

Electronic Supplementary Information

Cu-catalyzed, electron-relayed three-component synthesis of 2-alkenylbenzothiazoles with cathode ammonia evolution

Chengxian Hu, Dan Wang, Lu Wang, Ying Fu, * Zhengyin Du *

* Email: clinton_du@126.com; fu_yingmail@126.com

*Key Laboratory of Eco-functional Polymer Materials of the Ministry of Education,
College of Chemistry and Chemical Engineering, Northwest Normal University,
Lanzhou 730070, P. R. China.*

Contents

1. General Information.....	2
2. General Procedure for the Synthesis of Product 5	2
3. Characterization Data of Product 5	3
4. Reference	9
5. NMR Spectra Copies of Product 5	10
6. HRMS Spectra Copies of Products.....	32

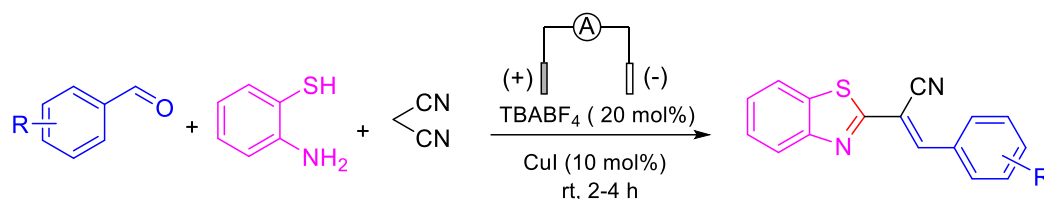
1. General Information

All chemicals were purchased from Energy Chemical Reagent, Ltd, Zane Chemical Technology company, Aladdin Ltd, Crystal pure bio-tech company and so forth. Unless otherwise stated, all experiments were conducted in a seal tube under argon atmosphere. Reactions were monitored by TLC or GC-MS analysis. Flash column chromatography was performed over silica gel (200-300 mesh).

$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectra were recorded in CDCl_3 on Nuclear Magnetic Resonance spectrometer (400 MHz for ^1H or 600 MHz for ^{13}C , 151 MHz for ^{13}C) at room temperature. Chemical shifts were reported in ppm on the scale relative to CDCl_3 ($\delta = 7.26$ for $^1\text{H-NMR}$, $\delta = 77.00$ for $^{13}\text{C-NMR}$) as an internal reference. High resolution mass spectra were recorded using ZAB-HS Bifocal high resolution mass spectrometer. Coupling constants (J) were reported in Hertz (Hz).

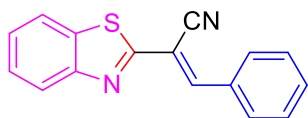
2. General Procedure for the Synthesis of Product 5

Ethanol (5 mL) was added into the beaker type electrolytic cell as the reaction solvent, and then malononitrile (0.5 mmol), 2-aminothiophenol (0.5 mmol), benzaldehyde (0.5 mmol) were successively added, TBABF_4 (32.2 mg, 20 mol%) as the electrolyte, after adding CuI (9.5 mg, 10 mol%), the reaction mixture is stirred at room temperature with a constant current of 12 mA and electrolyzed for 2-4 h. Real-time monitoring is carried out with TCL thin layer analysis. After the reaction is complete, then petroleum ether: ethyl acetate (15:1) was used to prepare the eluent and column chromatography was used to obtain the crystalline target product.



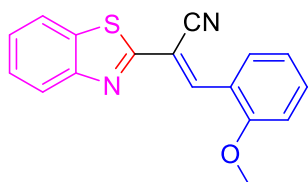


3. Characterization Data of Product 5



(E)-2-(Benzothiazol-2-yl)-3-phenylacrylonitrile (5a)

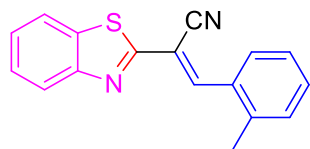
Yellow solid, 110.1 mg (84%). M.p. 148-149 °C (154-155 °C).¹ ¹H NMR (400 MHz, CDCl₃) δ 8.16 (s, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.99-7.96 (m 2H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.51-7.45 (m, 4H), 7.39 (t, *J* = 7.2 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 162.7, 153.6, 146.9, 134.9, 132.3, 132.2, 130.3, 129.7, 129.2, 128.6, 126.9, 126.0, 123.6, 121.7, 116.4, 105.6. HRMS (ESI) *m/z* calcd for C₁₆H₁₀N₂S⁺, (M+H)⁺ 263.0637, Found 263.0644.



(E)-2-(Benzothiazol-2-yl)-3-(2-methoxyphenyl)acrylonitrile (5b)

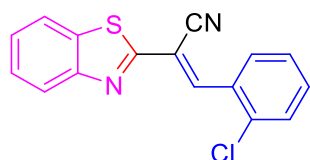
Yellow solid. 130.0 mg (89%). M.p. 154-155 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.65 (s, 1H), 8.33 (d, *J* = 8.6 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H),

7.55(dd, $J = 8.4, 18.4$ Hz, 2H), 7.43 (t, $J = 8.0$ Hz, 1H), 7.10 (t, $J = 7.6$ Hz, 1H), 7.00 (d, $J = 8.4$ Hz, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 163.5, 158.7, 153.7, 142.1, 134.8, 133.8, 128.9, 126.8, 125.9, 123.7, 121.6, 121.5, 121.0, 116.6, 111.0, 105.6, 55.8. HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{12}\text{N}_2\text{OS}^+$, (M+H) $^+$ 293.0743, Found 293.0742.



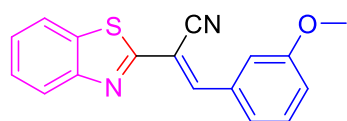
(E)-2-(Benzothiazol-2-yl)-3-(2-methylphenyl)acrylonitrile (5c)

Yellow solid. 118.7 mg (86%). M.p. 101-103 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.06-8.03 (m, 3H), 7.47-7.41 (m, 2H), 7.26-7.18 (m, 3H), 7.11-7.08 (m, 1H), 2.34 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 162.6, 153.6, 145.5, 138.9, 134.9, 131.8, 130.9, 130.3, 128.3, 126.9, 126.7, 126.0, 123.7, 121.7, 116.3, 107.3, 20.0. HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{12}\text{N}_2\text{S}^+$, (M+H) $^+$ 277.0794, Found 277.0795.



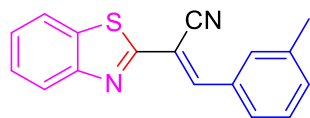
(E)-2-(Benzothiazol-2-yl)-3-(2-chlorophenyl)acrylonitrile (5d)

Yellow solid. 100.6 mg (68%). M.p. 177-178 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.58 (s, 1H), 8.28-8.226 (m, 1H), 8.13 (d, $J = 8.4$ Hz, 1H), 7.92 (d, $J = 3.6$ Hz, 1H), 7.56-7.40 (m, 5H). ^{13}C NMR (151 MHz, CDCl_3) δ 162.1, 153.6, 143.2, 135.8, 135.0, 132.8, 130.8, 130.3, 129.6, 127.4, 127.0, 126.4, 124.0, 121.7, 115.7, 108.8. HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_9\text{ClN}_2\text{S}^+$, (M+H) $^+$ 297.0248, Found 297.0248.



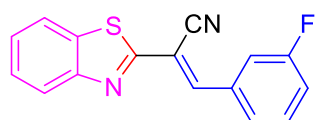
(E)-2-(Benzothiazol-2-yl)-3-(3-methoxyphenyl)acrylonitrile (5e)

Yellow solid. 121.2 mg (83%). M.p. 135-136 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.16 (s, 1H), 8.07 (d, $J = 8.0$ Hz, 1H), 7.89 (d, $J = 8.4$ Hz, 1H), 7.59 (s, 1H), 7.54-7.49(m, 2H), 7.43 (dd, $J = 8.0$ Hz, 12.8 Hz, 2H), 7.06-7.04 (m, 1H), 3.87 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 162.7, 159.9, 153.5, 146.8, 134.9, 133.5, 130.2, 126.9, 126.0, 123.6, 123.4, 121.6, 118.9, 116.5, 114.1, 105.7, 55.4. HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{12}\text{N}_2\text{OS}^+$, (M+H) $^+$ 293.0743, Found 293.0742.



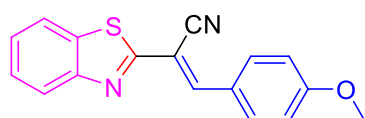
(E)-2-(Benzothiazol-2-yl)-3-(3-methylphenyl)acrylonitrile (5f)

Yellow solid. 113.2 mg (82%). M.p. 143-144 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.10 (s, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.85 (dd, *J* = 8.0, 14.0 Hz, 2H), 7.75 (s, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.40 (dd, *J* = 8.0 Hz, 16.8 Hz, 2H), 7.30 (d, *J* = 7.2 Hz, 1H), 2.40 (s, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 162.8, 153.6, 147.1, 139.0, 134.9, 133.2, 132.3, 131.0, 129.1, 127.5, 126.9, 126.0, 123.6, 121.6, 116.4, 105.2, 21.4. HRMS (ESI) *m/z* calcd for C₁₇H₁₂N₂S⁺, (M+H)⁺ 277.0794, Found 277.0794.



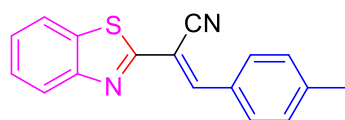
(E)-2-(Benzothiazol-2-yl)-3-(3-fluorophenyl)acrylonitrile (5g)

Yellow solid. 93.8 mg (67%). M.p. 171-172 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.22 (s, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 7.2 Hz, 1H), 7.57-7.44 (m, 3H), 7.26-7.21 (m, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 163.6, 162.0 (d, *J*_{C-F} = 13.59 Hz), 153.5, 145.1 (d, *J*_{C-F} = 3.02 Hz), 135.1, 134.3 (d, *J*_{C-F} = 9.06 Hz), 130.8 (d, *J*_{C-F} = 9.06 Hz), 127.1, 126.2 (d, *J*_{C-F} = 3.02 Hz), 123.7, 121.7, 119.2 (d, *J*_{C-F} = 21.14 Hz), 116.6 (d, *J*_{C-F} = 22.65 Hz), 116.0, 107.0. ¹⁹F NMR (376 MHz, CDCl₃) δ -110.8. HRMS (ESI) *m/z* calcd for C₁₆H₉N₂FS⁺, (M+H)⁺ 281.0543, Found 281.0543.



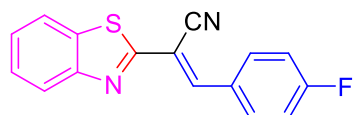
(E)-2-(Benzothiazol-2-yl)-3-(4-methoxyphenyl)acrylonitrile (5h)

Yellow solid. 121.2 mg (91%). M.p. 186-188 °C (194-196 °C).¹ ¹H NMR (400 MHz, CDCl₃) δ 8.17 (s, 1H), 8.07-8.02 (m, 3H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.02 (d, *J* = 8.8 Hz, 2H), 3.89 (s, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 163.4, 162.9, 153.6, 146.5, 134.8, 132.7, 126.8, 125.7, 125.2, 123.3, 121.6, 117.1, 114.7, 114.2, 102.3, 85.2, 55.6. HRMS (ESI) *m/z* calcd for C₁₇H₁₂N₂OS⁺, (M+H)⁺ 293.0743, Found 293.0746.



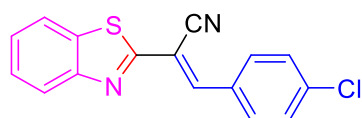
(E)-2-(Benzothiazol-2-yl)-3-(4-methylphenyl)acrylonitrile (5i)

Yellow solid. 117.3 mg (85%). M.p. 152-154 °C (159-161 °C).¹ ¹H NMR (400 MHz, CDCl₃) δ 8.16 (s, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 2H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.51 (t, *J* = 7.2 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 2.42 (s, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 163.0, 153.6, 146.9, 143.4, 134.9, 130.5, 130.0, 129.7, 129.3, 126.8, 125.9, 124.0, 123.5, 121.6, 116.7, 104.3, 21.8. HRMS (ESI) *m/z* calcd for C₁₇H₁₂N₂S⁺, (M+H)⁺ 277.0794, Found 277.0794.



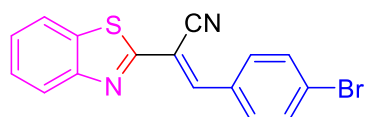
(E)-2-(Benzothiazol-2-yl)-3-(4-fluorophenyl)acrylonitrile (5j)

Yellow solid. 96.6 mg (69%). M.p. 120-121 °C. ¹H NMR (600 MHz, CDCl₃) δ 8.19 (s, 1H), 8.06 (m, 2H), 7.92-7.87 (m, 1H), 7.58-7.34 (m, 3H), 7.25-7.16 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 162.5, 153.5, 145.3, 134.9, 132.7(d, *J*_{C-F} = 9.06 Hz), 132.2(d, *J*_{C-F} = 9.06 Hz), 128.7(d, *J*_{C-F} = 3.02 Hz), 127.0, 126.4(d, *J*_{C-F} = 7.55 Hz), 126.0, 124.0, 123.6, 121.7, 116.6(d, *J*_{C-F} = 22.65 Hz), 116.4, 115.7(d, *J*_{C-F} = 21.14 Hz). ¹⁹F NMR (376 MHz, CDCl₃) δ -104.8. HRMS (ESI) *m/z* calcd for C₁₆H₉N₂FS⁺, (M+H)⁺ 281.0543, Found 281.0544.



(E)-2-(Benzo[d]thiazol-2-yl)-3-(4-chlorophenyl)acrylonitrile (5k)

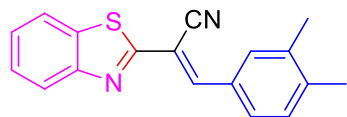
Yellow solid. 105.1 mg (71%). M.p. 224-225 °C (235-237 °C).¹ ¹H NMR (600 MHz, CDCl₃) δ 8.18 (s, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.52 (t, *J* = 7.2 Hz, 2H), 7.48 (t, *J* = 8.4 Hz, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 162.3, 153.5, 145.1, 138.4, 135.0, 131.5, 130.8, 129.6, 128.8, 127.0, 126.1, 123.6, 121.7, 116.2, 111.8, 106.0. HRMS (ESI) *m/z* calcd for C₁₆H₉N₂ClS⁺, (M+H)⁺ 297.0248, Found 297.0247.



(E)-2-(Benzothiazol-2-yl)-3-(4-bromophenyl)acrylonitrile (5l)

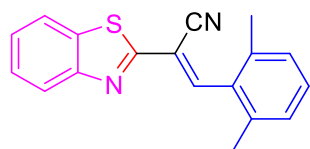
Yellow solid. 113.9 mg (67%). M.p. 207-209 °C (210-211 °C).¹ ¹H NMR (400 MHz, CDCl₃) δ 8.16 (s, 1H), 8.08 (d, *J* = 8.0 Hz, 1H), 7.91-7.86 (m, 2H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ

162.3, 153.5, 145.2, 137.0, 135.0, 132.6, 131.6, 131.5, 131.2, 127.0, 126.9, 126.1, 123.7, 121.7, 116.2, 106.1. HRMS (ESI) m/z calcd for $C_{16}H_9N_2BrS^+$, (M+H)⁺ 340.9743, Found 340.9742.



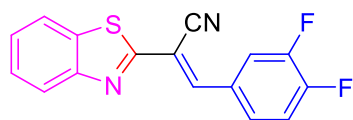
(E)-2-(Benzo[d]thiazol-2-yl)-3-(3,4-dimethylphenyl)acrylonitrile (5m)

Yellow solid. 127.6 mg (88%). M.p. 145-146 °C. ¹H NMR (600 MHz, CDCl₃) δ 8.11 (s, 1H), 8.04 (d, $J = 8.4$ Hz, 1H), 7.86 (d, $J = 7.8$ Hz, 1H), 7.78 (d, $J = 7.8$ Hz, 1H), 7.75 (s, 1H), 7.49 (t, $J = 7.2$ Hz, 1H), 7.48 (t, $J = 8.4$ Hz, 1H), 7.26-7.24 (m, 1H), 2.30 (s, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 163.2, 153.6, 147.1, 144.3, 142.2, 137.6, 134.8, 131.7, 130.5, 128.0, 126.8, 123.5, 121.6, 116.7, 104.0, 20.1, 19.8. HRMS (ESI) m/z calcd for $C_{18}H_{14}N_2S^+$, (M+H)⁺ 291.0950, Found 291.0950.



(E)-2-(Benzothiazol-2-yl)-3-(2,6-dimethylphenyl)acrylonitrile (5n)

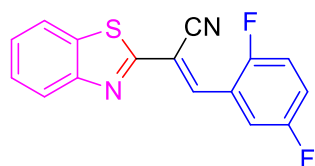
Yellow solid. 114.6 mg (79%). M.p. 125-126 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.40 (s, 1H), 8.14 (d, $J = 8.0$ Hz, 1H), 7.94 (d, $J = 8.0$ Hz, 1H), 7.56 (d, $J = 7.2$ Hz, 1H), 7.47 (t, $J = 8.4$ Hz, 1H), 7.26 (t, $J = 7.2$ Hz, 1H), 7.16-7.14 (m, 2H), 2.40 (s, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 161.2, 153.5, 148.9, 136.3, 134.9, 132.2, 130.0, 129.6, 128.6, 128.1, 127.0, 126.3, 123.9, 121.7, 115.1, 113.5, 20.4, 20.0. HRMS (ESI) m/z calcd for $C_{18}H_{14}N_2S^+$, (M+H)⁺ 291.0950, Found 291.0949.



(E)-2-(Benzothiazol-2-yl)-3-(3,4-difluorophenyl)acrylonitrile (5o)

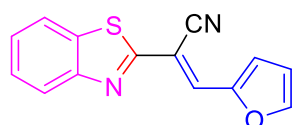
Yellow solid. 98.4 mg (66%). M.p. 102-103 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.16 (s, 1H), 8.08 (d, $J = 8.2$ Hz, 1H), 7.92 (d, $J = 7.6$ Hz, 2H), 7.77 (d, $J = 5.0$ Hz, 1H), 7.55 (t, $J = 7.7$ Hz, 1H), 7.45 (t, $J = 7.6$ Hz, 1H), 7.31 (q, $J = 8.7$ Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 161.9, 153.5, 151.5, 149.7 (d, $J_{C-F} = 13.59$ Hz), 143.9, 135.0, 127.5 (d, $J_{C-F} = 3.02$ Hz), 127.5 (d, $J_{C-F} = 4.53$ Hz), 127.1, 126.2, 123.7, 121.7, 118.8 (d, $J_{C-F} = 18.12$ Hz), 118.3 (d, $J_{C-F} = 18.12$ Hz), 116.0, 106.5 (d, $J_{C-F} = 3.02$ Hz). ¹⁹F NMR (376 MHz, CDCl₃) δ -134.5, -139.8. HRMS (ESI) m/z calcd for $C_{16}H_8F_2N_2S^+$, (M+H)⁺

299.0449, Found 299.0449.



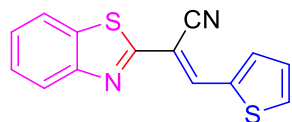
(E)-2-(Benzothiazol-2-yl)-3-(2,5-difluorophenyl)acrylonitrile (5p).

Yellow solid. 80.5 mg (54%). M.p. 131-132 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.24 (s, 1H), 8.06 (d, *J* = 8.2 Hz, 1H), 7.89 (dd, *J* = 23.7, 7.7 Hz, 2H), 7.59 - 7.55 (m, 1H), 7.52 - 7.46 (m, 2H), 7.42 - 7.37 (m, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 166.3, 162.7, 153.2 (d, *J*_{C-F} = 55.87 Hz), 135.5 (d, *J*_{C-F} = 61.96 Hz), 131.0, 129.7, 126.5 (d, *J*_{C-F} = 6.04 Hz), 126.2, 125.7, 124.1, 123.6, 121.6 (d, *J*_{C-F} = 43.79 Hz), 117.8 (d, *J*_{C-F} = 7.55 Hz), 117.6 (d, *J*_{C-F} = 9.06 Hz), 116.8. ¹⁹F NMR (376 MHz, CDCl₃) δ -123.1, -123.3. HRMS (ESI) *m/z* calcd for C₁₆H₈F₂N₂S⁺, (M+Na)⁺ 321.0268, Found 321.0269.



(E)-2-(Benzothiazol-2-yl)-3-(furan-2-yl)acrylonitrile (5q).

Yellow solid. 73.1 mg (58%). M.p. 141-142 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.02-8.03 (m, 2H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.72 (s, 1H), 7.50 (t, *J* = 8.4 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 7.4 Hz, 1H), 6.65-6.64 (m, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 162.2, 153.6, 149.2, 147.1, 135.0, 131.7, 126.9, 125.8, 123.3, 121.6, 119.6, 116.3, 113.6, 101.4. HRMS (ESI) *m/z* calcd for C₁₄H₈N₂SO⁺, (M+H)⁺ 253.0430, Found 253.0431.



