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Synthetic Manifestation of Trinitro-Pyrazolo-2H-1,2,3-Triazoles (TNPT) as Insensitive Energetic Materials

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SUPPORTING INFORMATION

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General Experimental

All the reactions has beencarried out in an oven-dried round bottomed flask. Commercial grade solvents were distilled prior to use. Column chromatography has been performed using silica gel (100-200 Mesh) with hexanes and ethyl acetate mixture. Thin layer chromatography (TLC) has beenchecked on silica gel GF254 plates. The spots on TLC plate have been visualized with UV light (254 nm) and/or staining over I_2 chamber.

Proton and carbon nuclear magnetic resonance spectra (^{1}H NMR,^{13}C NMR) are recorded on a 400 MHz (^{13}C NMR, 101 MHz), 500 MHz (^{13}C NMR, 126 MHz) spectrometer (spectra are recorded with a BRUKER-DMX-NMR) and 600 MHz (^{1}H NMR, 600 MHz; ^{13}C NMR, 151 MHz; ^{15}N NMR, 61 MHz; spectra are recorded with a JEOL JNM-ECZ-600R/M1) spectrometer, having solvent resonance as internal standard (^{1}H NMR: $CDCl_3$ at 7.26 ppm, DMSO-d_6 at 2.49 ppm, Acetone-d_6 at 2.04 ppm, CD_3CN at 1.93 ppm; ^{13}C NMR: $CDCl_3$ at 77.0 ppm, DMSO-d_6 at 39.5 ppm, Acetone-d_6 at 29.8 & 206.5 ppm, CD_3CN at 1.3 & 118.3 ppm). Few cases tetramethylsilane (TMS) at 0.00 ppm has been used as reference standard. The chemical shift values (ppm) are expressed relative to the chemical shift of [deuterated] solvent or to the external standard liq. NH_3 without correction (^{15}N NMR). Data for ^{1}H NMR are reported as follows: chemical shift (ppm), multiplicity (s = singlet; bs = broad singlet; d=doublet; bd = broad doublet; dd = doublet of doublet; dt = doublet of triplet; tt= triplet of triplet; t = triplet; bt= broad triplet; q = quartet; pent =pentet, m =multiplet), coupling constants *J* in (Hz), and integration. ^{13}C NMR is reported in terms of chemical shift (ppm). Melting points and decomposition temperatures are determined by DSC and TG-DSC measurements. IR spectra are recorded on FT/IR spectrometer and are reported in cm^{-1}. High resolution mass spectra (HRMS) are obtained in ESI mode. X-ray data are collected on a 'Bruker D8 VENTURE Photon III detector' and Rigaku Oxford Hypix-3000 diffractometer using Mo-Kα radiation (0.71073 Å) and Cu-Kα radiation (1.54 Å).

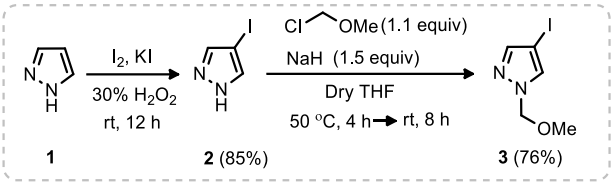
Caution! All the TNPT and its derivatives are energetic materials and they tend to explode under certain conditions unpredictably. However, none of the compounds described herein has exploded or detonated in the course of this research. Caution should be exercised at all times during the synthesis, characterization, and handling of any of these materials, and mechanical actions involving scratching or scraping must be avoided. Ignoring safety precautions can lead to serious injuries.

Materials: Unless otherwise noted, all the reagents and intermediates are obtained commercially and used without purification. Pyrazole, 1,2,3-triazole, iodine, chloromethyl methyl ether, silver nitrate, 30% H_2O_2, *O-p*-toluenesulfonylhydroxylamine, dimethyl sulfate, 70% perchloric acid, sodium hydride, sodium bicarbonate ($NaHCO_3$), tripotassium phosphate (K_3PO_4), copper(I) oxide (Cu_2O), aqueous ammonia, THF, methanol, acetonitrile, dichloromethane, and *N,N′*-dimethylformamide (DMF)are commercially available and used as received. Commercially available H_2SO_4 and $HNO_3$are used for nitration reactions.

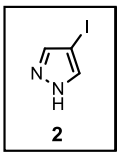
ExperimentalProcedures

General procedure for the preparation of precursors 2 and 3 (GP-1):

Physical characterization data are exactly matching with the reported values of the respective compounds **2** and **3**.



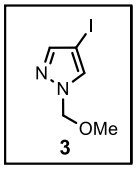
4-Iodo pyrazole (2):[1]



To a solution of pyrazole (**1**; 15.0 g, 220.58 mmol) and iodine (27.9 g, 110.29 mmol) in water (85.0 mL) was added 30% H_2O_2 (16.4 mL, 132.34 mmol). The reaction mixture was stirred for 12 h at room temperature. Upon reaction completion, a cold solution of 5% $NaHSO_3$ (50 mL) was added to the mixture. The compound strated precipitated providing off-white slurry. The product was filtered and washed with water to provide **2** (36.5 g, 85%) as an off-white crystalline solid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 11.25 (bs, 1H), 7.65 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 138.6, 56.6 ppm.

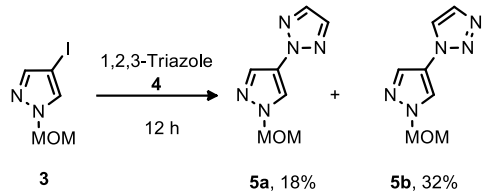
4-Iodo-1-(methoxymethyl)-1*H*-pyrazole (3):[2]



Sodium hydride (928 mg, 23.2 mmol, 60% wt in mineral oil) was suspended in 25 mL dry THF and stirred for 15 minutes. Then a solution of 4-iodopyrazole (**2**; 3.0 g, 15.54 mmol) in 25 mL dry THF was added drop wise at 0 °C and the resulting mixture was stirred at 40 °C for 1 h. Chloromethyl methyl ether (1.29 mL, 17.01 mmol) was added drop wise and the mixture was allowed to stir at 50 °C for 4 h and then at room temperature for 8 h. The mixture was quenched with saturated solution of $NaHCO_3$ and extracted with ethyl acetate. The organic fractions were washed with brine, dried over sodium sulfate, and concentrated in vacuo to afford **3** (2.82 g, 76%) as pale-yellow oil.

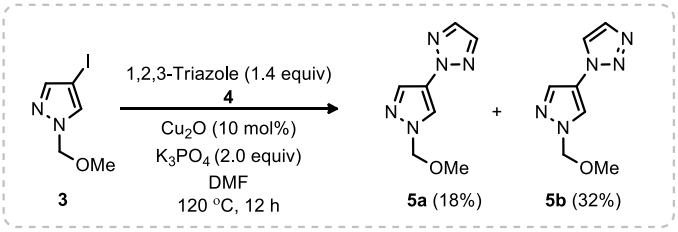
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.62 (s, 1H), 7.56 (s, 1H), 5.36 (s, 2H), 3.31 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 145.0, 134.1, 82.1, 58.1, 56.9 ppm.

Table S1: Optomization for synthesis of compounds **5a** and **5b**



entry	Catalyst(10 mol%)	Base (2 equiv.)	solvent	Temp(° C)	Yield (%)
1	CuI	Cs_2CO_3	DMF	120	NR
2	CuCl	Cs_2CO_3	DMF	120	NR
3	CuBr	Cs_2CO_3	DMF	120	NR
4	CuOAc	Cs_2CO_3	DMF	120	NR
5	$Fe(acac)_3$(30 mol %) + $Cu(acac)_2$(10 mol %)	Cs_2CO_3	DMF	120	8% (**5a**), 19% (**5b**)
6	$Fe(acac)_3$ + $Cu(acac)_2$	K_3PO_4	DMF	120	12% (**5a**), 22% (**5b**)
7	Cu_2O	Cs_2CO_3	CH_3CN	80	NR
8	Cu_2O	Cs_2CO_3	DMF	80	NR
9	Cu_2O	Cs_2CO_3	DMF	120	18% (**5a**), 32% (**5b**)
10	Cu_2O	Cs_2CO_3	DMSO	120	10% (**5a**), 15% (**5b**)

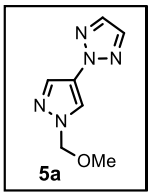
General procedure for the preparation of compounds 5a and 5b (GP-2):[3]



A mixture of Cu_2O (0.301 g, 2.10 mmol), K_3PO_4 (8.95 g, 42.18 mmol), 1,2,3-triazole (**4**; 2.03 g, 29.52 mmol), and the 4-iodo-1-(methoxymethyl)-pyrazole (**3**; 5.0 g, 21.09 mmol) in DMF (25 mL) was placed in a 100 mL screw capped Schlenk tube under an argon atmosphere. The resulting mixture was

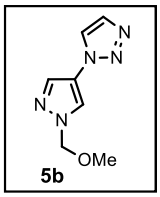
stirred at 120 °C for 12 h. The reaction mixture was diluted with EtOAc and filtered through a small plug of silica gel. The filtrate was washed with water and the aqueous layer was extracted withEtOAc. The combined organic extracts were washed with water and brine and dried over Na_2SO_4. The solvent was evaporated under reduced pressure. The crude residue was purified by column chromatography on silica gel using hexane-ethyl acetate. Isolation using 10% ethyl acetate in hexane led to separation of **5a** (700 mg, 18%) and 70% ethyl acetate in hexane **5b** (1.24 g, 32%) as pale-yellow liquids.

2-(1-(Methoxymethyl)-1*H*-pyrazol-4-yl)-2*H*-1,2,3-triazole (**5a**):



Following the general procedure (GP–2), compound **5a** (700 mg) was synthesized in 18% yield as pale-yellow liquid.^{1}H NMR (600 MHz, $CDCl_3$): δ 8.07 (s, 1H), 8.03 (s, 1H), 7.73 (s, 2H), 5.41 (s, 2H), 3.36 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 134.9, 131.6, 127.4, 121.0, 82.7, 56.9 ppm; IR (Neat)ν_{max} 3124, 2998, 2938, 2832, 1604, 1518, 1431, 1342, 1292, 1094, 935, 819, 750 cm^{-1}; HRMS (ESI) m/z $(M+H)^+$ calcd for $C_7H_{10}N_5O^+$ 180.0880, found 180.0885.

