Supporting Information

Electrochemical Synthesis of Cyanated Imidazo[1,5-a]pyridines

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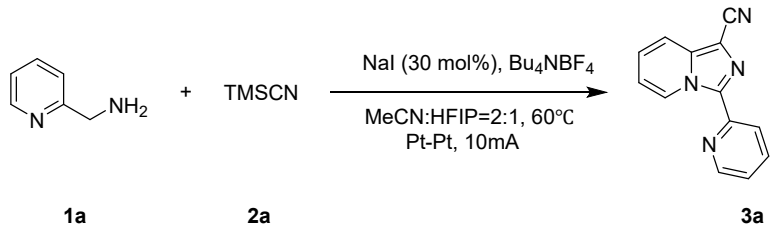
General Information

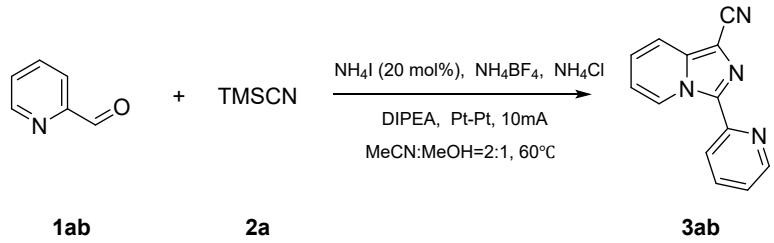
Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. NMR spectra were recorded on a Bruker AV-500 (1H: 500 MHz, 13C: 125 MHz, 19F NMR: 470 MHz) spectrometer using TMS as internal reference. Chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz, respectively. GC-MS was Shimadzu QP-5050 GC-MS system. All substances were known available compounds. High resolution mass spectra (HRMS) were measured using electrospray ionization (ESI) and the time-of-flight (TOF) mass analyzer. The instrument for electrolysis is dual display potentiostat (CJS-292) (made in China). The electrodes are commercially available from GaossUnion, China. Cyclic voltammetry data were measured with a Shanghai Chenhua potentiostat (CHI760E). Working electrode: The working electrode is a 3 mm diameter Pt disk working electrode. Polished with 0.3 μm aluminum oxide and then sonicated in distilled water before drying. Reference electrode: The reference electrode consisted of a silver wire covered with silver chloride immersed in a saturated solution of potassium chloride. Counter electrode: The counter electrode is a platinum wire that was polished with sand paper.

Experimental Procedure



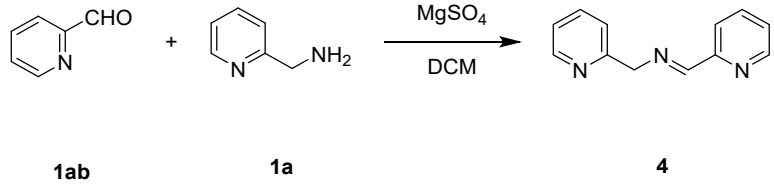
Scheme S1. Experimental procedure for **3a**.

Typical synthesis steps of 3-(pyridin-2-yl) imidazo[1,5-a]pyridine-1-carbonitrile (3a): A mixture of 2-picolylamine (0.6 mmol), trimethylsilyl cyanide (TMSCN) (0.9 mmol), sodium iodide (0.09 mmol), tetrabutylammonium tetrafluoroborate (0.3 mmol), and 3 mL of mixed solvent (MeCN/HFIP = 2:1) was added to an undivided electrolytic cell equipped with two platinum electrodes serving as both anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 60°C for approximately 6 hours. Upon completion, the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel (PE/EtOAc = 6:1) to afford the desired product.



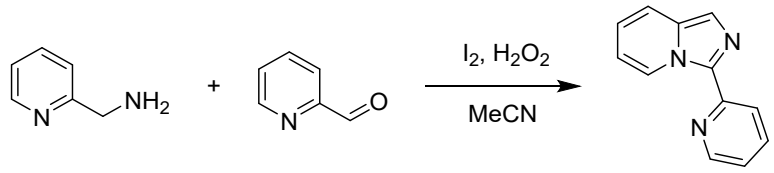
Scheme S2. Experimental procedure for **3ab**.

Typical synthesis of 3-(pyridin-2-yl) imidazo[1,5-a]pyridine-1-carbonitrile (3ab): A mixture of 2-pyridinecarboxaldehyde (0.6 mmol), trimethylsilyl cyanide (0.9 mmol), ammonium iodide (0.06 mmol), ammonium tetrafluoroborate (0.3 mmol), N,N-diisopropylethylamine (0.3 mmol), ammonium chloride (1.2 mmol), and 3 mL of a mixed solvent (MeCN/MeOH = 2:1) was added to an undivided electrolytic cell. The electrolytic cell was equipped with two platinum electrodes serving as both anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA at 60 °C for approximately 6 hours. Upon completion of the reaction, the solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 6:1) to afford the desired product.



Scheme S3. Experimental procedure for **4**.

Typical synthesis of (E)-N-benzyl-1-phenylmethanimine (4)[S1]: To a suspension of anhydrous $MgSO_4$ (5equiv, 10.5 mmol, 1.26 g) in anhydrous DCM (4 mL) was added 2-pyridinecarboxaldehyde (1equiv, 2.1 mmol, 0.2 mL), followed by dropwise addition of 2-picolylamine (1equiv, 2.1 mmol, 0.22 mL). The reaction mixture was stirred at room temperature for 3 h, then filtered under reduced pressure. The solvent was removed via rotary evaporation to afford the product.



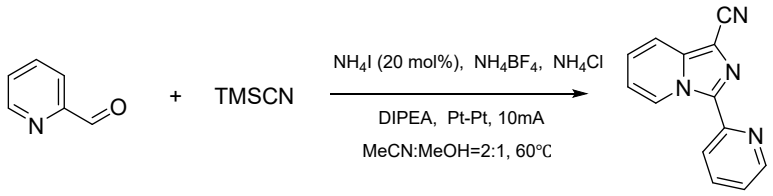
1a **1ab** **4a**

Scheme S4. Experimental procedure for **4a**.

Typical synthesis of 3-(pyridine-2-yl)imidazo[1,5-a]pyridine (4a)[S2]: 2-Picolylamine (0.8 mmol, 2 equiv), 2-pyridinecarboxaldehyde (0.4 mmol, 1 equiv), iodine (10.2 mg, 10 mol%), 30% hydrogen peroxide (3 mmol), and acetonitrile (5 mL) were added sequentially to a 25 mL round-bottom flask equipped with a spherical condenser. The reaction flask was placed in a preheated heating block at 60 °C and stirred for 3 hours. The reaction progress was monitored by thin-layer chromatography (TLC). After completion, the reaction mixture was allowed to cool to room temperature. The mixture was then concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (gradient elution with PE/EA, v/v = 20:1 to 5:1) to afford the target product, 3-(pyridin-2-yl)imidazo[1,5-a]pyridine.

Optimization of Reaction Conditions

Table S1. Optimization of reaction conditions for **3a** from **1ab**.[a]



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

Entry	Variations from standard conditions	Yields(%) [b]
1	None [a]	78
2	MeCN as solvent	34
3	DMSO as solvent	29
4	DMF as solvent	24
5	MeCN: H_2O=2:1	67
6	MeCN: EtOH=2:1	73
7	10mol%, 30mol%, 40mol%, 100mol% NH_4I	52, 61, 48, 37
8	n-Bu_4NBF_4 and n-Bu_4NPF_6 instead of NH_4BF_4	65,62
9	NaI, KI, Me_4NI instead of NH_4I	68, 57, 49
10	5mA, 15mA, 20mA instead of 15mA	59, 49, 32
11	50℃, 40℃, 18℃ instead of 60℃	63,51,45
12	no electricity and no I^-	n.d.[c]
13	DABCO, DBU, ^{t}BuOK instead of DIPEA	54, 42, 28
14	NH_4Br, NH_4OAC instead of NH_4Cl	trace, 34

[a] Reaction conditions: **1ab** (0.6 mmol), **2a** (0.9 mmol), NH_4I (0.06 mmol), NH_4BF_4 (0.3 mmol), MeCN:MeOH=2:1 (3.0 mL), DIPEA (0.3 mmol) 10 mA, 60 ℃, undivided cell. The platinum plate (10 mm × 10 mm × 0.2 mm). [b] isolated yield. [c] not detected. The reaction time was determined by TLC and GC-MS.

Theoretical charge calculation

1. Self-coupling reaction starting from 2-picolylamine **(1a)**

According to our proposed mechanism, the formation of one molecule of the final product **3a** requires two molecules of the starting material **1a**. one molecule of **1a** undergoes a two-electron oxidation process at the anode to form an imine intermediate through dehydrogenation, while the other molecule of 1a is not oxidized but instead serves as a nucleophile and condenses with the oxidized 1a to form intermediate **4**.The electron transfer process can be broken down as follows:

Oxidative Step A**:** One molecule of **1a** undergoes a 2-electron oxidation at the anode to generate an imine intermediate(-2e$^-$)

Condensation Step: Another molecule of **1a** acts as a nucleophile to condense with the generated imine, forming intermediate **4**. This step does not involve electron transfer (0e$^-$).

Oxidative Step B: Intermediate **4** undergoes a subsequent 4-electron oxidative dehydrogenation during the cyclization and aromatization process (-4e$^-$).

Total: A total of 6 moles of electrons is required to produce 1 mole of product **3a**.

Theoretical Charge Calculation:

$$Q_{theo} = \frac{n(e^-) \times n(product)}{n(substrate)} = \frac{6\,F \times 1\,mol}{2\,mol} = 3.0\,F/mol$$

2. Reaction starting from pyridine-2-carboxaldehyde (**1ab**)

For the system starting from the aldehyde, the process involves a convergent paired electrolysis logic in an undivided cell:

Reduction Step: At the cathode, one molecule of 1ab accepts 2 electrons to be reduced to 2-picolylamine (+2e$^-$).

Condensation Step: The freshly generated amine condenses with another unreduced 1ab molecule in the system to form intermediate 4 (0e$^-$).

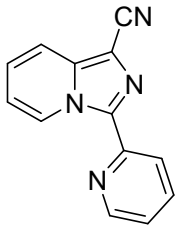
Oxidation Step: Intermediate 4 undergoes a 4-electron oxidation at the anode to complete the cyclization and aromatization (-4e$^-$).

Charge Balance: In an undivided cell, the total charge passed is dictated by the half-reaction with the higher electron demand—in this case, the 4-electron oxidation at the anode.

Theoretical Charge Calculation:

$$Q_{theo} = \frac{n(e^-)_{anodic} \times n(product)}{n\ (substrate)} = \frac{4F \times 1\,mol}{2\,mol} = 2.0\,F/mol$$

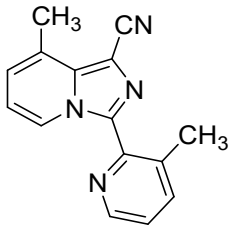
Detail Descriptions for Products



(3a)

3-(pyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3a)[S3] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 75% yield, 49.5 mg from amine. 78% yield, 51.5 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.05 (d, *J* = 7.3 Hz, 1H), 8.63 – 8.58 (m, 1H), 8.27 (d, *J* = 8.1 Hz, 1H), 7.79 (td, *J* = 7.8, 1.8 Hz, 1H), 7.68 (d, *J* = 9.1 Hz, 1H), 7.29 – 7.26 (m, 1H), 7.20 (ddd, *J* = 9.0, 6.6, 0.8 Hz, 1H), 6.93 – 6.88 (m, 1H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.5, 148.2, 138.4, 136.9, 136.7, 127.7, 125.5, 123.2, 122.5, 116.5, 115.4, 115.0, 103.3.

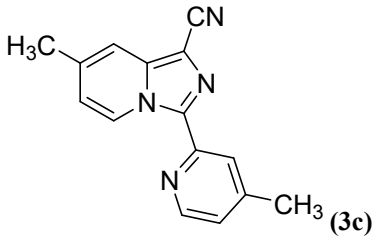
HRMS (ESI) *m/z*: calcd for $C_{13}H_8N_4[M+H]^+$ 221.0822, found 221.0823. mp = 201–203℃.



(3b)

8-methyl-3-(3-methylpyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3b)[S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 62% yield, 46.1 mg from amine. 61% yield, 45.4 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.15 (d, *J* = 7.1 Hz, 1H), 8.54 (d, *J* = 4.1 Hz, 1H), 7.70 (d, *J* = 7.7 Hz, 1H), 7.29 – 7.26 (m, 1H), 6.93 (d, *J* = 6.6 Hz, 1H), 6.76 (t, *J* = 6.9 Hz, 1H), 2.76 (s, 3H), 2.67 (s, 3H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 147.1, 146.1, 140.0, 137.5, 137.1, 134.7, 127.8, 125.0, 124.3, 123.5, 117.4, 114.8, 102.4, 20.7, 18.3.

HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_4[M+H]^+$ 249.1135, found 249.1138. mp = 205–207℃.

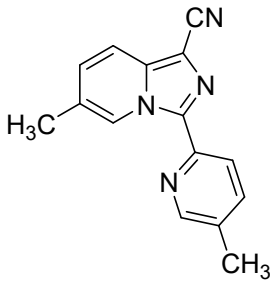


(3c)

7-methyl-3-(4-methylpyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3c) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid 67% yield, 49.9 mg from amine. 58% yield, 43.2 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.98 (d, *J* = 7.3 Hz, 1H), 8.49 (d, *J* = 5.0 Hz, 1H), 8.16 (s, 1H), 7.47 (s, 1H), 7.11 (d, *J* = 4.4 Hz, 1H), 6.75 (dd, *J* = 7.3, 1.5 Hz, 1H), 2.43 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.4, 148.3, 148.1, 139.2, 136.9, 136.6, 127.2, 124.3, 123.1, 117.9, 115.8,

114.7, 101.8, 21.5, 21.3.

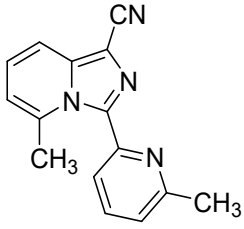
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_4[M+H]^+$ 249.1135, found 249.1143. mp = 188–190℃.



(3d)

6-methyl-3-(5-methylpyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3d) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 61% yield, 45.4 mg from amine. 63% yield, 46.9 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.80 (d, *J* = 1.2 Hz 1H), 8.46 (dd, *J* = 1.3, 0.7 Hz, 1H), 8.17 (d, *J* = 8.1 Hz, 1H), 7.60 (dd, *J* = 8.8, 1.2 Hz, 2H), 7.00 (dd, *J* = 9.2, 1.3 Hz 1H), 2.41 (s, 3H), 2.38 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 148.5, 147.2, 137.6, 137.5, 136.6, 133.0, 128.6, 125.0, 124.8, 122.3, 122.2, 115.7, 102.8, 18.7, 18.5.

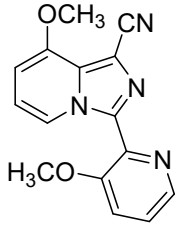
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_4[M+H]^+$ 249.1135, found 249.1142. mp = 148–150℃.



(3e)

5-methyl-3-(6-methylpyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3e)[S3] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 71% yield, 52.8 mg from amine. 57% yield, 42.4 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.73 (t, *J* = 7.7 Hz, 1H), 7.62 (d, *J* = 7.9 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 1H), 7.18 – 7.08 (m, 1H), 6.62 (d, *J* = 6.1 Hz, 1H), 2.60 (s, 3H), 2.31 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.5, 150.0, 139.9, 139.5, 136.9, 136.2, 125.5, 123.7, 123.4, 116.0, 115.5, 114.9, 103.1, 24.5, 22.2.

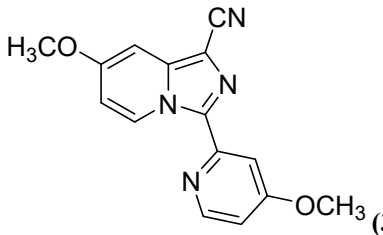
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_4[M+H]^+$ 249.1135, found 249.1136. mp = 163–164℃.



(3f)

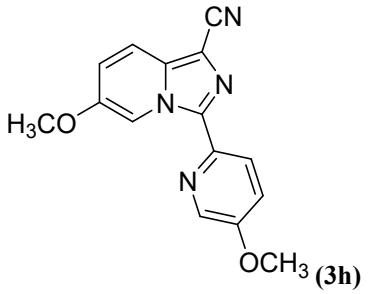
8-methoxy-3-(3-methoxypyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3f) was prepared

according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 62% yield, 52.1 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.40 (d, *J* = 6.9 Hz, 1H), 8.32 (d, *J* = 3.6 Hz, 1H), 7.48 – 7.35 (m, 2H), 6.72 (t, *J* = 7.1 Hz, 1H), 6.39 (d, *J* = 7.3 Hz, 1H), 4.01 (s, 3H), 3.92 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.9, 150.3, 140.9, 137.6, 136.2, 131.7, 125.2, 119.7, 118.3, 116.2, 114.9, 103.0, 100.6, 56.1, 56.1.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_4O_2[M+H]^+$ 281.1033, found 281.1039. mp = 162–164℃.



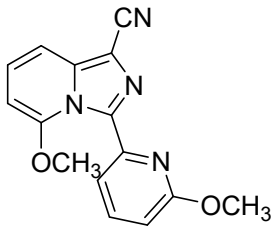
(3g)

7-methoxy-3-(4-methoxypyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3g) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 59% yield, 49.6 mg from amine. 66% yield, 55.5 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.02 (d, *J* = 7.8 Hz, 1H), 8.41 (d, *J* = 5.7 Hz, 1H), 7.83 (d, *J* = 2.4 Hz, 1H), 6.89 (d, *J* = 2.3 Hz, 1H), 6.83 (dd, *J* = 5.7, 2.5 Hz, 1H), 6.64 (dd, *J* = 7.8, 2.5 Hz, 1H), 3.96 (s, 3H), 3.93 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 166.4, 158.0, 151.3, 149.4, 141.1, 136.0, 129.4, 116.2, 111.3, 110.7, 106.4, 100.9, 92.6, 56.0, 55.6.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_4O_2[M+H]^+$ 281.1033, found 281.1035. mp = 218–220℃.



(3h)

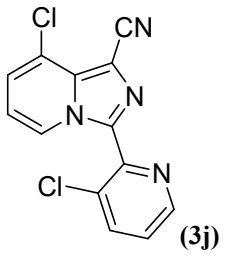
6-methoxy-3-(5-methoxypyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3h) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 81% yield, 68.1 mg from amine. 81% yield, 68.1 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.66 (s, 1H), 8.36 – 8.30 (m, 2H), 7.62 (d, *J* = 9.7 Hz, 1H), 7.37 (dd, *J* = 8.8, 2.7 Hz, 1H), 7.02 (d, *J* = 9.7 Hz, 1H), 3.94 (s, 3H), 3.92 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 155.4, 150.9, 142.8, 137.1, 135.7, 135.5, 123.8, 121.9, 121.3, 116.6, 115.8, 108.1, 103.3, 56.1, 55.9.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_4O_2[M+H]^+$ 281.1033, found 281.1034. mp = 218–220℃.



(3i)

5-methoxy-3-(6-methoxypyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3i) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 77% yield, 64.7 mg from amine. 84% yield, 70.6 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65 (t, *J* = 7.8 Hz, 1H), 7.32 (d, *J* = 8.9 Hz, 1H), 7.23 (d, *J* = 7.2 Hz, 1H), 7.20 – 7.14 (m, 1H), 6.81 (d, *J* = 8.3 Hz, 1H), 6.04 (d, *J* = 7.3 Hz, 1H), 3.89 (s, 3H), 3.84 (s, 3H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.8, 150.5, 147.9, 139.9, 138.3, 138.2, 127.2, 118.4, 115.6, 111.2, 108.7, 102.6, 90.3, 56.5, 53.5.

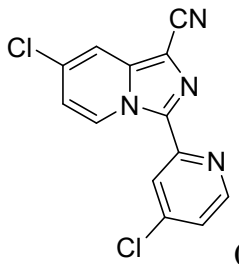
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_4O_2[M+H]^+$ 281.1033, found 281.1035. mp = 205–207℃.



(3j)

8-chloro-3-(3-chloropyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3j) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 47% yield, 40.6 mg from amine. 51% yield, 44.1 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.89 (d, *J* = 7.1 Hz, 1H), 8.64 (dd, *J* = 4.6, 1.4 Hz, 1H), 7.97 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.40 (dd, *J* = 8.2, 4.6 Hz, 1H), 7.24 (d, *J* = 7.1 Hz, 1H), 6.83 (t, *J* = 7.2 Hz, 1H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 147.1, 145.1, 139.7, 135.9, 134.5, 132.2, 125.1, 124.8, 124.6, 124.2, 115.3, 114.8, 104.6.

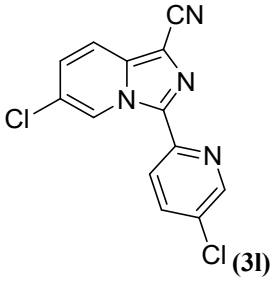
HRMS (ESI) *m/z*: calcd for $C_{13}H_6Cl_2N_4[M+H]^+$ 289.0042, found 289.0043. mp = 233–235℃.



(3k)

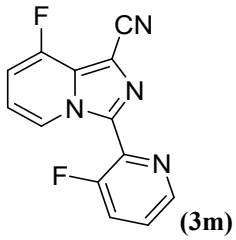
7-chloro-3-(4-chloropyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3k) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 52% yield, 45.8mg from amine. **^{1}H NMR** (500 MHz, $CDCl_3$)

δ 10.06 (d, *J* = 7.5 Hz, 1H), 8.55 (d, *J* = 5.1 Hz, 1H), 8.39 (s, 1H), 7.76 (s, 1H), 7.34 (d, *J* = 4.0 Hz, 1H), 6.93 (d, *J* = 7.1 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.4, 149.4, 145.4, 138.7, 136.0, 133.1, 128.4, 123.9, 122.8, 117.3, 115.5, 114.6, 103.8.
HRMS (ESI) *m/z*: calcd for $C_{13}H_6Cl_2N_4[M+H]^+$ 289.0042, found 289.0043. mp = 256–258℃.



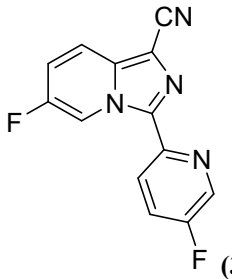
(3l)

6-chloro-3-(5-chloropyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3l) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 43% yield, 37.2mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.14 (s, 1H), 8.66 (d, *J* = 1.9 Hz, 1H), 8.33 (d, *J* = 8.6 Hz, 1H), 7.84 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.73 (d, *J* = 9.5 Hz, 1H), 7.23 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 147.4, 147.3, 137.3, 136.7, 136.1, 132.1, 127.2, 125.4, 124.2, 123.7, 117.2, 114.7, 105.1.
HRMS (ESI) *m/z*: calcd for $C_{13}H_6Cl_2N_4[M+H]^+$ 289.0042, found 289.0046. mp = 256–258℃.



(3m)

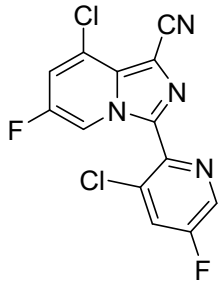
8-fluoro-3-(3-fluoropyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3m) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 53% yield, 40.7 mg from amine. 82% yield, 63.0mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.46 (d, *J* = 6.9 Hz, 1H), 8.55 (d, *J* = 4.4 Hz, 1H), 7.66 (t, *J* = 9.4 Hz, 1H), 7.45 (dt, *J* = 8.2, 4.1 Hz, 1H), 6.89–6.94 (m, 2H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ157.4 (d, *J* = 275.0 Hz), 152.4 (d, *J* = 250.0 Hz), 144.5 (d, *J* = 5.4 Hz), 136.9 (d, *J* = 8.4 Hz), 134.5 (d, *J* = 9.6 Hz), 130.2 (d, *J* = 37.5 Hz), 125.4 (dd, *J* = 11.8, 7.3 Hz), 123.1 (d, *J* = 5.4 Hz), 114.8 (d, *J* = 6.0 Hz), 114.6 (s), 108.3 (d, *J* = 16.0 Hz), 102.9 (s). **^{19}F NMR** (470 MHz, $CDCl_3$) δ -116.96, -123.24.
HRMS (ESI) *m/z*: calcd for $C_{13}H_6F_2N_4[M+H]^+$ 257.0633, found 257.0639. mp = 155–157℃.



