Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Palladium-Catalyzed Regio- and Stereoselective Access to Allyl Ureas/Carbamates: Facile Synthesis of Imidazolidinones and Oxazepinones

Irshad Maajid Taily, Debarshi Saha, and Prabal Banerjee*

Department of Chemistry, Indian Institute of Technology Ropar,

Nangal Road, Rupnagar, Punjab 140001, India,

E-mail: prabal@iitrpr.ac.in

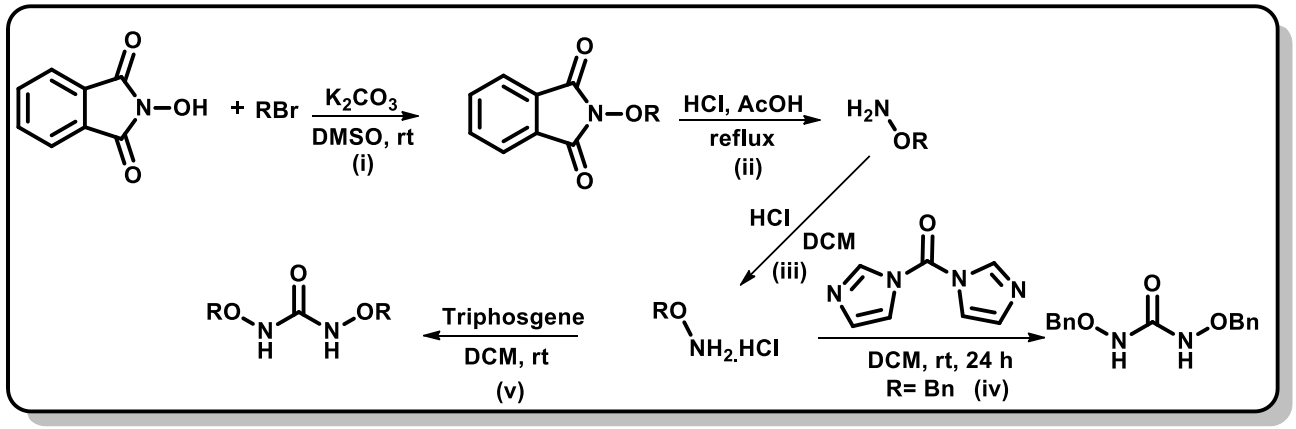
Contents

1. General Information

All reactions were carried out under an inert atmosphere with oven-dried glass wares. All solvents and reagents were obtained from commercial sources and were purified following the standard procedure before use. The developed chromatogram was analyzed by UV lamp (254 nm) or *p*-anisaldehyde solution. Products were purified by silica gel (mesh size 230–400) column chromatography. The ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ and DMSO as per requirement. Chemical shifts of ^{1}H and ^{13}C NMR spectra are expressed in parts per million (ppm). All coupling constants are absolute values and are expressed in hertz. The description of the signals includes the following: s = singlet, d = doublet, dd = doublet of doublet, t = triplet, dt = doublet of triplet, q = quartet, dq = doublet of quartet, br = broad, and m = multiplet.

2. General procedure for the synthesis symmetrical urea[1,2]

(i) To a mixed solution of 2-hydroxyisoindoline-1,3-dione (10 mmol) in DMSO (15 mL) and anhydrous potassium carbonate (8 mmol) benzyl bromide (20 mmol) was added and the resulting mixture was stirred for 24 h at room temperature. After that, 30 mL of cool water was added and the resulting mixture was allowed to stand for 30 minutes. The obtained precipitate was filtered and washed with water (3×5 mL). Then the precipitate was recrystallized from ethanol and gives the product *N*-benzyloxyphthalimide as white needle like crystals.



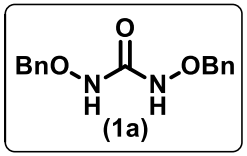
(ii) A mixture of *N*-Benzyloxyphthalimide (4 mmol), acetic acid (4 mL) and hydrochloric acid (aq. 37 %) (1.5 mL) was refluxed for 1.5 hours. The reaction mixture was cooled to room temperature and concentrated. Then cold water (10 mL) was added to the solid residue and the suspension was adjusted to alkaline by addition of 10% sodium hydroxide solution. The obtained solution was subsequently extracted with CH_2Cl_2 (3×15 mL) and the combined organic phases were dried over anhydrous Na_2SO_4 and concentrated to a final volume of 10 ml.

(iii) To the final concentrate obtained above 6M HCl (5 mL) was added to it under stirring at 0-5°C. After further stirring for another 1 hour at room temperature, the solid was filtered, washed with CH_2Cl_2 (10 mL) and dried extensively in vacuo at 45°C. The product was obtained as a white solid.

(iv)To a solution of O-Benzylhydroxylamine hydrochloride (125.30 mmol) in dichloromethane (313 ml) was added triethylamine (125.305 mmol) at 0 °C and stirred for 10 minutes before the addition of 1,1′-Carbonyldiimidazole (62.651 mmol) over a period of 15 minutes in 3 portions. The reaction mixture was stirred at room temperature for 24 hours. The reaction was quenched with water (100 ml) and extracted with dichloromethane (3 x 400 ml). The combined organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified via column chromatography (4:1 to 3:2, hexanes: ethyl acetate) to provide the white solid product. (**1a** was prepared by using this method)

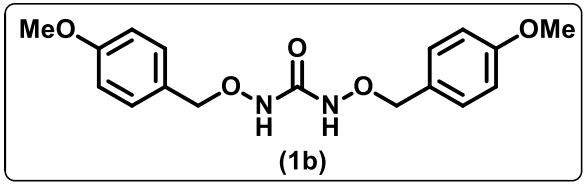
(v) To a stirring solution of amine in DCM was added base and stirred for 5-10 minutes at 0 ^{0}C. Triphosgene was added dropwise this this temperature and then allowed to stirred at rt until the completion of reaction as monitored by TLC. After completion the reaction was quenched by adding aq. NH_4Cl solution and then washed with water. The DCM layer was extracted and concentrated to dryness under reduced pressure. The residue was purified by means of silica gel column chromatography. (**1b-1f** were prepared by using this method)

1,3-bis(benzyloxy)urea:



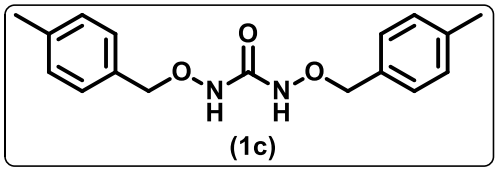
(1a)

^{1}H NMR (400 MHz, CDCl3): δ 7.59 (brs, 2H), 7.41–7.27 (m, 10H), 4.78 (s, 4H)



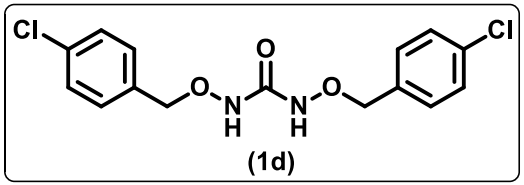
(1b)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.26 (s, 2H), 7.00 (d, *J* = 7.6 Hz, 4H), 6.63 (d, *J* = 8.4 Hz, 4H), 4.47 (s, 4H), 3.57 (s, 6H)



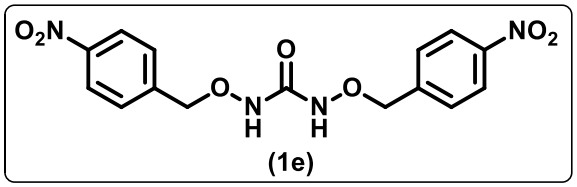
(1c)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.48 (s, 2H), 7.22-7.14 (m, 8H), 4.74 (s, 4H), 2.37 (s, 6H)



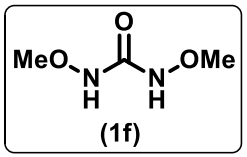
(1d)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.56 (s, 2H), 7.35 (d, *J* = 8.4 Hz, 4H), 7.26 (d, *J* = 8.3 Hz, 4H), 4.75 (s, 4H)



(1e)

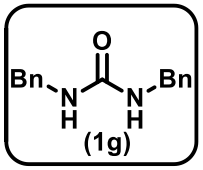
^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.23 (d, *J* = 8.5 Hz, 4H), 7.66 (s, 2H), 7.26 (d, *J* = 8.5 Hz, 4H), 4.93 (s, 4H)



(1f)

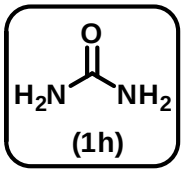
^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.81 (s, 2H), 3.75 (s, 6H)

Procedure for preparation of 1, 3-dibenzylurea: To a solution of amine (1.0 equiv.) in CH_2Cl_2 was added successively DABCO (0.1 equiv.) and a solution of $(Boc)_2O$ (0.5 equiv.). After the completion of the reaction as detected by TLC, the reaction mixture was cooled to 0 °C, n-hexane was then added, the resulting solid was collected and further washed with cold water and diethyl ether to afford the corresponding product.



(1g)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.33-7.20 (m, 10H), 6.43 (t, *J* = 5.8 Hz, 2H), 4.23 (d, *J* = 6.4 Hz, 4H)



(1h)

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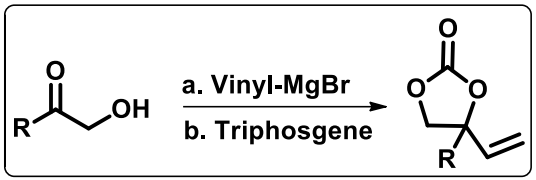
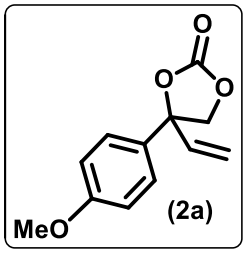
3. General procedure for the synthesis of substituted VECs 2[3]

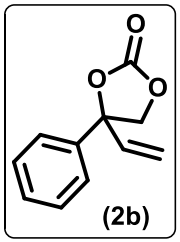


a) To a solution of hydroxyl methyl ketone (1 equiv.) in THF (20 mL) was added vinylmagnesium bromide (1.0 M in THF, 2.5 equiv.) at 0 °C. The reaction was stirred under N_2 atmosphere at room temperature for 2 h. The reaction mixture was then quenched with saturated aqueous NH_4Cl, and extracted with EtOAc. The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by flash chromatography on silica to afford corresponding diols.

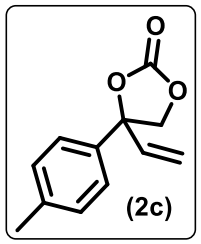
b) To a solution of diol (1 equiv.) and pyridine (4 equiv.) in CH_2Cl_2 (20 mL) was added triphosgene (0.5 equiv., 1.0 M in CH_2Cl_2) at 0 °C. The reaction was stirred under N_2 atmosphere at room temperature for 2 h. The reaction mixture was then quenched with saturated aqueous NH_4Cl, and extracted with CH_2Cl_2. The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by flash chromatography on silica to afford corresponding VECs.



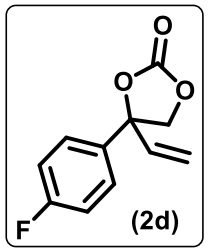
^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.29 (d, *J* = 8.7 Hz, 2H), 6.94 (d, *J* = 8.6 Hz, 2H), 6.14 (dd, *J* = 17.5, 10.5 Hz, 1H), 5.43 (d, *J* = 3.5 Hz, 1H), 5.39 (d, *J* = 9.1 Hz, 1H), 4.61 (d, *J* = 8.6 Hz, 1H), 4.56 (d, *J* = 8.5 Hz, 1H), 3.82 (s, 3H)



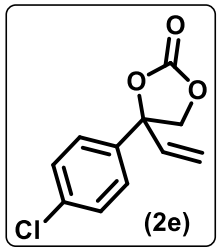
^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.46-7.34 (m, 5H), 6.16 (dd, *J* = 17.8, 10.6 Hz, 1H), 5.44 (s, 1H), 5.40 (d, *J* = 6.3 Hz, 1H), 4.66 (d, *J* = 8.2 Hz, 1H), 4.58 (d, *J* = 8.3 Hz, 1H)



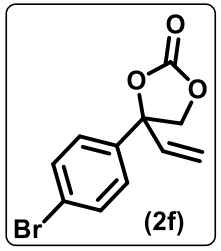
^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.24-7.21 (m, 4H), 6.14 (dd, *J* = 17.2, 10.4 Hz, 1H), 5.42 (d, *J* = 2.1 Hz, 1H), 5.39 (d, *J* = 4.2 Hz, 1H), 4.62 (d, *J* = 8.5 Hz, 1H), 4.56 (d, *J* = 8.4 Hz, 1H), 2.36 (s, 3H)



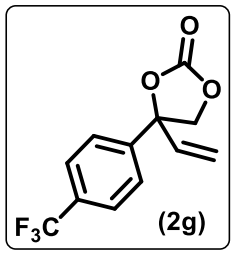
^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.38-7.32 (m, 2H), 7.12 (t, *J* = 8.8 Hz, 2H), 6.14 (dd, *J* = 17.5, 10.7 Hz, 1H), 5.45 (d, *J* = 10.6 Hz, 1H), 5.40 (d, *J* = 17.2 Hz, 1H), 4.65 (d, *J* = 8.5 Hz, 1H), 4.55 (d, *J* = 8.6 Hz, 1H)



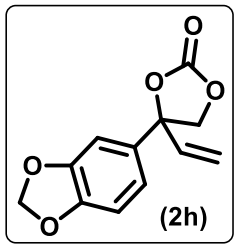
^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.41 (d, *J* = 8.7 Hz, 2H), 7.30 (d, *J* = 8.7 Hz, 2H), 6.13 (dd, *J* = 17.8, 10.8 Hz, 1H), 5.45 (d, *J* = 10.8 Hz, 1H), 5.41 (d, *J* = 17.1 Hz, 1H), 4.65 (d, *J* = 8.3 Hz, 1H), 4.53 (d, *J* = 8.6 Hz, 1H)



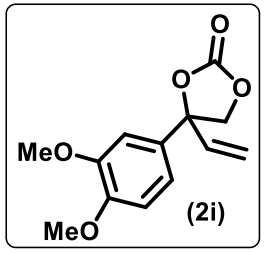
^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.5 Hz, 2H), 7.24 (d, *J* = 8.6 Hz, 2H), 6.12 (dd, *J* = 18.0, 10.4 Hz, 1H), 5.44 (d, *J* = 10.6 Hz, 1H), 5.40 (d, *J* = 17.1 Hz, 1H), 4.64 (d, *J* = 8.4 Hz, 1H), 4.53 (d, *J* = 8.7 Hz, 1H)



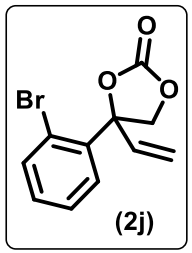
^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 2H), 6.15 (dd, *J* = 17.7, 10.5 Hz, 1H), 5.48 (d, *J* = 10.4 Hz, 1H), 5.43 (d, *J* = 17.3 Hz, 1H), 4.71 (d, *J* = 8.8 Hz, 1H), 4.56 (d, *J* = 8.5 Hz, 1H)



^{1}H-NMR (400 MHz, $CDCl_3$): δ 6.85-6.81 (m, 3H), 6.11 (dd, *J* = 16.4, 10.7 Hz, 1H), 6.00 (s, 2H), 5.44 (d, *J* = 3.1 Hz, 1H), 5.40 (d, *J* = 3.4 Hz, 1H), 4.60 (d, *J* = 8.5 Hz, 1H), 4.53 (d, *J* = 8.5 Hz, 1H)

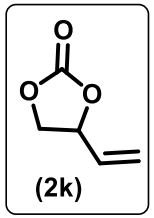


^{1}H-NMR (400 MHz, $CDCl_3$): δ 6.90-6.84 (m, 3H), 6.14 (dd, *J* = 17.0, 10.7 Hz, 1H), 5.44 (s, 1H), 5.41 (d, *J* = 5.5 Hz, 1H), 4.62 (d, *J* = 8.4 Hz, 1H), 4.58 (d, *J* = 8.4 Hz, 1H), 3.89 (s, 6H)



(2j)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 7.8 Hz, 1H), 7.59 (d, *J* =8.3 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.26 (m, 1H), 6.34 (dd, *J* = 17.0, 10.9 Hz, 1H), 5.39 (d, *J* = 2.6 Hz, 1H), 5.36 (d, *J* = 3.9 Hz, 1H), 4.96 (d, *J* = 9.2 Hz, 1H), 4.71 (d, *J* = 8.8 Hz, 1H)



(2k)

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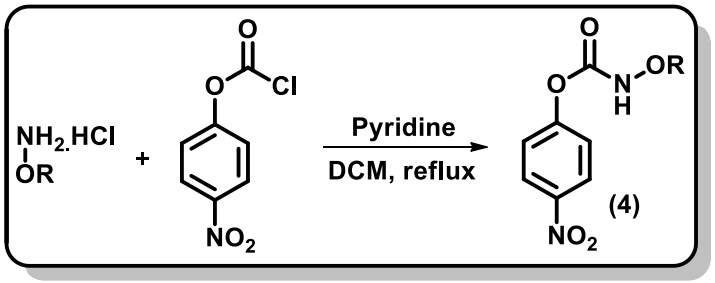
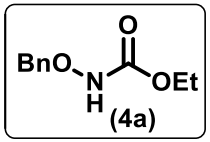
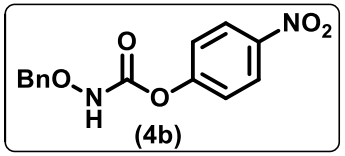
4. General procedure for the synthesis of carbamates[4]



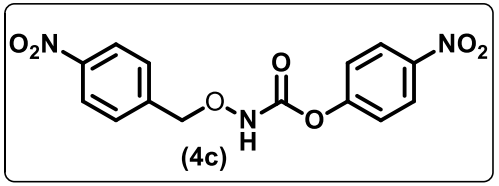
Amine hydrochloride was suspended in dry dichloromethane (DCM) (20 mL) and pyridine (10 mmol). 4-Nitrophenylchloroformate (10 mmol) dissolved in DCM (10 mL) was added dropwise while stirring at room temperature for 45 min. After the addition was completed, the reaction mixture was refluxed for 6 h and then cooled to rt, diluted with DCM (20 mL), washed sequentially with 1N HCl, H_2O, 1M sodium bicarbonate solution, water and brine. The DCM layer was dried over sodium sulfate and evaporated under vacuum. The crude product was purified by flash chromatography using a mixture of ethyl acetate/hexane.



^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.2-7.32 (m, 5H), 7.22 (brs, 1H), 4.87 (s, 2H), 4.24 (q, *J* = 7.1 Hz, 2H), 1.28 (t, *J* = 7.1 Hz, 3H)

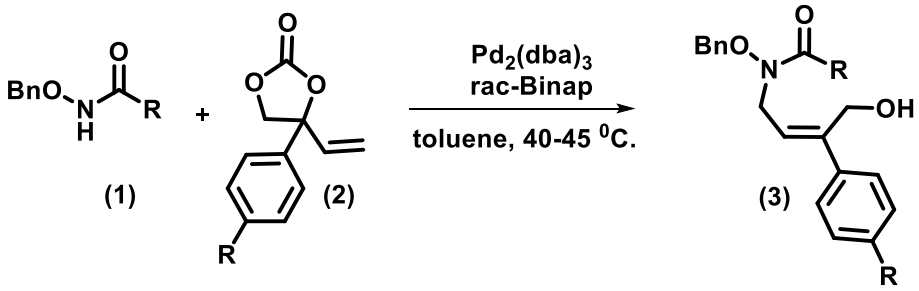


^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.26 (d, *J* = 9.3 Hz, 4H), 7.66 (brs, 2H), 7.46-7.36 (m, 5H), 7.32 (d, *J* = 9.1 Hz, 4H), 4.98 (s, 2H)



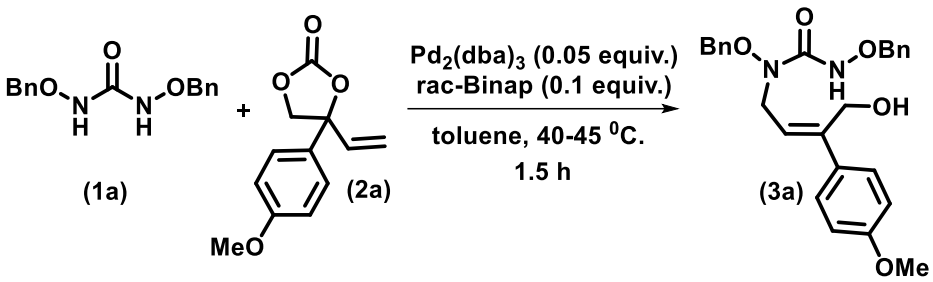
^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.30-8.25 (m, 4H), 7.78 (brs, 2H), 7.62 (d, *J* = 8.5 Hz, 2H), 7.34 (d, *J* = 9.2 Hz, 2H), 5.09 (s, 2H)

5. Representative procedure and Substrate scope for the synthesis of substituted Allyl-ureas/carbamates



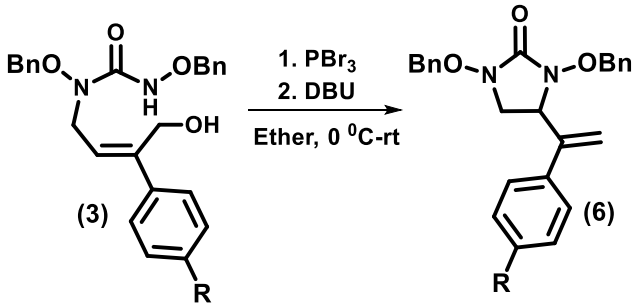
A round-bottom flask equipped with a magnetic stir bar was charged with urea/carbamate **1**, VEC **2**, catalyst and ligand. Toluene was added as a solvent to the reaction mixture and stirred at specified temperature until completion of the reaction (as monitored by TLC) and further purified by silica gel column chromatography with ethyl acetate/hexane as eluent.

Detailed procedure for the synthesis of 3a



A round-bottom flask equipped with a magnetic stir bar was charged with **1a** (0.100 g, 0.367 mmol), **2a** (0.080 g, 0.367 mmol) catalyst (0.05 equiv.) and ligand (0.1 equiv.) under nitrogen atmosphere. Toluene (2 ml) was added as a solvent to the reaction mixture and stirred at 40-45 ^{0}C until completion of the reaction (as monitored by TLC) and further purified by silica gel column chromatography taking ethyl acetate/hexane (2:8 v/v) as eluent to afford **3a** (0.141 g, 86% yield).

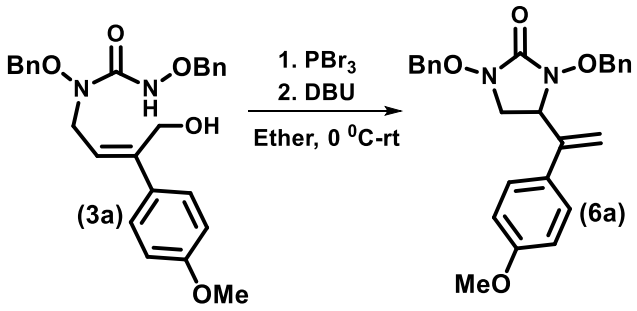
6. Representative procedure for the synthesis of substituted vinyl imidazolidinones



Procedure: To a round-bottom flask wrapped with aluminium foil and equipped with a magnetic stir bar was charged allyl urea **3** (1 equiv.), ether as solvent and stirred at 0 ^{0}C for 5-10 minutes. PBr_3 (1.1 equiv.) was added slowly and stirred at the same temperature until the completion of reaction (as

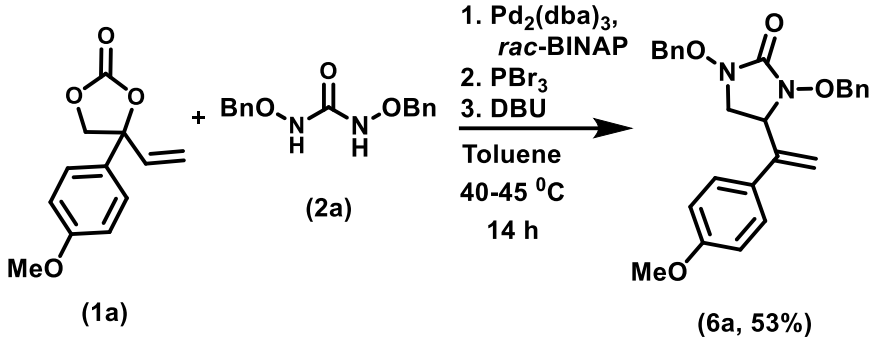
monitored by TLC). DBU (3 equiv.) was added and stirred at room temperature in open air until completion of the reaction (as monitored by TLC). The reaction mixture was washed with aqueous sodium thiosulphate solution and extracted with ether (3 times). The combined organic layers were evaporated on a rotary evaporator and further purified by silica gel column chromatography with ethyl acetate/hexane as eluent.

Detailed procedure for the synthesis of 6a



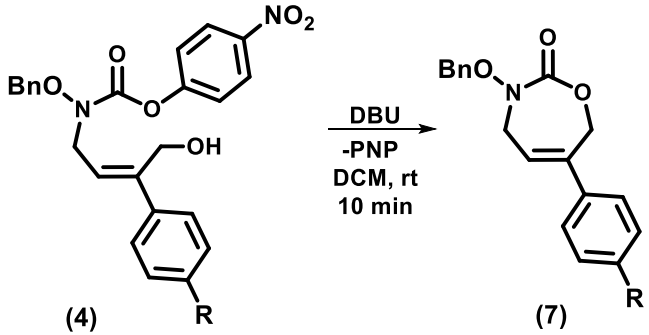
Procedure: To a round-bottom flask wrapped with aluminium foil and equipped with a magnetic stir bar was charged allyl urea **3a** (1 equiv.), ether as solvent and stirred at 0 ^{0}C for 5-10 minutes. PBr_3 (1.1 equiv.) was added slowly and stirred at the same temperature until the completion of reaction (as monitored by TLC). DBU (3 equiv.) was added and stirred at room temperature in open air until completion of the reaction (as monitored by TLC). The reaction mixture was washed with aqueous sodium thiosulphate solution and extracted with ether (3 times). The combined organic layers were evaporated on a rotary evaporator and further purified by silica gel column chromatography with ethyl acetate/hexane as eluent to afford pure **6a** (0.057 g, 80% yield).

7. Representative procedure for the sequential one pot synthesis of 6a



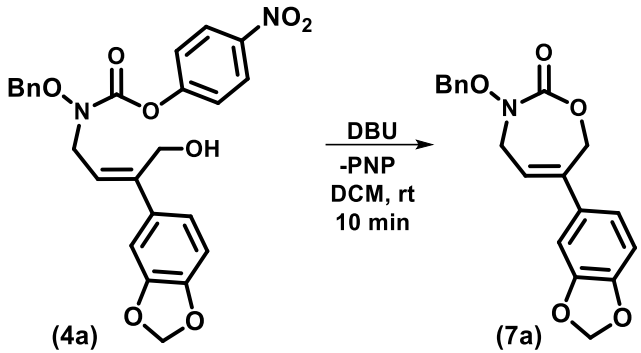
A round-bottom flask equipped with a magnetic stir bar was charged with **1a** (0.100 g, 0.367 mmol), **2a** (0.080 g, 0.367 mmol), Pd catalyst (0.05 equiv.) and ligand (0.1 equiv.). Toluene (2 ml) was added as a solvent to the reaction mixture and stirred at specified temperature until completion of the reaction (as monitored by TLC). PBr_3 (1.1 equiv.) was added slowly and stirred at 0 ^{0}C until the completion of reaction (as monitored by TLC). DBU (3 equiv.) was added and allowed to stir until completion of the reaction (as monitored by TLC). The reaction mixture was further purified by silica gel column chromatography taking ethyl acetate/hexane (2:8 v/v) as eluent to afford **6a** (53% yield).

8. Representative procedure for the synthesis of substituted Oxazepinones



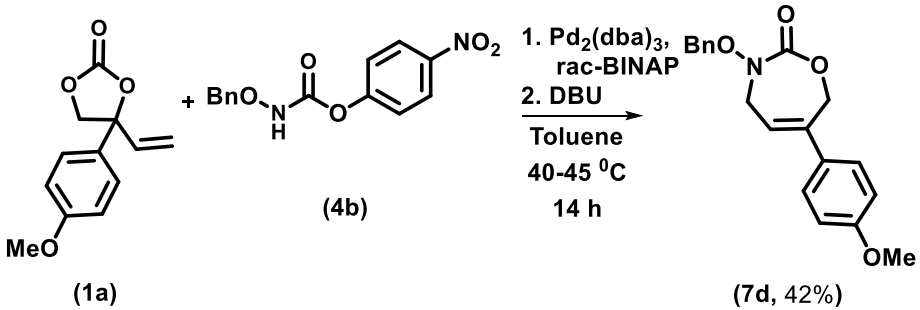
Procedure: To a round-bottom flask equipped with a magnetic stir bar was charged **4** (1 equiv.) and DBU (1.5 equiv.). DCM was added as a solvent and stirred at room temperature in open air until completion of the reaction (as monitored by TLC). The solvent was evaporated on a rotary evaporator and further purified by silica gel column chromatography with ethyl acetate/hexane as eluent.

Detailed procedure for the synthesis of 7a



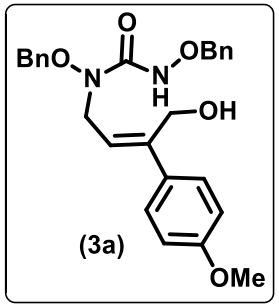
Procedure: To a round-bottom flask equipped with a magnetic stir bar was charged **4a** (0.070 g, 0.146 mmol) and DBU (1.5 equiv.). DCM (2 ml) was added as a solvent and stirred at room temperature in open air until completion of the reaction (as monitored by TLC). The solvent was evaporated on a rotary evaporator and further purified by silica gel column chromatography taking ethyl acetate/hexane as eluent to afford **7a** (0.070 g, 67% yield).

9. Representative procedure for the sequential one pot synthesis of 7d



A round-bottom flask equipped with a magnetic stir bar was charged with **1a** (1 equiv.), **4b** (1 equiv.), Pd catalyst (0.05 equiv.) and ligand (0.1 equiv.). Toluene (2 ml) was added as a solvent to the reaction mixture and stirred at specified temperature until completion of the reaction (as monitored by TLC). DBU (1.5 equiv.) were added and allowed to stir until completion of the reaction (as monitored by TLC). The reaction mixture was further purified by silica gel column chromatography taking ethyl acetate/hexane (2:8 v/v) as eluent to afford **7d** (42% yield).

(*Z*)-1,3-bis(benzyloxy)-1-(4-hydroxy-3-(4-methoxyphenyl)but-2-en-1-yl)urea:



Reaction time: 2 h

1a (0.100 g, 0.367 mmol), **2a** (0.080 g, 0.367 mmol), **3a** (0.141 g, 0.315 mmol)

Yield: 86 %

Nature: Yellow viscous liquid

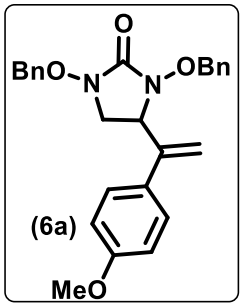
R_f = 0.55 (ethyl acetate/hexane 35:65)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.07 (s, 1H), 7.44 (d, *J* = 8.7 Hz, 2H), 7.37-7.30 (m, 8H), 7.20 (d, *J* = 7.6 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 5.87 (t, *J* = 7.7 Hz, 1H), 4.81 (s, 2H), 4.72 (s, 2H), 4.48 (d, *J* = 5.6 Hz, 2H), 4.27 (d, *J* = 7.7 Hz, 2H), 3.80 (s, 3H), 3.07 (brt, *J* = 6.0 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.5, 159.3, 143.6, 135.4, 134.3, 133.3, 129.6, 129.3, 128.9, 128.7, 128.6, 127.5, 121.3, 113.8, 78.4, 77.5, 59.8, 55.4, 47.7

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{29}N_2O_5$ 449.2076, found 449.2068

1,3-bis(benzyloxy)-4-(1-(4-methoxyphenyl)vinyl)imidazolidin-2-one:



Reaction time: 5 min.

3a (0.075 g, 0.167 mmol), **6a** (0.057 g, 0.0.133 mmol)

Yield: 80 %

Nature: Yellow viscous liquid

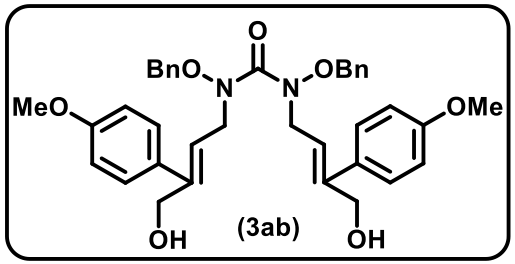
R_f = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.40-7.26 (m, 12H), 6.84 (d, *J* = 8.8 Hz, 2H), 5.45 (s, 1H), 5.40 (s, 1H), 5.19 (d, *J* = 9.9 Hz, 1H), 5.01 (d, *J* = 11.4 Hz, 1H), 4.95-4.90 (m, 2H), 4.21 (dd, *J* = 9.3, 6.9 Hz, 1H), 3.81 (s, 3H), 3.28 (t, *J* = 7.7 Hz, 1H), 3.02 (dd, *J* = 10.3, 7.8 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 162.0, 159.6, 143.2, 135.9, 135.5, 131.2, 129.4, 129.3, 128.6, 128.5, 128.4, 128.1, 117.0, 113.9, 78.8, 78.1, 60.1, 55.4, 50.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{27}N_2O_4$ 431.1971, found 431.1967

1,3-bis(benzyloxy)-1,3-bis((Z)-4-hydroxy-3-(4-methoxyphenyl)but-2-en-1-yl)urea:



Reaction time: 24 h (for more details see manuscript, Table 1, entry 8)

1a (0.100 g, 0.367 mmol), **2a** (0.080 g, 0.367 mmol), **3ab** (0.068 g, 0.110 mmol)

Yield: 30 %

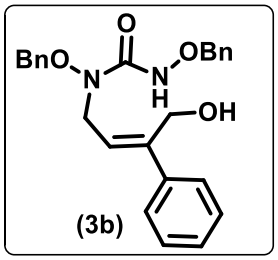
Nature: White viscous liquid

R_f = 0.55 (ethyl acetate/hexane 40:60)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.36-7.24 (m, 14H), 6.80 (d, *J* = 8.6 Hz, 4H), 5.85 (t, *J* = 7.6 Hz, 2H), 4.79 (s, 4H), 4.40 (s, 4H), 4.24 (d, *J* = 7.5 Hz, 4H), 3.78 (s, 6H)

D-Mass (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{37}H_{41}N_2O_7$ 625.29, found 625.30

(Z)-1,3-bis(benzyloxy)-1-(4-hydroxy-3-phenylbut-2-en-1-yl)urea:



Reaction time: 3.5 h

1a (0.075 g, 0.179 mmol), **2b** (0.070 g, 0.367 mmol), **3b** (0.121 g, 0.289 mmol)

Yield: 79 %

Nature: White viscous liquid

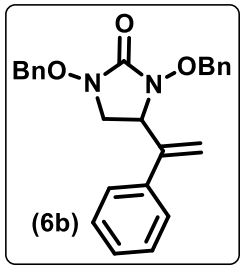
R_f = 0.55 (ethyl acetate/hexane 30:70)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.07 (s, 1H), 7.49 (d, *J* = 8.3 Hz, 2H), 7.37-7.27 (m, 11H), 7.21 (d, *J* = 7.6 Hz, 2H), 5.94 (t, *J* = 7.7 Hz, 1H), 4.81 (s, 2H), 4.72 (s, 2H), 4.50 (brs, 2H), 4.29 (d, *J* = 7.6 Hz, 2H), 3.12 (brs, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.5, 144.2, 140.9, 135.4, 134.3, 129.6, 129.3, 128.9, 128.7, 128.6, 128.5, 127.7, 126.4, 123.0, 78.4, 77.6, 59.8, 47.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{27}N_2O_4$ 419.1971, found 419.1949

1,3-bis(benzyloxy)-4-(1-phenylvinyl)imidazolidin-2-one:



Reaction time: 5 min.

3b (0.100 g, 0.239 mmol), **6b** (0.075 g, 0.188 mmol)

Yield: 79 %

Nature: White viscous liquid

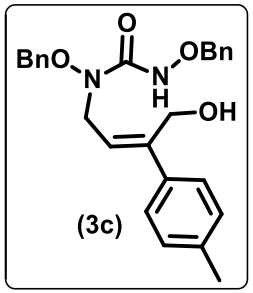
R_f = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.40-7.28 (m, 15H), 5.51 (s, 1H), 5.48 (s, 1H), 5.20 (d, *J* = 9.7 Hz, 1H), 5.01 (d, *J* = 11.4 Hz, 1H), 4.96-4.90 (m, 2H), 4.23 (dd, *J* = 9.6, 7.2 Hz, 1H), 3.29 (t, *J* = 7.4 Hz, 1H), 3.02 (dd, *J* = 9.7, 7.7 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 162.0, 143.9, 138.9, 135.9, 135.5, 129.5, 129.3, 128.6, 128.6, 128.5, 128.4, 128.2, 127.0, 118.3, 99.9, 78.8, 78.1, 60.0, 50.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{25}N_2O_3$ 401.1865, found 401.1862

(Z)-1,3-bis(benzyloxy)-1-(4-hydroxy-3-(p-tolyl)but-2-en-1-yl)urea:



Reaction time: 2.5 h

1a (0.080 g, 0.293 mmol), **2c** (0.060 g, 0.293 mmol), **3c** (0.103 g, 0.240 mmol)

Yield: 82 %

Nature: White viscous liquid

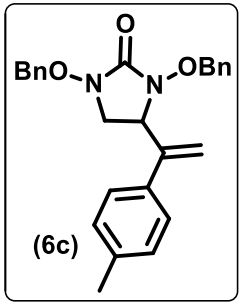
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 30:70)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.09 (s, 1H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.36-7.28 (m, 8H), 7.20 (d, *J* = 7.8 Hz, 2H), 7.14 (d, *J* = 8.2 Hz, 2H), 5.92 (t, *J* = 7.8 Hz, 1H), 4.81 (s, 2H), 4.72 (s, 2H), 4.49 (brs, 2H), 4.28 (d, *J* = 7.9 Hz, 2H), 3.09 (brs, 1H), 2.34 (s, 3H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.5, 144.0, 137.9, 137.5, 135.4, 134.3, 129.6, 129.3, 129.3, 129.2, 128.9, 128.7, 128.6, 126.3, 122.2, 78.4, 77.5, 59.8, 47.6, 21.1

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{29}N_2O_4$ 433.2127, found 433.2125

1,3-bis(benzyloxy)-4-(1-(p-tolyl)vinyl)imidazolidin-2-one:



Reaction time: 5 min.

3c (0.100 g, 0.231 mmol), **6c** (0.079 g, 0.192 mmol)

Yield: 83 %

Nature: White viscous liquid

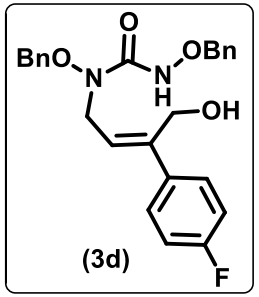
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 15:85)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.41-7.29 (m, 10H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 5.49 (s, 1H), 5.44 (s, 1H), 5.20 (d, *J* = 9.8 Hz, 1H), 5.02 (d, *J* = 11.2 Hz, 1H), 4.93(d, *J* = 10.6 Hz, 2H), 4.23 (dd, *J* = 9.5, 6.9 Hz, 1H), 3.29 (t, *J* = 7.2 Hz, 1H), 3.02 (dd, *J* = 9.4, 7.7 Hz, 1H), 2.35(s, 3H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 162.0, 143.7, 138.1, 135.9, 135.9, 135.5, 129.4, 129.3, 129.2, 128.6, 128.6, 128.5, 128.4, 126.8, 117.6, 78.8, 78.1, 60.0, 50.6, 21.2

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{27}N_2O_3$ 415.2022, found 415.2019

(Z)-1,3-bis(benzyloxy)-1-(3-(4-fluorophenyl)-4-hydroxybut-2-en-1-yl)urea:



(3d)

Reaction time: 4 h

1a (0.100 g, 0.367 mmol), **2d** (0.067 g, 0.367 mmol), **3d** (0.120 g, 0.275 mmol)

Yield: 75 %

Nature: White viscous liquid

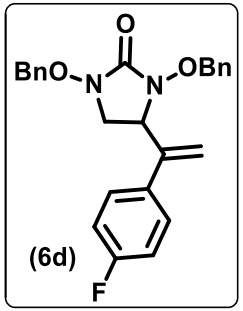
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 35:65)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.49-7.44 (m, 2H), 7.38-7.30 (m, 2H), 7.21 (d, *J* = 7.7 Hz, 2H), 7.00 (t, *J* = 8.5 Hz, 2H), 5.87 (t, *J* = 7.8 Hz, 1H), 4.81 (s, 2H), 4.72 (s, 2H), 4.46 (d, *J* = 6.3 Hz, 2H), 4.26 (d, *J* = 8.0 Hz, 2H), 3.19 (t, *J* = 6.6 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 163.7, 161.3, 160.5, 143.3, 137.0, 135.3, 134.3, 129.6, 129.3, 128.9, 128.7, 128.6, 128.1, 128.0, 122.8, 115.4, 115.1, 78.4, 77.5, 59.8, 47.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{26}FN_2O_4$ 437.1877, found 437.1875

1,3-bis(benzyloxy)-4-(1-(4-fluorophenyl)vinyl)imidazolidin-2-one:



Reaction time: 5 min.

3d (0.100 g, 0.229 mmol), **6d** (0.077 g, 0.185 mmol)

Yield: 81 %

Nature: White viscous liquid

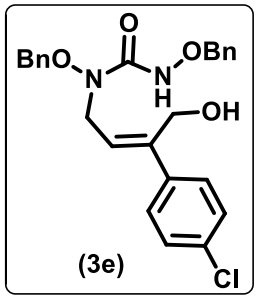
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.38-7.23 (m, 12H), 6.98 (t, *J* = 8.4 Hz, 2H), 5.43 (s, 1H), 5.43 (s, 1H), 5.17 (d, *J* = 10.1 Hz, 1H), 4.98 (d, *J* = 11.5 Hz, 1H), 4.94-4.88 (m, 2H), 4.16 (dd, *J* = 9.3, 7.3 Hz, 1H), 3.24 (t, *J* = 7.3 Hz, 1H), 2.97 (dd, *J* = 9.8, 7.7 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 163.9, 161.9, 161.4, 142.9, 135.8, 135.4, 134.8, 129.5, 129.3, 128.8, 128.7, 128.7, 128.7, 128.5, 128.4, 118.7, 115.6, 115.4, 78.8, 78.2, 60.1, 50.3

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{24}FN_2O_3$ 419.1771, found 419.1774

(Z)-1,3-bis(benzyloxy)-1-(3-(4-chlorophenyl)-4-hydroxybut-2-en-1-yl)urea:



Reaction time: 3.5 h

1a (0.100 g, 0.367 mmol), **2e** (0.082 g, 0.367 mmol), **3e** (0.121 g, 0.267 mmol)

Yield: 73 %

Nature: White viscous liquid

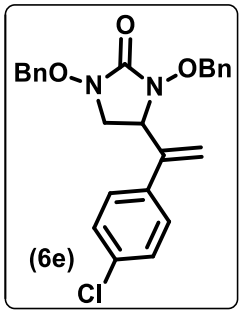
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 30:70)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.43 (d, *J* = 8.6 Hz, 2H), 7.38-7.30 (m, 8H), 7.28 (d, *J* = 8.7 Hz, 2H), 7.21 (d, *J* = 7.7 Hz, 2H), 5.90 (t, *J* = 7.8 Hz, 1H), 4.81 (s, 2H), 4.72 (s, 2H), 4.45 (d, *J* = 5.8 Hz, 2H), 4.26 (d, *J* = 7.6 Hz, 2H), 3.23 (t, *J* = 6.3 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.4, 143.2, 139.4, 135.3, 134.2, 133.5, 129.6, 129.3, 129.3, 128.9, 128.7, 128.6, 128.5, 127.7, 123.3, 78.4, 77.6, 59.6, 47.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{26}ClN_2O_4$ 453.1581, found 453.1578

1,3-bis(benzyloxy)-4-(1-(4-chlorophenyl)vinyl)imidazolidin-2-one:



Reaction time: 5 min.

3e (0.080 g, 0.176 mmol), **6e** (0.064 g, 0.146 mmol)

Yield: 83 %

Nature: White viscous liquid

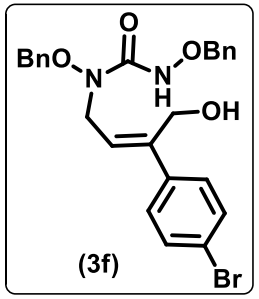
R_f = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.40-7.21 (m, 14H), 5.47 (s, 1H), 5.46 (s, 1H), 5.18 (d, *J* = 10.1 Hz, 1H), 5.00 (d, *J* = 11.4 Hz, 1H), 4.92 (d, *J* = 11.1 Hz, 2H), 4.17 (dd, *J* = 9.3, 7.2 Hz, 1H), 3.26 (t, *J* = 7.5 Hz, 1H), 2.98 (dd, *J* = 9.6, 7.9 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 161.8, 142.9, 137.2, 135.8, 135.4, 134.2, 129.5, 129.3, 128.7, 128.7, 128.5, 128.4, 128.4, 119.1, 78.8, 78.2, 59.9, 50.3

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{24}ClN_2O_3$ 435.1475, found 435.1473

(Z)-1,3-bis(benzyloxy)-1-(3-(4-bromophenyl)-4-hydroxybut-2-en-1-yl)urea:



Reaction time: 3 h

1h (0.100 g, 0.367 mmol), **2a** (0.098 g, 0.367 mmol), **3h** (0.139 g, 0.278 mmol)

Yield: 76 %

Nature: Yellow viscous liquid

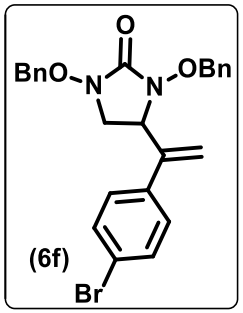
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 25:75)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.10 (s, 1H), 7.44 (d, *J* = 8.6 Hz, 2H), 7.38-7.30 (m, 10H), 7.21 (d, *J* = 8.0 Hz, 2H), 5.90 (t, *J* = 7.7 Hz, 1H), 4.80 (s, 2H), 4.72 (s, 2H), 4.44 (s, 2H), 4.25 (d, *J* = 7.7 Hz, 2H), 3.27 (brs, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.4, 143.2, 139.9, 135.3, 134.3, 131.5, 129.6, 129.3, 129.3, 128.9, 128.7, 128.6, 128.1, 123.4, 121.7, 78.5, 77.6, 59.6, 47.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{26}BrN_2O_4$ 497.1076, found 497.1072

1,3-bis(benzyloxy)-4-(1-(4-bromophenyl)vinyl)imidazolidin-2-one:



Reaction time: 5 min.

3f (0.070 g, 0.141 mmol), **6f** (0.053 g, 0.111 mmol)

Yield: 79 %

Nature: White viscous liquid

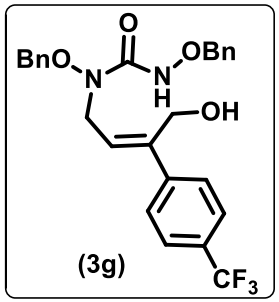
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 15:75)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.43 (d, *J* = 8.6 Hz, 2H), 7.39-7.29 (m, 10H), 7.17 (d, *J* = 8.4 Hz, 2H), 5.48 (s, 1H), 5.46 (s, 1H), 5.17 (d, *J* = 10.1 Hz, 1H), 5.00 (d, *J* = 11.2 Hz, 1H), 4.95-4.90 (m, 2H), 4.16 (dd, *J* = 9.3, 7.2 Hz, 1H), 3.26 (t, *J* = 7.7 Hz, 1H), 2.97 (dd, *J* = 9.4, 7.7 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 161.8, 142.9, 137.7, 135.8, 135.4, 131.7, 129.5, 129.3, 128.7, 128.7, 128.5, 128.4, 122.4, 119.1, 78.8, 78.2, 59.8, 50.3

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{24}BrN_2O_3$ 479.0970, found 479.1072

(Z)-1,3-bis(benzyloxy)-1-(4-hydroxy-3-(4-(trifluoromethyl)phenyl)but-2-en-1-yl)urea:



Reaction time: 4 h

1a (0.100 g, 0.367 mmol), **2g** (0.095 g, 0.367 mmol), **3g** (0.139 g, 0.286 mmol)

Yield: 78 %

Nature: White viscous liquid

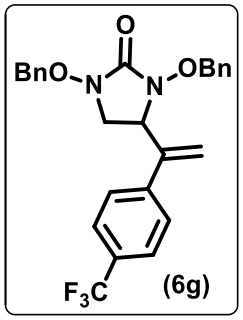
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 35:65)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.07 (s, 1H), 7.59 (q, *J* = 8.6 Hz, 4H), 7.39-7.29 (m, 8H), 7.21 (d, *J* = 7.6 Hz, 2H), 5.97 (t, *J* = 7.8 Hz, 1H), 4.81 (s, 2H), 4.73 (s, 2H), 4.48 (d, *J* = 6.3 Hz, 2H), 4.28 (d, *J* = 7.5 Hz, 2H), 3.31 (t, *J* = 6.7 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.4, 144.6, 143.2, 135.3, 134.2, 129.6, 129.4, 129.3, 129.0, 128.8, 128.6, 126.7, 125.4, 125.3, 124.7, 78.5, 77.6, 59.6, 47.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{26}F_3N_2O_4$ 487.1845, found 487.1852

1,3-bis(benzyloxy)-4-(1-(4-(trifluoromethyl)phenyl)vinyl)imidazolidin-2-one:



Reaction time: 5 min.

3g (0.090 g, 0.185 mmol), **6g** (0.071 g, 0.151 mmol)

Yield: 82 %

Nature: White viscous liquid

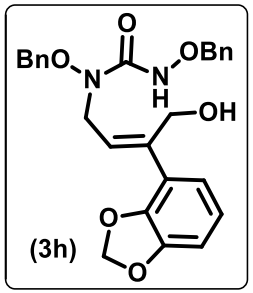
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.2 Hz, 2H), 7.42-7.28 (m, 12H), 5.53 (s, 1H), 5.52 (s, 1H), 5.18 (d, *J* = 10.2 Hz, 1H), 4.99 (d, *J* = 11.5 Hz, 1H), 4.95-4.89 (m, 2H), 4.19 (dd, *J* = 9.1, 7.1 Hz, 1H), 3.27 (t, *J* = 7.5 Hz, 1H), 2.97 (dd, *J* = 9.2, 7.9 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 161.8, 142.9, 142.4, 135.8, 135.4, 129.5, 129.3, 128.8, 128.7, 128.5, 128.5, 127.4, 125.5, 125.5, 120.4, 78.8, 78.2, 59.8, 50.3

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{24}F_3N_2O_3$ 469.1739, found 469.1738

(Z)-1-(3-(benzo[d][1,3]dioxol-4-yl)-4-hydroxybut-2-en-1-yl)-1,3-bis(benzyloxy)urea:



Reaction time: 2.3 h

1a (0.100 g, 0.367 mmol), **2h** (0.086 g, 0.367 mmol), **3h** (0.139 g, 0.300 mmol)

Yield: 82 %

Nature: White viscous liquid

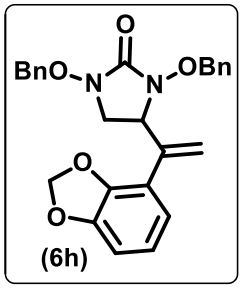
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 35:65)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.44-7.26 (m, 8H), 7.19 (d, *J* = 7.2 Hz, 2H), 7.01-6.93 (m, 2H), 6.74 (d, *J* = 7.7 Hz, 1H), 5.91(s, 2H), 5.82 (t, *J* = 7.7 Hz, 1H), 4.79 (s, 2H), 4.70 (s, 2H), 4.42 (brs, 2H), 4.23 (d, *J* = 7.8 Hz, 2H), 3.14 (brs, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.5, 147.8, 147.2, 143.7, 135.4, 135.2, 134.3, 129.6, 129.3, 128.9, 128.7, 128.6, 121.9, 120.0, 108.2, 107.0, 101.1, 78.4, 77.5, 59.8, 47.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{27}N_2O_6$ 463.1869, found 463.2221

4-(1-(benzo[d][1,3]dioxol-4-yl)vinyl)-1,3-bis(benzyloxy)imidazolidin-2-one:



Reaction time: 5 min.

3h (0.080 g, 0.173 mmol), **6h** (0.065 g, 0.147 mmol)

Yield: 85 %

Nature: White viscous liquid

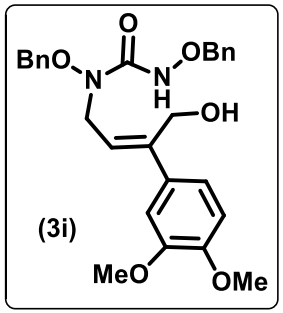
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.44-7.27 (m, 10H), 6.85-6.71 (m, 3H), 5.96 (s, 2H), 5.42 (s, 1H), 5.40 (s, 1H), 5.19 (d, *J* = 10.1 Hz, 1H), 5.02(d, *J* = 11.4 Hz, 1H), 4.97-4.89 (m, 2H), 4.16 (t, *J* = 8.0 Hz, 1H), 3.27 (t, *J* = 8.1 Hz, 1H), 3.00 (t, *J* = 8.3 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 161.9, 147.8, 147.6, 143.3, 135.9, 135.5, 132.9, 129.4, 129.3, 128.6, 128.5, 128.4, 120.6, 117.6, 108.3, 107.6, 101.2, 78.8, 78.1, 60.1, 50.5

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{25}N_2O_5$ 445.1763, found 445.1754

(Z)-1,3-bis(benzyloxy)-1-(3-(3,4-dimethoxyphenyl)-4-hydroxybut-2-en-1-yl)urea:



Reaction time: 1.8 h

1a (0.100 g, 0.367 mmol), **2i** (0.092 g, 0.367 mmol), **3i** (0.152 g, 0.319 mmol)

Yield: 87 %

Nature: White viscous liquid

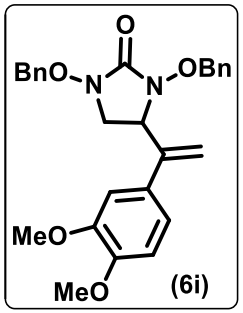
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 35:65)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.38-7.30 (m, 8H), 7.21 (d, *J* = 7.7 Hz, 2H), 7.08-7.03 (m, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 5.87 (t, *J* = 7.6 Hz, 1H), 4.81 (s, 2H), 4.72 (s, 2H), 4.47 (d, *J* = 5.6 Hz, 2H), 4.28 (d, *J* = 7.8 Hz, 2H), 3.88 (s, 3H),3.87 (s, 3H), 3.13 (t, *J* = 6.2 Hz, 2H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.5, 148.8, 148.8, 143.8, 135.4, 134.3, 133.9, 129.6, 129.3, 128.9, 128.7, 128.6, 121.7, 118.9, 110.9, 109.6, 78.4, 77.5, 59.9, 56.0, 47.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{27}H_{31}N_2O_6$ 479.2182, found 479.2184

1,3-bis(benzyloxy)-4-(1-(3,4-dimethoxyphenyl)vinyl)imidazolidin-2-one:



Reaction time: 5 min.

3i (0.100 g, 0.209 mmol), **6i** (0.080 g, 0.175 mmol)

Yield: 84 %

Nature: White viscous liquid

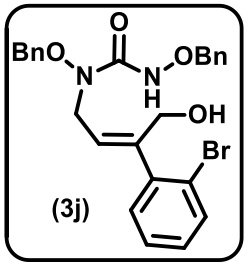
$\mathbf{R_f}$ = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.40-7.29 (m, 10H), 6.91-6.84 (m, 2H), 6.80 (d, *J* = 8.2 Hz, 1H), 5.46 (s, 1H), 5.41 (s, 1H), 5.21 (d, *J* = 10.0 Hz, 1H), 5.00 (d, *J* = 11.3 Hz, 1H), 4.97-4.91 (m, 2H), 4.21 (dd, *J* = 9.5, 7.1 Hz, 1H), 3.88 (s, 3H), 3.82 (s, 3H), 3.27 (t, *J* = 7.6 Hz, 1H), 3.02 (dd, *J* = 9.4, 7.7 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 161.9, 149.1, 148.8, 143.5, 135.9, 135.5, 131.6, 129.4, 129.4, 128.6, 128.5, 128.4, 119.4, 117.1, 110.9, 110.2, 78.9, 78.1, 60.0, 56.0, 55.9, 50.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{27}H_{29}N_2O_5$ 461.2076, found 461.2077

(Z)-1,3-bis(benzyloxy)-1-(3-(2-bromophenyl)-4-hydroxybut-2-en-1-yl)urea:



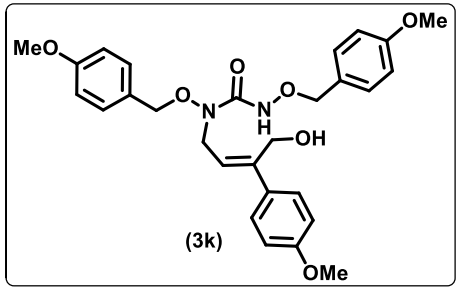
Reaction time: 24 h

R_f = 0.55 (ethyl acetate/hexane 35:65)

(**Note:** Since the desired molecule was determined by **HRMS** only, Stereoselectivity is not defined)

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{25}BrN_2O4$ 519.0895, found 519.0875

(Z)-1-(4-hydroxy-3-(4-methoxyphenyl)but-2-en-1-yl)-1,3-bis((4-methoxybenzyl)oxy)urea:



Reaction time: 2.1 h

1b (0.100 g, 0.299 mmol), **2a** (0.066 g, 0.299 mmol), **3k** (0.128 g, 0.251 mmol)

Yield: 84 %

Nature: White viscous liquid

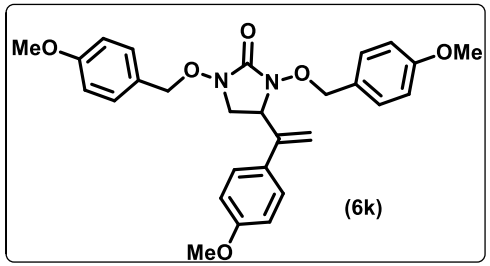
R_f = 0.55 (ethyl acetate/hexane 35:65)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.02 (s, 1H), 7.44 (d, *J* = 8.9 Hz, 2H), 7.24 (d, *J* = 8.5 Hz, 2H), 7.14 (d, *J* = 8.7 Hz, 2H), 6.88-6.82 (m, 4H), 6.80 (d, *J* = 8.7 Hz, 2H), 5.86 (t, *J* = 7.8 Hz, 1H), 4.75 (s, 2H), 4.66 (s, 2H), 4.47 (brs, 2H), 4.24 (d, *J* = 7.7 Hz, 2H), 3.80 (s, 3H), 3.79 (s, 3H), 3.78 (s, 3H), 3.15 (brs, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.5, 160.3, 160.0, 159.3, 143.5, 133.4, 131.3, 131.1, 127.5, 127.4, 126.5, 121.4, 114.2, 113.9, 113.8, 77.9, 59.7, 55.3, 55.3, 47.7

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{28}H_{33}N_2O_7$ 509.2288, found 509.2282

1,3-bis((4-methoxybenzyl)oxy)-4-(1-(4-methoxyphenyl)vinyl)imidazolidin-2-one:



(6k)

Reaction time: 5 min.

3k (0.100 g, 0.196 mmol), **6k** (0.083 g, 0.169 mmol)

Yield: 86 %

Nature: White viscous liquid

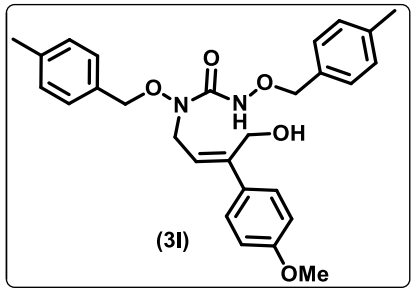
R_f = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.33-7.27 (m, 6H), 6.88-6.80 (m, 6H), 5.45 (s, 1H), 5.40 (s, 1H), 5.12 (d, *J* = 9.5 Hz, 1H), 4.94 (d, *J* = 10.9 Hz, 1H), 4.88-4.83 (m, 2H), 4.19 (dd, *J* = 9.7, 7.2 Hz, 1H), 3.81 (s, 3H), 3.80 (s, 3H), 3.78 (s, 3H), 3.24 (t, *J* = 7.3 Hz, 1H), 2.99 (dd, *J* = 9.7, 7.8 Hz, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 162.0, 159.9, 159.6, 143.2, 131.2, 131.1, 131.0, 128.2, 128.0, 127.7, 117.0, 113.9, 113.8, 113.8, 78.4, 77.7, 60.1, 55.4, 55.3, 50.5

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{28}H_{31}N_2O_6$ 491.2182, found 491.2175

(Z)-1-(4-hydroxy-3-(4-methoxyphenyl)but-2-en-1-yl)-1,3-bis((4-methylbenzyl)oxy)urea:



Reaction time: 2 h

1c (0.100 g, 0.333 mmol), **2a** (0.073 g, 0.333 mmol), **3l** (0.130 g, 0.273 mmol)

Yield: 82 %

Nature: White viscous liquid

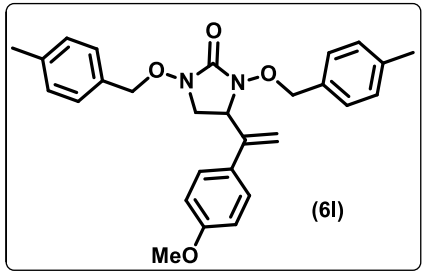
R_f = 0.55 (ethyl acetate/hexane 30:70)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.04 (s, 1H), 7.43 (d, *J* = 8.2 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.15-7.04 (m, 6H), 6.85 (d, *J* = 8.8 Hz, 2H), 5.86 (t, *J* = 7.6 Hz, 1H), 4.77 (s, 2H), 4.67 (s, 2H), 4.47 (s, 2H), 4.25 (d, *J* = 7.8 Hz, 2H), 3.80 (s, 3H), 3.08 (brs, 1H), 2.35 (s, 6H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.5, 159.3, 143.5, 139.3, 138.5, 133.3, 132.4, 131.3, 129.7, 129.5, 129.4, 129.3, 127.5, 121.4, 113.8, 78.2, 59.7, 55.4, 47.7, 21.3

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{28}H_{33}N_2O_5$ 477.2389, found 477.2387

4-(1-(4-methoxyphenyl)vinyl)-1,3-bis((4-methylbenzyl)oxy)imidazolidin-2-one:



Reaction time: 5 min.

3l (0.100 g, 0.210 mmol), **6l** (0.078 g, 0.172 mmol)

Yield: 82 %

Nature: White viscous liquid

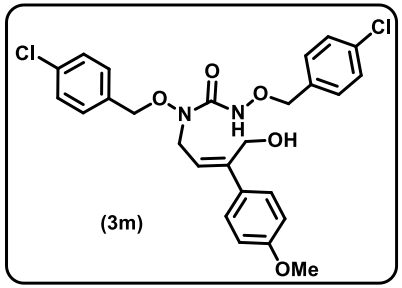
R_f = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.30-7.23 (m, 7H), 7.13 (t, *J* = 7.4 Hz, 3H), 6.84 (d, *J* = 8.5 Hz, 2H), 5.45 (s, 1H), 5.41 (s, 1H), 5.15 (d, *J* = 9.5 Hz, 1H), 4.96 (d, *J* = 11.0 Hz, 1H), 4.91-4.85 (m, 2H), 4.20 (dd, *J* = 9.6, 7.1 Hz, 1H), 3.81 (s, 3H), 3.26 (t, *J* = 7.2 Hz, 1H), 3.00 (dd, *J* = 9.9, 7.4 Hz, 1H), 2.33 (s, 3H), 2.32 (s, 3H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 162.0, 159.6, 143.2, 138.4, 132.9, 132.5, 131.3, 129.5, 129.4, 129.2, 129.1, 128.2, 117.0, 113.9, 78.6, 77.9, 60.1, 55.4, 50.6, 21.3

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{28}H_{31}N_2O_4$ 459.2284, found 459.2281

(Z)-1,3-bis((4-chlorobenzyl)oxy)-1-(4-hydroxy-3-(4-methoxyphenyl)but-2-en-1-yl)urea:



Reaction time: 3 h

1d (0.100 g, 0.294 mmol), **2a** (0.065 g, 0.294 mmol), **3m** (0.120 g, 0.232 mmol)

Yield: 79 %

Nature: White viscous liquid

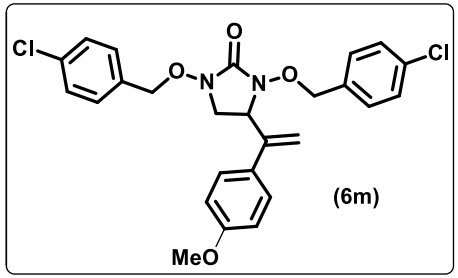
R_f = 0.55 (ethyl acetate/hexane 35:65)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.01 (s, 1H), 7.43 (d, *J* = 8.7 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 7.29-7.21 (m, 4H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 5.84 (t, *J* = 7.7 Hz, 1H), 4.77 (s, 2H), 4.70 (s, 2H), 4.48 (brs, 2H), 4.25 (d, *J* = 7.6 Hz, 2H), 3.81 (s, 3H), 3.00 (brs, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.6, 159.4, 143.7, 135.4, 134.6, 133.9, 133.1, 132.8, 130.9, 130.6, 129.1, 128.8, 127.5, 121.0, 113.9, 77.5, 76.6, 59.7, 55.4, 47.8

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{27}Cl_2N_2O_5$ 517.1297, found 517.1284

1,3-bis((4-chlorobenzyl)oxy)-4-(1-(4-methoxyphenyl)vinyl)imidazolidin-2-one:



Reaction time: 5 min.

3m (0.100 g, 0.193 mmol), **6m** (0.071 g, 0.143 mmol)

Yield: 74 %

Nature: White viscous liquid

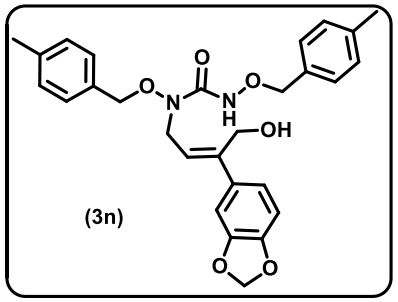
R_f = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.31 (s, 4H), 7.30-7.25 (m, 6H), 6.85 (d, *J* = 8.9 Hz, 2H), 5.46 (s, 1H), 5.39 (s, 1H), 5.12 (d, *J* = 10.2 Hz, 1H), 4.96 (d, *J* = 11.2 Hz, 1H), 4.92-4.86 (m, 2H), 4.23 (dd, *J* = 9.4, 7.4 Hz, 1H), 3.81 (s, 3H), 3.31 (t, *J* = 7.2 Hz, 1H), 3.04 (dd, *J* = 9.9, 7.8 Hz, 1H),

^{13}C-NMR (100 MHz, $CDCl_3$): δ 162.0, 159.7, 143.0, 134.6, 134.5, 134.4, 134.0, 131.0, 130.7, 130.6, 128.7, 128.6, 128.1, 117.1, 113.9, 77.9, 77.2, 60.1, 55.4, 50.5

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{25}Cl_2N_2O_4$ 499.1191, found 499.1178

(Z)-1-(3-(benzo[d][1,3]dioxol-5-yl)-4-hydroxybut-2-en-1-yl)-1,3-bis((4-methylbenzyl)oxy)urea:



Reaction time: 1.8 h

1e (0.100 g, 0.333 mmol), **2h** (0.078 g, 0.333 mmol), **3n** (0.139 g, 0.283 mmol)

Yield: 85 %

Nature: White viscous liquid

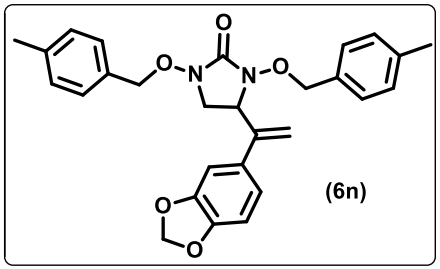
R_f = 0.55 (ethyl acetate/hexane 35:65)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.04 (s, 1H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.12 (d, *J* = 7.5 Hz, 4H), 7.07 (d, *J* = 8.1 Hz, 2H), 6.99-6.95 (m, 2H), 6.75 (d, *J* = 7.9 Hz, 1H), 5.92 (s, 2H), 5.81 (t, *J* = 7.7 Hz, 1H), 4.76 (s, 2H), 4.66 (s, 2H), 4.42 (d, *J* = 6.1 Hz, 2H), 4.22 (d, *J* = 7.7 Hz, 2H), 3.11 (t, *J* = 6.5 Hz, 1H), 2.34 (s, 6H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.4, 147.8, 147.2, 143.7, 139.3, 138.5, 135.3, 132.3, 131.3, 129.7, 129.5, 129.4, 129.3, 122.0, 120.0, 108.2, 107.0, 101.1, 78.2, 59.8, 47.7, 21.3

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{28}H_{31}N_2O_6$ 491.2182, found 491.2174

4-(1-(benzo[d][1,3]dioxol-5-yl)vinyl)-1,3-bis((4-methylbenzyl)oxy)imidazolidin-2-one:



Reaction time: 5 min.

