

Supporting Information

Modular Synthesis of Unsymmetrical Indolyl diketones from Ynediones via Sequential *aza*-Micheal Addition/C-H Functionalization

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1. General Methods:

Materials: All glassware was oven-dried (90 °C). Unless mentioned, chemicals & solvents were purchased in high purity grade from commercial suppliers and used without further purification. 1,2-alkynyldiketones were prepared according known procedures previously reported.

Chromatography: Thin layer chromatography (TLC) carried out on Merck silica plates (60F-254) and components were visualized by observation under UV light or by treating the plates with p-anisaldehyde followed by heating. Silica gel chromatography was performed using silica gel (60-120 or 100-200 mesh).

Characterization: NMR spectra for characterization of compounds were recorded on Bruker Avance DPX FT-NMR 400 MHz instrument (¹H) at 400 MHz and (¹³C) at 100 MHz respectively. ¹⁹F NMR were recorded at 376 MHz Chemical shifts (δ) are reported in ppm, using the residual solvent peak in CDCl₃ (δ H = 7.26 and δ C 77.16 ppm) and DMSO-d₆ (δ H = 2.50 and δ C = 39.52 ppm) as internal reference and coupling constants (*J*) are given in hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. High- Resolution Mass Spectra (HRMS) were recorded using Waters XEVO-G2-XS-Q-TOF mass spectrometer.

Experimental details. Unless mentioned, reactions were performed at refluxing temperature in 5 mL glass vial. Ynedione used in this study were synthesized following the previously known literature procedures. Solvent used for the reaction purpose are of commercial grade and used without further purification. N-protection of indole was done following the previously reported methods.

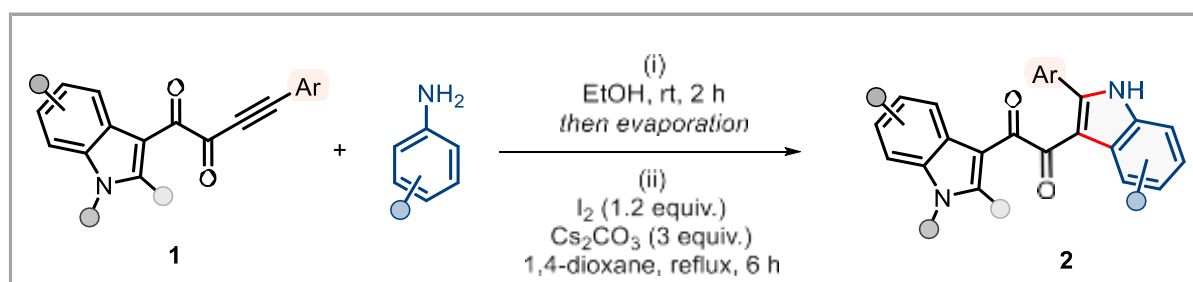
2. Synthesis of Starting Materials:

Ynedione used in this study were synthesized following the previously known literature procedure. ^[1] *N*-substituted indoles (1.0 equiv.) in dry THF (25 mL) were placed under argon atmosphere in a two-neck round-bottom flask, degassed with argon and cooled to 0 °C (water/ice) for 15 min. Then, oxalyl chloride (1.0 equiv.) was added dropwise to the reaction mixture maintaining the temperature 0 °C. The mixture was allowed to come to room temperature (water bath) and was stirred for 4 h. Then,

5 mol% CuI, 2.0 equiv. of terminal alkyne and dry triethylamine (4 equiv.) were successively added to the mixture and stirring at room temperature was continued for 12h. After complete conversion (product monitored by TLC) water was added, the phases were separated and the aqueous phase was extracted with dichloromethane. The combined organic. layers were dried with anhydrous sodium sulfate, concentrated and the residue was subjected to silica gel column chromatography by using petroleum ether/ethyl acetate to provide the desired ynedione.

3. General Experimental Procedure:

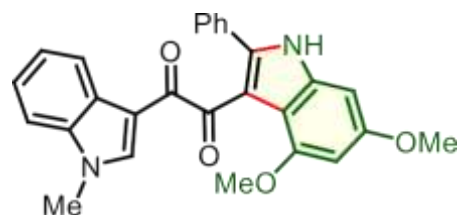
General procedure for the one-pot synthesis of indolyl-diketone (GP1):



Aniline was added to the solution of indole-tethered ynedione **1** (1.0 equiv.) in ethanol, and the resulting mixture was stirred at room temperature for 2 h. After completion, ethanol was evaporated. The resulting mixture was redissolved in 1,4-dioxane followed by addition of 1.2 equiv. of iodine and 3 equiv. of Cs₂CO₃. The resulting mixture was stirred at a refluxing temperature for 6 hrs. Upon completion, the reaction mixture was concentrated under reduced pressure and directly subjected to silica gel column purification using ethyl acetate and petroleum ether as eluent.

4. Characterization Data of Synthesized Compounds:

1-(4,6-dimethoxy-2-phenyl-1*H*-indol-3-yl)-2-(1-methyl-1*H*-indol-3-yl)ethane-1,2-

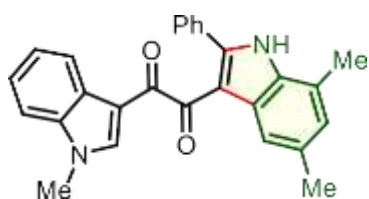


7.48-7.28 (m, 6H), 6.55 (d, $J = 1.62$ Hz, 1H), 6.16 (d, $J = 1.66$ Hz, 1H), 3.92 (s, 3H), 3.77 (s,

dione (2a): The title compound was isolated as a pale yellow solid (119 mg, 78% yield); R_f : 0.50 (30% ethyl acetate-petroleum ether); ¹H NMR (400 MHz, DMSO- *d*₆) δ 12.09 (s, 1H), 8.22-8.16 (m, 2H), 7.73-7.66 (m, 2H),

3H), 3.08 (s, 3H), ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) δ 192.2, 187.1, 158.5, 153.7, 142.7, 138.8, 137.4, 136.9, 131.5, 129.1, 129.0, 128.7, 128.5, 127.3, 123.5, 122.8, 112.5, 112.1, 111.2, 109.7, 94.0, 87.2, 55.7, 54.7, 33.7 ppm; HRMS (ESI): calcd. for $\text{C}_{27}\text{H}_{23}\text{N}_2\text{O}_2[\text{M}+\text{H}]^+$: 439.1658, found 439.1655.

1-(5,7-dimethyl-2-phenyl-1H-indol-3-yl)-2-(1-methyl-1H-indol-3-yl)ethane-1,2-dione



(2b): The title compound was isolated as a pale yellow solid (104 mg, 74% yield); R_f : 0.50 (30% ethyl acetate-petroleum ether); ^1H NMR (400 MHz, DMSO- d_6) δ 12.06 (s, 1H), 8.07 (s, 1H), 7.84-7.74 (m, 2H), 7.56-7.50 (m, 1H), 7.46-7.40 (m, 2H),

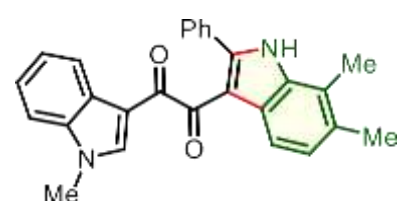
7.30-7.12 (m, 5H) 7.06-7.00 (m, 1H), 3.84 (s, 3H), 2.44 (s, 3H), 2.33 (s, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$

NMR (100 MHz, DMSO- d_6) δ 190.8, 189.0, 147.9, 139.8, 137.5, 136.2, 131.4, 131.0 130.2,

129.1, 127.7, 125.8, 125.5, 125.1, 123.4, 122.6, 121.3, 119.9, 118.1, 112.3, 110.9, 110.2, 33.4,

19.3, 13.45 ppm; HRMS (ESI): calcd. for $\text{C}_{27}\text{H}_{23}\text{N}_2\text{O}_2[\text{M}+\text{H}]^+$: 407.1760, found 407.1757.

1-(6,7-dimethyl-2-phenyl-1H-indol-3-yl)-2-(1-methyl-1H-indol-3-yl) ethane-1,2-dione



(2c): The title compound was isolated as a pale yellow solid (99 mg, 70% yield); R_f : 0.52 (30% ethyl acetate- petroleum ether); ^1H NMR (400 MHz, DMSO- d_6) δ 12.08 (s, 1H), 8.08 (s, 1H), 7.87-7.77 (m, 2H), 7.56-7.50 (m, 1H),

7.48-7.41 (m, 2H) 7.31-7.13 (m, 5H), 7.08-7.01 (m, 1H), 3.84 (s, 3H), 2.45 (s, 3H), 2.34 (s,

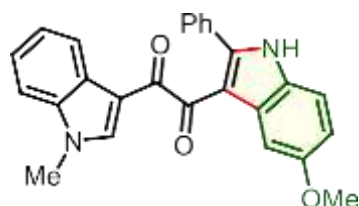
3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) δ 190.9, 189.0, 147.9, 139.8, 137.5, 136.2,

131.4, 131.0, 130.2, 129.1, 127.7, 125.8, 125.5, 125.2, 123.4, 122.6, 121.4, 119.9, 118.1, 112.4,

110.9, 110.3, 33.4, 19.3, 13.4 ppm; HRMS (ESI):calcd. for $\text{C}_{27}\text{H}_{23}\text{N}_2\text{O}_2[\text{M}+\text{H}]^+$: 407.1760,

found 407.1757.

1-(5-methoxy-2-phenyl-1H-indol-3-yl)-2-(1-methyl-1H-indol-3-yl) ethane-1,2-dione

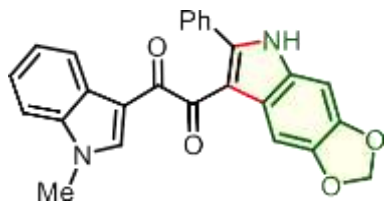


(2d): The title compound was isolated as a yellow solid (98 mg, 69% yield); R_f : 0.50 (30% ethyl acetate-petroleum ether); ^1H NMR (400 MHz, DMSO- d_6) δ 12.36 (s, 1H), 8.14 (s, 1H), 7.87-7.83 (m, 1H), 7.59-7.59 (m, 1H), 7.57-7.52 (m,

1H), 7.49-7.44 (m, 2H), 7.41-7.38 (m, 1H) 7.31-7.13 (m, 5H), 6.91 (dd, $J = 8.75, 2.42$ Hz,

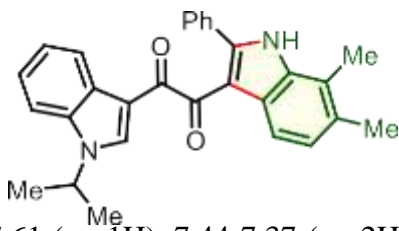
1H), 3.86 (s, 3H) 3.71 (s, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 190.9, 188.9, 156.6, 148.3, 139.2, 137.5, 131.2, 130.9, 129.2, 129.0, 128.9, 128.2, 126.5, 123.7, 122.9, 122.5, 113.9, 113.5, 113.1, 110.4, 109.7, 103.3, 55.8, 33.7 ppm; HRMS (ESI): calcd. for $\text{C}_{26}\text{H}_{21}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$: 409.1552, found 409.1553.

1-(1-methyl-1H-indol-3-yl)-2-(6-phenyl-5H-[1,3]dioxolo[4,5-f]indol-7-yl)ethane-1,2-



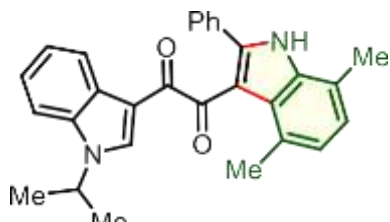
dione (2e): The title compound as off dark yellow solid (119 mg, 81% yield); R_f : 0.56 (30% ethyl acetate-petroleum ether); ^1H NMR (400 MHz, DMSO-d_6) δ 12.31 (s, 1H), 8.13-8.12 (m, 1H), 7.86-7.84 (m, 1H), 7.58-7.51 (m, 1H), 7.45-7.44 (m, 3H), 7.31-7.12 (m, 5H), 7.00-6.99 (m, 1H), 6.02 (s, 2H), 3.86 (s, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 190.5, 188.6, 146.0, 145.2, 144.6, 140.0, 137.5, 131.4, 130.9, 129.6, 128.9, 127.8, 125.7, 123.4, 122.6, 121.5, 121.2, 112.2, 110.9, 109.9, 101.0, 99.8, 92.9, 33.4 ppm; HRMS (ESI): calcd. for $\text{C}_{26}\text{H}_{19}\text{N}_2\text{O}_4$ $[\text{M}+\text{H}]^+$: 423.1345, found 423.1346.

1-(6,7-dimethyl-2-phenyl-1H-indol-3-yl)-2-(1-isopropyl-1H-indol-3-yl)ethane-1,2-



dione (2f): The title compound was isolated as a pale yellow solid (91 mg, 66% yield); R_f : 0.56 (30% ethyl acetate - petroleum ether); ^1H NMR (400 MHz, DMSO-d_6) δ 12.04 (s, 1H), 8.07 (s, 1H), 7.83-7.77 (m, 2H), 7.66-7.61 (m, 1H), 7.44-7.37 (m, 2H), 7.29-7.23 (m, 1H), 7.18-7.13 (m, 2H), 7.10-7.03 (m, 3H), 4.85-4.79 (m, 1H) 2.44 (s, 3H), 2.34 (s, 3H), 2.49 (d, $J = 6.55$ Hz, 6H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 191.3, 188.0, 146.8, 136.5, 135.6, 134.0, 131.8, 131.6, 129.5, 129.3, 128.2, 126.8, 125.8, 125.6, 123.4, 122.9, 122.8, 119.3, 118.3, 113.8, 111.8, 109.9, 48.2, 22.6, 19.4, 13.2 ppm; HRMS (ESI): calcd. For $\text{C}_{29}\text{H}_{27}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$: 435.2073, found 435.2057.

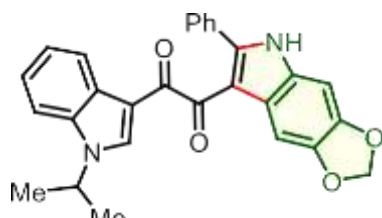
1-(4,7-dimethyl-2-phenyl-1H-indol-3-yl)-2-(1-isopropyl-1H-indol-3-yl)ethane-1,2-



dione (2g): The title compound was isolated as a yellow solid (96 mg, 70% yield); R_f : 0.56 (30% ethyl acetate - petroleum ether); ^1H NMR (400 MHz, DMSO-d_6) δ 11.99 (s, 1H), 8.24-8.23 (m, 1H), 7.82-7.79 (m, 1H), 7.63-7.60 (m, 1H), 7.40-7.39 (m, 2H), 7.26-7.21 (m, 1H), 7.15-7.10 (m, 1H), 7.00-6.88 (m, 5H), 4.87-4.80

(m, 1H), 3.35 (s, 3H), 2.55 (s, 3H), 1.55-1.52 (m, 6H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 192.4, 187.1, 145.3, 136.2, 135.5, 134.1, 131.1, 129.8, 129.7, 128.9, 127.9, 127.1, 126.0, 124.5, 124.4, 123.2, 122.8, 122.7, 117.8, 114.7, 113.7, 109.8, 48.1, 22.6, 22.2, 16.4 ppm; HRMS (ESI): calcd. For $\text{C}_{29}\text{H}_{27}\text{N}_2\text{O}_2[\text{M}+\text{H}]^+$: 435.2073 found 435.2067.

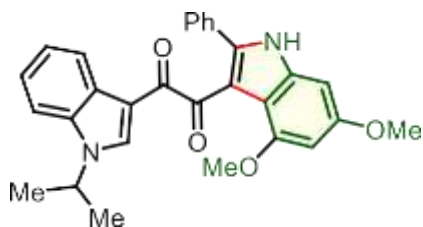
1-(1-isopropyl-1*H*-indol-3-yl)-2-(6-phenyl-5*H*-[1,3]dioxolo[4,5-*f*]indol-7-yl)ethane-



1,2-dione (2h): The title compound was isolated as a yellow solid (111 mg, 78% yield); R_f : 0.58 (30% ethyl acetate-petroleum ether); ^1H NMR (400 MHz, DMSO-d_6) δ

12.27 (m, 1H), 8.13 (s, 1H), 7.87-7.77 (m, 1H), 7.68-7.61 (m, 1H), 7.56-7.46 (m, 1H), 7.45-7.36 (m, 2H), 7.30-7.24 (m, 1H), 7.18-6.99 (m, 5H), 6.03 (s, 2H), 4.85-4.82 (m, 1H), 1.49 (d, $J = 5.98$ Hz, 6H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 190.6, 188.6, 145.9, 145.1, 144.5, 136.1, 135.1, 131.2, 130.8, 129.6, 128.8, 127.6, 125.8, 123.2, 122.4, 121.4, 121.3, 112.7, 111.0, 110.2, 100.9, 99.7, 92.8, 47.9, 22.0 ppm; HRMS (ESI): calcd. For $\text{C}_{28}\text{H}_{23}\text{N}_2\text{O}_4[\text{M}+\text{H}]^+$: 451.1658, found 451.1650.

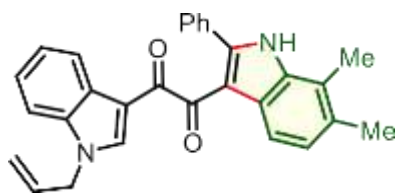
1-(4,6-dimethoxy-2-phenyl-1*H*-indol-3-yl)-2-(1-isopropyl-1*H*-indol-3-yl)ethane-1,2-



dione (2i): The title compound was isolated as a yellow solid (93 mg, 63% yield); R_f : 0.54 (30% ethyl acetate-petroleum ether); ^1H NMR (400 MHz, DMSO-d_6) δ 12.08 (s, 1H), 8.22-8.15 (m, 1H), 7.71-7.68 (m, 3H), 7.48-7.39 (m,

3H), 7.33-7.23 (m, 3H), 6.55 (d, $J = 1.75$, 1H), 6.15 (d, $J = 1.80$ Hz, 1H), 4.94-4.86 (m, 1H), 3.77 (s, 3H), 3.05 (s, 3H), 1.52 (d, $J = 6.63$ Hz, 6H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 192.5, 187.2, 158.5, 153.7, 142.5, 136.9, 136.3, 134.2, 131.5, 129.0, 128.6, 127.6, 123.2, 123.0, 122.7, 112.9, 112.1, 111.4, 110.0, 93.9, 87.1, 55.7, 54.6, 48.1, 22.7 ppm; HRMS (ESI): calcd. for $\text{C}_{29}\text{H}_{27}\text{N}_2\text{O}_4[\text{M}+\text{H}]^+$: 467.1971, found 467.1968.

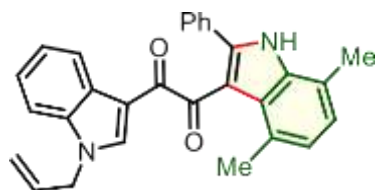
1-(1-allyl-1*H*-indol-3-yl)-2-(6,7-dimethyl-2-phenyl-1*H*-indol-3-yl)ethane-1,2-dione



(2j): The title compound was isolated as a yellow solid (81 mg, 59% yield); R_f : 0.57 (30% ethyl acetate - petroleum ether); ^1H NMR (400 MHz, DMSO-d_6) δ 12.07 (s, 1H), 8.07 (s, 1H), 7.86-7.76 (m, 2H), 7.54-7.48 (m, 1H),

7.44-7.37 (m, 2H), 7.29-7.16 (m, 3H), 7.14-7.03 (m, 3H), 6.06-5.96 (m, 1H) 5.20 (d, $J = 10.33$ Hz, 1H) 5.03(d, $J = 17.04$ Hz, 1H), 4.92-4.91 (m, 2H), 2.44 (s, 3H), 2.34 (s, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 191.2, 188.6, 146.8, 137.7, 136.9, 135.6, 131.9, 131.7, 129.5, 129.4, 128.3, 126.7, 125.9, 125.6, 123.6, 122.9, 122.8, 119.4, 118.8, 118.2, 113.9, 110.8, 49.6, 29.8, 19.4, 13.3 ppm; HRMS (ESI): calcd. For $\text{C}_{29}\text{H}_{27}\text{N}_2\text{O}_2[\text{M}+\text{H}]^+$: 433.1916, found 433.1894.

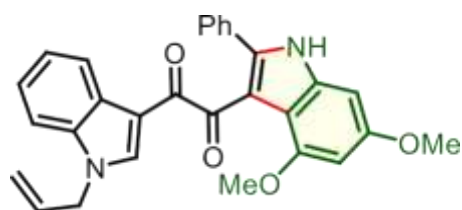
1-(1-allyl-1H-indol-3-yl)-2-(4,7-dimethyl-2-phenyl-1H-indol-3-yl) ethane-1,2-dione



(2k): The title compound was isolated as a greenish yellow solid (106 mg, 77% yield); R_f : 0.57 (30% ethyl acetate - petroleum ether); ^1H NMR (400 MHz, DMSO-d_6) δ 12.01 (s, 1H), 8.24 (s, 1H), 7.81-7.77 (m, 1H), 7.52-7.47 (m, 1H),

7.38-7.35 (m, 2H), 7.24-7.21 (m, 1H), 7.14-7.11 (m, 1H), 7.07-7.00 (m, 3H) 6.98-6.94 (m, 1H) 6.91-6.86 (m, 1H), 6.11-6.01 (m, 1H), 5.25 (dd, $J = 10.36, 1.28$ Hz, 1H), 5.08 (dd, $J = 17.05, 1.42$ Hz, 1H), 4.49 (d, $J = 5.22$ Hz, 2H), 3.33 (s, 3H), 2.54 (s, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 192.1, 187.1, 145.5, 138.0, 136.6, 135.5, 133.5, 131.9, 129.9, 129.7, 129.1, 129.0, 128.1, 127.6, 127.0, 124.6, 124.5, 123.5, 122.8, 118.7, 117.8, 114.5, 113.7, 110.0, 49.5, 22.3, 16.4 ppm; HRMS (ESI): calcd. For $\text{C}_{29}\text{H}_{25}\text{N}_2\text{O}_2[\text{M}+\text{H}]^+$: 433.1916, found 433.1909.

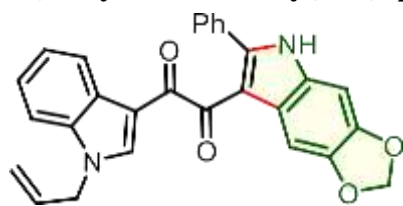
1-(1-allyl-1H-indol-3-yl)-2-(4,6-dimethoxy-2-phenyl-1H-indol-3-yl) ethane-1,2-dione



(2l): The title compound was isolated as a yellow solid (80 mg, 54% yield); R_f : 0.52 (30% ethyl acetate - petroleum ether); ^1H NMR (400 MHz, DMSO-d_6) δ 12.11 (s, 1H), 8.23-8.19 (m, 2H), 7.74-7.67 (m, 2H),

7.62-7.56 (m, 1H), 7.48-7.43 (m, 3H), 7.32-7.25 (m, 2H), 6.56 (d, $J = 1.68$ Hz, 1H), 6.16 (d, $J = 1.70$ Hz, 1H) 6.10-6.00 (m, 1H), 5.20 (d, $J = 10.36$ Hz, 1H), 5.06 (dd, $J = 17.09, 1.16$ Hz, 1H), 4.95 (d, $J = 5.07$ Hz, 2H), 3.77 (s, 3H), 3.08 (s, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 192.3, 187.4, 158.6, 153.7, 142.8, 138.0, 137.0, 136.8, 132.1, 131.6, 129.2, 129.1, 128.6, 127.6, 123.6, 123.0, 122.9, 118.8, 113.0, 112.2, 111.3, 110.3, 94.0, 87.3, 55.8, 54.8, 49.7 ppm; HRMS (ESI): calcd. for $\text{C}_{29}\text{H}_{25}\text{N}_2\text{O}_4[\text{M}+\text{H}]^+$: 465.1814, found 465.1807.

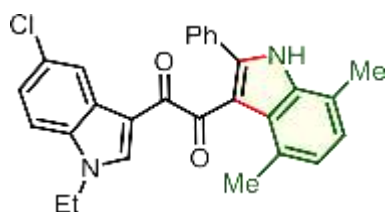
1-(1-allyl-1*H*-indol-3-yl)-2-(6-phenyl-5*H*-[1,3]dioxolo[4,5-*f*]indol-7-yl)ethane-1,2-



dione (2m): The title compound was isolated as a yellow solid (106 mg, 74% yield); R_f : 0.53 (30% ethyl acetate - petroleum ether); $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 12.31 (s, 1H), 8.12 (s, 1H), 7.82 (d, $J = 7.74$ Hz, 1H), 7.53-7.49 (m,

2H), 7.44-7.36 (m, 2H), 7.28-7.08 (m, 5H), 6.99 (s, 1H), 6.07-5.99 (m, 3H), 5.20 (dd, $J = 10.20$, 1.03 Hz, 1H) 5.03 (dd, $J = 17.10$, 1.22 Hz, 1H), 4.93 (d, $J = 5.72$ Hz, 2H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{DMSO-}d_6$) δ 190.6 189.0, 146.3, 145.3, 144.7, 139.1, 136.7, 133.6, 131.3, 131.0, 129.7, 129.0, 127.9, 125.9, 123.6, 122.7, 121.4, 117.6, 112.7, 111.4, 110.1, 101.1, 99.9, 93.0, 48.8, ppm; HRMS (ESI): calcd. for $\text{C}_{28}\text{H}_{21}\text{N}_2\text{O}_4$ $[\text{M}+\text{H}]^+$: 449.1501, found 449.1497.

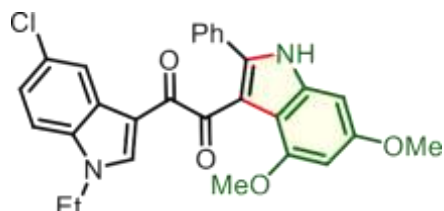
1-(5-chloro-1-ethyl-1*H*-indol-3-yl)-2-(5,7-dimethyl-2-phenyl-1*H*-indol-3-yl)ethane-



1,2-dione (2n): The title compound was isolated as a yellow solid (96 mg, 71% yield); R_f : 0.51 (30% ethyl acetate -petroleum ether); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 12.06 (s, 1H), 8.31 (s, 1H), 7.70 (d, $J = 1.88$ Hz, 1H), 7.66-7.59 (m,

1H), 7.40-7.32 (m, 2H), 7.26 (dd, $J = 8.69$, 1.93 Hz, 1H), 7.06-6.89 (m, 5H) 4.31(q, $J = 7.17$ Hz, 2H), 2.57(s, 3H), 2.48 (s, 3H), 1.40 (t, $J = 7.19$ Hz, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 191.8, 186.6, 145.6, 137.7, 135.5, 134.6, 131.6, 129.9, 129.7, 129.1, 128.7, 128.2, 128.1, 126.0, 124.7, 124.6, 123.8, 122.3, 117.8, 114.5, 113.2, 110.6, 42.1, 22.3, 16.4, 15.2 ppm; HRMS (ESI): calcd. for $\text{C}_{28}\text{H}_{24}\text{N}_2\text{O}_2\text{Cl}$ $[\text{M}+\text{H}]^+$: 455.1526, found 455.1526.

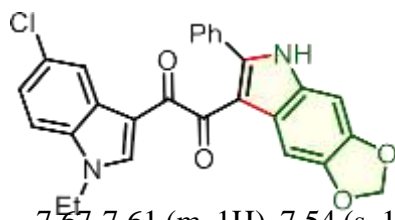
1-(5-chloro-1-ethyl-1*H*-indol-3-yl)-2-(4,6-dimethoxy-2-phenyl-1*H*-indol-3-yl)ethane-



1,2-dione (2o): The title compound was isolated as a yellow solid (93 mg, 64% yield); R_f : 0.59 (30% ethyl acetate -petroleum ether); $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 12.14 (s, 1H), 8.34 (s, 1H), 8.13 (s, 1H), 7.72-7.69

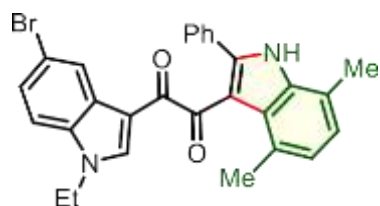
(m, 3H), 7.48-7.42 (m, 3H), 7.36-7.32 (m, 1H), 6.56 (s, 1H), 6.18 (s, 1H), 4.36 (q, $J = 7.19$ Hz, 2H), 3.77 (s, 3H), 3.09 (s, 3H), 1.39 (t, $J = 7.26$ Hz, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{DMSO-}d_6$) δ 191.2, 186.8, 157.6, 152.9, 142.4, 138.9, 137.0, 134.6, 131.4, 124.2, 128.7, 128.1, 127.7, 127.0, 123.0, 120.4, 112.7, 111.3, 111.2, 109.8, 93.3, 87.4, 55.4, 54.3, 41.4, 15.2 ppm; HRMS (ESI): calcd. for $\text{C}_{28}\text{H}_{24}\text{N}_2\text{O}_4\text{Cl}$ $[\text{M}+\text{H}]^+$: 487.1425, found 487.1418.

1-(5-chloro-1-ethyl-1*H*-indol-3-yl)-2-(6-phenyl-5*H*-[1,3]dioxolo[4,5-*f*]indol-7-



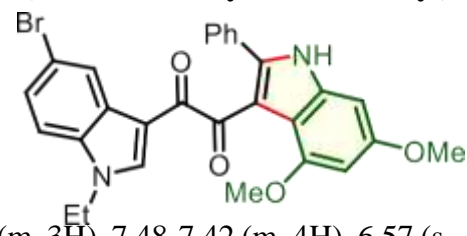
yl)ethane-1,2-dione (2p): The title compound was isolated as a greenish yellow solid (94 mg, 67% yield); R_f : 0.51 (30% ethyl acetate-petroleum ether); $^1\text{H NMR}$ (400 MHz, DMSO-d_6) δ 12.32 (s, 1H), 8.21 (s, 1H), 7.71 (s, 1H), 7.67-7.61 (m, 1H), 7.54 (s, 1H), 7.36-7.28 (m, 3H), 7.20-7.14 (m, 1H), 7.11-7.04 (m, 2H), 6.99 (s, 1H), 6.04 (s, 2H), 4.29 (q, $J = 7.16$ Hz, 2H) 1.36 (t, $J = 7.14$ Hz, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 190.3, 188.4, 146.3, 145.2, 144.6, 139.5, 134.8, 131.2, 130.8, 129.6, 128.7, 127.6, 127.1, 126.9, 123.2, 121.4, 120.4, 112.6, 112.0, 110.1, 100.9, 99.8, 92.8, 41.5, 15.2 ppm; HRMS (ESI): calcd. for $\text{C}_{27}\text{H}_{20}\text{N}_2\text{O}_4\text{Cl}[\text{M}+\text{H}]^+$: 471.1112, found 471.1103.

1-(5-bromo-1-ethyl-1*H*-indol-3-yl)-2-(5,7-dimethyl-2-phenyl-1*H*-indol-3-yl)ethane-



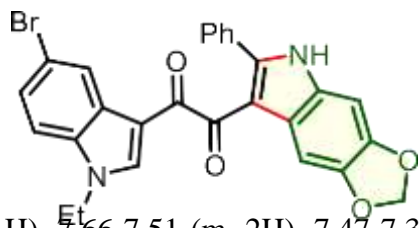
1,2-dione (2q): The title compound was isolated as a yellow solid (92 mg, 70% yield); R_f : 0.51 (30% ethyl acetate-petroleum ether); $^1\text{H NMR}$ (400 MHz, DMSO-d_6) δ 12.07 (s, 1H), 8.31 (s, 1H), 7.87 (d, $J = 1.81$ Hz, 1H), 7.62-7.59 (m, 1H), 7.04-7.35 (m, 3H), 7.06-6.91 (m, 5H), 4.32 (q, $J = 7.20$ Hz, 2H), 2.59 (s, 3H), 2.51 (s, 3H), 1.41 (t, $J = 7.14$ Hz, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 191.1, 187.4, 146.7, 139.6, 135.8, 134.7, 131.2, 130.4, 128.6, 128.1, 127.9, 127.3, 125.6, 125.5, 124.0, 123.4, 119.0, 115.0, 113.2, 112.9, 111.9, 41.5, 21.9, 16.7, 15.3 ppm; HRMS (ESI): calcd. for $\text{C}_{28}\text{H}_{24}\text{N}_2\text{O}_2\text{Br}[\text{M}+\text{H}]^+$: 499.1021, found 499.1020.

1-(5-bromo-1-ethyl-1*H*-indol-3-yl)-2-(4,6-dimethoxy-2-phenyl-1*H*-indol-3-yl)ethane-



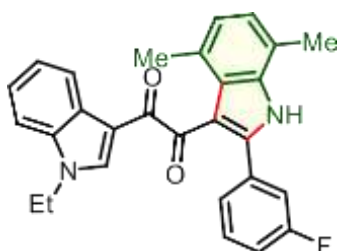
1,2-dione (2r): The title compound was isolated as a yellow solid (103 mg, 74% yield); R_f : 0.55 (30% ethyl acetate-petroleum ether); $^1\text{H NMR}$ (400 MHz, DMSO-d_6) δ 12.14 (s, 1H), 8.32-8.29 (m, 2H), 7.71-7.65 (m, 3H), 7.48-7.42 (m, 4H), 6.57 (s, 1H), 6.19 (s, 1H), 4.37 (q, $J = 6.98$ Hz, 2H), 3.77 (s, 3H), 3.09 (s, 3H), 1.38 (t, $J = 7.12$ Hz, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 191.9, 187.0, 158.5, 153.5, 142.9, 137.6, 136.9, 153.1, 131.3, 129.0, 128.5, 126.4, 126.0, 125.4, 116.4, 112.2, 112.0, 111.3, 110.9, 94.0, 87.2, 55.7, 54.7, 42.1, 15.1 ppm; HRMS (ESI): calcd. for $\text{C}_{28}\text{H}_{24}\text{N}_2\text{O}_4\text{Br}[\text{M}+\text{H}]^+$: 531.0919, found 531.0916.

1-(5-chloro-1-ethyl-1*H*-indol-3-yl)-2-(6-phenyl-5*H*-[1,3]dioxolo[4,5-*f*]indol-7-



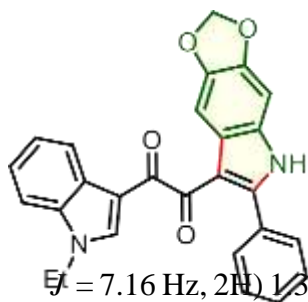
yl)ethane-1,2-dione (2s): The title compound was isolated as a yellow solid (100 mg, 74% yield); R_f : 0.51 (30% ethyl acetate-petroleum ether); $^1\text{H NMR}$ (400 MHz, DMSO-d_6) δ 12.32 (s, 1H), 8.21 (s, 1H), 7.87 (s, 1H), 7.66-7.51 (m, 2H), 7.47-7.30 (m, 3H), 7.22-6.96 (m, 4H) 6.04 (s, 2H), 4.29 (q, $J = 7.14$ Hz, 2H) 1.36 (t, $J = 7.14$ Hz, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 190.3, 188.4, 146.3, 145.2, 144.6, 139.5, 134.8, 131.2, 130.8, 129.6, 128.7, 127.6, 127.1, 126.9, 123.2, 121.4, 120.4, 112.6, 112.0, 110.1, 100.9, 99.8, 92.8, 41.5, 15.2 ppm; HRMS (ESI): calcd. for $\text{C}_{27}\text{H}_{20}\text{N}_2\text{O}_4^{79}\text{Br}[\text{M}+\text{H}]^+$: 513.0450, found 513.0445.

1-(1-ethyl-1*H*-indol-3-yl)-2-(2-(2-fluorophenyl)-4,7-dimethyl-1*H*-indol-3-yl)ethane-



1,2-dione (2t): The title compound was isolated as a yellow solid (85 mg, 62% yield); R_f : 0.51 (30% ethyl acetate -petroleum ether); $^1\text{H NMR}$ (400 MHz, DMSO-d_6) δ 12.08 (s, 1H), 8.30 (s, 1H), 7.82 (d, $J = 7.60$ Hz, 1H), 7.65-7.51 (m, 1H), 7.27-6.83 (m, 8H), 4.31 (q, $J = 7.09$ Hz, 2H), 2.57 (s, 3H), 2.49 (s, 3H), 1.41 (t, $J = 6.82$ Hz, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 191.4, 187.3, 162.1 (d, $J = 247.27$ Hz), 144.4, 138.8, 135.9, 133.3 (d, $J = 8.32$ Hz), 133.4, 129.8, 129.78, 129.74, 127.0, 125.9, 125.3 (d, $J = 2.82$ Hz), 124.68 (d, $J = 5.59$ Hz), 123.5, 122.8, 122.7 (d, $J = 10.85$ Hz), 116.9 (d, $J = 22.70$ Hz), 115.8 (d, $J = 21.04$ Hz), 114.9, 113.4, 110.0, 41.2, 21.8, 16.6, 15.1 ppm; ^{19}F NMR (376 MHz, DMSO-d_6) δ -133.2 ppm; HRMS (ESI): calcd. for $\text{C}_{28}\text{H}_{24}\text{N}_2\text{O}_2\text{F} [\text{M}+\text{H}]^+$: 439.1822, found 439.1813.

