Supporting Information

Switching between α-Alkenylation and α-Alkylation of Nitriles by Coupling Multiple Electrochemical Methods

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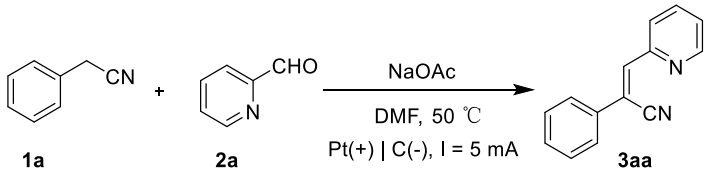
General Information

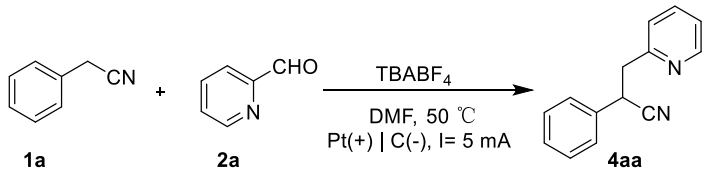
Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. NMR spectra were recorded on a Bruker AV-500 (1H: 500 MHz, 13C: 125 MHz, 19F NMR: 470 MHz) spectrometer using TMS as internal reference. Chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz, respectively. GC-MS was Shimadzu QP-5050 GC-MS system. Commercially available compounds were used without further purification. 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. Single crystal data was collected at room temperature on a Rigaku Oxford Diffraction SuperNova with an AtlasS2 CCD using Cu Kα radiation.

Experimental Procedure



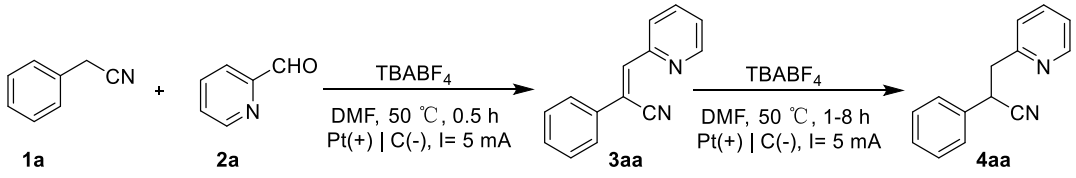
Scheme S1. Experimental procedure for **3aa**.

Typical synthesis steps of (*Z*)-2-phenyl-3-(pyridin-2-yl)acrylonitrile (3aa): A mixture of phenylacetonitrile (0.36 mmol), 2-picolinaldehyde (0.3 mmol), NaOAc (0.6 mmol) and DMF = 5mL were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for corresponding time. When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered. 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 S2. Experimental procedure for **4aa**.

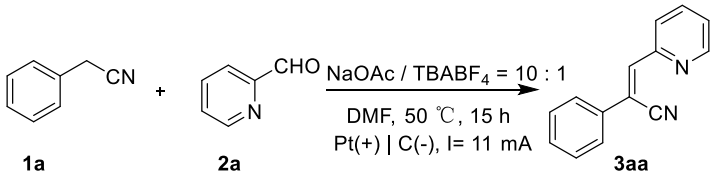
Typical synthesis of 2-phenyl-3-(pyridin-2-yl)propanenitrile (4aa): A mixture of phenylacetonitrile (0.36 mmol), 2-picolinaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol) and DMF = 5mL were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for corresponding time. When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 4:1) to afford the desired product.



Scheme S3. The ratio of **3aa** generating **4aa** with the time extension

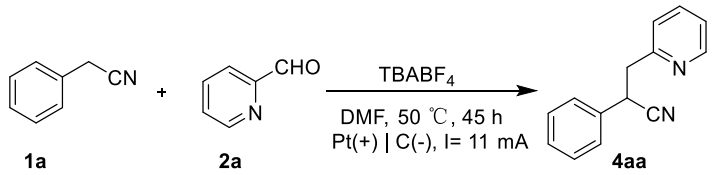
A mixture of phenylacetonitrile (0.36 mmol), 2-picolinaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol) and DMF = 5mL were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for corresponding time (1, 2, 3, 4, 5, 6, 7, 8h). When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The

residue was purified by column chromatography on silica gel (PE/EtOAc = 4:1) to afford the desired product.



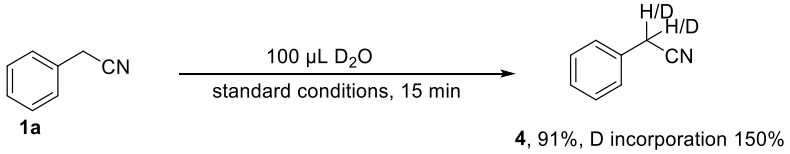
Scheme S4. Experimental procedure of gram scale for **3aa**.

Gram-scale synthesis of (*Z*)-2-phenyl-3-(pyridin-2-yl)acrylonitrile (3aa): A mixture of phenylacetonitrile (6 mmol), 2-picolinaldehyde (5 mmol), NaOAc (10 mmol)，$TBABF_4$ (1 mmol) and DMF = 85mL were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 11 mA under 50℃ for 15 h. When the reaction was finished, the solution was extracted with EtOAc (3×100 mL). The combined organic layer was dried with Na_2SO_4, filtered. 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.



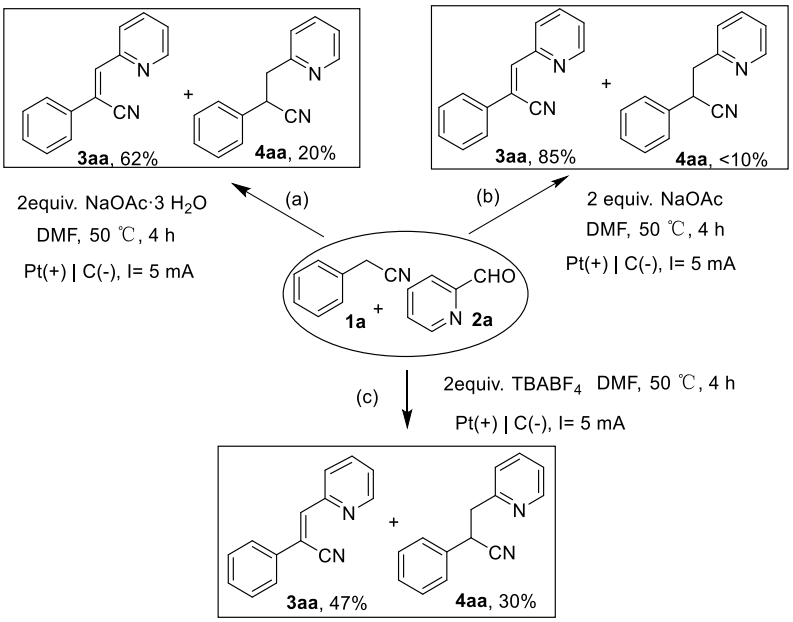
Scheme S5. Experimental procedure of gram scale for **4aa**.

Gram-scale synthesis of 2-phenyl-3-(pyridin-2-yl)propanenitrile (4aa): A mixture of phenylacetonitrile (6 mmol), 2-picolinaldehyde (5 mmol), $TBABF_4$ (5 mmol) and DMF = 85mL were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 11 mA under 50℃ for 45 h. When the reaction was finished, the solution was extracted with EtOAc (3×100 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 4:1) to afford the desired product.



Scheme S6. Deuterium exchange experiment.

A mixture of phenylacetonitrile (0.3 mmol), $TBABF_4$ (0.3 mmol), D_2O (100μL) and DMF (5mL) were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for 0.25h. **4** was isolated in 91% yield with 150% D-incorporation at α-position of cyano group as revealed by ^{1}H NMR.

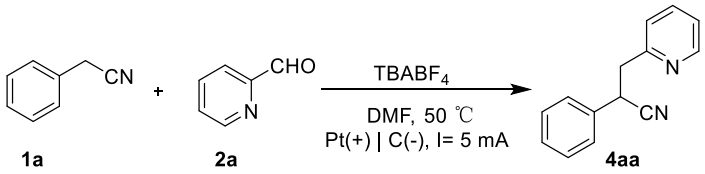


Scheme S7. The electrolytes effect on the reaction.

A mixture of phenylacetonitrile (0.36 mmol), 2-picolinaldehyde (0.3 mmol), $TBABF_4$ or NaOAc or $NaOAc·3H_2O$ (0.6 mmol) and DMF = 5mL were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for 4h. When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 4:1) to afford the desired product.

Optimization of Reaction Conditions

Table S1. Optimization of reaction conditions for α-alkylation of nitriles.[a]

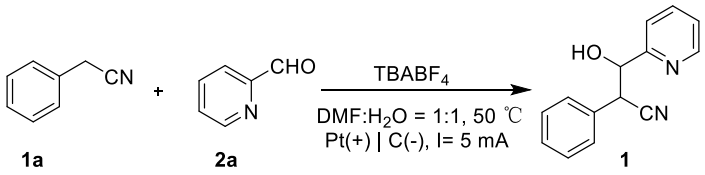


1a 2a 4aa

Entry	Variations from standard conditions	Yields [b]
1	None [a]	89%
2	KNO_3 + 5μL H_2O instead of $TBABF_4$	82%
3	*n*-Bu_4NPF_6 as electrolyte	77%
4	Me_4NI as electrolyte	n.d.[c]
5	DMSO as solvent	25%
6	CH_3CN as solvent	trace
7	DABCO (1 equiv.) as additive	61%
8	Pt-Pt	69%
9	10 mA	65%
10	no electricity	n.d.[c]

[a] Reaction conditions: **1a** (0.36 mmol), **2a** (0.3mmol), $TBABF_4$ (0.3 mmol), DMF (5.0 mL), 5 mA, 50 °C, undivided cell. [b] isolated yield. [c] not detected. The reaction time was determined by TLC and GC-MS.

Preparation of intermediate 1



Scheme S8. Experimental procedure for **1**.

Typical synthesis of 3-hydroxy-2-phenyl-3-(pyridin-2-yl)propanenitrile (1): A mixture of phenylacetonitrile (3.6 mmol), 2-picolinaldehyde (3 mmol), $TBABF_4$ (3 mmol) and DMF:H_2O （25mL:25mL） were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for corresponding time. When the reaction was finished, the solution was extracted with EtOAc (3×50 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 3:1) to afford the desired product.

Crystal data of 1

Recrystallization solvent: chloroform; Method for crystal growth: the crystal was prepared from the solution of **1** in chloroform. Dissolved 20 mg **1** with 1 mL of chloroform and volatilized slowly at 25℃ for 15 days. (CCDC : 2425206)

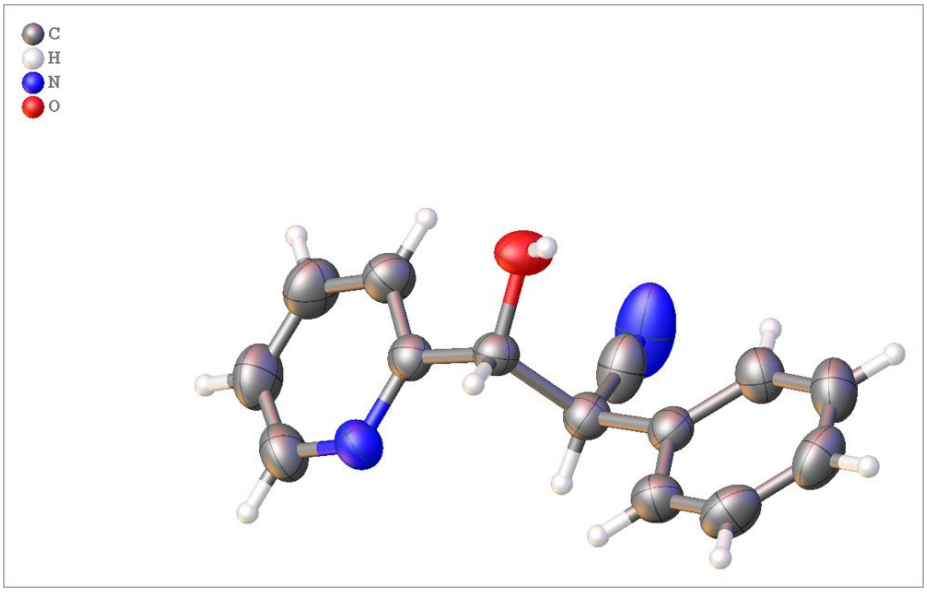


Figure S1. Crystal structure for **1**.

Table S2. Crystal data and structure refinement for LK-2-EA_aut**o.**

Identification code	LK-2-EA_auto
Empirical formula	$C_{14}H_{12}N_2O$
Formula weight	224.26

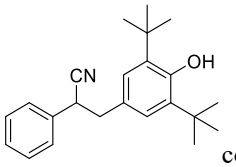
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.0084(3)
b/Å	8.7513(2)
c/Å	15.7194(4)
α/°	90
β/°	99.743(3)
γ/°	90
Volume/Å^3	1221.37(6)
Z	4
ρ_{calc}g/cm^3	1.220
μ/mm^{-1}	0.628
F(000)	472.0
Crystal size/mm^3	0.22 × 0.19 × 0.18
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.962 to 145.774
Index ranges	$-10 \leq h \leq 10$, $-3 \leq k \leq 10$, $-19 \leq l \leq 19$
Reflections collected	4213
Independent reflections	2345 [R_{int} = 0.0166, R_{sigma} = 0.0199]
Data/restraints/parameters	2345/0/156
Goodness-of-fit on F^2	1.061
Final R indexes [I>=2σ (I)]	R_1 = 0.0382, wR_2 = 0.0948
Final R indexes [all data]	R_1 = 0.0495, wR_2 = 0.1025
Largest diff. peak/hole / e Å^{-3}	0.16/-0.11

Mechanistic Studies

(1) BHT capturing the radicals in the reaction to afford 2.

A mixture of phenylacetonitrile (0.36 mmol), 2-picolinaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol), butylated hydroxytoluene (BHT, 0.6 mmol) and DMF （5 mL） were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for corresponding time.

HRMS (ESI) *m/z*: calcd for $C_{23}H_{29}NO[M+H]^+$ 336.2322, found 336.2331.



compound **2**

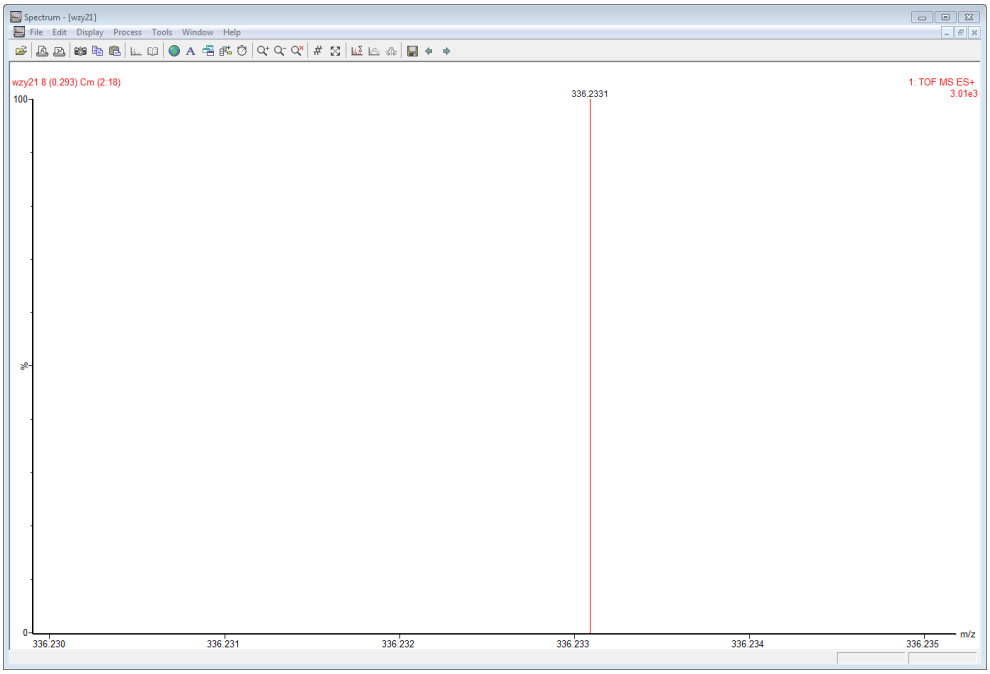
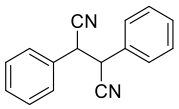


Figure S2. HRMS for **2**.

(2) The self-coupling product of 1a to afford 1aa.

A mixture of phenylacetonitrile (0.36 mmol), 2-picolinaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol), butylated hydroxytoluene (BHT, 0.6 mmol) and DMF （5 mL） were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for corresponding time.

HRMS (ESI) *m/z*: calcd for $C_{16}H_{12}N_2[M+H]^+$ 233.1073, found 233.1074.



compound **1aa**

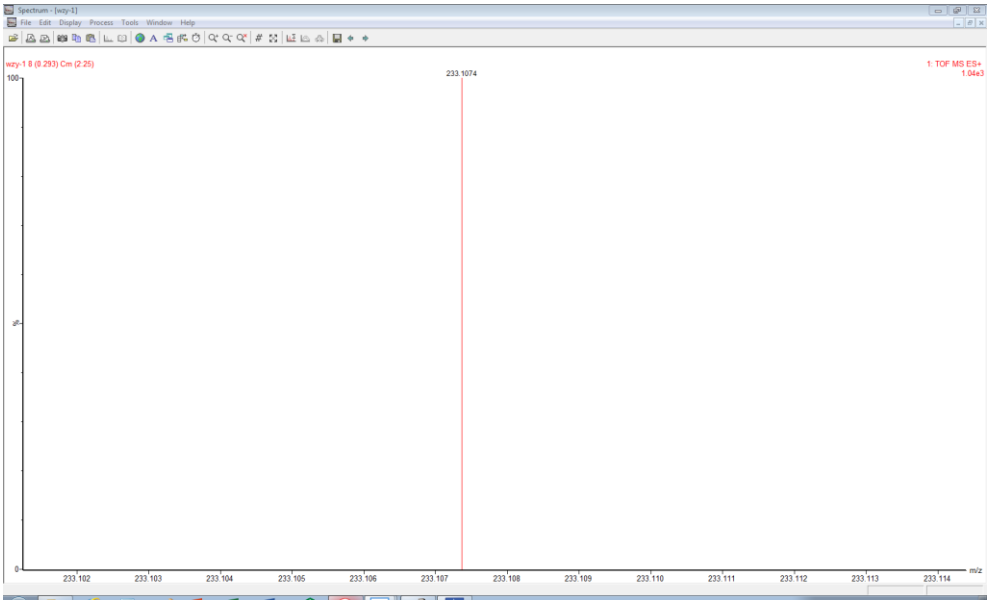
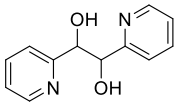


Figure S3. HRMS for **1aa**.

(3) The self-coupling product of 2a to afford 2aa..

A mixture of phenylacetonitrile (0.36 mmol), 2-picolinaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol), butylated hydroxytoluene (BHT, 0.6 mmol) and DMF （5 mL） were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50°C for corresponding time.

HRMS (ESI) *m/z*: calcd for $C_{12}H_{12}N_2O_2[M+H]^+$ 217.0972, found 217.0978.



compound **2aa**

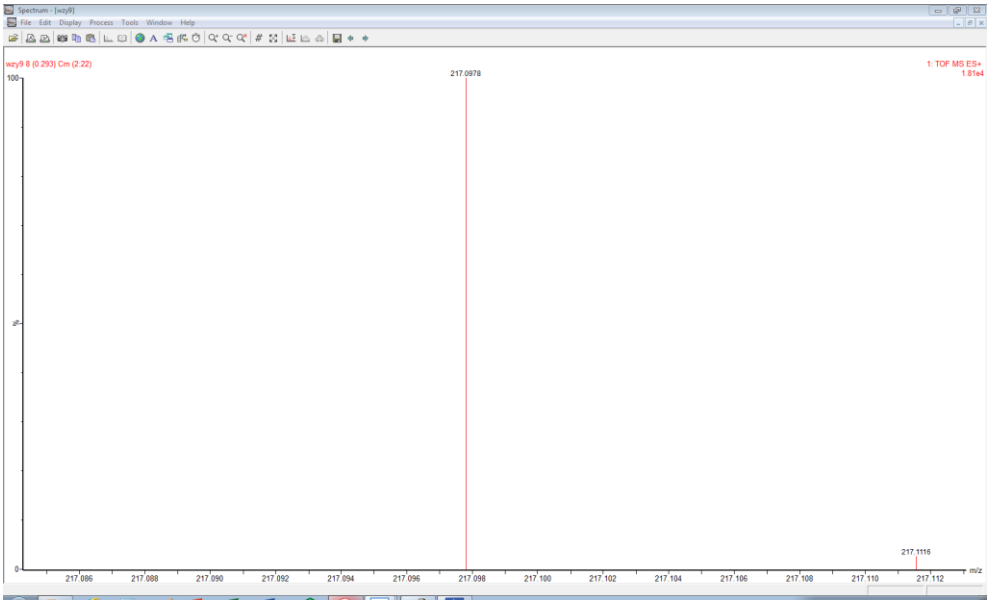
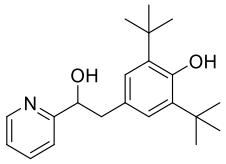


Figure S4. HRMS for **2aa**.

(4) BHT capturing the radicals in the reaction to afford 3.

A mixture of phenylacetonitrile (0.36 mmol), 2-picolinaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol), butylated hydroxytoluene (BHT, 0.6 mmol) and DMF （5 mL） were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for corresponding time.

HRMS (ESI) *m/z*: calcd for $C_{21}H_{29}NO_2[M+H]^+$ 328.2271, found 328.2276.



compound **3**

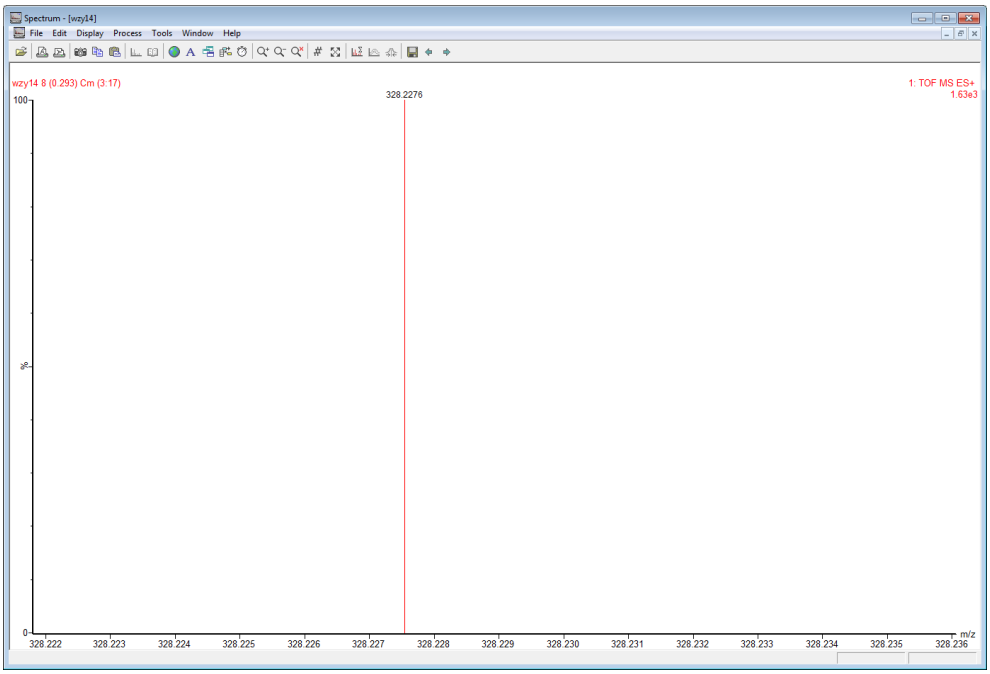


Figure S5. HRMS for **3**.

(5) The ration of 3aa generating 4aa with the time extension

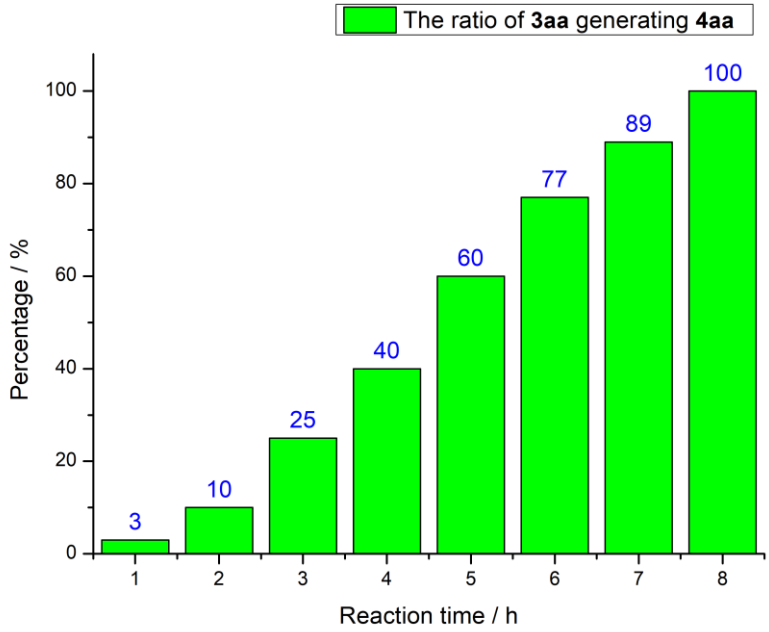


Figure S6. The ration of **3aa** generating **4aa**.

(6) Deuterium exchange of phenylacetonitrile to give D-incorporation product 4.

A mixture of phenylacetonitrile (0.3 mmol), $TBABF_4$ (0.3 mmol), D_2O (100μL) and DMF (5mL) were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for 0.25h. **4** was isolated in 91% yield with 150% D-incorporation at *α* position of cyano group as revealed by ^1H NMR.

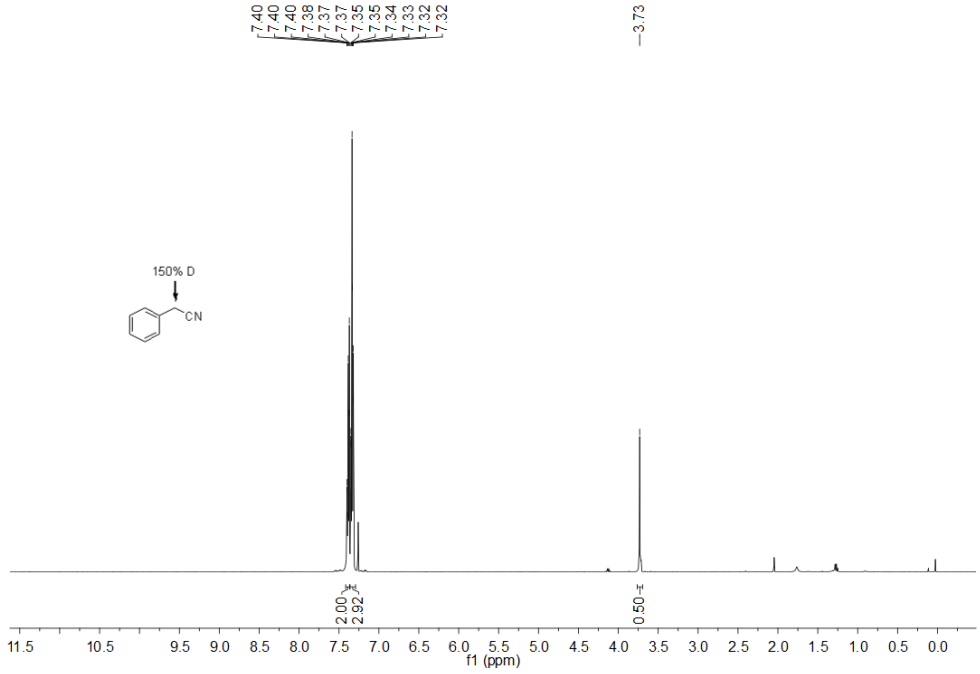
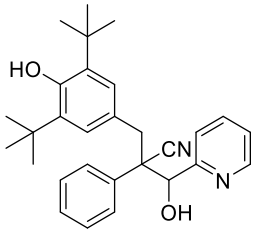


Figure S7. ^{1}H NMR of **4.**

(7) BHT capturing the radical from 1 to afford 5

A mixture of **1** (0.3 mmol), $TBABF_4$ (0.3 mmol), butylated hydroxytoluene (BHT, 0.6 mmol) and DMF = 5mL were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for 0.25h.

HRMS (ESI) *m/z*: calcd for $C_{29}H_{34}N_2O_2[M+H]^+$ 443.2693, found 443.2701.



compound **5**

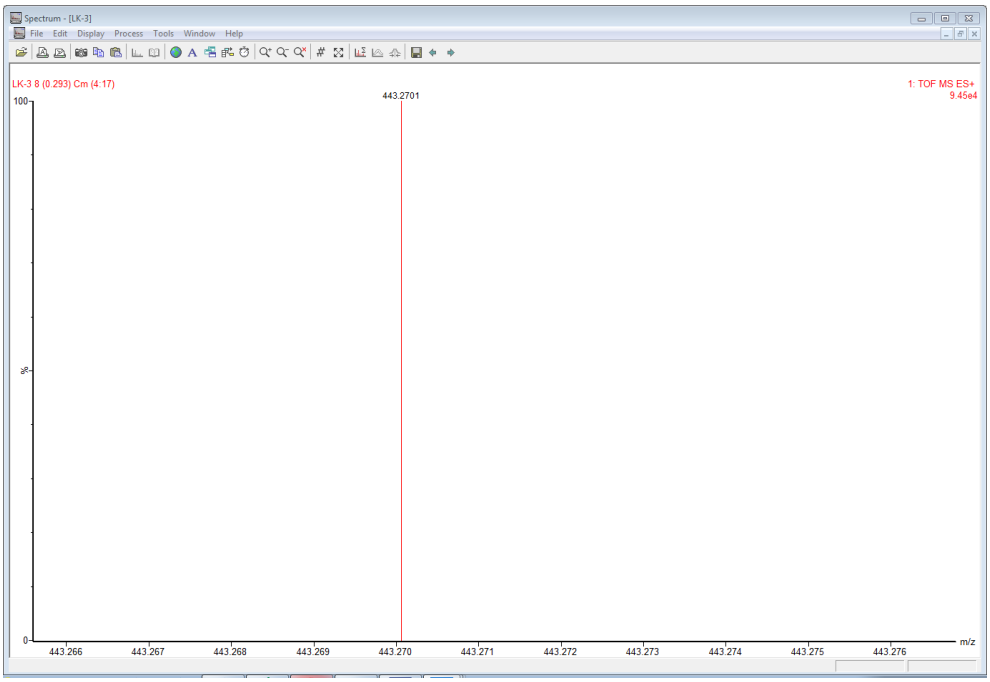


Figure S8. HRMS of **5.**

(8) The Deuterium exchange of 6 to afford 7 (2-phenylpropanenitrile).

A mixture of 2-phenylpropanenitrile (0.3 mmol), $TBABF_4$ (0.3 mmol), D_2O (100μL) and DMF = 5mL were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for 0.5h. **7** was isolated in 95% yield with 58% D-incorporation at α position of cyano group as revealed by ^{1}H NMR.

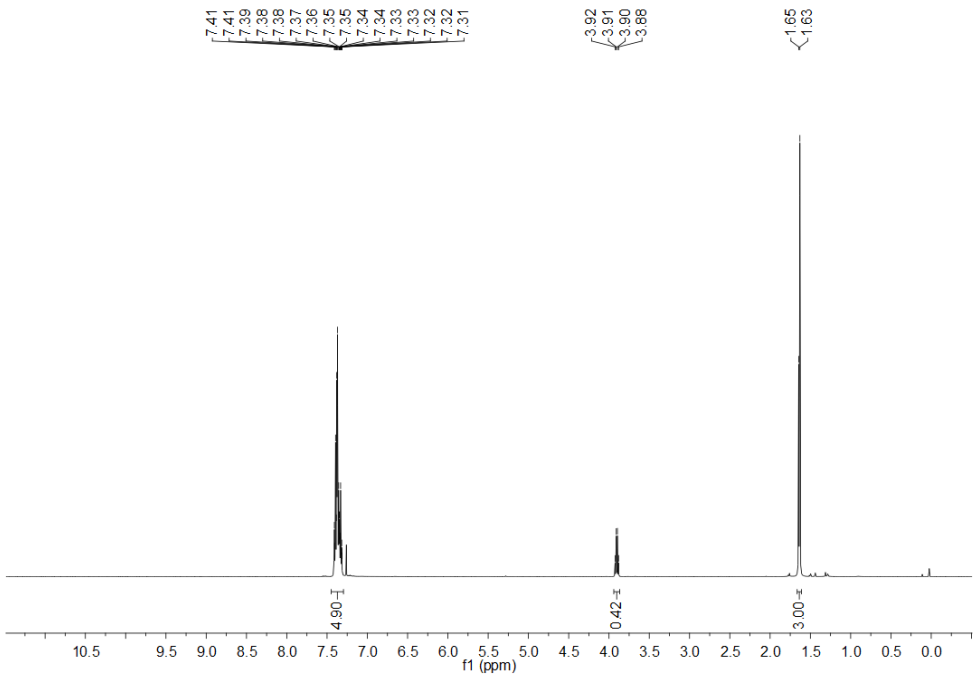


Figure S9. ^{1}H NMR of **7.**

(9) Deuterium incorporation of 3aa to afford 8.

A mixture of phenylacetonitrile (0.36 mmol), 2-picolinaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol), D_2O (100μL) and DMF = 5mL were added to an undivided electrolytic cell under N_2 atmosphere. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for corresponding time. **8** was isolated in 20% yield with 86% D-incorporation at *α*-position and 75% D-incorporation at *β*-position of cyano group as revealed by ^{1}H NMR.

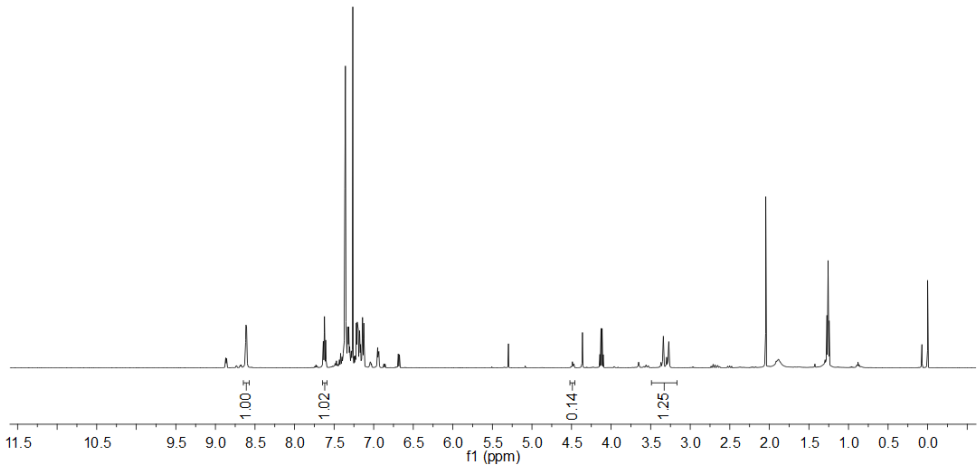


Figure S10. ^{1}H NMR of **8.**

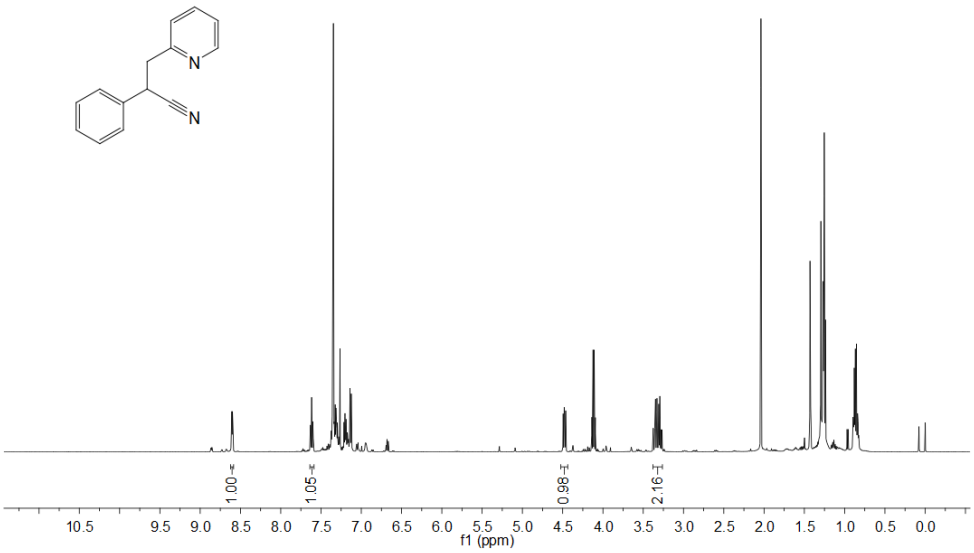
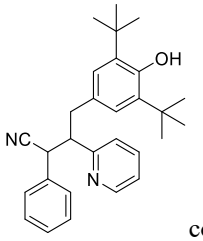


Figure S11. ^{1}H NMR of **3aa.**

(10) The BHT capturing the radial in the reduction of 3aa to afford 10.

A mixture of **3aa** (0.3 mmol), $TBABF_4$ (0.3 mmol), butylated hydroxytoluene (BHT, 0.6 mmol) and DMF (5mL) were added to an undivided electrolytic cell. The electrolytic cell was equipped with a platinum electrode as anode and a carbon electrode as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA under 50℃ for 1h.

HRMS (ESI) *m/z*: calcd for $C_{29}H_{34}N_2O_2[M+H]^+$ 427.2744, found 427.2750.



compound **10**

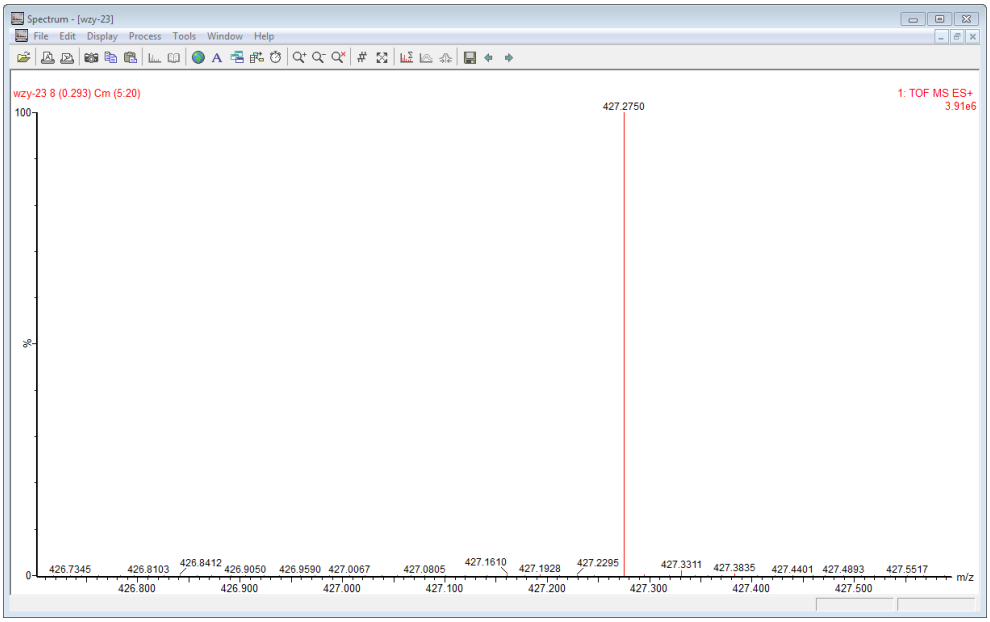
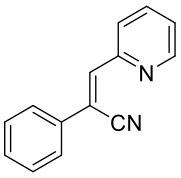
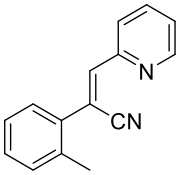


Figure S12. HRMS of **10.**

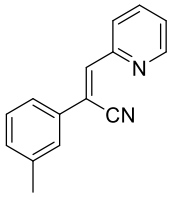
Detail Descriptions for Products



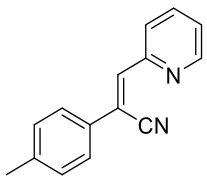
(*Z*)-2-phenyl-3-(pyridin-2-yl)acrylonitrile (3aa) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 95% yield, 58.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.75 (d, *J* = 4.6 Hz, 1H), 7.94 (d, *J* = 7.9 Hz, 1H), 7.79 (td, *J* = 7.8, 1.7 Hz, 1H), 7.77 – 7.72 (m, 2H), 7.65 (s, 1H), 7.47 – 7.40 (m, 3H), 7.32-7.29 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.2, 150.1, 141.1, 136.9, 134.1, 129.9, 129.2, 126.4, 124.4, 124.2, 117.5, 115.0.



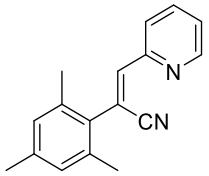
(*Z*)-3-(pyridin-2-yl)-2-(o-tolyl)acrylonitrile (3ba) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 58% yield, 38.3mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.76 (d, *J* = 4.3 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.81 (td, *J* = 7.7, 1.8 Hz, 1H), 7.37 – 7.31 (m, 3H), 7.28 (s, 1H), 7.26 (d, *J* = 4.2 Hz, 2H), 2.51 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.0, 150.0, 145.8, 136.9, 136.3, 135.1, 131.0, 129.5, 129.4, 126.6, 124.5, 124.0, 117.5, 114.8, 20.2.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_2[M+H]^+$ 221.1073, found 221.1077.



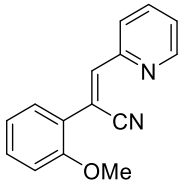
(*Z*)-3-(pyridin-2-yl)-2-(m-tolyl)acrylonitrile (3ca) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 58% yield, 60.7mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 4.6 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.76 (td, *J* = 7.8, 1.7 Hz, 1H), 7.61 (s, 1H), 7.54 (s, 1H), 7.53 (d, *J* = 8.3 Hz, 1H), 7.34 – 7.27 (m, 2H), 7.21 (d, *J* = 7.5 Hz, 1H), 2.39 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.2, 149.9, 140.7, 138.9, 136.7, 133.9, 130.6, 129.0, 127.0, 124.2, 124.1, 123.4, 117.5, 114.8, 21.4.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_2[M+H]^+$ 221.1073, found 221.1084.



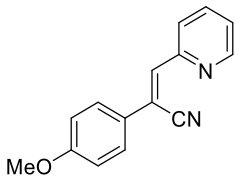
(*Z*)-3-(pyridin-2-yl)-2-(p-tolyl)acrylonitrile (3da) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a yellow solid. 94% yield, 62.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 4.2 Hz, 1H), 7.92 (d, *J* = 7.9 Hz, 1H), 7.78 (td, *J* = 7.8, 1.5 Hz, 1H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.60 (s, 1H), 7.29 (dd, *J* = 7.1, 5.1 Hz, 1H), 7.25 (d, *J* = 8.0 Hz, 2H), 2.39 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.4, 150.0, 140.2, 140.0, 136.8, 131.2, 129.9, 126.3, 124.1, 124.0, 117.6, 114.9, 21.3.



2-mesityl-3-(pyridin-2-yl)acrylonitrile (3ea, *Z*: *E*= 5: 2) 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 colorless oil. 27% yield, 20.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.76 (d, *J* = 3.0 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.80 (td, *J* = 7.8, 1.7 Hz, 1H), 7.33 (dd, *J* = 6.9, 4.9 Hz, 1H), 7.06 (s, 1H), 6.94 (s, 2H), 2.34 (s, 6H), 2.31 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.0, 150.0, 146.4, 138.8, 136.9, 136.4, 129.3, 128.9, 124.5, 123.8, 117.3, 113.0, 21.1, 20.2.
HRMS (ESI) *m/z*: calcd for $C_{17}H_{16}N_2[M+H]^+$ 249.1386, found 249.1395.

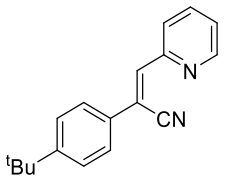


(*Z*)-2-(2-methoxyphenyl)-3-(pyridin-2-yl)acrylonitrile (3fa) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 45% yield, 31.2mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.75 (t, *J* = 5.8 Hz, 1H), 8.00 (d, *J* = 7.9 Hz, 1H), 7.79 (td, *J* = 7.8, 1.7 Hz, 1H), 7.63 (s, 1H), 7.50 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.39 (td, *J* = 8.3, 1.6 Hz, 1H), 7.30 (ddd, *J* = 7.5, 4.8, 0.7 Hz, 1H), 7.03 (td, *J* = 7.6, 0.8 Hz, 1H), 6.98 (d, *J* = 8.3 Hz, 1H), 3.93 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.3, 152.7, 150.0, 145.1, 136.9, 131.0, 130.2, 124.2, 124.1, 124.0, 121.2, 117.7, 112.5, 111.7, 55.9.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_2O[M+H]^+$ 237.1022, found 237.1029.

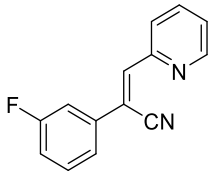


(*Z*)-2-(4-methoxyphenyl)-3-(pyridin-2-yl)acrylonitrile (3ga) [S2] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 59% yield, 41.8mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.55 (d, *J* = 5.7 Hz, 1H), 7.77 – 7.72 (m, 2H), 7.66 (s, 1H), 7.57 (d, *J* = 2.3 Hz, 1H), 7.48 – 7.41 (m, 3H), 6.86 (dd, *J* = 5.7, 2.4 Hz, 1H), 3.93 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 166.6, 153.5, 150.8, 140.9, 133.9, 130.0, 129.3,

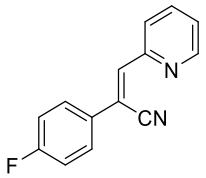
126.5, 117.5, 115.4, 110.7, 110.2, 55.6.



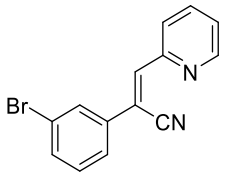
(*Z*)-2-(4-(*tert*-butyl)phenyl)-3-(pyridin-2-yl)acrylonitrile (3ha) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 90% yield, 70.8mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.72 (d, *J* = 4.6 Hz, 1H), 7.91 (d, *J* = 7.9 Hz, 1H), 7.75 (td, *J* = 7.8, 1.7 Hz, 1H), 7.71 – 7.65 (m, 2H), 7.62 (s, 1H), 7.49 – 7.44 (m, 2H), 7.27 (ddd, *J* = 5.9, 4.7, 0.7 Hz, 1H), 1.33 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 153.2, 152.3, 149.9, 139.9, 136.7, 131.1, 126.1, 124.1, 124.0, 117.5, 114.6, 34.8, 31.1.
HRMS (ESI) *m/z*: calcd for $C_{18}H_{18}N_2[M+H]^+$ 263.1543, found 263.1550.



(*Z*)-2-(3-fluorophenyl)-3-(pyridin-2-yl)acrylonitrile (3ia) [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 yellow solid. 75% yield, 50.2mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.76 (d, *J* = 4.3 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.81 (td, *J* = 7.8, 1.6 Hz, 1H), 7.64 (s, 1H), 7.54 (dd, *J* = 7.8, 0.6 Hz, 1H), 7.43 (ddd, *J* = 10.6, 5.9, 4.1 Hz, 2H), 7.33 (ddd, *J* = 7.7, 4.8, 0.7 Hz, 1H), 7.12 (td, *J* = 8.2, 2.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 163.1 (d, *J* = 247.6 Hz), 151.7, 150.1, 141.8, 136.9, 136.2 (d, *J* = 8.0 Hz), 130.8 (d, *J* = 8.4 Hz), 124.5 (d, *J* = 18.2 Hz), 122.2 (d, *J* = 2.7 Hz), 117.1, 116.7 (d, *J* = 21.3 Hz), 113.7 (d, *J* = 2.7 Hz), 113.5, 113.3. **^{19}F NMR** (470 MHz, $CDCl_3$) δ -111.52.

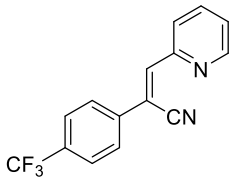


(*Z*)-2-(4-fluorophenyl)-3-(pyridin-2-yl)acrylonitrile (3ja) [S2] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a yellow solid. 93% yield, 62.4mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.72 (d, *J* = 4.6 Hz, 1H), 7.87 (d, *J* = 7.9 Hz, 1H), 7.77 (td, *J* = 7.8, 1.7 Hz, 1H), 7.73 – 7.67 (m, 2H), 7.55 (s, 1H), 7.30 (ddd, *J* = 7.6, 4.9, 0.6 Hz, 1H), 7.17 – 7.09 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 163.6 (d, *J* = 251.1 Hz), 152.0, 150.0, 140.8, 136.9, 130.2 (d, *J* = 3.4 Hz), 128.3 (d, *J* = 8.7 Hz), 124.3 (d, *J* = 26.7 Hz), 117.4, 116.4, 116.2, 113.8. **^{19}F NMR** (470 MHz, $CDCl_3$) δ -110.61.



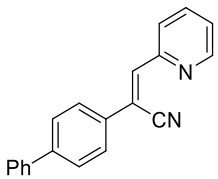
(*Z*)-2-(3-bromophenyl)-3-(pyridin-2-yl)acrylonitrile (3ka) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 65% yield, 55.3mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.77 (d, *J* = 4.3 Hz, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.89 (t, *J* = 1.8 Hz, 1H), 7.83 (td, *J* = 7.8, 1.8 Hz, 1H), 7.68 (ddd, *J* = 7.9, 1.5, 0.7 Hz, 1H), 7.65 (s, 1H), 7.56 (ddd, *J* = 8.0, 1.7, 0.9 Hz, 1H), 7.37 – 7.32 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.8, 150.1, 142.0, 137.1, 136.1, 132.9, 130.7, 129.4, 125.2, 124.8, 124.6, 123.4, 117.1, 113.7.

HRMS (ESI) *m/z*: calcd for $C_{14}H_9BrN_2[M+H]^+$ 285.0022, found 285.0031.

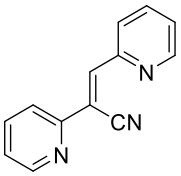


(*Z*)-3-(pyridin-2-yl)-2-(4-(trifluoromethyl)phenyl)acrylonitrile (3la) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 40% yield, 32.9mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.79 (d, *J* = 4.4 Hz, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.90 – 7.82 (m, 3H), 7.73 (d, *J* = 8.6 Hz, 3H), 7.38 (ddd, *J* = 7.5, 4.7, 0.8 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.5, 150.0, 142.7, 137.4, 137.1, 131.6 (q, *J* = 32.9 Hz), 126.8, 126.2 (q, *J* = 3.6 Hz), 124.9, 124.6, 122.7, 116.9, 113.7. **^{19}F NMR** (470 MHz, $CDCl_3$) δ -62.79.

HRMS (ESI) *m/z*: calcd for $C_{15}H_9F_3N_2[M+H]^+$ 275.0791, found 275.0800.

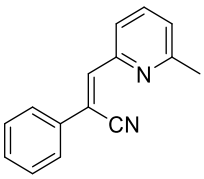


(*Z*)-2-([1,1'-biphenyl]-4-yl)-3-(pyridin-2-yl)acrylonitrile (3ma) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a yellow solid. 60% yield, 50.7mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.76 (d, *J* = 4.2 Hz, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.85 – 7.78 (m, 3H), 7.70 (d, *J* = 3.1 Hz, 2H), 7.68 (s, 1H), 7.63 (d, *J* = 7.4 Hz, 2H), 7.54 – 7.43 (m, 3H), 7.39 (t, *J* = 7.4 Hz, 1H), 7.32 (dd, *J* = 7.0, 4.9 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.2, 150.0, 142.6, 140.5, 139.9, 136.9, 132.8, 129.0, 128.0, 127.7, 127.1, 126.8, 124.3, 124.2, 117.4, 114.6.



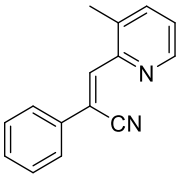
2,3-di(pyridin-2-yl)acrylonitrile (3na, *Z*: *E*=10: 3) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 4:1) to give the product as a yellow oil. 70% yield, 43.5mg. **^{1}H NMR** (500 MHz, Acetone) δ 8.82 – 8.75 (m, 1H), 8.70 (ddd, *J* = 4.7, 1.7, 0.9 Hz, 1H), 8.53 (s, 1H), 8.02 – 7.95 (m, 2H), 7.95 – 7.87 (m, 2H), 7.51 – 7.44 (m, 2H). **^{13}C NMR** (125 MHz, Acetone) δ 154.7, 151.0, 149.9, 148.9, 142.9, 137.7, 137.0, 125.9, 125.0, 124.5, 124.2, 121.4, 116.6.

HRMS (ESI) *m/z*: calcd for $C_{13}H_9N_3[M+H]^+$ 208.0869, found 208.0878.



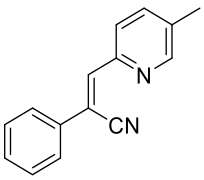
(*Z*)-3-(6-methylpyridin-2-yl)-2-phenylacrylonitrile (3ab) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 88% yield, 58.2mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.76 – 7.72 (m, 3H), 7.66 (t, *J* = 7.7 Hz, 1H), 7.61 (s, 1H), 7.46 – 7.39 (m, 3H), 7.16 (d, *J* = 7.7 Hz, 1H), 2.62 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 158.9, 151.5, 141.3, 137.0, 134.1, 129.7, 129.1, 126.3, 124.1, 121.2, 117.5, 114.6, 24.3.

HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_2[M+H]^+$ 221.1073, found 221.1076.

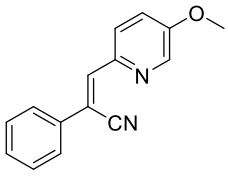


(*Z*)-3-(3-methylpyridin-2-yl)-2-phenylacrylonitrile (3ac) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 69% yield, 45.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.60 (dd, *J* = 4.6, 1.0 Hz, 1H), 7.78 – 7.72 (m, 2H), 7.70 (s, 1H), 7.54 (dd, *J* = 7.7, 0.7 Hz, 1H), 7.48 – 7.39 (m, 3H), 7.22 (dd, *J* = 7.7, 4.7 Hz, 1H), 2.43 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.5, 147.2, 138.4, 137.5, 134.7, 133.0, 129.7, 129.1, 126.6, 124.5, 117.7, 116.4, 18.7.

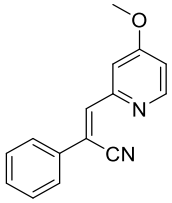
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_2[M+H]^+$ 221.1073, found 221.1073.



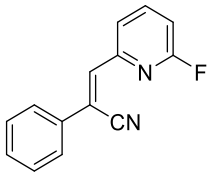
(*Z*)-3-(5-methylpyridin-2-yl)-2-phenylacrylonitrile (3ad) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 58% yield, 38.3mg. **^{1}H NMR** (500 MHz, Acetone) δ 8.45 (s, 1H), 7.71 (s, 1H), 7.70 (t, *J* = 1.7 Hz, 1H), 7.69 – 7.67 (m, 1H), 7.61 (t, *J* = 1.5 Hz, 2H), 7.41 – 7.36 (m, 2H), 7.35 – 7.31 (m, 1H), 2.27 (s, 3H). **^{13}C NMR** (125 MHz, Acetone) δ 150.3, 149.6, 140.7, 137.1, 134.8, 134.7, 129.5, 129.1, 126.2, 124.7, 117.2, 113.1, 17.6.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_2[M+H]^+$ 221.1073, found 221.1075.



(*Z*)-3-(5-methoxypyridin-2-yl)-2-phenylacrylonitrile (3ae) 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 colorless oil. 42% yield, 29.8mg. **^{1}H NMR** (500 MHz, Acetone) δ 8.30 (d, *J* = 3.0 Hz, 1H), 7.72 (d, *J* = 8.7 Hz, 1H), 7.69 (s, 1H), 7.68 – 7.66 (m, 2H), 7.34 (dddd, *J* = 10.3, 6.1, 5.5, 3.6 Hz, 4H), 2.73 (s, 3H). **^{13}C NMR** (125 MHz, Acetone) δ 156.4, 144.7, 140.2, 138.1, 134.9, 129.2, 129.1, 126.3, 126.0, 120.0, 117.4, 111.4, 55.4.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_2O[M+H]^+$ 237.1022, found 237.1028.



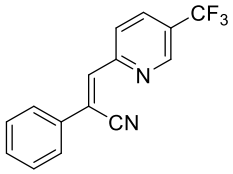
(*Z*)-3-(4-methoxypyridin-2-yl)-2-phenylacrylonitrile (3af) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 54% yield, 38.3mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.55 (d, *J* = 5.7 Hz, 1H), 7.74 (d, *J* = 7.1 Hz, 2H), 7.65 (s, 1H), 7.57 (d, *J* = 2.2 Hz, 1H), 7.49 – 7.41 (m, 3H), 6.86 (dd, *J* = 5.7, 2.3 Hz, 1H), 3.93 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 166.5, 153.6, 150.9, 141.0, 134.0, 130.0, 129.3, 126.5, 117.5, 115.4, 110.7, 110.2, 55.6.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{12}N_2O[M+H]^+$ 237.1022, found 237.1025.