(3n)

6-fluoro-3-(5-fluoropyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3n) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 44% yield, 33.8 mg from amine. 74% yield, 56.9 mg from aldehyde. **^{1}H NMR** (500 MHz, DMSO) δ 9.84 (dd, *J* = 5.4, 1.5 Hz, 1H), 8.69 (d, *J* = 2.8 Hz, 1H), 8.23 (dd, *J* = 8.9, 4.5 Hz, 1H), 7.99 (dd, *J* = 9.8, 5.3 Hz, 1H), 7.90 (td, *J* = 8.8, 2.9 Hz, 1H), 7.52 (ddd, *J* = 9.8, 7.7, 2.1 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 159.2 (d, *J* = 250.0 Hz), 154.7 (d, *J* = 237.5 Hz), 145.8 (s), 136.8 (d, *J* = 3.5 Hz), 136.7 (m), 136.3 (d, *J* = 50.0 Hz), 124.6 (d, *J* = 18.8 Hz), 124.2 (d, *J* = 5.0 Hz), 118.4 (d, *J* = 37.5 Hz), 117.5 (d, *J* = 9.5 Hz), 114.8 (s), 114.1 (d, *J* = 50.0 Hz), 104.8 (s). **^{19}F NMR** (470 MHz, $CDCl_3$) δ -124.97, -134.84.

HRMS (ESI) *m/z*: calcd for $C_{13}H_6F_2N_4[M+H]^+$ 257.0633, found 257.0641. mp = 206–208℃.

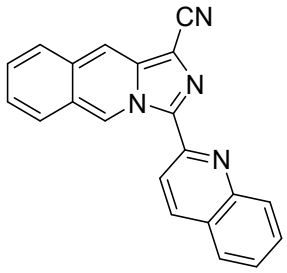


(3o)

8-chloro-3-(3-chloro-5-fluoropyridin-2-yl)-6-fluoroimidazo[1,5-a]pyridine-1-carbonitrile (3o) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 41% yield, 39.8 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.57 (s, 1H), 8.56 (s, 1H), 7.73 (dd, *J* = 9.8, 1.3 Hz, 1H), 7.00 (d, *J* = 8.8 Hz, 1H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.7 (d, *J* = 275.0 Hz), 151.5 (d, *J* = 250.0 Hz), 143.6 (d, *J* = 5.0 Hz), 134.8 (d, *J* = 8.4 Hz), 133.8 (d, *J* = 10.1 Hz), 132.9 (d, *J* = 3.9 Hz), 128.6 (d, *J* = 37.5 Hz), 125.9 (d, *J* = 12.5 Hz), 123.5 (d, *J* = 8.1 Hz), 121.0 (d, *J* = 5.9 Hz), 113.7 (s), 110.9 (d, *J* = 19.0 Hz), 104.3 (s).

^{19}F NMR (470 MHz, $CDCl_3$) δ -113.59, -121.29.

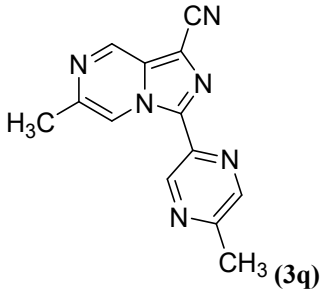
HRMS (ESI) *m/z*: calcd for $C_{13}H_4Cl_2F_2N_4[M+H]^+$ 324.9854 found 324.9855. mp = 167–169℃.



(3p)

3-(quinolin-2-yl)imidazo[1,5-b]isoquinoline-1-carbonitrile (3p) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a white solid. 64% yield, 61.5 mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.3 Hz, 1H), 8.06 (t, *J* = 8.4 Hz, 2H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.88 (d, *J* = 8.6 Hz, 1H), 7.79 (d, *J* = 7.6 Hz, 2H), 7.71 – 7.61 (m, 2H), 7.56 – 7.45 (m, 2H), 7.32 (t, *J* = 7.7 Hz, 1H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.7, 147.3, 143.0, 138.2, 137.8, 132.2, 130.7, 129.6, 129.3, 128.8, 128.3, 128.1, 128.1, 128.1, 126.9, 125.6, 122.7, 119.2, 115.0, 114.6, 106.6.

HRMS (ESI) *m/z*: calcd for $C_{21}H_{12}N_4[M+H]^+$ 321.1135, found 321.1137. mp = 283–285℃.



(3q)

6-methyl-3-(5-methylpyrazin-2-yl)imidazo[1,5-a]pyrazine-1-carbonitrile (3q) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a white solid. 64% yield, 51.0mg from aldehyde. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.47 (s, 1H), 9.42 (s, 1H) 9.24 (s, 1H), 8.53 (s, 1H), 2.68 (s, 3H), 2.61 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.0, 143.7, 143.1, 142.4, 141.9, 141.5, 135.5, 130.9, 115.2, 113.7, 107.3, 21.9, 21.4.

HRMS (ESI) *m/z*: calcd for $C_{13}H_{10}N_6[M+H]^+$ 251.1040, found 251.1035. mp = 202–204℃.

Reference

[S1] C. Incarvito, M. Lam, B. Rhatigan, A. L. Rheingold, C. J. Qin, A. L. Gavrilova and B. Bosnich, *J. Chem. Soc., Dalton Trans.*, 2001, **2001**, 3478–3488.

[S2] H. Li, C. Gao, Q. Liu, Y. Guo and Y. Zhao, *Chem. Sel.*, 2024, **9**, e202401875.

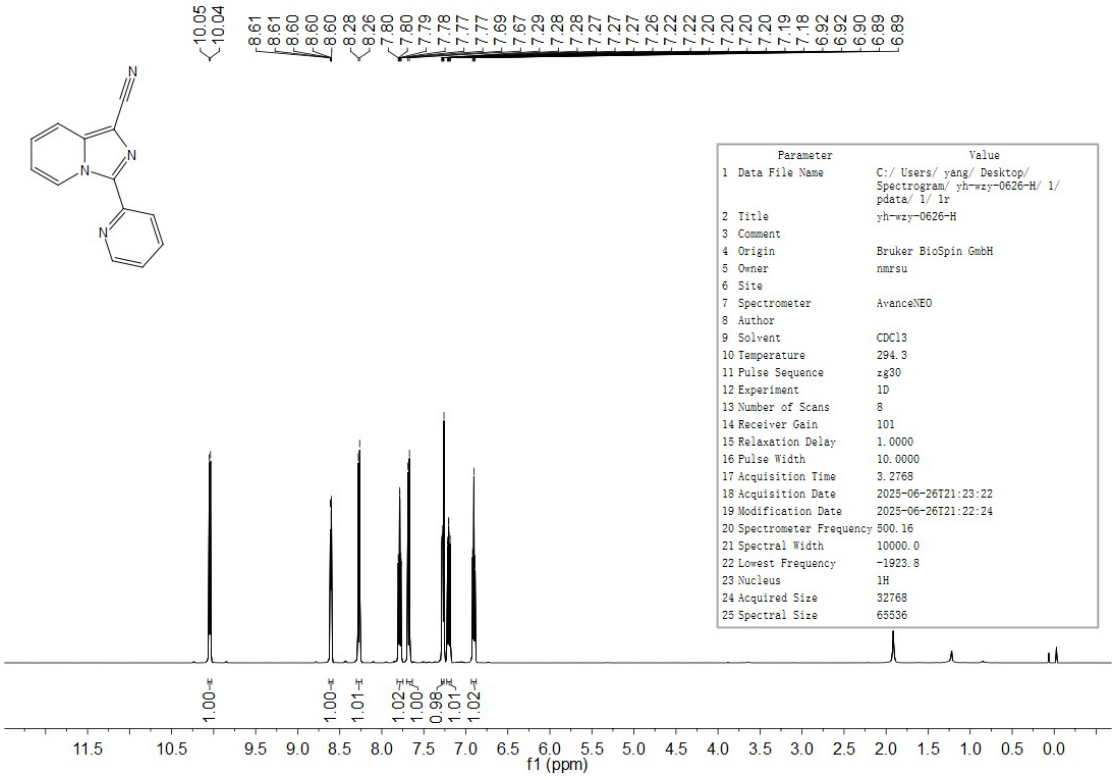
[S3] S. S. Grishin, A. O. Ustyuzhanin, V. A. Vil and A. O. Terent'ev, *Chem. Eur. J.*, 2025, **31**, e202404051.

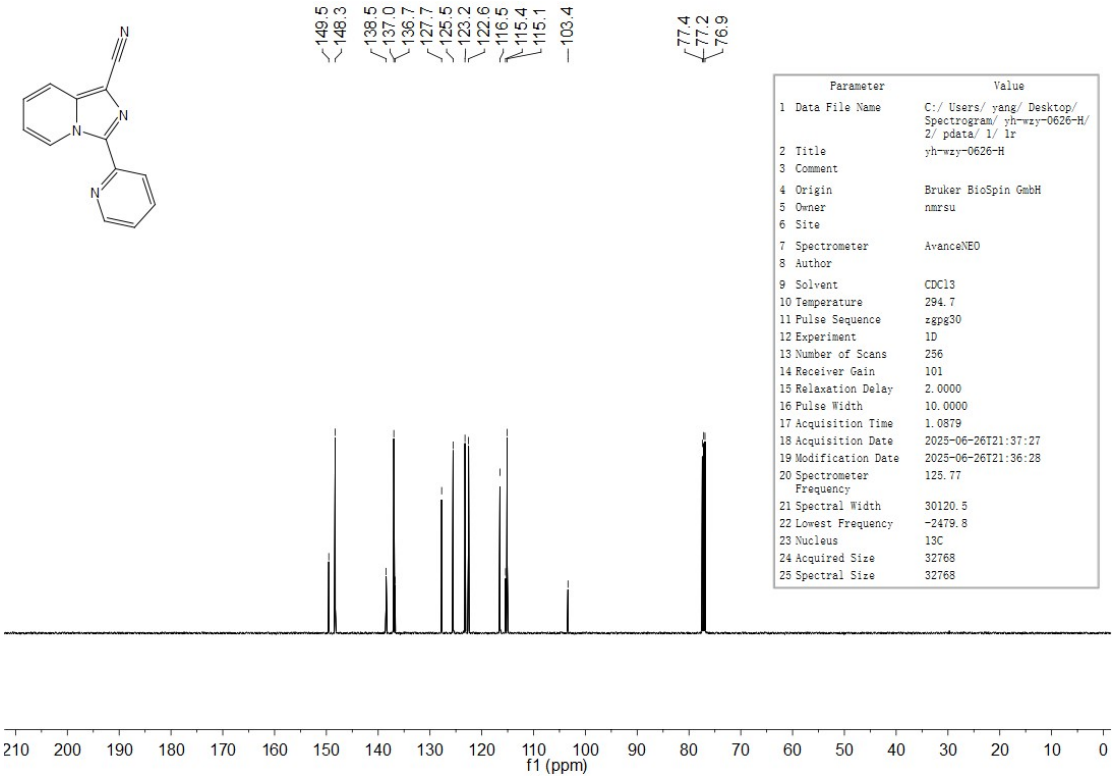
Copies of NMR spectra and HRMS.

Note: It was observed that some compounds exhibit relatively low signal intensities and diminished signal-to-noise (S/N) ratios in their ^{1}H NMR and ^{13}C NMR spectra. This is intrinsically attributed to the exceptionally poor solubility of these planar aromatic heterocycles in common deuterated solvents (e.g., $CDCl_3$, DMSO-d_6, Acetone-d_6) at room temperature. To acquire the characterization data, the NMR tubes were heated with a heat gun to achieve transient supersaturation prior to insertion into the spectrometer. However, during the data acquisition period (typically 20-40 minutes), partial precipitation of the products occurred as the samples cooled down within the probe, leading to a decrease in the effective concentration and a subsequent reduction in signal intensity.

The products 3f, 3g, 3h, 3j, 3k, 3l, 3m, 3n, and 3p are all slightly soluble compounds.

3-(pyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3a)

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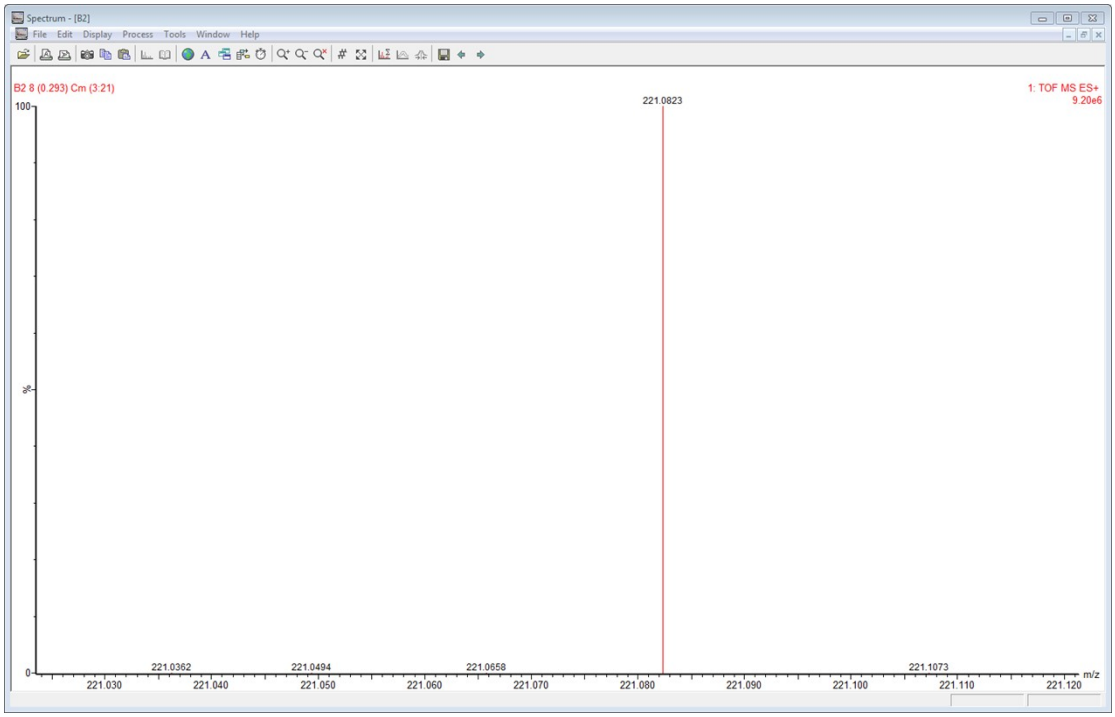
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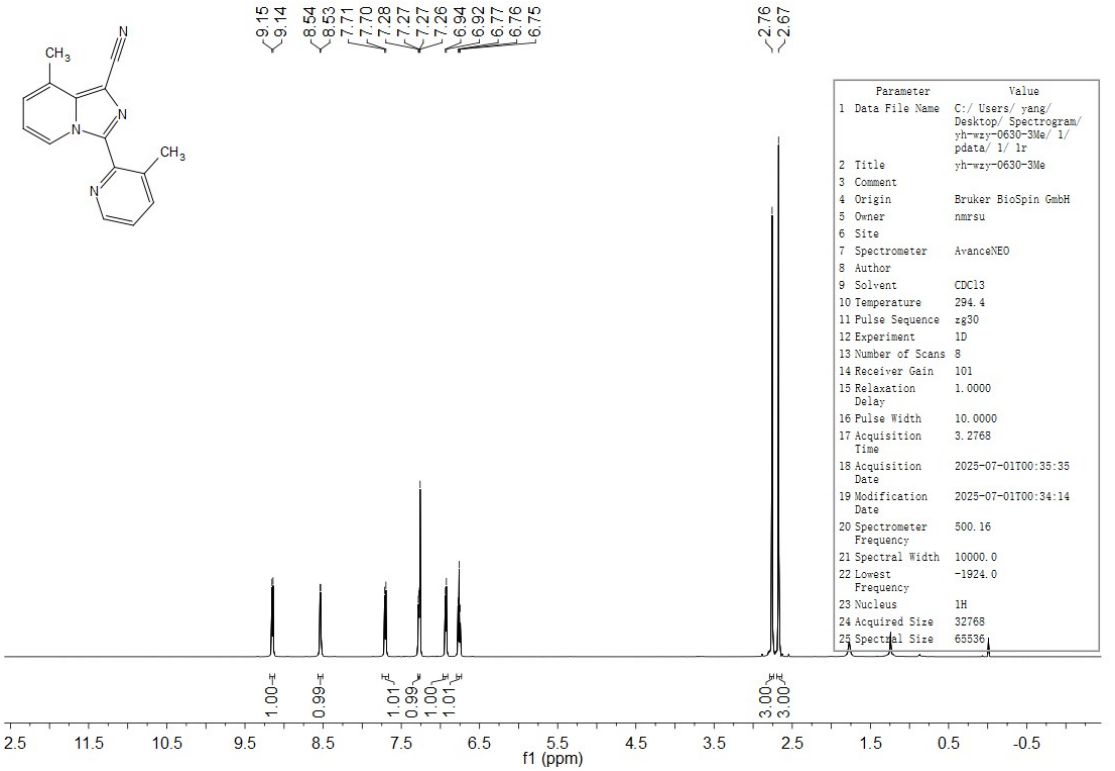
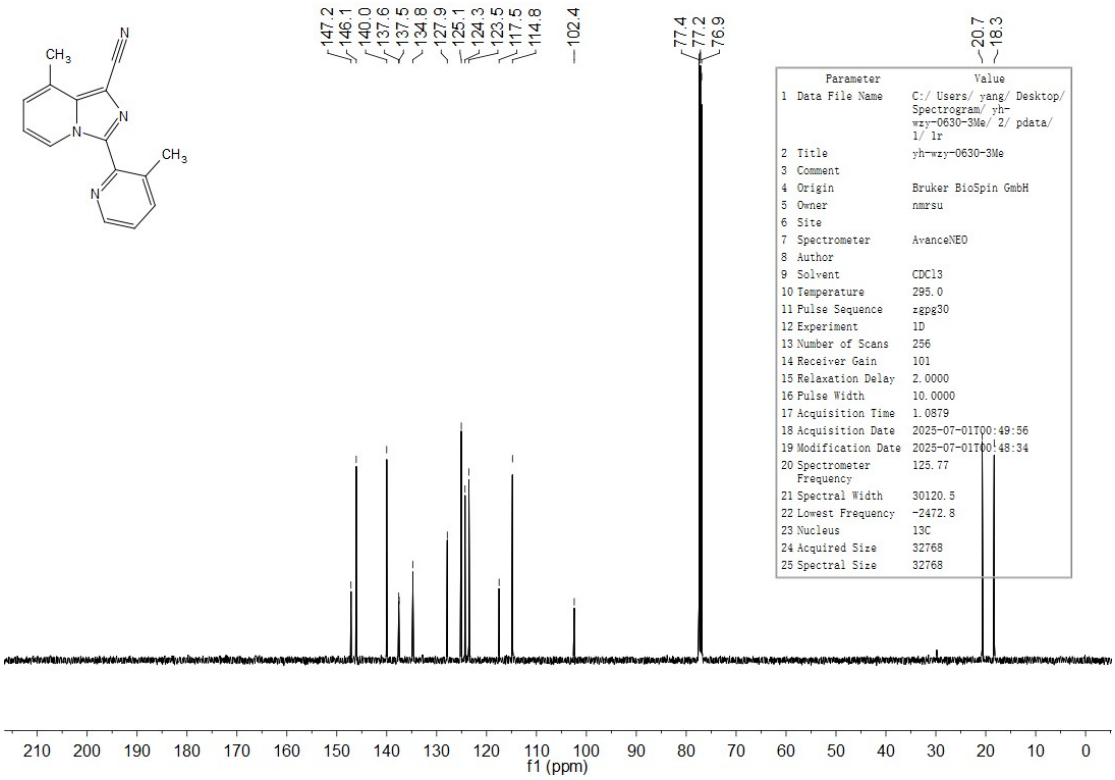
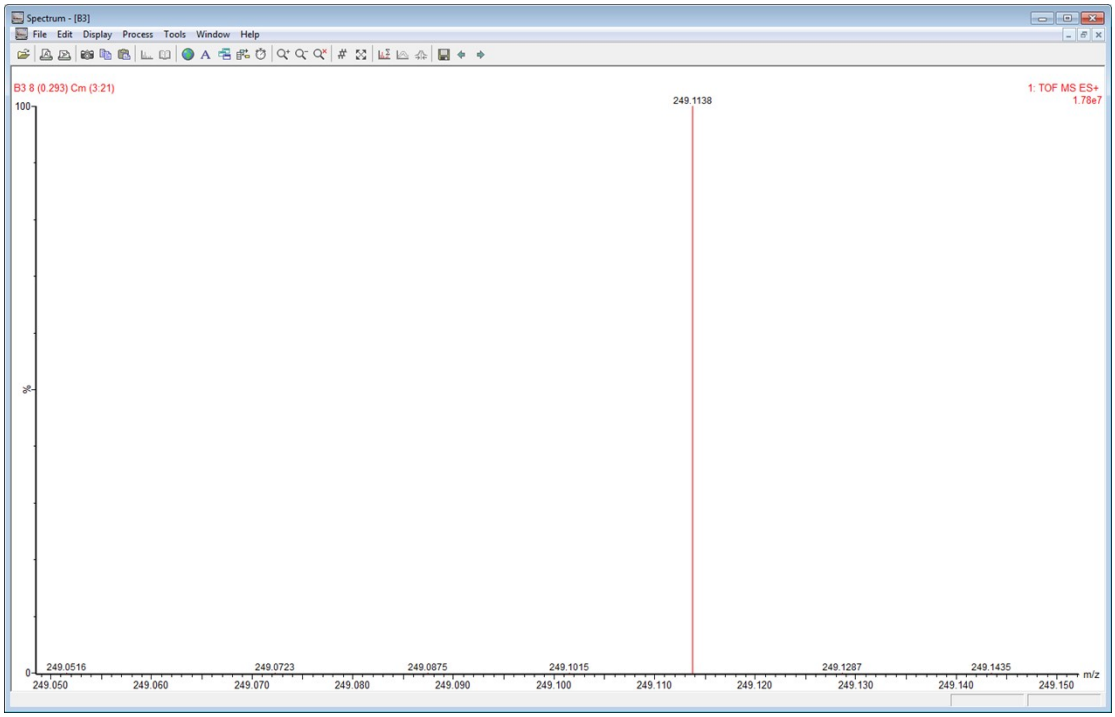
m/z

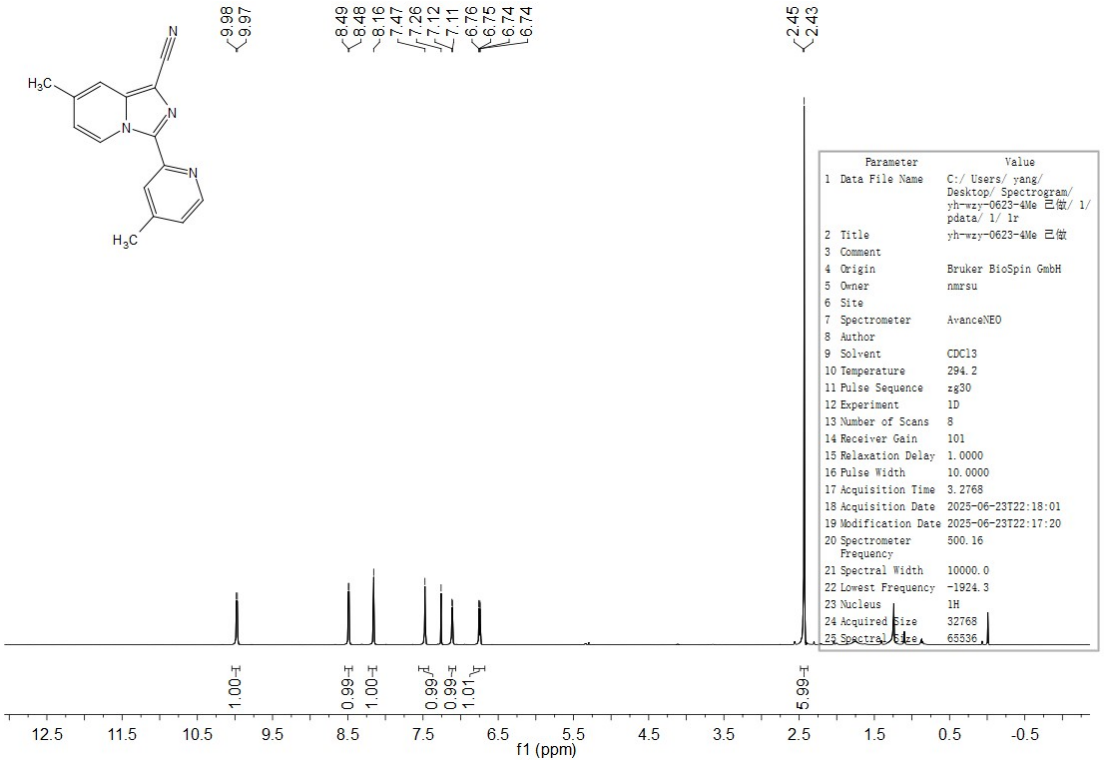
8-methyl-3-(3-methylpyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3b)

