37 (s, 0.75H), 1.47 (s, 3H), 1.86-2.03 (m, 2.75H), 2.24-2.31 (m, 1.25H), 2.36-2.42 (m, 4.75H), 3.196 (s, 0.75H), 3.205 (s, 3H), 6.70-6.73 (m, 1.25H), 6.87 (d, J = 8.0 Hz, 1H), 6.91 (d, J = 7.6 Hz, 0.25H), 7.06 (d, J = 7.6 Hz, 0.25H), 7.21 (t, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 13.2, 18.3, 21.9, 22.0, 23.7, 26.4, 26.5, 31.6, 33.6, 47.3, 48.5, 106.4, 109.6, 118.8, 119.0, 122.4, 123.6, 125.7, 128.2, 128.6, 128.8, 134.5, 139.0, 143.3, 143.6, 179.0, 179.3 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{16}N_2ONa$ $[M+Na]^+$ 251.1160, found 251.1166.



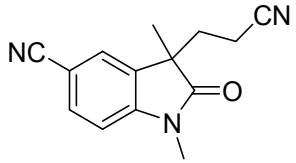
3-(5-Methoxy-1,3-dimethyl-2-oxoindolin-3-yl)propanenitrile (3k): A white solid (47 mg, 77% yield). M.p.: 83-85 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.38 (s, 3H), 1.96-2.13 (m, 3H), 2.28-2.35 (m, 1H), 3.19 (s, 3H), 3.81 (s, 3H), 6.76-6.84 (m, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 23.7, 26.5, 33.6, 47.9, 56.0, 109.0, 110.4, 112.7, 118.9, 133.2, 136.7, 156.5, 178.6 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{16}N_2O_2Na$ $[M+Na]^+$ 267.1109, found 267.1111.



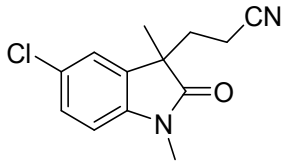
3-(1,3,5-Trimethyl-2-oxoindolin-3-yl)propanenitrile (3l): A white solid (46 mg, 81% yield). M.p.: 90-92 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.38 (s, 3H), 1.95-2.10 (m, 3H), 2.29-2.34 (m, 1H), 2.36 (s, 3H), 3.20 (s, 3H), 6.76 (d, J = 8.0 Hz, 1H), 7.00 (s, 1H), 7.11 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 21.3, 23.7, 26.5, 33.6, 47.6, 108.4, 119.0, 123.6, 129.0, 131.8, 132.8, 140.9, 178.9 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{16}N_2ONa$ $[M+Na]^+$ 251.1160, found 251.1158.



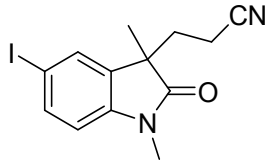
Ethyl 3-(2-cyanoethyl)-1,3-dimethyl-2-oxoindoline-5-carboxylate (3m): A white solid (36 mg, 50% yield). M.p.: 125 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.40-1.43 (m, 6H), 2.02-2.16 (m, 3H), 2.32-2.39 (m, 1H), 3.26 (s, 3H), 4.39 (q, J = 7.2 Hz, 2H), 6.92 (d, J = 8.4 Hz, 1H), 7.86 (d, J = 1.2 Hz, 1H), 8.08 (dd, J = 8.0 Hz, 1.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 14.5, 23.6, 26.7, 33.4, 47.3, 61.2, 108.2, 118.6, 124.0, 125.6, 131.5, 131.8, 147.3, 166.3, 179.4 ppm. HRMS (ESI$^+$): calcd for $C_{16}H_{18}N_2O_3Na$ $[M+Na]^+$ 309.1215, found 309.1217.



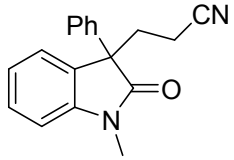
3-(2-Cyanoethyl)-1,3-dimethyl-2-oxoindoline-5-carbonitrile (3n): A pale yellow solid (38 mg, 63% yield). M.p.: 153-156 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.42 (s, 3H), 2.03-2.15 (m, 3H), 2.31-2.37 (m, 1H), 3.26 (s, 3H), 6.96 (d, J = 8.0 Hz, 1H), 7.46 (d, J = 1.6 Hz, 1H), 7.66 (dd, J = 8.0 Hz, 1.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 12.9, 23.5, 26.7, 33.1, 47.2, 106.4, 109.1, 118.2, 118.9, 126.2, 133.0, 134.2, 147.1, 178.7 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{13}N_3ONa$ $[M+Na]^+$ 262.0956, found 262.0955.



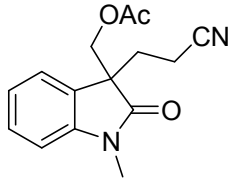
3-(5-Chloro-1,3-dimethyl-2-oxoindolin-3-yl)propanenitrile (3o): Pale yellow oil (58 mg, 92% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.40 (s, 3H), 2.01-2.13 (m, 3H), 2.28-2.36 (m, 1H), 3.21 (s, 3H), 6.81 (d, J = 8.0 Hz, 1H), 7.17 (d, J = 2.0 Hz, 1H), 7.30 (dd, J = 8.0 Hz, 2.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 23.6, 26.6, 33.4, 47.7, 109.6, 118.6, 123.4, 128.6, 128.8, 133.6, 141.9, 178.5 ppm. HRMS (ESI$^+$): calcd for $C_{13}H_{13}ClN_2ONa$ $[M+Na]^+$ 271.0614, found 271.0613.



3-(5-Iodo-1,3-dimethyl-2-oxoindolin-3-yl)propanenitrile (3p): A pale yellow solid (55 mg, 65% yield). M.p.: 84-86 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.39 (s, 3H), 2.00-2.11 (m, 3H), 2.28-2.35 (m, 1H), 3.19 (s, 3H), 6.66 (d, J = 8.4 Hz, 1H), 7.47 (d, J = 1.6 Hz, 1H), 7.64 (dd, J = 8.4 Hz, 1.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 23.6, 26.5, 33.4, 47.5, 85.7, 110.7, 118.6, 131.6, 134.3, 137.7, 143.0, 178.2 ppm. HRMS (ESI^+): calcd for $C_{13}H_{13}IN_2ONa$ $[M+Na]^+$ 362.9970, found 362.9976.

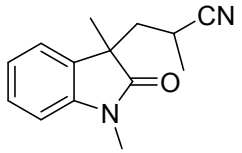


3-(1-Methyl-2-oxo-3-phenylindolin-3-yl)propanenitrile (4b): A pale yellow solid (33 mg, 48% yield). M.p.: 152-154 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.08-2.22 (m, 2H), 2.46-2.53 (m, 1H), 2.79-2.87 (m, 1H), 3.25 (s, 3H), 6.94 (d, J = 7.6 Hz, 1H), 7.17 (t, J = 7.2 Hz, 1H), 7.26-7.41 (m, 7H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.3, 26.7, 33.4, 55.5, 109.0, 118.8, 123.3, 124.9, 126.8, 128.0, 129.0, 129.3, 130.1, 138.5, 143.8, 177.2 ppm. HRMS (ESI^+): calcd for $C_{18}H_{16}N_2ONa$ $[M+Na]^+$ 299.1160, found 299.1163.

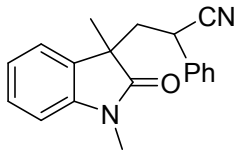


(3-(2-Cyanoethyl)-1-methyl-2-oxoindolin-3-yl)methyl acetate (4c): Colorless oil (38 mg, 54% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.94 (s, 3H), 1.98-2.21 (m, 3H), 2.36-2.43 (m, 1H), 3.24 (s, 3H), 4.13 (d, J = 10.8 Hz, 1H), 4.46 (d, J = 10.8 Hz, 1H), 6.90 (d, J = 7.6 Hz, 1H), 7.12 (td, J = 7.6 Hz, 0.8 Hz, 1H), 7.24 (d, J = 7.2 Hz, 1H), 7.36 (td, J = 7.6 Hz, 1.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 12.6, 20.7,

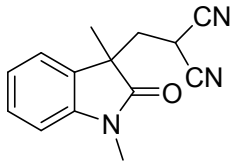
26.6, 29.1, 51.4, 66.7, 108.8, 118.5, 123.3, 123.8, 127.5, 129.6, 144.0, 170.2, 175.8 ppm. HRMS (ESI^+): calcd for $C_{15}H_{16}N_2O_3Na$ $[M+Na]^+$ 295.1059, found 295.1057.



3-(1,3-Dimethyl-2-oxoindolin-3-yl)-2-methylpropanenitrile (4d): Colorless oil (54 mg, 94% yield). ^1H NMR (400 MHz, $CDCl_3$): δ = 1.18 (d, J = 6.4 Hz, 3H), 1.42 (s, 3H), 1.84 (q, J = 9.6 Hz, 1H), 2.35-2.42 (m, 2H), 3.23 (s, 3H), 6.90 (d, J = 8.0 Hz, 1H), 7.09 (t, J = 7.2 Hz, 1H), 7.15 (d, J = 6.8 Hz, 1H), 7.32 (td, J = 8.0 Hz, 0.8 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 19.3, 21.8, 24.6, 26.5, 41.7, 47.2, 108.8, 121.9, 122.6, 122.8, 128.7, 132.3, 143.6, 179.3 ppm. HRMS (ESI^+): calcd for $C_{14}H_{16}N_2ONa$ $[M+Na]^+$ 251.1160, found 251.1162.

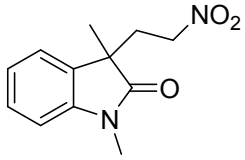


3-(1,3-Dimethyl-2-oxoindolin-3-yl)-2-phenylpropanenitrile (4e): Pale yellow oil (66 mg, 91% yield). ^1H NMR (400 MHz, $CDCl_3$): δ = 1.45 (s, 3H), 2.14 (dd, J = 14.4 Hz, 4.4 Hz, 1H), 2.70 (dd, J = 14.4 Hz, 10.8 Hz, 1H), 3.25 (s, 3H), 3.57 (dd, J = 10.4 Hz, 4.4 Hz, 1H), 6.88 (d, J = 8.0 Hz, 1H), 7.08 (td, J = 7.6 Hz, 0.4 Hz, 1H), 7.14-7.16 (m, 3H), 7.24-7.33 (m, 4H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 24.8, 26.5, 33.5, 43.5, 47.3, 108.8, 120.0, 122.7, 122.9, 127.3, 128.2, 128.8, 129.2, 132.0, 136.1, 143.6, 179.1 ppm. HRMS (ESI^+): calcd for $C_{19}H_{18}N_2ONa$ $[M+Na]^+$ 313.1317, found 313.1313.

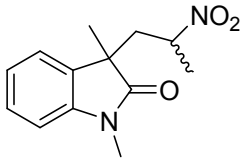


2-((1,3-Dimethyl-2-oxoindolin-3-yl)methyl)malononitrile (4f): Brown oil (43 mg, 72% yield). ^1H NMR (400 MHz, $CDCl_3$): δ = 1.49 (s, 3H), 2.36 (dd, J = 14.0 Hz, 5.2

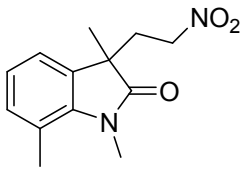
Hz, 1H), 2.76 (dd, J = 14.0 Hz, 8.8 Hz, 1H), 3.25 (s, 3H), 3.78-3.82 (m, 1H), 6.93 (d, J = 8.0 Hz, 1H), 7.16 (t, J = 7.2 Hz, 1H), 7.23 (d, J = 7.2 Hz, 1H), 7.38 (t, J = 7.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 18.6, 24.1, 26.7, 37.8, 46.3, 109.3, 112.16, 112.19, 123.0, 123.5, 129.7, 130.2, 143.3, 178.0 ppm. HRMS (ESI^+): calcd for $C_{14}H_{13}N_3ONa$ $[M+Na]^+$ 262.0956, found 262.0953.



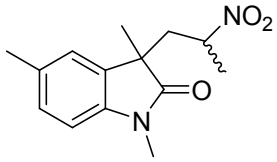
1,3-Dimethyl-3-(2-nitroethyl)indolin-2-one (5a): Pale yellow oil (40 mg, 68% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.43 (s, 3H), 2.45-2.52 (m, 1H), 2.59-2.66 (m, 1H), 3.24 (s, 3H), 4.04-4.11 (m, 1H), 4.18-4.25 (m, 1H), 6.88 (d, J = 8.0 Hz, 1H), 7.10 (t, J = 7.2 Hz, 1H), 7.21 (d, J = 7.2 Hz, 1H), 7.32 (td, J = 8.0 Hz, 0.8 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 23.7, 26.5, 34.6, 46.3, 71.5, 108.7, 122.8, 123.3, 128.9, 131.8, 143.0, 179.0 ppm. HRMS (ESI^+): calcd for $C_{12}H_{14}N_2O_3Na$ $[M+Na]^+$ 257.0902, found 257.0902.



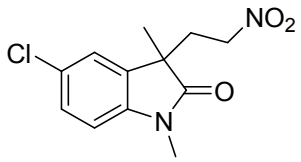
1,3-Dimethyl-3-(2-nitropropyl)indolin-2-one (5b): A mixture of isomers of *cis*-**5b** and *trans*-**5b** as yellow oil (57 mg, 92% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.31-1.39 (m, 12H), 2.02 (dd, J = 14.8 Hz, 3.2 Hz, 1H), 2.29 (dd, J = 14.8 Hz, 4.0 Hz, 1H), 2.73 (dd, J = 14.8 Hz, 8.4 Hz, 1H), 2.82 (dd, J = 15.2 Hz, 8.0 Hz, 1H), 3.22 (d, J = 22.8 Hz, 6H), 4.14-4.18 (m, 1H), 4.44-4.48 (m, 1H), 6.87 (t, J = 8.4 Hz, 2H), 7.04-7.18 (m, 4H), 7.28-7.34 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 20.9, 21.1, 24.1, 25.2, 26.3, 26.5, 41.7, 42.1, 46.5, 47.2, 80.1, 80.7, 108.5, 108.7, 122.6, 123.0, 123.1, 123.5, 128.7, 128.8, 130.7, 132.4, 143.1, 143.3, 178.8, 179.4 ppm. HRMS (ESI^+): calcd for $C_{13}H_{16}N_2O_3Na$ $[M+Na]^+$ 271.1059, found 271.1064.



1,3,7-Trimethyl-3-(2-nitroethyl)indolin-2-one (5c): Yellow oil (45 mg, 72% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.40 (s, 3H), 2.39-2.46 (m, 1H), 2.56-2.64 (m, 4H), 3.50 (s, 3H), 4.02-4.09 (m, 1H), 4.16-4.23 (m, 1H), 6.96-7.04 (m, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 19.1, 24.1, 29.8, 35.0, 45.5, 71.5, 120.4, 120.6, 123.2, 132.5, 132.6, 140.8, 179.6 ppm. HRMS (ESI$^+$): calcd for $C_{13}H_{16}N_2O_3Na$ $[M+Na]^+$ 271.1059, found 271.1060.

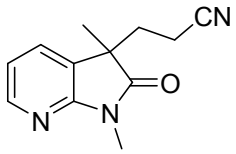


1,3,5-Trimethyl-3-(2-nitropropyl)indolin-2-one (5d): A mixture of isomers of *cis*-**5d** and *trans*-**5d** as yellow oil (62 mg, 94% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.31-1.38 (m, 12H), 1.98 (dd, J = 15.2 Hz, 3.6 Hz, 1H), 2.29 (dd, J = 14.8 Hz, 4.8 Hz, 1H), 2.33 (s, 3H), 2.35 (s, 3H), 2.69 (dd, J = 14.8 Hz, 8.0 Hz, 1H), 2.80 (dd, J = 15.2 Hz, 8.4 Hz, 1H), 3.17 (s, 3H), 3.22 (s, 3H), 4.12-4.21 (m, 1H), 4.45-4.53 (m, 1H), 6.75 (t, J = 8.4 Hz, 2H), 6.96 (d, J = 10.0 Hz, 2H), 7.10 (t, J = 7.6 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 20.8, 21.2, 21.26, 21.27, 24.1, 25.3, 26.4, 26.5, 41.8, 42.2, 46.6, 47.2, 80.1, 80.7, 108.2, 108.4, 123.4, 124.2, 128.95, 129.02, 130.9, 132.55, 132.63, 132.7, 140.8, 140.9, 178.8, 179.4 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{18}N_2O_3Na$ $[M+Na]^+$ 285.1215, found 285.1211.

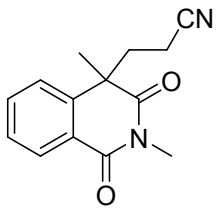


5-Chloro-1,3-dimethyl-3-(2-nitroethyl)indolin-2-one (5e): Yellow oil (54 mg, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.42 (s, 3H), 2.40-2.48 (m, 1H), 2.58-2.65 (m, 1H), 3.21 (s, 3H), 4.09-4.16 (m, 1H), 4.20-4.27 (m, 1H), 6.80 (d, J = 8.0 Hz, 1H),

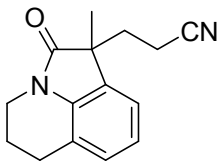
7.19 (d, J = 2.0 Hz, 1H), 7.30 (dd, J = 8.4 Hz, 2.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 23.6, 26.6, 34.5, 46.5, 71.3, 109.6, 123.4, 128.7, 128.9, 133.7, 141.6, 178.4 ppm. HRMS (ESI$^+$): calcd for $C_{12}H_{13}ClN_2O_3Na$ $[M+Na]^+$ 291.0512, found 291.0510.



3-(1,3-Dimethyl-2-oxo-2,3-dihydro-1H-pyrrolo[2,3-b]pyridin-3-yl)propanenitrile (3q): Orange oil (30 mg, 56% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.43 (s, 3H), 2.04-2.12 (m, 2H), 2.16-2.25 (m, 1H), 2.30-2.38 (m, 1H), 3.31 (s, 3H), 7.02 (dd, J = 7.2 Hz, 5.2 Hz, 1H), 7.45 (dd, J = 7.6 Hz, 1.6 Hz, 1H), 8.24 (dd, J = 5.6 Hz, 1.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 23.1, 25.6, 33.1, 47.2, 118.6, 126.3, 130.4, 147.8, 156.8, 178.7 ppm. HRMS (ESI$^+$): calcd for $C_{12}H_{13}N_3ONa$ $[M+Na]^+$ 238.0956, found 238.0959.



3-(2,4-Dimethyl-1,3-dioxo-1,2,3,4-tetrahydroisoquinolin-4-yl)propanenitrile (3r): Pale yellow oil (28 mg, 46% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.65 (s, 3H), 1.89-2.08 (m, 2H), 2.23-2.30 (m, 1H), 2.73-2.81 (m, 1H), 3.40 (s, 3H), 7.42 (d, J = 8.0 Hz, 1H), 7.49-7.53 (m, 1H), 7.71 (td, J = 7.6 Hz, 1.2 Hz, 1H), 8.29 (dd, J = 8.0 Hz, 1.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.7, 27.5, 30.3, 36.9, 47.2, 118.3, 125.0, 125.2, 128.4, 129.7, 134.7, 141.2, 163.9, 175.2 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{14}N_2O_2Na$ $[M+Na]^+$ 265.0953, found 265.0950.

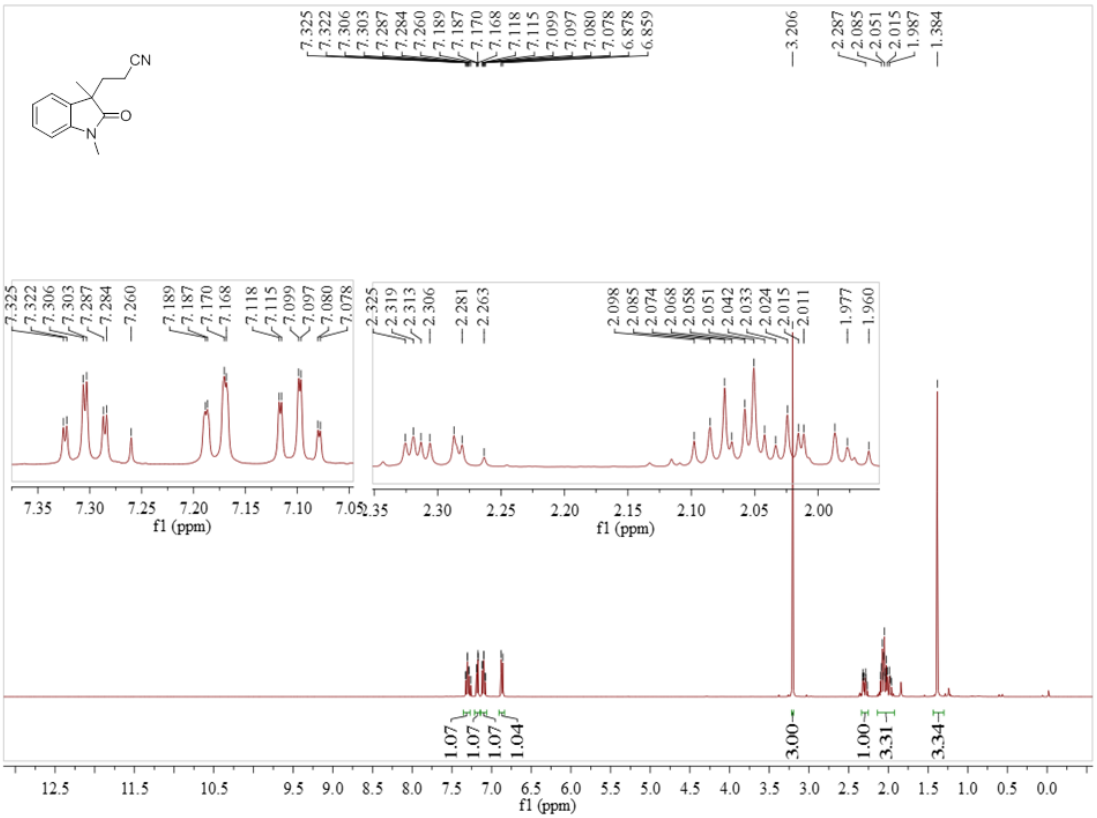


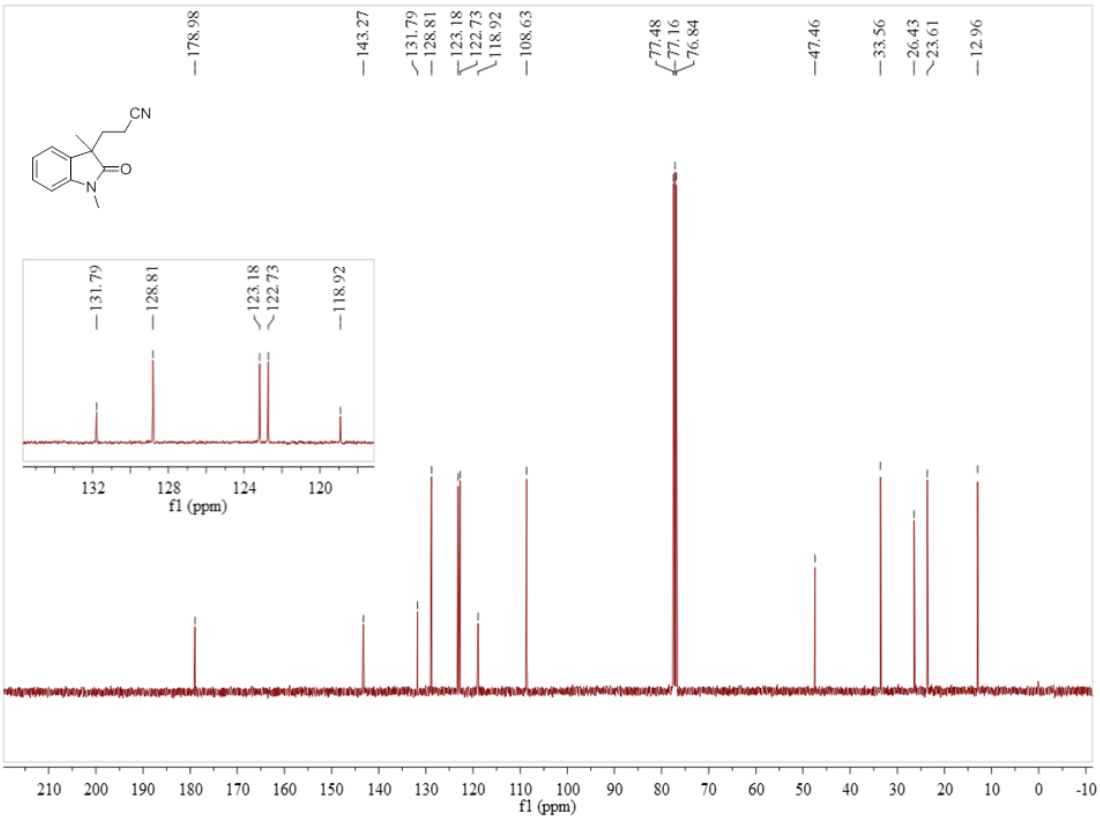
3-(1-Methyl-2-oxo-2,4,5,6-tetrahydro-1H-pyrrolo[3,2,1-ij]quinolin-1-yl)propanenitrile (3s): Yellow oil (44 mg, 73% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.40 (s, 3H), 1.98-2.14 (m, 5H), 2.27-2.34 (m, 1H), 2.80 (t, J = 6.0 Hz, 2H), 3.66-3.77 (m, 2H), 6.97-7.03 (m, 2H), 7.06 (dt, J = 6.8 Hz, 0.8 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.1, 21.3, 23.3, 24.7, 33.4, 39.0, 48.8, 119.0, 120.6, 120.8, 122.6, 127.6, 130.4, 139.1, 177.9 ppm. HRMS (ESI$^+$): calcd for $C_{15}H_{16}N_2ONa$ $[M+Na]^+$ 263.1160, found 263.1165.

