Supporting Information

Synthesis and antifungal evaluation of new azole derivatives containing 1,2,3-triazole

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1. Experimental section

1.1 General information

Starting reagents and solvents were commercially available and analytically pure without further purification. Nuclear Magnetic Resonance (NMR) spectra were performed recorded on a Bruker AV 400 spectrometer (Bruker Company, Germany). High Performance Liquid Chromatography-Mass Spectrometry (HRMS) spectra were carried out on a Triple TOF 5600^+ spectrometer (AB Sciex, United States). *Candida albicans* SC5314 was purchased from ATCC Culture Preservation Center (United States). FLC-resistant SC5314-FR was induced by SC5314 with FLC. All strains were frozen in 30% glycerol at -80 ℃ for use. Axio Vert. A1 Inverted Fluorescence Microscope (Zeiss, Germany), Centrifuge 5810R High Speed Refrigerated Centrifuge (Eppendorf, Germany) and Tecan Spark 10M multimode microplate reader (Tecan) were used for biological pharmacological analysis.

The purity of all compounds was no less than 95% by HPLC analysis. HPLC conditions: Solvent, CH_3CN/water=90:10, flow rate=1.0 mL/min; Column type: Thermo C18 Column 4.6×250 mm; Column temperature: 30 ℃; wavelength=210 nm.

1.2 General procedure for the preparation of compound **1**

To a stirred solution of 2'-chloro-2,4-dichloroacetophenone (4.47 g, 20 mmol) in acetonitrile (60 mL), potassium carbonate (3.31 g, 24 mmol) and imidazole (1.63 g, 24 mmol) was added, the mixture was refluxed for 4 h. After completion of the reaction as indicated by TLC (PE/EA 3:1, Rf=0.3), the mixture was poured into dichloromethane (DCM, 150 mL) and washed with water (3×150 mL). The organic layer was dried by anhydrous Na_2SO_4, concentrated *in vacuo* and purified by column chromatography (PE/EA 5:1) to afford white solid (4.39 g, 86% yield).

1.3 General procedure for the preparation of compound **2**

To a stirred solution of compound **1** (5.10 g, 20 mmol) in methanol solution (60 mL), sodium borohydride (2.27 g, 60 mmol) was added slowly on an ice bath and left to react at rt for 12 h. After completion of the reaction as indicated by TLC (PE/EA 1:1, Rf=0.5), the water (10 mL) was carefully added to the mixture and stirred for 15 minutes. The mixture was extracted with DCM (3×150 mL). The organic layer was dried by anhydrous Na_2SO_4, concentrated in vacuo and purified by column chromatography (DCM) to afford white solid (4.53 g, 88% yield).

1.4 General procedure for the preparation of compound **3**

To a stirred solution of compound **2** (5.14 g, 20 mmol) in THF (60 mL), sodium hydride (0.96 g, 40 mmol) was added and the mixture was reacted at 0℃ for 1 h. Following that 3-bromopropyl (3.5 mL, 40 mmol) and potassium iodide (0.3 g, 1.8 mmol) was added and the mixture was reacted at rt for 12 h. After completion of the reaction as indicated by TLC (PE/EA 2:1, Rf=0.4), the mixture was added saturated NH_4Cl solution (5 mL) to stir 10 min at 0 ℃, until the excess sodium hydride was completely consumed. Then the mixture was extracted with DCM (3×150 mL). The organic layer was dried by anhydrous Na_2SO_4, concentrated in vacuo and purified by column chromatography (PE/EA 3:1) to afford brown oil (5.12 g, 86.5% yield).

1.5 General procedure for synthesis of compound **4a**-**4w**

To a stirred solution of compound **3** (0.1 g, 0.35 mmol) and R-X (0.525 mmol) in ethanol: water =1:1 (4 mL), sodium azide (34 mg, 0.525 mmol), sodium ascorbate (84 mg, 0.42 mmol) and copper acetate (14 mg, 0.07 mmol) were added and the mixture was reacted at 65 ℃ for 12 h. After completion of the reaction as indicated by TLC (DCM/MeOH 30:1, Rf=0.4), H_2O (5 mL) was added, and then the mixture was extracted with DCM (3×5 mL). The organic layer was dried by anhydrous Na_2SO_4, concentrated in vacuo and purified by column chromatography (DCM/MeOH/TEA 100:1:0.5) to afford compound **4a-4w** (65-84% yields).

Compound 4a: ^{1}H NMR(400MHz, $CDCl_3$) δ: 7.18~7.49 (m, 11H), 5.47(s, 2H), 4.94(s, 1H), 4.59(d, *J* = 11.9 Hz, 1H), 4.37(d, *J* = 11.6 Hz, 1H), 4.18(s, 1H), 3.97(s, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 144.10, 134.64, 134.44,133.70, 133.04, 129.36, 128.91, 128.56, 128.40, 127.94, 127.74, 122.48, 77.48, 77.16, 76.84, 76.43, 62.79, 53.89.

Compound 4b: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.13~7.41(m, 10H), 5.51(q, *J* = 14.9 Hz, 2H), 4.93~4.95(m, 1H), 4.61(d, *J* = 12.4 Hz, 1H), 4.37(d, *J* = 12.5 Hz, 1H), 4.20(s, 1H), 3.97(s, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 144.54, 134.96, 134.79, 133.79, 133.25, 133.11, 129.63, 129.53, 129.30, 128.49, 127.98, 122.51, 77.48, 77.16, 76.84, 76.69, 63.02, 53.36.

Compound 4c: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.23(d, *J* = 8.6 Hz, 2H), 7.31-7.44(m, 5H), 7.30(t, *J* = 6.5 Hz, 1H), 7.21(s, 1H), 6.95(s, 1H), 5.68(q, *J* = 15.5 Hz, 2H), 4.96(d, *J* = 7.4 Hz, 1H), 4.66(d, *J* = 12.8 Hz, 1H), 4.40(d, *J* = 12.8 Hz, 1H), 4.00(d, *J* = 8.1 Hz, 1H), 3.95~3.97(m, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 147.94, 144.84, 141.69, 134.96, 133.66, 133.22, 129.61, 128.75, 128.43, 127.96, 124.20, 122.86, 77.48, 77.36, 77.16, 76.92, 76.84, 62.97, 52.97; HRMS-ESI calcd for $C_{21}H_{19}Cl_2N_6O_3$ $(M+H)^+$ 473.0890, found 473.0893.

Compound 4d: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.69(d, *J* = 8.3 Hz, 2H), 7.29~7.42(m, 5H), 7.14(s, 1H), 6.90(s, 2H), 5.62(q, *J* = 15.4 Hz, 2H), 4.95(d, *J* = 1.9 Hz, 1H), 4.93(d, *J* = 2.0 Hz, 1H), 4.66(d, *J* = 12.8 Hz, 1H), 4.39(d, *J* = 12.8 Hz, 1H), 3.93~4.20(m, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 144.77, 139.76, 134.94, 133.65, 133.21, 132.81, 129.60, 128.51, 128.42, 127.95, 122.76, 118.17, 112.60, 77.48, 77.16, 76.93, 76.84, 62.94, 53.25.

Compound 4e: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.65(d, *J* = 7.8 Hz, 2H), 7.39-7.41(m, 4H), 7.30(d, *J* = 8.4 Hz, 1H), 7.20(s, 1H), 6.92(s, 1H), 5.62(q, *J* = 15.2 Hz, 2H), 4.96(d, *J* = 6.7 Hz, 1H), 4.64(d, *J* = 12.6 Hz, 1H), 4.38(d, *J* = 12.6 Hz, 1H), 4.19(s, 1H), 3.97(s, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 144.65, 138.62, 135.02, 133.70, 133.27, 129.66, 128.48, 128.38, 128.01, 126.08, 126.04, 126.01, 122.78, 77.48, 77.16, 76.84, 63.01, 53.40.

Compound 4f: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.05~7.42(m, 10H), 5.51(q, *J* = 15.0 Hz, 2H), 4.95(d, *J* = 6.3 Hz, 1H), 4.64(d, *J* = 12.6 Hz, 1H), 4.38(d, *J* = 12.7 Hz, 1H), 4.21(s, 1H), 3.98(s, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 151.88, 151.84, 151.76, 151.71, 149.39, 149.35, 149.23, 144.74, 135.08, 133.76, 133.32, 131.70, 131.65, 131.61, 129.72, 128.51, 128.06, 124.49, 124.45, 124.42, 124.39, 122.59, 118.13, 117.96, 117.45, 117.27, 77.48, 77.16, 76.84, 63.07, 53.00. HRMS-ESI calcd for $C_{22}H_{19}Cl_2F_3N_5O$ $(M+H)^+$ 496.0913, found 496.0918.

Compound 4g: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.25~7.42(m, 5H), 7.01(s, 1H), 5.95~6.04(m, 1H), 5.28~5.38(dd, *J* = 9.6 Hz, 9.6 Hz, 2H), 4.98(d, *J* = 15.6 Hz, 3H), 4.64(d, *J* = 12.6 Hz, 1H), 4.41(d, *J* = 12.6 Hz, 1H), 4.22(s, 1H), 4.02(s, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 144.04, 134.86, 133.77, 133.21, 131.06, 129.55, 128.51, 127.91, 122.48, 120.26, 77.48, 77.16, 76.84, 76.63, 62.95, 52.65.

Compound 4h: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.47(s, 1H), 7.40~7.44(m, 2H), 7.30~7.33(m, 1H), 7.28(s, 1H), 7.02(s, 1H), 6.90(s, 1H), 4.95~4.98(dd, *J* = 2.6 Hz, 2.5 Hz, 1H), 4.63~4.68(m, 3H), 4.42(d, *J* = 12.7 Hz, 1H), 4.17~4.21(dd, *J* = 2.6 Hz, 2.6 Hz, 1H), 3.90~4.01(m, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 144.12, 137.97, 135.12, 133.83, 133.40, 129.79, 128.98, 128.59, 128.12, 123.68, 120.00, 77.48, 77.16, 77.05, 76.84, 63.09, 51.77, 51.45, 42.46; HRMS-ESI calcd for $C_{16}H_{17}Cl_3N_5O(M+H)^+$ 400.0493, found 400.0496.

Compound 4i: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.67(s, 1H), 7.29~7.44(m, 4H), 6.95(s, 1H), 5.17~5.21(m, 2H), 5.02(d, *J* = 7.4 Hz, 1H), 4.69(d, *J* = 12.5 Hz, 1H), 4.42(d, *J* = 12.6 Hz, 1H), 4.23~4.30(m, 2H), 4.01~4.06(dd, *J* = 7.7 Hz, 8.0 Hz, 1H), 3.82(s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 166.89, 144.29, 135.20, 133.54, 133.37, 129.80, 128.62, 128.15, 124.45, 77.48, 77.16, 76.84, 76.66, 63.02, 62.55, 53.17, 50.93, 50.78.

Compound 4j: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.22~7.51(m, 10H), 5.51(s, 2H), 5.00(s, 1H), 4.60(d, *J* = 9.8 Hz, 1H), 4.70(s, 2H), 4.05(s, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 144.28, 134.89, 133.68, 133.14, 132.11, 129.82, 129.51, 128.45, 127.89, 122.75, 122.71, 77.48, 77.16, 76.84, 62.89, 53.28, 46.03; HRMS-ESI calcd for $C_{21}H_{19}BrCl_2N_5O$ $(M+H)^+$ 508.0122, found 508.0126.

Compound 4k: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.03(s, 2H), 7.31~7.68(m, 9H), 5.95(s, 2H), 5.02(s, 1H), 4.67(d, *J* = 10.6 Hz, 1H), 4.40(d, *J* = 10.6 Hz, 2H), 4.03(s, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 190.52, 144.10, 134.93, 134.55, 133.93, 133.26, 129.59, 129.13, 128.57, 128.17, 127.98, 124.82, 77.48, 77.16, 76.84, 63.01, 55.63, 46.00; HRMS-ESI calcd for $C_{22}H_{20}Cl_2N_5O_2(M+H)^+$ 456.0989, found 456.0987.

Compound 4l: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.89(d, *J* = 8.1 Hz, 2H), 7.67(d, *J* = 8.2 Hz, 2H), 7.42~7.46(m, 4H), 7.29~7.32(m, 1H), 5.92(s, 2H), 5.00(s, 1H), 4.68(d, *J* = 12.4 Hz, 1H), 4.40(d, *J* = 12.4 Hz, 1H), 4.24(s, 1H), 4.01(s, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 189.78, 144.08, 134.91, 133.69, 133.22, 132.60, 132.41, 129.83, 129.63, 129.57, 128.51, 127.96, 124.80, 77.48, 77.16, 76.84, 76.50, 62.95, 55.55, 45.97; HRMS-ESI calcd for $C_{22}H_{19}BrCl_2N_5O_2(M+H)^+$ 536.0072, found 536.0068.

Compound 4m: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.04~8.07(m, 2H), 7.42~7.44(m, 3H), 7.21~7.33(m, 4H), 6.96(d, *J* = 24.2 Hz, 2H), 5.89(q, *J* = 17.7 Hz, 2H), 4.97~5.00(dd, *J* = 2.5 Hz, 2.5 Hz, 1H), 4.72(d, *J* = 12.6 Hz, 1H), 4.43(d, *J* = 12.6 Hz, 1H), 4.17~4.21(dd, *J* = 2.5 Hz, 2.5 Hz, 1H), 3.94~4.00(dd, *J* = 8.2 Hz, 8.2 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 188.84, 167.90, 165.34, 144.48, 135.05, 133.86, 133.38, 131.11, 131.01, 130.47, 130.44, 129.74, 128.91, 128.60, 128.09, 124.65, 120.06, 116.69, 116.47, 77.48, 77.16, 77.02, 76.84, 63.18, 55.39, 51.41.

Compound 4n: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.71(d, *J* = 8.4 Hz, 1H), 7.54(d, *J* = 2.0 Hz, 1H), 7.39~7.48(m, 4H), 7.26~7.33(m, 2H), 6.99(s, 1H), 6.91(s, 1H), 5.85(q, *J* = 18.1 Hz, 2H),

4.96~4.99(dd, *J* = 2.5 Hz, 2.5 Hz, 1H), 4.71(d, *J* = 12.6 Hz, 1H), 4.43(d, *J* = 12.6 Hz, 1H), 4.17~4.21(dd, *J* = 2.6 Hz, 2.6 Hz, 1H), 3.94~4.00(dd, *J* = 8.2 Hz, 8.2 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 144.54, 139.83, 135.16, 133.83, 133.49, 133.44, 133.17, 131.74, 131.13, 129.82, 128.63, 128.16, 128.12, 124.59, 77.48, 77.16, 77.03, 76.84, 63.21, 58.34, 51.51.

Compound 4o: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.19~7.59(m, 7H), 6.87(d, *J* = 7.6 Hz, 2H), 5.80(s, 2H), 4.92(s, 1H), 4.58(d, *J* = 10.9 Hz, 1H), 4.32(d, *J* = 11.0 Hz, 1H), 4.14(s, 1H), 3.81~3.87(m, 7H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 154.30, 149.27, 143.89, 134.75, 133.71, 133.12, 129.43, 128.48, 127.84, 126.91, 124.72, 122.95, 110.31, 110.00, 77.48, 77.16, 76.84, 76.45, 62.88, 56.10, 55.95, 55.14, 45.94.

Compound 4p: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.41~7.44(m, 3H), 7.30~7.33(m, 1H), 7.22(s, 1H), 6.97(d, *J* = 22.4 Hz, 2H), 5.28(q, *J* = 18.2 Hz, 2H), 4.95~4.97(dd, *J* = 2.1 Hz, 2.2 Hz, 1H), 4.69(d, *J* = 12.6 Hz, 1H), 4.40(d, *J* = 12.6 Hz, 1H), 4.20(d, *J* = 14.2 Hz, 1H), 3.94~3.99(dd, *J* = 8.2 Hz, 8.3 Hz,1H), 2.27(s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 199.06, 144.38, 135.03, 133.77, 133.33, 129.70, 128.55, 128.06, 124.28, 77.48, 77.16, 76.84, 63.07, 58.47, 51.44, 27.28.

Compound 4q: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.69(d, *J* = 16.0 Hz, 1H), 7.55(d, *J* = 7.4 Hz, 2H), 7.27~7.40(m, 7H), 6.47(d, *J* = 16.0 Hz, 1H), 5.55(s, 2H), 4.97(s, 1H), 4.62(d, *J* = 11.8 Hz, 1H), 4.38(d, *J* = 11.9 Hz, 1H), 4.26(s, 1H), 3.99(s, 1H), 3.81(s, 4H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 167.21, 144.44, 143.78, 136.70, 135.01, 134.83, 133.79, 133.25, 129.65, 128.70, 128.67, 128.52, 128.00, 122.77, 118.77, 77.48, 77.16, 76.84, 63.02, 53.69, 51.84, 46.07.

Compound 4r: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.92(d, *J* = 7.4 Hz, 2H), 7.29~7.42(m, 8H), 5.89(s, 2H), 5.02(s, 1H), 4.68(d, *J* = 11.9 Hz, 1H), 4.40(d, *J* = 11.9 Hz, 1H), 4.25(s, 1H), 4.00(s, 1H), 2.44(s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 190.07, 145.70, 144.04, 135.00, 133.31, 131.51, 129.84, 129.66, 128.60, 128.32, 128.04, 124.89, 77.48, 77.16, 76.84, 63.05, 55.58, 21.87.

Compound 4s: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.55(s, 1H), 7.91~8.03(m, 4H), 7.60~7.70(m, 2H), 7.30~7.44(m, 5H), 6.98(d, *J* = 28.8 Hz, 2H), 6.05(q, *J* = 17.6 Hz, 2H), 4.99~5.02(dd, *J* = 2.6 Hz, 2.6 Hz, 1H), 4.73(d, *J* = 12.6 Hz, 1H), 4.45(d, *J* = 12.6 Hz, 1H), 4.17~4.21(dd, *J* = 2.6 Hz, 2.6 Hz, 1H), 3.94~4.00(dd, *J* = 8.1 Hz, 8.1 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 144.47, 136.28, 135.07, 133.92, 133.41, 132.48, 131.34, 130.38, 129.87, 129.76, 129.52, 129.35, 128.66, 128.12, 128.08, 127.49, 124.74, 123.36, 77.48, 77.16, 77.02, 76.84, 63.23, 55.61, 51.45; HRMS-ESI calcd for $C_{26}H_{22}Cl_2N_5O_2$ $(M+H)^+$ 506.1145, found 506.1137.

Compound 4t: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.49(s, 1H), 7.33~7.46(m, 6H), 7.26~7.31(m, 2H), 7.00(s, 1H), 6.90(s, 1H), 6.74(d, *J* = 15.8Hz, 1H), 6.32-6.39(m, 1H), 5.11~5.14(m, 2H), 4.98~5.01(dd, *J* = 2.6 Hz, 2.6 Hz, 1H), 4.67(d, *J* = 12.6Hz, 1H), 4.44(d, *J* = 12.6Hz, 1H), 4.18~4.23(dd, *J* = 2.6 Hz, 2.7 Hz, 1H), 3.97~4.03(dd, *J* = 8.0 Hz, 8.0 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 144.37, 135.73, 135.62, 135.08, 133.91, 133.39, 129.75, 128.89, 128.71, 128.64, 128.09, 126.88, 122.42, 121.83, 77.48, 77.16, 76.99, 76.84, 63.18, 52.50, 51.44; HRMS-ESI calcd for $C_{23}H_{22}Cl_2N_5O$ $(M+H)^+$ 454.1196, found 454.1197.

Compound 4u: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.69~7.71(m, 1H), 7.40~7.51(m, 6H), 7.26~7.33(m, 2H), 7.00(s, 1H), 6.91(s, 1H), 5.86(q, *J* = 18.1Hz, 2H), 4.97~5.00(dd, *J* = 2.5 Hz, *J* = 2.5 Hz, 1H), 4.70(d, *J* = 12.6 Hz, 1H), 4.43(d, *J* = 12.6 Hz, 1H), 4.17~4.21(dd, *J* = 2.5 Hz, *J* =2.6 Hz, 1H), 3.95~4.00(dd, *J* = 8.1 Hz, 8.04 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 192.77, 144.43, 135.39, 135.11, 133.87, 133.71, 133.42, 131.99, 131.16, 130.42, 129.78, 128.66, 128.12, 127.59, 124.59, 77.48, 77.16, 76.99, 76.84, 63.18, 58.35, 51.50.

Compound 4v: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.90~7.96(m, 3H), 7.47~7.54(m, 4H), 7.32~7.37(m, 2H), 7.22~7.30(m, 2H), 6.97(s, 1H), 6.85(s, 1H), 6.68(s, 1H), 5.89~6.00(q, *J* = 14.8 Hz, 2H), 4.85~4.88((dd, *J* = 2.7 Hz, 2.7 Hz, 1H), 4.54(d, *J* = 12.6 Hz, 1H), 4.32(d, *J* = 12.6 Hz, 1H), 4.07~4.11(dd, *J* = 2.7 Hz, 2.7 Hz, 1H), 3.86~3.92(dd, *J* = 8.0 Hz, 8.0 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 144.27, 135.01, 134.07, 133.84, 133.35, 131.31, 130.24, 129.83, 129.69, 129.08, 128.62, 128.26, 128.03, 127.41, 126.53, 125.56, 123.02, 122.61, 77.48, 77.16, 76.84, 76.71, 63.02, 52.50, 51.32; HRMS-ESI calcd for $C_{25}H_{22}Cl_2N_5O$ $(M+H)^+$ 478.1196, found 478.1191.

Compound 4w: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.03~8.09(m, 1H), 7.42~7.46(m, 3H), 7.28~7.33(m, 2H), 6.98~7.09(m, 3H), 6.91(s, 1H), 5.82(q, *J* = 18.5 Hz, 2H), 4.98~5.01(dd, *J* = 2.6 Hz, 2.4 Hz, 1H), 4.73(d, *J* = 12.6 Hz, 1H),4.45(d, *J* = 12.6 Hz, 1H), 4.18~4.22(dd, *J* = 2.6 Hz, 2.6 Hz, 1H), 3.96~4.01(dd, *J* = 8.1 Hz, 8.2 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 187.23, 162.09, 144.43, 138.04, 135.11, 133.90, 133.43, 133.38, 133.34, 133.27, 133.23, 129.79, 129.00, 128.66, 128.13, 124.72, 120.02, 119.14, 113.49, 113.28, 113.25, 105.48, 105.21, 104.96, 77.48, 77.16, 77.03, 76.84, 63.25, 59.05, 58.91, 51.46; HRMS-ESI calcd for $C_{22}H_{18}Cl_2F_2N_5O_2$ $(M+H)^+$ 492.0800, found 492.0799.

1.6 Antifungal activity

The minimum inhibitory concentration (MIC_{50}) of a series of compounds (4a-4w) against *C. albicans* were determined by Microdilution method recommended by Clinical and Laboratory Standards Institute (CLSI) M27-A3. The logarithmic growth stage of *C. albicans* was adjusted to 1×10^5 CFU/mL by using Sand's liquid medium (SDB). All drugs were successively diluted by 5 times of SDB on a 96-well flat plate to achieve a final concentration of 200-0.064 μg/mL. The final concentration of DMSO per well was less than 0.1%. Growth control group (only added fungi), blank control group, single drug group (single drug + fungi) and fluconazole group (FLC+ fungi) were set up. Each compound was arranged in parallel with three multiple pores per concentration, with a final volume of 200 μL. The 96-well culture plate was cultured in an incubator at 30 °C for 24 h, and the OD value was detected at 630 nm with a multifunctional enzyme marker. The experiment was repeated three times.

1.7 Time-sterilization curve test

Logarithmic growth of *C. albicans* was taken and the concentration of SDB was adjusted to 1×10^5 CFU/mL. Control group (Control), FLC group, **4s** low dose group (L, 0.27 μg/mL), **4s** medium dose group (M, 0.53 μg/mL), **4s** high dose group (H, 1.06 μg/mL) were set. The system of each group was 10 mL. The strains and drugs were co-cultured on a constant temperature shaking

table at 150 r/min at 30 ºC. After culture for 0, 4, 8, 12, 24, 36, 48 h, the solution of each group was fully mixed, and 200 μL samples were taken from a super-clear workbench and placed on a 96-well plate. Then the absorbance at 630 nm was determined by enzyme labeling instrument. The remaining fungil solution was sealed with a sterile breathable sealing film and then placed back on the shaking table for culture. Each group is provided with three multiple holes. The time-sterilization curve was drawn with the time point as the horizontal coordinate and the absorbance measured at different time points as the vertical coordinate.

1.8 Cell morphology test

Mycelia induction SD+10% FBS and Spider were used to induce mycelia respectively. The *C. albicans* in the logarithmic growth stage were adjusted into a fungil suspension with a final concentration of 1×10^5 CFU/mL using SD+10% FBS or Spider medium. FLC group, **4s** low dose group (L, 0.27 μg/mL), **4s** medium dose group (M, 0.53 μg/mL), **4s** high dose group (H, 1.06 μg/mL) and control group without drugs were added to the corresponding 24-well plates, respectively, with a total system of 1mL per well and 3 multiple Wells in each group. Then it was cultured in a constant temperature and humidity incubator at 30 ºC. After 4 h and 8 h, the 24-well plate was taken out and the mycelium formation was observed under an inverted microscope and photographed.

1.9 Biofilm formation test

The culture medium of *C. albicans* in logarithmic growth stage (RPMI1640+10%FBS) was adjusted to 1×10^5 CFU/mL, which was added to the 24-well plate and cultured in an incubator at 30 ºC for 90 min, so that *C. albicans* adhered to the bottom of the culture plate, and the excess culture medium was slowly removed. The FLC group and **4s** low-dose group (L, 0.27 μg/mL), **4s** medium dose group (M, 0.53 μg/mL) and **4s** high dose group (H, 1.06 μg/mL) were added into 1 mL drug-containing and drug-free medium and cultured in an incubator at 30 ºC for 24 h. Then, the medium was discarded and stained with crystal violet solution for 30 min, the excess dye was washed 3 times with 1×PBS, and 200 μL PBS was added to observe the formation of *C. albicans* biofilm with an inverted microscope.

1.10 Membrane permeability test

FLC group, **4s** low dose group (L, 0.27 μg/mL), **4s** medium dose group (M, 0.53 μg/mL), **4s** high dose group (H, 1.06 μg/mL) and control group without drugs were set. The concentration of *C. albicans* was adjusted to 1×10^5 CFU/mL with SDB, and the corresponding drugs were added to the corresponding groups and cultured at 30 ºC and 150 r/min in a constant temperature shaking table for 16-24 hours, then was washed with aseptic PBS and resuspension to 2×10^6 CFU/mL. The strains were then incubated with PI dye (final concentration of 5 μg/mL) at room temperature for 30 min away from light, the dye was removed by centrifugation, and the cells were washed with sterile 1×PBS to remove the excess dye. Pictures were taken under a fluorescence microscope and their fluorescence intensity was measured.

1.11 Strain morphological change experiment

FLC group, **4s** low dose group (L, 0.27 μg/mL), **4s** medium dose group (M, 0.53 μg/mL), **4s** high dose group (H, 1.06 μg/mL) and control group without drugs were set up. The final concentration of Candida albicans with SDB was adjusted to 5×10^5 CFU/mL. The strains and drugs were placed on a constant temperature shaking table at 150 r/min at 30 °C for 16-24 hours. Cell precipitate was collected by centrifugation, sterilized by 1×PBS for three times, prefixed with pre-cooled 3% paraformaldehyde and 2.5% glutaraldehyde at 4 °C, and then refixed with 1% osmium tetroxide. Then dehydration with acetone step by step; The dehydrating agent and Epon-812 embedding agent were infiltrated in sequence according to the ratio of 3:1, 1:1 and 1:3, respectively. The 60-90 nm ultra-thin sections were prepared by the ultra-thin section mechanism using Epon-812 embedding method. The sections were stained with uranium acetate for 10-15 min and then with lead citrate for 1-2 min at room temperature. Images were then taken under a transmission electron microscope.