3n (0.100 g, 0.204 mmol), **6n** (0.073 g, 0.155 mmol)

Yield: 76 %

Nature: White viscous liquid

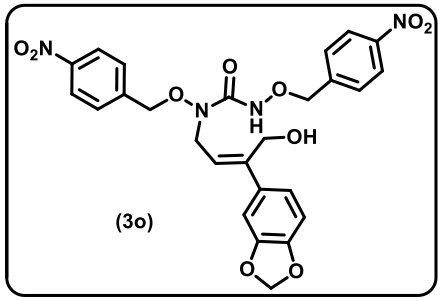
R_f = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.29-7.24 (m, 4H), 7.13 (t, *J* = 7.2 Hz, 4H), 6.82-6.72 (m, 3H), 5.96 (s, 2H), 5.42 (s, 1H), 5.40 (s, 1H), 5.15 (d, *J* = 9.9 Hz, 1H), 4.96 (d, *J* = 11.1 Hz, 1H), 4.92-4.86 (m, 2H), 4.14 (dd, *J* = 9.7, 7.1 Hz, 1H), 3.24 (t, *J* = 7.4 Hz, 1H), 2.97 (dd, *J* = 10.2, 7.8 Hz, 1H), 2.33 (s, 3H), 2.32 (s, 3H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 161.9, 147.8, 147.6, 143.4, 138.5, 132.9, 132.9, 132.5, 129.5, 129.4, 129.2, 129.1, 120.6, 117.6, 108.2, 107.6, 101.2, 78.6, 78.0, 60.1, 50.5, 21.3

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{28}H_{29}N_2O_5$ 473.2076, found 473.2064

(Z)-1-(3-(benzo[d][1,3]dioxol-5-yl)-4-hydroxybut-2-en-1-yl)-1,3-bis((4-nitrobenzyl)oxy)urea:



Reaction time: 5 h

1f (0.100 g, 0.276 mmol), **2h** (0.065 g, 0.276 mmol), **3o** (0.112 g, 0.204 mmol)

Yield: 74 %

Nature: Yellow viscous liquid

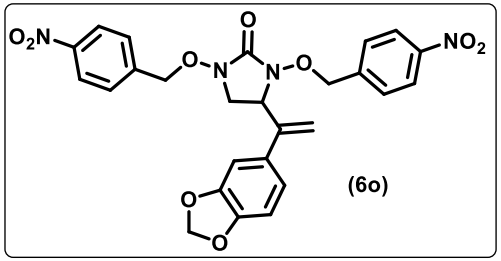
R_f = 0.55 (ethyl acetate/hexane 45:55)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.27 (s, 1H), 8.19 (d, *J* = 8.5 Hz, 2H), 8.11 (d, *J* = 8.8 Hz, 2H), 7.50-7.46 (m, 4H), 6.99-6.93 (m, 2H), 6.77 (d, *J* = 7.9 Hz, 1H), 5.96 (s, 2H), 5.79 (t, *J* = 7.7 Hz, 1H), 4.92 (s, 2H), 4.88 (s, 2H), 4.44 (s, 2H), 4.26 (d, *J* = 7.5 Hz, 2H), 2.98 (brs, 1H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.7, 148.3, 148.0, 147.9, 147.5, 144.2, 142.5, 141.3, 134.7, 130.0, 129.5, 124.0, 123.7, 121.2, 120.0, 108.3, 106.8, 101.3, 75.9, 59.8, 47.9

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{25}N_4O_{10}$ 553.1571, found 553.1565

4-(1-(benzo[d][1,3]dioxol-5-yl)vinyl)-1,3-bis((4-nitrobenzyl)oxy)imidazolidin-2-one:



(6o)

Reaction time: 5 min.

3o (0.100 g, 0.181 mmol), **6o** (0.069 g, 0.130 mmol)

Yield: 72 %

Nature: Yellow viscous liquid

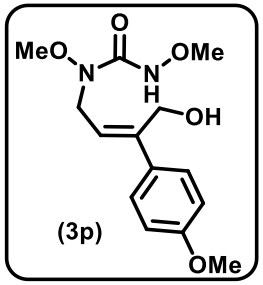
R_f = 0.55 (ethyl acetate/hexane 30:70)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.22 (d, *J* = 8.4 Hz, 2H), 8.17 (d, *J* = 8.6 Hz, 2H), 7.57 (d, *J* = 8.6 Hz, 2H), 7.54 (d, *J* = 8.6 Hz, 2H), 6.82-6.73 (m, 3H), 5.97 (s, 2H), 5.47 (s, 1H), 5.42 (s, 1H), 5.24 (d, *J* = 11.8 Hz, 1H), 5.10 (d, *J* = 12.3 Hz, 1H), 5.04 (d, *J* = 11.6 Hz, 2H), 4.26 (dd, *J* = 9.8, 6.9 Hz, 1H), 3.44 (t, *J* = 7.4 Hz, 1H), 3.12 (dd, *J* = 10.1, 8.1 Hz, 1H),

^{13}C-NMR (100 MHz, $CDCl_3$): δ 161.9, 148.0, 147.9, 147.9, 143.0, 142.6, 132.3, 129.6, 129.5, 123.8, 123.6, 120.5, 118.0, 108.4, 107.3, 101.4, 76.6, 60.3, 50.3

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{23}N_4O_9$ 535.1465, found 535.1445

(Z)-1-(4-hydroxy-3-(4-methoxyphenyl)but-2-en-1-yl)-1,3-dimethoxyurea:



Reaction time: 5 h

1g (0.060 g, 0.500 mmol), **2a** (0.110 g, 0.500 mmol), **3p** (0.115 g, 0.390 mmol)

Yield: 78 %

Nature: White viscous liquid

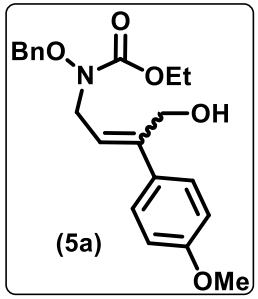
R_f = 0.55 (ethyl acetate/hexane 45:55)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.32 (s, 1H), 7.42 (d, *J* = 8.8 Hz, 2H), 6.84 (d, *J* = 8.5 Hz, 2H), 5.87 (t, *J* = 7.9 Hz, 1H), 4.49 (s, 2H), 4.30 (d, *J* = 7.6 Hz, 2H), 3.78 (s, 3H), 3.72 (s, 3H), 3.70 (s, 3H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.5, 159.3, 143.7, 133.3, 127.6, 121.3, 113.8, 64.9, 62.4, 59.8, 55.4, 55.3, 46.3

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{14}H_{21}N_2O_5$ 297.1450, found 297.1441

Ethyl benzyloxy(4-hydroxy-3-(4-methoxyphenyl)but-2-en-1-yl)carbamate:



Reaction time: 12 h

4a (0.100 g, 0.512 mmol), **2a** (0.112 g, 0.512 mmol), **5a** (0.135 g, 0.364 mmol)

Yield: 71 %

Nature: White viscous liquid

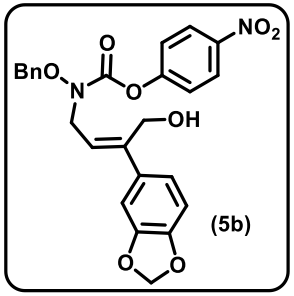
R_f = 0.55 (ethyl acetate/hexane 30:70)

^{1}H-NMR (400 MHz, $CDCl_3$) (only for *E* isomer): δ 7.44-7.34 (m, 7H), 6.86 (d, *J* = 9.0 Hz, 2H), 5.83 (t, *J* = 7.8 Hz, 1H), 4.89 (s, 2H), 4.45 (d, *J* = 6.5 Hz, 2H), 4.26-4.17 (m, 4H), 3.80 (s, 3H), 2.67 (t, *J* = 6.1 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 159.3, 158.1, 142.9, 135.1, 133.1, 131.2, 129.7, 129.7, 128.9, 128.6, 128.6, 127.5, 122.1, 113.8, 77.8, 62.6, 59.6, 55.3, 48.2, 30.3, 14.5

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{21}H_{26}NO_5$ 372.1811, found 372.1798

(Z)-4-nitrophenyl (3-(benzo[d][1,3]dioxol-5-yl)-4-hydroxybut-2-en-1-yl)(benzyloxy)carbamate



Reaction time: 10 h

4b (0.100 g, 0.347 mmol), **2h** (0.081 g, 0.347 mmol), **5b** (0.112 g, 0.236 mmol)

Yield: 68 %

Nature: White viscous liquid

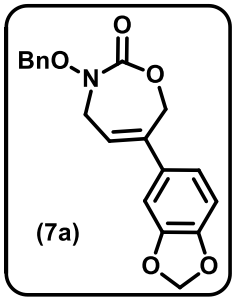
R_f = 0.55 (ethyl acetate/hexane 35:65)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.26 (d, *J* = 9.1 Hz, 2H), 7.47-7.37 (m, 5H), 7.27 (d, *J* = 9.0 Hz, 2H), 6.99-6.95 (m, 2H), 6.79 (d, *J* = 8.7 Hz, 1H), 5.96 (s, 2H), 5.90 (t, *J* = 7.6 Hz, 1H), 5.01 (s, 2H), 4.47 (d, *J* = 5.1 Hz, 2H), 4.36 (d, *J* = 7.9 Hz, 2H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 155.5, 154.5, 147.9, 147.5, 145.3, 143.8, 134.5, 134.4, 129.8, 129.3, 128.8, 125.3, 122.3, 121.8, 120.1, 108.3, 107.0, 101.2, 78.1, 59.8, 48.1

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{23}N_2O_8$ 479.1454, found 479.1442

6-(benzo[d][1,3]dioxol-4-yl)-3-(benzyloxy)-3,4-dihydro-1,3-oxazepin-2(7H)-one:



Reaction time: 10 min.

5b (0.070 g, 0.146 mmol), **7a** (0.033 g, 0.098 mmol)

Yield: 67 %

Nature: White viscous liquid

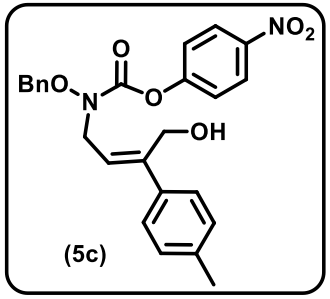
R_f = 0.55 (ethyl acetate/hexane 25:75)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.45-7.34 (m, 5H), 6.77 (d, *J* = 7.9 Hz, 1H), 6.71-6.65 (m, 2H), 5.97 (s, 2H), 5.72 (t, *J* = 4.6 Hz, 1H), 4.90 (s, 2H), 4.83 (s, 2H), 4.14-4.10 (m, 2H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 159.5, 148.0, 147.7, 137.5, 135.3, 132.5, 129.6, 128.8, 128.6, 121.1, 119.6, 108.4, 106.6, 101.4, 76.6, 69.6, 53.2

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{19}H_{18}NO_5$ 340.1185, found 340.1175

(Z)-4-nitrophenyl benzyloxy(4-hydroxy-3-(p-tolyl)but-2-en-1-yl)carbamate:



Reaction time: 12 h

4b (0.100 g, 0.347 mmol), **2c** (0.071 g, 0.347 mmol), **5c** (0.146 g, 0.326 mmol)

Yield: 64 %

Nature: White viscous liquid

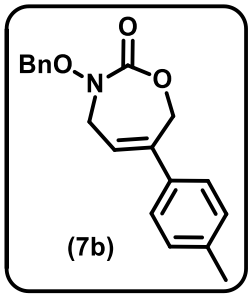
R_f = 0.55 (ethyl acetate/hexane 30:70)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.26 (d, *J* = 9.0 Hz, 2H), 7.46-7.36 (m, 7H), 7.27 (d, *J* = 8.9 Hz, 2H), 7.16 (d, *J* = 8.2 Hz, 1H), 5.98 (t, *J* = 7.5 Hz, 1H), 5.02 (s, 2H), 4.52 (d, *J* = 5.4 Hz, 2H), 4.39 (d, *J* = 7.8 Hz, 2H), 2.35 (s, 3H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 155.5, 154.4, 145.3, 144.1, 137.9, 137.2, 134.4, 129.8, 129.3, 129.2, 128.8, 126.3, 125.2, 122.3, 122.1, 78.1, 59.7, 48.1, 21.2

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{25}N_2O_6$ 449.1713, found 449.1696

3-(benzyloxy)-6-(p-tolyl)-3,4-dihydro-1,3-oxazepin-2(7H)-one:



Reaction time: 10 min.

5c (0.080 g, 0.178 mmol), **7b** (0.036 g, 0.117 mmol)

Yield: 66 %

Nature: White viscous liquid

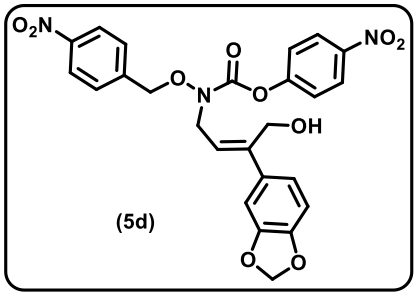
R_f = 0.55 (ethyl acetate/hexane 20:80)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.45-7.33 (m, 5H), 7.13 (q, *J* = 9.3 Hz, 4H), 5.79 (t, *J* = 4.6 Hz, 1H), 4.90 (s, 2H), 4.88 (brs, 2H), 4.16-4.12 (m, 2H), 2.34 (s, 3H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 159.6, 138.2, 137.7, 135.5, 135.3, 129.6, 129.4, 128.8, 128.5, 125.9, 121.2, 76.6, 69.6, 53.3, 21.2

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{19}H_{20}NO_3$ 310.1443, found 310.1424

(Z)-4-nitrophenyl (3-(benzo[d][1,3]dioxol-5-yl)-4-hydroxybut-2-en-1-yl)((4-nitrobenzyl)oxy)carbamate:



Reaction time: 12 h

4c (0.100 g, 0.300 mmol), **2h** (0.070 g, 0.300 mmol), **5d** (0.097 g, 0.186 mmol)

Yield: 62 %

Nature: Brownish viscous liquid

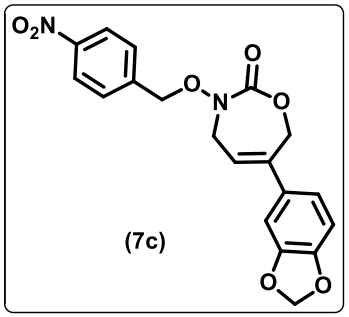
R_f = 0.55 (ethyl acetate/hexane 45:55)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.28 (d, *J* = 9.1 Hz, 2H), 8.23 (d, *J* = 8.5 Hz, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.8 Hz, 2H), 6.97-6.93 (m, 2H), 6.79 (d, *J* = 8.6 Hz, 1H), 5.97 (s, 2H), 5.88 (t, *J* = 7.4 Hz, 1H), 5.12 (s, 2H), 4.50 (s, 2H), 4.45 (d, *J* = 7.3 Hz, 2H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 155.2, 154.5, 148.2, 148.1, 147.7, 145.5, 144.0, 141.5, 134.2, 129.9, 125.4, 123.9, 122.2, 121.7, 120.0, 108.4, 106.9, 101.3, 76.6, 59.8, 48.4

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{25}H_{22}N_3O_{10}$ 524.1305, found 524.1284

6-(benzo[d][1,3]dioxol-4-yl)-3-((4-nitrobenzyl)oxy)-3,4-dihydro-1,3-oxazepin-2(7H)-one:



(7c)

Reaction time: 10 min.

5d (0.075 g, 0.143 mmol), **7c** (0.036 g, 0.093 mmol)

Yield: 65 %

Nature: Yellow viscous liquid

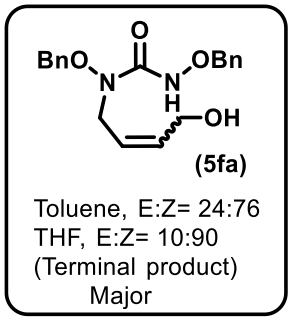
R_f = 0.55 (ethyl acetate/hexane 25:75)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.24 (d, *J* = 8.5 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 2H), 6.78 (d, *J* = 8.2 Hz, 1H), 6.74-6.67 (m, 2H), 5.98 (s, 2H), 5.82 (t, *J* = 4.5 Hz, 1H), 5.00 (s, 2H), 4.86 (brs, 2H), 4.24-4.21 (m, 2H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 159.8, 148.1, 148.0, 147.8, 142.6, 137.6, 132.3, 129.6, 123.8, 121.0, 119.6, 108.5, 106.5, 101.4, 75.1, 69.6, 53.5

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{19}H_{17}N_2O_7$ 385.1036, found 385.1024

1,3-bis(benzyloxy)-1-(4-hydroxybut-2-en-1-yl)urea:



Reaction time: 2 h

1a (0.100 g, 0.367 mmol), **3k** (0.042 g, 0.367 mmol), **5fa** (0.062 g, 0.191 mmol)

Yield: 52 %

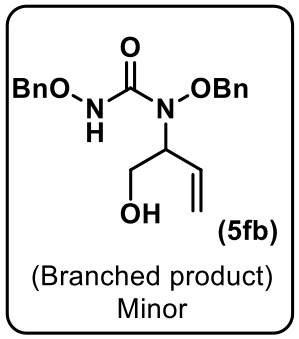
Nature: White viscous liquid

R_f = 0.55 (ethyl acetate/hexane 35:65)

^{1}H-NMR (400 MHz, $CDCl_3$) (For *Z*-isomer only): δ 8.08 (s, 1H), 7.40-7.27 (m, 8H), 7.15 (d, *J* = 7.0 Hz, 2H), 5.90-5.78 (m, 1H), 5.76-5.59 (m, 1H), 4.83 (s, 2H), 4.65 (s, 2H), 4.11 (d, *J* = 4.5 Hz, 2H), 4.06 (d, *J* = 6.4 Hz, 2H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.1, 135.7, 134.5, 134.0, 129.5, 129.2, 129.1, 128.8, 128.6, 125.0, 78.4, 77.5, 62.9, 51.0

HRMS (ESI, Q-TOF) m/z: $[M + H]^+$ Calculated for $C_{19}H_{23}N_2O_4$ 343.1658, found 343.1643



Reaction time: 2 h

1a (0.100 g, 0.367 mmol), **3k** (0.042 g, 0.367 mmol), **5fb** (0.031 g, 0.095 mmol)

Yield: 31 %

Nature: White viscous liquid

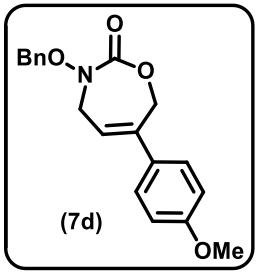
R_f = 0.55 (ethyl acetate/hexane 25:75)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.18 (s, 1H), 7.43-7.28 (m, 8H), 7.12 (d, *J* = 7.5 Hz, 2H), 5.95-5.86 (m, 1H), 5.35-5.26 (m, 2H), 4.86 (s, 2H), 4.71 (s, 2H), 4.57-4.50 (m, 1H), 3.92-3.78 (m, 2H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ 161.0, 135.6, 134.2, 132.1, 129.4, 129.3, 129.2, 128.8, 128.7, 119.7, 78.6, 78.4, 65.4, 62.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{19}H_{23}N_2O_4$ 343.1658, found 343.1654

3-(benzyloxy)-6-(4-methoxyphenyl)-3,4-dihydro-1,3-oxazepin-2(7H)-one:



Reaction time: 4 h

4b (0.100 g, 0.347 mmol), **2a** (0.076 g, 0.347 mmol), **7d** (0.055 g, 0.170 mmol)

Yield: 49 %

Nature: White viscous liquid

R_f = 0.55 (ethyl acetate/hexane 25:75)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.45-7.41 (m, 2H), 7.38-7.34 (m, 3H), 7.16 (d, *J* = 8.7 Hz, 2H), 6.87 (d, *J* = 8.5 Hz, 2H), 5.74 (t, *J* = 4.3 Hz, 1H), 4.90 (s, 2H), 4.87 (brs, 2H), 4.15-4.12 (m, 2H), 3.81 (s, 3H)

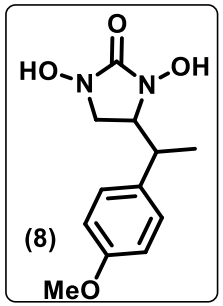
^{13}C-NMR (100 MHz, $CDCl_3$): δ 159.6, 159.6, 137.4, 135.3, 130.7, 129.6, 128.8, 128.5, 127.2, 120.5, 114.1, 76.6, 69.6, 55.4, 53.3

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{19}H_{20}NO_4$ 326.1392, found 326.1366

10. Procedure for the debenzylation of 6a[5]

To the solution of **6a** (0.100 g, 0.232 mmol) in methanol (3 ml) was added 10% Pd/C and then hydrogenated at 45 psi. The reaction was monitored by TLC. After completion of the reaction, the mixture was filtered over a bed of celite, washed with methanol (5 ml) and concentrated in vacuo. The crude product was further purified by column chromatograph on silica gel (60–120 mesh) using 30% methanol/chloroform (1:9 v/v) as eluent to afford **8** (0.037 g, 63% yield).

1,3-dihydroxy-4-(1-(4-methoxyphenyl)ethyl)imidazolidin-2-one:



dr ratio: 60:40

Reaction time: 6 h

6a (0.100 g, 0.232 mmol), **8** (0.037 g, 0.146 mmol)

Yield: 63 %

Nature: Colorless solid

R_f = 0.55 ($MeOH/CHCl_3$ 5:95)

^{1}H-NMR (400 MHz, $CDCl_3$) (for major isomer only): δ 7.04 (d, *J* = 8.4 Hz, 2H), 6.80 (d, *J* = 8.4 Hz, 2H), 3.74 (s, 3H), 3.62-3.53 (m, 1H), 3.35-3.27 (m, 1H), 3.15-3.05 (m, 1H), 2.87 (t, *J* = 9.4 Hz, 1H), 1.37 (d, *J* = 7.2 Hz, 3H)

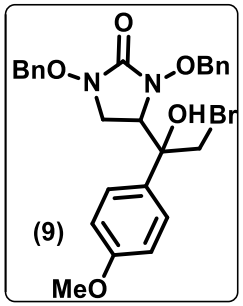
^{13}C-NMR (100 MHz, $CDCl_3$) (for major isomer only): δ 166.1, 158.6, 132.9, 128.9, 114.0, 62.0, 55.3, 48.8, 40.5, 18.2

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{12}H_{17}N_2O_4$ 253.1188, found 253.1161

11. Procedure for the synthesis of 9[6]

To the solution of **6a** (0.100 g, 1 equiv.) in nitromethane (2 ml) was added oxone (2 equiv.) and KBr (1.5 equiv.) and stirred at 45-50 °C. The reaction was monitored by TLC. After completion of the reaction, the crude product was further purified by column chromatography on silica gel (60–120 mesh) using 30% ethyl-acetate/hexane (2:8 v/v) as eluent to afford **9** (0.090 g, 74% yield)

1,3-bis(benzyloxy)-4-(2-bromo-1-hydroxy-1-(4-methoxyphenyl)ethyl)imidazolidin-2-one:



Reaction time: 24 h

6a (0.100 g, 0.232 mmol), **9** (0.090 g, 0.171 mmol)

Yield: 74 %

Nature: Colorless solid

R_f = 0.55 (ethyl acetate/hexane 30:70)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.40-7.27 (m, 12H), 6.86 (d, *J* = 8.6 Hz, 2H), 5.10 (d, *J* = 9.5 Hz, 1H), 4.83 (d, *J* = 9.6 Hz, 1H), 4.77 (s, 2H), 3.95 (t, *J* = 6.8 Hz, 1H), 3.84 (d, *J* = 10.7 Hz, 1H), 3.80 (s, 3H), 3.77 (d, *J* = 10.7 Hz, 1H), 3.18 (t, *J* = 8.1 Hz, 1H), 3.07 (t, *J* = 7.0 Hz, 1H), 2.77 (s, 1H),

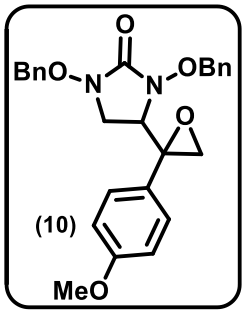
^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.7, 159.5, 130.0, 129.2, 129.1, 128.6, 128.6, 128.5, 127.6, 113.8, 78.0, 77.6, 74.8, 60.1, 55.3, 46.3, 42.6

HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{28}BrN_2O_5$ 527.1182, found 527.1180

12. Procedure for the synthesis of 10

To the solution of **9** (0.065 g, 0.123 mmol.) in DCM (1 ml) was added DBU (1.5 equiv.) and stirred at Room temperature until the completion of the reaction (as monitored by TLC). The crude product was further purified by column chromatography on silica gel (60–120 mesh) using 20% ethyl-acetate/hexane (2:8 v/v) as eluent to afford **10** (0.038 g, 7% yield)

1,3-bis(benzyloxy)-4-(2-(4-methoxyphenyl)oxiran-2-yl)imidazolidin-2-one:



Reaction time: 10 min.

6a (0.065 g, 0.123 mmol), **10** (0.038 g, 0.086 mmol)

Yield: 70 %

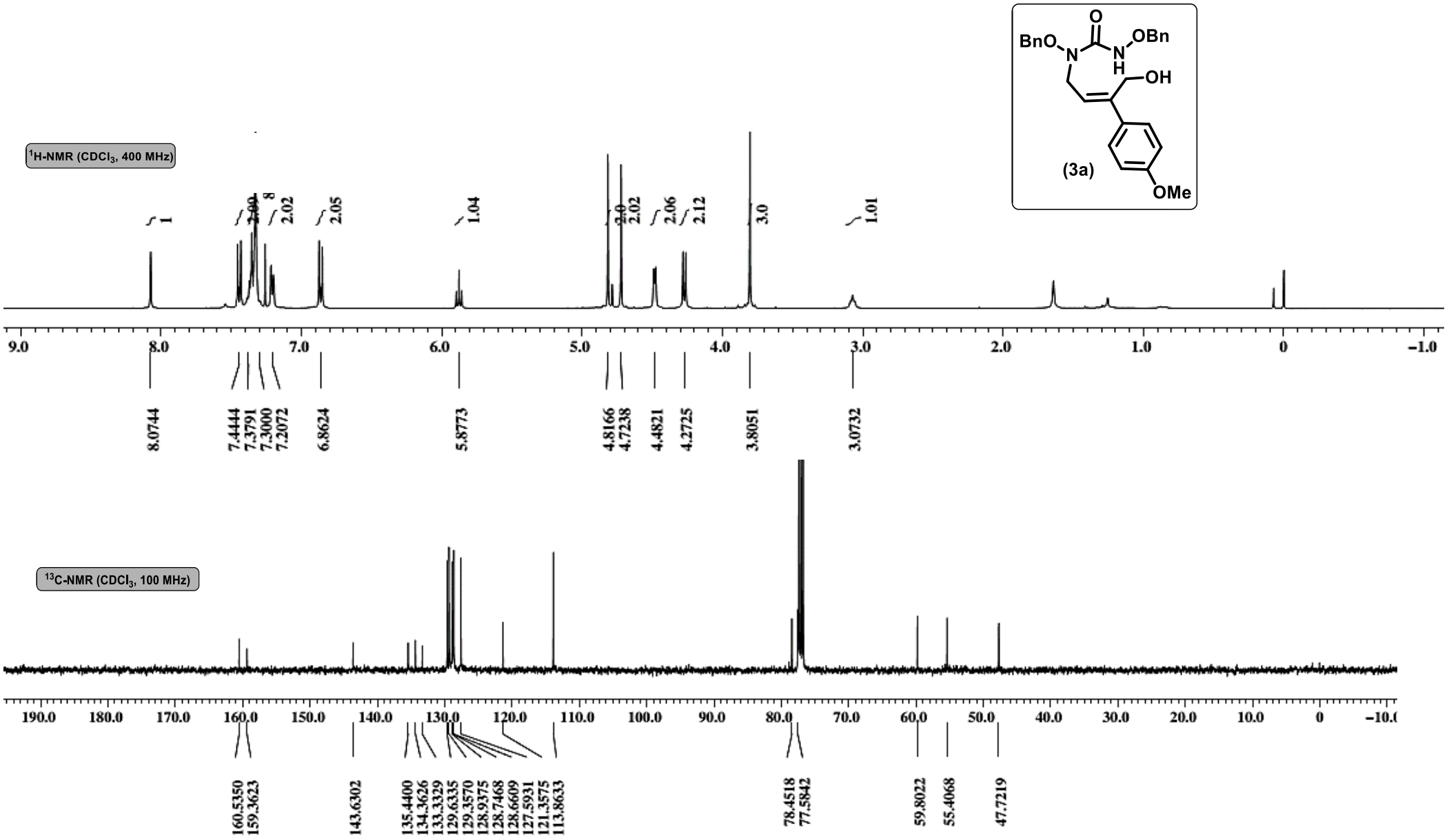
Nature: White viscous liquid

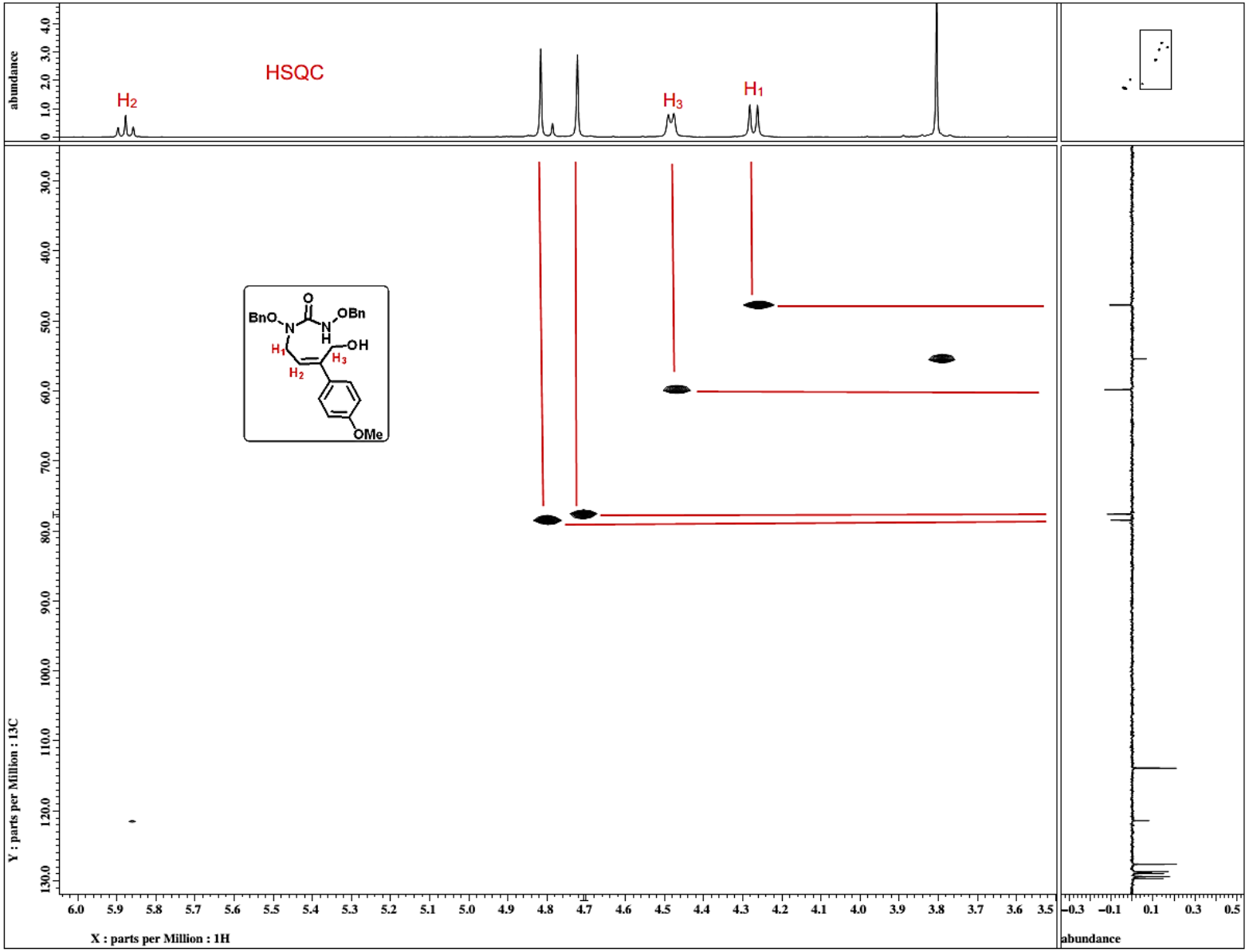
R_f = 0.55 (ethyl acetate/hexane 30:70)

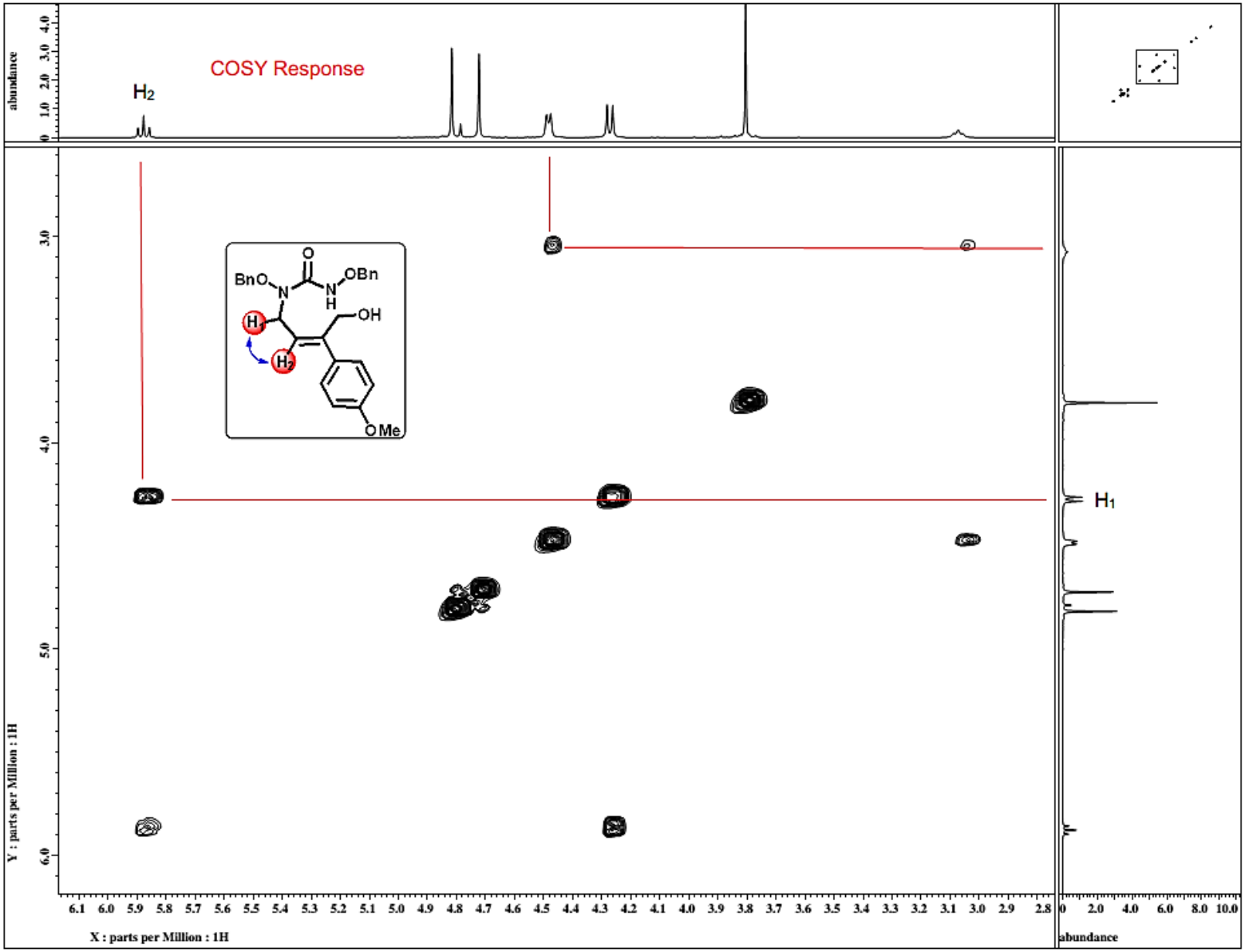
^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.40-7.23 (m, 12H), 6.82 (d, *J* = 8.9 Hz, 2H), 5.14 (d, *J* = 9.9 Hz, 1H), 4.97 (d, *J* = 9.9 Hz, 1H), 4.78 (s, 2H), 3.78 (s, 3H), 3.29 (t, *J* = 7.3 Hz, 1H), 3.17 (t, *J* = 7.5 Hz, 1H), 3.04 (t, *J* = 7.5 Hz, 1H), 2.92 (d, *J* = 5.2 Hz, 1H), 2.74 (d, *J* = 5.3 Hz, 1H)

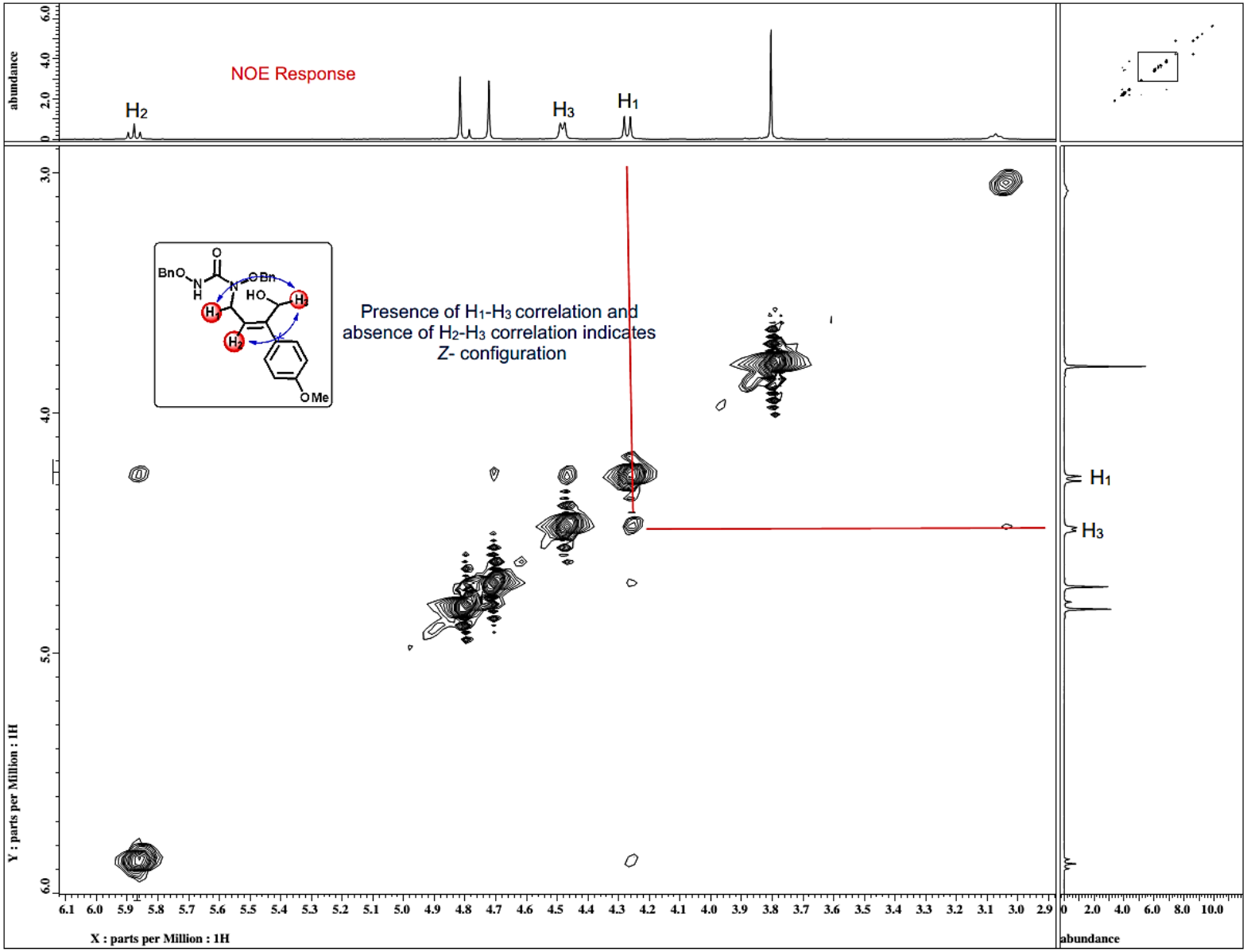
^{13}C-NMR (100 MHz, $CDCl_3$): δ 161.4, 159.6, 135.7, 135.3, 129.6, 129.2, 128.9, 128.7, 128.6, 128.5, 128.3, 128.1, 127.4, 113.9, 78.5, 78.1, 61.1, 57.6, 55.3, 33.5, 46.8

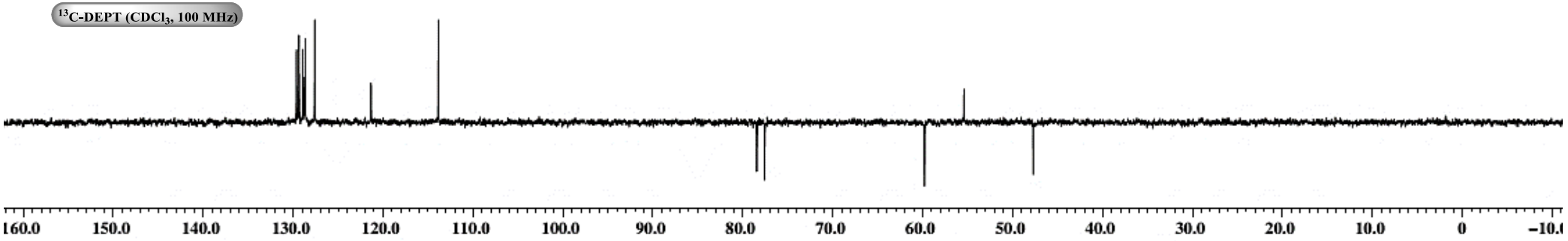
HRMS (ESI, Q-TOF) m/z: [M + H]+ Calculated for $C_{26}H_{27}N_2O_5$ 447.1920, found 447.1902


(3a)
BnO
OBn
OH
OMe
^{1}H-NMR (CDCl$_3$, 400 MHz)
1
2.00
8
2.02
2.05
1.04
2.0
2.02
2.06
2.12
3.0
1.01
8.0744
7.4444
7.3791
7.3000
7.2072
6.8624
5.8773
4.8166
4.7238
4.4821
4.2725
3.8051
3.0732
^{13}C-NMR (CDCl$_3$, 100 MHz)
160.5350
159.3623
143.6302
135.4400
134.3626
133.3329
129.6335
129.3570
128.9375
128.7468
128.6609
127.5931
121.3575
113.8633
78.4518
77.5842
59.8022
55.4068
47.7219


HSQC
H2
H3
H1
abundance
Y : parts per Million : 13C
X : parts per Million : 1H
abundance
BnO
OBn
OH
OMe


COSY Response
H2
H1
BnO
OBn
OH
OMe
abundance
Y : parts per Million : 1H
X : parts per Million : 1H
abundance


NOE Response
H2
H3
H1
abundance
Presence of H1-H3 correlation and
absence of H2-H3 correlation indicates
Z- configuration
BnO
N
H
O
N
OBn
HO
H1
H2
H3
OMe
H1
H3
Y : parts per Million : 1H
X : parts per Million : 1H
abundance


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

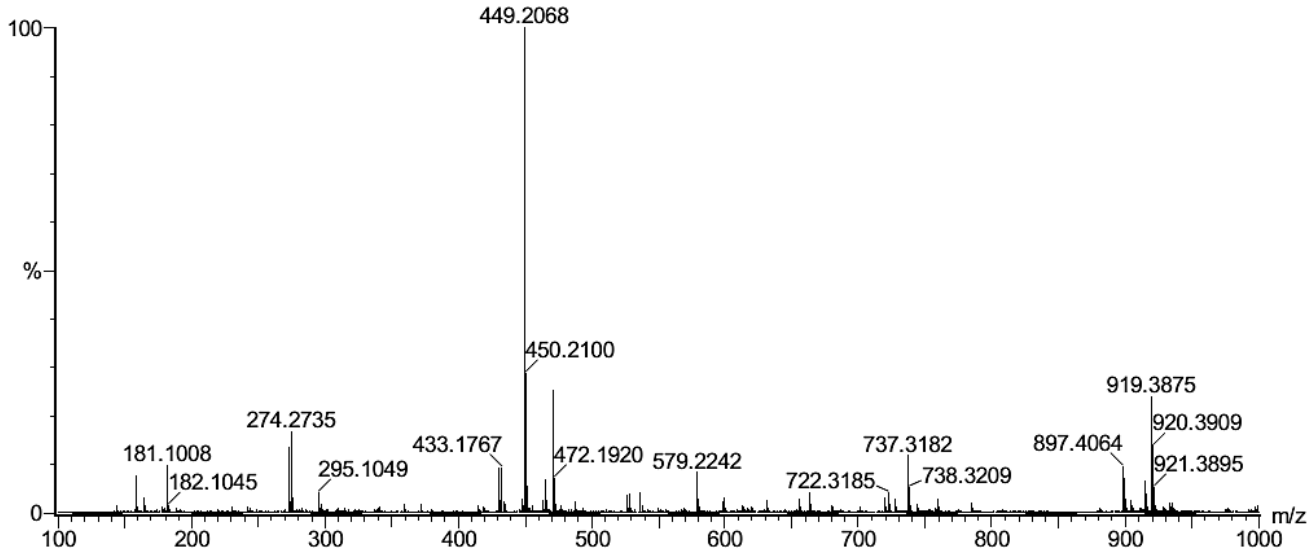
Monoisotopic Mass, Even Electron Ions
62 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 6-35 N: 0-3 O: 0-8

Sample Name : 15-01-288
Test Name : HRMS-1
130120-15-01-288 18 (0.183)

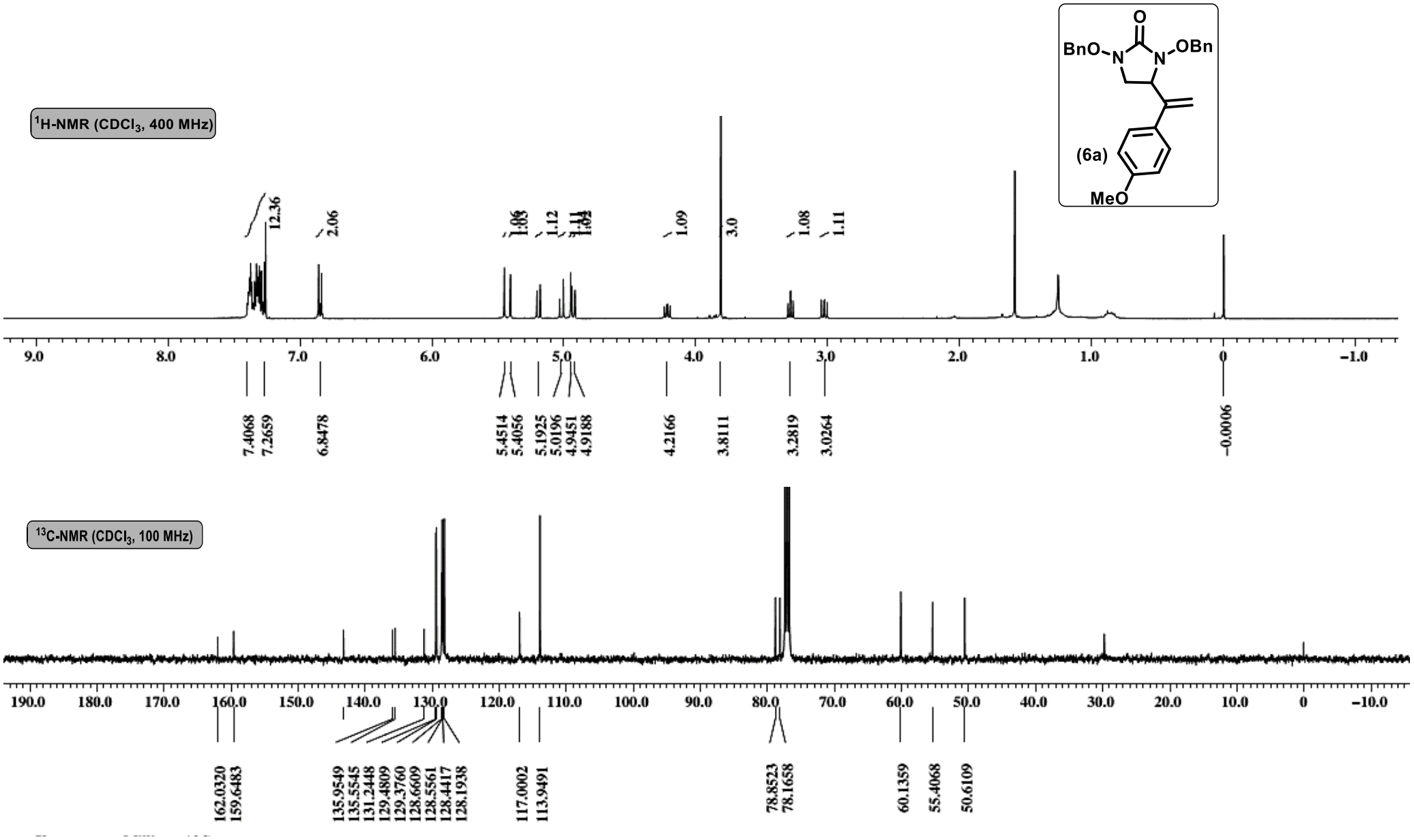
IITRPR

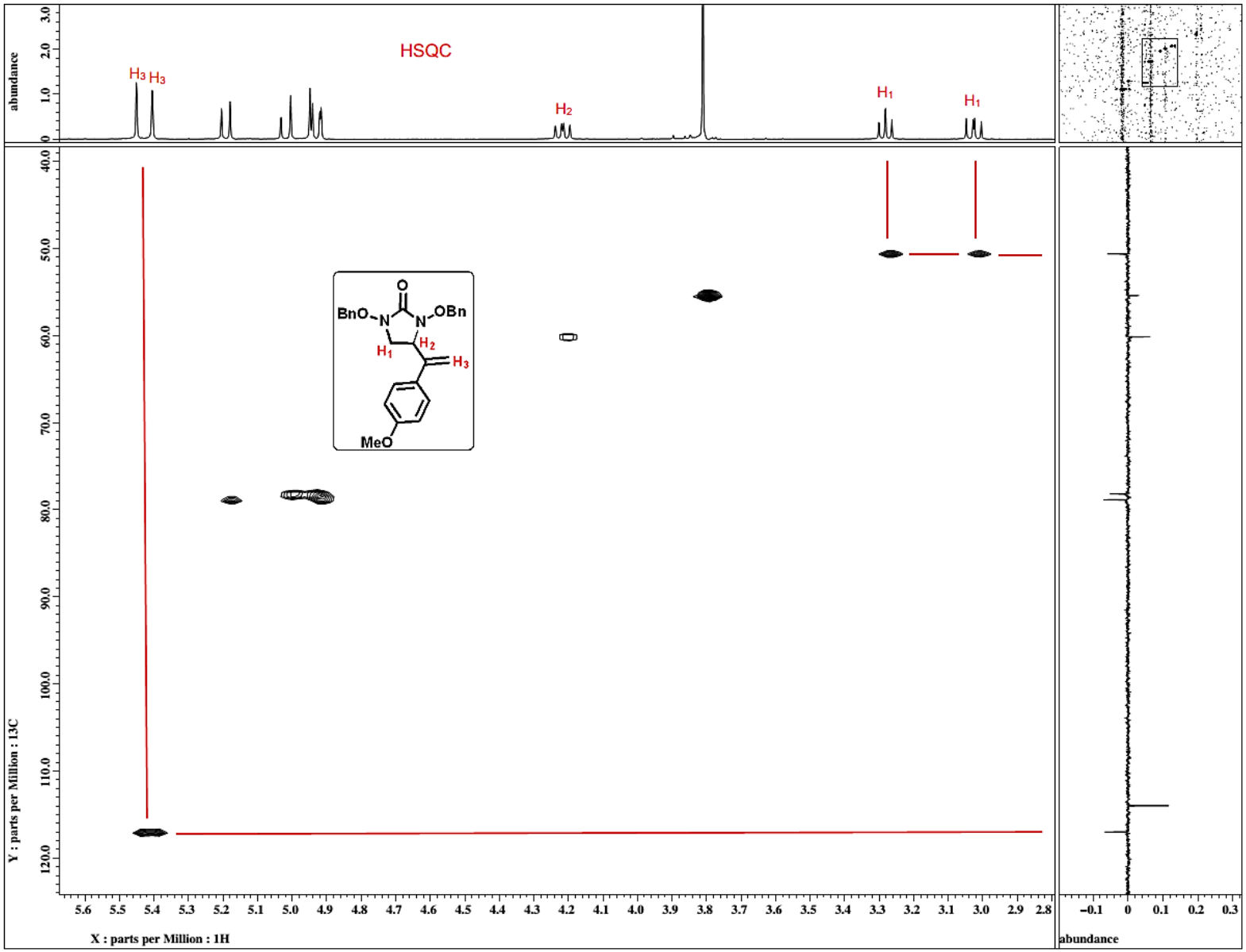
XEVO G2-XS QTOF

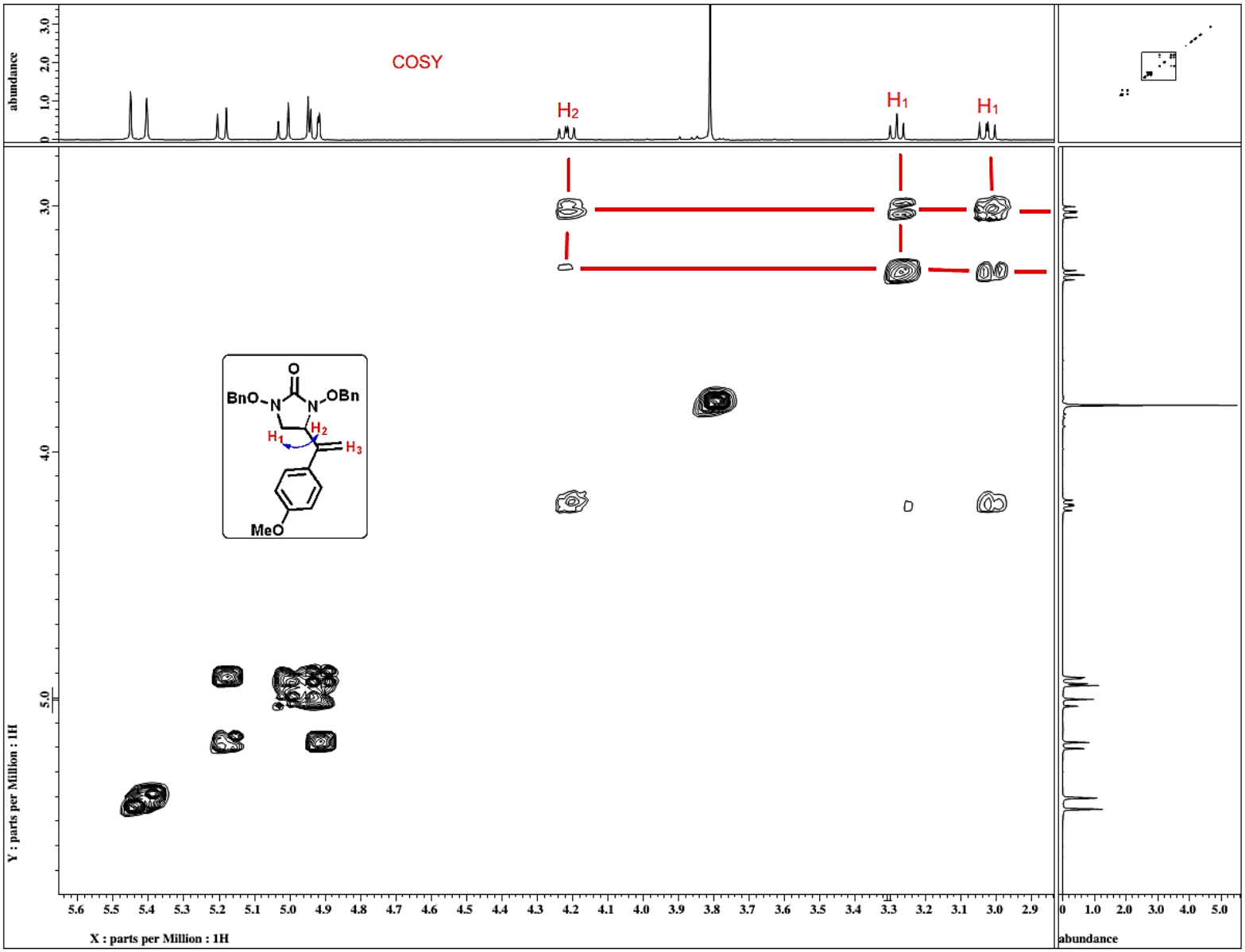
1: TOF MS ES+
1.81e+007

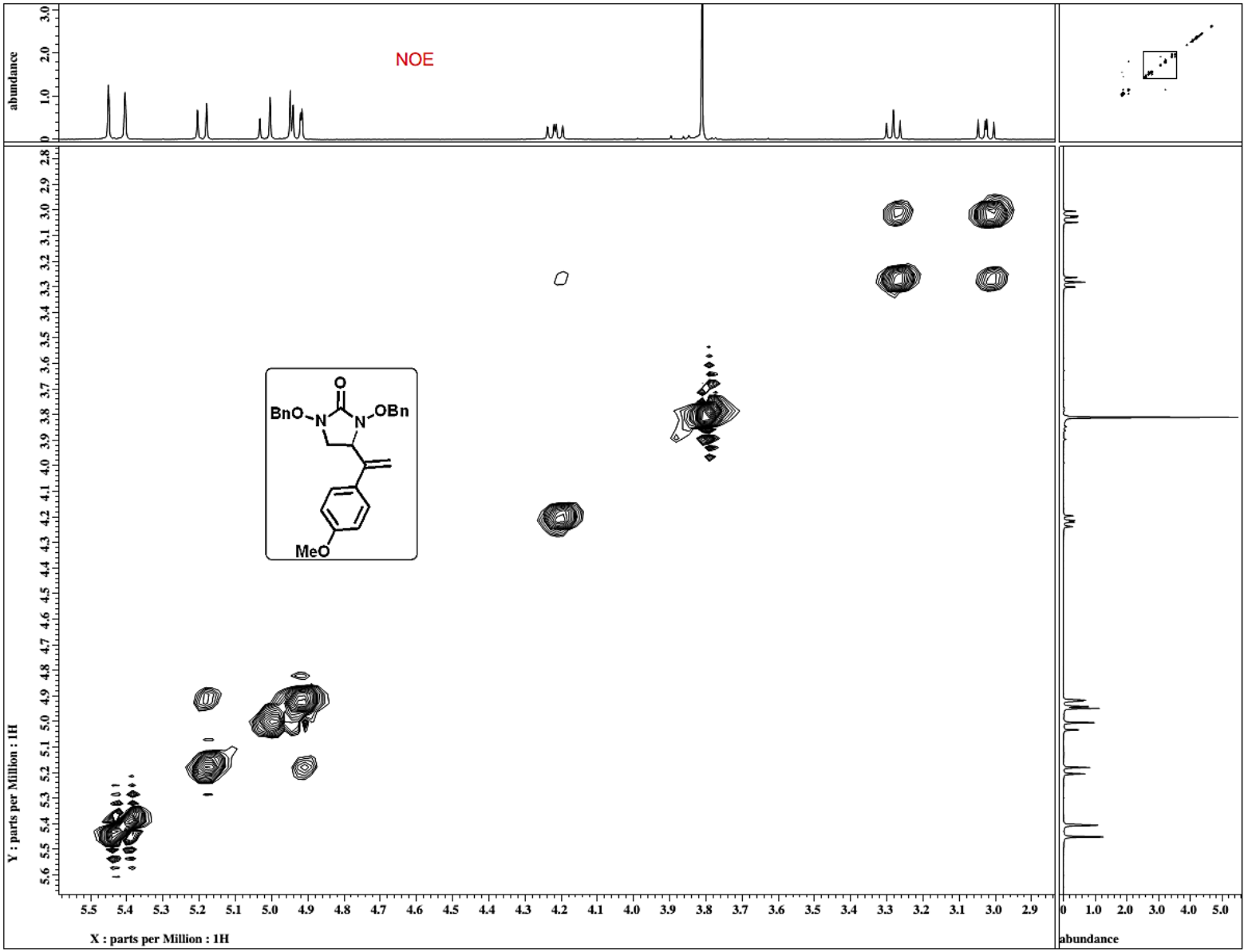


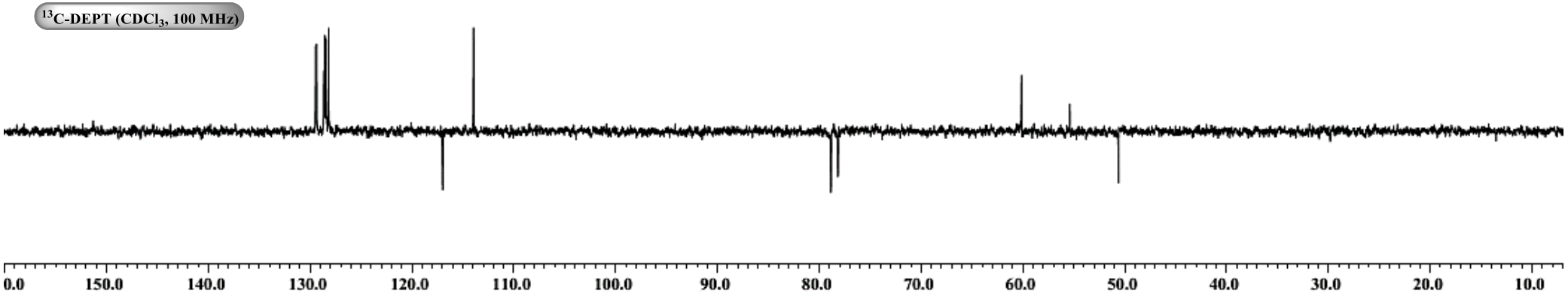
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
449.2068	449.2076	-0.8	-1.8	13.5	1177.4	n/a	n/a	C26 H29 N2 O5


^{1}H-NMR ($CDCl_3$, 400 MHz)
BnO
N
O
N
OBn
(6a)
MeO
12.36
2.06
1.09
3.0
1.08
1.11
7.4068
7.2659
6.8478
5.4514
5.4056
5.1925
5.0196
4.9451
4.9188
4.2166
3.8111
3.2819
3.0264
−0.0006
^{13}C-NMR ($CDCl_3$, 100 MHz)
162.0320
159.6483
135.9549
135.5545
131.2448
129.4809
129.3760
128.6609
128.5561
128.4417
128.1938
117.0002
113.9491
78.8523
78.1658
60.1359
55.4068
50.6109


HSQC
abundance
H3 H3
H2
H1
H1
BnO
N
O
N
OBn
H1
H2
H3
MeO
Y : parts per Million : 13C
X : parts per Million : 1H
abundance


COSY
H2
H1
H1
abundance
Y : parts per Million : 1H
X : parts per Million : 1H
abundance
BnO
OBn
MeO
H1
H2
H3


NOE
abundance
BnO
N
N
OBn
O
MeO
Y : parts per Million : 1H
X : parts per Million : 1H
abundance


^{13}C-DEPT ($CDCl_3$, 100 MHz)
0.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0

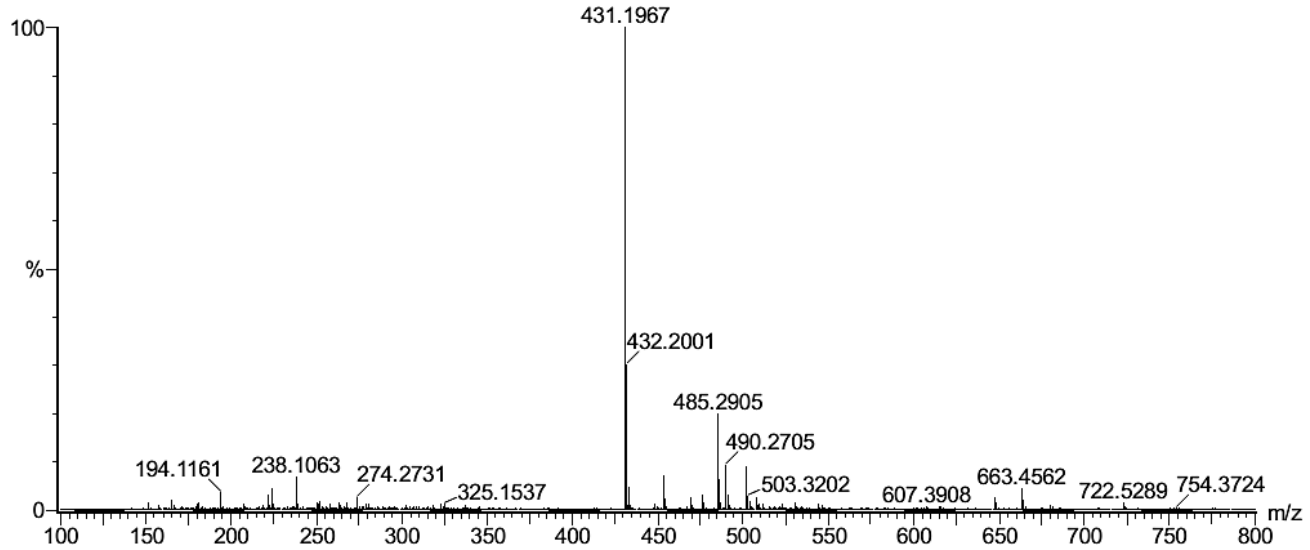
Elemental Composition Report

Single Mass Analysis

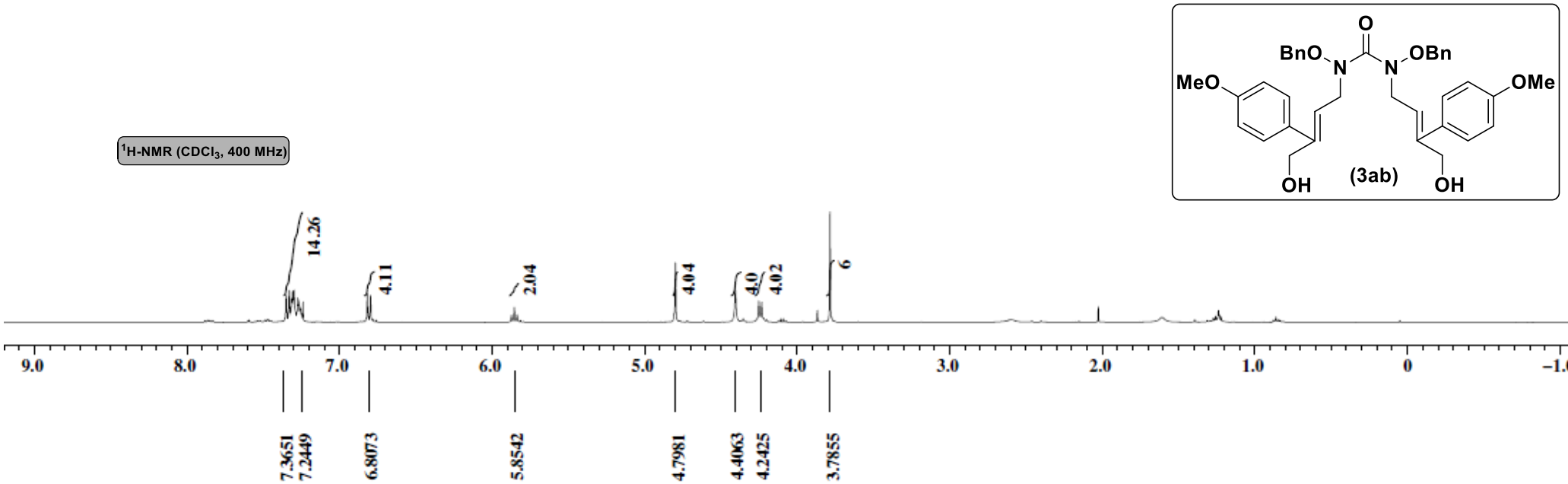
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

