Supporting Information

Synthesis of α-alkenylated nitriles via an electrochemical generation of ketyl radicals

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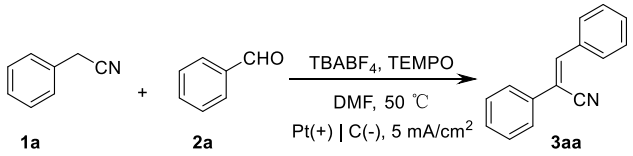
General Information

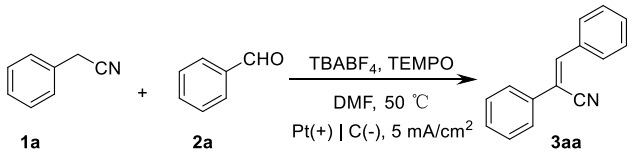
Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. NMR spectra were recorded on a Bruker AV-500 (1H: 500 MHz, 13C: 125 MHz, 19F NMR: 470 MHz) spectrometer using TMS as internal reference. Chemical shifts (δ) and coupling constants (J) were 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. Single crystals of $C_{15}H_{10}BrN$: A suitable crystal was selected and on a Bruker D8 VENTURE diffractometer. The crystal was kept at 170.00 K during data collection. Using Olex2, the structure was solved with the SHELXT structure solution program using Intrinsic Phasing and refined with the SHELXL refinement package using Least Squares minimisation.

Experimental Procedure



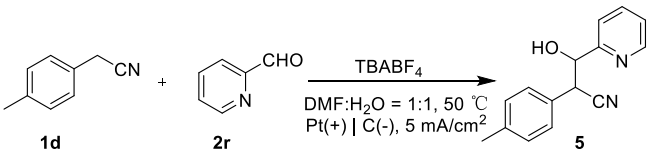
Scheme S1. Experimental procedure for **3aa**.

Typical synthesis steps of (*Z*)-2,3-diphenylacrylonitrile (3aa): A mixture of phenylacetonitrile (0.54 mmol), benzaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol), TEMPO(0.3mmol) 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 density of 5 mA/cm^2 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 = 50:1) to afford the desired product.



Scheme S2. Experimental procedure of gram scale for **3aa**.

Gram-scale synthesis of (*Z*)-2,3-diphenylacrylonitrile (3aa): A mixture of phenylacetonitrile (9 mmol), benzaldehyde (5 mmol), $TBABF_4$ (5 mmol), TEMPO(3mmol) 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 density of 5 mA/cm^2 under 50℃ for corresponding time. 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 = 50:1) to afford the desired product.



Scheme S3. Experimental procedure for **5**.

Typical synthesis of 3-hydroxy-3-(pyridin-2-yl)-2-(p-tolyl)propanenitrile (5): A mixture of 4-methylbenzyl cyanide (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/cm^2 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 3ha

Recrystallization solvent: chloroform; Method for crystal growth: the crystal was prepared from the solution of **3ha** in chloroform. Dissolved 20 mg **3ha** with 1 mL of chloroform and volatilized slowly at 25℃ for 15 days. (CCDC: 2516622)

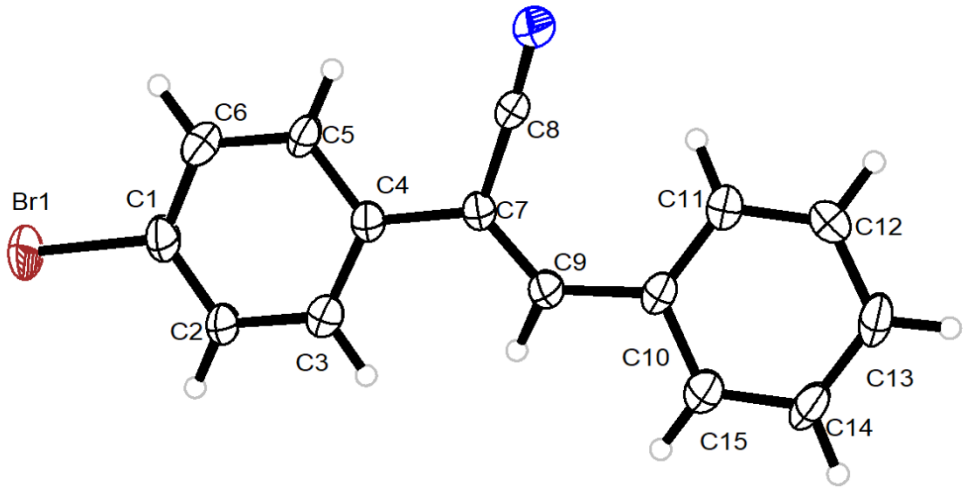


Figure S1. Crystal structure for **3ha**.

Table S1 Crystal data and structure refinement for LK-1214-1.

Identification code	LK-1214-1
Empirical formula	$C_{15}H_{10}BrN$
Formula weight	284.15
Temperature/K	170.00
Crystal system	triclinic
Space group	P-1
a/Å	6.8584(5)
b/Å	13.9916(9)
c/Å	14.6230(12)
α/°	116.987(4)
β/°	92.240(5)
γ/°	101.866(4)

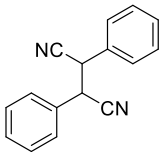
Volume/$Å^3$	1209.52(16)
Z	4
$\rho_{calc}g/cm^3$	1.560
μ/mm^{-1}	4.408
F(000)	568.0
Crystal size/mm^3	0.12 × 0.11 × 0.1
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.862 to 137.524
Index ranges	$-8 \leq h \leq 8$, $-16 \leq k \leq 15$, $-17 \leq l \leq 17$
Reflections collected	14636
Independent reflections	4341 [R_{int} = 0.0659, R_{sigma} = 0.0743]
Data/restraints/parameters	4341/0/307
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0691, wR_2 = 0.1914
Final R indexes [all data]	R_1 = 0.0931, wR_2 = 0.2052
Largest diff. peak/hole / e $Å^{-3}$	1.25/-0.89

Mechanistic Studies

(1) HRMS for 1.

A mixture of phenylacetonitrile (0.54 mmol), benzaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol), TEMPO(0.3mmol) 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 233.1077.



compound **1**

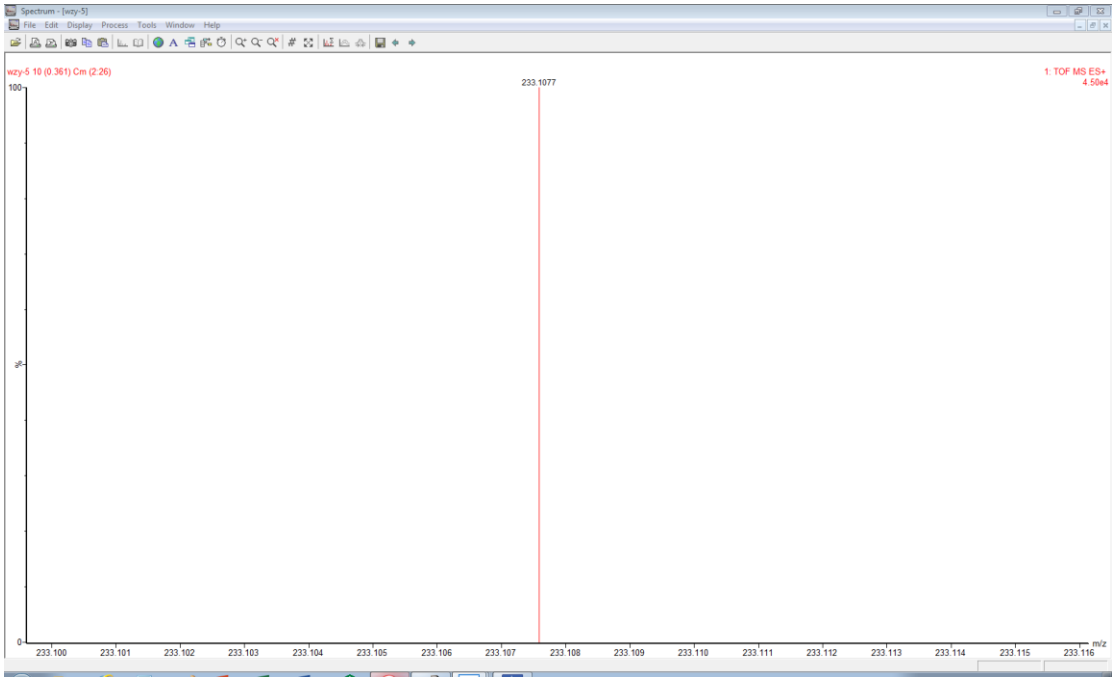
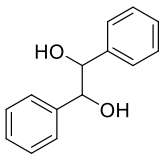


Figure S2. HRMS for **1**.

(2) HRMS for 2.

A mixture of phenylacetonitrile (0.54 mmol), benzaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol), TEMPO(0.3mmol) 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 $C_{14}H_{14}O_2[M+Na]^+$ 237.0886, found 237.0884.



compound **2**

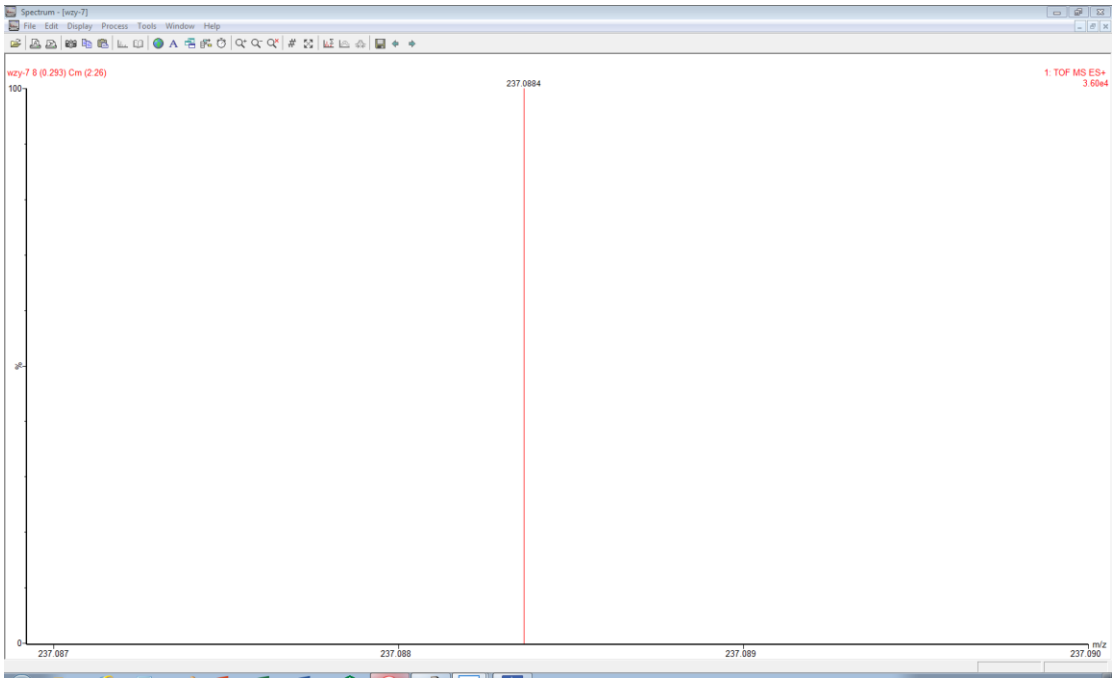
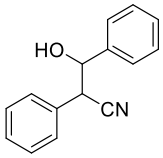


Figure S3. HRMS for **2**.

(3) HRMS for 3.

A mixture of phenylacetonitrile (0.54 mmol), benzaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol), TEMPO(0.3mmol) 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 $C_{15}H_{13}NO[M+Na]^+$ 246.0889, found 246.0896.



compound **3**

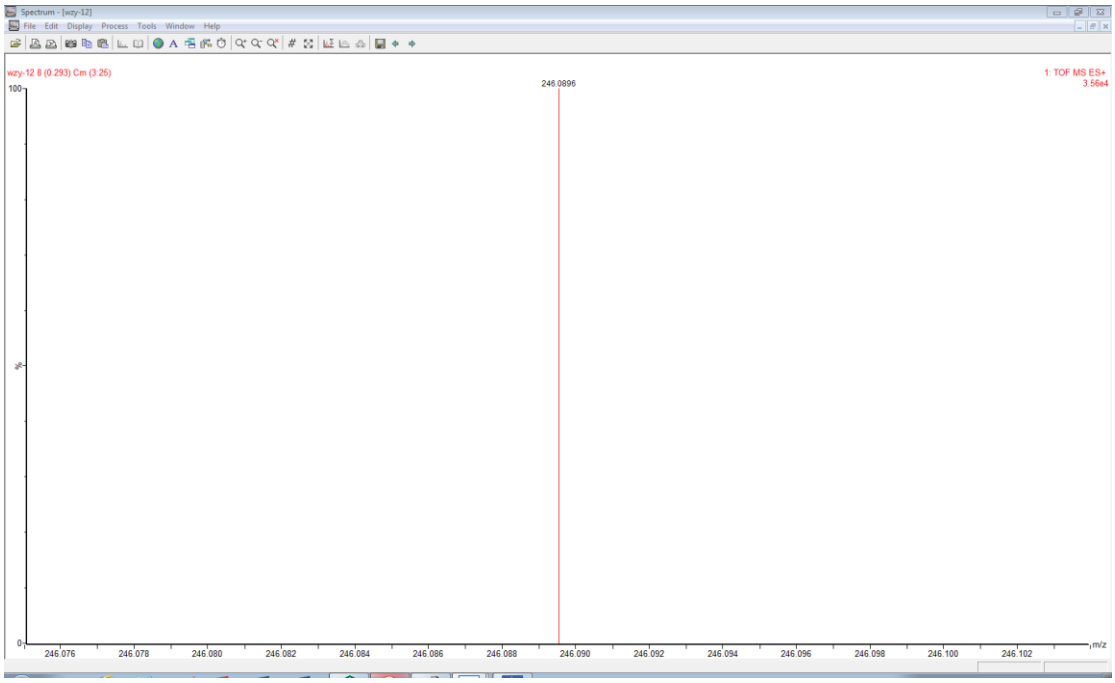


Figure S4. HRMS for **3**.

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

A mixture of phenylacetonitrile (0.54 mmol), $TBABF_4$ (0.3 mmol), D_2O (100μL)，TEMPO (0.3mmol) 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 3.5h. **4** was isolated in 96% yield with 190% D-incorporation at *α*-position of cyano group as revealed by ^1H NMR.

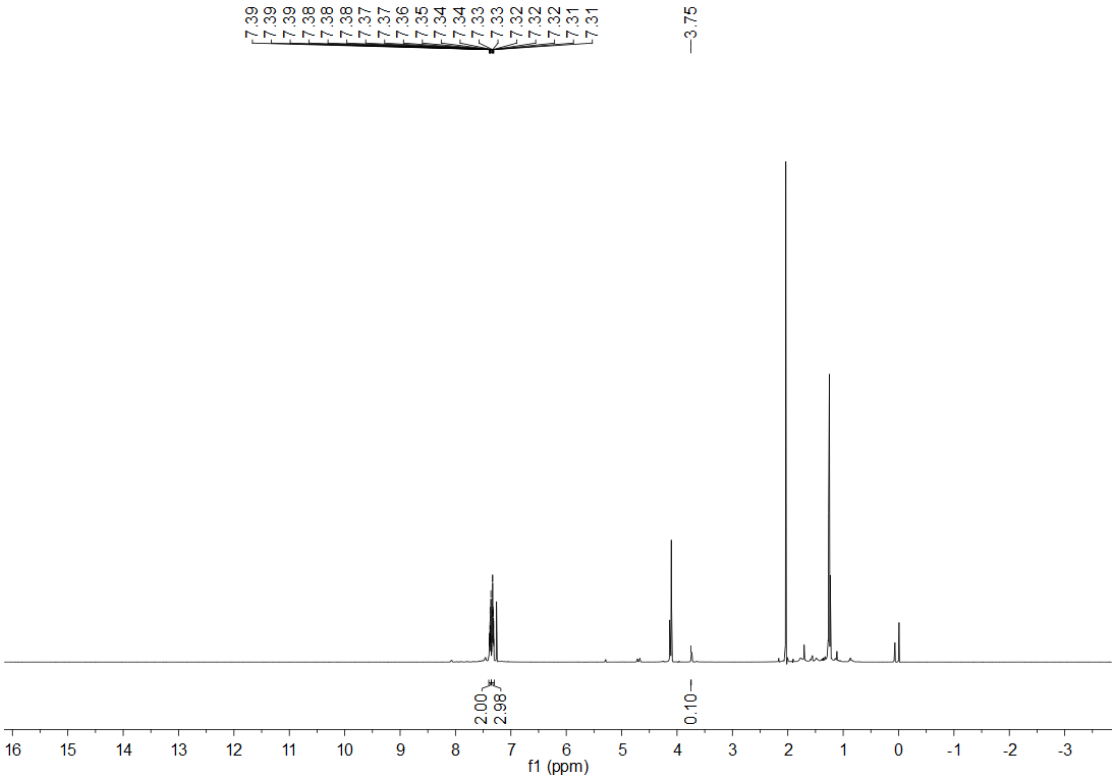


Figure S5. ^{1}H NMR of **4** for Scheme 5a (standard conditions).

A mixture of phenylacetonitrile (0.54 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 3.5h. **4** was isolated in 92% yield with 150% D-incorporation at α-position of cyano group as revealed by ^{1}H NMR.

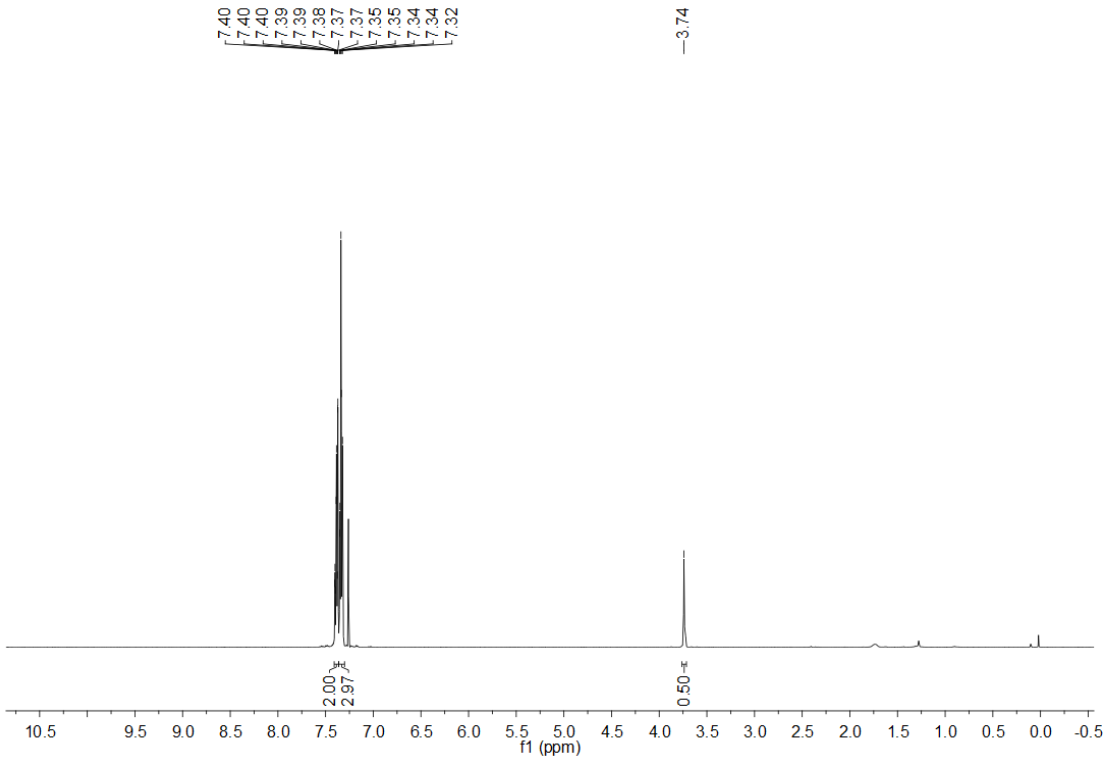


Figure S6. ^{1}H NMR of **4** for Scheme 5a (without TEMPO).

(5) HRMS for 7.

A mixture of phenylacetonitrile (0.54 mmol), benzaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol), TEMPO(0.3mmol) 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 $C_{15}H_{13}NO[M+Na]^+$ 467.1730, found 467.1727.

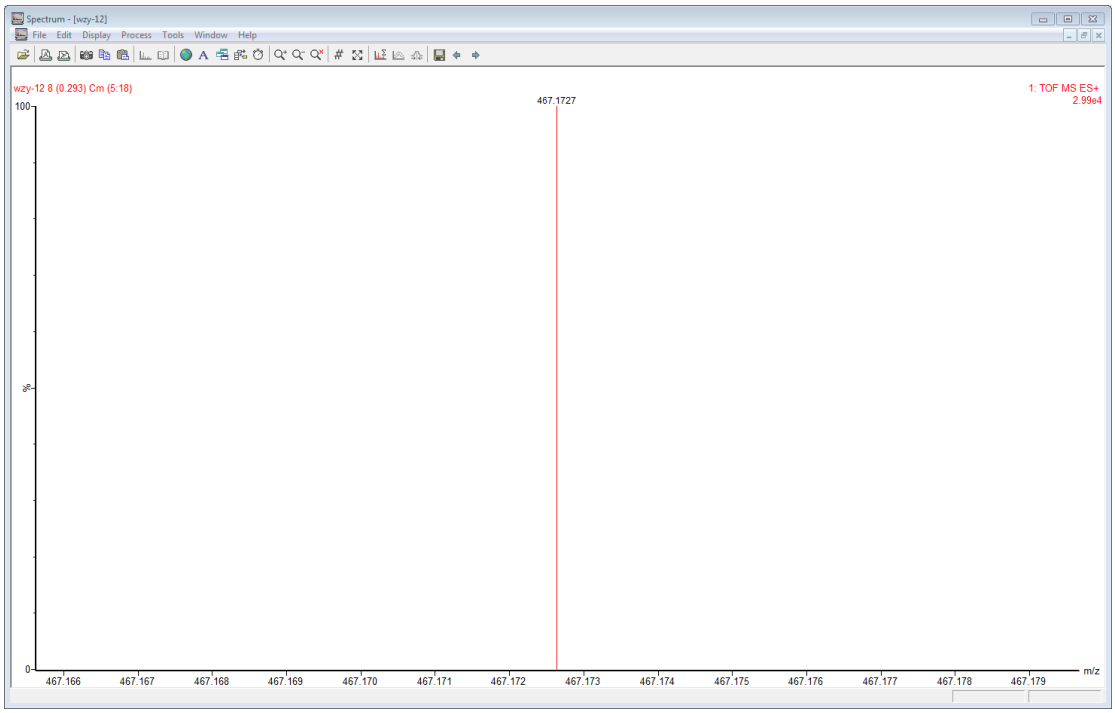


Figure S7. HRMS of **7.**

(6) Deuterium exchange of 2-phenylpropanenitrile to give D-incorporation product 9.

A mixture of 2-phenylpropanenitrile (0.54 mmol), $TBABF_4$ (0.3 mmol), D_2O (100μL), TEMPO(0.3mmol) 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 3.5h. **2** was isolated in 90% yield with 75% D-incorporation at *α* position of cyano group as revealed by ^1H NMR.

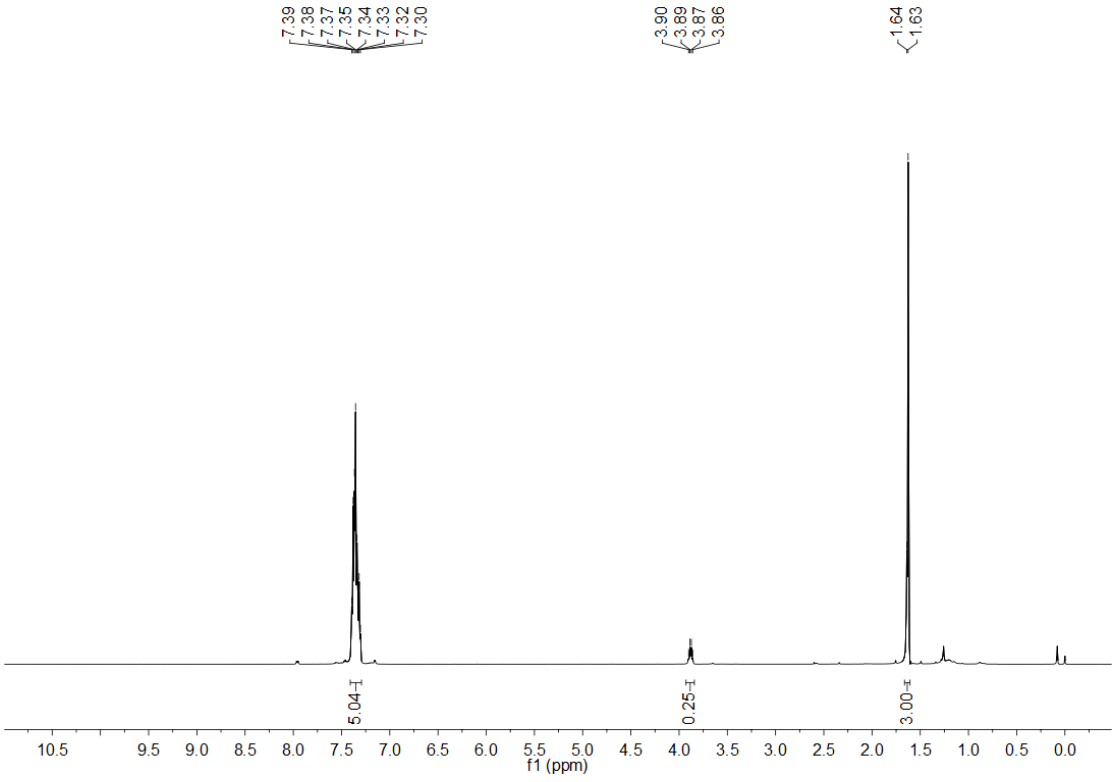


Figure S8. ^{1}H NMR of **9.**

(7) HRMS for II.

A mixture of phenylacetonitrile (0.54 mmol), benzaldehyde (0.3 mmol), $TBABF_4$ (0.3 mmol), TEMPO(0.3mmol) 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 $C_9H_{19}NO[M+H]^+$ 158.1539, found 158.1547.

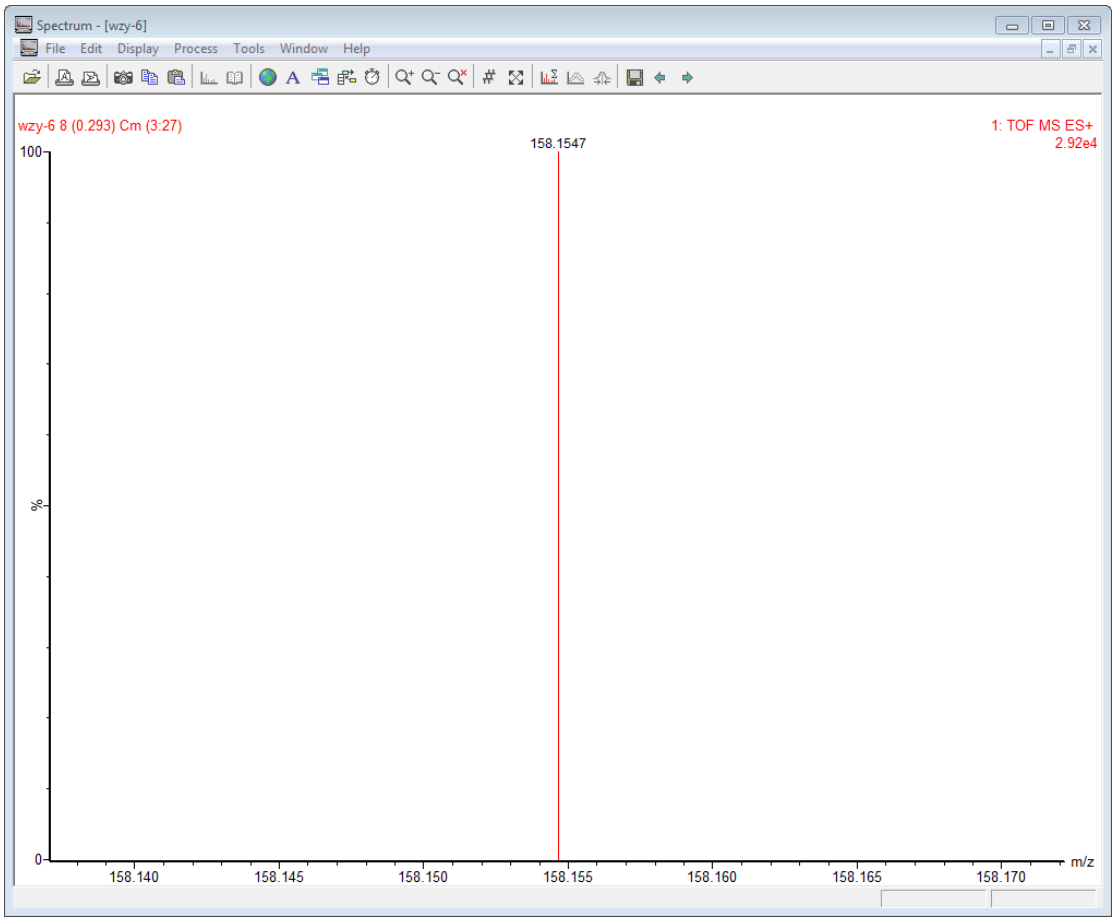


Figure S9. HRMS for **II**.

(8) Cyclic voltammetry experiments.

To gain insight into the reaction mechanism, we conducted a series of cyclic voltammograms. First, the electrochemical properties of reaction components were investigated (Figure S9), while the oxidation peaks from TEMPO (1.02V) [vs Ag/AgCl] and **1a** (1.40V) were found. These results indicate that TEMPO are first oxidized on the anode surface. Then, we treated **1a** with equal amounts of TEMPO, and found that the oxidation peak of TEMPO did not generate any significant catalytic current, indicating that TEMPO has no obvious catalytic effect on **1a**.

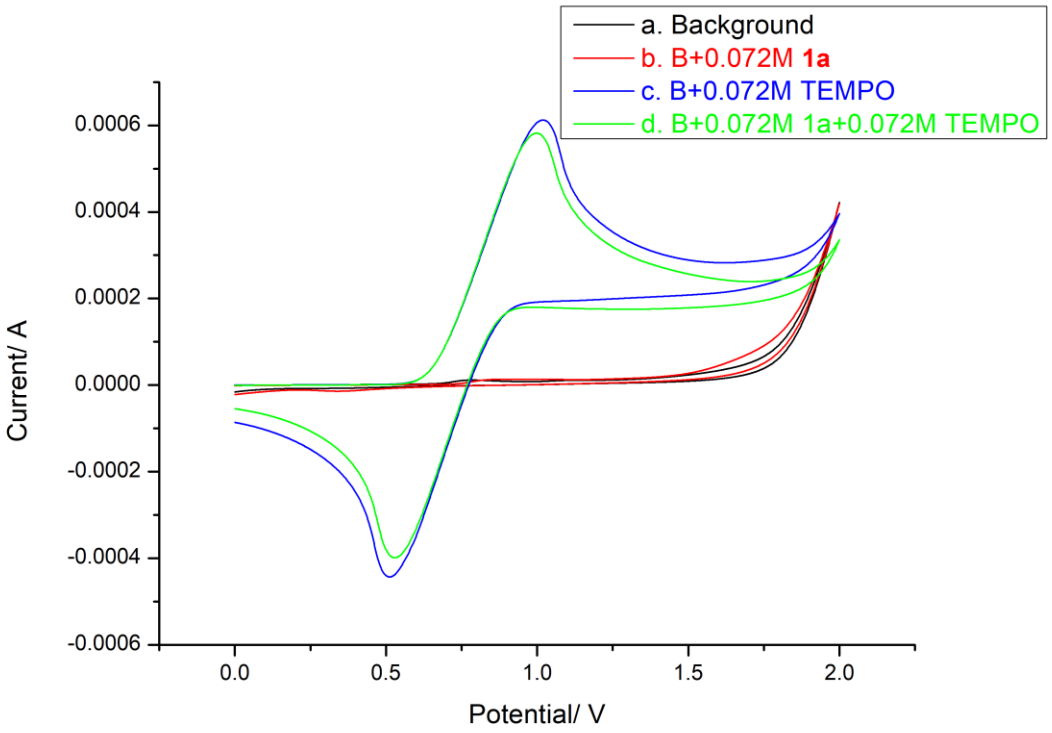


Figure S10. Cyclic voltammetry of **1a** and TEMPO in 0.1 M $TBABF_4$/DMF (10 mL) at room temperature using a Pt disk as the working electrode and Pt wire and Ag/AgCl as the counter and reference electrodes with a scan rate at 100 mV/s. background (curve a), **1a** (0.072M) (curve b), TEMPO (0.072M) (curve c) and **1a** (0.072M) TEMPO (0.072M) (curve d).