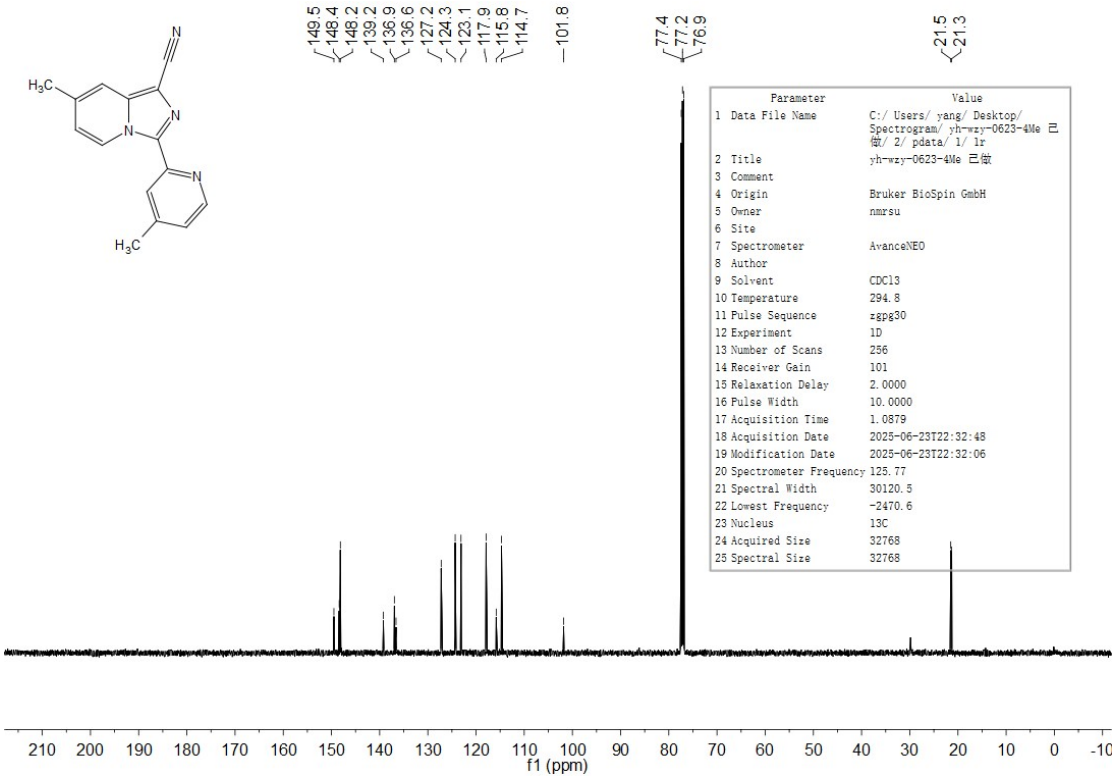






7-methyl-3-(4-methylpyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3c)

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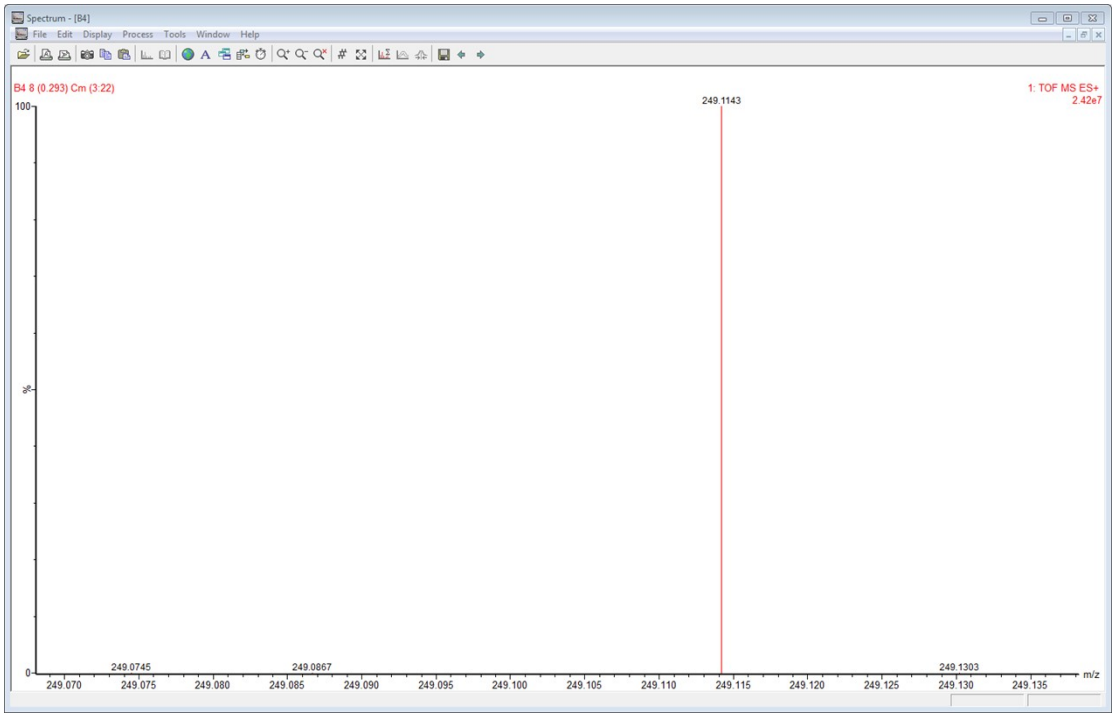
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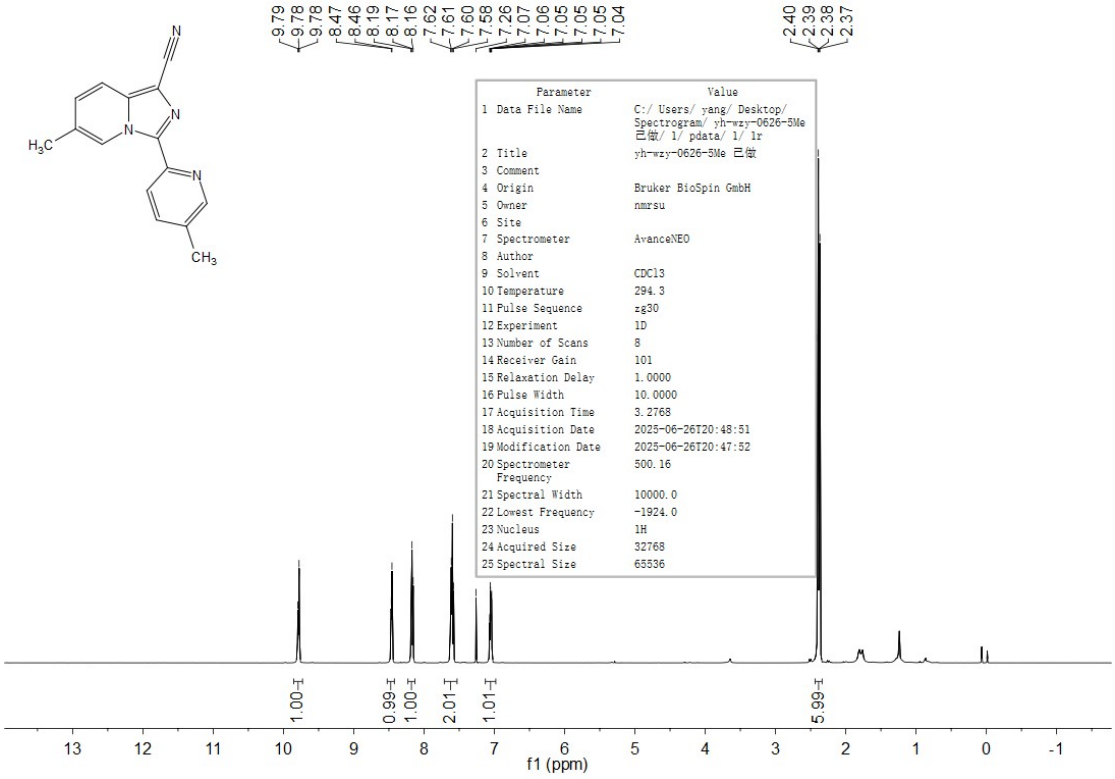
m/z

6-methyl-3-(5-methylpyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3d)



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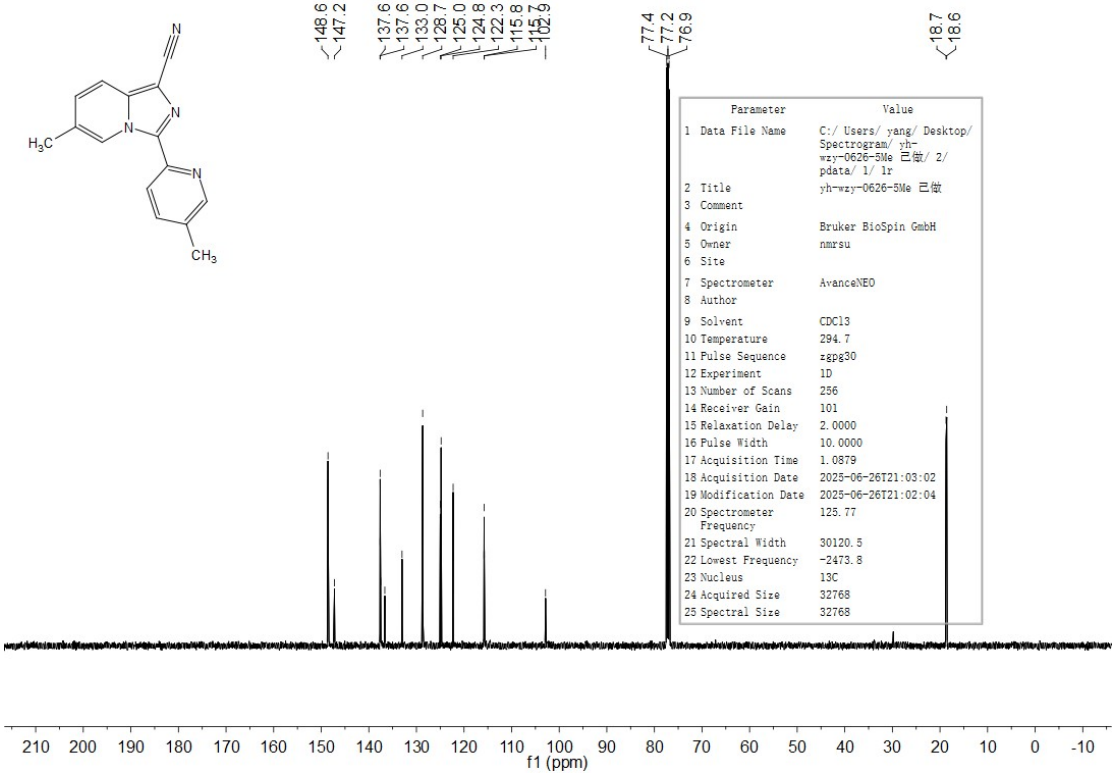

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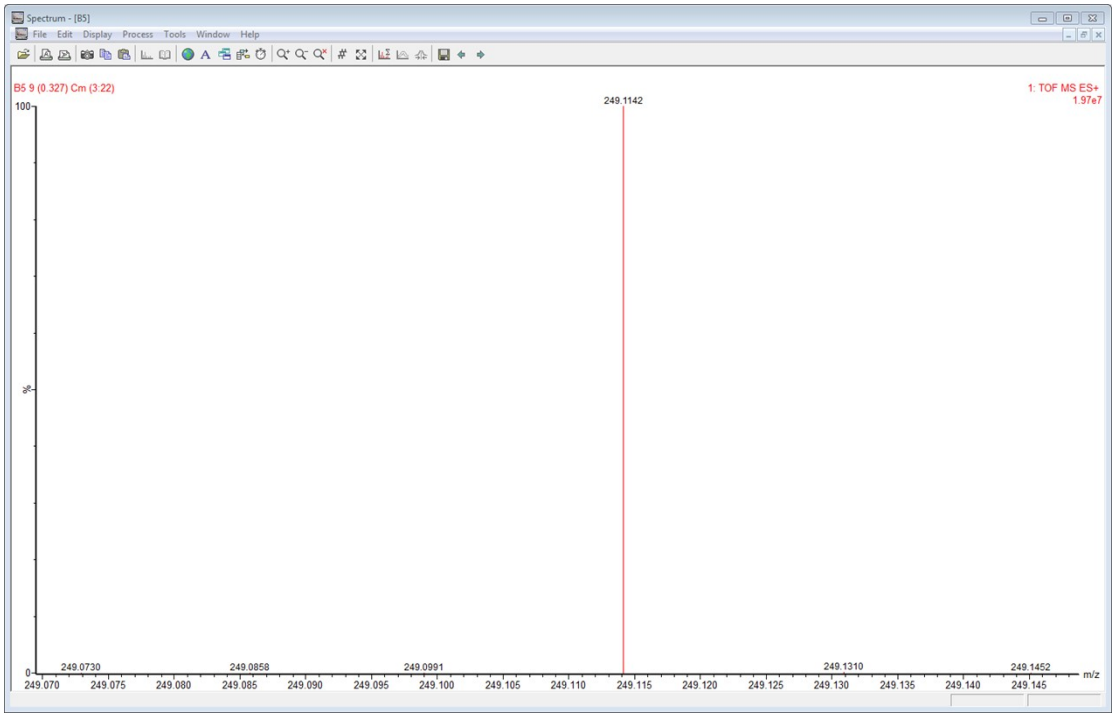
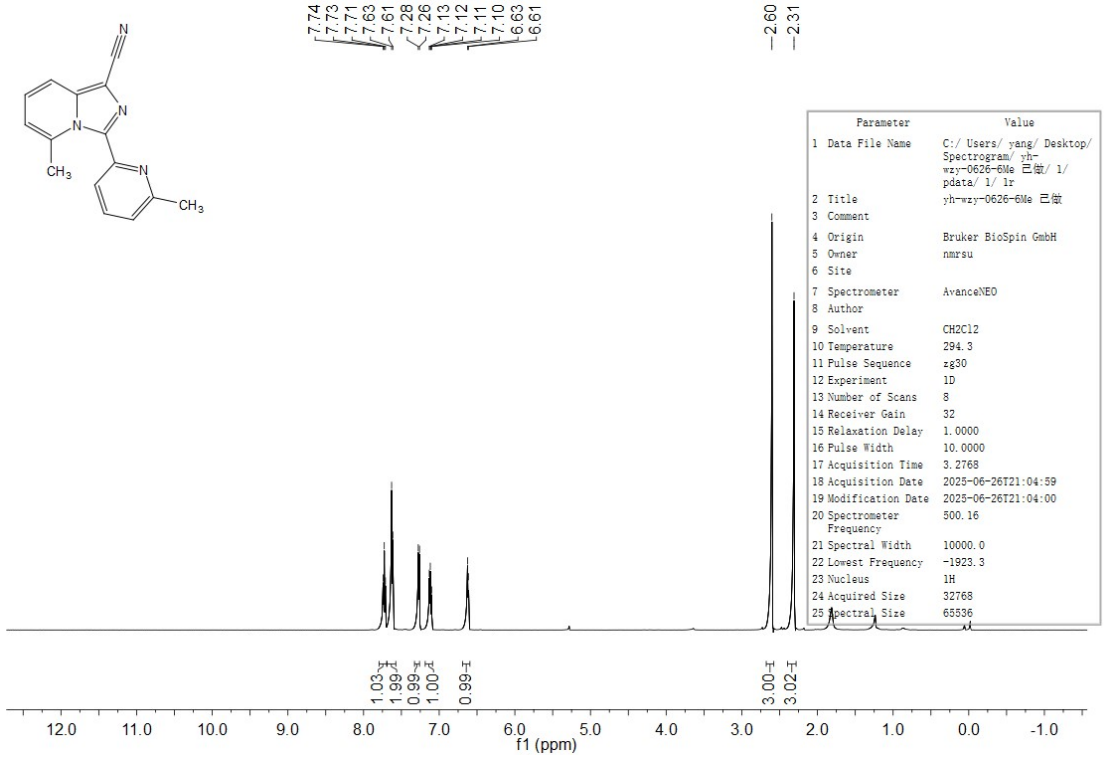
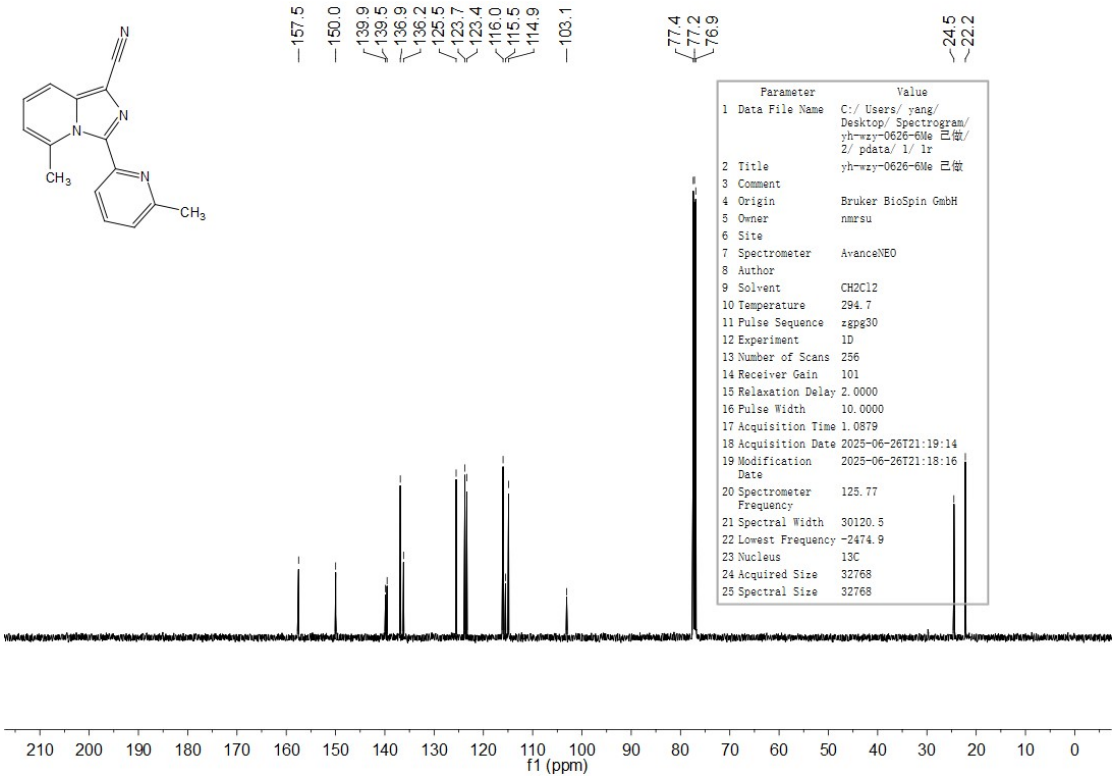


5-methyl-3-(6-methylpyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3e)

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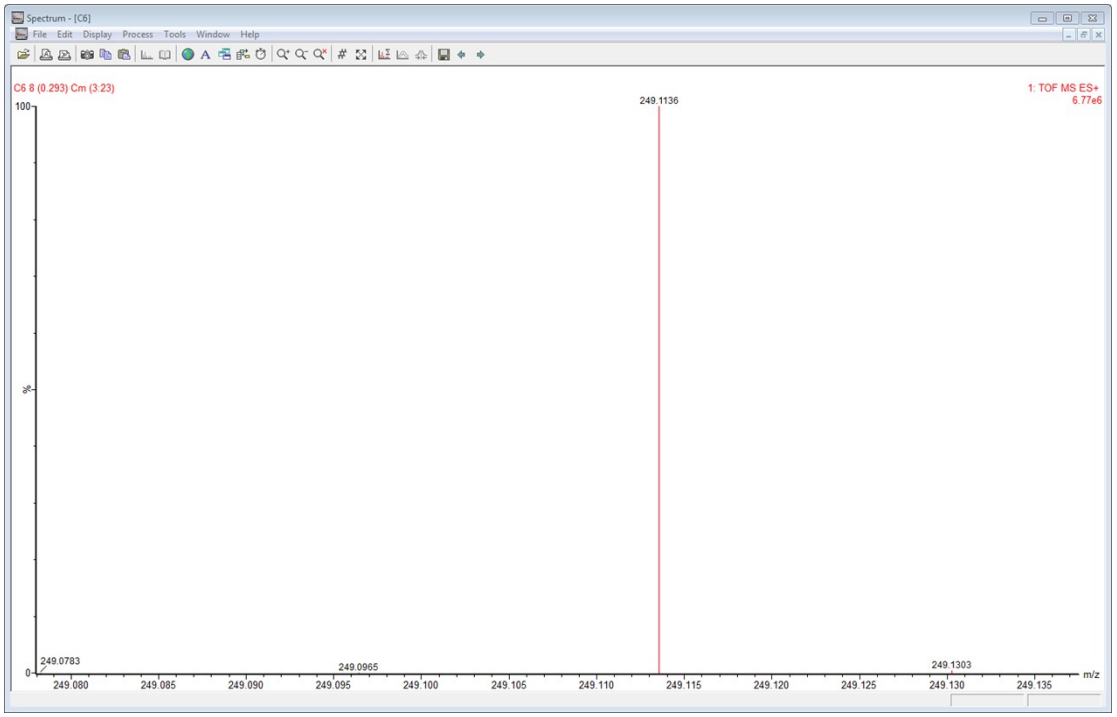
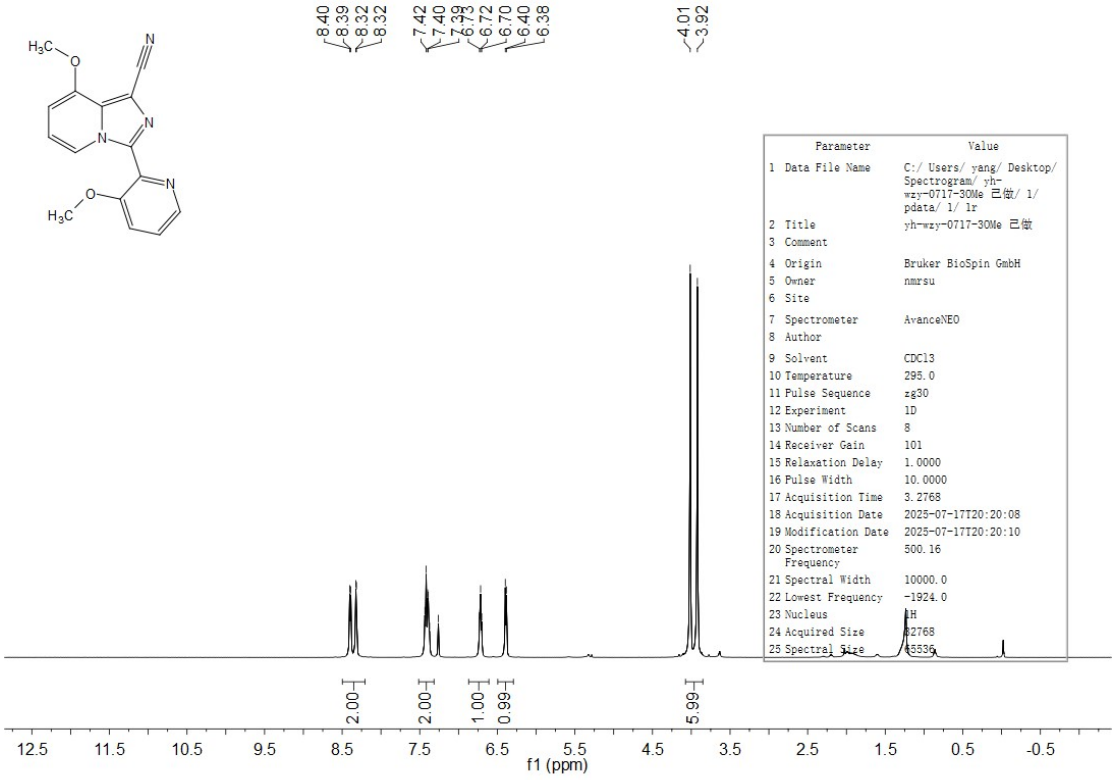
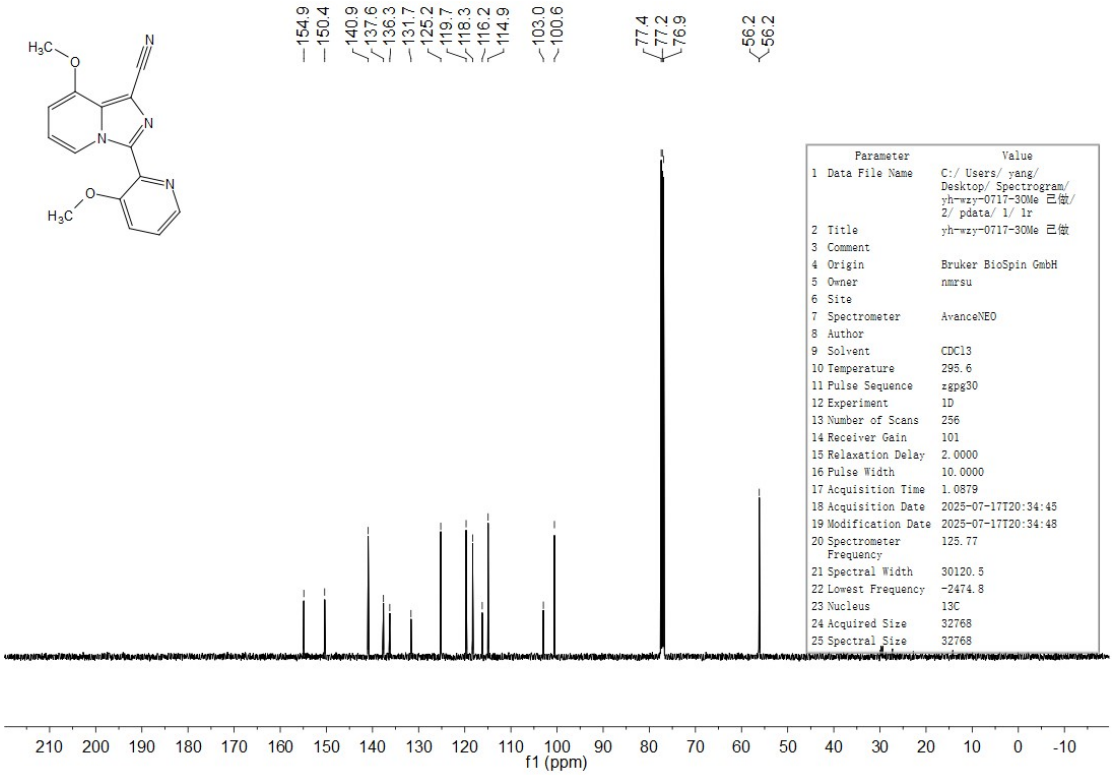
f1 (ppm)


