Trimethylindolenines as C-N synthons for the assembly of spiro[oxindole-thioxoimidazolidine-indoline] hybrids in formal [3+2] cycloadditions

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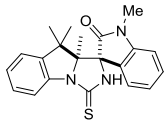
1. General information

Reactions were monitored by thin layer chromatography using UV light to visualize the course of reaction. Purification of reaction products was carried out by flash chromatography on silica gel or just by simple filtration and washing. ^{1}H and ^{13}CNMR spectra were obtained using a Bruker DPX-400 spectrometer. ^{1}H NMR chemical shifts are reported in ppm (δ) relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz) and integration. ^{13}C NMR chemical shifts are reported in ppm (δ) from tetramethylsilane (TMS) with the solvent resonance as the internal standard. Melting points were measured on an electrothermal digital melting point apparatus.

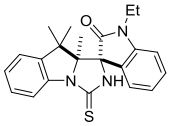
2. The 0.2 mmol scale synthesis of spiro[oxindole-thioxoimidazolidine-indoline] hybrids 3

In a sealed tube equipped with a magnetic stirring bar, a mixture of 3-isothiocyanato oxindole **1** (0.2 mmol), trimethylindolenine **2** (0.3 mmol) in 1.0 mL of DCM was stirred under catalyst-free condition at rt for 5 h, and then was directly loaded onto a silica gel and purified by flash chromatography to give the desired product **3**, using hexane/EtOAc (8/1, v/v) as the eluent.

3. Characterization data of compounds 3

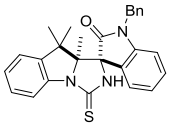


3aa: Light yellow solid, m.p. 200.3-201.5 ^{o}C; yield 85% (61.7 mg), >20:1 dr; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.61 (s, 3H), 1.15 (s, 3H), 1.45 (s, 3H), 3.15 (s, 3H), 6.48 (s, 1H), 6.76 (d, J = 8.0 Hz, 1H), 6.84-6.87 (m, 1H), 6.93 (d, J = 7.6 Hz, 1H), 6.98-7.02 (m, 1H), 7.16-7.26 (m, 3H), 8.16 (d, J = 7.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 18.6, 22.1, 26.1, 28.5, 46.7, 70.3, 81.7, 107.6, 114.3, 121.0, 121.6, 123.7, 125.8, 126.4, 126.5, 129.7, 136.0, 141.9, 143.4, 173.2, 177.0; HRMS (ESI-TOF) m/z: Calcd. for $C_{21}H_{21}N_3NaOS$ $[M+Na]^+$: 386.1298; Found: 386.1287.

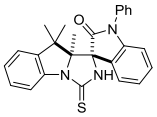


3ab: Light yellow solid, m.p. 180.4-181.3 ^{o}C; yield 75% (56.6 mg), >20:1 dr; ^{1}H NMR ($CDCl_3$,

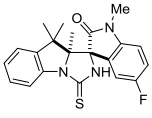
400 MHz) δ: 0.60 (s, 3H), 1.17 (s, 3H), 1.21-1.25 (m, 3H), 1.51 (s, 3H), 3.50-3.55 (m, 1H), 3.85-3.90 (m, 1H), 6.16-6.24 (m, 1H), 6.77 (d, J = 8.0 Hz, 1H), 6.84-6.88 (m, 1H), 6.95 (d, J = 7.6 Hz, 1H), 7.00-7.03 (m, 1H), 7.19-7.26 (m, 3H), 8.20 (d, J = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 12.6, 19.6, 23.1, 29.5, 35.3, 47.7, 71.3, 82.8, 108.5, 115.3, 122.0, 122.5, 124.8, 127.0, 127.6, 127.7, 130.7, 137.0, 141.9, 144.4, 173.4, 178.0; HRMS (ESI-TOF) m/z: Calcd. for $C_{22}H_{23}N_3NaOS$ $[M+Na]^+$: 400.1454; Found: 400.1448.



3ac: Light yellow solid, m.p. 155.4-156.0 ^{o}C; yield 92% (80.8 mg), 10:1 dr; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.54 (s, 3H), 1.11 (s, 3H), 1.48 (s, 3H), 4.50 (d, J = 15.6 Hz, 1H), 5.12 (d, J = 15.2 Hz, 1H), 6.55-6.61 (m, 1H), 6.69 (d, J = 7.6 Hz, 1H), 6.80-6.83 (m, 1H), 6.93 (d, J = 6.4 Hz, 1H), 6.97-7.01 (m, 1H), 7.14-7.27 (m, 8H), 8.19 (d, J = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.8, 23.0, 29.8, 44.5, 47.6, 71.3, 82.9, 109.4, 115.2, 122.1, 122.7, 124.7, 126.9, 127.5, 127.6, 127.8, 128.0, 128.9, 129.0, 130.6, 135.5, 136.9, 142.1, 144.4, 173.9, 177.6; HRMS (ESI-TOF) m/z: Calcd. for $C_{27}H_{25}N_3NaOS$ $[M+Na]^+$: 462.1611; Found: 462.1606.

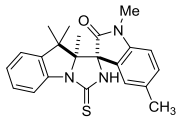


3ad: Light yellow solid, m.p. 214.6-215.5 ^{o}C; yield 84% (71.4 mg), >20:1 dr; ^{1}H NMR (DMSO-d_6, 400 MHz) δ: 0.95 (s, 3H), 1.19 (s, 3H), 1.46 (s, 3H), 6.71 (d, J = 8.0 Hz, 1H), 7.01-7.05 (m, 1H), 7.10-7.18 (m, 2H), 7.25-7.34 (m, 3H), 7.42-7.45 (m, 2H), 7.49-7.53 (m, 1H), 7.60-7.64 (m, 2H), 7.96 (d, J = 7.6 Hz, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ: 19.7, 23.2, 28.4, 48.7, 71.7, 82.8, 109.9, 116.3, 122.6, 123.1, 125.3, 126.3, 127.2, 127.3, 127.5, 129.1, 130.4, 130.9, 134.3, 139.2, 143.8, 144.6, 173.9, 181.9; HRMS (ESI-TOF) m/z: Calcd. for $C_{26}H_{23}N_3NaOS$ $[M+Na]^+$: 448.1454; Found: 448.1448.

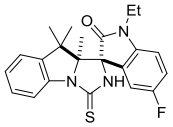


3ae: Light yellow solid, m.p. 192.3-193.0 ^{o}C; yield 90% (68.6 mg), >20:1 dr; ^{1}H NMR ($CDCl_3$,

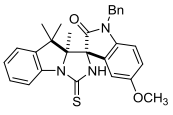
400 MHz) δ: 0.74 (s, 3H), 1.25 (s, 3H), 1.54 (s, 3H), 3.24 (s, 3H), 6.71-6.75 (m, 1H), 6.78-6.81 (m, 1H), 7.03-7.13 (m, 4H), 7.26-7.30 (m, 1H), 8.23 (d, J = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.6, 23.2, 27.4, 29.5, 47.7, 71.4, 82.9, 109.3 (d, J_{CF} = 8.2 Hz), 114.9 (d, J_{CF} = 25.1 Hz), 115.3, 117.1 (d, J_{CF} = 23.2 Hz), 122.1, 125.0, 127.7, 129.0 (d, J_{CF} = 7.5 Hz), 137.0, 139.0, 144.2, 158.7 (d, J_{CF} = 241.4 Hz), 173.9, 178.0; HRMS (ESI-TOF) m/z: Calcd. for $C_{21}H_{20}FN_3NaOS$ $[M+Na]^+$: 404.1203; Found: 404.1198.



3af: Light yellow solid, m.p. 168.3-169.2 ^{o}C; yield 85% (64.1 mg), >20:1 dr; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.67 (s, 3H), 1.24 (s, 3H), 1.55 (s, 3H), 2.20 (s, 3H), 3.22 (s, 3H), 6.48 (s, 1H), 6.73 (d, J = 8.0 Hz, 1H), 7.02-7.04 (m, 1H), 7.07 (s, 1H), 7.09-7.12 (m, 2H), 7.26-7.30 (m, 1H), 8.28 (d, J = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.7, 21.0, 23.2, 27.2, 29.5, 47.6, 71.4, 82.7, 108.4, 115.2, 122.1, 124.7, 127.5, 127.6, 130.9, 132.4, 137.1, 140.5, 144.4, 174.1, 177.8; HRMS (ESI-TOF) m/z: Calcd. for $C_{22}H_{23}N_3NaOS$ $[M+Na]^+$: 400.1454; Found: 400.1447.

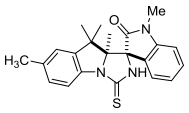


3ag: Light yellow solid, m.p. 228.3-228.3 ^{o}C; yield 77% (60.8 mg), >20:1 dr; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.73 (s, 3H), 1.27 (s, 3H), 1.29-1.33 (m, 3H), 1.58 (s, 3H), 3.58-3.63 (m, 1H), 3.93-3.98 (m, 1H), 6.51-6.54 (m, 1H), 6.79-6.82 (m, 1H), 7.03-7.14 (m, 4H), 7.28-7.32 (m, 1H), 8.26 (d, J = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 12.6, 19.6, 23.2, 29.5, 35.5, 47.6, 71.3, 83.0, 109.2 (d, J_{CF} = 8.3 Hz), 115.0, 115.3, 117.0 (d, J_{CF} = 23.1 Hz), 122.1, 124.9, 127.7, 129.2 (d, J_{CF} = 7.1 Hz), 136.9, 137.9, 144.1, 158.6 (d, J_{CF} = 242.4 Hz), 173.1, 177.9; HRMS (ESI-TOF) m/z: Calcd. for $C_{22}H_{22}FN_3NaOS$ $[M+Na]^+$: 418.1360; Found: 418.1361.

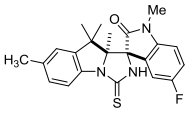


3ah: Light yellow solid, yield 84% (78.8 mg), >20:1 dr; ^{1}H NMR (DMSO-d_6, 400 MHz) δ: 0.77 (s, 3H), 1.12 (s, 3H), 1.50 (s, 3H), 3.48 (s, 3H), 4.86 (d, J = 15.6 Hz, 1H), 4.95 (d, J = 15.6 1H),

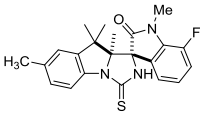
6.49 (s, 1H), 6.83-6.88 (m, 2H), 7.06-7.13 (m, 2H), 7.24-7.30 (m, 2H), 7.33-7.39 (m, 4H), 8.04 (d, J = 7.6 Hz, 1H), 9.68 (br s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ: 24.4, 29.9, 31.7, 48.5, 52.2, 60.6, 77.0, 87.4, 115.5, 118.3, 119.8, 119.9, 127.5, 132.7, 133.4, 133.8, 140.7, 141.1, 144.6, 148.8, 160.2, 178.0, 187.0; HRMS (ESI-TOF) m/z: $C_{28}H_{28}N_3O_2S$ $[M+H]^+$: 470.1897; Found: 470.1890.



3ba: Light yellow solid, m.p. 245.3-246.2 ^{o}C; yield 85% (64.1 mg), >20:1 dr; ^{1}H NMR (DMSO-d_6, 400 MHz) δ: 0.94 (s, 3H), 1.15 (s, 3H), 1.39 (s, 3H), 2.34 (s, 3H), 3.23 (s, 3H), 7.02 (s, 1H), 7.05-7.08 (m, 1H), 7.11-7.16 (m, 2H), 7.30 (d, J = 7.2 Hz, 1H), 7.44-7.48 (m, 1H), 7.84 (d, J = 8.0 Hz, 1H), 9.37 (br s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ: 19.6, 21.4, 22.6, 27.0, 28.8, 48.8, 71.4, 82.6, 109.6, 116.2, 122.4, 123.0, 126.4, 126.8, 127.8, 130.9, 134.5, 136.8, 144.1, 144.9, 174.7, 181.6; HRMS (ESI-TOF) m/z: Calcd. for $C_{22}H_{23}N_3NaOS$ $[M+Na]^+$: 400.1454; Found: 400.1448.

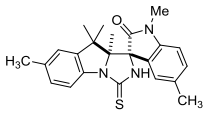


3bb: Light yellow solid, m.p. 231.3-231.5 ^{o}C; yield 90% (71.1 mg), 14:1 dr; ^{1}H NMR (DMSO-d_6, 400 MHz) δ: 0.86 (s, 3H), 1.11 (s, 3H), 1.36 (s, 3H), 2.27 (s, 3H), 3.15 (s, 3H), 6.88-6.91 (m, 1H), 6.96 (s, 1H), 7.06-7.13 (m, 2H), 7.24-7.30 (m, 1H), 7.79 (d, J = 8.0 Hz, 1H), 9.35 (br s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ: 24.3, 26.1, 28.0, 32.0, 33.0, 60.1, 76.4, 87.5, 115.4 (d, J_{CF} = 8.2 Hz), 119.2 (d, J_{CF} = 26.2 Hz), 120.6, 121.8 (d, J_{CF} = 23.1 Hz), 127.8, 132.6, 133.2 (d, J_{CF} = 8.1 Hz), 139.3, 141.6, 145.1, 149.3, 162.8 (d, J_{CF} = 237.3 Hz), 179.0, 186.5; HRMS (ESI-TOF) m/z: Calcd. for $C_{22}H_{22}FN_3NaOS$ $[M+Na]^+$: 418.1360; Found: 418.1352.

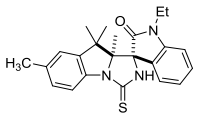


3bc: Light yellow solid, m.p. 231.2-232.0 ^{o}C; yield 73% (57.7 mg), >20:1 dr; ^{1}H NMR (DMSO-d_6, 400 MHz) δ: 0.81 (s, 3H), 1.13 (s, 3H), 1.36 (s, 3H), 2.28 (s, 3H), 3.33 (s, 3H), 6.97-7.07 (m, 4H), 7.27-7.32 (m, 1H), 7.82 (d, J = 8.0 Hz, 1H), 9.25 (br s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ: 19.7, 21.4, 23.0, 28.8, 29.5, 48.4, 71.3, 82.7, 115.6, 118.7 (d, J_{CF} = 18.4

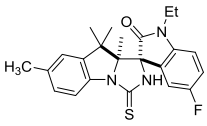
Hz), 123.1 (d, J_{CF} = 15.3 Hz), 123.5, 127.9, 130.0, 130.4, 134.4, 136.2, 144.8, 147.3 (d, J_{CF} = 239.0 Hz), 174.1, 180.5; HRMS (ESI-TOF) m/z: Calcd. for $C_{22}H_{22}FN_3NaOS$ $[M+Na]^+$: 418.1360; Found: 418.1353.



3bd: Light yellow solid, m.p. 180.6-181.2 °C; yield 81% (63.3 mg), 20:1 dr; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.59 (s, 3H), 1.14 (s, 3H), 1.45 (s, 3H), 2.12 (s, 3H), 2.24 (s, 3H), 3.13 (s, 3H), 6.24-6.29 (m, 1H), 6.64 (d, J = 7.6 Hz, 1H), 6.75 (s, 1H), 6.98-7.04 (m, 3H), 8.04-8.06 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.7, 21.0, 21.4, 23.0, 27.2, 29.6, 47.7, 71.4, 82.9, 108.3, 115.0, 122.7, 127.5, 128.0, 130.8, 132.3, 134.5, 134.8, 140.5, 144.6, 174.2, 177.5; HRMS (ESI-TOF) m/z: Calcd. for $C_{23}H_{25}N_3NaOS$ $[M+Na]^+$: 414.1611; Found: 414.1600.

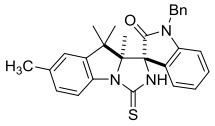


3be: Light yellow solid, m.p. 212.3-212.3 °C; yield 84% (65.7 mg), 19:1 dr; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.60 (s, 3H), 1.13 (s, 3H), 1.20-1.24 (m, 3H), 1.45 (s, 3H), 2.24 (s, 3H), 3.49-3.54 (m, 1H), 3.84-3.89 (m, 1H), 6.35 (br s, 1H), 6.75 (s, 1H), 6.76 (d, J = 7.6 Hz, 1H), 6.83-6.87 (m, 1H), 6.98 (d, J = 8.0 Hz, 1H), 7.21-7.27 (m, 2H), 8.05 (d, J = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 11.6, 18.5, 20.3, 21.8, 28.6, 34.3, 46.7, 70.2, 81.9, 107.5, 114.2, 121.4, 121.7, 126.0, 126.5, 127.0, 129.6, 133.5, 140.9, 143.5, 172.6, 176.7; HRMS (ESI-TOF) m/z: Calcd. for $C_{23}H_{25}N_3NaOS$ $[M+Na]^+$: 414.1611; Found: 414.1605.

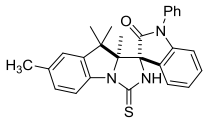


3bf: Light yellow solid, m.p. 207.5-208.1 °C; yield 83% (67.9 mg), 17:1 dr; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.74 (s, 3H), 1.25 (s, 3H), 1.27-1.34 (m, 3H), 1.57 (s, 3H), 2.34 (s, 3H), 3.58-3.61 (m, 1H), 3.93-3.97 (m, 1H), 6.41 (s, 1H), 6.79-6.81 (m, 1H), 6.85 (s, 1H), 7.03-7.06 (m, 1H), 7.09-7.13 (m, 2H), 8.12 (d, J = 5.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 11.0, 18.0, 19.8, 21.4, 28.1, 33.9, 46.1, 69.7, 81.6, 107.5 (d, J_{CF} = 8.1 Hz), 113.5 (d, J_{CF} = 25.0 Hz), 113.6, 115.4 (d, J_{CF} = 23.2 Hz), 121.1, 126.6, 127.6, 127.7, 133.0, 133.2, 136.4, 142.7, 157.2 (d, J_{CF} = 241.3 Hz),

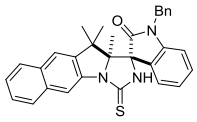
171.6, 176.0; HRMS (ESI-TOF) m/z: Calcd. for $C_{23}H_{24}FN_3NaOS$ $[M+Na]^+$: 432.1516; Found: 432.1506.



3bg: Light yellow solid, m.p. 158.5-159.3 ^oC; yield 90% (81.5 mg), 10:1 dr; ^1H NMR ($CDCl_3$, 400 MHz) δ: 0.55 (s, 3H), 1.09 (s, 3H), 1.47 (s, 3H), 2.22 (s, 3H), 4.50 (d, J = 15.6 Hz, 1H), 5.15 (d, J = 15.6 Hz, 1H), 6.47-6.58 (m, 1H), 6.69 (d, J = 7.6 Hz, 1H), 6.73 (s, 1H), 6.79-6.83 (m, 1H), 6.97 (d, J = 8.0 Hz, 1H), 7.10-7.14 (m, 1H), 7.20-7.26 (m, 6H), 8.05 (d, J = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.8, 21.4, 22.8, 30.0, 44.5, 47.7, 71.3, 83.1, 109.4, 115.1, 122.7, 122.8, 127.0, 127.5, 128.0, 128.1, 129.0, 130.5, 134.6, 135.6, 142.1, 144.6, 174.1, 177.3; HRMS (ESI-TOF) m/z: Calcd. for $C_{28}H_{27}N_3NaOS$ $[M+Na]^+$: 476.1767; Found: 476.1766.

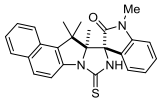


3bh: Light yellow solid, m.p. 290.0-291.1 ^oC; yield 78% (68.5 mg), >20:1 dr; ^1H NMR (DMSO-d_6, 400 MHz) δ: 1.04 (s, 3H), 1.23 (s, 3H), 1.49 (s, 3H), 2.36 (s, 3H), 6.78 (d, J = 8.0 Hz, 1H), 7.06 (s, 1H), 7.11-7.15 (m, 2H), 7.38-7.42 (m, 2H), 7.49 (d, J = 8.0 Hz, 2H), 7.56-7.60 (m, 1H), 7.67-7.71 (m, 2H), 7.85 (d, J = 8.0 Hz, 1H), 9.46 (br s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ: 19.7, 21.4, 22.6, 28.7, 49.0, 71.6, 83.0, 109.9, 116.4, 123.1, 127.2, 127.8, 130.4, 130.9, 134.6, 136.8, 143.9, 144.8, 174.1, 181.9; HRMS (ESI-TOF) m/z: Calcd. for $C_{27}H_{25}N_3NaOS$ $[M+Na]^+$: 462.1611; Found: 462.1604.

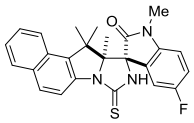


3ca: Light yellow solid, m.p. 236.2-236.7 ^oC; yield 76% (74.3 mg), >20:1 dr; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.11 (s, 3H), 1.29 (s, 3H), 1.75 (s, 3H), 4.65 (d, J = 15.2 Hz, 1H), 5.15 (d, J = 7.6 Hz, 1H), 6.88 (d, J = 7.6 Hz, 1H), 7.12-7.16 (m, 2H), 7.22 (d, J = 8.4 Hz, 1H), 7.28-7.39 (m, 6H), 7.45-7.49 (m, 1H), 7.53-7.57 (m, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.83 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 7.2 Hz, 1H), 8.63 (d, J = 8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.0, 19.6, 29.2, 29.7, 44.7, 71.5, 86.9, 110.0, 118.8, 122.2, 122.4, 125.6, 125.9, 126.6, 126.8, 127.7, 127.8, 127.9, 128.0,

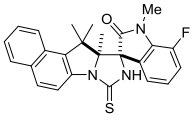
128.9, 131.0, 133.8, 135.2, 141.0, 144.8, 176.8, 188.4; HRMS (ESI-TOF) m/z: Calcd. for $C_{31}H_{27}N_3NaOS$ $[M+Na]^+$: 512.1767; Found: 512.1762.



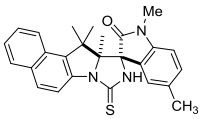
3da: Light yellow solid, m.p. 141.3-142.0 ^oC; yield 75% (62.0 mg), >20:1 dr; ^1H NMR ($CDCl_3$, 400 MHz) δ: 0.88 (s, 3H), 1.52 (s, 3H), 1.59 (s, 3H), 3.18 (s, 3H), 6.42-6.46 (m, 1H), 6.76 (d, J = 7.6 Hz, 1H), 6.80-6.84 (m, 1H), 7.18-7.33 (m, 4H), 7.72-7.83 (m, 3H), 8.56 (d, J = 8.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.3, 25.2, 27.1, 27.8, 49.8, 71.4, 83.0, 108.6, 115.3, 122.1, 122.7, 126.6, 126.8, 129.0, 129.8, 130.7, 142.9, 174.2, 178.7; HRMS (ESI-TOF) m/z: Calcd. for $C_{25}H_{23}N_3NaOS$ $[M+Na]^+$: 436.1454; Found: 436.1444.



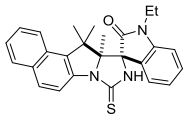
3db: Light yellow solid, m.p. 171.5-172.5 ^oC; yield 90% (77.6 mg), 20:1 dr; ^1H NMR ($CDCl_3$, 400 MHz) δ: 0.92 (s, 3H), 1.52 (s, 3H), 1.56 (s, 3H), 3.17 (s, 3H), 6.69-6.72 (m, 1H), 6.74-6.77 (m, 1H), 6.91-6.97 (m, 2H), 7.25-7.35 (m, 2H), 7.72 (d, J = 8.8 Hz, 1H), 7.76-7.83 (m, 2H), 8.51-8.53 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.3, 25.2, 27.4, 27.9, 49.8, 71.4, 83.1, 109.3 (d, J_{CF} = 8.1 Hz), 115.0 (d, J_{CF} = 25.2 Hz), 115.2, 117.0 (d, J_{CF} = 23.4 Hz), 122.0, 124.3, 126.7, 129.1, 129.6, 129.9, 132.2, 135.2, 135.8, 139.0, 158.8 (d, J_{CF} = 242.0 Hz), 173.9, 178.5; HRMS (ESI-TOF) m/z: Calcd. for $C_{25}H_{22}FN_3NaOS$ $[M+Na]^+$: 454.1360; Found: 454.1363.



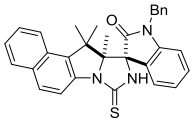
3dc: Light yellow solid, m.p. 244.6-245.1 ^oC; yield 70% (60.3 mg), 20:1 dr; ^1H NMR ($CDCl_3$, 400 MHz) δ: 0.86 (s, 3H), 1.56 (s, 3H), 1.62 (s, 3H), 3.39 (s, 3H), 6.42 (br s, 1H), 6.74-6.79 (m, 1H), 6.94-7.01 (m, 2H), 7.27-7.36 (m, 2H), 7.73 (d, J = 8.8 Hz, 1H), 7.78-7.83 (m, 2H), 8.58-8.61 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 18.3, 24.4, 26.7, 28.6, 48.5, 70.3, 82.1, 113.9, 117.5 (d, J_{CF} = 19.4 Hz), 121.0, 121.7 (d, J_{CF} = 3.1 Hz), 122.3 (d, J_{CF} = 7.1 Hz), 123.2, 125.6, 128.1, 128.4 (d, J_{CF} = 9.1 Hz), 128.6, 128.8, 129.5, 131.1, 134.2, 134.6, 146.8 (d, J_{CF} = 244.1 Hz), 172.6, 176.9; HRMS (ESI-TOF) m/z: Calcd. for $C_{25}H_{22}FN_3NaOS$ $[M+Na]^+$: 454.1360; Found: 454.1356.



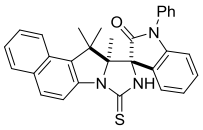
3dd: Light yellow solid, m.p. 175.6-176.3 ^{o}C; yield 80% (68.3 mg), 19:1 dr; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.86 (s, 3H), 1.53 (s, 3H), 1.61 (s, 3H), 2.03 (s, 3H), 3.16 (s, 3H), 6.36 (s, 3H), 6.64 (d, J = 8.0 Hz, 1H), 6.92 (s, 1H), 7.01 (d, J = 8.0 Hz, 1H), 7.28-7.33 (m, 2H), 7.73-7.83 (m, 3H), 8.60 (d, J = 8.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.3, 20.9, 25.3, 27.2, 27.7, 49.6, 71.5, 82.9, 108.4, 115.1, 122.1, 124.1, 126.6, 127.5, 127.6, 129.0, 129.6, 129.8, 130.9, 132.1, 132.4, 135.4, 136.0, 140.5, 174.0, 178.5; HRMS (ESI-TOF) m/z: Calcd. for $C_{26}H_{25}N_3NaOS$ $[M+Na]^+$: 450.1611; Found: 450.1600.



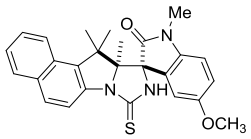
3de: Light yellow solid, m.p. 182.3-183.0 ^{o}C; yield 70% (59.8 mg), 20:1 dr; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.96 (s, 3H), 1.33-1.37 (m, 3H), 1.63 (s, 3H), 1.70 (s, 3H), 3.63-3.68 (m, 1H), 3.96-4.02 (m, 1H), 6.47 (s, 1H), 6.88-6.93 (m, 2H), 7.29-7.45 (m, 4H), 7.83-7.93 (m, 3H), 8.67 (d, J = 8.85 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 12.7, 19.3, 25.2, 27.8, 49.8, 71.4, 83.0, 108.6, 115.2, 122.1, 122.5, 124.2, 126.6, 127.1, 127.5, 129.0, 129.7, 129.9, 130.7, 132.1, 135.4, 135.8, 141.9, 173.5, 178.5; HRMS (ESI-TOF) m/z: Calcd. for $C_{26}H_{25}N_3NaOS$ $[M+Na]^+$: 450.1611; Found: 450.1608.



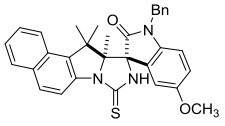
3df: Light yellow solid, m.p. 183.9-184.5 ^{o}C; yield 88% (86.1 mg), 19:1 dr; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.93 (s, 3H), 1.60 (s, 3H), 1.72 (s, 3H), 4.65 (d, J = 15.6 Hz, 1H), 5.24 (d, J = 15.2 Hz, 1H), 6.52-6.65 (m, 1H), 6.82 (d, J = 7.6 Hz, 1H), 6.88-6.92 (m, 1H), 7.22-7.26 (m, 1H), 7.31-7.43 (m, 8H), 7.83-7.93 (m, 3H), 8.71 (d, J = 8.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.4, 25.1, 28.0, 44.6, 49.7, 71.4, 83.1, 109.5, 115.1, 122.1, 122.8, 124.2, 126.6, 127.0, 127.6, 128.1, 129.0, 129.1, 129.9, 130.6, 135.4, 135.5, 142.1, 173.9, 178.1; HRMS (ESI-TOF) m/z: Calcd. for $C_{31}H_{27}N_3NaOS$ $[M+Na]^+$: 512.1767; Found: 512.1765.



3dg: Light yellow solid, m.p. 203.7-204.2 ^{o}C; yield 70% (66.5 mg), >20:1 dr; ^{1}H NMR (DMSO-d_6, 400 MHz) δ: 1.22 (s, 3H), 1.53 (s, 3H), 1.60 (s, 3H), 6.73 (d, J = 8.0 Hz, 1H), 6.92-6.96 (m, 1H), 7.12 (d, J = 7.6 Hz, 1H), 7.26-7.30 (m, 1H), 7.39-7.54 (m, 5H), 7.62-7.66 (m, 2H), 7.90-8.00 (m, 3H), 8.36 (d, J = 8.4 Hz, 1H), 9.66 (br s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ: 19.4, 25.3, 26.7, 50.4, 72.0, 83.3, 109.9, 116.2, 122.6, 123.1, 124.7, 126.6, 127.2, 127.3, 128.8, 129.1, 129.5, 130.0, 130.4, 130.9, 132.2, 134.3, 135.1, 138.2, 143.8, 173.7, 182.8; HRMS (ESI-TOF) m/z: Calcd. for $C_{30}H_{25}N_3NaOS$ $[M+Na]^+$: 498.1611; Found: 498.1594.

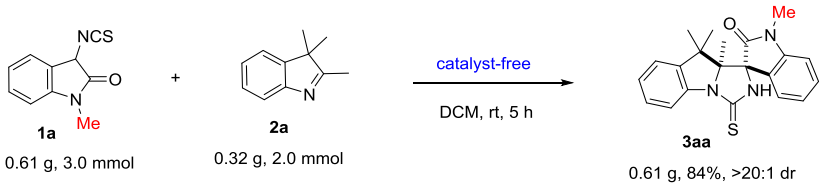


3dh: Light yellow solid, yield 71% (62.9 mg), >20:1 dr; ^{1}H NMR (DMSO-d_6, 400 MHz) δ: 1.11 (s, 3H), 1.44 (s, 3H), 1.61 (s, 3H), 3.17 (s, 3H), 3.26 (s, 3H), 6.31 (d, J = 2.4 Hz, 1H), 6.86-6.89 (m, 1H), 6.97 (d, J = 8.8 Hz, 1H), 7.37-7.47 (m, 2H), 7.89-7.95 (m, 3H), 8.42 (d, J = 8.8 Hz, 1H), 9.68 (br s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ: 24.0, 30.2, 31.2, 32.0, 53.8, 60.4, 77.4, 87.9, 114.8, 117.8, 120.3, 120.5, 127.3, 132.0, 133.5, 133.6, 134.2, 134.7, 136.8, 139.2, 141.9, 143.9, 160.1, 178.0, 188.6; HRMS (ESI-TOF) m/z: Calcd. for $C_{26}H_{26}N_3O_2S$ $[M+H]^+$: 444.1740; Found: 444.1734.



3di: Light yellow solid, yield 72% (74.7 mg), >20:1 dr; ^{1}H NMR (DMSO-d_6, 400 MHz) δ: 1.06 (s, 3H), 1.44 (s, 3H), 1.66 (s, 3H), 3.21 (s, 3H), 4.89-4.99 (m, 2H), 6.29 (d, J = 2.4 Hz, 1H), 6.76-6.79 (m, 1H), 6.84 (d, J = 8.8 Hz, 1H), 7.29-7.45 (m, 7H), 7.90-7.94 (m, 3H), 8.47 (d, J = 8.4 Hz, 1H), 9.91 (br s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ: 24.0, 30.2, 31.4, 48.6, 53.6, 60.4, 77.4, 88.1, 115.5, 117.9, 120.0, 120.4, 132.1, 132.7, 133.7, 133.8, 134.2, 136.7, 139.1, 140.7, 141.0, 143.8, 160.1, 177.8, 188.4; HRMS (ESI-TOF) m/z: Calcd. for $C_{32}H_{30}N_3O_2S$ $[M+H]^+$: 520.2053; Found: 520.2047.

4. Preparative scale synthesis of the product 3aa

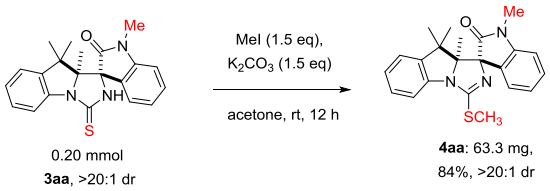


In a sealed tube equipped with a magnetic stirring bar, a mixture of 3-isothiocyanato oxindole **1a** (2.0 mmol), trimethylindolenine **2a** (3.0 mmol) in 10.0 mL of DCM was stirred under catalyst-free at rt for 5 h, and then was directly loaded onto a silica gel and purified by flash chromatography (hexane/EtOAc, 8/1, v/v) to give the desired product **3aa** (0.61 g, 84%, >20:1 dr).

5. General experimental procedures for in vitro cytotoxicity assay

Two human cancer cell lines, K562 and A549 were purchased from Chinese Academy of Sciences. All the cells were cultured in RPMI-1640 medium (GIBICO, USA), supplemented with 10% fetal bovine serum (Hyclone, USA) and Penicillin-Streptomycin (respectively 100 U/mL) in 5% CO_2 at 37℃. The cytotoxicity assay was performed according to the MTT (3-(4,5-dimethylthiazol-2-yl)-2, 5-diphenyl tetrazolium bromide) method in 96-well microplates. Briefly, 5000 cells were seeded into each well of 96-well cell culture plates and allowed to grow for 24 h before drug addition. The K562 tumor cell line was exposed to test compounds **3ab**, **3ac**, **3af**, **3be**, **3bg** and **3bh** at the concentrations of 10, 20, 40, 80, and 100 μmol·L^{-1} in triplicates for 48 h, comparable to cisplatin (Aladdin, China). Then the MTT reagent was added to reaction with the cancer cells for 4 hours. At least, measure the OD value at 490 wavelengths. IC_{50} of all the compounds were calculated by IBM SPSS Statistics (version 19).

6. Further investigation of transformation of 3aa

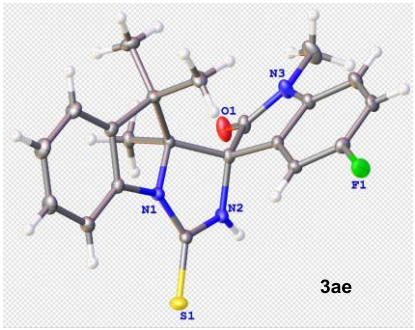


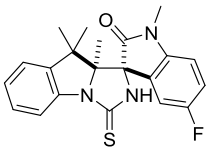
To a stirred solution of **3aa** (72.6 mg, 0.20 mmol) in acetone (1.0 mL) was added K_2CO_3 (41 mg, 0.30 mmol) at 0 ℃. Then iodomethane (43 mg, 0.30 mmol) in 2.0 mL acetone was added dropwise into the stirred reaction mixture. The reaction mixture was allowed to stir at room temperature for another 12 h, and was directly loaded onto a silica gel and purified by flash

chromatography (hexane/EtOAc, 10/1, v/v) to give the desired product **4aa**.

4aa: Light yellow solid, yield 84% (63.3 mg), >20:1 dr; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.72 (s, 3H), 1.03 (s, 3H), 1.65 (s, 3H), 2.47 (s, 3H), 3.12 (s, 3H), 5.58-5.60 (m, 1H), 6.43-6.47 (m, 1H), 6.58 (d, J = 7.6 Hz, 1H), 6.69-6.71 (m, 1H), 6.88-6.92 (m, 1H), 7.01-7.06 (m, 1H), 7.12-7.16 (m, 1H), 7.37 (d, J = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 14.7, 18.4, 19.8, 26.6, 30.9, 45.3, 81.1, 86.3, 107.3, 113.3, 121.8, 122.4, 123.3, 126.4, 127.4, 129.1, 141.8, 143.5, 145.2, 171.1, 176.0; HRMS (ESI-TOF) m/z: Calcd. for $C_{22}H_{23}N_3NaOS$ $[M+Na]^+$: 400.1454; Found: 400.1451.

