Supporting Information

Electrochemical Site-Selective direct C-H Sulfenylation and Selenylation of Chromone-Fused-Indolizine (CFI) Skeleton

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General information:

All the chemicals and reagents were purchased from commercially suppliers and used without prior any purification. Column chromatography was performed over silica-gel (particle size: 100-200 Mesh) using hexanes and ethyl acetate as eluent. The aluminium supported silica plate Si 60 F_{254} was used for the thin layer chromatography. ^{1}H NMR, ^{13}C NMR, and HRMS techniques were used for the analysis of synthesized compounds. ^{1}H NMR and ^{13}C NMR spectra were recorded on JEOL ECS-400 instrument in $CDCl_3$ solvent. Chemical shifts reported in parts per million (ppm) with referencing the TMS at 0.00 ppm and coupling constants (J) were given in Hz. ^{1}H NMR peak signals were reported as s (singlet), d (doublet), dd (double doublet), td (triplet of doublet), ddd (doublet of double doublet), and m (multiplet). In the ^{13}C NMR, Chemical shifts were reported in ppm with referencing the center line of a triplet of Chloroform-d at 77.10 ppm. High-resolution mass spectra (HRMS) were recorded on a Xevo G2-S Q Tof (Waters, USA) mass spectrometer and Agilent technologies Q-TOF B.06.01 mass spectrometer. All electrocatalytic reactions were carried out in IKA ElectraSyn 2.0 instrument. All the starting precursors were synthesized using reported literature.[1]

General procedure for Table 2

In an undivided Electrasyn 2.0 cell equipped with a graphite anode and a platinum cathode was charged with chromone-fused-indazoline **1** (0.25 mmol), disulfides **2** (0.20 mmol), KI (50 mol %), and *n*-Bu_4NPF_6 (50 mol %) in acetonitrile (4 mL) solvent. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA at room temperature for the 4-6 h *via* the manual programming of IKA ElectraSyn 2.0 instrument. After the completion of the reaction, the acetonitrile solvent was evaporated and the crude was diluted with water (20 mL) followed by extracted with chloroform (3x20 mL). The combined organic layers were concentrated under reduced to get crude product which were further purified by trituration process in EtOAc: Hexanes to afford the corresponding products **3** except **3ai**, **3aj**, **3ed, 3ak, 3al, 3am, 3gb, 3hb** which were purified through column chromatography using EtOAc: Hexanes as an eluent.

General Procedure for and results of Cyclic Voltammetry (CV):

Cyclic voltammetry was performed in a three electrode cell at room temperature. The working electrode was a glassy electrode and the counter electrode was a platinum electrode. The reference was an Ag/AgCl electrode submerged in 3M KCl solution, and separated from the reaction by a salt bridge. 8 mL of CH_3CN containing 0.05 M and 0.025 M KI were used in the all electrochemical cyclic voltammograms experiments. The scan rate is 0.2 V/s.

The CV of *n*-Bu_4NPF_6 (0.5 M) showed no oxidation peak. The CV of *n*-Bu_4NPF_6 (0.5 M) and KI 0.025 M showed a oxidation peak at +1.27 V which indicates that iodide ion gets oxidized into iodine radical or iodine (curve blank). The CV of the **2a** (5 mM), KI (0.025M), and *n*-Bu_4NPF_6 (0.05 M) demonstrated an apparent oxidation peak at +2.30 V (curve 2a) whereas the CV of the **1a** (5 mM), KI (0.025M), and *n*-Bu_4NPF_6 (0.05 M) showed an apparent oxidation peak at +2.64V (curve 1a). The CV of the mixture of **1a**, **2a**, KI (0.025 M) and *n*-Bu_4NPF_6 (0.05 M) demonstrated apparent oxidation peaks at +2.06 and +2.75 V (curve 1a+2a), due to the possible chemical interaction between the compounds **1a** and **2a**.

Cyclic Voltammograms graph for KI

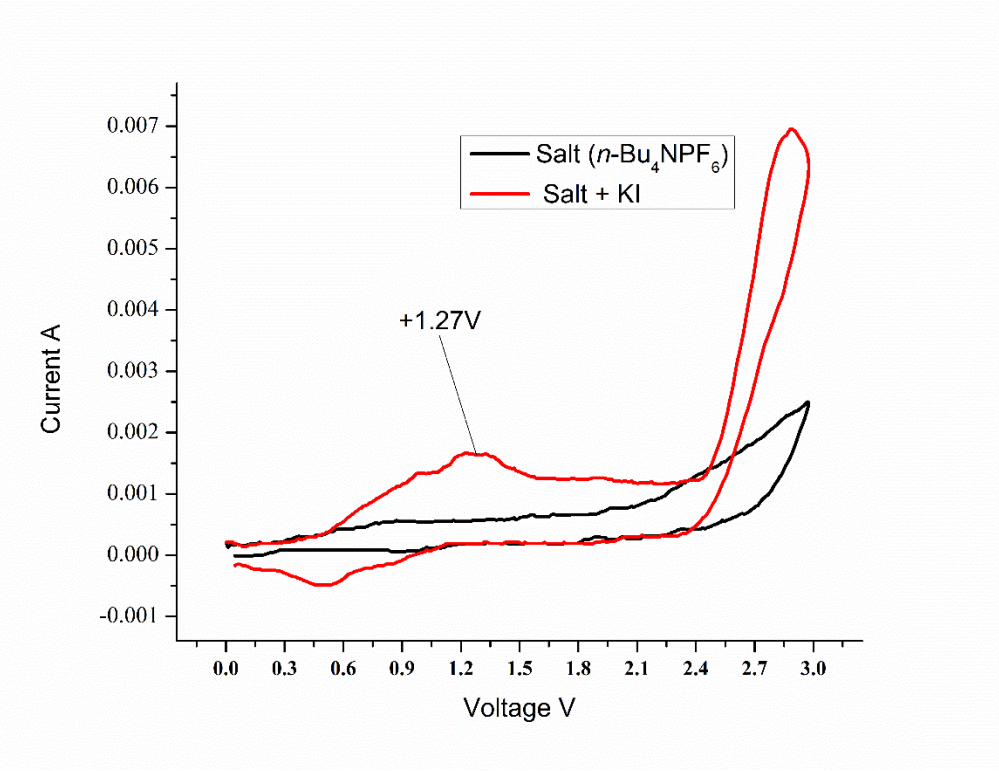


Figure S1. Cyclic voltammograms of reactants and mixture in 0.1 M *n*-Bu_4NPF_6/ CH_3CN (3:2) using a glassy carbon disk electrode, Pt electrode as counter electrode and Ag/AgCl as reference

electrode; Cyclic voltammograms of salt and salt with KI at a 200 mVS^{-1} (curve-salt): *n*-Bu_4NPF_6 (0.05 M); (curve salt+KI): *n*-Bu_4NPF_6 (0.05 M), KI (0.025M).

Cyclic Voltammograms graph of 2a

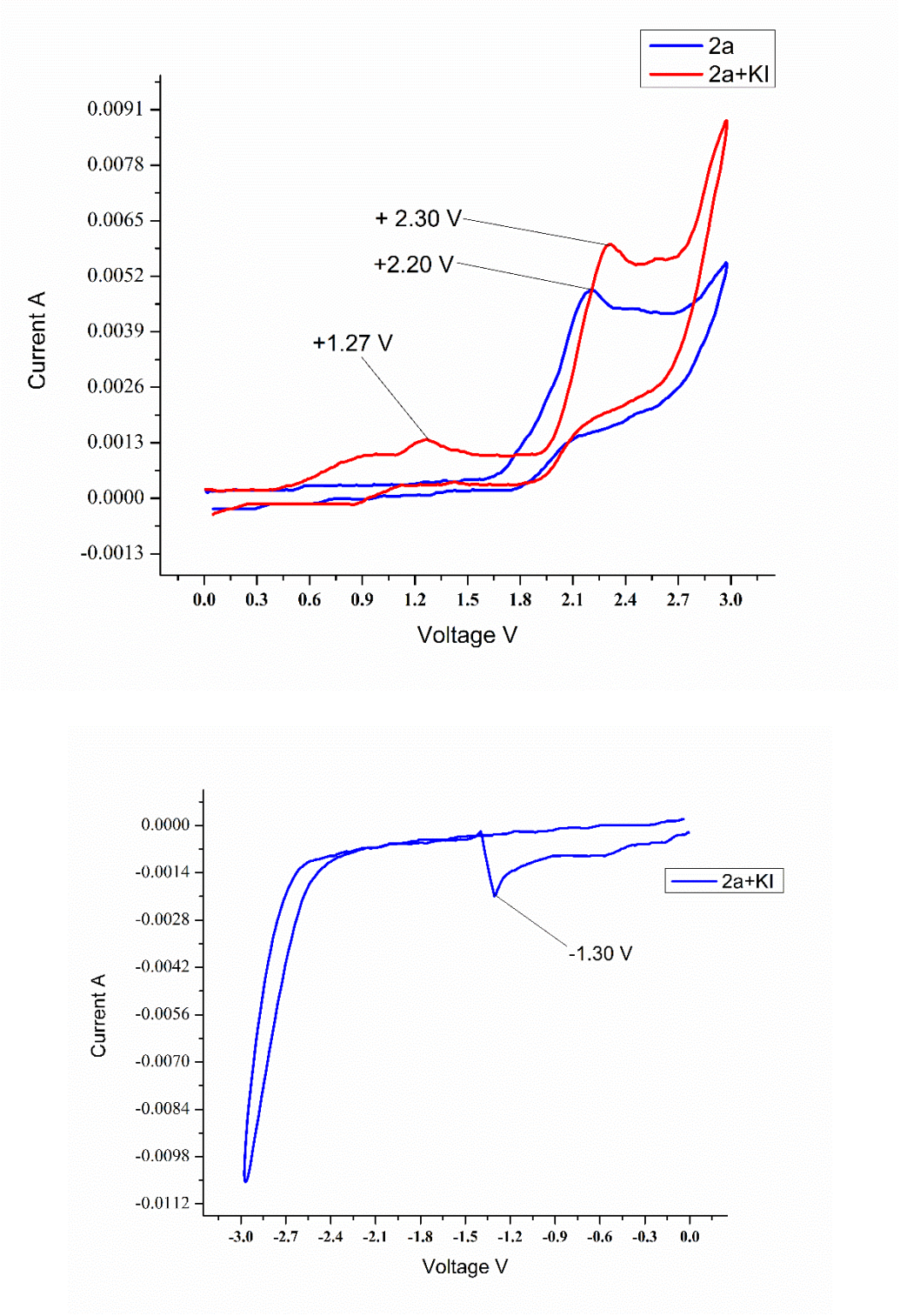


Figure S2. Cyclic voltammograms of reactants and mixture in 0.1 M *n*-Bu_4NPF_6/ CH_3CN using

a glassy carbon disk electrode, Pt electrode as counter electrode and Ag/AgCl as reference electrode, at a 200 mVS^{-1}; (curve 2a+KI): *n*-Bu_4NPF_6 (0.05 M), KI (0.025M)

Cyclic Voltammograms graph for 1a

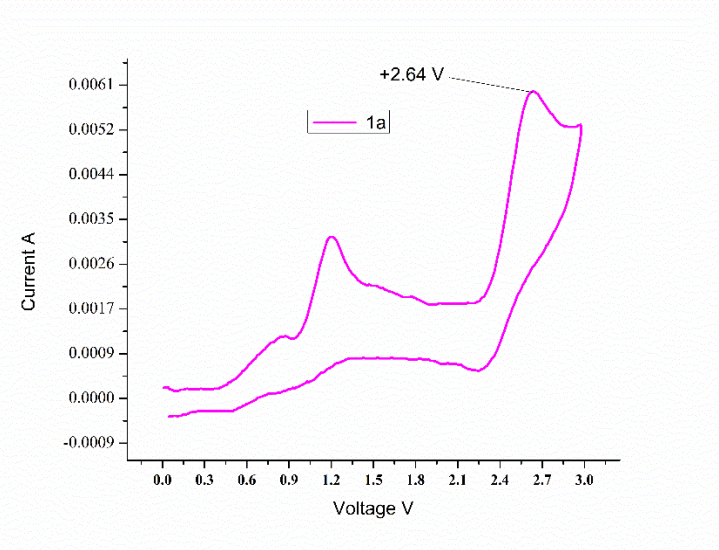


Figure S3. Cyclic voltammograms of reactants and mixture in 0.1 M *n*-Bu_4NPF_6/ CH_3CN using a glassy carbon disk electrode, Pt electrode as counter electrode and Ag/AgCl as reference electrode, at a 200 mVS^{-1} (Curve **1a**): **1a** (5 mM) + *n*-Bu_4NPF_6 (0.05 M), KI (0.025M)

Cyclic Voltammograms graph for 1a+2a

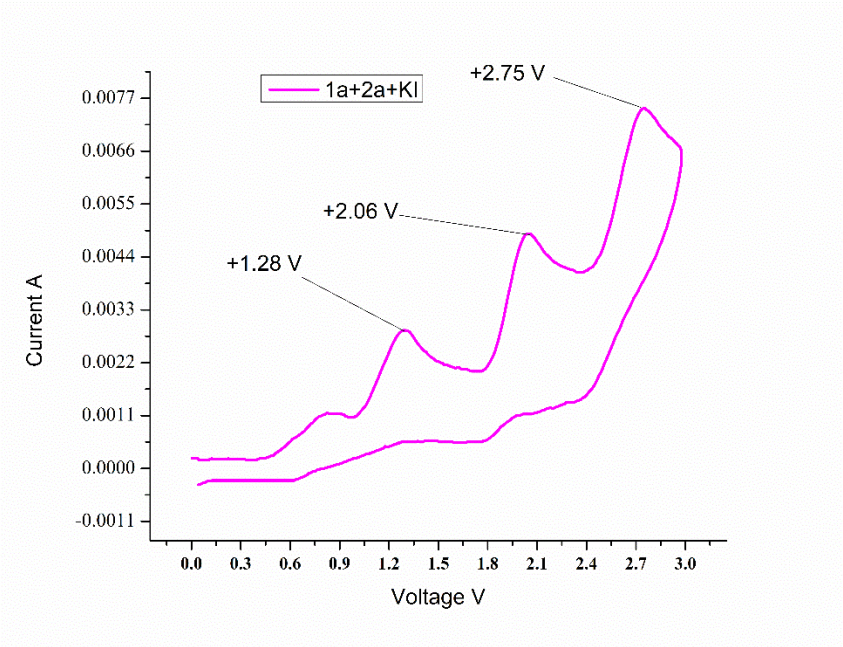


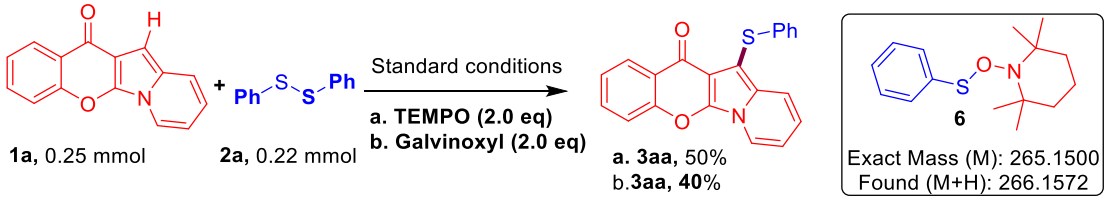
Figure S4. Cyclic voltammograms of reactants and mixture in 0.1 M *n*-Bu_4NPF_6/ CH_3CN (3:2)

using a glassy carbon disk electrode, Pt electrode as counter electrode and Ag/AgCl as reference electrode, at a 200 mVS^{-1}; (Curve 1a+2a): **1a** (5 mM) + **2a** (5 mM)+ *n*-Bu_4NPF_6 (0.05 M), KI (0.025M) .

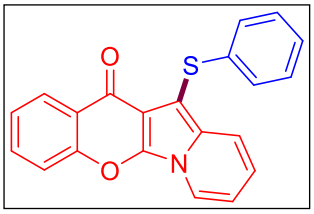
Control experiments

To gain the intrinsic reaction pathway of this interesting electrochemical C-H chalcogenation protocol, we carried out some control experiments as shown in Scheme 1. The essential role of electricity and iodo source were already established during optimization studies (Table 1, entries 2-3). To check the radical involvement in this C-H chalcogenation process, radical scavenger experiments were conducted. The reaction of **1a** with **2a** was performed in the presence of TEMPO or galvinoxyl free radicals under optimized reaction conditions which provided the **3aa** in 50% and 40% respectively. The formation of TEMPO-adduct **6** was also confirmed by HRMS data analysis which supports the possible radical pathway. However, since the reactions were not fully quenched, ionic pathway also cannot be ruled out.

Scheme 1



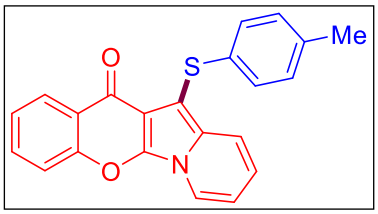
11-(Phenylthio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3aa)*:



The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and diphenyl disulfide **2a** (0.2 mmol, 0.044 g), after trituration process in 10-15% EtOAc/Hexanes) obtained **3aa** as a yellow solid; Yield: 0.079 g, 92%; M.P.: 182 °C ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.29 (dd, J = 8.0 & 1.6 Hz, 1H), 8.02 (d, J = 7.2 Hz, 1H), 7.62-7.57 (m, 2H), 7.48 (d, J = 8.4 Hz, 1H), 7.32 (td, J = 8.0 & 1.2 Hz, 1H), 7.15-7.13 (m, 2H), 7.10-7.06 (m, 2H), 6.99-6.95 (m, 1H), 6.80-6.76 (m, 1H), 6.64 (td, J = 7.2 & 1.2, 1H); ^{13}C NMR

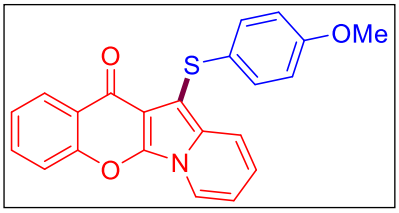
(100 MHz, $CDCl_3$): δ 174.1, 153.7, 141.5, 139.3, 133.1, 132.0, 128.7, 127.0, 126.9, 125.3, 124.6, 123.7, 121.2, 120.6, 118.8, 117.3, 112.8, 109.4, 92.6; HRMS (ESI) exact mass calcd for $C_{21}H_{13}NO_2S$ + H (M + H), 344.0740; Found: 344.0741.

11-(*p*-Tolylthio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ab)*:



The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(4-methylphenyl) disulfide **2b** (0.2 mmol, 0.049 g), after trituration process in 10-15% EtOAc/Hexanes) obtained **3ab** as a yellow solid; Yield: 0.083 g, 93%; M.P.: 164 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40 (dd, *J* = 8.0 & 1.7 Hz, 1H), 8.12 (d, *J* = 7.2 Hz, 1H), 7.74-7.67 (m, 2H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 6.89-6.85 (m, 1H), 6.73 (t, *J* = 7.2 Hz, 1H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.2, 153.8, 141.6, 135.6, 135.3, 133.2, 131.8, 129.6, 127.6, 127.1, 124.6, 123.8, 121.0, 120.5, 119.0, 117.3, 112.8, 109.4, 93.6, 21.0; HRMS (ESI) exact mass calcd for $C_{22}H_{15}NO_2S$ + H (M + H), 358.0896; Found: 358.0892.

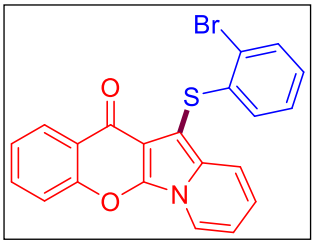
11-((4-Methoxyphenyl)thio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ac)*:



The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(4-methoxyphenyl) disulfide **2c** (0.2 mmol, 0.056 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3ac** as a yellow solid; Yield: 0.090 g, 96%; M.P.: 182 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41 (dd, *J* = 8.0 & 1.6 Hz, 1H), 8.08 (d, *J* = 7.2 Hz, 1H), 7.77 (d, *J* = 9.2 Hz, 1H), 7.70-7.66 (m, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.42 (td, *J* = 8.0 & 1.2 Hz, 1H), 7.38-7.34 (m, 2H), 6.88-6.85 (m, 1H), 6.75-6.69 (m, 3H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.3, 158.3, 153.8, 141.5,

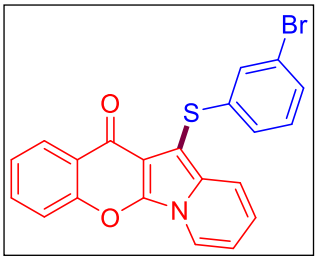
113.1, 131.5, 130.6, 129.7, 127.1, 124.6, 123.8, 120.9, 120.5, 119.0, 117.3, 114.5, 112.7, 109.3, 95.2, 55.3.

11-((2-Bromophenyl)thio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ad)*:



The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(2-bromophenyl) disulfide **2d** (0.2 mmol, 0.075 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3ad** as a yellow solid; Yield: 0.087 g, 82%; M.P.: 194 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (dd, J = 8.0 & 1.6 Hz, 1H), 8.12 (d, J = 7.2 Hz, 1H), 7.67-7.62 (m, 2H), 7.55 (d, J = 7.6 Hz, 1H), 7.43 (dd, J = 8.0 & 1.6 Hz, 1H), 7.39-7.35 (m, 1H), 6.90 (td, J = 7.6 & 1.2 Hz, 1H), 6.87-6.81 (m, 2H), 6.74-6.70 (m, 1H), 6.62 (dd, J = 7.6 & 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.1, 153.9, 141.9, 140.7, 133.3, 132.6, 132.4, 127.5, 127.2, 126.7, 125.9, 124.8, 123.8, 121.6, 120.8, 120.1, 119.0, 117.4, 113.1, 109.6, 91.1; HRMS (ESI) exact mass calcd for $C_{21}H_{12}BrNO_2S$ + H (M + H), 421.9845; Found: 421.9844.

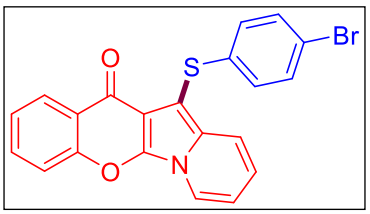
11-((3-Bromophenyl)thio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ae)*:



The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(3-bromophenyl) disulfide **2e** (0.2 mmol, 0.075 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3ae** as a yellow solid; Yield: 0.093 g, 88%; M.P.: 152 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.39 (dd, J = 8.0 & 1.6 Hz, 1H), 8.16 (dt, J = 7.2 & 1.2 Hz, 1H), 7.73-7.66 (m, 2H), 7.60 (dd, J = 8.4 & 1.2 Hz, 1H), 7.45-7.41 (m, 1H), 7.24-7.23 (m, 1H), 7.19-7.13 (m, 2H), 7.03 (t, J = 8.0 Hz, 1H), 6.95-6.90 (m, 1H), 6.80-6.76 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.2, 153.8, 142.0, 141.8, 133.3, 132.3, 130.1, 128.8, 128.2, 127.1, 125.0, 124.8, 123.8, 122.9, 121.7, 120.8, 118.7, 117.4,

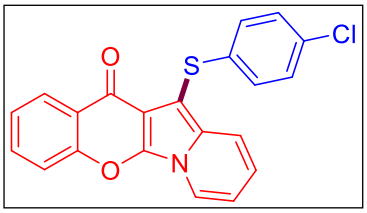
113.0, 109.3, 91.1; HRMS (ESI) exact mass calcd for $C_{21}H_{12}BrNO_2S$ + H (M + H), 421.9845; Found: 421.9854.

11-((4-Bromophenyl)thio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3af)*:



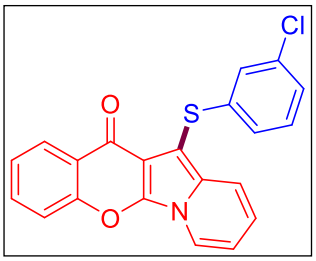
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(4-bromophenyl) disulfide **2f** (0.2 mmol, 0.075 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3af** as a yellow solid; Yield: 0.095 g, 90%; M.P.: 184 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (d, J = 8.0 Hz, 1H), 8.11 (d, J = 7.2 Hz, 1H), 7.69-7.63 (m, 2H), 7.56 (d, J = 10.0 Hz, 1H), 7.41-7.38 (m, 1H), 7.26-7.23 (m, 2H), 7.06-7.04 (m, 2H), 6.89-6.86 (m, 1H), 6.75-6.72 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.2, 153.8, 141.7, 138.7, 133.3, 132.0, 131.7, 128.3, 127.0, 124.8, 123.7, 121.5, 120.7, 118.9, 118.7, 117.4, 113.0, 109.3, 91.8; HRMS (ESI) exact mass calcd for $C_{21}H_{12}BrNO_2S$ + H (M + H), 421.9845; Found: 421.9850.

11-((4-Chlorophenyl)thio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ag)*:



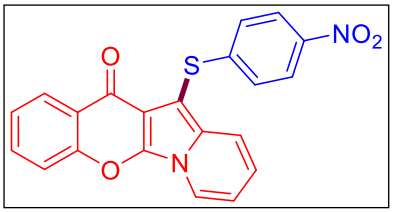
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(4-chlorophenyl) disulfide **2g** (0.2 mmol, 0.057 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3ag** as a yellow solid; Yield: 0.085 g, 90%; M.P.: 182 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (dd, J = 8.0 & 2.0 Hz, 1H), 8.08 (d, J = 7.2 Hz, 1H), 7.66-7.61 (m, 2H), 7.52 (d, J = 8.4 Hz, 1H), 7.36 (t, J = 8.0, 1H), 7.09-7.04 (m, 4H), 6.84 (t, J = 8.0 Hz, 1H), 6.70 (t, J = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.2, 153.8, 141.7, 137.9, 133.3, 132.0, 131.1, 128.8, 128.1, 127.1, 124.8, 123.8, 121.5, 120.7, 118.7, 117.4, 113.0, 109.3, 92.1; HRMS (ESI) exact mass calcd for $C_{21}H_{12}ClNO_2S$ + H (M + H), 378.0350; Found: 378.0351.

11-((3-Chlorophenyl)thio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ah)*:



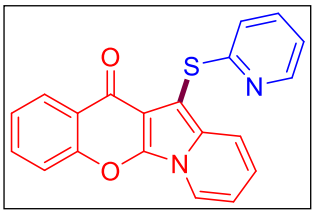
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(3-chlorophenyl) disulfide **2h** (0.2 mmol, 0.057 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3ah** as a yellow solid; Yield: 0.082 g, 87%; M.P.: 156 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.37 (d, J = 8.0 Hz, 1H), 8.15 (d, J = 7.2 Hz, 1H), 7.72-7.65 (m, 2H), 7.59 (d, J = 8.4 Hz, 1H), 7.42 (t, J = 8.0 Hz, 1H), 7.09-7.06 (m, 3H), 7.03-6.99 (m, 1H), 6.91 (t, J = 6.8 Hz, 1H), 6.77 (t, J = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.1, 153.8, 141.79, 141.74, 134.6, 133.3, 132.3, 129.7, 127.0, 125.9, 125.3, 124.8, 124.5, 123.7, 121.7, 120.7, 118.7, 117.4, 113.0, 109.3, 91.1; HRMS (ESI) exact mass calcd for $C_{21}H_{12}ClNO_2S$ + H (M + H), 378.0350; Found: 378.0351.

11-((4-Nitrophenyl)thio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ai)*:



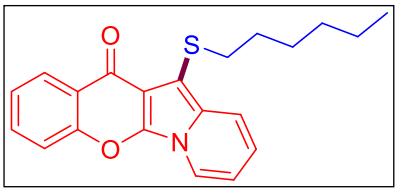
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(4-nitrophenyl) disulfide **2i** (0.2 mmol, 0.062 g), after column chromatography (20-25% EtOAc/Hexanes) obtained **3ai** as a yellow solid; Yield: 0.074 g, 76%; M.P.: 210 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, J = 8.0 Hz, 1H), 8.23 (d, J = 7.2 Hz, 1H), 8.01 (d, J = 8.8 Hz, 2H), 7.74 (t, J = 8.0 Hz, 1H), 7.66-7.64 (m, 2H), 7.46 (t, J = 7.6 Hz, 1H), 7.19 (d, J = 8.8 Hz, 2H), 7.00-6.96 (m, 1H), 6.84 (t, J = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.2, 153.9, 149.8, 145.1, 142.0, 133.6, 132.4, 127.1, 125.3, 125.0, 124.0, 123.7, 122.3, 121.0, 118.4, 117.5, 113.2, 109.3, 89.1; HRMS (ESI) exact mass calcd for $C_{21}H_{12}N_2O_4S$ + H (M + H), 389.0591; Found: 389.0591.

11-(Pyridin-2-ylthio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3aj)*:



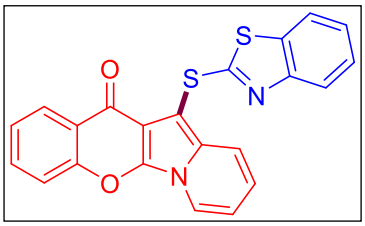
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and 2,2-dipyridyl disulfide **2j** (0.2 mmol, 0.044 g), after column chromatography (25-30% EtOAc/Hexanes) obtained **3aj** as a yellow solid; Yield: 0.060 g, 70%; M.P.: 88 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.38-8.34 (m, 2H), 8.15 (dt, J = 7.2 & 1.2 Hz, 1H), 7.72-7.66 (m, 2H), 7.60 (dd, J = 8.4 & 1.2 Hz, 1H), 7.43-7.35 (m, 2H), 6.94-6.87 (m, 3H), 6.78-6.74 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.2, 162.2, 153.8, 149.3, 141.8, 136.5, 133.2, 132.1, 127.0, 124.7, 123.8, 121.4, 120.7, 120.1, 119.5, 118.9, 117.4, 112.9, 109.4, 90.3; HRMS (ESI) exact mass calcd for $C_{20}H_{12}N_2O_2S$ + H (M + H), 345.0692; Found: 345.0691.

11-(Hexylthio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ak)*:



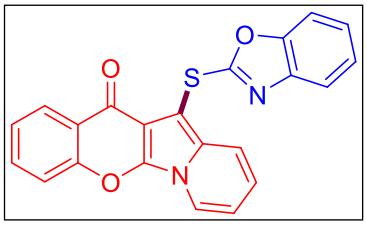
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and and 1,2-dihexyldisulfane **2k** (0.2 mmol, 0.047 g), after column chromatography process in 20-25% EtOAc/Hexanes) obtained **3ak** as a yellow solid; Yield: 0.051 g, 58%; M.P.: 52 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.37 (dd, J = 8.0 & 1.6 Hz, 1H), 7.99 (br, 1H), 7.64-7.60 (m, 2H), 7.51 (d, J = 9.6 Hz, 1H), 7.39-7.35 (m, 1H), 6.71 (br, 1H), 6.59 (t, J = 7.2 Hz, 1H), 2.96 (br, 2H), 1.47-1.39 (m, 2H), 1.34-1.27 (m, 2H), 1.17-1.11 (m, 4H), 0.75 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.6, 153.8, 141.5, 133.1, 130.9, 127.0, 124.6, 123.8, 120.2, 119.8, 119.4, 117.3, 112.5, 109.6, 96.5, 37.0, 31.5, 29.4, 28.4, 22.6, 14.0; HRMS (ESI) exact mass calcd for $C_{21}H_{21}NO_2S$ + H (M + H), 352.1366; Found: 352.1365.

11-(Benzo[*d*]thiazol-2-ylthio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3al)*:



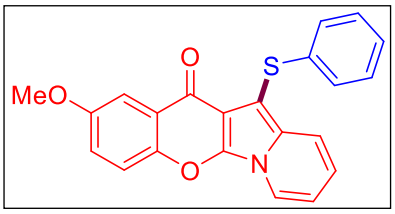
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and 2-mercaptobenzothiazole **2l** (0.38 mmol, 0.063 g), after column chromatography process in 25-30% EtOAc/Hexanes) obtained **3al** as a yellow solid; Yield: 0.075 g, 75%; M.P.: 210 °C ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (dd, J = 8.0 & 1.6 Hz, 1H), 8.18 (d, J = 7.2 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.68-7.65 (m, 2H), 7.57 (d, J = 8.4 Hz, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.40-7.36 (m, 1H), 7.30-7.26 (m, 1H), 7.13-7.09 (m, 1H), 6.98- (ddd, J = 9.2, 6.4 & 1.2 Hz, 1H), 6.79 (td, J = 6.8, & 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.0, 154.0, 153.0, 142.1, 135.1, 133.6, 133.0, 127.1, 126.2, 125.0, 124.1, 123.8, 123.0, 121.5, 121.1, 120.8, 118.4, 117.5, 113.5, 109.0, 88.6; HRMS (ESI) exact mass calcd for $C_{22}H_{12}N_2O_2S_2$ + H (M + H), 401.0413; Found: 401.0412.

11-(Benzo[*d*]oxazol-2-ylthio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3am)*:



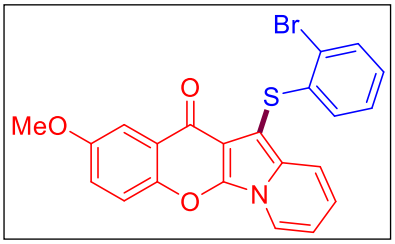
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and 2-mercaptobenzoxazole **2m** (0.38 mmol, 0.057 g), after column chromatography process in 25-30% EtOAc/Hexanes) **3am** as a yellow solid; Yield: 0.067 g, 70%; M.P.: 230 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.31 (dd, J = 8.0 & 1.6 Hz, 1H), 8.15 (d, J = 6.8 Hz, 1H), 7.68-7.64 (m, 2H), 7.56 (d, J = 8.4 Hz, 1H), 7.45-7.43 (m, 1H), 7.38 (td, J = 7.2 & 1.2 Hz, 1H), 7.32-7.29 (m, 1H), 7.15-7.09 (m, 2H), 6.94 (ddd, J = 9.2, 6.4 & 1.2 Hz, 1H), 6.76 (td, J = 7.2 & 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.1, 154.0, 152.0, 142.1, 141.7, 133.4, 132.3, 131.8, 127.1, 125.3, 124.2, 123.9, 122.5, 121.1, 119.3, 118.5, 117.1, 113.1, 110.1, 109.2., 84.11; HRMS (ESI) exact mass calcd for $C_{22}H_{12}N_2O_3S$ + H (M + H), 385.0642; Found: 385.0643.

2-Methoxy-11-(phenylthio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ba)*:



The title compound was prepared following the general procedure for Table 2, using 2-methoxy-12*H*-chromeno[3,2-*b*]indolizin-12-one **1b** (0.25 mmol, 0.067 g) and diphenyl disulfide **2a** (0.2 mmol, 0.044 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3ba** as a yellow solid; Yield: 0.088 g, 94%; M.P.: 220 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, J = 7.2 Hz, 1H), 7.78 (d, J = 3.2 Hz, 1H), 7.71 (d, J = 9.6 Hz, 1H), 7.52 (d, J = 8.8 Hz, 1H), 7.29-7.26 (m, 1H), 7.24-7.22 (m, 2H), 7.18-7.14 (m, 2H), 7.06 (t, J = 7.6 Hz, 1H), 6.90-6.86 (m, 1H), 6.73 (t, J = 7.6 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.1, 156.5, 148.4, 141.9, 139.4, 132.1, 128.8, 126.9, 125.3, 124.3, 122.7, 121.2, 120.6, 119.0, 118.6, 112.7, 109.0, 106.7, 92.5, 55.9; HRMS (ESI) exact mass calcd for $C_{22}H_{15}NO_3S$ + H (M + H), 374.0846; Found: 374.0847.

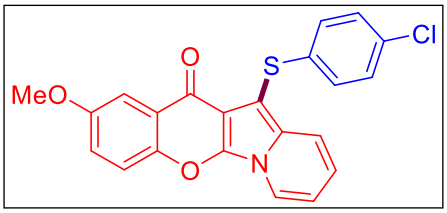
11-((2-Bromophenyl)thio)-2-methoxy-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3bd)*:



The title compound was prepared following the general procedure for Table 2, using 2-methoxy-12*H*-chromeno[3,2-*b*]indolizin-12-one **1b** (0.25 mmol, 0.067 g) and bis(2-bromophenyl) disulfide **2d** (0.2 mmol, 0.075 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3bd** as a yellow solid; Yield: 0.095 g, 84%; M.P.: 88 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, J = 7.2 Hz, 1H), 7.77 (d, J = 2.8 Hz, 1H), 7.70 (d, J = 9.2 Hz, 1H), 7.55 (d, J = 8.8 Hz, 1H), 7.50 (dd, J = 8.0 & 1.6 Hz, 1H), 7.29 (dd, J = 9.2, 3.2 Hz, 1H), 6.98 (td, J = 7.6 & 1.6 Hz, 1H), 6.94-6.88 (m, 2H), 6.78 (t, J = 7.6 Hz, 1H), 6.70 (dd, J = 7.6 & 1.6 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.9, 156.6, 148.5, 142.2, 140.7, 132.6, 132.4, 127.5, 126.7, 125.9, 124.3, 122.8, 121.6, 120.8, 120.1, 118.9, 118.6, 112.9, 109.1, 106.7, 90.8, 55.9; HRMS (ESI) exact mass calcd for $C_{22}H_{14}BrNO_3S$ + H (M + H),

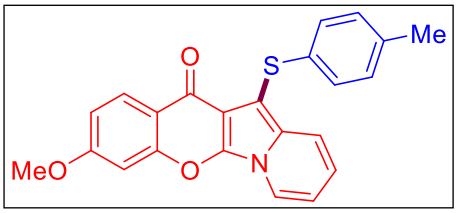
451.9951; Found: 451.9955.

11-((4-Chlorophenyl)thio)-2-methoxy-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3bg)*:



The title compound was prepared following the general procedure for Table 2, using 2-methoxy-12*H*-chromeno[3,2-*b*]indolizin-12-one **1b** (0.25 mmol, 0.067 g) and bis(4-chlorophenyl) disulfide **2g** (0.2 mmol, 0.057 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3bg** as a yellow solid; Yield: 0.094 g, 92%; M.P.: 174 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (dt, J = 7.2 & 1.2 Hz, 1H), 7.76 (d, J = 3.2 Hz, 1H), 7.69 (dt, J = 9.6 & 1.2 Hz, 1H), 7.52 (d, J = 9.2 Hz, 1H), 7.29-7.26 (m, 1H), 7.16-7.11 (m, 4H), 6.93-6.89 (m, 1H), 6.75 (td, J = 7.2 & 1.2 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.0, 156.6, 148.4, 142.0, 138.0, 132.1, 131.1, 128.8, 128.1, 124.3, 122.8, 121.5, 120.7, 118.7, 118.6, 112.8, 108.8, 106.7, 91.9, 55.9; HRMS (ESI) exact mass calcd for $C_{22}H_{14}ClNO_3S$ + H (M + H), 408.0456; Found: 408.0457.

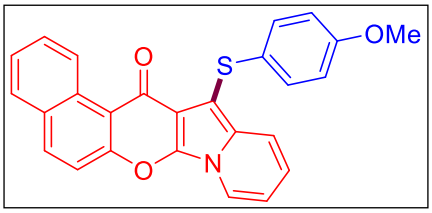
3-Methoxy-11-(*p*-tolylthio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3cb)*:



The title compound was prepared following the general procedure for Table 2, using 3-methoxy-12*H*-chromeno[3,2-*b*]indolizin-12-one **1c** (0.25 mmol, 0.067 g) and bis(4-methylphenyl) disulfide **2b** (0.2 mmol, 0.049 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3cb** as a yellow solid; Yield: 0.093 g, 96%; M.P.: 182 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.29 (d, J = 8.8 Hz, 1H), 8.07 (d, J = 7.2 Hz, 1H), 7.72 (d, J = 9.6 Hz, 1H), 7.18 (d, J = 8.0 Hz, 2H), 6.99-6.95 (m, 4H), 6.85 (ddd, J = 9.2, 6.4 & 1.2 Hz, 1H), 6.73-6.69 (m, 1H), 3.94 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.9, 163.7, 155.4, 141.5, 135.7, 135.2, 131.5, 129.5, 128.4, 127.6, 120.7, 120.4, 119.0, 117.7, 113.0, 112.7, 109.3, 100.5, 93.6, 55.9, 21.0; HRMS (ESI) exact mass calcd for $C_{23}H_{17}NO_3S$ + H (M + H), 388.1002; Found:

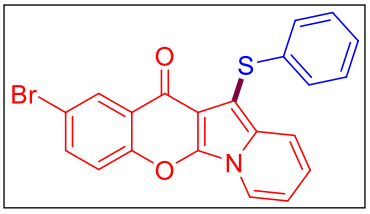
388.1005.

13-((4-Methoxyphenyl)thio)-14*H*-benzo[5,6]chromeno[3,2-*b*]indolizin-14-one *(3dc)*:



The title compound was prepared following the general procedure for Table 2, using 14*H*-benzo[5,6]chromeno[3,2-*b*]indolizin-14-one **1d** (0.25 mmol, 0.072 g) and bis(4-methoxyphenyl) disulfide **2c** (0.2 mmol, 0.056 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3dc** as a yellow solid; Yield: 0.102 g, 96%; M.P.: 232 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.33 (d, J = 8.8 Hz, 1H), 8.16 (d, J = 7.2 Hz, 1H), 8.11 (d, J = 9.2 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.80 (d, J = 9.2 Hz, 1H), 7.77-7.73 (m, 1H), 7.67 (d, J = 9.2 Hz, 1H), 7.60 (td, J = 8.0 & 1.2 Hz, 1H), 7.36 (d, J = 8.4 Hz, 2H), 6.93-6.89 (m, 1H), 6.77-6.74 (m, 3H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.4, 157.6, 154.7, 139.4, 135.5, 132.4, 131.7, 130.7, 130.0, 129.1, 128.1, 127.5, 125.8, 121.0, 120.6, 118.6, 117.2, 114.5, 112.2, 107.0, 91.8, 55.8; HRMS (ESI) exact mass calcd for $C_{26}H_{17}NO_3S$ + H (M + H), 424.1002; Found: 424.1007.

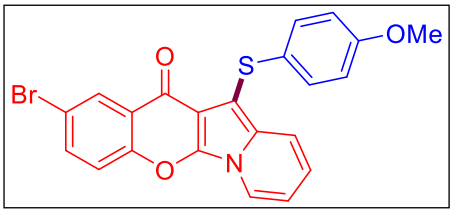
2-Bromo-11-(phenylthio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ea)*:



The title compound was prepared following the general procedure for Table 2, using 2-bromo-12*H*-chromeno[3,2-*b*]indolizin-12-one **1e** (0.25 mmol, 0.079 g) and diphenyl disulfide **2a** (0.2 mmol, 0.044 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3ea** as a yellow solid; Yield: 0.087 g, 82%; M.P.: 192 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.51 (d, J = 2.4 Hz, 1H), 8.13 (d, J = 6.8 Hz, 1H), 7.78 (dd, J = 8.8 & 2.4 Hz, 1H), 7.74 (d, J = 9.2 Hz, 1H), 7.50 (d, J = 8.8 Hz, 1H), 7.23-7.15 (m, 4H), 7.07 (t, J = 7.2 Hz, 1H), 6.94-6.70 (m, 1H), 6.78 (t, J = 6.8 Hz, 1H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.0, 152.6, 141.3, 139.0, 136.0, 132.2, 129.8, 128.8, 127.1, 125.5, 124.9, 121.5, 120.6, 119.3, 119.1, 118.0, 113.1, 109.4, 93.2; HRMS (ESI) exact

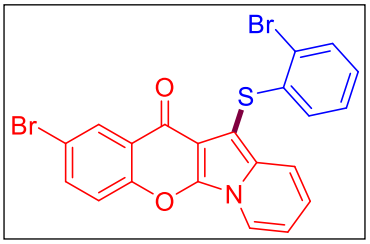
mass calcd for $C_{21}H_{12}BrNO_2S$ + H (M + H), 421.9845; Found: 421.9847.

2-Bromo-11-((4-methoxyphenyl)thio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ec)*:



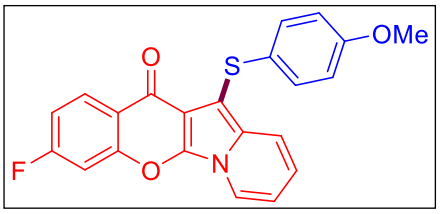
The title compound was prepared following the general procedure for Table 2, using 2-bromo-12*H*-chromeno[3,2-*b*]indolizin-12-one **1e** (0.25 mmol, 0.079 g) and bis(4-methoxyphenyl) disulfide **2c** (0.2 mmol, 0.056 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3ec** as a yellow solid; Yield: 0.096 g, 85%; M.P.: 139 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (d, J = 2.4 Hz, 1H), 8.03 (d, J = 7.2 Hz, 1H), 7.76-7.70 (m, 2H), 7.43 (d, J = 8.8 Hz, 1H), 7.32 (d, J = 8.8 Hz, 2H), 6.90-6.84 (m, 1H), 6.72-6.68 (m, 3H), 3.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.6, 166.5, 163.9, 158.9, 154.5, 141.6, 133.4, 131.4, 129.5, 123.6, 120.8, 120.4, 120.1, 114.7, 112.8, 109.5, 104.4, 104.2, 89.5, 55.2.

2-Bromo-11-((2-bromophenyl)thio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3ed)*:



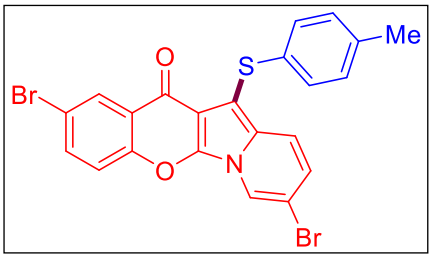
The title compound was prepared following the general procedure for Table 2, using 2-bromo-12*H*-chromeno[3,2-*b*]indolizin-12-one **1e** (0.25 mmol, 0.079 g) and bis(2-bromophenyl) disulfide **2d** (0.2 mmol, 0.075 g), after column chromatography (20-25% EtOAc/Hexanes) obtained **3ed** as a yellow solid; Yield: 0.093 g, 74%; M.P.: 158 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.45 (d, J = 2.4 Hz, 1H), 8.15 (d, J = 7.2 Hz, 1H), 7.77 (dd, J = 8.8 & 2.4 Hz, 1H), 7.68 (d, J = 9.2 Hz, 1H), 7.52-7.49 (m, 2H), 6.99-6.89 (m, 3H), 6.81(t, J = 8.0 Hz, 1H), 6.68 (dd, J = 8.0 & 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.6, 152.6, 141.7, 140.4, 136.1, 132.7, 132.5, 129.7, 127.5, 126.8, 126.1, 125.1, 121.9, 120.7, 120.3, 119.3, 118.9, 118.1, 109.5, 91.4; HRMS (ESI) exact mass calcd for $C_{21}H_{11}Br_2NO_2S$ + H (M + H), 499.8950; Found: 499.8946.

3-Fluoro-11-((4-methoxyphenyl)thio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3fc)*:



The title compound was prepared following the general procedure for Table 2, using 3-fluoro-12*H*-chromeno[3,2-*b*]indolizin-12-one **1f** (0.25 mmol, 0.064 g) and bis(4-methoxyphenyl) disulfide **2c** (0.2 mmol, 0.056 g), after trituration process in 10-15% EtOAc/Hexanes obtained **3fc** as a yellow solid; Yield: 0.090 g, 92%; M.P.: 182 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.44-8.40 (m, 1H), 8.06 (d, J = 7.2 Hz, 1H), 7.78 (d, J = 9.6 Hz, 1H), 7.35 (d, J = 8.8 Hz, 2H), 7.28-7.25 (m, 1H), 7.18-7.13 (m, 1H), 6.88 (t, J = 8.0 Hz, 1H), 6.78-6.72 (m, 3H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 173.4, 165.2 ($J_{C\text{-}F}$ = 253.0 Hz), 158.4, 154.6 ($J_{C\text{-}F}$ = 13.0 Hz), 141.4, 131.5, 130.7, 129.4 ($J_{C\text{-}F}$ = 10.0 Hz), 121.0, 120.7, 120.4, 119.0, 114.5, 113.1 ($J_{C\text{-}F}$ = 22.0 Hz), 113.0, 109.2, 104.3 ($J_{C\text{-}F}$ = 25.0 Hz), 104.2, 95.4, 55.3; ^{19}F NMR (376 MHz, $CDCl_3$): -103.8; HRMS (ESI) exact mass calcd for $C_{22}H_{14}FNO_3S$ + H (M + H), 392.0751; Found: 392.0752.

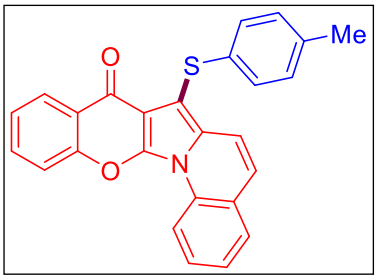
2,8-Dibromo-11-(*p*-tolylthio)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(3gb)*:



The title compound was prepared following the general procedure for Table 2, using 2,8-dibromo-12*H*-chromeno[3,2-*b*]indolizin-12-one **1g** (0.25 mmol, 0.098 g) and bis(4-methylphenyl) disulfide **2b** (0.2 mmol, 0.049 g), after column chromatography process in 20-25% EtOAc/Hexanes) obtained **3gb** as a yellow solid; Yield: 0.084 g, 65%; M.P.: 200 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.38 (d, J = 2.4 Hz, 1H), 8.17 (s, 1H), 7.69 (dd, J = 8.8 & 2.4 Hz, 1H), 7.56 (d, J = 9.6 Hz, 1H), 7.38 (d, J = 8.8 Hz, 1H), 7.09 (d, J = 8.0 Hz, 2H), 6.92 (d, J = 8.0 Hz, 2H), 6.85 (dd, J = 9.6 & 1.6 Hz, 1H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.5, 152.5, 140.9, 136.3, 135.9, 134.6, 129.9, 129.79, 129.72, 128.2, 125.1, 124.8, 120.2, 119.8, 119.2, 118.2, 109.4, 108.5, 96.6, 21.0; HRMS (ESI) exact

mass calcd for $C_{22}H_{13}Br_2NO_2S$ + H (M + H), 513.9107; Found: 513.9108.

7-(*p*-Tolylthio)-8*H*-chromeno[3',2':4,5]pyrrolo[1,2-*a*]quinolin-8-one *(3hb)*:

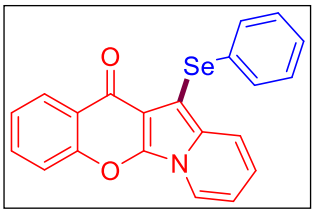


The title compound was prepared following the general procedure for Table 2, using 8*H*-chromeno[3',2':4,5]pyrrolo[1,2-*a*]quinolin-8-one **1h** (0.25 mmol, 0.071 g) and bis(4-methylphenyl) disulfide **2b** (0.2 mmol, 0.049 g), after column chromatography process in 25-30% EtOAc/Hexanes) obtained **3hb** as a yellow solid; Yield: 0.061 g, 60%; M.P.: 218 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.96 (d, J = 8.4 Hz, 1H), 8.43 (d, J = 8.8 Hz, 1H), 7.75-7.72 (m, 2H), 7.69-7.64 (m, 3H), 7.49-7.45 (m, 2H), 7.21 (d, J = 8.0 Hz, 2H), 7.15 (d, J = 9.6 Hz, 1H), 6.99 (d, J = 8.0 Hz, 2H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.6, 153.9, 145.5, 135.4, 135.1, 133.1, 131.3, 129.6, 128.8, 128.7, 127.8, 127.0, 125.7, 125.3, 125.0, 123.3, 117.6, 117.2, 110.2, 98.1, 21.0; HRMS (ESI) exact mass calcd for $C_{26}H_{17}NO_2S$ + H (M + H), 408.1053; Found: 408.1052.

General procedure for Table 3

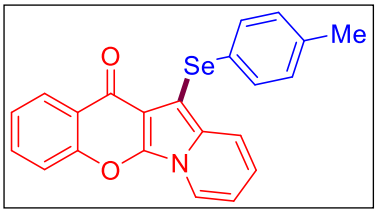
In an undivided Electrasyn 2.0 cell equipped with a graphite anode and a platinum cathode was charged chromone-fused-indazoline **1** (0.25 mmol), diselenides **4** (0.20 mmol), KI (50 mol%), and *n*-Bu_4NPF_6 (50 mol%) in acetonitrile (4 mL) solvent. The reaction mixture was stirred and electrolyzed at a constant current of 5 mA at room temperature for the 4-7 h *via* the manual programming of IKA ElectraSyn 2.0 instrument. After the completion of the reaction, the acetonitrile solvent was evaporated and the crude was diluted with water (20 mL) followed by extracted with chloroform (3x20 mL). The combined organic layers were concentrated under reduced to get crude product which were further purified by trituration process in EtOAc:Hexanes to afford the corresponding products **5** except **5cc**, **5ec, 5ga** which were purified through column chromatography using EtOAc: Hexanes as an eluent.

11-(Phenylselanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5aa)*:



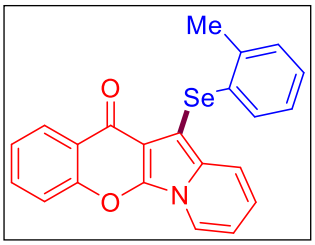
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and diphenyl diselenide **4a** (0.2 mmol, 0.062 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5aa** as a yellow solid; Yield: 0.090 g, 92%; M.P.: 180 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40 (d, J = 8.0 Hz, 1H), 8.07 (d, J = 7.2 Hz, 1H), 7.69-7.65 (m, 2H), 7.56 (d, J = 8.4 Hz, 1H), 7.41 (d, J = 7.6 Hz, 1H), 7.38 (d, J = 7.2 Hz, 2H), 7.15-7.07 (m, 3H), 6.85-6.81 (m, 1H), 6.70 (t, J = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.4, 153.7, 141.7, 134.0, 133.1, 131.9, 129.9, 129.0, 127.1, 126.1, 124.6, 123.8, 121.0, 120.6, 119.9, 117.3, 112.7, 109.7, 87.4; HRMS (ESI) exact mass calcd for $C_{21}H_{13}NO_2Se$ + H (M + H), 392.0185; Found: 392.0183.

11-(*p*-Tolylselanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5ab)*:



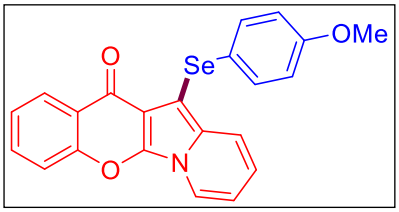
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(*p*-tolyl) diselenide **4b** (0.2 mmol, 0.068 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5ab** as a yellow solid; Yield: 0.095 g, 94%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.33 (dd, J = 8.0 & 2.0 Hz, 1H), 7.98 (d, J = 6.8 Hz, 1H), 7.62-7.57 (m, 2H), 7.48 (d, J = 8.4 Hz, 1H), 7.33 (t, J = 6.8 Hz, 1H), 7.27 (d, J = 8.0 Hz, 2H), 6.88 (d, J = 8.0 Hz, 2H), 6.75-6.71(m, 1H), 6.60 (t, J = 8.0 Hz, 1H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.4, 153.7, 141.7, 136.1, 133.0, 131.6, 130.6, 130.0, 129.8, 127.1, 124.5, 123.8, 120.8, 120.5, 120.0, 117.3, 112.6, 109.7, 88.2, 21.0.

11-(*o*-Tolylselanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5ac)*:



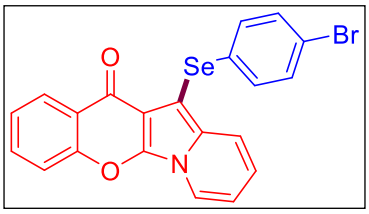
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(*o*-tolyl) diselenide **4c** (0.2 mmol, 0.068 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5ac** as a yellow solid; Yield: 0.081 g, 80%; M.P.: 154 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40 (dd, J = 8.0 & 1.6 Hz, 1H), 8.12 (d, J = 7.2 Hz, 1H), 7.71-7.70 (m, 1H), 7.62-7.58 (m, 2H), 7.44-7.40 (m, 1H), 7.11 (d, J = 7.2 Hz, 1H), 6.99 (td, J = 7.2 & 1.6 Hz, 1H), 6.89 (dd, J = 8.0 & 1.6 Hz, 1H), 6.86-6.81 (m, 2H), 6.74-6.70 (m, 1H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.4, 153.8, 141.9, 136.6, 134.8, 133.1, 132.1, 129.9, 128.6, 127.1, 126.4, 125.7, 124.6, 123.8, 121.0, 120.7, 120.0, 117.3, 112.7, 110.0, 86.2, 21.5; HRMS (ESI) exact mass calcd for $C_{22}H_{15}NO_2Se$ + H (M + H), 406.0341; Found: 406.0342.

11-((4-Methoxyphenyl)selanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5ad)*:



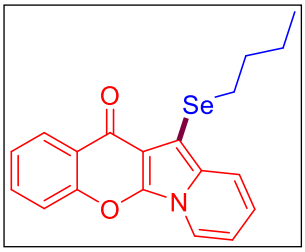
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(4-methoxyphenyl) diselenide **4d** (0.2 mmol, 0.074 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5ad** as a yellow solid; Yield: 0.099 g, 94%; M.P.: 178 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.44 (dd, J = 8.0 & 1.6 Hz, 1H), 8.06 (d, J = 6.4 Hz, 1H), 7.74 (d, J = 9.2 Hz, 1H), 7.71-7.66 (m, 1H), 7.57 (d, J = 8.4 Hz, 1H), 7.51 (d, J = 8.8 Hz, 2H), 7.43 (t, J = 7.6 Hz, 1H), 6.81 (br, 1H), 6.73-6.67 (m, 3H), 3.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.6, 158.8, 153.7, 141.7, 133.3, 133.1, 131.4, 127.1, 124.6, 123.8, 120.7, 120.5, 120.1, 117.3, 114.7, 112.6, 109.6, 89.3, 55.2; HRMS (ESI) exact mass calcd for $C_{22}H_{15}NO_3Se$ + H (M + H), 422.0290; Found: 422.0285.

11-((4-Bromophenyl)selanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5ae)*:



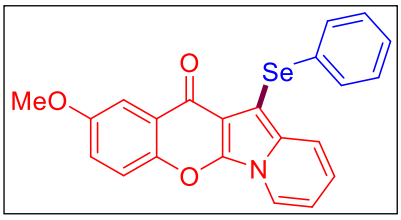
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(4-bromophenyl) diselenide **4e** (0.2 mmol, 0.094 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5ae** as a yellow solid; Yield: 0.106 g, 90%; M.P.: 156 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.39 (dd, J = 8.0 & 1.6 Hz, 1H), 8.10 (d, J = 7.2 Hz, 1H), 7.71-7.67 (m, 1H), 7.64 (d, J = 9.2 Hz, 1H), 7.57 (d, J = 8.8 Hz, 1H), 7.42 (t, J = 8.0 Hz, 1H), 7.23 (br, 4H), 6.88-6.84 (m, 1H), 6.74-6.71 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.4, 153.7, 141.8, 133.2, 133.1, 131.9, 131.4, 127.0, 124.7, 123.7, 121.3, 120.7, 120.1, 119.7, 117.4, 112.8, 109.6, 86.8; HRMS (ESI) exact mass calcd for $C_{21}H_{12}BrNO_2Se$ + H (M + H), 469.9290; Found: 469.9291.