Spectrum - [C6]
File Edit Display Process Tools Window Help
C6 8 (0.293) Cm (3:23)
1: TOF MS ES+
6.77e6
100
%
0
249.1136
249.0783
249.0965
249.1303
249.080 249.085 249.090 249.095 249.100 249.105 249.110 249.115 249.120 249.125 249.130 249.135
m/z

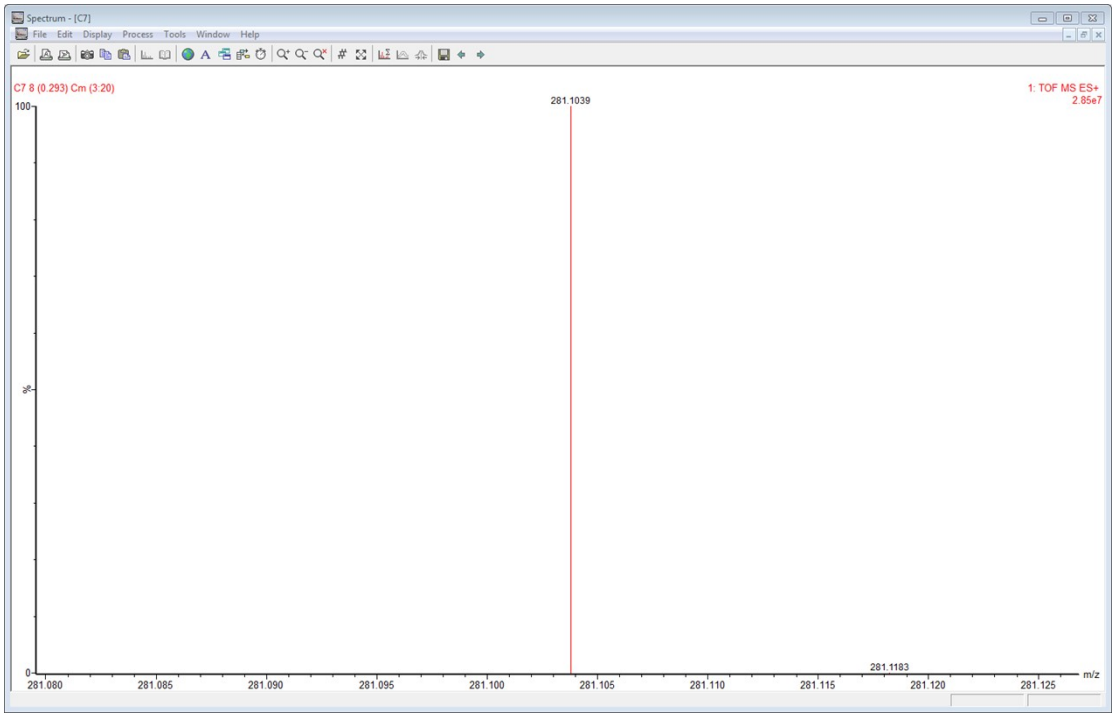
8-methoxy-3-(3-methoxypyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3f)



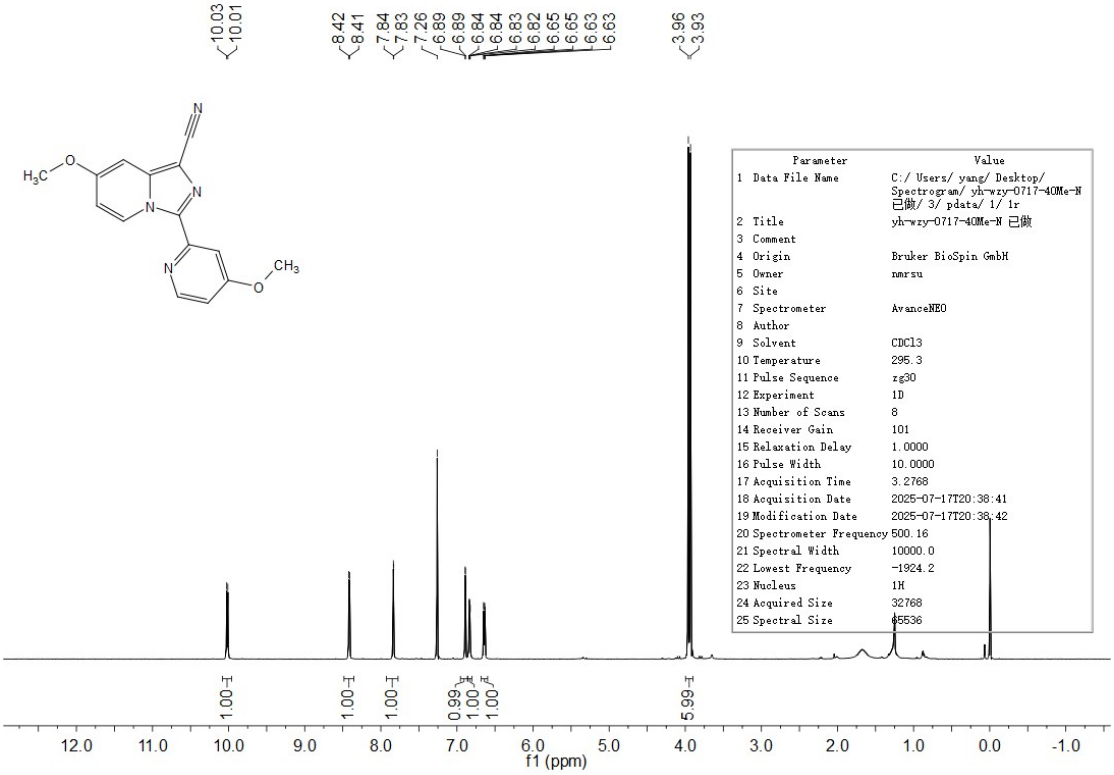
Parameter	Value
1 Data File Name	C:/ Users/ yang/ Desktop/ Spectrogram/ yh-wzy-0717-30Me 已做/ 1/ pdata/ 1/ 1r
2 Title	yh-wzy-0717-30Me 已做
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	295.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2025-07-17T20:20:08
19 Modification Date	2025-07-17T20:20:10
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1924.0
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

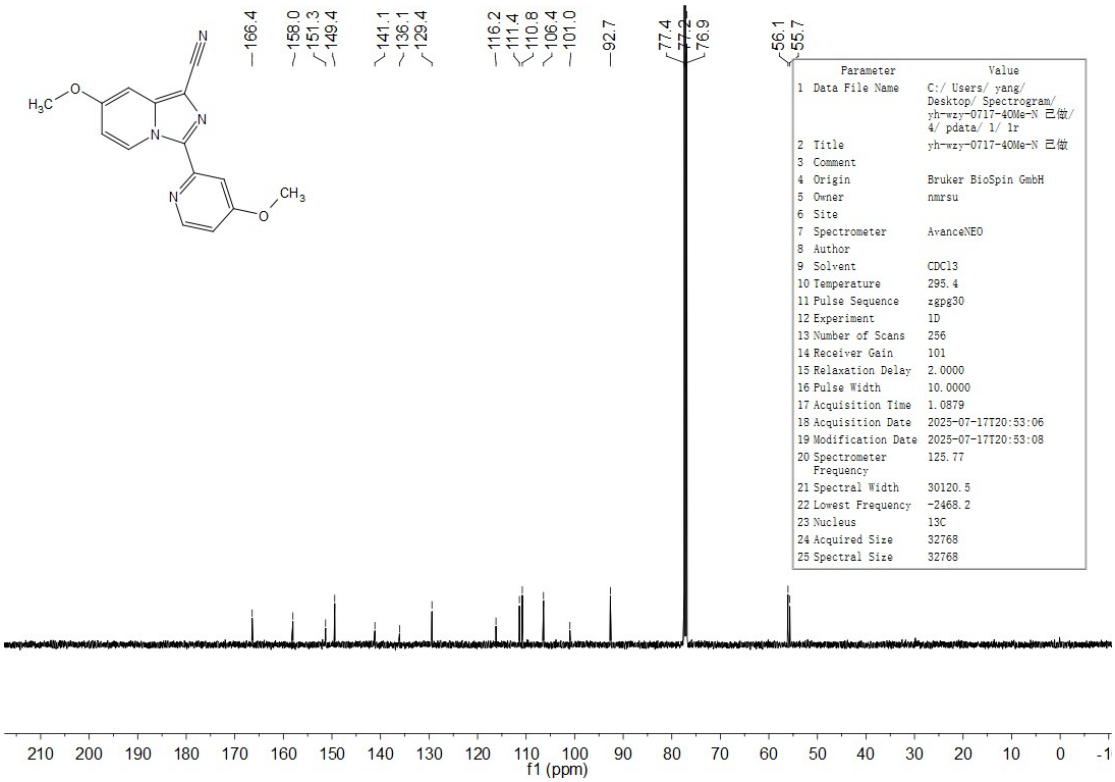


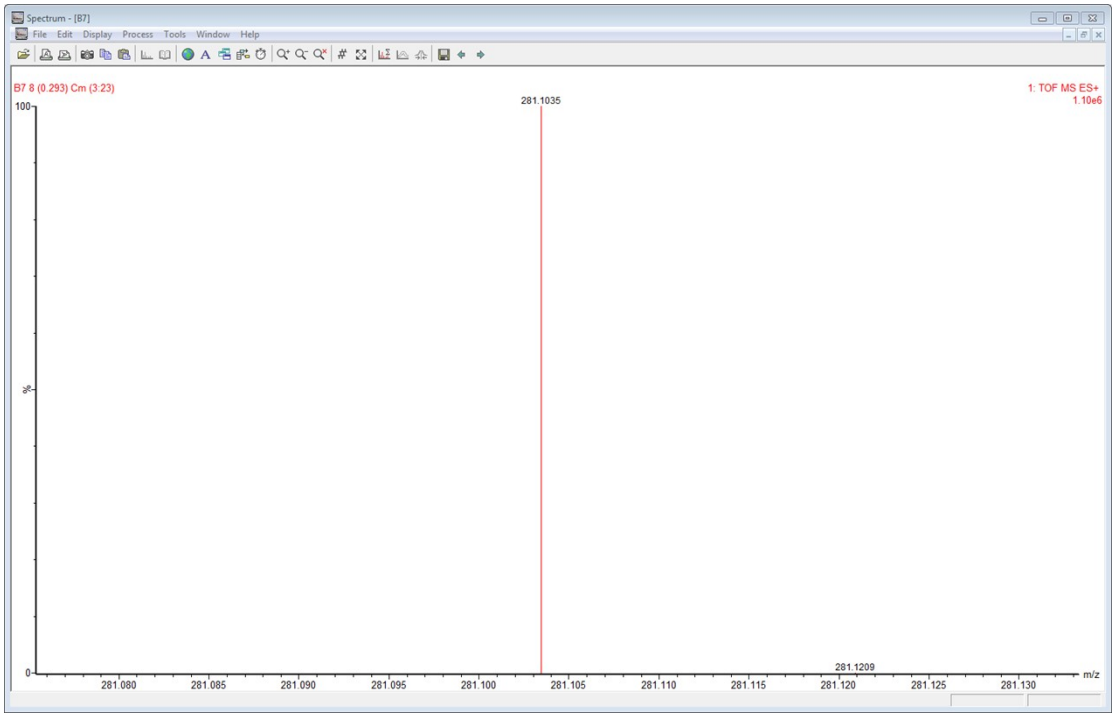
Parameter	Value
1 Data File Name	C:/ Users/ yang/ Desktop/ Spectrogram/ yh-wzy-0717-30Me 已做/ 2/ pdata/ 1/ 1r
2 Title	yh-wzy-0717-30Me 已做
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	295.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2025-07-17T20:34:45
19 Modification Date	2025-07-17T20:34:48
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2474.8
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768



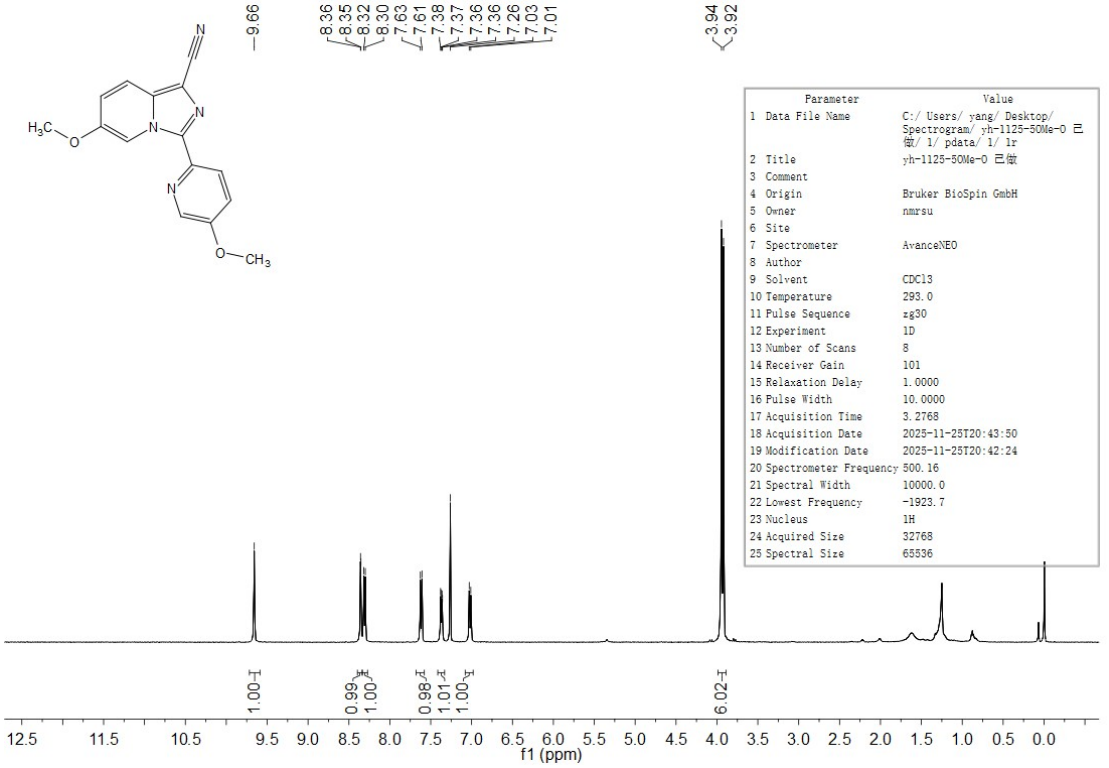
7-methoxy-3-(4-methoxypyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3g)



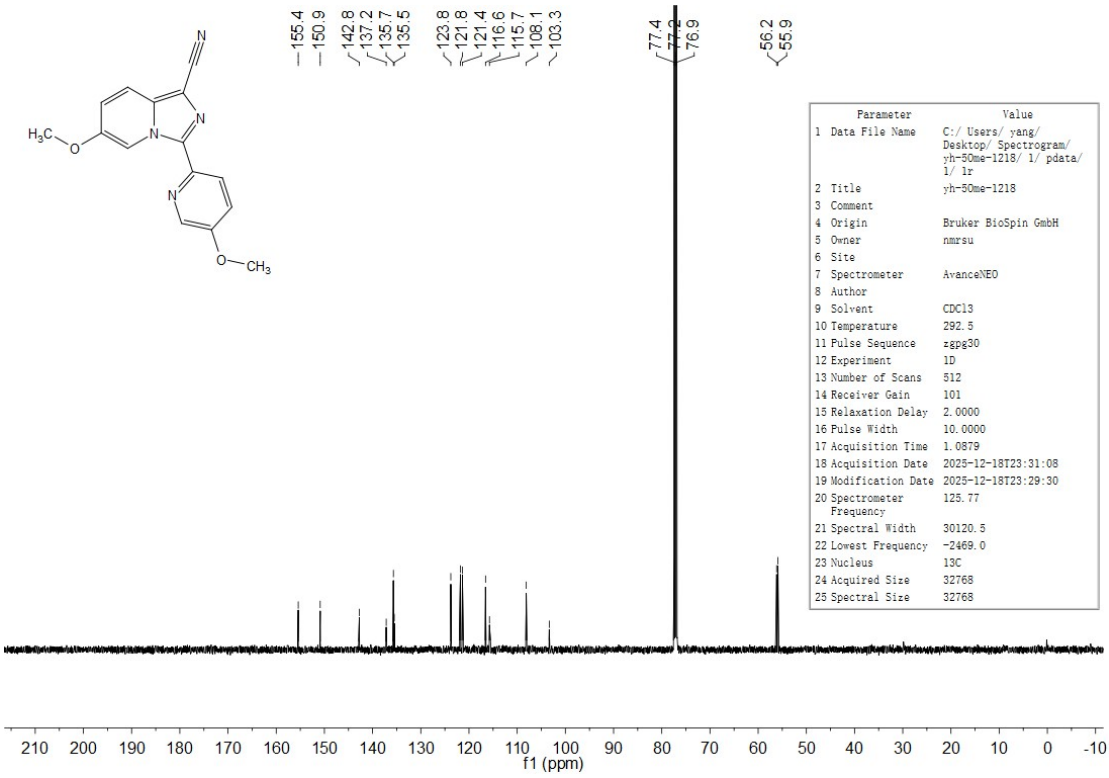

166.4
158.0
151.3
149.4
141.1
136.1
129.4
116.2
111.4
110.8
106.4
101.0
92.7
77.4
77.2
76.9
56.1
55.7
Parameter Value
1 Data File Name C:/ Users/ yang/ Desktop/ Spectrogram/ yh-wzy-0717-4OMe-N 已做/ 4/ pdata/ 1/ 1r
2 Title yh-wzy-0717-4OMe-N 已做
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 295.4
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2025-07-17T20:53:06
19 Modification Date 2025-07-17T20:53:08
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2468.2
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


Spectrum - [B7]
File Edit Display Process Tools Window Help
B7 8 (0.293) Cm (3:23)
1: TOF MS ES+
1.10e6
281.1035
100
%
0
281.1209
281.080 281.085 281.090 281.095 281.100 281.105 281.110 281.115 281.120 281.125 281.130
m/z

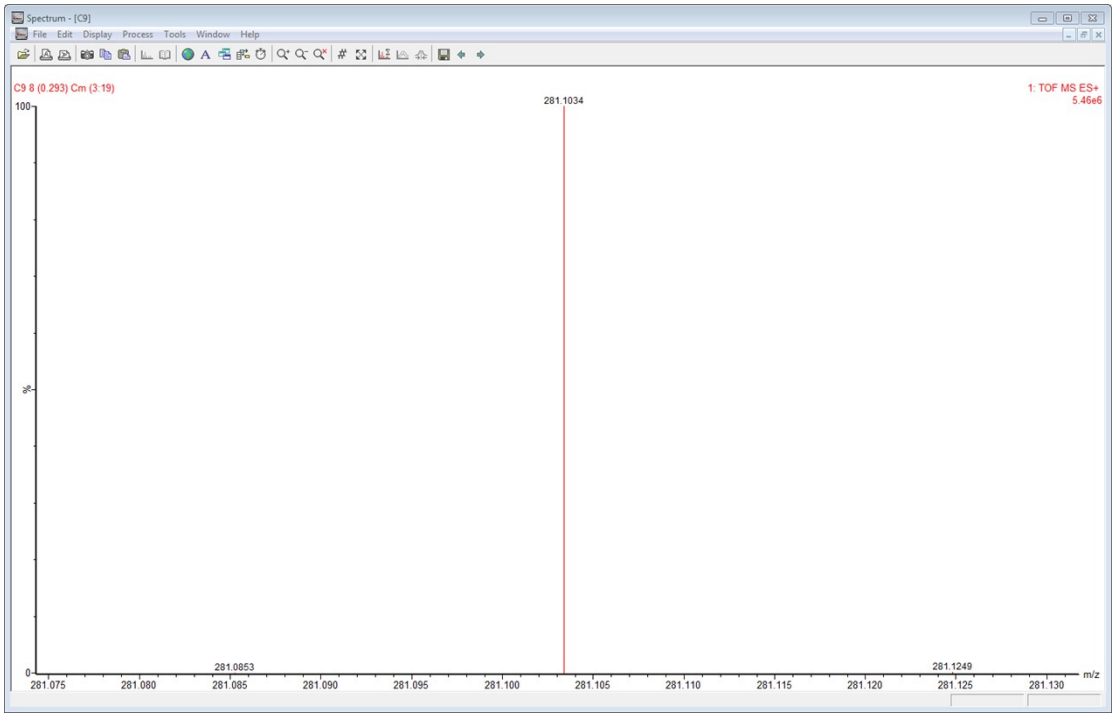
6-methoxy-3-(5-methoxypyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3h)



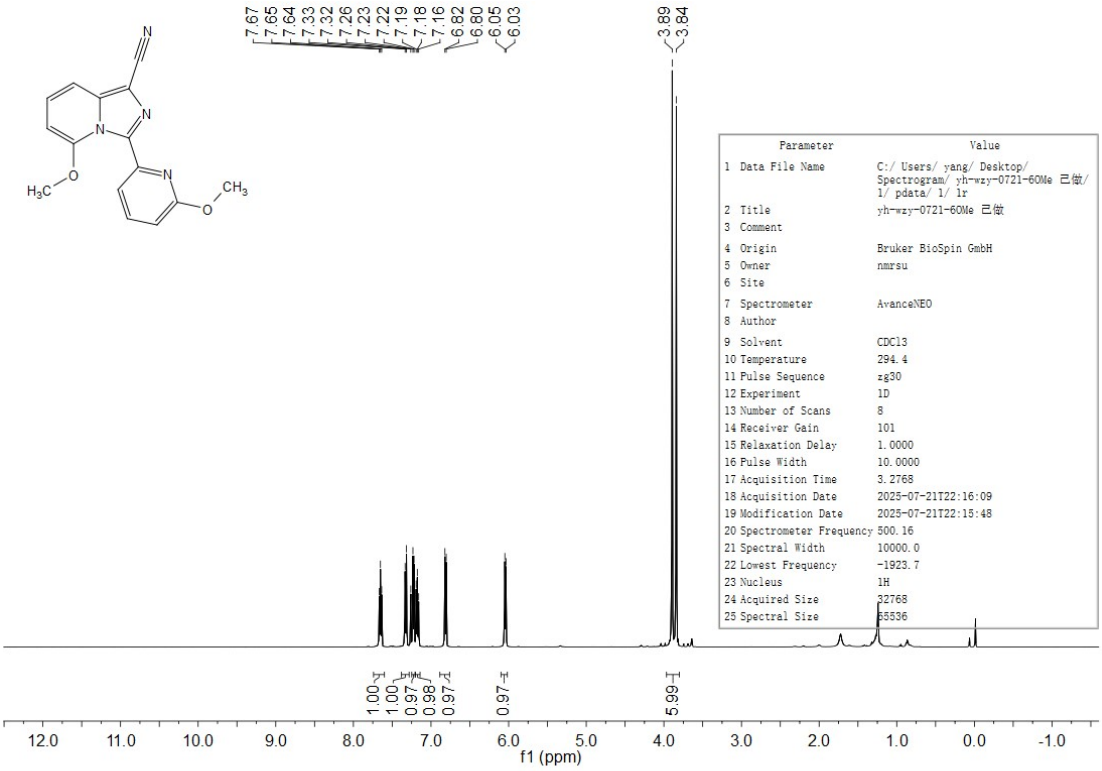
Parameter	Value
1 Data File Name	C:/ Users/ yang/ Desktop/ Spectrogram/ yh-1125-50Me-0 已做/ 1/ pdata/ 1/ 1r
2 Title	yh-1125-50Me-0 已做
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	293.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2025-11-25T20:43:50
19 Modification Date	2025-11-25T20:42:24
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1923.7
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