7. X-ray crystal data for compound 3ae





3ae

CCDC 2233242

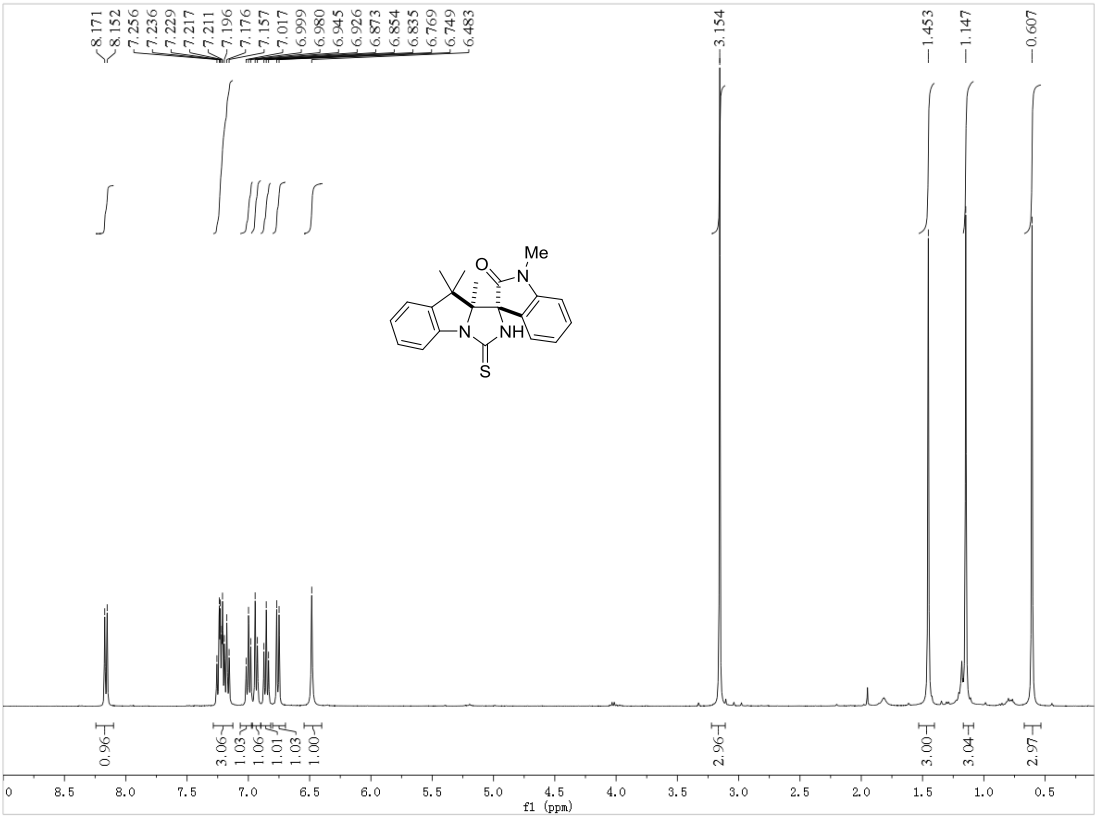
Table S1 Crystal data and structure refinement for 3ae

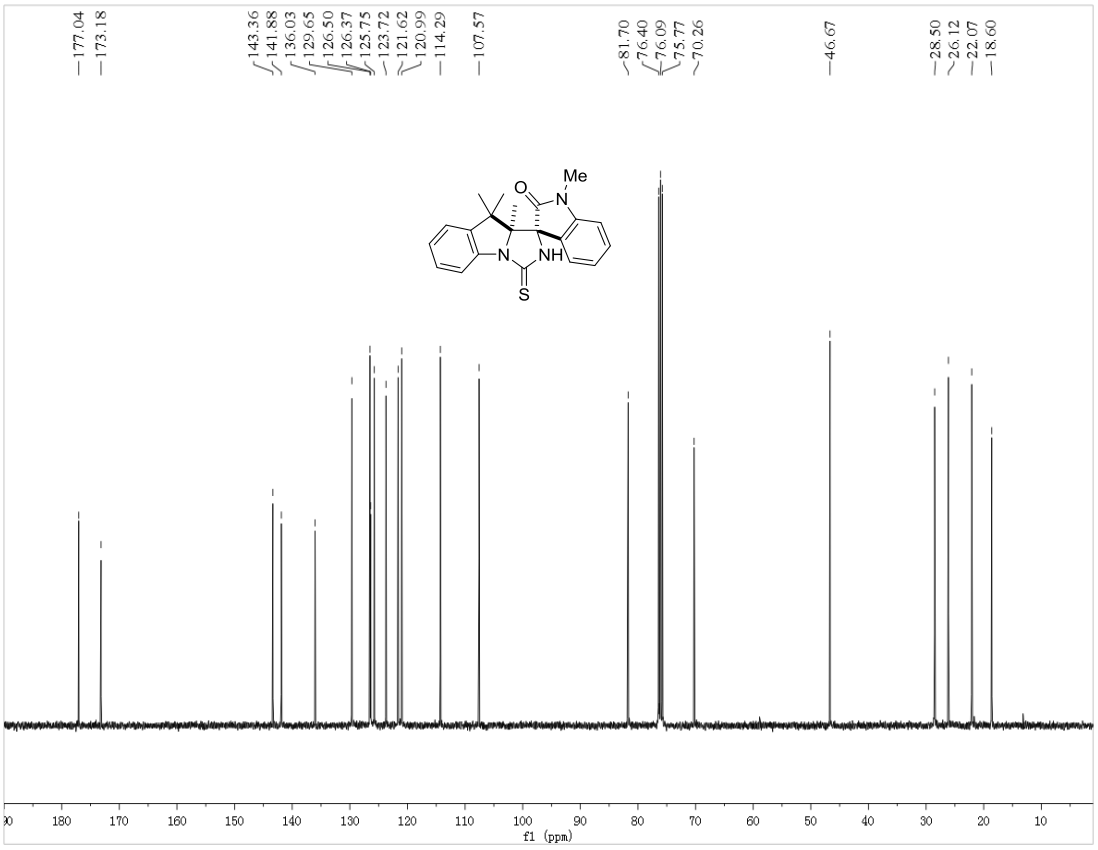
Identification code	**3ae**
Empirical formula	$C_{21}H_{20}FN_3OS$
Formula weight	381.46
Temperature/K	150.00(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å, b/Å, c/Å	8.0518(2), 17.6500(4), 26.8891(6)
α/°, β/°, γ/°,	90, 90, 90
Volume/Å^3	3821.32(15)
Z	8
ρ_{calc}g/cm^3	1.326
μ/mm^{-1}	1.715
F(000)	1600.0
Radiation	Cu Kα (λ = 1.54178)
Crystal size/mm^3	0.15 × 0.13 × 0.12
2Θ range for data collection/°	6.574 to 147.152
Index ranges	-9 ≤ h ≤ 9, -21 ≤ k ≤ 16, -33 ≤ l ≤ 31
Reflections collected	17499
Independent reflections	3807 [R_{int} = 0.0466, R_{sigma} = 0.0288]
Data/restraints/parameters	3807/0/248
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0512, wR_2 = 0.1384
Final R indexes [all data]	R_1 = 0.0542, wR_2 = 0.1418
Largest diff. peak/hole / e Å^{-3}	0.48/-0.53

Crystal Data for $C_{21}H_{20}FN_3OS$ (*M* =381.46 g/mol): orthorhombic, space group Pbca (no. 61), *a* = 8.0518(2) Å, *b* = 17.6500(4) Å, *c* = 26.8891(6) Å, *V* = 3821.32(15) Å^3, *Z* = 8, *T* = 150.00(10) K, μ(Cu Kα) = 1.715 mm^{-1}, *Dcalc* = 1.326 g/cm^3, 17499 reflections measured (6.574 ° ≤ 2Θ ≤ 147.152°), 3807 unique (R_{int} = 0.0466, R_{sigma} = 0.0288) which were used in all calculations. The final R_1 was 0.0512 (I > 2σ(I)) and wR_2 was 0.1418 (all data).

8. The copies of ^{1}H NMR and ^{13}C NMR spectra for compounds 3 and 4

^{1}H and ^{13}C NMR of 3aa

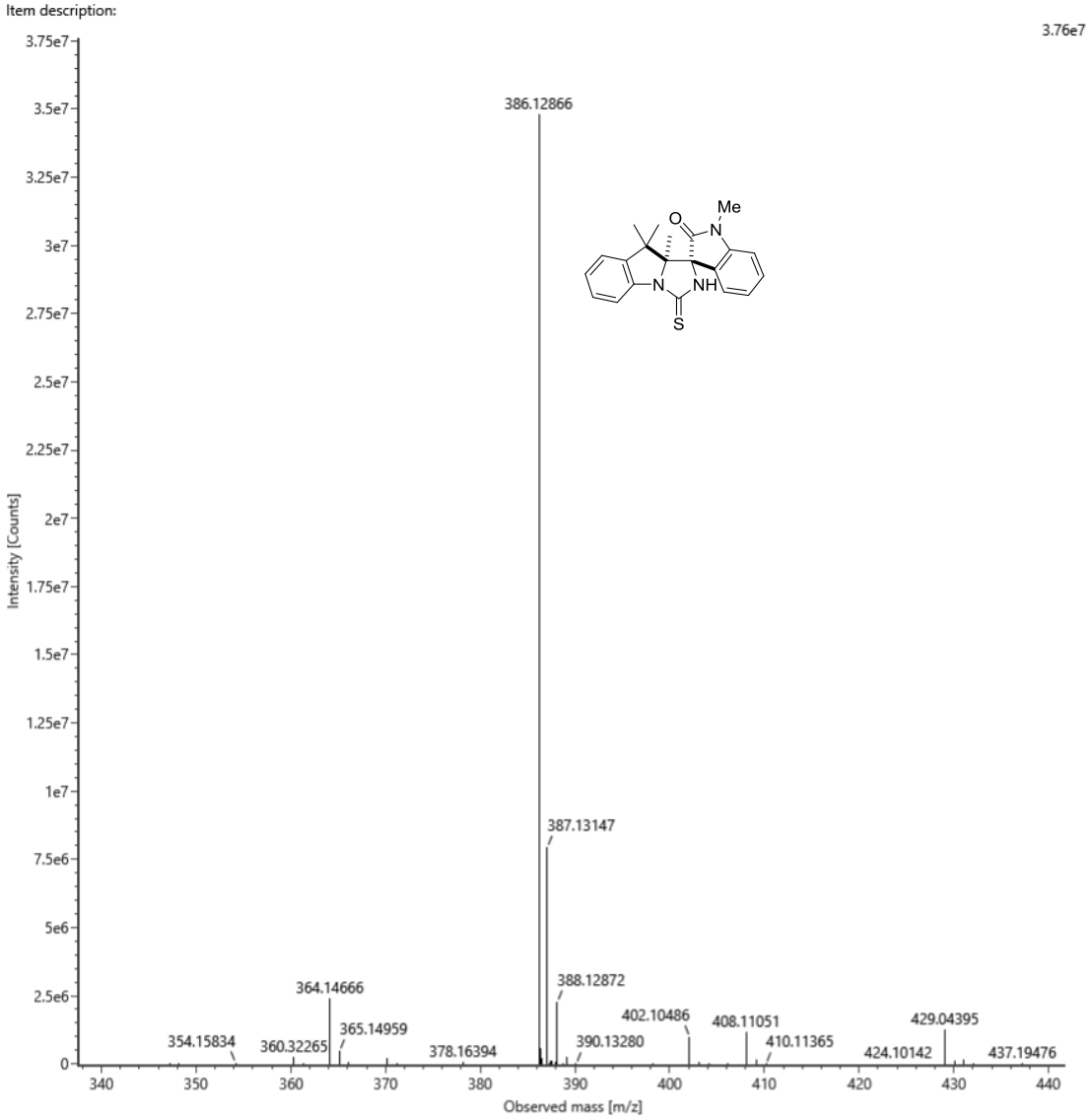




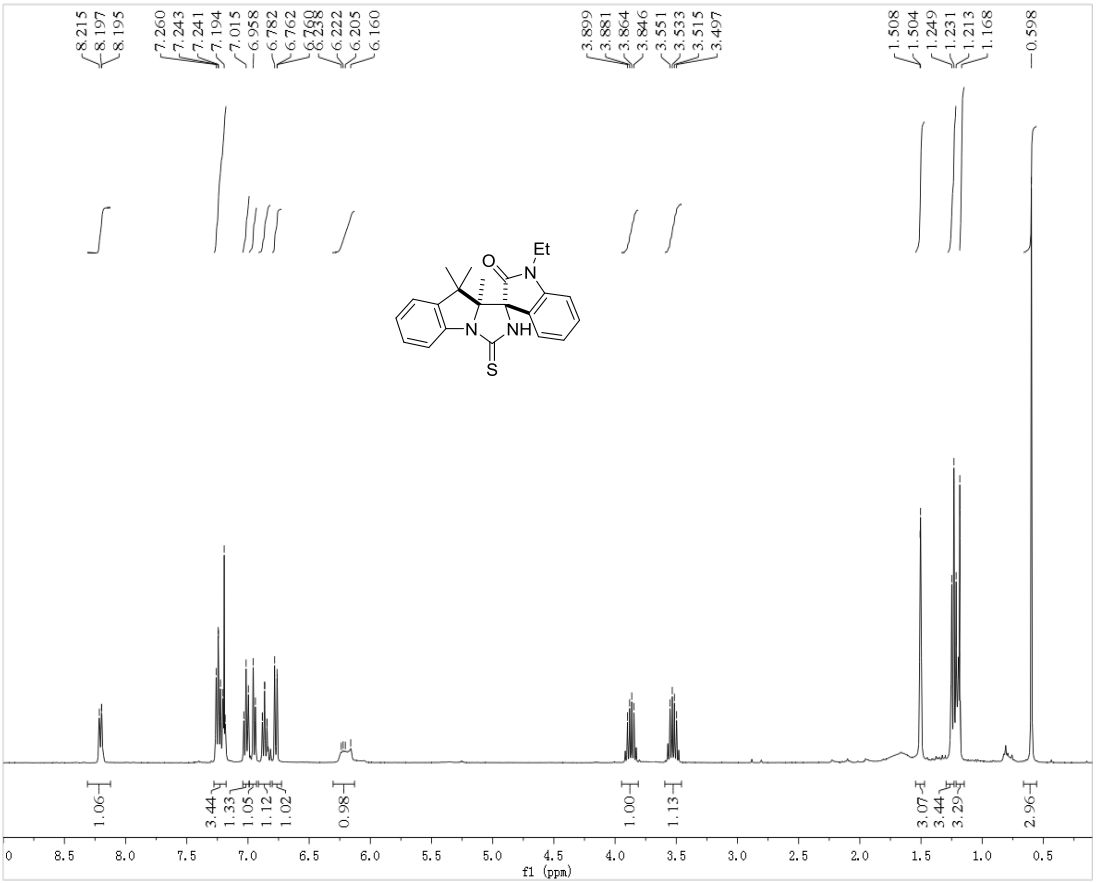
HRMS of 3aa

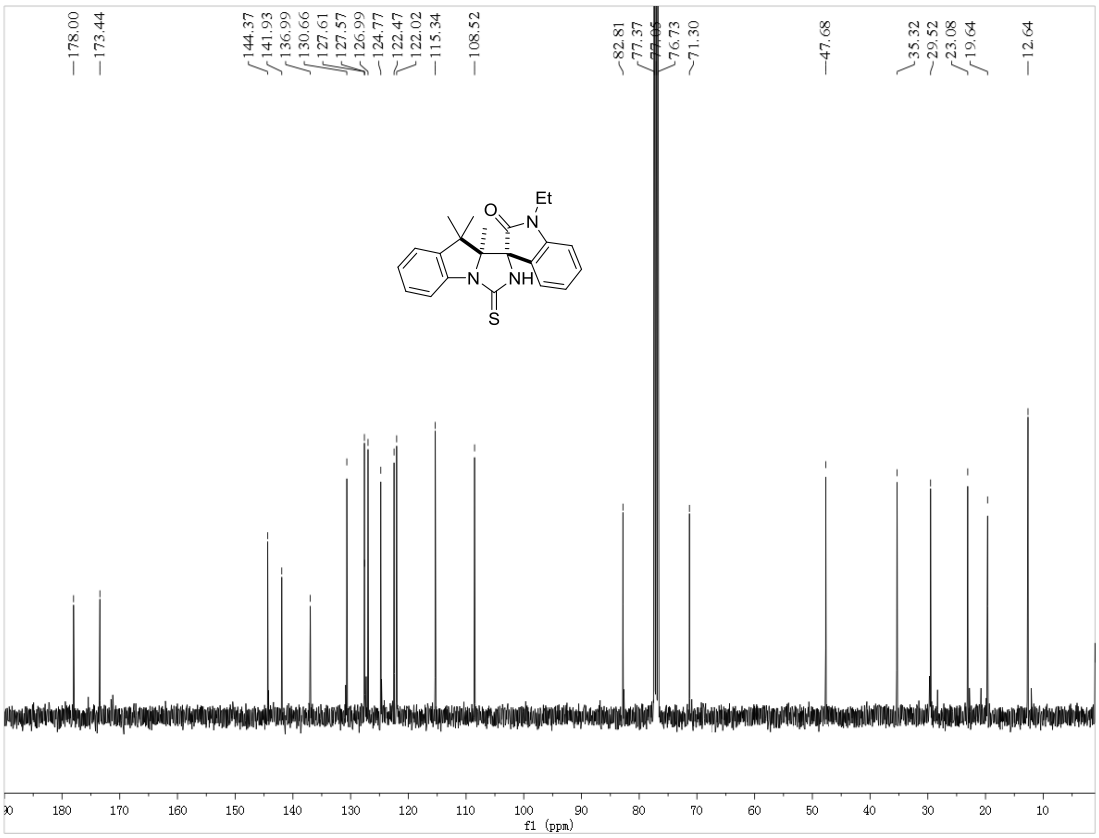
Item name: LRM-BS20-3aa
Item description:

Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined



^{1}H and ^{13}C NMR of 3ab

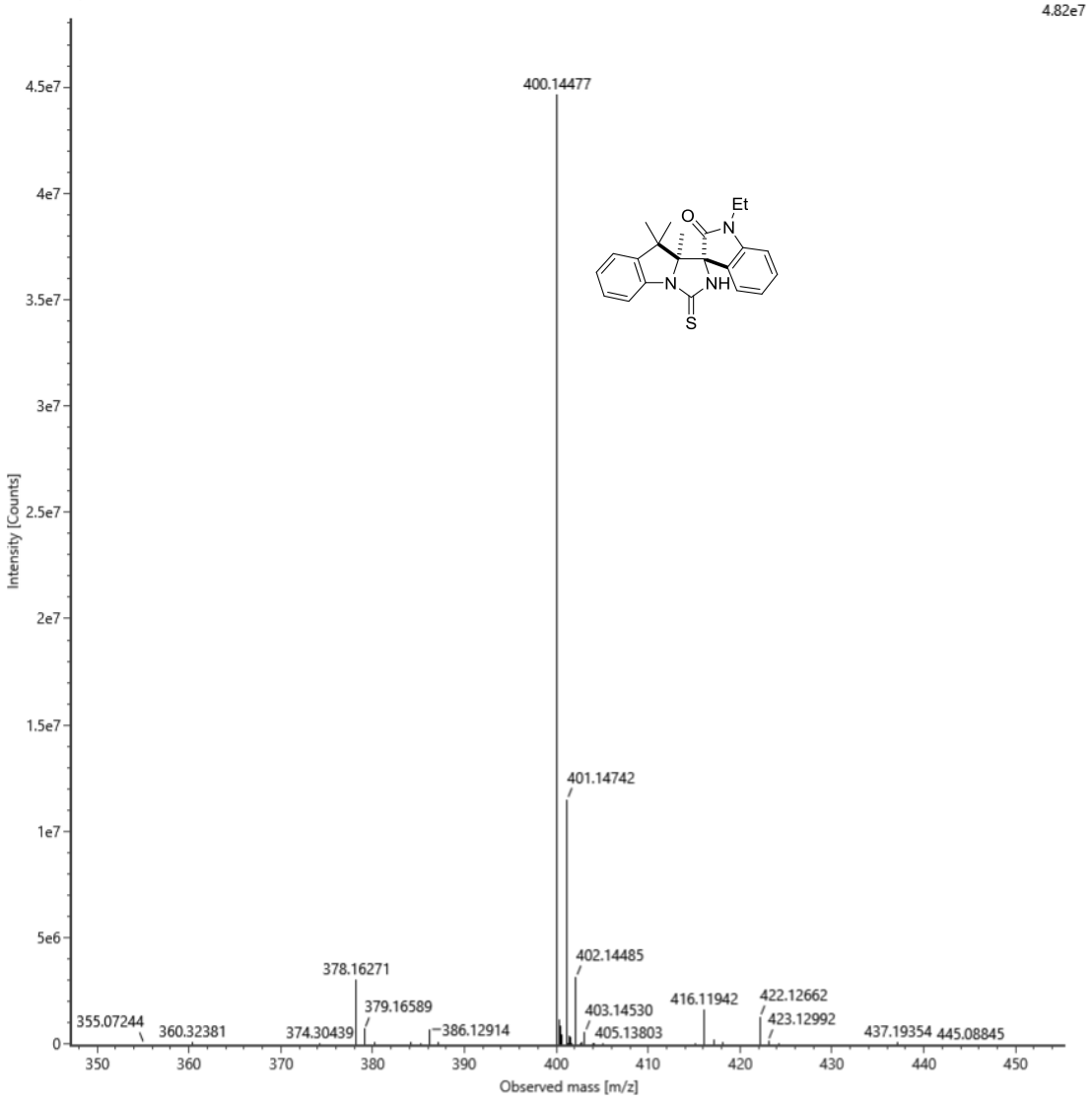




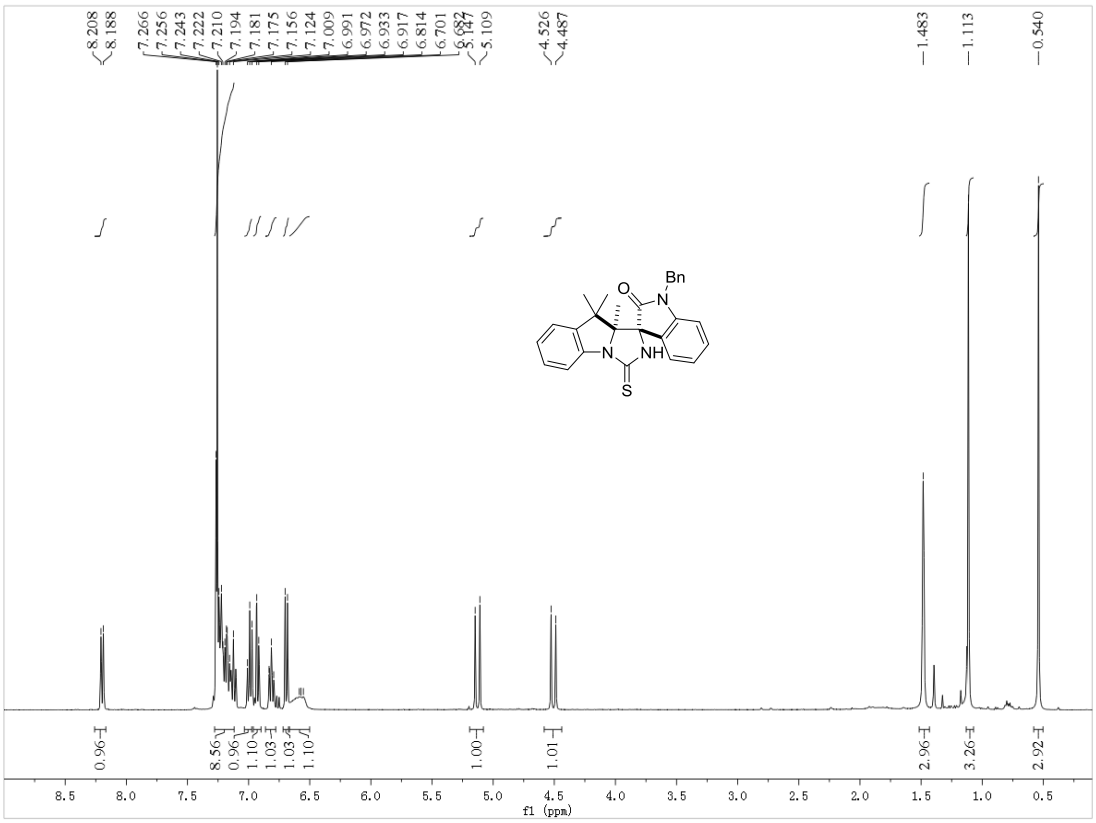
HRMS of 3ab

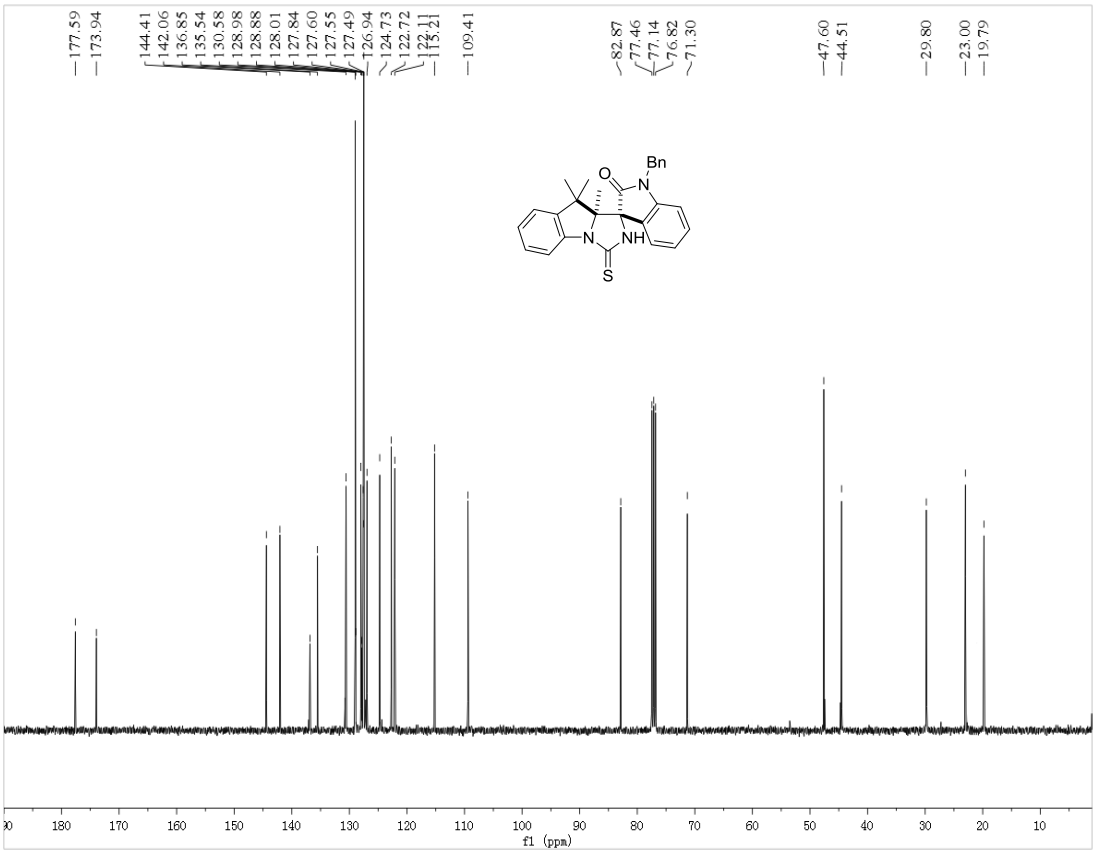
Item name: LRM-B5-3ab
Item description:

Channel name: 1: Average Time 0.1089 min : TOF MS (50-1500) ESI+ : Centroided : Combined

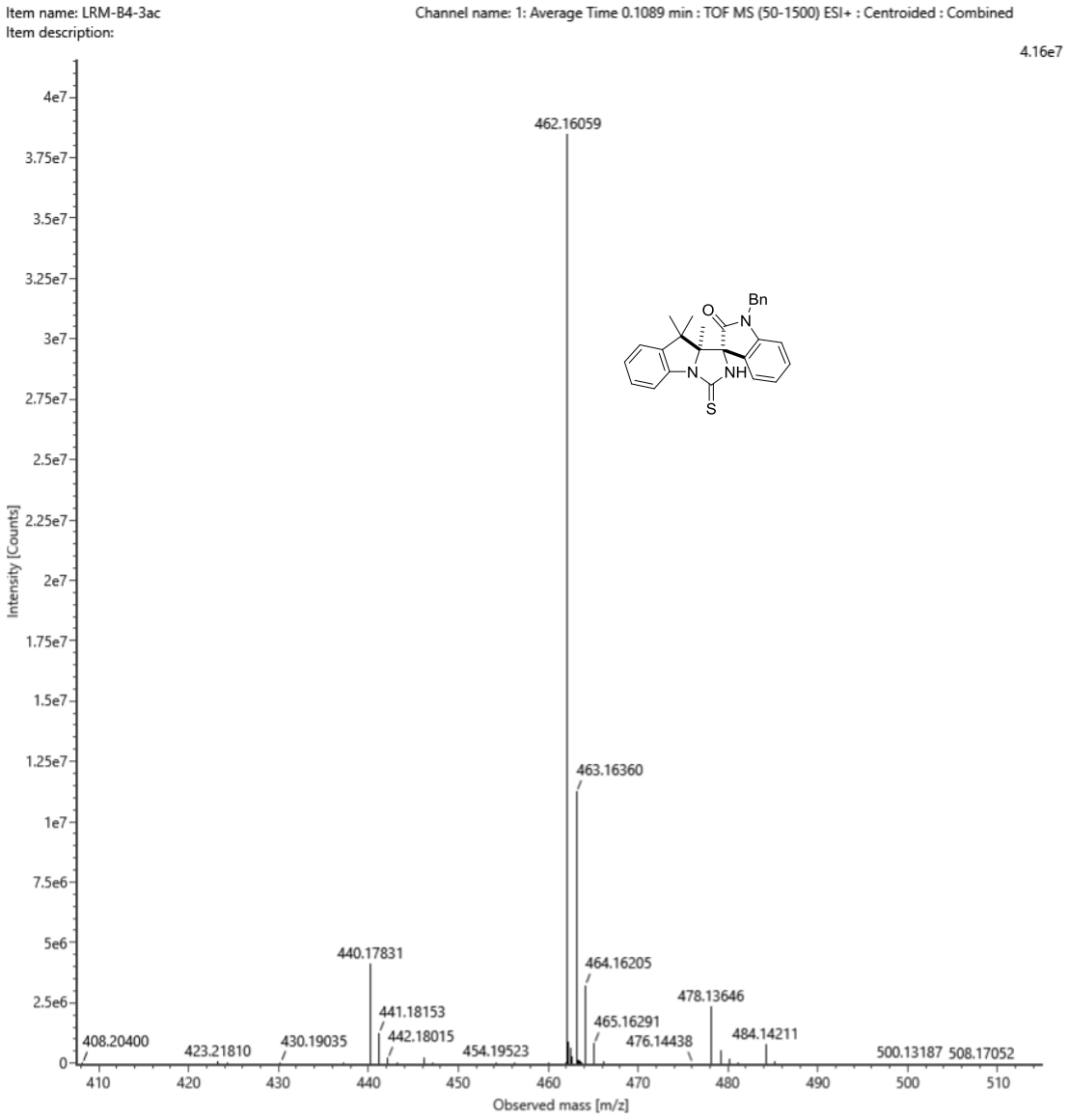


^{1}H and ^{13}C NMR of 3ac

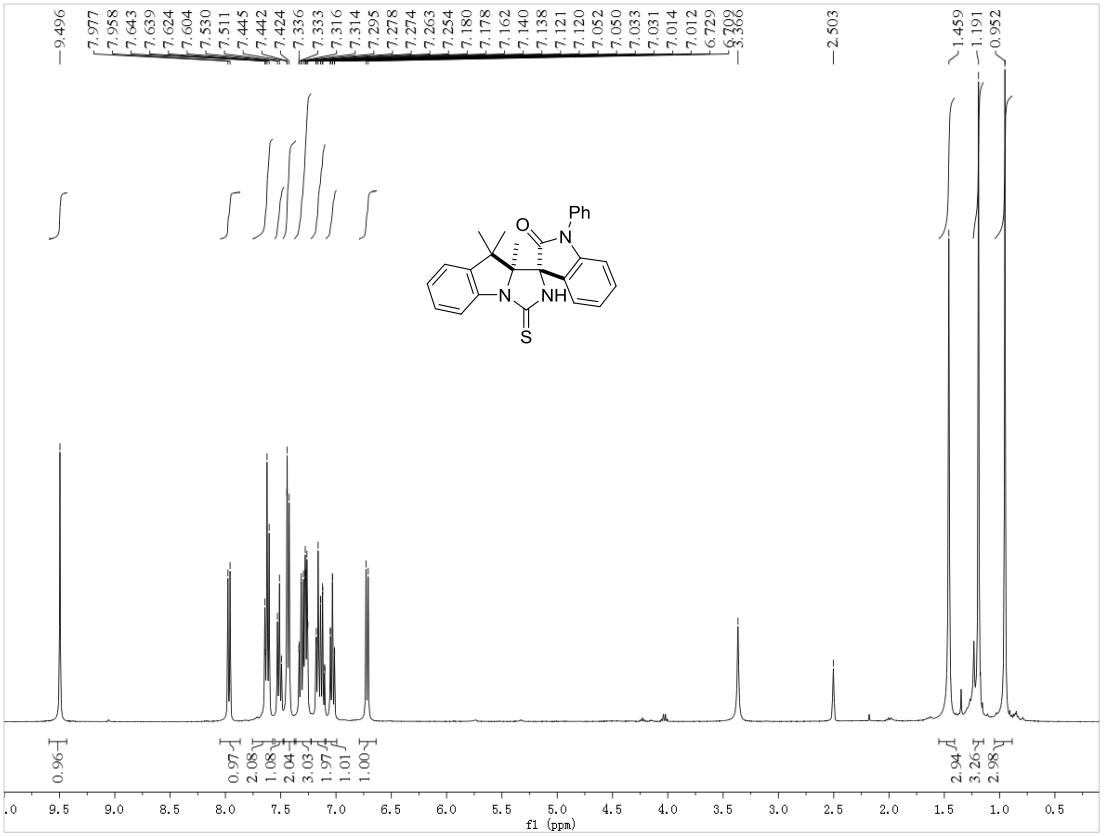


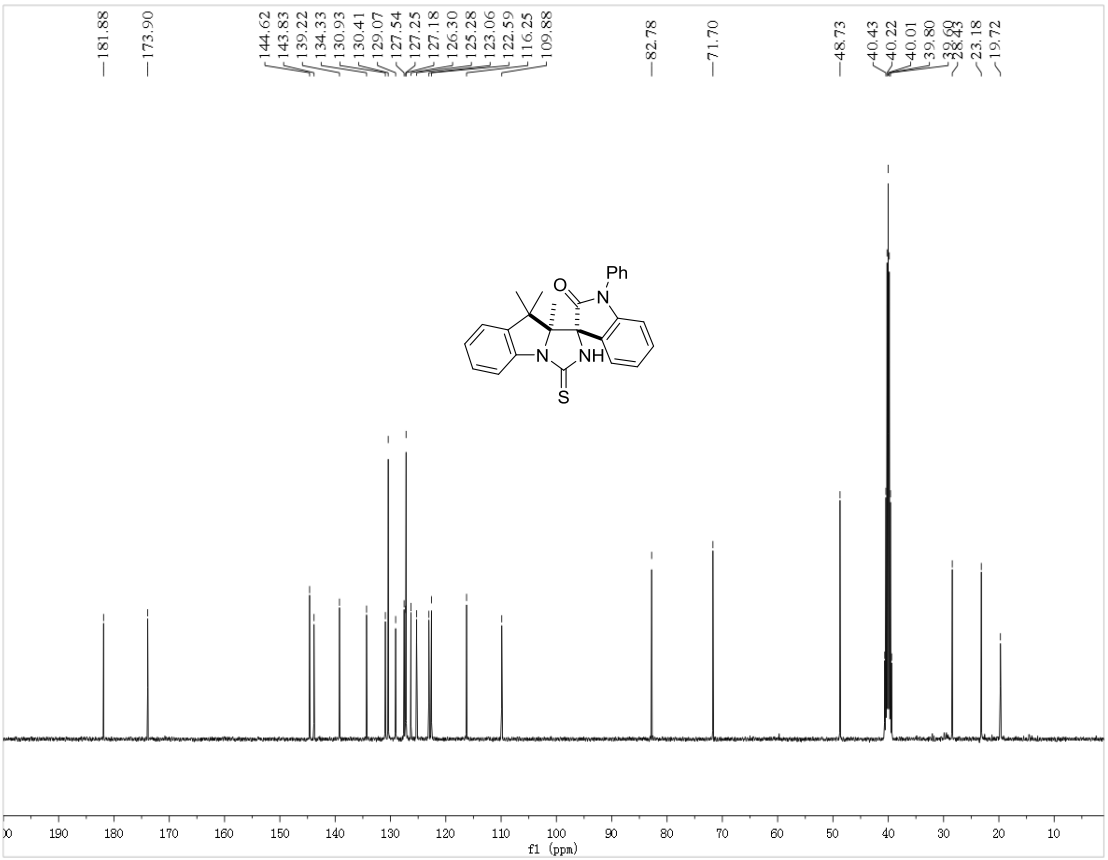


HRMS of 3ac

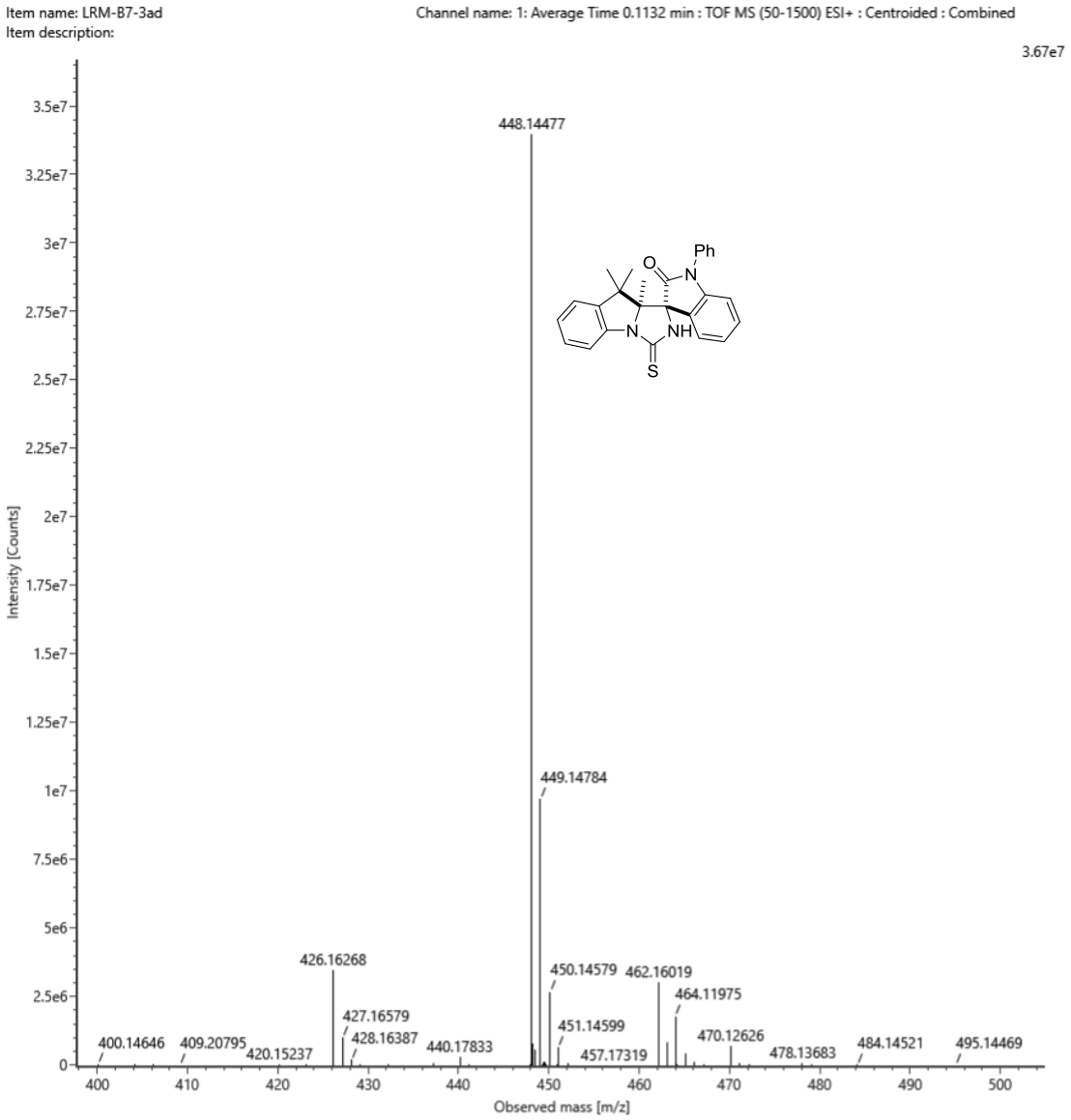

Item name: LRM-B4-3ac
Item description:
Channel name: 1: Average Time 0.1089 min : TOF MS (50-1500) ESI+ : Centroided : Combined
4.16e7
462.16059
463.16360
440.17831
464.16205
478.13646
441.18153
465.16291
484.14211
442.18015
476.14438
408.20400
423.21810
430.19035
454.19523
500.13187
508.17052
Intensity [Counts]
Observed mass [m/z]
Bn
O
N
NH
N
S