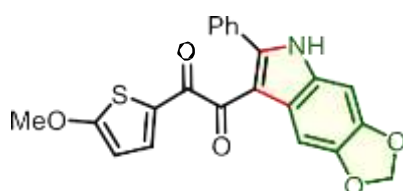
1-(1-ethyl-1*H*-indol-3-yl)-2-(6-(2-fluorophenyl)-5*H*-[1,3]dioxolo[4,5-*f*]indol-7-



yl)ethane-1,2-dione (2u): The title compound was isolated as a yellow solid (96 mg, 68% yield); R_f : 0.51 (30% ethyl acetate -petroleum ether); $^1\text{H NMR}$ (400 MHz, DMSO-d_6) δ 12.39 (s, 1H), 8.16 (s, 1H), 7.90-7.85 (m, 1H), 7.63-7.57 (m, 1H), 7.48 (s, 1H), 7.30-7.12 (m, 5H), 7.01-6.97 (m, 2H) 6.03 (s, 2H), 4.29 (q, $J = 7.16$ Hz, 2H) 1.37 (t, $J = 7.20$ Hz, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 190.7,

188.8, 161.3 (d, $J = 244.15$ Hz), 145.2 (d, $J = 70.15$ Hz), 144.3 (d, $J = 1.91$ Hz), 138.7, 136.5, 133.4 (d, $J = 8.44$ Hz), 131.0, 129.9 (d, $J = 8.52$ Hz), 125.8 (t, $J = 2.61$ Hz), 123.6, 122.7, 121.5, 121.4, 116.7 (d, $J = 22.77$ Hz), 115.9, 115.8, 112.5, 111.0, 110.5, 101.1, 99.9, 93.0, 41.5, 15.3 ppm; ^{19}F NMR (376 MHz, DMSO- d_6) δ -113.7 ppm; HRMS (ESI): calcd. for $\text{C}_{27}\text{H}_{20}\text{N}_2\text{O}_4\text{F}$ $[\text{M}+\text{H}]^+$: 455.1407, found 455.1400.

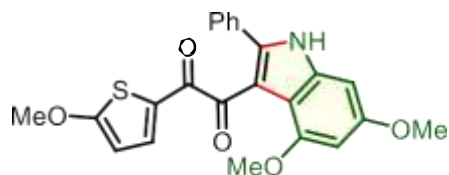
1-(5-methoxythiophen-2-yl)-2-(6-phenyl-5H-[1,3]dioxolo[4,5-f]indol-7-yl)ethane-1,2-



dione (2v): The title compound was isolated as a dark yellow solid (93 mg, 62% yield); R_f : 0.54 (30% ethyl acetate - petroleum ether); ^1H NMR (400 MHz, DMSO- d_6) δ 12.38 (s, 1H), 7.54-7.50 (m, 2H), 7.37-7.27 (m, 5H),

7.01-7.00 (m, 1H), 6.49-6.47 (m, 1H), 6.04 (s, 2H), 3.96 (s, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) δ 188.6, 185.4, 175.4, 146.6, 145.3, 144.7, 137.4, 130.9, 130.8, 129.7, 129.3, 127.9, 126.7, 121.2, 110.1, 107.2, 101.0, 99.7, 92.9, 61.0 ppm; HRMS (ESI): calcd. for $\text{C}_{22}\text{H}_{16}\text{NO}_5\text{S}$ $[\text{M}+\text{H}]^+$: 406.0749, found 406.0733.

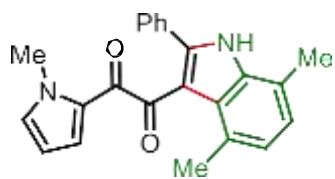
1-(4,6-dimethoxy-2-phenyl-1H-indol-3-yl)-2-(5-methoxythiophen-2-yl)ethane-1,2-



dione (2w): The title compound was isolated as a dark yellow solid (107 mg, 69% yield); R_f : 0.54 (30% ethyl acetate -petroleum ether); ^1H NMR (400 MHz, DMSO- d_6) δ 12.20 (s, 1H), 7.66-7.60 (m, 3H), 7.49-7.44

(m, 3H), 6.56-6.55 (m, 2H), 6.24 (s, 1H), 4.01 (s, 3H), 3.78 (s, 3H), 3.38 (s, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 190.0, 184.0, 175.3, 158.6, 153.6 143.0, 136.8, 136.4, 131.2, 129.2, 129.1, 128.5, 111.9, 110.8, 106.7, 94.0, 87.2, 60.6, 55.8, 54.8 ppm; HRMS (ESI): calcd. for $\text{C}_{23}\text{H}_{20}\text{NO}_5\text{S}$ $[\text{M}+\text{H}]^+$: 422.1062, found 422.1050.

1-(4,7-dimethyl-2-phenyl-1H-indol-3-yl)-2-(1-methyl-1H-pyrrol-2-yl)ethane-1,2-dione (2x):

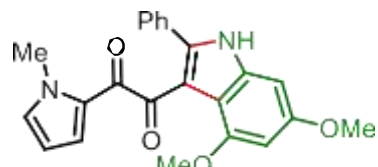


The title compound was isolated as a dark yellow solid (96 mg, 64% yield); R_f : 0.54 (30% ethyl acetate-petroleum ether); ^1H NMR (400 MHz, DMSO- d_6) δ 12.09 (s, 1H), 7.34 (t, J = 7.03 Hz, 1H), 7.24-7.17 (m, 5H), 7.08 (s, 1H), 6.98-6.90 (m, 2H),

6.81-6.80 (m, 1H), 6.10-6.08 (m, 1H), 3.30 (s, 3H), 2.64 (s, 3H), 2.45 (s, 3H) ppm; $^{13}\text{C}\{^1\text{H}\}$

NMR (100 MHz, DMSO- d₆) δ 189.8, 183.1, 147.6, 135.8, 132.6, 131.0, 130.5, 128.9, 128.4, 128.2, 126.9, 125.2, 124.2, 124.1, 122.5, 118.8, 113.2, 108.7, 36.3, 22.2, 16.5 ppm; HRMS (ESI): calcd. for C₂₃H₁₉N₂O₂ [M-H]⁻: 355.1447, found 355.1439.

1-(4,6-dimethoxy-2-phenyl-1H-indol-3-yl)-2-(1-methyl-1H-pyrrol-2-yl)ethane-1,2-



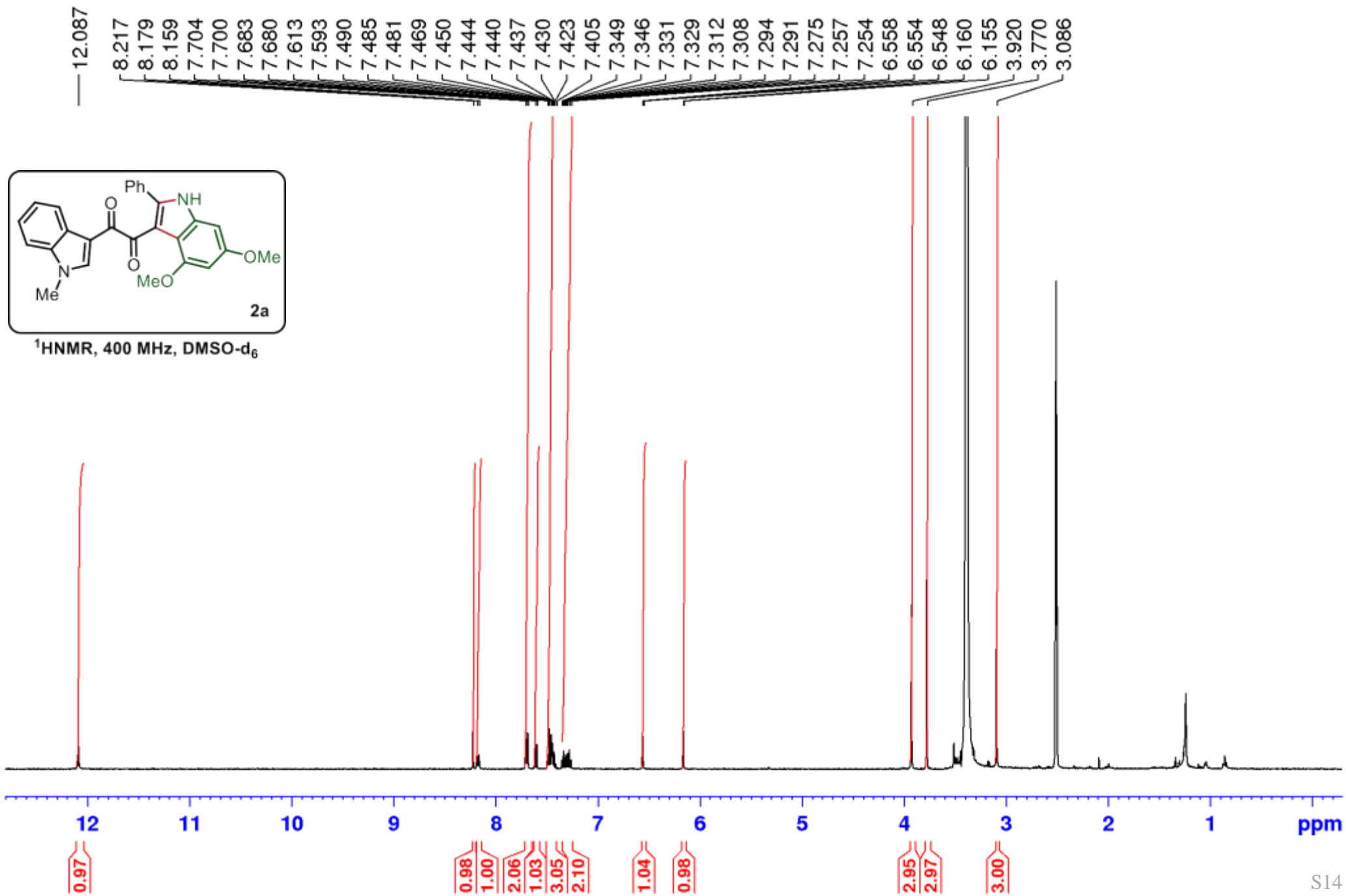
dione (2y): The title compound was isolated as a yellow solid (111 mg, 68% yield); R_f: 0.54 (30% ethyl acetate - petroleum ether); ¹H NMR (400 MHz, DMSO-d₆) δ 12.10 (s,

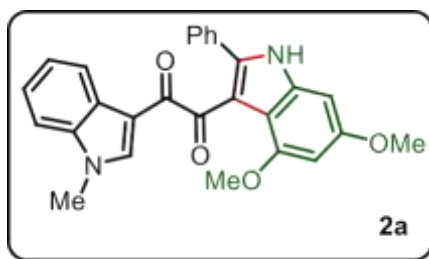
1H), 7.63 (d, *J* = 5.82 Hz, 2H), 7.45-7.44 (m, 2H), 7.25 (s, 2H), 6.87(s, 1H) 6.54 (s, 1H), 6.21-6.19 (m, 2H), 3.90 (s, 3H), 3.77 (s, 3H), 3.30 (s, 3H) ppm; ¹³C{¹H} NMR (100 MHz, DMSO-d₆) δ 190.1, 182.6, 157.6, 153.0, 142.8, 137.0, 132.2, 131.4, 129.3, 128.7, 128.1, 127.8, 121.8, 111.0, 109.8, 108.6, 93.3, 87.4, 55.4, 54.5, 36.8 ppm; HRMS (ESI): calcd. for C₂₃H₁₉N₂O₄ [M-H]⁻: 387.1335, found 387.1345.

5. References:

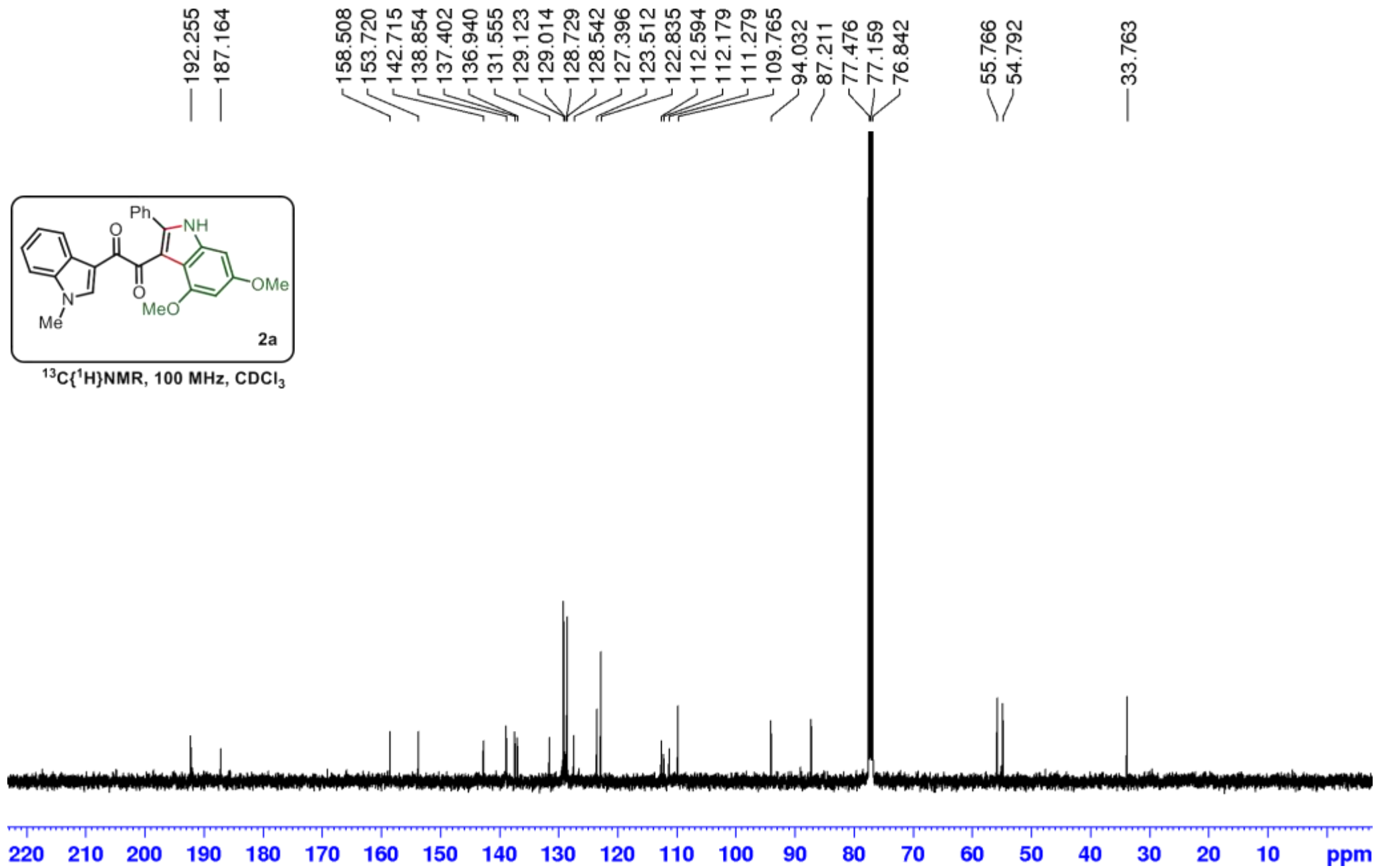
- [1] E. Merkul, J. Dohe, C. Gers, F. Rominger, T. J. J. Müller, *Angew. Chem. Int. Ed.* **2011**, *50*, 2966-2969.
- [2] D. Bag, S. D. Sawant, *Org. Lett.* **2022**, *24*, 27, 4930-4934.

6. NMR Spectra





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

24 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

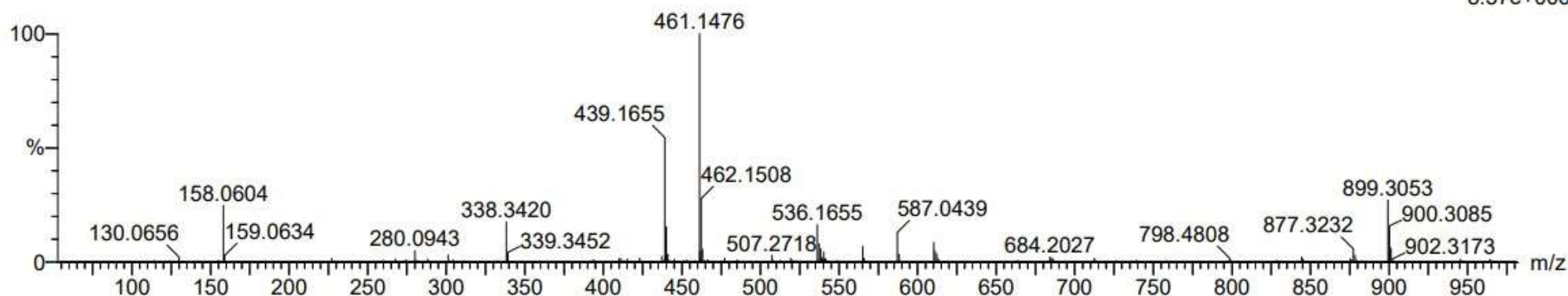
C: 0-27 H: 0-100 N: 0-2 O: 0-4

NVD-41

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

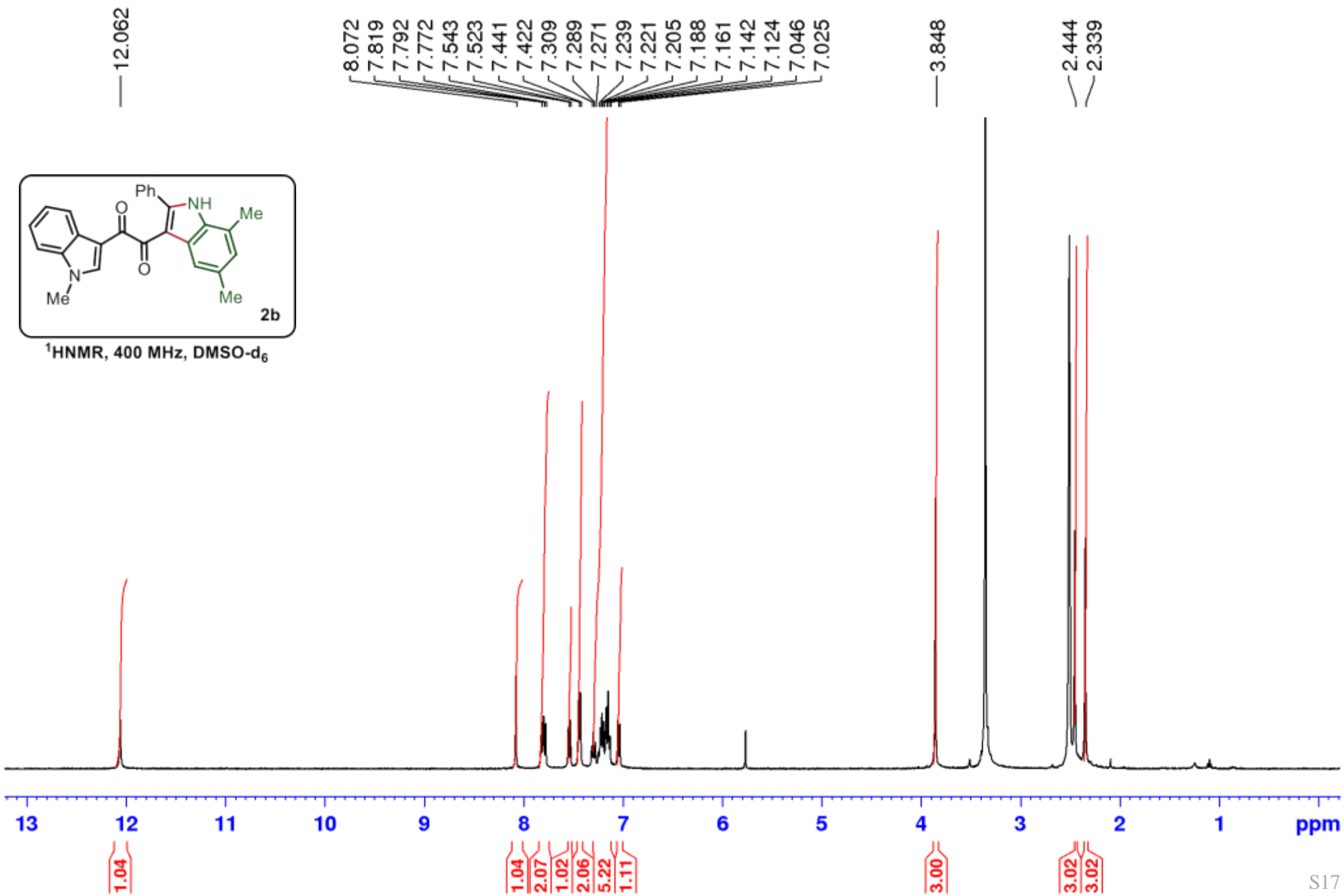
13-Apr-2023
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8.57e+006

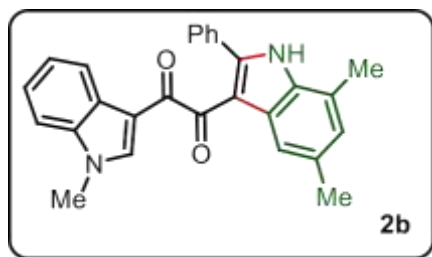
130423_09 6 (0.138)



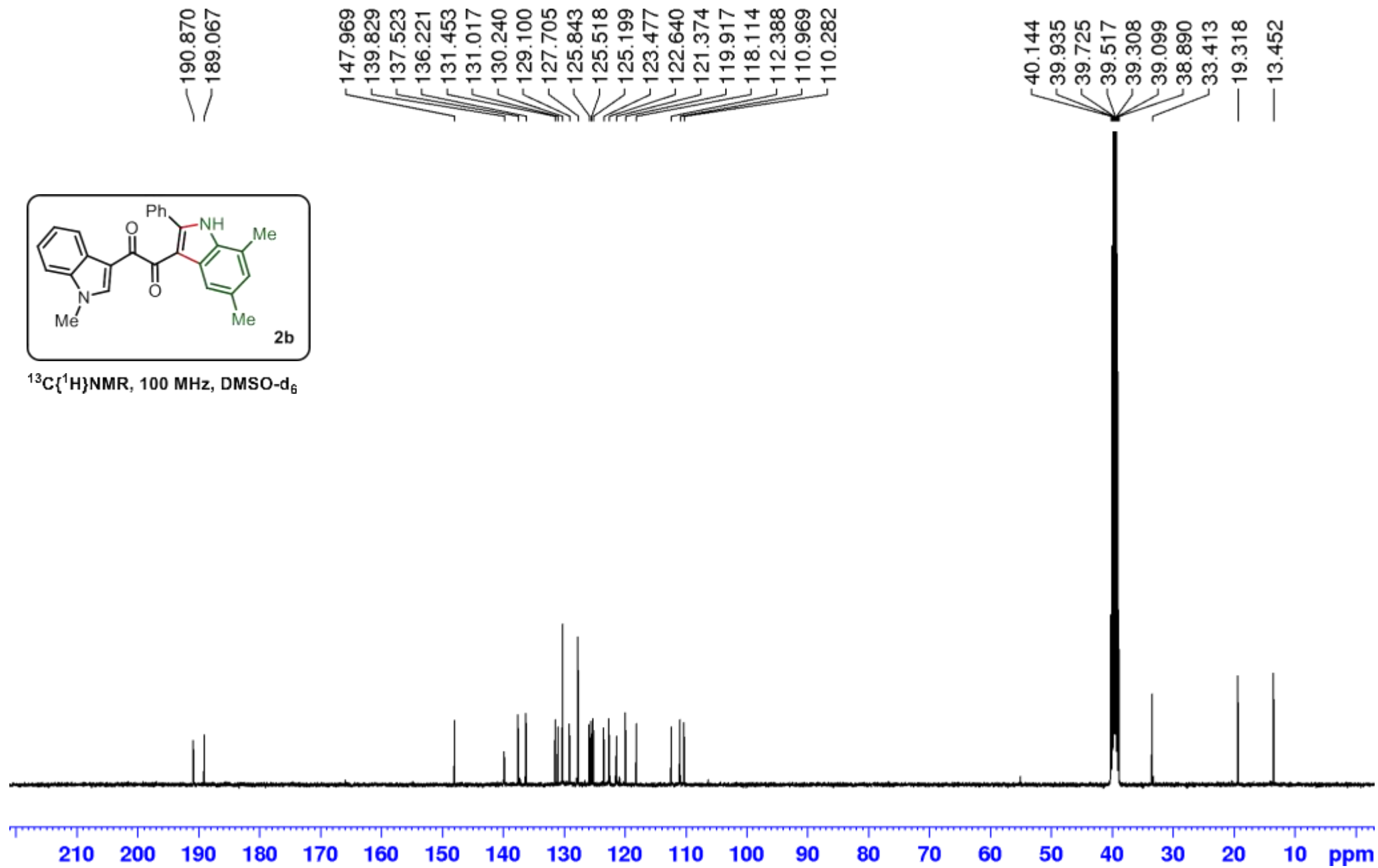
Minimum: -1.5
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
439.1655	439.1658	-0.3	-0.7	17.5	919.9	n/a	n/a	C27 H23 N2 O4





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, DMSO- d_6



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

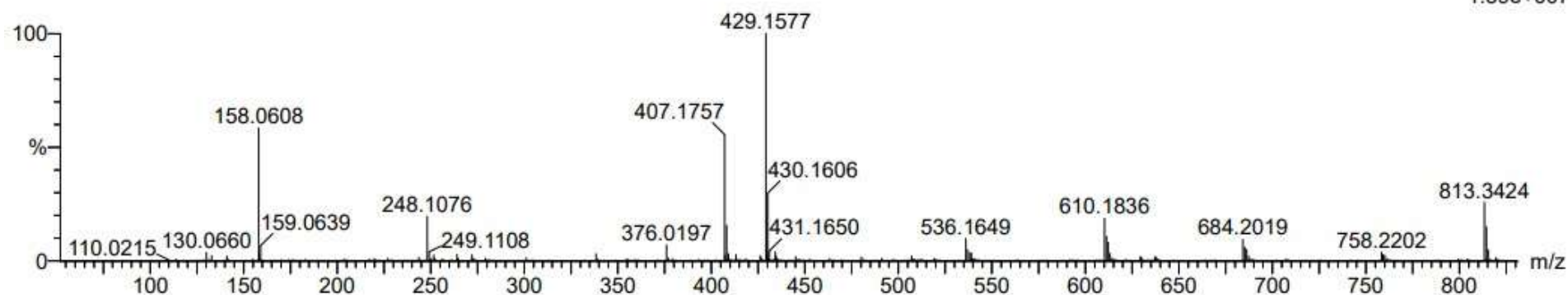
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NVD-43

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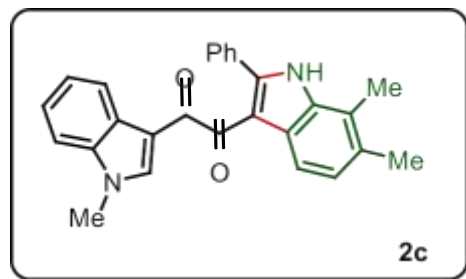
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

24-Apr-2023
12:14:11
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1.59e+007

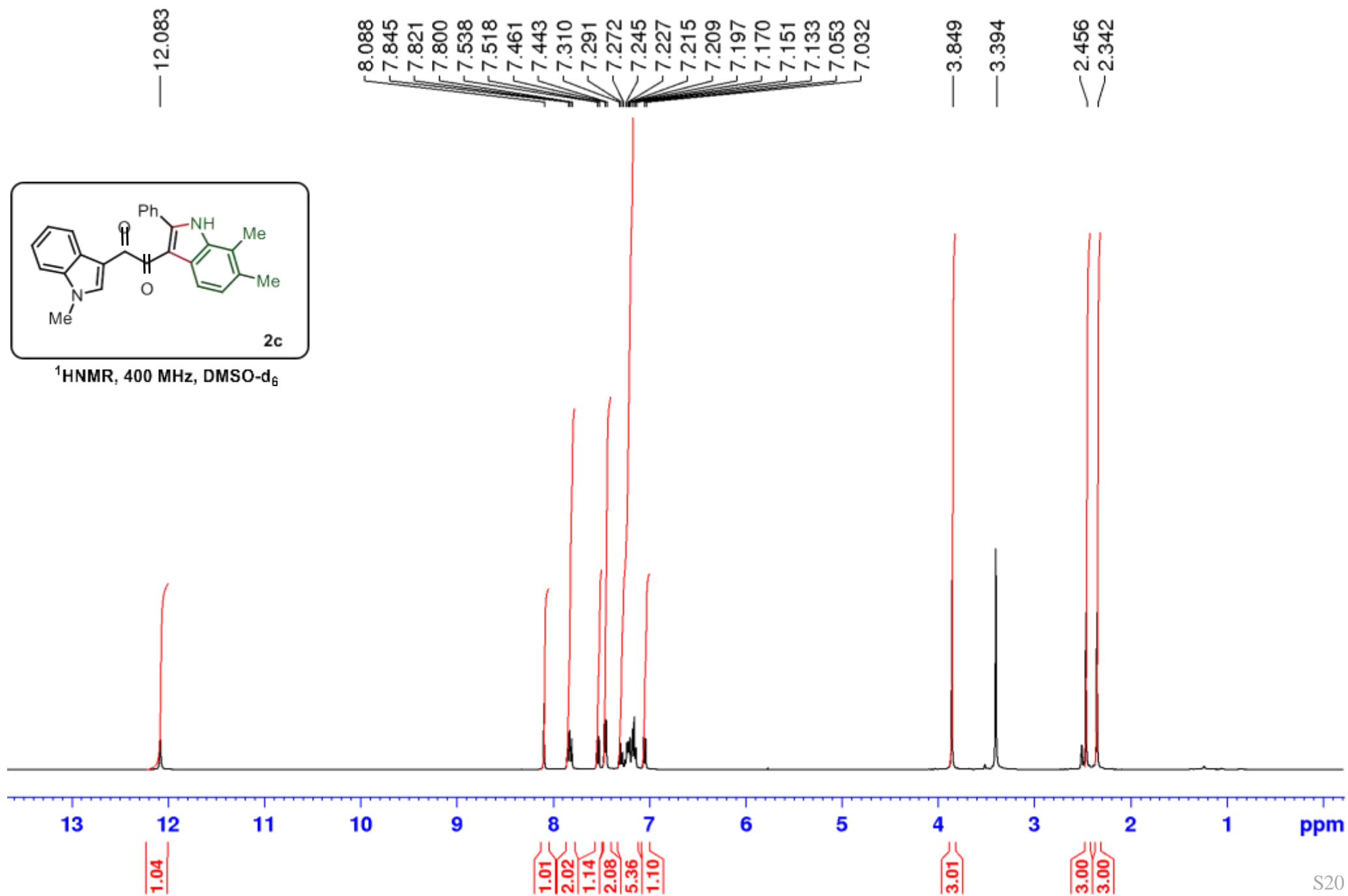


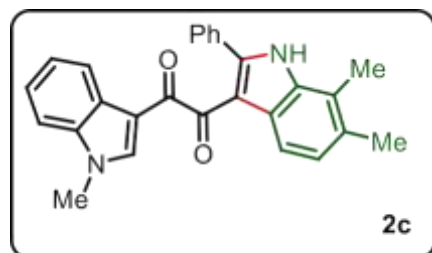
Minimum: -1.5
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
407.1757	407.1760	-0.3	-0.7	17.5	1016.5	n/a	n/a	C27 H23 N2 O2

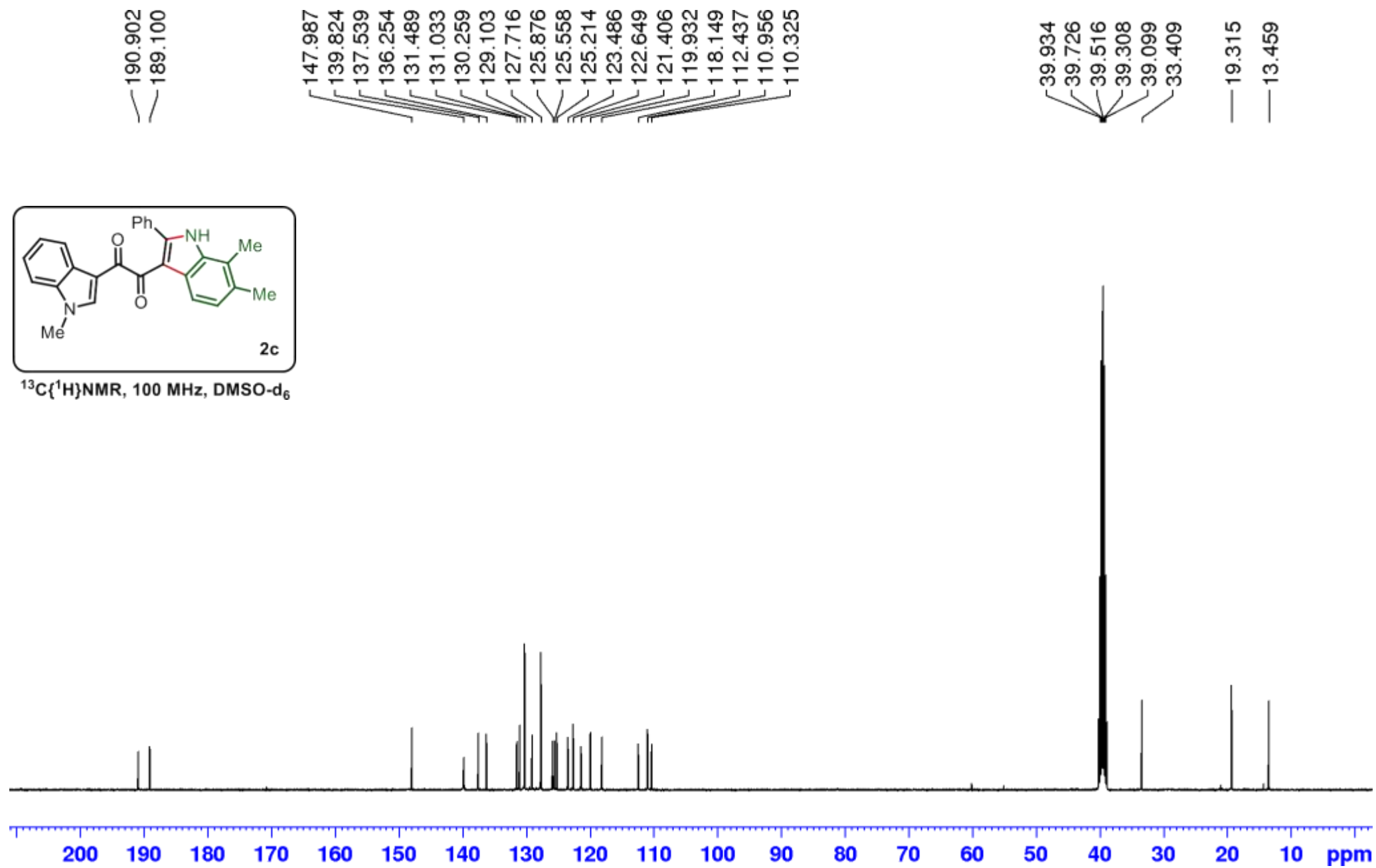


¹HNMR, 400 MHz, DMSO-d₆





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, DMSO- d_6



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

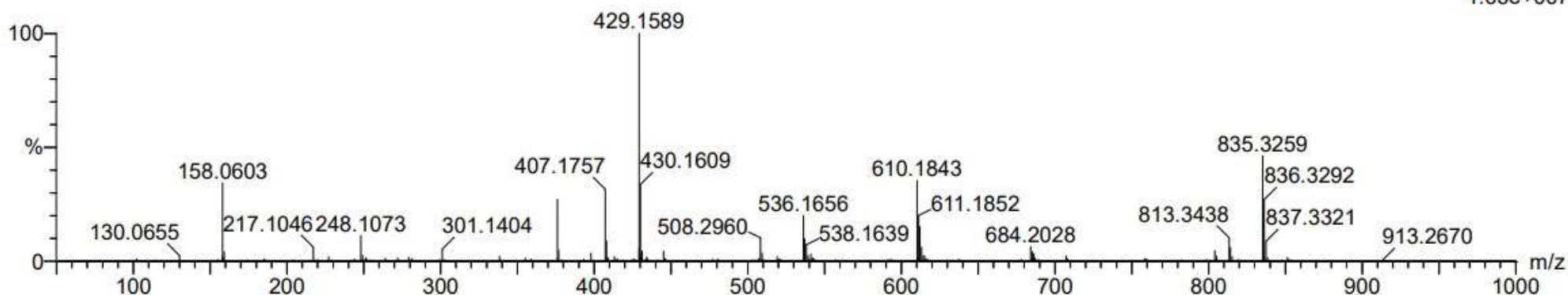
C: 0-27 H: 0-100 N: 0-2 O: 0-2

NVD 52

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

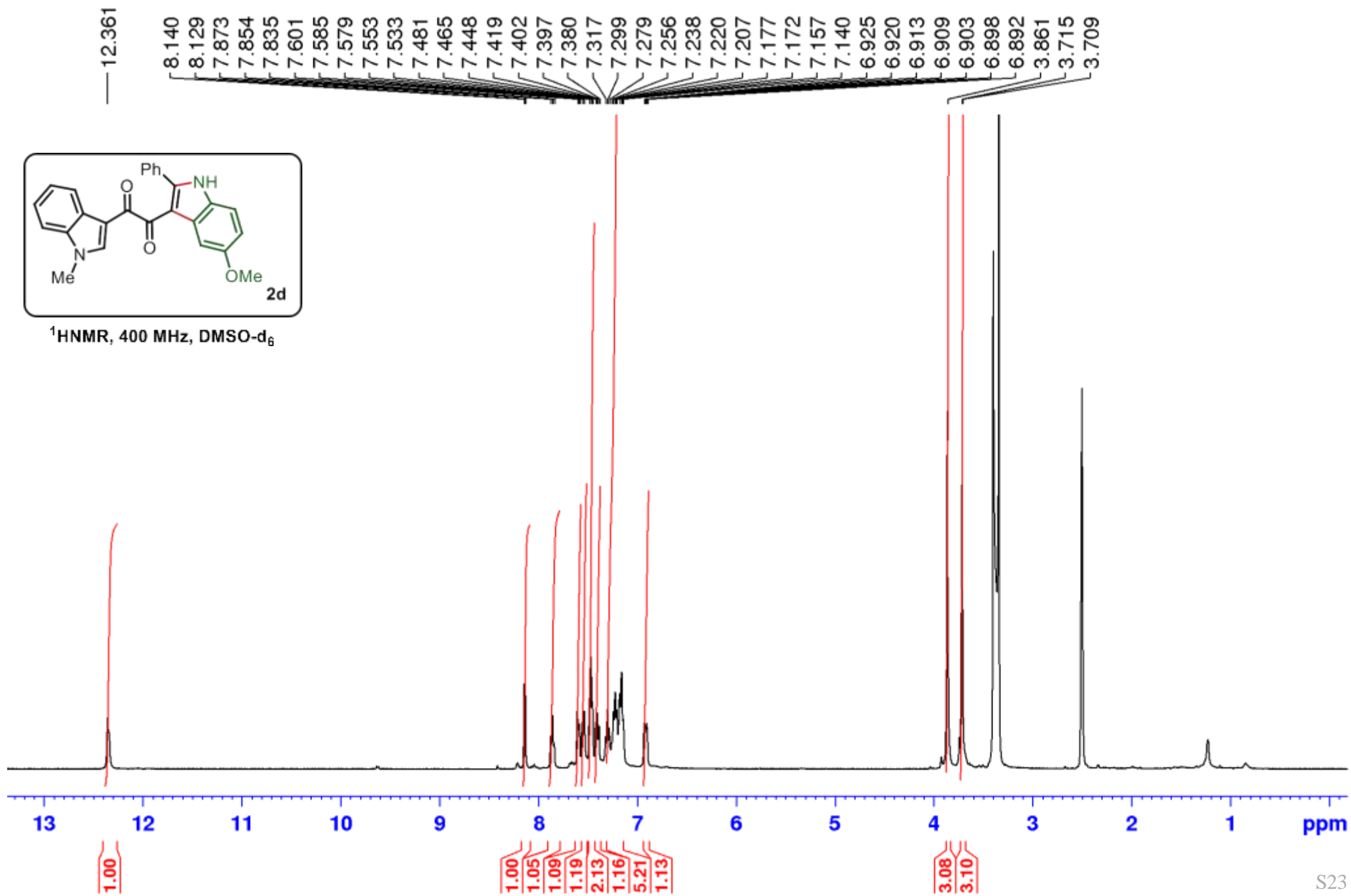
17-May-2023
11:52:01
1: TOF MS ES+
1.63e+007