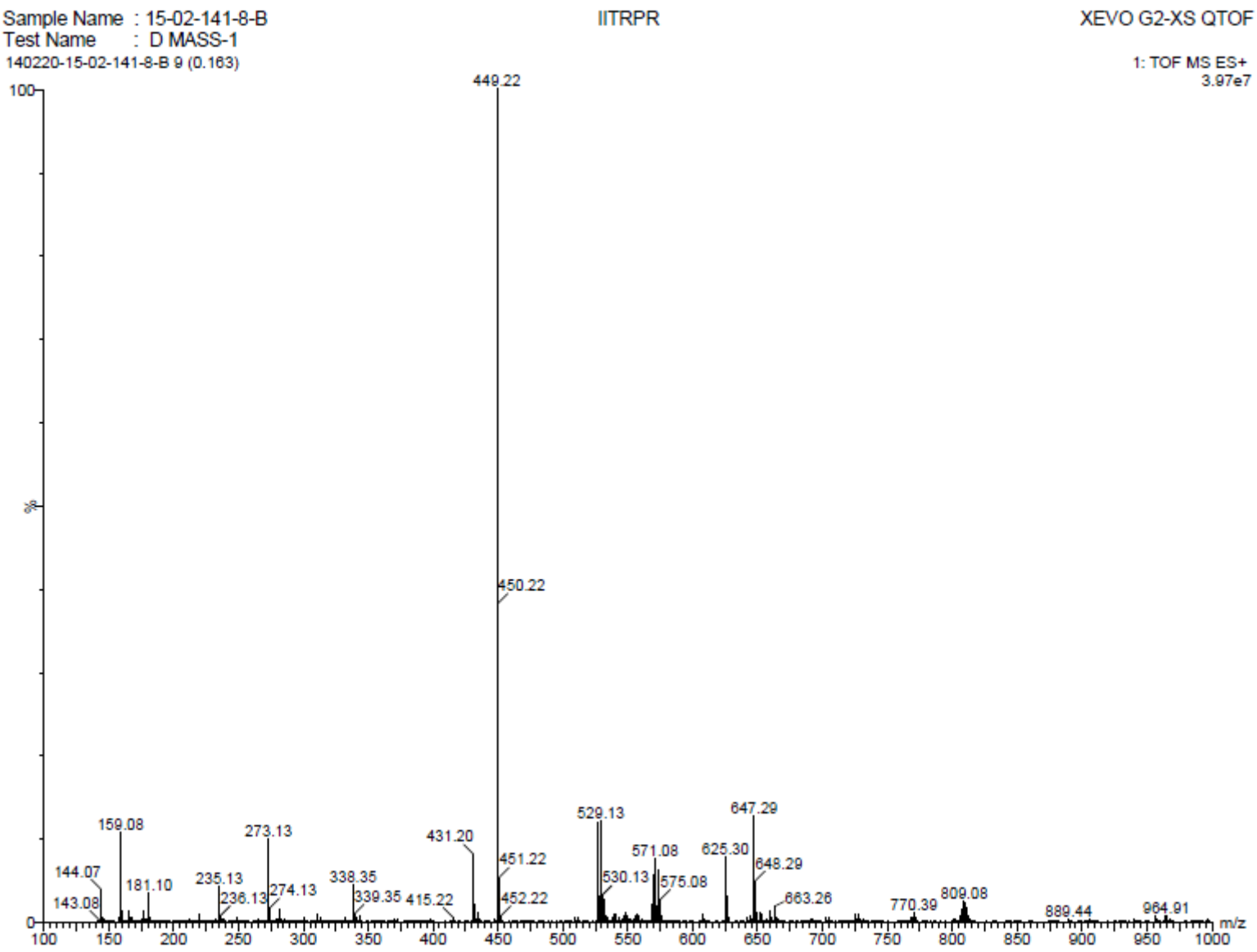
Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 25-30 H: 25-30 N: 0-2 O: 0-5 Cl: 0-1

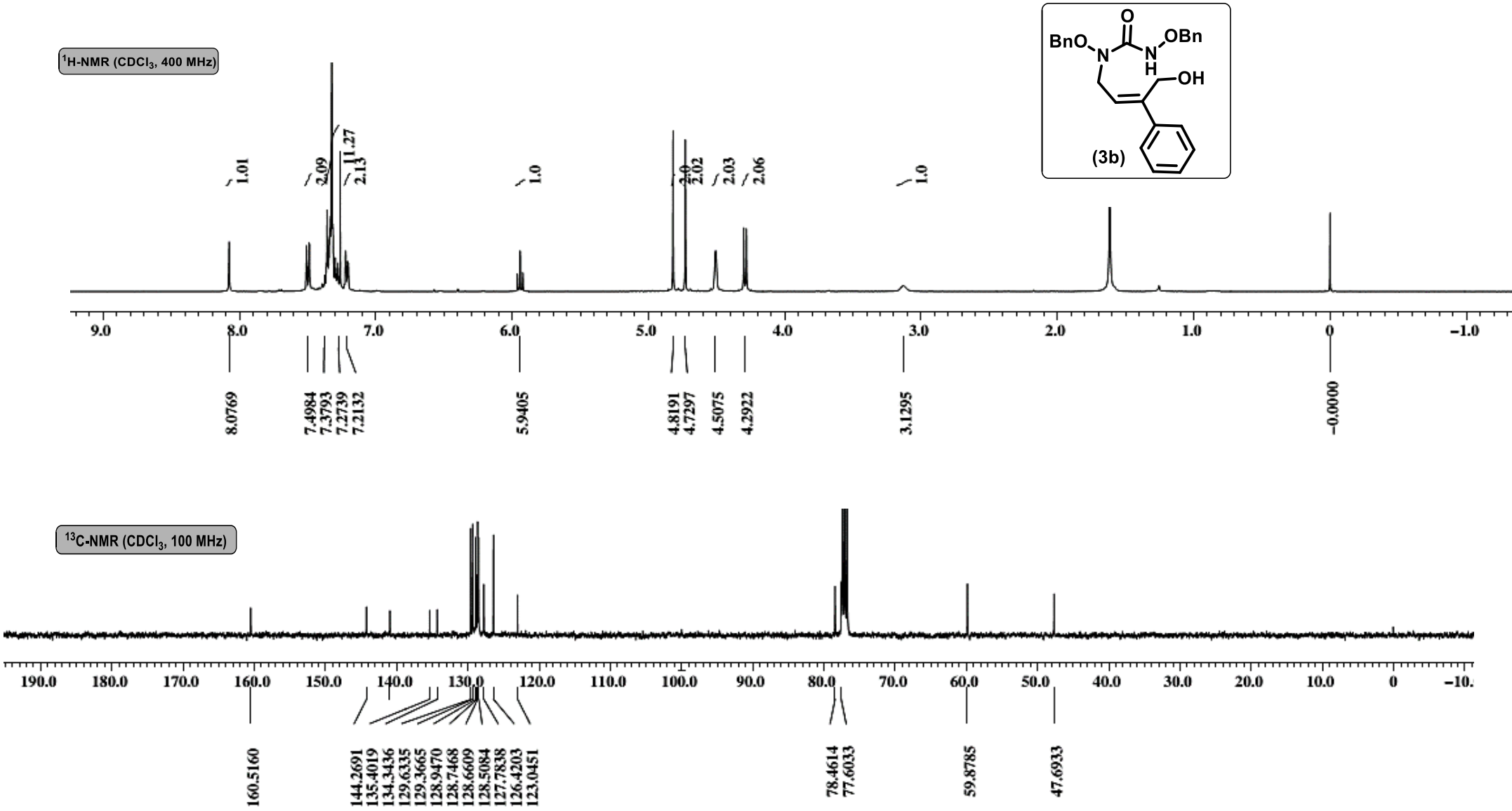
Sample Name : 15-01-310 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
110619-15-01-310 17 (0.174) AM (Cen,4, 85.00, Ar,10000.0,0.00,0.00); Sm (SG, 1x3.00); Cm (17:20) 1: TOF MS ES+
2.64e+007

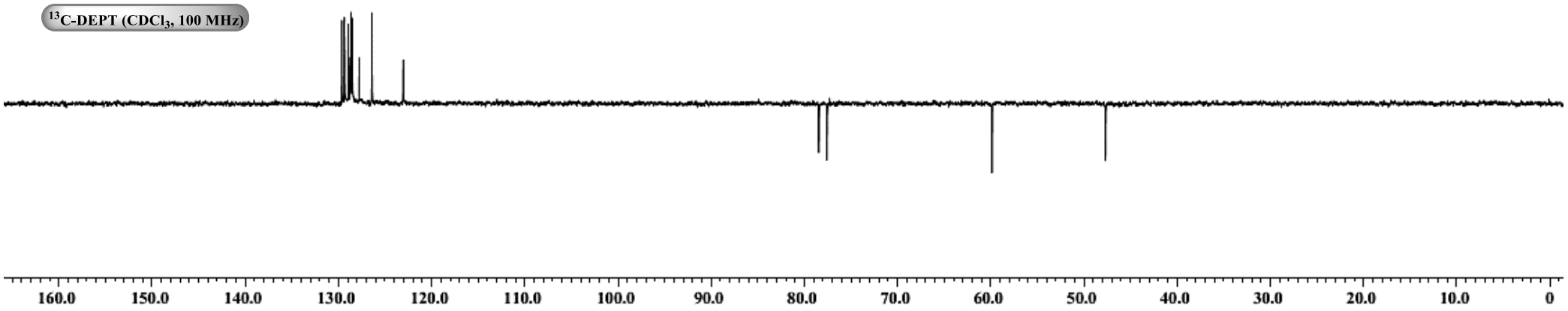


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
431.1967	431.1971	-0.4	-0.9	14.5	907.0	n/a	n/a	C26 H27 N2 O4


^{1}H-NMR ($CDCl_3$, 400 MHz)
BnO
N
O
N
OBn
MeO
OMe
OH
(3ab)
OH
14.26
4.11
2.04
4.04
4.0
4.02
6
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.3651
7.2449
6.8073
5.8542
4.7981
4.4063
4.2425
3.7855


Sample Name : 15-02-141-8-B
Test Name : D MASS-1
140220-15-02-141-8-B 9 (0.163)
IITRPR
XEVO G2-XS QTOF
1: TOF MS ES+
3.97e7
100
%
0
449.22
450.22
159.08
273.13
431.20
529.13
647.29
571.08
625.30
451.22
648.29
144.07
181.10
235.13
274.13
338.35
530.13
575.08
236.13
339.35
415.22
452.22
663.26
770.39
809.08
889.44
964.91
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000


^{1}H-NMR ($CDCl_3$, 400 MHz)
BnO
N
O
N
H
OBn
OH
(3b)
1.01
2.09
1.27
2.13
1.0
2.0
2.02
2.03
2.06
1.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.0769
7.4984
7.3793
7.2739
7.2132
5.9405
4.8191
4.7297
4.5075
4.2922
3.1295
−0.0000
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
160.5160
144.2691
135.4019
134.3436
129.6335
129.3665
128.9470
128.7468
128.6609
128.5084
127.7838
126.4203
123.0451
78.4614
77.6033
59.8785
47.6933


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

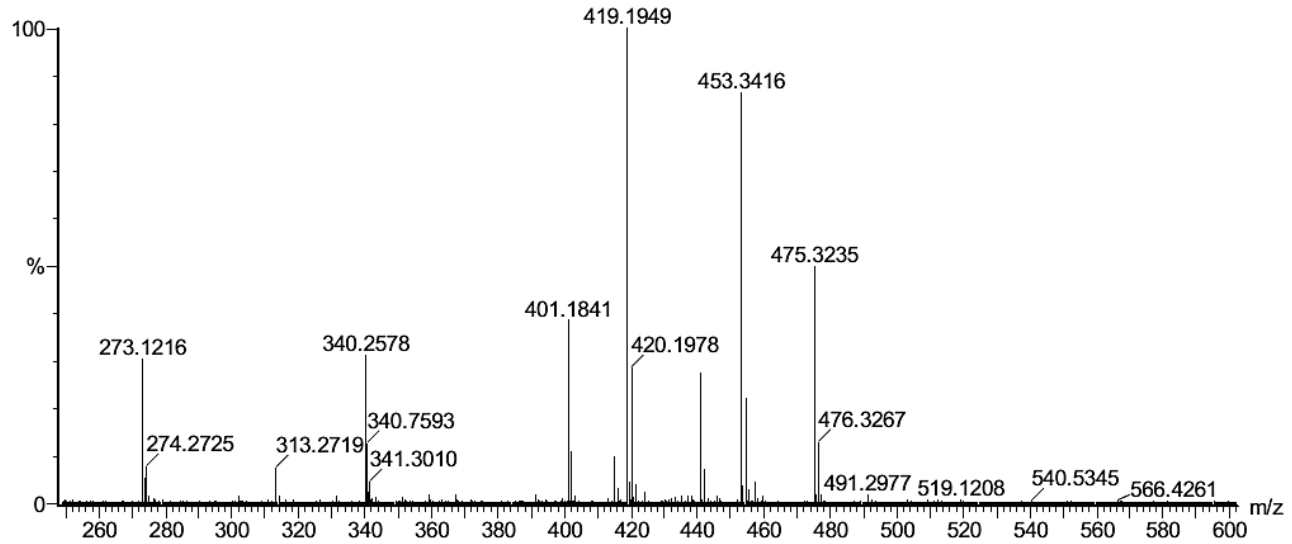
Elemental Composition Report

Single Mass Analysis

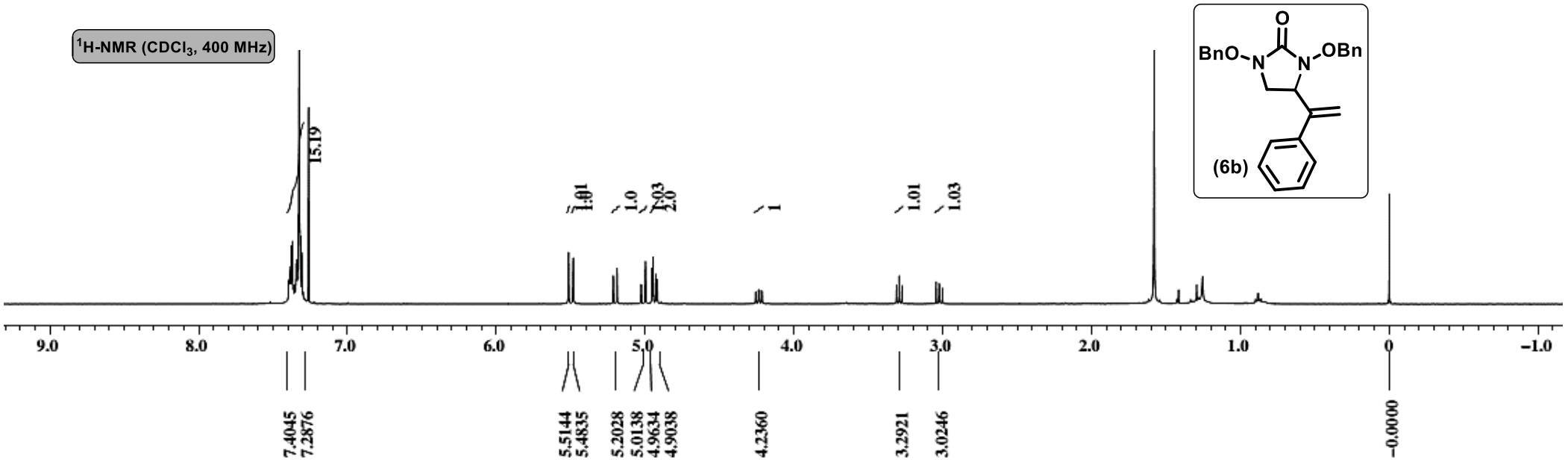
Tolerance = 6.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

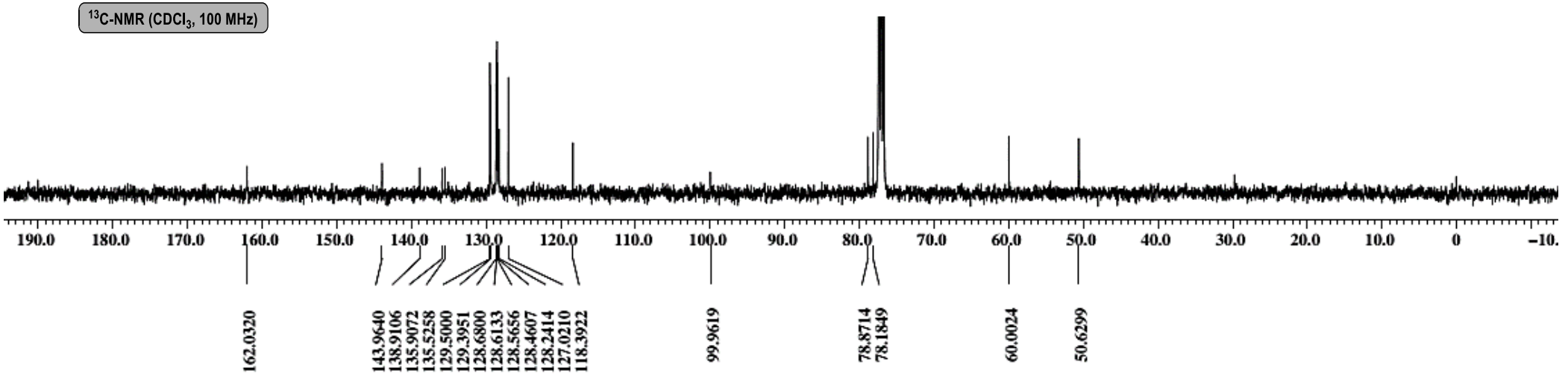
Monoisotopic Mass, Even Electron Ions
99 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 5-30 H: 5-30 N: 0-5 O: 1-4 Br: 0-1

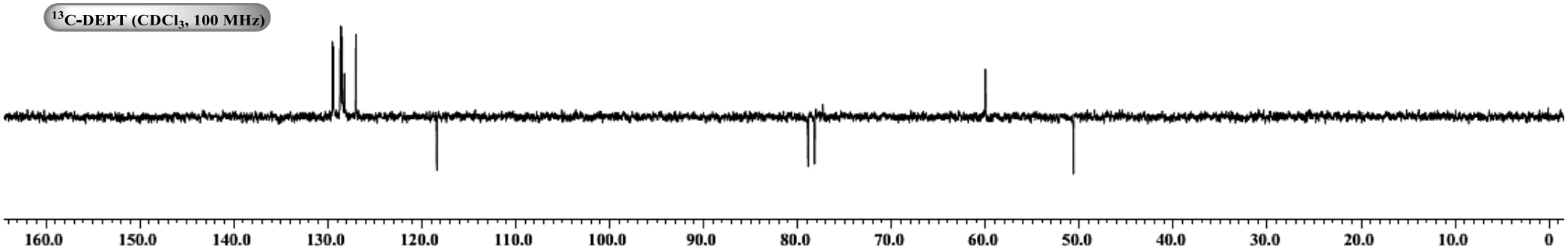
Sample Name : 15-02-26 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
290819-15-02-26 13 (0.140) AM2 (Ar,22000.0,0.00,0.00); Cm (13:18) 1: TOF MS ES+
4.14e+007



Minimum:				-1.5				
Maximum:		5.0	6.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
419.1949	419.1971	-2.2	-5.2	13.5	839.8	n/a	n/a	C25 H27 N2 O4


^{1}H-NMR (CDCl$_3$, 400 MHz)
BnO
N
O
N
OBn
(6b)
15.19
1.01
1.01
1.0
1.03
2.0
1
1.01
1.03
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.4045
7.2876
5.5144
5.4835
5.2028
5.0138
4.9634
4.9038
4.2360
3.2921
3.0246
−0.0000


^{13}C-NMR (CDCl$_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.
162.0320
143.9640
138.9106
135.9072
135.5258
129.5000
129.3951
128.6800
128.6133
128.5656
128.4607
128.2414
127.0210
118.3922
99.9619
78.8714
78.1849
60.0024
50.6299


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

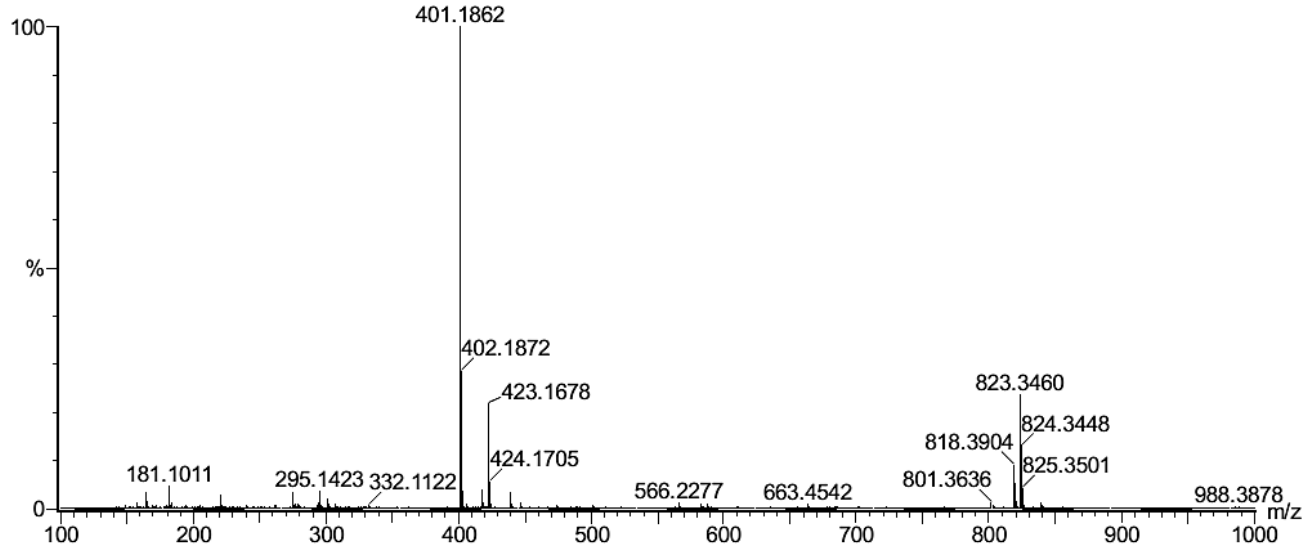
Elemental Composition Report

Single Mass Analysis

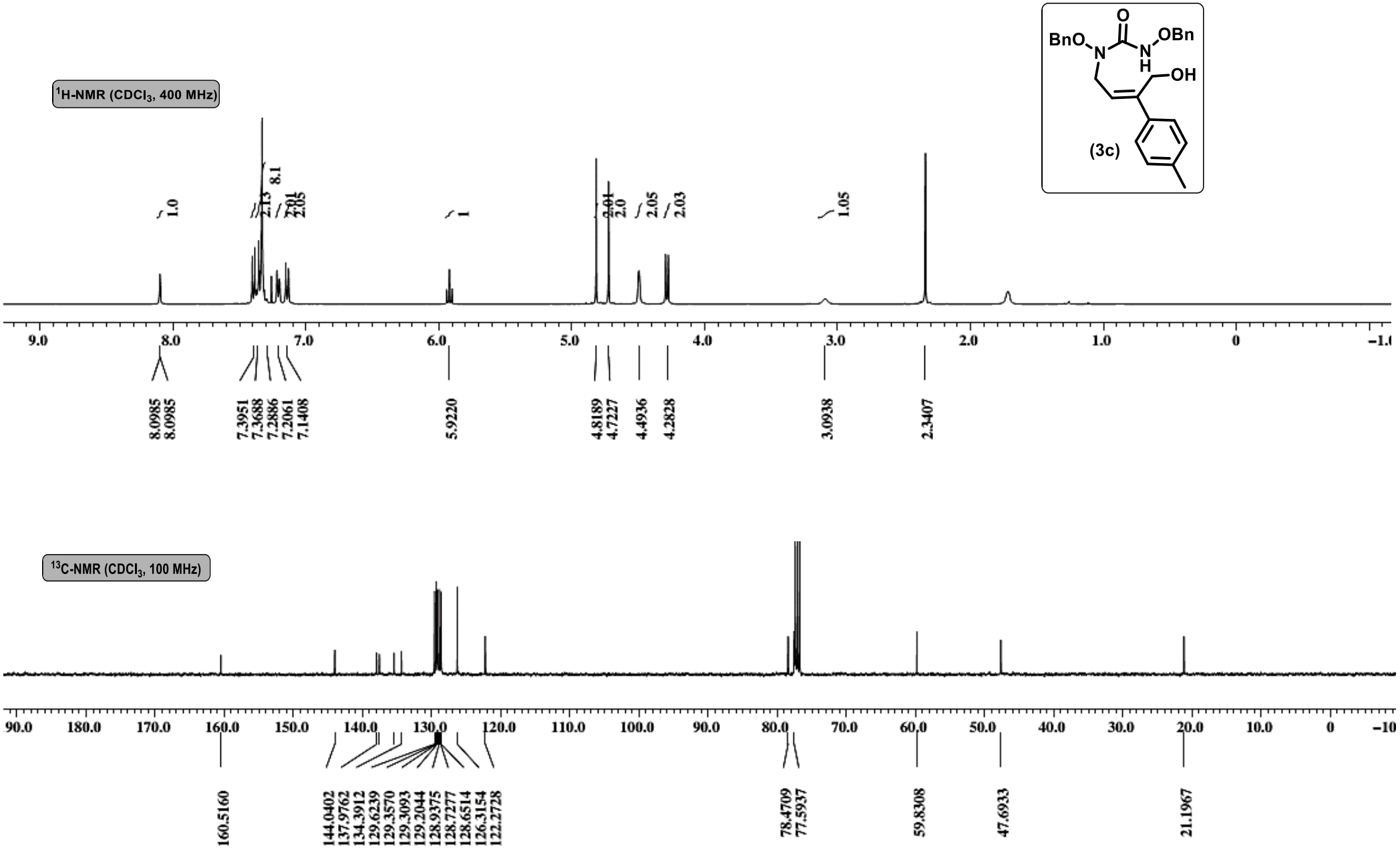
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

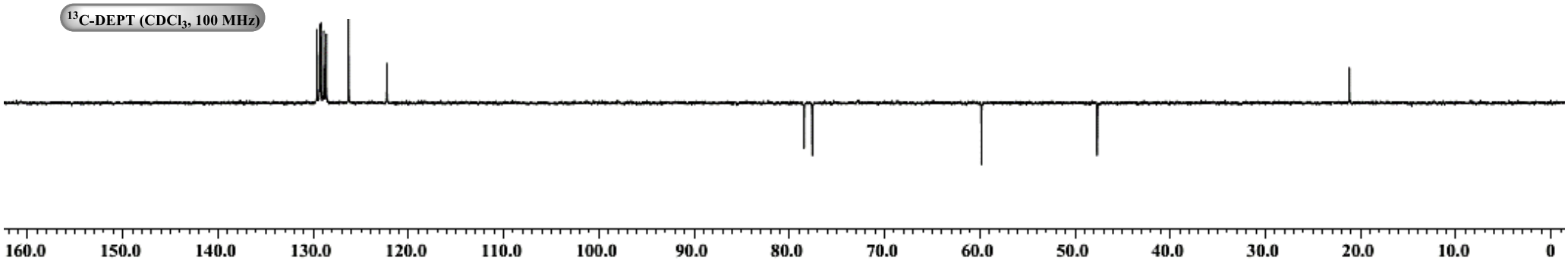
Monoisotopic Mass, Even Electron Ions
35 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 6-35 N: 0-3 O: 0-3

Sample Name : 15-02-32 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
130120-15-02-32 17 (0.174) 1: TOF MS ES+
2.36e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
401.1862	401.1865	-0.3	-0.7	14.5	1338.2	n/a	n/a	C25 H25 N2 O3


(3c)
^{1}H-NMR (CDCl$_3$, 400 MHz)
^{13}C-NMR (CDCl$_3$, 100 MHz)


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

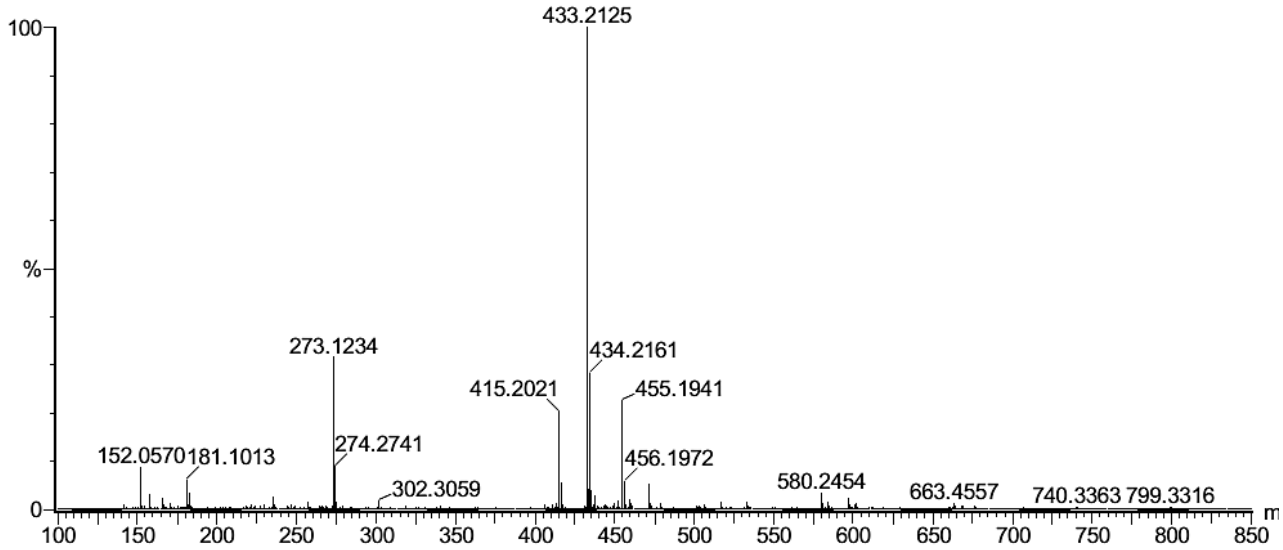
Elemental Composition Report Page

Single Mass Analysis

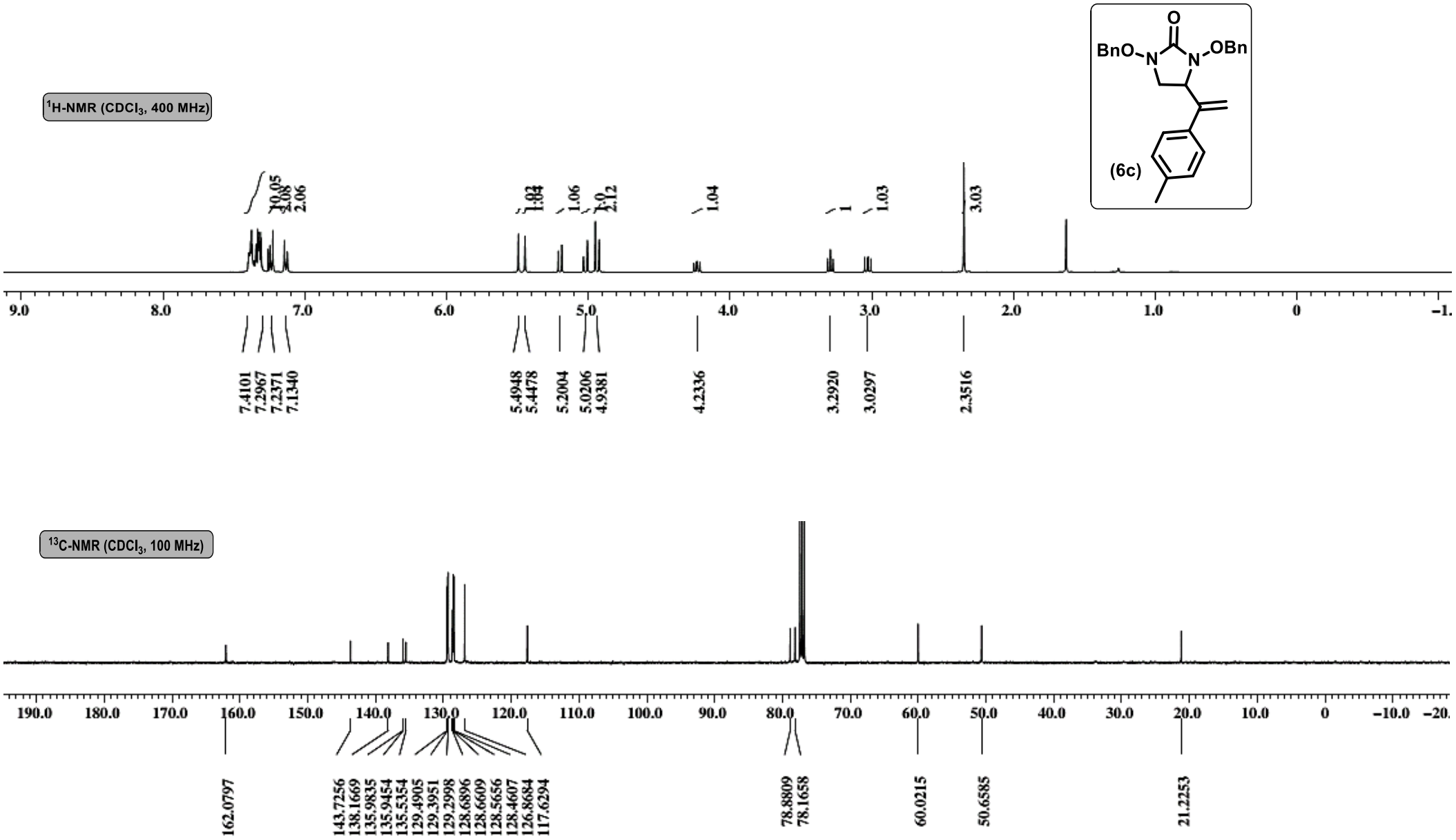
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

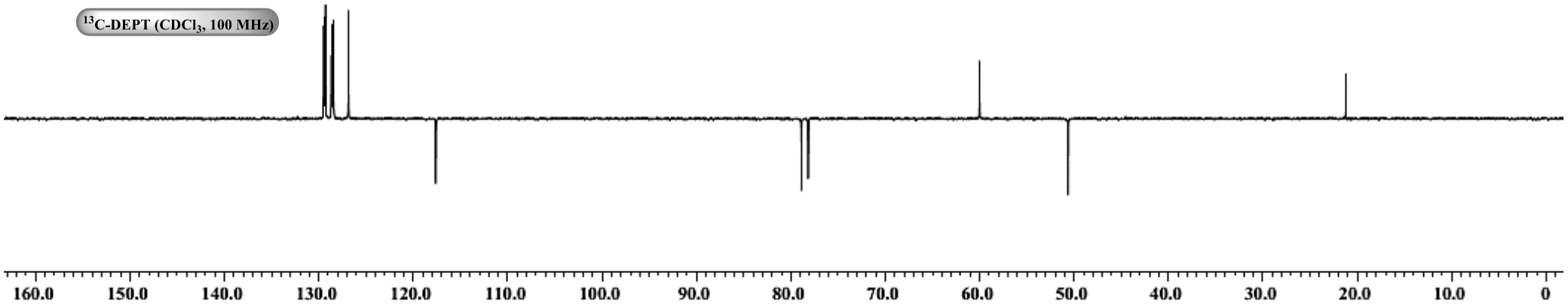
Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 5-30 H: 5-30 N: 0-3 O: 1-4

Sample Name : 15-02-35 IITRPR XEVO G2-XS QT
Test Name : HRMS-1
060919-15-02-35 17 (0.174) AM2 (Ar,22000.0,0.00,0.00); Cm (17:19) 1: TOF MS ES
1.43e+0



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
433.2125	433.2127	-0.2	-0.5	13.5	747.4	n/a	n/a	C26 H29 N2 O4


^{1}H-NMR (CDCl$_3$, 400 MHz)
BnO
N
O
N
OBn
(6c)
10.05
2.08
2.06
1.06
2.12
1.04
1
1.03
3.03
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.4101
7.2967
7.2371
7.1340
5.4948
5.4478
5.2004
5.0206
4.9381
4.2336
3.2920
3.0297
2.3516
^{13}C-NMR (CDCl$_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
162.0797
143.7256
138.1669
135.9835
135.9454
135.5354
129.4905
129.3951
129.2998
128.6896
128.6609
128.5656
128.4607
126.8684
117.6294
78.8809
78.1658
60.0215
50.6585
21.2253


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

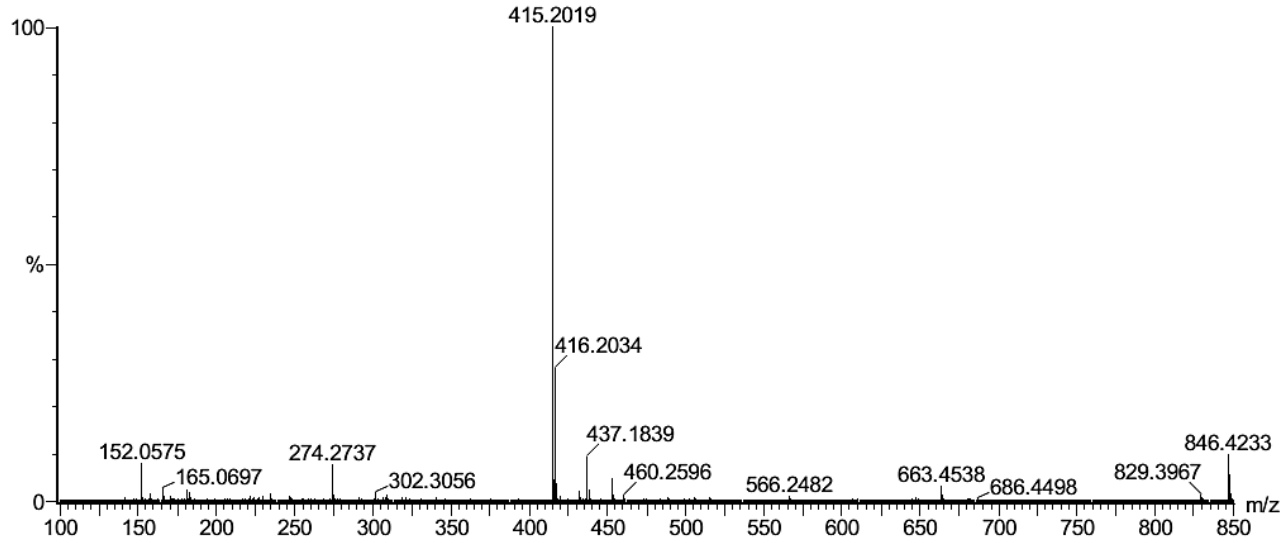
Elemental Composition Report

Single Mass Analysis

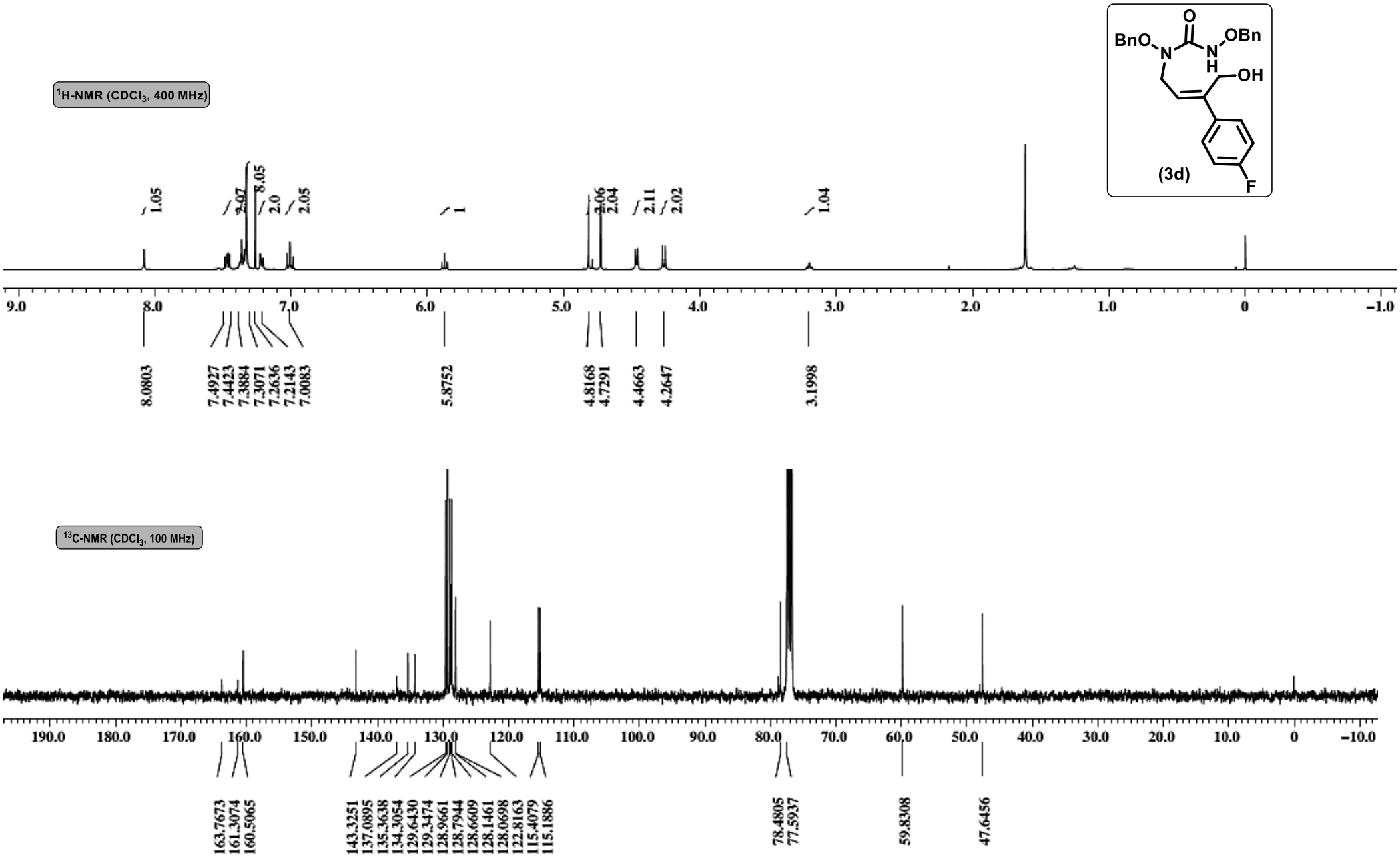
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

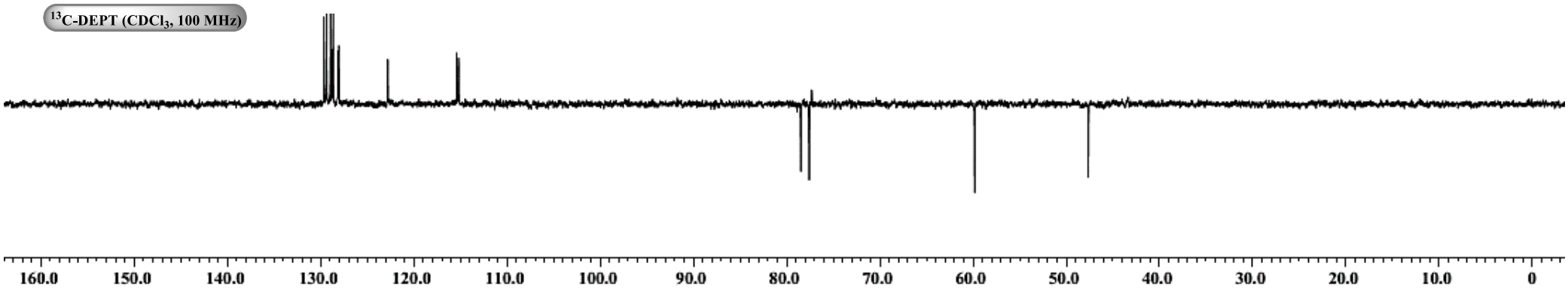
Monoisotopic Mass, Even Electron Ions
65 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 5-30 H: 5-30 N: 0-3 O: 1-4 Br: 0-1

Sample Name : 15-02-39 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
060919-15-02-39 20 (0.211) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (20:22) 1: TOF MS ES+
1.88e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
415.2019	415.2022	-0.3	-0.7	14.5	994.4	n/a	n/a	C26 H27 N2 O3


^{1}H-NMR (CDCl$_3$, 400 MHz)
BnO
N
O
N
H
OBn
OH
F
(3d)
1.05
3.07
8.05
2.0
2.05
1
3.06
2.04
2.11
2.02
1.04
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.0803
7.4927
7.4423
7.3884
7.3071
7.2636
7.2143
7.0083
5.8752
4.8168
4.7291
4.4663
4.2647
3.1998
^{13}C-NMR (CDCl$_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
163.7673
161.3074
160.5065
143.3251
137.0895
135.3638
134.3054
129.6430
129.3474
128.9661
128.7944
128.6609
128.1461
128.0698
122.8163
115.4079
115.1886
78.4805
77.5937
59.8308
47.6456


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

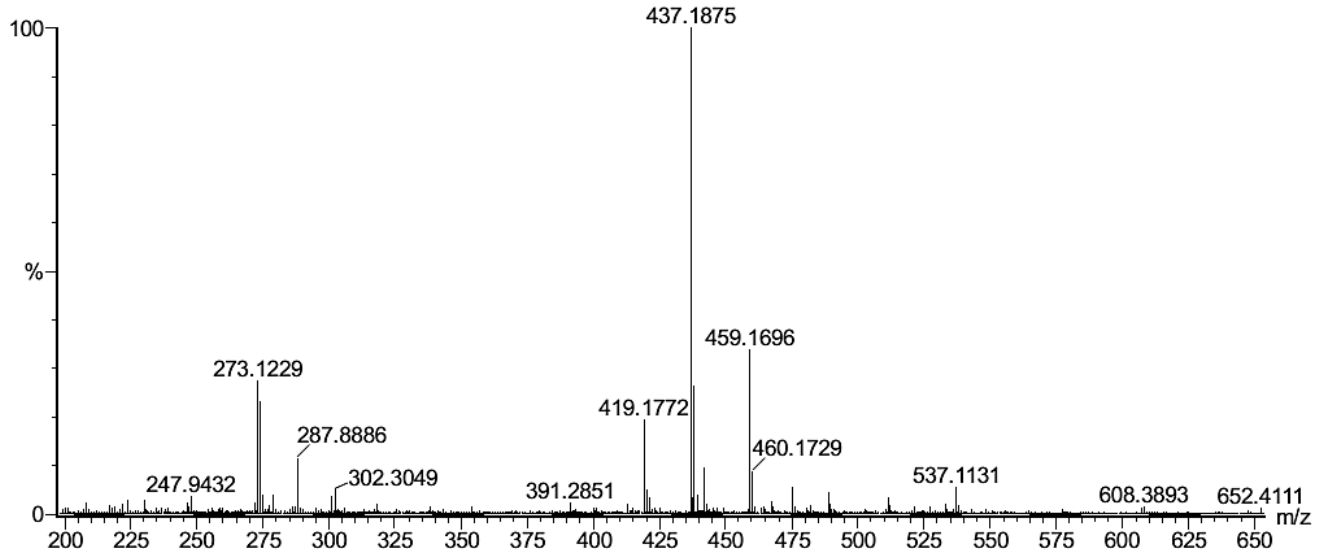
Elemental Composition Report

Single Mass Analysis

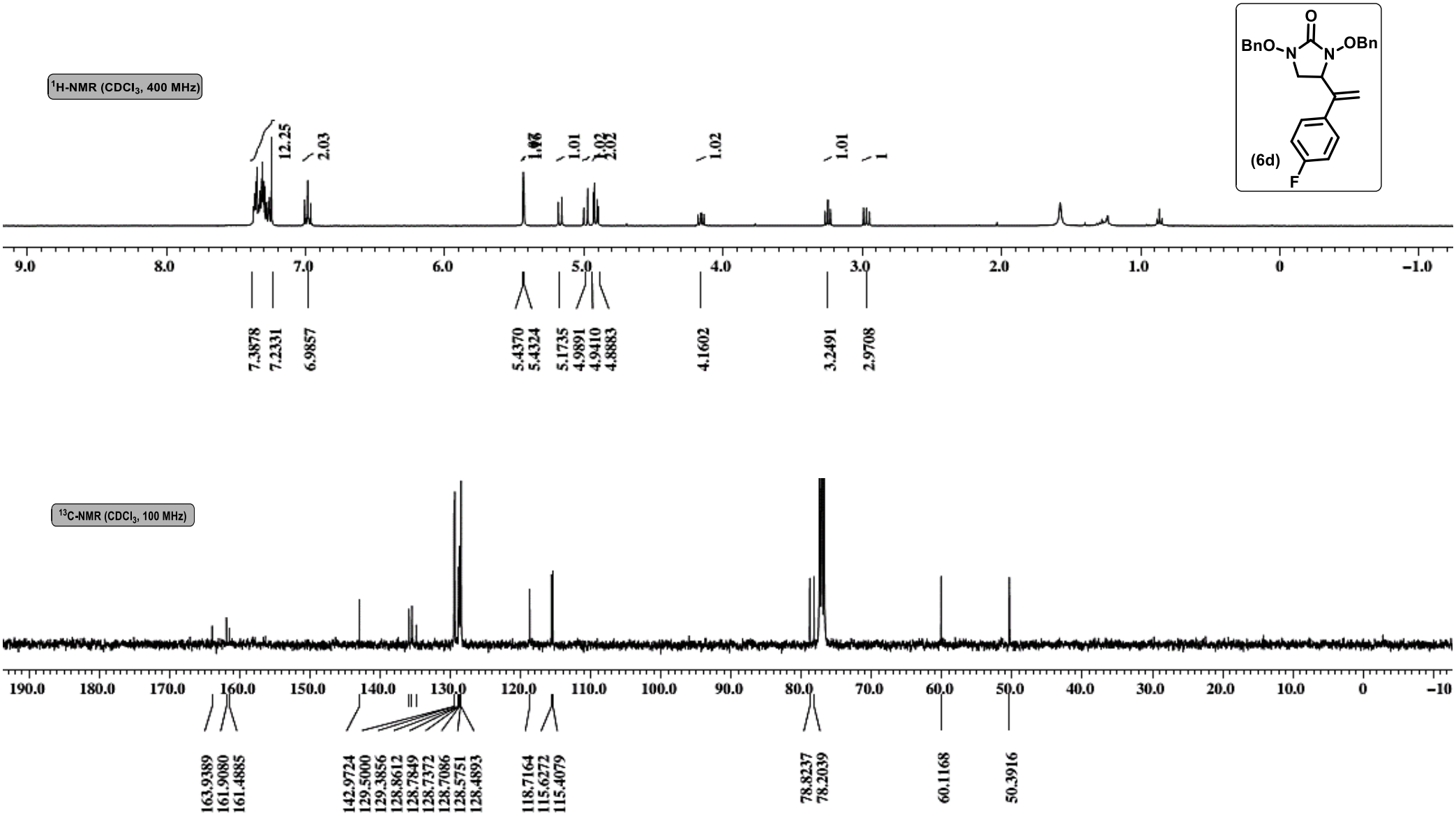
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

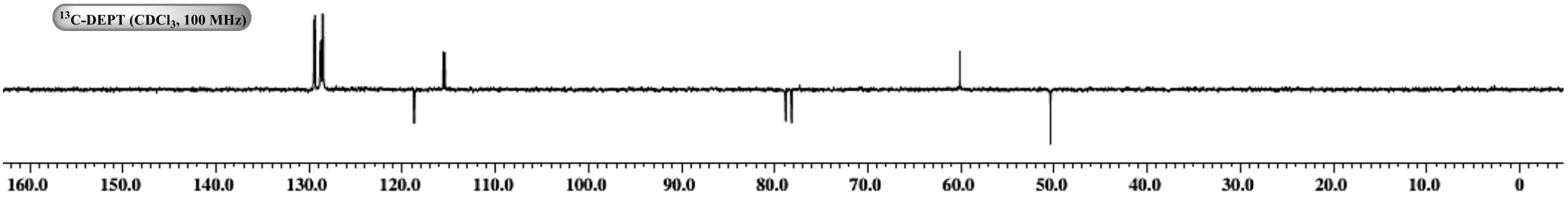
Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 11-25 H: 8-30 N: 0-3 O: 1-4 F: 0-1

Sample Name : 15-02-16 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
260819-15-02-16 18 (0.183) AM2 (Ar,22000.0,0.00,0.00); Cm (18:21) 1: TOF MS ES+
6.92e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
437.1875	437.1877	-0.2	-0.5	13.5	693.4	n/a	n/a	C25 H26 N2 O4 F


^{1}H-NMR (CDCl$_3$, 400 MHz)
12.25
2.03
1.01
1.02
1.01
1
7.3878
7.2331
6.9857
5.4370
5.4324
5.1735
4.9891
4.9410
4.8883
4.1602
3.2491
2.9708
BnO
N
O
N
OBn
(6d)
F
^{13}C-NMR (CDCl$_3$, 100 MHz)
163.9389
161.9080
161.4885
142.9724
129.5000
129.3856
128.8612
128.7849
128.7372
128.7086
128.5751
128.4893
118.7164
115.6272
115.4079
78.8237
78.2039
60.1168
50.3916


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

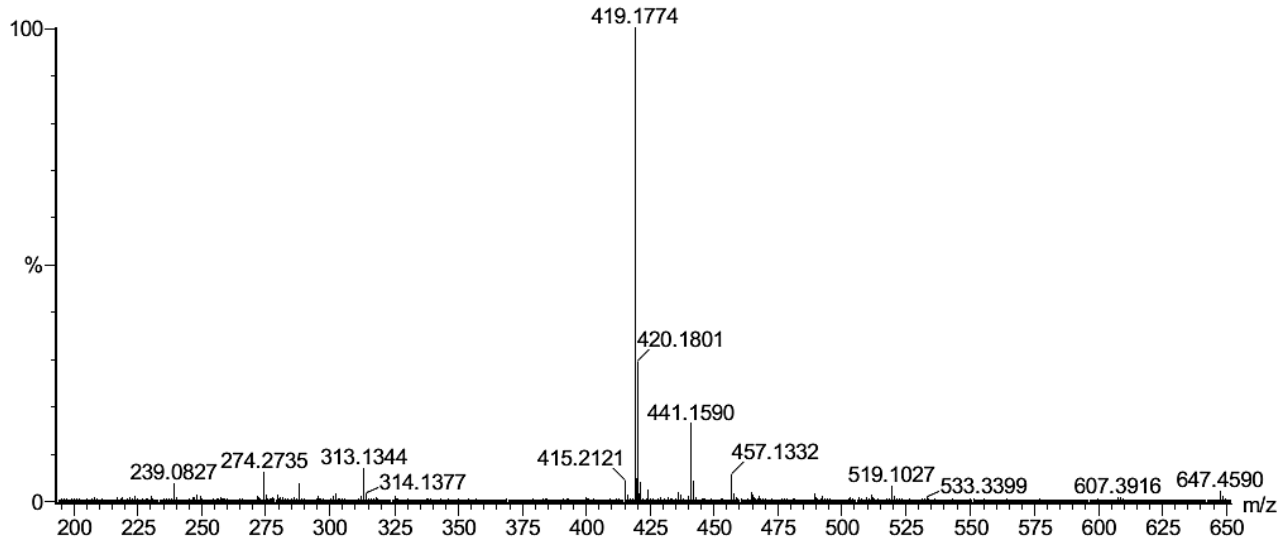
Elemental Composition Report

Single Mass Analysis

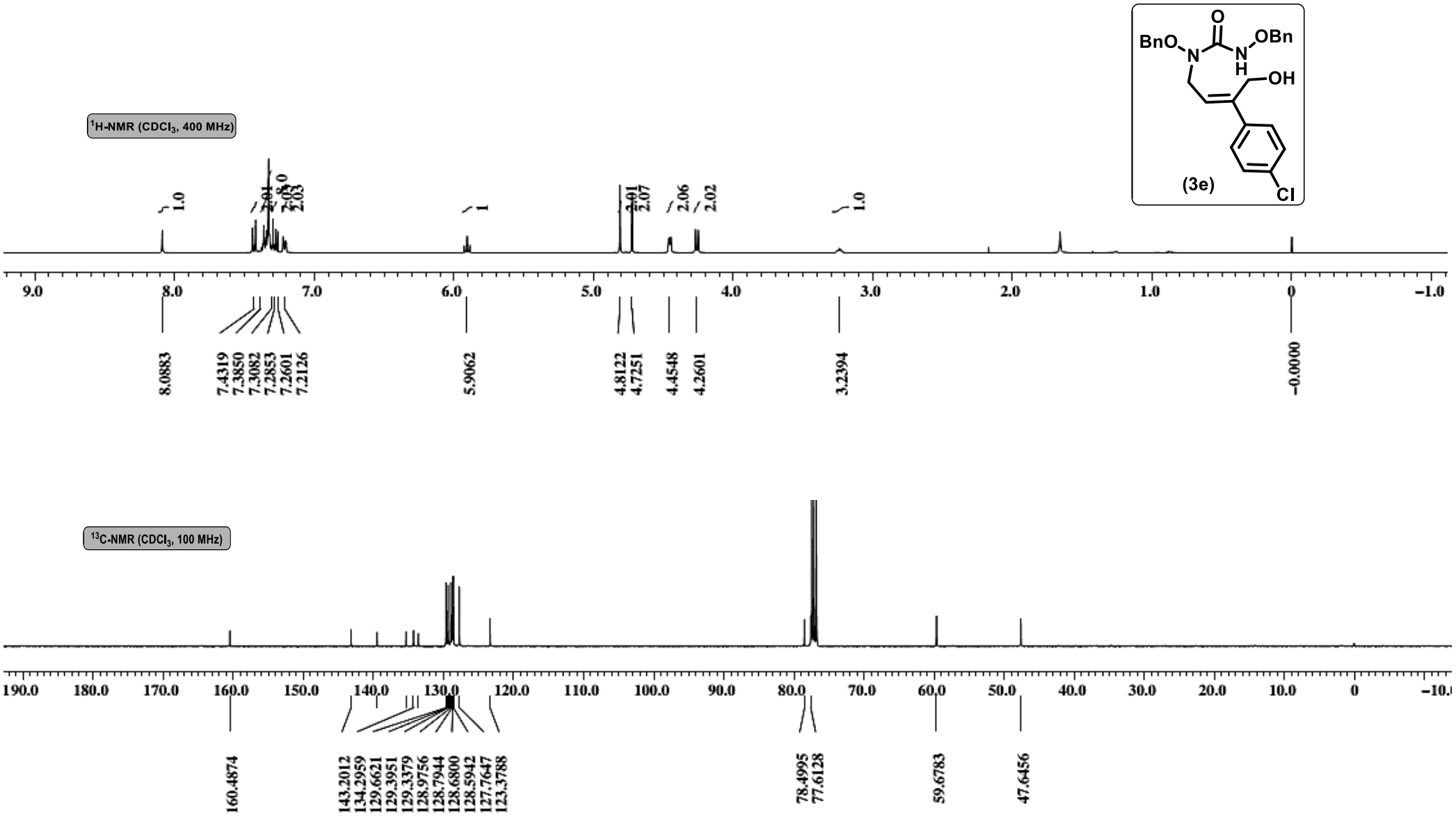
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

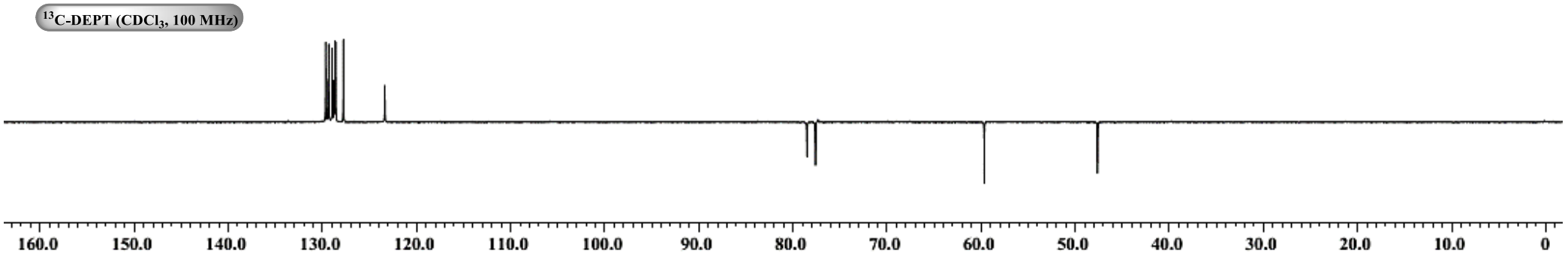
Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 11-25 H: 8-25 N: 0-3 O: 1-3 F: 0-1

Sample Name : 15-02-23 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
260819-15-02-23 17 (0.174) AM2 (Ar,22000.0,0.00,0.00); Cm (17:20) 1: TOF MS ES+
2.27e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
419.1774	419.1771	0.3	0.7	14.5	871.0	n/a	n/a	C25 H24 N2 O3 F


^{1}H-NMR ($CDCl_3$, 400 MHz)
BnO
N
O
N
H
OBn
OH
Cl
(3e)
1.0
2.01
2.00
2.08
2.03
1
2.01
2.07
2.06
2.02
1.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.0883
7.4319
7.3850
7.3082
7.2853
7.2601
7.2126
5.9062
4.8122
4.7251
4.4548
4.2601
3.2394
−0.0000
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
160.4874
143.2012
134.2959
129.6621
129.3951
129.3379
128.9756
128.7944
128.6800
128.5942
127.7647
123.3788
78.4995
77.6128
59.6783
47.6456


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

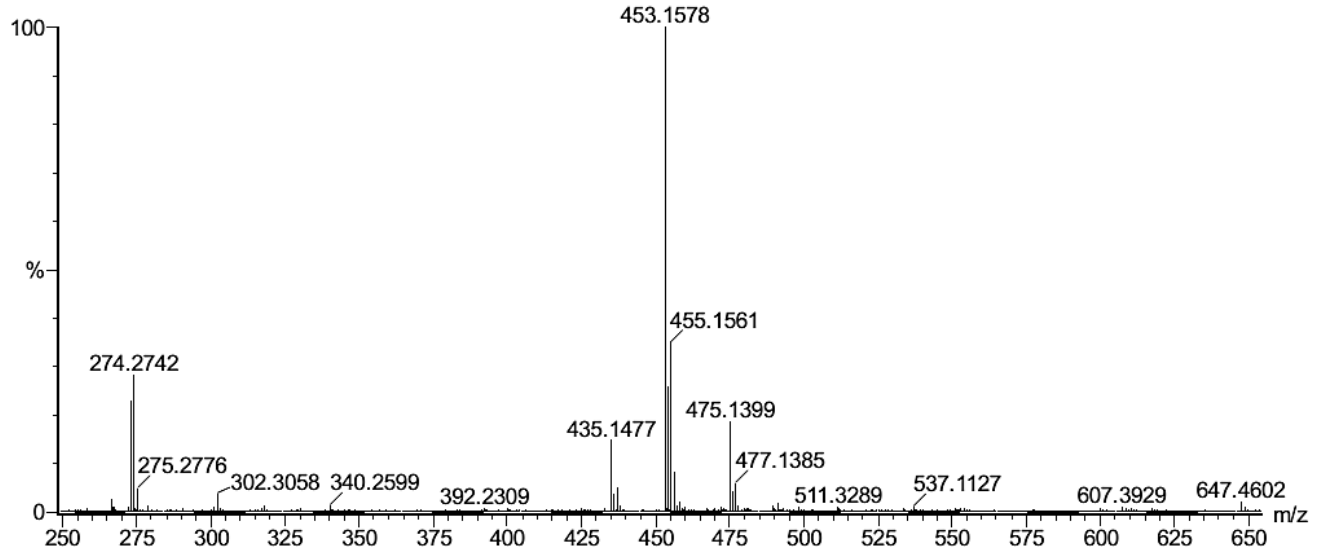
Elemental Composition Report

Single Mass Analysis

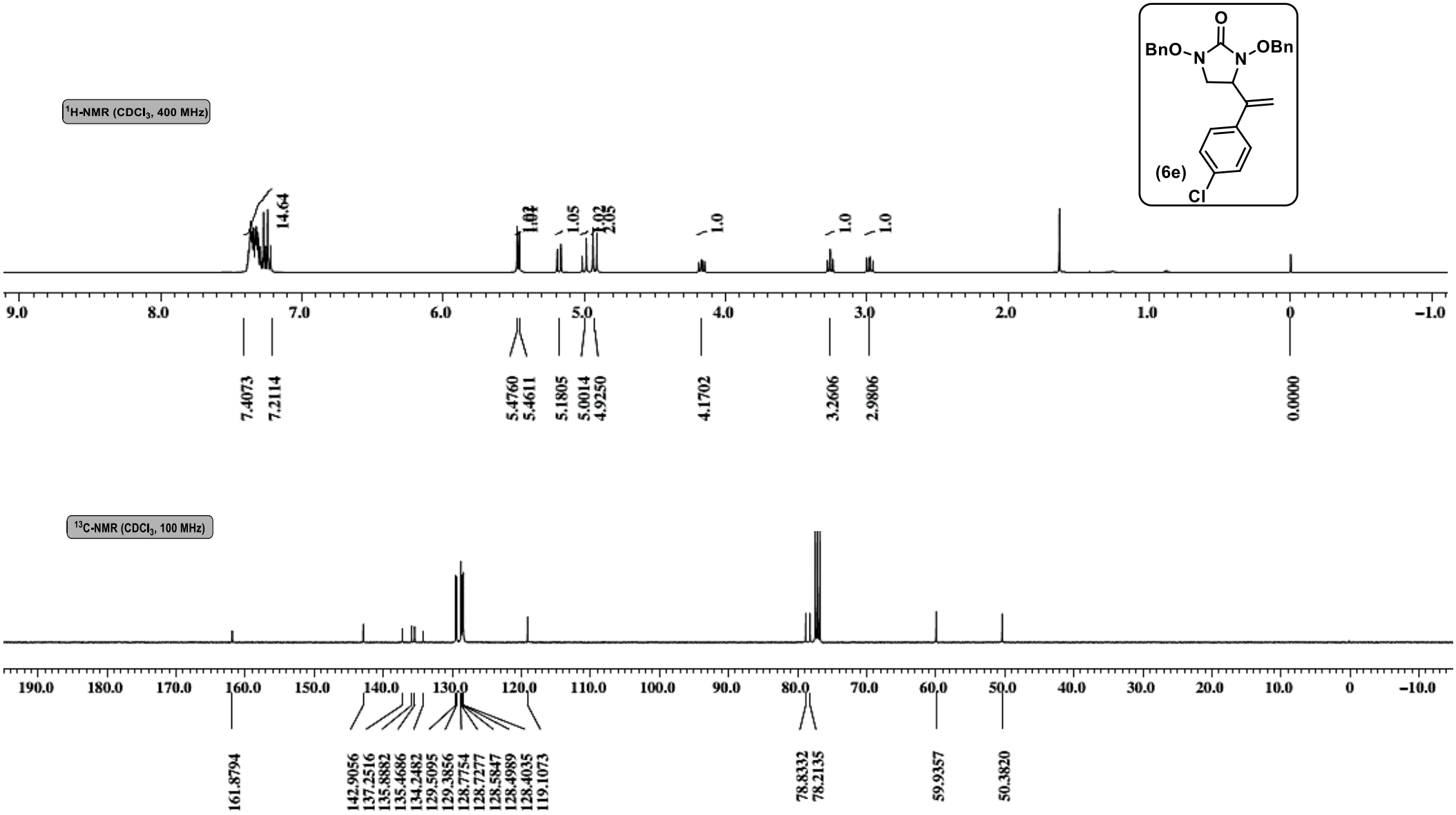
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

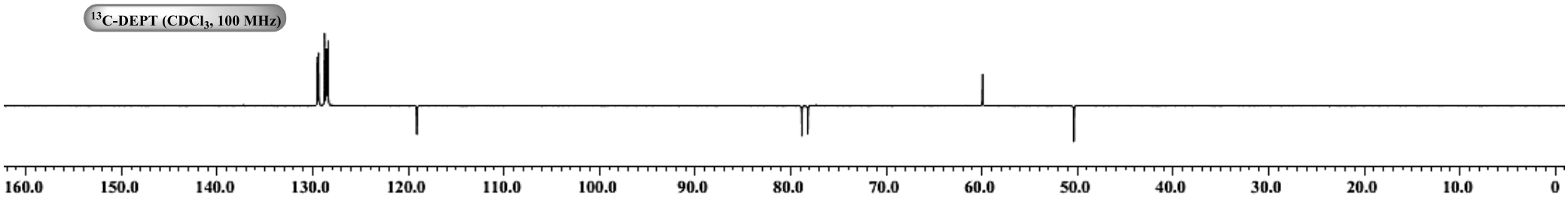
Monoisotopic Mass, Even Electron Ions
78 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 11-35 N: 0-3 O: 1-6 Cl: 0-1