^{1}H and ^{13}C NMR of 3ad

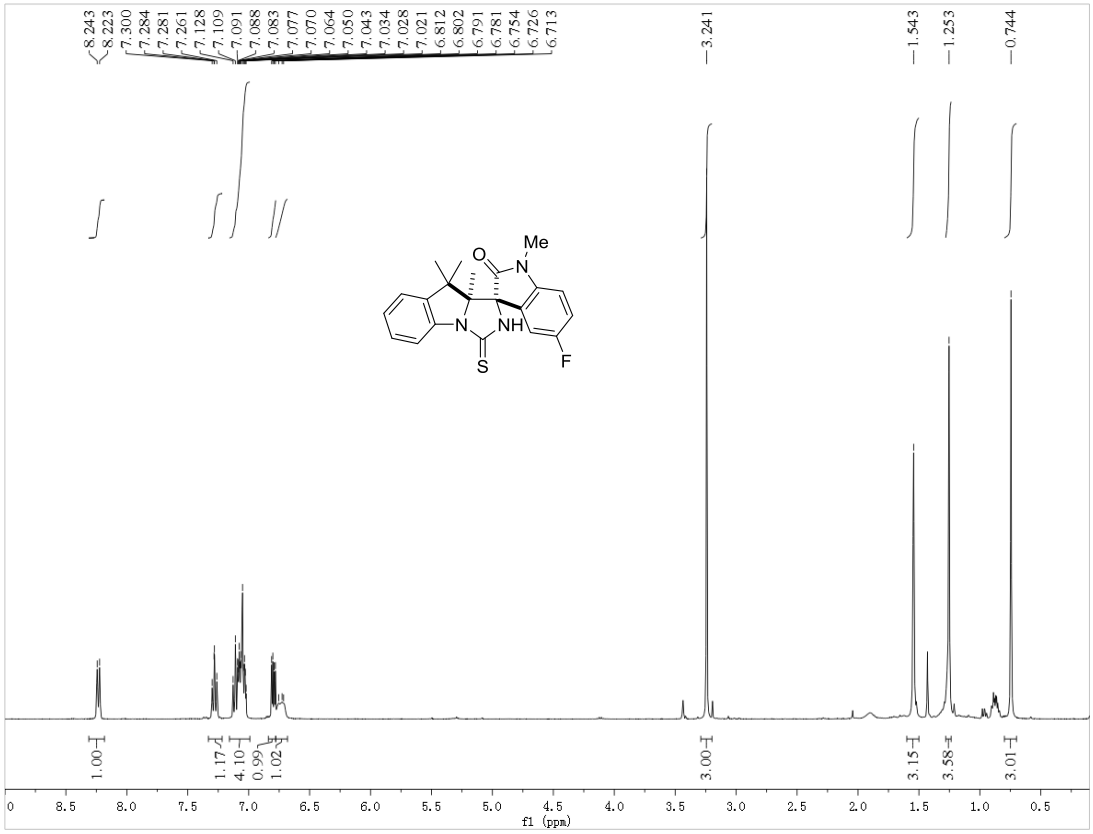


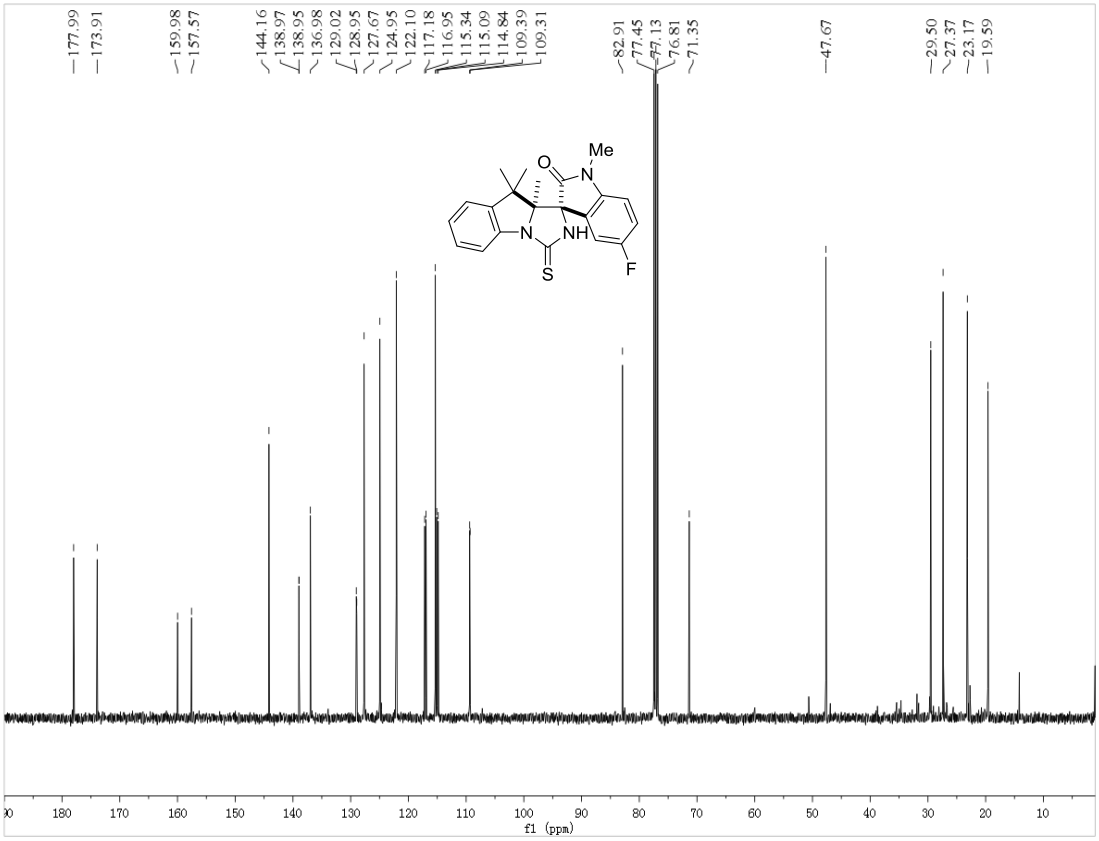


HRMS of 3ad

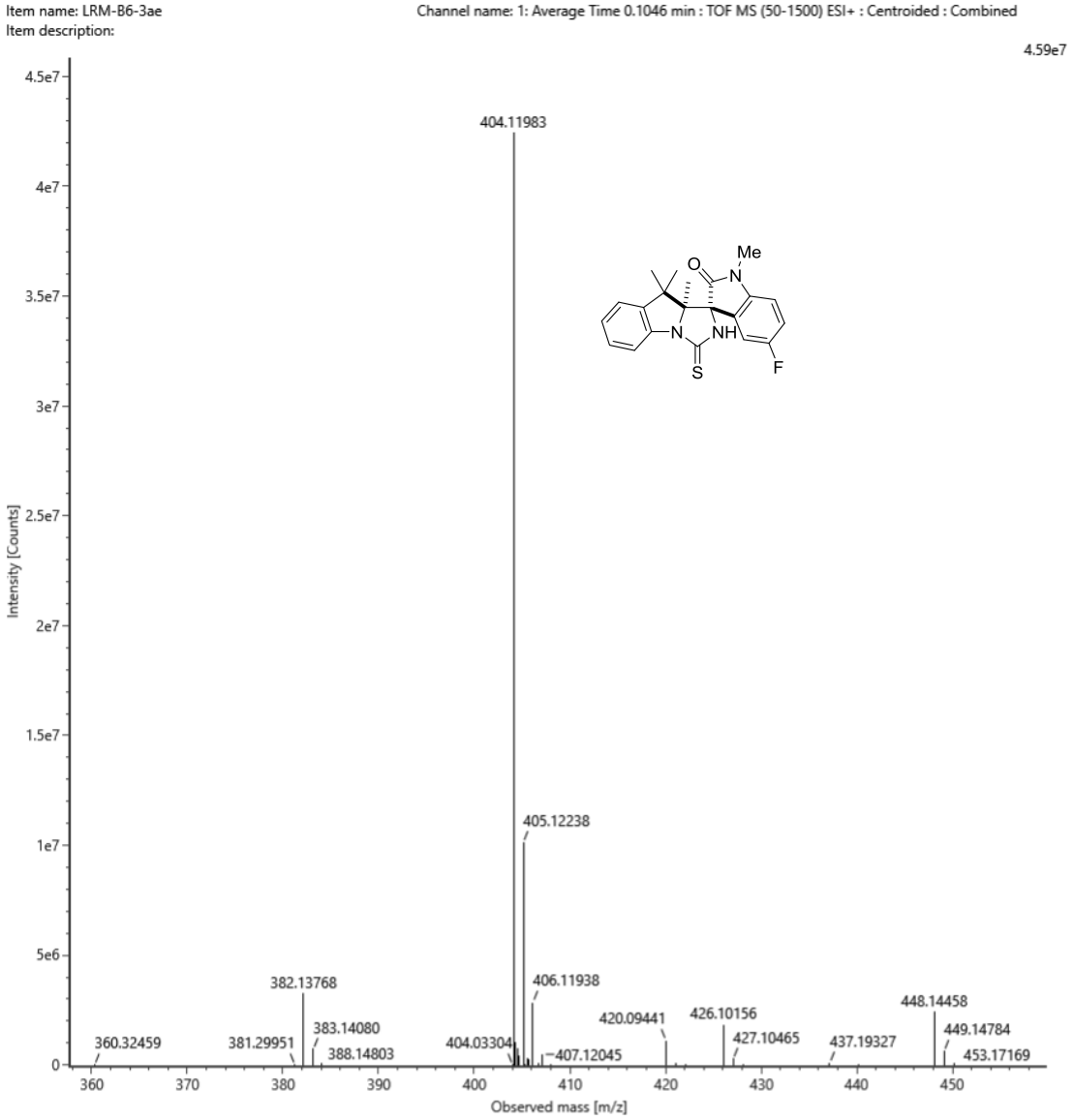

Item name: LRM-B7-3ad
Item description:
Channel name: 1: Average Time 0.1132 min : TOF MS (50-1500) ESI+ : Centroided : Combined
3.67e7
Intensity [Counts]
Observed mass [m/z]
448.14477
449.14784
426.16268
450.14579
462.16019
464.11975
427.16579
428.16387
451.14599
470.12626
400.14646
409.20795
420.15237
440.17833
457.17319
478.13683
484.14521
495.14469
Ph
O
N
NH
S

^{1}H and ^{13}C NMR of 3ae

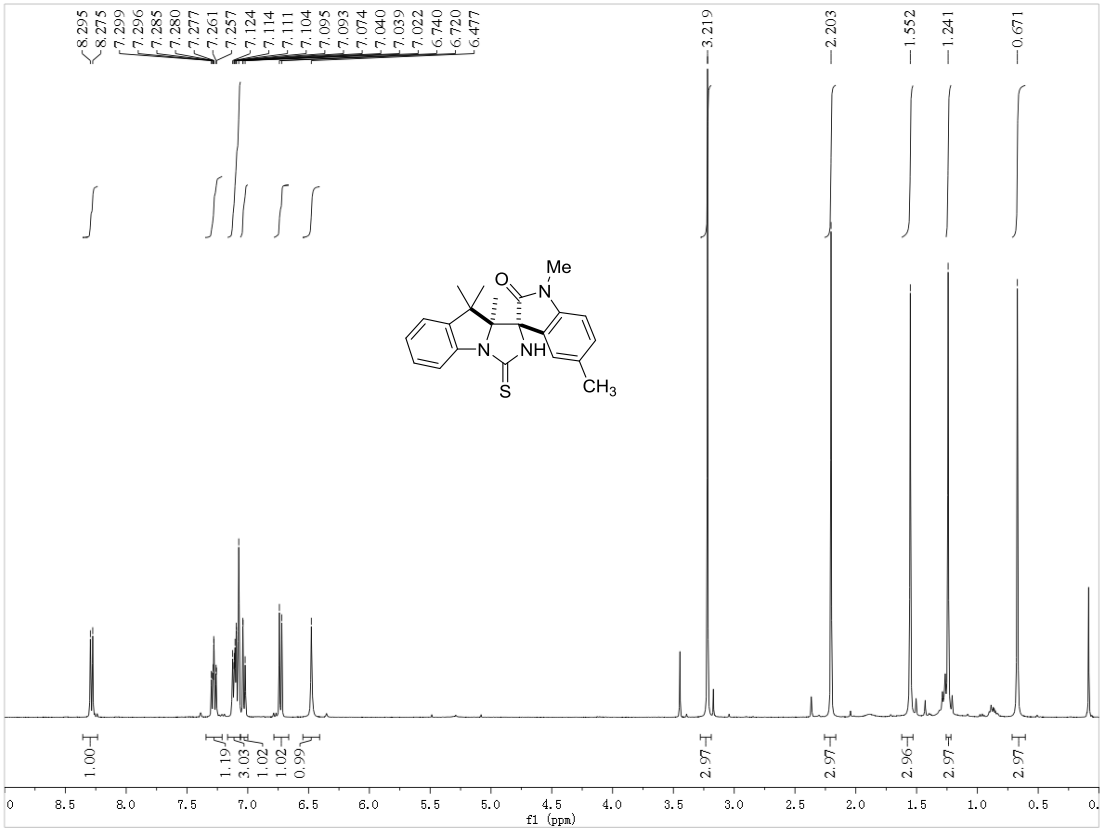


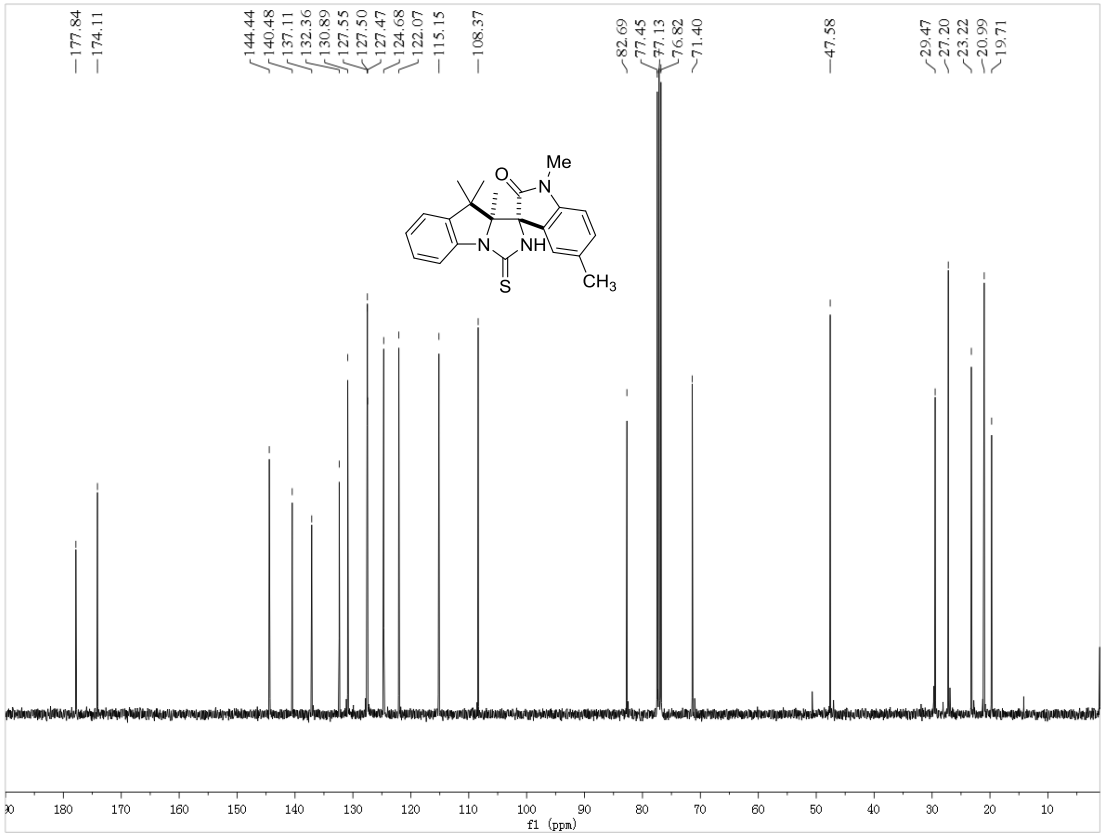


HRMS of 3ae

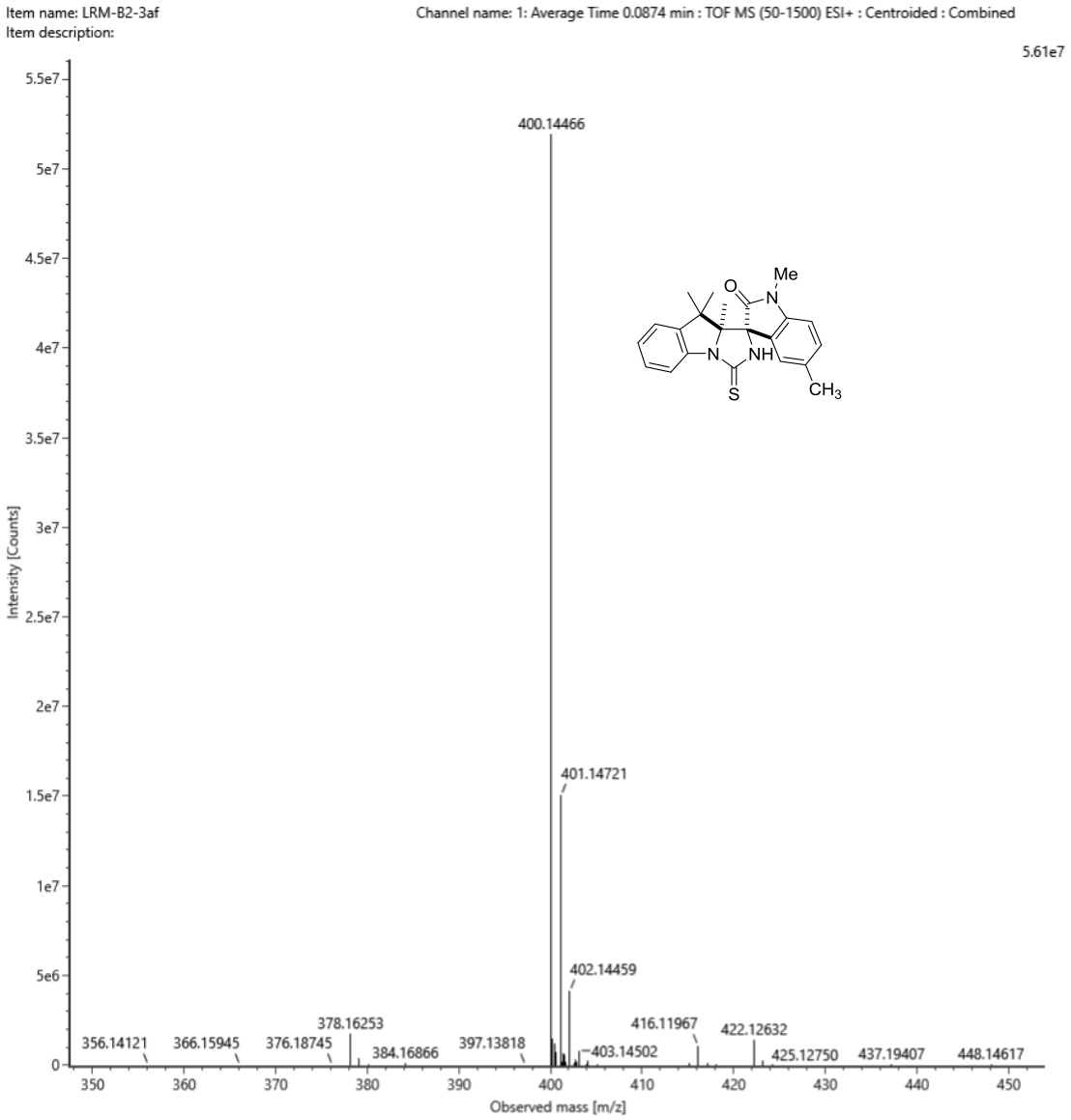

Item name: LRM-B6-3ae
Item description:
Channel name: 1: Average Time 0.1046 min : TOF MS (50-1500) ESI+ : Centroided : Combined
4.59e7
Intensity [Counts]
Observed mass [m/z]
404.11983
405.12238
406.11938
382.13768
383.14080
360.32459
381.29951
388.14803
404.03304
407.12045
420.09441
426.10156
427.10465
437.19327
448.14458
449.14784
453.17169
Me
O
N
NH
S
F

^{1}H and ^{13}C NMR of 3af

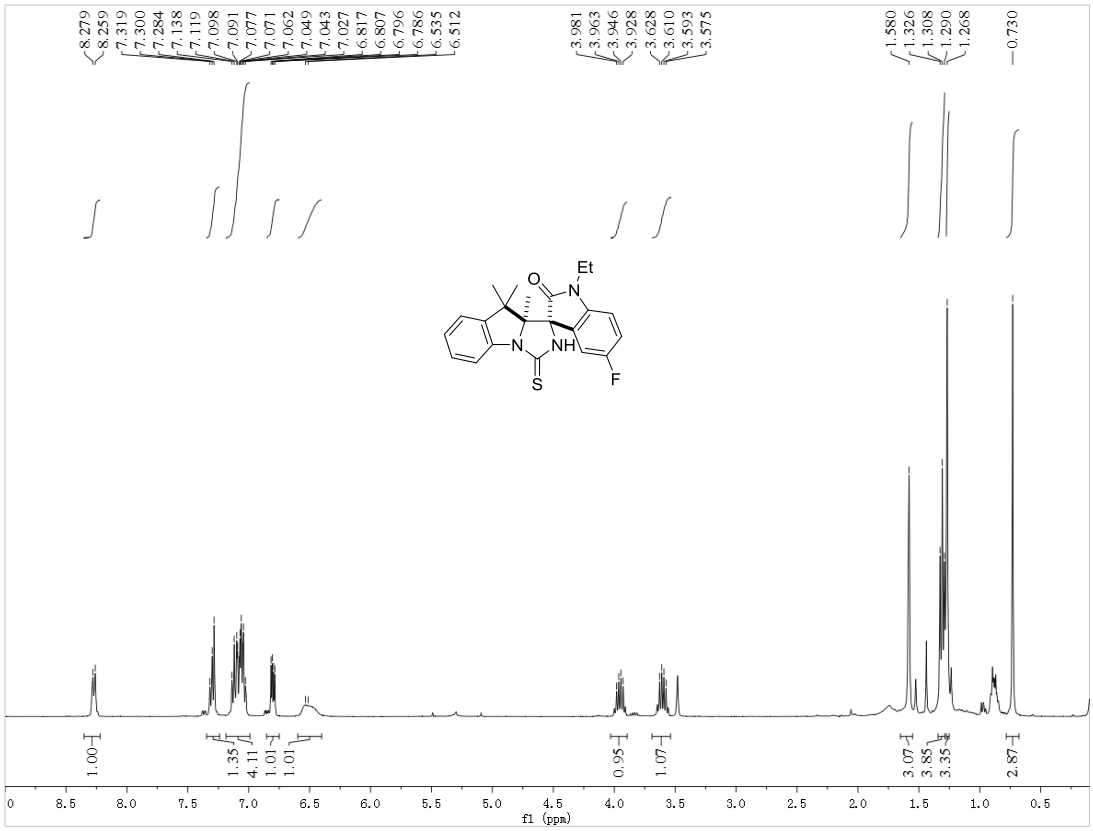


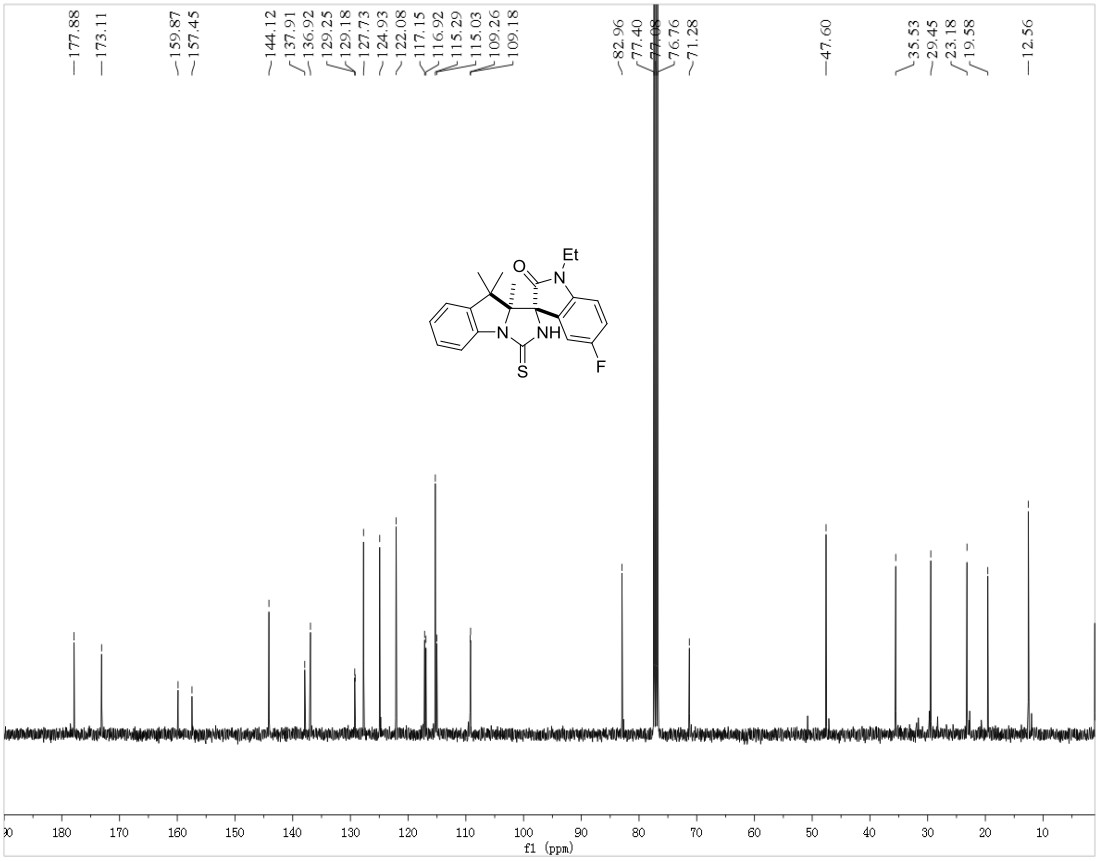


HRMS of 3af


Item name: LRM-B2-3af
Item description:
Channel name: 1: Average Time 0.0874 min : TOF MS (50-1500) ESI+ : Centroided : Combined
5.61e7
Intensity [Counts]
Observed mass [m/z]
400.14466
401.14721
402.14459
403.14502
356.14121
366.15945
376.18745
378.16253
384.16866
397.13818
416.11967
422.12632
425.12750
437.19407
448.14617
Me
O
N
NH
S
CH3

^{1}H and ^{13}C NMR of 3ag

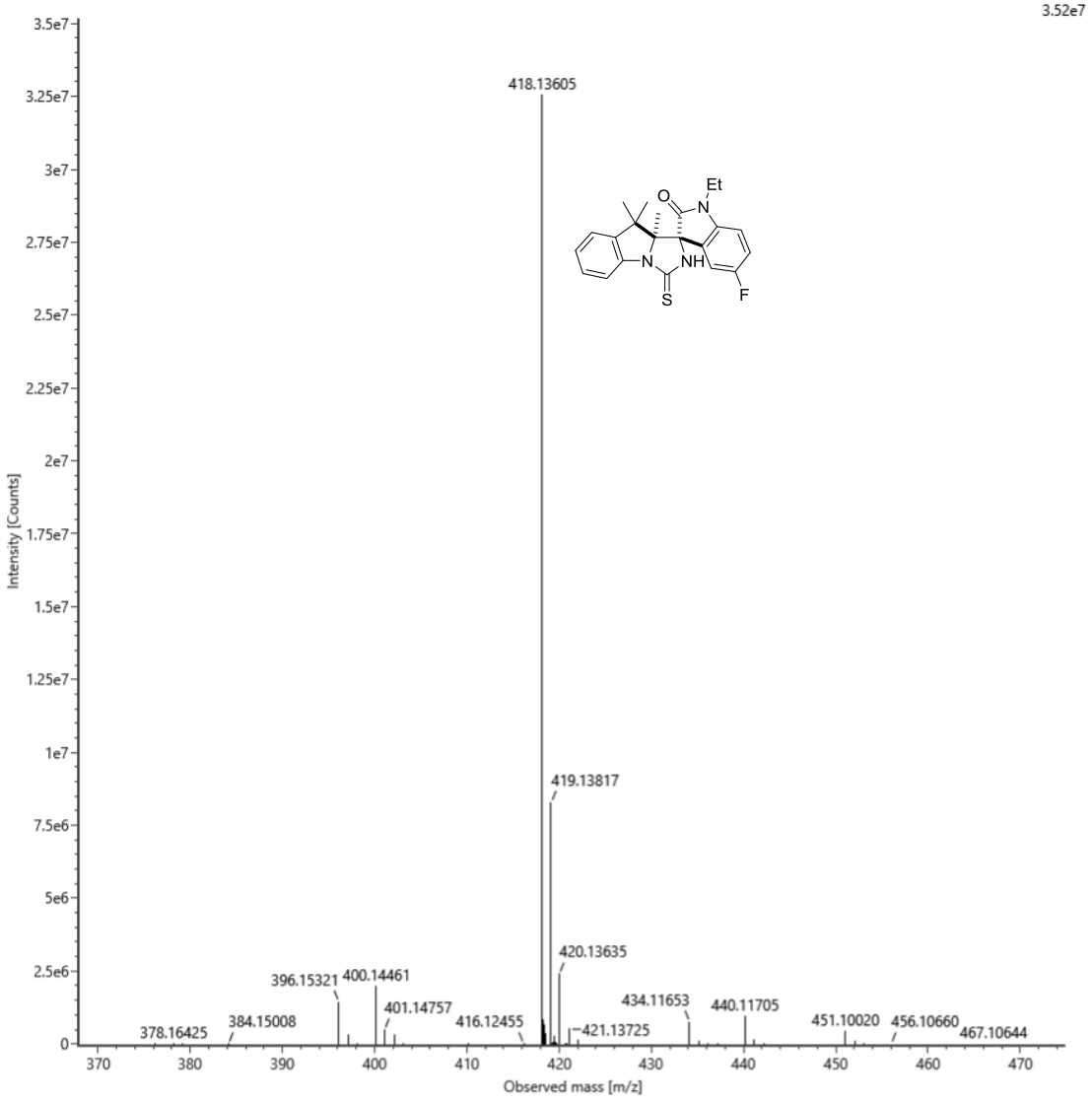




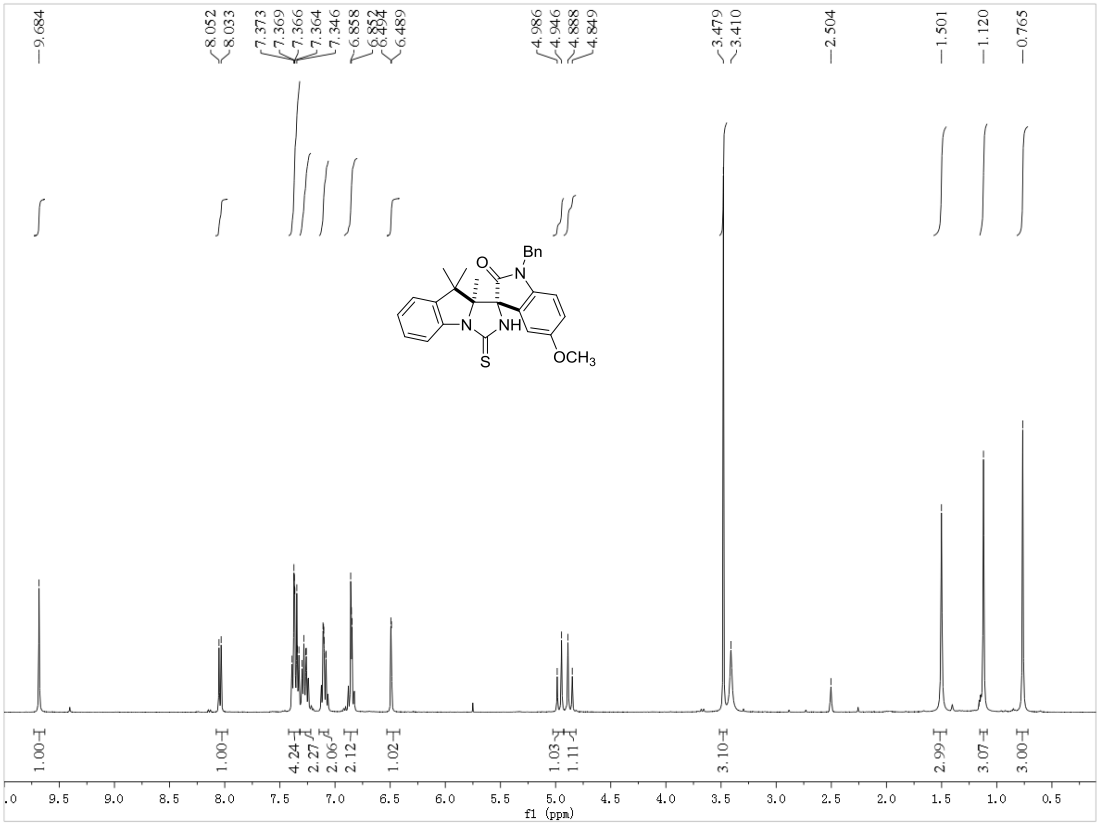
HRMS of 3ag

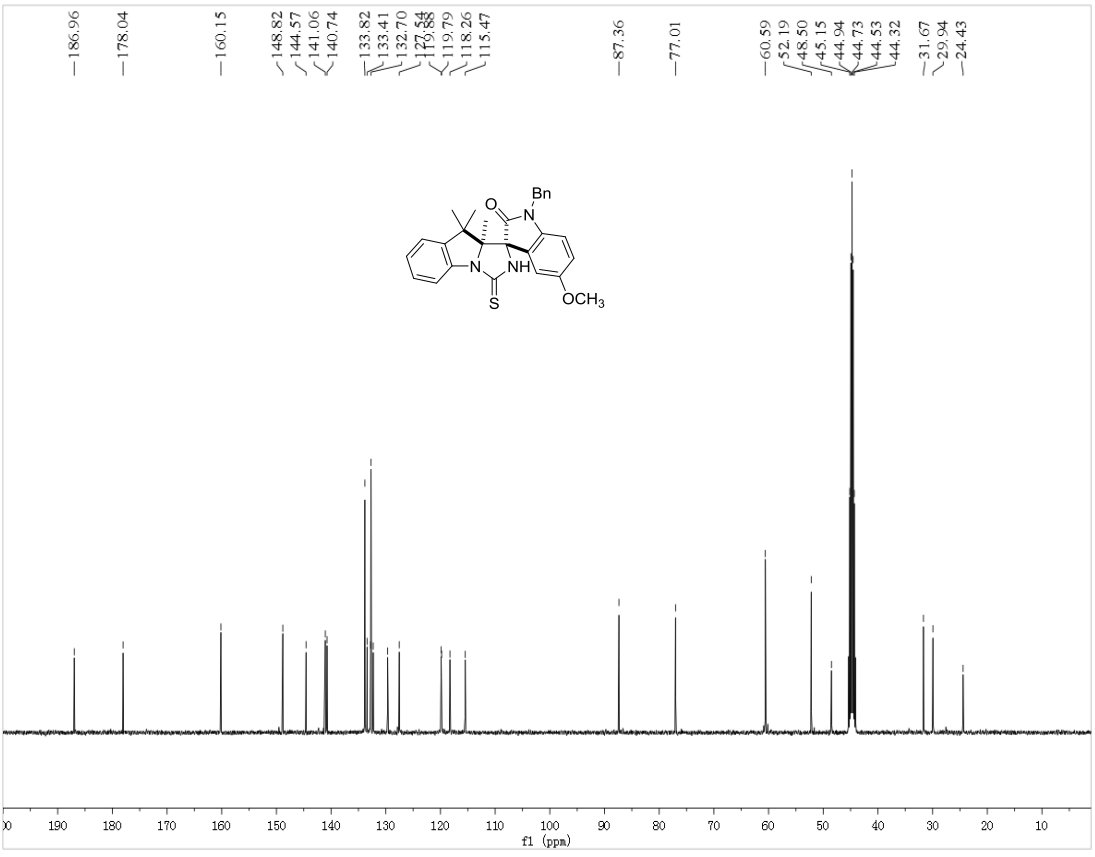
Item name: LRM-B3-3ag
Item description:

Channel name: 1: Average Time 0.0831 min : TOF MS (50-1500) ESI+ : Centroided : Combined



^{1}H and ^{13}C NMR of 3ah

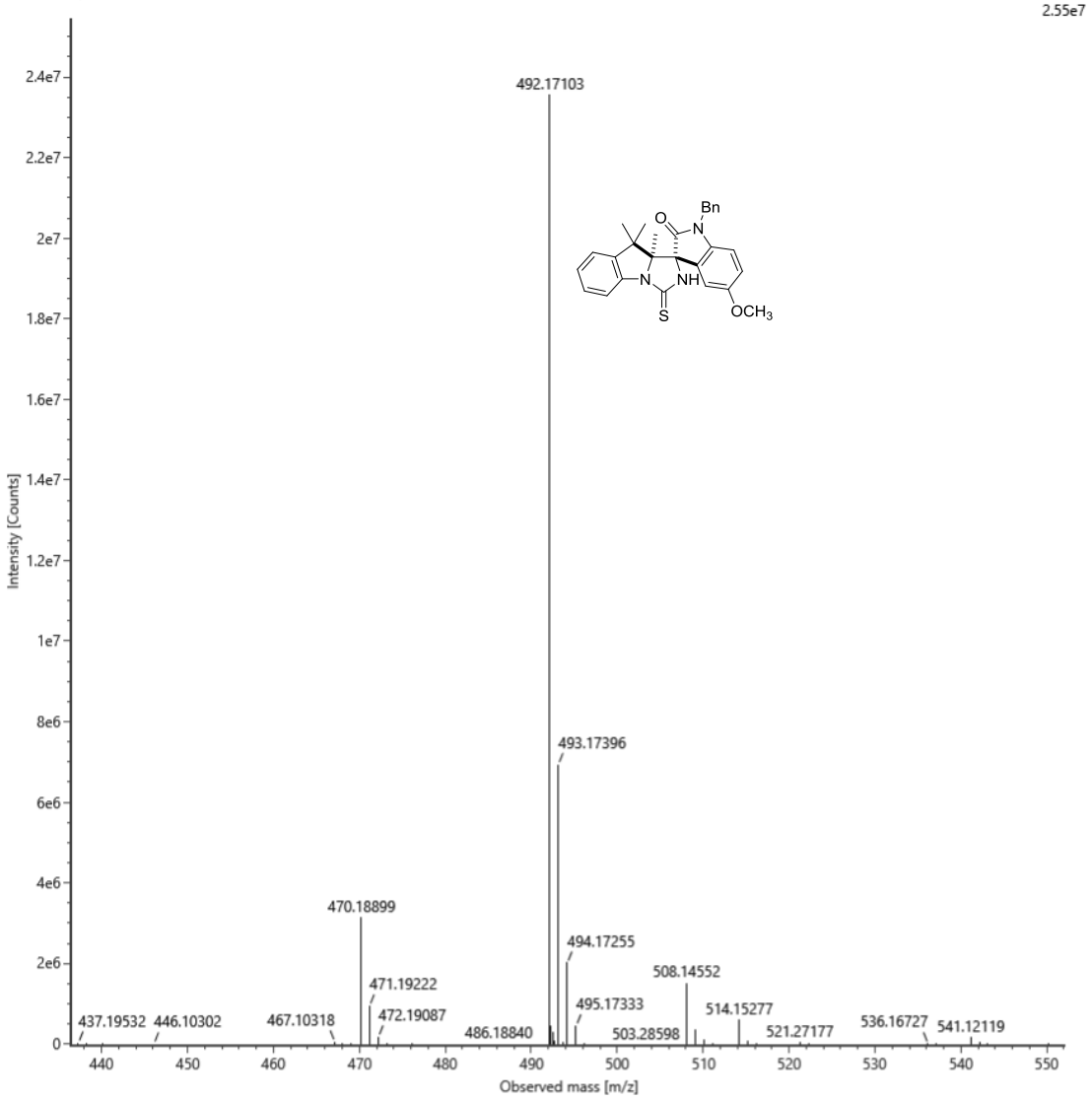




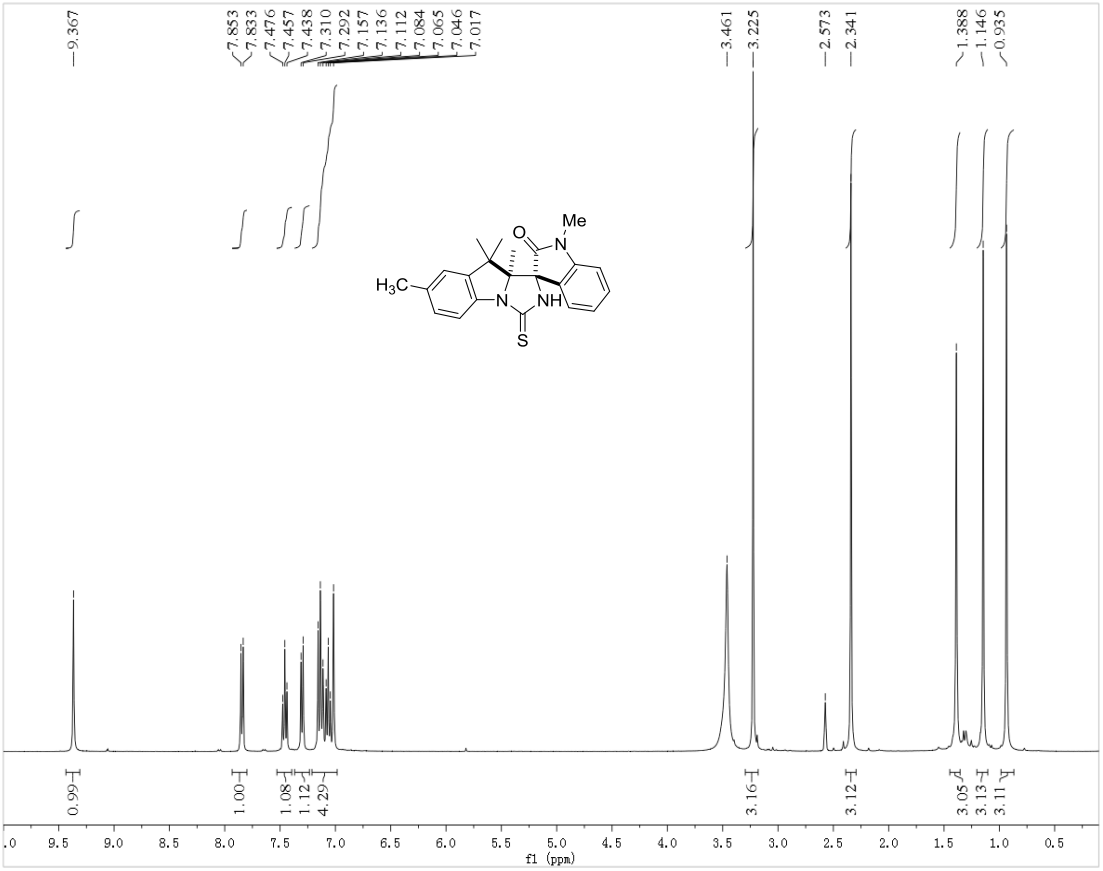
HRMS of 3ah

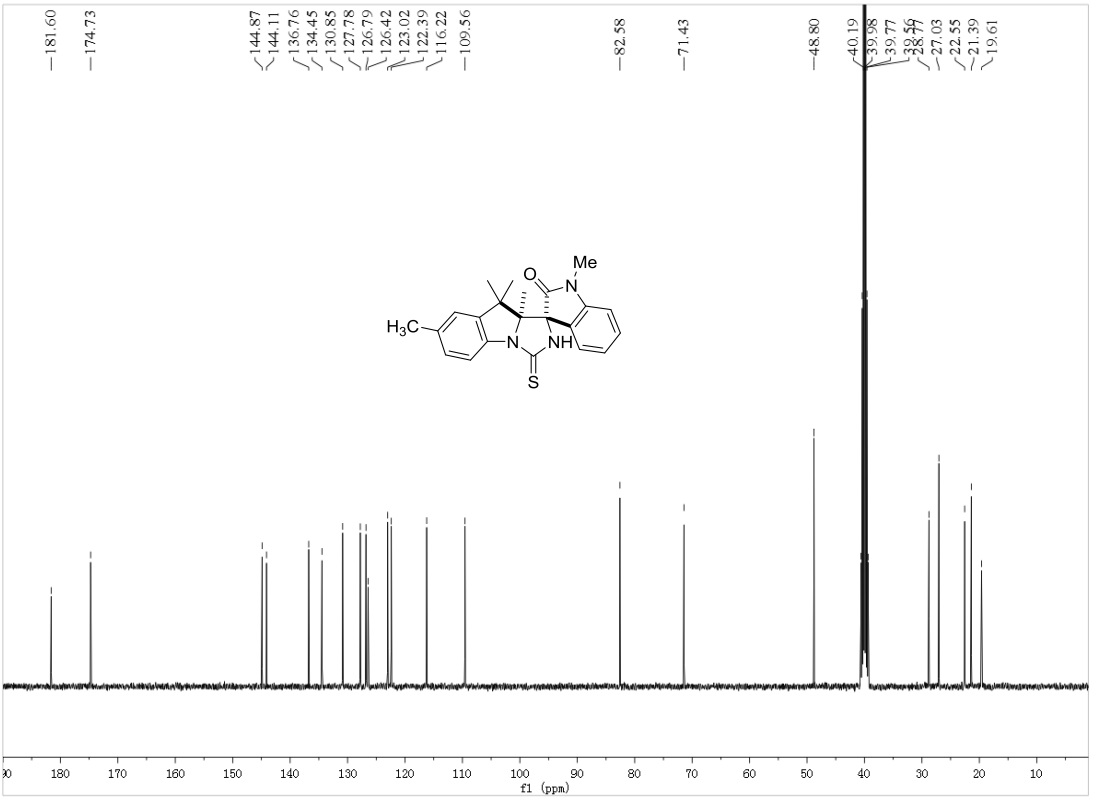
Item name: LRM-H23-3ah
Item description:

Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined

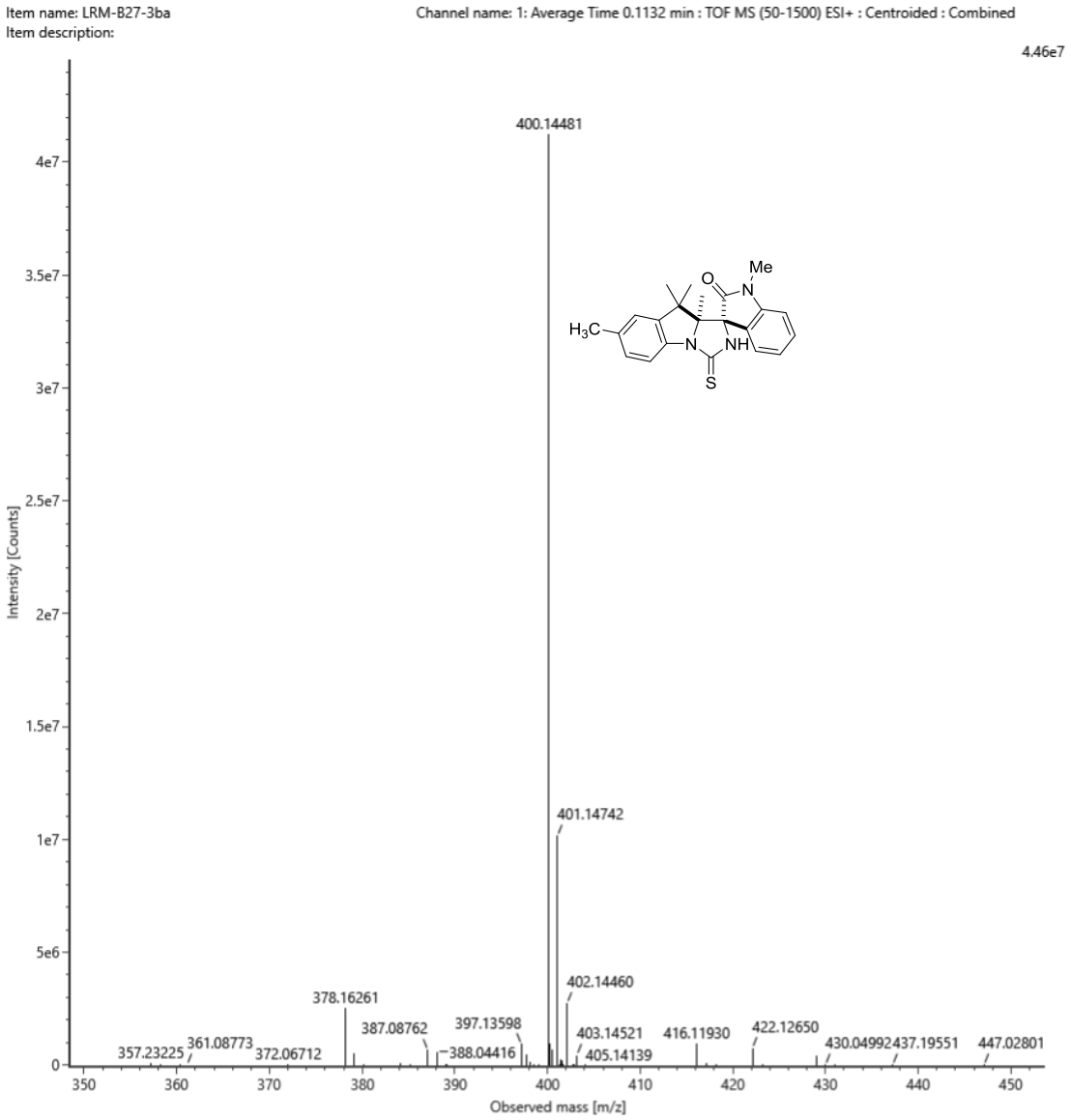


^{1}H and ^{13}C NMR of 3ba

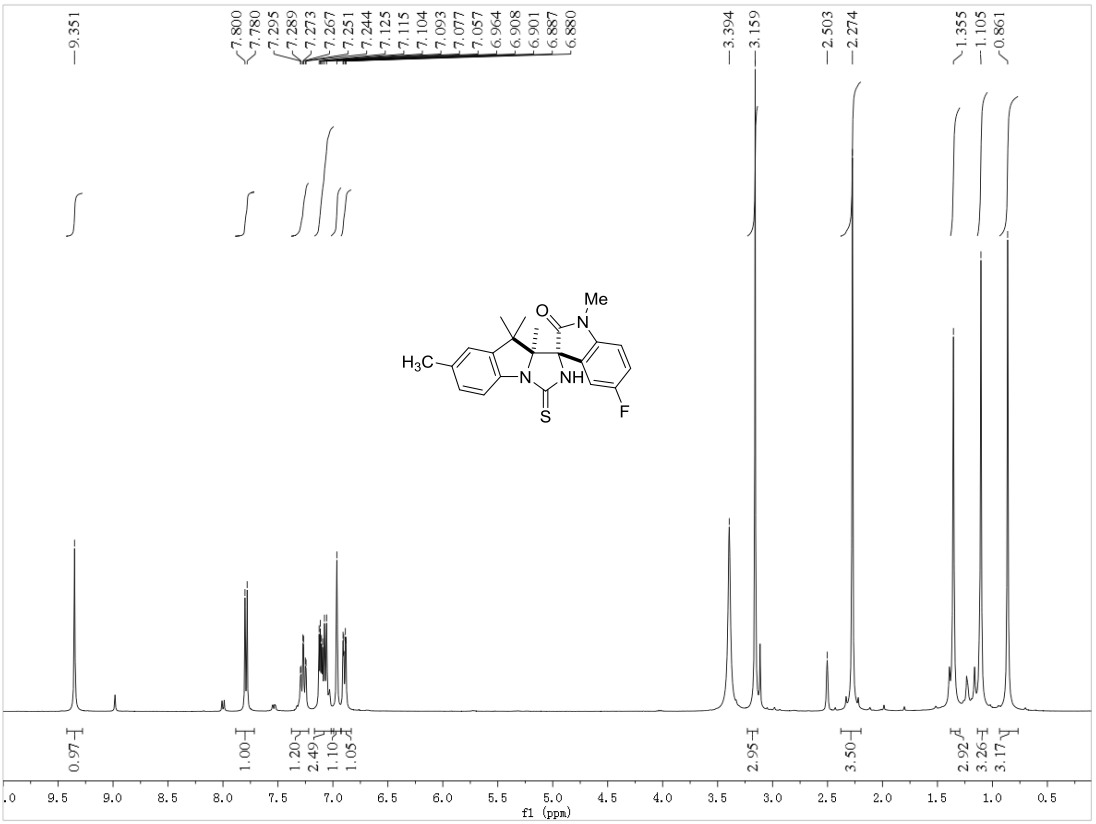


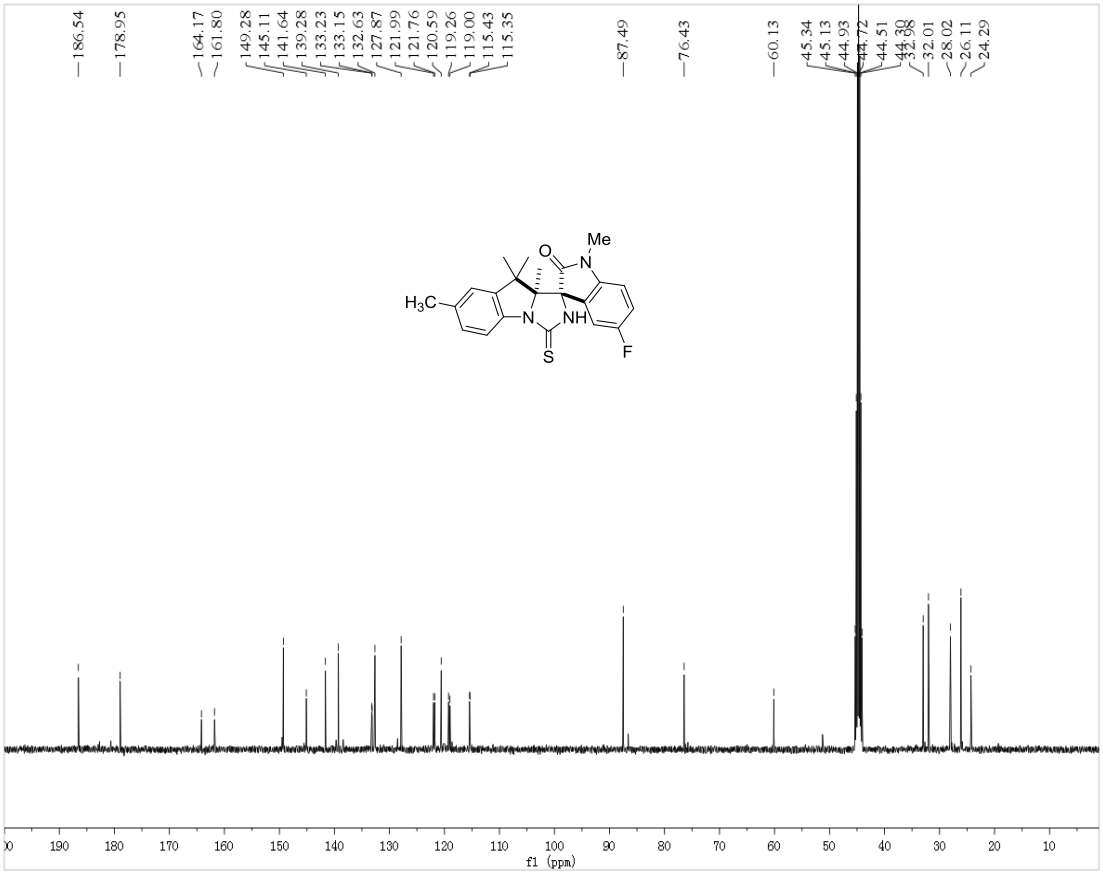


HRMS of 3ba


Item name: LRM-B27-3ba
Item description:
Channel name: 1: Average Time 0.1132 min : TOF MS (50-1500) ESI+ : Centroided : Combined
4.46e7
400.14481
401.14742
402.14460
378.16261
387.08762
397.13598
403.14521
416.11930
422.12650
430.04992
437.19551
447.02801
357.23225
361.08773
372.06712
388.04416
405.14139
Intensity [Counts]
Observed mass [m/z]
Me
O
N
H3C
NH
S

^{1}H and ^{13}C NMR of 3bb

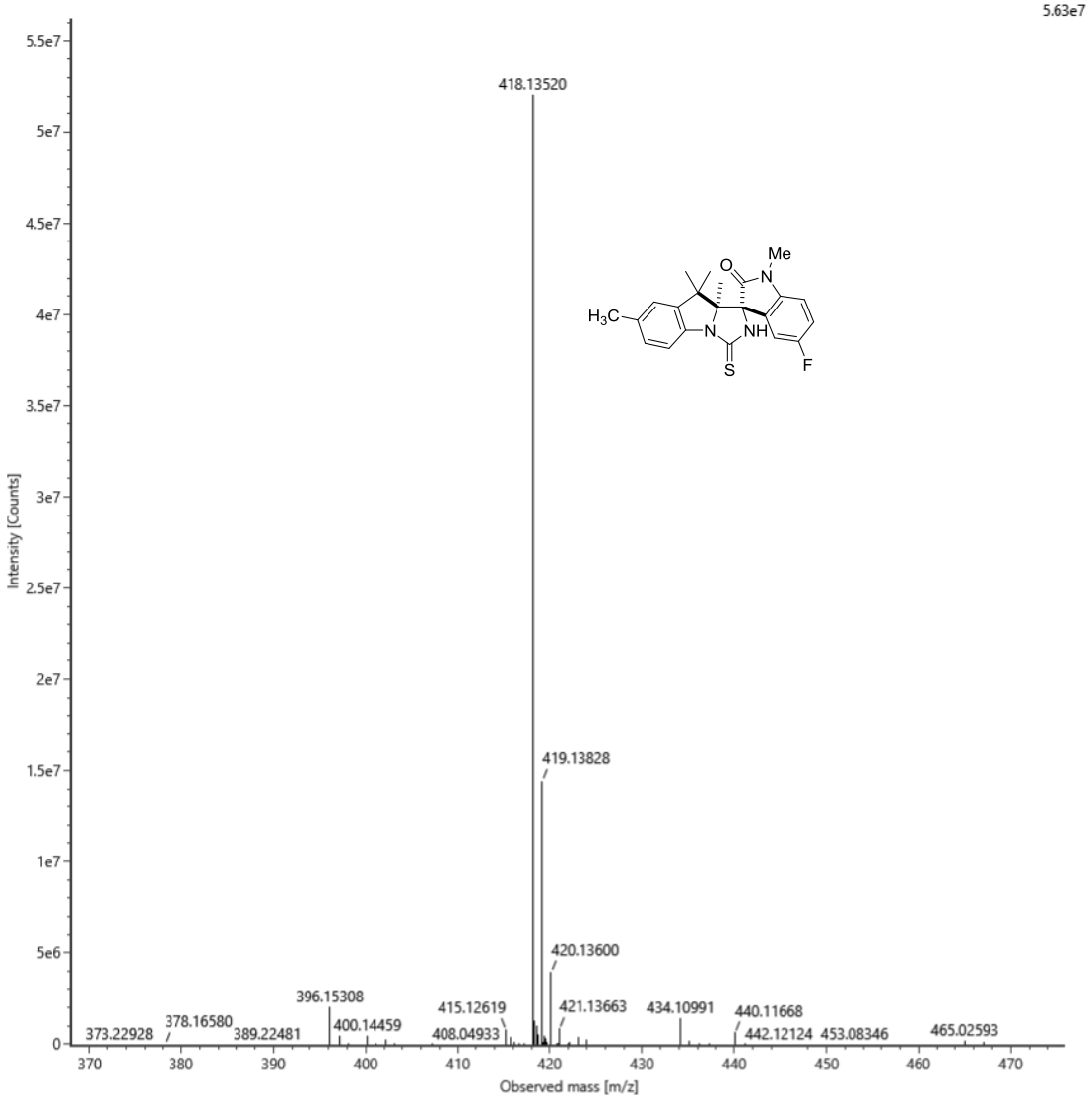




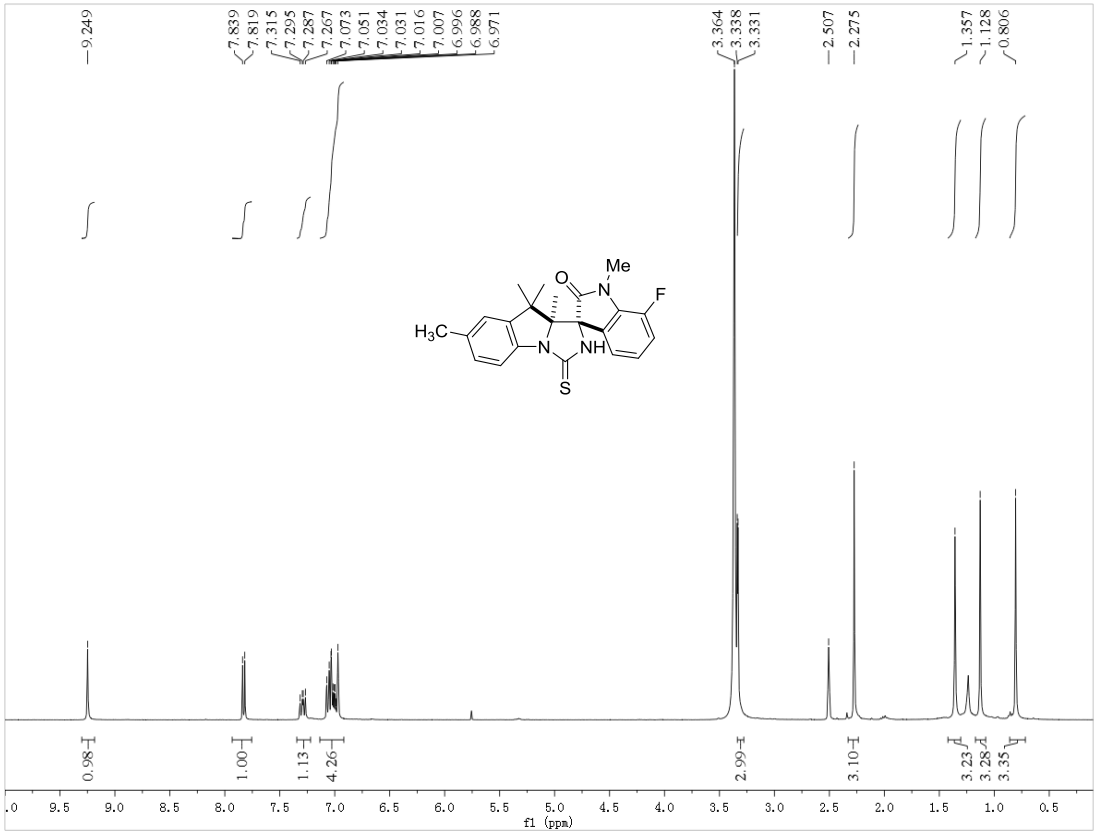
HRMS of 3bb

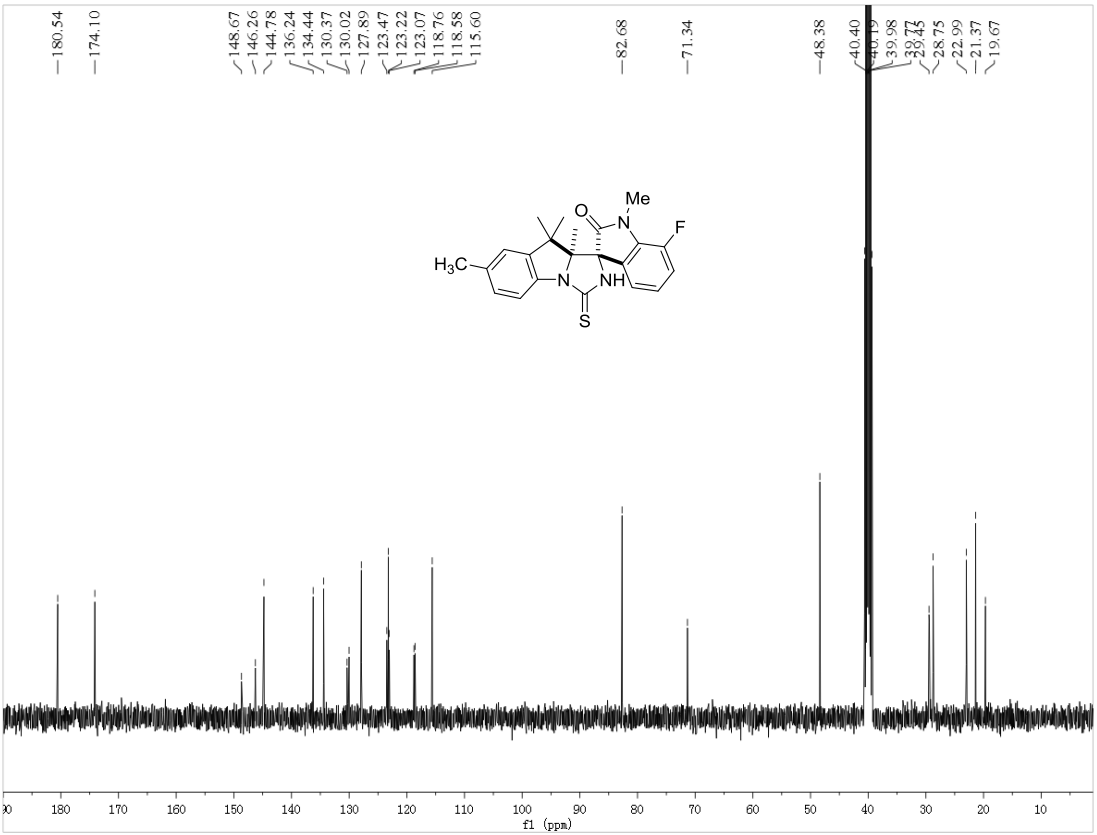
Item name: LRM-B20-3bb
Item description:

Channel name: 1: Average Time 0.1046 min : TOF MS (50-1500) ESI+ : Centroided : Combined



^{1}H and ^{13}C NMR of 3bc

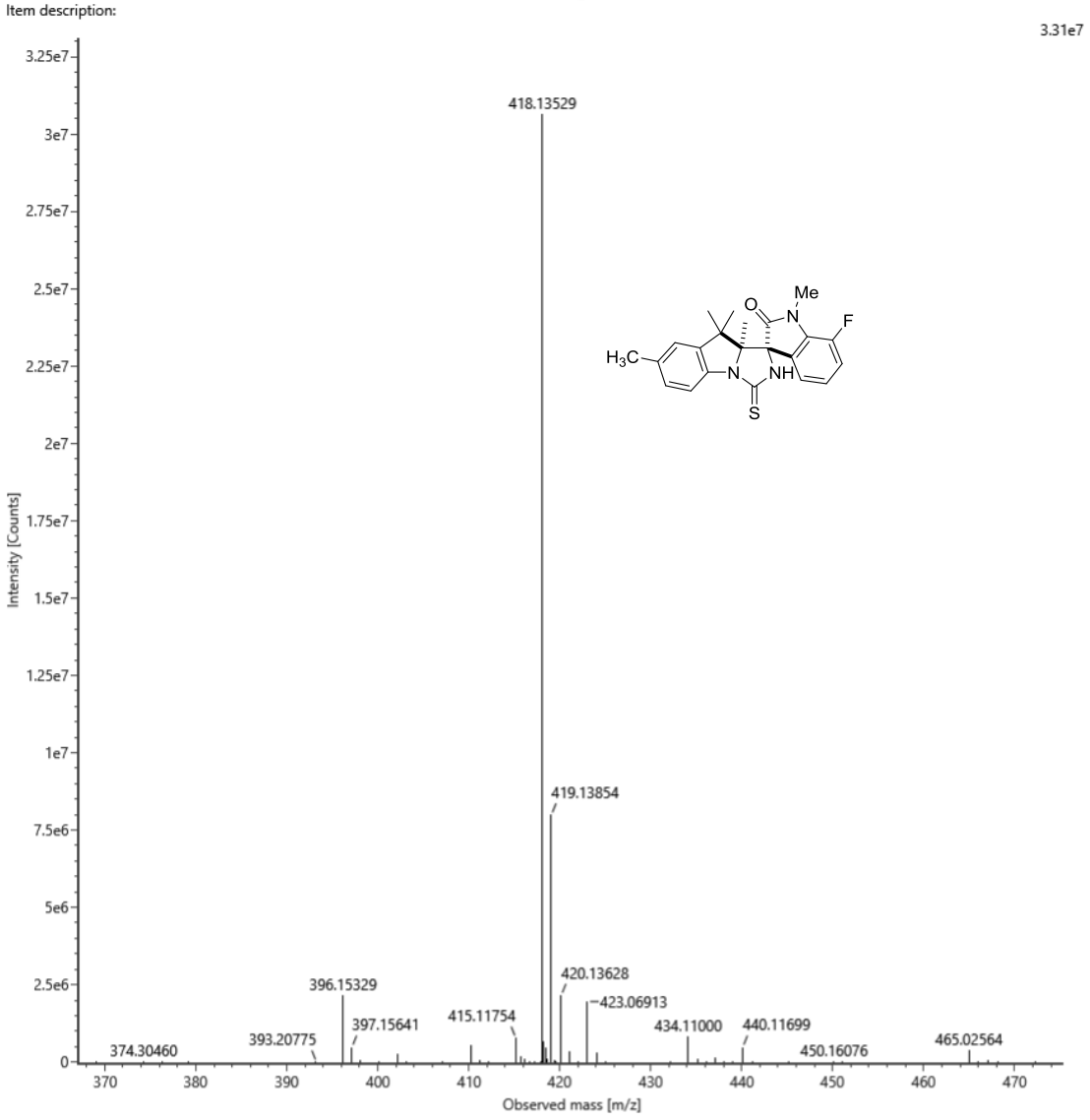




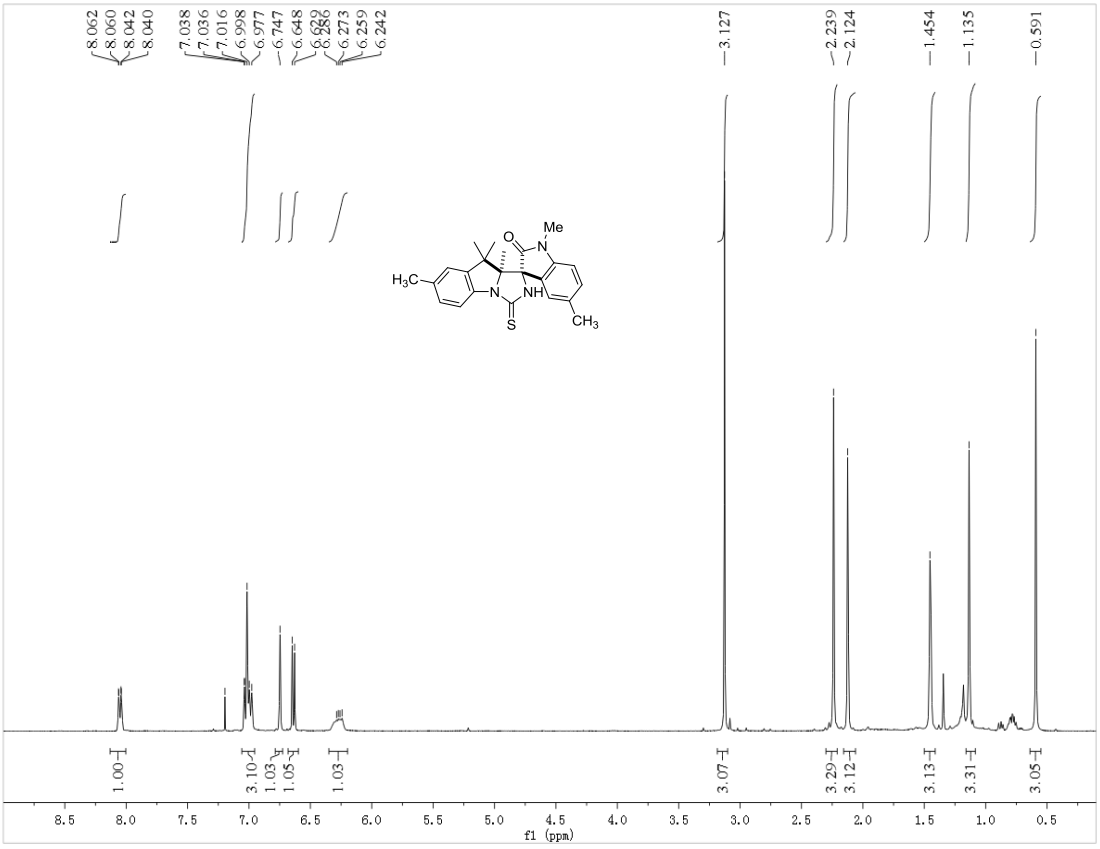
HRMS of 3bc

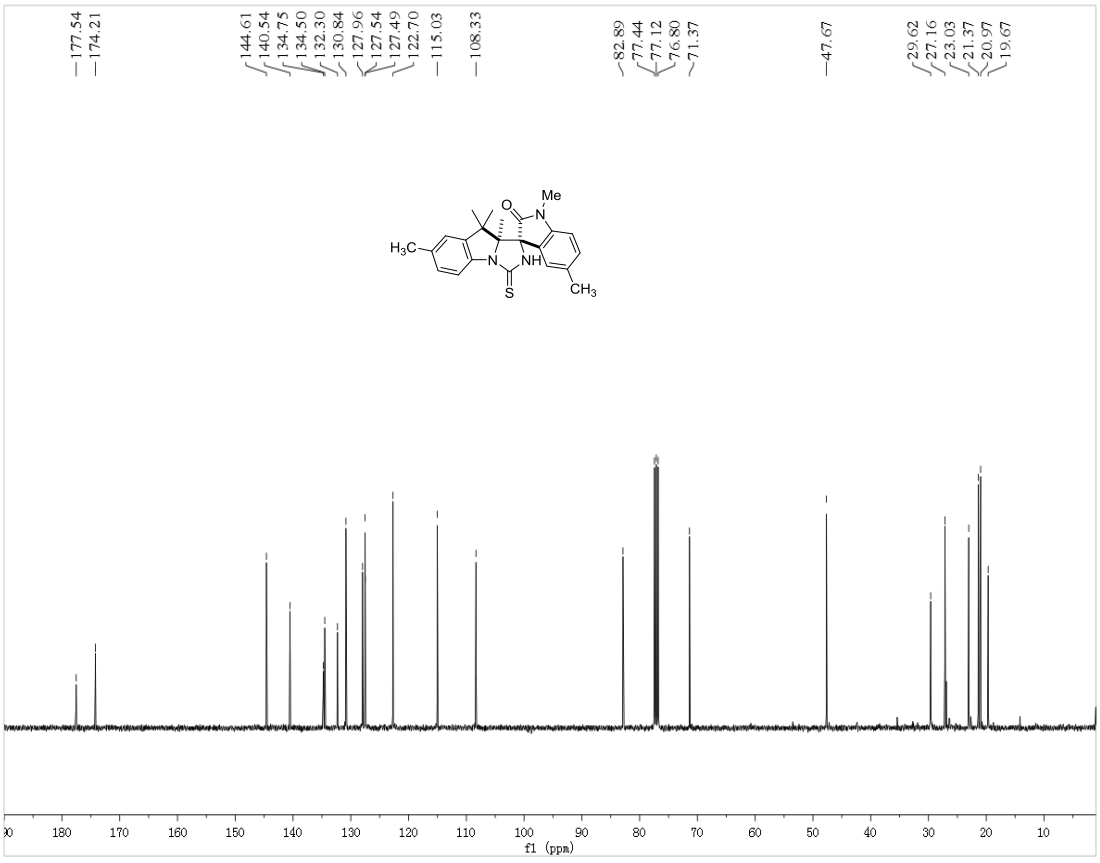
Item name: LRM-B31-3bc
Item description:

Channel name: 1: Average Time 0.1046 min : TOF MS (50-1500) ESI+ : Centroided : Combined



^{1}H and ^{13}C NMR of 3bd

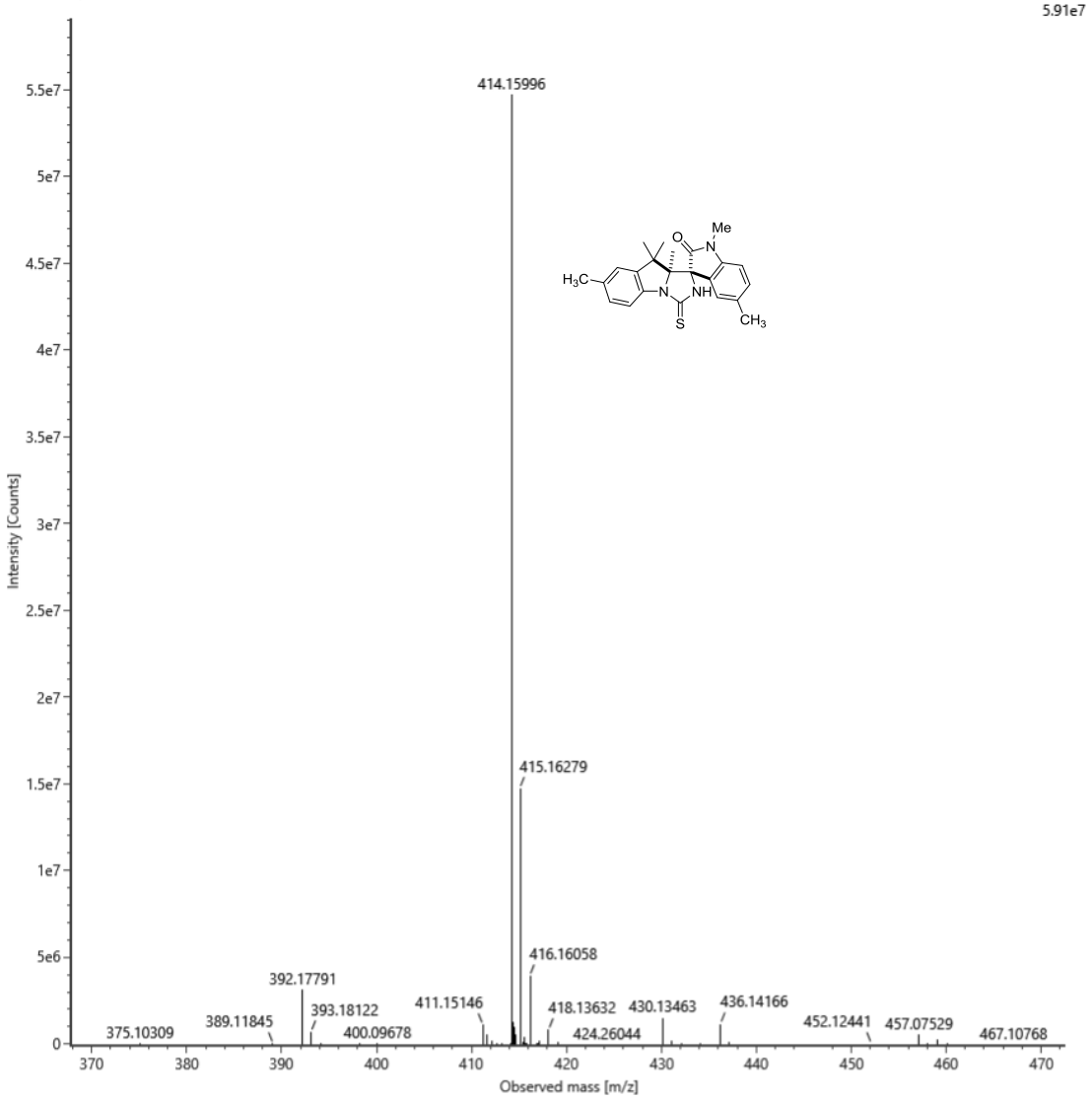




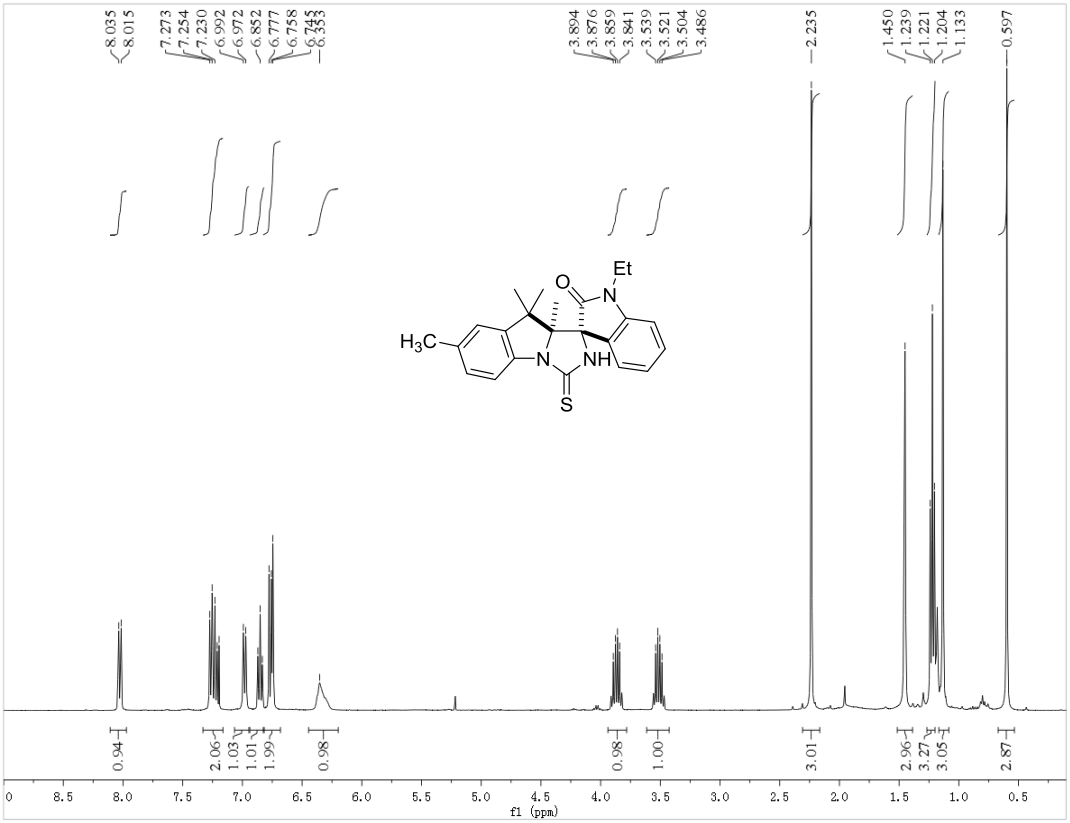
HRMS of 3bd

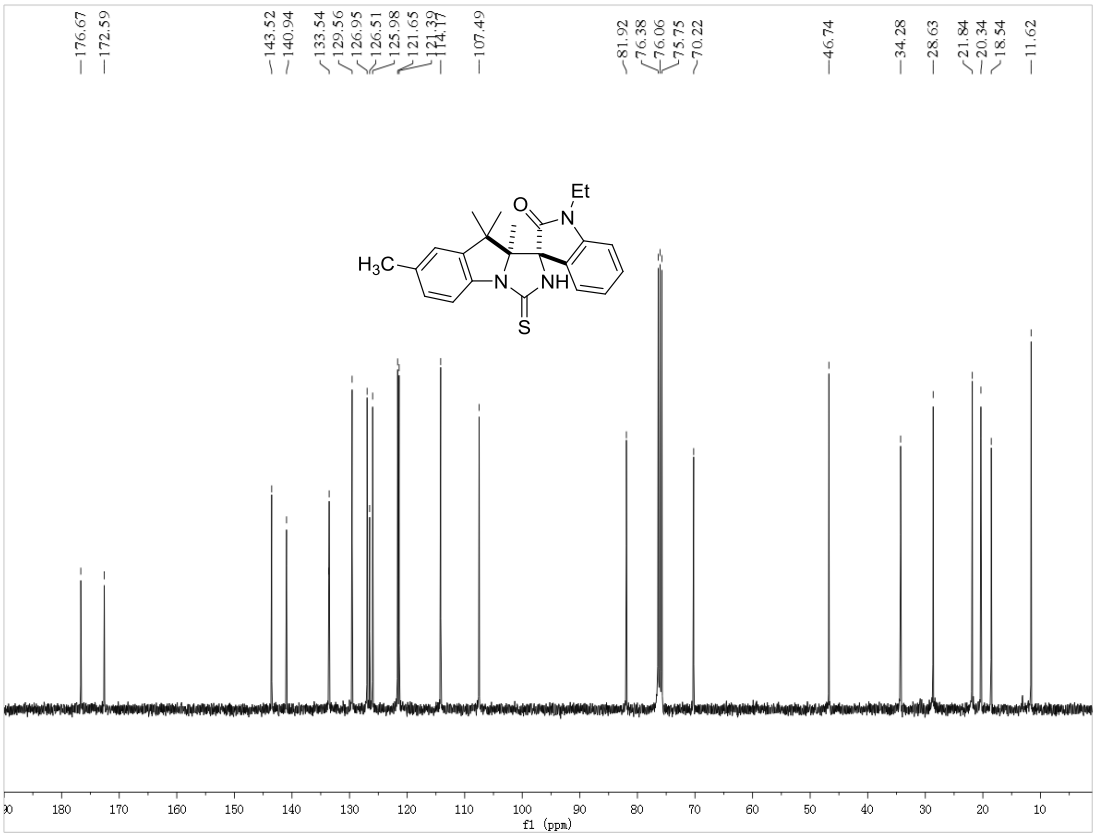
Item name: LRM-B25-3bd
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

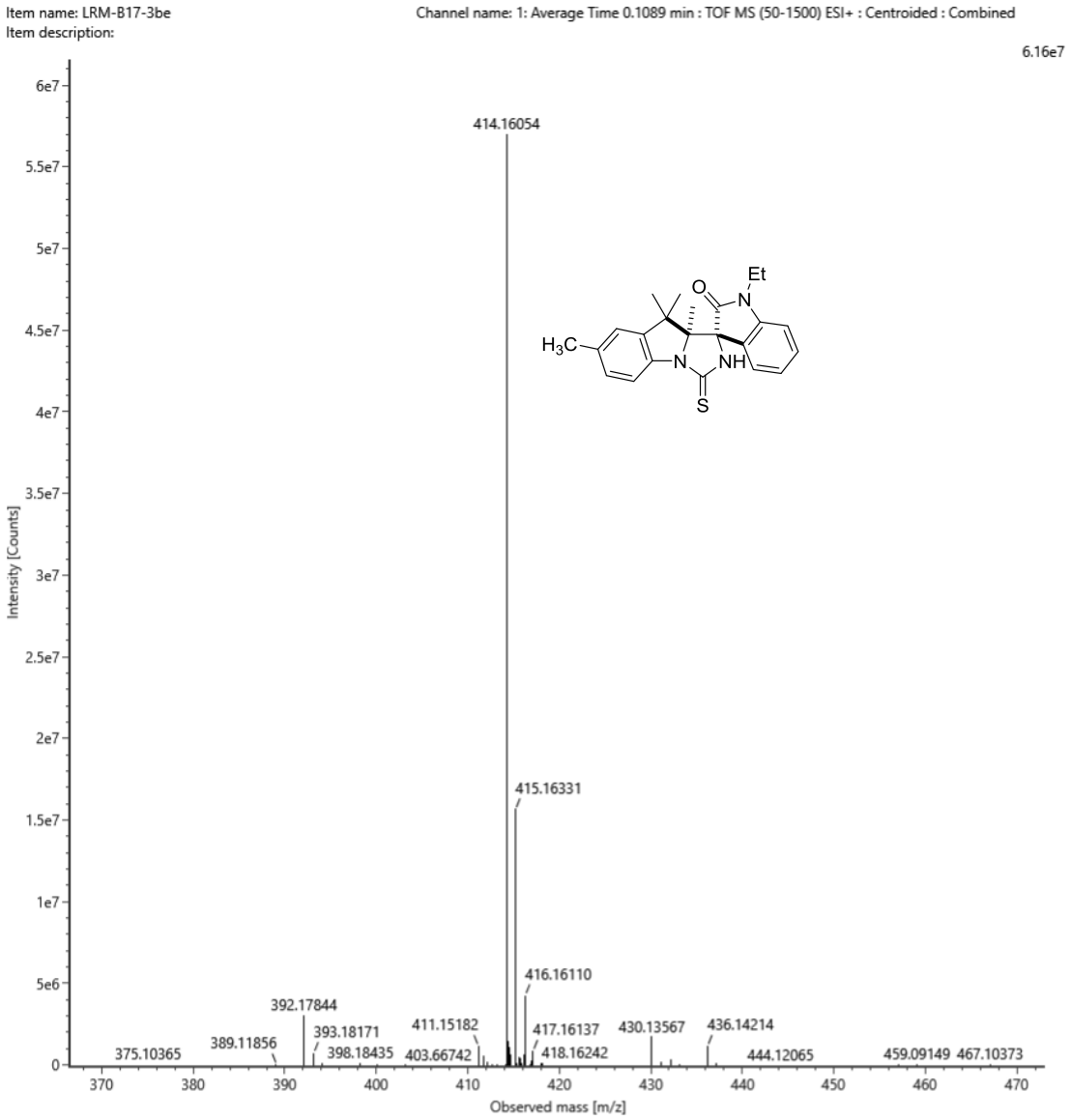


^{1}H and ^{13}C NMR of 3be

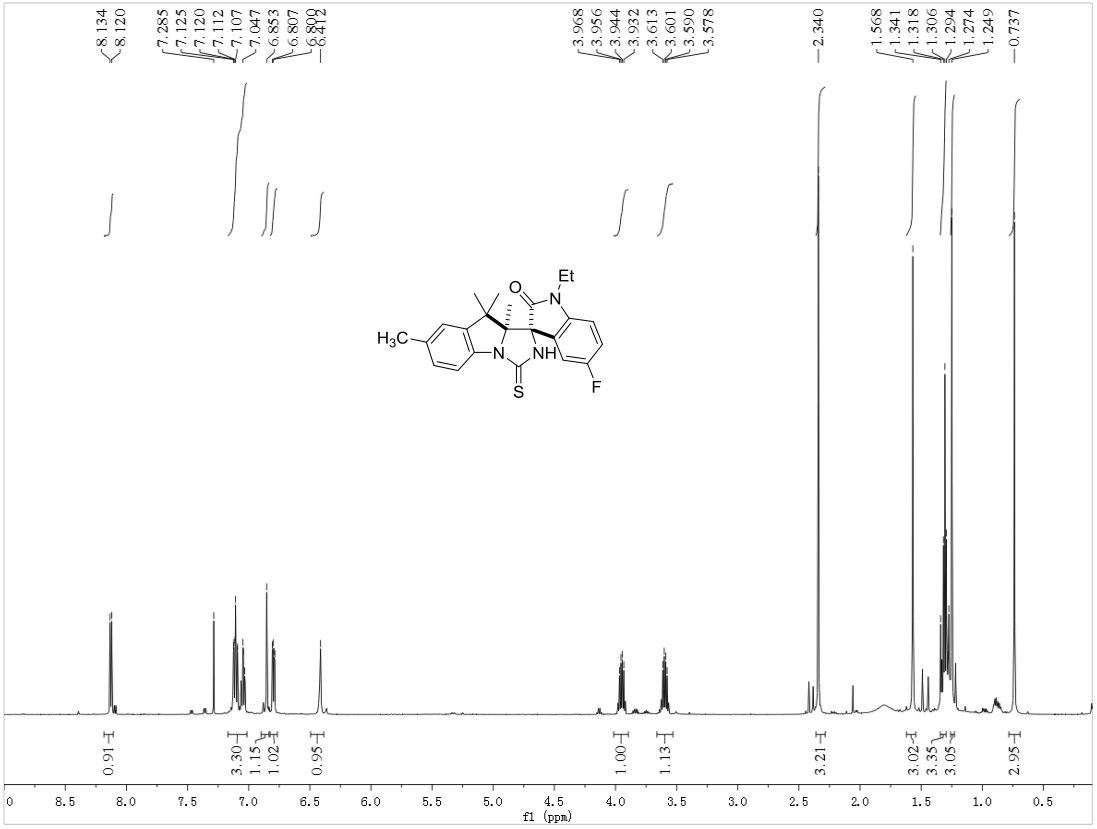


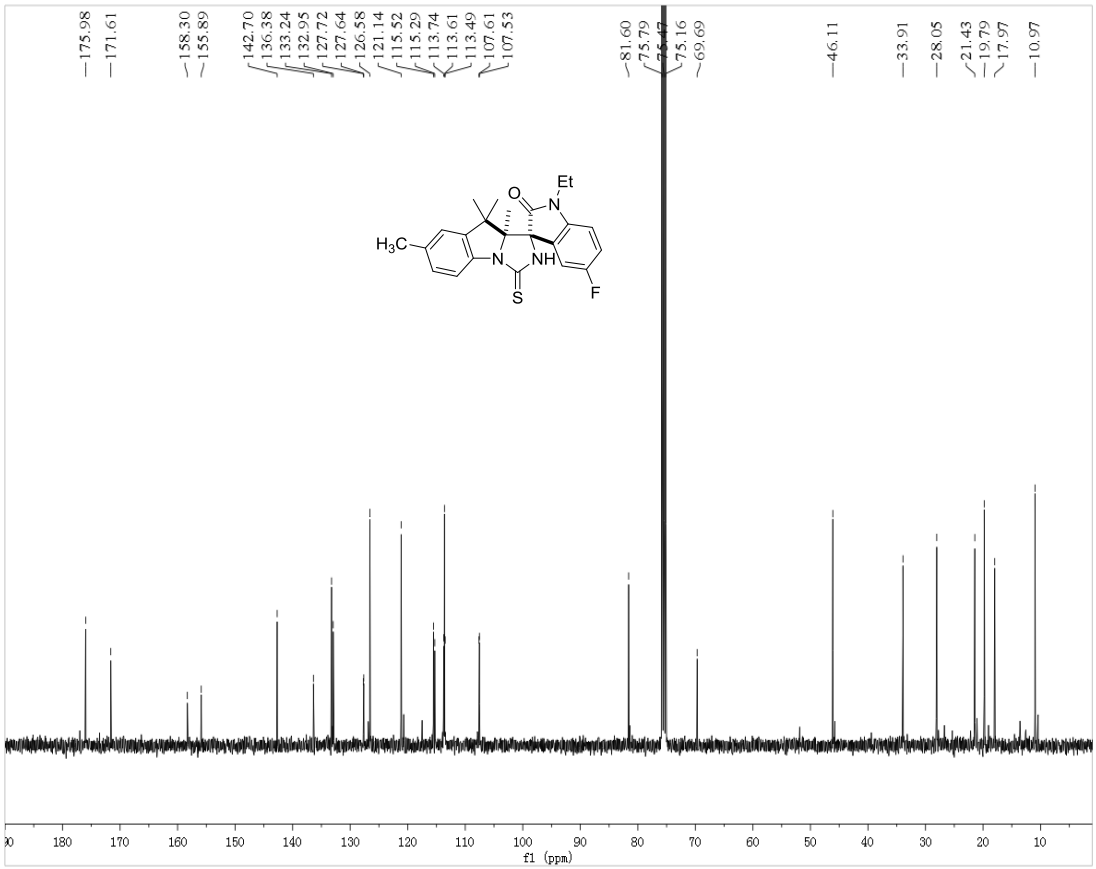


HRMS of 3be

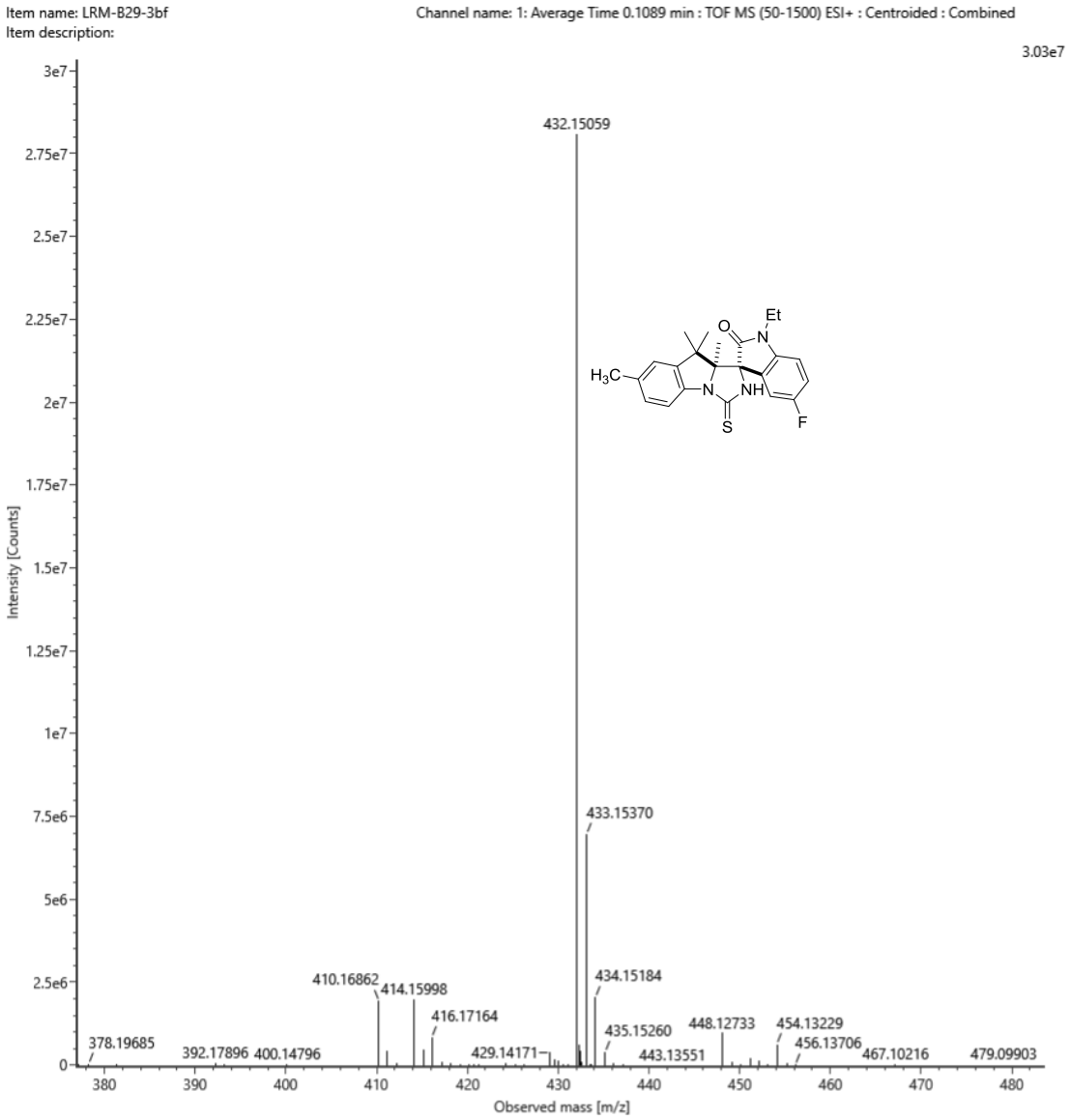

Item name: LRM-B17-3be
Item description:
Channel name: 1: Average Time 0.1089 min : TOF MS (50-1500) ESI+ : Centroided : Combined
6.16e7
Intensity [Counts]
Observed mass [m/z]
414.16054
415.16331
416.16110
392.17844
393.18171
411.15182
417.16137
430.13567
436.14214
375.10365
389.11856
398.18435
403.66742
418.16242
444.12065
459.09149
467.10373
Et
O
N
H3C
N
NH
S

^{1}H and ^{13}C NMR of 3bf

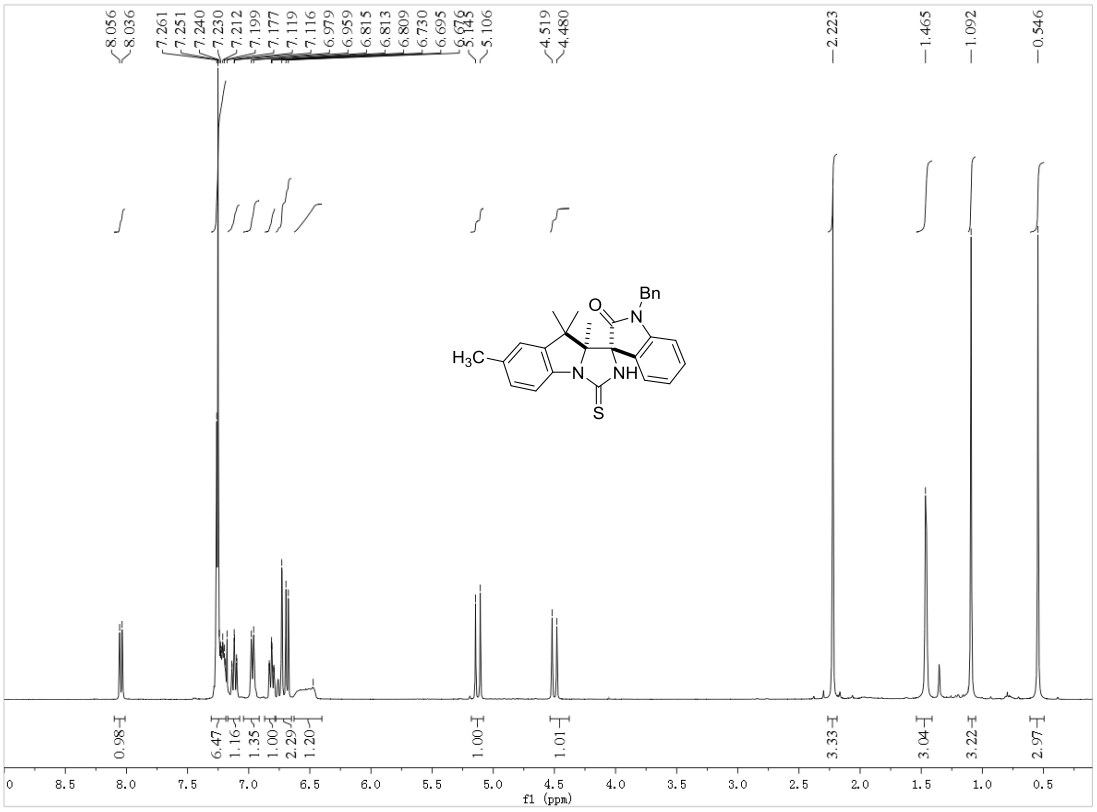


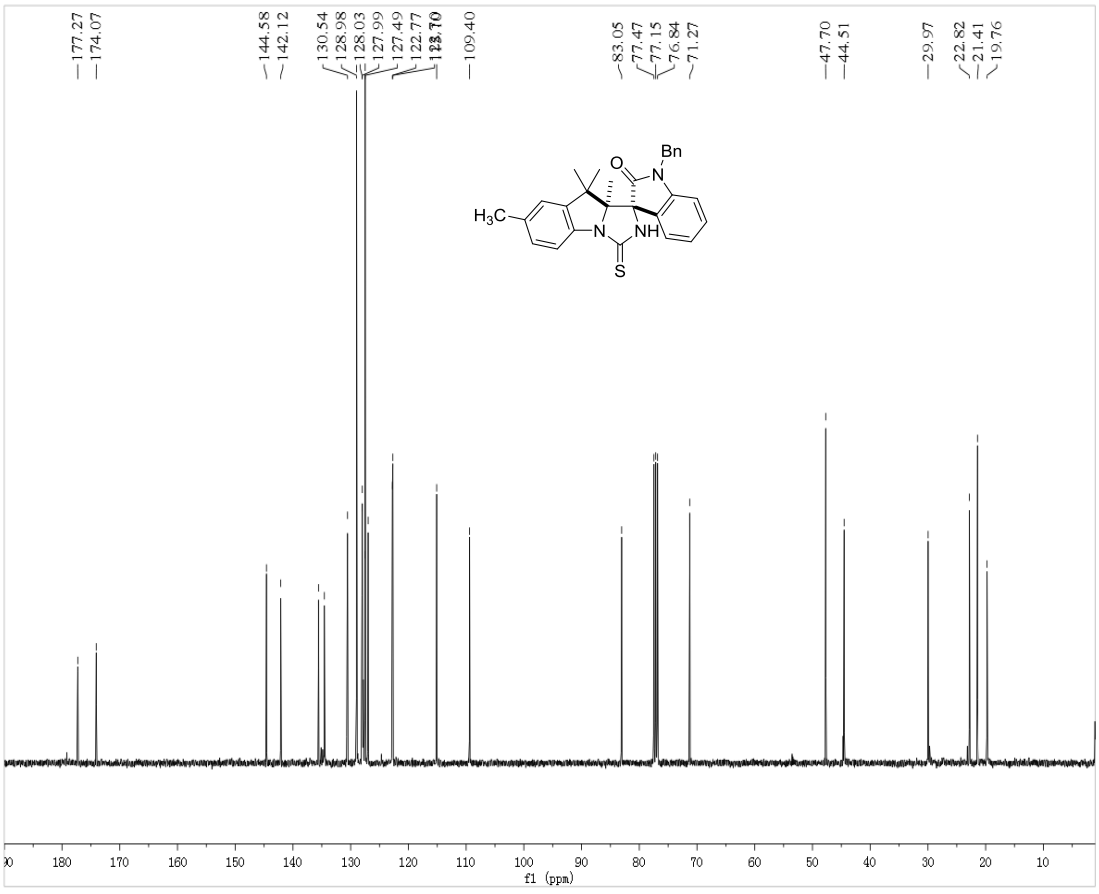


HRMS of 3bf

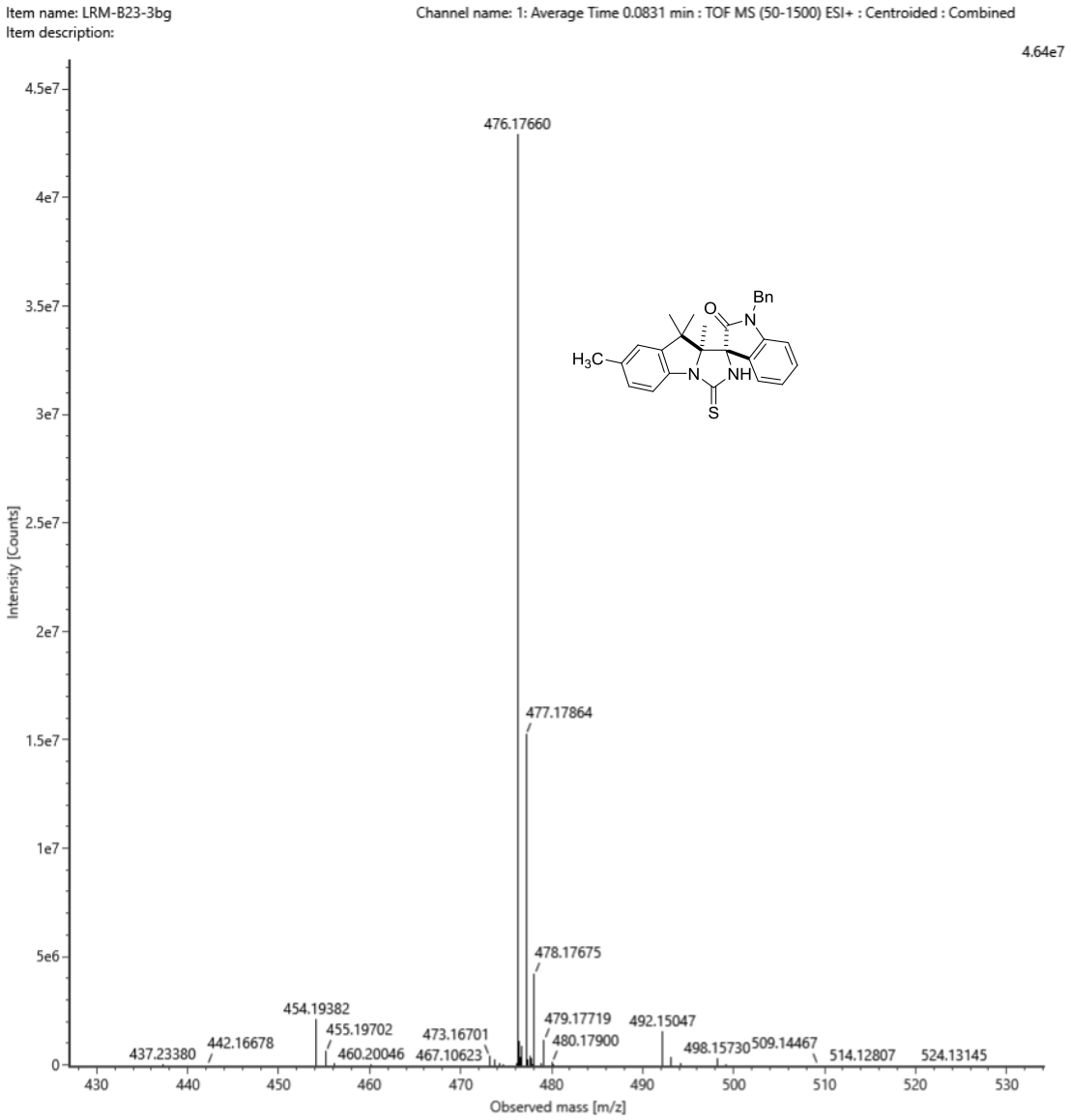

Item name: LRM-B29-3bf
Item description:
Channel name: 1: Average Time 0.1089 min : TOF MS (50-1500) ESI+ : Centroided : Combined
3.03e7
Intensity [Counts]
Observed mass [m/z]
432.15059
433.15370
434.15184
410.16862
414.15998
416.17164
378.19685
392.17896
400.14796
429.14171
435.15260
443.13551
448.12733
454.13229
456.13706
467.10216
479.09903
Et
O
N
H3C
N
NH
S
F