(*Z*)-3-(6-fluoropyridin-2-yl)-2-phenylacrylonitrile (3ag) 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 colorless oil. 57% yield, 38.3mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.94 – 7.85 (m, 2H), 7.76 – 7.70 (m, 2H), 7.54 (s, 1H), 7.47 (dt, *J* = 14.8, 4.9 Hz, 3H), 6.98 (dd, *J* = 7.8, 2.6 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.8 (d, *J* = 241.5 Hz), 150.7 (d, *J* = 13.8 Hz), 142.0 (d, *J* = 7.7 Hz), 139.0,

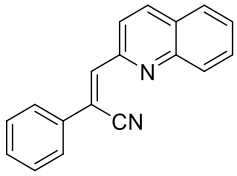
133.6, 130.1, 129.2, 126.4, 121.4 (d, *J* = 3.8 Hz), 117.0, 116.1, 110.8 (d, *J* = 37.1 Hz). **^{19}F NMR** (470 MHz, $CDCl_3$) δ -64.99.

HRMS (ESI) *m/z*: calcd for $C_{14}H_9FN_2[M+H]^+$ 225.0823, found 225.0828.

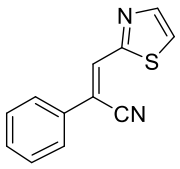


(*Z*)-2-phenyl-3-(5-(trifluoromethyl)pyridin-2-yl)acrylonitrile (3ah) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 48% yield, 39.5mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.00 (d, *J* = 0.8 Hz, 1H), 8.06 – 7.99 (m, 2H), 7.79 – 7.74 (m, 2H), 7.67 (s, 1H), 7.52 – 7.46 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 155.4, 146.9 (q, *J* = 3.9 Hz), 138.9, 134.2 (q, *J* = 3.5 Hz), 133.5, 130.5, 129.4, 126.6, 126.6 (q, *J* = 33.2 Hz), 124.4, 123.7, 117.5, 117.0. **^{19}F NMR** (470 MHz, CDCl3) δ -62.51.

HRMS (ESI) *m/z*: calcd for $C_{15}H_9F_3N_2[M+H]^+$ 275.0791, found 275.0794.

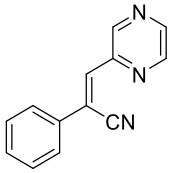


(*Z*)-2-phenyl-3-(quinolin-2-yl)acrylonitrile (3ai) [S4] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a yellow solid. 67% yield, 51.5mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.6 Hz, 1H), 8.19 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.90 – 7.85 (m, 2H), 7.84 – 7.80 (m, 2H), 7.80 – 7.75 (m, 1H), 7.64 – 7.59 (m, 1H), 7.52 – 7.43 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.2, 148.1, 141.3, 137.3, 134.1, 130.6, 130.1, 129.7, 129.3, 128.1, 128.0, 127.7, 126.6, 120.9, 117.5, 116.4.

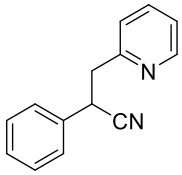


(*Z*)-2-phenyl-3-(thiazol-2-yl)acrylonitrile (3aj) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a yellow solid. M.P. 112- 114 ℃. 85% yield, 54.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 2.8 Hz, 1H), 7.90 (s, 1H), 7.76 – 7.69 (m, 2H), 7.58 (d, *J* = 2.4 Hz, 1H), 7.46 (ddd, *J* = 9.1, 7.2, 1.7 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.6, 144.2, 133.9, 132.9, 130.2, 129.3, 126.2, 122.3, 117.1, 114.3.

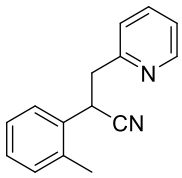
HRMS (ESI) *m/z*: calcd for $C_{12}H_8N_2S[M+H]^+$ 213.0481, found 213.0489.



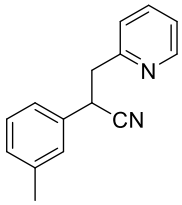
(*Z*)-2-phenyl-3-(pyrazin-2-yl)acrylonitrile (3ak) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 53% yield, 32.9mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.97 (s, 1H), 8.79 – 8.72 (m, 1H), 8.59 (d, *J* = 2.0 Hz, 1H), 7.82 – 7.75 (m, 2H), 7.60 (s, 1H), 7.53 – 7.44 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 148.1, 145.4, 144.8, 144.6, 136.3, 133.6, 130.4, 129.3, 126.5, 117.4, 116.9.
HRMS (ESI) *m/z*: calcd for $C_{13}H_9N_3[M+H]^+$ 208.0869, found 208.0868.



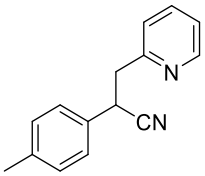
2-phenyl-3-(pyridin-2-yl)propanenitrile (4aa) [S3] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 89% yield, 55.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.2 Hz, 1H), 7.59 (td, *J* = 7.7, 1.8 Hz, 1H), 7.34 (d, *J* = 4.4 Hz, 4H), 7.32 – 7.28 (m, 1H), 7.17 (dd, *J* = 6.8, 5.0 Hz, 1H), 7.11 (d, *J* = 7.7 Hz, 1H), 4.49 (dd, *J* = 9.2, 6.6 Hz, 1H), 3.31 (ddd, *J* = 20.4, 13.9, 7.9 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.1, 149.6, 136.8, 135.4, 129.1, 128.2, 127.4, 123.9, 122.4, 120.6, 44.1, 37.3.



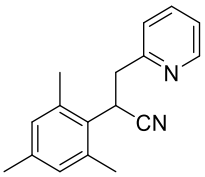
3-(pyridin-2-yl)-2-(o-tolyl)propanenitrile (4ba) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 48% yield, 31.8mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 4.2 Hz, 1H), 7.63 (td, *J* = 7.7, 1.8 Hz, 1H), 7.50 (dd, *J* = 7.4, 1.5 Hz, 1H), 7.26 – 7.14 (m, 5H), 4.64 (dd, *J* = 9.5, 6.0 Hz, 1H), 3.29 (ddd, *J* = 19.9, 13.9, 7.8 Hz, 2H), 2.36 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.4, 149.8 137.0, 135.5, 133.9, 131.1, 128.4, 127.6, 127.0, 124.0, 122.5, 121.0, 42.9, 34.3, 19.2.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{14}N_2[M+H]^+$ 223.1230, found 223.1231.



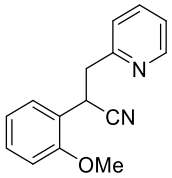
3-(pyridin-2-yl)-2-(m-tolyl)propanenitrile (4ca) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 86% yield, 57.3mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.53 (d, *J* = 4.4 Hz, 1H), 7.55 (td, *J* = 7.7, 1.7 Hz, 1H), 7.19 – 7.11 (m, 3H), 7.09 – 7.03 (m, 3H), 4.37 (dd, *J* = 9.3, 6.5 Hz, 1H), 3.23 (m, 2H), 2.27 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.3, 149.7, 139.0, 137.0, 135.4, 129.1, 129.0, 128.2, 124.5, 124.1, 122.5, 120.8, 44.3, 37.4, 21.5.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{14}N_2[M+H]^+$ 223.1230, found 223.1228.



3-(pyridin-2-yl)-2-(p-tolyl)propanenitrile (4da) 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 colorless oil. 87% yield, 58.0mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 3.7 Hz, 1H), 7.61 (td, *J* = 7.7, 1.7 Hz, 1H), 7.24 (d, *J* = 8.1 Hz, 2H), 7.19 (dd, *J* = 7.2, 5.2 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 1H), 4.44 (dd, *J* = 9.2, 6.6 Hz, 1H), 3.30 (ddd, *J* = 20.4, 13.8, 7.9 Hz, 2H), 2.33 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.3, 149.6, 138.0, 136.9, 132.4, 129.8, 127.3, 124.1, 122.4, 120.8, 44.2, 37.0, 21.2.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{14}N_2[M+H]^+$ 223.1230, found 223.1230.



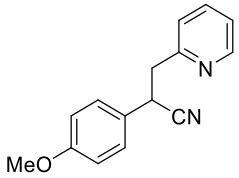
2-mesityl-3-(pyridin-2-yl)propanenitrile (4ea) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 50% yield, 37.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.1 Hz, 1H), 7.60 (td, *J* = 7.7, 1.8 Hz, 1H), 7.19 (ddd, *J* = 7.5, 4.9, 0.8 Hz, 1H), 7.10 (d, *J* = 7.7 Hz, 1H), 6.86 (s, 2H), 4.84 (dd, *J* = 9.2, 6.4 Hz, 1H), 3.31 (ddd, *J* = 20.2, 13.8, 7.8 Hz, 2H), 2.44 (s, 6H), 2.26 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.7, 149.9, 137.8, 136.7, 136.5, 130.3, 128.7, 123.8, 122.4, 120.5, 40.6, 31.4, 20.9, 20.6.
HRMS (ESI) *m/z*: calcd for $C_{17}H_{18}N_2[M+H]^+$ 251.1543, found 251.1544.



2-(2-methoxyphenyl)-3-(pyridin-2-yl)propanenitrile (4fa) 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 colorless oil. 38% yield, 27.2mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.5 Hz,

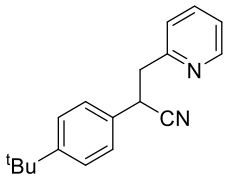
1H), 7.61 (td, *J* = 7.7, 1.8 Hz, 1H), 7.37 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.19 – 7.14 (m, 2H), 6.95 (td, *J* = 7.5, 0.9 Hz, 1H), 6.90 (d, *J* = 8.2 Hz, 1H), 4.74 (dd, *J* = 9.3, 6.2 Hz, 1H), 3.85 (s, 3H), 3.31 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.9, 156.4, 149.6, 136.7, 129.7, 128.8, 123.9, 123.7, 122.3, 121.0, 120.8, 111.0, 55.7, 41.7, 32.2.

HRMS (ESI) *m/z*: calcd for $C_{15}H_{14}N_2O[M+H]^+$ 239.1179, found 239.1180.



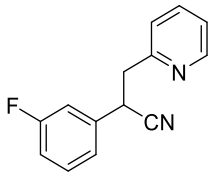
2-(4-methoxyphenyl)-3-(pyridin-2-yl)propanenitrile (4ga) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 50% yield, 35.7mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 4.2 Hz, 1H), 7.61 (td, *J* = 7.7, 1.8 Hz, 1H), 7.28 – 7.24 (m, 2H), 7.19 (ddd, *J* = 7.4, 4.9, 0.7 Hz, 1H), 7.12 (d, *J* = 7.7 Hz, 1H), 6.90 – 6.85 (m, 2H), 4.43 (dd, *J* = 9.0, 6.7 Hz, 1H), 3.79 (s, 3H), 3.29 (ddd, *J* = 20.5, 13.8, 7.9 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 159.5, 156.4, 149.7, 136.9, 128.7, 127.5, 124.1, 122.4, 121.0, 114.5, 55.4, 44.4, 36.6.

HRMS (ESI) *m/z*: calcd for $C_{15}H_{14}N_2O[M+H]^+$ 239.1179, found 239.1171.



2-(4-(*tert*-butyl)phenyl)-3-(pyridin-2-yl)propanenitrile (4ha) 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 colorless oil. 74% yield, 58.7mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 4.2 Hz, 1H), 7.61 (td, *J* = 7.7, 1.8 Hz, 1H), 7.41 – 7.36 (m, 2H), 7.33 – 7.29 (m, 2H), 7.19 (dd, *J* = 6.8, 4.9 Hz, 1H), 7.16 (d, *J* = 7.8 Hz, 1H), 4.46 (dd, *J* = 9.3, 6.6 Hz, 1H), 3.35 – 3.25 (m, 2H), 1.31 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.4, 151.3, 149.7, 136.8, 132.5, 127.1, 126.1, 124.0, 122.4, 120.8, 44.2, 37.0, 34.6, 31.3.

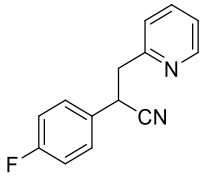
HRMS (ESI) *m/z*: calcd for $C_{18}H_{20}N_2[M+H]^+$ 265.1699, found 265.1706.



2-(3-fluorophenyl)-3-(pyridin-2-yl)propanenitrile (4ia) 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 colorless oil. 60% yield, 40.7mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 4.1 Hz, 1H), 7.63 (td, *J* = 7.7, 1.8 Hz, 1H), 7.33 (td, *J* = 8.0, 5.9 Hz, 1H), 7.21 (ddd, *J* = 7.5, 4.9, 0.8 Hz, 1H), 7.16 – 7.12 (m, 2H), 7.09 – 7.06 (m, 1H), 7.01 (tdd, *J* = 8.5, 2.5, 0.8 Hz, 1H), 4.52 (dd, *J* = 9.0, 6.7 Hz,

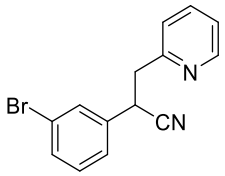
1H), 3.32 (ddd, *J* = 20.6, 13.9, 7.8 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 163.0 (d, *J* = 247.9 Hz), 155.7, 149.7, 137.8 (d, *J* = 7.5 Hz), 136.9, 130.7 (d, *J* = 8.3 Hz), 123.9, 123.2 (d, *J* = 3.2 Hz), 122.5, 120.1, 115.3 (d, *J* = 21.1 Hz), 114.7 (d, *J* = 22.6 Hz), 43.9, 36.9 (d, *J* = 1.5 Hz). **^{19}F NMR** (470 MHz, $CDCl_3$) δ -111.53.

HRMS (ESI) *m/z*: calcd for $C_{14}H_{11}FN_2[M+H]^+$ 227.0979, found 227.0981.



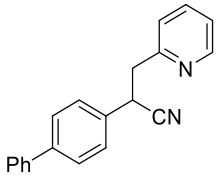
2-(4-fluorophenyl)-3-(pyridin-2-yl)propanenitrile (4ja) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 88% yield, 59.7mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.1 Hz, 1H), 7.61 (td, *J* = 7.7, 1.8 Hz, 1H), 7.34 – 7.29 (m, 2H), 7.20 (ddd, *J* = 7.5, 4.9, 0.8 Hz, 1H), 7.11 (d, *J* = 7.7 Hz, 1H), 7.07 – 7.00 (m, 2H), 4.50 (dd, *J* = 8.9, 6.8 Hz, 1H), 3.31 (ddd, *J* = 20.7, 13.9, 7.8 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.5 (d, *J* = 247.8 Hz), 156.0, 149.8, 136.9, 131.3 (d, *J* = 3.2 Hz), 129.3 (d, *J* = 8.3 Hz), 124.0, 122.5, 120.6, 116.1 (d, *J* = 22.0 Hz), 44.2, 36.5. **^{19}F NMR** (470 MHz, $CDCl_3$) δ -113.58.

HRMS (ESI) *m/z*: calcd for $C_{14}H_{11}FN_2[M+H]^+$ 227.0979, found 227.0980.



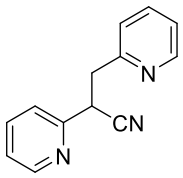
2-(3-bromophenyl)-3-(pyridin-2-yl)propanenitrile (4ka) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 46% yield, 39.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.62 (d, *J* = 2.5 Hz, 1H), 7.66 (td, *J* = 7.9, 1.4 Hz, 1H), 7.53 (s, 1H), 7.49 – 7.44 (m, 1H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.24 (t, *J* = 7.8 Hz, 2H), 7.16 (d, *J* = 7.6 Hz, 1H), 4.51 (dd, *J* = 8.7, 6.9 Hz, 1H), 3.33 (ddd, *J* = 20.3, 13.9, 7.9 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 155.7, 149.7, 137.6, 137.3, 131.6, 130.8, 130.7, 126.3, 124.2, 123.2, 122.8, 120.1, 43.9, 36.9.

HRMS (ESI) *m/z*: calcd for $C_{14}H_{11}BrN_2[M+H]^+$ 287.0178, found 287.0178.

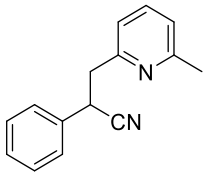


2-([1,1'-biphenyl]-4-yl)-3-(pyridin-2-yl)propanenitrile (4la) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 40% yield, 34.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.3 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.59 (dd, *J* = 8.3, 6.9 Hz, 4H), 7.47 – 7.43 (m, 4H), 7.39 – 7.35 (m, 1H),

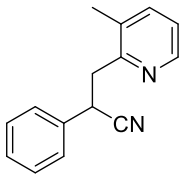
7.25 (d, *J* = 4.9 Hz, 1H), 7.21 (d, *J* = 7.7 Hz, 1H), 4.58 (m, 1H), 3.42 – 3.35 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 155.9, 149.3, 141.2, 140.2, 137.4, 134.3, 128.9, 127.9, 127.8, 127.7, 127.1, 124.3, 122.7, 120.5, 43.9, 37.1.
HRMS (ESI) *m/z*: calcd for $C_{20}H_{16}N_2[M+H]^+$ 285.1386, found 285.1395.



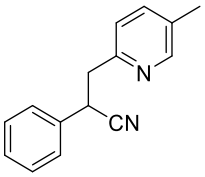
2,3-di(pyridin-2-yl)propanenitrile (4ma) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 4:1) to give the product as a yellow oil. 63% yield, 39.4mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.3 Hz, 1H), 8.59 (d, *J* = 4.6 Hz, 1H), 7.68 (td, *J* = 7.7, 1.7 Hz, 1H), 7.62 (td, *J* = 7.7, 1.7 Hz, 1H), 7.35 (d, *J* = 7.8 Hz, 1H), 7.25 (dd, *J* = 7.2, 5.2 Hz, 1H), 7.22 – 7.17 (m, 2H), 4.68 (dd, *J* = 9.1, 6.3 Hz, 1H), 3.51 (ddd, *J* = 23.2, 14.0, 7.7 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.2, 154.6, 150.1, 149.5, 137.3, 136.9, 124.0, 123.1, 122.4, 122.4, 119.9, 41.7, 39.4.
HRMS (ESI) *m/z*: calcd for $C_{13}H_{11}N_3[M+H]^+$ 210.1026, found 210.1029.



3-(6-methylpyridin-2-yl)-2-phenylpropanenitrile (4ab) 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 colorless oil. 51% yield, 34.0mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 (t, *J* = 7.7 Hz, 1H), 7.38 – 7.29 (m, 5H), 7.05 (d, *J* = 7.7 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 1H), 4.48 (dd, *J* = 9.1, 6.7 Hz, 1H), 3.28 (ddd, *J* = 20.4, 13.7, 8.0 Hz, 2H), 2.57 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 158.6, 155.5, 137.0, 135.7, 129.1, 128.2, 127.6, 122.1, 121.0, 120.8, 44.2, 37.5, 24.6.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{14}N_2[M+H]^+$ 223.1230, found 223.1230.

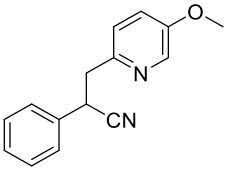


3-(3-methylpyridin-2-yl)-2-phenylpropanenitrile (4ac) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 58% yield, 38.7mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 4.0 Hz, 1H), 7.42 (d, *J* = 7.4 Hz, 1H), 7.39 – 7.31 (m, 5H), 7.11 (dd, *J* = 7.6, 4.9 Hz, 1H), 4.63 (dd, *J* = 9.2, 6.5 Hz, 1H), 3.32 (ddd, *J* = 21.2, 14.8, 7.8 Hz, 2H), 2.18 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.6, 146.9, 138.1, 136.0, 131.9, 129.1, 128.2, 127.5, 122.3, 121.2, 40.7, 36.3, 18.7.
HRMS (ESI) *m/z*: calcd for $C_{15}H_{14}N_2[M+H]^+$ 223.1230, found 223.1234.



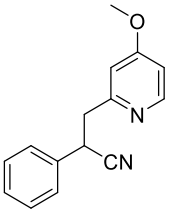
3-(5-methylpyridin-2-yl)-2-phenylpropanenitrile (4ad) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 50% yield, 33.3mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.43 (s, 1H), 7.44 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.38 – 7.30 (m, 5H), 7.05 (d, *J* = 7.8 Hz, 1H), 4.46 (dd, *J* = 8.9, 6.9 Hz, 1H), 3.36 – 3.23 (m, 2H), 2.33 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 153.2, 150.0, 137.7, 135.6, 132.1, 129.2, 128.3, 127.5, 123.6, 120.7, 43.8, 37.7, 29.8.

HRMS (ESI) *m/z*: calcd for $C_{15}H_{14}N_2[M+H]^+$ 223.1230, found 223.1231.



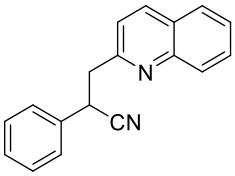
3-(5-methoxypyridin-2-yl)-2-phenylpropanenitrile (4ae) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 34% yield, 24.3mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.39 – 7.31 (m, 5H), 7.13 (dd, *J* = 8.5, 2.9 Hz, 1H), 7.06 (d, *J* = 8.5 Hz, 1H), 4.42 (dd, *J* = 8.9, 6.7 Hz, 1H), 3.86 (s, 3H), 3.27 (m, 2H). **^{13}C NMR** (125MHz, $CDCl_3$) δ 154.8, 148.0, 137.3, 135.5, 129.1, 128.2, 127.4, 124.2, 121.1, 120.7, 55.7, 43.3, 37.8.

HRMS (ESI) *m/z*: calcd for $C_{15}H_{14}N_2O[M+H]^+$ 239.1179, found 239.1178.



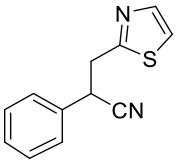
3-(4-methoxypyridin-2-yl)-2-phenylpropanenitrile (4af) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 40% yield, 28.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.42 (d, *J* = 5.7 Hz, 1H), 7.41 – 7.31 (m, 5H), 6.74 (dd, *J* = 5.8, 2.4 Hz, 1H), 6.66 (d, *J* = 2.3 Hz, 1H), 4.50 (dd, *J* = 8.9, 6.9 Hz, 1H), 3.82 (s, 3H), 3.33 – 3.22 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 166.4, 157.6, 150.6, 135.4, 129.1, 128.2, 127.4, 120.6, 110.2, 108.7, 55.3, 44.3, 37.3.

HRMS (ESI) *m/z*: calcd for $C_{15}H_{14}N_2O[M+H]^+$ 239.1179, found 239.1178.



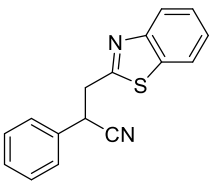
2-phenyl-3-(quinolin-2-yl)propanenitrile (4ag) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 54% yield, 41.8mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.5 Hz, 1H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.75 – 7.68 (m, 1H), 7.55 – 7.49 (m, 1H), 7.40 (d, *J* = 7.1 Hz, 2H), 7.36 – 7.27 (m, 3H), 7.20 (d, *J* = 8.4 Hz, 1H), 4.70 (dd, *J* = 8.9, 6.7 Hz, 1H), 3.52 (ddd, *J* = 21.0, 14.4, 7.8 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.6, 148.0, 136.9, 135.7, 129.9, 129.2, 129.0, 128.3, 127.7, 127.6, 127.2, 126.5, 121.8, 120.9, 44.5, 36.8.

HRMS (ESI) *m/z*: calcd for $C_{18}H_{14}N_2[M+H]^+$ 259.1230, found 259.1232.



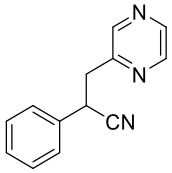
2-phenyl-3-(thiazol-2-yl)propanenitrile (4ah) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give the product as a colorless oil. 70% yield, 45.0mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 3.3 Hz, 1H), 7.42 – 7.32 (m, 5H), 7.27 – 7.25 (m, 1H), 4.45 (dd, *J* = 8.8, 6.6 Hz, 1H), 3.57 (ddd, *J* = 21.5, 14.9, 7.7 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 164.3, 143.0, 134.5, 129.4, 128.7, 127.5, 120.0, 119.6, 38.9, 37.7.

HRMS (ESI) *m/z*: calcd for $C_{12}H_{10}N_2S[M+H]^+$ 215.0637, found 215.0635.



3-(benzo[*d*]thiazol-2-yl)-2-phenylpropanenitrile (4ai) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 4:1) to give the product as a colorless oil. 44% yield, 34.8mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.53 – 7.48 (m, 1H), 7.43 – 7.34 (m, 6H), 4.60 (dd, *J* = 8.8, 6.6 Hz, 1H), 3.67 (ddd, *J* = 21.7, 15.2, 7.7 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 165.1, 153.0, 135.2, 134.5, 129.4, 128.7, 127.5, 126.4, 125.4, 123.0, 121.7, 119.8, 39.9, 37.0.

HRMS (ESI) *m/z*: calcd for $C_{16}H_{12}N_2S[M+H]^+$ 265.0794, found 265.0790.



2-phenyl-3-(pyrazin-2-yl)propanenitrile (4aj) was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 4:1) to give the product as a colorless oil. 38% yield, 23.9mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.88 (s, 1H), 7.86 (dd, *J* = 8.1, 2.0 Hz, 1H), 7.41 – 7.32 (m, 5H), 7.27 (s, 1H), 4.53 (dd, *J* = 9.1, 6.5 Hz, 1H), 3.41 (ddd, *J* = 20.6, 14.1, 7.8 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.1, 146.6, 135.0, 134.0, 129.3, 128.5, 127.4, 123.7, 120.2, 43.9, 36.8.

HRMS (ESI) *m/z*: calcd for $C_{13}H_{11}N_3[M+Na]^+$ 232.0845, found 232.0841.

Reference

S1 R.-N. Wang, S.-W. Wang, D.-Y. Li, F.-Y. Ye, Y.-T. Leng, Y.-J. Wu, J.-b. Chang, Y.-S. Wu, *Tetrahedron* **75** (2019) 2298-2305.

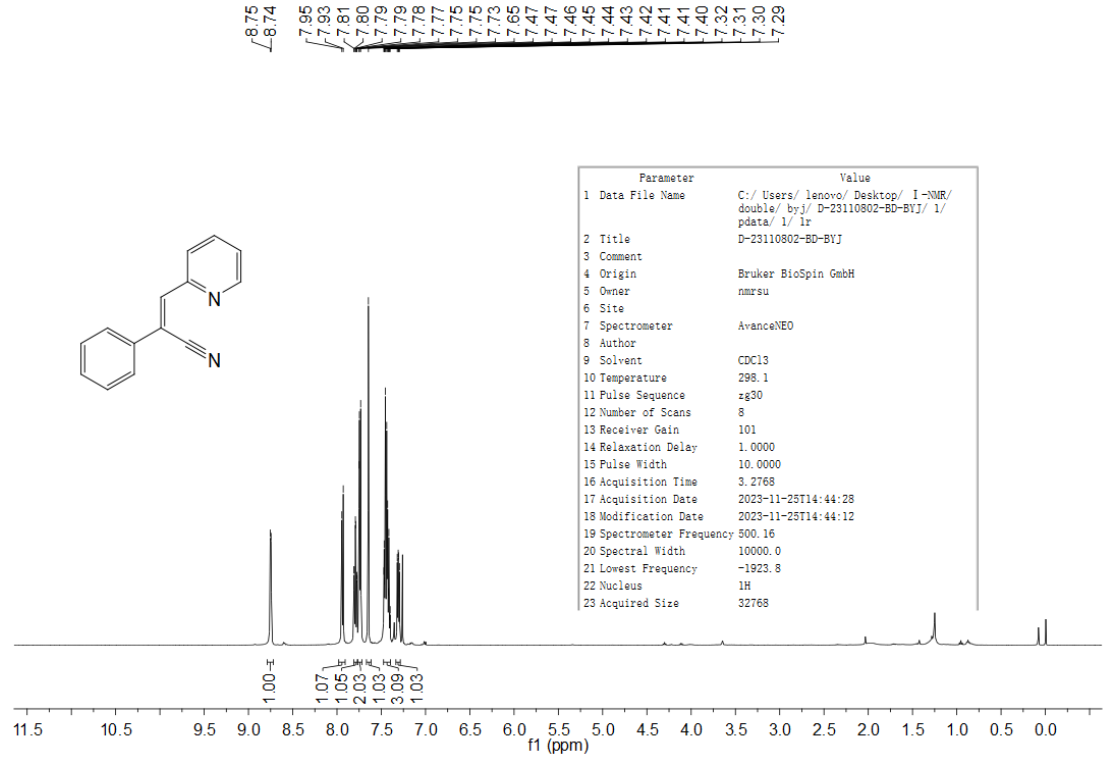
S2 W.-H. Liu, R.-J. Liu, X.-Y. Liu, H.-Q. Zhao, Z.-H. Xi. *Asian J. Org. Chem*. 2023, **12**, e202300247.

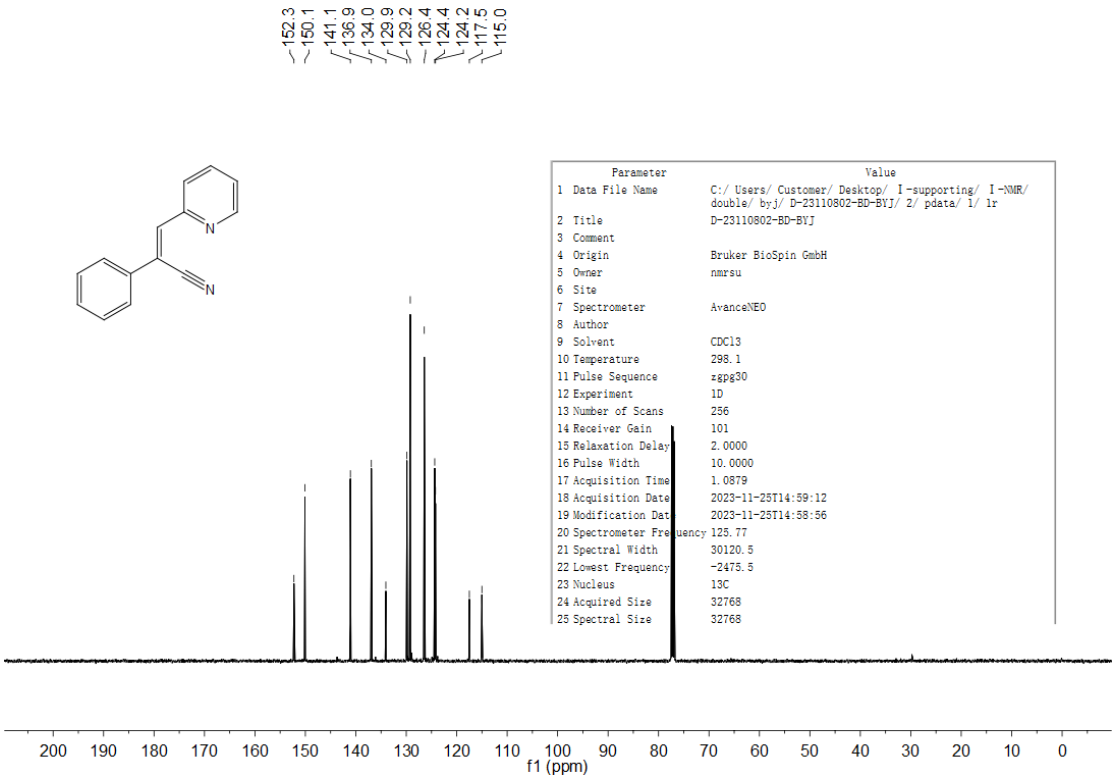
S3 C. Li, L. Bai, M.-T. Ge, A.-B. Xia, Y. Wang, Y.-R. Qiu, D.-Q. Xu. *New J. Chem*., 2021, **45**, 15200.

S4 N. Moreira, L. Martelli, Kiyara. Julio, J. Zukerman-Schpector, T. Opatz, A. Corrêa. *Eur. J. Org. Chem*. 2020, 4563–4570.

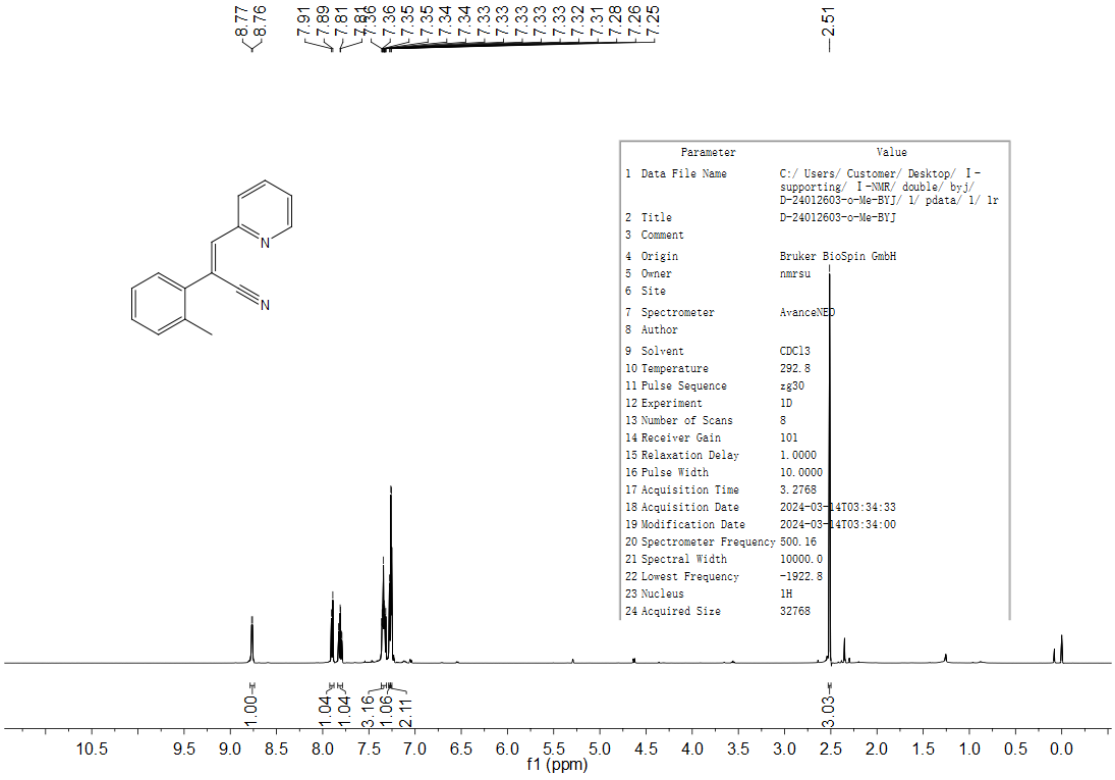
Copies of NMR spectra and HRMS.

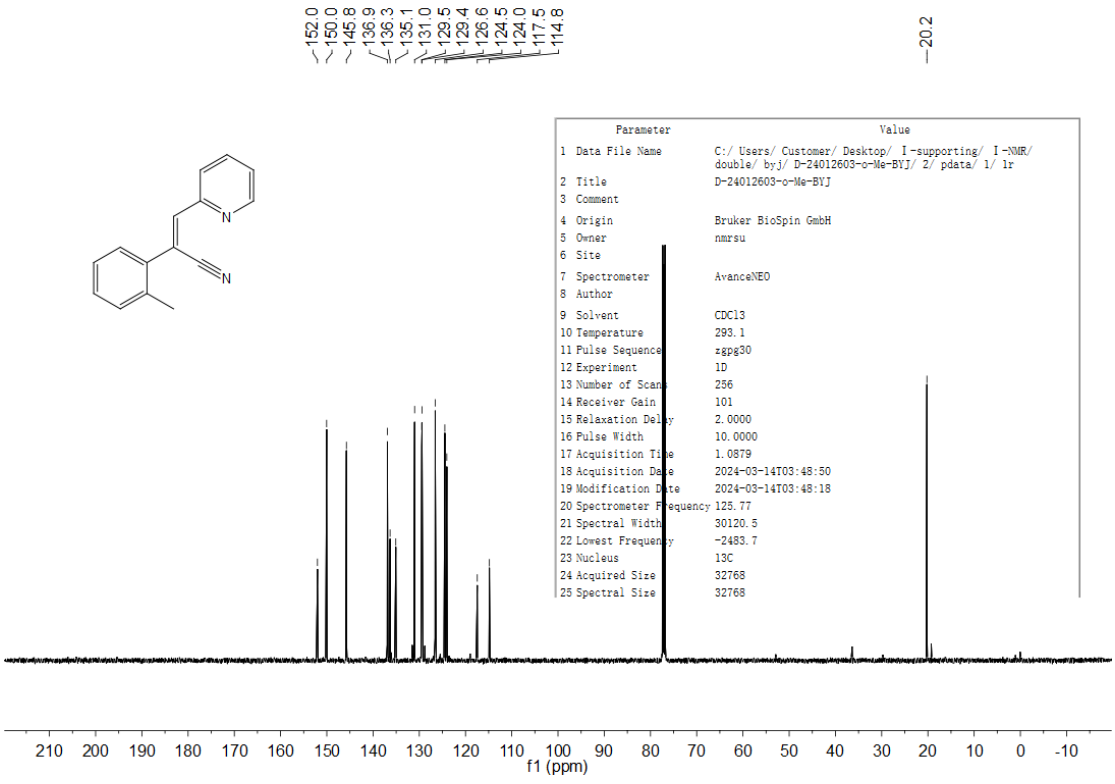
(*Z*)-2-phenyl-3-(pyridin-2-yl)acrylonitrile (3aa)

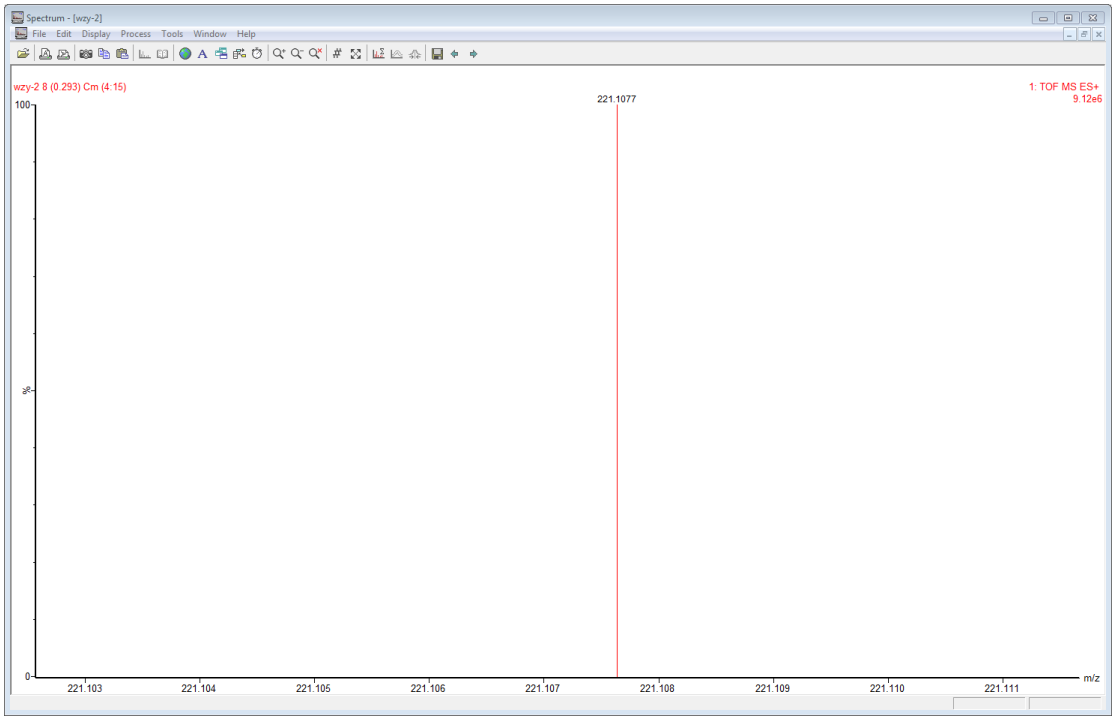




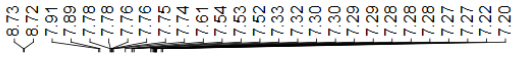
(*Z*)-3-(pyridin-2-yl)-2-(o-tolyl)acrylonitrile (3ba)

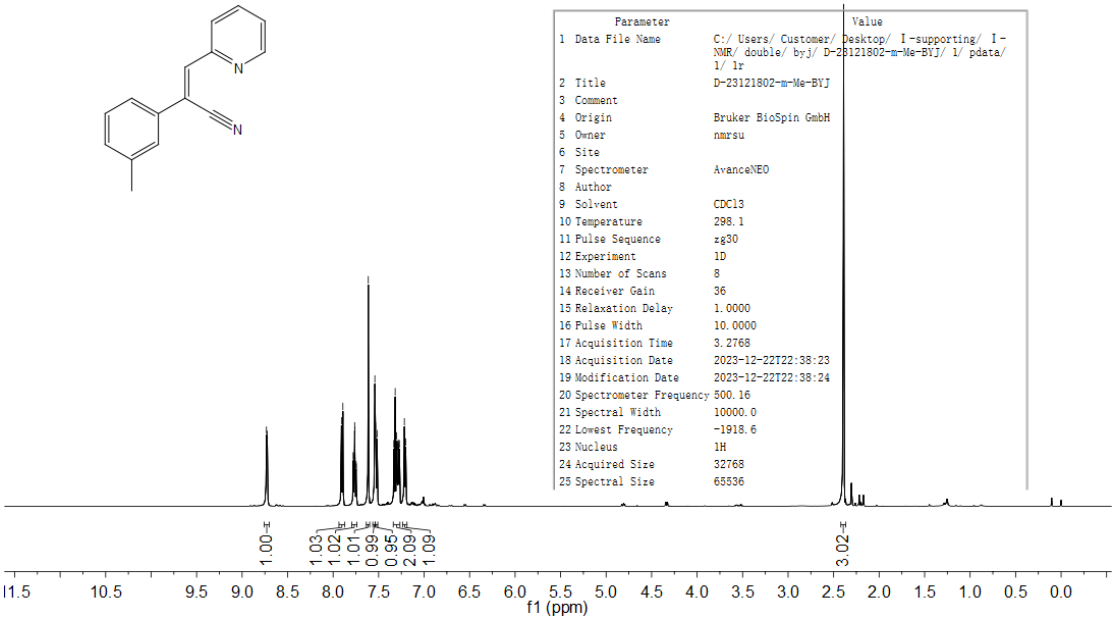


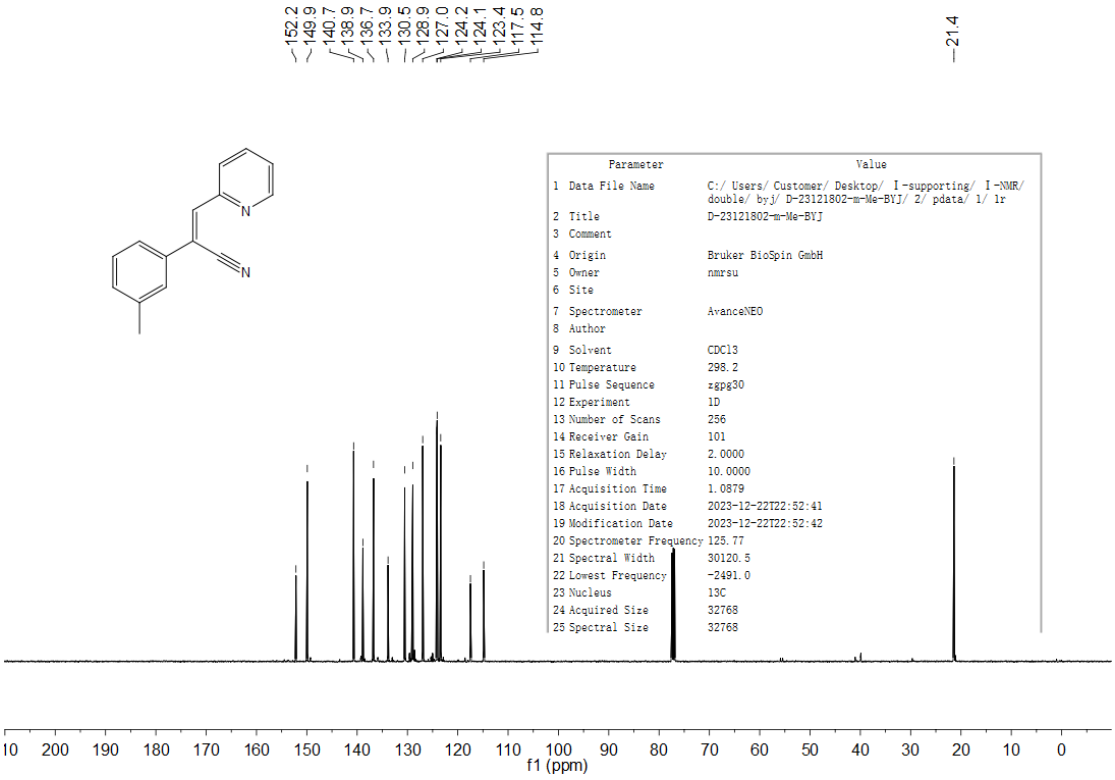


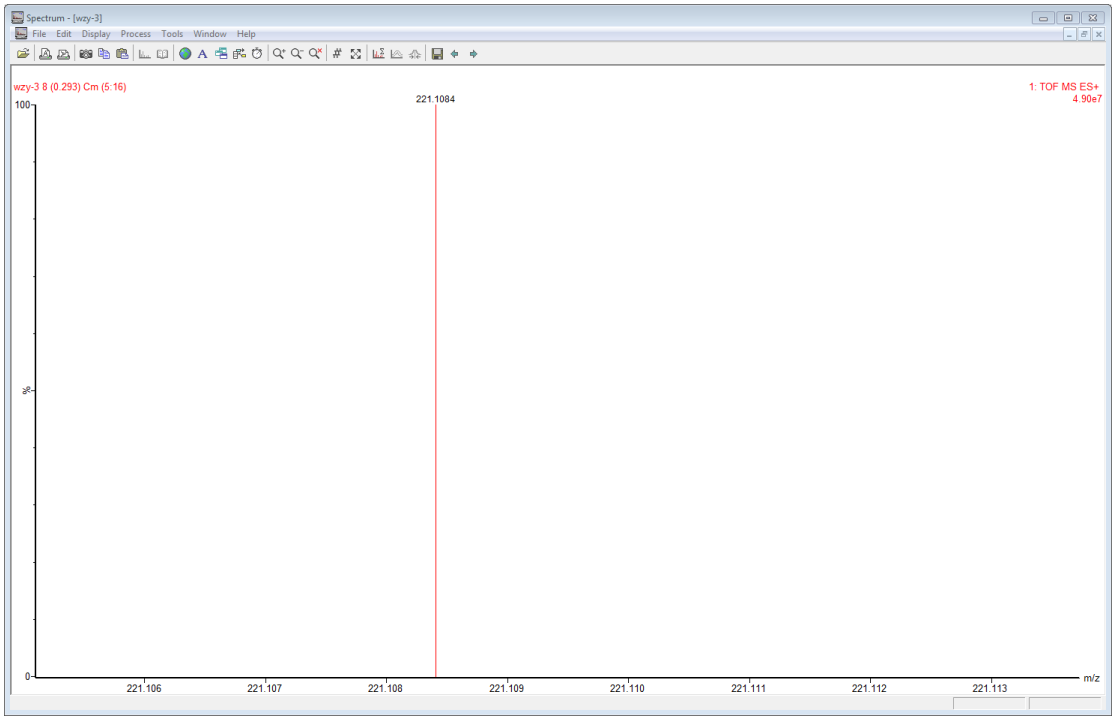


(*Z*)-3-(pyridin-2-yl)-2-(m-tolyl)acrylonitrile (3ca)

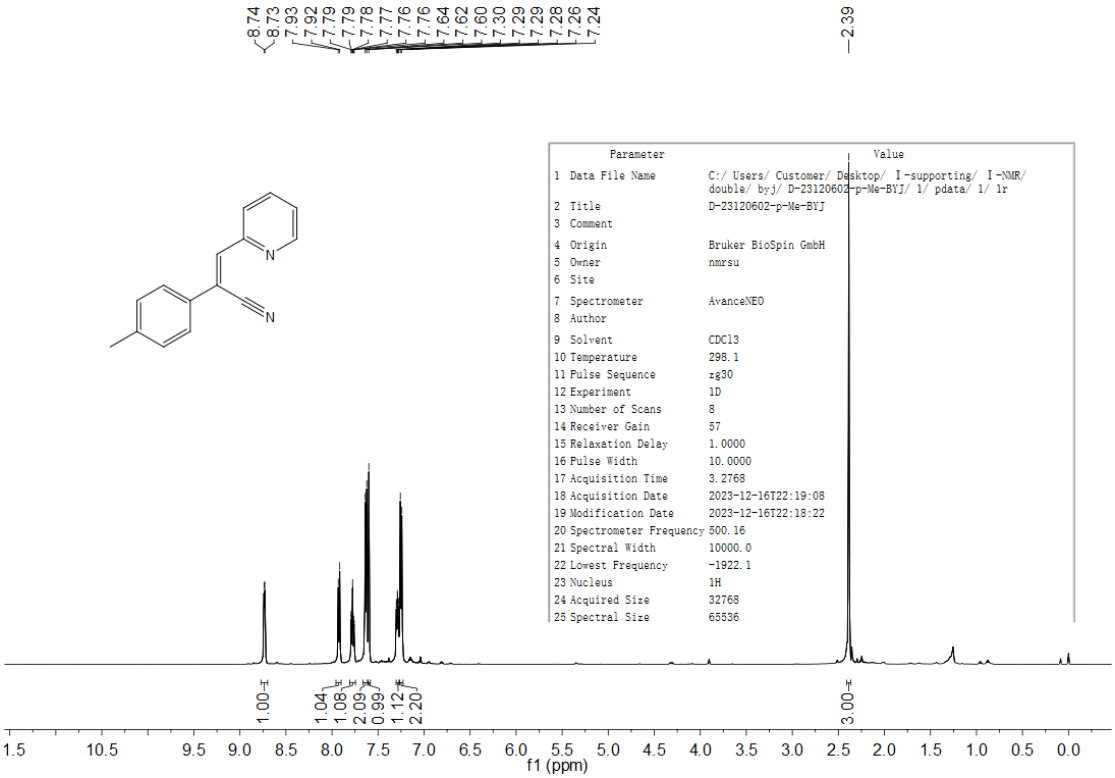


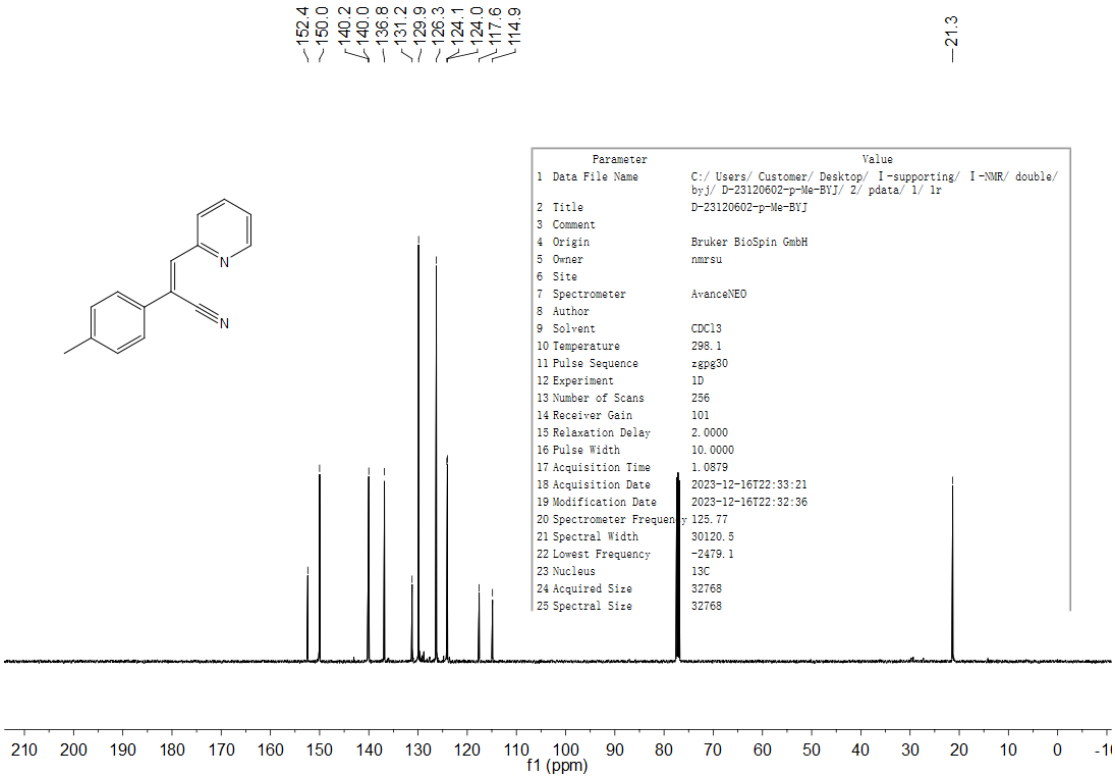




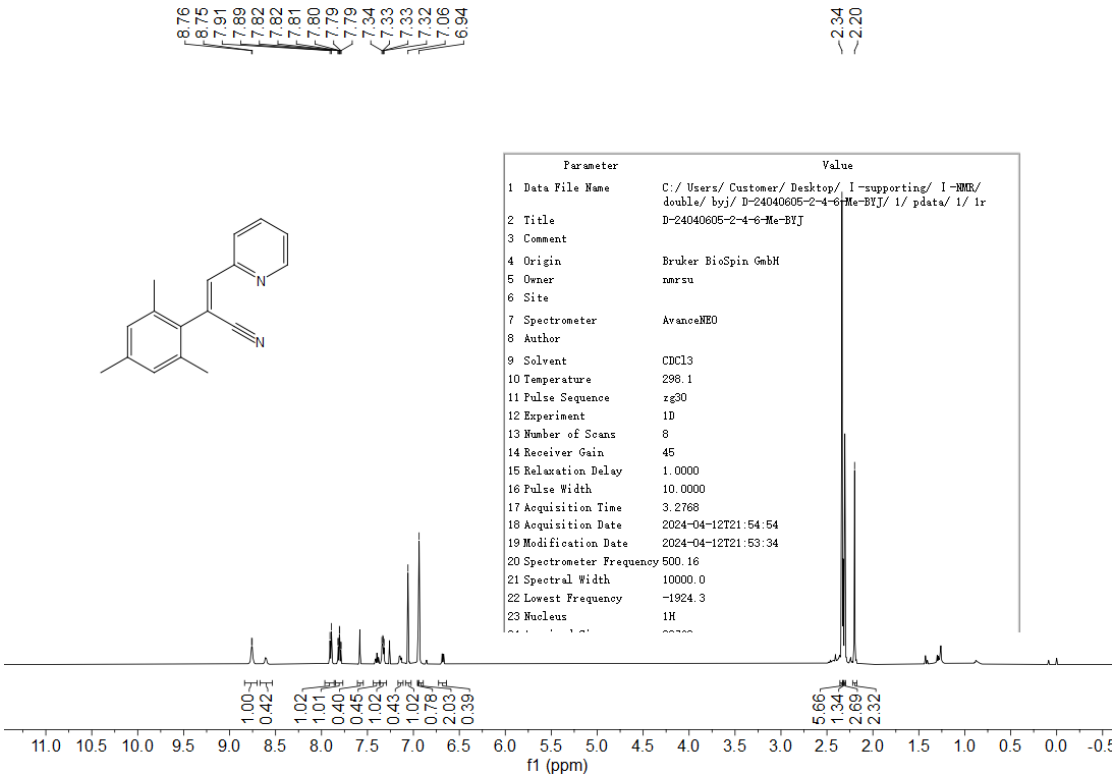


(*Z*)-3-(pyridin-2-yl)-2-(p-tolyl)acrylonitrile (3da)





(*Z*)-2-mesityl-3-(pyridin-2-yl)acrylonitrile (3ea)