Sample Name : 15-2-59 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
270919-15-2-59 19 (0.203) AM2 (Ar,22000.0,0.00,0.00); Cm (19:23) 1: TOF MS ES+
1.19e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
453.1578	453.1581	-0.3	-0.7	13.5	646.0	n/a	n/a	C25 H26 N2 O4 Cl


^{1}H-NMR ($CDCl_3$, 400 MHz)
BnO
N
O
N
OBn
(6e)
Cl
14.64
1.04
1.05
2.02
2.05
1.0
1.0
1.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.4073
7.2114
5.4760
5.4611
5.1805
5.0014
4.9250
4.1702
3.2606
2.9806
0.0000
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
161.8794
142.9056
137.2516
135.8882
135.4686
134.2482
129.5095
129.3856
128.7754
128.7277
128.5847
128.4989
128.4035
119.1073
78.8332
78.2135
59.9357
50.3820

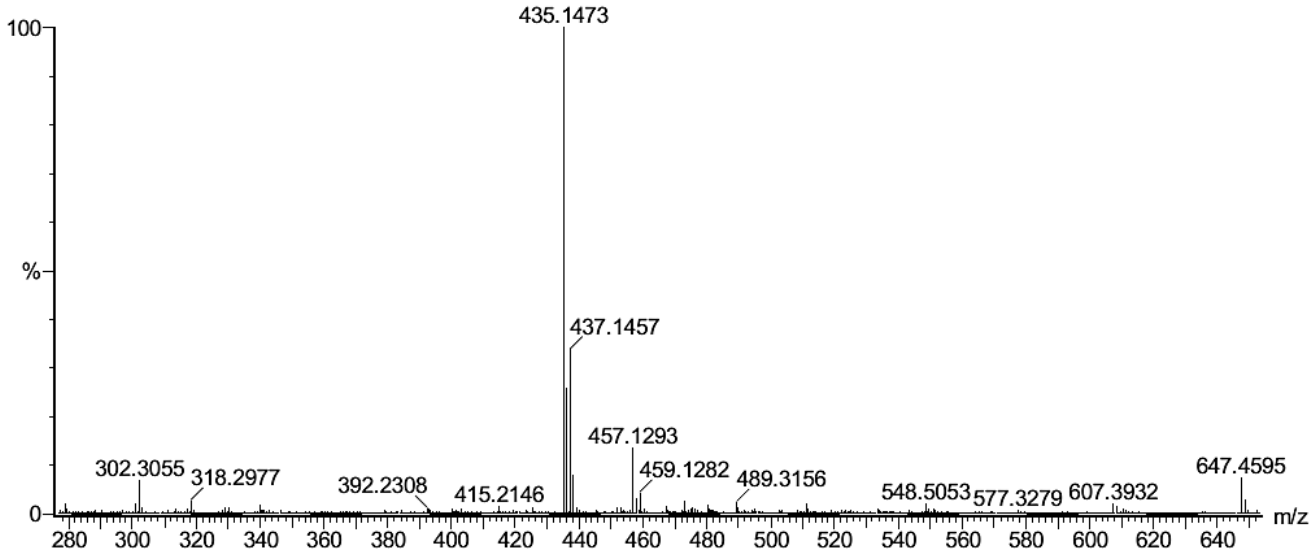

^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Single Mass Analysis

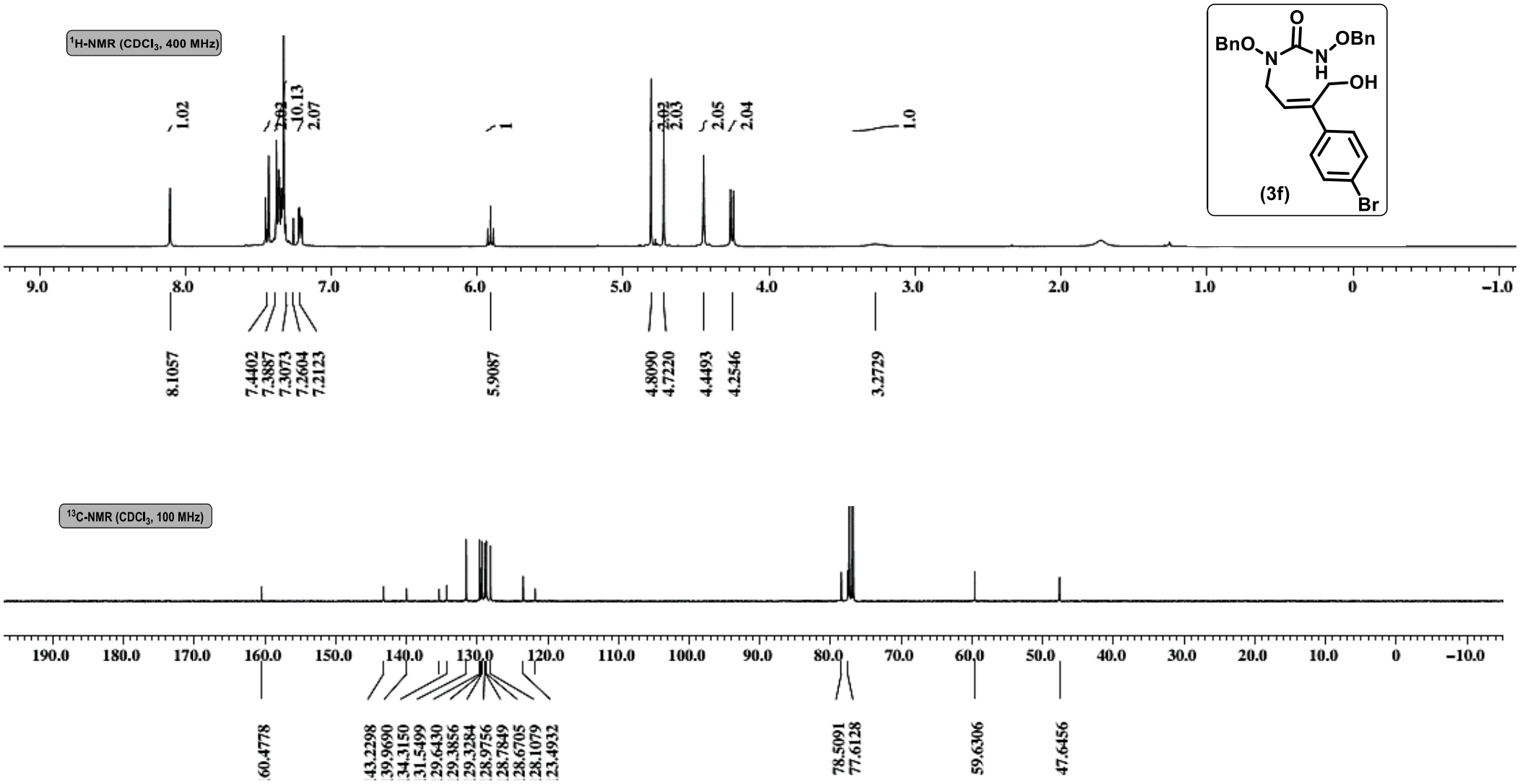
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

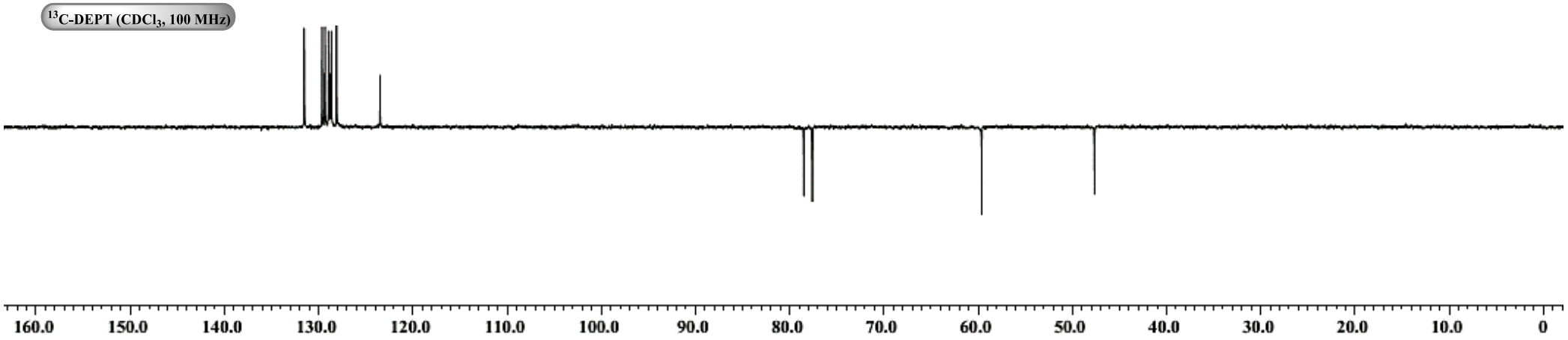
Monoisotopic Mass, Even Electron Ions
89 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 11-35 N: 0-3 O: 1-6 Cl: 0-1

Sample Name : 15-2-61 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
270919-15-2-61 19 (0.203) AM2 (Ar,22000.0,0.00,0.00); Cm (19:24) 1: TOF MS ES+
7.62e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
435.1473	435.1475	-0.2	-0.5	14.5	660.6	n/a	n/a	C25 H24 N2 O3 Cl


^{1}H-NMR ($CDCl_3$, 400 MHz)
1.02
2.03
10.13
2.07
1
3.02
2.03
2.05
2.04
1.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.1057
7.4402
7.3887
7.3073
7.2604
7.2123
5.9087
4.8090
4.7220
4.4493
4.2546
3.2729
BnO
N
O
N
H
OBn
OH
Br
(3f)
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
60.4778
43.2298
39.9690
34.3150
31.5499
29.6430
29.3856
29.3284
28.9756
28.7849
28.6705
28.1079
23.4932
78.5091
77.6128
59.6306
47.6456


^{13}C-DEPT (CDCl$_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

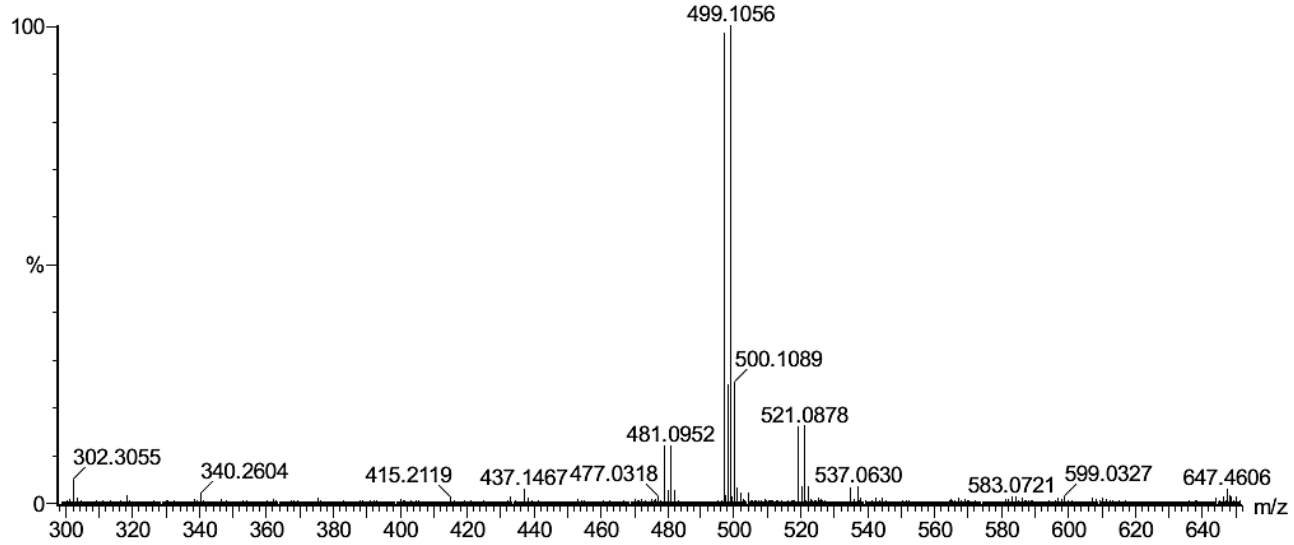
Elemental Composition Report

Single Mass Analysis

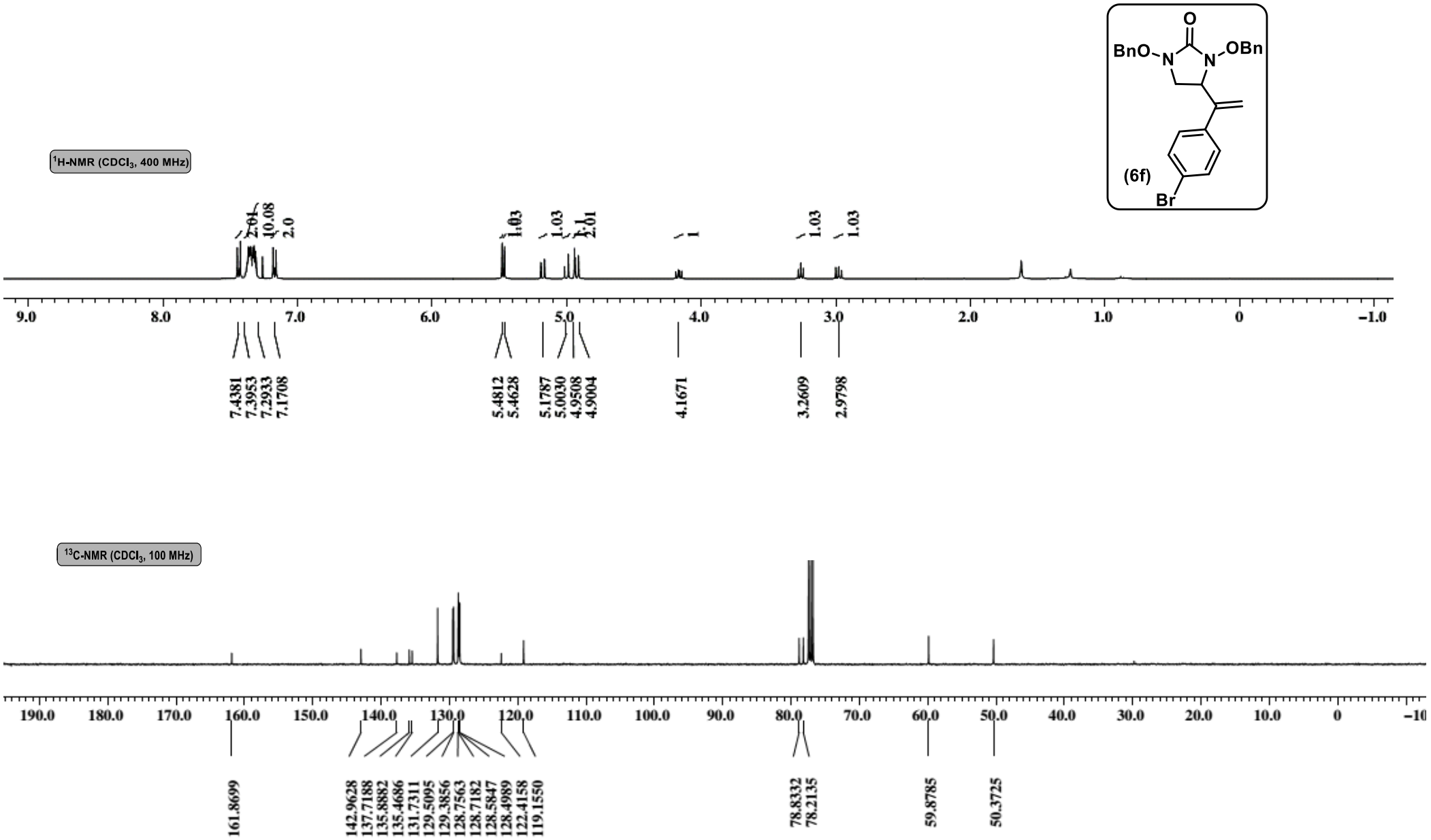
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

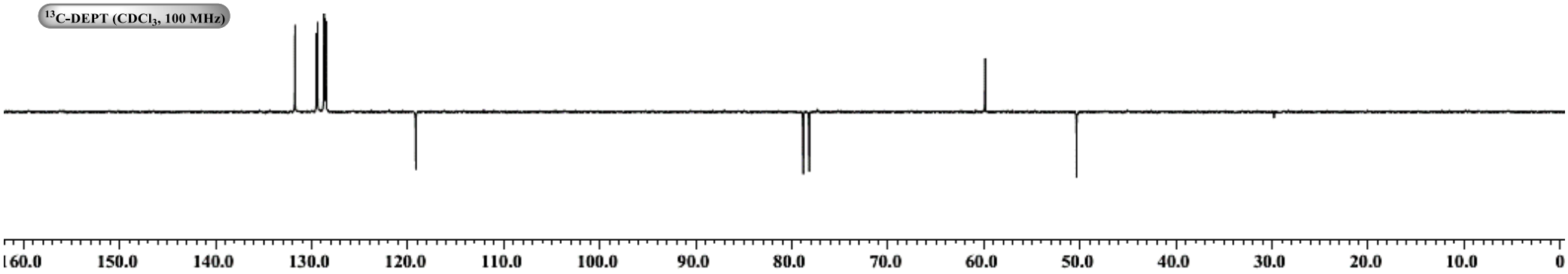
Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 5-30 H: 5-30 N: 0-3 O: 1-4 Br: 0-1

Sample Name : 15-02-36 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
060919-15-02-36 19 (0.203) AM2 (Ar,22000.0,0.00,0.00); Cm (19:21) 1: TOF MS ES+
5.43e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
497.1072	497.1076	-0.4	-0.8	13.5	628.7	n/a	n/a	C25 H26 N2 O4 Br


(6f)
BnO
OBn
Br
^{1}H-NMR (CDCl$_3$, 400 MHz)
2.04
10.08
2.0
1.03
1.03
2.01
1
1.03
1.03
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.4381
7.3953
7.2933
7.1708
5.4812
5.4628
5.1787
5.0030
4.9508
4.9004
4.1671
3.2609
2.9798
^{13}C-NMR (CDCl$_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.8699
142.9628
137.7188
135.8882
135.4686
131.7311
129.5095
129.3856
128.7563
128.7182
128.5847
128.4989
122.4158
119.1550
78.8332
78.2135
59.8785
50.3725


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

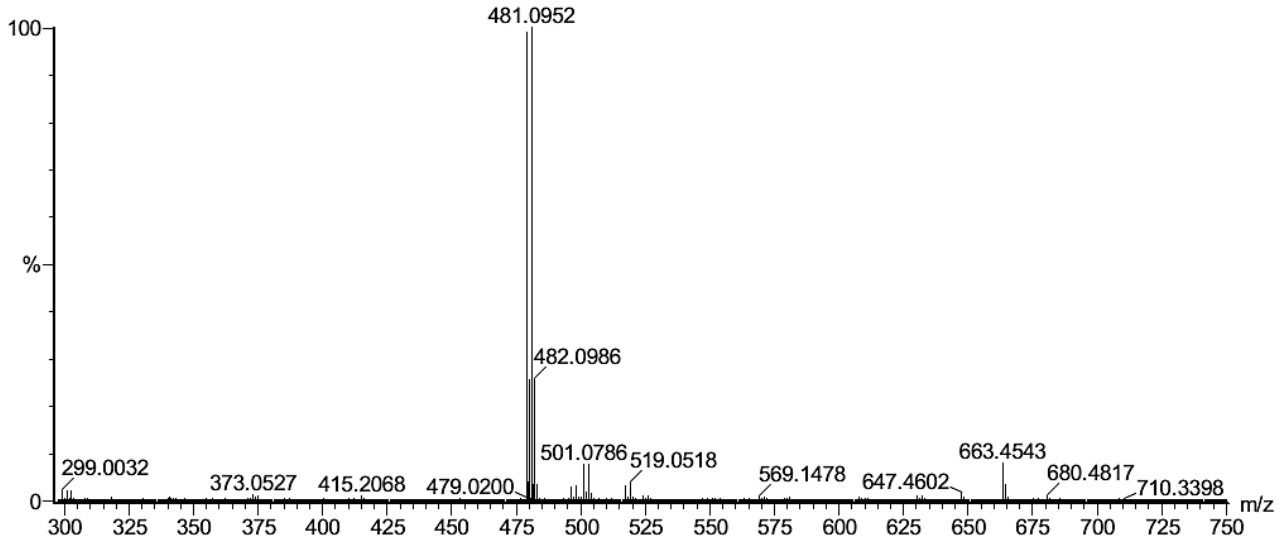
Elemental Composition Report

Single Mass Analysis

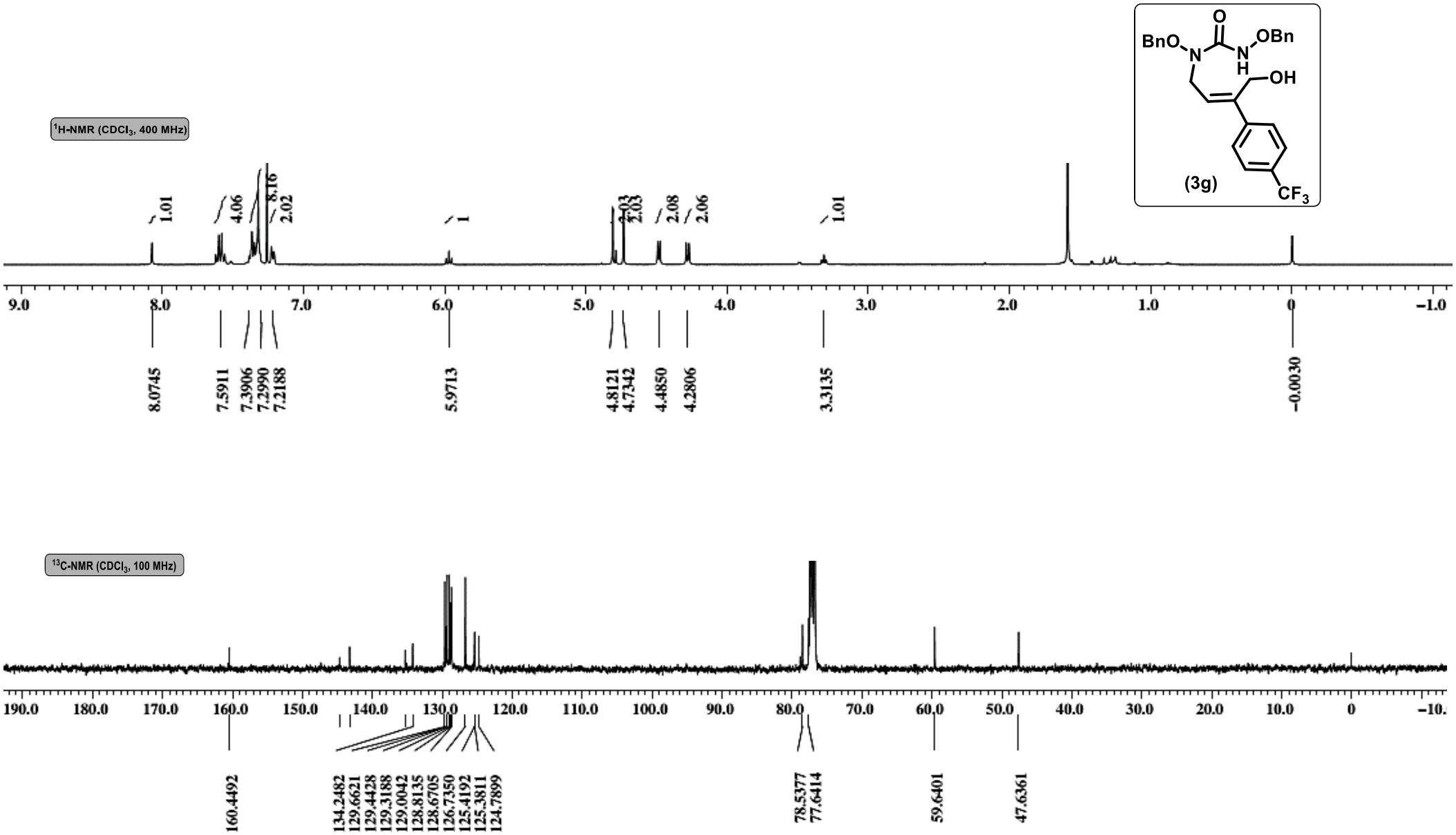
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

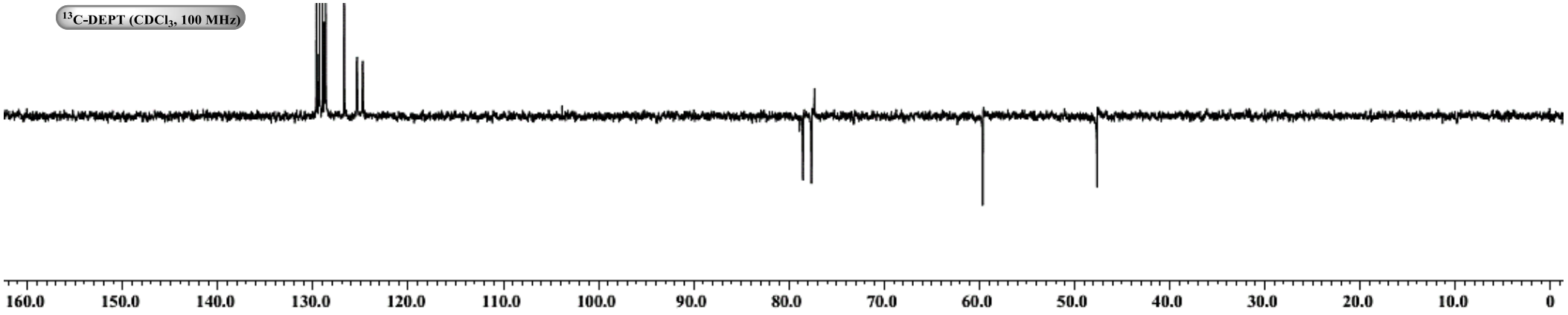
Monoisotopic Mass, Even Electron Ions
42 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 5-30 H: 5-30 N: 0-3 O: 1-4 Br: 0-1

Sample Name : 15-02-40 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
060919-15-02-40 19 (0.203) AM2 (Ar,22000.0,0.00,0.00); Cm (19:21) 1: TOF MS ES+
1.49e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
479.0969	479.0970	-0.1	-0.2	14.5	713.4	n/a	n/a	C25 H24 N2 O3 Br


^{1}H-NMR ($CDCl_3$, 400 MHz)
BnO
N
O
N
H
OBn
OH
(3g)
CF_3
1.01
4.06
8.16
2.02
1
2.03
2.03
2.08
2.06
1.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.0745
7.5911
7.3906
7.2990
7.2188
5.9713
4.8121
4.7342
4.4850
4.2806
3.3135
−0.0030
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
160.4492
134.2482
129.6621
129.4428
129.3188
129.0042
128.8135
128.6705
126.7350
125.4192
125.3811
124.7899
78.5377
77.6414
59.6401
47.6361

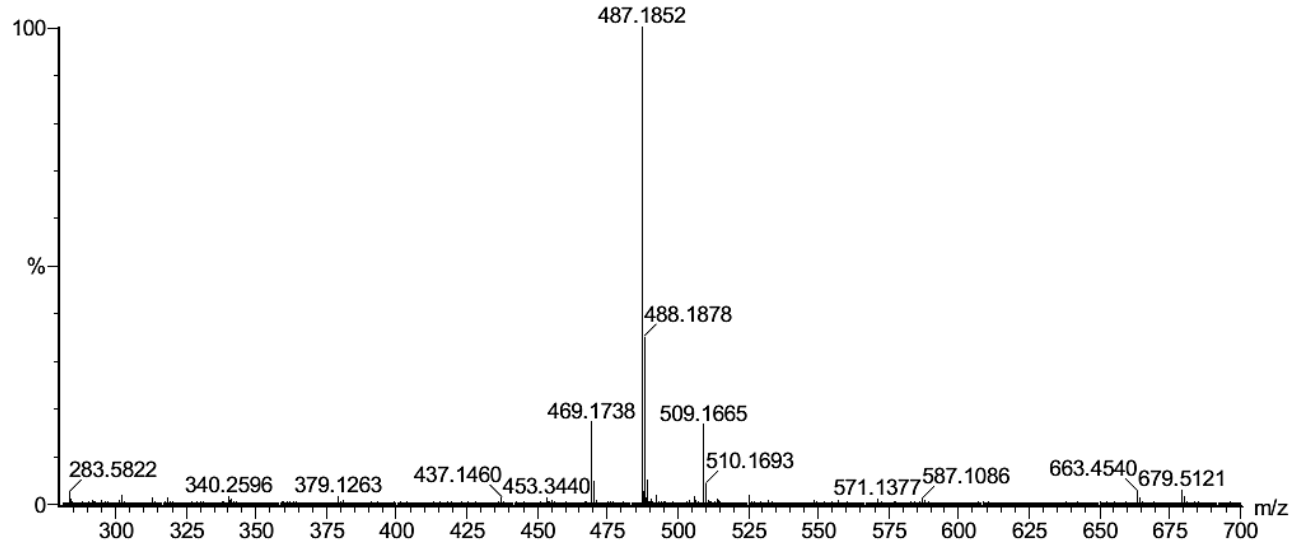

^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Single Mass Analysis

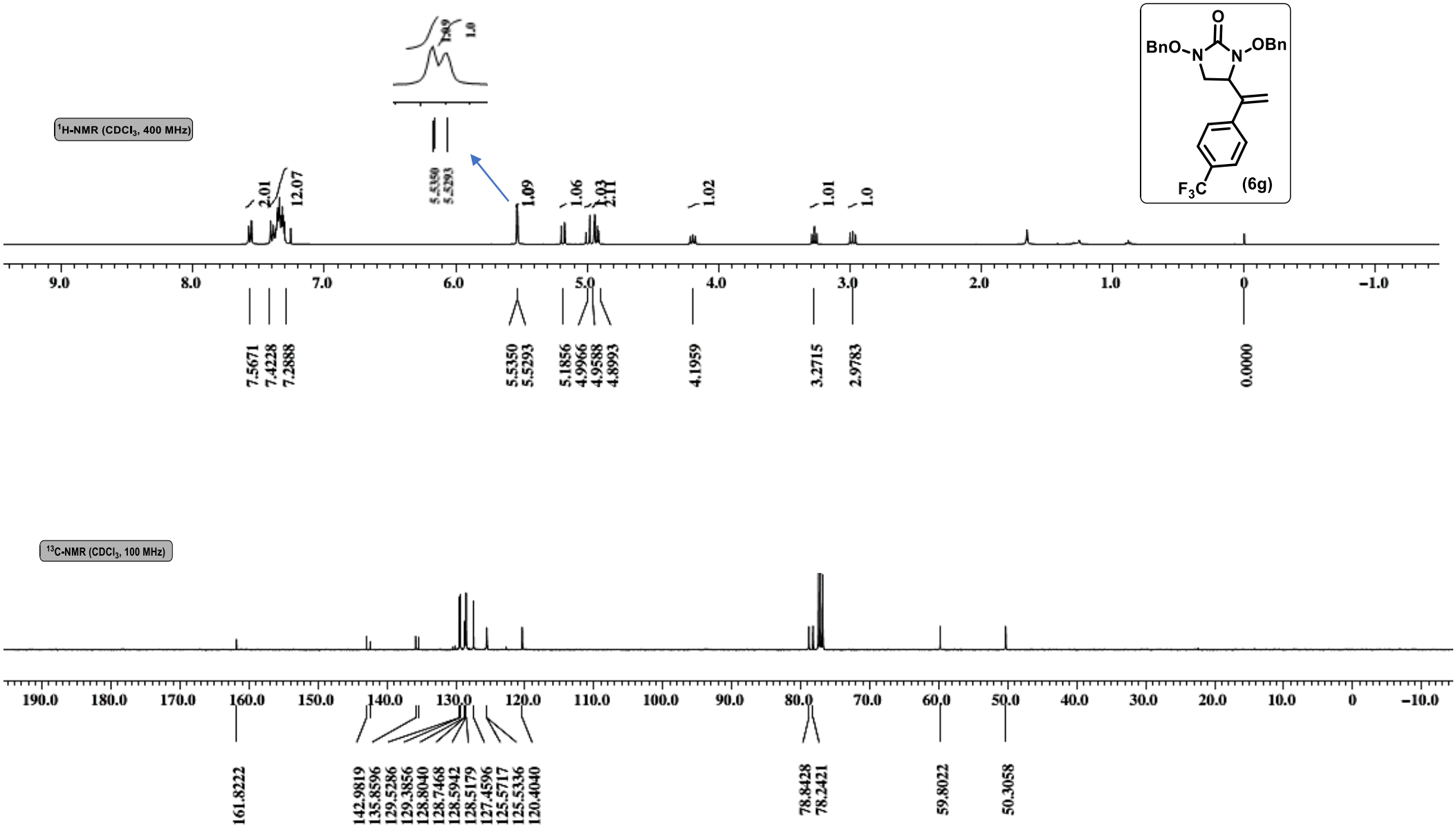
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

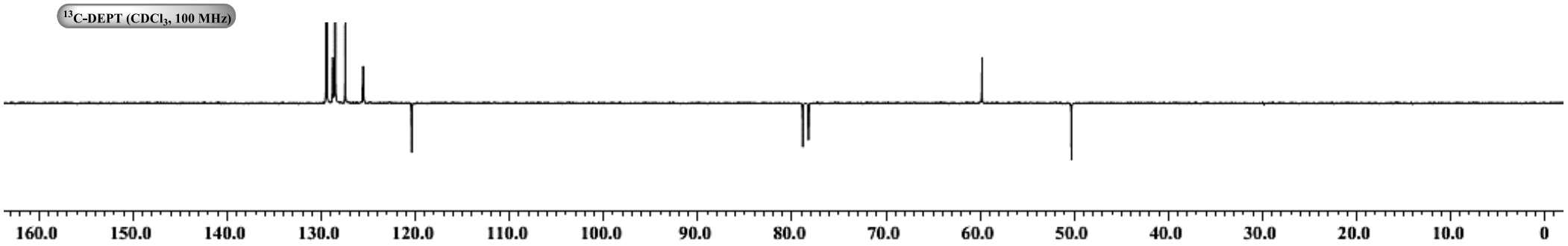
Monoisotopic Mass, Even Electron Ions
38 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-28 H: 11-30 N: 0-3 O: 1-4 F: 0-3

Sample Name : 15-02-66 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
141019-15-02-66- 17 (0.174) AM (Cen,4, 85.00, Ar,10000.0,0.00,0.00); Cm (17:21) 1: TOF MS ES+
2.98e+007



Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
487.1852	487.1845	0.7	1.4	13.5	1022.2	n/a	n/a	C26 H26 N2 O4 F3


^{1}H-NMR ($CDCl_3$, 400 MHz)
BnO
N
O
N
OBn
F_3C
(6g)
2.01
12.07
1.09
1.06
1.03
2.11
1.02
1.01
1.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.5671
7.4228
7.2888
5.5350
5.5293
5.1856
4.9966
4.9588
4.8993
4.1959
3.2715
2.9783
0.0000
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
161.8222
142.9819
135.8596
129.5286
129.3856
128.8040
128.7468
128.5942
128.5179
127.4596
125.5717
125.5336
120.4040
78.8428
78.2421
59.8022
50.3058


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

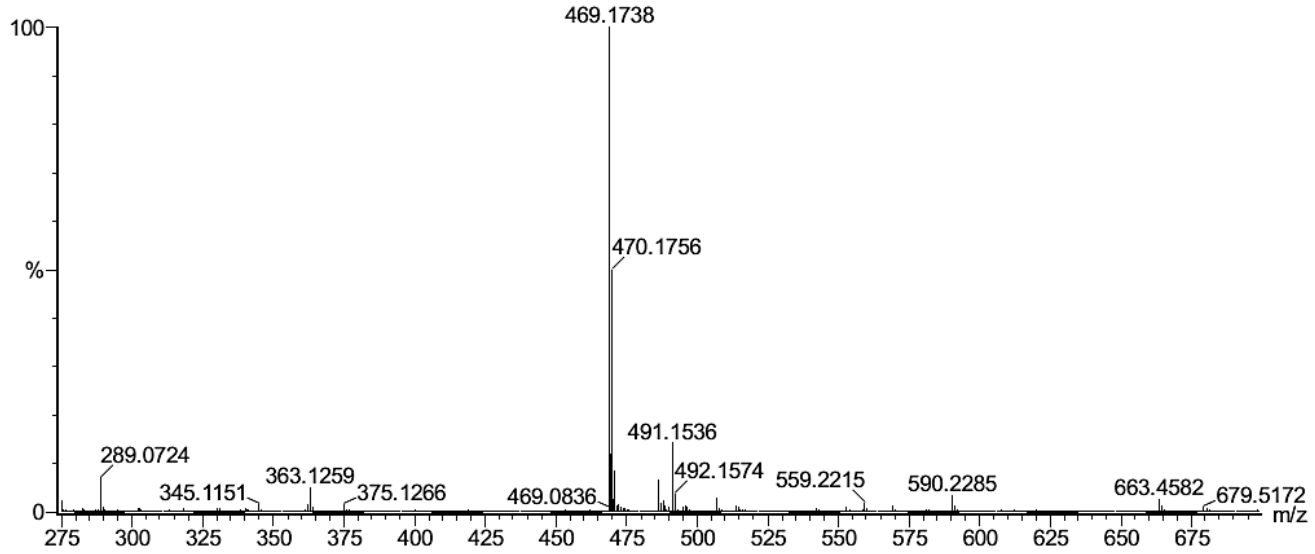
Elemental Composition Report

Single Mass Analysis

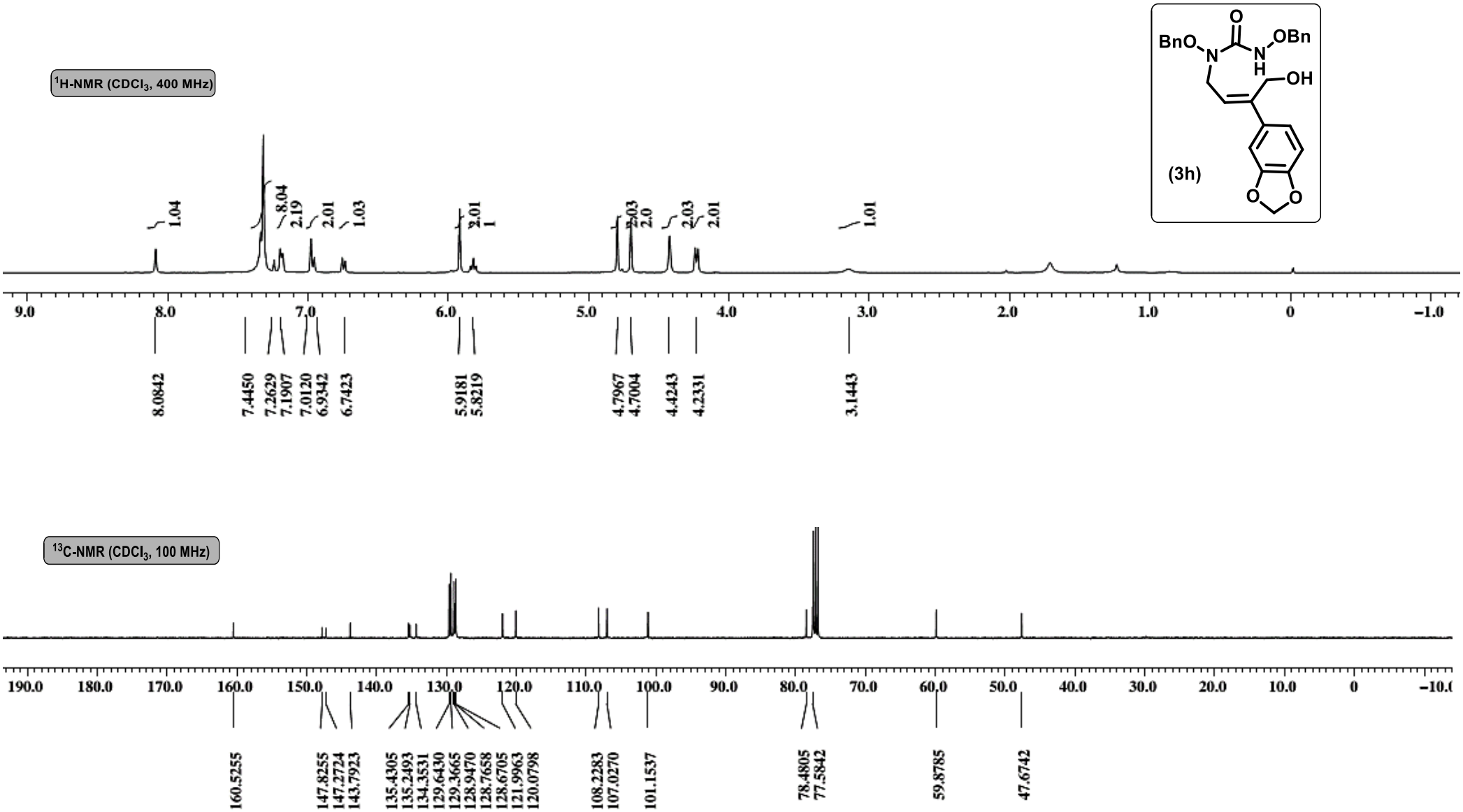
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

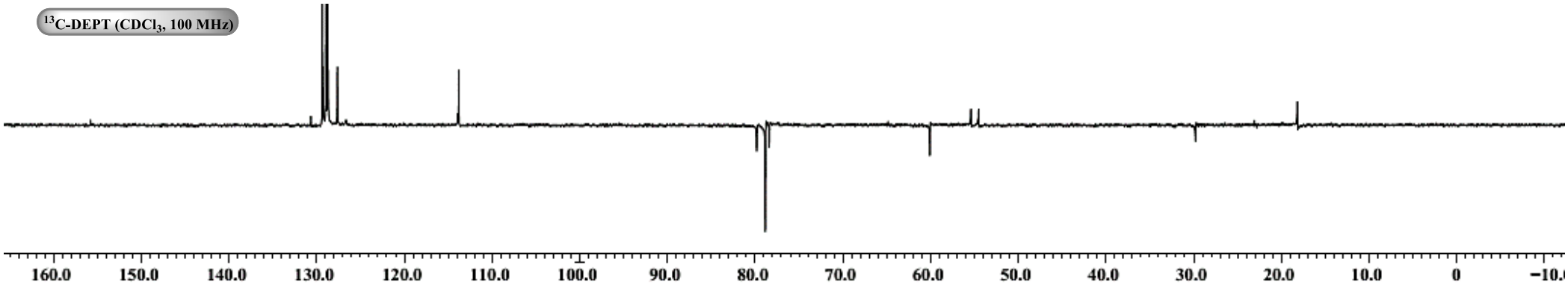
Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 25-28 H: 21-28 N: 0-3 O: 1-4 F: 0-3

Sample Name : 15-02-73 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
141019-15-02-73 18 (0.183) AM2 (Ar,22000.0,0.00,0.00); Cm (18:20) 1: TOF MS ES+
4.56e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
469.1738	469.1739	-0.1	-0.2	14.5	898.6	n/a	n/a	C26 H24 N2 O3 F3


^{1}H-NMR ($CDCl_3$, 400 MHz)
BnO
N
O
N
H
OBn
OH
(3h)
1.04
8.04
2.19
2.01
1.03
2.01
1
2.03
2.0
2.03
2.01
1.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.0842
7.4450
7.2629
7.1907
7.0120
6.9342
6.7423
5.9181
5.8219
4.7967
4.7004
4.4243
4.2331
3.1443
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
160.5255
147.8255
147.2724
143.7923
135.4305
135.2493
134.3531
129.6430
129.3665
128.9470
128.7658
128.6705
121.9963
120.0798
108.2283
107.0270
101.1537
78.4805
77.5842
59.8785
47.6742


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

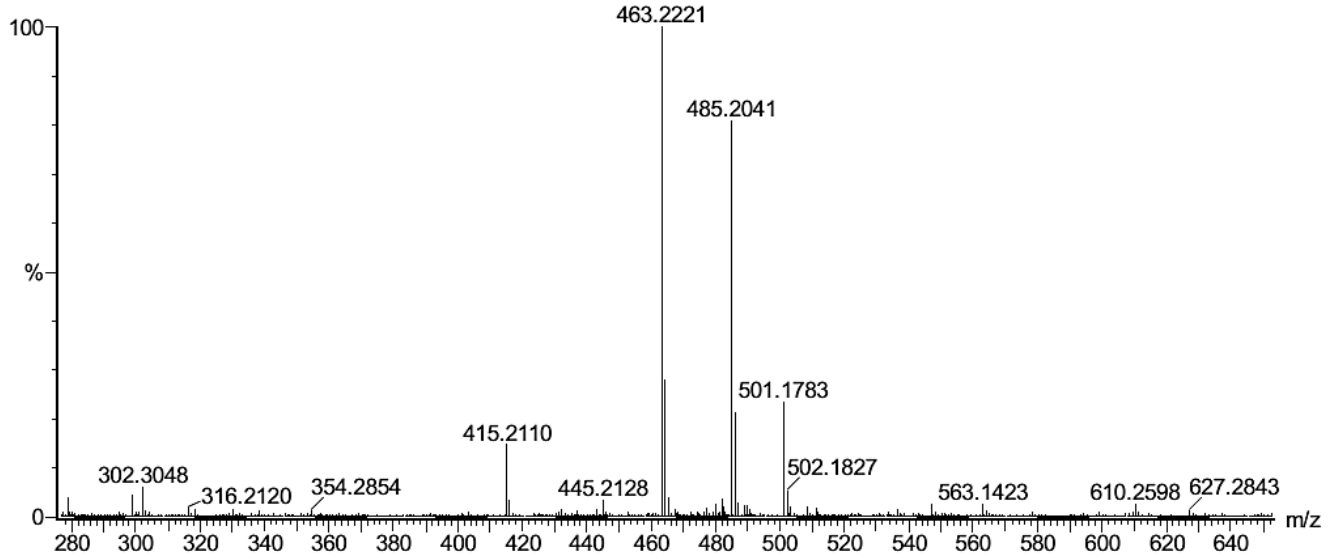
Elemental Composition Report

Single Mass Analysis

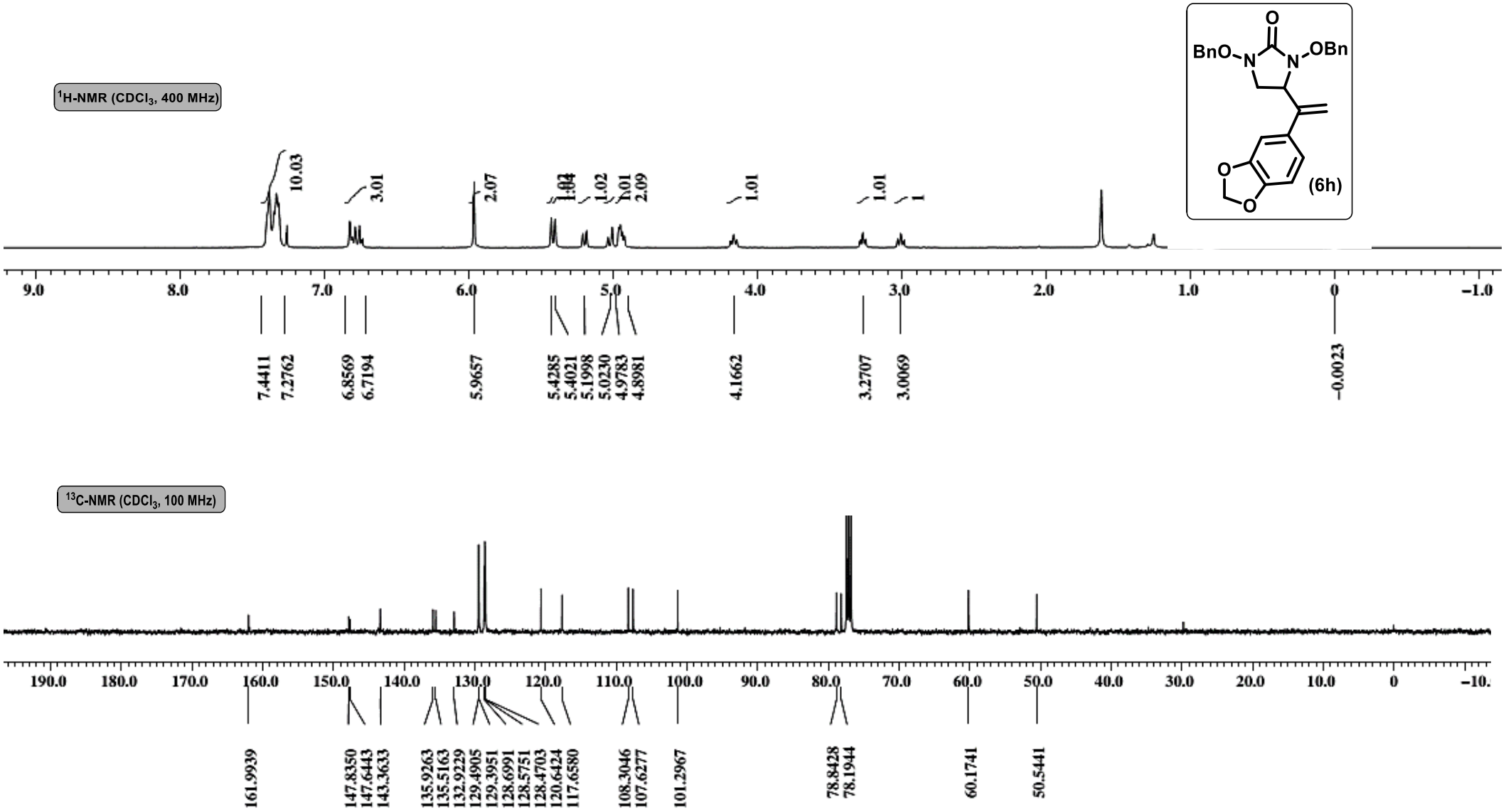
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

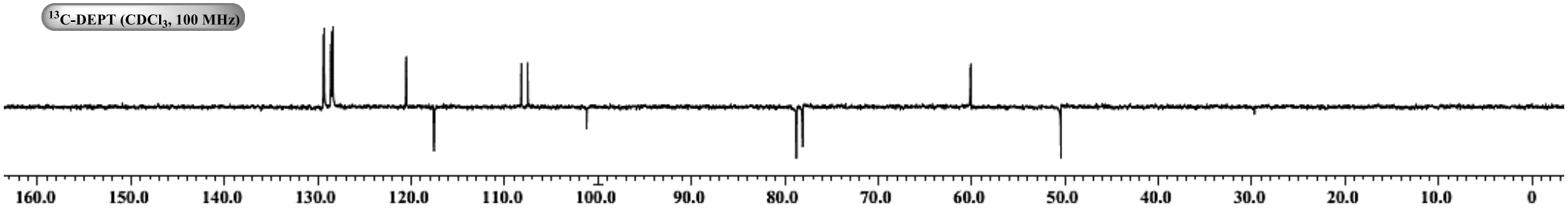
Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-30 H: 10-35 N: 0-4 O: 1-6

Sample Name : 15-02-86 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
161019-15-02-86 15 (0.157) AM2 (Ar,22000.0,0.00,0.00); Cm (15:19) 1: TOF MS ES+
4.04e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
463.2221	463.2233	-1.2	-2.6	13.5	567.9	n/a	n/a	C27 H31 N2 O5


^{1}H-NMR ($CDCl_3$, 400 MHz)
BnO
N
O
N
OBn
O
O
O
(6h)
10.03
3.01
2.07
1.02
2.09
1.01
1.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.4411
7.2762
6.8569
6.7194
5.9657
5.4285
5.4021
5.1998
5.0230
4.9783
4.8981
4.1662
3.2707
3.0069
−0.0023
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.9939
147.8350
147.6443
143.3633
135.9263
135.5163
132.9229
129.4905
129.3951
128.6991
128.5751
128.4703
120.6424
117.6580
108.3046
107.6277
101.2967
78.8428
78.1944
60.1741
50.5441

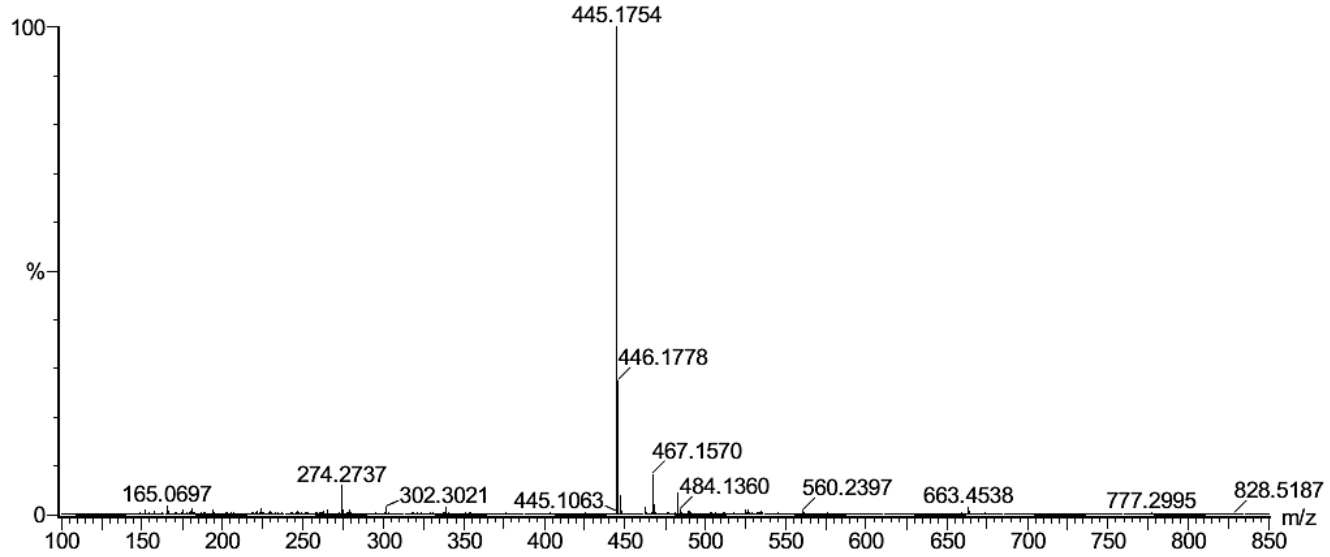

^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Single Mass Analysis

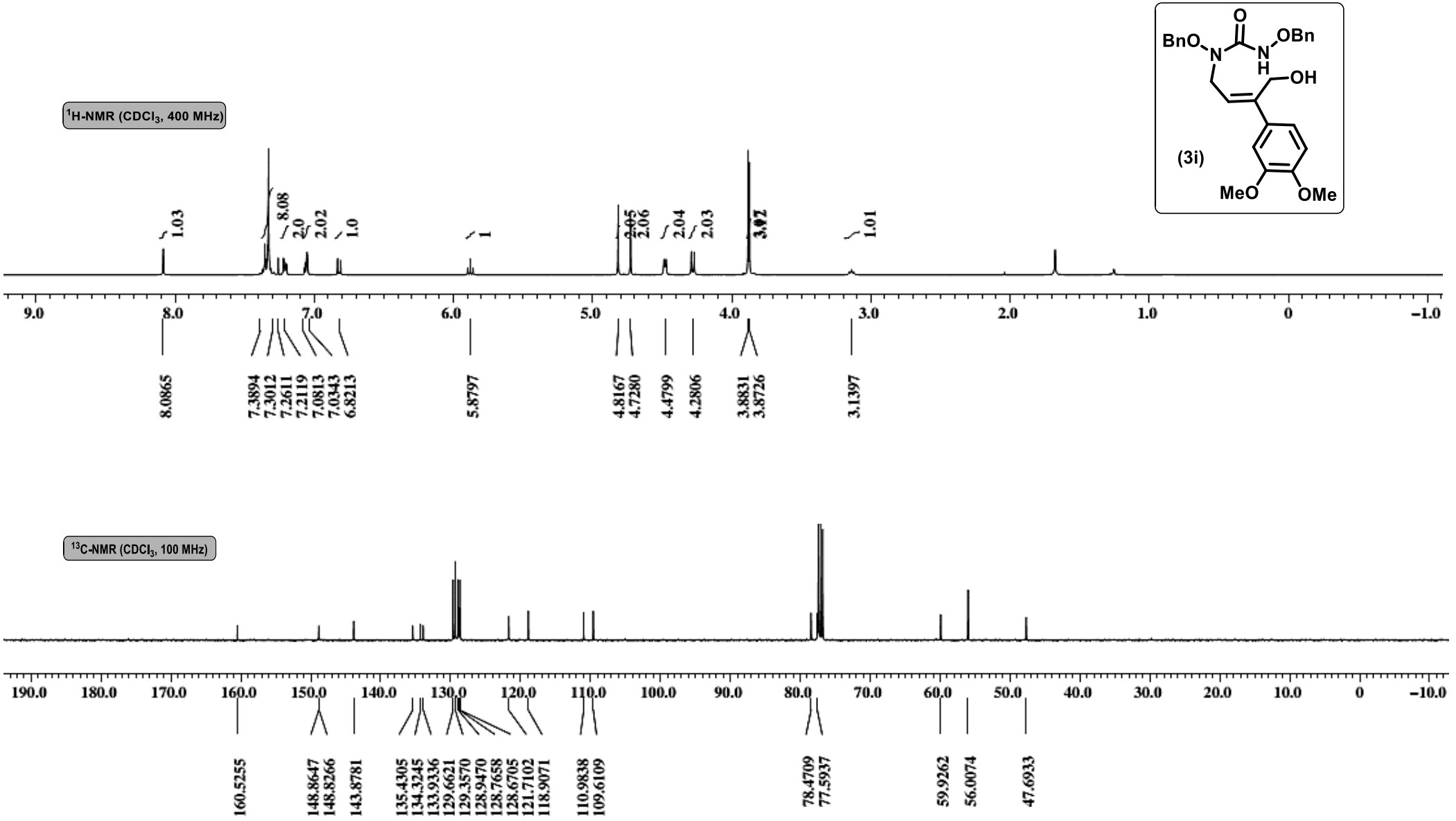
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

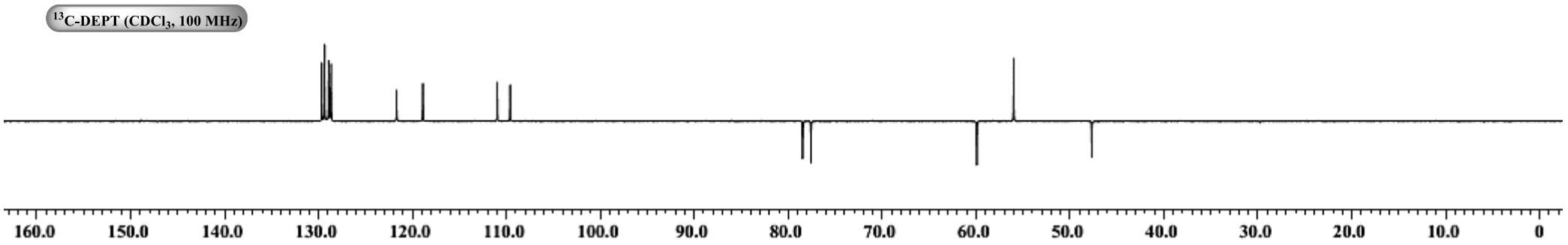
Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 20-35 H: 11-25 N: 0-4 O: 1-5

Sample Name : 15-02-83-A IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
181019-15-02-83-A 19 (0.203) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (19:22) 1: TOF MS ES+
1.47e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
445.1754	445.1763	-0.9	-2.0	15.5	765.0	n/a	n/a	C26 H25 N2 O5


^{1}H-NMR ($CDCl_3$, 400 MHz)
BnO
N
O
N
H
OBn
OH
MeO
OMe
(3i)
1.03
8.08
2.0
2.02
1.0
1
2.05
2.06
2.04
2.03
3.07
1.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.0865
7.3894
7.3012
7.2611
7.2119
7.0813
7.0343
6.8213
5.8797
4.8167
4.7280
4.4799
4.2806
3.8831
3.8726
3.1397
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
160.5255
148.8647
148.8266
143.8781
135.4305
134.3245
133.9336
129.6621
129.3570
128.9470
128.7658
128.6705
121.7102
118.9071
110.9838
109.6109
78.4709
77.5937
59.9262
56.0074
47.6933


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

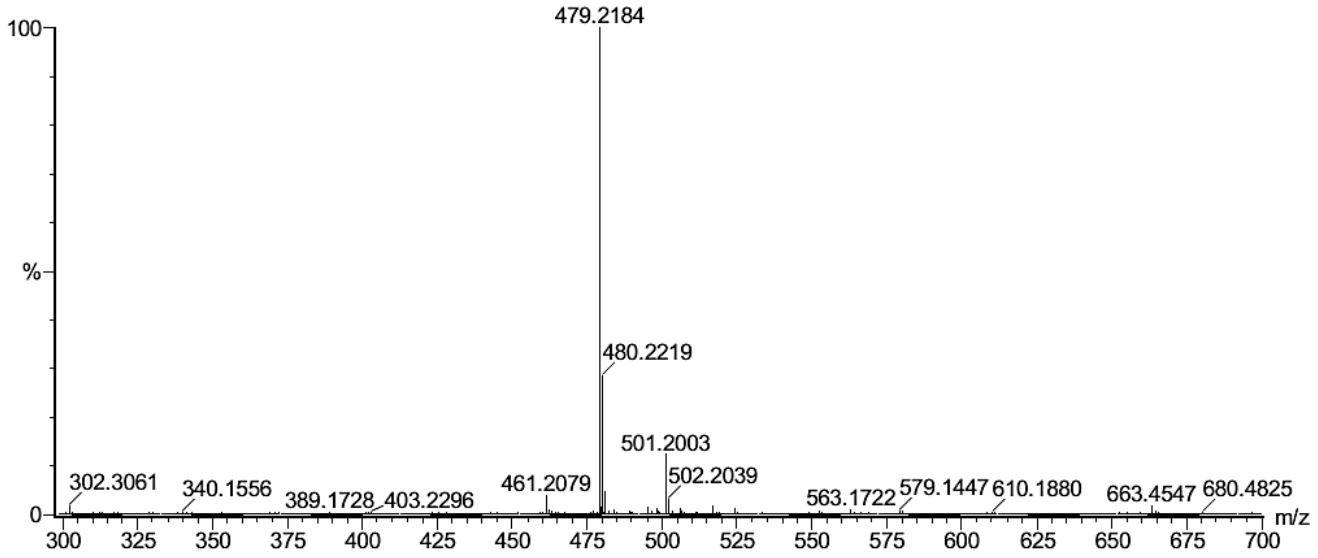
Elemental Composition Report

Single Mass Analysis

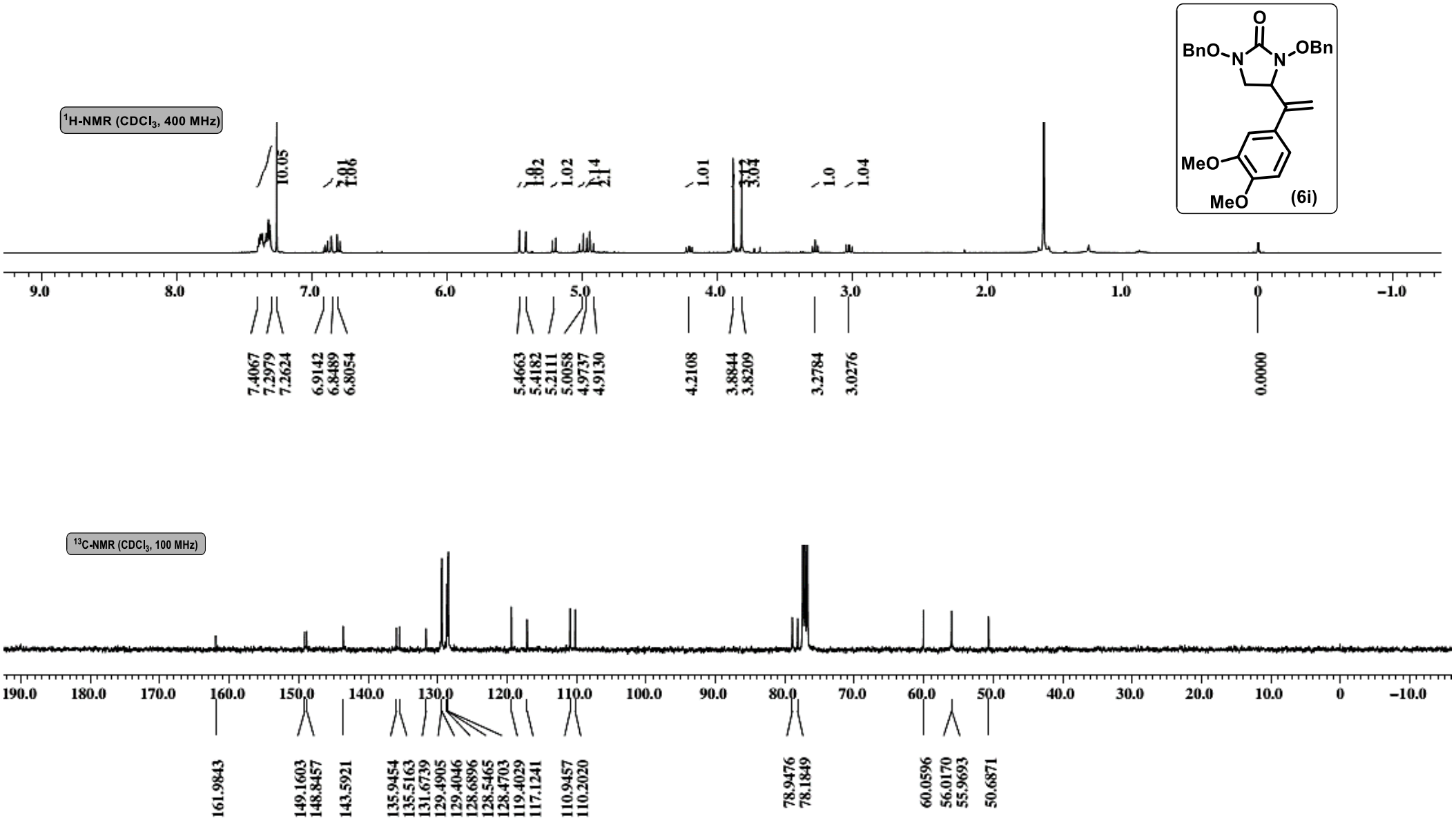
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

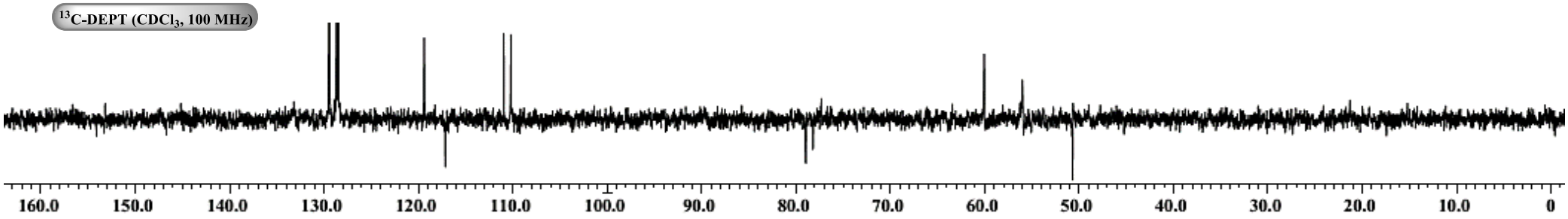
Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 11-35 N: 0-3 O: 1-6

Sample Name : 15-2-44 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
270919-15-2-44 19 (0.203) AM2 (Ar,22000.0,0.00,0.00); Cm (19:22) 1: TOF MS ES+
1.99e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
479.2184	479.2182	0.2	0.4	13.5	673.7	n/a	n/a	C27 H31 N2 O6


^{1}H-NMR (CDCl$_3$, 400 MHz)
BnO
N
O
N
OBn
MeO
MeO
(6i)
10.05
2.01
2.06
1.02
1.02
1.14
2.1
1.01
3.12
3.04
1.0
1.04
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.4067
7.2979
7.2624
6.9142
6.8489
6.8054
5.4663
5.4182
5.2111
5.0058
4.9737
4.9130
4.2108
3.8844
3.8209
3.2784
3.0276
0.0000
^{13}C-NMR (CDCl$_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
161.9843
149.1603
148.8457
143.5921
135.9454
135.5163
131.6739
129.4905
129.4046
128.6896
128.5465
128.4703
119.4029
117.1241
110.9457
110.2020
78.9476
78.1849
60.0596
56.0170
55.9693
50.6871