11-(Butylselanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5af)*:



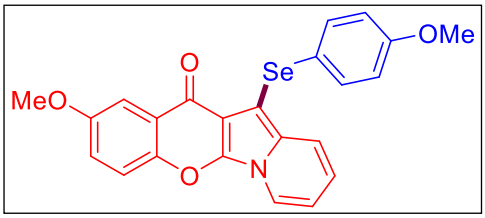
The title compound was prepared following the general procedure for Table 2, using 12*H*-chromeno[3,2-*b*]indolizin-12-one **1a** (0.25 mmol, 0.059 g) and bis(butyl) diselenide **4f** (0.2 mmol, 0.055 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5af** as a yellow solid; Yield: 0.078 g, 84%; M.P.: 80 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.44 (d, J = 8.0 Hz, 1H), 8.03 (dd, J = 7.2 & 1.2 Hz, 1H), 7.71-7.65 (m, 2H), 7.57 (d, J = 8.0 Hz, 1H), 7.43 (t, J = 8.0 Hz, 1H), 6.80-6.77 (m, 1H), 6.67-6.64 (m, 1H), 2.98 (t, J = 6.8 Hz, 2H), 1.57 (quint, J = 7.2 Hz, 2H), 1.39 (sext, J = 7.6 Hz, 2H), 0.83 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.7, 153.7, 141.7, 133.0, 131.0, 127.0, 124.5, 123.8, 120.3, 119.8, 117.3, 112.4, 110.0, 88.4, 32.2, 29.7, 22.8, 13.7; HRMS (ESI) exact mass calcd for $C_{19}H_{17}NO_2Se$ + H (M + H), 372.0498; Found: 372.0043.

2-Methoxy-11-(phenylselanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5ba)*:



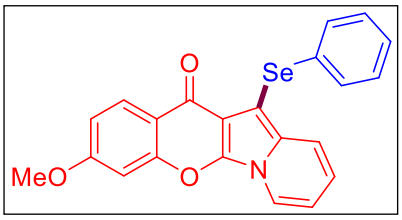
The title compound was prepared following the general procedure for Table 2, using 2-methoxy-12*H*-chromeno[3,2-*b*]indolizin-12-one **1b** (0.25 mmol, 0.067 g) and diphenyl diselenide **4a** (0.2 mmol, 0.062 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5ba** as a yellow solid; Yield: 0.099 g, 94%; M.P.: 202 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09 (d, J = 7.2 Hz, 1H), 7.80 (d, J = 3.2 Hz, 1H), 7.70 (d, J = 9.2 Hz, 1H), 7.52 (d, J = 9.2 Hz, 1H), 7.40-7.37 (m, 2H), 7.29-7.28 (m, 1H), 7.16-7.08 (m, 3H), 6.87-6.83 (m, 1H), 6.73-6.69 (m, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.4, 156.5, 148.4, 142.2, 134.1, 132.0, 129.9, 129.0, 126.1, 124.3, 122.6, 121.0, 120.7, 120.1, 118.6, 112.6, 109.3, 106.8, 87.3, 55.9; HRMS (ESI) exact mass calcd for $C_{22}H_{15}NO_3Se$ + H (M + H), 422.0290 Found: 422.0290.

2-Methoxy-11-((4-methoxyphenyl)selanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5bd)*:



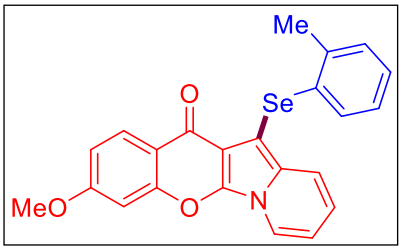
The title compound was prepared following the general procedure for Table 2, using 2-methoxy-12*H*-chromeno[3,2-*b*]indolizin-12-one **1b** (0.25 mmol, 0.067 g) and bis(4-methoxyphenyl) diselenide **4d** (0.2 mmol, 0.074 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5bd** as a yellow solid; Yield: 0.099 g, 88%; M.P.: 180 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, J = 7.2 Hz, 1H), 7.81 (d, J = 3.2 Hz, 1H), 7.73 (d, J = 9.6 Hz, 1H), 7.52-7.47 (m, 3H), 7.26 (dd, J = 8.8 & 3.2 Hz, 1H), 6.83 (dd, J = 10.4 & 6.4 Hz, 1H), 6.72 (d, J = 9.2 Hz, 2H), 6.67 (t, J = 6.8 Hz, 1H), 3.91 (s, 3H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.4, 158.8, 156.4, 148.3, 141.9, 133.3, 131.5, 124.3, 123.8, 122.6, 120.7, 120.6, 120.1, 118.6, 114.7, 112.4, 109.2, 106.7, 89.0, 55.9, 55.2; HRMS (ESI) exact mass calcd for $C_{23}H_{17}NO_4Se$ + H (M + H), 452.0396; Found: 452.0389.

3-Methoxy-11-(phenylselanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5ca)*:



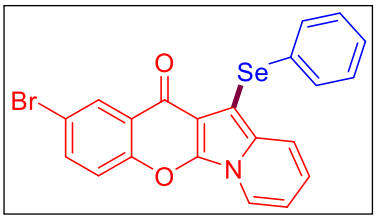
The title compound was prepared following the general procedure for Table 2, using 3-methoxy-12*H*-chromeno[3,2-*b*]indolizin-12-one **1c** (0.25 mmol, 0.067 g) and diphenyl diselenide **4a** (0.2 mmol, 0.062 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5ca** as a yellow solid; Yield: 0.097 g, 92%; M.P.: 178 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.27 (d, J = 9.2 Hz, 1H), 8.00 (d, J = 6.8 Hz, 1H), 7.64 (d, J = 9.6 Hz, 1H), 7.38 (d, J = 6.4 Hz, 2H), 7.15-7.07 (m, 3H), 6.94-6.92 (m, 2H), 6.82-6.78 (m, 1H), 6.67 (d, J = 7.2 Hz, 1H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.1, 163.6, 155.3, 141.6, 134.1, 131.5, 129.9, 128.9, 128.3, 126.1, 120.6, 120.4, 119.9, 117.5, 113.0, 112.6, 109.5, 100.4, 87.4, 55.9; HRMS (ESI) exact mass calcd for $C_{22}H_{15}NO_3Se$ + H (M + H), 422.0290; Found: 422.0298.

3-Methoxy-11-(*o*-tolylselanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5cc)*:



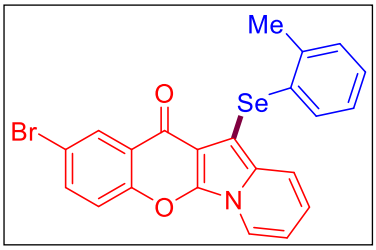
The title compound was prepared following the general procedure for Table 2, using 3-methoxy-12*H*-chromeno[3,2-*b*]indolizin-12-one **1c** (0.25 mmol, 0.067 g) and bis(*o*-tolyl) diselenide **4c** (0.2 mmol, 0.068 g), after column chromatography (20-25% EtOAc/Hexanes) obtained **5cc** as a yellow solid; Yield: 0.092 g, 85%; M.P.: 168 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.30 (d, J = 8.8 Hz, 1H), 8.09 (dt, J = 7.2 & 1.2 Hz, 1H), 7.61 (dt, J = 9.6 & 1.2 Hz, 1H), 7.11 (d, J = 6.0 Hz, 1H), 7.01-6.97 (m, 3H), 6.89 (dd, J = 8.0 & 1.6 Hz, 1H), 6.85 (d, J = 8.0 Hz, 1H), 6.83-6.80 (m, 1H), 6.72 (td, J = 8.0 & 1.2 Hz, 1H), 3.94 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.1, 163.7, 155.4, 141.8, 136.6, 134.9, 131.8, 129.9, 128.6, 128.4, 126.4, 125.6, 120.6, 120.5, 120.1, 117.7, 112.9, 112.7, 109.8, 100.5, 86.2, 55.5, 21.5; HRMS (ESI) exact mass calcd for $C_{23}H_{17}NO_3Se$ + H (M + H), 436.0447; Found: 436.0455.

2-Bromo-11-(phenylselanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5ea)*:



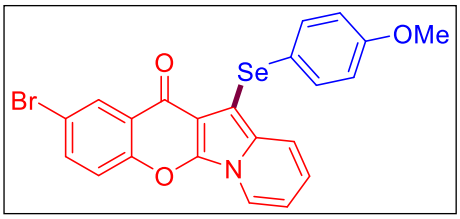
The title compound was prepared following the general procedure for Table 2, using 2-bromo-12*H*-chromeno[3,2-*b*]indolizin-12-one **1e** (0.25 mmol, 0.079 g) and diphenyl diselenide **4a** (0.2 mmol, 0.062 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5ea** as a yellow solid; Yield: 0.101 g, 86%; M.P.: 186 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.50-8.49 (m, 1H), 8.08 (d, J = 6.8 Hz, 1H), 7.77-7.74 (m, 1H), 7.69 (d, J = 9.2 Hz, 1H), 7.47 (dd, J = 9.2 & 3.2 Hz, 1H), 7.39-7.36 (m, 2H), 7.16-7.08 (m, 3H), 6.89-6.85 (m, 1H), 6.76-6.71 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.0, 152.5, 141.6, 135.9, 133.7, 132.1, 130.2, 129.7, 129.0, 126.3, 125.2, 121.3, 120.6, 120.1, 119.2, 117.9, 113.0, 109.6, 87.8; HRMS (ESI) exact mass calcd for $C_{21}H_{12}BrNO_2Se$ + H (M + H), 469.9290; Found: 469.9284.

2-Bromo-11-(*o*-tolylselanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5ec)*:



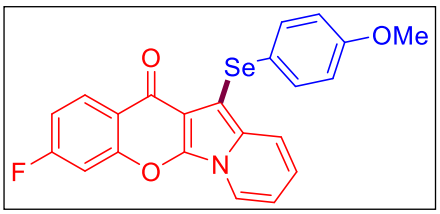
The title compound was prepared following the general procedure for Table 2, using 2-bromo-12*H*-chromeno[3,2-*b*]indolizin-12-one **1e** (0.25 mmol, 0.079 g) and bis(*o*-tolyl) diselenide **4c** (0.2 mmol, 0.068 g), after column chromatography (20-25% EtOAc/Hexanes) obtained **5ec** as a yellow solid; Yield: 0.099 g, 82%; M.P.: 174 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.43 (d, J = 2.4 Hz, 1H), 8.06 (d, J = 7.2 Hz, 1H), 7.72 (dd, J = 8.8 & 2.8 Hz, 1H), 7.58 (d, J = 9.2 Hz, 1H), 7.44 (d, J = 8.8 Hz, 1H), 7.11 (d, J = 7.6 Hz, 1H), 7.02-6.98 (m, 1H), 6.89 (d, J = 6.4 Hz, 1H), 6.86-6.82 (m, 2H), 6.73(t, J = 6.8 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.8, 152.4, 141.6, 136.8, 135.9, 134.5, 132.2, 129.9, 129.6, 128.9, 126.4, 125.9, 125.0, 121.3, 120.6, 120.0, 119.2, 117.9, 113.0, 109.8, 86.5, 21.6; HRMS (ESI) exact mass calcd for $C_{22}H_{14}BrNO_2Se$ + H (M + H), 483.9446; Found: 483.9448.

2-Bromo-11-((4-methoxyphenyl)selanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-one *(5ed)*:



The title compound was prepared following the general procedure for Table 2, using 2-bromo-12*H*-chromeno[3,2-*b*]indolizin-12-one **1e** (0.25 mmol, 0.079 g) and bis(4-methoxyphenyl) diselenide **4d** (0.2 mmol, 0.074 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5ed** as a yellow solid; Yield: 0.112 g, 90%; M.P.: 136 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52 (d, J = 2.4 Hz, 1H), 8.03 (dt, J = 7.2 & 1.2 Hz, 1H), 7.76-7.73 (m, 2H), 7.53-7.49 (m, 2H), 7.45 (d, J = 8.8 Hz, 1H), 6.86 (ddd, J = 9.2, 6.4 & 1.2 Hz, 1H), 6.74-6.69 (m, 3H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.1, 158.9, 152.4, 141.5, 135.9, 133.6, 131.6, 129.7, 125.2, 123.5, 121.0, 120.5, 120.1, 119.2, 117.9, 114.7, 112.9, 109.5, 89.6, 55.2; HRMS (ESI) exact mass calcd for $C_{22}H_{14}BrNO_3Se$ + H (M + H), 499.9395; Found: 499.9393.

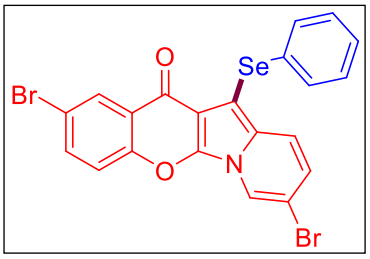
3-Fluoro-11-((4-methoxyphenyl)selanyl)-12*H*-chromeno[3,2-b]indolizin-12-one *(5fd)*:



The title compound was prepared following the general procedure for Table 2, using 3-fluoro-12*H*-chromeno[3,2-*b*]indolizin-12-one **1f** (0.25 mmol, 0.064 g) and bis(4-methoxyphenyl) diselenide **4d** (0.2 mmol, 0.074 g), after trituration process in 10-15% EtOAc/Hexanes obtained **5fd** as a yellow solid; Yield: 0.090 g, 82%; M.P.: 162 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.44 (dd, J = 8.8 & 6.4, Hz, 1H), 8.03 (d, J = 7.2 Hz, 1H), 7.73 (d, J = 9.2 Hz, 1H), 7.50 (d, J = 8.8 Hz, 2H), 7.26 (d, J = 8.8, 2.4 Hz, 1H), 7.18-7.14 (m, 1H), 6.85 (ddd, J = 9.2, 6.4 & 1.2, Hz, 1H), 6.74-6.69 (m, 3H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.6, 165.2 ($J_{C\text{-}F}$ = 252.0 Hz), 158.9, 154.5 ($J_{C\text{-}F}$ = 13.0 Hz), 141.6, 133.4, 131.4, 129.4 ($J_{C\text{-}F}$ = 11.0 Hz), 123.6, 120.8, 120.7, 120.4, 120.1, 114.7, 113.1 ($J_{C\text{-}F}$ = 22.0 Hz), 112.8, 109.5, 104.3 ($J_{C\text{-}F}$ = 26.0 Hz), 89.5, 55.2; ^{19}F NMR (376 MHz, $CDCl_3$): -103.8; HRMS (ESI) exact mass calcd for

$C_{22}H_{14}FNO_3Se$ + H (M + H), 440.0196; Found: 440.0192.

2,8-Dibromo-11-(phenylselanyl)-12*H*-chromeno[3,2-*b*]indolizin-12-ones *(5ga)*:

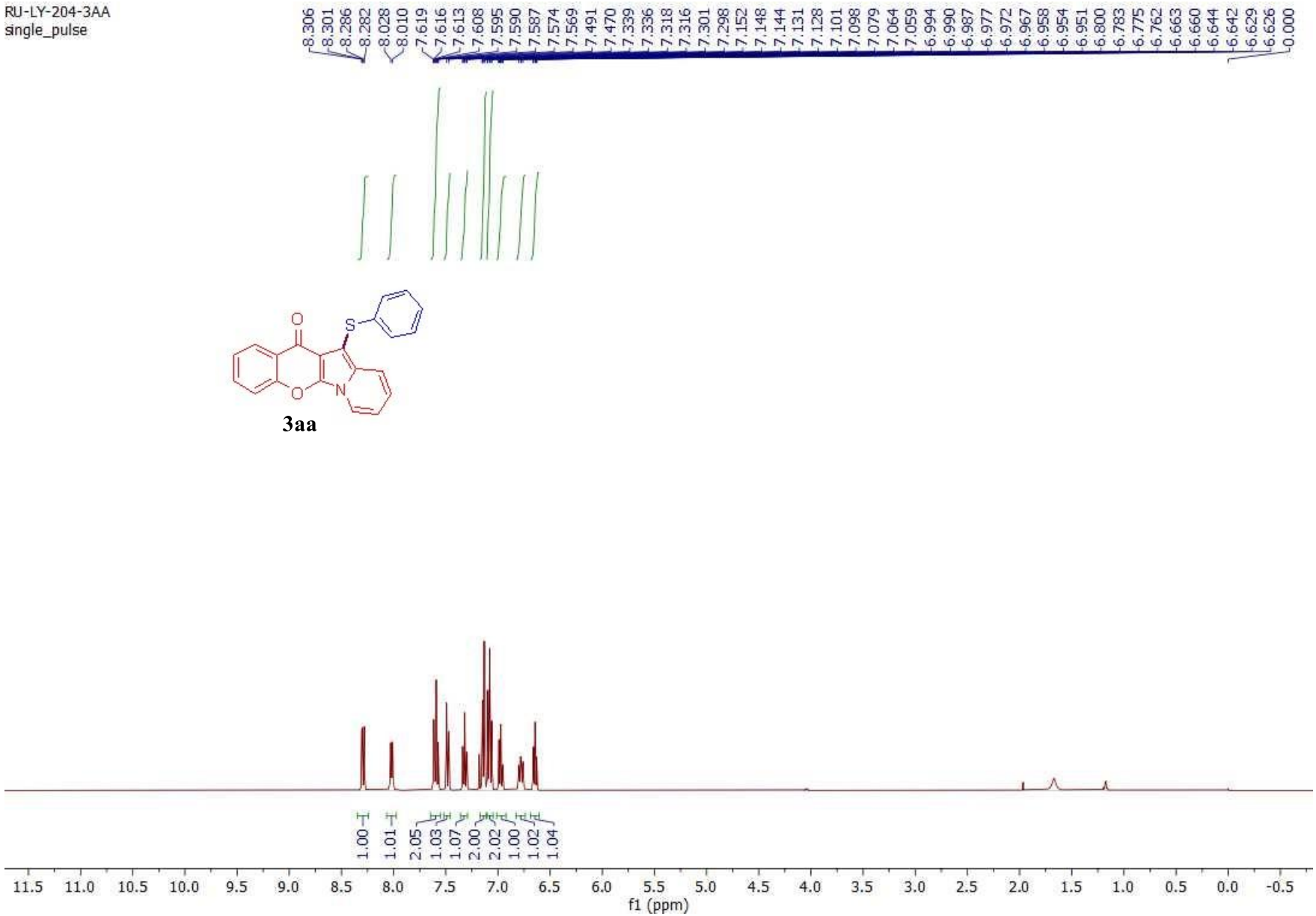


The title compound was prepared following the general procedure for Table 3, using 2,8-dibromo-12*H*-chromeno[3,2-*b*]indolizin-12-one **1g** (0.25 mmol, 0.098 g) and diphenyl diselenide **4a** (0.2 mmol, 0.062 g), after column chromatography process in 20-25% EtOAc/Hexanes) obtained **5ga** as a yellow solid; Yield: 0.084 g, 61%; M.P.: 190 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.48 (d, J = 2.8 Hz, 1H), 8.25 (s, 1H), 7.78 (dd, J = 8.8 & 2.4 Hz, 1H), 7.60 (dd, J = 9.6 & 1.2 Hz, 1H), 7.47 (d, J = 9.2 Hz, 1H), 7.39-7.36 (m, 2H), 7.17-7.12 (m, 3H), 6.90 (dd, J = 9.6 & 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.8, 152.5, 141.2, 136.3, 133.2, 130.5, 130.0, 129.8, 129.1, 126.6, 125.1, 124.8, 120.9, 120.3, 119.2, 118.2, 109.8, 108.5, 90.1; HRMS (ESI) exact mass calcd for $C_{21}H_{11}Br_2NO_2Se$ + H (M + H), 547.8395; Found: 547.8396.

References:

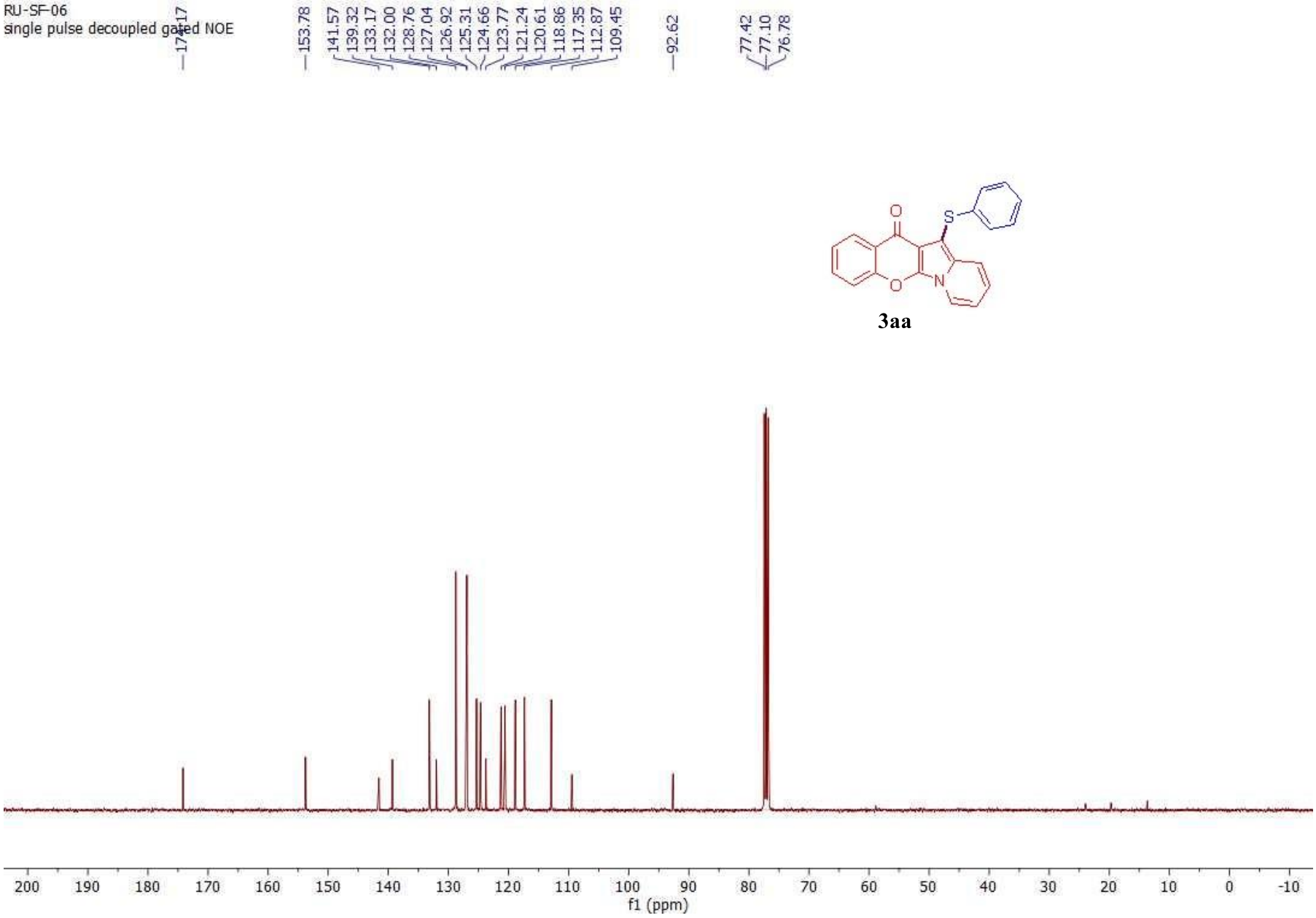
1. D. Basavaiah and A. J. Rao, *Tetrahedron Lett.* 2003. **44**, 4365.

^{1}H NMR spectrum of 3aa (400 MHz, $CDCl_3$)



3aa

^{13}C NMR spectrum of 3aa (100 MHz, $CDCl_3$)

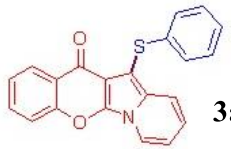


3aa

Mass spectrum of 3aa

Data File	SJ-LY-204.d	**Sample Name**	SJ-LY-204
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 6:56:47 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



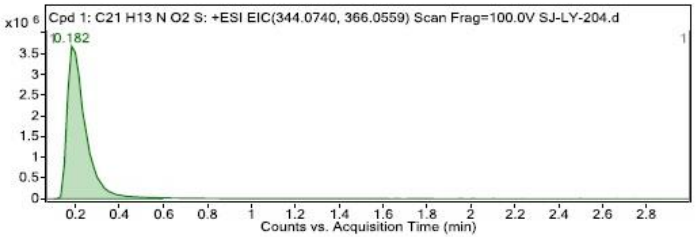
3aa

Chemical Formula (M): $C_{21}H_{13}NO_2S$
Exact Mass: 343.0667
Found (M+H) = 344.0741

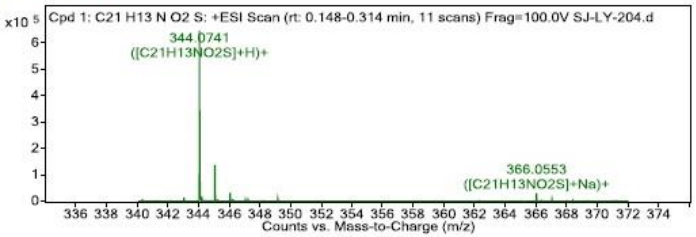
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C21 H13 N O2 S	0.182	343.0668	652803	C21 H13 N O2 S	343.0667	0.16

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H13 N O2 S	344.0741	0.182	Find By Formula	343.0668



MS Zoomed Spectrum



MS Spectrum Peak List

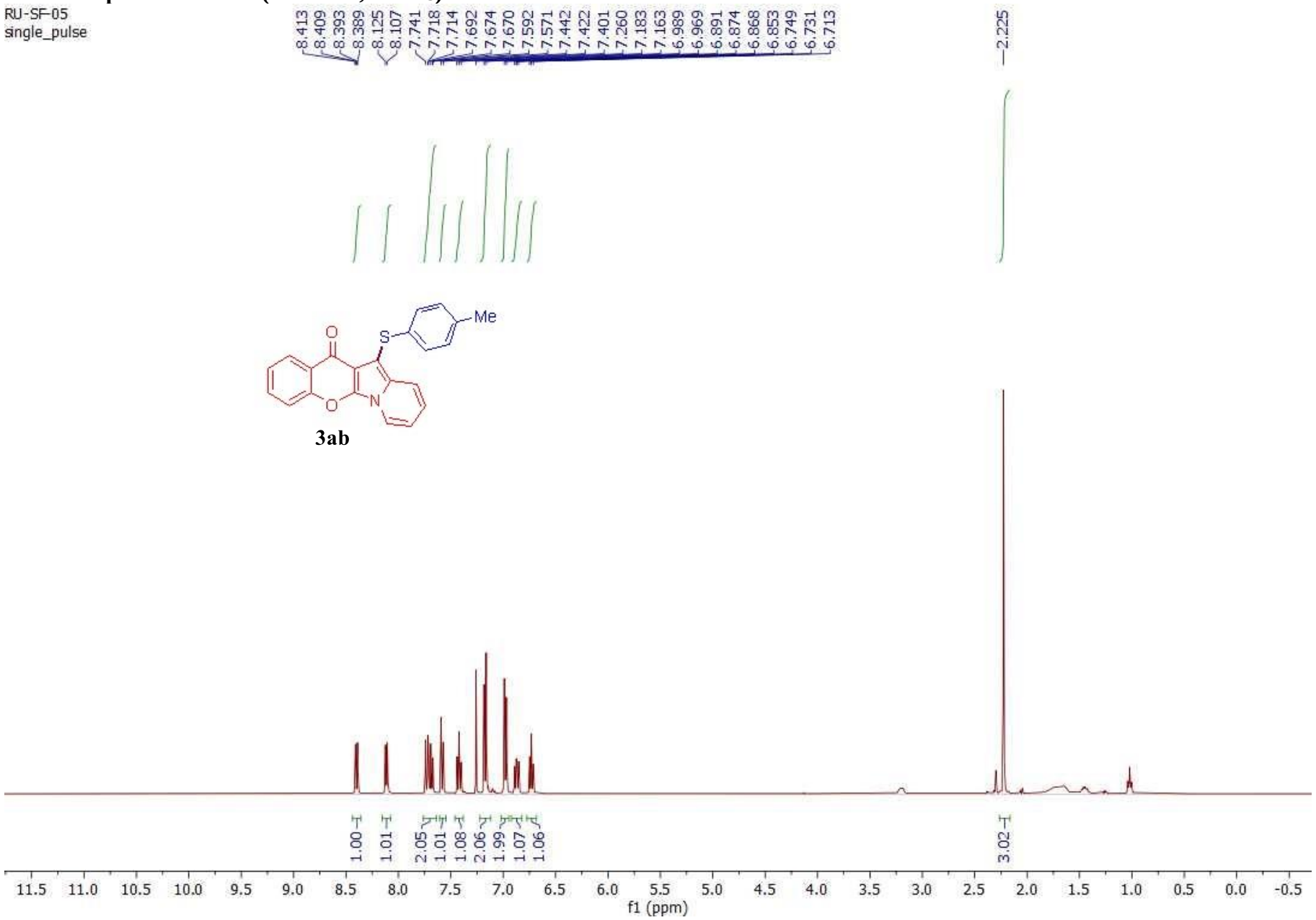
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
344.0741	344.074	-0.36	1	652802.62	C21H13NO2S	(M+H)+
345.0769	345.0771	0.59	1	142673.69	C21H13NO2S	(M+H)+
346.0745	346.074	-1.41	1	31869.94	C21H13NO2S	(M+H)+
366.0553	366.0559	1.59	1	30756.65	C21H13NO2S	(M+Na)+
367.0587	367.0591	0.92	1	6922.59	C21H13NO2S	(M+Na)+
368.0556	368.056	0.92	1	1566.83	C21H13NO2S	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

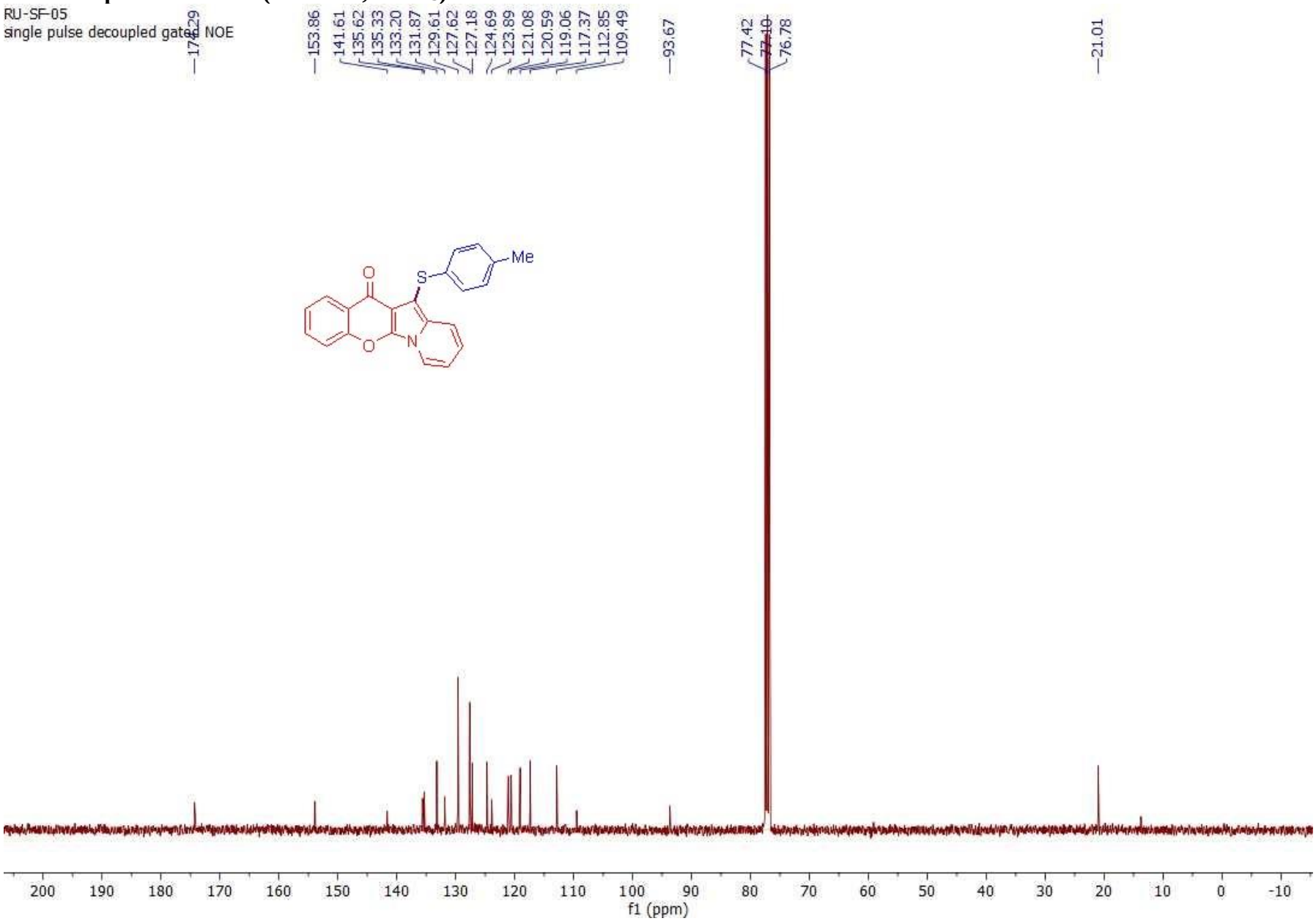
---End Of Report---

^{1}H NMR spectrum of 3ab (400 MHz, $CDCl_3$)

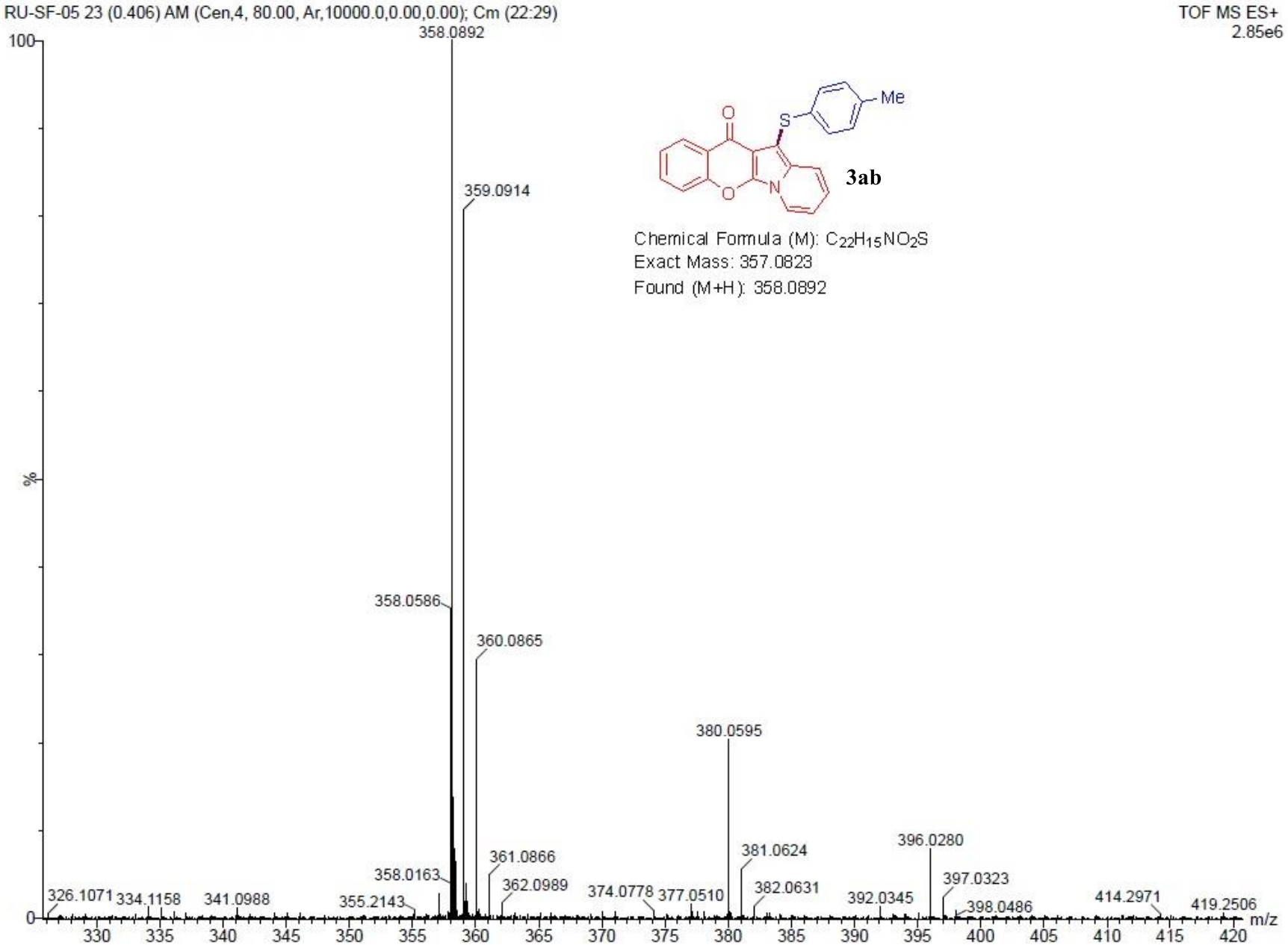


3ab

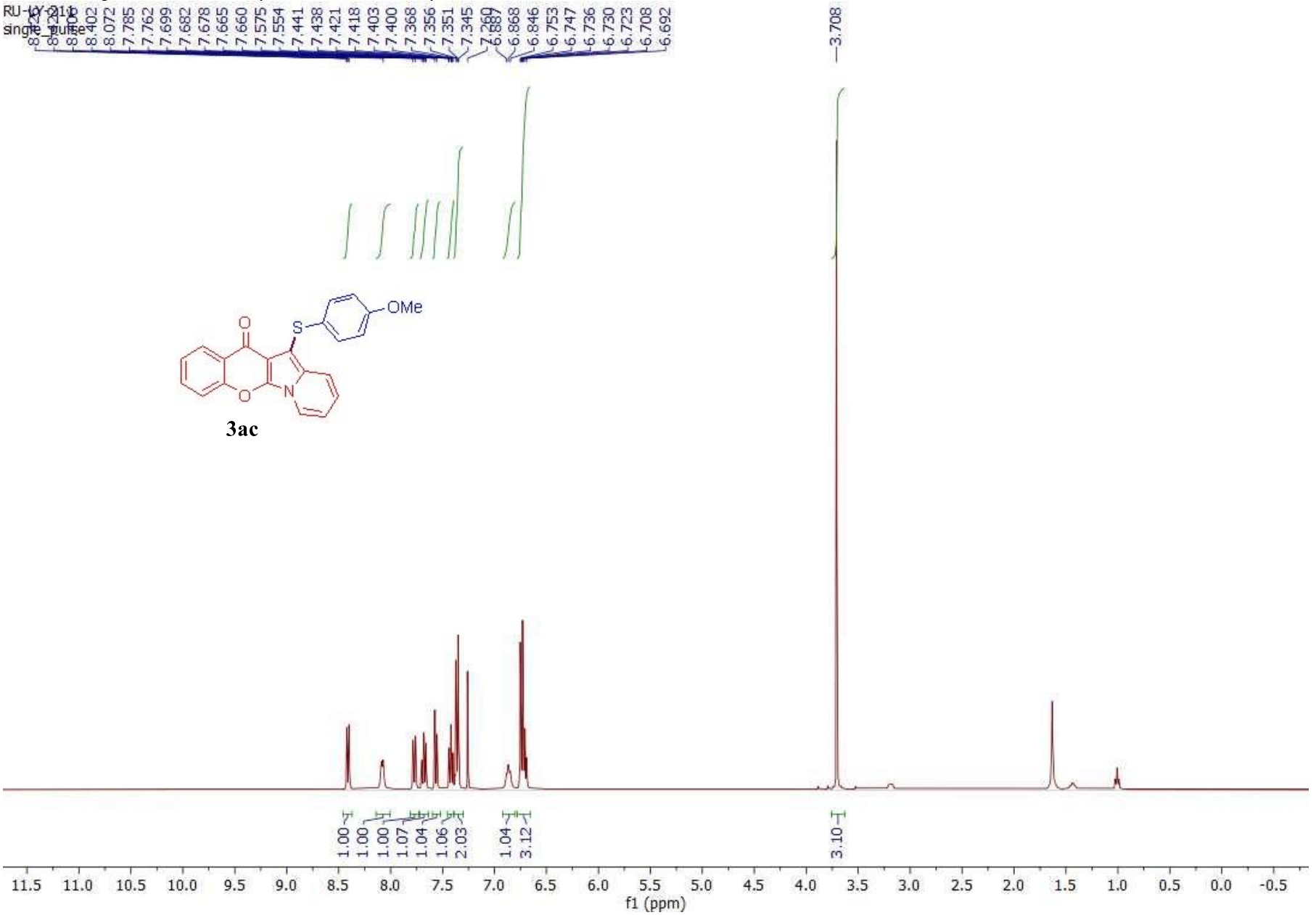
^{13}C NMR spectrum of 3ab (100 MHz, $CDCl_3$)



Mass spectrum of 3ab

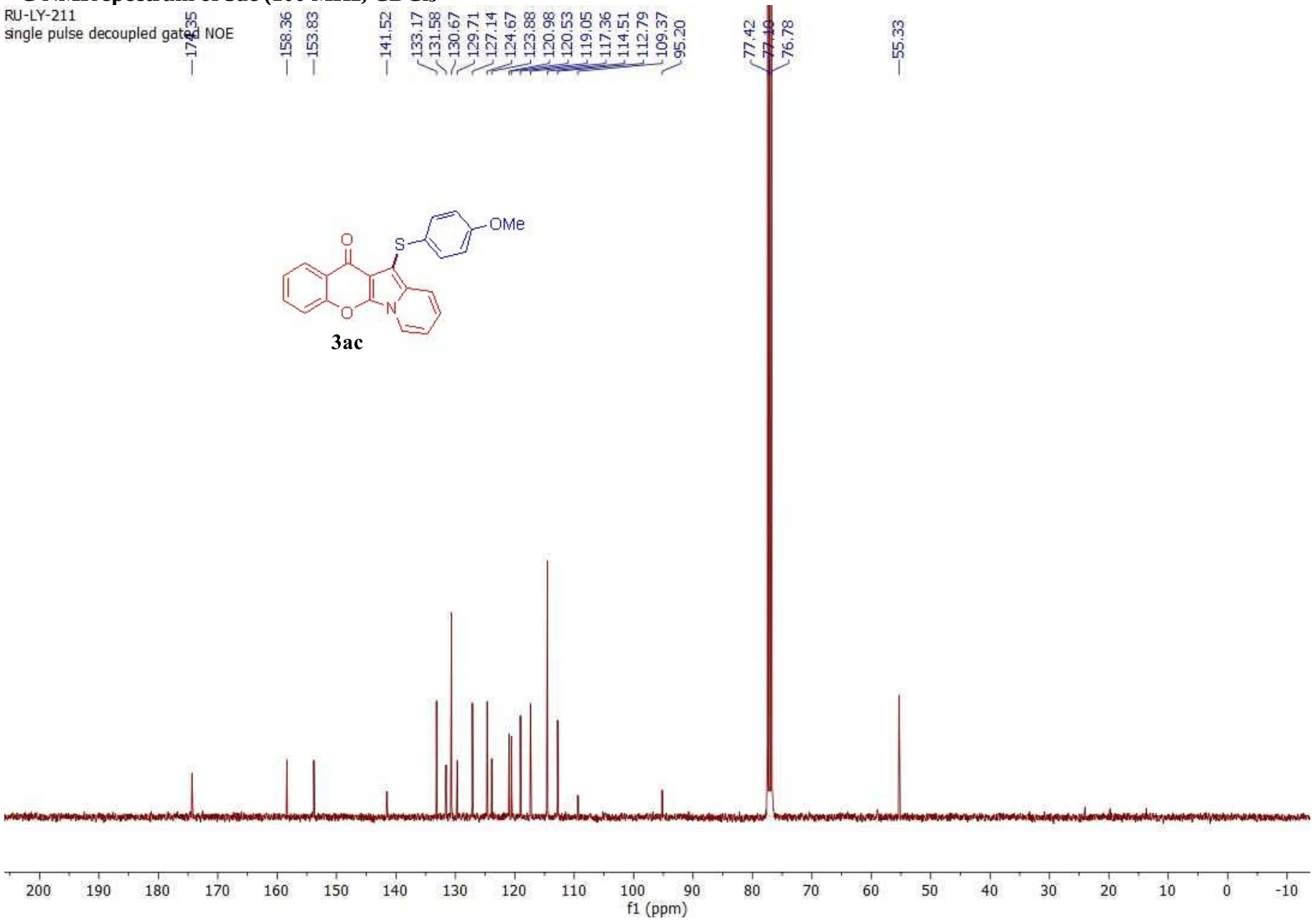


^{1}H NMR spectrum of 3ac (400 MHz, $CDCl_3$)



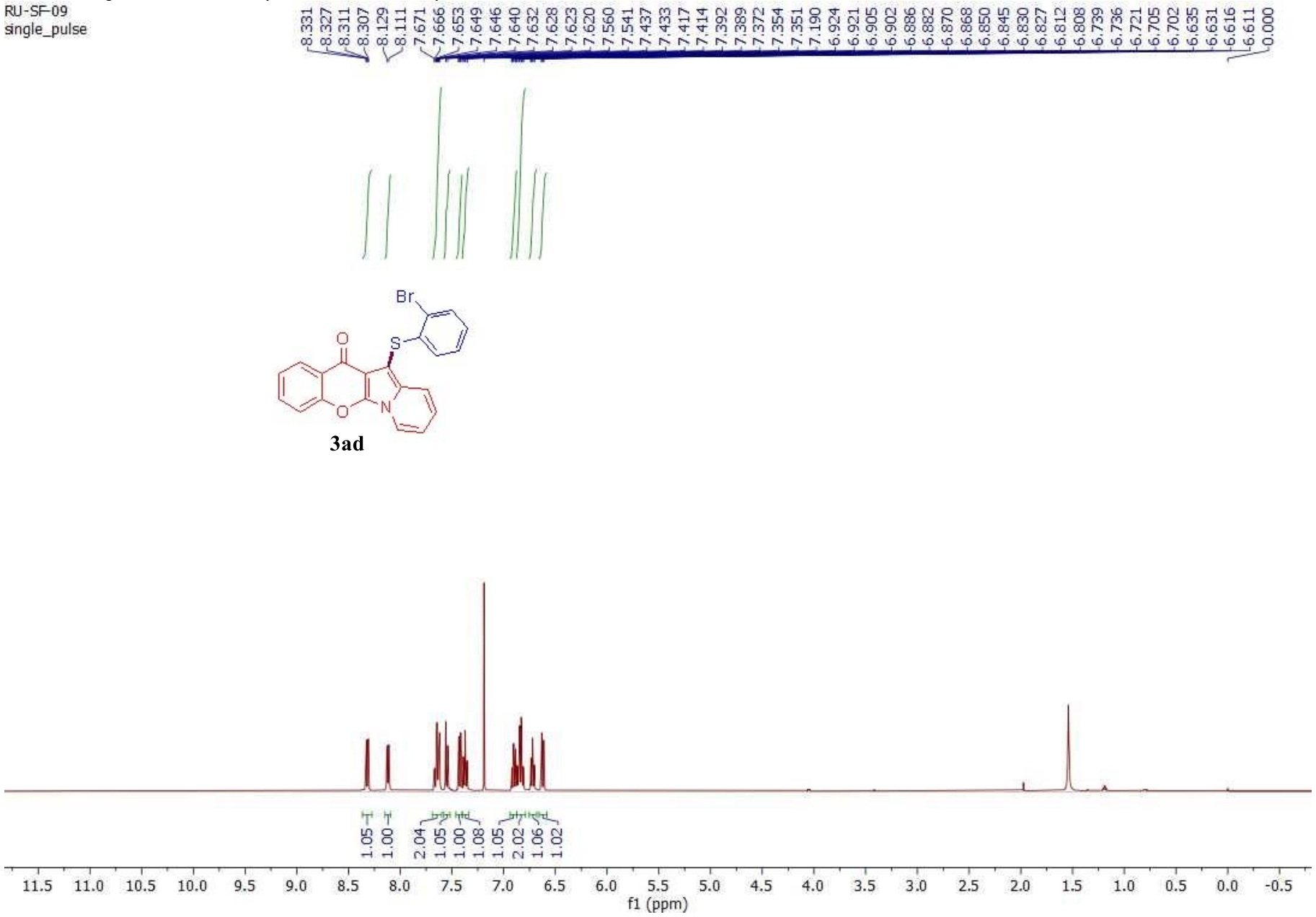
3ac

^{13}C NMR spectrum of 3ac (100 MHz, $CDCl_3$



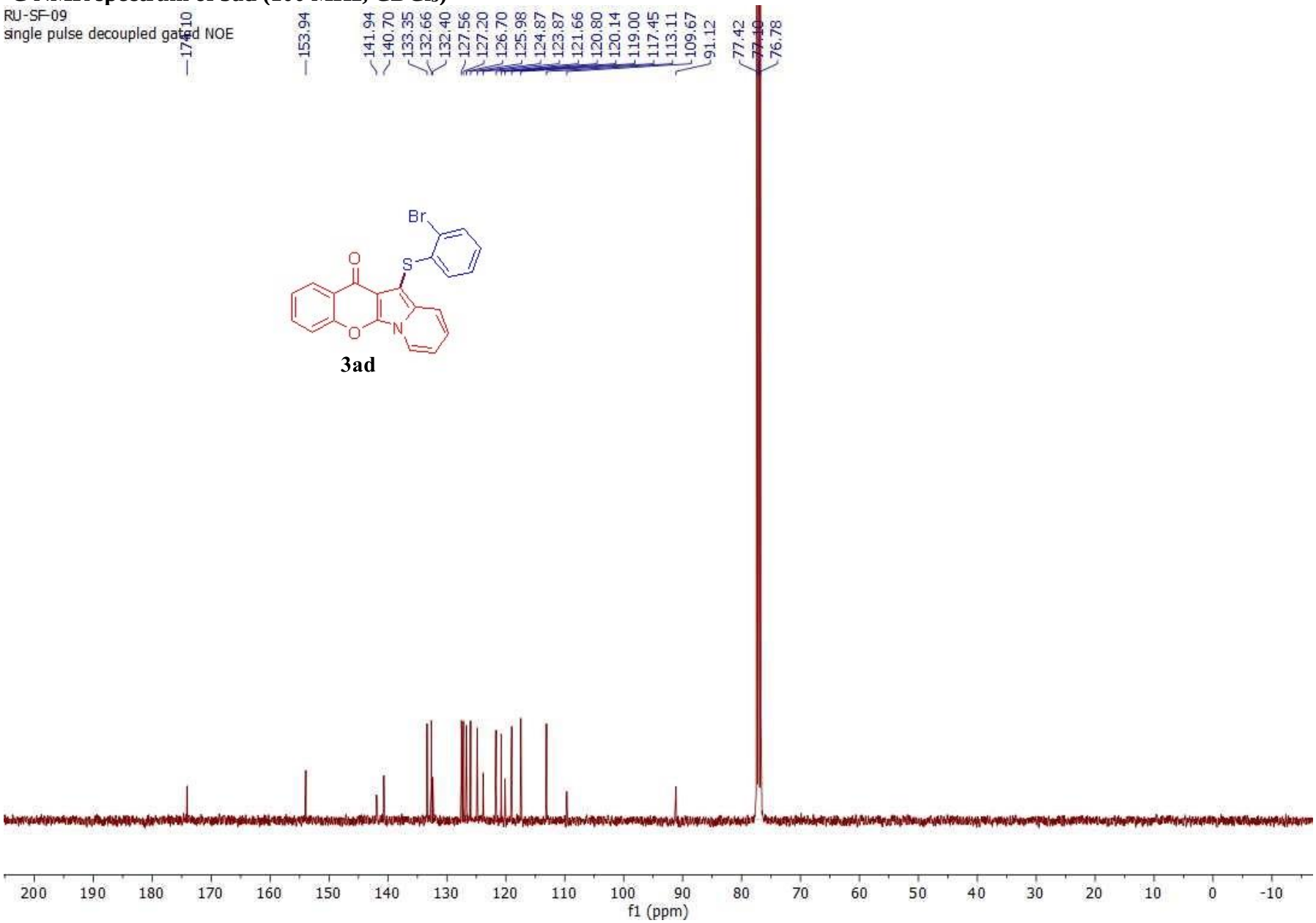
3ac

^{1}H NMR spectrum of 3ad (400 MHz, $CDCl_3$)



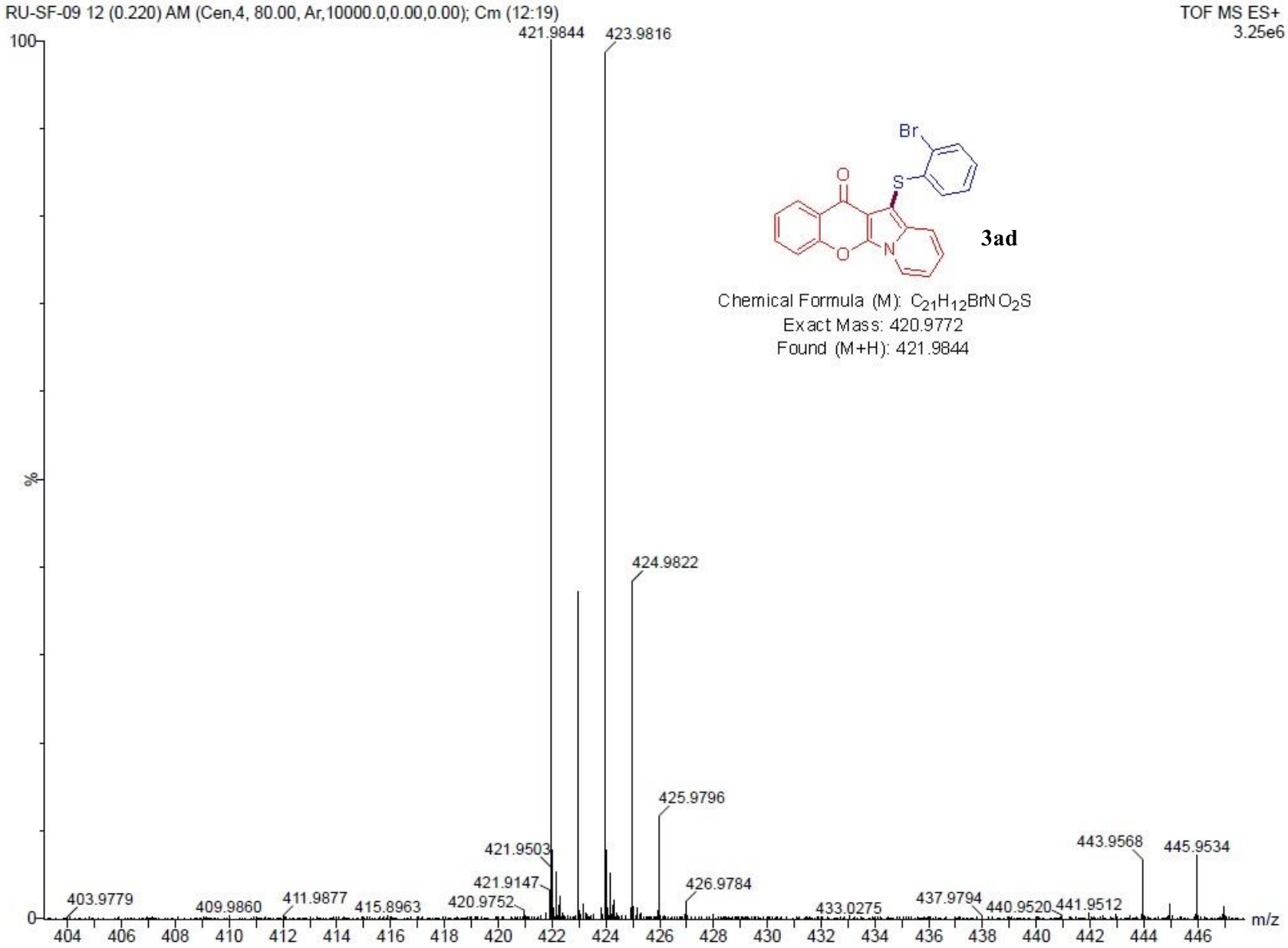
3ad

^{13}C NMR spectrum of 3ad (100 MHz, $CDCl_3$)