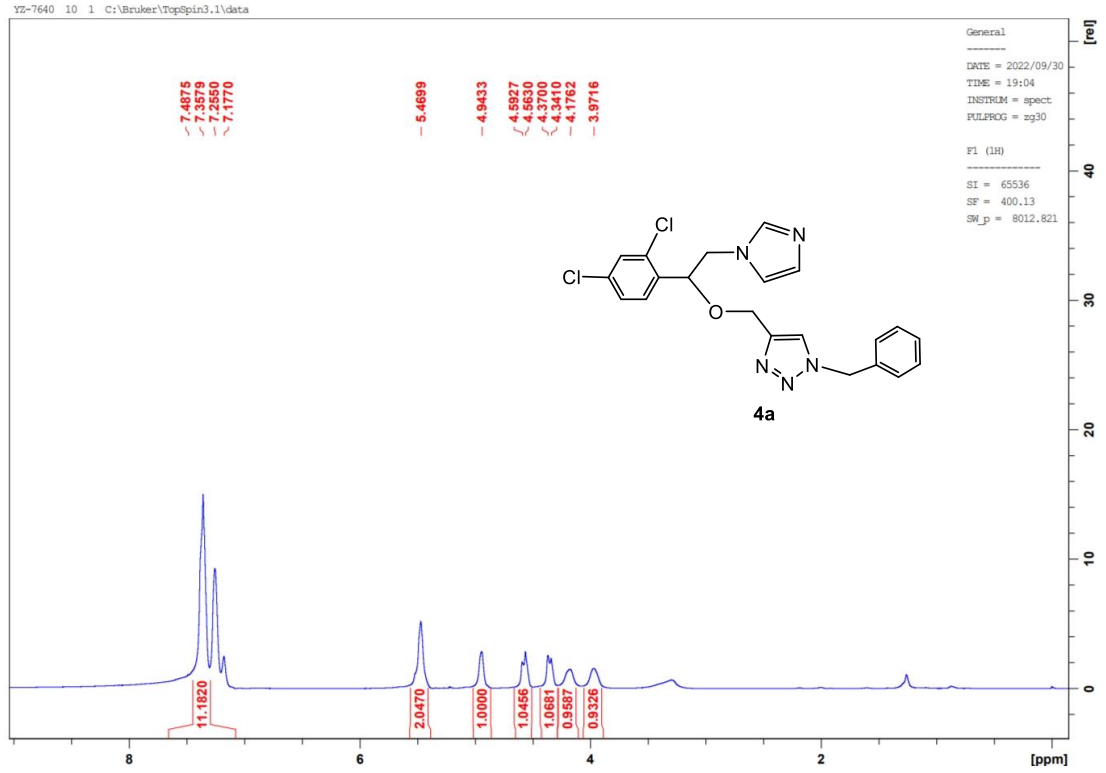
1.12 Toxicity test

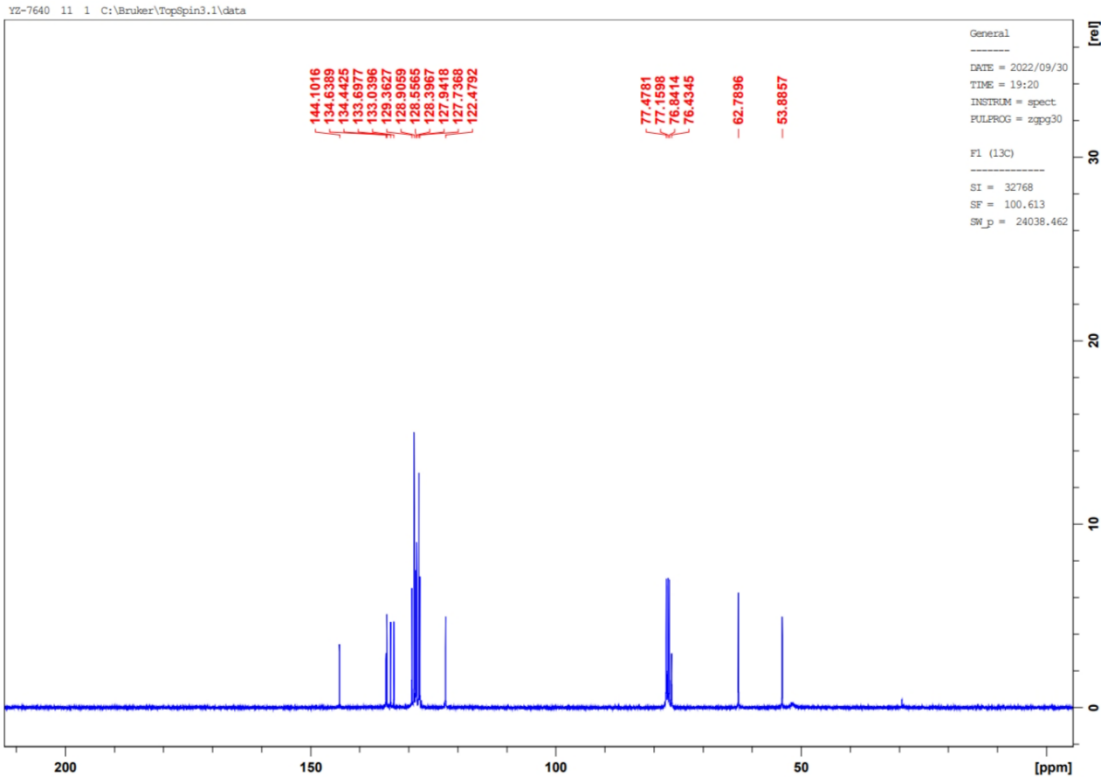
16HBE cells at logarithmic growth stage were inoculated into 96-well plates, and the cell concentration was adjusted to 1×10^5 CFU/mL with complete medium (RPMI1640 medium plus 10%FBS and 1% double antibody). The cells were cultured at 37 °C in a cell incubator for 24 h, so that the cells were uniformly attached to the bottom of the 96-well plates. After 24 h, the culture medium was removed, and the FLC group, **4s** drug group, growth control group and blank control group were set up. The drug was continuously diluted from 100 μg/mL by 5 times gradient with complete culture medium. Only cells were added to the growth control group, and the blank control group only contained the culture medium. The corresponding drugs were added according to the groups and incubated in the incubator for 48 h. After that, the culture plate was taken out in strict accordance with the instructions of the CCK8 test kit, and appropriate amount of CCK8 working liquid was added to each hole and placed in the incubator for incubation. OD values of each group were detected and cell viability was calculated at 450 nm wavelength by enzyme-labeler.

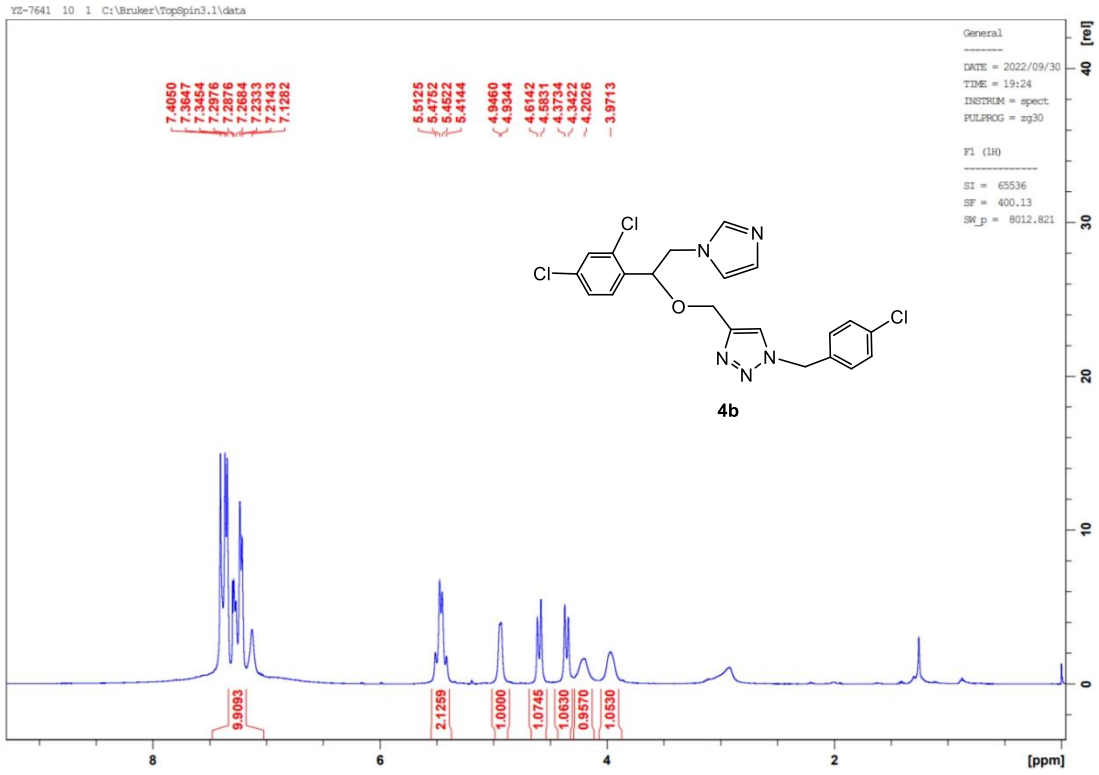
1.13 Molecular docking study

Firstly, 2D planar structure of the desired compound **4s** was drawn and saved as a mol format file. Then the three-dimensional crystal structure of CYP51 in PDB format was obtained from PDB database (https://www.rcsb.org/), and 5TL8 fragment was selected as the intended target protein of the synthesized drug. The protein was hydrotreated with water removal at Discovery Studio and saved as a PBD file. The software was used to dock compound **4s** with the target protein 5TL8, formed and visualized the score result. Finally, the interaction diagram of the docking site between compound and target protein was given.