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

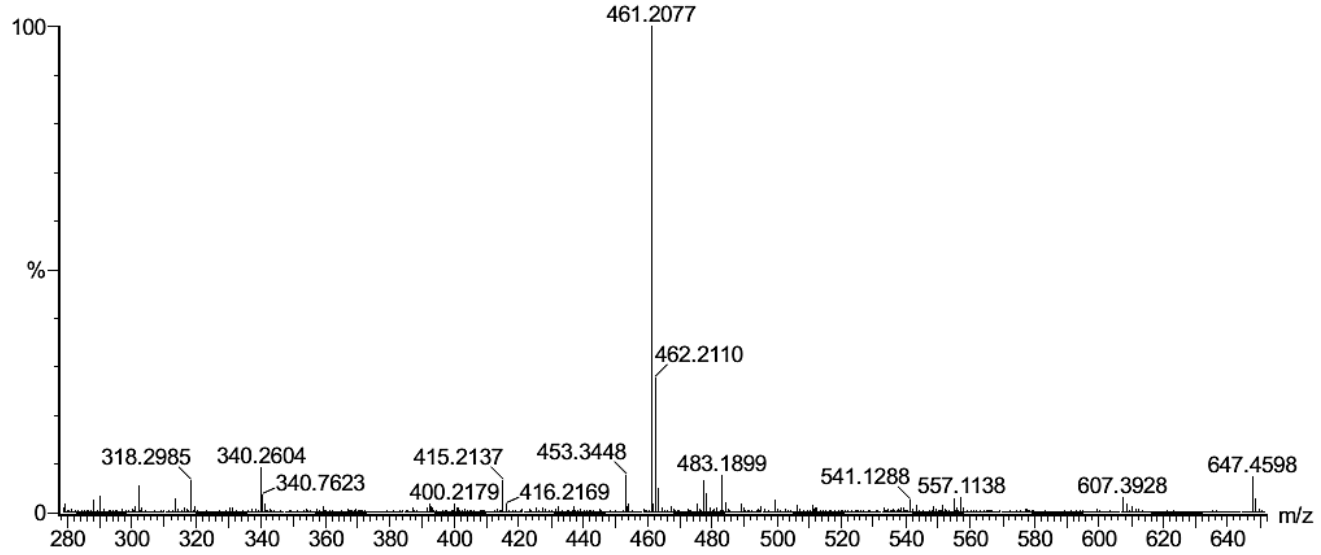
Elemental Composition Report

Single Mass Analysis

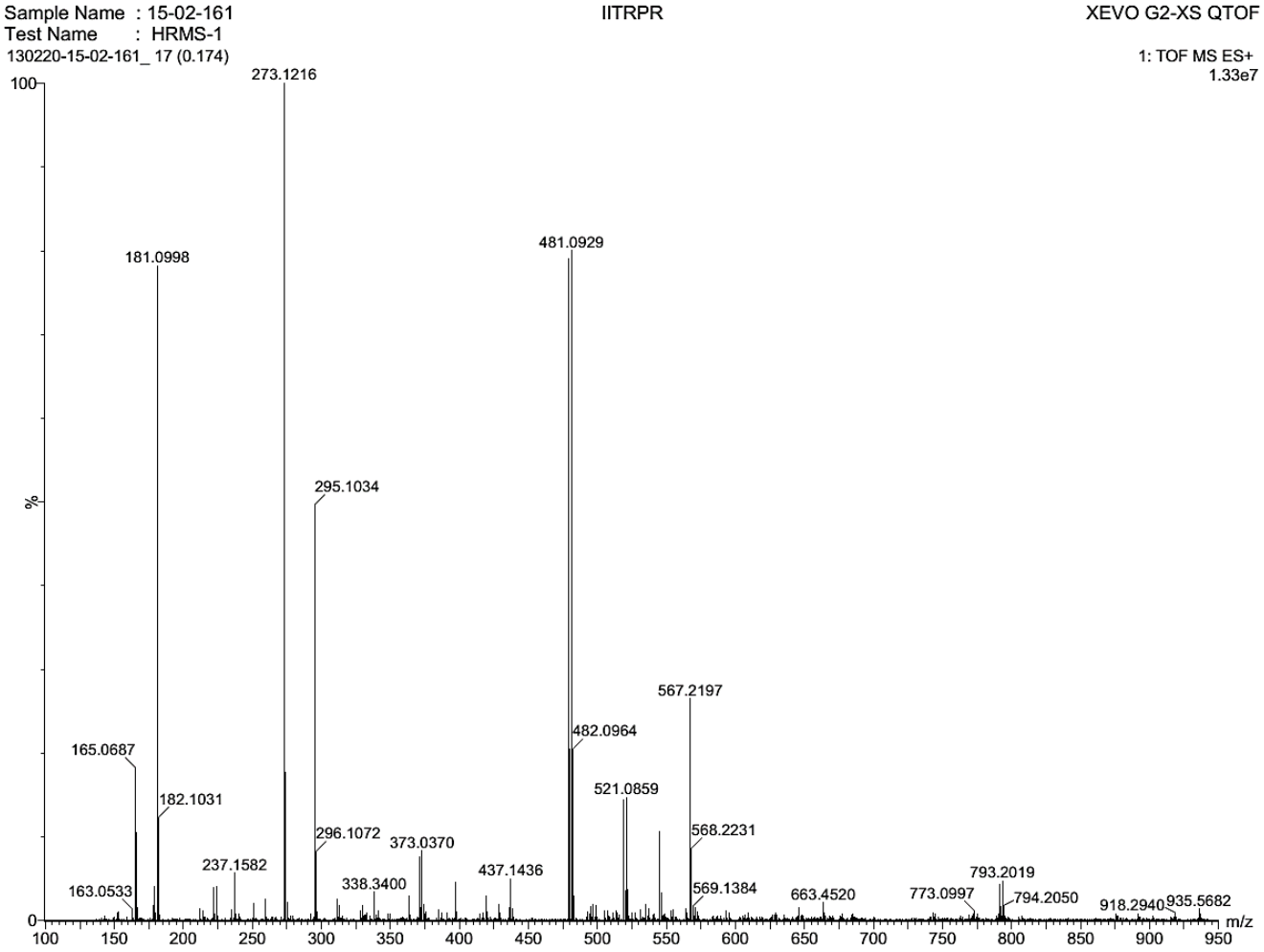
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

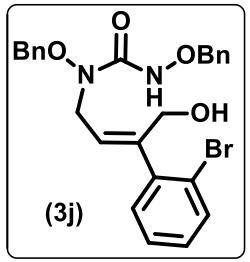
Monoisotopic Mass, Even Electron Ions
29 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 11-35 N: 0-3 O: 1-6

Sample Name : 15-2-47 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
270919-15-2-47 18 (0.183) AM2 (Ar,22000.0,0.00,0.00); Cm (18:19) 1: TOF MS ES+
3.01e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
461.2077	461.2076	0.1	0.2	14.5	639.5	n/a	n/a	C27 H29 N2 O5


Sample Name : 15-02-161
Test Name : HRMS-1
130220-15-02-161_ 17 (0.174)
IITRPR
XEVO G2-XS QTOF
1: TOF MS ES+
1.33e7
273.1216
181.0998
481.0929
295.1034
567.2197
482.0964
165.0687
521.0859
182.1031
568.2231
296.1072
373.0370
237.1582
437.1436
793.2019
163.0533
338.3400
569.1384
663.4520
773.0997
794.2050
918.2940
935.5682
%
m/z


BnO
N
O
N
H
OBn
OH
Br
(3j)

Elemental Composition Report

Single Mass Analysis

Tolerance = 6.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

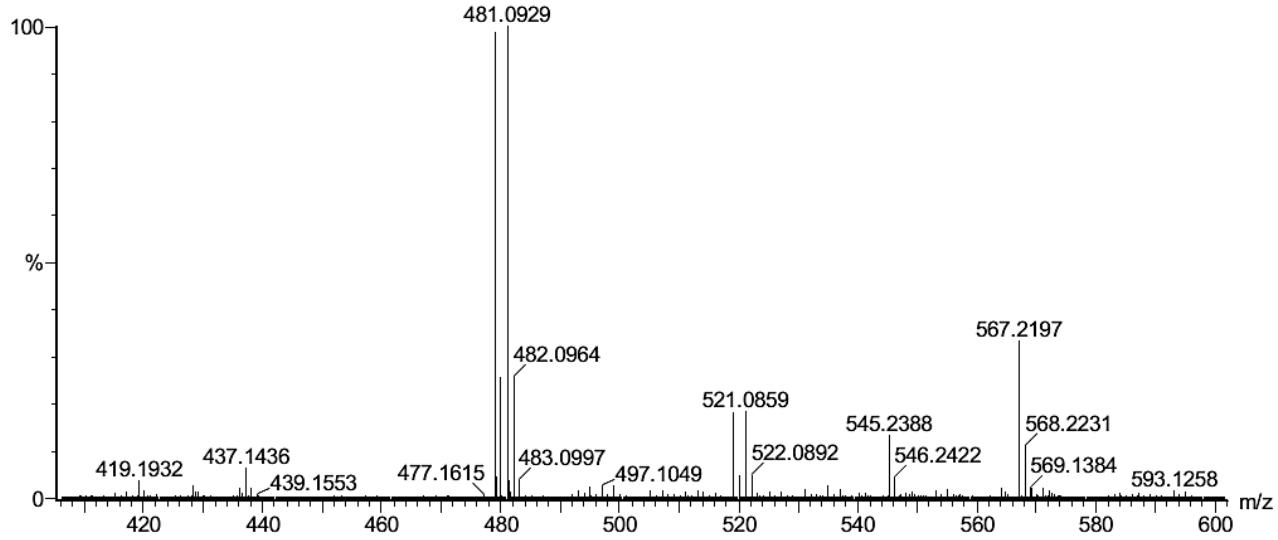
Monoisotopic Mass, Even Electron Ions
29 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 10-30 N: 0-2 O: 0-4 Br: 0-1

Sample Name : 15-02-161
Test Name : HRMS-1
130220-15-02-161_ 17 (0.174)

IITRPR

XEVO G2-XS QTOF

1: TOF MS ES+
1.06e+007



Minimum:				-1.5				
Maximum:		5.0	6.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
497.1049	497.1076	-2.7	-5.4	13.5	861.6	n/a	n/a	C25 H26 N2 O4 Br

Elemental Composition Report

Single Mass Analysis

Tolerance = 6.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

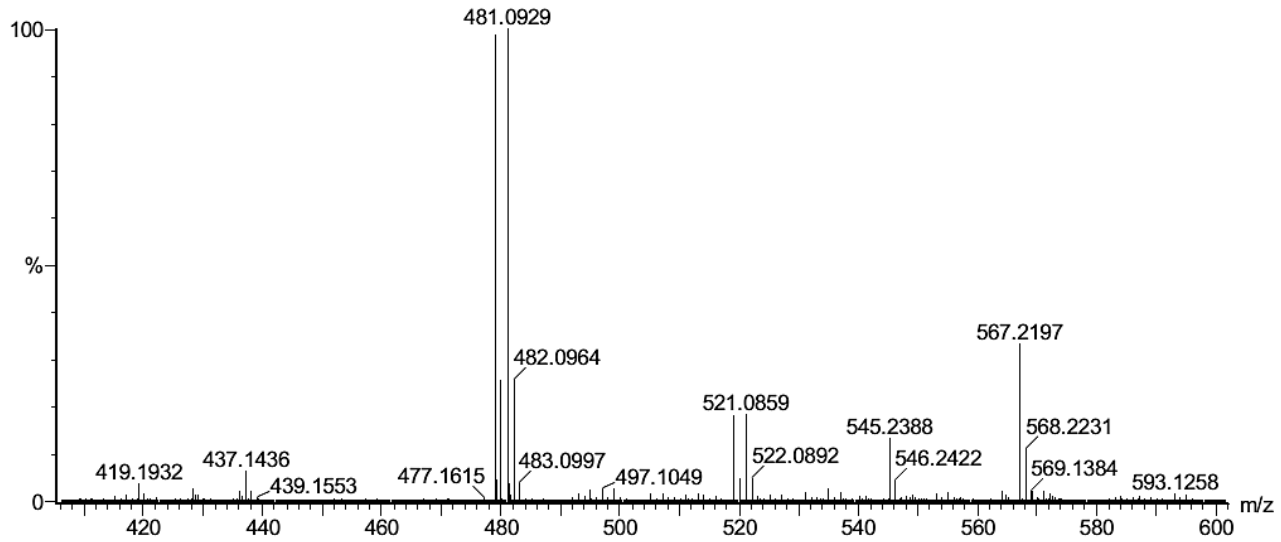
Monoisotopic Mass, Even Electron Ions
53 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 10-30 N: 0-2 O: 0-4 Br: 0-1 Na: 0-1

Sample Name : 15-02-161
Test Name : HRMS-1
130220-15-02-161_ 17 (0.174)

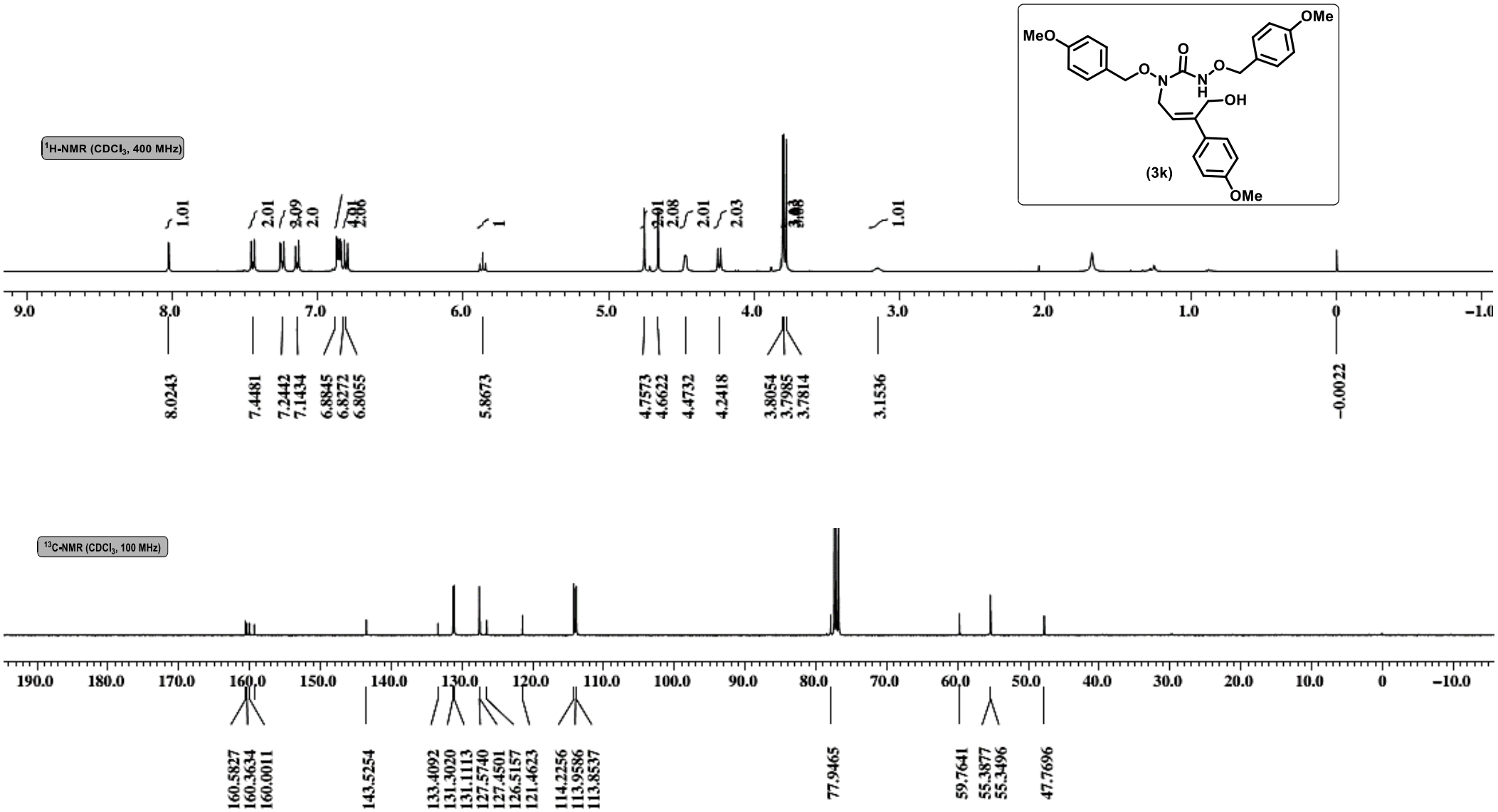
IITRPR

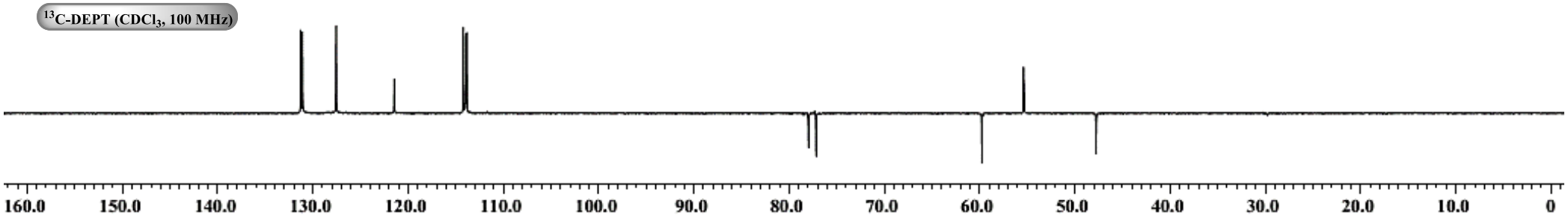
XEVO G2-XS QTOF

1: TOF MS ES+
1.06e+007



Minimum:				-1.5				
Maximum:		5.0	6.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
519.0875	519.0895	-2.0	-3.9	13.5	971.4	n/a	n/a	C25 H25 N2 O4 Br Na


MeO
OMe
O
N
O
N
H
OH
O
OMe
(3k)
^{1}H-NMR ($CDCl_3$, 400 MHz)
1.01
2.01
3.09
2.0
1
2.01
2.08
2.01
2.03
1.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.0243
7.4481
7.2442
7.1434
6.8845
6.8272
6.8055
5.8673
4.7573
4.6622
4.4732
4.2418
3.8054
3.7985
3.7814
3.1536
−0.0022
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
160.5827
160.3634
160.0011
143.5254
133.4092
131.3020
131.1113
127.5740
127.4501
126.5157
121.4623
114.2256
113.9586
113.8537
77.9465
59.7641
55.3877
55.3496
47.7696

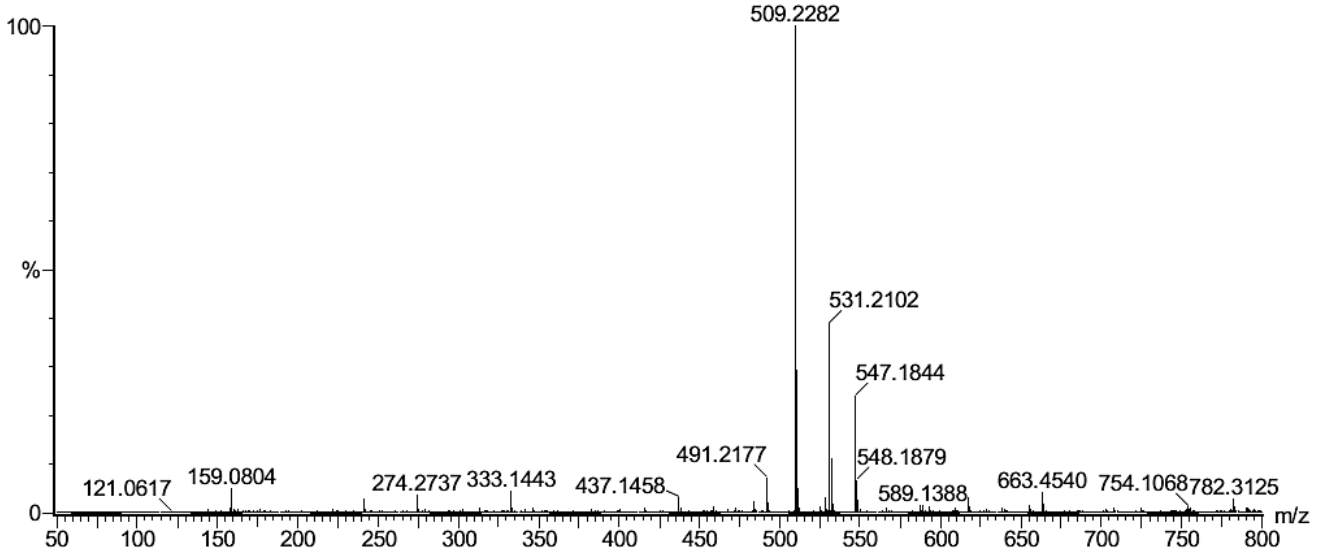

^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Single Mass Analysis

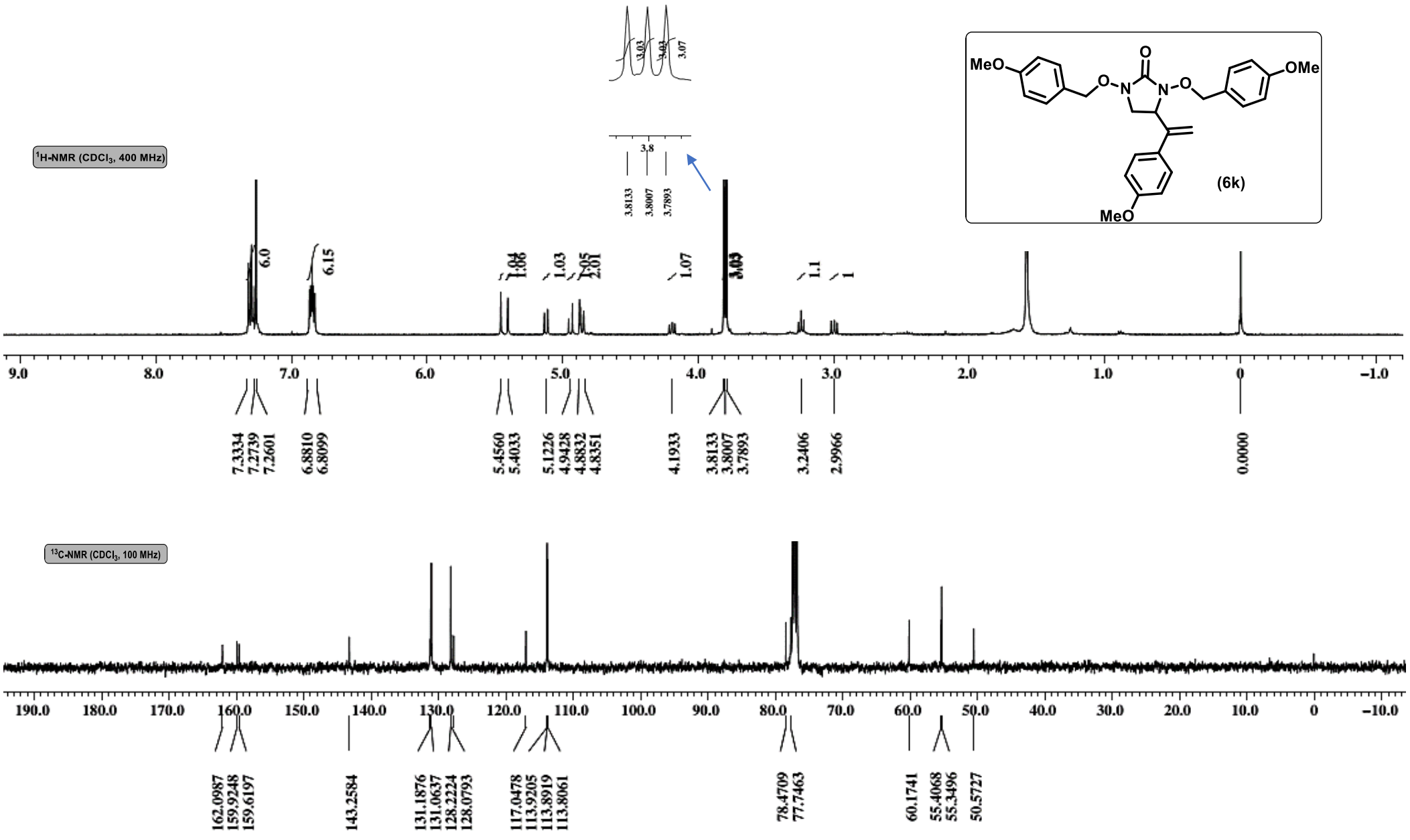
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

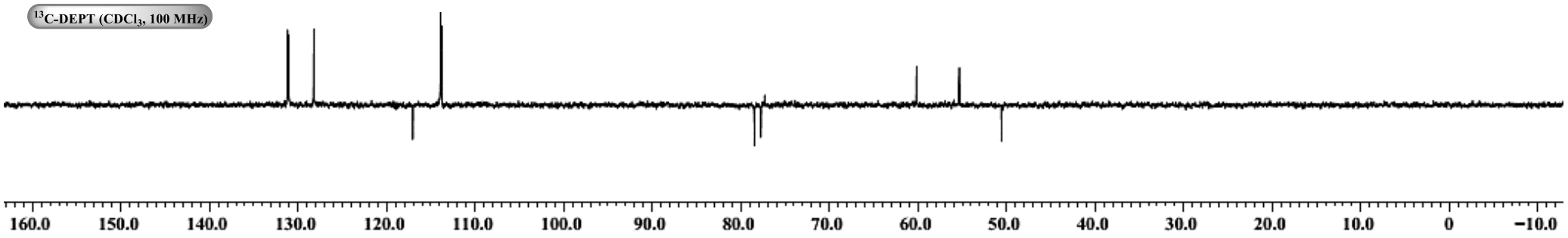
Monoisotopic Mass, Even Electron Ions
90 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-35 H: 11-35 N: 0-4 O: 1-10

Sample Name : 15-02-103 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
061119-15-02-103 17 (0.174) AM2 (Ar,22000.0,0.00,0.00); Cm (17:20) 1: TOF MS ES+
1.61e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
509.2282	509.2288	-0.6	-1.2	13.5	575.1	n/a	n/a	C28 H33 N2 O7


^{1}H-NMR ($CDCl_3$, 400 MHz)
^{13}C-NMR ($CDCl_3$, 100 MHz)
MeO
OMe
MeO
(6k)
7.3334
7.2739
7.2601
6.8810
6.8099
5.4560
5.4033
5.1226
4.9428
4.8832
4.8351
4.1933
3.8133
3.8007
3.7893
3.2406
2.9966
0.0000
162.0987
159.9248
159.6197
143.2584
131.1876
131.0637
128.2224
128.0793
117.0478
113.9205
113.8919
113.8061
78.4709
77.7463
60.1741
55.4068
55.3496
50.5727


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0

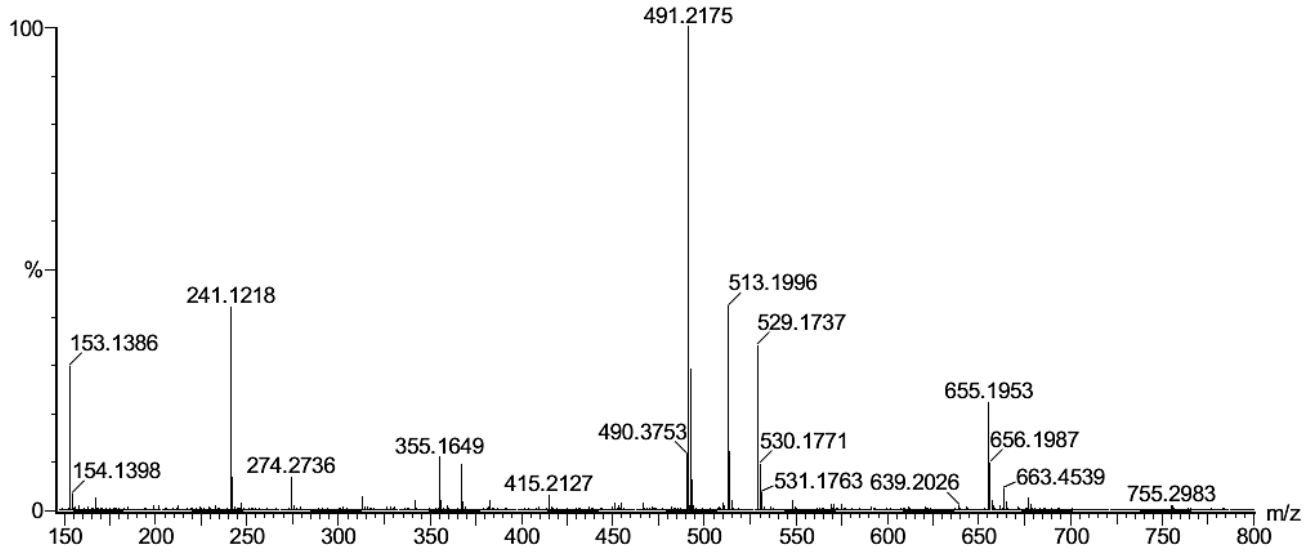
Elemental Composition Report

Single Mass Analysis

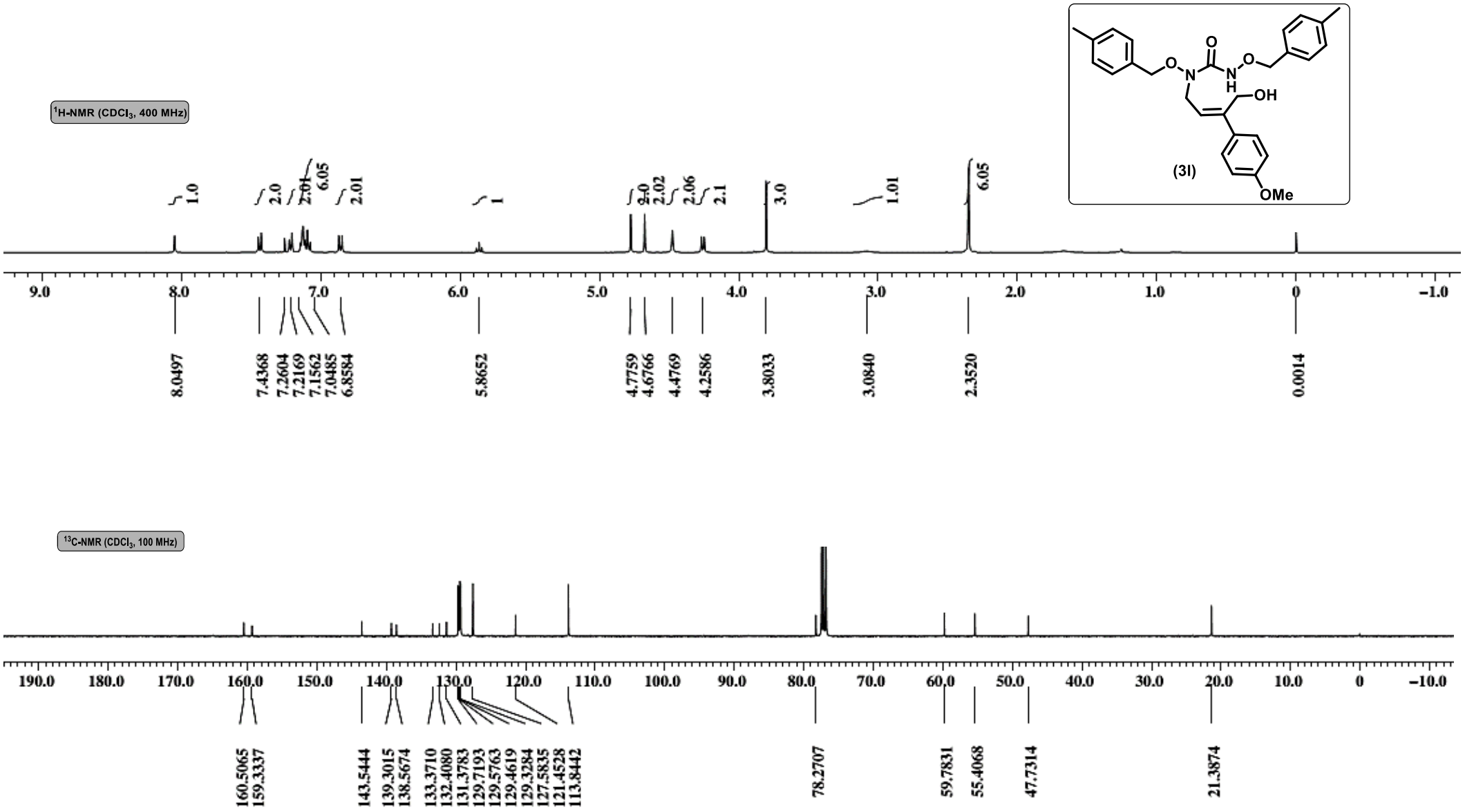
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

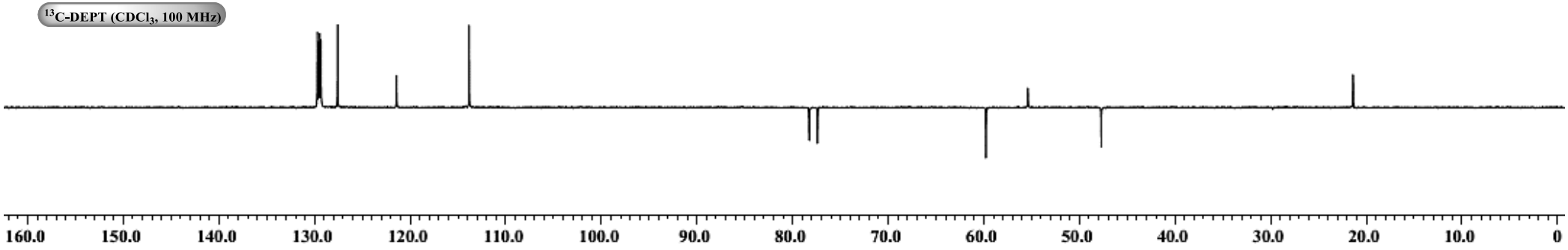
Monoisotopic Mass, Even Electron Ions
101 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-35 H: 11-35 N: 0-4 O: 1-10

Sample Name : 15-02-103-B IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
061119-15-02-103-B 16 (0.165) AM2 (Ar,22000.0,0.00,0.00); Cm (16:18) 1: TOF MS ES+
1.09e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
491.2175	491.2182	-0.7	-1.4	14.5	666.2	n/a	n/a	C28 H31 N2 O6


^{1}H-NMR (CDCl$_3$, 400 MHz)
1.0
2.0
2.01
6.05
2.01
1
2.0
2.02
2.06
2.1
3.0
1.01
6.05
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.0497
7.4368
7.2604
7.2169
7.1562
7.0485
6.8584
5.8652
4.7759
4.6766
4.4769
4.2586
3.8033
3.0840
2.3520
0.0014
(3l)
OMe
OH
^{13}C-NMR (CDCl$_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
160.5065
159.3337
143.5444
139.3015
138.5674
133.3710
132.4080
131.3783
129.7193
129.5763
129.4619
129.3284
127.5835
121.4528
113.8442
78.2707
59.7831
55.4068
47.7314
21.3874


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

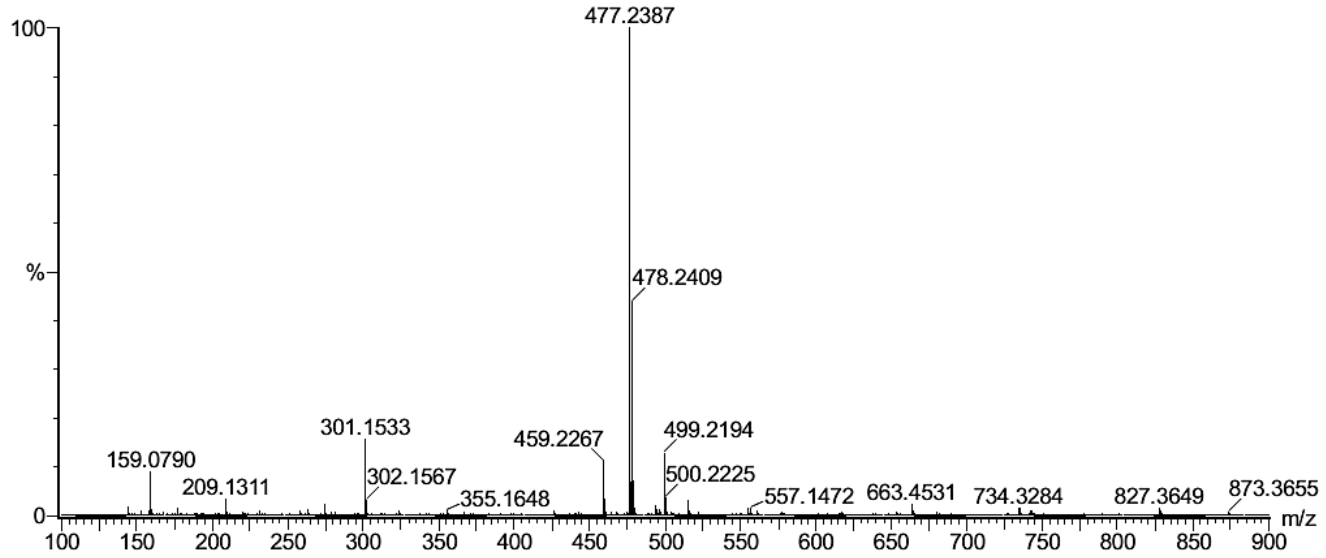
Elemental Composition Report

Single Mass Analysis

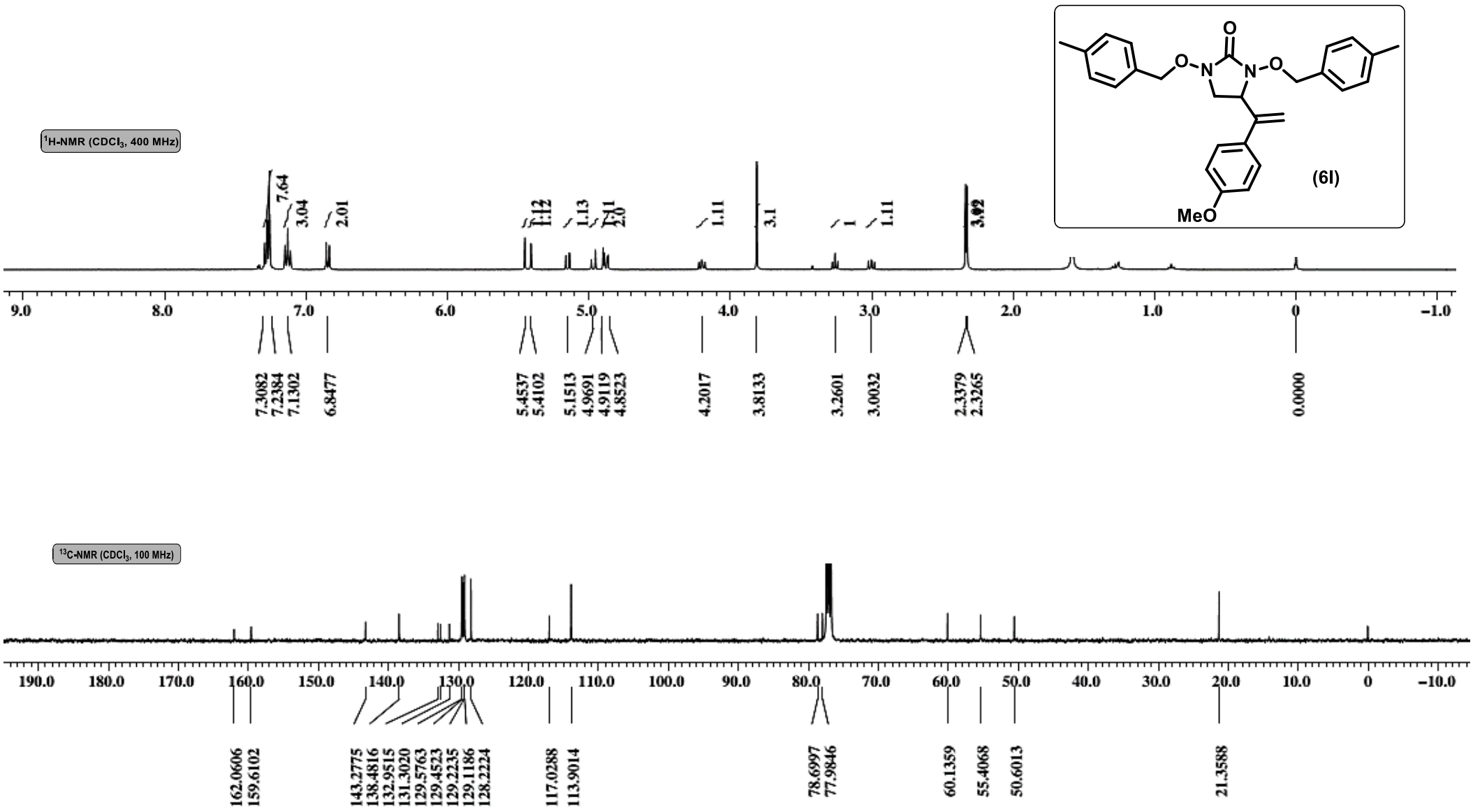
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

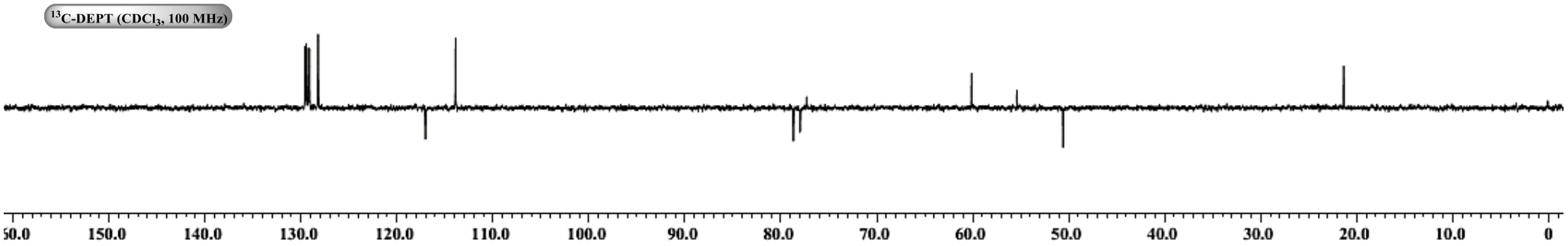
Monoisotopic Mass, Even Electron Ions
19 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 8-30 H: 7-35 N: 0-3 O: 0-5

Sample Name : 15-02-129 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
161219-15-02-129 17 (0.174) AM2 (Ar,22000.0,0.00,0.00); Cm (17:22) 1: TOF MS ES+
4.78e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
477.2387	477.2389	-0.2	-0.4	13.5	906.9	n/a	n/a	C28 H33 N2 O5


^{1}H-NMR (CDCl$_3$, 400 MHz)
7.64
3.04
2.01
1.12
1.13
1.11
3.1
1
1.11
3.02
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.3082
7.2384
7.1302
6.8477
5.4537
5.4102
5.1513
4.9691
4.9119
4.8523
4.2017
3.8133
3.2601
3.0032
2.3379
2.3265
0.0000
O
O-N
N-O
MeO
(6l)
^{13}C-NMR (CDCl$_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
162.0606
159.6102
143.2775
138.4816
132.9515
131.3020
129.5763
129.4523
129.2235
129.1186
128.2224
117.0288
113.9014
78.6997
77.9846
60.1359
55.4068
50.6013
21.3588

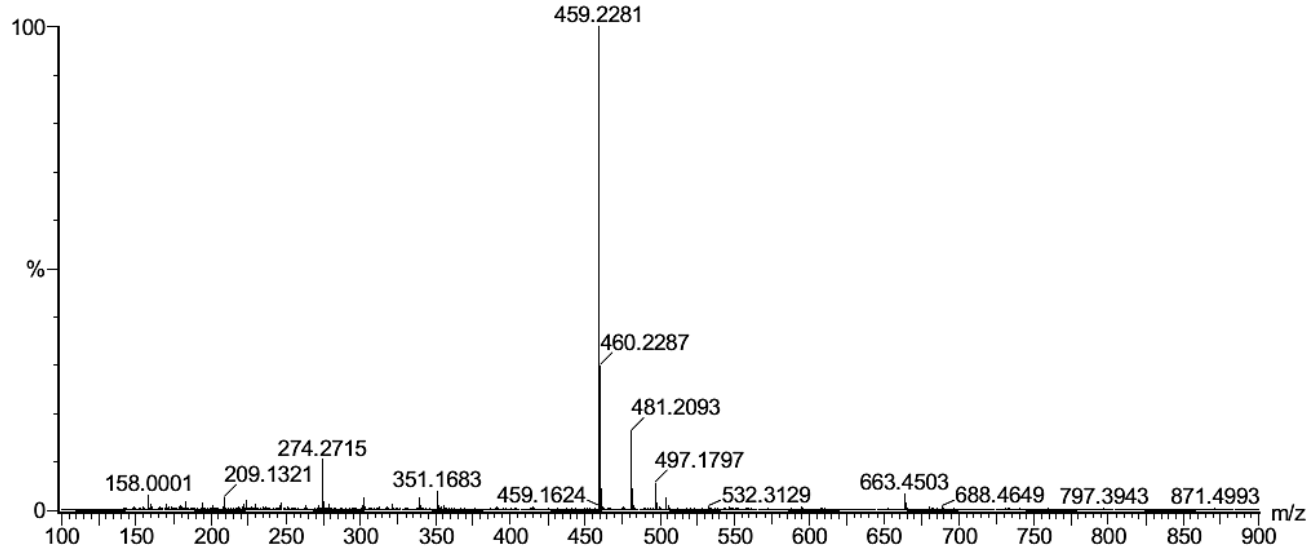

^{13}C-DEPT (CDCl$_3$, 100 MHz)
50.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Single Mass Analysis

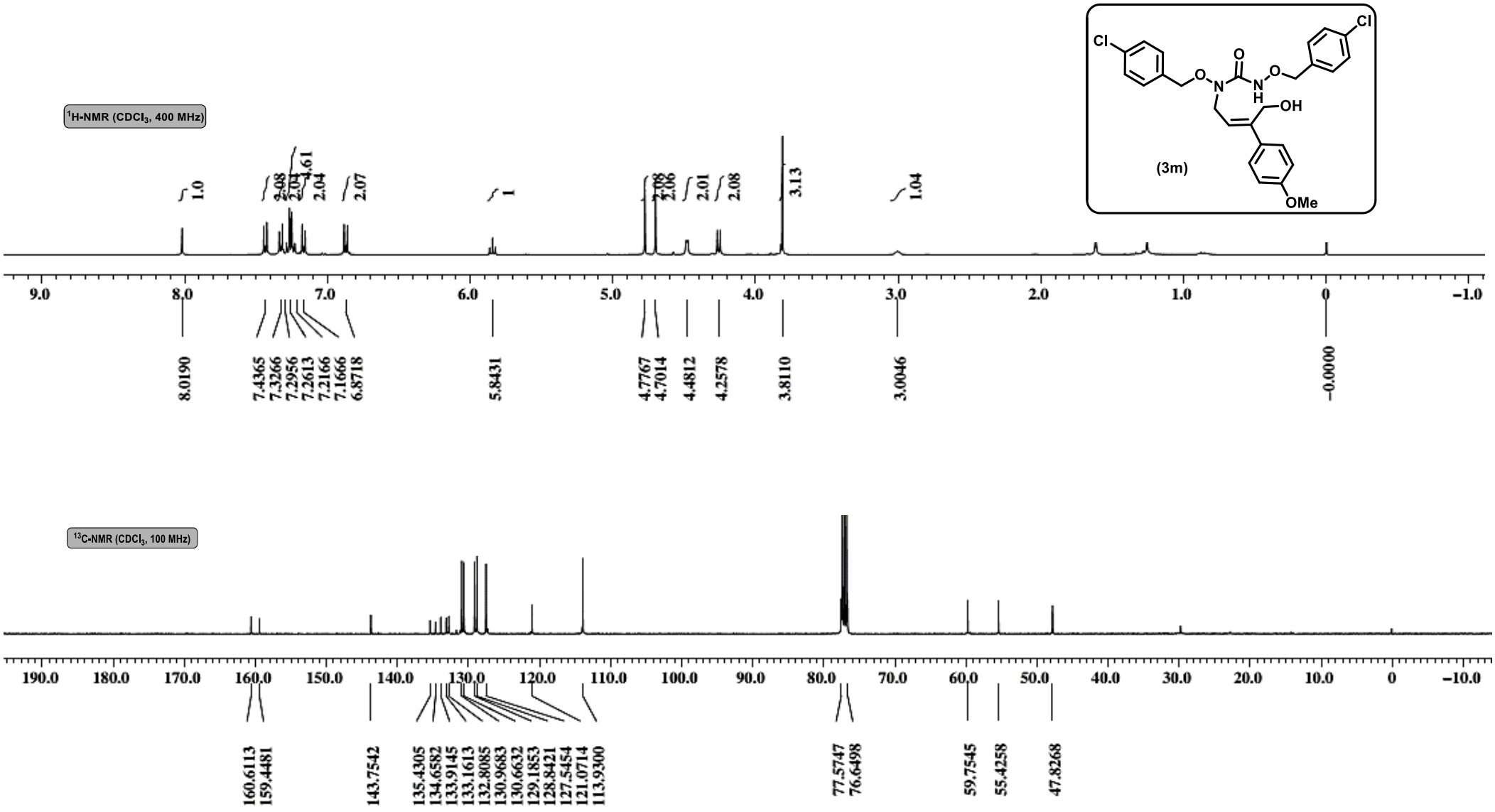
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

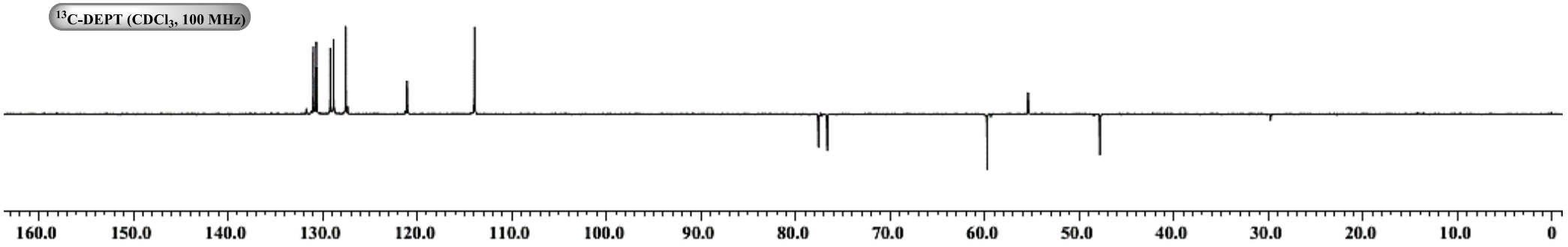
Monoisotopic Mass, Even Electron Ions
56 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 15-35 N: 0-3 O: 0-5 S: 0-1

Sample Name : 15-02-129-F IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
161219-15-02-129-F 19 (0.203) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (19:20) 1: TOF MS ES+
4.21e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
459.2281	459.2284	-0.3	-0.7	14.5	471.3	n/a	n/a	C28 H31 N2 O4


^{1}H-NMR ($CDCl_3$, 400 MHz)
1.0
2.08
2.04
4.61
2.04
2.07
1
2.08
2.06
2.01
2.08
3.13
1.04
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.0190
7.4365
7.3266
7.2956
7.2613
7.2166
7.1666
6.8718
5.8431
4.7767
4.7014
4.4812
4.2578
3.8110
3.0046
−0.0000
Cl
Cl
O
O
N
N
H
O
OH
OMe
(3m)
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
160.6113
159.4481
143.7542
135.4305
134.6582
133.9145
133.1613
132.8085
130.9683
130.6632
129.1853
128.8421
127.5454
121.0714
113.9300
77.5747
76.6498
59.7545
55.4258
47.8268


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

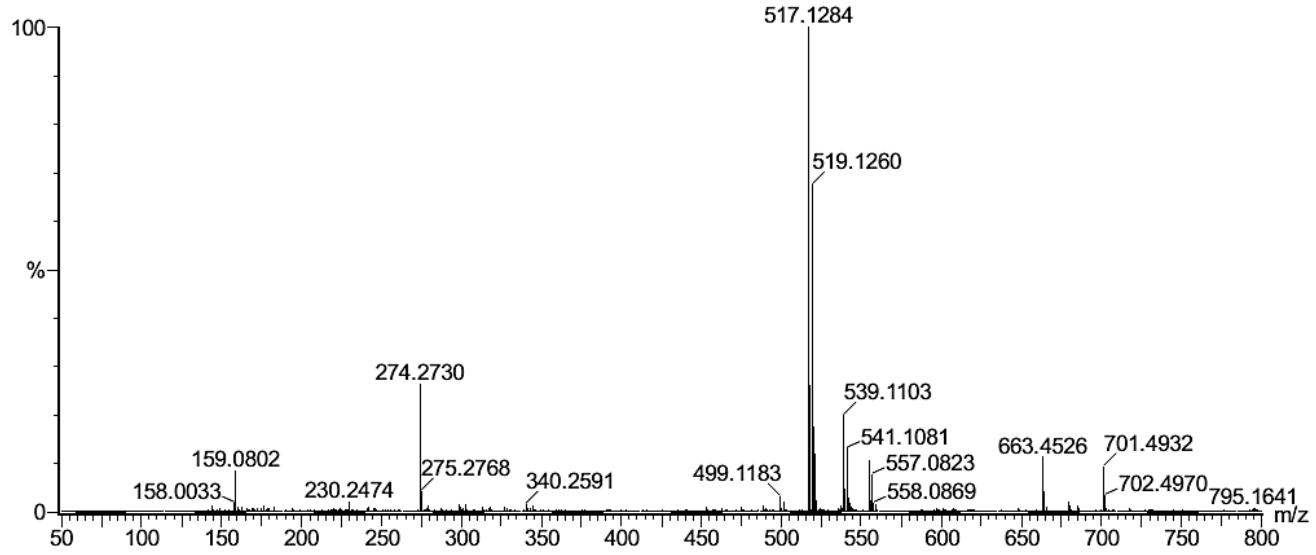
Elemental Composition Report

Single Mass Analysis

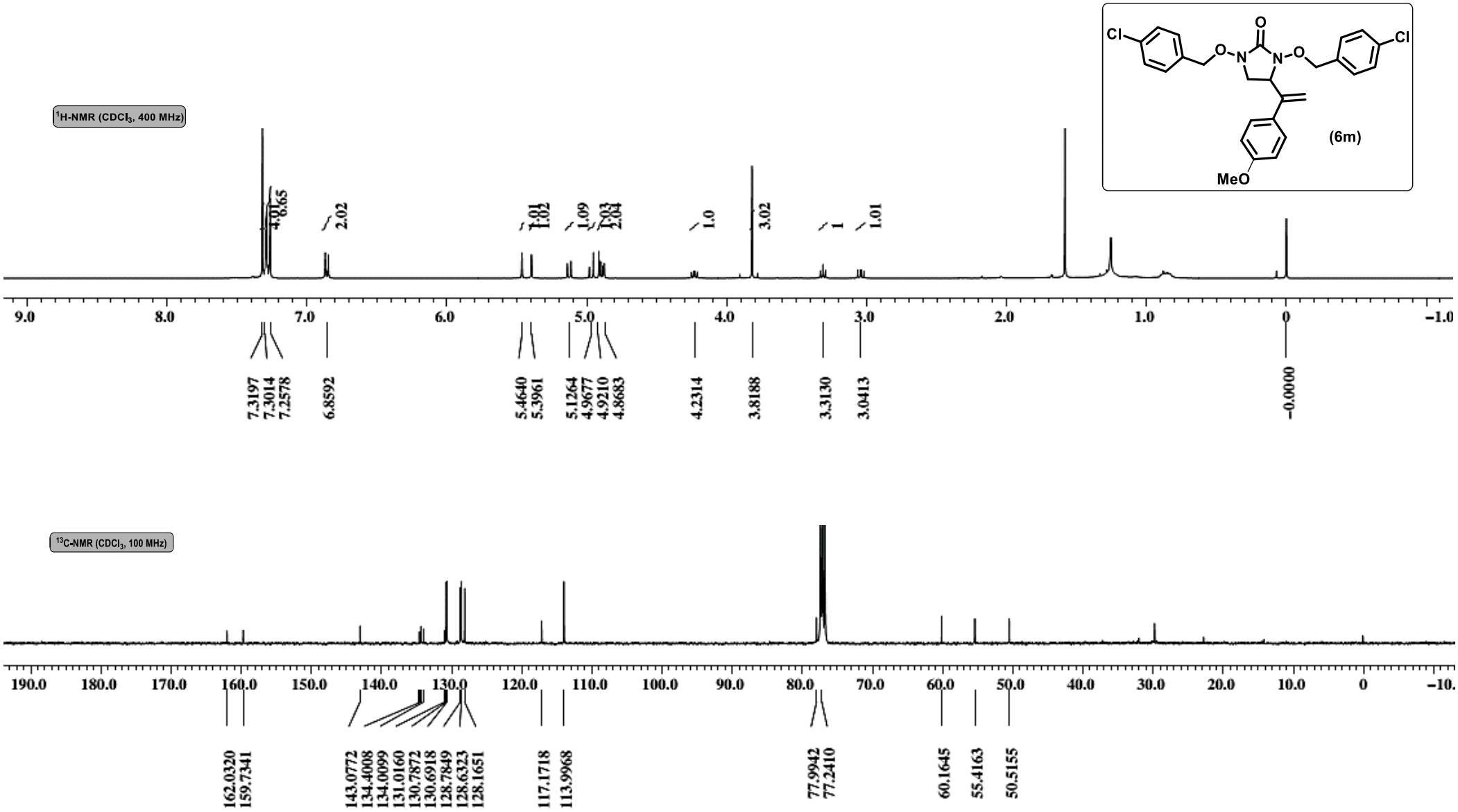
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

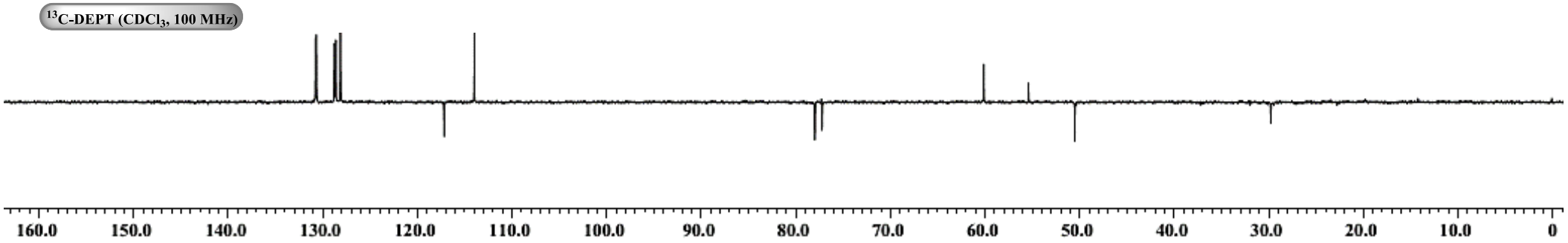
Monoisotopic Mass, Even Electron Ions
102 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-35 H: 11-35 N: 0-3 O: 1-5 Cl: 0-2

Sample Name : 15-02-107 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
071119-15-02-107 18 (0.183) AM2 (Ar,22000.0,0.00,0.00); Cm (18:21) 1: TOF MS ES+
8.85e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
517.1284	517.1297	-1.3	-2.5	13.5	587.0	n/a	n/a	C26 H27 N2 O5 Cl2


^{1}H-NMR ($CDCl_3$, 400 MHz)
Cl
Cl
O
N
N
O
O
MeO
(6m)
4.00
0.65
2.02
1.01
1.02
1.09
2.03
2.04
1.0
3.02
1
1.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.3197
7.3014
7.2578
6.8592
5.4640
5.3961
5.1264
4.9677
4.9210
4.8683
4.2314
3.8188
3.3130
3.0413
−0.0000
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.
162.0320
159.7341
143.0772
134.4008
134.0099
131.0160
130.7872
130.6918
128.7849
128.6323
128.1651
117.1718
113.9968
77.9942
77.2410
60.1645
55.4163
50.5155


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

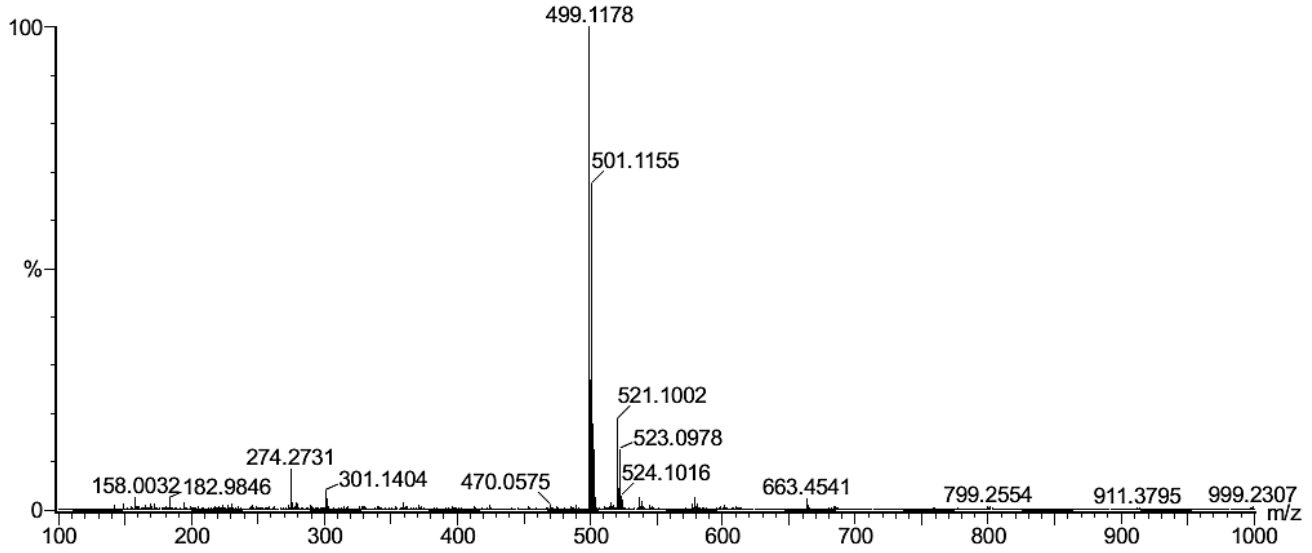
Elemental Composition Report

Single Mass Analysis

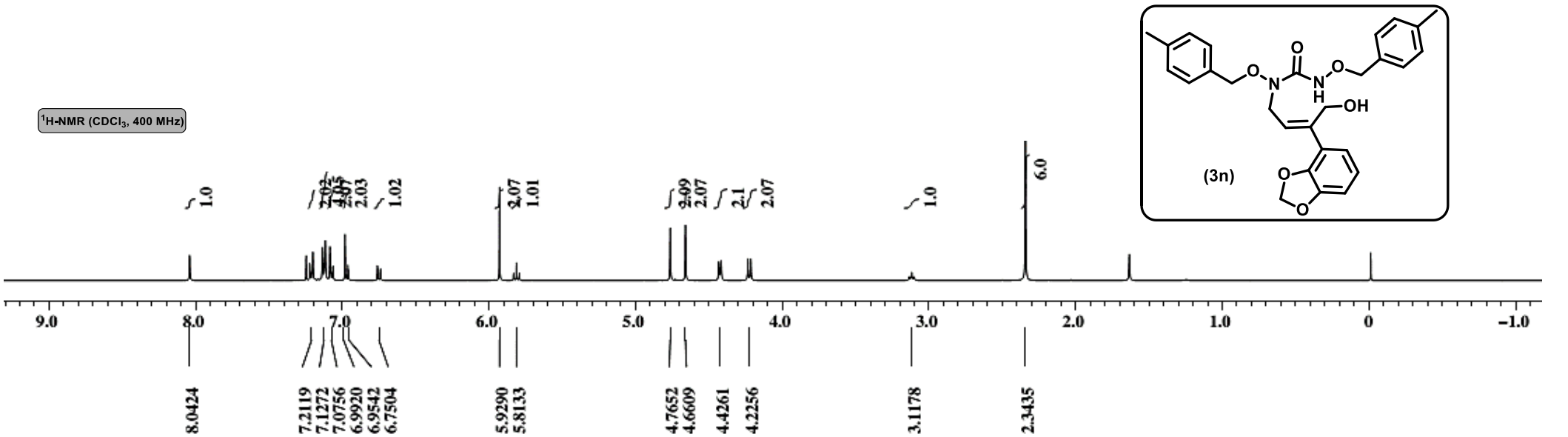
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

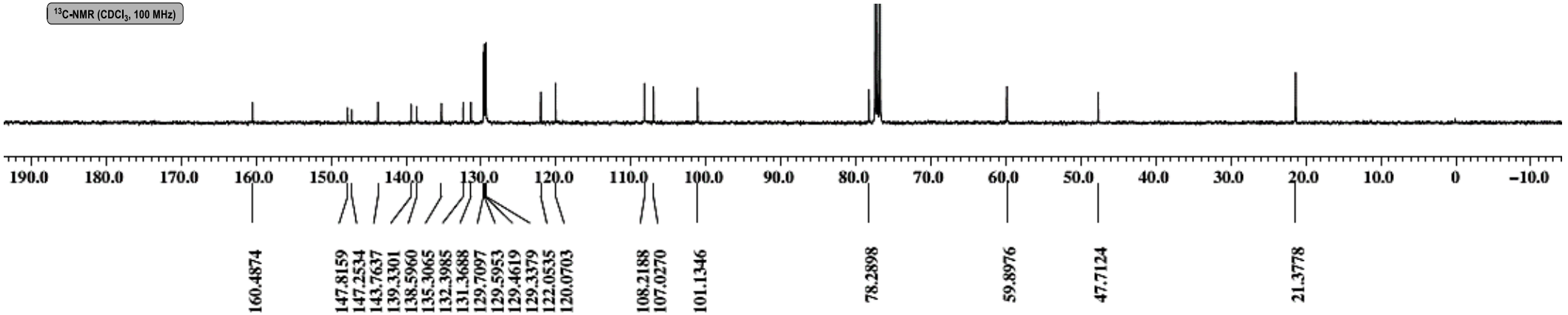
Monoisotopic Mass, Even Electron Ions
110 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 6-35 N: 0-3 O: 0-6 Cl: 0-2

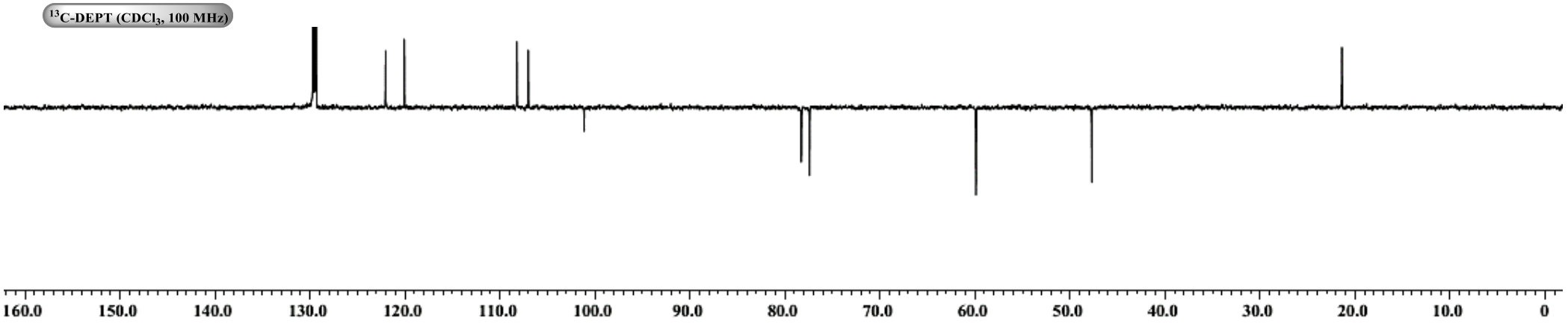
Sample Name : 15-02-107-F IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
130120-15-02-107-F 18 (0.183) 1: TOF MS ES+
3.82e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
499.1178	499.1191	-1.3	-2.6	14.5	970.1	n/a	n/a	C26 H25 N2 O4 Cl2


^{1}H-NMR ($CDCl_3$, 400 MHz)
(3n)
8.0424
7.2119
7.1272
7.0756
6.9920
6.9542
6.7504
5.9290
5.8133
4.7652
4.6609
4.4261
4.2256
3.1178
2.3435


^{13}C-NMR ($CDCl_3$, 100 MHz)
160.4874
147.8159
147.2534
143.7637
139.3301
138.5960
135.3065
132.3985
131.3688
129.7097
129.5953
129.4619
129.3379
122.0535
120.0703
108.2188
107.0270
101.1346
78.2898
59.8976
47.7124
21.3778