8.76
8.75
7.91
7.89
7.82
7.81
7.80
7.79
7.79
7.34
7.33
7.33
7.32
7.06
6.94
2.34
2.20
N
N
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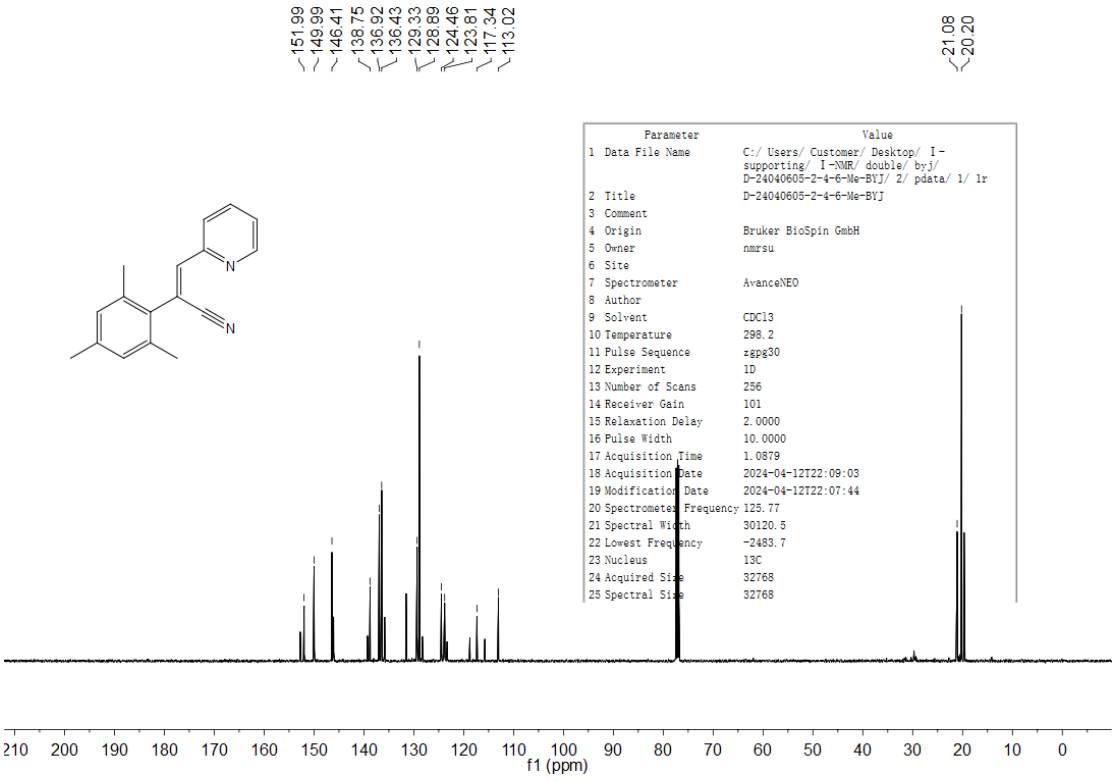
2 Title D-24040605-2-4-6-Me-BYJ
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.1
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 8
14 Receiver Gain 45
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2024-04-12T21:54:54
19 Modification Date 2024-04-12T21:53:34
20 Spectrometer Frequency 500.16
21 Spectral Width 10000.0
22 Lowest Frequency -1924.3
23 Nucleus 1H
1.00
0.42
1.02
1.01
0.40
0.45
1.02
0.43
1.02
0.78
2.03
0.39
5.66
1.34
2.69
2.32
f1 (ppm)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149.99
146.41
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128.89
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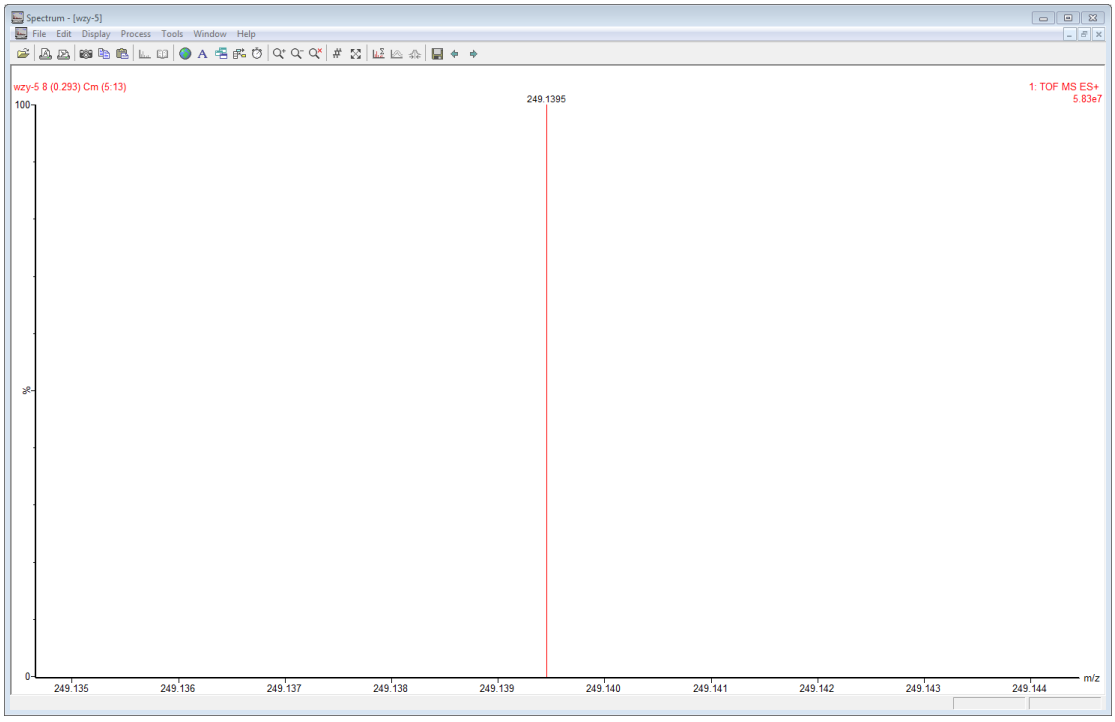
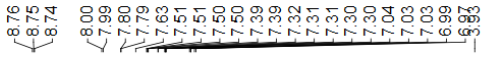
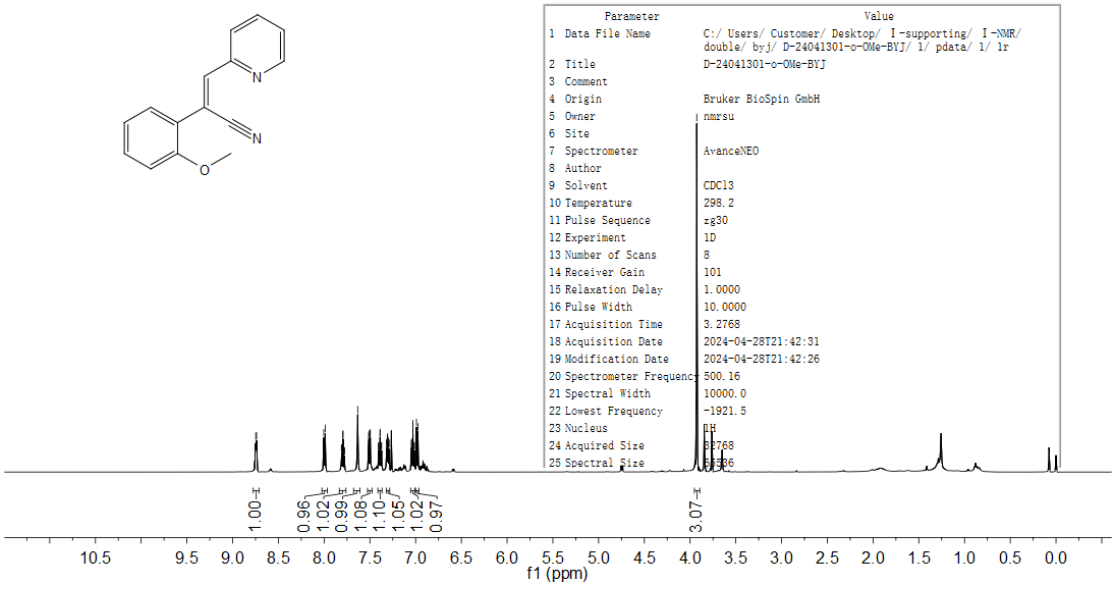
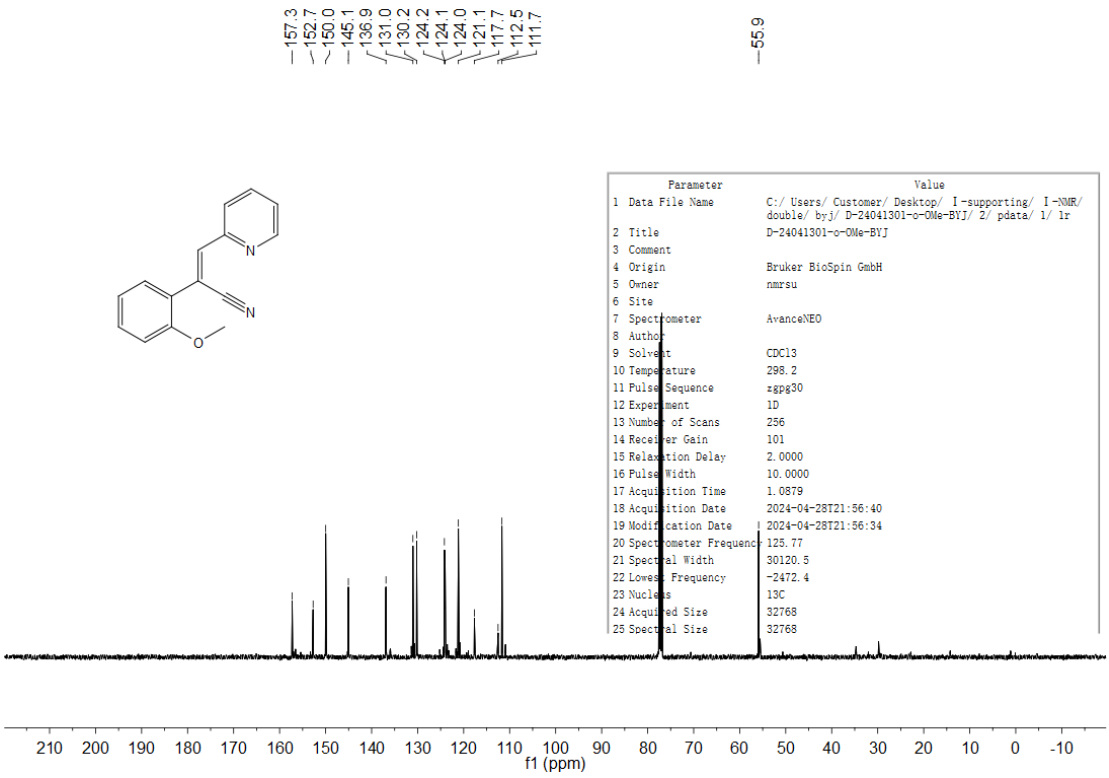
123.81
117.34
113.02
21.08
20.20
N
N
Parameter Value
1 Data File Name C:/ Users/ Customer/ Desktop/ I-supporting/ I-NMR/ double/ byj/ D-24040605-2-4-6-Me-BYJ/ 2/ pdata/ 1/ 1r
2 Title D-24040605-2-4-6-Me-BYJ
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.2
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 2024-04-12T22:09:03
19 Modification Date 2024-04-12T22:07:44
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2483.7
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
f1 (ppm)

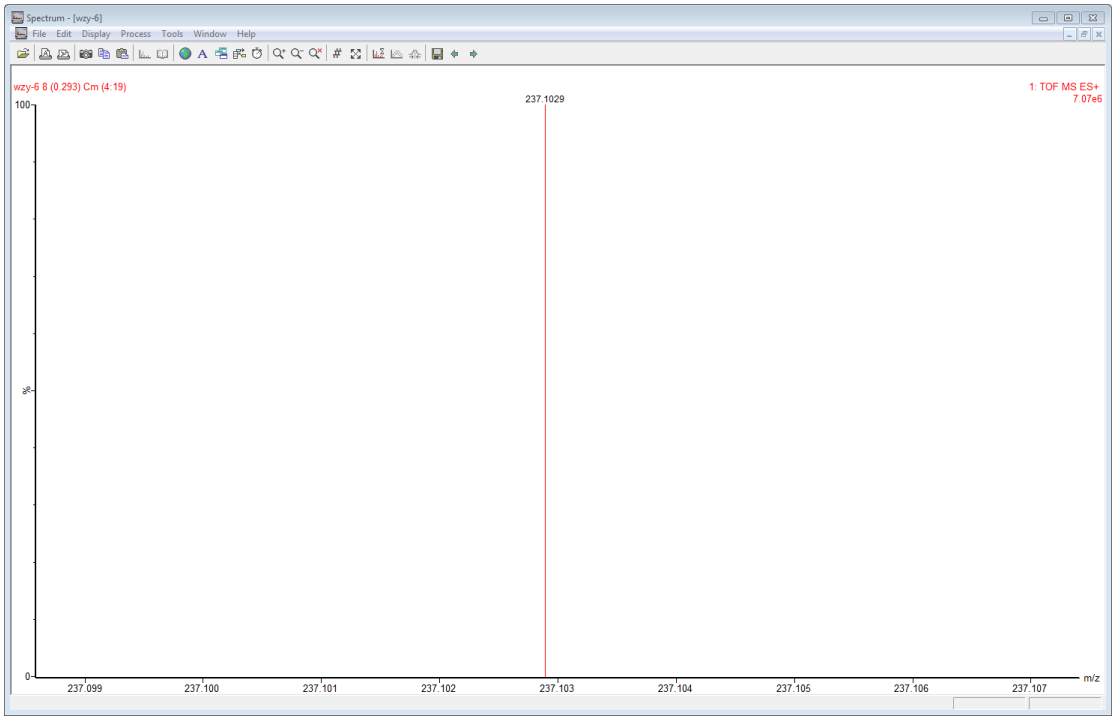


(*Z*)-2-(2-methoxyphenyl)-3-(pyridin-2-yl)acrylonitrile (3fa)

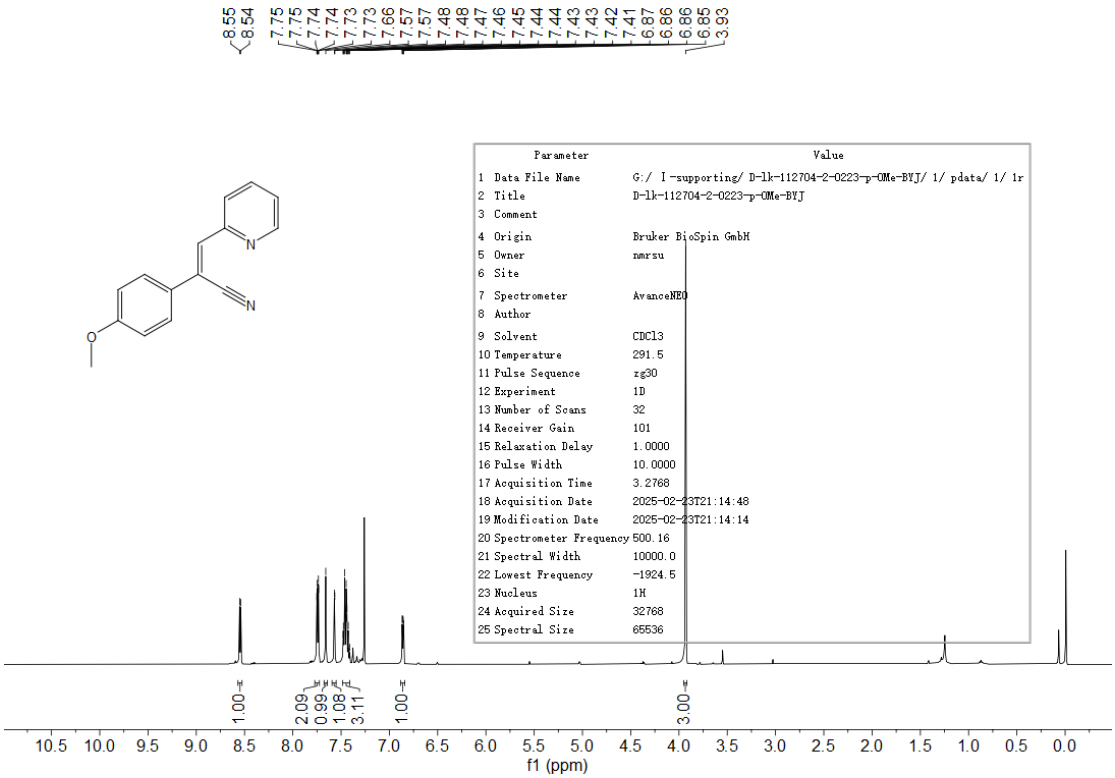


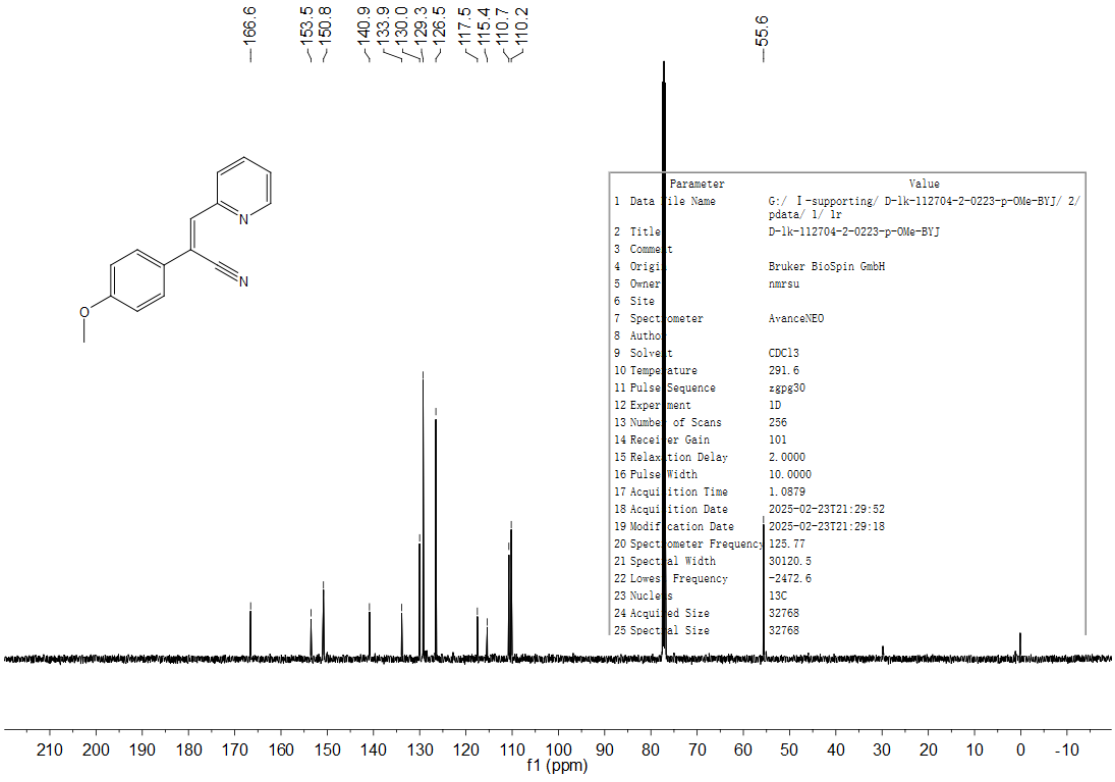




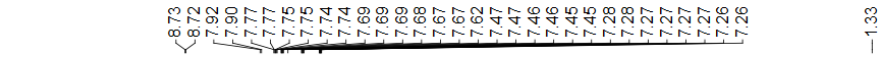


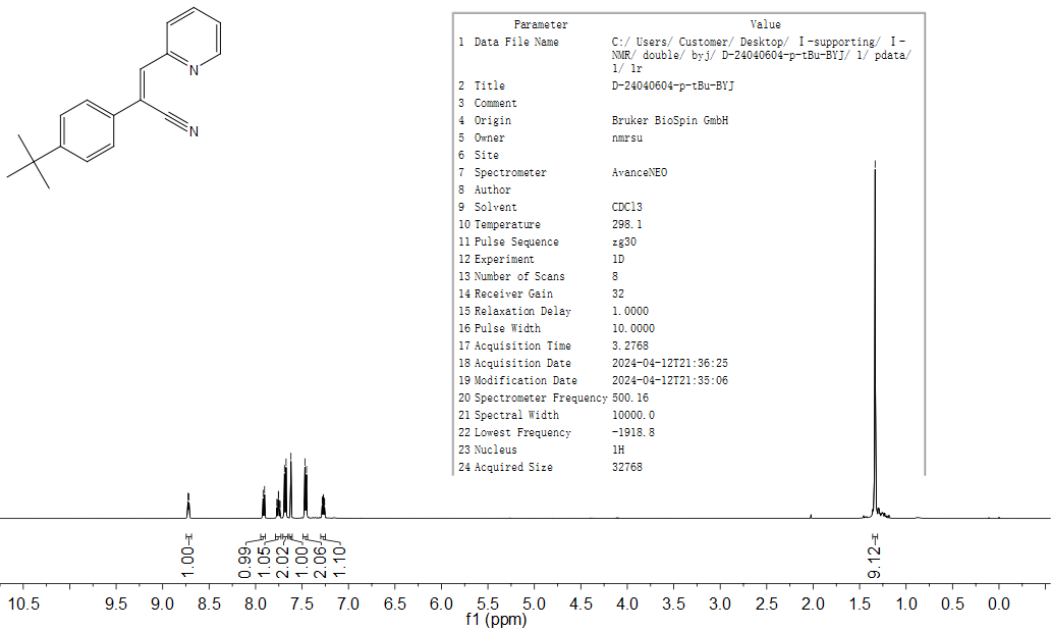
(*Z*)-2-(4-methoxyphenyl)-3-(pyridin-2-yl)acrylonitrile (3ga)





(*Z*)-2-(4-(*tert*-butyl)phenyl)-3-(pyridin-2-yl)acrylonitrile (3ha)





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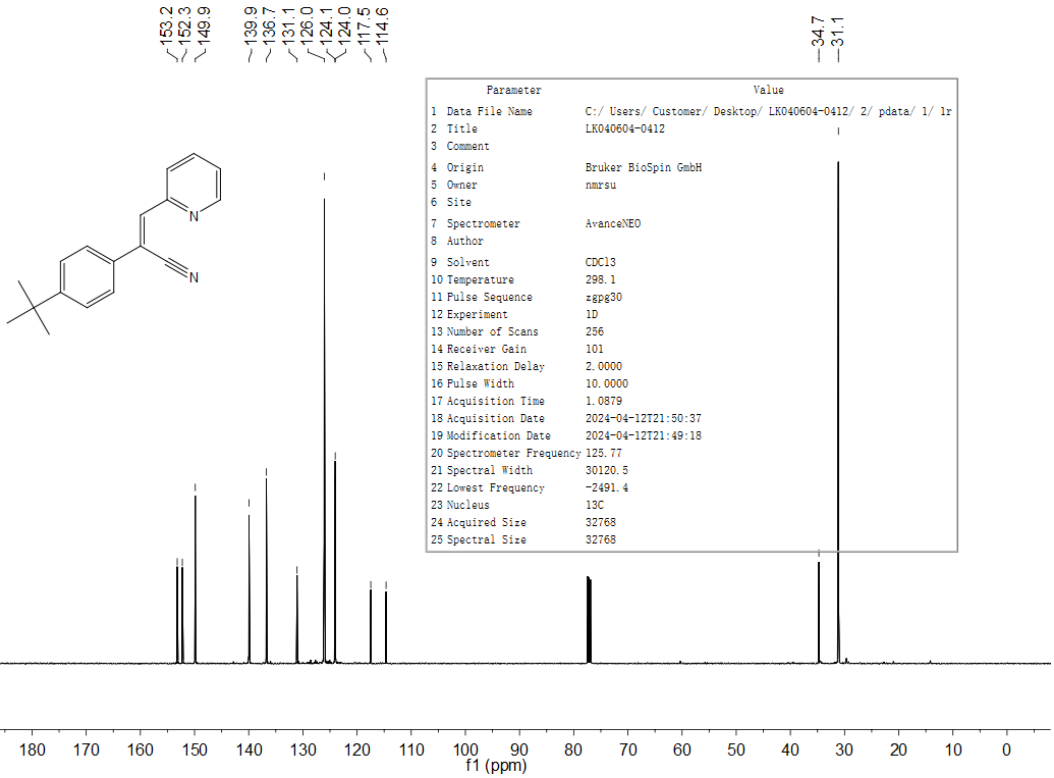
2 Title	D-24040604-p-tBu-BYJ
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	32
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2024-04-12T21:36:25
19 Modification Date	2024-04-12T21:35:06
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1918.8
23 Nucleus	1H
24 Acquired Size	32768



Parameter	Value
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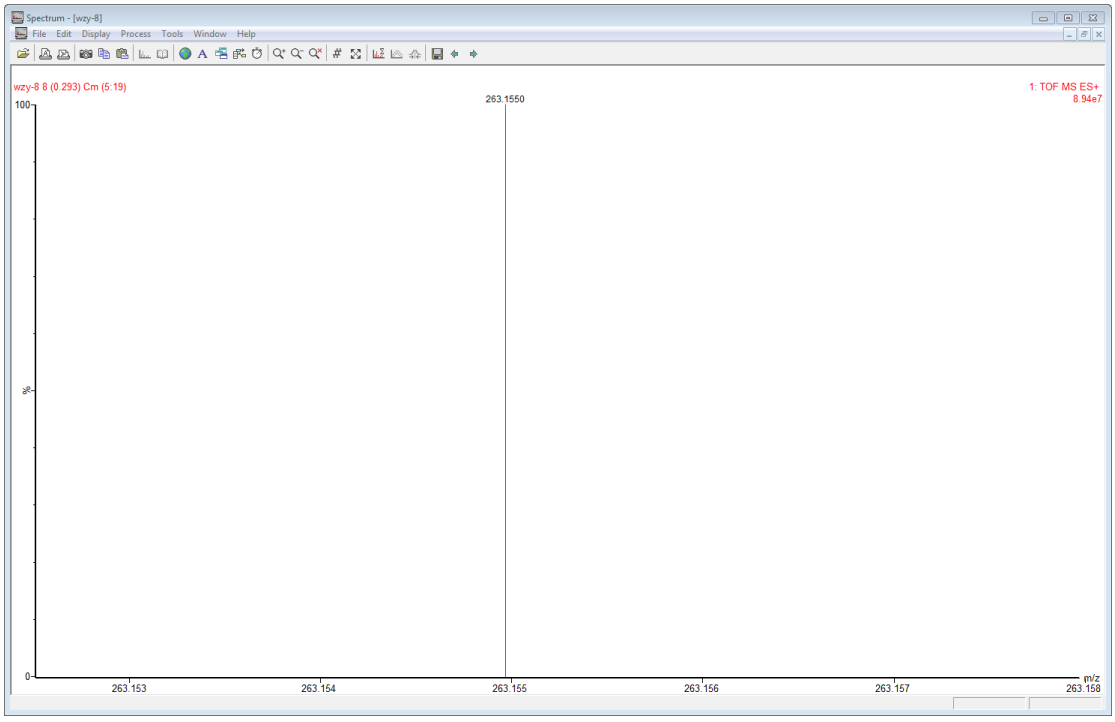
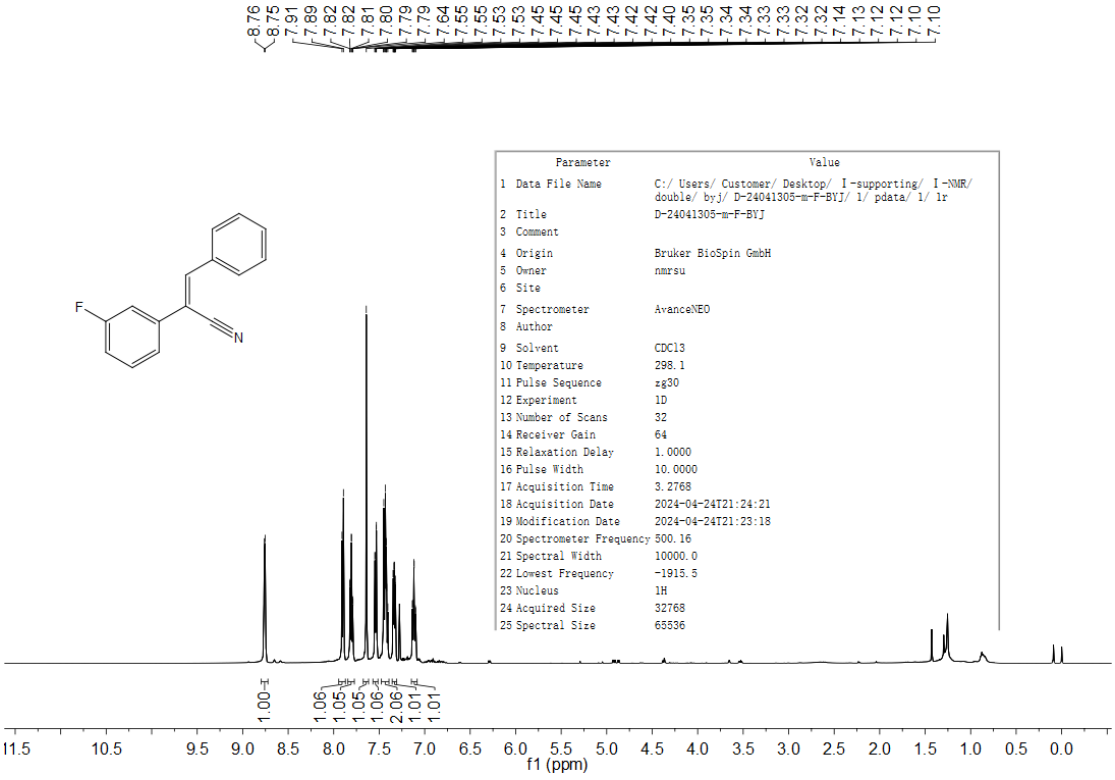
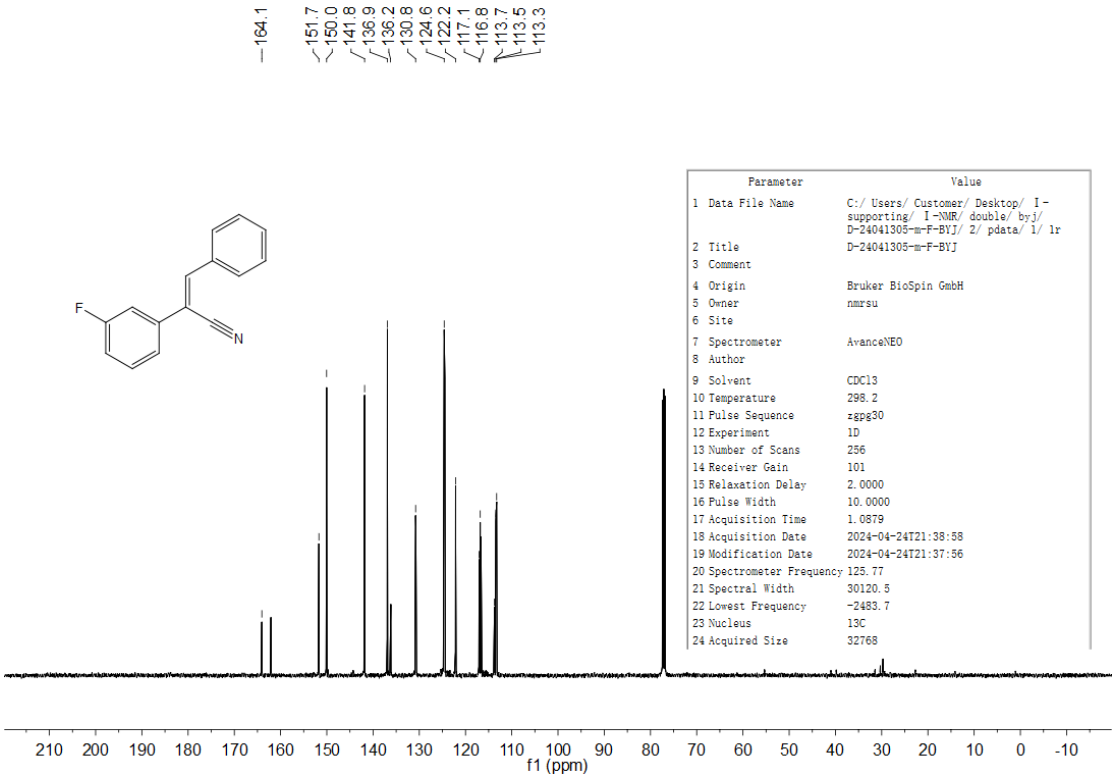
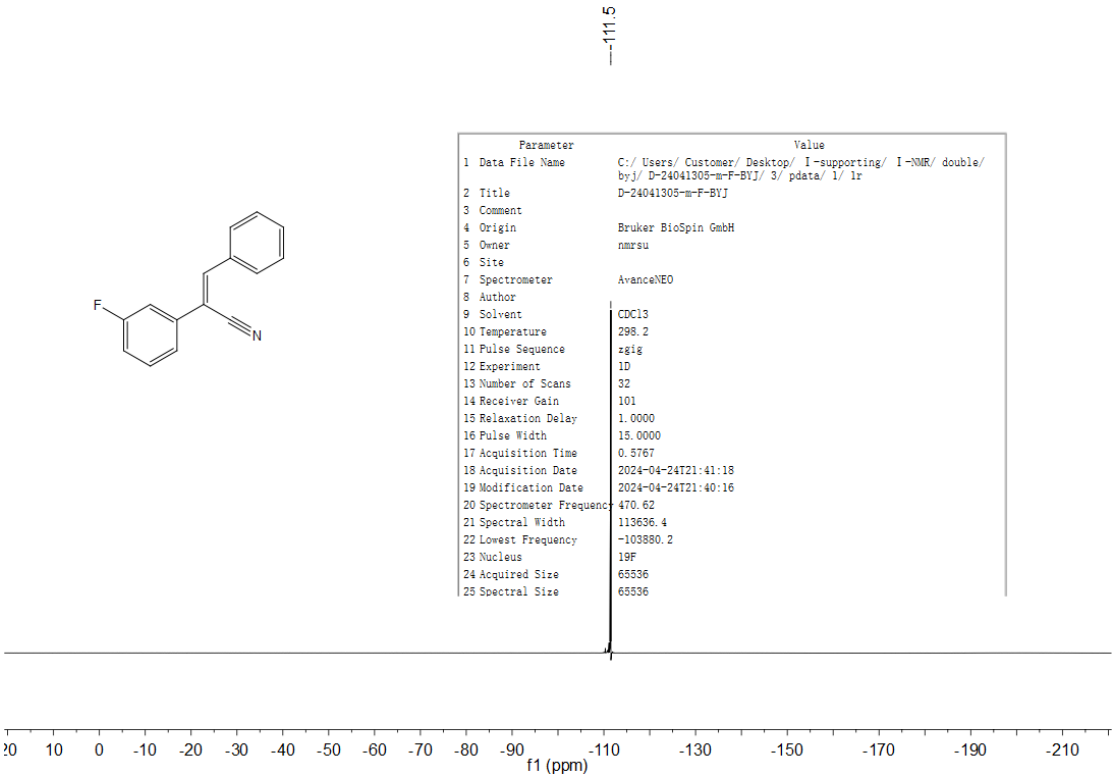
2 Title	LK040604-0412
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2024-04-12T21:50:37
19 Modification Date	2024-04-12T21:49:18
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2491.4
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768



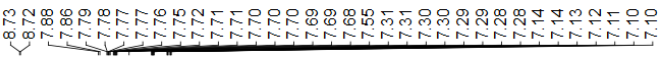
(*Z*)-2-(3-fluorophenyl)-3-(pyridin-2-yl)acrylonitrile (3ia)

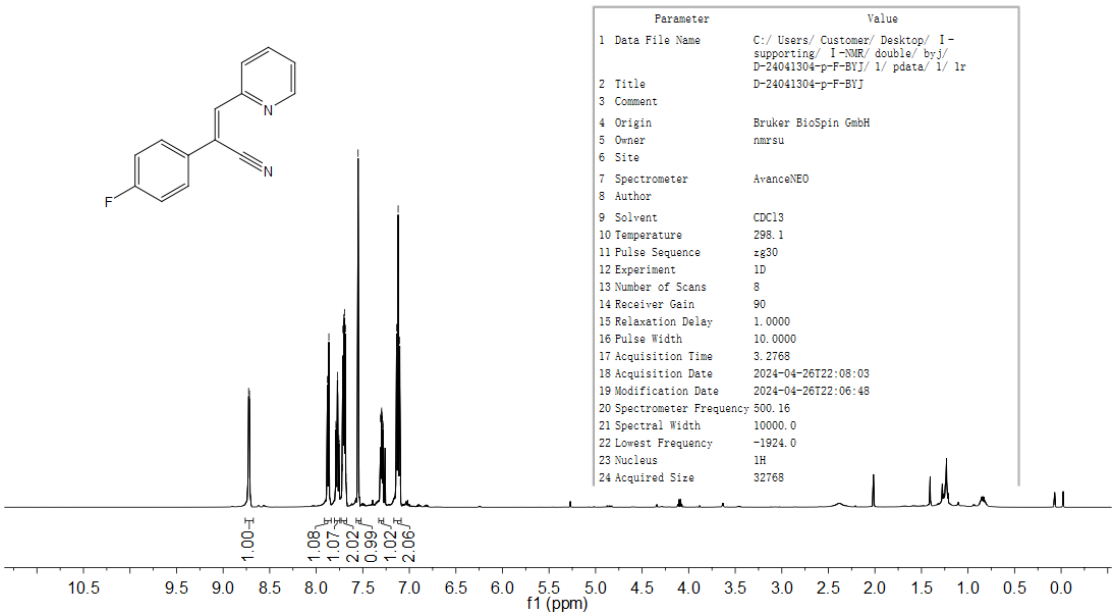






(*Z*)-2-(4-fluorophenyl)-3-(pyridin-2-yl)acrylonitrile (3ja)





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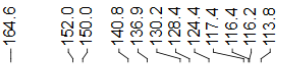
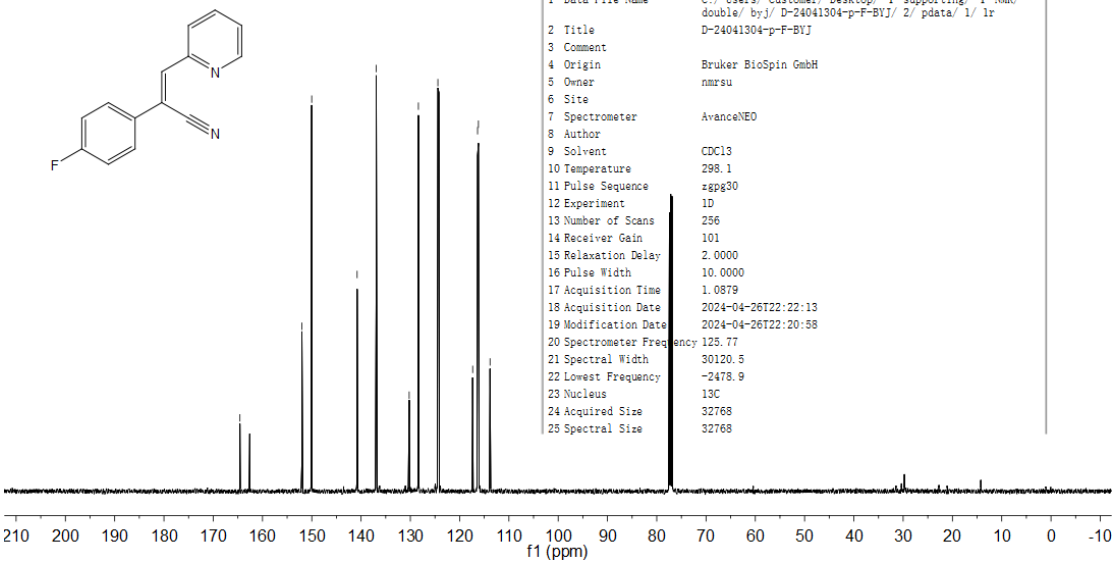
2 Title	D-24041304-p-F-BYJ
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	90
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2024-04-26T22:08:03
19 Modification Date	2024-04-26T22:06:48
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1924.0
23 Nucleus	1H
24 Acquired Size	32768





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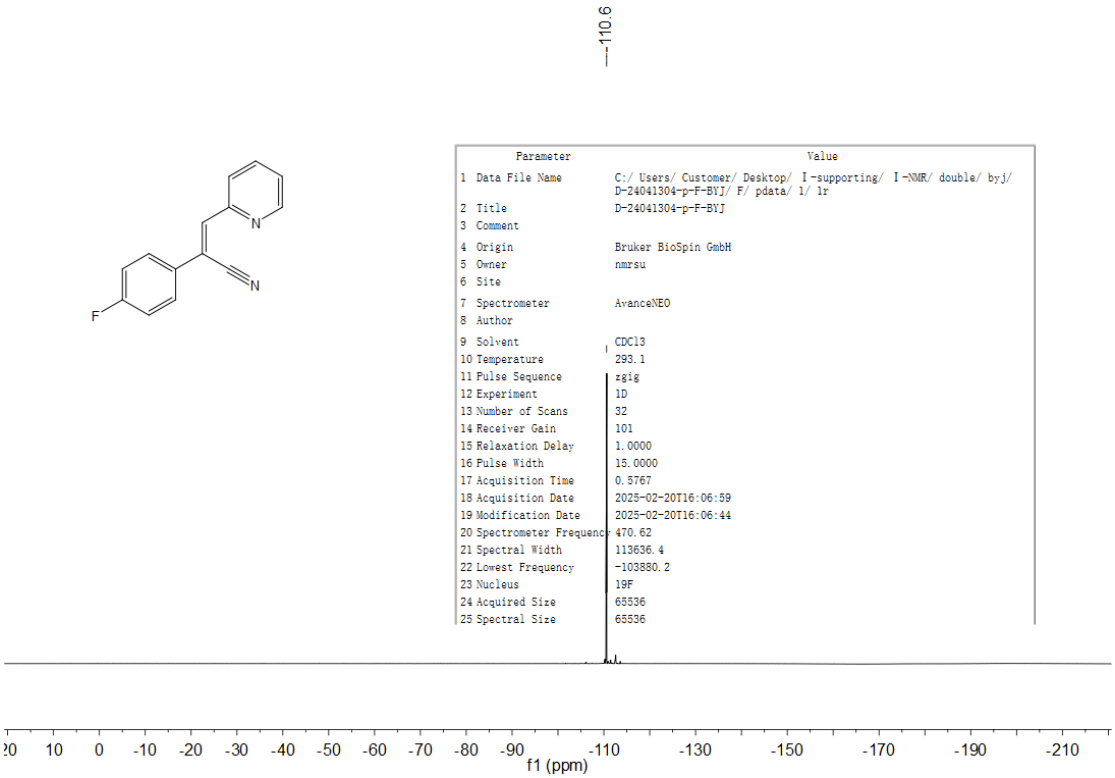
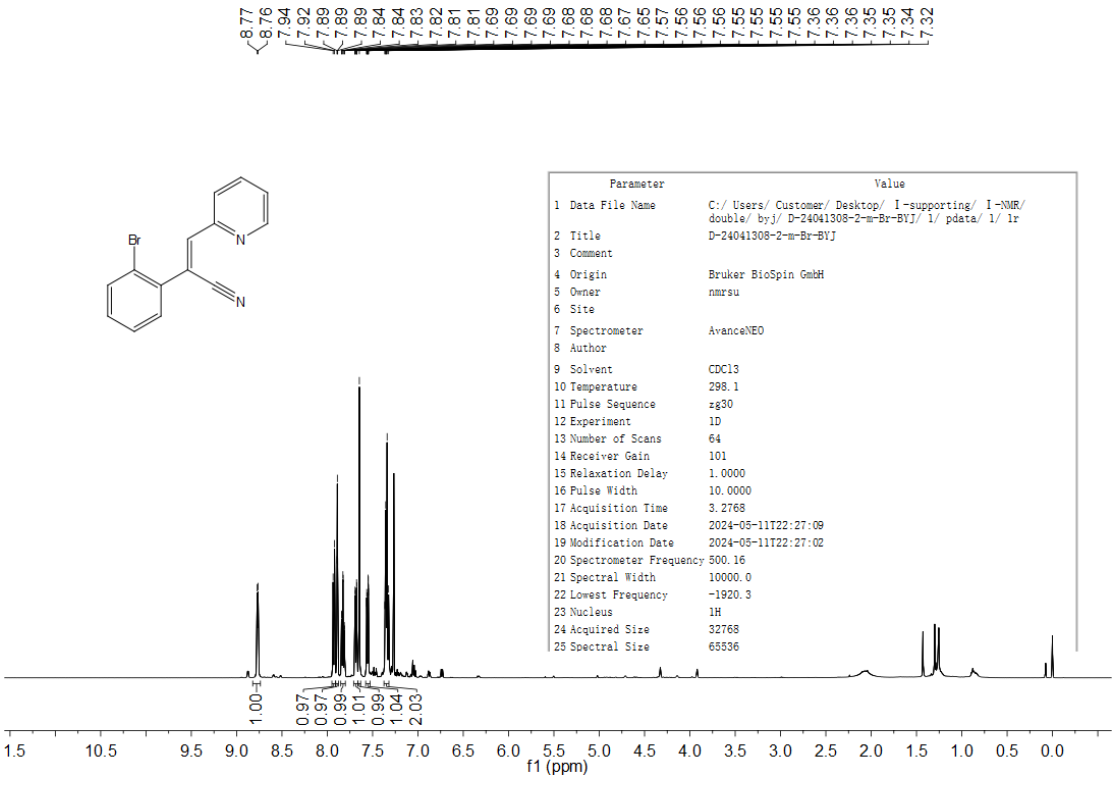
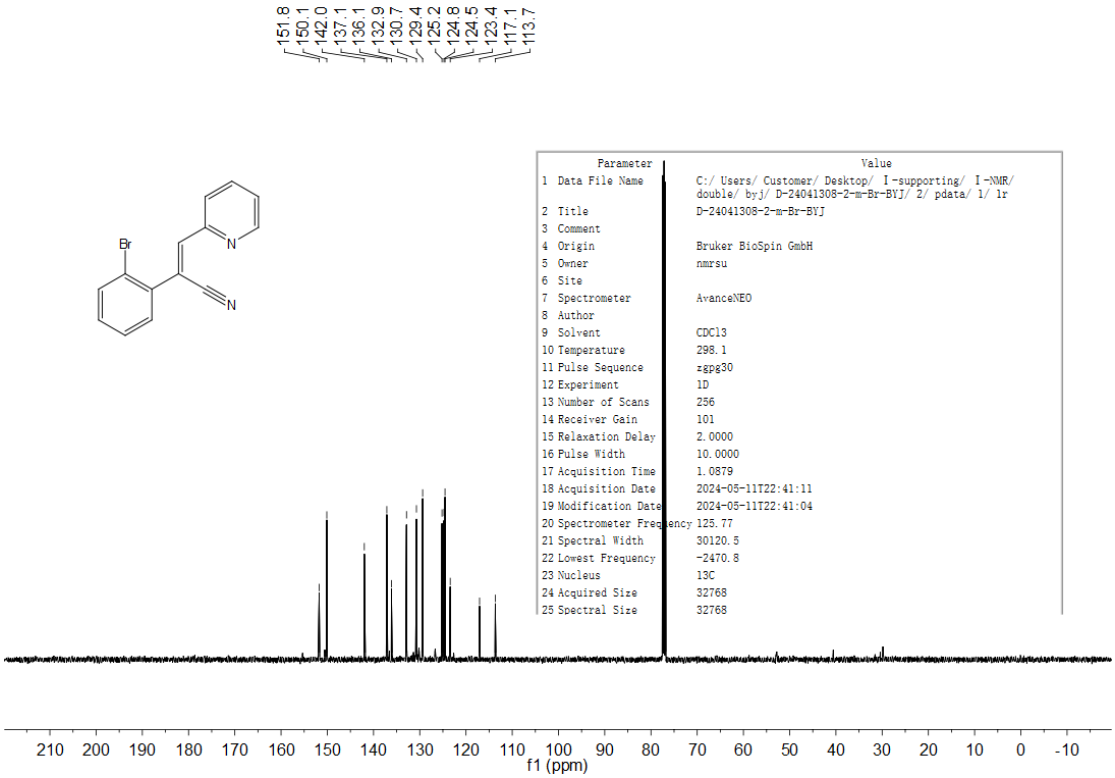
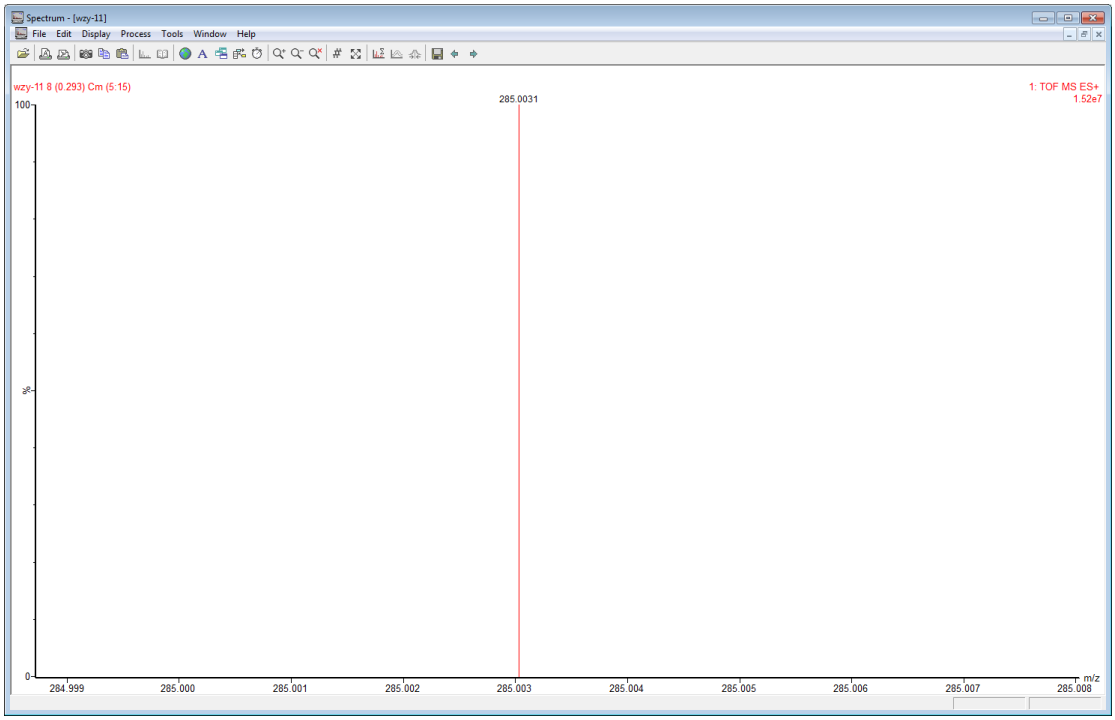
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2024-04-26T22:22:13
19 Modification Date	2024-04-26T22:20:58
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2478.9
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768



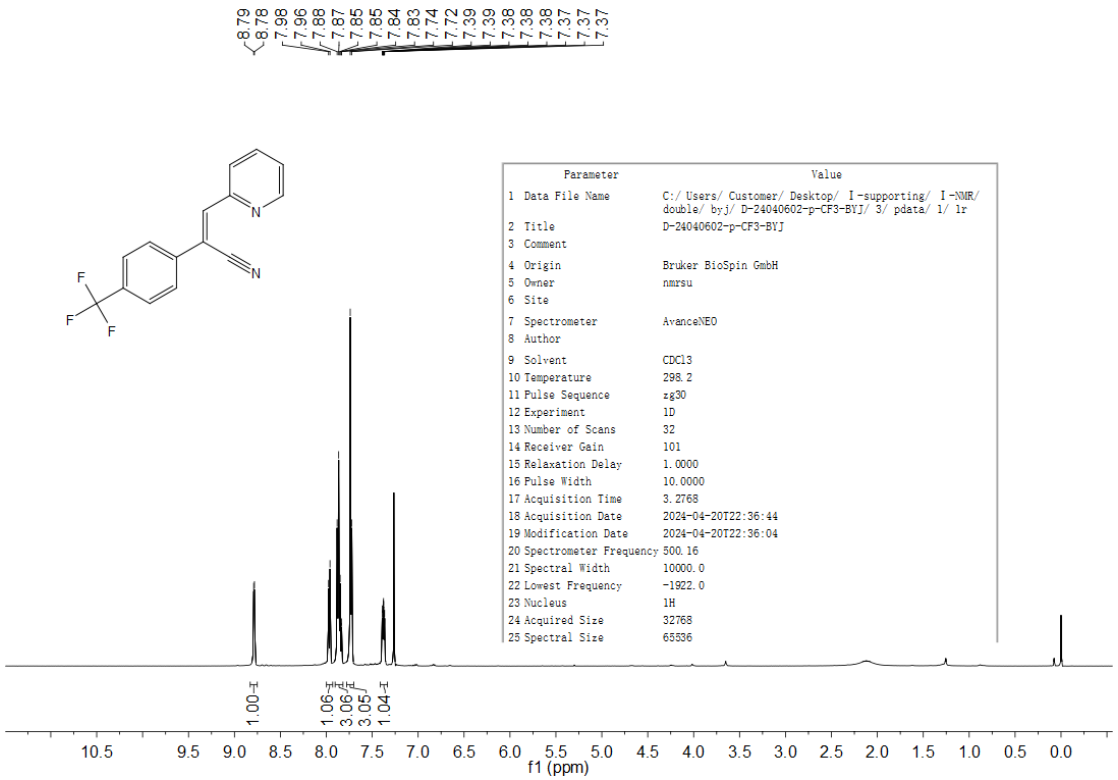
(*Z*)-2-(3-bromophenyl)-3-(pyridin-2-yl)acrylonitrile (3ka)







(*Z*)-3-(pyridin-2-yl)-2-(4-(trifluoromethyl)phenyl)acrylonitrile (3la)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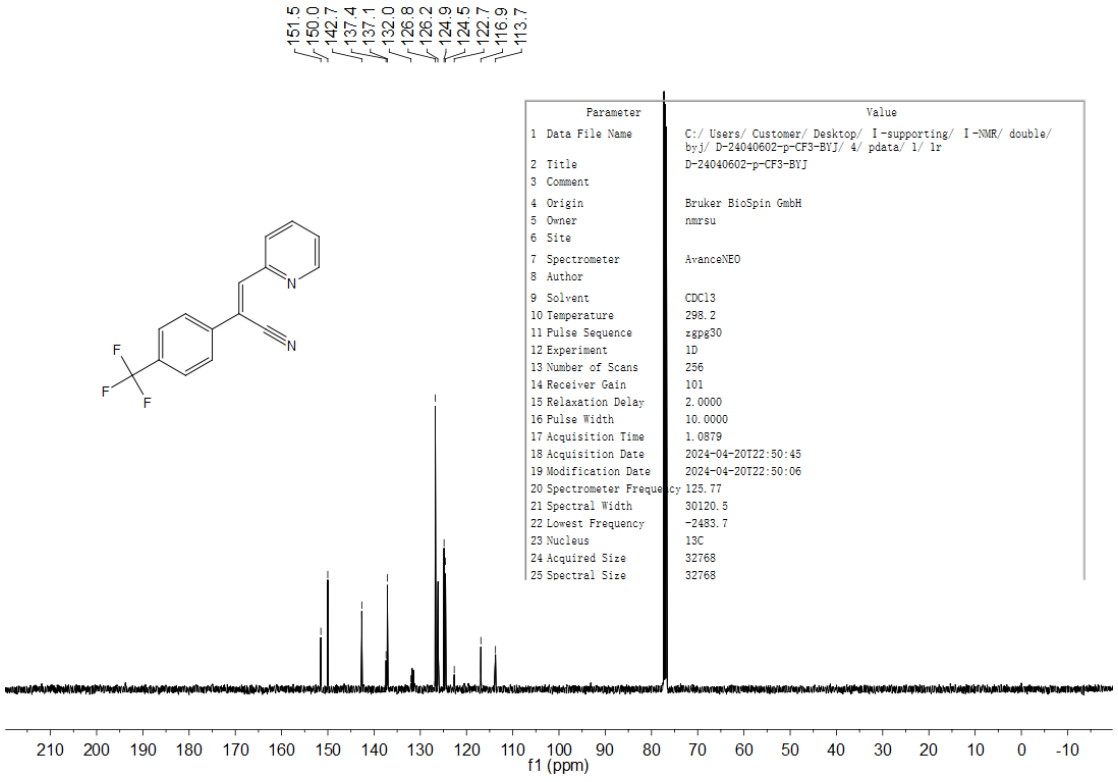
8.78
7.98
7.96
7.88
7.87
7.85
7.85
7.84
7.83
7.74
7.72
7.39
7.38
7.38
7.37
7.37
7.37
N
N
F
F
F
Parameter Value
1 Data File Name C:/ Users/ Customer/ Desktop/ I-supporting/ I-NMR/ double/ byj/ D-24040602-p-CF3-BYJ/ 3/ pdata/ 1/ 1r
2 Title D-24040602-p-CF3-BYJ
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.2
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 32
14 Receiver Gain 101
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2024-04-20T22:36:44
19 Modification Date 2024-04-20T22:36:04
20 Spectrometer Frequency 500.16
21 Spectral Width 10000.0
22 Lowest Frequency -1922.0
23 Nucleus 1H
24 Acquired Size 32768
25 Spectral Size 65536
1.00
1.06
3.06
3.05
1.04
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)