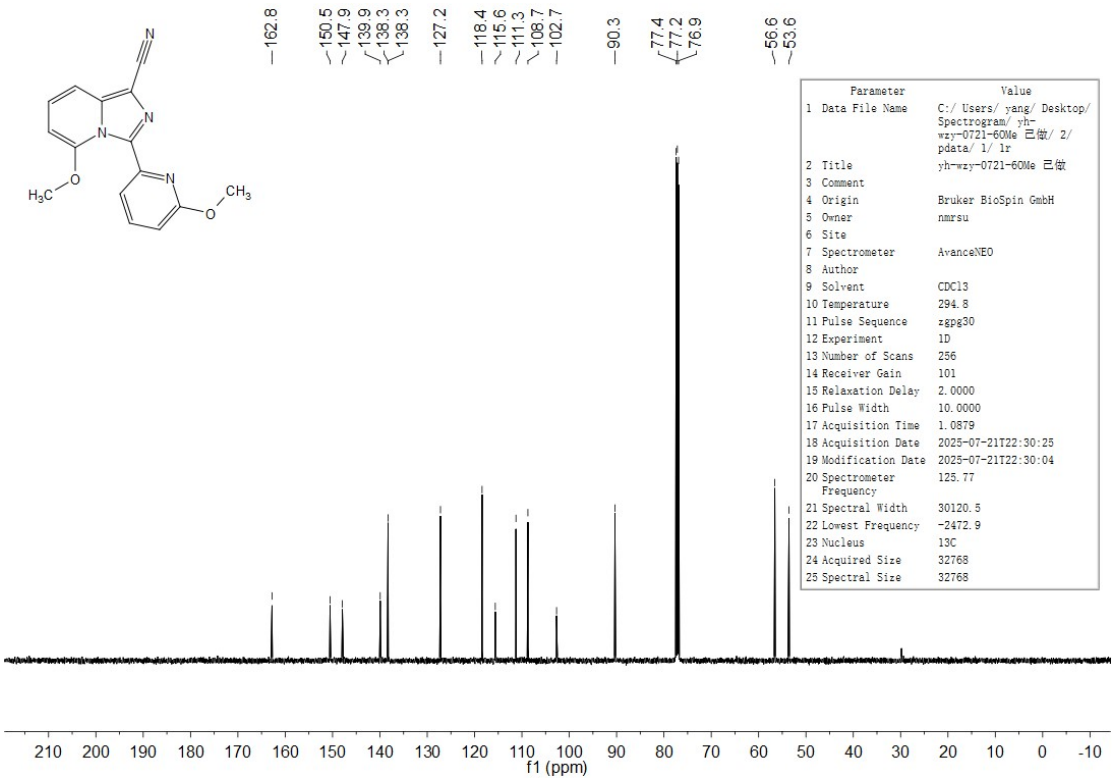


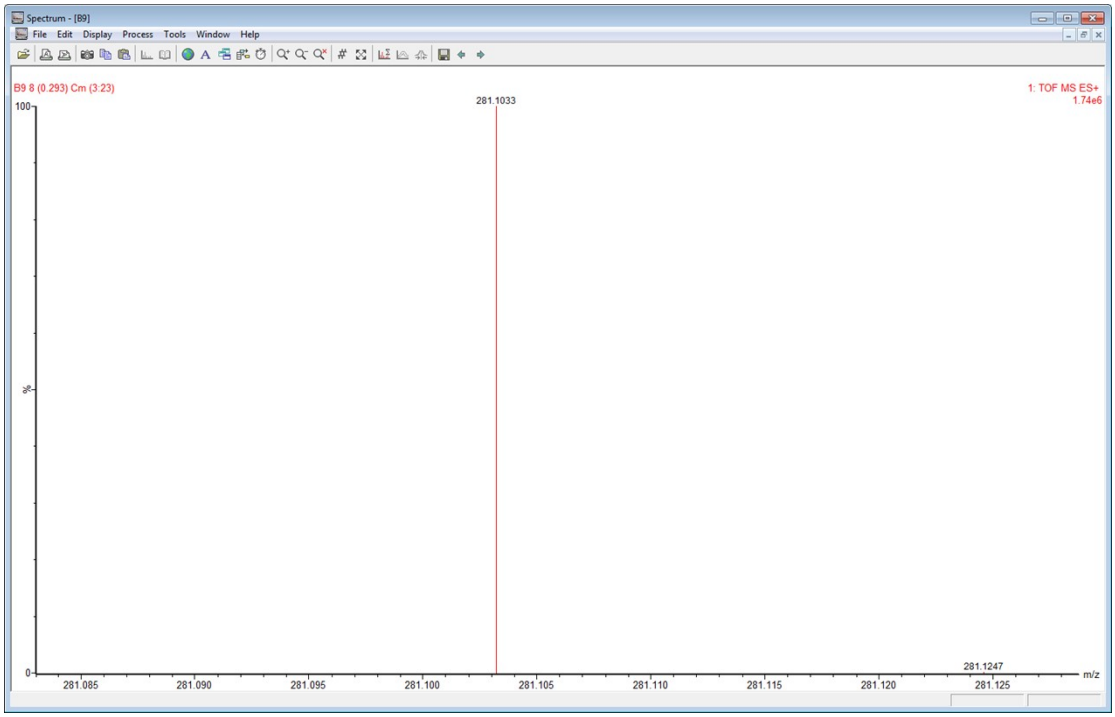
Parameter	Value
1 Data File Name	C:/ Users/ yang/ Desktop/ Spectrogram/ yh-50me-1218/ 1/ pdata/ 1/ 1r
2 Title	yh-50me-1218
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	292.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	512
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2025-12-18T23:31:08
19 Modification Date	2025-12-18T23:29:30
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2469.0
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768



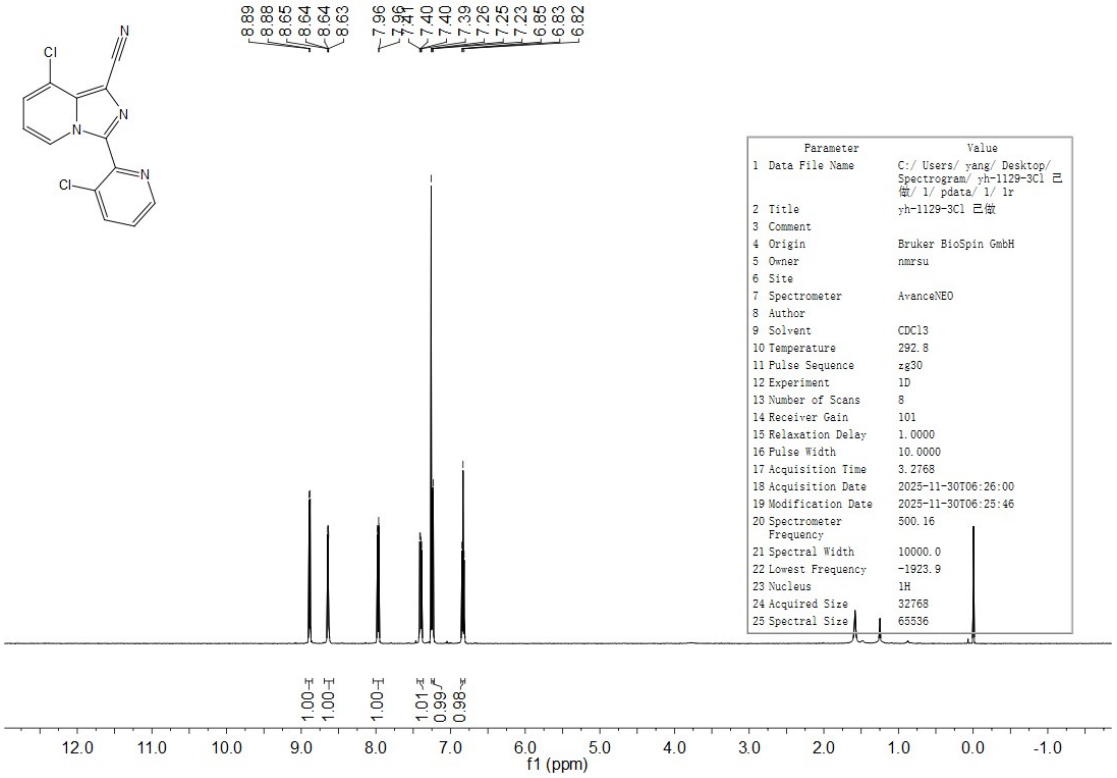
5-methoxy-3-(6-methoxypyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3i)

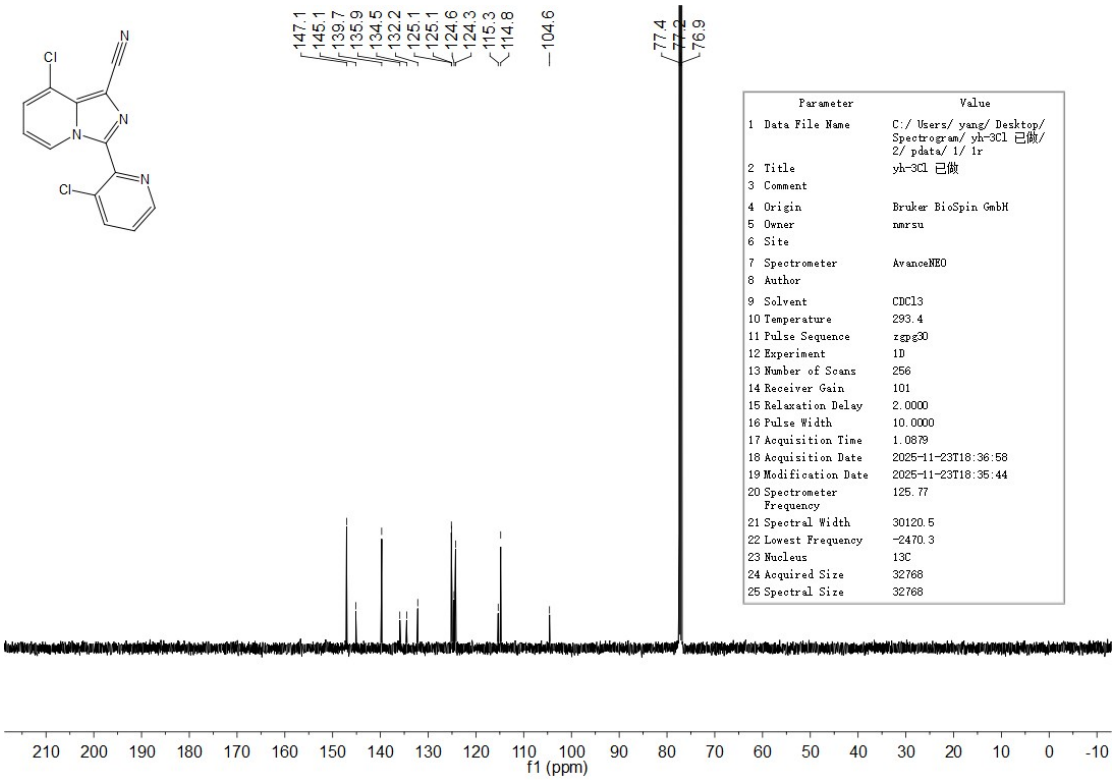


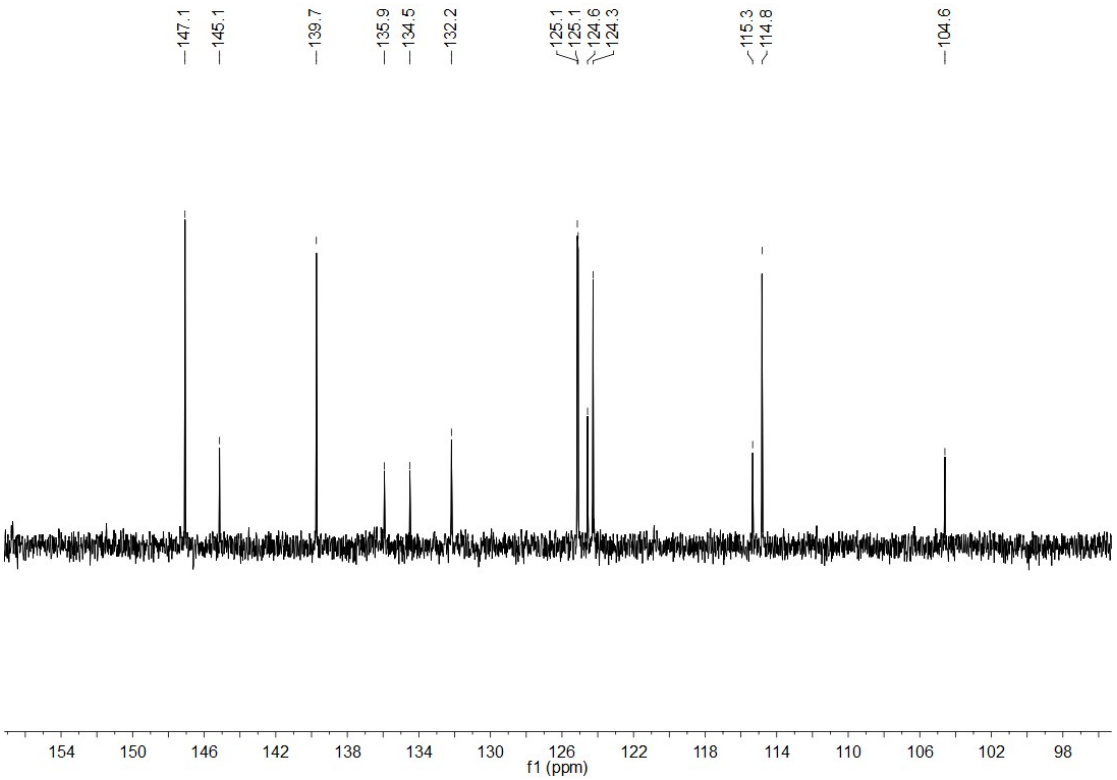

162.8
150.5
147.9
139.9
138.3
138.3
127.2
118.4
115.6
111.3
108.7
102.7
90.3
77.4
77.2
76.9
56.6
53.6
Parameter Value
1 Data File Name C:/ Users/ yang/ Desktop/ Spectrogram/ yh-wzy-0721-60Me 已做/ 2/ pdata/ 1/ 1r
2 Title yh-wzy-0721-60Me 已做
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 294.8
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2025-07-21T22:30:25
19 Modification Date 2025-07-21T22:30:04
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2472.9
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
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)

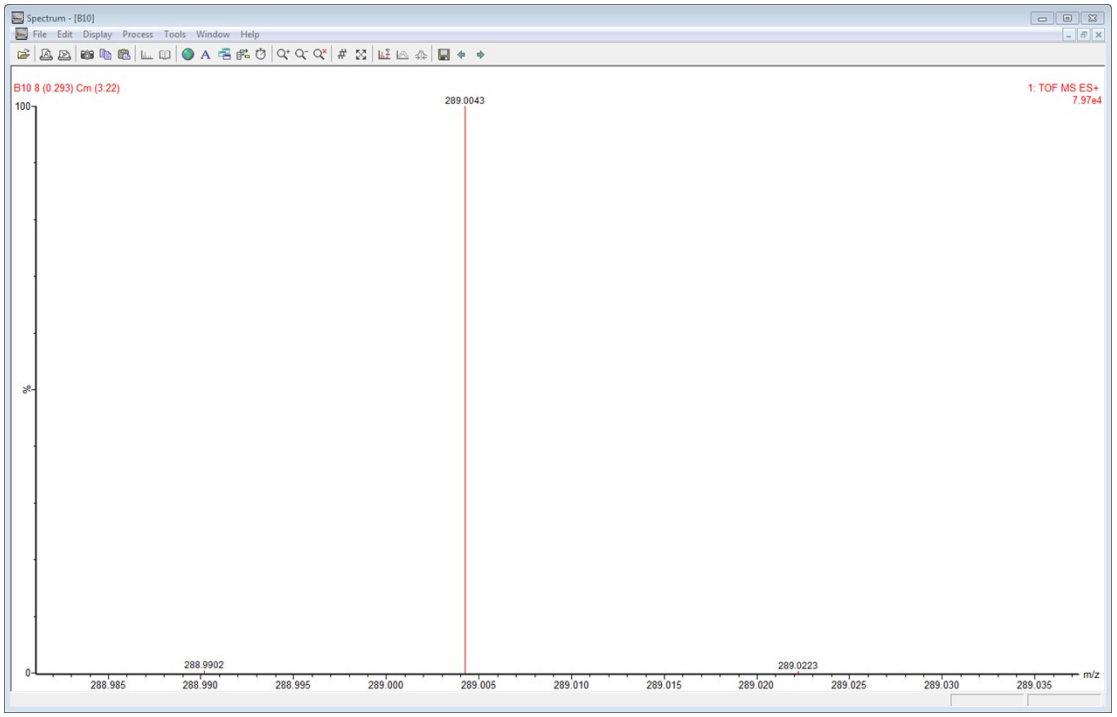

Spectrum - [B9]
File Edit Display Process Tools Window Help
B9 8 (0.293) Cm (3:23)
1: TOF MS ES+
1.74e6
281.1033
100
%
0
281.1247
281.085 281.090 281.095 281.100 281.105 281.110 281.115 281.120 281.125
m/z

8-chloro-3-(3-chloropyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3j)

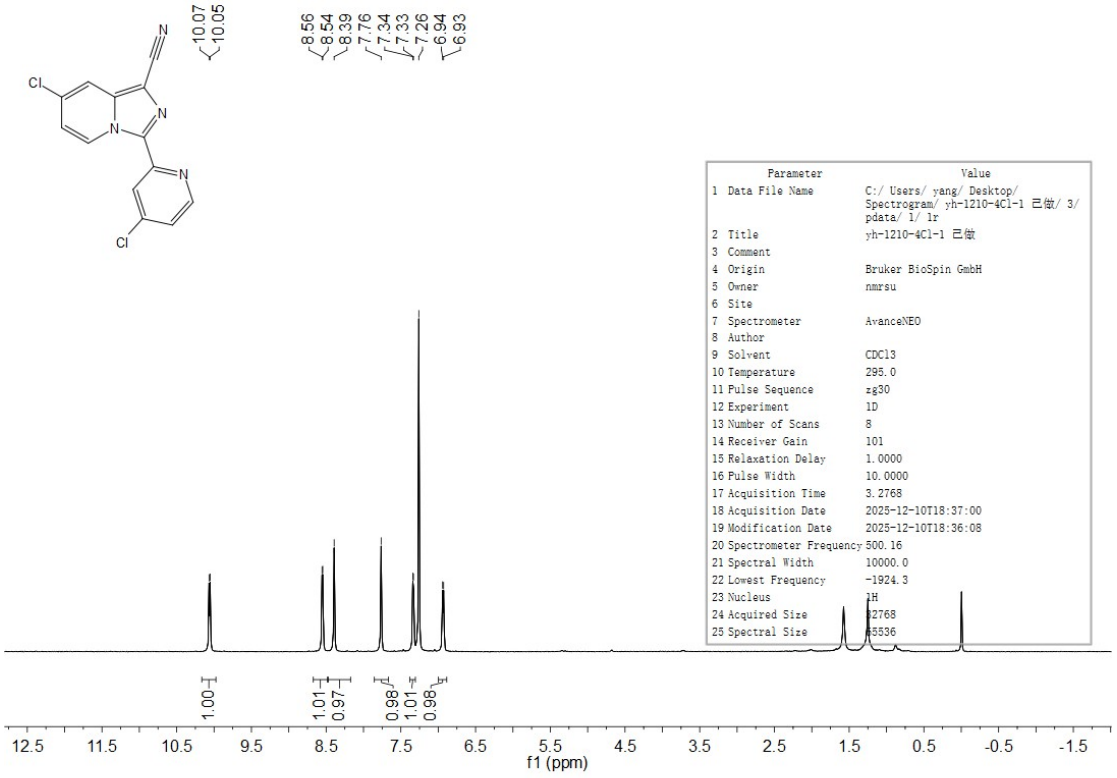


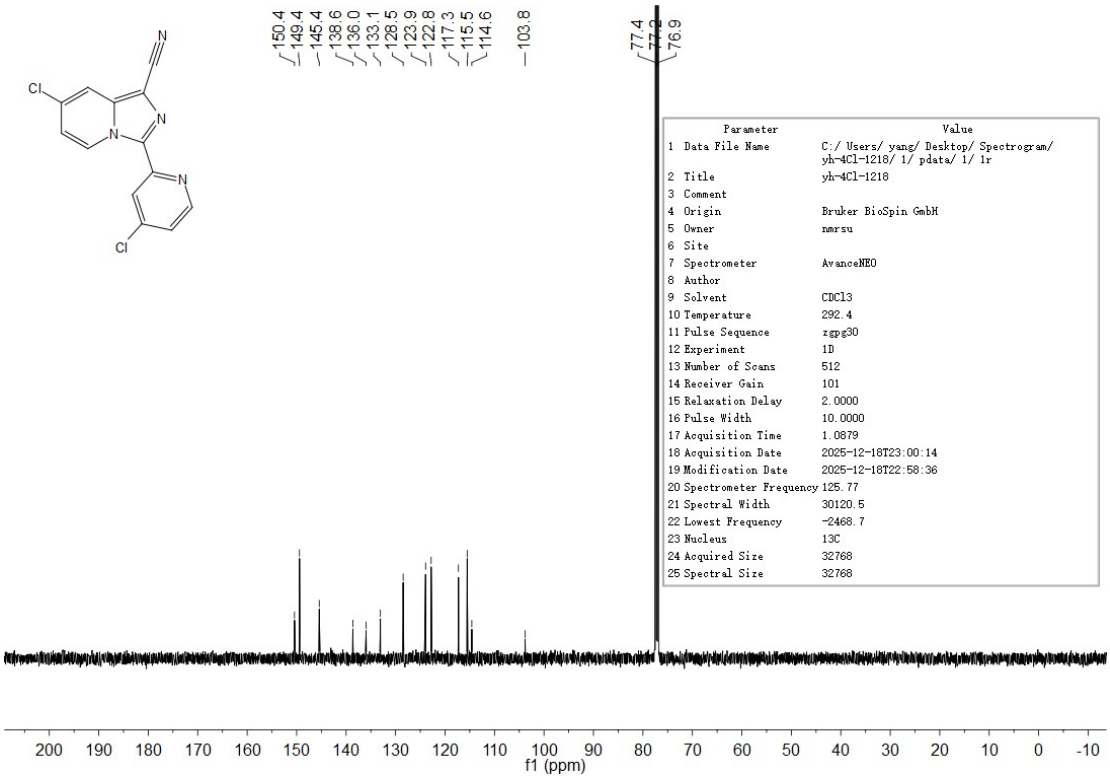


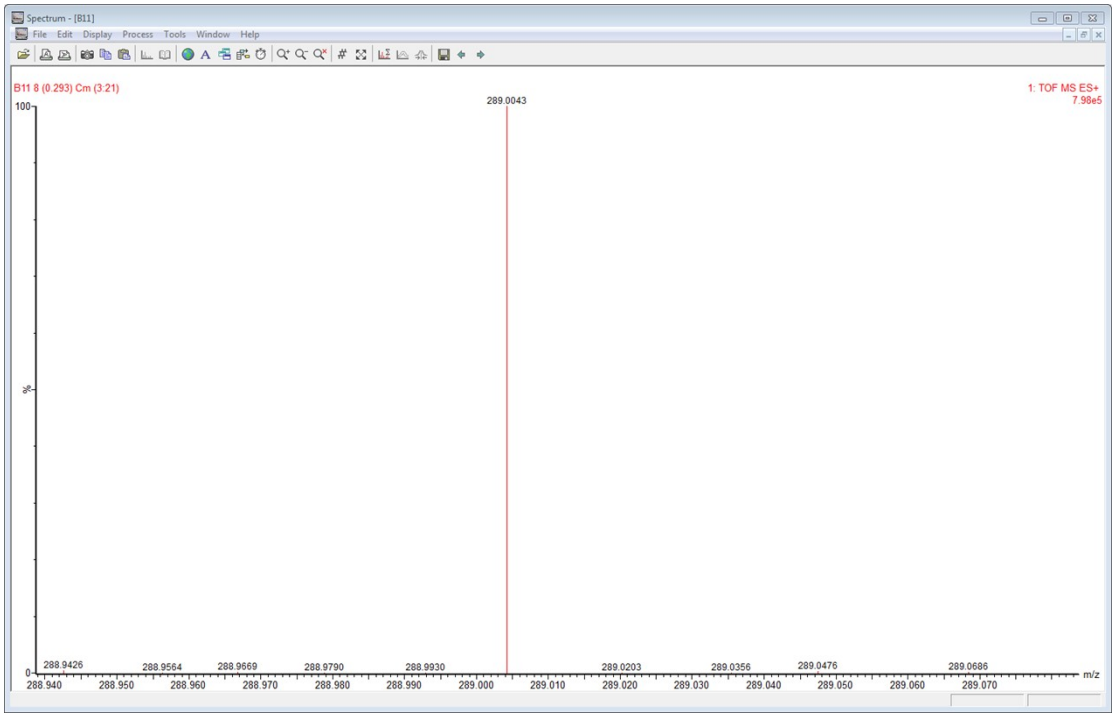

147.1
145.1
139.7
135.9
134.5
132.2
125.1
125.1
124.6
124.3
115.3
114.8
104.6
154
150
146
142
138
134
130
126
122
118
114
110
106
102
98
f1 (ppm)