^{13}C-DEPT (CDCl$_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

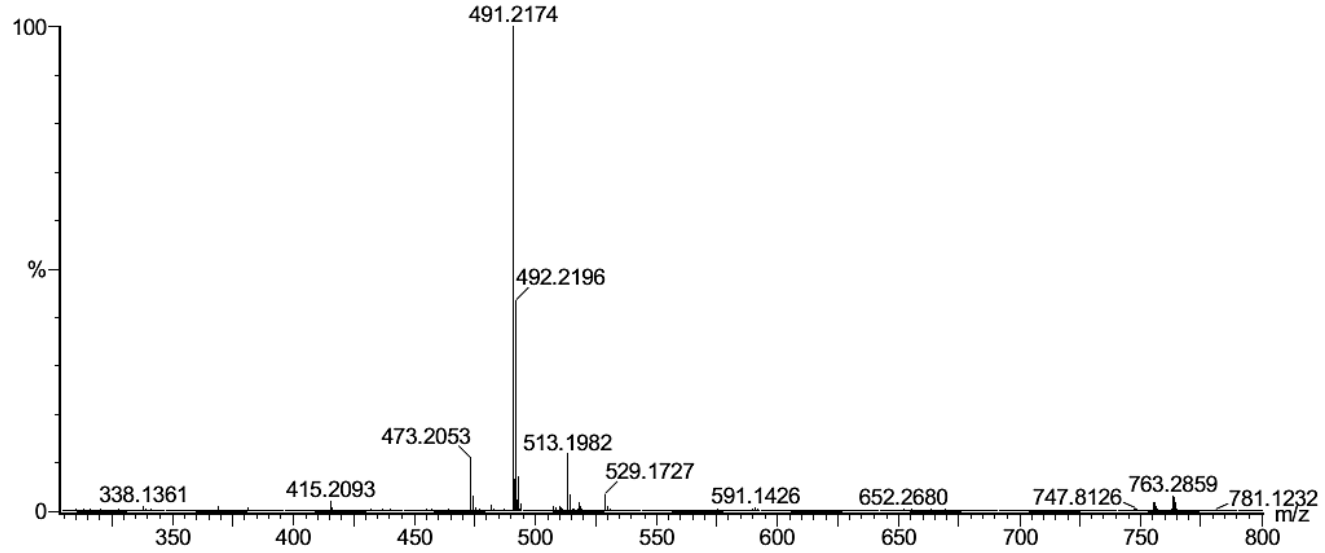
Elemental Composition Report

Single Mass Analysis

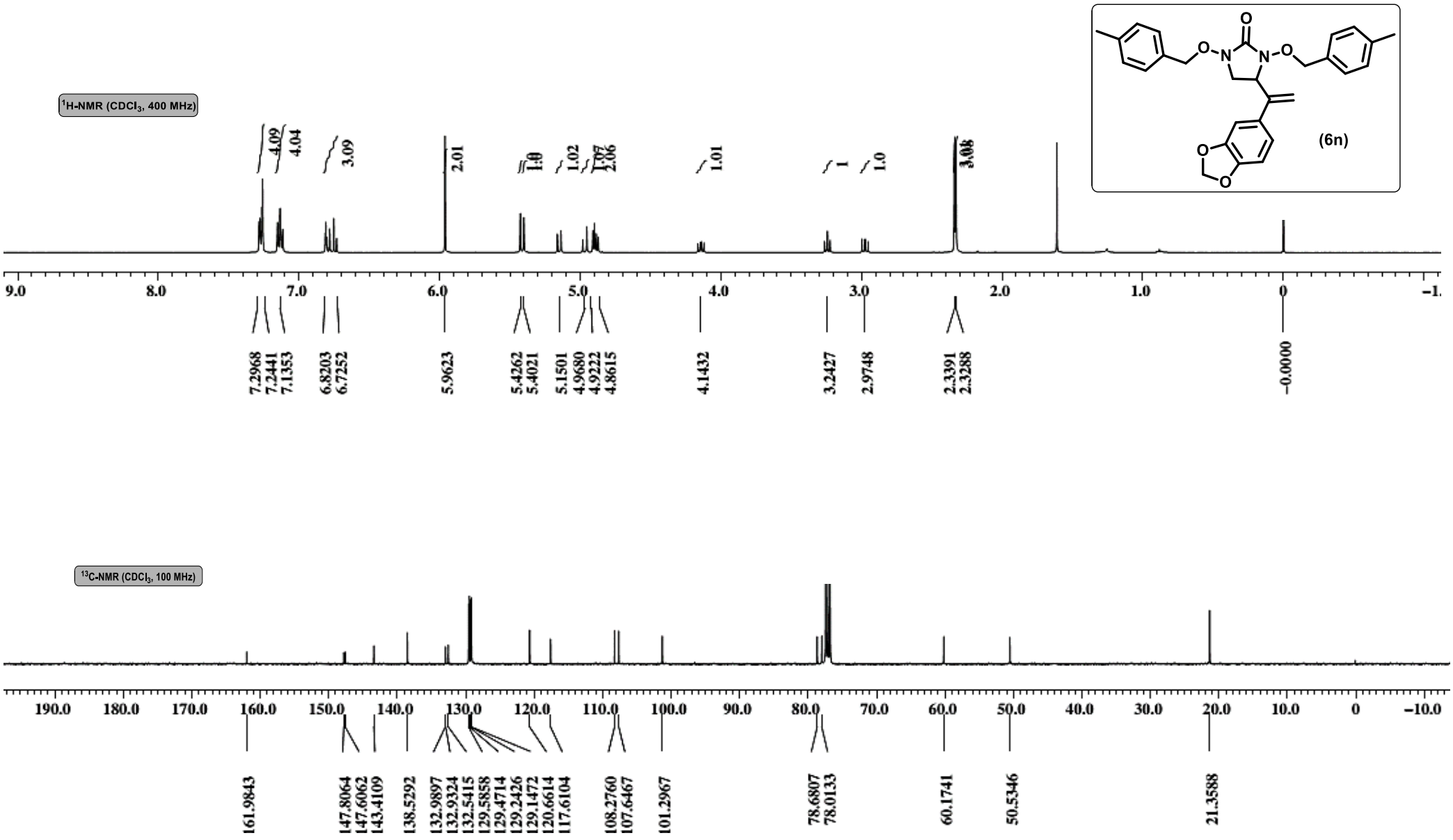
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

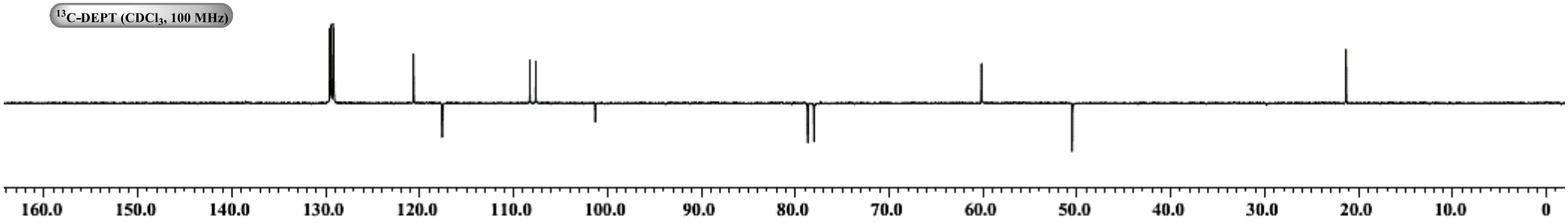
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-30 H: 20-35 N: 0-3 O: 1-6

Sample Name : 15-02-110 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
161119-15-02-110 11 (0.123) AM2 (Ar,22000.0,0.00,0.00); Cm (7:20) 1: TOF MS ES+
1.54e+008



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
491.2174	491.2182	-0.8	-1.6	14.5	907.5	n/a	n/a	C28 H31 N2 O6


^{1}H-NMR (CDCl$_3$, 400 MHz)
4.09
4.04
3.09
2.01
1.01
1
1.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2968
7.2441
7.1353
6.8203
6.7252
5.9623
5.4262
5.4021
5.1501
4.9680
4.9222
4.8615
4.1432
3.2427
2.9748
2.3391
2.3288
−0.0000
(6n)
^{13}C-NMR (CDCl$_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
161.9843
147.8064
147.6062
143.4109
138.5292
132.9897
132.9324
132.5415
129.5858
129.4714
129.2426
129.1472
120.6614
117.6104
108.2760
107.6467
101.2967
78.6807
78.0133
60.1741
50.5346
21.3588

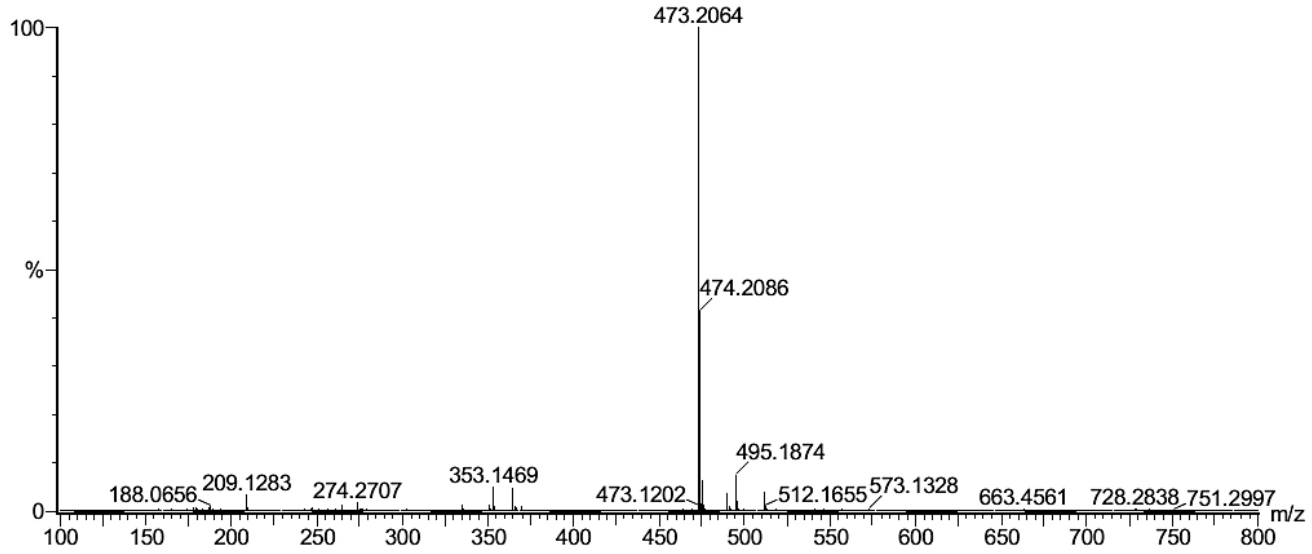

^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Single Mass Analysis

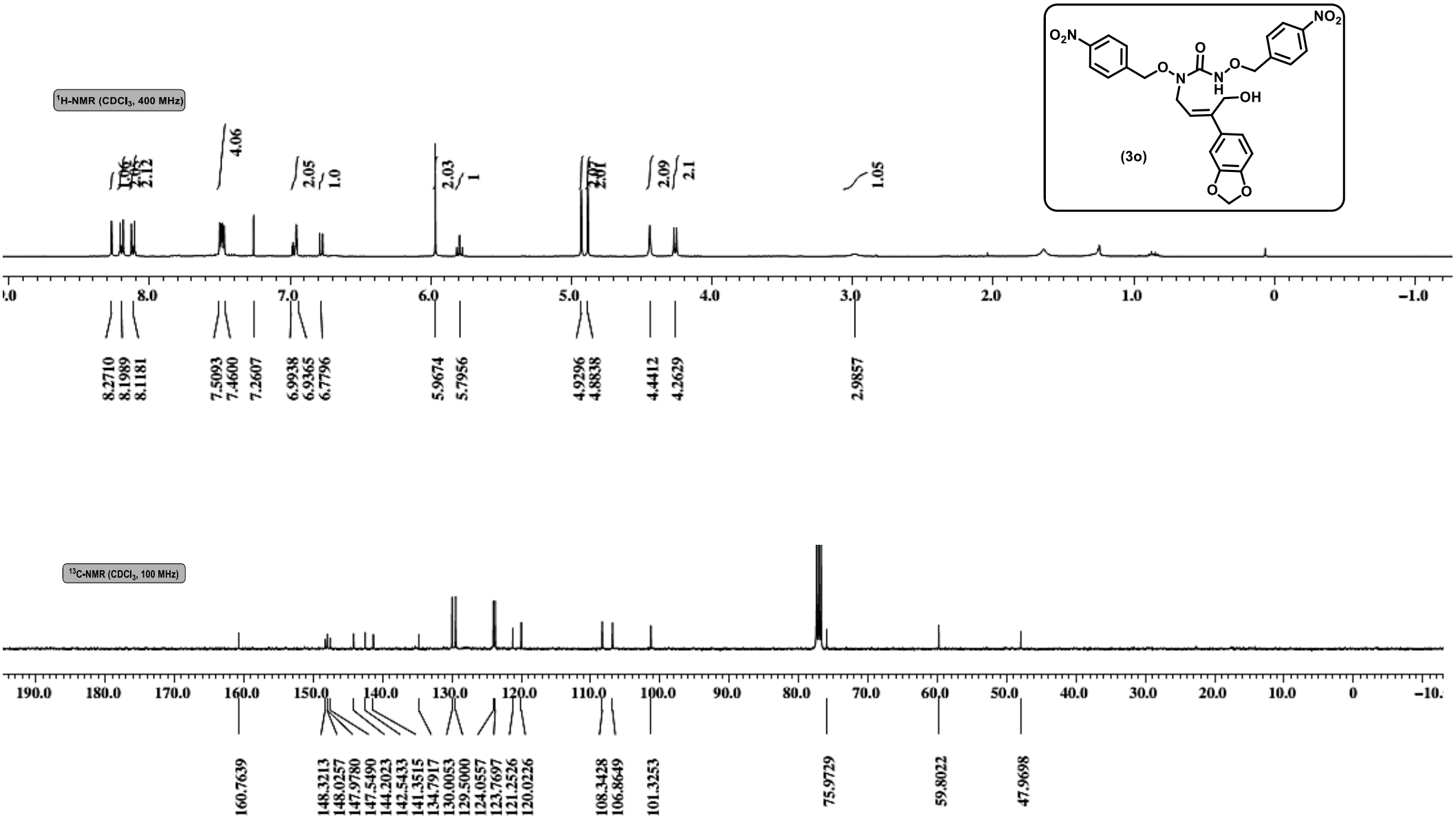
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

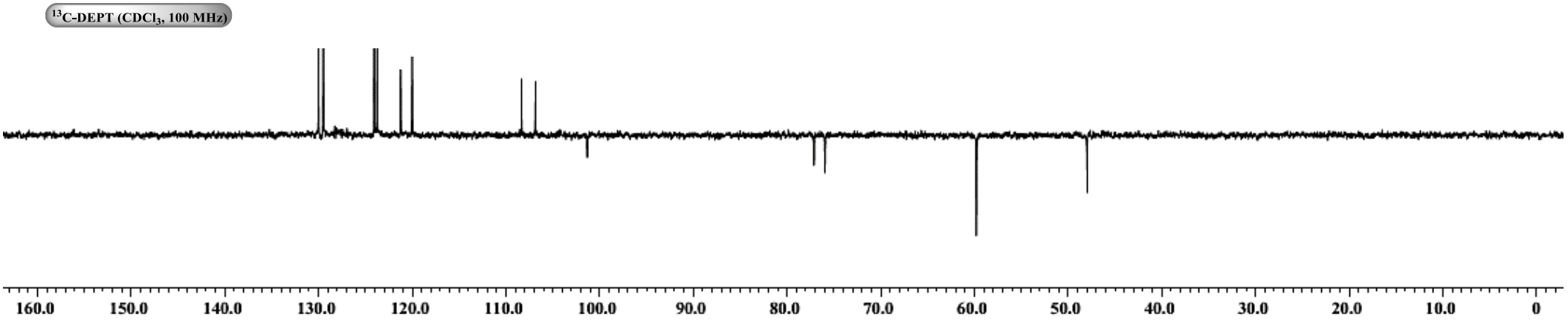
Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-30 H: 20-35 N: 0-3 O: 1-6

Sample Name : 15-02-110-B IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
161119-15-02-110-B 13 (0.140) AM2 (Ar,22000.0,0.00,0.00); Cm (13:22) 1: TOF MS ES+
8.68e+007



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
473.2064	473.2076	-1.2	-2.5	15.5	904.9	n/a	n/a	C28 H29 N2 O5


^{1}H-NMR ($CDCl_3$, 400 MHz)
4.06
2.05
1.0
2.03
1
2.09
2.1
1.05
8.2710
8.1989
8.1181
7.5093
7.4600
7.2607
6.9938
6.9365
6.7796
5.9674
5.7956
4.9296
4.8838
4.4412
4.2629
2.9857
(3o)
^{13}C-NMR ($CDCl_3$, 100 MHz)
160.7639
148.3213
148.0257
147.9780
147.5490
144.2023
142.5433
141.3515
134.7917
130.0053
129.5000
124.0557
123.7697
121.2526
120.0226
108.3428
106.8649
101.3253
75.9729
59.8022
47.9698


^{13}C-DEPT (CDCl$_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

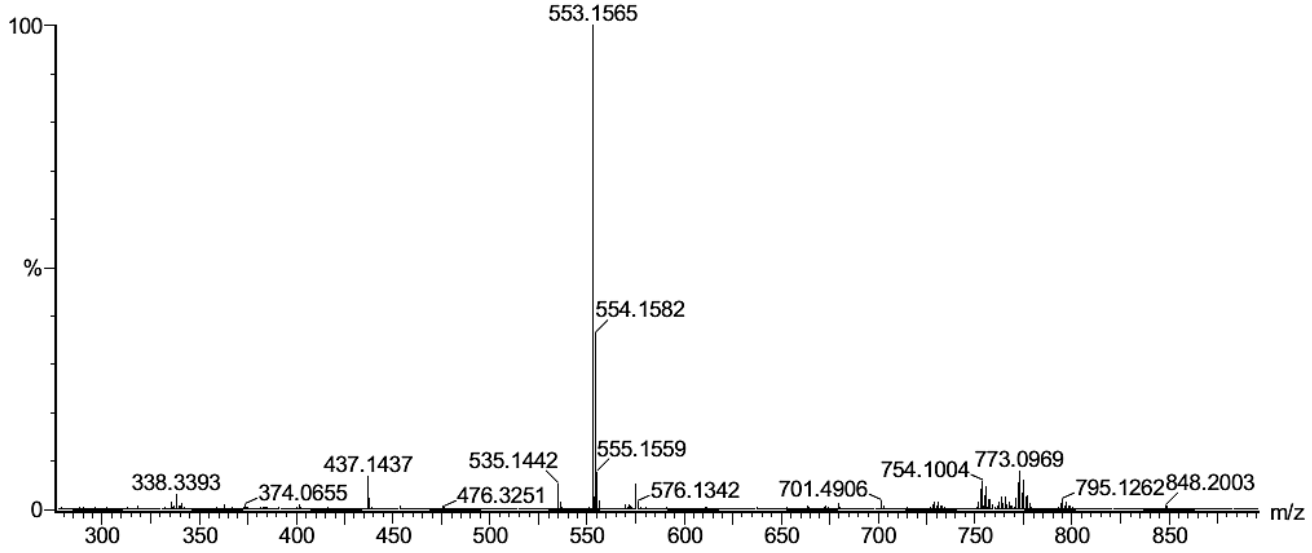
Elemental Composition Report

Single Mass Analysis

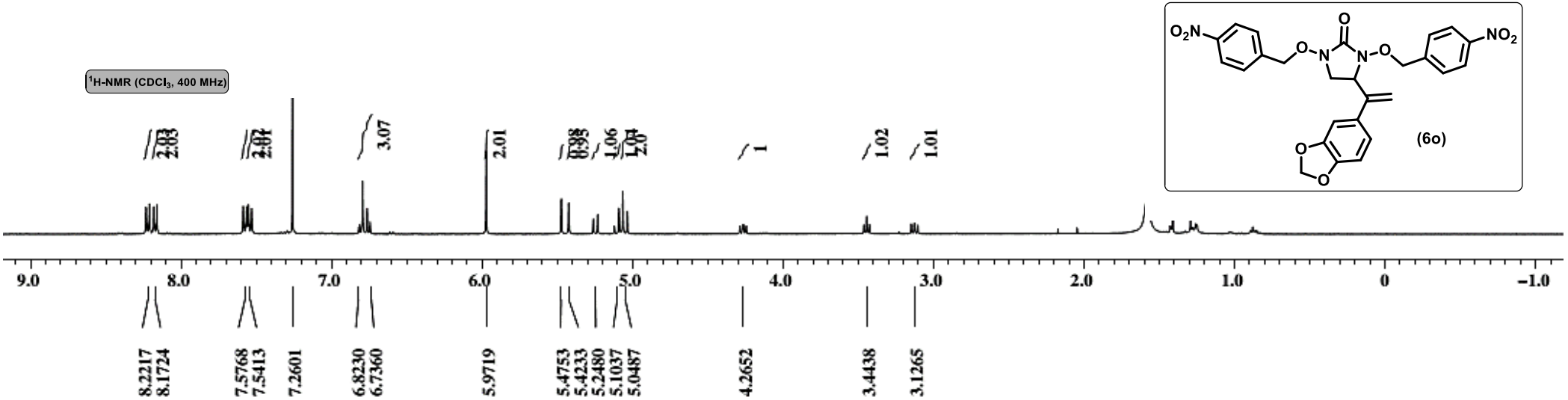
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

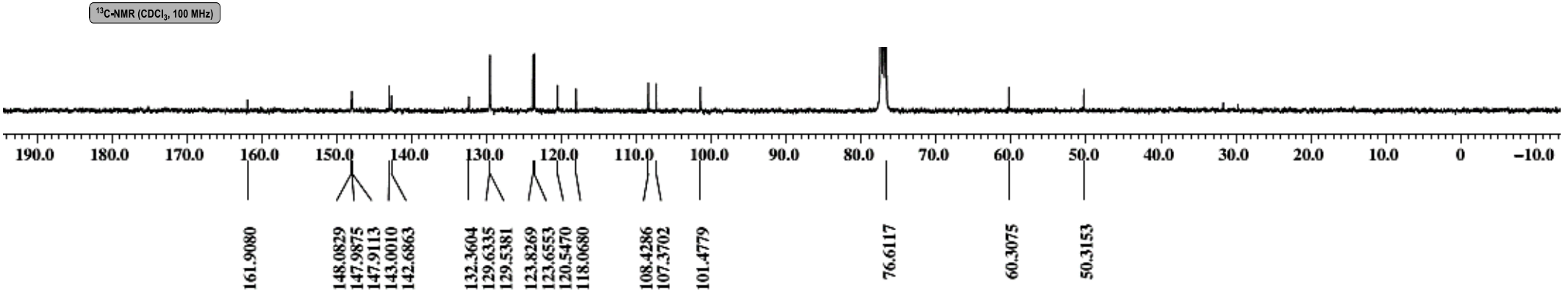
Monoisotopic Mass, Even Electron Ions
45 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 8-30 H: 4-25 N: 0-4 O: 0-10

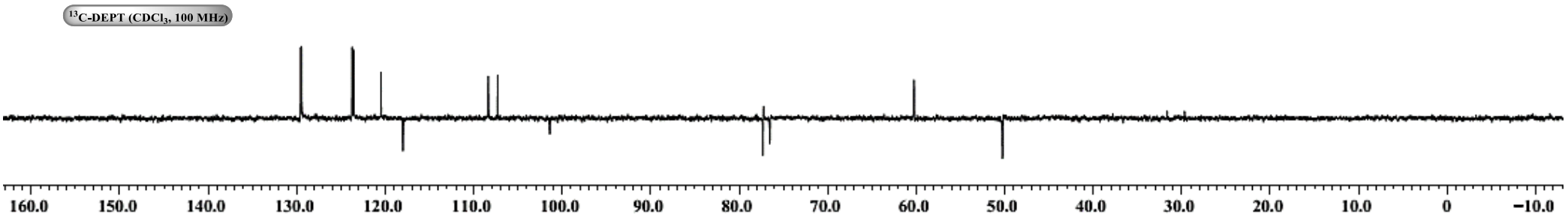
Sample Name : 15-02-097 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
040220-15-02-097 20 (0.211) 1: TOF MS ES+
8.10e+007



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
553.1565	553.1571	-0.6	-1.1	16.5	1668.0	n/a	n/a	C26 H25 N4 O10


^{1}H-NMR ($CDCl_3$, 400 MHz)
(6o)
8.2217
8.1724
7.5768
7.5413
7.2601
6.8230
6.7360
5.9719
5.4753
5.4233
5.2480
5.1037
5.0487
4.2652
3.4438
3.1265


^{13}C-NMR ($CDCl_3$, 100 MHz)
161.9080
148.0829
147.9875
147.9113
143.0010
142.6863
132.3604
129.6335
129.5381
123.8269
123.6553
120.5470
118.0680
108.4286
107.3702
101.4779
76.6117
60.3075
50.3153


^{13}C-DEPT (CDCl$_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0

Elemental Composition Report

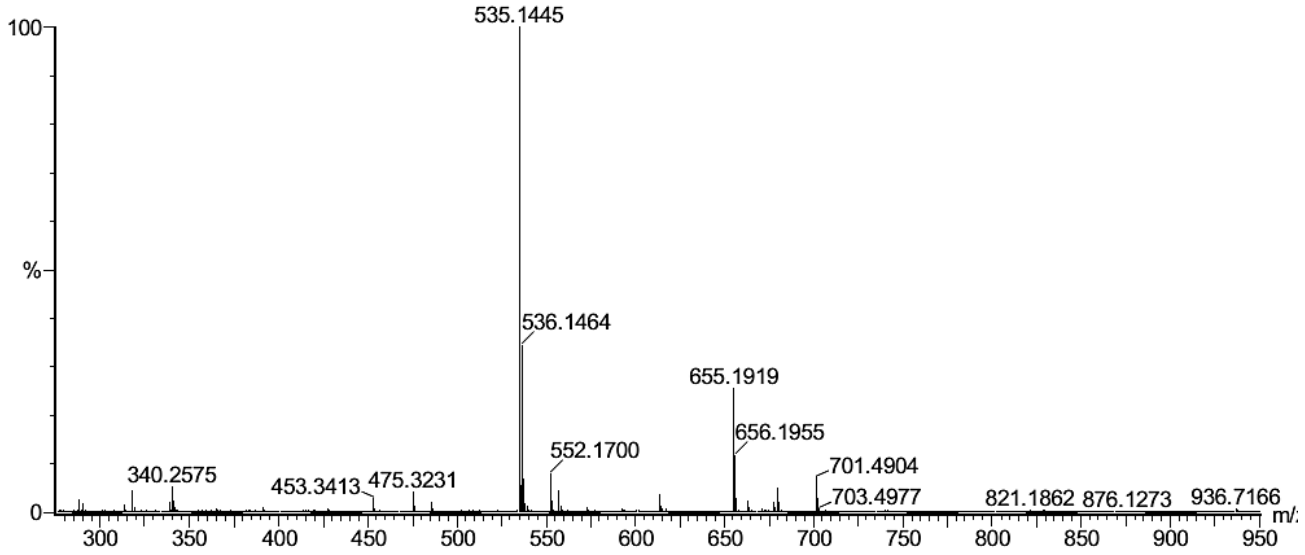
Page

Single Mass Analysis

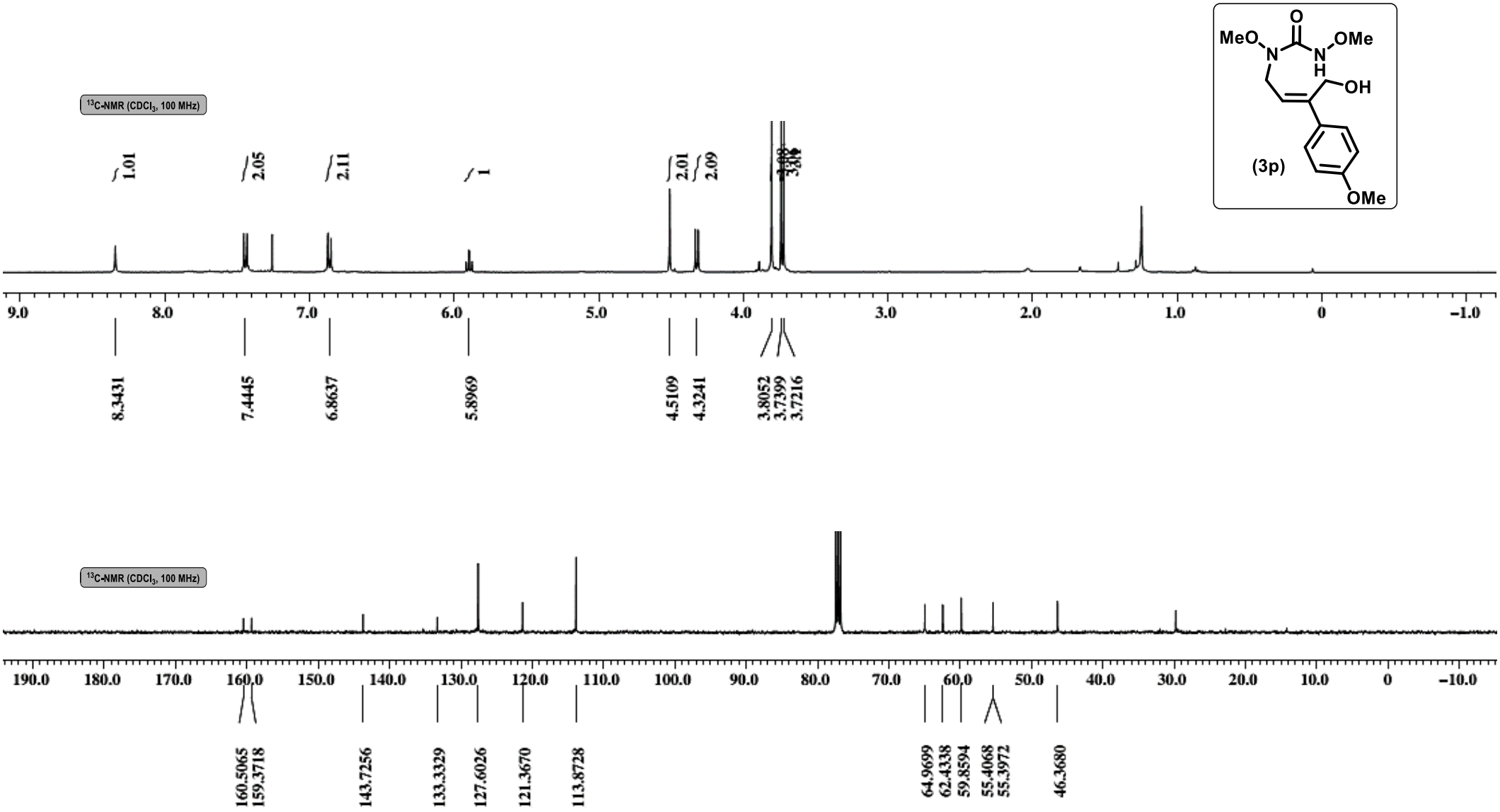
Tolerance = 15.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

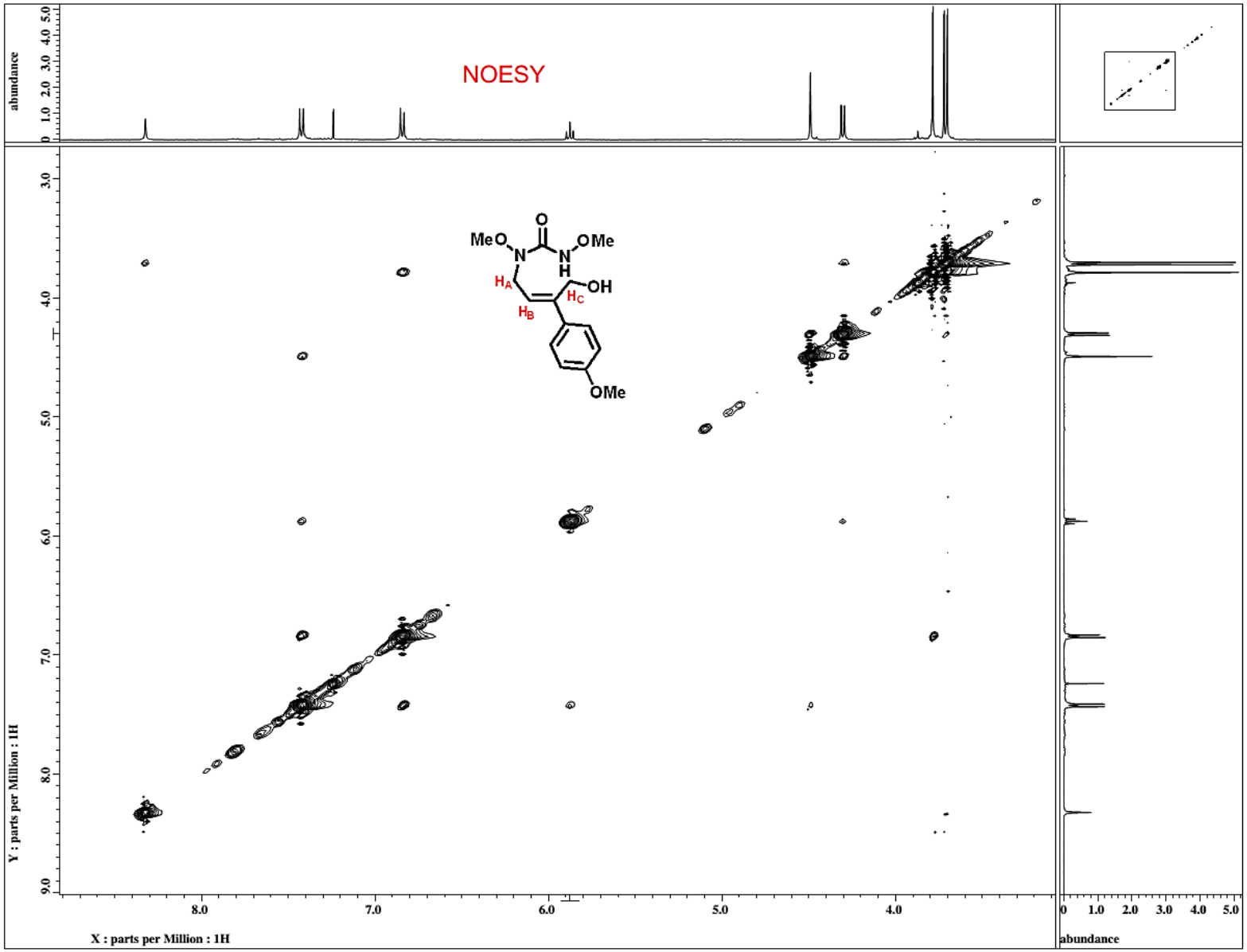
Monoisotopic Mass, Even Electron Ions
45 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 8-30 H: 8-25 N: 0-4 O: 0-10

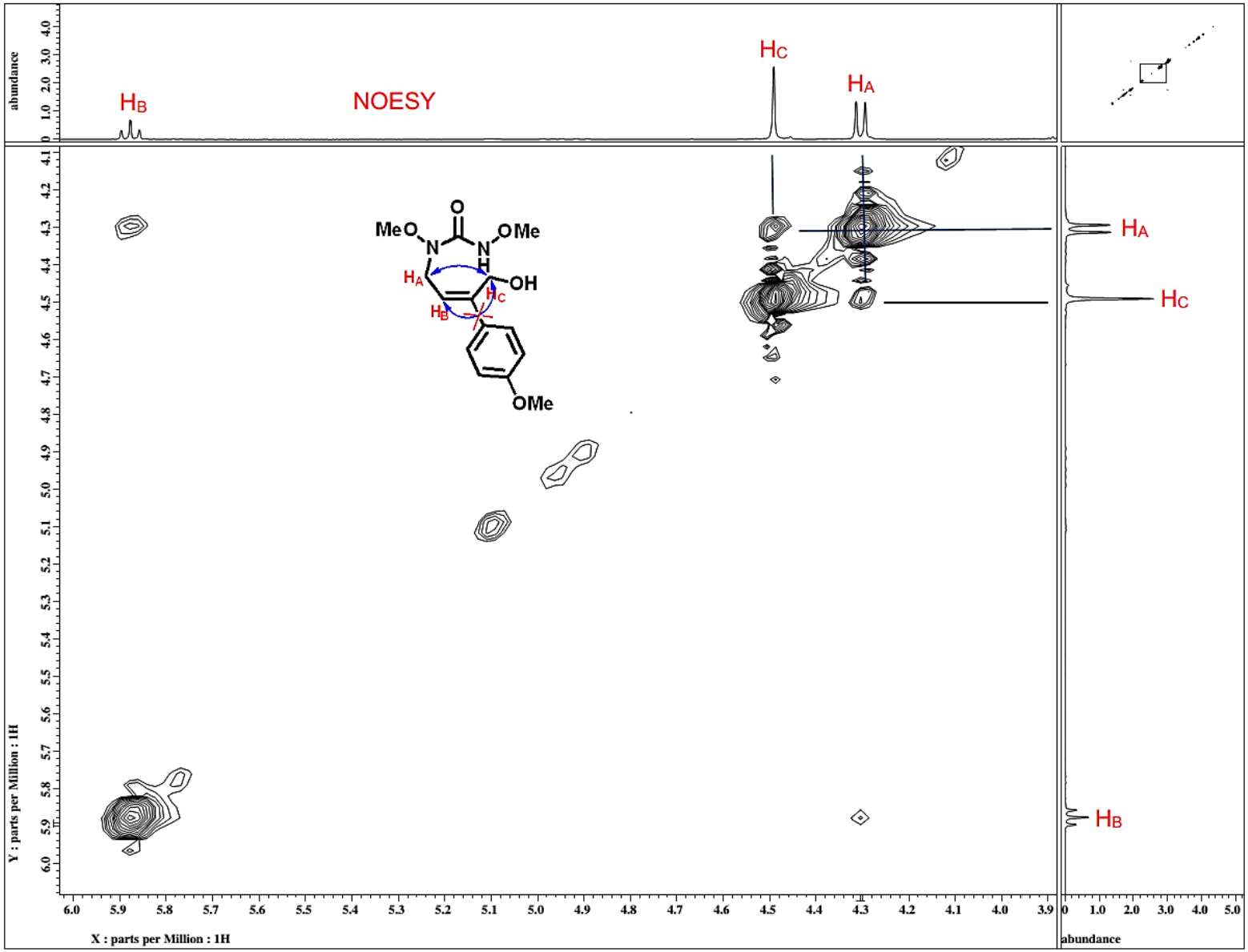
Sample Name : 15-02-098 IITRPR XEVO G2-XS QTC
Test Name : HRMS-1
040220-15-02-098 14 (0.148) 1: TOF MS ES-
7.62e+0C



Minimum:				-1.5				
Maximum:		5.0	15.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
535.1445	535.1465	-2.0	-3.7	17.5	1313.2	n/a	n/a	C26 H23 N4 O9


13C-NMR (CDCl3, 100 MHz)
1.01
2.05
2.11
1
2.01
2.09
3.08
3.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.3431
7.4445
6.8637
5.8969
4.5109
4.3241
3.8052
3.7399
3.7216
MeO
N
O
N
H
OMe
OH
(3p)
OMe
13C-NMR (CDCl3, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
160.5065
159.3718
143.7256
133.3329
127.6026
121.3670
113.8728
64.9699
62.4338
59.8594
55.4068
55.3972
46.3680


NOESY
abundance
MeO
OMe
N
N
H
O
HA
HB
HC
OH
OMe
Y : parts per Million : 1H
X : parts per Million : 1H
abundance


NOESY
HB
HC
HA
abundance
Y : parts per Million : 1H
X : parts per Million : 1H
MeO
OMe
N
N
H
OH
OMe
HA
HC
HB

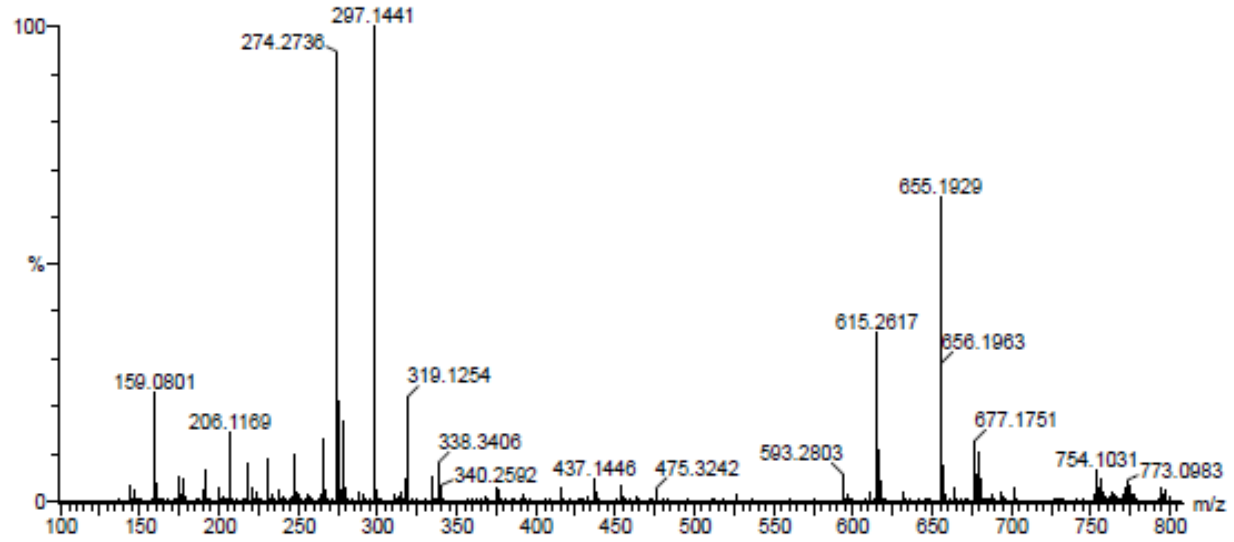
Elemental Composition Report

Single Mass Analysis

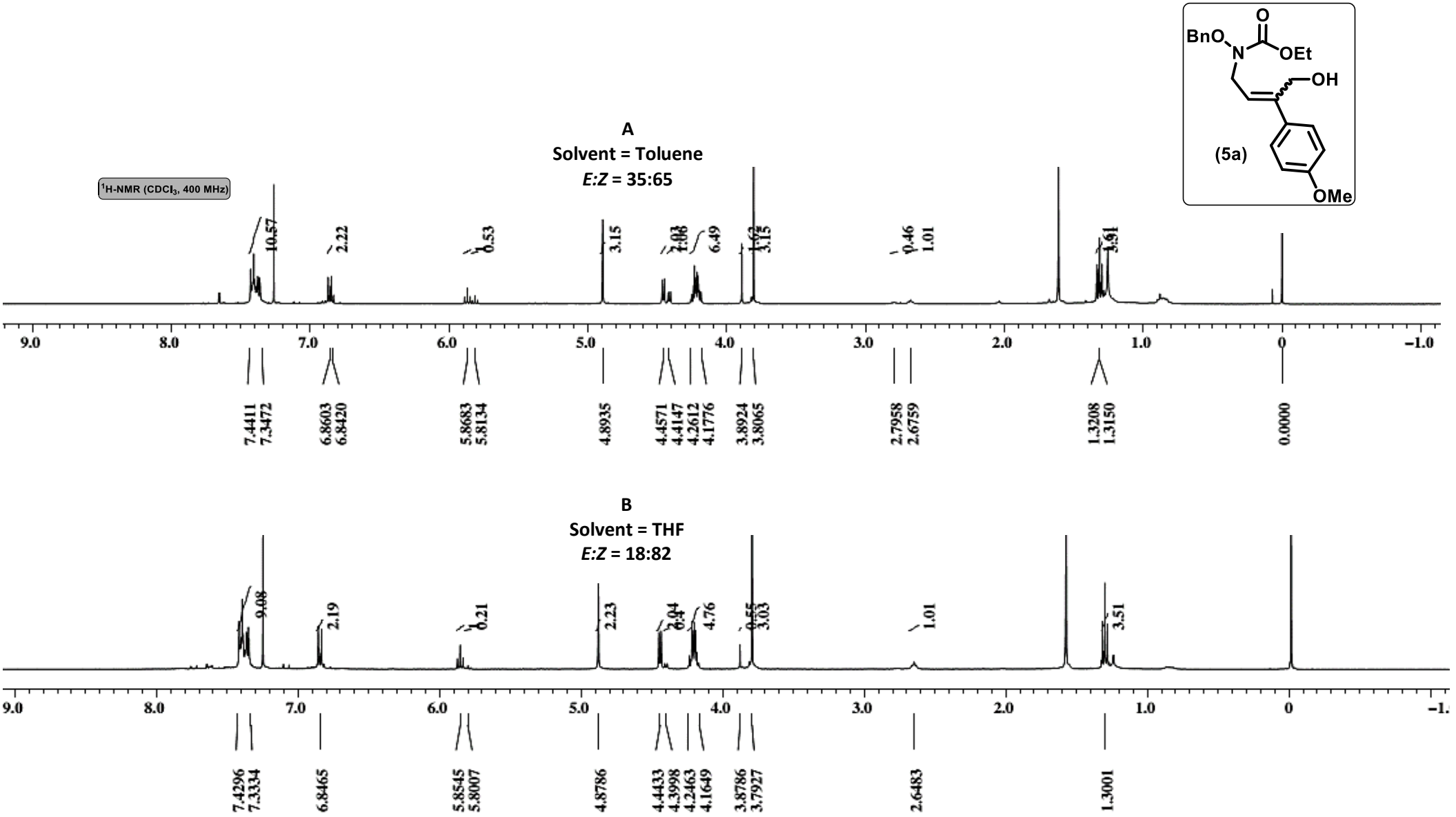
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

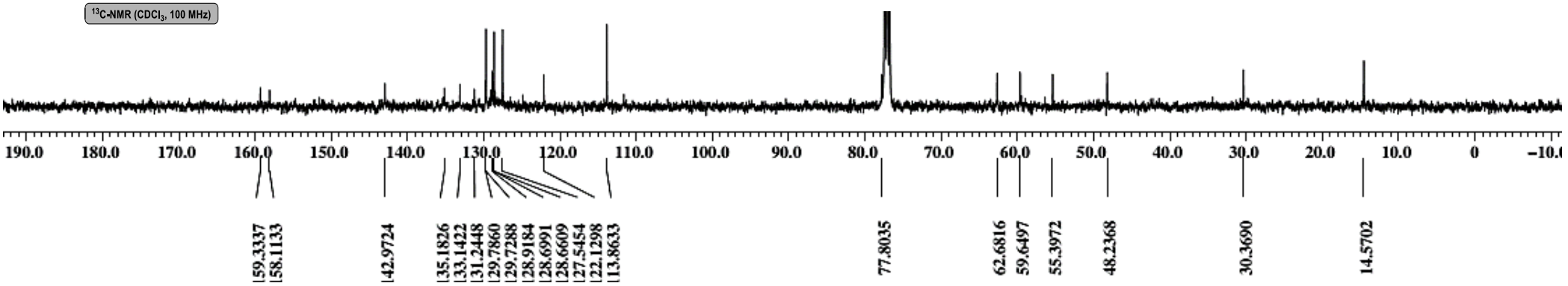
Monoisotopic Mass, Even Electron Ions
29 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-20 H: 11-35 N: 0-2 O: 0-5

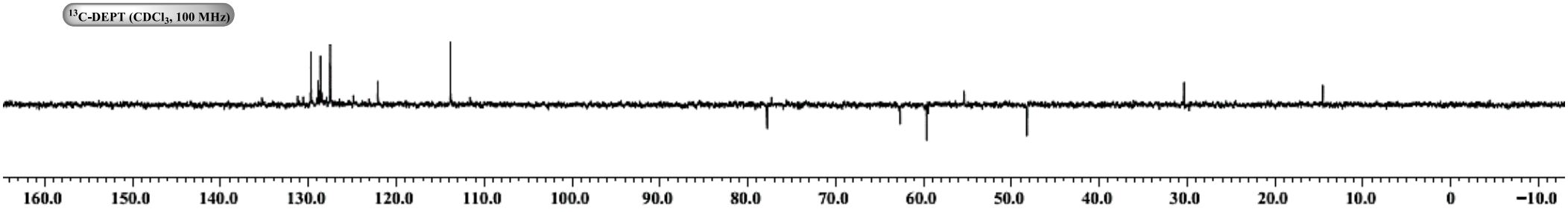
15-02-168 IITRPR UPLC-XEVOG2XSQTOF
060320-15-02-168 15 (0.157) AM2 (Ar,22000.0,0.00,0.00); Cm (9:26) 1: TOF MS ES+
1.31e+008

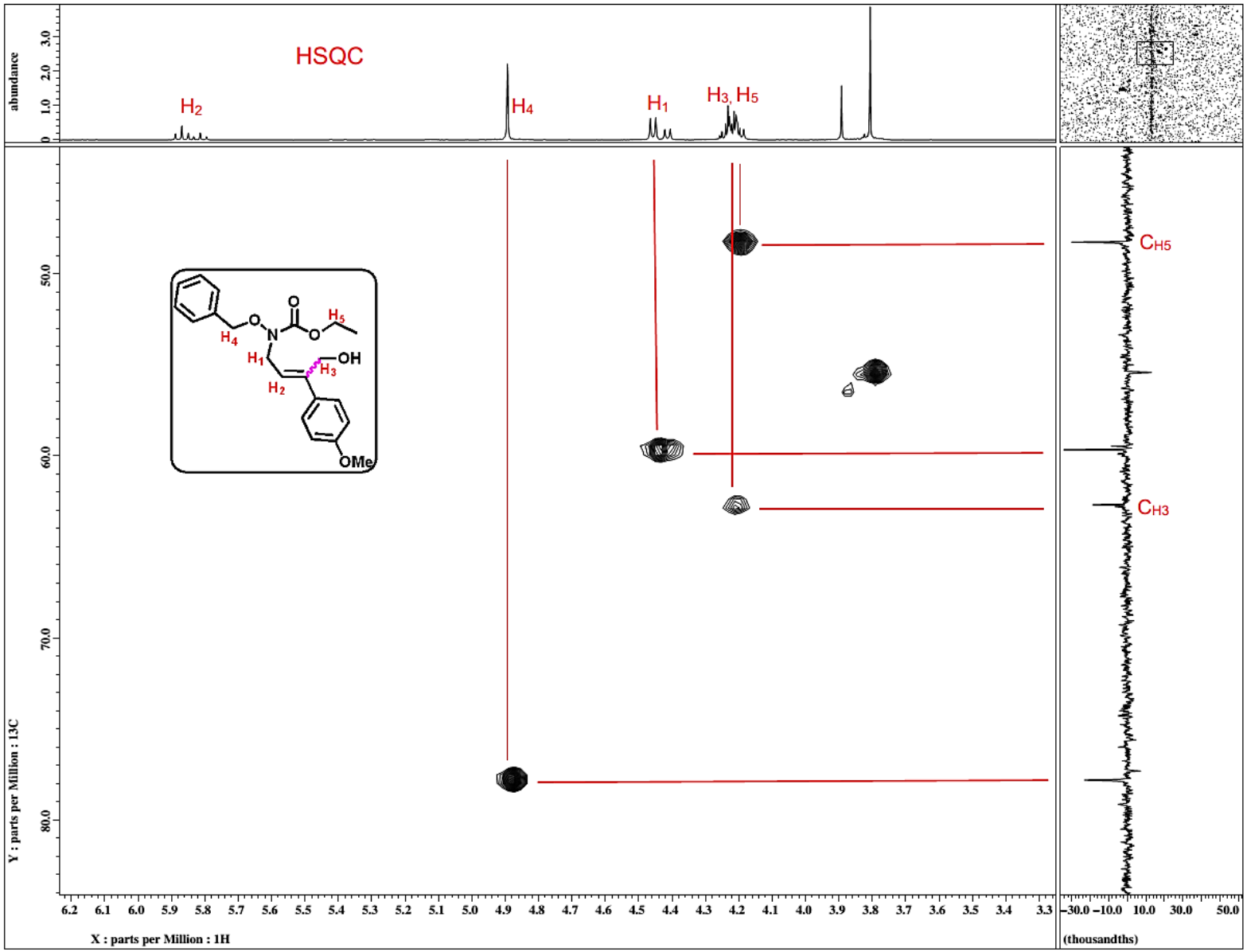


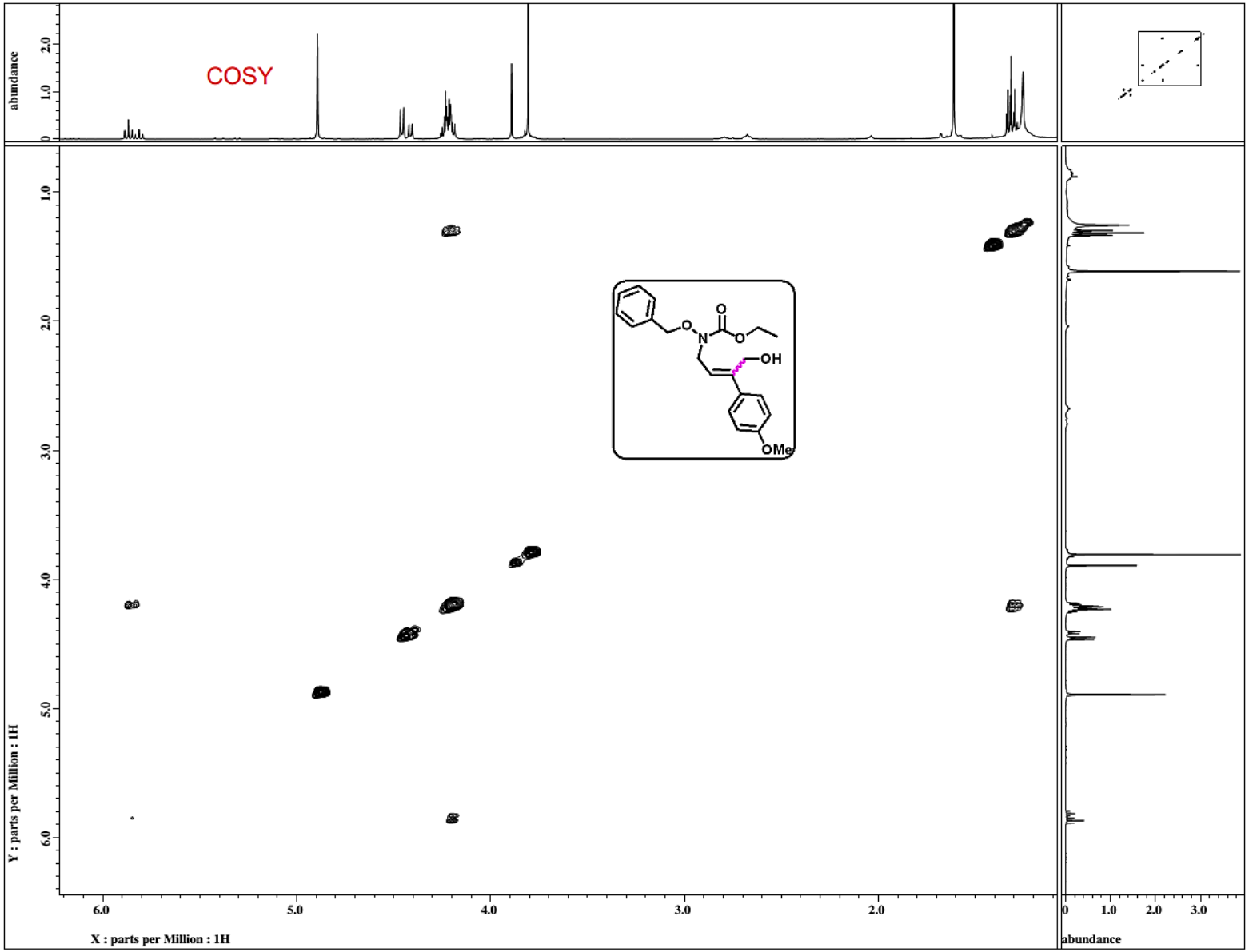
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
297.1441	297.1450	-0.9	-3.0	5.5	1104.6	n/a	n/a	C14 H21 N2 O5

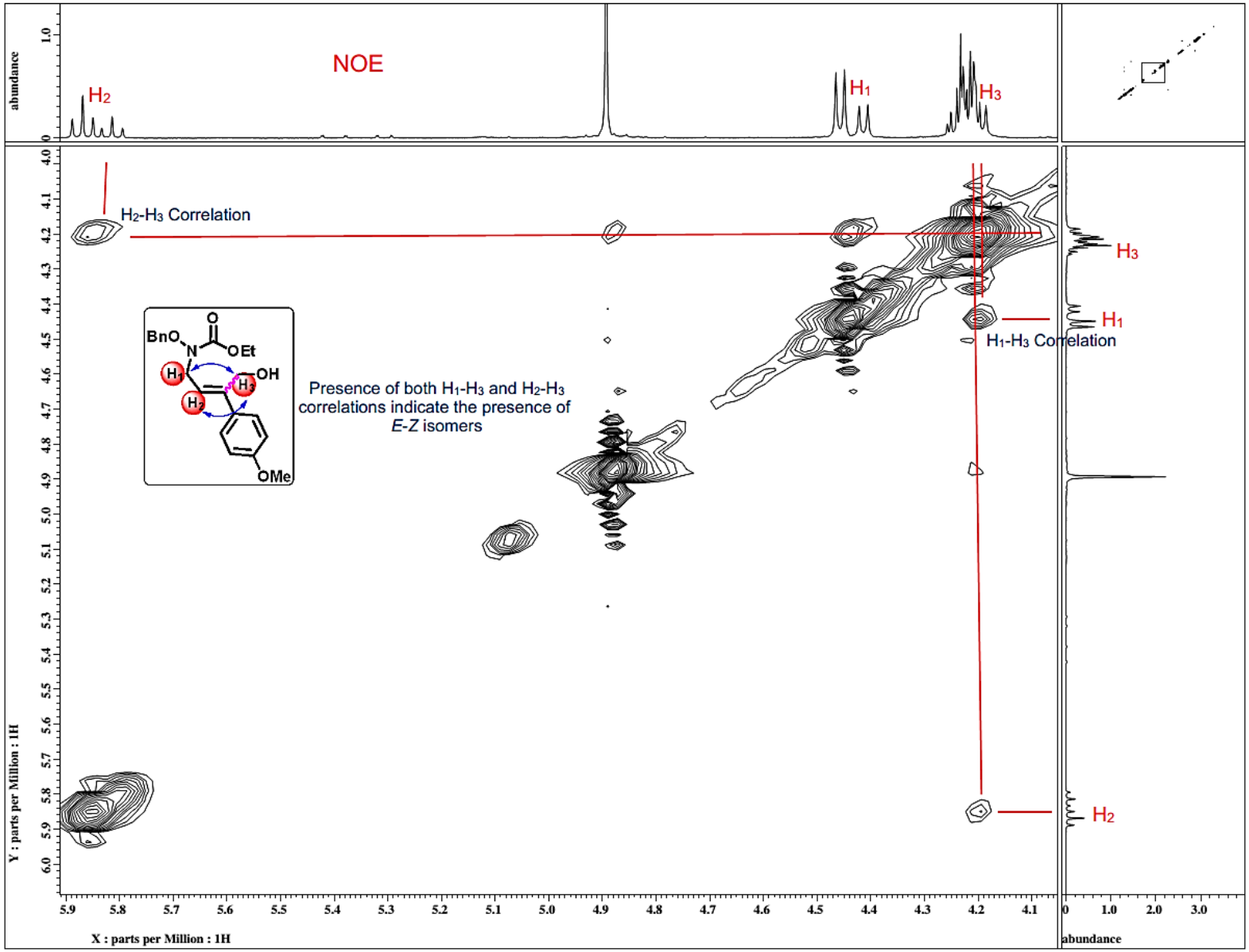

A
Solvent = Toluene
E:Z = 35:65
1H-NMR (CDCl3, 400 MHz)
BnO
N
O
OEt
OH
(5a)
OMe
10.57
2.22
0.53
3.15
6.49
0.46
1.01
7.4411
7.3472
6.8603
6.8420
5.8683
5.8134
4.8935
4.4571
4.4147
4.2612
4.1776
3.8924
3.8065
2.7958
2.6759
1.3208
1.3150
0.0000
B
Solvent = THF
E:Z = 18:82
9.08
2.19
0.21
2.23
4.76
1.01
3.51
7.4296
7.3334
6.8465
5.8545
5.8007
4.8786
4.4433
4.3998
4.2463
4.1649
3.8786
3.7927
2.6483
1.3001


^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
159.3337
158.1133
142.9724
135.1826
133.1422
131.2448
129.7860
129.7288
128.9184
128.6991
128.6609
127.5454
122.1298
113.8633
77.8035
62.6816
59.6497
55.3972
48.2368
30.3690
14.5702


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0


HSQC
abundance
H2
H4
H1
H3, H5
CH5
CH3
OH
OMe
Y : parts per Million : 13C
X : parts per Million : 1H
(thousandths)


COSY
abundance
Y : parts per Million : 1H
X : parts per Million : 1H
OH
OMe

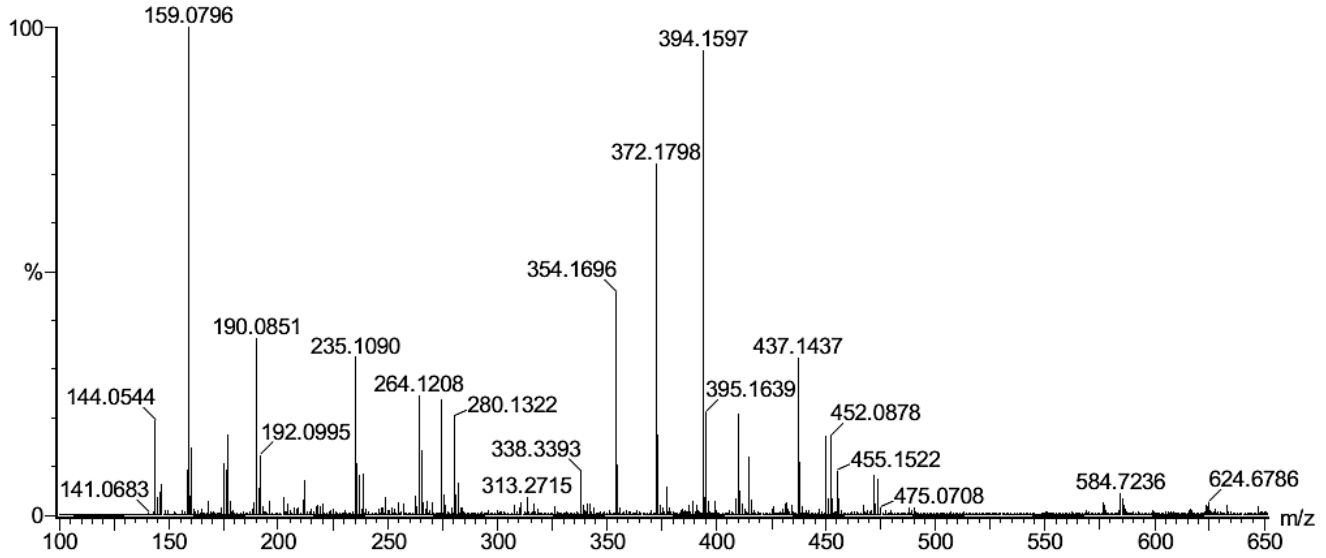

NOE
H2
H1
H3
abundance
H2-H3 Correlation
H1-H3 Correlation
Presence of both H1-H3 and H2-H3 correlations indicate the presence of E-Z isomers
BnO
N
OEt
O
OH
OMe
Y : parts per Million : 1H
X : parts per Million : 1H
abundance

Single Mass Analysis

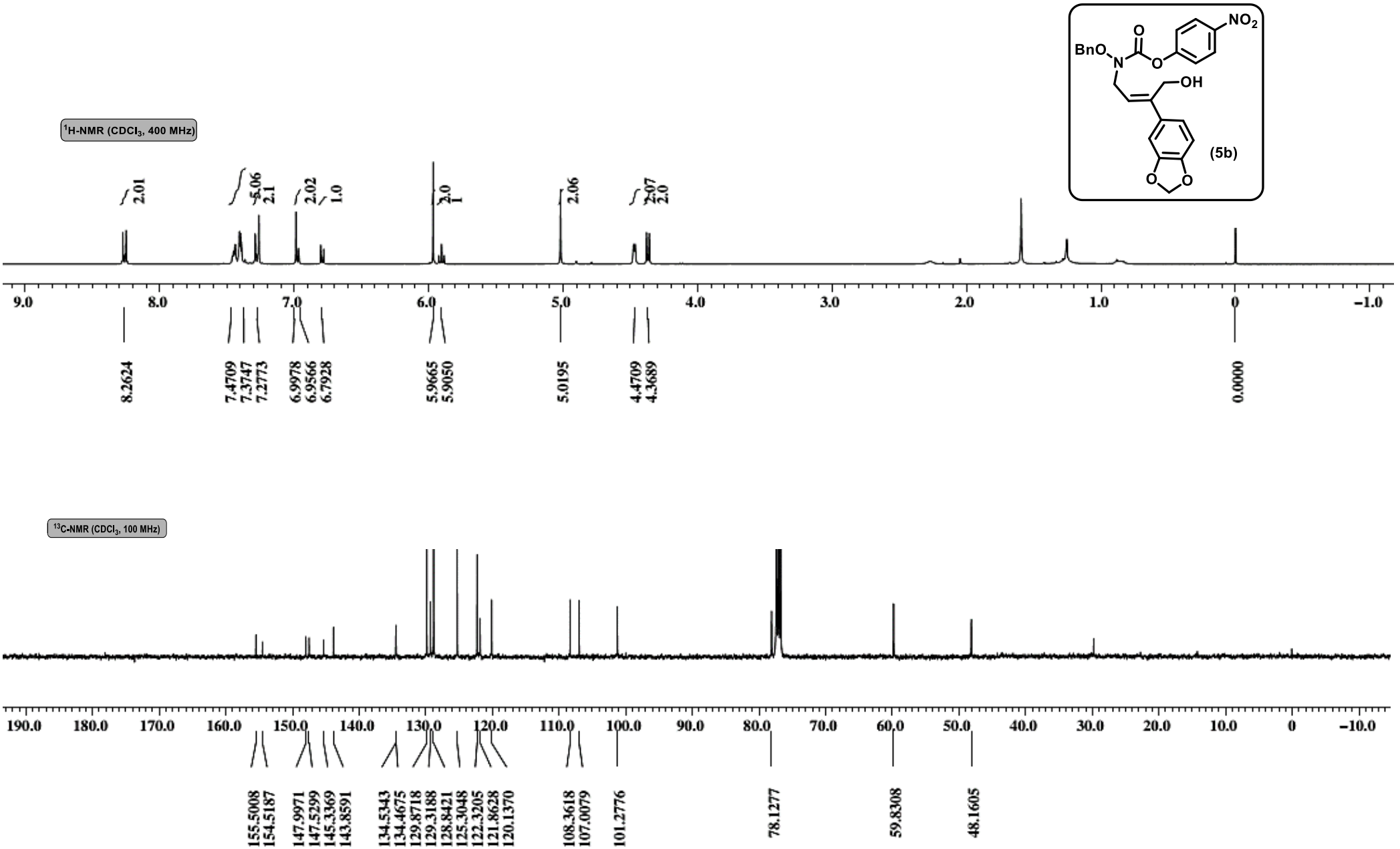
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

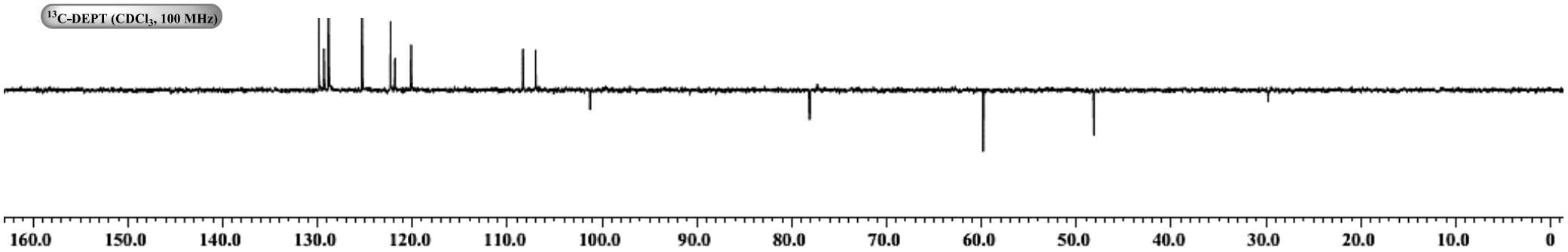
Monoisotopic Mass, Even Electron Ions
45 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-25 H: 8-30 N: 0-4 O: 0-5