2. NMR spectra



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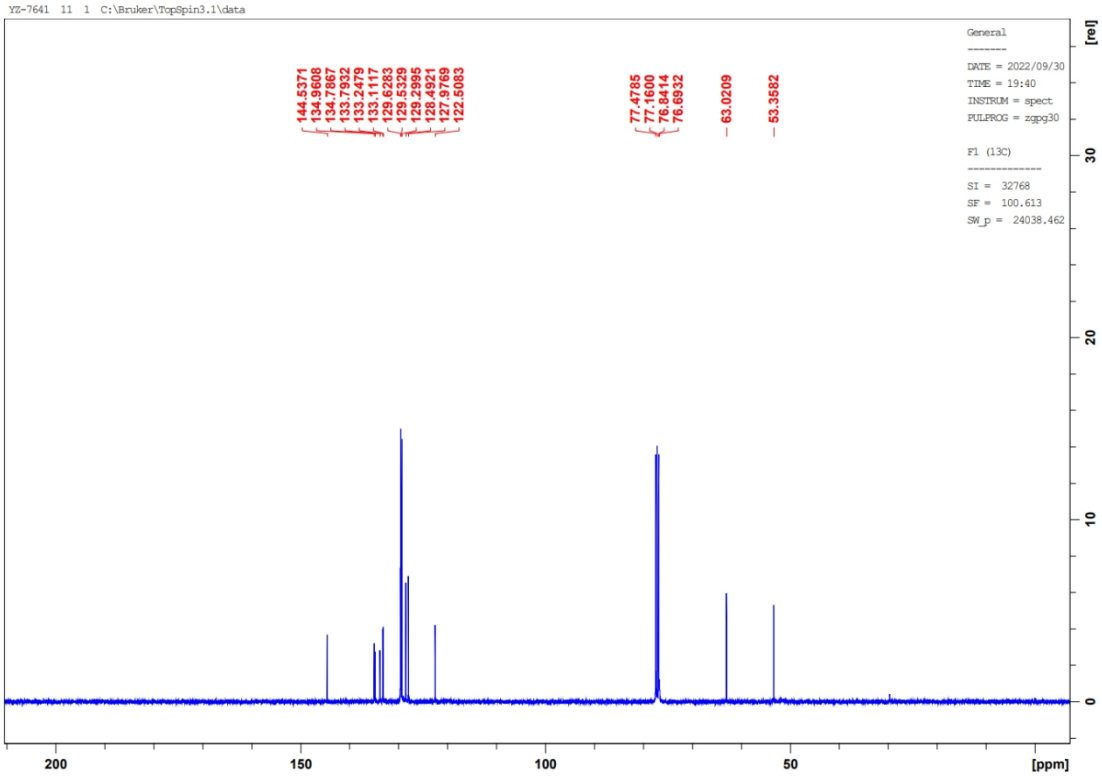
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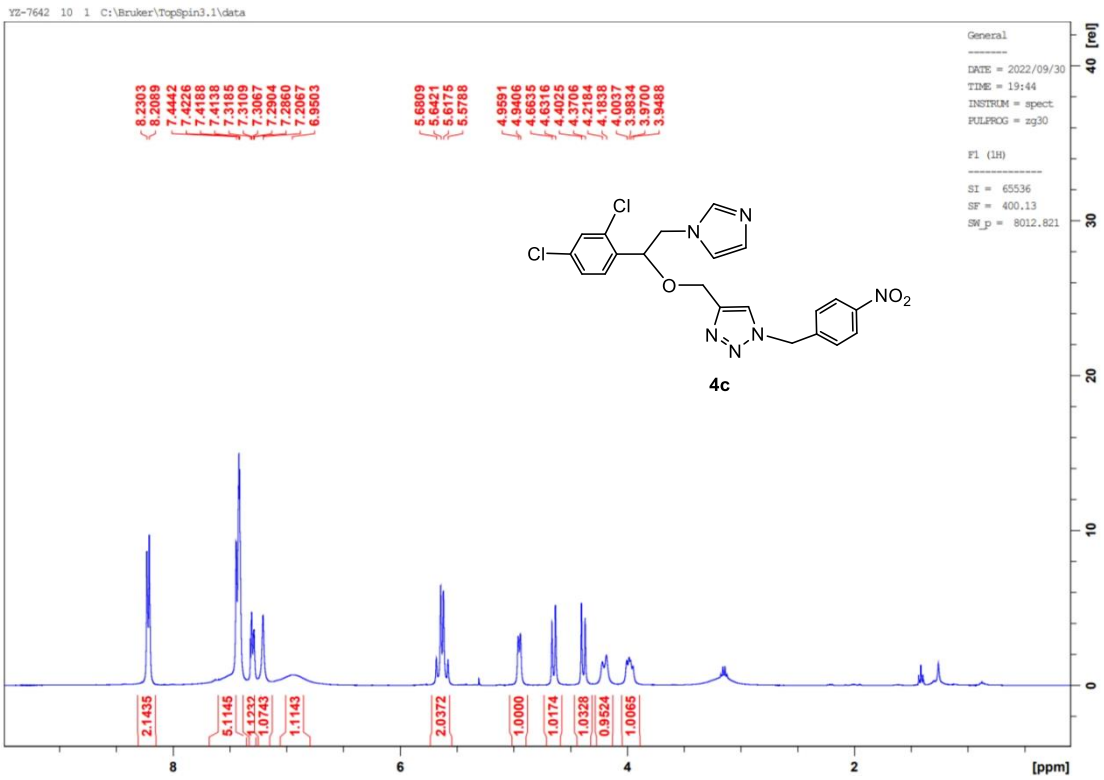
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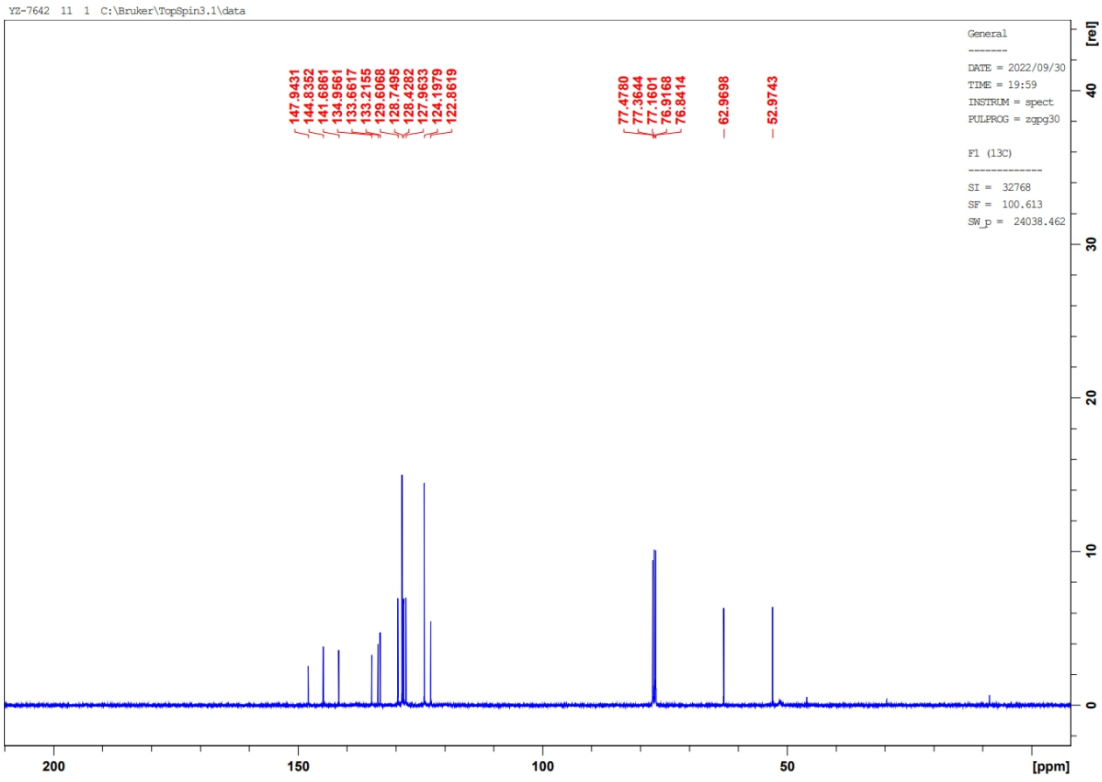
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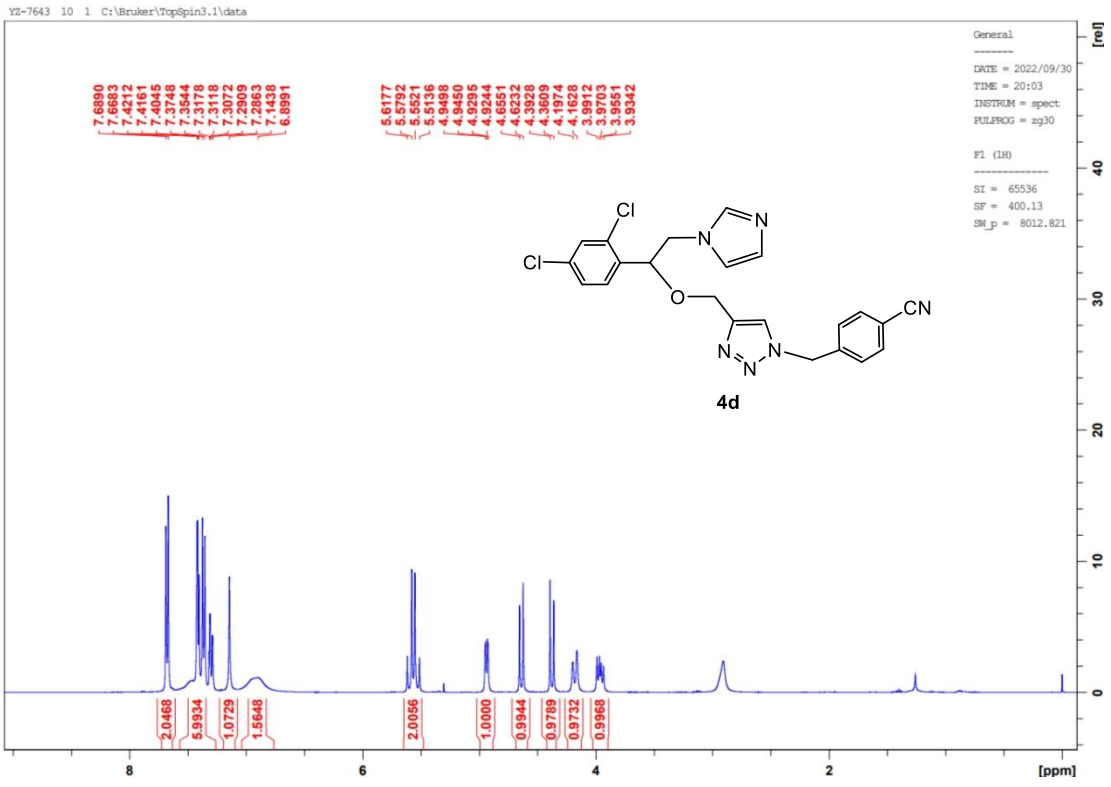
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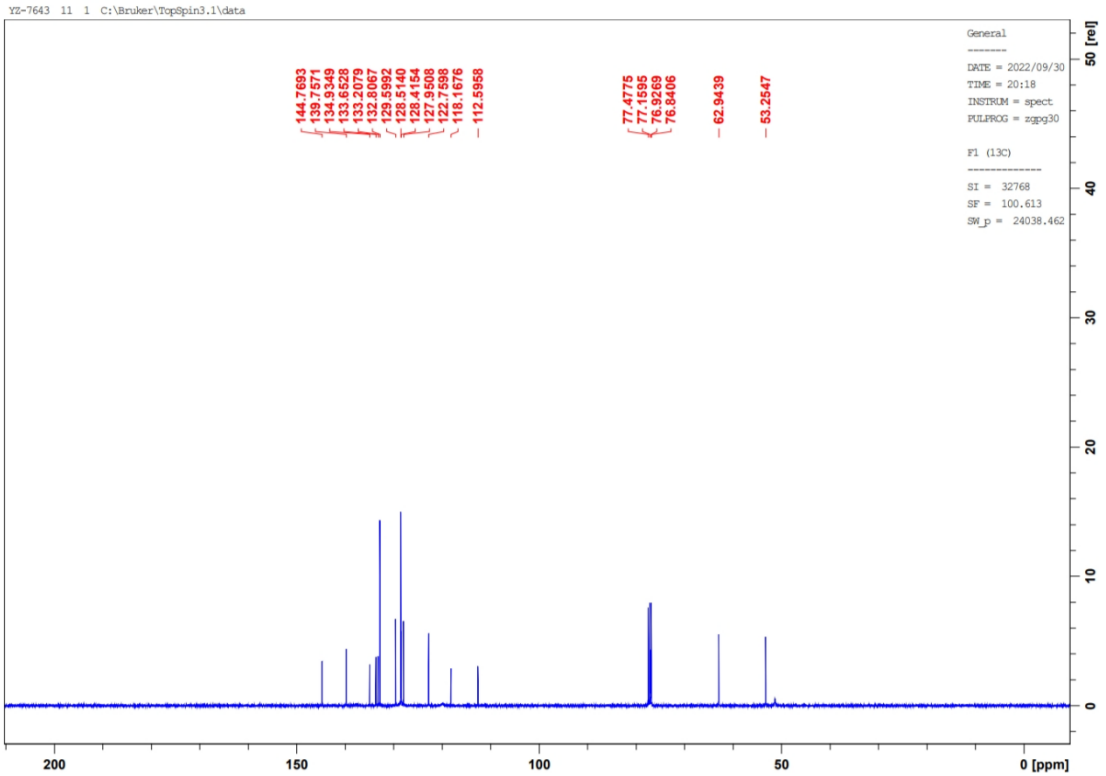
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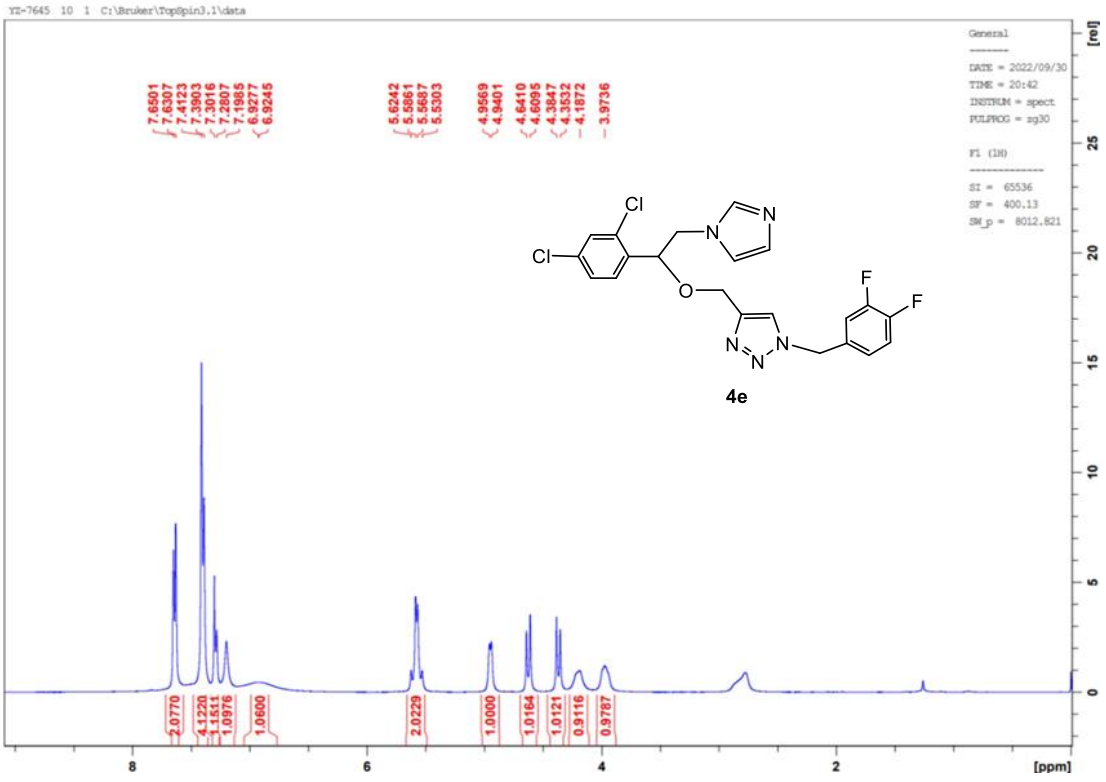
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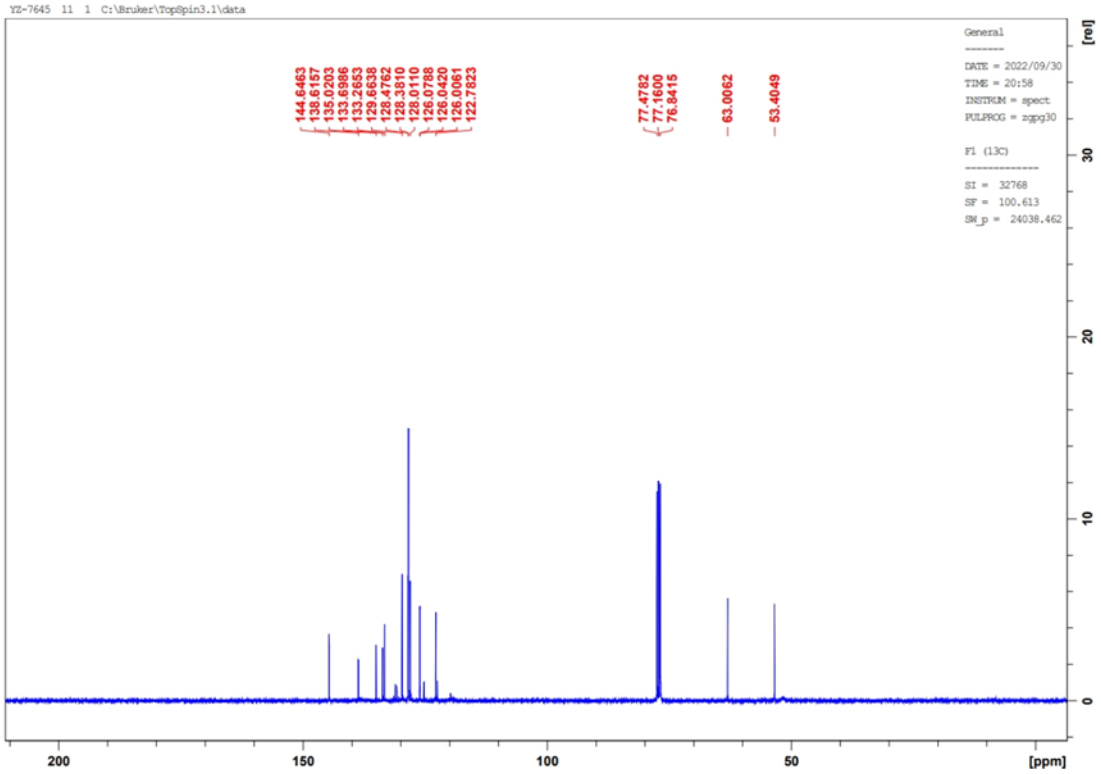
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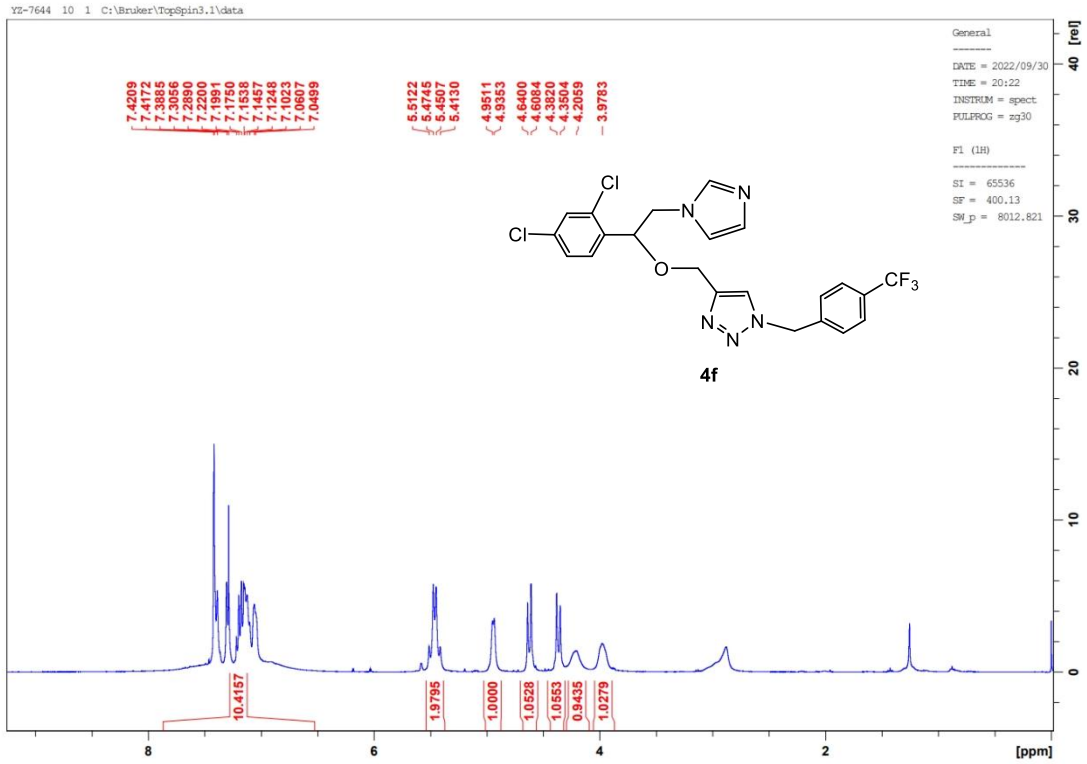
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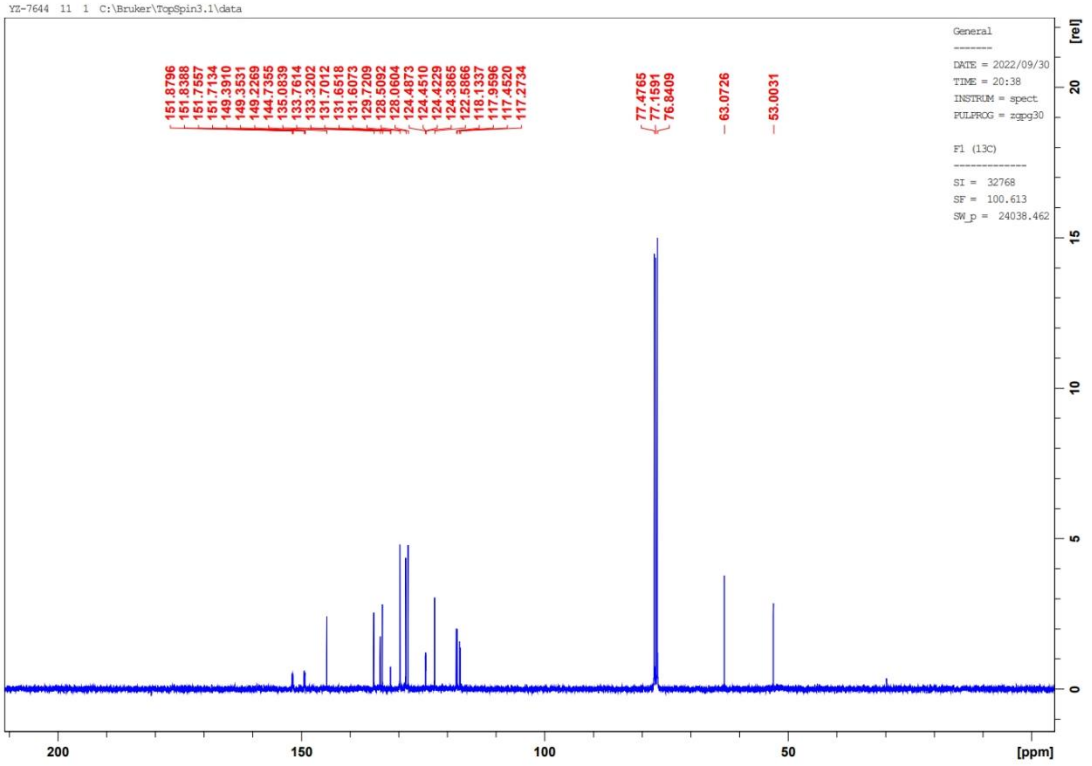
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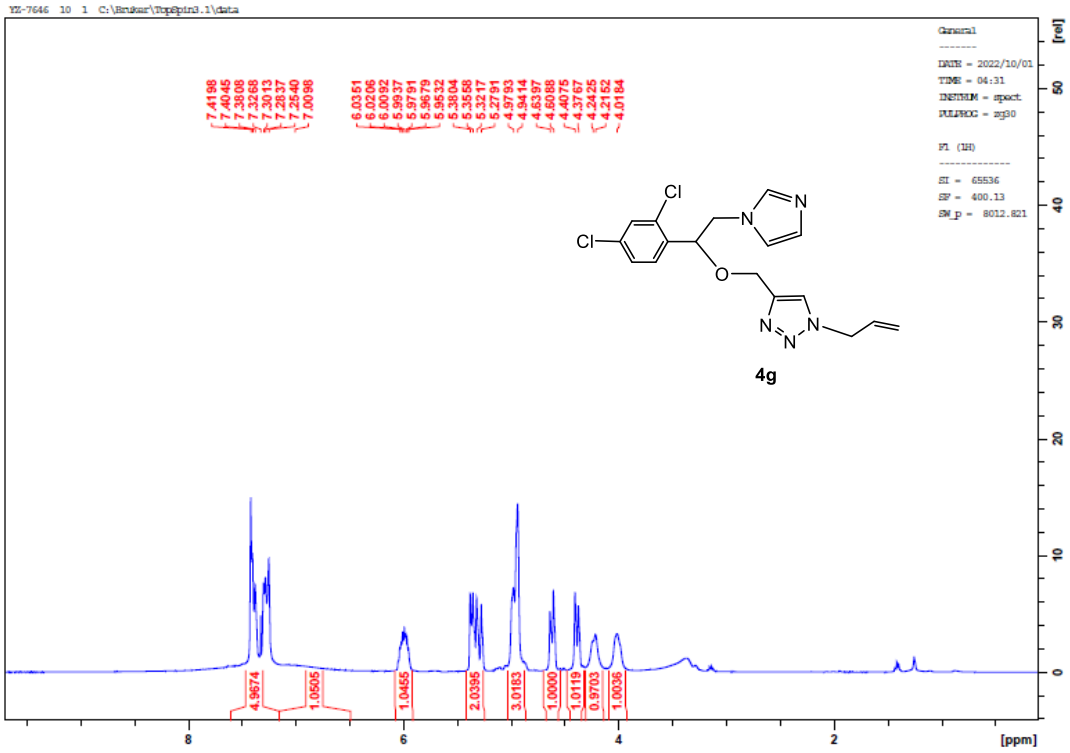
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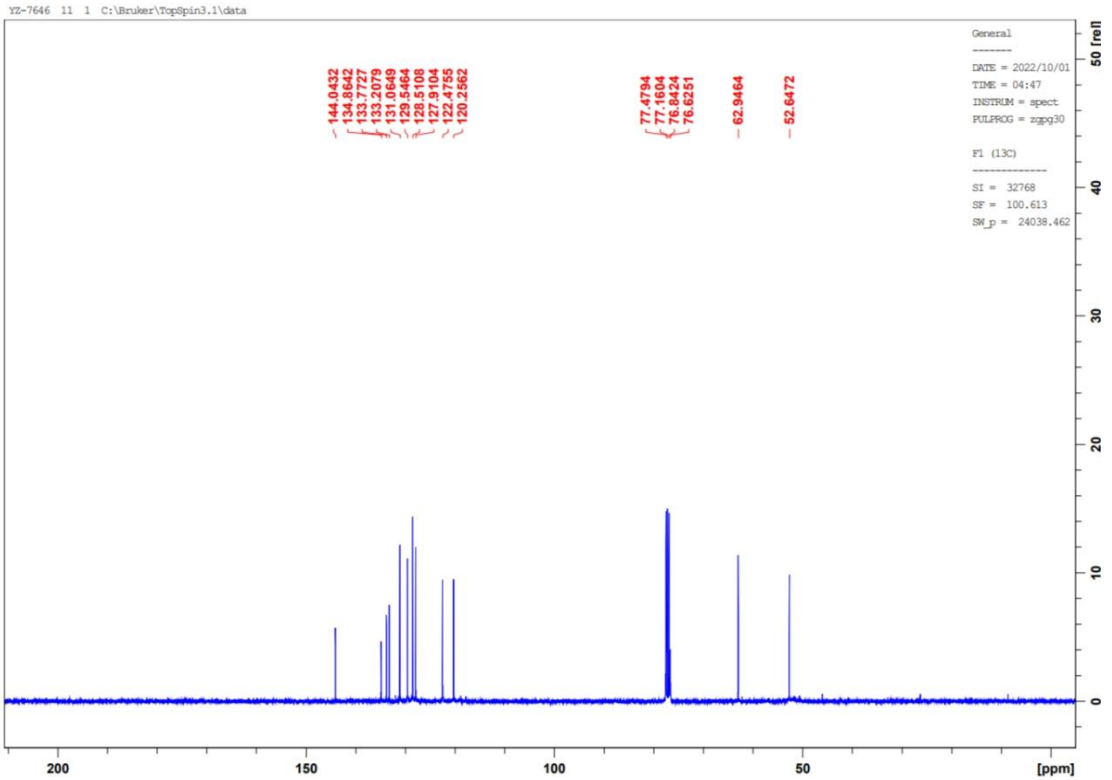
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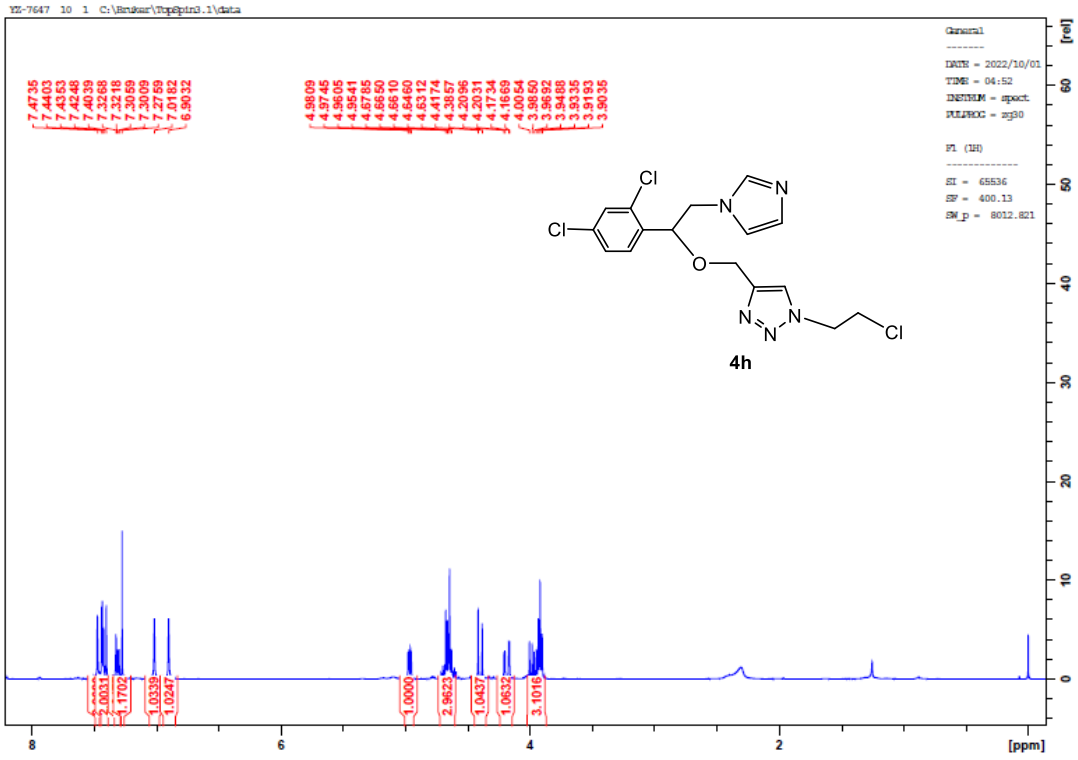
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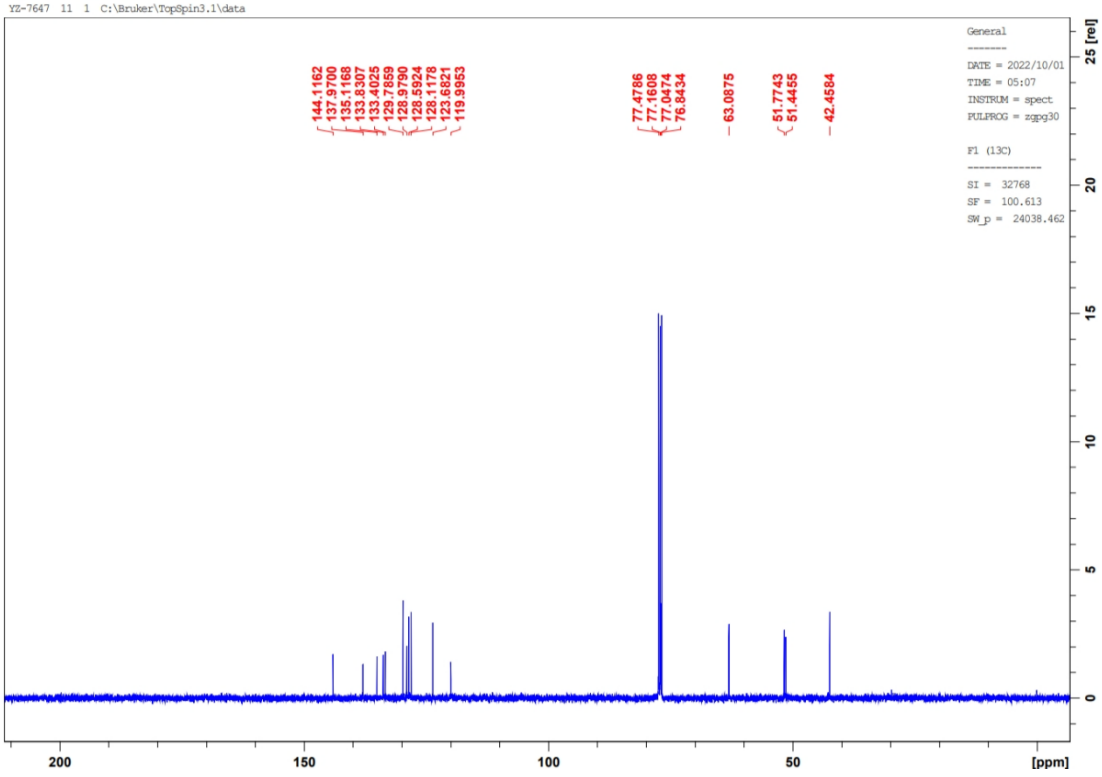
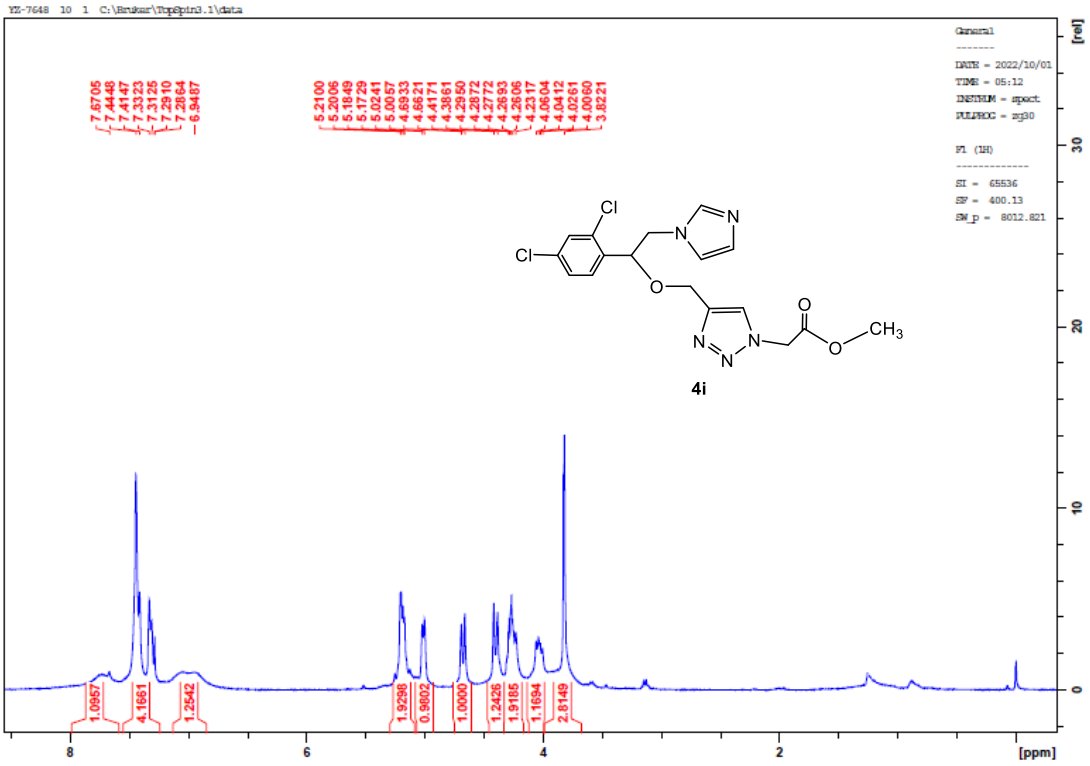
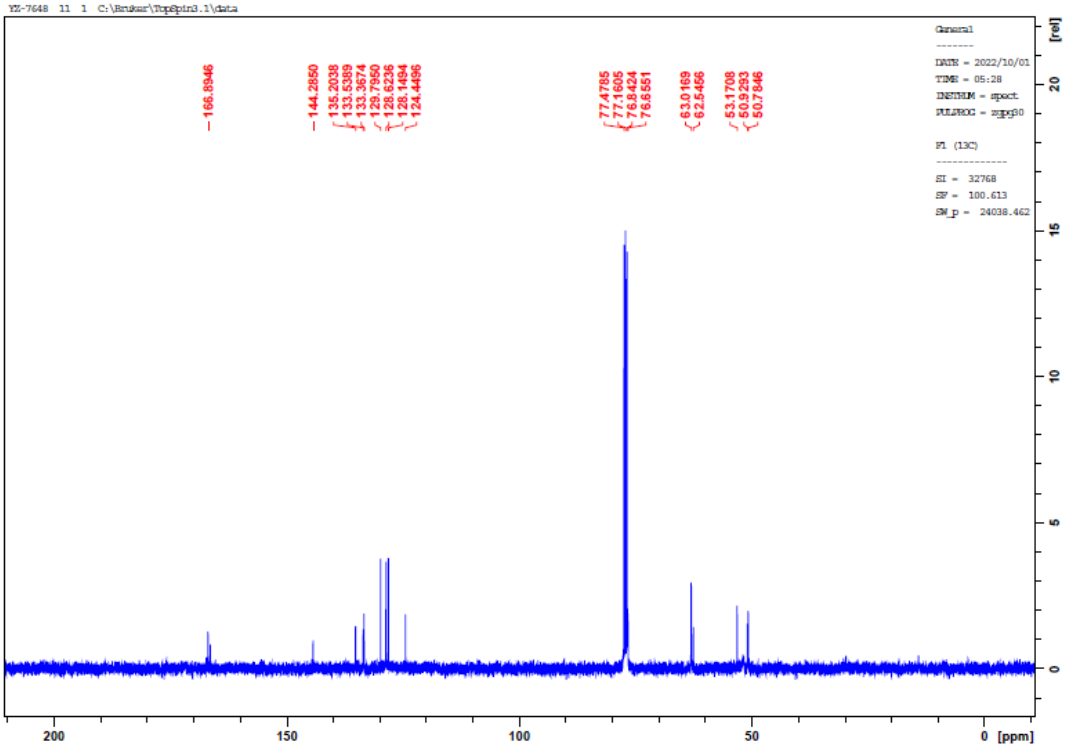
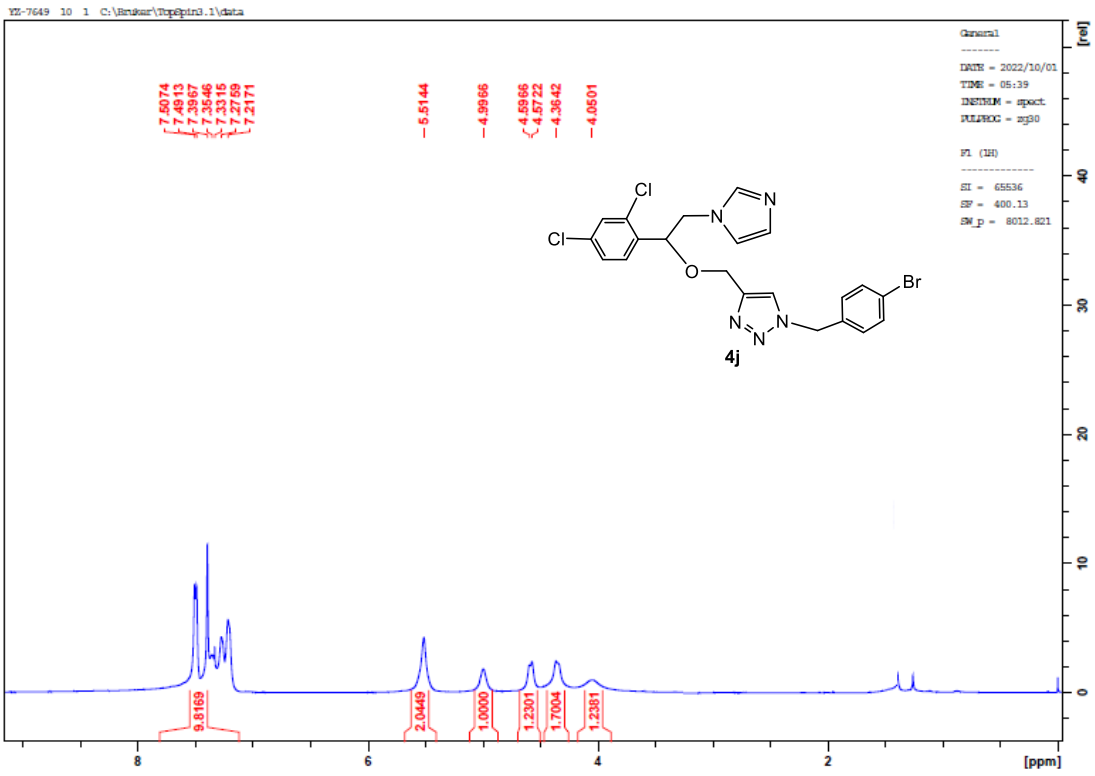
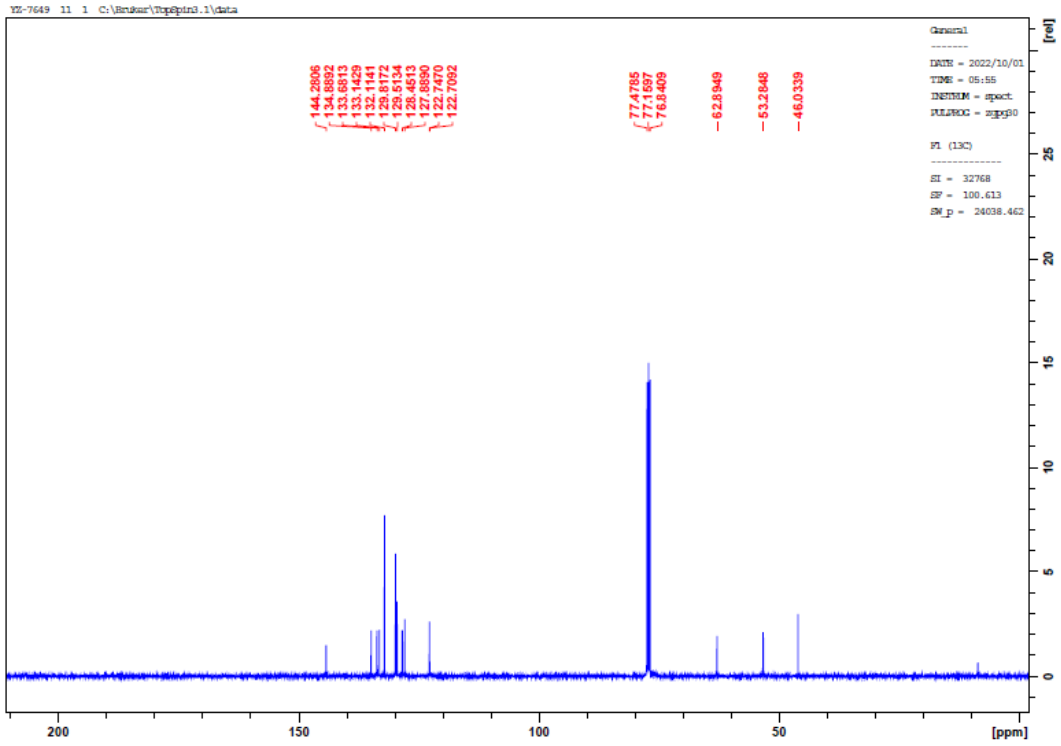
1.0632
3.1016
Cl
Cl
N
N
O
N
N
N
Cl
4h
General
DATE = 2022/10/01
TIME = 04:52
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
[rel]
[ppm]

