

Supporting Information

$Cu(II)/I_2$ Mediated $C_{sp^2} - C_{sp}$ Bond Cleavage of 1,2-Alkyndiones Followed by C-O Bond Formation

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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 (60 F-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.

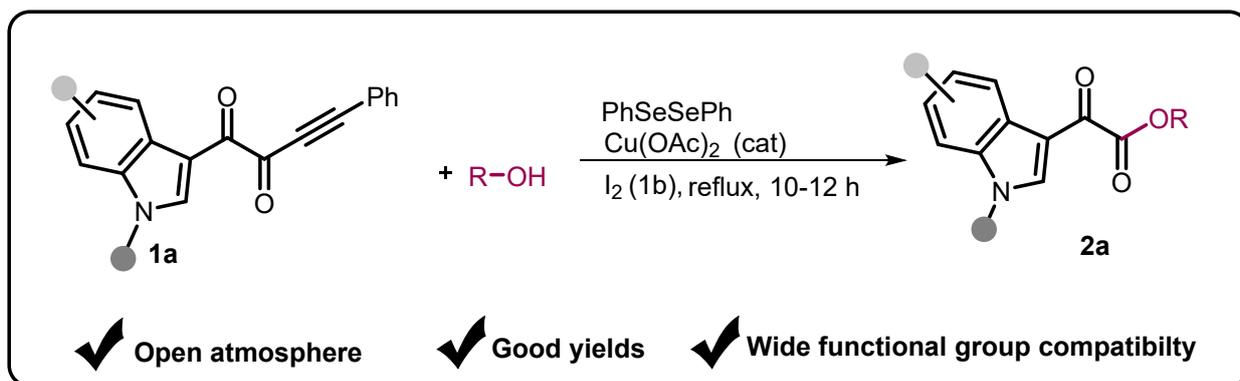
2. Synthesis of Starting Materials:

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 at 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 Procedures:

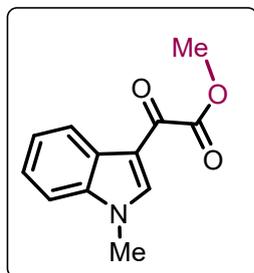
Procedure for the Cu/I_2 Catalysed $C_{sp^2}-C_{sp}$ bond cleavage of α -keto 1,2 Alkyneiones followed by C-O bond formation



To the solution of indole-tethered ynedione **1a** (1.0 equiv.) in alcohol, Iodine and diphenyldisilide was added, Cu(OAc)₂ (10 mol %). The resulting mixture was stirred at refluxing temperature. Progress of reaction was monitored periodically by TLC. Upon completion, the reaction mixture was concentrated under reduced pressure and directly subjected for silica gel column purification by using ethyl acetate and petroleum ether mixture as eluent.

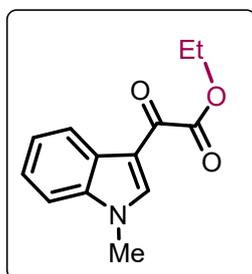
4. Characterization Data of Synthesized Compounds

Methyl 2-(1-methyl-1H-indol-3-yl)-2-oxoacetate (2a)²: The title compound as off white solid (60 mg, 79% yield); R_f: 0.50 (20% ethyl acetate -petroleum ether); ¹H NMR (400 MHz, CDCl₃)



δ 8.44-8.40 (m, 1H), 8.31 (s, 1H), 7.35-7.34 (m, 3H), 3.94 (s, 3H), 3.84 (s, 3H) ppm; ¹³C{¹H}NMR (100 MHz, CDCl₃) δ 176.9, 163.5, 140.6, 137.4, 127.1, 124.3, 123.7, 122.9, 112.9, 110.0, 52.8, 33.9 ppm; HRMS (ESI): calcd. for C₁₃H₁₁NO₃ [M+H]⁺: 218.0817 found 218.0812.

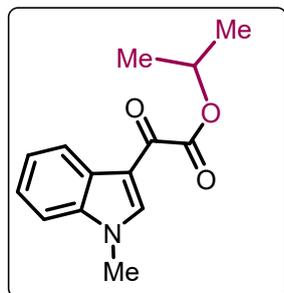
acetate -petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 8.41-8.37 (m, 1H), 8.20 (s, 2H), 3.76 (s, 3H),



Ethyl 2-(1-methyl-1H-indol-3-yl)-2-oxoacetate (2b)³: The title compound as off white solid (65 mg, 81% yield); R_f: 0.56 (20% ethyl acetate -petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 8.41-8.37 (m, 1H), 7.33-7.26 (m, 3H), 4.41-4.35 (q, *J*=7.12 Hz, 2H), 1.43-1.40 (d, *J*=7.15 Hz, 3H) ppm; ¹³C{¹H}NMR

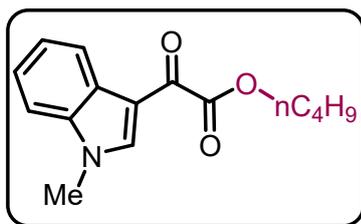
(100 MHz, CDCl₃) δ 177.4, 163.0, 140.3, 137.3, 127.0, 124.1, 123.5, 122.6, 112.7, 109.9, 62.0, 33.7, 14.1 ppm; HRMS (ESI): calcd. for C₁₃H₁₃NO₃ [M+H]⁺: 232.0974, found 232.0986.

Isopropyl 2-(1-methyl-1*H*-indol-3-yl)-2-oxoacetate (2c)⁴: The title compound as off orange solid (66 mg, 77% yield); R_f: 0.50 (20% ethyl acetate -petroleum ether); ¹H NMR (400 MHz,



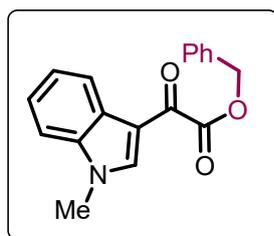
CDCl₃) δ 8.44-8.40 (m, 1H), 8.28 (s, 1H), 7.35-7.32 (m, 3H), 5.29-5.11 (m, 1H), 3.84 (s, 3H), 1.41 (d, *J*=6.28 Hz, 6H) ppm; ¹³C {¹H}NMR (100 MHz, CDCl₃) δ 177.8, 162.5, 140.0, 137.1, 126.7, 123.8, 123.2, 122.3, 112.4, 109.8, 69.8, 33.5, 21.6 ppm; HRMS (ESI): calcd. for C₁₄H₁₅NO₃ [M+H]⁺: 246.1130, found 246.1112.

Butyl 2-(1-methyl-1*H*-indol-3-yl)-2-oxoacetate (2d)⁵: The title compound as off white solid (61 mg, 72% yield); R_f: 0.52 (20% ethyl acetate -petroleum ether); ¹H NMR (400 MHz,



CDCl₃) δ 8.40-8.38 (m, 1H), 8.19 (s, 1H), 7.31-7.26 (m, 3H), 4.37-4.33 (t, *J*=6.89 Hz, 2H), 3.75 (s, 3H), 1.79-1.65 (m, 3H), 1.00-0.92 (m, 6H) ppm; ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 177.4, 163.1, 140.2, 140.2, 137.2, 126.9, 124.0, 123.4, 122.5, 112.0, 109.9, 64.6, 37.0, 33.7, 25.0, 24.4 ppm; HRMS (ESI): calcd. for C₁₅H₁₇NO₃ [M+H]⁺: 260.1287, found 260.1287.

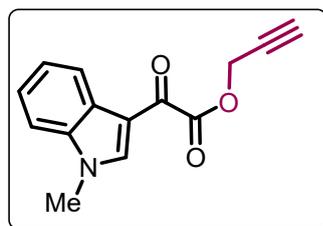
Benzyl 2-(1-methyl-1*H*-indol-3-yl)-2-oxoacetate (2e)⁶: The title compound as off white solid



(70 mg, 69% yield); R_f: 0.51 (20% ethyl acetate -petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 8.40-8.38 (m, 1H), 8.18 (s, 1H), 7.46-7.44 (m, 2H), 7.39-7.30 (m, 6H), 5.35 (s, 2H), 3.76 (s, 3H) ppm; ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 177.0, 162.8, 140.4, 137.3, 135.1, 128.7, 128.6, 128.5, 124.1, 123.5, 122.6, 112.7, 110.0, 67.5, 33.8 ppm; HRMS

(ESI): calcd. For C₁₈H₁₅NO₃ [M+H]⁺: 294.1130, found 294.1131.

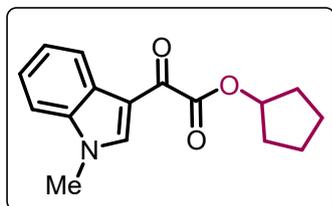
Prop-2-yn-1-yl 2-(1-methyl-1*H*-indol-3-yl)-2-oxoacetate (2f)⁷: The title compound as off brown solid (57 mg, 68 % yield); R_f: 0.54 (20% ethyl acetate -petroleum ether); ¹H NMR (400



MHz, CDCl₃) δ 8.43-8.39 (m, 1H), 8.31 (s, 1H), 7.37-7.34 (m, 3H), 4.92 (d, *J*=2.46 Hz, 2H), 3.87 (d, *J*=2.63 Hz, 1H), 7.23 (s, 1H), 7.17-7.13 (m, 1H), 7.10 (dd, *J*=8.67, 2.07 Hz, 1H), 6.98-6.94 (s, 3H), 2.56 (t, *J*=2.47 Hz, 1H) ppm; ¹³C {¹H}NMR (100 MHz, CDCl₃) δ 175.9, 161.9, 156.1, 140.5, 137.3, 126.9, 124.3, 123.6,

122.6, 112.6, 110.0, 75.9, 75.7, 54.4, 33.9 ppm; HRMS (ESI): calcd. for $C_{14}H_{11}NO_3$ $[M+H]^+$: 242.0817, found 242.0793.

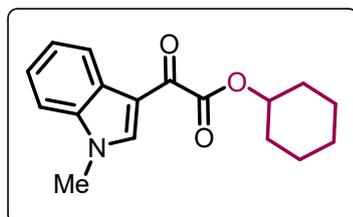
Cyclopentyl 2-(1-methyl-1*H*-indol-3-yl)-2-oxoacetate (2g)⁸: The title compound as off white solid (62 mg, 66% yield); R_f : 0.54 (20% ethyl acetate -petroleum ether); 1H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 8.18-8.11 (m, 1H), 7.50-7.10 (m, 3H), 5.38-



5.35 (m, 1H), 3.78(s, 3H), 2.00-1.63 (m, 8H) ppm; ^{13}C $\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 178.0, 163.1, 140.2, 137.3, 140.2, 137.3, 127.0, 124.1, 123.5, 122.7, 112.8, 109.9, 79.1, 33.8, 32.8, 32.7 ppm; HRMS (ESI): calcd. for $C_{16}H_{18}NO_3$ $[M+H]^+$: 272.1287, found

272.1288.

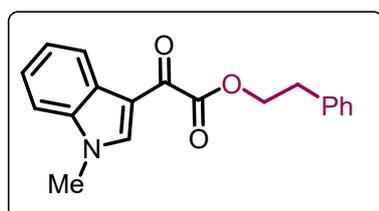
Cyclohexyl 2-(1-methyl-1*H*-indol-3-yl)-2-oxoacetate (2h)⁹: The title compound as off white solid (63 mg, 64% yield); R_f : 0.56 (20% ethyl acetate -petroleum ether); 1H NMR (400 MHz, $CDCl_3$) δ 8.42-8.40 (m, 1H), 8.23(s, 1H), 7.35-7.32 (m, 3H),



5.02-4.95 (m, 1H), 3.82 (s, 3H), 2.02-1.98 (m, 2H), 71.85-1.79 (m, 2H) 1.66-1.55 (m, 3H), 1.47-1.25 (m, 3H) ppm; ^{13}C $\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 178.1, 162.7, 140.2, 137.3, 127.1, 124.1, 123.5, 122.8, 112.9, 109.9, 75.0, 33.8, 31.5, 25.3, 23.9 ppm; HRMS

(ESI): calcd. for $C_{17}H_{19}NO_3$ $[M+H]^+$: 286.1443 found 286.1435.

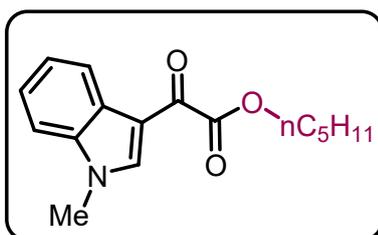
Phenethyl 2-(1-methyl-1*H*-indol-3-yl)-2-oxoacetate (2i)¹⁰: The title compound as off yellow



solid (75 mg, 70 % yield); R_f : 0.59 (20% ethyl acetate - petroleum ether); 1H NMR (400 MHz, $CDCl_3$) δ 8.42-8.38 (m, 1H), 7.88 (s, 1H), 7.33-7.14 (m, 9H), 4.55 (t, $J=7.00$ Hz, 2H), 3.69 (s, 3H), 3.08 (t, $J=6.92$ Hz, 2H) ppm; ^{13}C $\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 177.9, 162.9, 140.3, 137.4, 137.2, 129.1, 128.6,

126.9, 126.7, 124.1, 123.5, 122.6, 112.6, 109.9, 66.2, 34.9, 33.7 ppm; HRMS (ESI): calcd. for $C_{19}H_{17}NO_3$ $[M+H]^+$: 308.1287, found 308.1289.

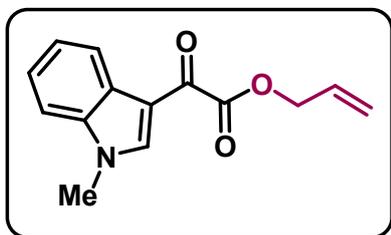
Pentyl 2-(1-methyl-1*H*-indol-3-yl)-2-oxoacetate (2j)¹¹: The title compound as off yellow liquid (75 mg, 79% yield); R_f : 0.55 (20% ethyl acetate -petroleum ether); 1H NMR (400 MHz, $CDCl_3$) δ 8.43-8.39 (m, 1H), 8.31(s, 1H), 7.37-7.34 (m, 3H),



4.92 (d, $J=2.84$ Hz, 2H), 3.87 (s, 3H), 2.56 (t, $J=2.47$ Hz, 1H) ppm; ^{13}C $\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 175.9, 161.9, 156.1, 140.5, 137.3, 126.9, 124.3, 123.6, 122.6, 112.6, 110.0, 54.4, 33.9 ppm; HRMS (ESI): calcd. for $C_{16}H_{19}NO_3$ $[M+H]^+$: 274.1443,

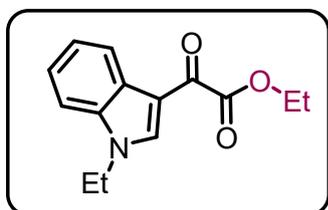
found 274.1438.

Allyl 2-(1-methyl-1*H*-indol-3-yl)-2-oxoacetate (2k)¹¹: The title compound as off brown solid (58 mg, 69 % yield); *R_f*: 0.55 (20% ethyl acetate -petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 8.44-8.42 (m, 1H), 8.32 (s, 1H), 7.37-7.35 (m, 3H), 6.09-5.99 (m, 1H), 5.47-5.43 (m, 1H), 5.35-5.32 (m, 1H), 4.85-4.83 (m, 2H), 3.87(s, 3H) ppm; ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 177.1, 162.7, 140.4, 137.4, 131.3, 127.1, 124.3, 123.7, 122.9, 119.6, 112.9, 110.0, 66.6, 33.9

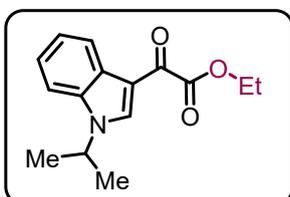


ppm; HRMS (ESI): calcd. for C₁₄H₁₃NO₃ [M+H]⁺: 244.0974, found 244.0979.

Ethyl 2-(1-ethyl-1*H*-indol-3-yl)-2-oxoacetate (2l)¹²: The title compound as off white solid (68 mg, 84 % yield); *R_f*: 0.53 (20% ethyl acetate -petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 8.45-8.41 (m, 1H), 8.34 (s, 1H), 7.37-7.29 (m, 3H), 4.40(q, *J*=14.33 Hz, 2H), 4.19 (t, *J*=14.60 Hz, 2H), 1.52 (t, *J*=7.32 Hz, 3H), 1.42 (t, *J*=7.15, 3H) ppm; ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 177.2, 162.8, 136.5, 136.1, 129.1, 126.9, 123.7, 123.1, 122.4, 112.5, 109.9, 61.7, 41.8, 14.6, 13.92 ppm; HRMS (ESI): calcd. for C₁₄H₁₆NO₃ [M+H]⁺: 246.1130, found 246.1136.

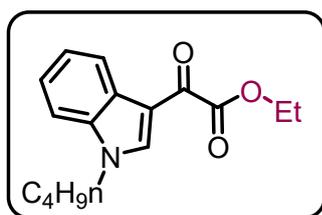


ppm; HRMS (ESI): calcd. for C₁₄H₁₆NO₃ [M+H]⁺: 246.1130, found 246.1136.



Ethyl 2-(1-isopropyl-1*H*-indol-3-yl)-2-oxoacetate (2m)¹²: The title compound as off yellow liquid (66 mg, 80% yield); *R_f*: 0.54 (20% ethyl acetate-petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 8.42-8.41(m, 1H), 7.38-7.37 (m, 1H), 7.32-7.27 (m, 3H), 4.67-4.60 (m, 1H), 4.38 (q, *J*=7.16 Hz, 2H), 1.54 (d, *J*=6.72 Hz, 6H), 1.41(t, *J*=7.12 Hz, 3H) ppm; ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 177.3, 163.0, 136.3, 135.7, 127.2, 123.8, 123.4, 122.7, 112.9, 110.2, 61.9, 48.3, 22.3, 14.0 ppm; HRMS (ESI): calcd. for C₁₅H₁₇NO₃ [M+H]⁺: 260.1287, found 260.1290.

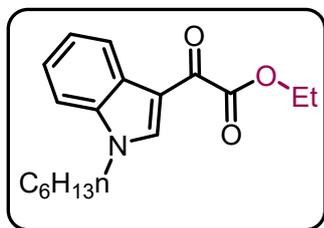
Ethyl 2-(1-butyl-1*H*-indol-3-yl)-2-oxoacetate (2n)¹²: The title compound as off yellow solid (82 mg, 82 % yield); *R_f*: 0.57 (20% ethyl acetate -petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 8.46-8.43 (m, 1H), 8.37 (s, 1H), 7.40-7.32 (m, 3H), 4.41(q, *J*=7.13 Hz, 2H), 4.18 (t, *J*=7.18, 2H), 1.92-1.85 (m, 2H), 1.45-1.36 (m, 5H) 0.96 (t, *J*=7.35 Hz, 3H) ppm; ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 177.9, 163.9, 140.3, 137.2, 129.1, 128.6, 126.9, 126.9, 124.1, 123.5, 122.6, 112.6, 109.9, 66.2, 34.9, 33.7



ppm; HRMS (ESI): calcd. for C₁₉H₂₃NO₃ [M+H]⁺: 323.1647, found 323.1647.

ppm; HRMS (ESI): calcd. for $C_{16}H_{19}NO_3$ $[M+H]^+$: 274.1443, found 274.1441.

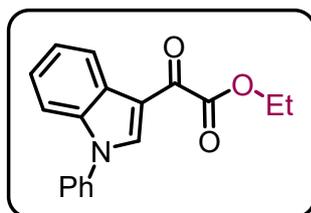
Ethyl 2-(1-hexyl-1H-indol-3-yl)-2-oxoacetate (2o)¹²: The title compound as off yellow solid (70 mg, 83 % yield); R_f : 0.58 (20% ethyl acetate -petroleum ether); 1H NMR (400 MHz,



$CDCl_3$) δ 8.46-8.42 (m, 1H), 8.33 (s, 1H), 7.37-7.29 (m, 3H), 4.40 (q, $J=7.15$ Hz, 2H), 4.12 (t, $J=7.16$ Hz, 2H), 1.90-1.83 (m, 2H), 1.42 (t, $J=7.15$ Hz, 3H), 1.36-1.26 (m, 6H), 0.87 (t, $J=6.92$ Hz, 3H) ppm; ^{13}C $\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 177.4, 163.0, 139.4, 136.6, 127.2, 124.0, 123.4, 122.8, 112.8, 110.2, 47.4, 31.2,

29.6, 26.4, 22.4, 14.1, 13.9 ppm; HRMS (ESI): calcd. for $C_{18}H_{23}NO_3$ $[M+H]^+$: 302.1756, found 302.1760.

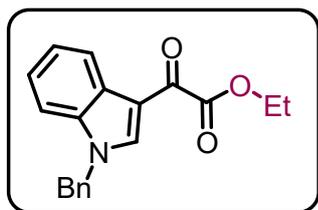
Ethyl 2-oxo-2-(1-phenyl-1H-indol-3-yl)acetate (2p)¹²: The title compound as off white solid (77 mg, 76 % yield); R_f : 0.52 (20% ethyl acetate -petroleum ether); 1H NMR (400 MHz,



$CDCl_3$) δ 8.56 (s, 1H), 8.52-8.50 (m, 1H), 7.60-7.46 (m, 6H), 7.43-7.7.31(m, 2H), 4.42 (q, $J=7.14$ Hz, 2H), 1.44 (t, $J=7.15$ Hz, 3H) ppm; ^{13}C $\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 178.1, 162.9, 139.2, 138.0, 137.0, 130.0, 128.6, 125.1, 124.7, 124.0, 123.0.9, 114.5, 111.2, 62.3, 14.2 ppm; HRMS (ESI): calcd. for $C_{18}H_{15}NO_3$

$[M+H]^+$: 294.1130, found 294.1128.

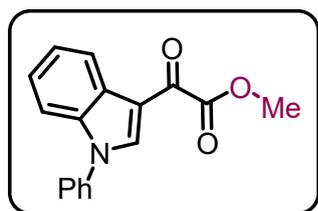
Ethyl 2-(1-benzyl-1H-indol-3-yl)-2-oxoacetate (2q)¹²: The title compound as off orange (59 mg, 70% yield); R_f : 0.58 (20% ethyl acetate -petroleum ether); 1H NMR (400 MHz, $CDCl_3$) δ



8.45 (d, $J=7.80$ Hz, 1H), 8.38 (s, 1H), 7.34-7.24 (m, 6H), 7.17-7.14 (m, 2H), 5.33 (s, 2H), 4.37 (q, $J=7.17$ Hz, 2H), 1.39 (t, $J=7.15$ Hz, 3H) ppm; ^{13}C $\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 177.6, 162.9, 139.8, 136.8, 135.2, 129.1, 128.3, 127.3, 127.0, 124.3, 123.6, 122.9, 113.3, 110.6, 62.1, 51.1, 14.1 ppm; HRMS (ESI): calcd. for $C_{19}H_{17}NO_3$

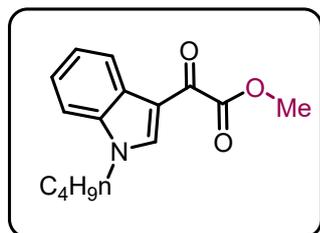
$[M+H]^+$: 308.1287, found 308.1291.

Methyl 2-oxo-2-(1-phenyl-1H-indol-3-yl)acetate (2r)¹²: The title compound as off white solid (60 mg, 75% yield); R_f : 0.56 (20% ethyl acetate -petroleum ether); 1H NMR (400 MHz,



$CDCl_3$) δ 8.57 (s, 1H), 8.52-8.50 (m, 1H), 7.61-7.46 (m, 6H), 7.42-7.32 (m, 2H), 3.96 (s, 3H) ppm; ^{13}C $\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 177.6, 163.2, 139.4, 138.0, 137.1, 130.0, 128.6, 127.3, 125.7, 124.8, 124.1, 123.0, 114.5, 111.2, 52.9 ppm; HRMS (ESI): calcd. for $C_{17}H_{13}NO_3$ $[M+H]^+$: 280.0974, found 280.0977.

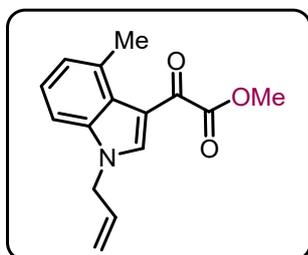
Methyl 2-(1-butyl-1*H*-indol-3-yl)-2-oxoacetate (2s)¹²: The title compound as off orange solid (52 mg, 67% yield); *R*_f: 0.54 (20 % ethyl acetate petroleum ether); ¹H NMR (400 MHz, CDCl₃)



δ 8.45-8.40 (m, 1H), 8.45-8.40 (m, 1H), 8.31(s, 1H), 7.35-7.29 (m, 3H), 4.10 (t, *J*=7.20Hz, 2H), 3.92 (s, 3H), 1.86-1.79 (m, 2H), 1.39-1.25 (m, 2H), 0.93 (t, *J*=7.21 Hz, 3H) ppm; ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 176.8, 163.3, 139.5, 136.6, 127.1, 124.0, 123.4, 122.7, 112.6, 110.2, 52.6, 47.1, 31.6, 20.0, 13.5 ppm; HRMS (ESI):

calcd. for C₁₅H₁₇NO₃ [M+H]⁺: 260.1287, found 260.1291.

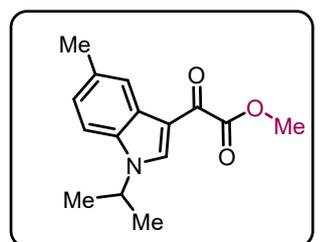
Methyl 2-(1-allyl-4-methyl-1*H*-indol-3-yl)-2-oxoacetate (2t): The title compound as off white solid (65 mg, 83% yield); m.p.= 84-86 °C; *R*_f: 0.54 (20 % ethyl acetate petroleum ether);



¹H NMR (400 MHz, CDCl₃) δ 8.18 (s, 1H), 7.26-7.15 (m, 2H), 7.09 (d, *J*=7.03 Hz, 1H), 6.04-5.94 (m, 1H), 5.31 (dd, *J*=0.82, 0.82 Hz, 1H), 5.18 (dd, *J*=0.79, 0.81Hz, 1H) 4.40 (q, *J*=7.14 Hz, 2H), 2.88 (s, 3H), 1.42 (t, *J*=7.09 Hz, 3H) ppm; ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 178.2, 164.7, 140.6, 137.9, 134.2, 131.5, 125.7, 125.5, 124.5, 119.2, 114.3, 62.1, 49.8, 23.2, 14.2 ppm; HRMS (ESI): calcd.

for C₁₆H₁₈NO₃ [M+H]⁺: 258.1130, found 258.1133.

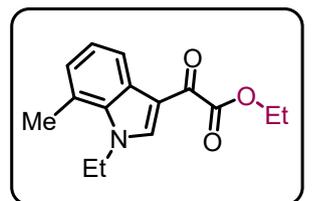
Methyl 2-(1-isopropyl-5-methyl-1*H*-indol-3-yl)-2-oxoacetate (2u): The title compound as off light yellow solid (66 mg, 84% yield); m.p.= 82-84 °C; *R*_f: 0.57 (20% ethyl acetate petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 8.41 (s, 1H), 8.26-8.25 (m,



1H), 7.31(s, *J*=8.37 Hz, 1H), 7.16 (dd, *J*=1.42, 1.43 Hz, 1H), 4.70-4.63 (m, 1H), 3.95(s, 3H), 2.40 (s, 3H), 1.60 (d, *J*=6.65 Hz, 6H) ppm; ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 176.9, 163.7, 136.0, 134.8, 133.5, 127.6, 125.5, 122.8, 112.8, 110.0, 52.7, 48.6, 22.6, 21.6ppm;

HRMS (ESI): calcd. for C₁₅H₁₇NO₃ [M+H]⁺: 260.1287, found 260.1293.

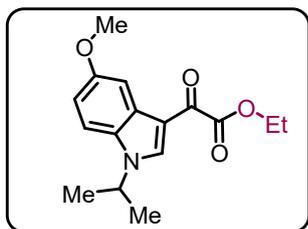
Ethyl 2-(1-ethyl-7-methyl-1*H*-indol-3-yl)-2-oxoacetate (2v): The title compound as off white solid (73 mg, 85% yield); m.p.= 78-80 °C; *R*_f: 0.51 (20% ethyl acetate -petroleum ether); ¹H



NMR (400 MHz, CDCl₃) δ 8.32 (d, *J*=7.98 Hz, 1H), 8.25 (s, 1H), 7.14 (t, *J*=7.59 Hz, 1H), 7.01 (d, *J*=7.07 Hz, 1H), 4.41-4.32 (m, 4H), 2.66 (s, 3H), 1.43-1.40 (m, 6H) ppm; ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 177.1, 162.9, 140.0, 134.9, 128.0, 126.9, 123.2, 121.3, 120.4, 112.3, 61.7, 44.4, 19.3, 16.9, 13.9 ppm; HRMS (ESI): calcd. for

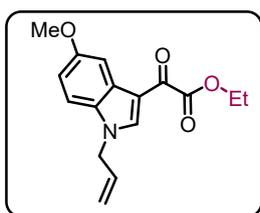
C₁₅H₁₇NO₃ [M+H]⁺: 260.1287, found 260.1286.

Ethyl 2-(1-isopropyl-5-methoxy-1*H*-indol-3-yl)-2-oxoacetate (2w): The title compound as off yellow liquid (67 mg, 80% yield); R_f : 0.54 (20% ethyl acetate -petroleum ether); ^1H NMR (400



MHz, CDCl_3) δ 8.29 (s, 1H), 7.87 (s, 1H), 7.19 (d, $J=8.66$ Hz, 1H), 6.85 (d, $J=8.92$ Hz, 1H), 4.55-4.47 (m, 1H), 4.30 (q, $J=7.12$ Hz, 2H), 3.79 (s, 3H), 1.48 (d, $J=6.65$ Hz, 6H) 1.33 (t, $J=7.09$ Hz, 3H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 177.3, 163.2, 157.0, 135.6, 131.1, 128.3, 114.0, 112.7, 111.1, 104.2, 61.9, 55.7, 48.6, 22.4, 14.1

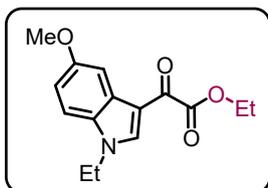
ppm; HRMS (ESI): calcd. for $\text{C}_{16}\text{H}_{19}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 290.1392, found 290.1395.



Ethyl 2-(1-allyl-5-methoxy-1*H*-indol-3-yl)-2-oxoacetate (2x): The title compound as off yellow solid (62 mg, 74% yield); m.p.= 76-78 °C; R_f : 0.56 (20% ethyl acetate -petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ 8.24 (s, 1H), 7.88 (d, $J=2.50$ Hz, 1H), 7.19-7.16 (m, 1H), 6.88 (dd, $J=2.54, 2.54$ Hz, 1H) 5.98-5.89 (m, 1H), 5.26-5.23 (m, 1H), 5.16-5.11

(m, 1H), 4.66-4.67 (m, 2H), 4.33 (q, $J=7.10$ Hz, 2H), 3.82 (s, 3H), 1.36 (t, $J=7.10$ Hz, 3H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 177.5, 163.1, 157.2, 139.3, 131.6, 128.3, 114.4, 113.0, 111.3, 104.3, 62.1, 55.8, 50.1, 14.2 ppm; HRMS (ESI): calcd. for $\text{C}_{16}\text{H}_{17}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 288.1236, found 288.1214.