Spectrum - [B10]
File Edit Display Process Tools Window Help
B10 8 (0.293) Cm (3:22)
1: TOF MS ES+
7.97e4
289.0043
100
%
0
288.9902
289.0223
m/z
288.985
288.990
288.995
289.000
289.005
289.010
289.015
289.020
289.025
289.030
289.035

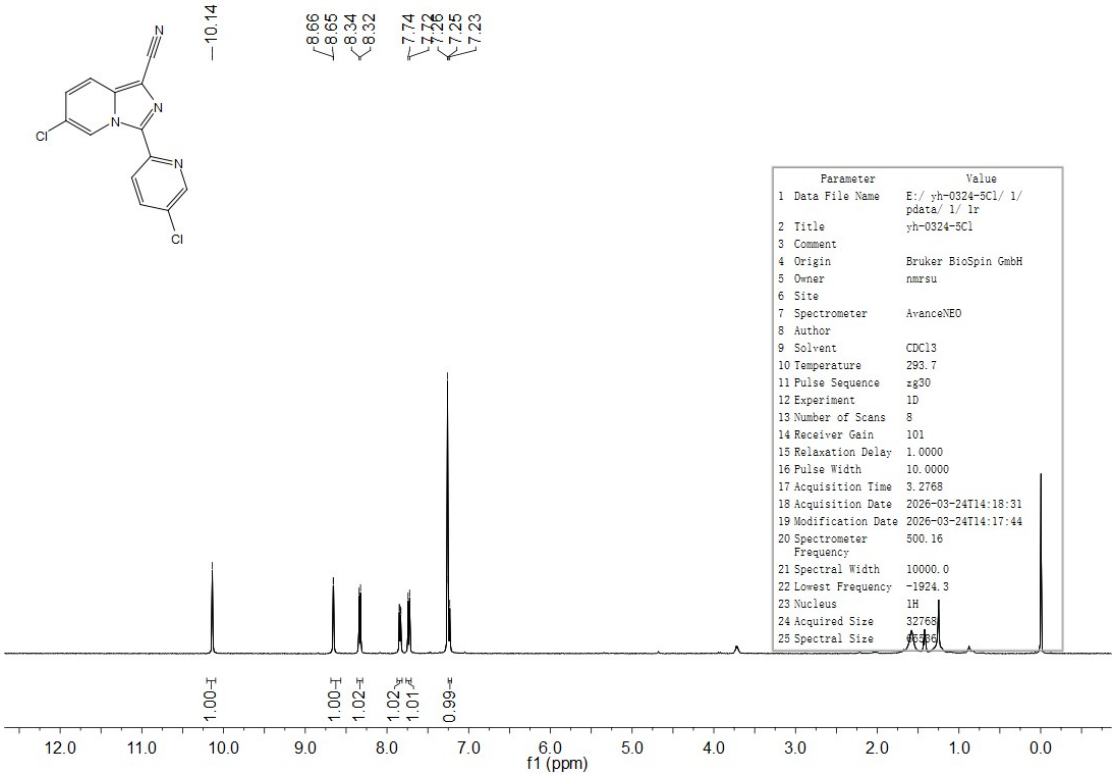
7-chloro-3-(4-chloropyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3k)

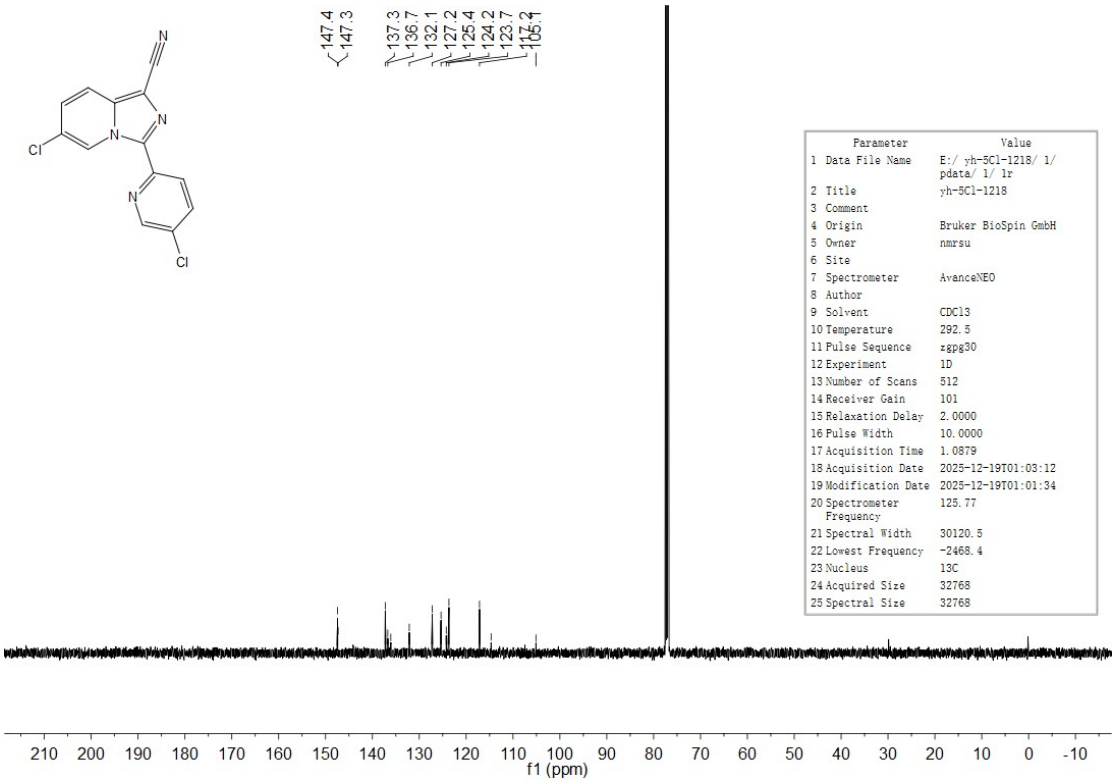


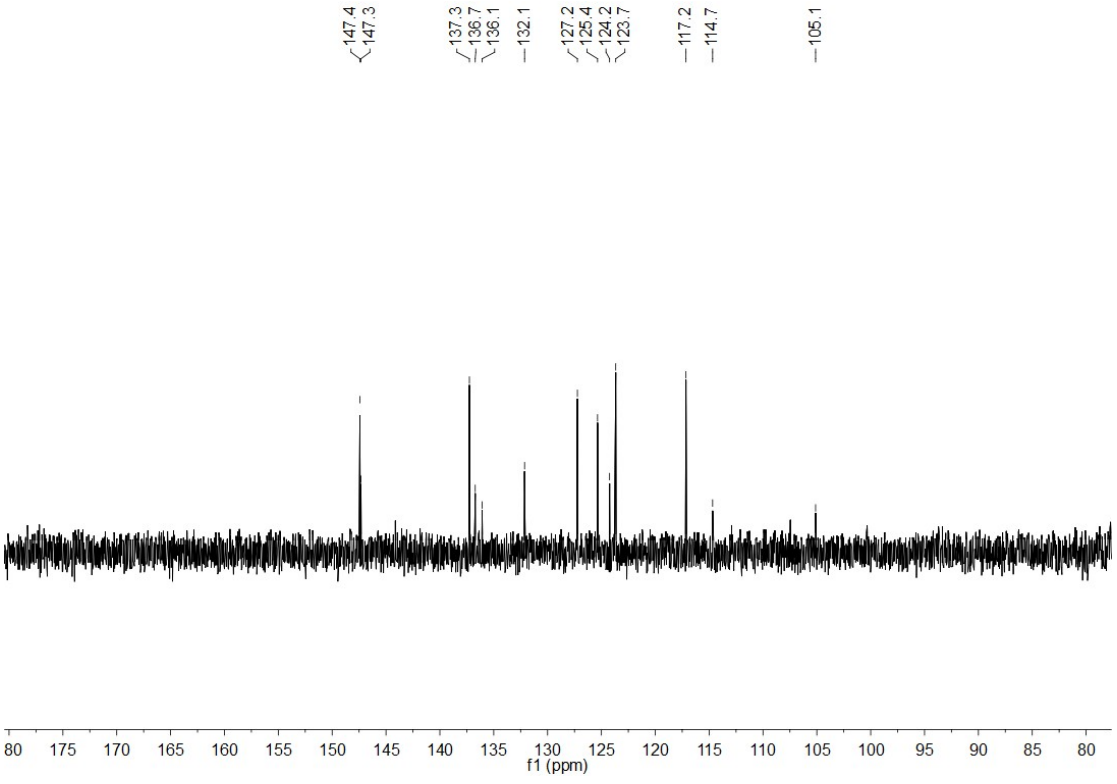


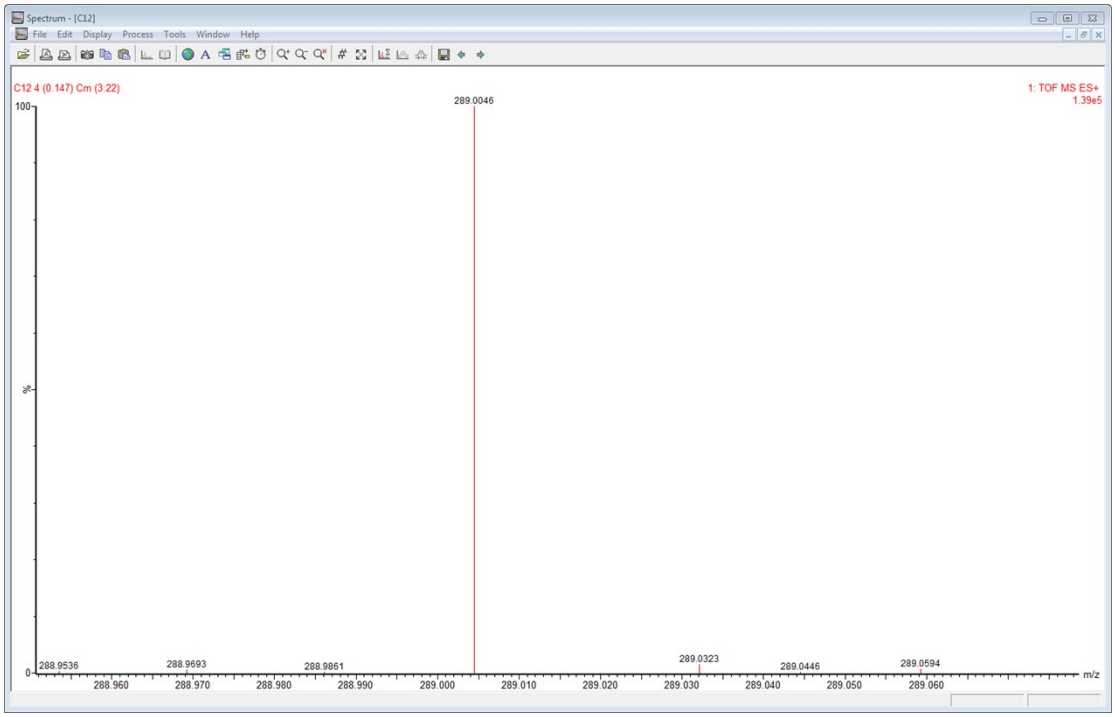


6-chloro-3-(5-chloropyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3l)

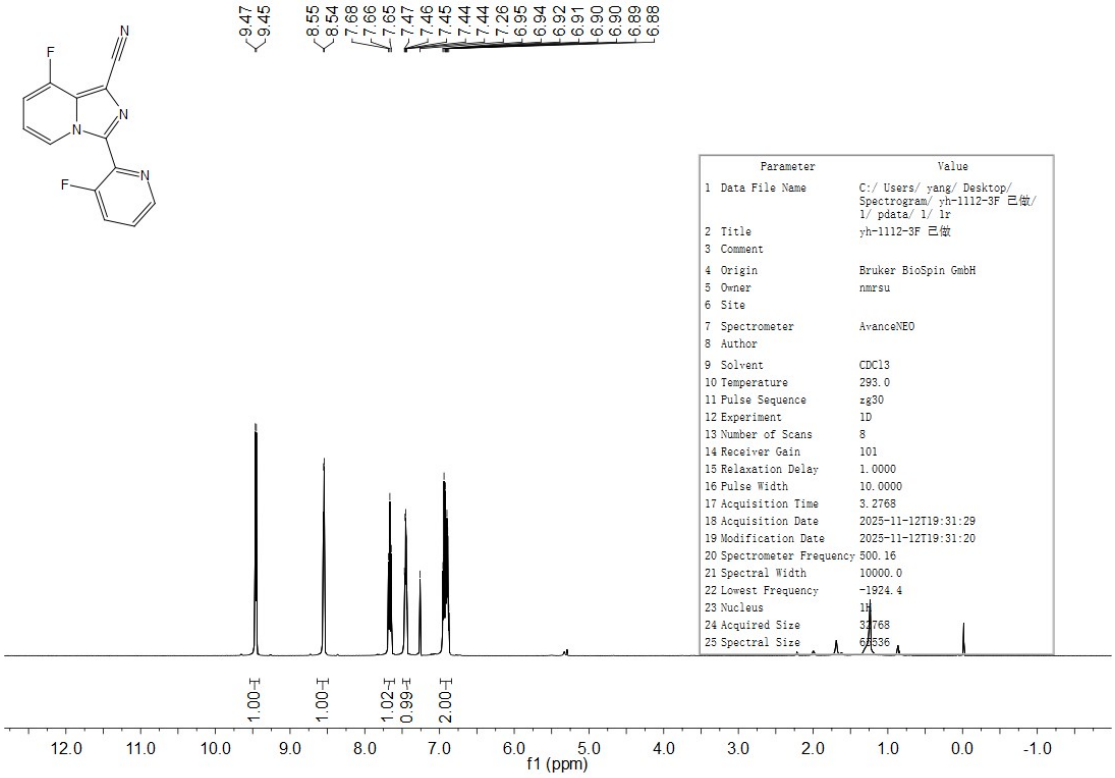


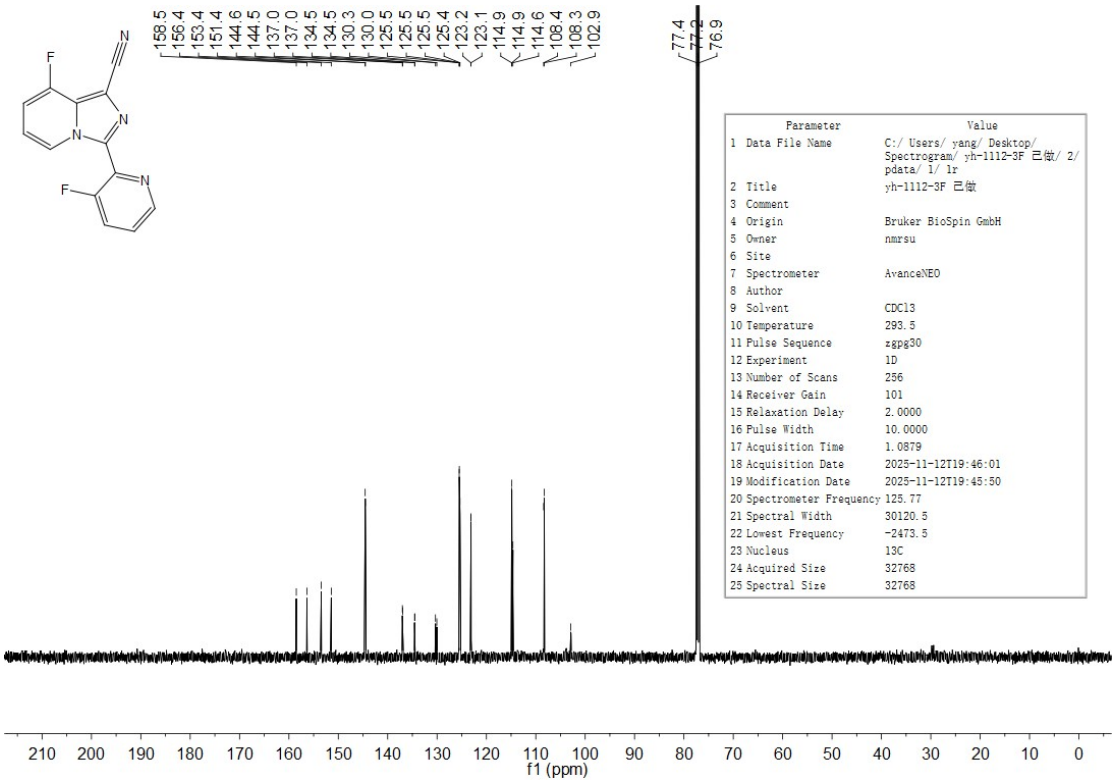

147.4
147.3
137.3
136.7
132.1
127.2
125.4
124.2
123.7
117.2
105.1
Cl
N
N
N
Cl
Parameter Value
1 Data File Name E:/ yh-5Cl-1218/ 1/ pdata/ 1/ 1r
2 Title yh-5Cl-1218
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 292.5
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 512
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2025-12-19T01:03:12
19 Modification Date 2025-12-19T01:01:34
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2468.4
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
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)

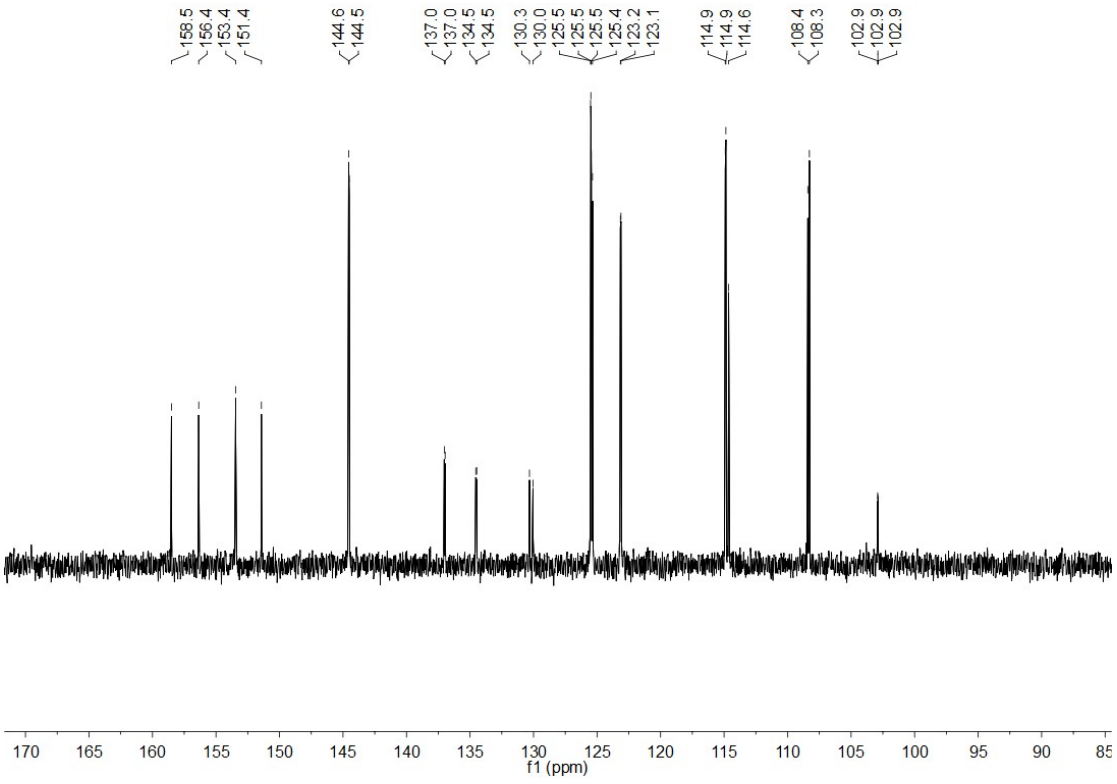

147.4
147.3
137.3
136.7
136.1
132.1
127.2
125.4
124.2
123.7
117.2
114.7
105.1
80 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80
f1 (ppm)

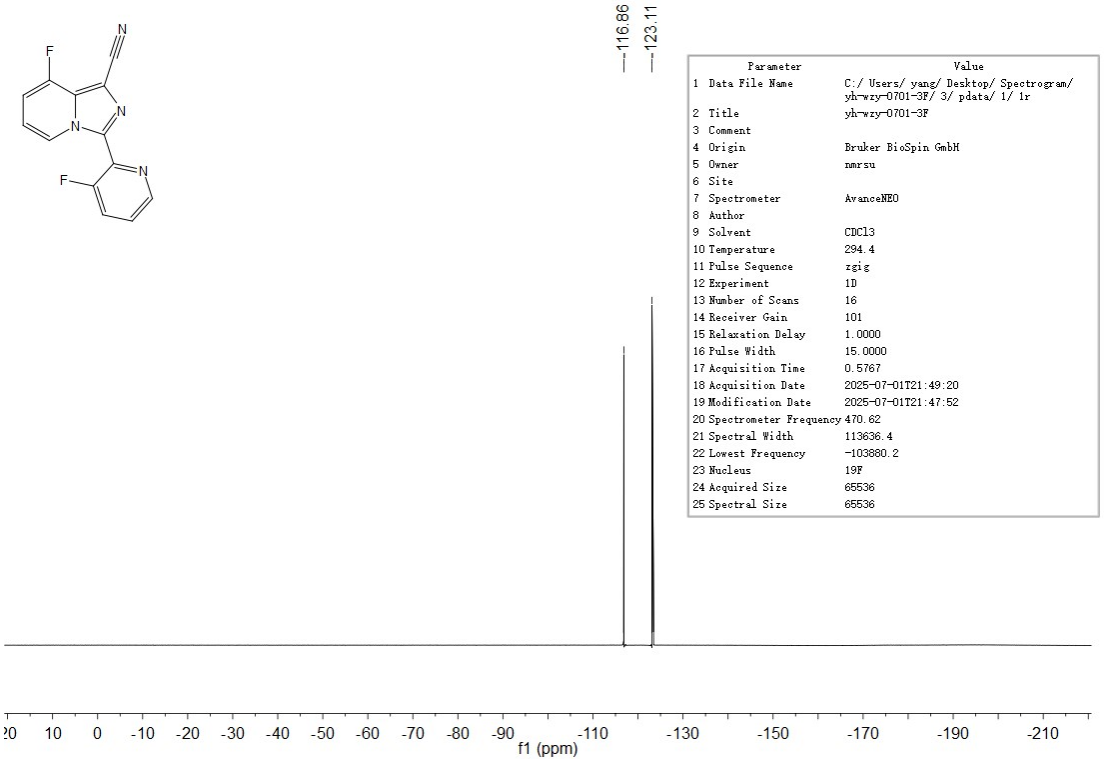


8-fluoro-3-(3-fluoropyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3m)