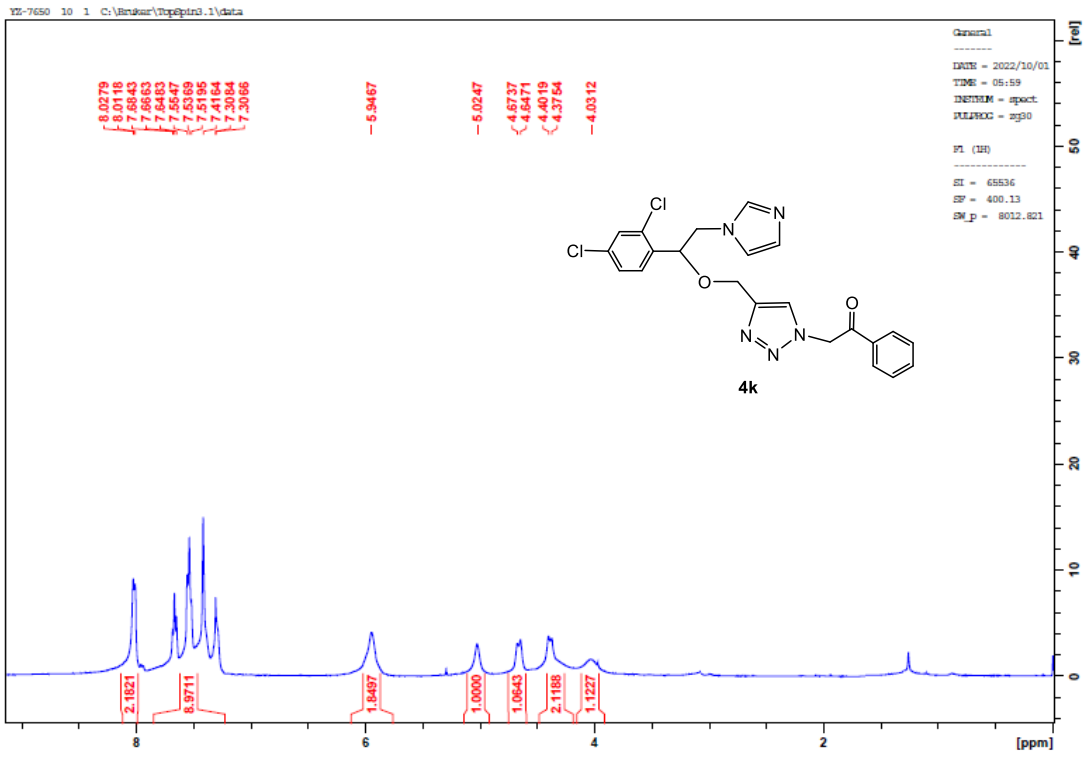

YZ-7647 11 1 C:\Bruker\TopSpin3.1\data
144.1162
137.9700
135.1168
133.8307
133.4025
129.7859
128.9790
128.5924
128.1178
123.6821
119.9953
77.4786
77.1608
77.0474
76.8434
63.0875
51.7743
51.4455
42.4584
General
DATE = 2022/10/01
TIME = 05:07
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
[rel]
[ppm]

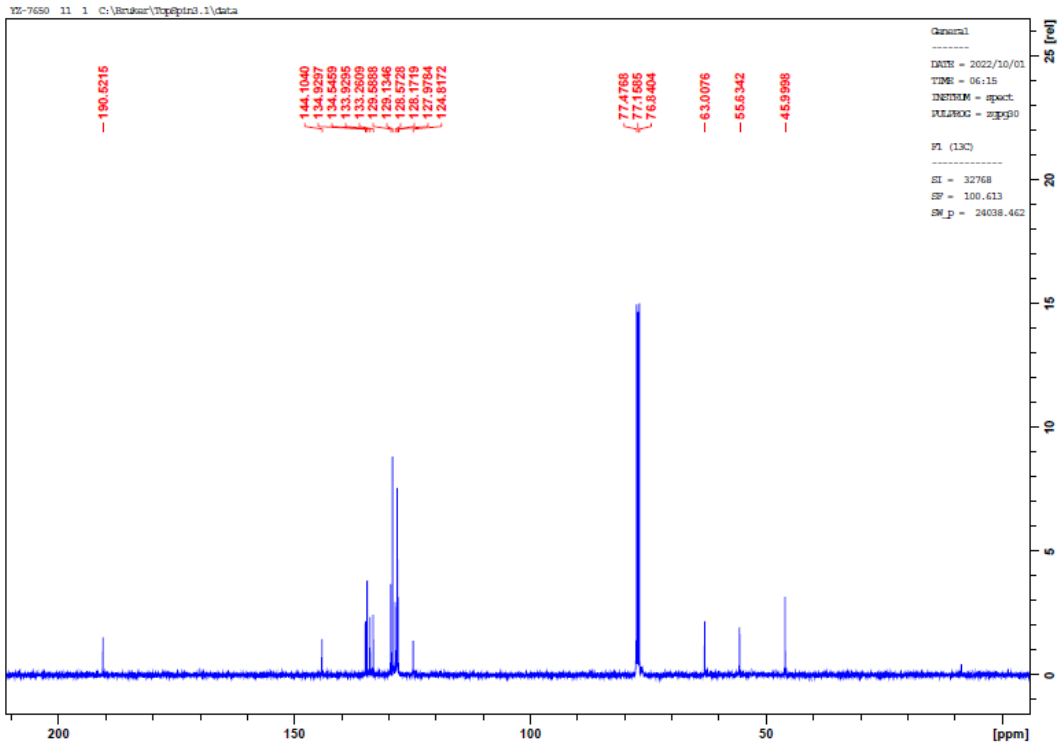

YZ-7648 10 1 C:\Bruker\TopSpin3.1\data
7.6705
7.4448
7.4147
7.3323
7.3125
7.2910
7.2864
6.9487
5.2100
5.2006
5.1849
5.1729
5.0241
5.0057
4.6933
4.6621
4.4171
4.3861
4.2950
4.2872
4.2772
4.2693
4.2606
4.2317
4.0604
4.0412
4.0261
4.0060
3.8221
Cl
Cl
N
N
O
N
N
N
O
O
CH3
4i
General
DATE = 2022/10/01
TIME = 05:12
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
1.0957
4.1661
1.2542
1.9298
0.9802
1.0000
1.2426
1.9185
1.1694
2.8149
8
6
4
2
[ppm]
[rel]

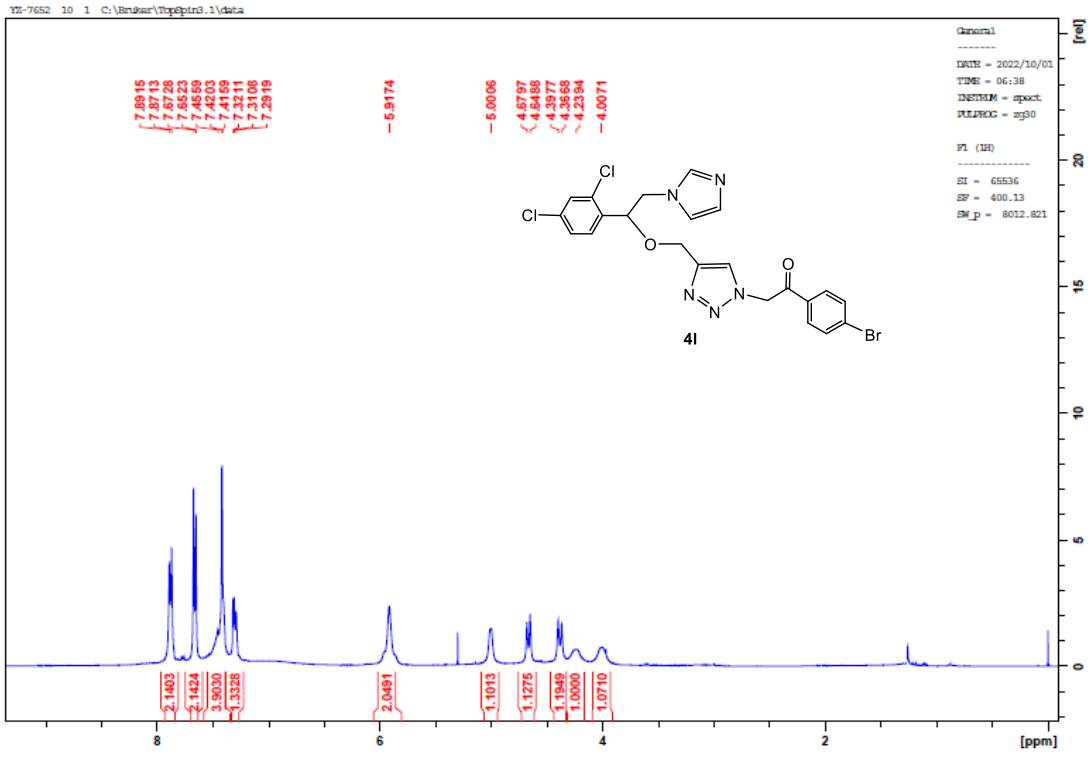

YZ-7648 11 1 C:\Bruker\TopSpin3.1\data
166.8946
144.2850
135.2038
133.5389
133.3674
129.7950
128.6236
128.1494
124.4496
77.4785
77.1605
76.8424
76.6551
63.0169
62.5456
53.1708
50.9293
50.7846
General
DATE = 2022/10/01
TIME = 05:28
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
200
150
100
50
0 [ppm]
[rel]

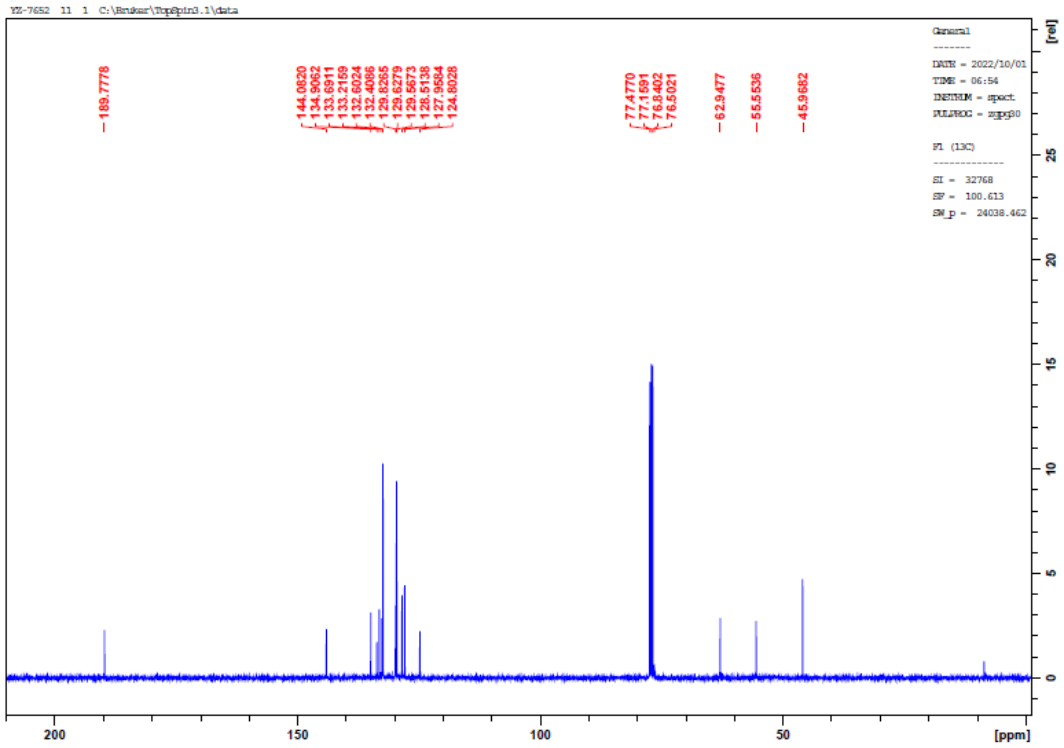

7.5074
7.4913
7.3967
7.3546
7.3315
7.2769
7.2171
5.5144
4.9966
4.5966
4.5722
4.3642
4.0501
9.8169
2.0449
1.0000
1.2301
1.7004
1.2381
8
6
4
2
[ppm]
[rel]
4j

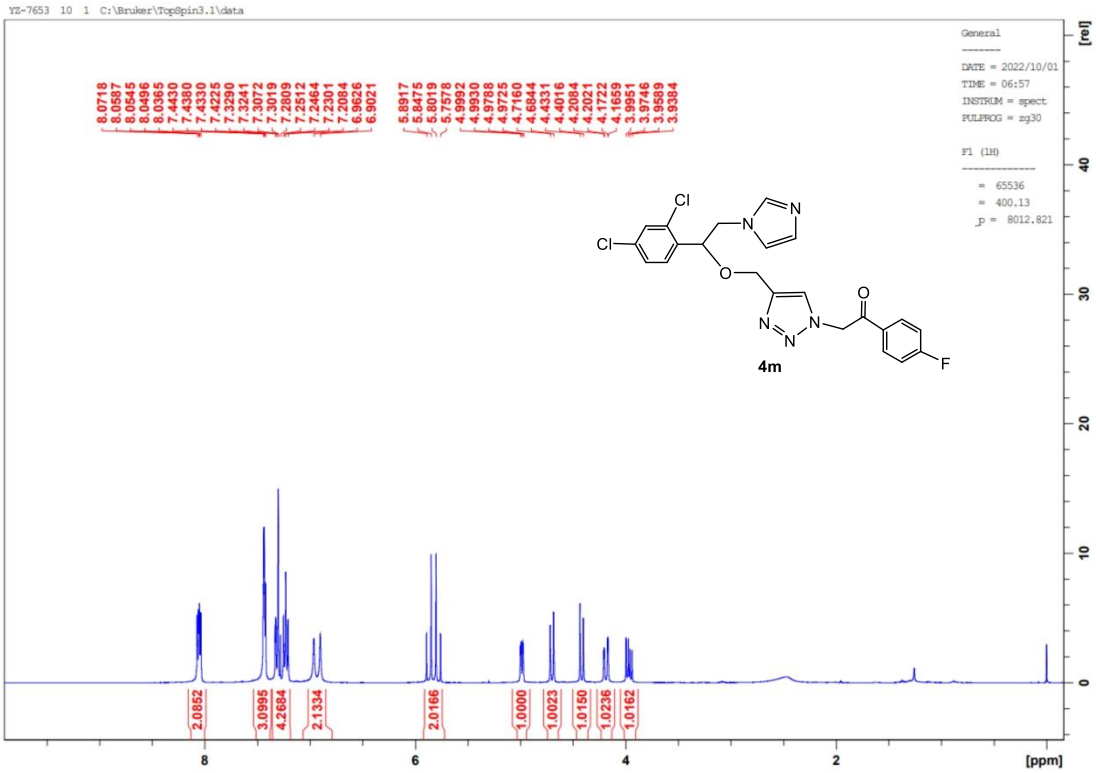

144.2806
134.8892
133.6813
133.1429
132.1141
129.8172
129.5134
128.4813
127.8880
122.7470
122.7092
77.4785
77.1567
76.8409
62.8949
53.2848
46.0339
200
150
100
50
[ppm]
[rel]

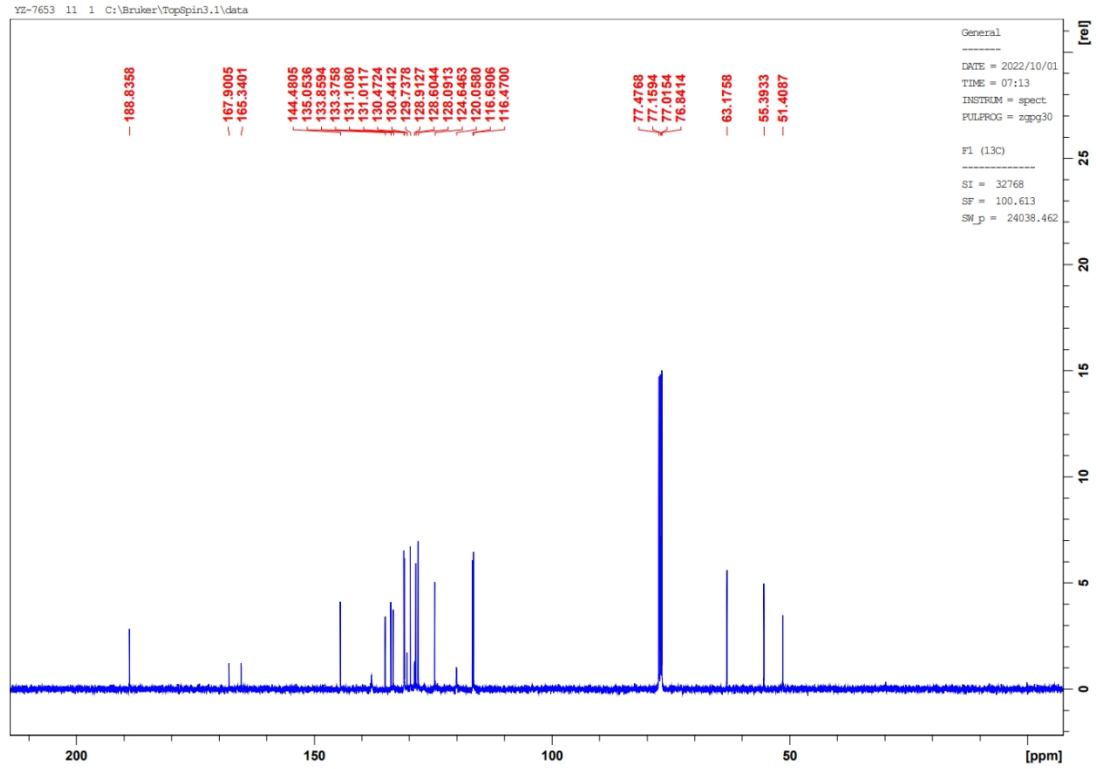

YZ-7650 10 1 C:\Bruker\TopSpin3.1\data
8.0279
8.0118
7.6843
7.6663
7.6483
7.5547
7.5369
7.5195
7.4164
7.3084
7.3066
5.9467
5.0247
4.6737
4.6471
4.4019
4.3754
4.0312
Cl
Cl
N
N
O
N
N
N
O
4k
General
DATE = 2022/10/01
TIME = 05:59
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
2.1821
8.9711
1.8497
1.0000
1.0643
2.1188
1.1227
8
6
4
2
[ppm]
[rel]

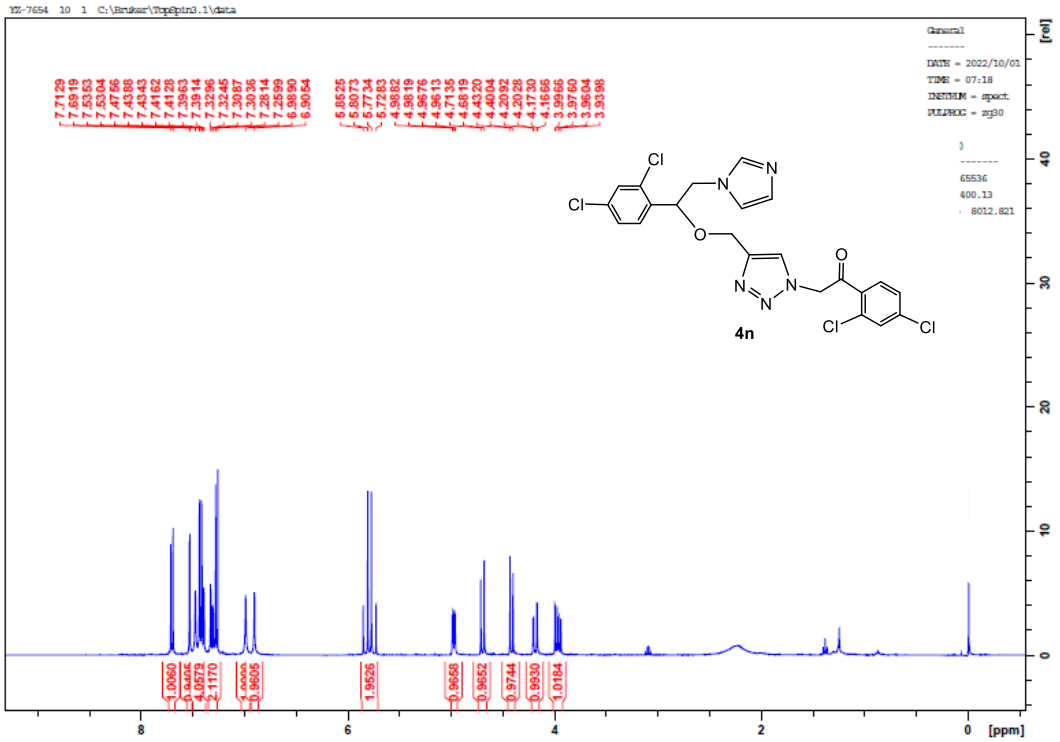

YZ-7650 11 1 C:\Bruker\TopSpin3.1\data
190.5215
144.1040
134.9297
134.5459
133.9295
133.2609
129.5888
129.1346
128.5728
128.1719
127.9784
124.8172
77.4768
77.1585
76.8404
63.0076
55.6342
45.9998
General
DATE = 2022/10/01
TIME = 06:15
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
200
150
100
50
[ppm]
[rel]

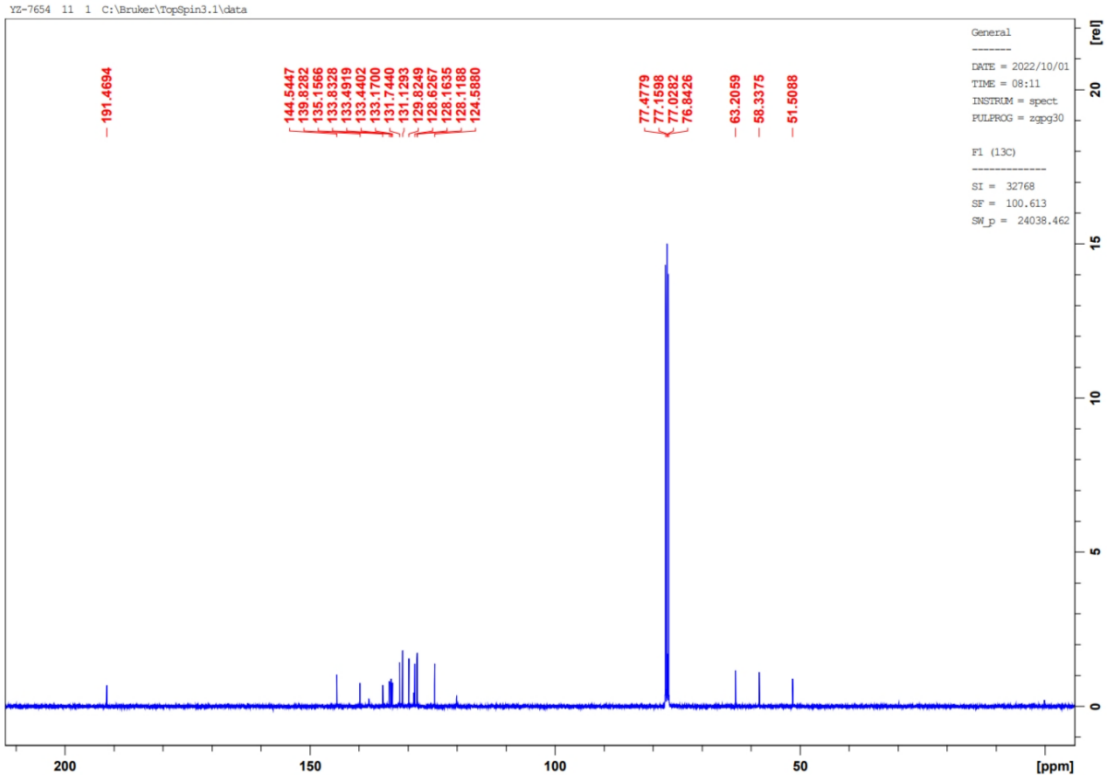

7.8915
7.8713
7.6728
7.6523
7.4659
7.4403
7.4169
7.3211
7.3108
7.2919
5.9174
5.0006
4.6797
4.6488
4.3977
4.3868
4.2394
4.0071
Cl
Cl
N
N
O
N
N
O
Br
4l
2.1403
2.1424
3.9030
1.3328
2.0491
1.1013
1.1275
1.1949
1.0000
1.0710
8
6
4
2
[ppm]
[rel]

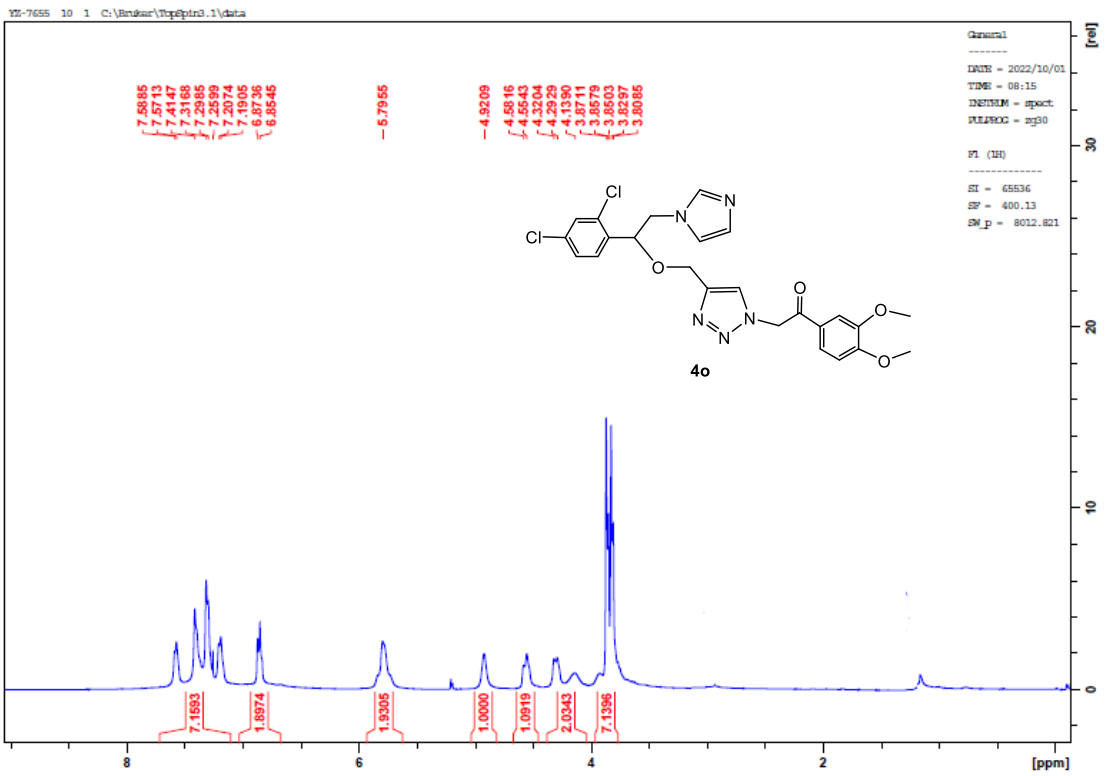

189.7778
144.0820
134.9062
133.6911
133.2169
132.6024
132.4086
129.6265
129.6279
129.5673
128.5138
127.9884
124.8028
77.4770
77.1591
76.8402
76.5021
62.9477
55.5536
45.9682
200
150
100
50
[ppm]
[rel]