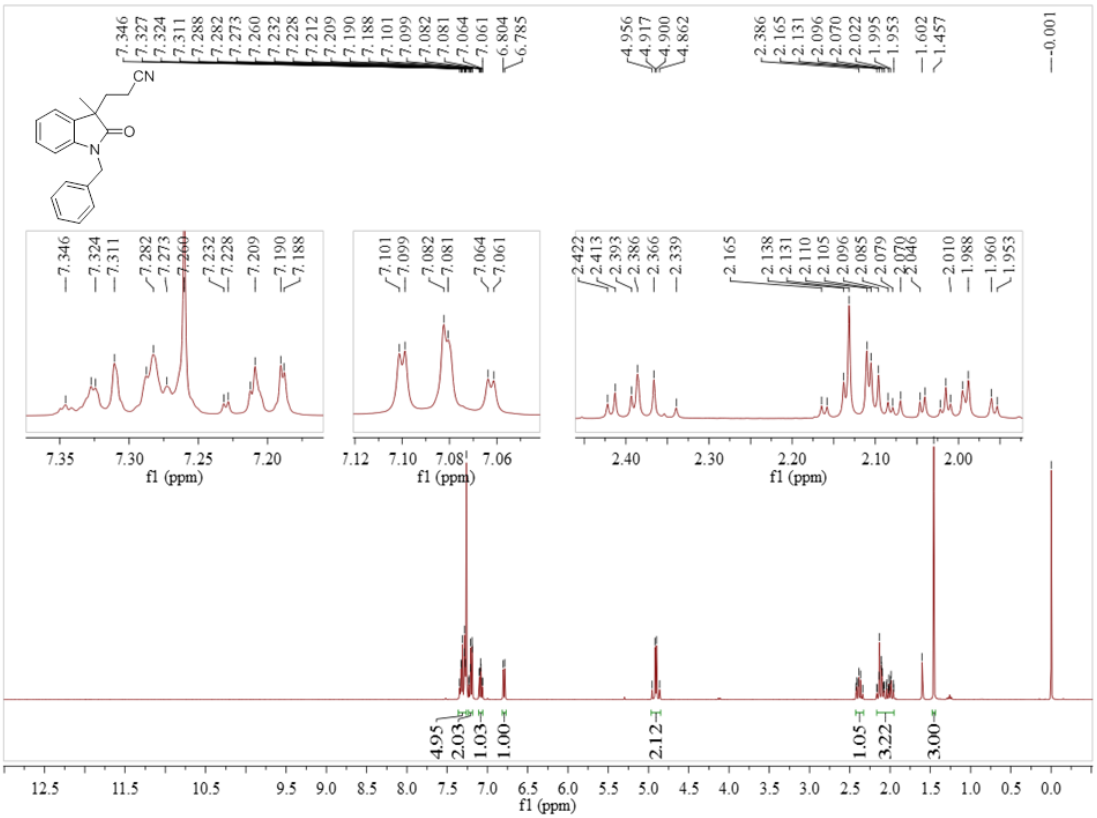
V. References

[1] (*a*) M. P. Sibi, Z. Ma, K. Itoh, N. Prabagaran and C. P. Jasperse, *Org. Lett*., 2005, **7**, 2349; (*b*) A. Pinto, Y. Jia, L. Neuville and J. Zhu, *Chem. Eur. J*., 2007, **13**, 961; (*c*) A. J.-L. Ayitou and J. Sivaguru, *Chem. Commun*., 2011, **47**, 2568; (*d*) Q.-Q. Zhang, J.-H. Xie, X.-H. Yang, J.-B. Xie and Q.-L. Zhou, *Org. Lett*., 2012, **14**, 6158.