Additionally, the electrochemical properties of TEMPO and **2a** were investigated (Figure S11), Cyclic voltammetry curves show that TEMPO has an obvious catalytic effect on **2a** (curve b *vs* curve d, curve c *vs* curve d). These results indicate that TEMPO would facilitate the reduction of **2a** on the cathode surface.

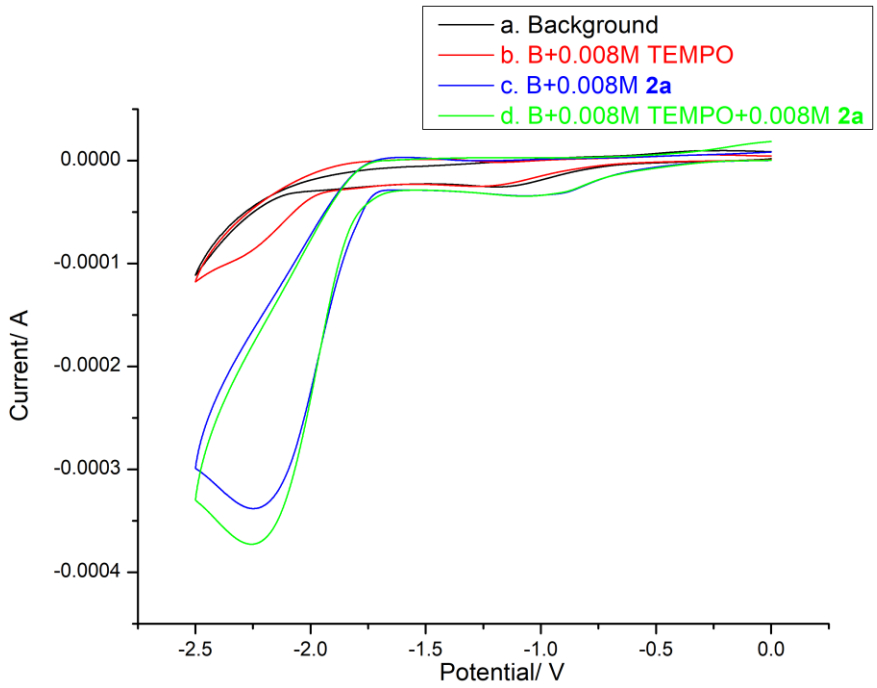


Figure S11. Cyclic voltammetry of **2a** and TEMPO in 0.1 M $TBABF_4$/DMF (10 mL) at room temperature using a Pt disk as the working electrode and Pt wire and Ag/AgCl as the counter and reference electrodes with a scan rate at 100 mV/s. background (curve a), TEMPO (0.008M) (curve b), **2a** (0.008M) (curve c),and **2a** (0.008M) TEMPO (0.008M) (curve d).

Finally, the electrochemical properties of **1a** were investigated (Figure S12), while the oxidation peaks of **1a** (1.35V) [vs Ag/AgCl]) was found.

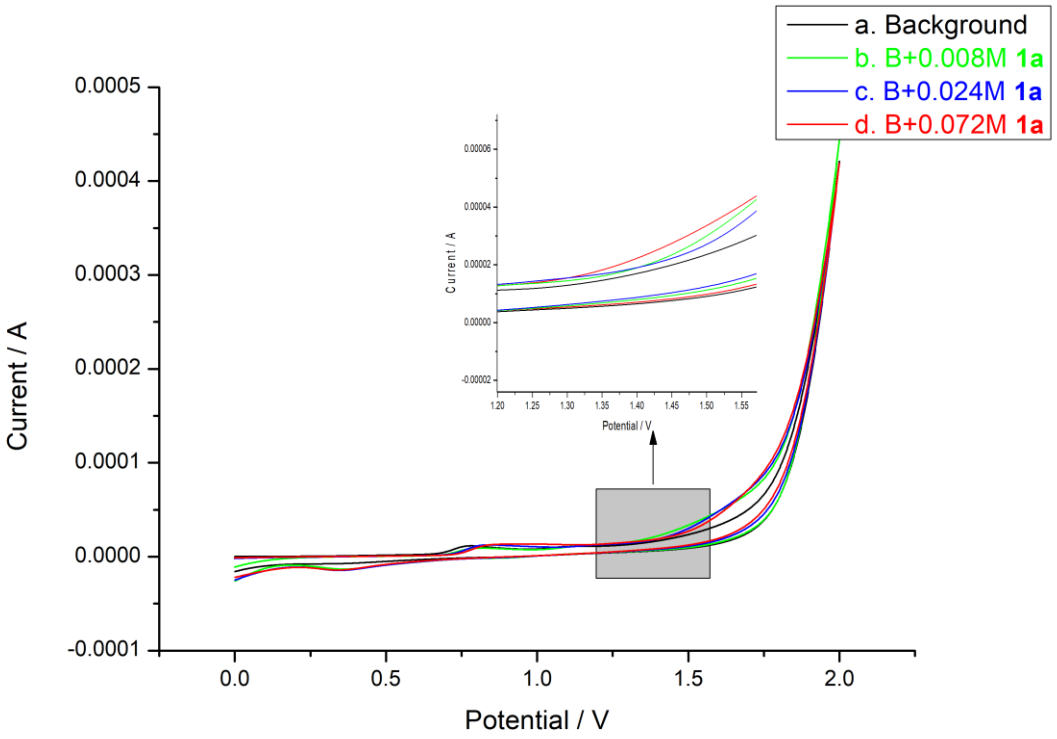
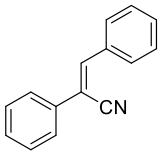
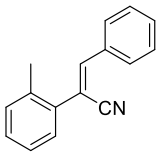


Figure S12. Cyclic voltammetry of **1a** in 0.1 M $TBABF_4$/DMF (10 mL) at room temperature using a Pt disk as the working electrode and Pt wire and Ag/AgCl as the counter and reference electrodes with a scan rate at 100 mV/s. background (curve a), **1a** (0.008M) (curve b), **1a** (0.024M) (curve c) and **1a** (0.072M) (curve d).

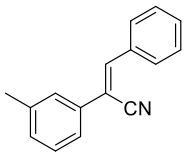
Detail Descriptions for Products



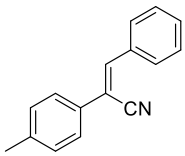
(*Z*)-2,3-diphenylacrylonitrile (3aa) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 95% yield, 58.4mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.4 Hz, 2H), 7.70 (d, *J* = 7.7 Hz, 2H), 7.55 (s, 1H), 7.50 – 7.39 (m, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.3, 134.5, 133.8, 130.6, 129.3, 129.2, 129.1, 129.0, 126.0, 118.0, 111.7.



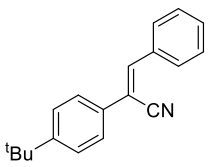
(*Z*)-3-phenyl-2-(*o*-tolyl)acrylonitrile (3ba) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 45% yield, 29.5mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92 – 7.85 (m, 2H), 7.49 – 7.44 (m, 3H), 7.33 – 7.25 (m, 4H), 7.15 (s, 1H), 2.49 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 147.0, 136.4, 135.6, 133.7, 131.0, 130.8, 129.5, 129.3, 129.2, 129.1, 126.6, 118.0, 111.3, 20.3.



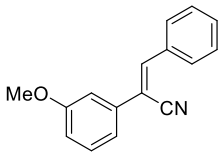
(*Z*)-3-phenyl-2-(*m*-tolyl)acrylonitrile (3ca) [S7] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 86% yield, 56.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.94 – 7.90 (m, 2H), 7.54 (s, 1H), 7.52 – 7.45 (m, 5H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 7.5 Hz, 1H), 2.44 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.0, 138.8, 134.3, 133.8, 130.5, 130.0, 129.3, 129.0, 128.9, 126.7, 123.1, 118.1, 111.6, 21.5.



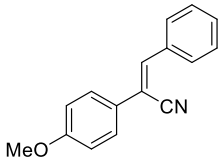
(*Z*)-3-phenyl-2-(*p*-tolyl)acrylonitrile (3da) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 94% yield, 61.7mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86 – 7.82 (m, 2H), 7.55 – 7.51 (m, 2H), 7.44 (s, 1H), 7.43 – 7.37 (m, 3H), 7.21 – 7.19 (m, 2H), 2.35 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 141.2, 139.4, 133.8, 131.6, 130.3, 129.8, 129.2, 128.9, 125.8, 118.1, 111.5, 21.2.



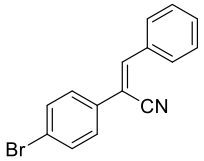
(*Z*)-2-(4-(*tert*-butyl)phenyl)-3-phenylacrylonitrile (3ea) [S7] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 81% yield, 60.2mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 – 7.72 (m, 2H), 7.50 – 7.46 (m, 2H), 7.36 (s, 1H), 7.33 – 7.26 (m, 5H), 1.21 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.6, 141.3, 133.8, 131.6, 130.4, 129.2, 128.9, 126.0, 125.7, 118.1, 111.4, 34.7, 31.2.



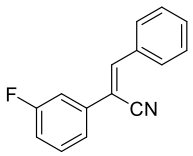
(*Z*)-2-(3-methoxyphenyl)-3-phenylacrylonitrile (3fa) [S8] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 84% yield, 59.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.89 – 7.84 (m, 2H), 7.51 (s, 1H), 7.46 – 7.41 (m, 3H), 7.33 (t, J = 8.0 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.18 – 7.17 (m, 1H), 6.94 – 6.90 (m, 1H), 3.83 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.1, 142.5, 135.9, 133.7, 130.6, 130.1, 129.4, 129.0, 118.4, 118.0, 114.8, 111.7, 111.5, 55.4.



(*Z*)-2-(4-methoxyphenyl)-3-phenylacrylonitrile (3ga) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 88% yield, 62.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.83 – 7.81 (m, 2H), 7.58 – 7.55 (m, 2H), 7.43 – 7.37 (m, 3H), 7.37 (s, 1H), 6.93 – 6.89 (m, 2H), 3.78 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.4, 140.0, 133.9, 130.1, 129.0, 128.8, 127.2, 126.8, 118.1, 114.4, 111.1, 55.3.

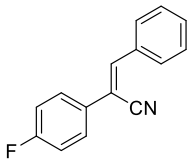


(*Z*)-2-(4-bromophenyl)-3-phenylacrylonitrile (3ha) [S7] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 69% yield, 58.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 – 7.87 (m, 2H), 7.59 – 7.52 (m, 5H), 7.49 – 7.45 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.7, 133.6, 133.5, 132.4, 131.0, 129.5, 129.2, 127.6, 123.6, 117.7, 110.7.

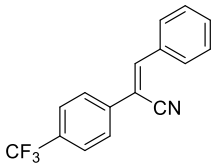


***(Z)*-2-(3-fluorophenyl)-3-phenylacrylonitrile (3ia)** [S12] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 81% yield, 54.2mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.93 – 7.88 (m, 2H), 7.54 (s, 1H), 7.50 – 7.45 (m, 4H), 7.44 – 7.40 (m, 1H), 7.40 – 7.36 (m, 1H), 7.12-7.08 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 163.2 (d, J = 247.2 Hz), 143.3, 136.7 (d, J = 8.0 Hz), 133.4, 131.0, 130.8 (d, J = 8.5 Hz), 129.5, 129.1, 121.9 (d, J = 2.8 Hz), 117.7, 116.2 (d, J = 21.3 Hz), 113.0 (d, J = 23.5 Hz), 110.5

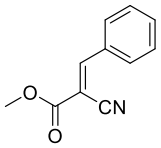
(d, *J* = 2.7 Hz).**^{19}F NMR** (470 MHz, $CDCl_3$) δ -111.7.



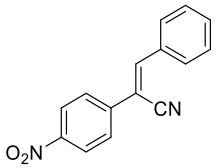
(*Z*)-2-(4-fluorophenyl)-3-phenylacrylonitrile (3ja) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 96% yield, 64.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.87 – 7.83 (m, 2H), 7.65 – 7.60 (m, 2H), 7.46 – 7.40 (m, 4H), 7.13 – 7.08 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.2 (d, *J* = 250.3 Hz), 142.2 (d, *J* = 1.6 Hz),133.6, 130.7, 130.6, 129.3, 129.0, 127.9 (d, *J* = 8.3 Hz), 117.9, 116.2 (d, *J* = 22.0 Hz), 110.5. **^{19}F NMR** (470 MHz, $CDCl_3$) δ -111.5.



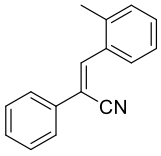
(*Z*)-3-phenyl-2-(4-(trifluoromethyl)phenyl)acrylonitrile (3ka) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 53% yield, 43.3mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.95 – 7.90 (m, 2H), 7.81 – 7.77 (m, 2H), 7.72 – 7.68 (m, 2H), 7.62 (s, 1H), 7.52 – 7.47 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 144.2, 137.9, 133.2, 131.3, 131.0 (q, *J* = 32.9 Hz),129.6, 129.1, 126.3, 126.1 (q, *J* = 3.6 Hz), 123.8 (q, *J* = 272.3 Hz), 117.5, 110.3. **^{19}F NMR** (470 MHz, $CDCl_3$) δ -62.7.



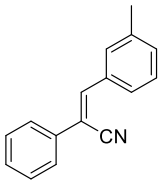
methyl (*Z*)-2-cyano-3-phenylacrylate (3la) [S11] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 43% yield, 24.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.27 (s, 1H), 8.02 – 7.98 (m, 2H), 7.59 – 7.55 (m, 1H), 7.53 – 7.49 (m, 2H), 3.94 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 163.1, 155.4, 133.5, 131.4, 131.2, 129.3, 115.5, 102.5, 53.5.



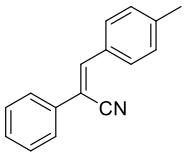
(*Z*)-2-(4-nitrophenyl)-3-phenylacrylonitrile (3na) [S14] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a yellow solid. 25% yield, 18.8mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.33 – 8.30 (m, 2H), 7.96 – 7.93 (m, 2H), 7.87 – 7.84 (m, 2H), 7.69 (s, 1H), 7.54 – 7.50 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 148.1, 145.7, 140.7, 133.0, 131.9, 129.9, 129.4, 126.1, 124.5, 117.3, 109.7.



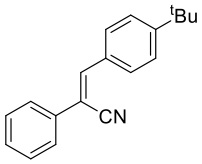
(*Z*)-2-phenyl-3-(*o*-tolyl)acrylonitrile (3ab) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 90% yield, 59.3mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.00 – 7.96 (m, 1H), 7.79 (s, 1H), 7.75 – 7.70 (m, 2H), 7.51 – 7.43 (m, 3H), 7.38 – 7.28 (m, 3H), 2.43 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 141.2, 137.6, 134.4, 133.2, 130.6, 130.3, 129.4, 129.2, 128.2, 126.5, 126.2, 117.8, 113.9, 20.0.



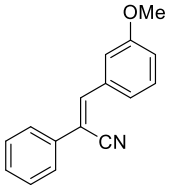
(*Z*)-2-phenyl-3-(*m*-tolyl)acrylonitrile (3ac) [S3] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 92% yield, 60.7mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71-7.68 (m, 1H), 7.67 – 7.62 (m, 3H), 7.47 (s, 1H), 7.44 – 7.39 (m, 2H), 7.38 – 7.31 (m, 2H), 7.24 – 7.20 (m, 1H), 2.39 (s, 3H).. **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.5, 138.7, 134.6, 133.7, 131.45, 130.0, 129.2, 129.1, 128.9, 126.4, 126.0, 118.1, 111.4, 21.5.



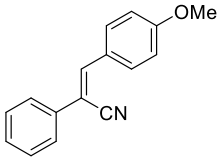
(Z)-2-phenyl-3-(*p*-tolyl)acrylonitrile (3ad) [S4] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 91% yield, 60.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84 – 7.80 (m, 2H), 7.70 – 7.66 (m, 2H), 7.51 (s, 1H), 7.47 – 7.43 (m, 2H), 7.42 – 7.37 (m, 1H), 7.30 – 7.27 (m, 2H), 2.42 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.3, 141.2, 134.7, 131.1, 129.7, 129.4, 129.1, 129.0, 125.9, 118.3, 110.5, 21.6.



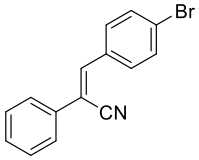
(*Z*)-3-(4-(*tert*-butyl)phenyl)-2-phenylacrylonitrile (3ae) [S4] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 83% yield, 65.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.89 – 7.84 (m, 2H), 7.71 – 7.67 (m, 2H), 7.53 (s, 1H), 7.52 – 7.49 (m, 2H), 7.47 – 7.39 (m, 3H), 1.37 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.3, 142.3, 134.8, 131.0, 129.3, 129.1, 129.0, 126.0, 125.9, 118.3, 110.6, 35.1, 31.2.



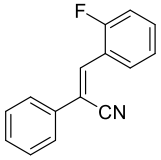
(*Z*)-3-(3-methoxyphenyl)-2-phenylacrylonitrile (3af) [S2] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 93% yield, 65.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 – 7.67 (m, 2H), 7.55 – 7.52 (m, 1H), 7.51 (s, 1H), 7.47 – 7.36 (m, 5H), 7.00 (dd, *J* = 8.1, 2.1 Hz, 1H), 3.88 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 159.9, 142.3, 135.0, 134.5, 130.0, 129.3, 129.1, 126.1, 122.3, 118.1, 117.1, 113.5, 111.9, 55.5.



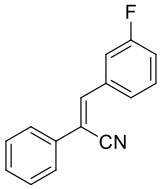
(*Z*)-3-(4-methoxyphenyl)-2-phenylacrylonitrile (3ag) [S4] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 89% yield, 62.8mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 – 7.88 (m, 2H), 7.67 – 7.64 (m, 2H), 7.46 (s, 1H), 7.45 – 7.37 (m, 3H), 6.99 – 6.97 (m, 2H), 3.86 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.4, 141.9, 134.9, 131.2, 129.0, 128.8, 126.5, 125.8, 118.6, 114.4, 108.6, 55.5.



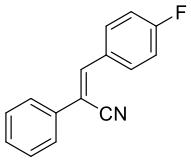
(*Z*)-3-(4-bromophenyl)-2-phenylacrylonitrile (3ah) [S2] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 78% yield, 66.5mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 – 7.74 (m, 2H), 7.69 – 7.66 (m, 2H), 7.62 – 7.59 (m, 2H), 7.48 – 7.41 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 140.9, 134.3, 132.7, 132.4, 130.8, 129.6, 129.3, 126.1, 125.0, 117.9, 112.5.



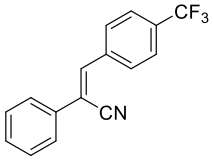
(*Z*)-3-(2-fluorophenyl)-2-phenylacrylonitrile (3ai) [S5] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 87% yield, 58.3mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.30 – 8.22 (m, 1H), 7.77 (s, 1H), 7.71 – 7.67 (m, 2H), 7.48 – 7.38 (m, 4H), 7.26 – 7.23 (m, 1H), 7.16 – 7.11 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.0 (d, *J* = 252.7 Hz), 134.2, 133.7 (d, *J* = 6.8 Hz), 132.3 (d, *J* = 9.0 Hz), 129.6, 129.2, 128.6, 126.2,124.7 (d, *J* = 3.7 Hz), 122.1 (d, *J* = 11.3 Hz), 117.7, 115.82 (d, *J* = 21.7 Hz),) δ 113.8 (d, *J* = 1.7 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ -114.5.



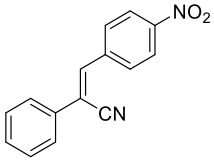
(*Z*)-3-(3-fluorophenyl)-2-phenylacrylonitrile (3aj) [S9] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 94% yield, 62.9mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.67 – 7.56 (m, 4H), 7.45 (s, 1H), 7.44 – 7.36 (m, 4H), 7.12 – 7.07 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.8 (d, *J* = 246.9 Hz), 140.6 (d, *J* = 2.6 Hz), 135.8 (d, *J* = 7.6 Hz), 134.0, 130.6 (d, *J* = 8.2 Hz), 129.6, 129.2, 126.1, 125.3 (d, *J* = 2.8 Hz), 117.6, 117.5 (d, *J* = 21.2 Hz), 115.7 (d, *J* = 22.9 Hz), 113.1. **^{19}F NMR** (470 MHz, $CDCl_3$) δ -111.5.



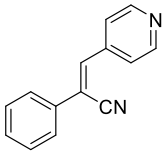
(*Z*)-3-(4-fluorophenyl)-2-phenylacrylonitrile (3ak) [S1] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 95% yield, 63.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92 – 7.88 (m, 2H), 7.69 – 7.65 (m, 2H), 7.49 (s, 1H), 7.47 – 7.40 (m, 3H), 7.17 – 7.13 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 163.7 (d, *J* = 252.8 Hz), 140.9, 134.3, 131.4 (d, *J* = 8.8 Hz), 130.0 (d, *J* = 2.9 Hz), 129.3 (d, *J* = 22.1 Hz), 126.0, 125.0, 118.0, 116.2 (d, *J* = 22.0 Hz), 111.4 (d, *J* = 1.9 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ -108.2.



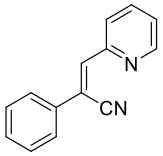
(*Z*)-2-phenyl-3-(4-(trifluoromethyl)phenyl)acrylonitrile (3al) [S2] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 91% yield, 74.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.5 Hz, 2H), 7.73 – 7.68 (m, 4H), 7.57 (s, 1H), 7.49 – 7.43 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 140.1, 137.1, 133.8, 131.8 (q, *J* = 32.6 Hz), 129.9, 129.5, 129.3, 126.2, 125.9 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 272.6 Hz), 117.5, 114.4. **^{19}F NMR** (470 MHz, $CDCl_3$) δ -62.8.



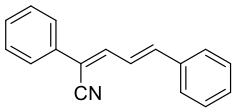
(*Z*)-3-(4-nitrophenyl)-2-phenylacrylonitrile (3am) [S14] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 35% yield, 26.3mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.32 – 8.27 (m, 2H), 8.05 – 8.00 (m, 2H), 7.74 – 7.69 (m, 2H), 7.60 (s, 1H), 7.51 – 7.45 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 148.3, 139.7, 139.0, 133.5, 130.3, 130.0, 129.4, 126.3, 124.2, 117.2, 116.0.



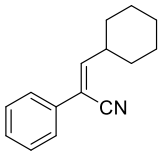
(*Z*)-2-phenyl-3-(pyridin-4-yl)acrylonitrile (3aq) [S6] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 96% yield, 59.4mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.73 – 8.70 (m, 2H), 7.71 – 7.66 (m, 4H), 7.47 (s, 1H), 7.46 – 7.42 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.5, 140.6, 138.7, 133.2, 130.1, 129.2, 126.2, 122.6, 116.8, 116.3.



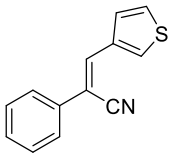
(*Z*)-2-phenyl-3-(pyridin-2-yl)acrylonitrile (3ar) [S15] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 6:1) to give the product as a colorless oil. 93% yield, 57.5mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.76 (d, *J* = 4.5 Hz, 1H), 7.96 (d, *J* = 7.9 Hz, 1H), 7.82-7.80 (m, 1H), 7.77 – 7.73 (m, 2H), 7.65 (s, 1H), 7.49 – 7.41 (m, 3H), 7.32 -7.29 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.4, 150.2, 141.2, 137.0, 134.1, 129.9, 129.3, 126.5, 124.4, 124.2, 117.6, 115.1.



(2*Z*,4*E*)-2,5-diphenylpenta-2,4-dienenitrile (3as) [S4] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 65% yield, 45.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.66 – 7.62 (m, 2H), 7.58 – 7.55 (m, 2H), 7.44 – 7.36 (m, 8H), 7.05 – 7.01 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 141.7, 141.3, 135.8, 133.3, 129.6, 129.2, 129.1, 129.0, 127.6, 125.7, 125.2, 117.1, 113.2.

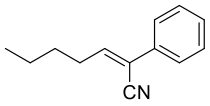


(*Z*)-3-cyclohexyl-2-phenylacrylonitrile (3at) [S10] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 94% yield, 59.6mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.57 – 7.50 (m, 2H), 7.40-7.38 (m, 2H), 7.37 – 7.32 (m, 1H), 6.66 (d, *J* = 10.0 Hz, 1H), 2.82 – 2.72 (m, 1H), 1.86 – 1.77 (m, 4H), 1.75-1.70 (m, 1H), 1.46 – 1.36 (m, 2H), 1.30 – 1.21 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.1, 133.3, 128.9, 128.8, 125.7, 116.7, 113.8, 41.4, 32.2, 25.6, 25.3.

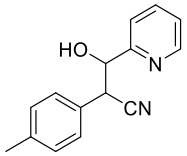


(*Z*)-2-phenyl-3-(thiophen-3-yl)acrylonitrile (3at) [S16] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 40% yield, 25.4mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.96 – 7.94 (m, 1H), 7.81 –

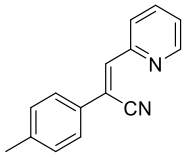
7.78 (m, 1H), 7.67 – 7.63 (m, 2H), 7.54 (s, 1H), 7.47 – 7.37 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 136.1, 135.4, 134.2, 129.6, 129.1, 129.0, 127.4, 126.7, 125.8, 118.5, 109.8.



(*Z*)-2-phenylhept-2-enenitrile (3ax) [S13] was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 50:1) to give the product as a white solid. 85% yield, 47.2mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.58 – 7.51 (m, 2H), 7.42 – 7.34 (m, 3H), 6.83 (t, *J* = 7.8 Hz, 1H), 2.60 (q, *J* = 7.6 Hz, 2H), 1.58 – 1.52 (m, 2H), 1.47 – 1.41 (m, 2H), 0.96 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 147.4, 133.5, 129.1, 129.0, 125.7, 116.8, 116.0, 32.0, 30.9, 22.4, 14.0.



3-hydroxy-3-(pyridin-2-yl)-2-(*p*-tolyl)propanenitrile (2:3 dr) (5) [S17] 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 white solid. 40% yield, 285.9mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.59 – 8.57 (m, 1H), 7.62 (td, *J* = 7.7, 1.7 Hz, 1H), 7.29-7.28 (m, 2H), 7.12 – 7.08 (m, 4H), 6.90 (d, *J* = 7.8 Hz, 1H), 5.06 (d, *J* = 5.7 Hz, 1H), 4.31 (d, *J* = 5.6 Hz, 1H), 2.34 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.2, 148.6, 138.5, 136.7, 129.7, 128.7, 128.6, 123.8, 122.2, 118.8, 74.6, 45.7, 21.3.



(*Z*)-3-(pyridin-2-yl)-2-(*p*-tolyl)acrylonitrile (6) [S15] 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. 97% yield, 64.1mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.74 (d, *J* = 4.1 Hz, 1H), 7.97 – 7.92 (m, 1H), 7.79 (td, *J* = 7.8, 1.7 Hz, 1H), 7.65 – 7.62 (m, 2H), 7.61 (s, 1H), 7.32-7.28 (m, 1H), 7.26 – 7.24 (m, 2H), 2.39 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.4, 150.0, 140.2, 140.0, 136.9, 131.2, 129.9, 126.3, 124.2, 124.0, 117.6, 115.0, 21.4.