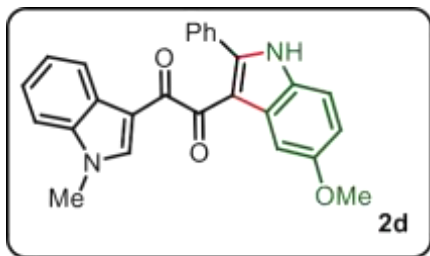
170523_06 6 (0.138)



Minimum: -1.5
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
407.1757	407.1760	-0.3	-0.7	17.5	982.5	n/a	n/a	C27 H23 N2 O2





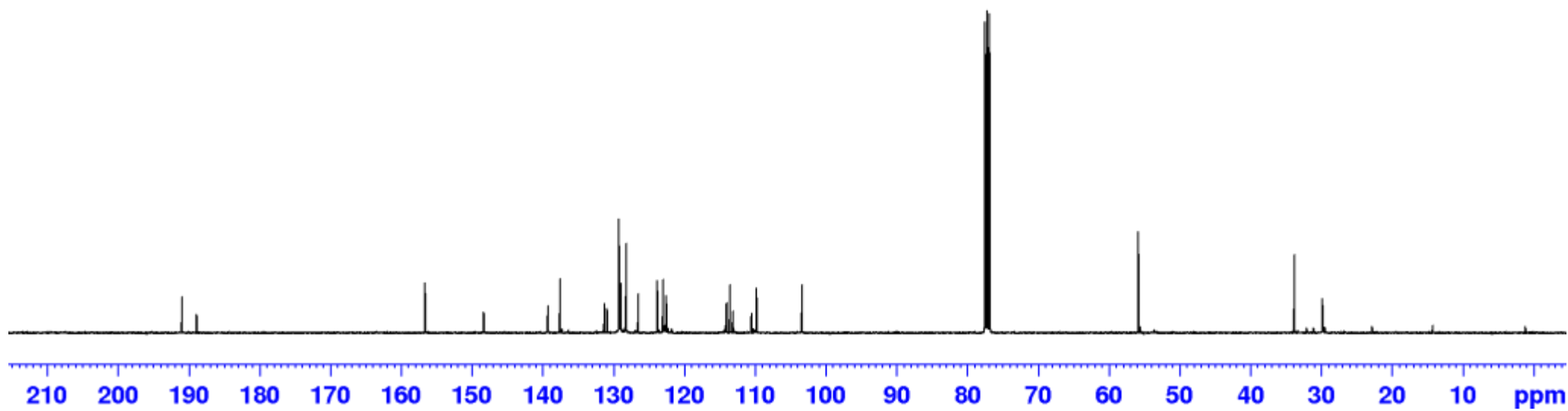
$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3

190.975
188.934

156.621
148.337
139.261
137.575
131.265
130.927
129.232
129.089
128.958
128.217
126.500
123.798
122.988
122.546
113.997
113.549
113.138
110.494
109.792
103.366

55.821

33.788



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

21 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

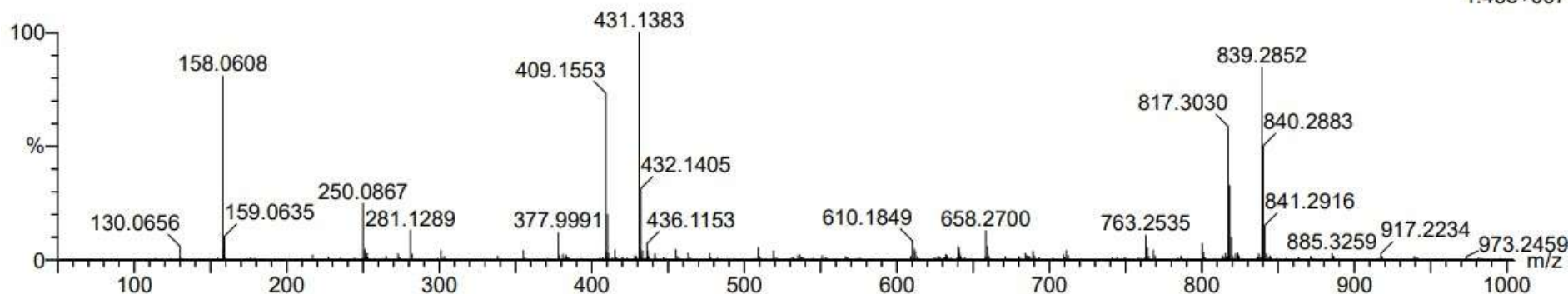
C: 0-26 H: 0-100 N: 0-2 O: 0-3

NVD 51

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

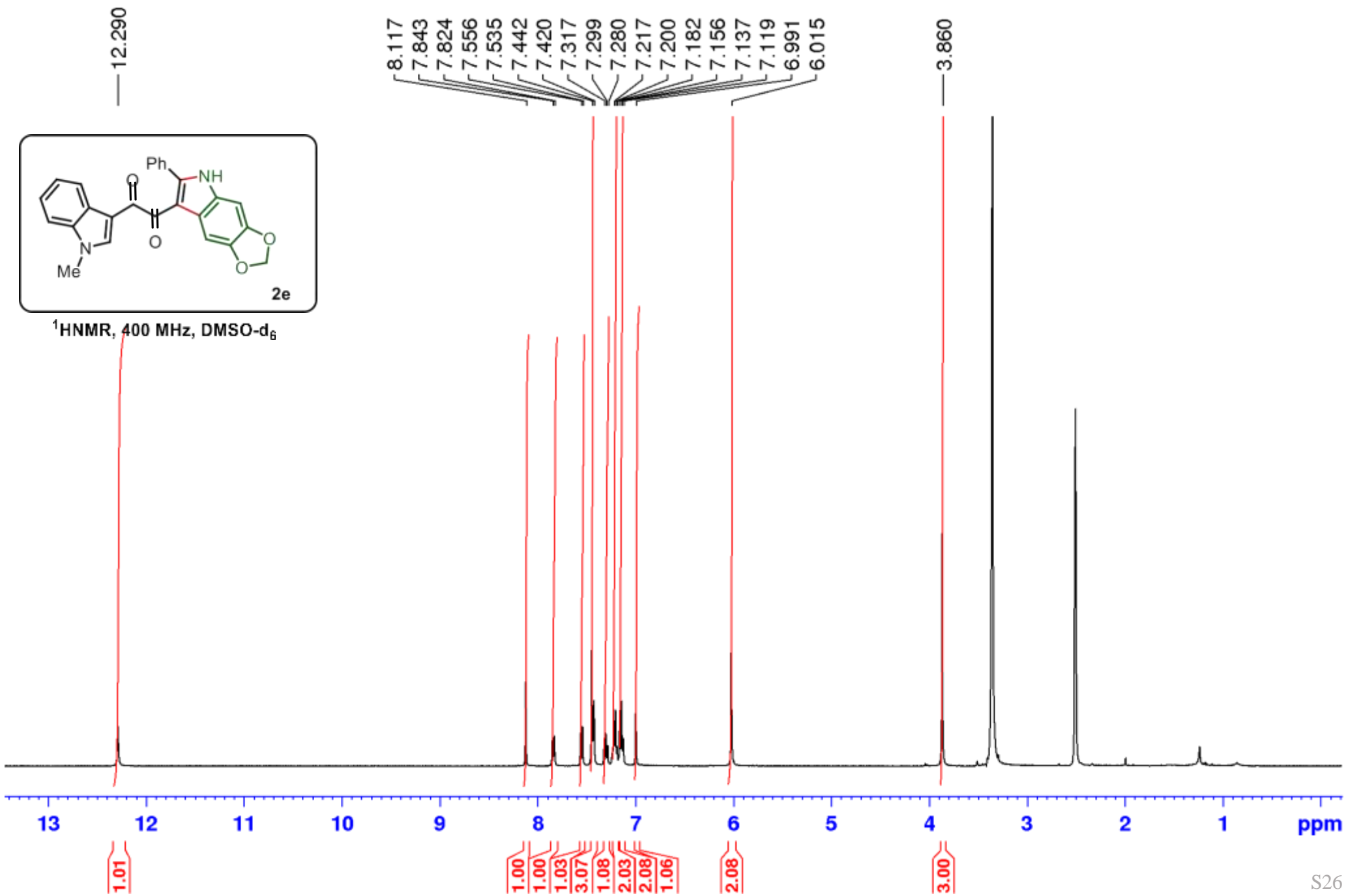
17-May-2023
11:41:45
1: TOF MS ES+
1.43e+007

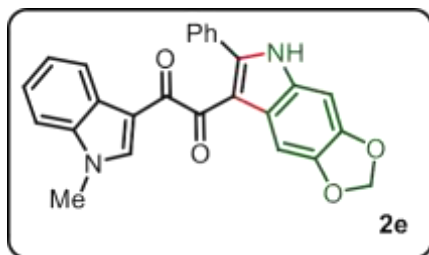
170523_02 5 (0.121)



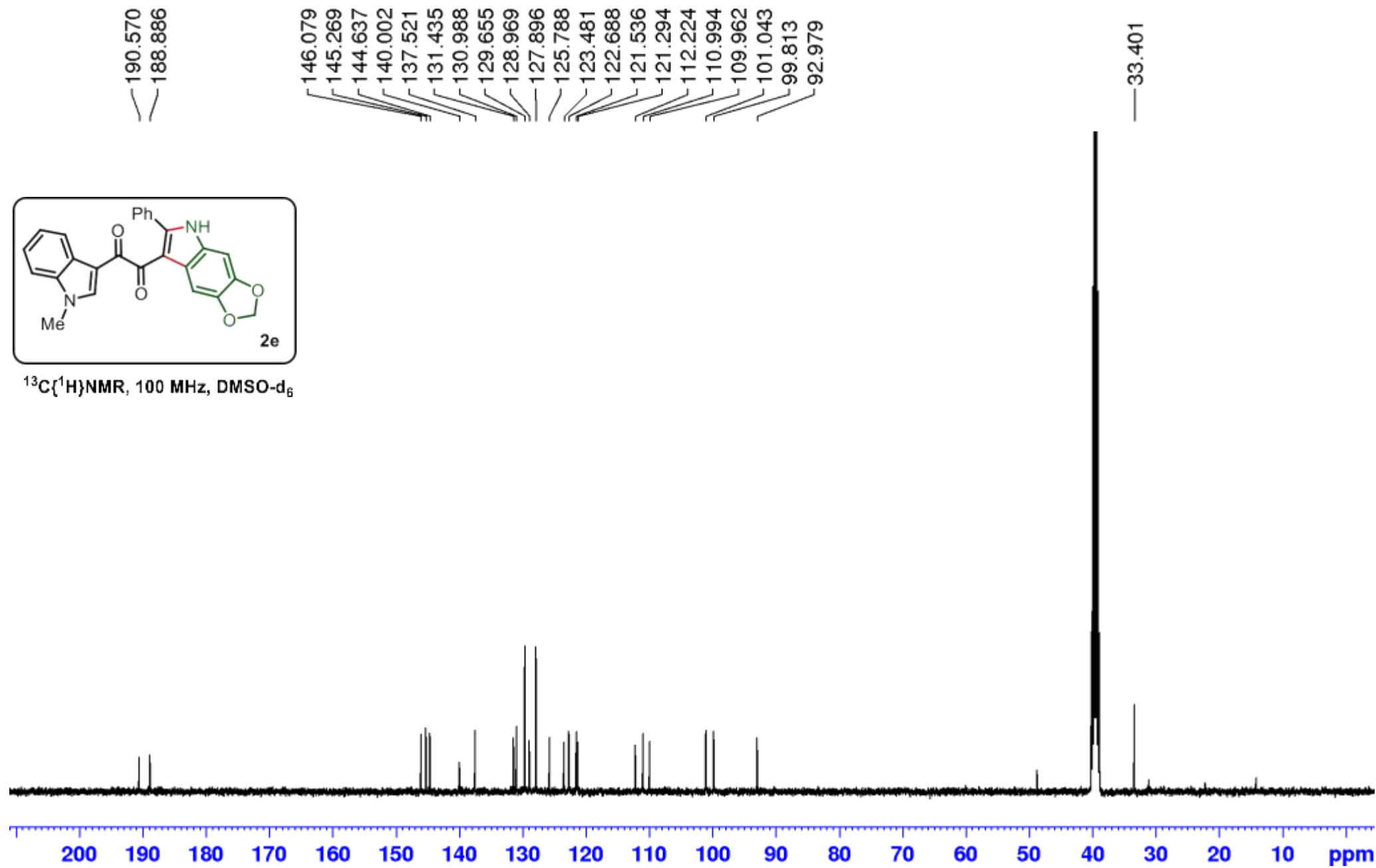
Minimum: -1.5
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
409.1553	409.1552	0.1	0.2	17.5	1021.9	n/a	n/a	C26 H21 N2 O3





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, DMSO- d_6



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-26 H: 0-100 N: 0-2 O: 0-4

NVD 46

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

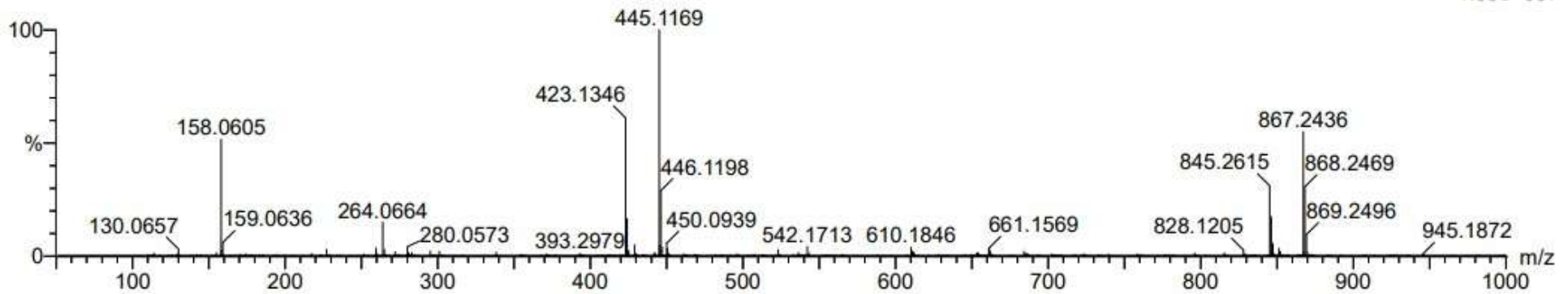
17-May-2023

11:49:28

1: TOF MS ES+

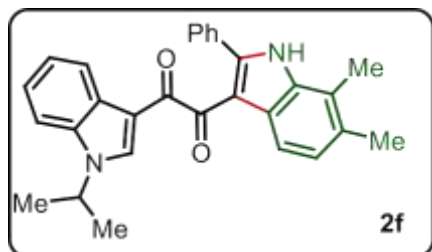
1.09e+007

170523_05 5 (0.121)

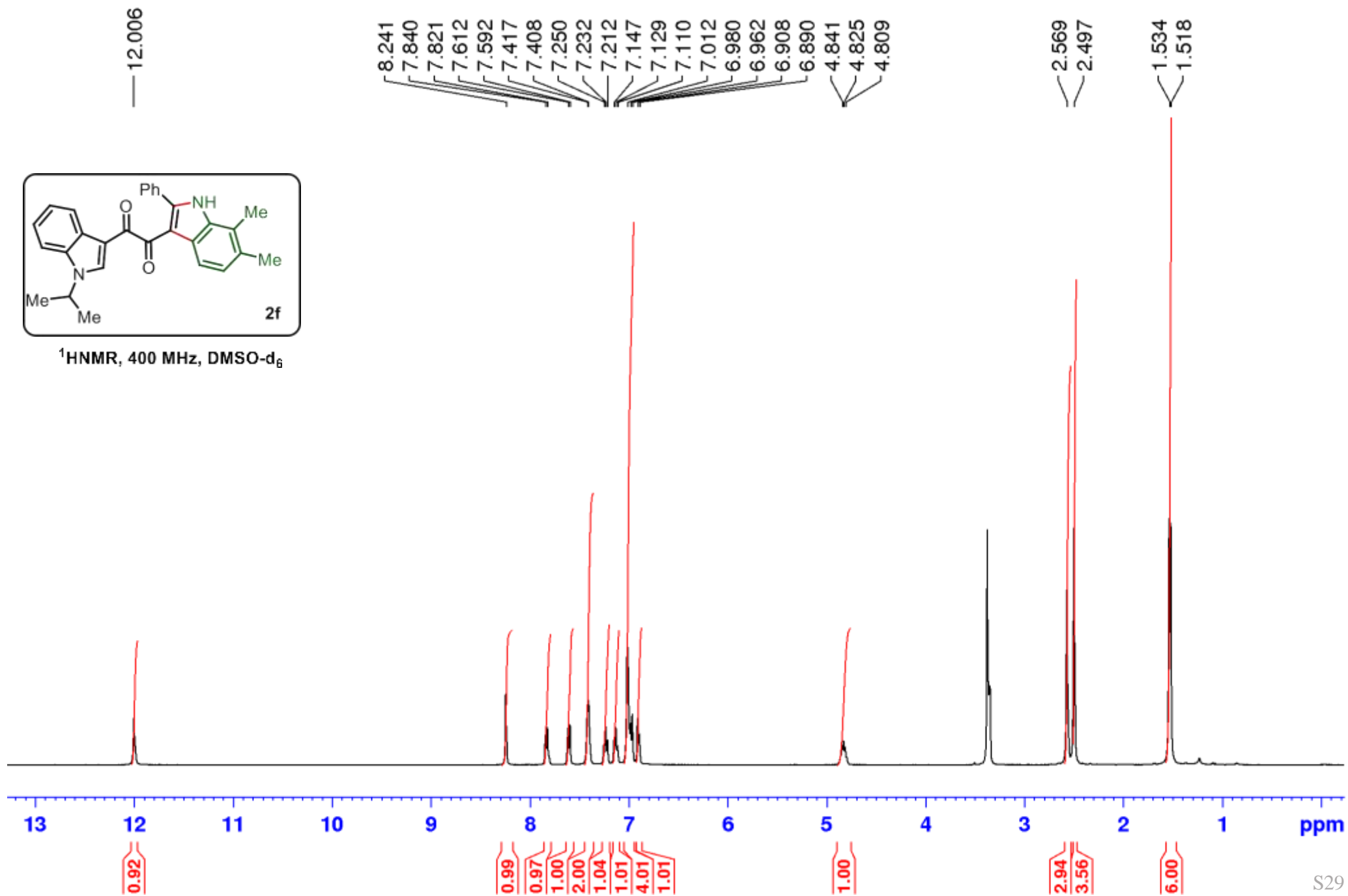


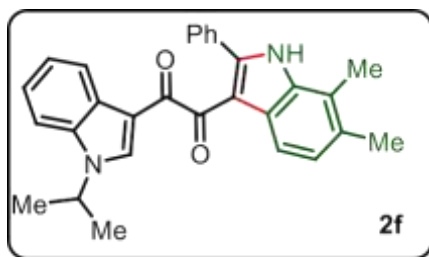
Minimum: -1.5
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
423.1346	423.1345	0.1	0.2	18.5	933.2	n/a	n/a	C26 H19 N2 O4



¹HNMR, 400 MHz, DMSO-d₆





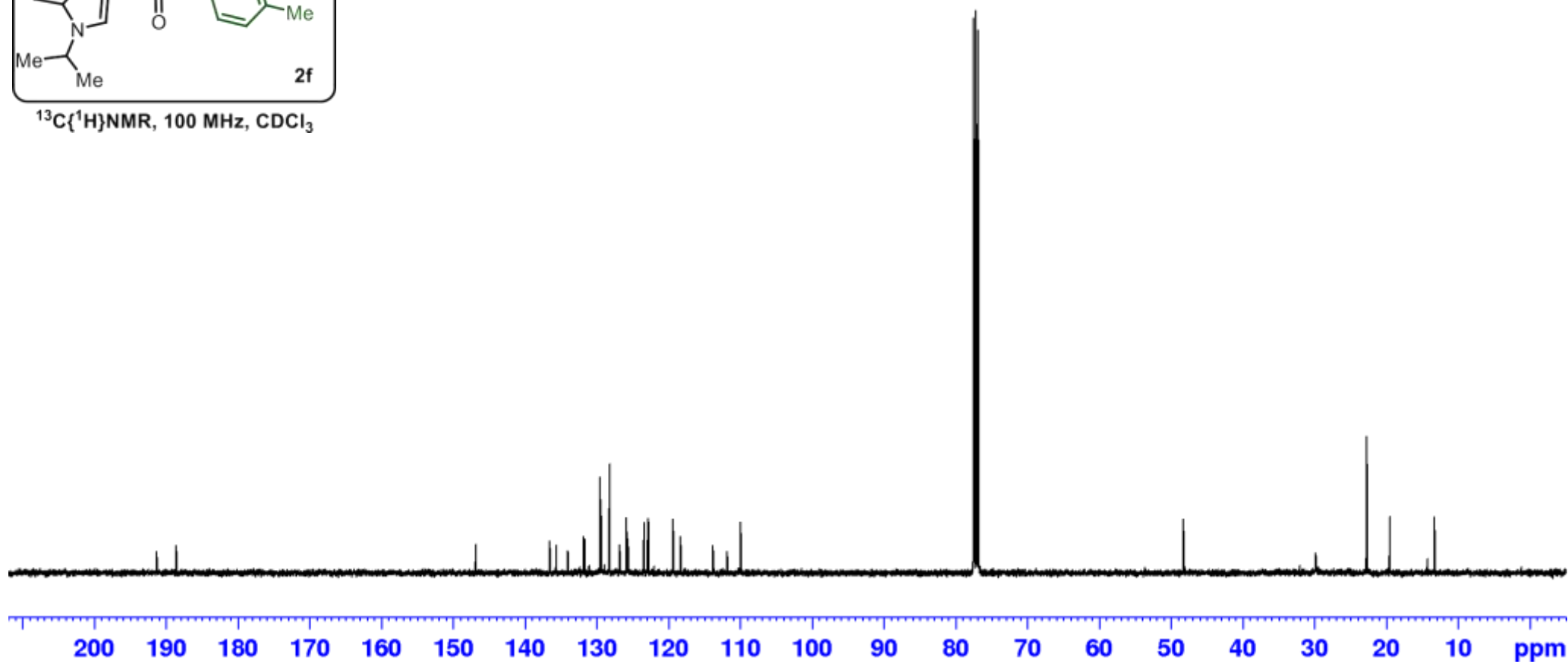
$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3

191.355
188.600

146.878
136.558
135.645
134.013
131.835
131.689
129.533
129.364
128.240
126.817
125.868
125.664
123.420
122.933
122.805
119.374
118.335
113.802
111.841
109.949

48.247

22.679
19.470
13.281



Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-29 H: 0-100 N: 0-2 O: 0-2

NVD-100

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

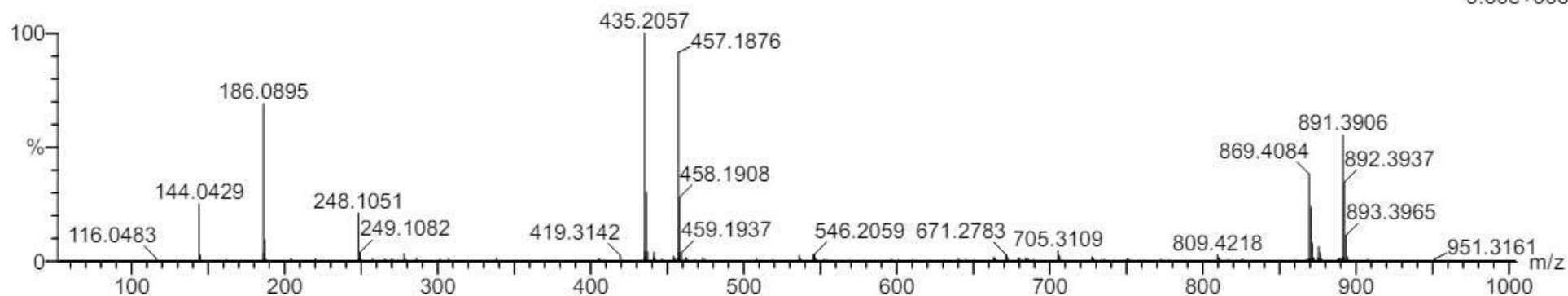
03-May-2024

14:04:06

1: TOF MS ES+

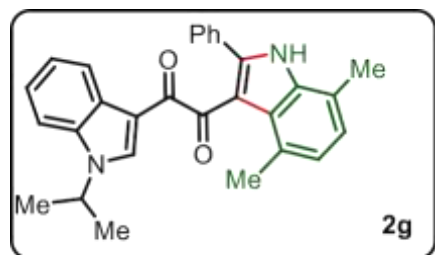
9.60e+006

030524_12 5 (0.121)

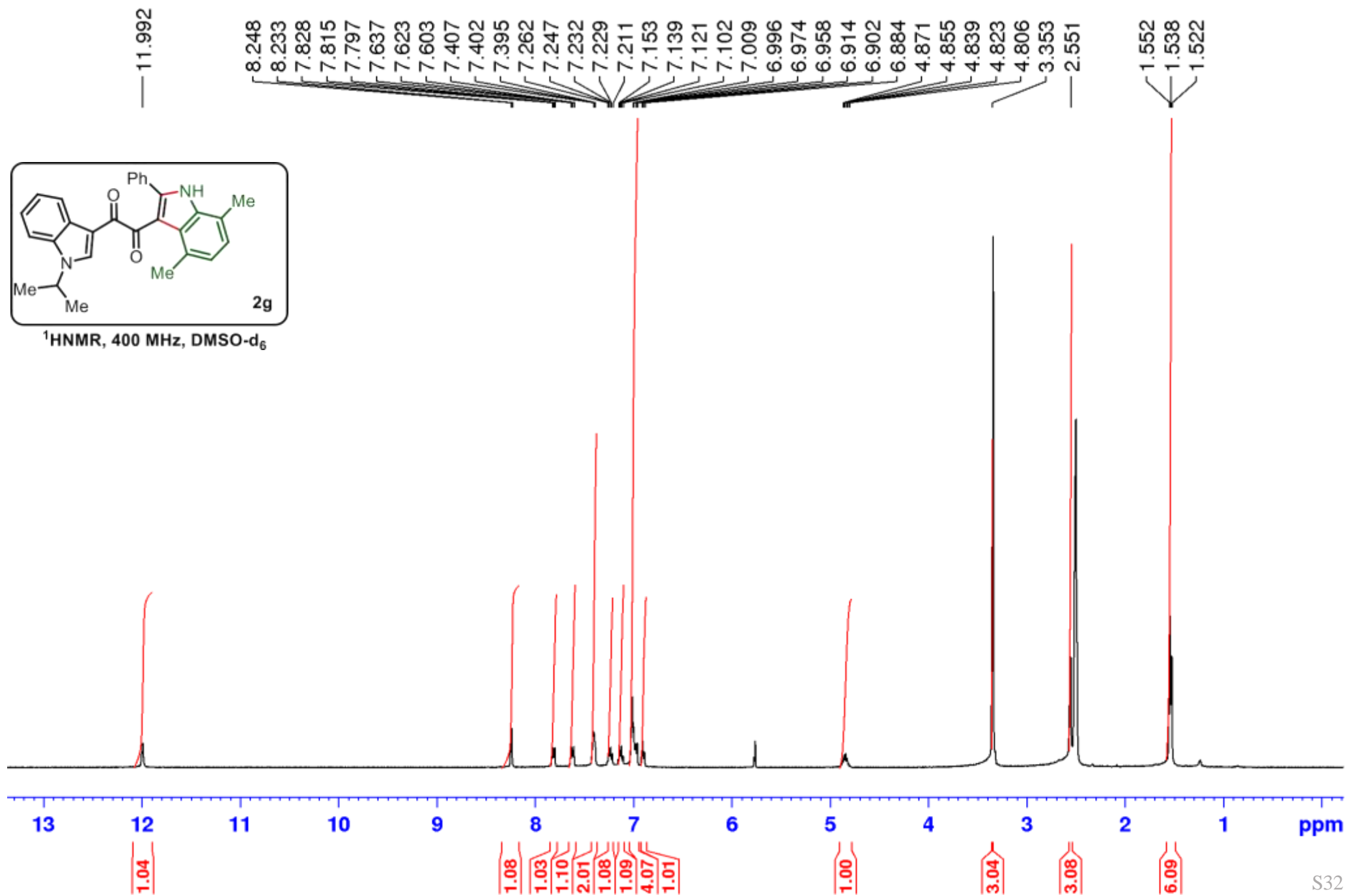


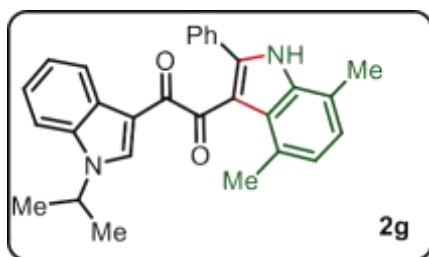
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
435.2057	435.2073	-1.6	-3.7	17.5	1029.8	n/a	n/a	C29 H27 N2 O2

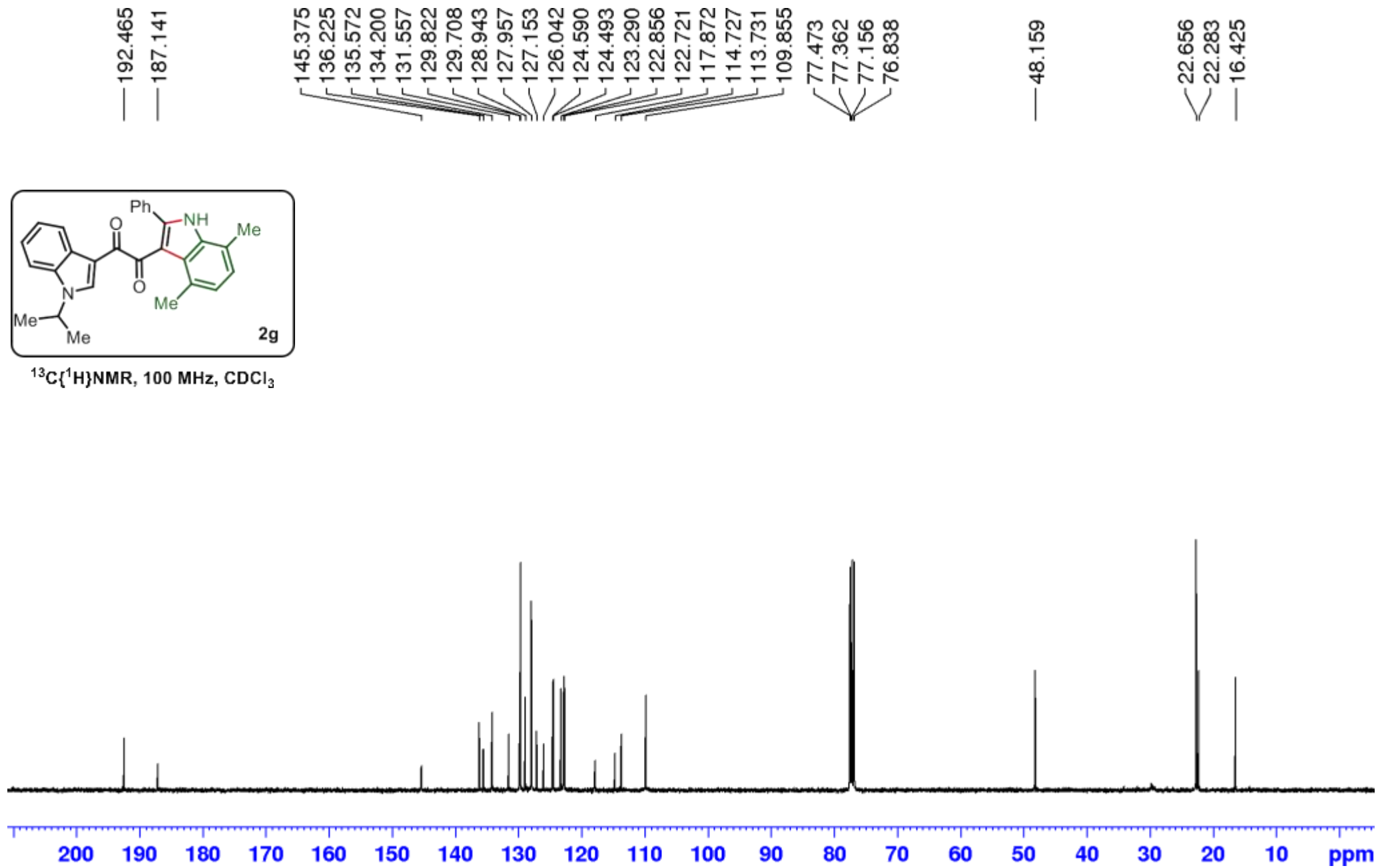


¹H NMR, 400 MHz, DMSO-d₆





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3



Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

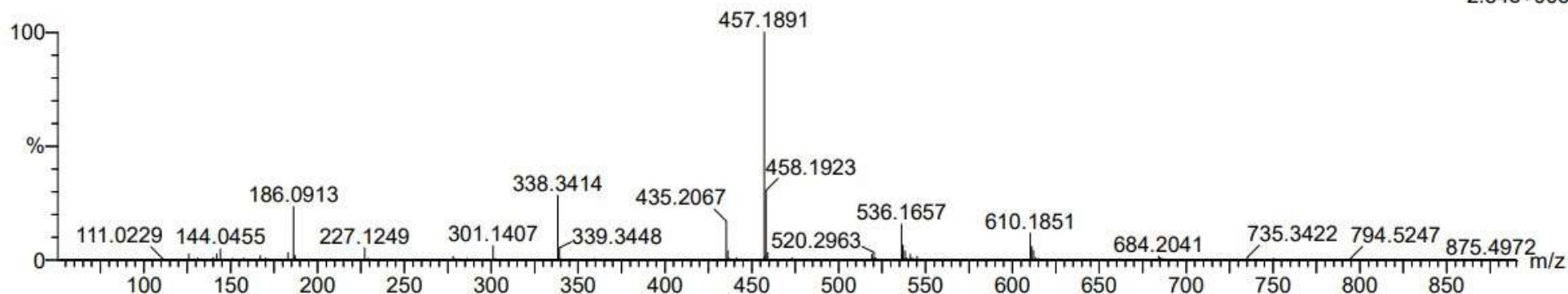
C: 0-29 H: 0-100 N: 0-2 O: 0-2

NVD-92

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

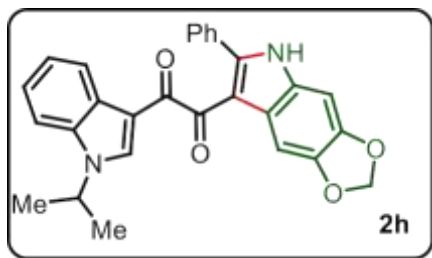
06-Oct-2023
13:59:10
1: TOF MS ES+
2.54e+006

061023_13 5 (0.121)