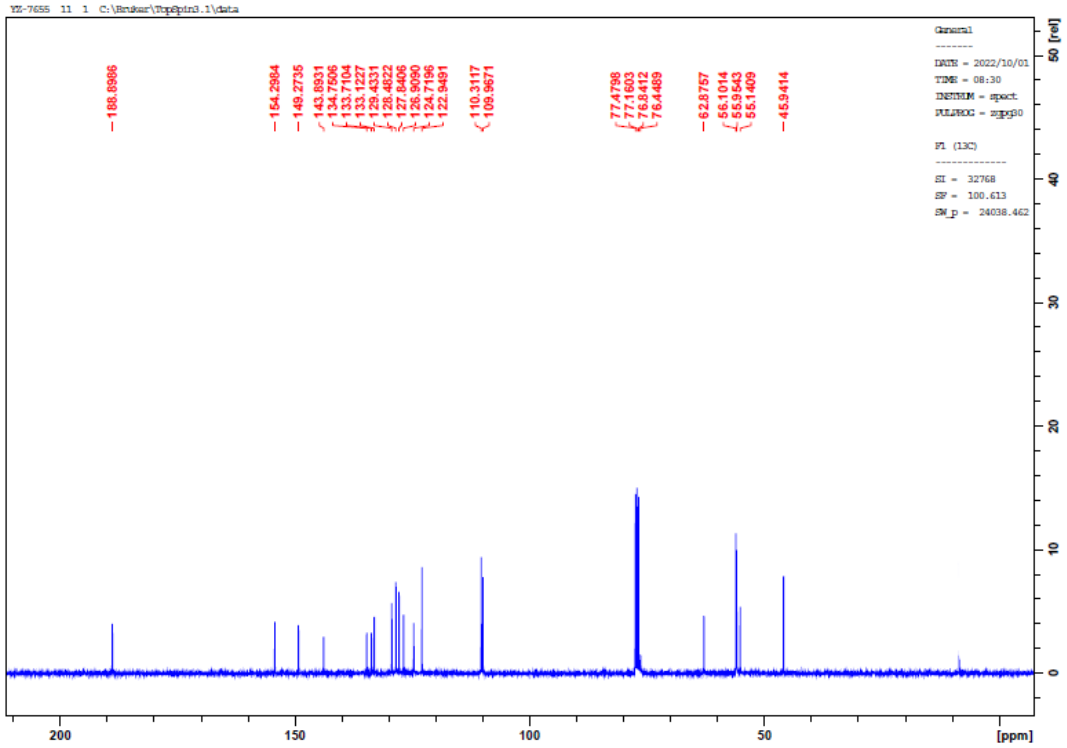

YZ-7653 10 1 C:\Bruker\TopSpin3.1\data
8.0718
8.0587
8.0545
8.0496
8.0365
7.4430
7.4380
7.4330
7.4225
7.3290
7.3241
7.3072
7.3019
7.2809
7.2512
7.2464
7.2301
7.2084
6.9626
6.9021
5.8917
5.8475
5.8019
5.7578
4.9992
4.9930
4.9788
4.9725
4.7160
4.6844
4.4331
4.4016
4.2084
4.2021
4.1722
4.1659
3.9951
3.9746
3.9589
3.9384
Cl
Cl
N
N
O
N
N
N
O
F
4m
General
DATE = 2022/10/01
TIME = 06:57
INSTRUM = spect
PULPROG = zg30
F1 (1H)
= 65536
= 400.13
p = 8012.821
2.0852
3.0995
4.2684
2.1334
2.0166
1.0000
1.0023
1.0150
1.0236
1.0162
8
6
4
2
[ppm]
[rel]

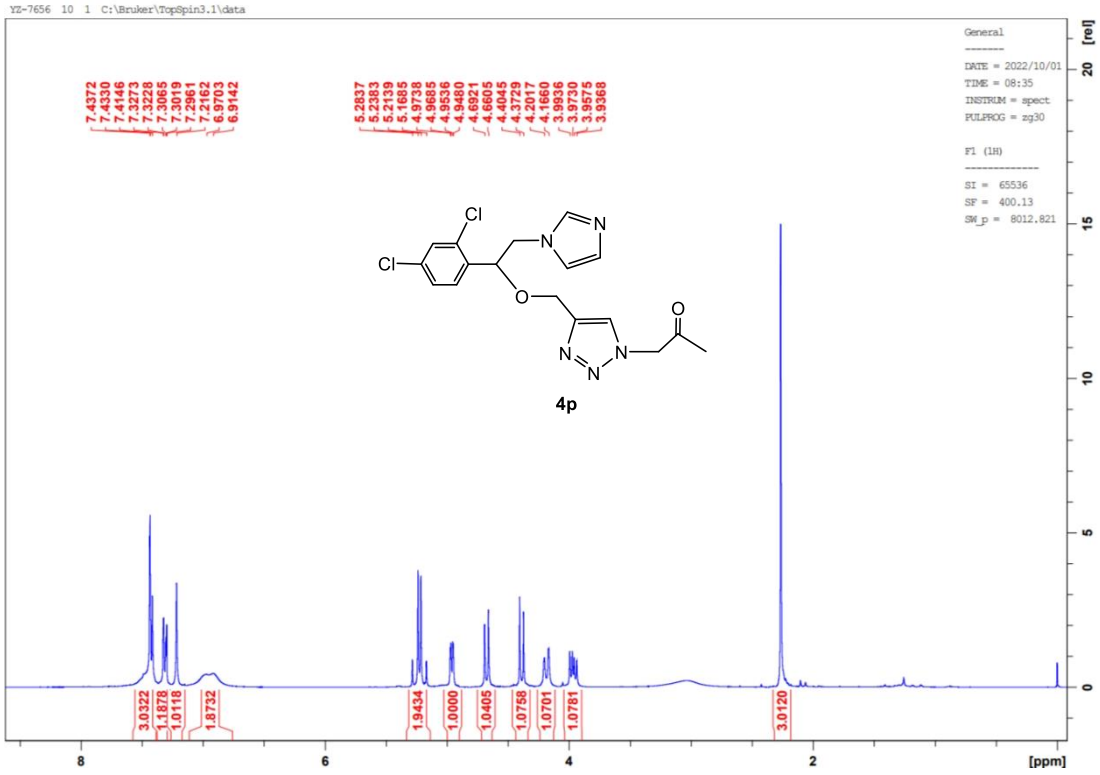

YZ-7653 11 1 C:\Bruker\TopSpin3.1\data
188.8358
167.9005
165.3401
144.4805
135.0536
133.8594
133.3758
131.1080
131.0117
130.4724
130.4412
128.7378
128.5127
128.0044
128.0013
124.6463
120.0580
116.6906
116.4700
77.4768
77.1594
77.0154
76.8414
63.1758
55.3933
51.4087
General
DATE = 2022/10/01
TIME = 07:13
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
200
150
100
50
[ppm]
[rel]

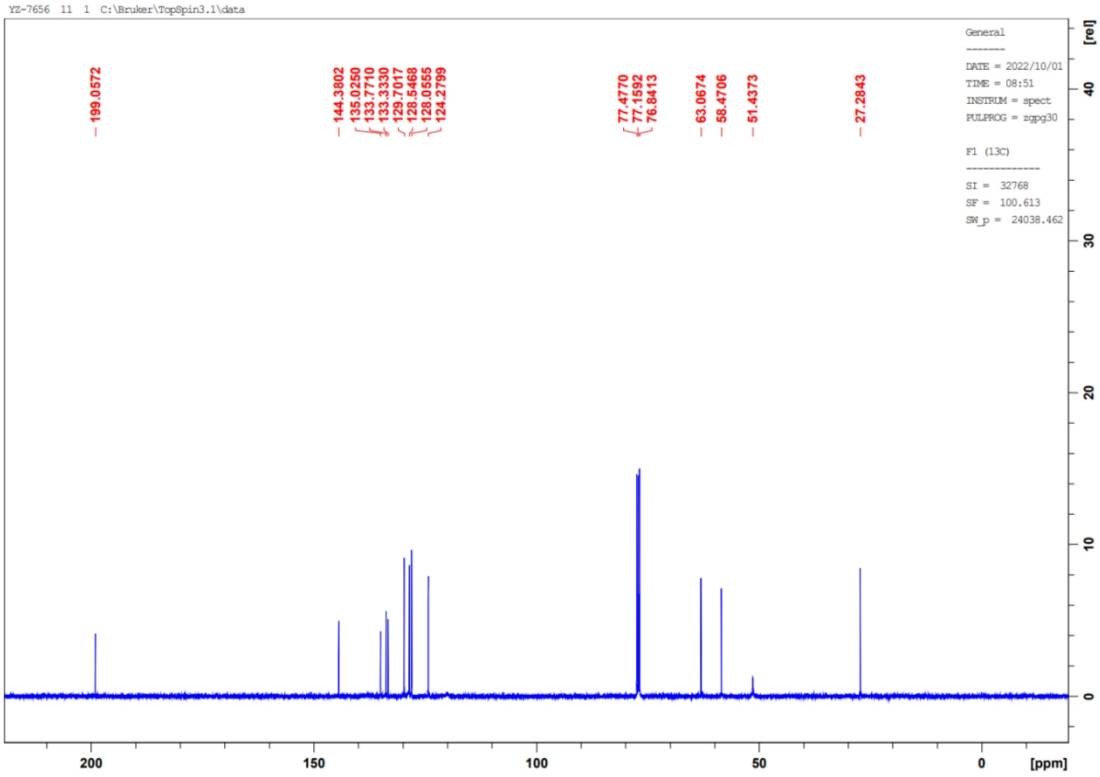

YZ-7654 10 1 C:\Bruker\TopSpin3.1\data
7.7129
7.6919
7.5353
7.5304
7.4756
7.4388
7.4343
7.4162
7.4128
7.3963
7.3914
7.3296
7.3245
7.3087
7.3036
7.2814
7.2599
6.9890
6.9054
5.8525
5.8073
5.7734
5.7283
4.9682
4.9619
4.9576
4.9613
4.7135
4.6819
4.4320
4.4004
4.2092
4.2028
4.1730
4.1666
3.9966
3.9760
3.9604
3.9398
General
DATE = 2022/10/01
TIME = 07:18
INSTRUM = spect
PULPROG = zg30
65536
400.13
8012.821
Cl
Cl
N
N
O
N
N
N
O
Cl
Cl
4n
1.0060
0.9605
4.0579
2.1170
1.9526
0.9658
0.9652
0.9744
0.9930
1.0164
8
6
4
2
0
[ppm]
[rel]

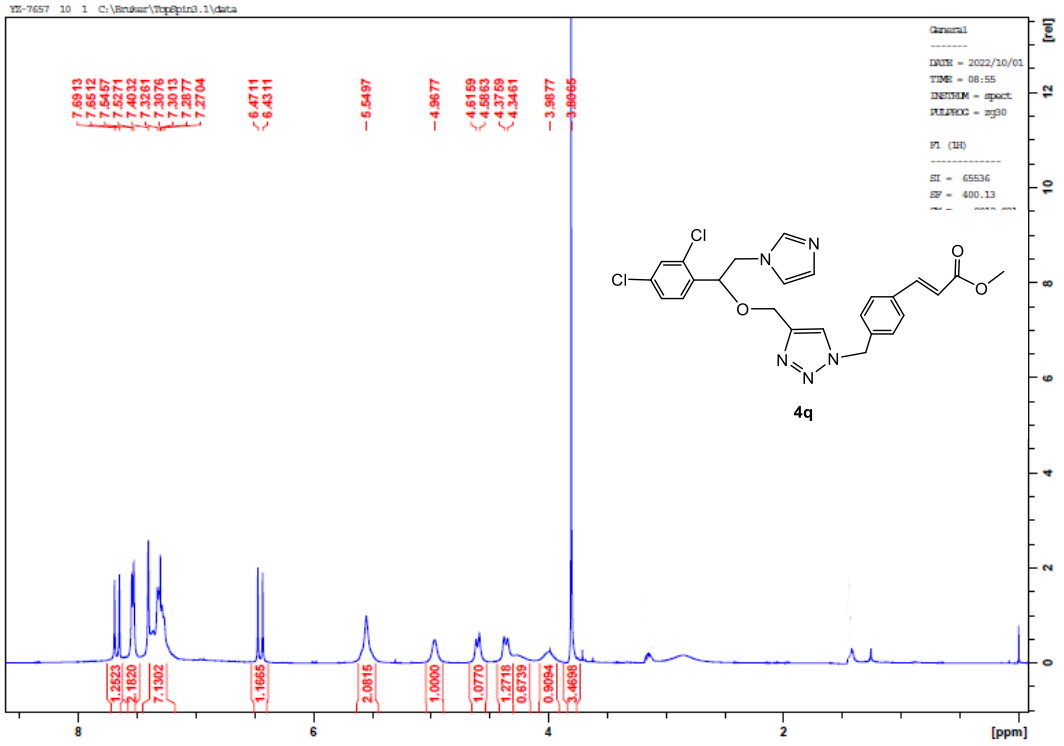

YZ-7654 11 1 C:\Bruker\TopSpin3.1\data
191.4694
144.5447
139.8282
135.1566
133.8328
133.4919
133.4402
133.1700
131.7440
131.1293
129.8249
128.6267
128.1635
128.1188
124.5880
77.4779
77.1598
77.0282
76.8426
63.2059
58.3375
51.5088
General
DATE = 2022/10/01
TIME = 08:11
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
200
150
100
50
[ppm]
[rel]

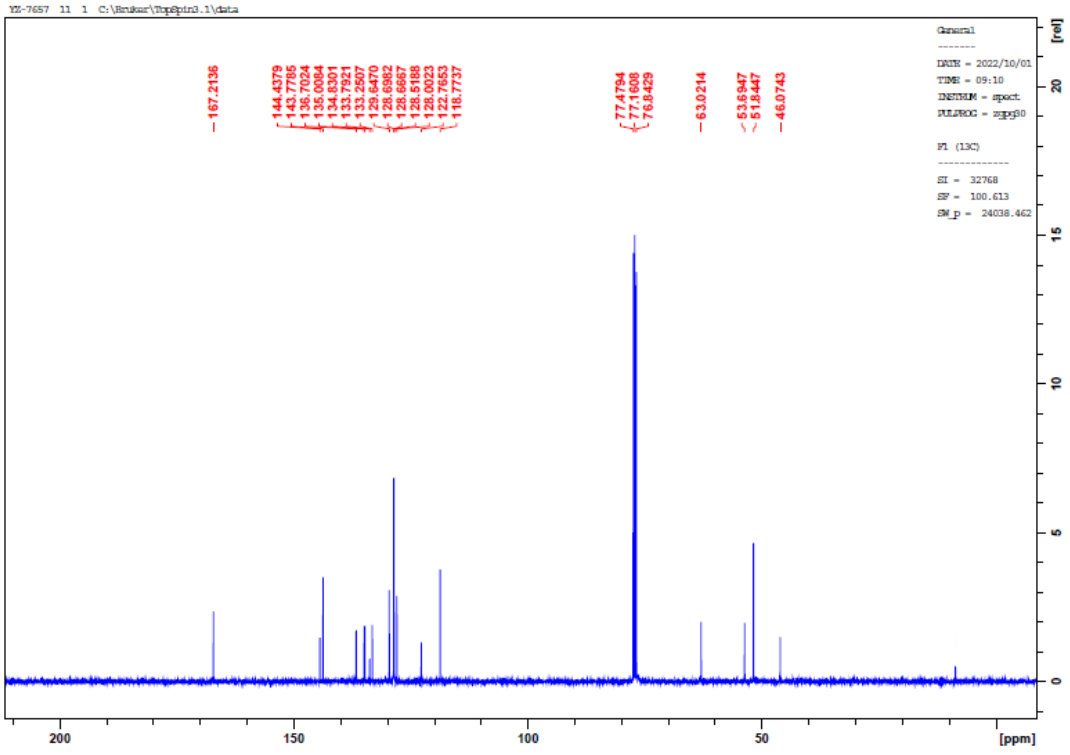

YZ-7655 10 1 C:\Bruker\TopSpin3.1\data
7.5885
7.5713
7.4147
7.3168
7.2985
7.2599
7.2074
7.1905
6.8736
6.8545
5.7955
4.9209
4.5816
4.5543
4.3204
4.2929
4.1390
3.8711
3.8579
3.8503
3.8297
3.8085
7.1683
1.8974
1.9305
1.0000
1.0919
2.0343
7.1396
8
6
4
2
[ppm]
[rel]
Cl
Cl
N
N
O
N
N
N
O
O
O
4o

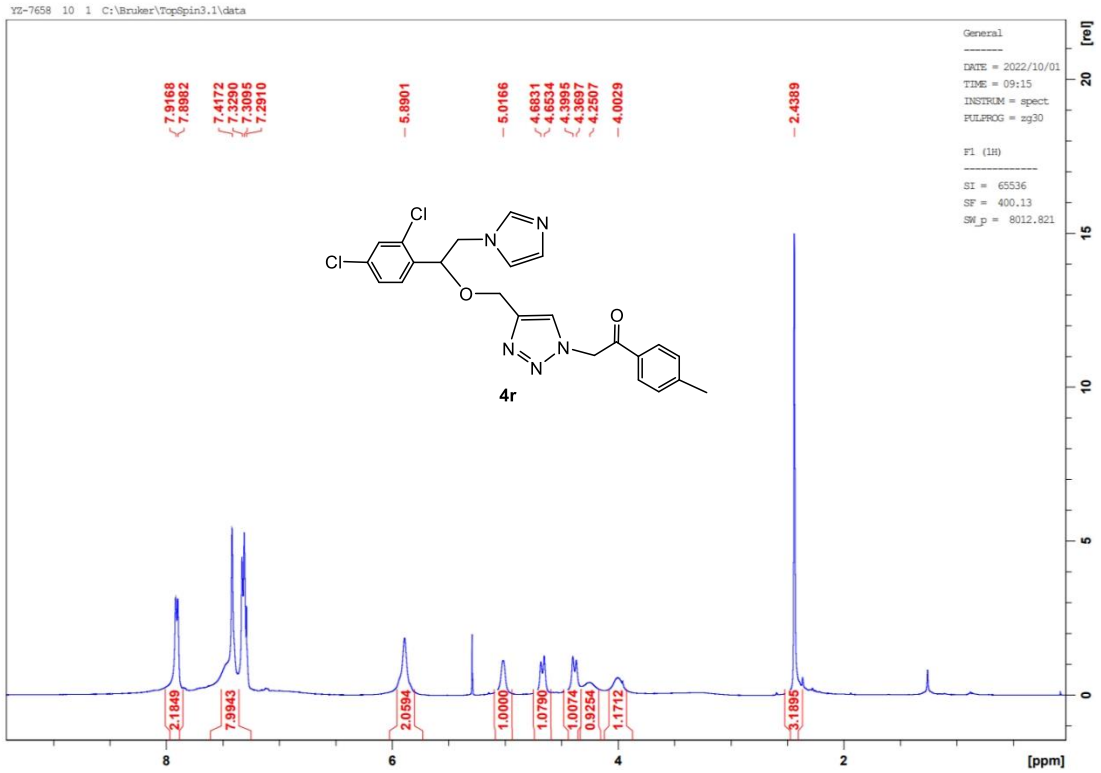

YZ-7655 11 1 C:\Bruker\TopSpin3.1\data
188.8986
154.2984
149.2735
143.8831
134.7606
133.7104
133.1227
129.4331
128.4822
127.8406
125.9096
124.7196
122.9491
110.3117
109.9671
77.4798
77.1603
76.8412
76.4489
62.8757
56.1014
55.9543
55.1409
45.9414
200
150
100
50
[ppm]
[rel]

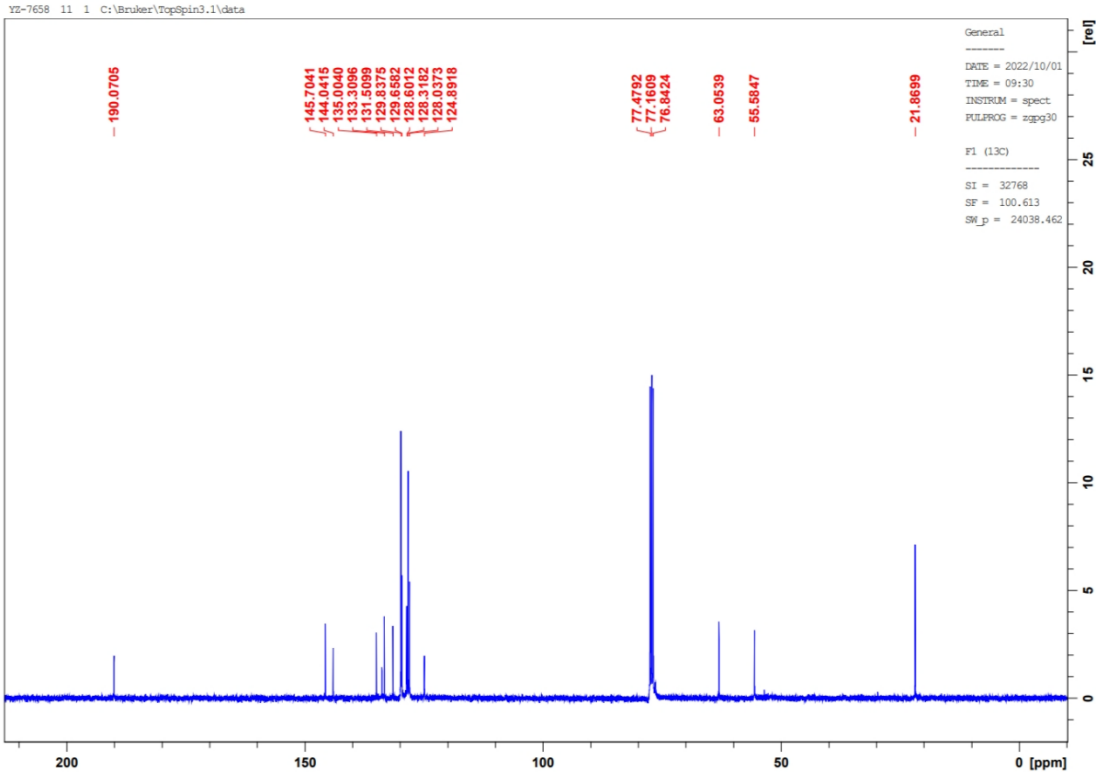

YZ-7656 10 1 C:\Bruker\TopSpin3.1\data
7.4372
7.4330
7.4146
7.3273
7.3228
7.3065
7.3019
7.2961
7.2162
6.9703
6.9142
5.2837
5.2383
5.2139
5.1685
4.9738
4.9685
4.9536
4.9480
4.6921
4.6605
4.4045
4.3729
4.2017
4.1660
3.9936
3.9730
3.9575
3.9368
General
DATE = 2022/10/01
TIME = 08:35
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
Cl
Cl
N
N
O
N
N
N
O
4p
3.0322
1.1878
1.0118
1.8732
1.9434
1.0000
1.0405
1.0758
1.0701
1.0781
3.0120
8
6
4
2
[ppm]
[rel]

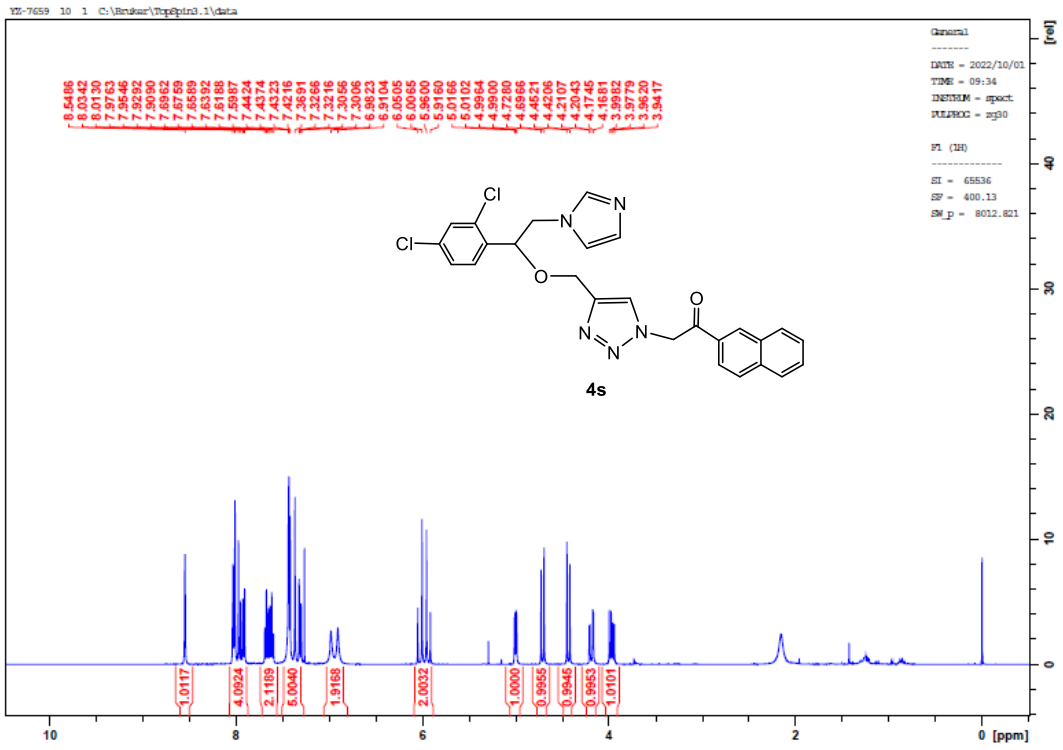

YZ-7656 11 1 C:\Bruker\TopSpin3.1\data
199.0572
144.3802
135.0250
133.7710
133.3330
129.7017
128.5468
128.0555
124.2799
77.4770
77.1592
76.8413
63.0674
58.4706
51.4373
27.2843
General
DATE = 2022/10/01
TIME = 08:51
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
200
150
100
50
0
[ppm]
[rel]

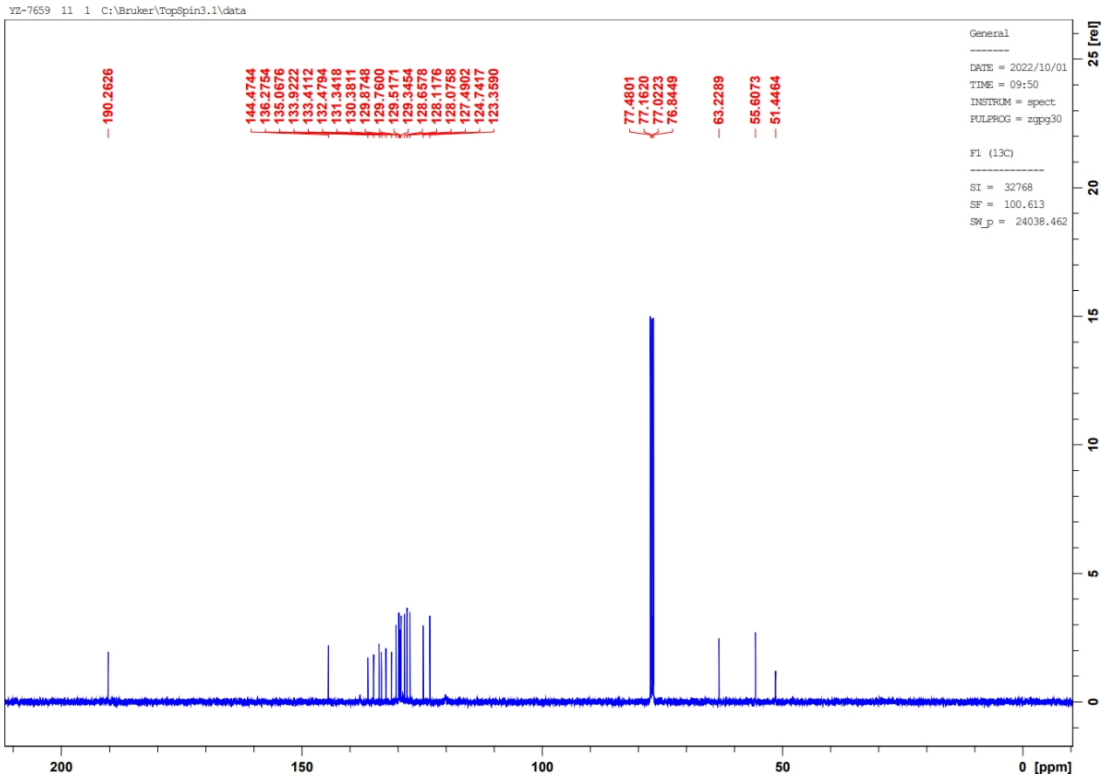

YZ-7657 10 1 C:\Bruker\TopSpin3.1\data
7.6913
7.6512
7.5457
7.5271
7.4032
7.3261
7.3076
7.3013
7.2877
7.2704
6.4711
6.4311
5.5497
4.9677
4.6159
4.5863
4.3759
4.3461
3.9877
3.8965
1.2523
2.1820
7.1302
1.1665
2.0815
1.0000
1.0770
1.2718
0.6739
0.5084
3.4698
8
6
4
2
[ppm]
[rel]
Cl
Cl
N
N
O
O
O
N
N
N
4q