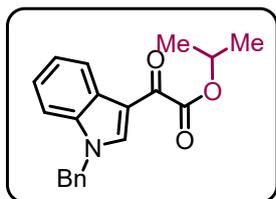
Ethyl 2-(1-ethyl-5-methoxy-1*H*-indol-3-yl)-2-oxoacetate (2y): The title compound as off yellow solid (69 mg, 83% yield); m.p.= 68-70 °C; R_f : 0.59 (20% ethyl acetate -petroleum



ether); ^1H NMR (400 MHz, CDCl_3) δ 8.32 (s, 1H), 7.95 (d, $J=2.50$ Hz, 1H), 7.26 (t, $J=5.27$, 1H), 6.96 (dd, $J=2.55, 2.56$, 1H), 4.40 (q, $J=7.16$ Hz, 2H), 4.19 (q, $J=7.32$ Hz, 3H), 3.90 (s, 3H), 1.54 (t, $J=7.31$ Hz, 3H), 1.43

(t, $J=7.13$ Hz, 3H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 177.4, 163.2, 157.1, 138.5, 131.3, 128.4, 114.2, 112.7, 110.9, 104.3, 62.0, 55.8, 42.3, 15.1, 14.2 ppm; HRMS (ESI) : calcd. for $\text{C}_{15}\text{H}_{17}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 276.1236, found 276.1233.

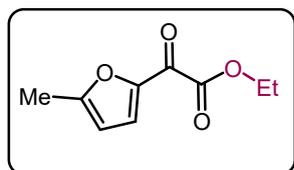
Isopropyl 2-(1-benzyl-1*H*-indol-3-yl)-2-oxoacetate (2z): The title compound as off light yellow solid (60 mg, 68% yield); m.p.= 95-97 °C; R_f : 0.58 (20% ethyl acetate -petroleum



ether); ^1H NMR (400 MHz, CDCl_3) δ 8.46-8.43 (m, 1H), 8.35 (s, 1H), 7.35-7.24 (m, 6H), 7.18-7.16 (m, 2H), 5.33 (s, 2H), 5.24-5.18 (m, 1H), 1.37 (d, $J=6.25$ Hz, 6H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 178.1, 162.6, 139.6, 136.8, 135.2, 129.1, 128.4, 127.3, 127.1, 124.2, 123.6, 122.9, 113.3, 110.5, 70.1, 51.1, 21.7 ppm; HRMS (ESI): calcd.

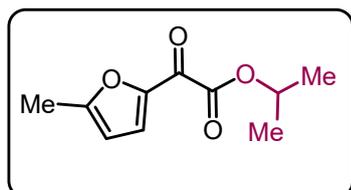
for $\text{C}_{20}\text{H}_{19}\text{NO}_3$ $[\text{M}+\text{H}]^+$: 222.1443, found 222.1449.

Ethyl 2-(5-methylfuran-2-yl)-2-oxoacetate (3a)¹³: The title compound as off yellow solid (53 mg, 70% yield); R_f : 0.40 (20% ethyl acetate -petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ



7.62 (dd, $J=1.95$ Hz, 1.72, 1H), 6.24 (dd, $J=3.85$, 3.82 Hz, 1H), 4.36 (q, $J=15.36$, 2H), 2.41 (s, 3H), 1.37 (t, $J=67.09$ Hz, 3H), ppm; ^{13}C { ^1H } NMR (100 MHz, CDCl_3) δ 170.2, 161.8, 161.4, 148.9, 127.2, 110.2, 62.6, 14.3, 14.0, ppm; HRMS (ESI): calcd. for $\text{C}_9\text{H}_{11}\text{O}_4$ $[\text{M}+\text{H}]^+$:

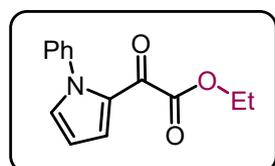
183.2553, found 183.2550



Isopropyl 2-(5-methylfuran-2-yl)-2-oxoacetate (3b)¹³: The title compound as off colorless liquid (61 mg, 74% yield); R_f : 0.44(20% ethyl acetate-petroleum ether); ^1H NMR (400 MHz, CDCl_3) 7.60 (dd, $J=3.60\text{Hz}$, 3.63, 1H), 6.24 (dd, $J=3.59\text{Hz}$, 3.59,

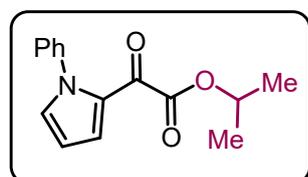
1H), 5.25-5.19 (m, 1H), 2.43 (s, 3H), 1.38 (d, $J=6.34\text{Hz}$, 6H) ppm; ^{13}C { ^1H } NMR (100 MHz, CDCl_3) 170.8, 161.6, 149.03, 126.9, 110.2, 70.9, 21.7, 21.5, ppm; HRMS(ESI): calcd. for $\text{C}_{14}\text{H}_{13}\text{NO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$: 219.0633 found 219.0600.

Ethyl 2-oxo-2-(1-phenyl-1H-pyrrol-3-yl)acetate (3c)¹⁴: The title compound as off white solid (56 mg, 69% yield); R_f : 0.53 (20% ethyl acetate -petroleum ether); ^1H NMR (400 MHz, CDCl_3)



δ 7.43-7.38 (m, 4H), 7.28-7.25 (m, 2H), 7.10 (t, $J=1.71$ Hz, 1H), 6.37 (q, $J=2.60$ Hz, 1H), 4.32 (q, $J=7.18$ Hz, 2H), 1.35 (t, $J=7.10$ Hz, 3H) ppm; ^{13}C { ^1H } NMR (100 MHz, CDCl_3) δ 173.4, 163.2, 139.8, 133.9, 128.7, 128.1, 126.0, 125.5, 110.8, 62.0, 14.0 ppm; HRMS (ESI): calcd. for $\text{C}_{14}\text{H}_{13}\text{NO}_3$ $[\text{M}+\text{H}]^+$: 244.0939 found 244.0974.

Isopropyl 2-oxo-2-(1-phenyl-1H-pyrrol-2-yl)acetate (3d)¹⁴: The title compound as off yellow solid (56 mg, 66% yield); R_f : 0.50 (20% ethyl acetate -petroleum ether); ^1H NMR (400



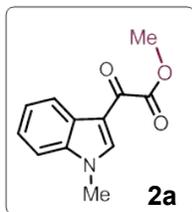
MHz, CDCl_3) δ 7.41-7.34 (m, 4H), 7.27-7.24 (m, 2H), 7.08-7.07 (m, 1H), 6.37-6.35 (m, 1H), 5.21-5.15 (m, 1H), 1.33 (d, $J=6.27$ Hz, 6H) ppm; ^{13}C { ^1H } NMR (100 MHz, CDCl_3) δ 173.8, 162.9, 139.8, 133.8, 128.7, 128.1, 128.0, 125.3, 110.7, 70.1, 21.6 ppm; HRMS

(ESI): calcd. for $\text{C}_{14}\text{H}_{13}\text{NO}_3$ $[\text{M}+\text{H}]^+$: 258.1130 found 258.1128.

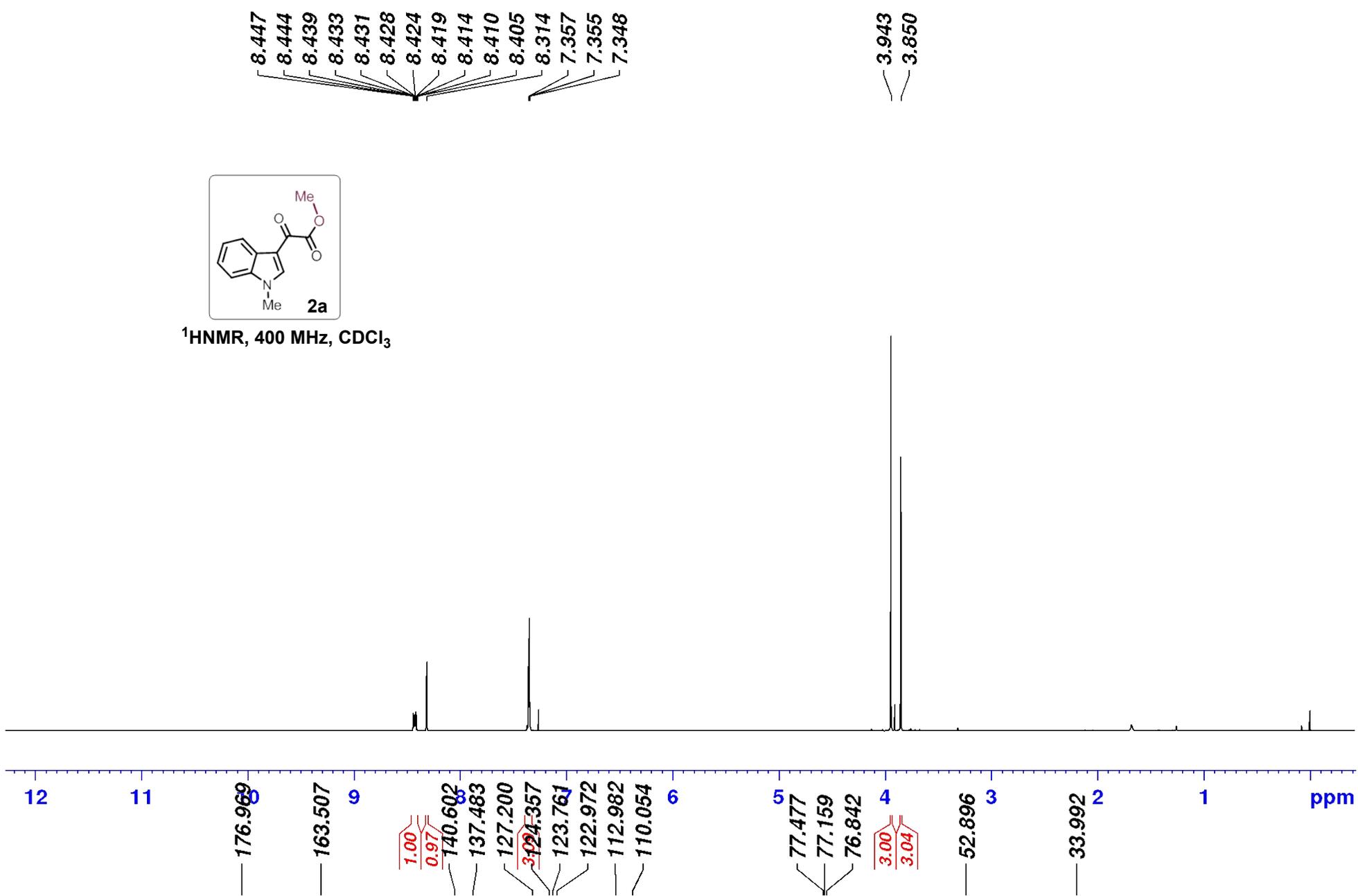
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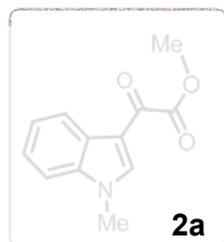
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¹HNMR, 400 MHz, CDCl₃





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

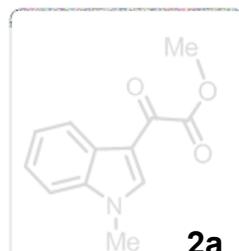
— 140.490

124.238
123.645
122.852

— 109.938

— 52.783

— 33.878



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

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

Elements Used:

C: 0-12 H: 0-100 N: 0-1 O: 0-3

NVD- 37

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

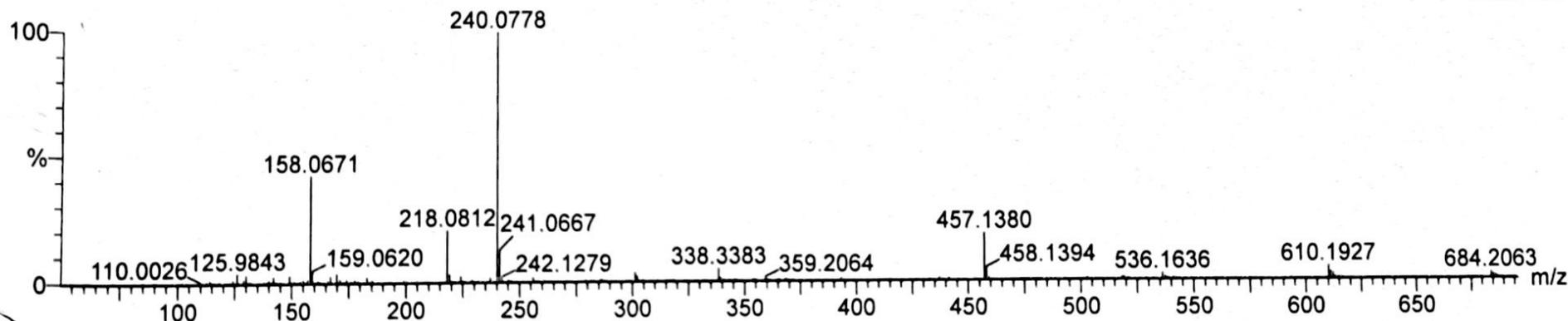
24-Jun-2022

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1: TOF MS ES+

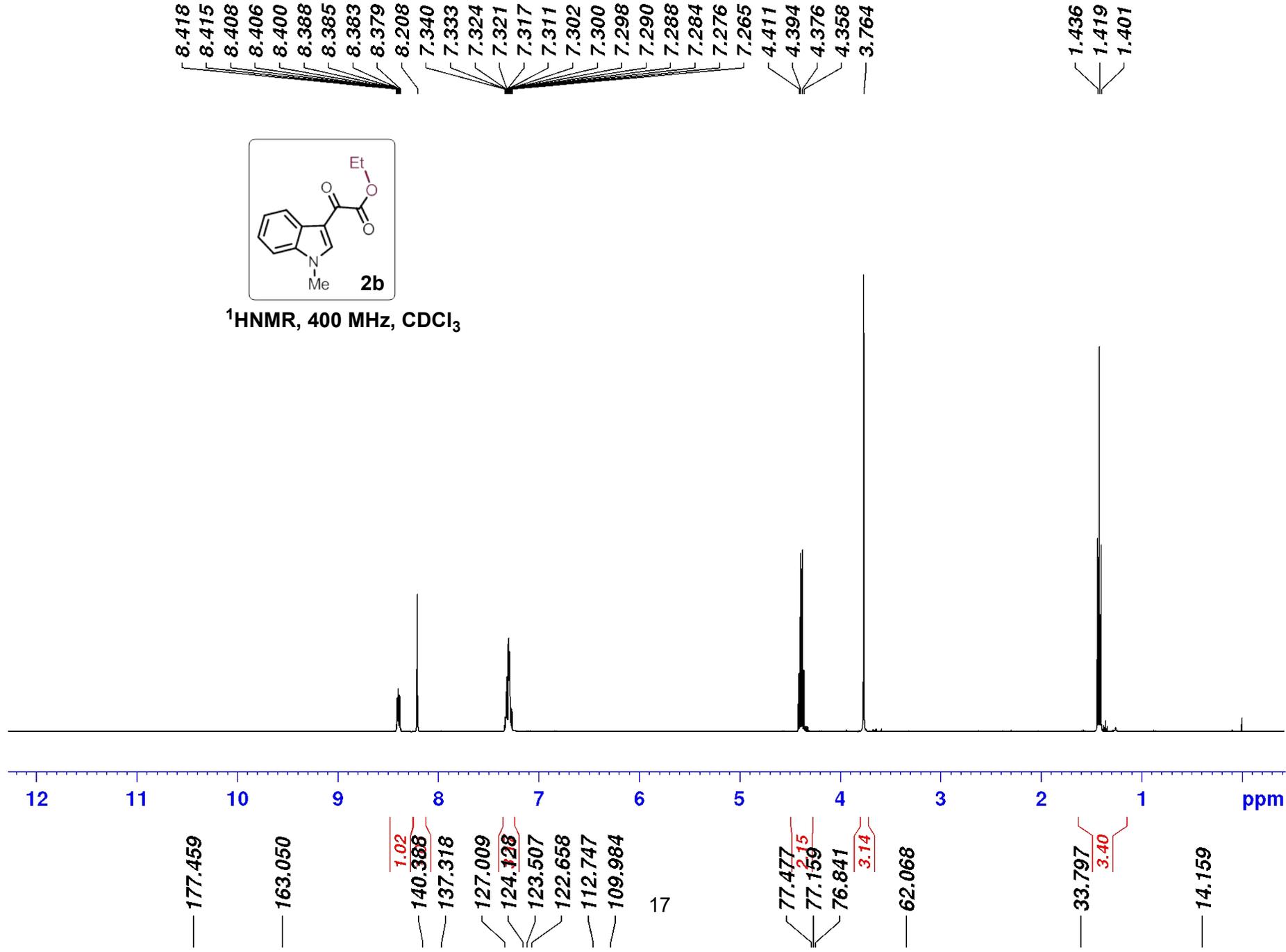
1.26e+007

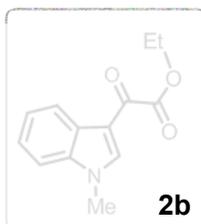
240622_07 7 (0.155) Cm (7)



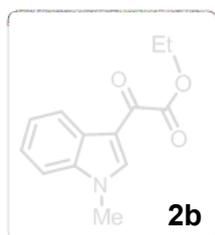
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
218.0812	218.0817	-0.5	-2.3	7.5	56.9	n/a	n/a	C12 H12 N O3





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



DEPT-135NMR, 101 MHz, CDCl_3

— 140.383

124.116
123.495
122.644

— 109.973

— 62.060

— 33.788

— 14.148

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

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

Elements Used:

C: 0-13 H: 0-100 N: 0-1 O: 0-3

NVD-39

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

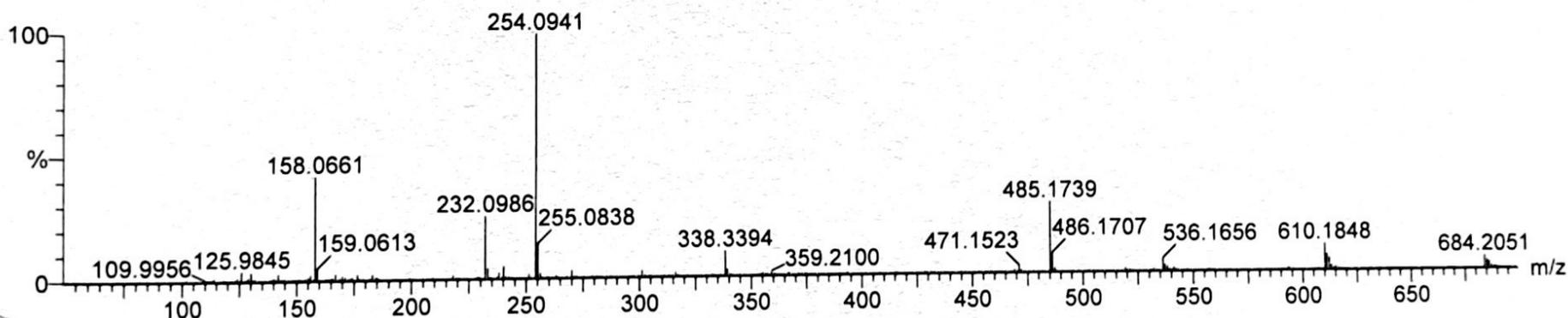
24-Jun-2022

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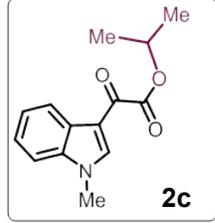
2.48e+007

240622_09 7 (0.155) Cm (7:8)

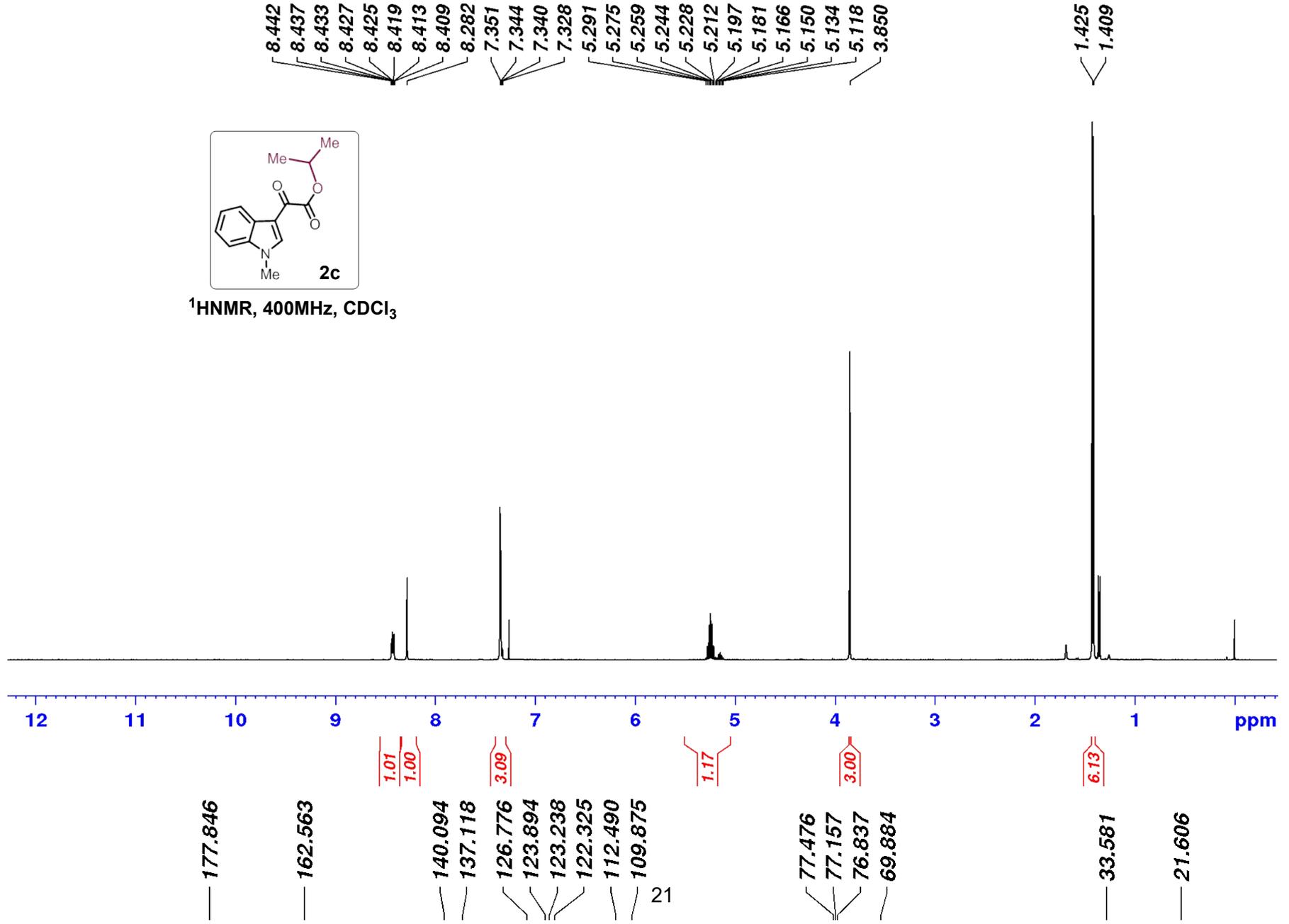


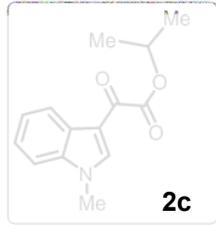
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
232.0986	232.0974	1.2	5.2	7.5	29.6	n/a	n/a	C13 H14 N O3



¹HNMR, 400MHz, CDCl₃





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

— 140.229

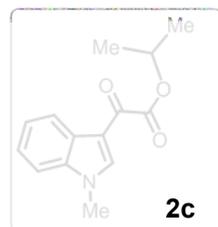
124.022
123.366
122.450

— 110.007

— 70.013

— 33.714

— 21.734



DEPT-135NMR, 101MHz, CDCl₃

Elemental Composition Report

Single Mass Analysis

Tolérance = 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

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

Elements Used:

C: 0-14 H: 0-100 N: 0-1 O: 0-3

NVD 103

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

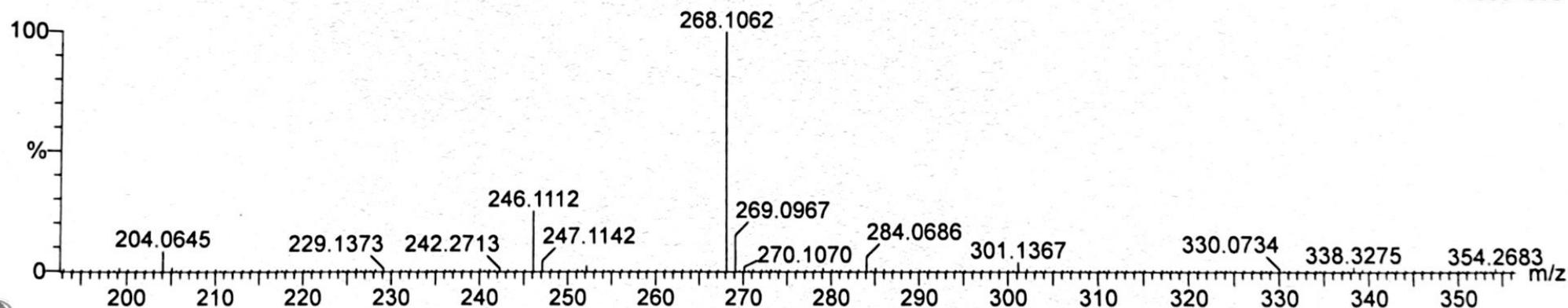
24-Jun-2022

13:20:20

1: TOF MS ES+

7.68e+006

240622_06 9 (0.208) Cm (9)



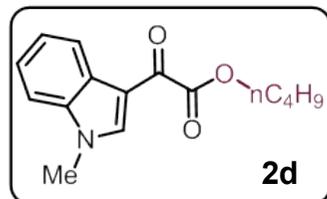
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
246.1112	246.1130	-1.8	-7.3	7.5	20.4	n/a	n/a	C14 H16 N O3

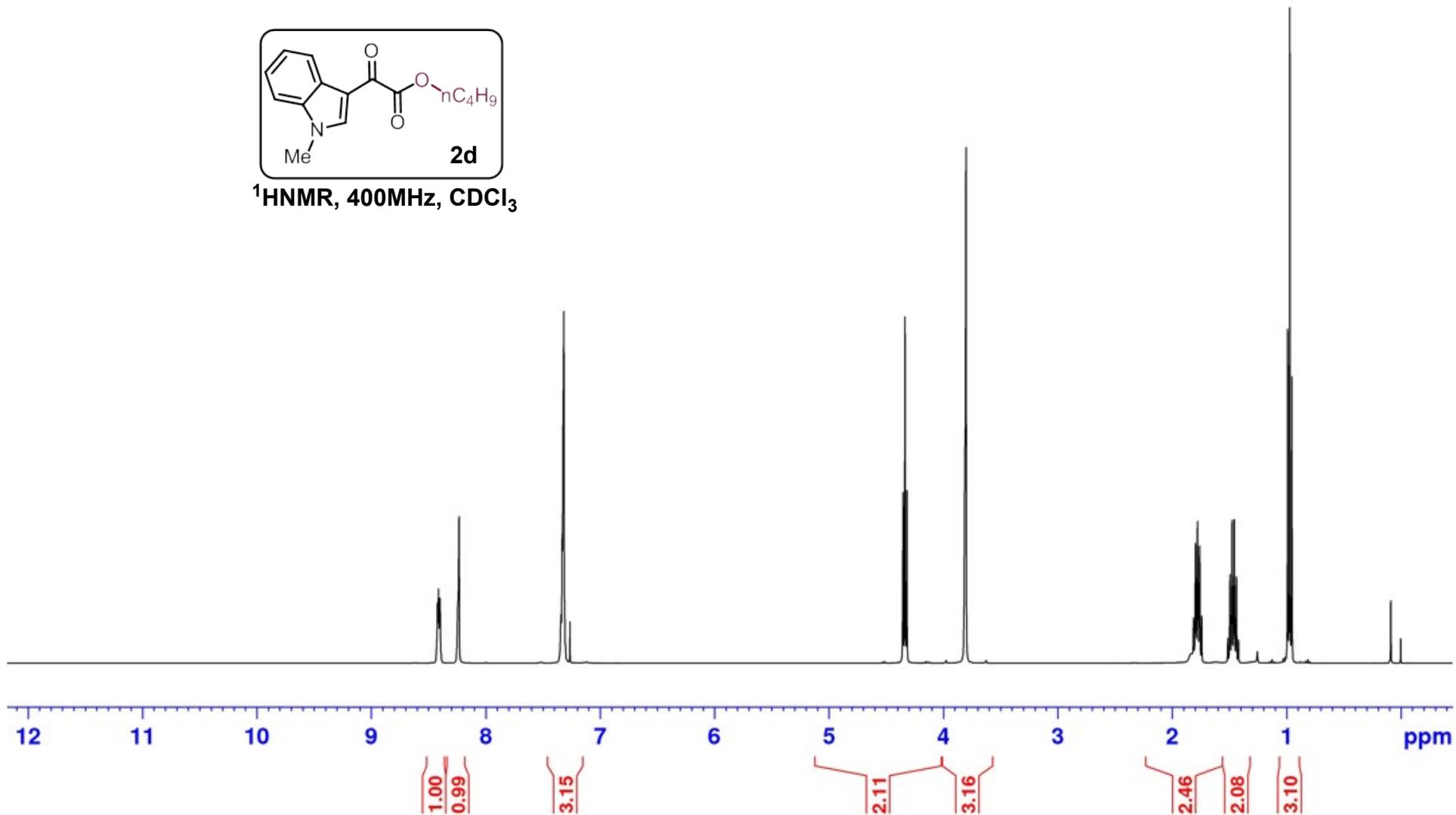
8.421
8.418
8.412
8.409
8.403
8.400
8.397
8.233
7.345
7.341
7.331
7.322
7.317
7.309

4.351
4.334
4.317
—
3.800

1.811
1.795
1.788
1.776
1.757
1.740
1.511
1.493
1.474
1.455
1.437
1.418
0.988
0.970
0.951