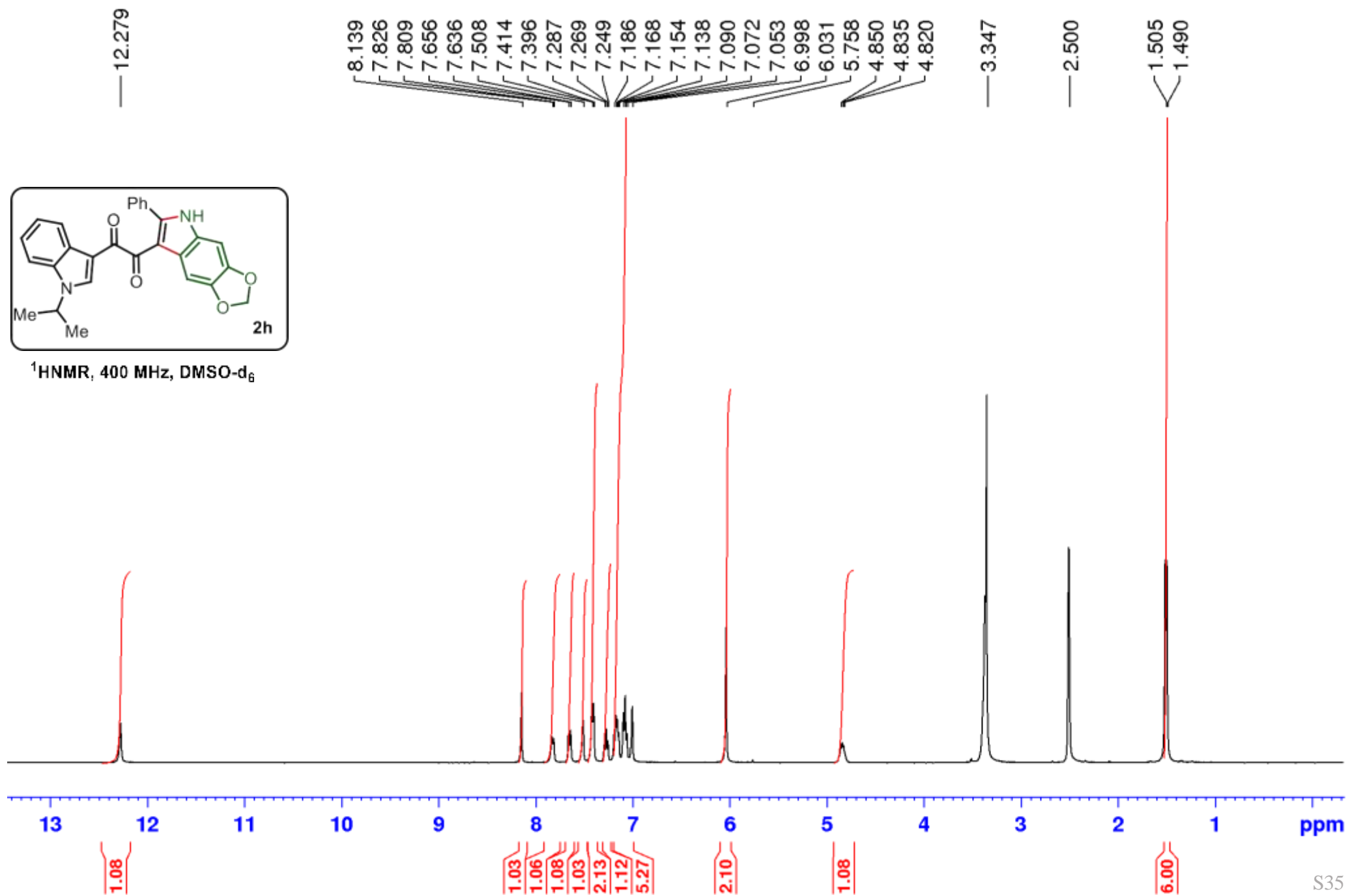


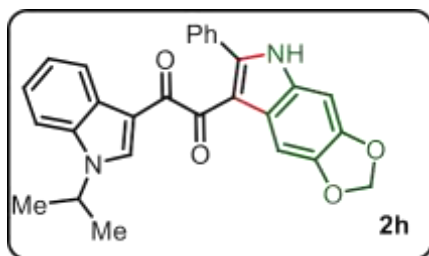
Minimum: -1.5
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
435.2067	435.2073	-0.6	-1.4	17.5	776.1	n/a	n/a	C29 H27 N2 O2

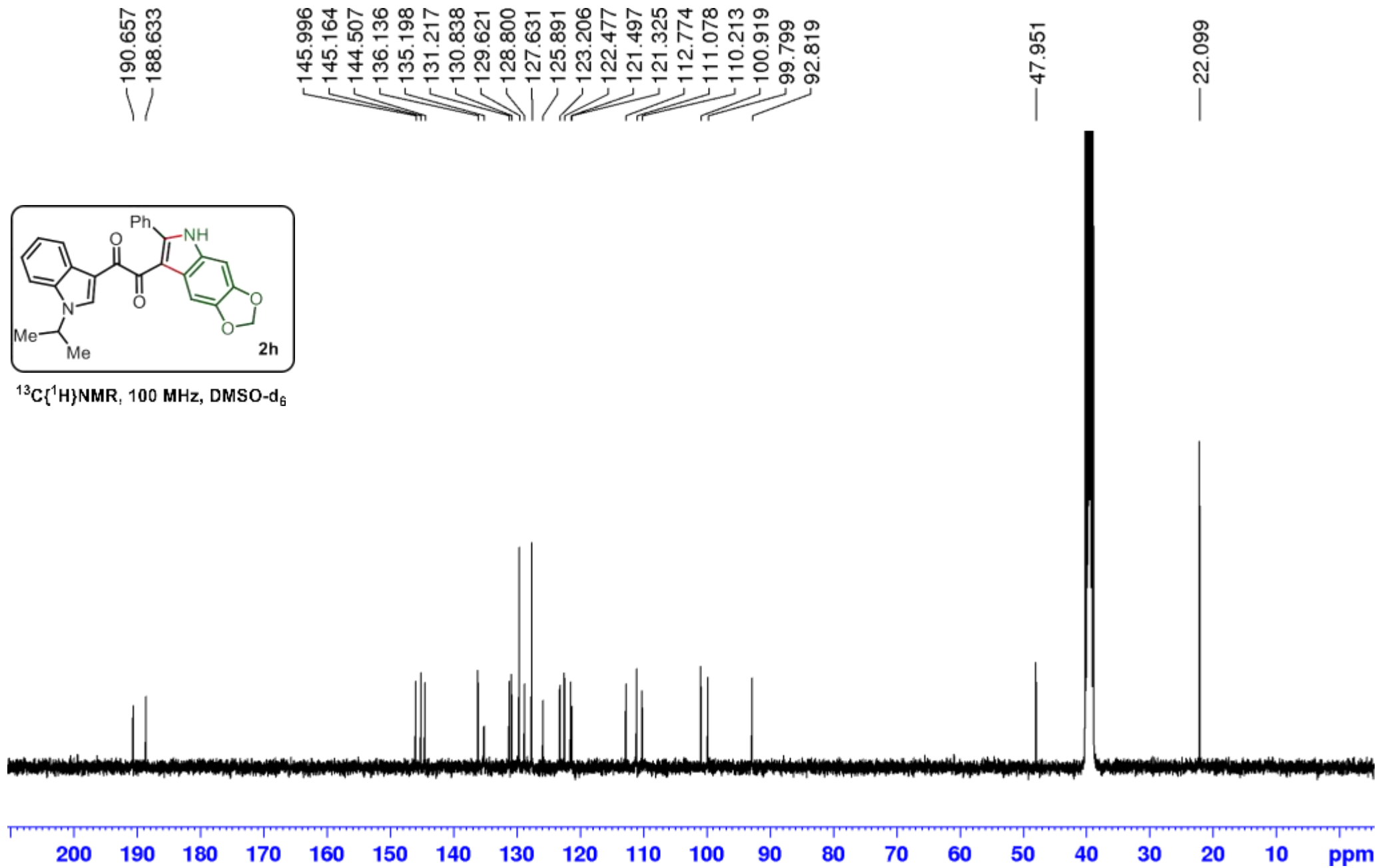


$^1\text{H NMR}$, 400 MHz, DMSO-d_6





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, DMSO-d_6



Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-28 H: 0-100 N: 0-2 O: 0-4

NVD-91

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

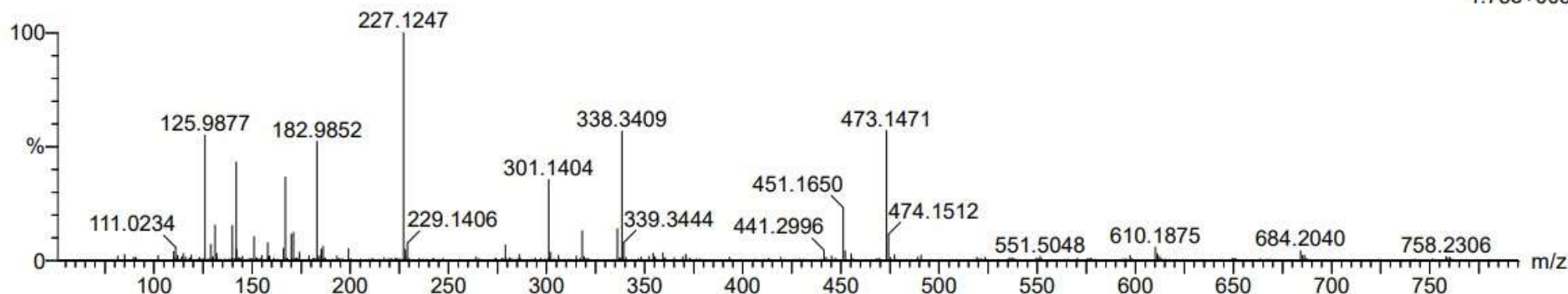
06-Oct-2023

13:51:19

1: TOF MS ES+

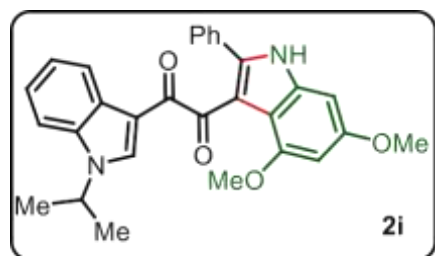
1.75e+005

061023_10 4 (0.104)

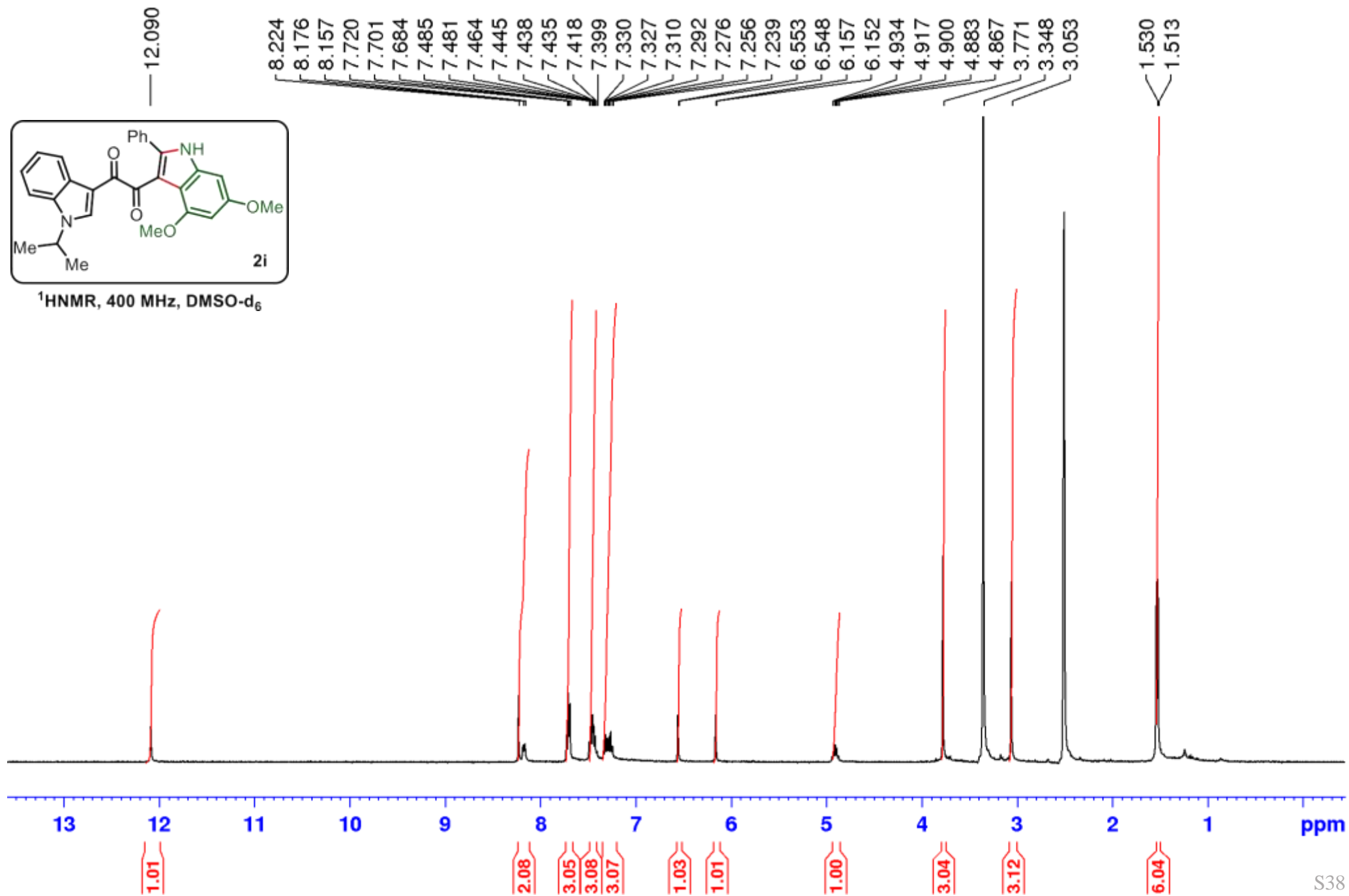


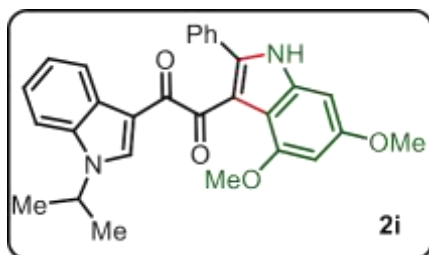
Minimum: -1.5
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
451.1650	451.1658	-0.8	-1.8	18.5	560.1	n/a	n/a	C28 H23 N2 O4

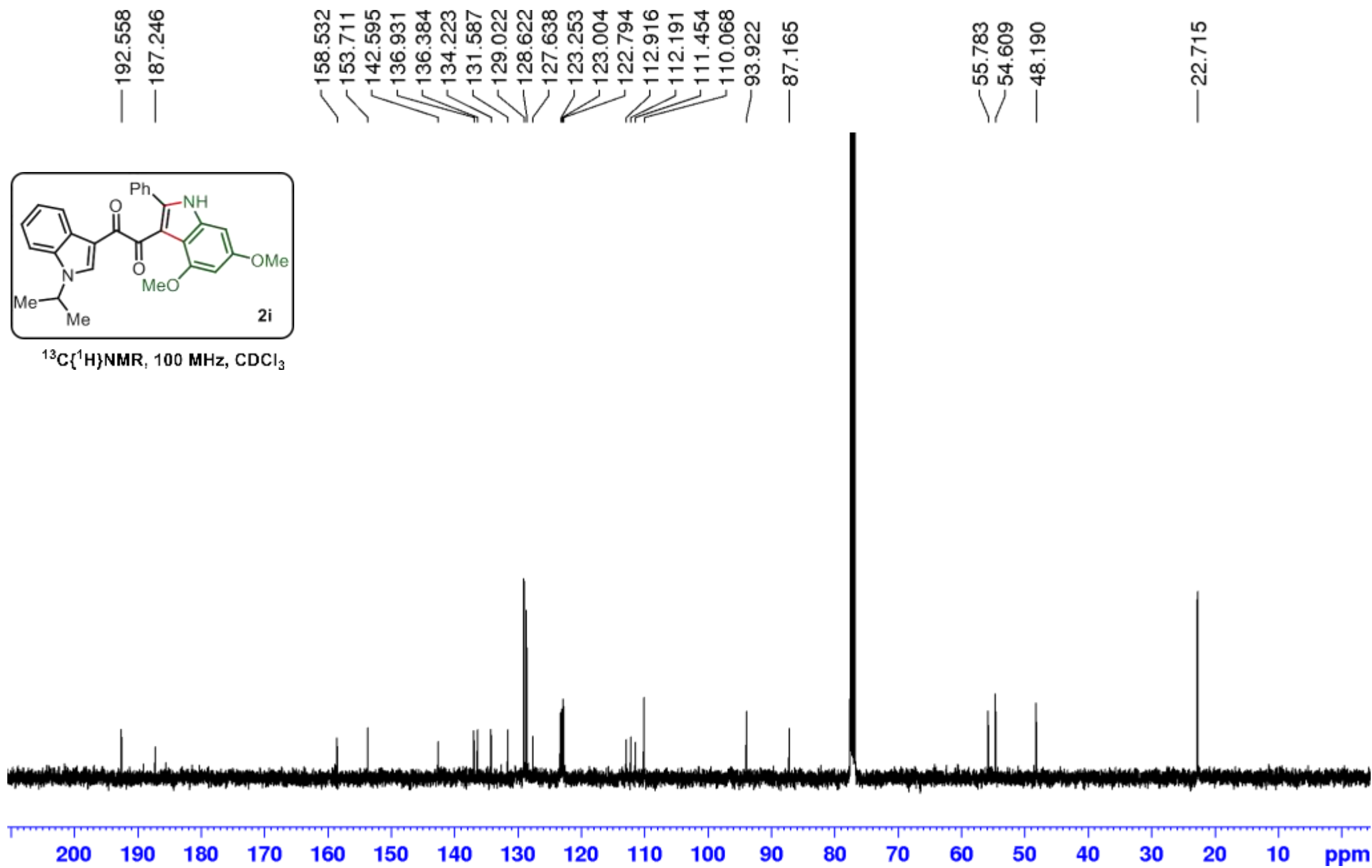


¹HNMR, 400 MHz, DMSO-d₆





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

24 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

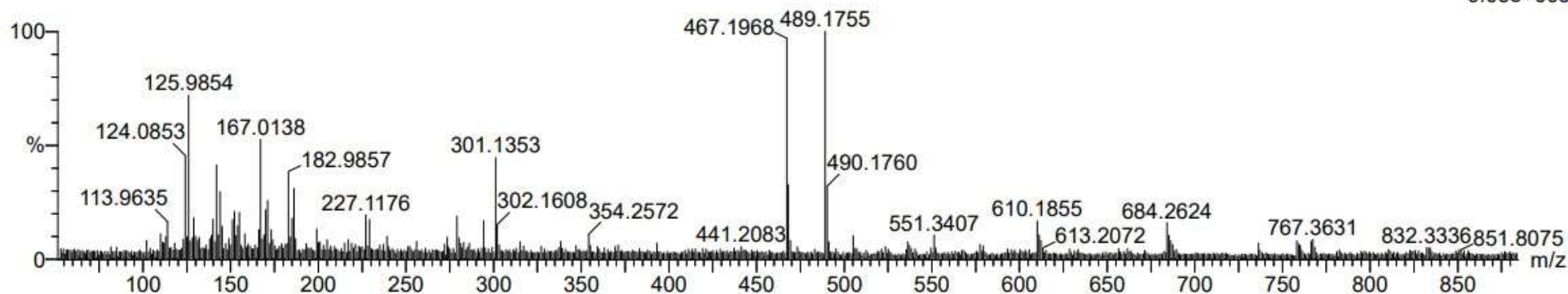
C: 0-29 H: 0-100 N: 0-2 O: 0-4

NVD-67

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

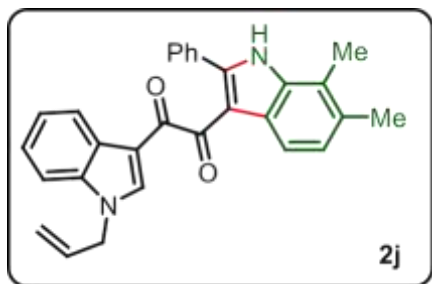
04-Mar-2024
13:41:47
1: TOF MS ES+
9.05e+005

040324_12 8 (0.172) Cm (8)

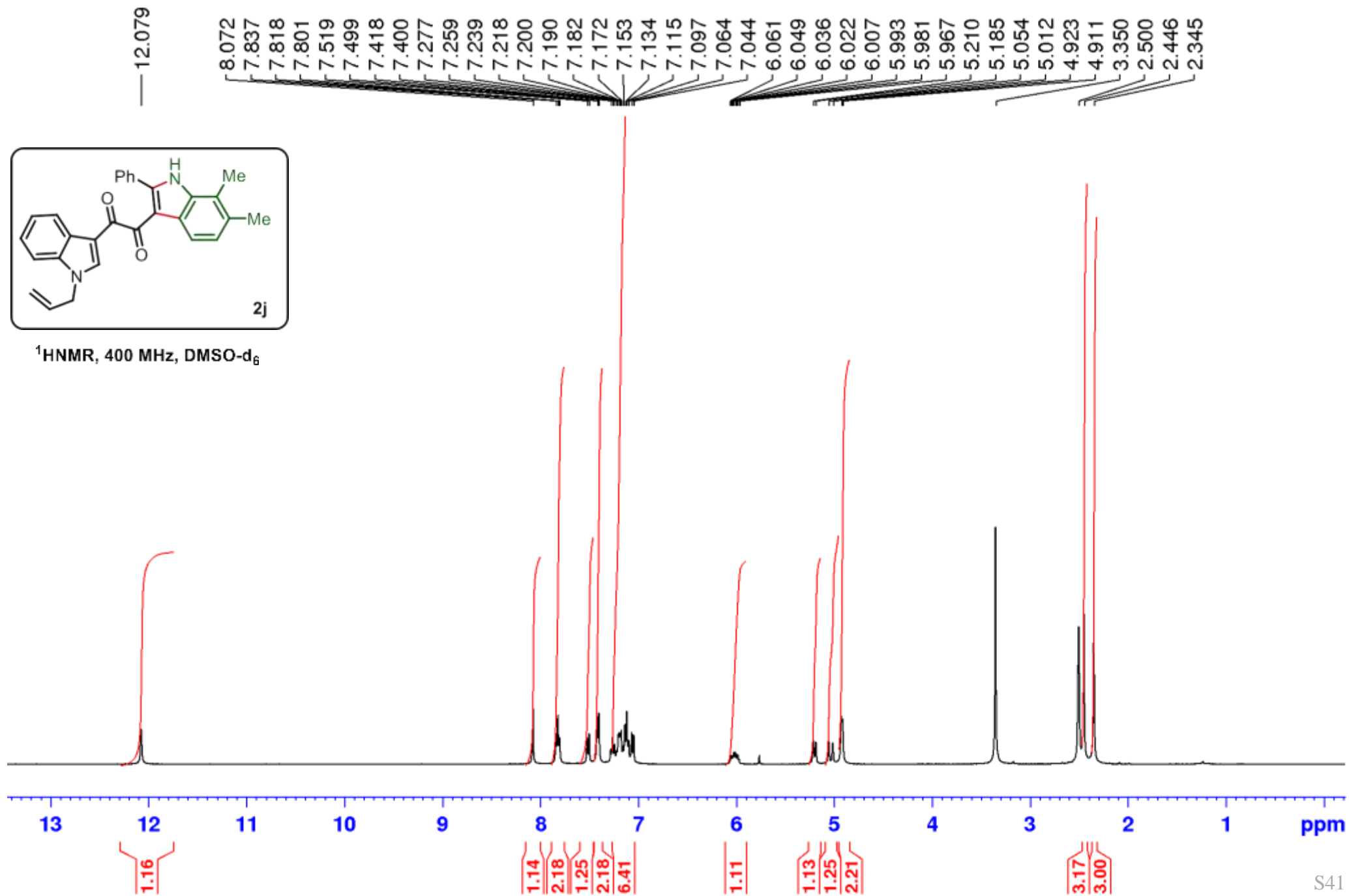


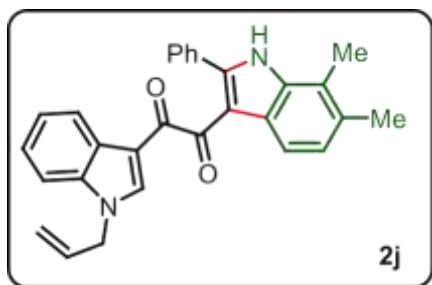
Minimum: -1.5
Maximum: 2.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
467.1968	467.1971	-0.3	-0.6	17.5	31.9	n/a	n/a	C29 H27 N2 O4

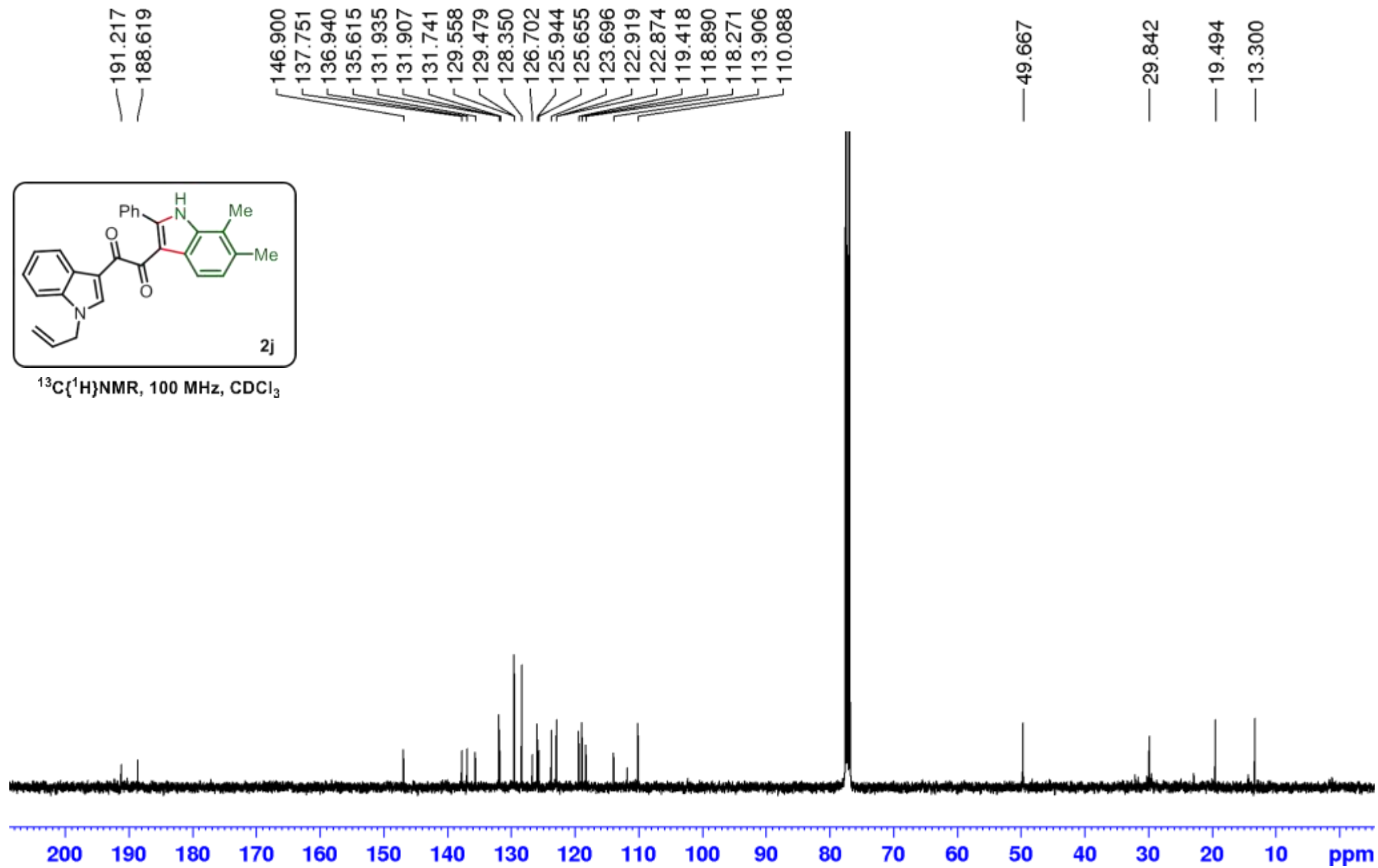


$^1\text{H NMR}$, 400 MHz, DMSO-d_6





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3



Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-29 H: 0-100 N: 0-2 O: 0-2

NVD-99

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

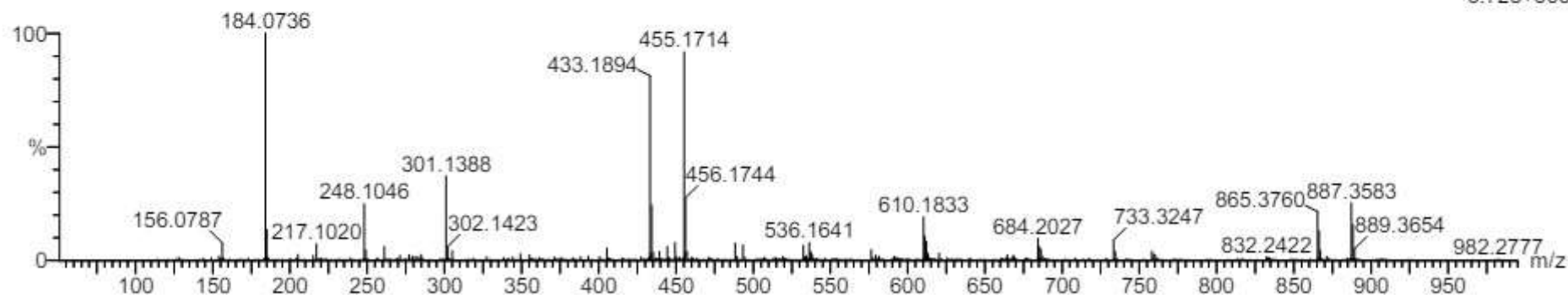
03-May-2024

14:07:23

1: TOF MS ES+

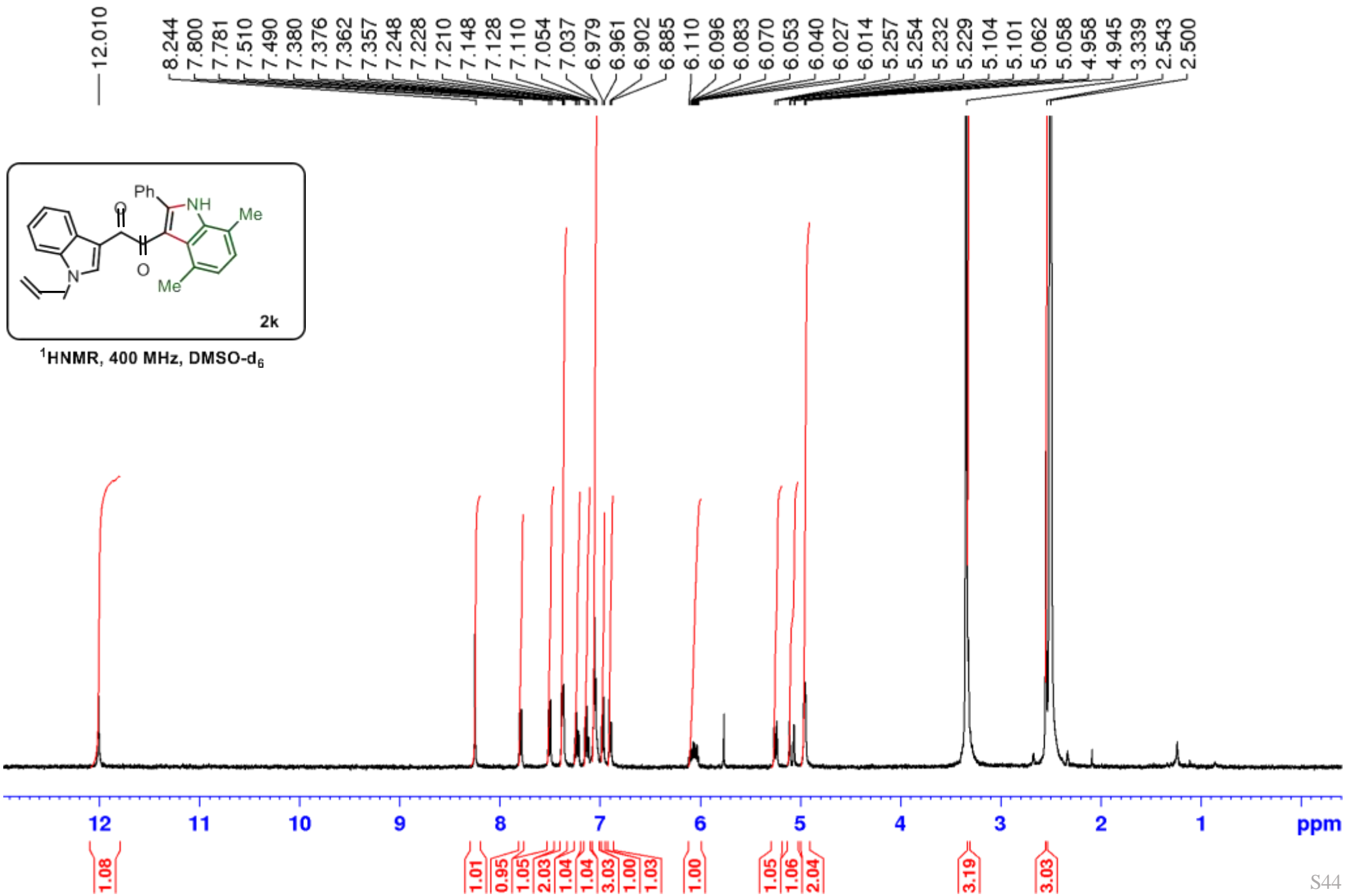
6.72e+006

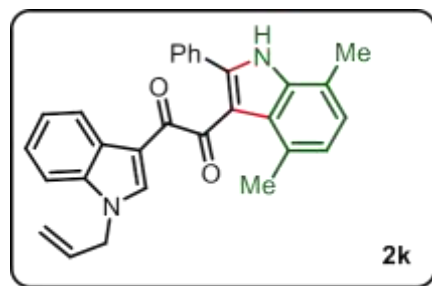
030524_13 5 (0.121)



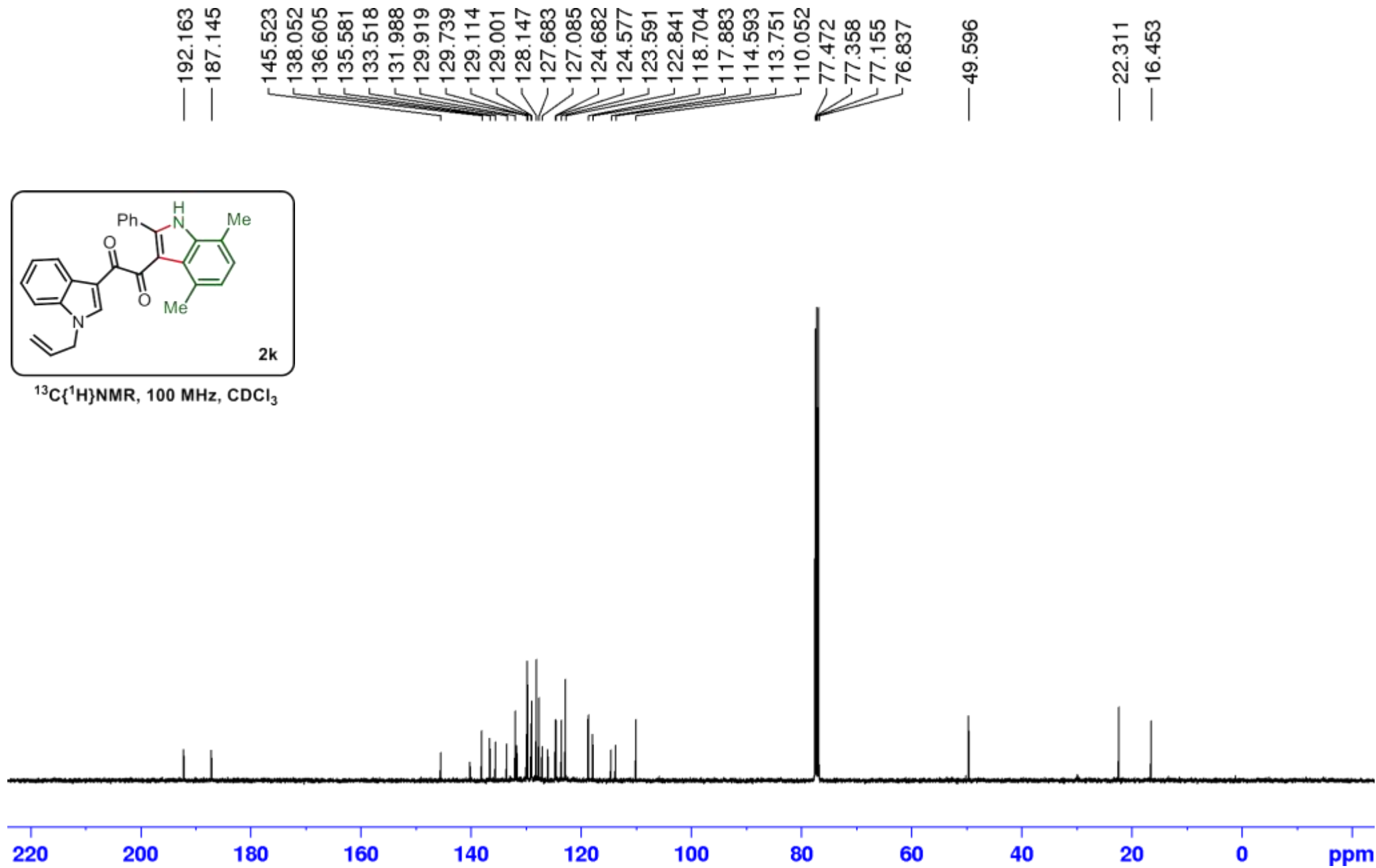
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
433.1894	433.1916	-2.2	-5.1	18.5	1064.0	n/a	n/a	C29 H25 N2 O2