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Copies of NMR spectra

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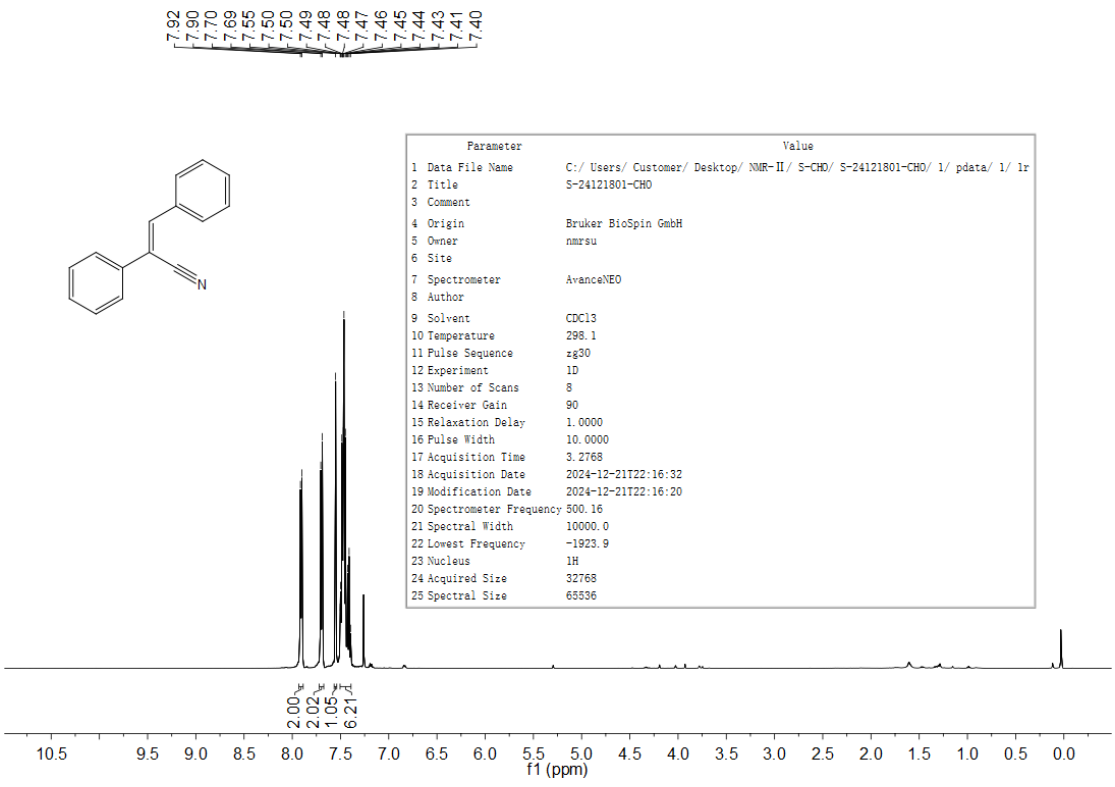

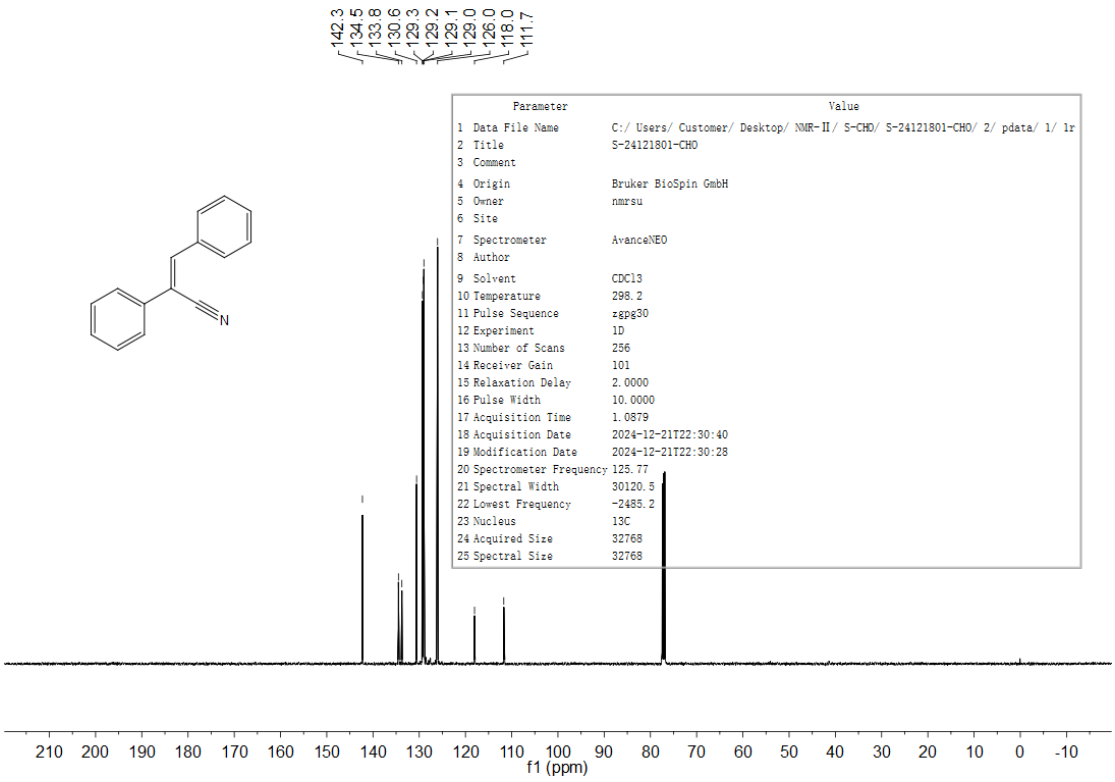

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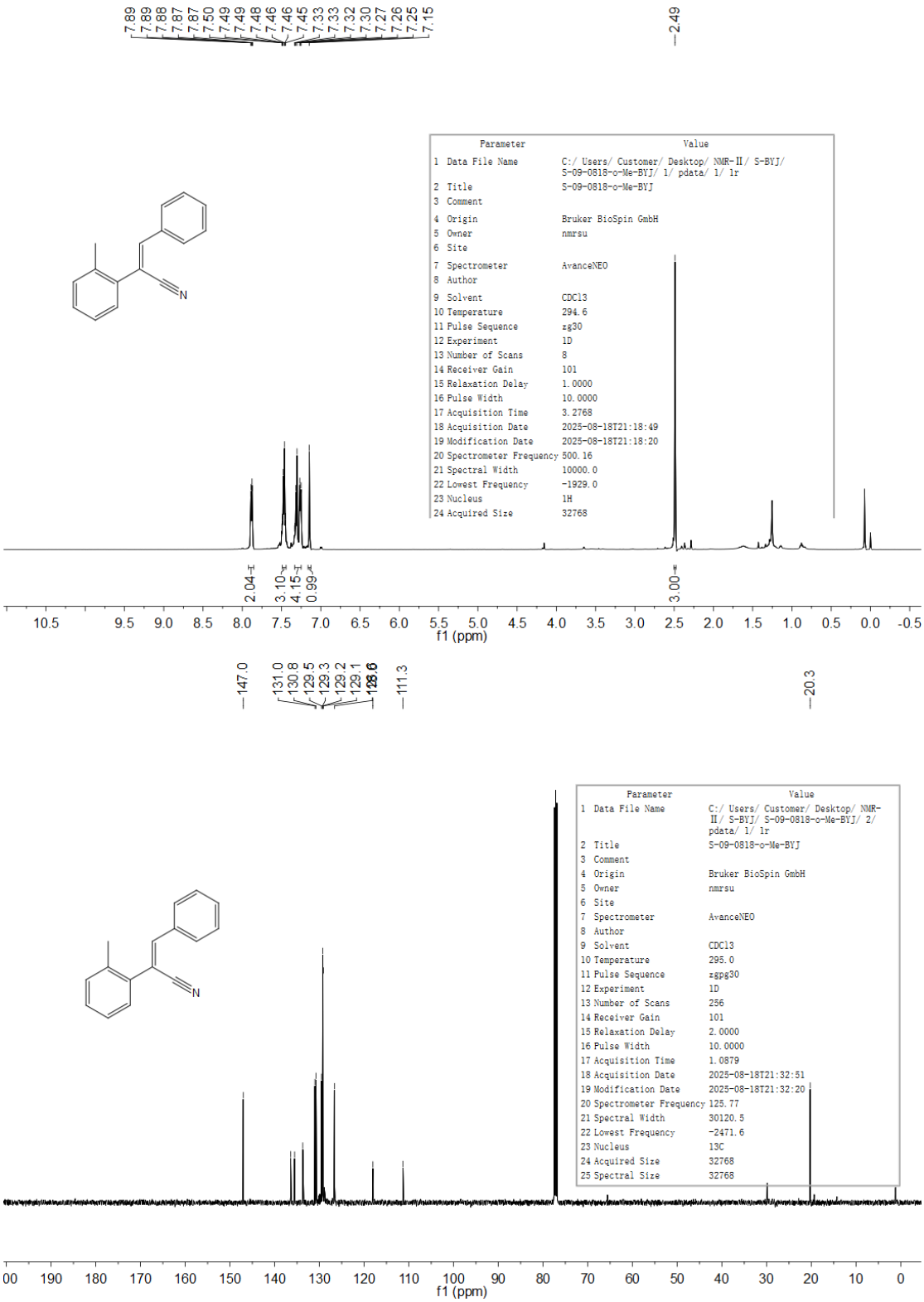

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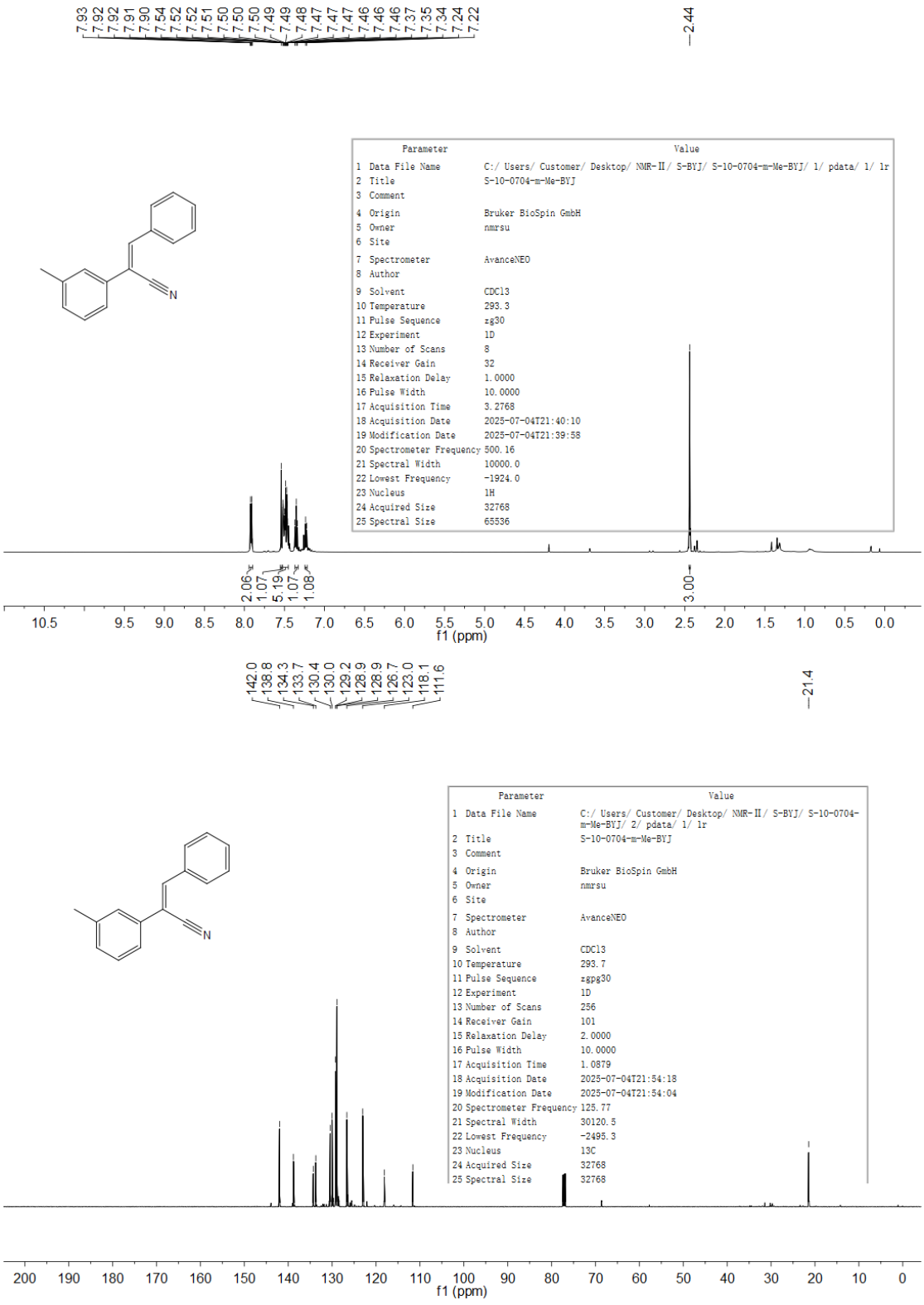

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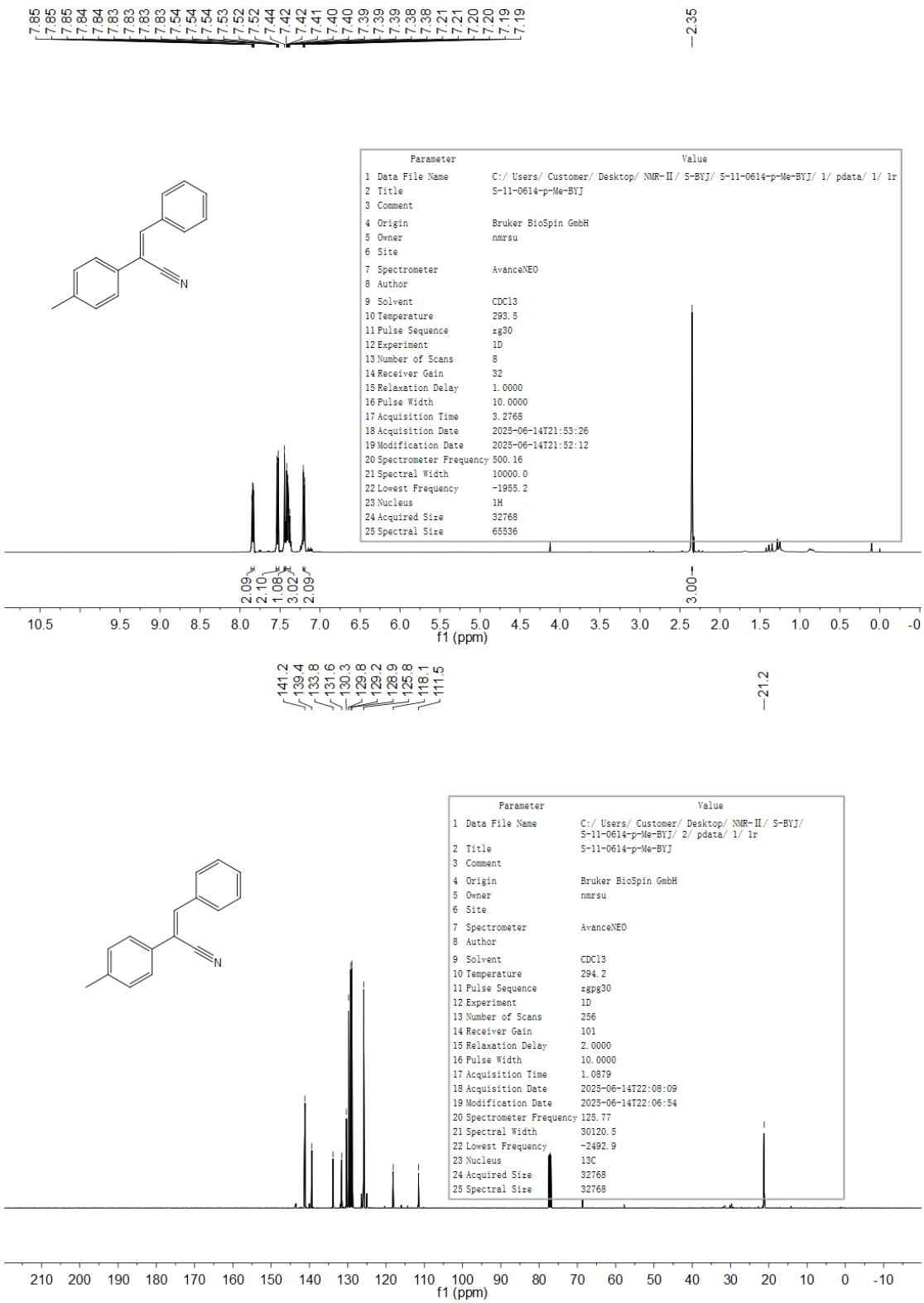

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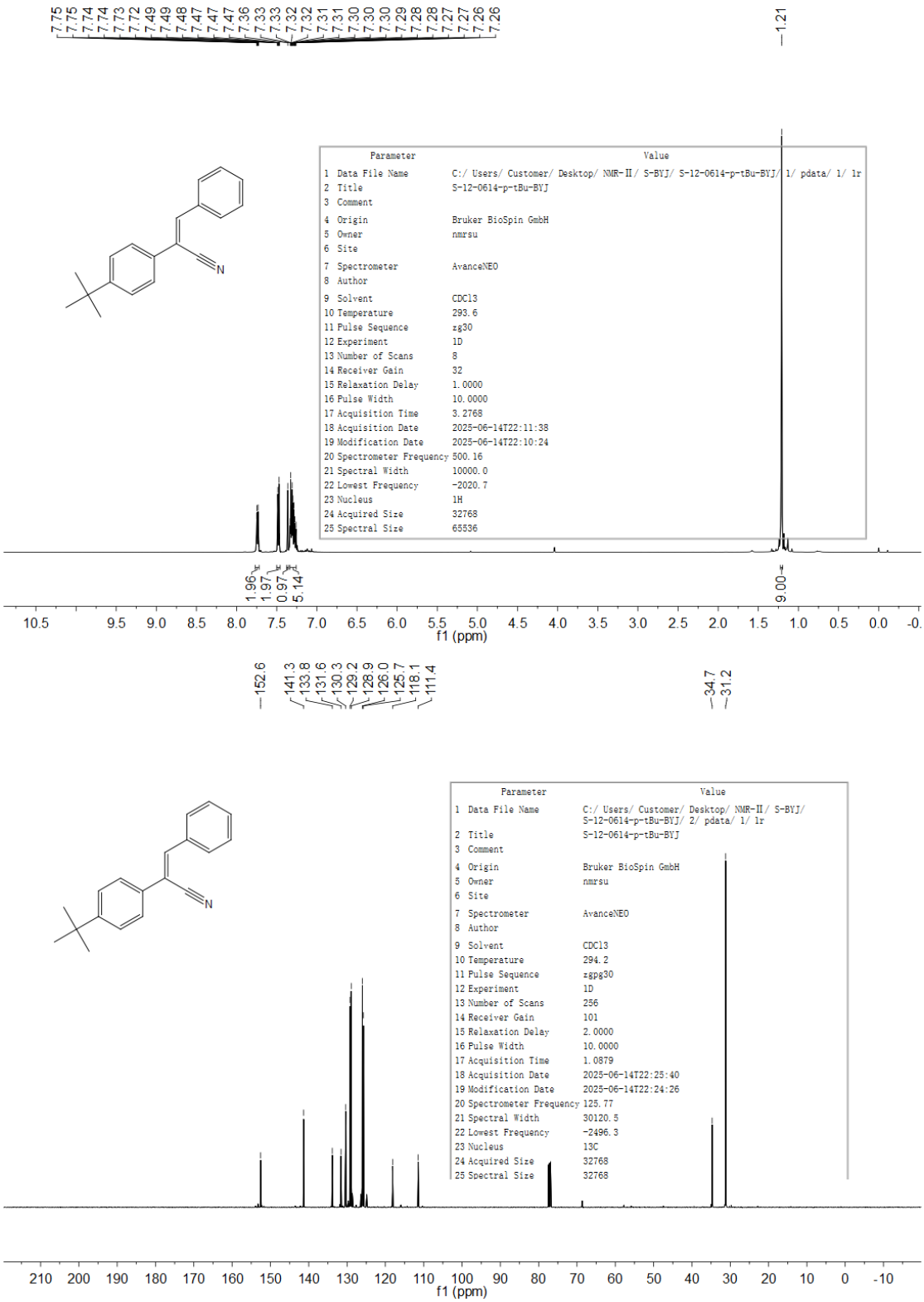

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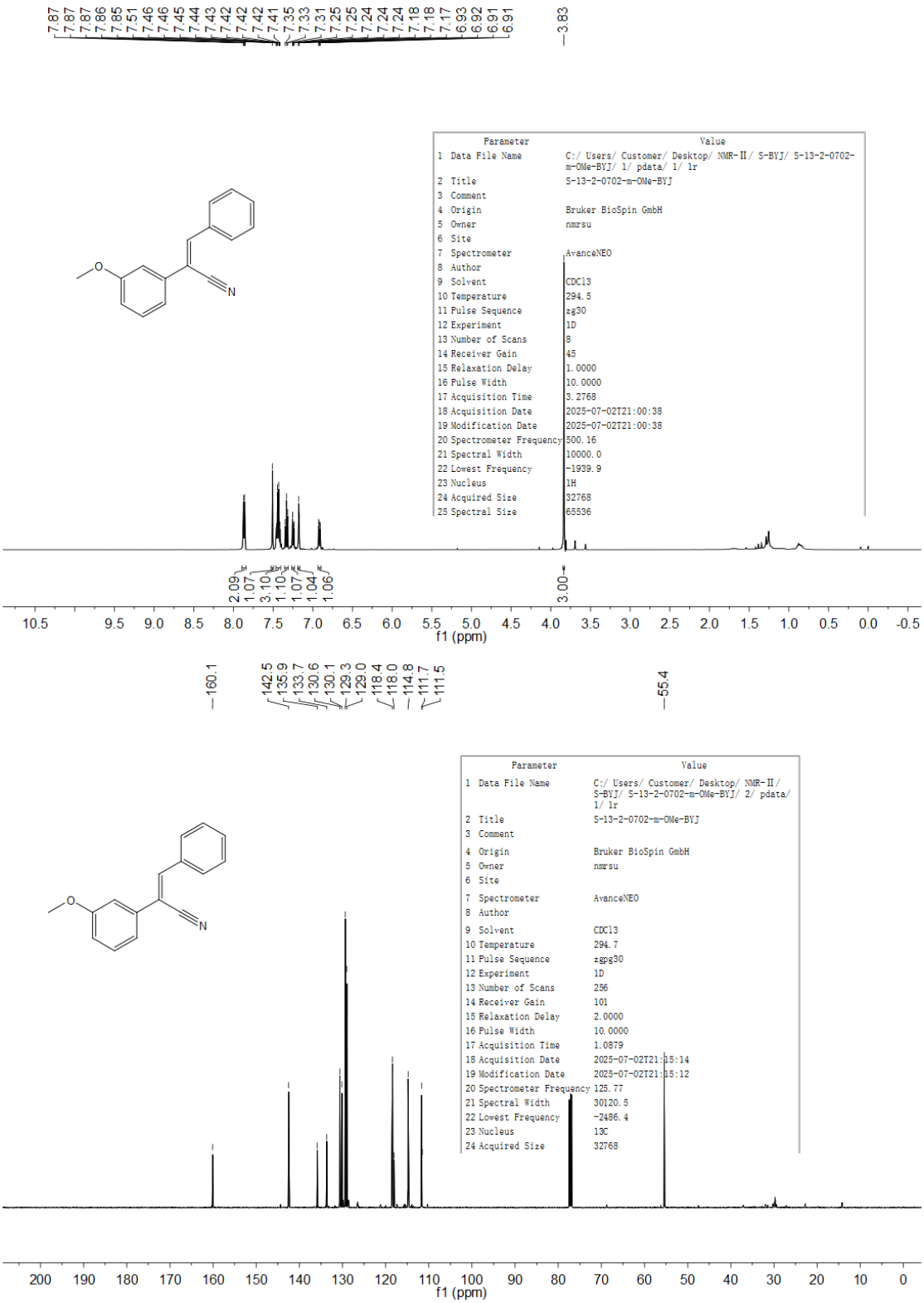

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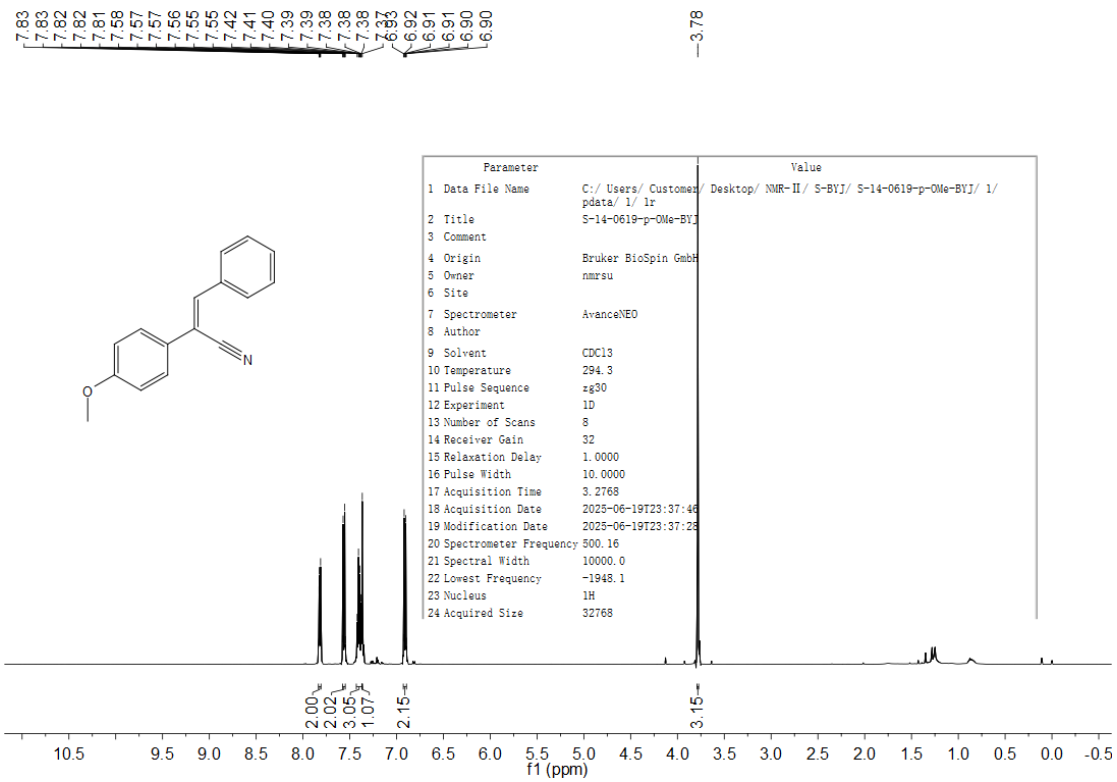

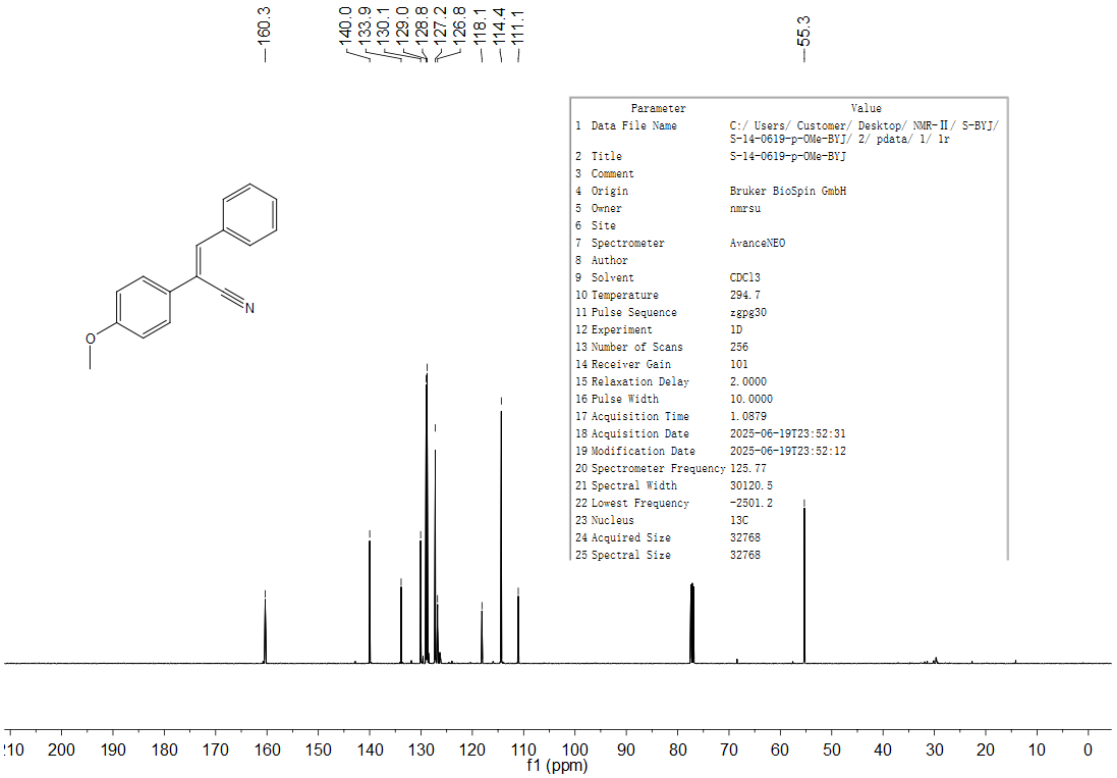

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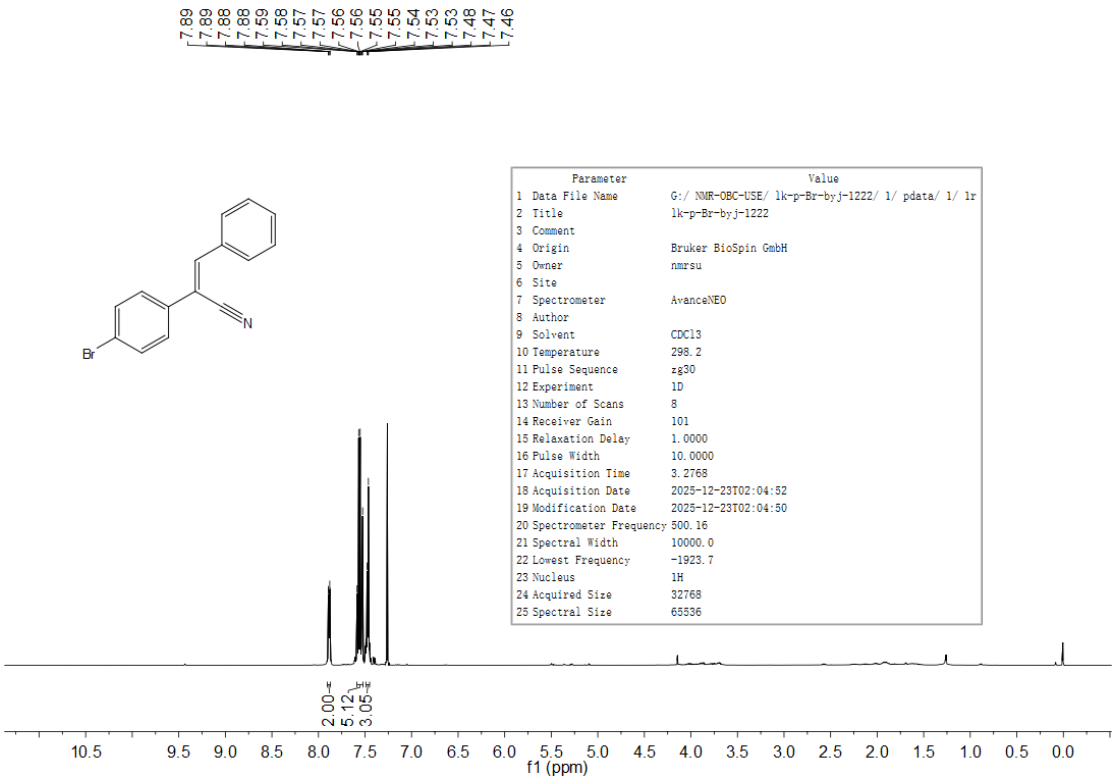
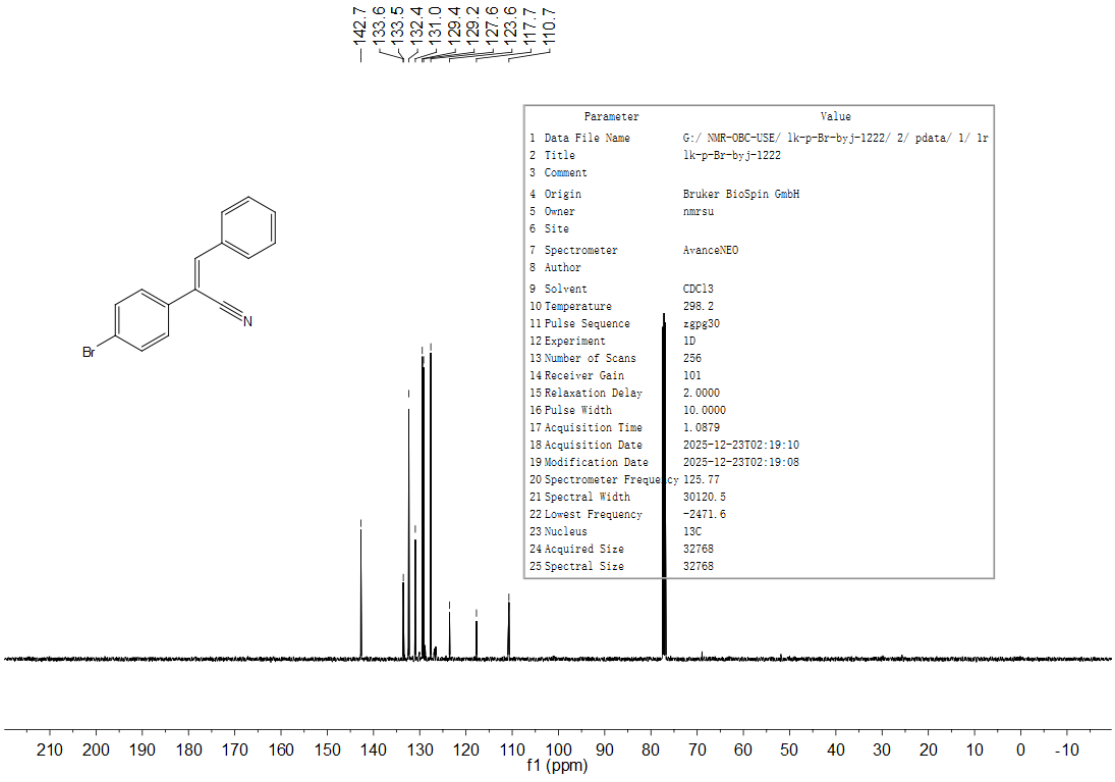
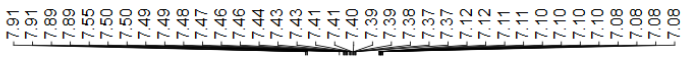
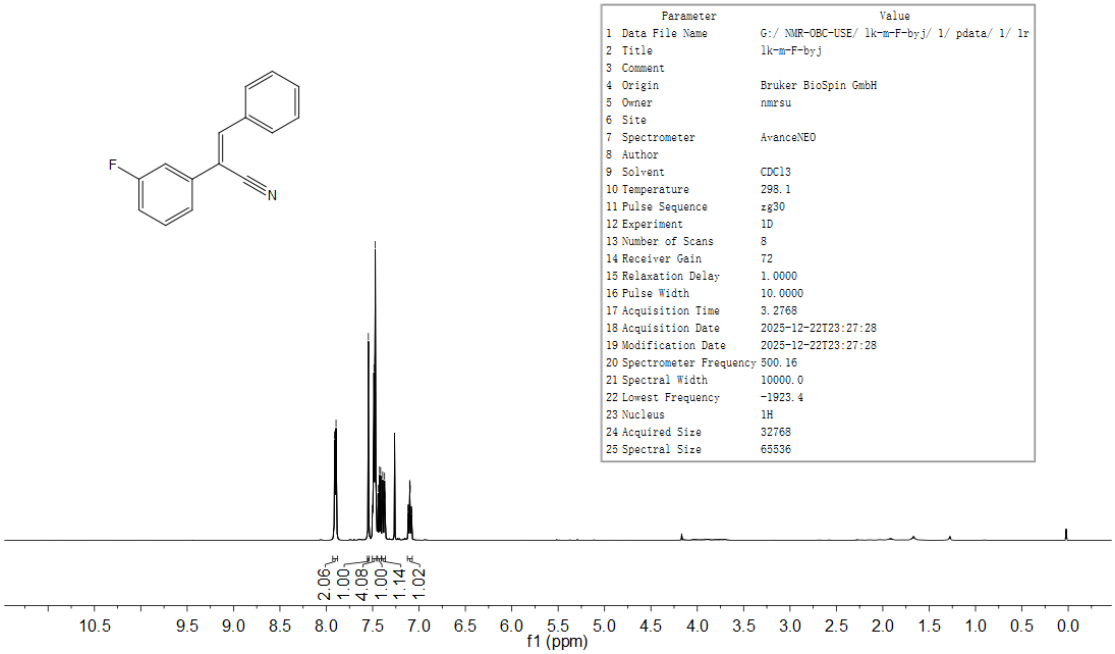