¹HNMR, 400MHz, CDCl₃



— 177.530

— 163.220

— 140.358

— 137.339

— 127.021

— 124.146

— 123.527

— 122.683

— 112.805

— 109.988

— 77.478

— 77.160

— 76.842

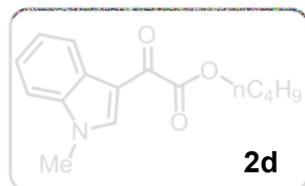
— 65.891

— 33.827

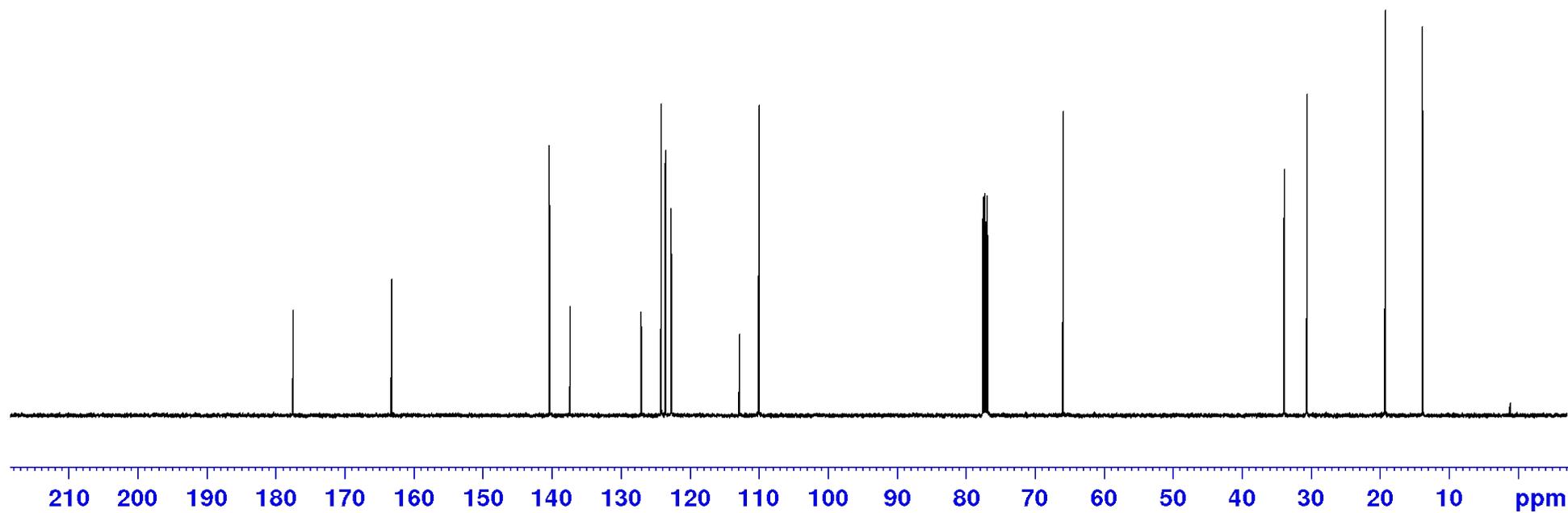
— 30.534

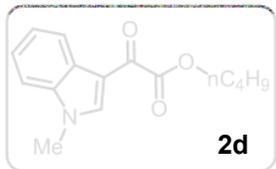
— 19.167

— 13.763



¹³C{¹H}NMR, 100MHz, CDCl₃





DEPT-135NMR, 101MHz, CDCl₃

140.342

124.124

123.506

122.657

109.970

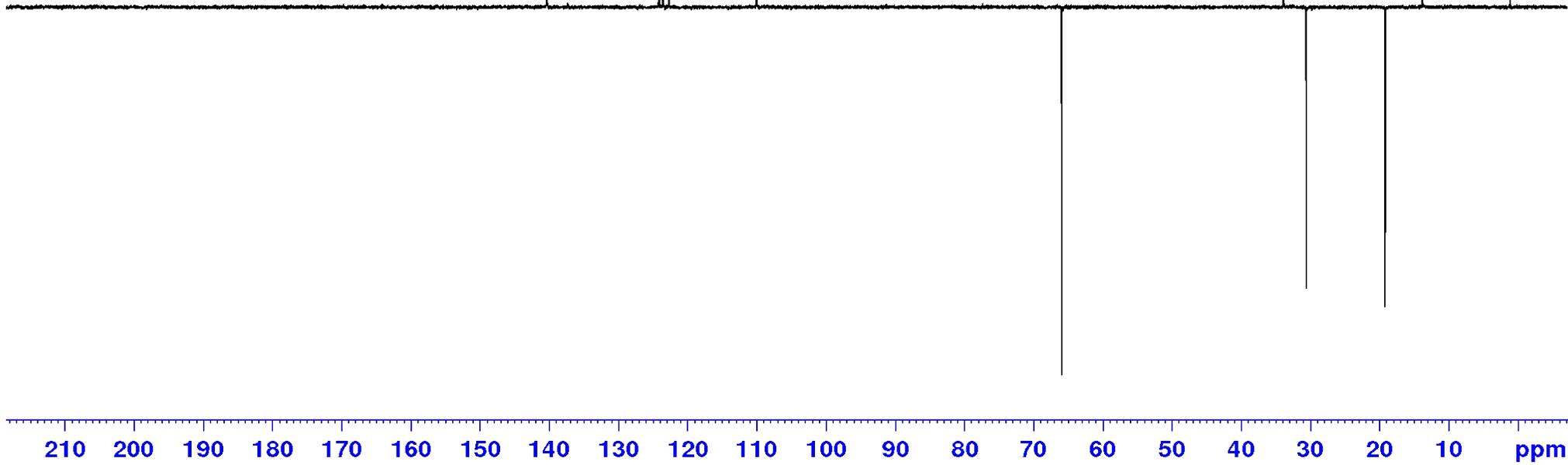
65.872

33.809

30.508

19.145

13.742



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

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

Elements Used:

C: 0-18 H: 0-100 N: 0-1 O: 0-3

NVD-104

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

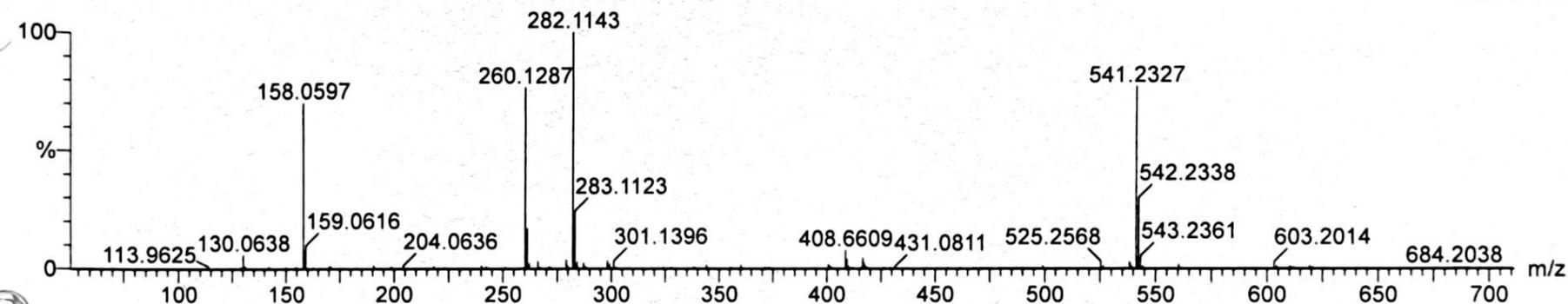
22-Aug-2022

12:14:46

1: TOF MS ES+

2.67e+007

220822_19 7 (0.155)

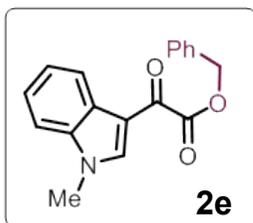


Minimum: -1.5
Maximum: 2.0 50.0 50.0

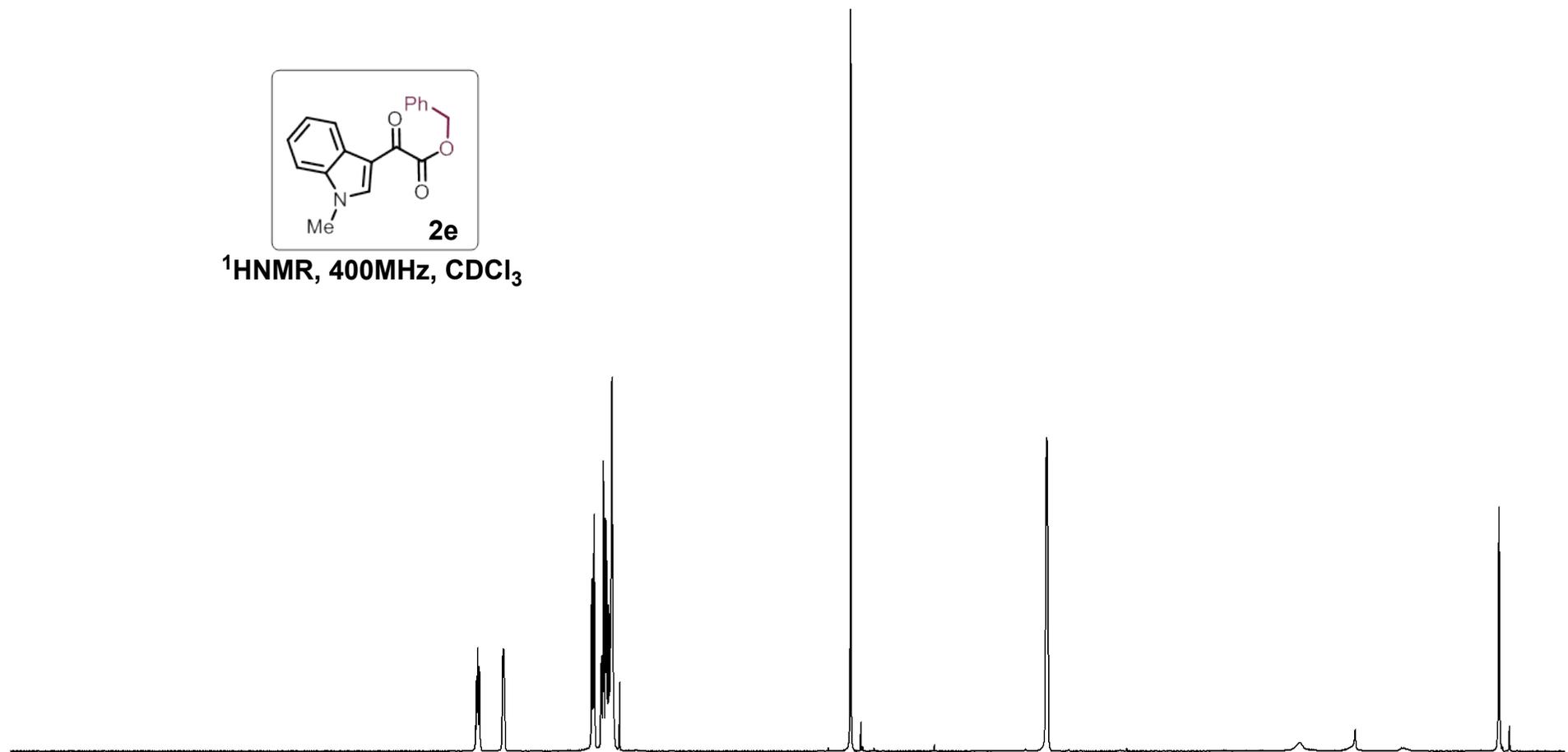
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
260.1287	260.1287	0.0	0.0	7.5	1075.7	n/a	n/a	C15 H18 N O3

8.405
8.403
8.396
8.384
8.381
8.188
7.469
7.465
7.449
7.446
7.394
7.388
7.384
7.372
7.368
7.357
7.353
7.347
7.343
7.337
7.330
7.319
7.316
7.303
5.360

3.766



¹HNMR, 400MHz, CDCl₃



12 11 10 9 8 7 6 5 4 3 2 1 ppm

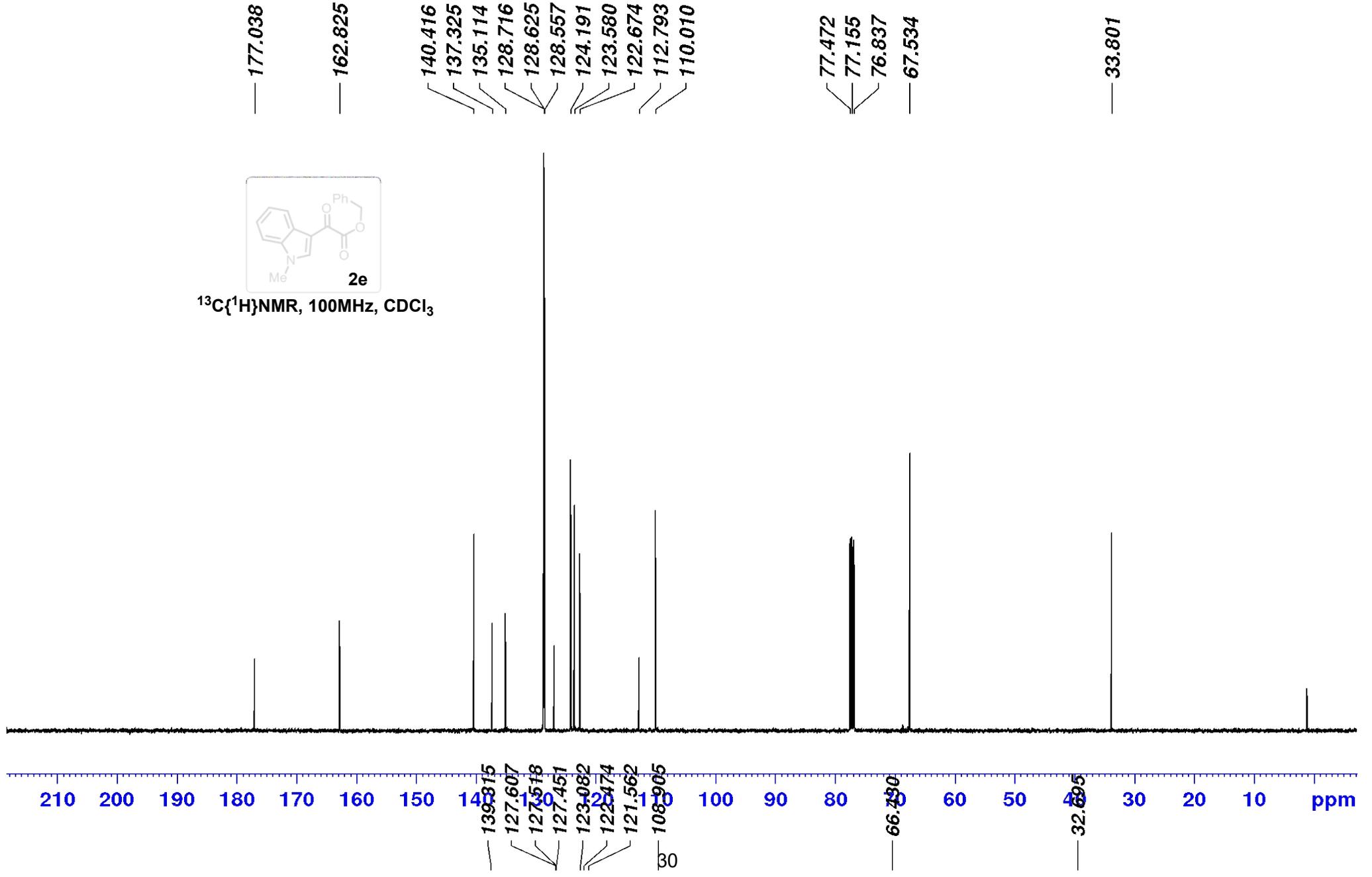
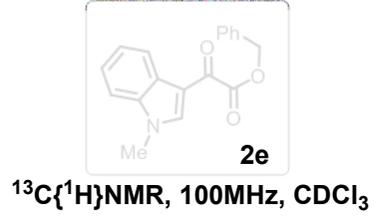
0.98
0.96

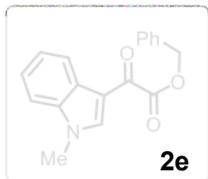
1.92
6.17

29

1.97

3.00





DEPT-135NMR, 101MHz, CDCl₃

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

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

Elements Used:

C: 0-18 H: 0-100 N: 0-1 O: 0-3

NVD-82

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

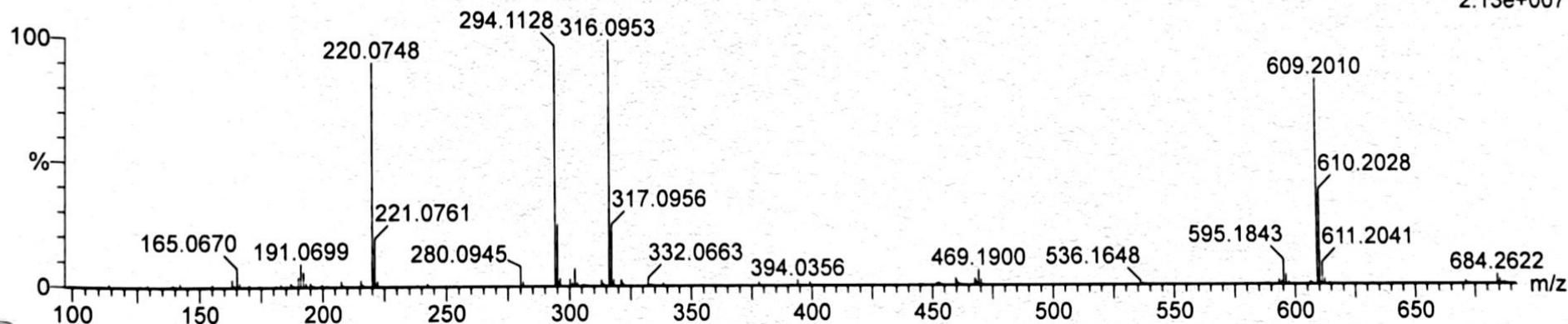
23-Aug-2022

11:41:18

1: TOF MS ES+

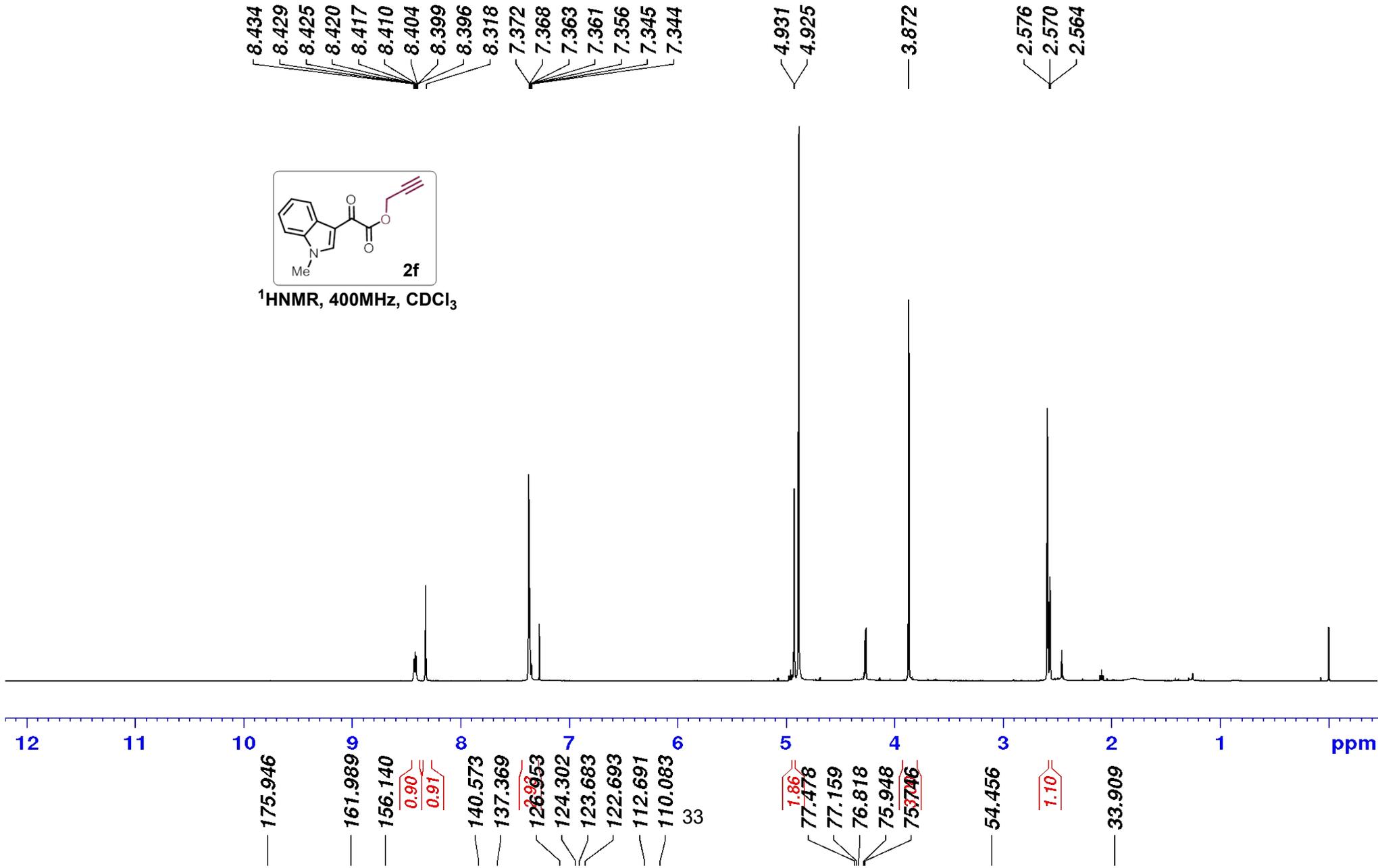
2.13e+007

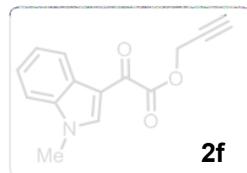
230822_11 8 (0.172)



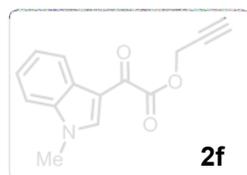
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
294.1128	294.1130	-0.2	-0.7	11.5	970.5	n/a	n/a	C18 H16 N O3





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



DEPT-135NMR, 101MHz, CDCl_3

— 140.549

124.274

123.656

122.664

— 110.056

34

— 76.791

— 54.428

— 33.884

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

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

Elements Used:

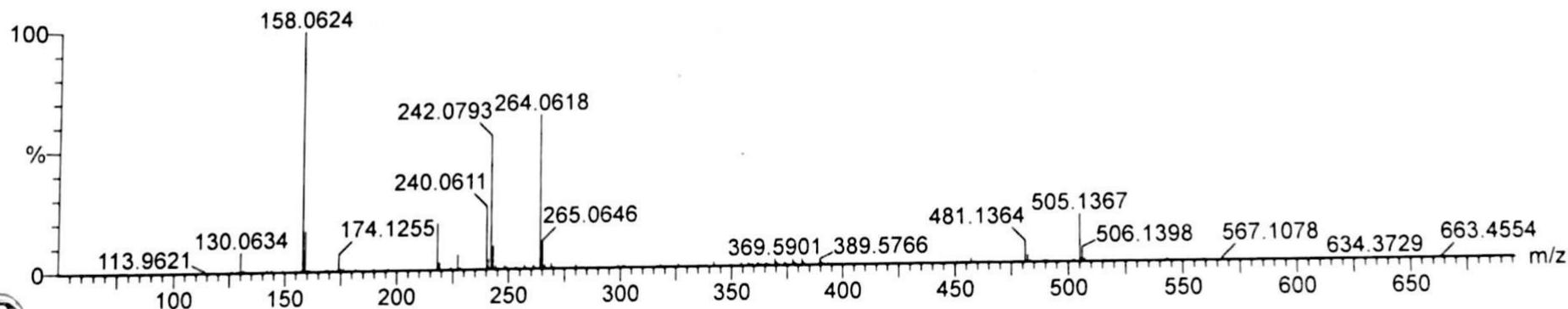
C: 0-19 H: 0-100 N: 0-1 O: 0-3

NVD-102

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

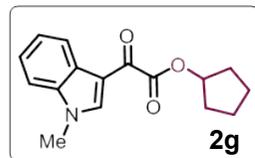
29-Aug-2022
12:45:02
1: TOF MS ES+
2.70e+007

290822_25 6 (0.138)

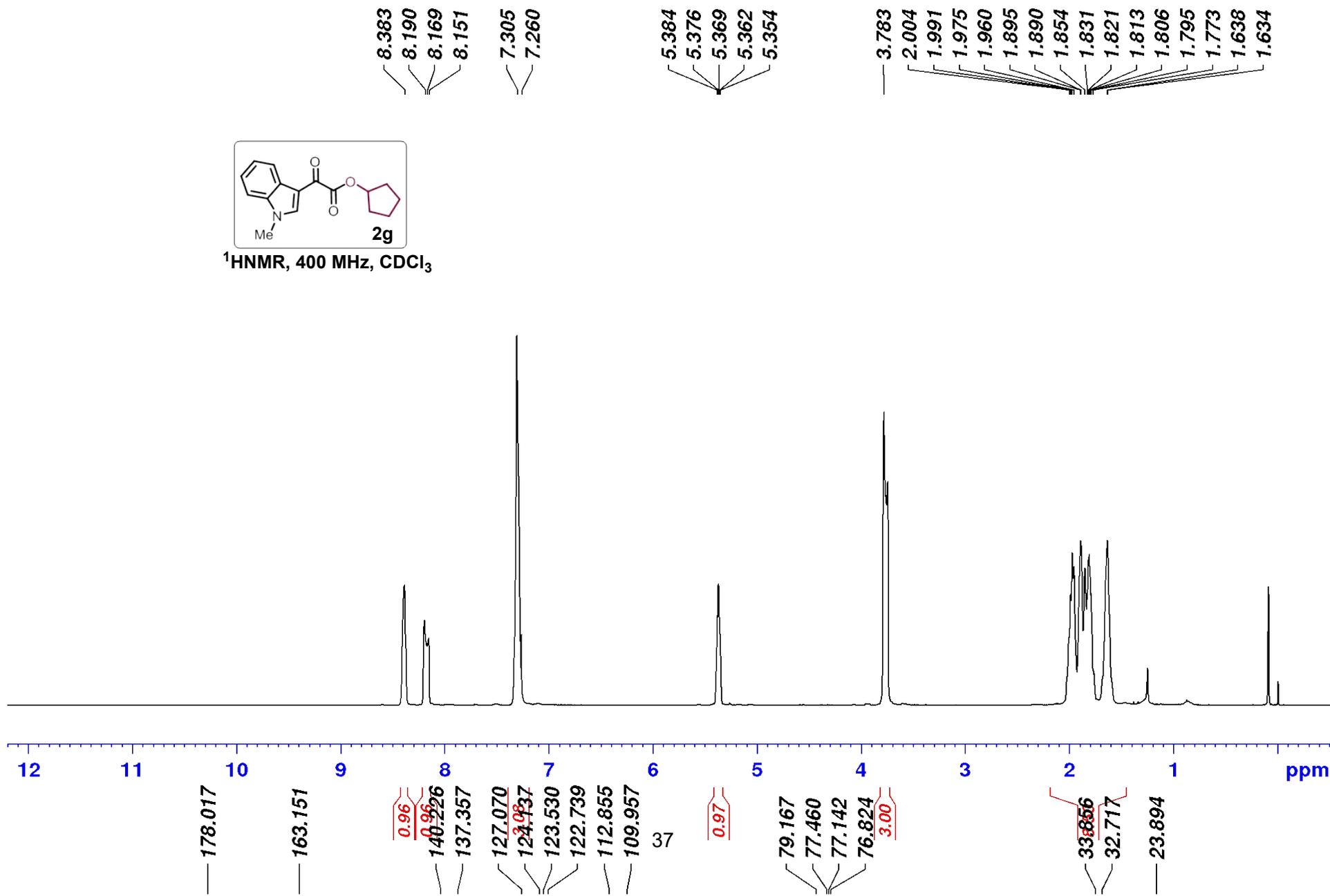


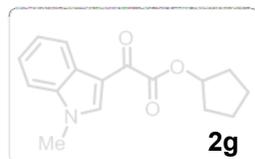
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
242.0793	242.0817	-2.4	-9.9	9.5	1108.9	n/a	n/a	C14 H12 N O3

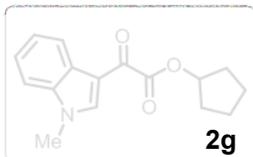


¹HNMR, 400 MHz, CDCl₃

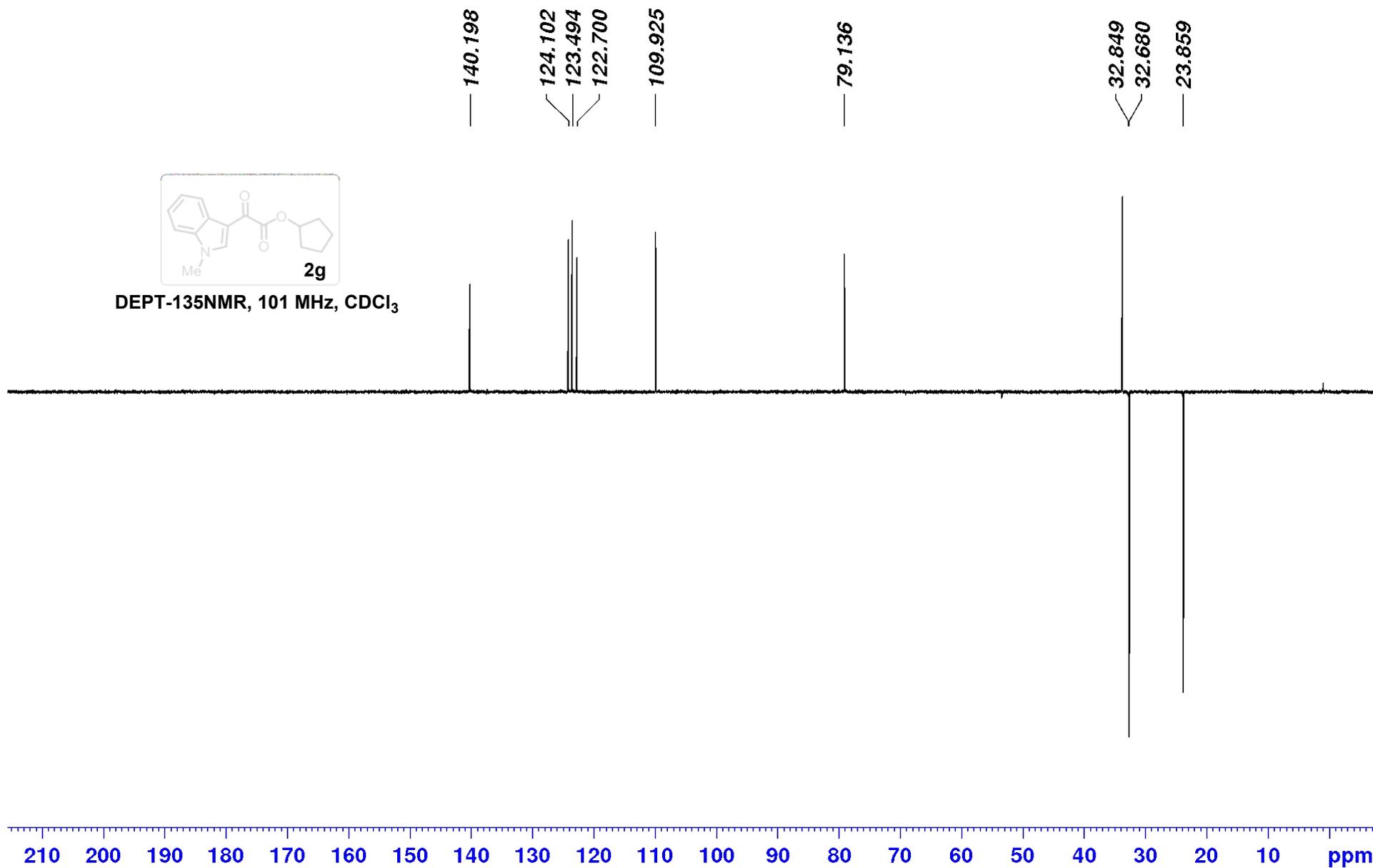




$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3



DEPT-135NMR, 101 MHz, CDCl₃



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

44 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: 0-3

NVD-118

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

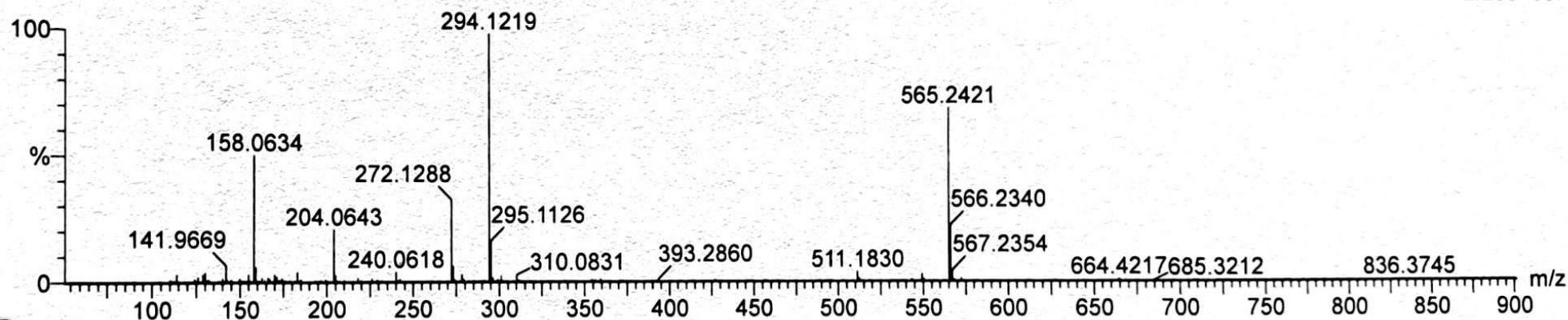
17-Aug-2022

12:37:40

1: TOF MS ES+

2.26e+007

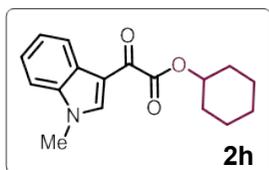
170822_08 10 (0.225) Cm (10:12)