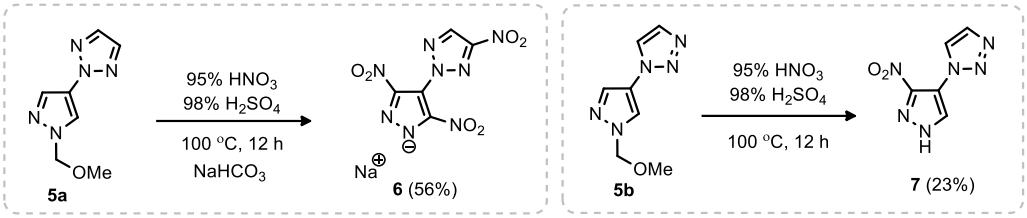
1-(1-(Methoxymethyl)-1*H*-pyrazol-4-yl)-1*H*-1,2,3-triazole (5b):



Following the general procedure (GP–2), compound **5b** (1.24 g) was synthesized in 32% yield as pale-yellow liquid.^{1}H NMR (600 MHz, $CDCl_3$): δ 8.06 (s, 1H), 7.87 (s, 1H), 7.85 (s, 1H), 7.82 (s, 1H), 5.44 (s, 2H), 3.38 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 133.9, 132.3, 123.0, 122.8, 122.6, 82.9, 57.1 ppm; IR (Neat)ν_{max} 3119, 2937, 1716, 1662, 1467, 1388, 1227, 1098, 933, 852, 750 cm^{-1}; HRMS (ESI) m/z $(M–H)^-$ calcd for $C_7H_8N_5O^-$ 178.0734, found 178.0701.

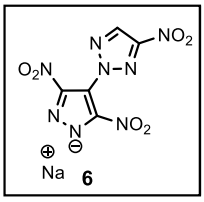
General procedure for the preparation of compound 6 and 7 (GP-3):

A mixture of 98% sulphuric acid and fuming nitric acid (95%) was independently added to compound **5a** and **5b** at 0 °C. Later the resulting mixture was stirred at 100 °C for 8-12h. The reaction progress was motinored by TLC. Upon reaction completion, the mixture was poured into ice cold water and neutralized with saturated aqueous $NaHCO_3$ solution. After neutralization, the reaction mixture was extracted with EtOAc. The organic layer was separated and dried over Na_2SO_4. The solvent was evaporated under reduced pressure. The crude residue was purified by column chromatography on silica gel eluting with hexane: ethyl acetate to afford the desired nitration products **6** and **7**.[4]



Sodium 3, 5-dinitro-4-(4-nitro-2*H*-1,2,3-triazol-2-yl)pyrazol-1-ide (6):

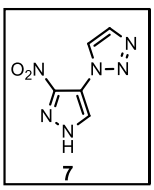
Following the general procedure (GP–3), compound **5a** (1.00 g, 5.58 mmol) was dissolved in sulphuric acid (10 mL), and fuming nitric acid (7 mL) was added dropwise to the reaction mixture at 0 °C. The resulting mixture was stirred at 100 °C for 8h. The reaction progress was motinored by TLC. Upon reaction completion, the mixture was poured into ice cold water and neutralized with saturated aqueous $NaHCO_3$ solution. After neutralization, the reaction mixture was extracted with EtOAc. The organic layer was separated and dried over Na_2SO_4. The solvent was evaporated under reduced pressure. The crude residue was purified by column chromatography on silica gel eluting with hexane: ethyl acetate to afford the desired product **6** (840 mg, 56%) as yellow solid.[4]



DSC (10 °C min^{-1}, °C): 290 °C (T_d); ^{1}H NMR (600 MHz, DMSO–d_6): δ 9.04 (s, 1H); ^{13}C NMR (151 MHz, DMSO–d_6): δ 154.2, 150.2, 132.8, 110.0; IR (Neat)ν_{max} 1621, 1523, 1447, 1359, 1325, 1074, 968, 828, 757 cm^{-1}; HRMS (ESI) m/z $(M–Na)^-$calcd for $C_5HN_8O_6^-$269.0024, found 269.0019.

1-(3-Nitro-1*H*-pyrazol-4-yl)-1*H*-1,2,3-triazole (7):

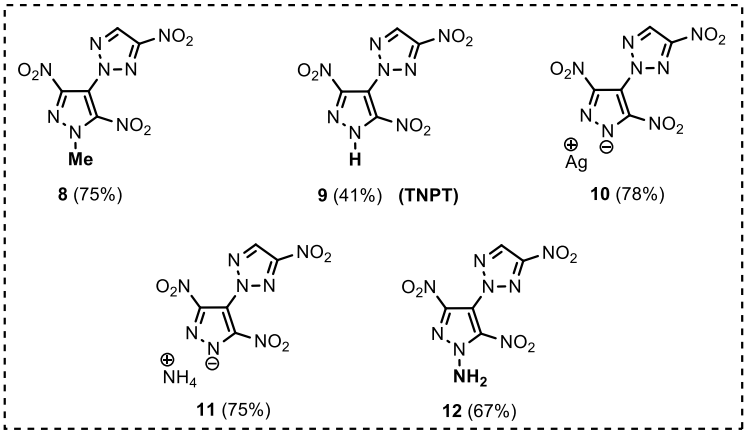
Following the general procedure (GP–3), compound **5b** (0.6 g, 3.35 mmol) was dissolved in sulphuric acid (7.5 mL), and fuming nitric acid (2.5 mL) was added dropwise to the reaction mixture at 0 °C. The resulting mixture was stirred at 100 °C for 12h. The reaction progress was motinored by TLC. Upon reaction completion, the mixture was poured into ice cold water and neutralized with saturated aqueous $NaHCO_3$solution. After neutralization, the reaction mixture was extracted with EtOAc. The organic layer was separated and dried over Na_2SO_4. The solvent was evaporated under reduced pressure. The crude residue was purified by column chromatography on silica gel eluting with hexane: ethyl acetate to afford the desired nitration product**7** (136 mg, 23%) as colorless solid.[4,5]



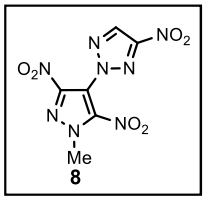
DSC (10 °C min^{-1}, °C): 135 °C (T_m) & 177 °C (T_d); ^{1}H NMR (600 MHz, CD_3CN): δ 12.20 (bs, 1H), 8.18 (s, 1H), 8.16 (d, J= 0.6 Hz, 1H), 7.82 (d, J= 1.2 Hz, 1H);^{13}C NMR (101 MHz, CD_3CN): δ 134.4, 130.7, 128.4, 115.8, 79.1 ppm;IR

(Neat)ν_{max}3161, 3118, 2925, 1721, 1613, 1528, 1445, 1354, 1242, 1121, 1077, 975, 827, 782 cm^{-1};HRMS (ESI) m/z $(M+H)^+$ calcd for $C_5H_5N_6O_2^+$ 181.0469, found 181.0471.

Synthesis of compounds 8, 9, 10, 11, and 12 from sodium salt of TNPT derivative (6):



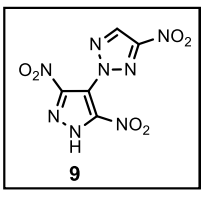
2-(1-Methyl-3,5-dinitro-1*H*-pyrazol-4-yl)-4-nitro-2*H*-1,2,3-triazole (8):



To a solution of compound **6** (520 mg, 1.78 mmol) in water (5.0 mL) was added dimethyl sulfate (270 mg, 2.13 mmol). The reaction mixture was stirred at room temperature for 8 h. The precipitate was collected by filtration and washed with distilled water to yield **8** (380 mg, 75%)as colorless solid.[6]

DSC–TGA (10 °C min^{-1}, °C): 134°C (T_m) & 230 °C (T_d); ^{1}H NMR (600 MHz, CD_3CN): δ 8.66 (s, 1H), 4.36 (s, 3H); ^{13}C NMR (151 MHz, CD_3CN):δ 156.5, 147.1, 142.4, 134.3 (d, *J*= 10Hz), 113.5, 44.3 (d, *J*= 4.4 Hz);^{15}N NMR (61 MHz, Acetone–d_6): δ –26.1, –28.2, –31.7, –32.9, –46.5, –75.0, –151.0, –180.3 ppm; IR (Neat)ν_{max} 3149, 1622, 1539, 1468, 1444, 1367, 1332, 1228, 1137, 1041, 961, 826, 756 cm^{-1}; HRMS (ESI) m/z $(M+Na)^+$ calcd for $C_6H_4N_8NaO_6^+$ 307.0146, found 307.0148.

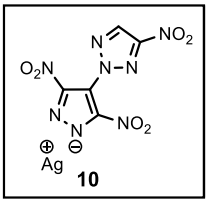
2-(3,5-Dinitro-1*H*-pyrazol-4-yl)-4-nitro-2*H*-1,2,3-triazole (9):



A solution of the corresponding pyrazole **6**(300 mg, 1.0 mmol) in concentrated HCl (10 mL) was stirred for 24 h at room temperature. The solvent was evaporated at reduced pressure and the residue was recrystallized from H_2O to obtain desired product **9** (113 mg, 41%) as colorless solid.[7]

DSC (10 °C min^{-1}, °C): 204 °C (T_m) & 261 °C (T_d); ^{1}H NMR (600 MHz, DMSO–d_6): δ 9.03 (s, 1H); ^{13}C NMR (151 MHz, DMSO–d_6): δ 154.2, 150.2, 132.8, 110.1; ^{15}NNMR (61 MHz, DMSO–d_6): δ –19.5, –24.5, –32.4, –47.5, –141.9 ppm;IR (Neat)ν_{max} 3641, 3502, 3148, 1628, 1542, 1480, 1453, 1370, 1225, 1067, 960, 829, 759 cm^{-1}; HRMS (ESI) m/z $(M–H)^–$ calcd for $C_5HN_8O_6^–$ 269.0024, found 269.0016.

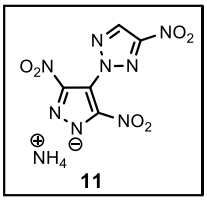
Silver (I) 3,5-dinitro-4-(4-nitro-2*H*-1,2,3-triazol-2-yl)pyrazol-1-ide (10):



A solution of silver nitrate (410 mg, 2.44 mmol) in distilled water (4.0 mL) was added dropwise to a suspension of **6** (600 mg, 2.2 mmol) in methanol (4.0 mL). The reaction mixture was stirred at room temperature for 12 h, then **10** (650 mg, 78%) was collected by filtration, washed with water, and dried in vacuum.[6]

DSC (10 °C min^{-1}, °C): T_d : 302 °C; ^{1}H NMR (600 MHz, CD_3CN): δ 8.58 (s, 1H); ^{13}C NMR (151 MHz, CD_3CN): δ 155.8, 150.9, 133.3, 111.5 ppm; IR (Neat)ν_{max} 1616, 1523, 1452, 1364, 1326, 1024, 975, 829, 756 cm^{-1}; HRMS (ESI) m/z $(M-Ag)^-$ calcd for $C_5HN_8O_6^-$ 269.0024, found 269.0038.