***(Z)*-2-(3-fluorophenyl)-3-phenylacrylonitrile (3ia)**





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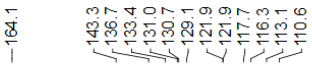

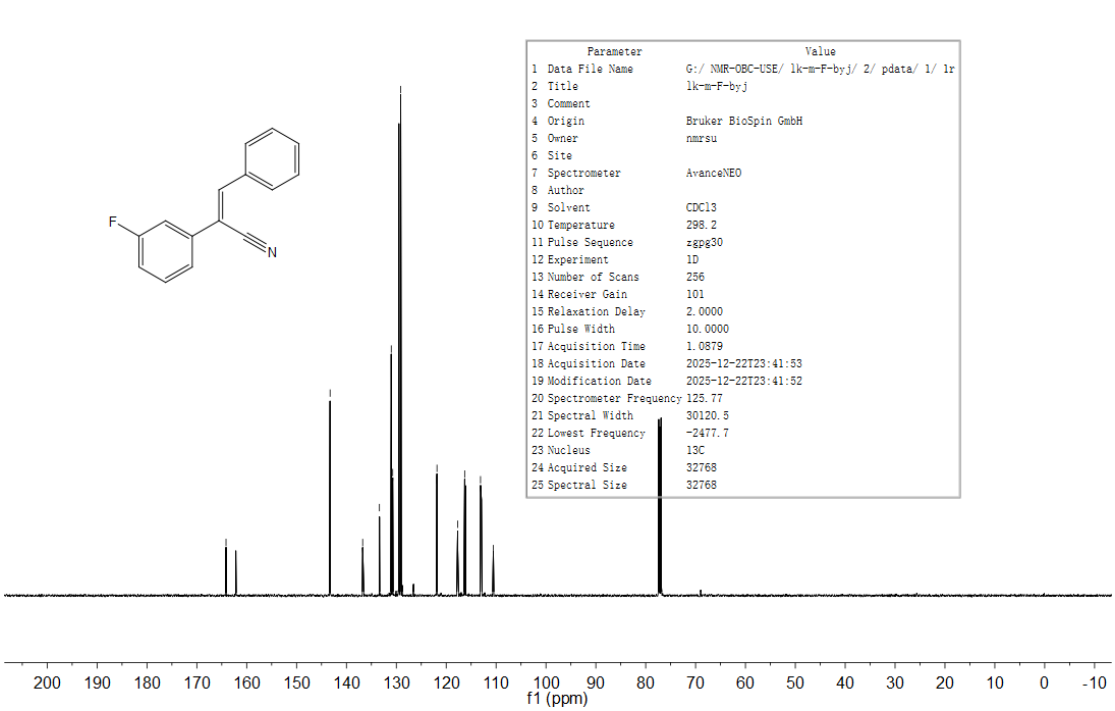

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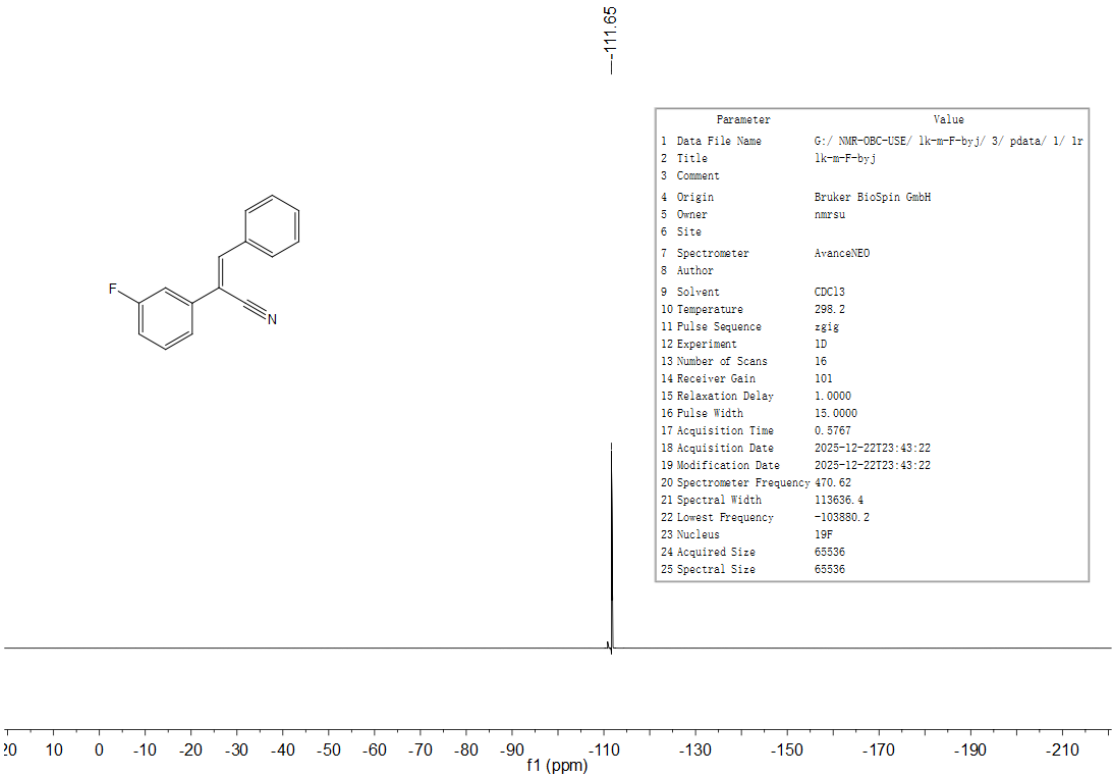

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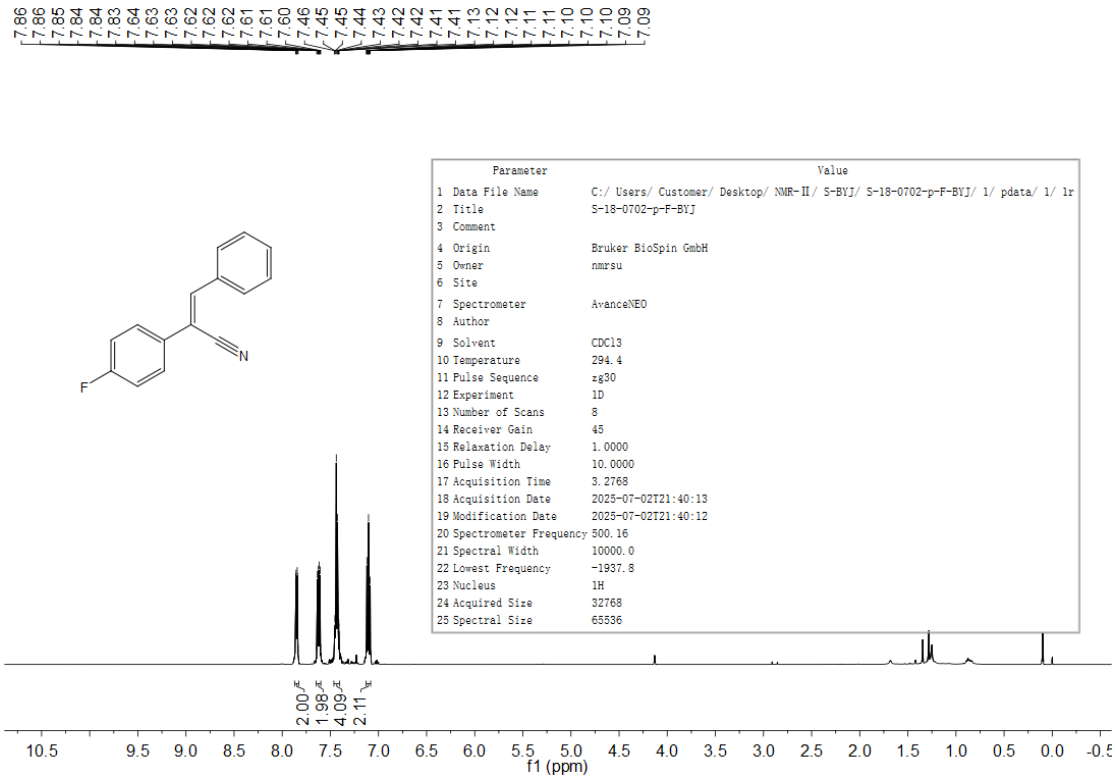
(*Z*)-2-(4-fluorophenyl)-3-phenylacrylonitrile (3ja)



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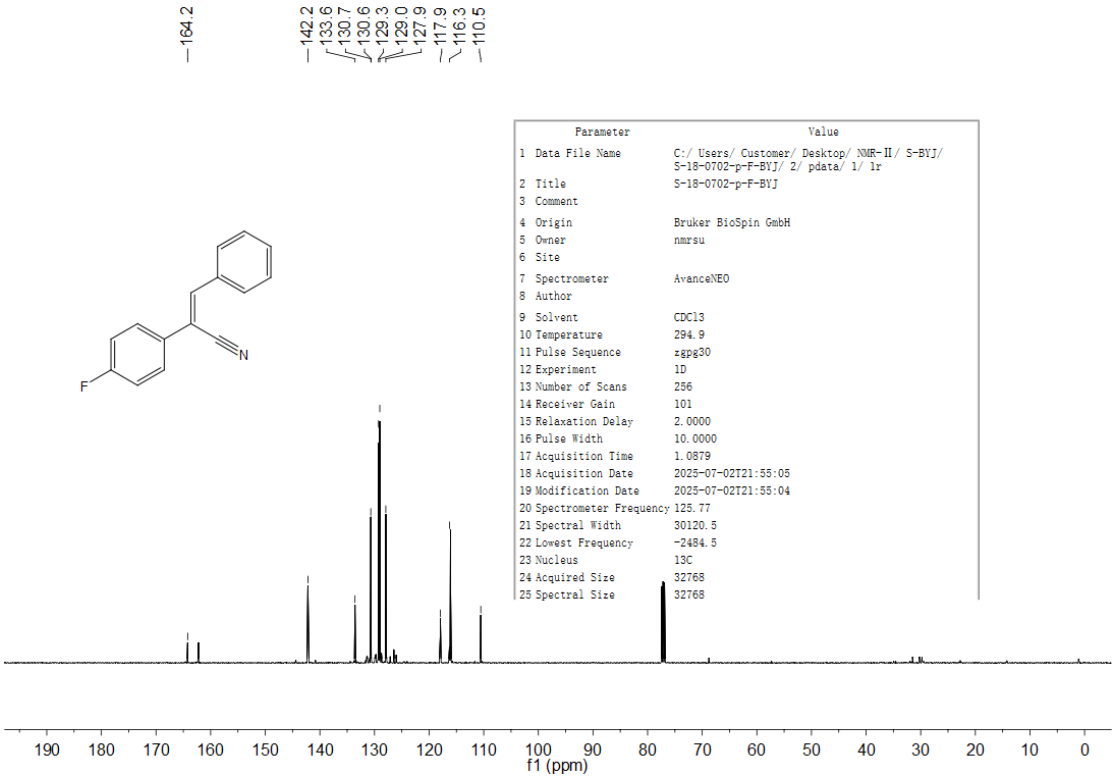

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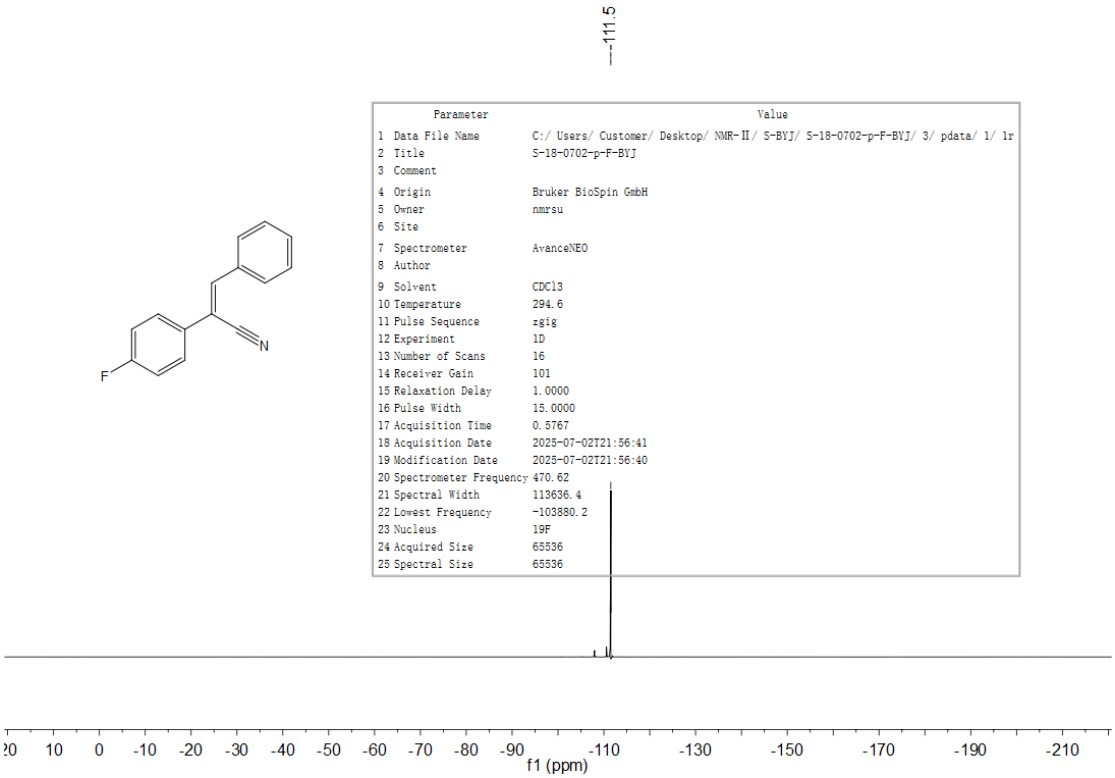
25 Spectral Size	32768



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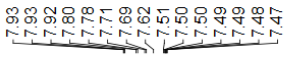
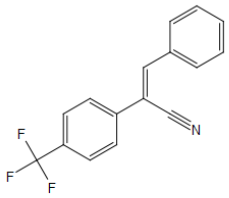
2 Title	S-18-0702-p-F-BYJ
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	294.6
11 Pulse Sequence	zgig
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	15.0000
17 Acquisition Time	0.5767
18 Acquisition Date	2025-07-02T21:56:41
19 Modification Date	2025-07-02T21:56:40
20 Spectrometer Frequency	470.62
21 Spectral Width	113636.4
22 Lowest Frequency	-103880.2
23 Nucleus	19F
24 Acquired Size	65536
25 Spectral Size	65536

(*Z*)-3-phenyl-2-(4-(trifluoromethyl)phenyl)acrylonitrile (3ka)





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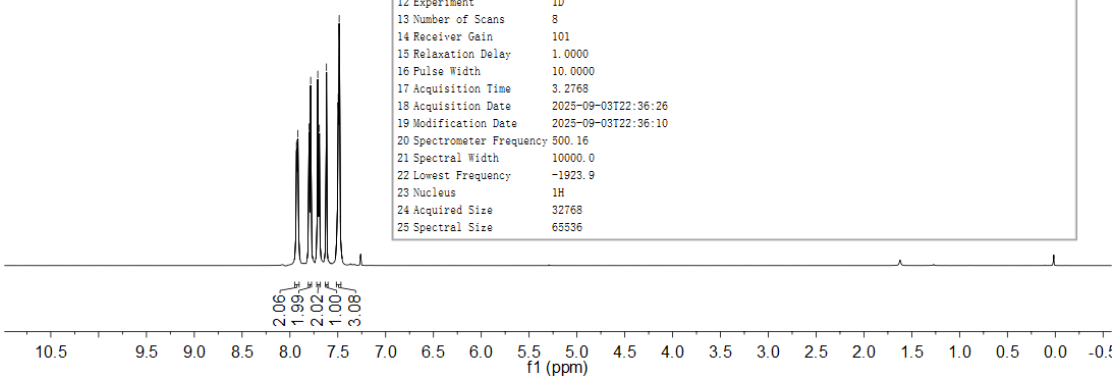
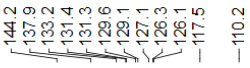
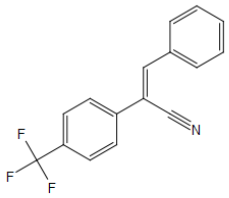
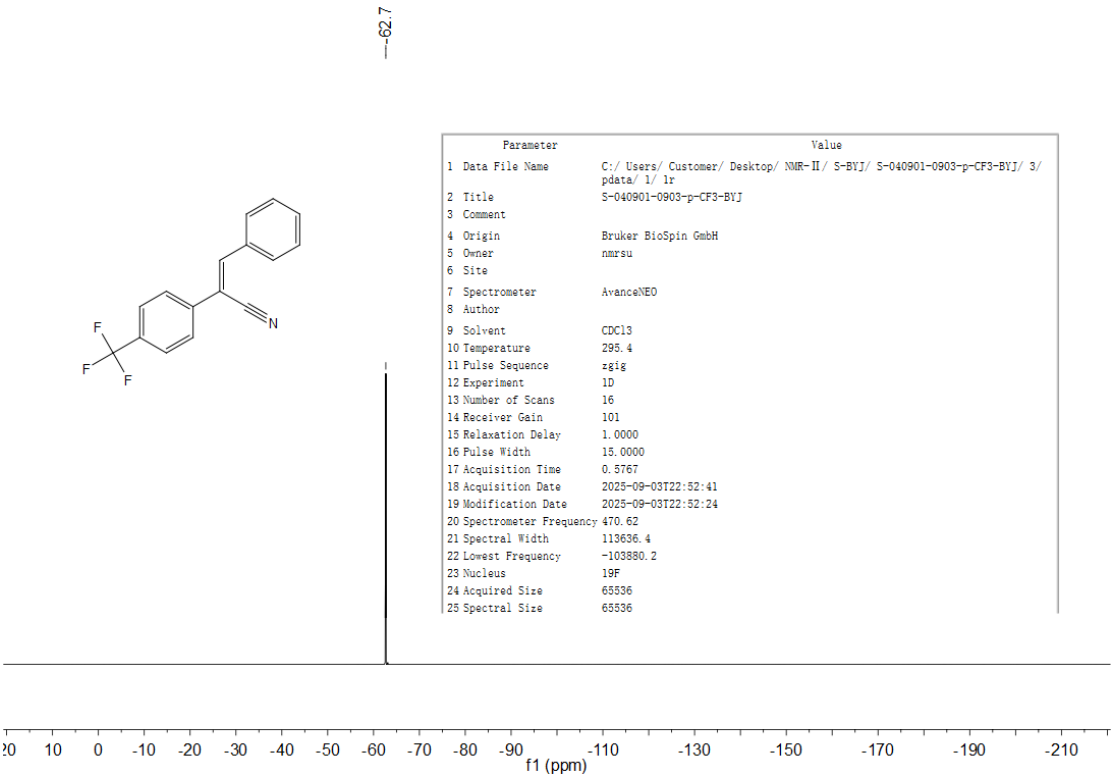
2 Title	S-040901-0903-p-CF3-BYJ
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	295.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2025-09-03T22:36:26
19 Modification Date	2025-09-03T22:36:10
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





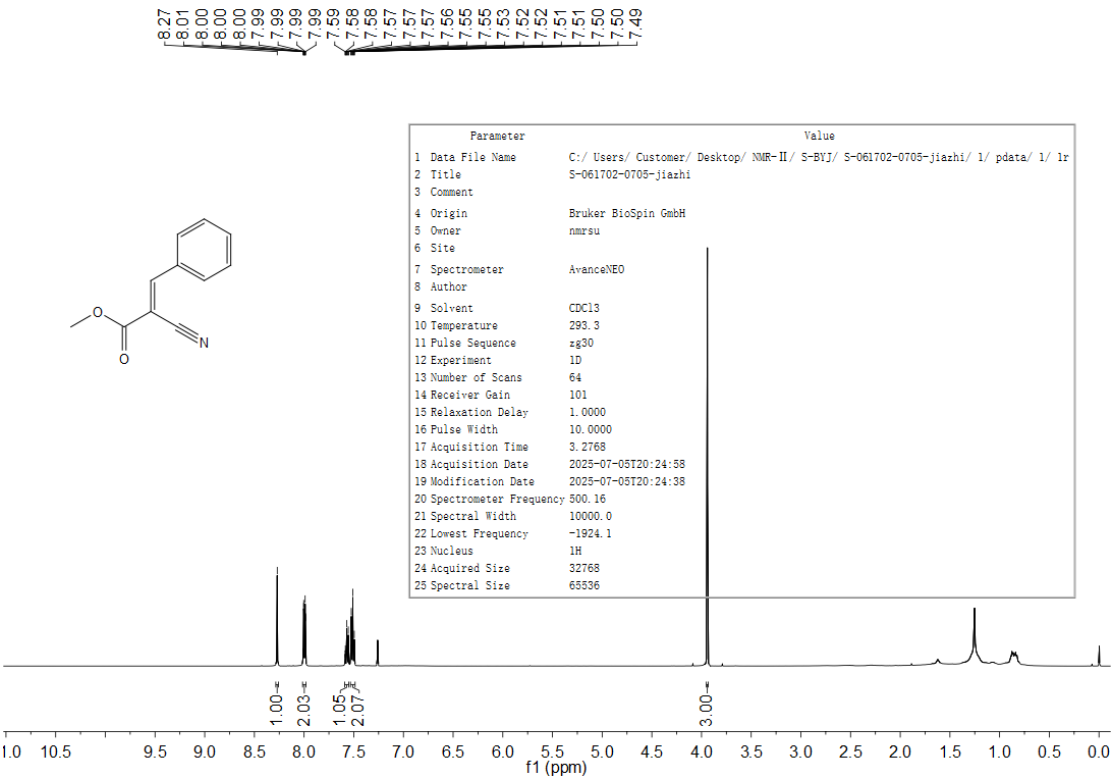


Parameter	Value
1 Data File Name	C:/ Users/ Customer/ Desktop/ NMR-Ⅱ/ S-BYJ/ S-040901-0903-p-CF3-BYJ/ 2/ pdata/ 1/ 1r
2 Title	S-040901-0903-p-CF3-BYJ
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	295.7
11 Pulse Sequence	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	2025-09-03T22:50:47
19 Modification Date	2025-09-03T22:50:30
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



Parameter	Value
1 Data File Name	C:/ Users/ Customer/ Desktop/ NMR-Ⅱ/ S-BYJ/ S-040901-0903-p-CF3-BYJ/ 3/ pdata/ 1/ 1r
2 Title	S-040901-0903-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	295.4
11 Pulse Sequence	zgig
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	15.0000
17 Acquisition Time	0.5767
18 Acquisition Date	2025-09-03T22:52:41
19 Modification Date	2025-09-03T22:52:24
20 Spectrometer Frequency	470.62
21 Spectral Width	113636.4
22 Lowest Frequency	-103880.2
23 Nucleus	19F
24 Acquired Size	65536
25 Spectral Size	65536

methyl (*Z*)-2-cyano-3-phenylacrylate (3la)



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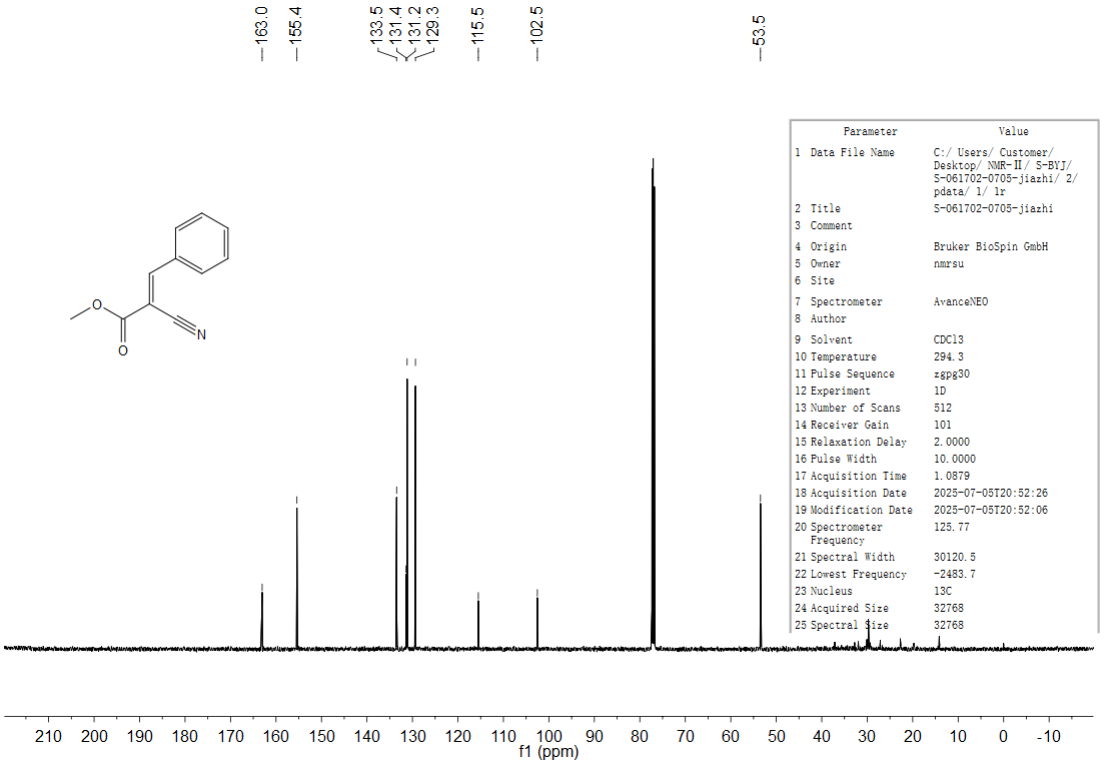
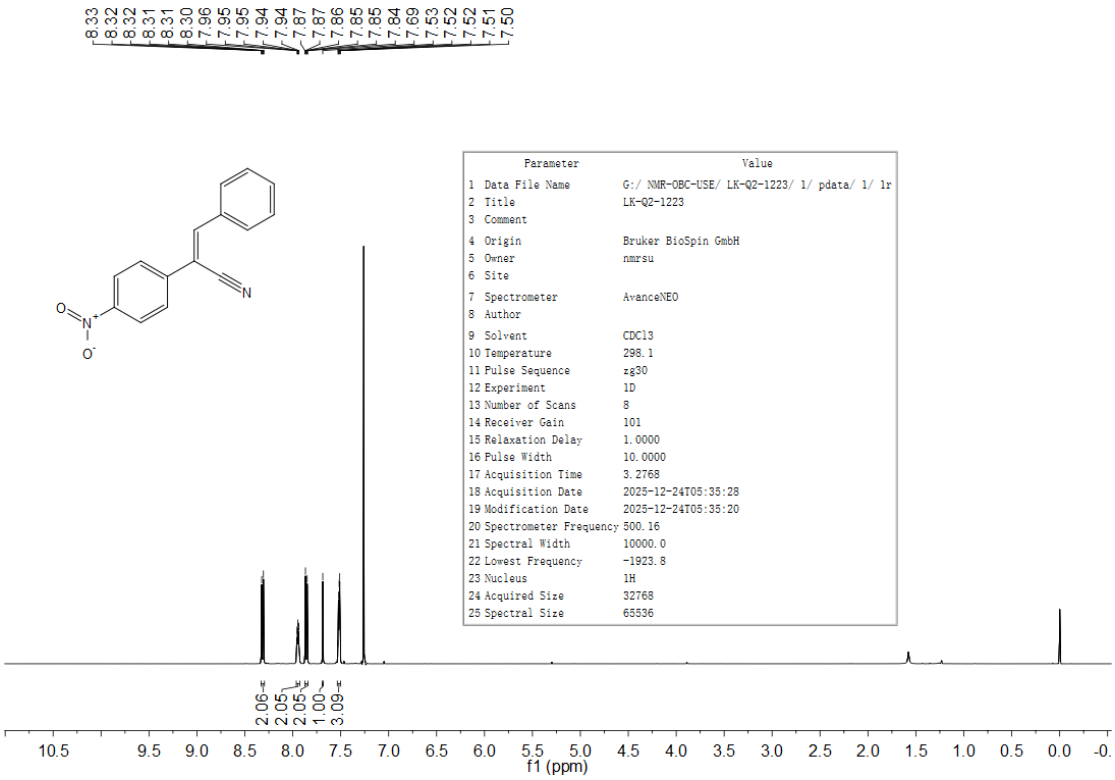
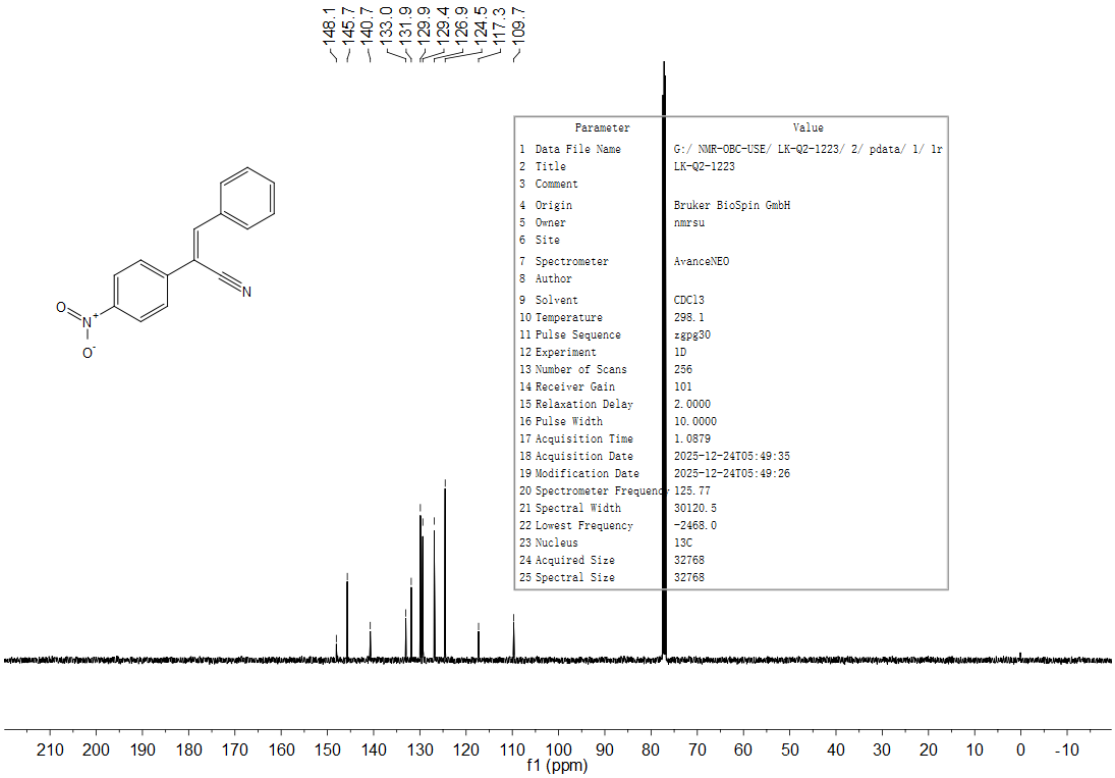
2 Title	S-061702-0705-jiazhi
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	293.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	64
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2025-07-05T20:24:58
19 Modification Date	2025-07-05T20:24:38
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1924.1
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