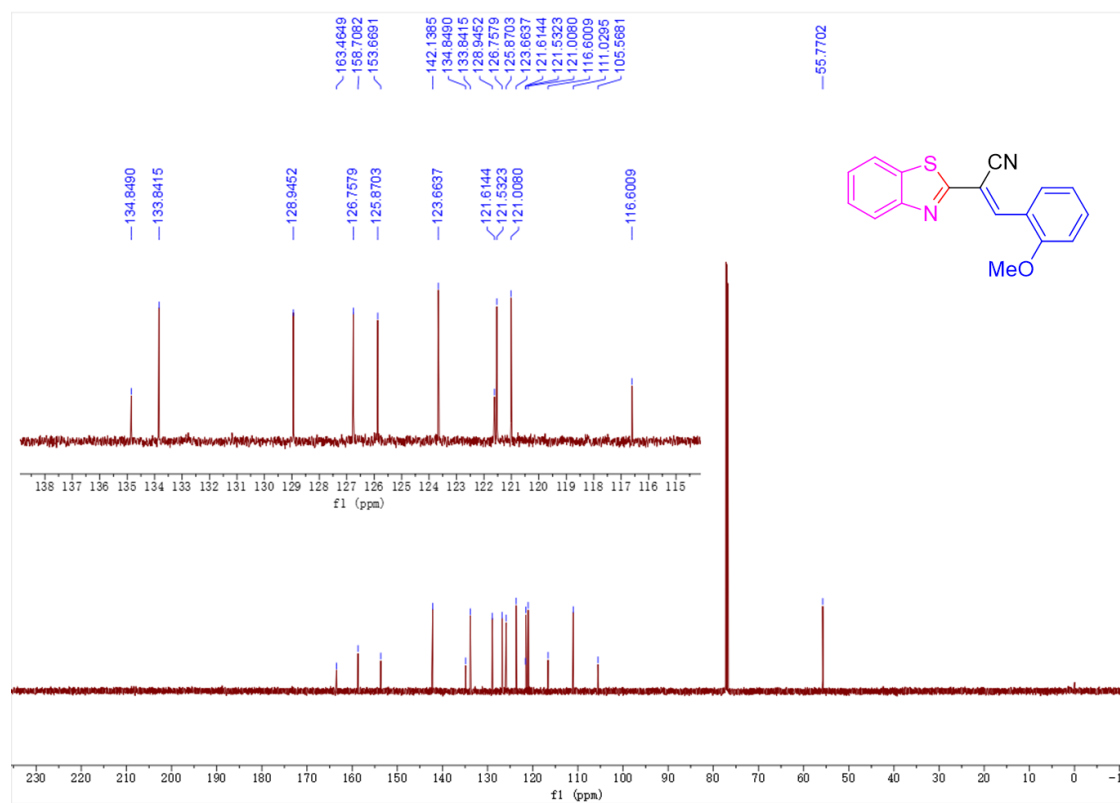
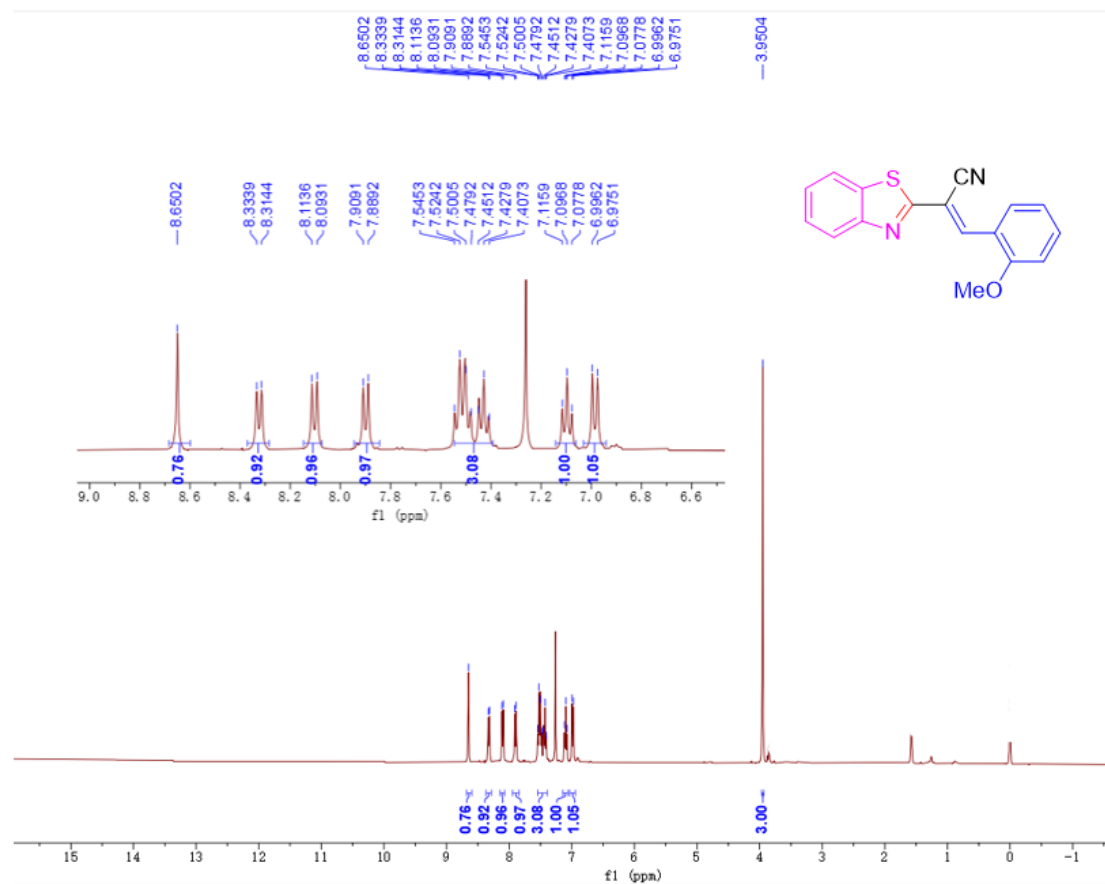
(E)-2-(Benzothiazol-2-yl)-3-(thiophen-2-yl)acrylonitrile (5r)

Yellow solid. 89.8 mg (67%). M.p. 170-173 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.40 (s, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.91 (d, *J* = 4.4 Hz, 1H), 7.83 (d, *J* = 3.6 Hz, 1H), 7.73 (d, *J* = 5.2 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.24-7.21 (m, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 162.3, 153.6, 138.8, 136.9, 135.4, 135.0, 133.3, 128.5, 126.9, 125.8, 123.3, 121.7, 116.6, 102.1. HRMS (ESI) *m/z* calcd for C₁₄H₈N₂S₂⁺, (M+Na)⁺ 291.0021, Found 291.0021.

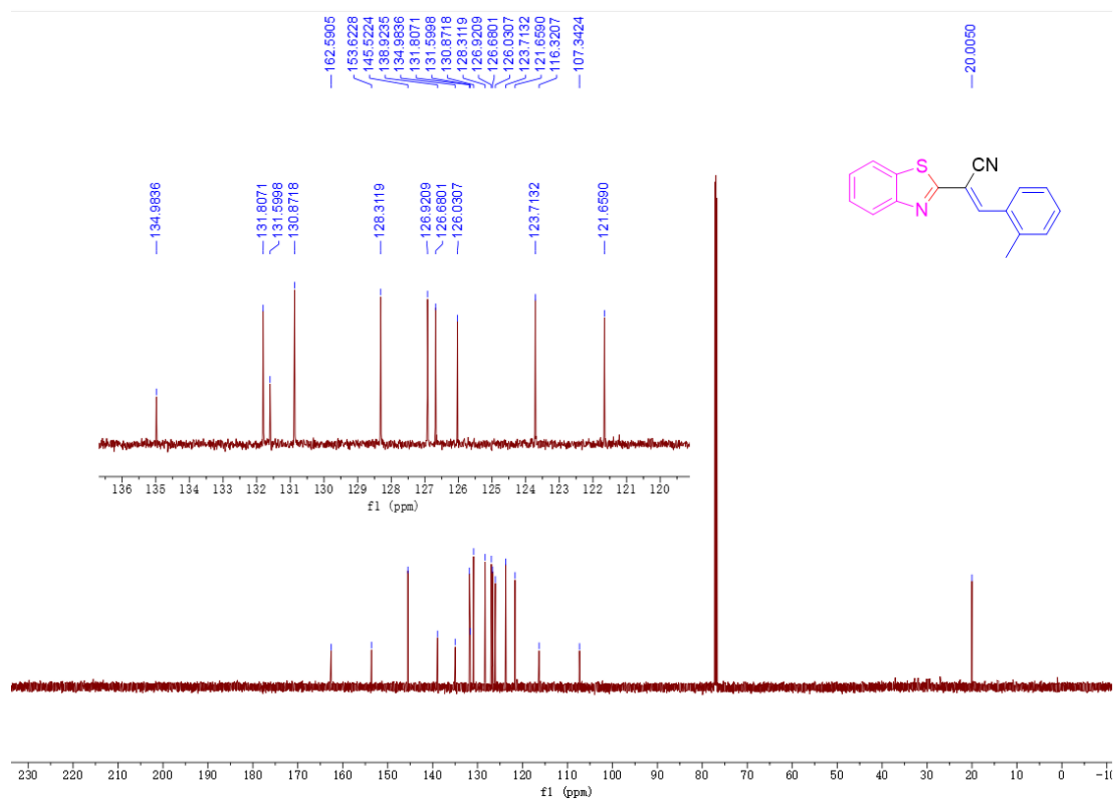
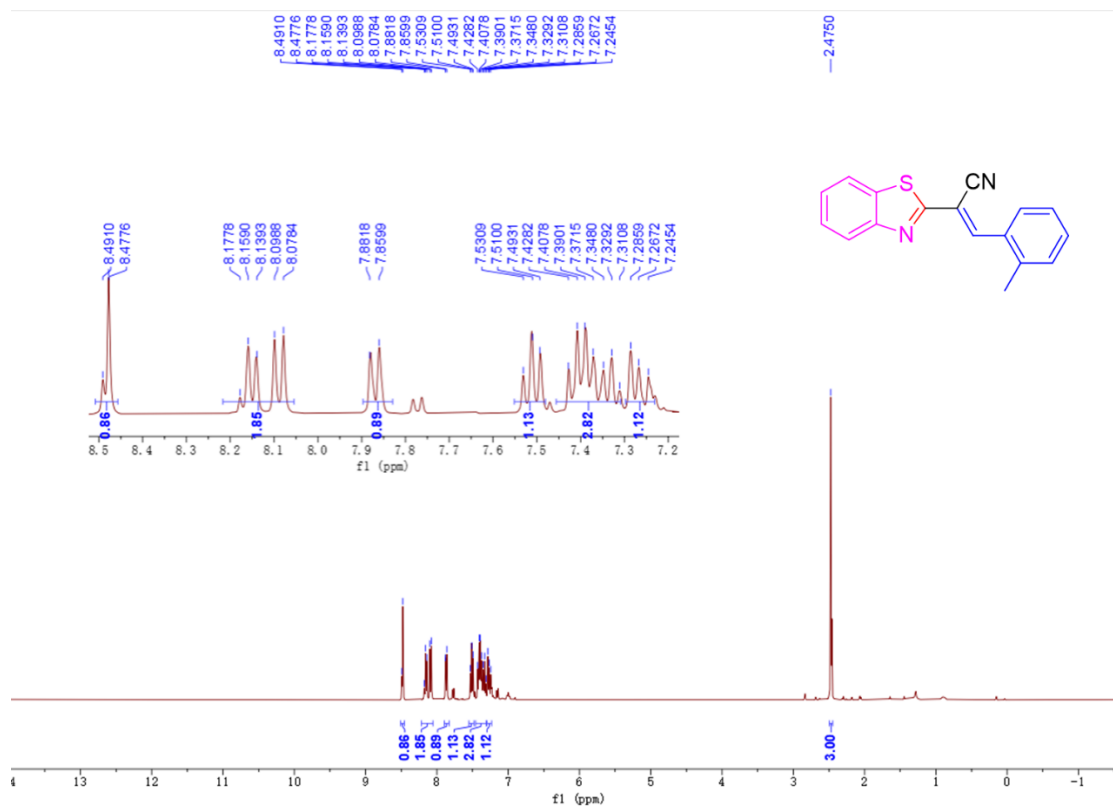
4. Reference

[1] S. Maddila, S. B. Jonnalagadda, Bull. Chem. Soc. Ethiop. 2012, 26, 3, 467-471.

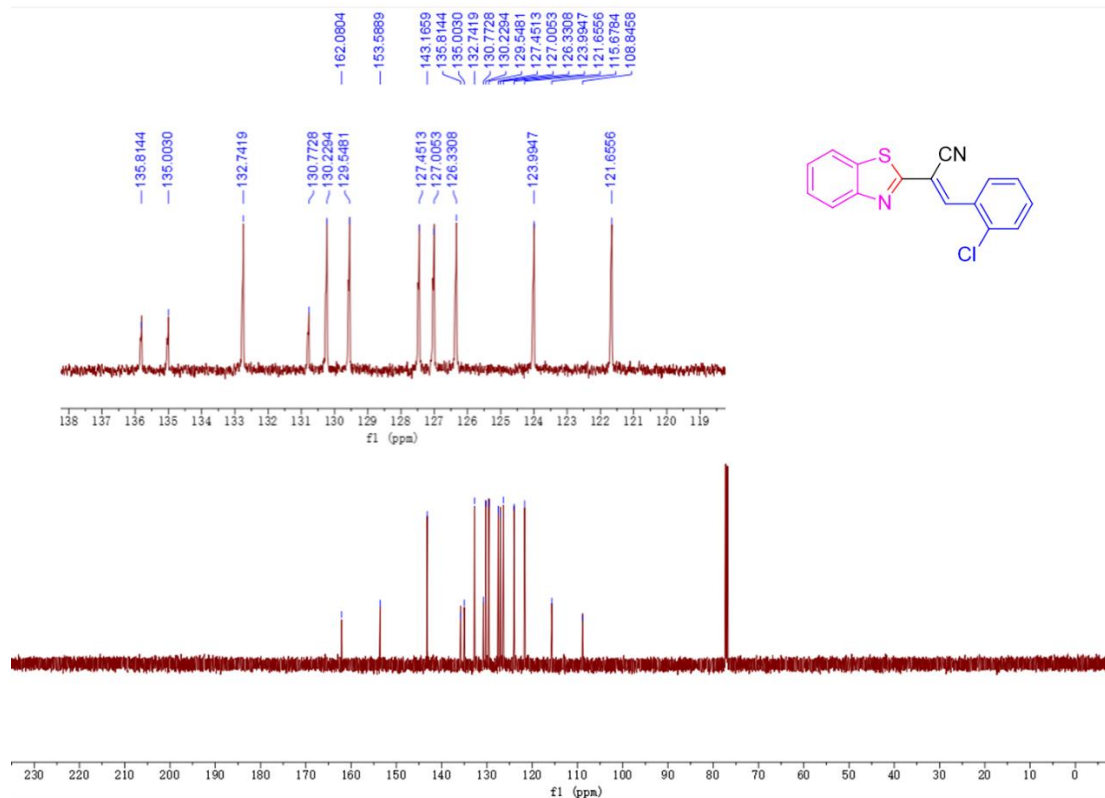
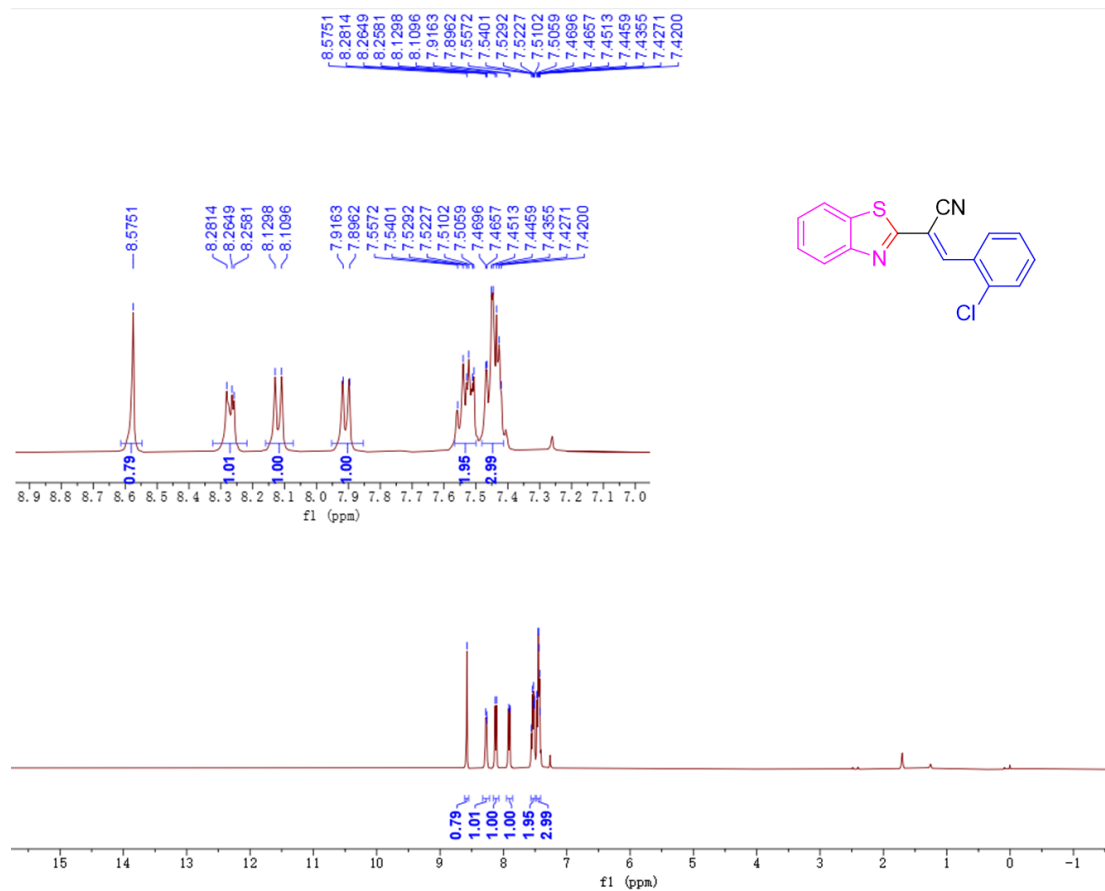
(E)-2-(Benzothiazol-2-yl)-3-(2-methoxyphenyl)acrylonitrile (5b)