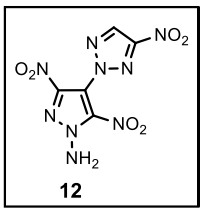
Ammonium 3,5-dinitro-4-(4-nitro-2*H*-1,2,3-triazol-2-yl)pyrazol-1-ide(11):



A solution of **10** (500 mg, 1.71 mmol) in methanol (8.0 mL) was addedammonium chloride (100mg, 1.88 mmol). The reaction mixture was stirred at room temperature for 12 h.The suspension was filtered, washed with water, and dried in vacuum to yield **11** (370mg, 75%)as yellow solid. [6,8]

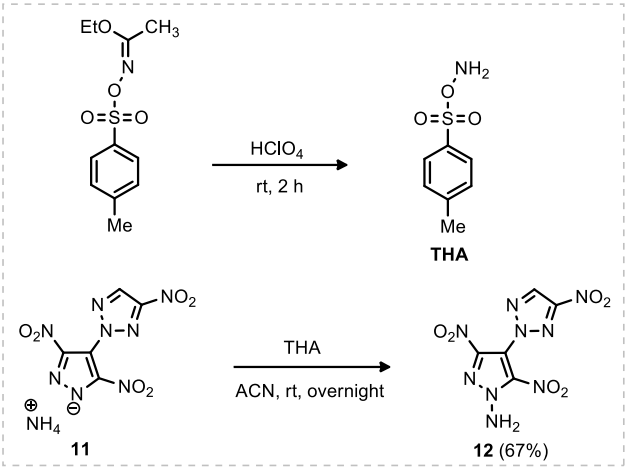
DSC (10 °C min^{-1}, °C): T_d :268 °C; ^{1}H NMR (600 MHz, CD_3CN): δ 8.55 (s, 1H), 6.47 (bs, 4H); ^{13}C NMR (151 MHz, CD_3CN): δ 155.6, 151.4, 133.1, 111.1; ^{15}NNMR (61 MHz, DMSO–d_6): δ –19.1, –24.4, –32.5, –47.7, –51.5, –141.6, –352.4 ppm; IR (Neat)ν_{max} 3289, 3247, 3161, 2795, 1614, 1523, 1441, 1408, 1354, 1324, 1231, 1155, 1071, 966, 836, 757 cm^{-1}; HRMS (ESI) m/z $(M+H)^+$ calcd for $C_5H_6N_9O_6^+$ 288.0436, found 288.0432.

3,5-Dinitro-4-(4-nitro-2*H*-1,2,3-triazol-2-yl)-1*H*-pyrazol-1-amine (12):



To a freshly prepared pulverized ethyl *O*-*p*-tolylsulphonylacetohydroximate (1.34 g, 5.22 mmol) was added 70% perchloric acid (12.5 mL) at room temperature and stirred at ambient conditions for 2 h. The tosylhydroxylamine suspension was poured into 80 mL of ice/water slurry.The mixture was extracted with dichloromethane (3 × 20 mL). The combined dichloromethane extracts were dried over sodium sulfate and filtered. Next, a solution of **11**(1.0 g, 3.48 mmol) in acetonitrile (50 mL) was added dropwise to the freshly prepraredtosylhydroxylamine in dichloromethane. The resulting mixture was stirred overnight under ambient conditions, evaporated to dryness, and resuspended in ethyl acetate.

The suspension was filtered and evaporated, and purified by silica gel chromatography eluting with hexane-ethyl acetate (70:30)to afford**12** (655 mg, 67%) as pink solid.[9]



DSC (10 ^{o}C min^{-1}, °C): 185 ^{o}C (T_m) & 280 ^{o}C (T_d);^{1}H NMR (600 MHz, Acetone–d_6): δ 8.88 (s, 1H), 7.91 (s, 2H);^{13}C NMR (151 MHz, Acetone–d_6): δ 156.2, 143.0, 137.9, 134.1, 111.8;^{15}N NMR (61 MHz, CD_3CN): δ –30.4, –32.9, –36.4, –37.9, –51.1, –88.8, –155.9, –168.6, –286.9 ppm;IR (Neat)ν_{max}3363, 3277, 1620, 1484, 1370, 1334, 1311, 1233, 1128, 1059, 968, 827, 758 cm^{-1};HRMS (ESI) m/z $(M+Na)^+$ calcd for $C_5H_3N_9NaO_6^+$ 308.0099, found 308.0078.

X-ray crystallography:[10]

Single crystal X-ray data for the compounds **6**, **7**, **9**, **11**, were collected using 'Bruker D8 VENTURE Photon III detector' system [**6**, **7**, **11** using λ (Mo–Kα) = 0.71073Å; **9** using λ (Cu-Kα) = 1.54 Å] at 108 K, 104 K, 296 K, 107 K, and **8**, **12** were collected using Rigaku Oxford Hypix-3000 system [**6, 7** using λ (Mo–Kα) = 0.71073Å; at 298 K, 298 K, graphite monochromator with a ω scan. Data reduction was performed using Bruker SAINT[2] software. Intensities for absorption were corrected using SADABS 2014/5. Structure solution and refinement were carried out using Bruker SHELX-TL/ Olex2 1.3 version. All non-hydrogen atoms were refined anisotropically. Thermal ellipsoid plots of all the compounds **6, 7, 8, 9, 11** and **12** with 50% probability and hydrogen atoms are unlabelled for clarity shown (Manuscript Figure 3).

CCDC-2241660 (**6**), CCDC-2241851 (**7**), CCDC-2289671 (**8**), CCDC-2241662 (**9**), CCDC-2241663 (**11**), and CCDC-2289806 (**12**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_ request/cif.

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Table S2 Crystallographic data for compounds **6**, **7**, and **8**

Compound	**6**	**7**	**8**
CCDC	2241660	2241851	2289671
Formula	C5 H3 N8 Na O7	$C_5H_4N_6O_2$	$C_6H_4N_8O_6$
M_w	310.14	180.14	284.17
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*C*2/*c*	*P*21	*P*21/*n*
T [K]	108 K	104 K	298 K
a [Å]	11.4210 (11)	6.6812 (10)	9.1552(5)
b [Å]	9.3158 (10)	7.0171 (11)	8.1515(4)
c [Å]	21.599 (2)	7.8472 (12)	15.7139(7)
α [°]	90	90	90
β [°]	96.498 (4)	104.571 (5)	106.884(5)
γ [°]	90	90	90
Z	8	2	4
V [Å^3]	2283.3 (4)	356.07 (9)	1122.16(10)
D_{calc} [g/cc]	1.804	1.68	1.682
μ [mm^{-1}]	0.196	0.136	0.151
Total reflns	2838	2082	-
Unique reflns	2829	1941	2347
Observed reflns	2553	1924	1974
$R_1[I > 2\sigma(I)]$	0.0290	0.0303	0.0427
wR_2 [all]	0.0789	0.0804	0.1329
GOF	1.060	1.064	1.065
Diffractometer	Bruker D8 VENTURE Photon III detector	Bruker D8 VENTURE Photon III detector	Rigaku Oxford Hypix-3000 detector

Table S3 Crystallographic data for compounds **9**, **11**, and**12**

Compound	**9**	**11**	**12**
CCDC	2241662	2241663	2289806
Formula	$C_5H_2N_8O_6$	$C_5H_5N_9O_6$	$C_5H_3N_9O_6$
M_w	270.15	287.18	285.16
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	*P*21/*c*	*P –1*	*P*21/*n*
T [K]	296 K	107 K	298 K
a [Å]	11.9516 (2)	5.1838 (8)	8.8502(4)
b [Å]	8.6036 (2)	9.1275 (12)	7.3093(4)
c [Å]	10.7241 (2)	12.3907 (18)	16.7588(7)
α [°]	90	107.311 (4)	90
β [°]	104.501 (1)	99.537 (5)	98.440(4)
γ [°]	90	102.736 (4)	90
Z	4	2	4
V [Å^3]	1067.6 (4)	528.83 (13)	1072.37(9)
D_{calc} [g/cc]	1.68	1.804	1.766
μ [mm^{-1}]	1.371	0.163	0.161
Total reflns	-	4021	-
Unique reflns	1926	3999	2204
Observed reflns	1779	3603	1129
$R_1[I > 2\sigma(I)]$	0.0352	0.0328	0.0686
wR_2 [all]	0.0993	0.0904	0.2247
GOF	1.057	1.051	1.011
Diffractometer	Bruker D8 VENTURE Photon III detector	Bruker D8 VENTURE Photon III detector	Rigaku Oxford Hypix-3000 detector

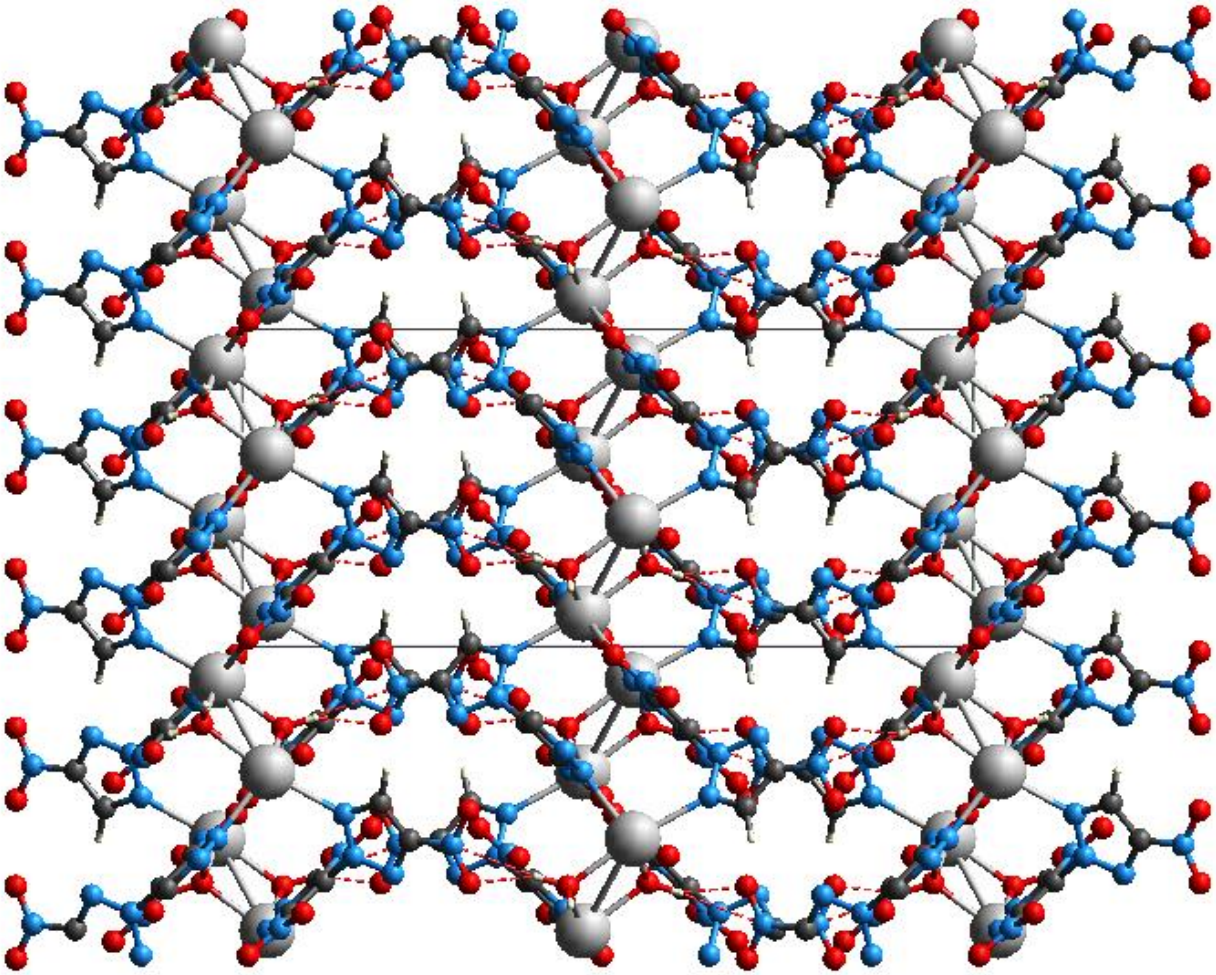


Figure S1: Ball and stick packing diagram of compound **6** viewed down the b axis. Dashed lines indicate hydrogen bonding.