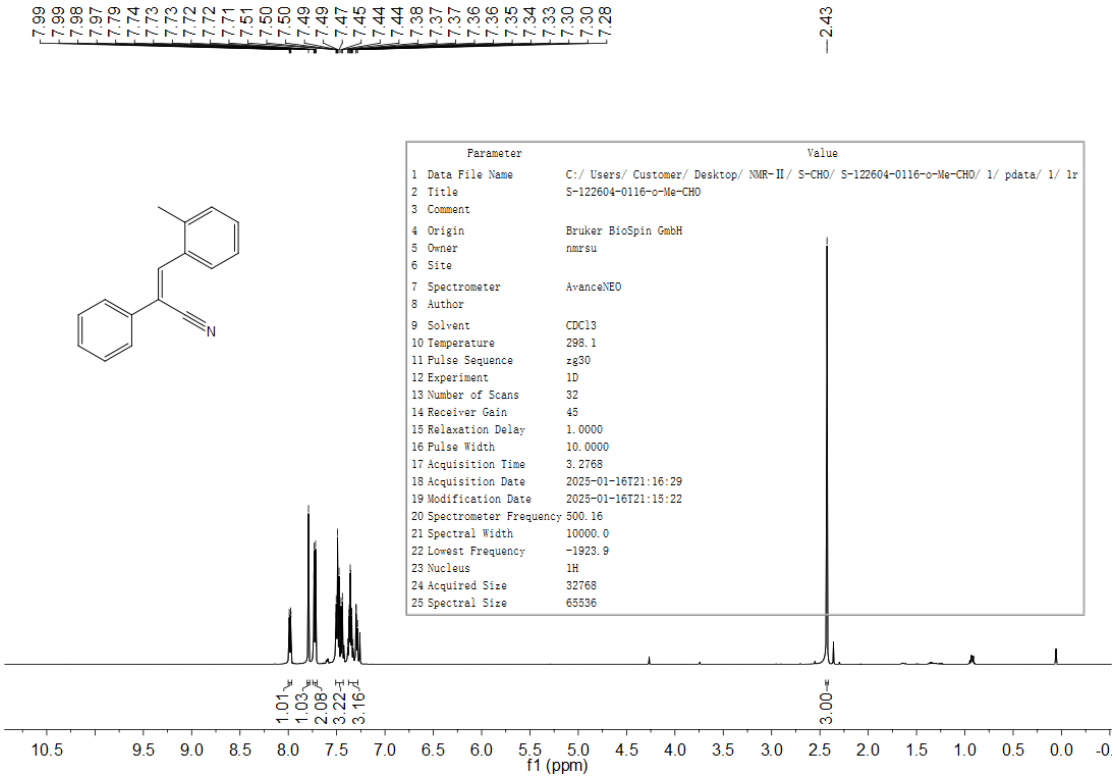


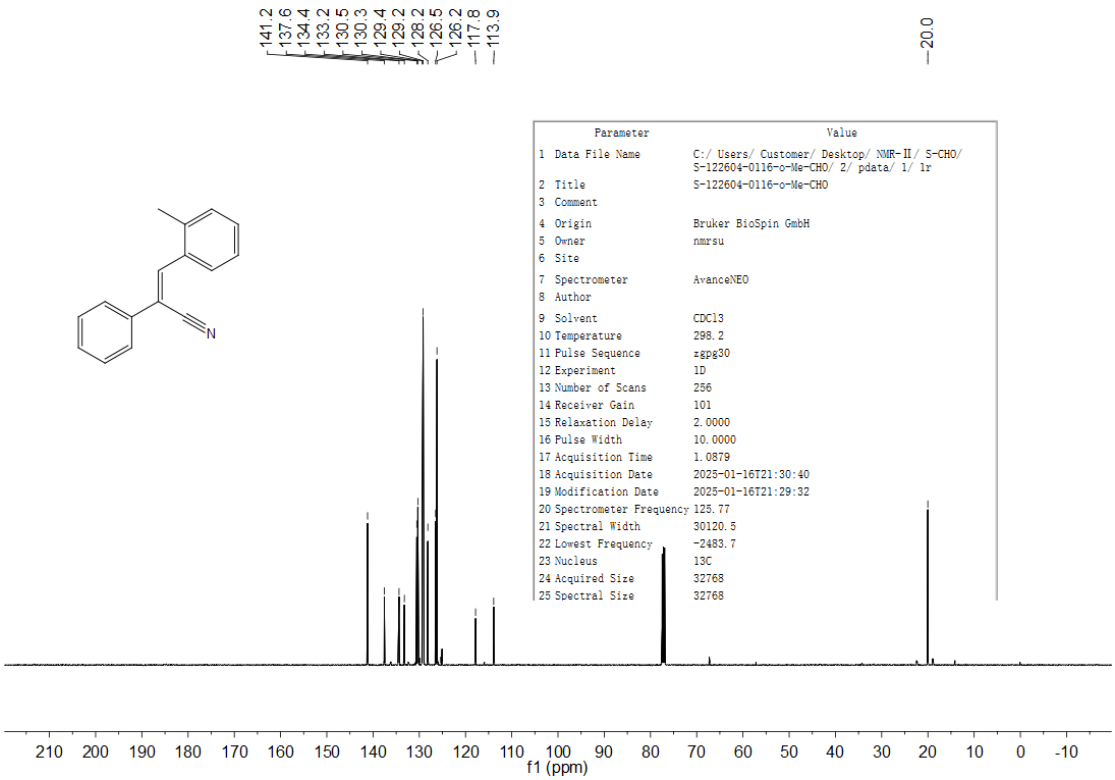
(*Z*)-2-(4-nitrophenyl)-3-phenylacrylonitrile (3na)



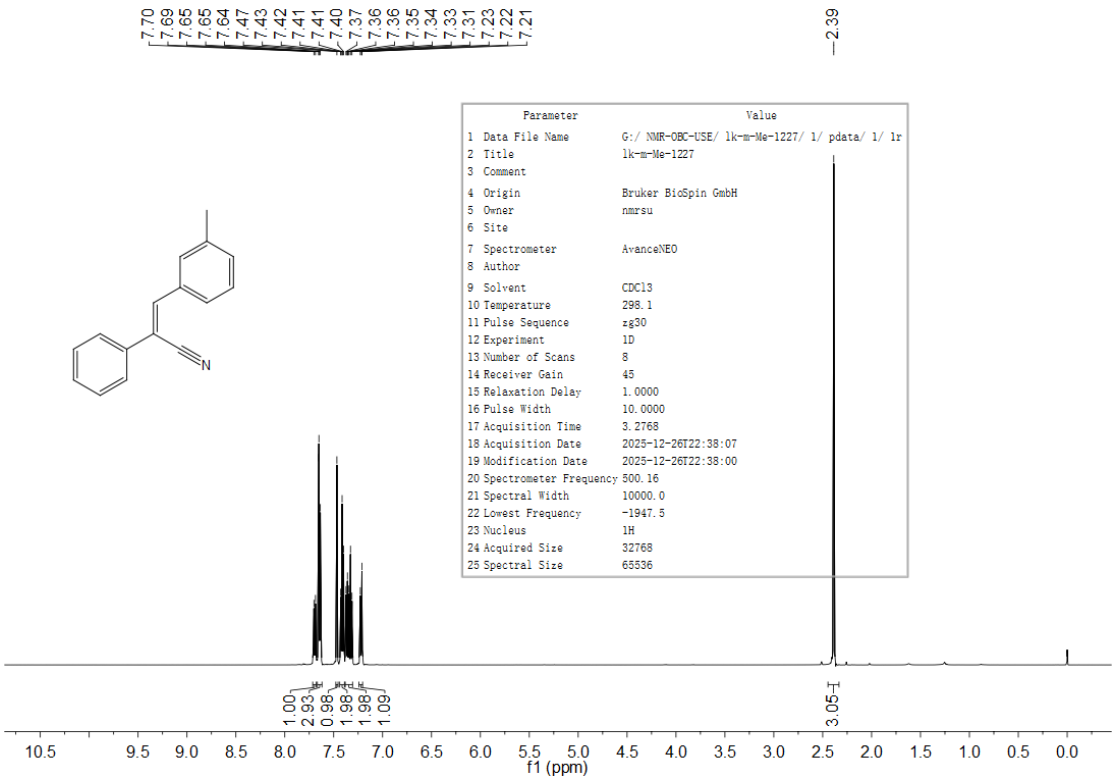


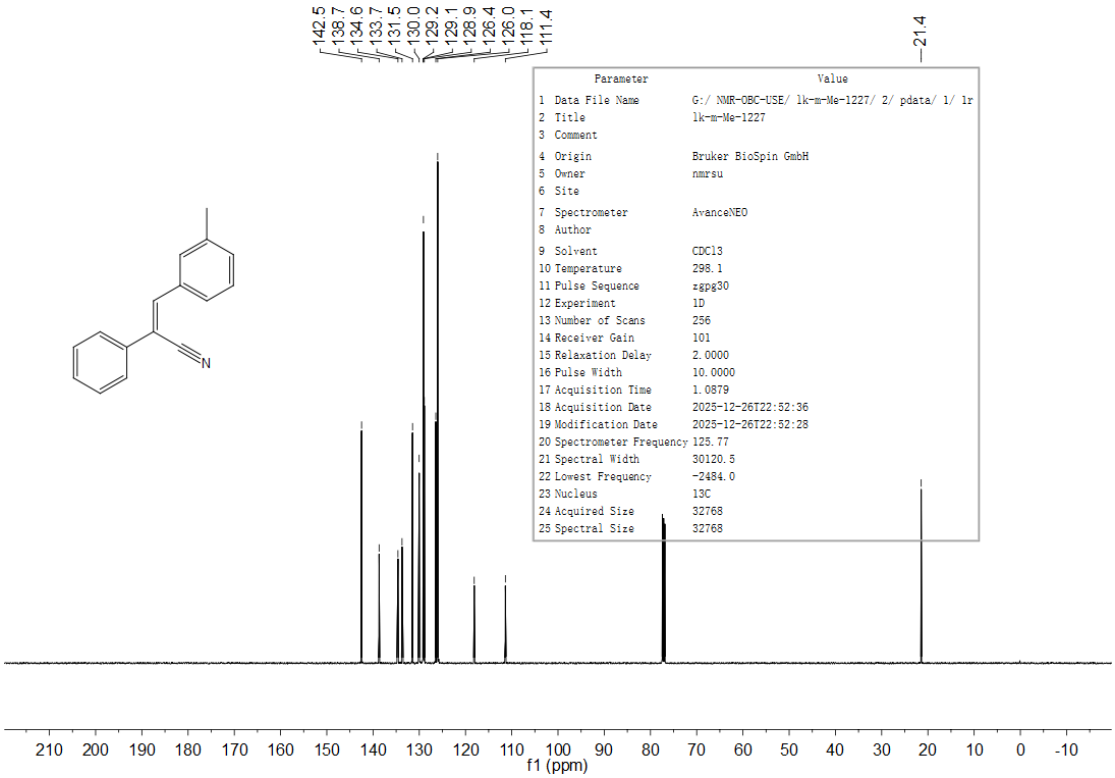
(*Z*)-2-phenyl-3-(*o*-tolyl)acrylonitrile (3ab)





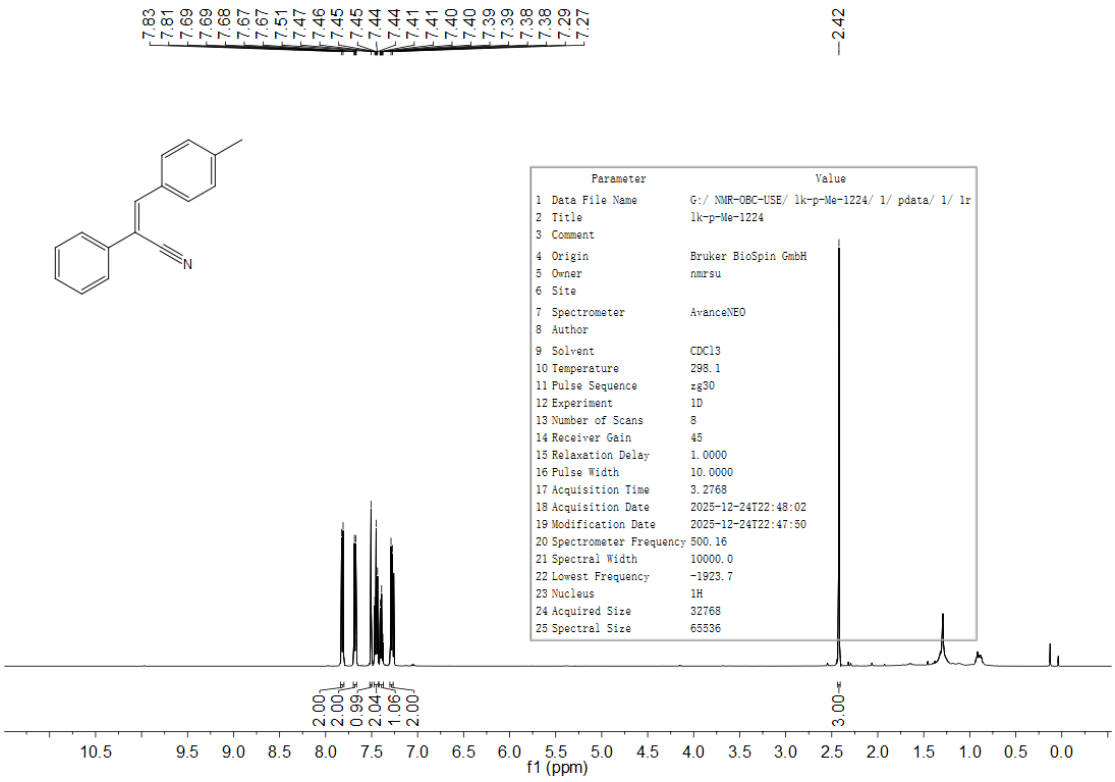
(*Z*)-2-phenyl-3-(*m*-tolyl)acrylonitrile (3ac)





Parameter	Value
1 Data File Name	G:/ NMR-OBC-USE/ lk-m-Me-1227/ 2/ pdata/ 1/ 1r
2 Title	lk-m-Me-1227
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	2025-12-26T22:52:36
19 Modification Date	2025-12-26T22:52:28
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2484.0
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768

(Z)-2-phenyl-3-(*p*-tolyl)acrylonitrile (3ad)



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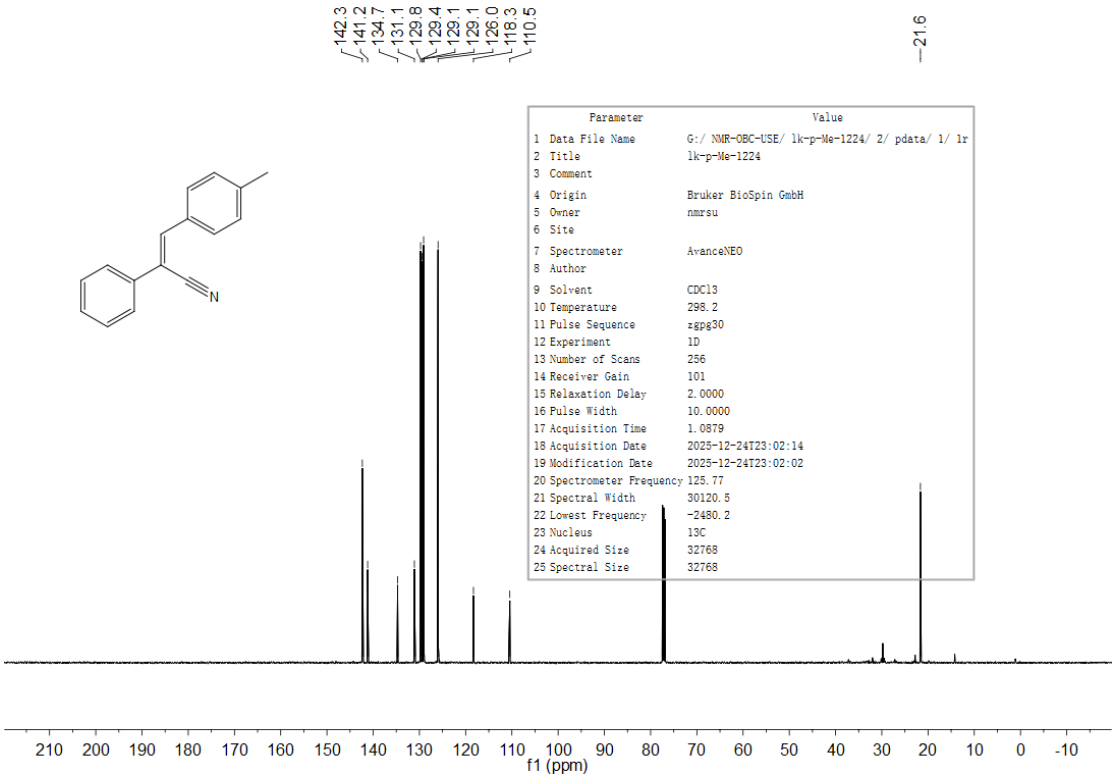
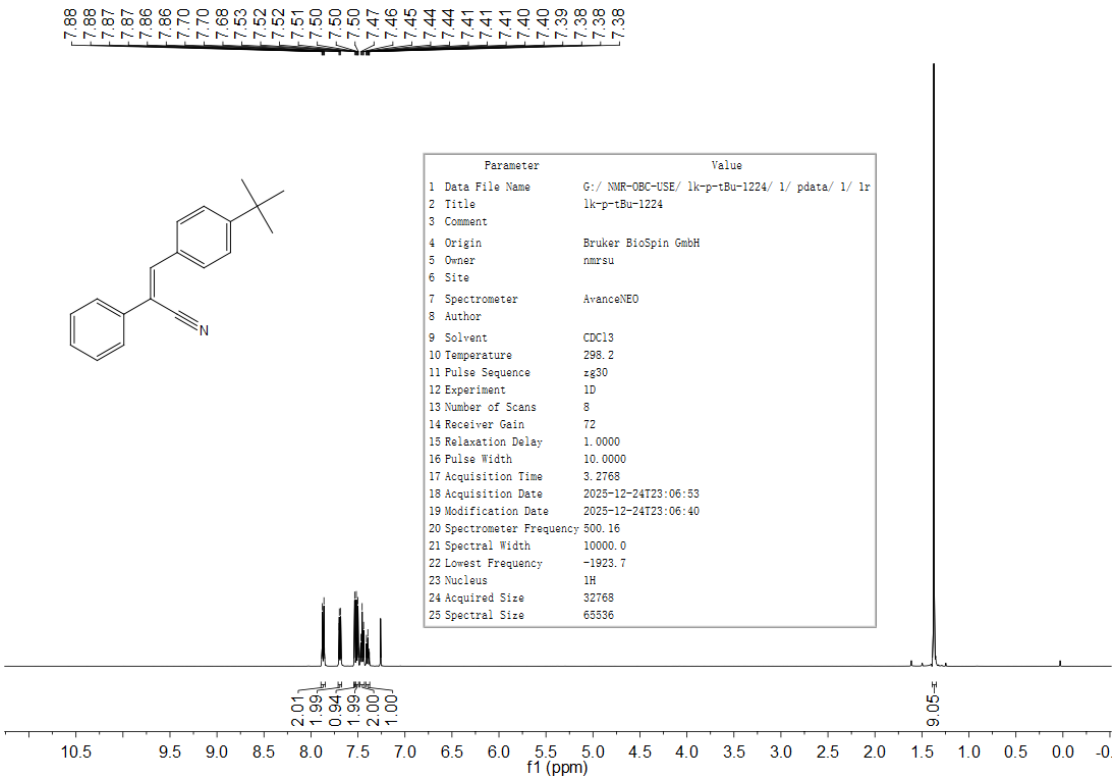
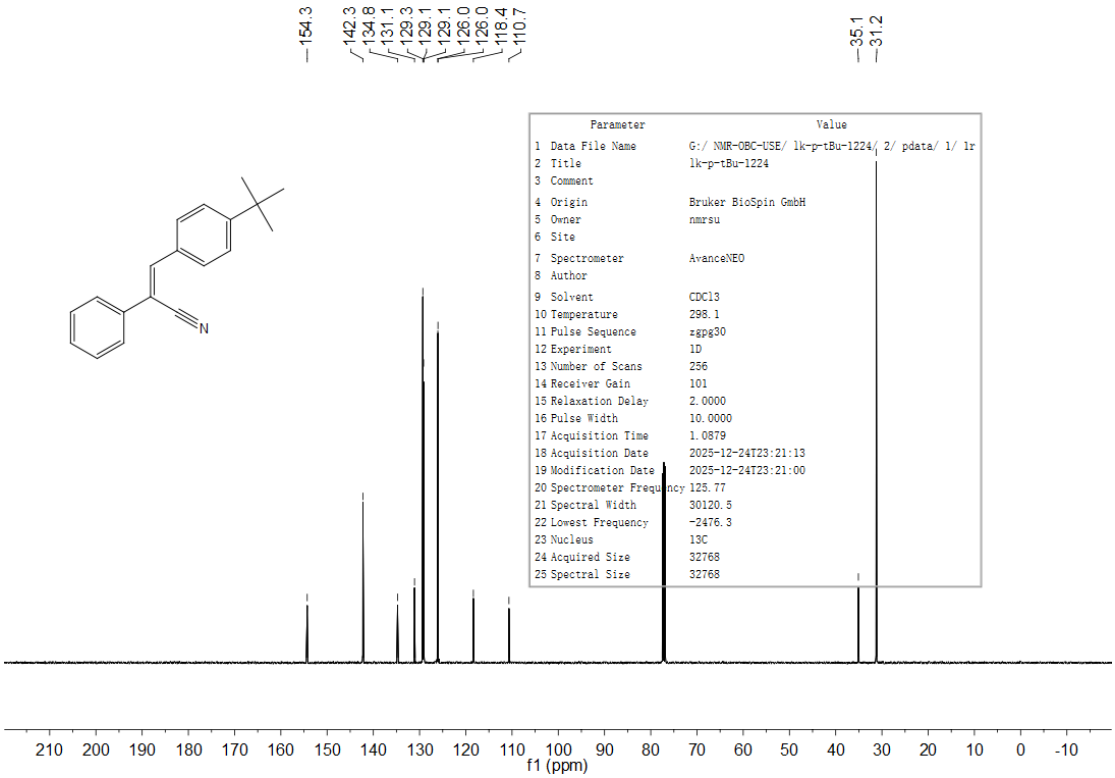
1 Data File Name	G:/ NMR-OBC-USE/ lk-p-Me-1224/ 1/ pdata/ 1/ 1r
2 Title	lk-p-Me-1224
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	45
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2025-12-24T22:48:02
19 Modification Date	2025-12-24T22:47:50
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1923.7
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

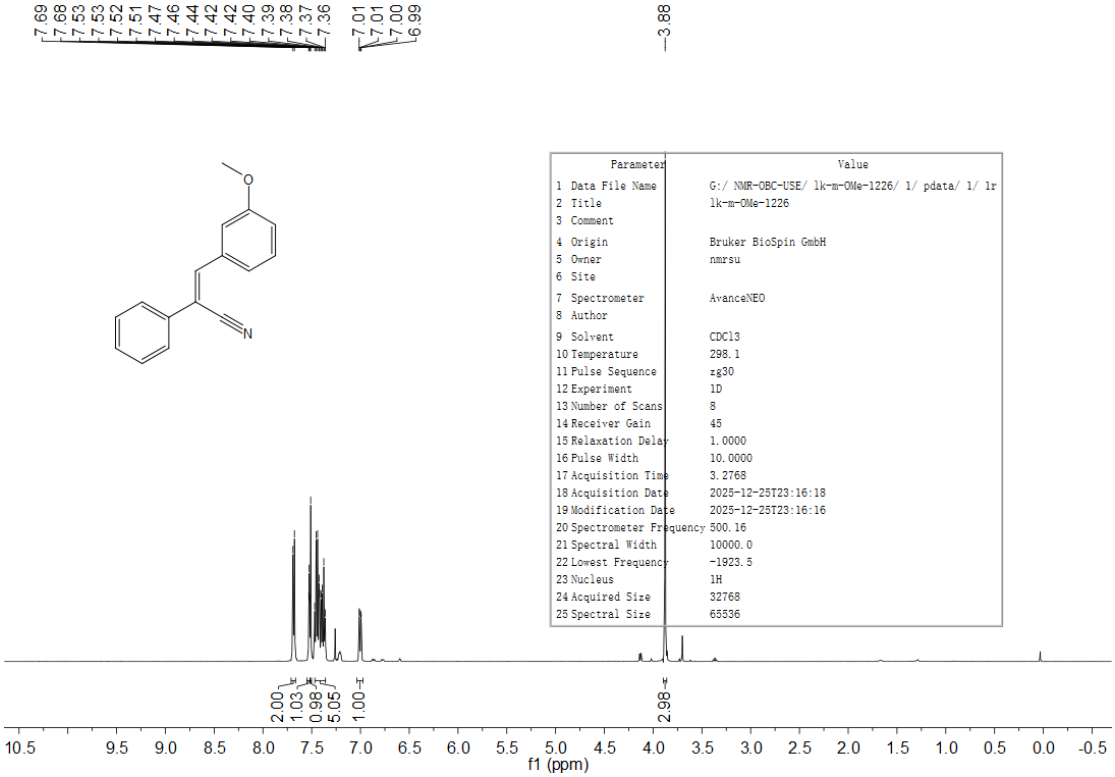


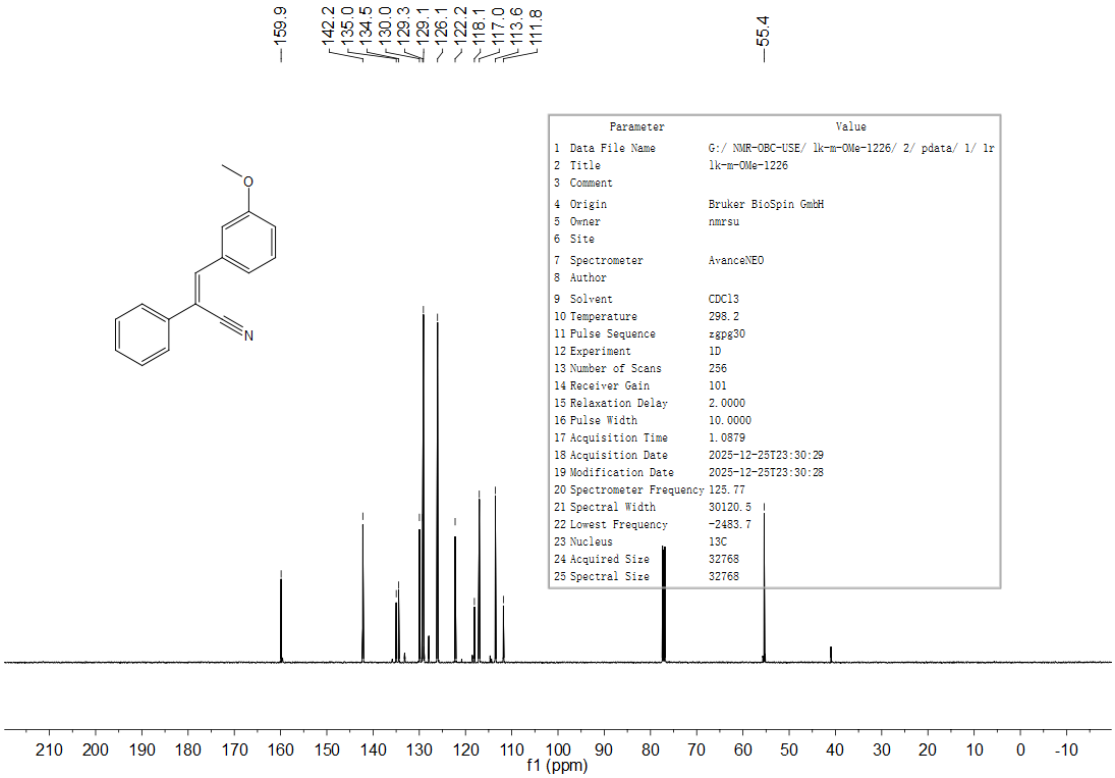
(*Z*)-3-(4-(*tert*-butyl)phenyl)-2-phenylacrylonitrile (3ae)