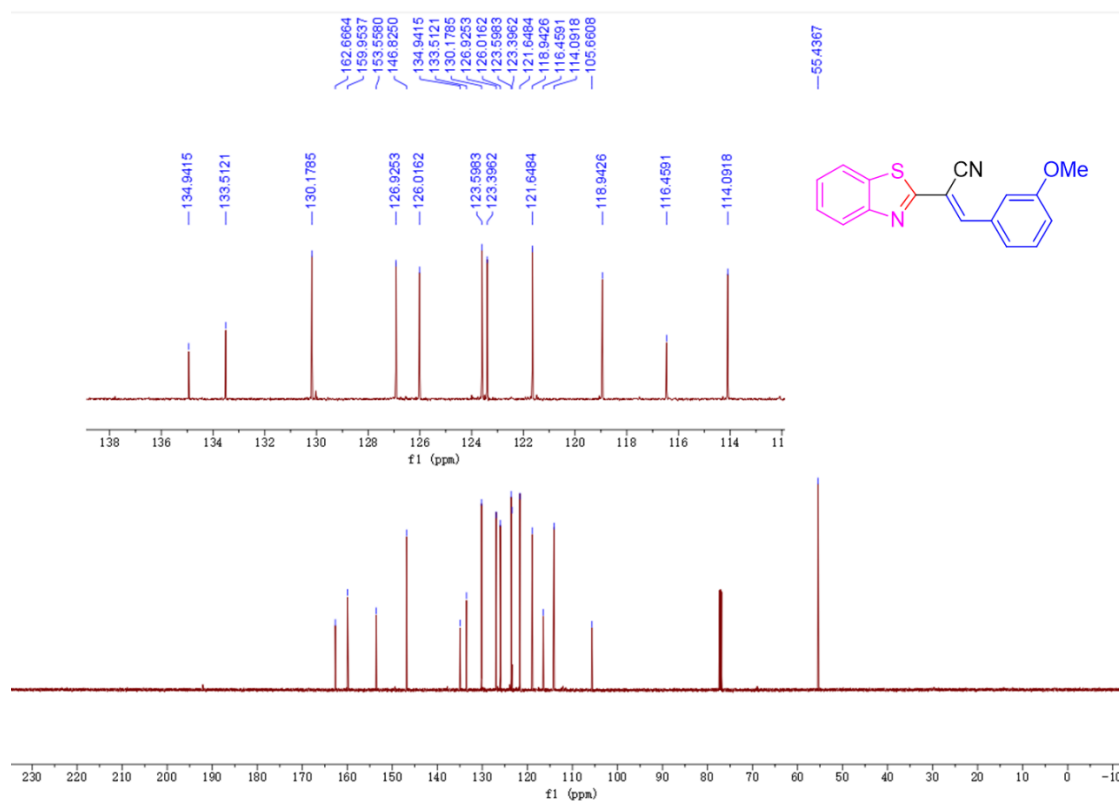
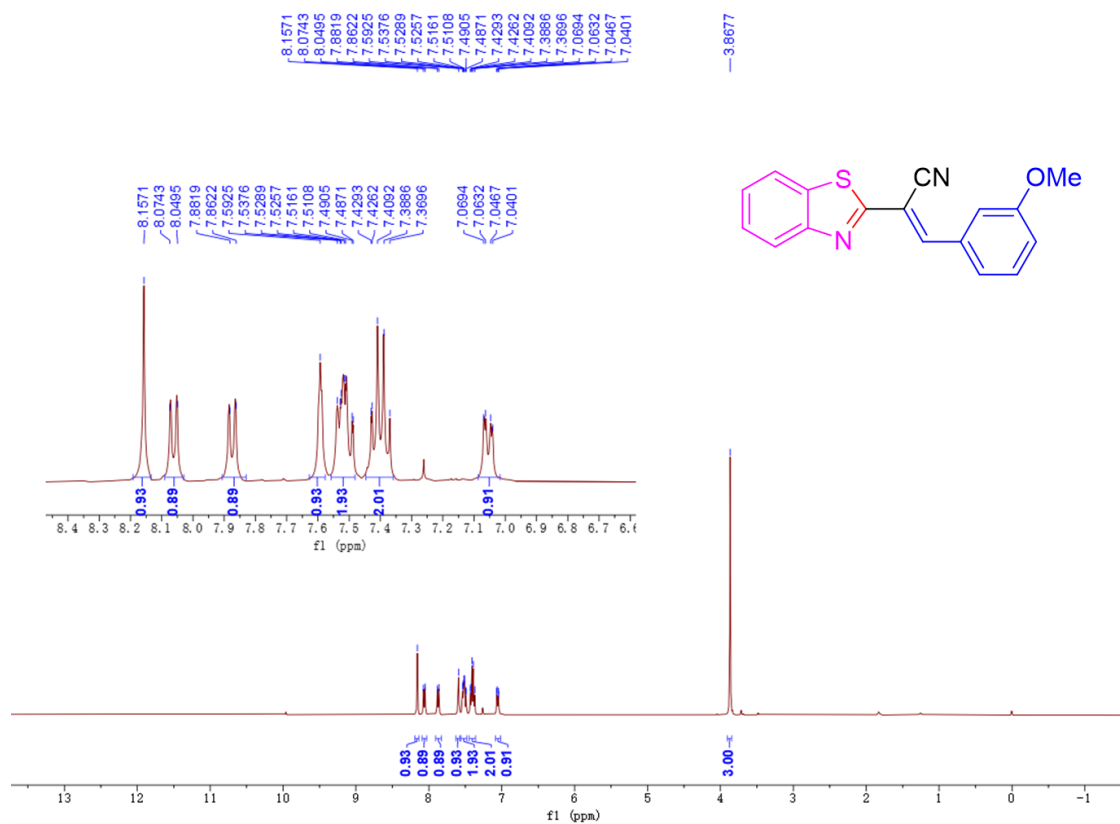
(E)-2-(Benzothiazol-2-yl)-3-(*o*-tolyl)acrylonitrile (5c)



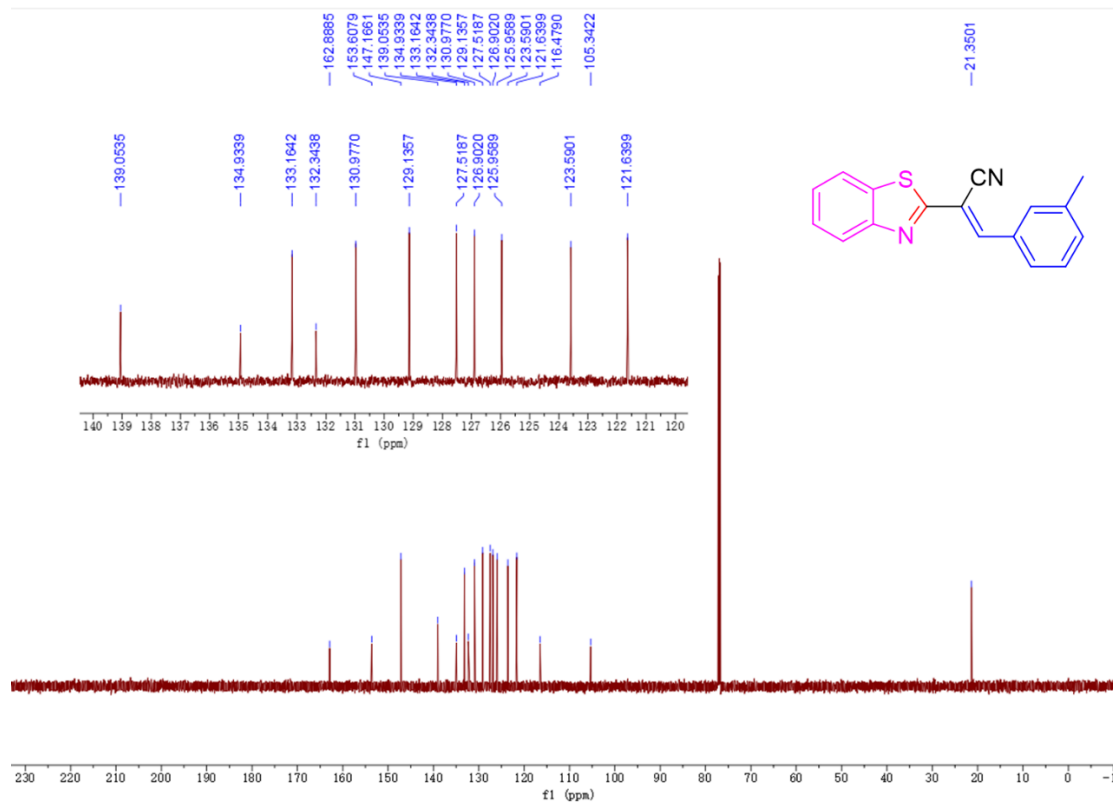
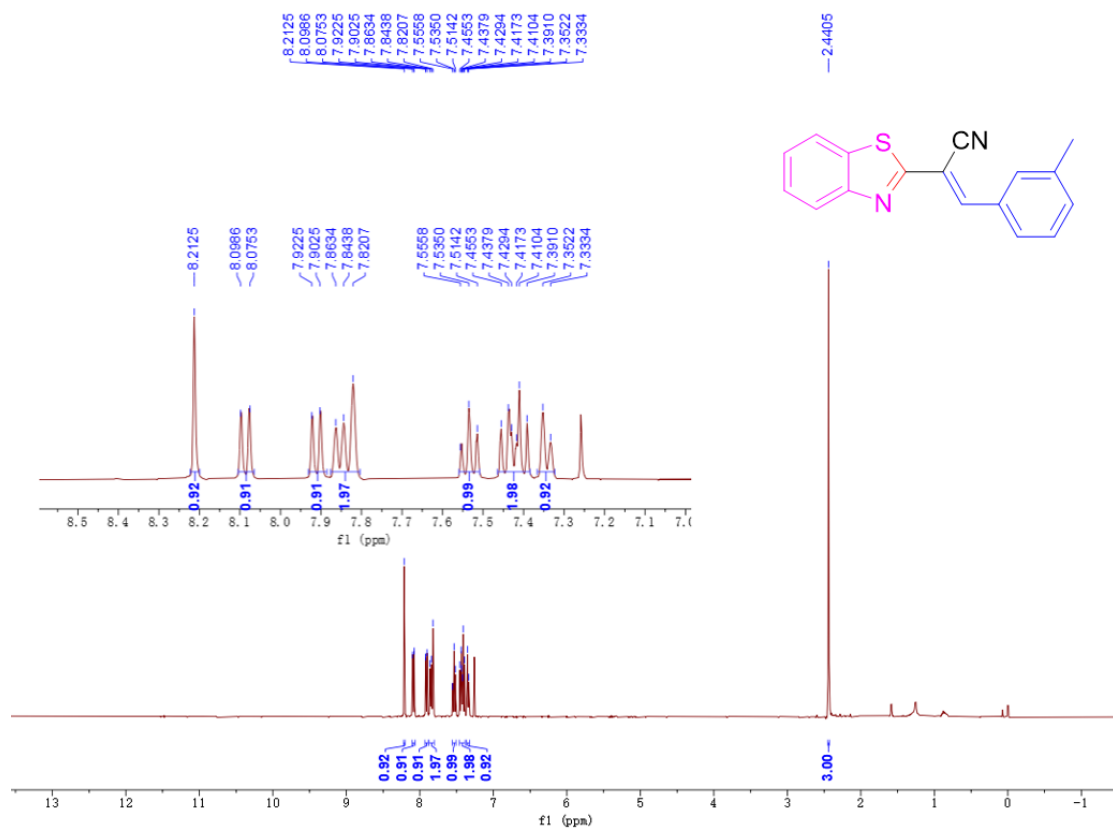
(E)-2-(Benzothiazol-2-yl)-3-(2-chlorophenyl)acrylonitrile (5d)



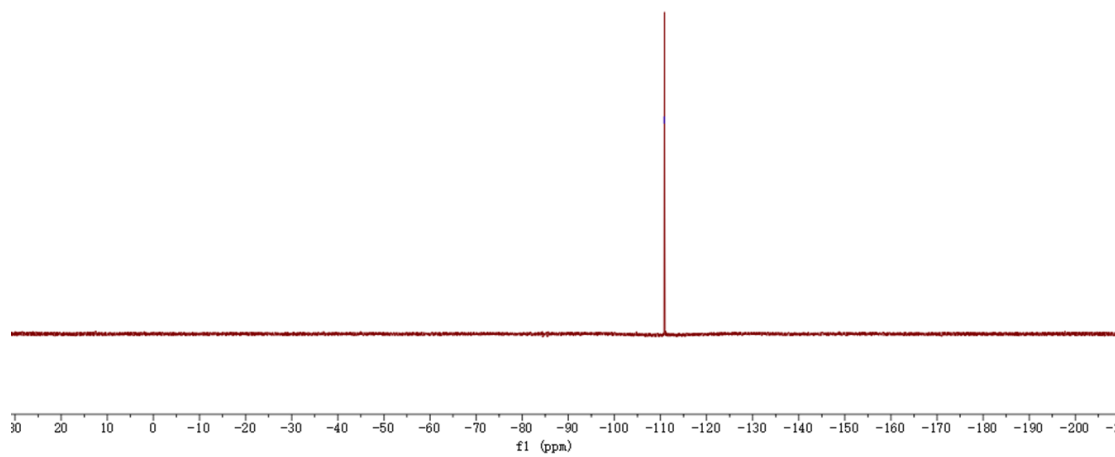
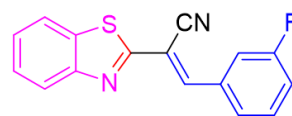
(E)-2-(Benzothiazol-2-yl)-3-(3-methoxyphenyl)acrylonitrile (5e)



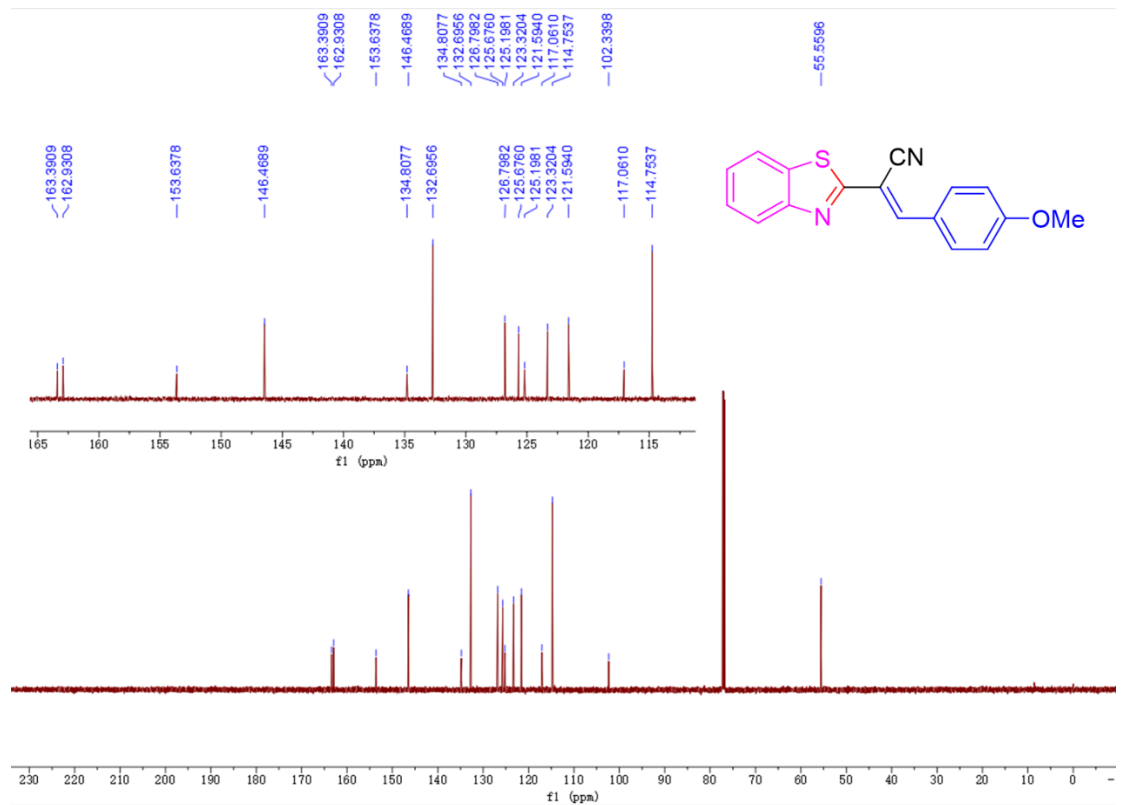
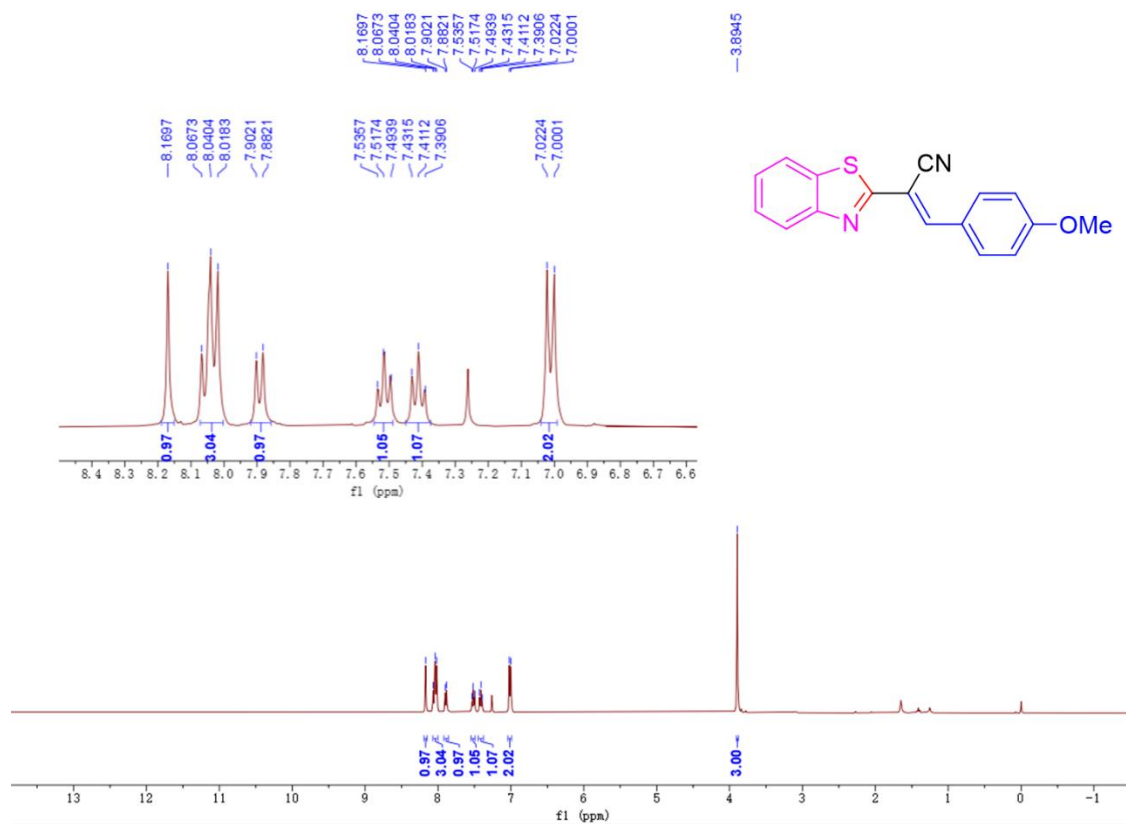
(E)-2-(Benzothiazol-2-yl)-3-(m-tolyl)acrylonitrile (5f)



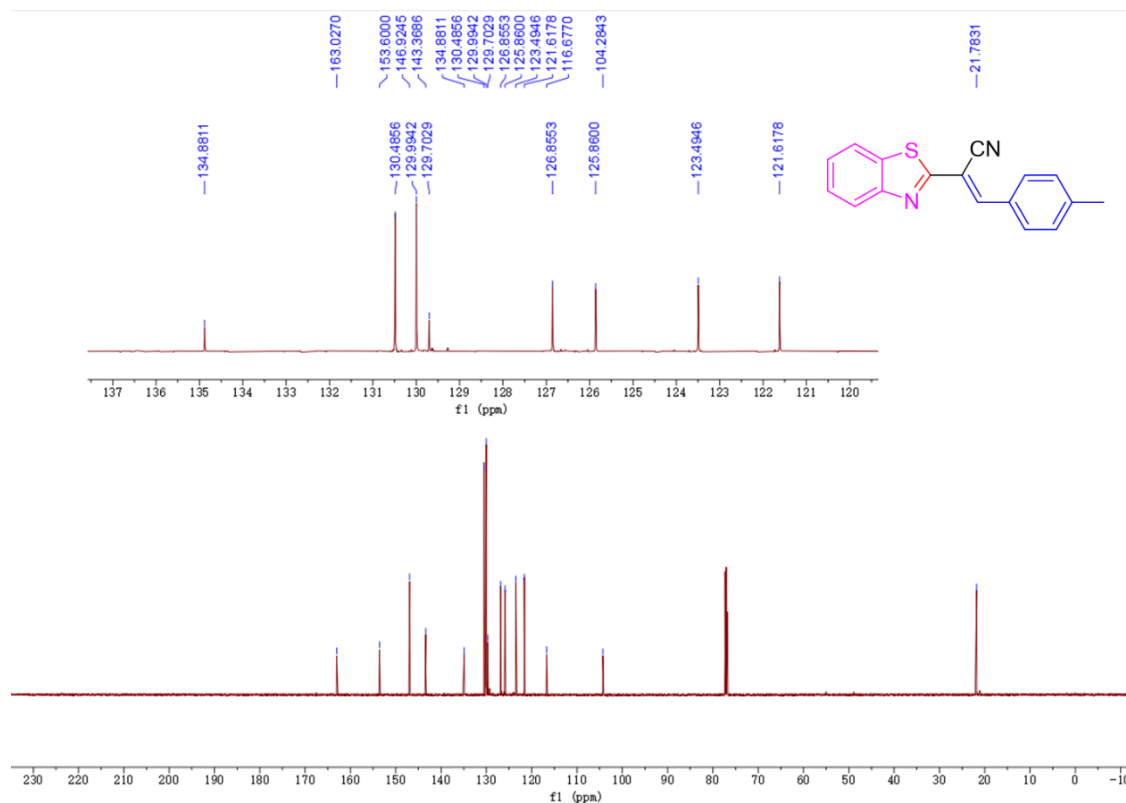
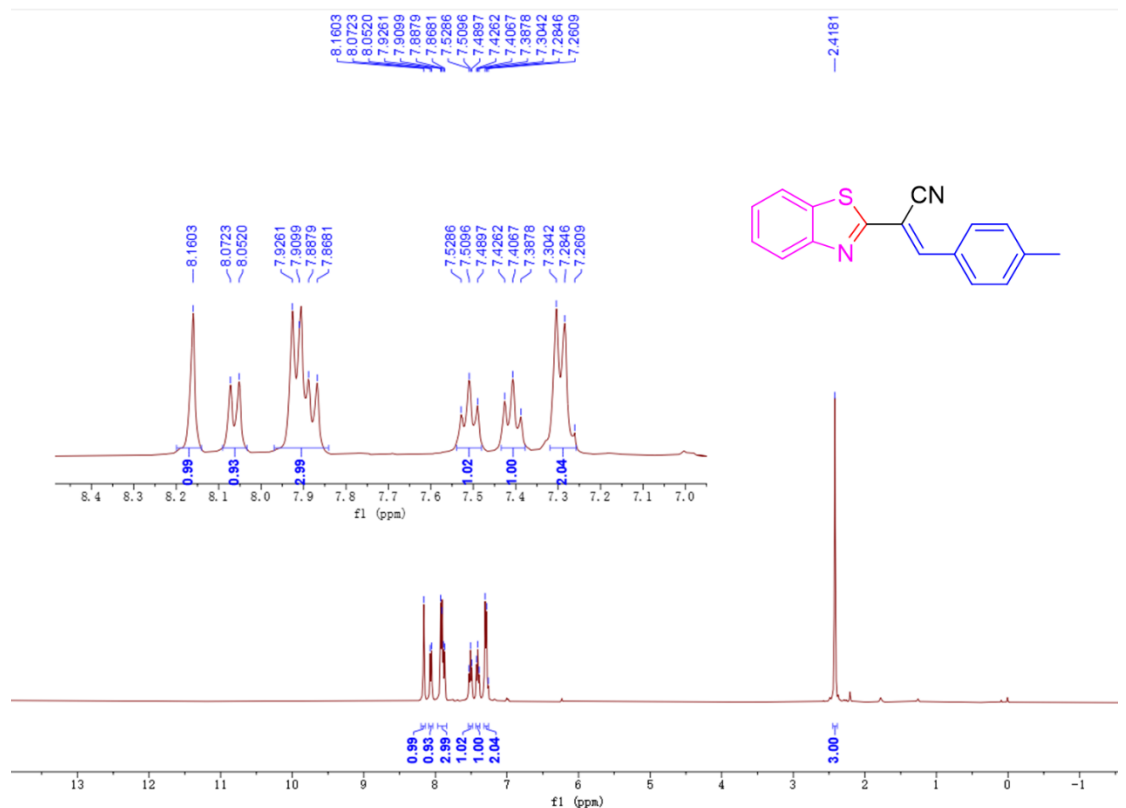
—110.8196