151.5
150.0
142.7
137.4
137.1
132.0
126.8
126.2
124.9
124.5
122.7
116.9
113.7
N
N
F
F
F
Parameter Value
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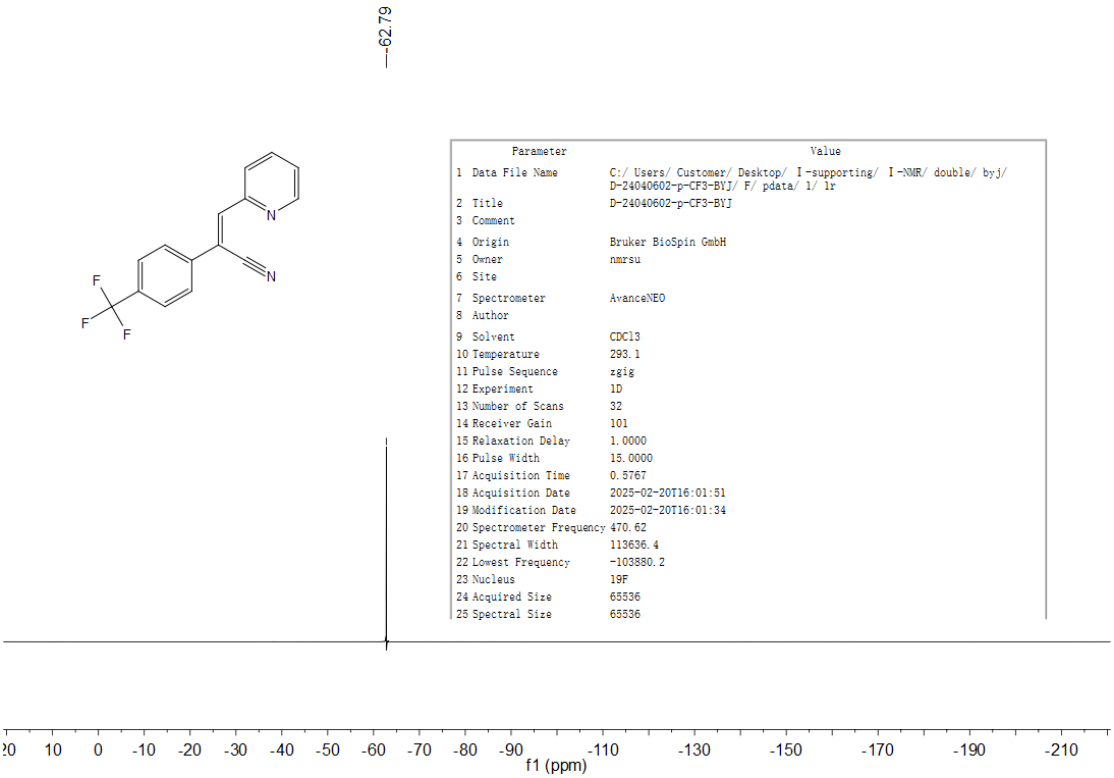
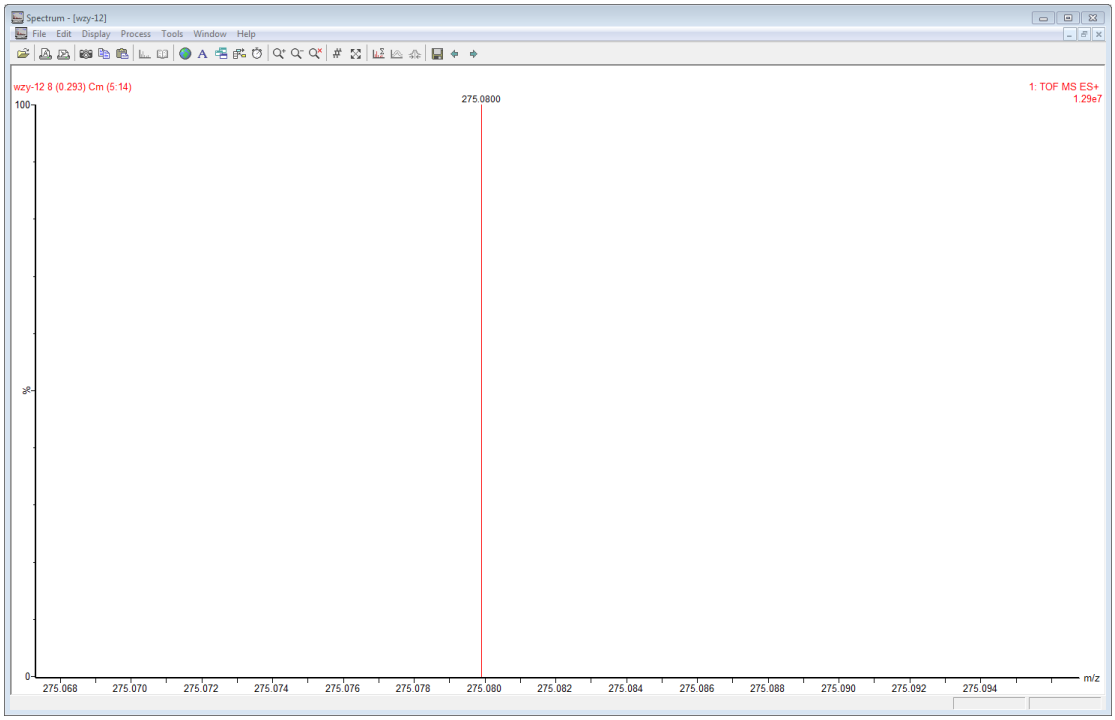
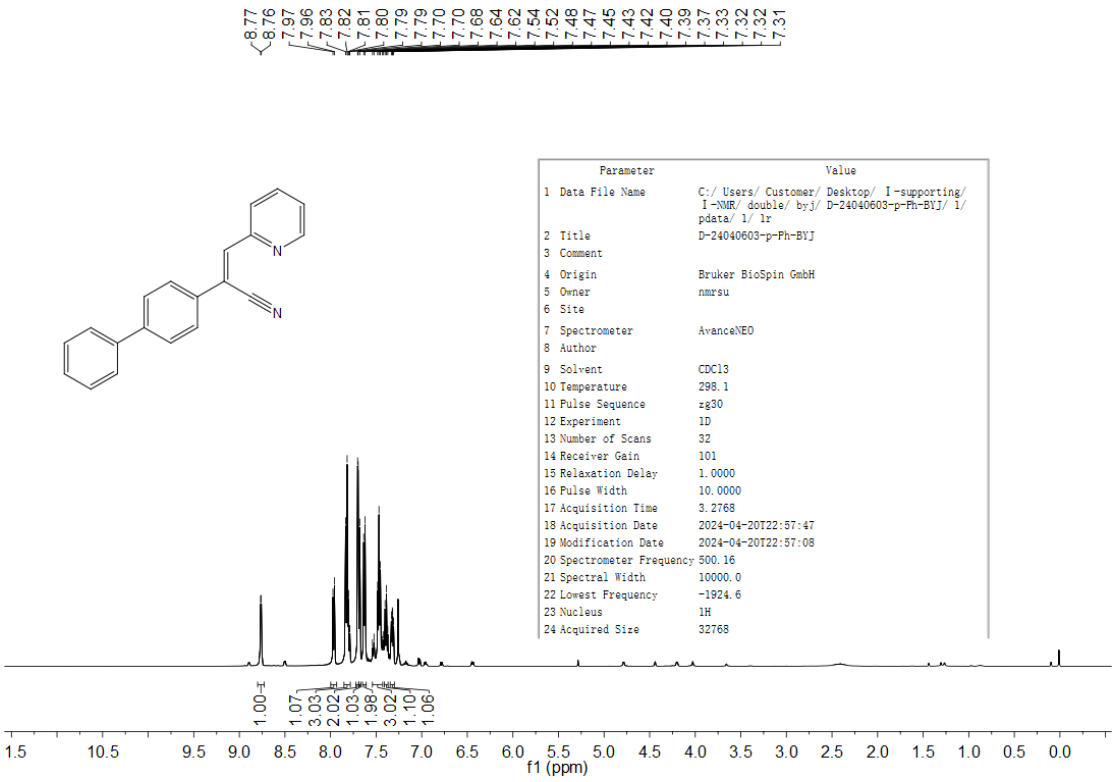
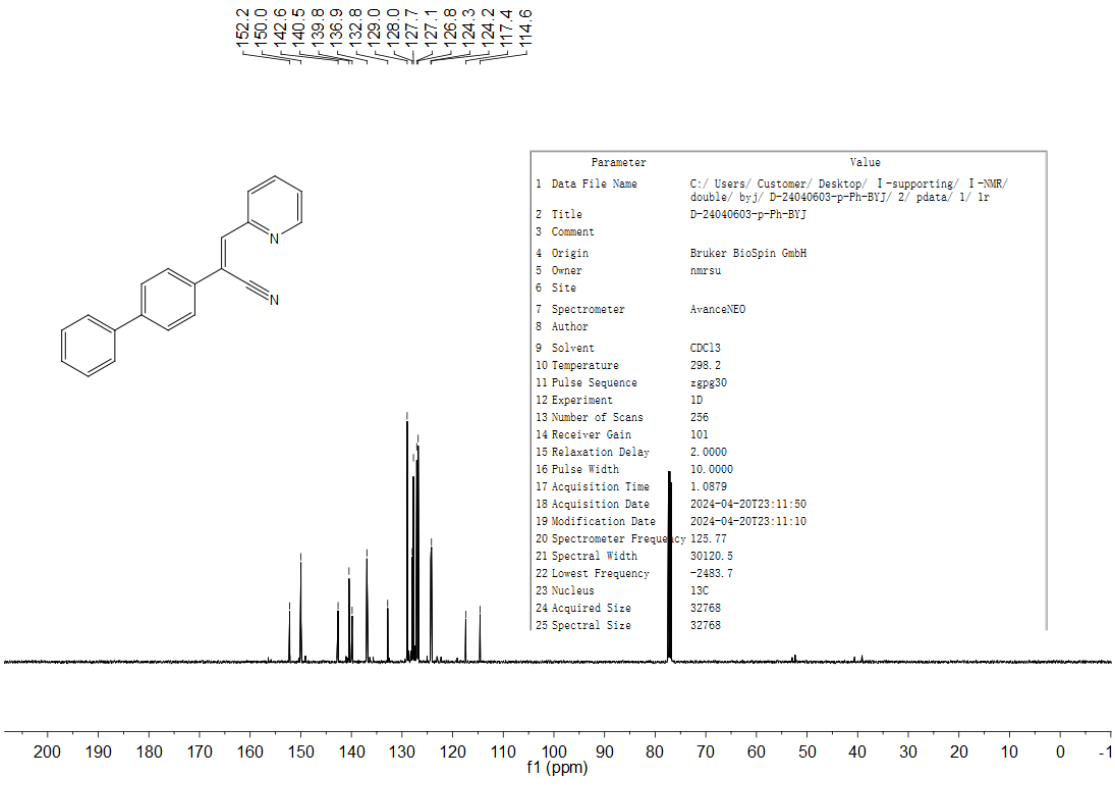
2 Title D-24040602-p-CF3-BYJ
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.2
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2024-04-20T22:50:45
19 Modification Date 2024-04-20T22:50:06
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2483.7
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)



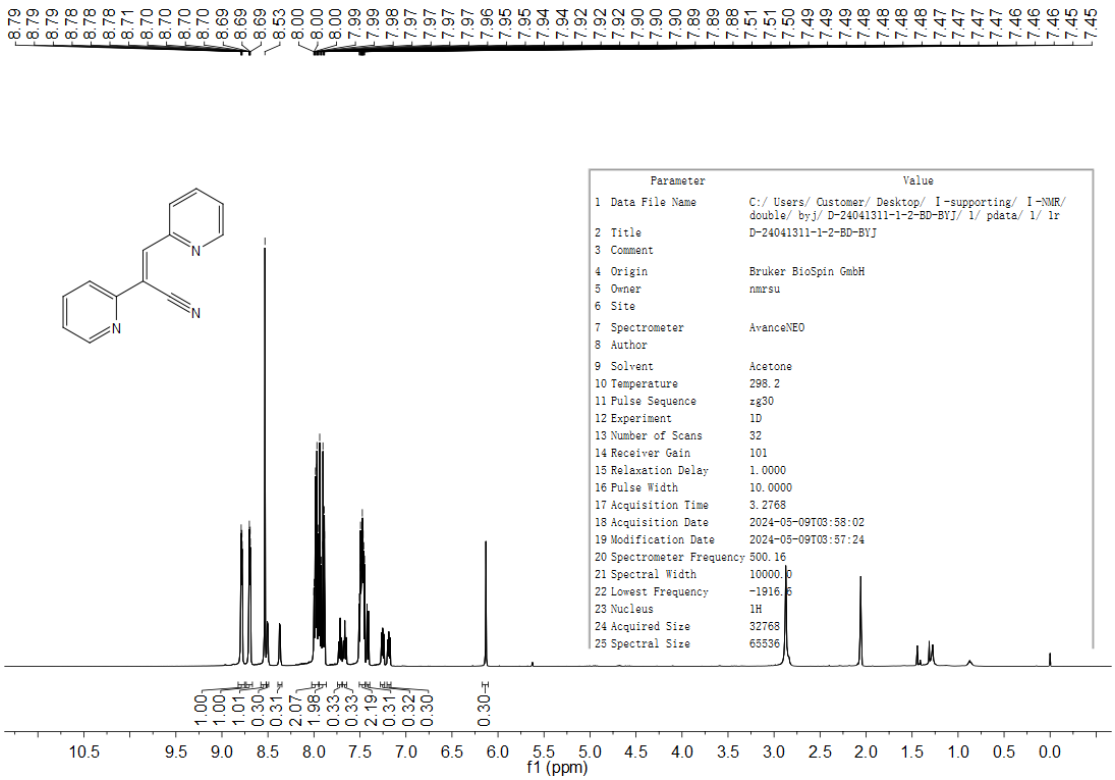


(*Z*)-2-([1,1'-biphenyl]-4-yl)-3-(pyridin-2-yl)acrylonitrile (3ma)





(*Z*)-2,3-di(pyridin-2-yl)acrylonitrile (3na)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N
N
N
Parameter Value
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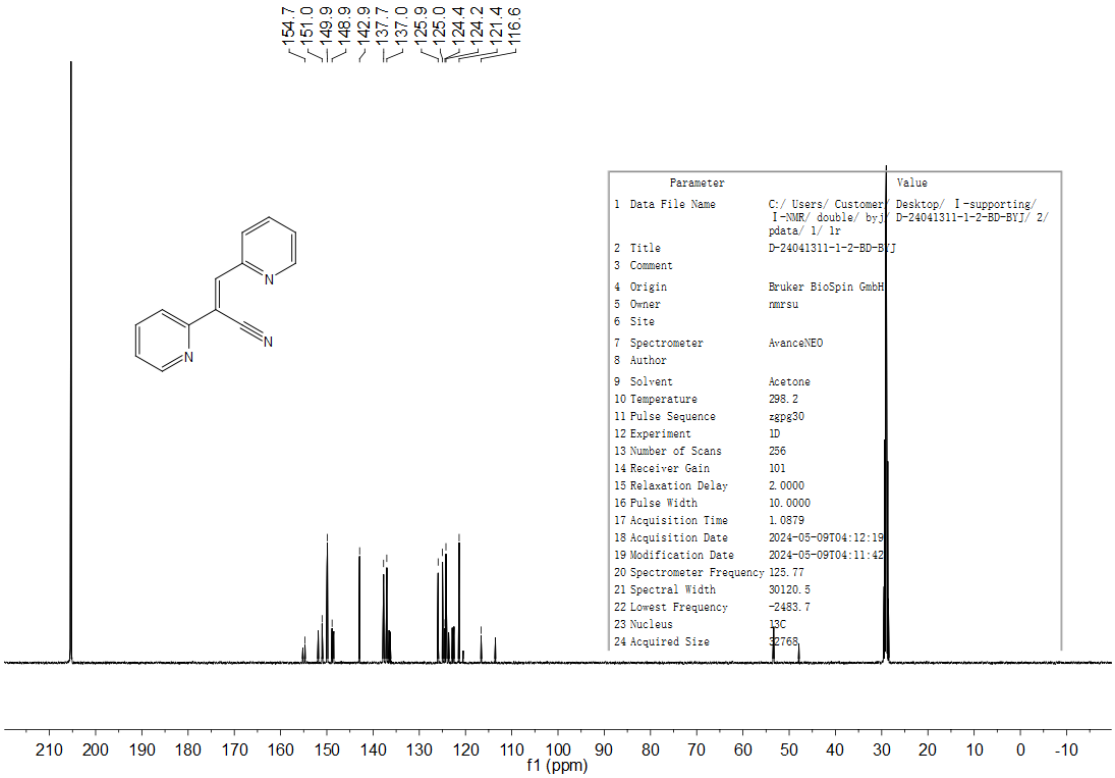
2 Title D-24041311-1-2-BD-BYJ
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent Acetone
10 Temperature 298.2
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 32
14 Receiver Gain 101
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2024-05-09T03:58:02
19 Modification Date 2024-05-09T03:57:24
20 Spectrometer Frequency 500.16
21 Spectral Width 10000.0
22 Lowest Frequency -1916.6
23 Nucleus 1H
24 Acquired Size 32768
25 Spectral Size 65536
1.00 1.00 1.01 0.30 0.31 2.07 1.98 0.33 0.33 2.19 0.31 0.32 0.30 0.30
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)


154.7 151.0 149.9 148.9 142.9 137.7 137.0 125.9 125.0 124.4 124.2 121.4 116.6
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N
N
Parameter Value
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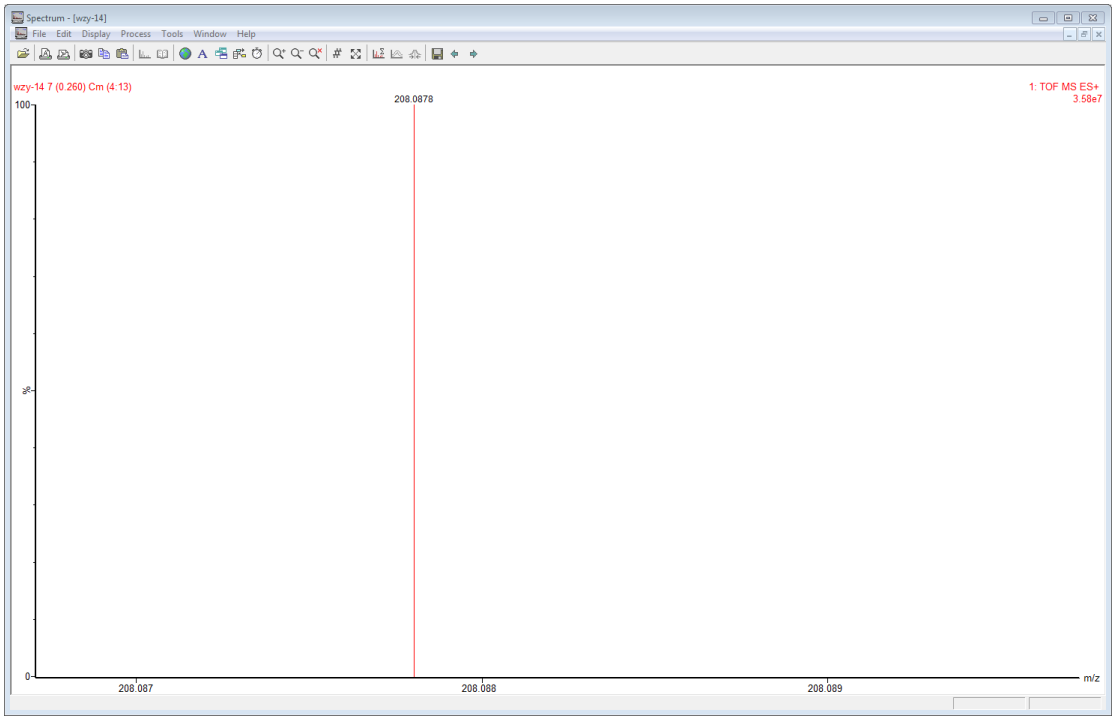
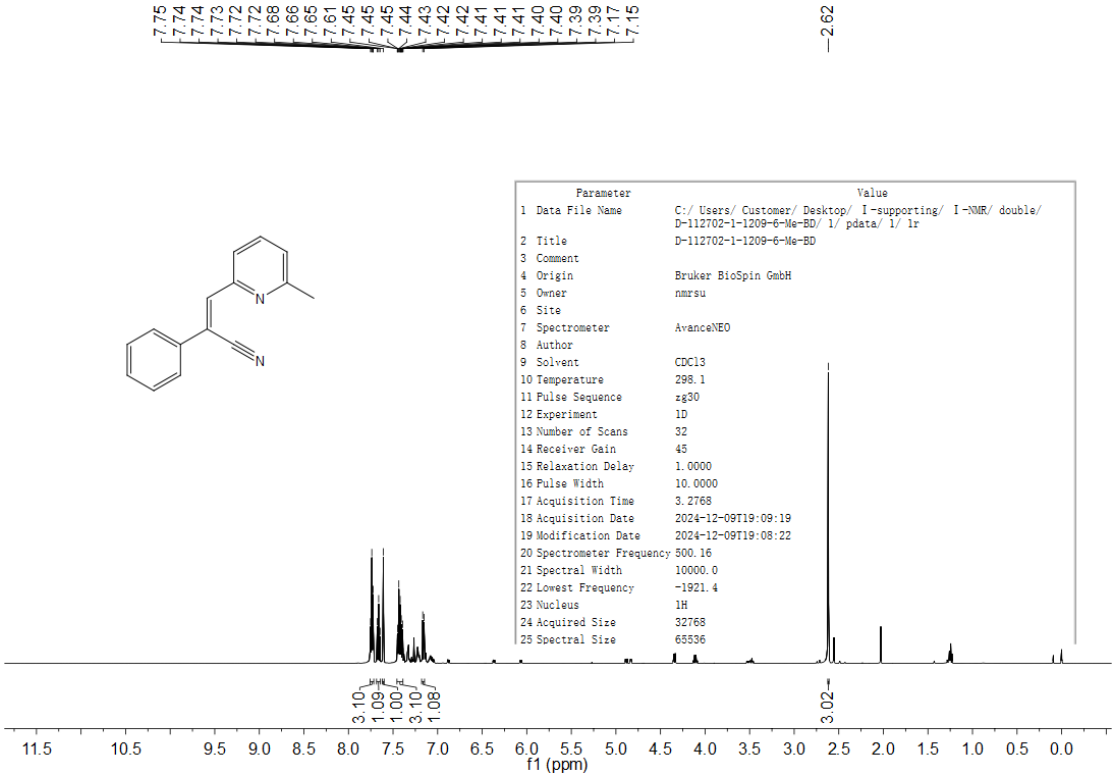
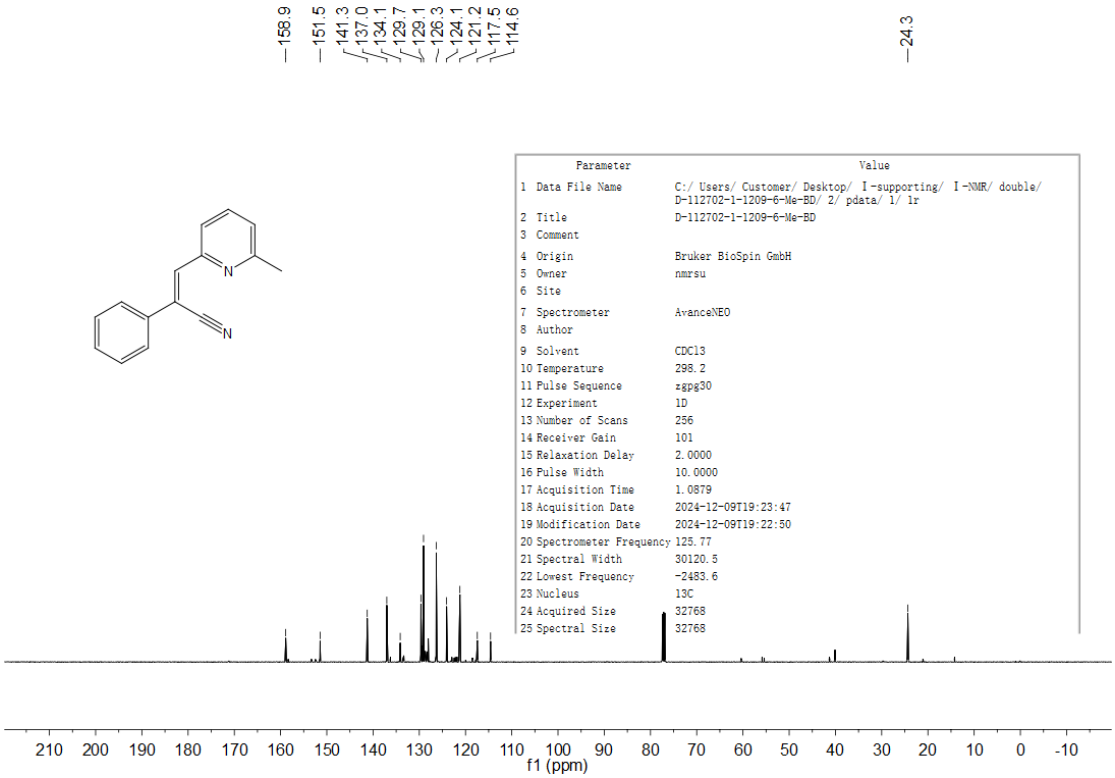
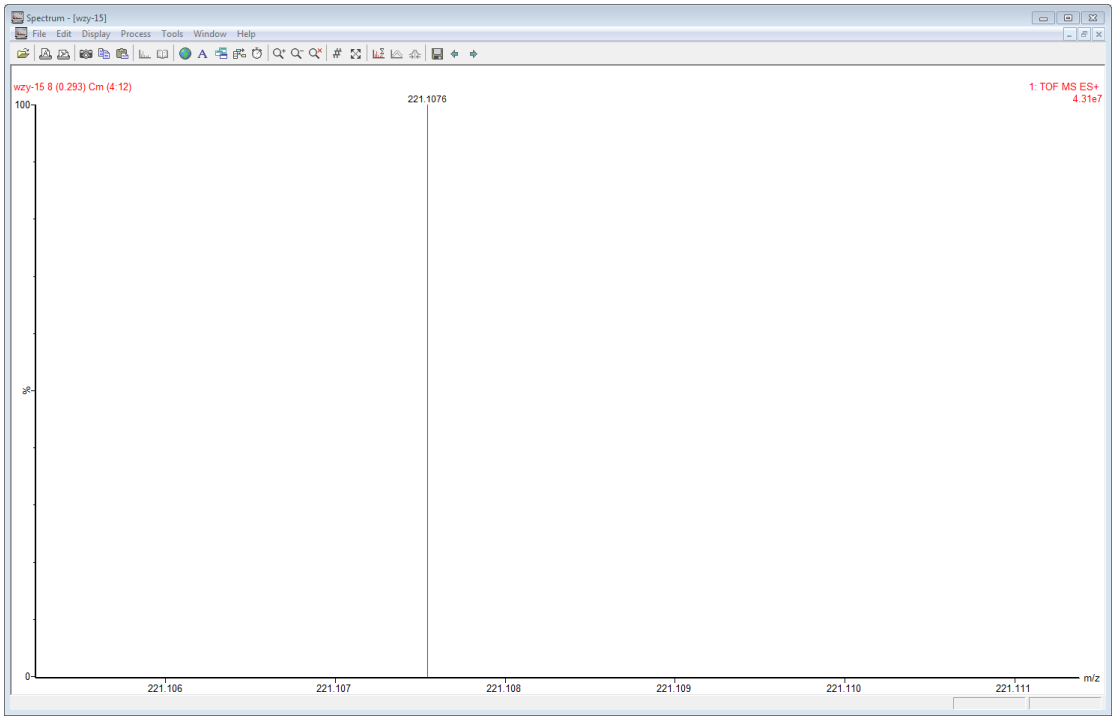
2 Title D-24041311-1-2-BD-BYJ
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent Acetone
10 Temperature 298.2
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2024-05-09T04:12:19
19 Modification Date 2024-05-09T04:11:42
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2483.7
23 Nucleus 13C
24 Acquired 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)



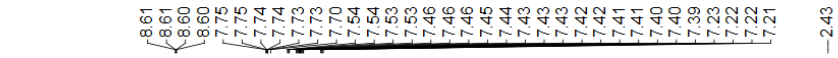
(*Z*)-3-(6-methylpyridin-2-yl)-2-phenylacrylonitrile (3ab)

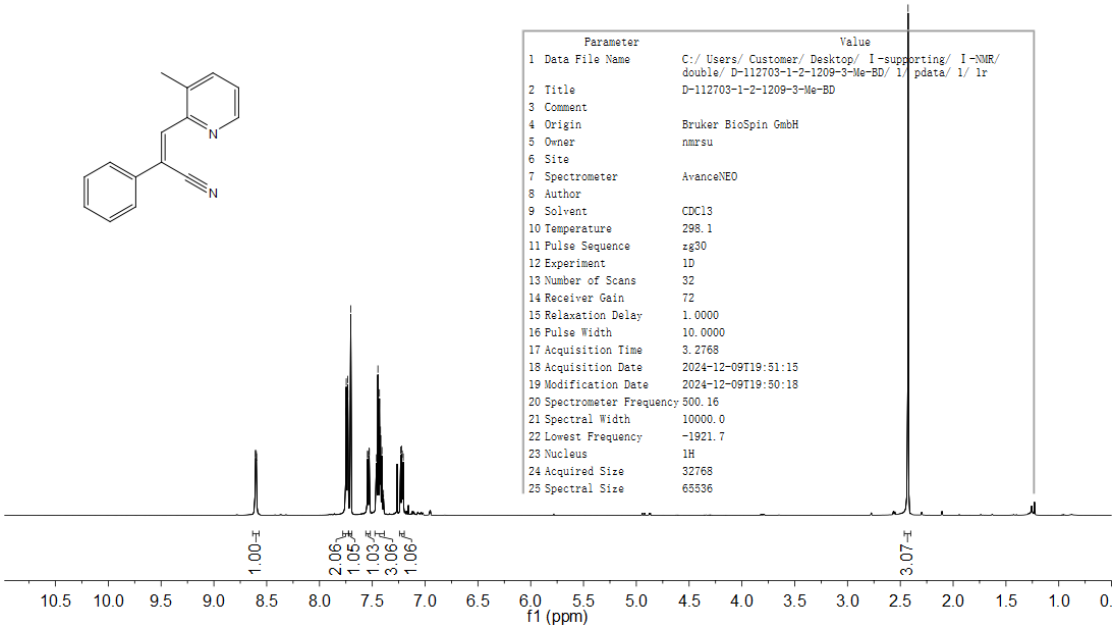






(*Z*)-3-(3-methylpyridin-2-yl)-2-phenylacrylonitrile (3ac)


8.61
8.61
8.60
8.60
7.75
7.75
7.74
7.74
7.73
7.73
7.70
7.54
7.54
7.53
7.53
7.46
7.46
7.45
7.44
7.43
7.43
7.43
7.42
7.42
7.41
7.41
7.40
7.40
7.39
7.23
7.22
7.22
7.21
2.43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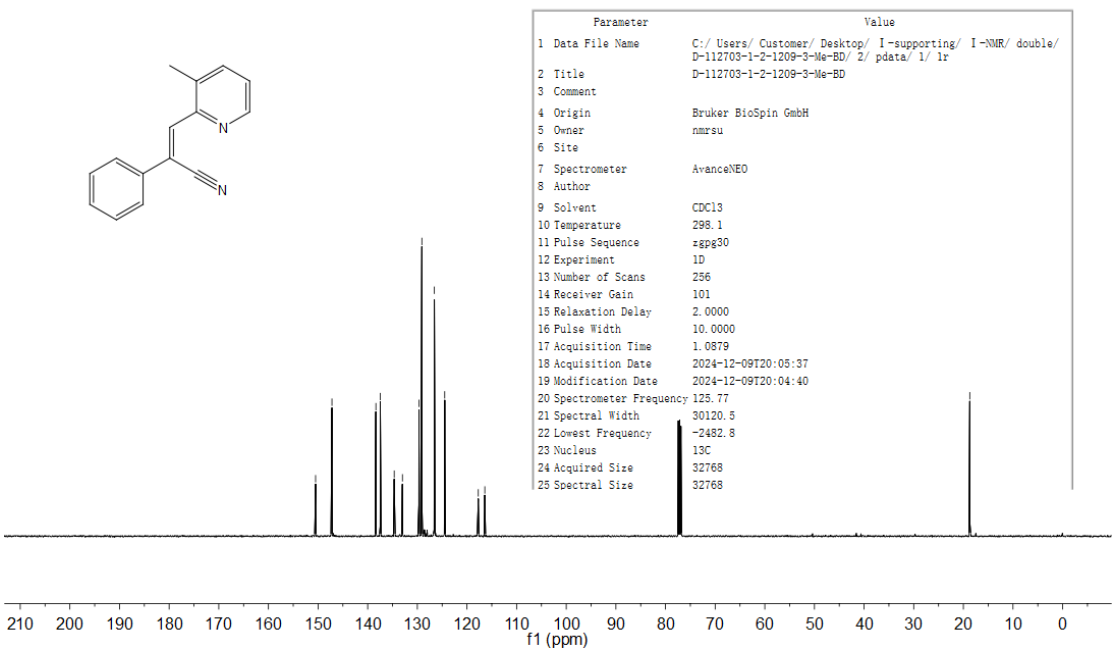
2 Title D-112703-1-2-1209-3-Me-BD
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.1
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 32
14 Receiver Gain 72
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2024-12-09T19:51:15
19 Modification Date 2024-12-09T19:50:18
20 Spectrometer Frequency 500.16
21 Spectral Width 10000.0
22 Lowest Frequency -1921.7
23 Nucleus 1H
24 Acquired Size 32768
25 Spectral Size 65536
1.00
2.06
1.05
1.03
3.06
1.06
3.07
10.5 10.0 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.
f1 (ppm)


150.5
147.2
138.3
137.5
134.7
133.0
129.7
129.1
126.6
124.5
117.7
116.4
18.7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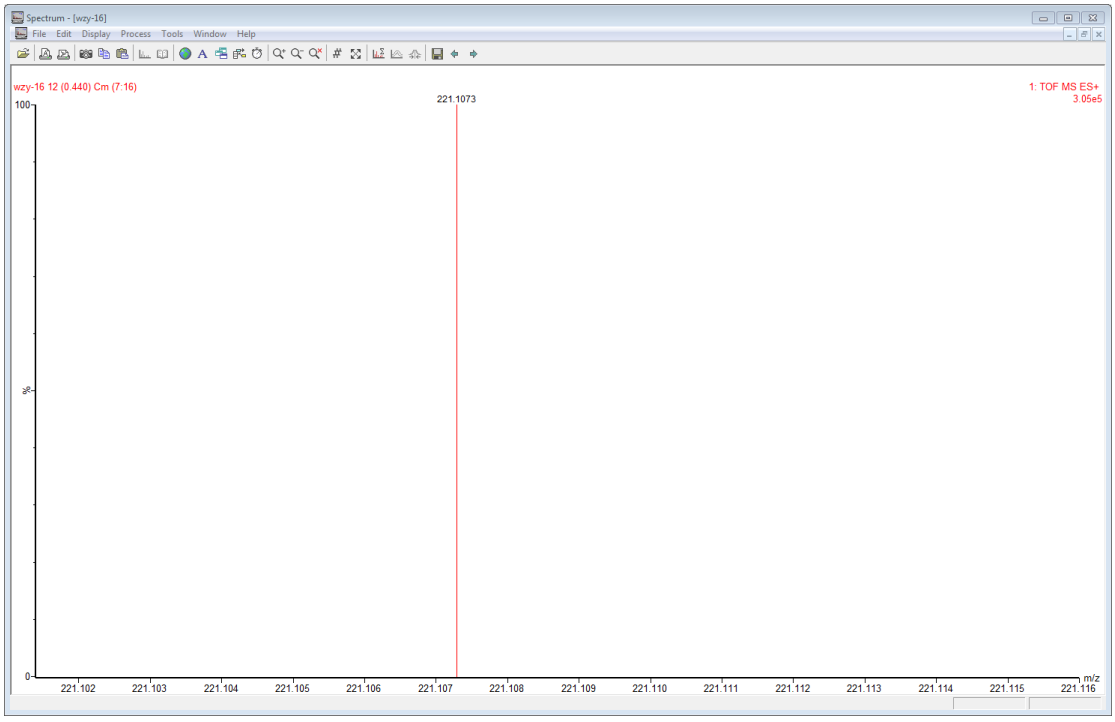
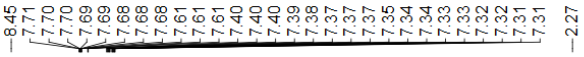
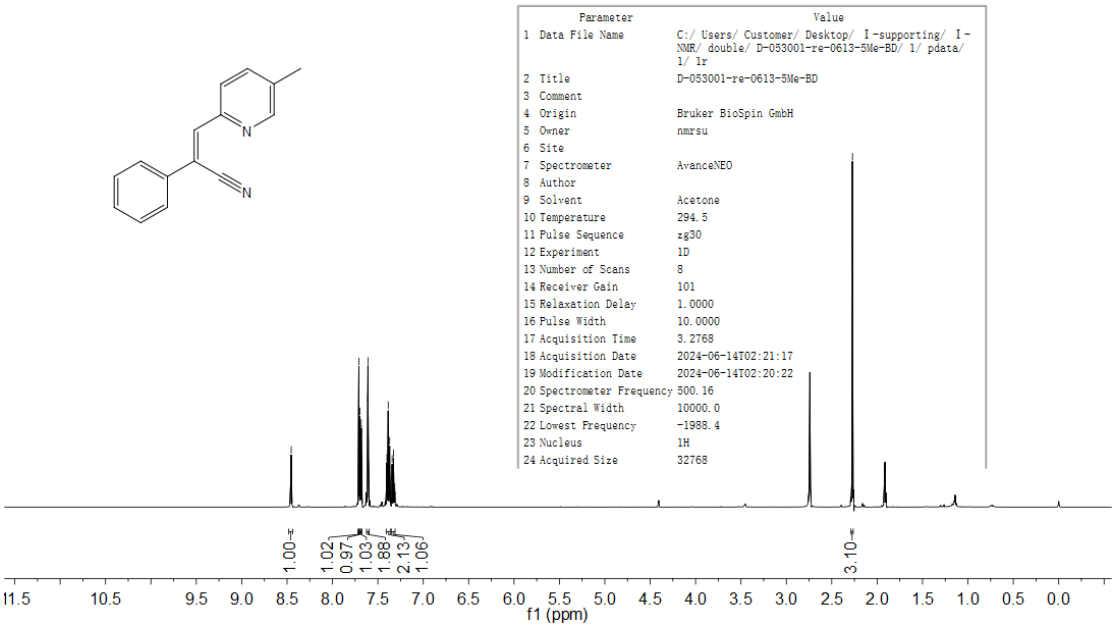
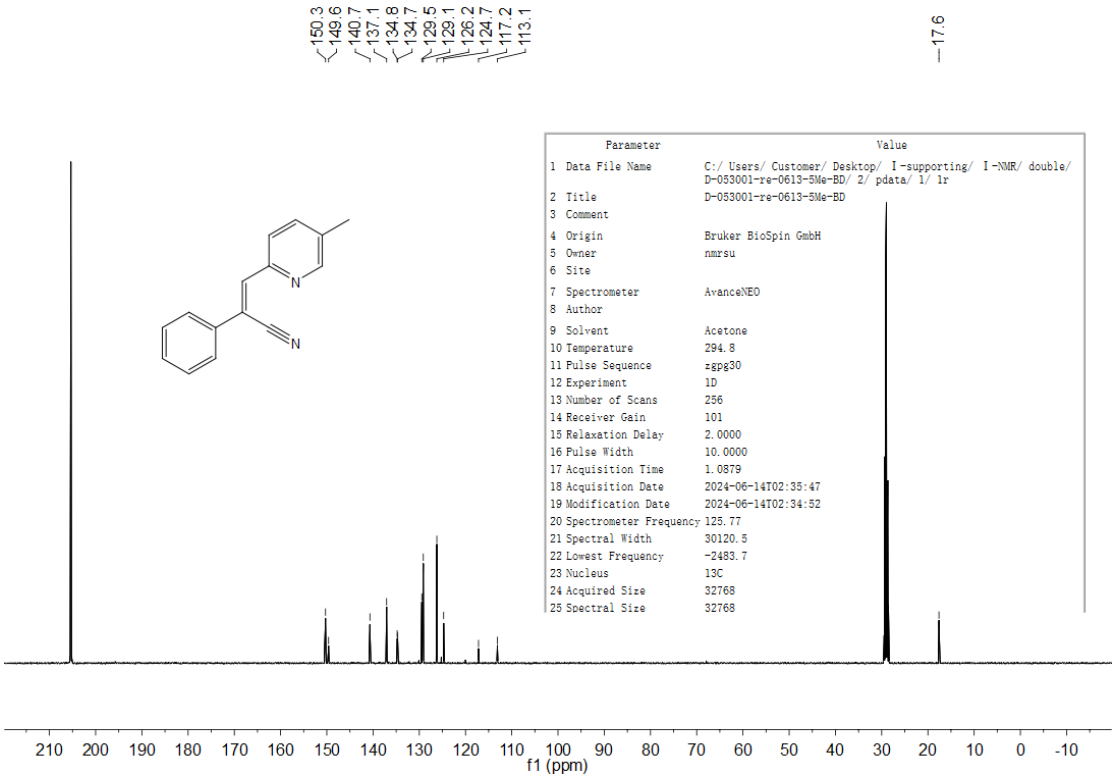
2 Title D-112703-1-2-1209-3-Me-BD
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.1
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2024-12-09T20:05:37
19 Modification Date 2024-12-09T20:04:40
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2482.8
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)

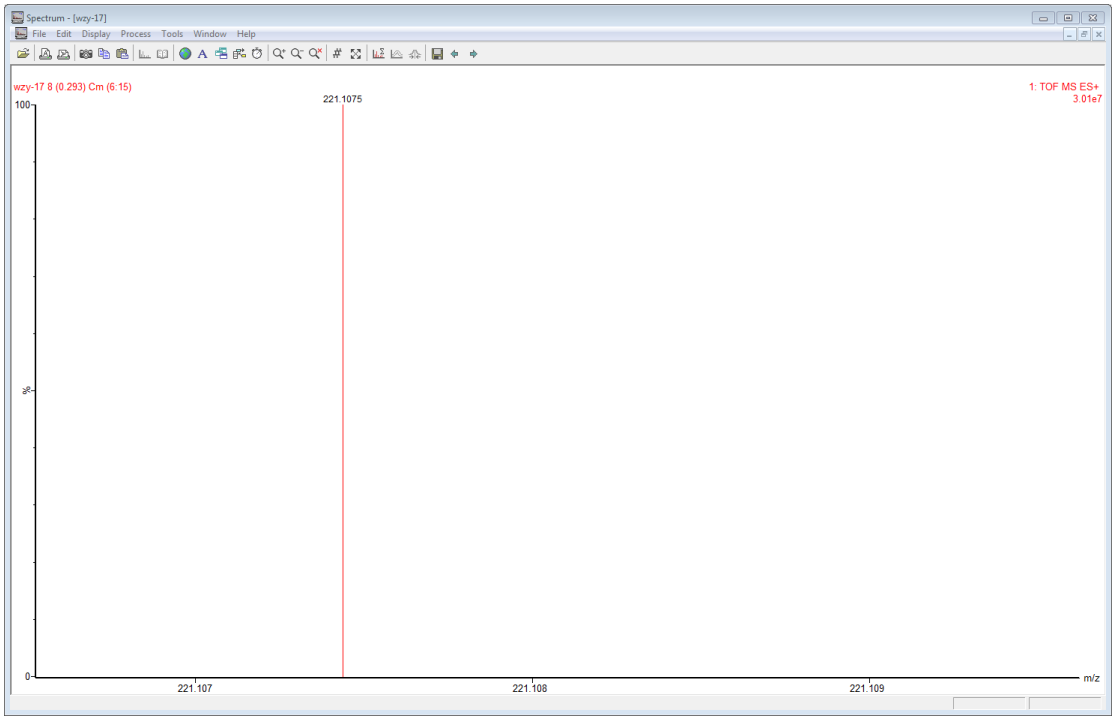


(*Z*)-3-(5-methylpyridin-2-yl)-2-phenylacrylonitrile (3ad)

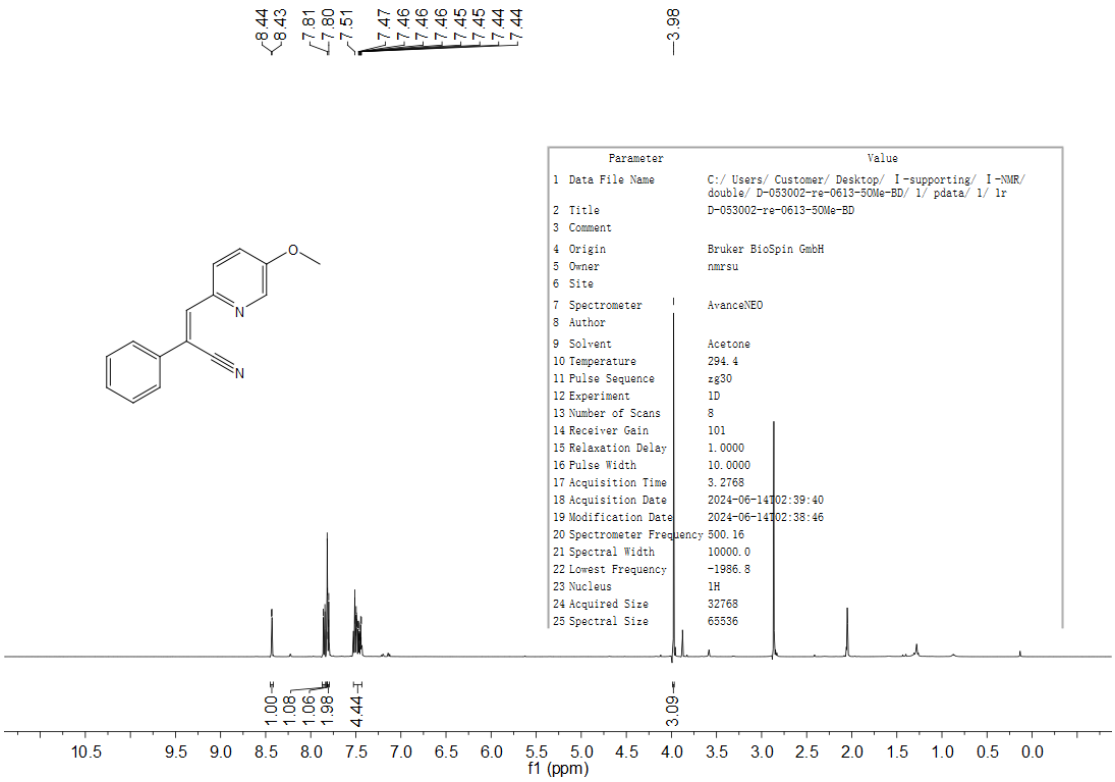








(*Z*)-3-(5-methoxypyridin-2-yl)-2-phenylacrylonitrile (3ae)


8.44
8.43
7.81
7.80
7.51
7.47
7.46
7.46
7.46
7.45
7.45
7.44
7.44
3.98
O
N
N
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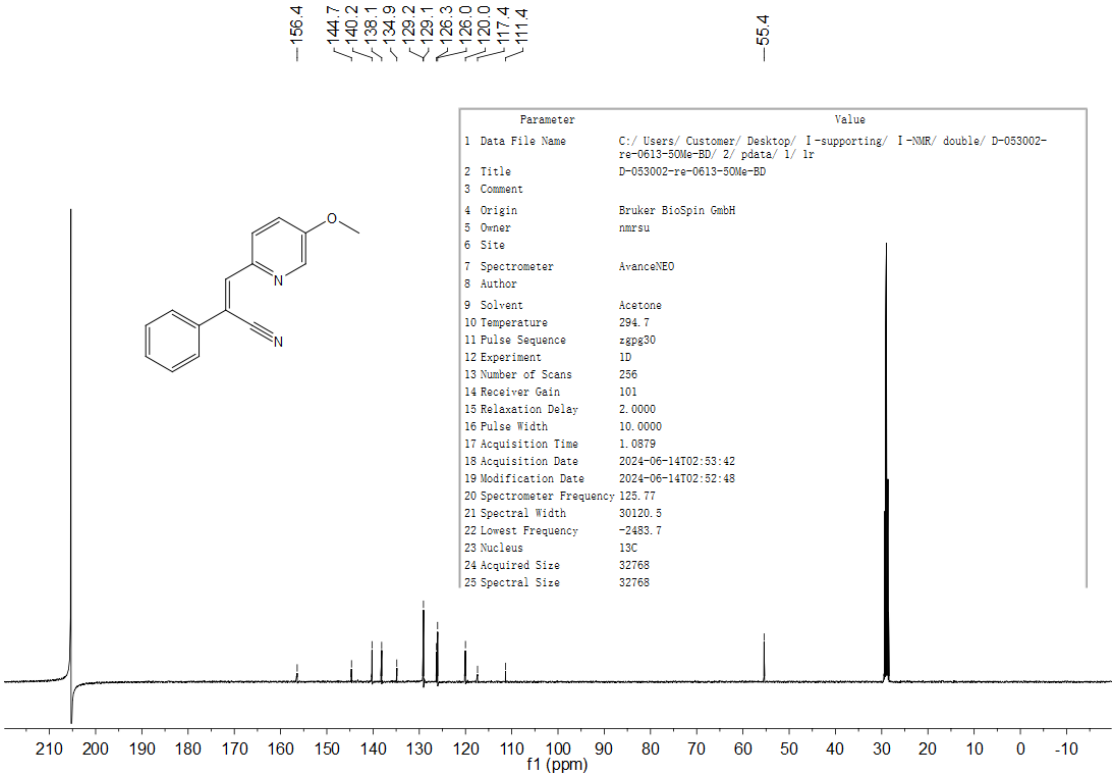
2 Title D-053002-re-0613-50Me-BD
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent Acetone
10 Temperature 294.4
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 8
14 Receiver Gain 101
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2024-06-14T02:39:40
19 Modification Date 2024-06-14T02:38:46
20 Spectrometer Frequency 500.16
21 Spectral Width 10000.0
22 Lowest Frequency -1986.8
23 Nucleus 1H
24 Acquired Size 32768
25 Spectral Size 65536
1.00
1.08
1.06
1.98
4.44
3.09
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)


156.4
144.7
140.2
138.1
134.9
129.2
129.1
126.3
126.0
120.0
117.4
111.4
55.4
O
N
N
Parameter Value
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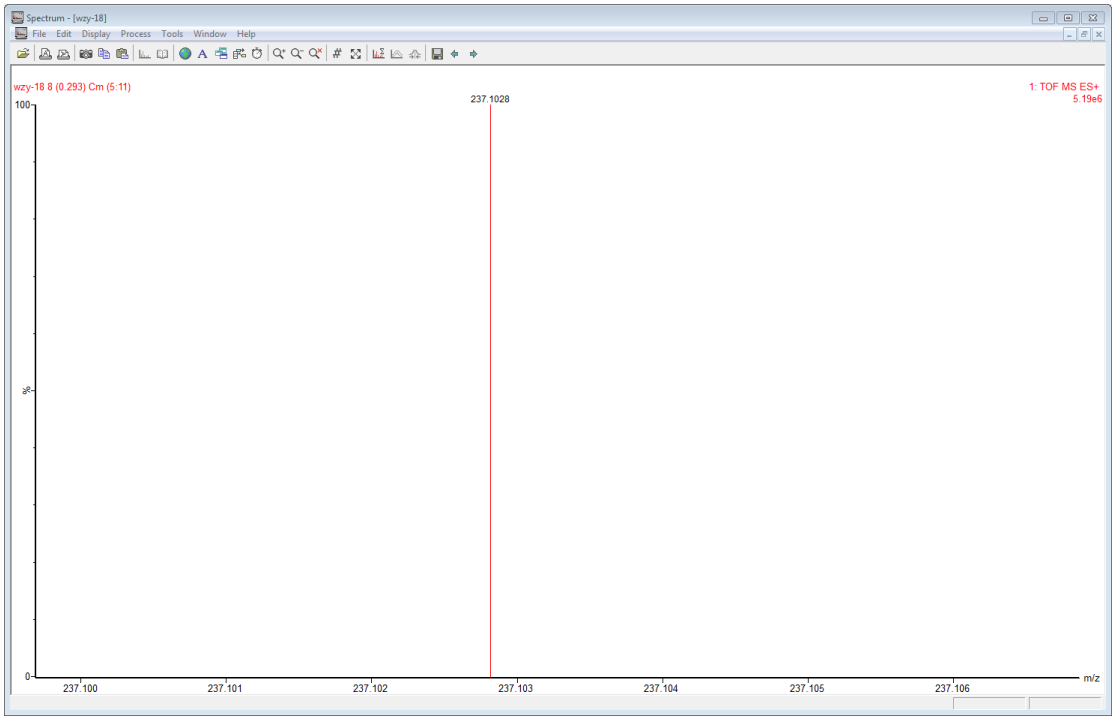
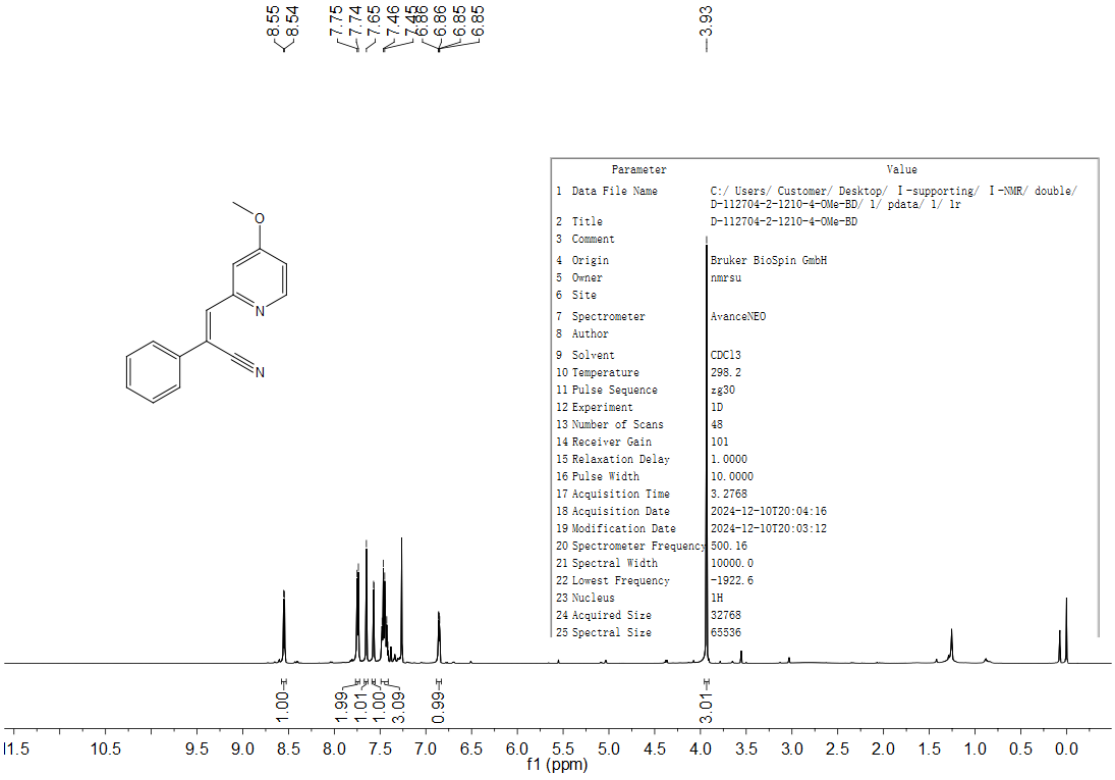
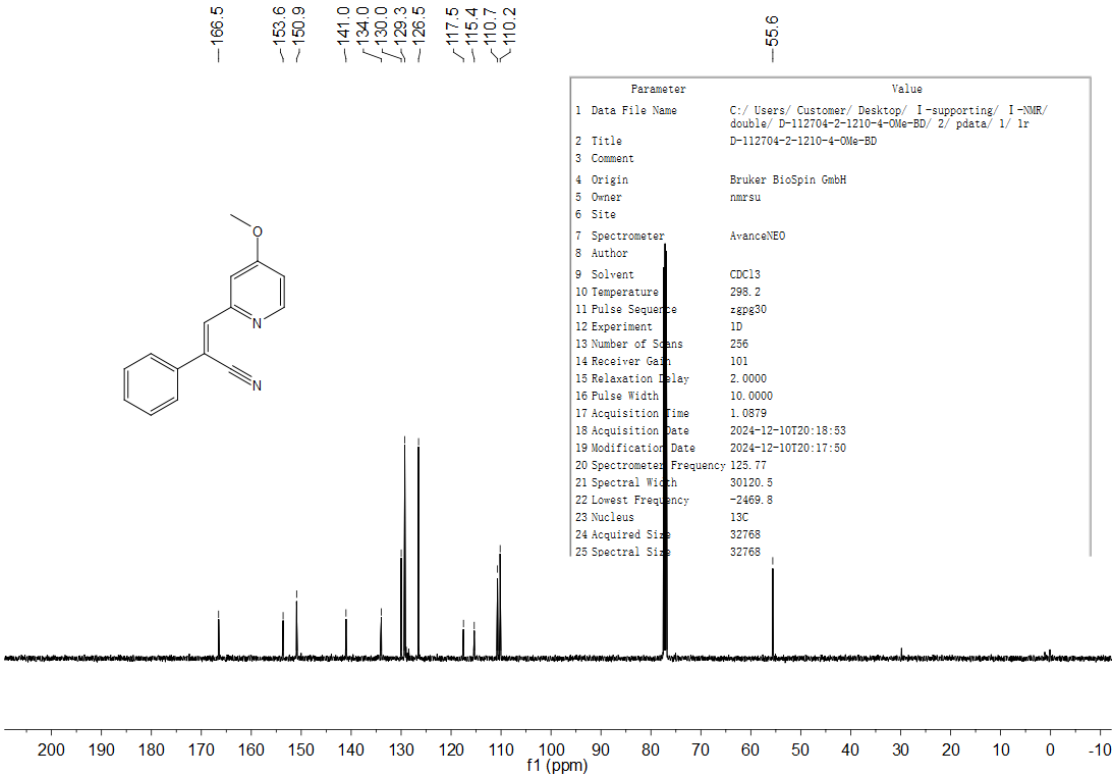
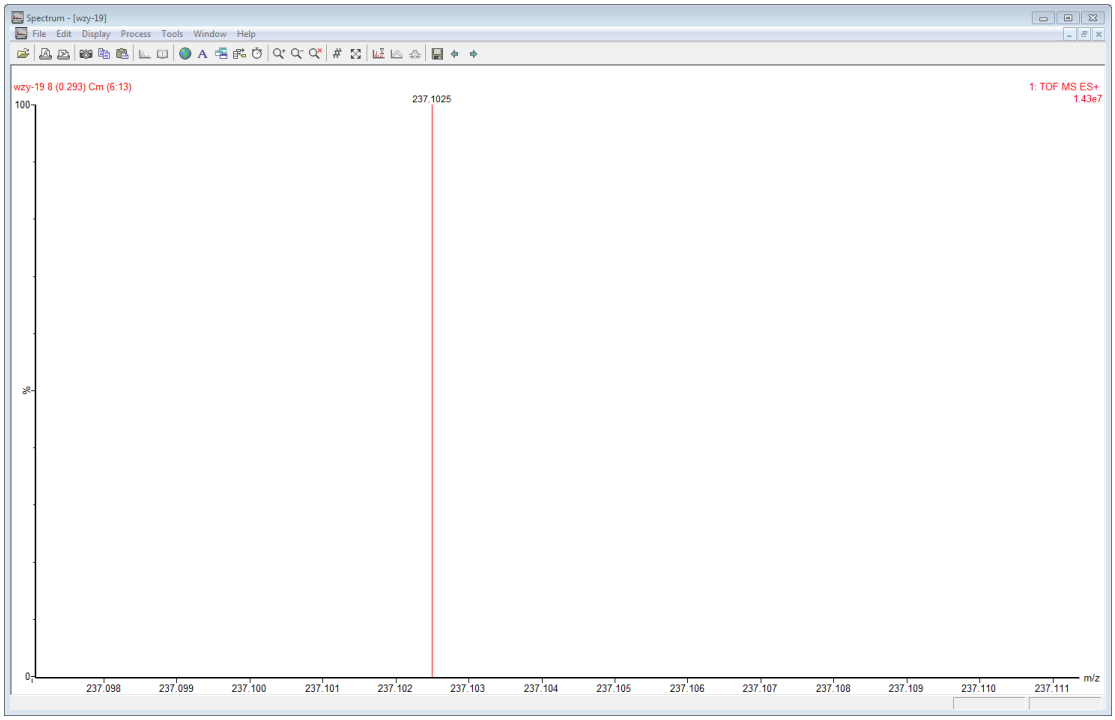
2 Title D-053002-re-0613-50Me-BD
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent Acetone
10 Temperature 294.7
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2024-06-14T02:53:42
19 Modification Date 2024-06-14T02:52:48
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2483.7
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)