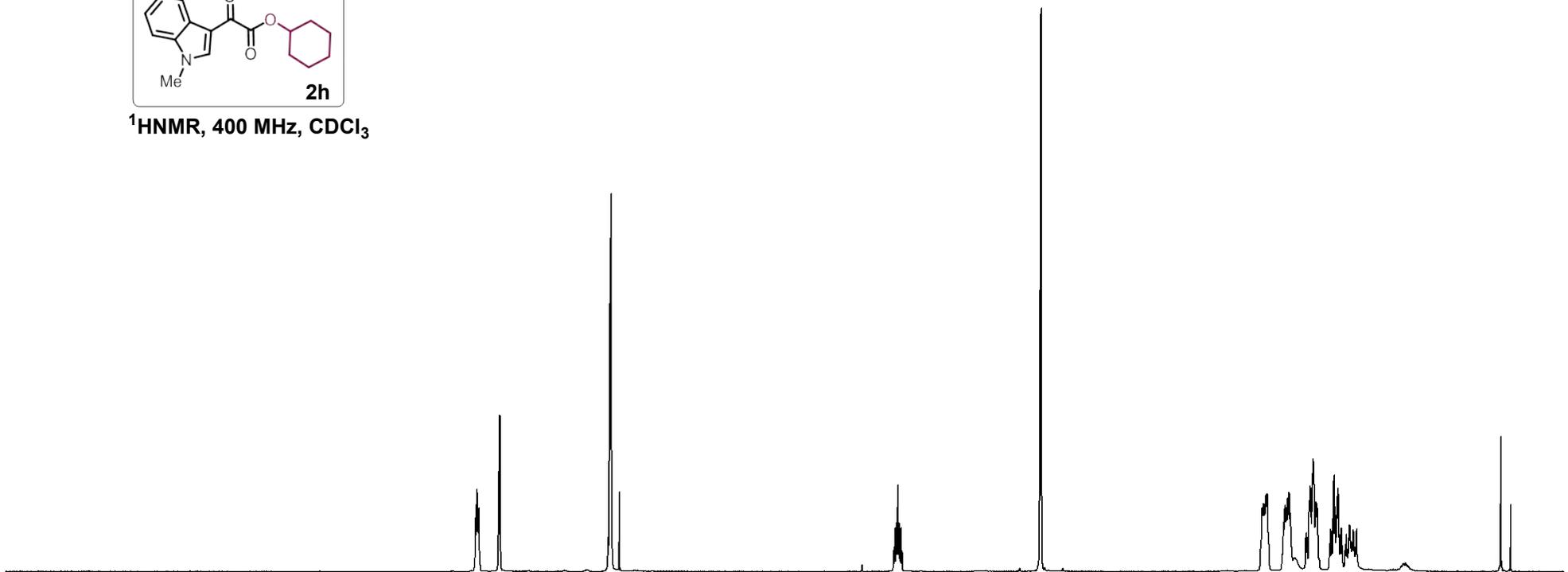
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
272.1288	272.1287	0.1	0.4	8.5	34.5	n/a	n/a	C16 H18 N O3

8.430
8.423
8.416
8.409
8.405
8.235
7.351
7.338
7.335
7.328
5.016
5.003
4.992
4.982
4.969
3.825
2.024
2.014
2.003
1.993
1.982
1.849
1.839
1.827
1.815
1.805
1.794
1.667
1.658
1.640
1.634
1.608
1.603
1.584
1.576
1.475
1.466
1.448
1.439
1.431
1.421
1.413
1.406
1.398
1.387
1.379
1.340
1.314
1.309
1.287
1.282
1.255



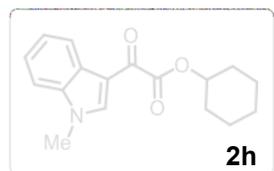
¹HNMR, 400 MHz, CDCl₃



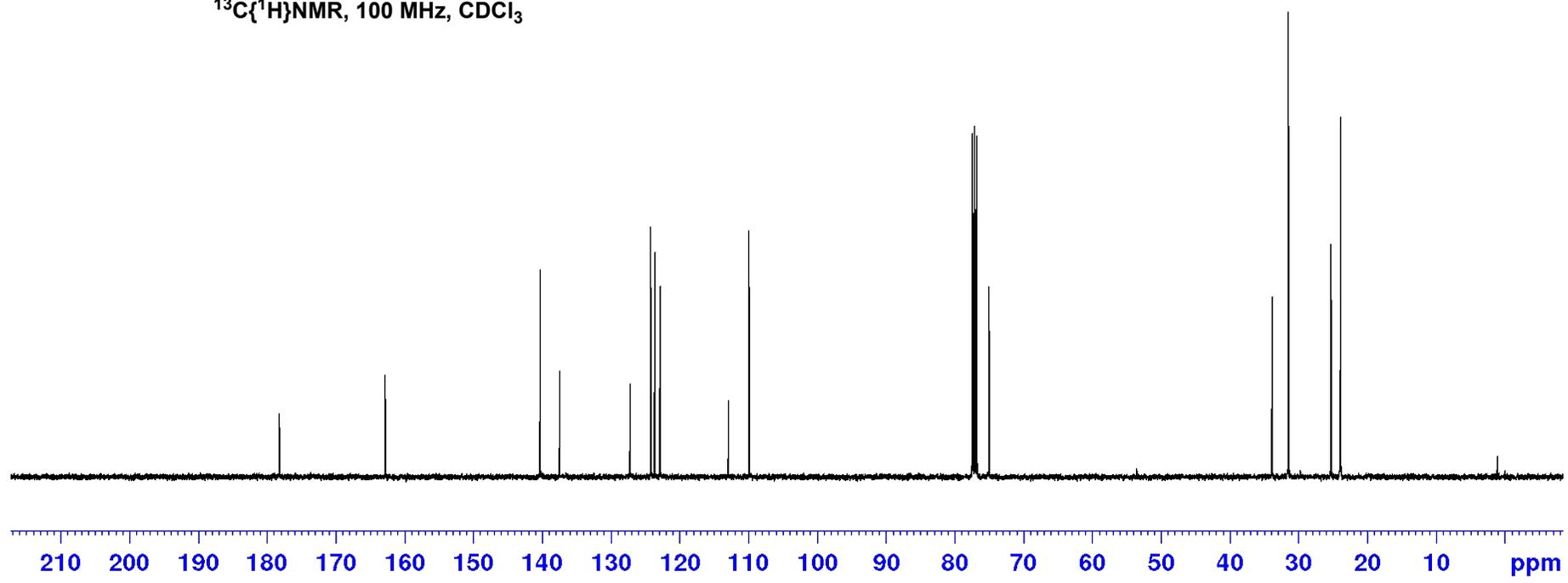
12 11 10 9 8 7 6 5 4 3 2 1 ppm

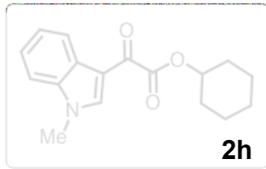
0.99
0.98
3.01
1.00
3.00
2.08
2.39
3.21
3.01

178.131
162.770
140.214
137.385
127.123
124.166
123.558
122.801
112.934
109.968
77.475
77.158
76.840
75.065
33.896
31.559
25.332
23.939

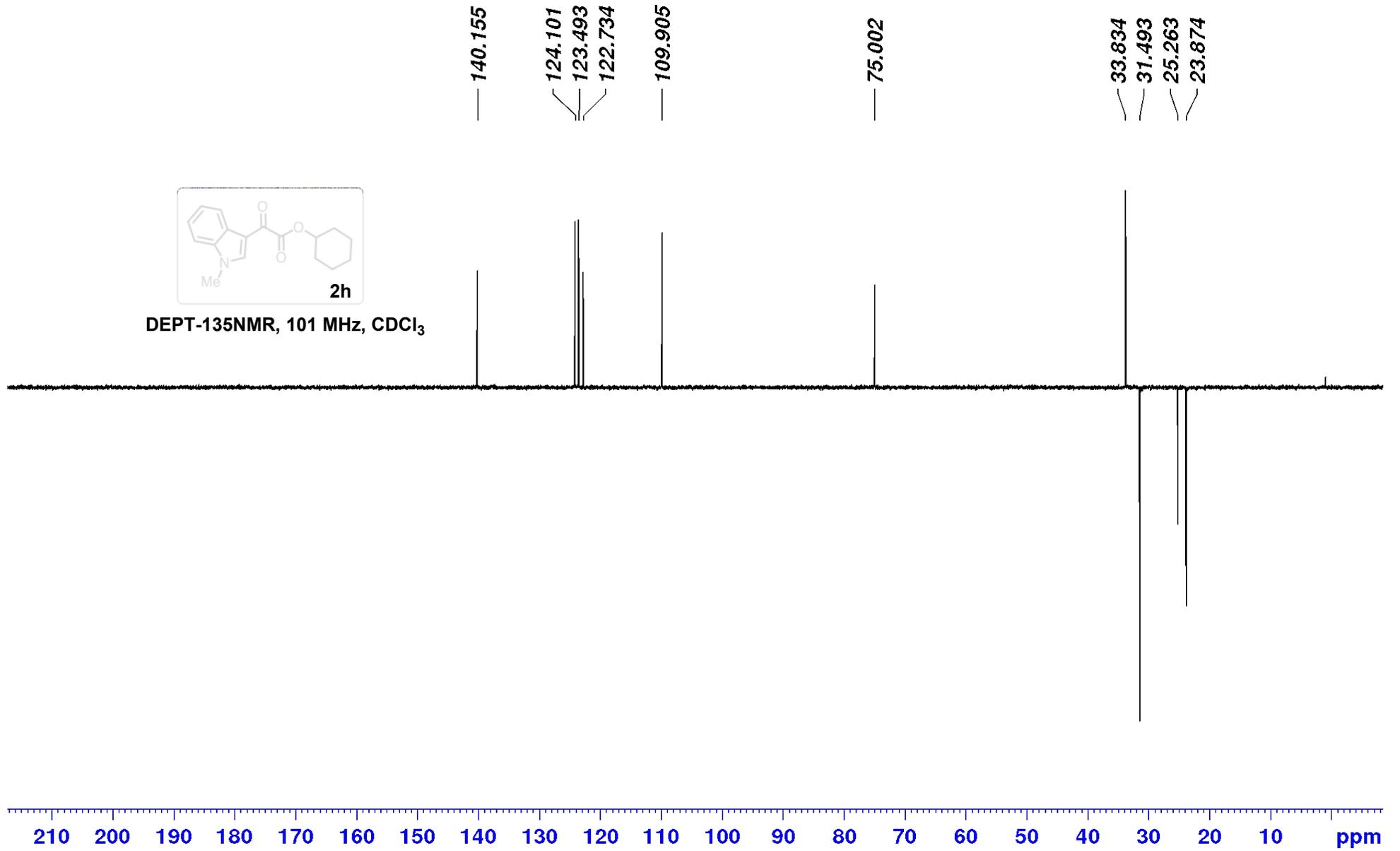


$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3





DEPT-135NMR, 101 MHz, CDCl₃



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

45 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: 0-3

NVD-117

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

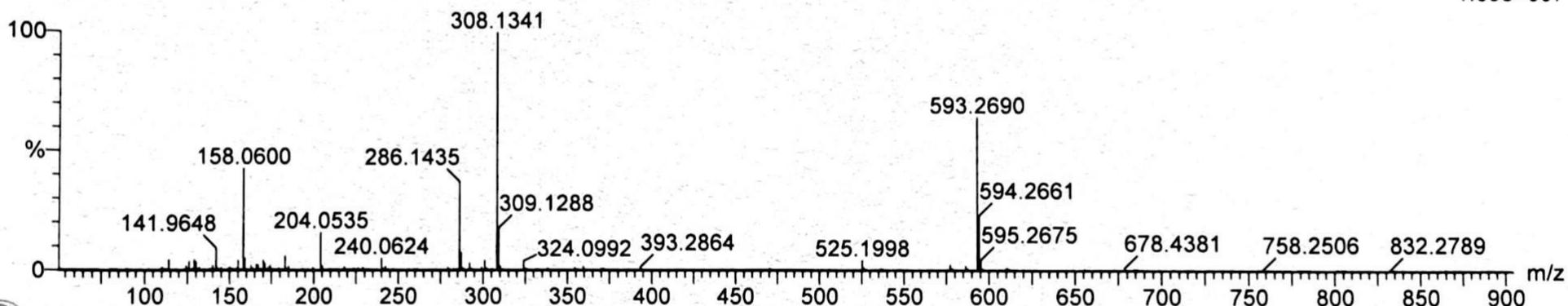
17-Aug-2022

12:32:32

1: TOF MS ES+

1.09e+007

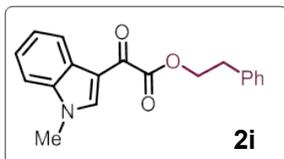
170822_06 10 (0.225) Cm (10:11)



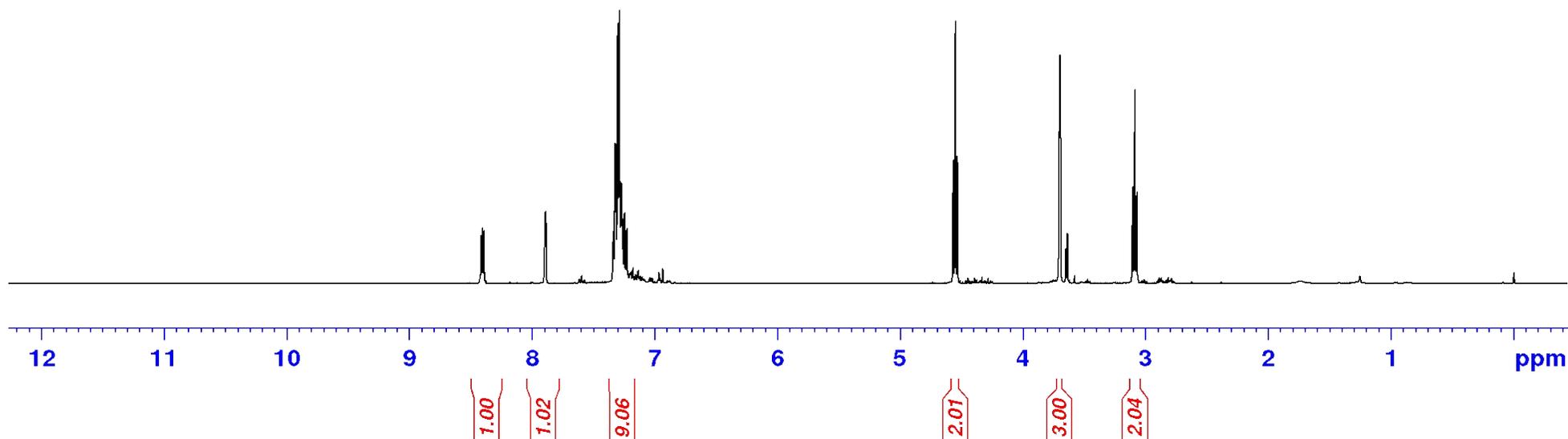
Minimum: -1.5
Maximum: 2.0 50.0 50.0

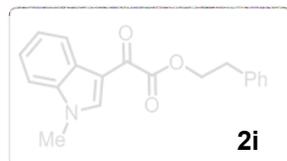
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
286.1435	286.1443	-0.8	-2.8	8.5	40.2	n/a	n/a	C17 H20 N O3

8.420
8.412
8.411
8.405
8.401
8.393
8.390
8.383
7.887
7.334
7.329
7.323
7.318
7.316
7.312
7.298
7.285
7.268
7.264
7.249
7.243
7.236
7.231
7.225
7.174
4.570
4.552
4.535
— 3.699
3.107
3.090
3.072

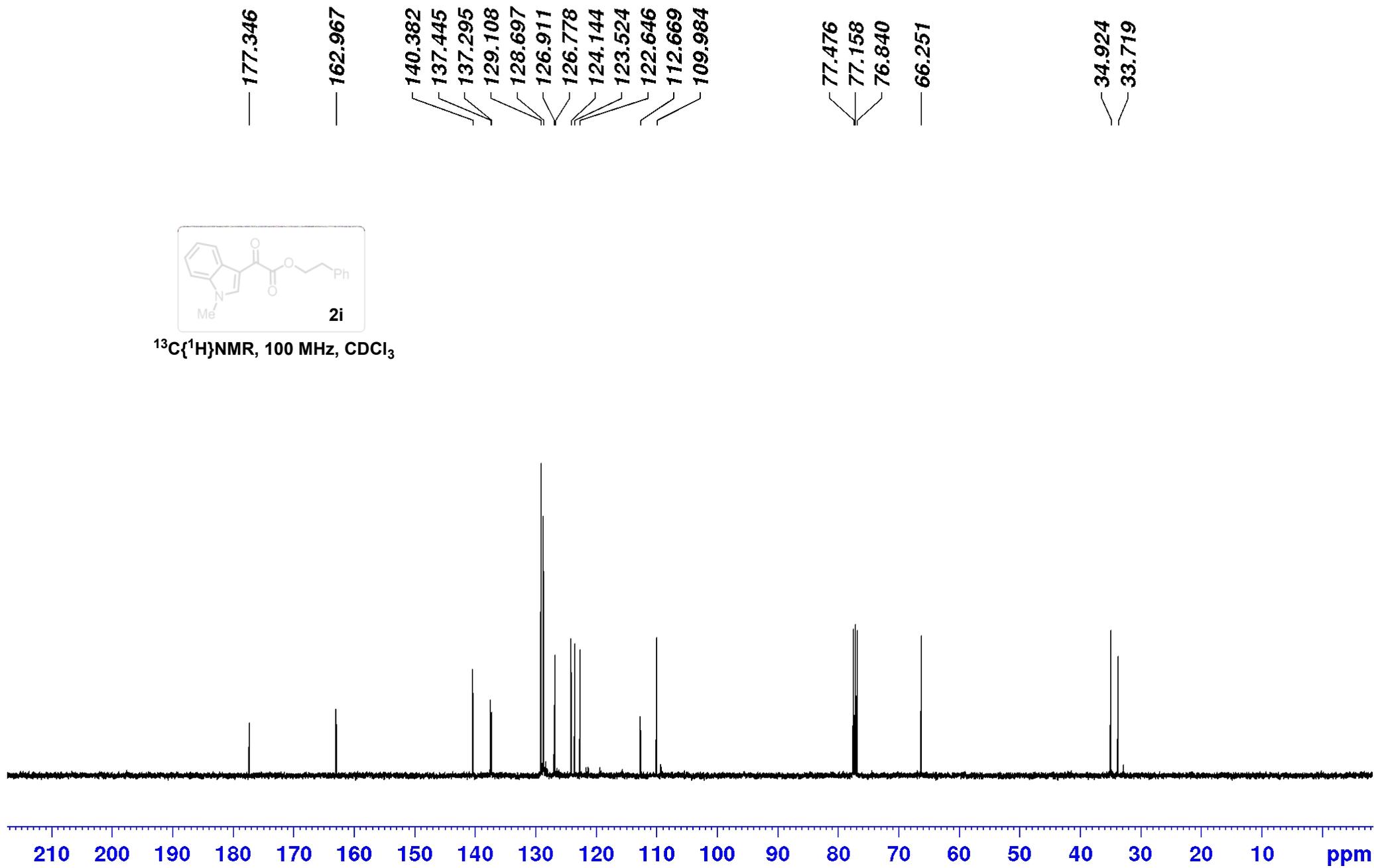


¹HNMR, 400 MHz, CDCl₃





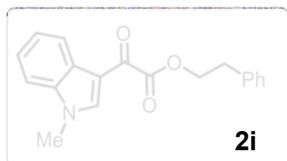
$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3



140.420
129.141
128.730
126.812
124.177
123.559
122.677
110.018

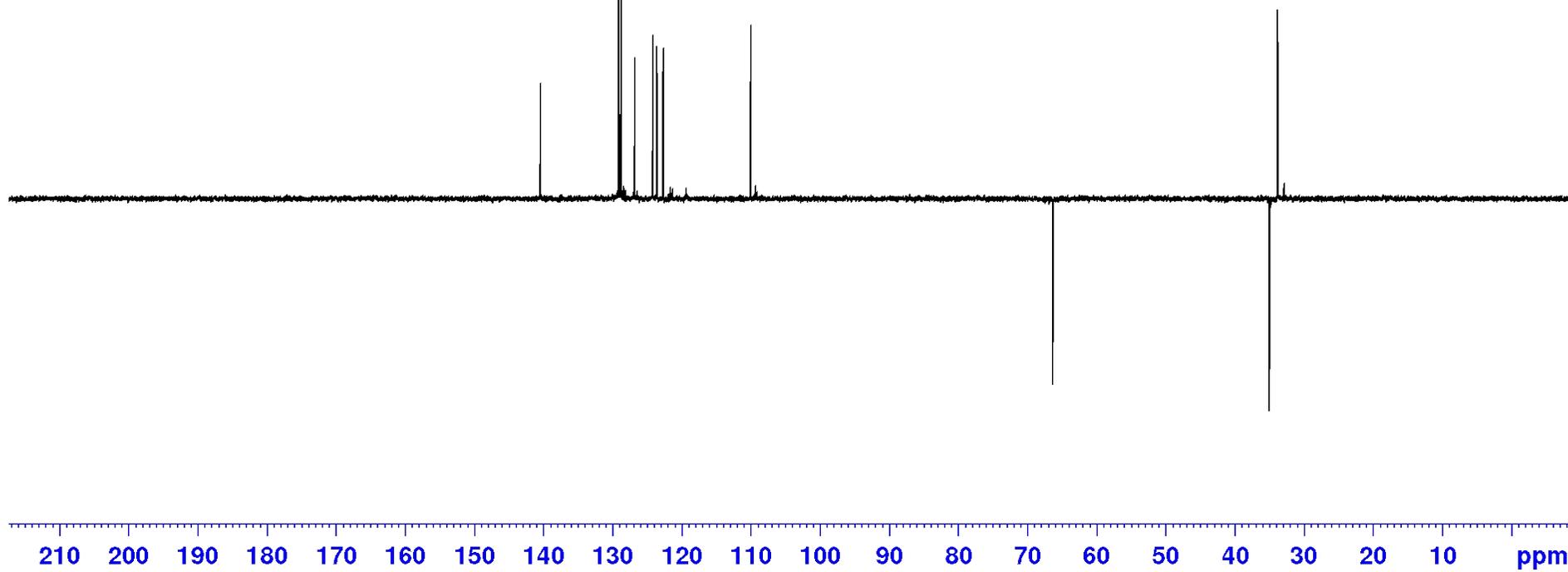
66.285

34.955
34.804



2i

DEPT-135NMR, 101 MHz, CDCl₃



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

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

Elements Used:

C: 0-19 H: 0-100 N: 0-1 O: 0-3

NVD-111

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

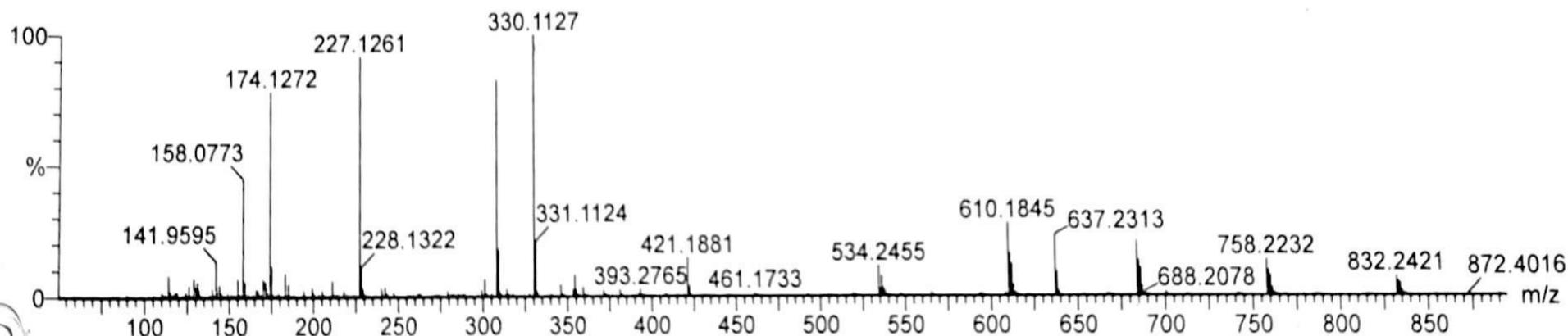
29-Aug-2022

12:42:27

1: TOF MS ES+

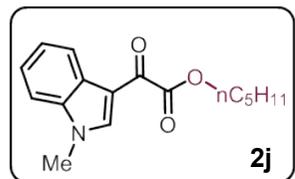
3.48e+006

290822_24 12 (0.259) Cm (12)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
308.1289	308.1287	0.2	0.6	11.5	32.4	n/a	n/a	C19 H18 N O3