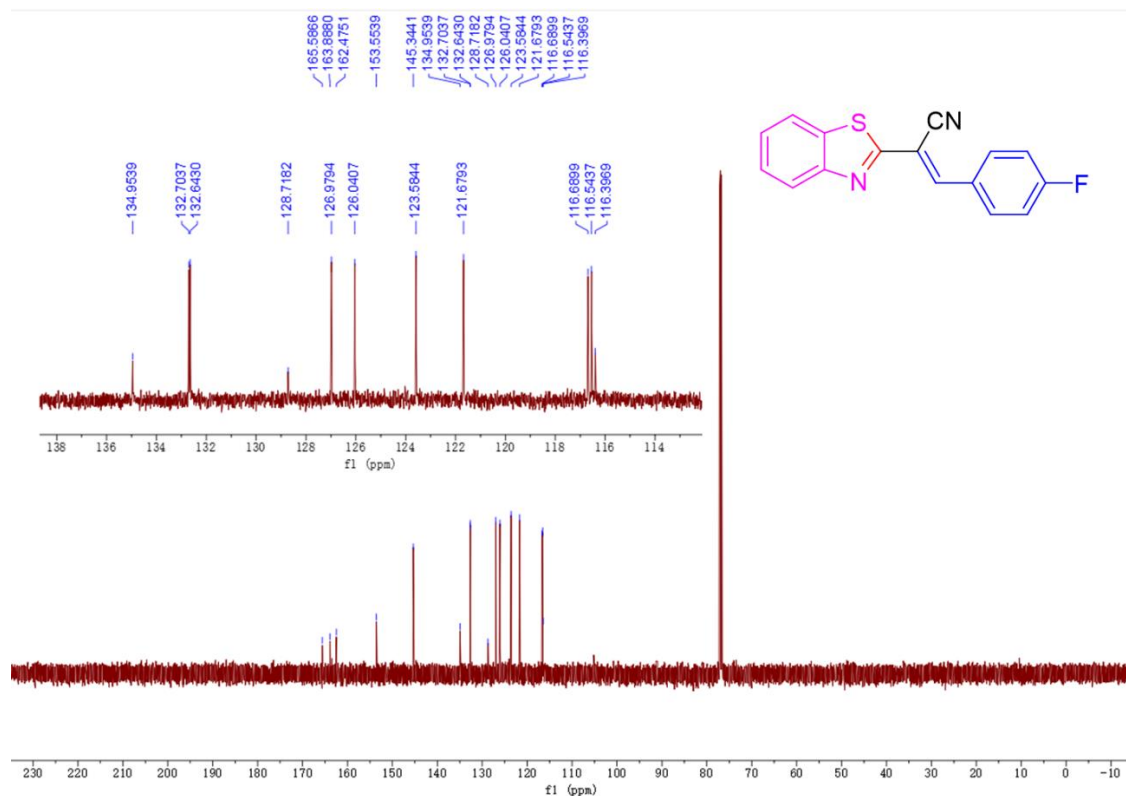
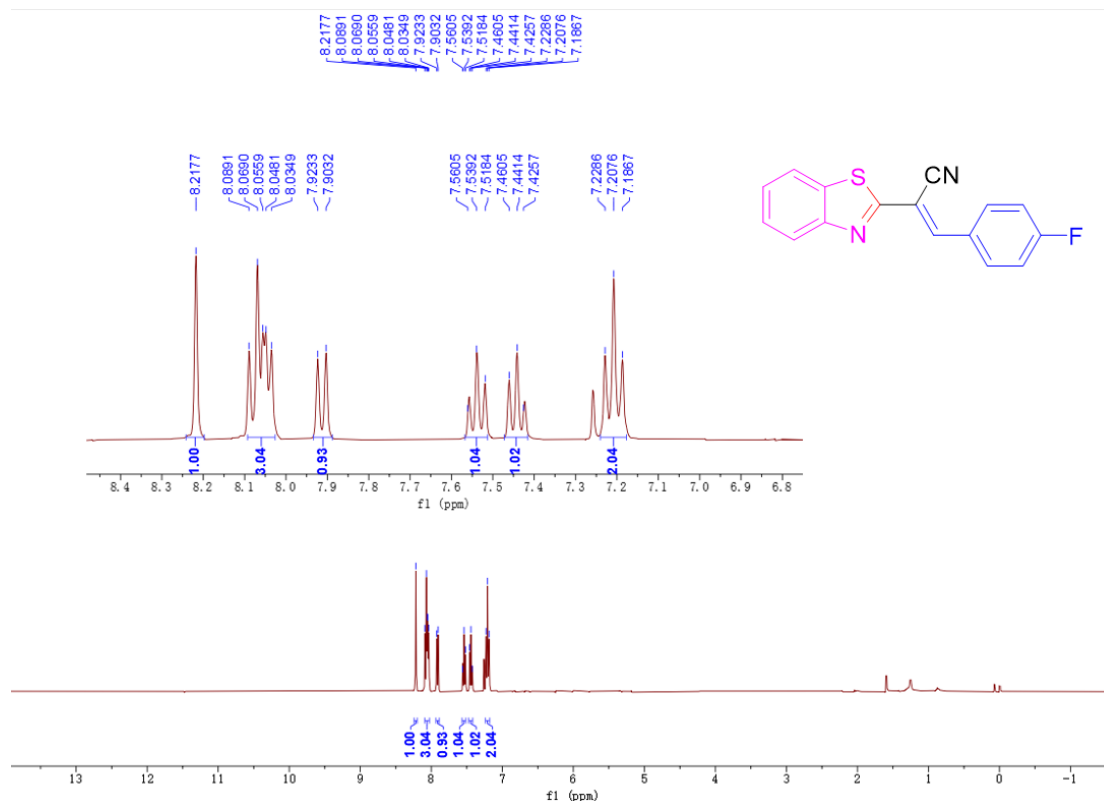
(E)-2-(Benzothiazol-2-yl)-3-(4-methoxyphenyl)acrylonitrile (5h)



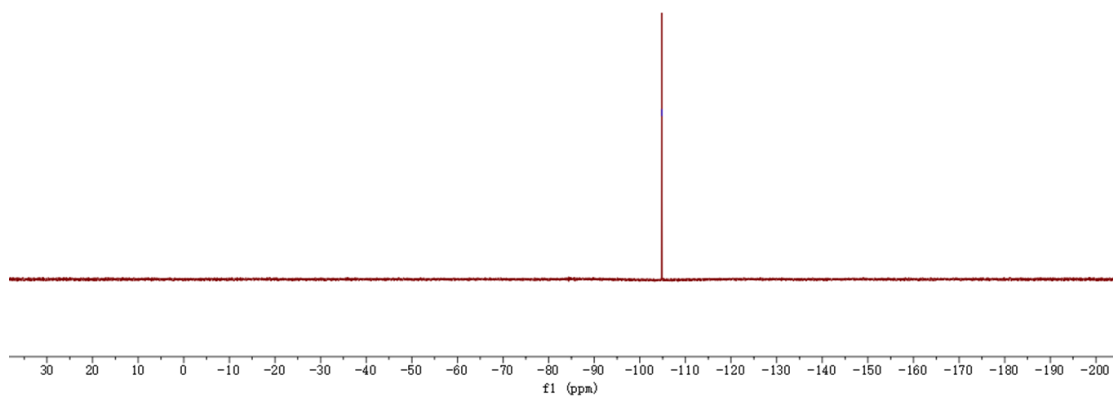
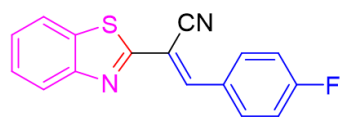
(E)-2-(Benzothiazol-2-yl)-3-(p-tolyl)acrylonitrile (5i)



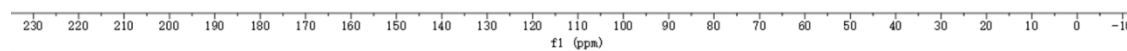
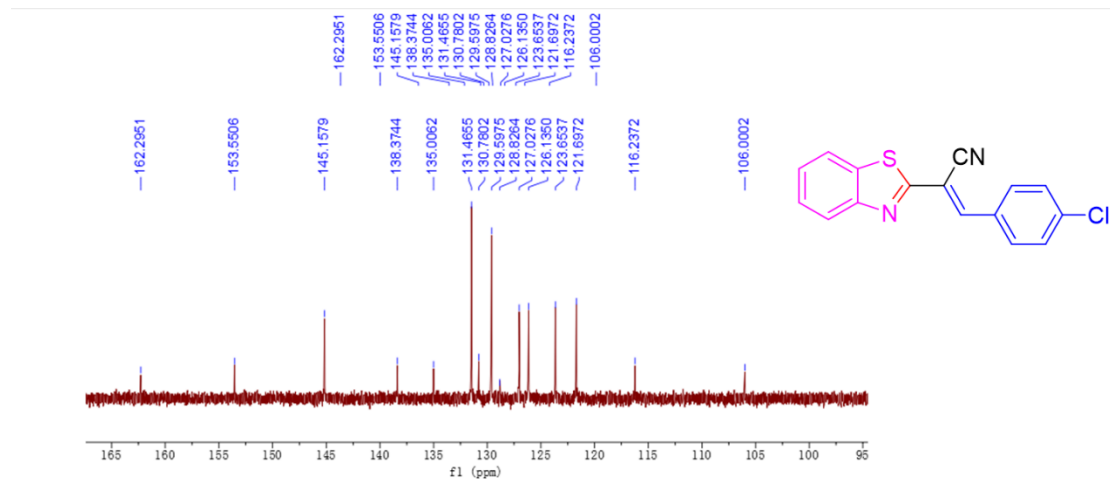
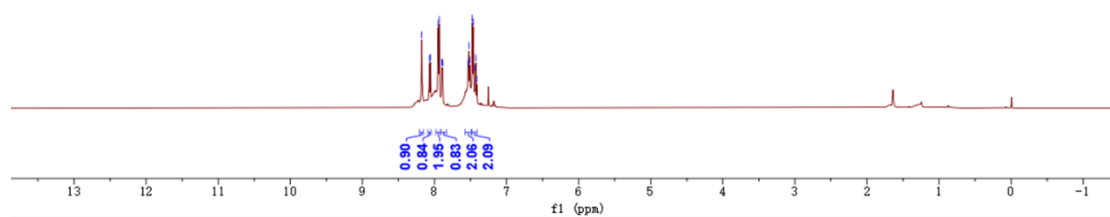
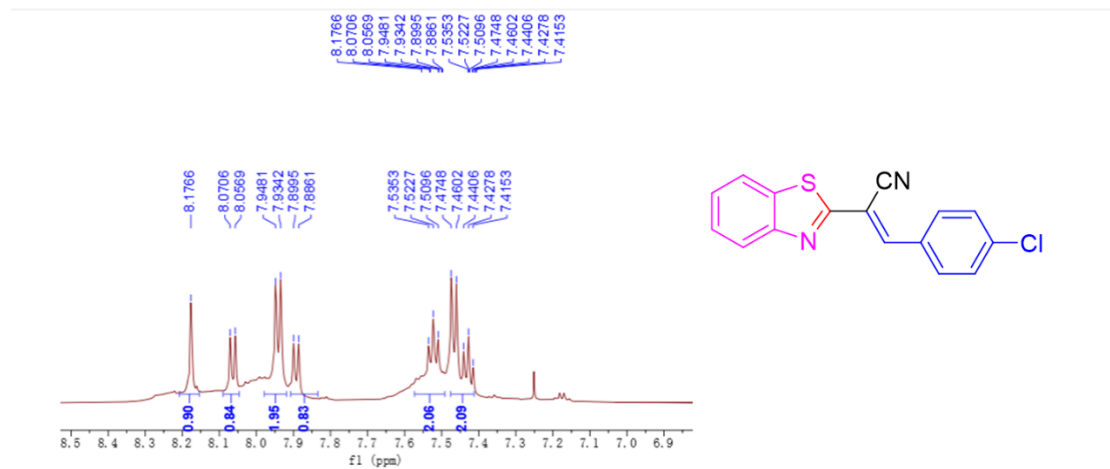
(E)-2-(Benzothiazol-2-yl)-3-(4-fluorophenyl)acrylonitrile (5j)



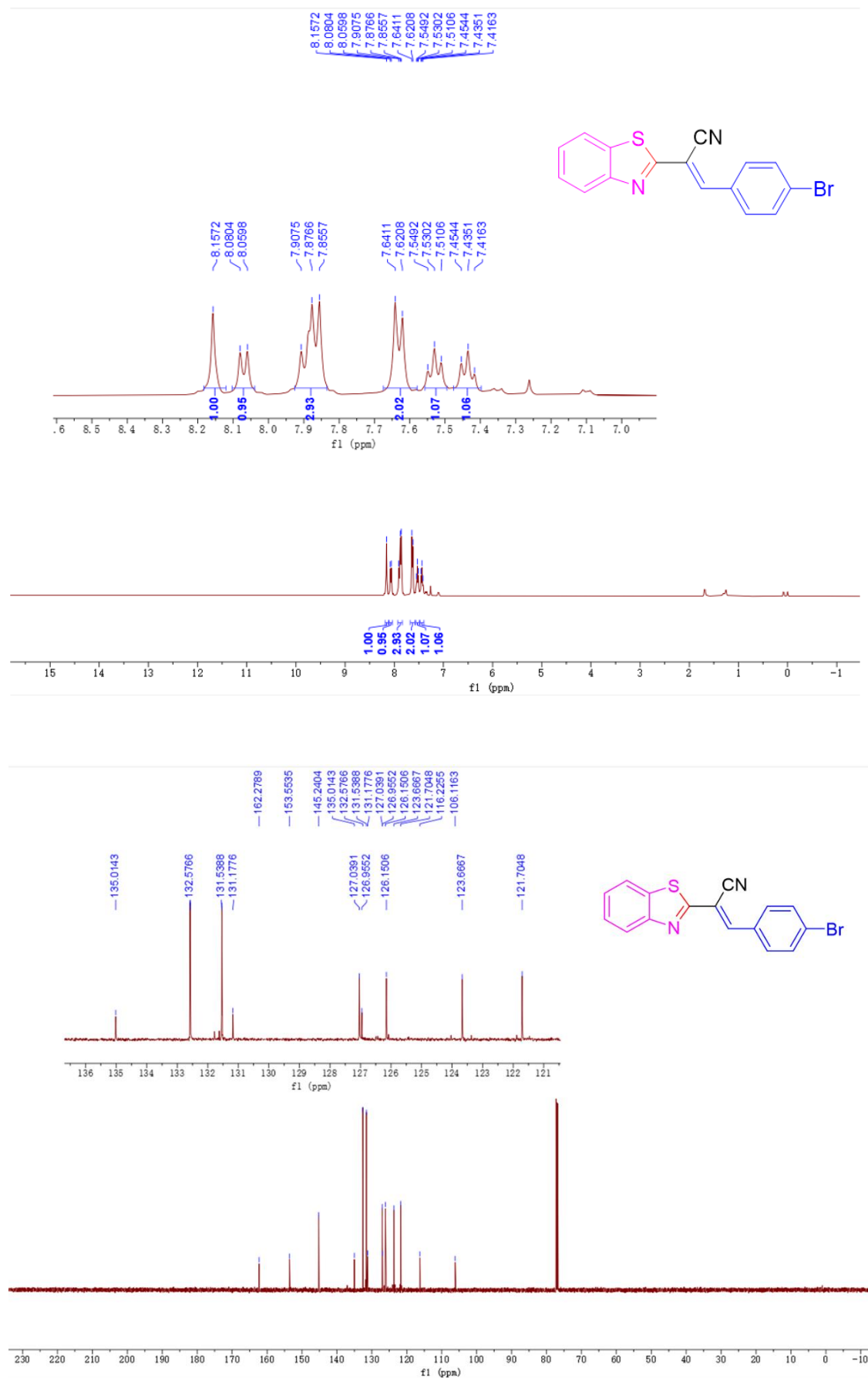
104.8089



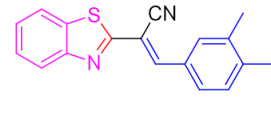
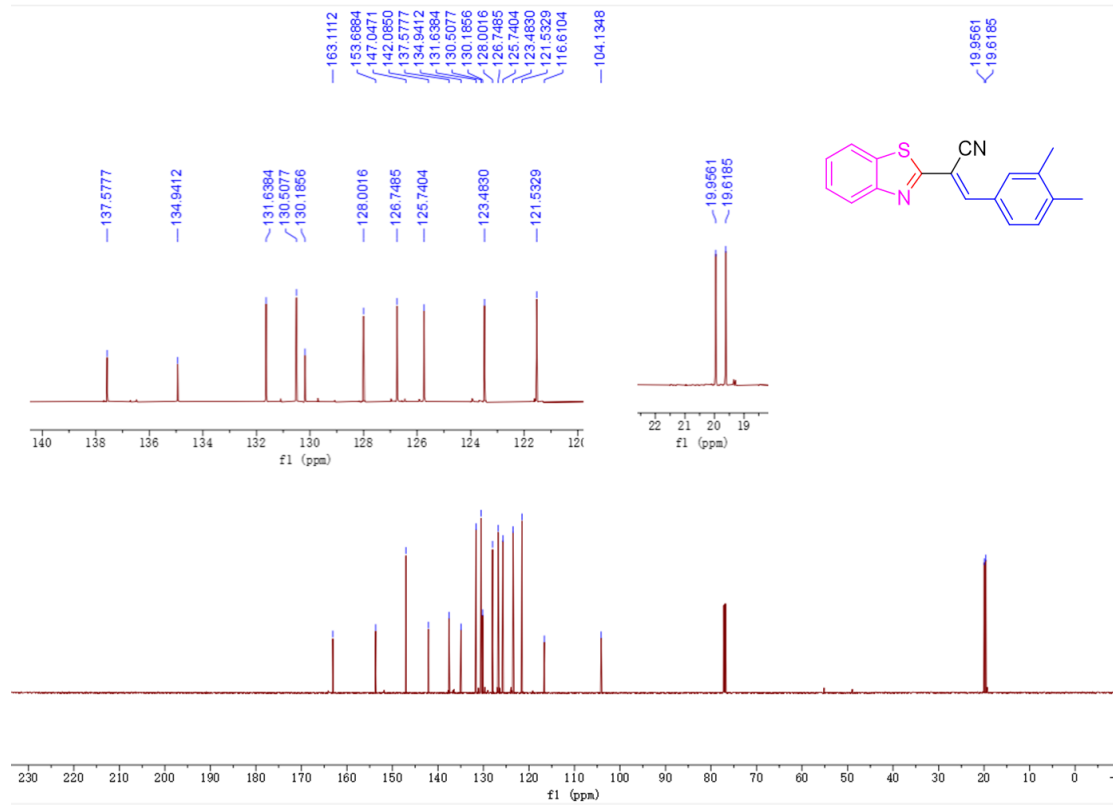
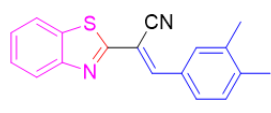
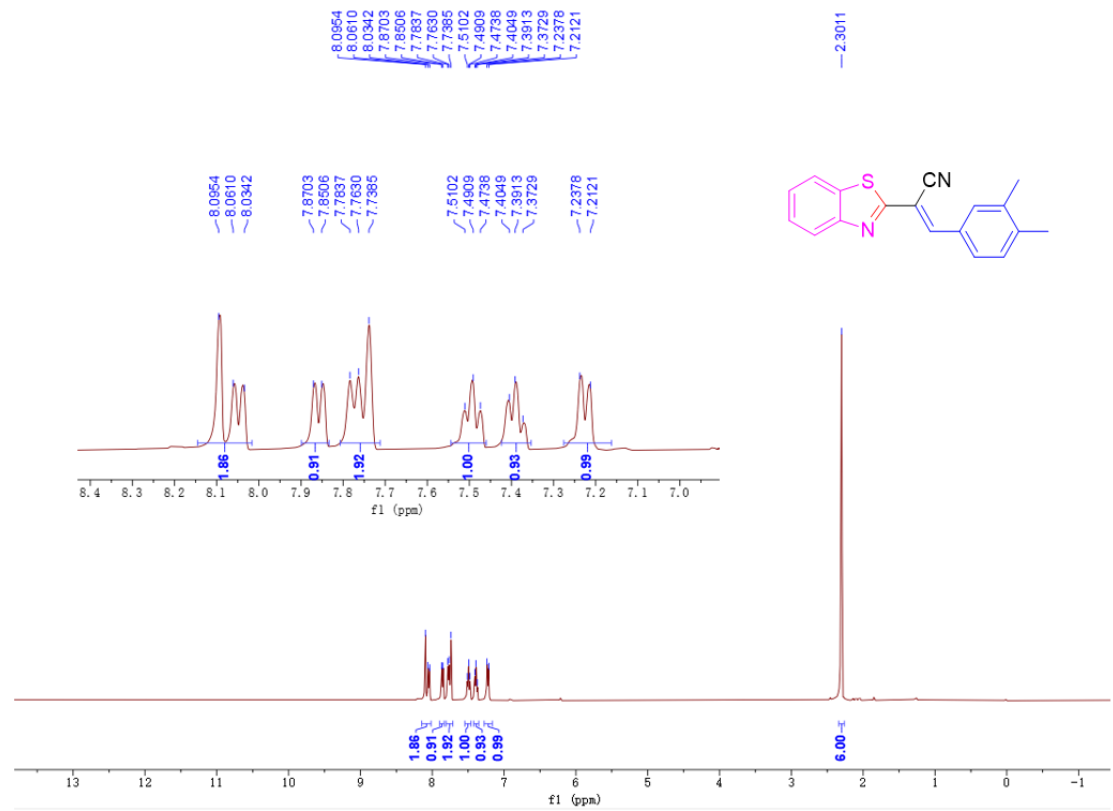
(E)-2-(Benzo[d]thiazol-2-yl)-3-(4-chlorophenyl)acrylonitrile (5k)