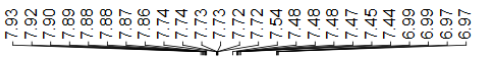
(*Z*)-3-(4-methoxypyridin-2-yl)-2-phenylacrylonitrile (3af)







(*Z*)-3-(6-fluoropyridin-2-yl)-2-phenylacrylonitrile (3ag)


7.93
7.92
7.90
7.89
7.88
7.88
7.87
7.86
7.74
7.74
7.73
7.73
7.72
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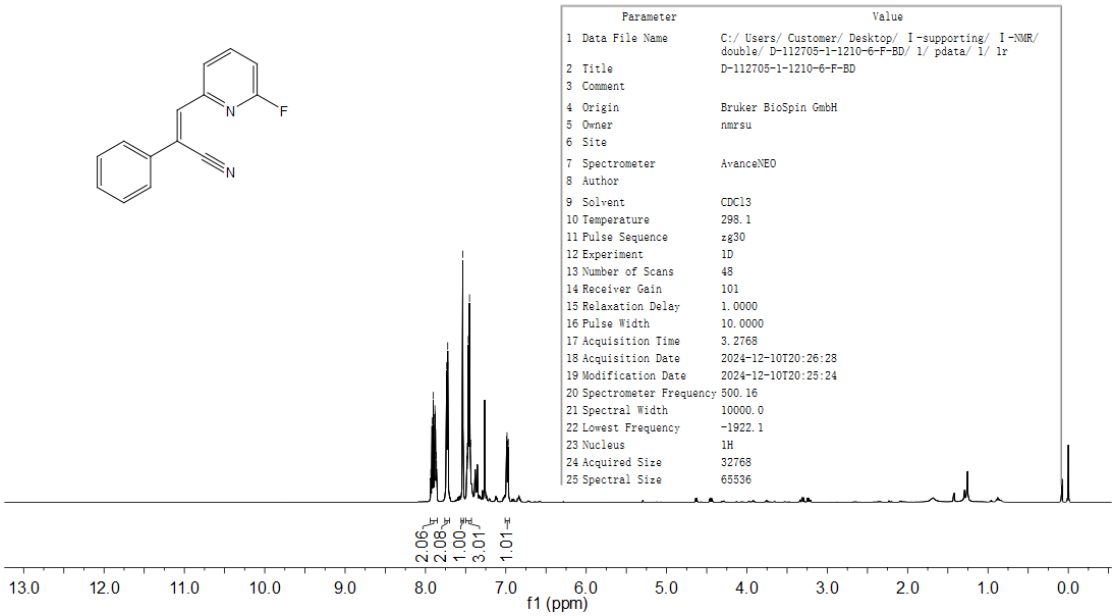
7.47
7.45
7.44
6.99
6.99
6.97
6.97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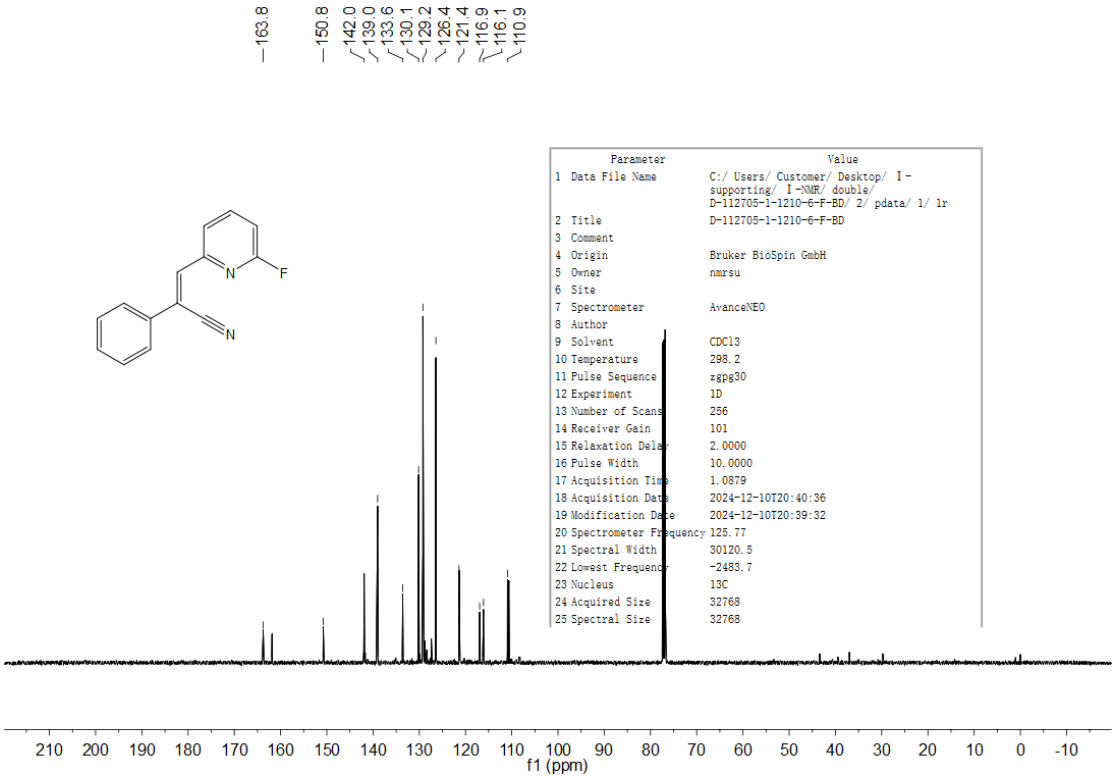
2 Title D-112705-1-1210-6-F-BD
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.1
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 48
14 Receiver Gain 101
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2024-12-10T20:26:28
19 Modification Date 2024-12-10T20:25:24
20 Spectrometer Frequency 500.16
21 Spectral Width 10000.0
22 Lowest Frequency -1922.1
23 Nucleus 1H
24 Acquired Size 32768
25 Spectral Size 65536
2.06
2.08
1.00
3.01
1.01
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)


163.8
150.8
142.0
139.0
133.6
130.1
129.2
126.4
121.4
116.9
116.1
110.9
N
F
N
Parameter Value
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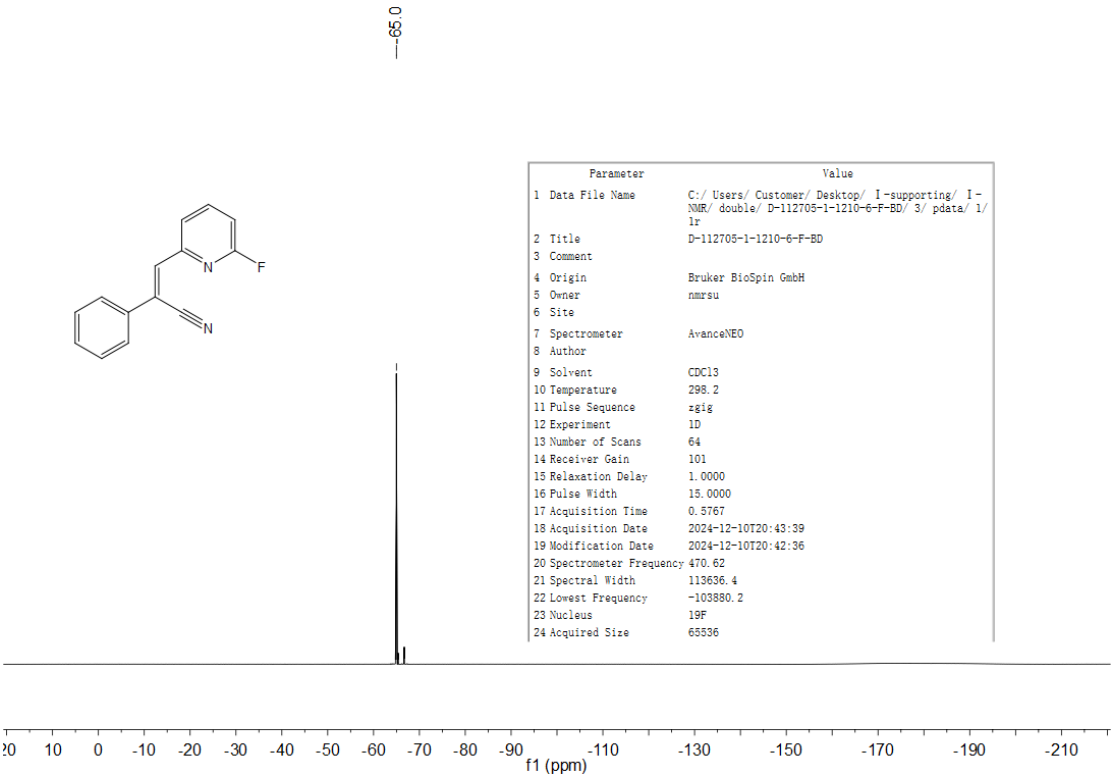
2 Title D-112705-1-1210-6-F-BD
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.2
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2024-12-10T20:40:36
19 Modification Date 2024-12-10T20:39:32
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2483.7
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)



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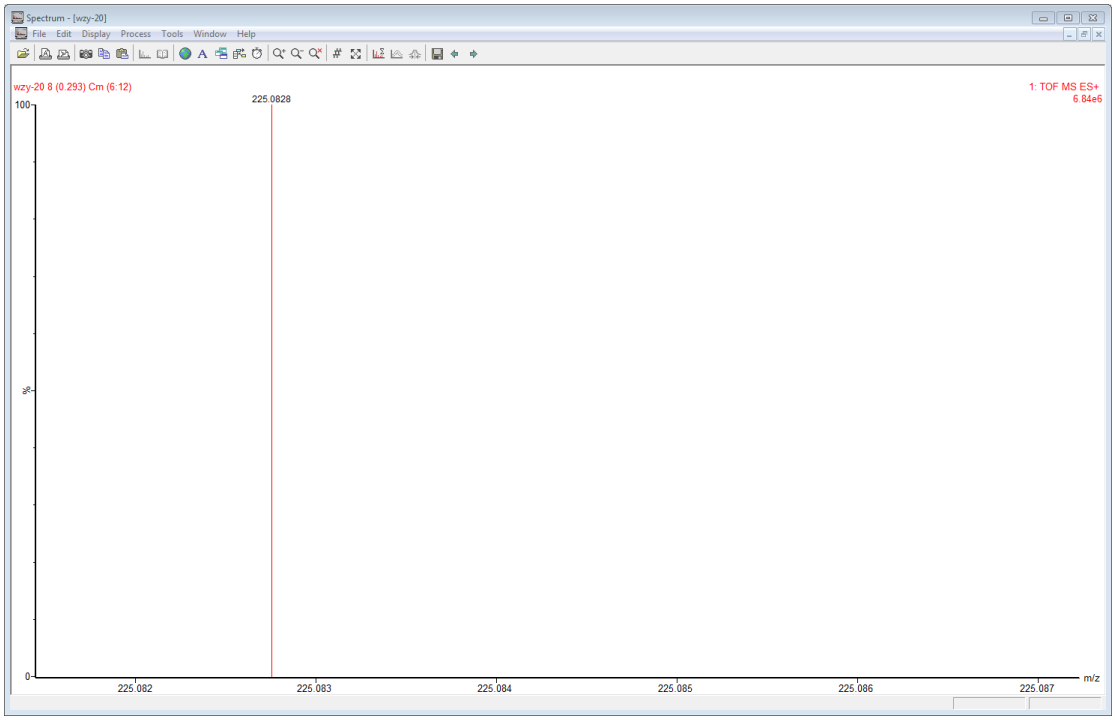
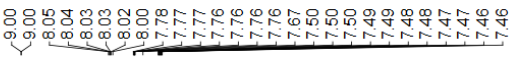
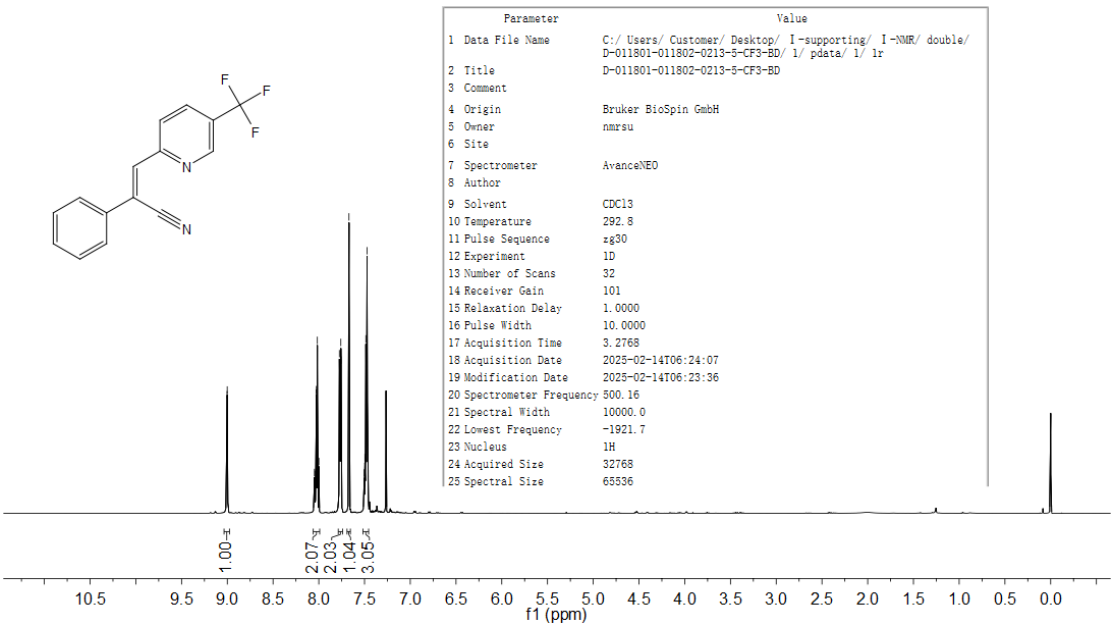
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgig
12 Experiment	1D
13 Number of Scans	64
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	15.0000
17 Acquisition Time	0.5767
18 Acquisition Date	2024-12-10T20:43:39
19 Modification Date	2024-12-10T20:42:36
20 Spectrometer Frequency	470.62
21 Spectral Width	113636.4
22 Lowest Frequency	-103880.2
23 Nucleus	19F
24 Acquired Size	65536



(*Z*)-2-phenyl-3-(5-(trifluoromethyl)pyridin-2-yl)acrylonitrile (3ah)





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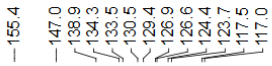
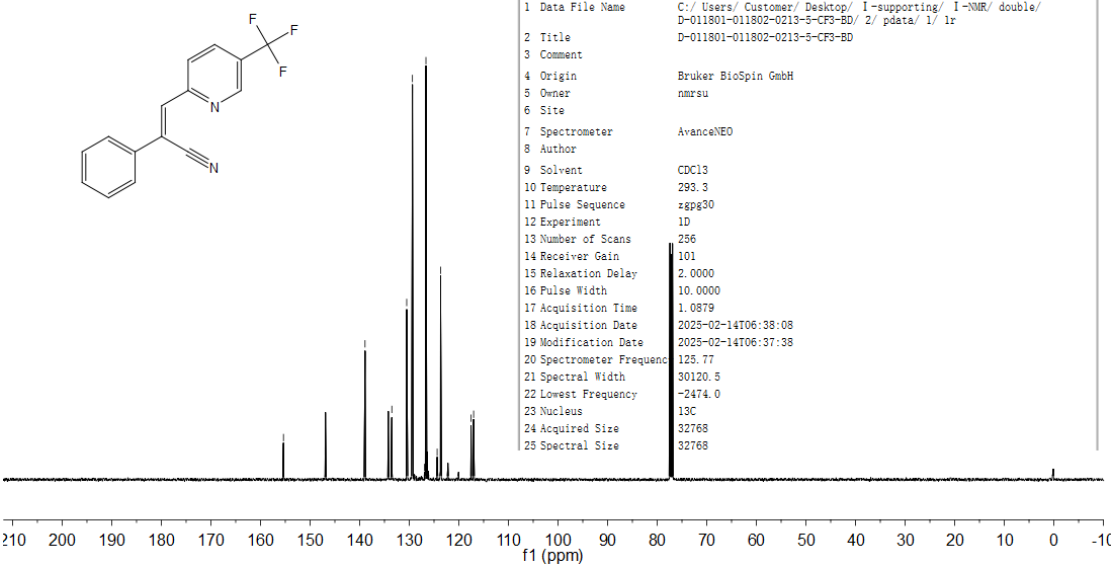
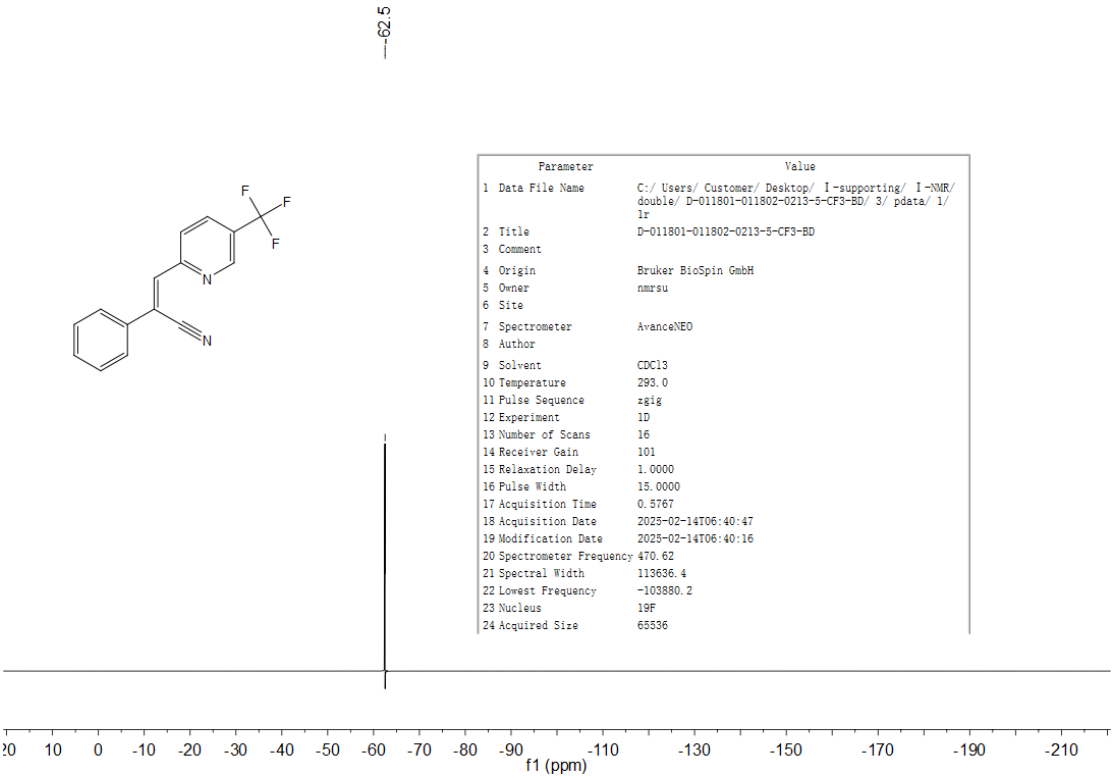
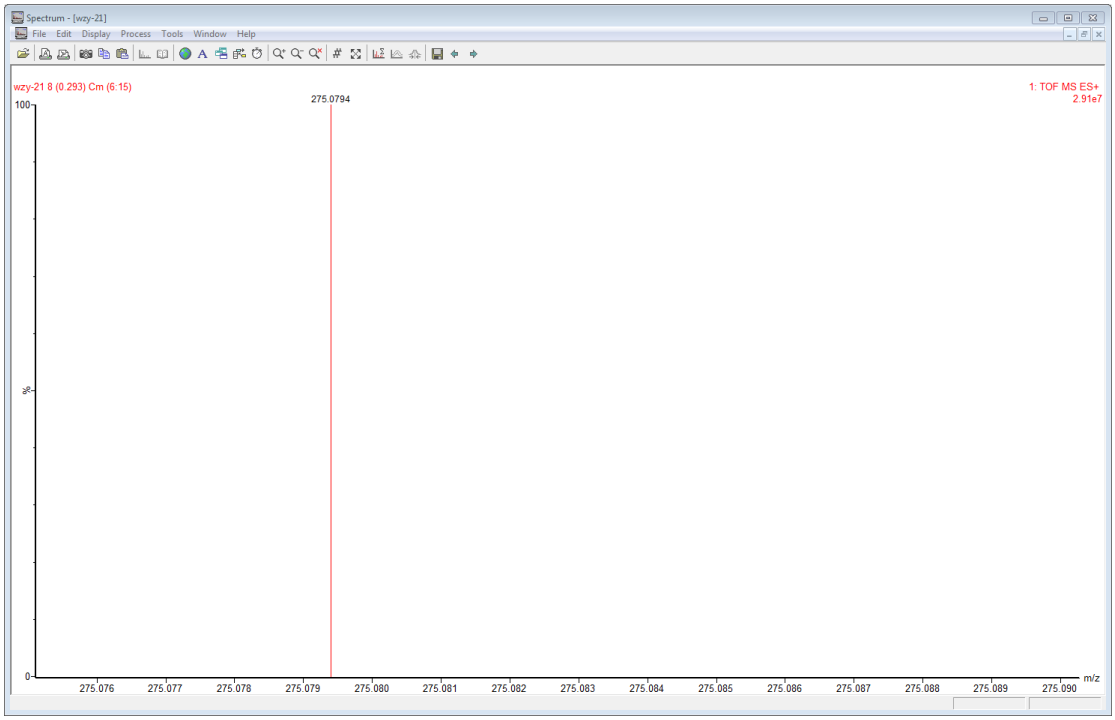
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	292.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	32
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2025-02-14T06:24:07
19 Modification Date	2025-02-14T06:23:36
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1921.7
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



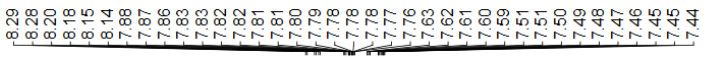


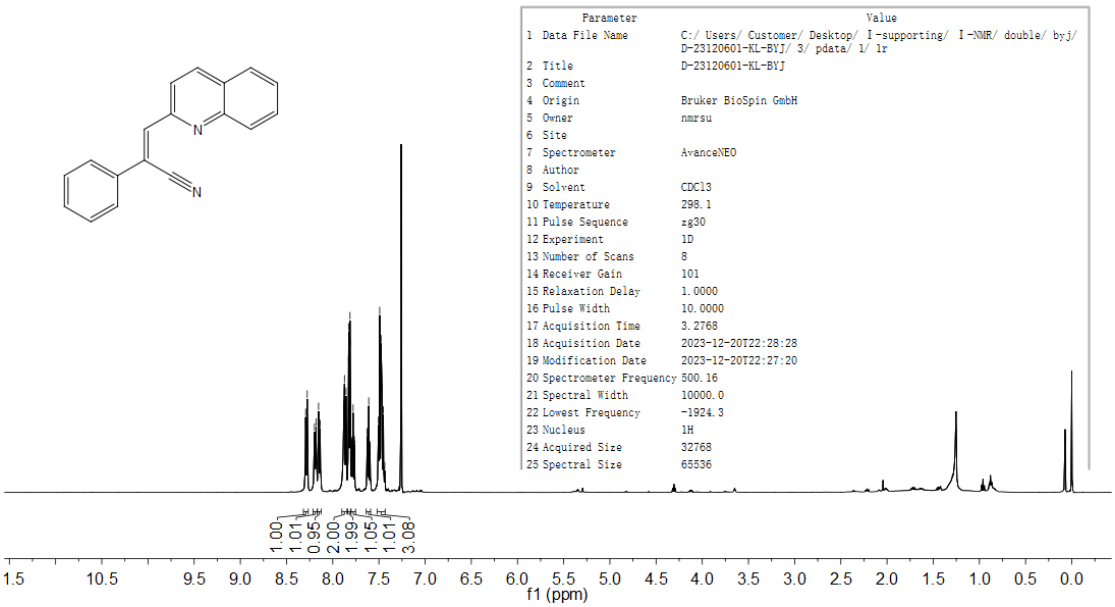
Parameter	Value
1 Data File Name	C:/ Users/ Customer/ Desktop/ I-supporting/ I-NMR/ double/ D-011801-011802-0213-5-CF3-BD/ 2/ pdata/ 1/ 1r
2 Title	D-011801-011802-0213-5-CF3-BD
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	293.3
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	2025-02-14T06:38:08
19 Modification Date	2025-02-14T06:37:38
20 Spectrometer Frequenc	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2474.0
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768

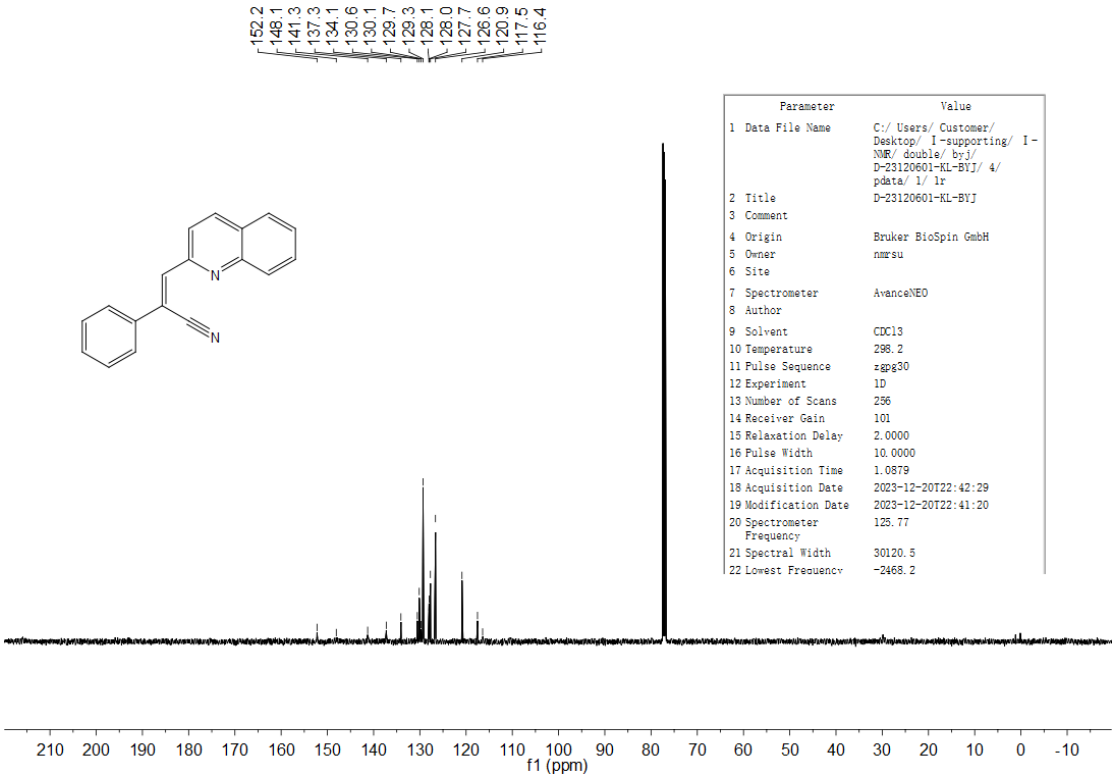




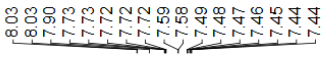
(*Z*)-2-phenyl-3-(quinolin-2-yl)acrylonitrile (3ai)

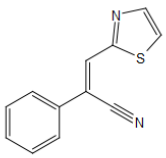






(*Z*)-2-phenyl-3-(thiazol-2-yl)acrylonitrile (3aj)





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2 Title	D-120202-1211-SZ
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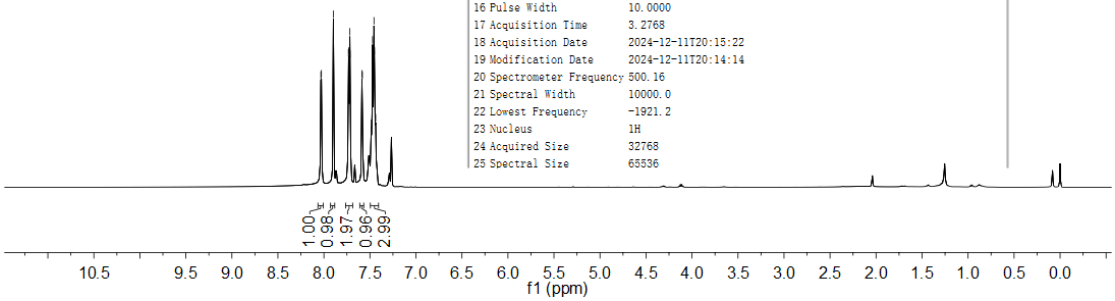
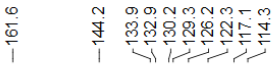
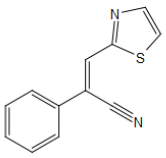
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	64
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2024-12-11T20:15:22
19 Modification Date	2024-12-11T20:14:14
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1921.2
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536







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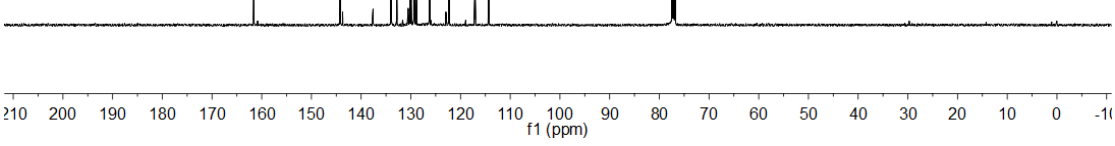
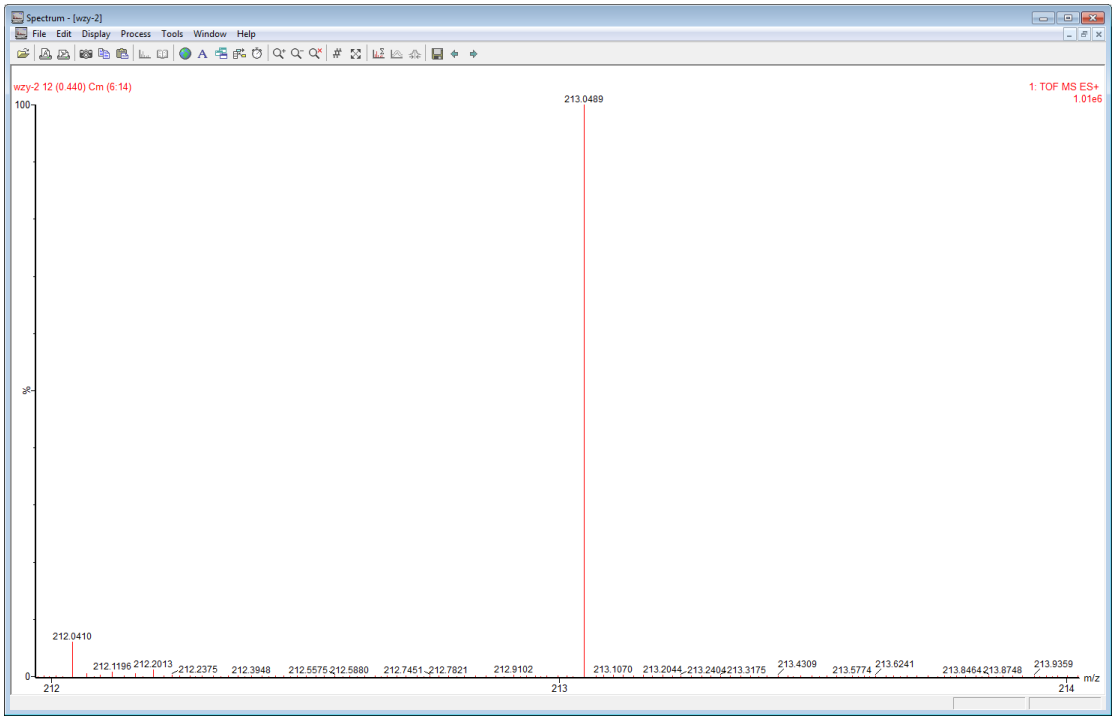
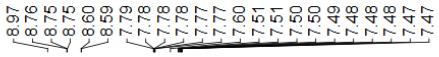
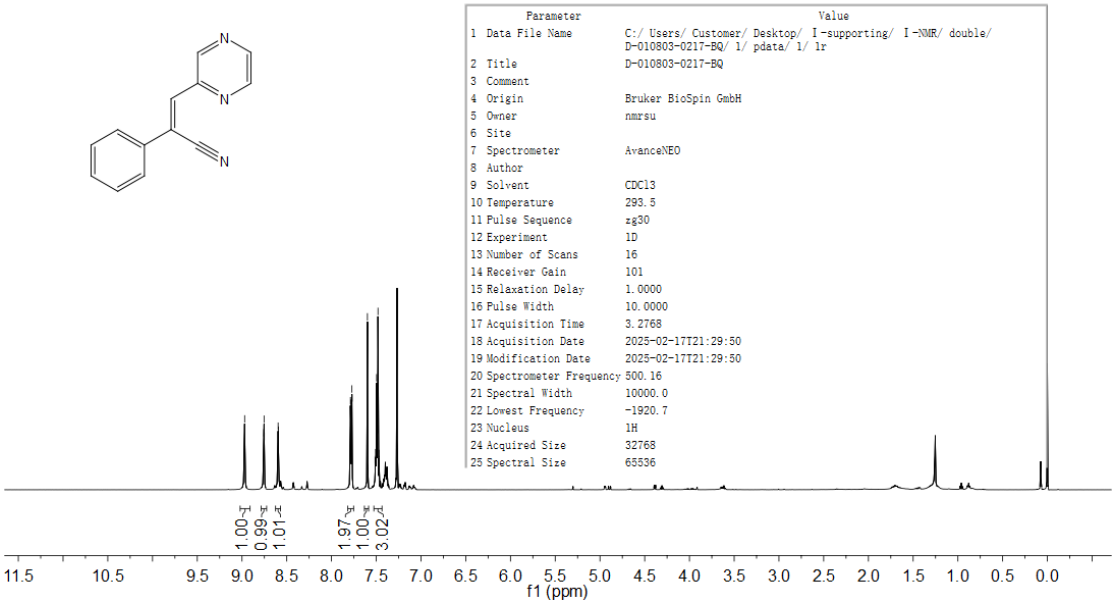
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	512
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2024-12-11T20:43:01
19 Modification Date	2024-12-11T20:41:52
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2483.7
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768

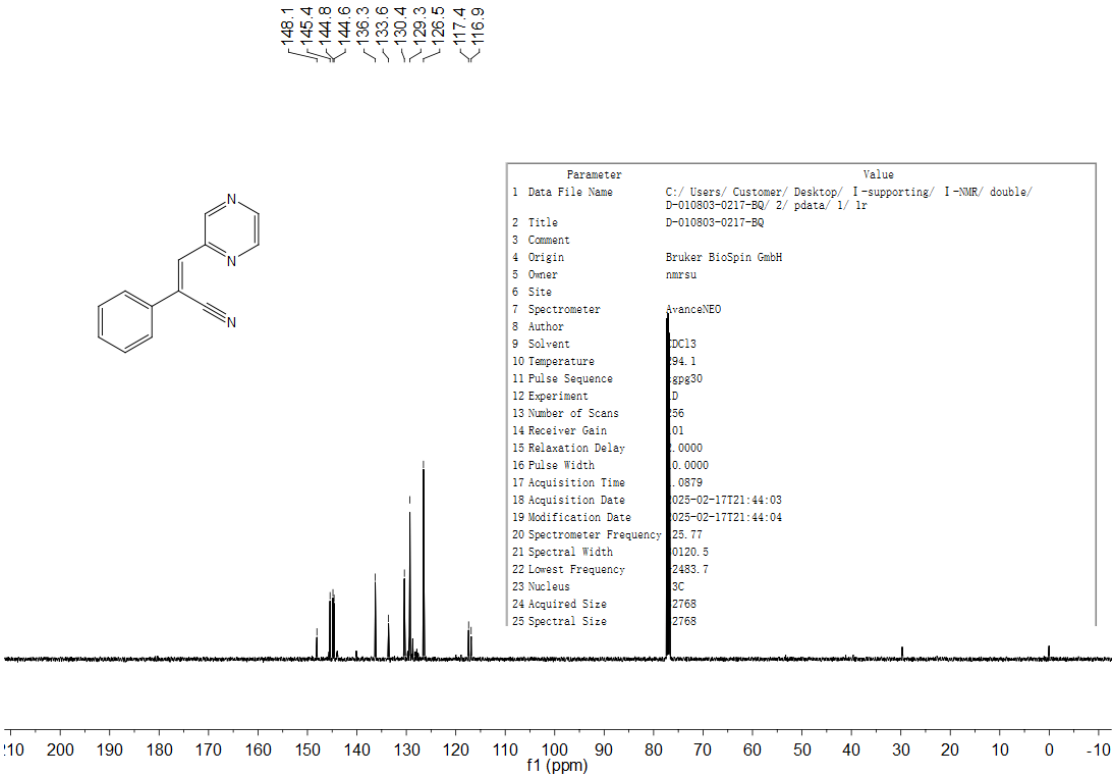


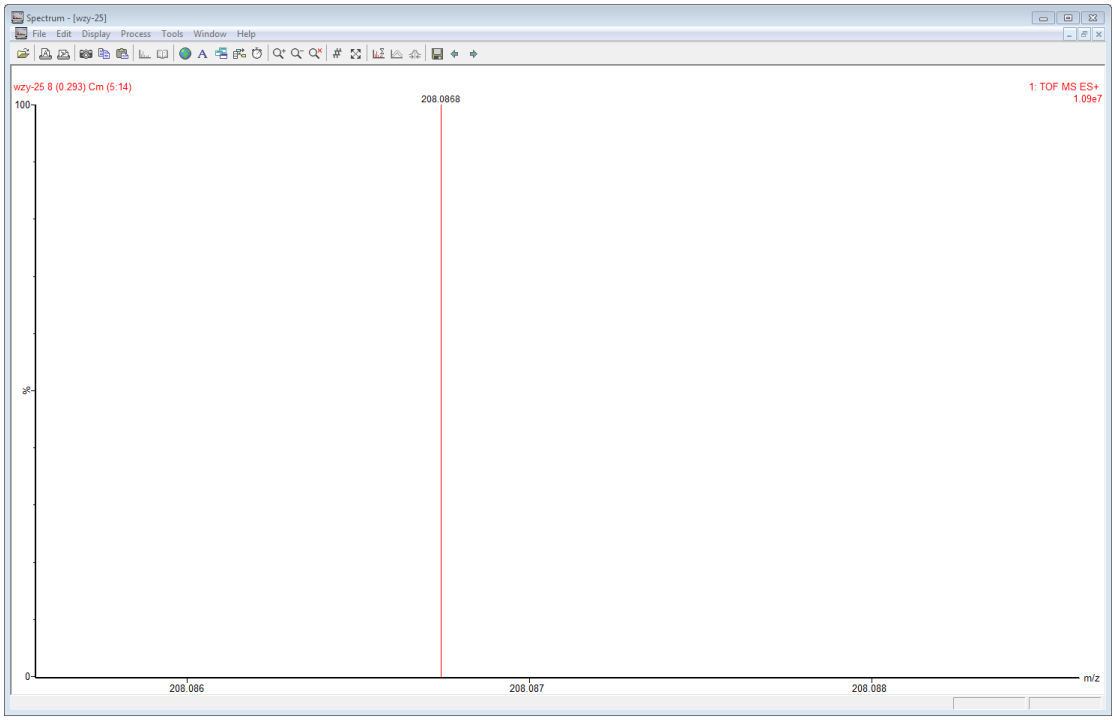


(*Z*)-2-phenyl-3-(pyrazin-2-yl)acrylonitrile (3ak)

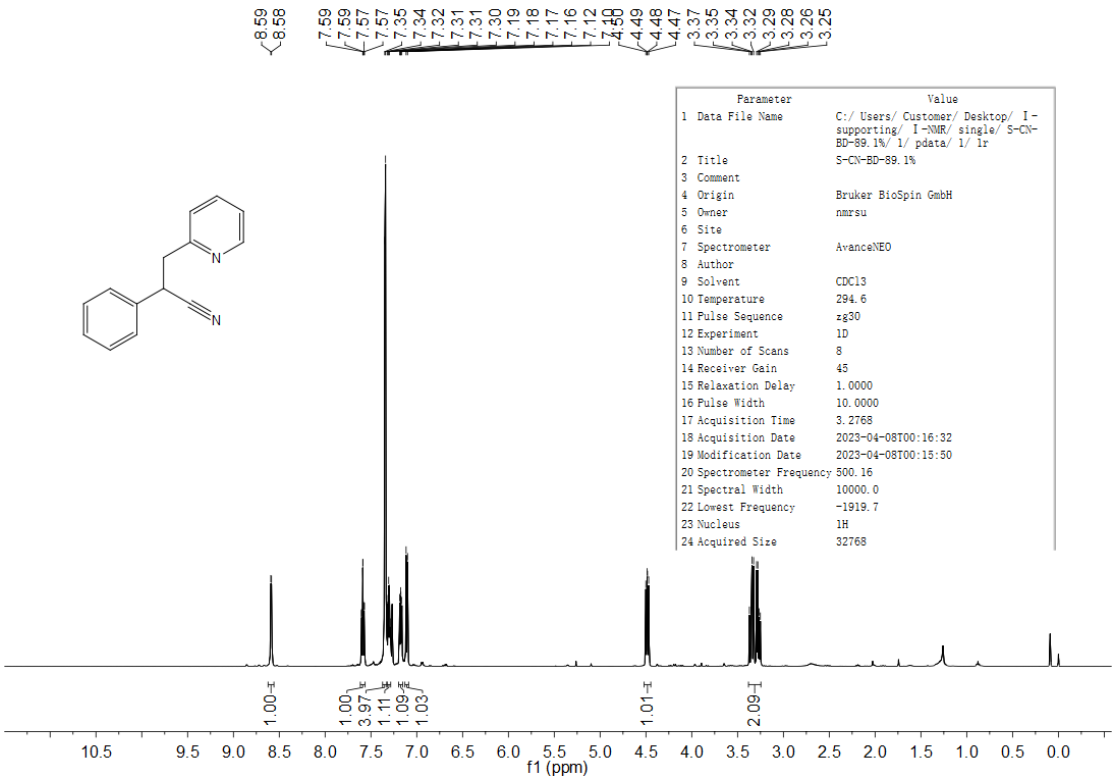


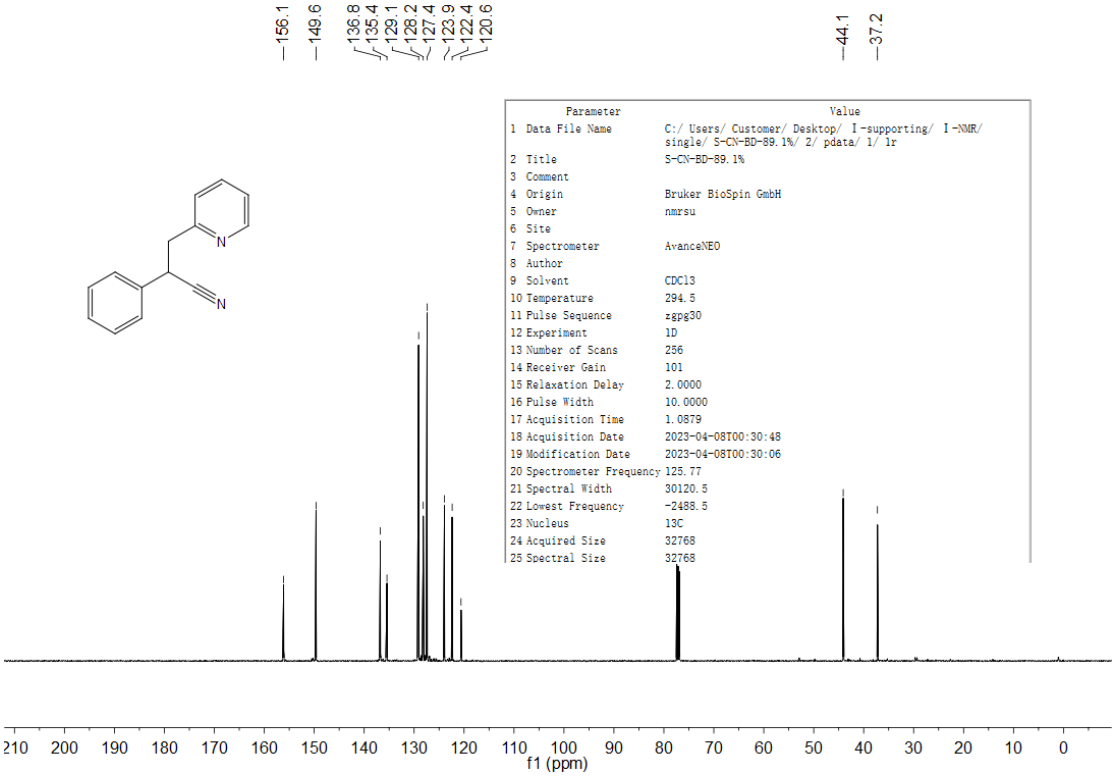




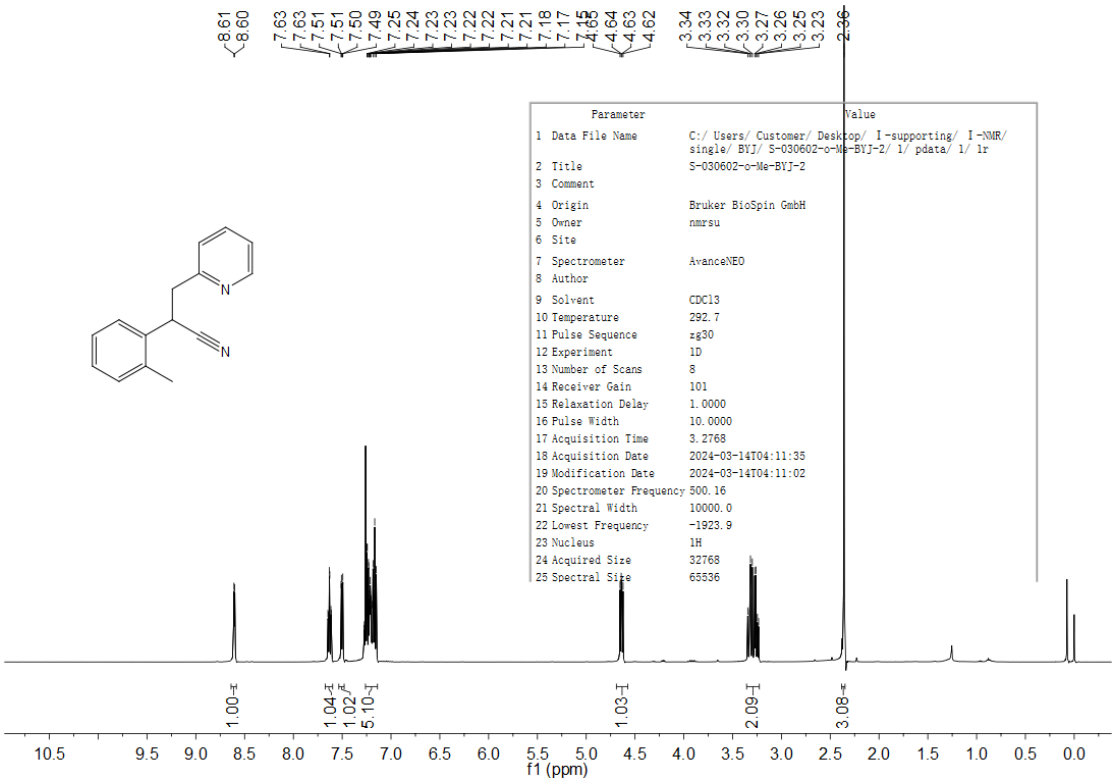


2-phenyl-3-(pyridin-2-yl)propanenitrile (4aa)





3-(pyridin-2-yl)-2-(o-tolyl)propanenitrile (4ba)



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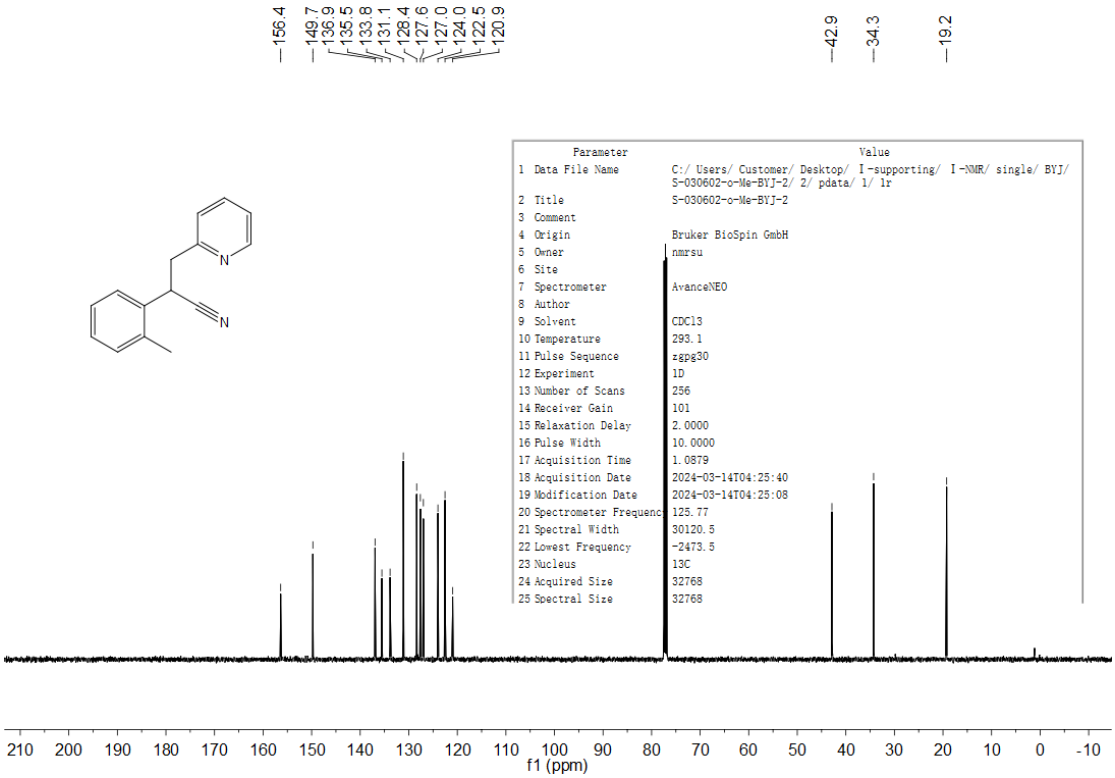
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	292.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2024-03-14T04:11:35
19 Modification Date	2024-03-14T04:11:02
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1923.9
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



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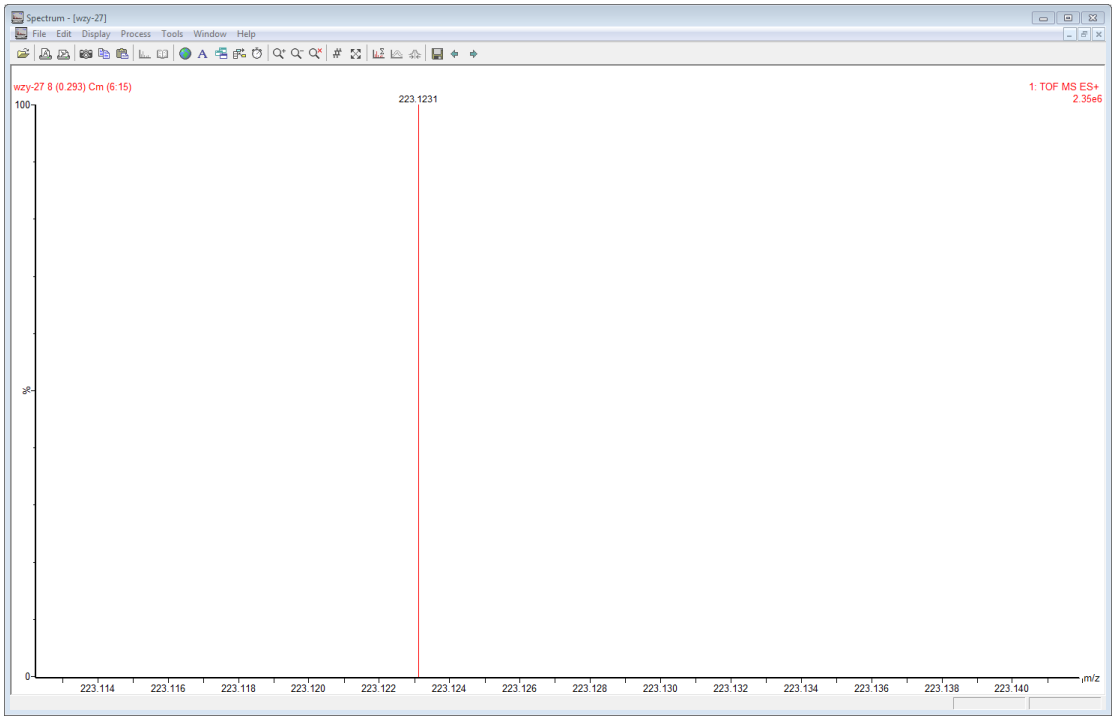
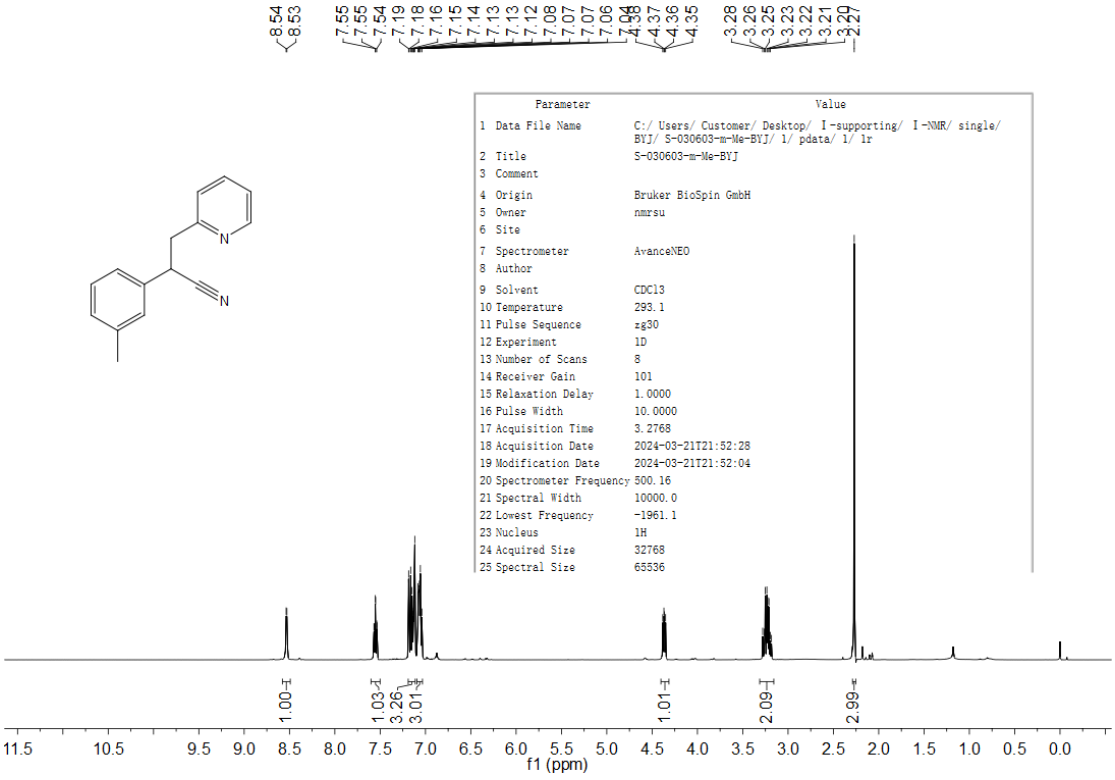
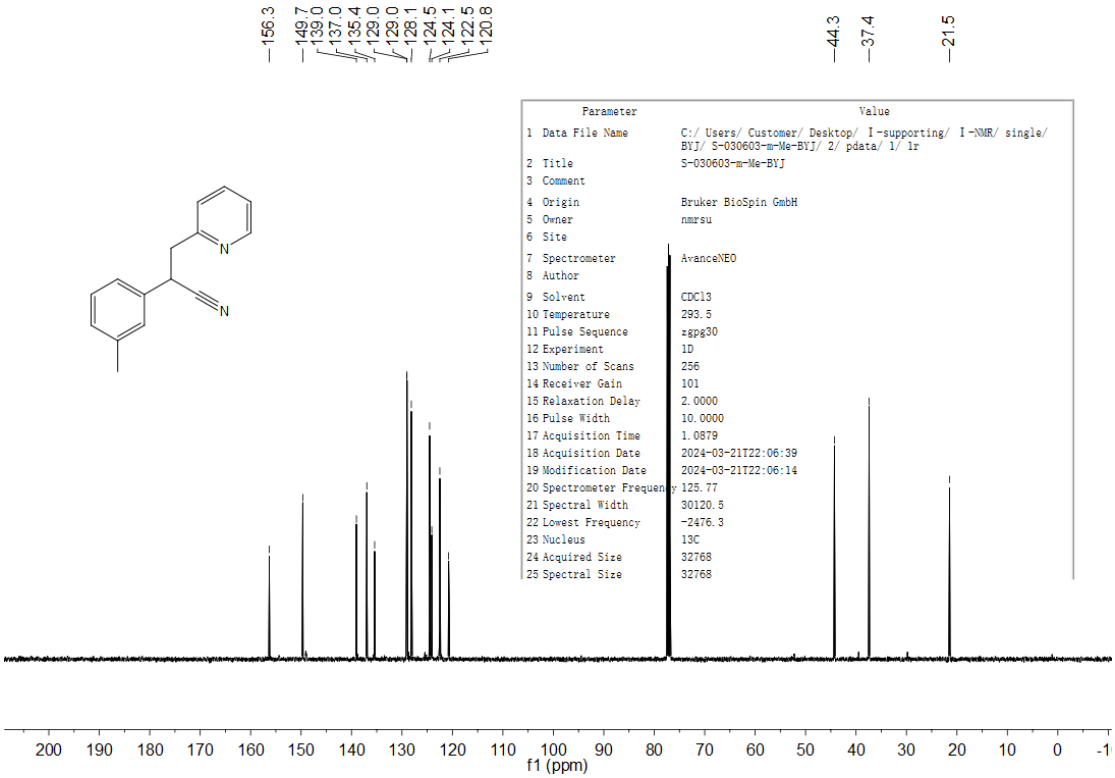
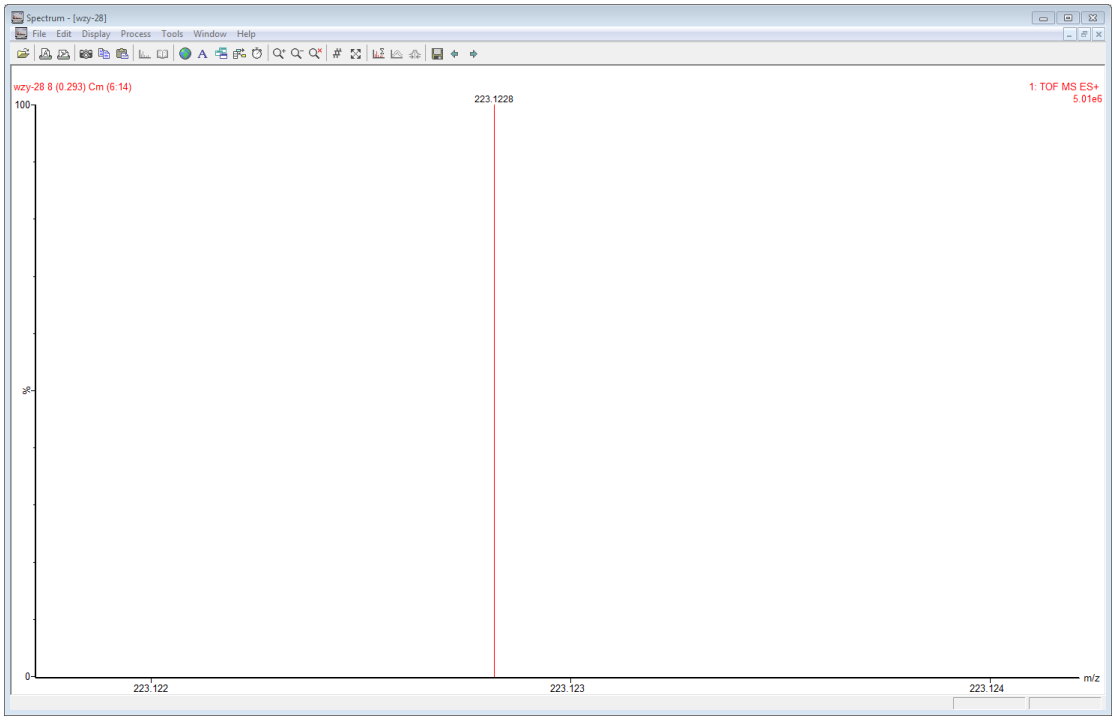
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	293.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2024-03-14T04:25:40
19 Modification Date	2024-03-14T04:25:08
20 Spectrometer Frequenc	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2473.5
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768