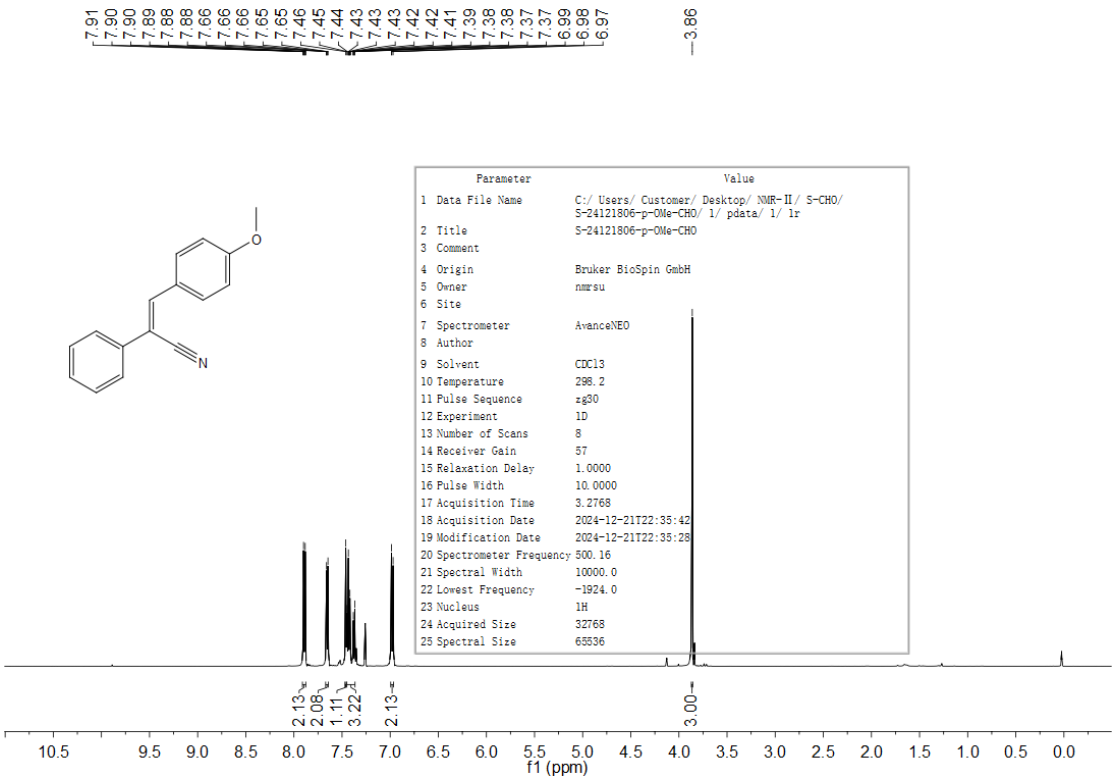


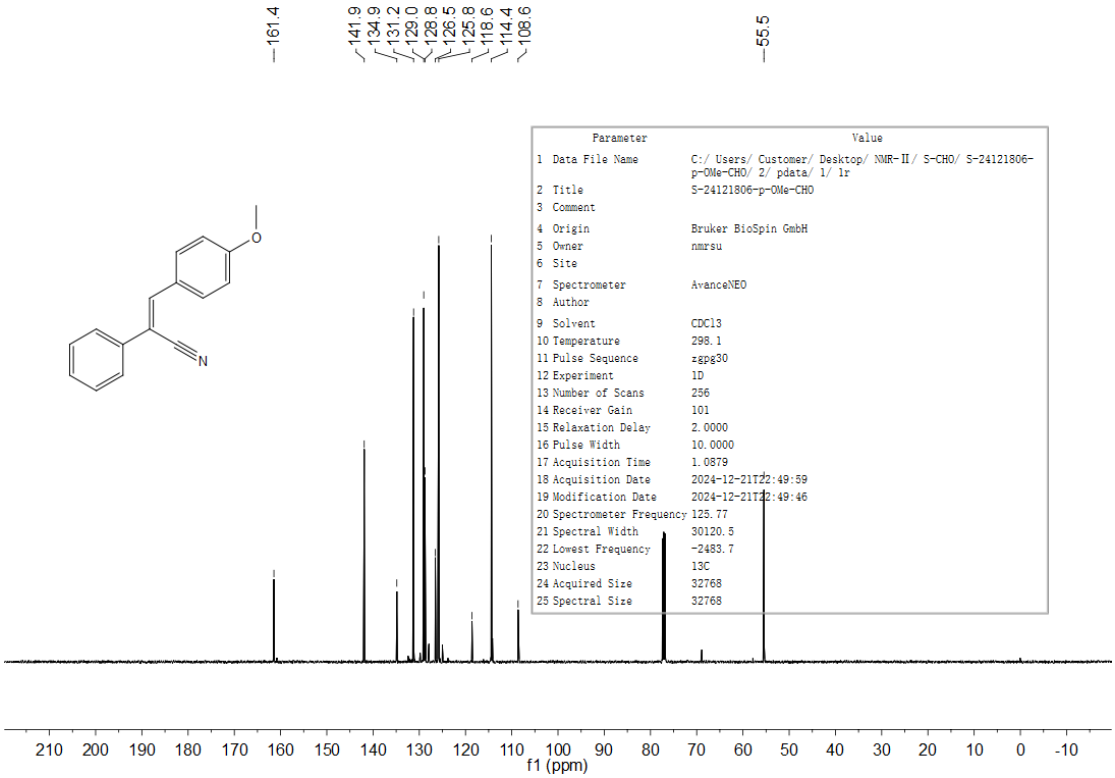
(*Z*)-3-(3-methoxyphenyl)-2-phenylacrylonitrile (3af)



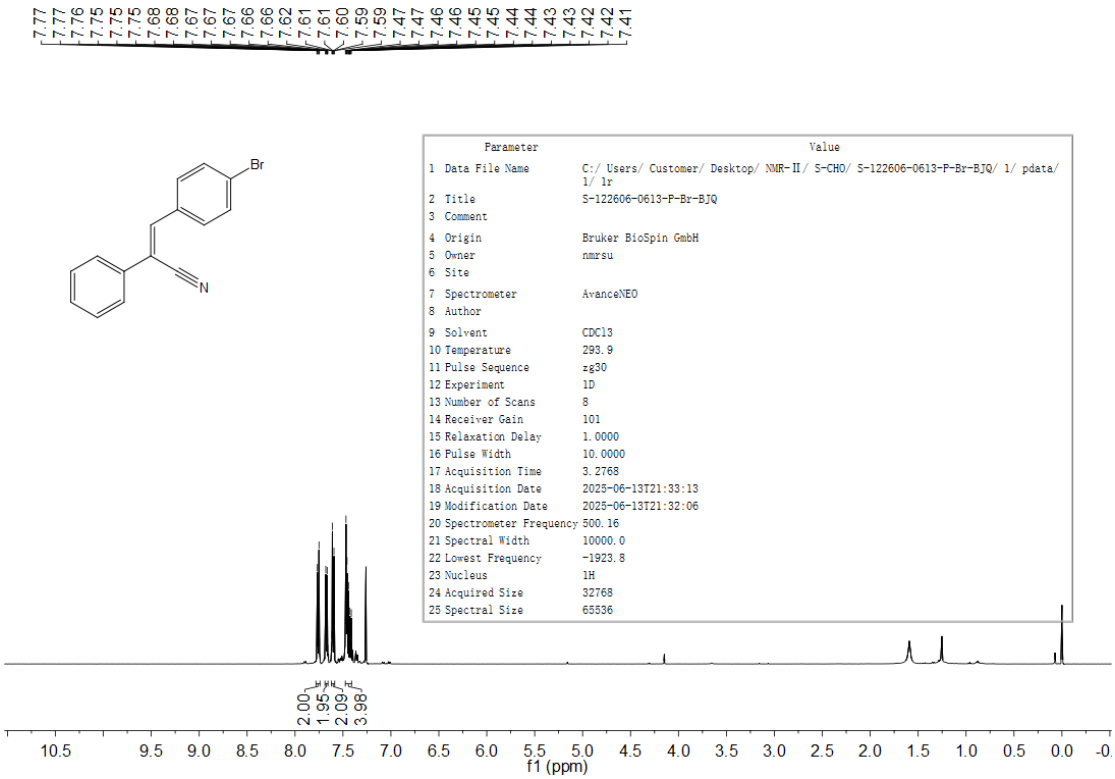


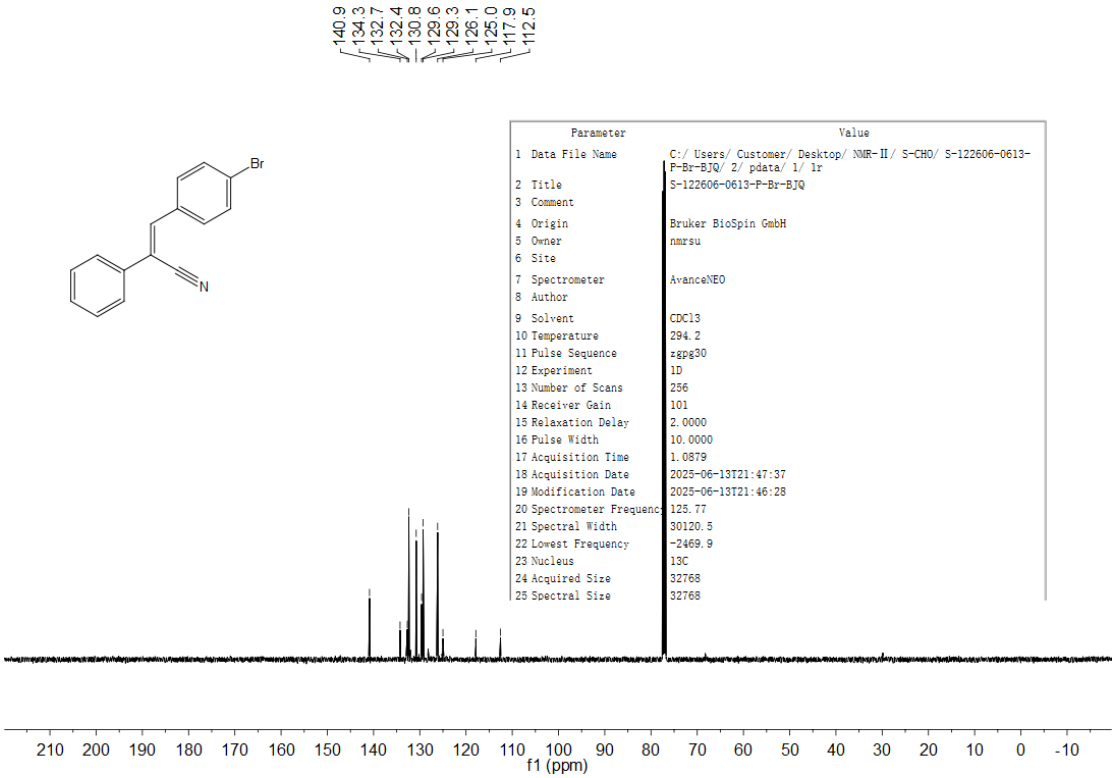
(*Z*)-3-(4-methoxyphenyl)-2-phenylacrylonitrile (3ag)



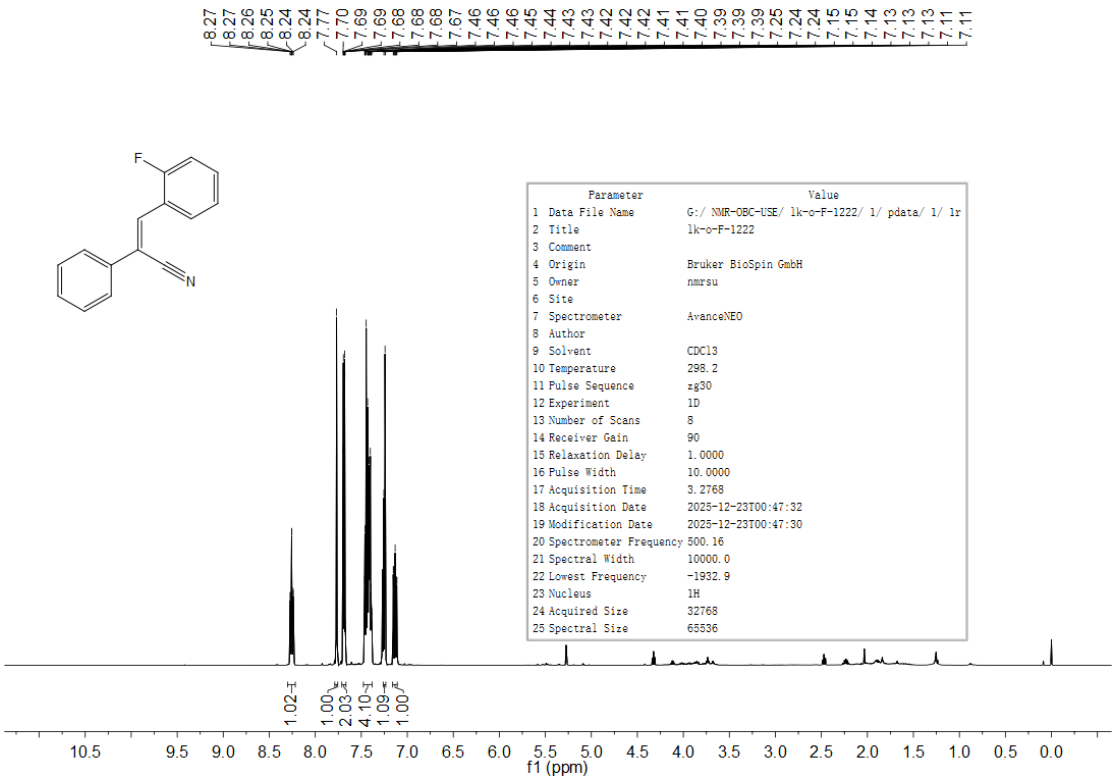


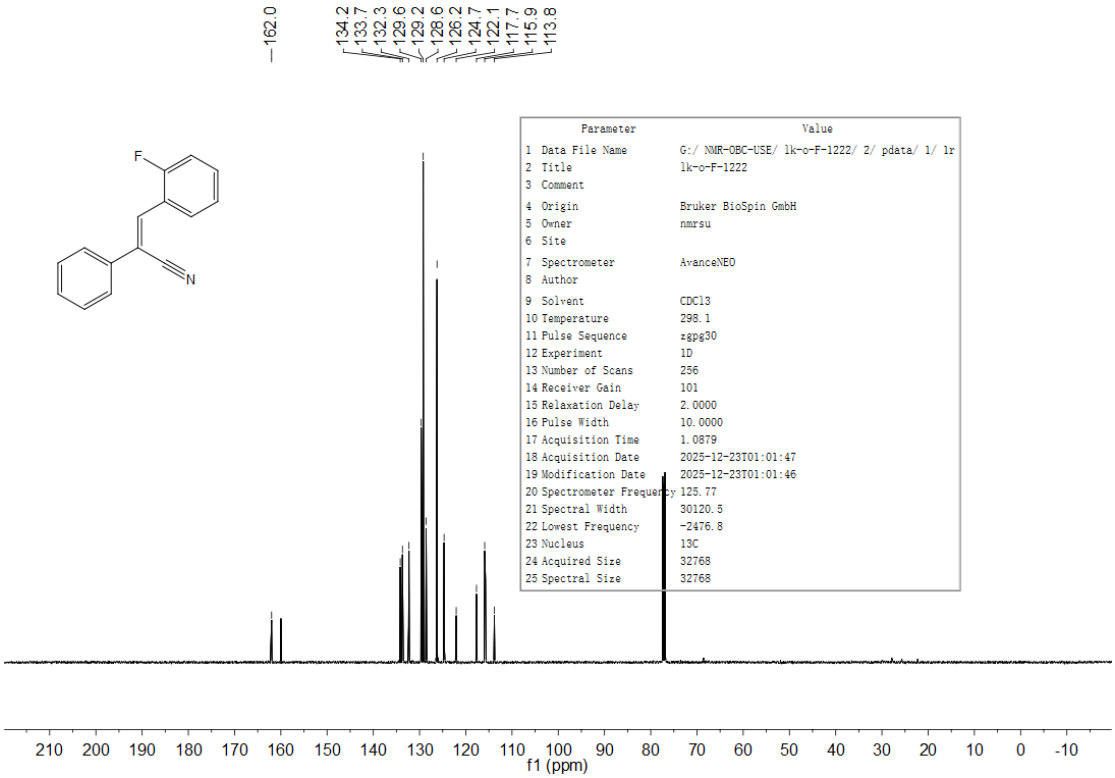
(*Z*)-3-(4-bromophenyl)-2-phenylacrylonitrile (3ah)

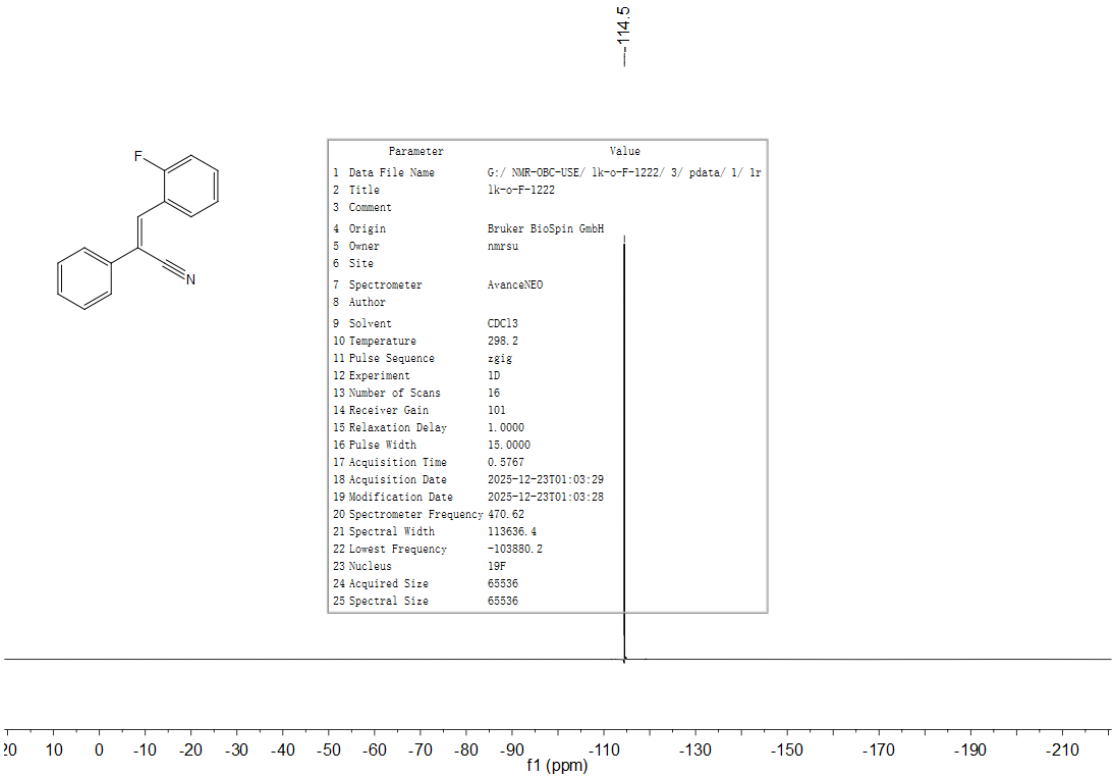




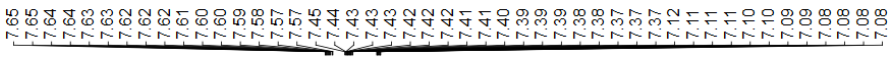
(*Z*)-3-(2-fluorophenyl)-2-phenylacrylonitrile (3ai)

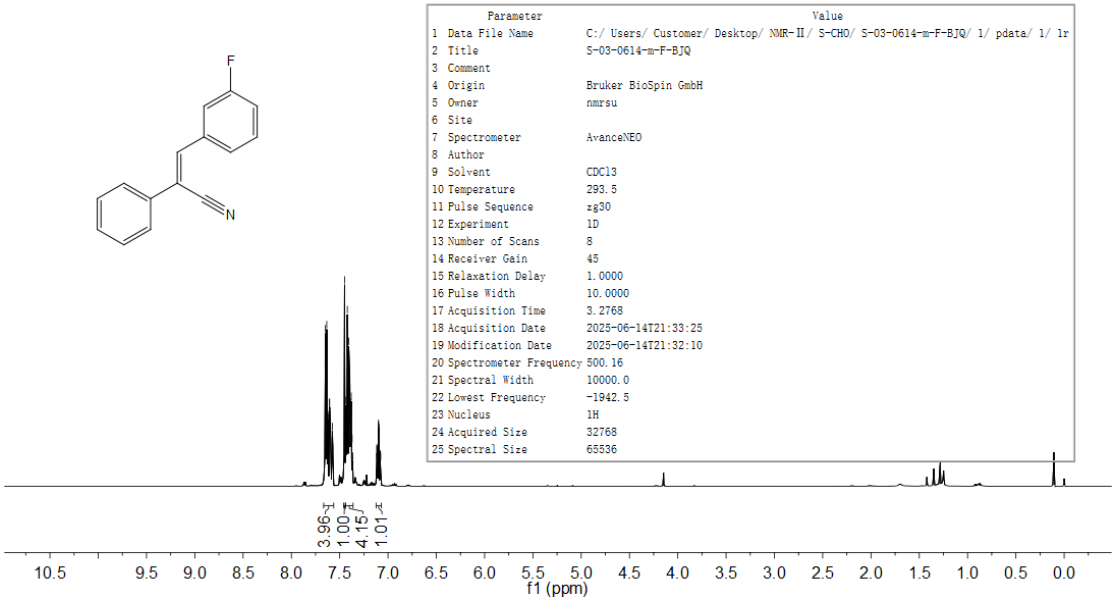




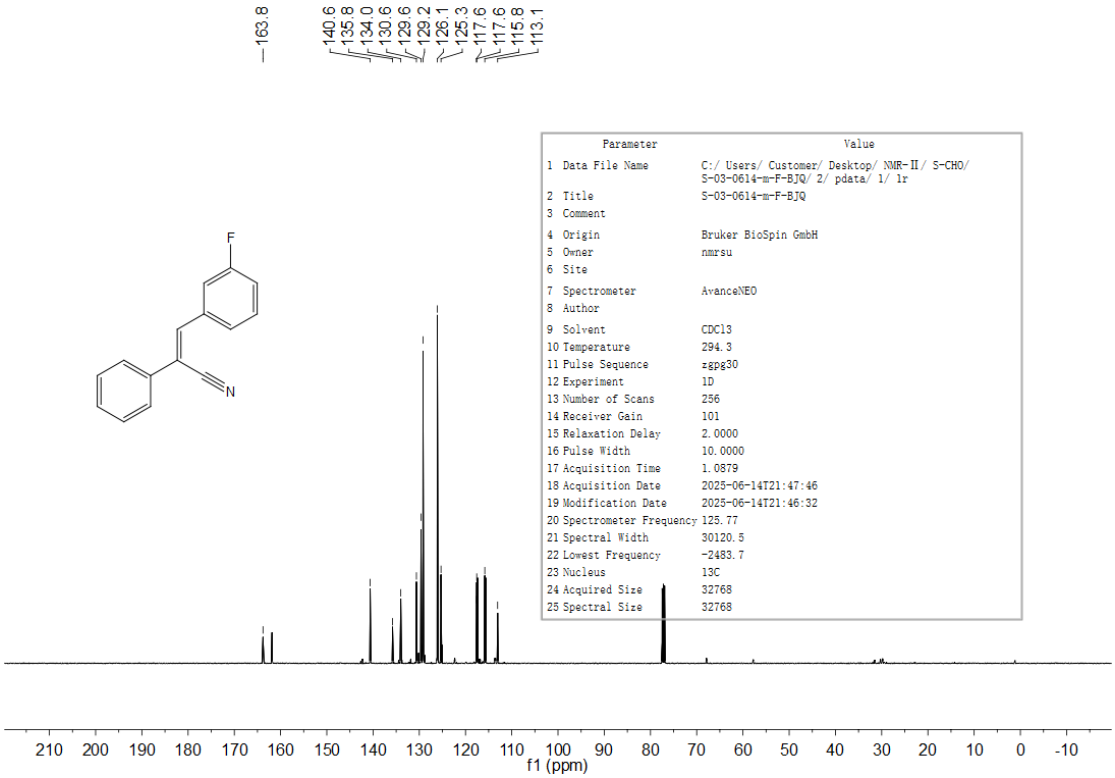


(*Z*)-3-(3-fluorophenyl)-2-phenylacrylonitrile (3aj)

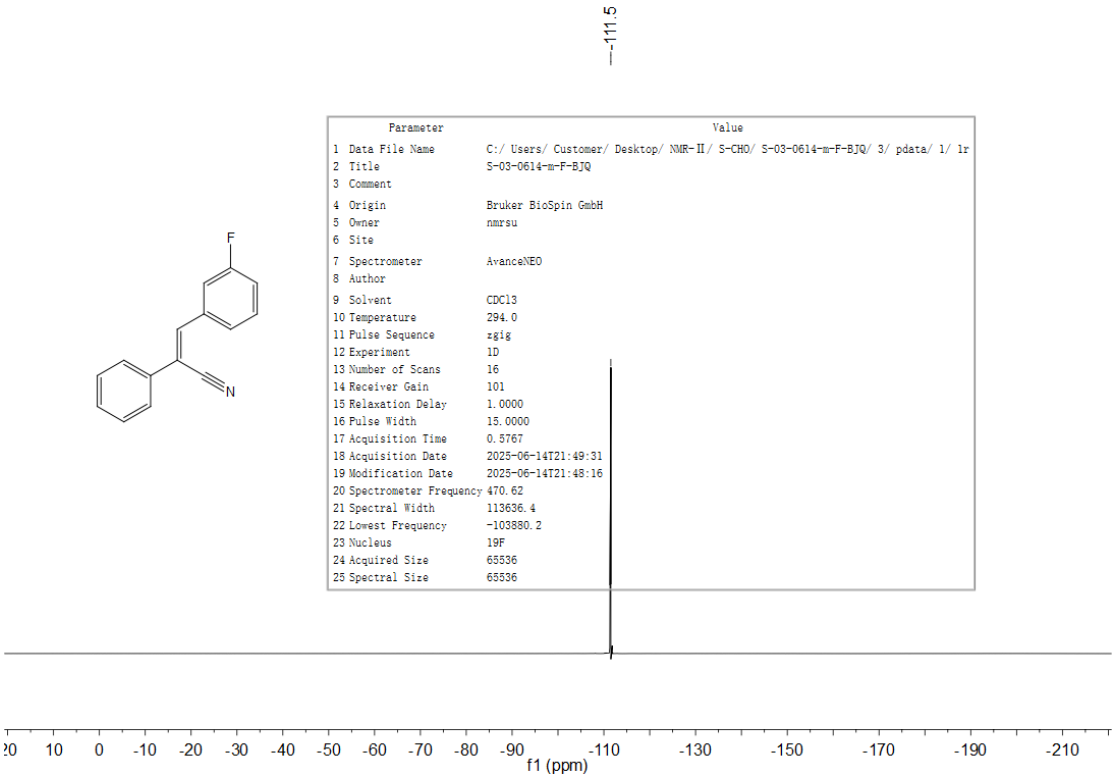




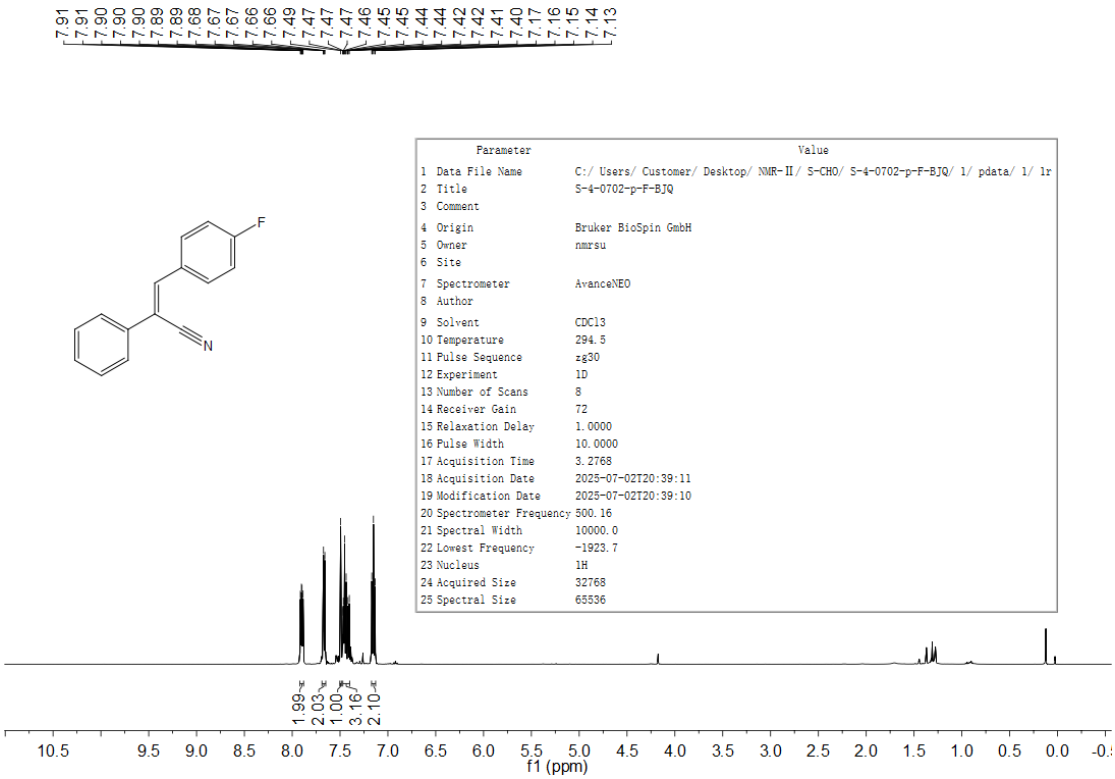
Parameter	Value
1 Data File Name	C:/ Users/ Customer/ Desktop/ NMR-Ⅱ/ S-CHO/ S-03-0614-m-F-BJQ/ 1/ pdata/ 1/ 1r
2 Title	S-03-0614-m-F-BJQ
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	293.5
11 Pulse Sequence	zg30
12 Experiment	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	2025-06-14T21:33:25
19 Modification Date	2025-06-14T21:32:10
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1942.5
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