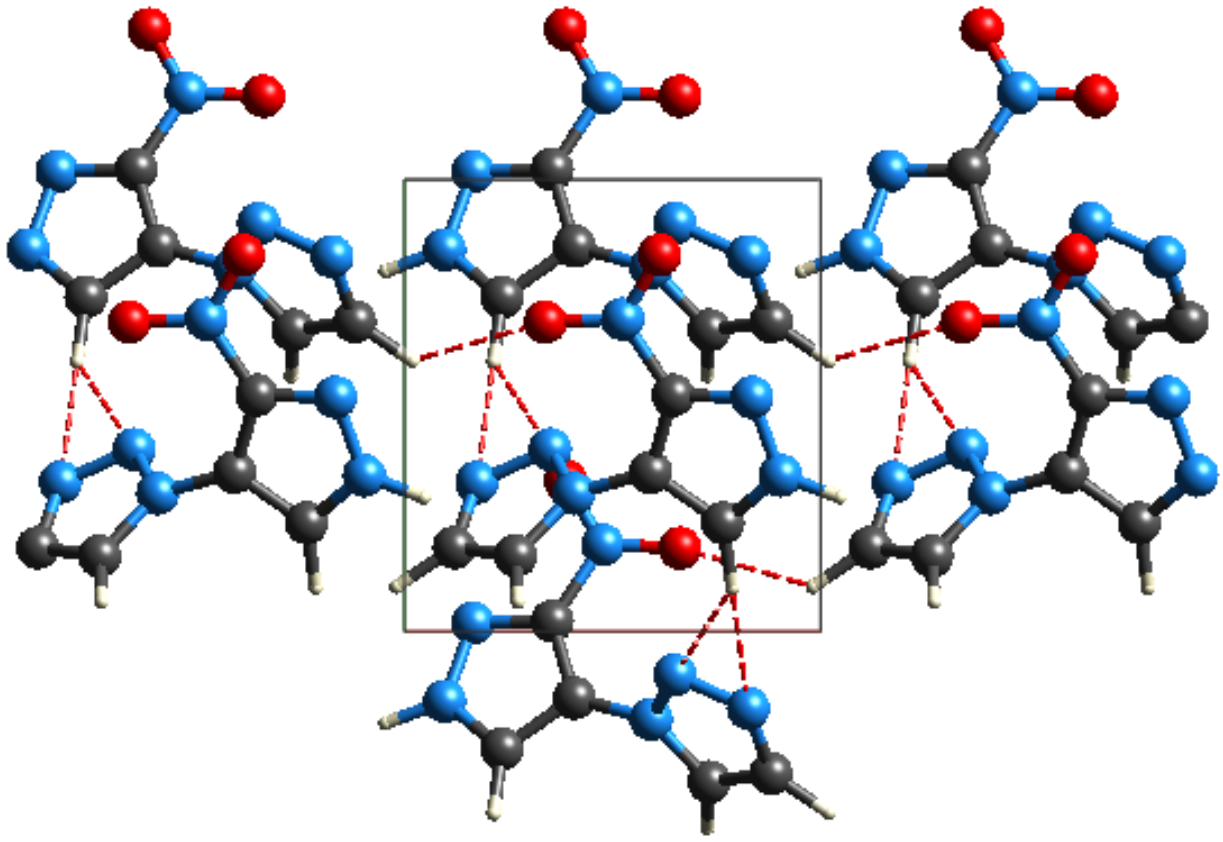


Figure S2: Ball and stick packing diagram of compound **7** viewed down the C axis. Dashed lines indicate hydrogen bonding.

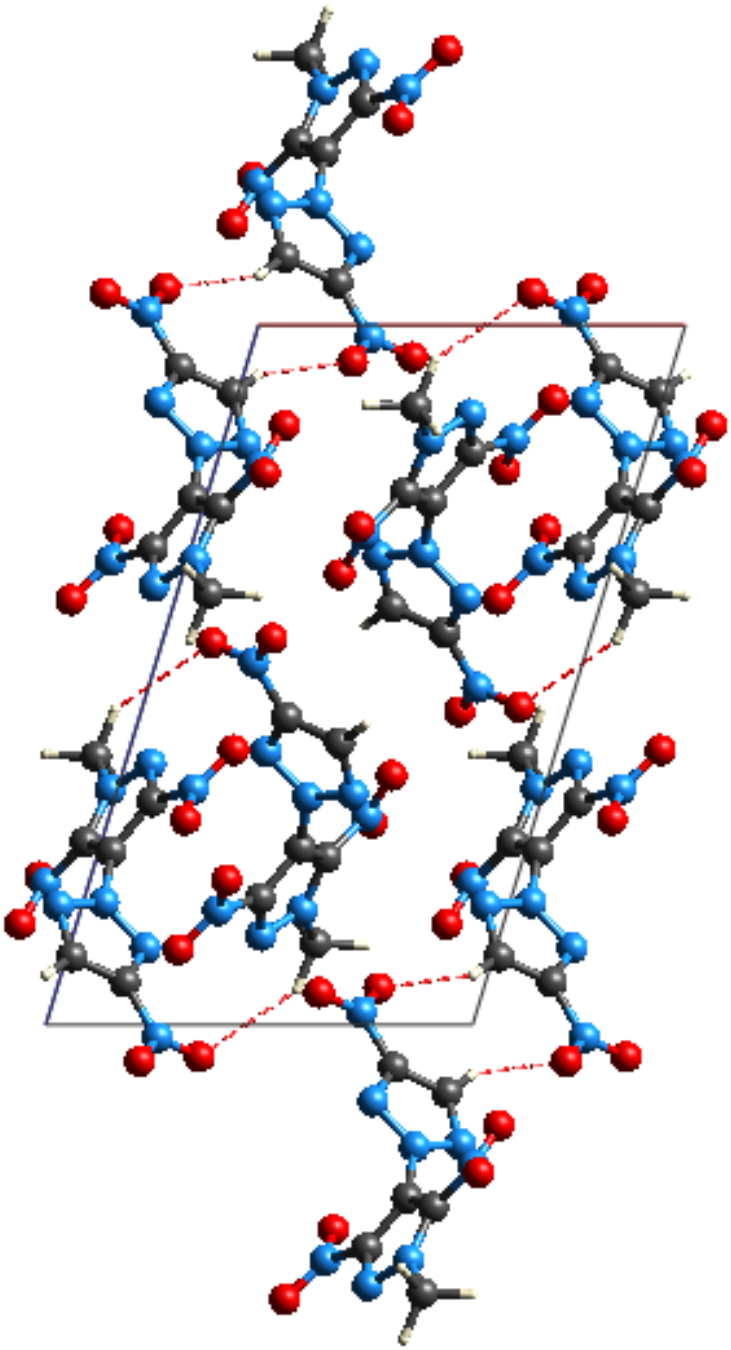


Figure S3: Ball and stick packing diagram of compound **8** viewed down the b axis. Dashed lines indicate hydrogen bonding.

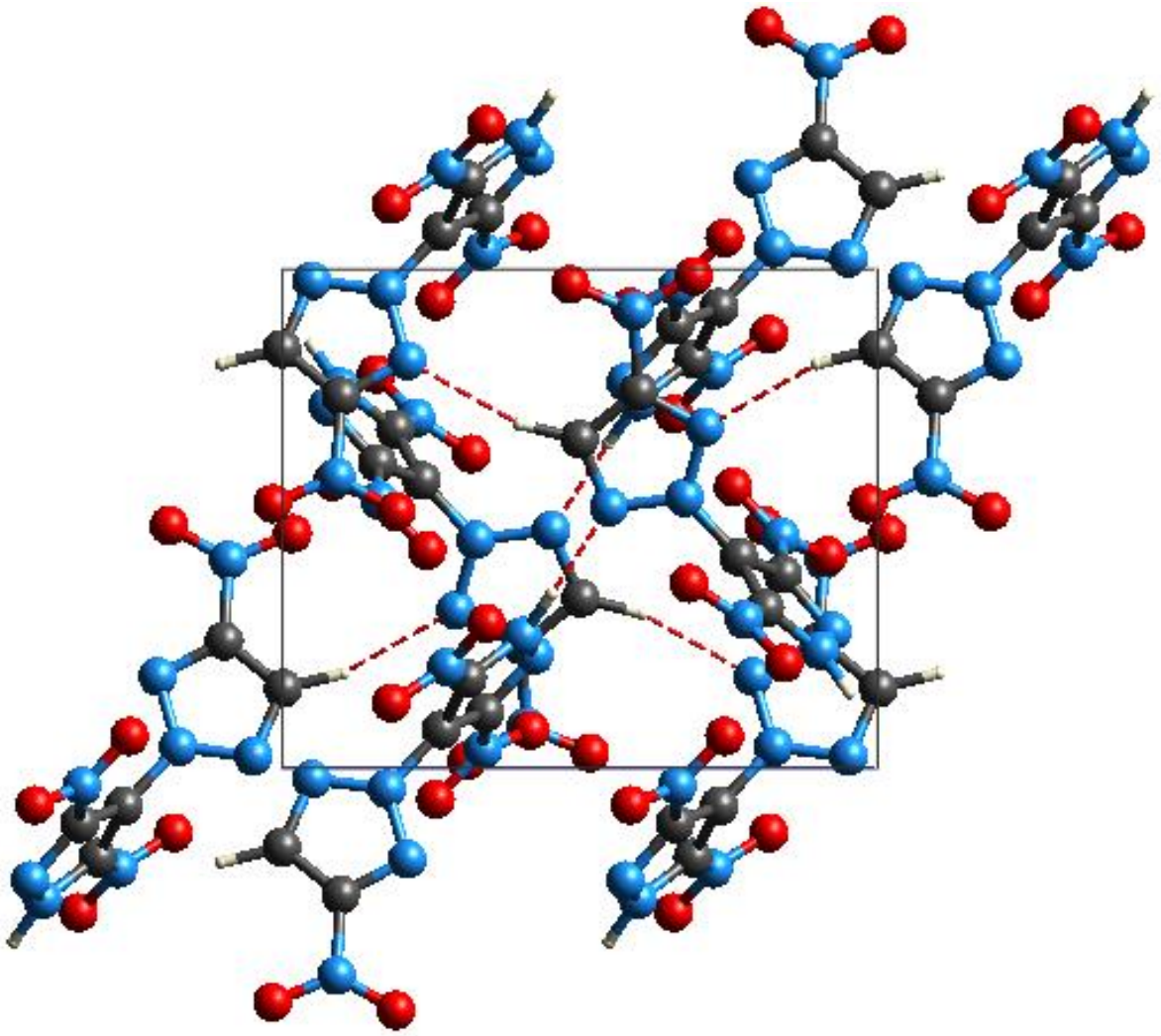


Figure S4: Ball and stick packing diagram of compound **9** viewed down the a axis. Dashed lines indicate hydrogen bonding.