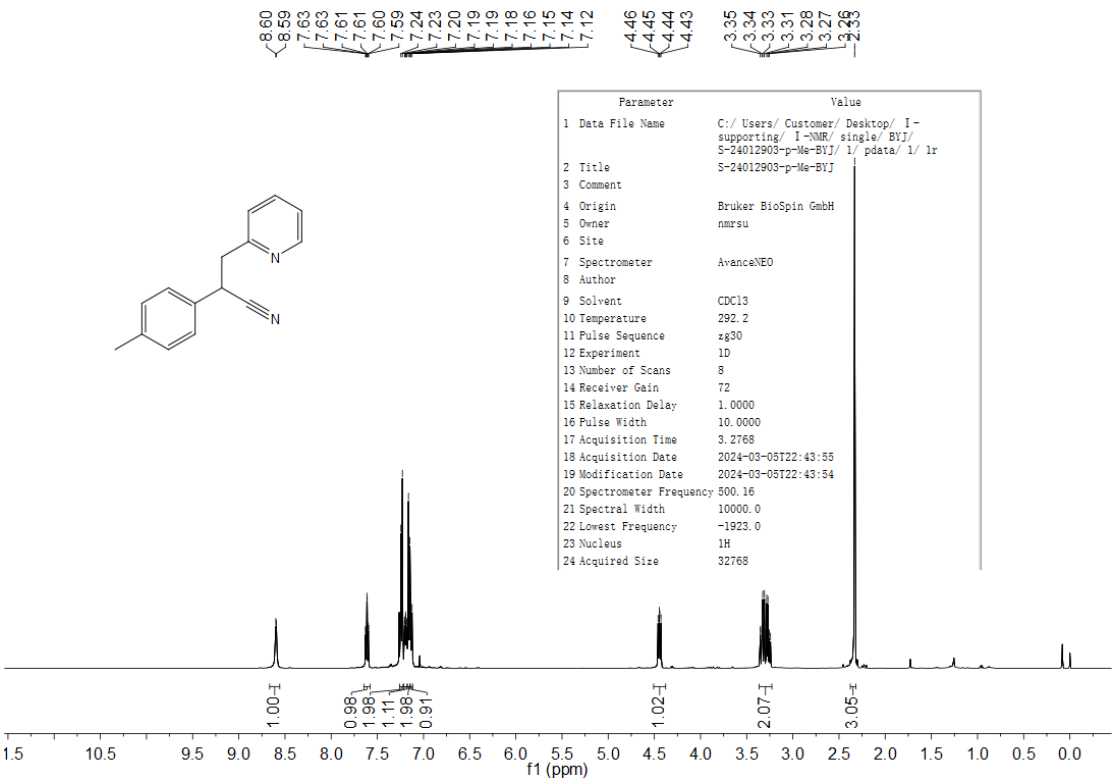
3-(pyridin-2-yl)-2-(m-tolyl)propanenitrile (4ca)







3-(pyridin-2-yl)-2-(p-tolyl)propanenitrile (4da)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7.63
7.61
7.61
7.60
7.59
7.24
7.23
7.20
7.19
7.19
7.18
7.16
7.15
7.14
7.12
4.46
4.45
4.44
4.43
3.35
3.34
3.33
3.31
3.28
3.27
2.33
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2 Title S-24012903-p-Me-BYJ
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 292.2
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 8
14 Receiver Gain 72
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2024-03-05T22:43:55
19 Modification Date 2024-03-05T22:43:54
20 Spectrometer Frequency 500.16
21 Spectral Width 10000.0
22 Lowest Frequency -1923.0
23 Nucleus 1H
24 Acquired Size 32768
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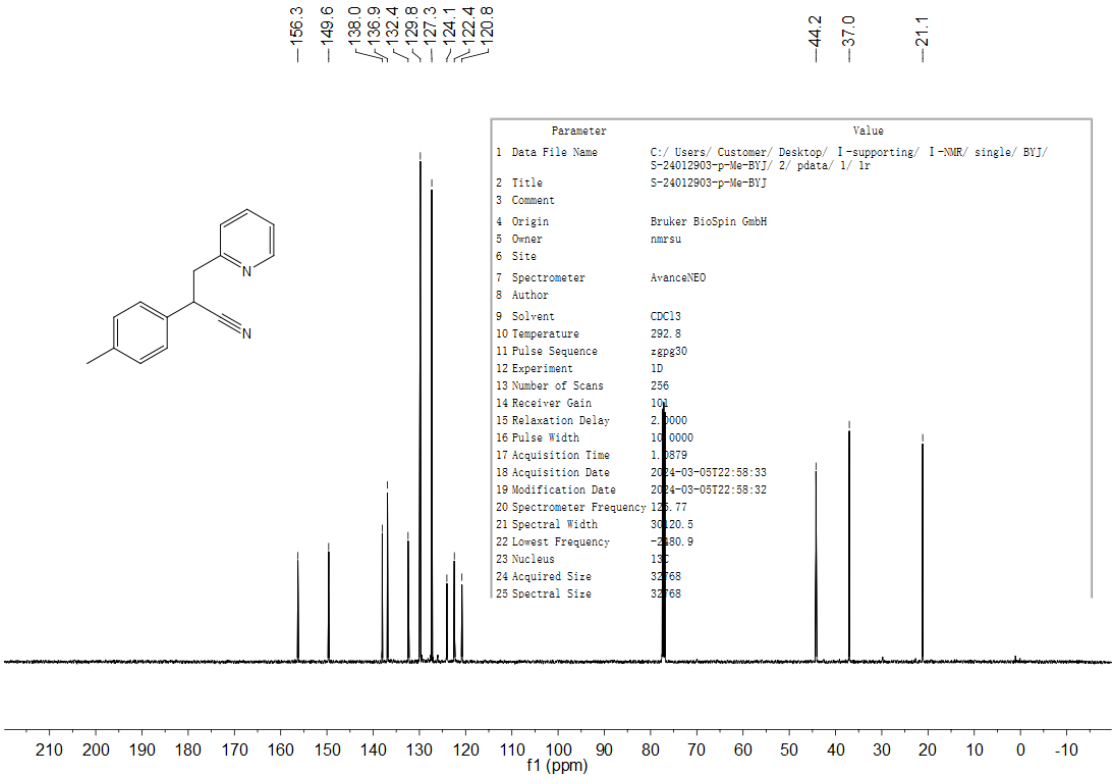
N
1.00
0.98
1.98
1.11
1.98
0.91
1.02
2.07
3.05
f1 (ppm)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149.6
138.0
136.9
132.4
129.8
127.3
124.1
122.4
120.8
44.2
37.0
21.1
Parameter Value
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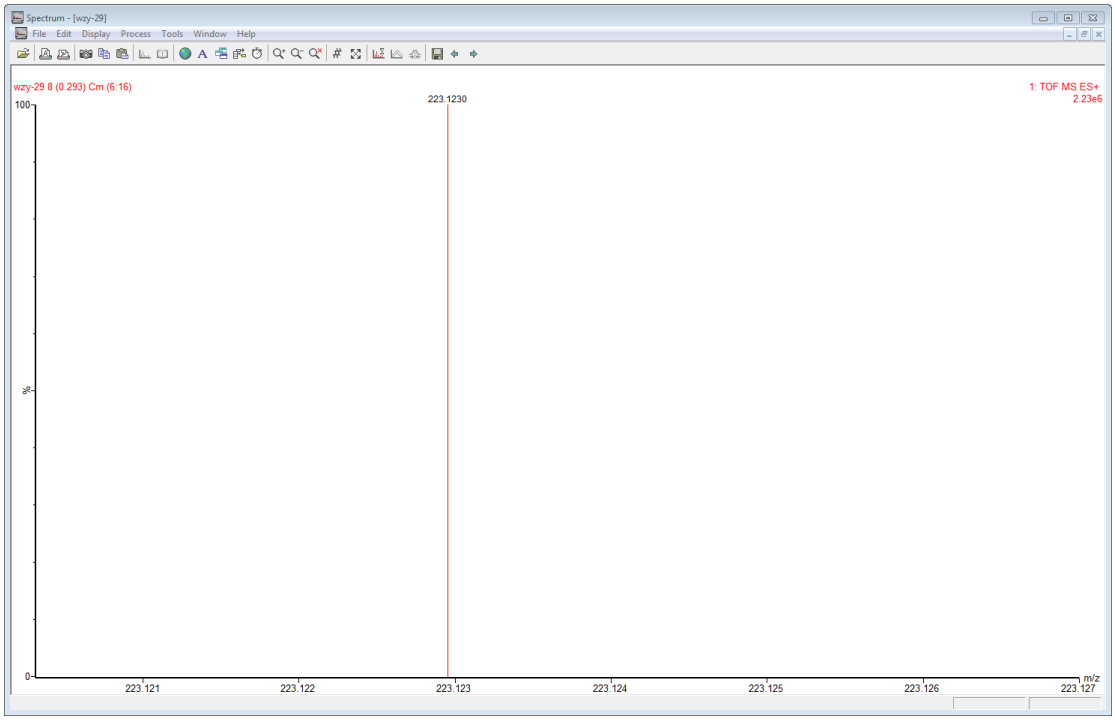
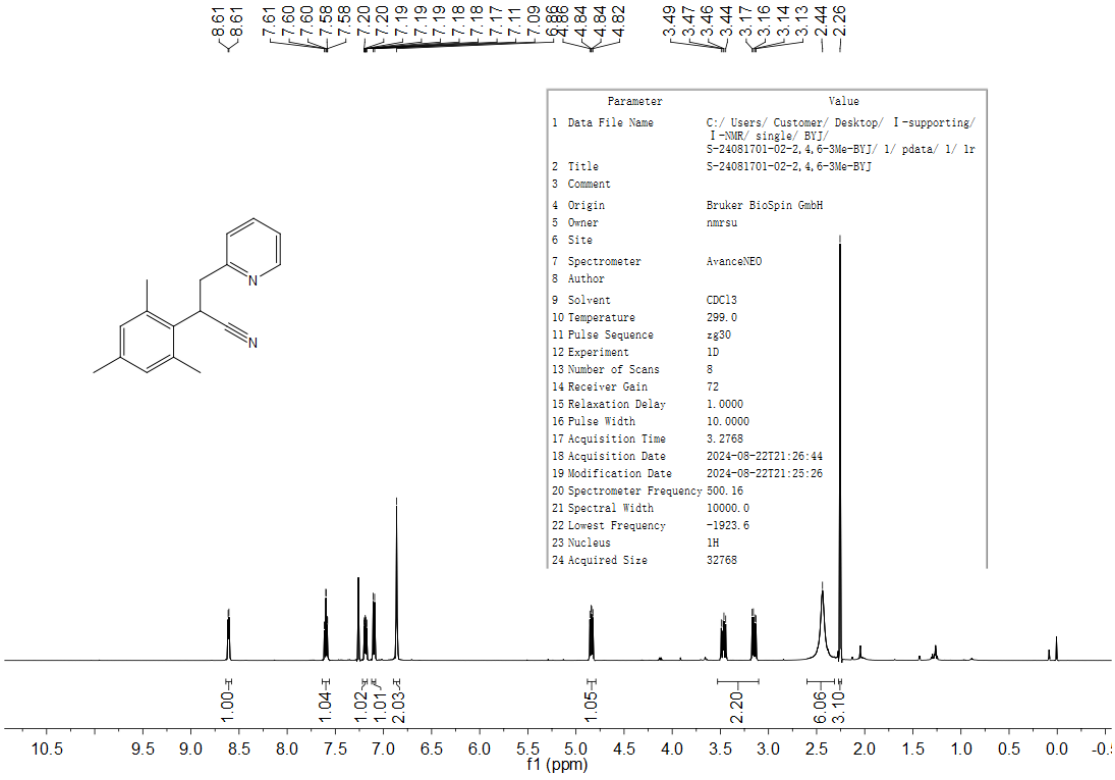
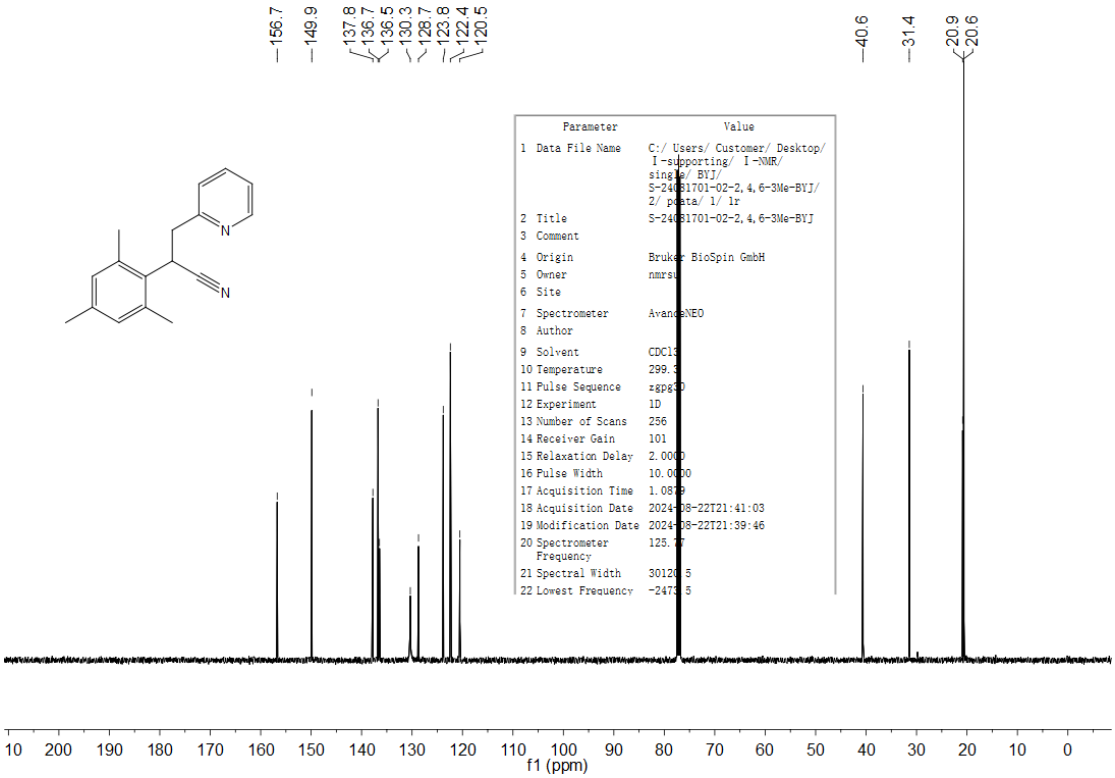
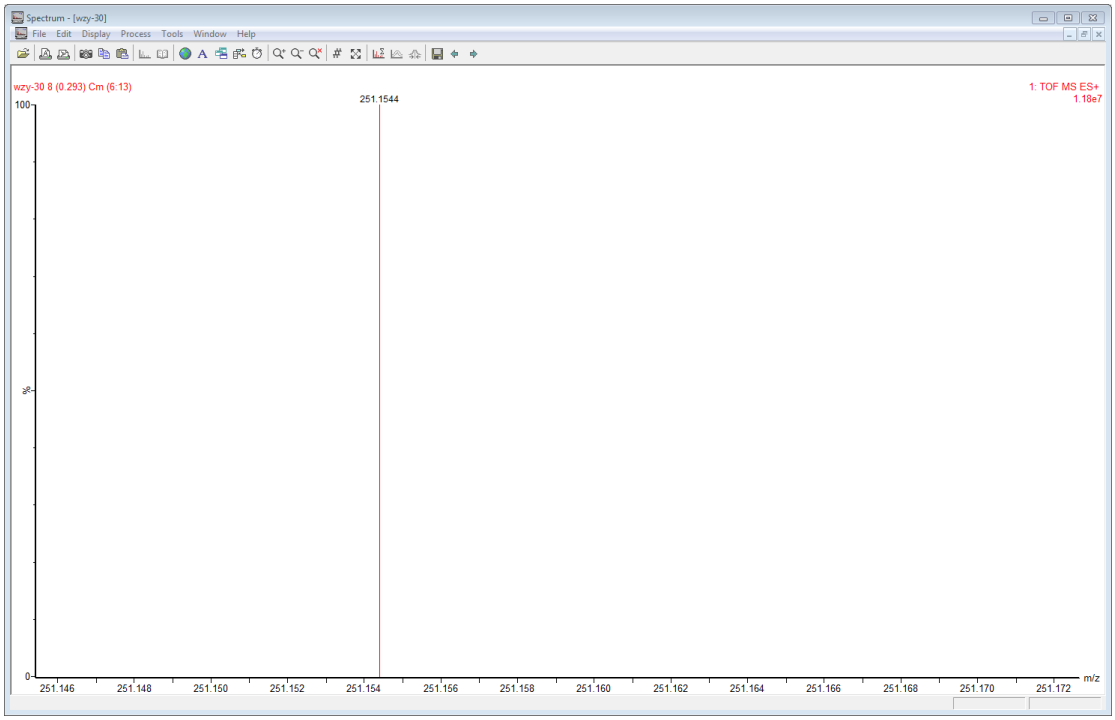
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 292.8
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2024-03-05T22:58:33
19 Modification Date 2024-03-05T22:58:32
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2480.9
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
N
N
f1 (ppm)



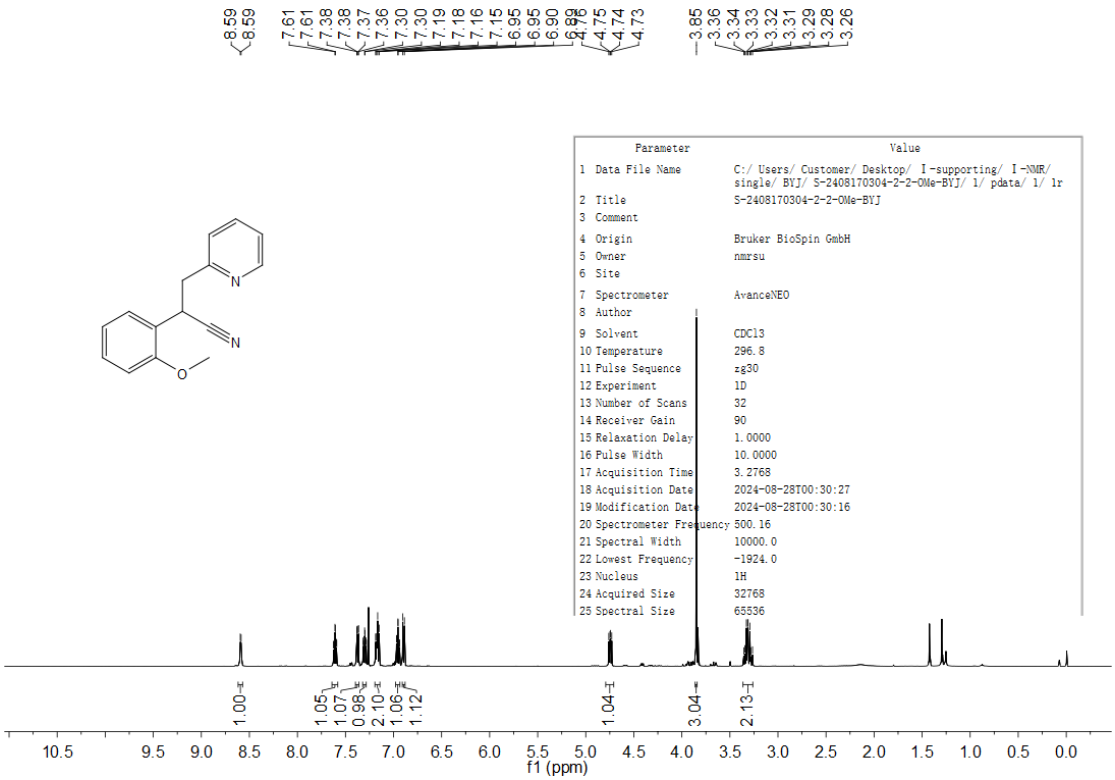
2-mesityl-3-(pyridin-2-yl)propanenitrile (4ea)







2-(2-methoxyphenyl)-3-(pyridin-2-yl)propanenitrile (4fa)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7.38
7.37
7.36
7.30
7.30
7.19
7.18
7.16
7.15
6.95
6.95
6.90
4.75
4.74
4.73
3.85
3.36
3.34
3.33
3.32
3.31
3.29
3.28
3.26
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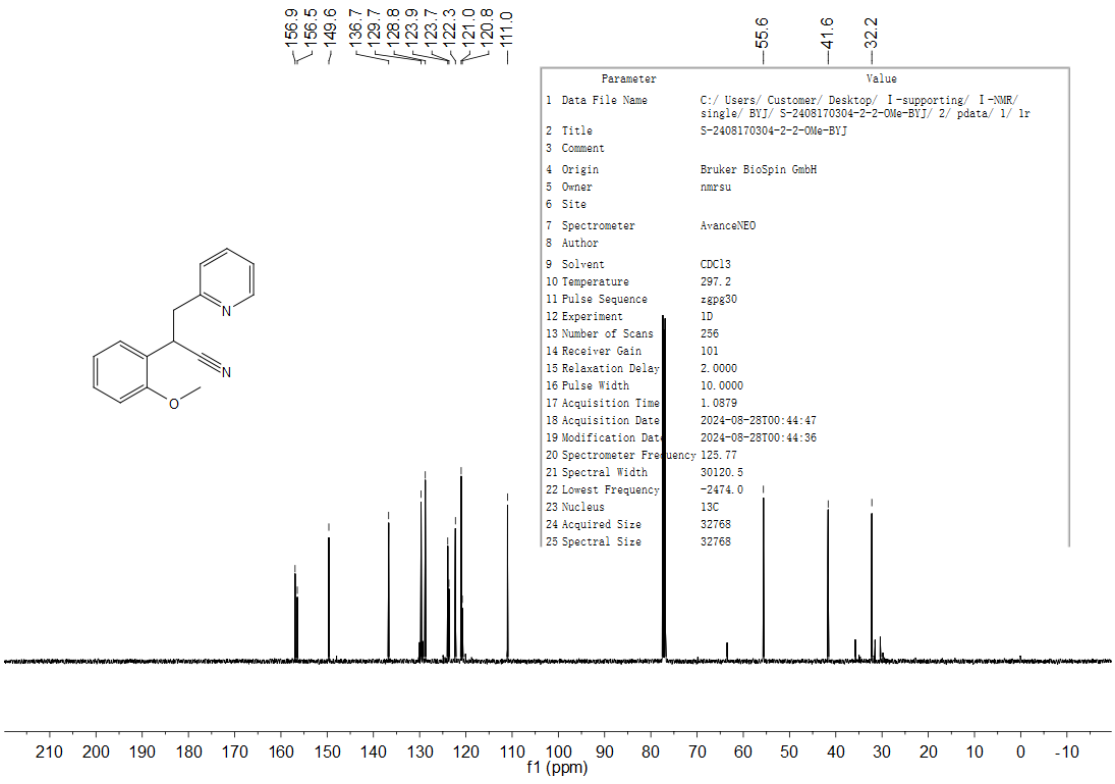
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 296.8
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 32
14 Receiver Gain 90
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2024-08-28T00:30:27
19 Modification Date 2024-08-28T00:30:16
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
N
N
O
1.00
1.05
1.07
0.98
2.10
1.06
1.12
1.04
3.04
2.13
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)


156.9
156.5
149.6
136.7
129.7
128.8
123.9
123.7
122.3
121.0
120.8
111.0
55.6
41.6
32.2
Parameter Value
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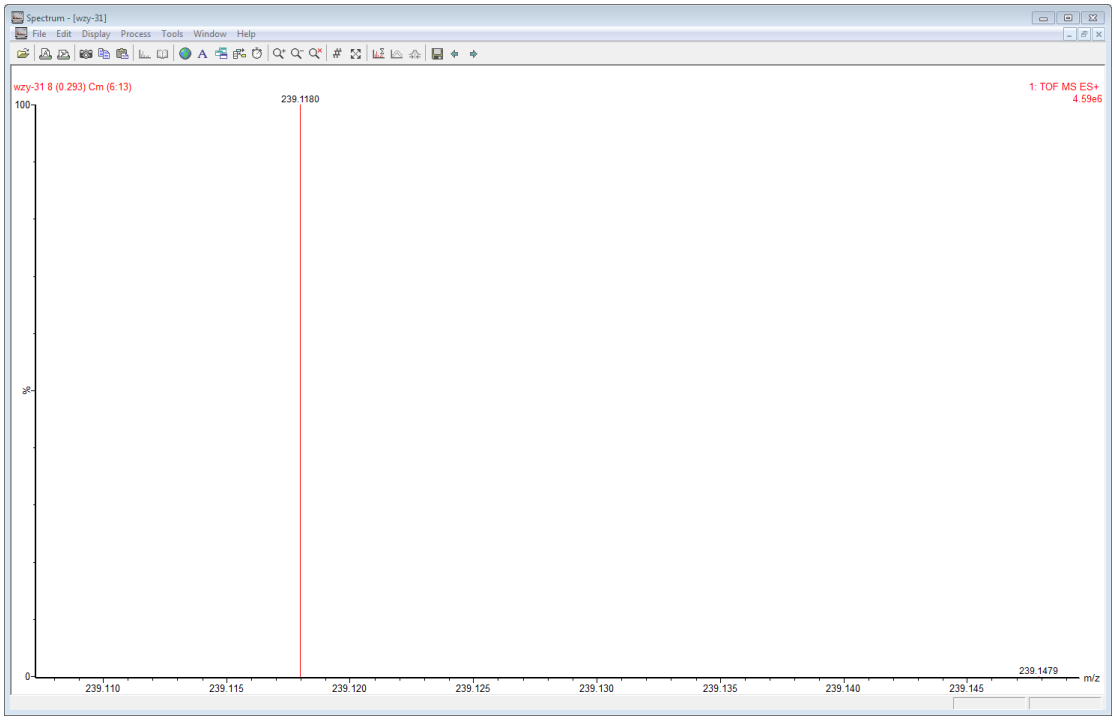
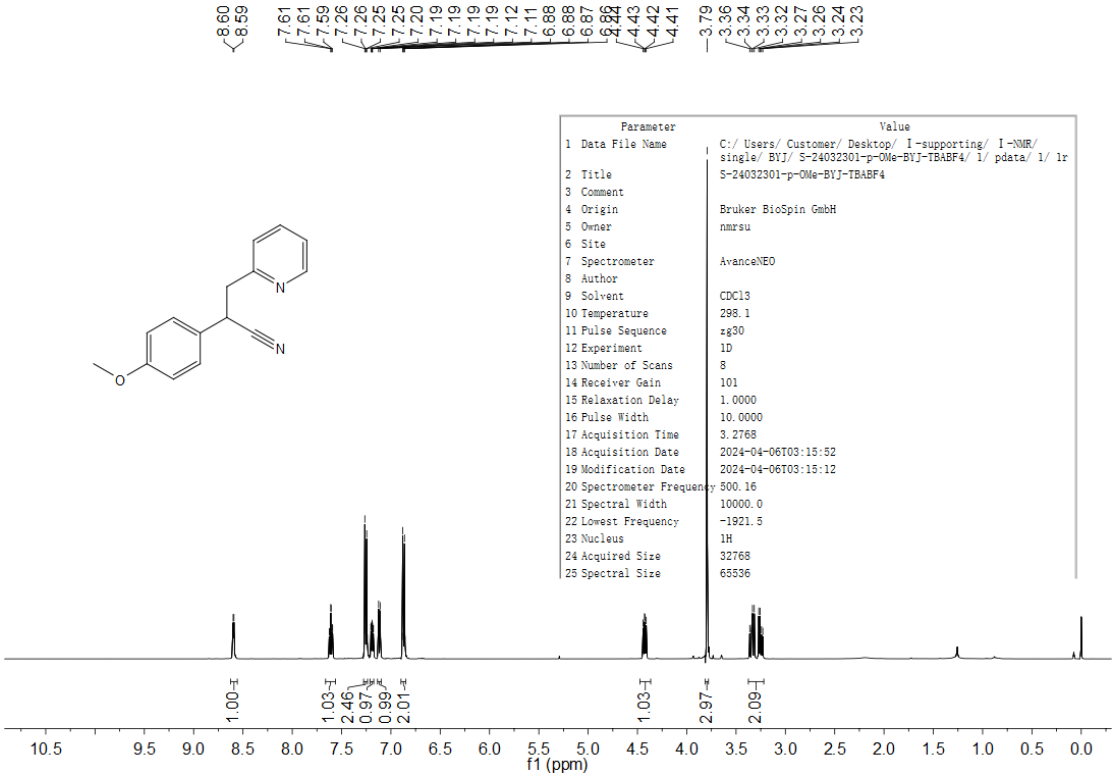
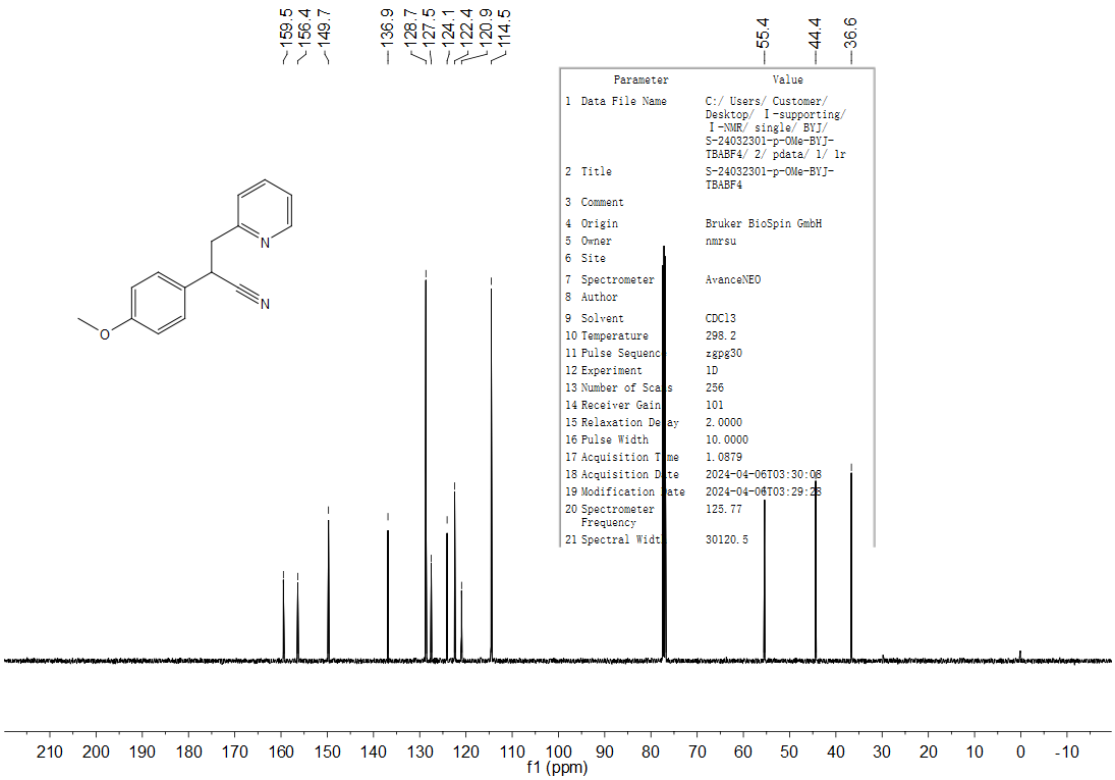
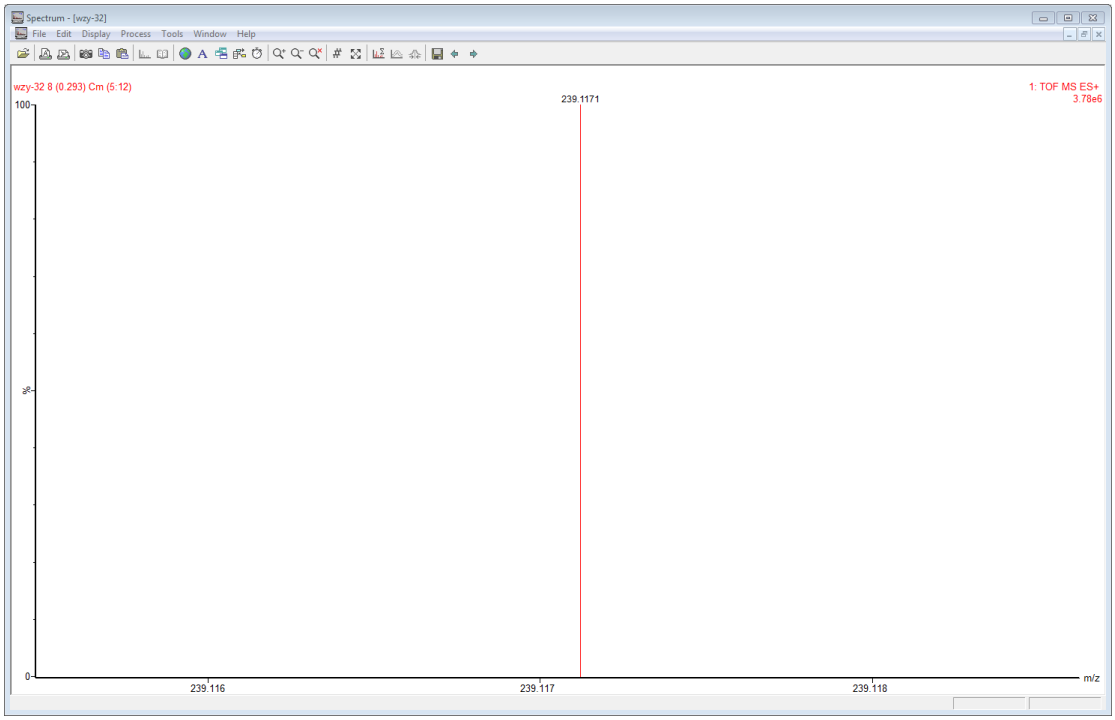
2 Title S-2408170304-2-2-OMe-BYJ
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 297.2
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2024-08-28T00:44:47
19 Modification Date 2024-08-28T00:44:36
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2474.0
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
N
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



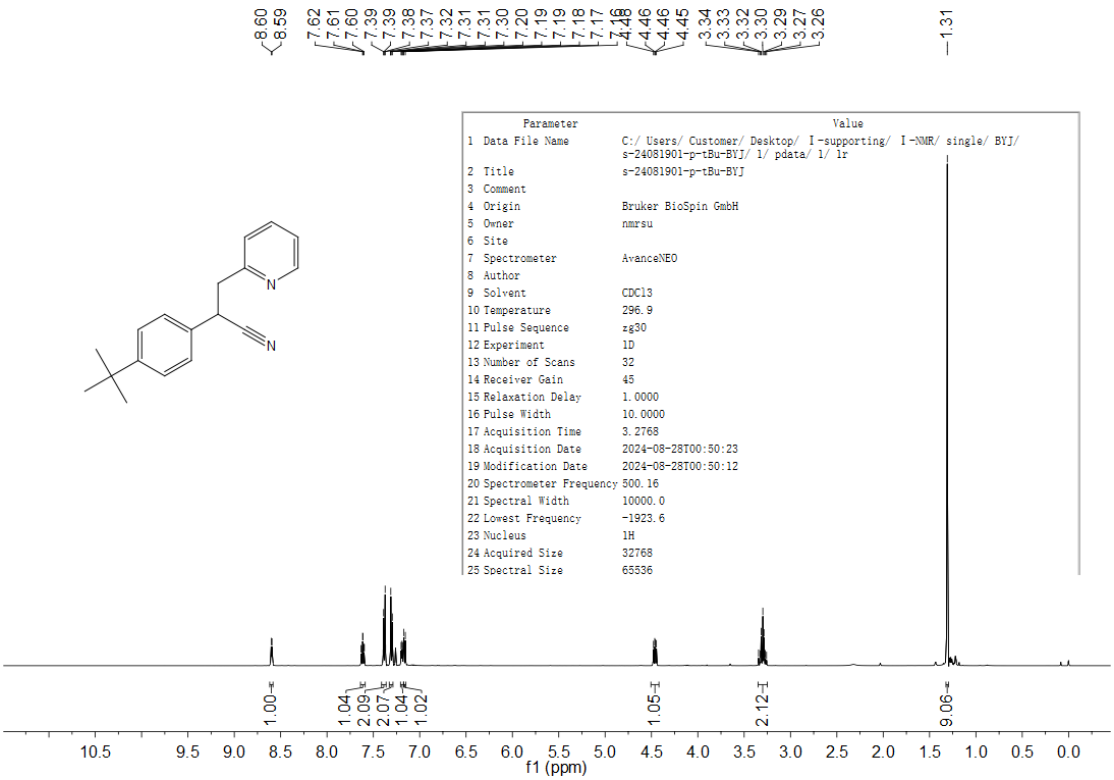
2-(4-methoxyphenyl)-3-(pyridin-2-yl)propanenitrile (4ga)







2-(4-(*tert*-butyl)phenyl)-3-(pyridin-2-yl)propanenitrile (4ha)


8.60
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7.61
7.60
7.39
7.39
7.38
7.37
7.32
7.31
7.31
7.30
7.20
7.19
7.19
7.18
7.17
7.16
4.48
4.46
4.46
4.45
3.34
3.33
3.32
3.30
3.29
3.27
3.26
1.31
Parameter Value
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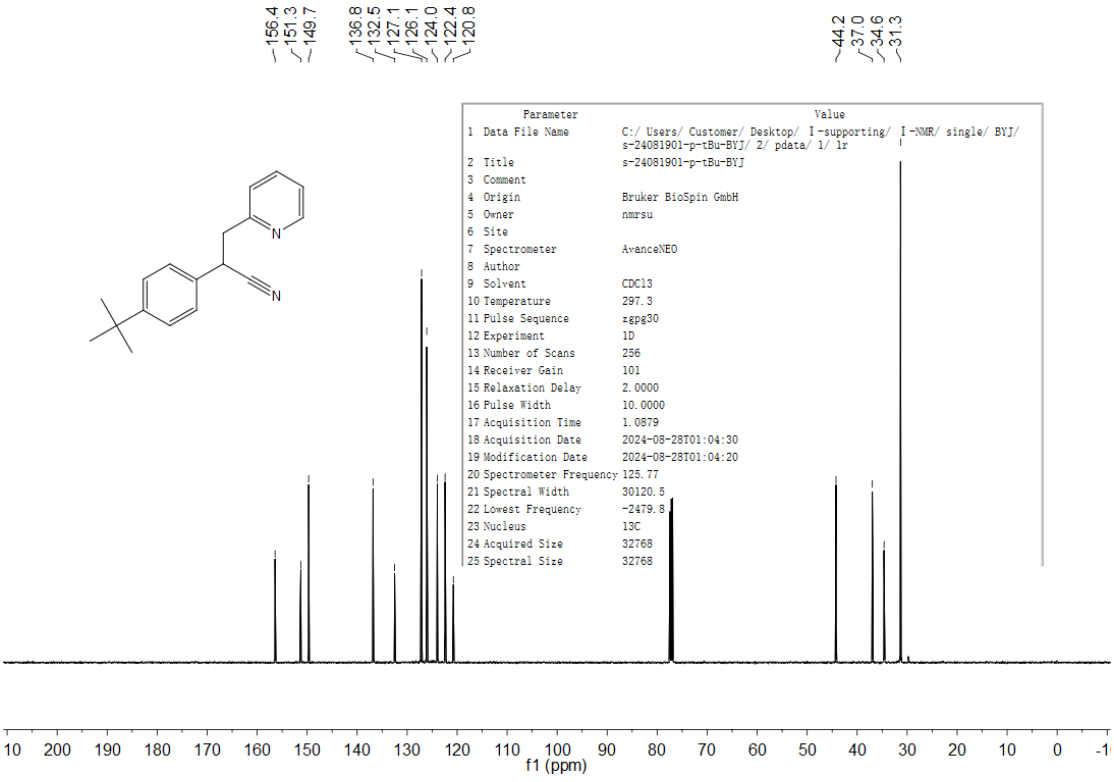
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 296.9
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 32
14 Receiver Gain 45
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2024-08-28T00:50:23
19 Modification Date 2024-08-28T00:50:12
20 Spectrometer Frequency 500.16
21 Spectral Width 10000.0
22 Lowest Frequency -1923.6
23 Nucleus 1H
24 Acquired Size 32768
25 Spectral Size 65536
N
N
1.00
1.04
2.09
2.07
1.04
1.02
1.05
2.12
9.06
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)


156.4
151.3
149.7
136.8
132.5
127.1
126.1
124.0
122.4
120.8
44.2
37.0
34.6
31.3
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2 Title s-24081901-p-tBu-BYJ
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 297.3
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 2024-08-28T01:04:30
19 Modification Date 2024-08-28T01:04:20
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2479.8
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
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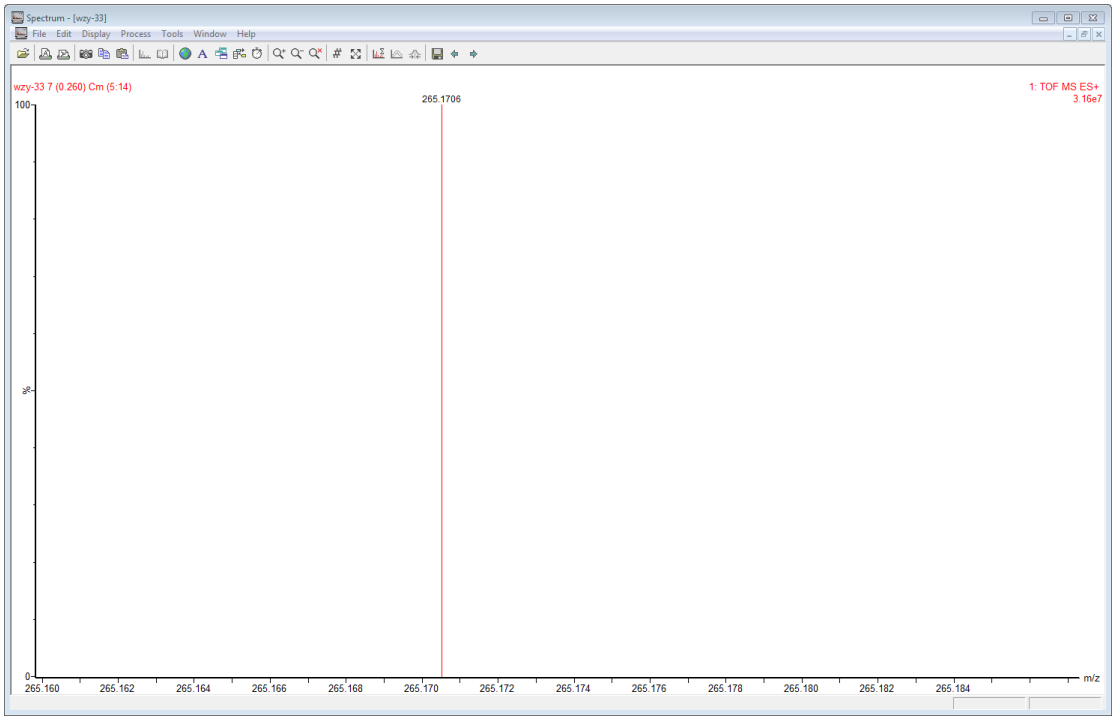
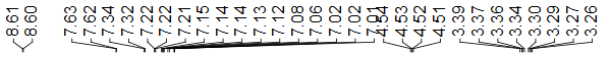
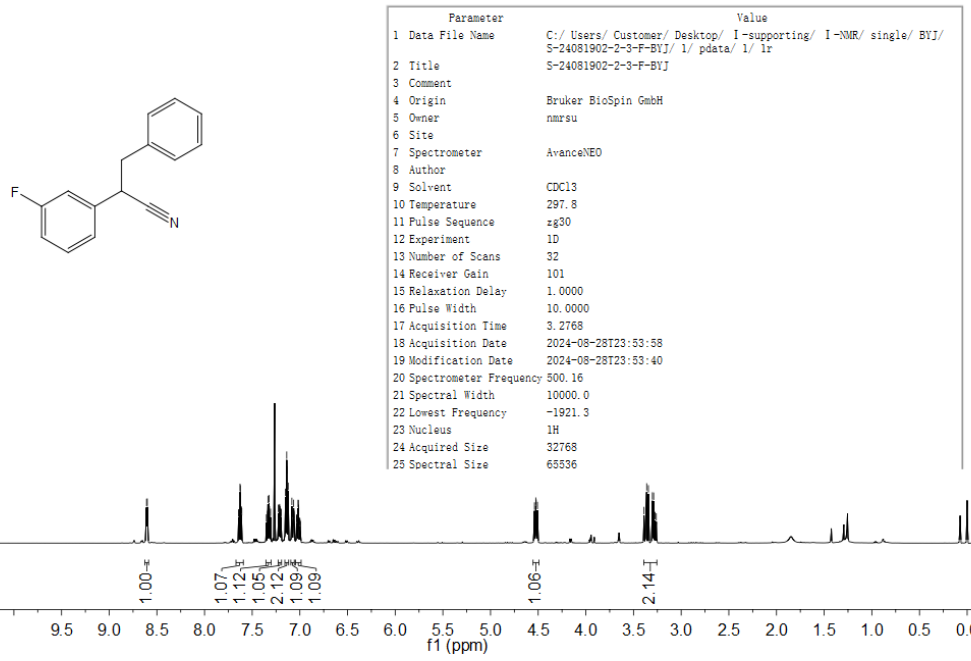
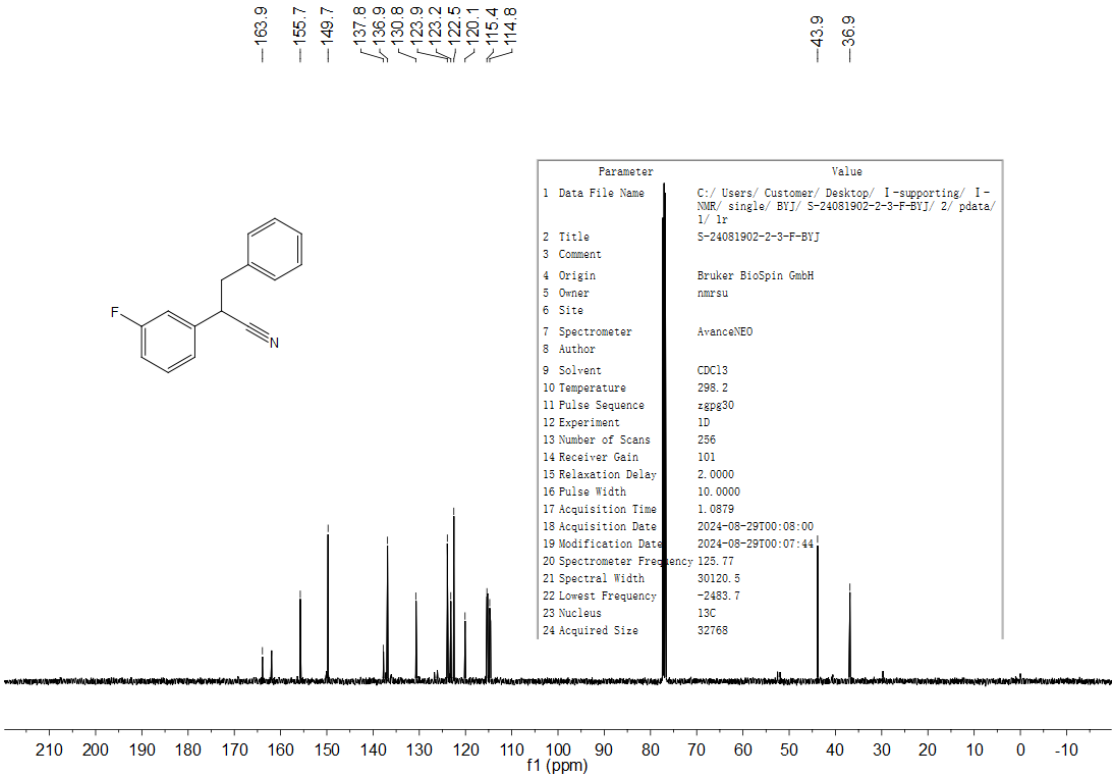
N
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

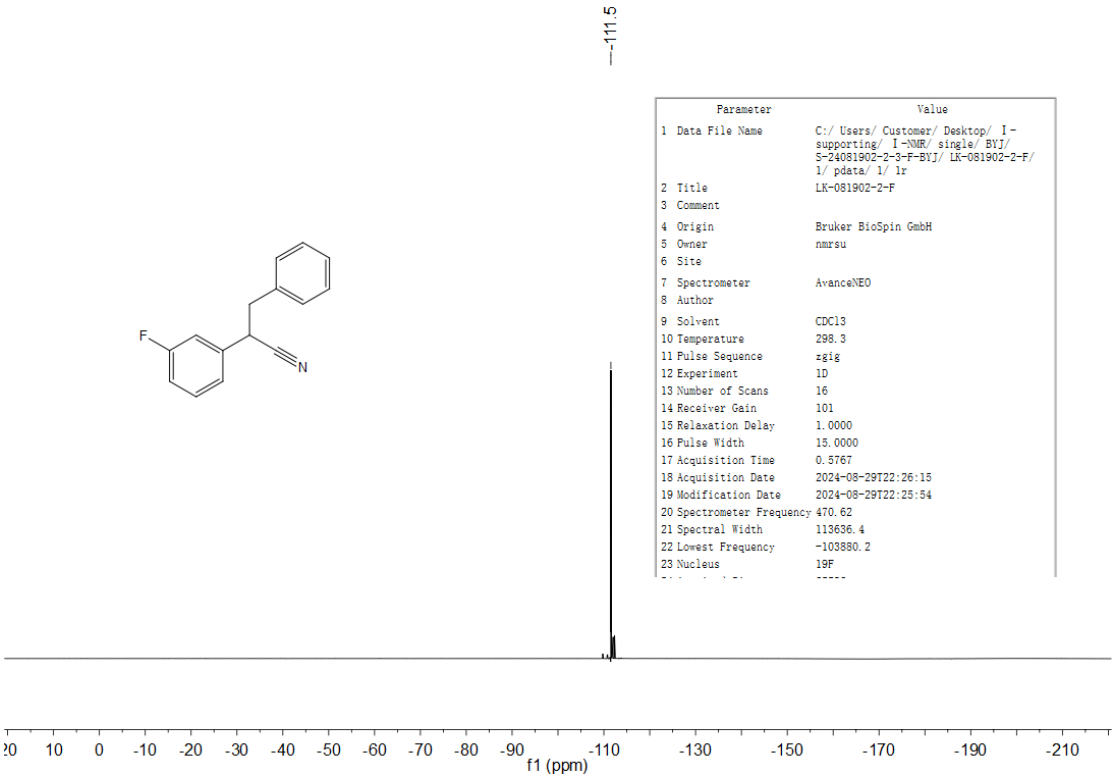


2-(3-fluorophenyl)-3-(pyridin-2-yl)propanenitrile (4ia)






163.9
155.7
149.7
137.8
136.9
130.8
123.9
123.2
122.5
120.1
115.4
114.8
43.9
36.9
F
N
Parameter
Value
1 Data File Name
C:/ Users/ Customer/ Desktop/ I-supporting/ I-NMR/ single/ BYJ/ S-24081902-2-3-F-BYJ/ 2/ pdata/ 1/ 1r
2 Title
S-24081902-2-3-F-BYJ
3 Comment
4 Origin
Bruker BioSpin GmbH
5 Owner
nmrsu
6 Site
7 Spectrometer
AvanceNEO
8 Author
9 Solvent
CDCl3
10 Temperature
298.2
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
2024-08-29T00:08:00
19 Modification Date
2024-08-29T00:07:44
20 Spectrometer Frequency
125.77
21 Spectral Width
30120.5
22 Lowest Frequency
-2483.7
23 Nucleus
13C
24 Acquired 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)