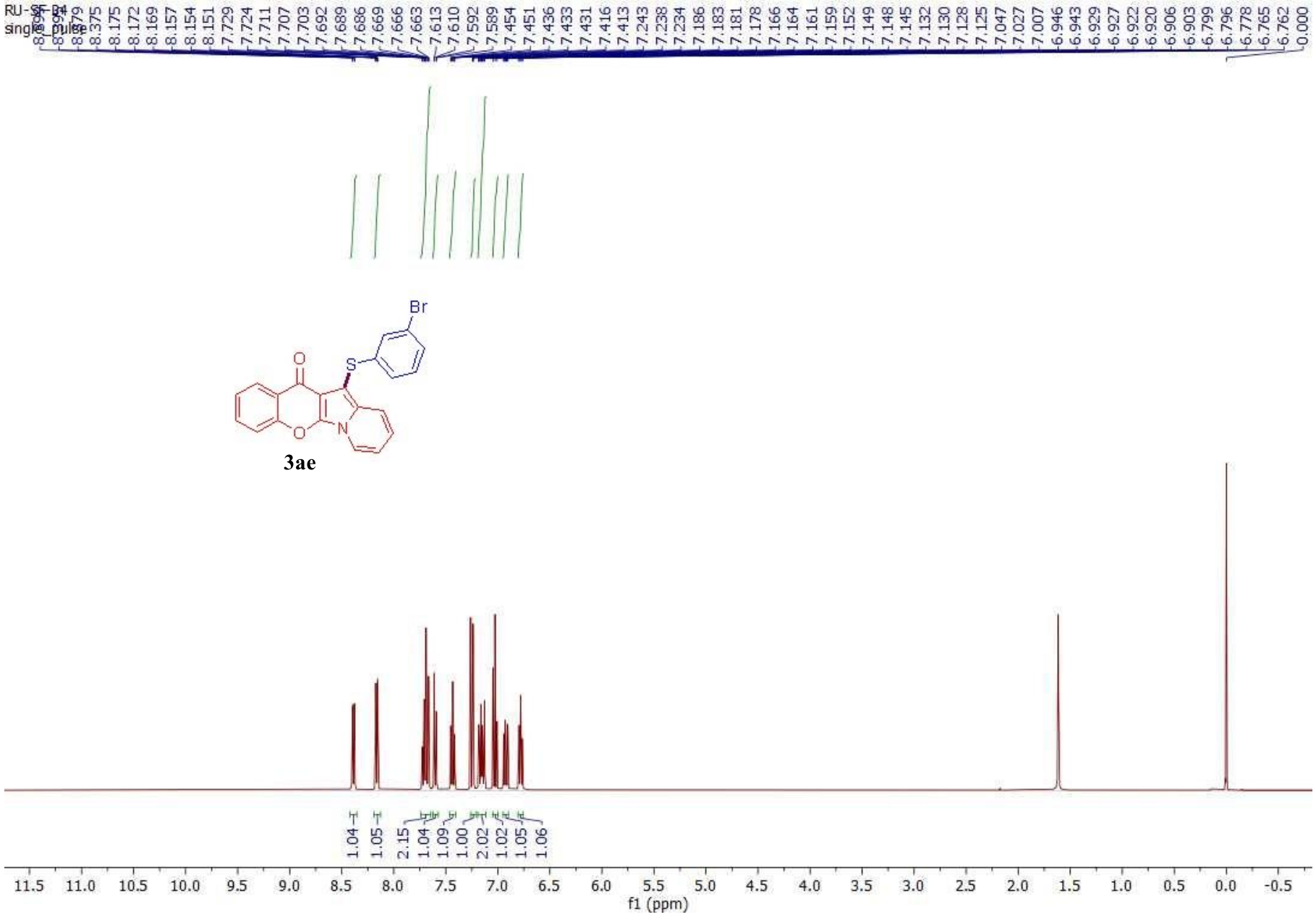


3ad

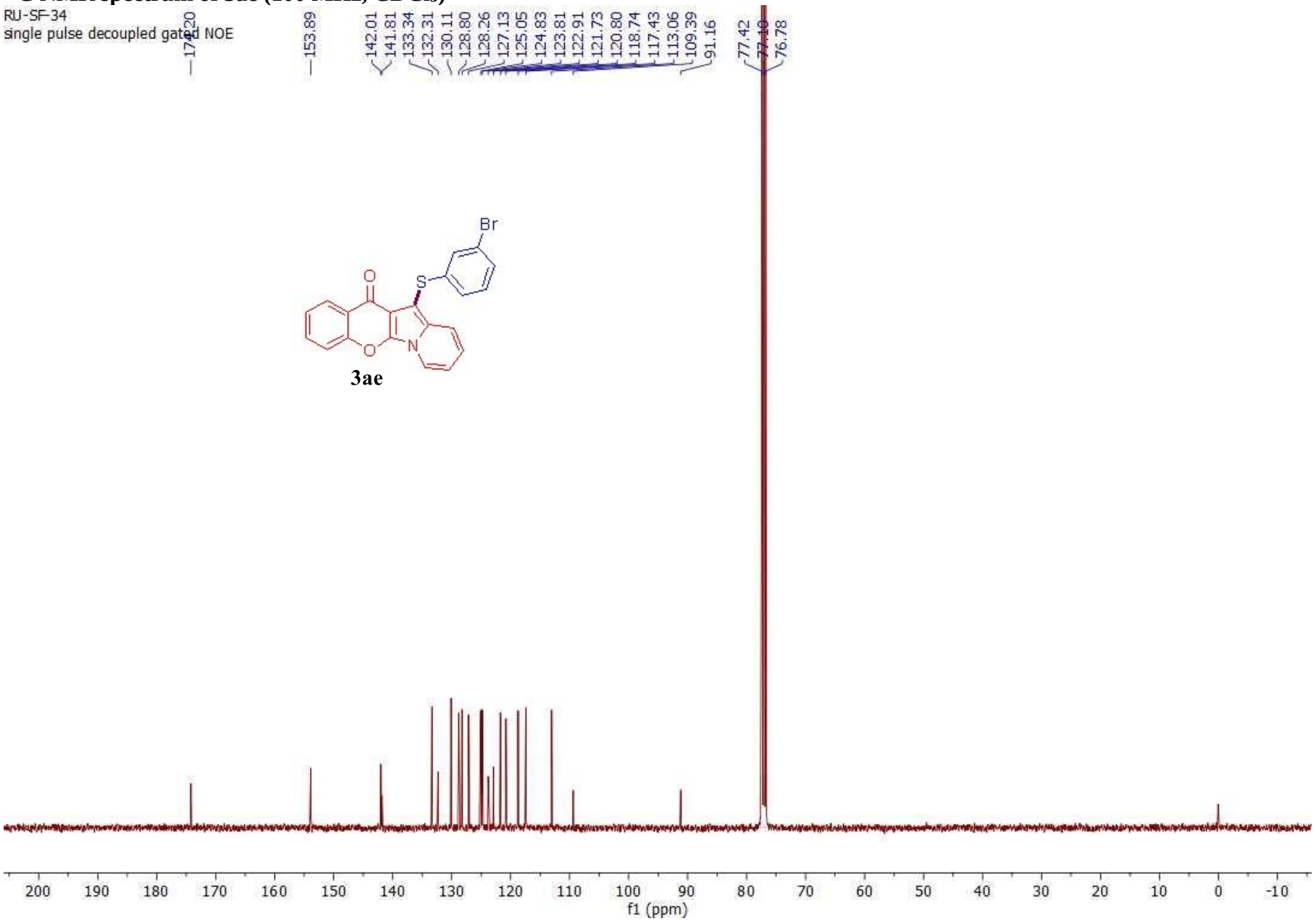
Mass spectrum of 3ad



^{1}H NMR spectrum of 3ae (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of 3ae (100 MHz, $CDCl_3$)

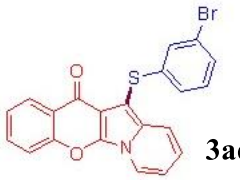


3ae

Mass spectrum of 3ae

Data File	SJ-SF-34.d	**Sample Name**	SJ-SF-34
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 8:45:19 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



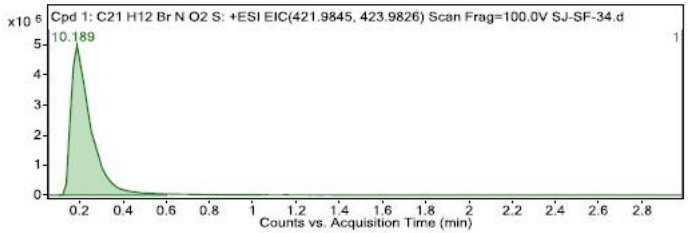
3ae

Chemical Formula (M): $C_{21}H_{12}BrNO_2S$
Exact Mass: 420.9772
Found (M+H): 421.9854

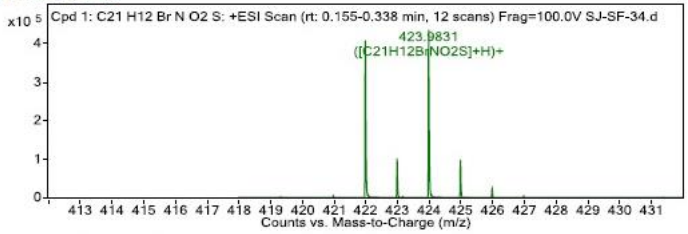
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C21 H12 Br N O2 S	0.189	420.9777	436508	C21 H12 Br N O2 S	420.9772	1.28

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H12 Br N O2 S	423.9831	0.189	Find By Formula	420.9777



MS Zoomed Spectrum



MS Spectrum Peak List

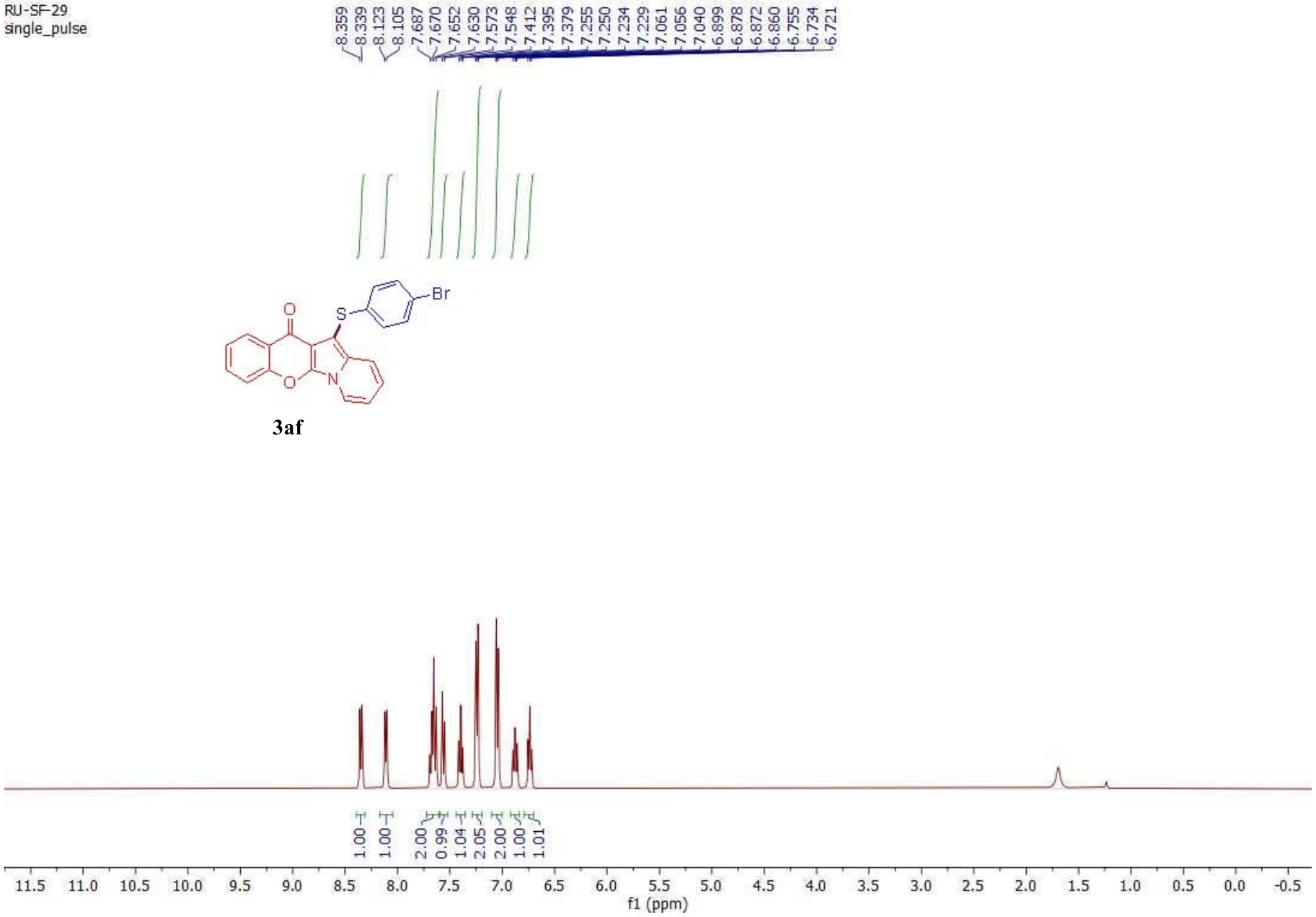
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
421.9854	421.9845	-2.1	1	409658.75	C21H12BrNO2S	(M+H)+
422.9874	422.9876	0.56	1	101527.19	C21H12BrNO2S	(M+H)+
423.9831	423.9826	-1.3	1	436507.94	C21H12BrNO2S	(M+H)+
424.9855	424.9856	0.2	1	98060.9	C21H12BrNO2S	(M+H)+
425.983	425.9826	-0.97	1	22249.11	C21H12BrNO2S	(M+H)+
426.983	426.9838	1.8	1	3972.86	C21H12BrNO2S	(M+H)+
427.9849	427.9853	1.13	1	522.57	C21H12BrNO2S	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

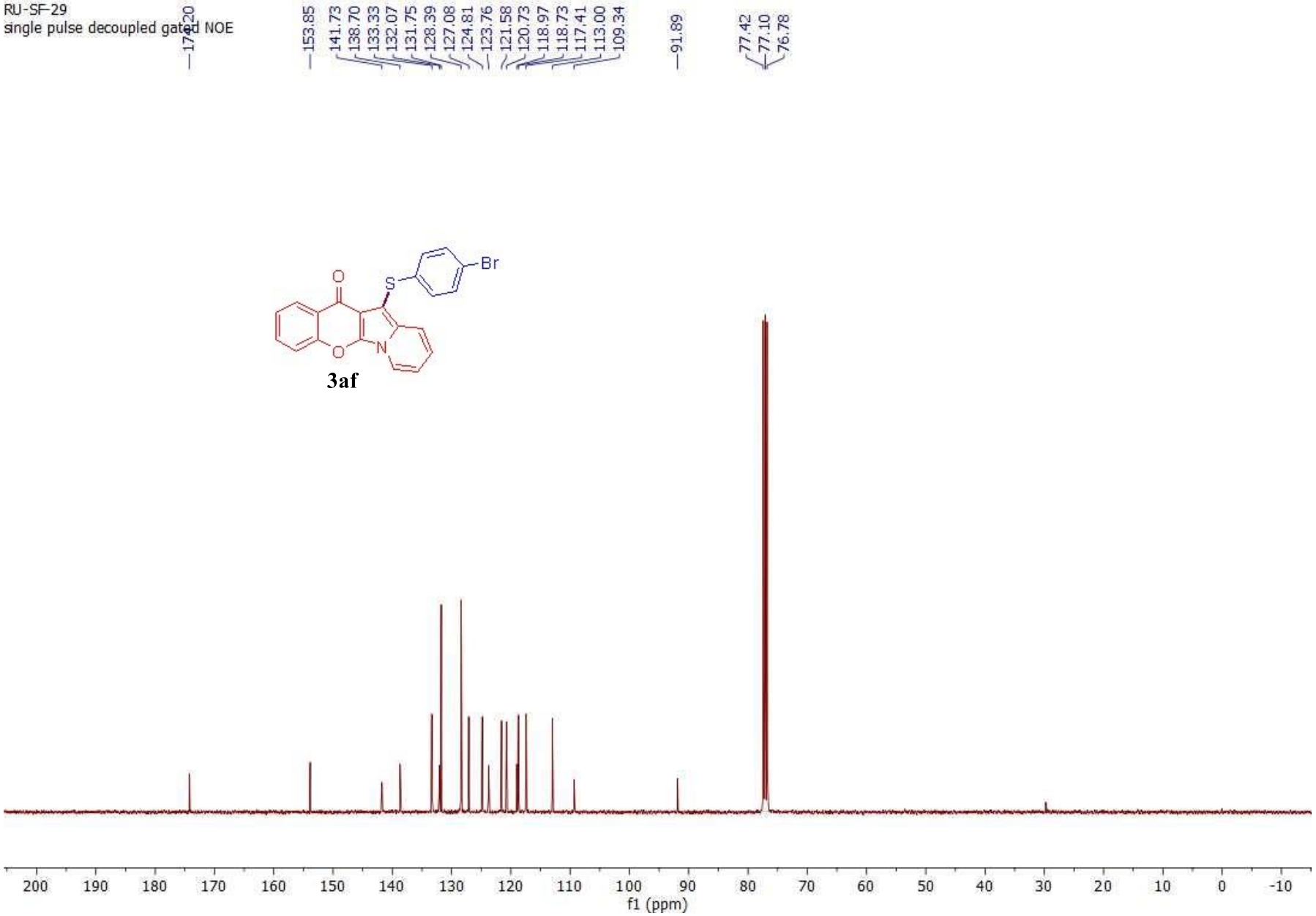
---End Of Report---

^{1}H NMR spectrum of 3af (400 MHz, $CDCl_3$)



3af

^{13}C NMR spectrum of 3af (100 MHz, $CDCl_3$)

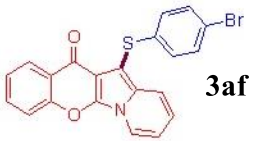


3af

Mass spectrum of 3af

Data File	SJ-SF-29.d	**Sample Name**	SJ-SF-29
Sample Type	Sample	**Position**	P1-B10
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 8:11:55 P
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



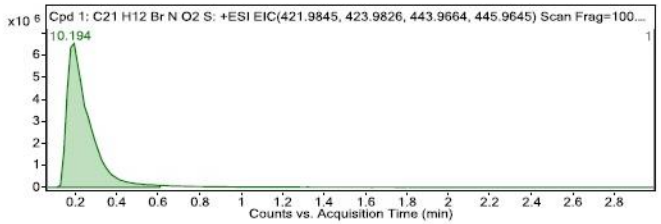
3af

Chemical Formula (M): $C_{21}H_{12}BrNO_2S$
Exact Mass: 420.9772
Found (M+H):421.9850

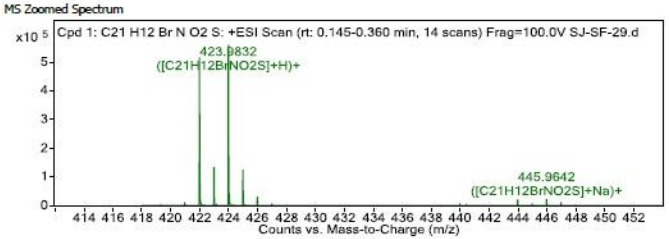
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C21 H12 Br N O2 S	0.194	420.9777	22405	C21 H12 Br N O2 S	420.9772	1.07

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H12 Br N O2 S	445.9642	0.194	Find By Formula	420.9777



MS Zoomed Spectrum



MS Spectrum Peak List

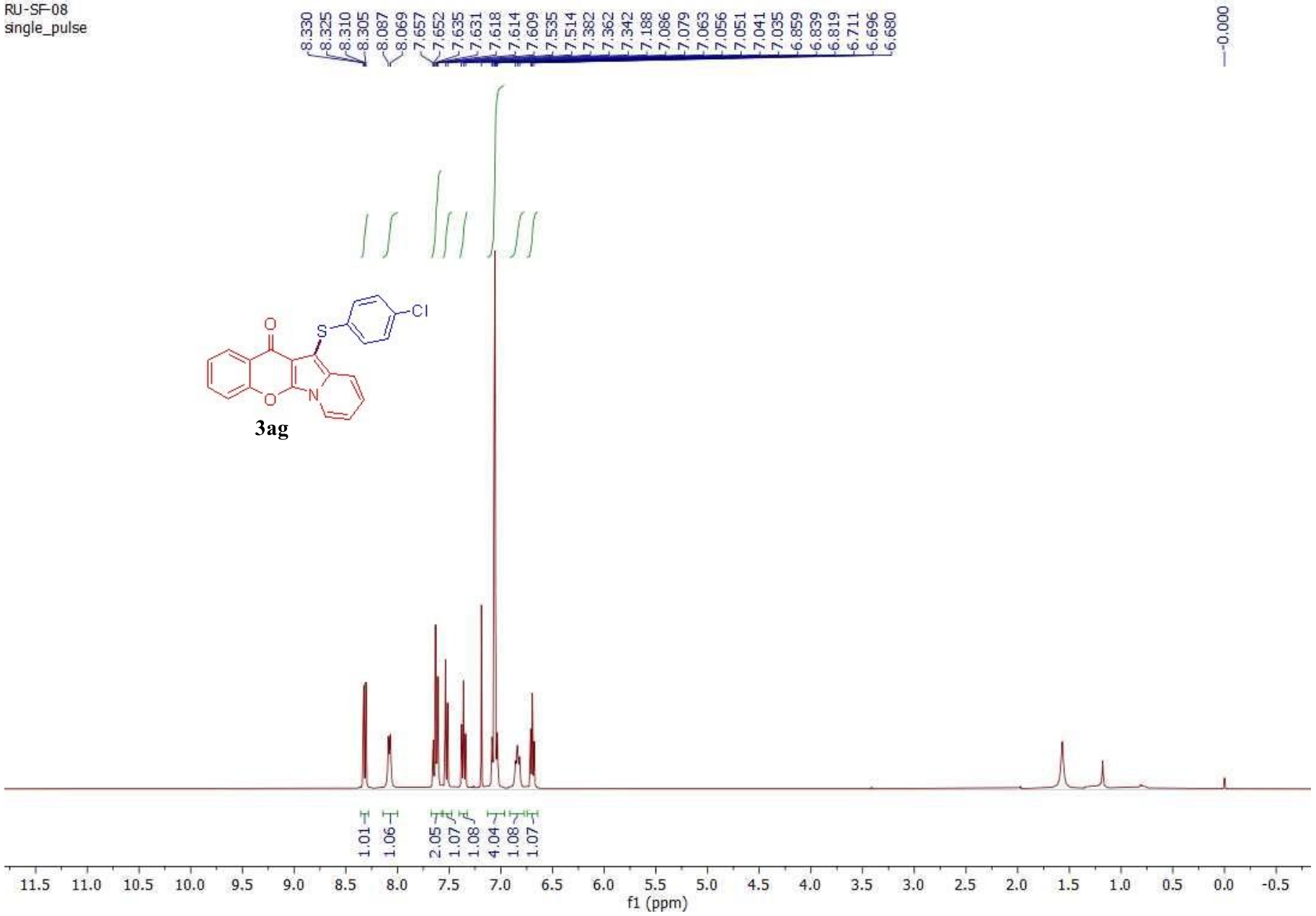
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
421.985	421.9845	-1.31	1	554982.23	C21H12BrNO2S	(M+H)+
422.9875	422.9876	0.27	1	134745.14	C21H12BrNO2S	(M+H)+
423.9832	423.9826	-1.53	1	571559.7	C21H12BrNO2S	(M+H)+
424.9857	424.9856	-0.26	1	130960.95	C21H12BrNO2S	(M+H)+
425.9831	425.9826	-1.24	1	29766.91	C21H12BrNO2S	(M+H)+
426.9832	426.9838	1.26	1	5244.5	C21H12BrNO2S	(M+H)+
443.9661	443.9664	0.75	1	21490.75	C21H12BrNO2S	(M+Na)+
444.9691	444.9696	1.07	1	5055.36	C21H12BrNO2S	(M+Na)+
445.9642	445.9645	0.84	1	22404.76	C21H12BrNO2S	(M+Na)+
446.9671	446.9675	0.94	1	5301.45	C21H12BrNO2S	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

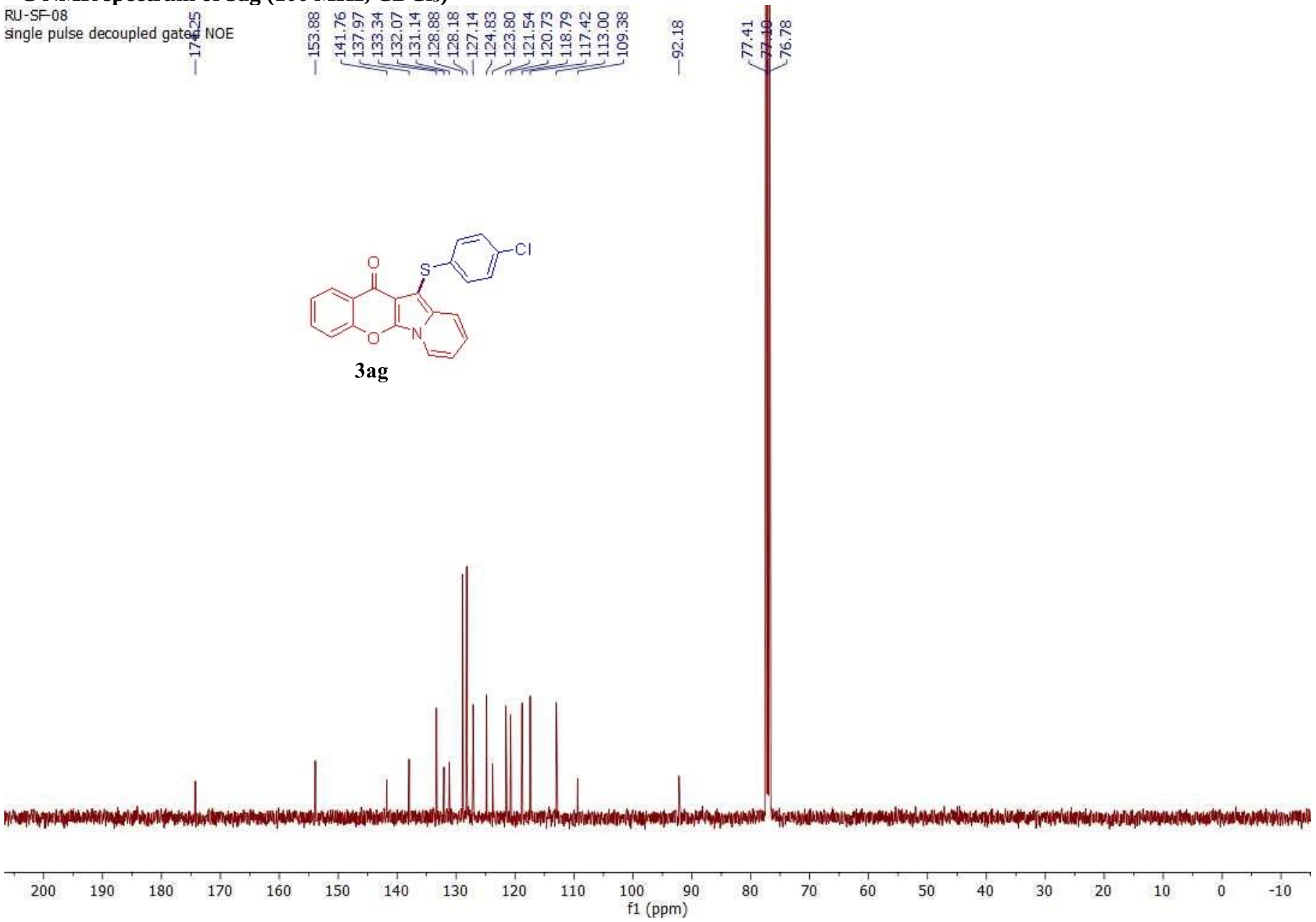
---End Of Report---

^{1}H NMR spectrum of 3ag (400 MHz, $CDCl_3$)



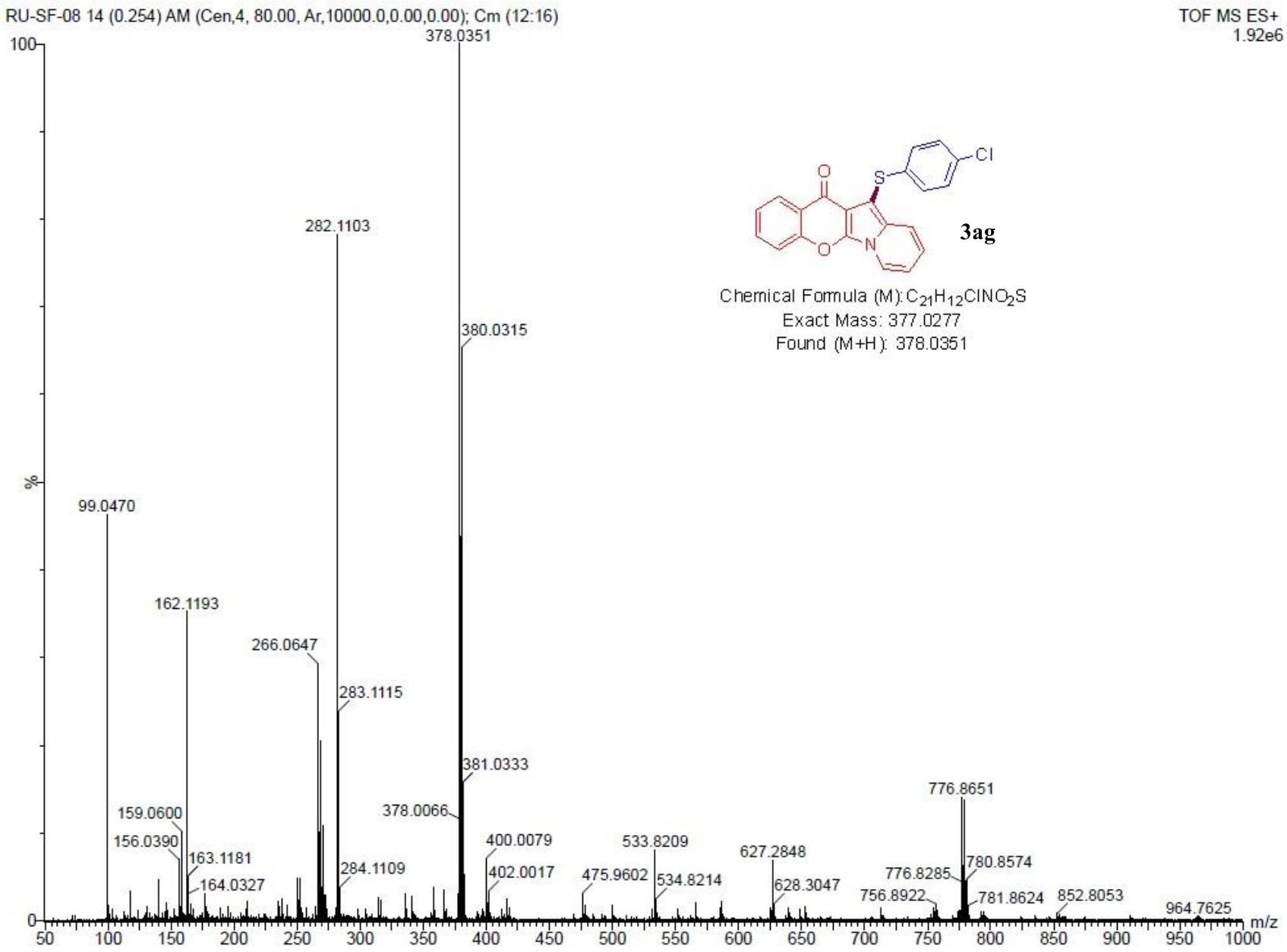
3ag

^{13}C NMR spectrum of 3ag (100 MHz, $CDCl_3$)

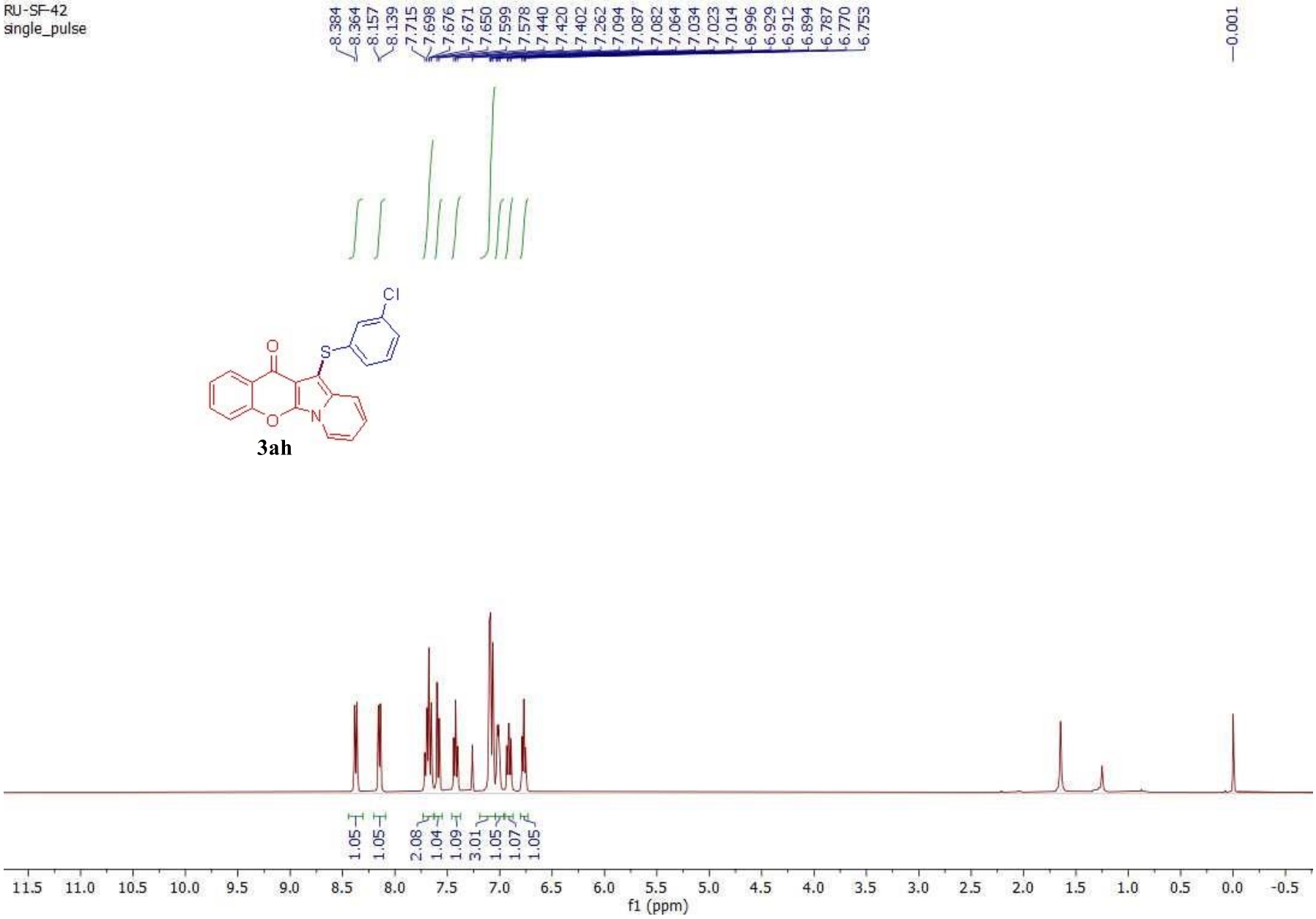


3ag

Mass spectrum of 3ag

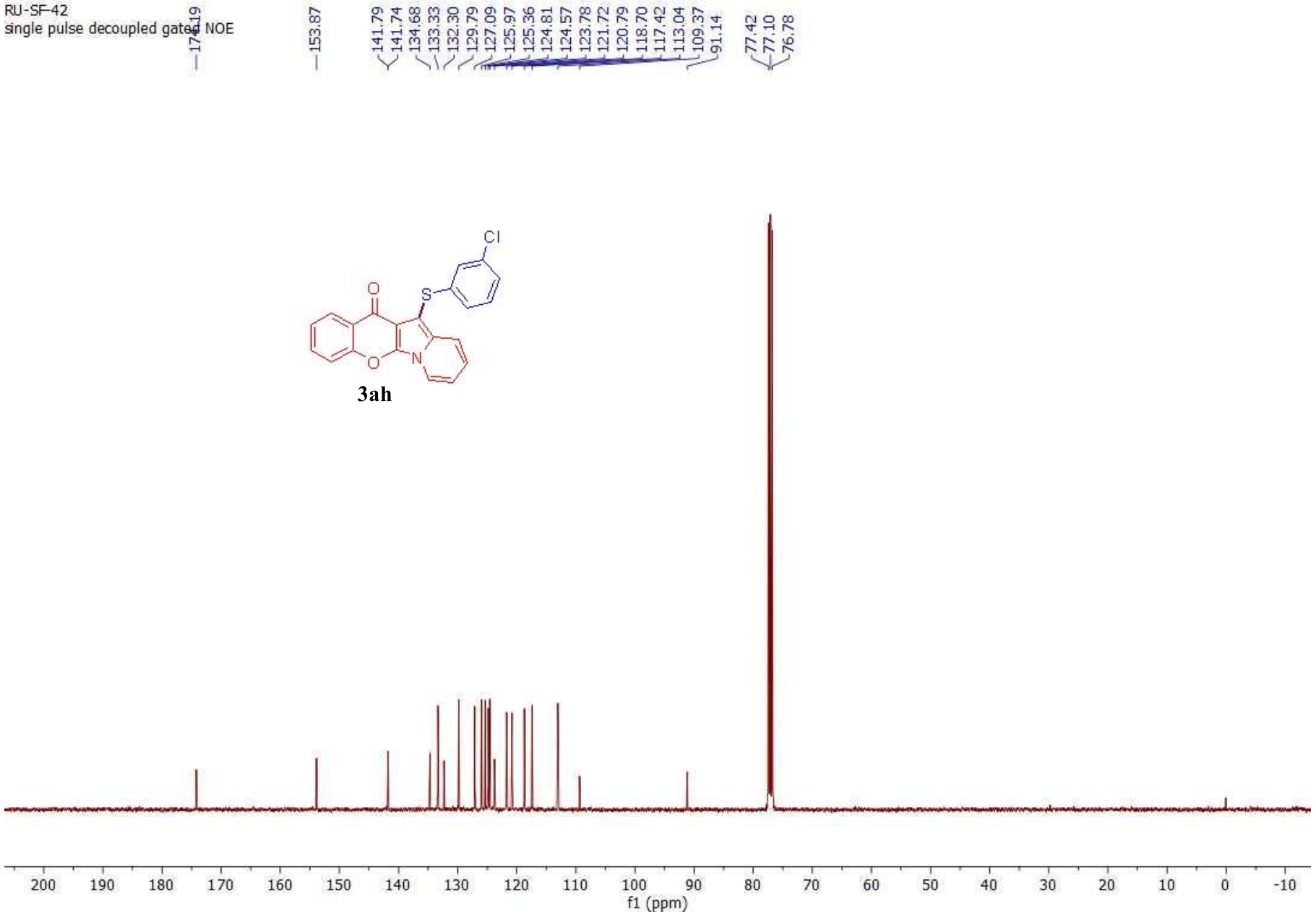


^{1}H NMR spectrum of 3ah (400 MHz, $CDCl_3$)



3ah

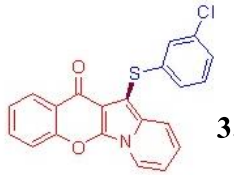
^{13}C NMR spectrum of 3ah (100 MHz, $CDCl_3$)



Mass spectrum of 3ah

Data File	SJ-SF-42.d	**Sample Name**	SJ-SF-42
Sample Type	Sample	**Position**	P1-C9
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 9:35:25 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



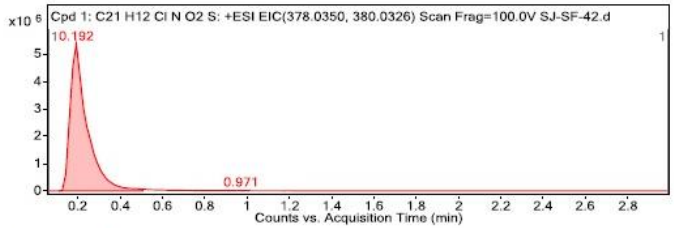
3ah

Chemical Formula (M): $C_{21}H_{12}ClNO_2S$
Exact Mass: 377.0277
Found (M+H): 378.0351

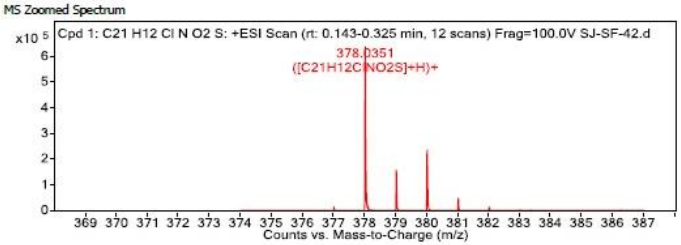
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C21 H12 Cl N O2 S	0.192	377.0278	645823	C21 H12 Cl N O2 S	377.0277	0.06

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H12 Cl N O2 S	378.0351	0.192	Find By Formula	377.0278



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
378.0351	378.035	-0.37	1	645823.14	C21H12ClNO2S	(M+H)+
379.0381	379.0382	0.25	1	157641.93	C21H12ClNO2S	(M+H)+
380.0325	380.0326	0.26	1	242298.13	C21H12ClNO2S	(M+H)+
381.0349	381.0354	1.08	1	50300.88	C21H12ClNO2S	(M+H)+
382.0322	382.0325	0.64	1	10904.26	C21H12ClNO2S	(M+H)+
383.0325	383.0335	2.74	1	2243.78	C21H12ClNO2S	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

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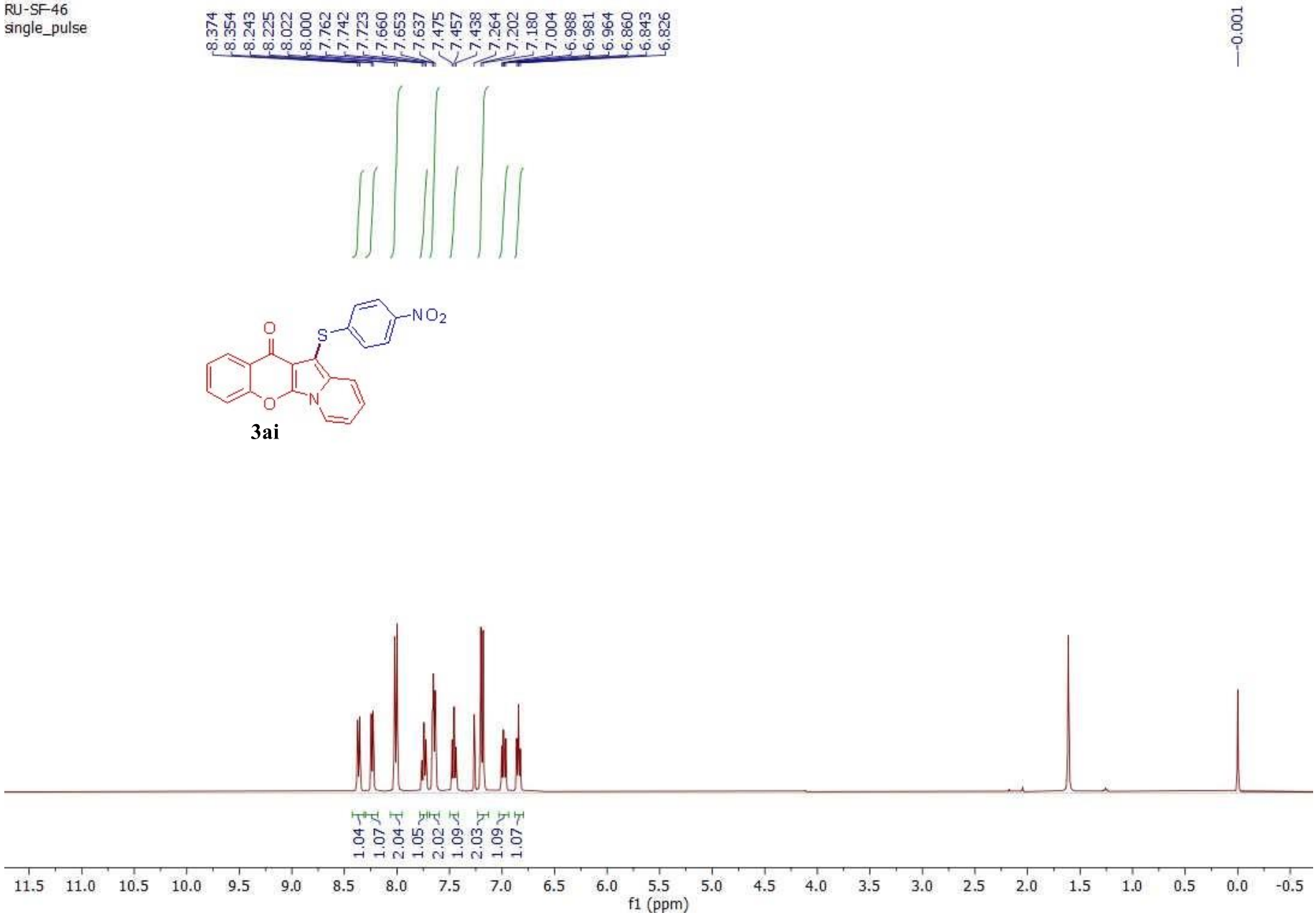
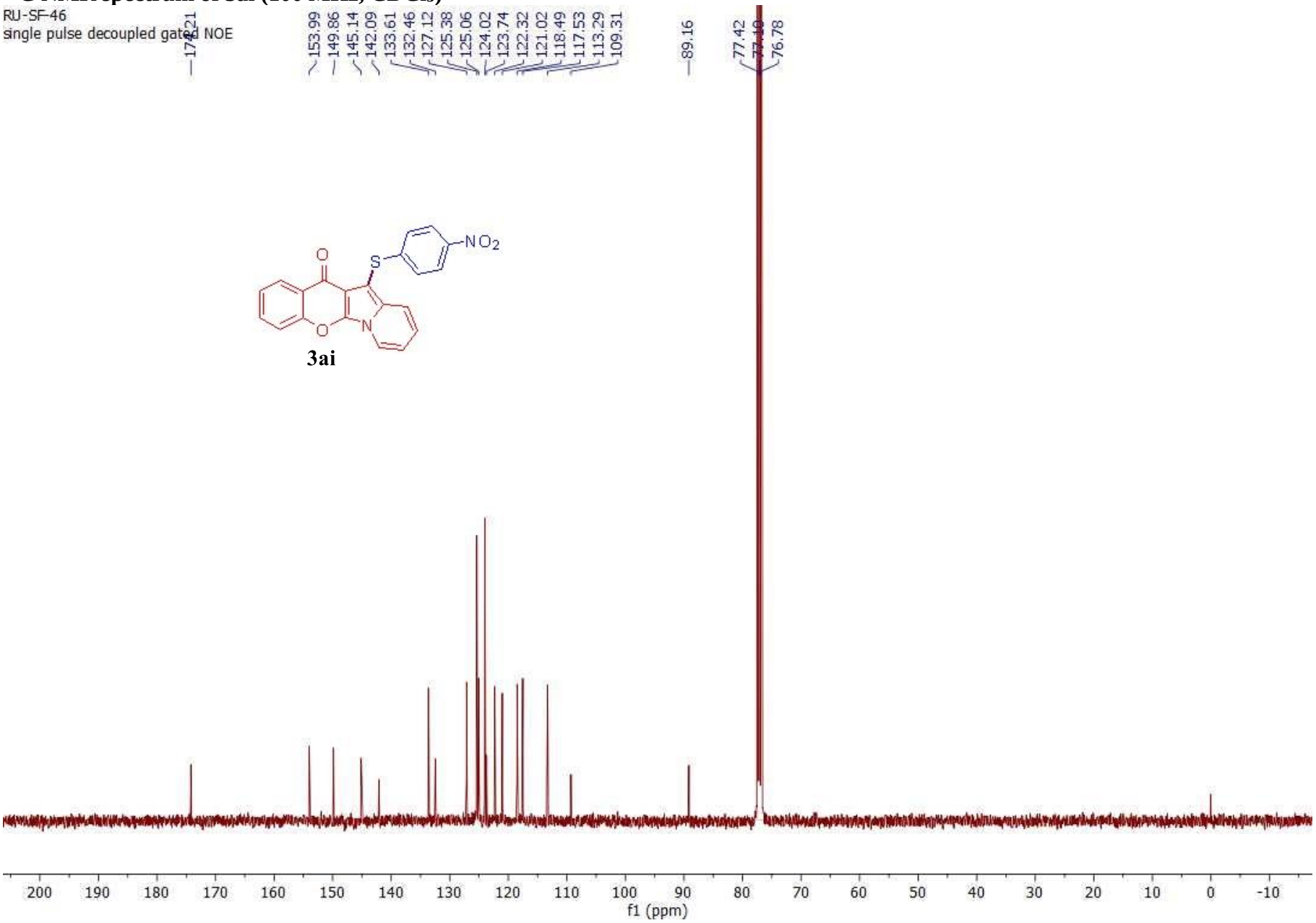
^{1}H NMR spectrum of 3ai (400 MHz, $CDCl_3$)



3ai

^{13}C NMR spectrum of 3ai (100 MHz, $CDCl_3$)

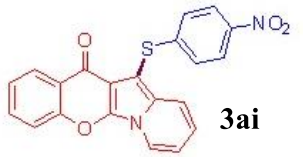


3ai

Mass spectrum of 3ai

Data File	SJ-SF-46.d	**Sample Name**	SJ-SF-46
Sample Type	Sample	**Position**	P1-D1
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 10:00:27 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



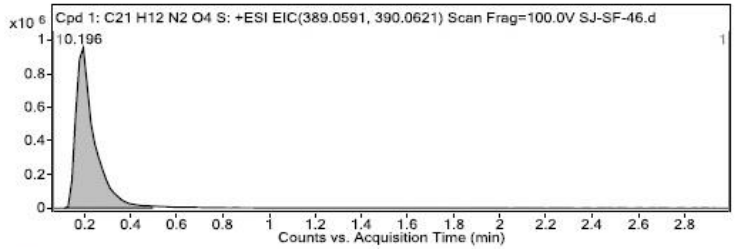
3ai

Chemical Formula (M): $C_{21}H_{12}N_2O_4S$
Exact Mass: 388.0518
Found (M+H): 389.0591

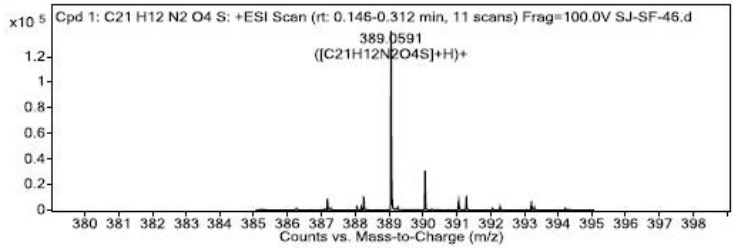
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C21 H12 N2 O4 S	0.196	388.0518	142218	C21 H12 N2 O4 S	388.0518	-0.03

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H12 N2 O4 S	389.0591	0.196	Find By Formula	388.0518



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
389.0591	389.0591	-0.01	1	142218.27	C21H12N2O4S	(M+H)+
390.0619	390.0621	0.5	1	31218.02	C21H12N2O4S	(M+H)+
391.0598	391.0593	-1.1	1	7934.48	C21H12N2O4S	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

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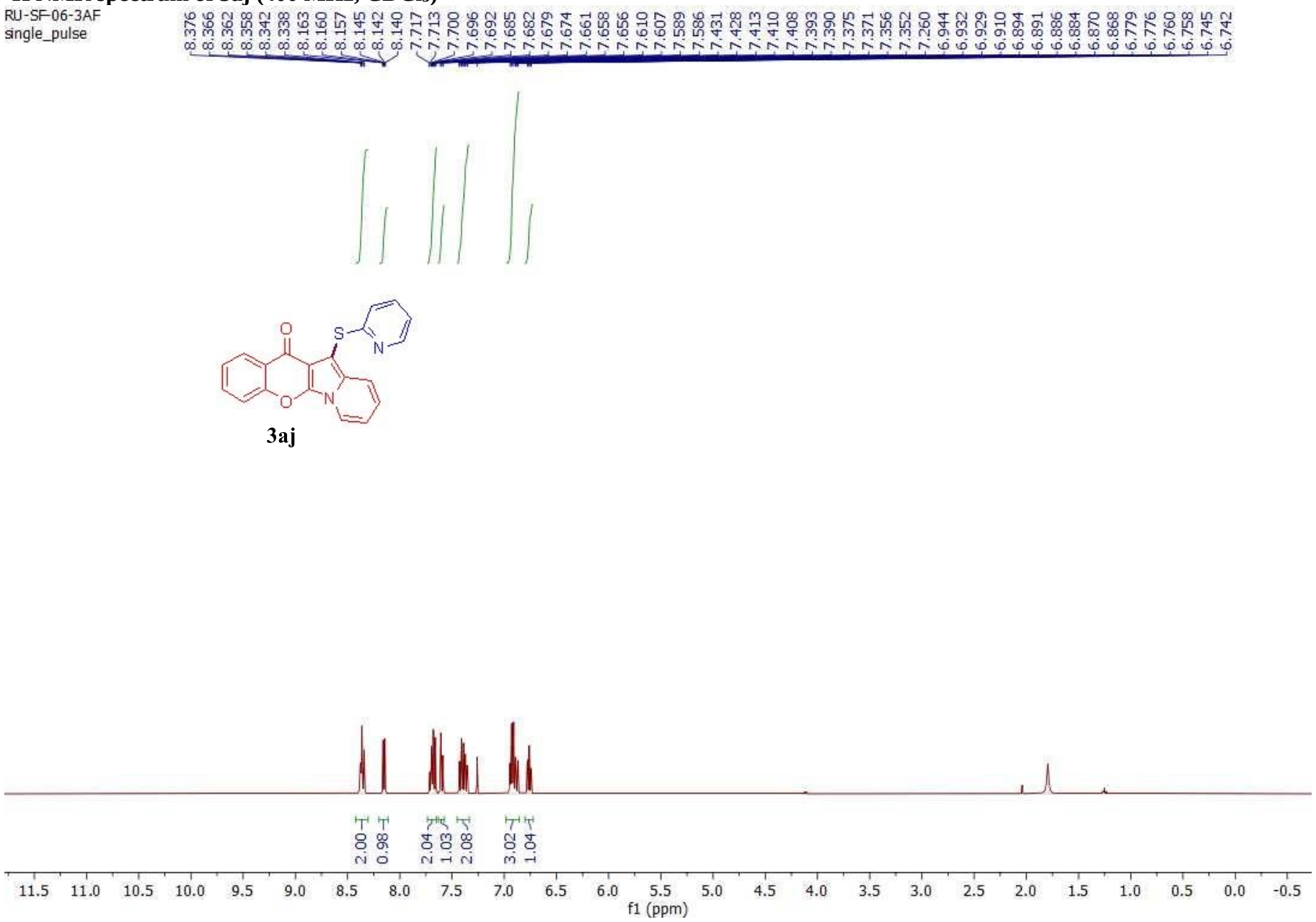
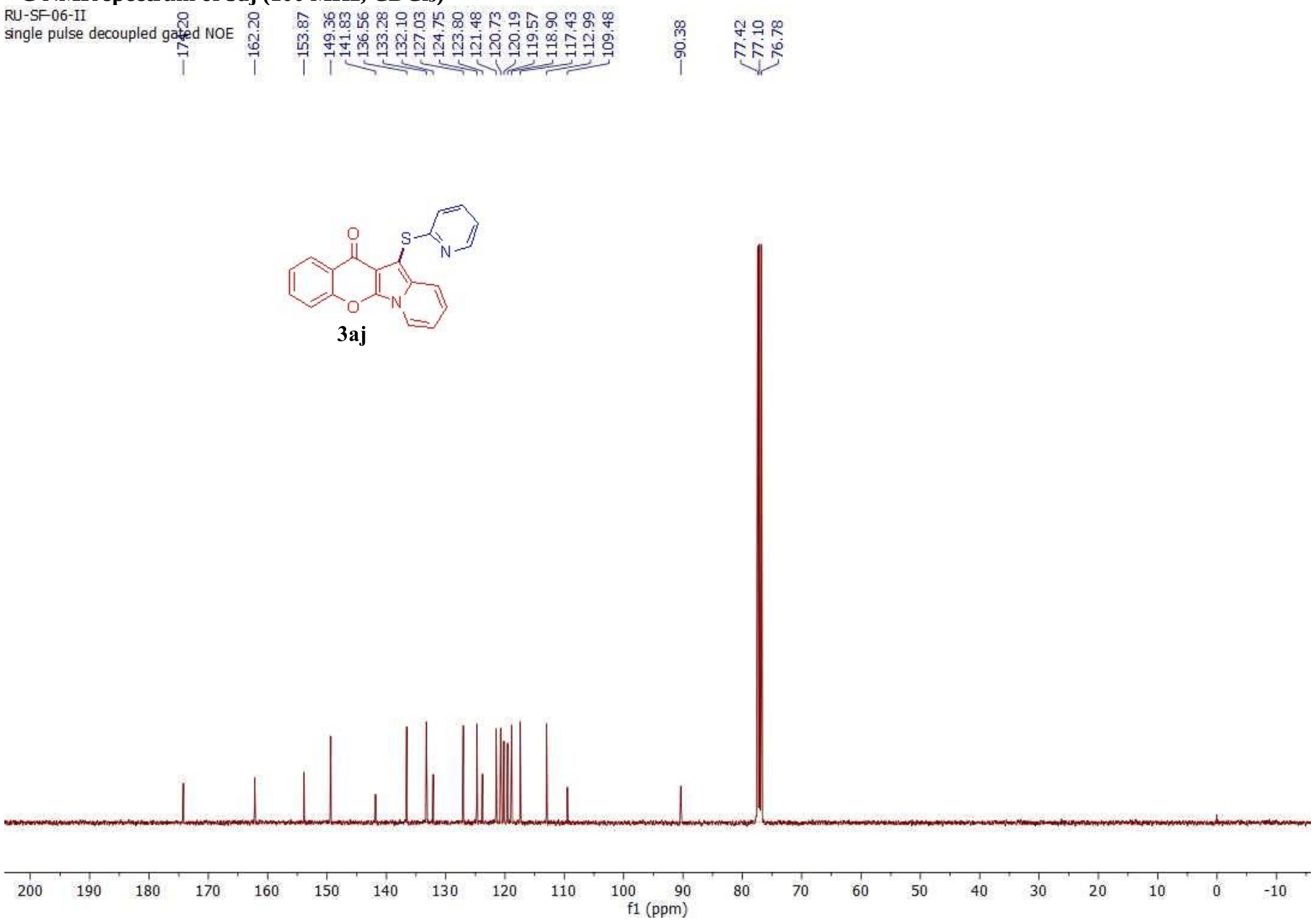
^{1}H NMR spectrum of 3aj (400 MHz, $CDCl_3$)



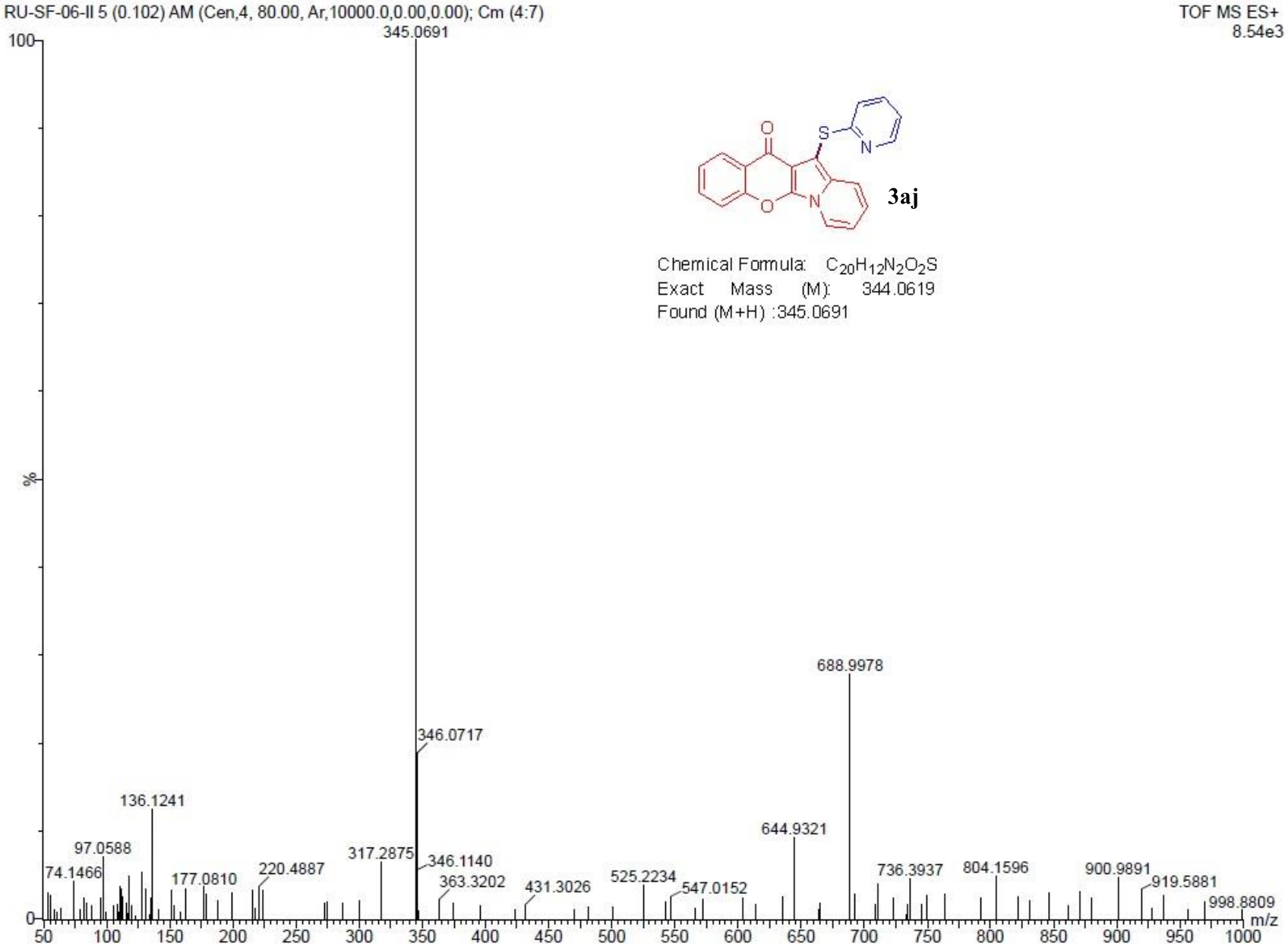
3aj

^{13}C NMR spectrum of 3aj (100 MHz, $CDCl_3$)