$^{13}\text{C}\{^1\text{H}\}\text{NMR}$, 100 MHz, CDCl_3



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-29 H: 0-100 N: 0-2 O: 0-2

NVD-89

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

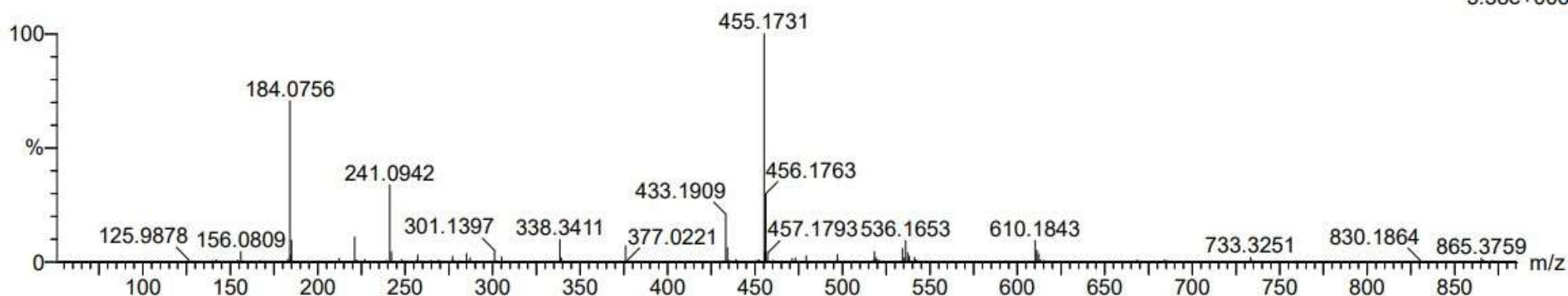
06-Oct-2023

13:56:35

1: TOF MS ES+

5.58e+006

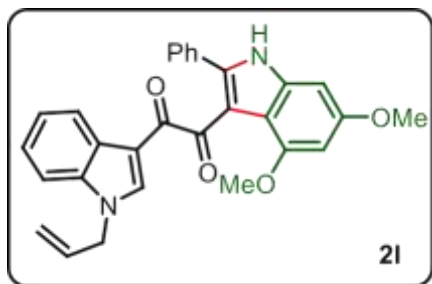
061023_12 5 (0.121)



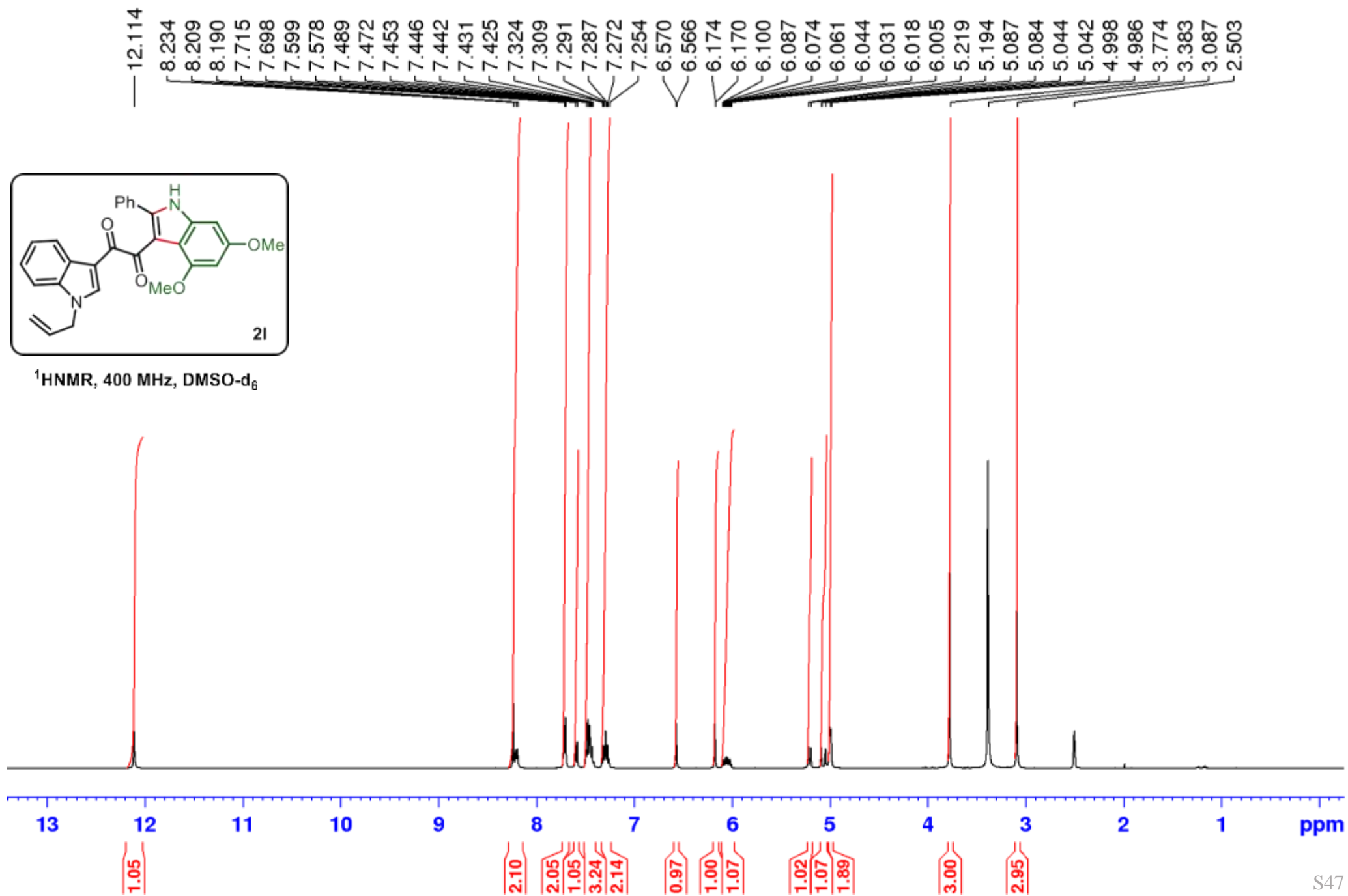
Minimum: -1.5

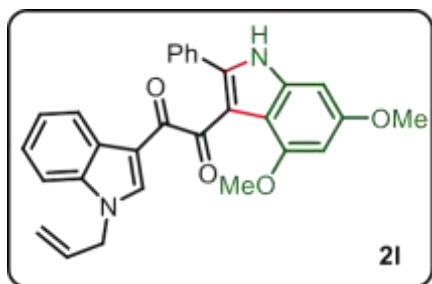
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
433.1909	433.1916	-0.7	-1.6	18.5	777.3	n/a	n/a	C29 H25 N2 O2

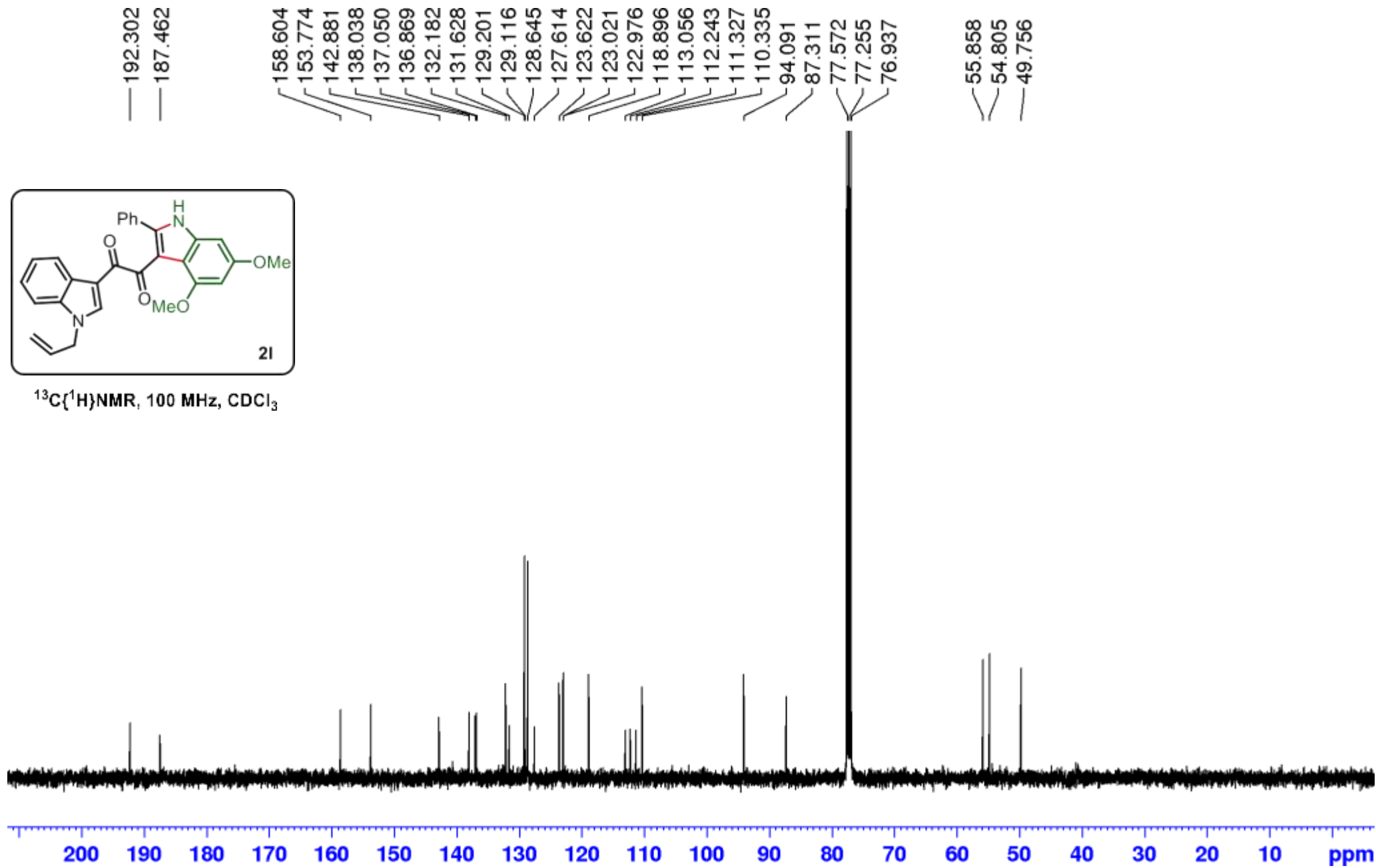


$^1\text{H NMR}$, 400 MHz, DMSO-d_6





$^{13}\text{C}\{^1\text{H}\}\text{NMR}$, 100 MHz, CDCl_3



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-29 H: 0-100 N: 0-2 O: 0-4

NVD-65

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

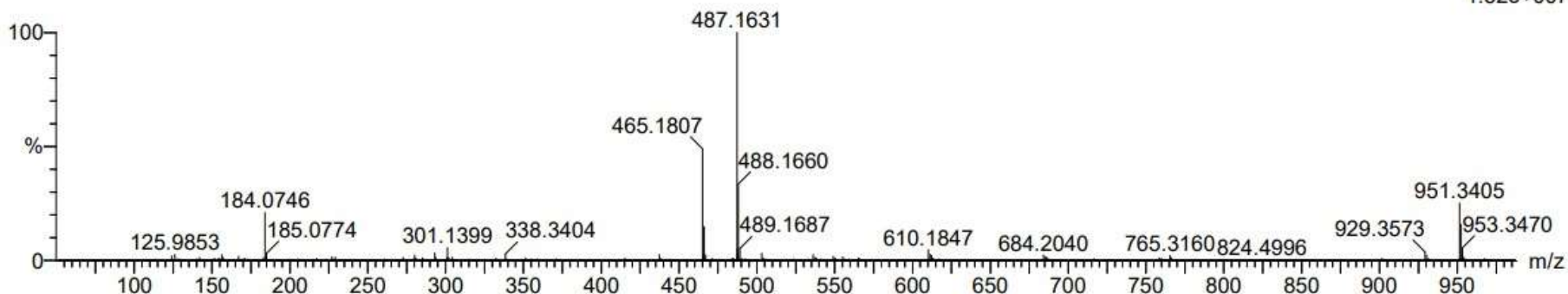
04-Mar-2024

13:28:40

1: TOF MS ES+

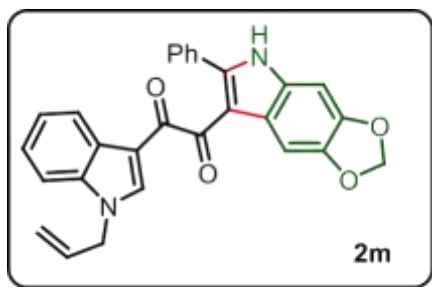
1.52e+007

040324_07 6 (0.138)

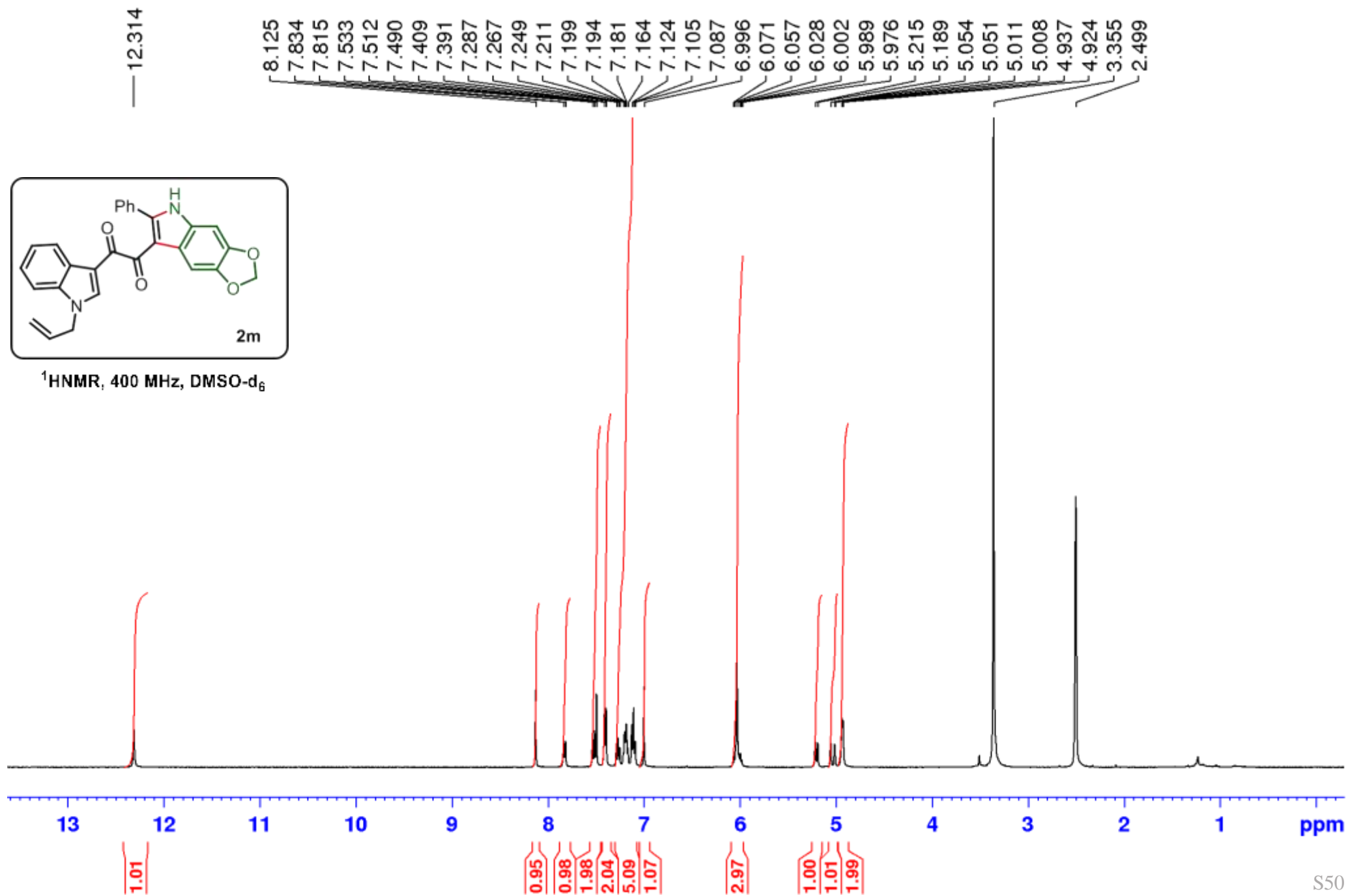


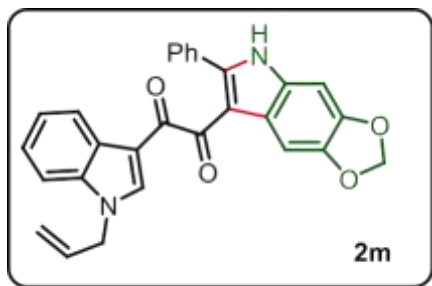
Minimum: -1.5
Maximum: 2.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
465.1807	465.1814	-0.7	-1.5	18.5	941.4	n/a	n/a	C29 H25 N2 O4

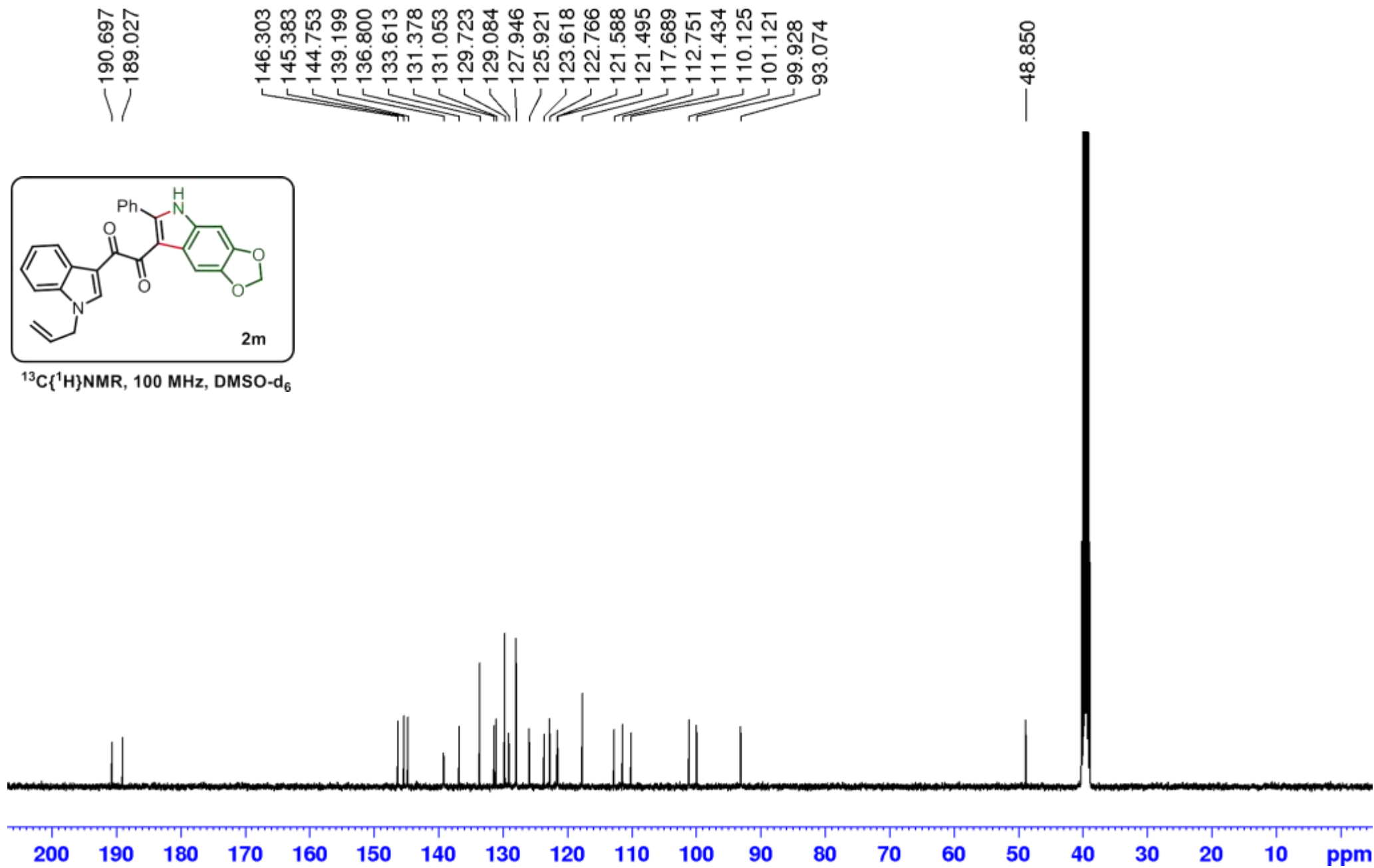


¹H NMR, 400 MHz, DMSO-d₆





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, DMSO-d_6



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-28 H: 0-100 N: 0-2 O: 0-4

NVD-88

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

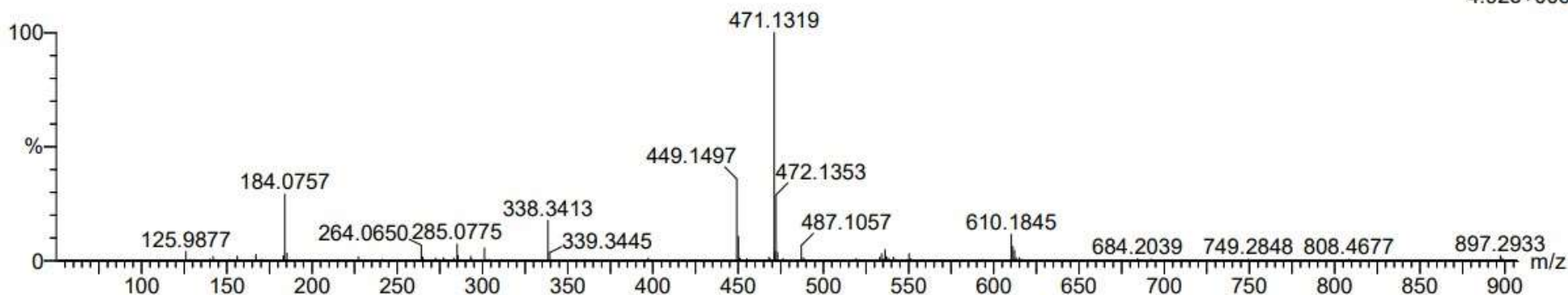
06-Oct-2023

14:04:17

1: TOF MS ES+

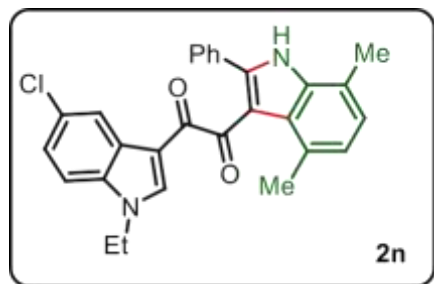
4.92e+006

061023_15 6 (0.138)

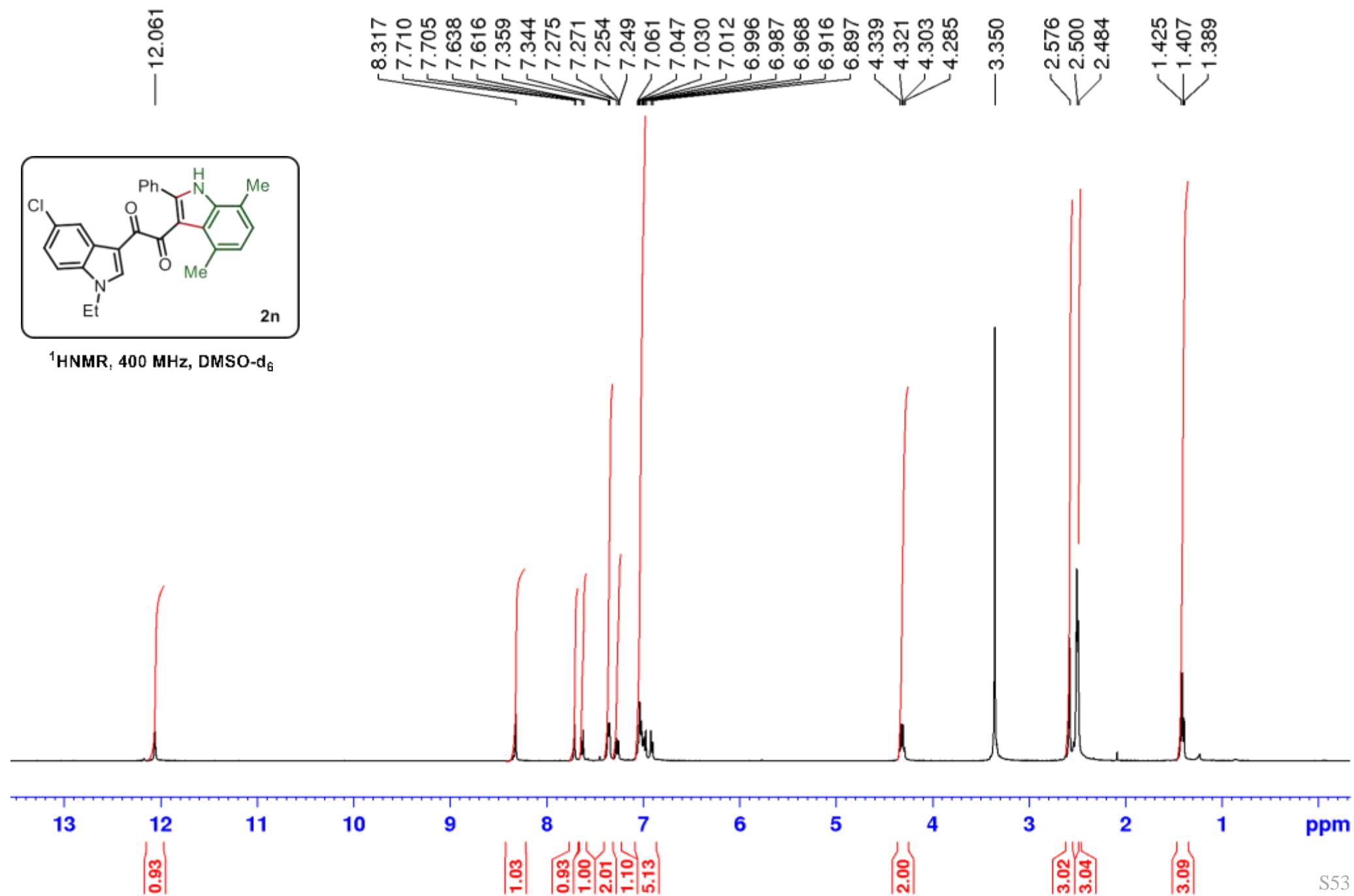


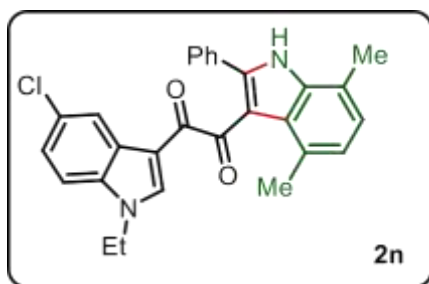
Minimum: -1.5
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
449.1497	449.1501	-0.4	-0.9	19.5	785.8	n/a	n/a	C28 H21 N2 O4

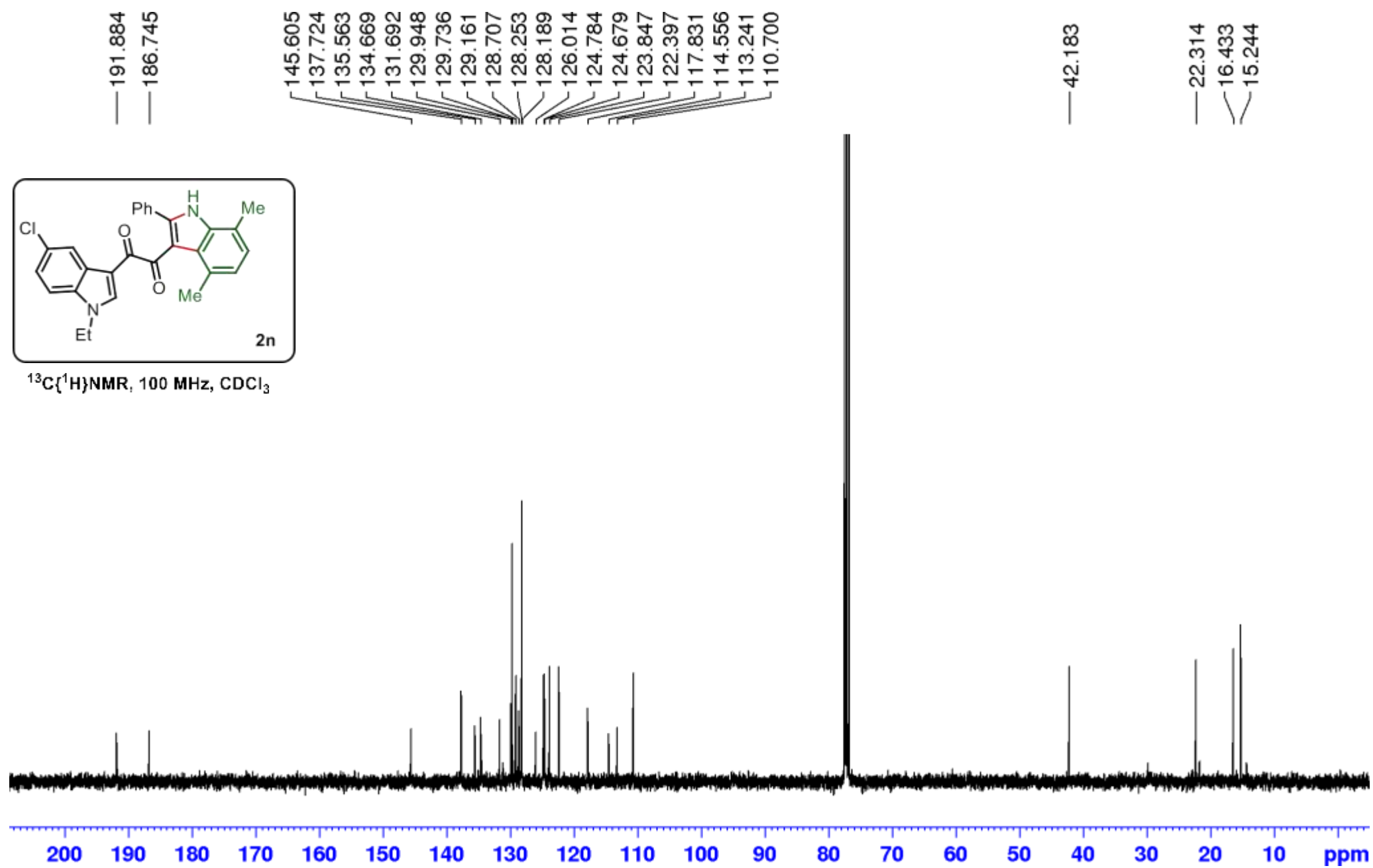


¹HNMR, 400 MHz, DMSO-d₆





$^{13}\text{C}\{^1\text{H}\}\text{NMR}$, 100 MHz, CDCl_3



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

27 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

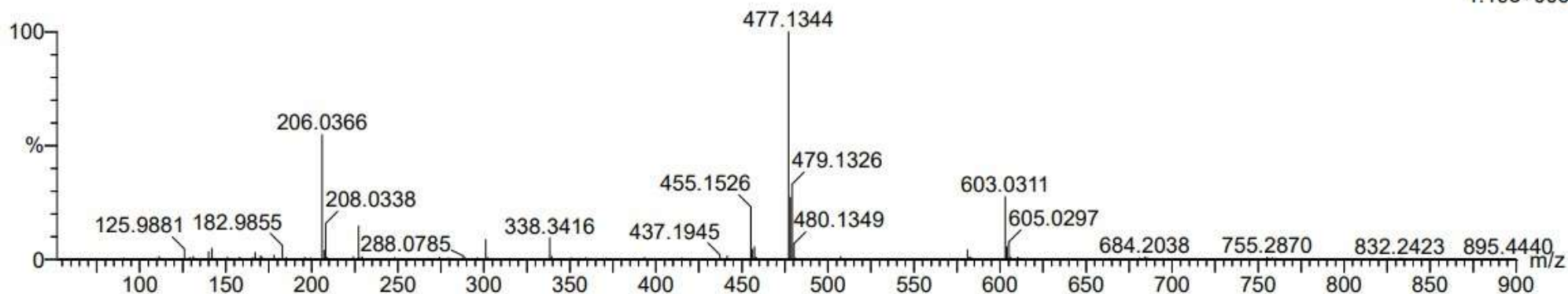
C: 0-28 H: 0-100 N: 0-2 O: 0-2 Cl: 0-1

NVD-96

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

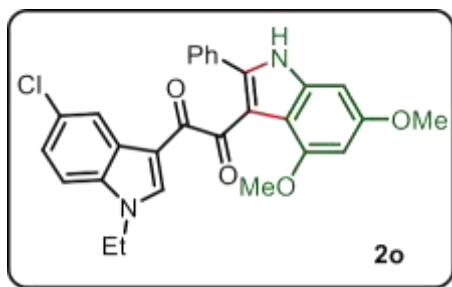
11-Oct-2023
13:17:40
1: TOF MS ES+
1.19e+006

111023_02 5 (0.121)

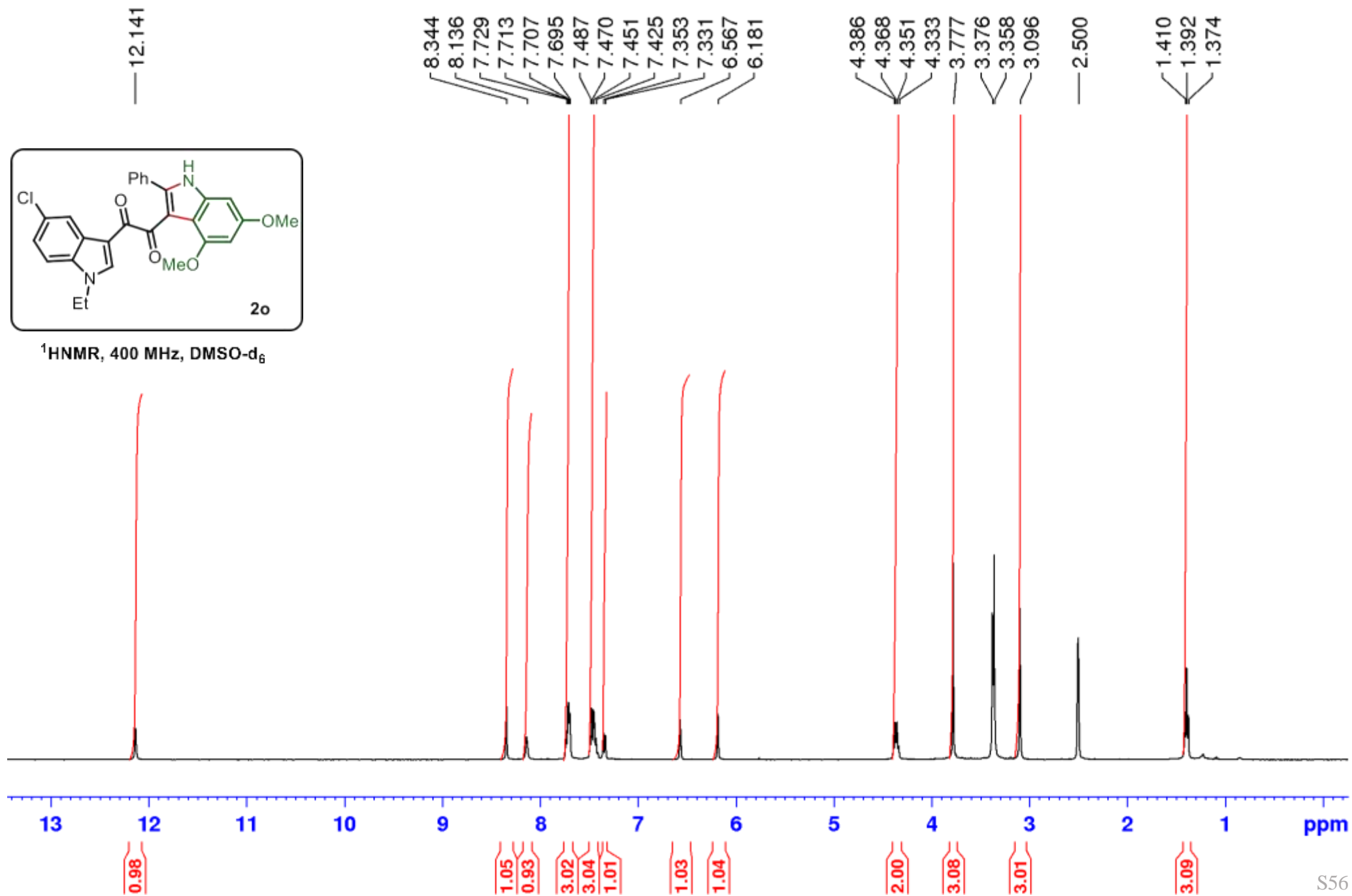


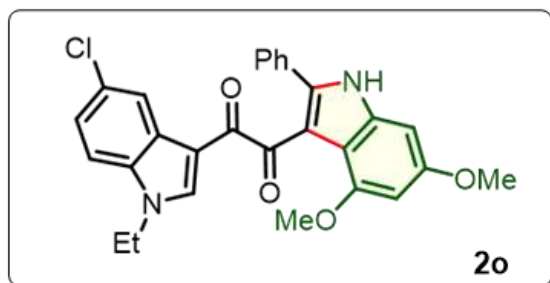
Minimum: -1.5
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
455.1526	455.1526	0.0	0.0	17.5	636.7	n/a	n/a	C28 H24 N2 O2 Cl