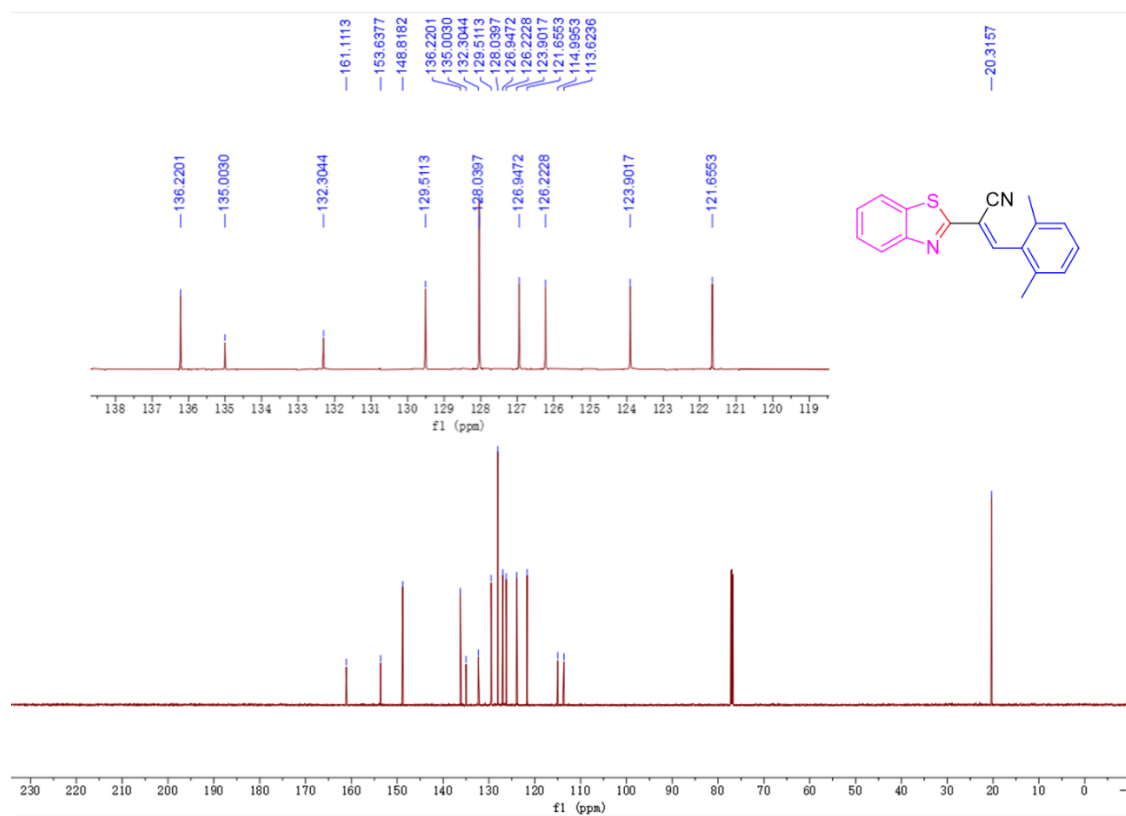
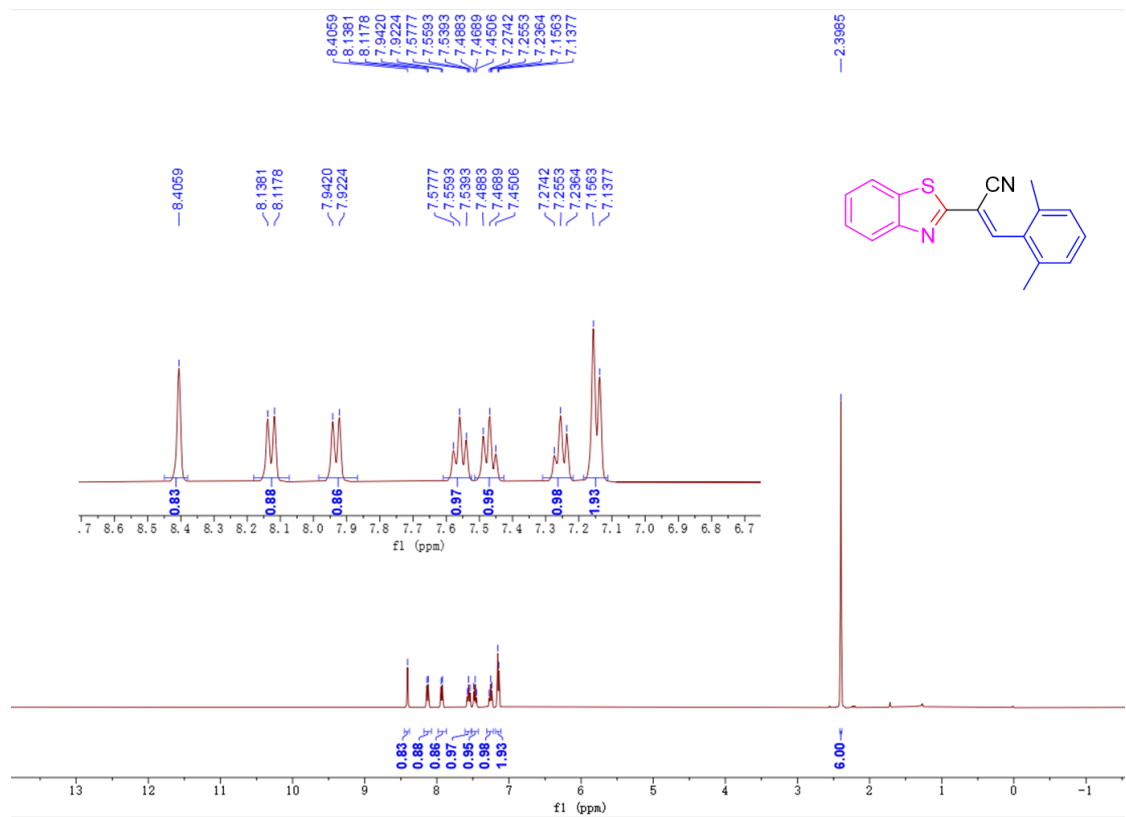
(E)-2-(Benzothiazol-2-yl)-3-(4-bromophenyl)acrylonitrile (5l)



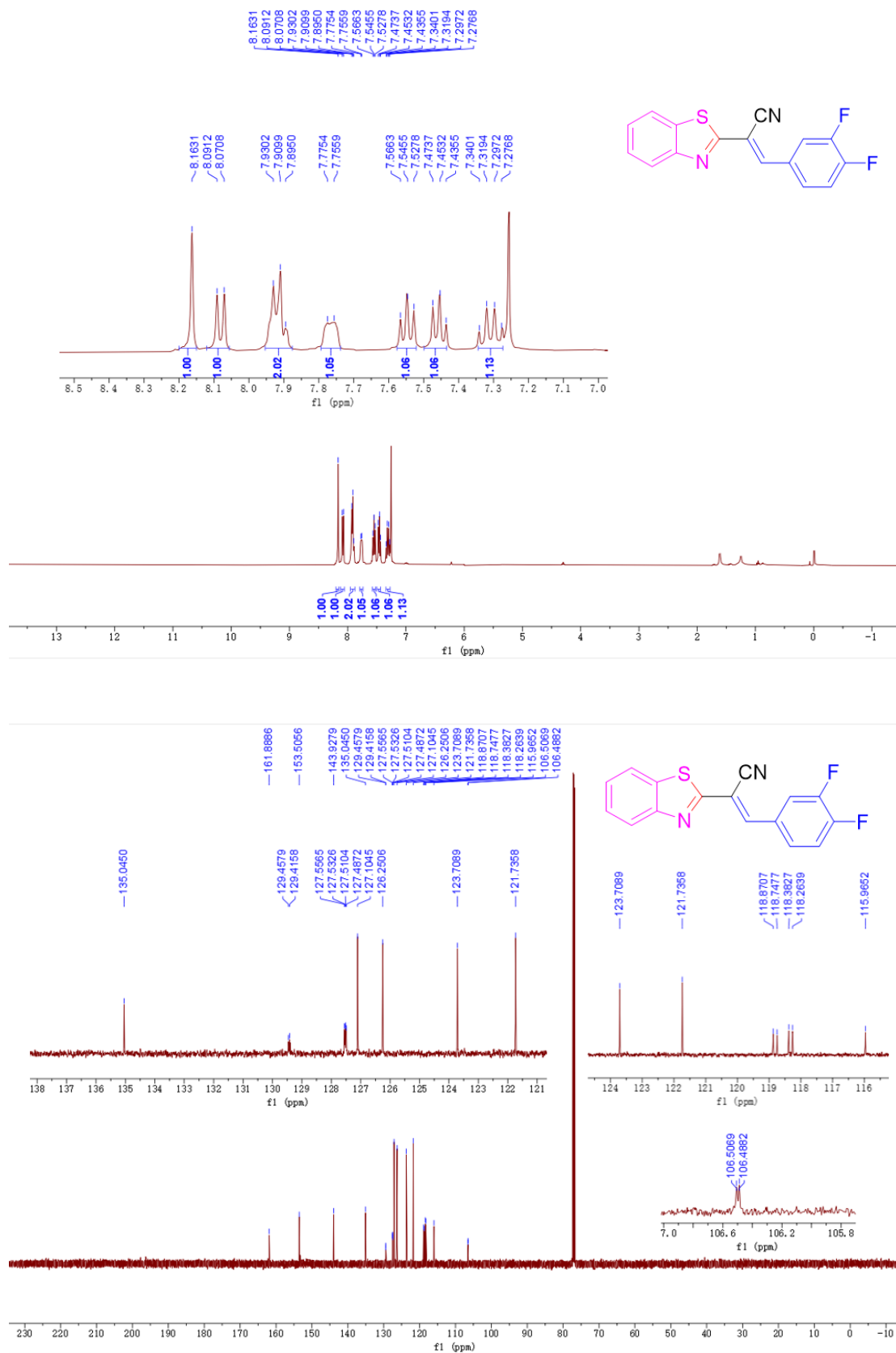
(E)-2-(Benzo[d]thiazol-2-yl)-3-(3,4-dimethylphenyl)acrylonitrile (5m)



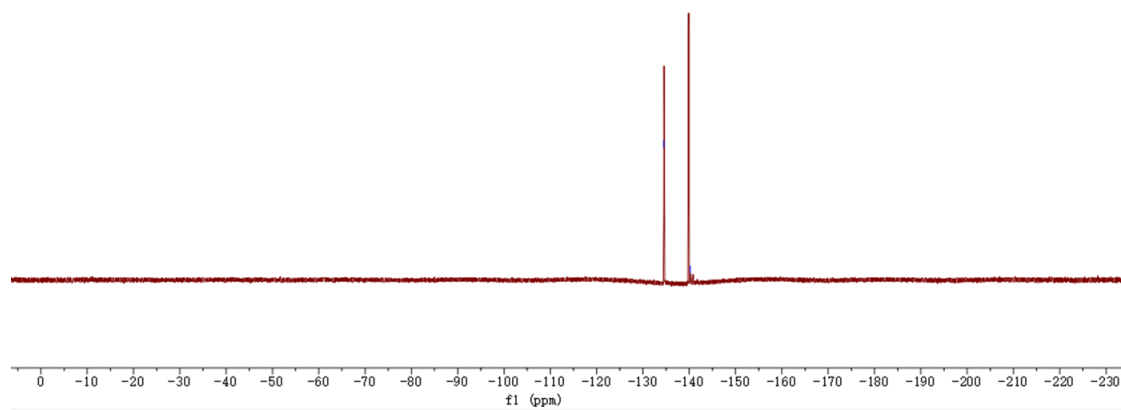
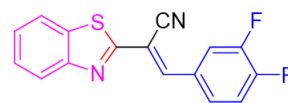
(E) -2-(Benzothiazol-2-yl)-3-(2,6-dimethylphenyl)acrylonitrile (5n)



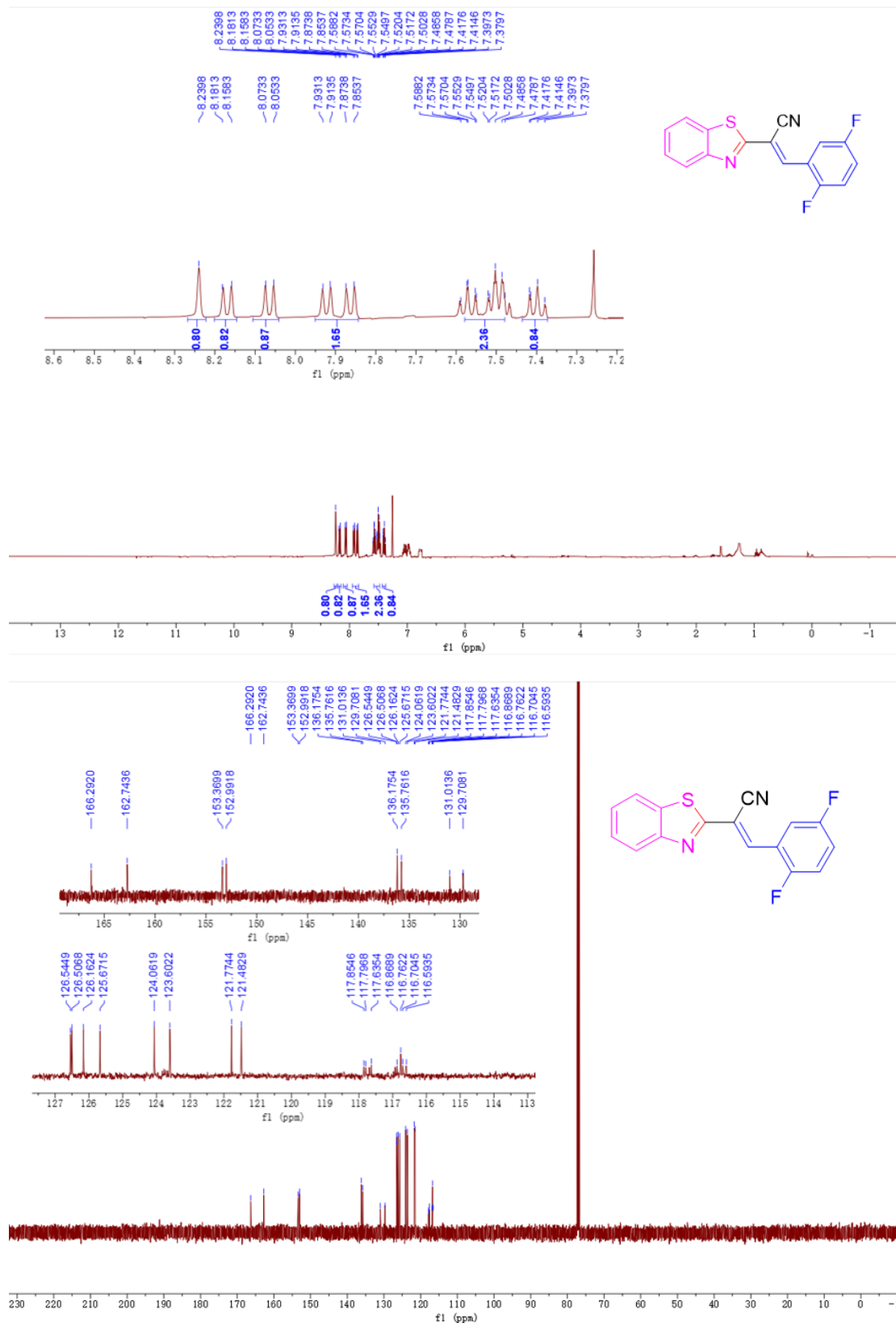
(E)-2-(Benzothiazol-2-yl)-3-(3,4-difluorophenyl)acrylonitrile (5o).