^{1}H and ^{13}C NMR of 3bg

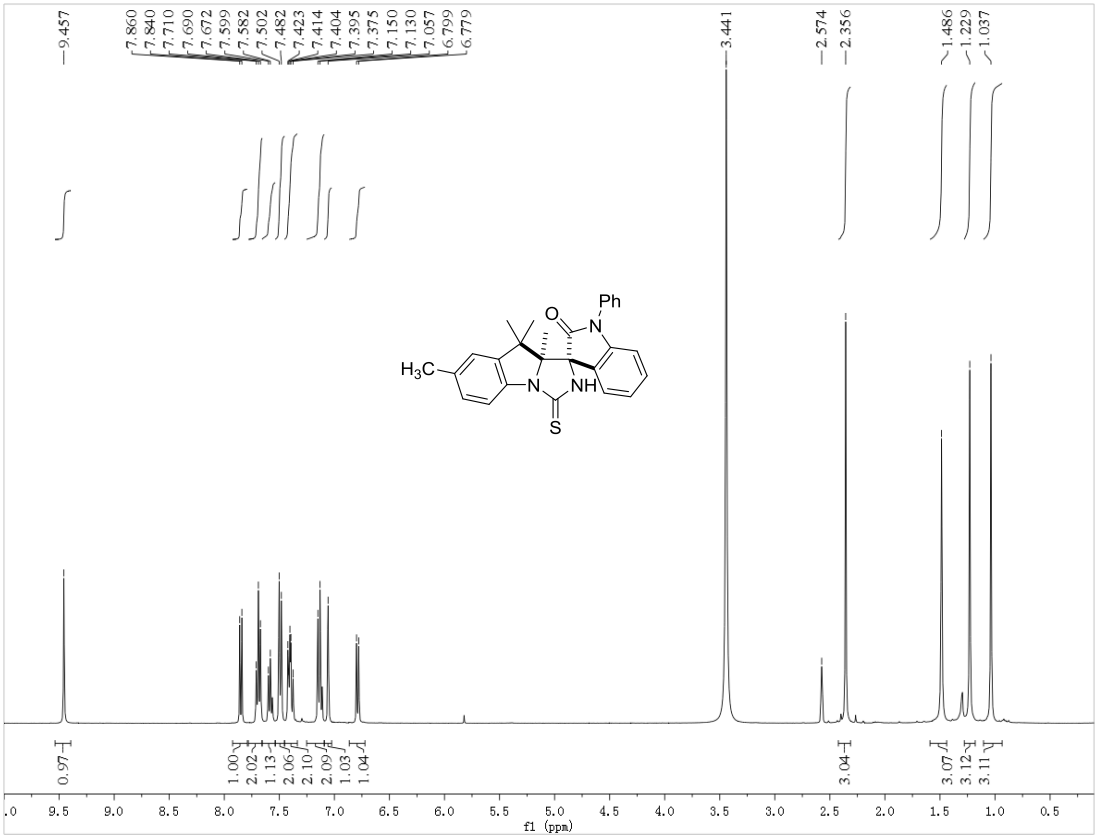


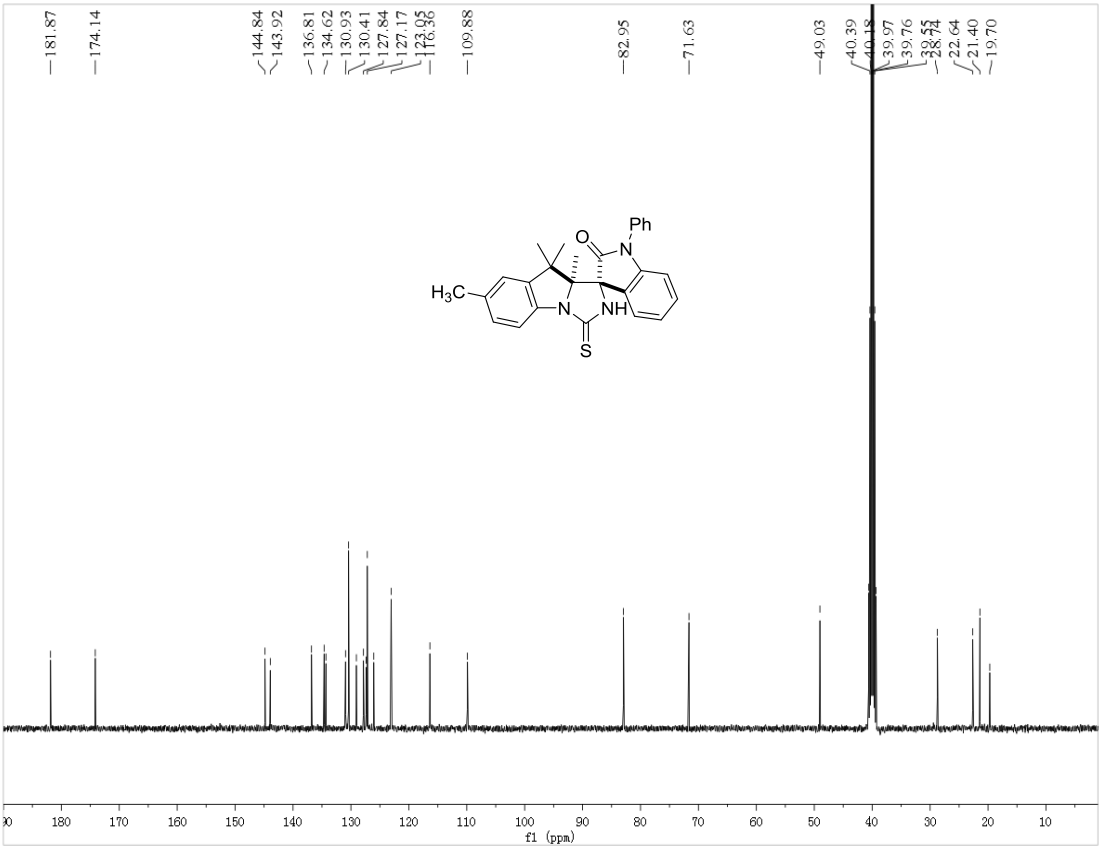


HRMS of 3bg

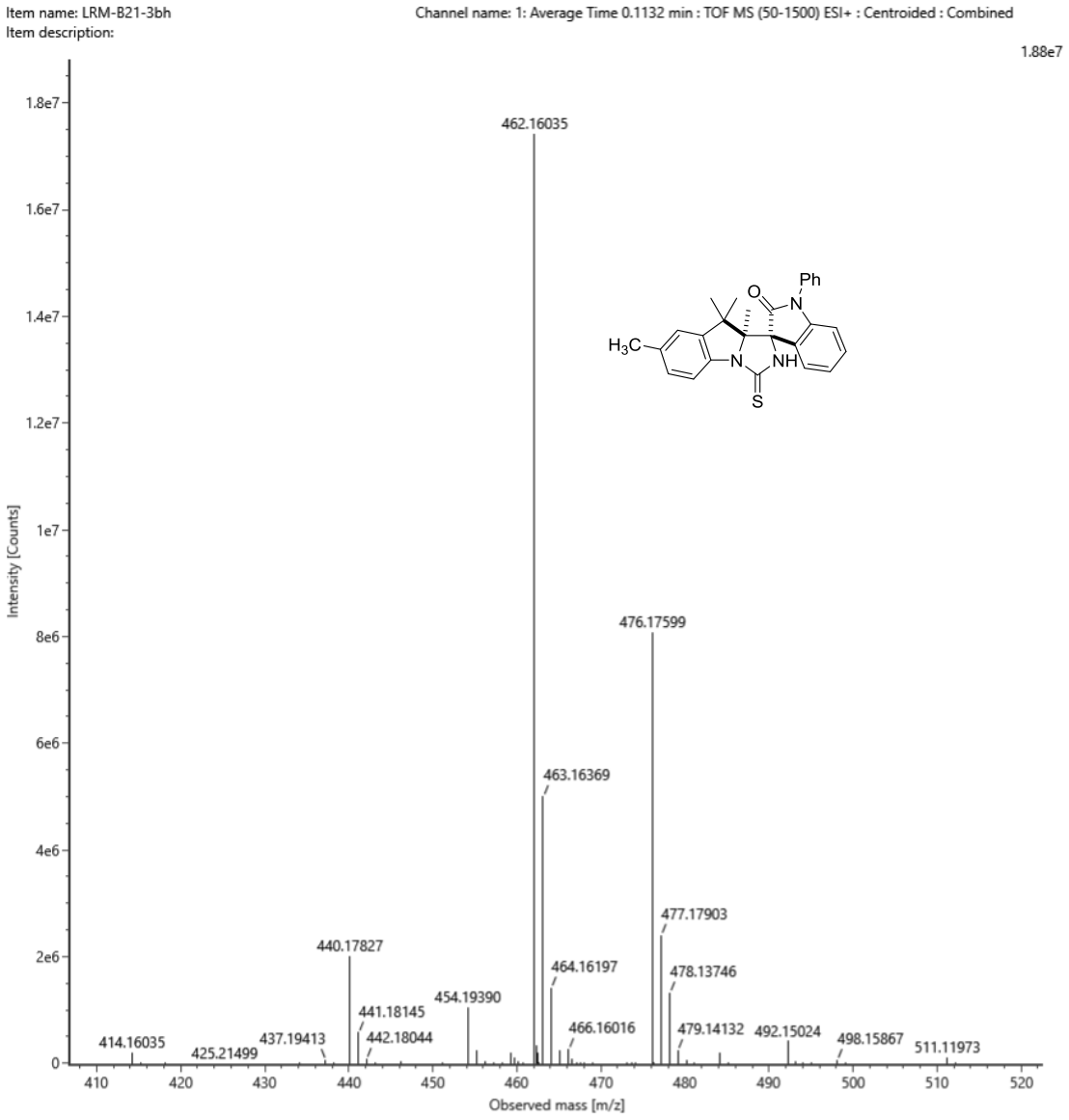

Item name: LRM-B23-3bg
Item description:
Channel name: 1: Average Time 0.0831 min : TOF MS (50-1500) ESI+ : Centroided : Combined
4.64e7
Intensity [Counts]
Observed mass [m/z]
476.17660
477.17864
478.17675
454.19382
455.19702
460.20046
473.16701
467.10623
479.17719
480.17900
492.15047
498.15730
509.14467
514.12807
524.13145
437.23380
442.16678
Bn
O
N
H3C
N
NH
S

^{1}H and ^{13}C NMR of 3bh

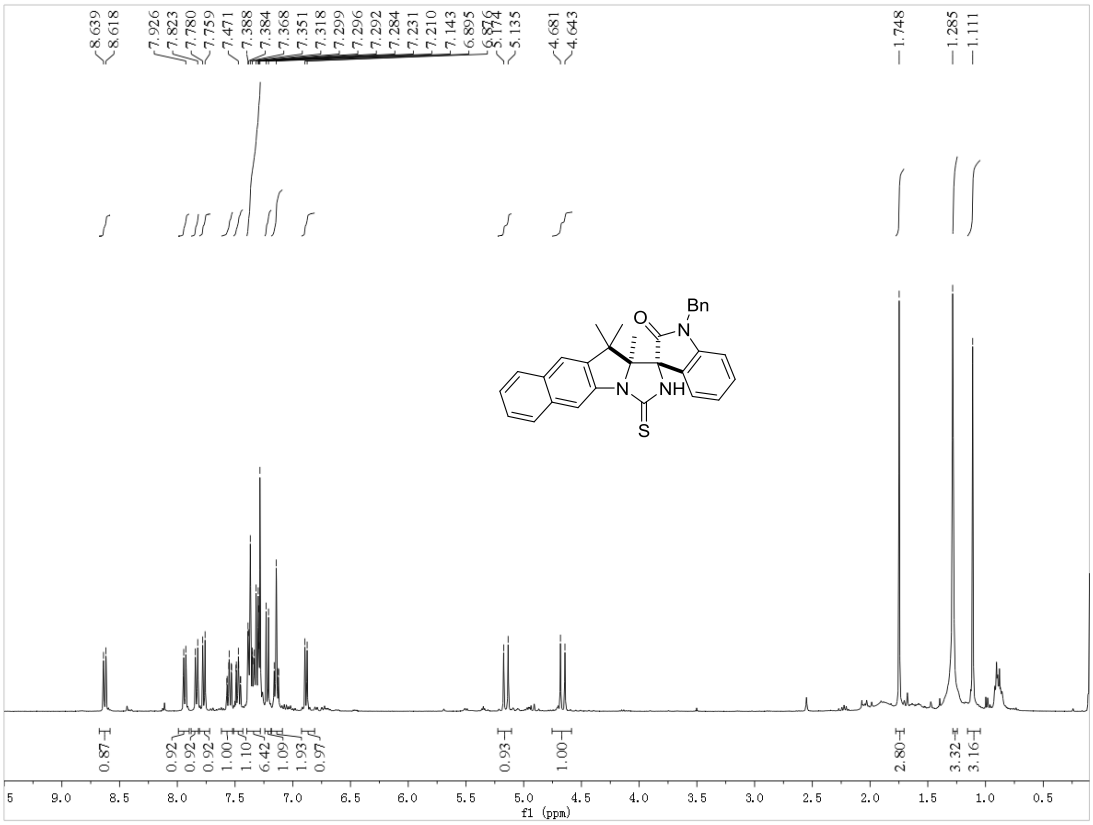


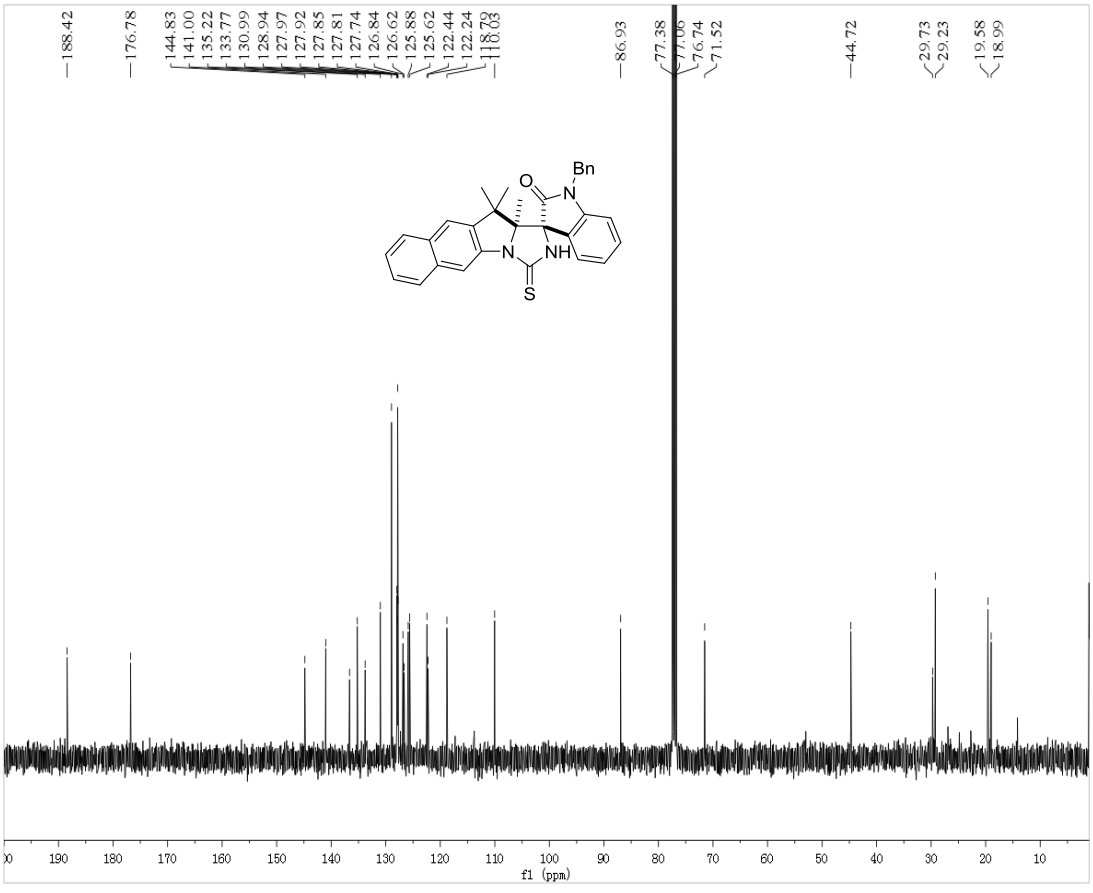


HRMS of 3bh

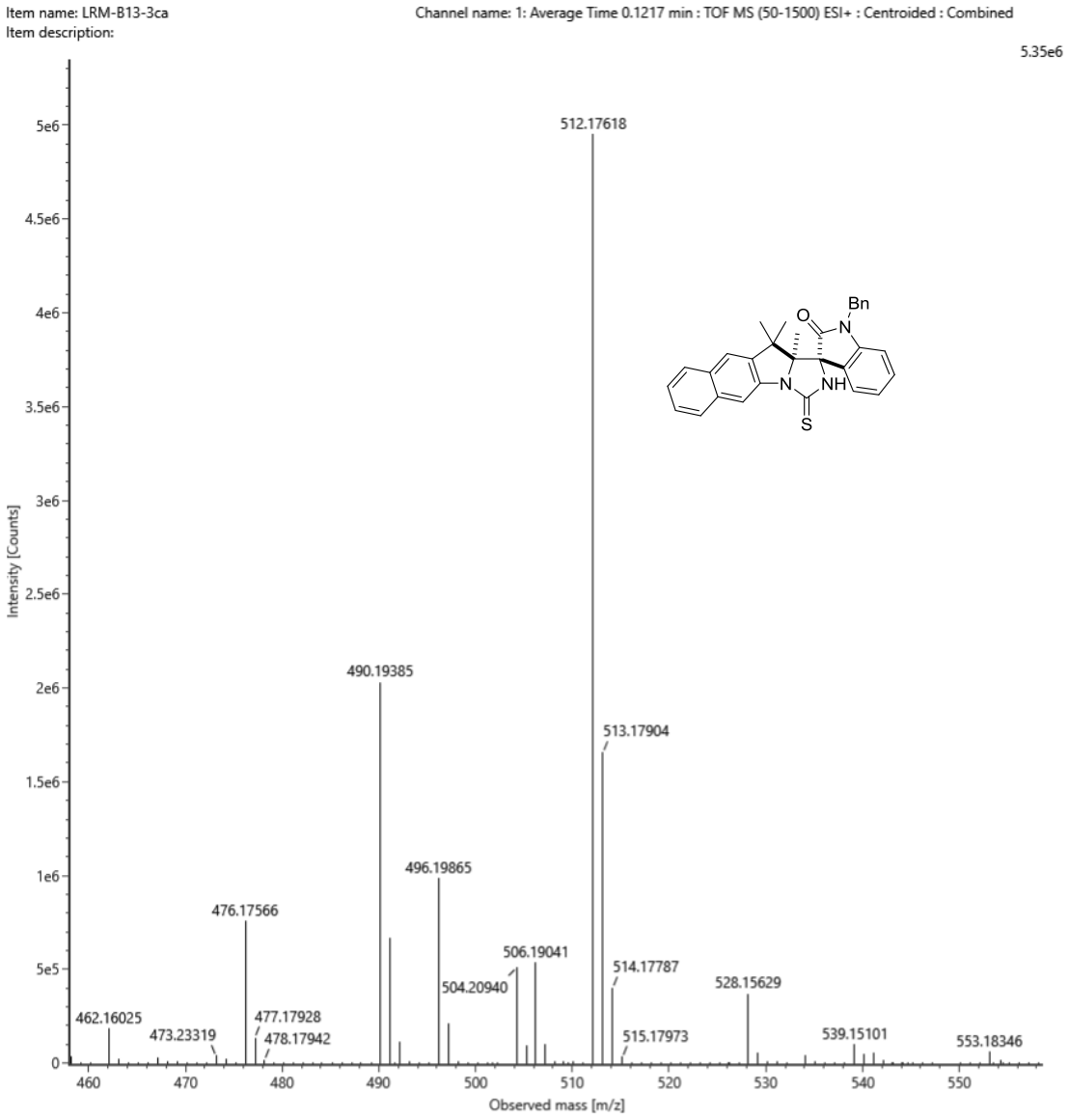

Item name: LRM-B21-3bh
Item description:
Channel name: 1: Average Time 0.1132 min : TOF MS (50-1500) ESI+ : Centroided : Combined
1.88e7
Intensity [Counts]
Observed mass [m/z]
462.16035
476.17599
463.16369
477.17903
440.17827
464.16197
478.13746
454.19390
441.18145
466.16016
479.14132
492.15024
498.15867
511.11973
414.16035
425.21499
437.19413
442.18044
Ph
O
N
H3C
N
NH
S

^{1}H and ^{13}C NMR of 3ca

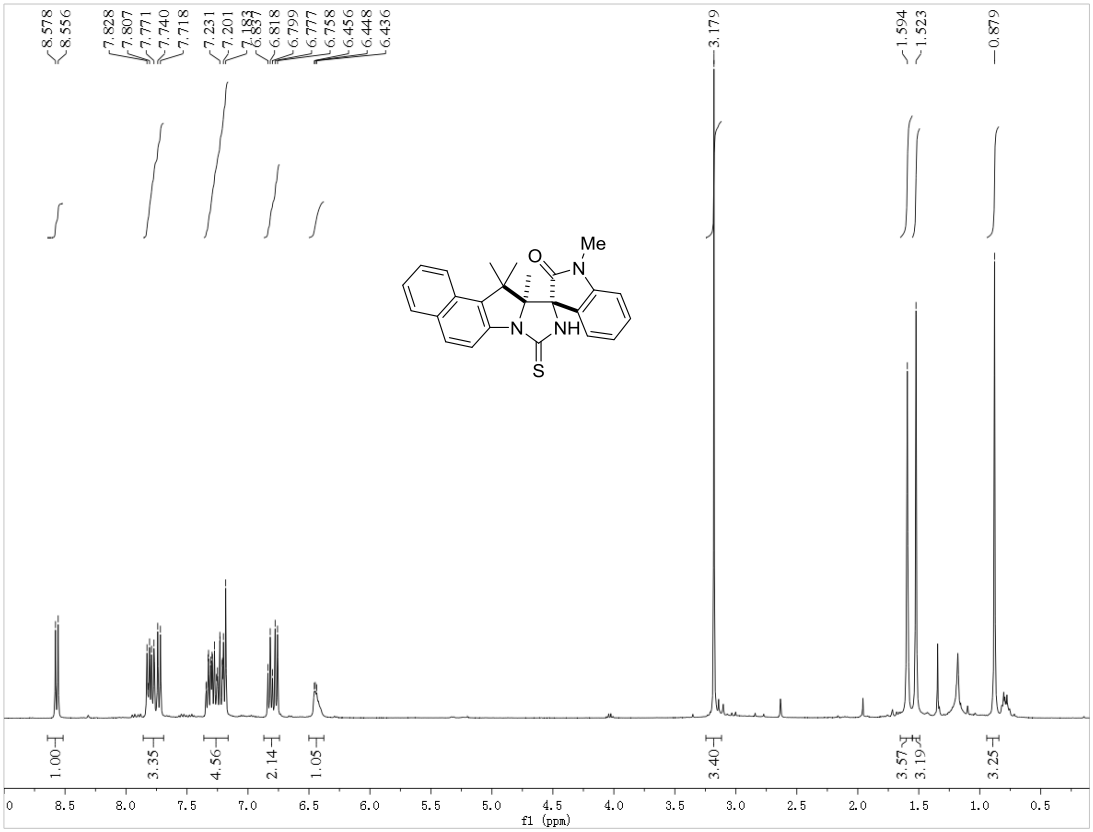


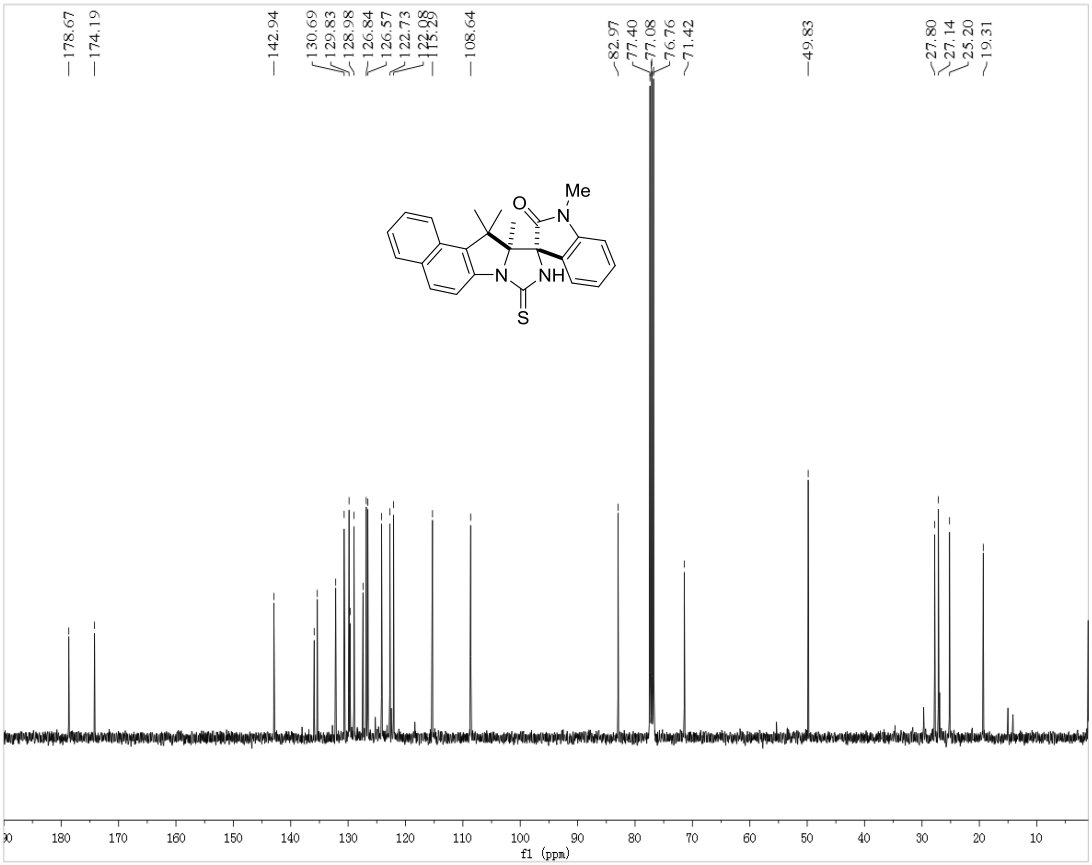


HRMS of 3ca

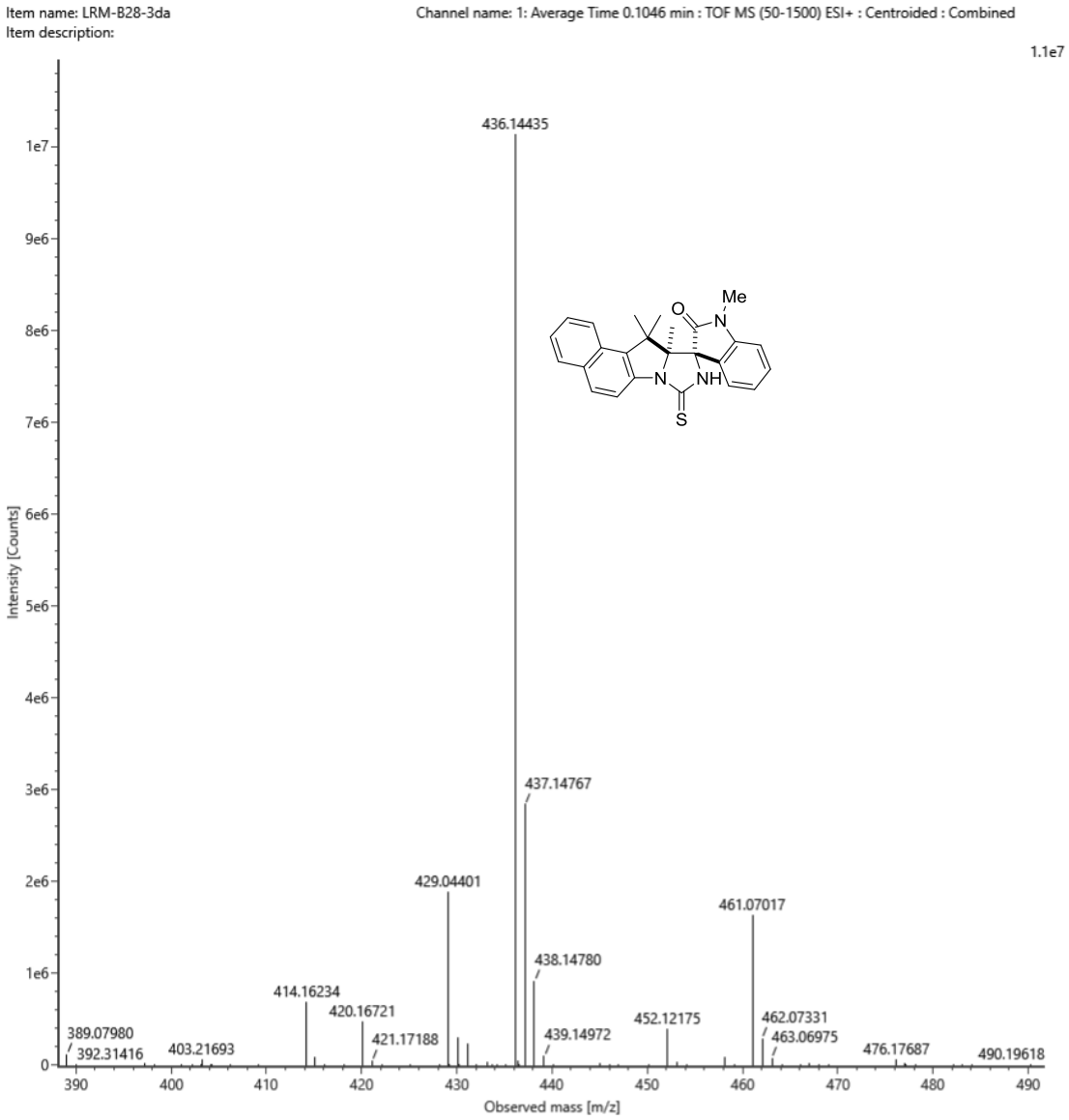

Item name: LRM-B13-3ca
Item description:
Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined
5.35e6
Intensity [Counts]
Observed mass [m/z]
512.17618
490.19385
513.17904
496.19865
476.17566
506.19041
514.17787
504.20940
528.15629
462.16025
473.23319
477.17928
478.17942
515.17973
539.15101
553.18346
Bn
O
N
N
NH
S

^{1}H and ^{13}C NMR of 3da

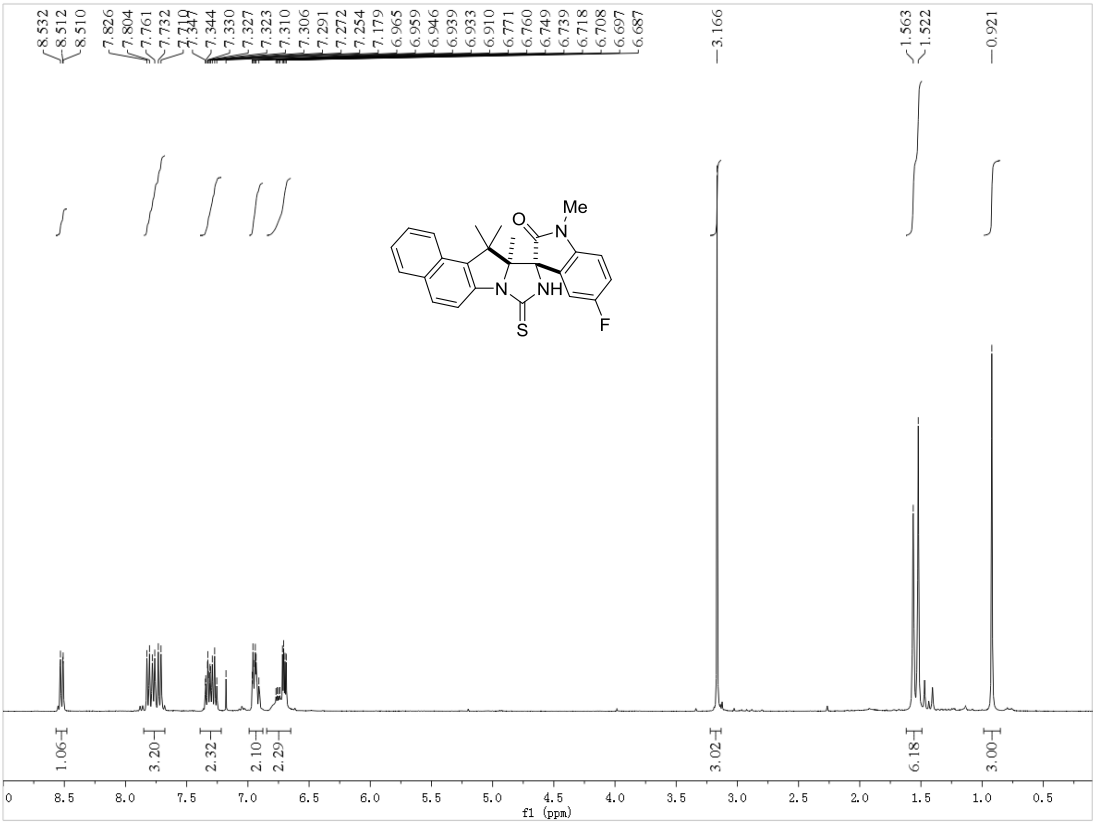


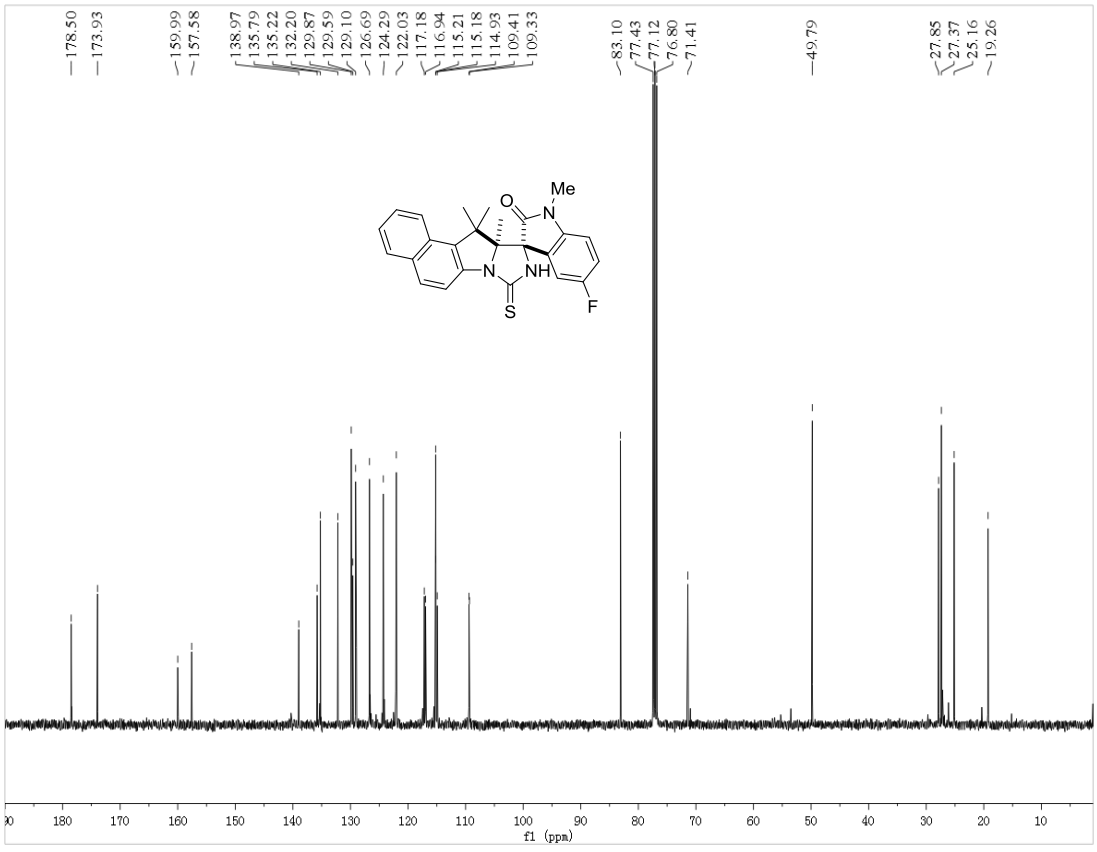


HRMS of 3da

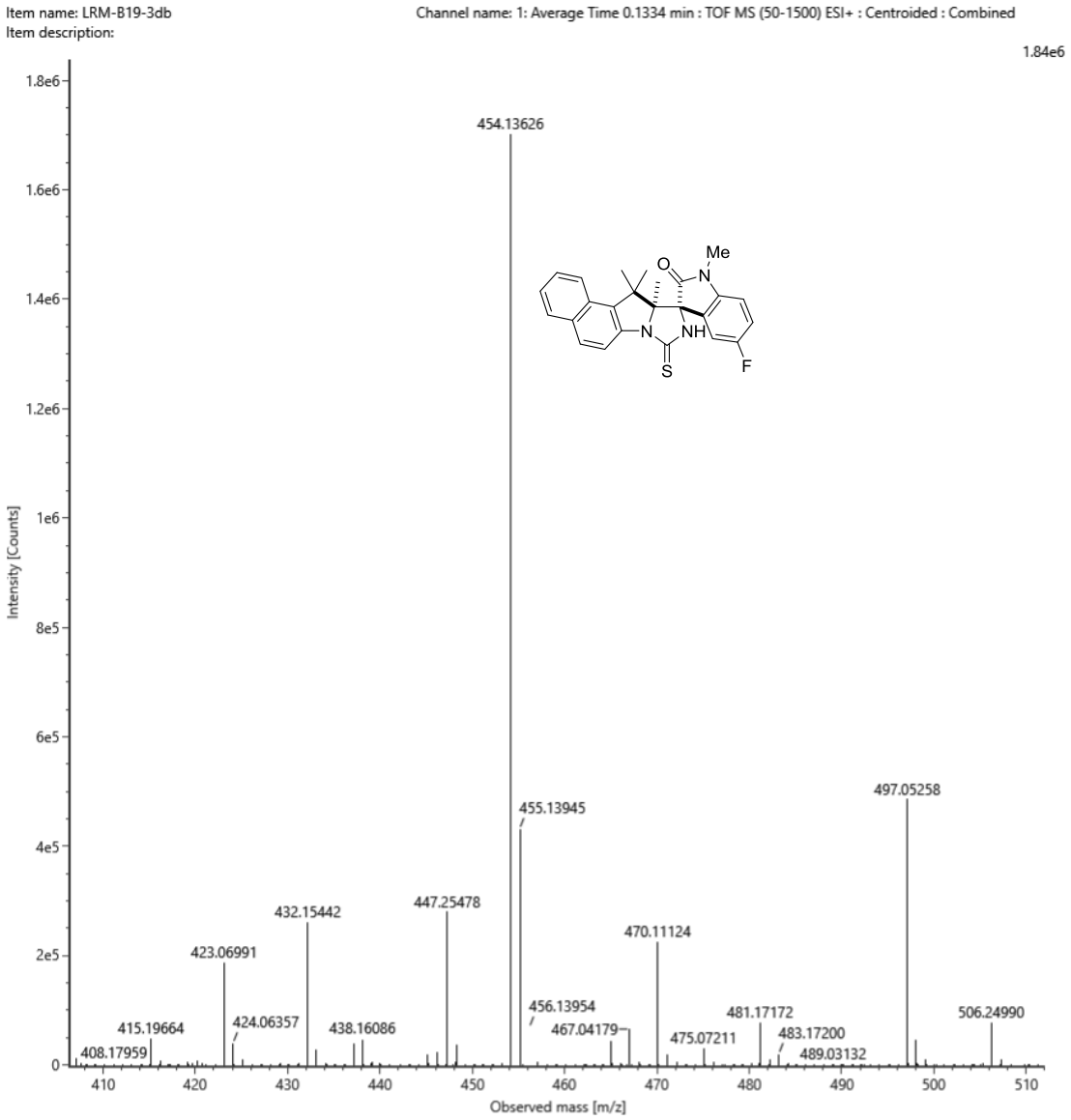

Item name: LRM-B28-3da
Item description:
Channel name: 1: Average Time 0.1046 min : TOF MS (50-1500) ESI+ : Centroided : Combined
1.1e7
436.14435
437.14767
429.04401
461.07017
438.14780
414.16234
420.16721
452.12175
462.07331
463.06975
389.07980
392.31416
403.21693
421.17188
439.14972
476.17687
490.19618
Intensity [Counts]
Observed mass [m/z]
Me
O
N
NH
S