¹HNMR, 400 MHz, DMSO-d₆





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100MHz, DMSO- d_6

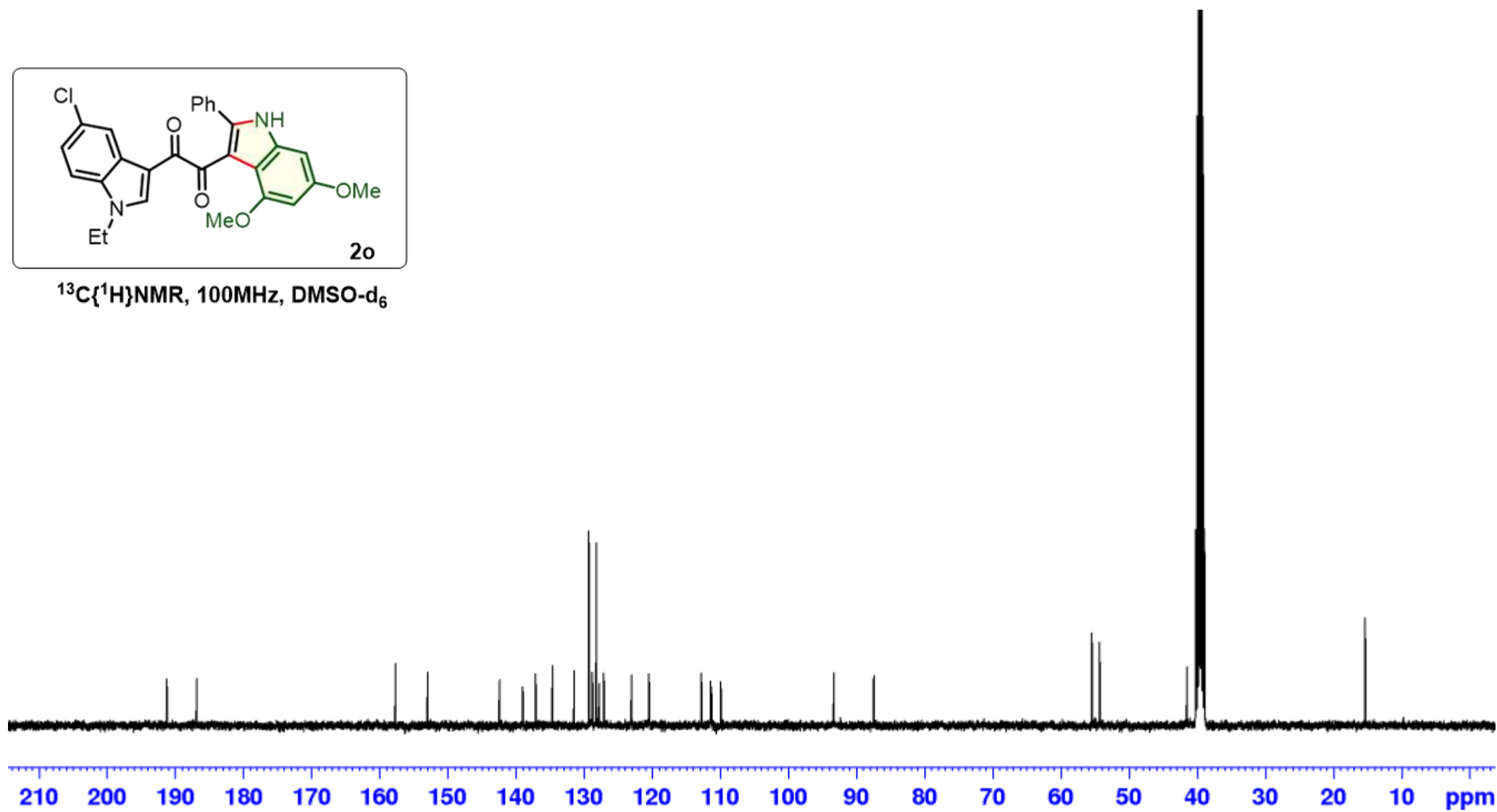
— 191.216
— 186.857

— 157.684
— 152.960
— 142.420
— 138.970
— 137.073
— 134.626
— 131.450
— 129.259
— 128.762
— 128.181
— 127.772
— 127.060
— 123.022
— 120.434
— 112.738
— 111.385
— 111.267
— 109.886
— 93.305
— 87.437

— 55.419
— 54.311

— 41.474

— 15.293



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

39 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-28 H: 0-100 N: 0-2 O: 0-4 Cl: 0-1

NVD-68

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

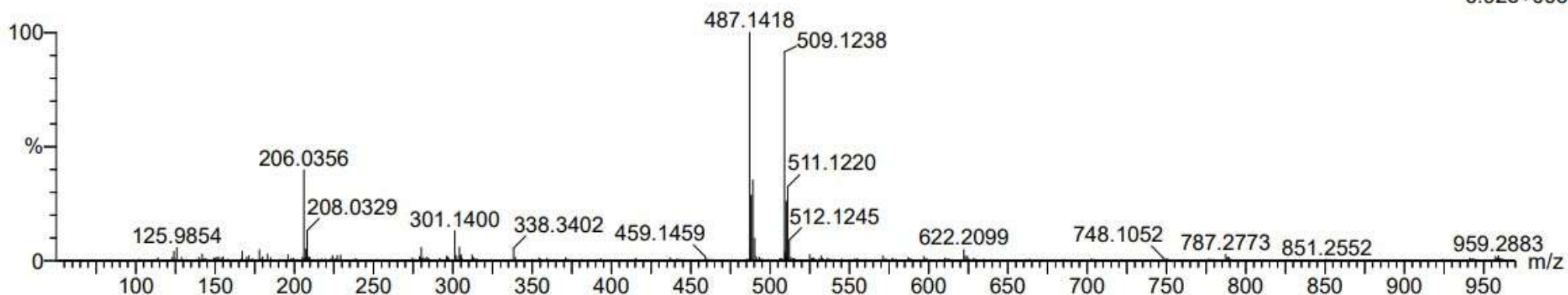
04-Mar-2024

13:26:06

1: TOF MS ES+

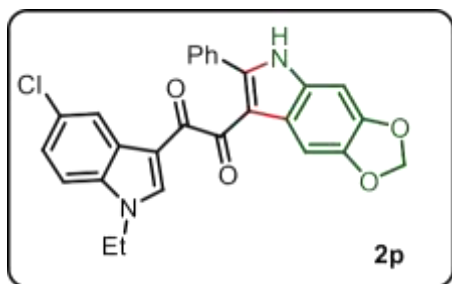
6.92e+006

040324_06 6 (0.138)

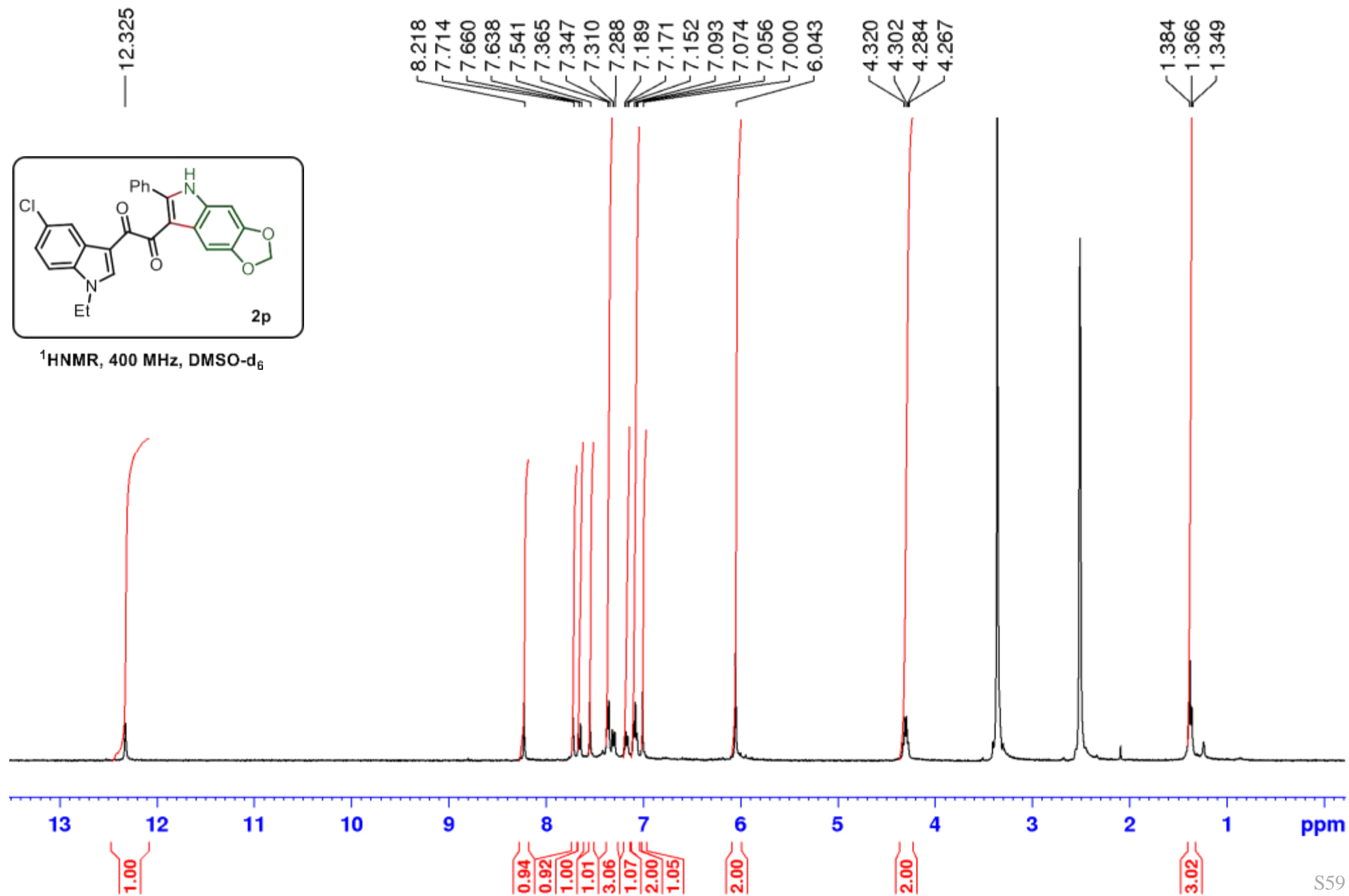


Minimum: -1.5
Maximum: 2.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
487.1418	487.1425	-0.7	-1.4	17.5	967.4	n/a	n/a	C28 H24 N2 O4 Cl



¹H NMR, 400 MHz, DMSO-d₆

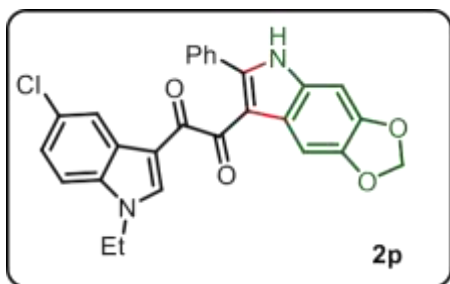


190.305
188.476

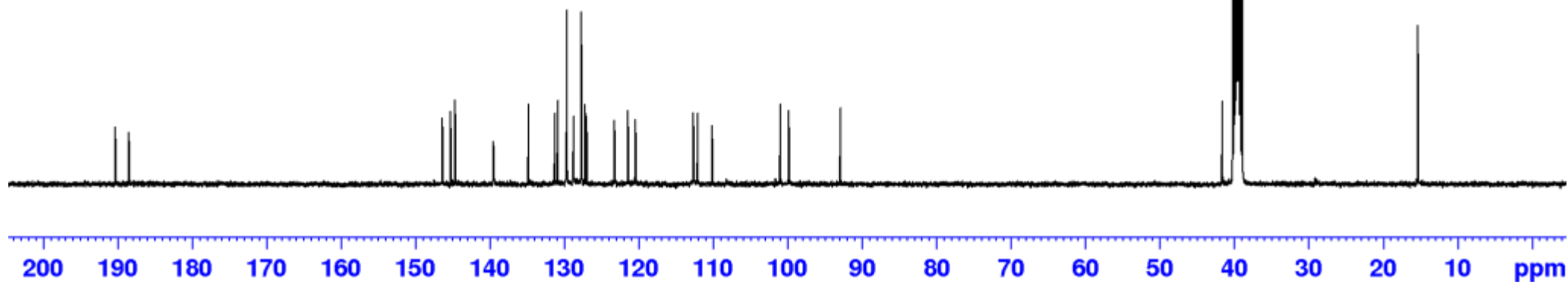
146.356
145.272
144.637
139.500
134.815
131.262
130.873
129.637
128.753
127.688
127.161
126.987
123.242
121.423
120.437
112.643
112.074
110.125
100.972
99.836
92.894

41.584

15.278



$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, DMSO-d_6



Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

49 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-28 H: 0-100 N: 0-2 O: 0-4 Cl: 0-1

NVD-95

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

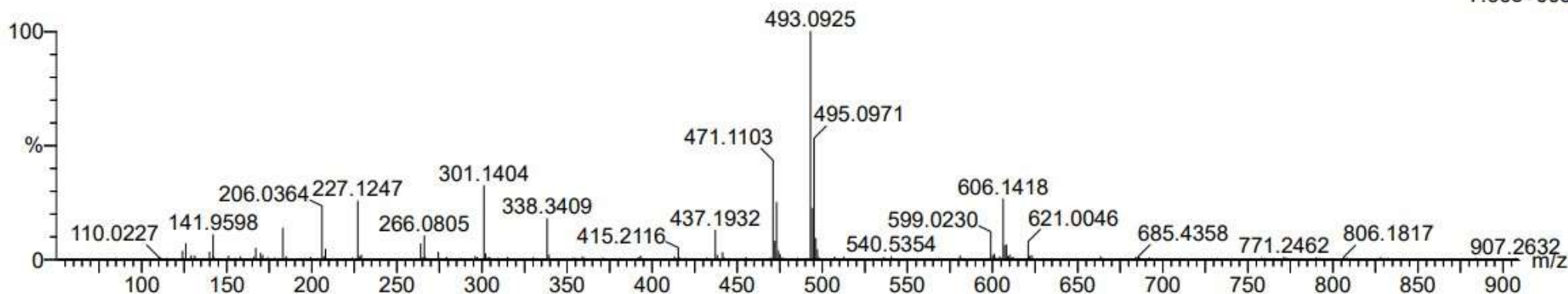
11-Oct-2023

13:20:22

1: TOF MS ES+

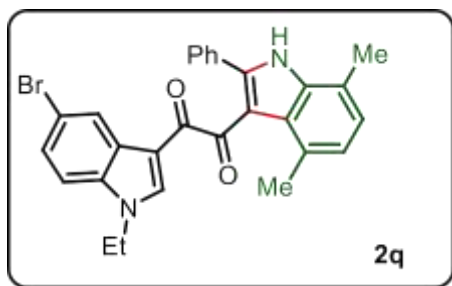
7.66e+005

111023_03 6 (0.138)

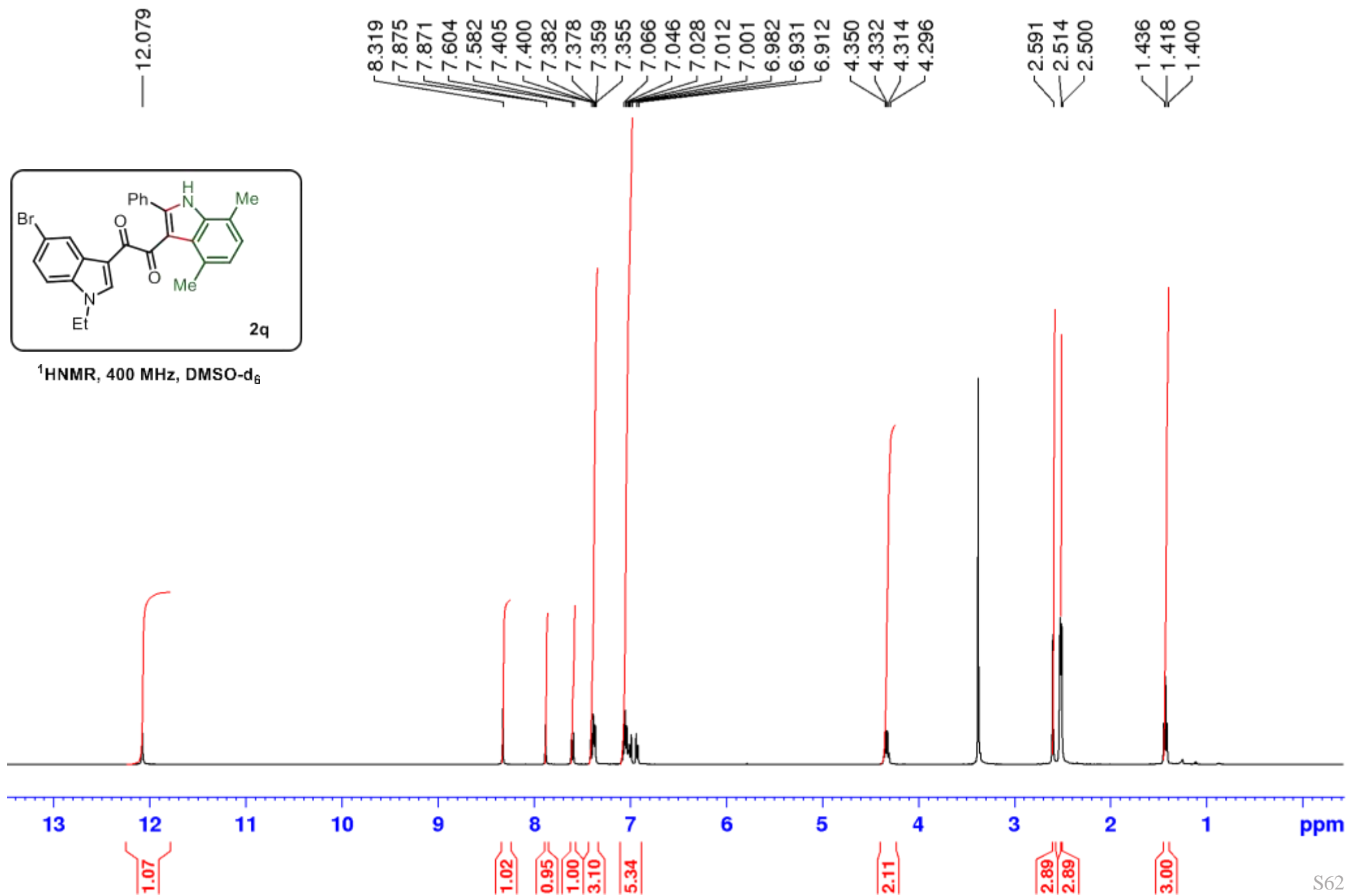


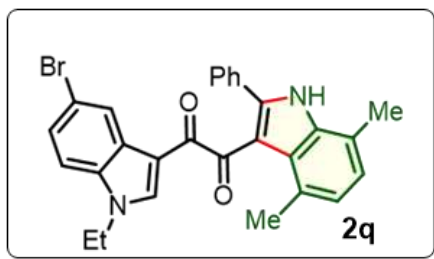
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
471.1103	471.1112	-0.9	-1.9	18.5	606.1	n/a	n/a	C27 H20 N2 O4 Cl

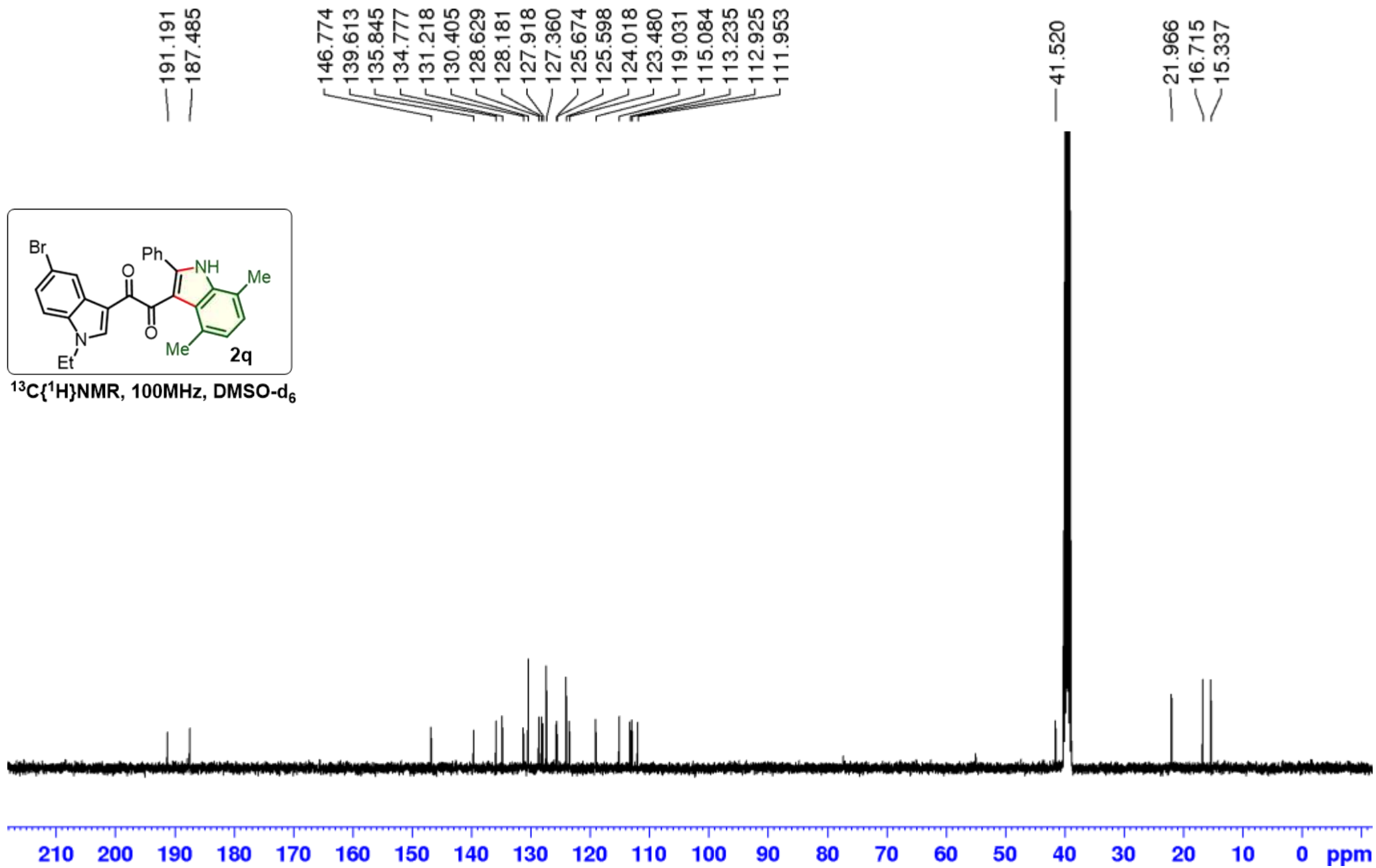


$^1\text{H NMR}$, 400 MHz, DMSO-d_6





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100MHz, DMSO- d_6



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

27 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-28 H: 0-100 N: 0-2 O: 0-2 Br: 0-1

NVD-94

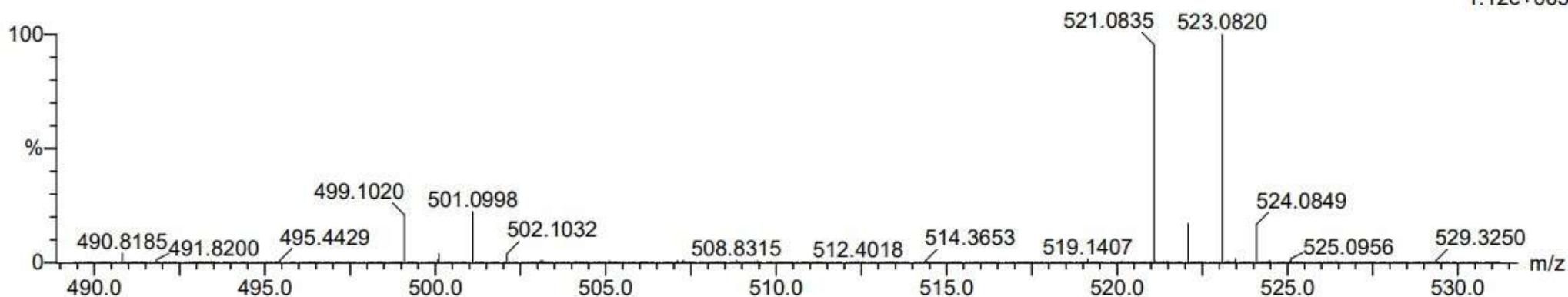
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

06-Oct-2023

14:01:43

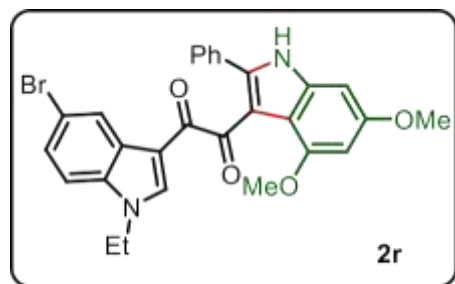
061023_14 4 (0.104)

1: TOF MS ES+
1.12e+005

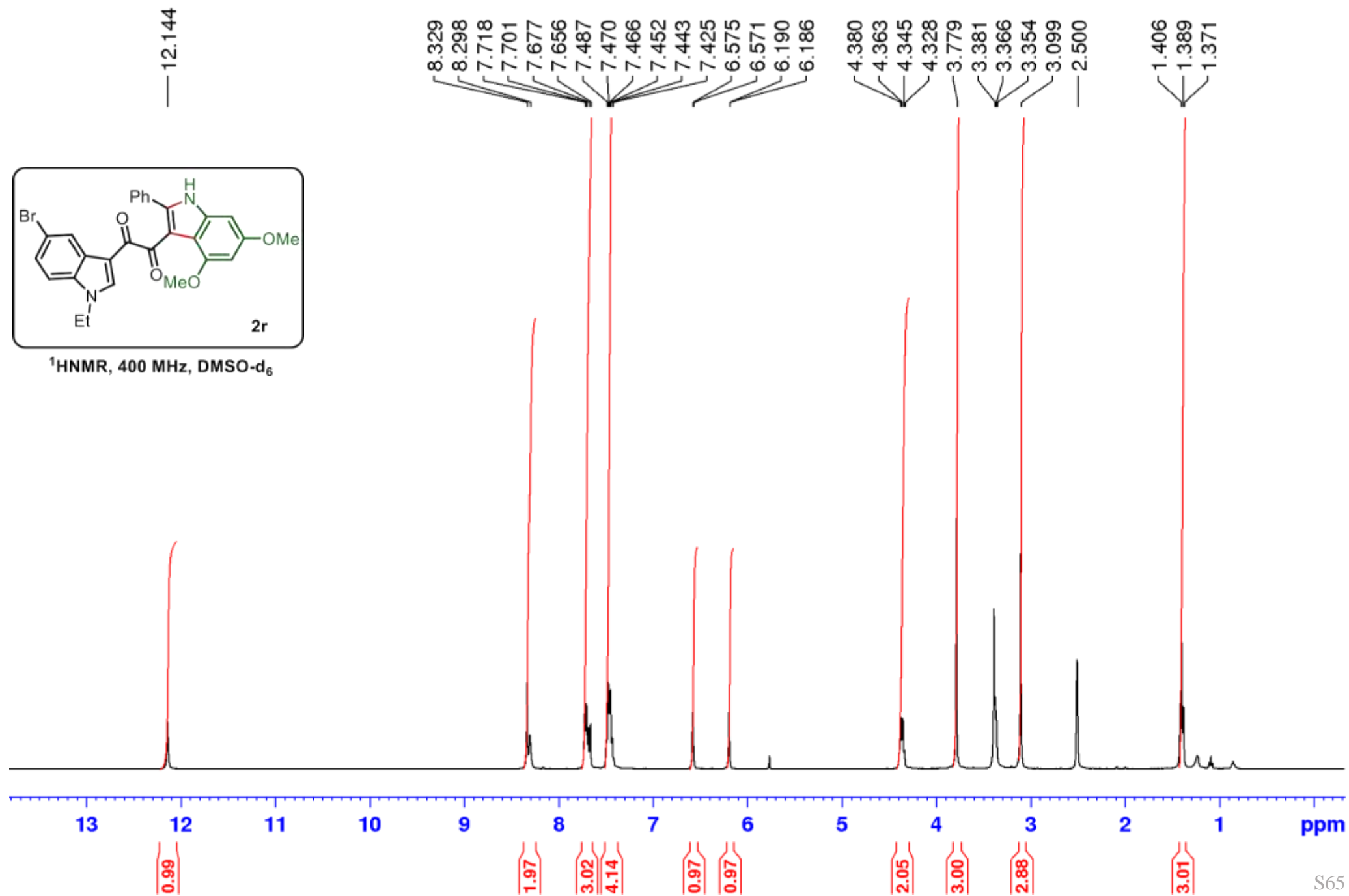


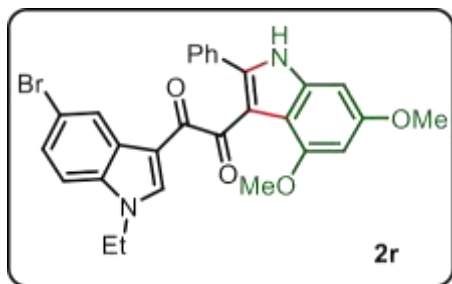
Minimum: -1.5
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
499.1020	499.1021	-0.1	-0.2	17.5	517.0	n/a	n/a	C28 H24 N2 O2 Br

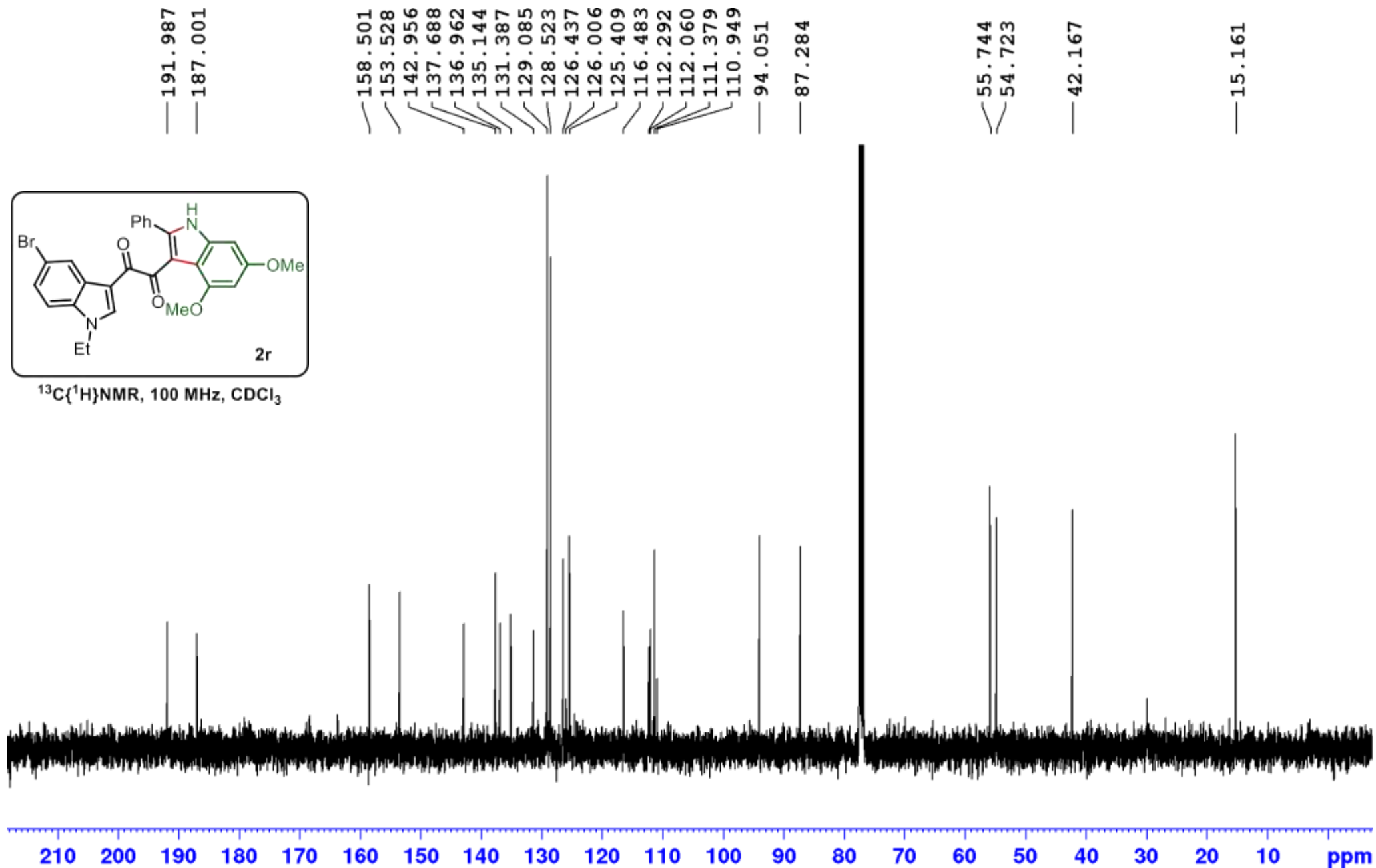


¹HNMR, 400 MHz, DMSO-d₆





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

39 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-28 H: 0-100 N: 0-2 O: 0-4 Br: 0-1

NVD-66

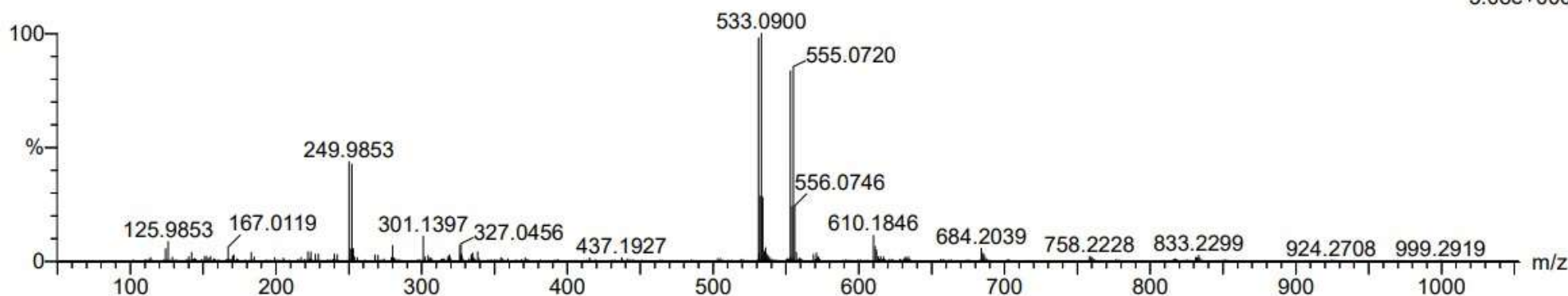
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

04-Mar-2024

13:31:14

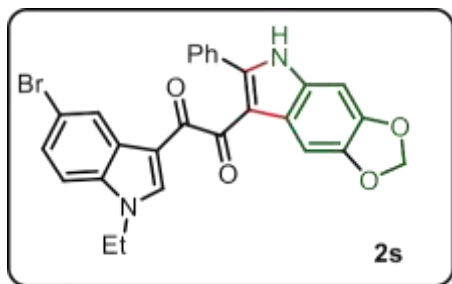
040324_08 6 (0.138)

1: TOF MS ES+
5.08e+006

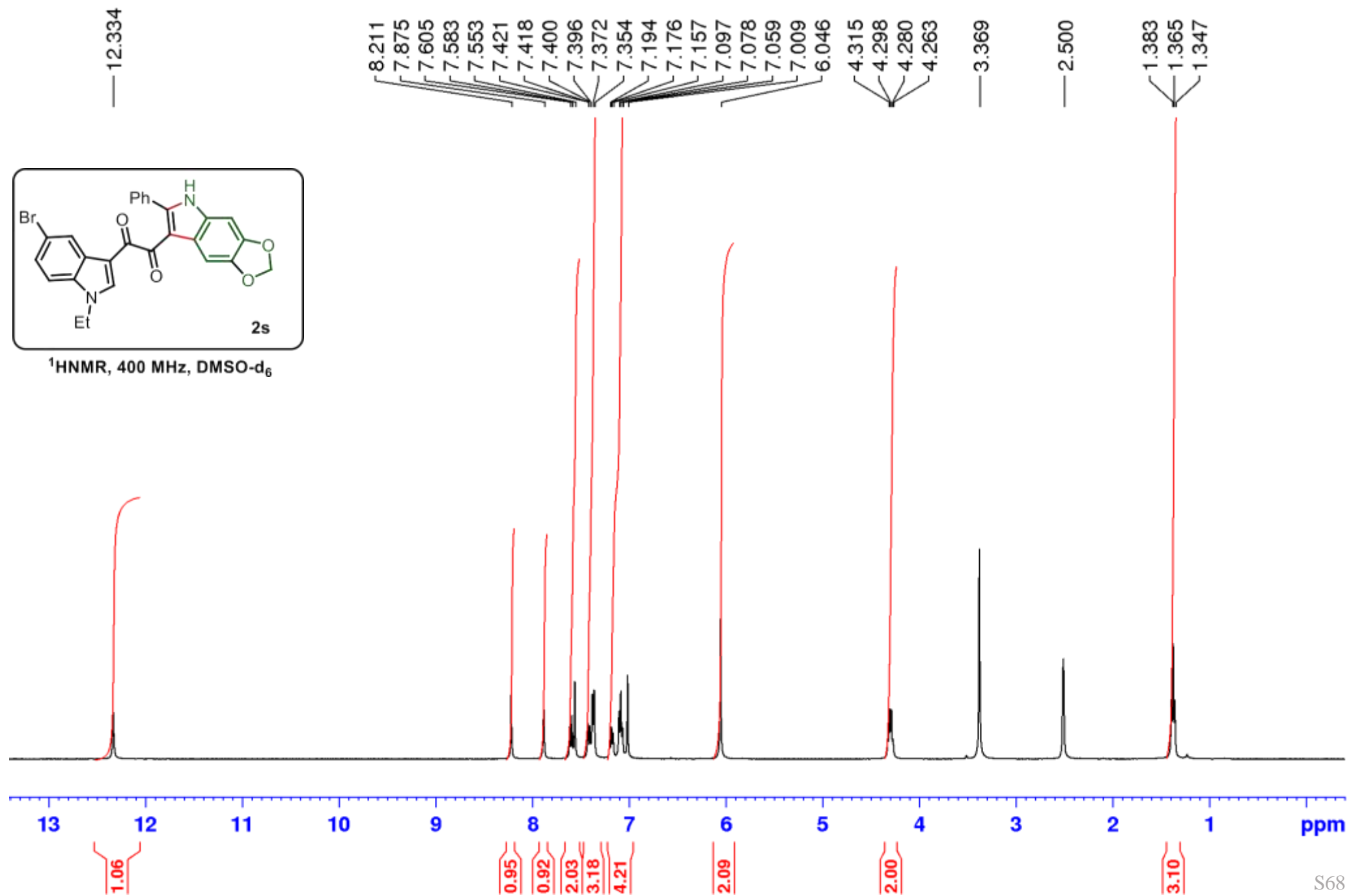


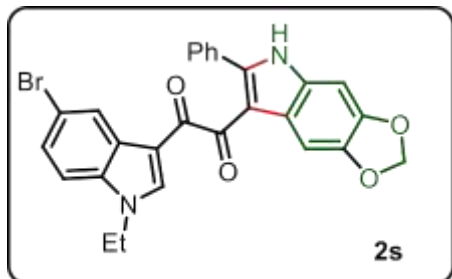
Minimum: -1.5
Maximum: 2.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
531.0916	531.0919	-0.3	-0.6	17.5	873.6	n/a	n/a	C28 H24 N2 O4 Br