-111.5
F
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Parameter
Value
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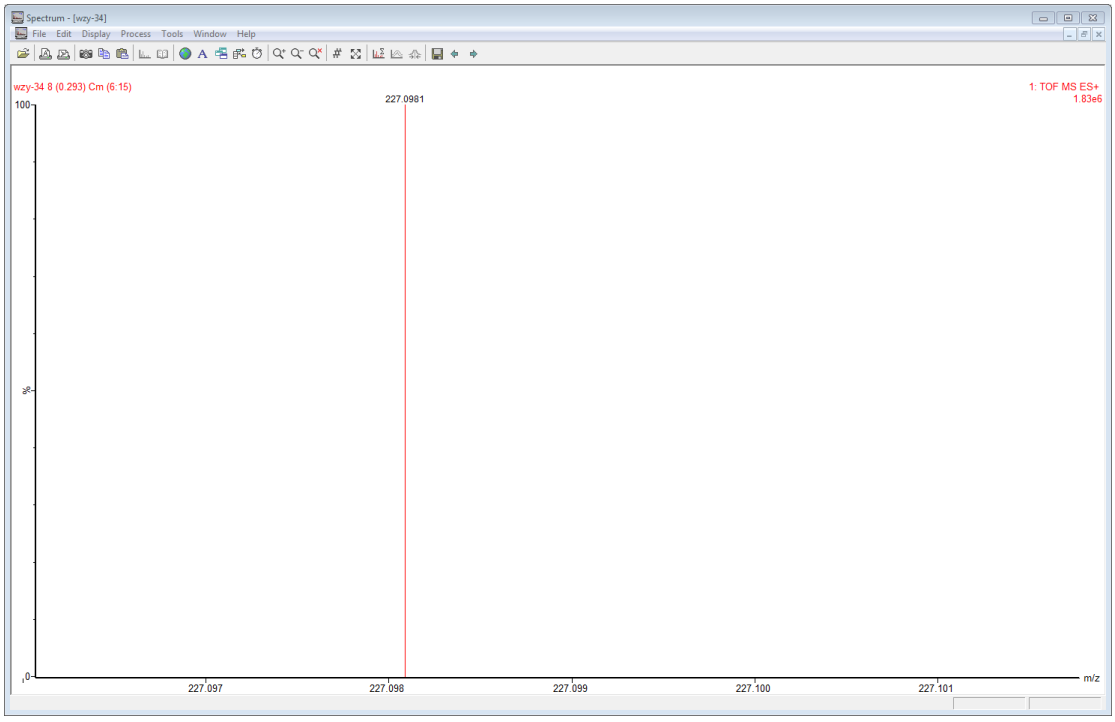
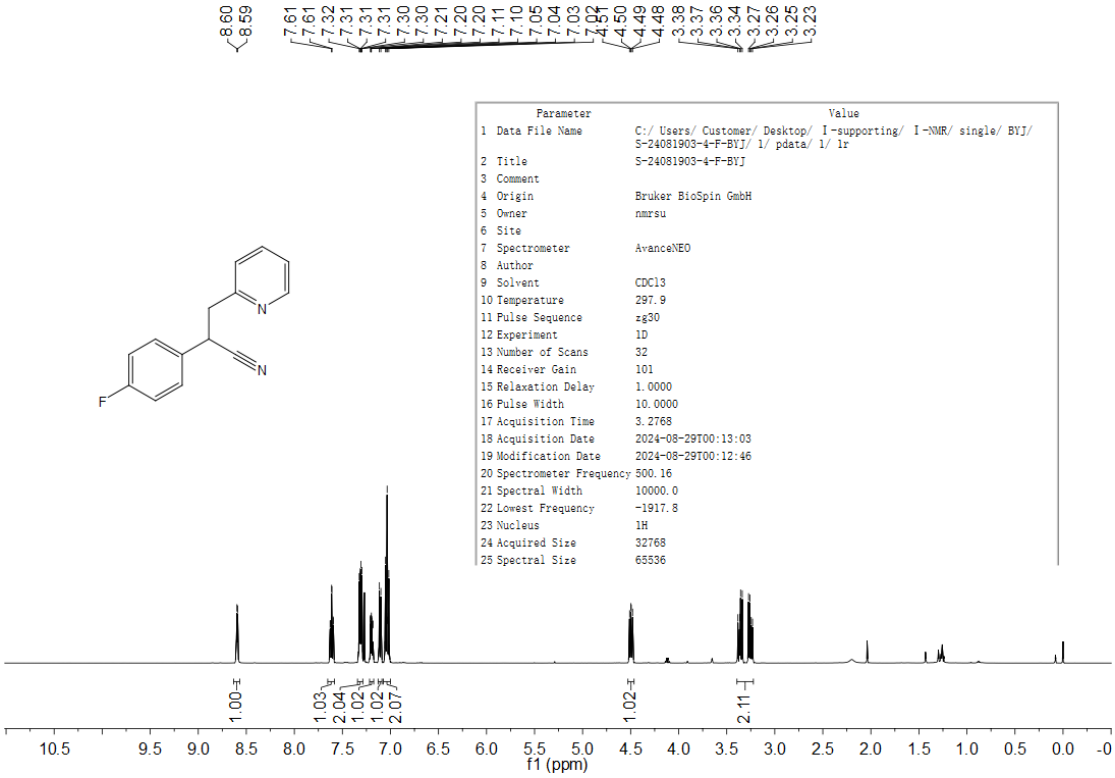
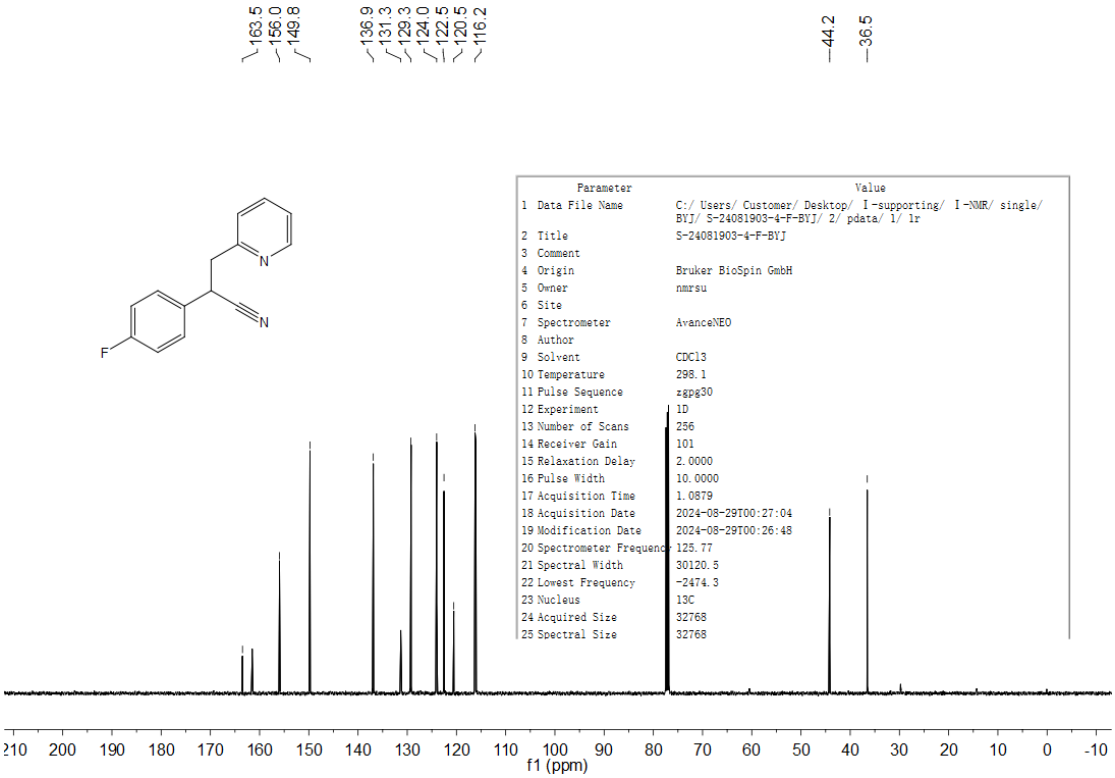
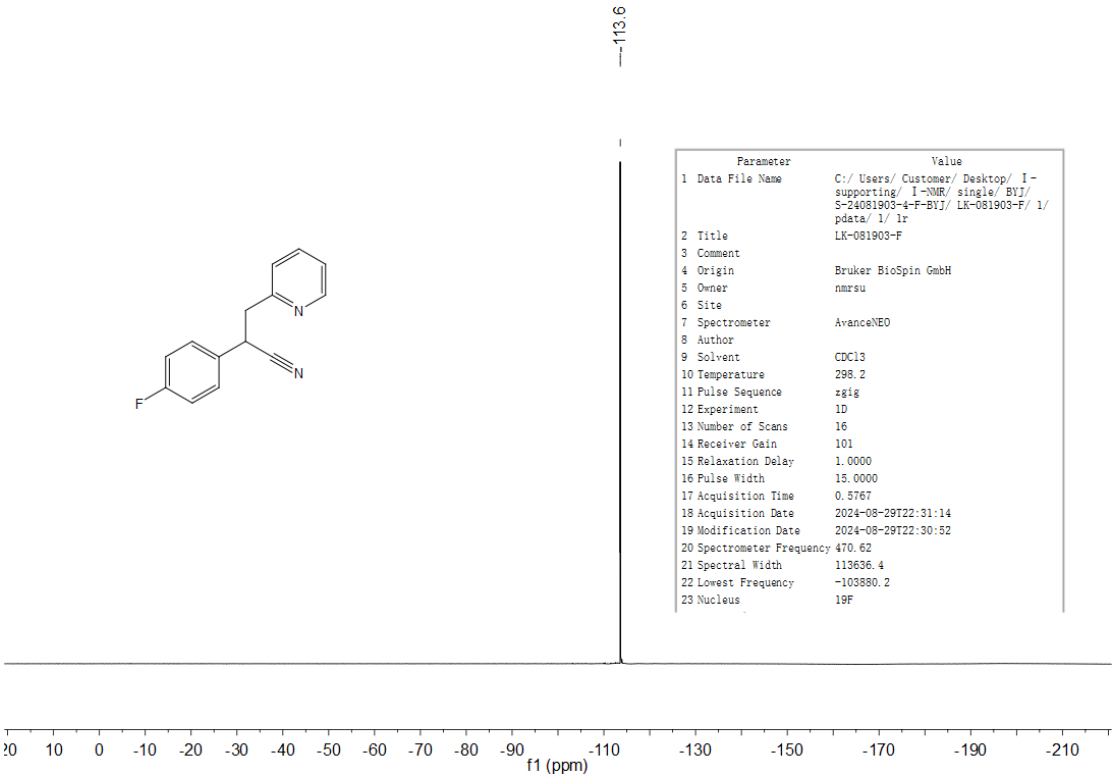
2 Title
LK-081902-2-F
3 Comment
4 Origin
Bruker BioSpin GmbH
5 Owner
nmrsu
6 Site
7 Spectrometer
AvanceNEO
8 Author
9 Solvent
CDCl3
10 Temperature
298.3
11 Pulse Sequence
zgig
12 Experiment
1D
13 Number of Scans
16
14 Receiver Gain
101
15 Relaxation Delay
1.0000
16 Pulse Width
15.0000
17 Acquisition Time
0.5767
18 Acquisition Date
2024-08-29T22:26:15
19 Modification Date
2024-08-29T22:25:54
20 Spectrometer Frequency
470.62
21 Spectral Width
113636.4
22 Lowest Frequency
-103880.2
23 Nucleus
19F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)



2-(4-fluorophenyl)-3-(pyridin-2-yl)propanenitrile (4ja)




163.5
156.0
149.8
136.9
131.3
129.3
124.0
122.5
120.5
116.2
44.2
36.5
N
N
F
Parameter Value
1 Data File Name C:/ Users/ Customer/ Desktop/ I-supporting/ I-NMR/ single/ BYJ/ S-24081903-4-F-BYJ/ 2/ pdata/ 1/ 1r
2 Title S-24081903-4-F-BYJ
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.1
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 2024-08-29T00:27:04
19 Modification Date 2024-08-29T00:26:48
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2474.3
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)


113.6
N
N
F
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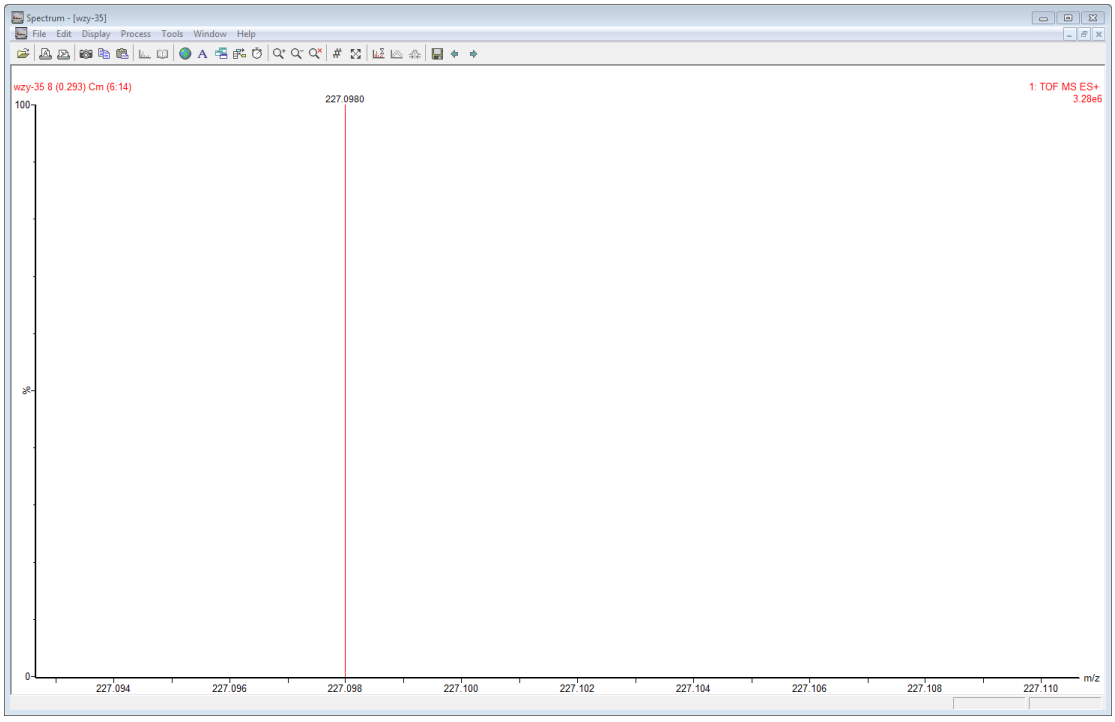
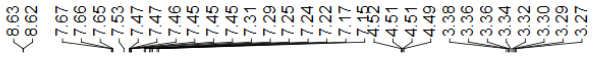
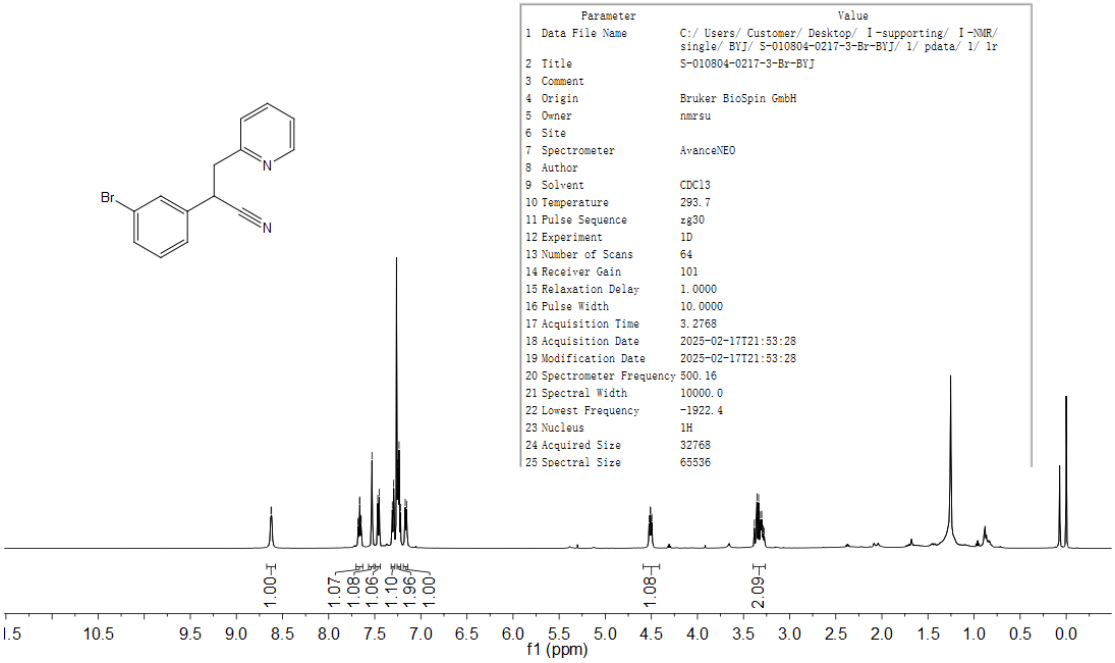
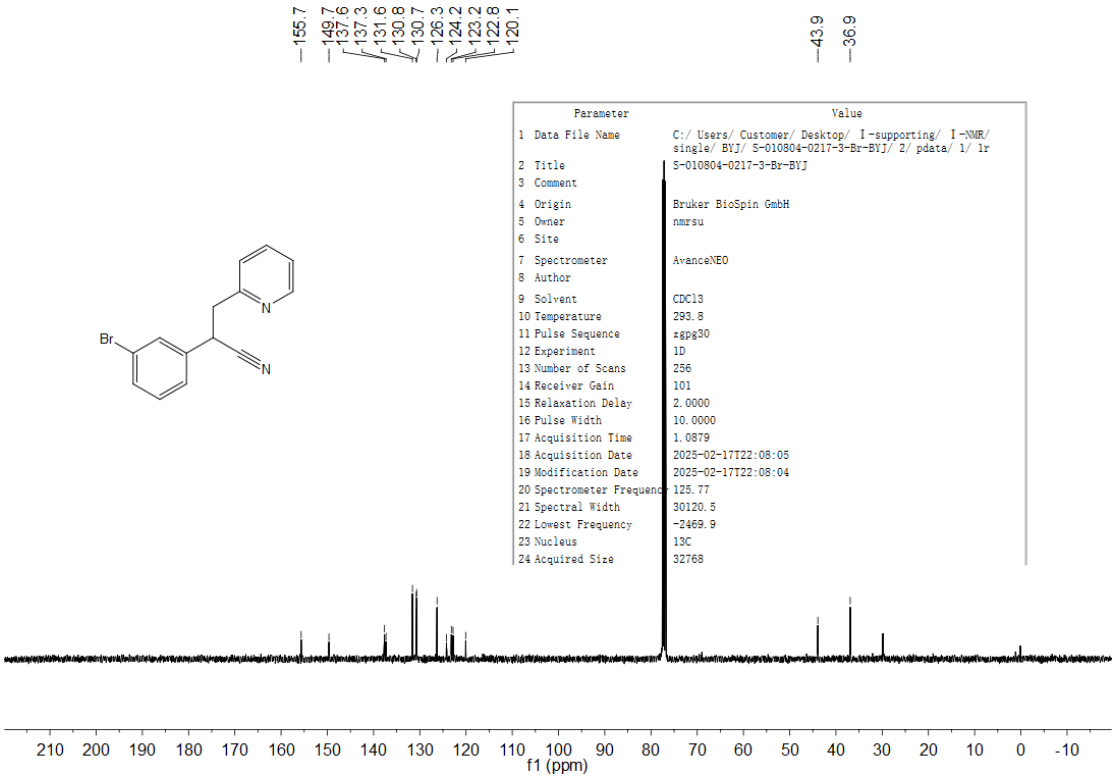
2 Title LK-081903-F
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.2
11 Pulse Sequence zgig
12 Experiment 1D
13 Number of Scans 16
14 Receiver Gain 101
15 Relaxation Delay 1.0000
16 Pulse Width 15.0000
17 Acquisition Time 0.5767
18 Acquisition Date 2024-08-29T22:31:14
19 Modification Date 2024-08-29T22:30:52
20 Spectrometer Frequency 470.62
21 Spectral Width 113636.4
22 Lowest Frequency -103880.2
23 Nucleus 19F
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

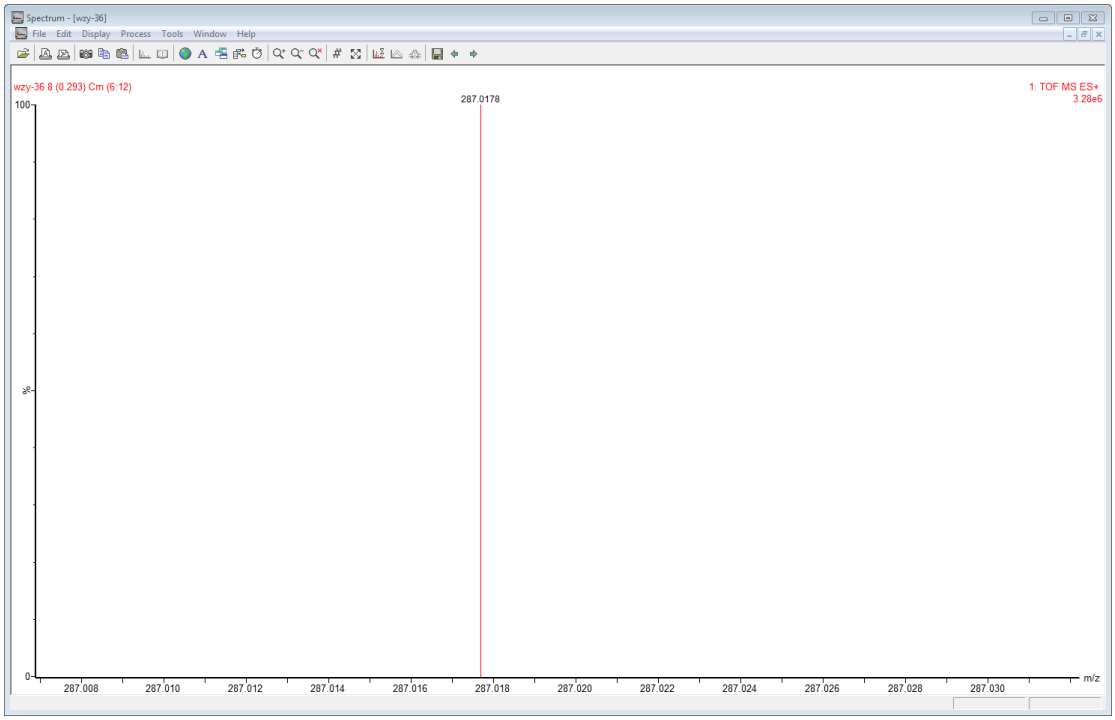


2-(3-bromophenyl)-3-(pyridin-2-yl)propanenitrile (4ka)

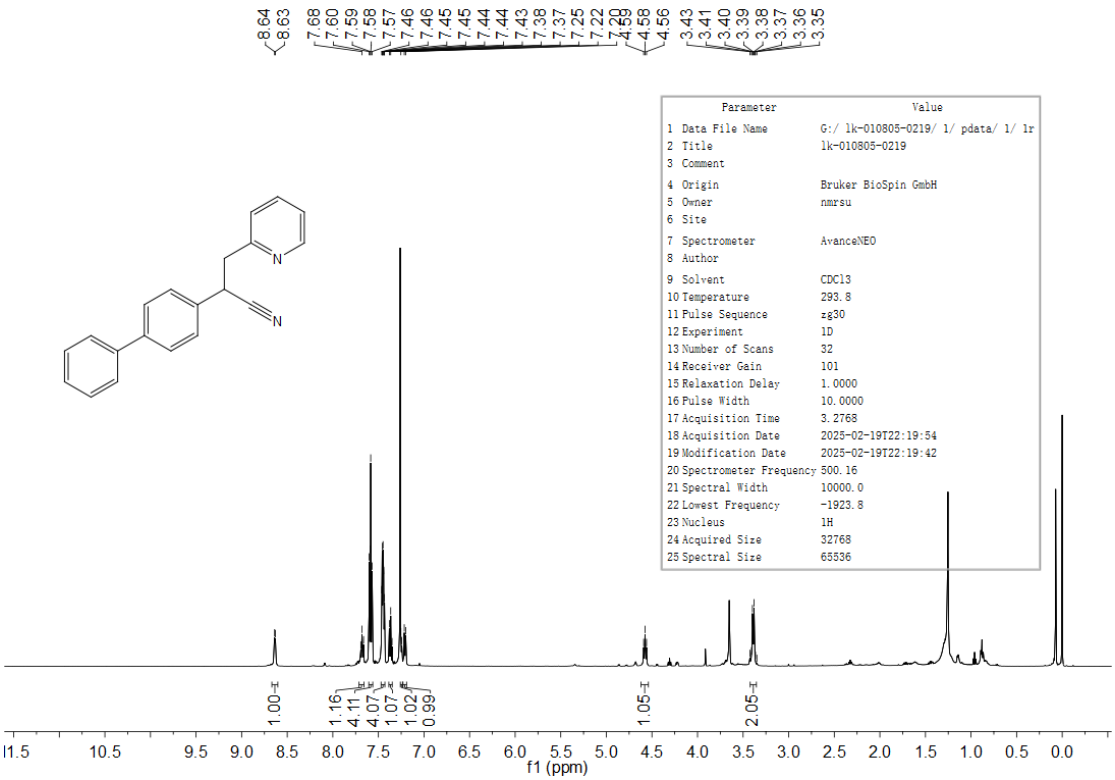








2-([1,1'-biphenyl]-4-yl)-3-(pyridin-2-yl)propanenitrile (4la)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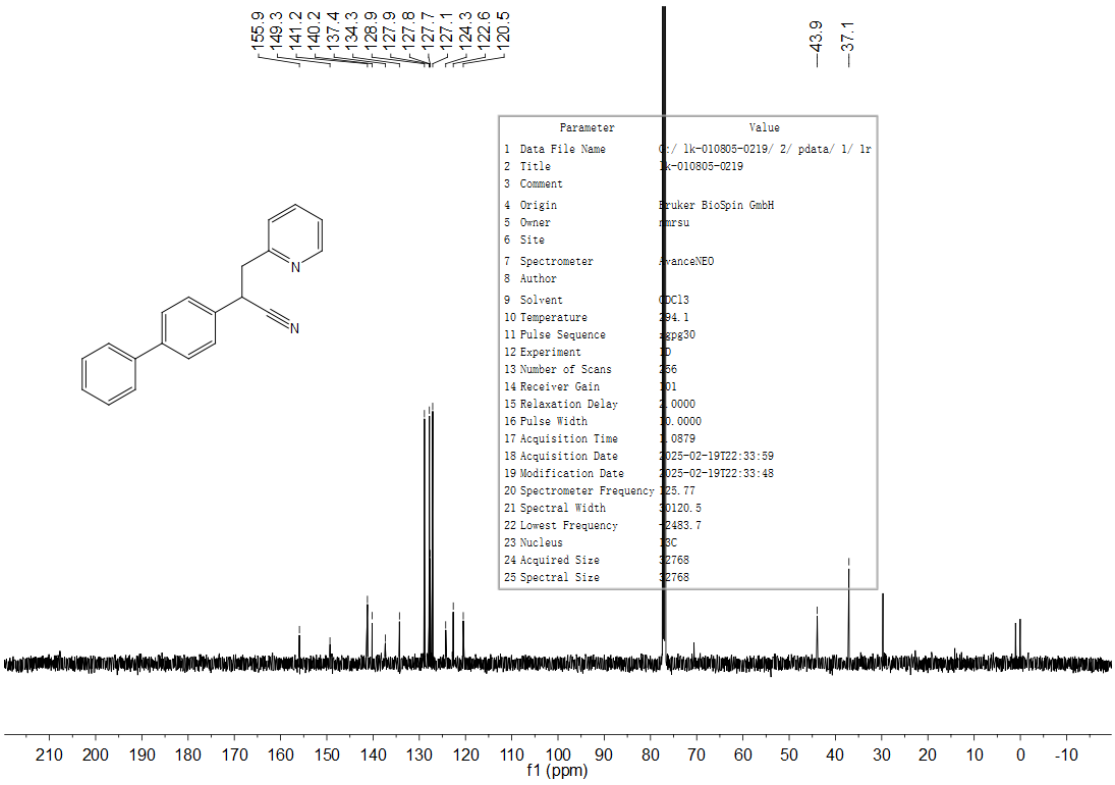
8.63
7.68
7.60
7.59
7.58
7.57
7.46
7.46
7.45
7.45
7.44
7.44
7.43
7.38
7.37
7.25
7.22
7.20
4.59
4.58
4.56
3.43
3.41
3.40
3.39
3.38
3.37
3.36
3.35
N
N
Parameter Value
1 Data File Name G:/ lk-010805-0219/ 1/ pdata/ 1/ 1r
2 Title lk-010805-0219
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 293.8
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 32
14 Receiver Gain 101
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2025-02-19T22:19:54
19 Modification Date 2025-02-19T22:19:42
20 Spectrometer Frequency 500.16
21 Spectral Width 10000.0
22 Lowest Frequency -1923.8
23 Nucleus 1H
24 Acquired Size 32768
25 Spectral Size 65536
1.00
1.16
4.11
4.07
1.07
1.02
0.99
1.05
2.05
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)


155.9
149.3
141.2
140.2
137.4
134.3
128.9
127.9
127.8
127.7
127.1
124.3
122.6
120.5
43.9
37.1
N
N
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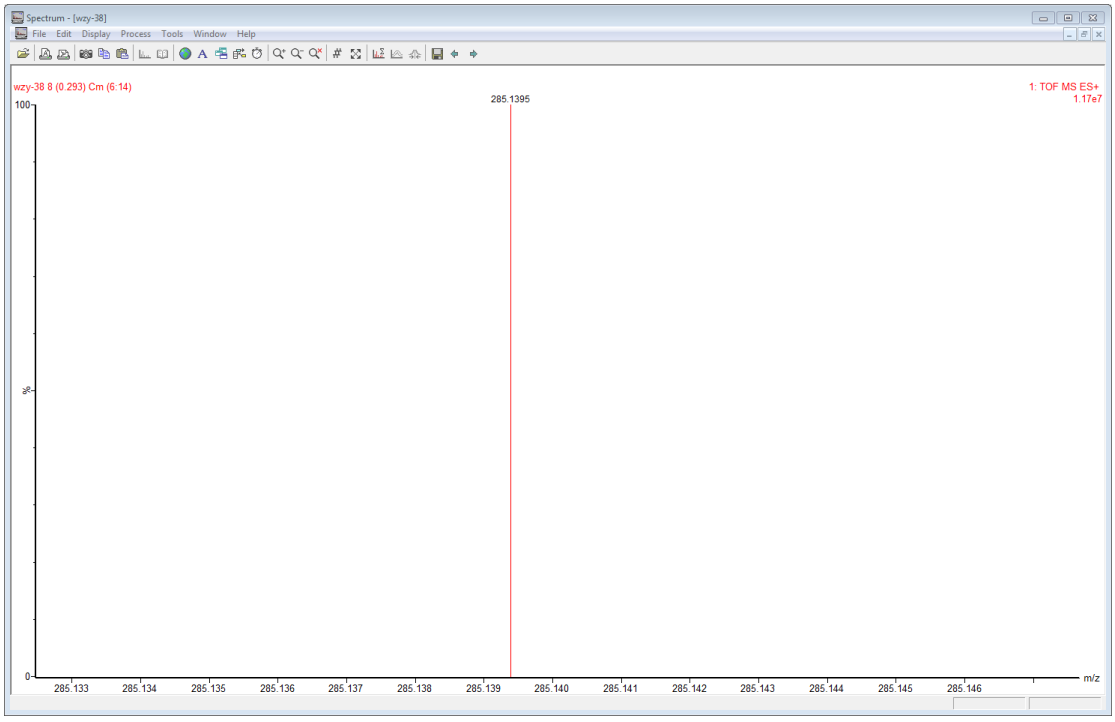
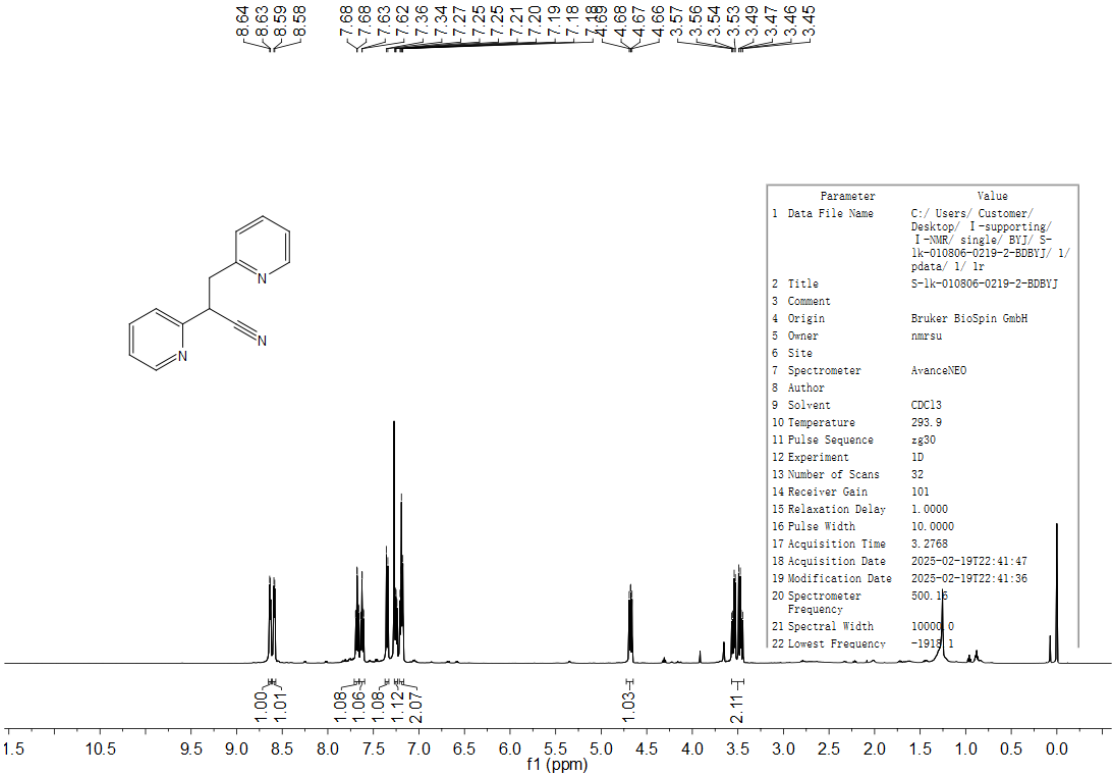
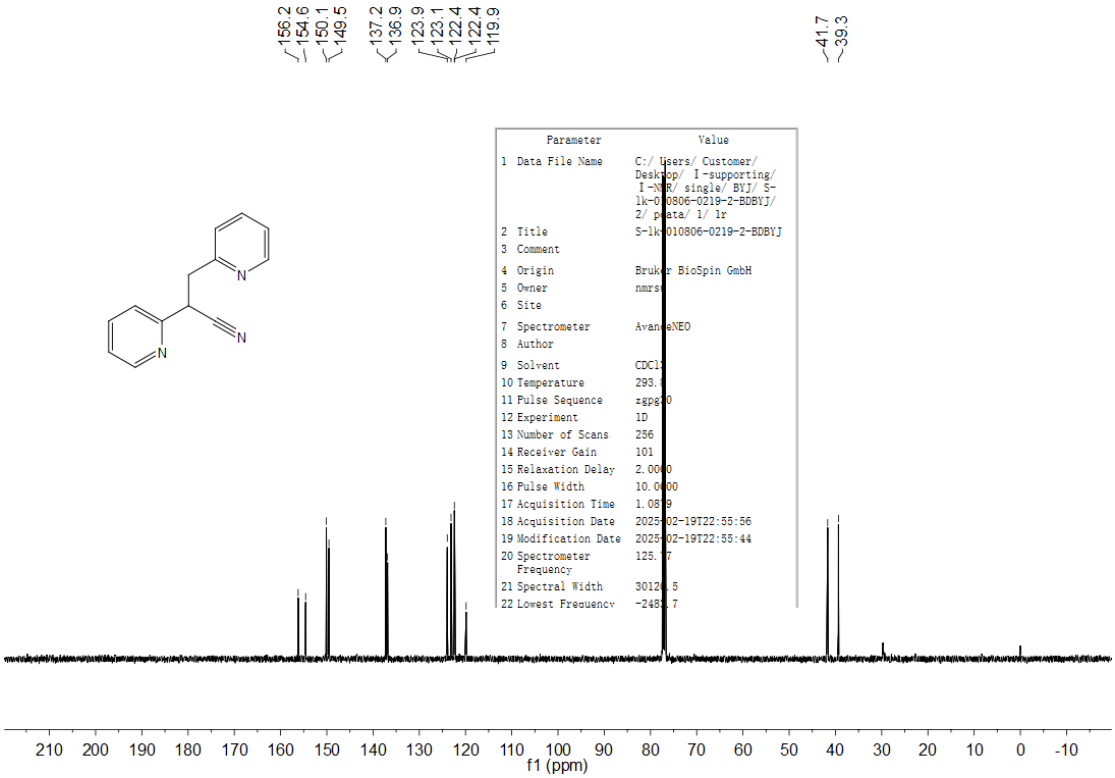
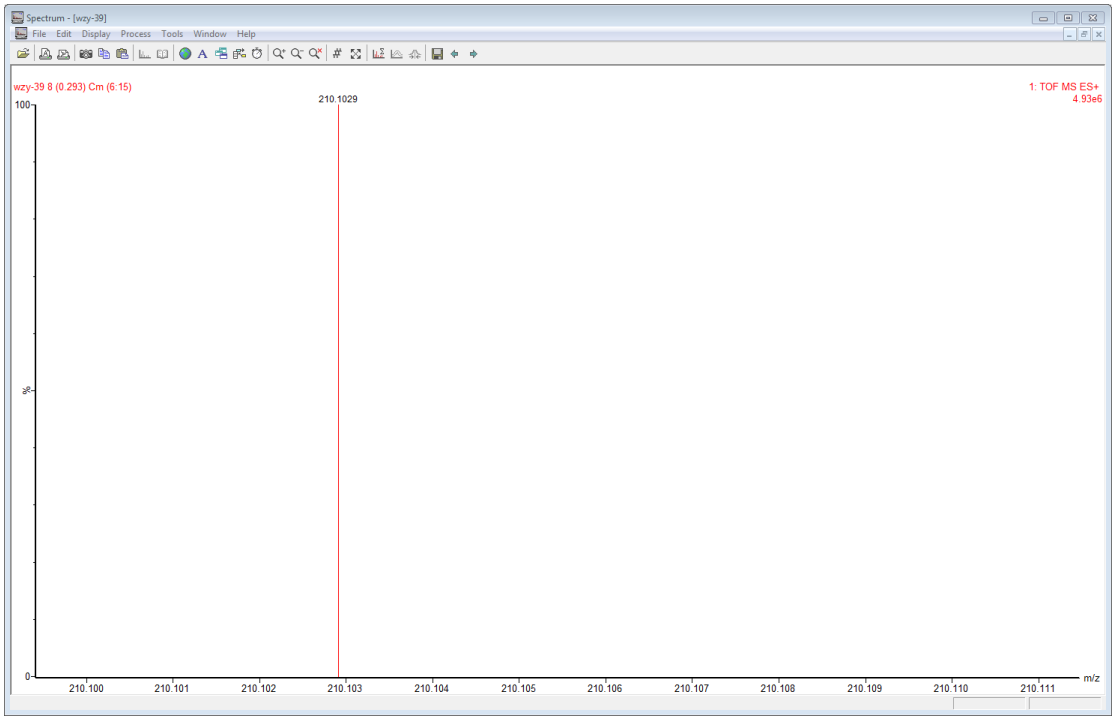
1 Data File Name G:/ lk-010805-0219/ 2/ pdata/ 1/ 1r
2 Title lk-010805-0219
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 294.1
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2025-02-19T22:33:59
19 Modification Date 2025-02-19T22:33:48
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2483.7
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)



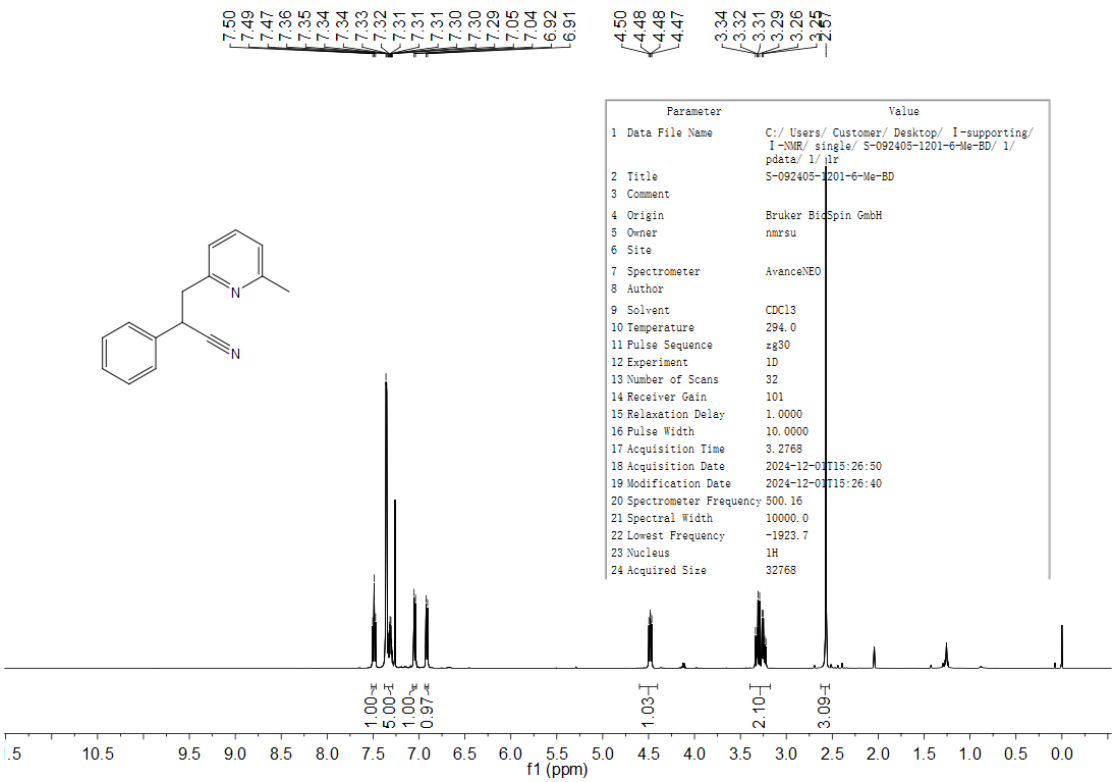
2,3-di(pyridin-2-yl)propanenitrile (4ma)







3-(6-methylpyridin-2-yl)-2-phenylpropanenitrile (4ab)


7.50
7.49
7.47
7.36
7.35
7.34
7.34
7.33
7.32
7.31
7.31
7.31
7.30
7.30
7.29
7.05
7.04
6.92
6.91
4.50
4.48
4.48
4.47
3.34
3.32
3.31
3.29
3.26
2.57
N
N
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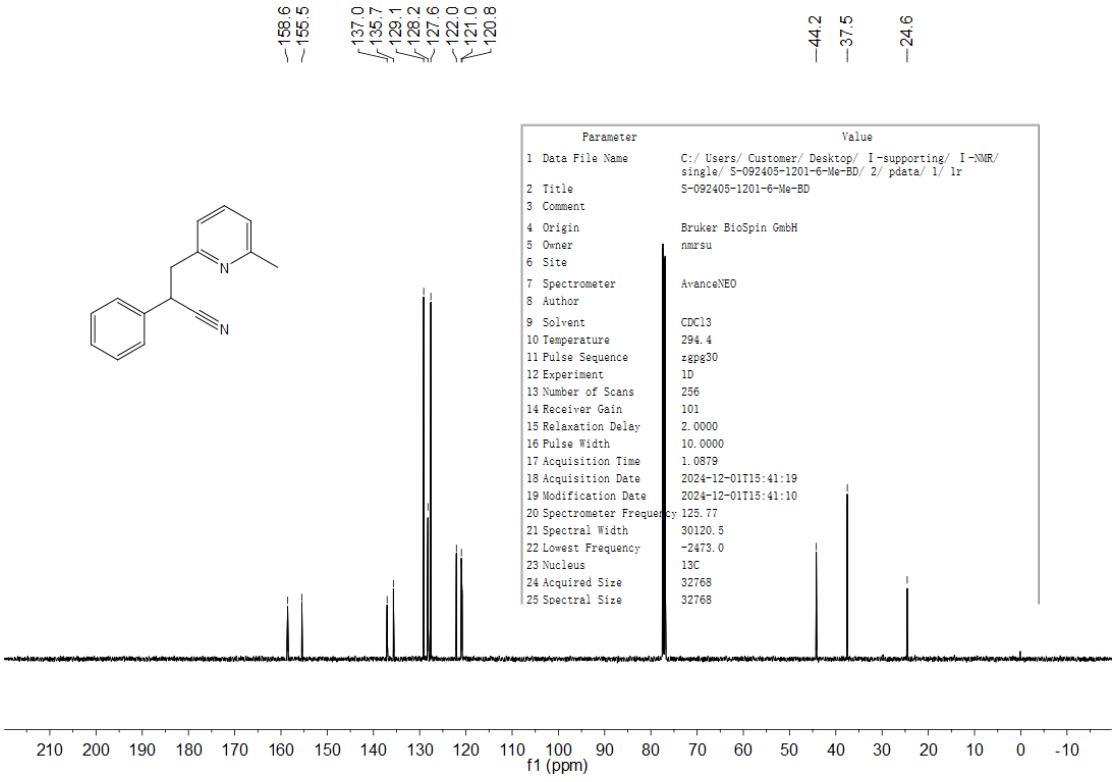
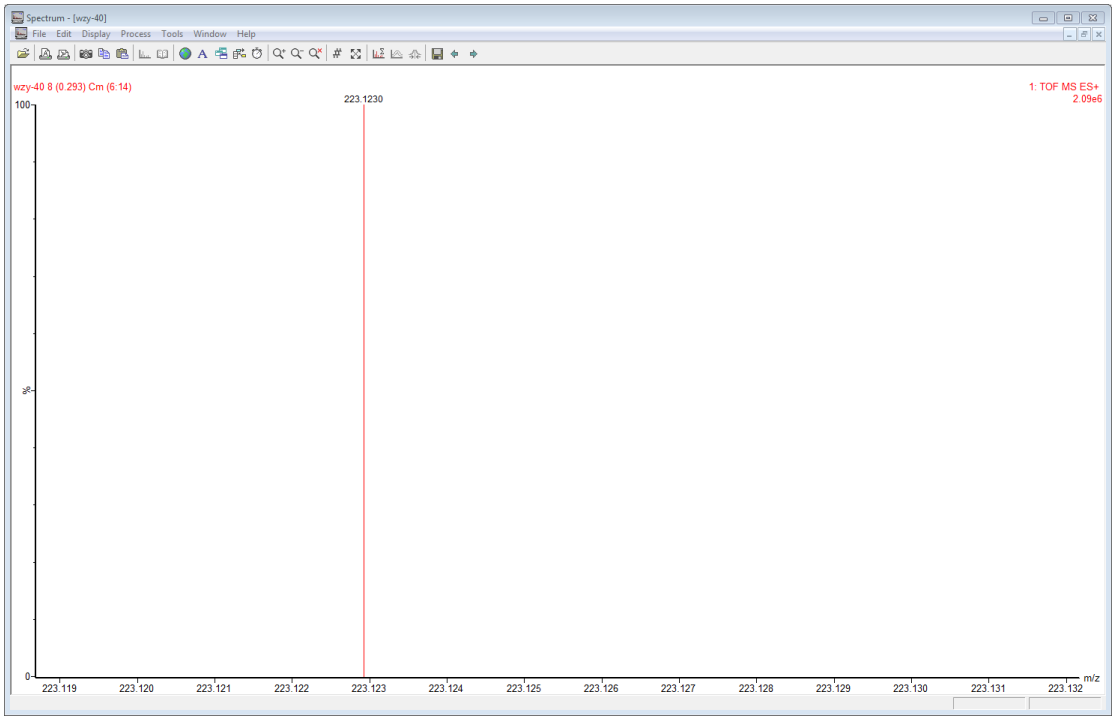
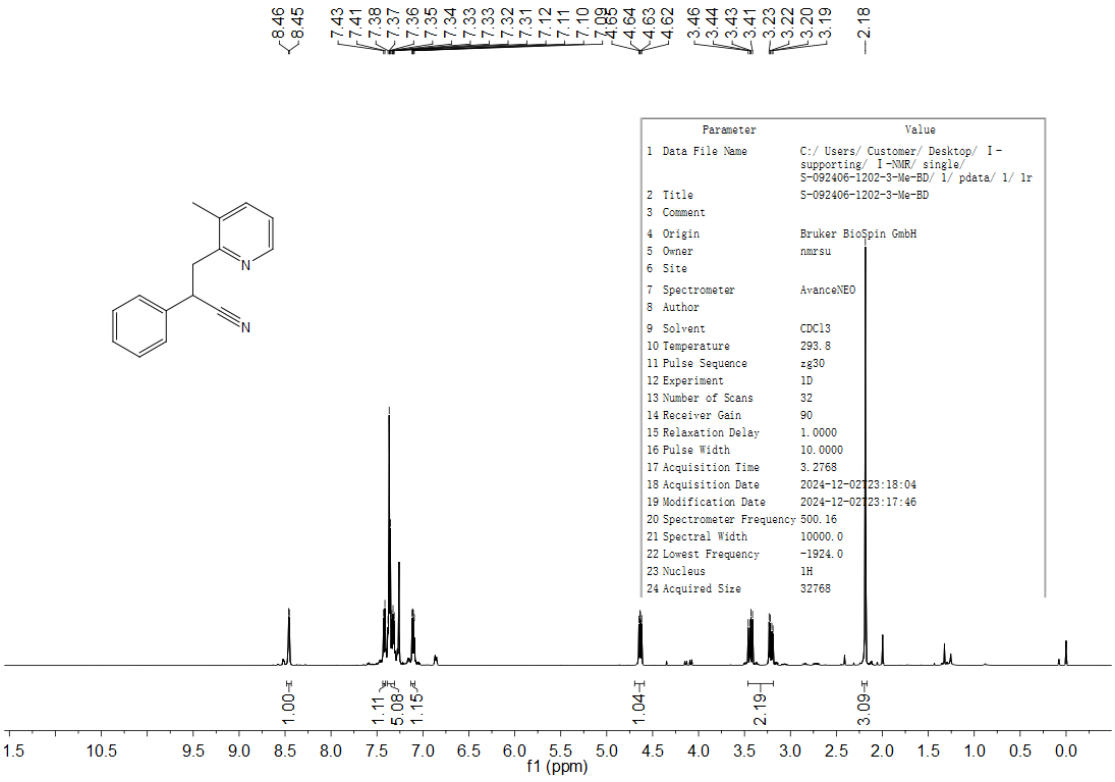
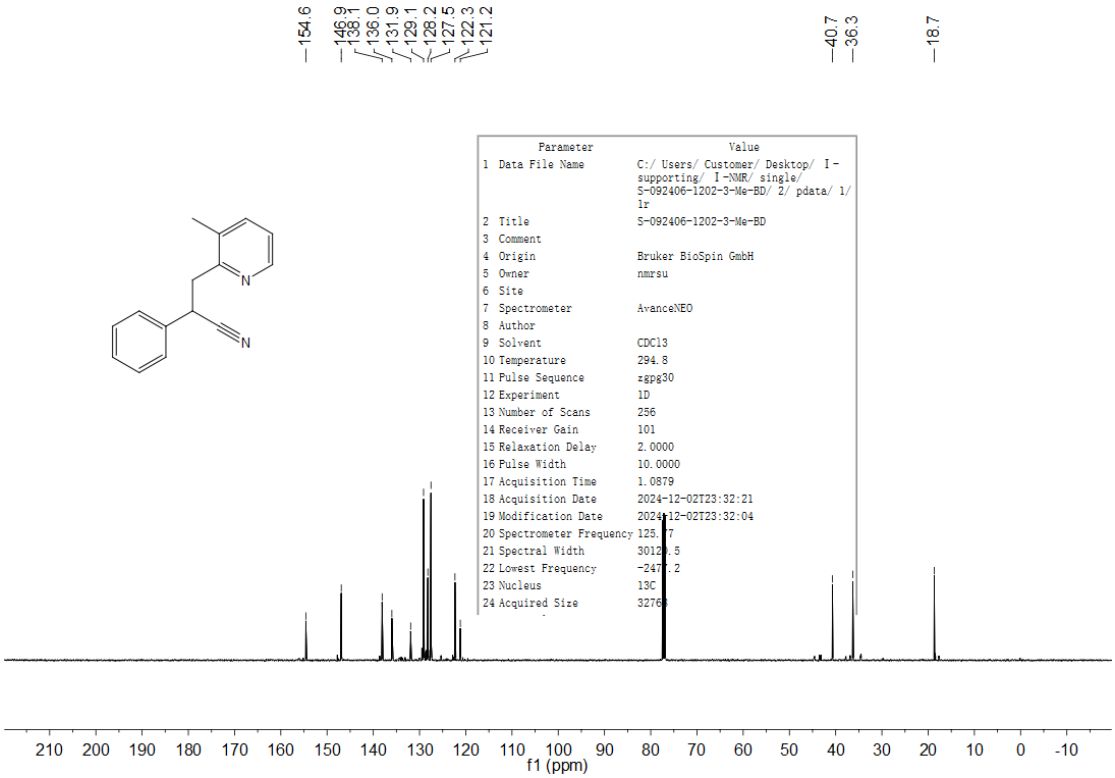
2 Title S-092405-1201-6-Me-BD
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 294.0
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 32
14 Receiver Gain 101
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2024-12-01T15:26:50
19 Modification Date 2024-12-01T15:26:40
20 Spectrometer Frequency 500.16
21 Spectral Width 10000.0
22 Lowest Frequency -1923.7
23 Nucleus 1H
24 Acquired Size 32768
1.00
5.00
1.00
0.97
1.03
2.10
3.09
f1 (ppm)

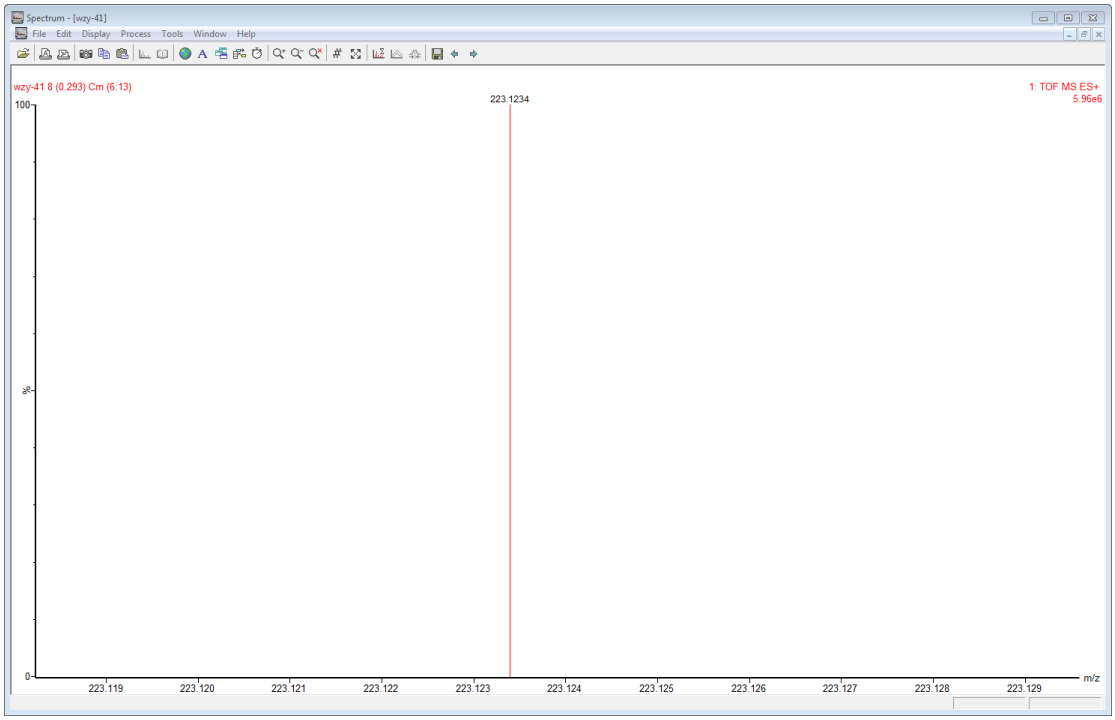

158.6
155.5
137.0
135.7
129.1
128.2
127.6
122.0
121.0
120.8
44.2
37.5
24.6
N
N
Parameter Value
1 Data File Name C:/ Users/ Customer/ Desktop/ I-supporting/ I-NMR/ single/ S-092405-1201-6-Me-BD/ 2/ pdata/ 1/ 1r
2 Title S-092405-1201-6-Me-BD
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 294.4
11 Pulse Sequence 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 2024-12-01T15:41:19
19 Modification Date 2024-12-01T15:41:10
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2473.0
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
f1 (ppm)



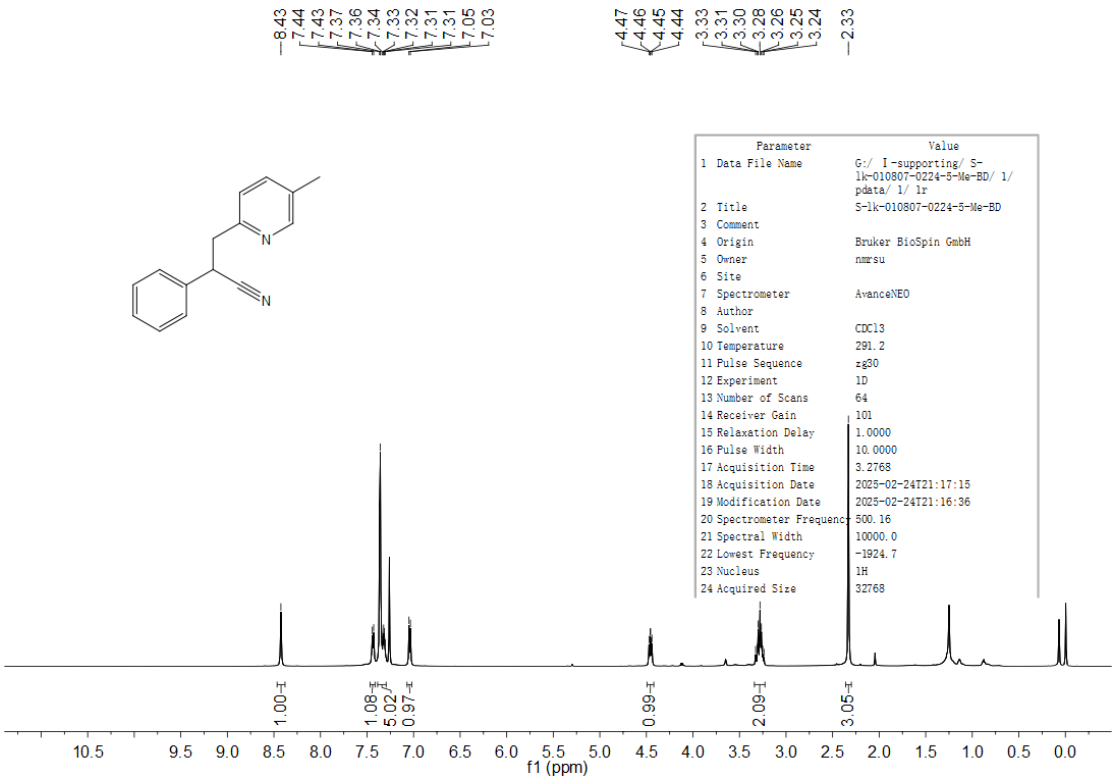
3-(3-methylpyridin-2-yl)-2-phenylpropanenitrile (4ac)