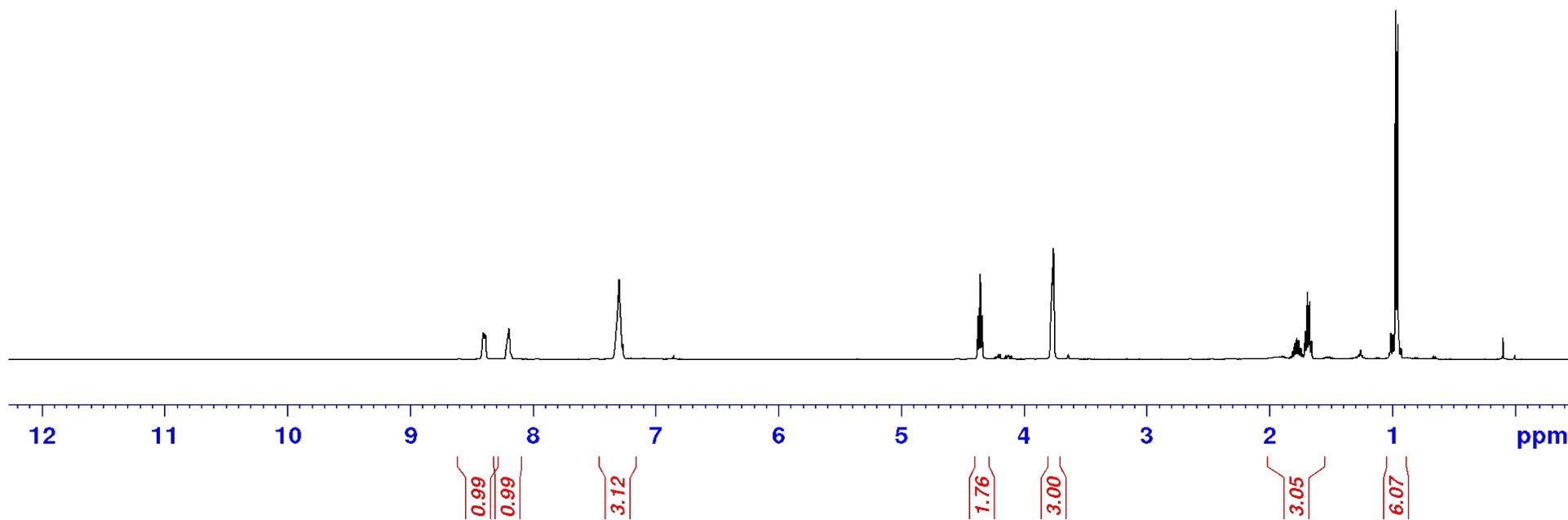


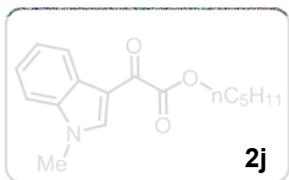
¹HNMR, 400 MHz, CDCl₃

8.404
8.399
8.396
8.387
8.384
8.195

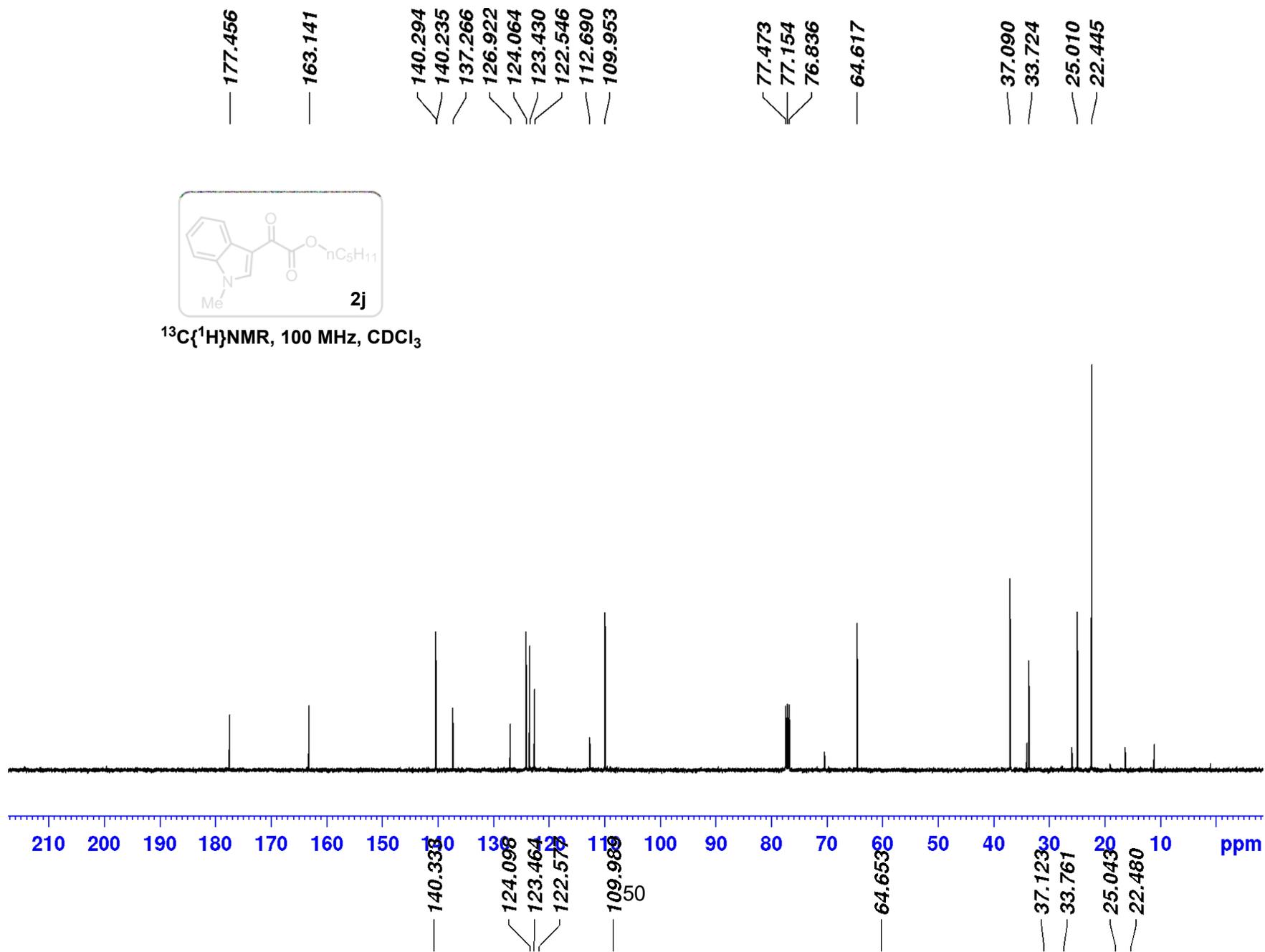
4.372
4.355
4.337
— 3.759

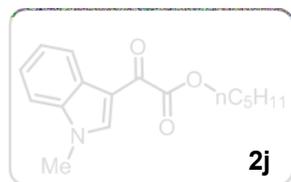
1.810
1.793
1.777
1.760
1.743
1.706
1.689
1.672
1.655
1.010
0.993
0.970
0.954
0.925





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





DEPT-135NMR, 101 MHz, CDCl₃

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

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

Elements Used:

C: 0-16 H: 0-100 N: 0-1 O: 0-3

NVD-106

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

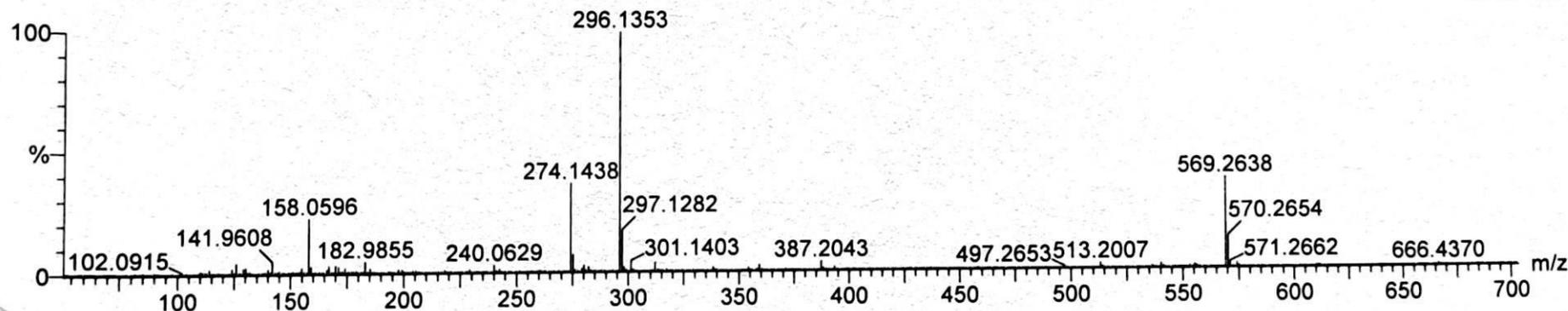
24-Jun-2022

13:30:36

1: TOF MS ES+

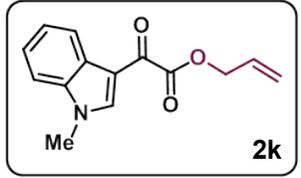
1.17e+007

240622_10 9 (0.208) Cm (9:10)

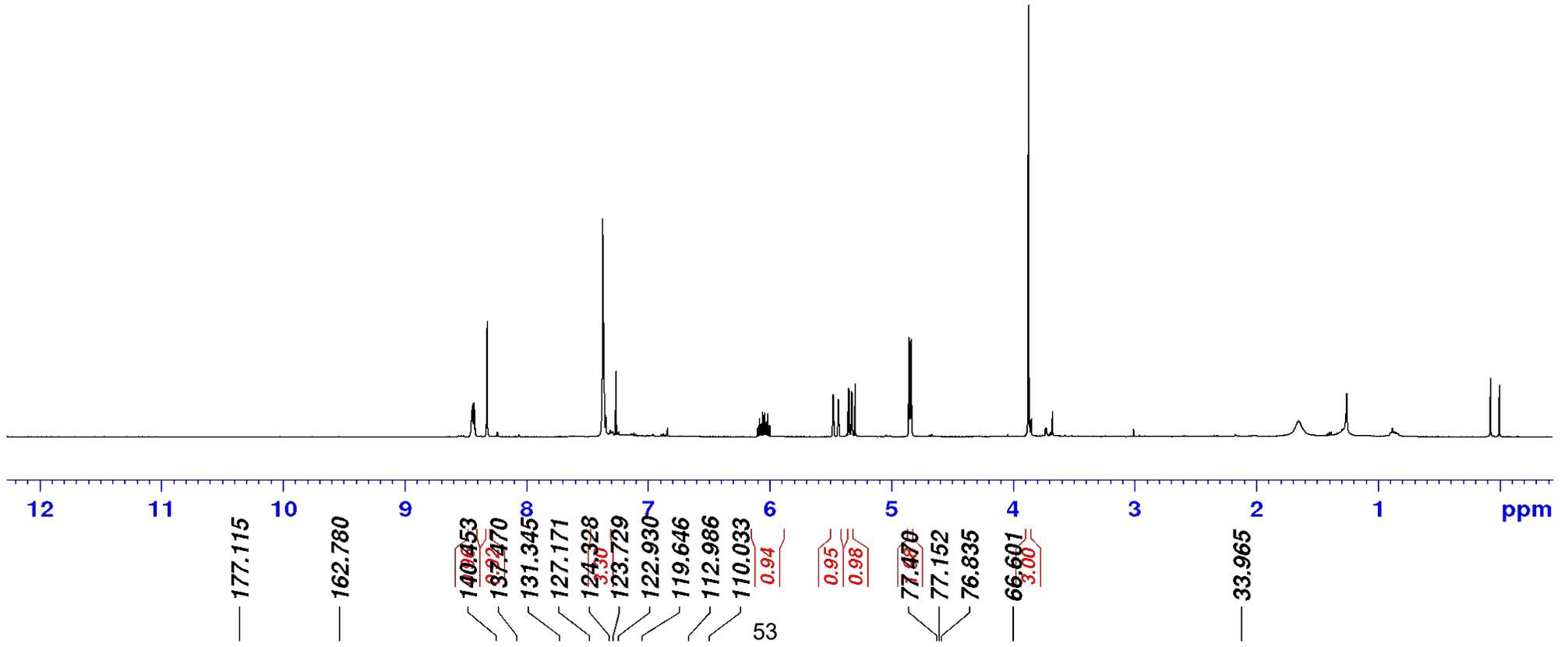


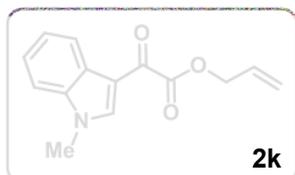
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
274.1438	274.1443	-0.5	-1.8	7.5	29.2	n/a	n/a	C16 H20 N O3



^1H NMR, 400 MHz, CDCl_3





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

— 140.353

— 131.234

— 124.222

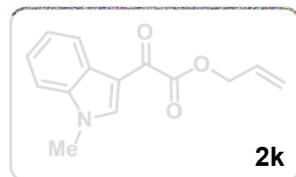
— 123.624

— 119.545

— 109.930

— 66.496

— 33.862



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

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

Elements Used:

C: 0-20 H: 0-100 N: 0-1 O: 0-3

NVD-155

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

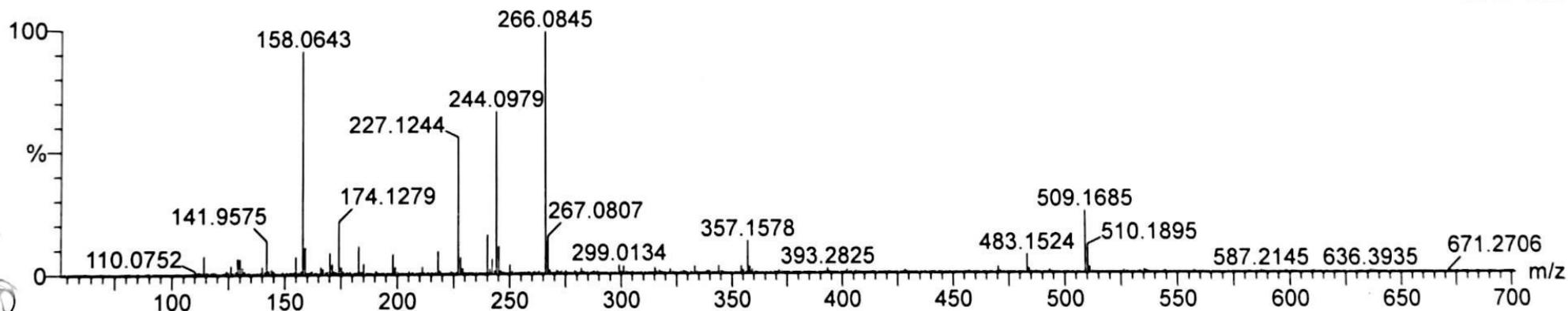
30-Aug-2022

11:46:50

1: TOF MS ES+

4.64e+006

300822_12 9 (0.208) Cm (9)



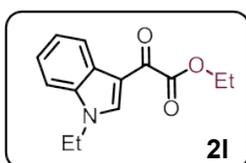
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
244.0979	244.0974	0.5	2.0	8.5	43.0	n/a	n/a	C14 H14 N O3

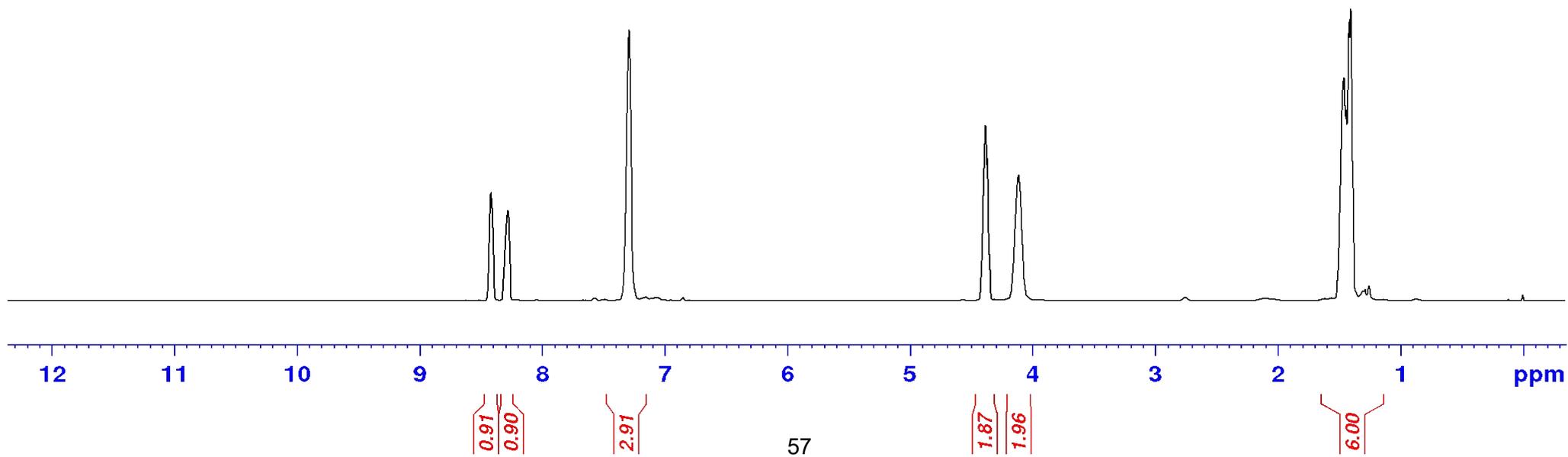
8.619
8.518
8.505
8.418
8.415
8.281
7.573
7.489
7.290
7.169
7.152
7.066
7.005
6.955
6.851

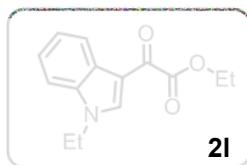
4.566
4.394
4.383
4.370
4.113

1.464
1.460
1.446
1.438
1.417
1.413
1.403
1.390
1.358
1.304
1.286
1.254

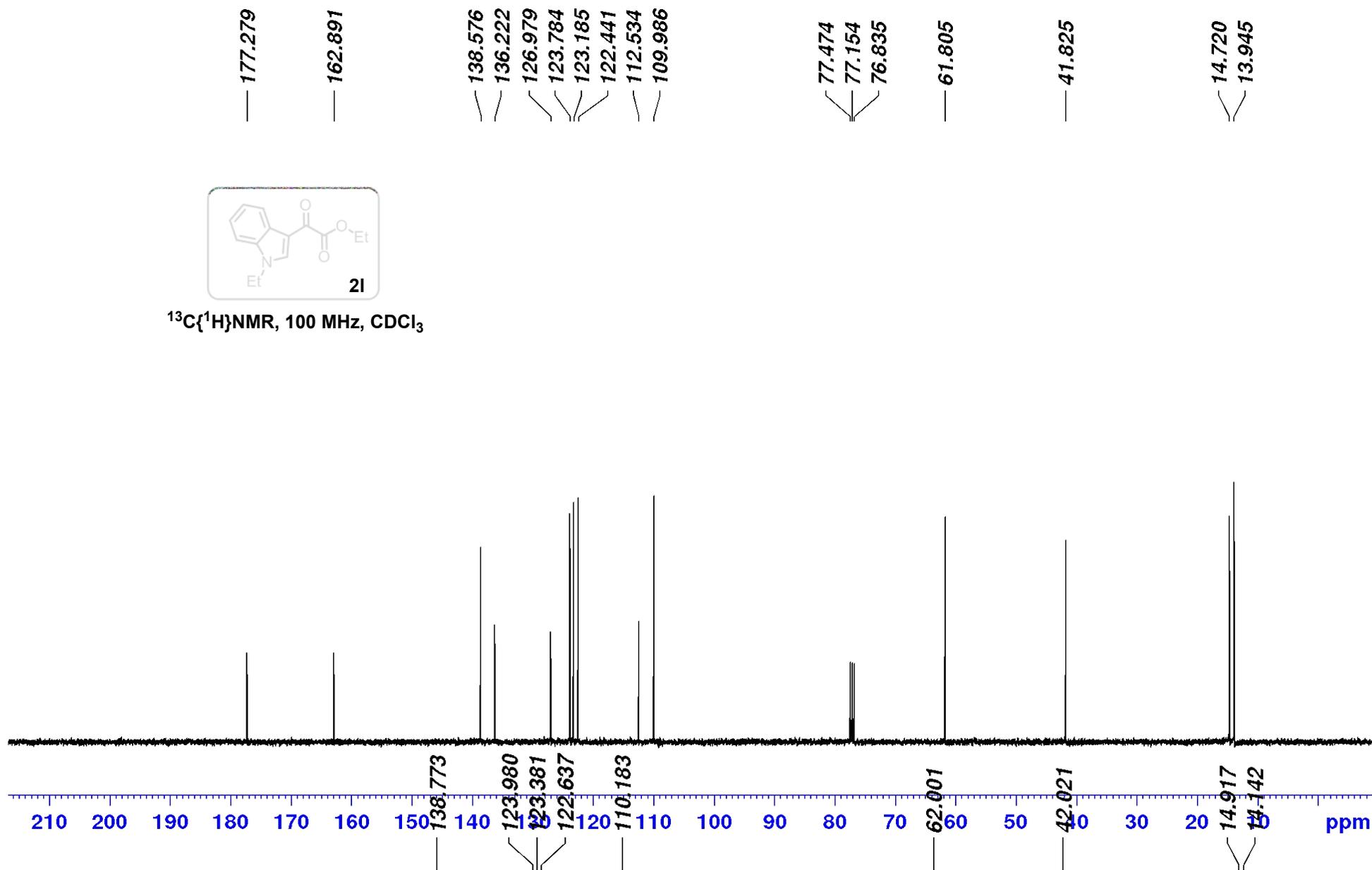


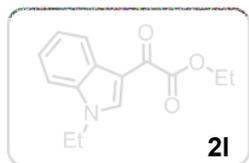
$^1\text{H NMR}$, 400 MHz, CDCl_3





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





DEPT-135NMR, 101 MHz, CDCl₃

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

41 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: 0-3

NVD-120

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

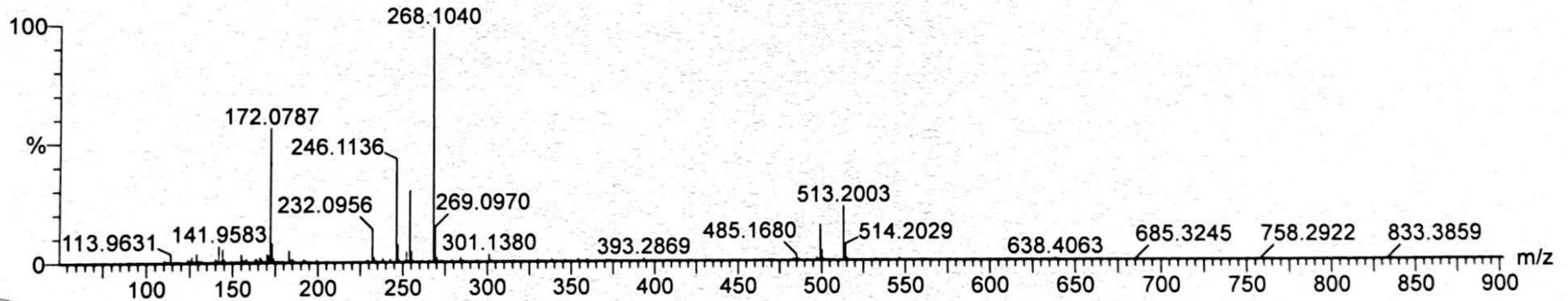
17-Aug-2022

12:35:06

1: TOF MS ES+

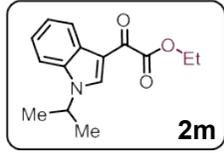
1.28e+007

170822_07 11 (0.242) Cm (11:12)

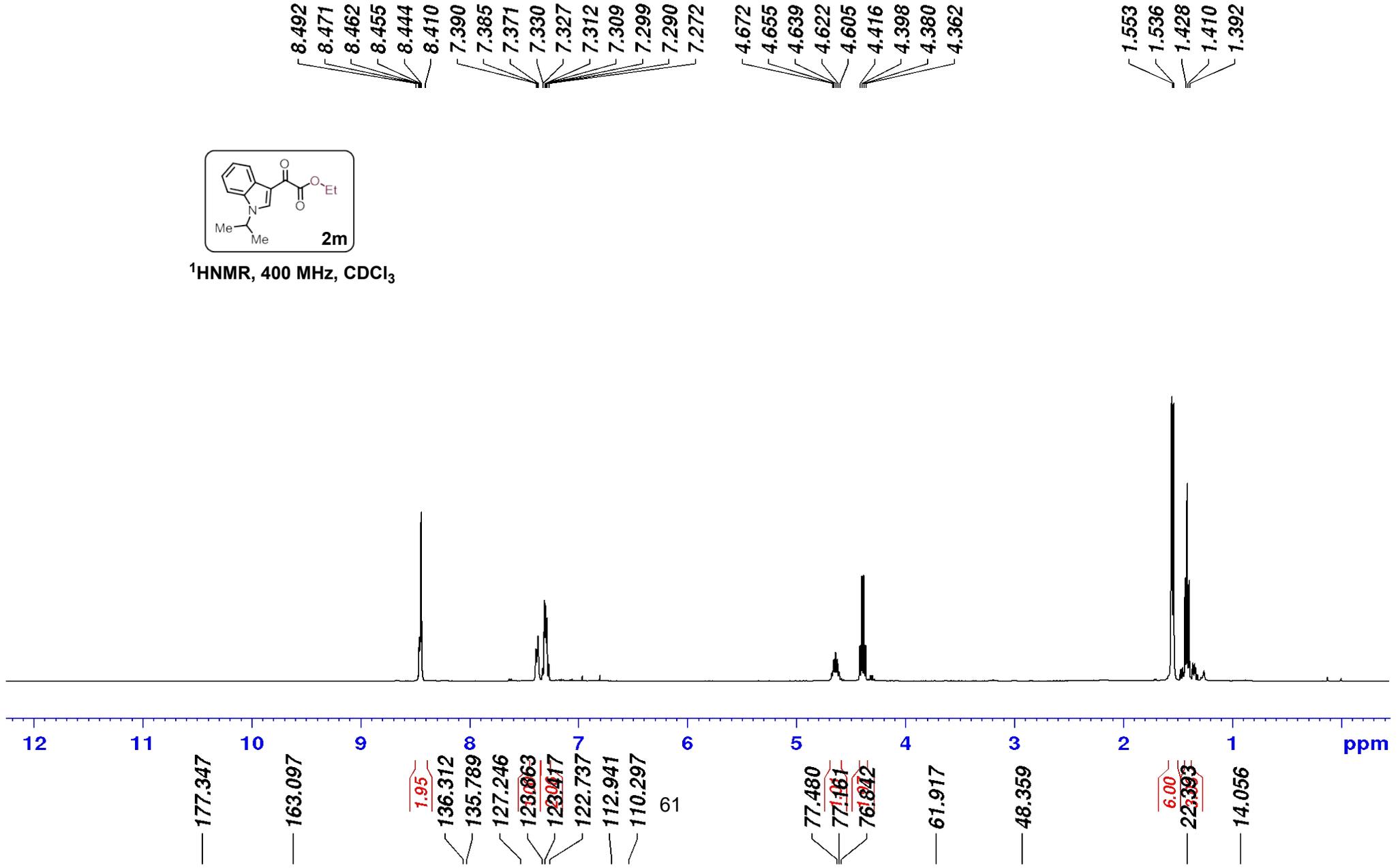


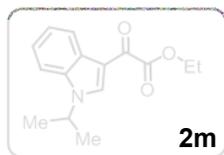
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
246.1136	246.1130	0.6	2.4	7.5	34.4	n/a	n/a	C14 H16 N O3



$^1\text{H NMR}$, 400 MHz, CDCl_3





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

— 135.886

— 123.955

— 123.509

— 122.827

— 110.389

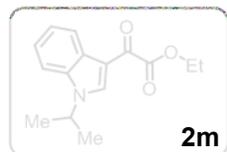
62

— 62.010

— 48.449

— 22.485

— 14.148



DEPT-135NMR, 101 MHz, CDCl₃

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

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

Elements Used:

C: 0-18 H: 0-100 N: 0-1 O: 0-3

NVD-112

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

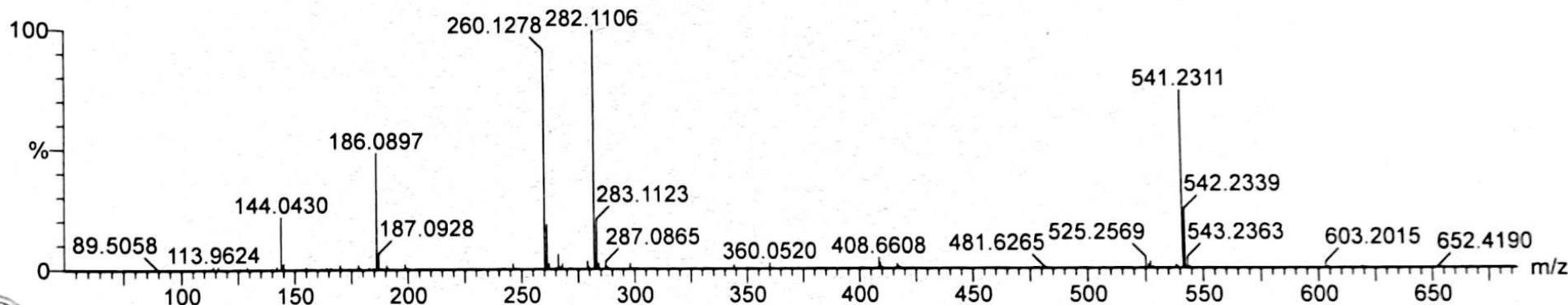
22-Aug-2022

12:12:12

1: TOF MS ES+

2.33e+007

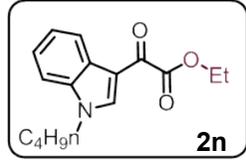
220822_18 10 (0.225)



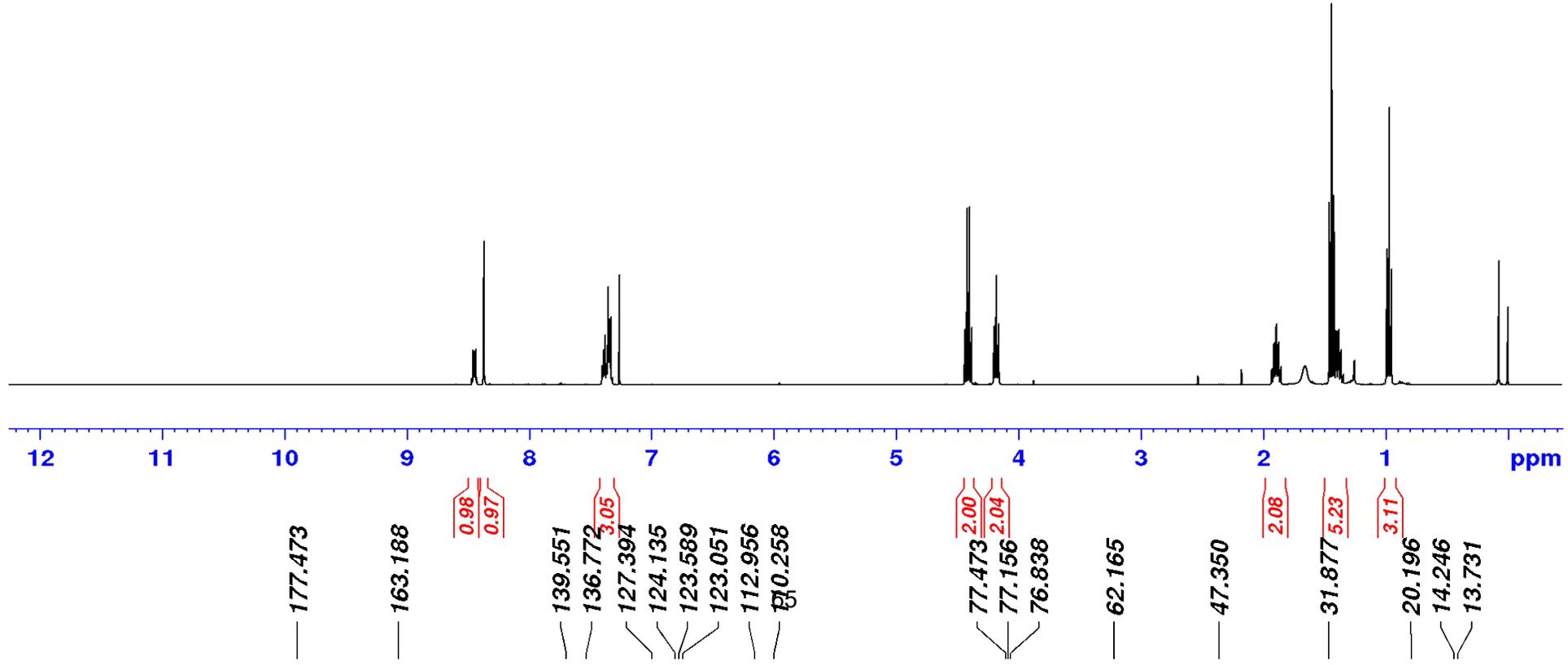
Minimum: -1.5
Maximum: 2.0 50.0 50.0

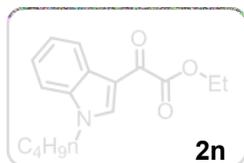
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
260.1278	260.1287	-0.9	-3.5	7.5	1067.7	n/a	n/a	C15 H18 N O3

8.461
8.459
8.452
8.451
8.448
8.442
8.438
8.436
8.370
7.403
7.398
7.392
7.389
7.381
7.380
7.371
7.370
7.367
7.363
7.355
7.349
7.346
7.342
7.338
7.332
7.325
7.320
4.438
4.421
4.403
4.385
4.199
4.181
4.163
1.929
1.910
1.904
1.892
1.886
1.873
1.854
1.458
1.440
1.423
1.401
1.382
1.363
0.967



¹HNMR, 400 MHz, CDCl₃





¹³C{¹H}NMR, 100 MHz, CDCl₃

— 139.455

124.031
123.486
122.946

— 110.156

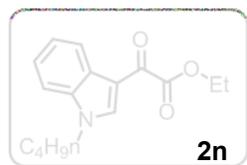
66

— 62.067

— 47.249

— 31.773

— 20.092
14.143
13.633



DEPT-135NMR, 101 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

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

Elements Used:

C: 0-16 H: 0-100 N: 0-1 O: 0-3

NVD-123

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

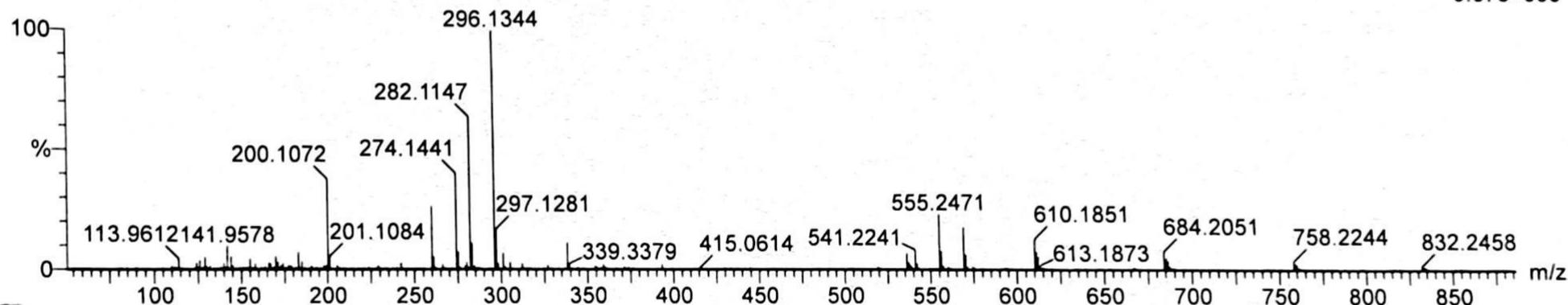
17-Aug-2022

12:42:48

1: TOF MS ES+

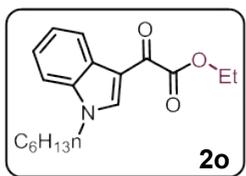
9.07e+006

170822_10 8 (0.172) Cm (8:9)

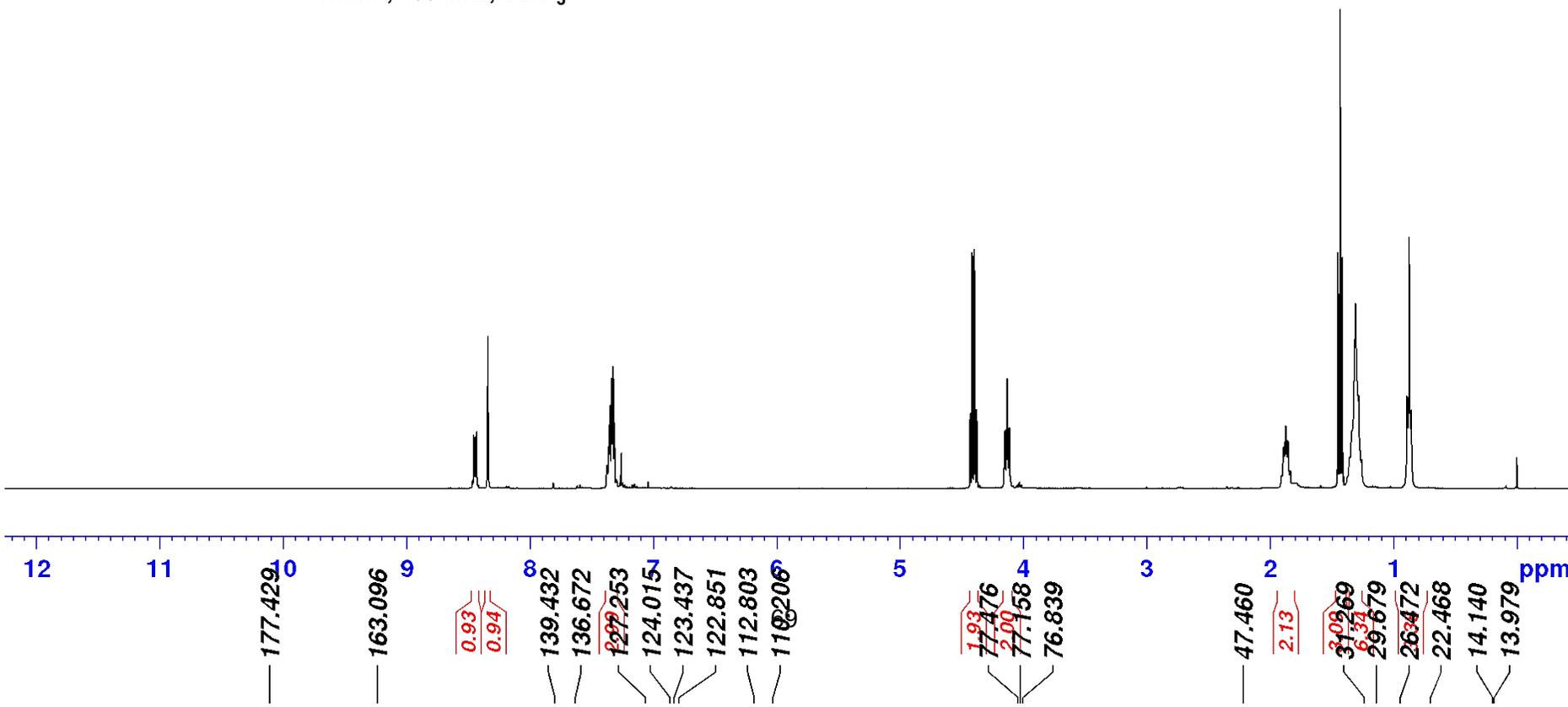


Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
274.1441	274.1443	-0.2	-0.7	7.5	29.6	n/a	n/a	C16 H20 N O3

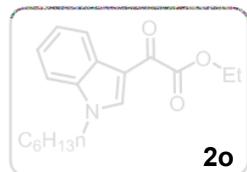


¹HNMR, 400 MHz, CDCl₃



- 8.463
- 8.455
- 8.453
- 8.447
- 8.444
- 8.435
- 8.432
- 8.430
- 8.424
- 8.338
- 7.374
- 7.369
- 7.360
- 7.350
- 7.336
- 7.333
- 7.324
- 7.313
- 7.298
- 7.292
- 4.429
- 4.411
- 4.394
- 4.376
- 4.147
- 4.129
- 4.111
- 1.905
- 1.888
- 1.871
- 1.853
- 1.835
- 1.447
- 1.429
- 1.412
- 1.400
- 1.395
- 1.367
- 1.354
- 1.350
- 1.333
- 1.305
- 1.294
- 1.290

- 177.429
- 163.096
- 139.432
- 136.672
- 127.253
- 124.015
- 123.437
- 122.851
- 112.803
- 110.206
- 77.476
- 77.158
- 76.839
- 47.460
- 31.269
- 29.679
- 26.472
- 22.468
- 14.140
- 13.979



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

— 139.429

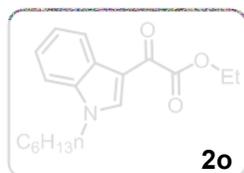
124.009
123.432
122.844

— 110.201

— 62.027

— 47.455

31.264
29.673
26.467
22.464
14.135
13.974



DEPT-135NMR, 101 MHz, CDCl₃

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

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

Elements Used:

C: 0-18 H: 0-100 N: 0-1 O: 0-3

NVD-121

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

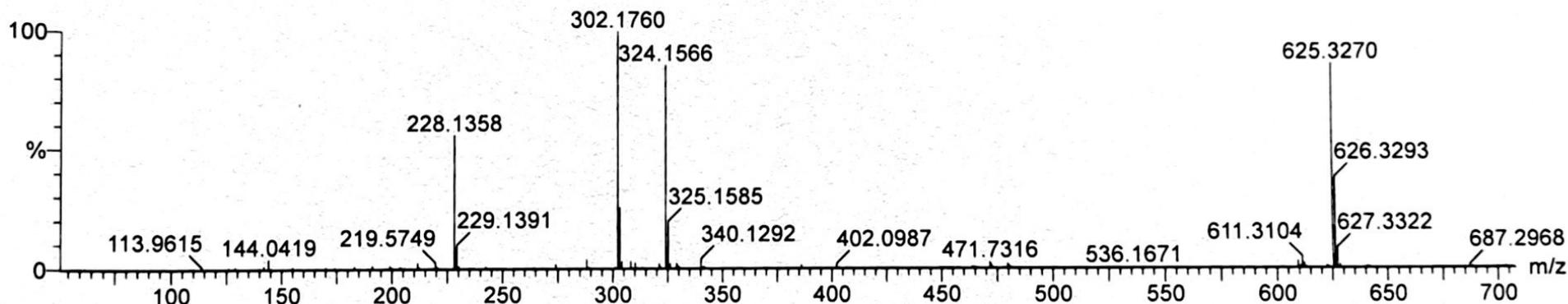
23-Aug-2022

11:38:44

1: TOF MS ES+

2.52e+007

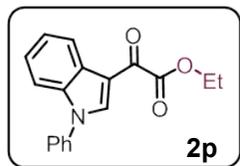
230822_10 8 (0.172)



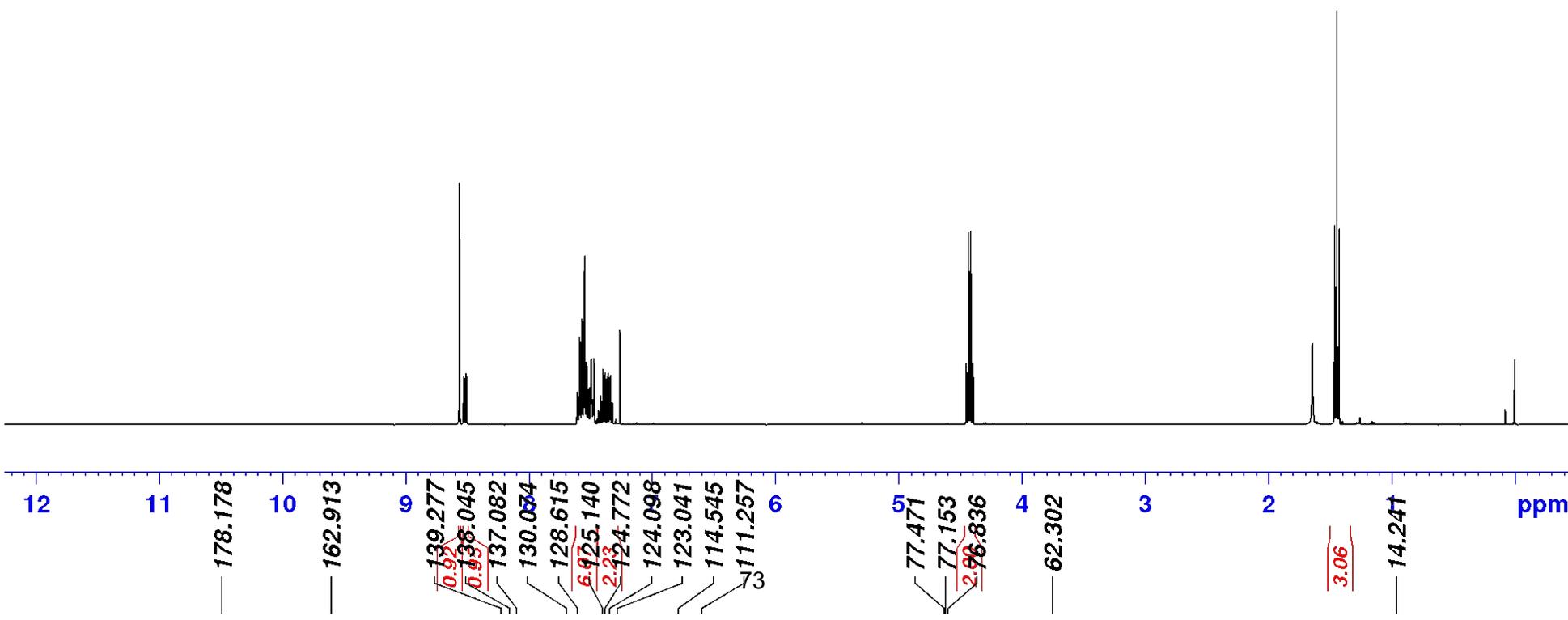
Minimum: -1.5
Maximum: 2.0 50.0 50.0

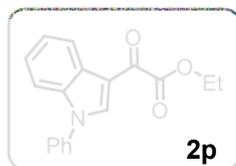
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
302.1760	302.1756	0.4	1.3	7.5	973.2	n/a	n/a	C18 H24 N O3

8.564
8.530
8.528
8.526
8.525
8.510
8.508
8.507
8.505
7.605
7.589
7.586
7.584
7.573
7.568
7.566
7.564
7.552
7.547
7.541
7.534
7.530
7.529
7.527
7.519
7.515
7.499
7.497
7.493
7.491
7.488
7.472
7.471
7.470
7.468
7.415
7.399
7.397
7.380
7.377
7.360
7.356
7.342
7.339
7.336
4.448
4.430
4.412
4.394
1.459
1.442
1.424



¹HNMR, 400 MHz, CDCl₃



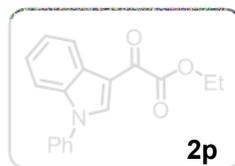


$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3

139.185
129.980
128.520
125.042
124.677
124.004
122.946
111.162

— 62.211

— 14.148



DEPT ^{13}C NMR, 101 MHz, CDCl_3

74

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

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

Elements Used:

C: 0-18 H: 0-100 N: 0-1 O: 0-3

NVD-82

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

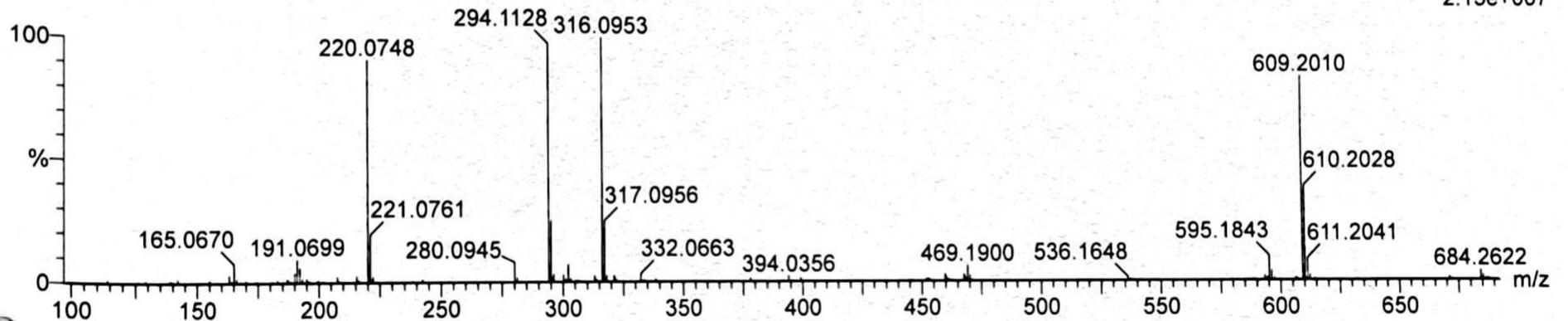
23-Aug-2022

11:41:18

1: TOF MS ES+

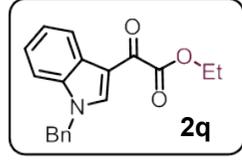
2.13e+007

230822_11 8 (0.172)

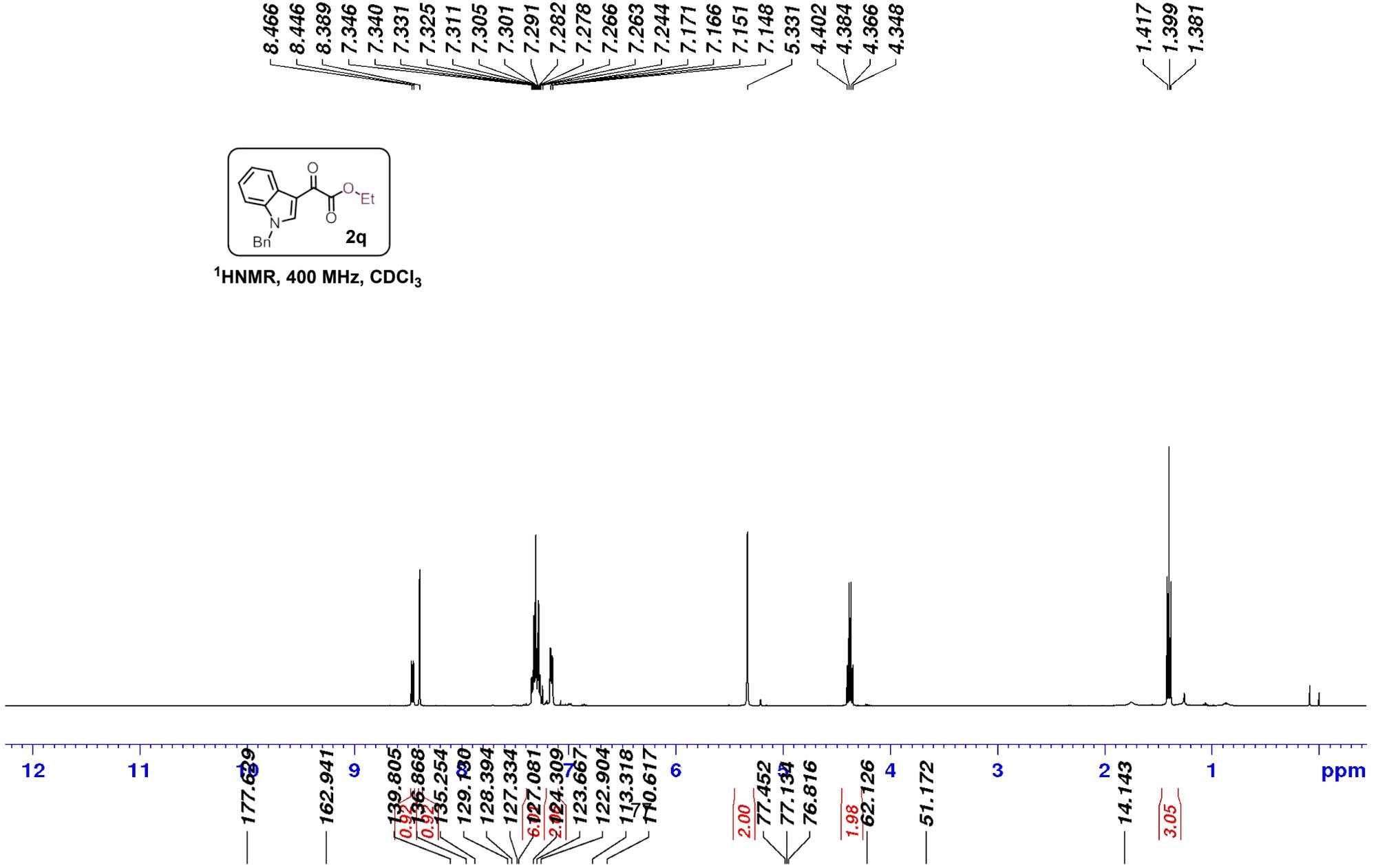


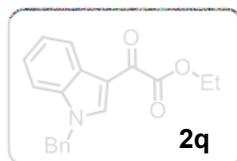
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
294.1128	294.1130	-0.2	-0.7	11.5	970.5	n/a	n/a	C18 H16 N O3



¹HNMR, 400 MHz, CDCl₃





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

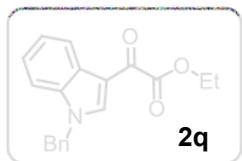
— 139.797
— 129.120
— 128.384
— 127.071
— 124.299
— 123.658
— 122.893
— 110.608

78

— 62.118

— 51.162

— 14.133



DEPT-135NMR, 101 MHz, CDCl₃

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

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

Elements Used:

C: 0-19 H: 0-100 N: 0-1 O: 0-3

NVD-156

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

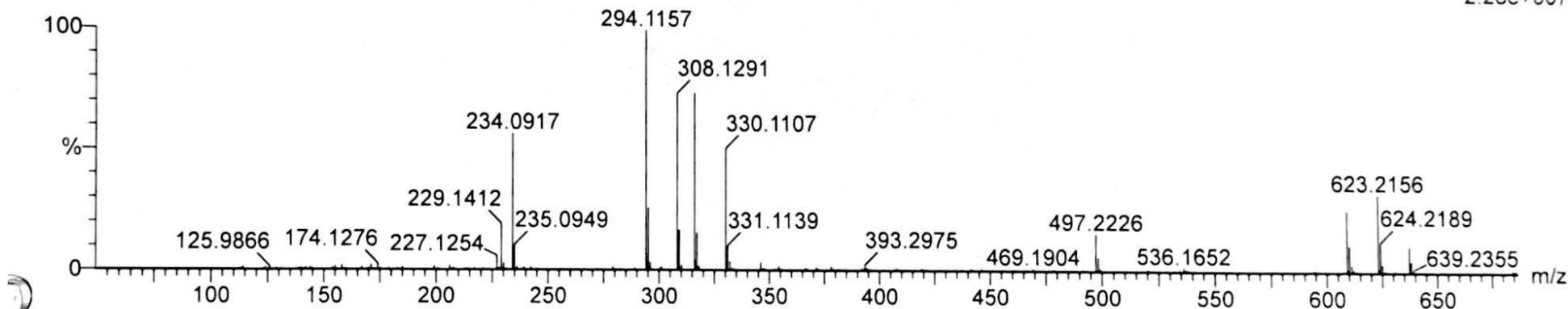
28-Sep-2022

12:52:44

1: TOF MS ES+

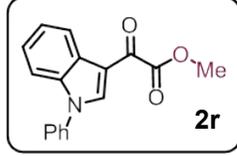
2.28e+007

280922_07 12 (0.259)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
308.1291	308.1287	0.4	1.3	11.5	1195.9	n/a	n/a	C19 H18 N O3



¹HNMR, 400 MHz, CDCl₃

8.577
8.529
8.511
8.509
7.611
7.608
7.590
7.571
7.553
7.550
7.536
7.532
7.522
7.519
7.502
7.493
7.484
7.473
7.462
7.422
7.404
7.385
7.364
7.362
7.344
7.326

— 3.963

— 177.660

— 163.271

139.409

138.030

137.136

130.094

128.670

127.320

125.176

124.837

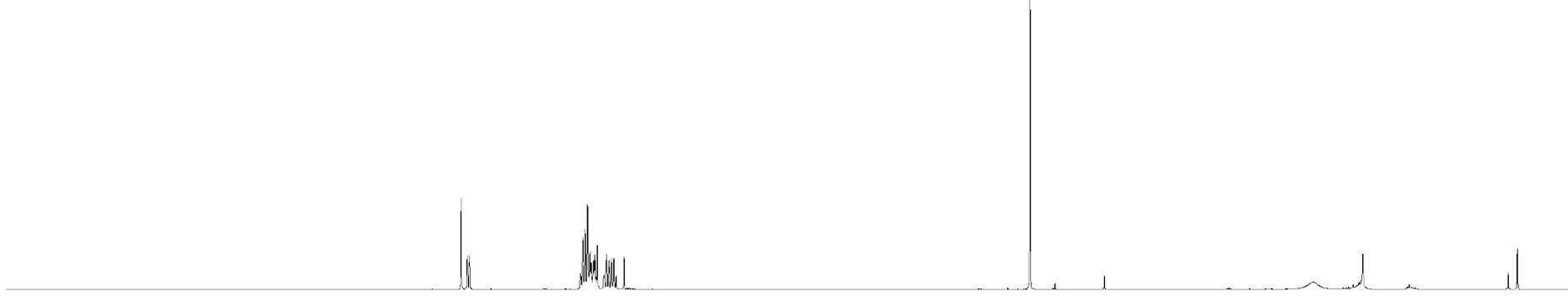
124.154

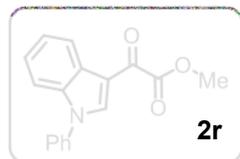
123.065

114.537

111.298

— 52.963





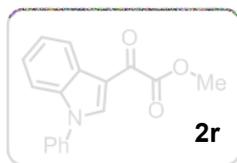
$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3

139.297
129.980
129.636
128.557
125.063
124.724
124.427
124.041
122.951
111.185

— 77.248

— 52.851
— 50.364

— 29.717



DEPT-135NMR, 101 MHz, CDCl₃

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

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

Elements Used:

C: 0-17 H: 0-100 N: 0-1 O: 0-3

NVD-175

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

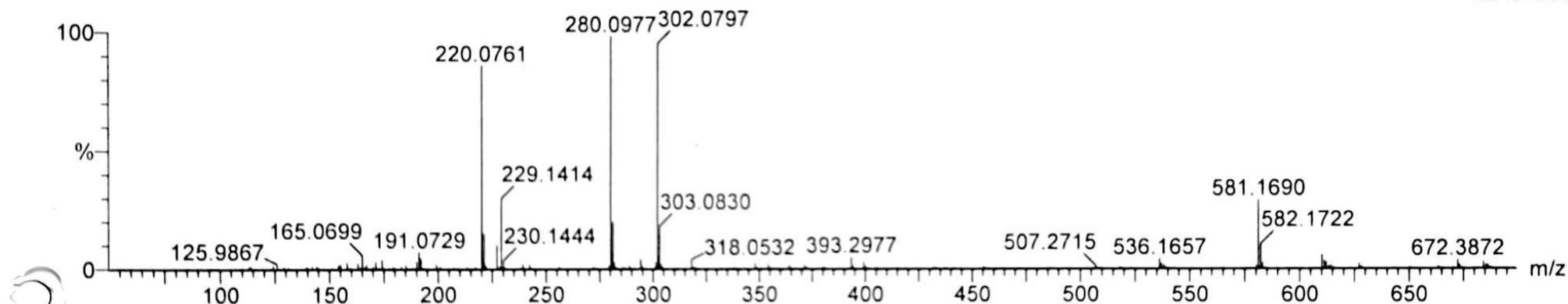
28-Sep-2022

12:50:01

1: TOF MS ES+

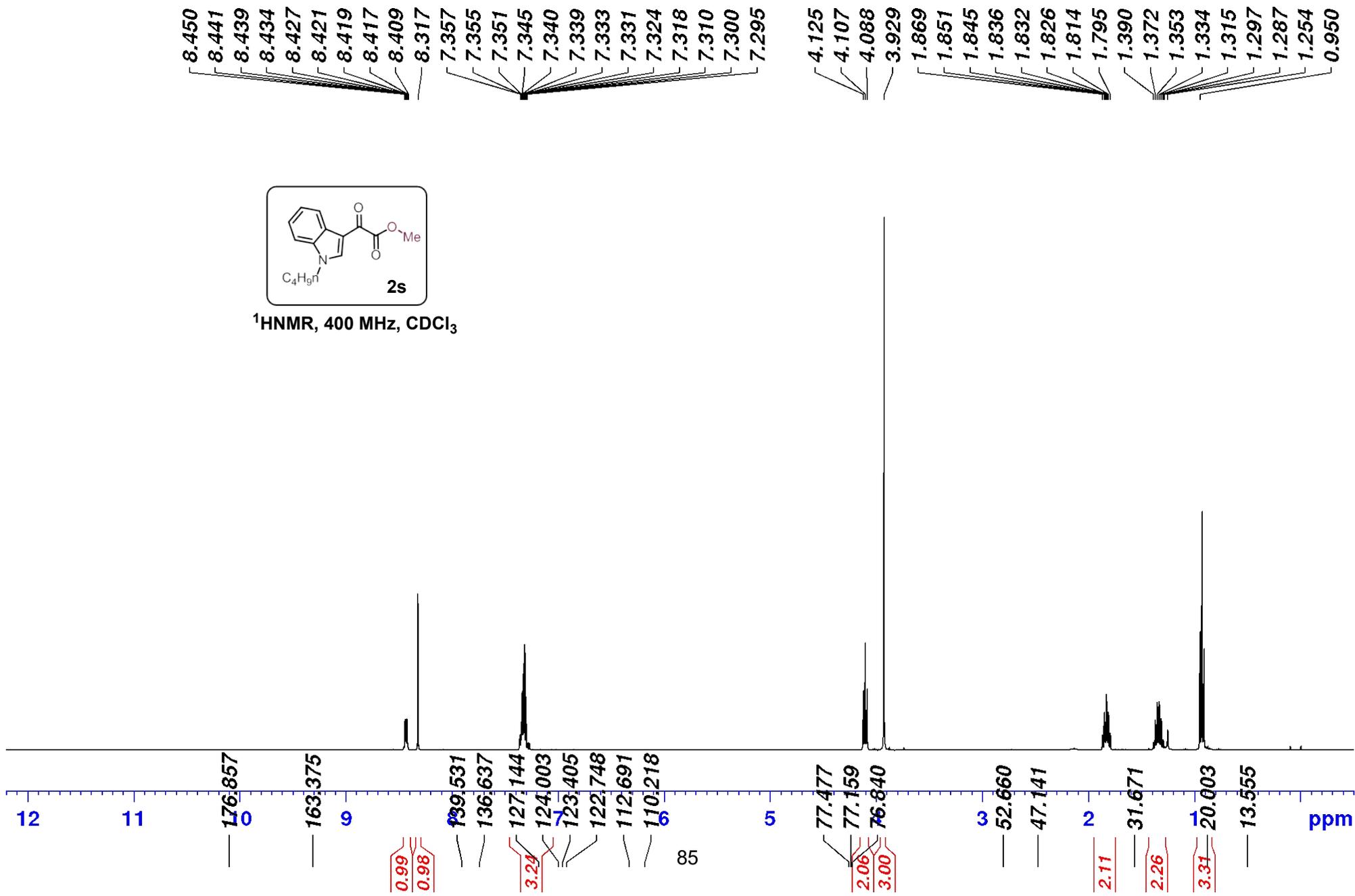
1.54e+007

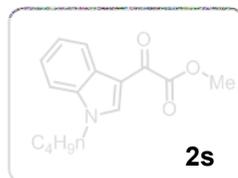
280922_06 9 (0.209)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
280.0977	280.0974	0.3	1.1	11.5	1347.8	n/a	n/a	C17 H14 N O3





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

— 139.584

124.046
123.448
122.789

— 110.263

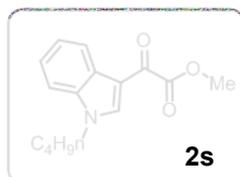
— 52.709

— 47.186

— 31.712

— 20.046

— 13.602



DEPT-135NMR, 101 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

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

Elements Used:

C: 0-15 H: 0-100 N: 0-1 O: 0-4

NVD-143

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

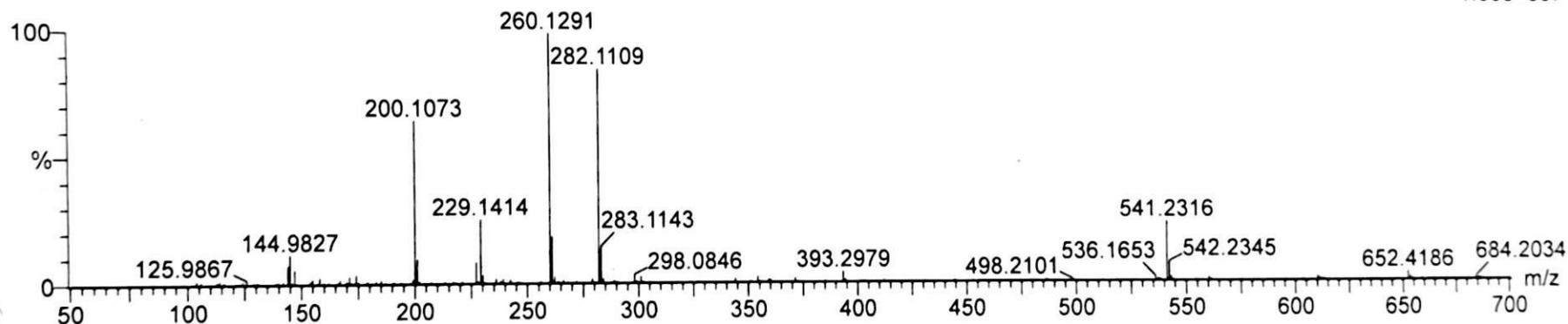
28-Sep-2022

13:00:32

1: TOF MS ES+

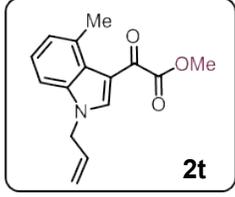
1.66e+007

280922_10 17 (0.364)

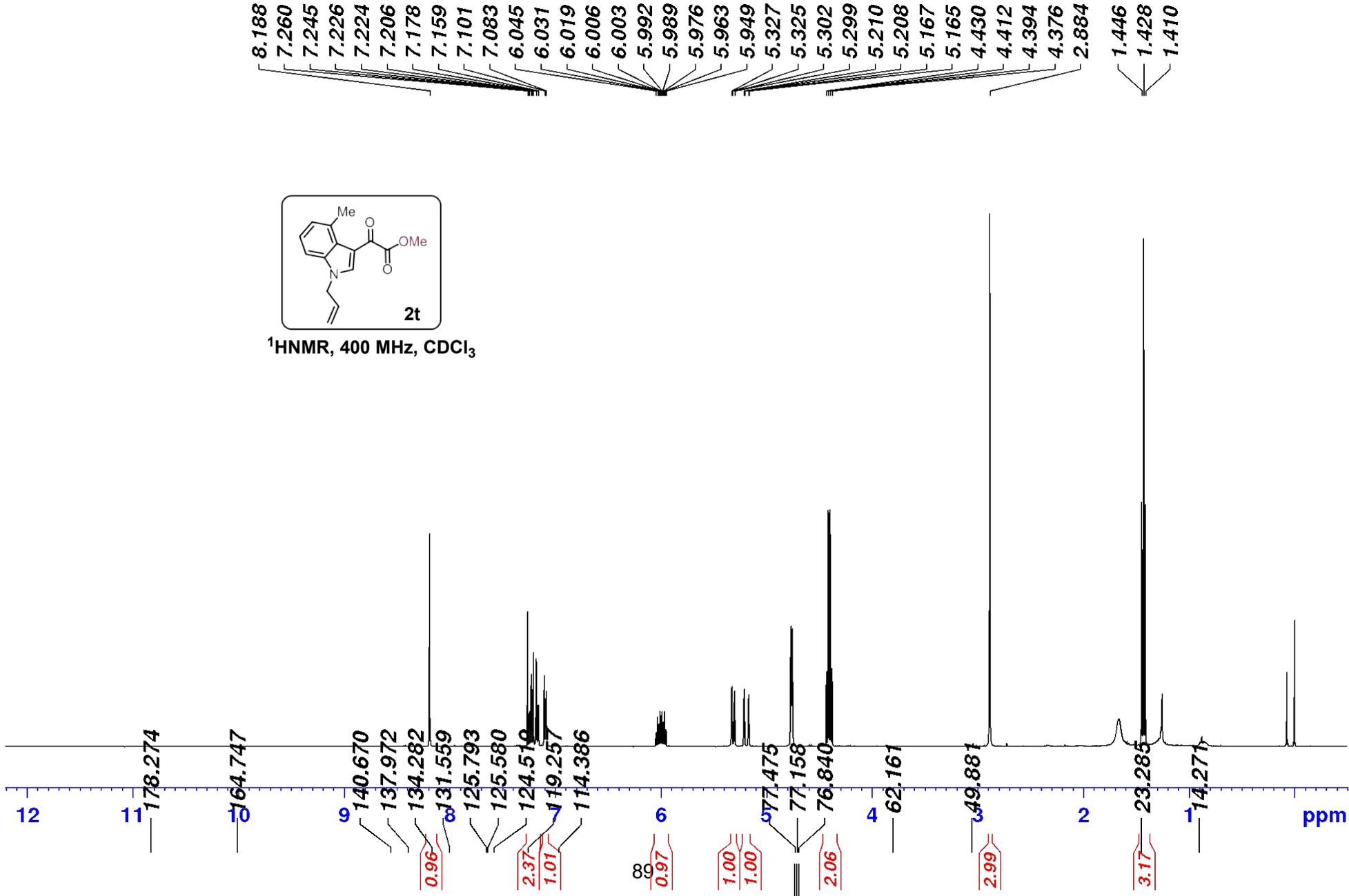


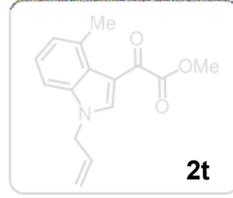
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
260.1291	260.1287	0.4	1.5	7.5	1508.9	n/a	n/a	C15 H18 N O3



¹HNMR, 400 MHz, CDCl₃





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

— 140.558

— 131.440

— 125.464

— 124.403

— 119.142

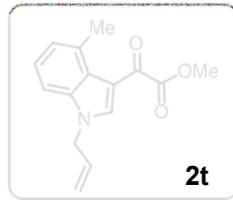
— 107.916

— 62.047

— 49.766

— 23.175

— 14.156



90

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

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

Elements Used:

C: 0-15 H: 0-100 N: 0-1 O: 0-3

NVD-122

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

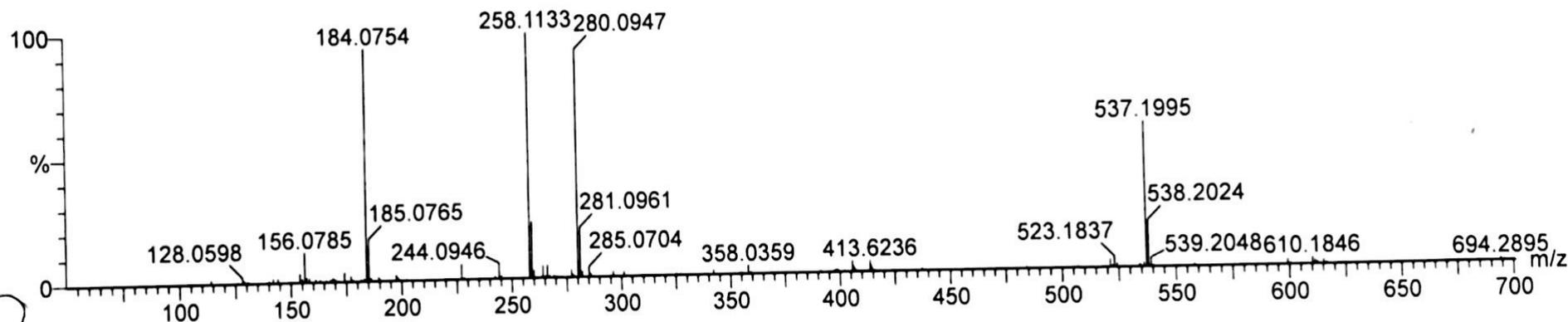
30-Aug-2022

11:49:24

1: TOF MS ES+

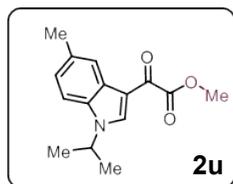
2.21e+007

300822_13 8 (0.172)

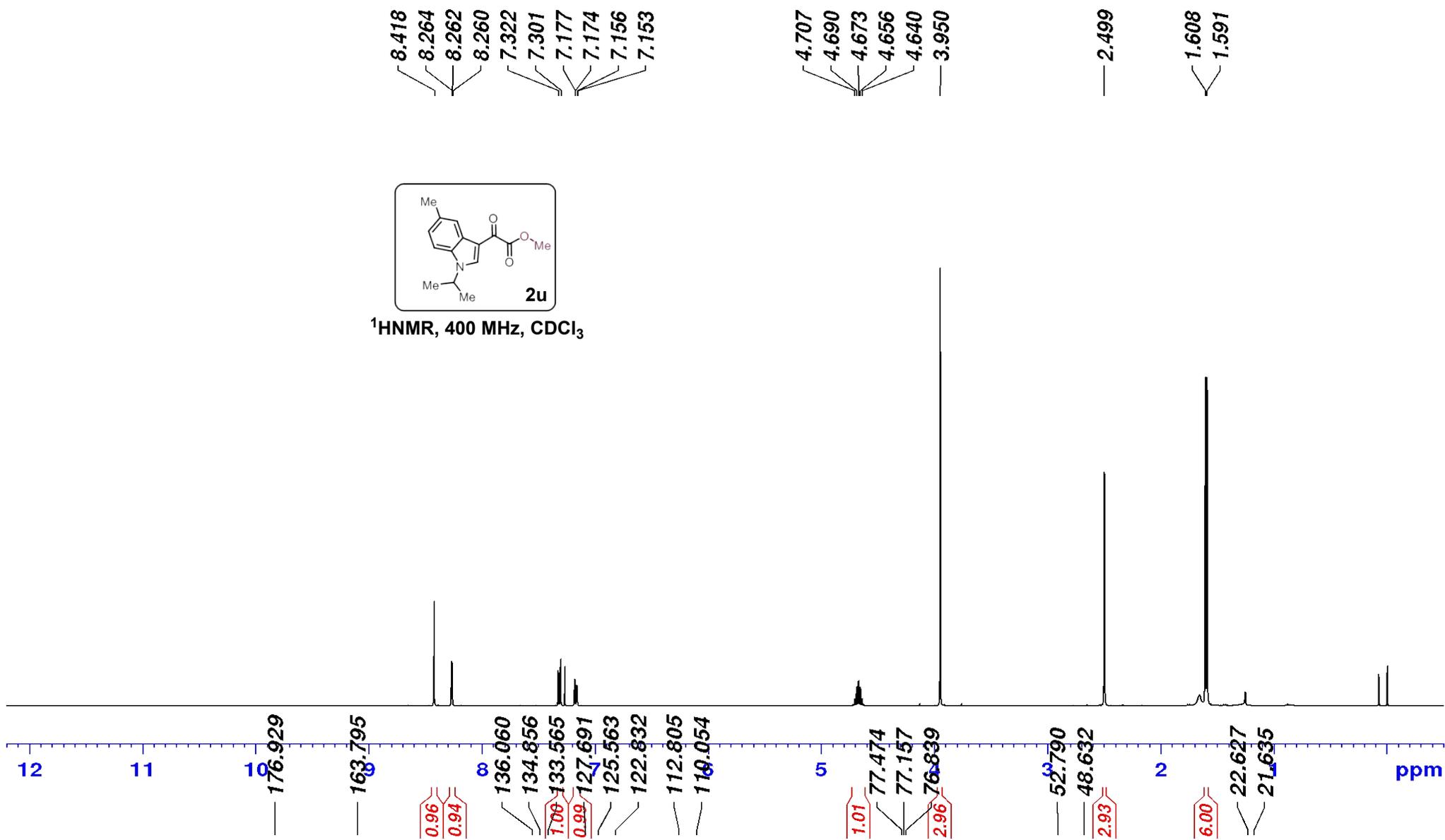


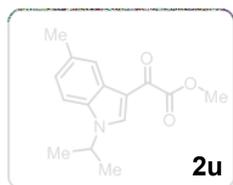
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
258.1133	258.1130	0.3	1.2	8.5	1013.5	n/a	n/a	C15 H16 N O3



¹HNMR, 400 MHz, CDCl₃





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

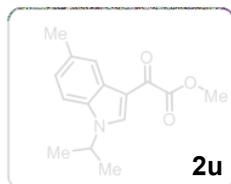
— 135.956

— 125.458
— 122.725

— 109.949

— 52.691
— 48.528

— 22.524
— 21.532



DEPT-135NMR, 101 MHz, CDCl₃

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

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

Elements Used:

C: 0-15 H: 0-100 N: 0-1 O: 0-3

NVD-147

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

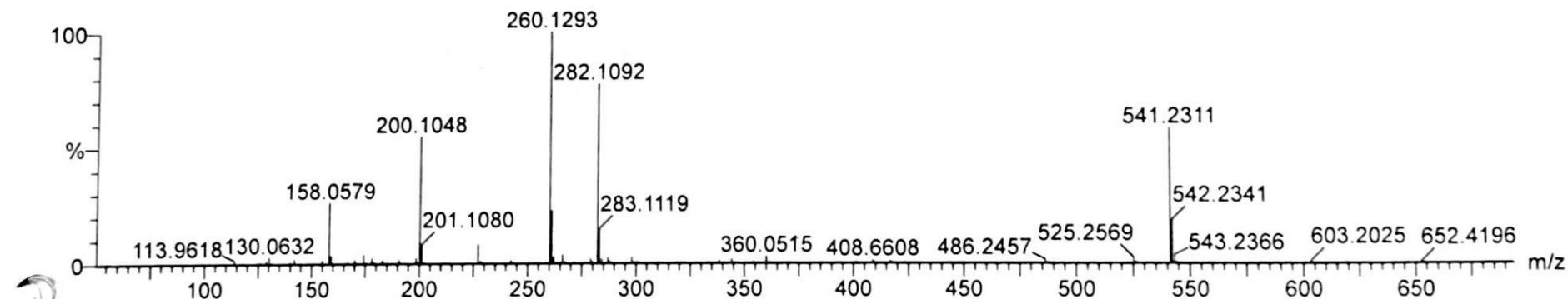
30-Aug-2022

11:41:41

1: TOF MS ES+

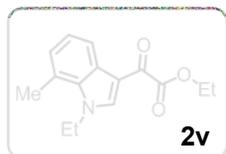
2.21e+007

300822_10 7 (0.155)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
260.1293	260.1287	0.6	2.3	7.5	1000.3	n/a	n/a	C15 H18 N O3



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

— **140.215**

— **127.158**

— **120.573**

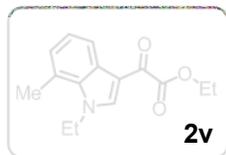
— **61.968**

— **44.586**

— **19.475**

— **17.114**

— **14.155**



DEPT-135NMR, 101 MHz, CDCl₃

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

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

Elements Used:

C: 0-18 H: 0-100 N: 0-1 O: 0-3

NVD-128

220822_16 9 (0.208)

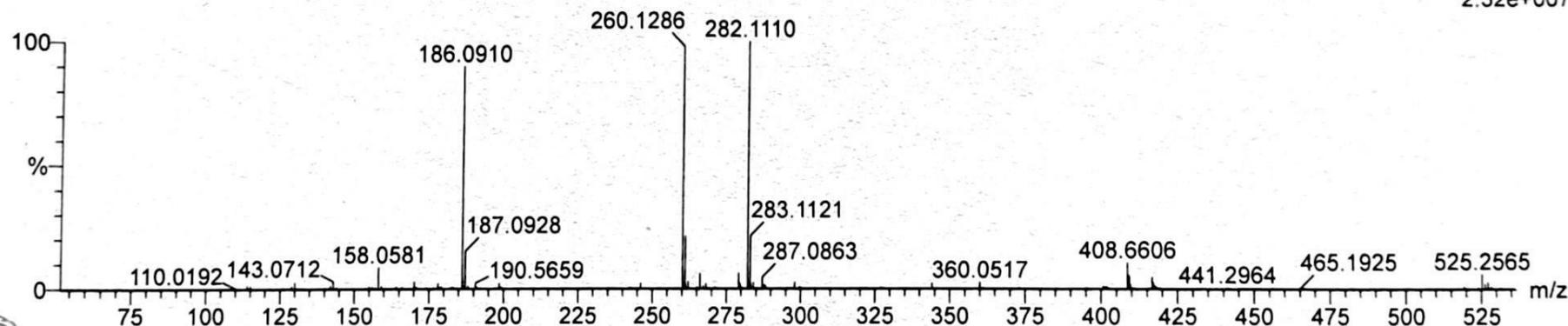
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

22-Aug-2022

12:07:03

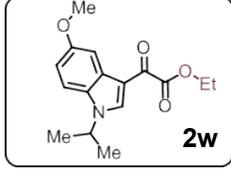
1: TOF MS ES+

2.32e+007

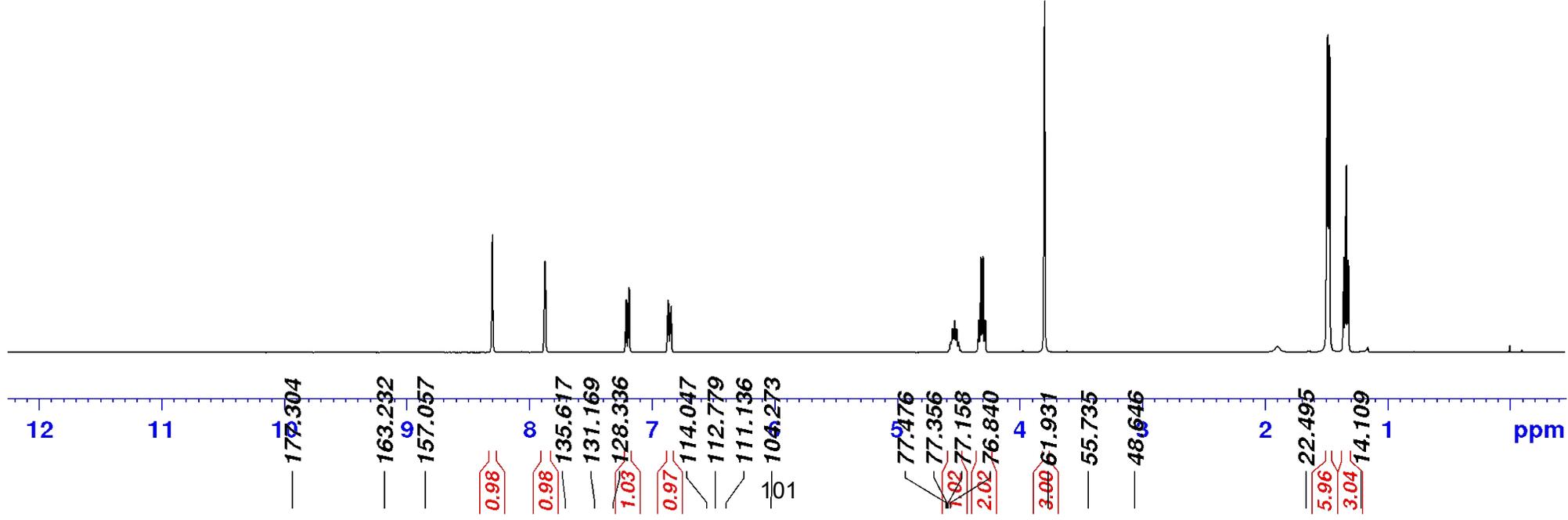


Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
260.1286	260.1287	-0.1	-0.4	7.5	1083.5	n/a	n/a	C15 H18 N O3



¹HNMR, 400 MHz, CDCl₃



177.304

163.232

157.057

0.98

0.98

135.617

131.169

128.336

1.03

114.047

112.779

111.136

104.273

1.01

77.476

77.356

77.158

76.840

1.02

76.840

2.02

61.931

3.00

55.735

48.646

22.495

5.96

3.04

14.109

8.300

7.871

7.207

7.186

6.865

6.843

4.560

4.546

4.529

4.513

4.496

4.480

4.332

4.315

4.297

4.279

3.795

1.488

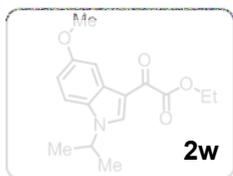
1.472

1.354

1.336

1.318

ppm



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

— 157.058

— 135.619

— 114.048

— 111.138

— 104.272

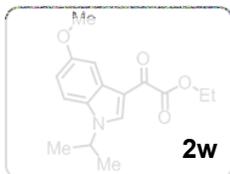
— 61.934

— 55.737

— 48.647

— 22.498

— 14.111



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

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

Elements Used:

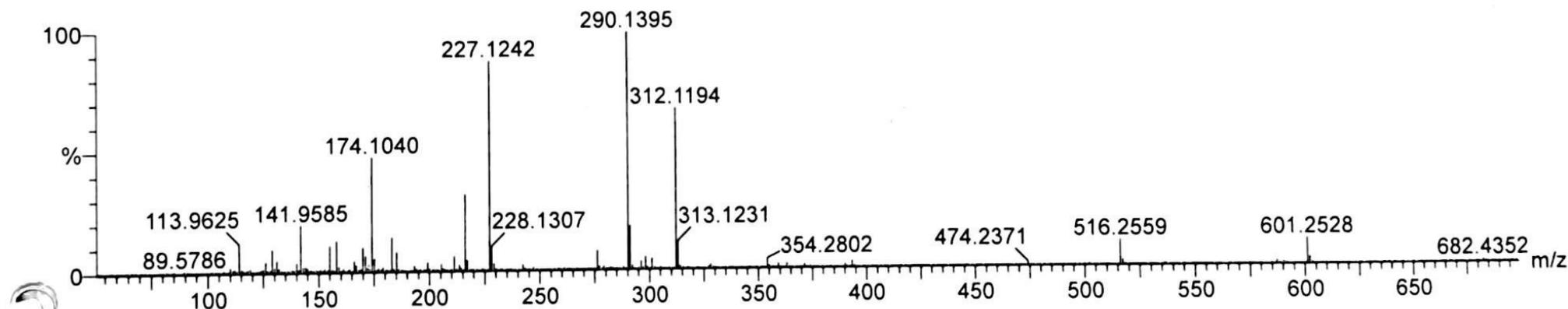
C: 0-16 H: 0-100 N: 0-1 O: 0-4

NVD-137

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

30-Aug-2022
11:51:58
1: TOF MS ES+
3.02e+006

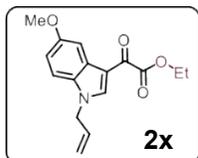
300822_14 16 (0.327) Cm (16)



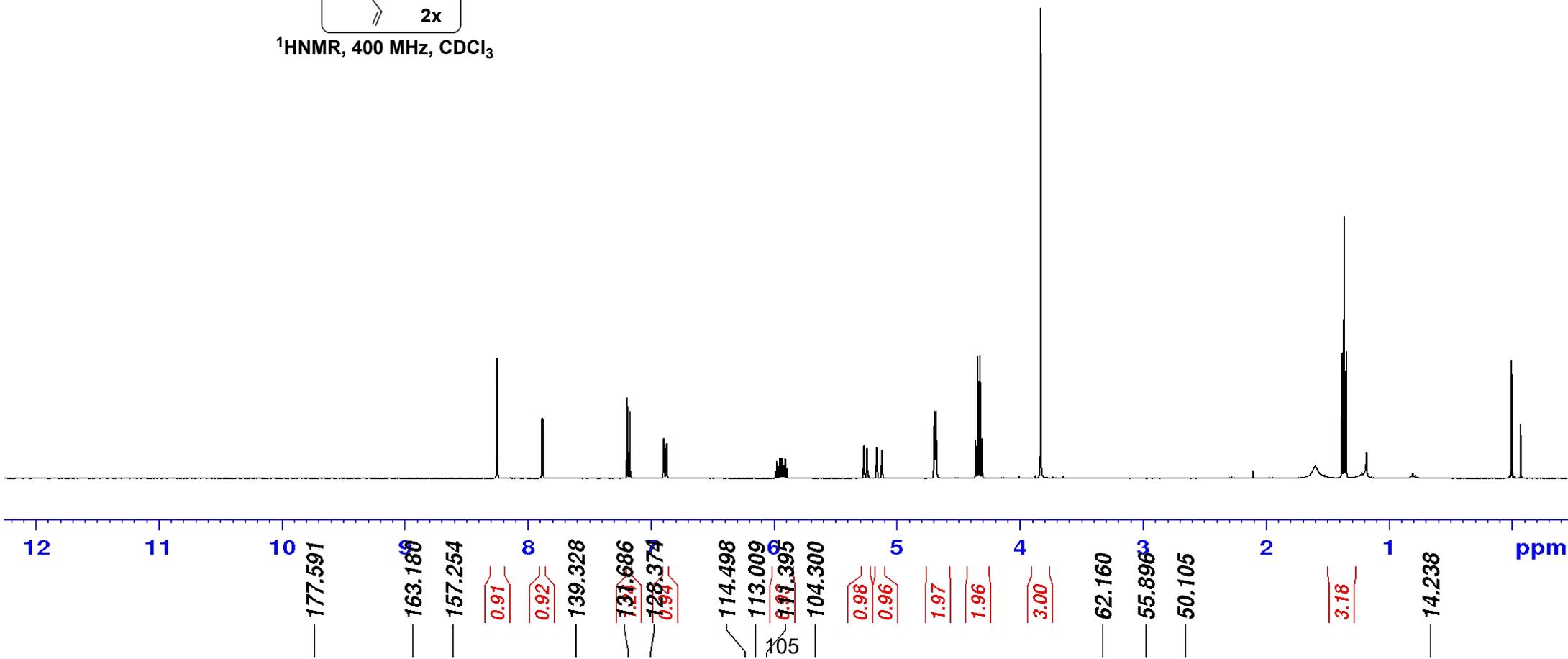
Minimum: -1.5
Maximum: 2.0 50.0 50.0

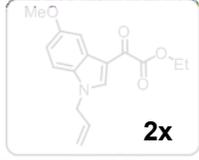
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
290.1395	290.1392	0.3	1.0	7.5	31.6	n/a	n/a	C16 H20 N O4

8.249
7.884
7.878
7.194
7.190
7.168
6.897
6.891
6.875
6.869
5.987
5.973
5.961
5.960
5.948
5.945
5.934
5.931
5.919
5.917
5.905
5.891
5.267
5.265
5.242
5.240
5.163
5.161
5.120
5.118
4.696
4.693
4.689
4.683
4.679
4.675
4.357
4.340
4.322
4.304
3.829
1.380
1.362
1.345



¹HNMR, 400 MHz, CDCl₃





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

— 139.221

— 131.573

— 119.218

— 114.385

— 111.285

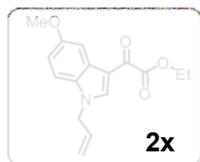
— 104.183

— 62.052

— 55.784

— 49.994

— 14.126



DEPT-135NMR, 101 MHz, CDCl₃

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

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

Elements Used:

C: 0-16 H: 0-100 N: 0-1 O: 0-4

NVD-138

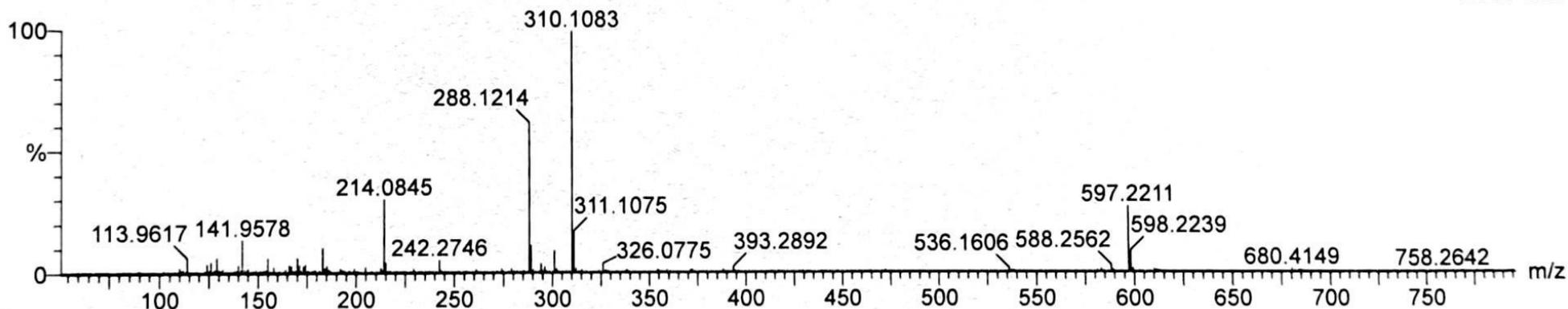
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

23-Aug-2022

11:33:36

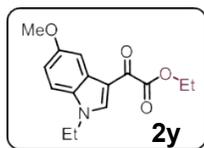
1: TOF MS ES+
3.69e+006

230822_08 9 (0.209) Cm (9)

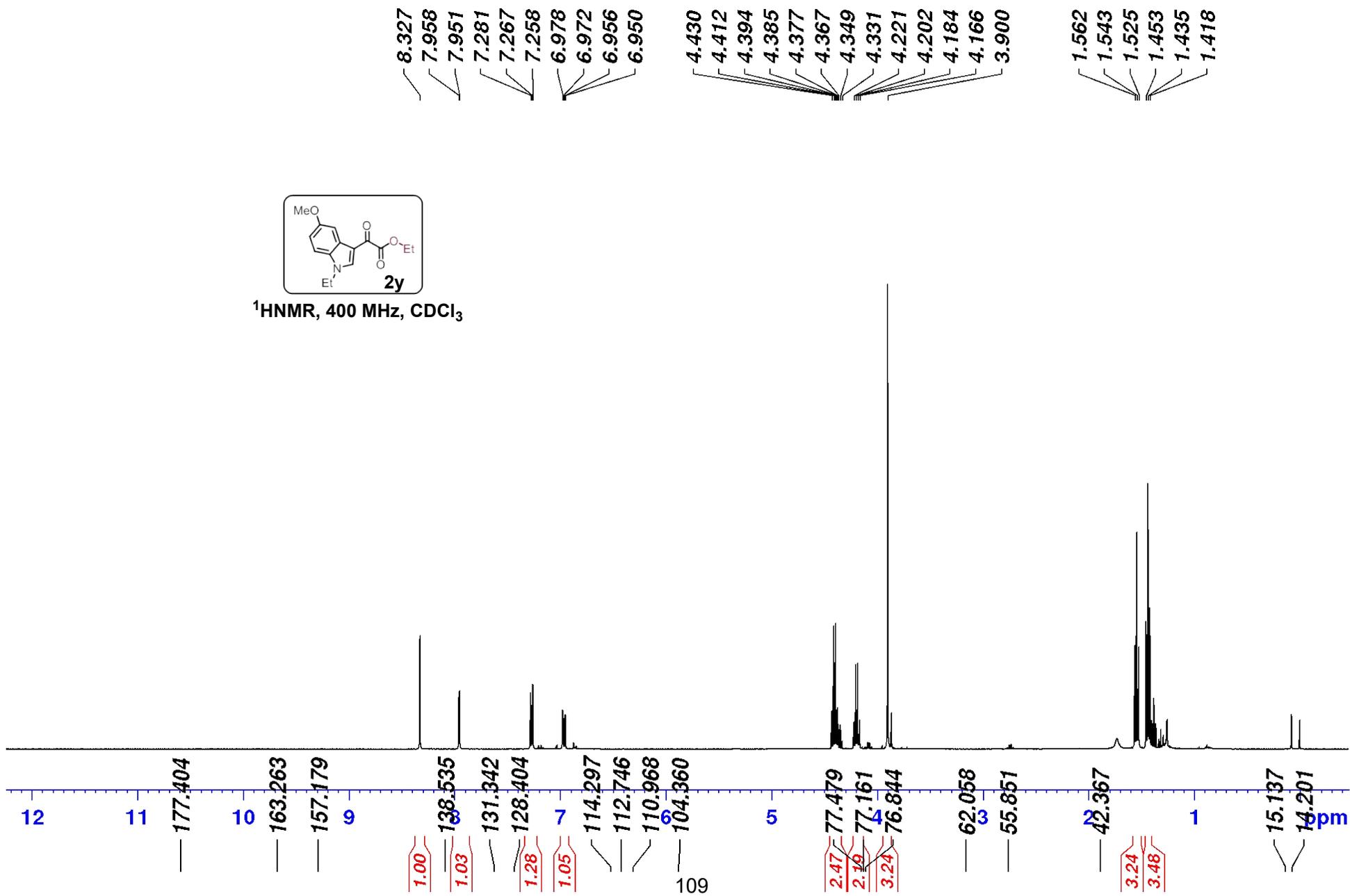


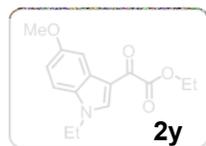
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
288.1214	288.1236	-2.2	-7.6	8.5	28.2	n/a	n/a	C16 H18 N O4