¹HNMR, 400 MHz, DMSO-d₆





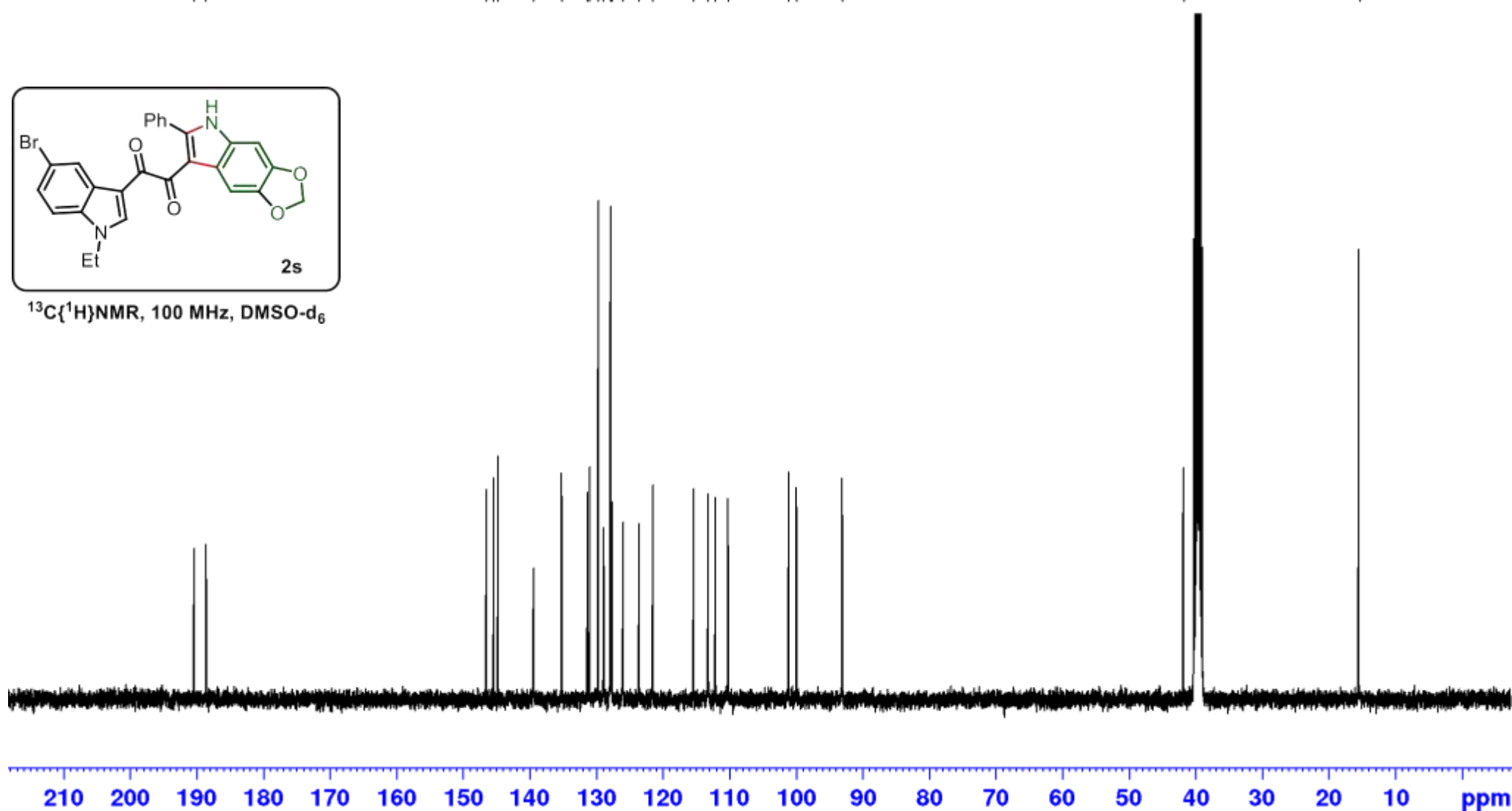
$^{13}\text{C}\{^1\text{H}\}\text{NMR}$, 100 MHz, DMSO-d_6

190.467
188.659

146.571
145.440
144.805
139.460
135.231
131.374
131.032
129.752
128.943
127.901
127.689
126.023
123.619
121.564
115.438
113.230
112.127
110.256
101.139
99.968
93.095

41.757

15.403



Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

40 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-27 H: 0-100 N: 0-2 O: 0-4 Br: 0-1

NVD-93

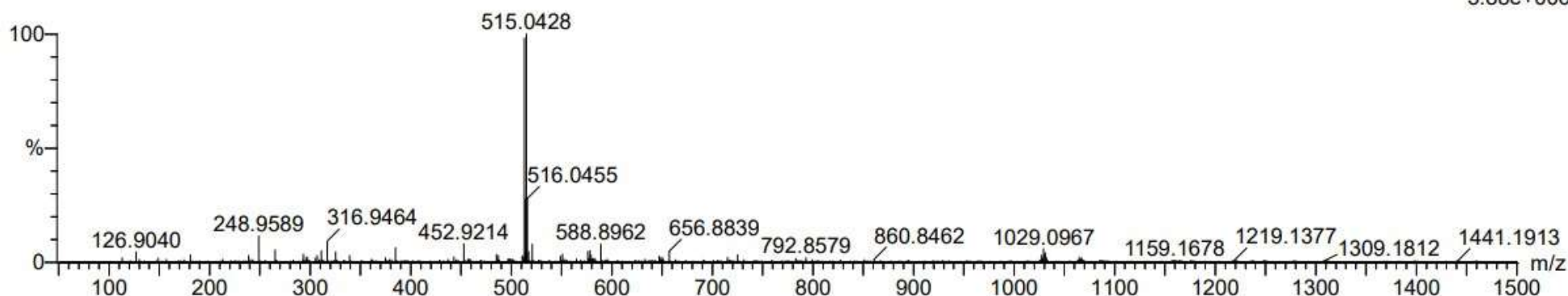
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

28-Mar-2024

15:27:49

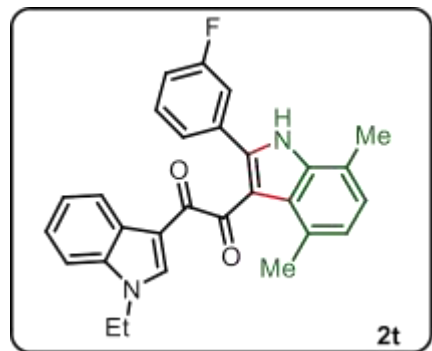
280324_03 6 (0.138)

1: TOF MS ES-
3.88e+006

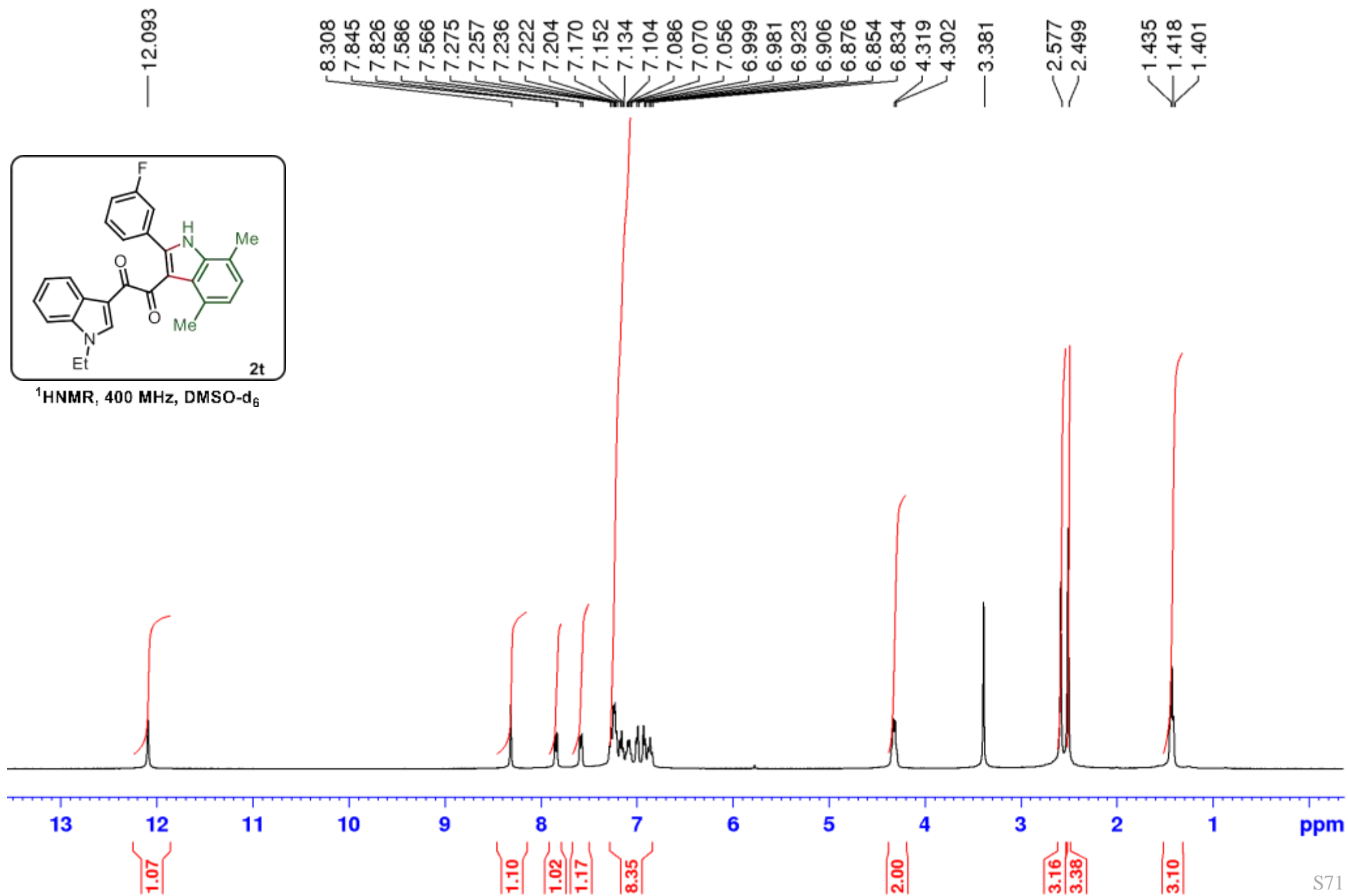


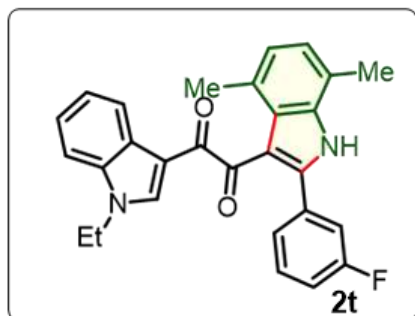
Minimum: -1.5
Maximum: 2.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
513.0445	513.0450	-0.5	-1.0	19.5	952.6	n/a	n/a	C27 H18 N2 O4 Br

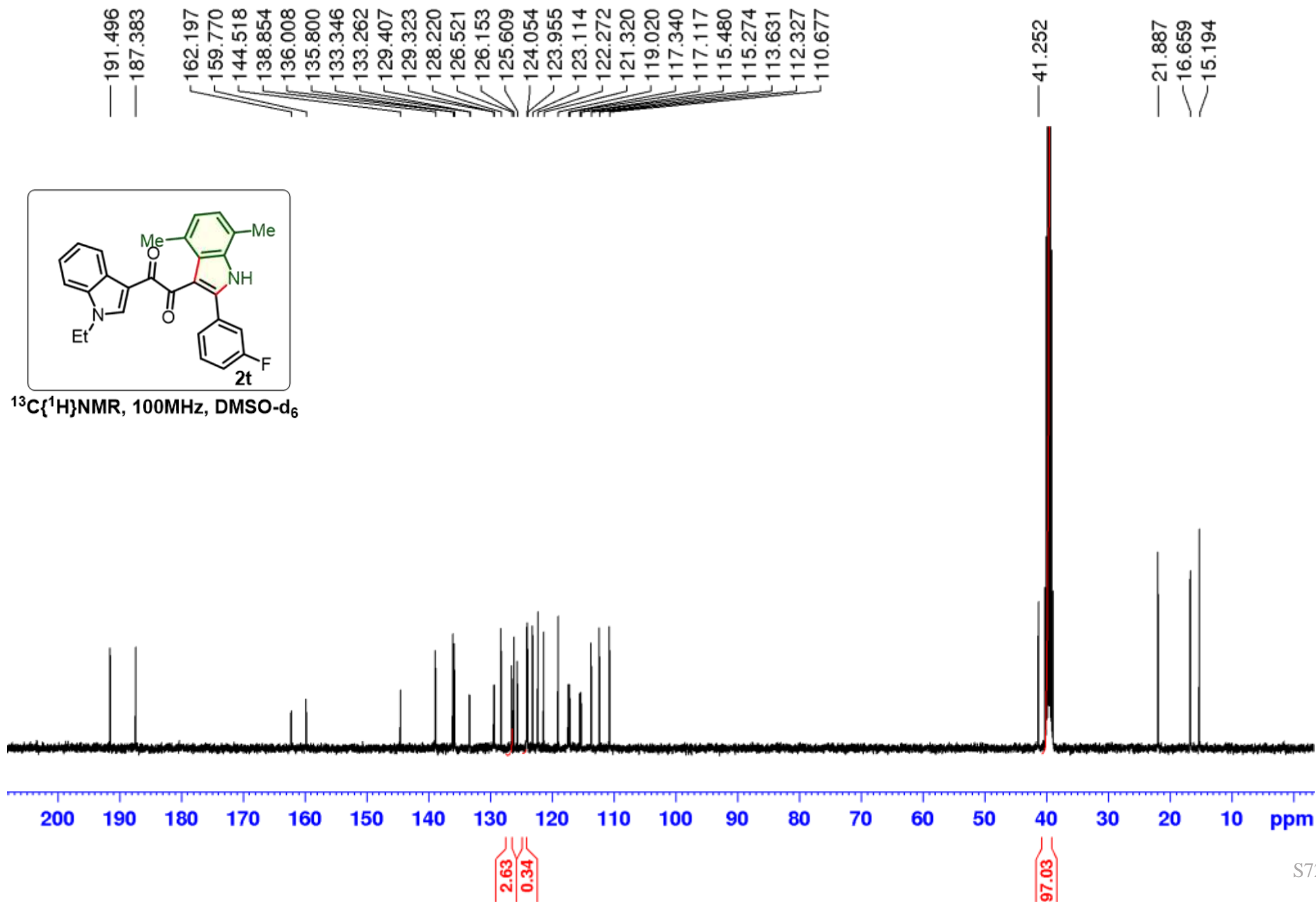


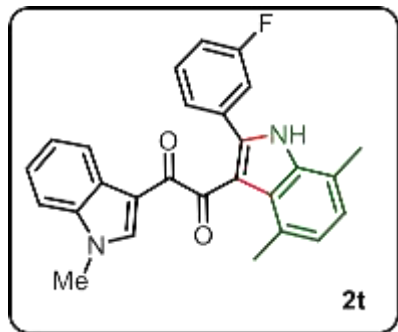
$^1\text{H NMR}$, 400 MHz, DMSO-d_6





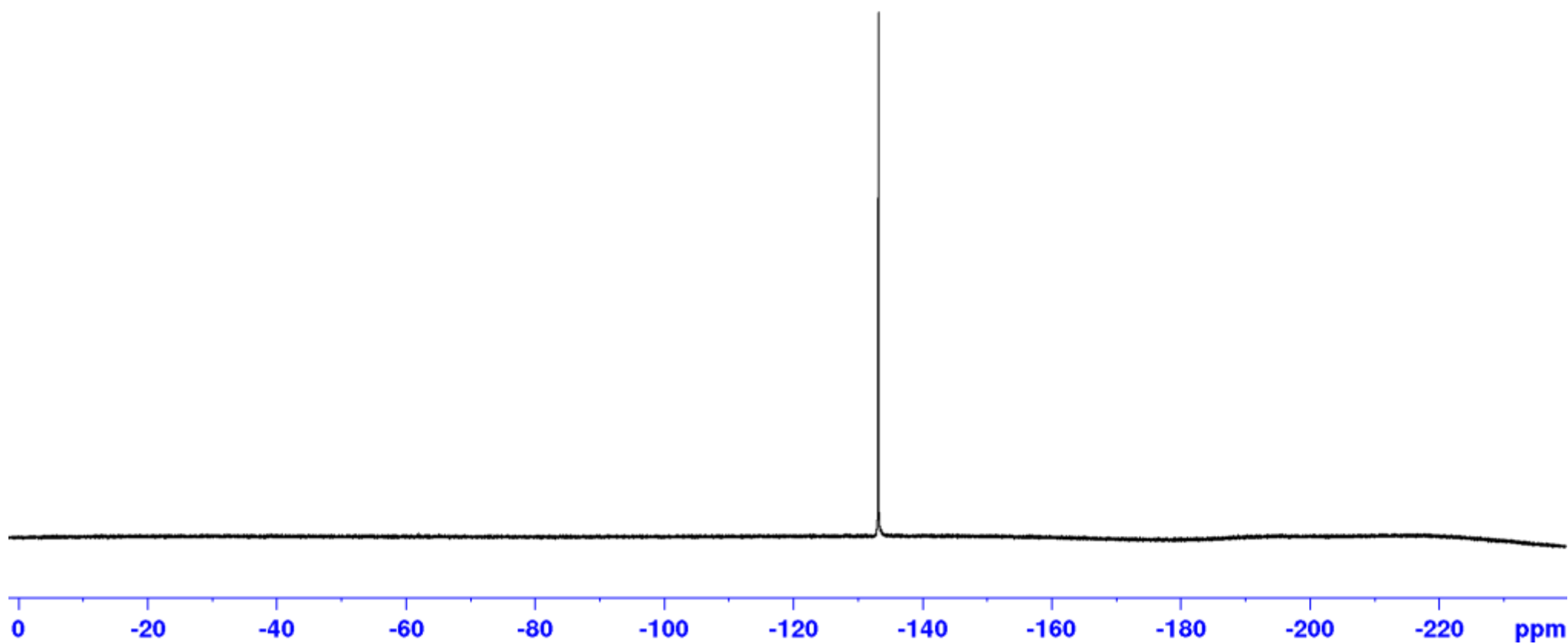
$^{13}\text{C}\{^1\text{H}\}$ NMR, 100MHz, DMSO- d_6





-133.161
-133.185
-133.201
-133.224

¹⁹F NMR, 376 MHz, DMSO-d₆



Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

28 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-28 H: 0-100 N: 0-2 O: 0-2 F: 0-1

NVD-98

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

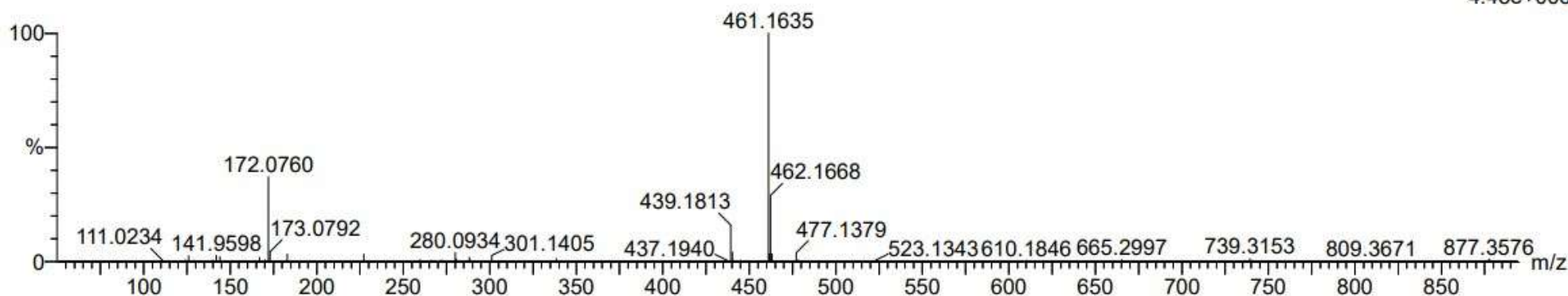
11-Oct-2023

13:23:05

1: TOF MS ES+

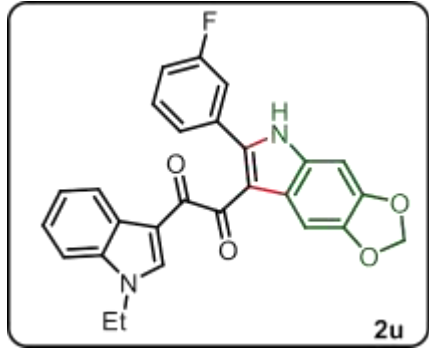
4.45e+006

111023_04 7 (0.155)

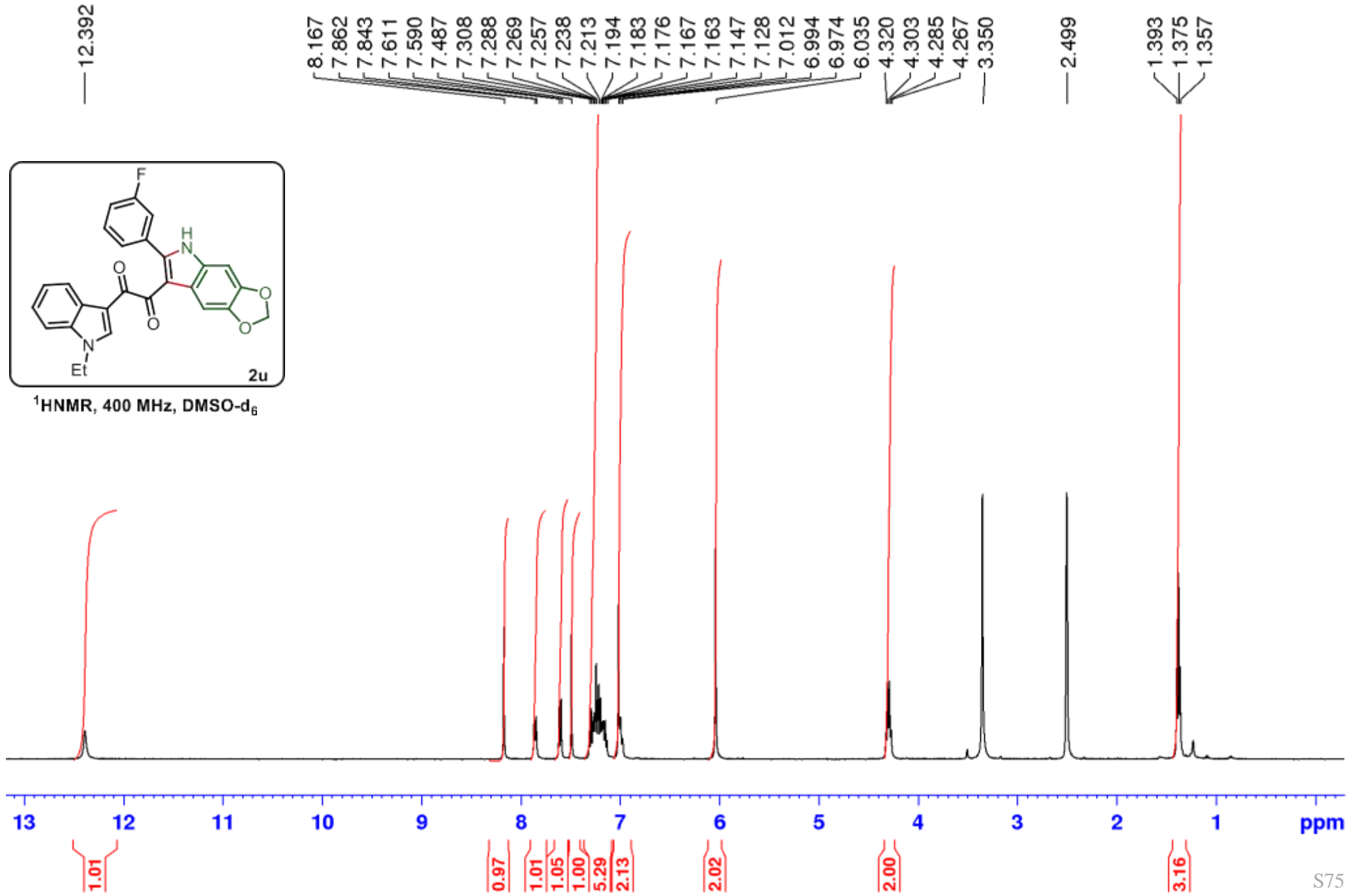


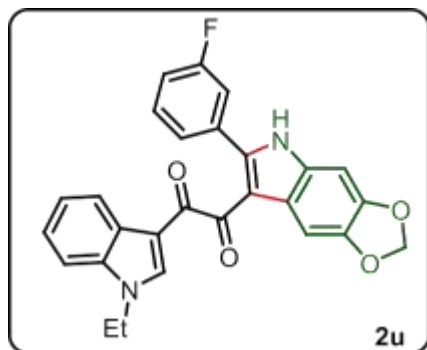
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
439.1813	439.1822	-0.9	-2.0	17.5	632.7	n/a	n/a	C28 H24 N2 O2 F



¹HNMR, 400 MHz, DMSO-d₆



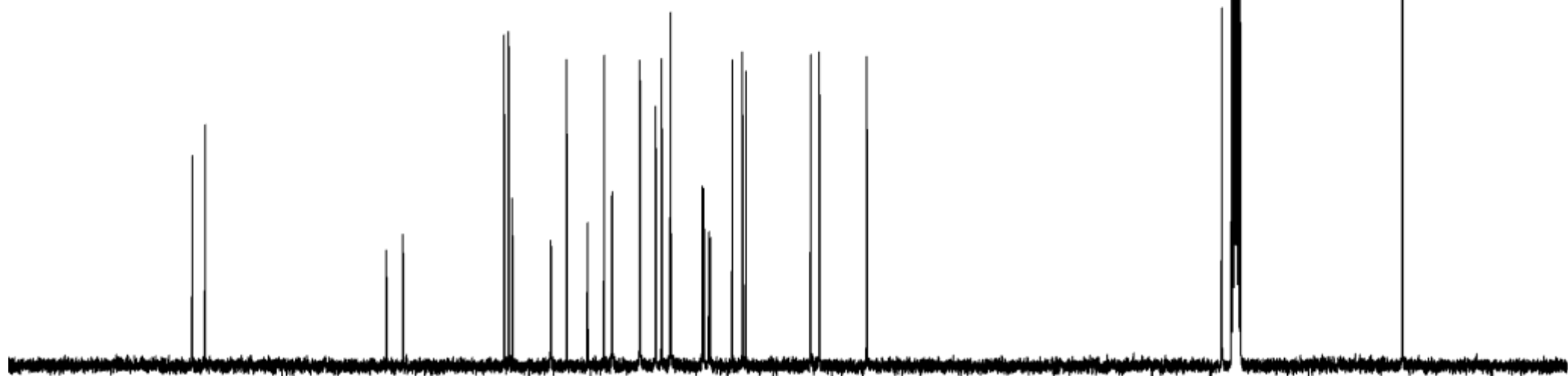


$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, DMSO-d_6

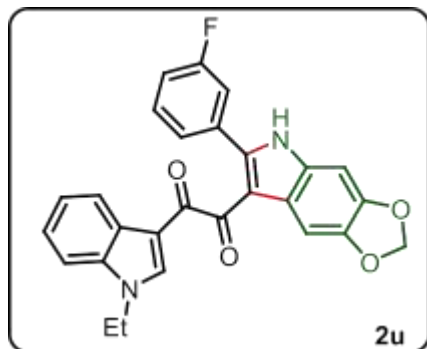
190.706
188.857
162.599
160.173
145.575
144.878
144.383
138.782
136.508
133.512
133.428
131.066
129.975
129.891
125.946
125.876
125.854
123.604
122.758
121.504
121.417
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115.909
115.701
112.530
111.060
110.545
101.172
99.903
93.071

41.540

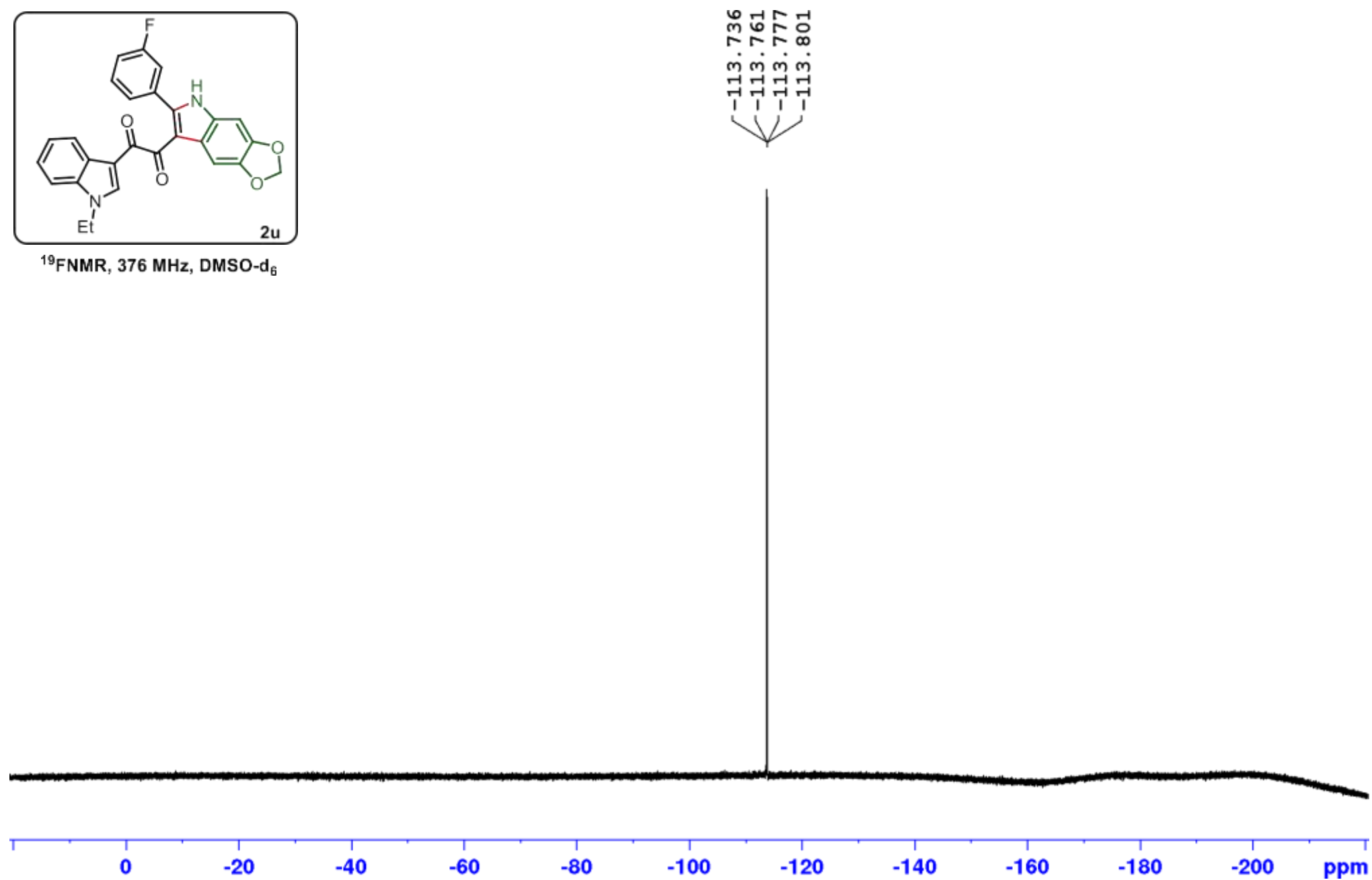
15.381



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



^{19}F NMR, 376 MHz, DMSO-d_6



Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

43 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

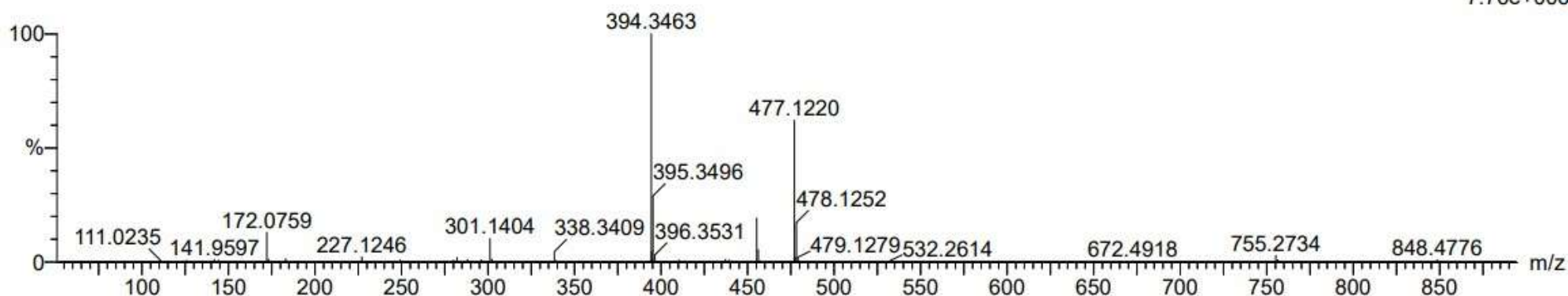
C: 0-27 H: 0-100 N: 0-2 O: 0-4 F: 0-1

NVD-97

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

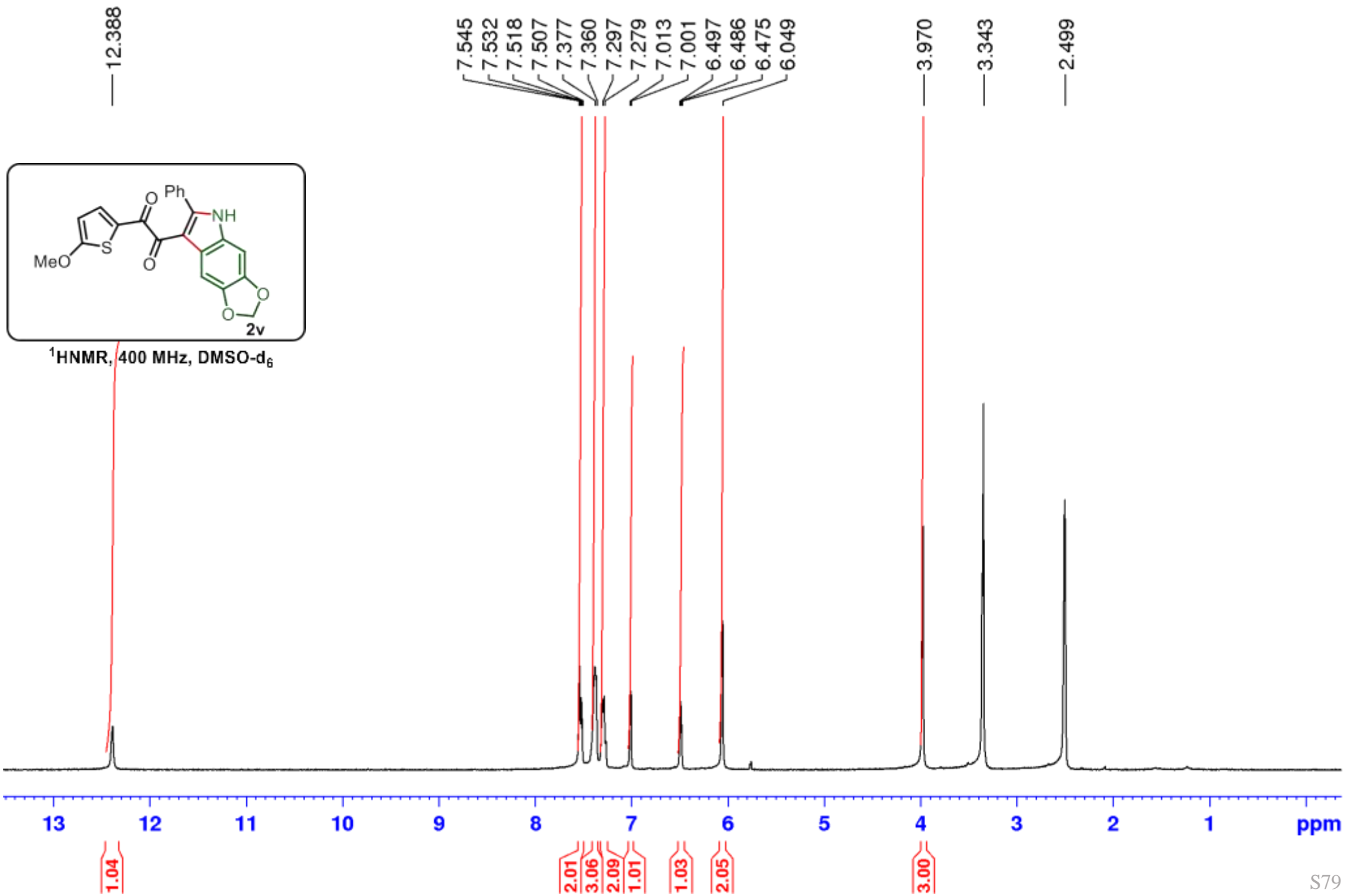
11-Oct-2023
13:25:49
1: TOF MS ES+
7.76e+006