VI. Copies of ^{1}H and ^{13}C NMR spectra



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2.165
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1.602
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CN
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N
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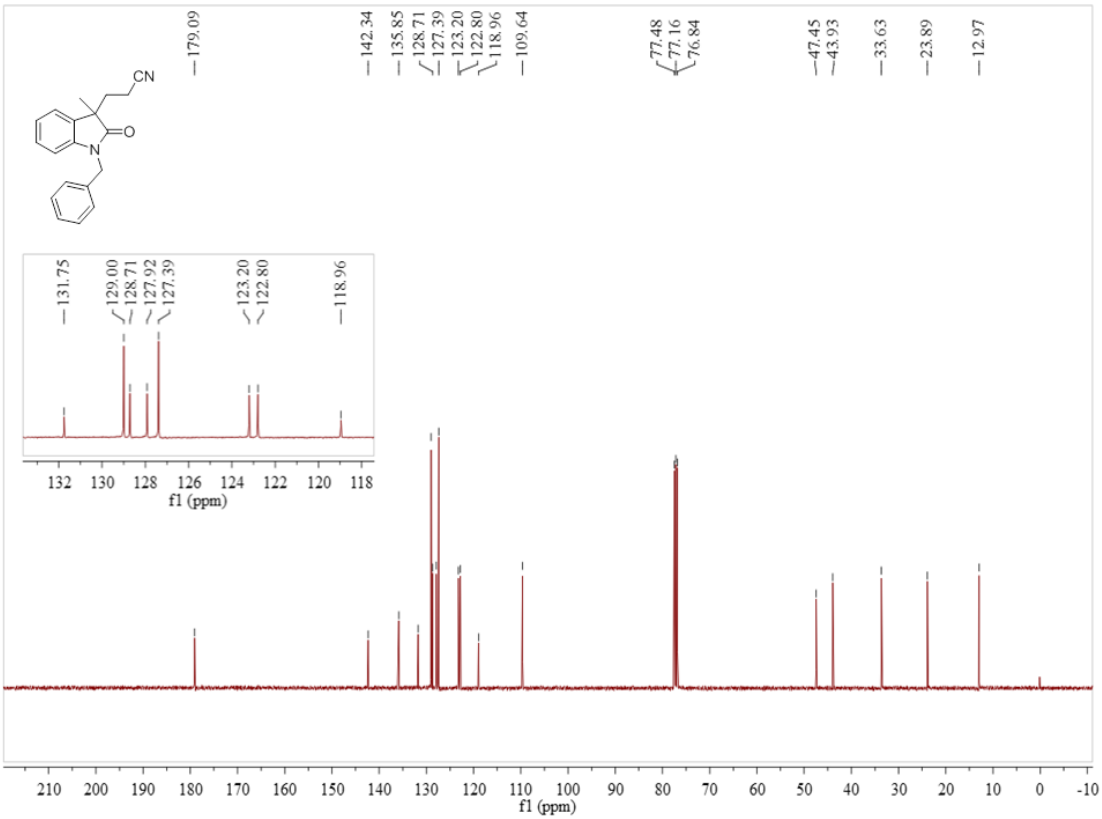
3.00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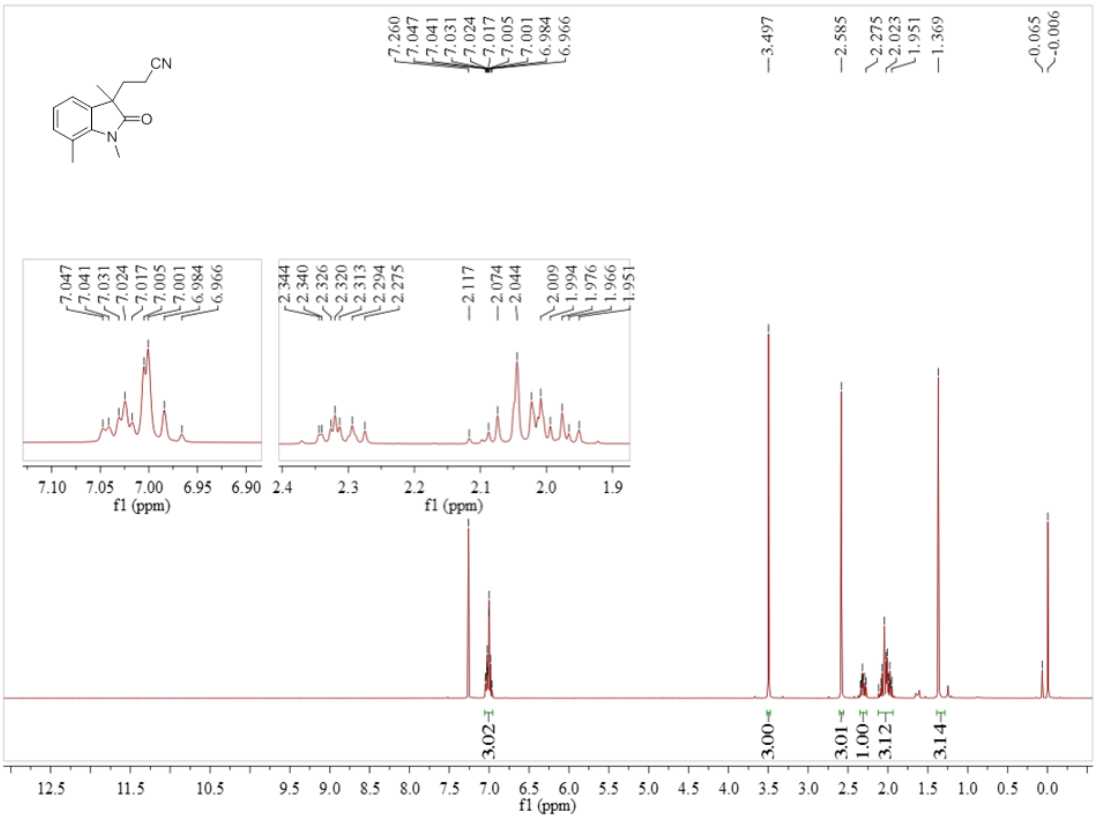
f1 (ppm)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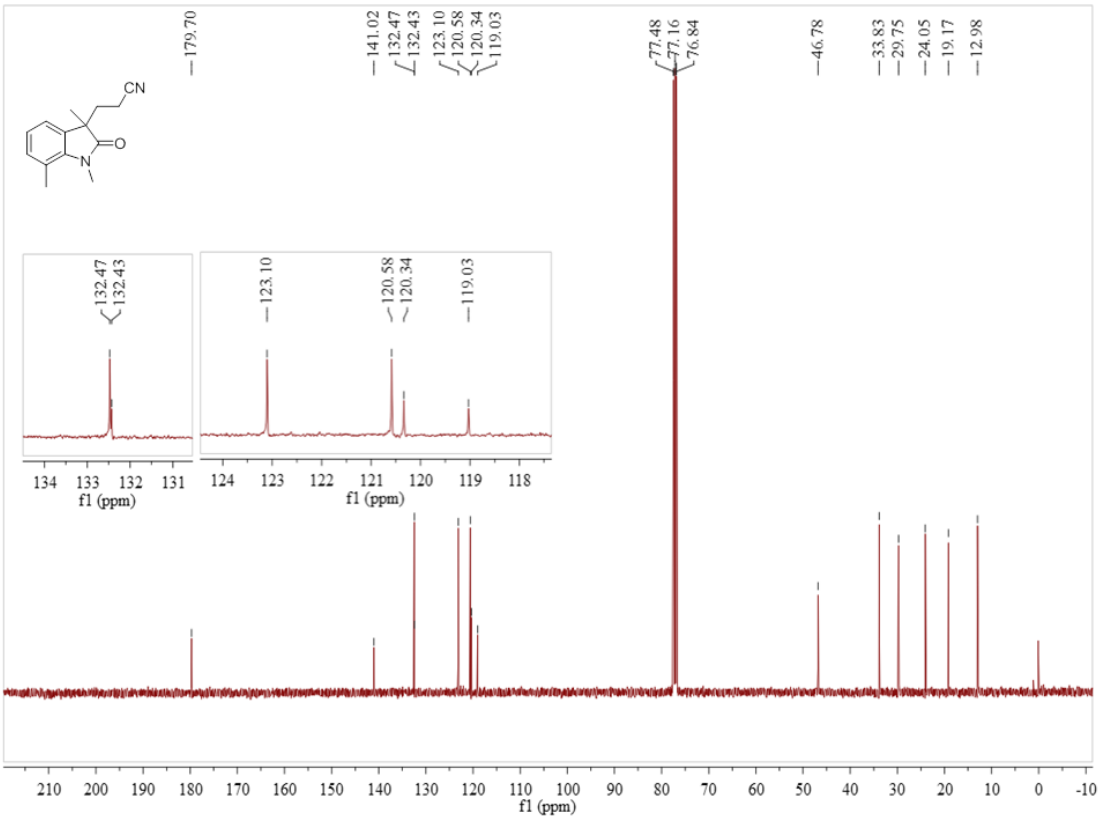
3.14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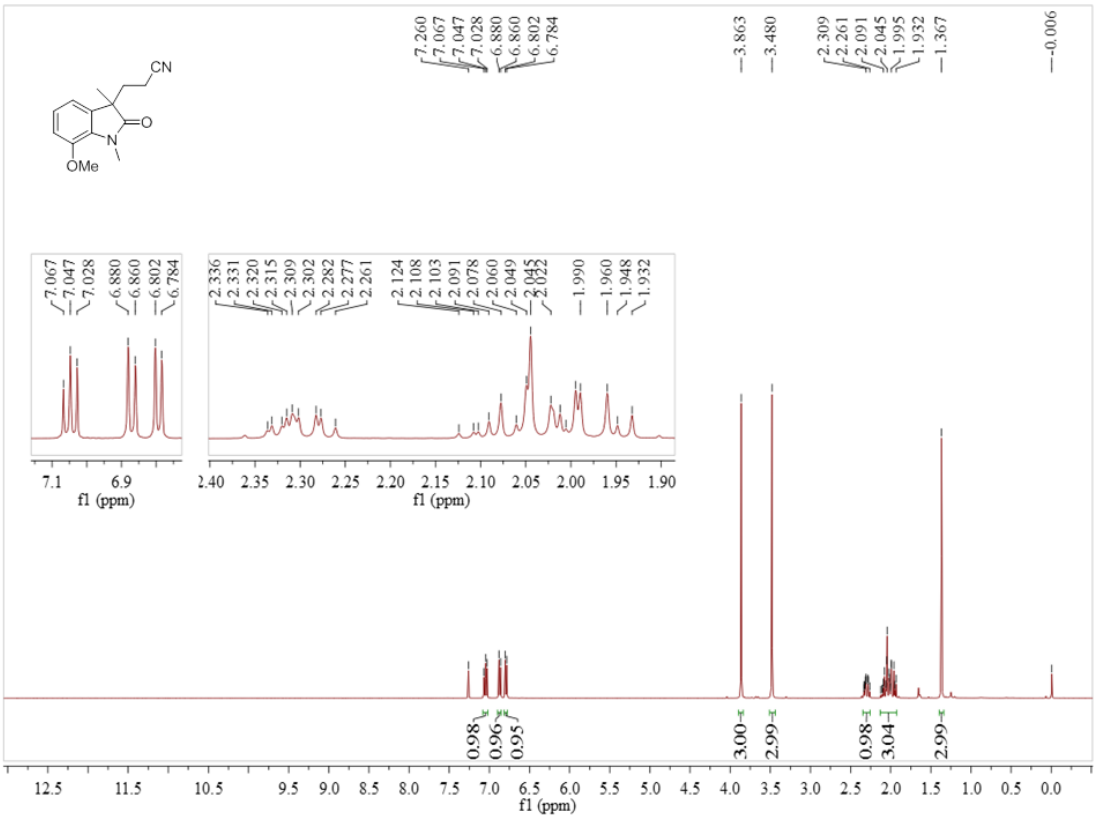
f1 (ppm)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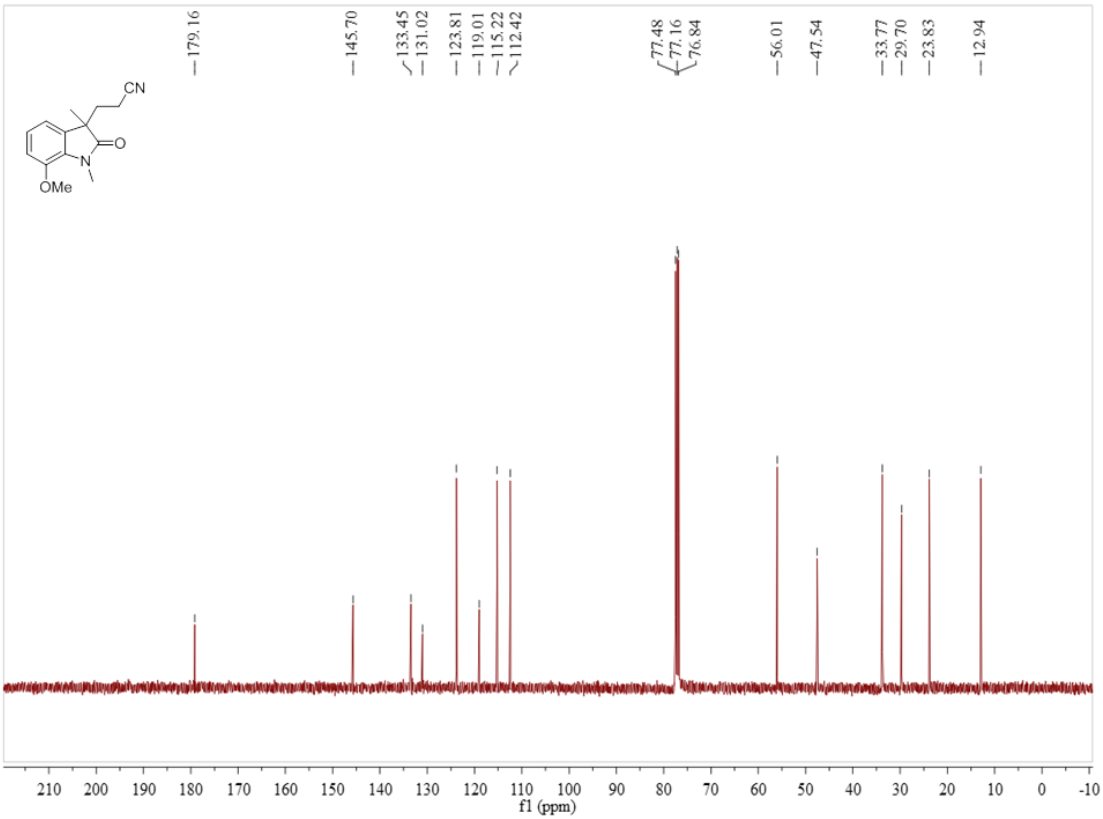
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N
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33.77
29.70
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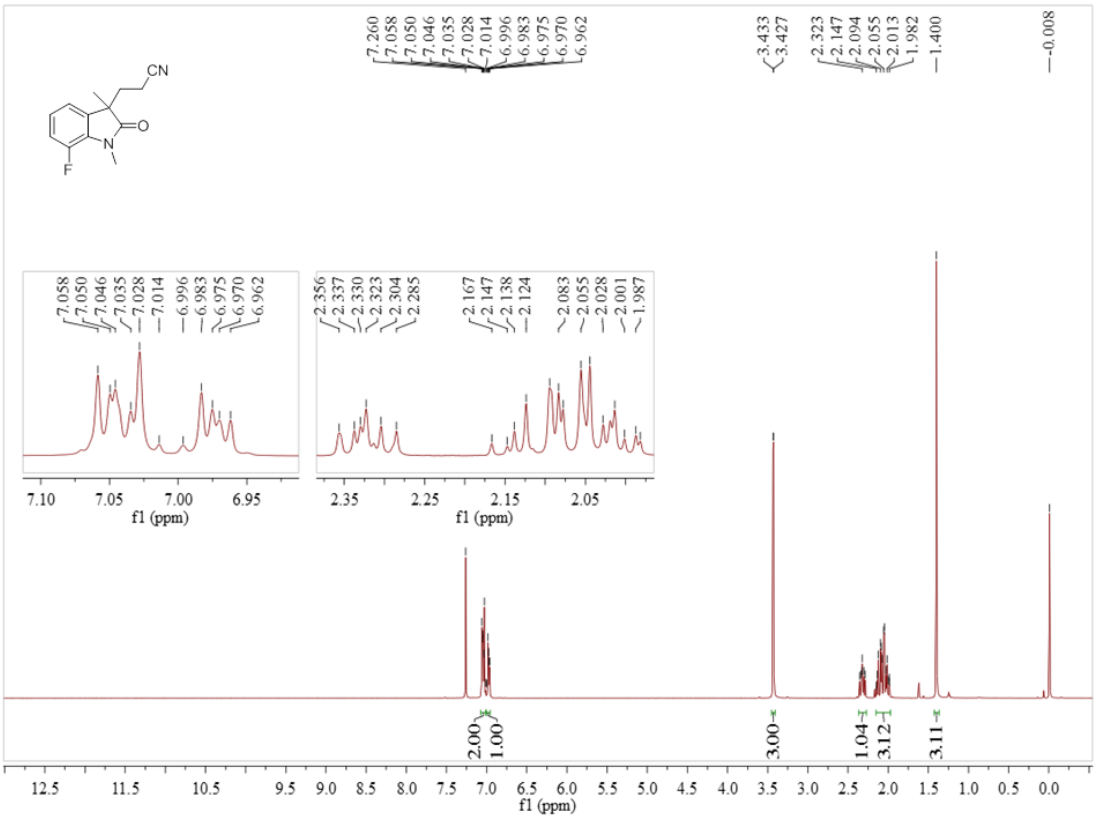
12.94
f1 (ppm)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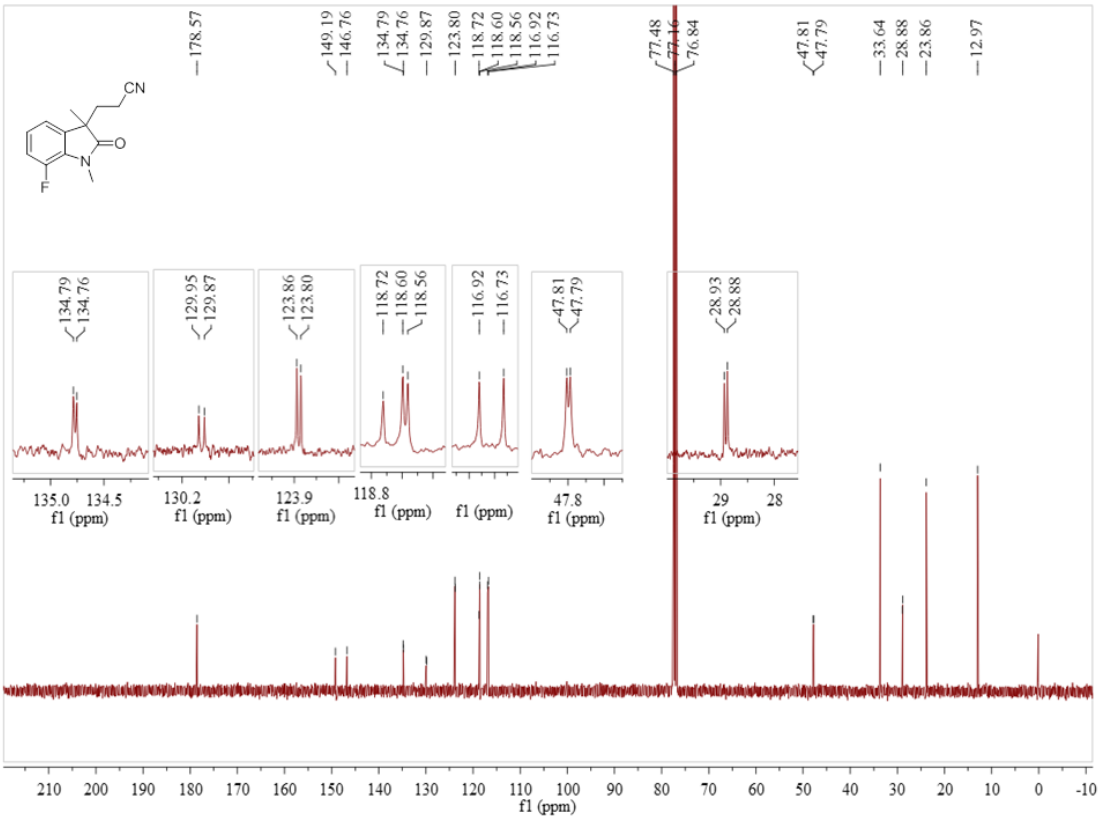
3.11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CN
O
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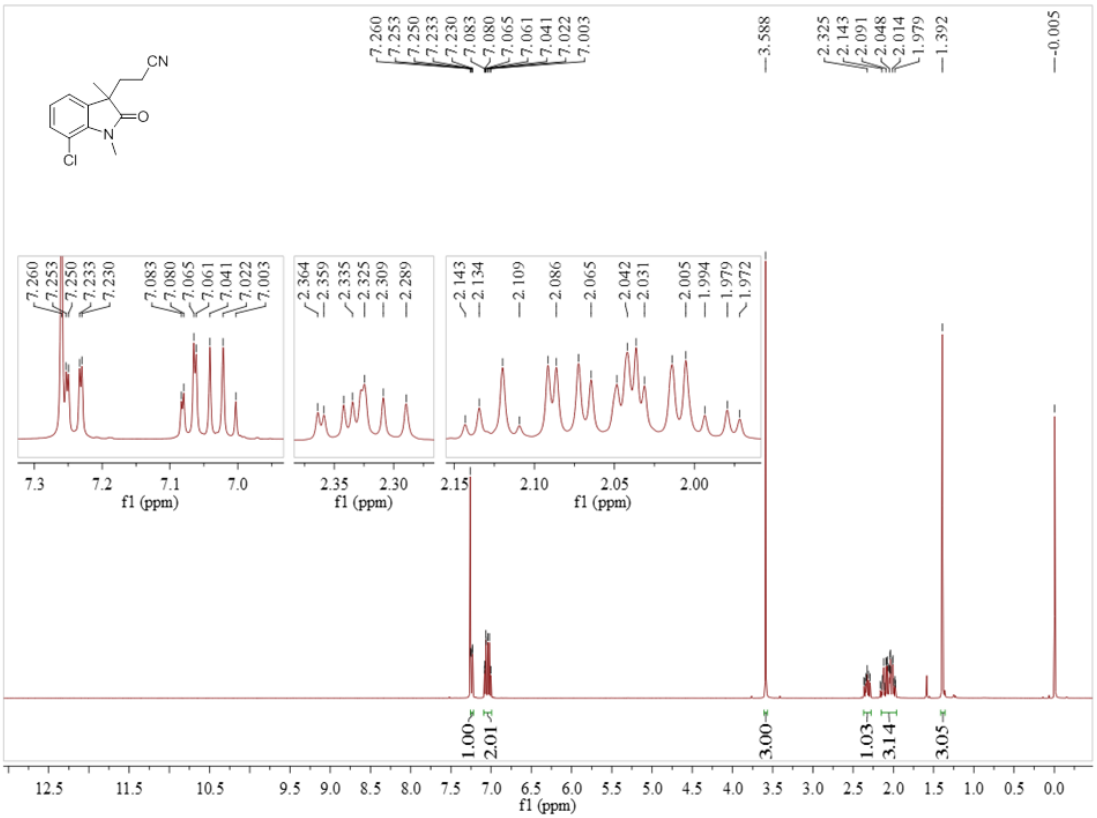
F
f1 (ppm)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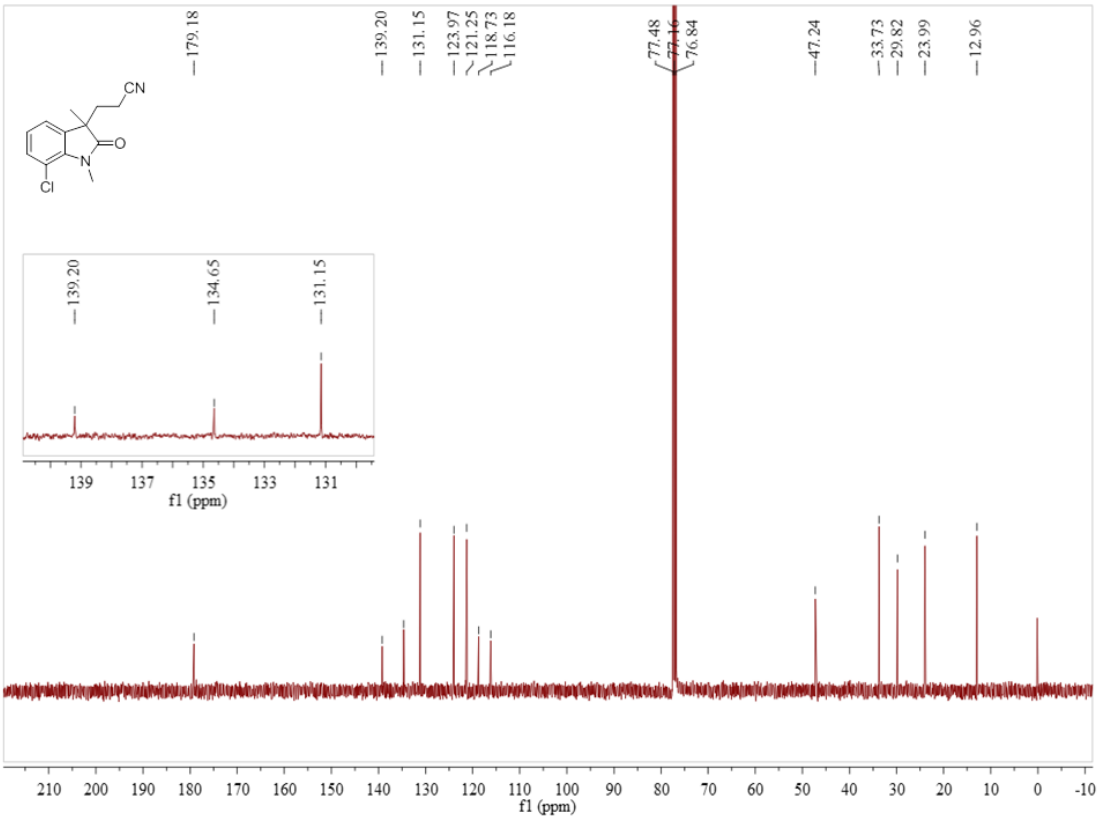
2.109
2.086
2.065
2.042
2.031
2.005
1.994
1.979
1.972
f1 (ppm)
1.00
2.01
3.00
1.03
3.14
3.05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O
N
Cl
179.18
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131.15
123.97
121.25
118.73
116.18
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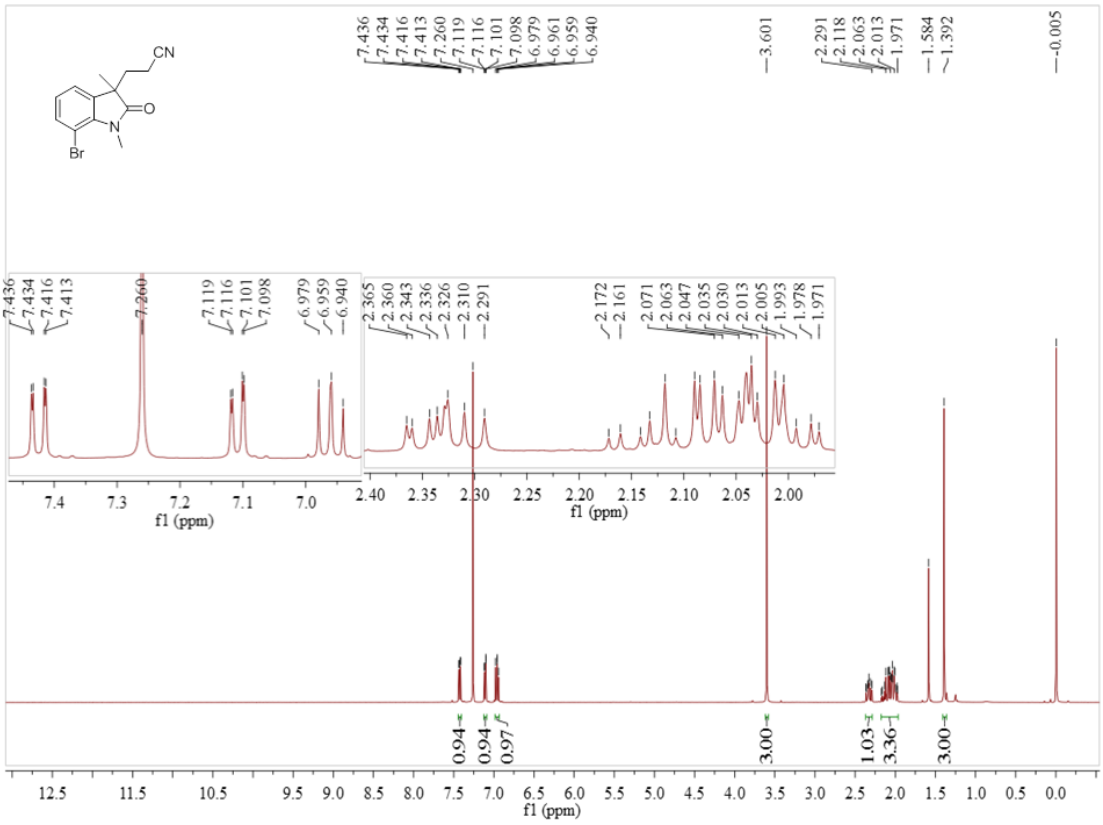
77.16
76.84
47.24
33.73
29.82
23.99
12.96
139.20
134.65
131.15
f1 (ppm)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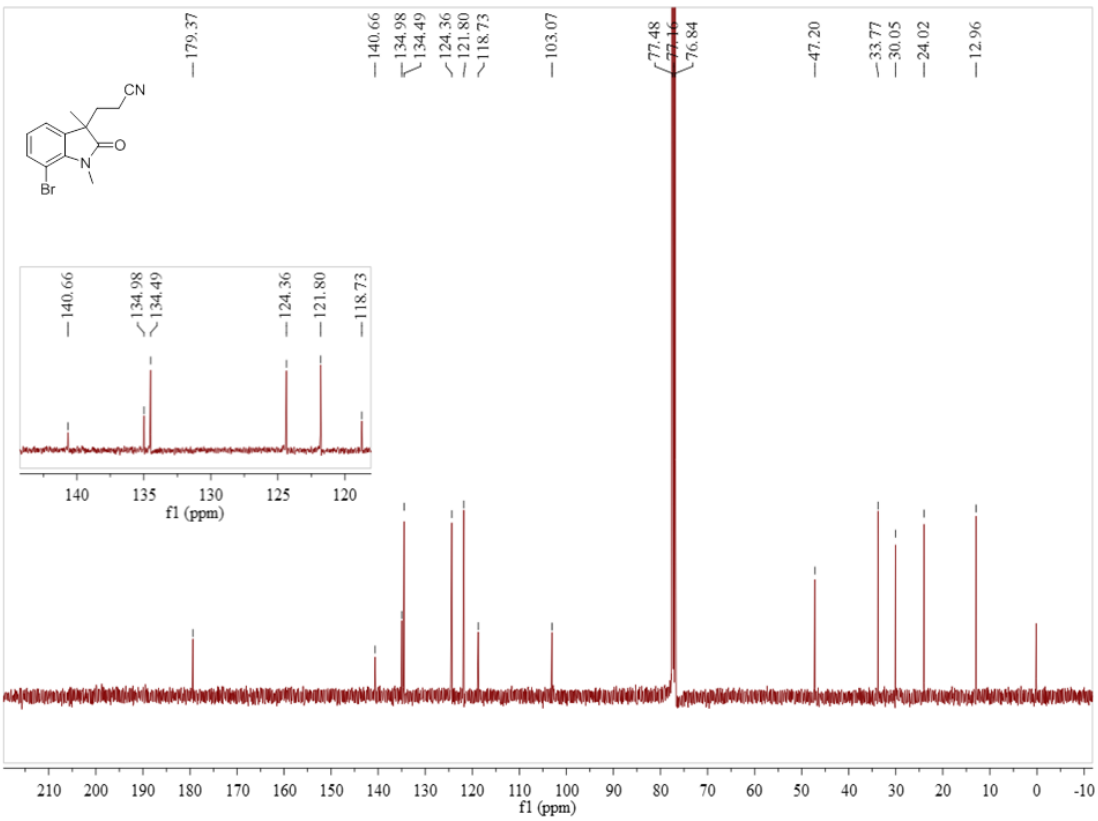
O
N
Br
7.436
7.434
7.416
7.413
7.260
7.119
7.116
7.101
7.098
6.979
6.961
6.959
6.940
3.601
2.291
2.118
2.063
2.013
1.971
1.584
1.392
-0.005
2.365
2.360
2.343
2.336
2.326
2.310
2.291
2.172
2.161
2.071
2.063
2.047
2.035
2.030
2.013
2.005
1.993
1.978
1.971
0.94
0.94
0.97
3.00
1.03
3.36
3.00
f1 (ppm)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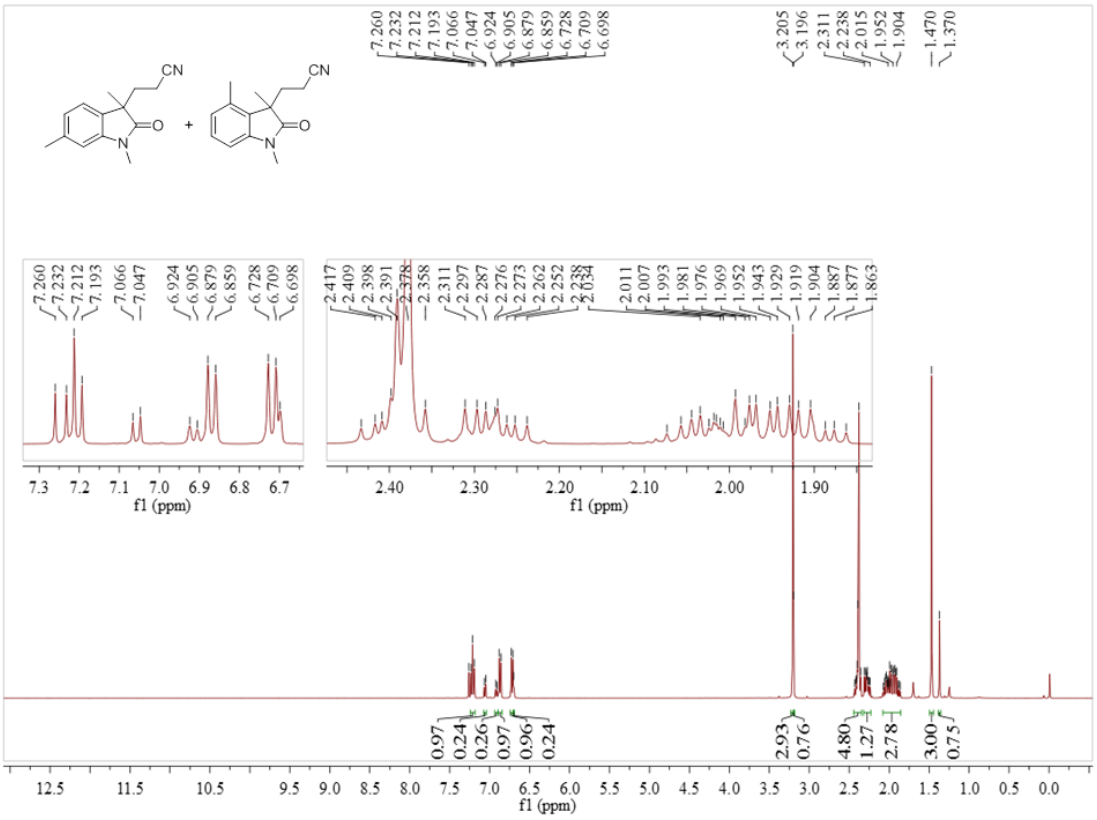
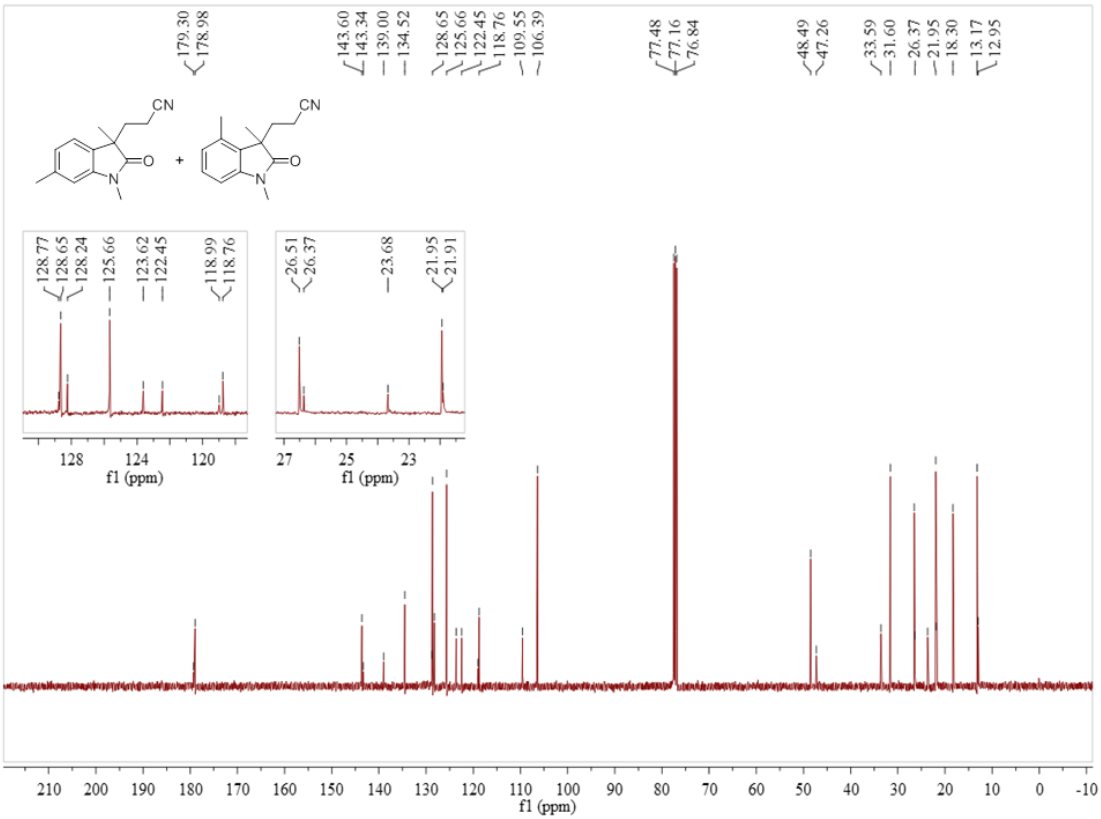
O
N
Br
179.37
140.66
134.98
134.49
124.36
121.80
118.73
103.07
77.48
77.16
76.84
47.20
33.77
30.05
24.02
12.96
f1 (ppm)


7.260
7.232
7.212
7.193
7.066
7.047
6.924
6.905
6.879
6.859
6.728
6.709
6.698
3.205
3.196
2.311
2.238
2.015
1.952
1.904
1.470
1.370
CN
O
N
+
f1 (ppm)
0.97
0.24
0.26
0.97
0.96
0.24
2.93
0.76
4.80
1.27
2.78
3.00
0.75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178.98
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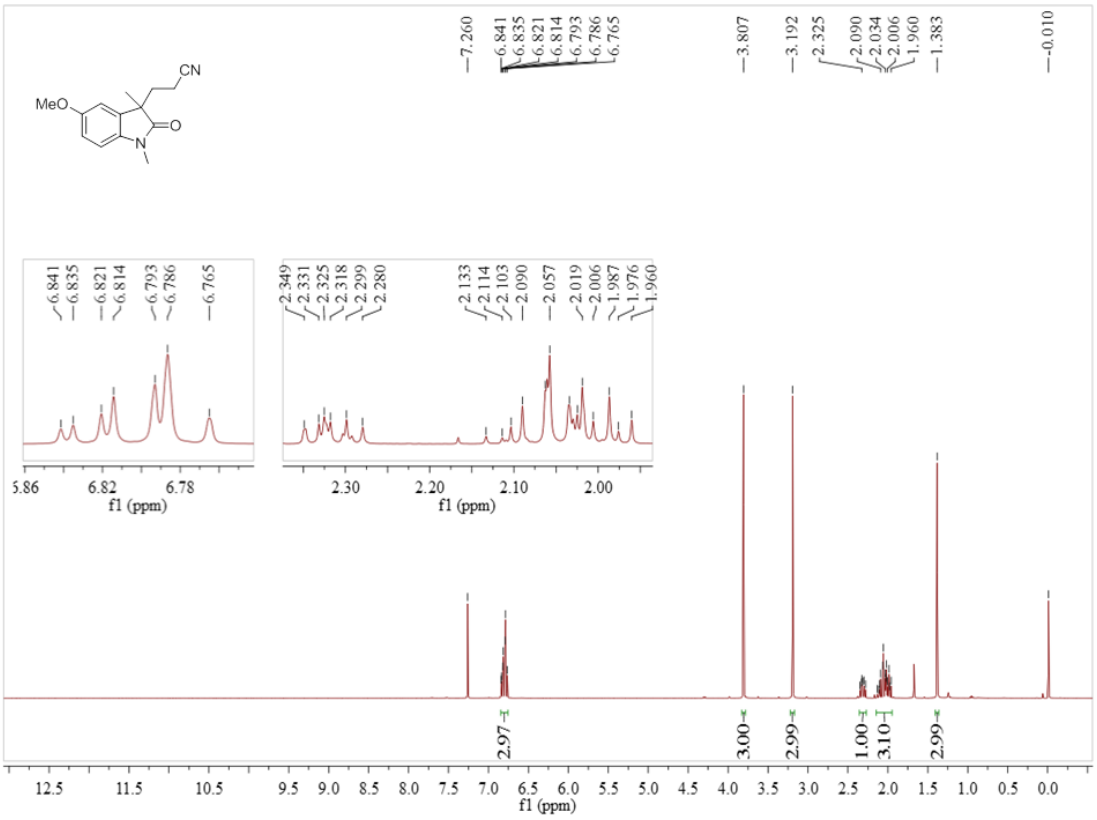
143.34
139.00
134.52
128.65
125.66
122.45
118.76
109.55
106.39
77.48
77.16
76.84
48.49
47.26
33.59
31.60
26.37
21.95
18.30
13.17
12.95
CN
O
N
+
f1 (ppm)