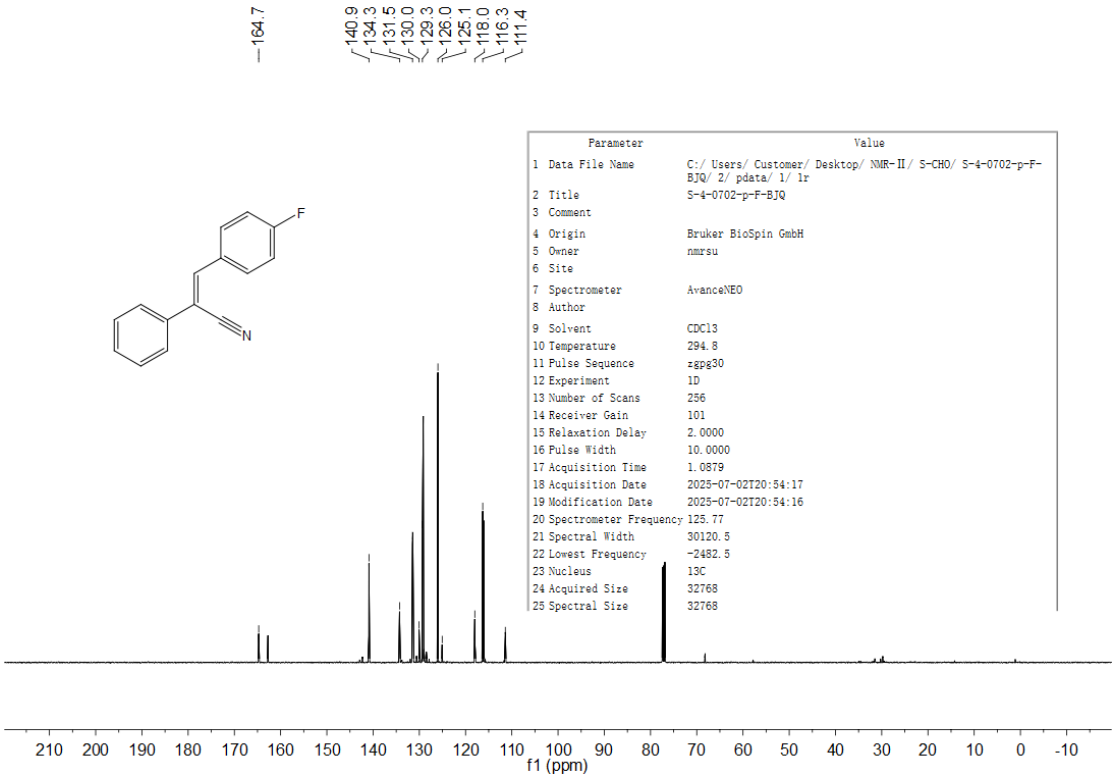


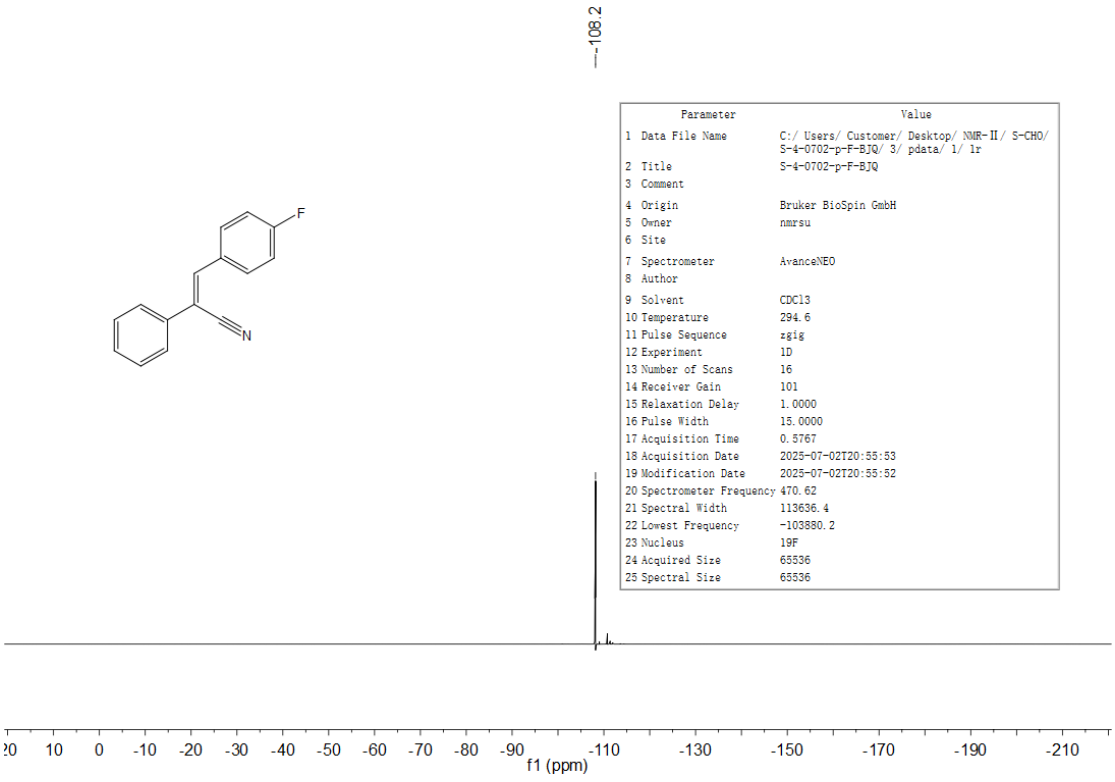
Parameter	Value
1 Data File Name	C:/ Users/ Customer/ Desktop/ NMR-Ⅱ/ S-CHO/ S-03-0614-m-F-BJQ/ 2/ pdata/ 1/ 1r
2 Title	S-03-0614-m-F-BJQ
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	294.3
11 Pulse Sequence	zgpg30
12 Experiment	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	2025-06-14T21:47:46
19 Modification Date	2025-06-14T21:46:32
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



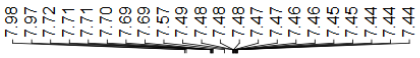
(*Z*)-3-(4-fluorophenyl)-2-phenylacrylonitrile (3ak)

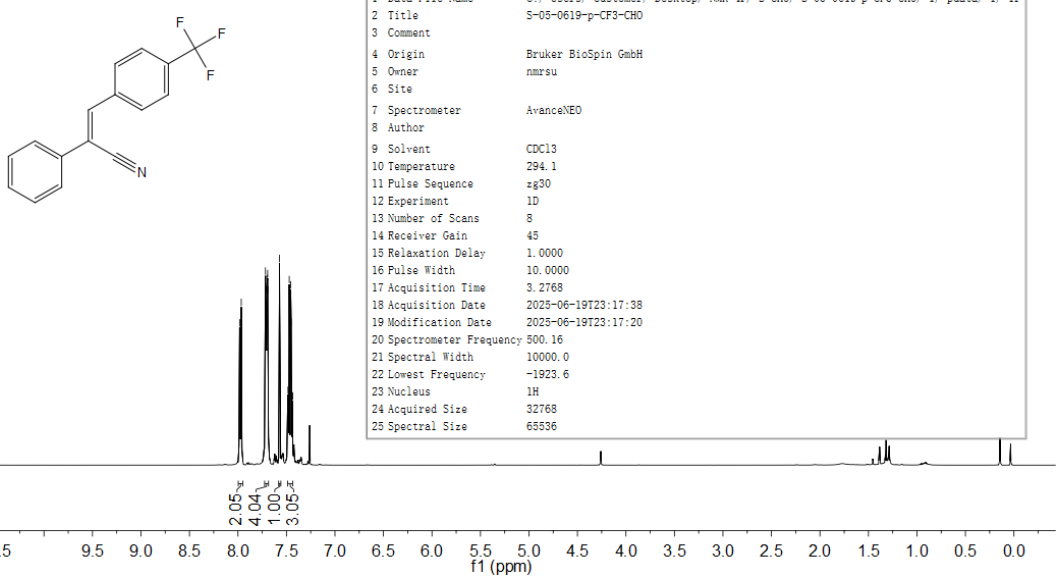




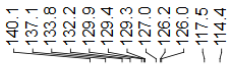


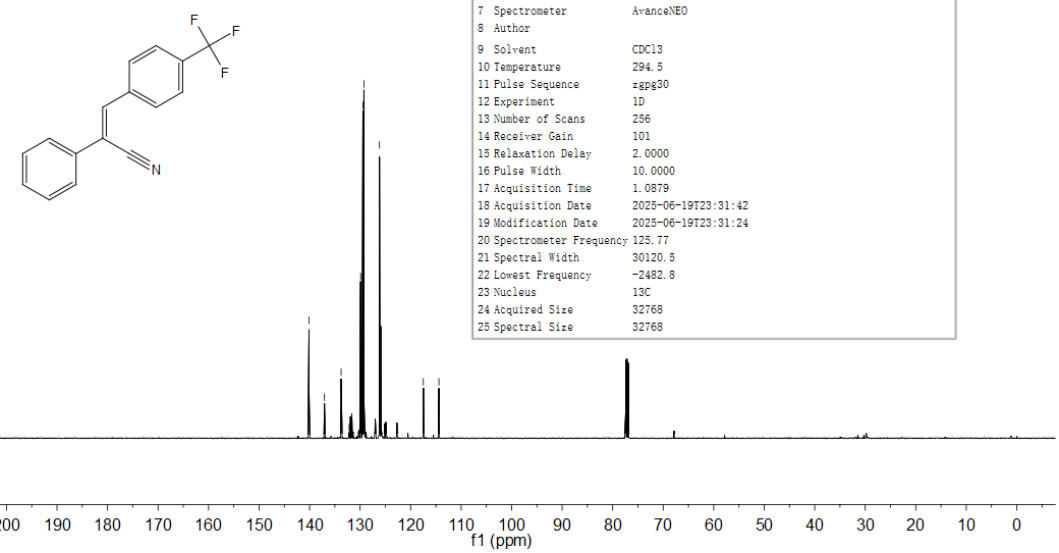
(*Z*)-2-phenyl-3-(4-(trifluoromethyl)phenyl)acrylonitrile (3al)



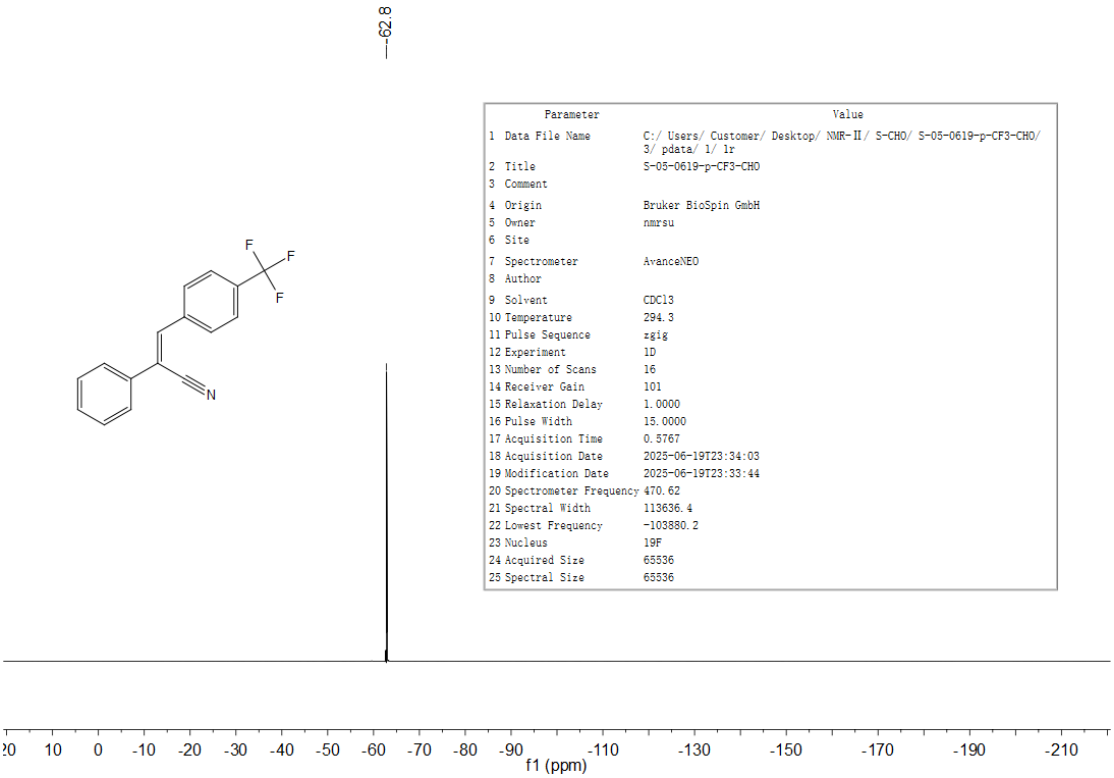


Parameter	Value
1 Data File Name	C:/ Users/ Customer/ Desktop/ NMR-Ⅱ/ S-CHO/ S-05-0619-p-CF3-CHO/ 1/ pdata/ 1/ 1r
2 Title	S-05-0619-p-CF3-CHO
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	294.1
11 Pulse Sequence	zg30
12 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	2025-06-19T23:17:38
19 Modification Date	2025-06-19T23:17:20
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



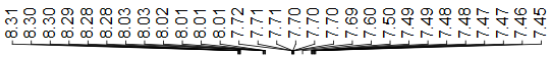


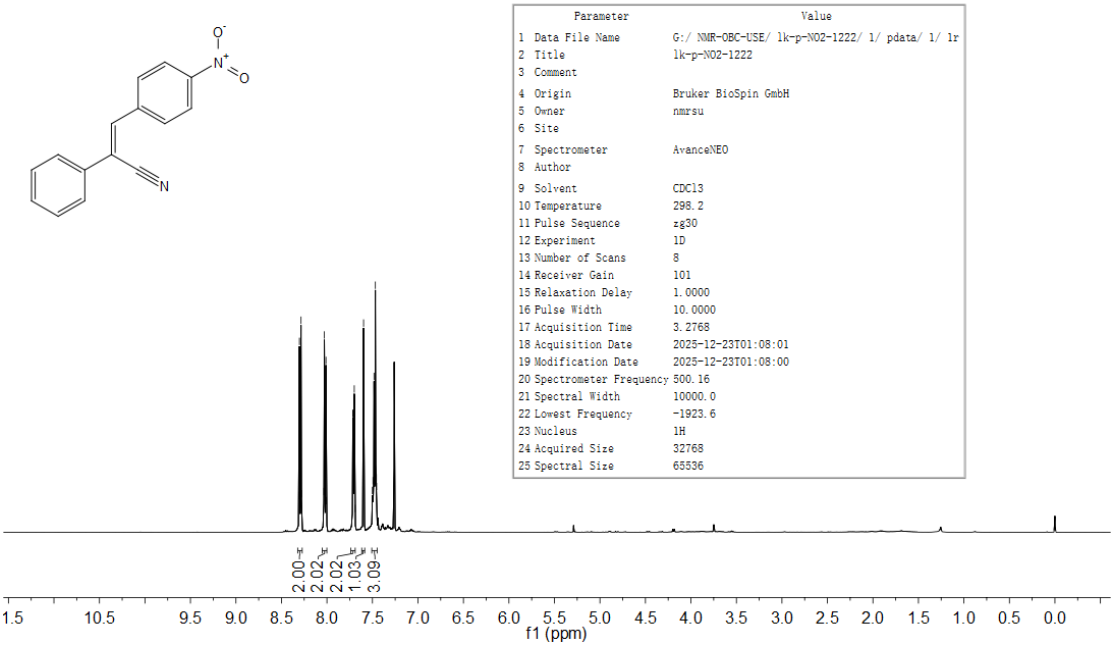
Parameter	Value
1 Data File Name	C:/ Users/ Customer/ Desktop/ NMR-Ⅱ/ S-CHO/ S-05-0619-p-CF3-CHO/ 2/ pdata/ 1/ 1r
2 Title	S-05-0619-p-CF3-CHO
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	294.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2025-06-19T23:31:42
19 Modification Date	2025-06-19T23:31:24
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



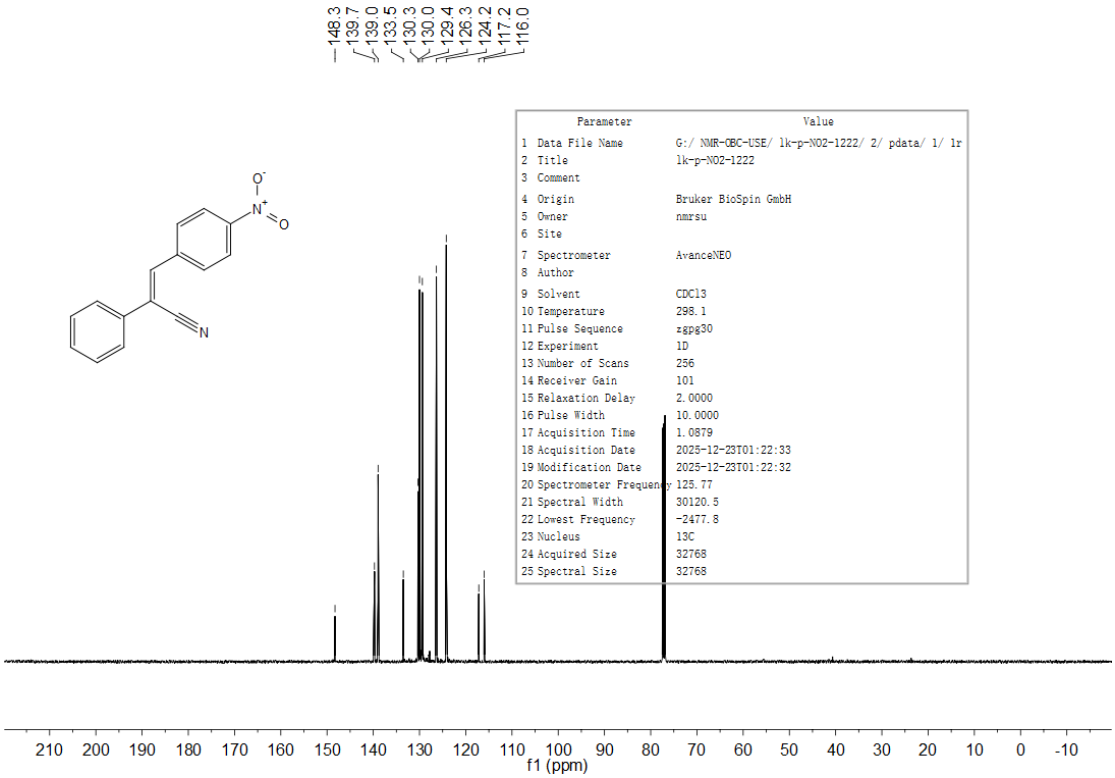
Parameter	Value
1 Data File Name	C:/ Users/ Customer/ Desktop/ NMR-Ⅱ/ S-CHO/ S-05-0619-p-CF3-CHO/ 3/ pdata/ 1/ 1r
2 Title	S-05-0619-p-CF3-CHO
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	294.3
11 Pulse Sequence	zgig
12 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	2025-06-19T23:34:03
19 Modification Date	2025-06-19T23:33:44
20 Spectrometer Frequency	470.62
21 Spectral Width	113636.4
22 Lowest Frequency	-103880.2
23 Nucleus	19F
24 Acquired Size	65536
25 Spectral Size	65536

(*Z*)-3-(4-nitrophenyl)-2-phenylacrylonitrile (3am)

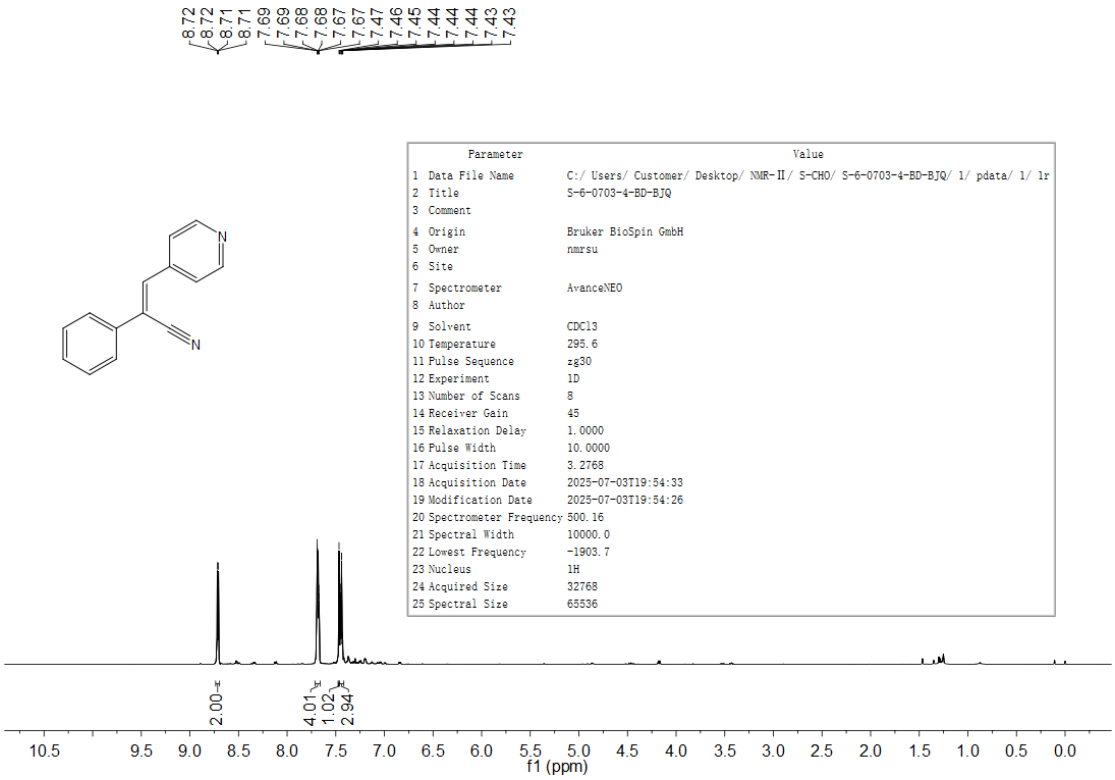


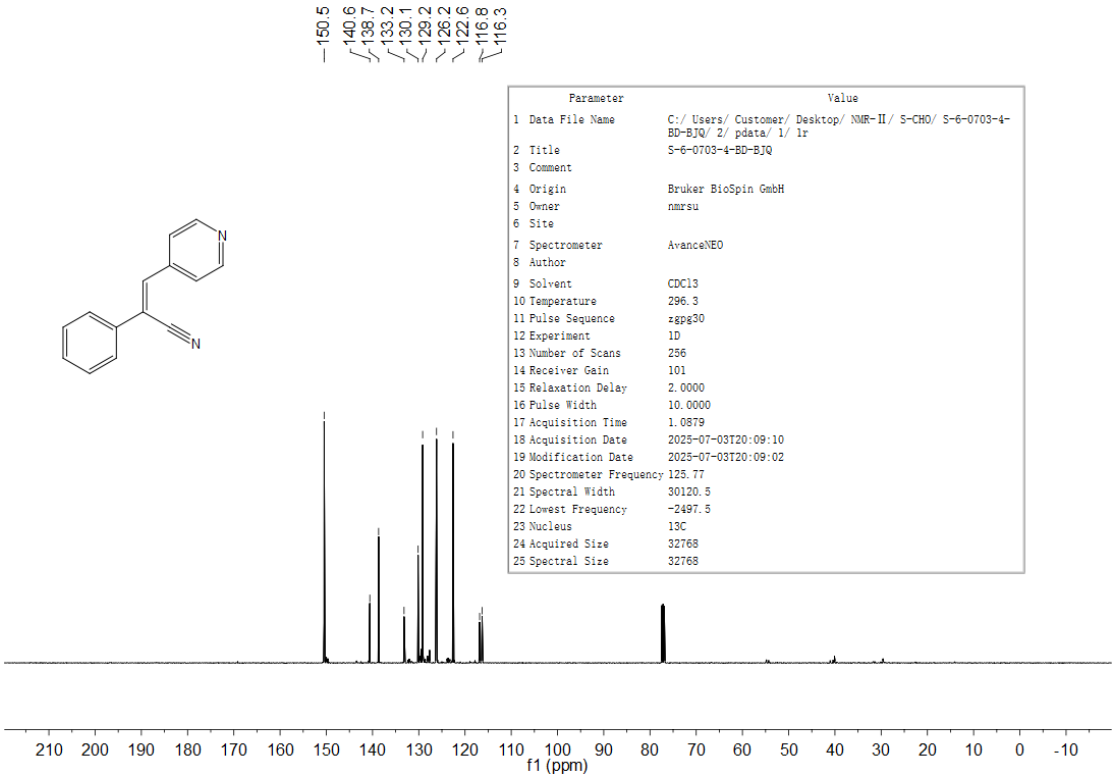


Parameter	Value
1 Data File Name	G:/ NMR-OBC-USE/ lk-p-NO2-1222/ 1/ pdata/ 1/ 1r
2 Title	lk-p-NO2-1222
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2025-12-23T01:08:01
19 Modification Date	2025-12-23T01:08:00
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



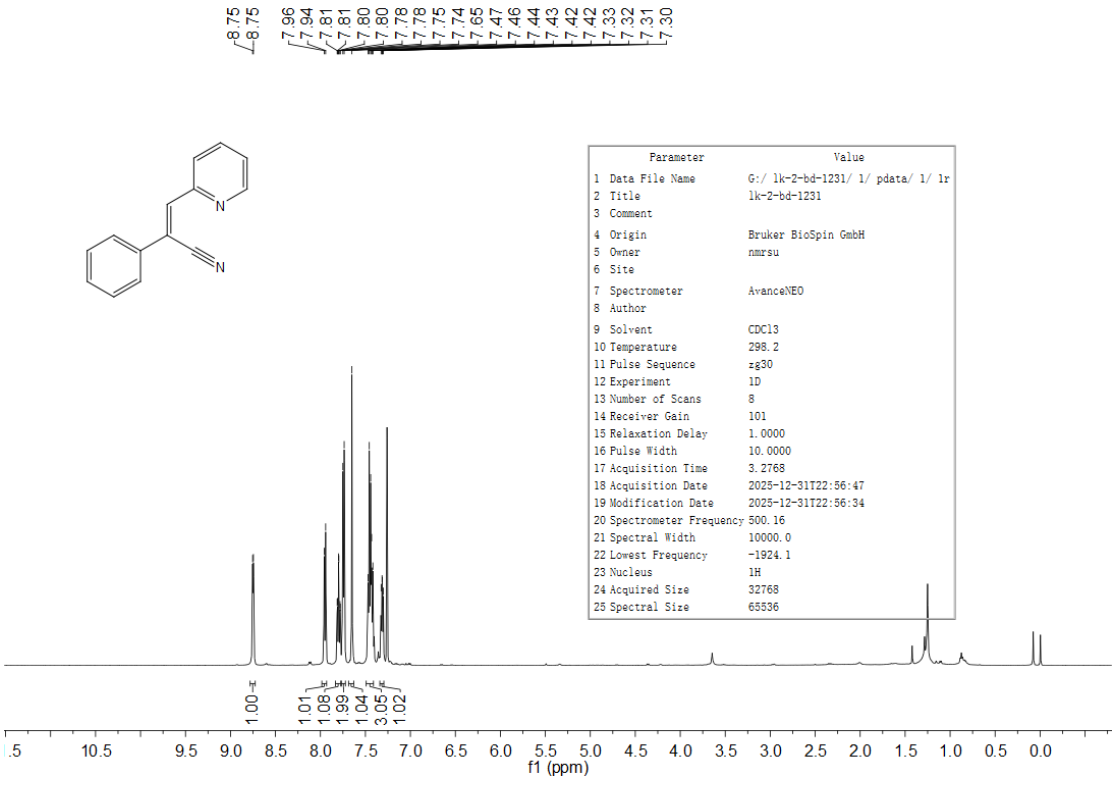
(*Z*)-2-phenyl-3-(pyridin-4-yl)acrylonitrile (3aq)



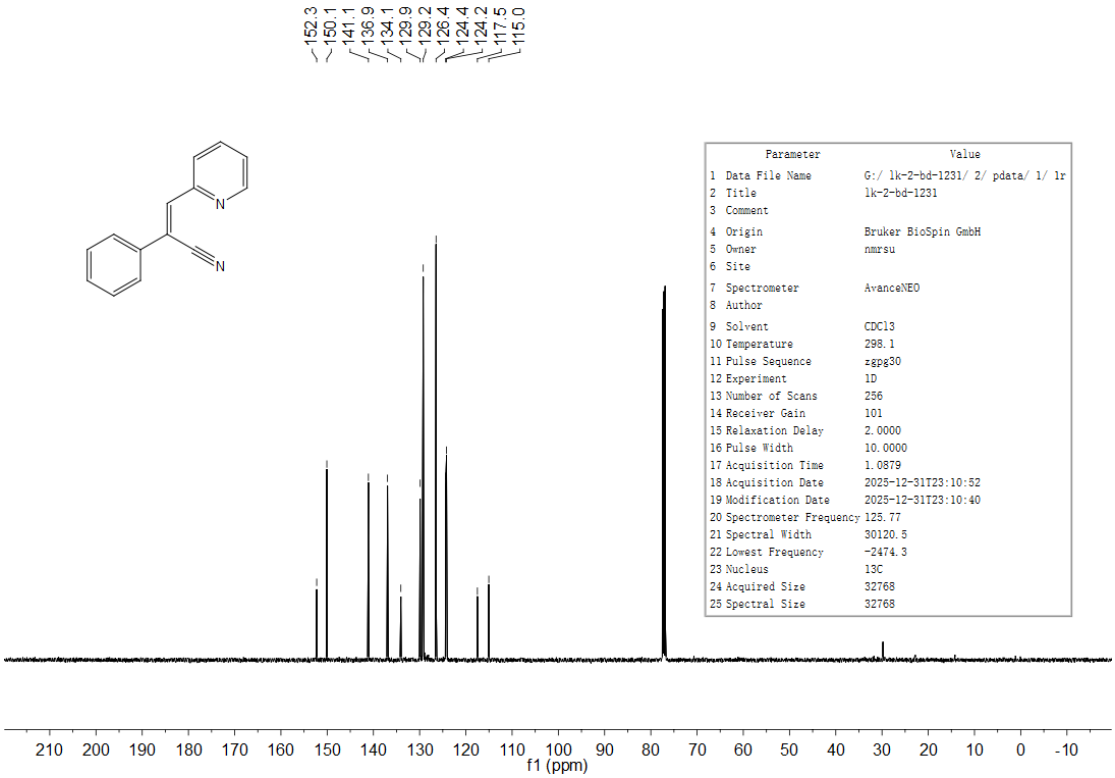


Parameter	Value
1 Data File Name	C:/ Users/ Customer/ Desktop/ NMR-II/ S-CHO/ S-6-0703-4-BD-BJQ/ 2/ pdata/ 1/ 1r
2 Title	S-6-0703-4-BD-BJQ
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	296.3
11 Pulse Sequence	zgpg30
12 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	2025-07-03T20:09:10
19 Modification Date	2025-07-03T20:09:02
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2497.5
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768

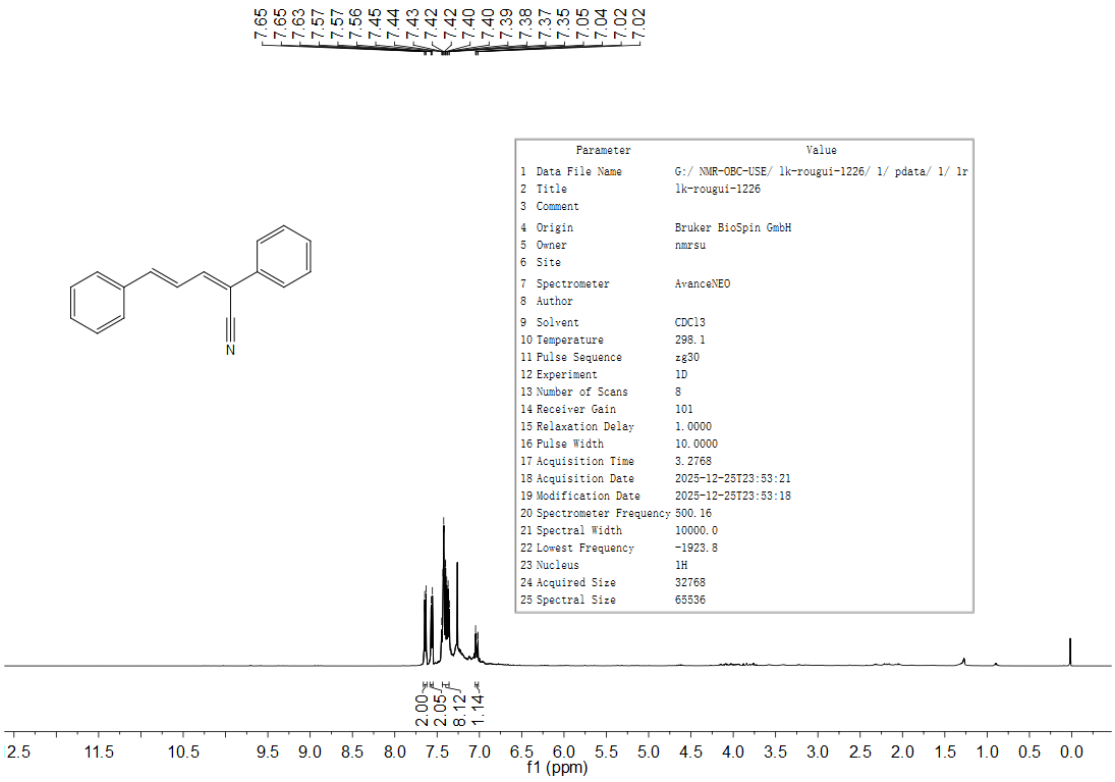
(*Z*)-2-phenyl-3-(pyridin-2-yl)acrylonitrile (3ar)