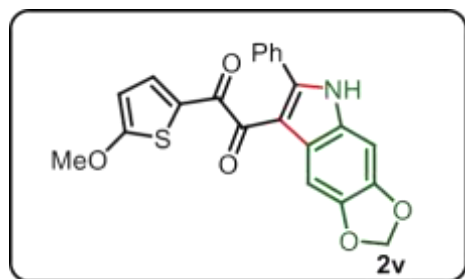
111023_05 6 (0.138)



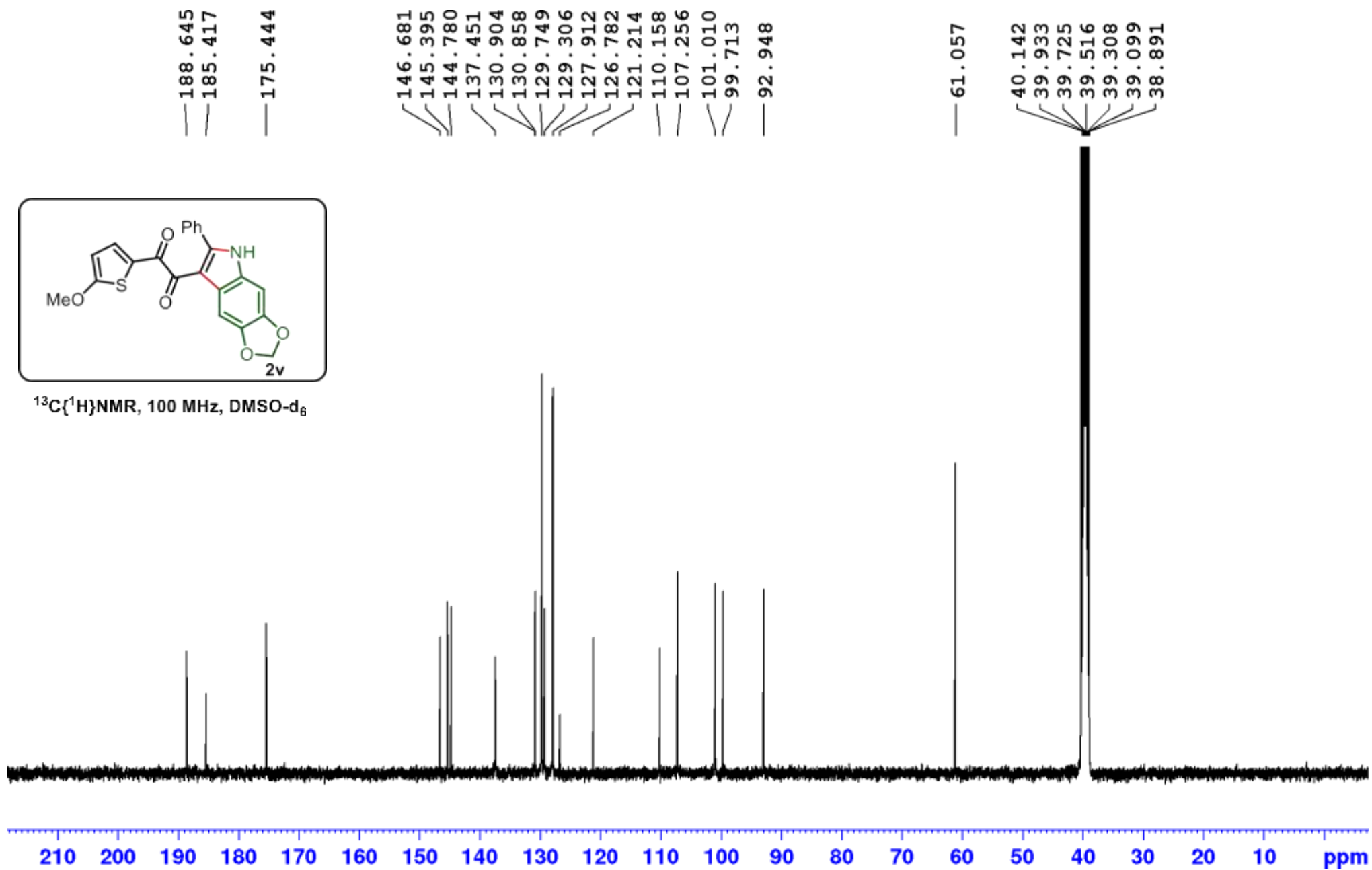
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
455.1400	455.1407	-0.7	-1.5	18.5	741.1	n/a	n/a	C27 H20 N2 O4 F





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, DMSO-d_6



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

28 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-22 H: 0-100 N: 0-1 O: 0-5 S: 0-1

NVD-116

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

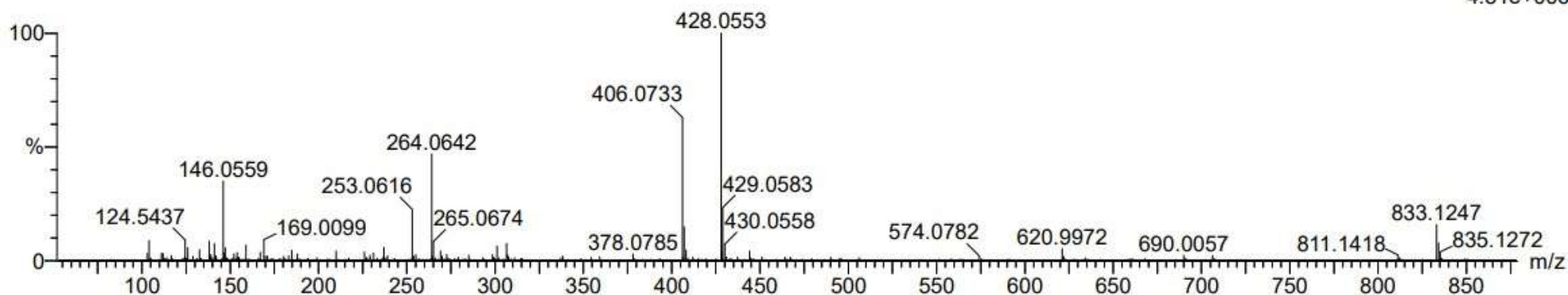
04-Mar-2024

13:39:05

1: TOF MS ES+

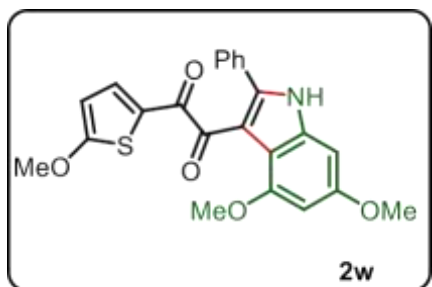
4.51e+006

040324_11 5 (0.121)

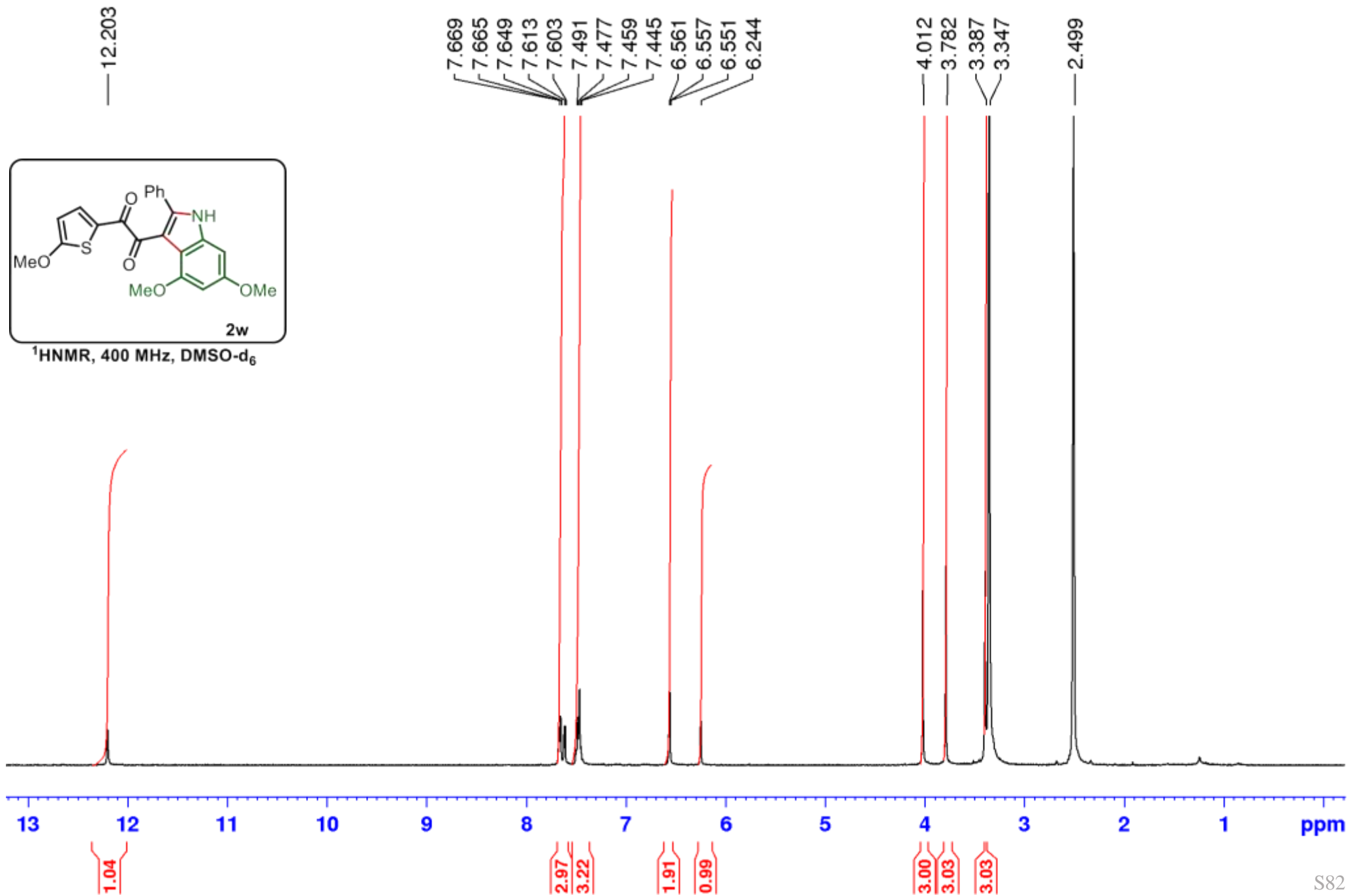


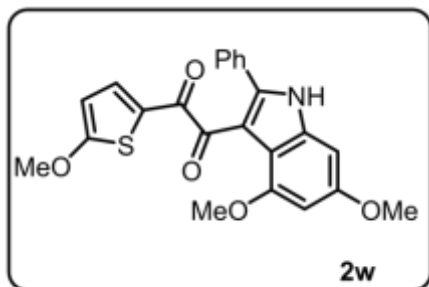
Minimum: -1.5
Maximum: 2.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
406.0733	406.0749	-1.6	-3.9	15.5	1036.7	n/a	n/a	C22 H16 N O5 S

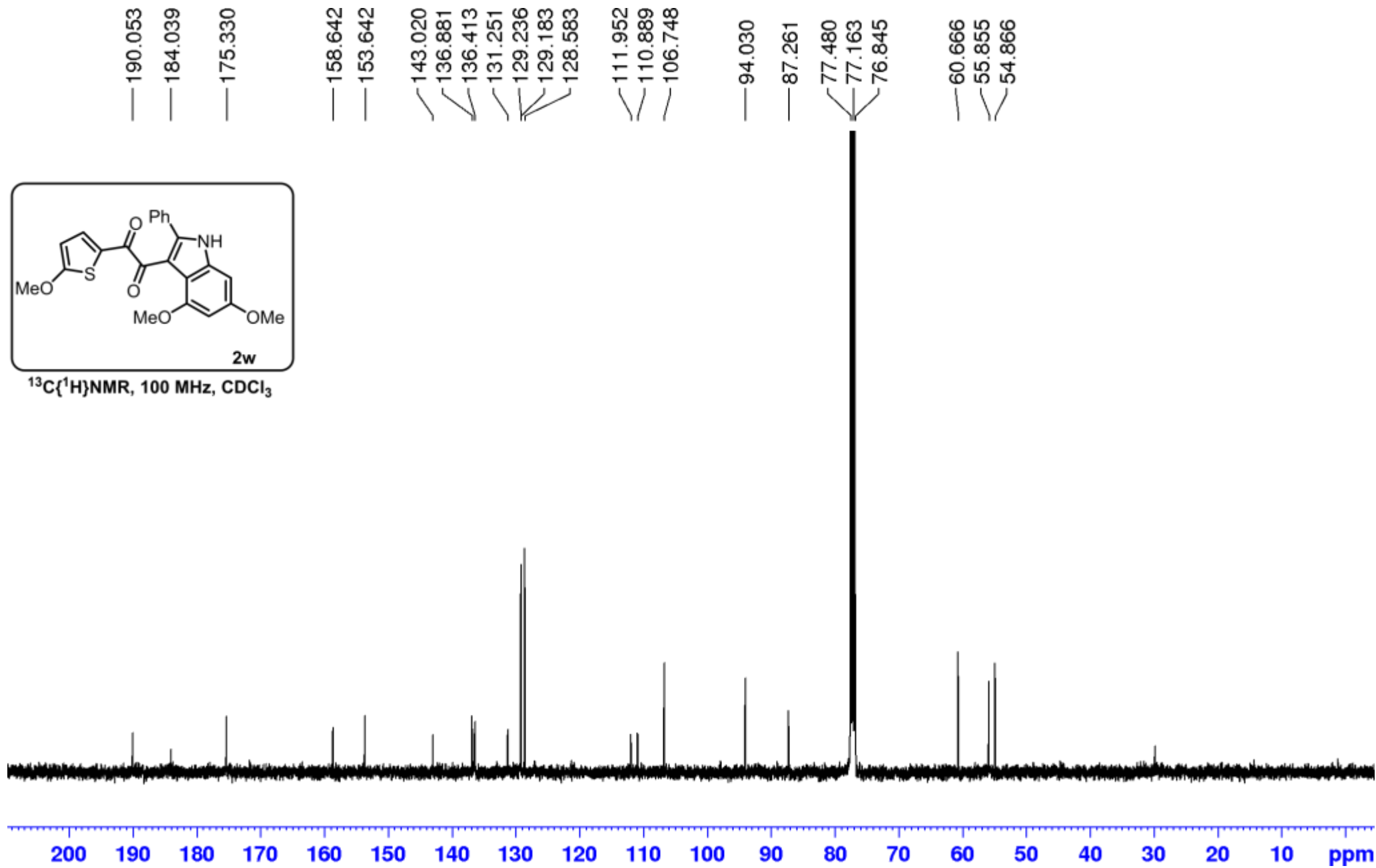


¹HNMR, 400 MHz, DMSO-d₆





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

28 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-23 H: 0-100 N: 0-1 O: 0-5 S: 0-1

NVD-117

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

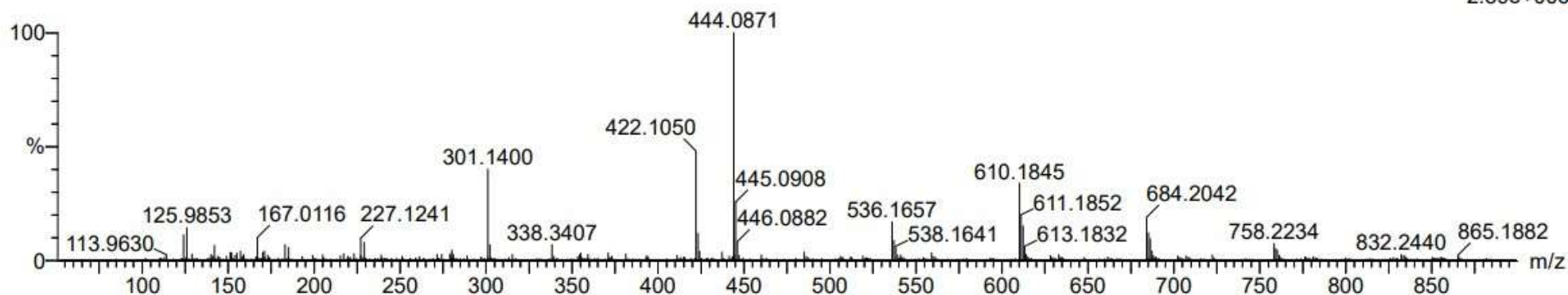
04-Mar-2024

13:33:57

1: TOF MS ES+

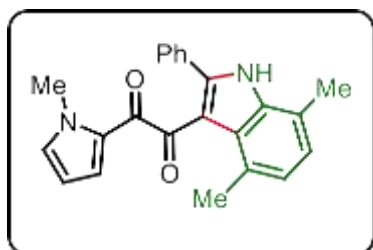
2.89e+006

040324_09 6 (0.138)

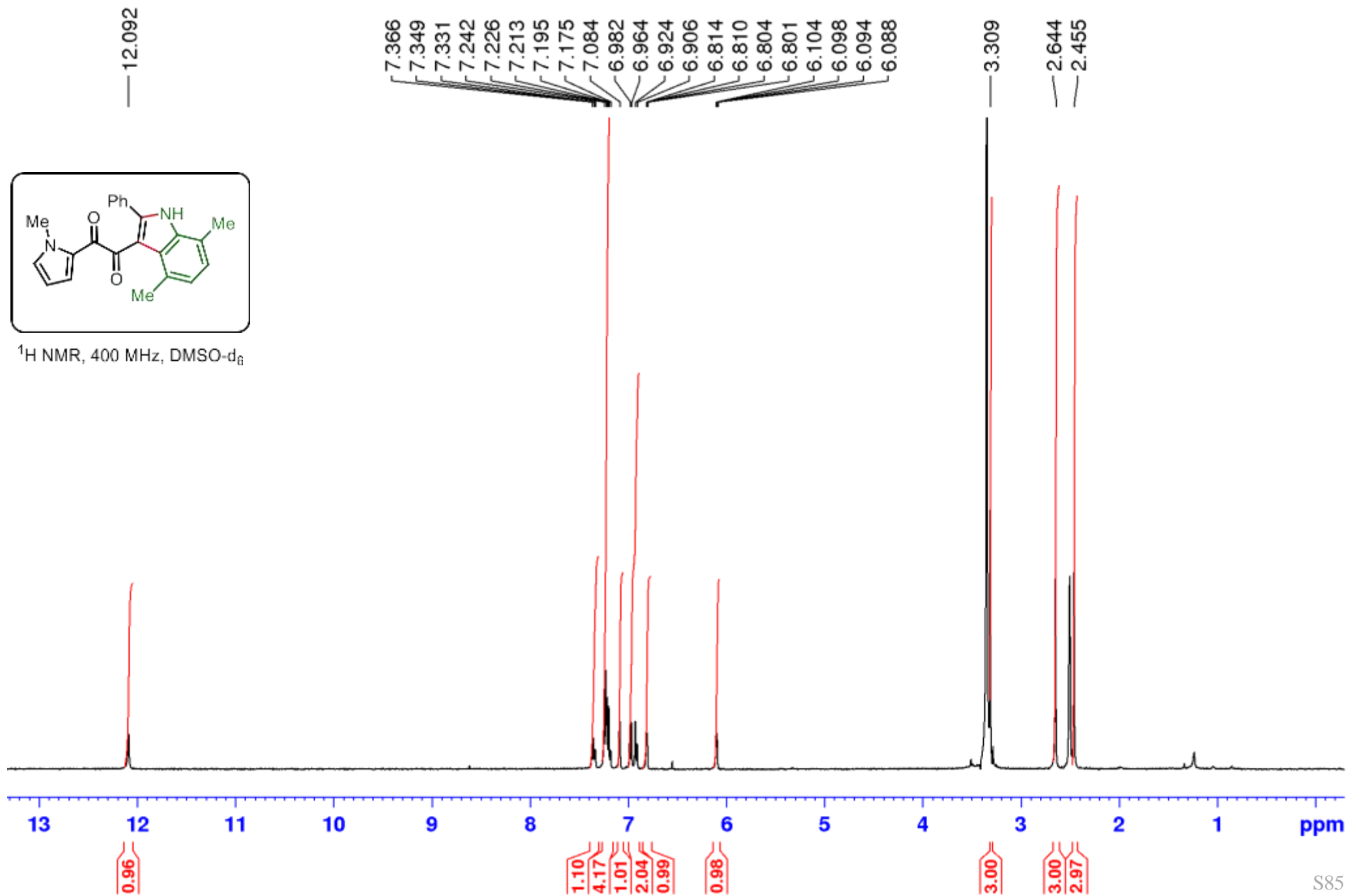


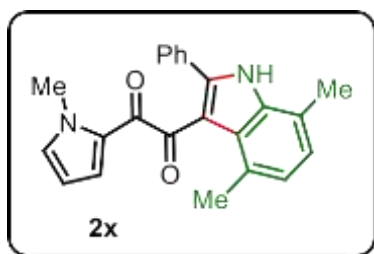
Minimum: -1.5
Maximum: 2.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
422.1050	422.1062	-1.2	-2.8	14.5	1092.4	n/a	n/a	C23 H20 N O5 S

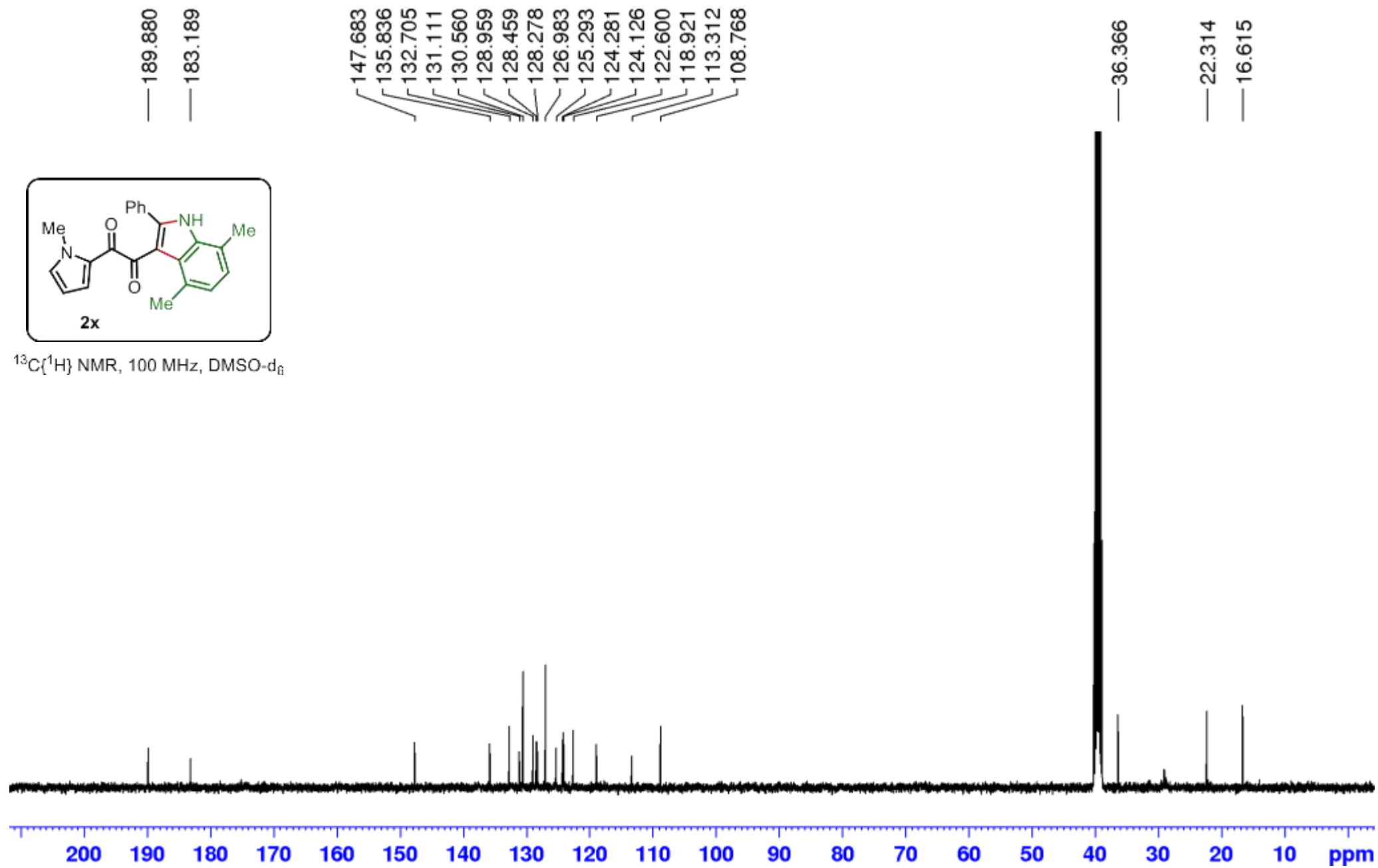


$^1\text{H NMR}$, 400 MHz, DMSO-d_6





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, DMSO-d_6



Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

C: 0-23 H: 0-100 N: 0-2 O: 0-2

NVD/B-16

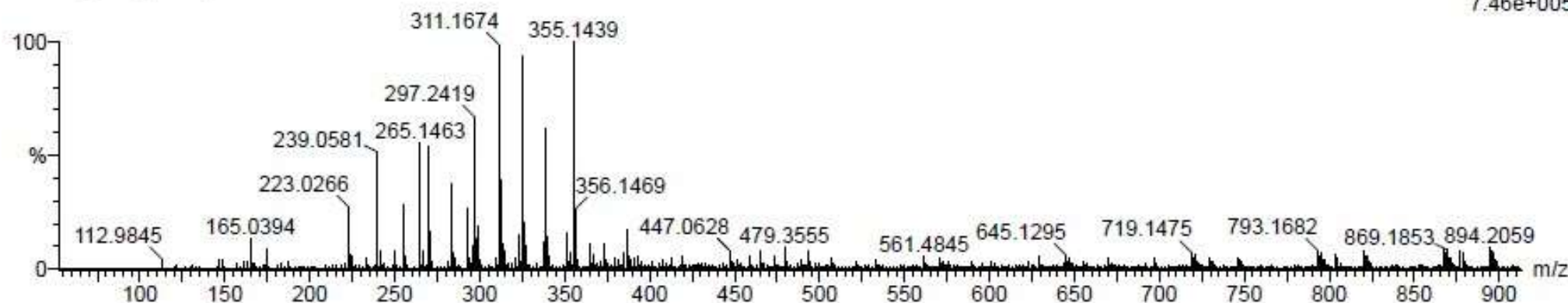
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

15-Jul-2024

14:51:53

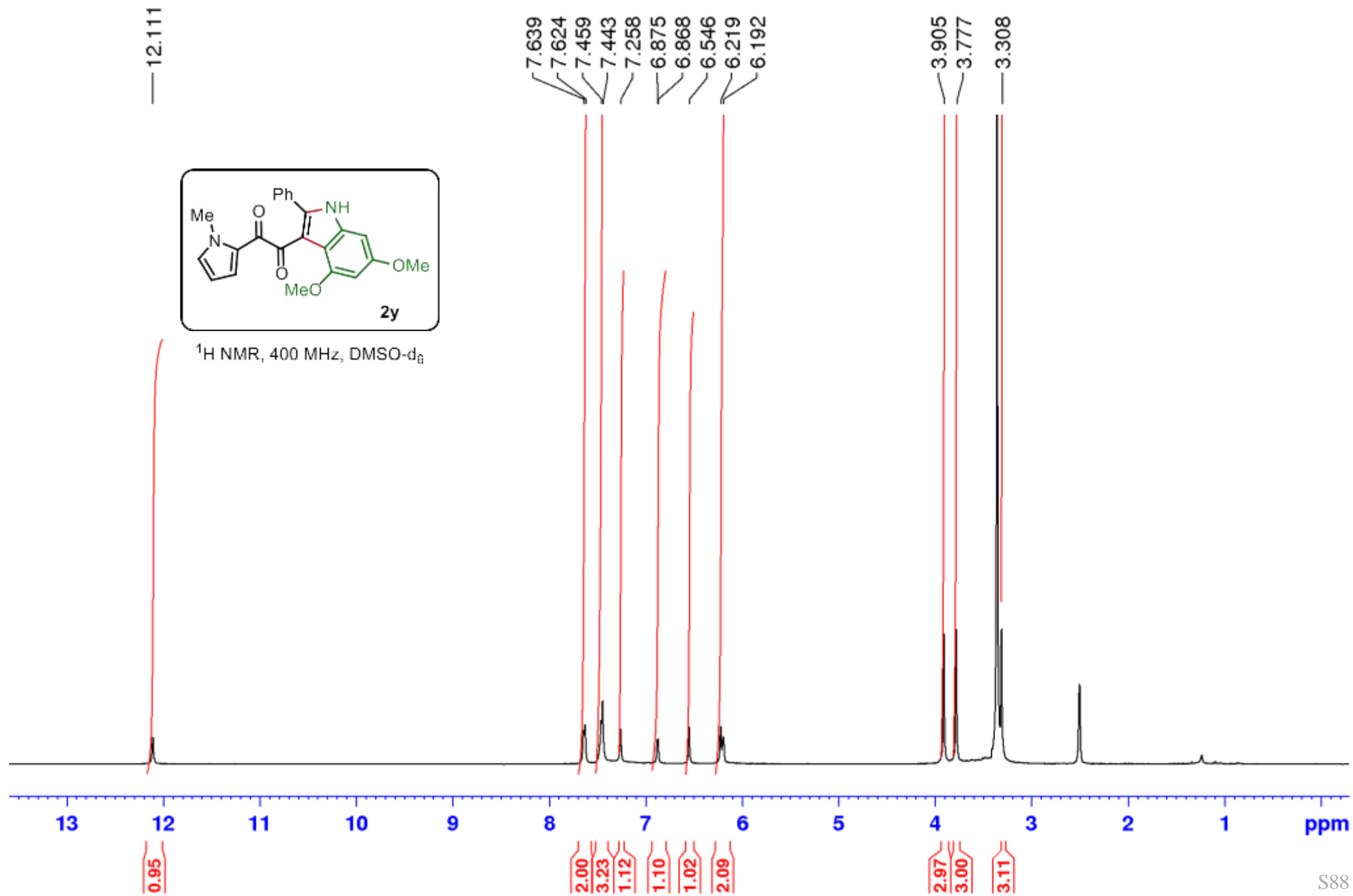
1: TOF MS ES-
7.46e+005

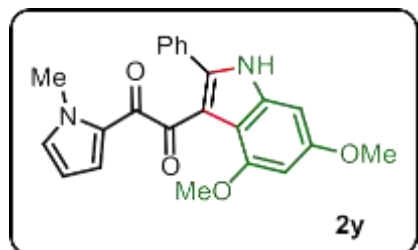
150724_13 5 (0.121)



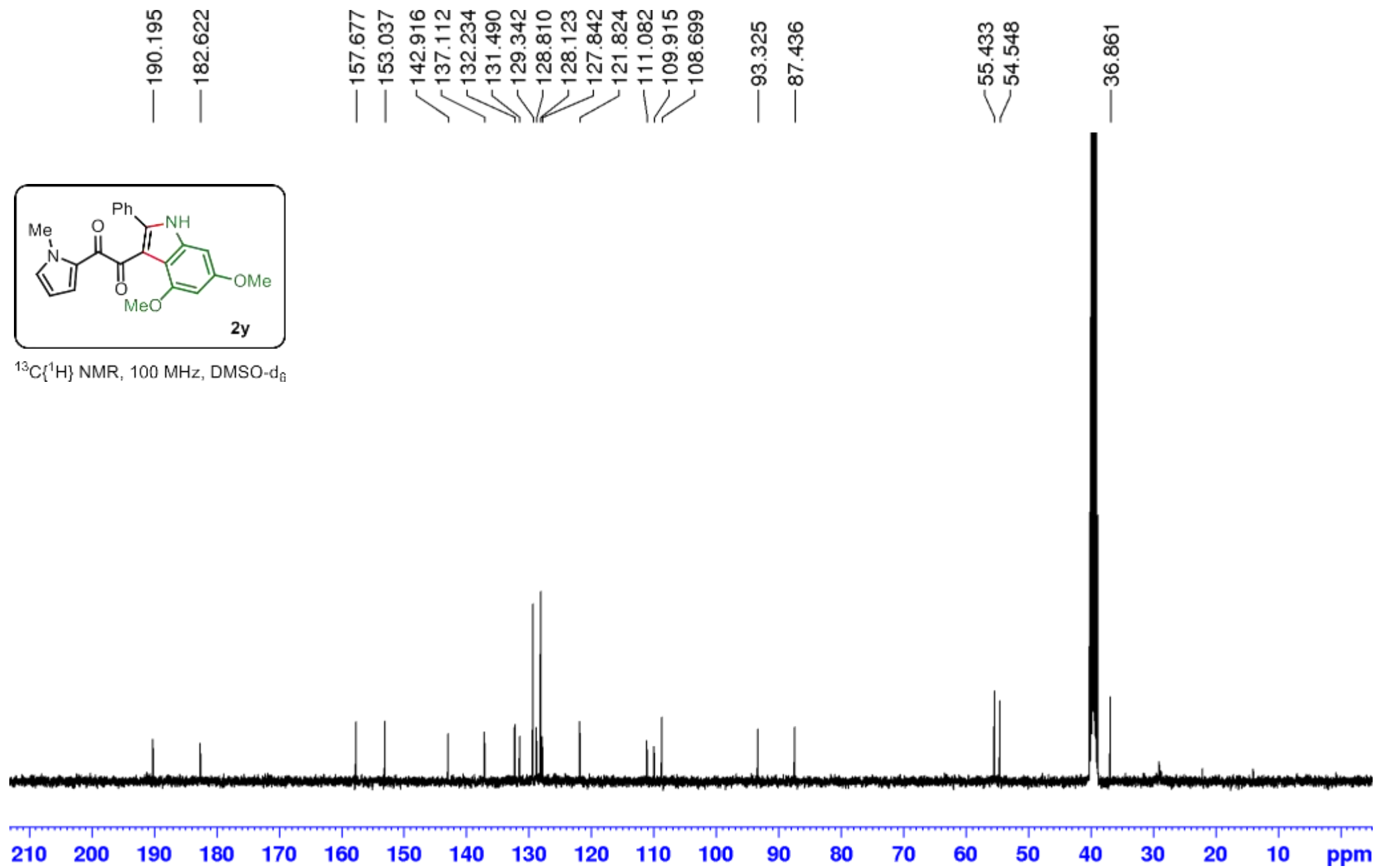
Minimum: -1.5
Maximum: 2.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
355.1439	355.1447	-0.8	-2.3	15.5	1190.6	n/a	n/a	C23 H19 N2 O2





$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, DMSO-d_6



Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)

Elements Used:

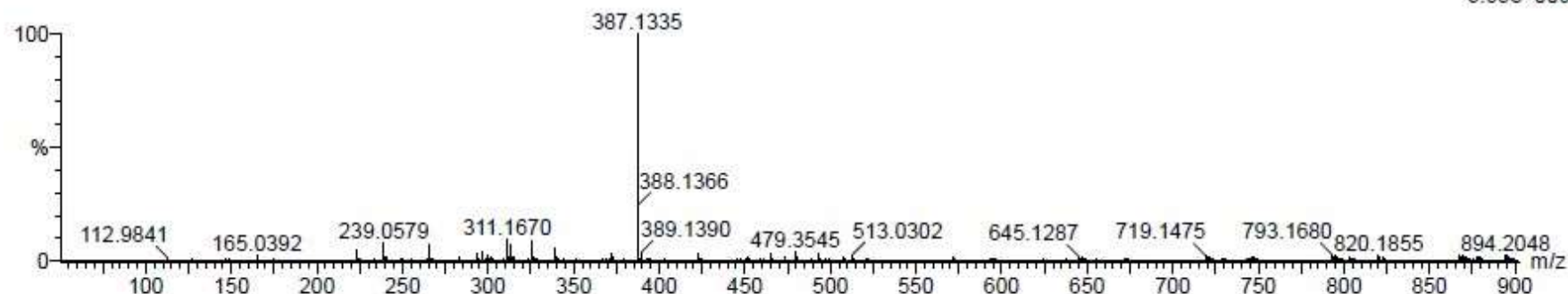
C: 0-23 H: 0-100 N: 0-2 O: 0-4

NVD/B-15

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

15-Jul-2024
14:54:37
1: TOF MS ES-
9.99e+006

150724_14 6 (0.138)



Minimum: -1.5
Maximum: 2.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
387.1335	387.1345	-1.0	-2.6	15.5	1166.9	n/a	n/a	C23 H19 N2 O4