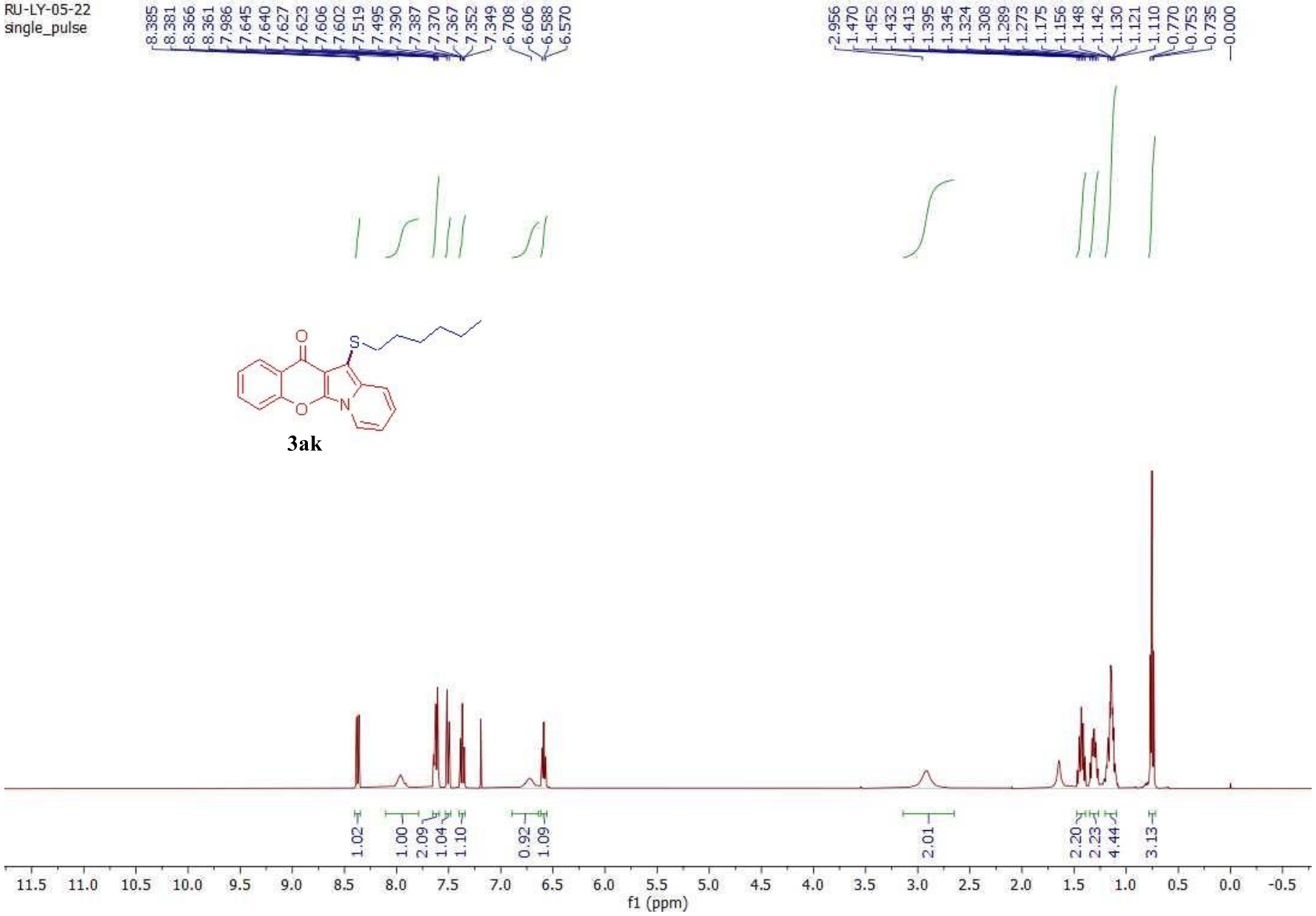


3aj

Mass spectrum of 3aj

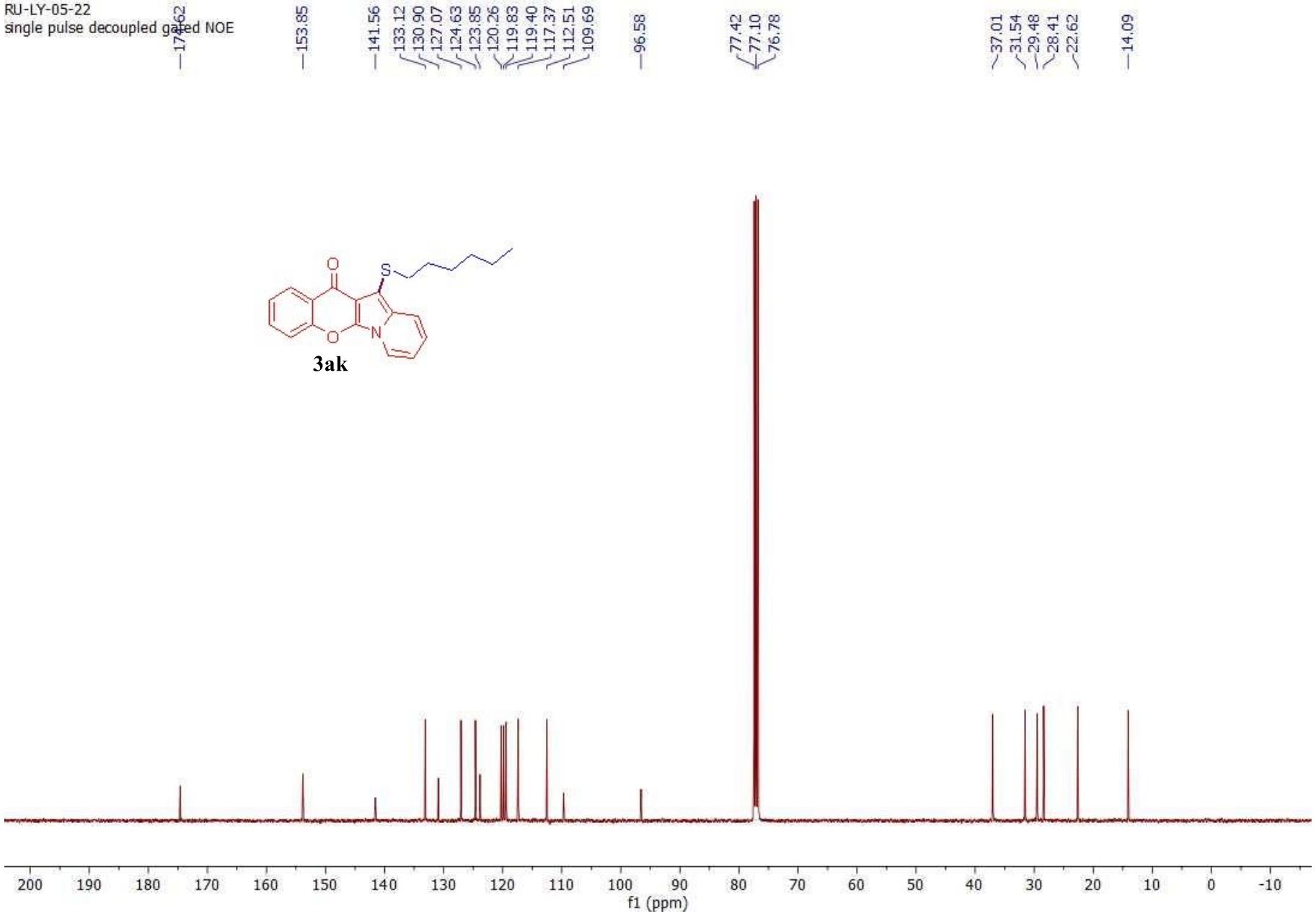


^{1}H NMR spectrum of 3ak (400 MHz, $CDCl_3$)

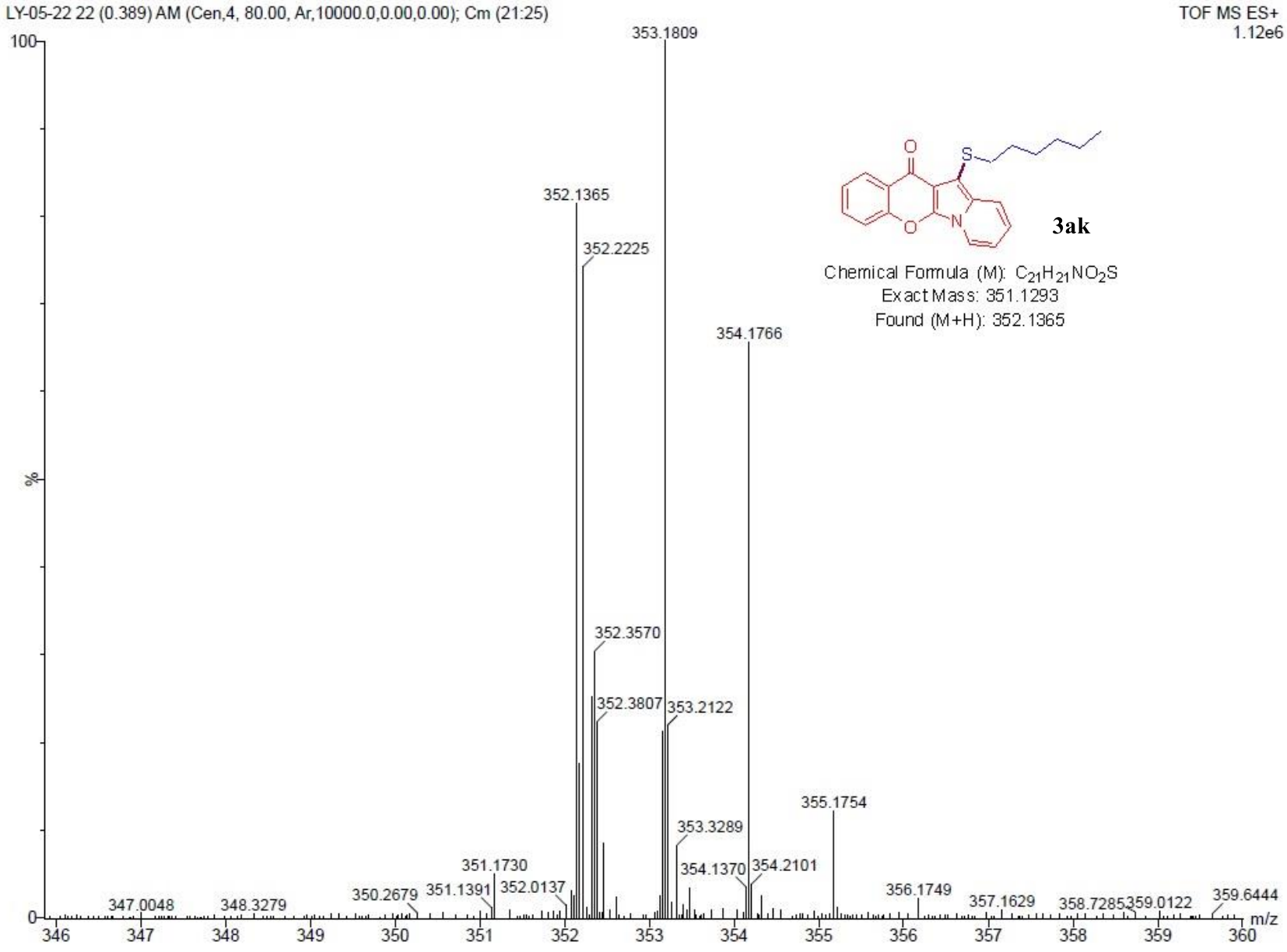


3ak

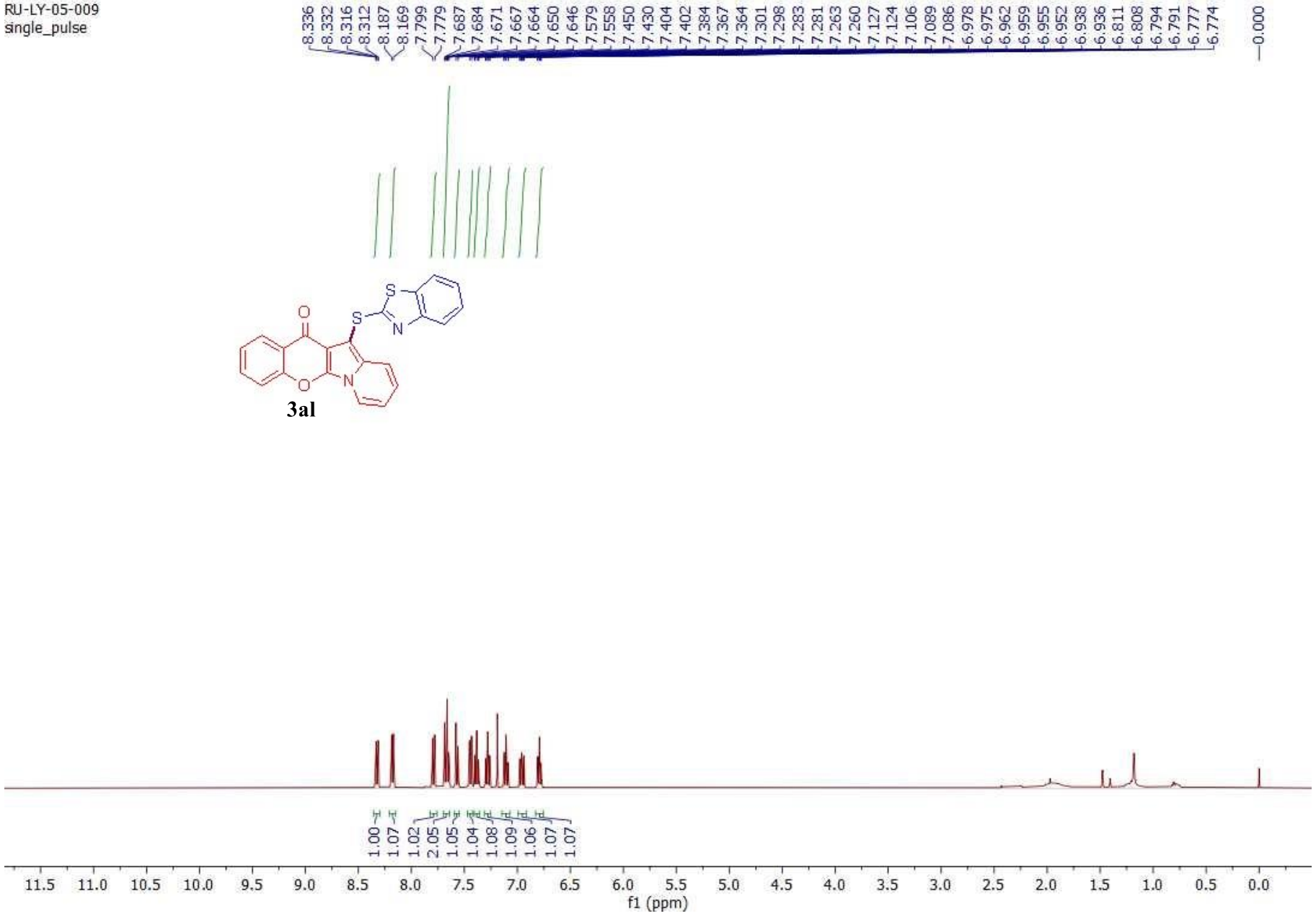
^{13}C NMR spectrum of 3ak (100 MHz, $CDCl_3$)



Mass spectrum of 3ak

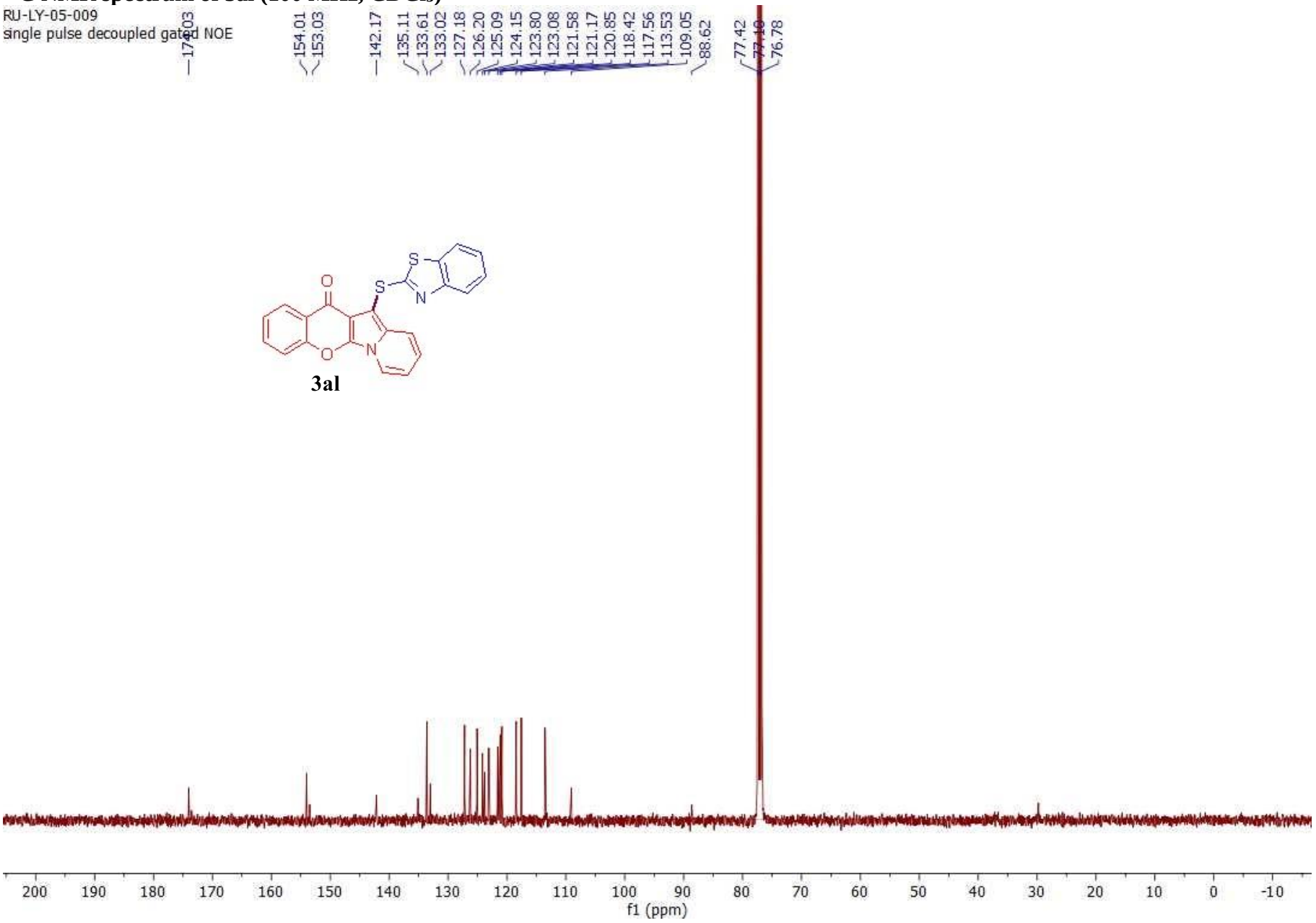


^{1}H NMR spectrum of 3al (400 MHz, $CDCl_3$)

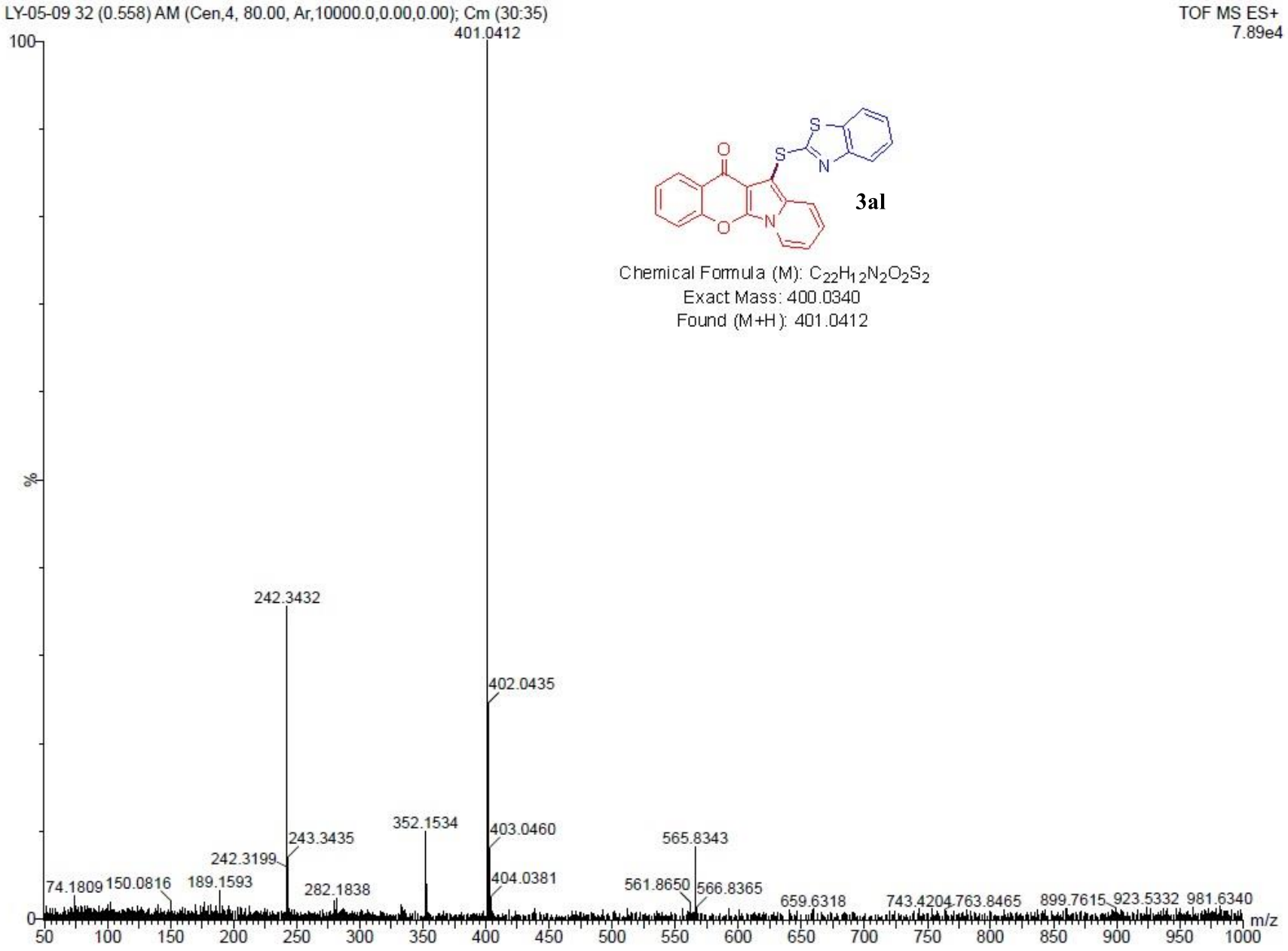


3al

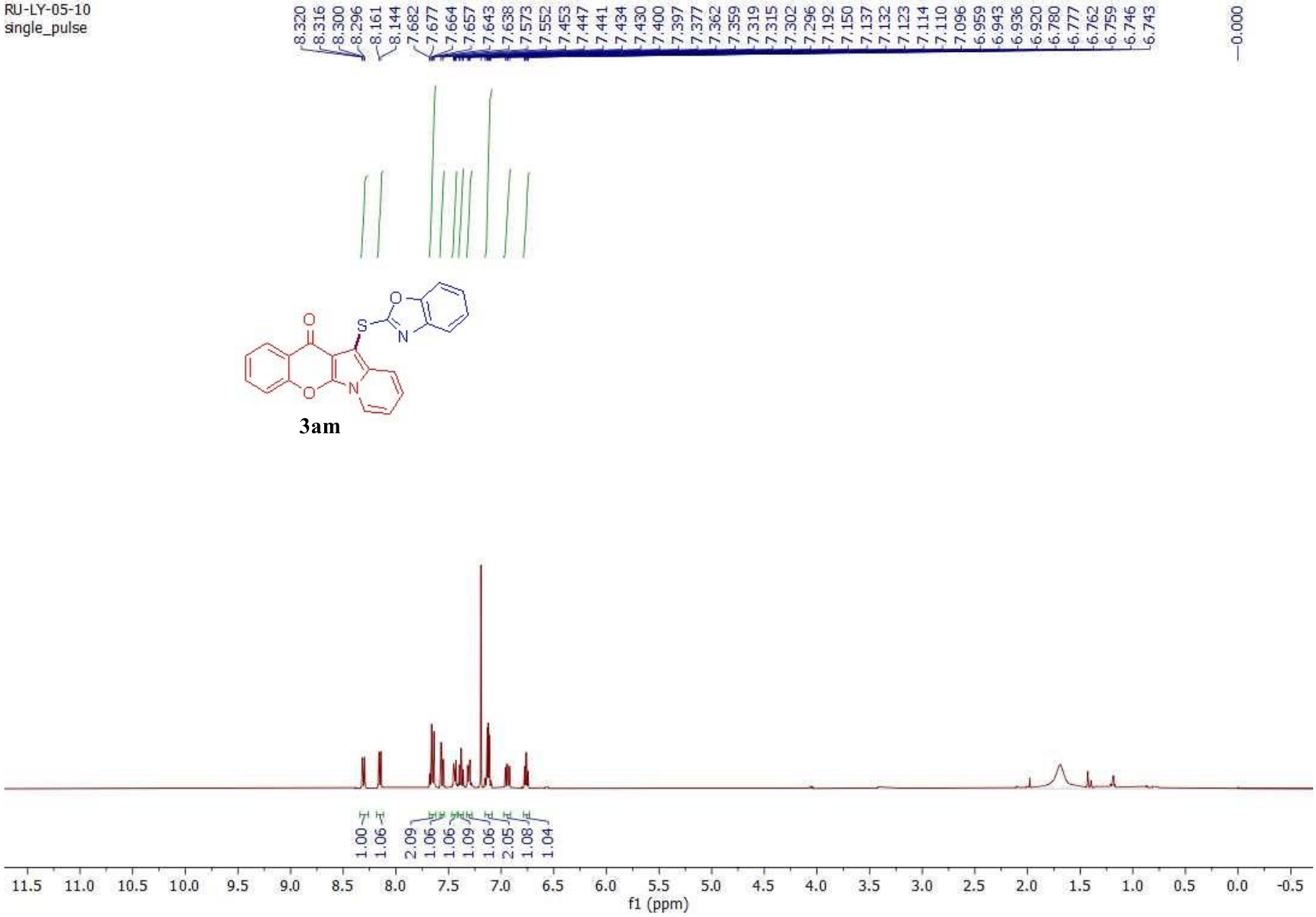
^{13}C NMR spectrum of 3al (100 MHz, $CDCl_3$)



Mass spectrum of 3al

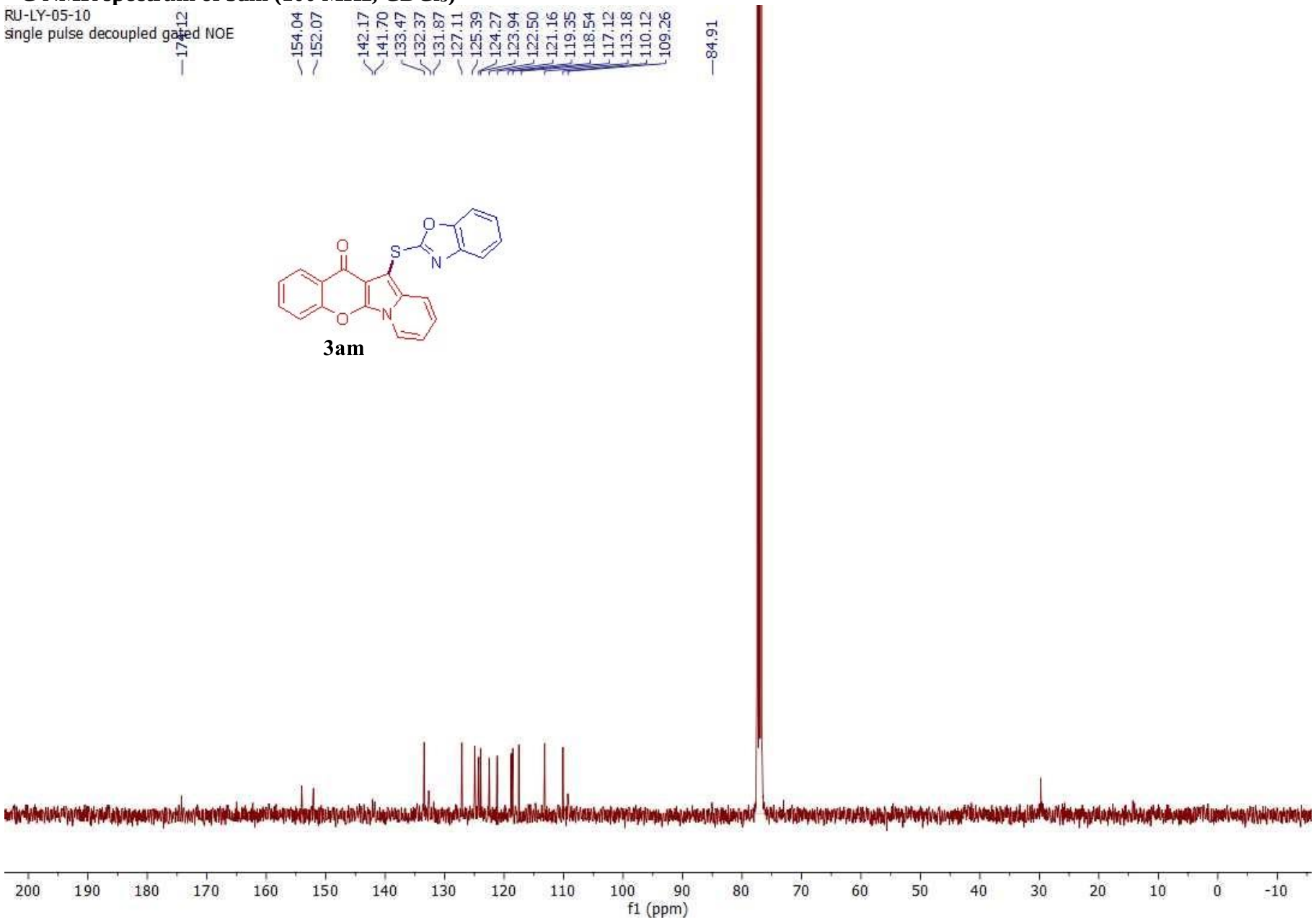


^{1}H NMR spectrum of 3am (400 MHz, $CDCl_3$)



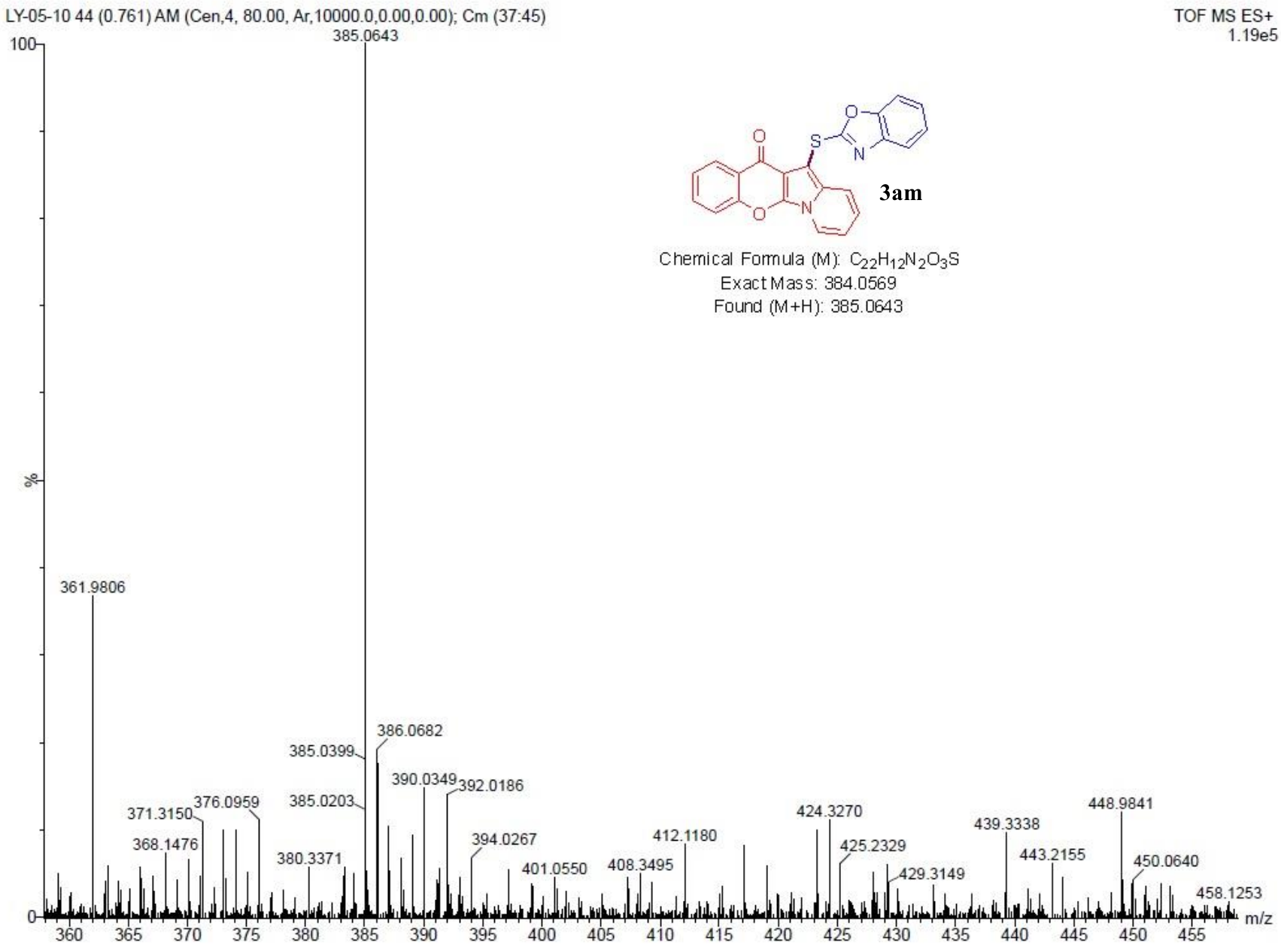
3am

^{13}C NMR spectrum of 3am (100 MHz, $CDCl_3$)

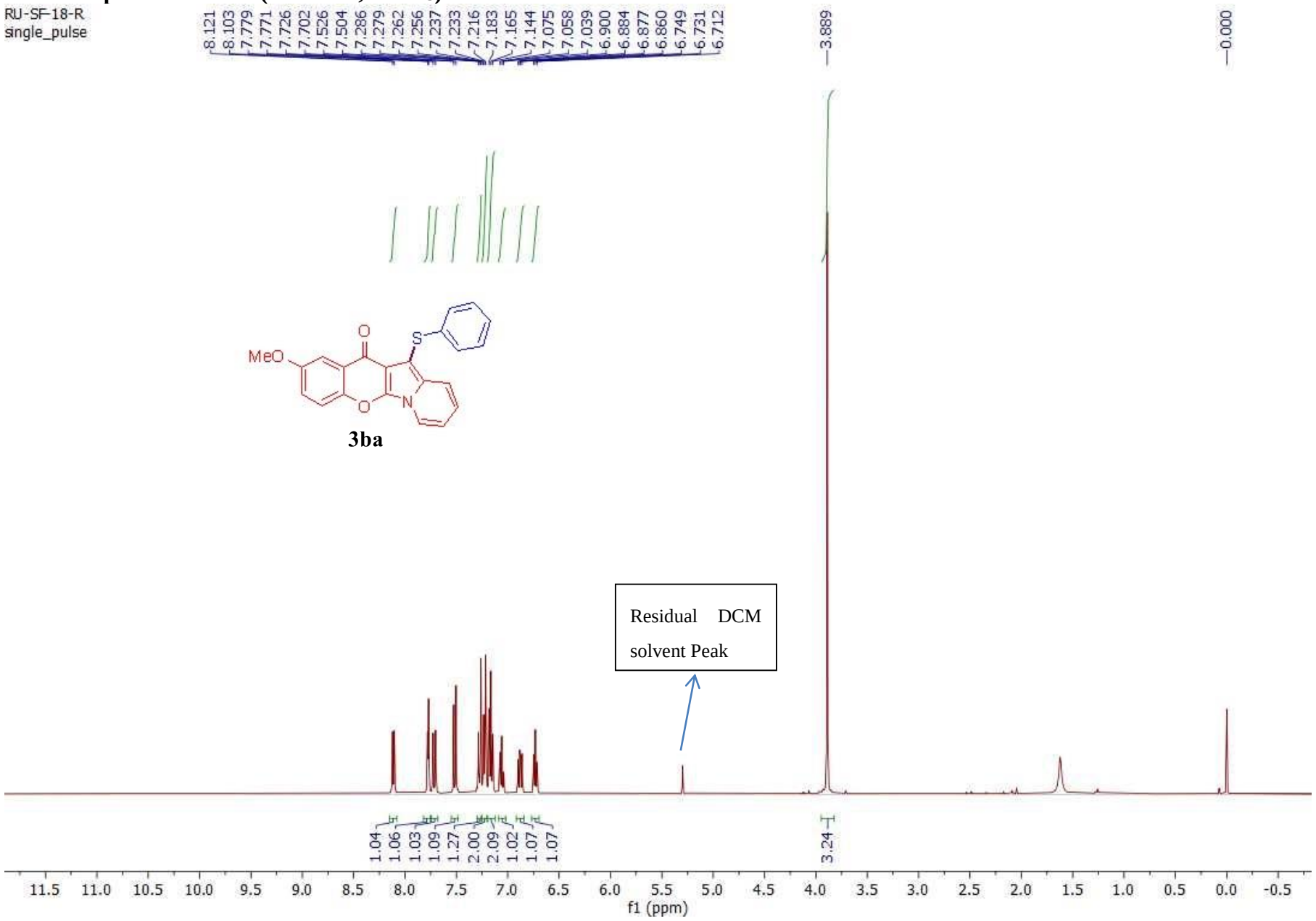


3am

Mass spectrum of 3am

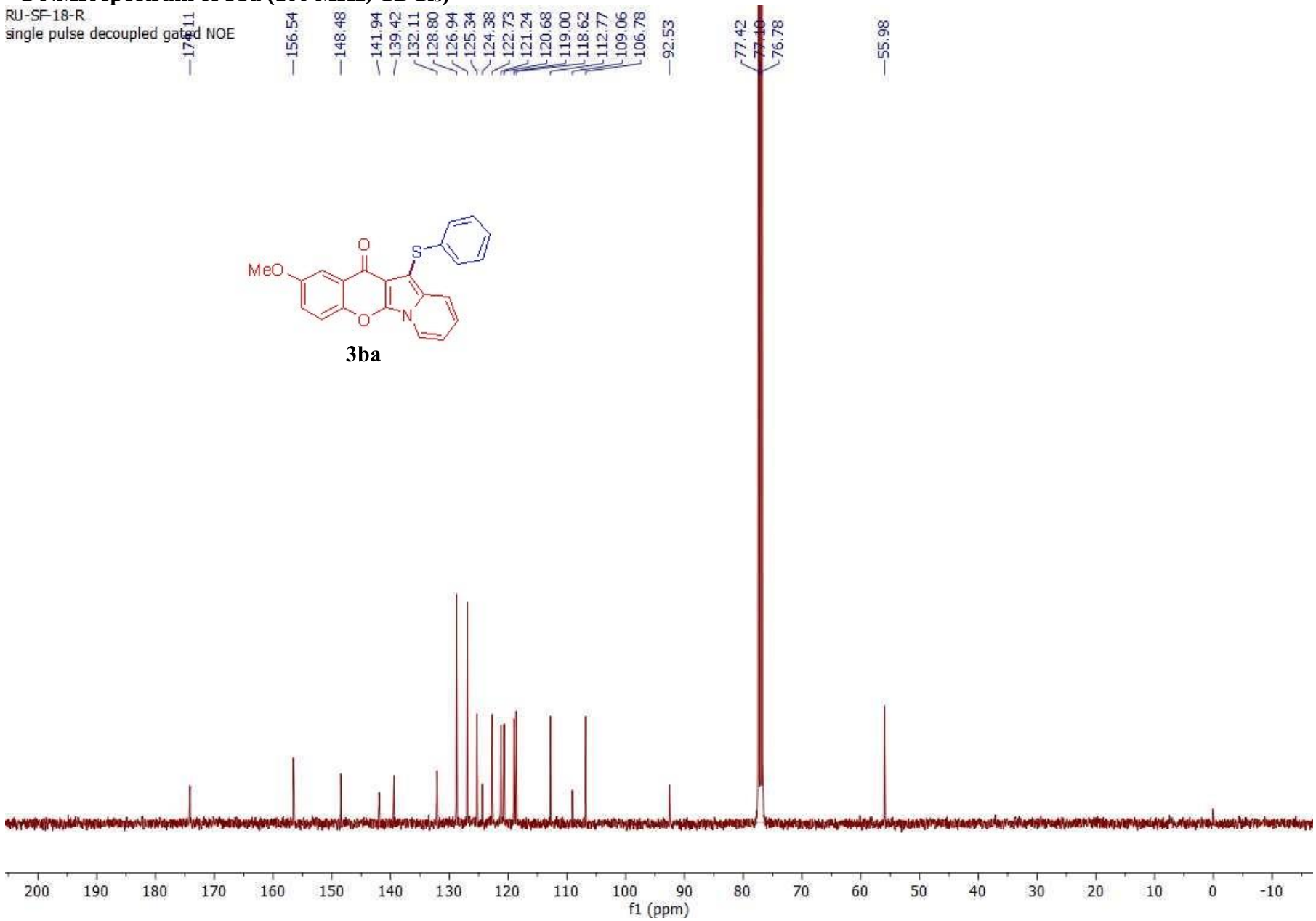


^{1}H NMR spectrum of 3ba (400 MHz, $CDCl_3$)



3ba

^{13}C NMR spectrum of 3ba (100 MHz, $CDCl_3$)

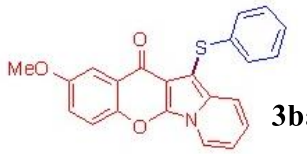


3ba

Mass spectrum of 3ba

Data File	SJ-SF-18.d	**Sample Name**	SJ-SF-18
Sample Type	Sample	**Position**	P1-B3
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 7:13:27 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



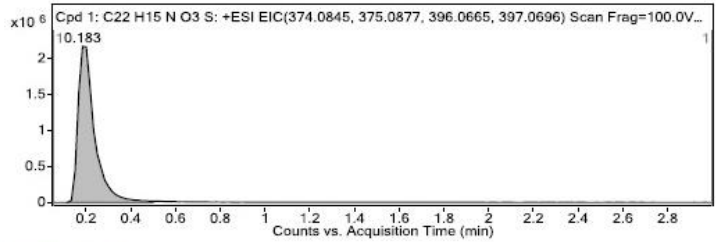
3ba

Chemical Formula (M): $C_{22}H_{15}NO_3S$
Exact Mass: 373.0773
Found (M+H): 374.0847

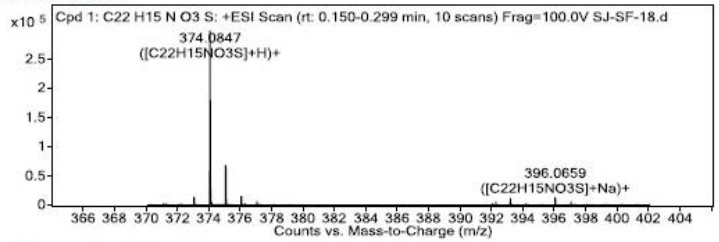
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H15 N O3 S	0.183	373.0773	13356	C22 H15 N O3 S	373.0773	0.07

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H15 N O3 S	396.0659	0.183	Find By Formula	373.0773



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
374.0847	374.0845	-0.34	1	300414.03	C22H15NO3S	(M+H)+
375.0874	375.0877	0.82	1	69123.15	C22H15NO3S	(M+H)+
376.0851	376.0849	-0.4	1	15488.28	C22H15NO3S	(M+H)+
396.0659	396.0665	1.43	1	13356.28	C22H15NO3S	(M+Na)+
397.0691	397.0696	1.49	1	3126.78	C22H15NO3S	(M+Na)+
398.067	398.0669	-0.23	1	849.97	C22H15NO3S	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

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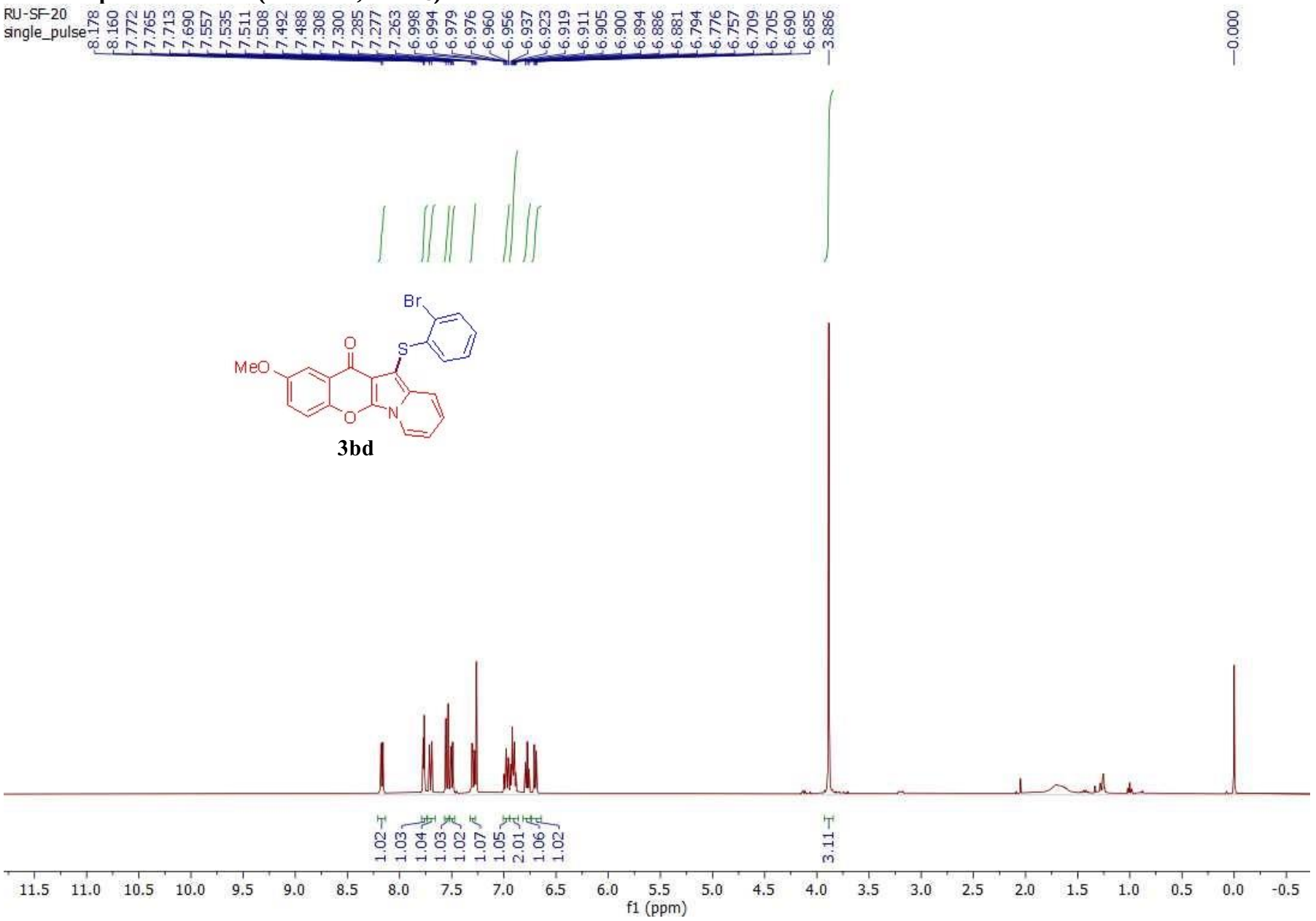
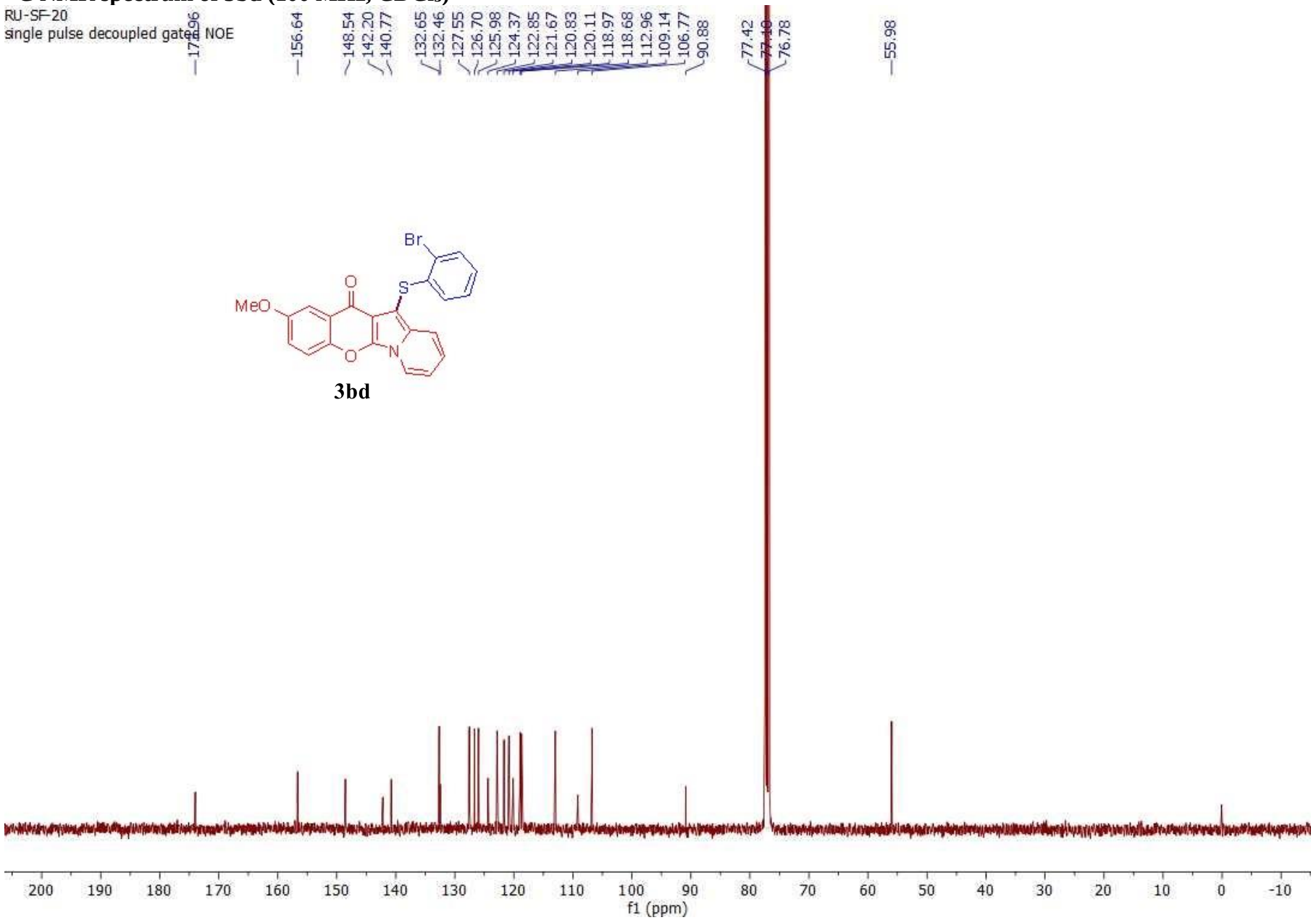
^{1}H NMR spectrum of 3bd (400 MHz, $CDCl_3$)



3bd

^{13}C NMR spectrum of 3bd (100 MHz, $CDCl_3$)



3bd

Mass spectrum of 3bd

Data File	SJ-SF-20.d	**Sample Name**	SJ-SF-20
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 7:30:10 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

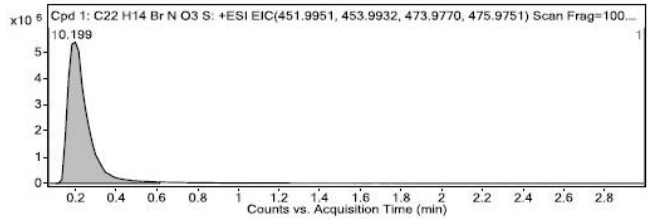
3bd

Chemical Formula (M): $C_{22}H_{14}BrNO_3S$
Exact Mass: 450.9878
Found (M+H): 451.9955

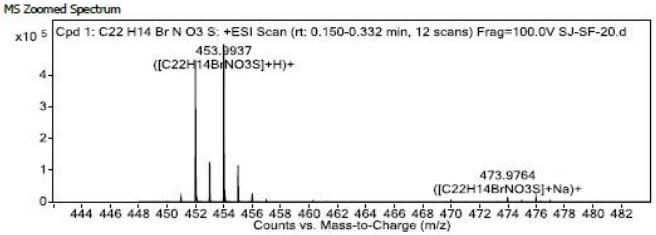
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H14 Br N O3 S	0.199	450.9881	505616	C22 H14 Br N O3 S	450.9878	0.61

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H14 Br N O3 S	453.9937	0.199	Find By Formula	450.9881



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
451.9955	451.9951	-0.89	1	459362.04	C22H14BrNO3S	(M+H)+
452.9976	452.9982	1.33	1	125609.95	C22H14BrNO3S	(M+H)+
453.9937	453.9932	-1.22	1	505616.25	C22H14BrNO3S	(M+H)+
454.996	454.9962	0.35	1	121038.36	C22H14BrNO3S	(M+H)+
455.9938	455.9935	-0.72	1	26791.32	C22H14BrNO3S	(M+H)+
456.9943	456.9947	0.82	1	4830.14	C22H14BrNO3S	(M+H)+
473.9764	473.977	1.36	1	14647.95	C22H14BrNO3S	(M+Na)+
474.9794	474.9802	1.66	1	3558.96	C22H14BrNO3S	(M+Na)+
475.9746	475.9751	1.23	1	14640.55	C22H14BrNO3S	(M+Na)+
476.9776	476.9781	1.1	1	3566.75	C22H14BrNO3S	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

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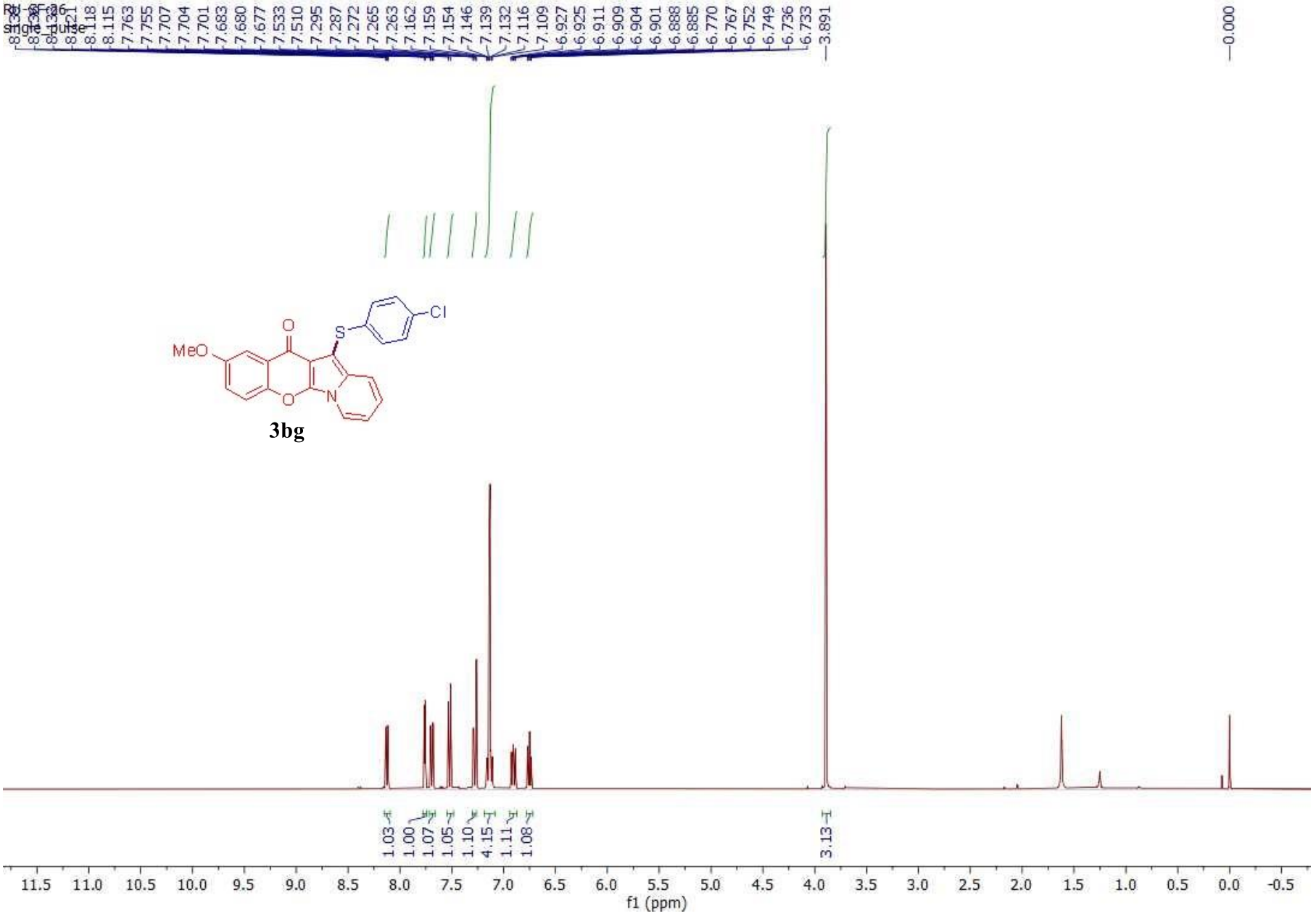
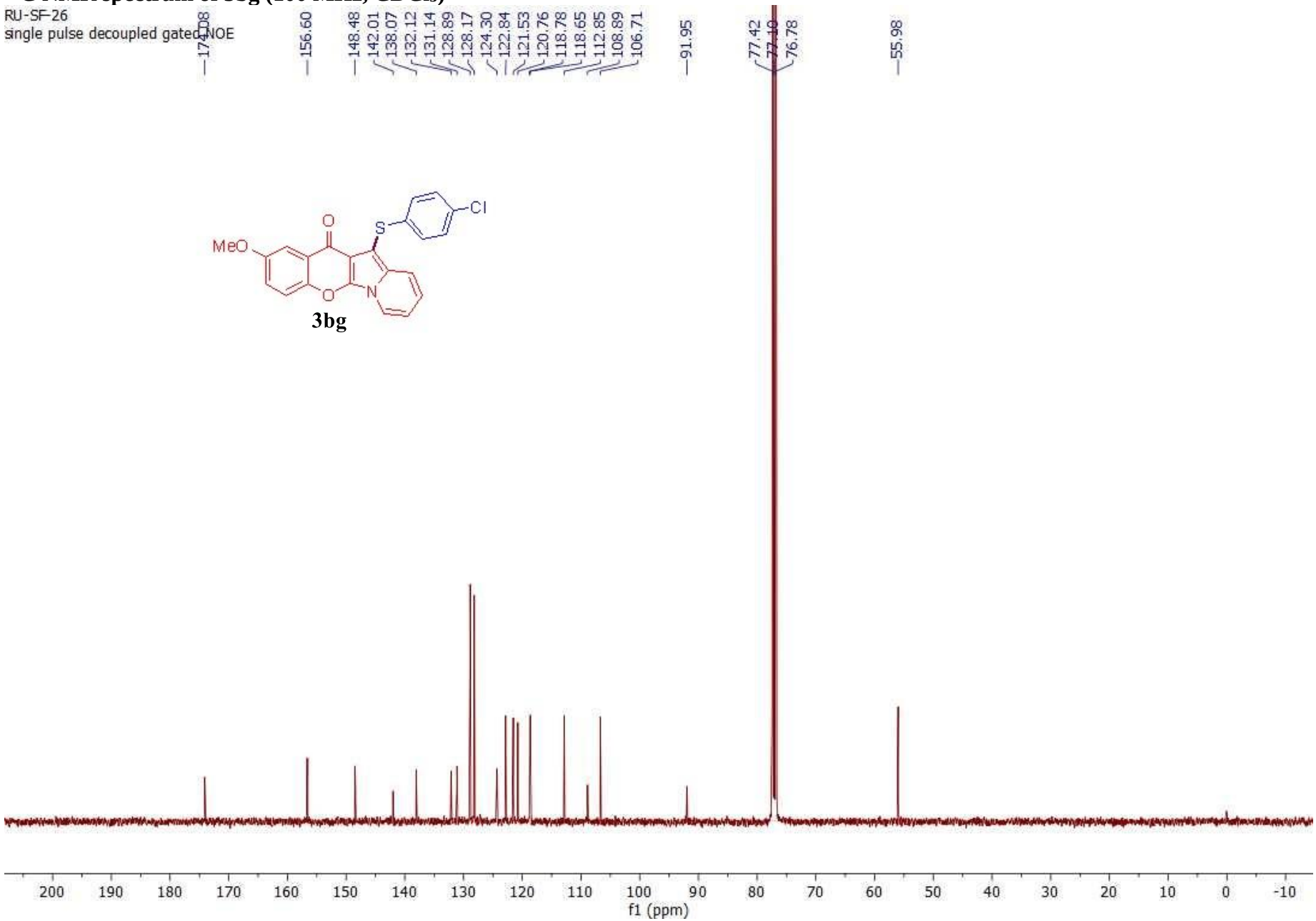
---End Of Report---