CN
MeO
O
N
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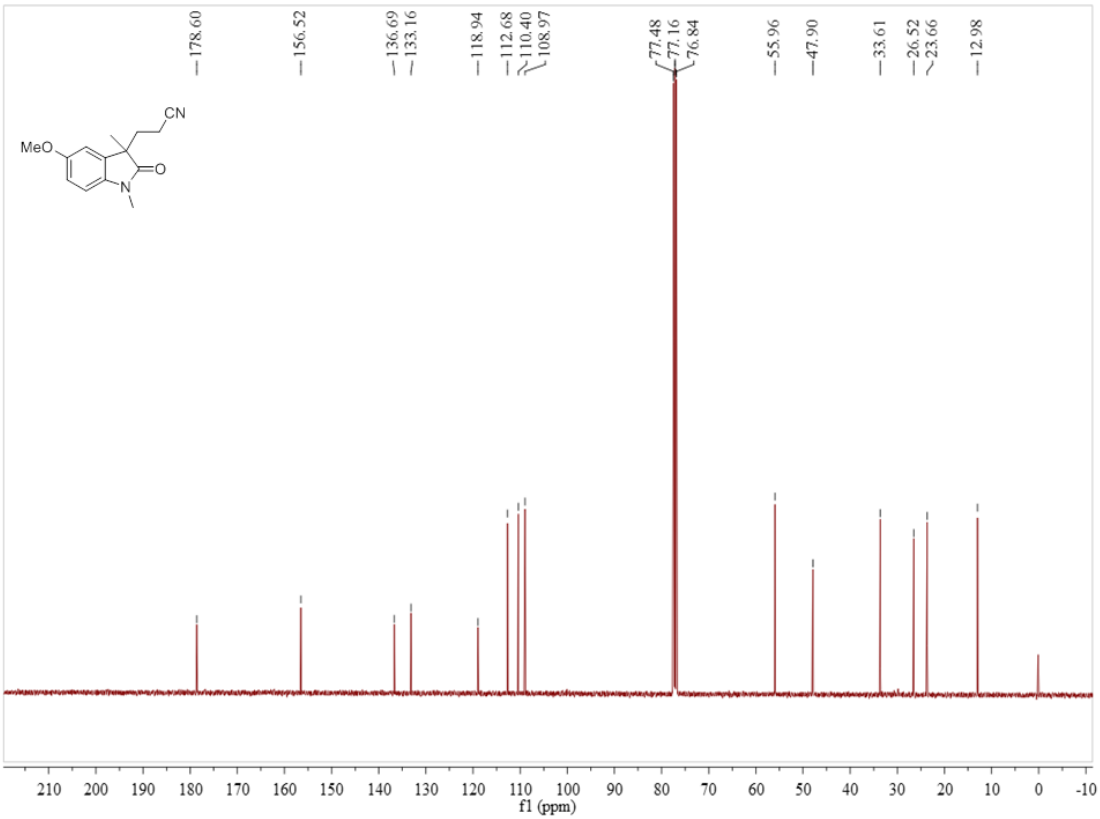
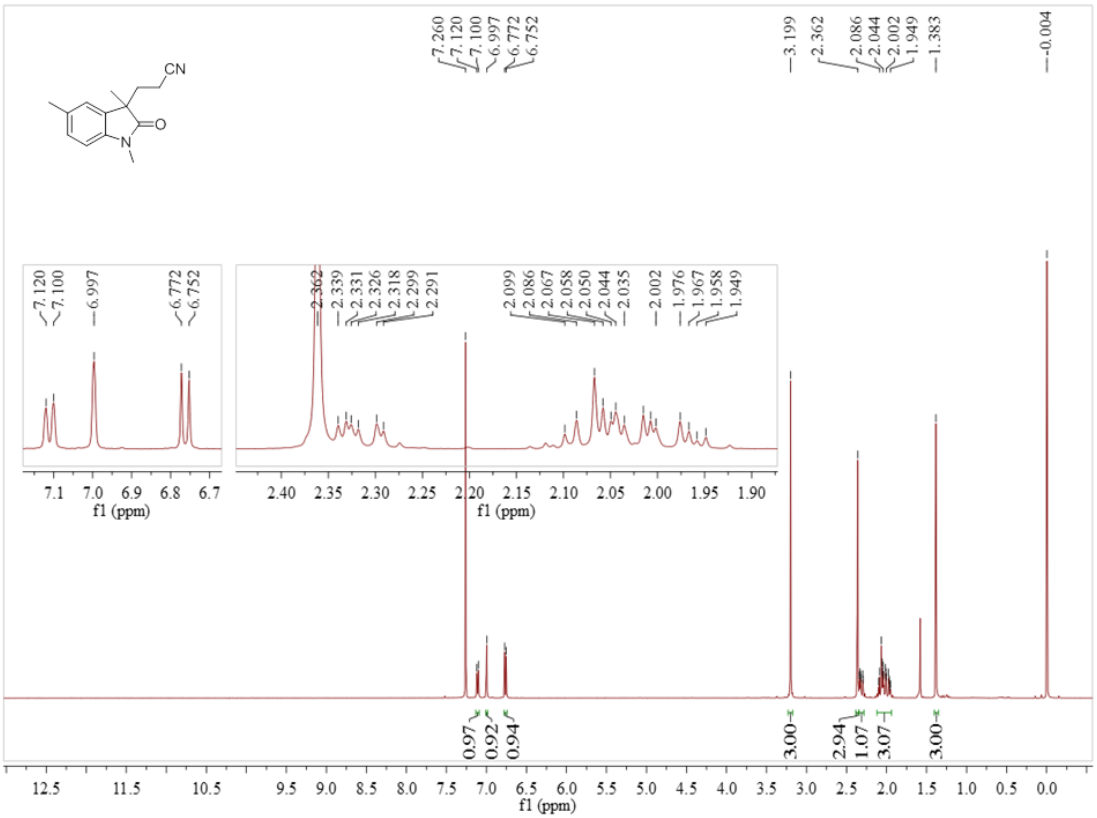
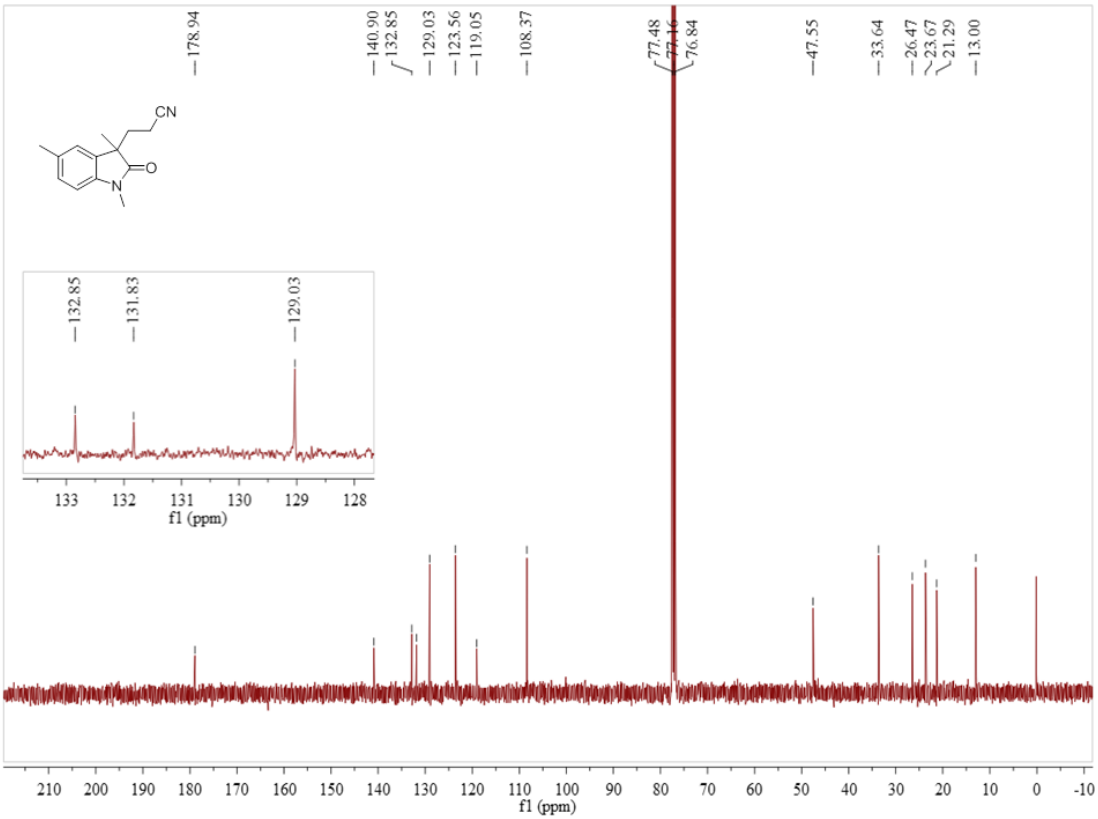
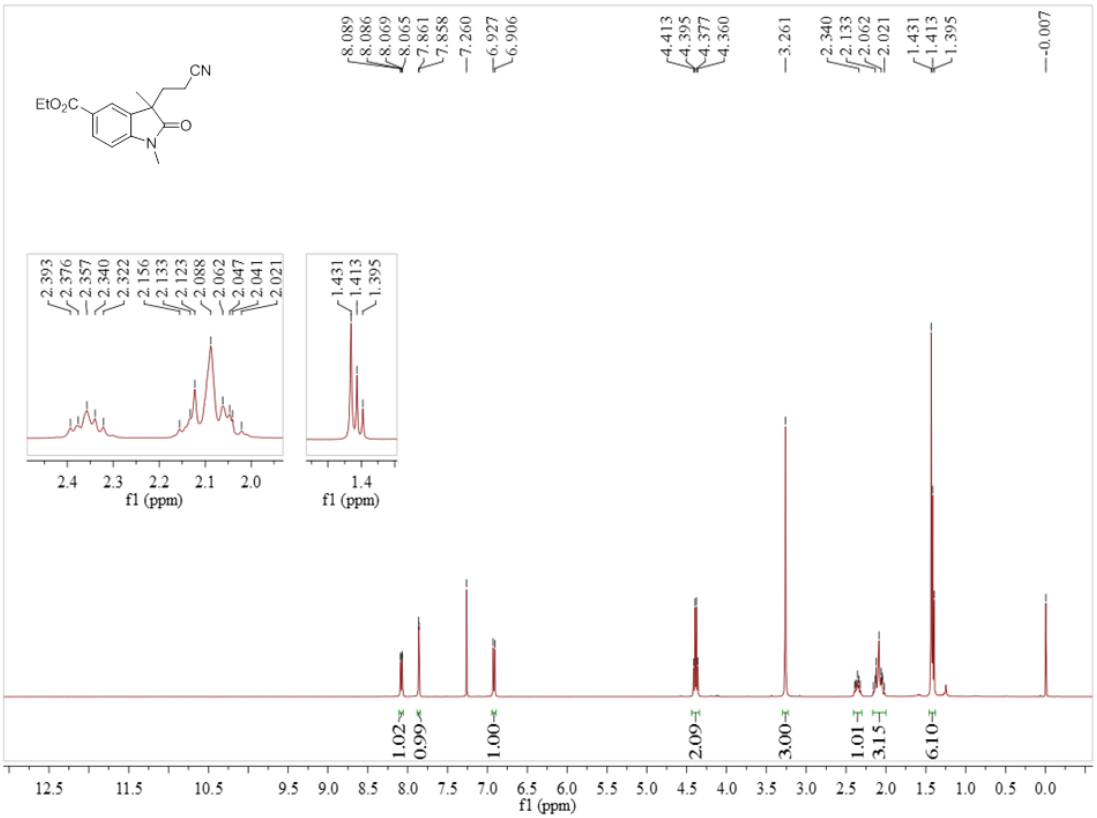
6.835
6.821
6.814
6.793
6.786
6.765
3.807
3.192
2.325
2.090
2.034
2.006
1.960
1.383
-0.010
2.349
2.331
2.325
2.318
2.299
2.280
2.133
2.114
2.103
2.090
2.057
2.019
2.006
1.987
1.976
1.960
5.86
6.82
6.78
f1 (ppm)
2.30
2.20
2.10
2.00
f1 (ppm)
2.97
3.00
2.99
1.00
3.10
2.99
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CN
MeO
O
N
178.60
156.52
136.69
133.16
118.94
112.68
110.40
108.97
77.48
77.16
76.84
55.96
47.90
33.61
26.52
23.66
12.98
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)


CN
O
N
7.260
7.120
7.100
6.997
6.772
6.752
3.199
2.362
2.086
2.044
2.002
1.949
1.383
-0.004
0.97
0.92
0.94
3.00
2.94
1.07
3.07
3.00
f1 (ppm)


CN
O
N
178.94
140.90
132.85
129.03
123.56
119.05
108.37
77.48
77.16
76.84
47.55
33.64
26.47
23.67
21.29
13.00
132.85
131.83
129.03
f1 (ppm)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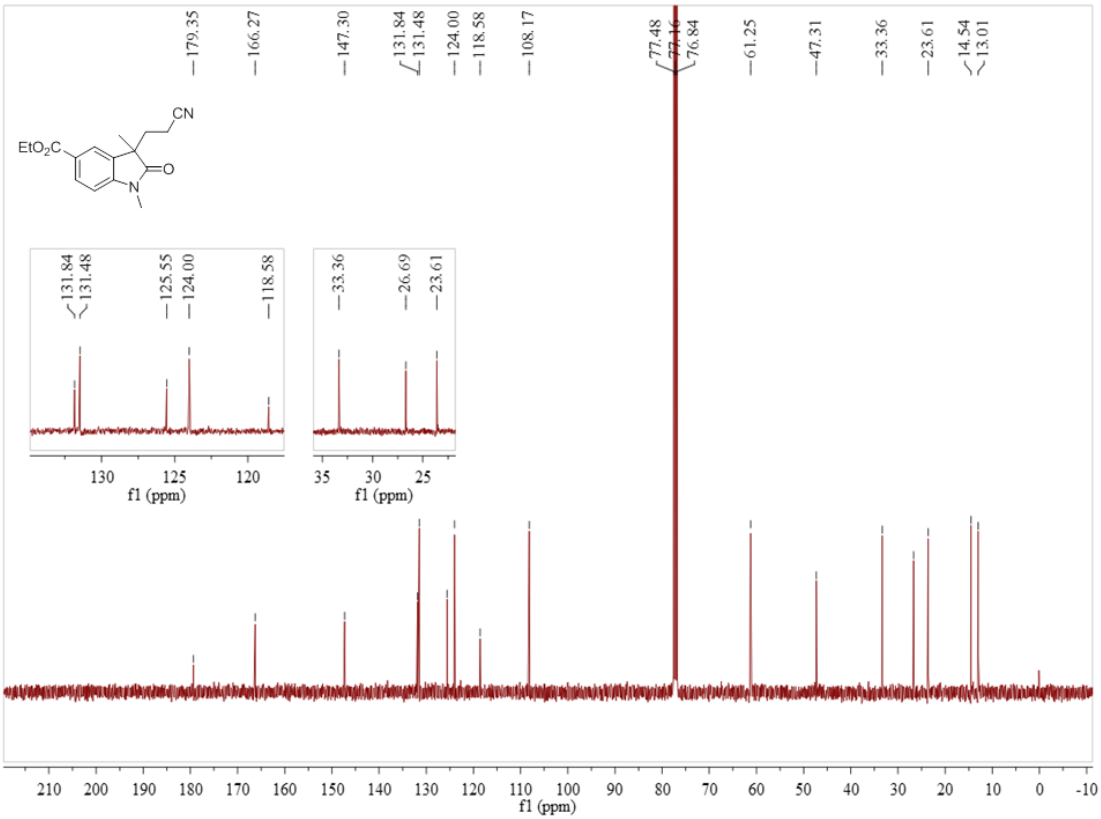
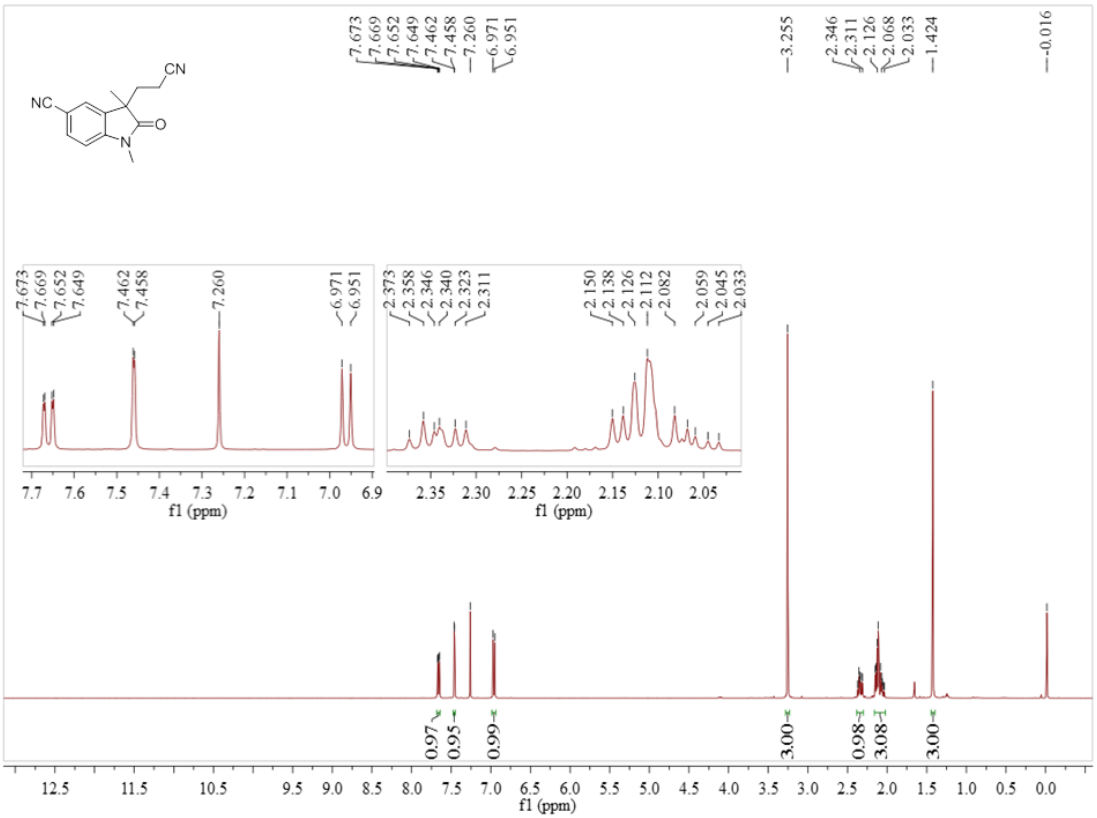
8.086
8.069
8.065
7.861
7.858
7.260
6.927
6.906
4.413
4.395
4.377
4.360
3.261
2.340
2.133
2.062
2.021
1.431
1.413
1.395
-0.007
CN
EtO2C
O
N
2.393
2.376
2.357
2.340
2.322
2.156
2.133
2.123
2.088
2.062
2.047
2.041
2.021
f1 (ppm)
1.431
1.413
1.395
f1 (ppm)
1.02
0.99
1.00
2.09
3.00
1.01
3.15
6.10
f1 (ppm)