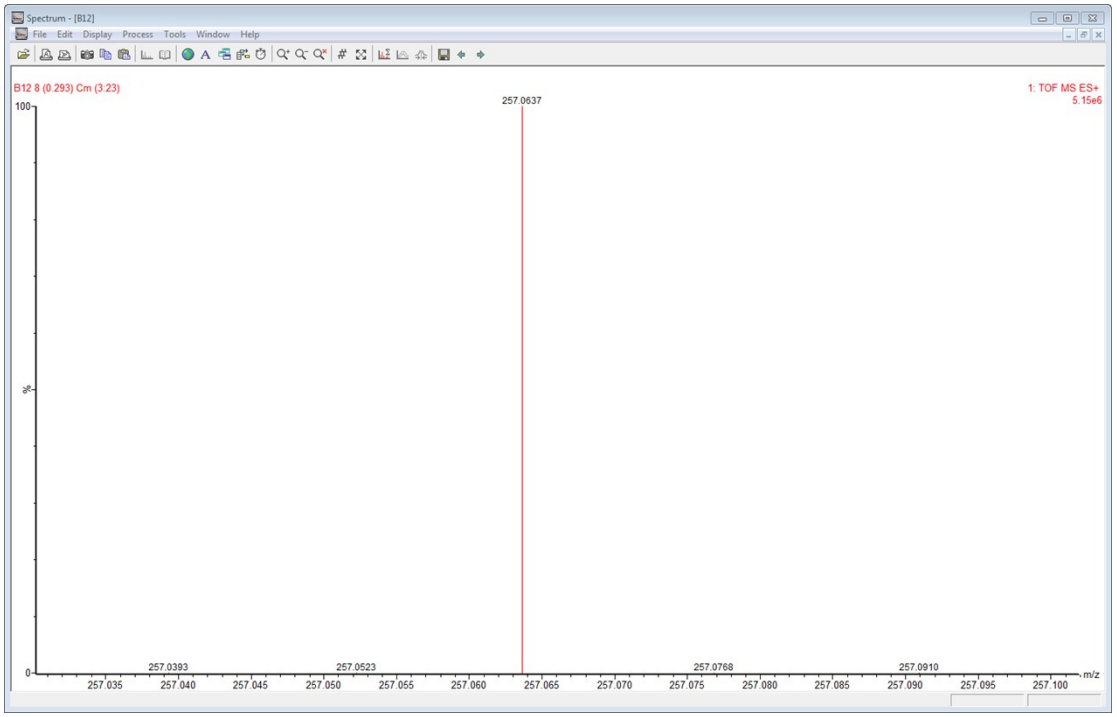



158.5
156.4
153.4
151.4
144.6
144.5
137.0
137.0
134.5
134.5
130.3
130.0
125.5
125.5
125.5
125.4
123.2
123.1
114.9
114.9
114.6
108.4
108.3
102.9
77.4
77.2
76.9
F
N
N
N
F
Parameter Value
1 Data File Name C:/ Users/ yang/ Desktop/ Spectrogram/ yh-1112-3F 已做/ 2/ pdata/ 1/ 1r
2 Title yh-1112-3F 已做
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 293.5
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2025-11-12T19:46:01
19 Modification Date 2025-11-12T19:45:50
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2473.5
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

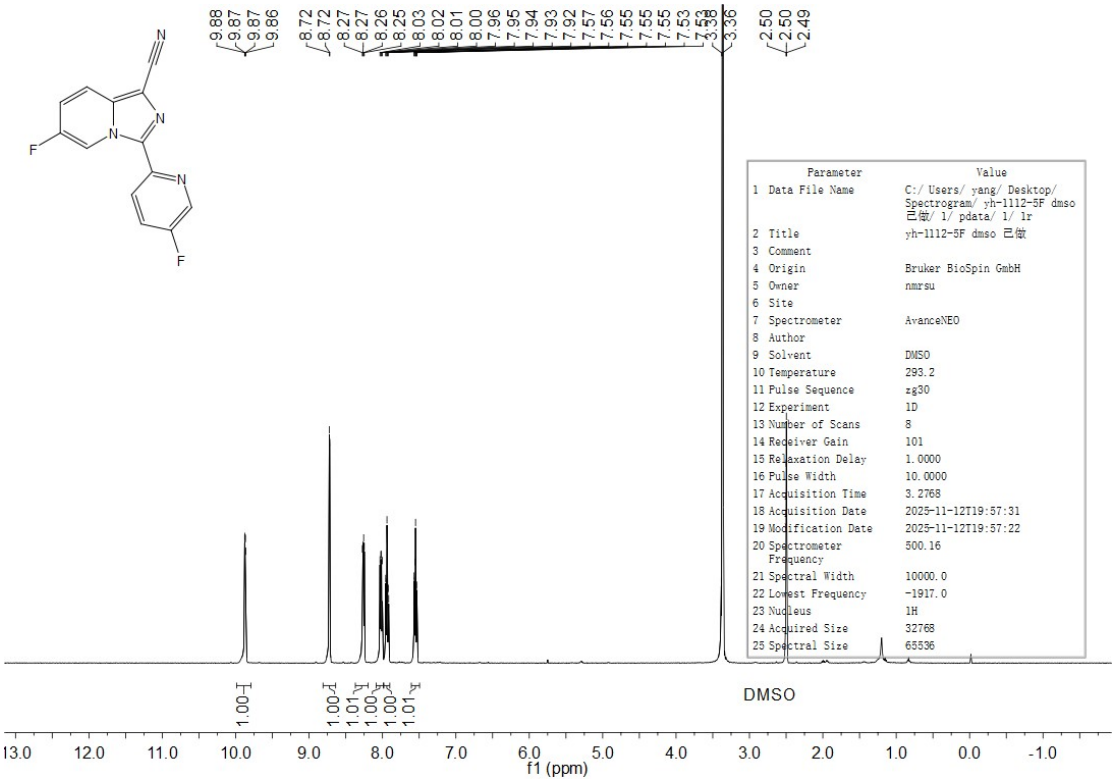

158.5
156.4
153.4
151.4
144.6
144.5
137.0
137.0
134.5
134.5
130.3
130.0
125.5
125.5
125.5
125.4
123.2
123.1
114.9
114.9
114.6
108.4
108.3
102.9
102.9
102.9
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85
f1 (ppm)



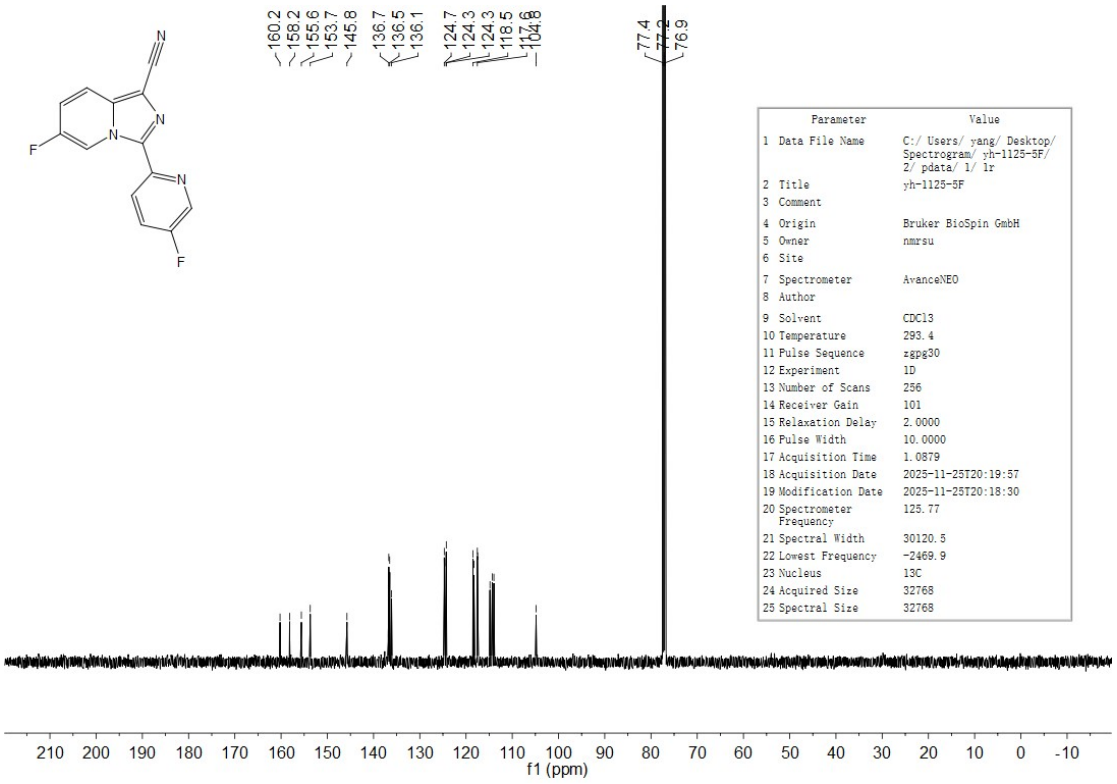
Parameter		Value
1	Data File Name	C:/ Users/ yang/ Desktop/ Spectrogram/ yh-wzy-0701-3F/ 3/ pdata/ 1/ 1r
2	Title	yh-wzy-0701-3F
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	294.4
11	Pulse Sequence	zgig
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	101
15	Relaxation Delay	1.0000
16	Pulse Width	15.0000
17	Acquisition Time	0.5767
18	Acquisition Date	2025-07-01T21:49:20
19	Modification Date	2025-07-01T21:47:52
20	Spectrometer Frequency	470.62
21	Spectral Width	113636.4
22	Lowest Frequency	-103880.2
23	Nucleus	19F
24	Acquired Size	65536
25	Spectral Size	65536



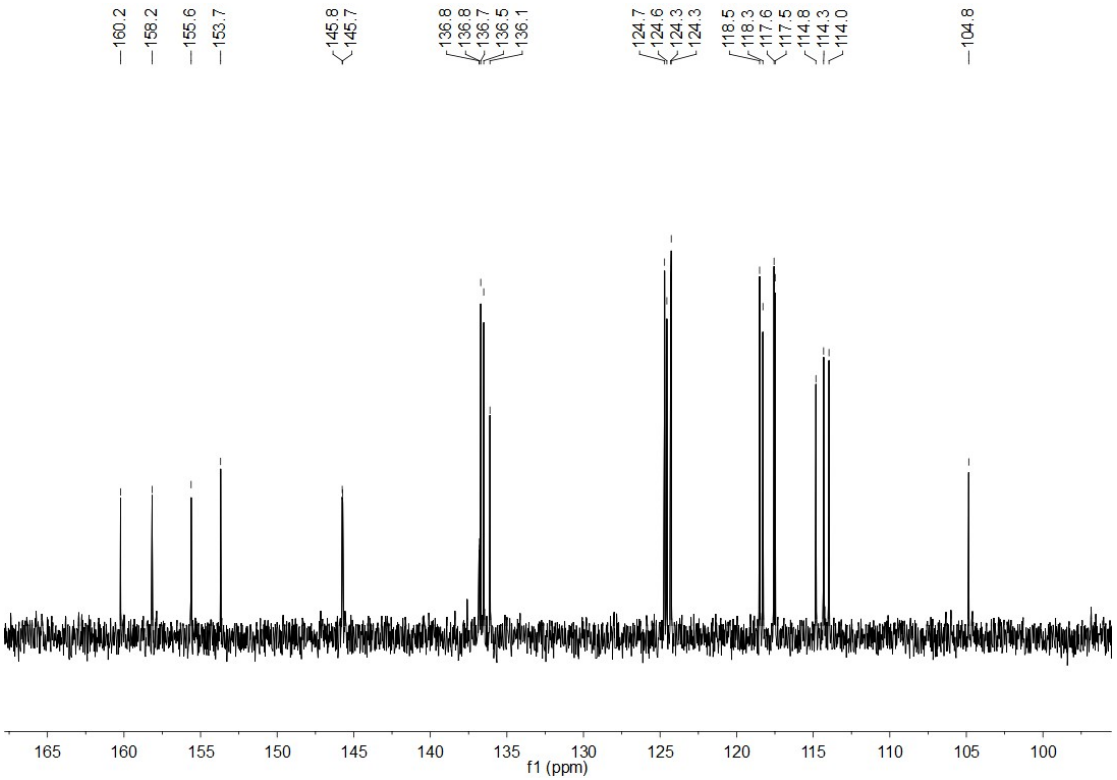
6-fluoro-3-(5-fluoropyridin-2-yl)imidazo[1,5-a]pyridine-1-carbonitrile (3n)

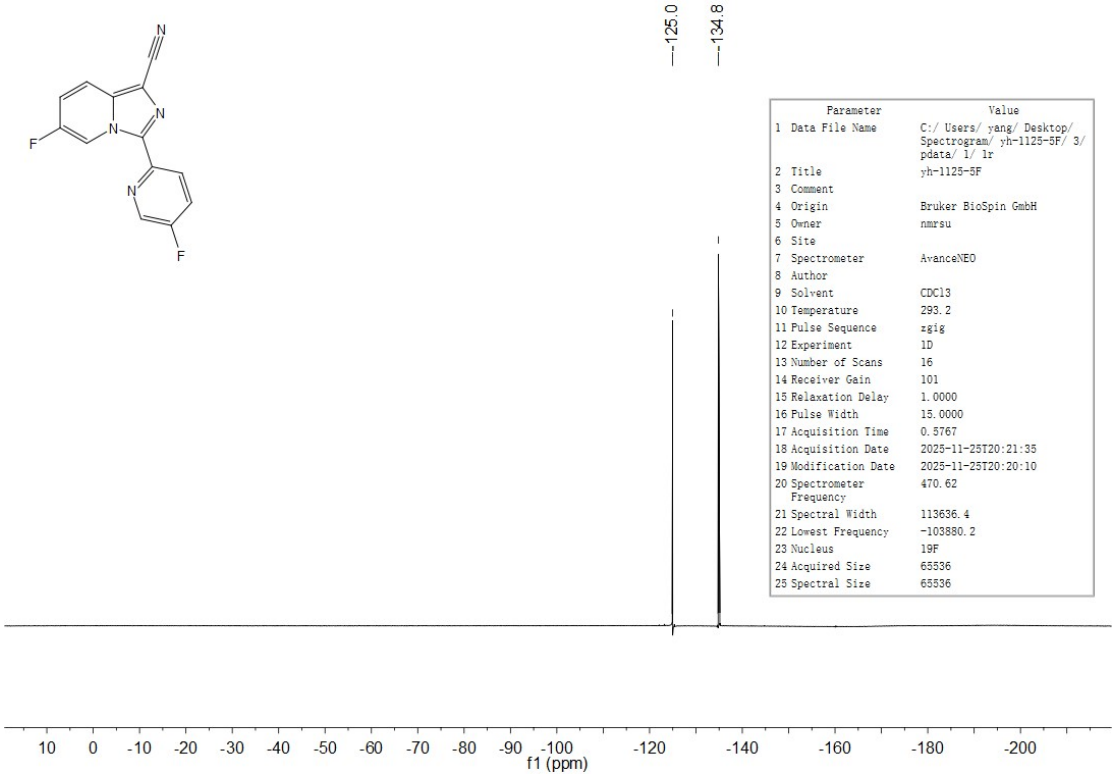


Parameter	Value
1 Data File Name	C:/ Users/ yang/ Desktop/ Spectrogram/ yh-1112-5F dmso 已做/ 1/ pdata/ 1/ 1r
2 Title	yh-1112-5F dmso 已做
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	DMSO
10 Temperature	293.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2025-11-12T19:57:31
19 Modification Date	2025-11-12T19:57:22
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1917.0
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

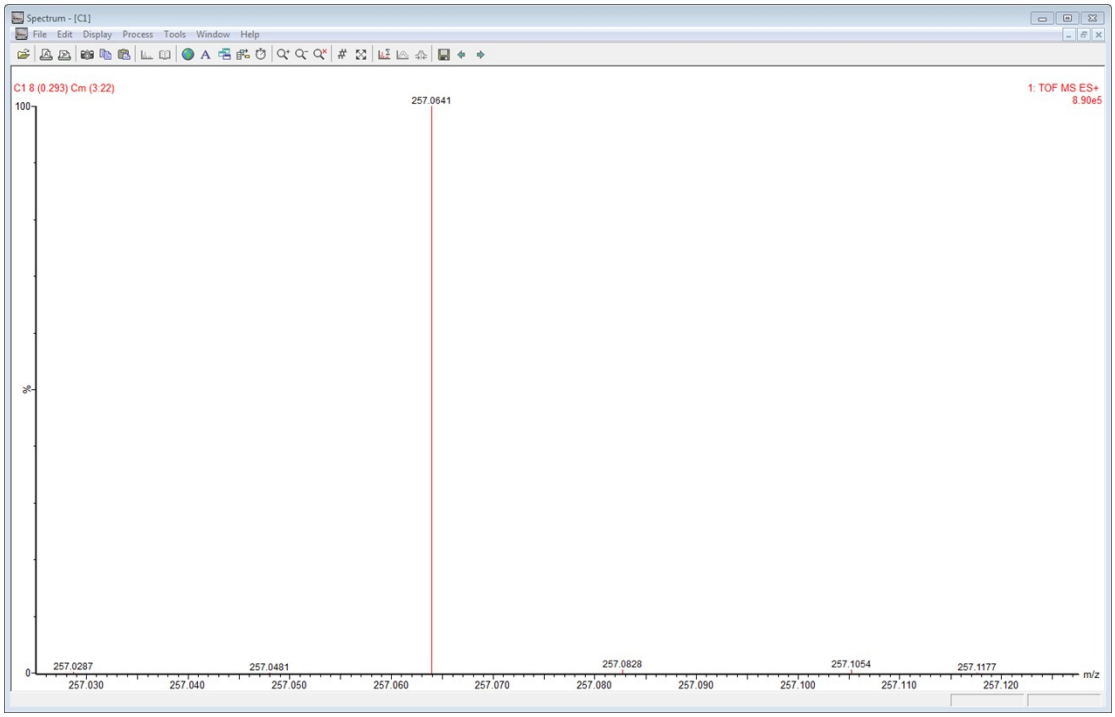


Parameter	Value
1 Data File Name	C:/ Users/ yang/ Desktop/ Spectrogram/ yh-1125-5F/ 2/ pdata/ 1/ 1r
2 Title	yh-1125-5F
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	293.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2025-11-25T20:19:57
19 Modification Date	2025-11-25T20:18:30
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2469.9
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768

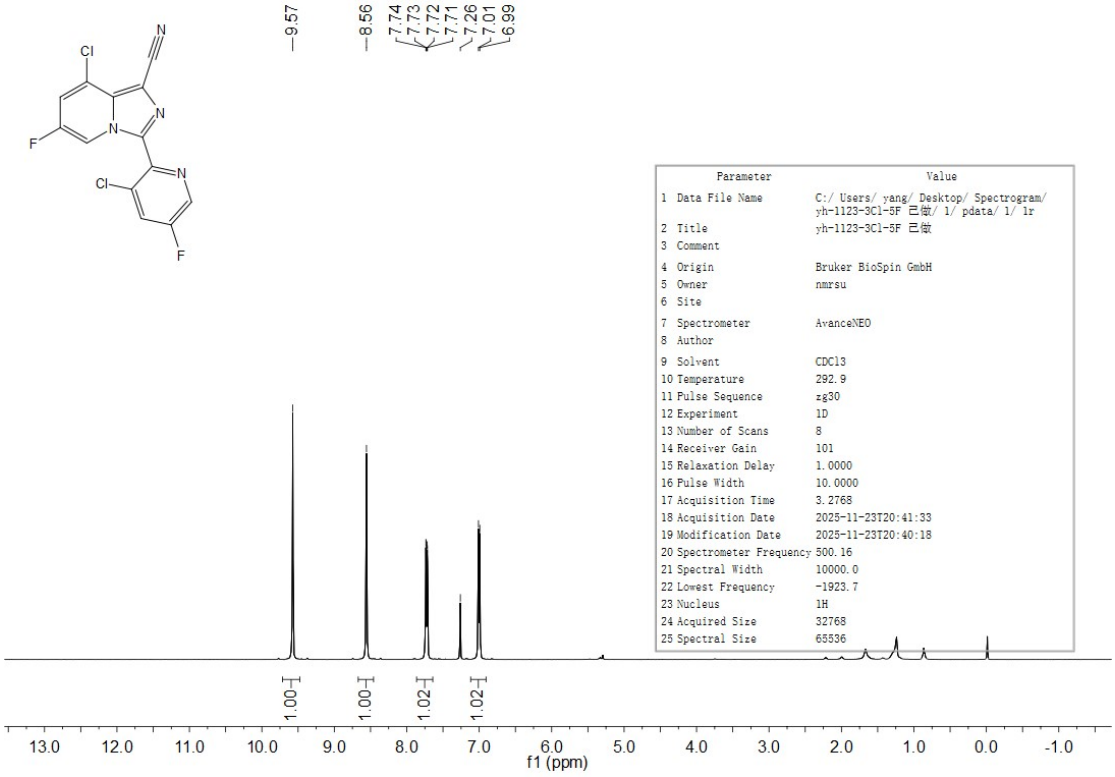


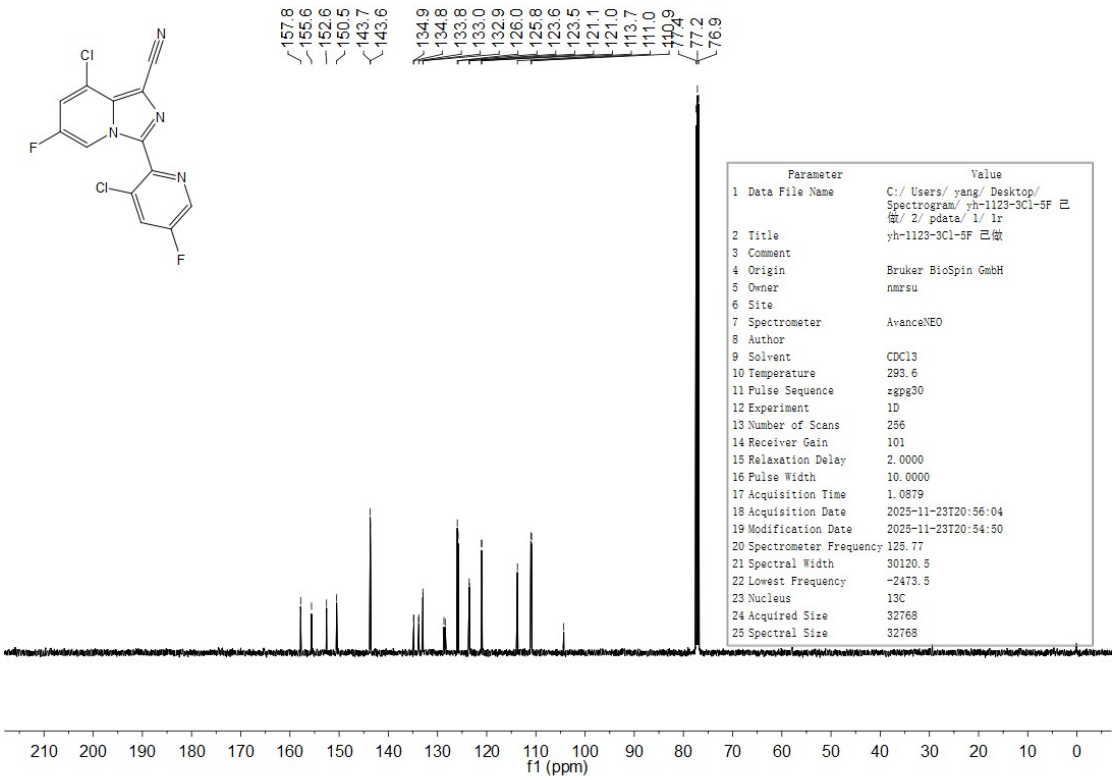


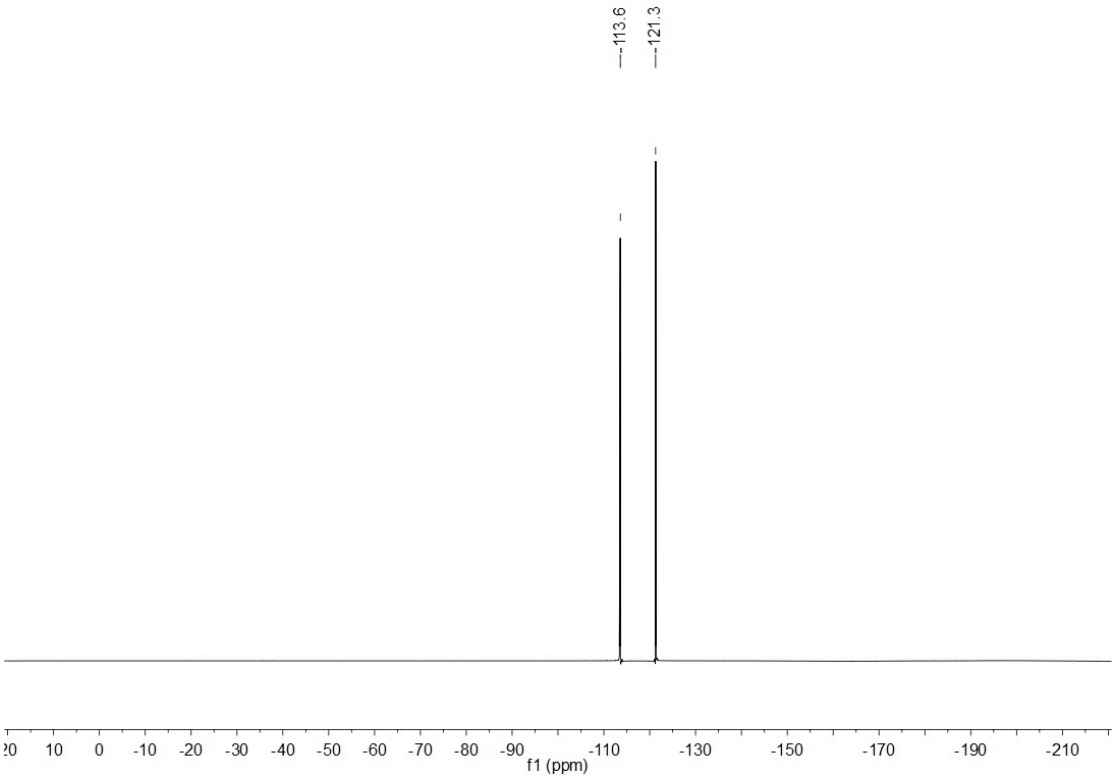
Parameter	Value
1 Data File Name	C:/ Users/ yang/ Desktop/ Spectrogram/ yh-1125-5F/ 3/ pdata/ 1/ 1r
2 Title	yh-1125-5F
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	293.2
11 Pulse Sequence	zgig
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	15.0000
17 Acquisition Time	0.5767
18 Acquisition Date	2025-11-25T20:21:35
19 Modification Date	2025-11-25T20:20:10
20 Spectrometer Frequency	470.62
21 Spectral Width	113636.4
22 Lowest Frequency	-103880.2
23 Nucleus	19F
24 Acquired Size	65536
25 Spectral Size	65536