^{1}H and ^{13}C NMR of 3db

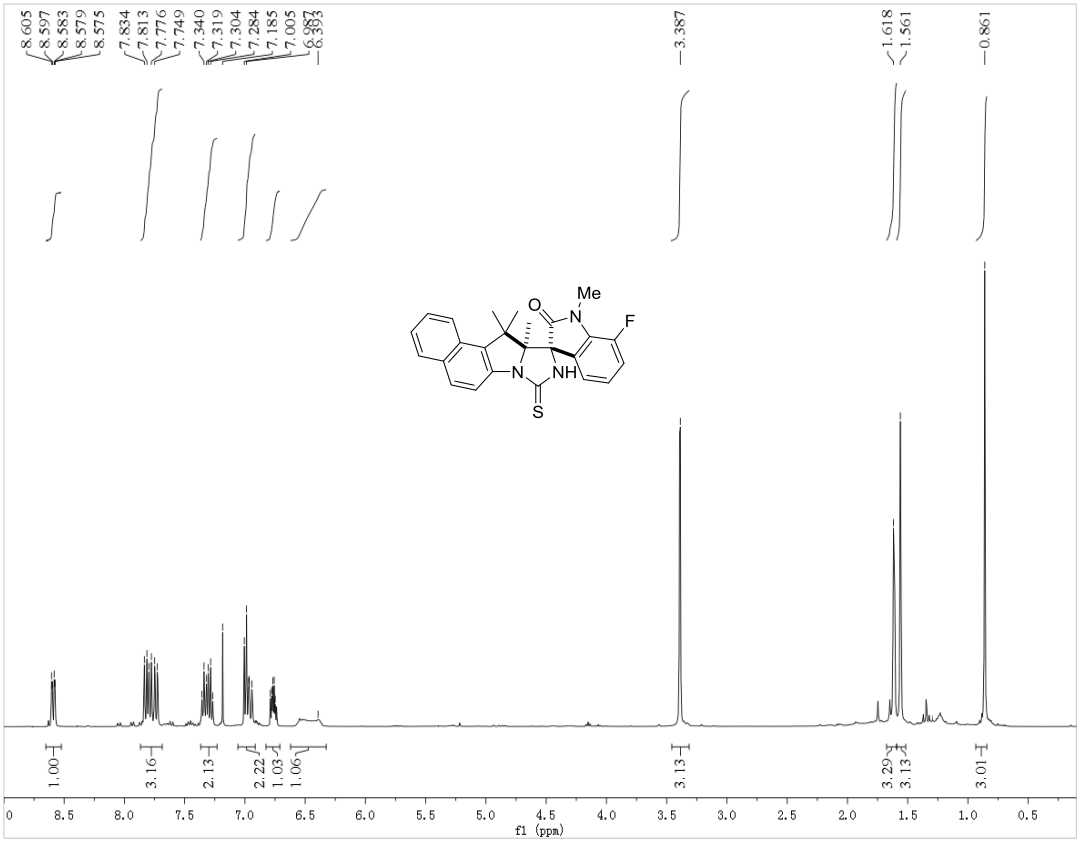


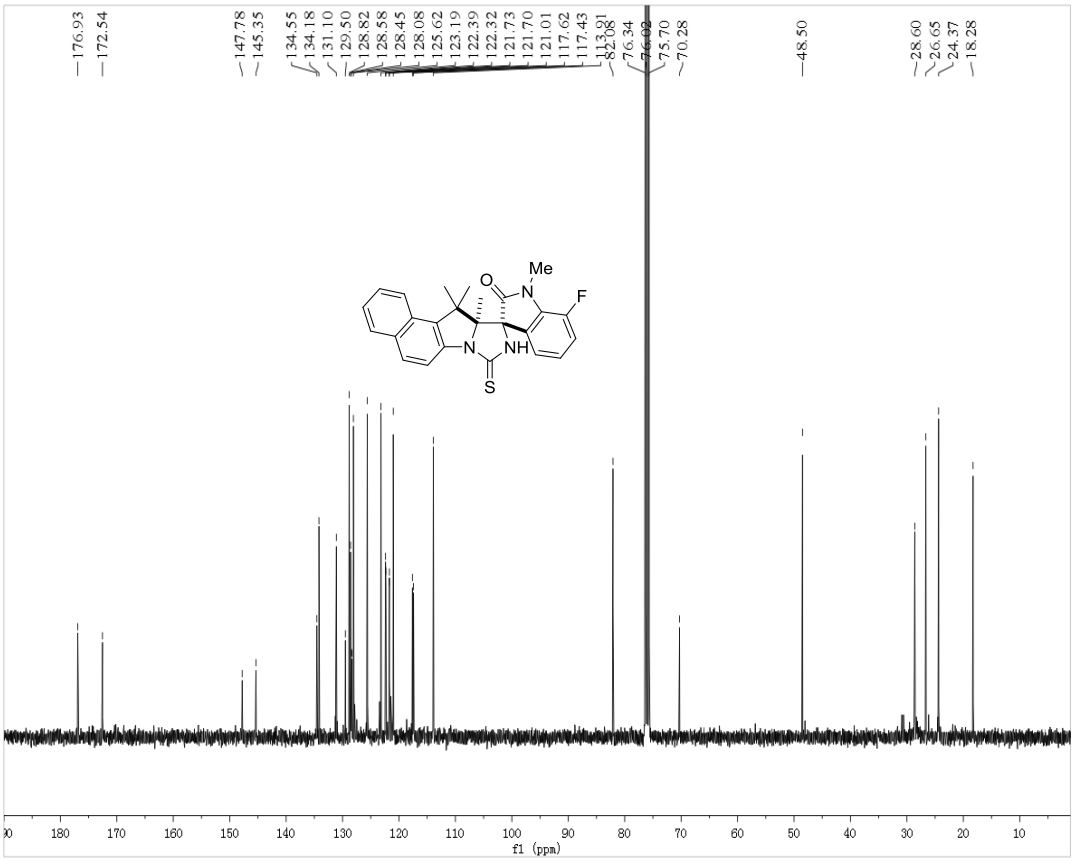


HRMS of 3db


Item name: LRM-B19-3db
Item description:
Channel name: 1: Average Time 0.1334 min : TOF MS (50-1500) ESI+ : Centroided : Combined
1.84e6
Intensity [Counts]
Observed mass [m/z]
454.13626
455.13945
497.05258
447.25478
432.15442
423.06991
470.11124
456.13954
467.04179
481.17172
483.17200
489.03132
475.07211
506.24990
415.19664
424.06357
438.16086
408.17959
Me
O
N
NH
S
F

^{1}H and ^{13}C NMR of 3dc

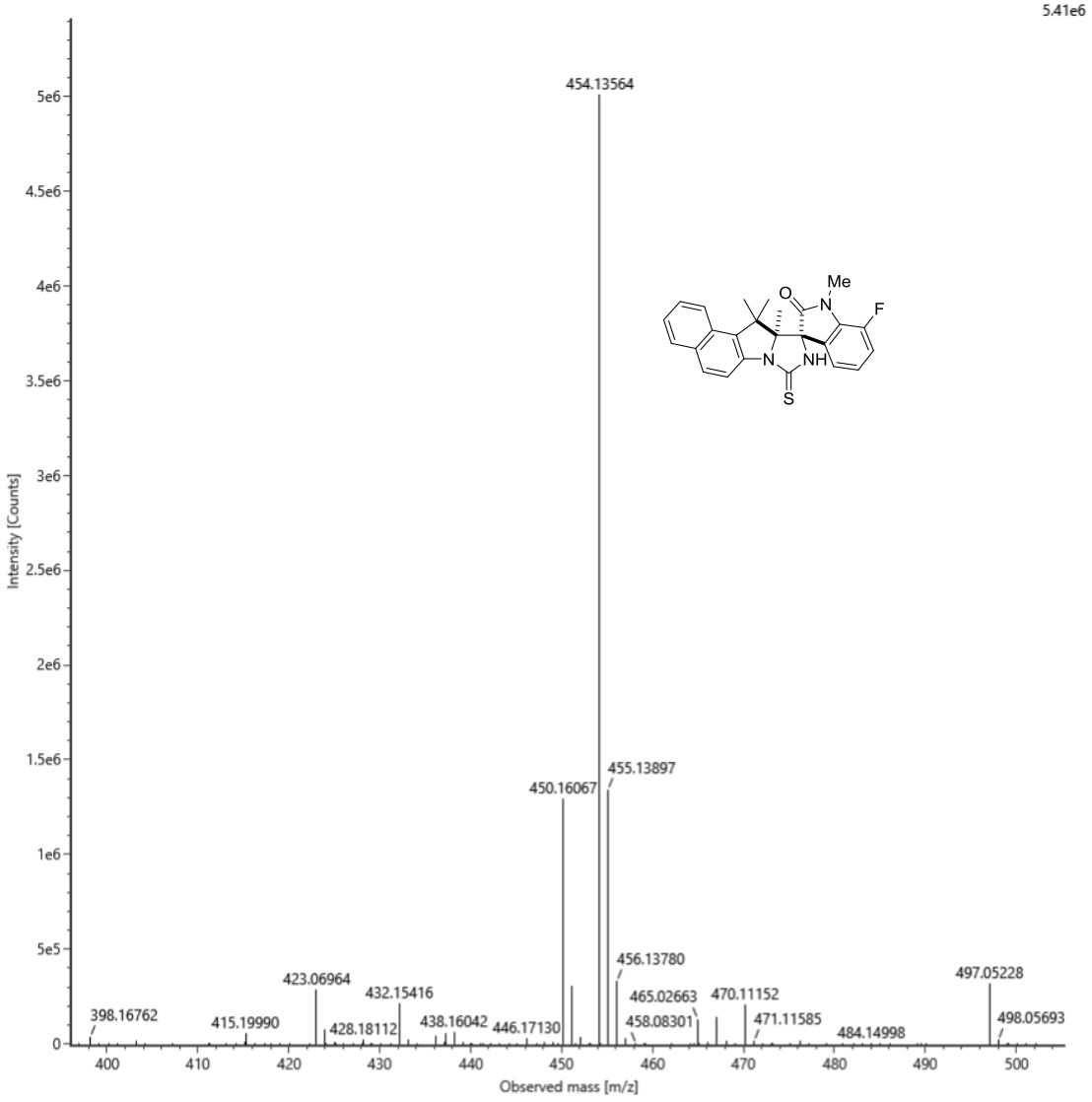




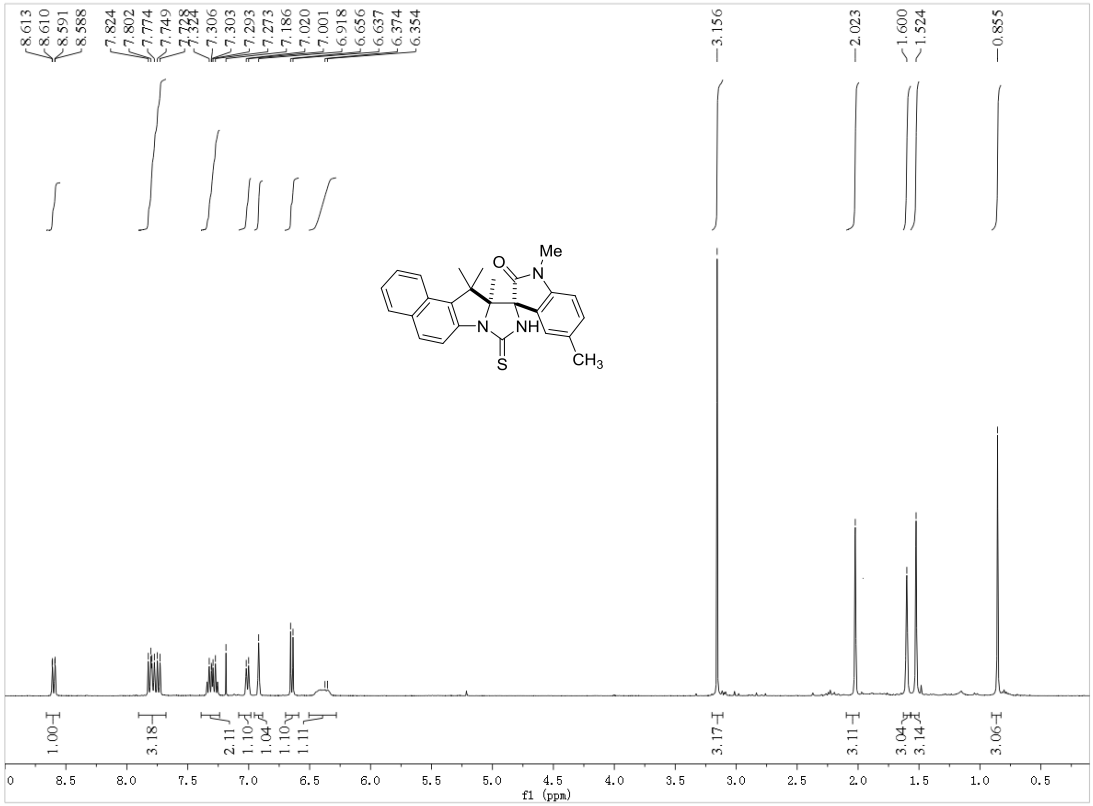
HRMS of 3dc

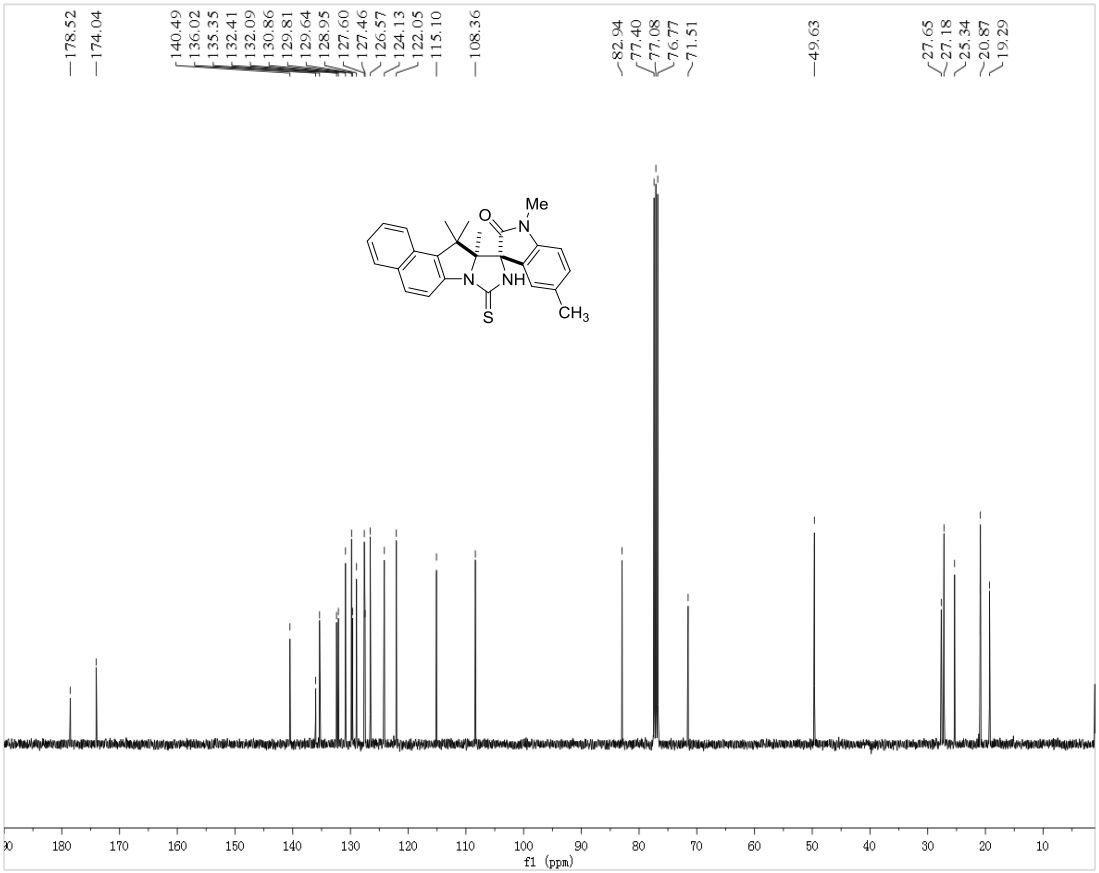
Item name: LRM-B32-3dc
Item description:

Channel name: 1: Average Time 0.1132 min : TOF MS (50-1500) ESI+ : Centroided : Combined



^{1}H and ^{13}C NMR of 3dd

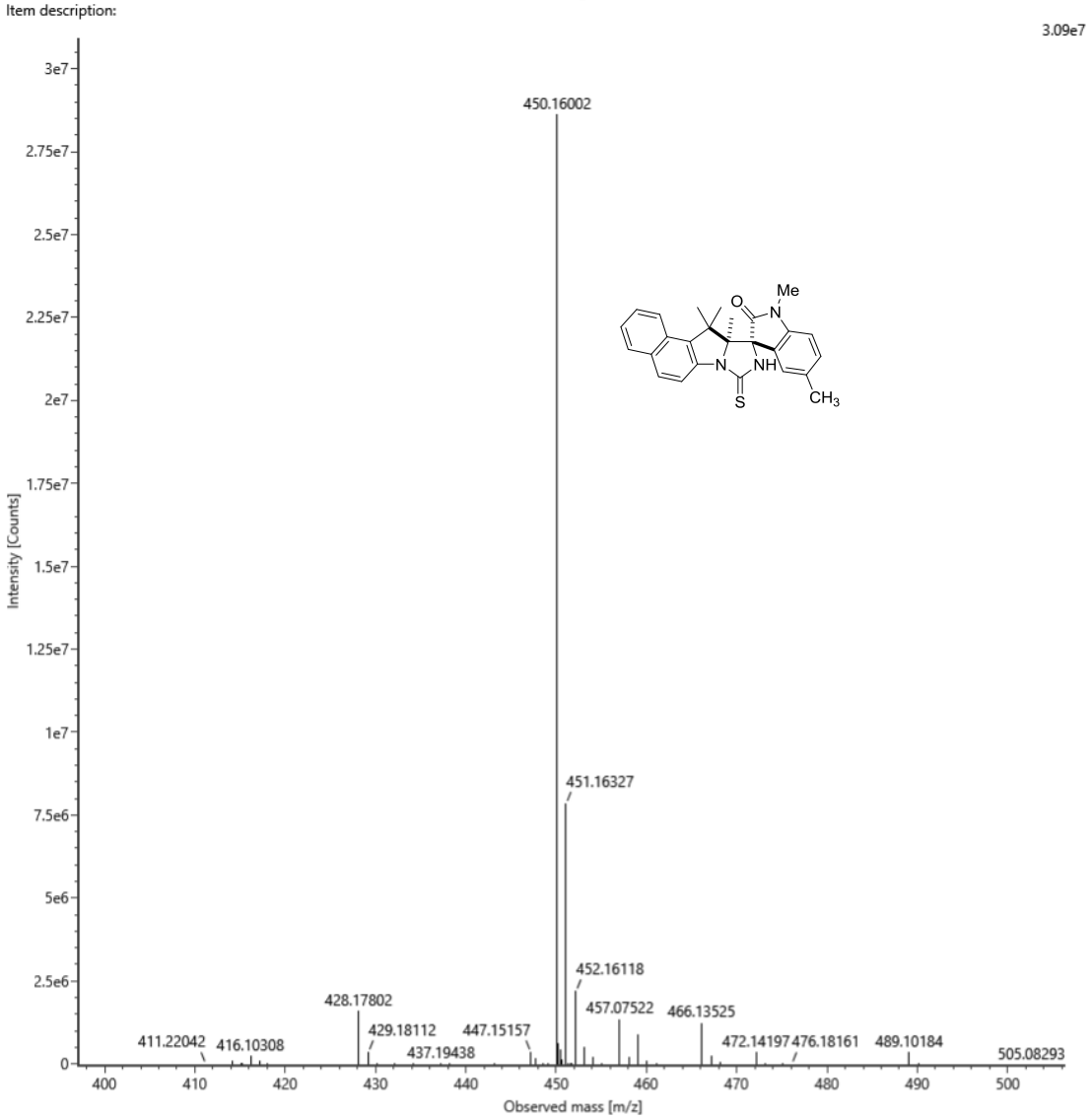




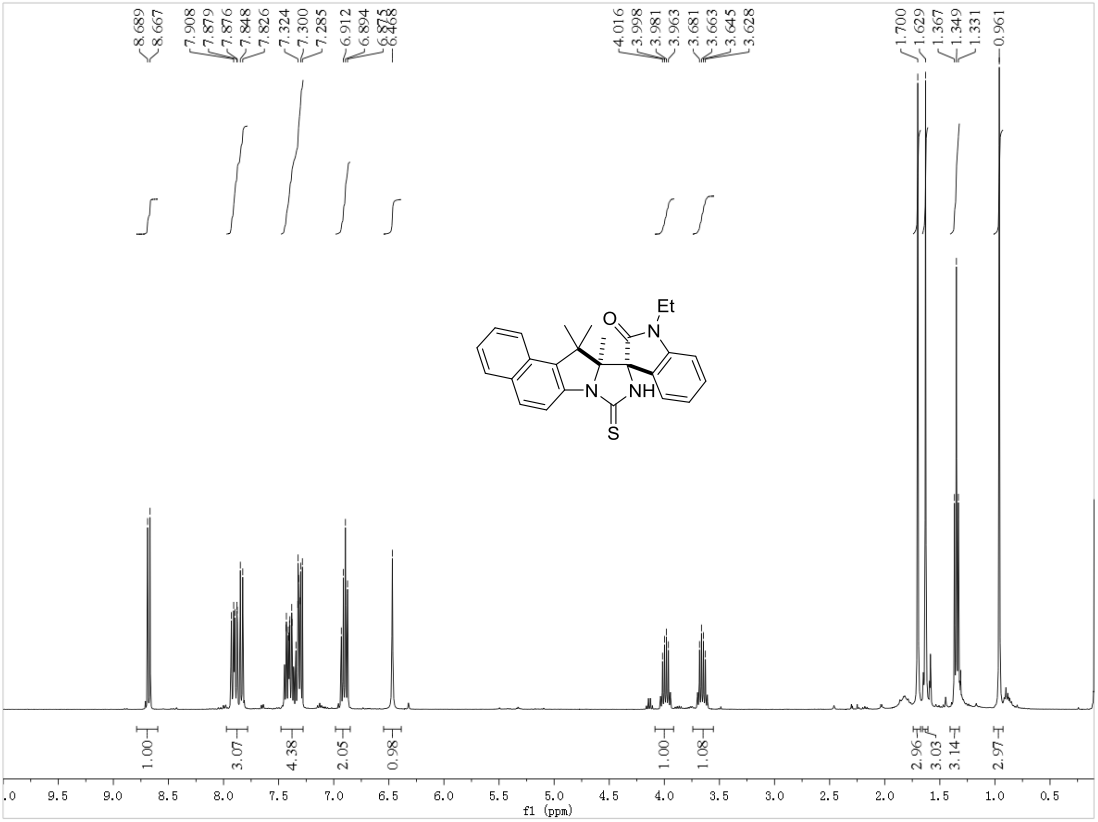
HRMS of 3dd

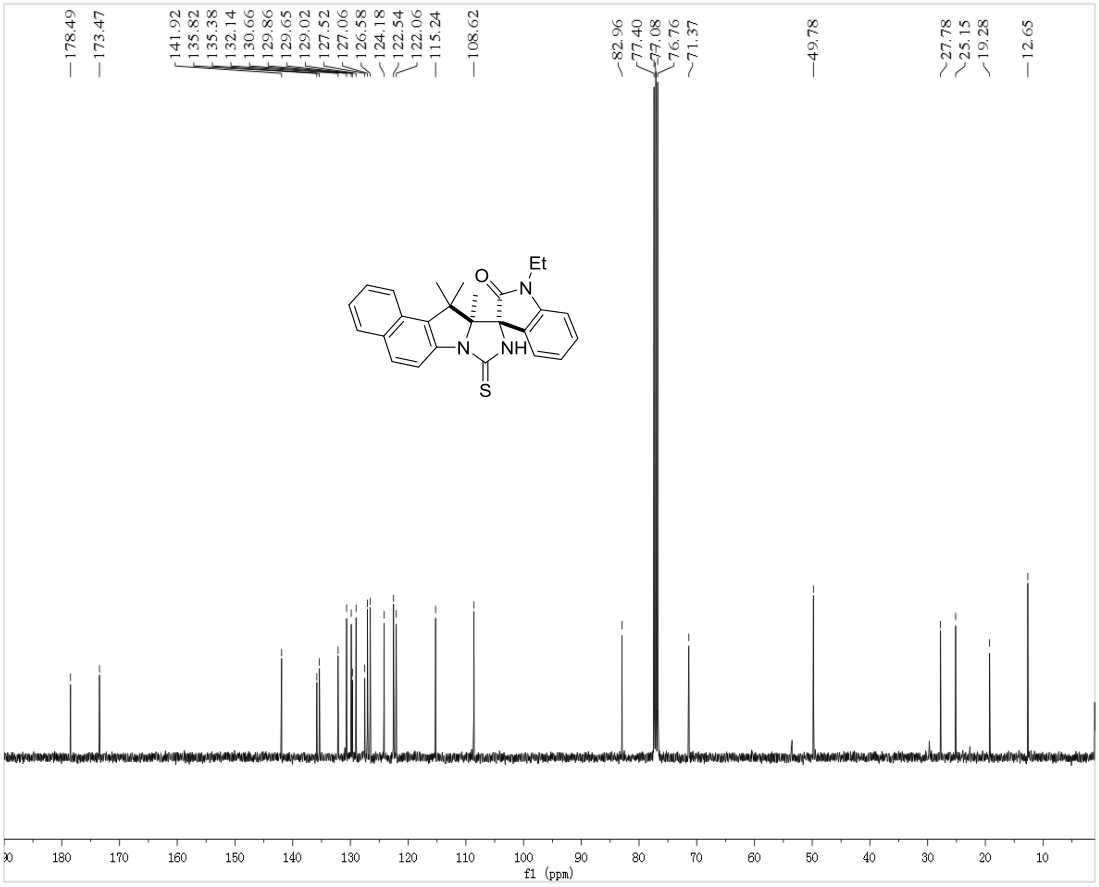
Item name: LRM-B26-3dd
Item description:

Channel name: 1: Average Time 0.1132 min : TOF MS (50-1500) ESI+ : Centroided : Combined



^{1}H and ^{13}C NMR of 3de

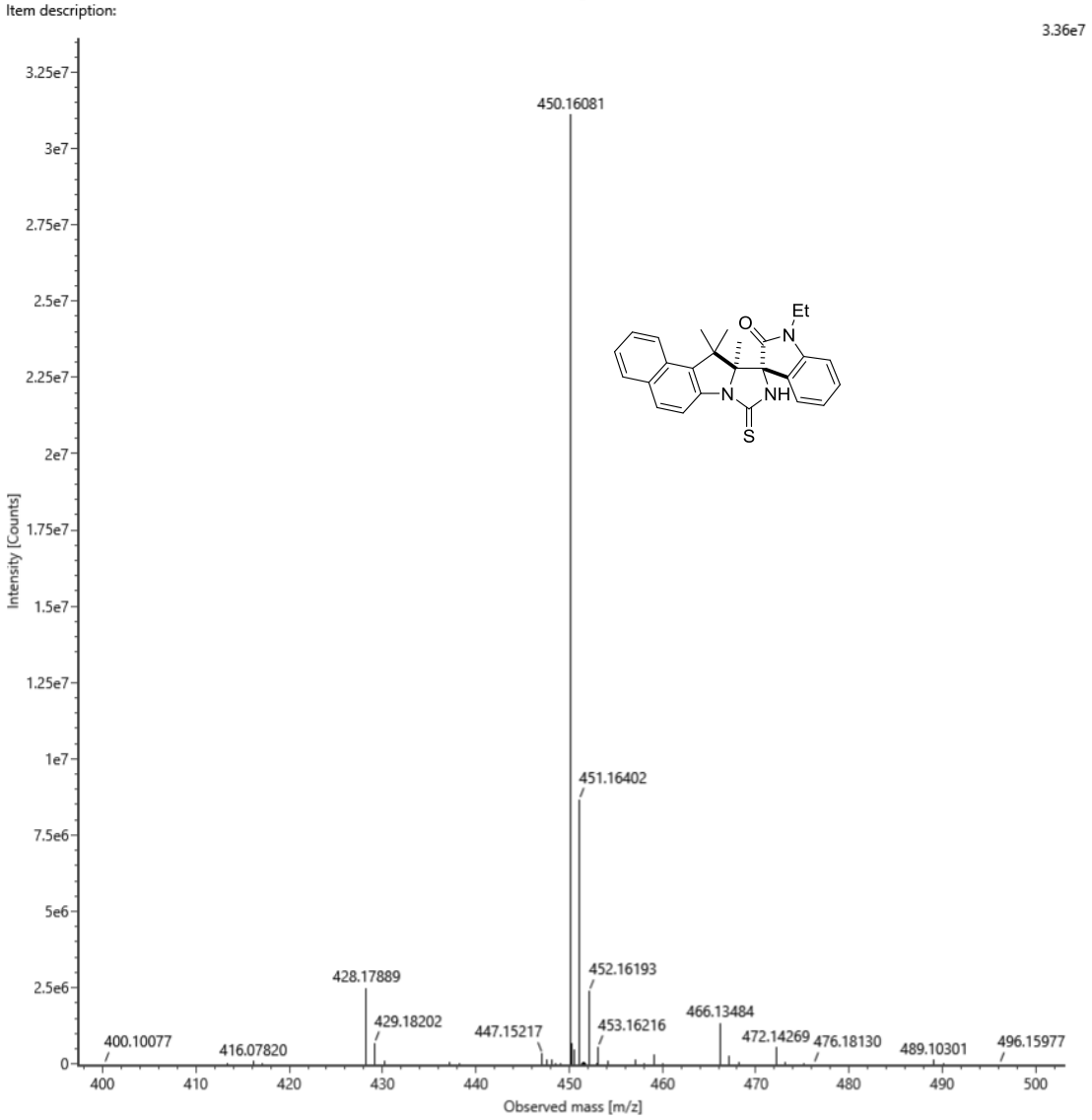




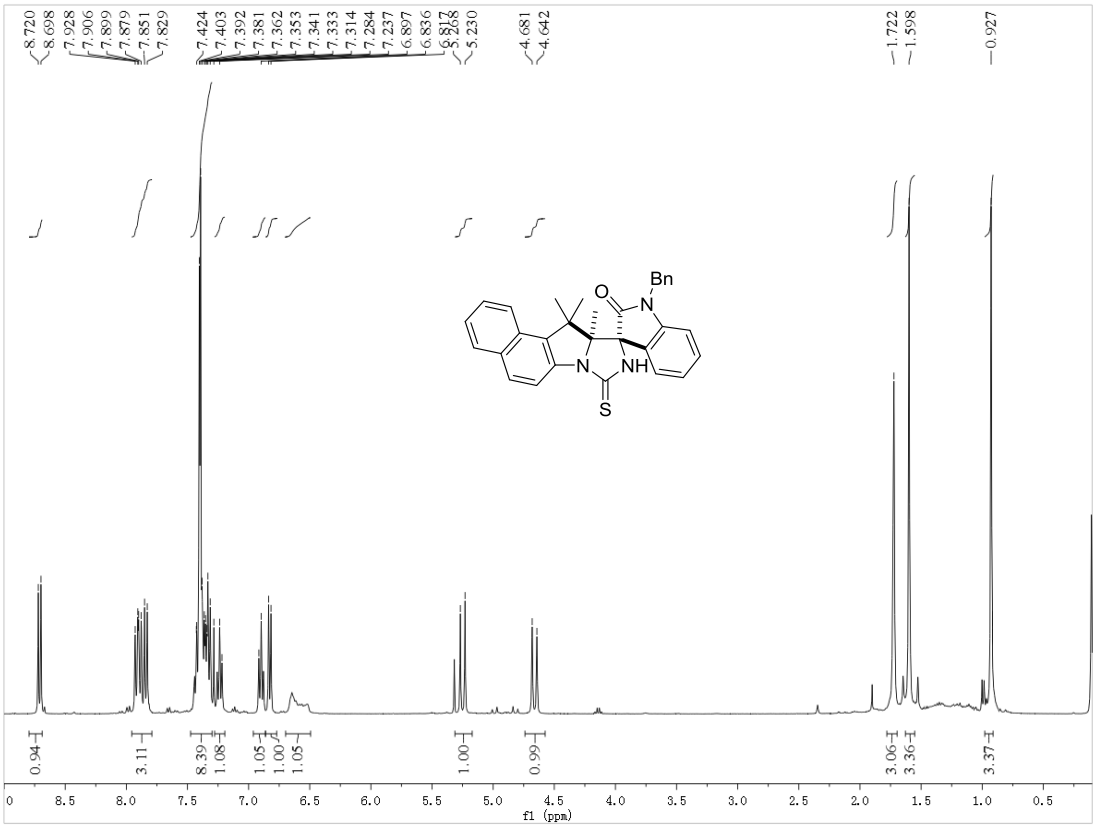
HRMS of 3de

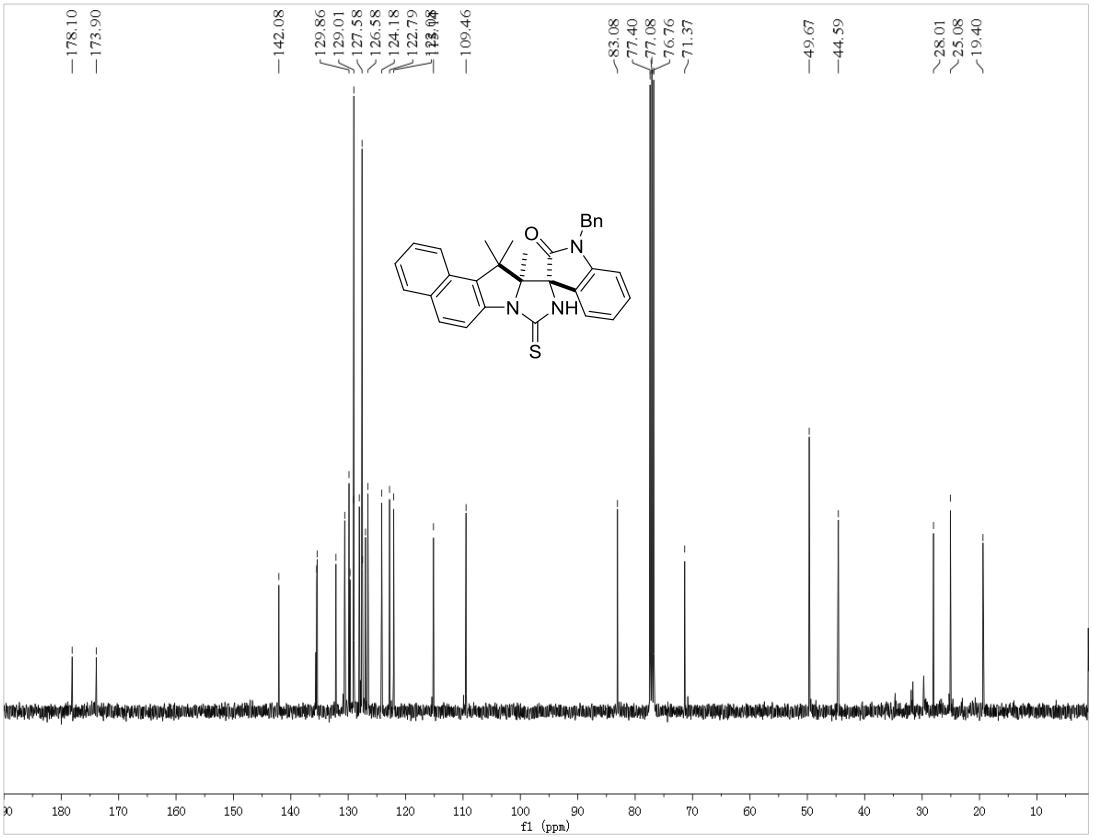
Item name: LRM-B18-3de
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