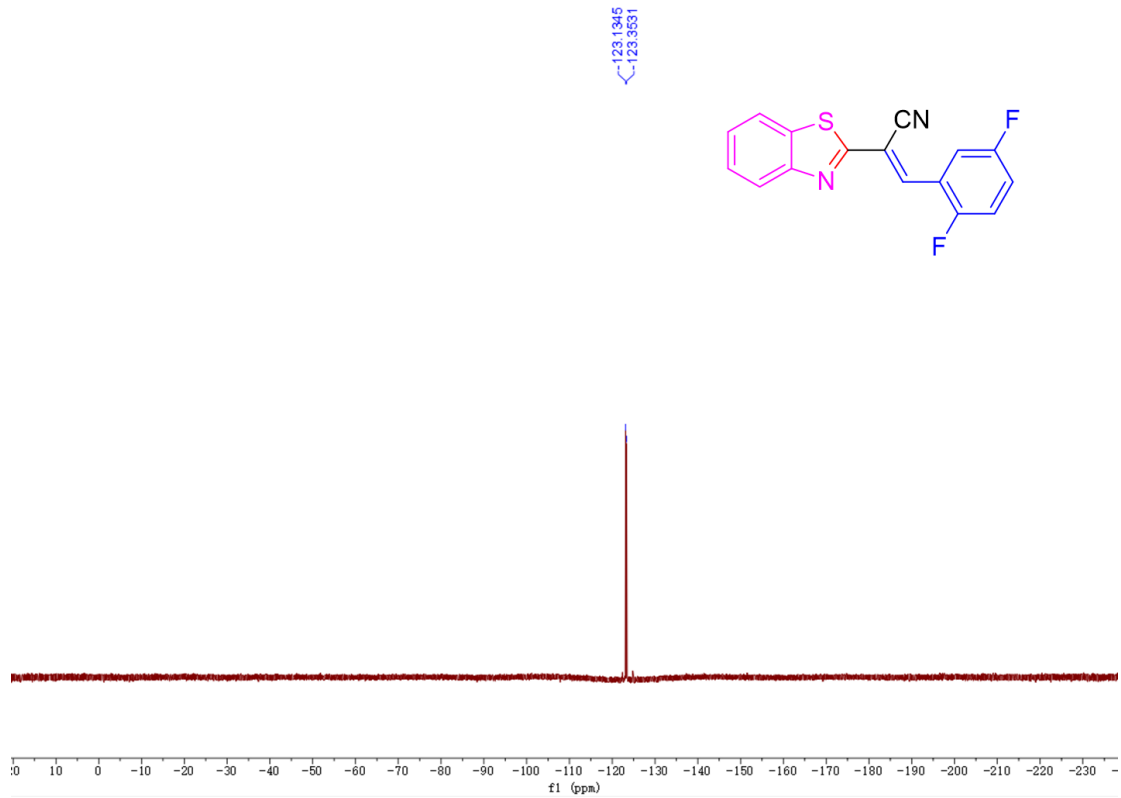


—134.5243
—140.2406

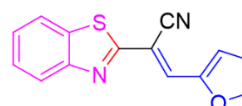
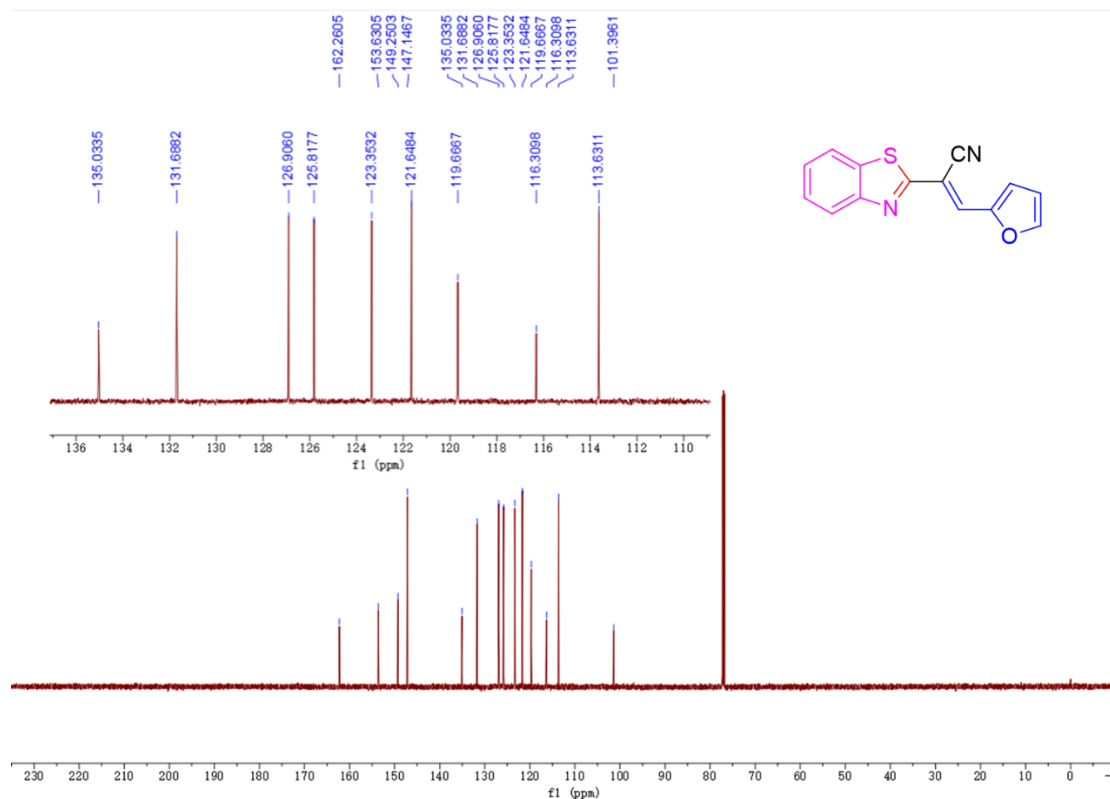
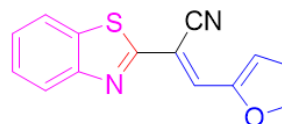
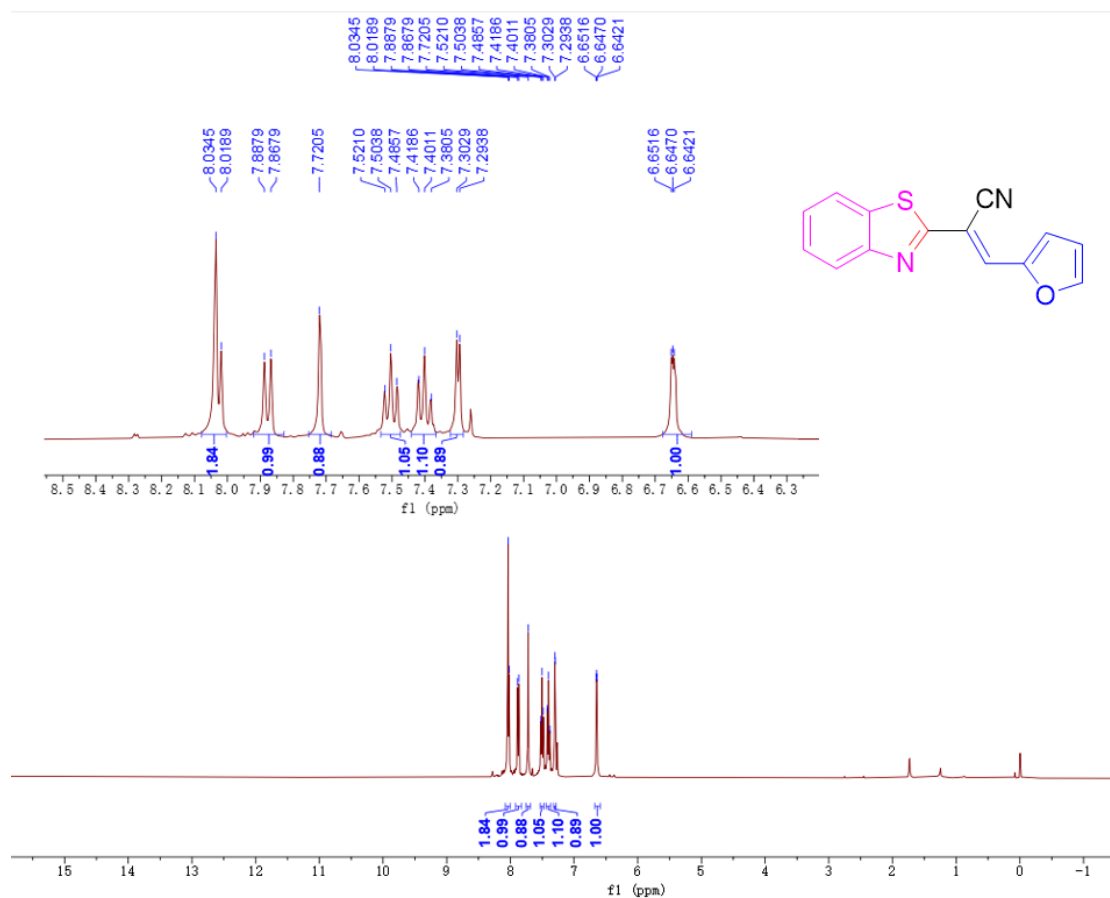


(E)-2-(Benzothiazol-2-yl)-3-(2,5-difluorophenyl)acrylonitrile (5p).

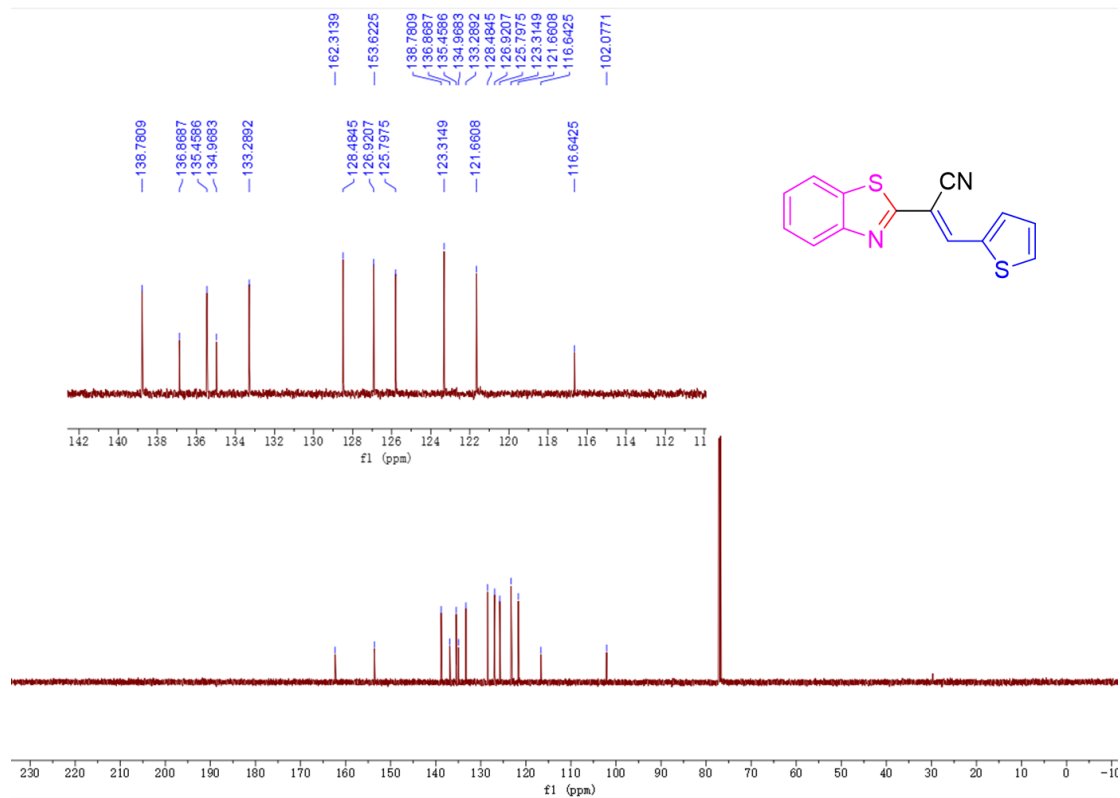
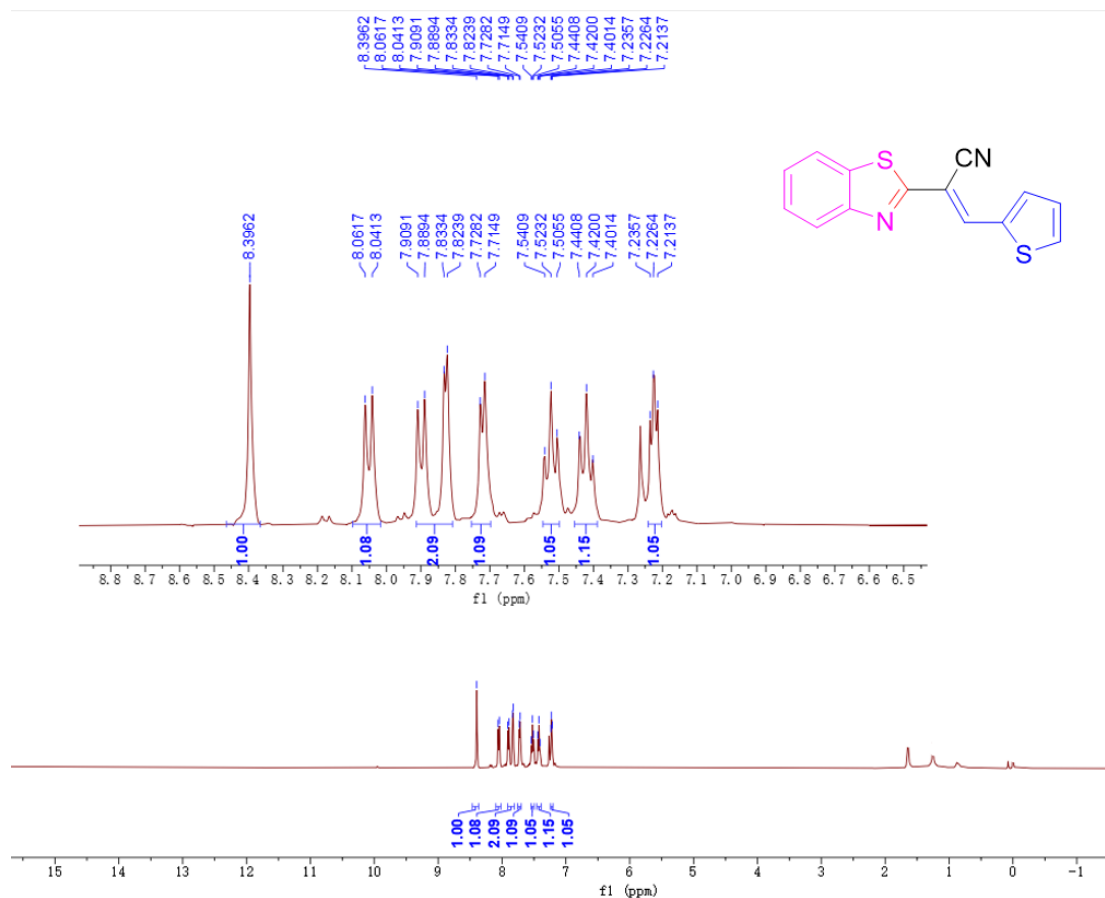




(E)-2-(Benzothiazol-2-yl)-3-(furan-2-yl)acrylonitrile (5q)



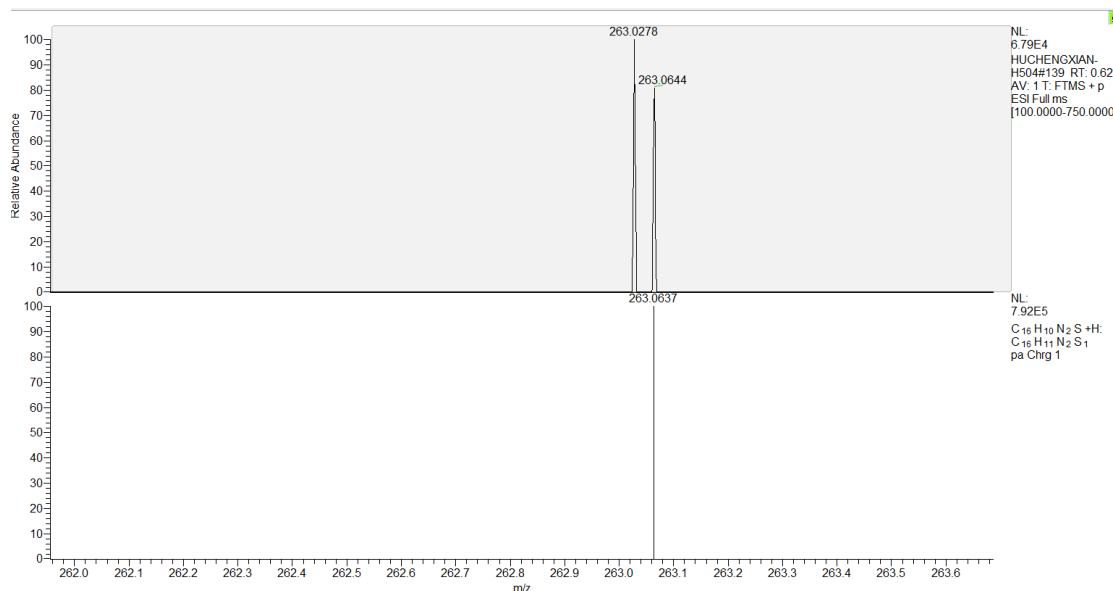
(E)-2-(Benzothiazol-2-yl)-3-(thiophen-2-yl)acrylonitrile (5r)



6. HRMS Spectra Copies of Products

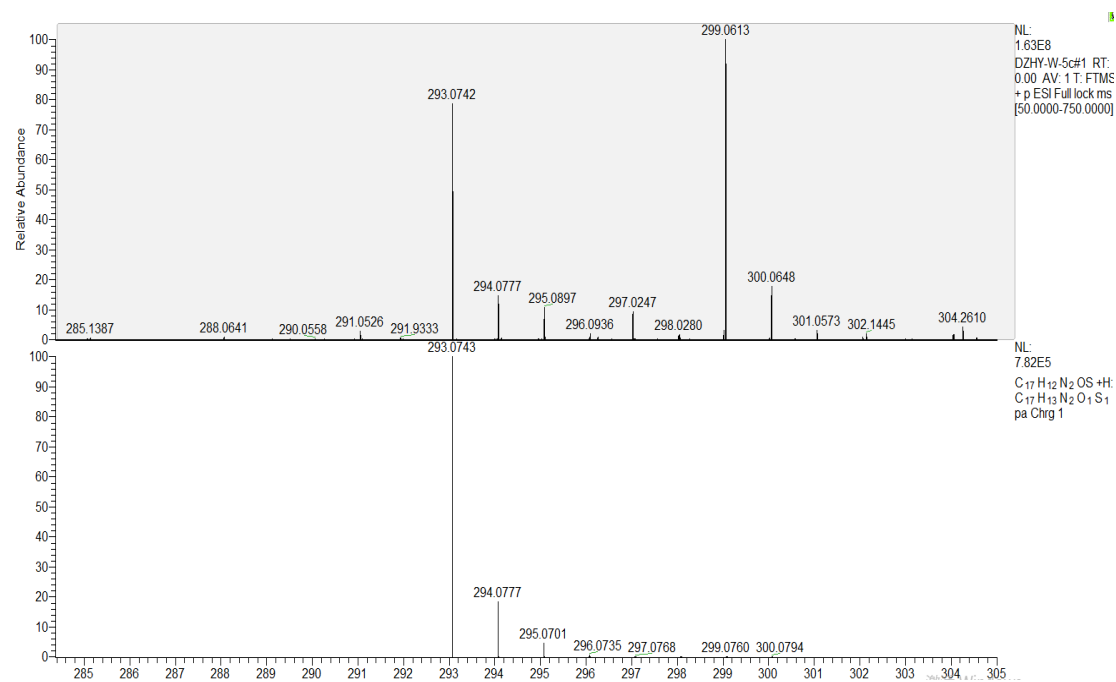
Product 5a

HRMS (ESI) m/z calcd for $C_{16}H_{10}N_2S^+$, (M+H)⁺ 263.0637, Found 263.0644.



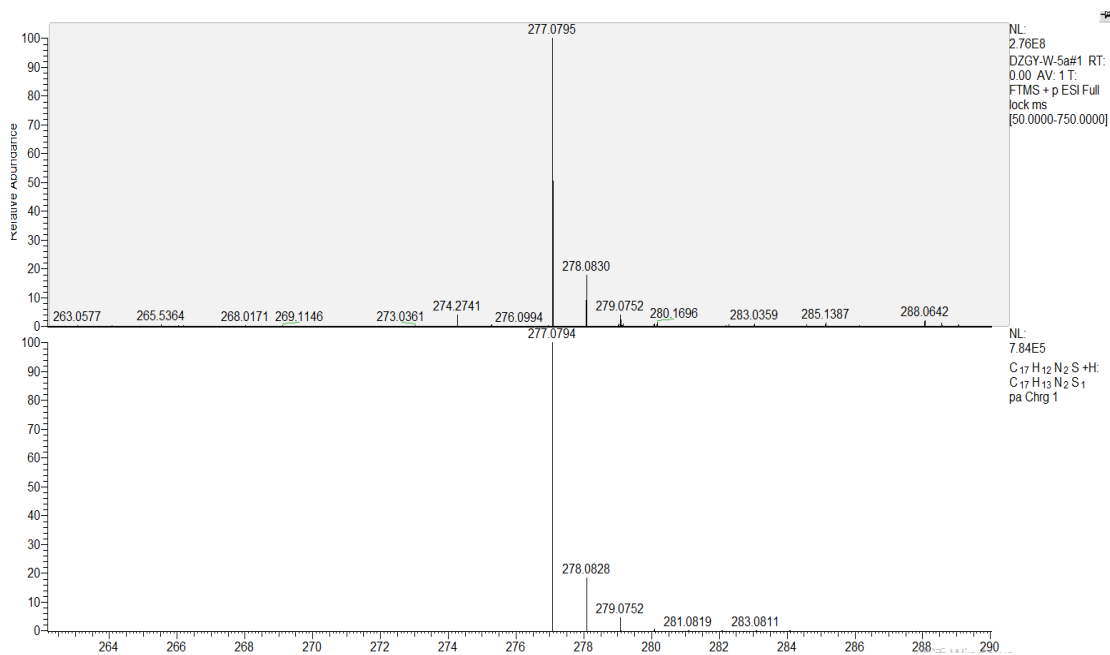
Product 5b

HRMS (ESI) m/z calcd for $C_{17}H_{12}N_2OS^+$, (M+H)⁺ 293.0743, Found 293.0742.



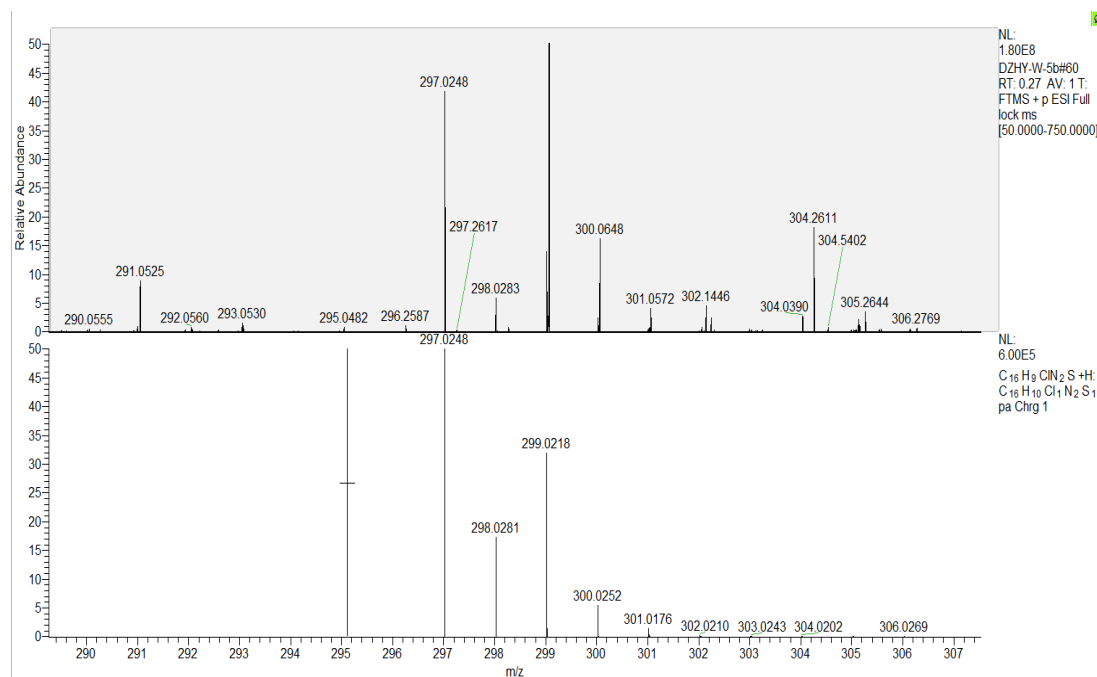
Product 5c

HRMS (ESI) m/z calcd for $C_{17}H_{12}N_2S^+$, $(M+H)^+$ 277.0794, Found 277.0795.