¹HNMR, 400 MHz, CDCl₃





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

— 138.466

— 114.222

— 110.896

— 104.278

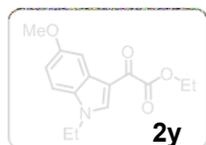
— 61.987

— 55.777

— 42.294

< 15.066

< 14.127



DEPT-135NMR, 101 MHz, CDCl_3

110

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

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

Elements Used:

C: 0-15 H: 0-100 N: 0-1 O: 0-4

NVD-130

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

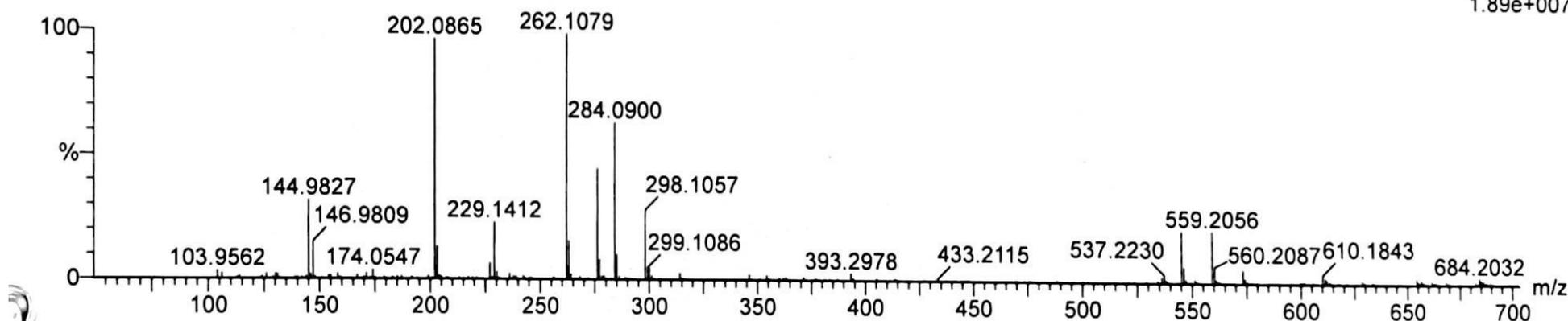
28-Sep-2022

12:57:59

1: TOF MS ES+

1.89e+007

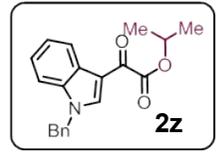
280922_09 9 (0.209)



Minimum: -1.5
Maximum: 2.0 50.0 50.0

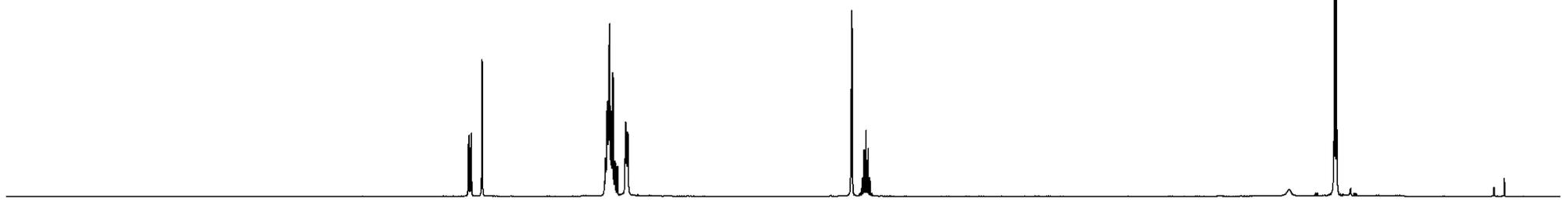
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
276.1236	276.1236	0.0	0.0	7.5	1384.4	n/a	n/a	C15 H18 N O4

8.464
8.462
8.459
8.445
8.442
8.439
8.352
7.353
7.345
7.340
7.330
7.324
7.318
7.313
7.305
7.299
7.296
7.287
7.284
7.268
7.265
7.246
7.182
7.177
7.162
5.332
5.247
5.231
5.215
5.200
5.184

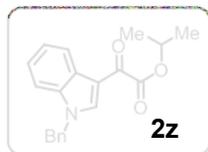


¹HNMR, 400 MHz, CDCl₃

1.386
1.370



12
11
1
178.127
162.601
0.97
1.39
6.16
0.98
136.890
135.249
129.164
128.436
127.383
127.199
124.289
123.659
122.926
113.367
110.587
2.00
0.98
5
77.470
77.152
76.834
70.149
3
51.185
2
1
6.01
21.767
ppm



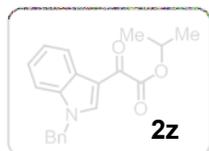
$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3

139.583
129.126
128.398
127.162
124.252
123.622
122.889
— 110.551

— 70.112

— 51.147

— 21.729



DEPT-135NMR, 101 MHz, CDCl₃

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

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

Elements Used:

C: 0-20 H: 0-100 N: 0-1 O: 0-3

NVD-157

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

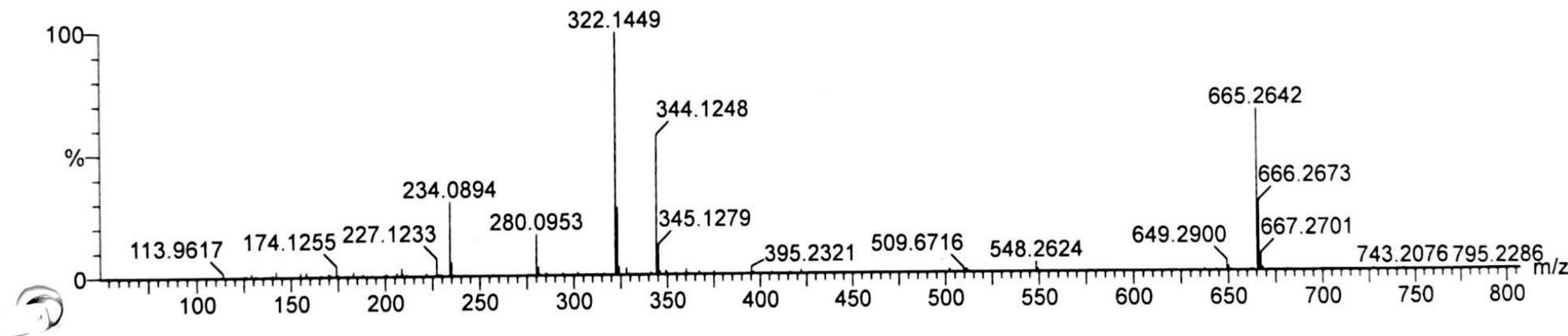
30-Aug-2022

11:44:15

1: TOF MS ES+

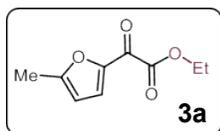
2.09e+007

300822_11 11 (0.242)

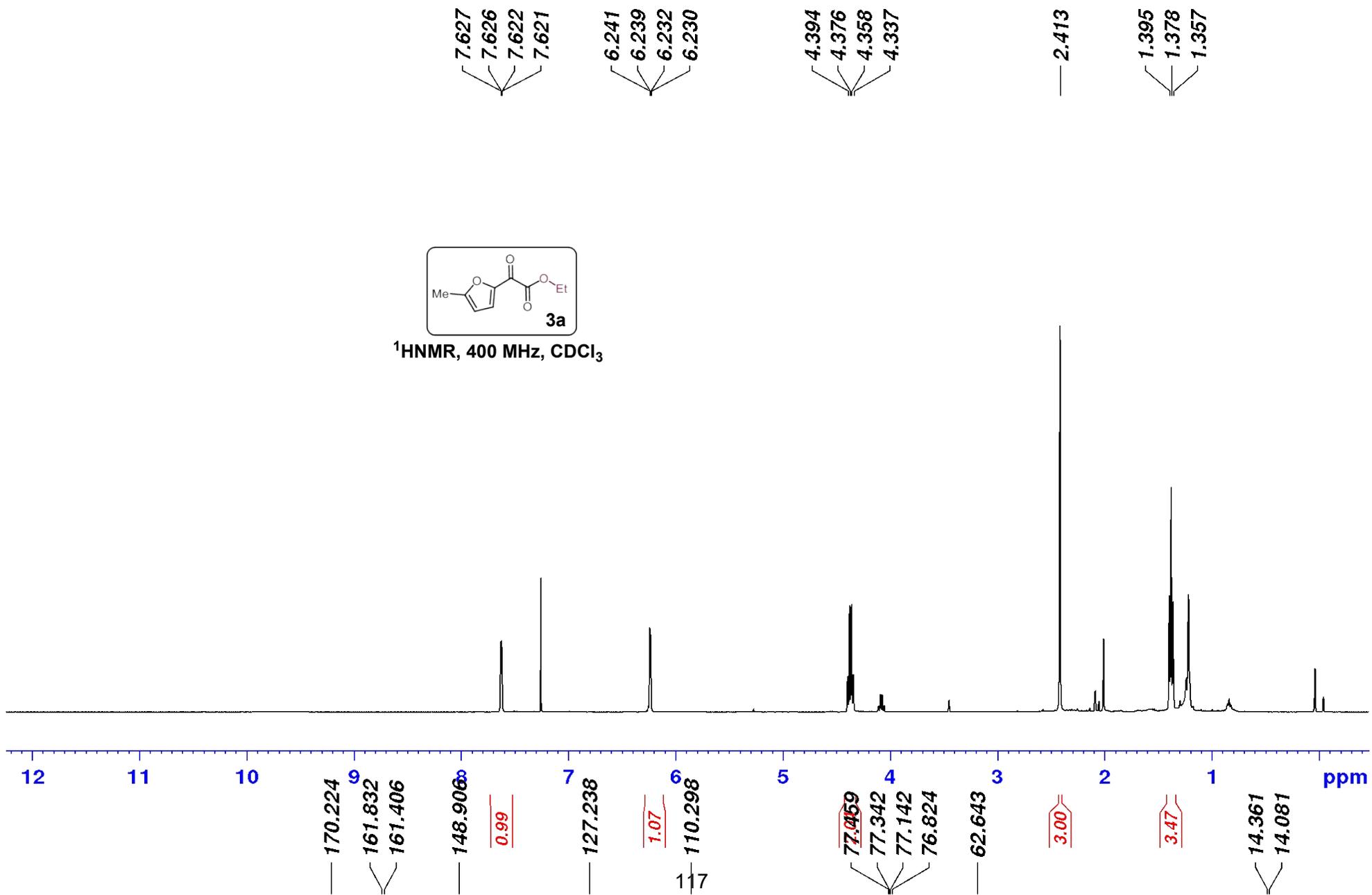


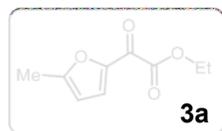
Minimum: -1.5
Maximum: 2.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
322.1449	322.1443	0.6	1.9	11.5	909.6	n/a	n/a	C20 H20 N O3



¹HNMR, 400 MHz, CDCl₃





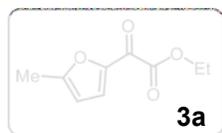
$^{13}\text{C}\{^1\text{H}\}$ NMR, 100 MHz, CDCl_3

— 127.191

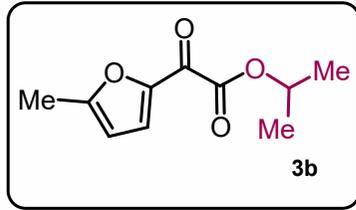
— 110.244

— 62.589

— 14.307
— 14.023



DEPT-135NMR, 101 MHz, CDCl₃



$^1\text{H NMR}$, 400MHz, CDCl_3

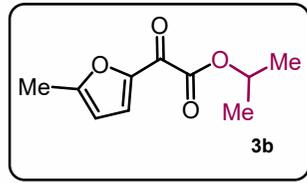
7.607
7.606
7.598
7.597
7.259

6.252
6.250
6.243
6.241

5.259
5.243
5.227
5.212
5.196

— 2.434

1.392
1.376



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

— 170.830

< 161.683

161.193

— 149.038

— 126.947

— 110.242

77.472

77.358

77.154

76.836

70.943

< 21.741

21.587

— 14.417

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 = 4

Monoisotopic Mass, Even Electron Ions

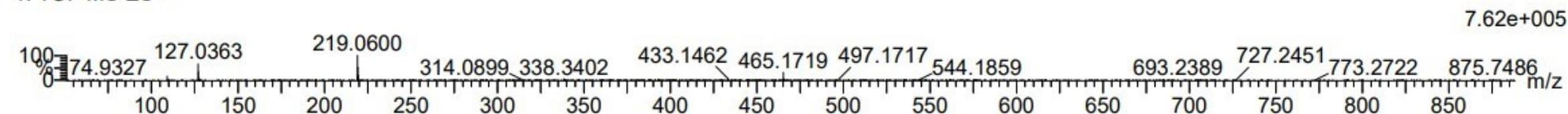
11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-10 H: 0-100 O: 0-4 Na: 0-1

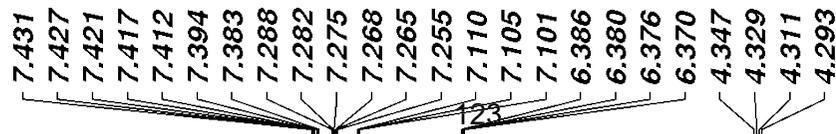
150623_04 6 (0.138)

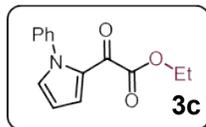
1: TOF MS ES+



Minimum: -1.5
Maximum: 5.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
219.0600	219.0633	-3.3	-15.1	4.5	216.2	n/a	n/a	C10 H12 O4 Na





¹HNMR, 400 MHz, CDCl₃

— 173.423

— 163.229

— 139.820

— 133.984

— 128.793

— 128.133

— 126.010

— 125.526

— 110.843

124

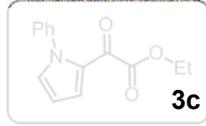
— 77.470

— 77.153

— 76.834

— 62.066

— 14.031

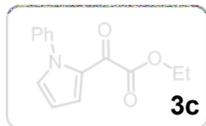


$^{13}\text{C}\{^1\text{H}\}\text{NMR}$, 100 MHz, CDCl_3

134.032
129.907
128.838
128.178
128.072
126.055
125.573
— 110.889

63.182
62.112

14.076
13.959



DEPT-135NMR, 101 MHz, CDCl_3

125

Elemental Composition Report

Page 1

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 = 4

Monoisotopic Mass, Even Electron Ions

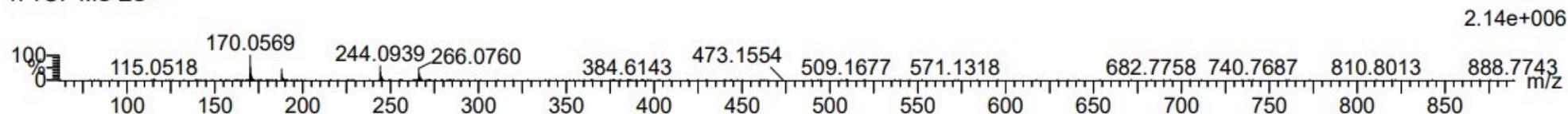
16 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-16 H: 0-100 N: 0-1 O: 0-3

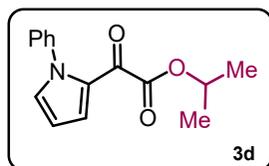
150623_03 17 (0.363)

1: TOF MS ES+

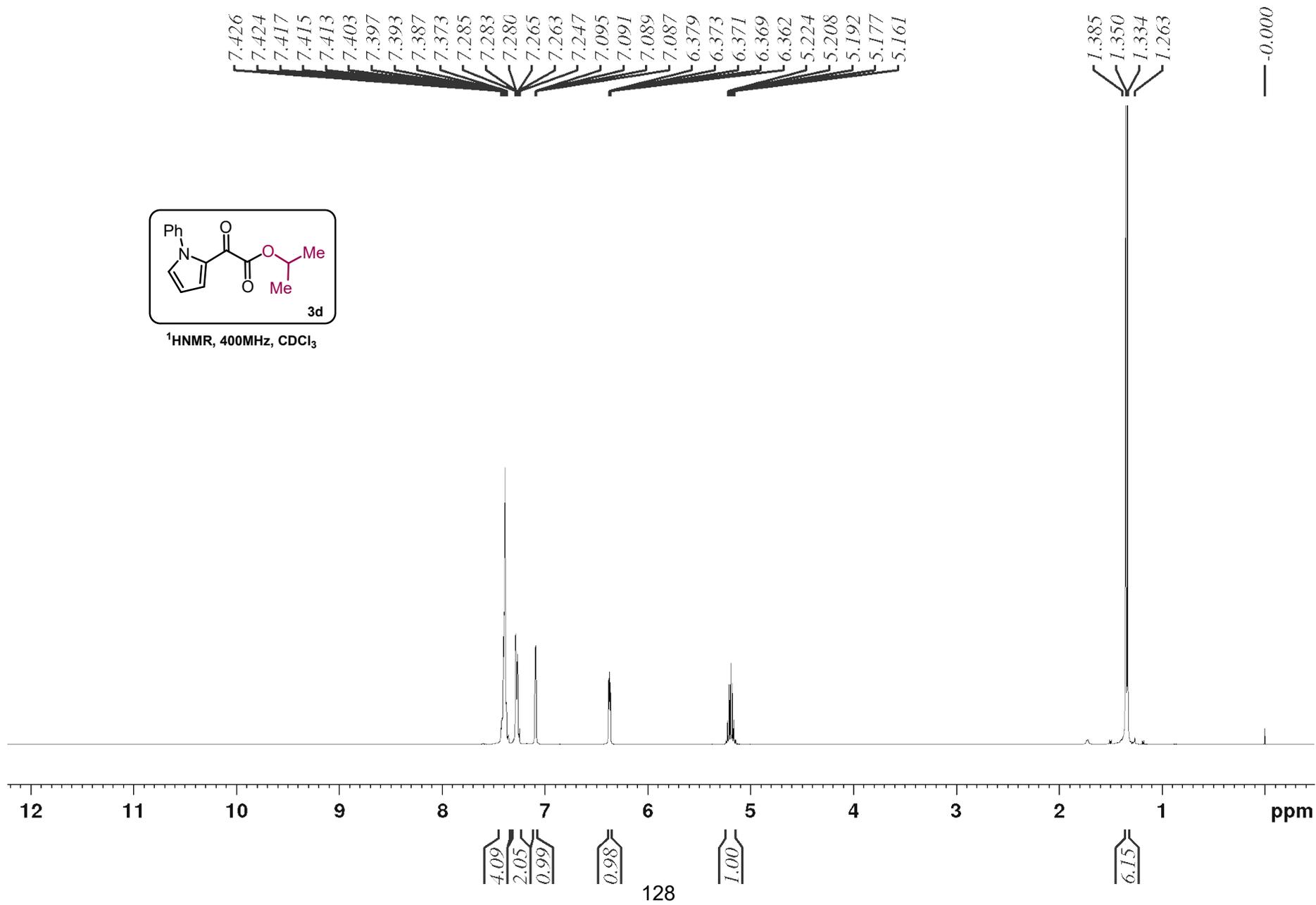


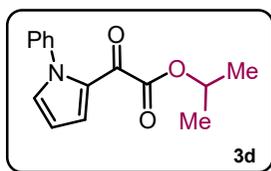
Minimum: -1.5
Maximum: 5.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
244.0939	244.0974	-3.5	-14.3	8.5	282.5	n/a	n/a	C14 H14 N O3

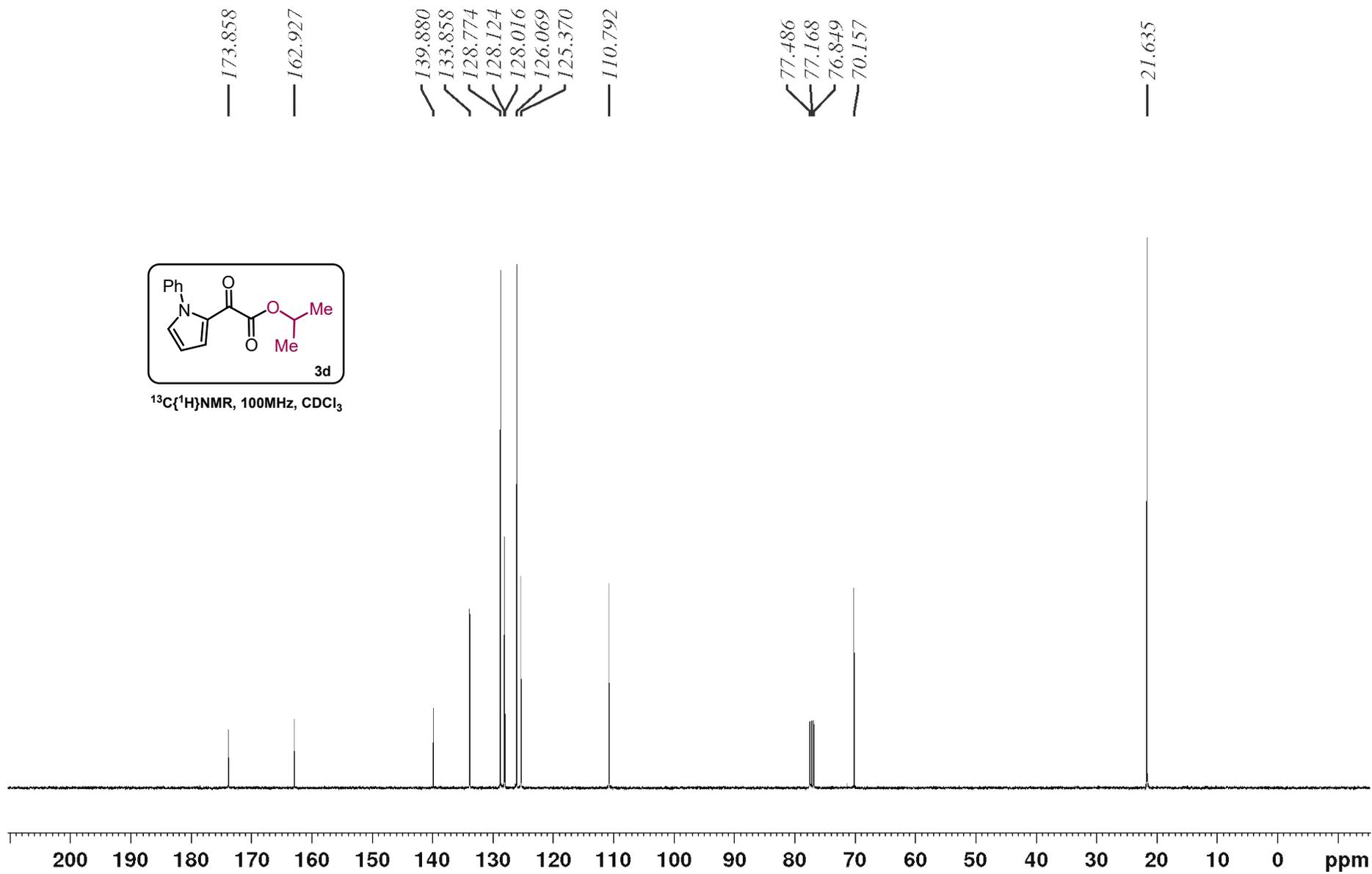


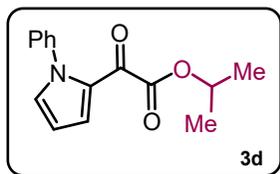
¹HNMR, 400MHz, CDCl₃



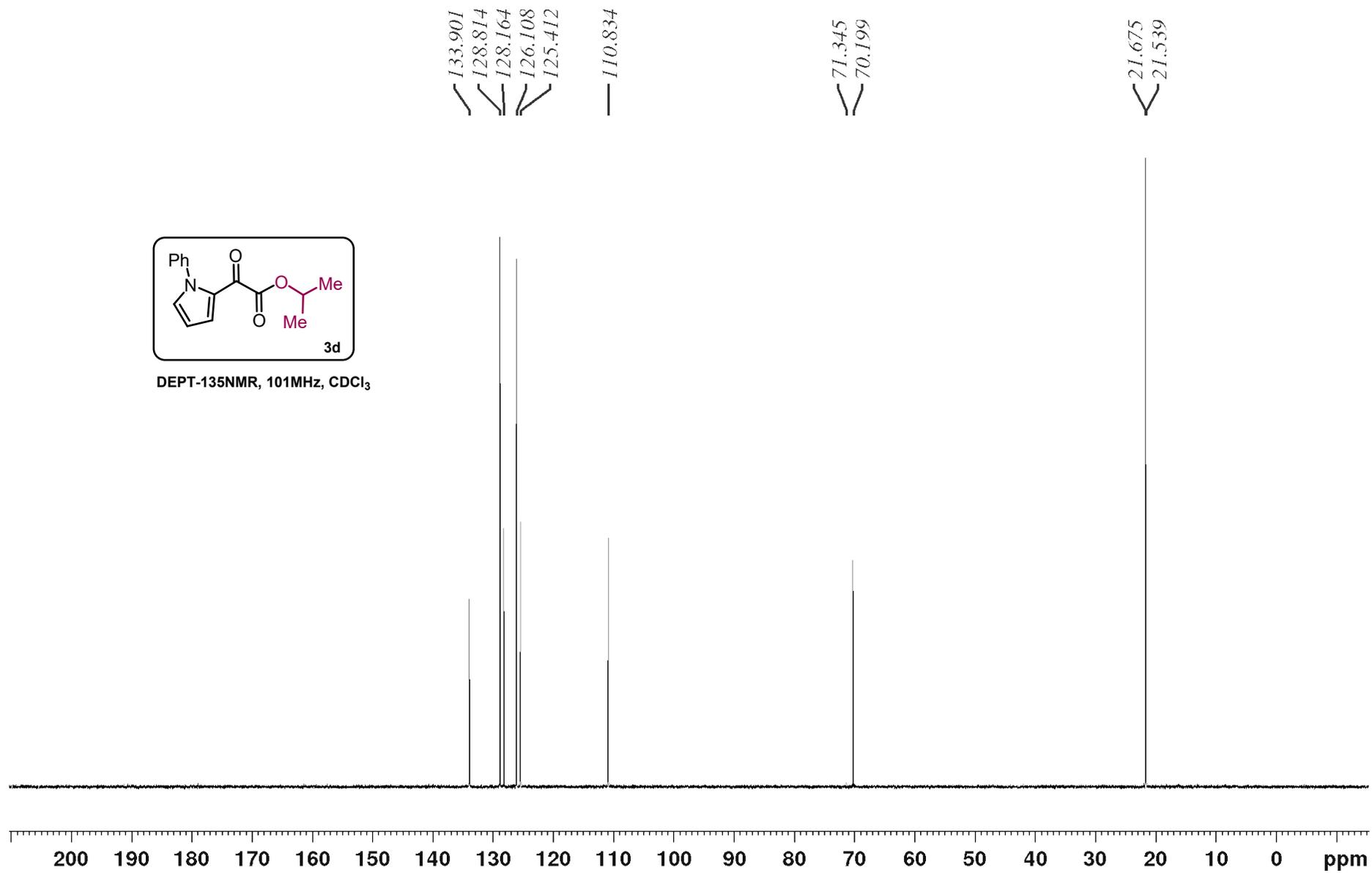


$^{13}\text{C}\{^1\text{H}\}$ NMR, 100MHz, CDCl_3





DEPT-135NMR, 101MHz, CDCl₃



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

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

Elements Used:

C: 0-15 H: 0-100 N: 0-1 O: 0-3

NVD 22

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

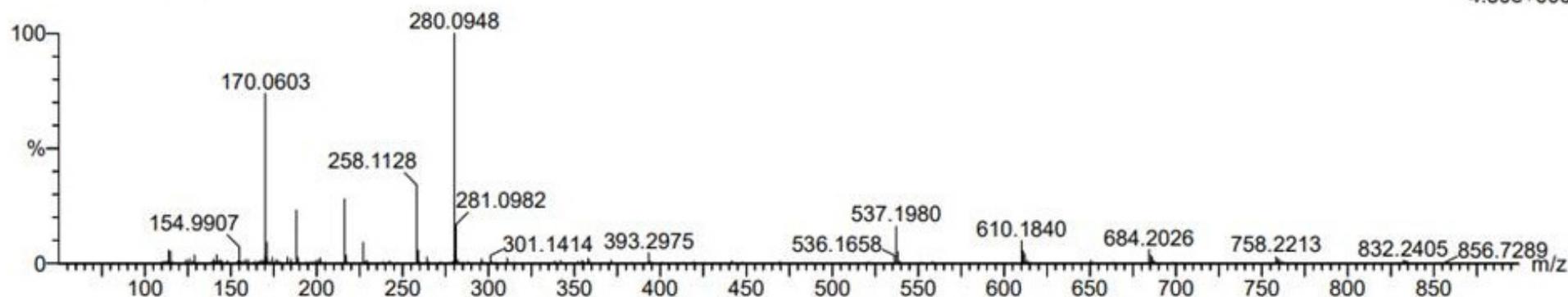
17-May-2023

11:44:20

1: TOF MS ES+

4.50e+006

170523_03 8 (0.172)



Minimum: -1.5
Maximum: 2.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
258.1128	258.1130	-0.2	-0.8	8.5	1130.8	n/a	n/a	C15 H16 N O3