^{1}H NMR spectrum of 3bg (400 MHz, $CDCl_3$)



3bg

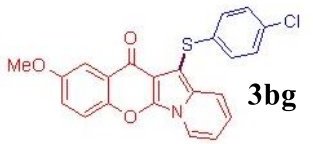
^{13}C NMR spectrum of 3bg (100 MHz, $CDCl_3$)



Mass spectrum of 3bg

Data File	SJ-SF-26.d	**Sample Name**	SJ-SF-26
Sample Type	Sample	**Position**	P1-B8
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 7:55:13 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



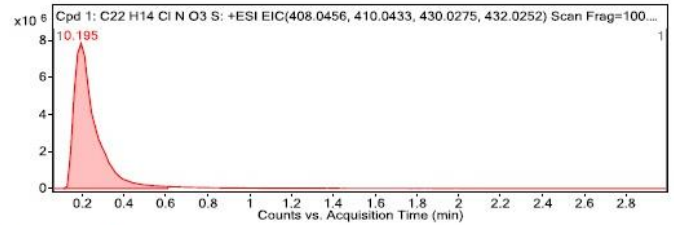
3bg

Chemical Formula (M): $C_{22}H_{14}ClNO_3S$
Exact Mass: 407.0383
Found (M+H): 408.0457

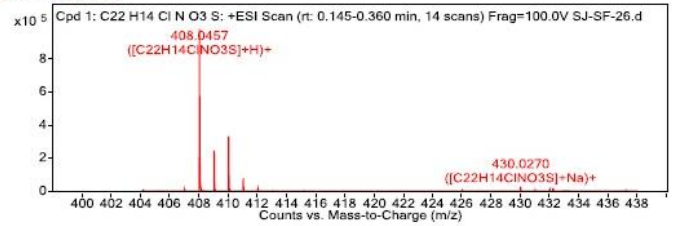
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H14 Cl N O3 S	0.195	407.0385	28892	C22 H14 Cl N O3 S	407.0383	0.48

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H14 Cl N O3 S	430.027	0.195	Find By Formula	407.0385



MS Zoomed Spectrum



MS Spectrum Peak List

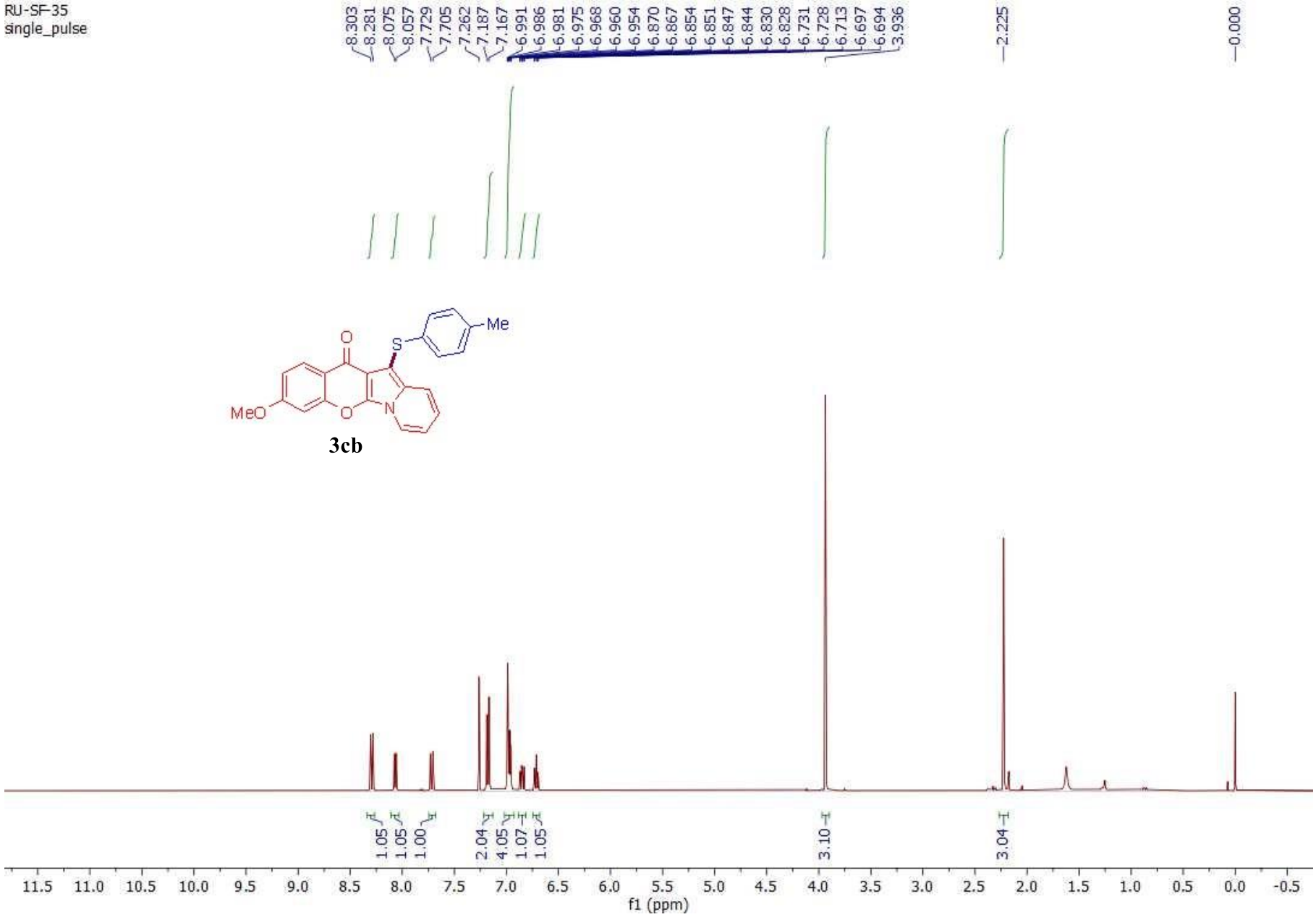
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
408.0457	408.0456	-0.42	1	993912.31	C22H14ClNO3S	(M+H)+
409.0488	409.0487	-0.1	1	251827.83	C22H14ClNO3S	(M+H)+
410.0439	410.0433	-1.39	1	352640.88	C22H14ClNO3S	(M+H)+
411.0458	411.046	0.58	1	79345.06	C22H14ClNO3S	(M+H)+
412.0437	412.0434	-0.7	1	17744.61	C22H14ClNO3S	(M+H)+
413.0441	413.0445	0.98	1	3092.75	C22H14ClNO3S	(M+H)+
430.027	430.0275	1.09	1	28892.43	C22H14ClNO3S	(M+Na)+
431.0301	431.0307	1.24	1	7015.09	C22H14ClNO3S	(M+Na)+
432.0247	432.0252	1.25	1	10529.43	C22H14ClNO3S	(M+Na)+
433.0271	433.0279	1.84	1	2483.43	C22H14ClNO3S	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

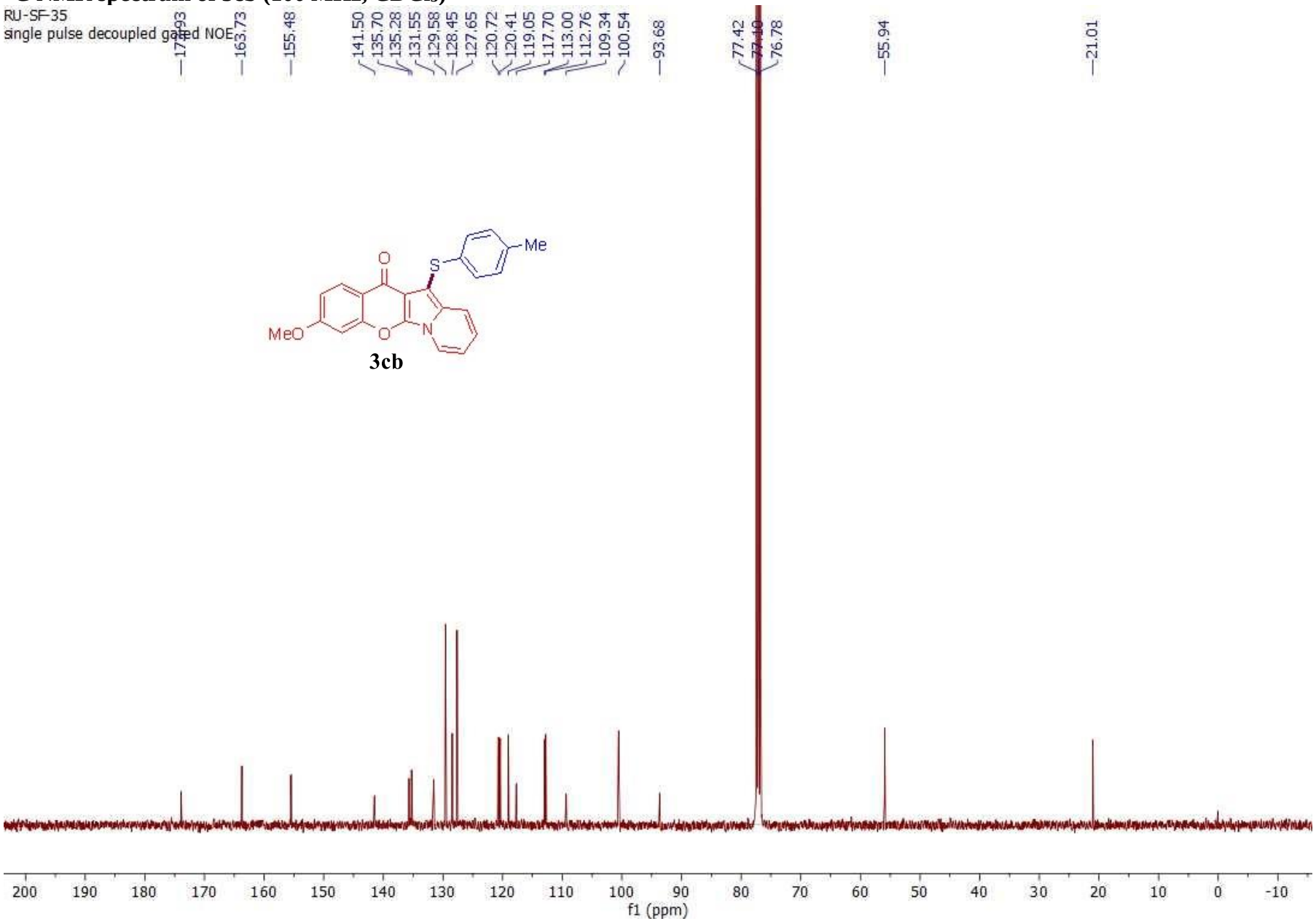
---End Of Report---

^{1}H NMR spectrum of 3cb (400 MHz, $CDCl_3$)



3cb

^{13}C NMR spectrum of 3cb (100 MHz, $CDCl_3$)

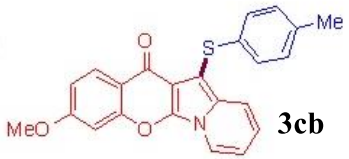


3cb

Mass spectrum of 3cb

Data File	SJ-SF-35.d	**Sample Name**	SJ-SF-35
Sample Type	Sample	**Position**	P1-C4
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 8:53:41 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



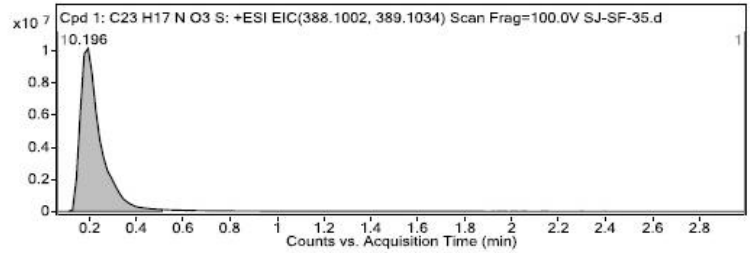
3cb

Chemical Formula (M): $C_{23}H_{17}NO_3S$
Exact Mass: 387.0929
Found (M+H):388.1005

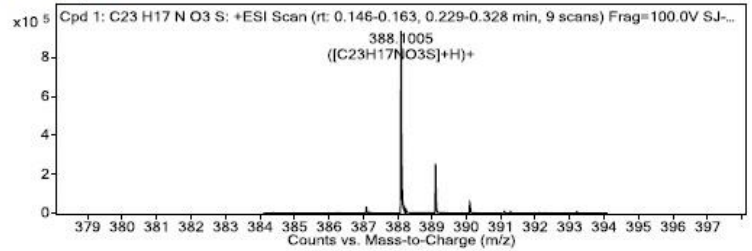
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C23 H17 N O3 S	0.196	387.0933	961104	C23 H17 N O3 S	387.0929	0.94

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H17 N O3 S	388.1005	0.196	Find By Formula	387.0933



MS Zoomed Spectrum



MS Spectrum Peak List

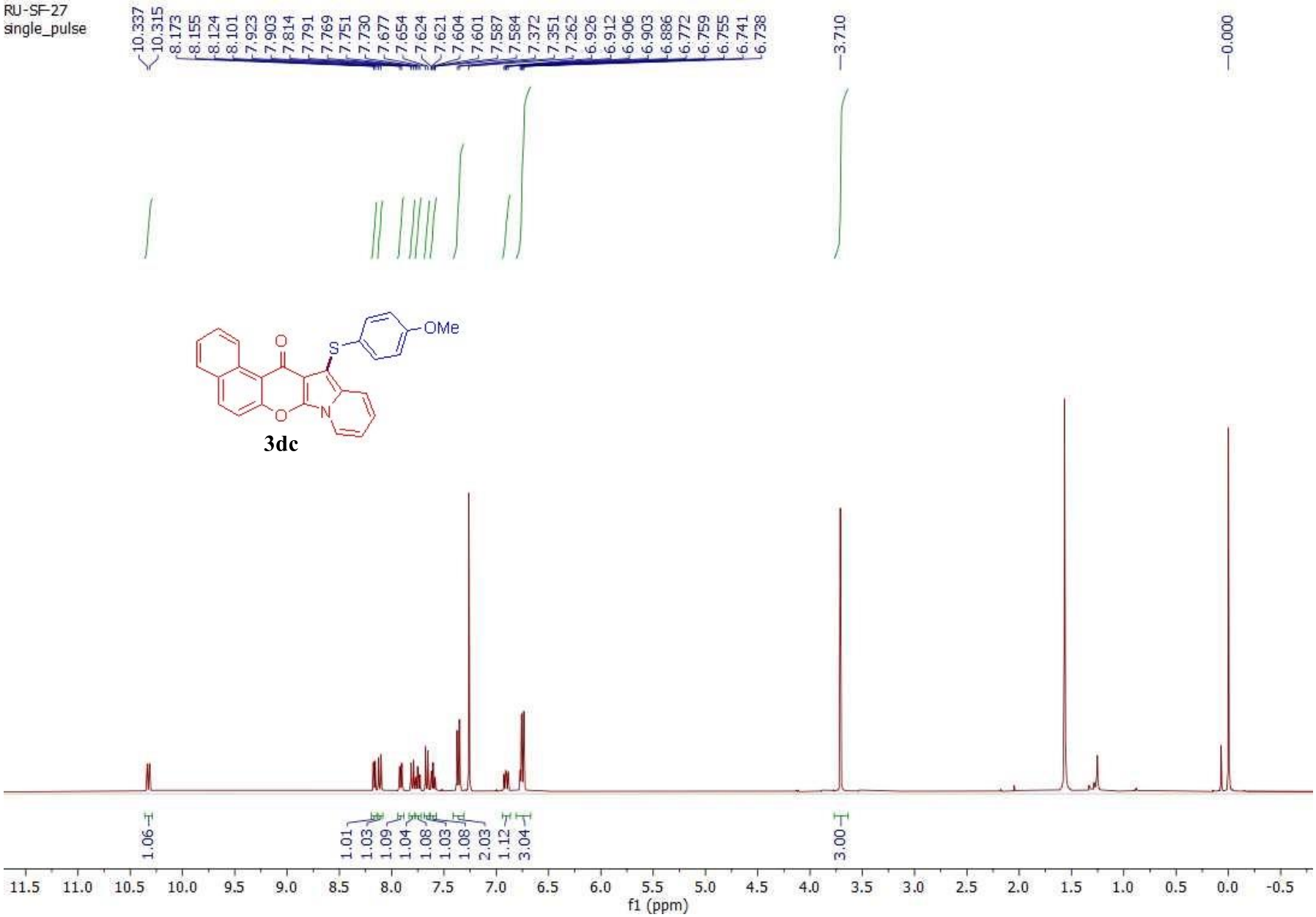
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
388.1005	388.1002	-0.86	1	961103.83	C23H17NO3S	(M+H)+
389.1037	389.1034	-0.84	1	254119.72	C23H17NO3S	(M+H)+
390.1018	390.1008	-2.72	1	55208.8	C23H17NO3S	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

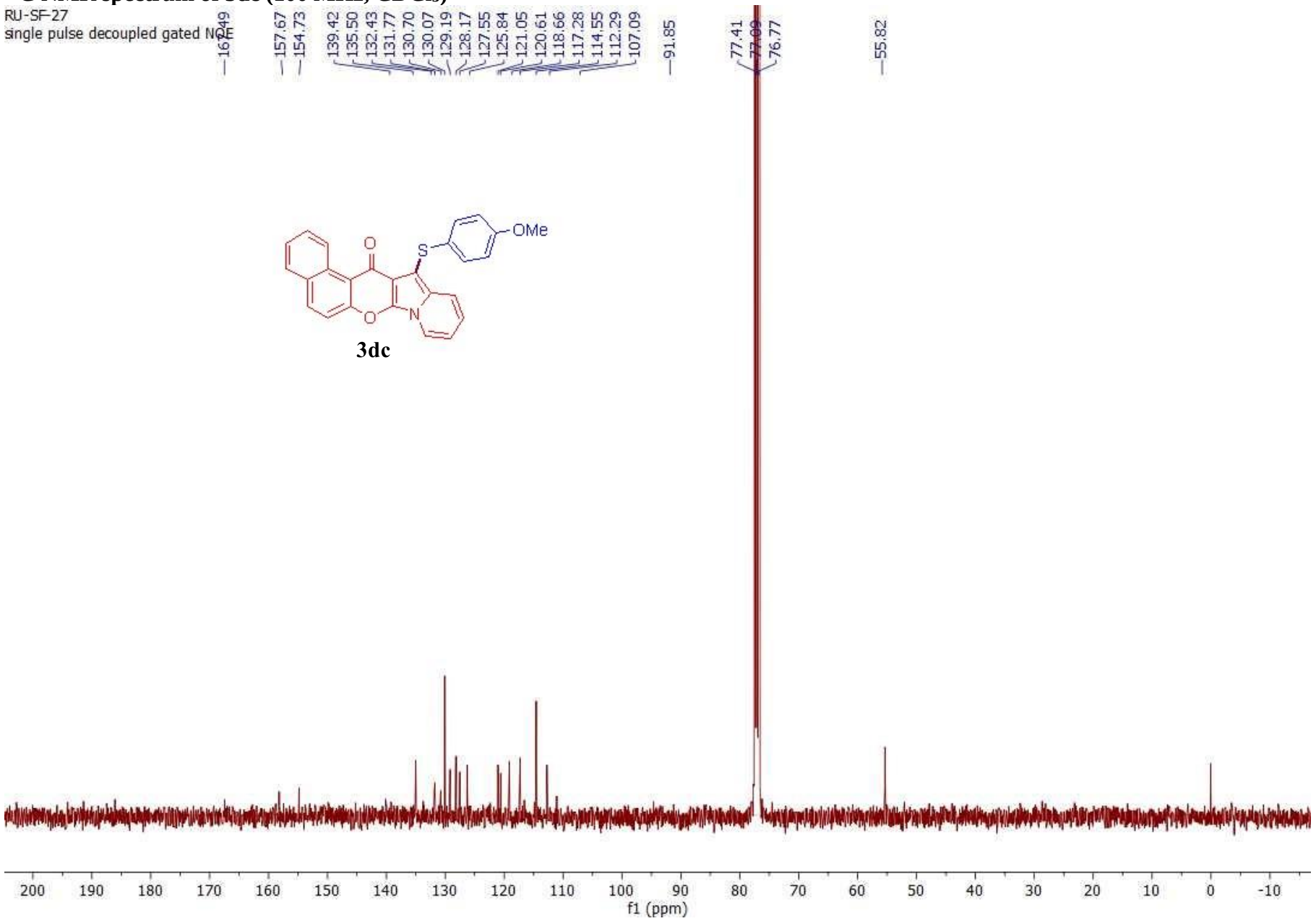
Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

---End Of Report---

^{1}H NMR spectrum of 3dc (400 MHz, $CDCl_3$)



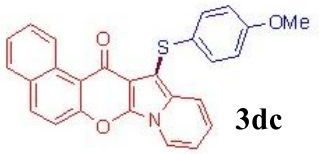
^{13}C NMR spectrum of 3dc (100 MHz, $CDCl_3$)



Mass spectrum of 3dc

Data File	SJ-SF-27.d	**Sample Name**	SJ-SF-27
Sample Type	Sample	**Position**	P1-B9
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 8:03:33 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



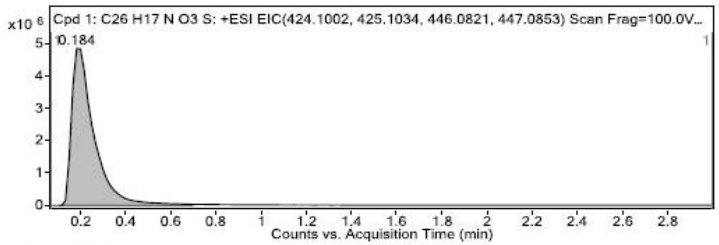
3dc

Chemical Formula (M): $C_{26}H_{17}NO_3S$
Exact Mass: 423.0929
Found (M+H): 424.1007

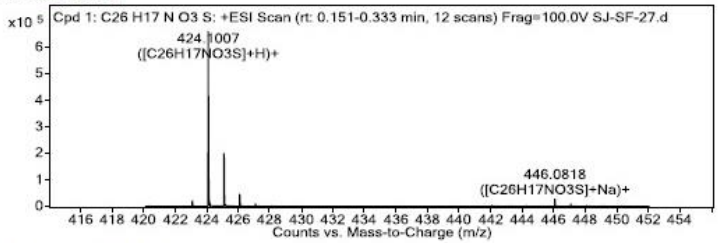
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C26 H17 N O3 S	0.184	423.0933	29070	C26 H17 N O3 S	423.0929	0.95

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C26 H17 N O3 S	446.0818	0.184	Find By Formula	423.0933



MS Zoomed Spectrum



MS Spectrum Peak List

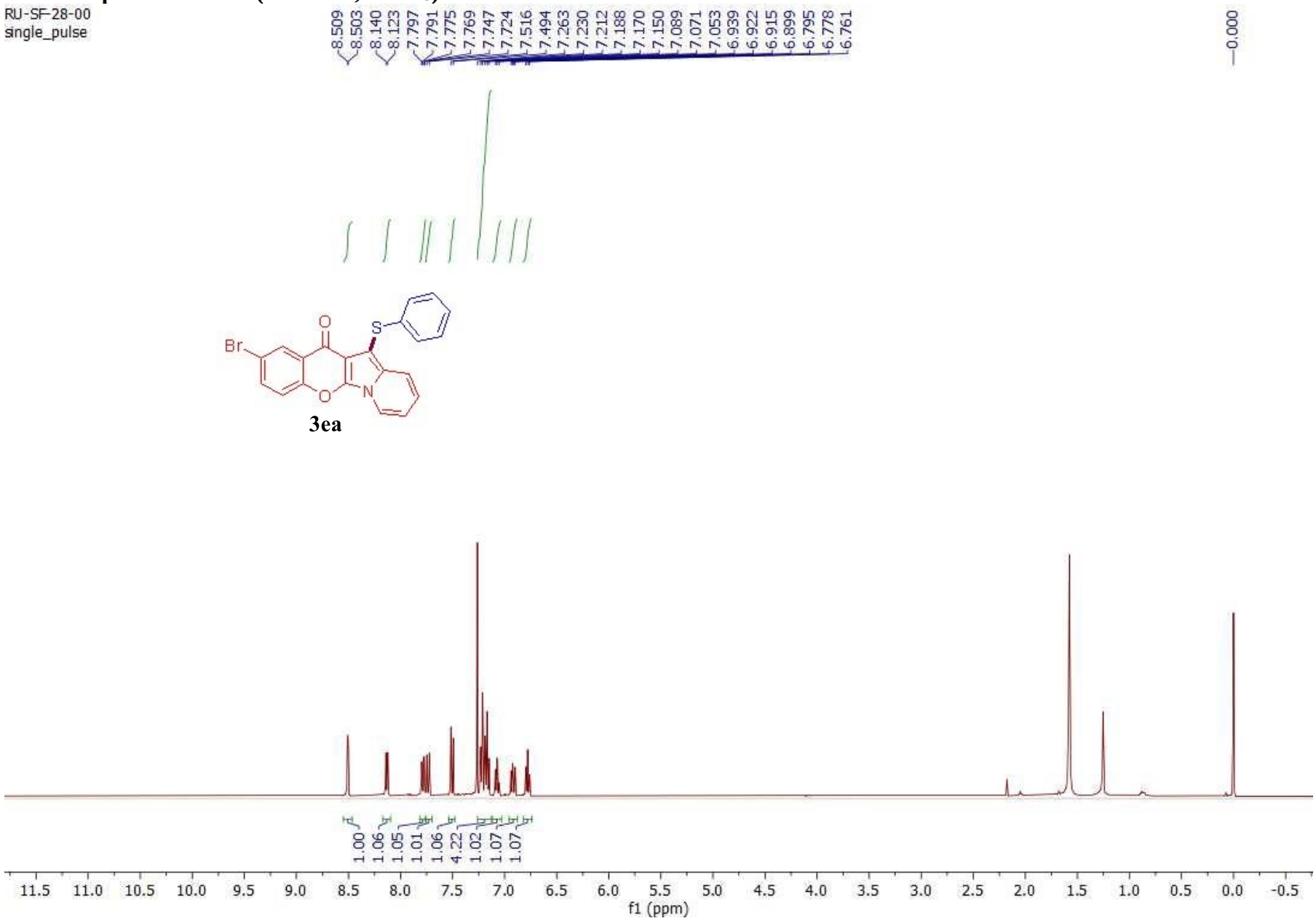
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
424.1007	424.1002	-1.12	1	688150.81	C26H17NO3S	(M+H)+
425.1036	425.1034	-0.4	1	205450.68	C26H17NO3S	(M+H)+
426.1023	426.1013	-2.16	1	44329.55	C26H17NO3S	(M+H)+
446.0818	446.0821	0.69	1	29070.21	C26H17NO3S	(M+Na)+
447.0851	447.0853	0.52	1	7703	C26H17NO3S	(M+Na)+
448.0837	448.0833	-0.97	1	2080.67	C26H17NO3S	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

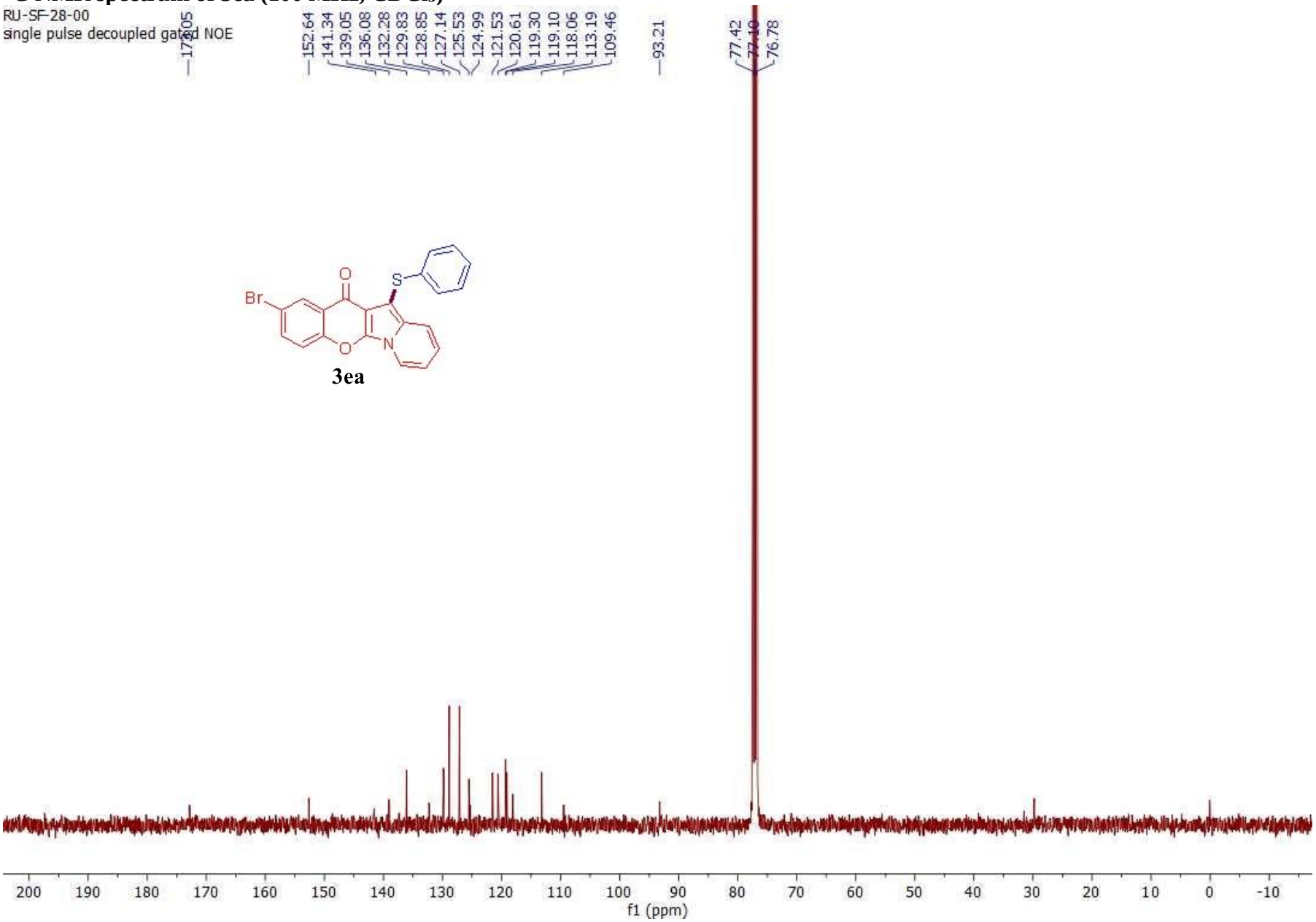
---End Of Report---

^{1}H NMR spectrum of 3ea (400 MHz, $CDCl_3$)



3ea

^{13}C NMR spectrum of 3ea (100 MHz, $CDCl_3$)

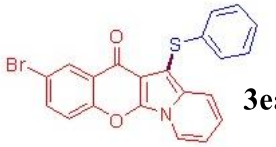


3ea

Mass spectrum of 3ea

Data File	SJ-SF-30.d	**Sample Name**	SJ-SF-30
Sample Type	Sample	**Position**	P1-B11
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 8:20:17 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



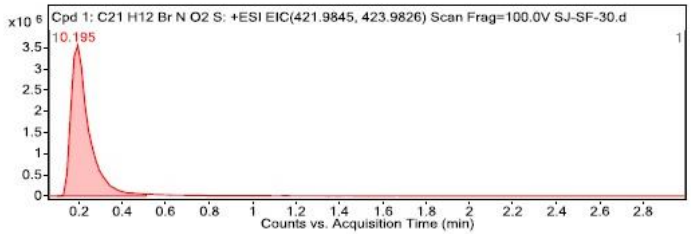
3ea

Chemical Formula (M): $C_{21}H_{12}BrNO_2S$
Exact Mass: 420.9772
Found (M+H): 421.9847

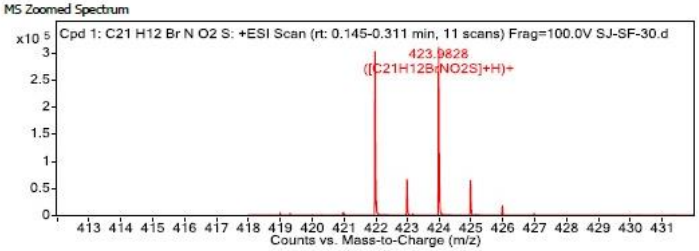
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C21 H12 Br N O2 S	0.195	420.9773	310931	C21 H12 Br N O2 S	420.9772	0.32

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H12 Br N O2 S	423.9828	0.195	Find By Formula	420.9773



MS Zoomed Spectrum



MS Spectrum Peak List

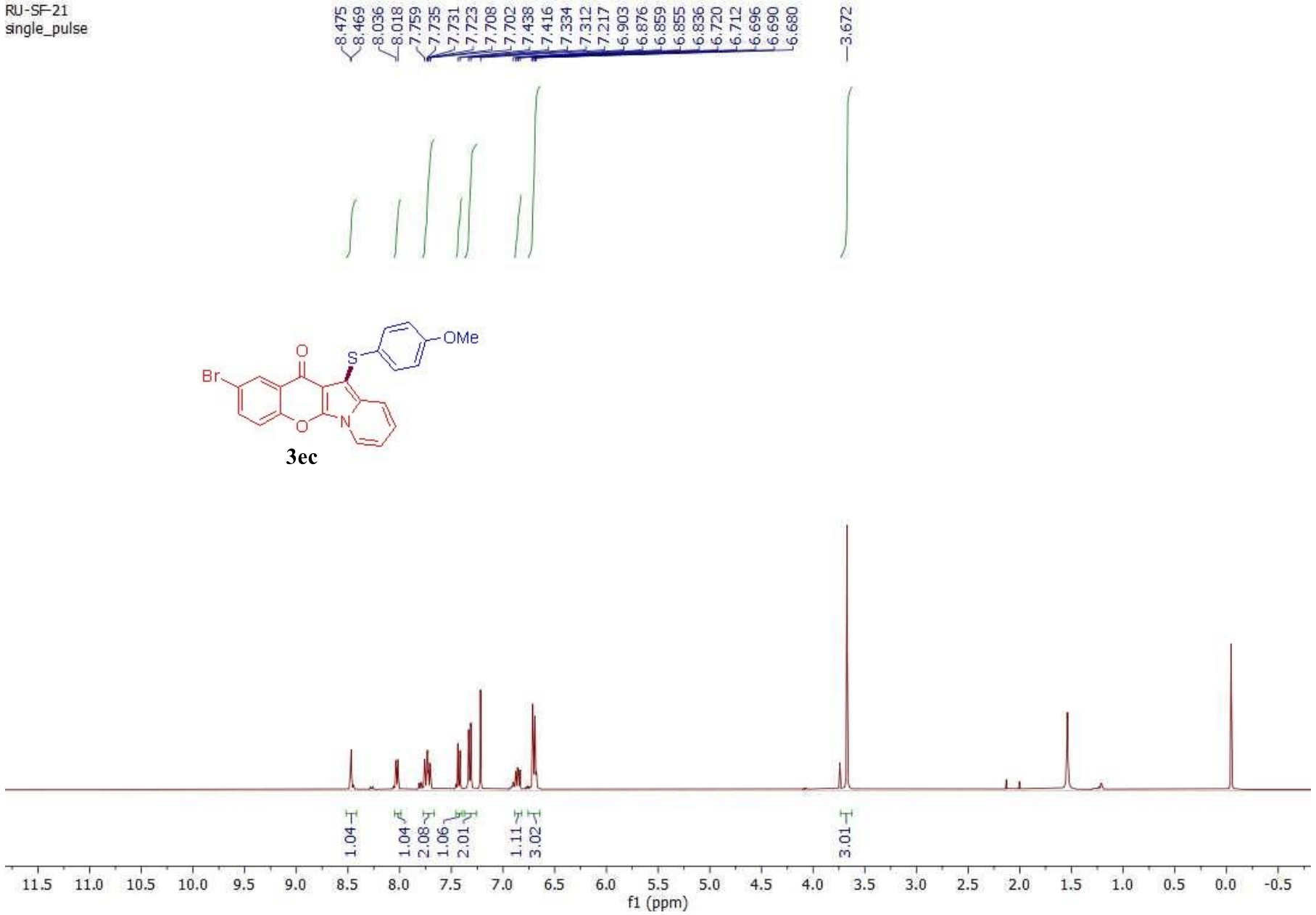
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
421.9847	421.9845	-0.49	1	304697.6	C21H12BrNO2S	(M+H)+
422.9873	422.9876	0.92	1	66944.09	C21H12BrNO2S	(M+H)+
423.9828	423.9826	-0.55	1	310930.96	C21H12BrNO2S	(M+H)+
424.9854	424.9856	0.36	1	64795.51	C21H12BrNO2S	(M+H)+
425.9829	425.9826	-0.66	1	14883.56	C21H12BrNO2S	(M+H)+
426.9832	426.9838	1.23	1	2677.73	C21H12BrNO2S	(M+H)+
427.985	427.9853	0.89	1	353.11	C21H12BrNO2S	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

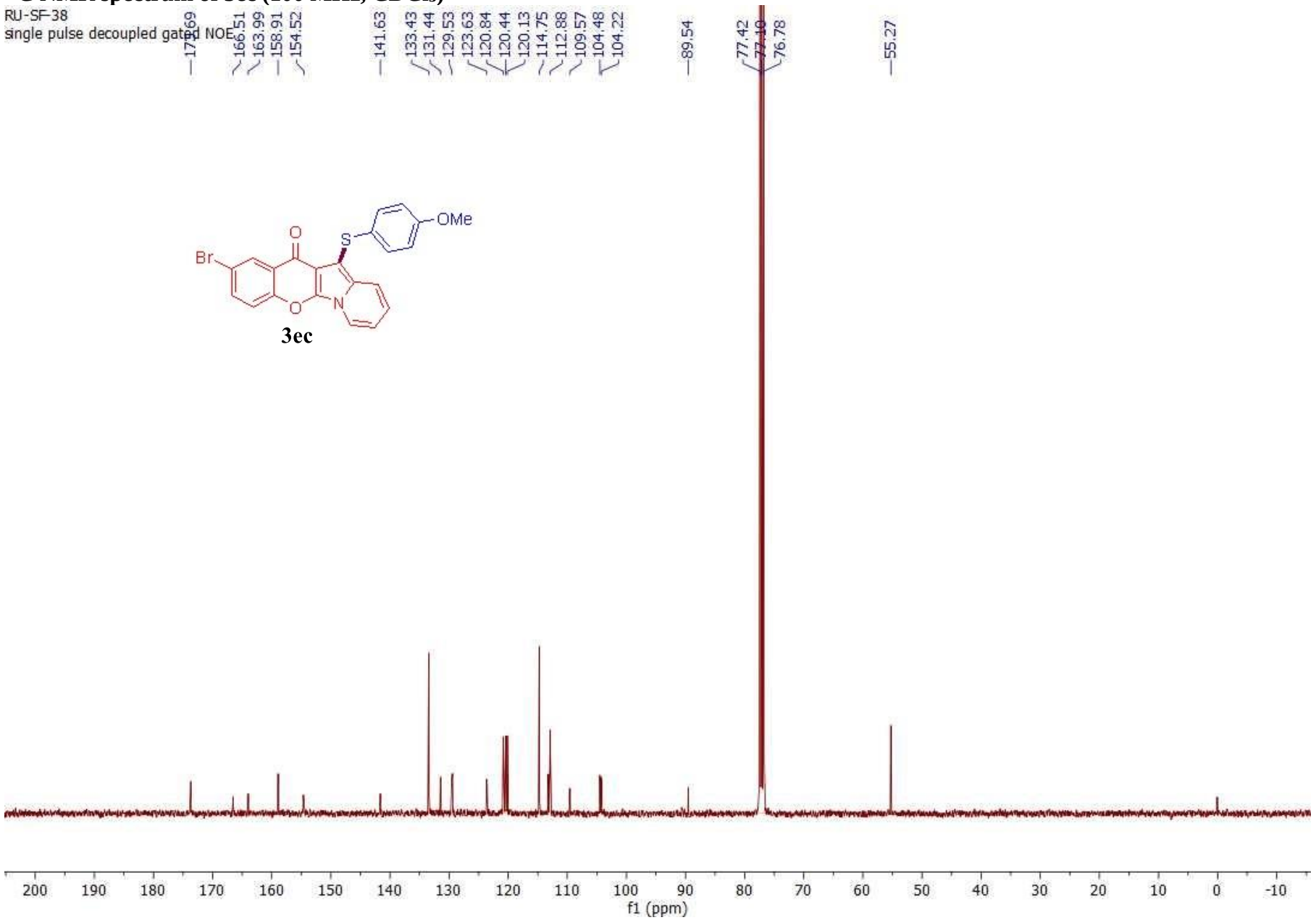
---End Of Report---

^{1}H NMR spectrum of 3ec (400 MHz, $CDCl_3$)



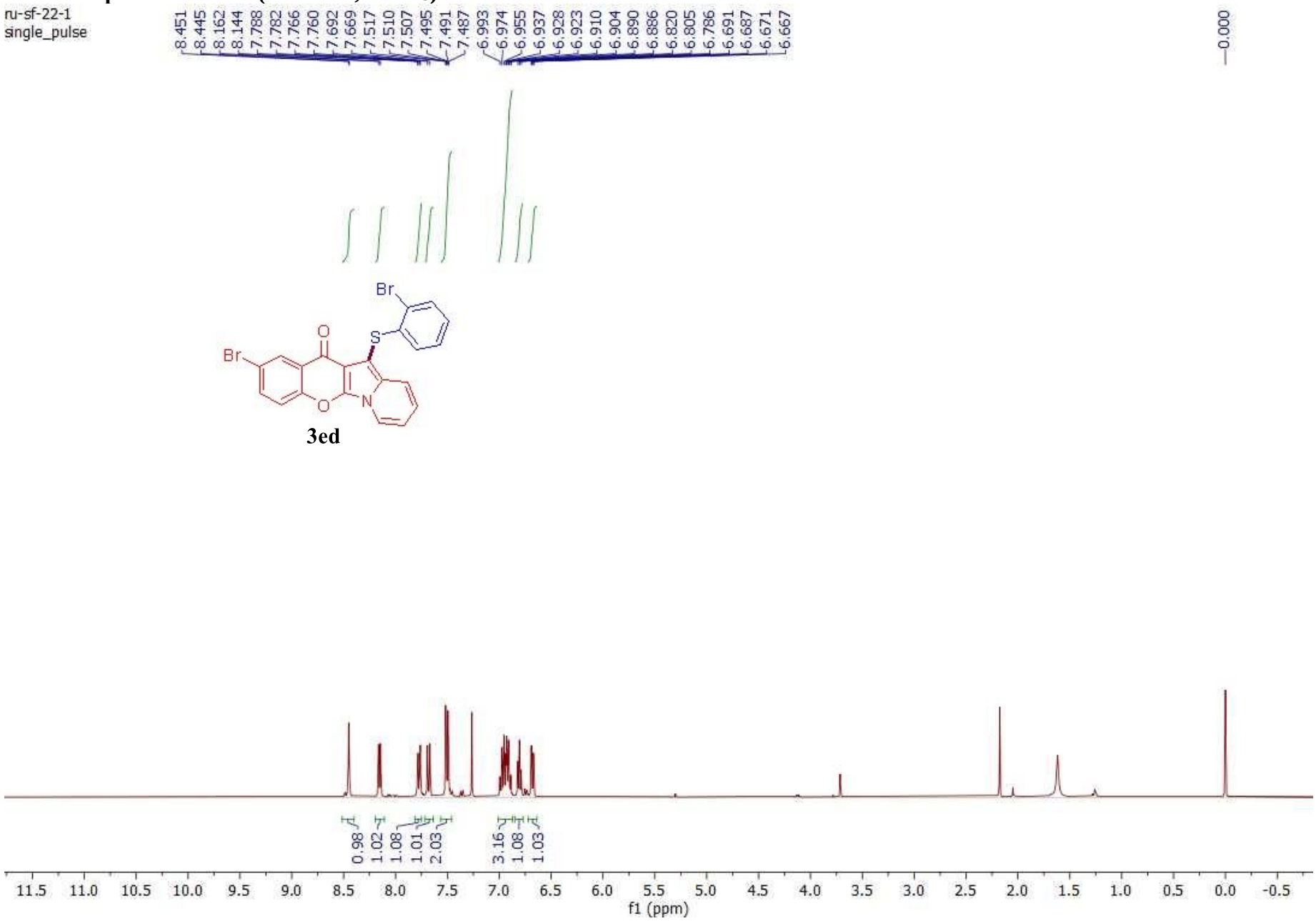
3ec

^{13}C NMR spectrum of 3ec (100 MHz, $CDCl_3$)



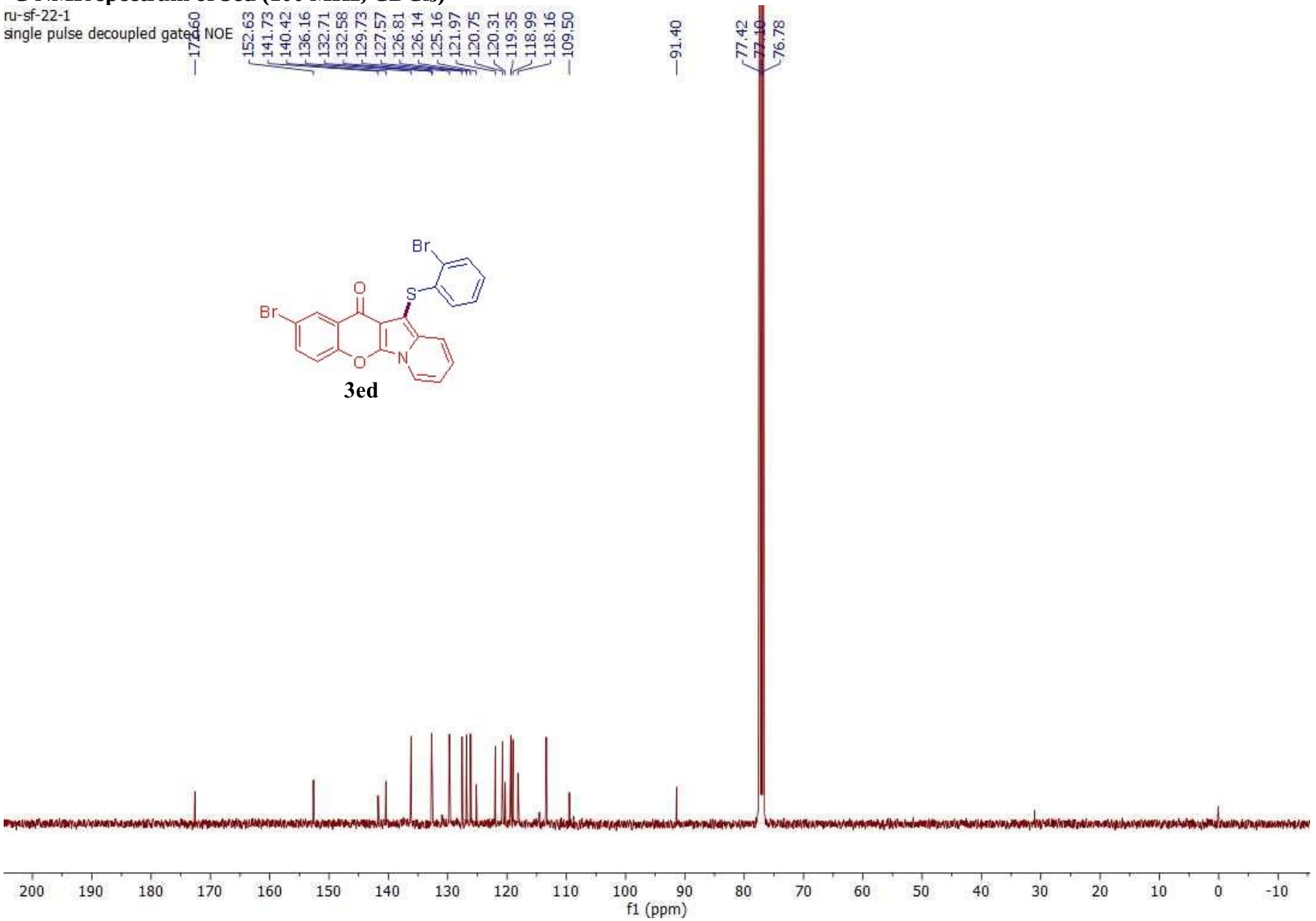
3ec

^{1}H NMR spectrum of 3ed (400 MHz, $CDCl_3$)



3ed

^{13}C NMR spectrum of 3ed (100 MHz, $CDCl_3$)



3ed

Mass spectrum of 3ed

Data File	SJ-SF-31.d	**Sample Name**	SJ-SF-31
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_C_H2O_60-40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 8:28:38 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

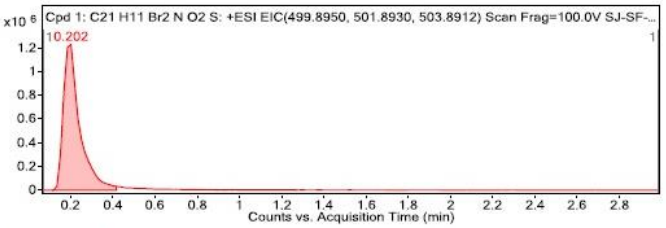
3ed

Chemical Formula (M): $C_{21}H_{11}Br_2NO_2S$
Exact Mass: 498.8877
Found (M+H): 499.8946

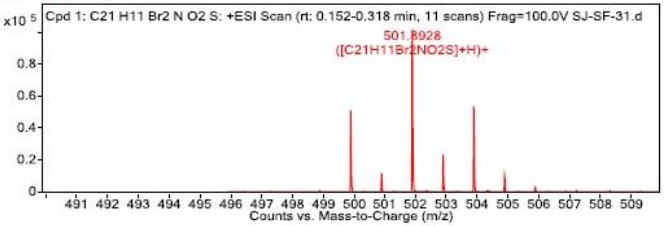
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C21 H11 Br2 N O2 S	0.202	498.8873	107517	C21 H11 Br2 N O2 S	498.8877	-0.8

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H11 Br2 N O2 S	501.8928	0.202	Find By Formula	498.8873



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
499.8946	499.895	0.86	1	51314.92	C21H11Br2NO2S	(M+H)+
500.8968	500.8981	2.74	1	11817.14	C21H11Br2NO2S	(M+H)+
501.8928	501.893	0.38	1	107517.41	C21H11Br2NO2S	(M+H)+
502.8954	502.8961	1.44	1	23450.6	C21H11Br2NO2S	(M+H)+
503.8908	503.8912	0.71	1	54695.79	C21H11Br2NO2S	(M+H)+
504.8934	504.8941	1.43	1	11399.37	C21H11Br2NO2S	(M+H)+
505.8909	505.8912	0.56	1	2841.11	C21H11Br2NO2S	(M+H)+
506.8915	506.8923	1.61	1	519.25	C21H11Br2NO2S	(M+H)+
507.8932	507.8938	1.28	1	73.63	C21H11Br2NO2S	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

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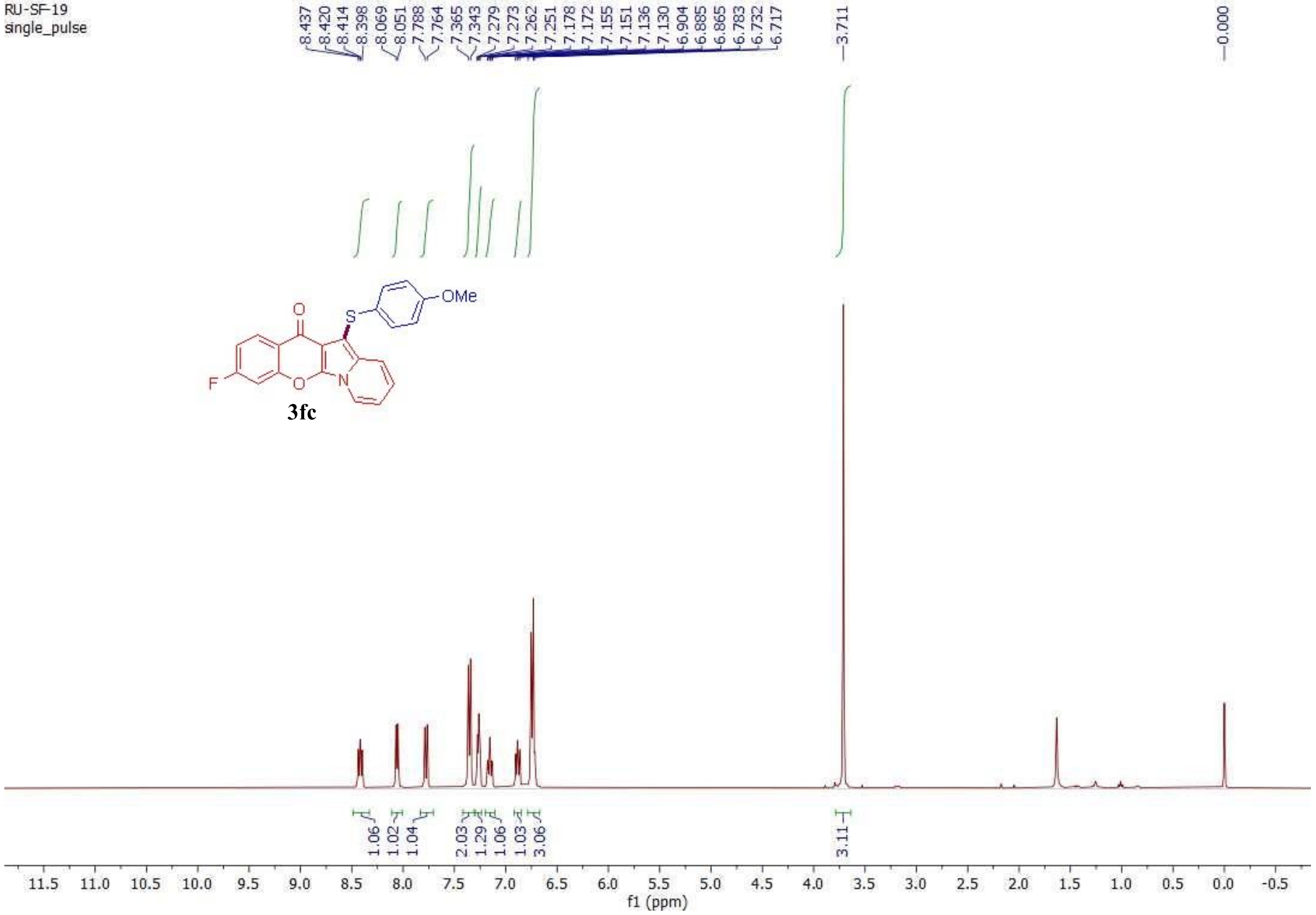
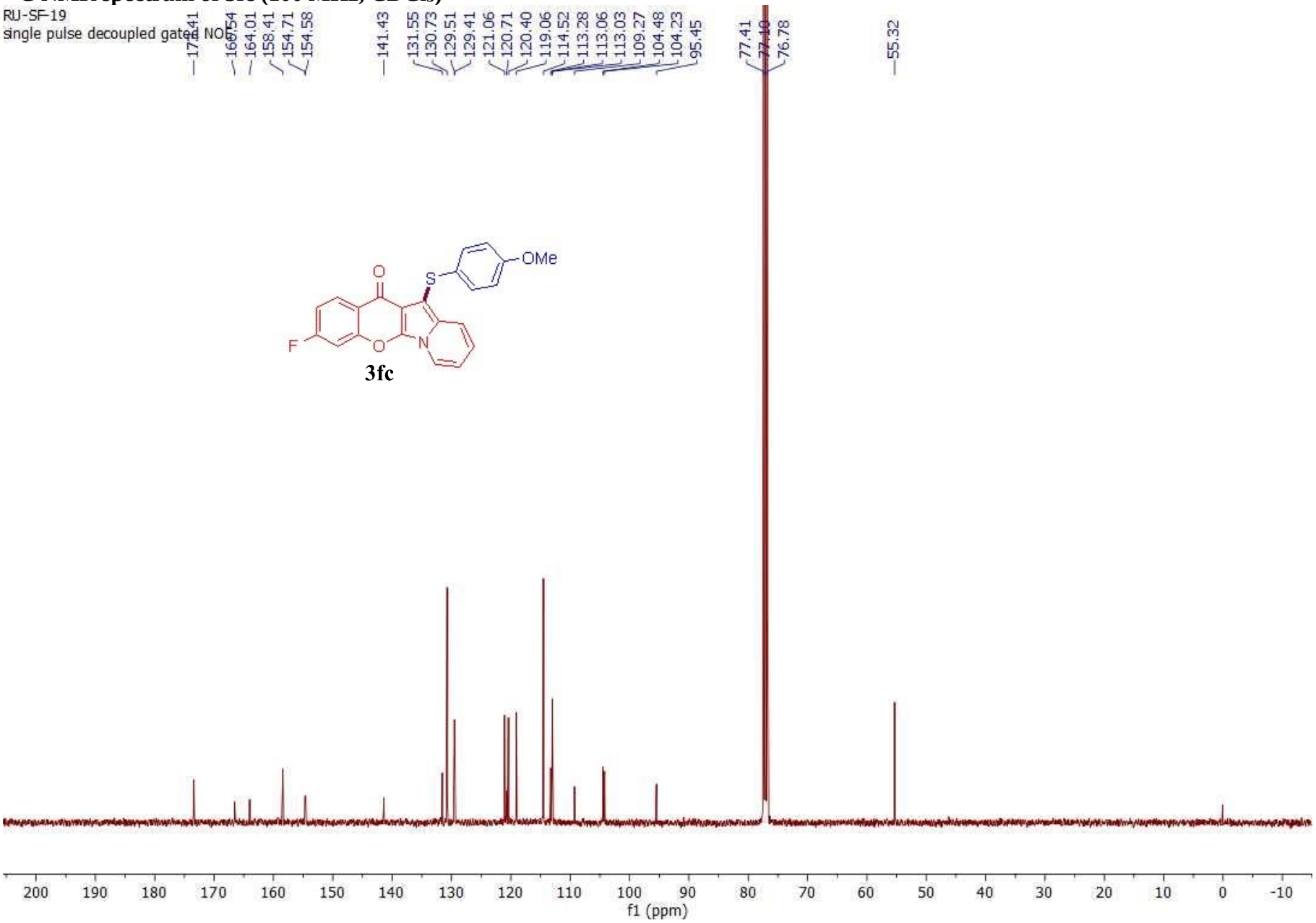
^{1}H NMR spectrum of 3fc (400 MHz, $CDCl_3$)