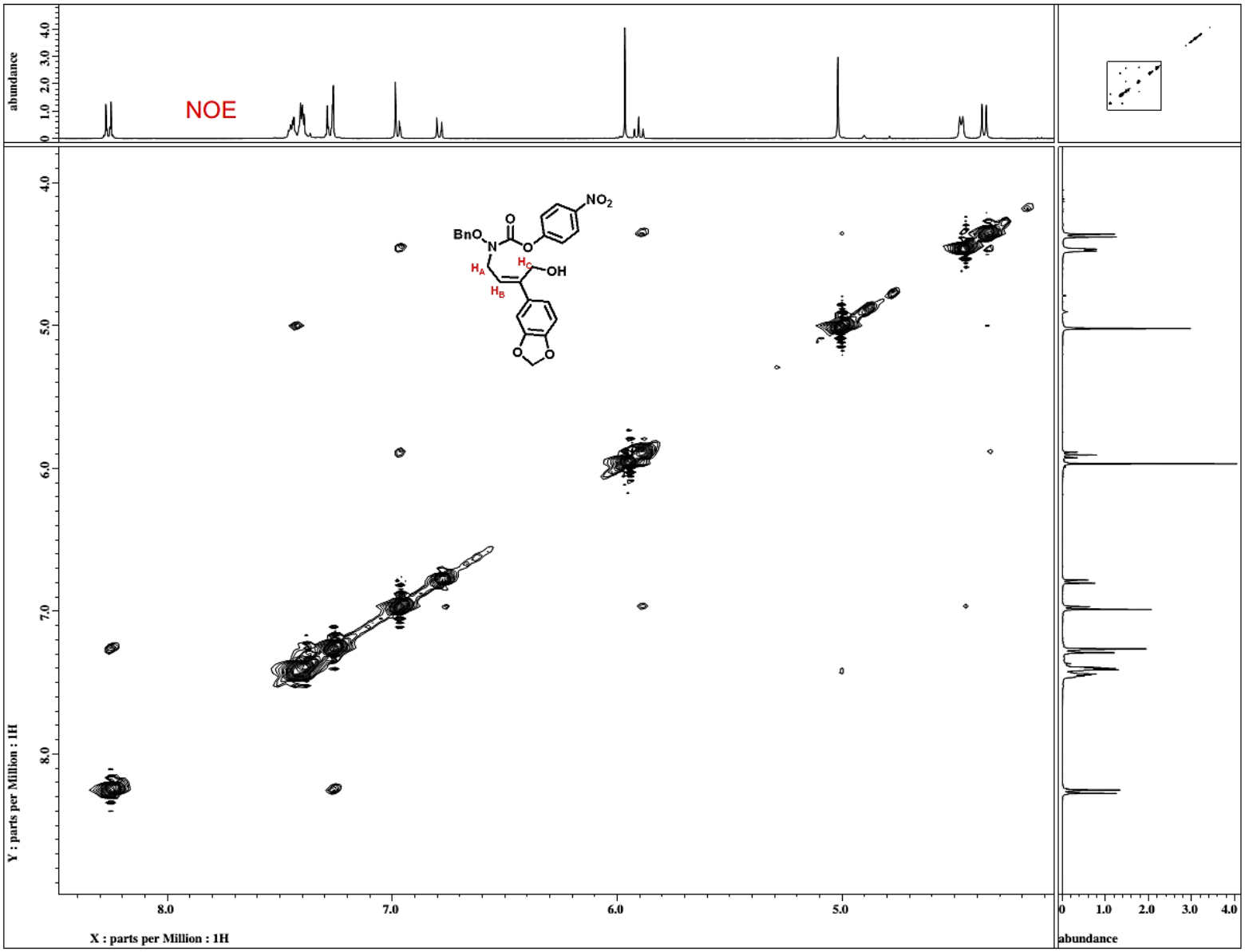
Sample Name : 15-02-067 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
120220-15-02-067 12 (0.131) 1: TOF MS ES+
4.99e+007

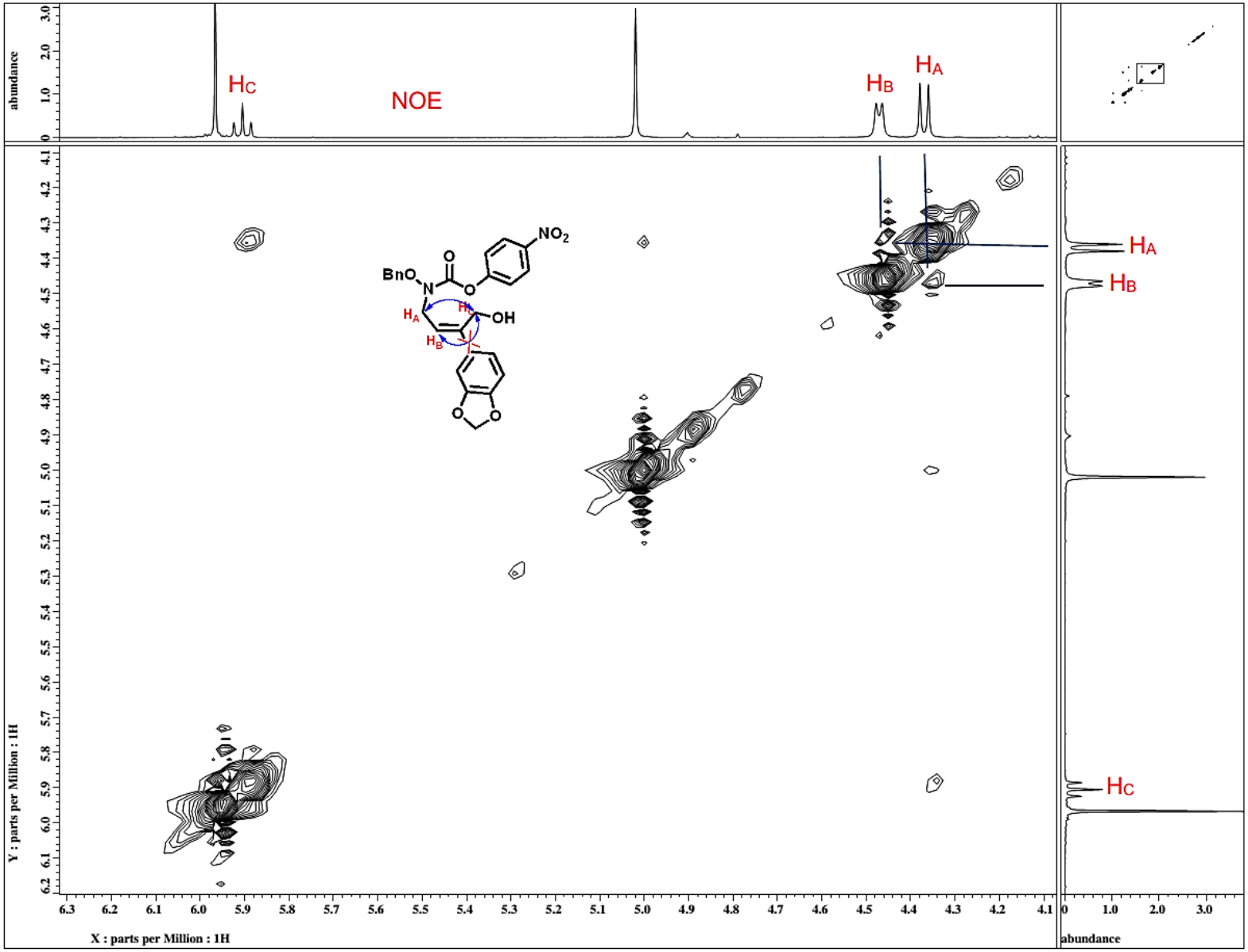


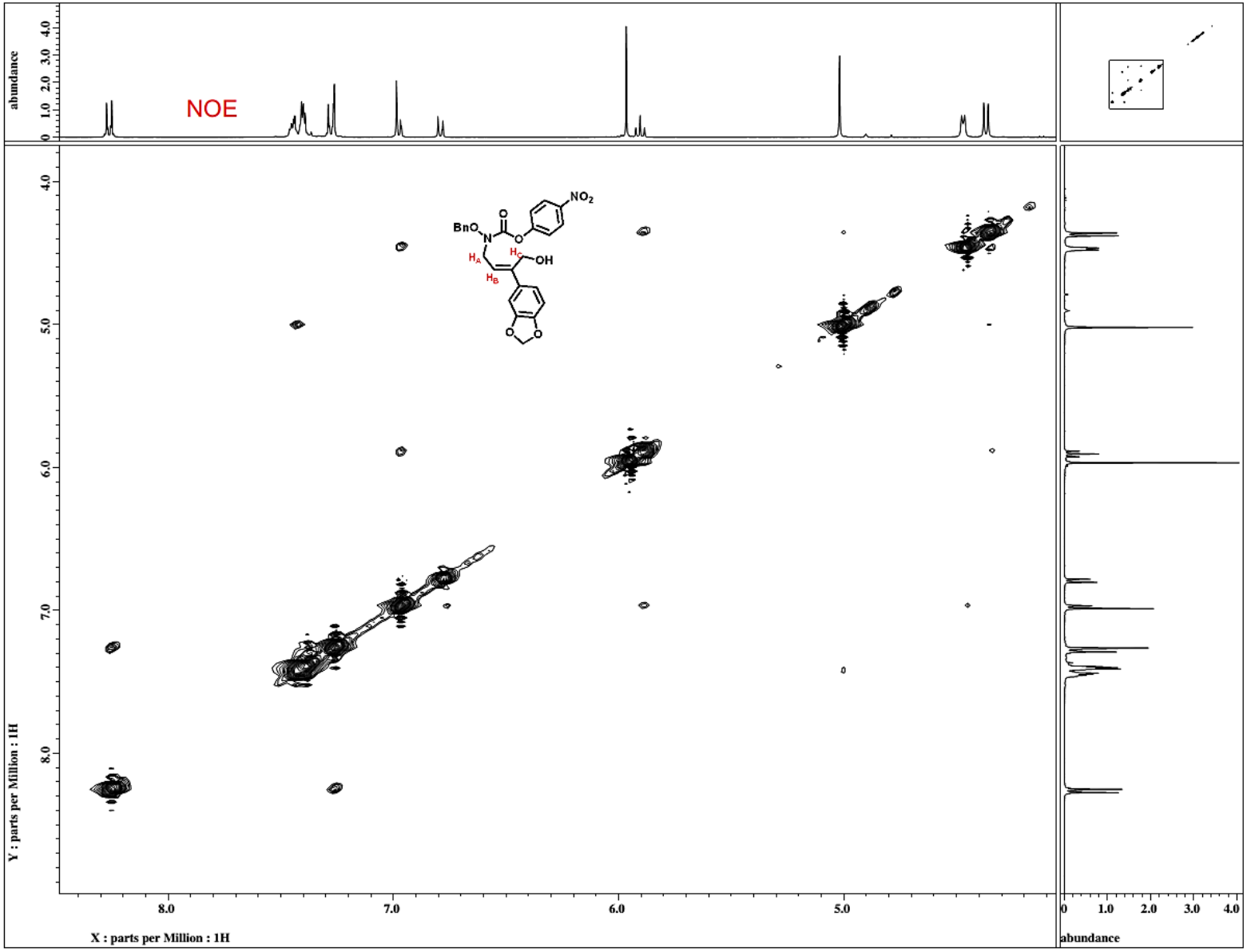
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
372.1798	372.1811	-1.3	-3.5	9.5	1566.8	n/a	n/a	C21 H26 N O5

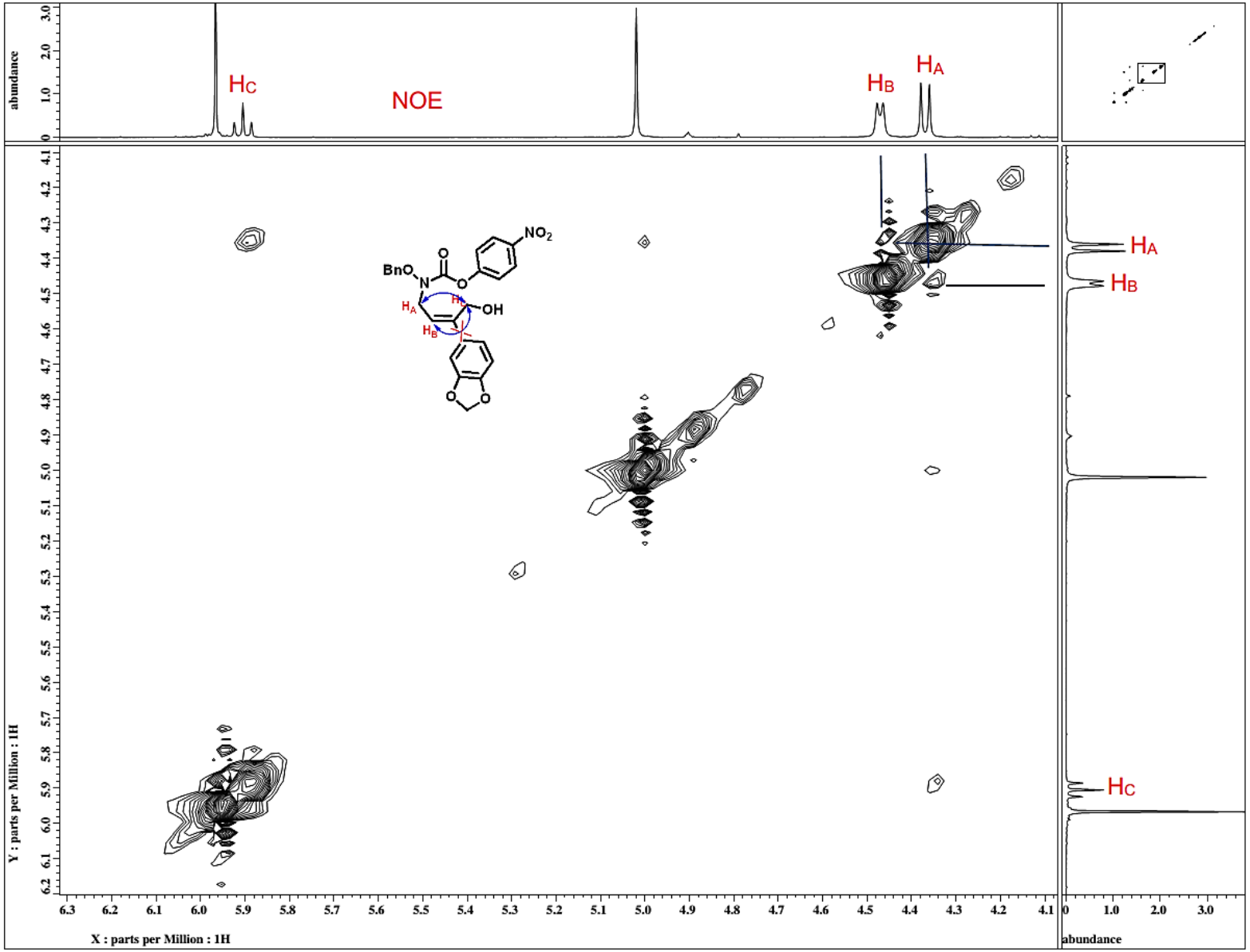

^{1}H-NMR ($CDCl_3$, 400 MHz)
^{13}C-NMR ($CDCl_3$, 100 MHz)
BnO
N
O
O
NO_2
OH
(5b)
2.01
5.06
2.1
2.02
1.0
2.0
1
2.06
2.07
2.0
8.2624
7.4709
7.3747
7.2773
6.9978
6.9566
6.7928
5.9665
5.9050
5.0195
4.4709
4.3689
0.0000
155.5008
154.5187
147.9971
147.5299
145.3369
143.8591
134.5343
134.4675
129.8718
129.3188
128.8421
125.3048
122.3205
121.8628
120.1370
108.3618
107.0079
101.2776
78.1277
59.8308
48.1605


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0


NOE
abundance
BnO
N
O
O
NO2
HA
HB
HC
OH
Y : parts per Million : 1H
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
abundance


abundance
HC
NOE
HB
HA
HA
HB
HC
Y : parts per Million : 1H
X : parts per Million : 1H
abundance
BnO
NO2
OH
HA
HB


NOE
abundance
Y : parts per Million : 1H
X : parts per Million : 1H
abundance
BnO
N
O
O
NO2
HA
HB
HC
OH


abundance
HC
NOE
HB
HA
NO2
BnO
N
O
OH
HA
HB
HA
HB
HC
Y : parts per Million : 1H
X : parts per Million : 1H
abundance

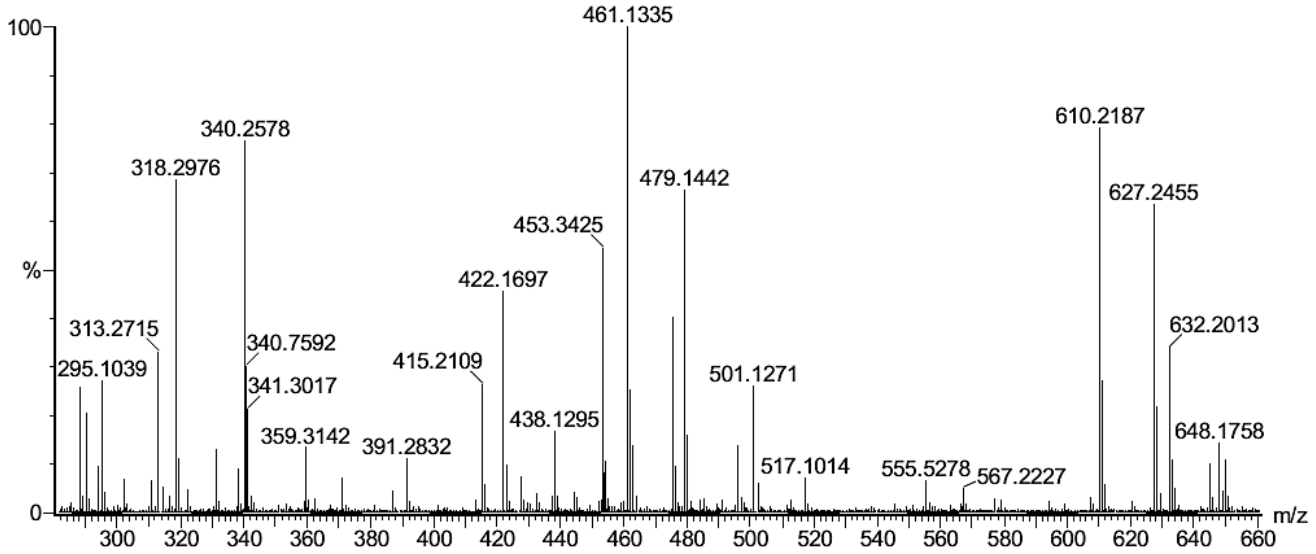
Elemental Composition Report

Single Mass Analysis

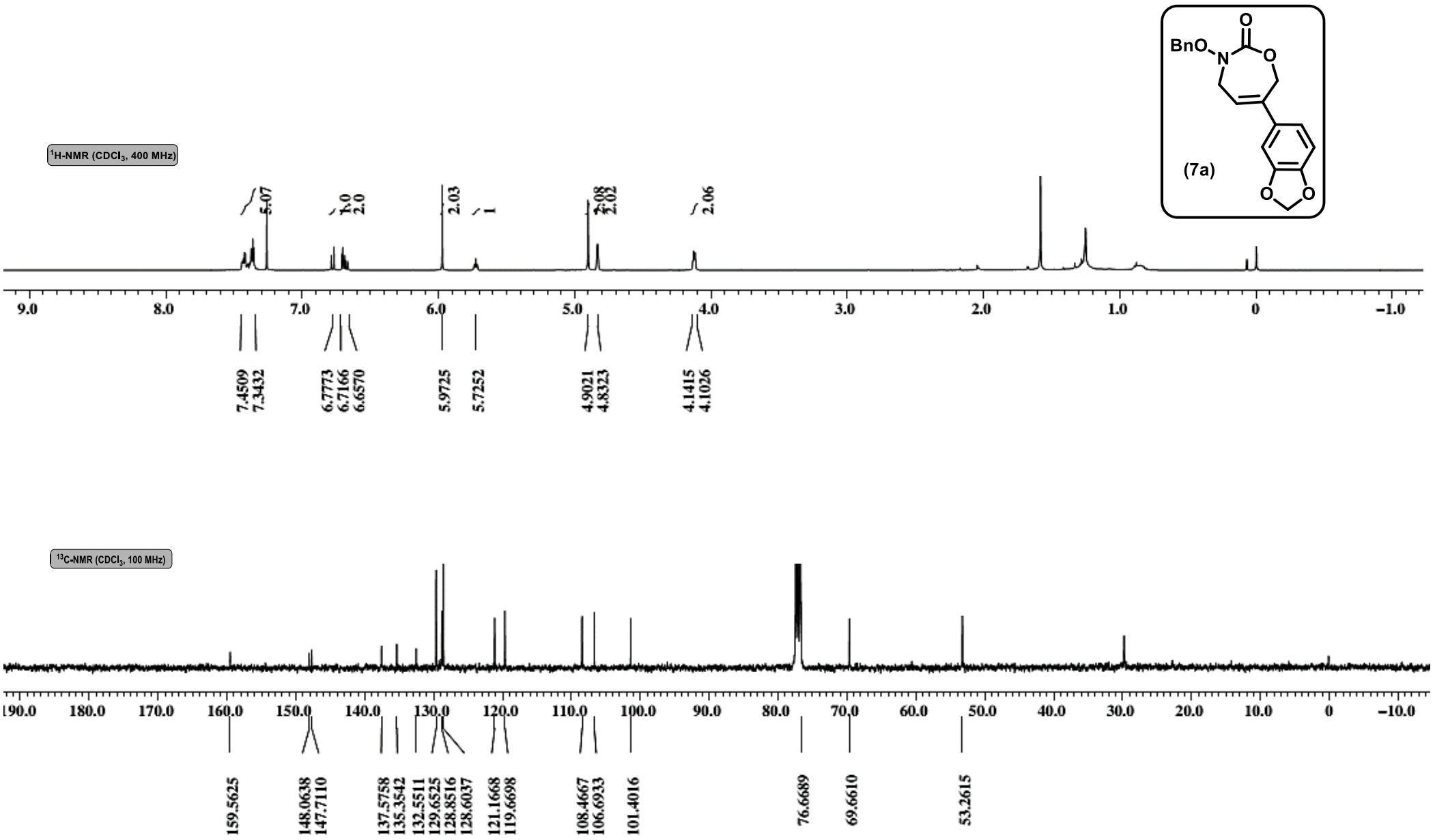
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

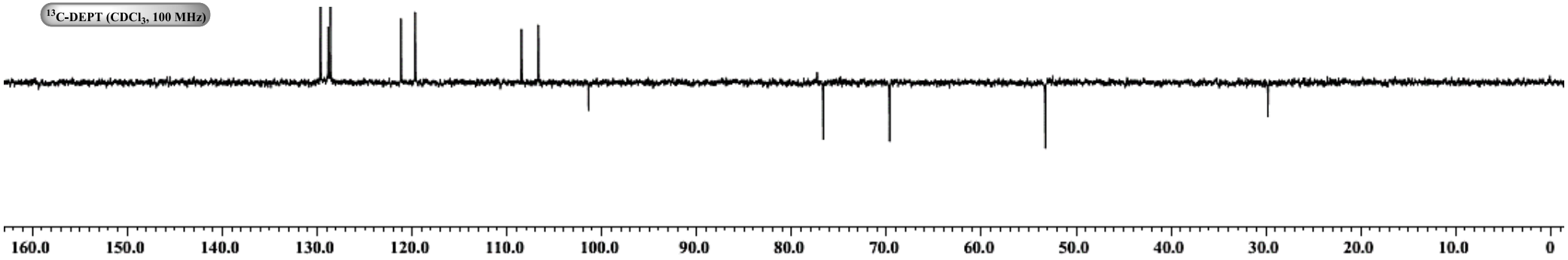
Monoisotopic Mass, Even Electron Ions
73 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-30 H: 9-35 N: 0-5 O: 1-8

Sample Name : 15-02-116 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
181119-15-02-116 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (8:19) 1: TOF MS ES+
9.24e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
479.1442	479.1454	-1.2	-2.5	15.5	515.1	n/a	n/a	C25 H23 N2 O8


BnO
N
O
O
O
O
O
(7a)
^{1}H-NMR (CDCl$_3$, 400 MHz)
5.07
1.0
2.0
2.03
1
2.08
2.02
2.06
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.4509
7.3432
6.7773
6.7166
6.6570
5.9725
5.7252
4.9021
4.8323
4.1415
4.1026
^{13}C-NMR (CDCl$_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
159.5625
148.0638
147.7110
137.5758
135.3542
132.5511
129.6525
128.8516
128.6037
121.1668
119.6698
108.4667
106.6933
101.4016
76.6689
69.6610
53.2615

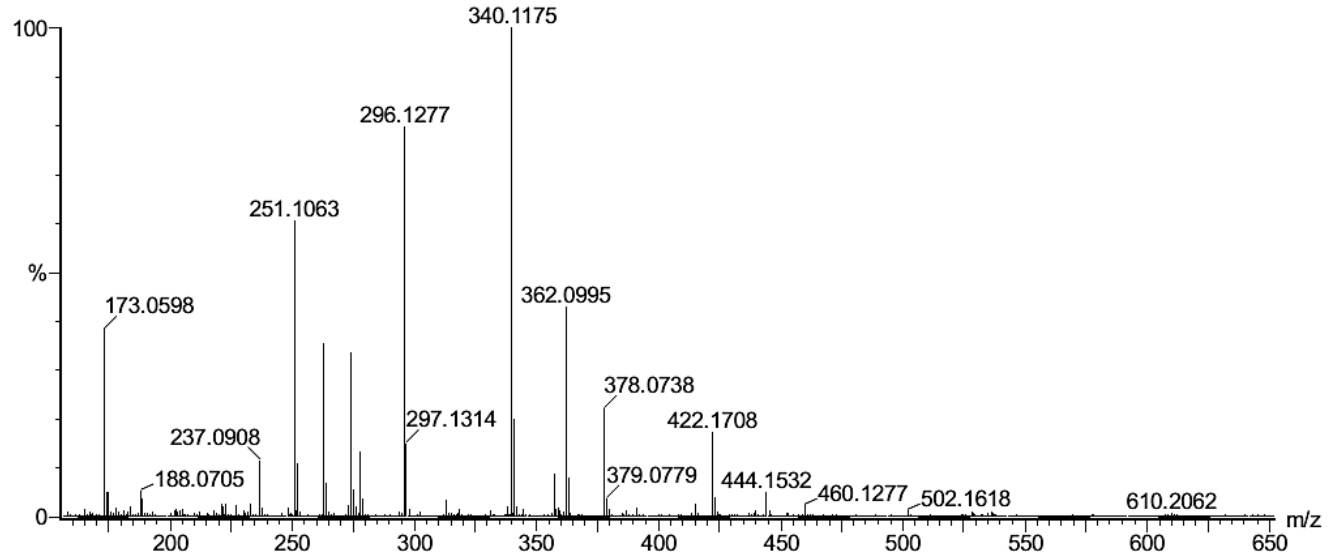

^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Single Mass Analysis

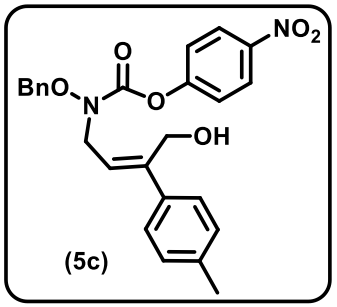
Tolerance = 40.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
56 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-30 H: 9-40 N: 0-2 O: 1-7

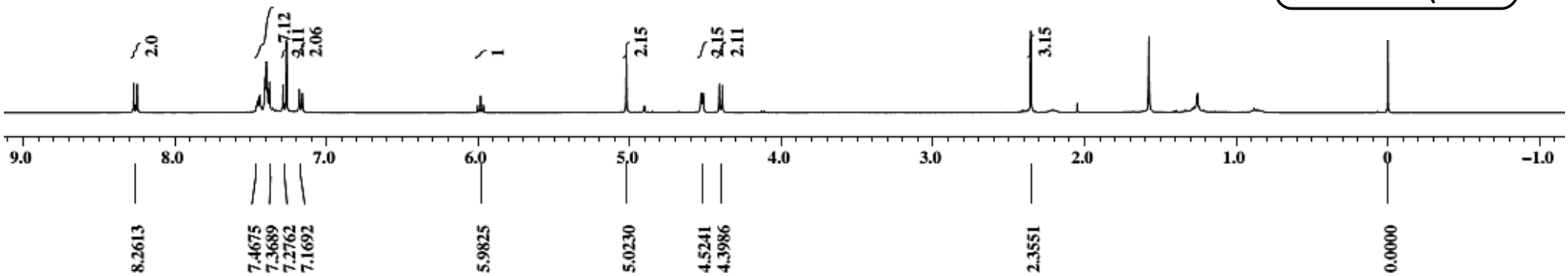
Sample Name : 15-02-117 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
191119-15-02-117 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (9:18) 1: TOF MS ES+
3.54e+007



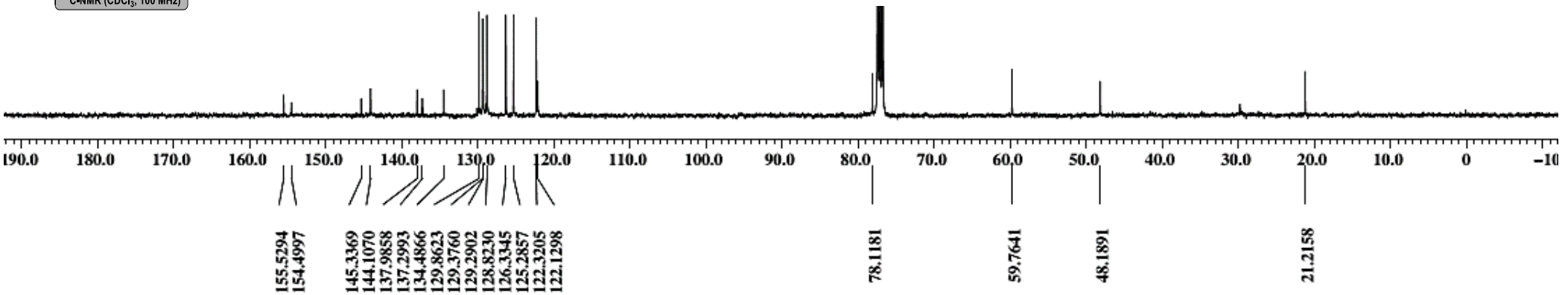
Minimum:				-1.5				
Maximum:		5.0	40.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
340.1175	340.1185	-1.0	-2.9	11.5	863.9	n/a	n/a	C19 H18 N O5

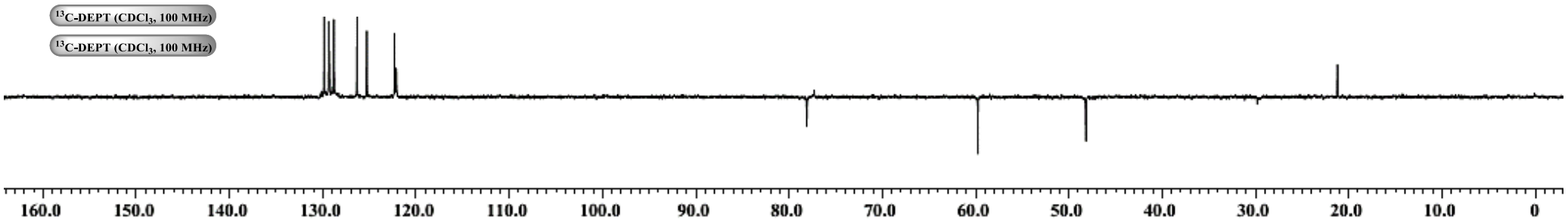


^{1}H-NMR ($CDCl_3$, 400 MHz)



^{13}C-NMR ($CDCl_3$, 100 MHz)



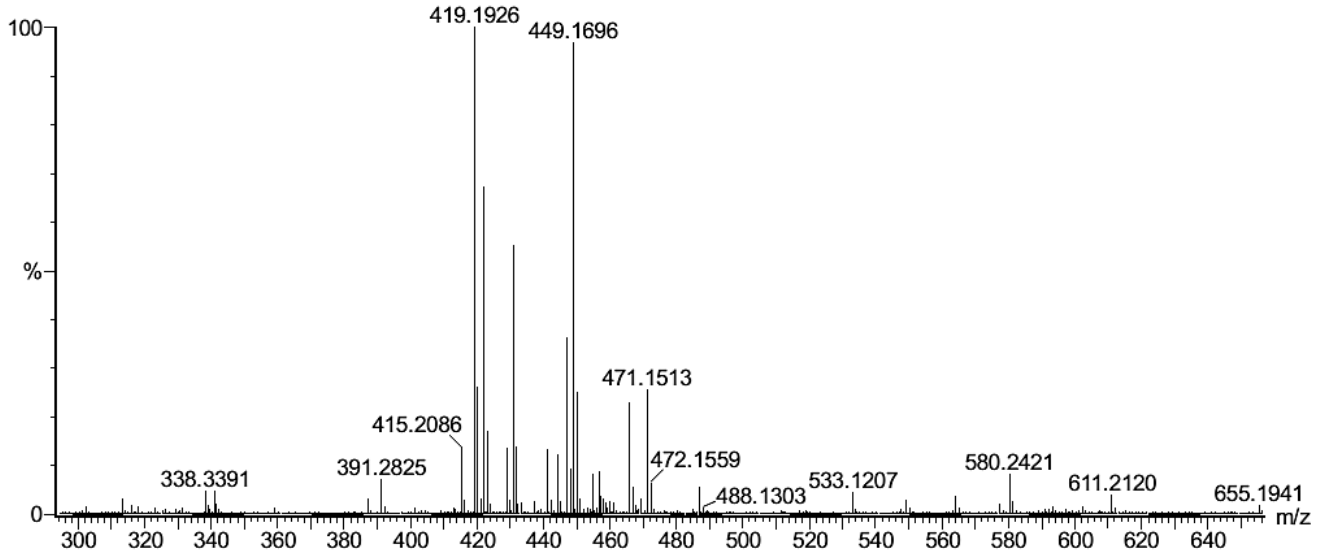

^{13}C-DEPT ($CDCl_3$, 100 MHz)
^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Single Mass Analysis

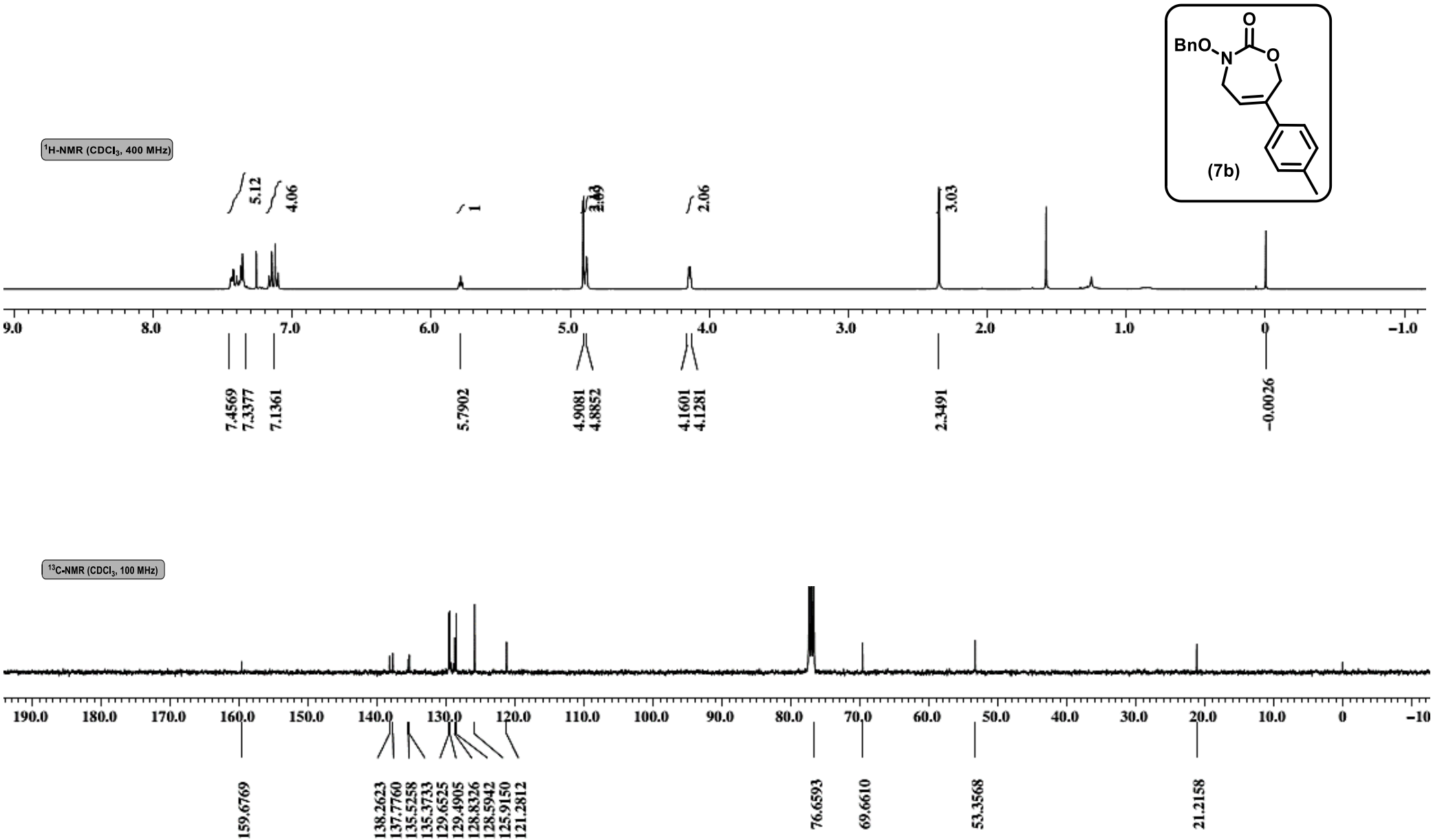
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

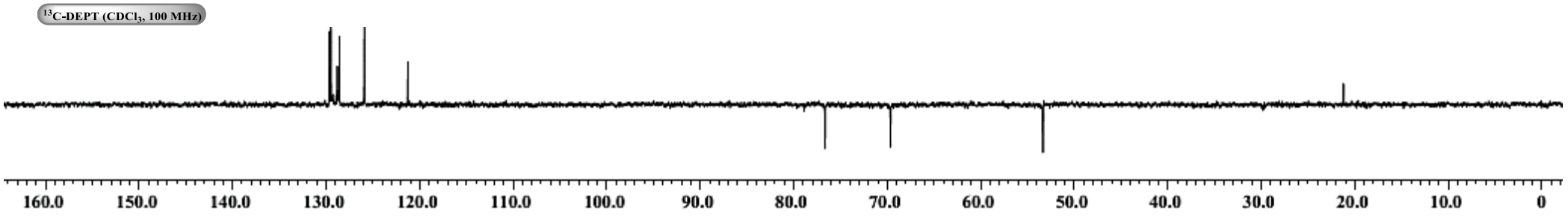
Monoisotopic Mass, Even Electron Ions
39 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-30 H: 7-35 N: 0-3 O: 1-6

Sample Name : 15-02-118 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
221119-15-02-118 12 (0.131) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (7:19) 1: TOF MS ES+
1.99e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
449.1696	449.1713	-1.7	-3.8	14.5	722.6	n/a	n/a	C25 H25 N2 O6


(7b)
^{1}H-NMR ($CDCl_3$, 400 MHz)
5.12
4.06
1
2.06
3.03
7.4569
7.3377
7.1361
5.7902
4.9081
4.8852
4.1601
4.1281
2.3491
−0.0026
^{13}C-NMR ($CDCl_3$, 100 MHz)
159.6769
138.2623
137.7760
135.5258
135.3733
129.6525
129.4905
128.8326
128.5942
125.9150
121.2812
76.6593
69.6610
53.3568
21.2158


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

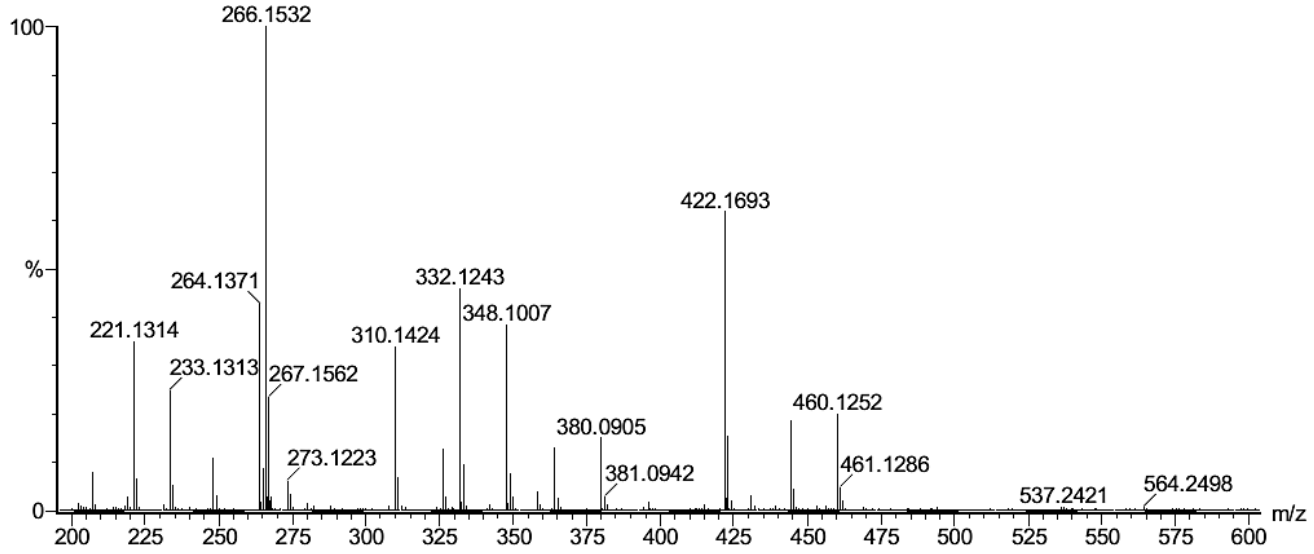
Elemental Composition Report

Single Mass Analysis

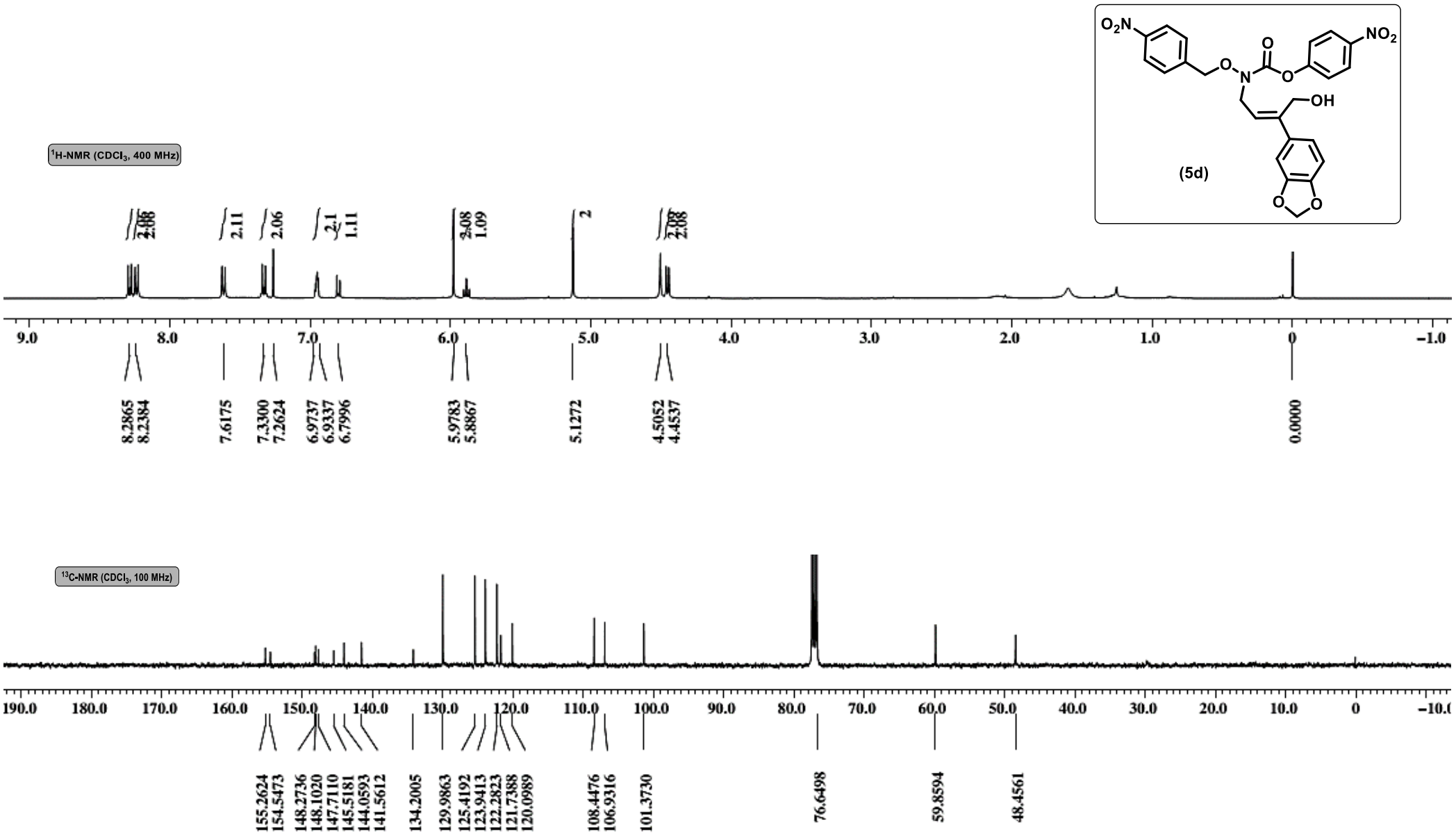
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

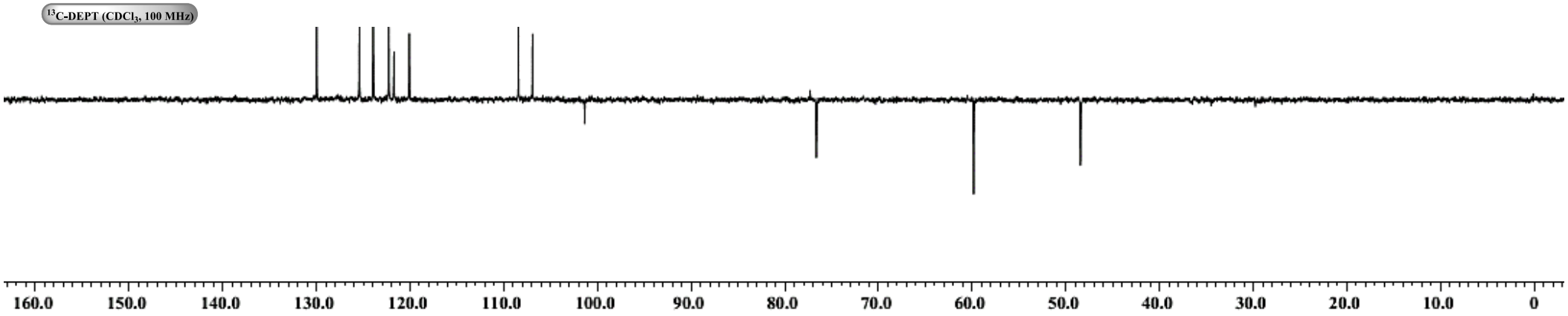
Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-25 H: 7-25 N: 0-3 O: 1-3

Sample Name : 18-01-120 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
251119-18-01-120 12 (0.131) AM2 (Ar,22000.0,0.00,0.00); Cm (8:18) 1: TOF MS ES+
1.00e+008



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
310.1424	310.1443	-1.9	-6.1	10.5	859.6	n/a	n/a	C19 H20 N O3


(5d)
^{1}H-NMR (CDCl$_3$, 400 MHz)
^{13}C-NMR (CDCl$_3$, 100 MHz)

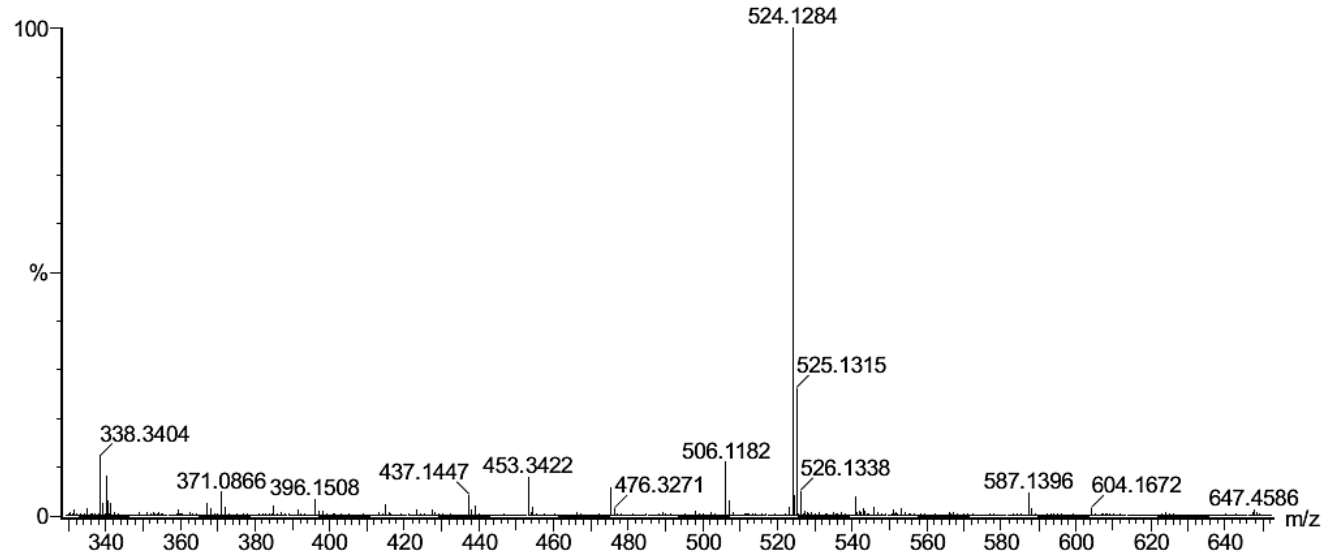

^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Single Mass Analysis

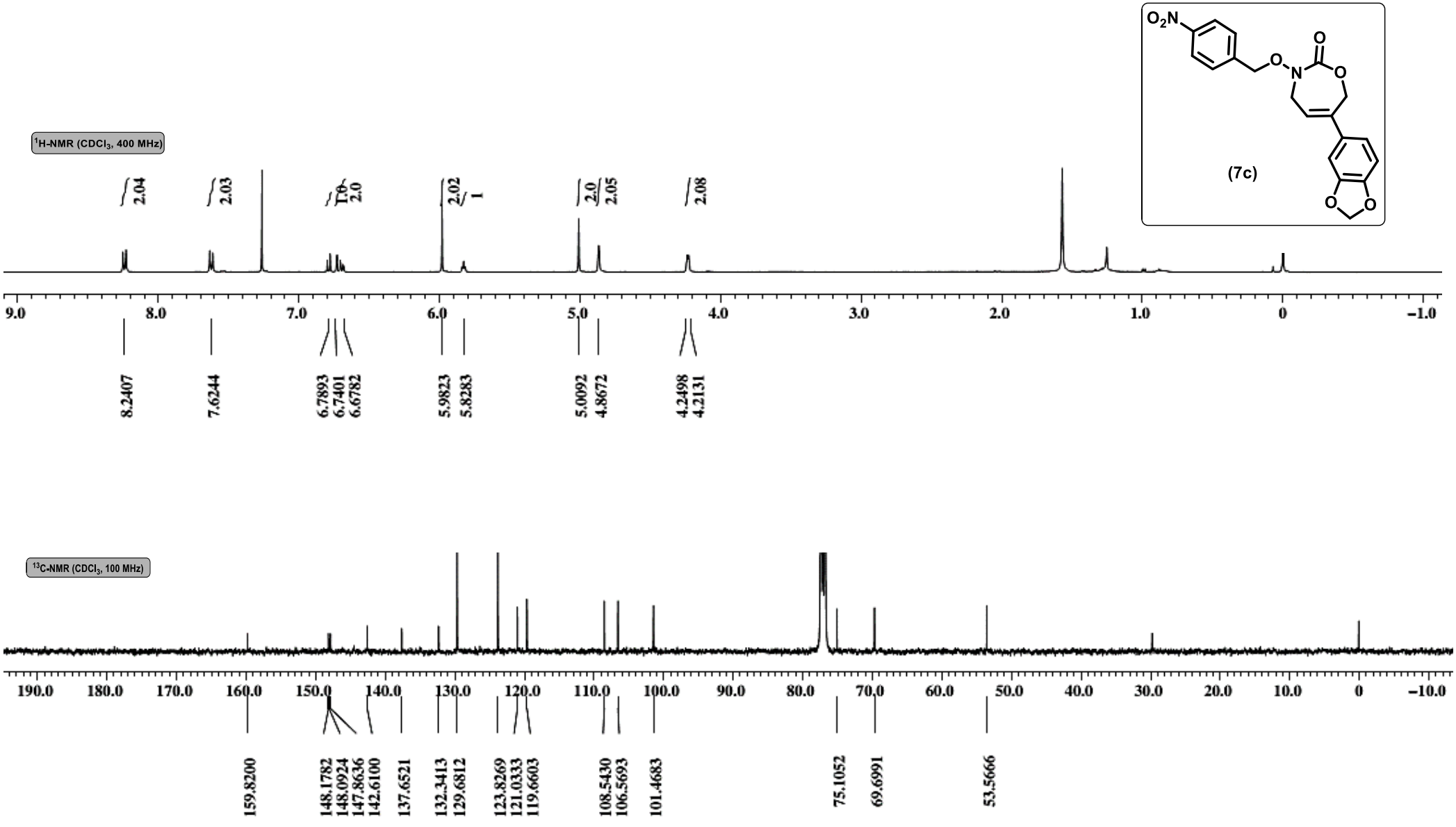
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 7

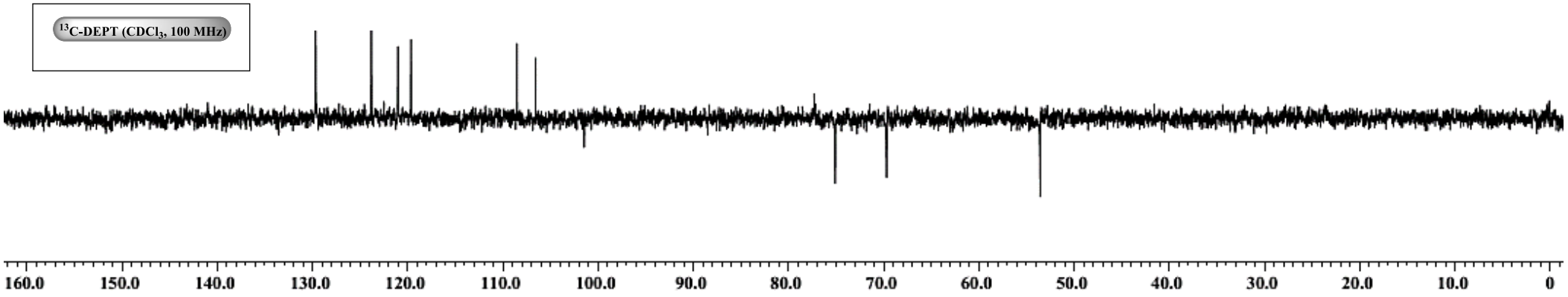
Monoisotopic Mass, Even Electron Ions
192 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 8-25 H: 7-35 B: 0-2 N: 0-5 O: 0-10

Sample Name : 15-02-136 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
231219-15-02-136 13 (0.140) AM2 (Ar,22000.0,0.00,0.00); Cm (13:20) 1: TOF MS ES+
3.08e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
524.1284	524.1305	-2.1	-4.0	16.5	1472.3	n/a	n/a	C25 H22 N3 O10


^{1}H-NMR ($CDCl_3$, 400 MHz)
2.04
2.03
1.0
2.0
2.02
1
2.0
2.05
2.08
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.2407
7.6244
6.7893
6.7401
6.6782
5.9823
5.8283
5.0092
4.8672
4.2498
4.2131
O_2N
O
N
O
O
O
O
(7c)
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
159.8200
148.1782
148.0924
147.8636
142.6100
137.6521
132.3413
129.6812
123.8269
121.0333
119.6603
108.5430
106.5693
101.4683
75.1052
69.6991
53.5666

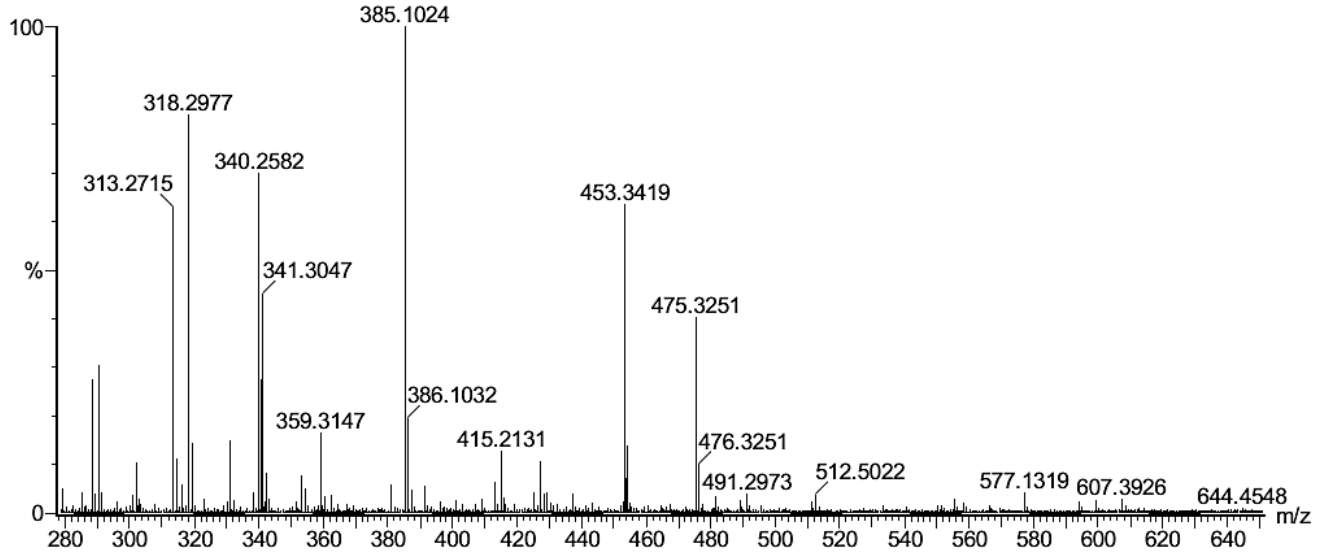

^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 7

Monoisotopic Mass, Even Electron Ions
291 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 8-25 H: 7-35 B: 0-2 N: 0-5 O: 0-7

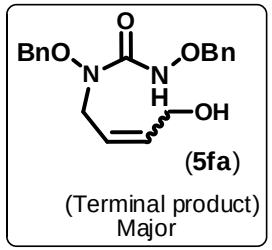
Sample Name : 15-02-137 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
231219-15-02-137 12 (0.131) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (6:19) 1: TOF MS ES+
9.65e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
385.1024	385.1036	-1.2	-3.1	12.5	2503.0	n/a	n/a	C19 H17 N2 O7

Reaction Solvent = Toluene

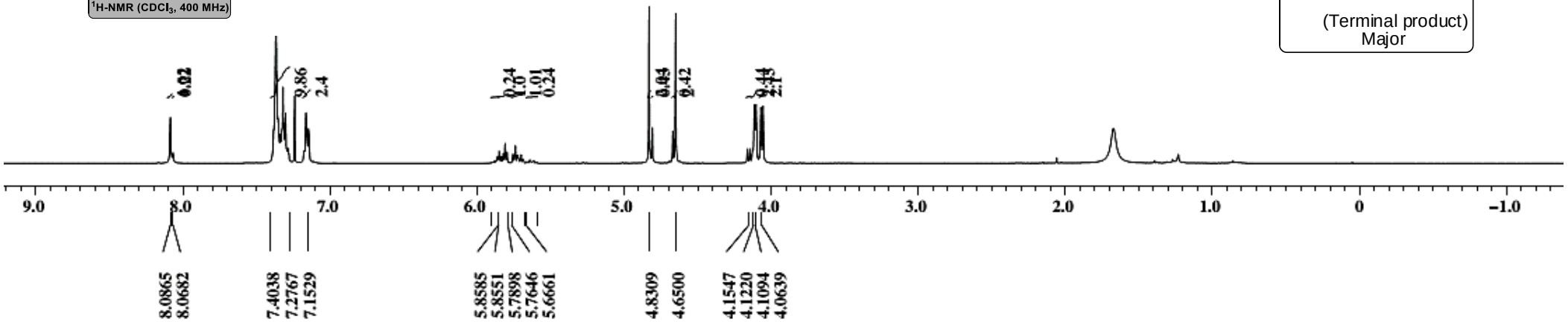
***E:Z* = 24:76**



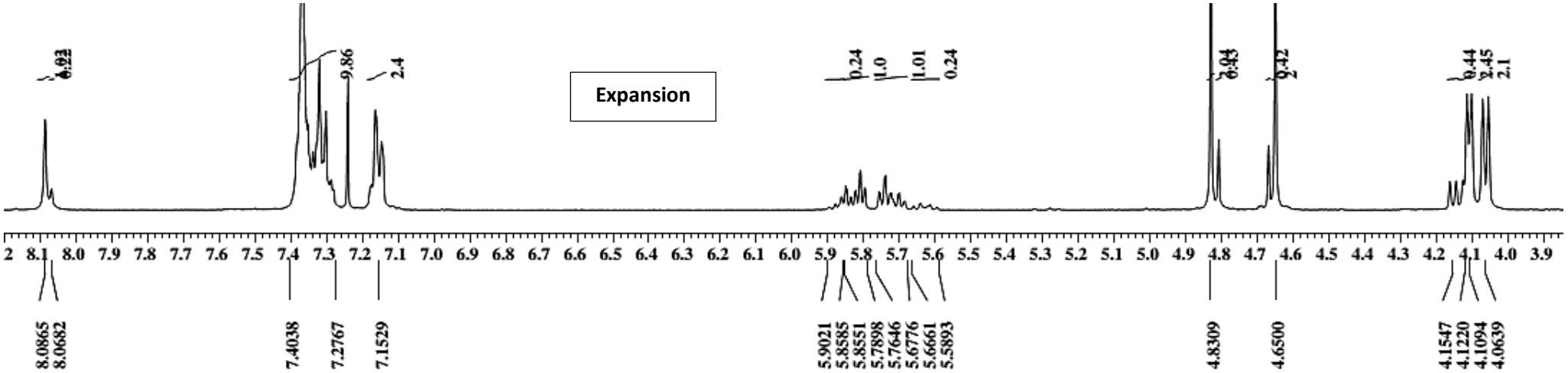
(**5fa**)

(Terminal product)
Major

^{1}H-NMR ($CDCl_3$, 400 MHz)

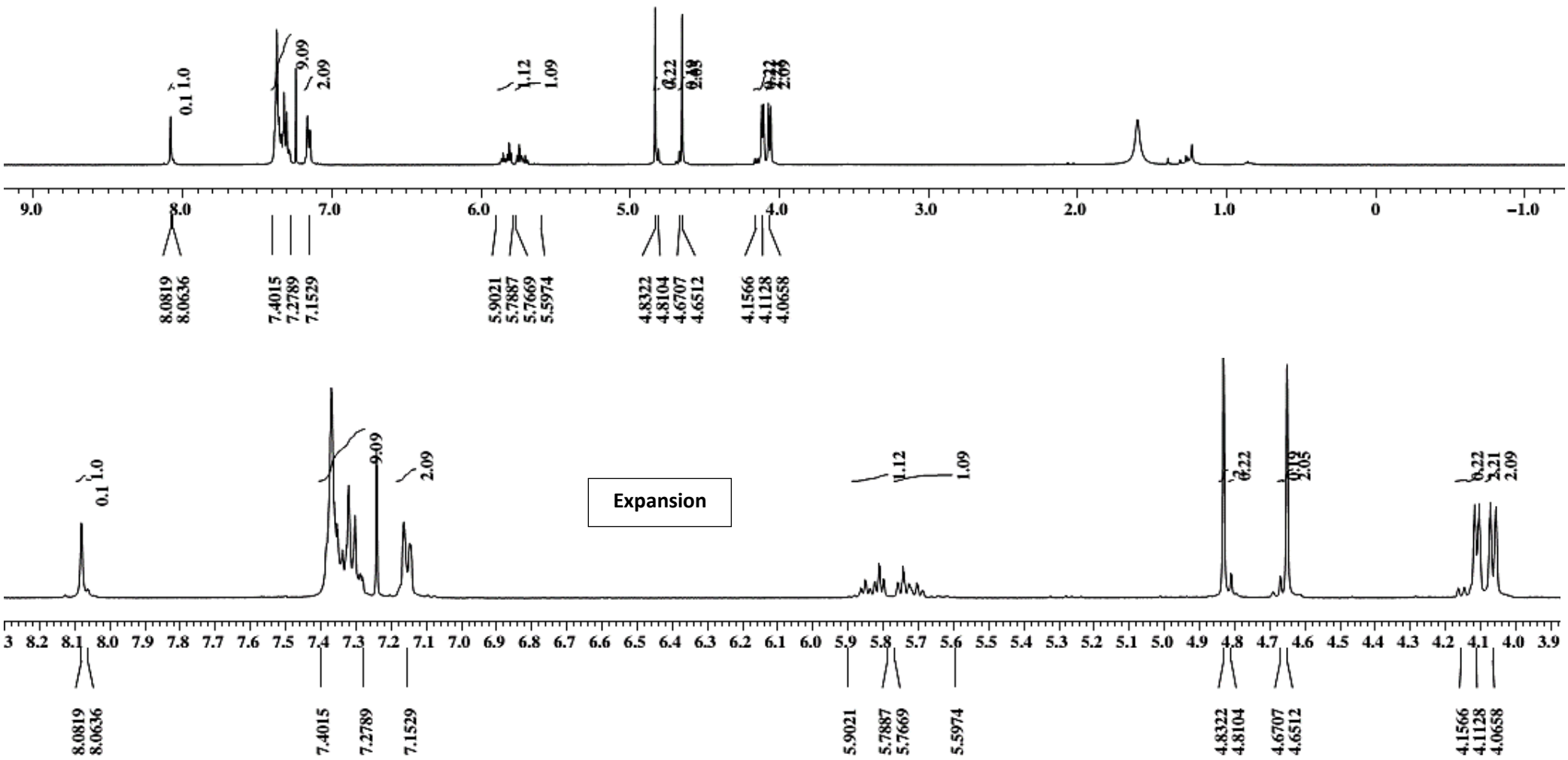


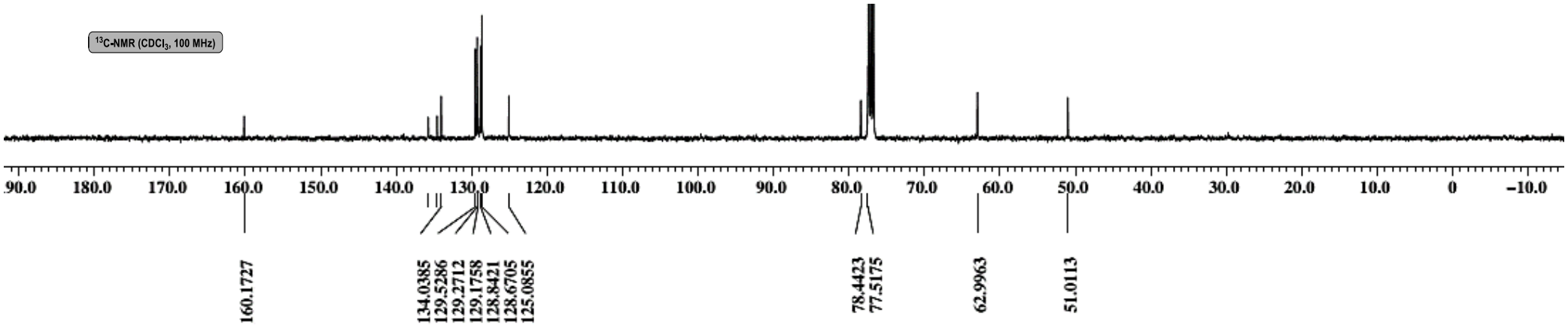
Expansion

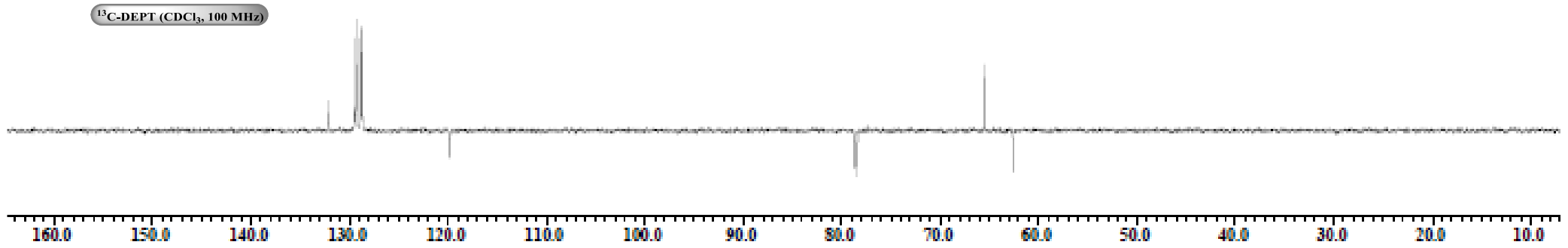


Reaction Solvent = THF

E:Z **=10:90**




^{13}C-NMR ($CDCl_3$, 100 MHz)
90.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0
160.1727
134.0385
129.5286
129.2712
129.1758
128.8421
128.6705
125.0855
78.4423
77.5175
62.9963
51.0113