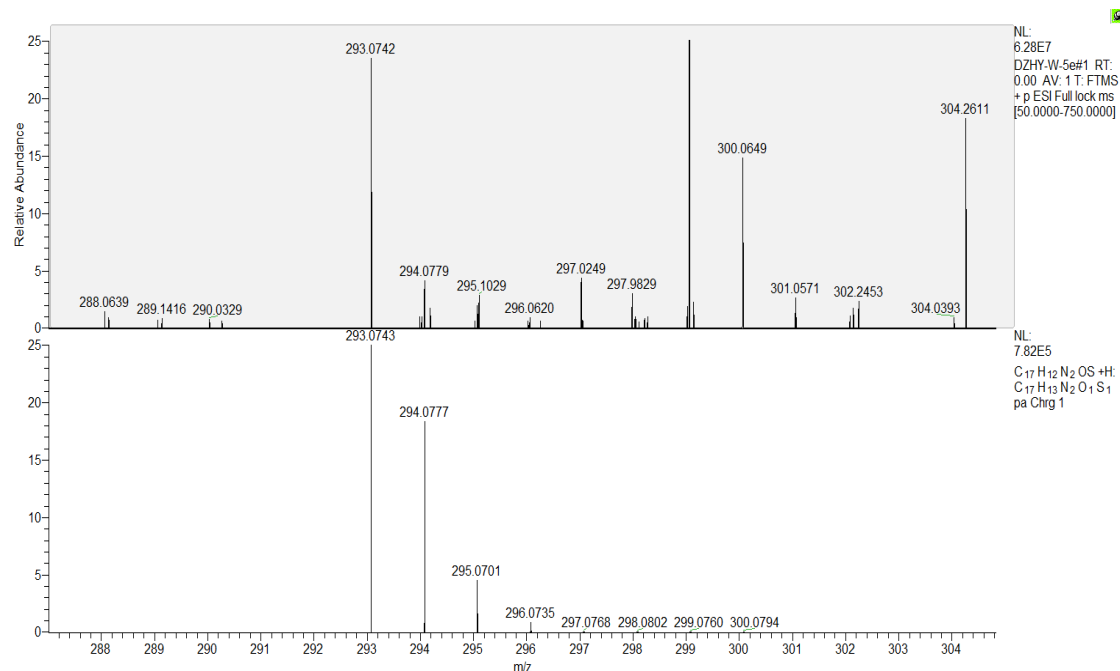
Product 5d

HRMS (ESI) m/z calcd for $C_{16}H_9ClN_2S^+$, $(M+H)^+$ 297.0248, Found 297.0248.



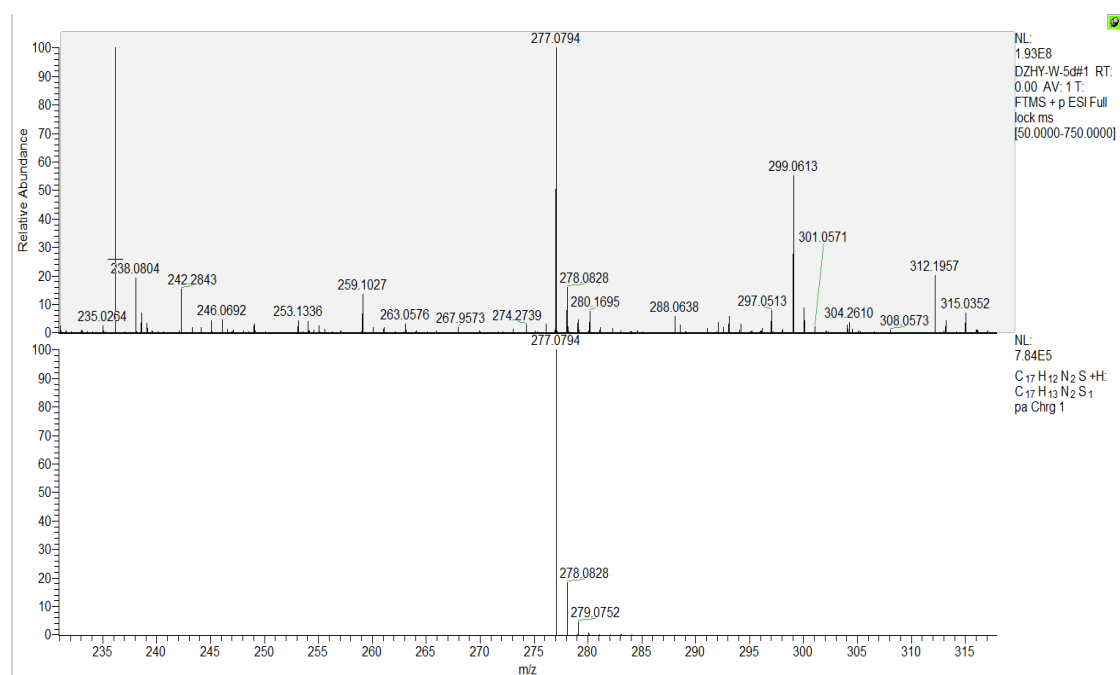
Product 5e

HRMS (ESI) m/z calcd for $C_{17}H_{12}N_2OS^+$, $(M+H)^+$ 293.0743, Found 293.0742.



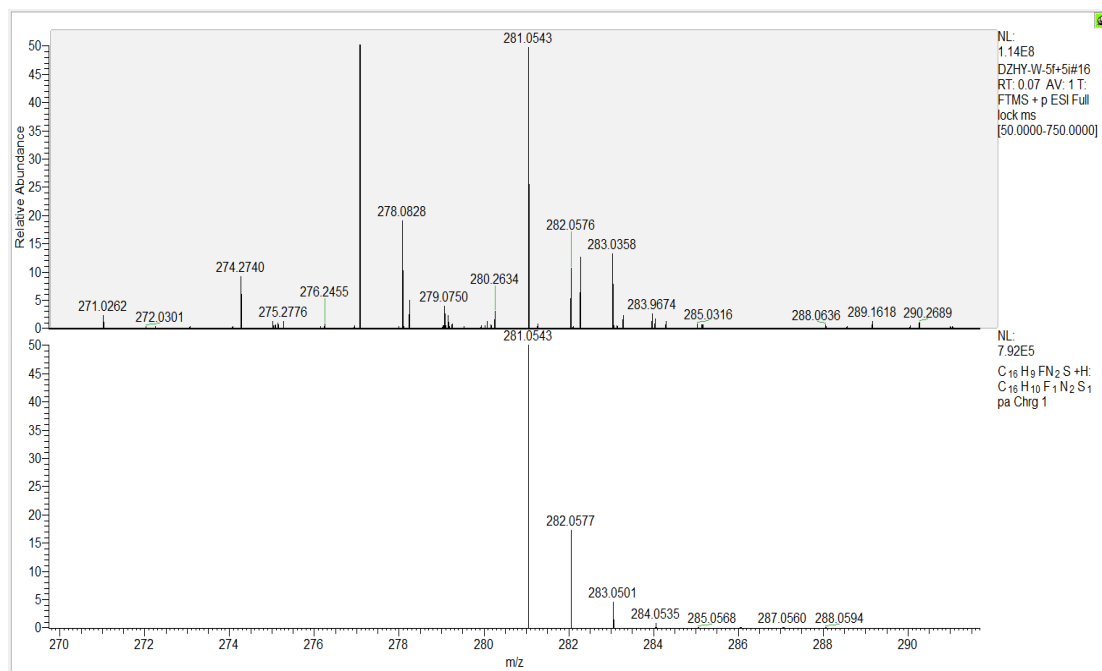
Product 5f

HRMS (ESI) m/z calcd for $C_{17}H_{12}N_2S^+$, $(M+H)^+$ 277.0794, Found 277.0794.



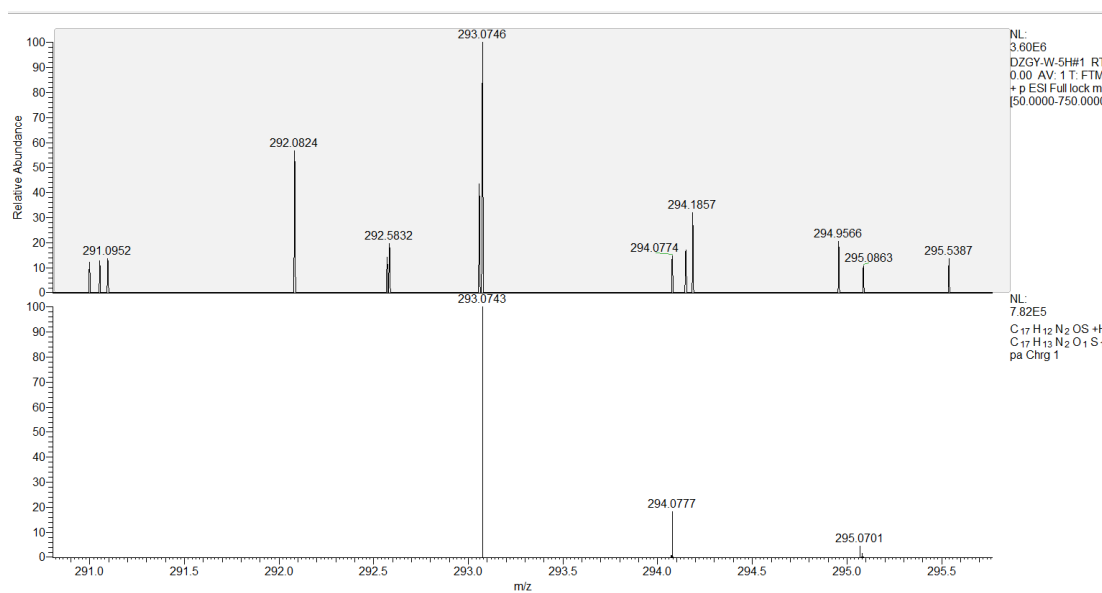
Product 5g

HRMS (ESI) m/z calcd for $C_{16}H_9N_2FS^+$, $(M+H)^+$ 281.0543, Found 281.0543.



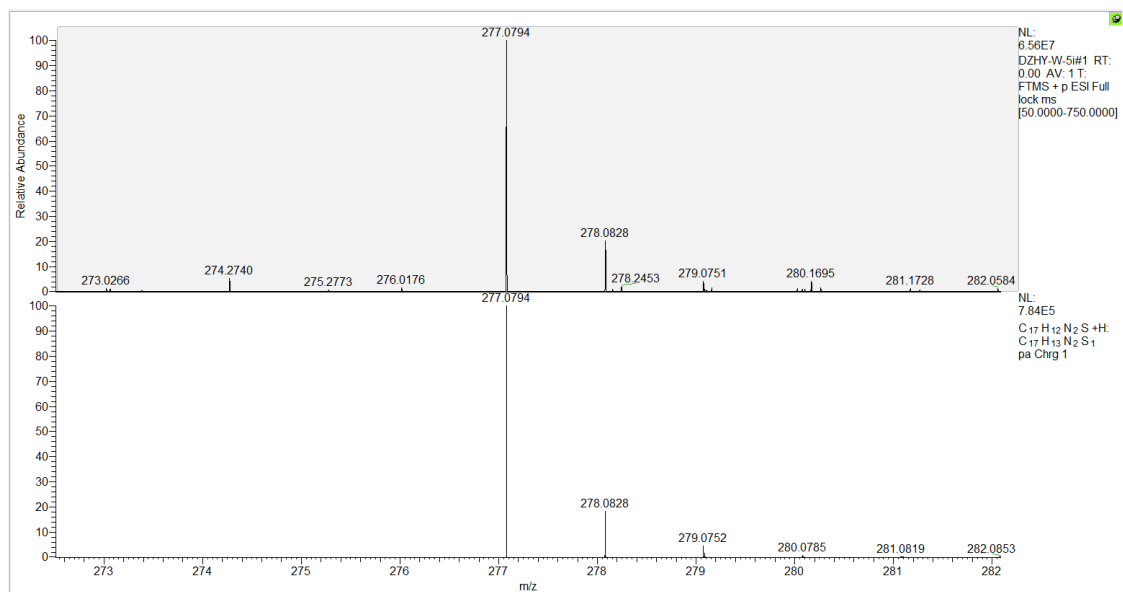
Product 5h

HRMS (ESI) m/z calcd for $C_{17}H_{12}N_2OS^+$, $(M+H)^+$ 293.0743, Found 293.0746.



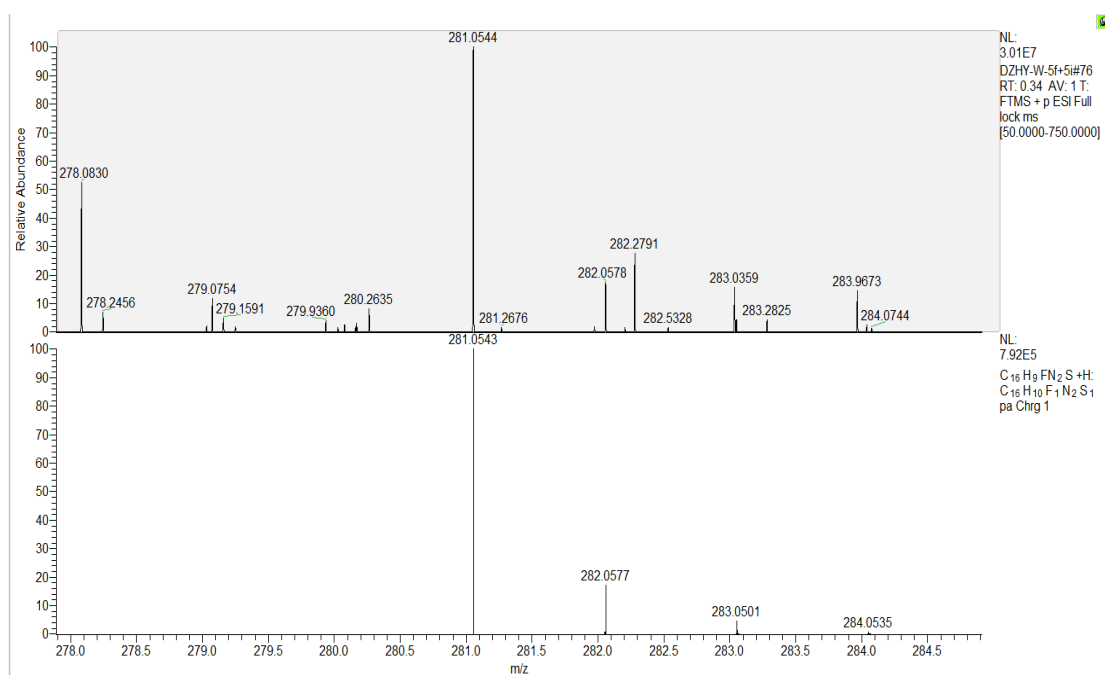
Product 5i

HRMS (ESI) m/z calcd for $C_{17}H_{12}N_2S^+$, $(M+H)^+$ 277.0794, Found 277.0794.



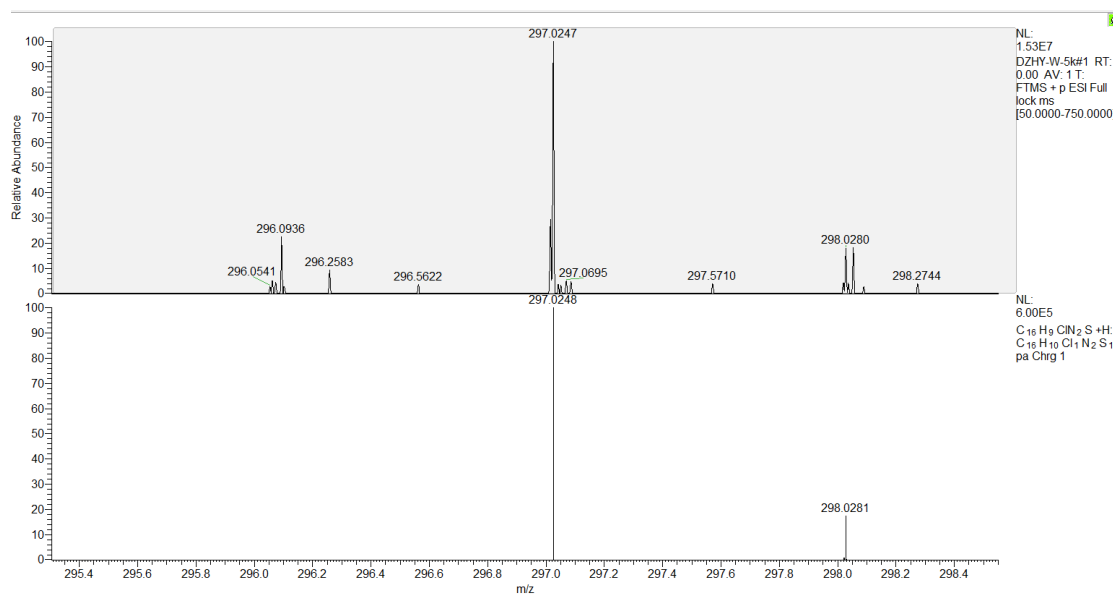
Product 5j

HRMS (ESI) m/z calcd for $C_{16}H_9N_2FS^+$, $(M+H)^+$ 281.0543, Found 281.0544.



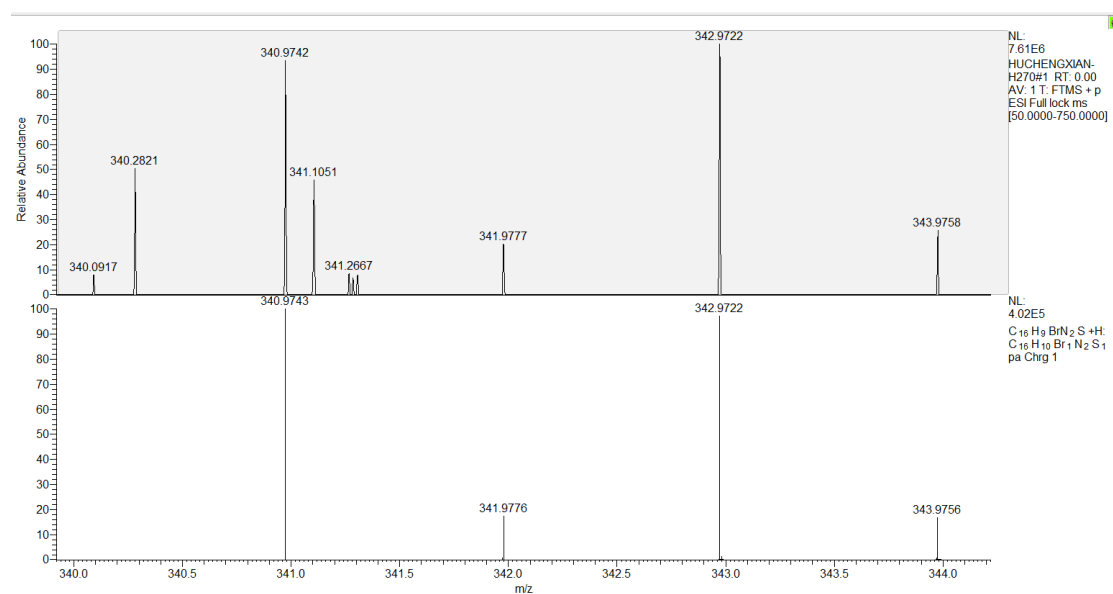
Product 5k

HRMS (ESI) m/z calcd for $C_{16}H_9N_2ClS^+$, (M+H)⁺ 297.0248, Found 297.0247.