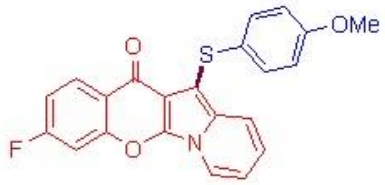
3fc

^{13}C NMR spectrum of 3fc (100 MHz, $CDCl_3$)



^{19}F NMR spectrum of 3fc (376 MHz, $CDCl_3$)

RU-SF-19
single_pulse

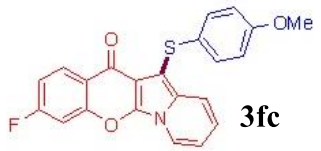


3fc

Mass spectrum of 3fc

Data File	SJ-SF-19.d	**Sample Name**	SJ-SF-19
Sample Type	Sample	**Position**	P1-B4
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 7:21:49 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



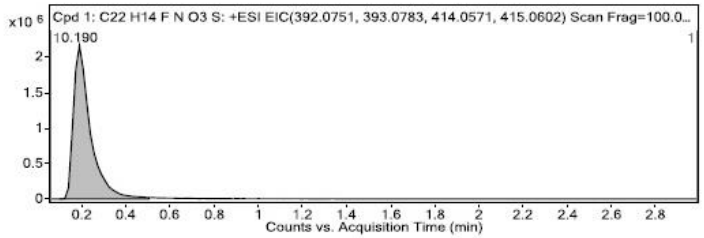
3fc

Chemical Formula (M): $C_{22}H_{14}FNO_3S$
Exact Mass: 391.0678
Found (M+H): 392.0752

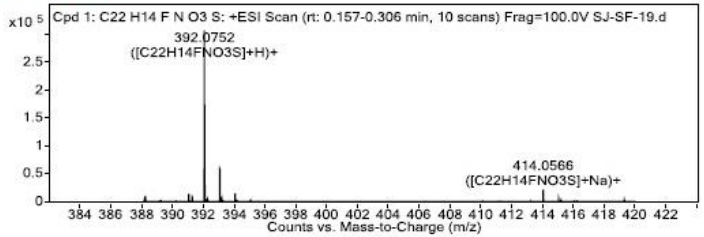
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H14 F N O3 S	0.19	391.0679	21933	C22 H14 F N O3 S	391.0678	0.03

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H14 F N O3 S	414.0566	0.19	Find By Formula	391.0679



MS Zoomed Spectrum



MS Spectrum Peak List

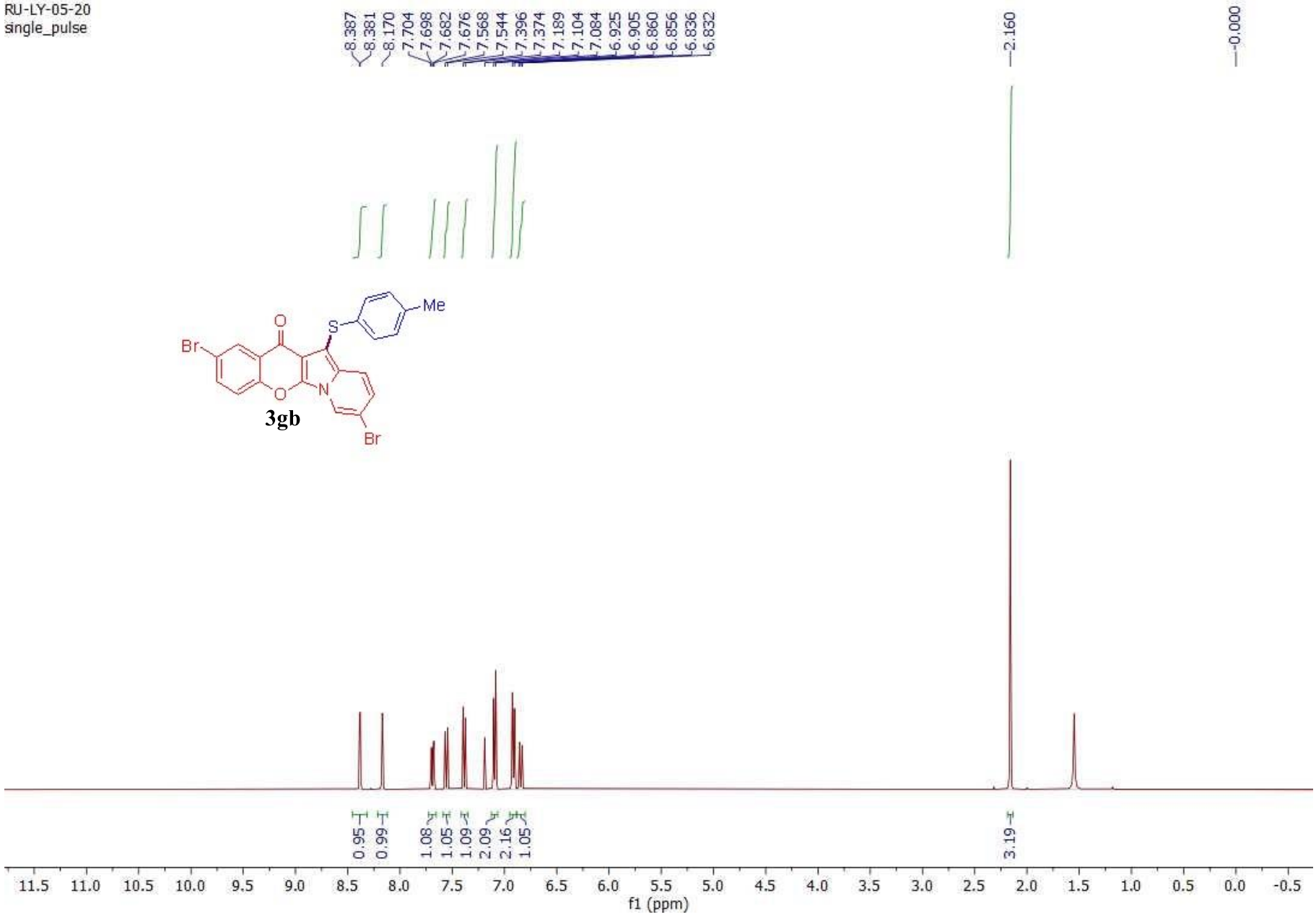
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
392.0752	392.0751	-0.27	1	308105.53	C22H14FNO3S	(M+H)+
393.0779	393.0783	1	1	63755.23	C22H14FNO3S	(M+H)+
394.0761	394.0755	-1.63	1	14919.7	C22H14FNO3S	(M+H)+
414.0566	414.0571	1.04	1	21932.94	C22H14FNO3S	(M+Na)+
415.0598	415.0602	1.12	1	5331.72	C22H14FNO3S	(M+Na)+
416.0575	416.0574	-0.13	1	1232.31	C22H14FNO3S	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

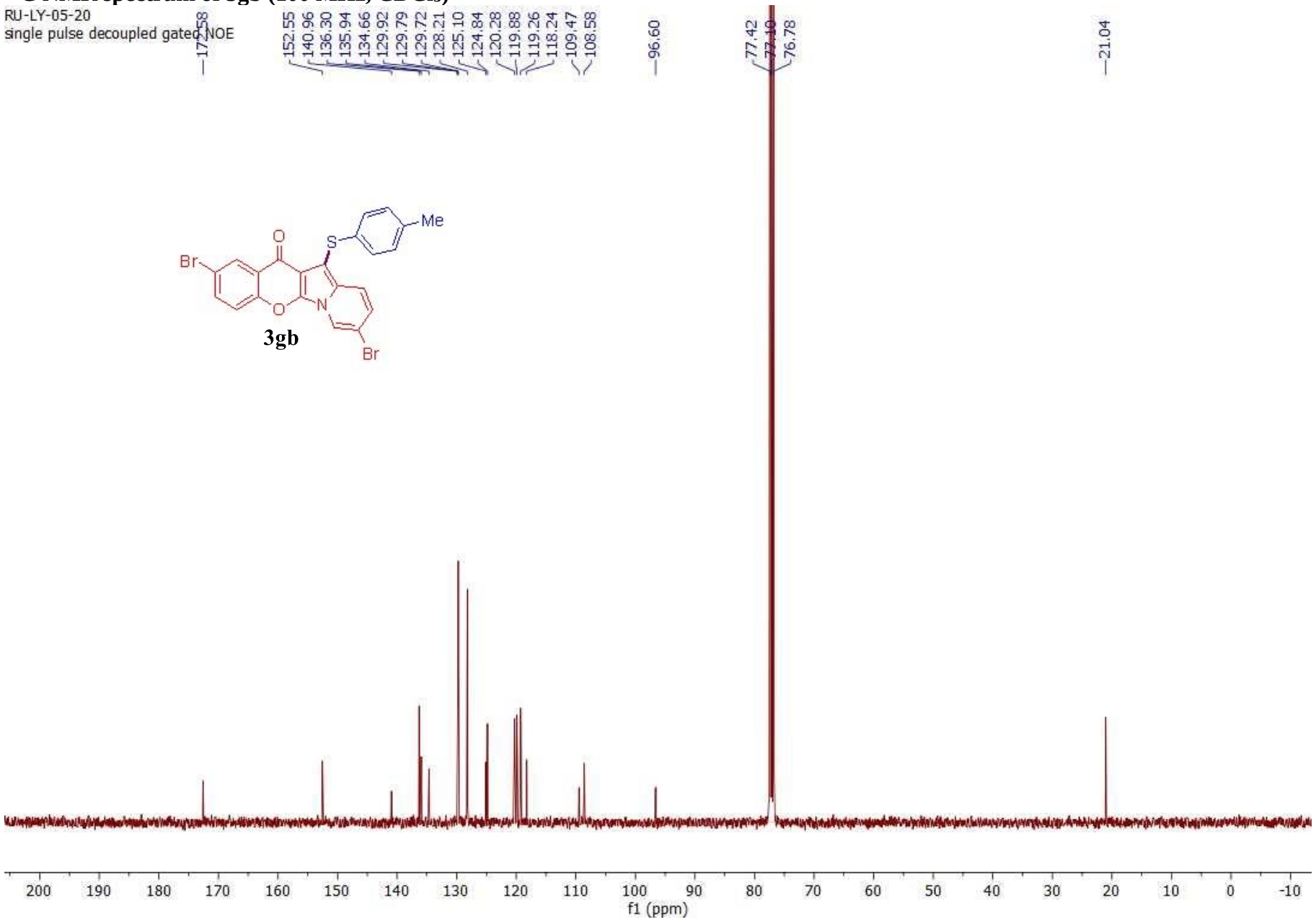
Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

---End Of Report---

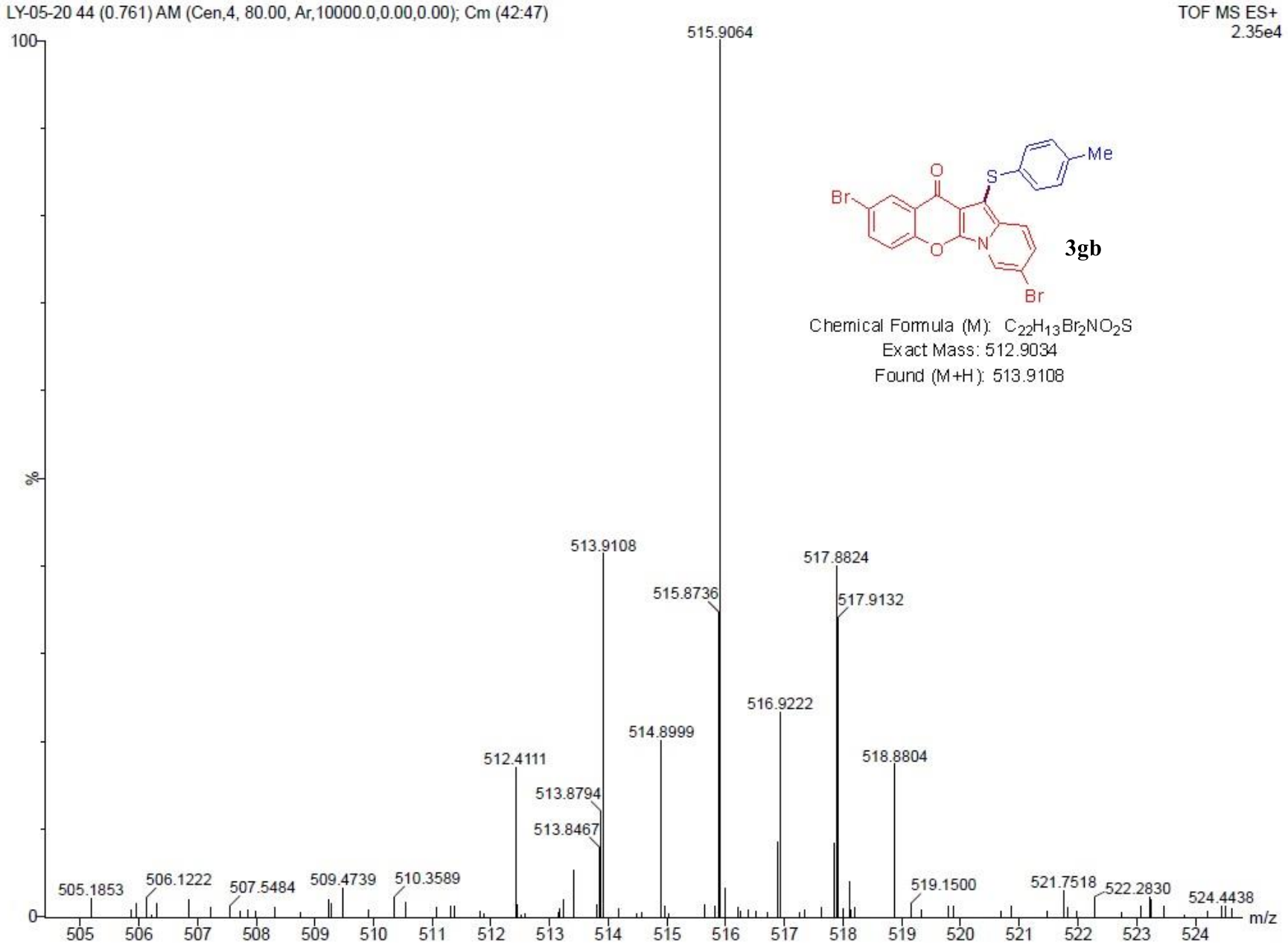
^{1}H NMR spectrum of 3gb (400 MHz, $CDCl_3$)



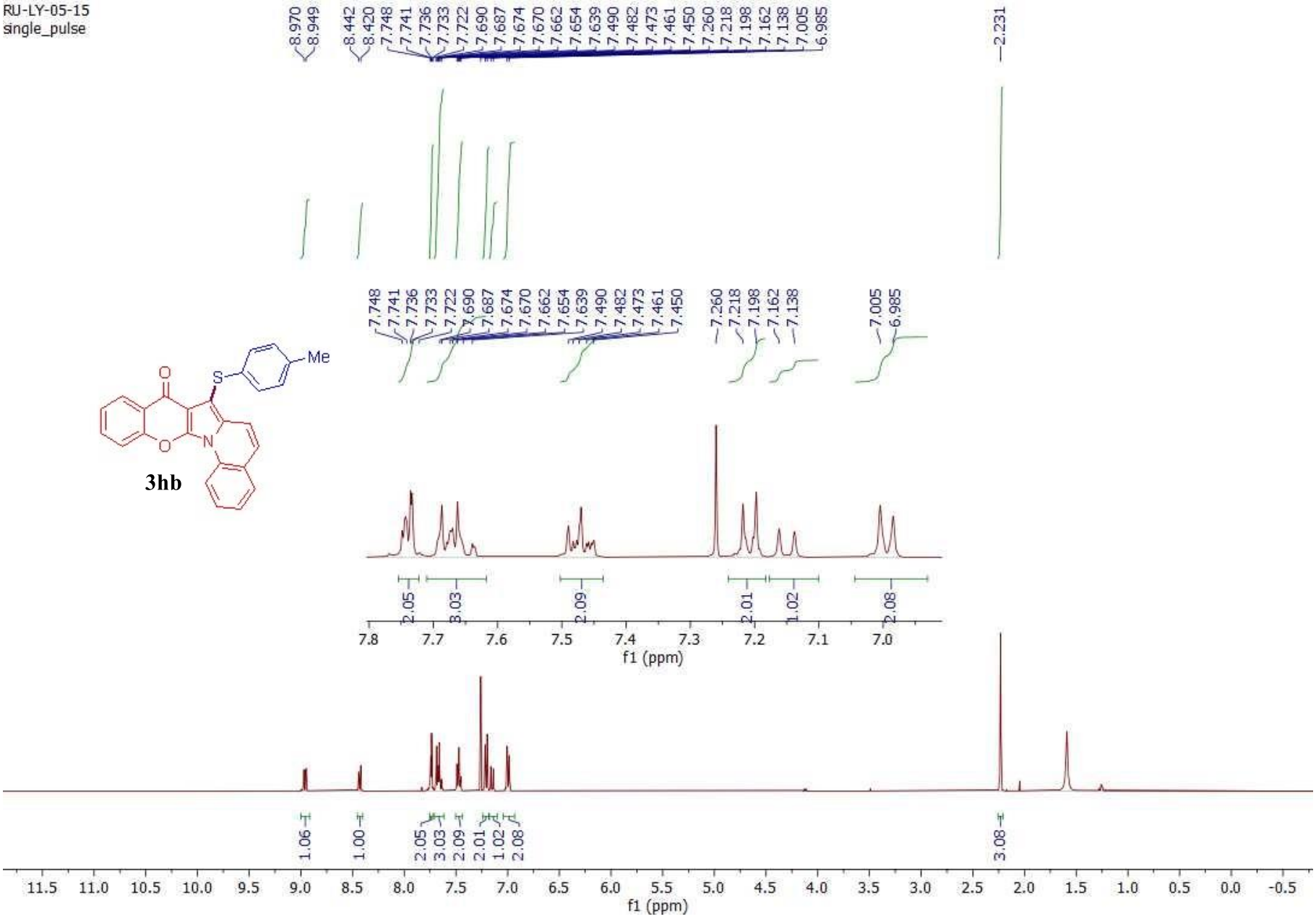
^{13}C NMR spectrum of 3gb (100 MHz, $CDCl_3$)



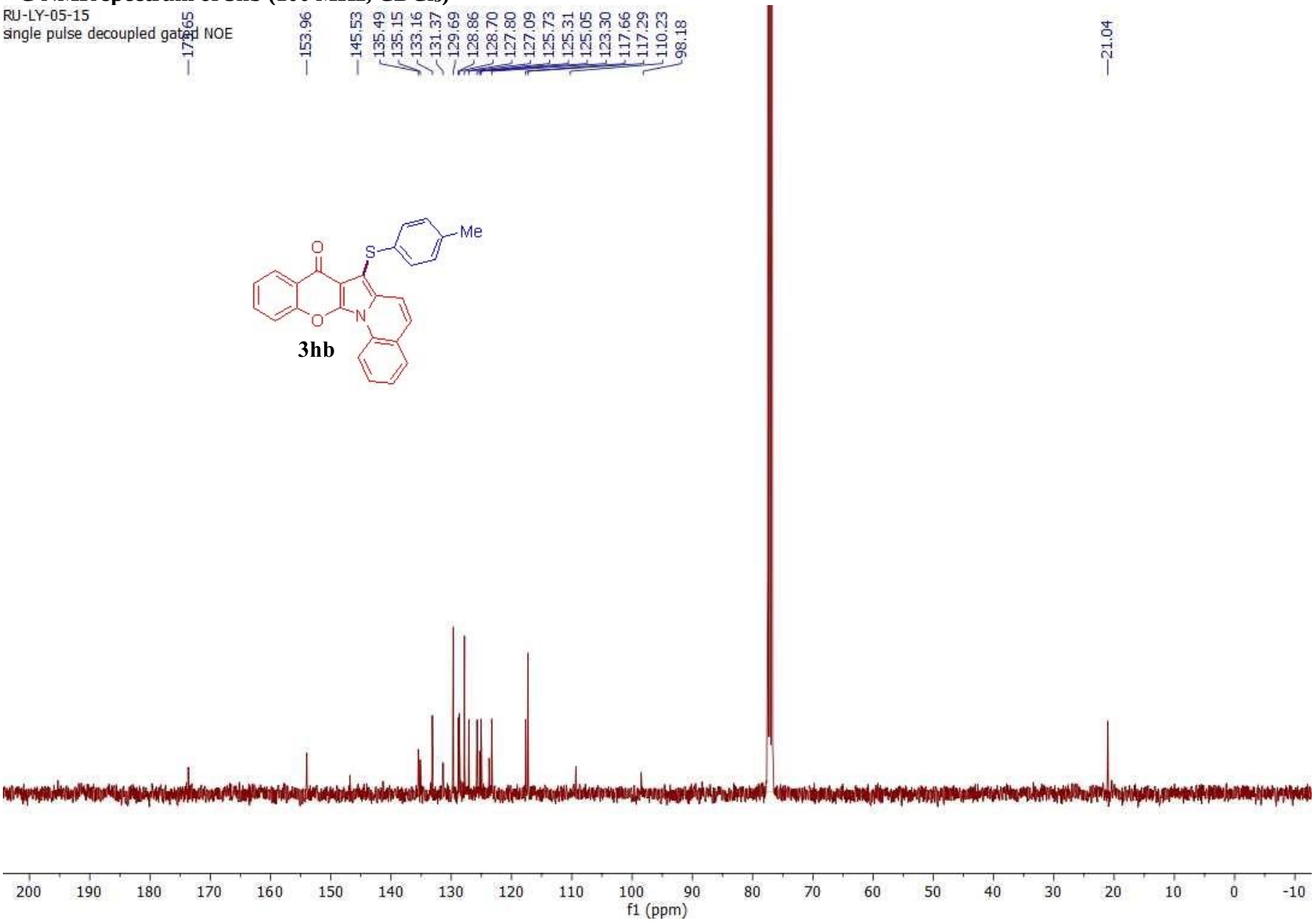
Mass spectrum of 3gb



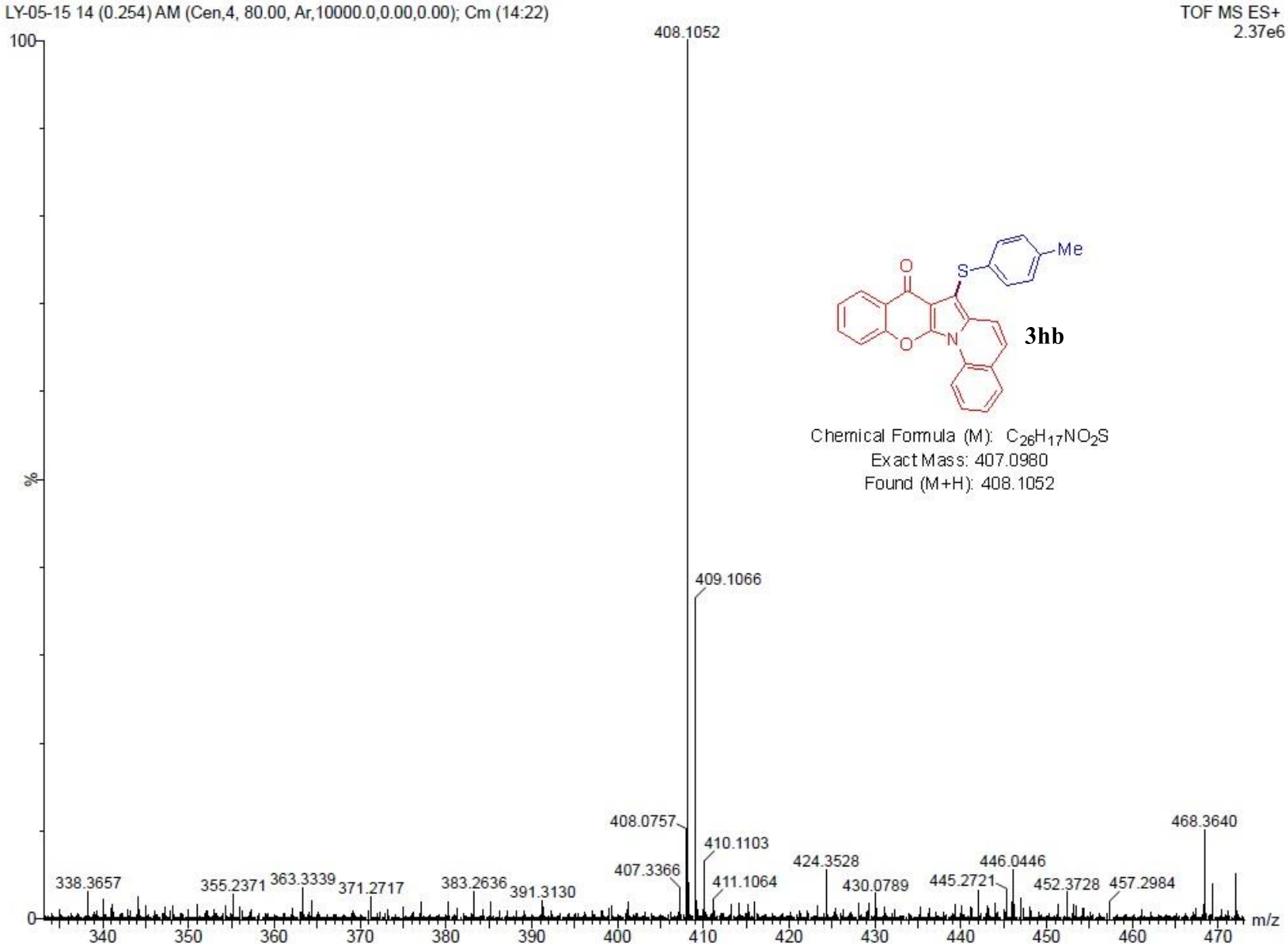
^{1}H NMR spectrum of 3hb (400 MHz, $CDCl_3$)



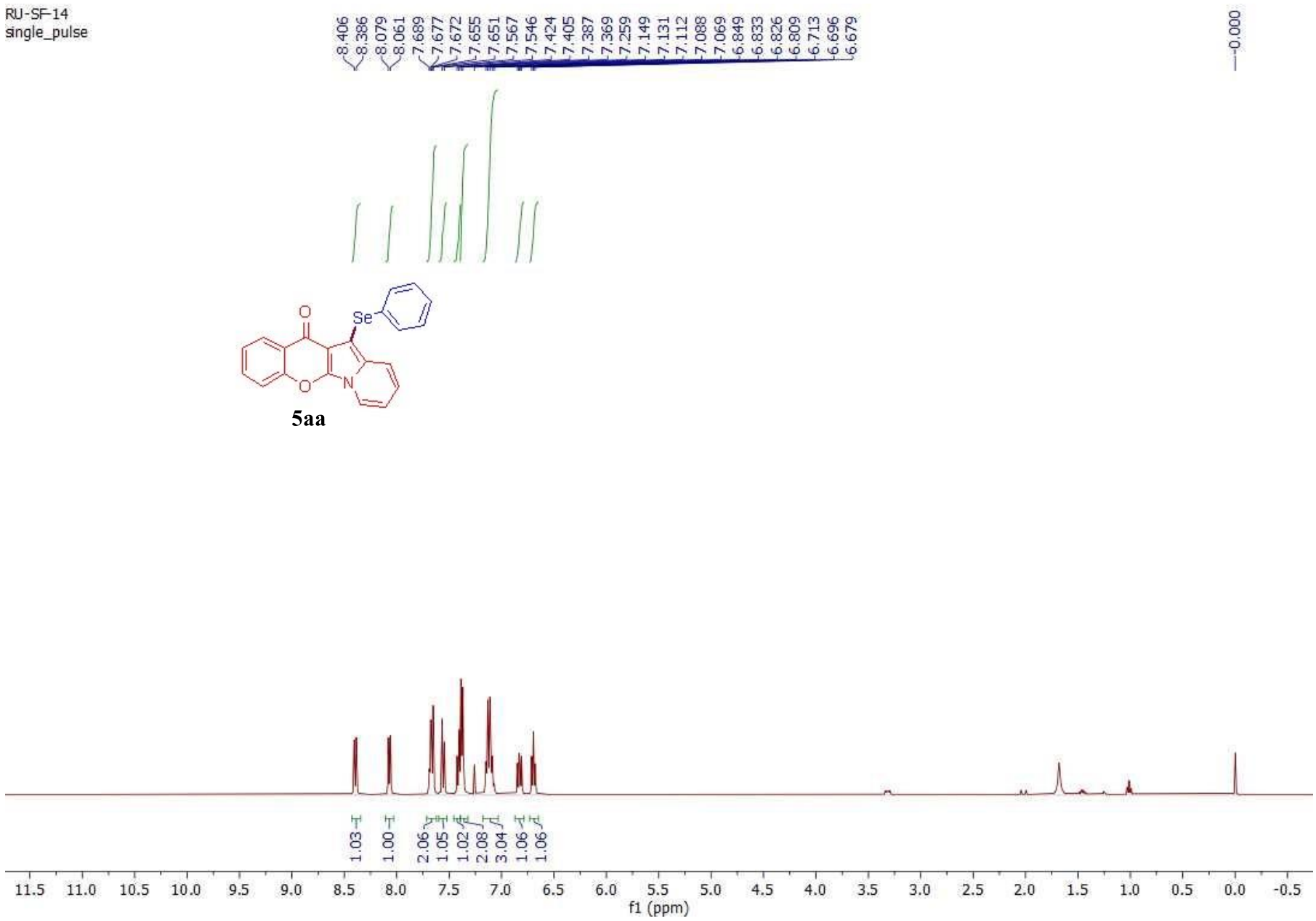
^{13}C NMR spectrum of 3hb (100 MHz, $CDCl_3$)



Mass spectrum of 3hb

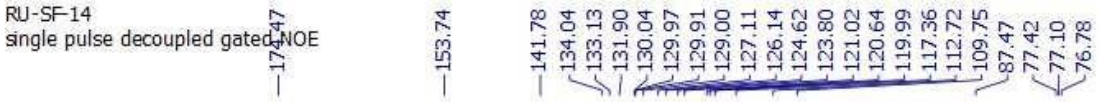


^{1}H NMR spectrum of 5aa (400 MHz, $CDCl_3$)



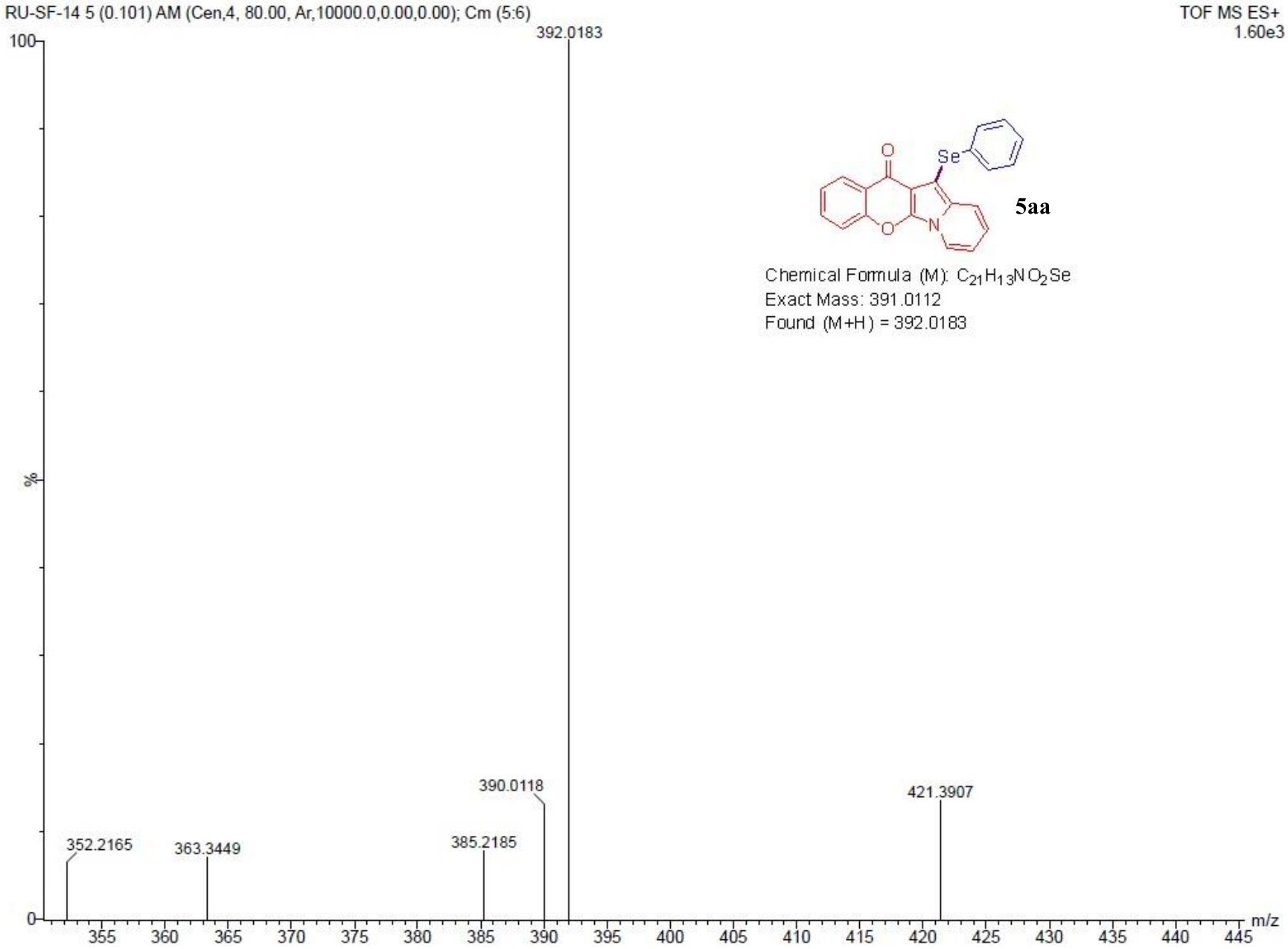
5aa

^{13}C NMR spectrum of 5aa (100 MHz, $CDCl_3$)

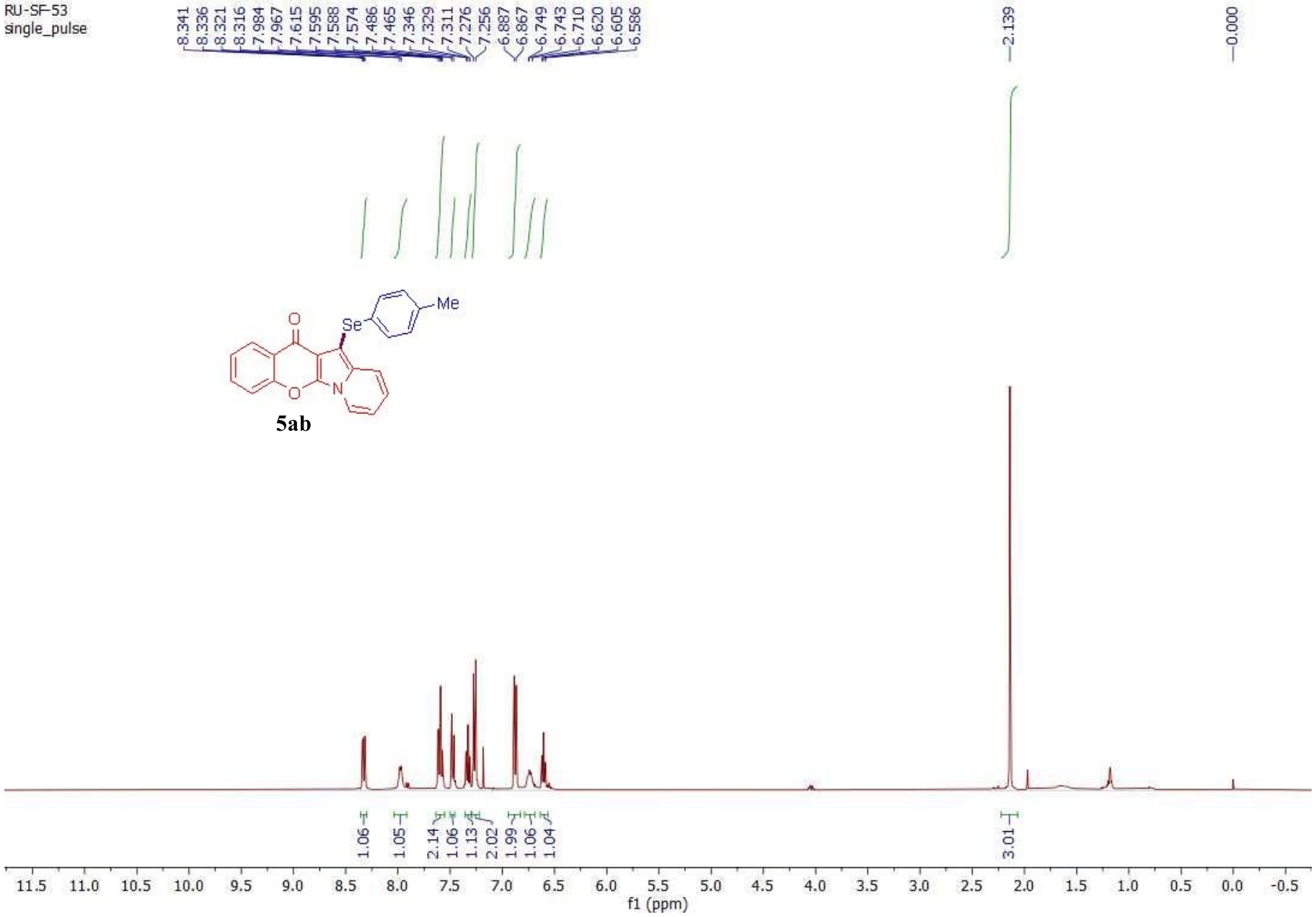


5aa

Mass spectrum of 5aa

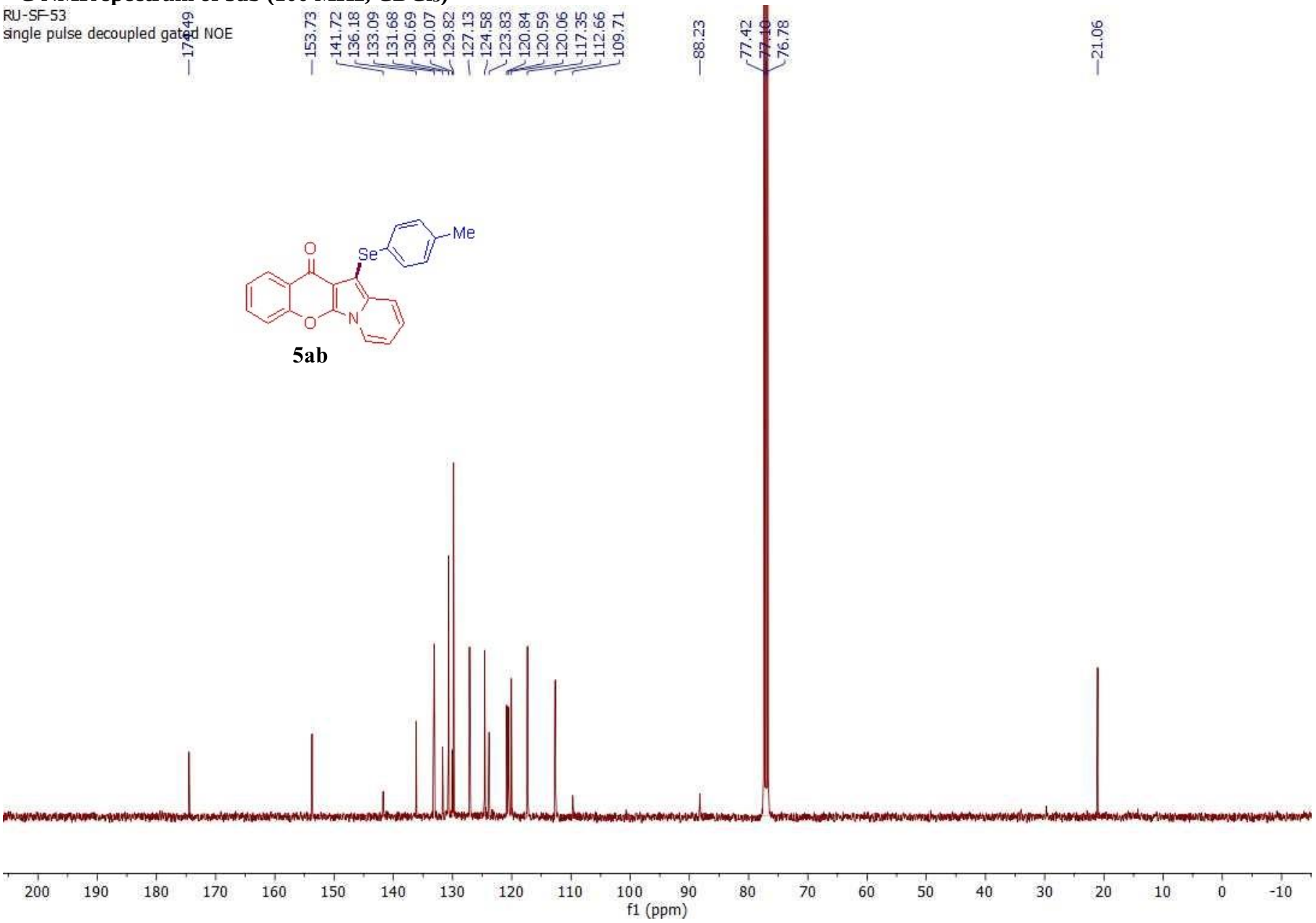


^{1}H NMR spectrum of 5ab (400 MHz, $CDCl_3$)



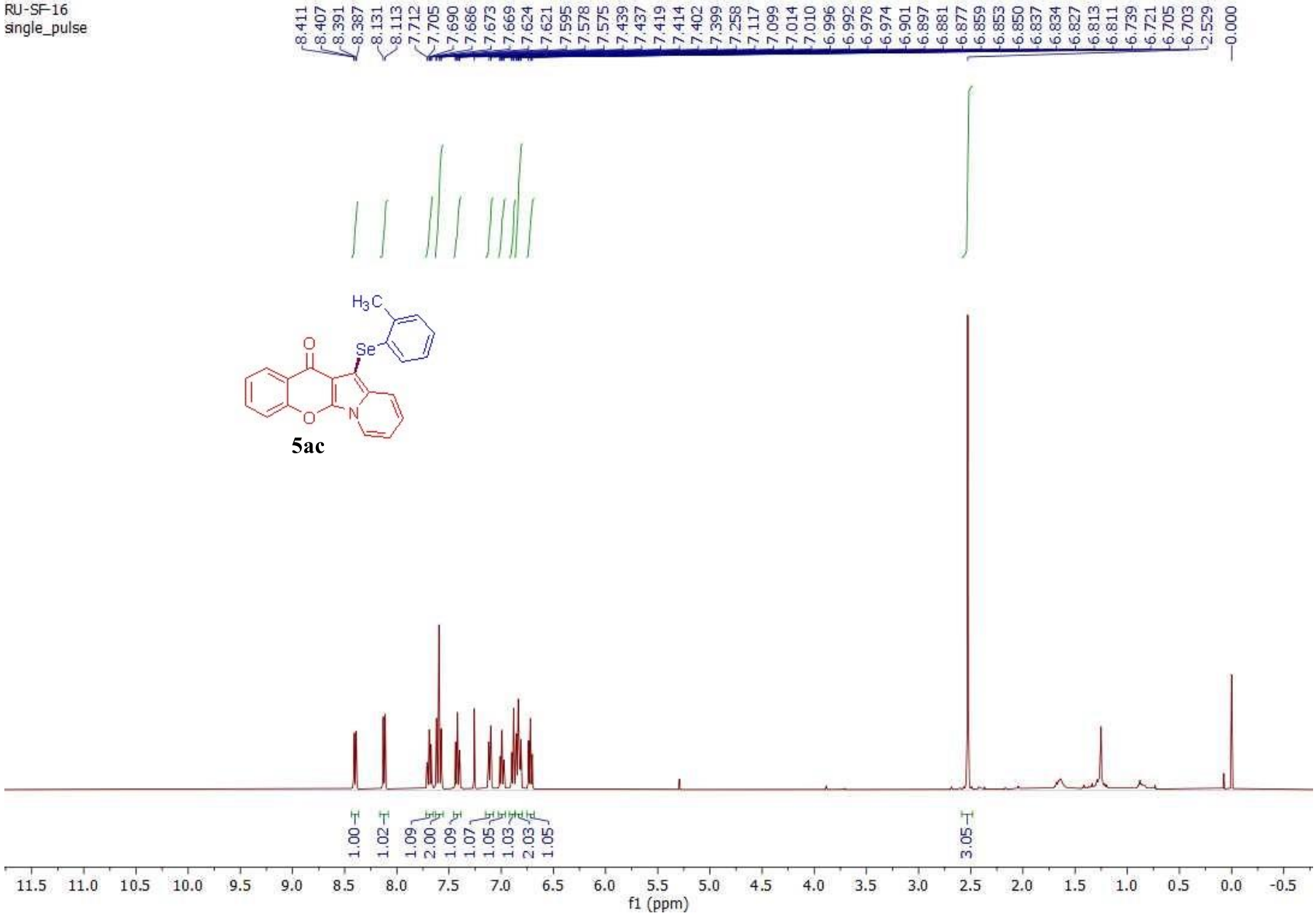
5ab

^{13}C NMR spectrum of 5ab (100 MHz, $CDCl_3$)

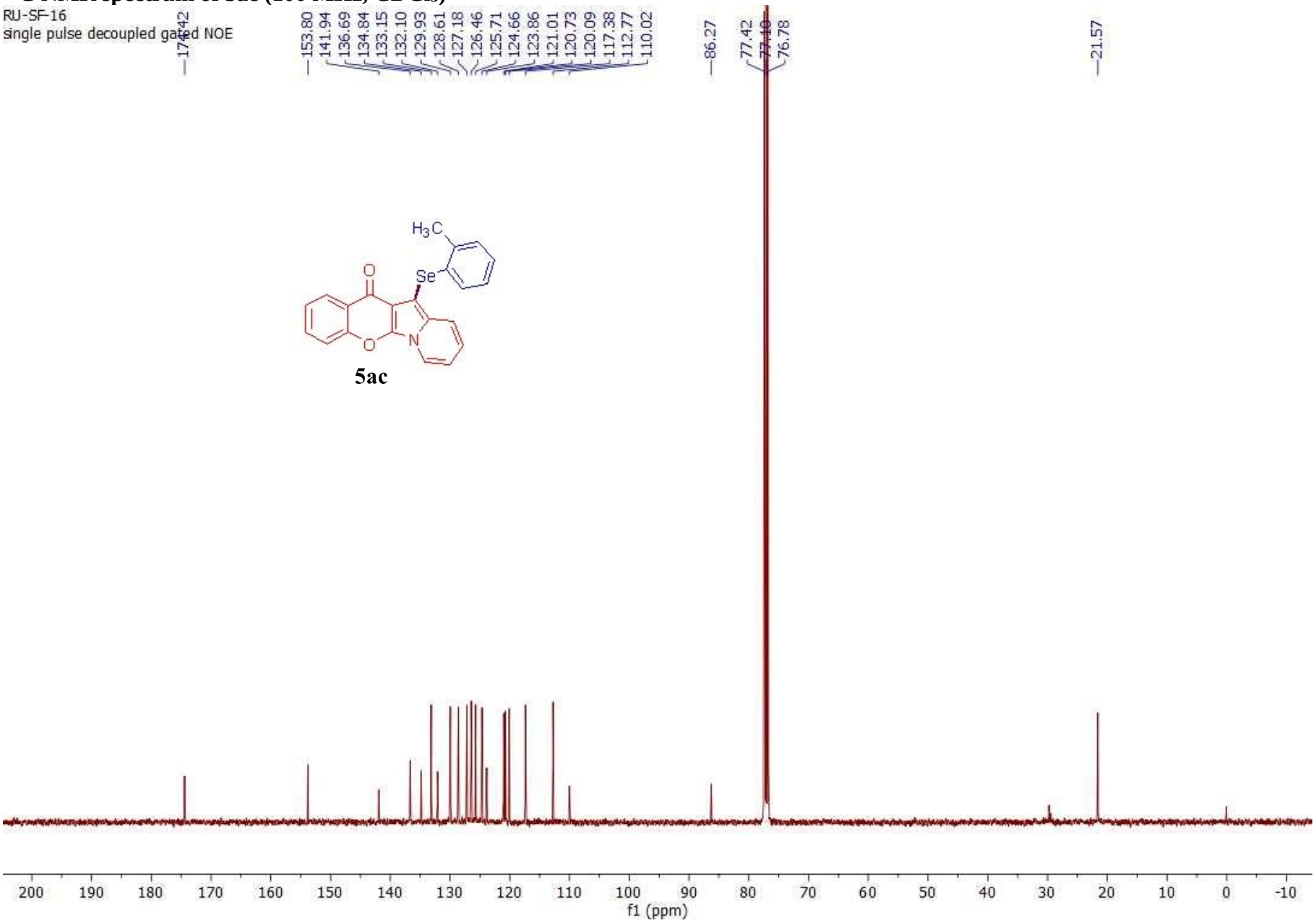


5ab

^{1}H NMR spectrum of 5ac (400 MHz, $CDCl_3$)

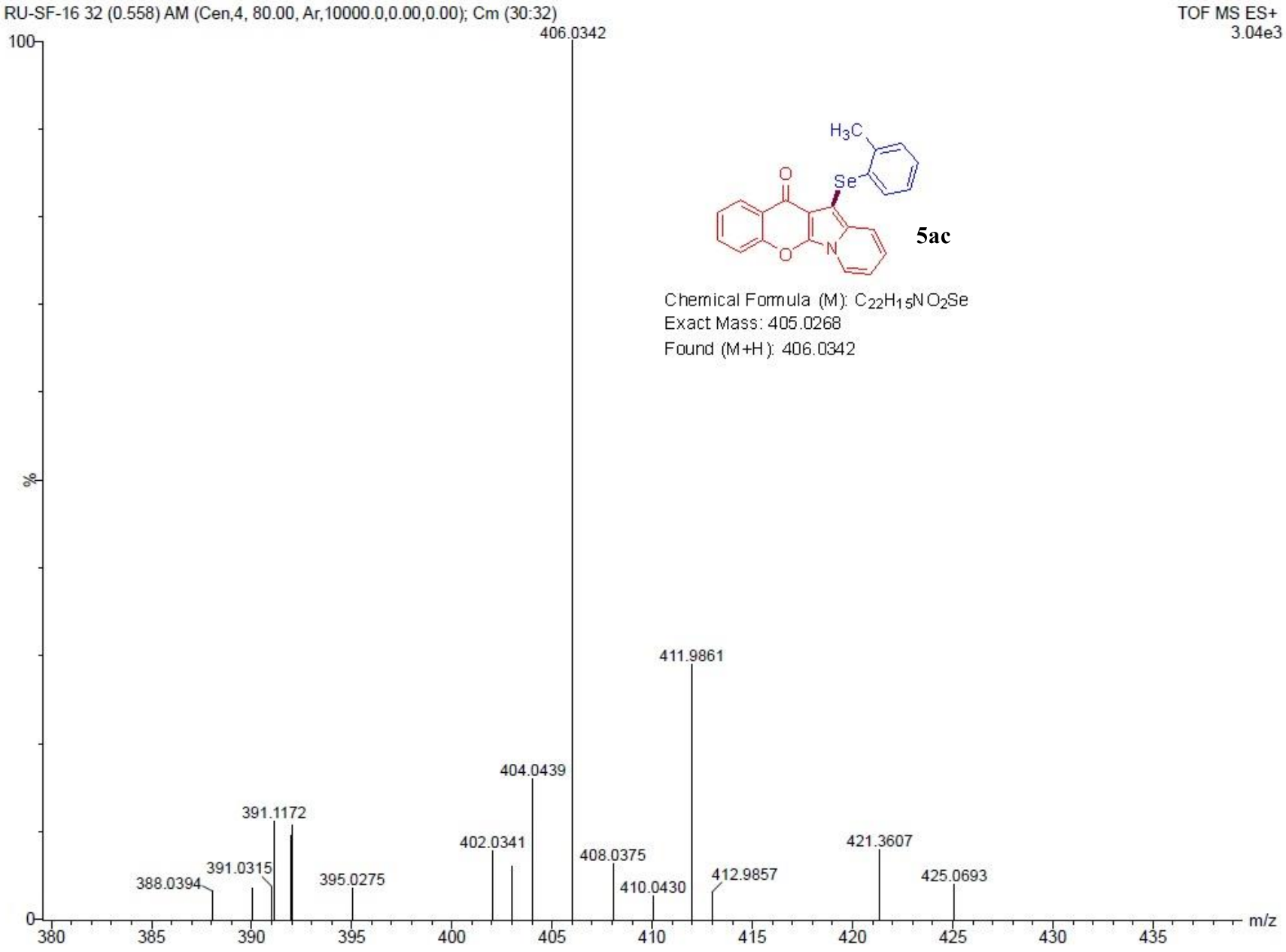


^{13}C NMR spectrum of 5ac (100 MHz, $CDCl_3$)

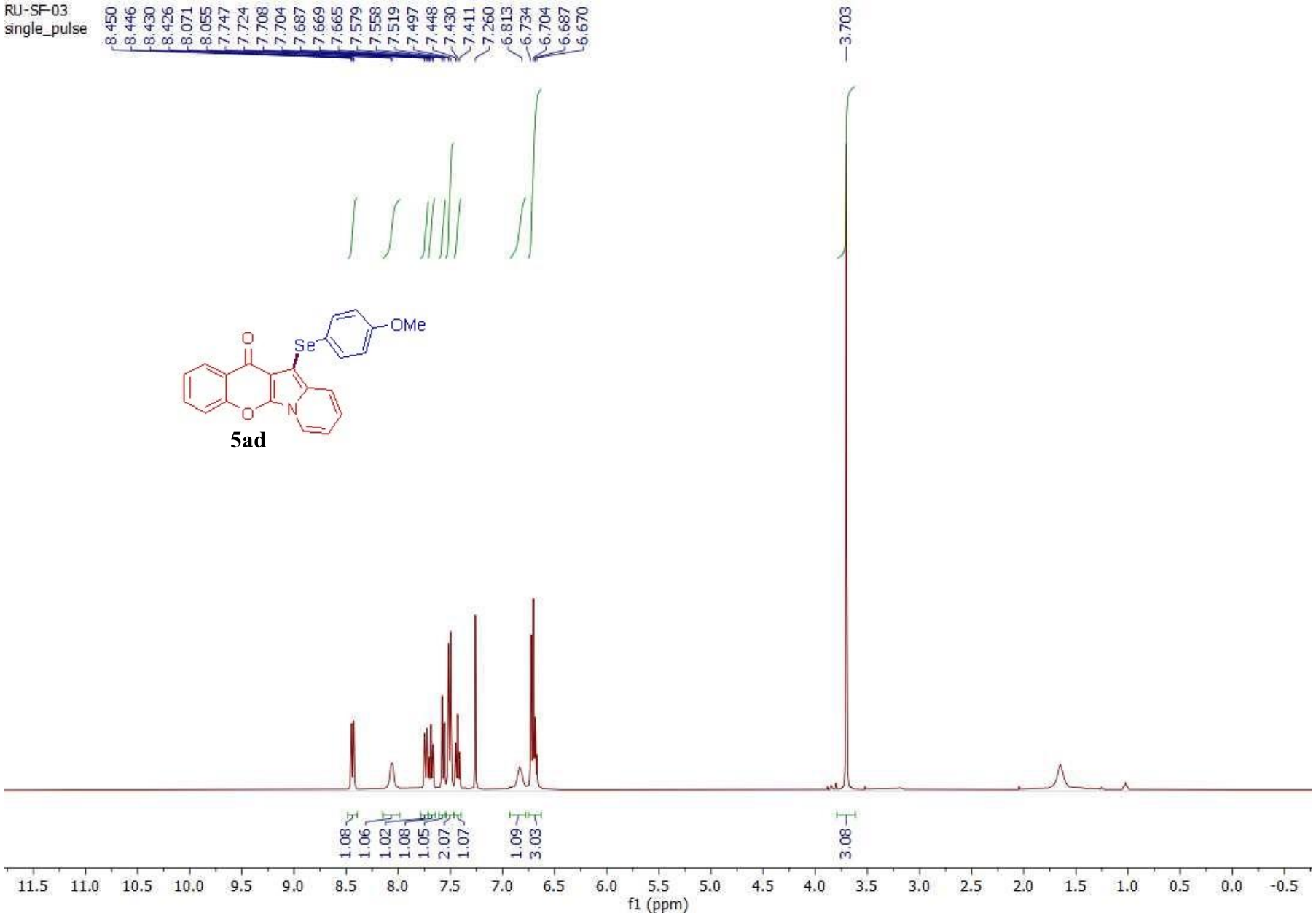


5ac

Mass spectrum of 5ac

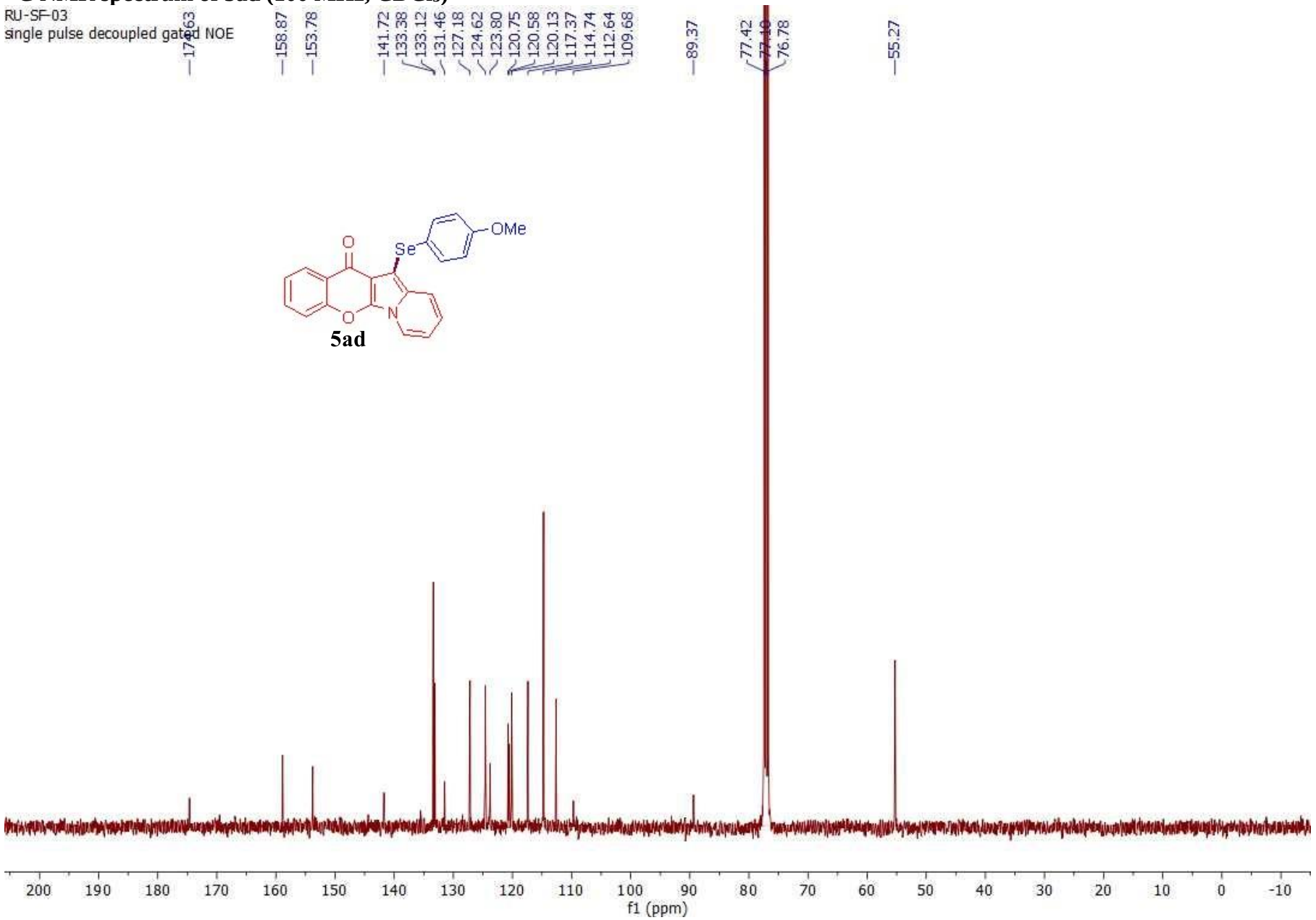


^{1}H NMR spectrum of 5ad (400 MHz, $CDCl_3$)