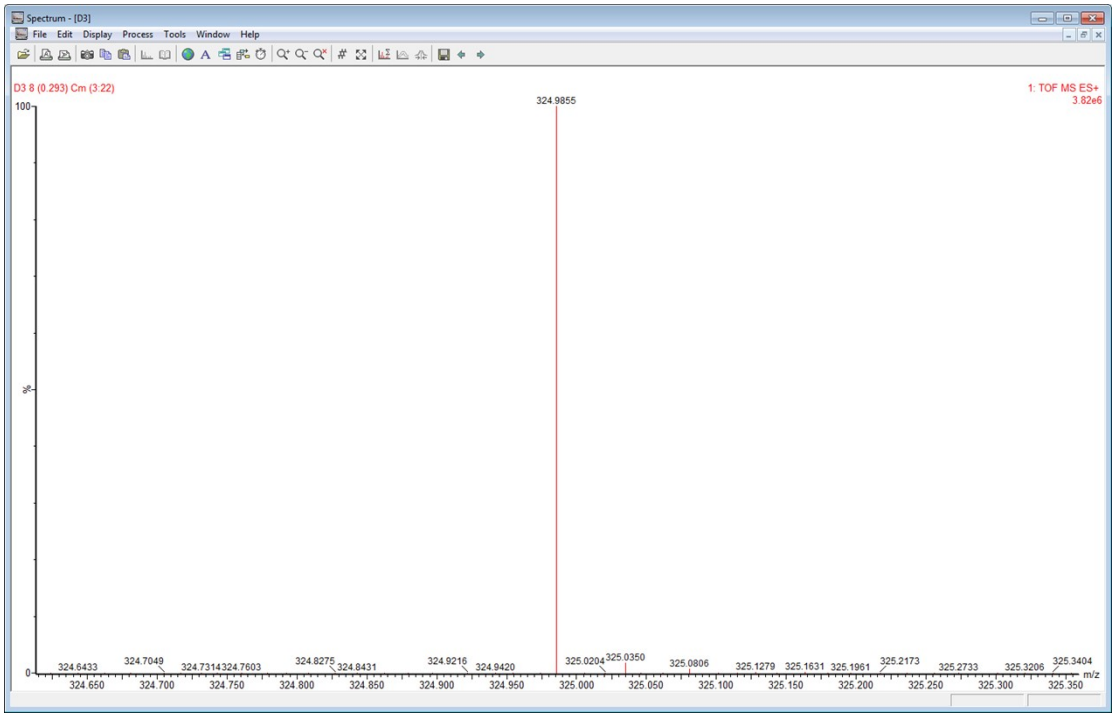


8-chloro-3-(3-chloro-5-fluoropyridin-2-yl)-6-fluoroimidazo[1,5-a]pyridine-1-carbonitrile (3o)

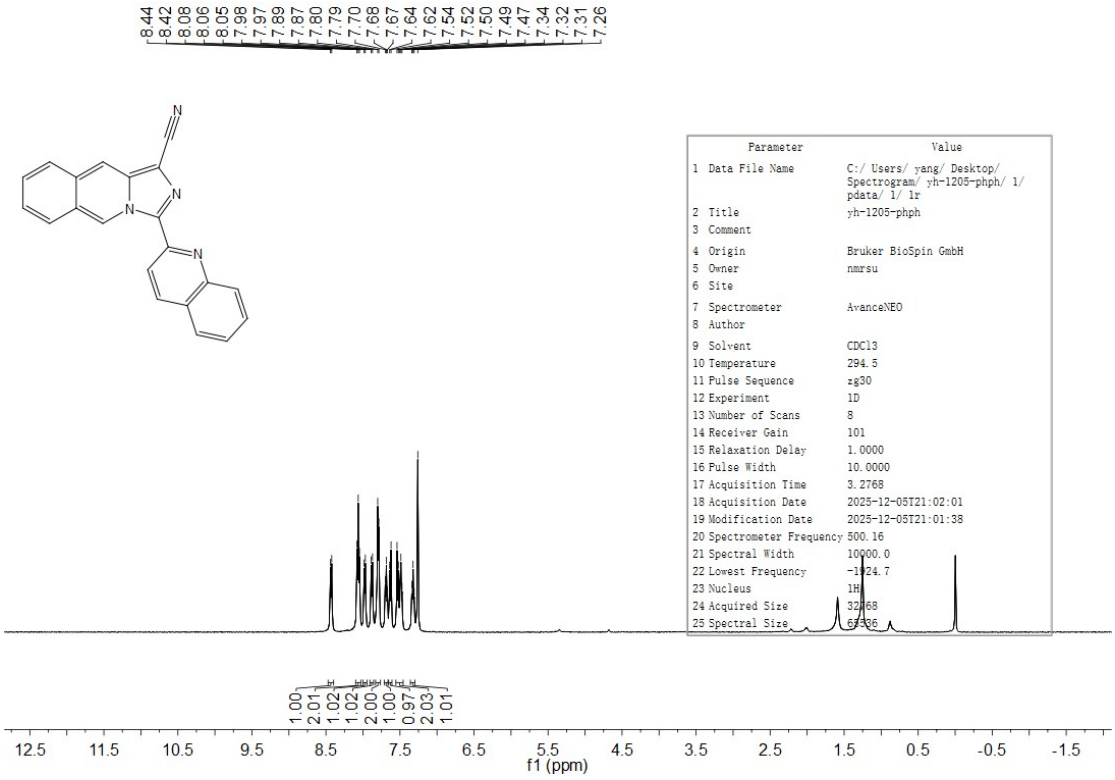


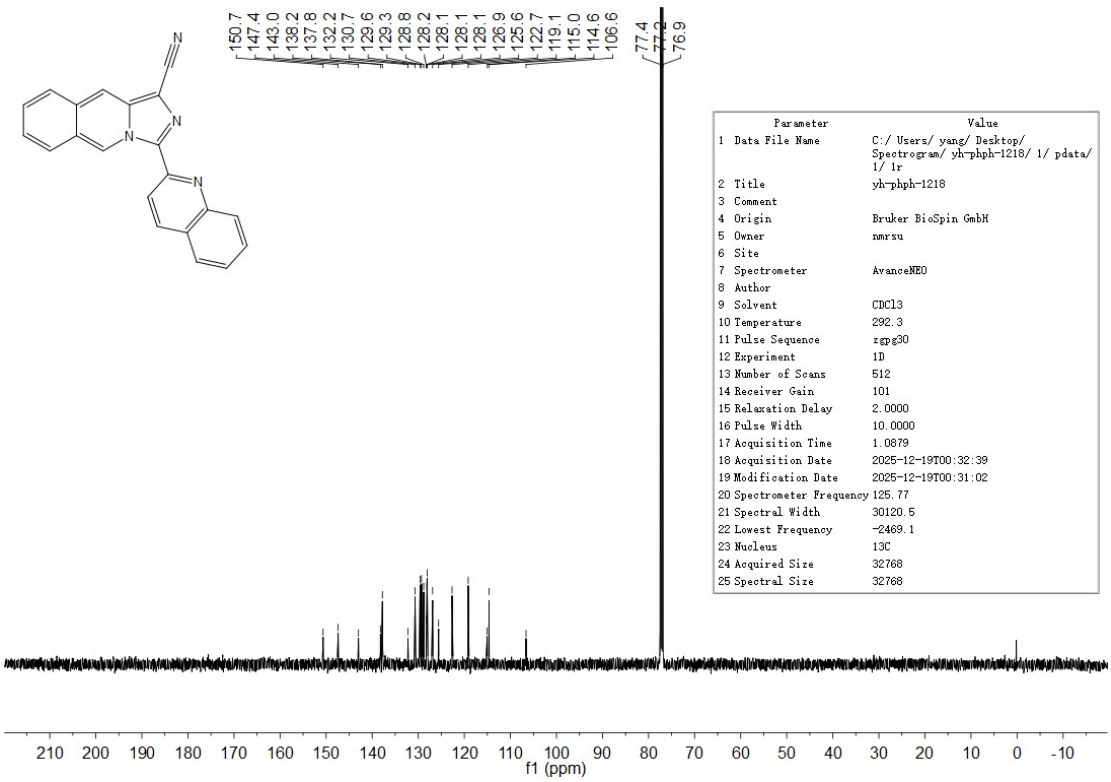

157.8
155.6
152.6
150.5
143.7
143.6
134.9
134.8
133.8
133.0
132.9
126.0
125.8
123.6
123.5
121.1
121.0
113.7
111.0
110.9
77.4
77.2
76.9
Cl
N
F
N
N
Cl
N
F
Parameter Value
1 Data File Name C:/ Users/ yang/ Desktop/ Spectrogram/ yh-1123-3Cl-5F 已做/ 2/ pdata/ 1/ 1r
2 Title yh-1123-3Cl-5F 已做
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 293.6
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2025-11-23T20:56:04
19 Modification Date 2025-11-23T20:54:50
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2473.5
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

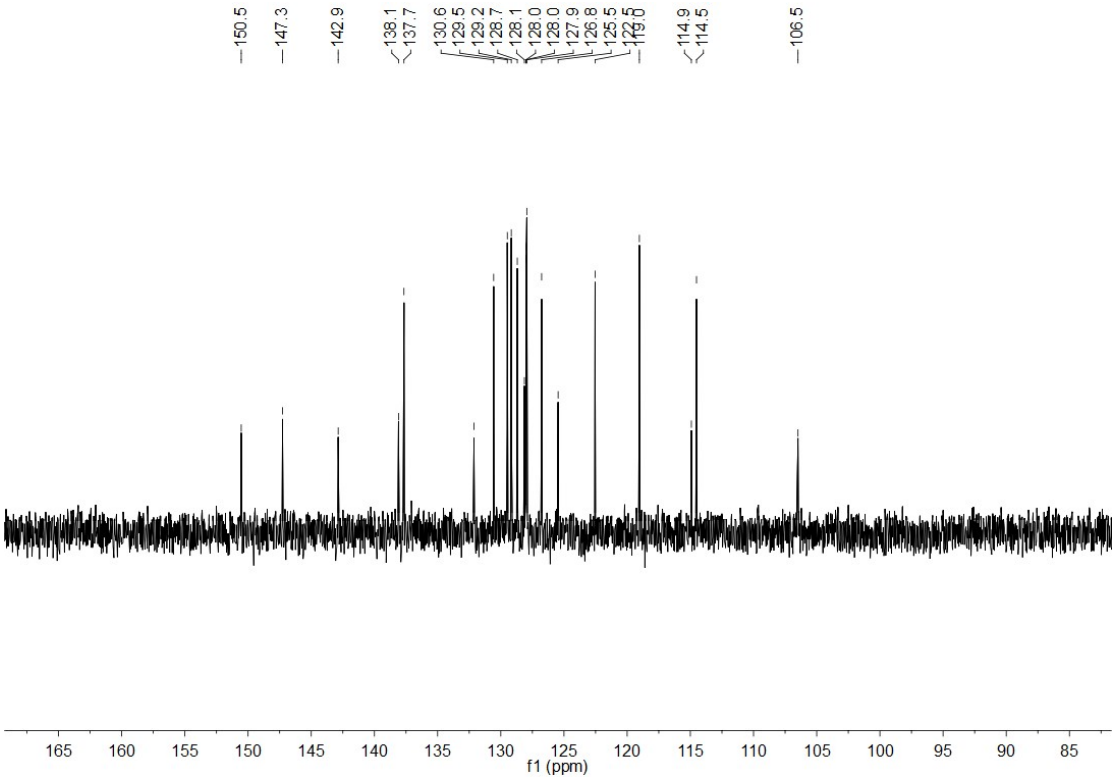

113.6
121.3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

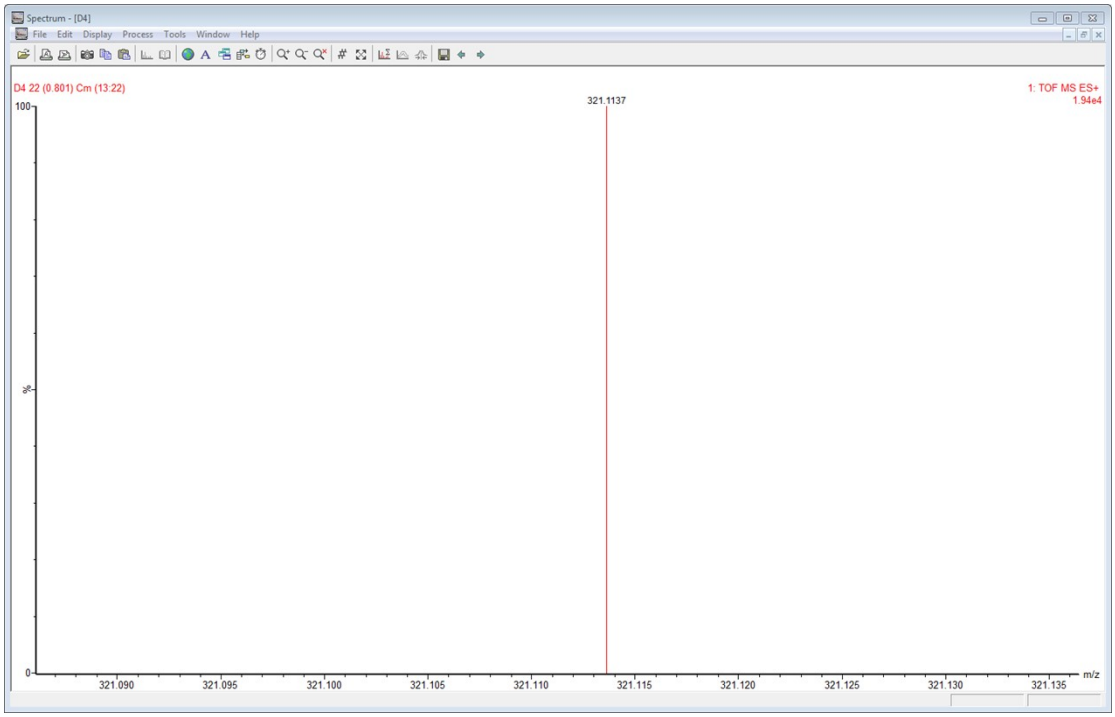


3-(quinolin-2-yl)imidazo[1,5-b]isoquinoline-1-carbonitrile (3p)

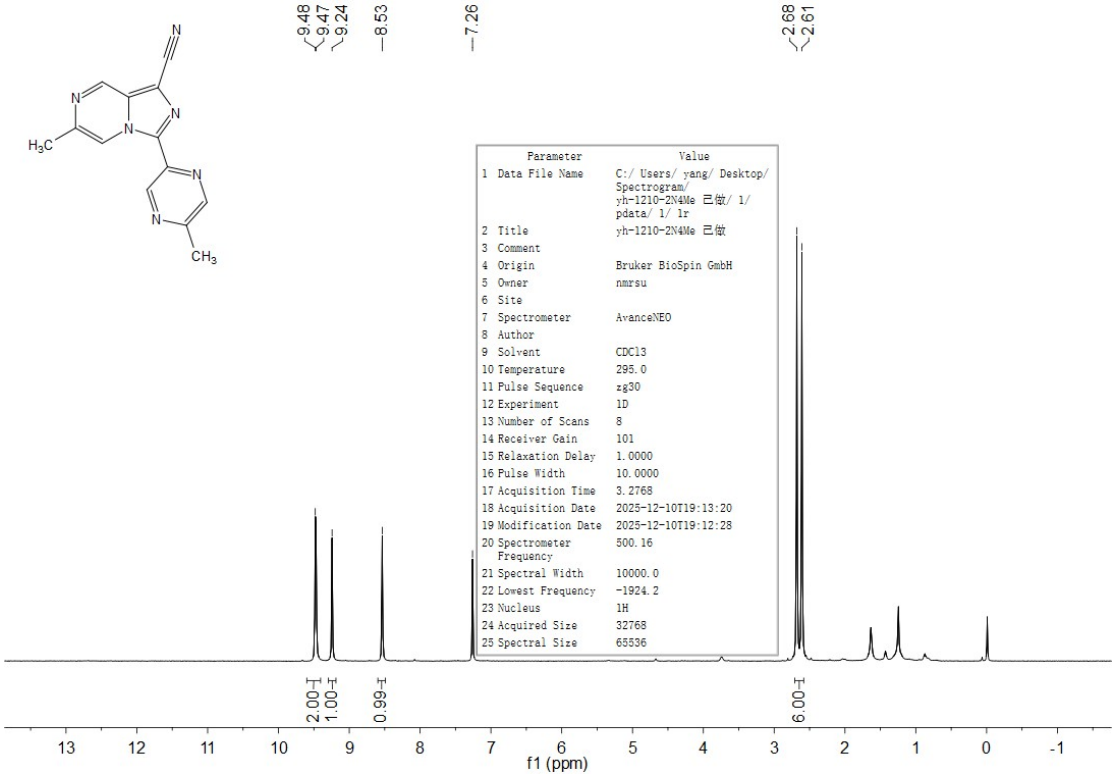


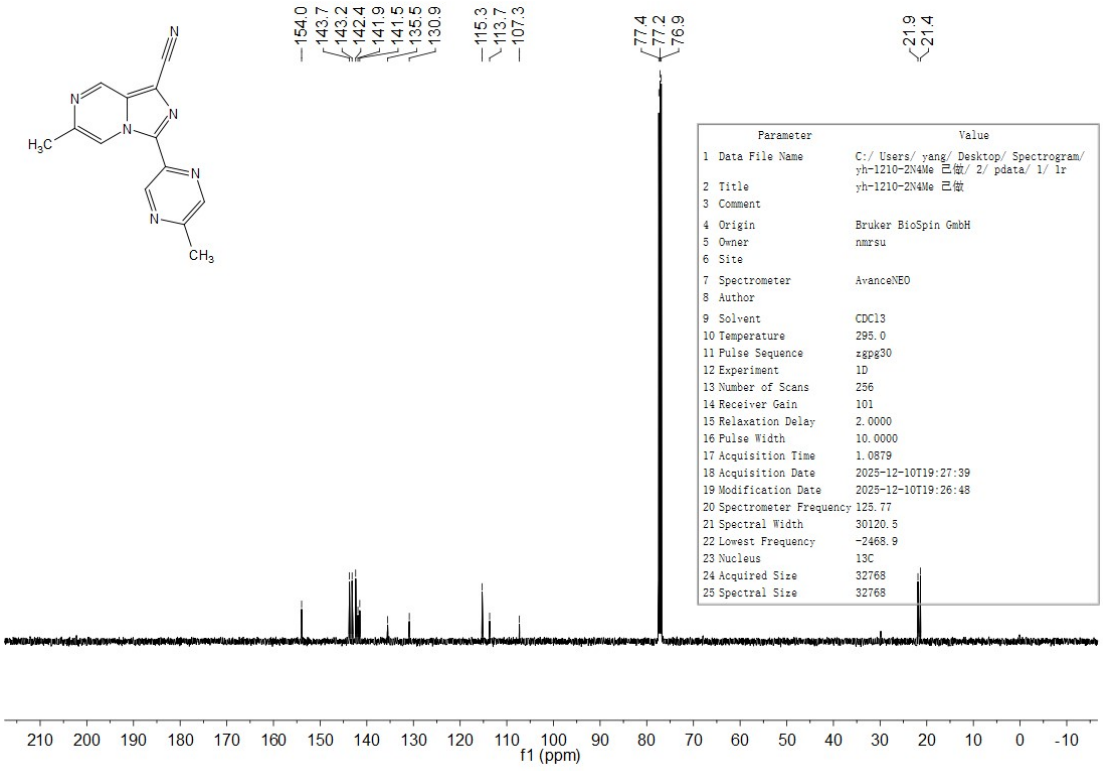

150.7
147.4
143.0
138.2
137.8
132.2
130.7
129.6
129.3
128.8
128.2
128.1
128.1
128.1
126.9
125.6
122.7
119.1
115.0
114.6
106.6
77.4
77.2
76.9
N
N
N
N
Parameter Value
1 Data File Name C:/ Users/ yang/ Desktop/ Spectrogram/ yh-phph-1218/ 1/ pdata/ 1/ 1r
2 Title yh-phph-1218
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 292.3
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 512
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2025-12-19T00:32:39
19 Modification Date 2025-12-19T00:31:02
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2469.1
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
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)

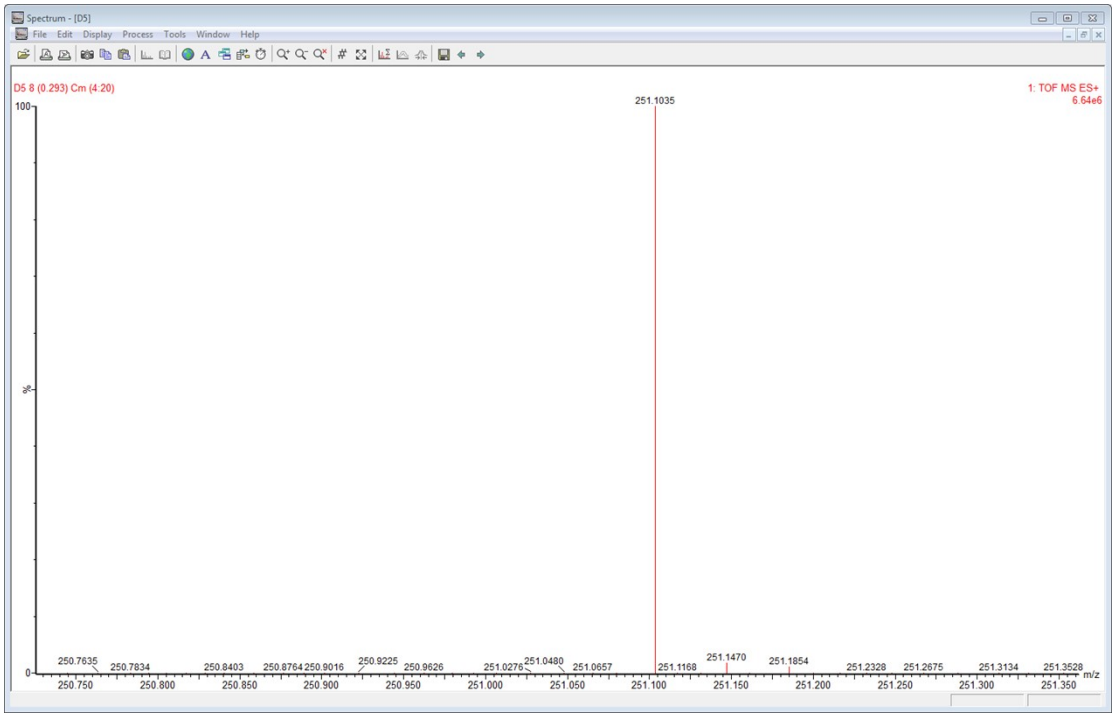

150.5
147.3
142.9
138.1
137.7
130.6
129.5
129.2
128.7
128.1
128.0
128.0
127.9
126.8
125.5
122.5
119.0
114.9
114.5
106.5
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85
f1 (ppm)



6-methyl-3-(5-methylpyrazin-2-yl)imidazo[1,5-a]pyrazine-1-carbonitrile (3q)




154.0
143.7
143.2
142.4
141.9
141.5
135.5
130.9
115.3
113.7
107.3
77.4
77.2
76.9
21.9
21.4
N
N
N
N
N
H3C
CH3
Parameter Value
1 Data File Name C:/ Users/ yang/ Desktop/ Spectrogram/ yh-1210-2N4Me 已做/ 2/ pdata/ 1/ 1r
2 Title yh-1210-2N4Me 已做
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 295.0
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2025-12-10T19:27:39
19 Modification Date 2025-12-10T19:26:48
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2468.9
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
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)


Spectrum - [D5]
File Edit Display Process Tools Window Help
D5 8 (0.293) Cm (4:20)
1: TOF MS ES+
6.64e6
251.1035
100
%
0
250.7635
250.7834
250.8403
250.8764
250.9016
250.9225
250.9626
251.0278
251.0480
251.0657
251.1168
251.1470
251.1854
251.2328
251.2675
251.3134
251.3528
m/z
250.750
250.800
250.850
250.900
250.950
251.000
251.050
251.100
251.150
251.200
251.250
251.300
251.350