179.35
166.27
147.30
131.84
131.48
124.00
118.58
108.17
77.48
77.16
76.84
61.25
47.31
33.36
23.61
14.54
13.01
CN
EtO2C
O
N
131.84
131.48
125.55
124.00
118.58
f1 (ppm)
33.36
26.69
23.61
f1 (ppm)
f1 (ppm)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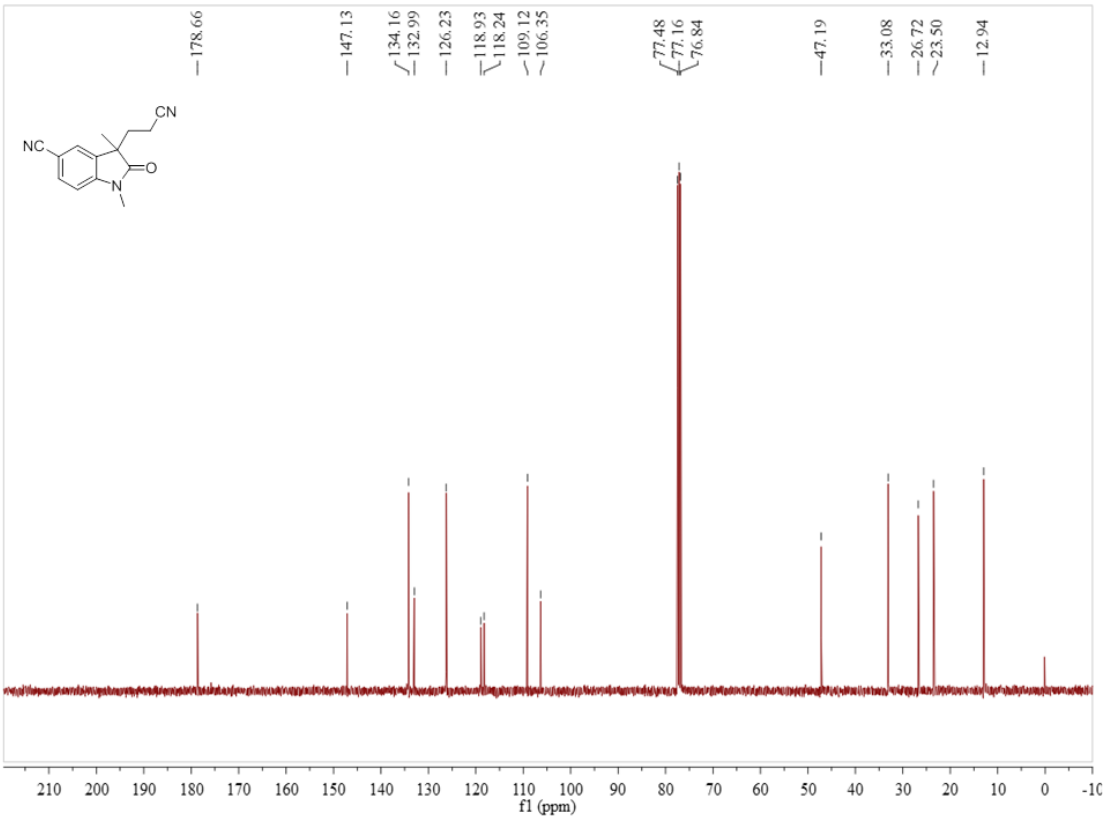
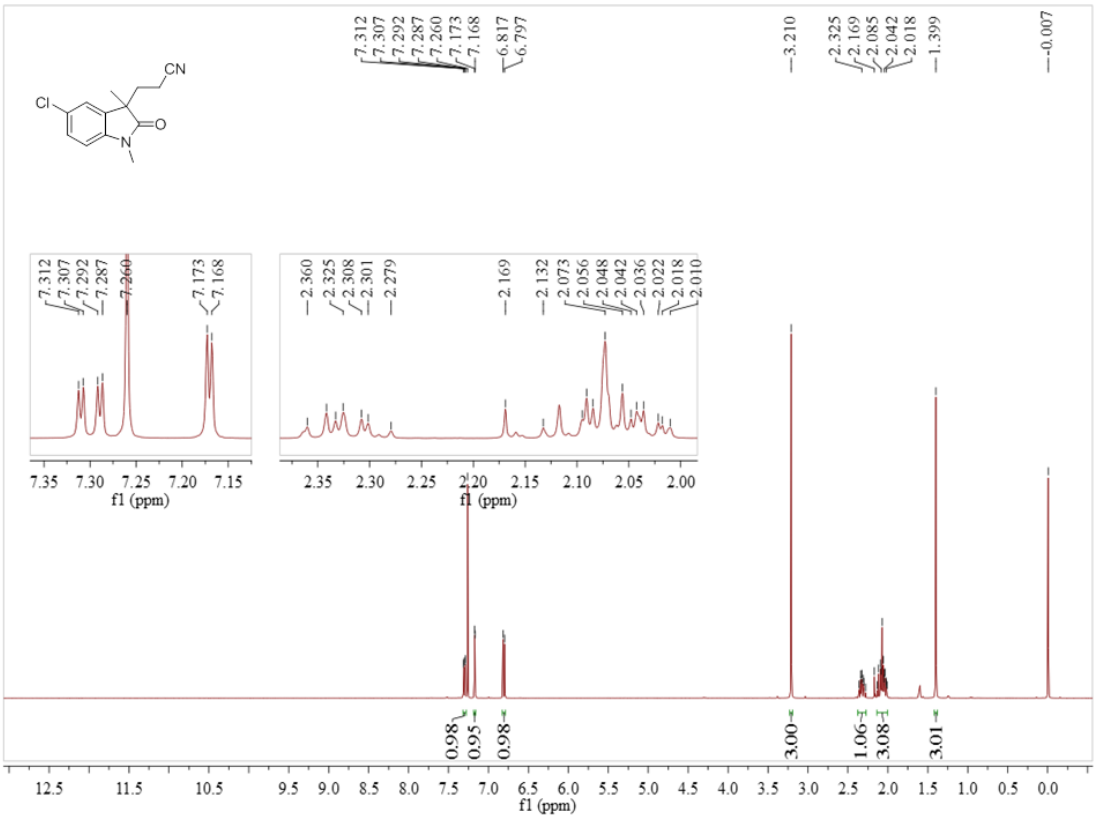
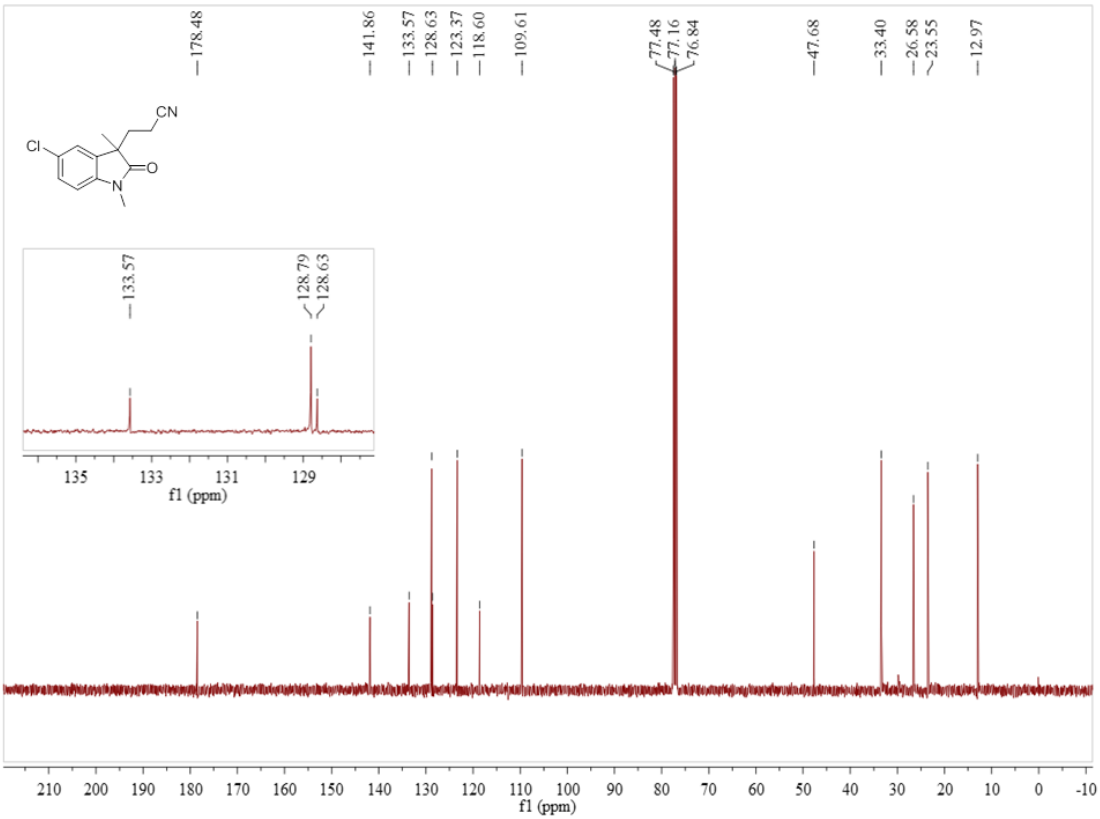
7.669
7.652
7.649
7.462
7.458
7.260
6.971
6.951
3.255
2.346
2.311
2.126
2.068
2.033
1.424
-0.016
2.373
2.358
2.346
2.340
2.323
2.311
2.150
2.138
2.126
2.112
2.082
2.059
2.045
2.033
0.97
0.95
0.99
3.00
0.98
3.08
3.00
f1 (ppm)


178.66
147.13
134.16
132.99
126.23
118.93
118.24
109.12
106.35
77.48
77.16
76.84
47.19
33.08
26.72
23.50
12.94
f1 (ppm)


CN
Cl
O
N
7.312
7.307
7.292
7.287
7.260
7.173
7.168
6.817
6.797
3.210
2.325
2.169
2.085
2.042
2.018
1.399
-0.007
2.360
2.325
2.308
2.301
2.279
2.169
2.132
2.073
2.056
2.048
2.042
2.036
2.022
2.018
2.010
f1 (ppm)
0.98
0.95
0.98
3.00
1.06
3.08
3.01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Cl
O
N
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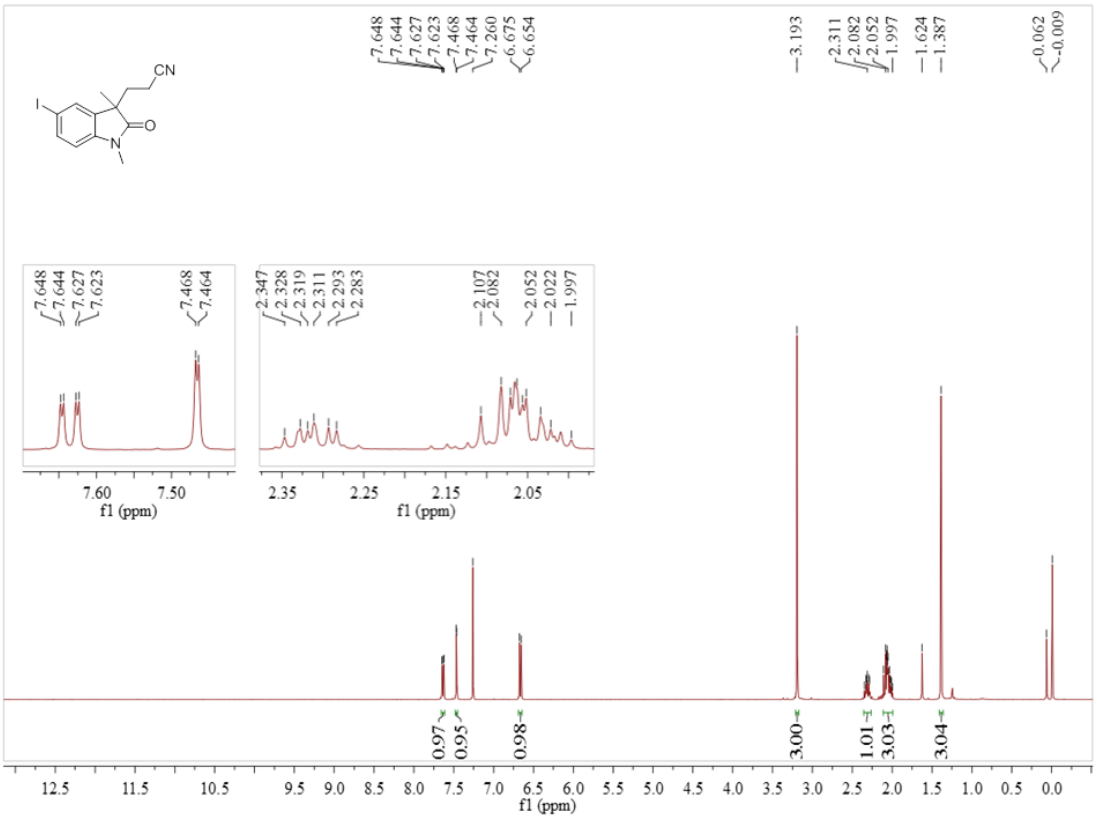
141.86
133.57
128.63
123.37
118.60
109.61
77.48
77.16
76.84
47.68
33.40
26.58
23.55
12.97
133.57
128.79
128.63
f1 (ppm)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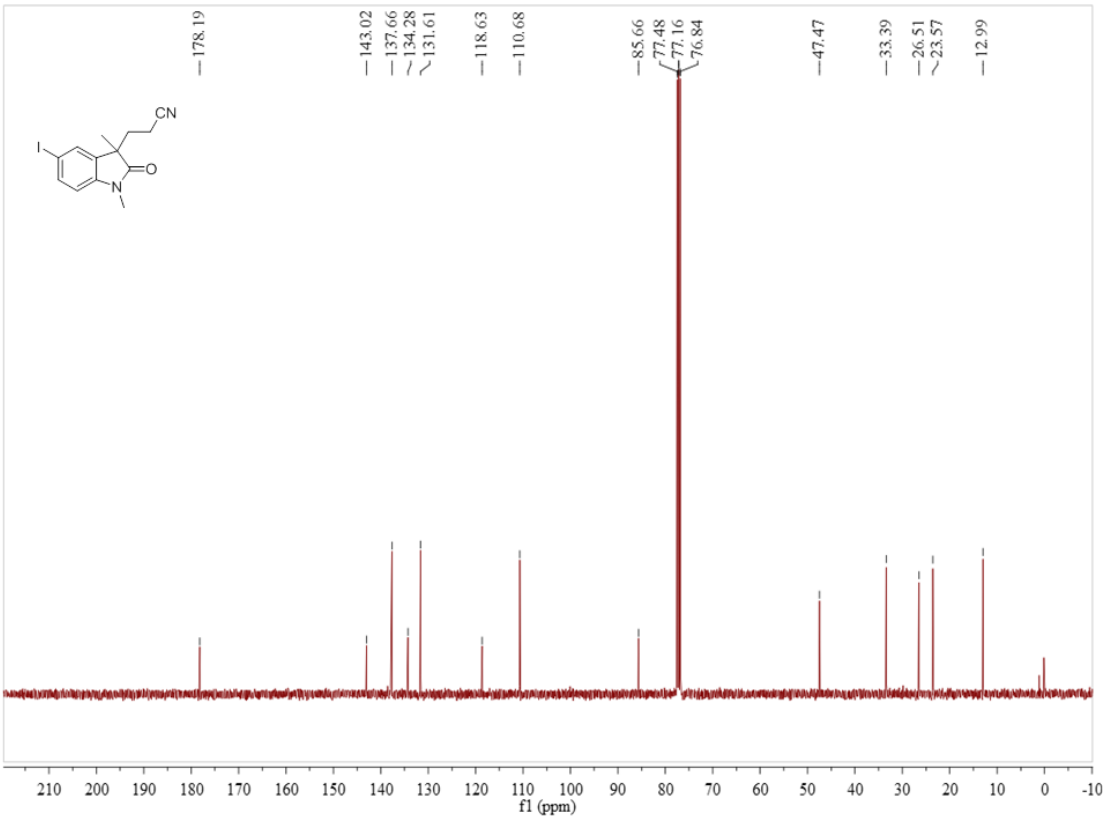
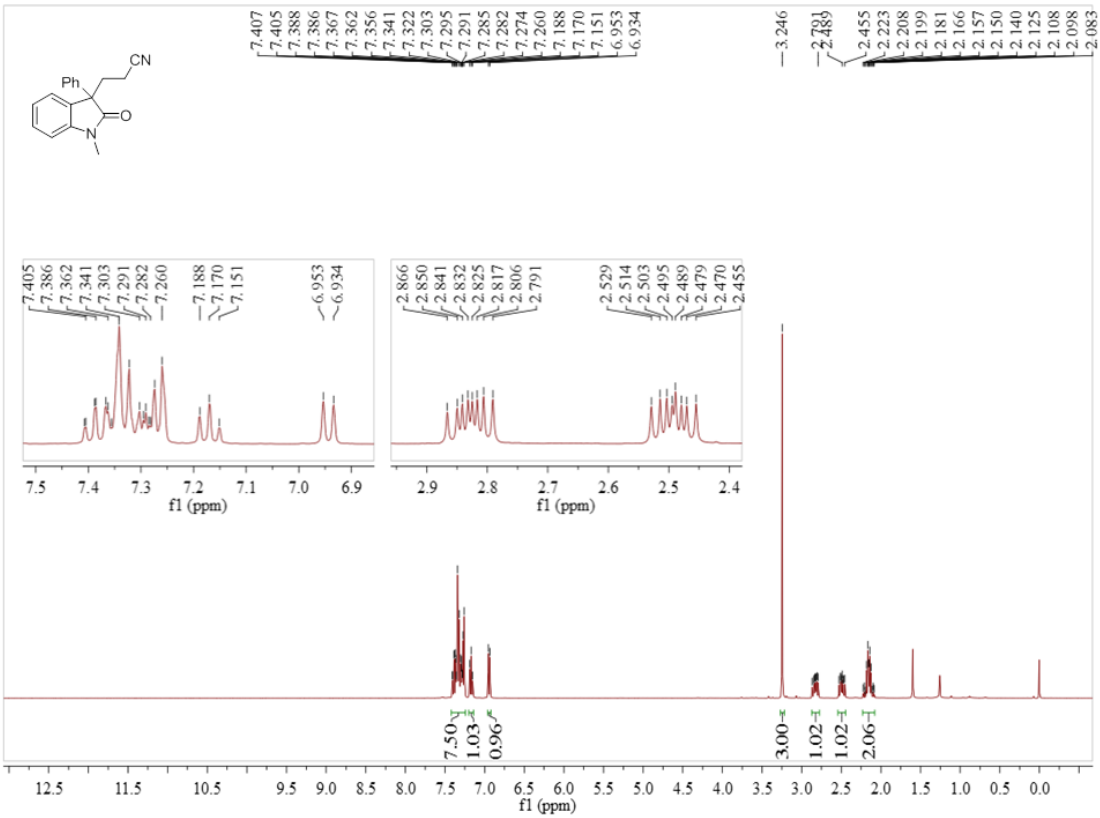
7.627
7.623
7.468
7.464
7.260
6.675
6.654
3.193
2.311
2.082
2.052
1.997
1.624
1.387
0.062
-0.009
CN
I
O
N
7.60
7.50
f1 (ppm)
2.35
2.25
2.15
2.05
f1 (ppm)
0.97
0.95
0.98
3.00
1.01
3.03
3.04
f1 (ppm)


178.19
143.02
137.66
134.28
131.61
118.63
110.68
85.66
77.48
77.16
76.84
47.47
33.39
26.51
23.57
12.99
CN
I
O
N
f1 (ppm)


CN
Ph
O
N
f1 (ppm)
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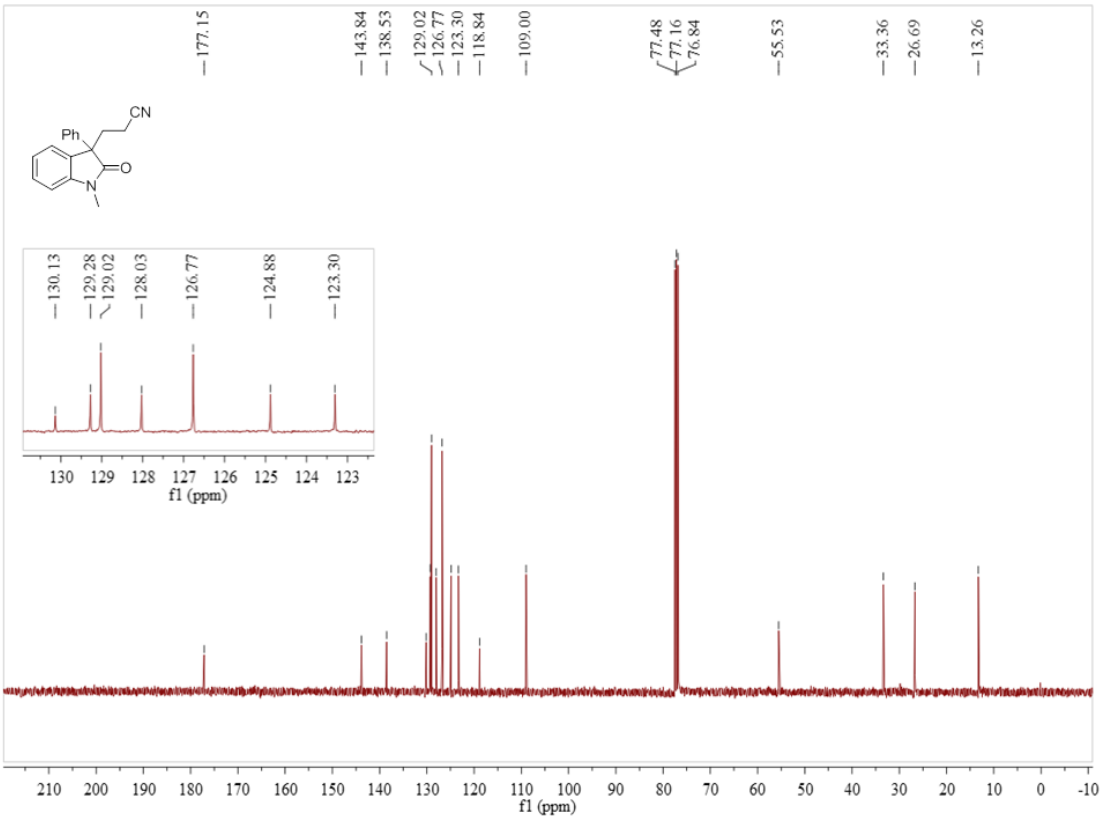
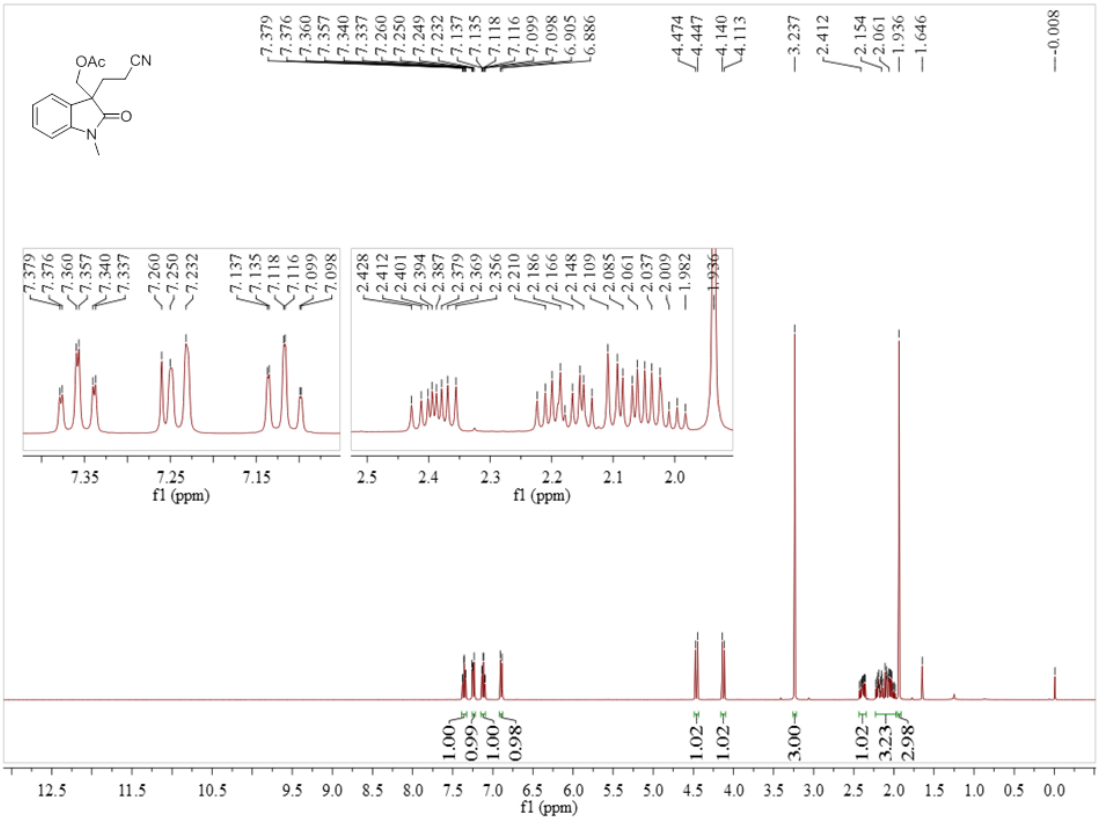
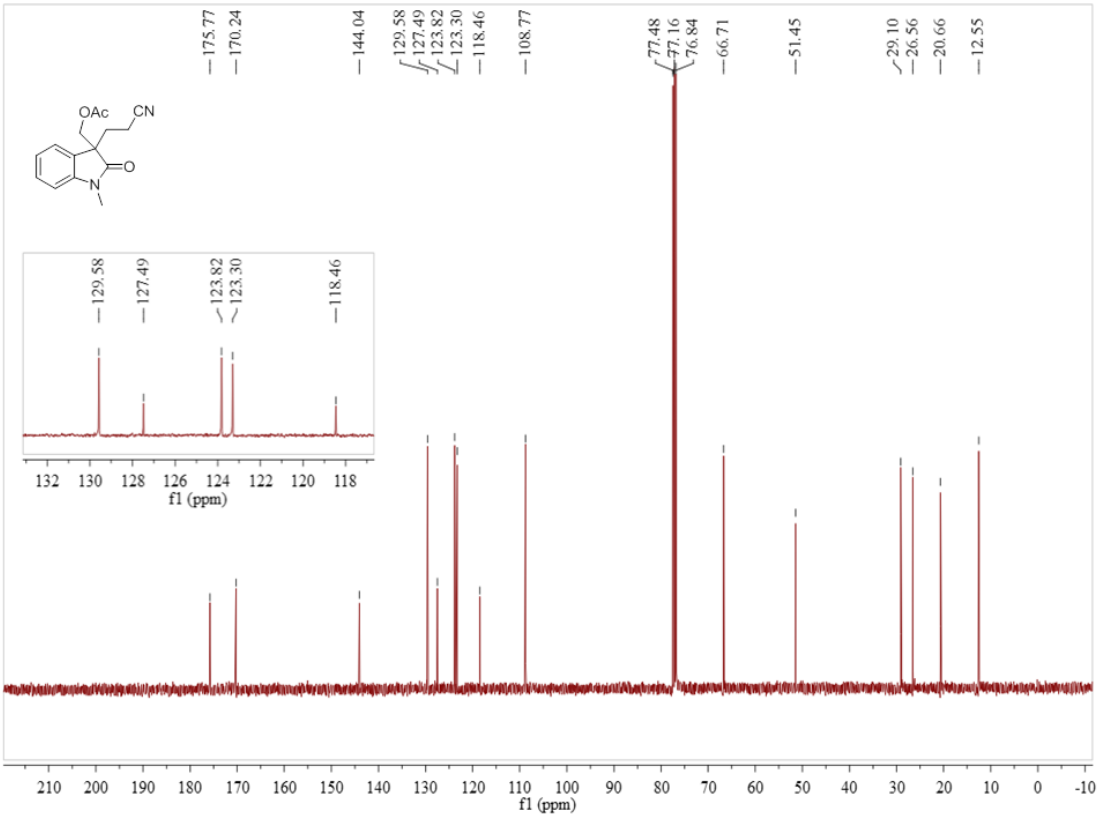
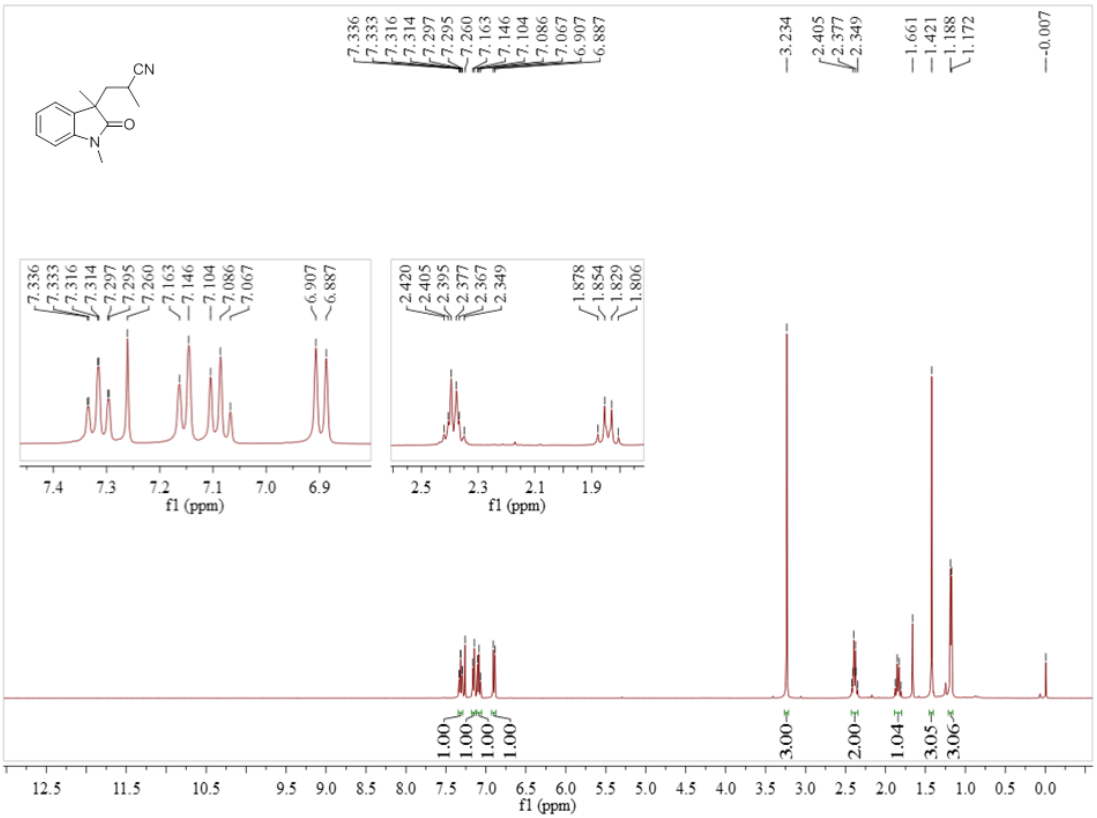
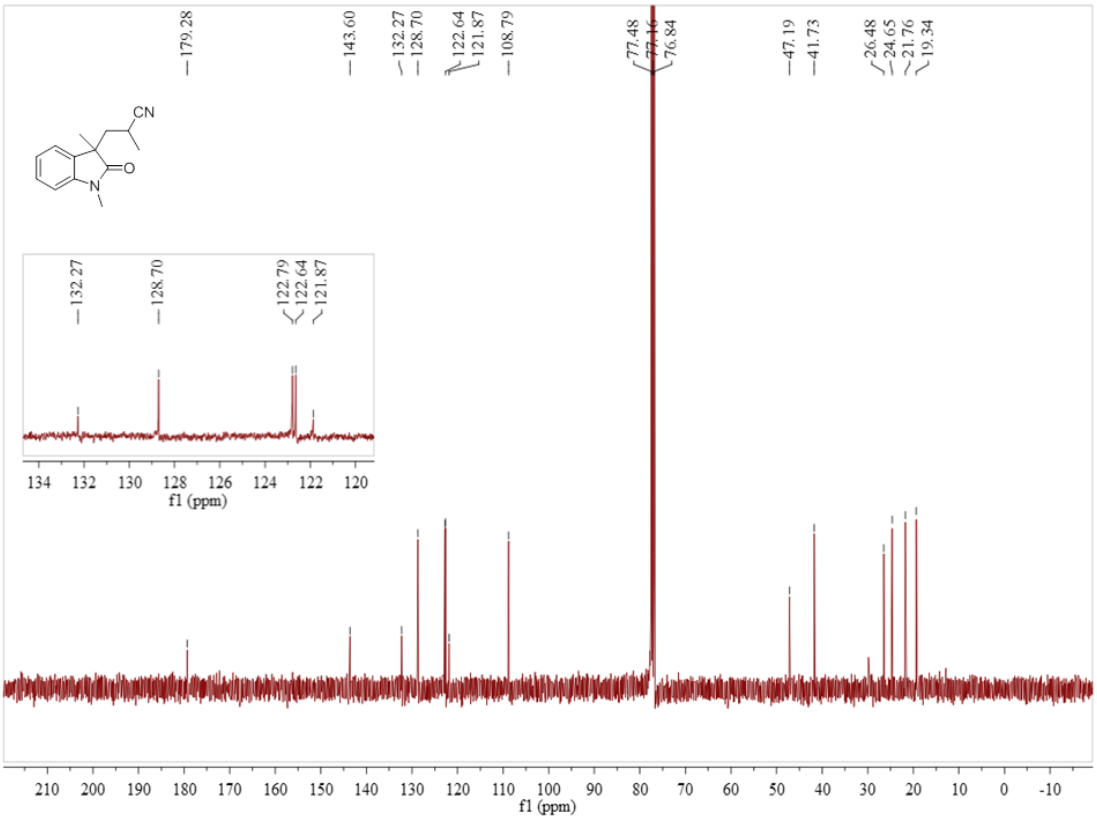
1.03
0.96
3.00
1.02
1.02
2.06