5ad

^{13}C NMR spectrum of 5ad (100 MHz, $CDCl_3$)



5ad

Mass spectrum of 5ad

Data File	SJ-SF-03.d	**Sample Name**	SJ-SF-03
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 7:05:07 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

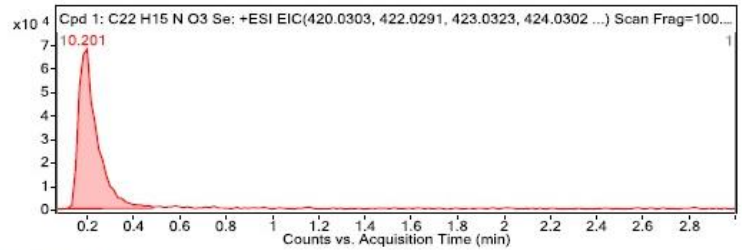
5ad

Chemical Formula (M): $C_{22}H_{15}NO_3Se$
Exact Mass: 421.0217
Found (M+H) = 422.0285

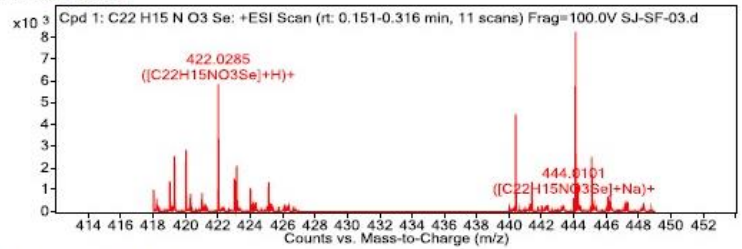
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H15 N O3 Se	0.201	415.027	5855	C22 H15 N O3 Se	415.0277	-1.58

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H15 N O3 Se	422.0285	0.201	Find By Formula	415.027



MS Zoomed Spectrum



MS Spectrum Peak List

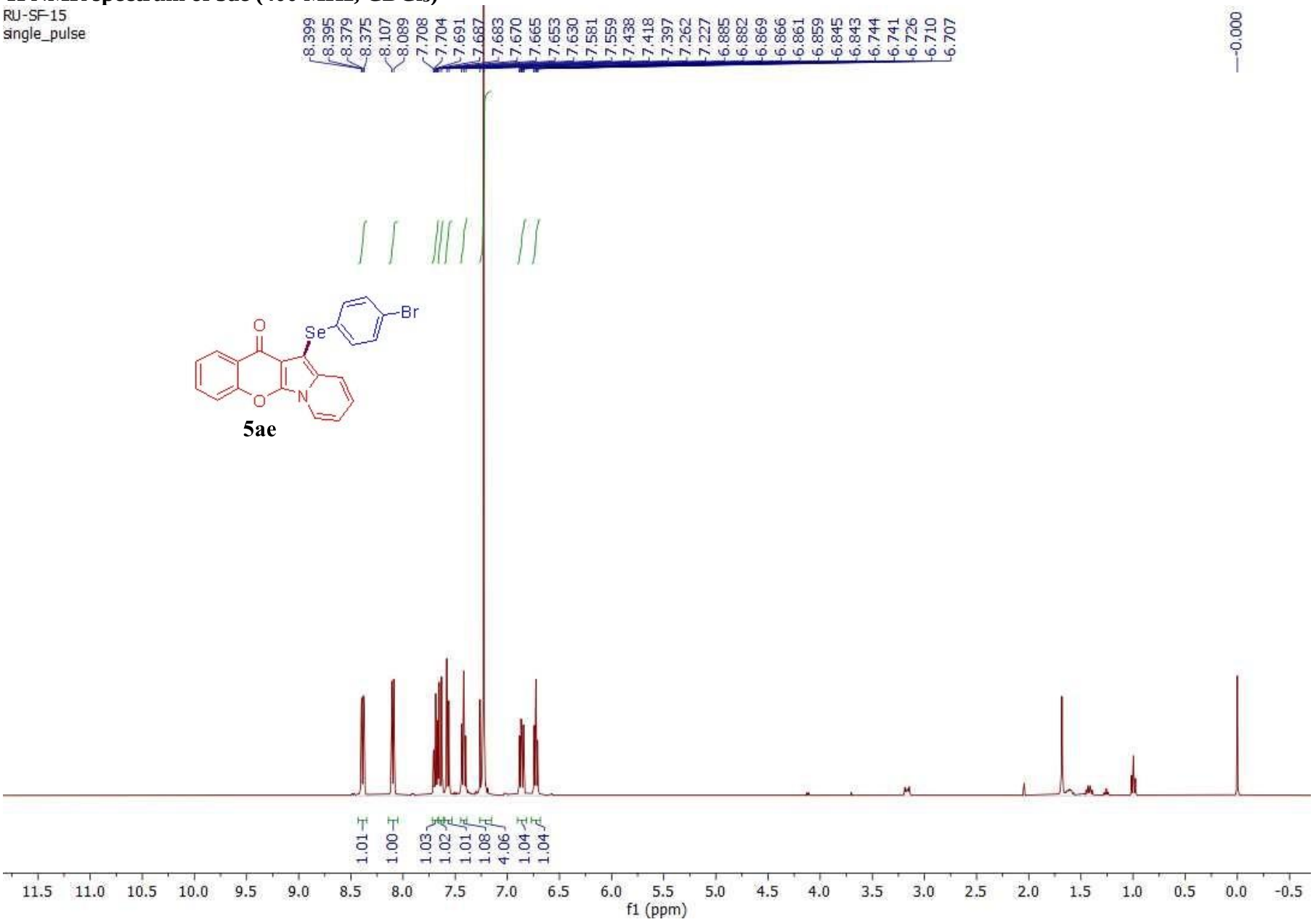
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
422.0285	422.0291	1.35	1	5854.59	C22H15NO3Se	(M+H)+
423.0316	423.0323	1.8	1	1532.32	C22H15NO3Se	(M+H)+
444.0101	444.0111	2.19	1	622.54	C22H15NO3Se	(M+Na)+
445.0126	445.0143	3.68	1	153.74	C22H15NO3Se	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

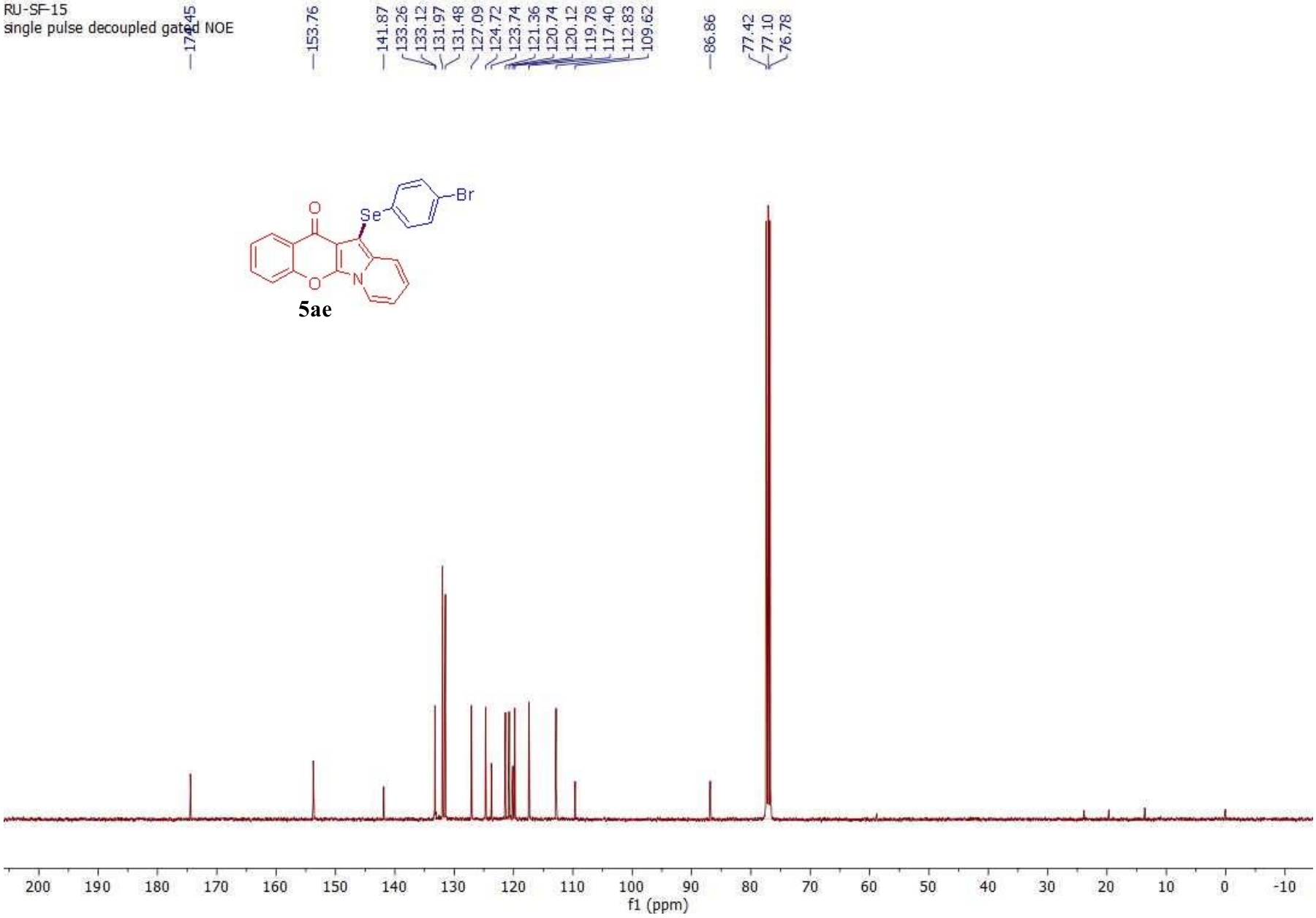
---End Of Report---

^{1}H NMR spectrum of 5ae (400 MHz, $CDCl_3$)



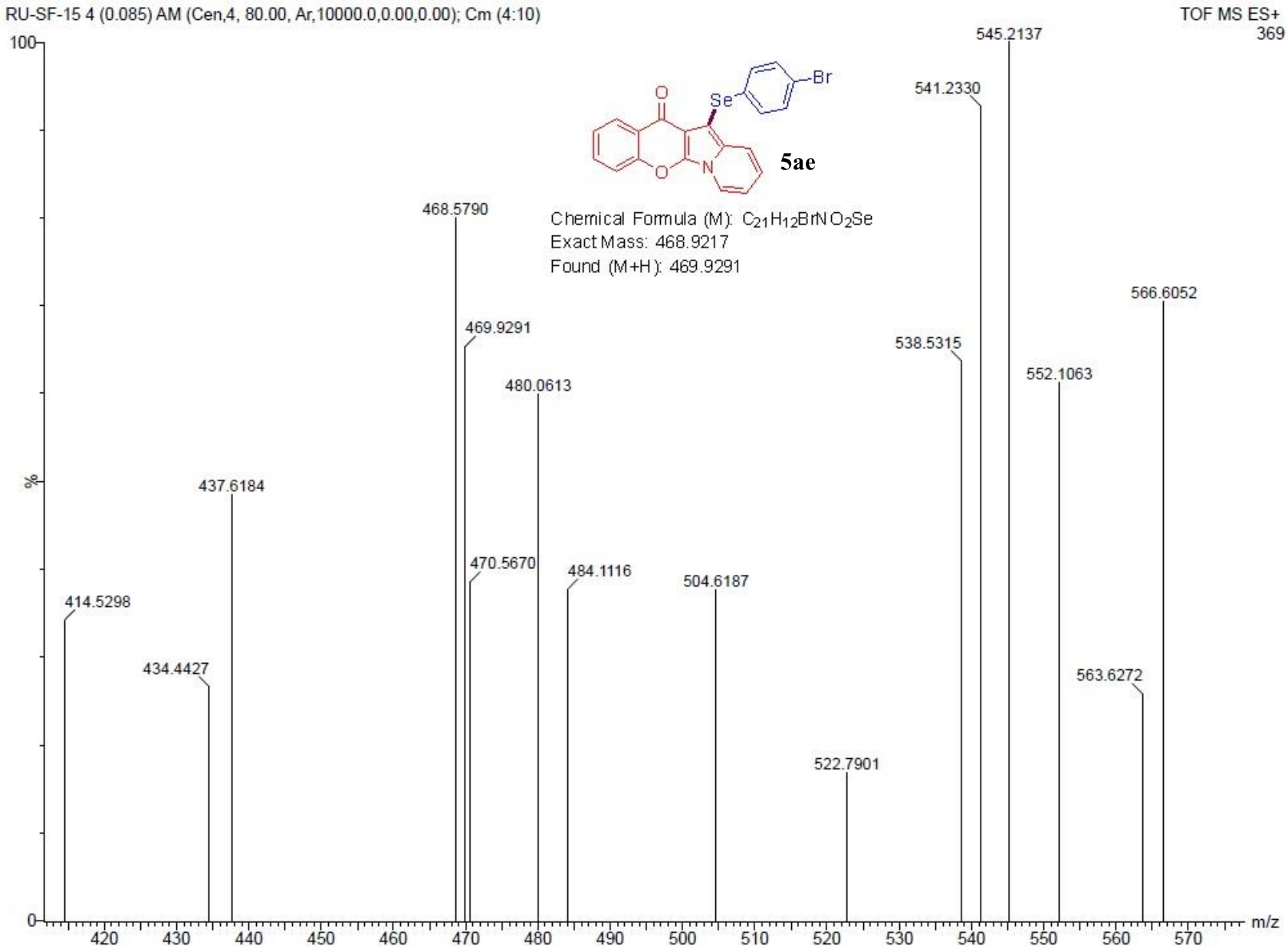
5ae

^{13}C NMR spectrum of 5ae (100 MHz, $CDCl_3$)

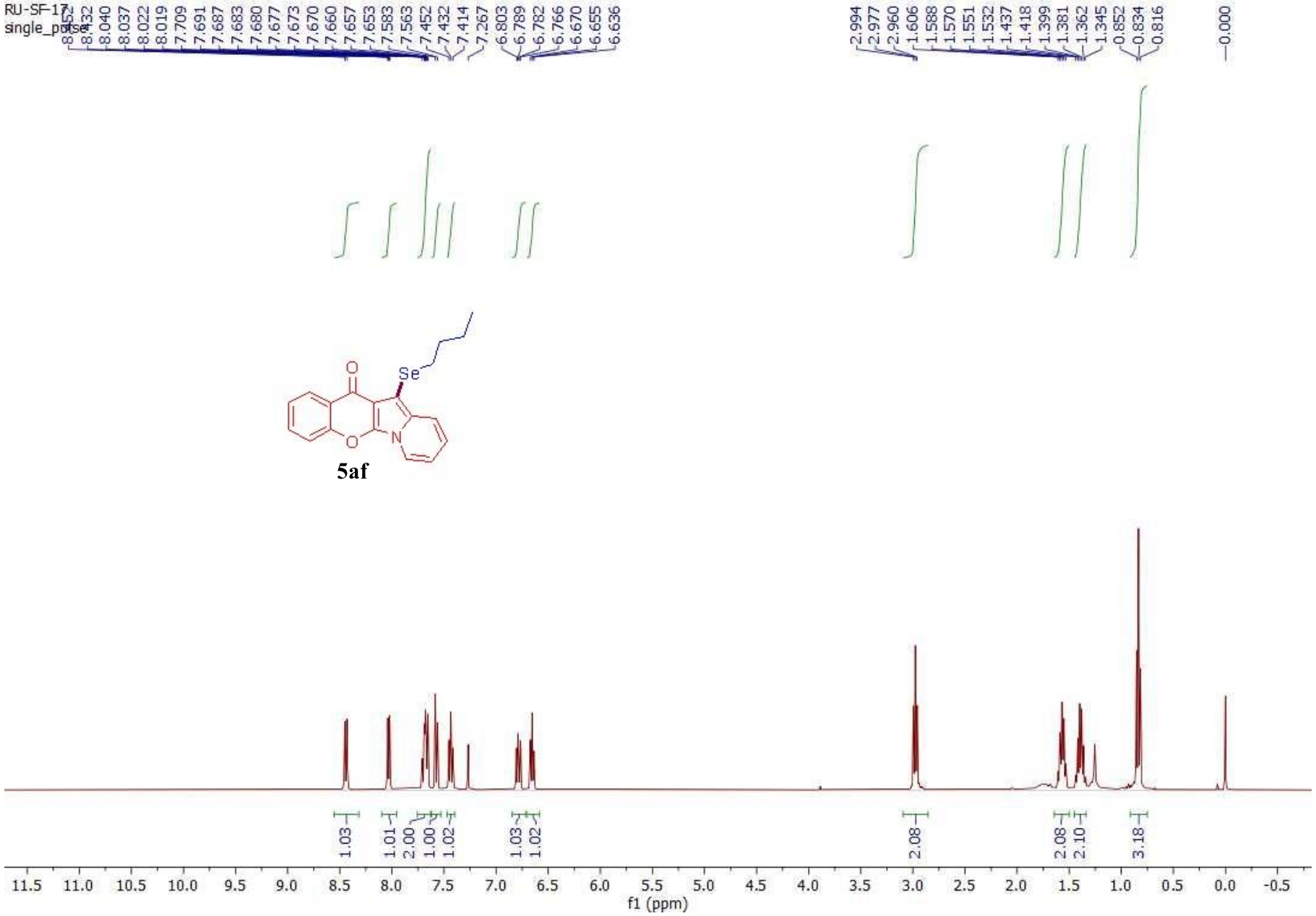


5ae

Mass spectrum of 5ae

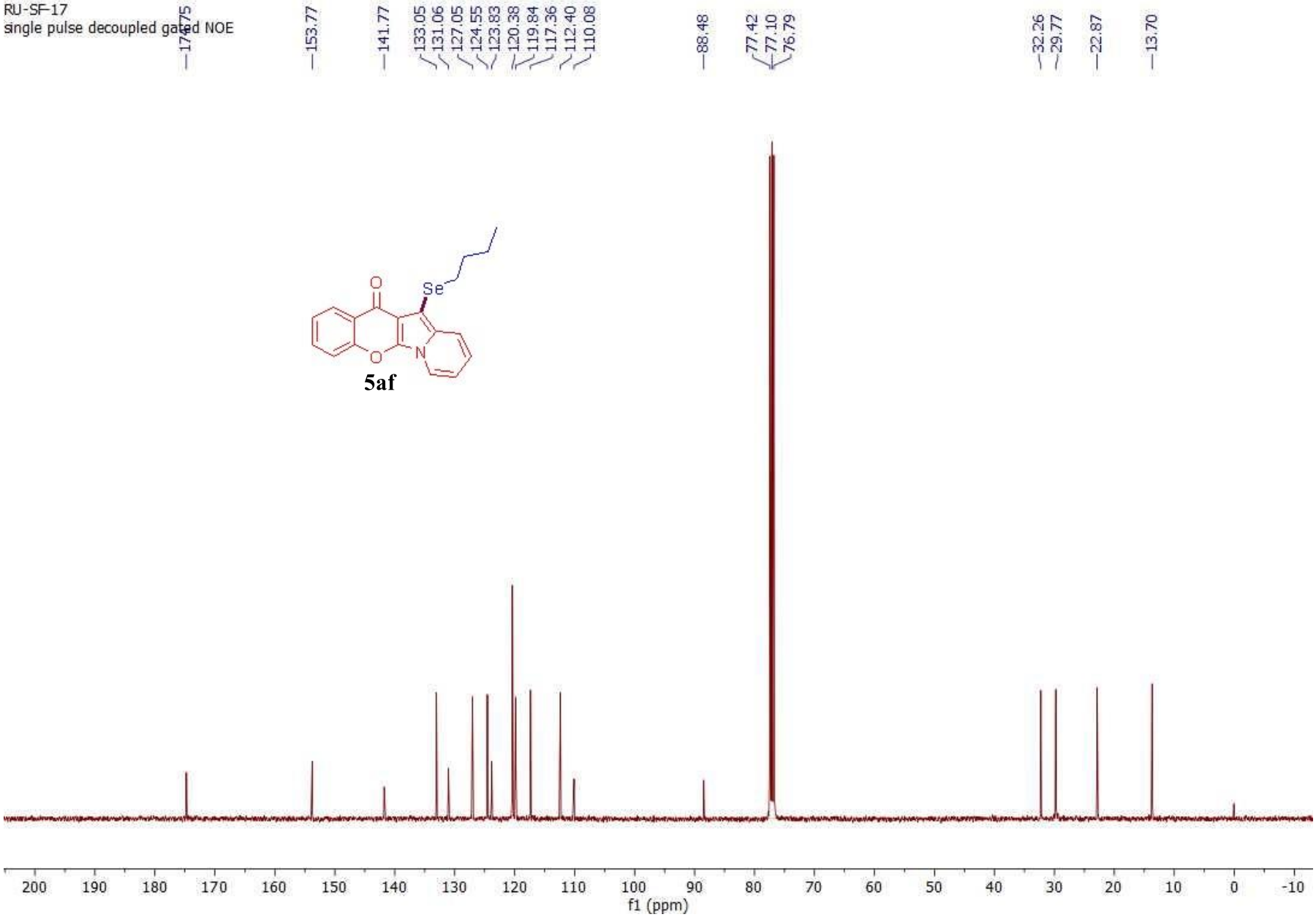


^{1}H NMR spectrum of 5af (400 MHz, $CDCl_3$)

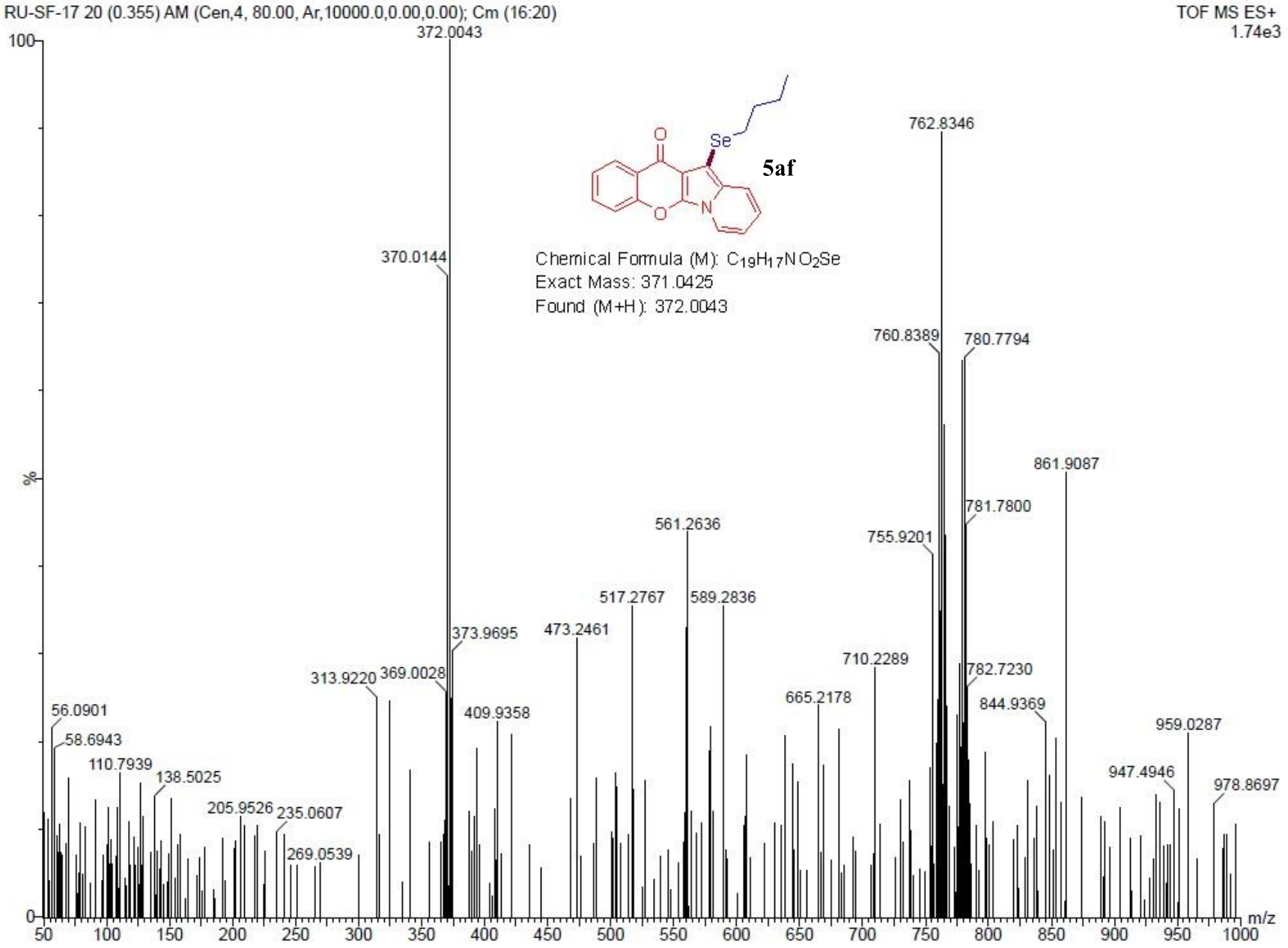


5af

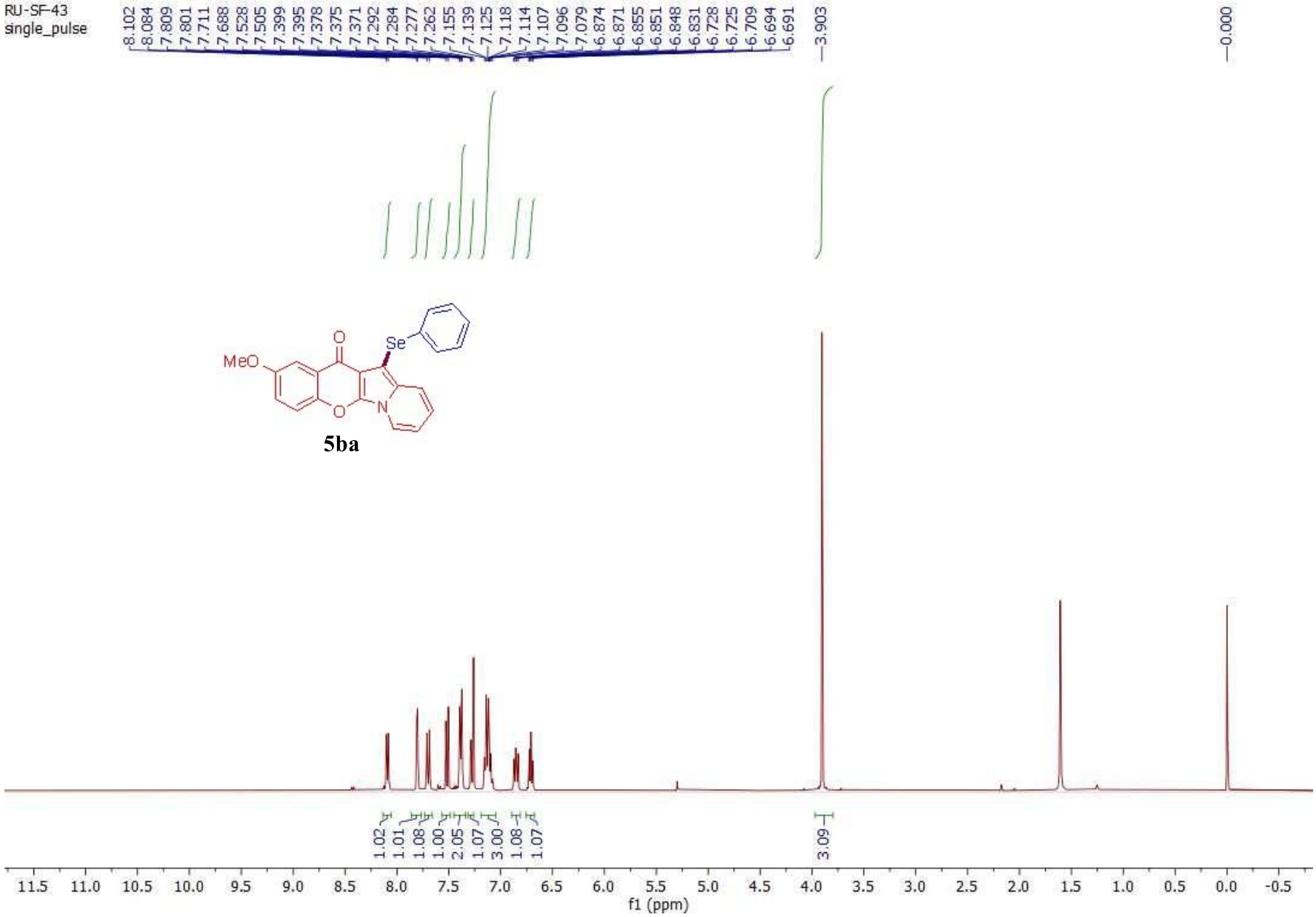
^{13}C NMR spectrum of 5af (100 MHz, $CDCl_3$)



Mass spectrum of 5af

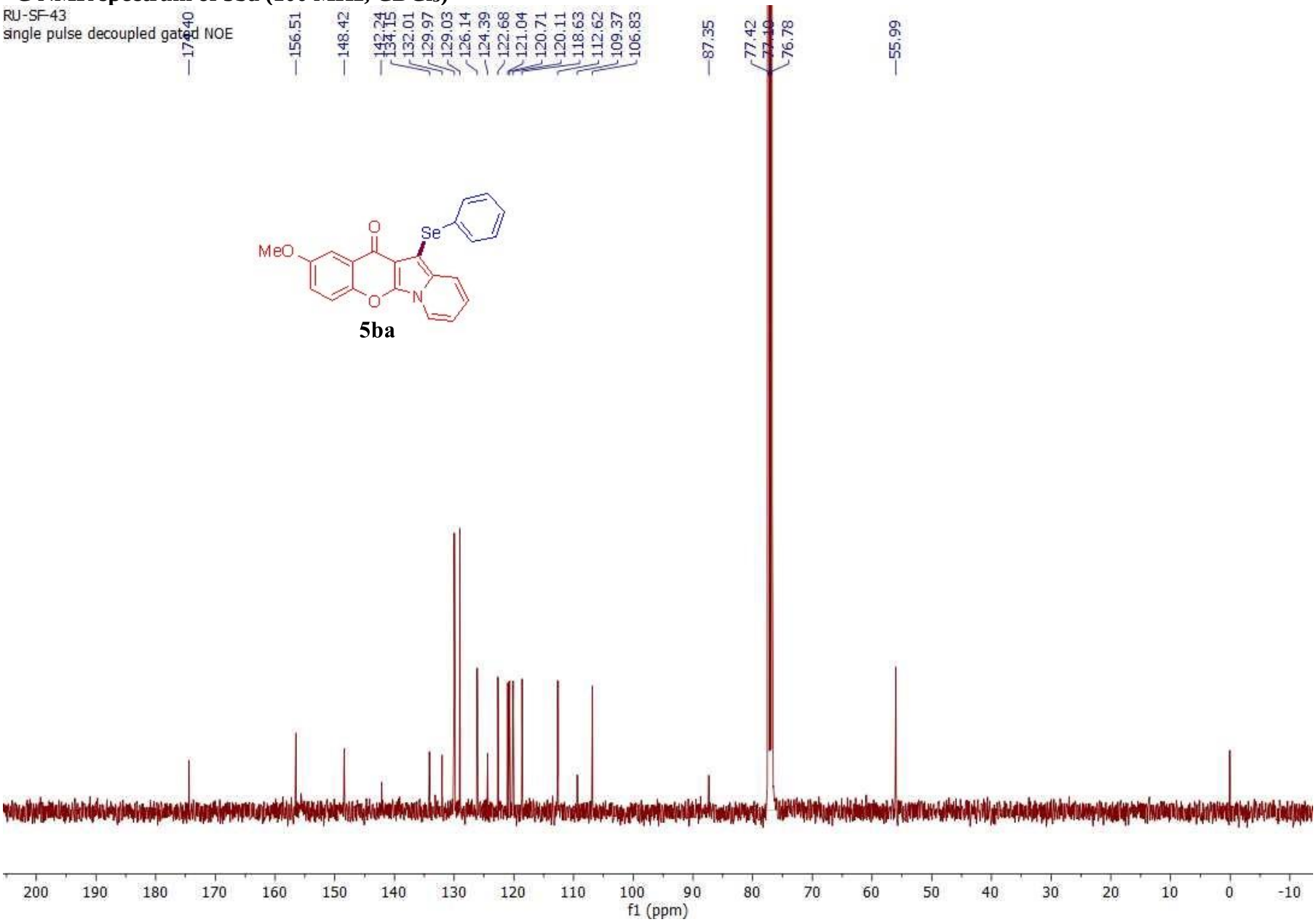


^{1}H NMR spectrum of 5ba (400 MHz, $CDCl_3$)



5ba

^{13}C NMR spectrum of 5ba (100 MHz, $CDCl_3$)

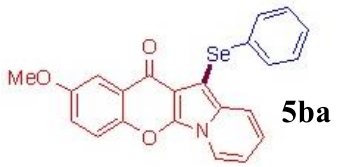


5ba

Mass spectrum of 5ba

Data File	SJ-SF-43.d	**Sample Name**	SJ-SF-43
Sample Type	Sample	**Position**	P1-C10
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 9:43:45 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



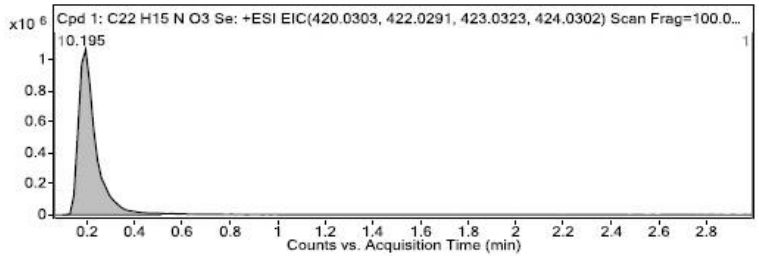
5ba

Chemical Formula (M): $C_{22}H_{15}NO_3Se$
Exact Mass: 421.0217
Found (M+H): 422.0290

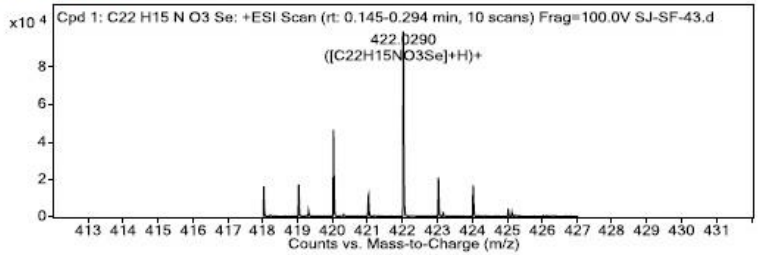
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H15 N O3 Se	0.195	415.0275	99826	C22 H15 N O3 Se	415.0277	-0.36

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H15 N O3 Se	422.029	0.195	Find By Formula	415.0275



MS Zoomed Spectrum



MS Spectrum Peak List

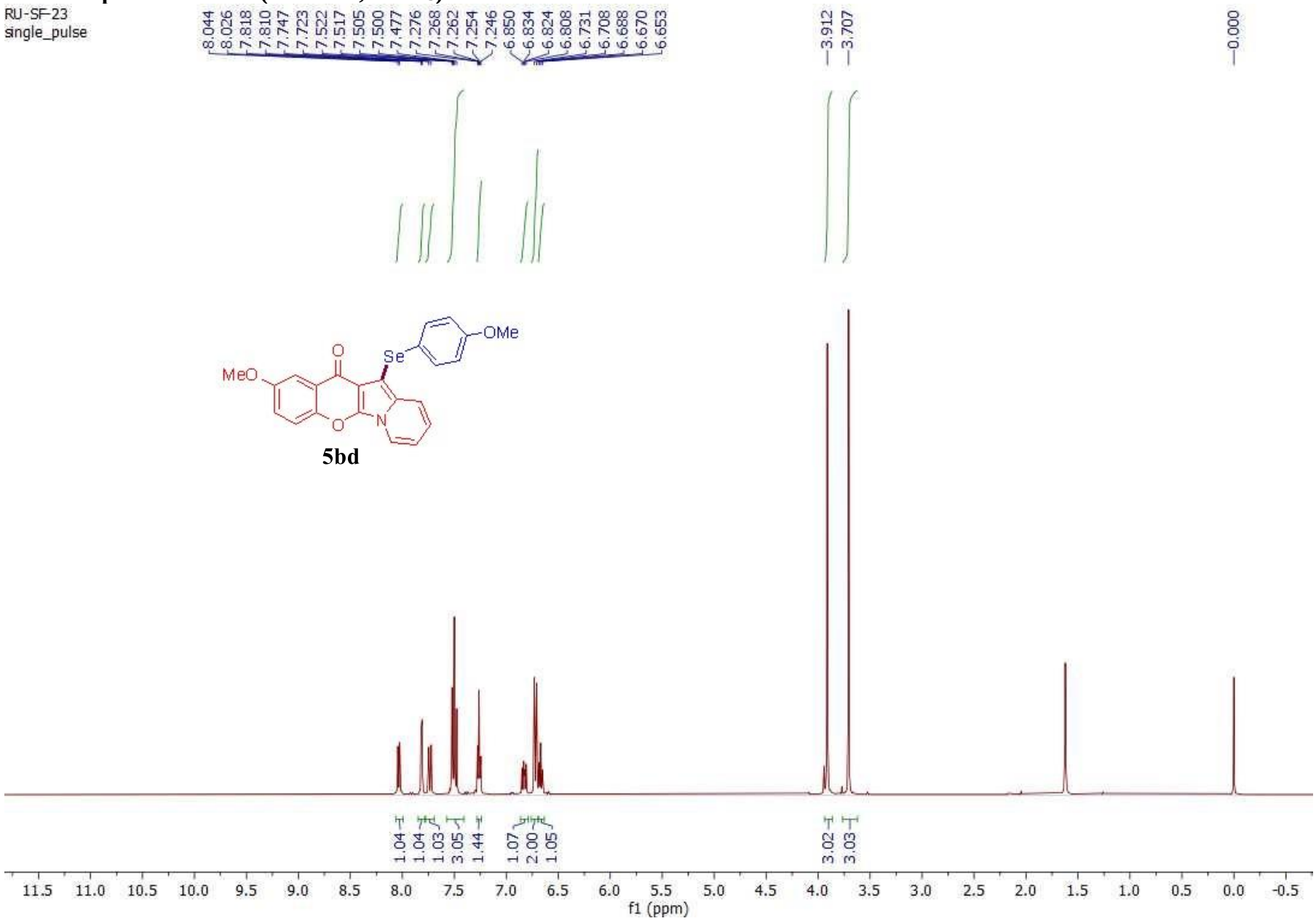
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
422.029	422.0291	0.21	1	99826.07	C22H15NO3Se	(M+H)+
423.0319	423.0323	1.05	1	21671.24	C22H15NO3Se	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

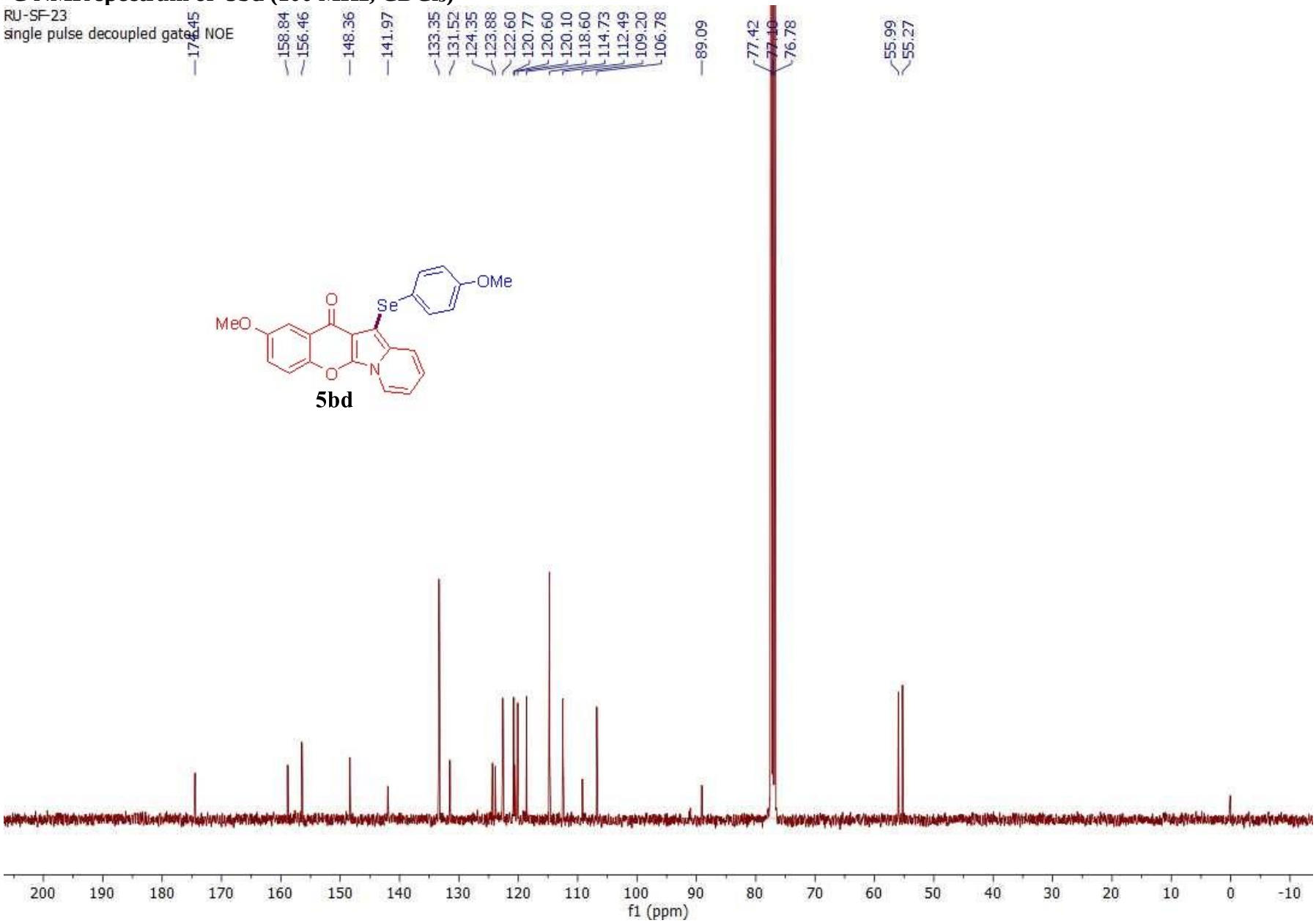
---End Of Report---

^{1}H NMR spectrum of 5bd (400 MHz, $CDCl_3$)



5bd

^{13}C NMR spectrum of 5bd (100 MHz, $CDCl_3$)



5bd

Mass spectrum of 5bd

Data File	SJ-SF-23.d	**Sample Name**	Unavailable
Sample Type	Unavailable	**Position**	Unavailable
Instrument Name	Unavailable	**User Name**	Unavailable
Acq Method		**Acquired Time**	Unavailable
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment	Sample information is unavailable		

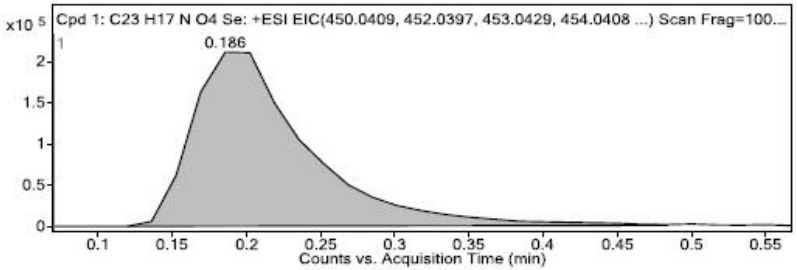
5bd

Chemical Formula (M): $C_{23}H_{17}NO_4Se$
Exact Mass: 451.0323
Found (M+H): 452.0389

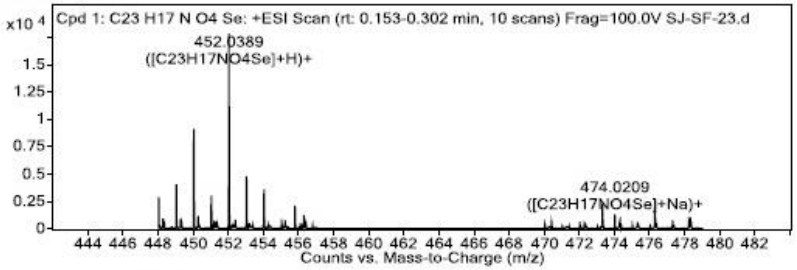
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C23 H17 N O4 Se	0.186	445.0375	1328	C23 H17 N O4 Se	445.0382	-1.67

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H17 N O4 Se	474.0209	0.186	Find By Formula	445.0375



MS Zoomed Spectrum



MS Spectrum Peak List

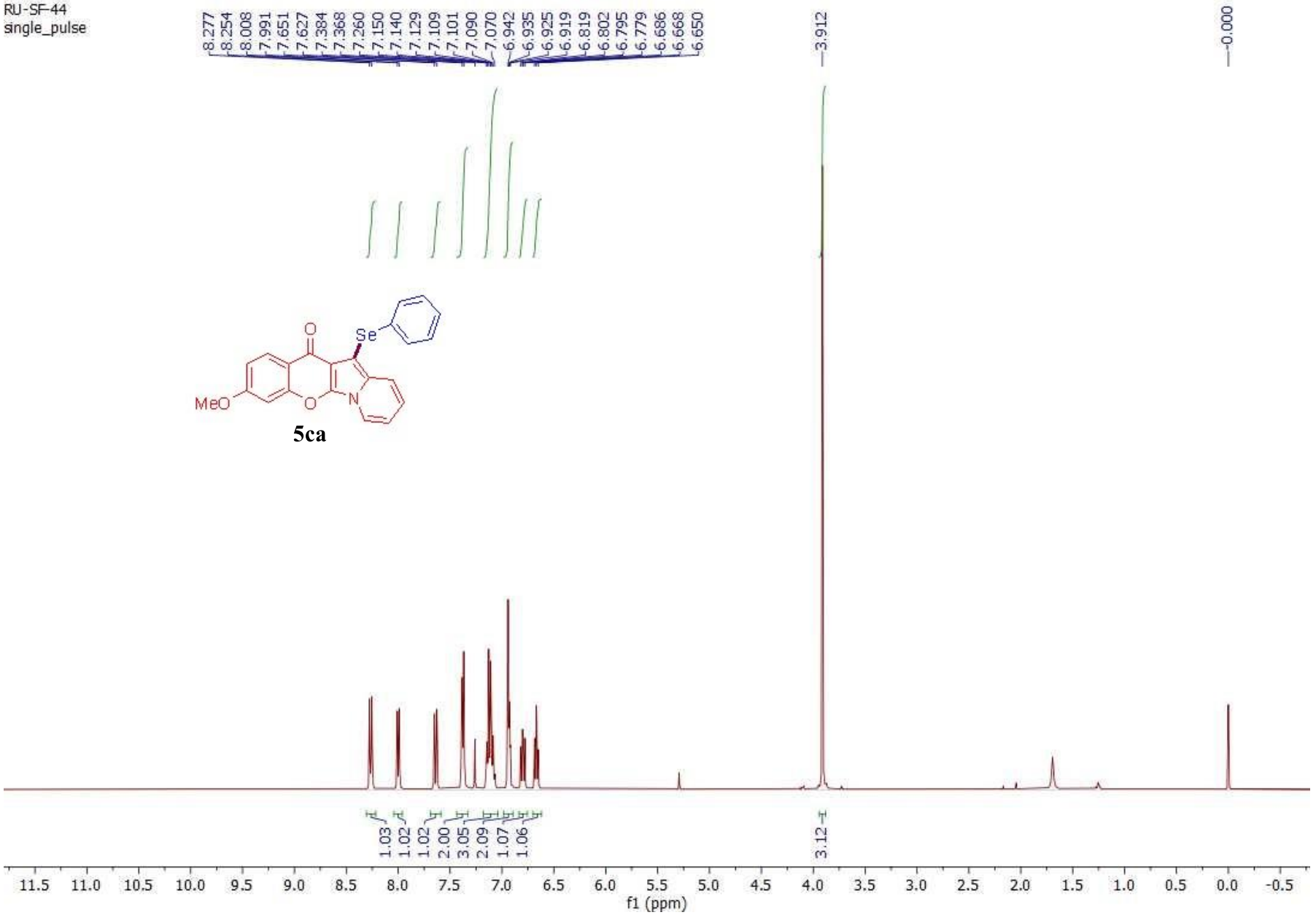
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
452.0389	452.0397	1.69	1	18257.4	C23H17NO4Se	(M+H)+
453.0422	453.0429	1.49	1	4823.93	C23H17NO4Se	(M+H)+
474.0209	474.0216	1.57	1	1328.15	C23H17NO4Se	(M+Na)+
475.0242	475.0248	1.47	1	341.7	C23H17NO4Se	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

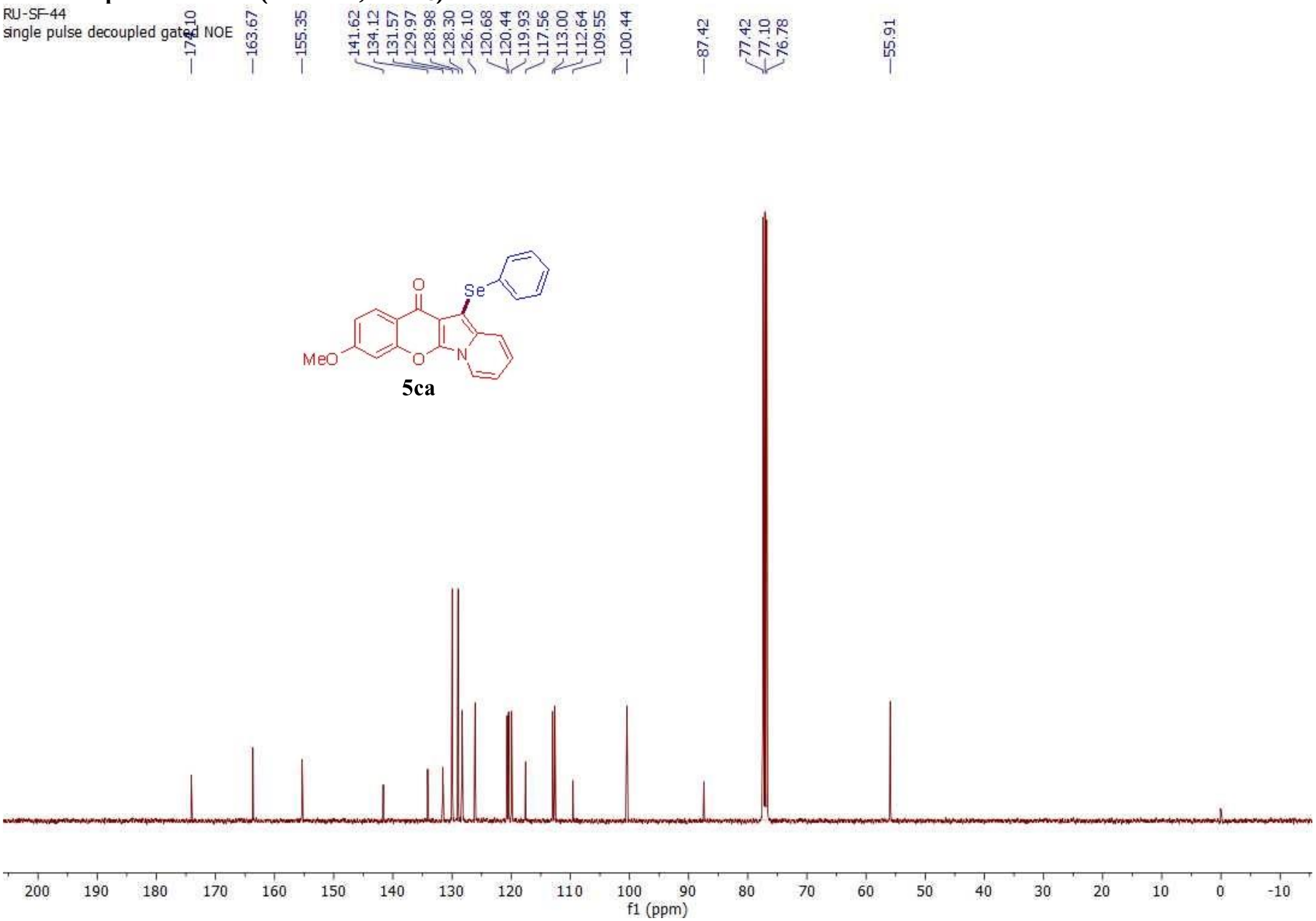
---End Of Report---

^{1}H NMR spectrum of 5ca (400 MHz, $CDCl_3$)



5ca

^{13}C NMR spectrum of 5ca (100 MHz, $CDCl_3$)



5ca

Mass spectrum of 5ca

Data File	SJ-SF-44.d	**Sample Name**	SJ-SF-44
Sample Type	Sample	**Position**	P1-C11
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 9:52:07 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

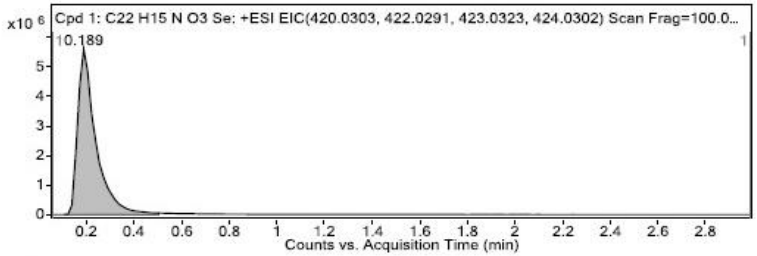
5ca

Chemical Formula (M): $C_{22}H_{15}NO_3Se$
Exact Mass: 421.0217
Found (M+H): 422.0298

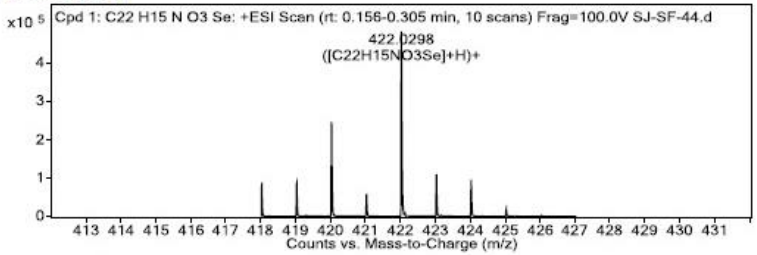
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H15 N O3 Se	0.189	415.0282	499437	C22 H15 N O3 Se	415.0277	1.32

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H15 N O3 Se	422.0298	0.189	Find By Formula	415.0282



MS Zoomed Spectrum



MS Spectrum Peak List

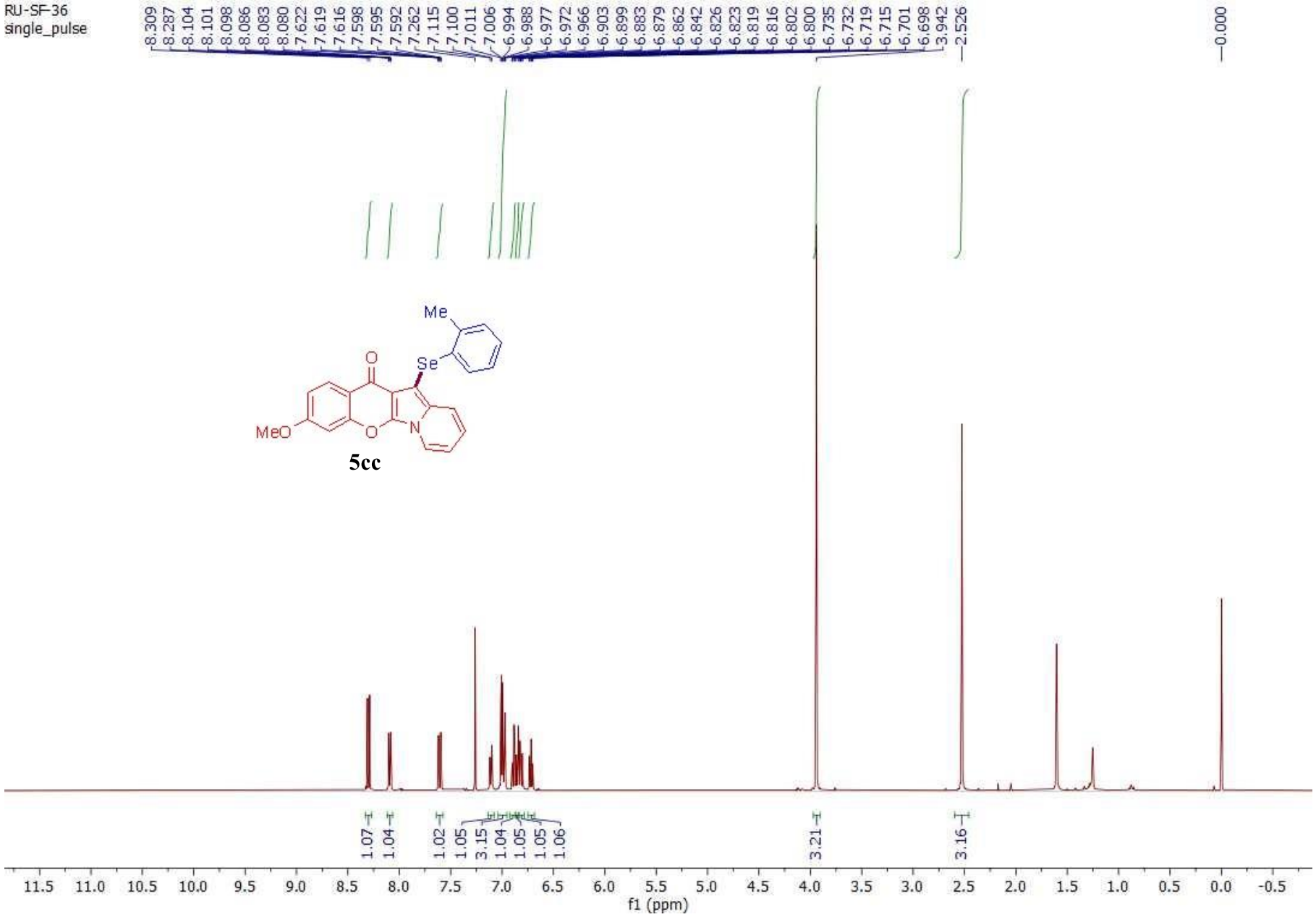
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
422.0298	422.0291	-1.68	1	499436.96	C22H15NO3Se	(M+H)+
423.0321	423.0323	0.42	1	113263.6	C22H15NO3Se	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