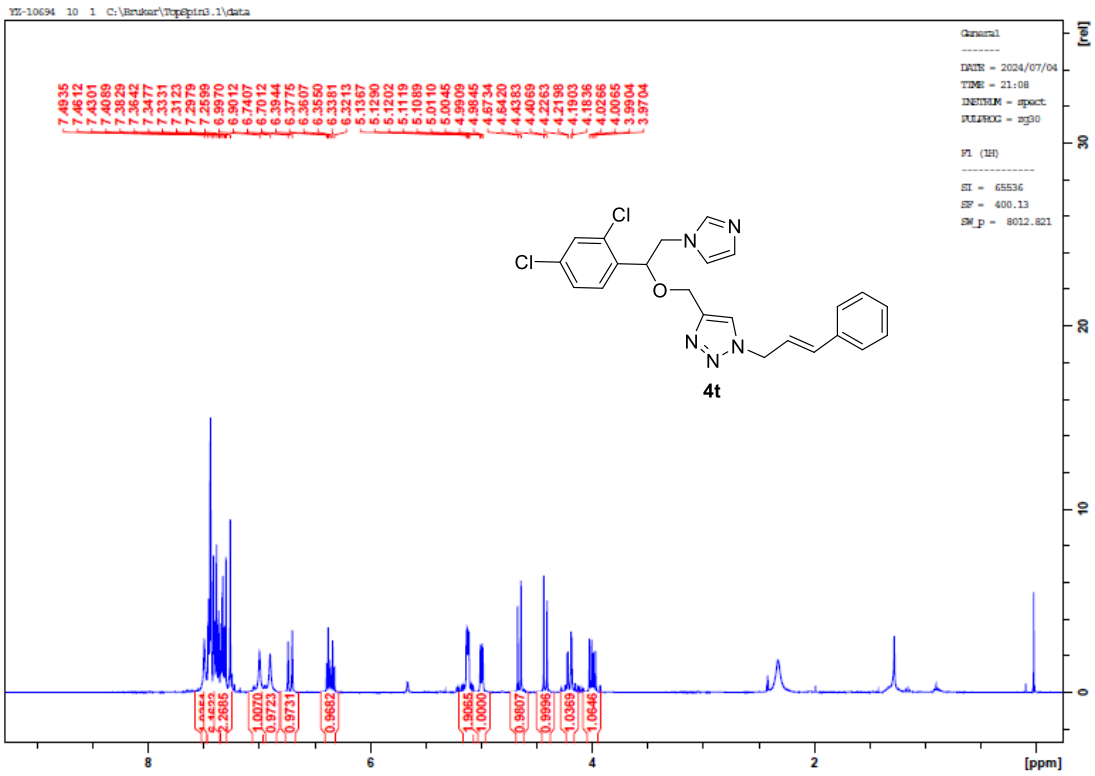

YZ-7657 11 1 C:\Bruker\TopSpin3.1\data
167.2136
144.4379
143.7785
136.7024
135.0084
134.8301
133.7921
133.2507
129.6470
128.6982
128.6667
128.5188
128.0023
122.7653
118.7737
77.4784
77.1608
76.8429
63.0214
53.6947
51.8447
46.0743
200
150
100
50
[ppm]
[rel]

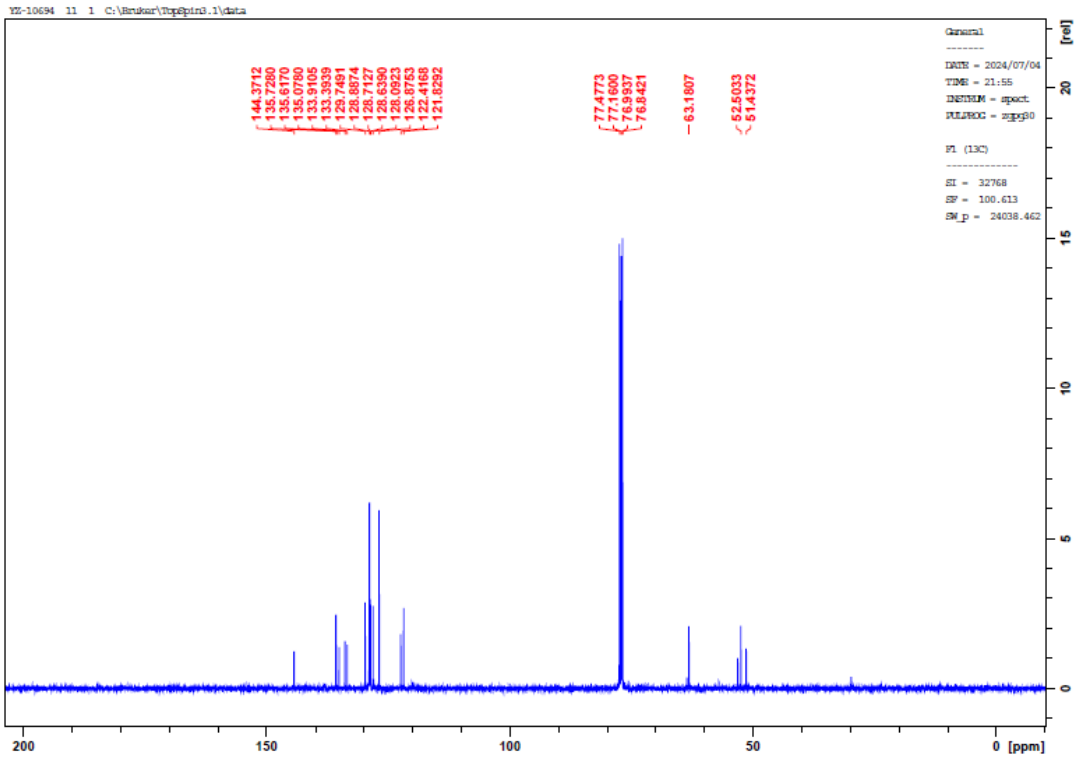

YZ-7658 10 1 C:\Bruker\TopSpin3.1\data
7.9168
7.8982
7.4172
7.3290
7.3095
7.2910
5.8901
5.0166
4.6831
4.6534
4.3995
4.3697
4.2507
4.0029
2.4389
Cl
Cl
N
N
O
N
N
N
O
4r
2.1849
7.9943
2.0594
1.0000
1.0790
1.0074
0.9254
1.1712
3.1895
8
6
4
2
[ppm]
General
DATE = 2022/10/01
TIME = 09:15
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
[rel]

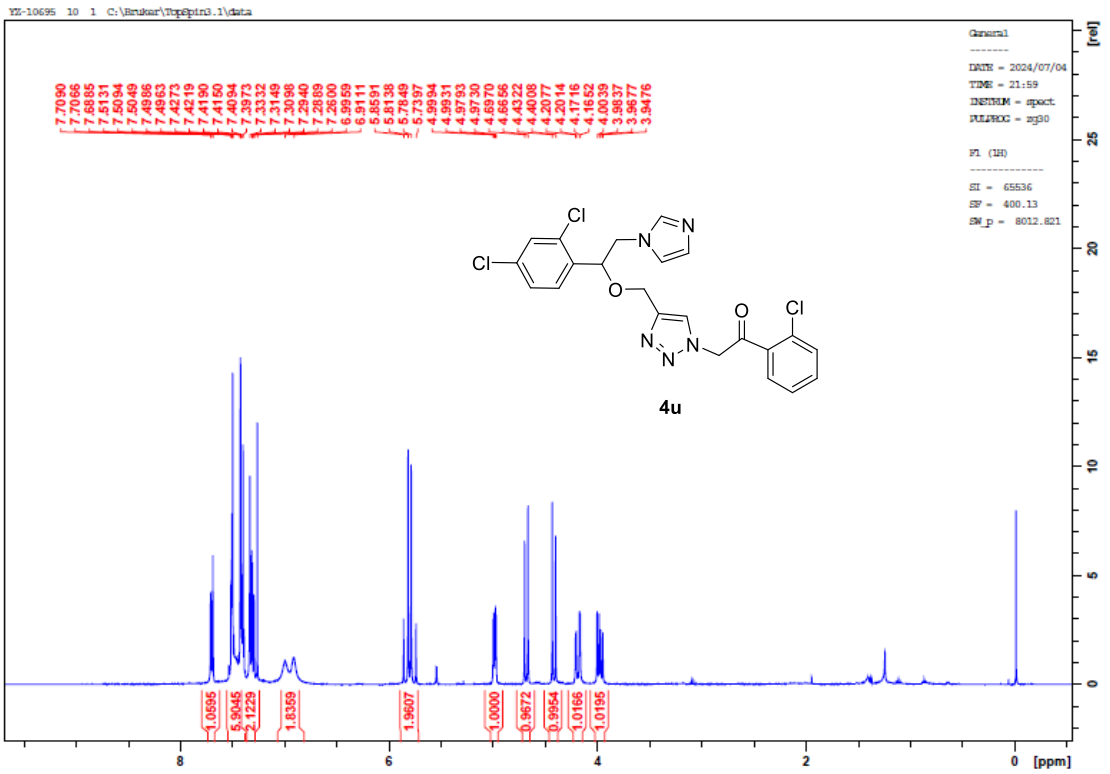

YZ-7658 11 1 C:\Bruker\TopSpin3.1\data
190.0705
145.7041
144.0415
135.0040
133.3096
131.5099
129.8375
129.6582
128.6012
128.3182
128.0373
124.8918
77.4792
77.1609
76.8424
63.0539
55.5847
21.8699
200
150
100
50
0 [ppm]
General
DATE = 2022/10/01
TIME = 09:30
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
[rel]

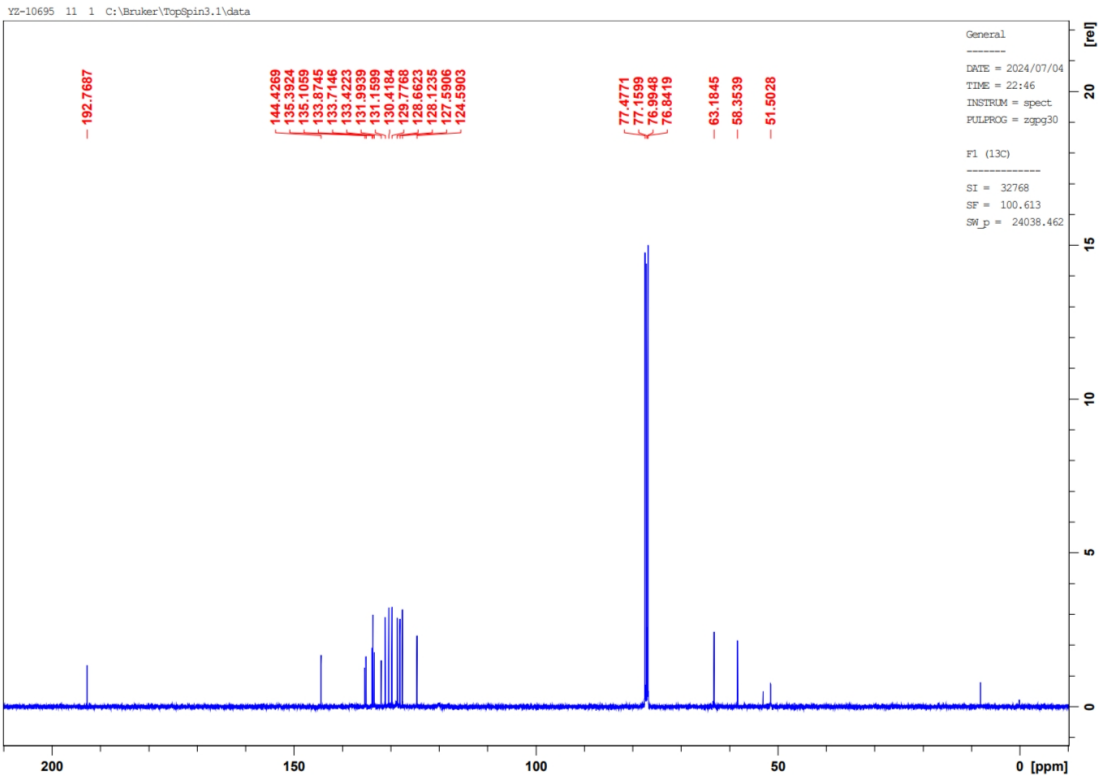

YZ-7659 10 1 C:\Bruker\TopSpin3.1\data
8.5486
8.0342
8.0130
7.9763
7.9546
7.9292
7.9096
7.6962
7.6759
7.6589
7.6392
7.6188
7.5987
7.4424
7.4374
7.4323
7.4216
7.3691
7.3266
7.3216
7.3056
7.3006
6.9823
6.9104
6.0505
6.0065
5.9600
5.9160
5.0166
5.0102
4.9964
4.9900
4.7280
4.6966
4.4621
4.4206
4.2107
4.2043
4.1745
4.1681
3.9982
3.9779
3.9620
3.9417
Cl
Cl
N
N
O
N
N
N
O
4s
1.0117
4.0924
2.1168
5.0040
1.9168
2.0032
1.0000
0.9955
0.9945
0.9953
1.0101
10
8
6
4
2
0 [ppm]
General
DATE = 2022/10/01
TIME = 09:34
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
[rel]

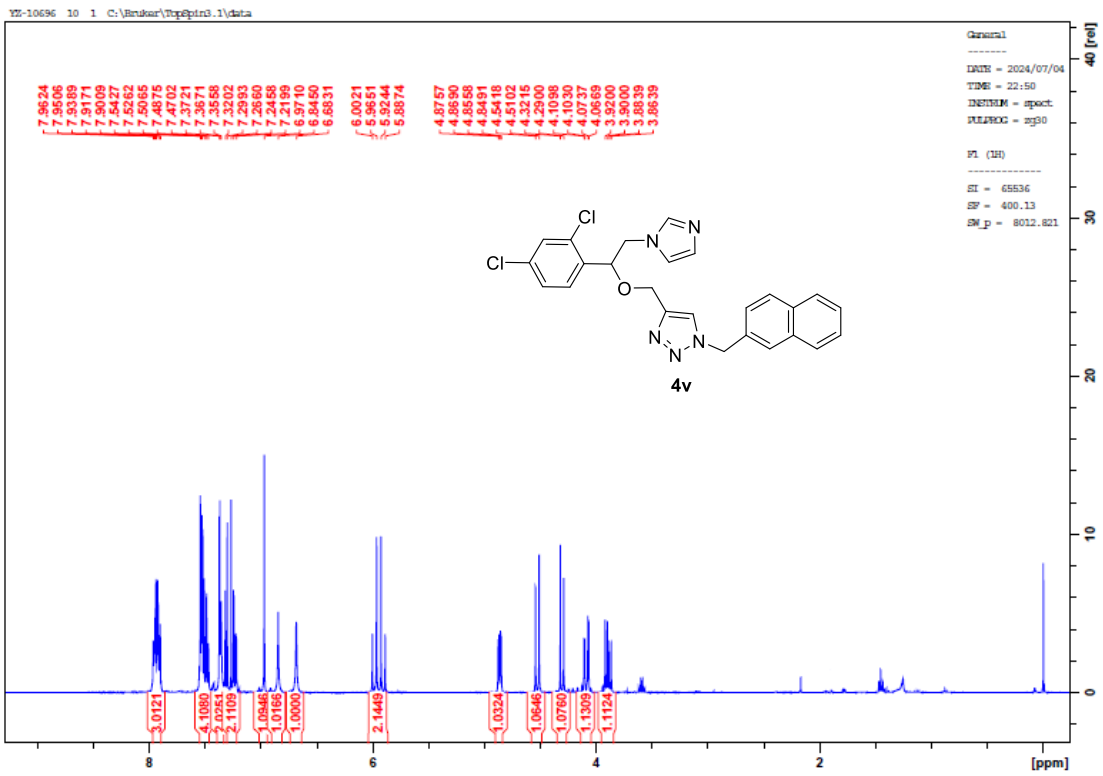

YZ-7659 11 1 C:\Bruker\TopSpin3.1\data
190.2626
144.4744
136.2754
135.0676
133.9222
133.4112
132.4794
131.3418
130.3811
129.8748
129.7600
129.5171
129.3454
128.6578
128.1176
128.0758
127.4902
124.7417
123.3590
77.4801
77.1620
77.0223
76.8449
63.2289
55.6073
51.4464
200
150
100
50
0 [ppm]
General
DATE = 2022/10/01
TIME = 09:50
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
25 [rel]

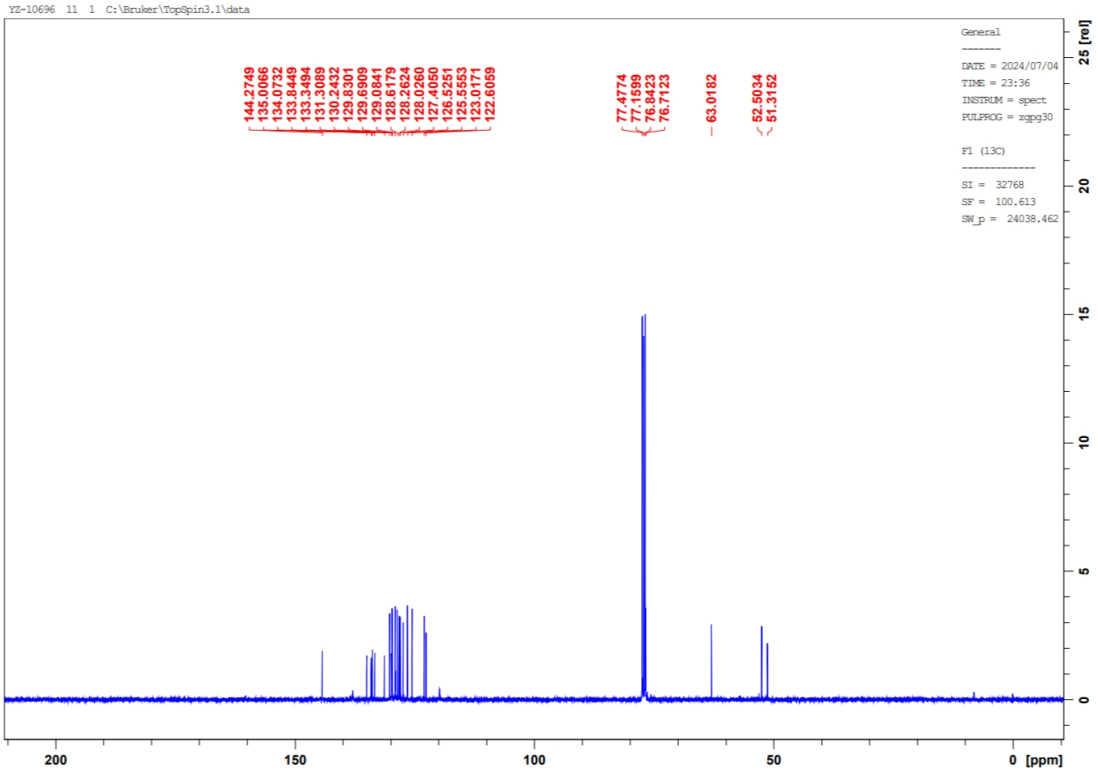

YZ-10694 10 1 C:\Bruker\TopSpin3.1\data
7.4935
7.4612
7.4301
7.4089
7.3829
7.3642
7.3477
7.3331
7.3123
7.2979
7.2599
6.9970
6.9012
6.7407
6.7012
6.3944
6.3775
6.3607
6.3550
6.3381
6.3213
5.1367
5.1290
5.1202
5.1119
5.1089
5.0110
5.0045
4.9909
4.9845
4.6734
4.6420
4.4383
4.4069
4.2263
4.2198
4.1903
4.1836
4.0266
4.0065
3.9904
3.9704
Cl
Cl
N
N
O
N
N
N
4t
General
DATE = 2024/07/04
TIME = 21:08
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
[rel]
30
20
10
0
8
6
4
2
[ppm]
1.0070
0.9723
0.9731
0.9682
1.9065
1.0000
0.9807
0.9996
1.0369
1.0646

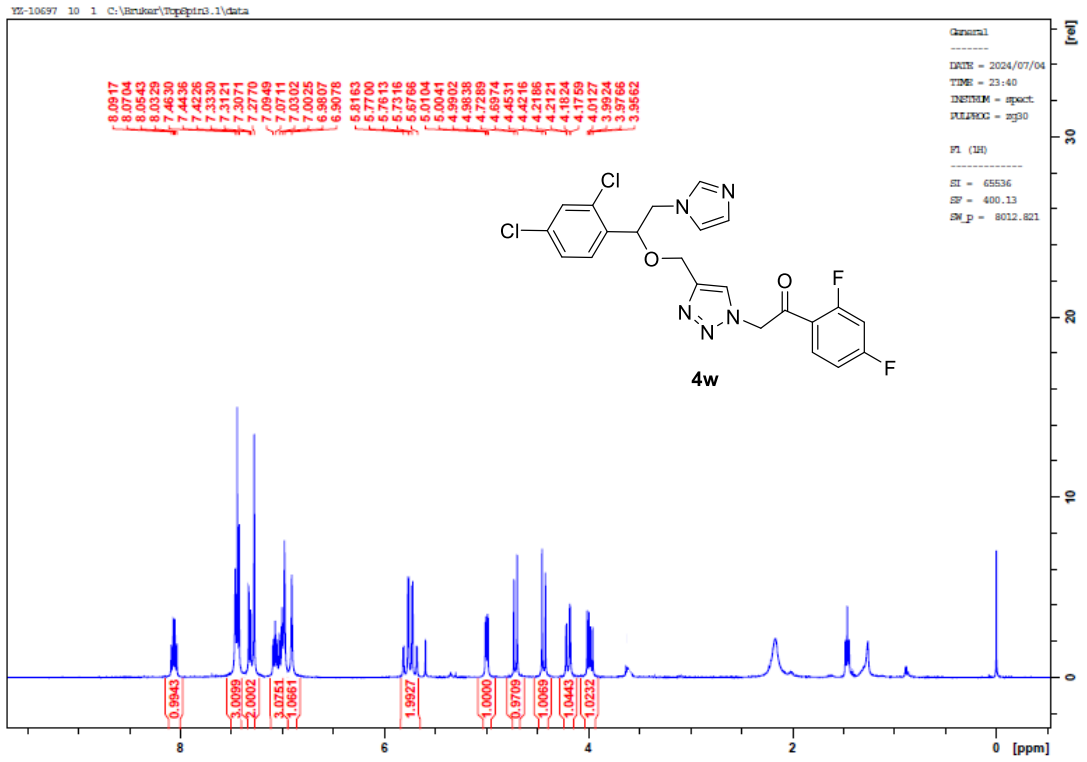

YZ-10694 11 1 C:\Bruker\TopSpin3.1\data
144.3712
135.7280
135.6170
135.0780
133.9105
133.3939
129.7491
128.8874
128.7127
128.6390
128.0923
126.8753
122.4168
121.8292
77.4773
77.1600
76.9937
76.8421
63.1807
52.5033
51.4372
General
DATE = 2024/07/04
TIME = 21:55
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
[rel]
20
15
10
5
0
200
150
100
50
0 [ppm]

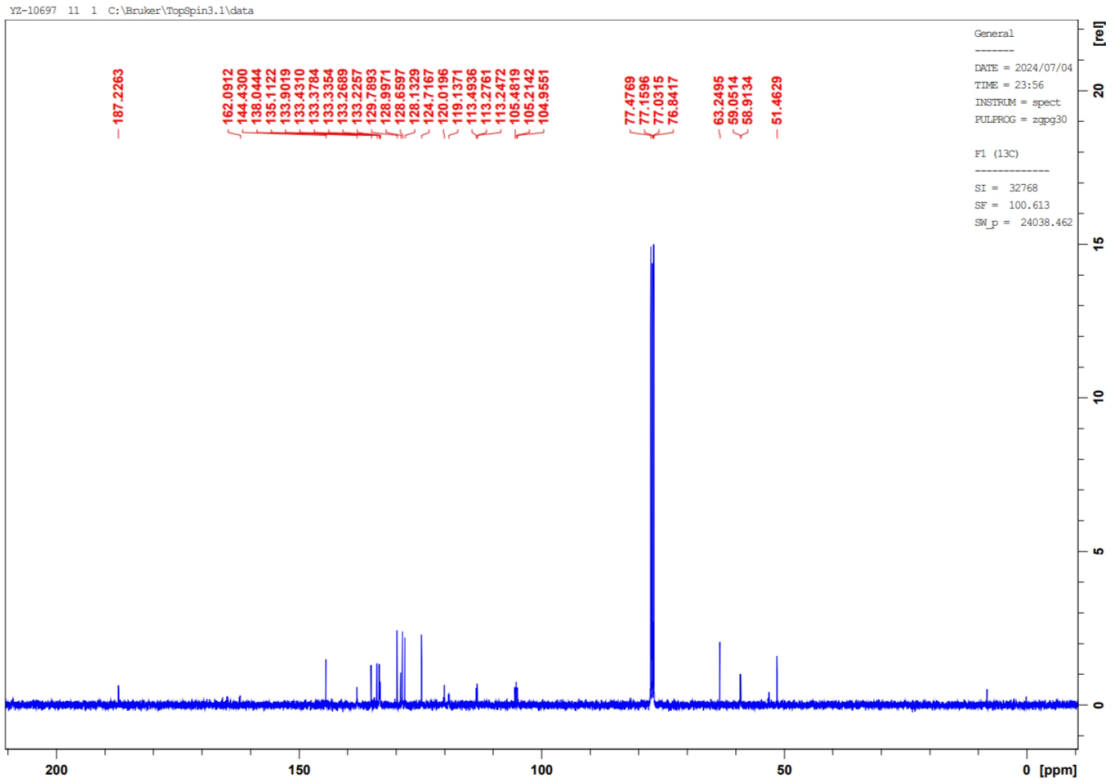

YZ-10695 10 1 C:\Bruker\TopSpin3.1\data
General
DATE = 2024/07/04
TIME = 21:59
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
[rel]
[ppm]
4u


YZ-10695 11 1 C:\Bruker\TopSpin3.1\data
General
DATE = 2024/07/04
TIME = 22:46
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
[rel]
[ppm]