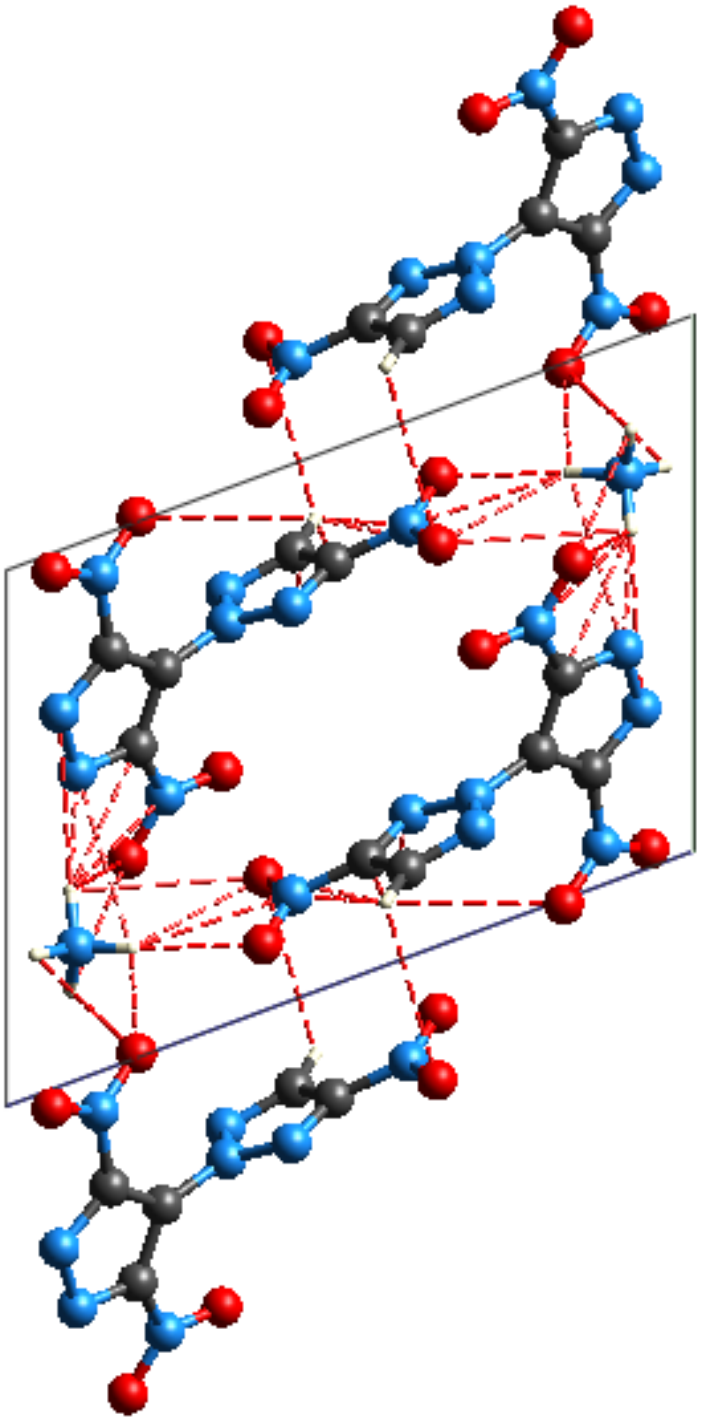


Figure S5: Ball and stick packing diagram of compound **11** viewed down the a axis. Dashed lines indicate hydrogen bonding.

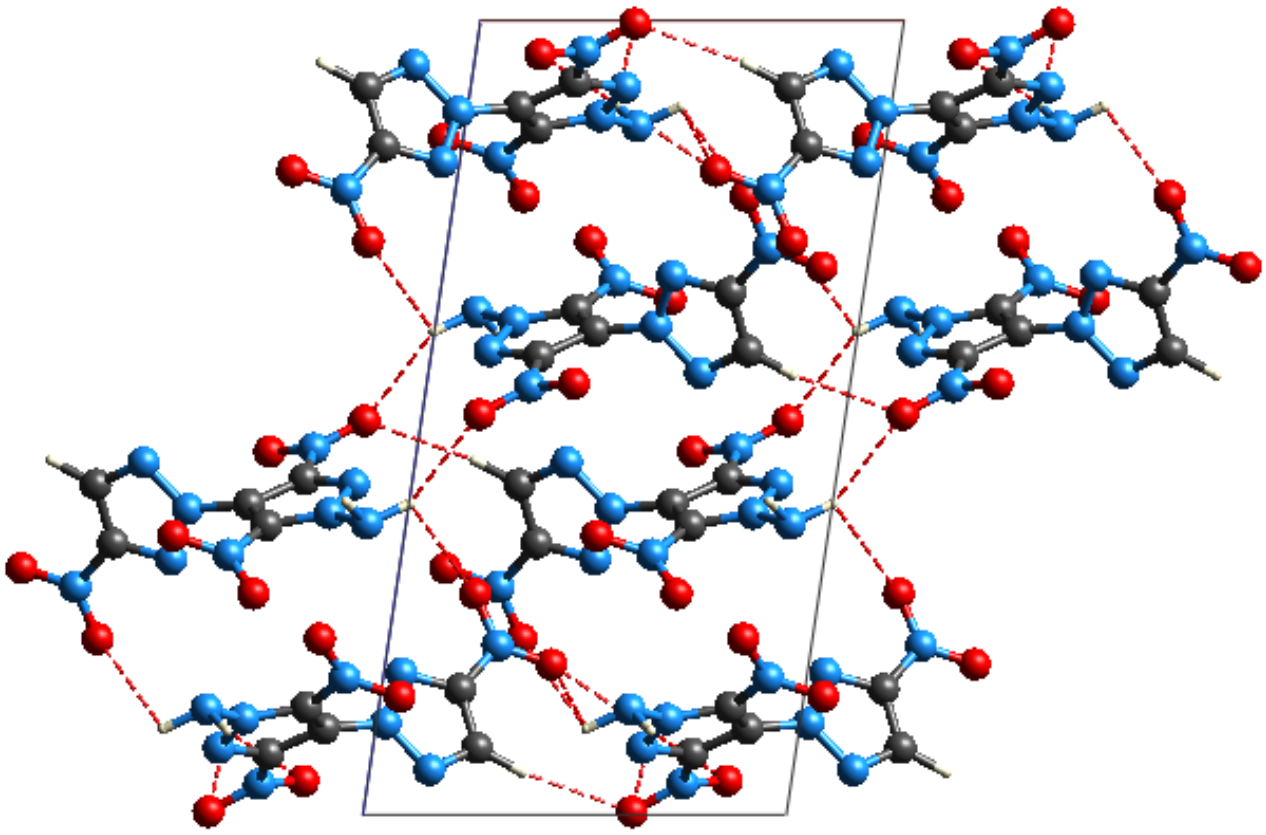


Figure S6 : Ball and stick packing diagram of compound **12** viewed down the b axis. Dashed lines indicate hydrogen bonding.

In most cases, the X-Ray crystallography data of the energetic compounds are collected at low temperature. The strong intermolecular interactions in the crystal unit cell affect the X-ray diffraction [see Effect of Strong Intermolecular Interaction in 2D Inorganic Molecular Crystals, Xin Feng, Xingliang Peng, Baixin Peng, Zexin Li, Wentao Huang, Sijie Yang, Ke Pei, Zongdong Sun, Fuqiang Huang, Huiqiao Li, Zhigang Shuai, and Tianyou Zhai, *Journal of the American Chemical Society* **2021,** *143* (48), 20192-20201]. Thus, most of the X-ray crystal data are collected in different temperature; we report the best diffraction results. Whereas X-ray data for compound **8** and **12** are collected at 298K.

The Hirschfield surfaces analysis of compound **12** was independently examined at low temperature and room temperature as shown in Table 1. We did not see significant variation of atomic interactions (listed in the table) in the crystal packing. We therefore believe that the thermal expansion is not greatly affected with respect to temperature.

Table 1:

S. No	**2D fingerprint plots of compound 12 at low temperature**		**2D fingerprint plots of compound 12 at room temperature**	
	Atomic interactions	**Percentage (%)**	**Atomic interactions**	**Percentage (%)**
1	O…H/H…O	27.2	O…H/H…O	25.9
2	N…H/H…N	9.7	N…H/H…N	6.7
3	N…O/O…N	22.7	N…O/O…N	23.3
4	C…O/O…C	11.7	C…O/O…C	11.6
5	C…N/N…C	4.6	C…N/N…C	4.6
6	O…O	17.7	O…O	19.4

Hirshfeld Surface Analysis[11]

The Hirshfeld surface image shown in Figure4 (in the manuscript body), the red spots signify the high contact populations, while blue and white spots are for low contact populations. This suggests that the negative (red) or positive value (blue and white) of d_{norm} depends on the intermolecular contacts being shorter (red) or longer (blue and white) than the Vander Waals separations. For each point on the Hirshfeld surface, the normalized contact distance (d_{norm}) was determined by the equation shown below.

$$[d_{norm}= (d_i – d_i^{vdW})/r_i^{vdW} + (d_e – d_e^{vdW}/r_e^{vdW}]$$

In which, d_i is measured from the surface to the nearest atom interior to the surface interior, while d_e is measured from the surface to the nearest atom exterior to the surface interior, where $r_i^{vdW}$and$r_e^{vdW}$are the Van der Waals radii of the atoms.Hirshfeld surface graphs and two-dimensional fingerprint plots of **8**, **9**, **11**, and **12**were analyzed using Crystalexplorer17.5 softwareand Hirshfeld surface calculation of **11**as shown in Figure S12 (Hirshfeldplots of **8**, **9**, and **12**are shown inFigure 4, manuscript body).