CN
Ph
O
N
f1 (ppm)


OAc
CN
O
N
f1 (ppm)


OAc
CN
O
N
f1 (ppm)


CN
O
N
7.336
7.333
7.316
7.314
7.297
7.295
7.260
7.163
7.146
7.104
7.086
7.067
6.907
6.887
3.234
2.405
2.377
2.349
1.661
1.421
1.188
1.172
-0.007
2.420
2.405
2.395
2.377
2.367
2.349
1.878
1.854
1.829
1.806
f1 (ppm)
1.00
1.00
1.00
1.00
3.00
2.00
1.04
3.05
3.06


CN
O
N
179.28
143.60
132.27
128.70
122.64
121.87
108.79
77.48
77.16
76.84
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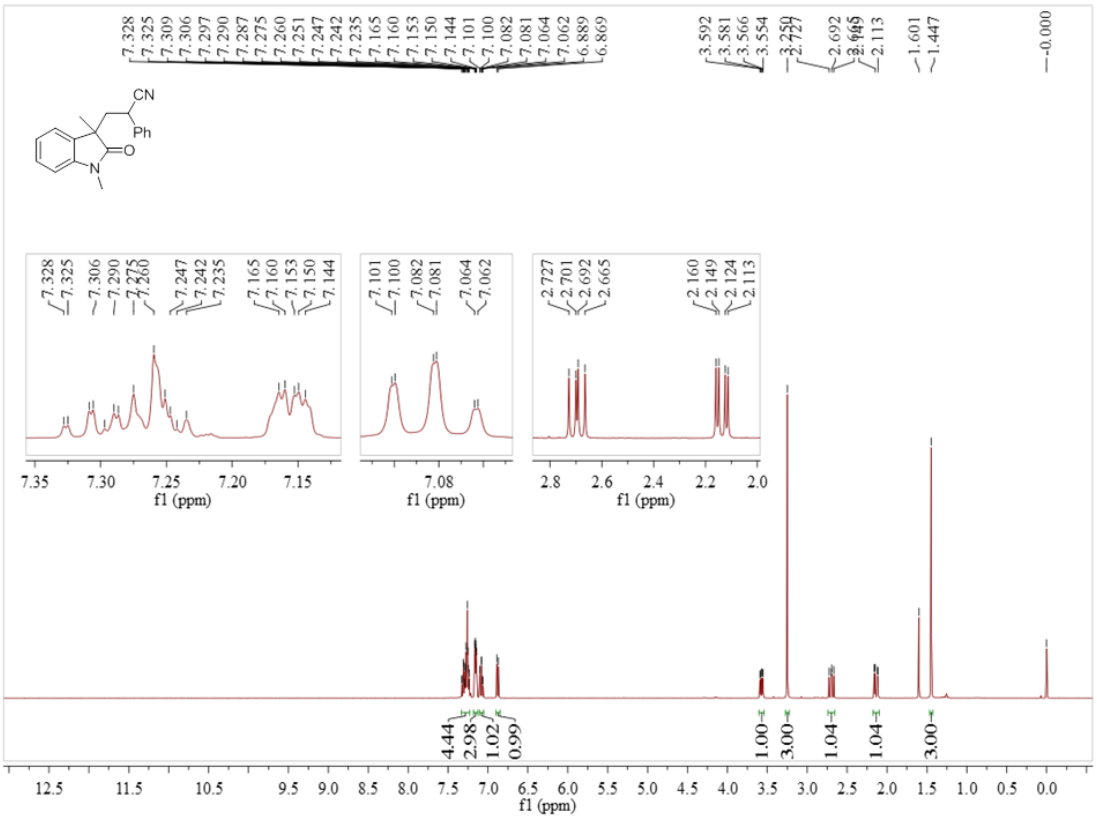
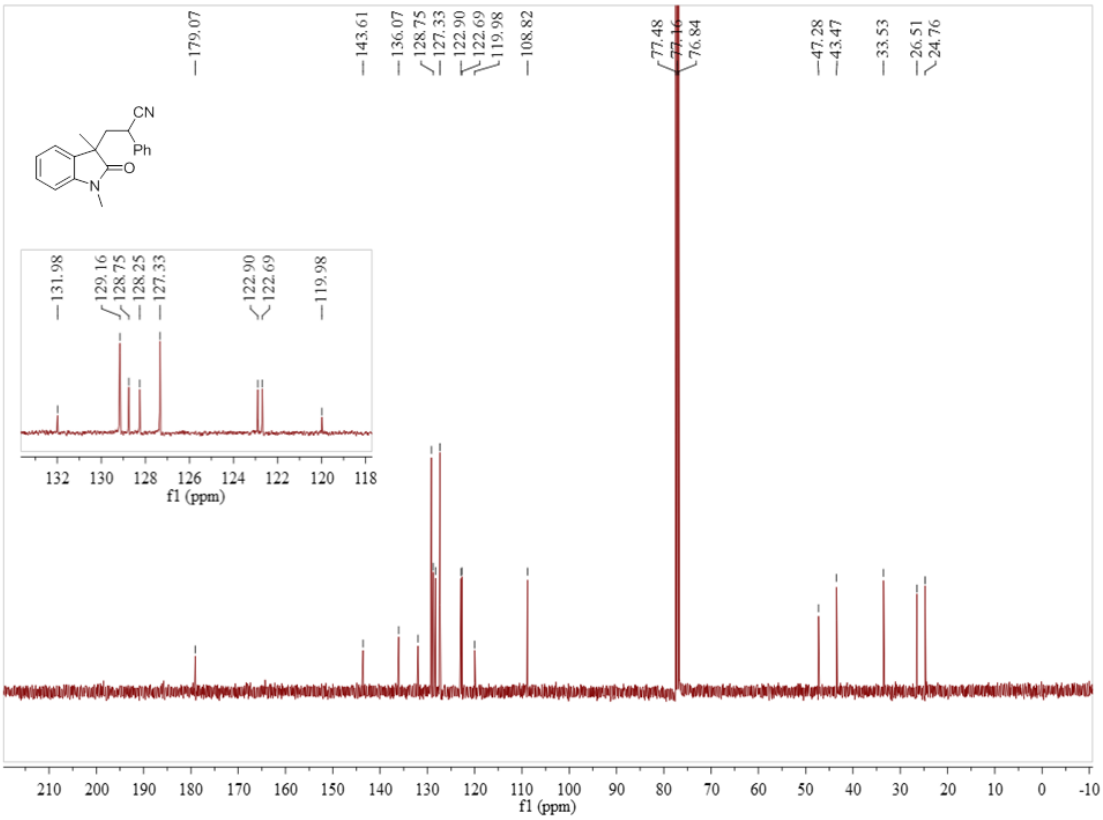
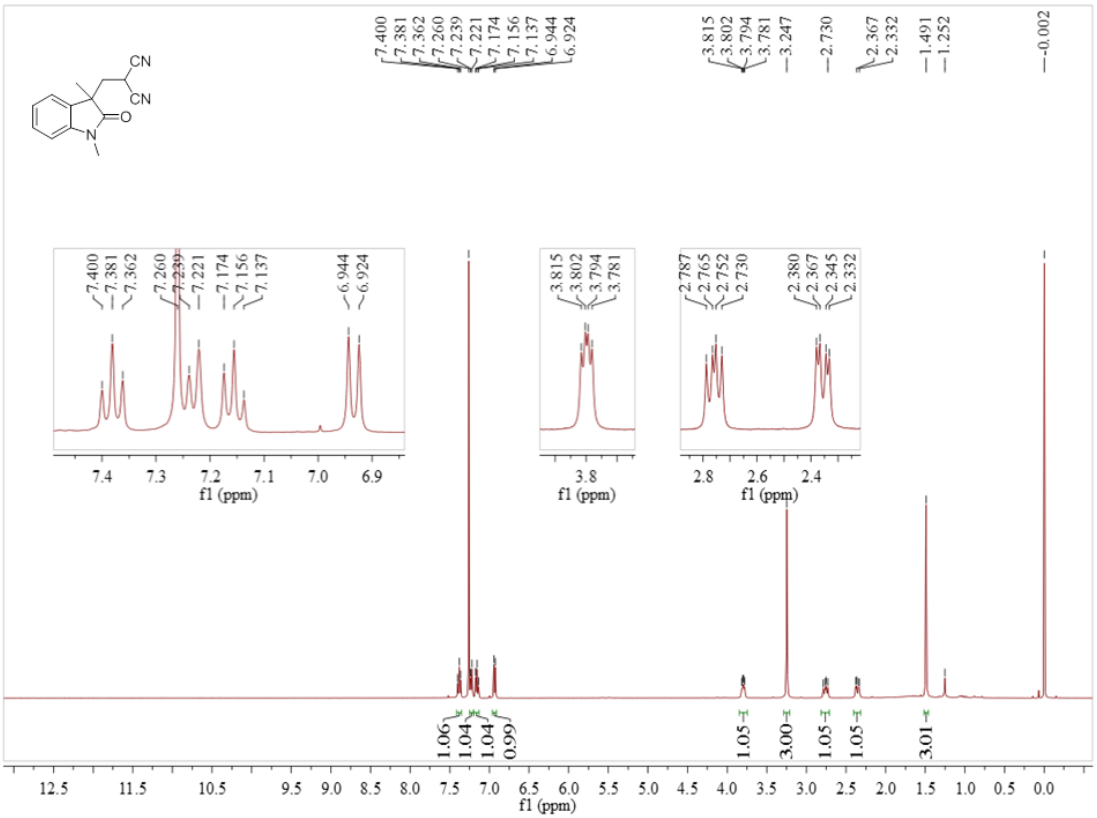
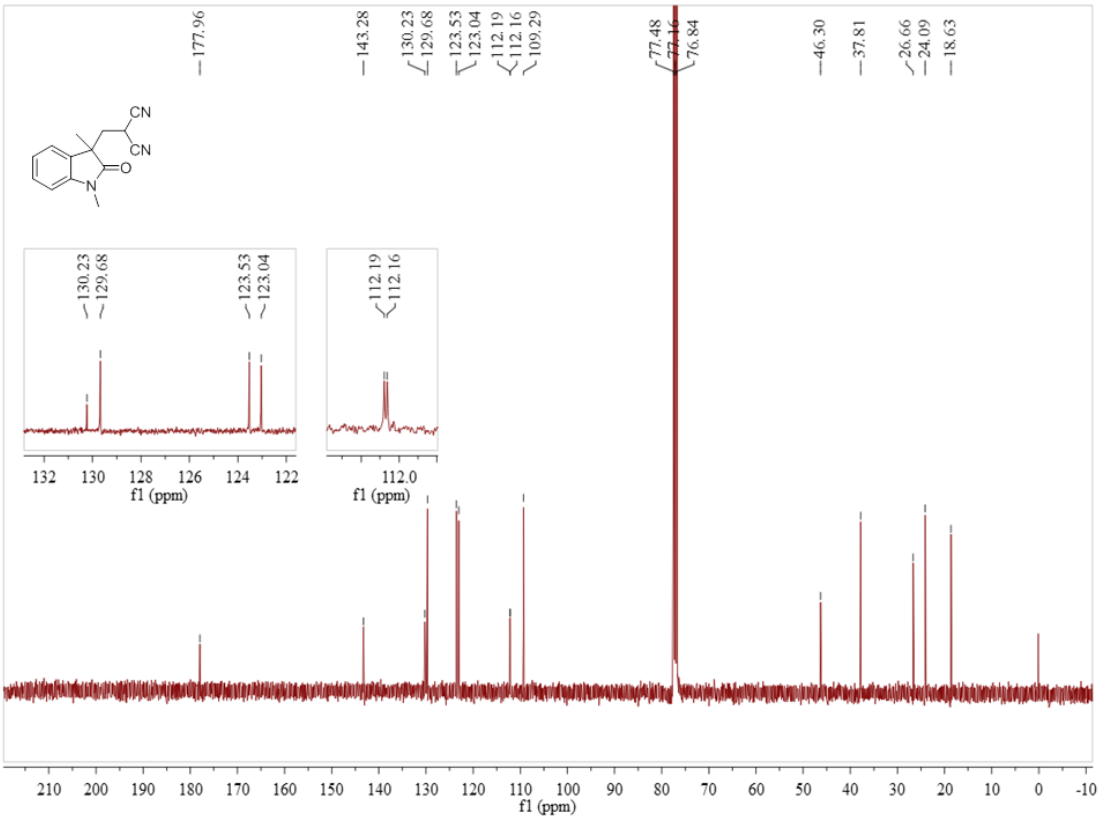
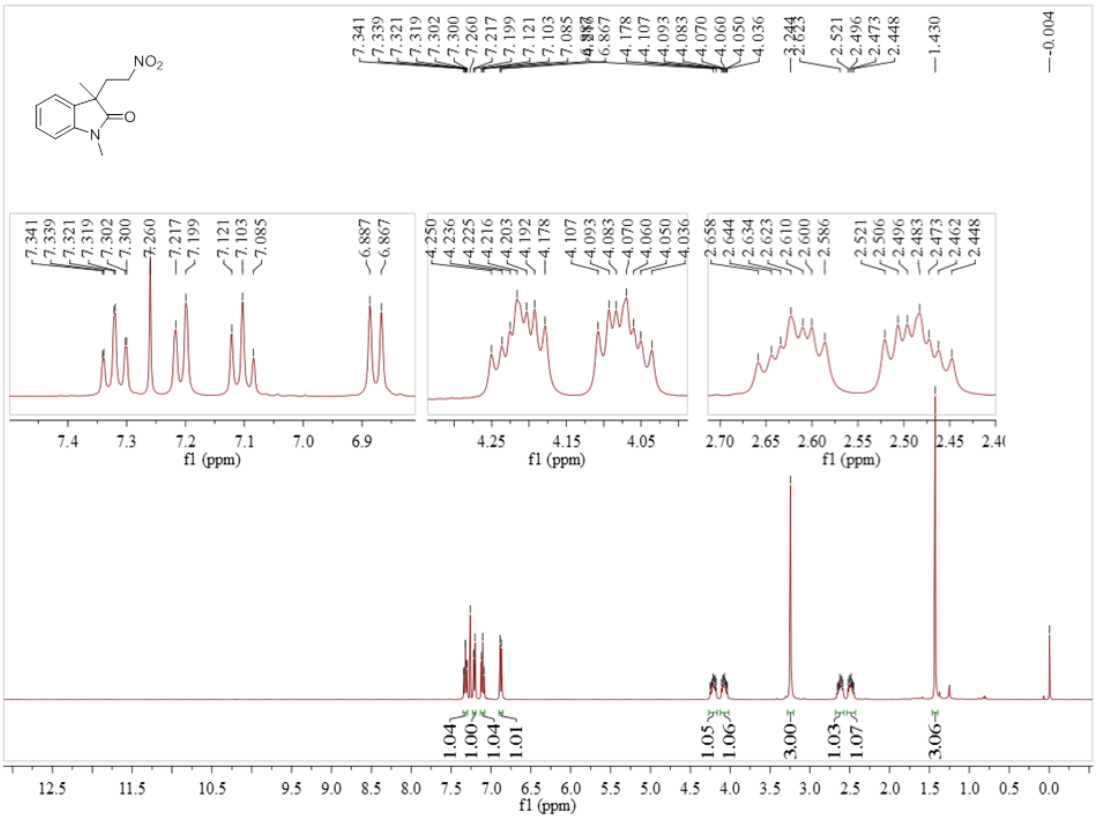
26.48
24.65
21.76
19.34
f1 (ppm)


CN
Ph
O
N
f1 (ppm)
4.44
2.98
1.02
0.99
1.00
3.00
1.04
1.04
3.00


CN
Ph
O
N
f1 (ppm)


CN
CN
O
N
7.400
7.381
7.362
7.260
7.239
7.221
7.174
7.156
7.137
6.944
6.924
3.815
3.802
3.794
3.781
3.247
2.730
2.367
2.332
1.491
1.252
-0.002
f1 (ppm)
1.06
1.04
1.04
0.99
1.05
3.00
1.05
1.05
3.01


CN
CN
O
N
177.96
143.28
130.23
129.68
123.53
123.04
112.19
112.16
109.29
77.48
77.16
76.84
46.30
37.81
26.66
24.09
18.63
f1 (ppm)