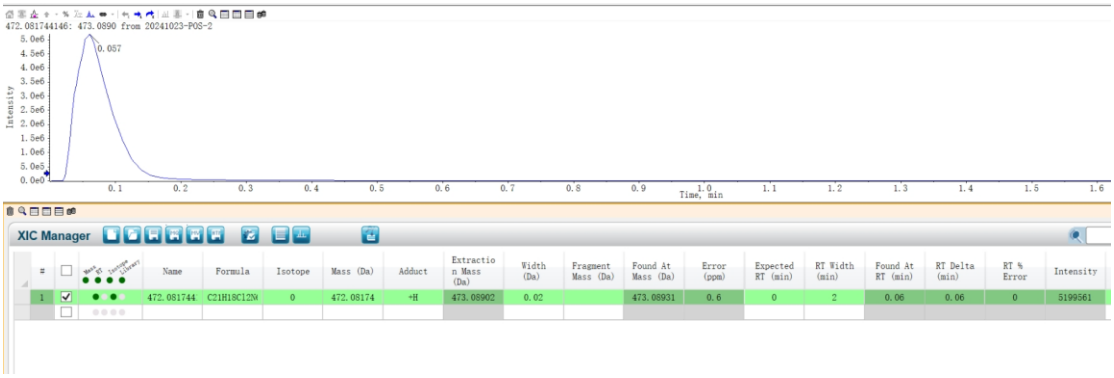

YZ-10696 10 1 C:\Bruker\TopSpin3.1\data
7.9624
7.9566
7.9389
7.9171
7.9009
7.5427
7.5262
7.5065
7.4875
7.4702
7.3721
7.3671
7.3558
7.3202
7.2993
7.2660
7.2468
7.2199
6.9710
6.8460
6.6831
6.0021
5.9651
5.9244
5.8874
4.8757
4.8690
4.8558
4.8491
4.5418
4.5102
4.3215
4.2900
4.1098
4.1030
4.0737
4.0669
3.9200
3.9000
3.8839
3.8639
Cl
Cl
N
N
O
N
N
N
4v
General
DATE = 2024/07/04
TIME = 22:50
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
3.0121
4.1080
2.0251
2.1109
1.0946
1.0166
1.0000
2.1449
1.0324
1.0646
1.0760
1.1309
1.1124
8
6
4
2
[ppm]
40 [rel]
30
20
10
0

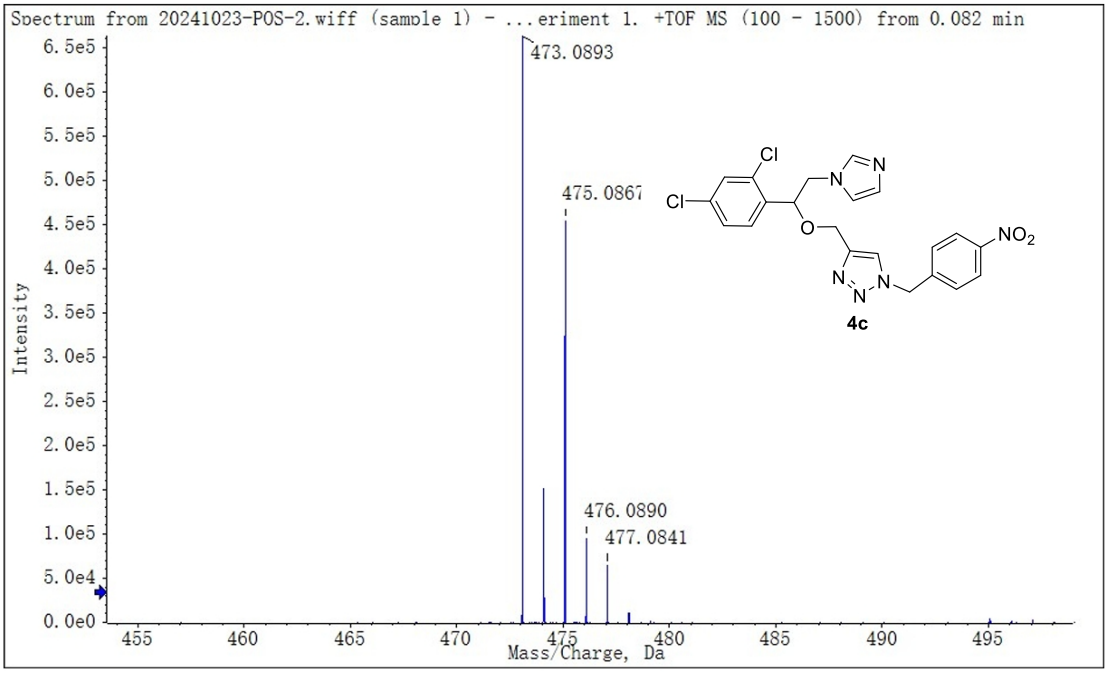

YZ-10696 11 1 C:\Bruker\TopSpin3.1\data
144.2749
135.0066
134.0732
133.8449
133.3494
131.3089
130.2432
129.8301
129.6909
129.0841
128.6179
128.2624
128.0260
127.4050
126.5251
125.5553
123.0171
122.6059
77.4774
77.1599
76.8423
76.7123
63.0182
52.5034
51.3152
General
DATE = 2024/07/04
TIME = 23:36
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
200
150
100
50
0 [ppm]
25 [rel]
20
15
10
5
0

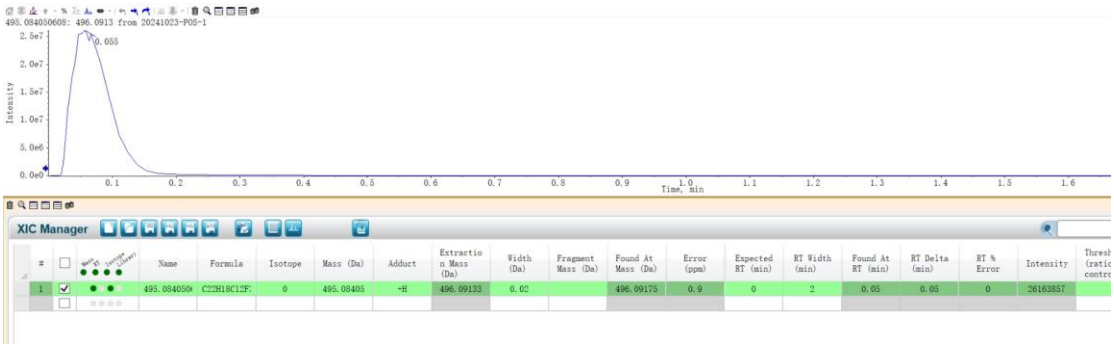

YZ-10697 10 1 C:\Bruker\TopSpin3.1\data
8.0917
8.0704
8.0543
8.0329
7.4630
7.4436
7.4226
7.3330
7.3121
7.3071
7.2770
7.0949
7.0711
7.0302
7.0025
6.9807
6.9078
5.8163
5.7700
5.7613
5.7316
5.6766
5.0104
5.0041
4.9902
4.9638
4.7269
4.6974
4.4531
4.4216
4.2166
4.2121
4.1824
4.1759
4.0127
3.9924
3.9766
3.9662
Cl
Cl
N
N
O
N
N
O
F
F
4w
0.9943
3.0099
2.0002
3.0751
1.0661
1.9927
1.0000
0.9709
1.0069
1.0443
1.0235
8
6
4
2
0
[ppm]
[rel]
General
DATE = 2024/07/04
TIME = 23:40
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821

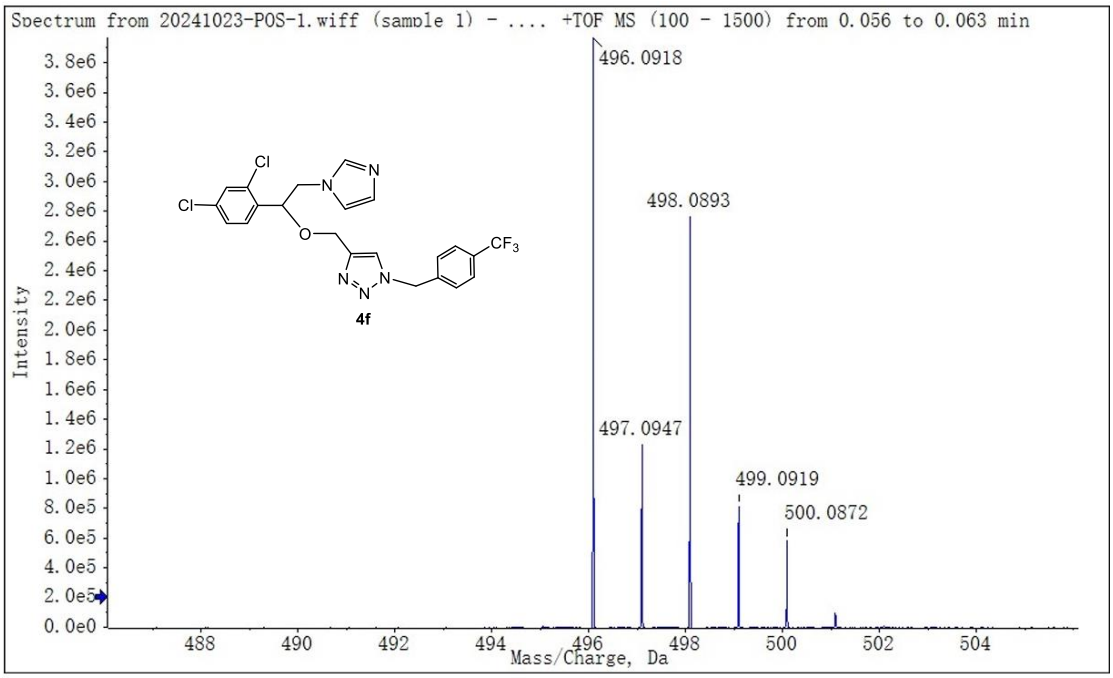

YZ-10697 11 1 C:\Bruker\TopSpin3.1\data
187.2263
162.0912
144.4300
138.0444
135.1122
133.9019
133.4310
133.3784
133.3354
133.2689
133.2257
129.7893
128.9971
128.6597
128.1329
124.7167
120.0196
119.1371
113.4936
113.2761
113.2472
105.4819
105.2142
104.9551
77.4769
77.1596
77.0315
76.8417
63.2495
59.0514
58.9134
51.4629
200
150
100
50
0
[ppm]
[rel]
General
DATE = 2024/07/04
TIME = 23:56
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462

3. HRMS spectra

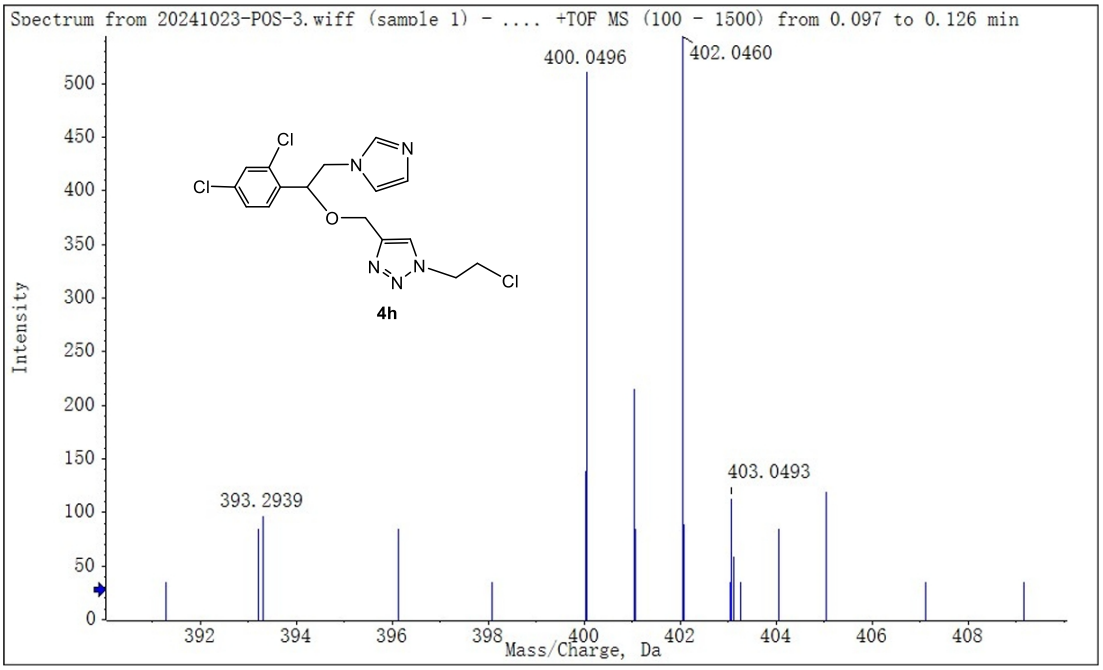




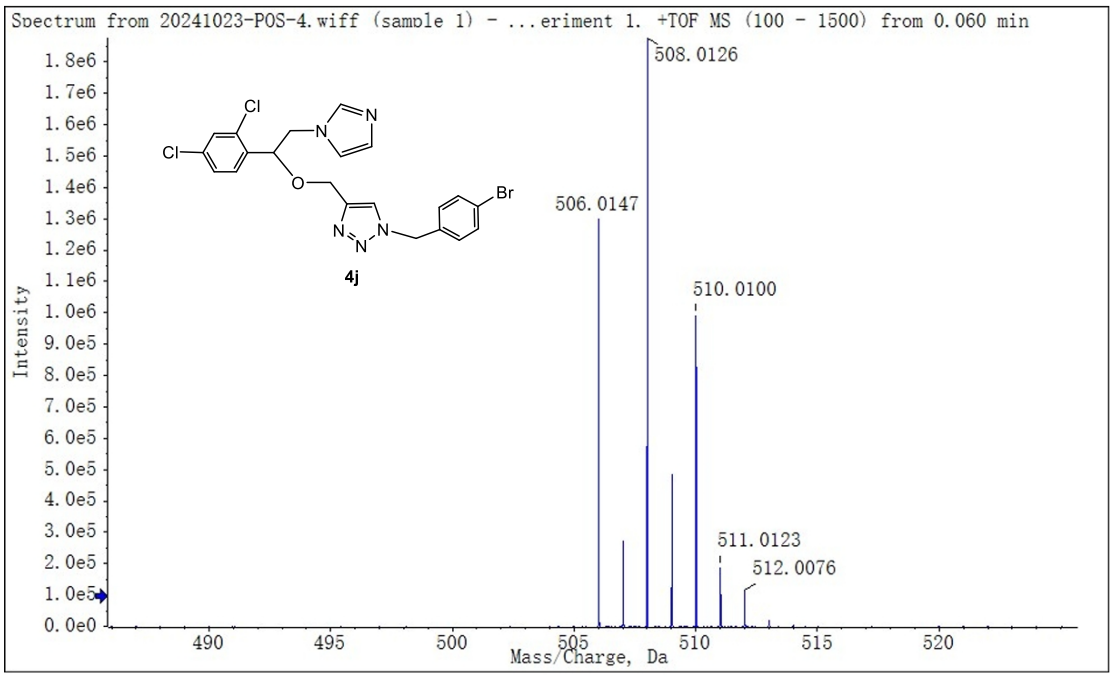

495.084050608: 496.0913 from 20241023-POS-1
0.055
Intensity
Time, min
XIC Manager
Name
Formula
Isotope
Mass (Da)
Adduct
Extraction Mass (Da)
Width (Da)
Fragment Mass (Da)
Found At Mass (Da)
Error (ppm)
Expected RT (min)
RT Width (min)
Found At RT (min)
RT Delta (min)
RT % Error
Intensity
495.084050
C22H18Cl2F
0
495.08405
+H
496.09133
0.02
496.09175
0.9
0
2
0.05
0.05
0
26163857


Spectrum from 20241023-POS-1.wiff (sample 1) - .... +TOF MS (100 - 1500) from 0.056 to 0.063 min
496.0918
498.0893
497.0947
499.0919
500.0872
Intensity
Mass/Charge, Da
4f

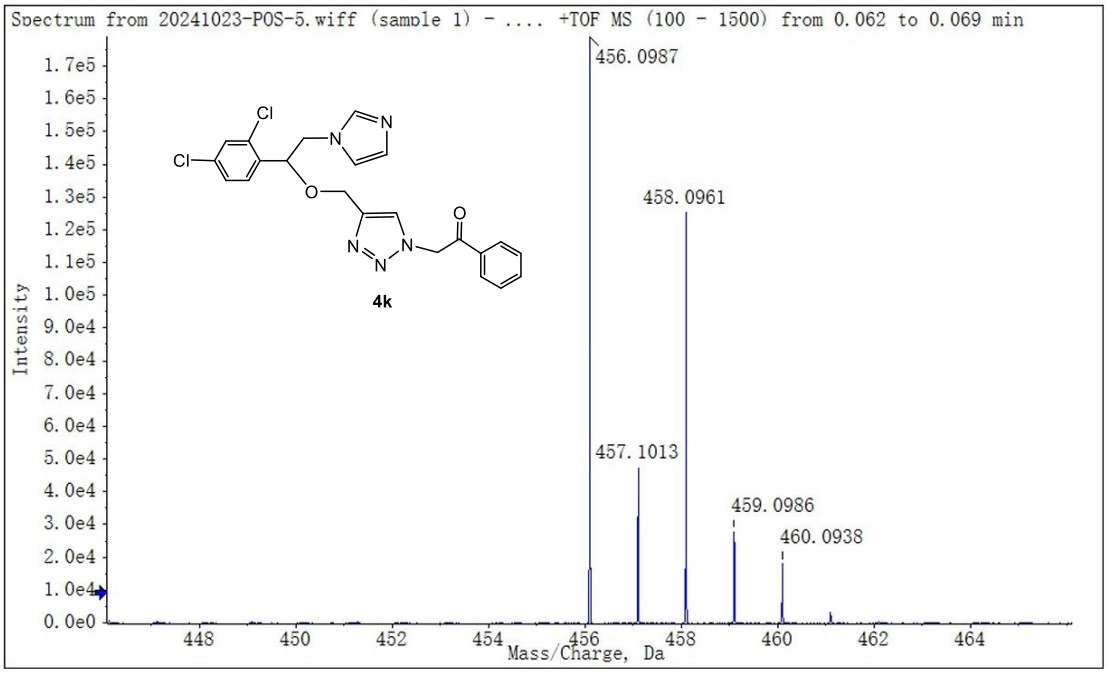

399.042043507: 400.0493 from 20241023-POS-3
0.061
Intensity
Time, min
XIC Manager
| Name | Formula | Isotope | Mass (Da) | Adduct | Extraction Mass (Da) | Width (Da) | Fragment Mass (Da) | Found At Mass (Da) | Error (ppm) | Expected RT (min) | RT Width (min) | Found At RT (min) | RT Delta (min) | RT % Error | Intensity
1 | 399.042043 | C16H16Cl3N | 0 | 399.04204 | +H | 400.04932 | 0.02 | | 400.0496 | 0.7 | 0 | 2 | 0.06 | 0.06 | 0 | 9143


Spectrum from 20241023-POS-3.wiff (sample 1) - .... +TOF MS (100 - 1500) from 0.097 to 0.126 min
400.0496
402.0460
403.0493
393.2939
Cl
Cl
N
N
O
N
N
Cl
4h
Intensity
Mass/Charge, Da

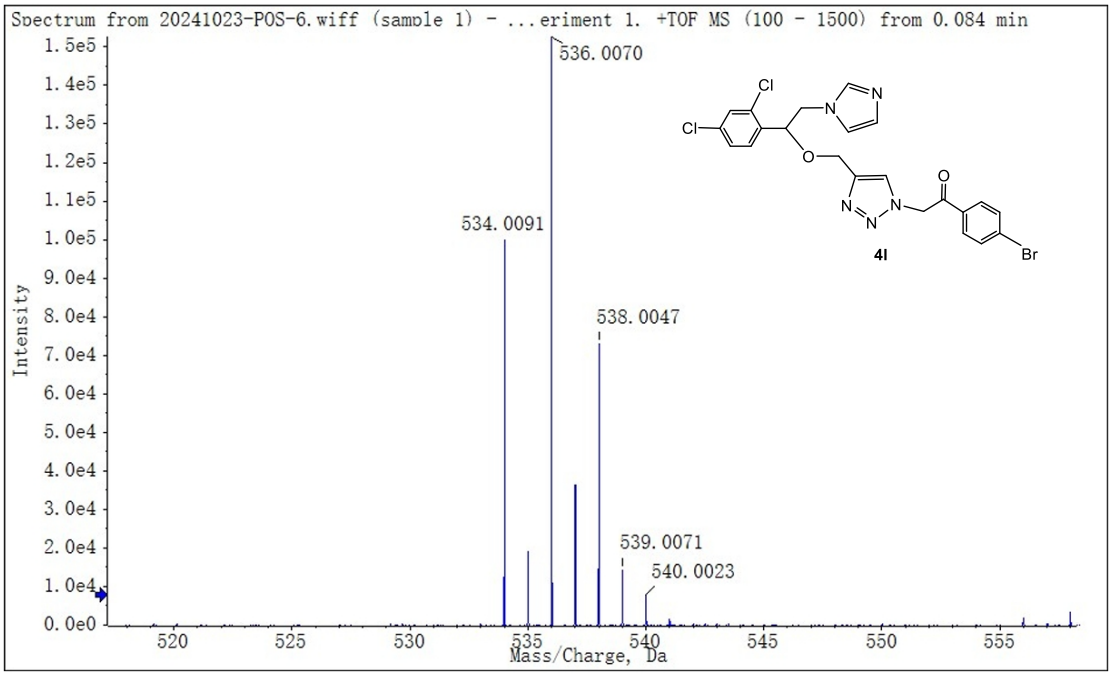

505.00717698: 508.0122 from 20241023-POS-4
0.057
Intensity
Time, min
XIC Manager
| Name | Formula | Isotope | Mass (Da) | Adduct | Extraction Mass (Da) | Width (Da) | Fragment Mass (Da) | Found At Mass (Da) | Error (ppm) | Expected RT (min) | RT Width (min) | Found At RT (min) | RT Delta (min) | RT % Error | Intensity
1 | 505.00717€ | C21H18BrCl | 3 | 507.00494 | +H | 508.01221 | 0.02 | | 508.01258 | 0.7 | 0 | 2 | 0.06 | 0.06 | 0 | 10605412

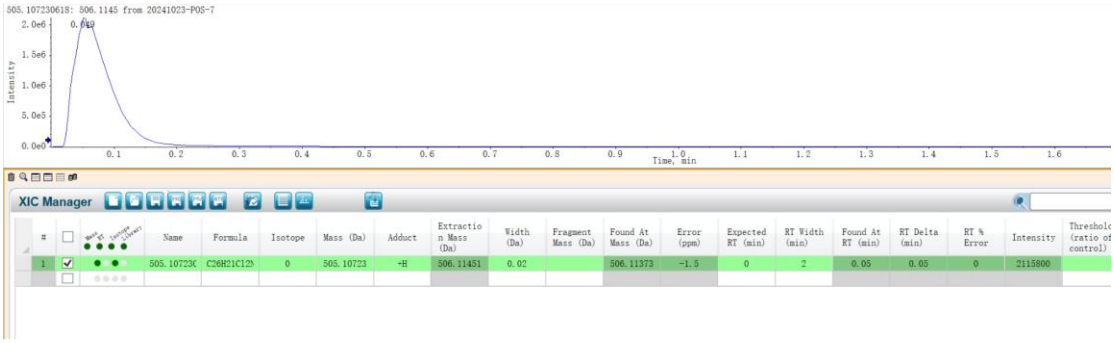

Spectrum from 20241023-POS-4.wiff (sample 1) - ...eriment 1. +TOF MS (100 - 1500) from 0.060 min
508.0126
506.0147
510.0100
511.0123
512.0076
Cl
Cl
N
N
O
N
N
N
Br
4j
Intensity
Mass/Charge, Da

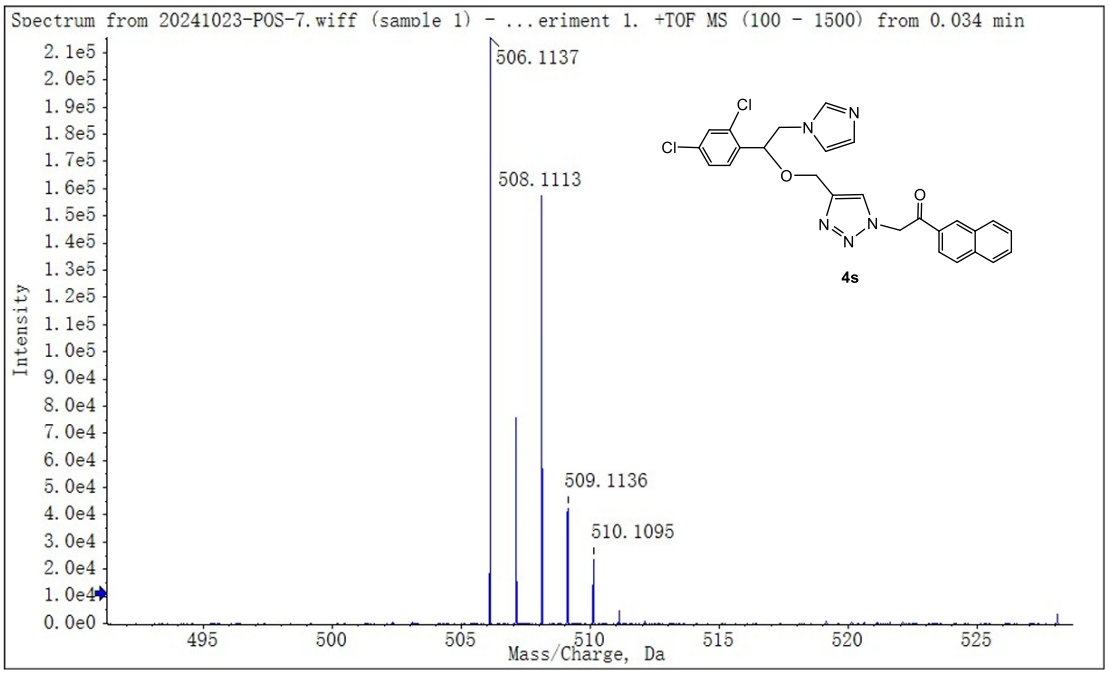

455.091580538: 456.0989 from 20241023-POS-5
0.067
Intensity
Time, min
XIC Manager
Name
Formula
Isotope
Mass (Da)
Adduct
Extraction Mass (Da)
Width (Da)
Fragment Mass (Da)
Found At Mass (Da)
Error (ppm)
Expected RT (min)
RT Width (min)
Found At RT (min)
RT Delta (min)
RT % Error
Intensity
455.09158
C22H19Cl2N
0
455.09158
-H
456.09886
0.02
456.0987
-0.3
0
2
0.07
0.07
0
994127


Spectrum from 20241023-POS-5.wiff (sample 1) - .... +TOF MS (100 - 1500) from 0.062 to 0.069 min
456.0987
458.0961
457.1013
459.0986
460.0938
Intensity
Mass/Charge, Da
Cl
Cl
N
N
O
N
N
O
4k

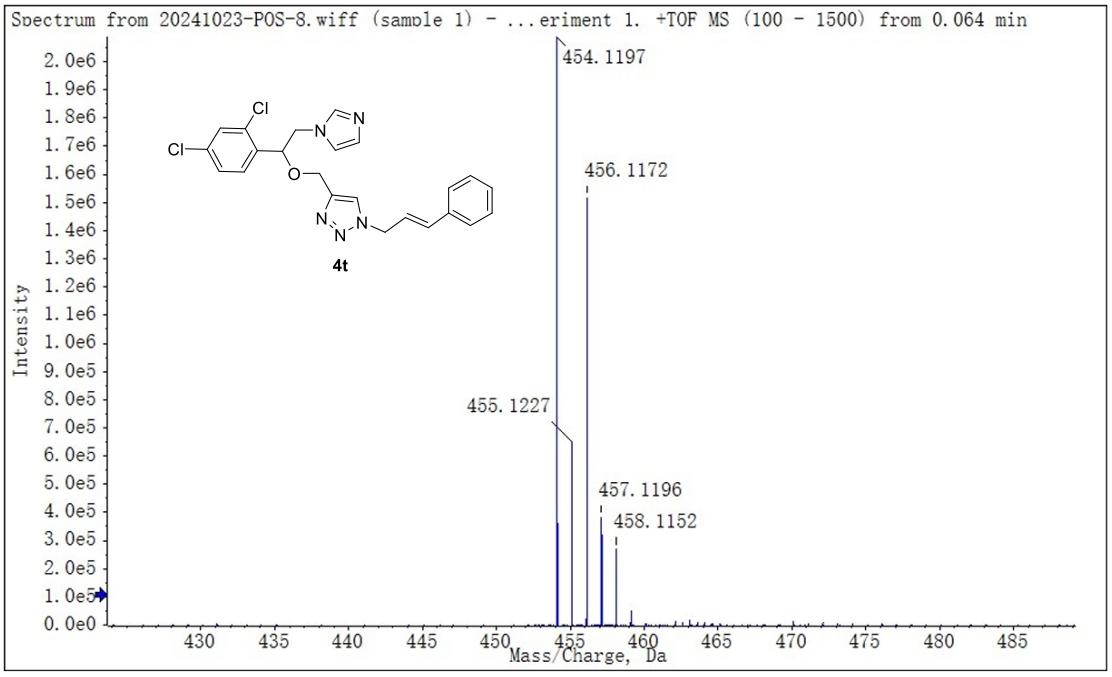

533.002091598: 536.0071 from 20241023-POS-6
Intensity
Time, min
XIC Manager
Name
Formula
Isotope
Mass (Da)
Adduct
Found At Mass (Da)
Error (ppm)
Expected RT (min)
RT Width (min)
Found At RT (min)
RT Delta (min)
RT % Error
Intensity
533.002091
C22H18BrCl
534.99987
+H
536.00715
536.00684
-0.6
911867