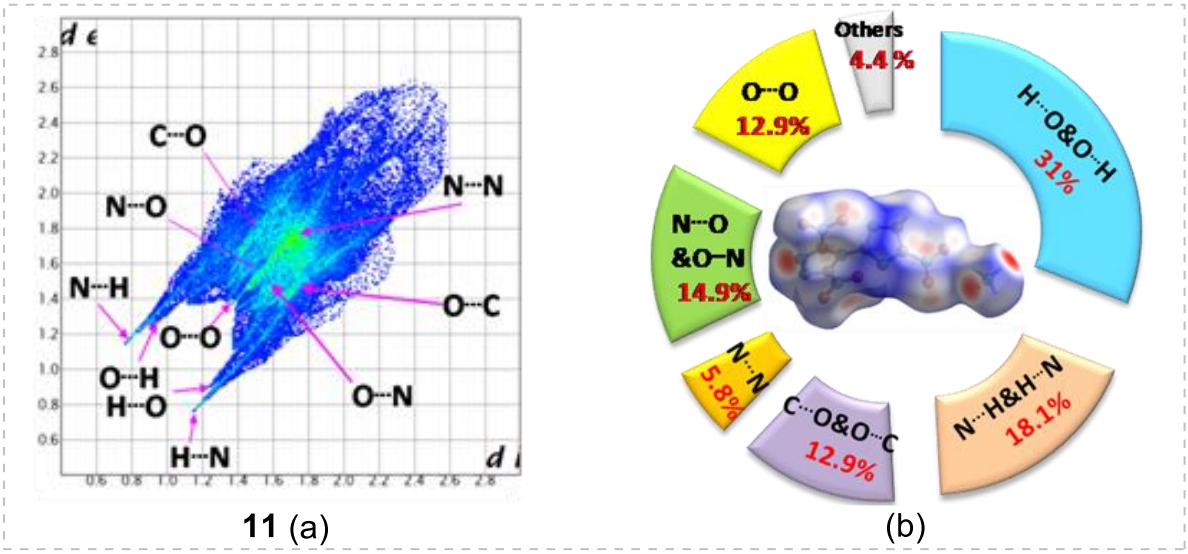
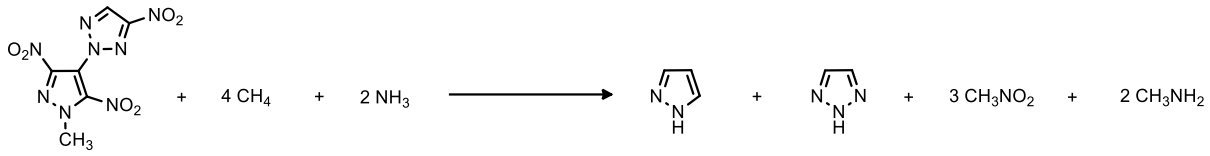


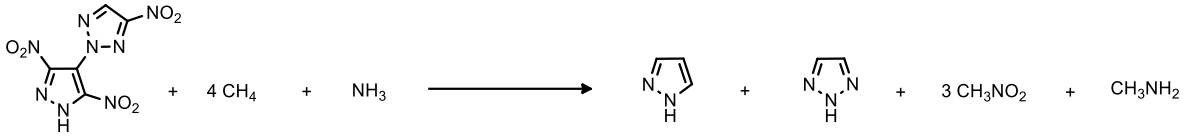
Figure S7: Hirshfeld surface calculation of **11** as well as two-dimensional finger print plot in the crystal structure. Hirshfeld surface graph (centre of pie graph) with proximity of close contacts around **11** molecules (white, d = Van der Waals (vdW) distance; blue, d >vdW distance; red, d <vdW distance). The pie graph (b) for **11** and show percentage contributions of the individual atomic contacts to the Hirshfeld surface.

Hirschfield surface and the related 2D fingerprint plots mainly reveals the intermolecular interactions [such as hydrogen bonding (HB), and π-stacking] of the energetic crystals; these interactions generally determine the packing structure and further the properties and performances of an energetic compound. In general, the large population of O...H/H...O and N...H/H...N interactions makes the molecule more stable and therefore is less sensitive. Accordingly, compound **8** (N-methyl trinitro-pyrazolo-triazole; IS: 40 J) and **12** (N-amino trinitro-pyrazolo-triazole; IS: 35 J) are relatively less sensitive than trinitro-pyrazolo-triazole (TNPT) (IS: 35 J) due to more O...H/H...O and N...H/H...N interactions in the crystal packing {see: Hirshfeld Surface Method and Its Application in Energetic Crystals, Shijie Li, Rupeng Bu, Rui-jun Gou, and Chaoyang Zhang, *Crystal Growth & Design*, **2021**, *21* (12), 6619-6634].

Isodesmic reactions for the prediction of heat of formation:[12]



8



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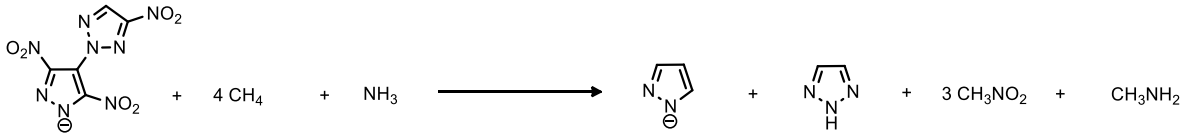
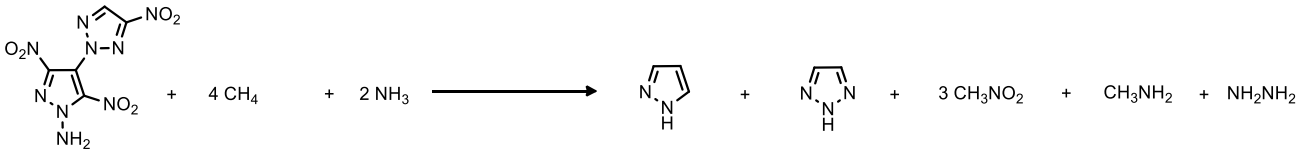
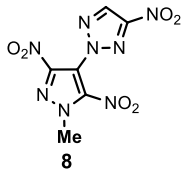


11 Anion



12

Impact Sensitivity Test Results

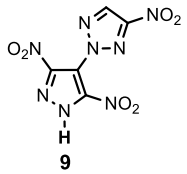


8

Table S4

Weight	Height	IS	1	2	3	4	5	6	Result
5 kg	100 cm	50 J	Negative	Positive	Positive				2 Out of 3
	90 cm	45 J	Negative	Negative	Negative	Positive	Negative	Positive	1 Out of 6
	80 cm	40 J	Negative	Negative	Negative	Negative	Negative	Negative	0 Out of 6

Final Result: Impact Sensitivity of 2-(1-Methyl-3,5-dinitro-1*H*-pyrazol-4-yl)-4-nitro-2*H*-1,2,3-triazole = 40 J

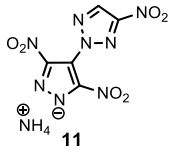


9

Table S5

Weight	Height	IS	1	2	3	4	5	6	Result
5 kg	100 cm	50 J	Negative	Positive	Negative	Positive			2 Out of 4
	80 cm	40 J	Positive	Negative	Negative	Negative	Positive		1 Out of 4
	70 cm	35 J	Negative	Negative	Negative	Negative	Negative	Negative	0 Out of 6

Final Result: Impact Sensitivity of 2-(3,5-Dinitro-1*H*-pyrazol-4-yl)-4-nitro-2*H*-1,2,3-triazole= 35 J

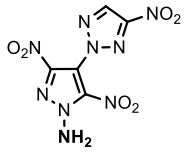


11

Table S6

Weight	Height	IS	1	2	3	4	5	6	Result
5 kg	100 cm	50 J	Positive	Positive					2 Out of 2
	80 cm	40 J	Negative	Positive	Negative	Negative	Positive		2 Out of 5
	70 cm	35 J	Negative	Negative	Negative	Negative	Negative	Positive	1 Out of 6
	60 cm	30 J	Negative	Negative	Negative	Negative	Negative	Negative	0 Out of 6

Final Result: Impact Sensitivity of Ammonium 3,5-dinitro-4-(4-nitro-2*H*-1,2,3-triazol-2-yl)pyrazol-1-ide= 30 J



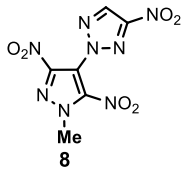
12

Table S7

Weight	Height	IS	1	2	3	4	5	6	Result
5 kg	100 cm	50 J	Negative	Positive	Positive				2 Out of 3
	80 cm	40 J	Positive	Negative	Negative	Negative	Positive		2 Out of 5
	70 cm	35 J	Negative	Negative	Negative	Negative	Negative	Negative	0 Out of 6

Final Result: Impact Sensitivity of 3,5-Dinitro-4-(4-nitro-2*H*-1,2,3-triazol-2-yl)-1*H*-pyrazol-1-amine = 35 J

Friction Sensitivity Results

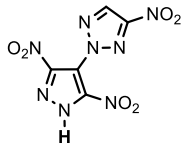


8

Table S8

Load	Notch No.	FS	1	2	3	4	5	6	Result
B9	6	360 N	Negative	Negative	Negative	Negative	Negative	Negative	0 Out of 6

Final Result: Friction Sensitivity of 2-(1-Methyl-3,5-dinitro-1*H*-pyrazol-4-yl)-4-nitro-2*H*-1,2,3-triazole = 360 N

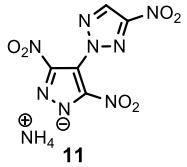


9

Table S9

Load	Notch No.	FS	1	2	3	4	5	6	Result
B9	5	324 N	Negative	Positive	Positive				2 Out of 3
B9	4	288 N	Negative	Negative	Positive	Negative	Positive		2 Out of 5
B9	3	252 N	Negative	Negative	Negative	Negative	Positive		1 Out of 5
B9	2	216 N	Negative	Negative	Negative	Negative	Negative	Negative	0 out of 6

Final Result: Friction Sensitivity of 2-(3,5-Dinitro-1*H*-pyrazol-4-yl)-4-nitro-2*H*-1,2,3-triazole= 216 N

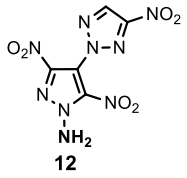


11

Table S10

Load	Notch No.	FS	1	2	3	4	5	6	Result
B9	5	324 N	Negative	Positive	Negative	Negative	Negative	Negative	1 Out of 6
B9	4	288 N	Negative	Negative	Negative	Negative	Negative	Negative	0 Out of 6

Final Result: Friction Sensitivity of Ammonium 3,5-dinitro-4-(4-nitro-2*H*-1,2,3-triazol-2-yl) pyrazol-1-ide= 288 N



12

Table S11

Load	**Notch No.**	**FS**	**1**	**2**	**3**	**4**	**5**	**6**	**Result**
B9	5	324 N	Positive	Positive					2 Out of 2
B9	4	288 N	Negative	Positive	Negative	Positive			2 Out of 4
B9	3	252 N	Negative	Negative	Positive	Negative	Negative	Negative	1 Out of6
B9	2	216 N	Negative	Negative	Negative	Negative	Negative	Positive	1 out of 6
B9	1	180 N	Negative	Negative	Negative	Negative	Negative	Negative	0 out of 6

Final Result: Friction Sensitivity of 3,5-Dinitro-4-(4-nitro-2*H*-1,2,3-triazol-2-yl)-1*H*-pyrazol-1-amine= 180 N