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0

Elemental Composition Report

Single Mass Analysis

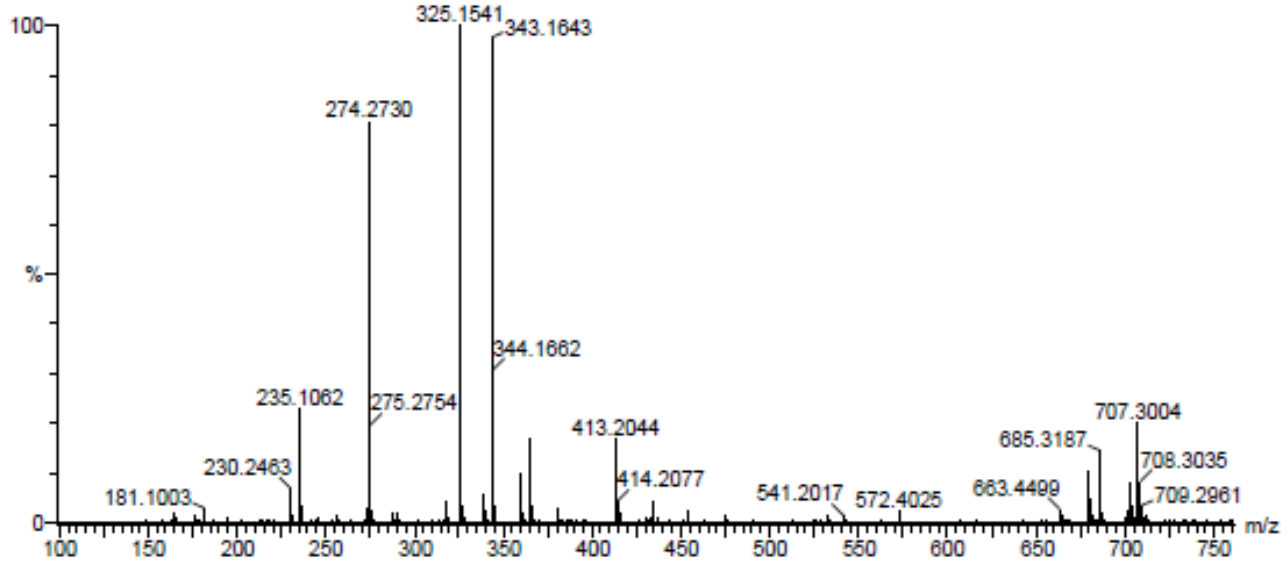
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-20 H: 11-35 N: 0-2 O: 0-5

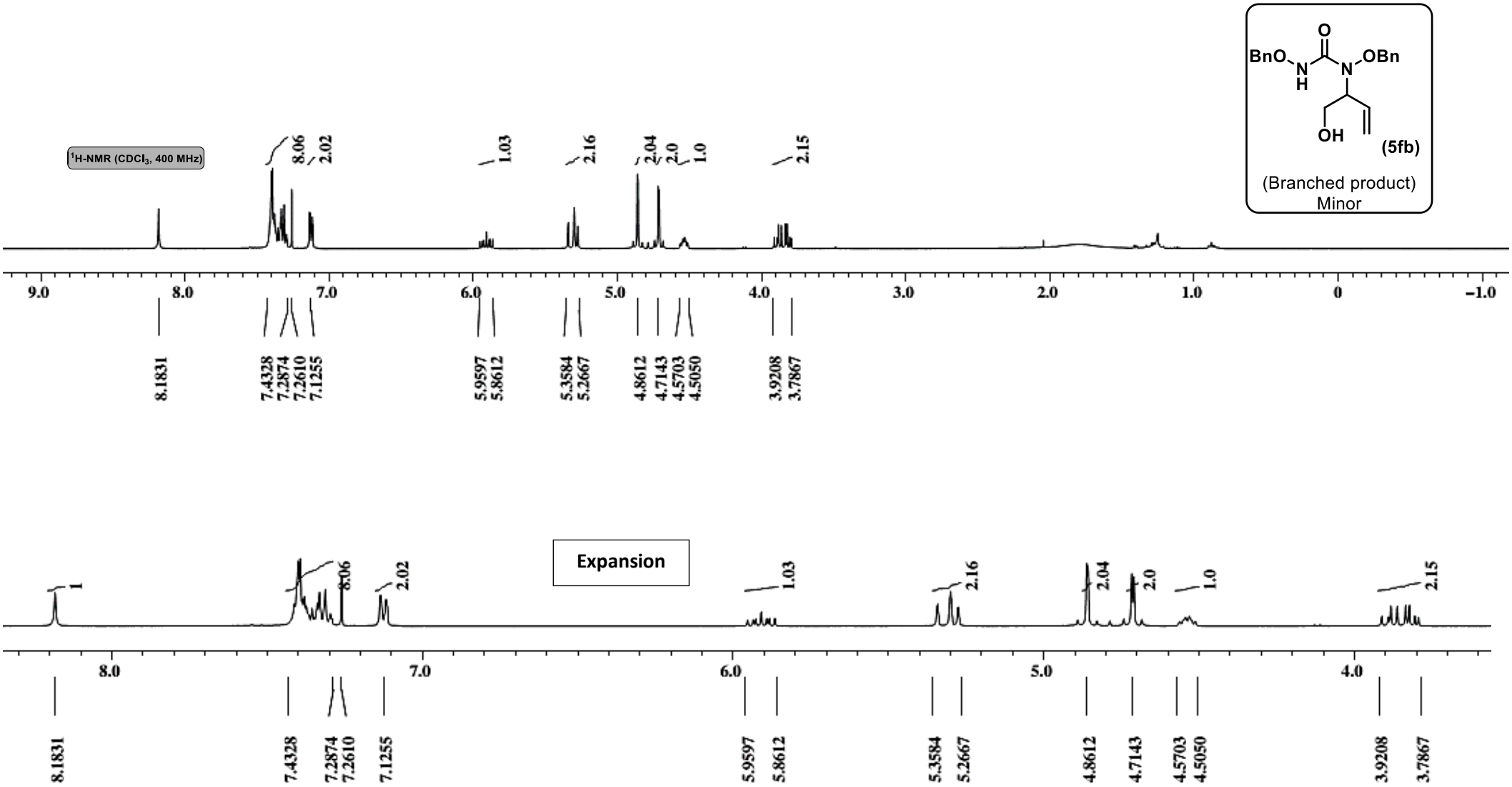
15-02-169-A
060320-15-02-169-A 15 (0.157) AM2 (Ar,22000.0,0.00,0.00); Cm (10:25)

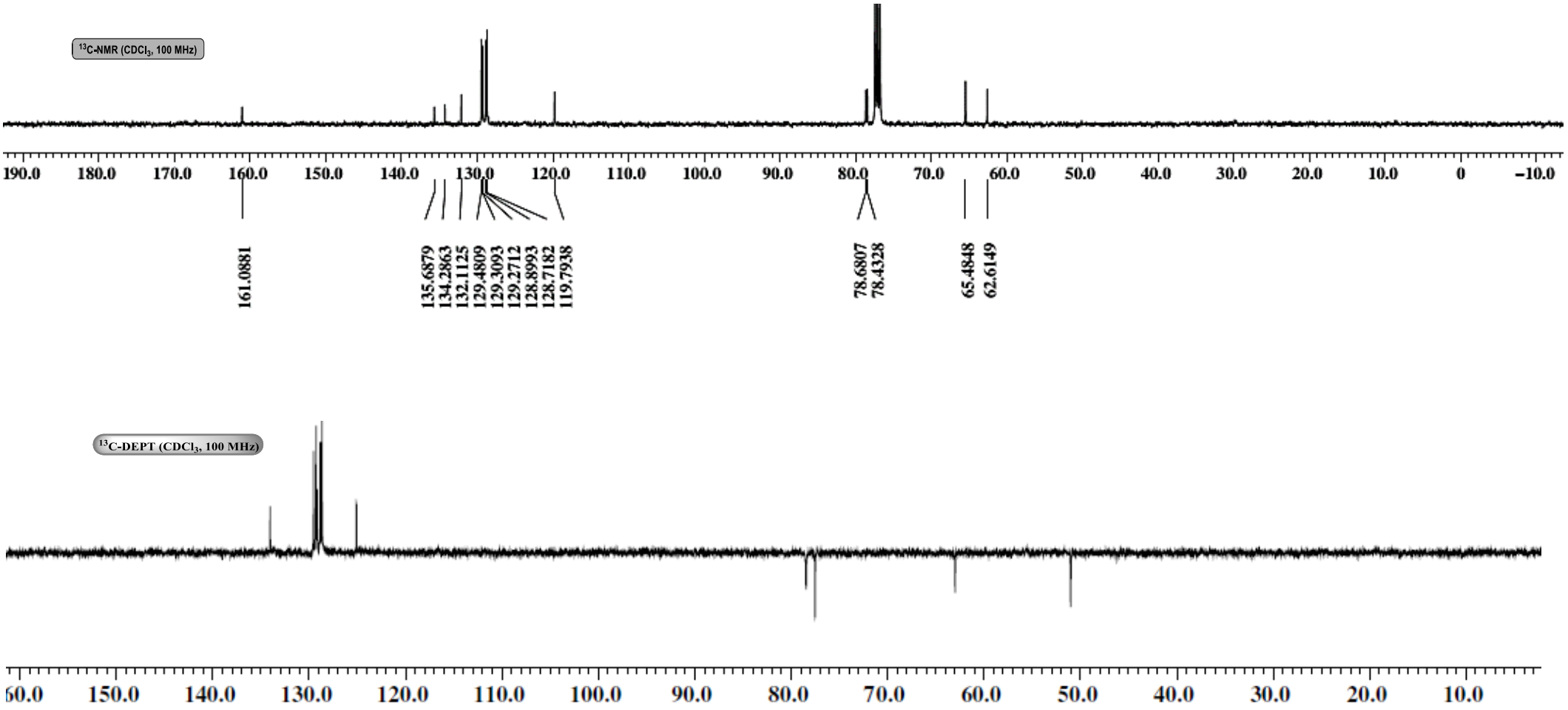
IITRPR

UPLC-XEVOG2XSQTOF
1: TOF MS ES+
1.68e+008



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
343.1643	343.1658	-1.5	-4.4	9.5	1144.0	n/a	n/a	C19 H23 N2 O4


^{1}H-NMR ($CDCl_3$, 400 MHz)
8.06
2.02
1.03
2.16
2.04
2.0
1.0
2.15
BnO
N
H
O
N
OBn
OH
(5fb)
(Branched product)
Minor
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.1831
7.4328
7.2874
7.2610
7.1255
5.9597
5.8612
5.3584
5.2667
4.8612
4.7143
4.5703
4.5050
3.9208
3.7867
Expansion
1
8.06
2.02
1.03
2.16
2.04
2.0
1.0
2.15
8.0
7.0
6.0
5.0
4.0
8.1831
7.4328
7.2874
7.2610
7.1255
5.9597
5.8612
5.3584
5.2667
4.8612
4.7143
4.5703
4.5050
3.9208
3.7867


^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0
161.0881
135.6879
134.2863
132.1125
129.4809
129.3093
129.2712
128.8993
128.7182
119.7938
78.6807
78.4328
65.4848
62.6149
^{13}C-DEPT ($CDCl_3$, 100 MHz)
60.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0

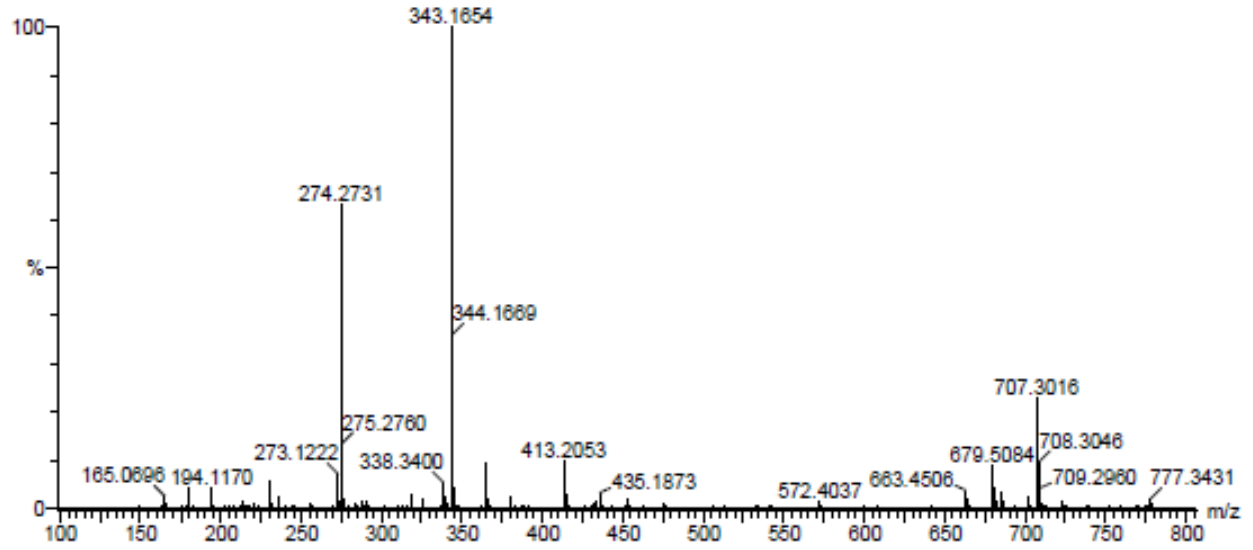
Elemental Composition Report

Single Mass Analysis

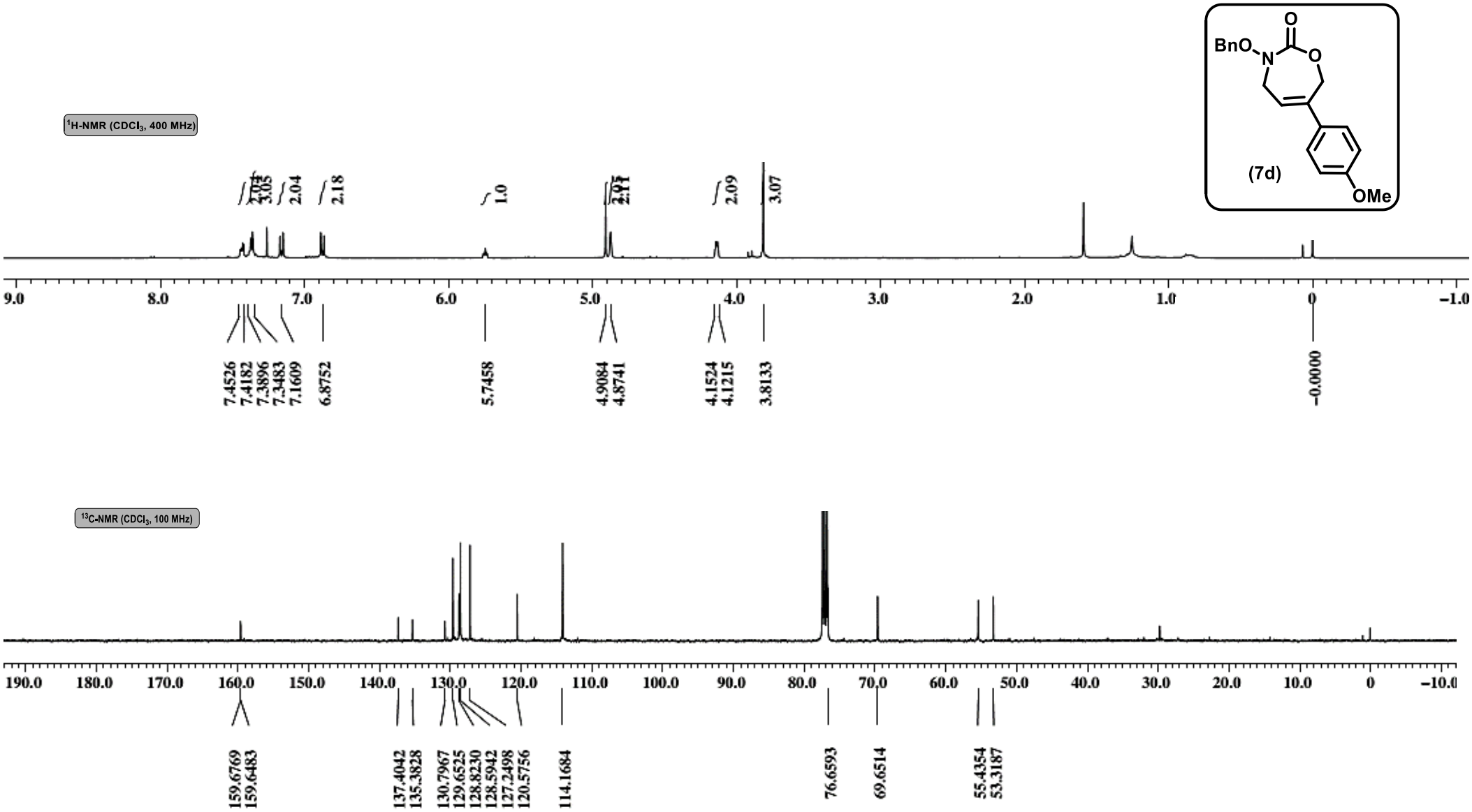
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

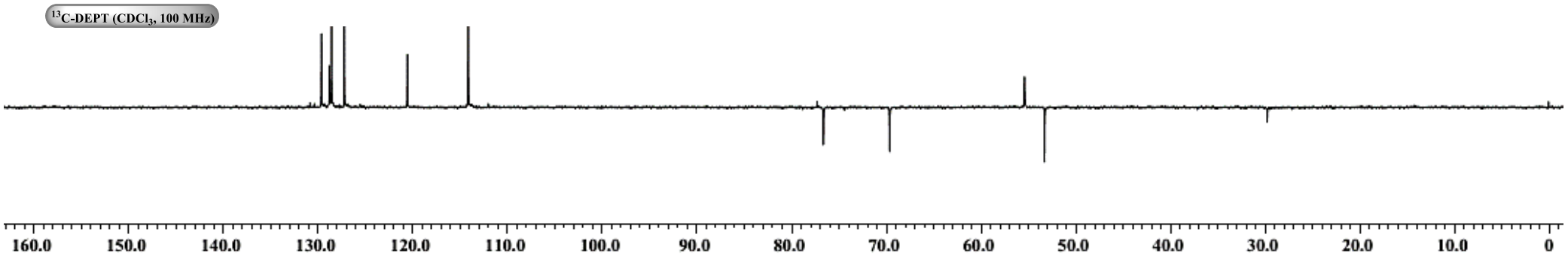
Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-20 H: 11-35 N: 0-2 O: 0-5

15-02-169-B IITRPR UPLC-XEVOG2XSQTOF
060320-15-02-169-B 17 (0.174) AM2 (Ar,22000.0,0.00,0.00); Cm (17:21) 1: TOF MS ES+
6.76e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
343.1654	343.1658	-0.4	-1.2	9.5	1055.2	n/a	n/a	C19 H23 N2 O4


(7d)
BnO
N
O
O
OMe
^{1}H-NMR (CDCl$_3$, 400 MHz)
2.04
2.18
1.0
2.09
3.07
7.4526
7.4182
7.3896
7.3483
7.1609
6.8752
5.7458
4.9084
4.8741
4.1524
4.1215
3.8133
−0.0000
^{13}C-NMR (CDCl$_3$, 100 MHz)
159.6769
159.6483
137.4042
135.3828
130.7967
129.6525
128.8230
128.5942
127.2498
120.5756
114.1684
76.6593
69.6514
55.4354
53.3187


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

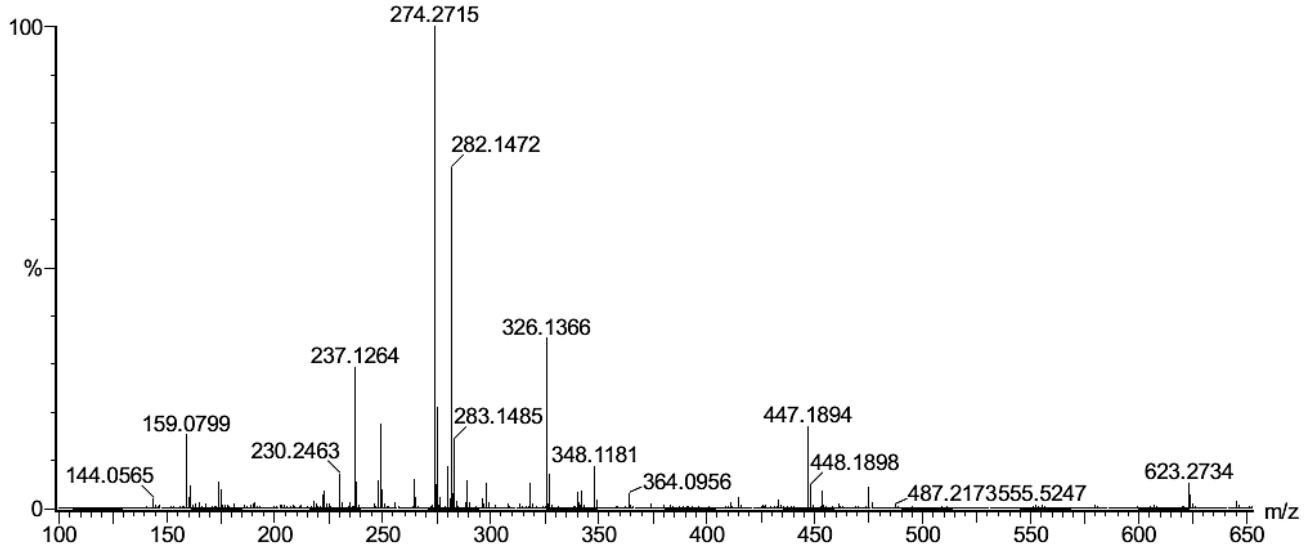
Elemental Composition Report

Single Mass Analysis

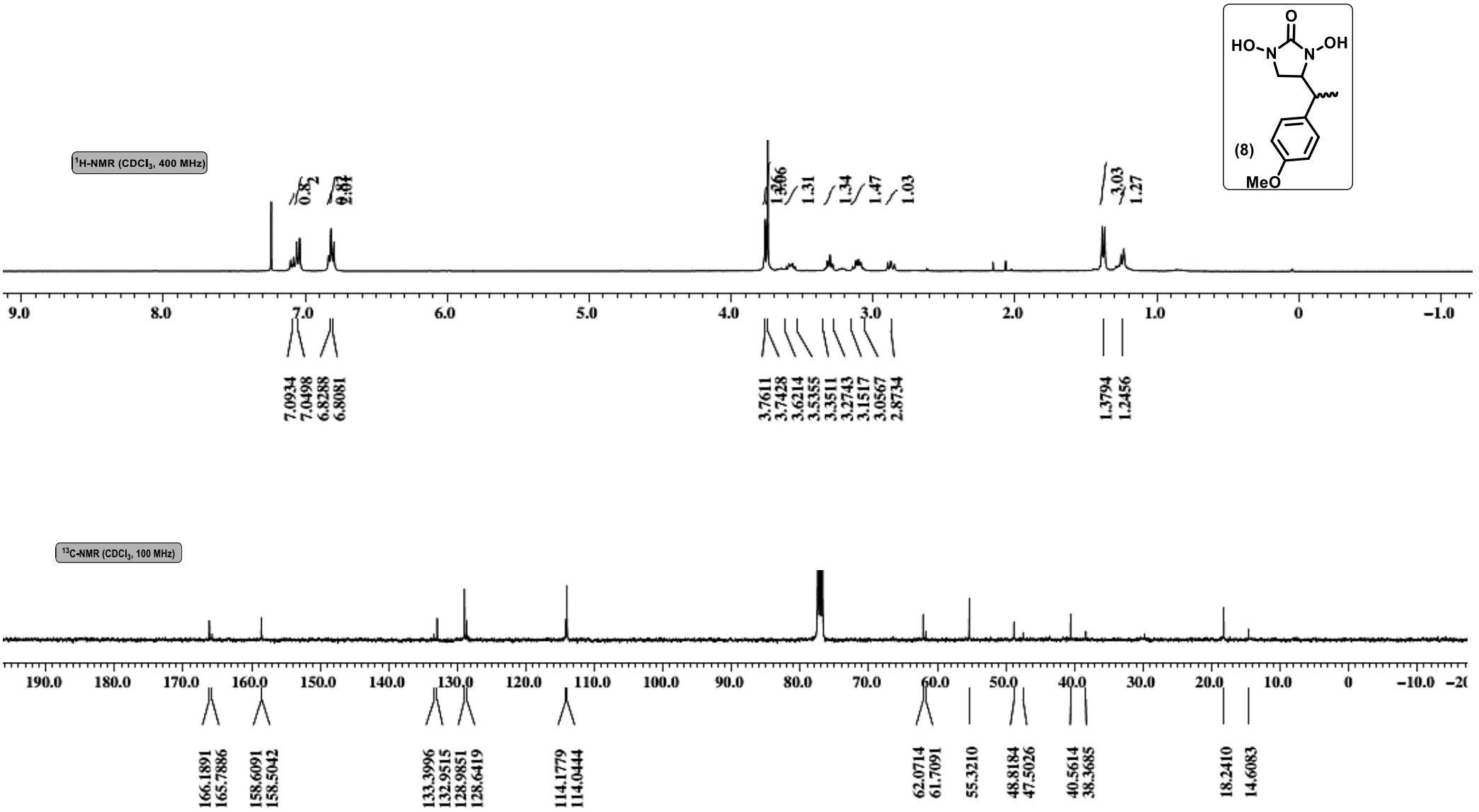
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

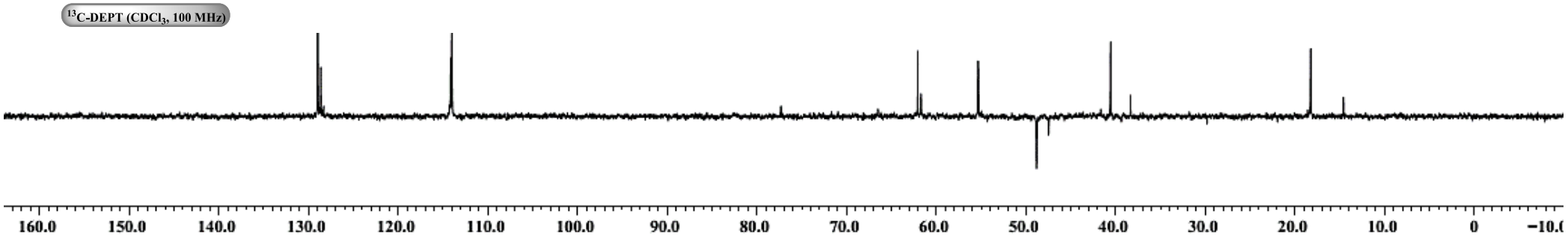
Monoisotopic Mass, Even Electron Ions
50 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 7-30 N: 0-4 O: 1-5

Sample Name : 15-01-121 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
271119-15-01-121 12 (0.131) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (7:18) 1: TOF MS ES+
8.99e+007



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
326.1366	326.1392	-2.6	-8.0	10.5	940.9	n/a	n/a	C19 H20 N O4


^{1}H-NMR ($CDCl_3$, 400 MHz)
HO
N
O
N
OH
(8)
MeO
0.85
1.31
1.34
1.47
1.03
3.03
1.27
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.0934
7.0498
6.8288
6.8081
3.7611
3.7428
3.6214
3.5355
3.3511
3.2743
3.1517
3.0567
2.8734
1.3794
1.2456
^{13}C-NMR ($CDCl_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
166.1891
165.7886
158.6091
158.5042
133.3996
132.9515
128.9851
128.6419
114.1779
114.0444
62.0714
61.7091
55.3210
48.8184
47.5026
40.5614
38.3685
18.2410
14.6083

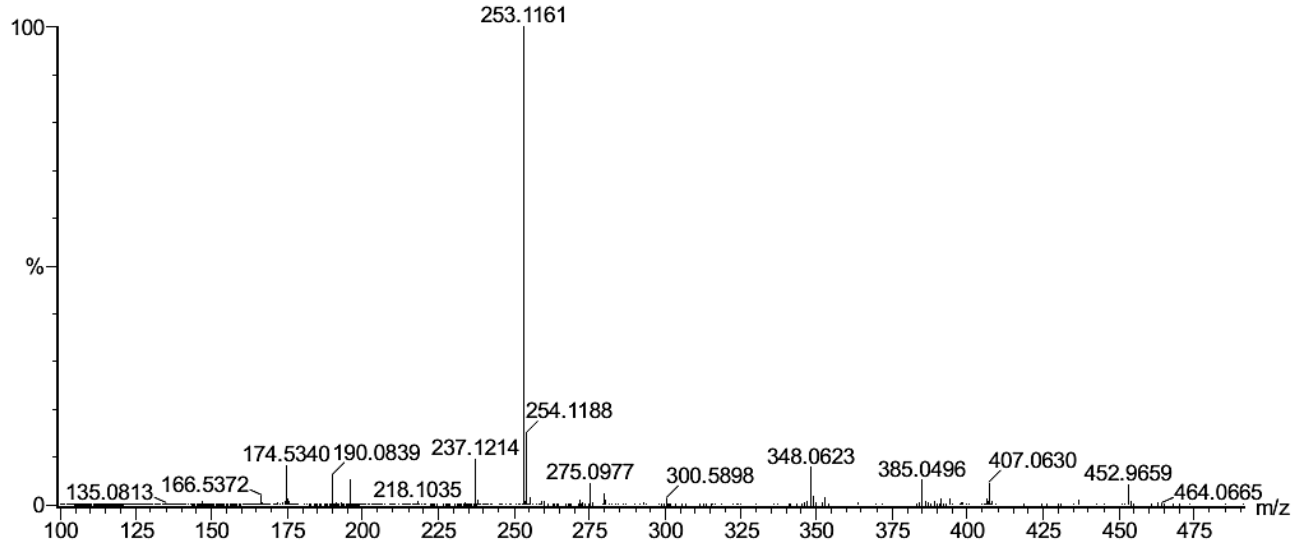

^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0

Single Mass Analysis

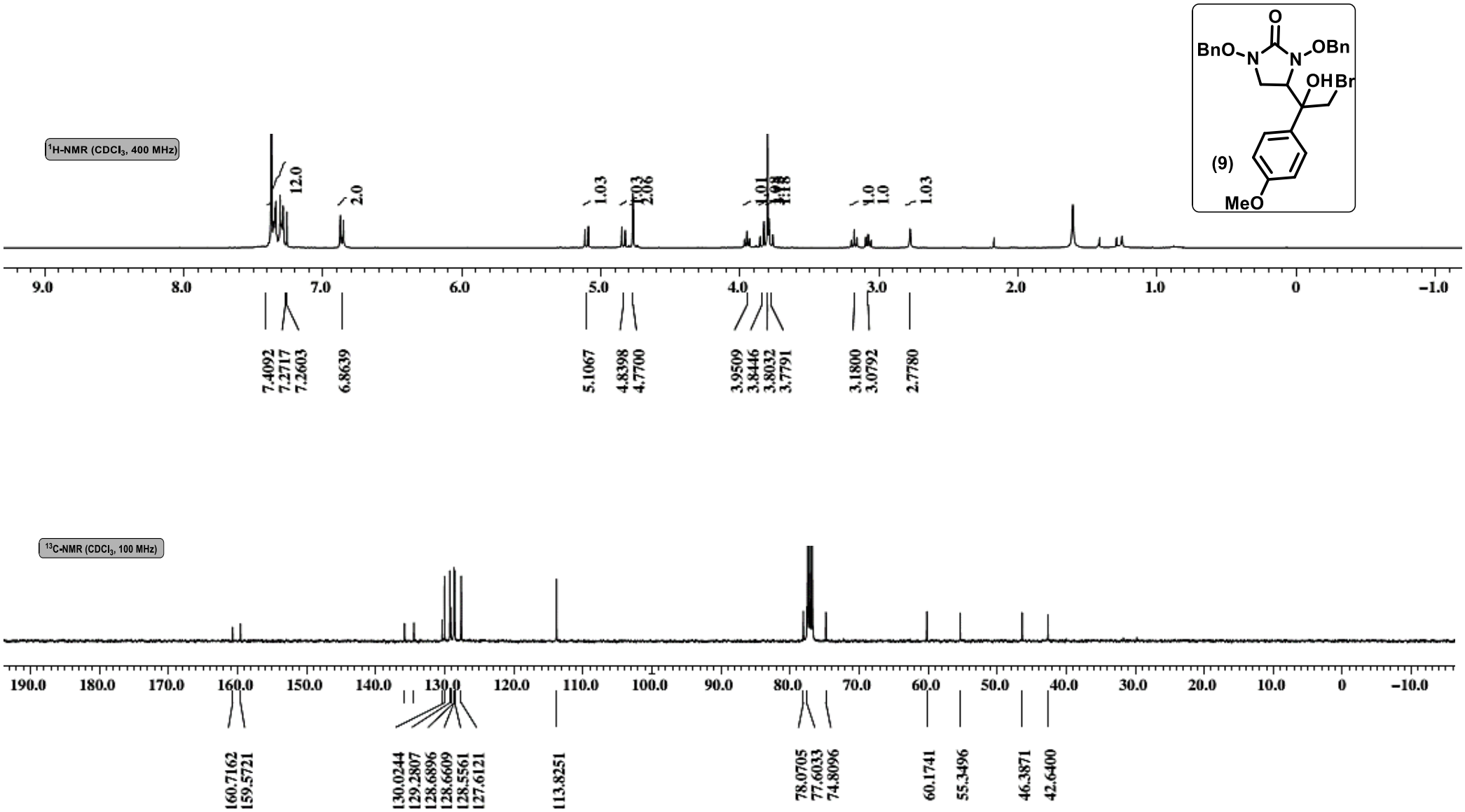
Tolerance = 15.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

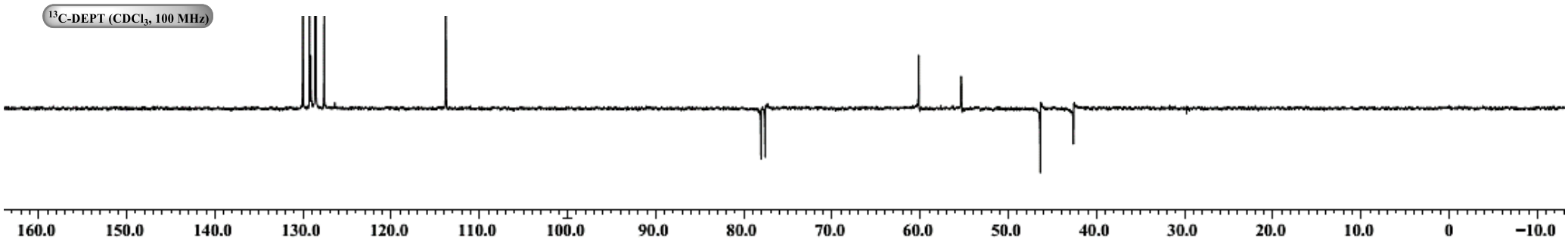
Monoisotopic Mass, Even Electron Ions
30 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 8-20 H: 8-25 N: 0-3 O: 0-4

Sample Name : 15-02-150 IITRPR XEVO G2-XS QTOF
Test Name : LCHRMS-4MIN
060220-15-02-150- 256 (2.578) 1: TOF MS ES+
3.69e+006



Minimum:				-1.5				
Maximum:		5.0	15.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
253.1161	253.1188	-2.7	-10.7	5.5	190.8	n/a	n/a	C12 H17 N2 O4


^{1}H-NMR (CDCl$_3$, 400 MHz)
12.0
2.0
1.03
1.03
2.08
1.01
1.98
1.18
1.0
1.0
1.03
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.4092
7.2717
7.2603
6.8639
5.1067
4.8398
4.7700
3.9509
3.8446
3.8032
3.7791
3.1800
3.0792
2.7780
BnO
N
O
N
OBn
OH
Br
(9)
MeO
^{13}C-NMR (CDCl$_3$, 100 MHz)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
160.7162
159.5721
130.0244
129.2807
128.6896
128.6609
128.5561
127.6121
113.8251
78.0705
77.6033
74.8096
60.1741
55.3496
46.3871
42.6400


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

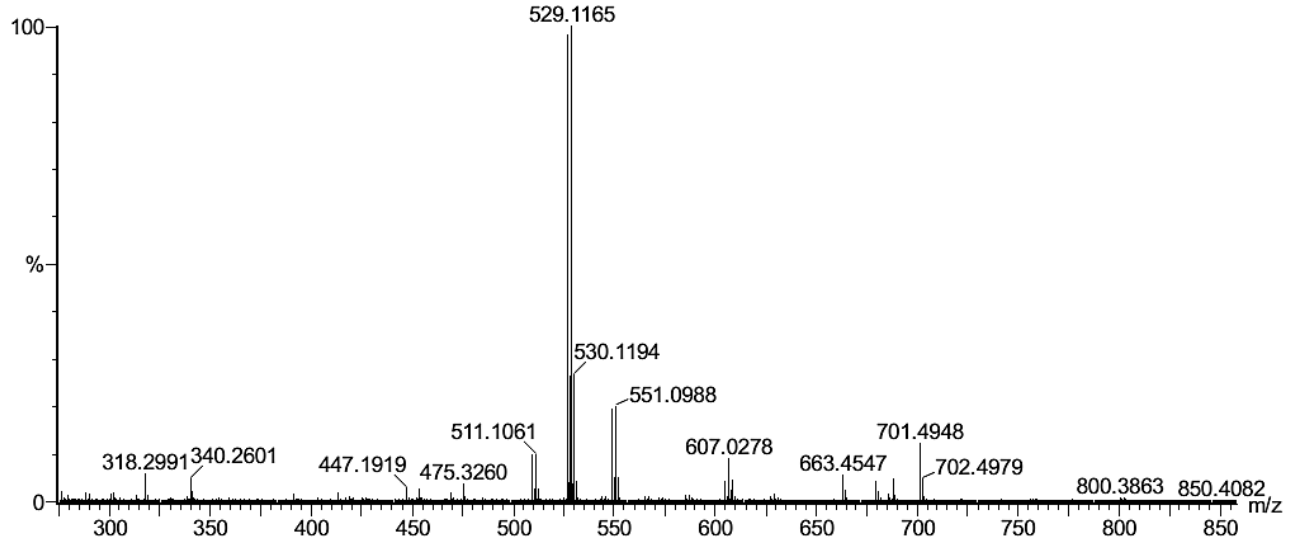
Monoisotopic Mass, Even Electron Ions
81 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 8-30 H: 10-30 N: 0-3 O: 0-5 Br: 0-2

Sample Name : 15-02-146
Test Name : HRMS-1
290120-15-02-146- 16 (0.165)

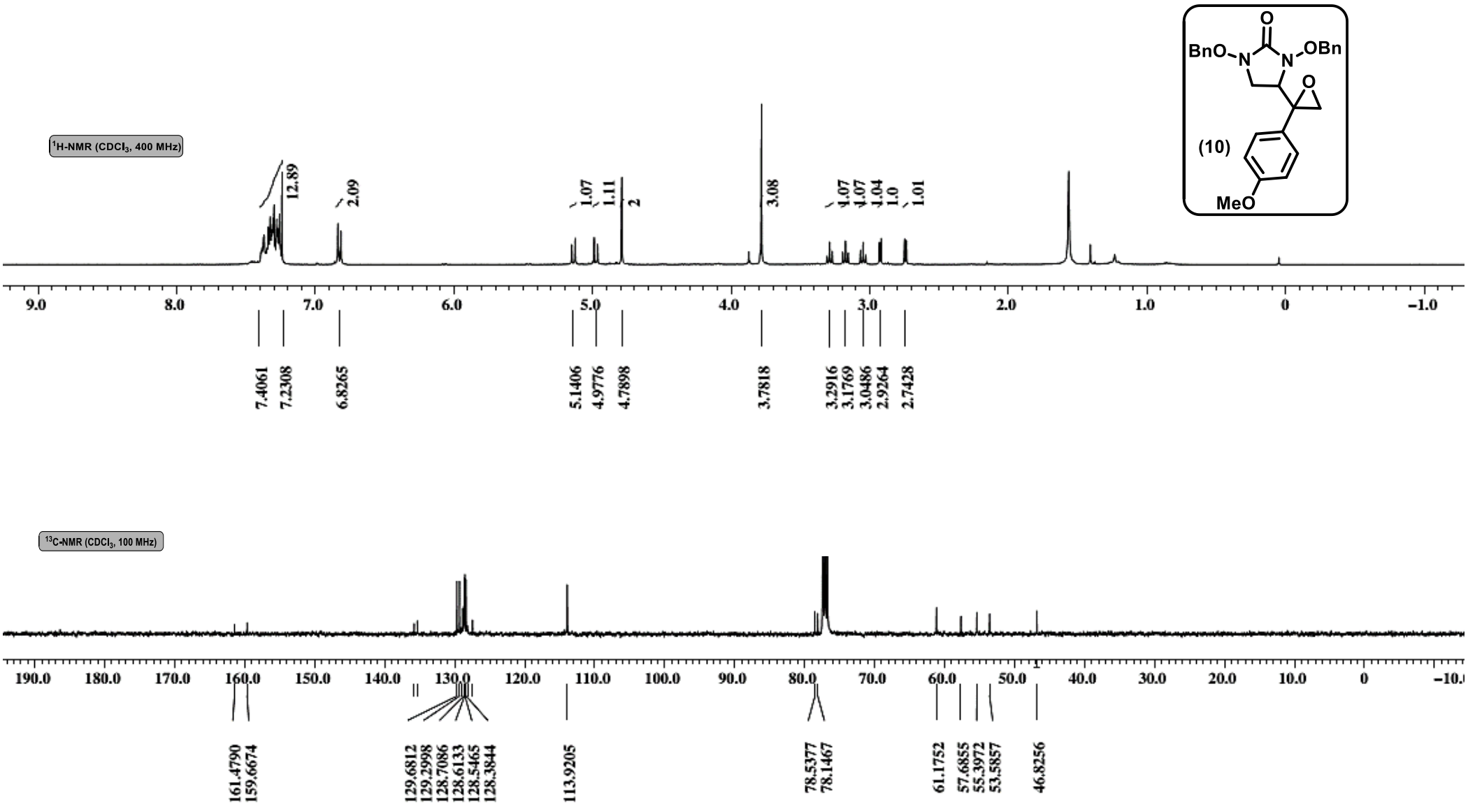
IITRPR

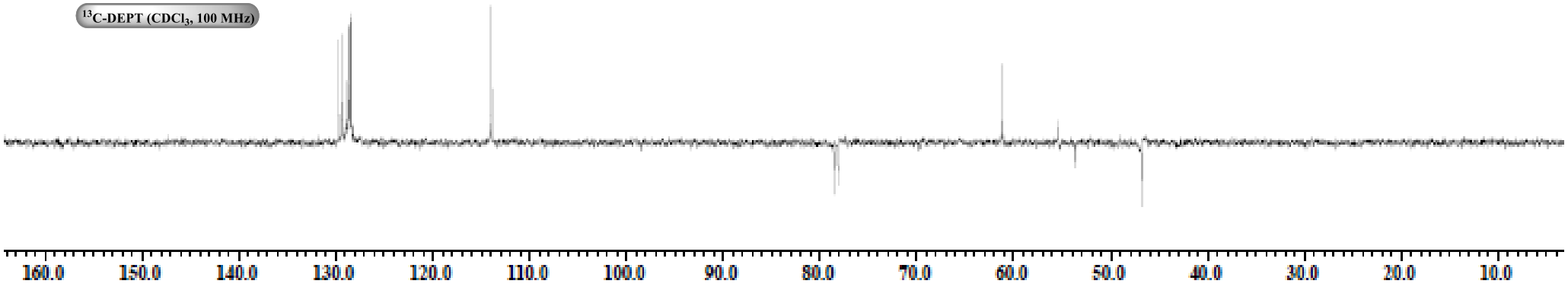
XEVO G2-XS QTOF

1: TOF MS ES+
1.90e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
527.1180	527.1182	-0.2	-0.4	13.5	1179.7	n/a	n/a	C26 H28 N2 O5 Br


(10)
BnO
OBn
MeO
^{1}H-NMR (CDCl$_3$, 400 MHz)
12.89
2.09
1.07
1.11
2
3.08
1.07
1.07
1.04
1.0
1.01
7.4061
7.2308
6.8265
5.1406
4.9776
4.7898
3.7818
3.2916
3.1769
3.0486
2.9264
2.7428
^{13}C-NMR (CDCl$_3$, 100 MHz)
161.4790
159.6674
129.6812
129.2998
128.7086
128.6133
128.5465
128.3844
113.9205
78.5377
78.1467
61.1752
57.6855
55.3972
53.5857
46.8256


^{13}C-DEPT ($CDCl_3$, 100 MHz)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

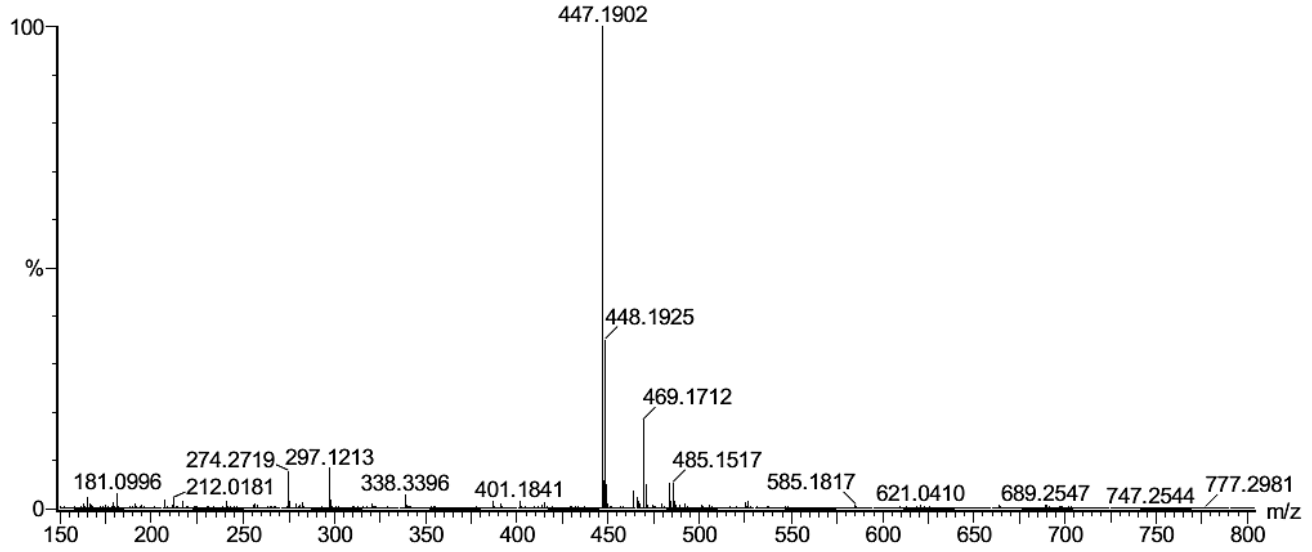
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 10-30 N: 0-2 O: 0-5

Sample Name : 15-02-epoxide
Test Name : HRMS-1
180220-15-02-epoxide 12 (0.131)

IITRPR

XEVO G2-XS QTOF

1: TOF MS ES+
1.12e+008



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
447.1902	447.1920	-1.8	-4.0	14.5	1549.2	n/a	n/a	C26 H27 N2 O5

13. Single-crystal X-Ray data of 8 and 9

For the determination of X-ray crystal structures of **8** and **9** a single crystal was selected and mounted with paratone oil on a glass fiber using gum. The data was collected at 293K on a CMOS based Bruker D8 Venture PHOTON 100 diffractometer equipped with a INCOATEC micro-focus source with graphite monochromatic Mo Kα radiation (λ = 0.71073 Å) operation at 50 kV and 30 mA. For the integration of diffraction profiles SAINT program[7] was used. Absorption correction was done applying SADABS program.[8] The crystal structure was solved by SIR 92[9] and refined by full matrix least square method using SHELXL-97[10] WinGX system, Ver 1.70.01.[11] All the non-hydrogen atoms in the structure were located the Fourier map and refined anisotropically. The hydrogen atoms were fixed by HFIX in their ideal positions and refined using riding model with isotropic thermal parameters. The crystal structure (excluding structure factor) has been deposited to Cambridge Crystallographic Data Centre and allocated deposition number**: 8:** CCDC **1985301** and **9:** CCDC **1989355**.[12]

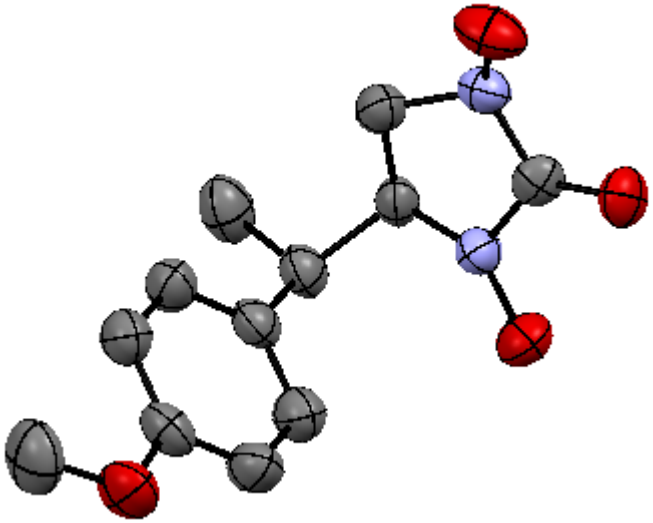


Figure S1. X-ray crystal structure of compound **8** (Hydrogen atoms are omitted for the sake of clarity)

CCDC No.	1985301
Formula	C24 H32 N4 O8
Formula weight	504.53
Crystal System	Orthorhombic
Space group	Pca21
a, b, c (Å)	9.621(2) 8.003(2) 33.196(9)
α, β, γ (°)	90, 90, 90
V ($Å^3$)	2556.0(11)
Z	4

Calculated Density (g/cm^3)	1.311
F(000)	1072
Crystal Size (mm^3)	0.25 x 0.31 x 0.36
Theta range for data collection:	2.5^o to 27.2°
Data set	-11: 12 ; -10: 10 ; -42: 37
Reflection	4988
Independent refl.	[R(int) = 0.033]
data [$I > 2\sigma(I)$]	3495
R indices (all data)	$R = 0.0603$, $wR_2 = 0.1688$
S	1.08
Min. and Max. Resd. Dens. ($e/Å^3$)	-0.31 and 0.28

Table S1: Selected bond lengths [Å] of 8

Atoms	Bond lengths [Å]	Atoms	Bond lengths [Å]
O1-N1	1.385(7)	C10-C11	1.385(10)
O2-C13	1.244(9)	C14-C15	1.526(9)
O3-N2	1.373(6)	C15-C16	1.547(8)
O4-C9	1.385(8)	C16-C17	1.525(10)
O4-C12	1.425(9)	C7-H7	0.9300
O1-H1	0.8200	C8-H8	0.9300
O3-H3	0.8200	C10-H10	0.9300
O5-N3	1.394(6)	C11-H11	0.9300
O6-C18	1.221(9)	C12-H12C	0.9600
O7-N4	1.391(6)	C12-H12B	0.9600
O8-C27	1.422(9)	C12-H12A	0.9600
O8-C26	1.388(8)	C14-H14B	0.9700
O5-H5	0.8200	C14-H14A	0.9700
O7-H100	0.8200	C15-H15	0.9800
N1-C14	1.453(8)	C16-H16	0.9800
N1-C13	1.365(8)	C17-H17A	0.9600
N2-C13	1.373(8)	C17-H17B	0.9600
N2-C15	1.450(7)	C17-H17C	0.9600
N3-C18	1.345(8)	C19-C20	1.533(9)
N3-C20	1.461(7)	C20-C21	1.526(8)
N4-C19	1.481(8)	C21-C22	1.539(10)
N4-C18	1.352(8)	C21-C23	1.517(9)
C6 -C16	1.530(9)	C23-C29	1.387(9)

C6-C7	1.374(9)	C23-C24	1.391(9)
C6-C11	1.401(10)	C24-C25	1.366(10)
C7-C8	1.393(9)	C25-C26	1.393(9)
C8-C9	1.382(10)	C26-C28	1.383(10)
C9-C10	1.375(9)	C28-C29	1.380(9)
C19-H19A	0.9700	C24-H24	0.9300
C19-H19B	0.9700	C25-H25	0.9300
C20-H20	0.9800	C27-H27A	0.9600
C21-H21	0.9800	C27-H27B	0.9600
C22-H22A	0.9600	C27-H27C	0.9600
C22-H22B	0.9600	C28-H28	0.9300
C22-H22C	0.9600	C29-H29	0.9300

Table S2: Selected bond angles [º] of 8

Atoms	**Bond angles[º]**	**Atoms**	**Bond angles[º]**
C9-O4-C12	117.8(5)	O2-C13-N2	126.1(6)
N1-O1-H1	109.00	O2-C13-N1	127.6(5)
N2-O3-H3	109.00	N1-C13-N2	106.4(6)
C26-O8-C27	117.2(5)	N1-C14-C15	101.5(5)
N3-O5-H5	110.00	C14-C15-C16	117.9(5)
N4-O7-H100	109.00	N2-C15-C16	114.5(5)
O1-N1-C13	115.6(5)	N2-C15-C14	98.5(5)
C13-N1-C14	109.7(5)	C15-C16-C17	108.4(5)
O1-N1-C14	115.2(5)	C6-C16-C17	114.1(5)
O3-N2 -C13	118.9(5)	C6-C16-C15	114.5(5)

O3-N2-C15	120.7(4)	C8-C7-H7	119.00
C13-N2-C15	111.2(5)	C6-C7-H7	119.00
O5-N3-C18	118.8(5)	C7-C8-H8	120.00
C18-N3-C20	111.8(5)	C9-C8-H8	120.00
O5-N3-C20	119.0(4)	C9-C10-H10	120.00
O7-N4-C18	116.8(5)	C11-C10-H10	120.00
C18-N4-C19	109.8(5)	C6-C11-H11	119.00
O7-N4-C19	115.6(5)	C10-C11-H11	119.00
C7-C6-C16	123.0(6)	O4-C12-H12A	109.00
C11-C6-C16	119.8(5)	H12A-C12-H12B	109.00
C7-C6-C11	117.2(6)	O4-C12-H12B	109.00
C6-C7-C8	122.1(6)	O4-C12-H12C	109.00
C7-C8-C9	119.4(6)	H12B-C12-H12C	110.00
O4-C9-C10	115.2(6)	H12A-C12-H12C	110.00
C8-C9-C10	120.0(6)	N1-C14-H14B	111.00
O4-C9-C8	124.8(6)	H14A-C14-H14B	109.00
C9 -C10-C11	119.9(6)	C15-C14-H14B	111.00
C6-C11-C10	121.5(6)	C15-C14-H14A	111.00
N1-C14-H14A	111.00	O8-C26-C28	125.0(6)
C16-C15-H15	108.00	O8-C26-C25	115.8(6)
C14-C15-H15	108.00	C25-C26-C28	119.2(6)
N2-C15-H15	108.00	C26-C28-C29	119.2(6)
C6-C16-H16	106.00	C23-C29-C28	123.2(6)
C15-C16-H16	106.00	N4-C19-H19A	112.00
C17 -C16-H16	106.00	N4-C19-H19B	112.00
C16-C17-H17B	109.00	C20-C19-H19A	112.00
C16-C17-H17A	109.00	C20-C19-H19B	112.00
H17A-C17-H17C	109.00	H19A-C19-H19B	110.00
H17B-C17-H17C	110.00	N3-C20-H20	109.00
H17A-C17-H17B	110.00	C19-C20-H20	109.00
C16-C17-H17C	109.00	C21-C20-H20	109.00

O6-C18-N4	126.3(5)	C20-C21-H21	107.00
O6-C18-N3	126.2(6)	C22-C21-H21	107.00
N3-C18-N4	107.4(6)	C23-C21-H21	107.00
N4-C19-C20	100.2(5)	C21-C22-H22A	109.00
N3-C20-C19	98.8(5)	C21-C22-H22B	109.00
C19-C20-C21	116.0(5)	C21-C22-H22C	109.00
N3-C20-C21	115.4(5)	H22A-C22-H22B	110.00
C20-C21-C23	114.1(5)	H22A-C22-H22C	109.00
C22-C21-C23	114.6(5)	H22B-C22-H22C	110.00
C20-C21-C22	107.8(5)	C23-C24-H24	119.00
C24-C23-C29	115.6(6)	C25-C24-H24	119.00
C21-C23-C24	120.6(5)	C24-C25-H25	120.00
C21-C23-C29	123.7(6)	C26-C25-H25	120.00
C23-C24-C25	122.9(6)	O8-C27-H27A	109.00
C24-C25-C26	119.8(7)	O8-C27-H27B	109.00
O8-C27-H27C	109.00	C26-C28-H28	120.00
H27A-C27-H27B	110.00	C29-C28-H28	120.00
H27A-C27-H27C	109.00	C23-C29-H29	118.00
H27B-C27-H27C	109.00	C28-C29-H29	118.00

Table S3: Selected hydrogen bonding geometry [Å, º] for a compound 8

D--H.. **A**	**D**..**H**	**H**..**A**	**D**..**A**	**D--H**..**A**
O1--H1..O2 0.8200	0.8200	2.4600	2.824(7)	108.00
O3--H3..O2	0.8200	2.4100	2.799(6)	110.00
O3--H3..O7	0.8200	2.4800	3.293(7)	171.00
O3--H3..N4	0.8200	2.3300	3.071(7)	151.00
O5--H5..O6	0.8200	2.4100	2.783(6)	108.00
O7--H100..O6	0.8200	2.4300	2.791(7)	108.00
C22--H22A..O7	0.9600	2.5900	3.537(9)	170.00

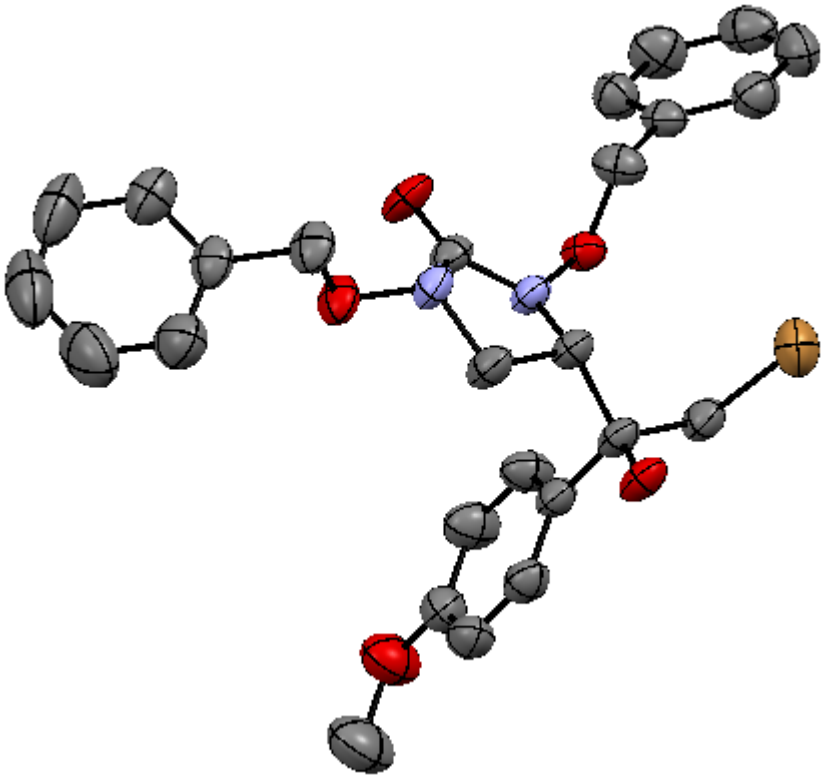


Figure S2. X-ray crystal structure of compound **9** (Hydrogen atoms are omitted for the sake of clarity)

CCDC No.	1989355
Formula	C26 H27 Br N2 O5
Formula weight	527.40
Crystal System	Monoclinic
Space group	P21/c
a, b, c (Å)	8.0617(6), 26.398(3), 11.8969(14)
α, β, γ (°)	90, 91.684(2), 90
V ($Å^3$)	2530.7(5)
Z	4
Calculated Density (g/cm^3)	1.384
F(000)	1088
Crystal Size (mm^3)	0.27 x 0.28 x 0.30
Theta range for data collection:	2.3^o to 26.4°
Data set	-9: 10 ; -32: 32 ; -14: 14
Reflection	5121
Independent refl.	[R(int) = 0.087]
data [$I > 2\sigma(I)$]	2964
R indices (all data)	$R = 0.0440$, $wR_2 = 0.0995$
S	1.01
Min. and Max. Resd. Dens. ($e/Å^3$)	-0.40 and 0.24

Table S1: Selected bond lengths [Å] of 9

Atoms	Bond lengths [Å]	Atoms	Bond lengths [Å]
Br1-C19	1.952(4)	C13-C15	1.350(9)
O1-N2	1.418(3	C14-C15	1.371(7)
O1-C9	1.438(4)	C17-C18	1.375(5)
O3-N1	1.399(3)	C20-C21	1.497(5)
O3-C20	1.457(4)	C21-C26	1.376(4)
O4-C16	1.219(3)	C21-C22	1.380(5)
O102-C6	1.424(3)	C22-C23	1.384(5)
O104-C1	1.398(5)	C23-C24	1.364(6)
O104-C2	1.367(4)	C24-C25	1.366(7)
N1-C7	1.460(3)	C25-C26	1.378(5)
N1-C16	1.364(3)	C1-H1	0.9600
N2-C8	1.469(3)	C1-H9	0.9600
N2-C16	1.381(4)	C1-H10	0.9600
O102-H102	0.8200	C3-H11	0.9300
C2-C3	1.377(5)	C4-H12	0.9300
C2-C17	1.374(5)	C7-H17	0.9800
C3-C4	1.392(5)	C8-H15	0.9700
C4-C5	1.382(5)	C8-H16	0.9700
C5-C6	1.525(5)	C9-H6	0.9700
C5-C18	1.396(4)	C9-H25	0.9700
C6-C19	1.524(5)	C11-H26	0.9300
C6-C7	1.547(4)	C12-H3	0.9300
C7-C8	1.531(5)	C13-H2	0.9300

C9-C10	1.504(5)	C14-H4	0.9300
C10-C14	1.377(6)	C15-H5	0.9300
C10-C11	1.369(5)	C17-H7	0.9300
C11-C12	1.393(7)	C18-H8	0.9300
C12-C13	1.364(8)	C19-H13	0.9700
C19-H14	0.9700	C23-H22	0.9300
C20-H18	0.9700	C24-H19	0.9300
C20-H24	0.9700	C25-H20	0.9300
C22-H23	0.9300	C26-H21	0.9300

Table S2: Selected bond angles [º] of 9

Atoms	**Bond angles[º]**	**Atoms**	**Bond angles[º]**
N2-O1-C9	108.5(2)	O1-C9-C10	107.6(3)
N1-O3-C20	111.2(2)	C9-C10-C11	119.8(3)
C1-O104-C2	117.7(3)	C11-C10-C14	119.3(3)
O3-N1 -C7	120.8(2)	C9-C10-C14	120.9(3)
O3-N1-C16	118.88(19)	C10-C11-C12	119.6(4)
C7-N1-C16	112.8(2)	C11-C12-C13	119.9(5)
O1-N2-C8	114.4(2)	C12-C13-C15	120.7(5)
O1-N2-C16	112.8(2)	C10-C14-C15	120.7(4)
C8-N2-C16	109.6(2)	C13-C15-C14	119.9(5)
C6-O102-H102	109.00	O4-C16-N2	126.9(3)
O104-C2-C3	124.9(3)	N1-C16-N2	106.7(2)
C3-C2-C17	119.2(3)	O4-C16-N1	126.4(3)
O104-C2-C17	115.9(3)	C2-C17-C18	120.4(3)

C2-C3-C4	119.9(3)	C5-C18-C17	122.0(3)
C3-C4-C5	122.0(3)	Br1-C19-C6	114.0(2)
C4-C5-C18	116.5(3)	O3-C20-C21	107.3(2)
C6-C5-C18	121.7(3)	C20-C21-C22	120.6(3)
C4-C5-C6	121.9(3)	C22-C21-C26	118.8(3)
O102-C6-C7	101.3(2)	C20-C21-C26	120.6(3)
O102-C6-C19	110.5(2)	C21-C22-C23	120.5(3)
O102-C6-C5	112.0(3)	C22-C23-C24	119.8(4)
C5-C6-C19	106.9(2)	C23-C24-C25	120.1(4)
C7-C6-C19	113.0(3)	C24-C25-C26	120.4(4)
C5-C6-C7	113.3(2)	C21-C26-C25	120.3(3)
N1-C7-C8	100.1(2)	O104-C1-H1	109.00
C6-C7-C8	112.9(3)	O104-C1-H9	109.00
N1-C7-C6	114.4(2)	O104-C1-H10	110.00
N2-C8-C7	101.8(2)	H1-C1-H9	109.00
H1-C1-H10	109.00	C13-C15-H5	120.00
H9-C1-H10	109.00	C14-C15-H5	120.00
C2-C3-H11	120.00	C2-C17-H7	120.00
C4-C3-H11	120.00	C18-C17-H7	120.00
C3-C4-H12	119.00	C5-C18-H8	119.00
C5-C4-H12	119.00	C17-C18-H8	119.00
N1-C7-H17	110.00	Br1-C19-H13	109.00
C6-C7-H17	110.00	Br1-C19-H14	109.00
C8-C7-H17	110.00	C6-C19-H13	109.00
N2-C8-H15	111.00	C6-C19-H14	109.00
N2-C8-H16	111.00	H13-C19-H14	108.00
C7-C8-H15	111.00	O3-C20-H18	110.00
C7-C8-H16	111.00	O3-C20-H24	110.00
H15-C8-H16	109.00	C21-C20-H18	110.00
O1-C9-H6	110.00	C21-C20-H24	110.00
O1-C9-H25	110.00	H18-C20-H24	109.00

C10-C9-H6	110.00	C21-C22-H23	120.00
C10-C9-H25	110.00	C23-C22-H23	120.00
H6-C9-H25	108.00	C22-C23-H22	120.00
C10-C11-H26	120.00	C24-C23-H22	120.00
C12-C11-H26	120.00	C23-C24-H19	120.00
C11-C12-H3	120.00	C25-C24-H19	120.00
C13-C12-H3	120.00	C24-C25-H20	120.00
C12-C13-H2	120.00	C26-C25-H20	120.00
C15-C13-H2	120.00	C21-C26-H21	120.00
C10-C14-H4	120.00	C25-C26-H21	120.00
C15-C14-H4	120.00		

Table S3: Selected hydrogen bonding geometry [Å, º] for a compound 9

D--H.. **A**	**D**..**H**	**H**..**A**	**D**..**A**	**D--H**..**A**
O102--H102..O4	0.8200	1.9500	2.731(2)	159.00
C18--H8..N1	0.9300	2.6000	3.026(4)	108.00
C4-- H12..O102	0.9300	2.4300	2.792(4)	103.00
C19--H13..O3	0.9700	2.5000	3.107(3)	120.00
C19--H14..O4	0.9700	2.5200	3.203(3)	127.00
C7--H17..Br1	0.9800	2.8400	3.315(3)	111.00
C24--H19..O4	0.9300	2.5900	3.446(5)	152.00

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