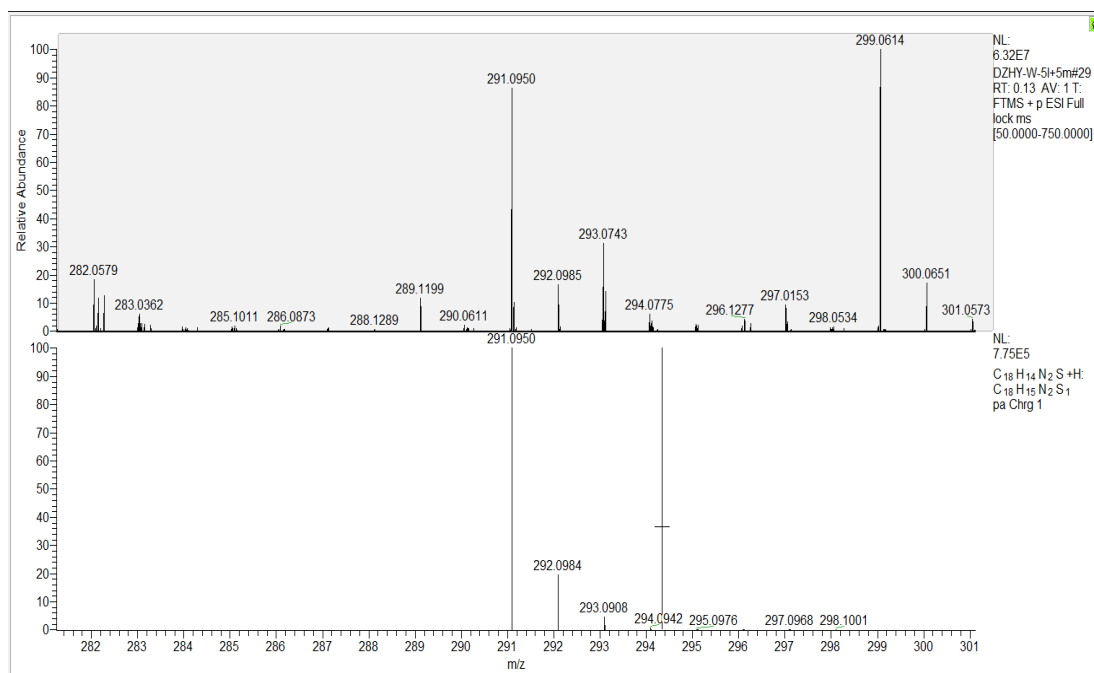
Product 5l

HRMS (ESI) m/z calcd for $C_{16}H_9N_2BrS^+$, (M+H)⁺ 340.9743, Found 340.9742.



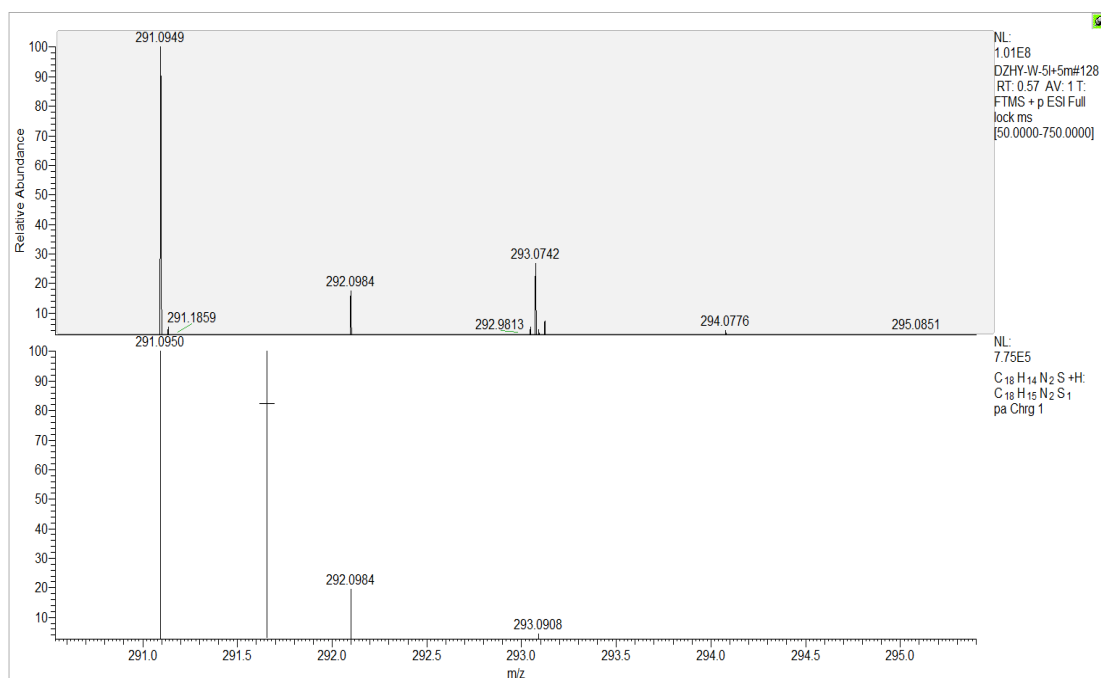
Product 5m

HRMS (ESI) m/z calcd for $C_{18}H_{14}N_2S^+$, $(M+H)^+$ 291.0950, Found 291.0950.



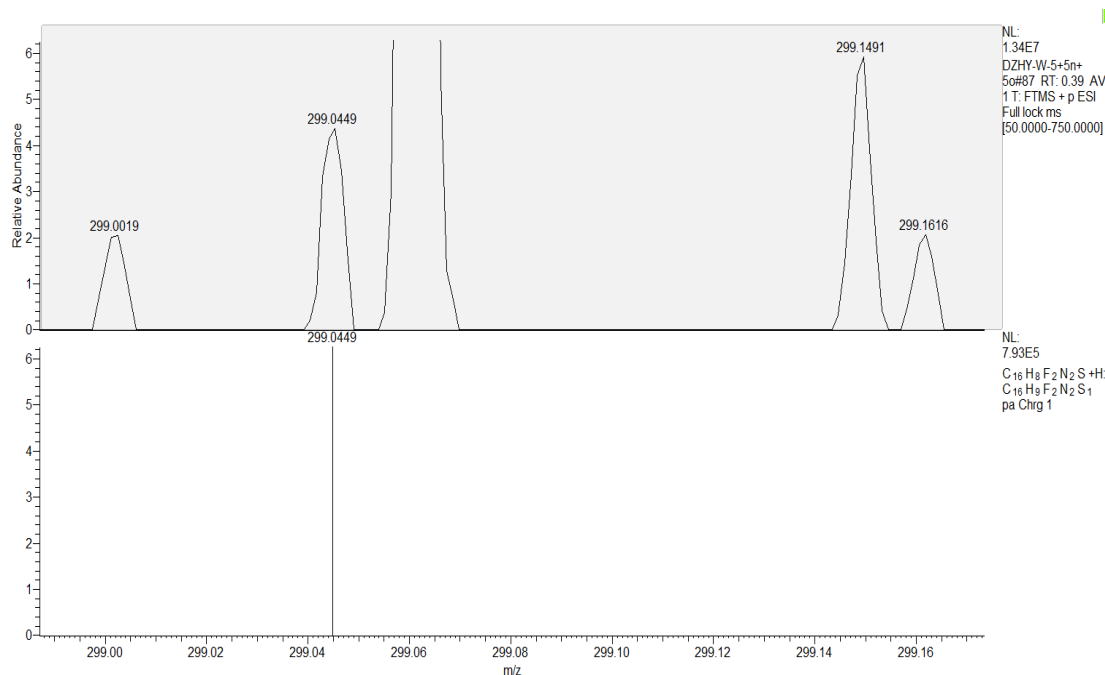
Product 5n

HRMS (ESI) m/z calcd for $C_{18}H_{14}N_2S^+$, $(M+H)^+$ 291.0950, Found 291.0949.



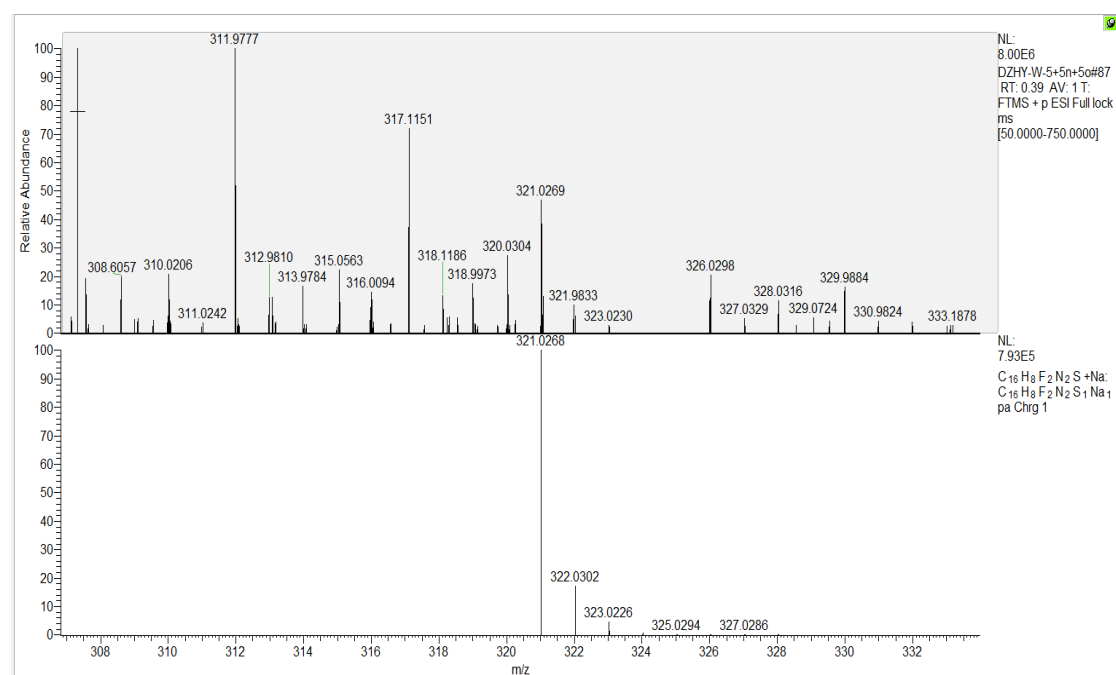
Product 5o

HRMS (ESI) m/z calcd for $C_{16}H_8F_2N_2S^+$, $(M+H)^+$ 299.0449, Found 299.0449.



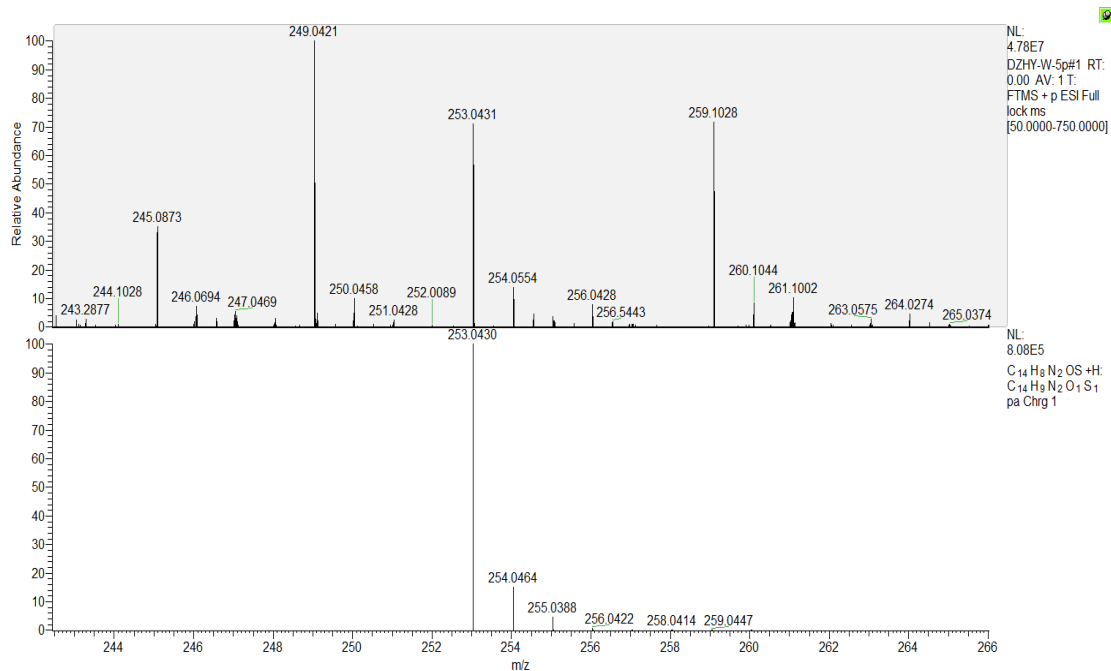
Product 5p

HRMS (ESI) m/z calcd for $C_{16}H_8F_2N_2S^+$, $(M+Na)^+$ 321.0268, Found 321.0269.



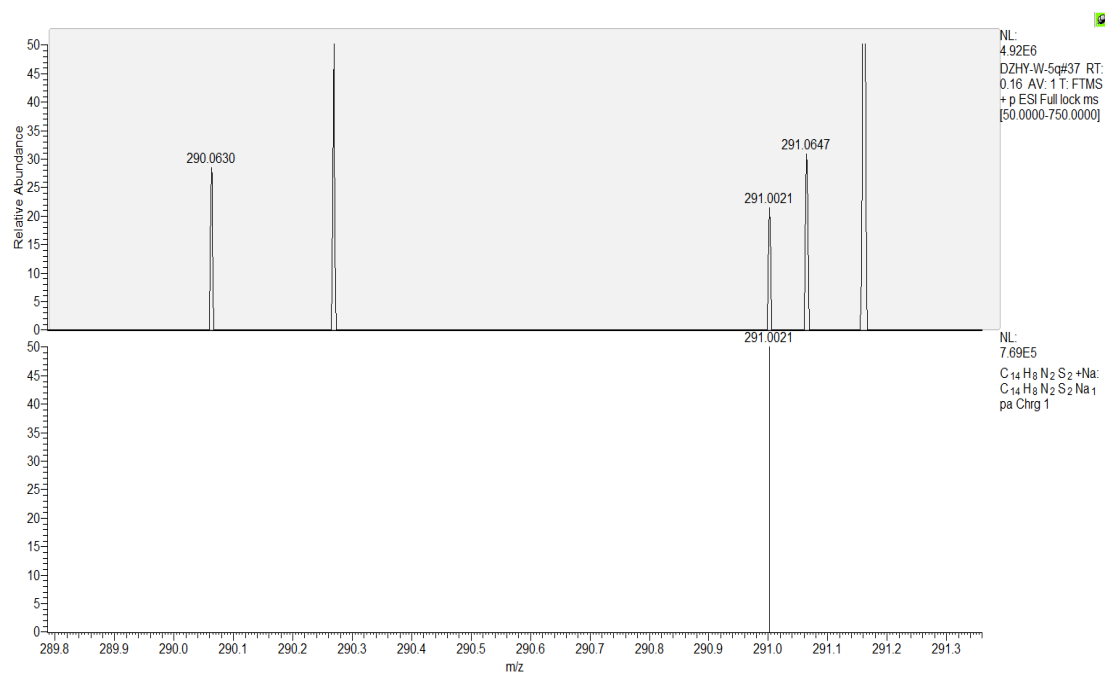
Product 5q

HRMS (ESI) m/z calcd for $C_{14}H_8N_2SO^+$, $(M+H)^+$ 253.0430, Found 253.0431.

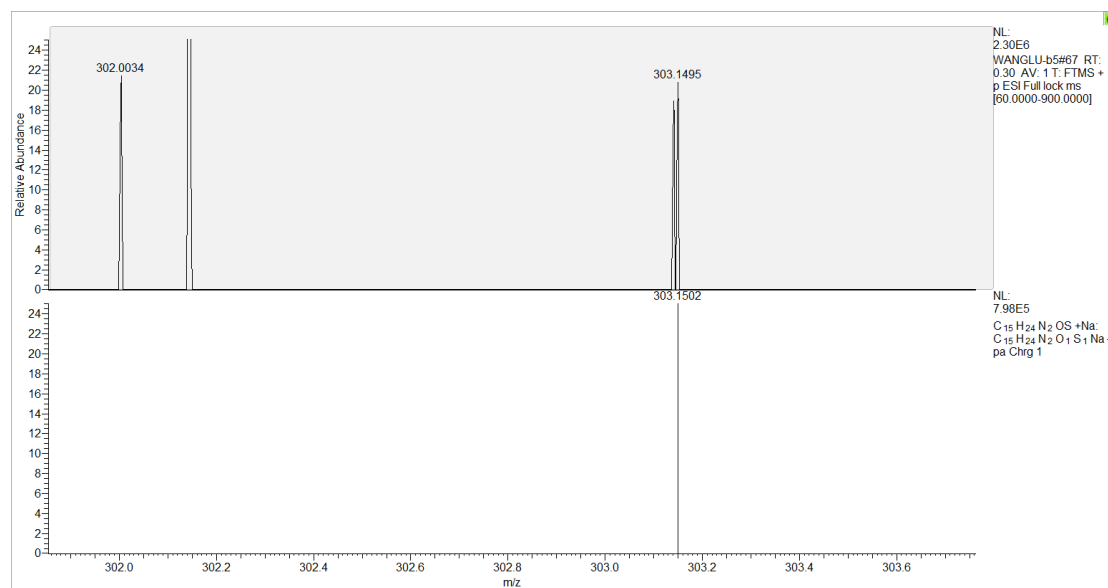


Product 5r

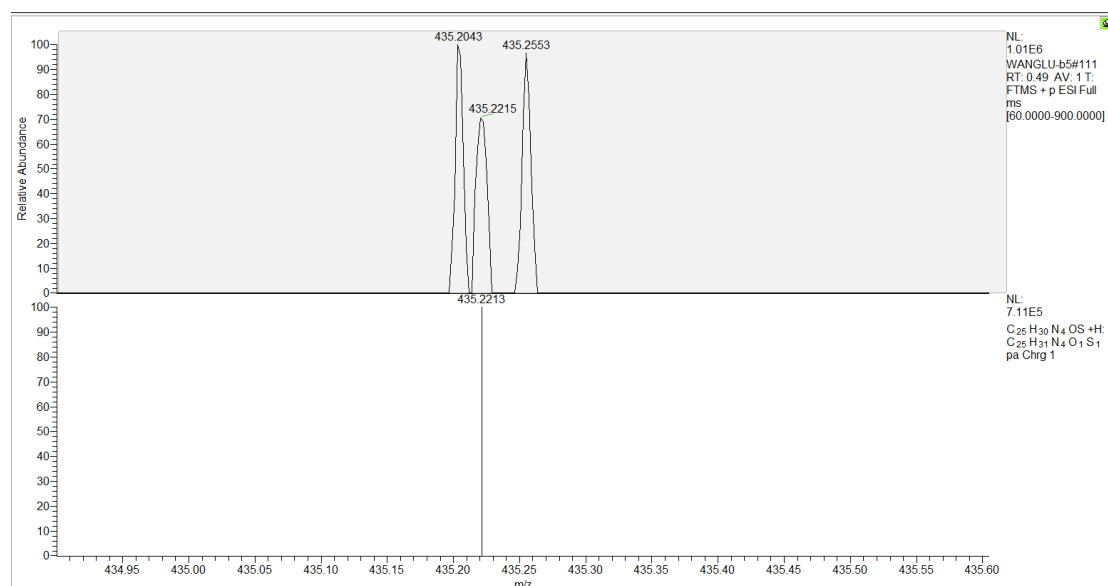
HRMS (ESI) m/z calcd for $C_{14}H_8N_2S_2^+$, $(M+Na)^+$ 291.0021, Found 291.0021.



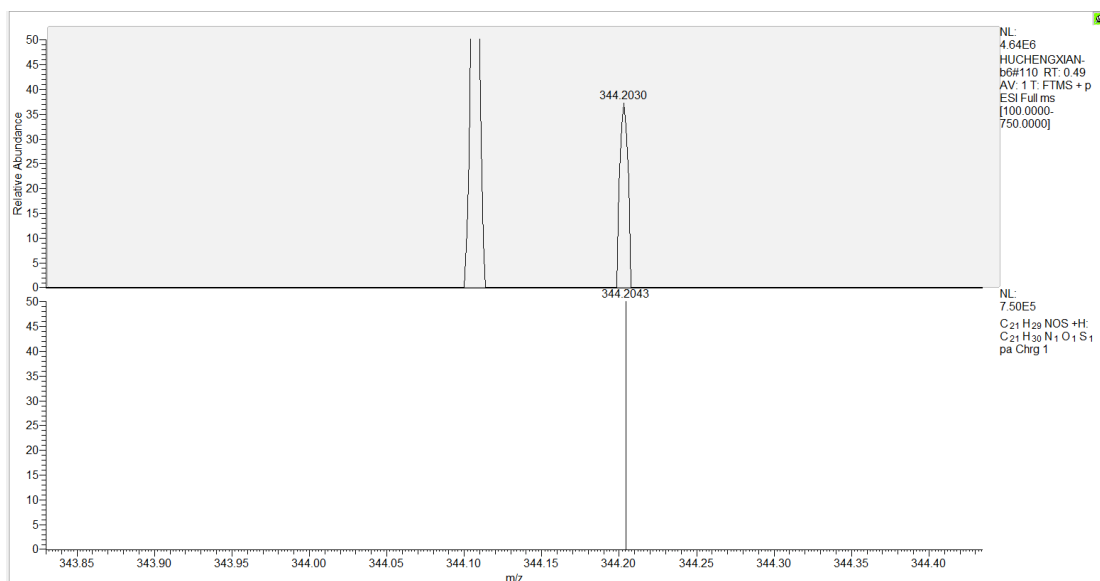
Product 7



Product 8



Product 9



Product 10