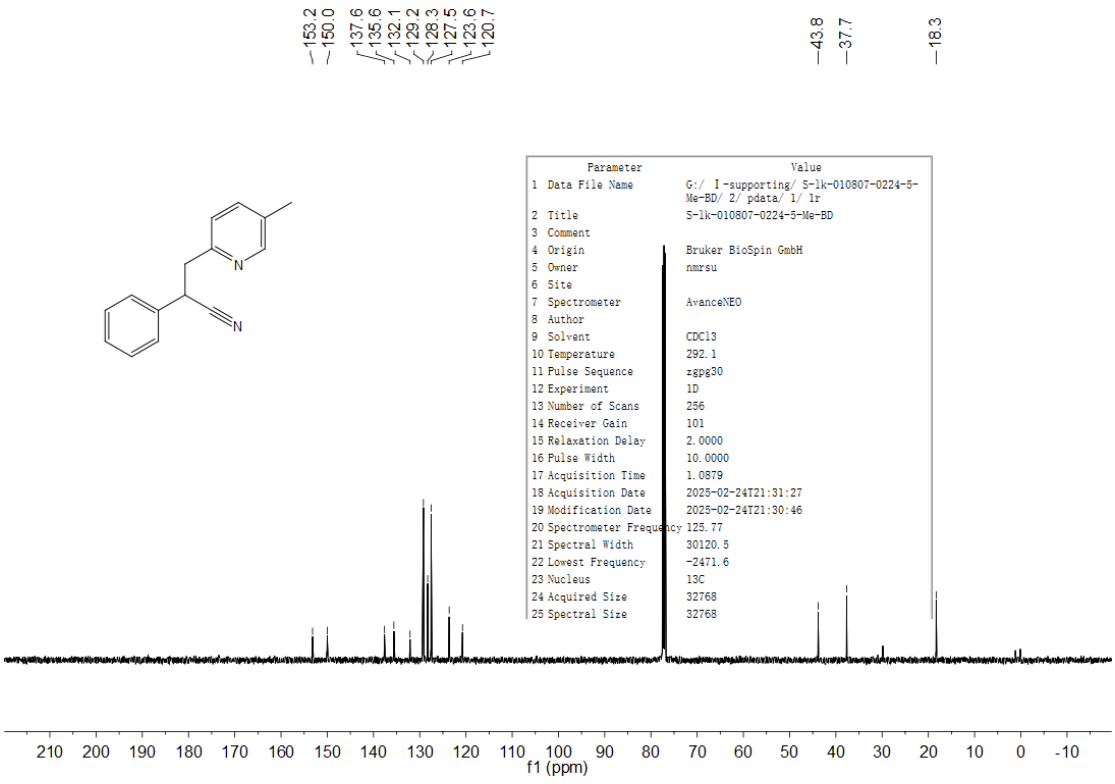






3-(5-methylpyridin-2-yl)-2-phenylpropanenitrile (4ad)


8.43
7.44
7.43
7.37
7.36
7.34
7.33
7.32
7.31
7.31
7.05
7.03
4.47
4.46
4.45
4.44
3.33
3.31
3.30
3.28
3.26
3.25
3.24
2.33
N
N
Parameter Value
1 Data File Name G:/ I-supporting/ S-1k-010807-0224-5-Me-BD/ 1/ pdata/ 1/ 1r
2 Title S-1k-010807-0224-5-Me-BD
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 291.2
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 64
14 Receiver Gain 101
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2025-02-24T21:17:15
19 Modification Date 2025-02-24T21:16:36
20 Spectrometer Frequency 300.16
21 Spectral Width 10000.0
22 Lowest Frequency -1924.7
23 Nucleus 1H
24 Acquired Size 32768
1.00
1.08
5.02
0.97
0.99
2.09
3.05
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)


153.2
150.0
137.6
135.6
132.1
129.2
128.3
127.5
123.6
120.7
43.8
37.7
18.3
N
N
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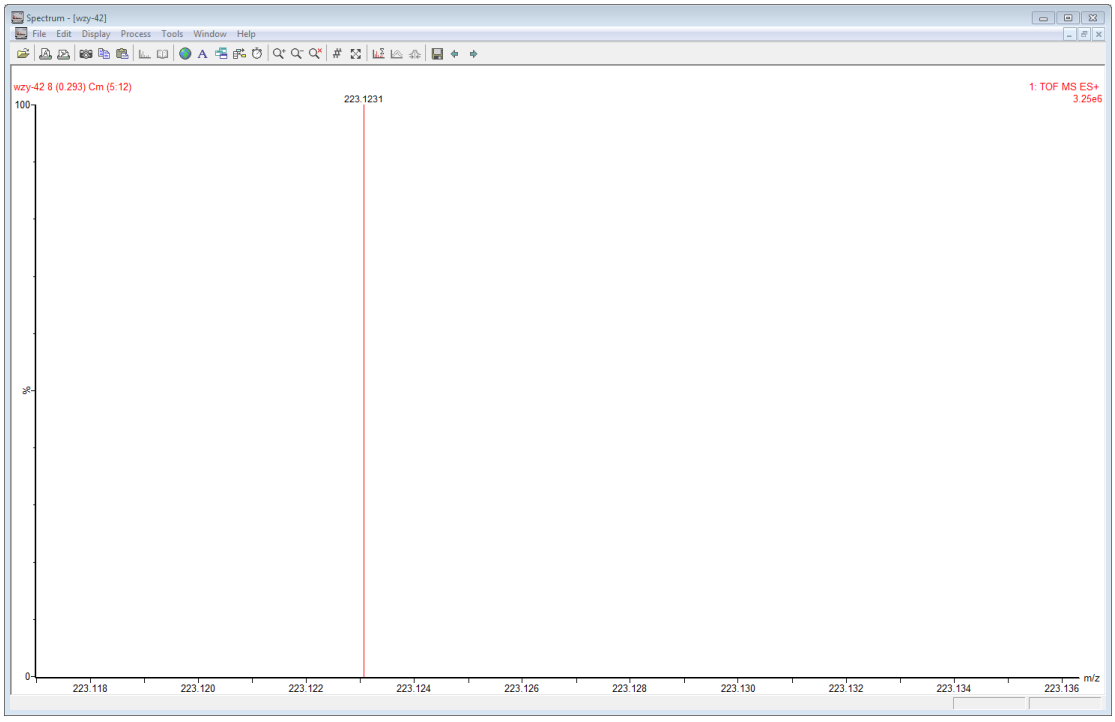
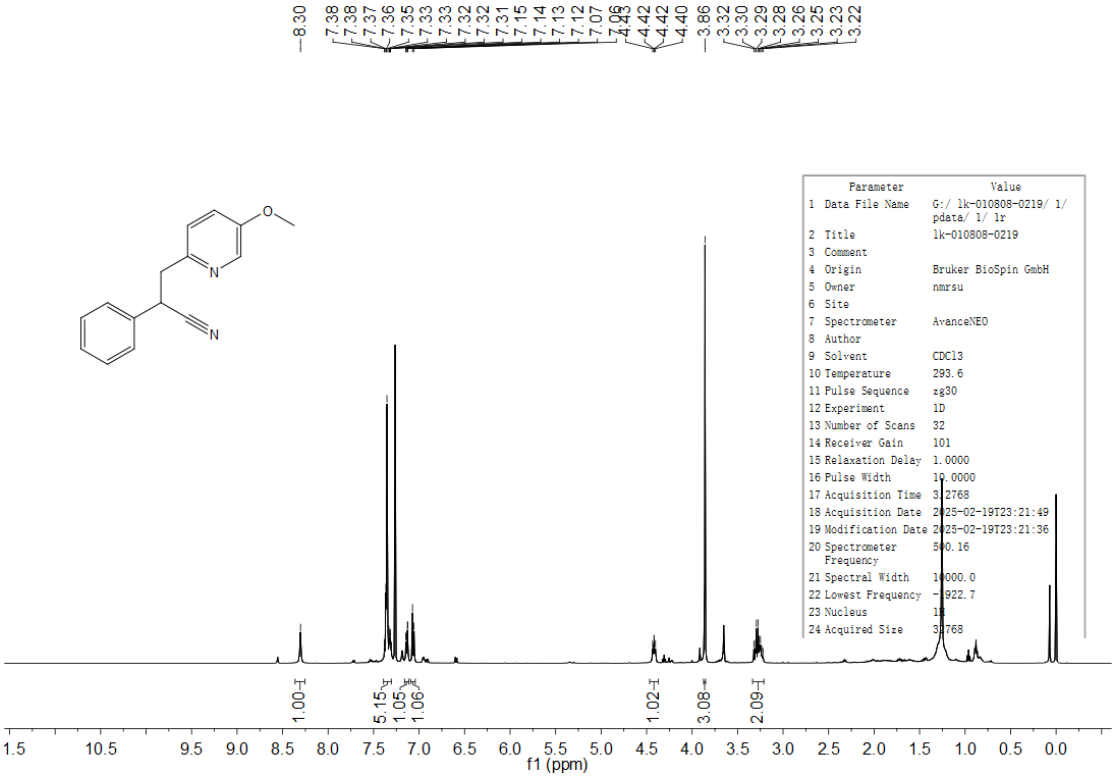
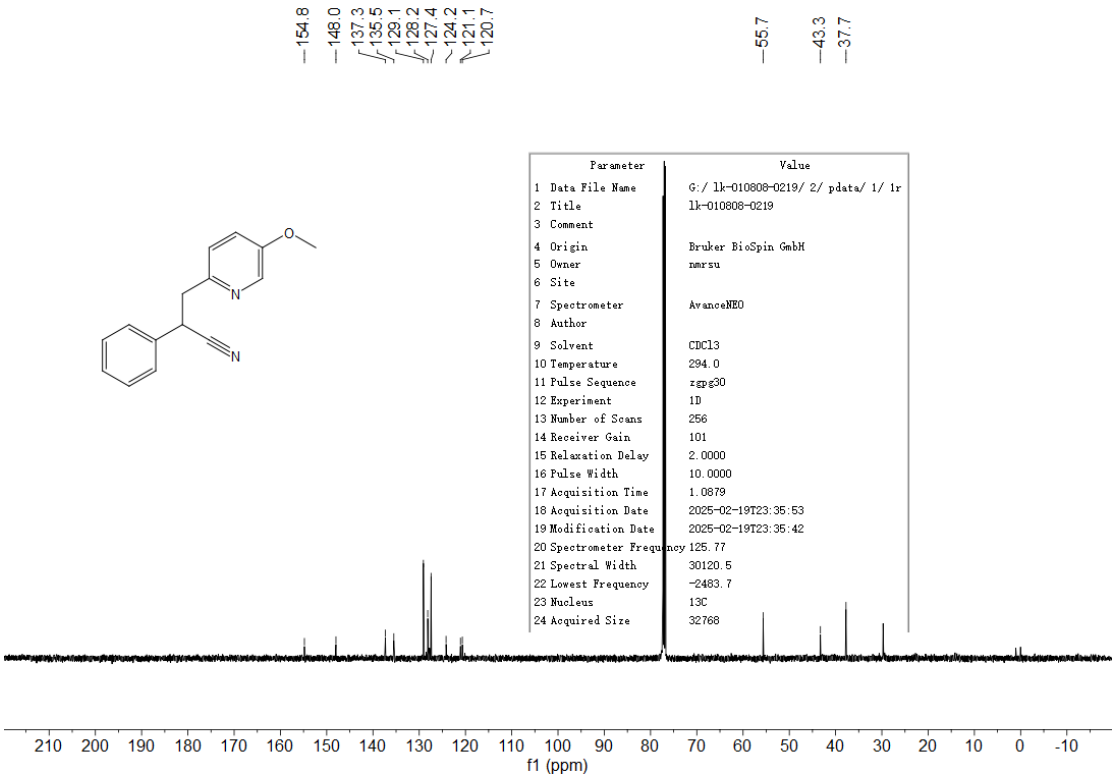
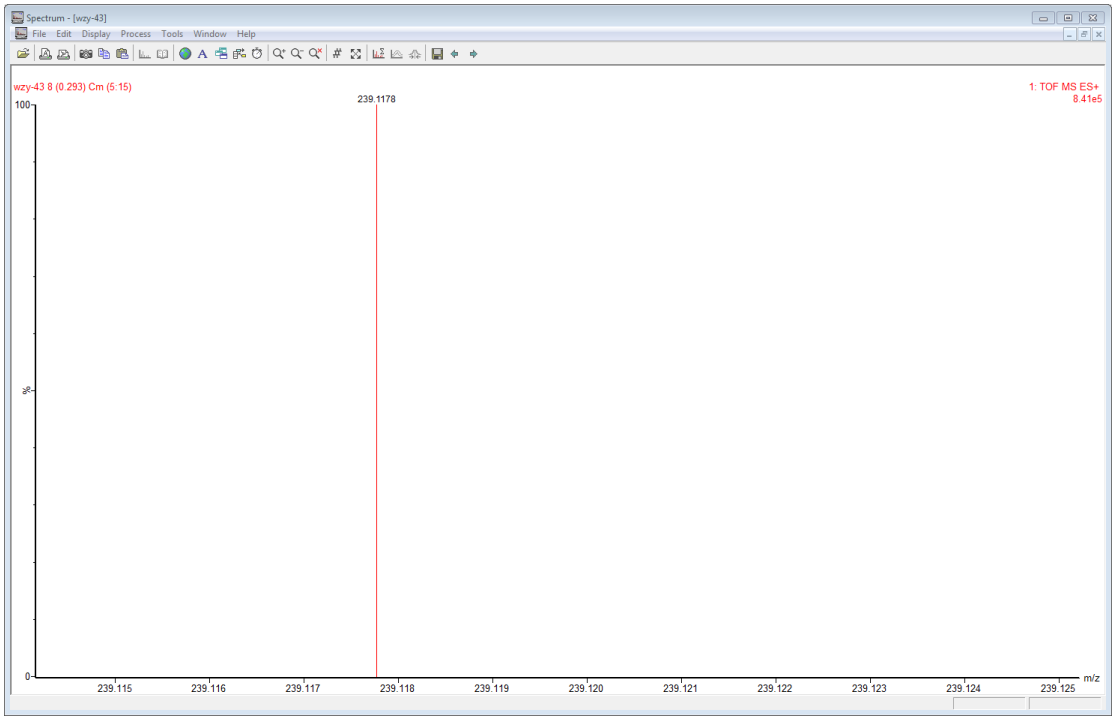
1 Data File Name G:/ I-supporting/ S-1k-010807-0224-5-Me-BD/ 2/ pdata/ 1/ 1r
2 Title S-1k-010807-0224-5-Me-BD
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 292.1
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2025-02-24T21:31:27
19 Modification Date 2025-02-24T21:30:46
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2471.6
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)



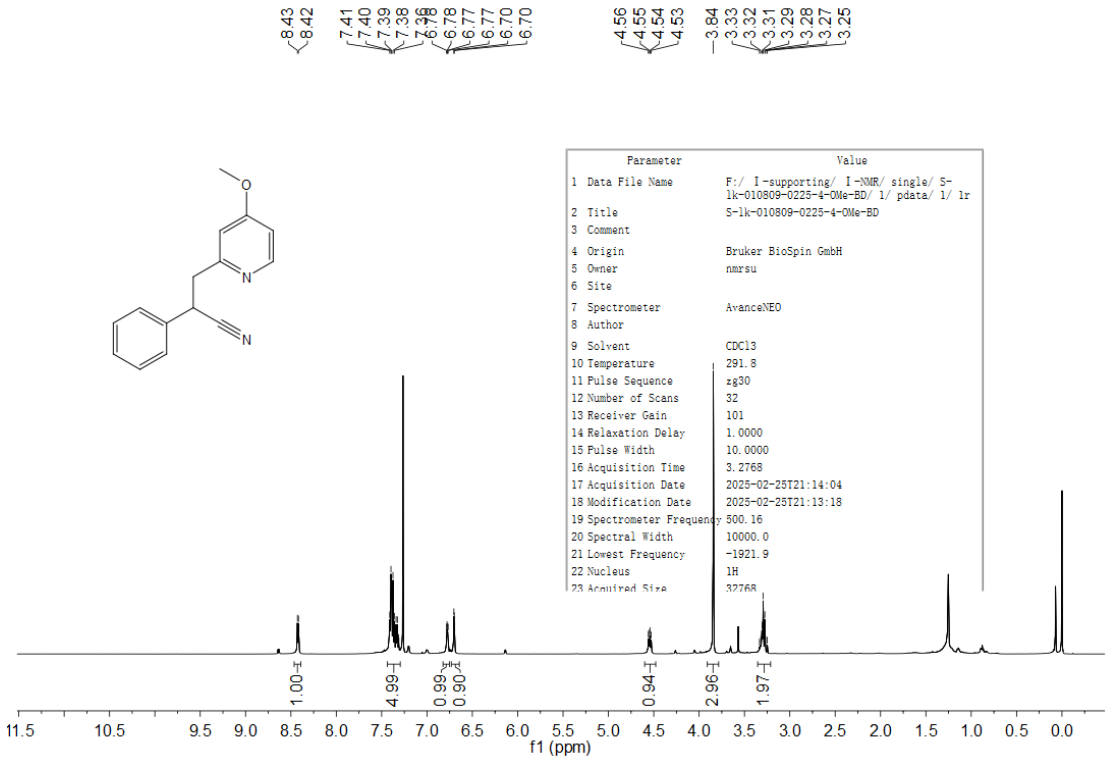
3-(5-methoxypyridin-2-yl)-2-phenylpropanenitrile (4ae)







3-(4-methoxypyridin-2-yl)-2-phenylpropanenitrile (4af)


8.43
8.42
7.41
7.40
7.39
7.38
7.36
6.78
6.77
6.77
6.70
6.70
4.56
4.55
4.54
4.53
3.84
3.33
3.32
3.31
3.29
3.28
3.27
3.25
O
N
N
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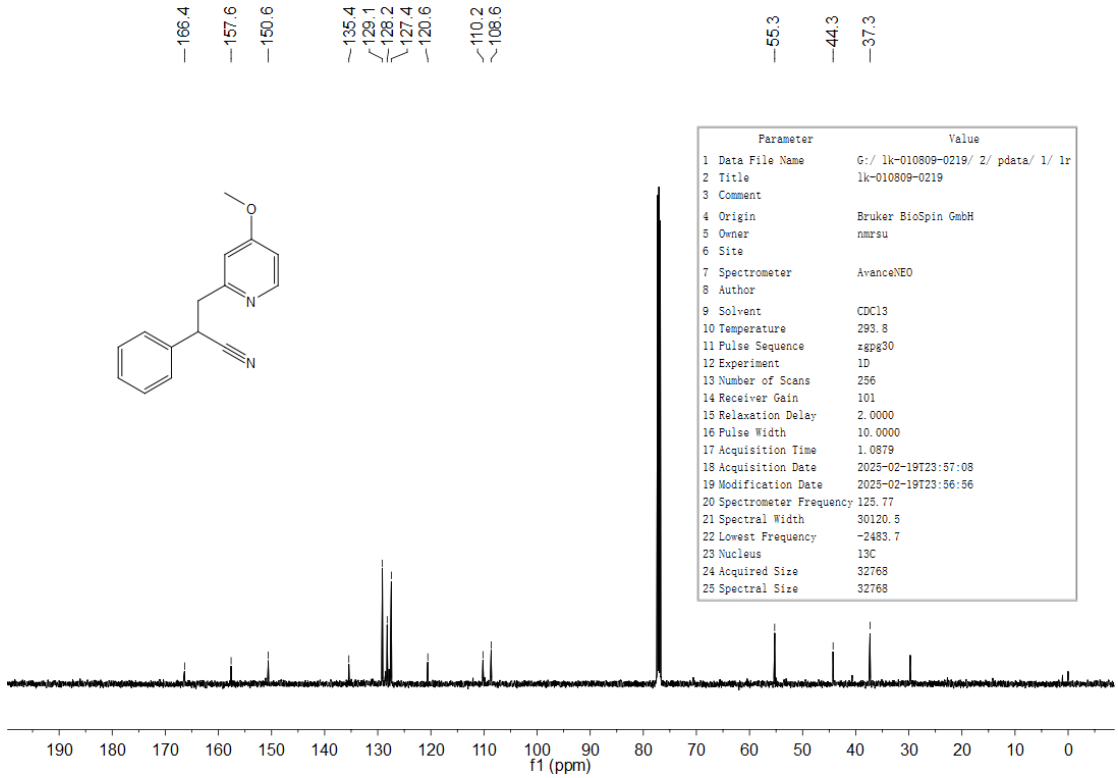
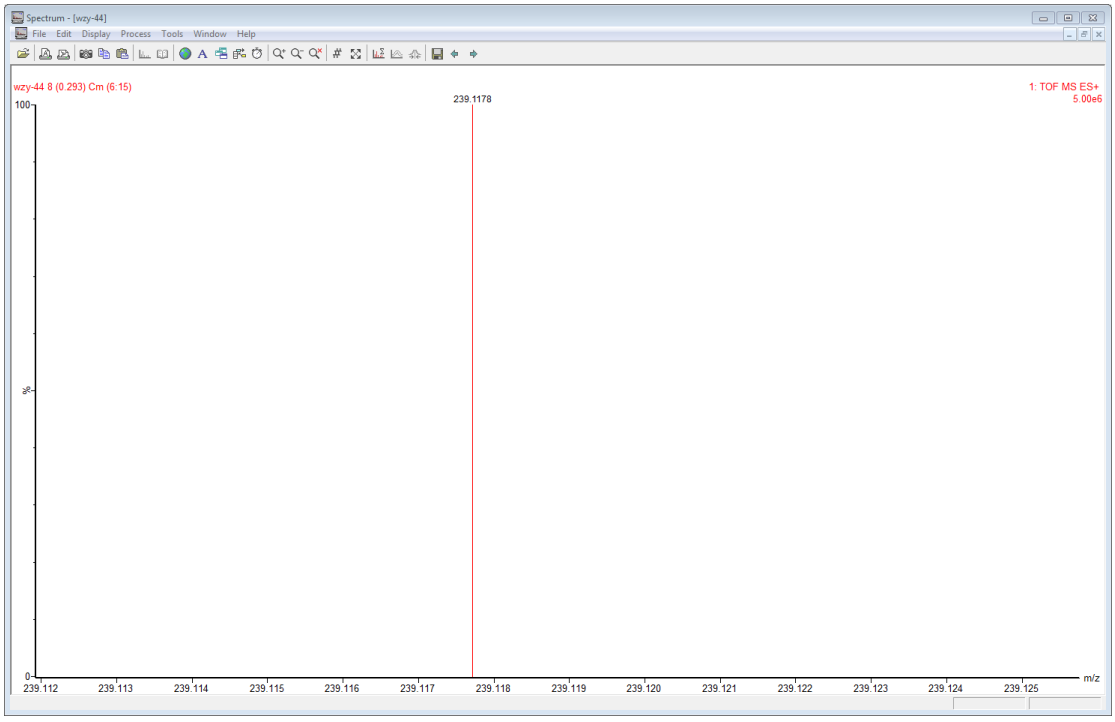
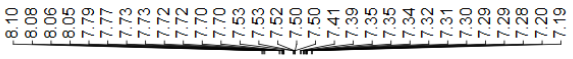
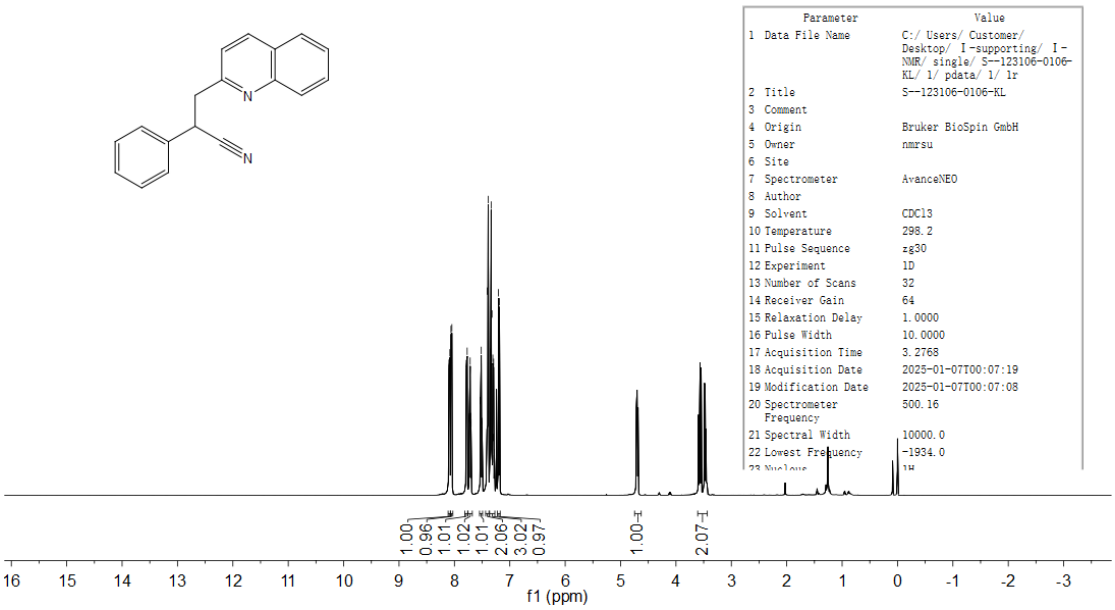
1 Data File Name F:/ I-supporting/ I-NMR/ single/ S-1k-010809-0225-4-OMe-BD/ 1/ pdata/ 1/ 1r
2 Title S-1k-010809-0225-4-OMe-BD
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 291.8
11 Pulse Sequence zg30
12 Number of Scans 32
13 Receiver Gain 101
14 Relaxation Delay 1.0000
15 Pulse Width 10.0000
16 Acquisition Time 3.2768
17 Acquisition Date 2025-02-25T21:14:04
18 Modification Date 2025-02-25T21:13:18
19 Spectrometer Frequency 500.16
20 Spectral Width 10000.0
21 Lowest Frequency -1921.9
22 Nucleus 1H
23 Acquired Size 32768
1.00
4.99
0.99
0.90
0.94
2.96
1.97
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)

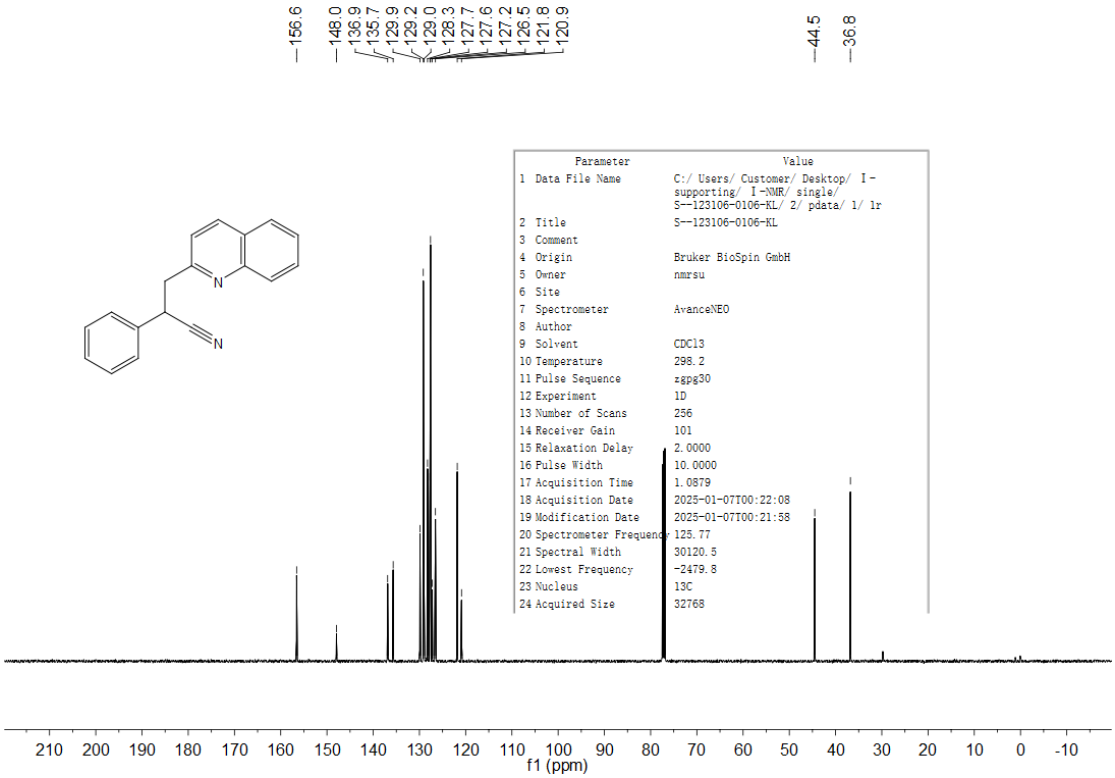

166.4
157.6
150.6
135.4
129.1
128.2
127.4
120.6
110.2
108.6
55.3
44.3
37.3
O
N
N
Parameter Value
1 Data File Name G:/ 1k-010809-0219/ 2/ pdata/ 1/ 1r
2 Title 1k-010809-0219
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 293.8
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 2025-02-19T23:57:08
19 Modification Date 2025-02-19T23:56:56
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2483.7
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

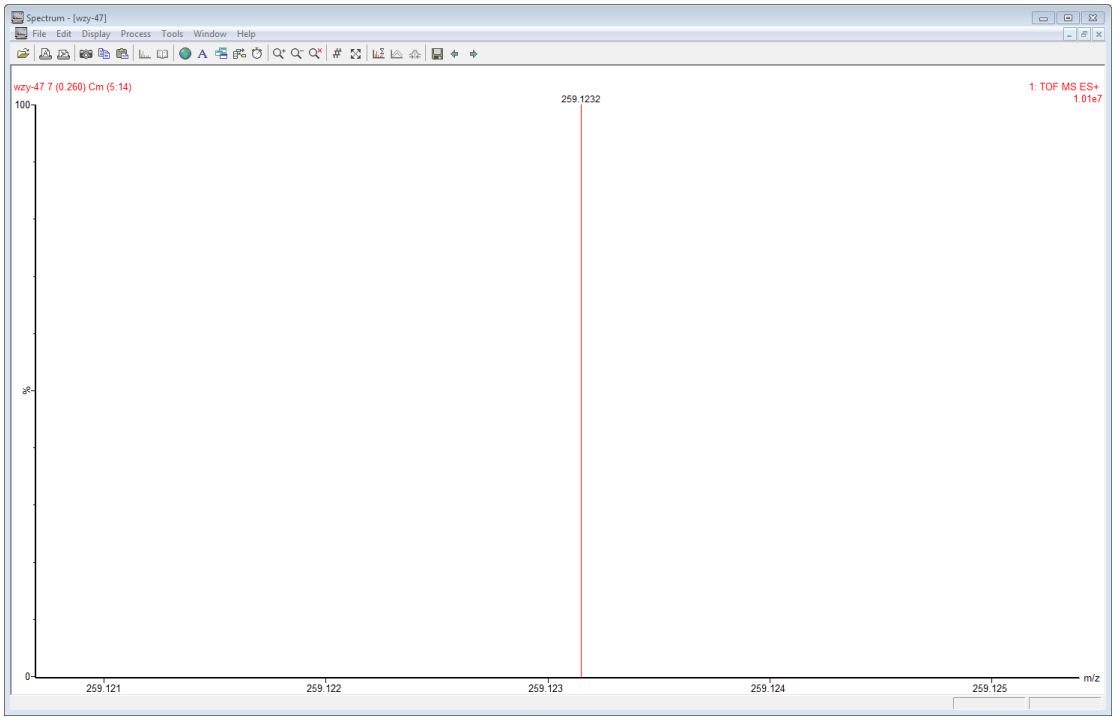


2-phenyl-3-(quinolin-2-yl)propanenitrile (4ag)

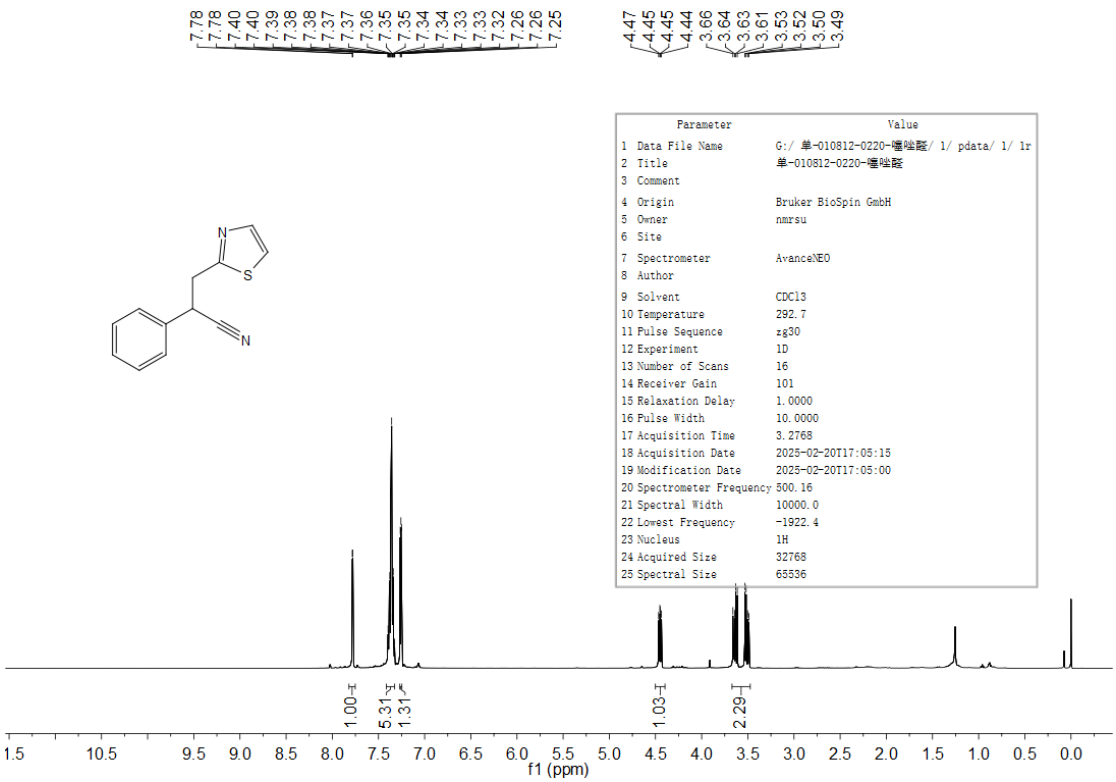








2-phenyl-3-(thiazol-2-yl)propanenitrile (4ah)


7.78
7.78
7.40
7.40
7.39
7.38
7.38
7.37
7.37
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.26
7.26
7.25
4.47
4.45
4.45
4.44
3.66
3.64
3.63
3.61
3.53
3.52
3.50
3.49
N
S
N
Parameter Value
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2 Title 单-010812-0220-噻唑醛
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 292.7
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 16
14 Receiver Gain 101
15 Relaxation Delay 1.0000
16 Pulse Width 10.0000
17 Acquisition Time 3.2768
18 Acquisition Date 2025-02-20T17:05:15
19 Modification Date 2025-02-20T17:05:00
20 Spectrometer Frequency 500.16
21 Spectral Width 10000.0
22 Lowest Frequency -1922.4
23 Nucleus 1H
24 Acquired Size 32768
25 Spectral Size 65536
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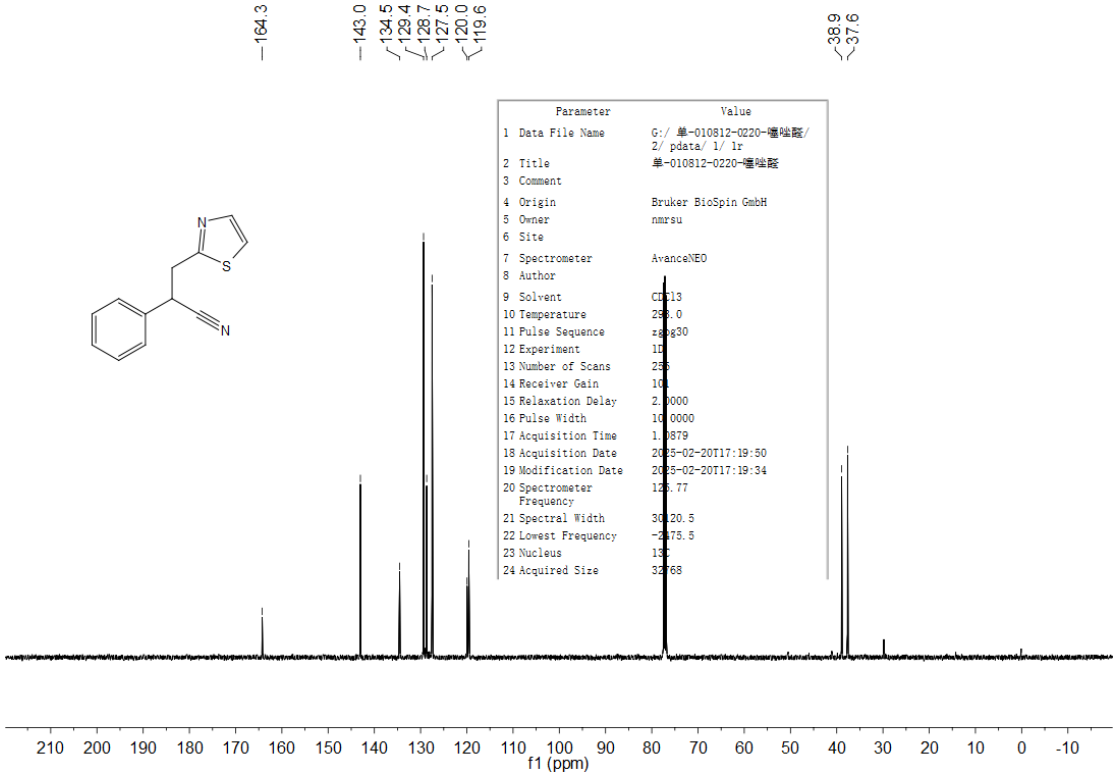
5.31
1.31
1.03
2.29
f1 (ppm)


164.3
143.0
134.5
129.4
128.7
127.5
120.0
119.6
38.9
37.6
N
S
N
Parameter Value
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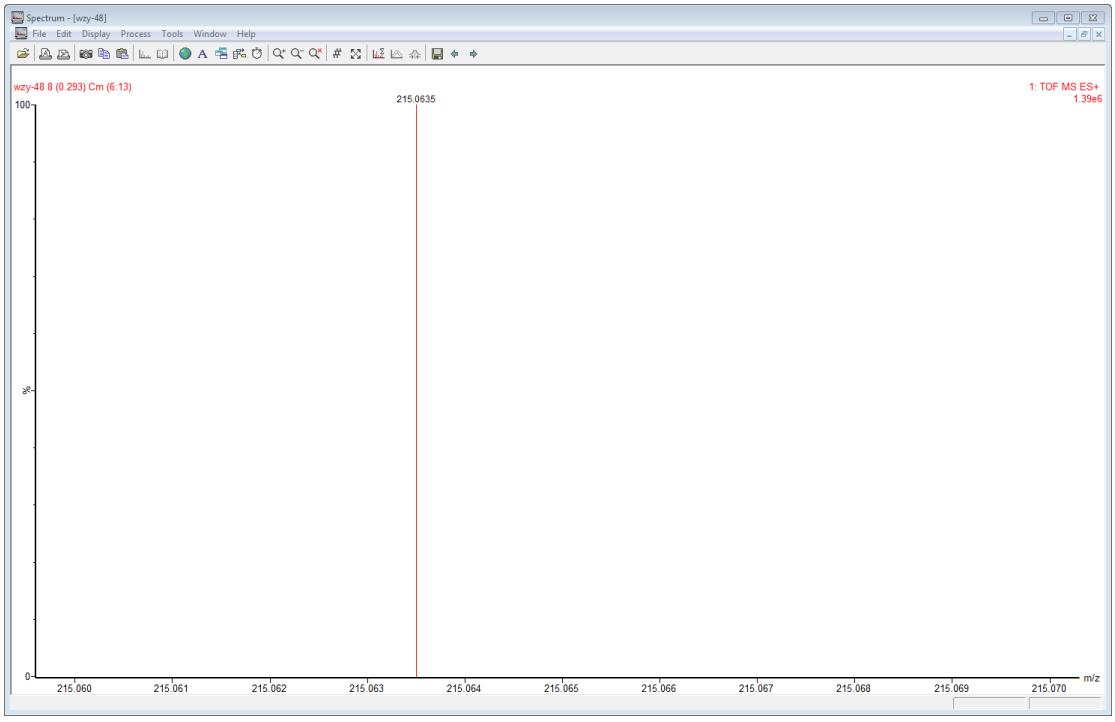
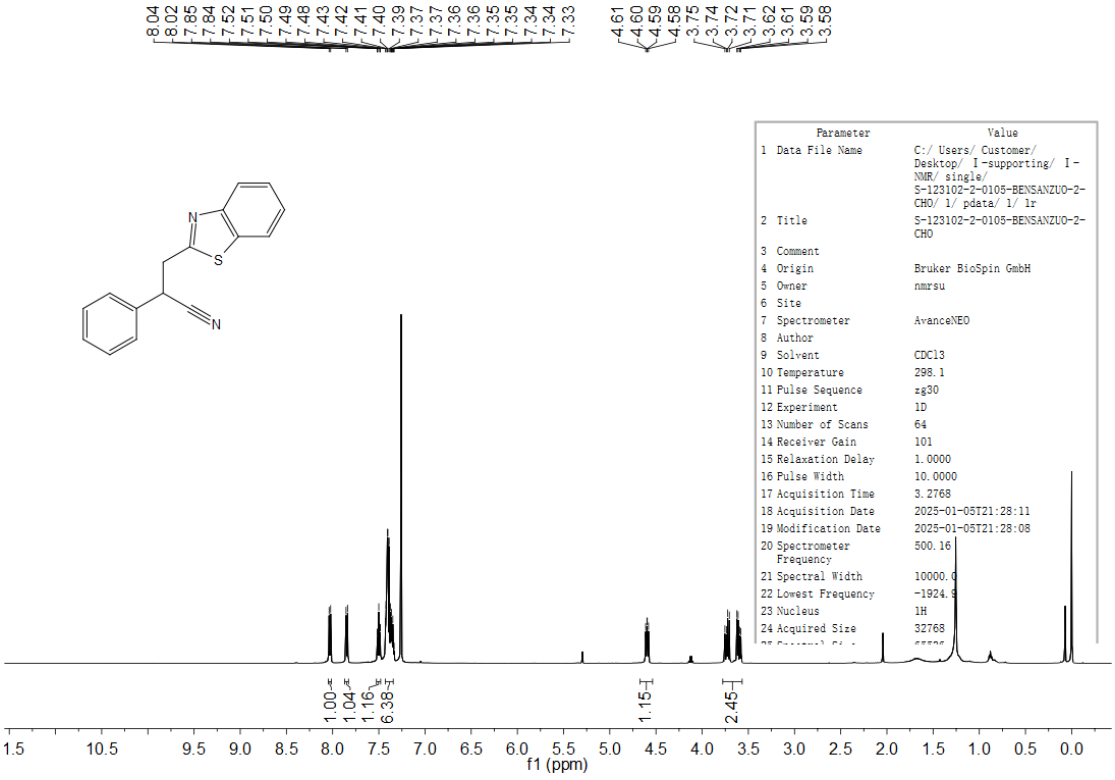
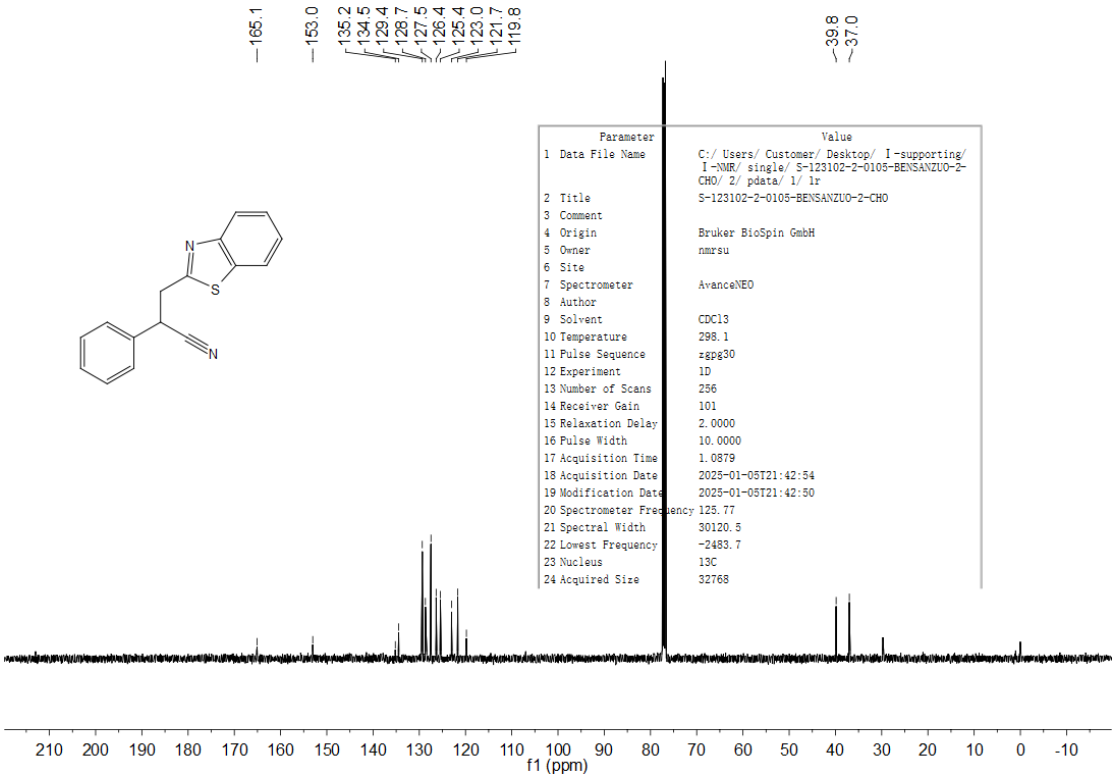
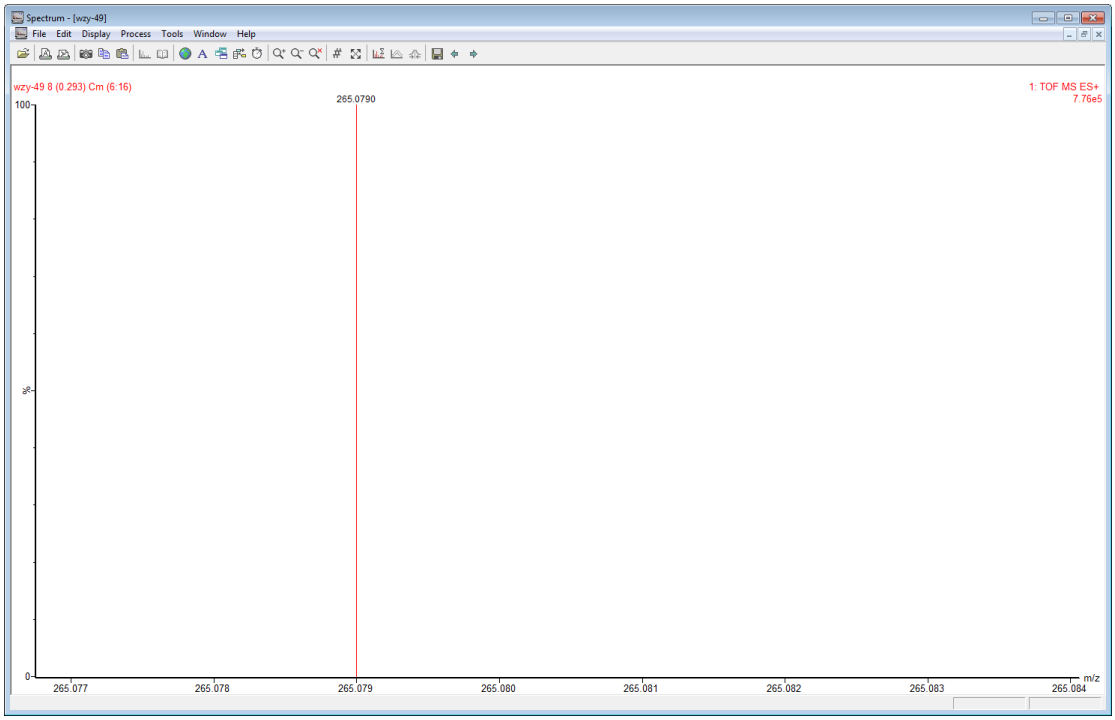
2 Title 单-010812-0220-噻唑醛
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.0
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2025-02-20T17:19:50
19 Modification Date 2025-02-20T17:19:34
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2475.5
23 Nucleus 13C
24 Acquired Size 32768
f1 (ppm)



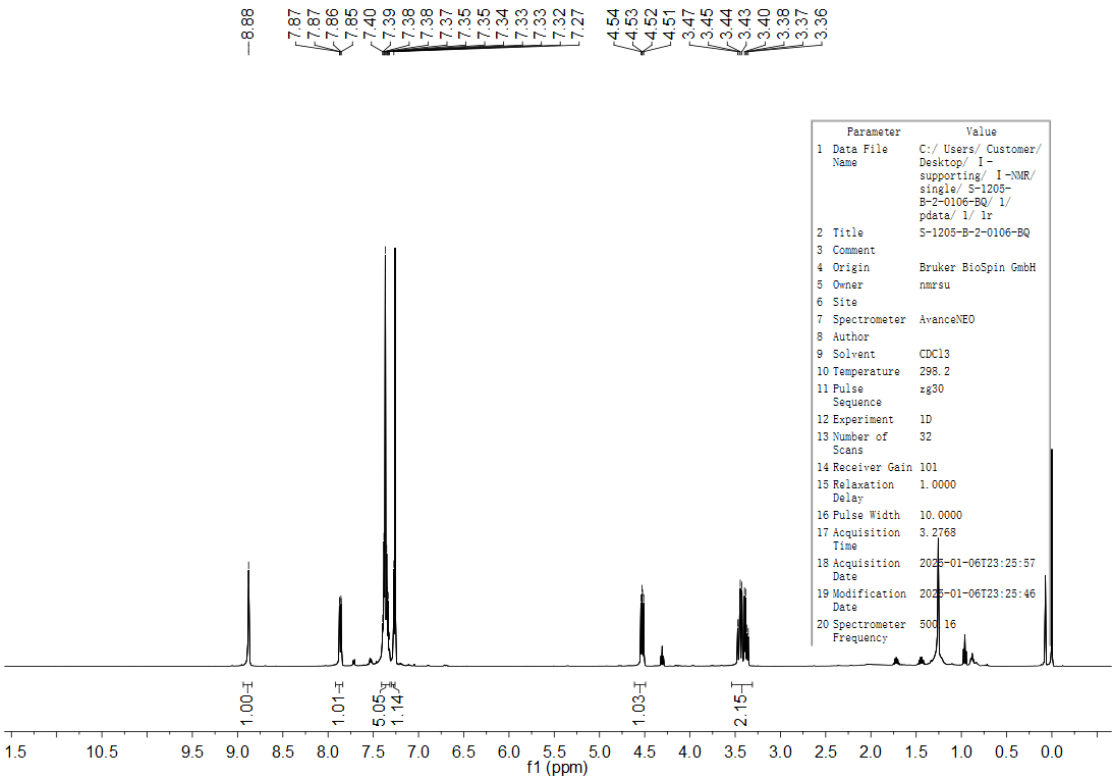
3-(benzo[*d*]thiazol-2-yl)-2-phenylpropanenitrile (4ai)







2-phenyl-3-(pyrazin-2-yl)propanenitrile (4aj)



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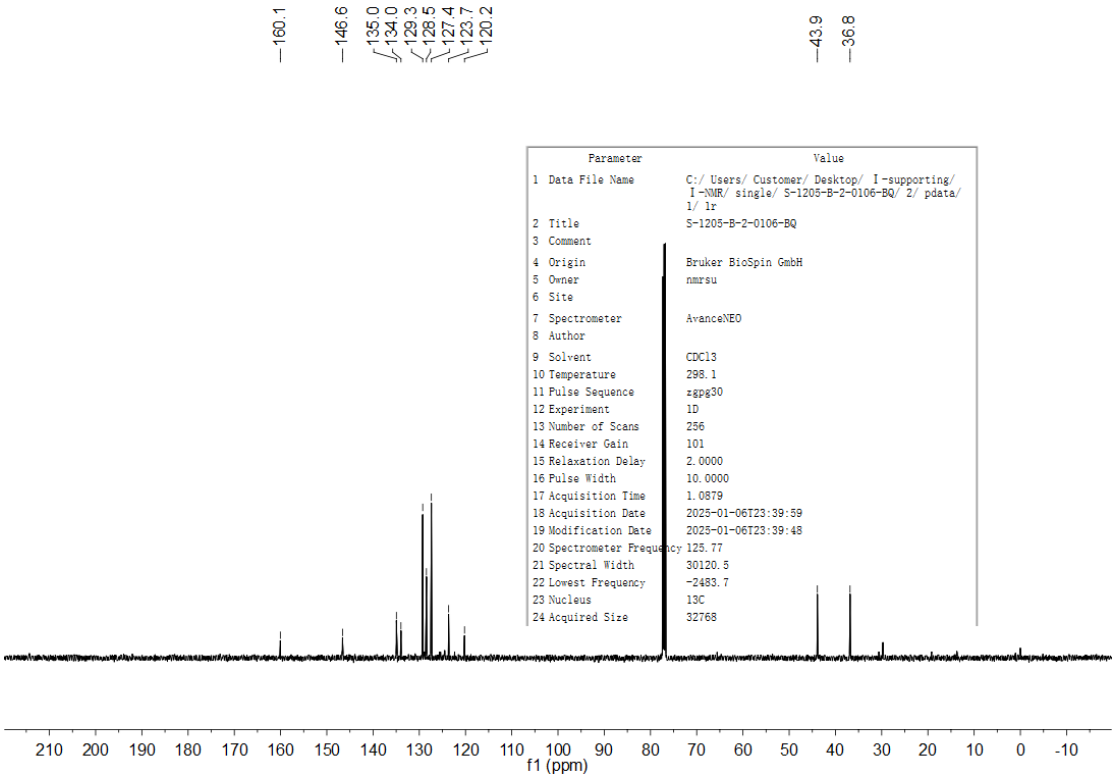
2	Title	S-1205-B-2-0106-BQ
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	298.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	32
14	Receiver Gain	101
15	Relaxation Delay	1.0000
16	Pulse Width	10.0000
17	Acquisition Time	3.2768
18	Acquisition Date	2025-01-06T23:25:57
19	Modification Date	2025-01-06T23:25:46
20	Spectrometer Frequency	500.16



	Parameter	Value
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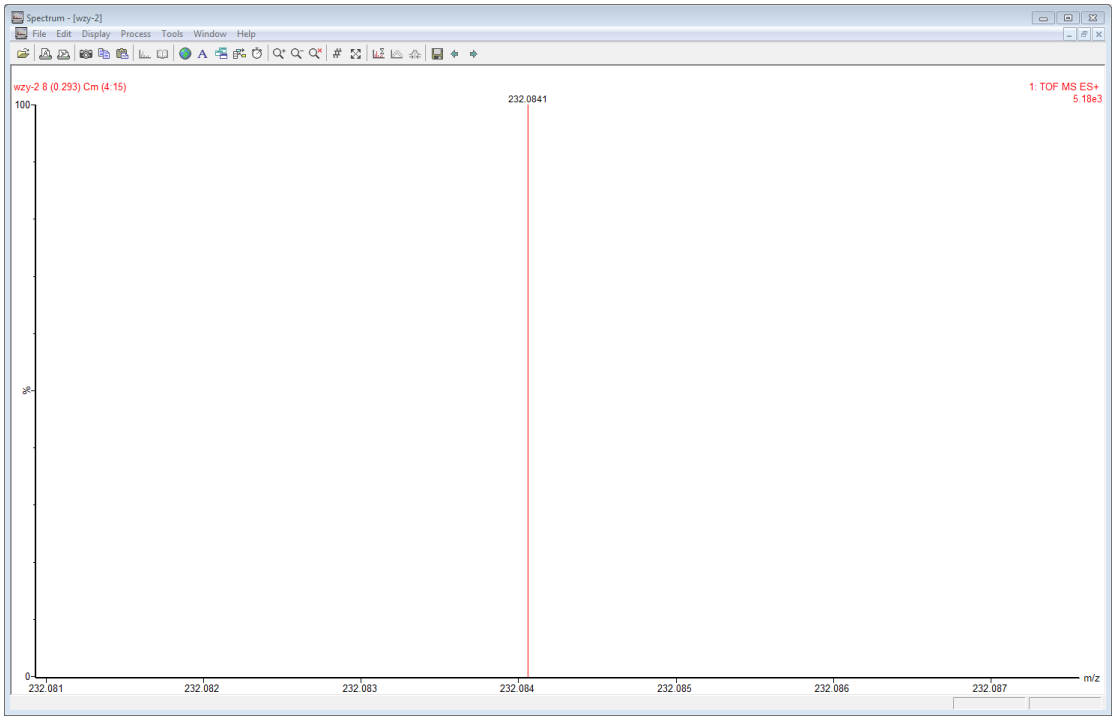
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	256
14	Receiver Gain	101
15	Relaxation Delay	2.0000
16	Pulse Width	10.0000
17	Acquisition Time	1.0879
18	Acquisition Date	2025-01-06T23:39:59
19	Modification Date	2025-01-06T23:39:48
20	Spectrometer Frequency	125.77
21	Spectral Width	30120.5
22	Lowest Frequency	-2483.7
23	Nucleus	13C
24	Acquired Size	32768


Spectrum - [wzy-2]
File Edit Display Process Tools Window Help
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5.18e3
232.0841
100
%
0
232.081
232.082
232.083
232.084
232.085
232.086
232.087
m/z