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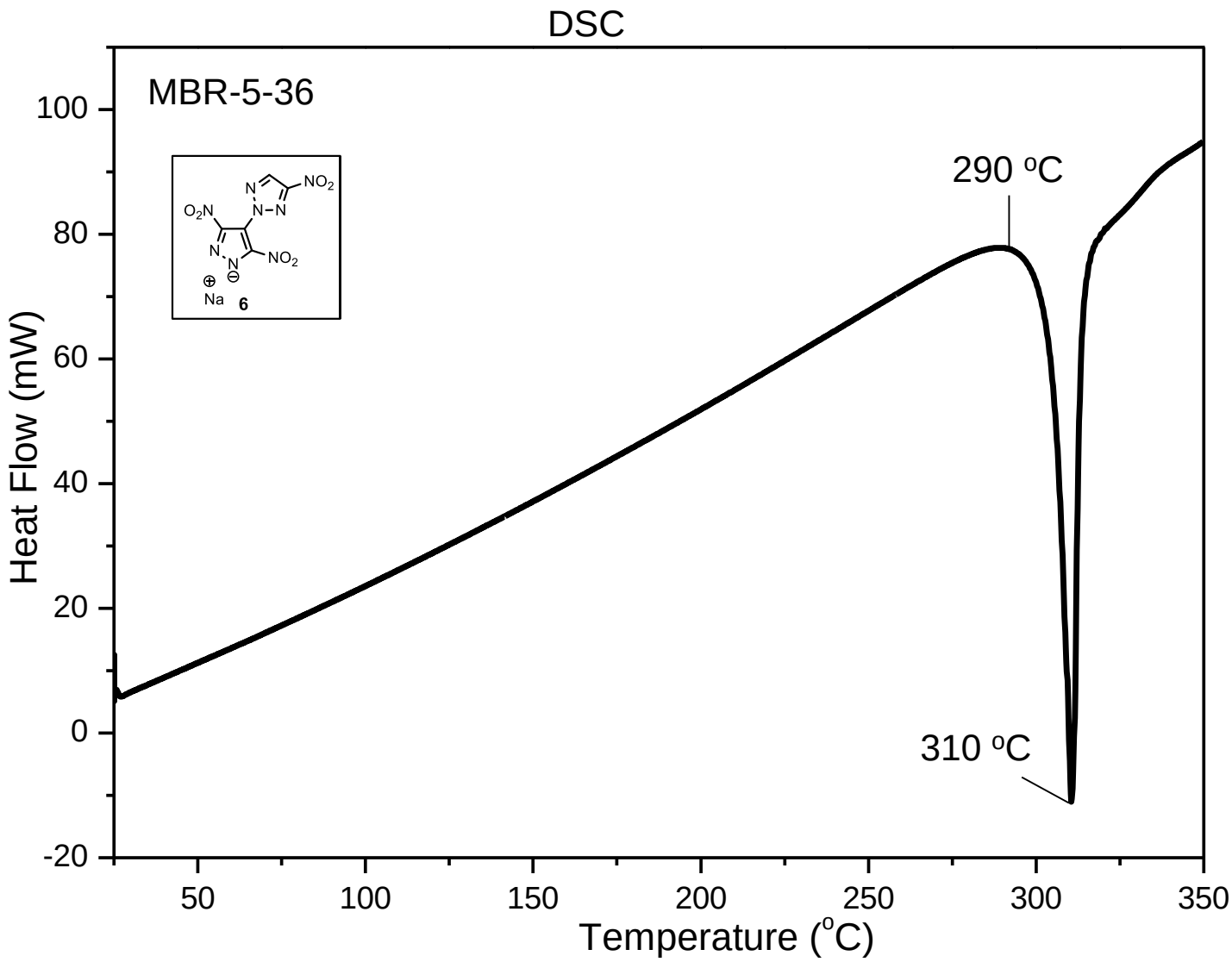
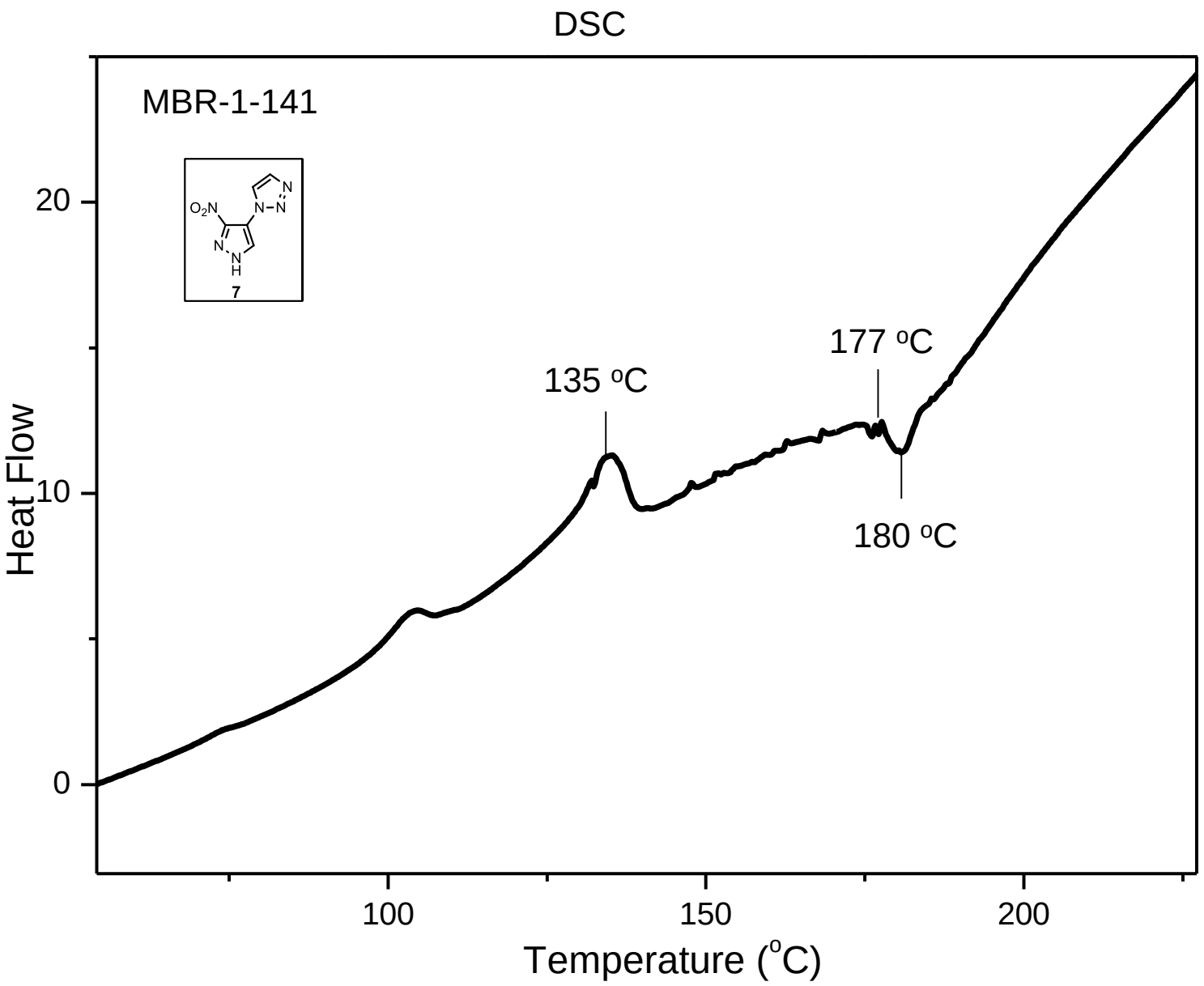
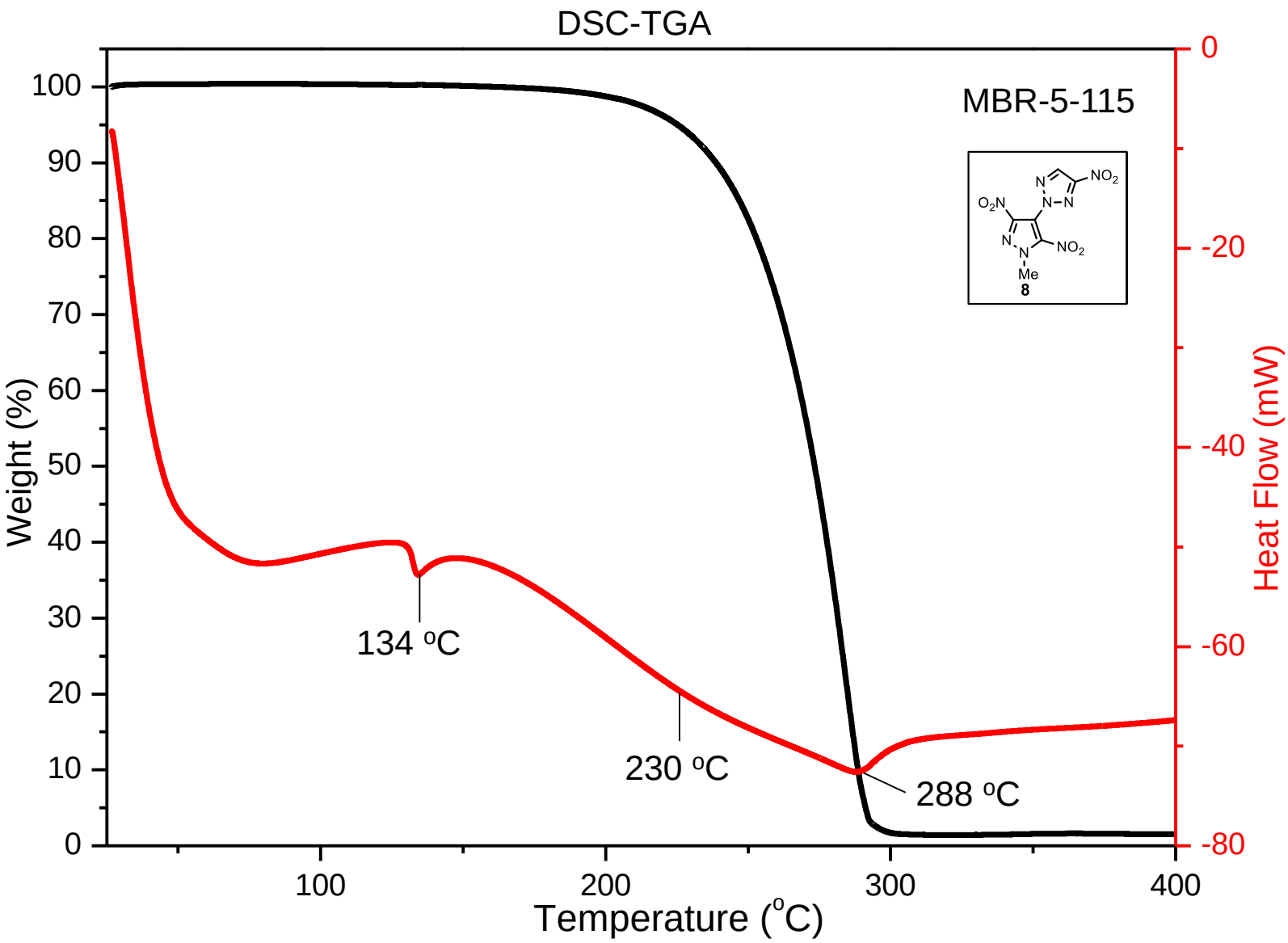
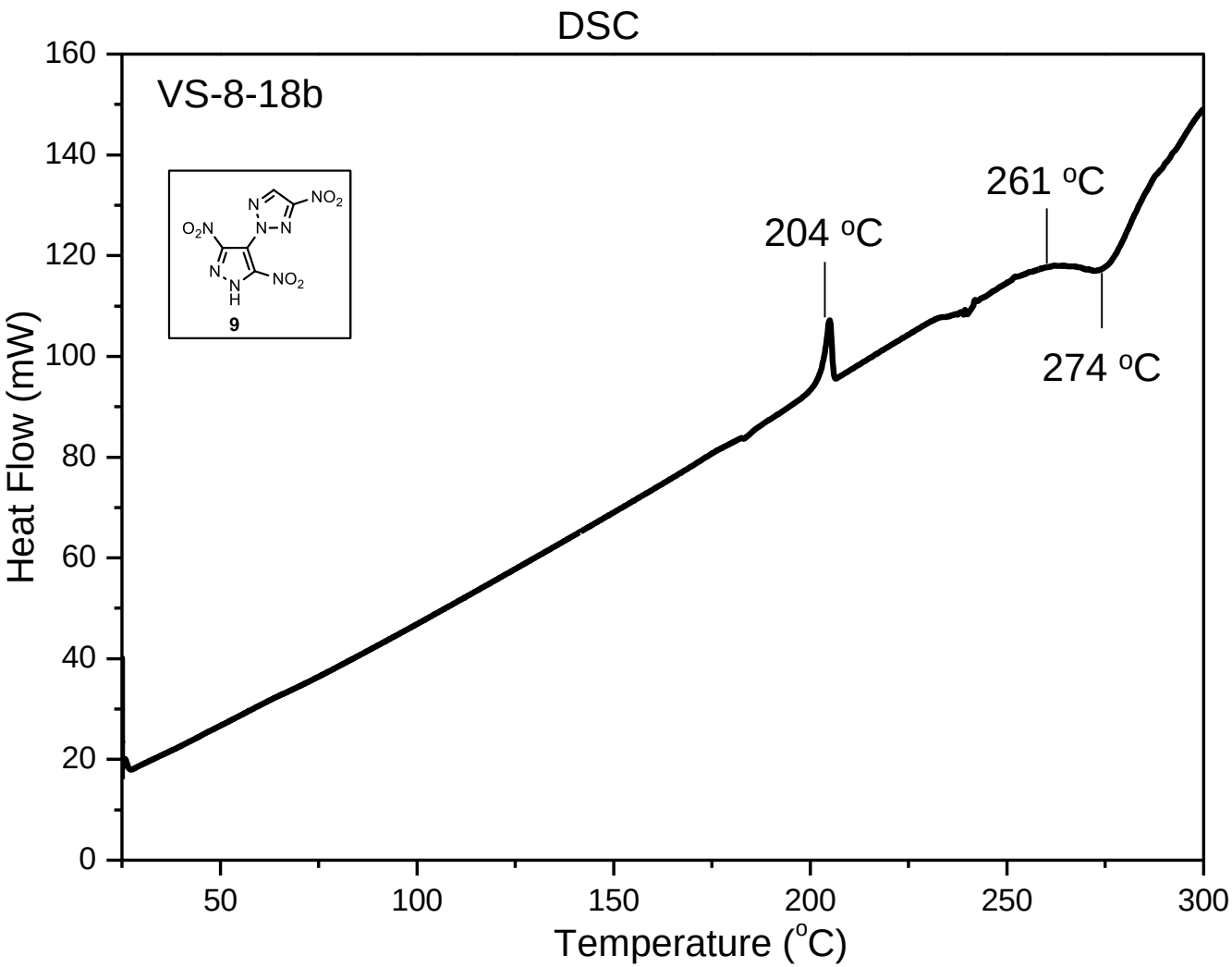
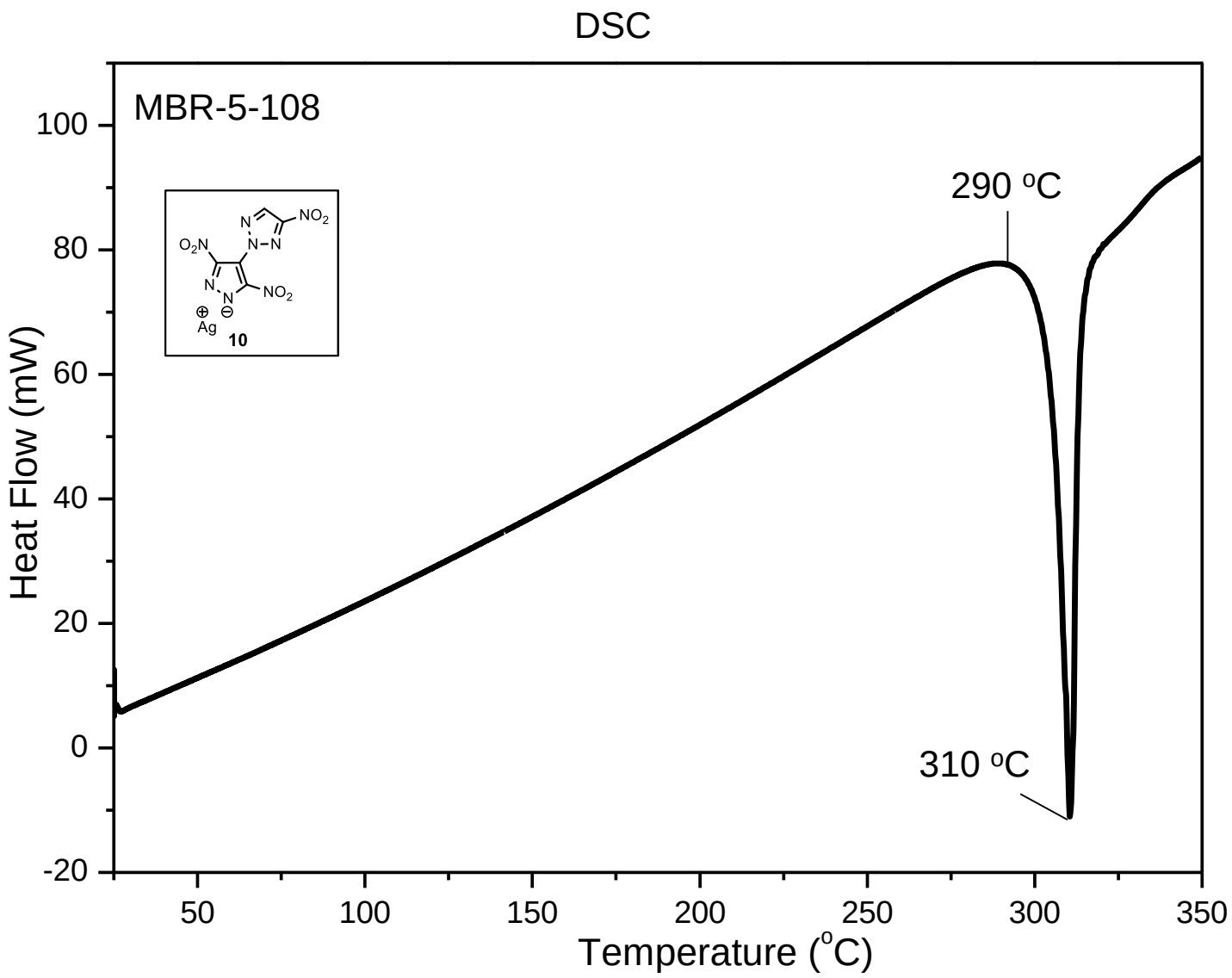
Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