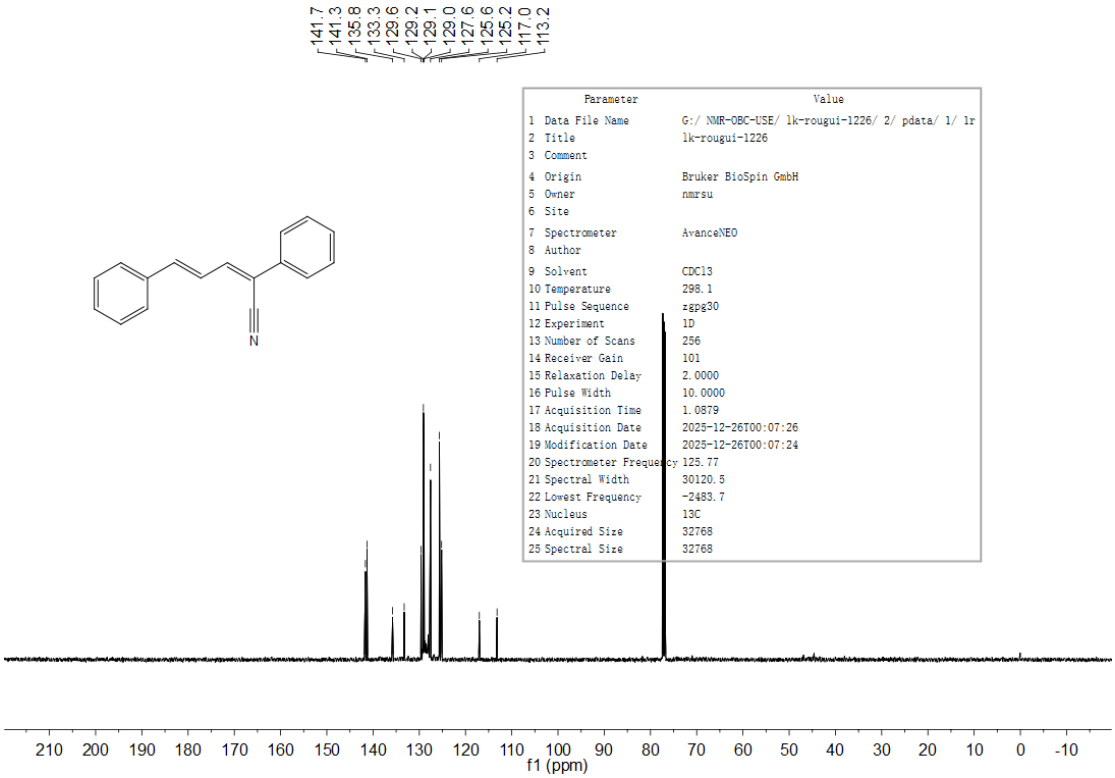


Parameter	Value
1 Data File Name	G:/ lk-2-bd-1231/ 1/ pdata/ 1/ 1r
2 Title	lk-2-bd-1231
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2025-12-31T22:56:47
19 Modification Date	2025-12-31T22:56:34
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1924.1
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

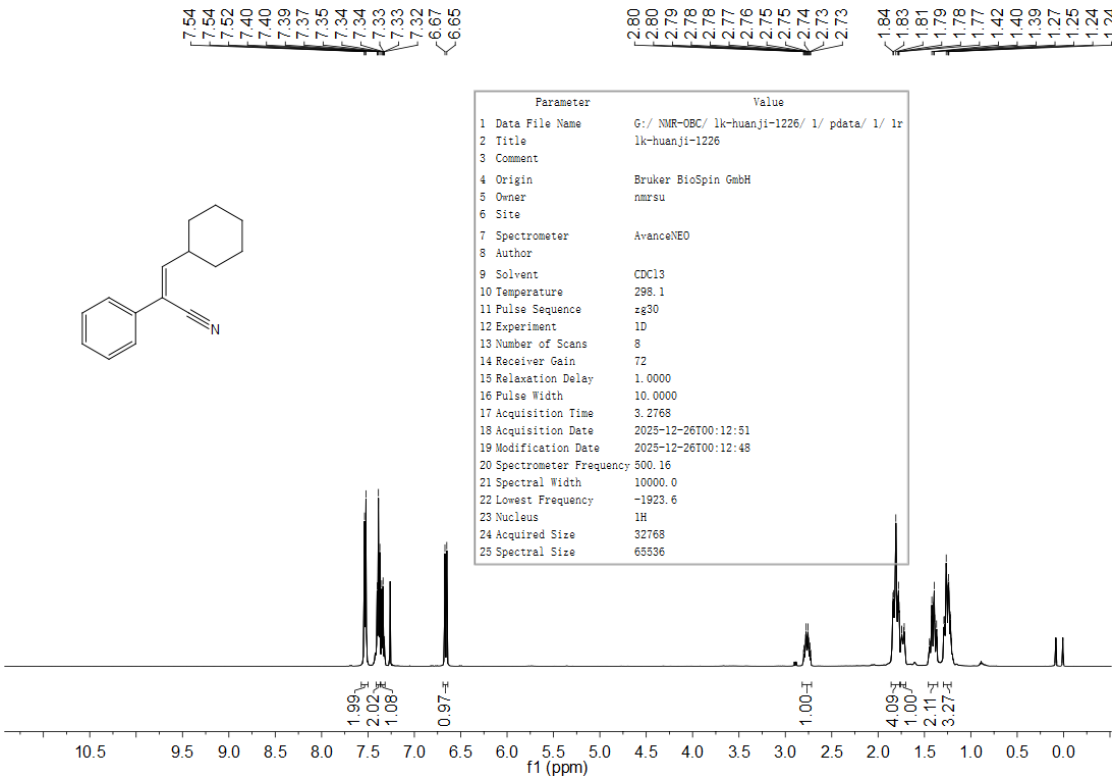


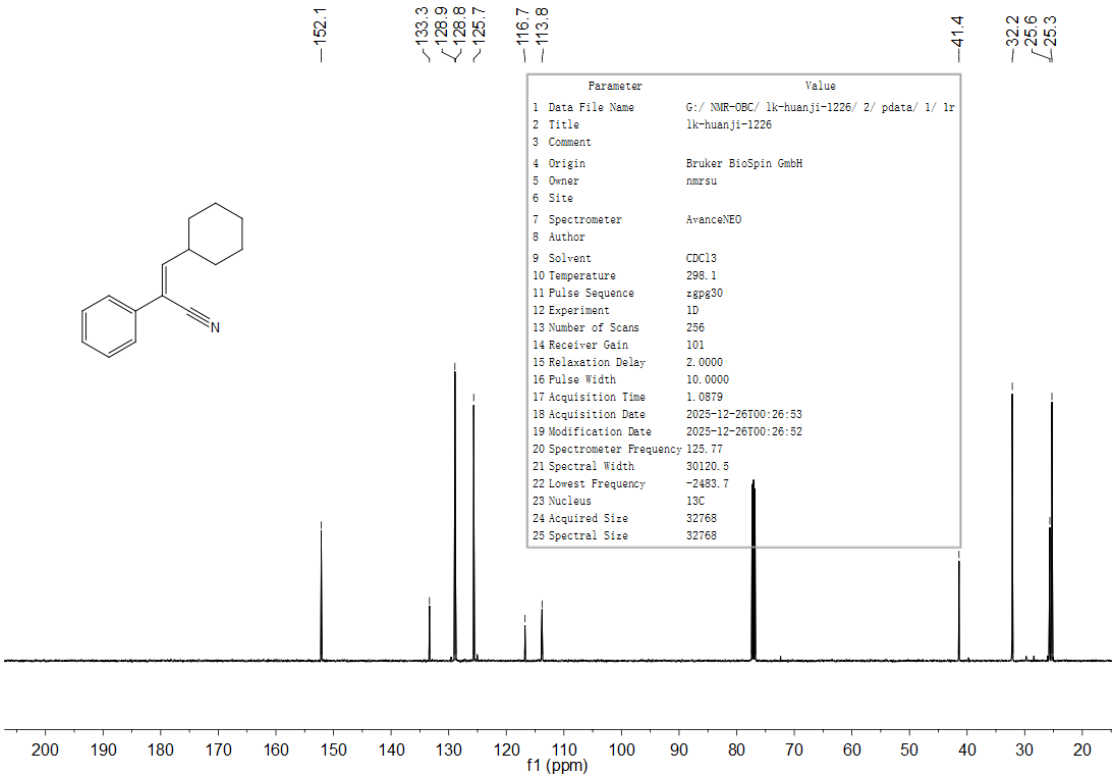
(2*Z*,4*E*)-2,5-diphenylpenta-2,4-dienenitrile (3as)



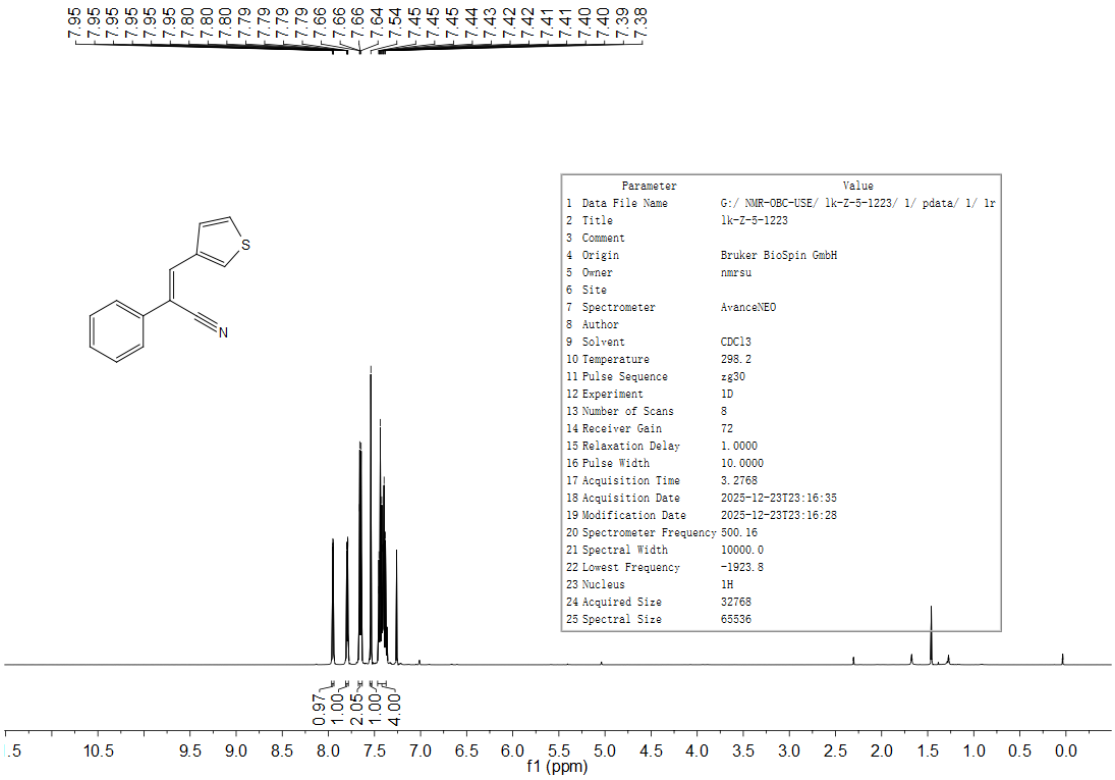


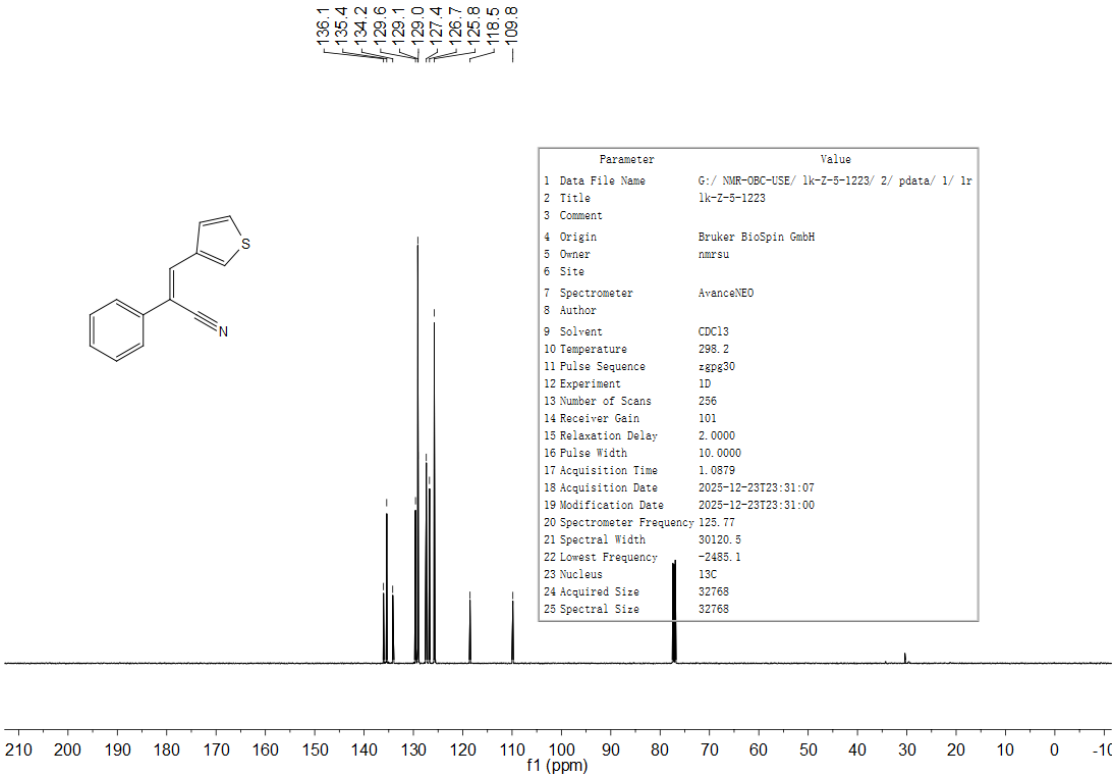
(*Z*)-3-cyclohexyl-2-phenylacrylonitrile (3at)



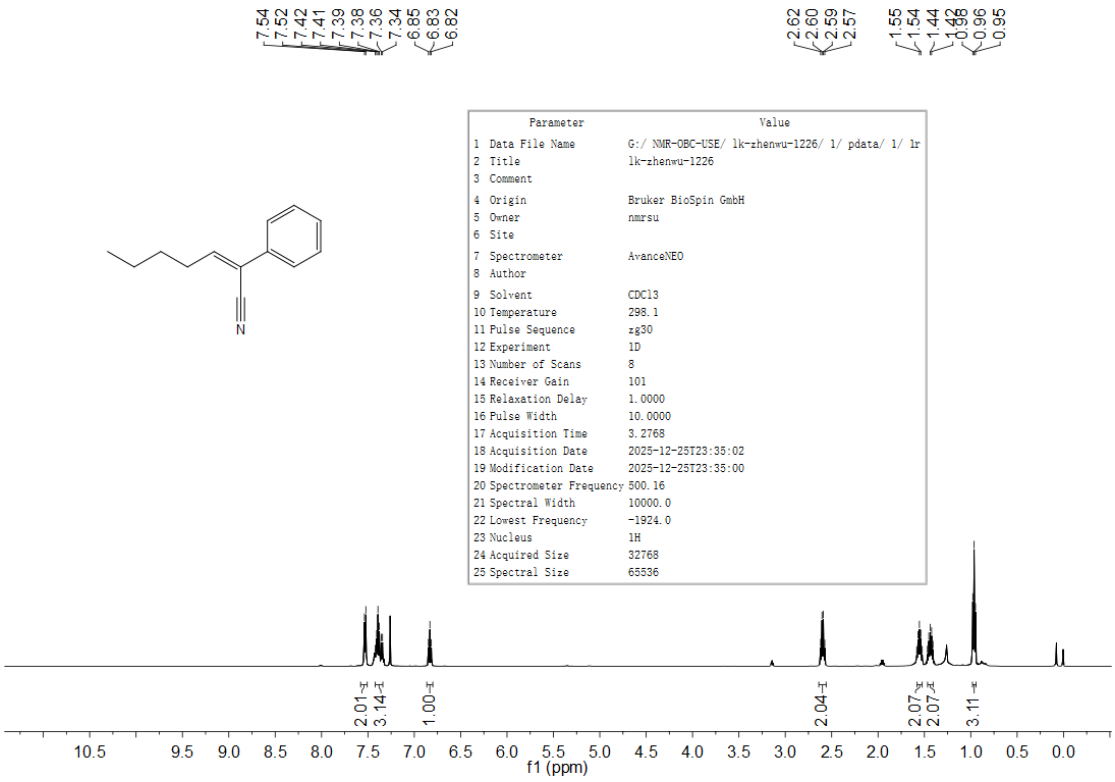


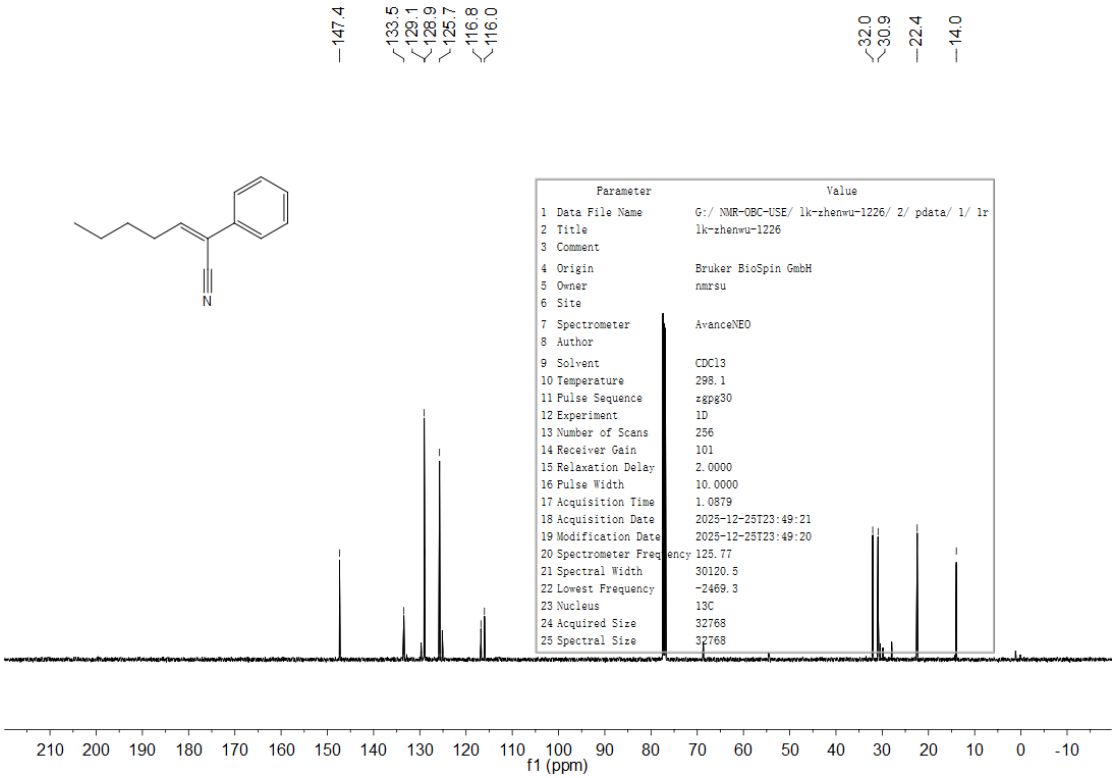
(*Z*)-2-phenyl-3-(thiophen-3-yl)acrylonitrile (3aw)



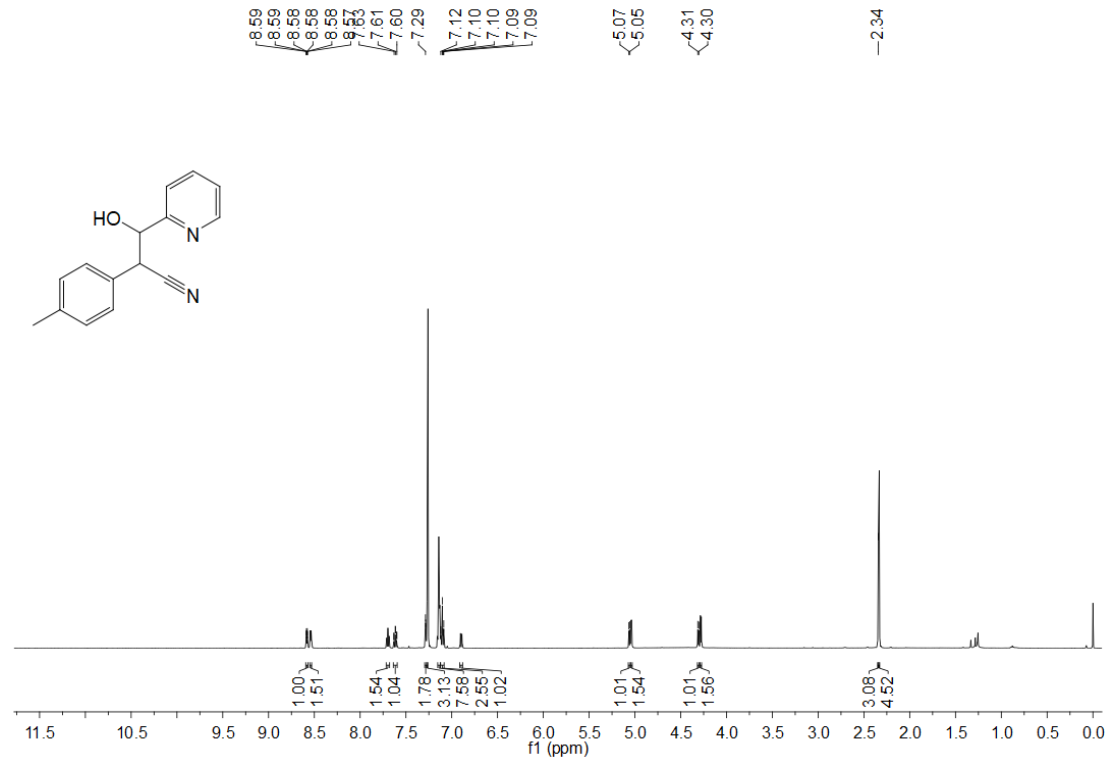


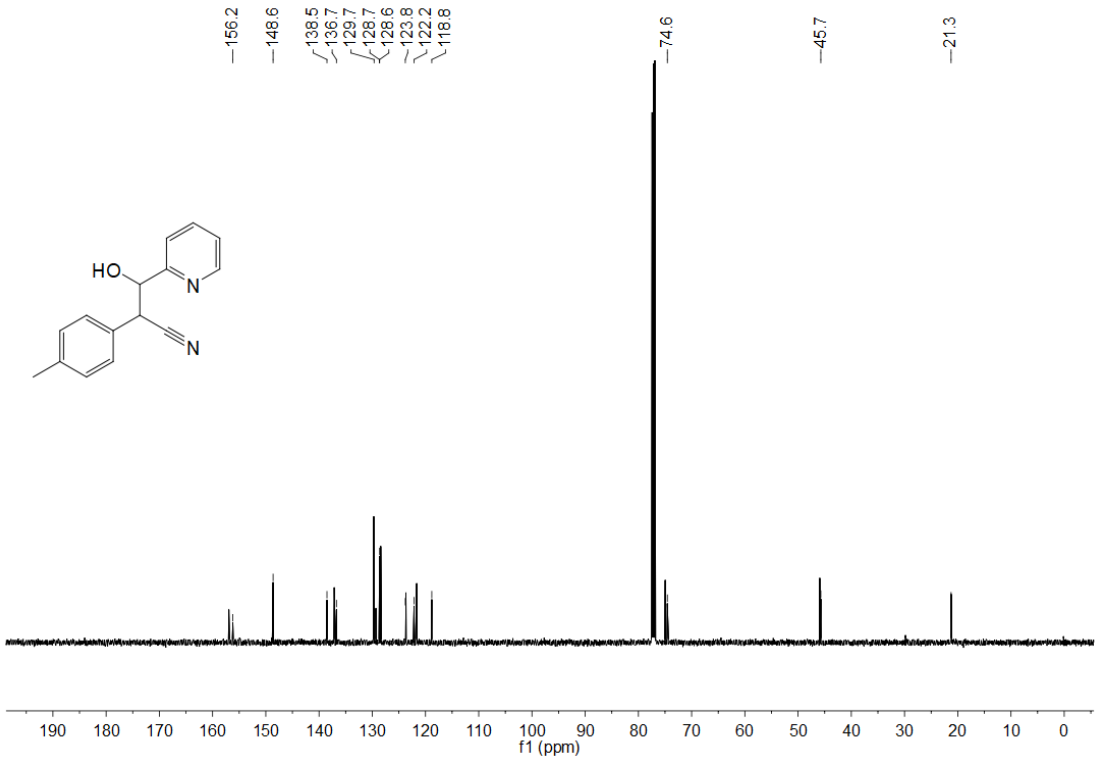
(*Z*)-2-phenylhept-2-enenitrile (3ax)



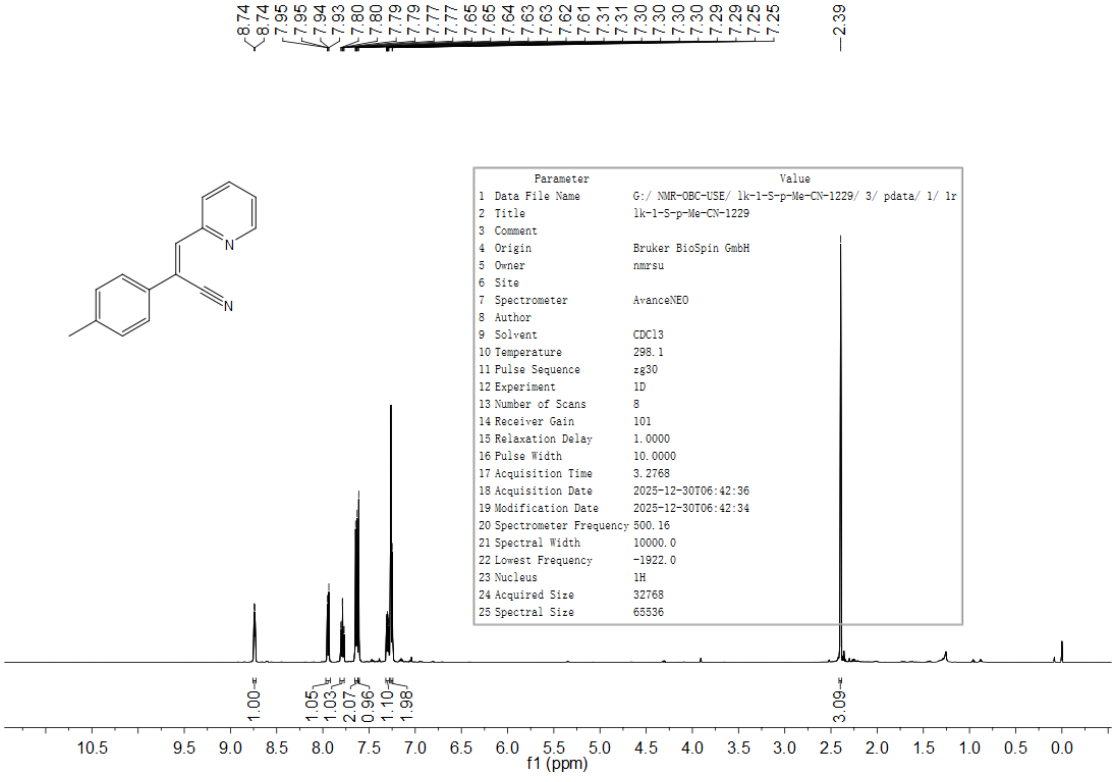


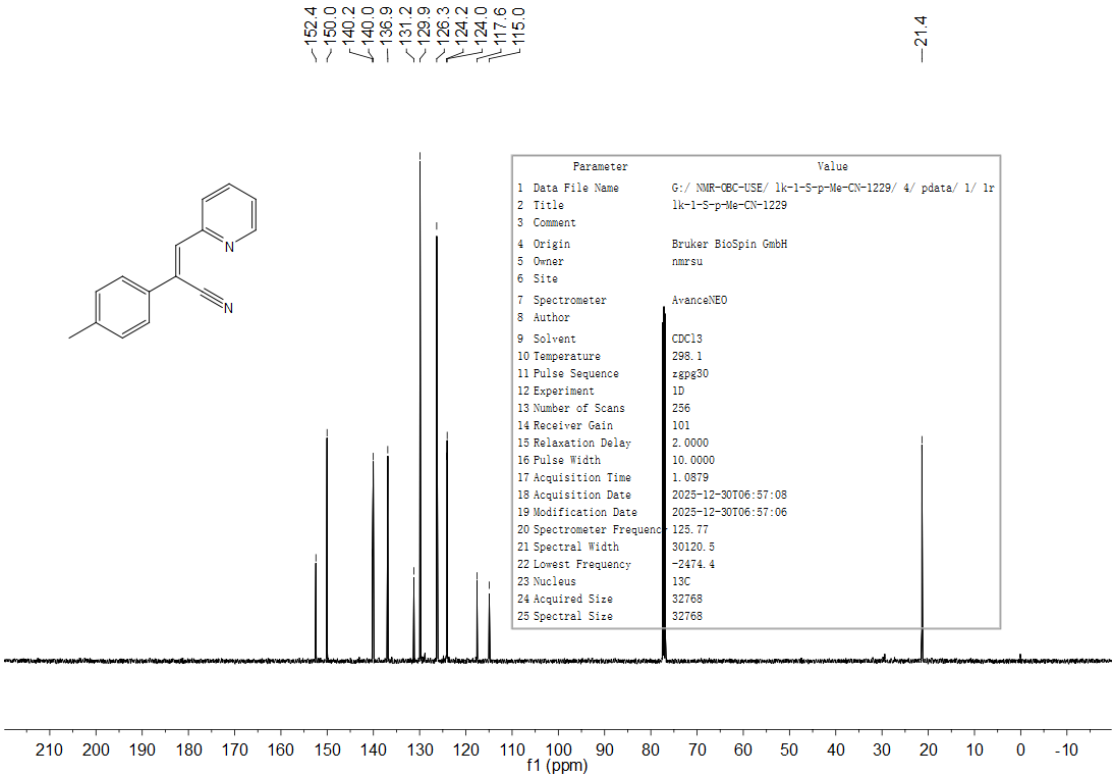
3-hydroxy-3-(pyridin-2-yl)-2-(*p*-tolyl)propanenitrile (2:3 dr)(5)





(Z)-3-(pyridin-2-yl)-2-(*p*-tolyl)acrylonitrile (6)




152.4
150.0
140.2
140.0
136.9
131.2
129.9
126.3
124.2
124.0
117.6
115.0
21.4
N
N
Parameter Value
1 Data File Name G:/ NMR-OBC-USE/ lk-1-5-p-Me-CN-1229/ 4/ pdata/ 1/ 1r
2 Title lk-1-5-p-Me-CN-1229
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 2025-12-30T06:57:08
19 Modification Date 2025-12-30T06:57:06
20 Spectrometer Frequenc 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2474.4
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)