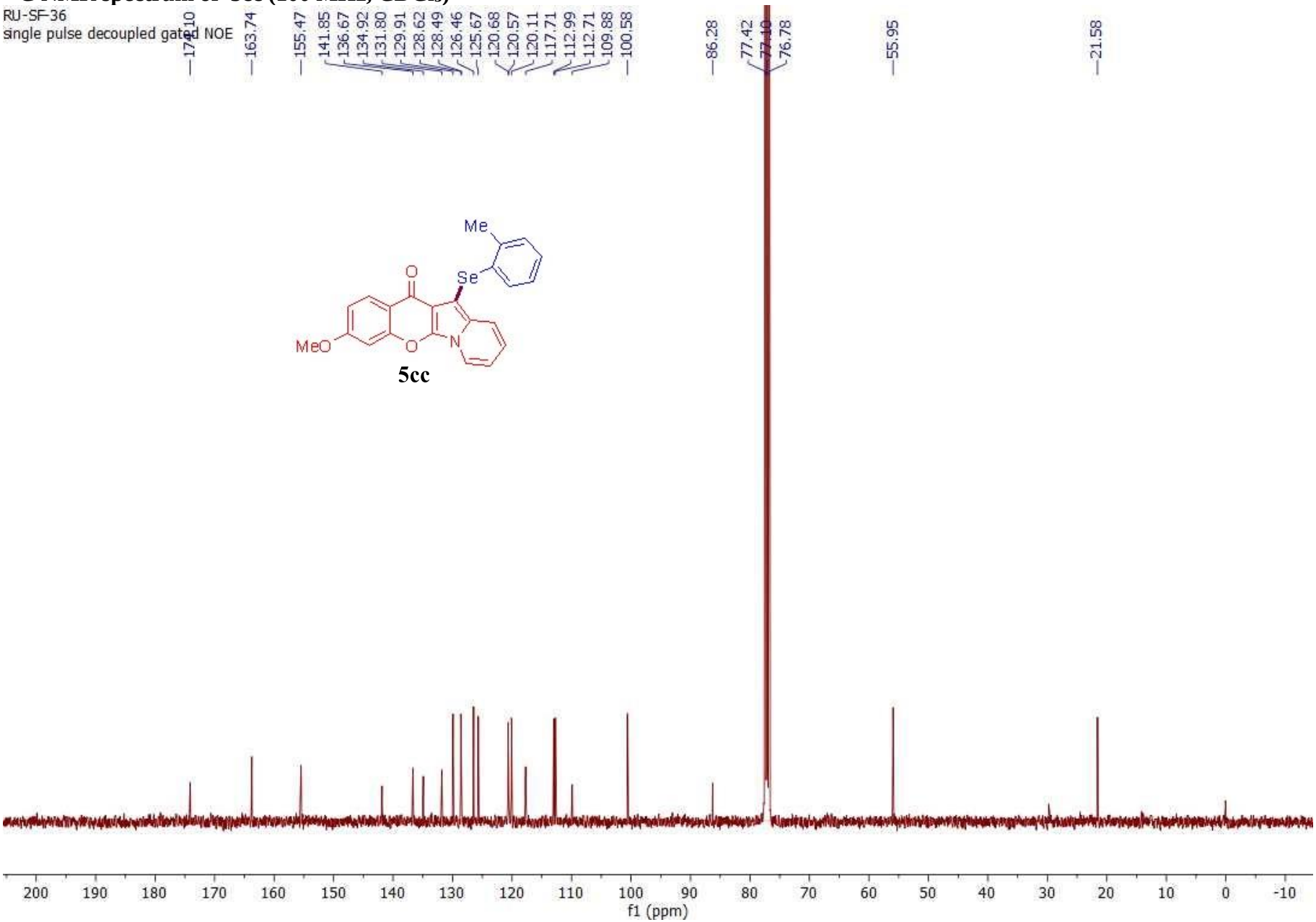
---End Of Report---

^{1}H NMR spectrum of 5cc (400 MHz, $CDCl_3$)



5cc

^{13}C NMR spectrum of 5cc (100 MHz, $CDCl_3$)



5cc

Mass spectrum of 5cc

Data File	SJ-SF-36.d	**Sample Name**	SJ-SF-36
Sample Type	Sample	**Position**	P1-C5
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 9:02:02 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

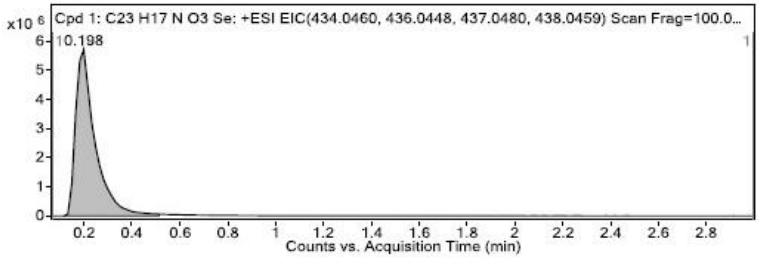
5cc

Chemical Formula (M): $C_{23}H_{17}NO_3Se$
Exact Mass: 435.0374
Found (M+H): 436.0455

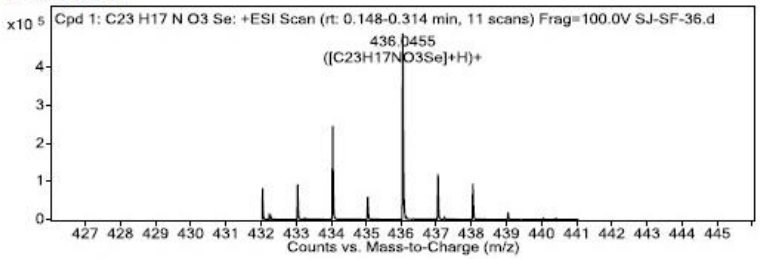
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C23 H17 N O3 Se	0.198	429.0439	489850	C23 H17 N O3 Se	429.0433	1.36

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H17 N O3 Se	436.0455	0.198	Find By Formula	429.0439



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
436.0455	436.0448	-1.7	1	489849.83	C23H17NO3Se	(M+H)+
437.0479	437.048	0.15	1	119283.4	C23H17NO3Se	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

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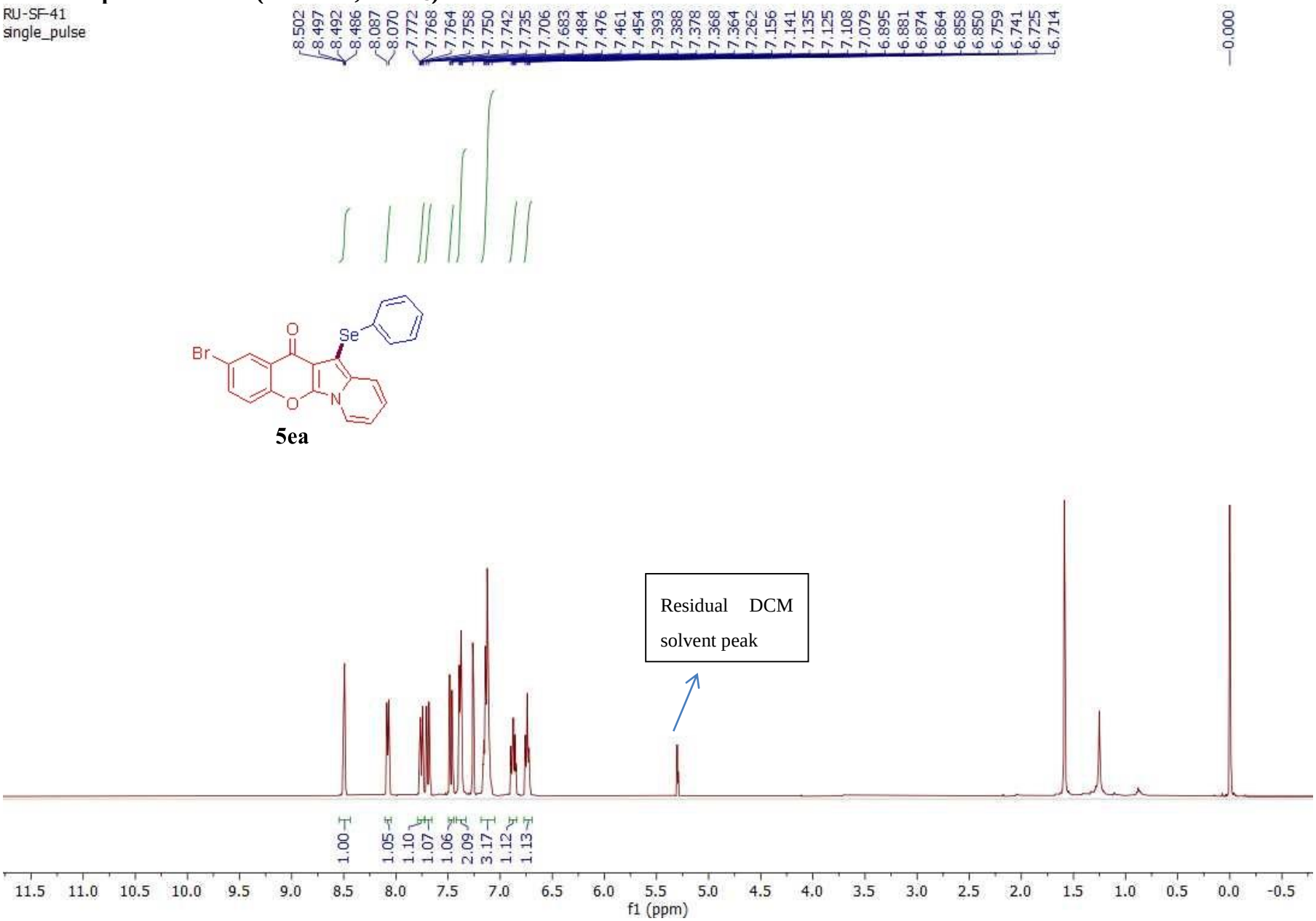
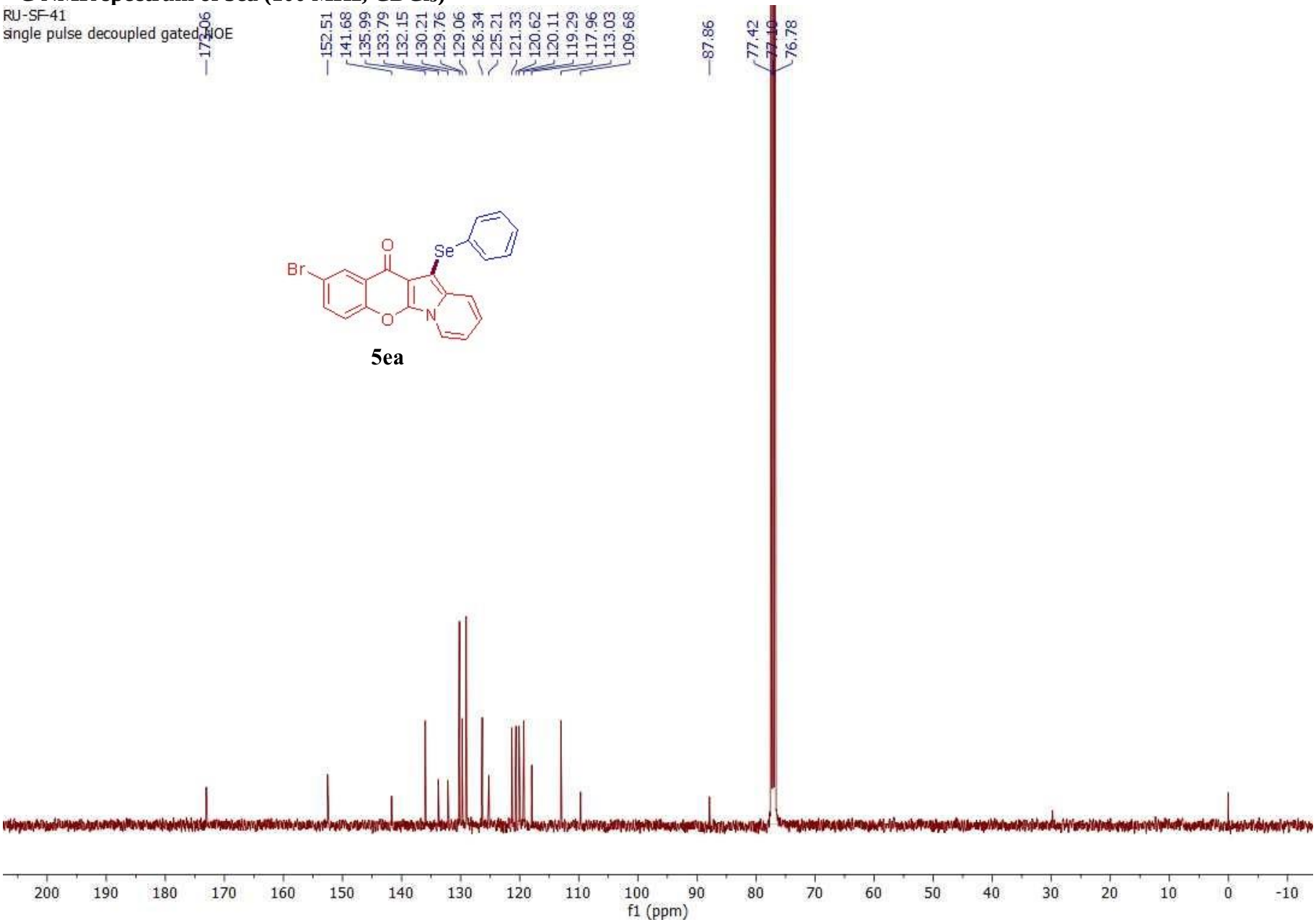
^{1}H NMR spectrum of 5ea (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of 5ea (100 MHz, $CDCl_3$)



5ea

Mass spectrum of 5ea

Data File	SJ-SF-41.d	**Sample Name**	SJ-SF-41
Sample Type	Sample	**Position**	P1-C8
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 9:27:04 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

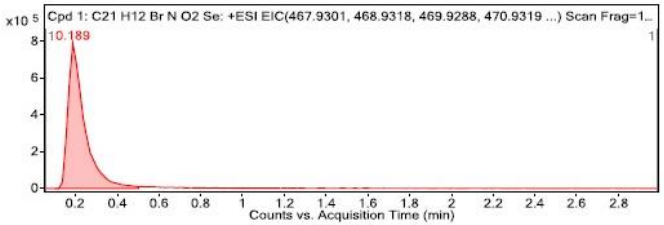
5ea

Chemical Formula (M): $C_{21}H_{12}BrNO_2Se$
Exact Mass: 468.9217
Found (M+H): 469.9284

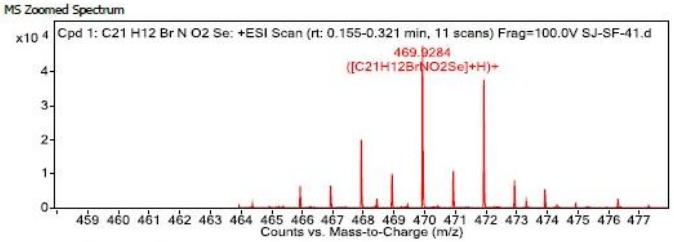
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C21 H12 Br N O2 Se	0.189	462.9269	48195	C21 H12 Br N O2 Se	462.9276	-1.46

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H12 Br N O2 Se	469.9284	0.189	Find By Formula	462.9269



MS Zoomed Spectrum



MS Spectrum Peak List

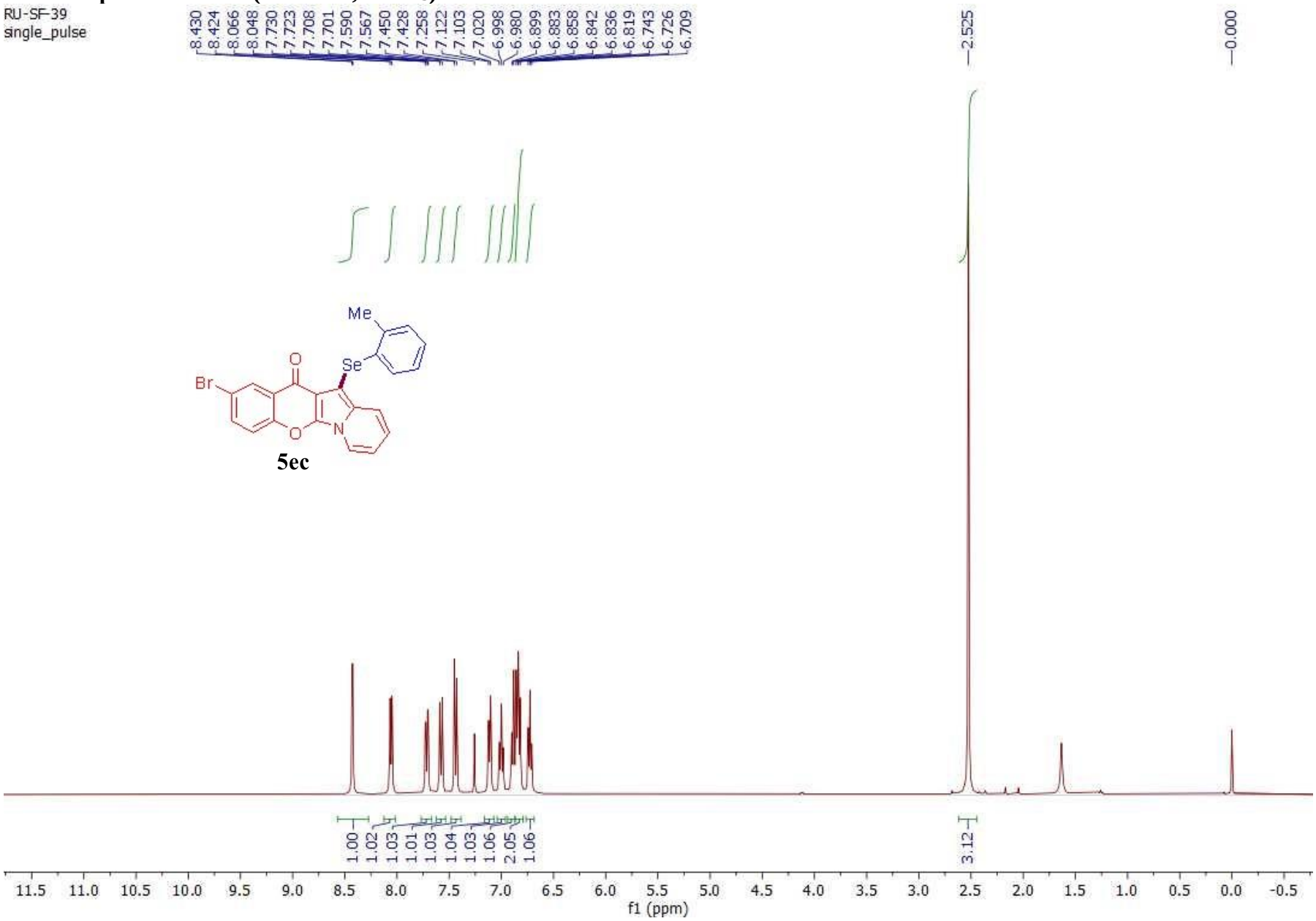
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
467.9295	467.9301	1.3	1	20554.23	C21H12BrNO2Se	(M+H)+
468.9298	468.9318	4.09	1	10429.06	C21H12BrNO2Se	(M+H)+
469.9284	469.9288	0.83	1	48194.97	C21H12BrNO2Se	(M+H)+
470.9305	470.9319	3	1	11377.8	C21H12BrNO2Se	(M+H)+
471.927	471.9275	1.11	1	38252.09	C21H12BrNO2Se	(M+H)+
472.9299	472.9306	1.46	1	8127.8	C21H12BrNO2Se	(M+H)+
473.9275	473.9282	1.44	1	5775.92	C21H12BrNO2Se	(M+H)+
474.9302	474.9308	1.24	1	1235.7	C21H12BrNO2Se	(M+H)+
475.9346	475.9336	-2.26	1	196.09	C21H12BrNO2Se	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

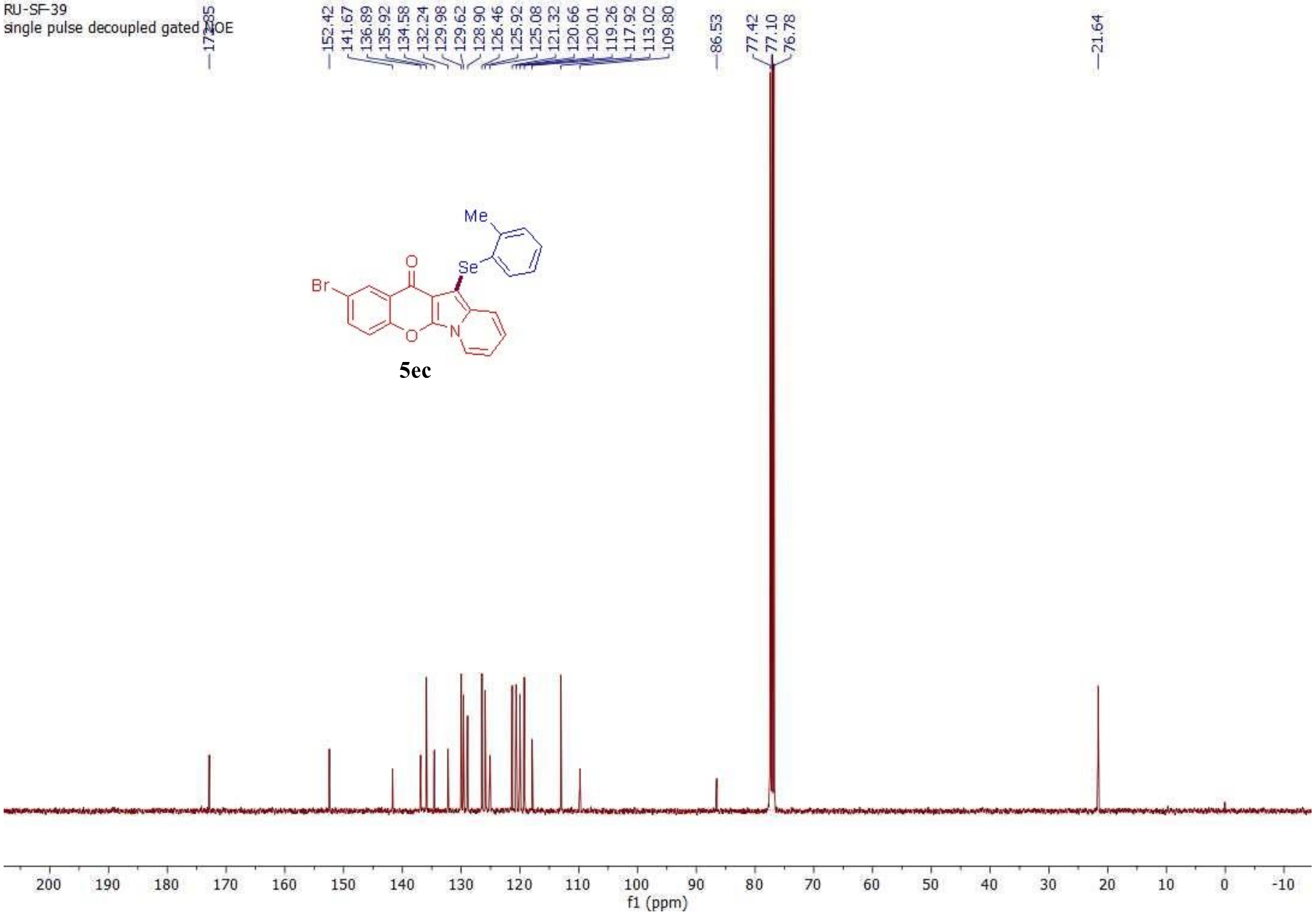
---End Of Report---

^{1}H NMR spectrum of 5ec (400 MHz, $CDCl_3$)



5ec

^{13}C NMR spectrum of 5ec (100 MHz, $CDCl_3$)



5ec

Mass spectrum of 5ec

Data File	SJ-SF-39.d	**Sample Name**	SJ-SF-39
Sample Type	Sample	**Position**	P1-C7
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 9:18:44 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

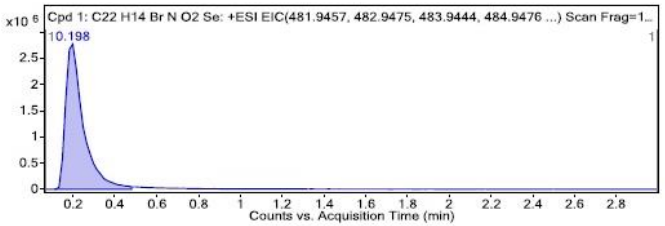
5ec

Chemical Formula (M): $C_{22}H_{14}BrNO_2Se$
Exact Mass: 482.9373
Found (M+H): 483.9448

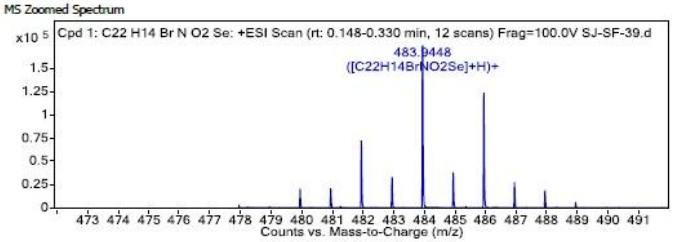
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H14 Br N O2 Se	0.198	476.9433	174333	C22 H14 Br N O2 Se	476.9433	0

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H14 Br N O2 Se	483.9448	0.198	Find By Formula	476.9433



MS Zoomed Spectrum



MS Spectrum Peak List

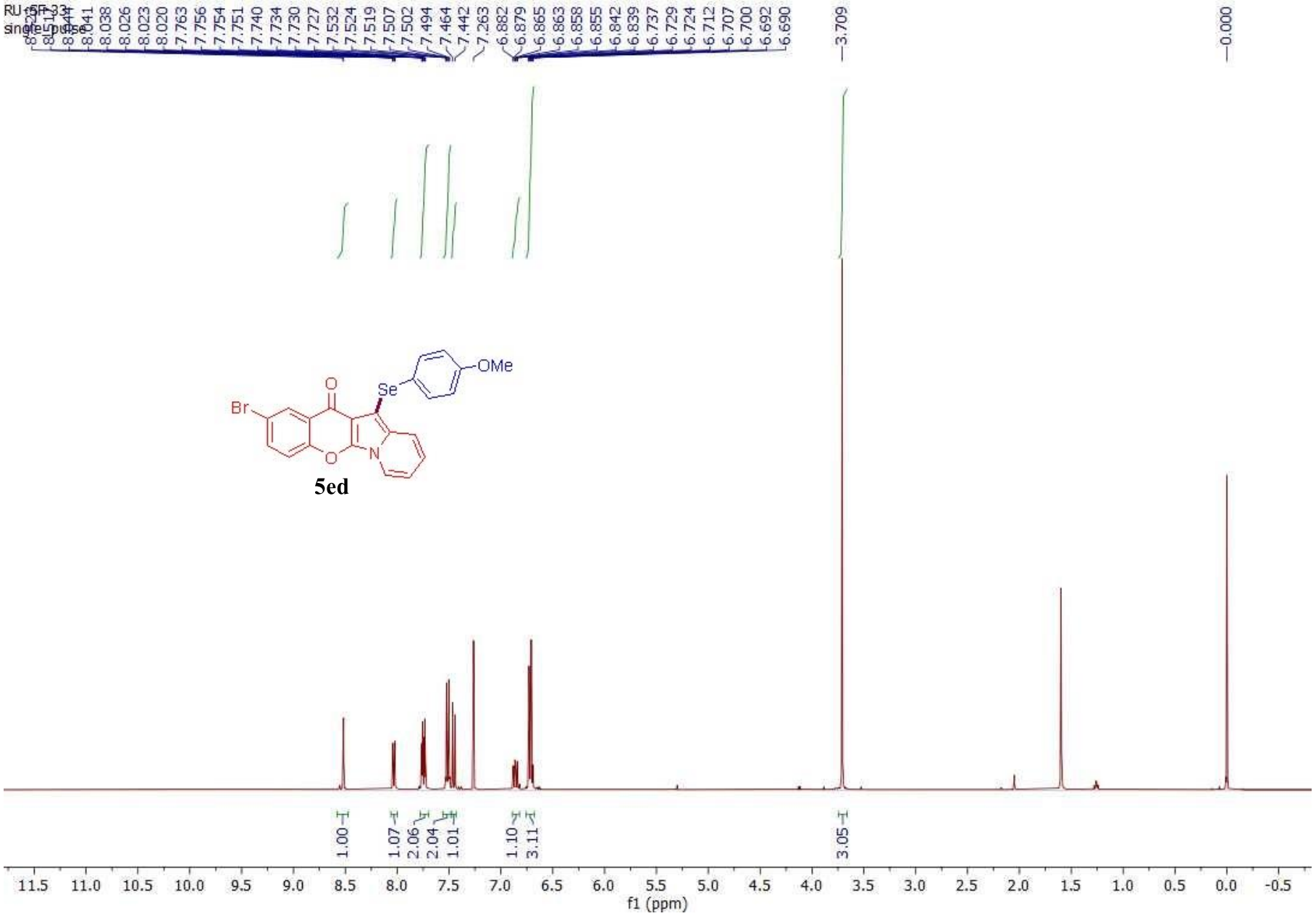
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
481.9458	481.9457	-0.08	1	72920.3	C22H14BrNO2Se	(M+H)+
482.9462	482.9475	2.59	1	33795.71	C22H14BrNO2Se	(M+H)+
483.9448	483.9444	-0.69	1	174332.63	C22H14BrNO2Se	(M+H)+
484.9468	484.9476	1.57	1	38335.4	C22H14BrNO2Se	(M+H)+
485.9434	485.9432	-0.36	1	127528.85	C22H14BrNO2Se	(M+H)+
486.946	486.9463	0.49	1	27863.78	C22H14BrNO2Se	(M+H)+
487.9438	487.9439	0.29	1	18790.2	C22H14BrNO2Se	(M+H)+
488.9461	488.9465	0.88	1	3981.69	C22H14BrNO2Se	(M+H)+
489.9487	489.9493	1.17	1	525.64	C22H14BrNO2Se	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

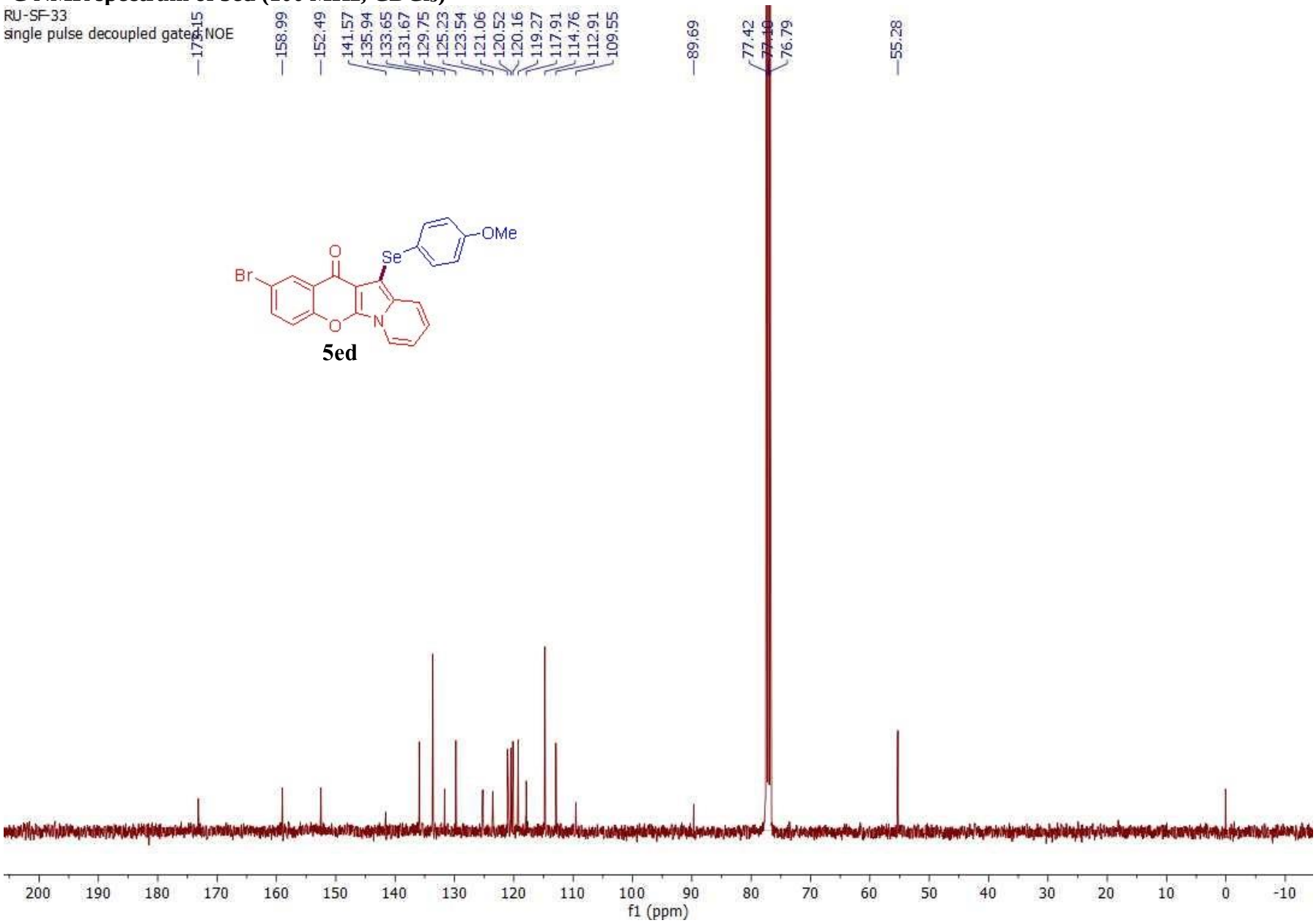
Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

---End Of Report---

^{1}H NMR spectrum of 5ed (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of 5ed (100 MHz, $CDCl_3$)



5ed

Mass spectrum of 5ed

Data File	SJ-SF-33.d	**Sample Name**	SJ-SF-33
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 8:36:58 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

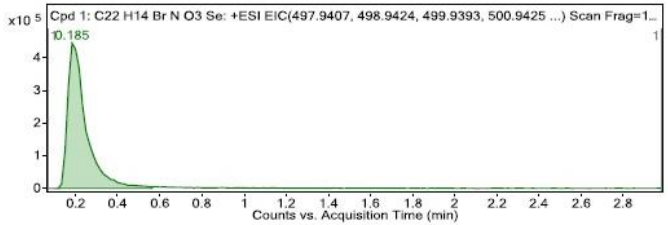
5ed

Chemical Formula (M): $C_{22}H_{14}BrNO_3Se$
Exact Mass: 498.9322
Found (M+H): 499.9393

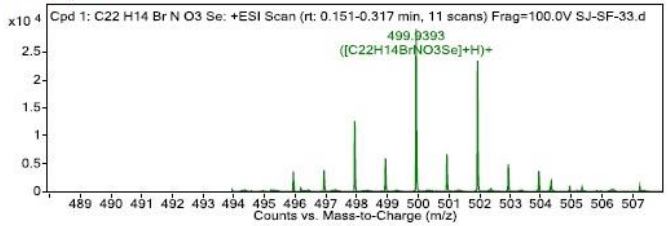
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H14 Br N O3 Se	0.185	492.9378	29411	C22 H14 Br N O3 Se	492.9382	-0.72

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H14 Br N O3 Se	499.9393	0.185	Find By Formula	492.9378



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
497.9402	497.9407	0.85	1	12736.99	C22H14BrNO3Se	(M+H)+
498.9409	498.9424	3.01	1	6163.89	C22H14BrNO3Se	(M+H)+
499.9393	499.9393	0.18	1	29411.38	C22H14BrNO3Se	(M+H)+
500.9414	500.9425	2.14	1	6968.28	C22H14BrNO3Se	(M+H)+
501.938	501.9381	0.29	1	23653.7	C22H14BrNO3Se	(M+H)+
502.941	502.9412	0.46	1	5036.89	C22H14BrNO3Se	(M+H)+
503.9384	503.9389	0.85	1	3772.04	C22H14BrNO3Se	(M+H)+
504.9406	504.9415	1.66	1	866.42	C22H14BrNO3Se	(M+H)+
505.9441	505.9441	0.07	1	120.73	C22H14BrNO3Se	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

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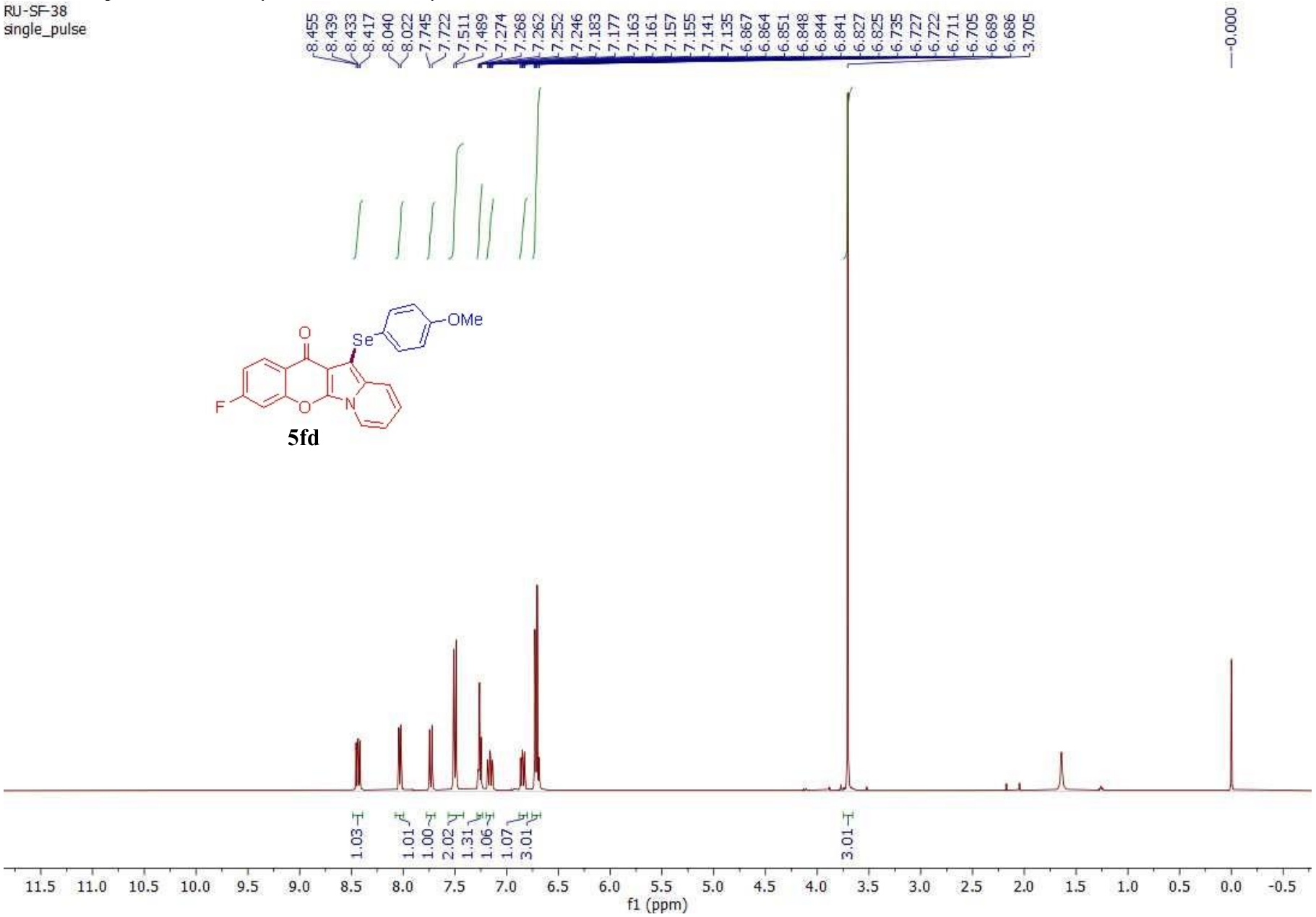
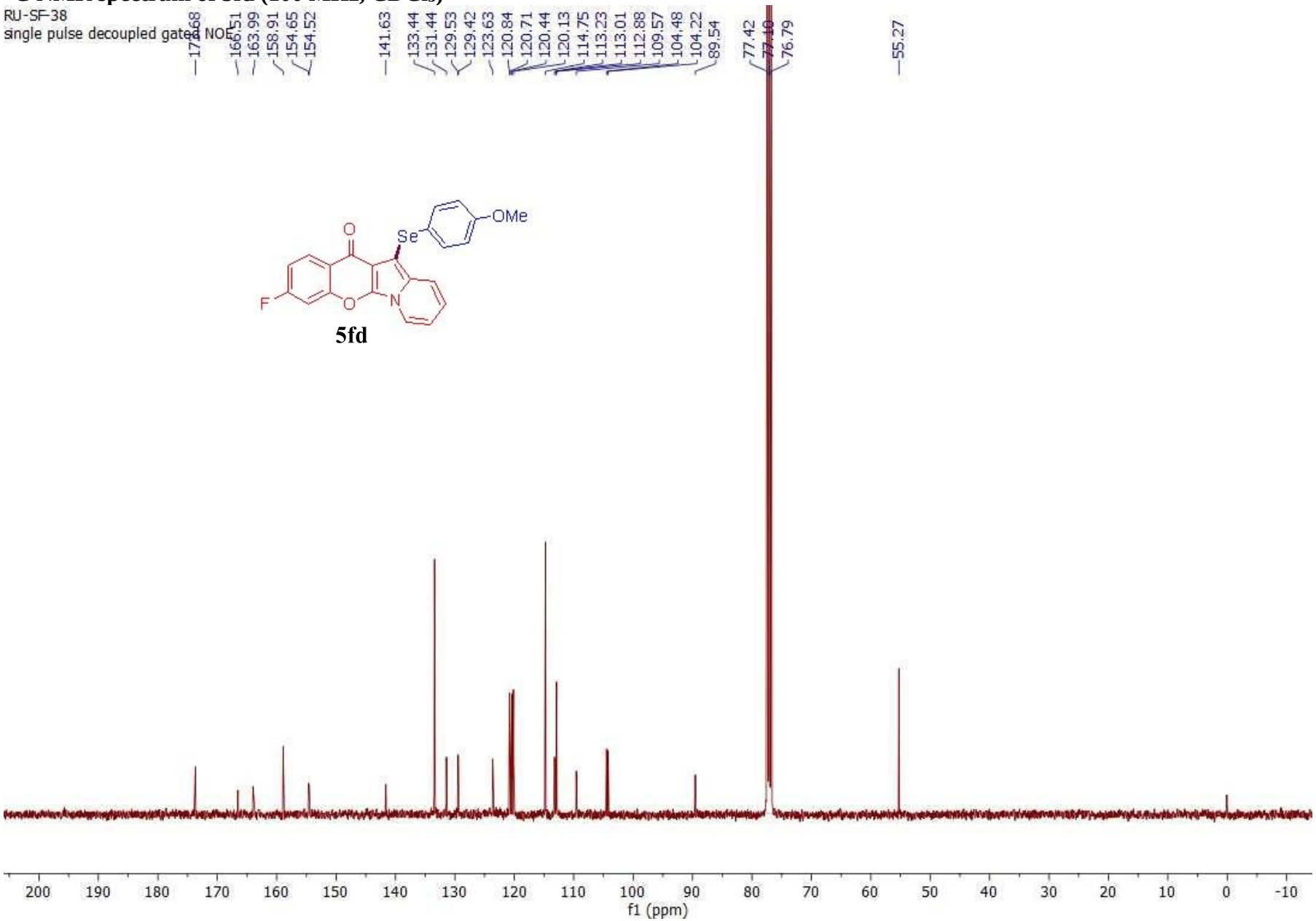
^{1}H NMR spectrum of 5fd (400 MHz, $CDCl_3$)



5fd

^{13}C NMR spectrum of 5fd (100 MHz, $CDCl_3$)



5fd

^{19}F NMR spectrum of 5fd (376 MHz, $CDCl_3$)

RU-SF-38
single_pulse

5fd

Mass spectrum of 5fd

Data File	SJ-SF-21.d	**Sample Name**	SJ-SF-21
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	A_ACN_ C_H2O _60 -40 ESI+VE.3MIN16022022_REF.m	**Acquired Time**	1/31/2023 7:38:30 PM
IRM Calibration Status	Success	**DA Method**	BTP.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

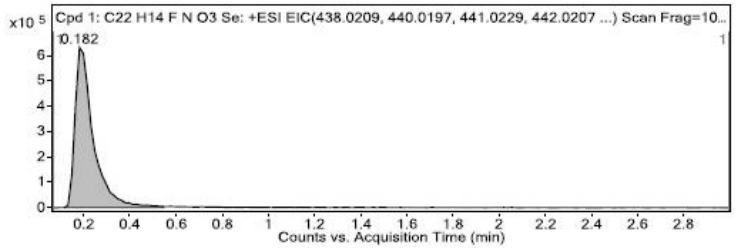
5fd

Chemical Formula (M): $C_{22}H_{14}FNO_3Se$
Exact Mass: 439.0123
Found (M+H): 440.0192

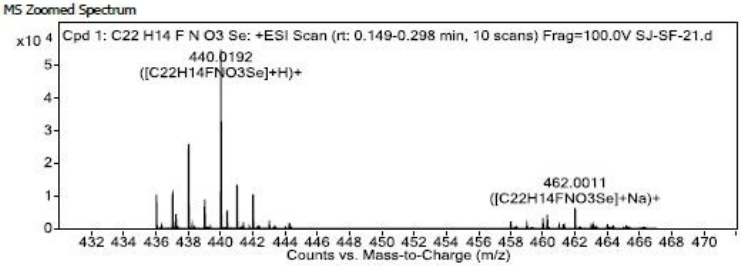
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H14 F N O3 Se	0.182	433.0177	6407	C22 H14 F N O3 Se	433.0182	-1.23

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H14 F N O3 Se	462.0011	0.182	Find By Formula	433.0177



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
440.0192	440.0197	1.03	1	55992.23	C22H14FNO3Se	(M+H)+
441.022	441.0229	1.98	1	13411.04	C22H14FNO3Se	(M+H)+
462.0011	462.0016	1.25	1	6406.74	C22H14FNO3Se	(M+Na)+
463.0047	463.0048	0.33	1	1522.92	C22H14FNO3Se	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

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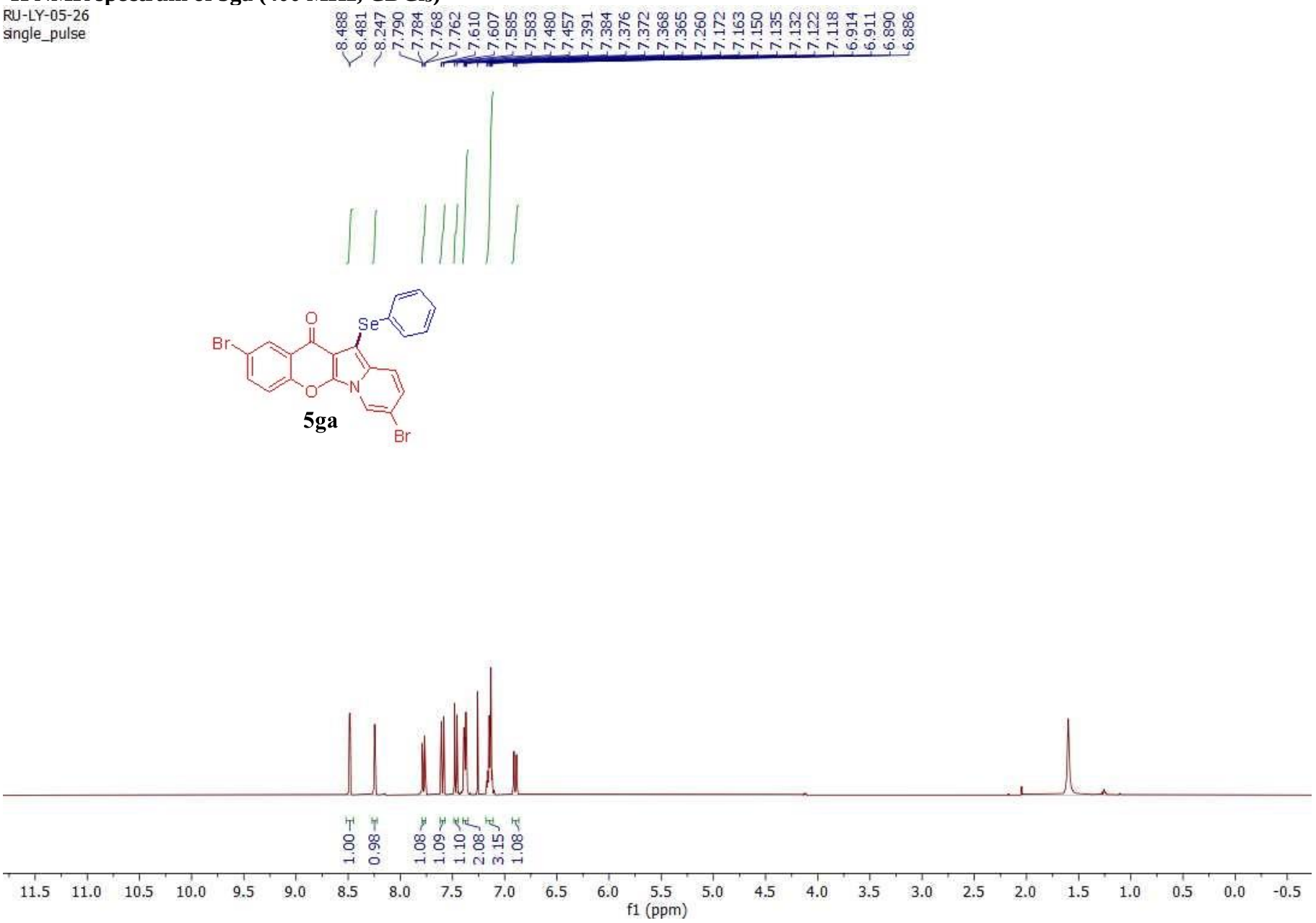
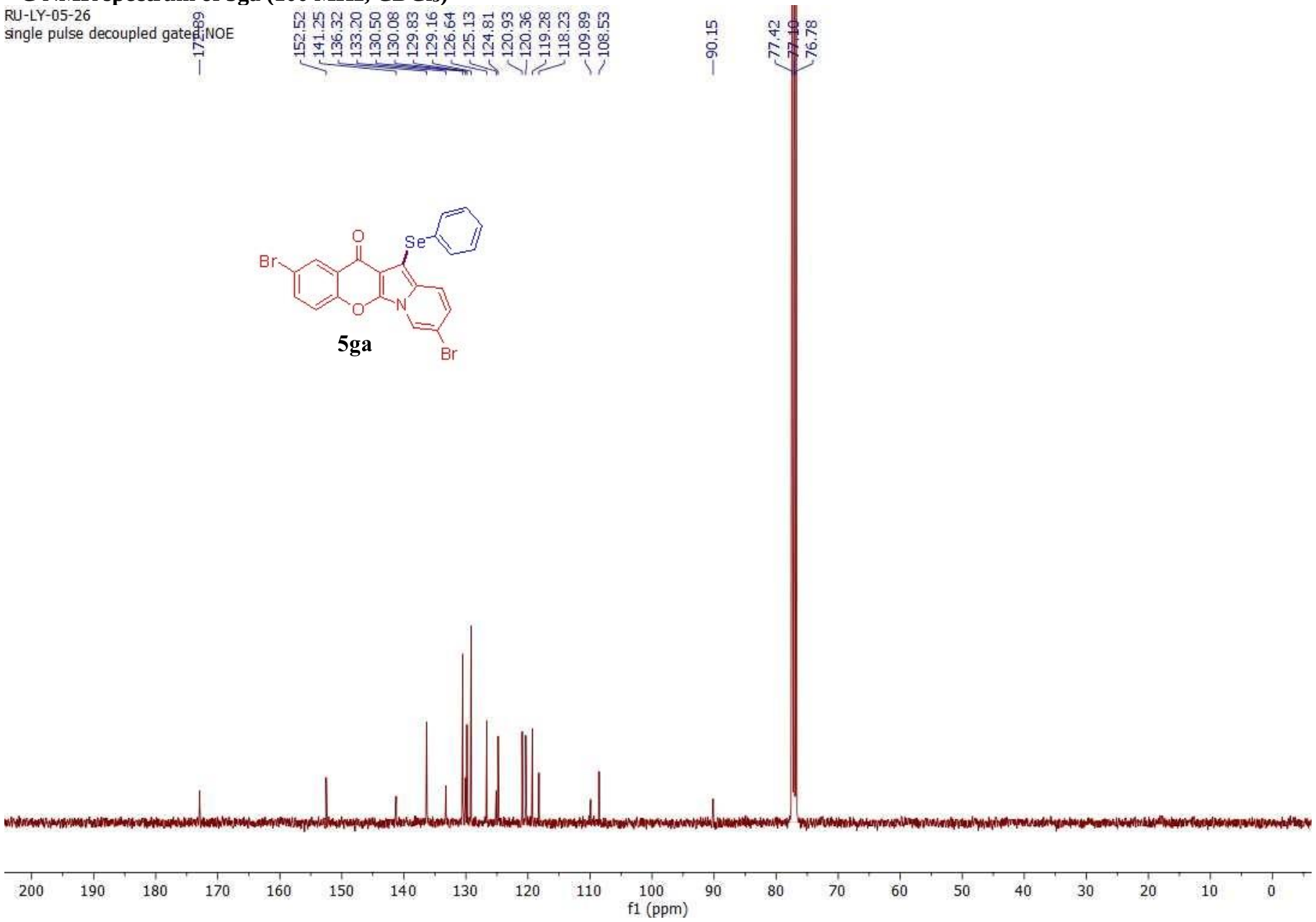
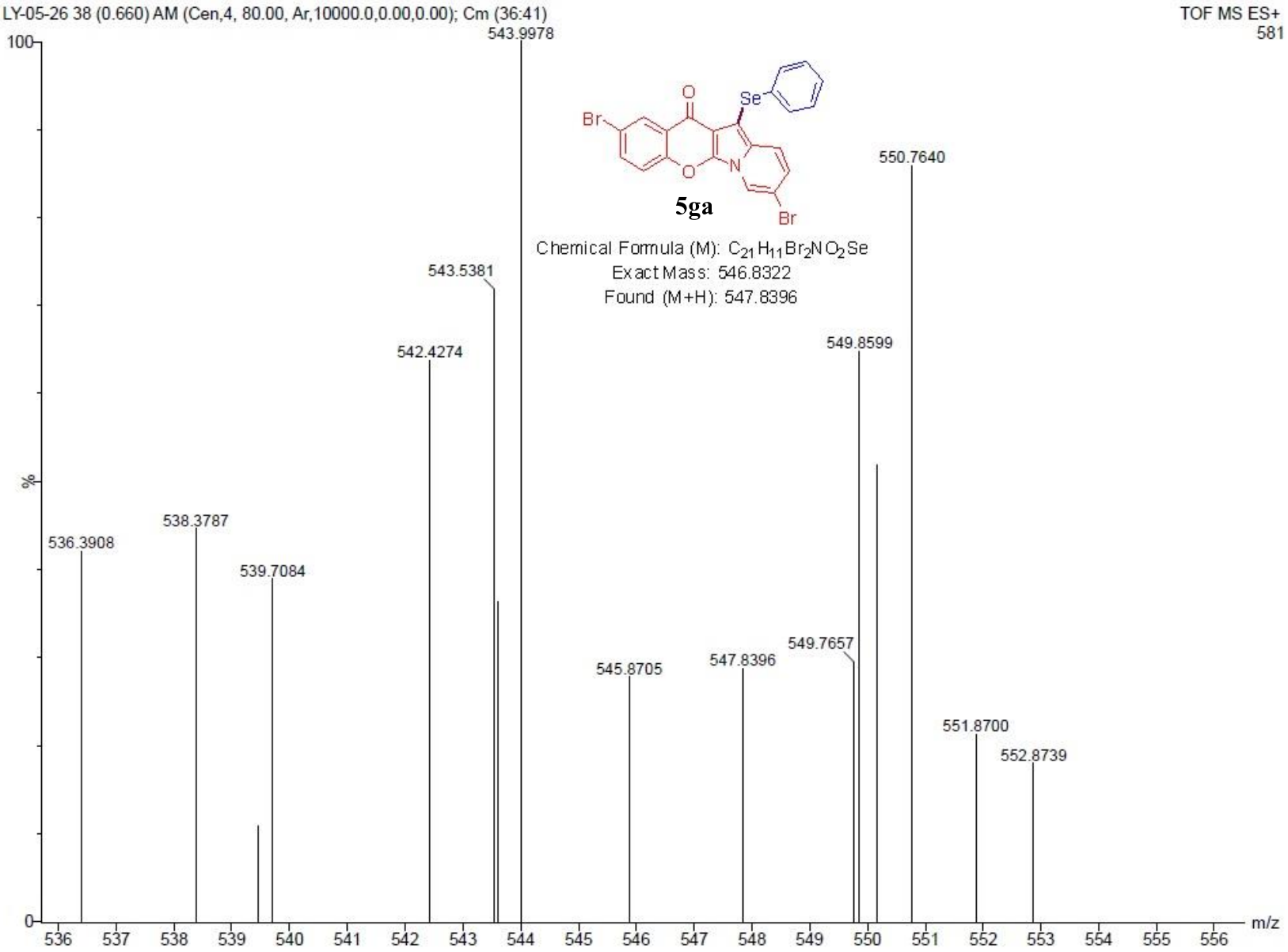
^{1}H NMR spectrum of 5ga (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of 5ga (100 MHz, $CDCl_3$)



Mass spectrum of 5ga



Mass spectrum of TEMPO-adduct (6)