NO2
O
N
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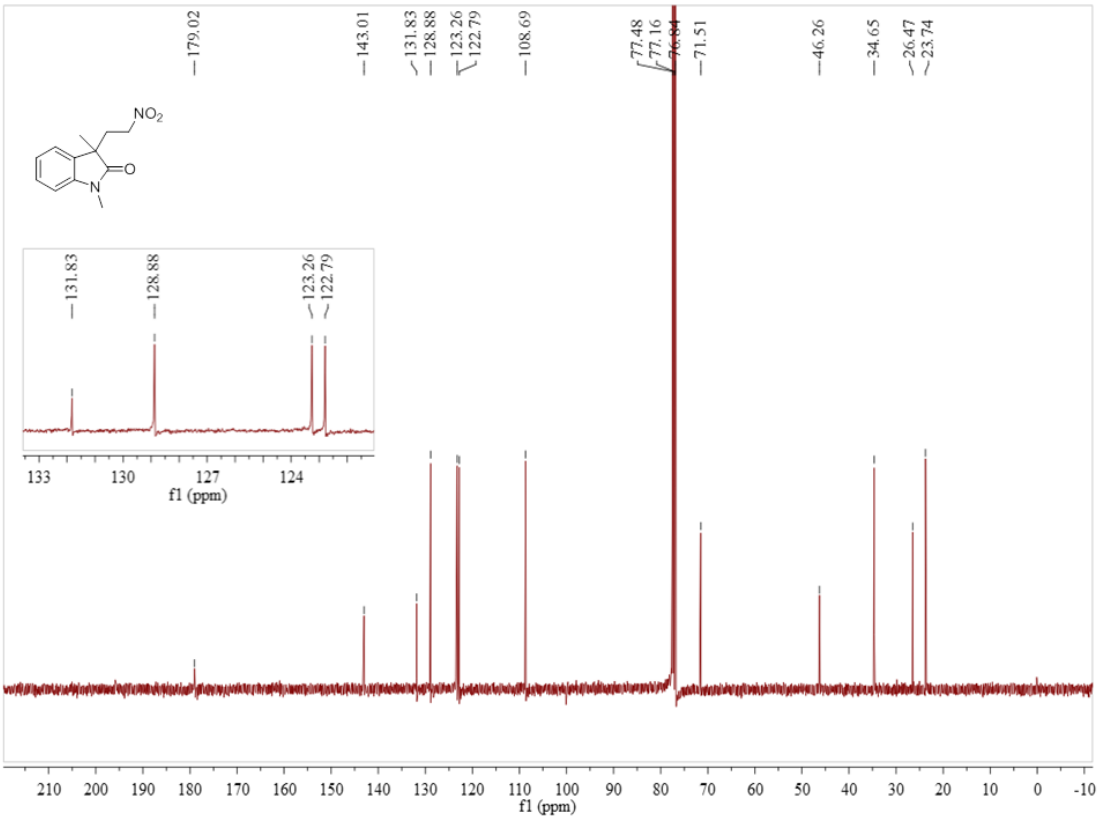
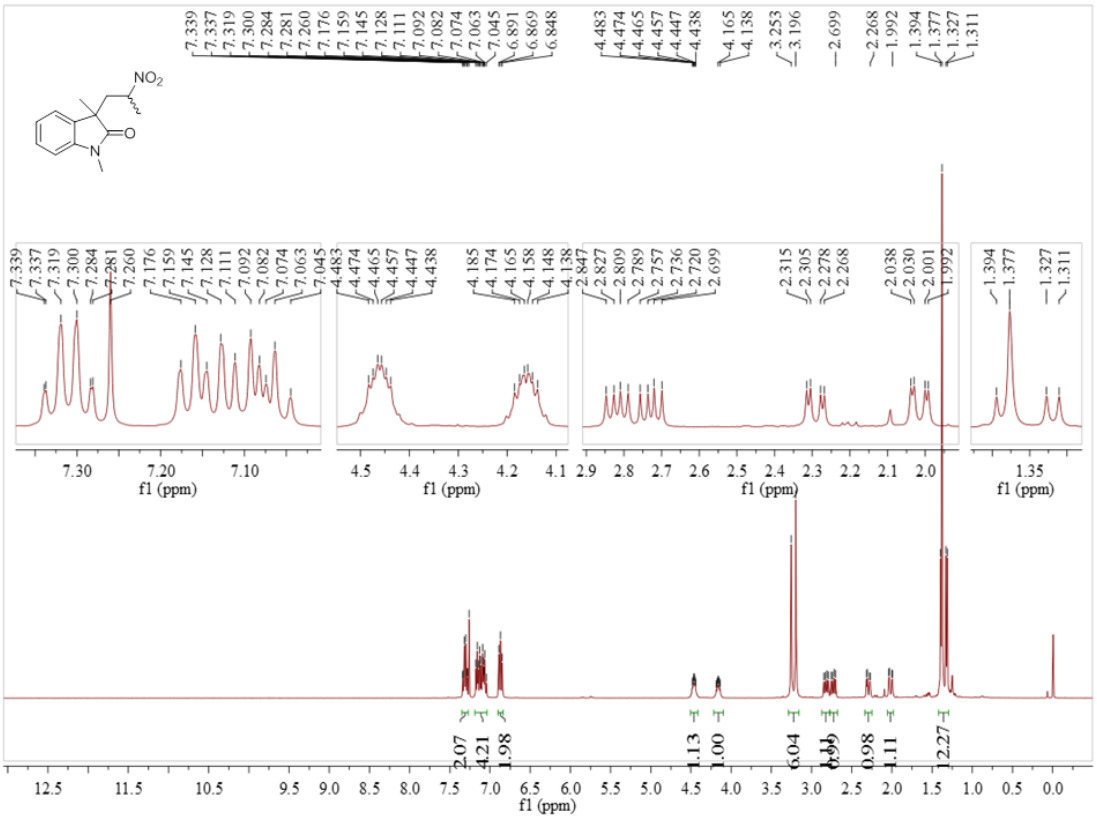
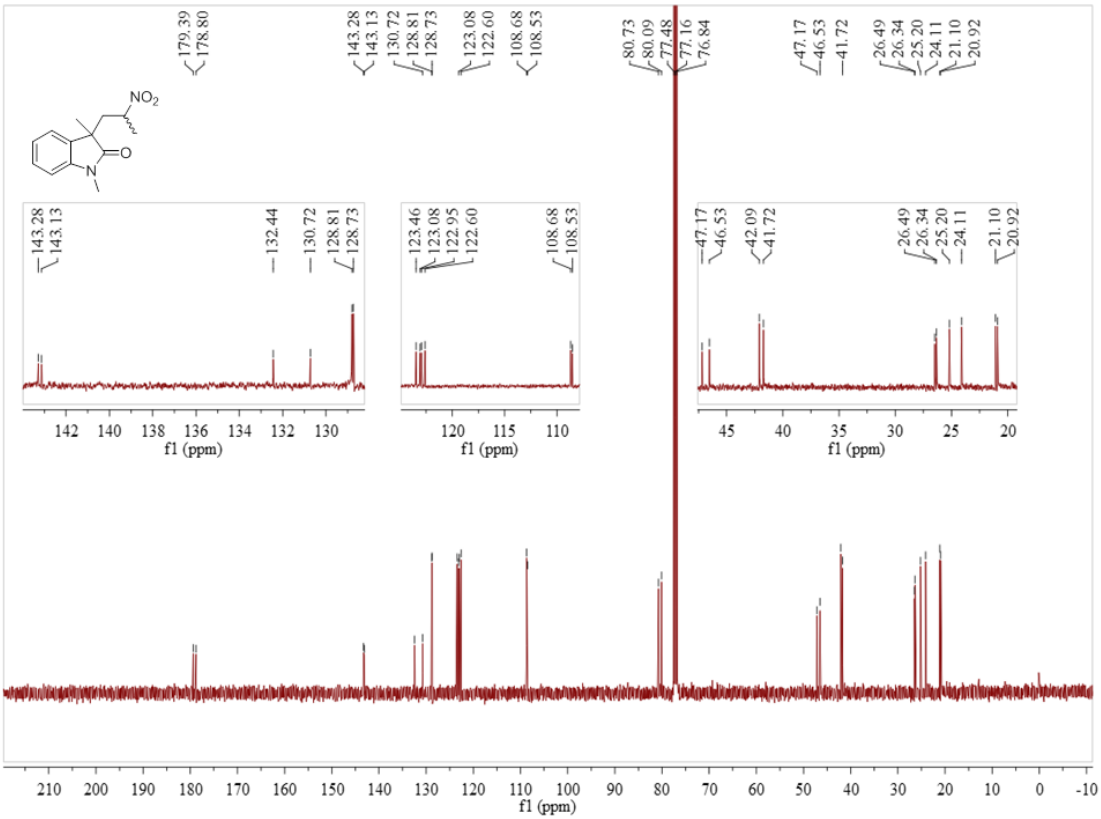
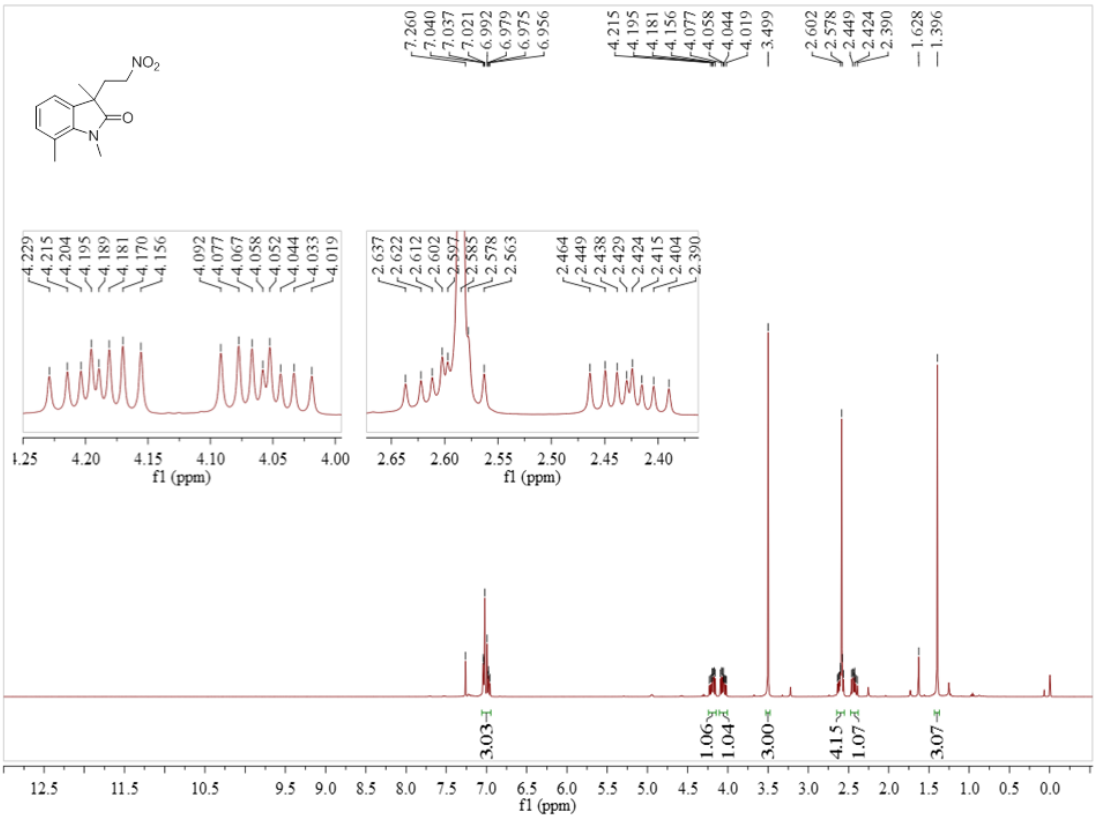
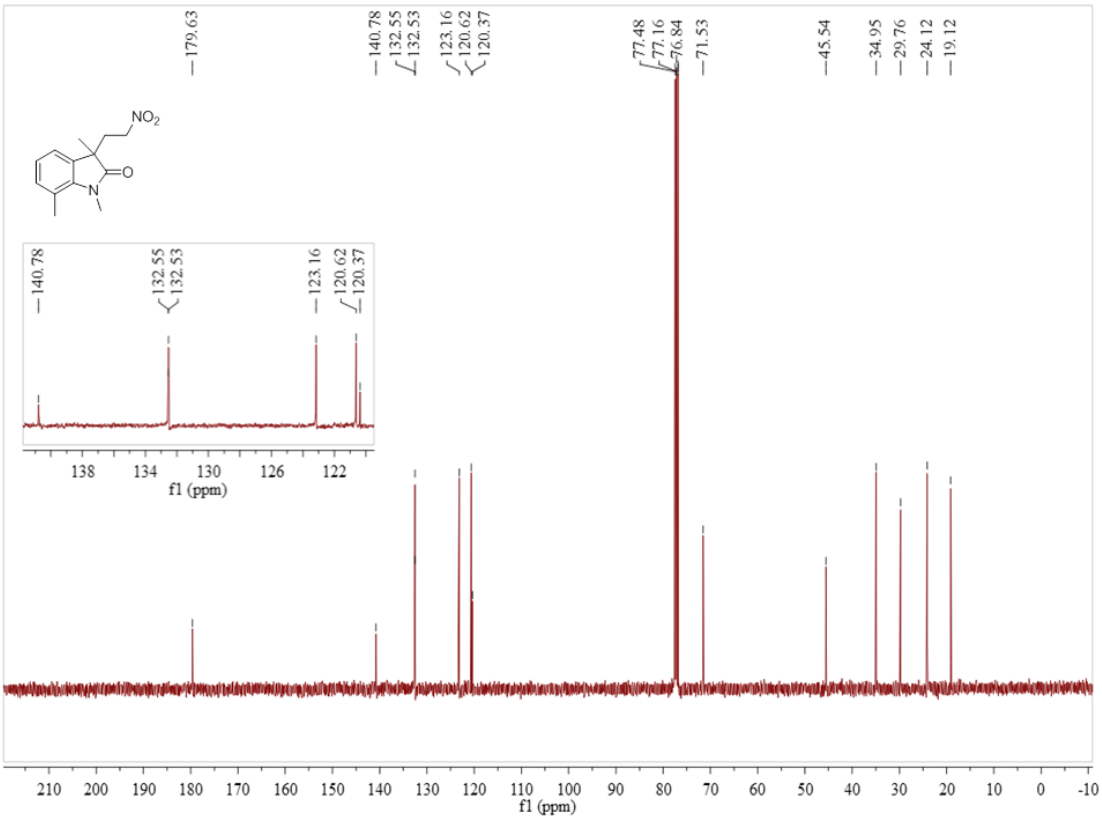
7.339
7.321
7.319
7.302
7.300
7.260
7.217
7.199
7.121
7.103
7.085
6.887
6.867
4.250
4.236
4.225
4.216
4.203
4.192
4.178
4.107
4.093
4.083
4.070
4.060
4.050
4.036
2.658
2.644
2.634
2.623
2.610
2.600
2.586
2.521
2.506
2.496
2.483
2.473
2.462
2.448
1.430
-0.004
f1 (ppm)
1.04
1.00
1.04
1.01
1.05
1.06
3.00
1.03
1.07
3.06

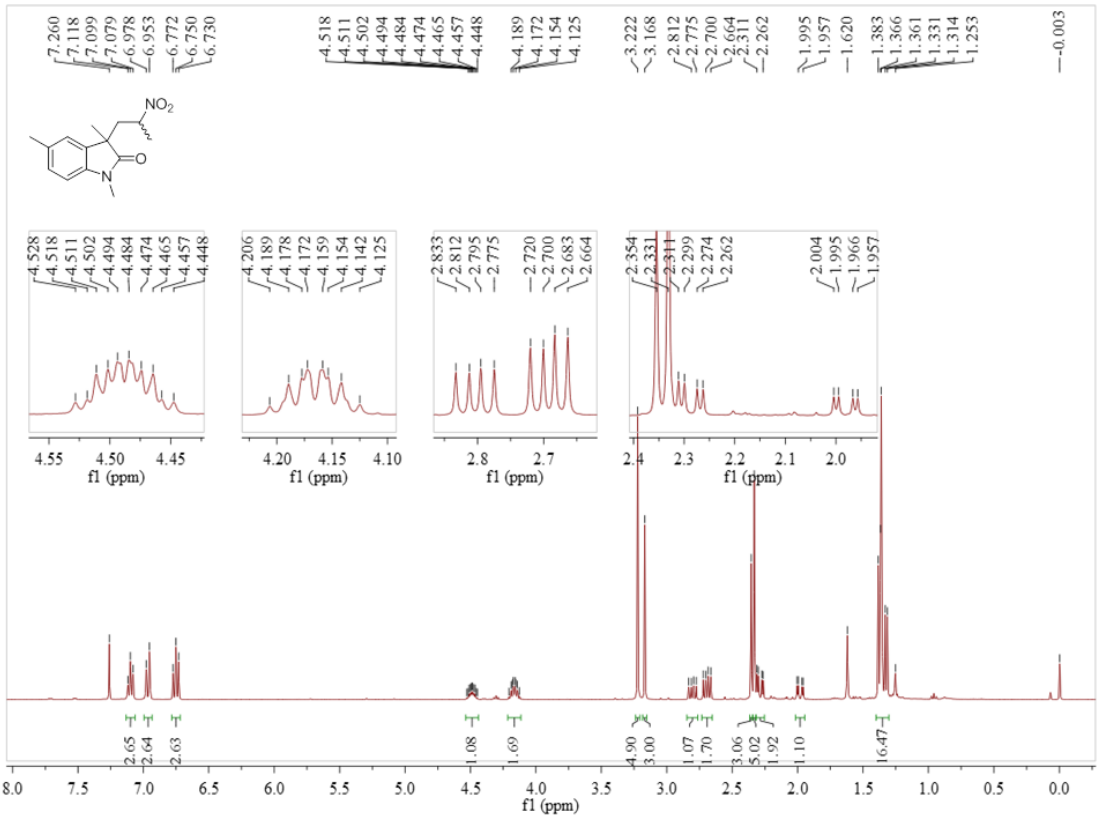

NO2
O
N
179.02
143.01
131.83
128.88
123.26
122.79
108.69
77.48
77.16
76.84
71.51
46.26
34.65
26.47
23.74
f1 (ppm)

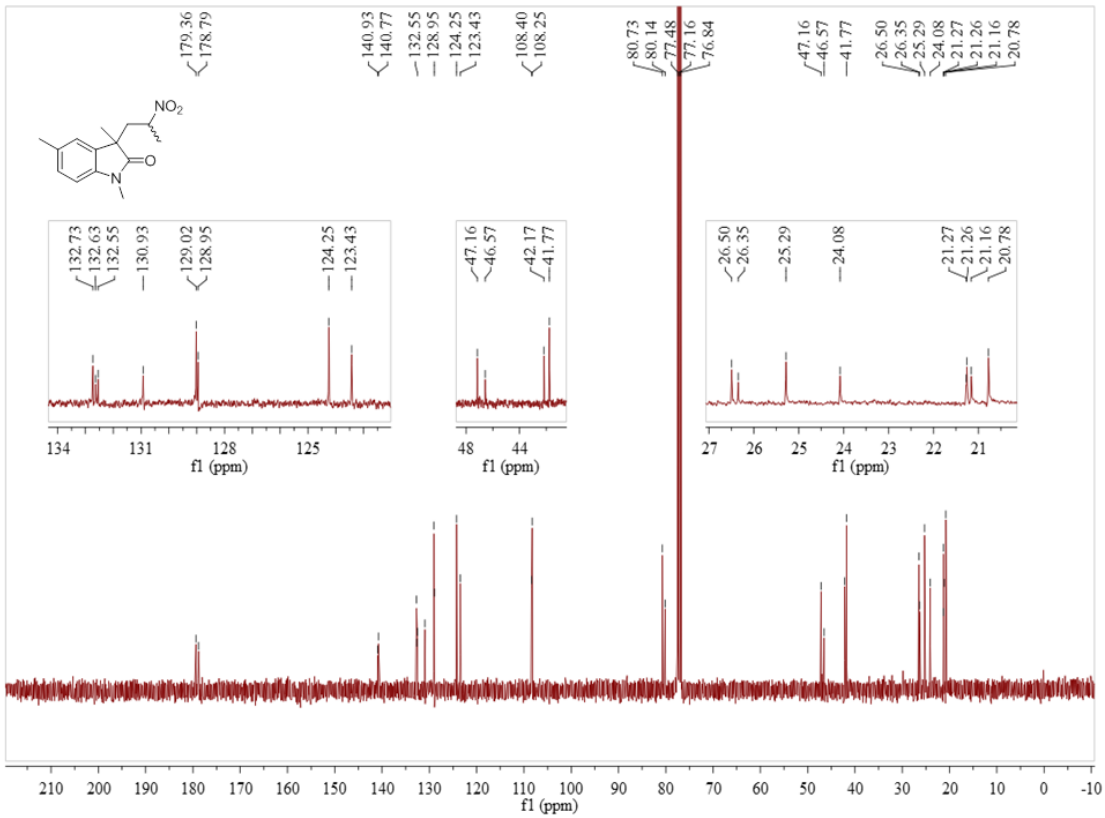

NO2
O
N
f1 (ppm)

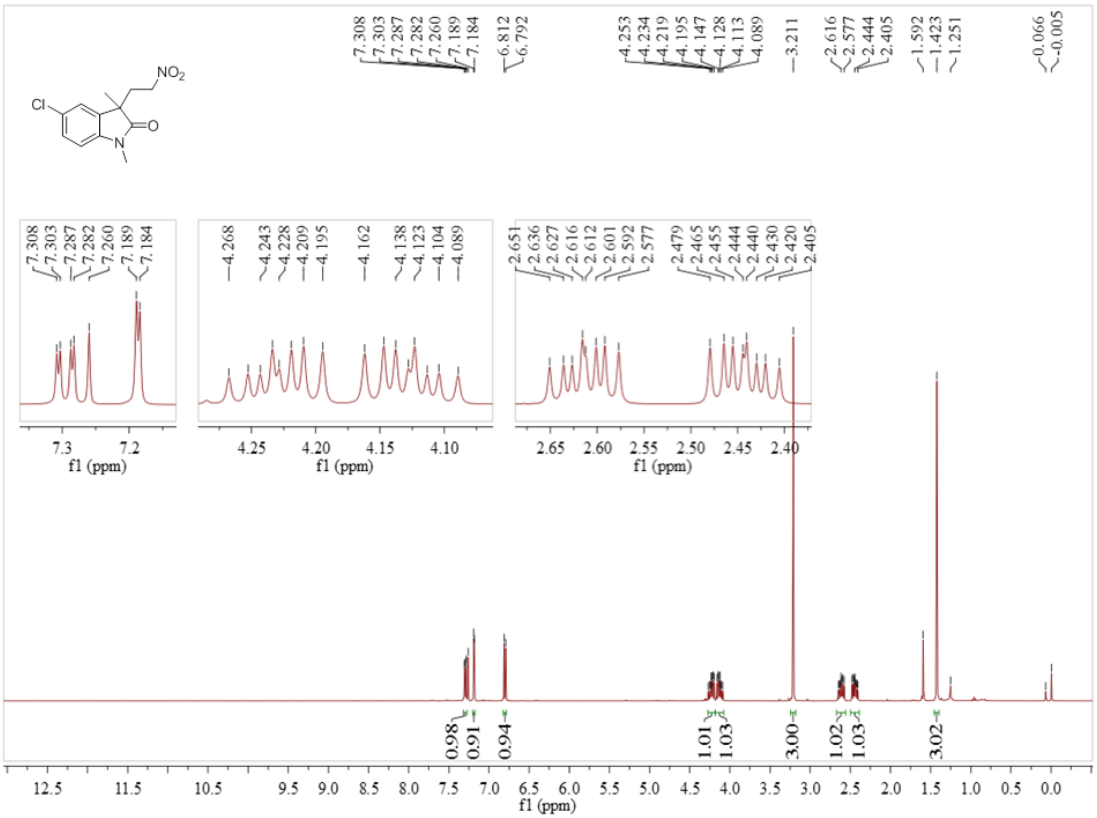

NO2
O
N
f1 (ppm)