Spectrum from 20241023-POS-6.wiff (sample 1) - ...eriment 1. +TOF MS (100 - 1500) from 0.084 min
536.0070
534.0091
538.0047
539.0071
540.0023
Intensity
Mass/Charge, Da
4l

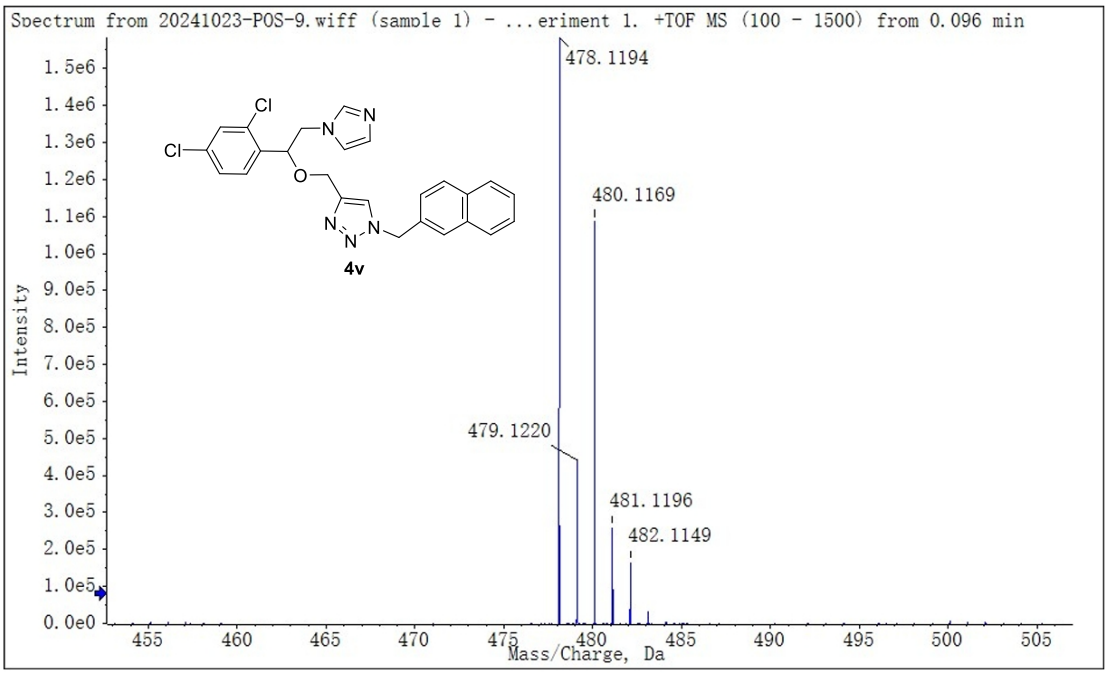

505.107230618: 506.1145 from 20241023-POS-7
Intensity
Time, min
XIC Manager
Name
Formula
Isotope
Mass (Da)
Adduct
Extraction Mass (Da)
Width (Da)
Fragment Mass (Da)
Found At Mass (Da)
Error (ppm)
Expected RT (min)
RT Width (min)
Found At RT (min)
RT Delta (min)
RT % Error
Intensity
506.11373
-1.5
2115800

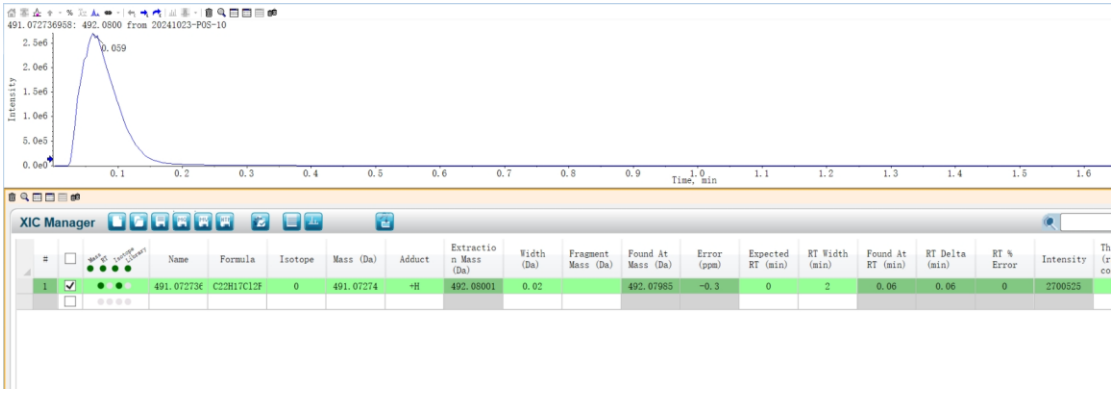

Spectrum from 20241023-POS-7.wiff (sample 1) - ...eriment 1. +TOF MS (100 - 1500) from 0.034 min
506.1137
508.1113
509.1136
510.1095
Intensity
Mass/Charge, Da
Cl
Cl
N
N
O
N
N
N
O
4s

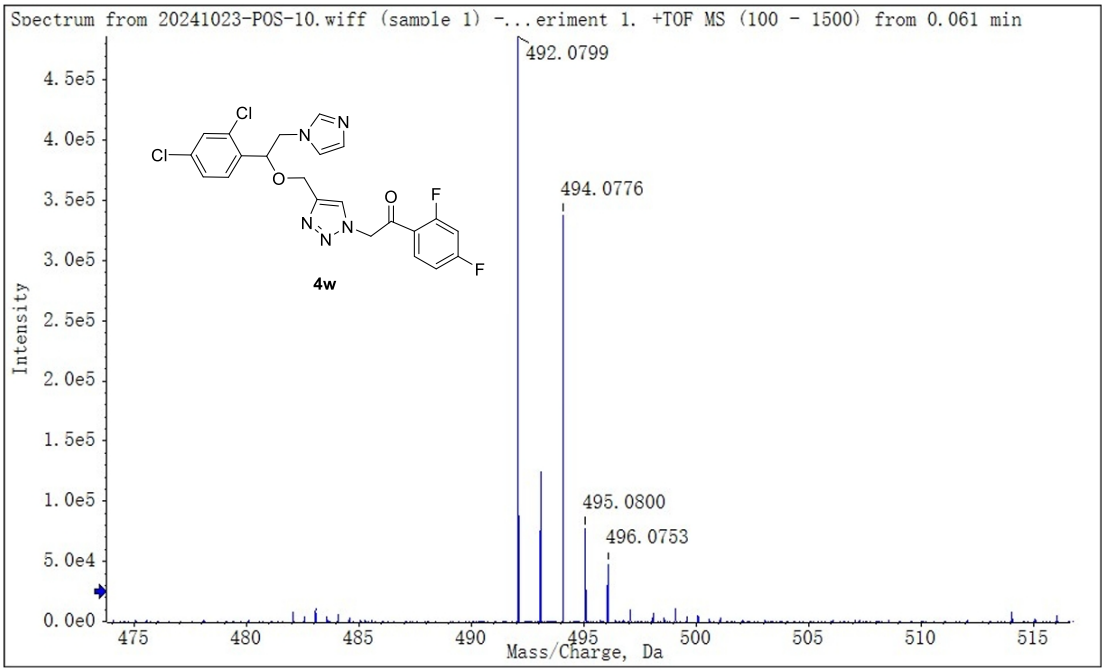

453.112318978: 454.1196 from 20241023-POS-8
0.059
Intensity
Time, min
XIC Manager
Name
Formula
Isotope
Mass (Da)
Adduct
Extraction Mass (Da)
Width (Da)
Fragment Mass (Da)
Found At Mass (Da)
Error (ppm)
Expected RT (min)
RT Width (min)
Found At RT (min)
RT Delta (min)
RT % Error
Intensity
453.112318(
C23H21Cl2N
454.11959
454.11973
12585990


Spectrum from 20241023-POS-8.wiff (sample 1) - ...eriment 1. +TOF MS (100 - 1500) from 0.064 min
454.1197
456.1172
455.1227
457.1196
458.1152
Cl
Cl
N
N
O
N
N
4t
Intensity
Mass/Charge, Da

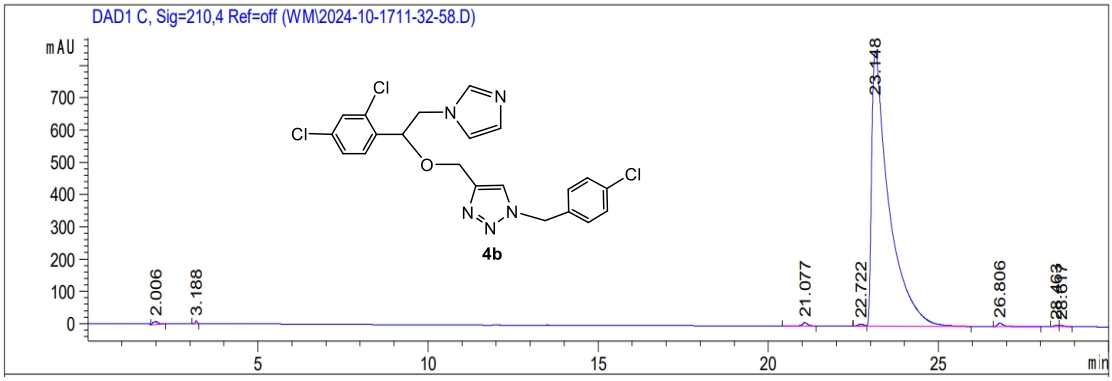

477.112319978: 478.1196 from 20241023-POS-9
0.063
Intensity
Time, min
XIC Manager
Name
Formula
Isotope
Mass (Da)
Adduct
Extraction Mass (Da)
Width (Da)
Fragment Mass (Da)
Found At Mass (Da)
Error (ppm)
Expected RT (min)
RT Width (min)
Found At RT (min)
RT Delta (min)
RT % Error
Intensity
1
477.11231
C25H21Cl2N
0
477.11232
+H
478.11959
0.02
478.11913
-1
0
2
0.06
0.06
0
13102035


Spectrum from 20241023-POS-9.wiff (sample 1) - ...eriment 1. +TOF MS (100 - 1500) from 0.096 min
478.1194
480.1169
479.1220
481.1196
482.1149
Cl
Cl
N
N
O
N
N
N
4v
Intensity
Mass/Charge, Da


491.072736958: 492.0800 from 20241023-POS-10
0.059
Intensity
Time, min
XIC Manager
Name
Formula
Isotope
Mass (Da)
Adduct
Extraction Mass (Da)
Width (Da)
Fragment Mass (Da)
Found At Mass (Da)
Error (ppm)
Expected RT (min)
RT Width (min)
Found At RT (min)
RT Delta (min)
RT % Error
Intensity
491.07273€
C22H17Cl2F
491.07274
+H
492.08001
0.02
492.07985
-0.3
2700525


Spectrum from 20241023-POS-10.wiff (sample 1) -...eriment 1. +TOF MS (100 - 1500) from 0.061 min
492.0799
494.0776
495.0800
496.0753
4w
Intensity
Mass/Charge, Da

4. HPLC spectra



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面积百分比报告

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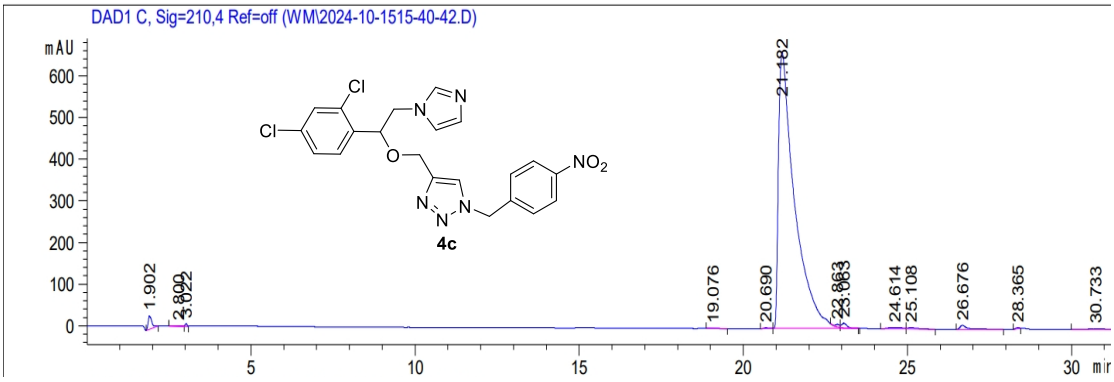
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

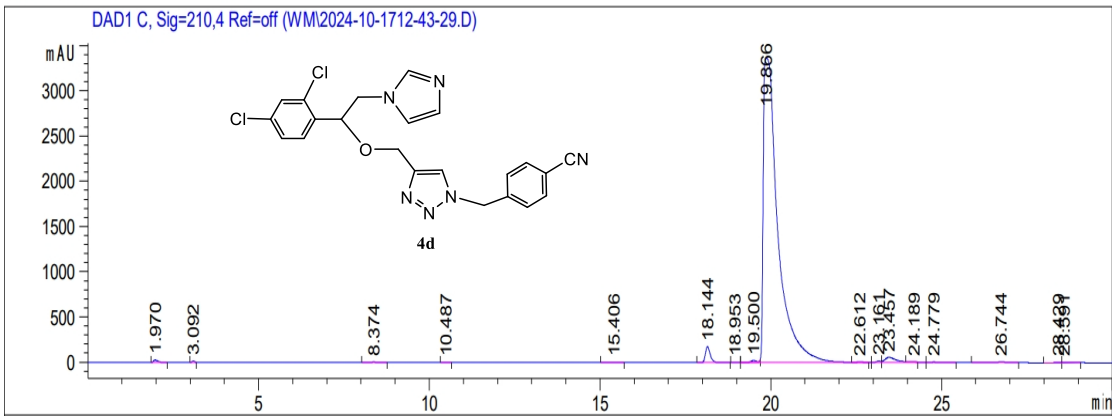
信号 1: DAD1 C, Sig=210,4 Ref=off

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	2.006	BB	0.1498	100.69322	9.18968	0.3299
2	3.188	BB	0.0563	34.33208	9.47926	0.1125
3	21.077	BB	0.1658	117.58685	10.41125	0.3853
4	22.722	BV E	0.1635	68.66209	6.48532	0.2250
5	23.148	VB R	0.4903	2.99671e4	852.08276	98.1908
6	26.806	BB	0.2051	158.75778	11.08436	0.5202
7	28.463	BV	0.1364	39.28884	4.38961	0.1287
8	28.617	VB	0.1521	32.84701	3.19162	0.1076
总量 :				3.05193e4	906.31386	



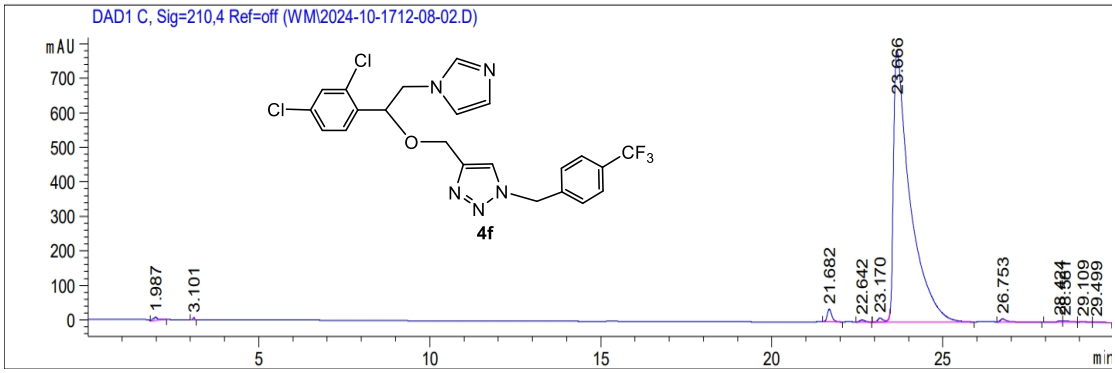
信号 1: DAD1 C, Sig=210,4 Ref=off

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	1.902	BB	0.1054	243.18951	31.73482	1.0342
2	2.800	BV E	0.1651	12.32899	1.00521	0.0524
3	3.022	VB R	0.0558	22.03857	6.15014	0.0937
4	19.076	BB	0.2045	16.96358	1.29784	0.0721
5	20.690	BB	0.1538	20.87162	2.10325	0.0888
6	21.182	BV R	0.4750	2.25898e4	663.77087	96.0689
7	22.863	VV E	0.1247	54.72068	6.46918	0.2327
8	23.063	VB E	0.1748	134.81682	11.49611	0.5733
9	24.614	BV	0.3909	102.33519	3.48204	0.4352
10	25.108	VB	0.2959	70.04793	3.32298	0.2979
11	26.676	BB	0.2206	151.84813	9.70290	0.6458
12	28.365	BB	0.1109	14.60383	2.10696	0.0621
13	30.733	BBA	0.4529	80.59692	2.33385	0.3428
总量：				2.35141e4	744.97614	



信号 1: DAD1 C, Sig=210,4 Ref=off

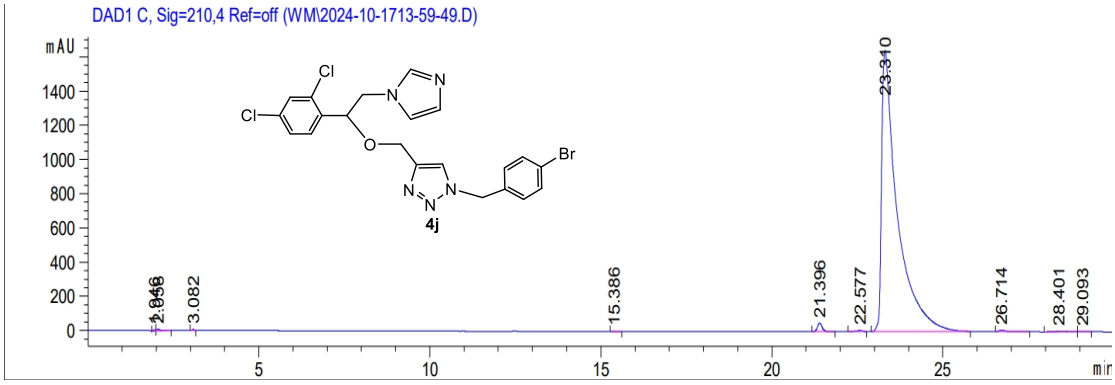
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	1.970	BB	0.1225	241.85104	27.52695	0.2302
2	3.092	BB	0.0595	51.01194	13.66936	0.0485
3	8.374	BB	0.1745	46.37060	3.79527	0.0441
4	10.487	BB	0.1228	9.54208	1.20019	9.081e-3
5	15.406	BB	0.1646	49.63017	4.36712	0.0472
6	18.144	BB	0.1486	1738.47498	176.93298	1.6544
7	18.953	BB	0.1250	14.11590	1.81018	0.0134
8	19.500	BV E	0.1904	274.25296	21.84788	0.2610
9	19.866	VV R	0.3784	1.00515e5	3365.65088	95.6545
10	22.612	VB E	0.1907	81.96693	6.43006	0.0780
11	23.161	BV	0.1445	131.08615	14.09306	0.1247
12	23.457	VV R	0.3714	1436.65112	56.73995	1.3672
13	24.189	VB E	0.1354	35.37079	4.15201	0.0337
14	24.779	BB	0.2343	88.32639	5.19716	0.0841
15	26.744	BB	0.2528	222.69290	12.09463	0.2119
16	28.429	BV	0.1494	58.93422	5.95963	0.0561
17	28.591	VB	0.2246	86.05263	5.43816	0.0819
总量 :				1.05081e5	3726.90548	



排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: DAD1 C, Sig=210,4 Ref=off

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	1.987	BB	0.1365	95.37249	9.54862	0.3486
2	3.101	BB	0.0579	22.85099	6.36651	0.0835
3	21.682	BB	0.1368	330.99994	36.84132	1.2099
4	22.642	BB	0.1602	57.51737	5.58180	0.2102
5	23.170	BV E	0.1761	133.35530	11.26667	0.4874
6	23.666	VB R	0.4627	2.64372e4	785.39117	96.6336
7	26.753	BB	0.1966	123.23627	9.06457	0.4505
8	28.424	BV	0.1432	43.25673	4.45755	0.1581
9	28.581	VV	0.2364	72.90102	4.20256	0.2665
10	29.109	VB	0.2314	29.76090	1.93501	0.1088
11	29.499	BBA	0.1528	11.73164	1.13261	0.0429
总量 :				2.73582e4	875.78838	



排序 : 信号

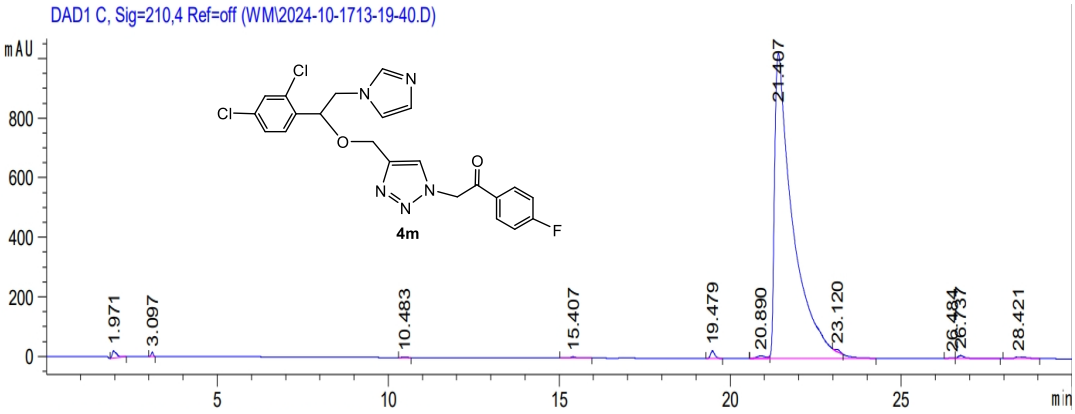
乘积因子 : 1.0000

稀释因子 : 1.0000

内标使用乘积因子和稀释因子

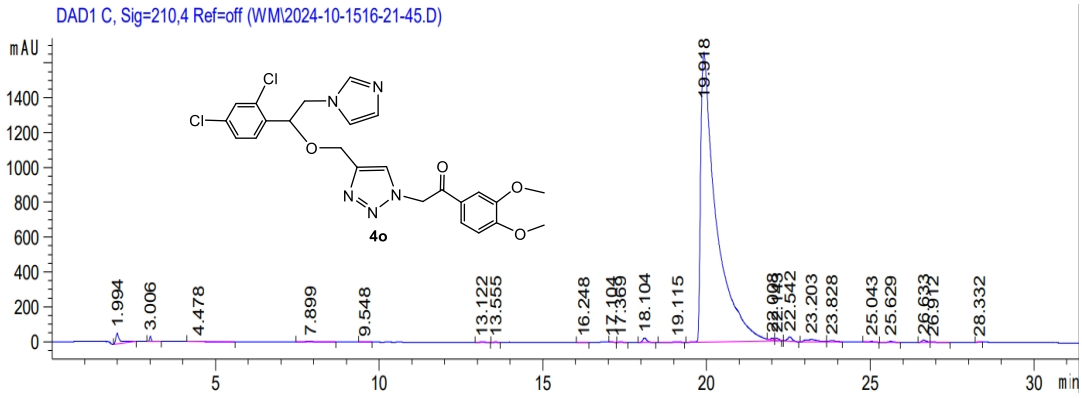
信号 1: DAD1 C, Sig=210,4 Ref=off

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	1.946	BV	0.0722	36.76105	7.91099	0.0693
2	2.058	VB	0.1342	91.71786	9.36775	0.1730
3	3.082	BB	0.0539	23.95029	6.99581	0.0452
4	15.386	BB	0.1260	9.54838	1.16015	0.0180
5	21.396	BB	0.1447	482.19165	50.81166	0.9095
6	22.577	BB	0.1976	71.22945	5.48082	0.1343
7	23.310	BB	0.4339	5.20481e4	1641.80090	98.1666
8	26.714	BB	0.1870	119.05479	9.31990	0.2245
9	28.401	BV	0.2831	121.66861	5.69952	0.2295
10	29.093	VB	0.2007	15.94857	1.23471	0.0301
总量 :				5.30201e4	1739.78221	



信号 1: DAD1 C, Sig=210,4 Ref=off

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	1.971	BB	0.1293	229.72830	24.52172	0.5850
2	3.097	BB	0.0564	50.33078	13.84075	0.1282
3	10.483	BB	0.1234	11.64093	1.45439	0.0296
4	15.407	BB	0.1629	46.38844	4.13454	0.1181
5	19.479	BB	0.1324	218.63318	25.39623	0.5568
6	20.890	BV E	0.2311	146.55904	8.94662	0.3732
7	21.407	VV R	0.5110	3.81503e4	1023.28461	97.1573
8	23.120	VB E	0.1539	80.05579	8.06092	0.2039
9	26.484	BV	0.1763	27.14244	2.39301	0.0691
10	26.737	VB	0.2170	156.55794	10.20642	0.3987
11	28.421	BB	0.2570	149.19028	7.87405	0.3799
总量：				3.92666e4	1130.11324	



信号 1: DAD1 C, Sig=210,4 Ref=off

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	1.994	BV R	0.1230	539.84772	59.95606	0.9429
2	3.006	BB	0.0603	116.17842	30.56993	0.2029
3	4.478	BB	0.2278	31.40068	1.95027	0.0548
4	7.899	BB	0.2225	84.46083	5.01549	0.1475
5	9.548	BB	0.1289	22.08710	2.60621	0.0386
6	13.122	BB	0.1663	16.48894	1.37095	0.0288
7	13.555	BB	0.1066	9.67875	1.40069	0.0169
8	16.248	BB	0.1177	10.48813	1.33396	0.0183
9	17.104	BB	0.1012	8.75416	1.35743	0.0153
10	17.369	BB	0.1136	26.90931	3.58354	0.0470
11	18.104	BB	0.1304	224.03717	26.04434	0.3913
12	19.115	VB R	0.2285	42.61397	2.91511	0.0744
13	19.918	BV R	0.4536	5.49551e4	1662.75623	95.9842
14	22.008	VV E	0.1032	68.70119	9.87467	0.1200
15	22.143	VB E	0.1242	99.94233	12.37137	0.1746
16	22.542	BB	0.1438	238.67291	24.90069	0.4169
17	23.203	BV	0.3662	334.31302	12.57497	0.5839
18	23.828	VB	0.2109	88.85822	6.28687	0.1552
19	25.043	BB	0.1931	48.92569	3.58842	0.0855
20	25.629	VB R	0.1957	62.81178	5.17077	0.1097
21	26.633	BV	0.1637	140.07114	13.00008	0.2446
22	26.912	VB	0.1821	59.00170	4.58585	0.1031
23	28.332	BB	0.1147	24.95971	3.52241	0.0436
总量 :				5.72543e4	1896.73629	