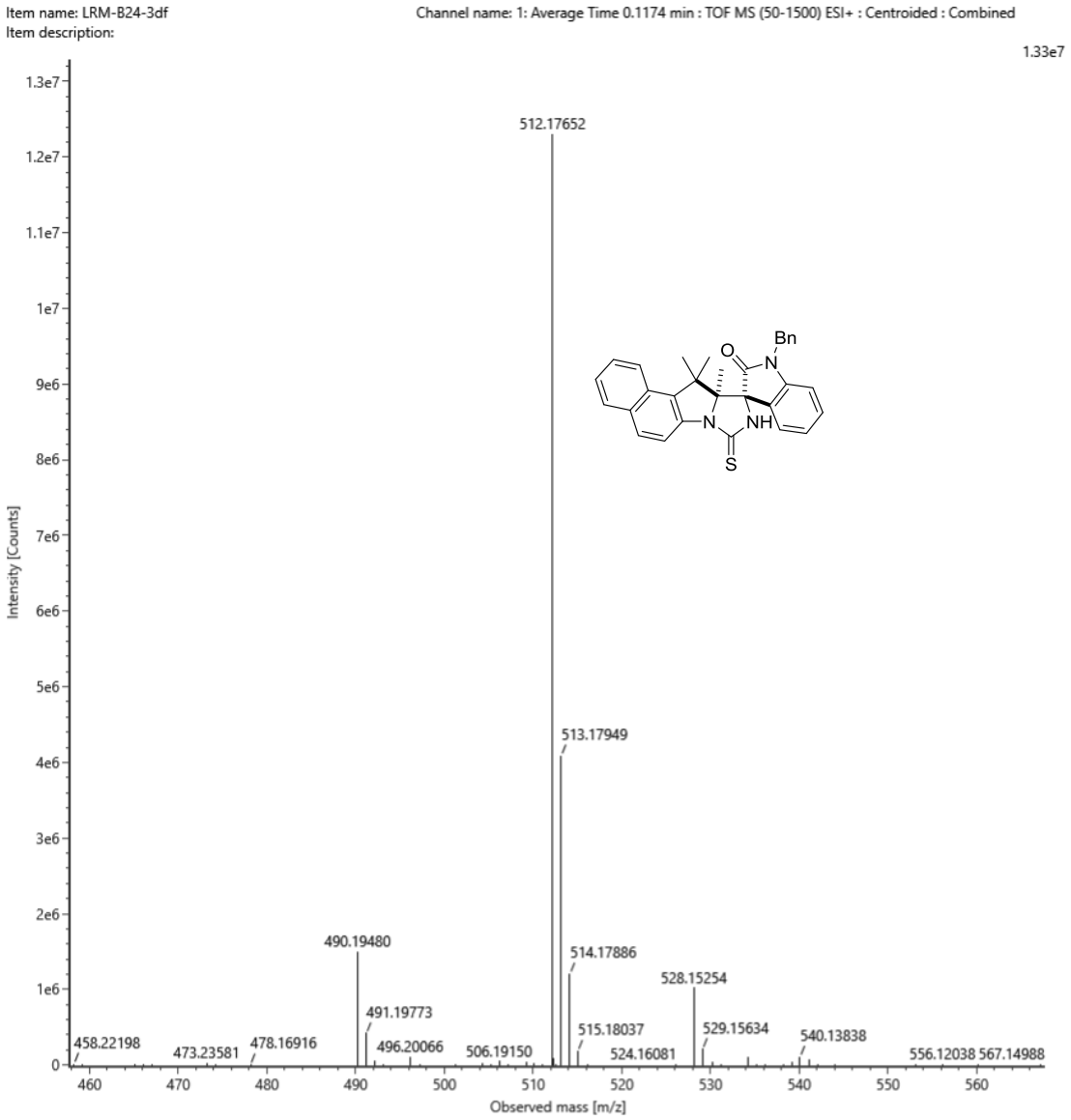


^{1}H and ^{13}C NMR of 3df

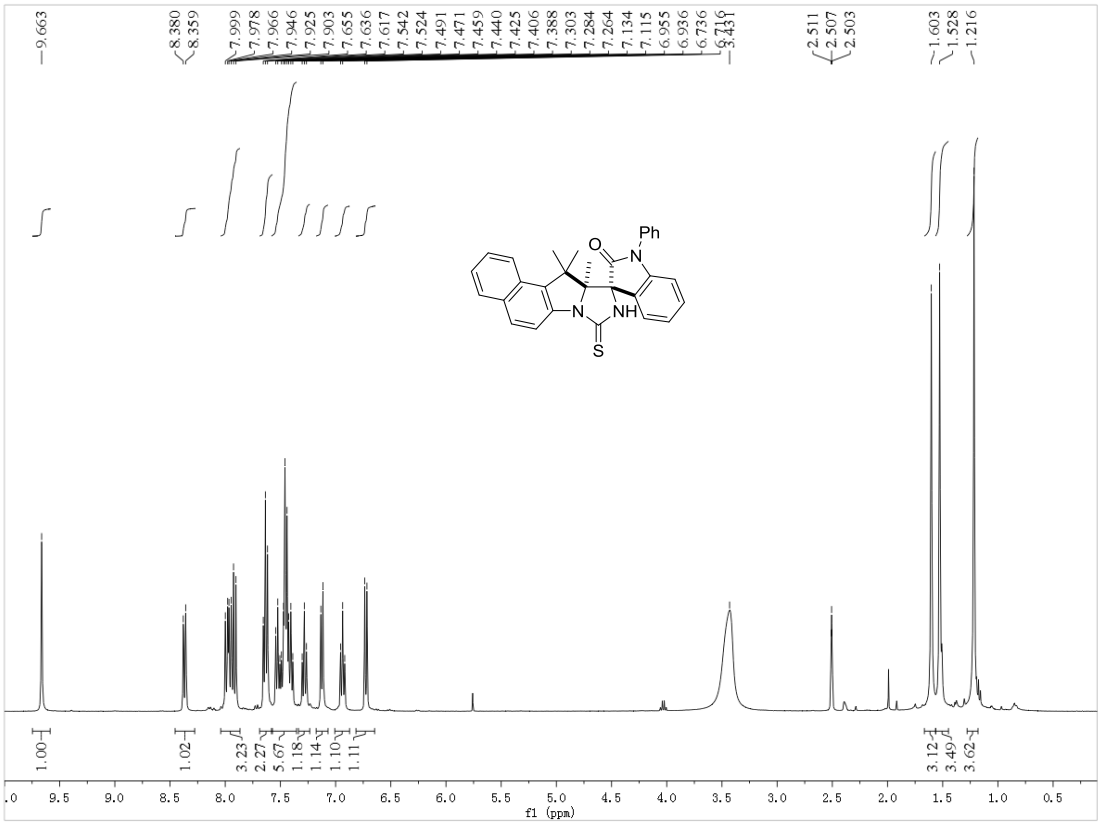


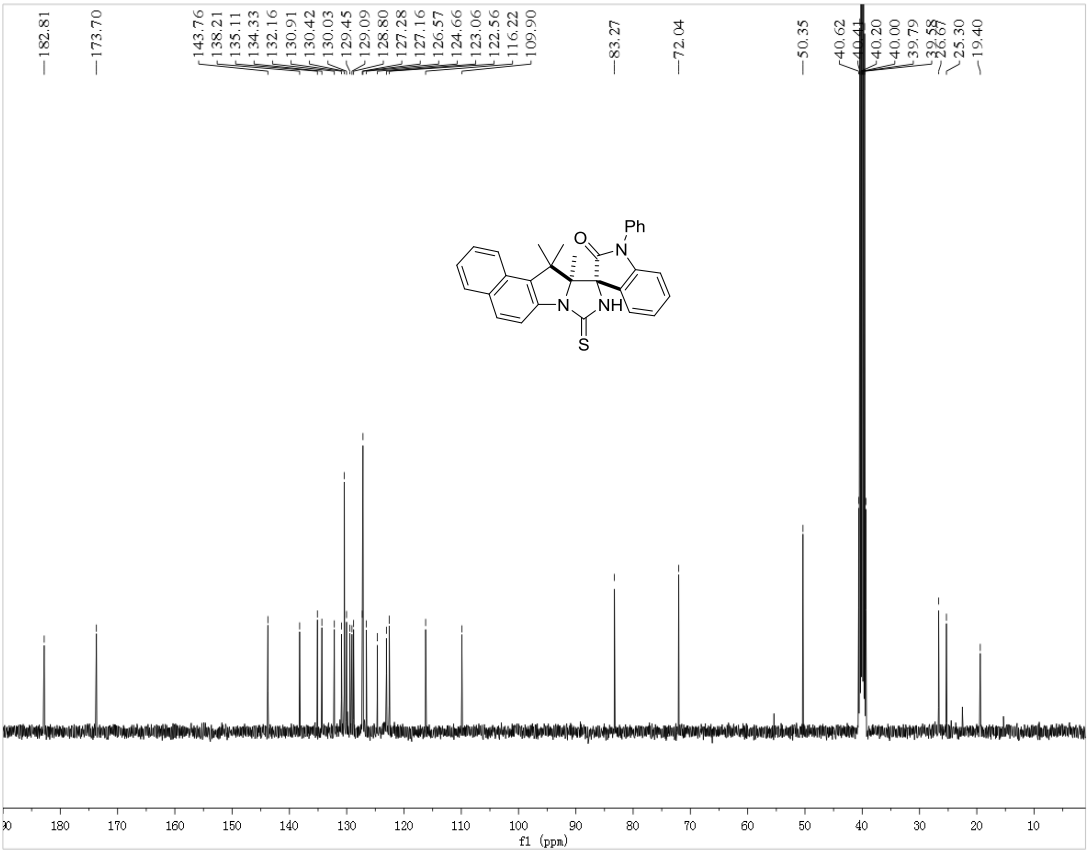


HRMS of 3df


Item name: LRM-B24-3df
Item description:
Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined
1.33e7
Intensity [Counts]
Observed mass [m/z]
512.17652
513.17949
490.19480
514.17886
528.15254
491.19773
515.18037
529.15634
540.13838
458.22198
473.23581
478.16916
496.20066
506.19150
524.16081
556.12038
567.14988
Bn
O
N
N
NH
S

^{1}H and ^{13}C NMR of 3dg

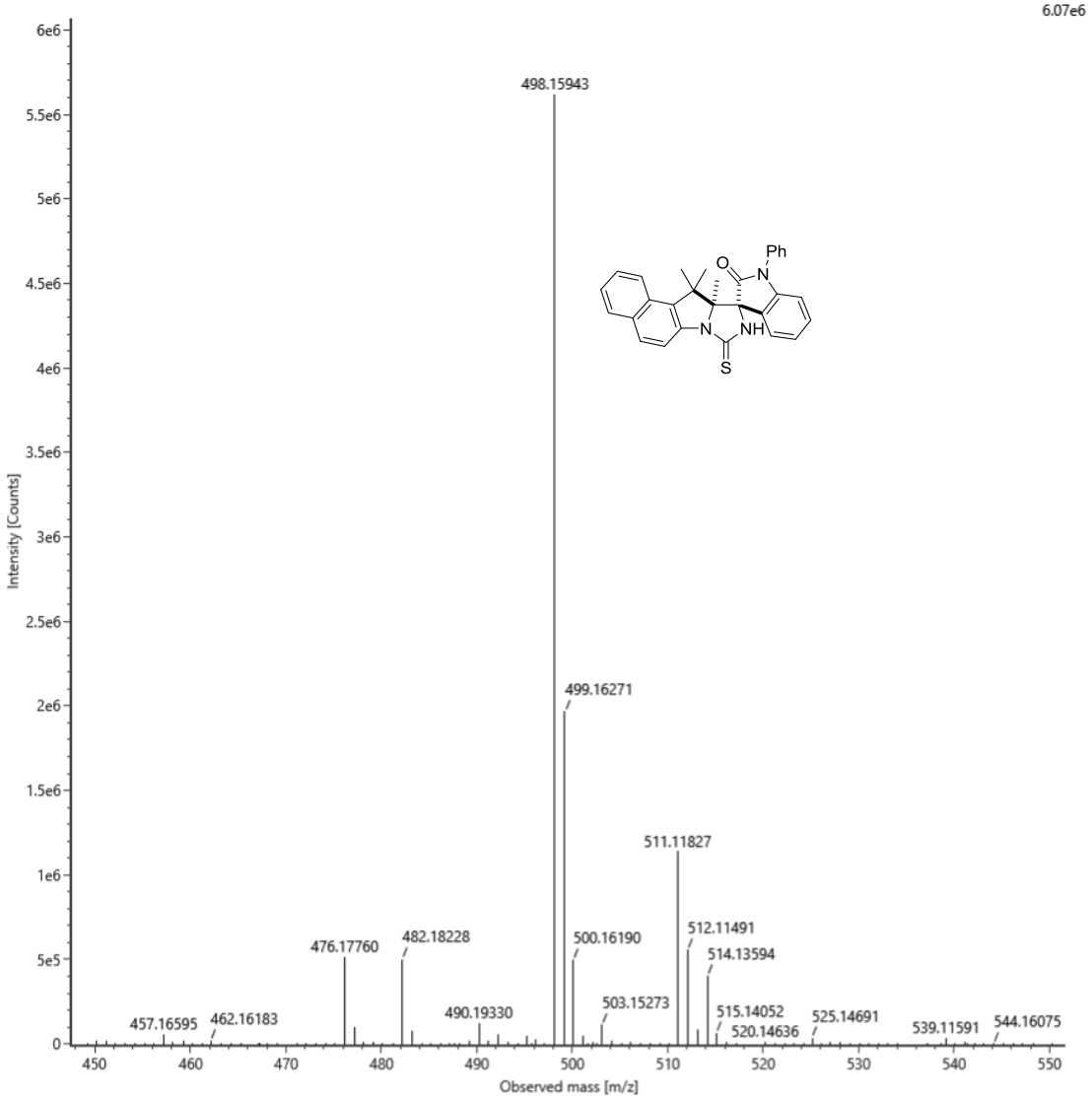




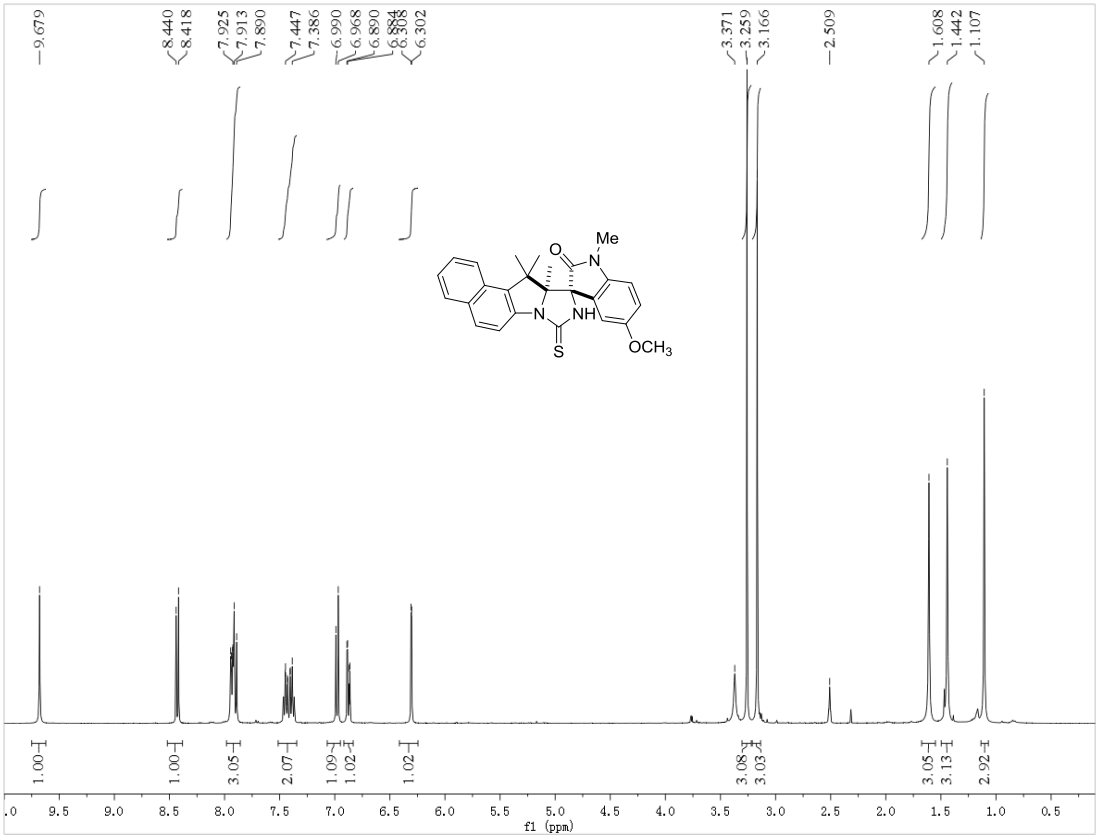
HRMS of 3dg

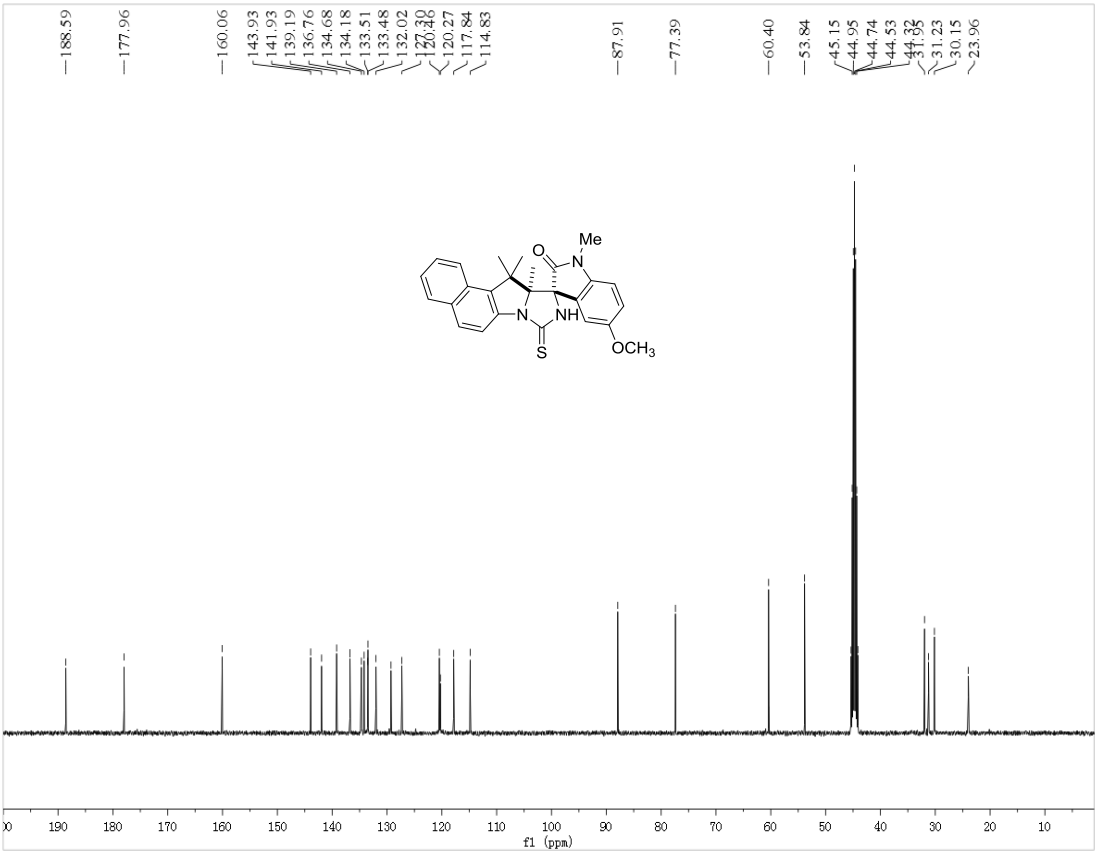
Item name: LRM-B22-3dg
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

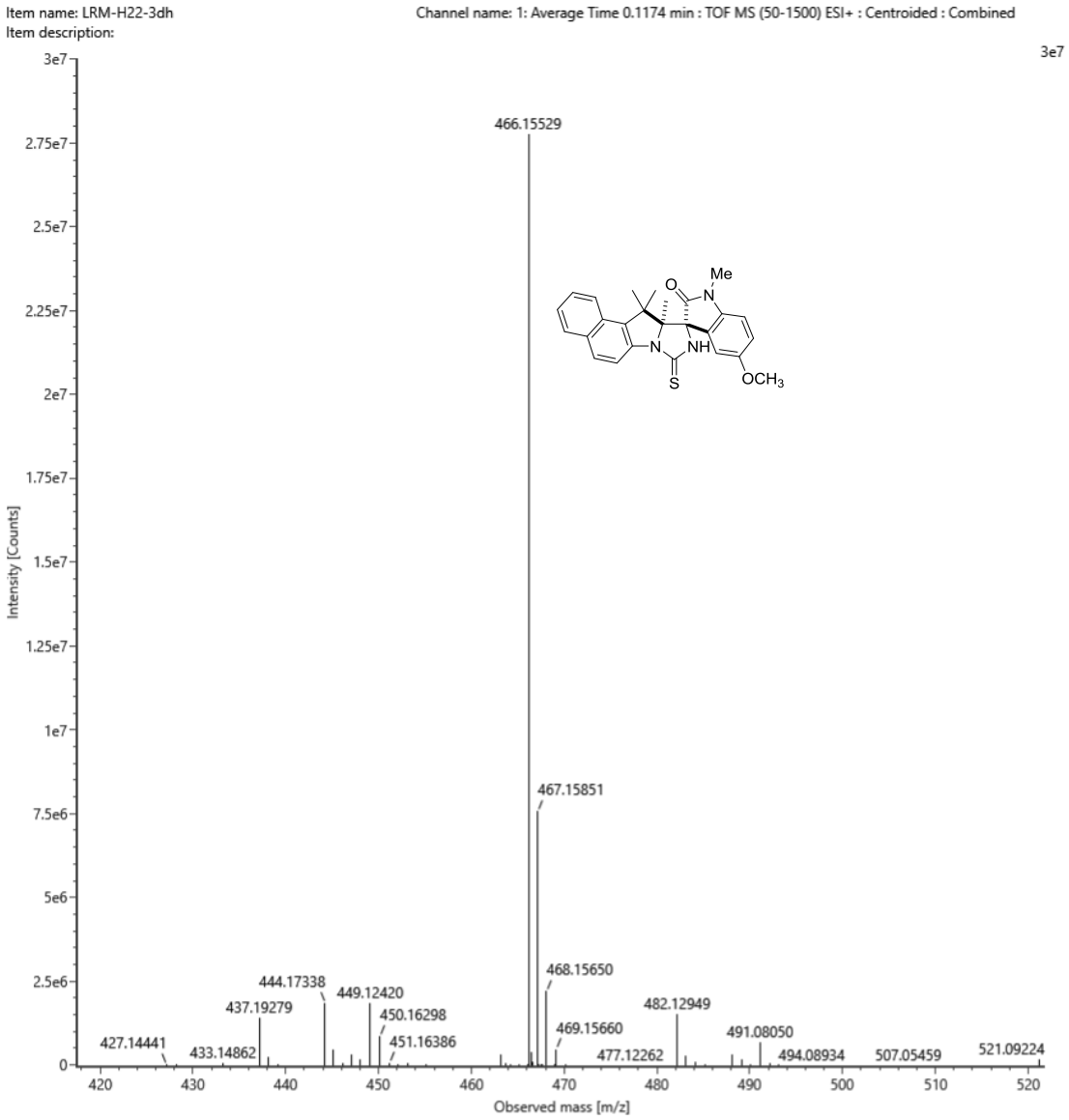


^{1}H and ^{13}C NMR of 3dh

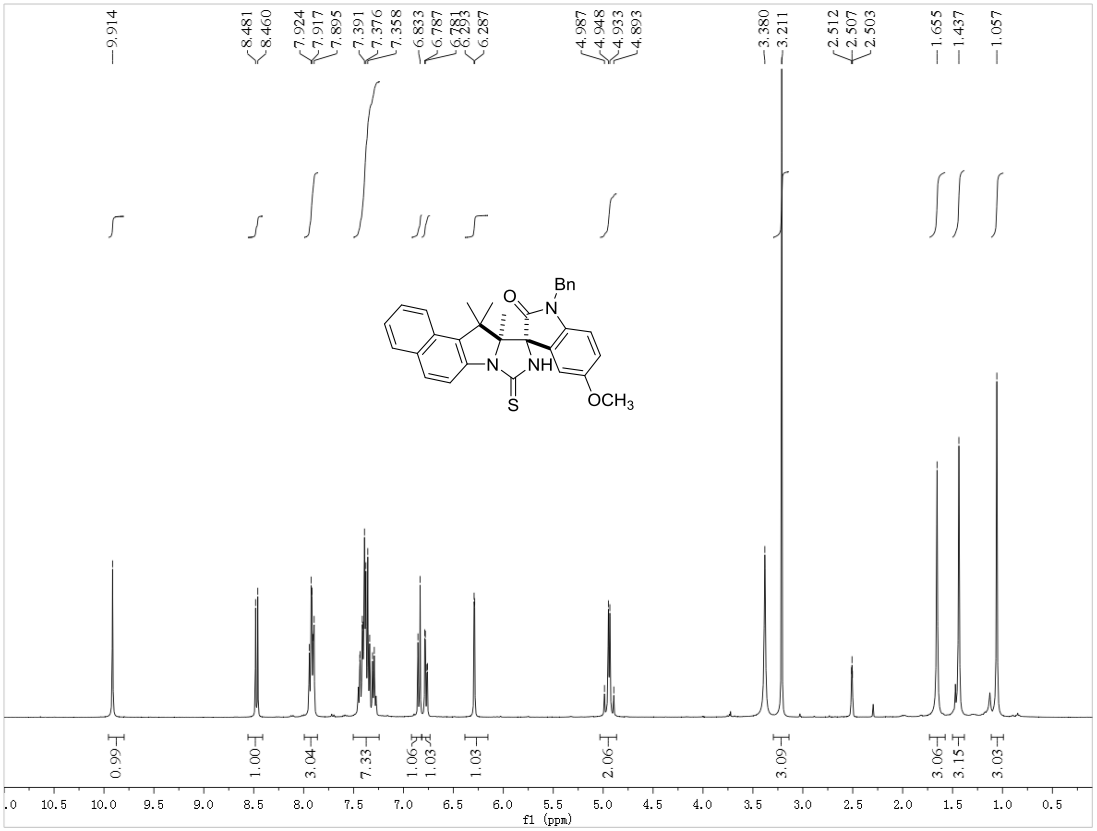


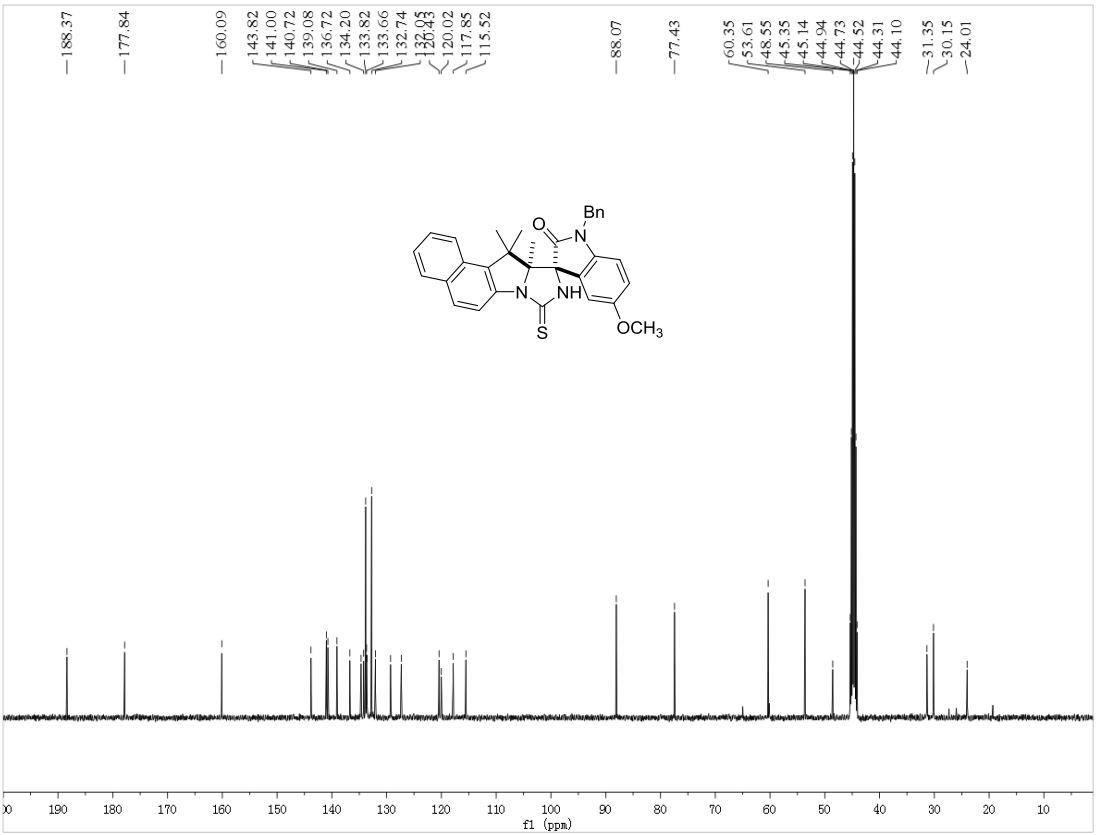


HRMS of 3dh


Item name: LRM-H22-3dh
Item description:
Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined
3e7
Intensity [Counts]
Observed mass [m/z]
466.15529
467.15851
468.15650
444.17338
449.12420
437.19279
450.16298
451.16386
427.14441
433.14862
469.15660
482.12949
491.08050
477.12262
494.08934
507.05459
521.09224
Me
O
N
NH
S
OCH3

^{1}H and ^{13}C NMR of 3di

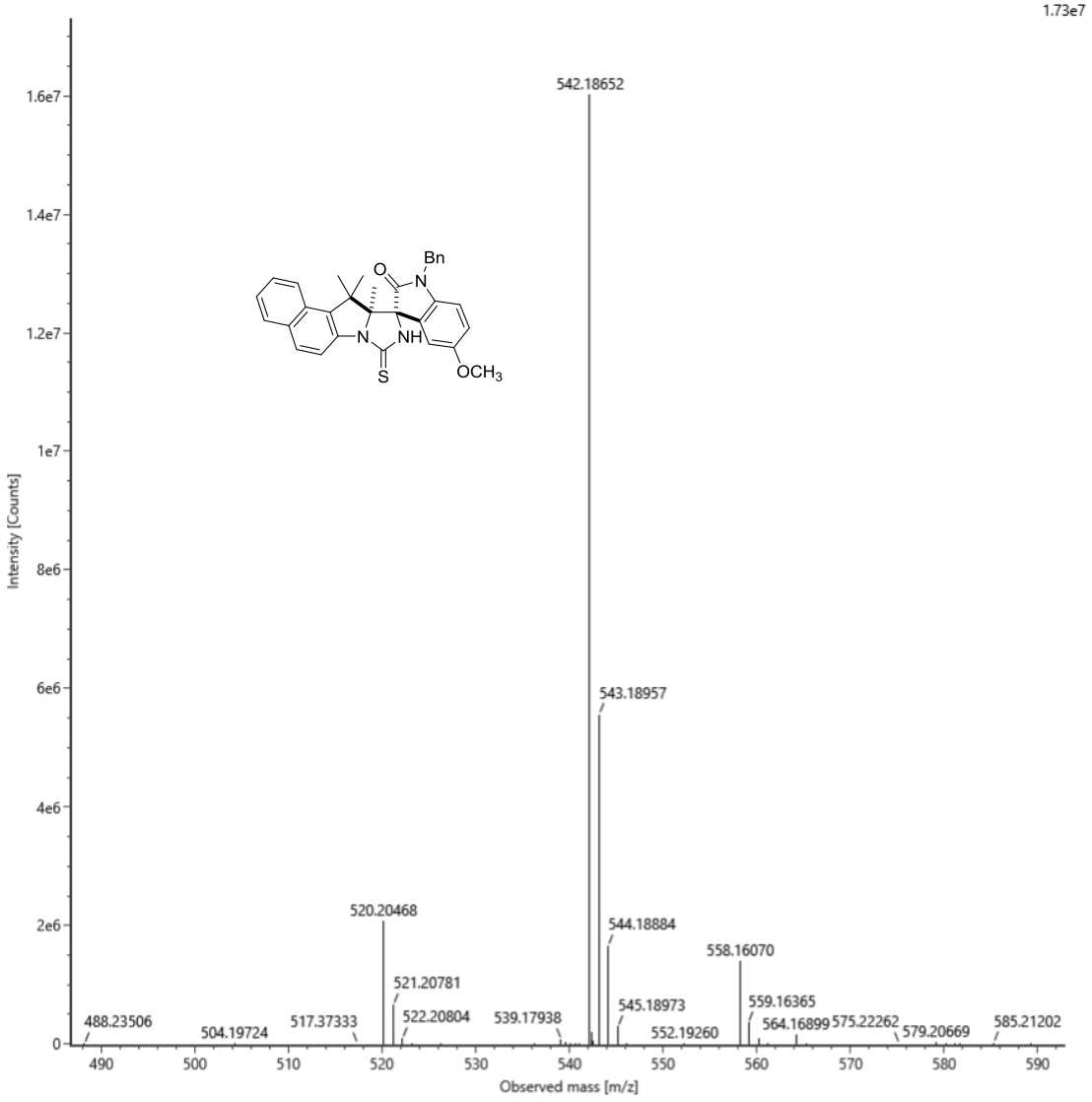




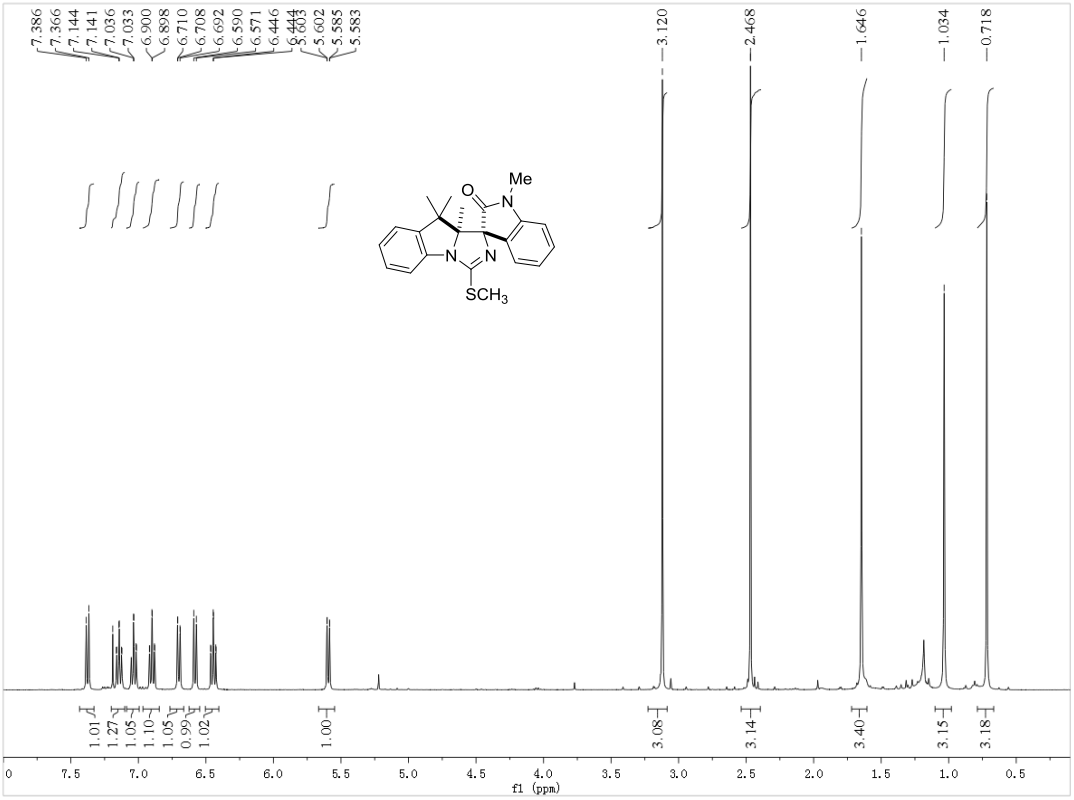
HRMS of 3di

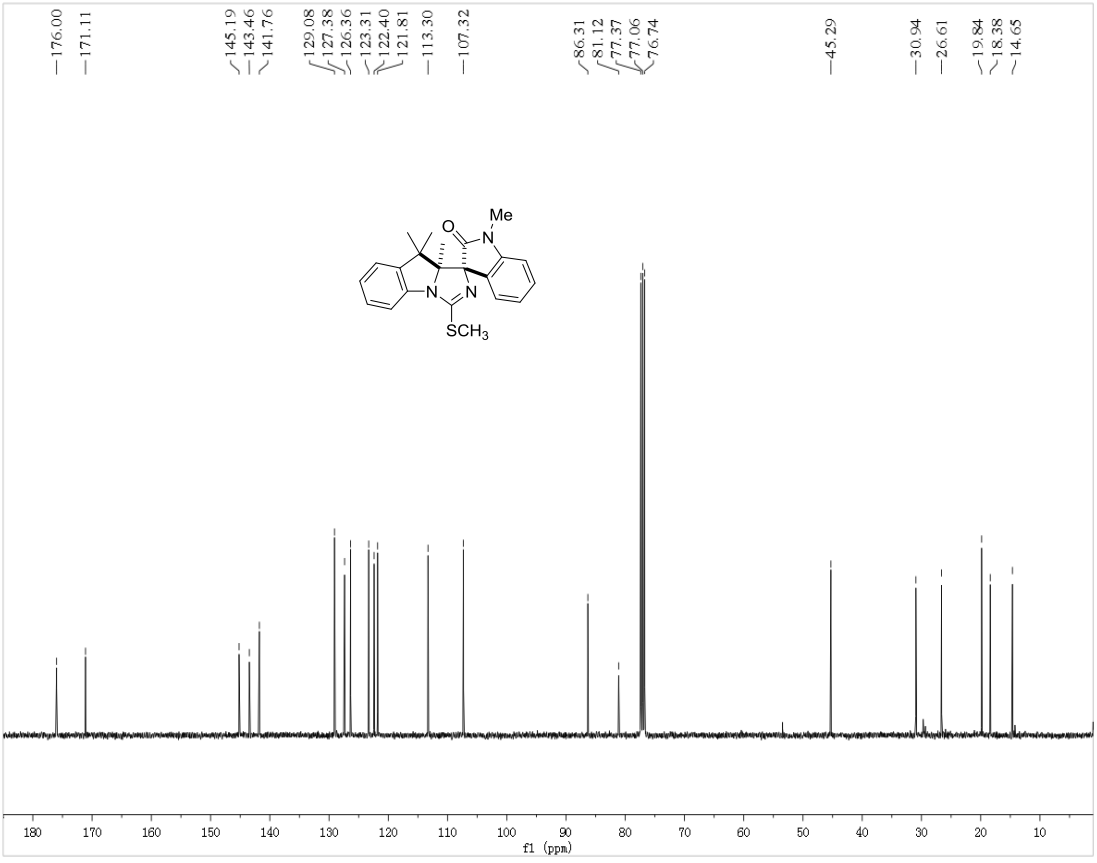
Item name: LRM-H24-3di
Item description:

Channel name: 1: Average Time 0.1132 min : TOF MS (50-1500) ESI+ : Centroided : Combined



^{1}H and ^{13}C NMR of 4aa





HRMS of 4aa

Item name: LRM-G68
Item description:

Channel name: 1: Average Time 0.0917 min : TOF MS (50-1500) ESI+ : Centroided : Combined