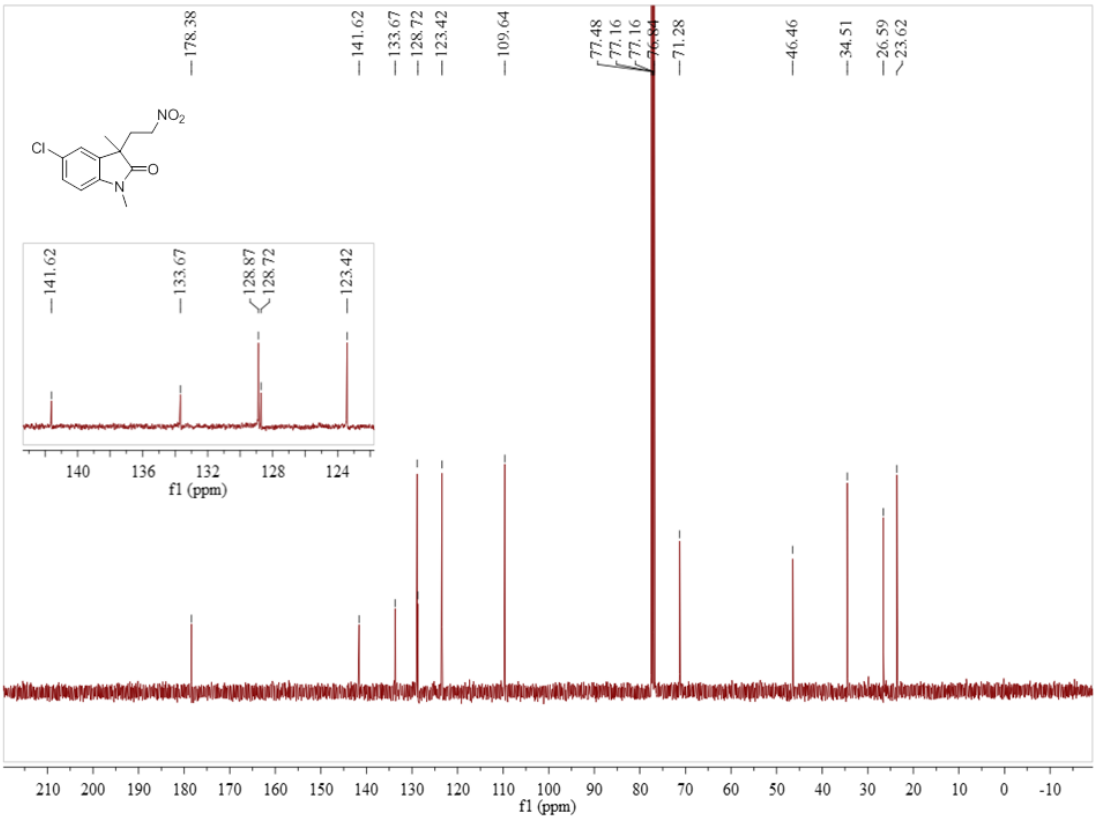

NO2
O
N
7.260
7.040
7.037
7.021
6.992
6.979
6.975
6.956
4.215
4.195
4.181
4.156
4.077
4.058
4.044
4.019
3.499
2.602
2.578
2.449
2.424
2.390
1.628
1.396
f1 (ppm)
3.03
1.06
1.04
3.00
4.15
1.07
3.07

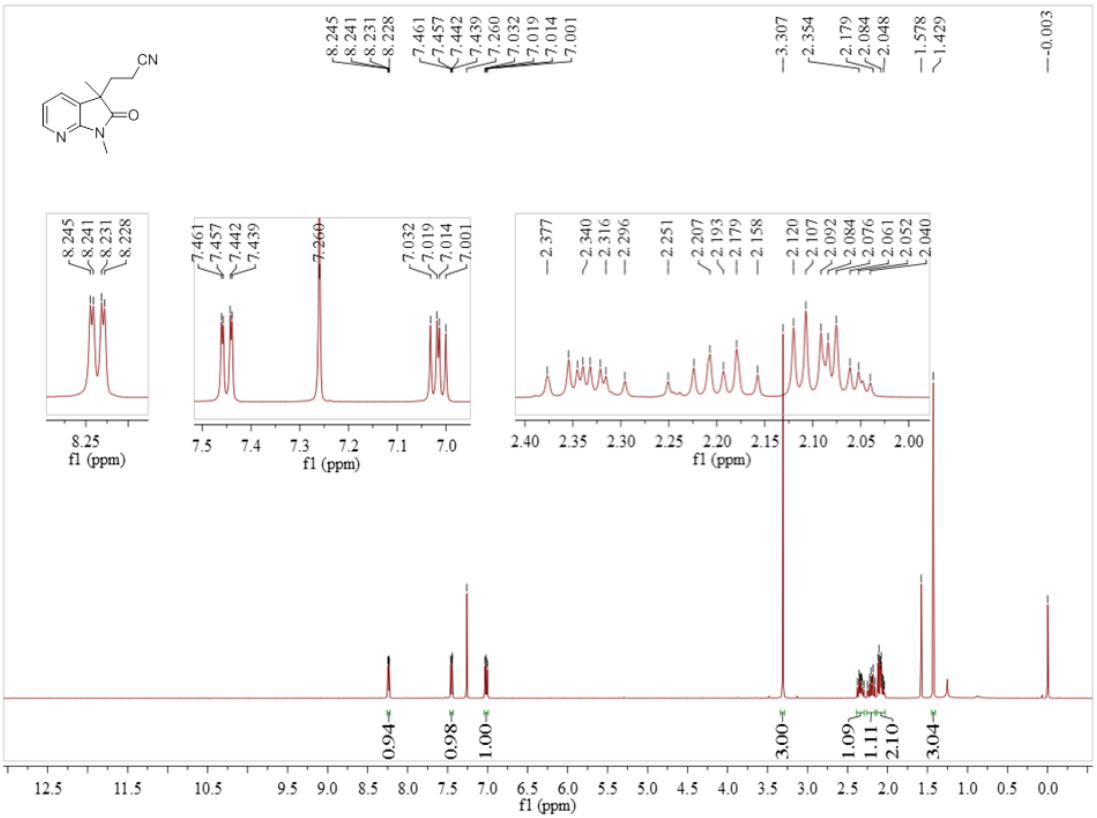

NO2
O
N
179.63
140.78
132.55
132.53
123.16
120.62
120.37
77.48
77.16
76.84
71.53
45.54
34.95
29.76
24.12
19.12
f1 (ppm)

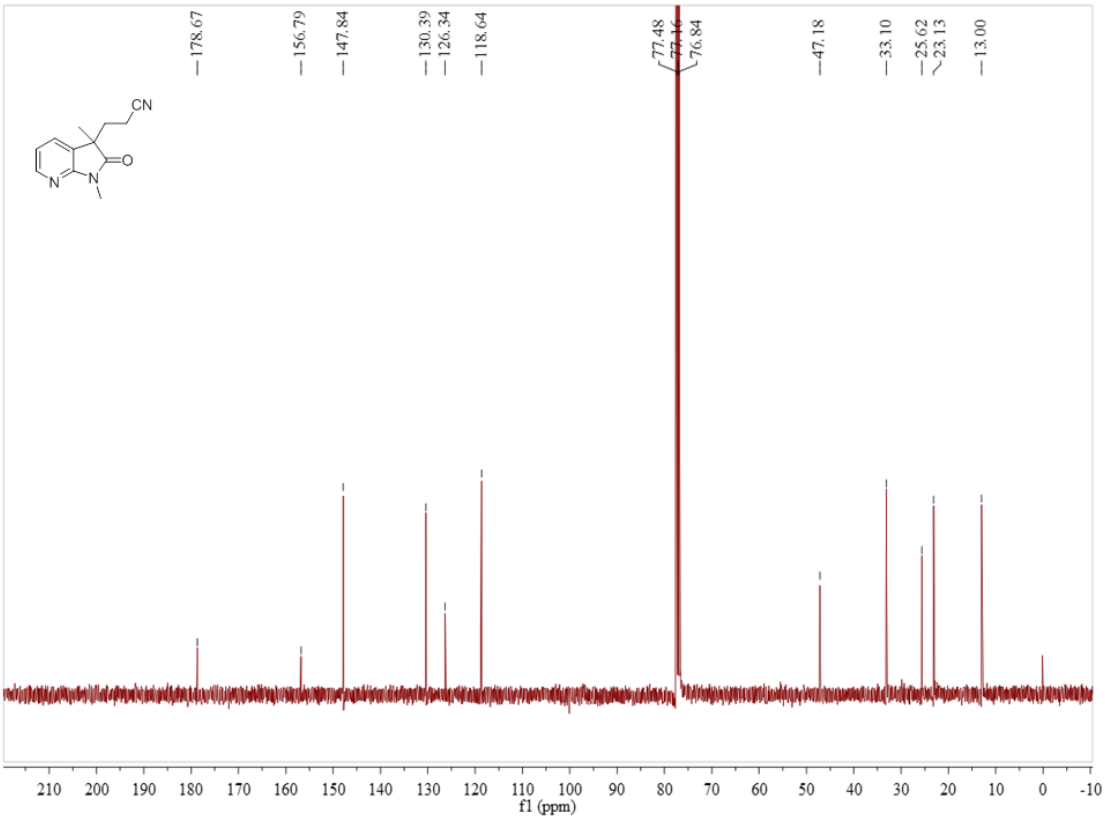

7.260
7.118
7.099
7.079
6.978
6.953
6.772
6.750
6.730
4.518
4.511
4.502
4.494
4.484
4.474
4.465
4.457
4.448
4.189
4.172
4.154
4.125
3.222
3.168
2.812
2.775
2.700
2.664
2.311
2.262
1.995
1.957
1.620
1.383
1.366
1.361
1.331
1.314
1.253
-0.003
NO2
O
N
f1 (ppm)
2.65
2.64
2.63
1.08
1.69
4.90
3.00
1.07
1.70
3.06
5.02
1.92
1.10
16.47

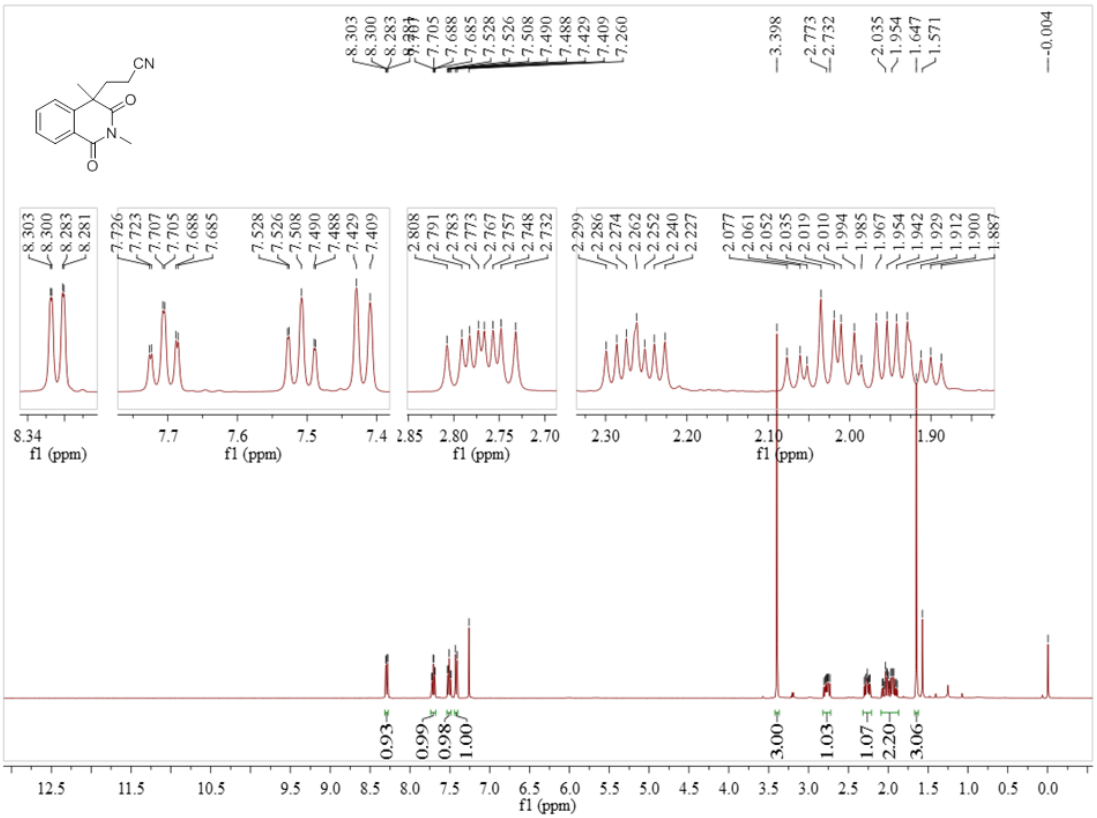

179.36
178.79
140.93
140.77
132.55
128.95
124.25
123.43
108.40
108.25
80.73
80.14
77.48
77.16
76.84
47.16
46.57
41.77
26.50
26.35
25.29
24.08
21.27
21.26
21.16
20.78
NO2
O
N
f1 (ppm)

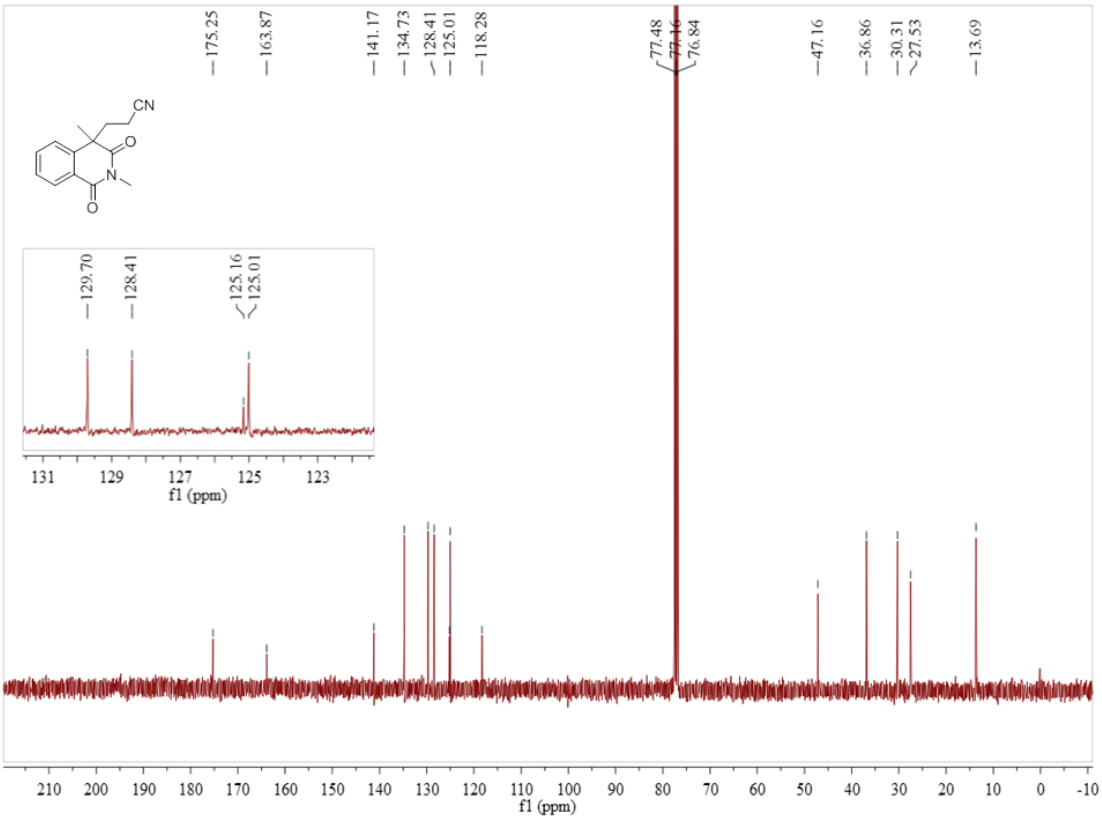

7.308
7.303
7.287
7.282
7.260
7.189
7.184
6.812
6.792
4.253
4.234
4.219
4.195
4.147
4.128
4.113
4.089
3.211
2.616
2.577
2.444
2.405
1.592
1.423
1.251
0.066
-0.005
NO2
Cl
O
N
f1 (ppm)
0.98
0.91
0.94
1.01
1.03
3.00
1.02
1.03
3.02

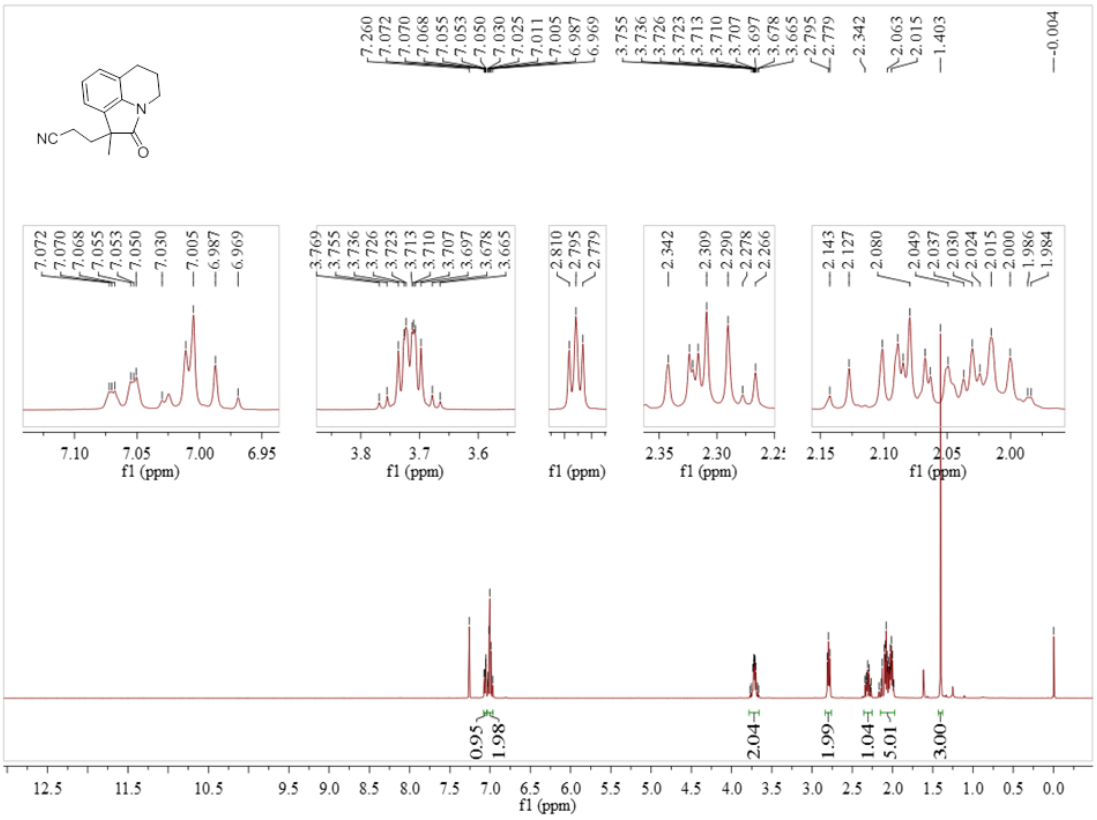

178.38
141.62
133.67
128.72
123.42
109.64
77.48
77.16
76.84
71.28
46.46
34.51
26.59
23.62
NO2
Cl
O
N
128.87
f1 (ppm)

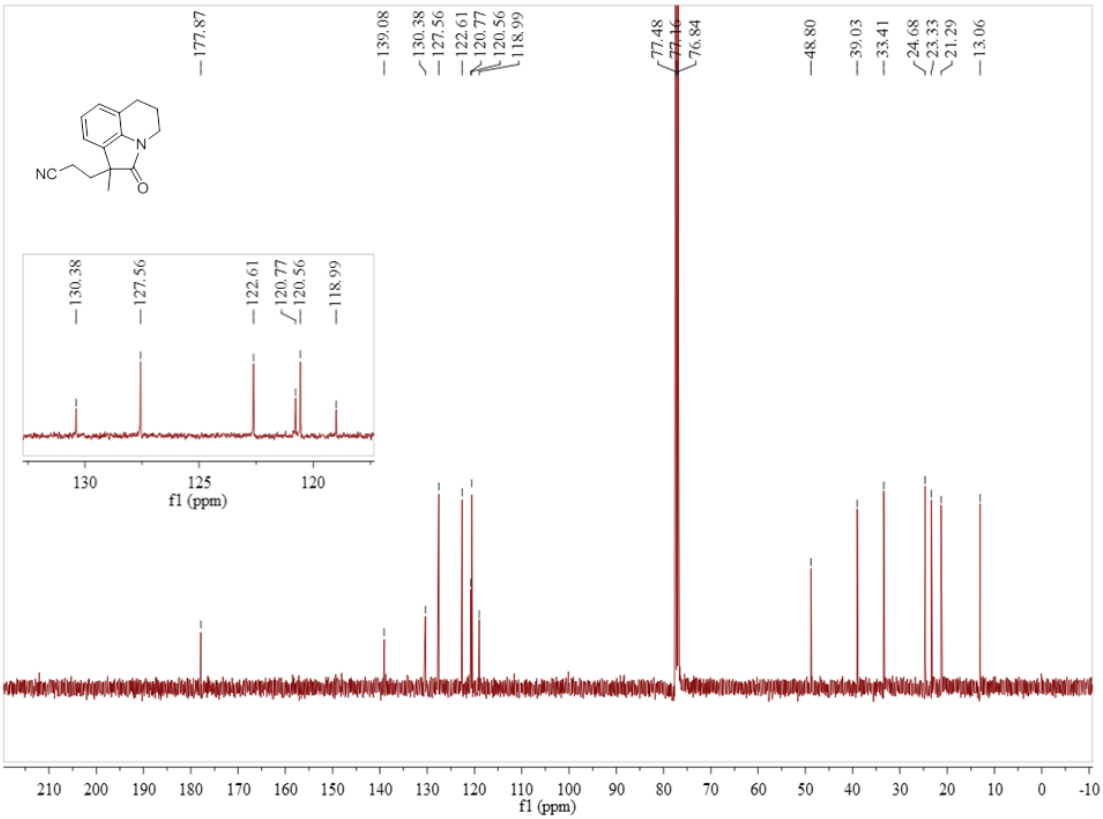

8.245
8.241
8.231
8.228
7.461
7.457
7.442
7.439
7.260
7.032
7.019
7.014
7.001
3.307
2.354
2.179
2.084
2.048
1.578
1.429
-0.003
2.377
2.340
2.316
2.296
2.251
2.207
2.193
2.179
2.158
2.120
2.107
2.092
2.084
2.076
2.061
2.052
2.040
f1 (ppm)
0.94
0.98
1.00
3.00
1.09
1.11
2.10
3.04


178.67
156.79
147.84
130.39
126.34
118.64
77.48
77.16
76.84
47.18
33.10
25.62
23.13
13.00
f1 (ppm)


8.303
8.300
8.283
8.281
7.726
7.723
7.707
7.705
7.688
7.685
7.528
7.526
7.508
7.490
7.488
7.429
7.409
7.260
3.398
2.808
2.791
2.783
2.773
2.767
2.757
2.748
2.732
2.773
2.732
2.299
2.286
2.274
2.262
2.252
2.240
2.227
2.077
2.061
2.052
2.035
2.019
2.010
1.994
1.985
1.967
1.954
1.942
1.929
1.912
1.900
1.887
2.035
1.954
1.647
1.571
-0.004
f1 (ppm)
0.93
0.99
0.98
1.00
3.00
1.03
1.07
2.20
3.06


175.25
163.87
141.17
134.73
128.41
125.01
118.28
77.48
77.16
76.84
47.16
36.86
30.31
27.53
13.69
129.70
128.41
125.16
125.01
f1 (ppm)


7.260
7.072
7.070
7.068
7.055
7.053
7.050
7.030
7.025
7.011
7.005
6.987
6.969
3.755
3.736
3.726
3.723
3.713
3.710
3.707
3.697
3.678
3.665
2.795
2.779
2.342
2.063
2.015
1.403
-0.004
NC
O
N
f1 (ppm)
0.95
1.98
2.04
1.99
1.04
5.01
3.00


177.87
139.08
130.38
127.56
122.61
120.77
120.56
118.99
77.48
77.16
76.84
48.80
39.03
33.41
24.68
23.33
21.29
13.06
NC
O
N
f1 (ppm)