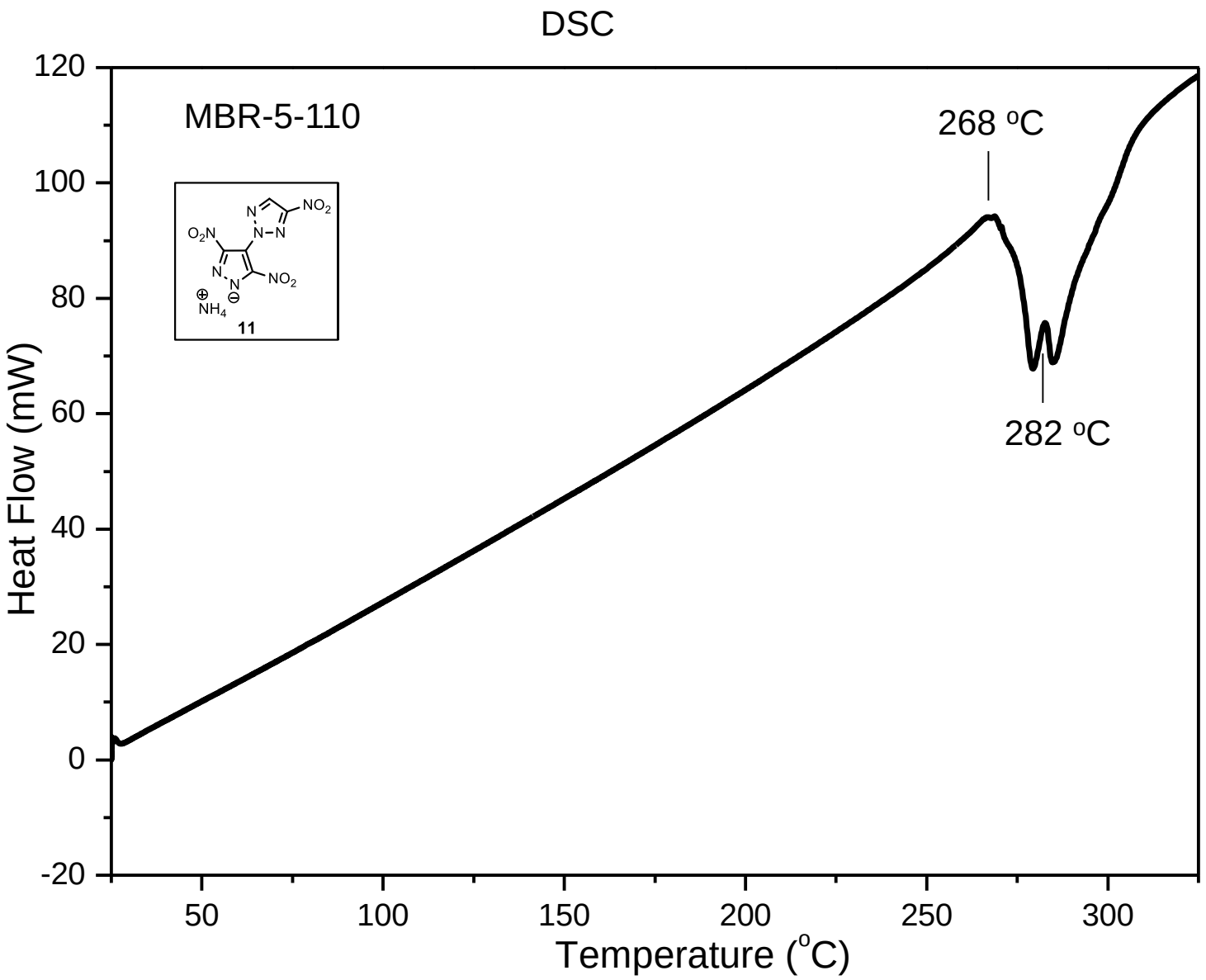

DSC
MBR-5-36
6
290 °C
310 °C
Heat Flow (mW)
Temperature (°C)
100
80
60
40
20
0
-20
50
100
150
200
250
300
350

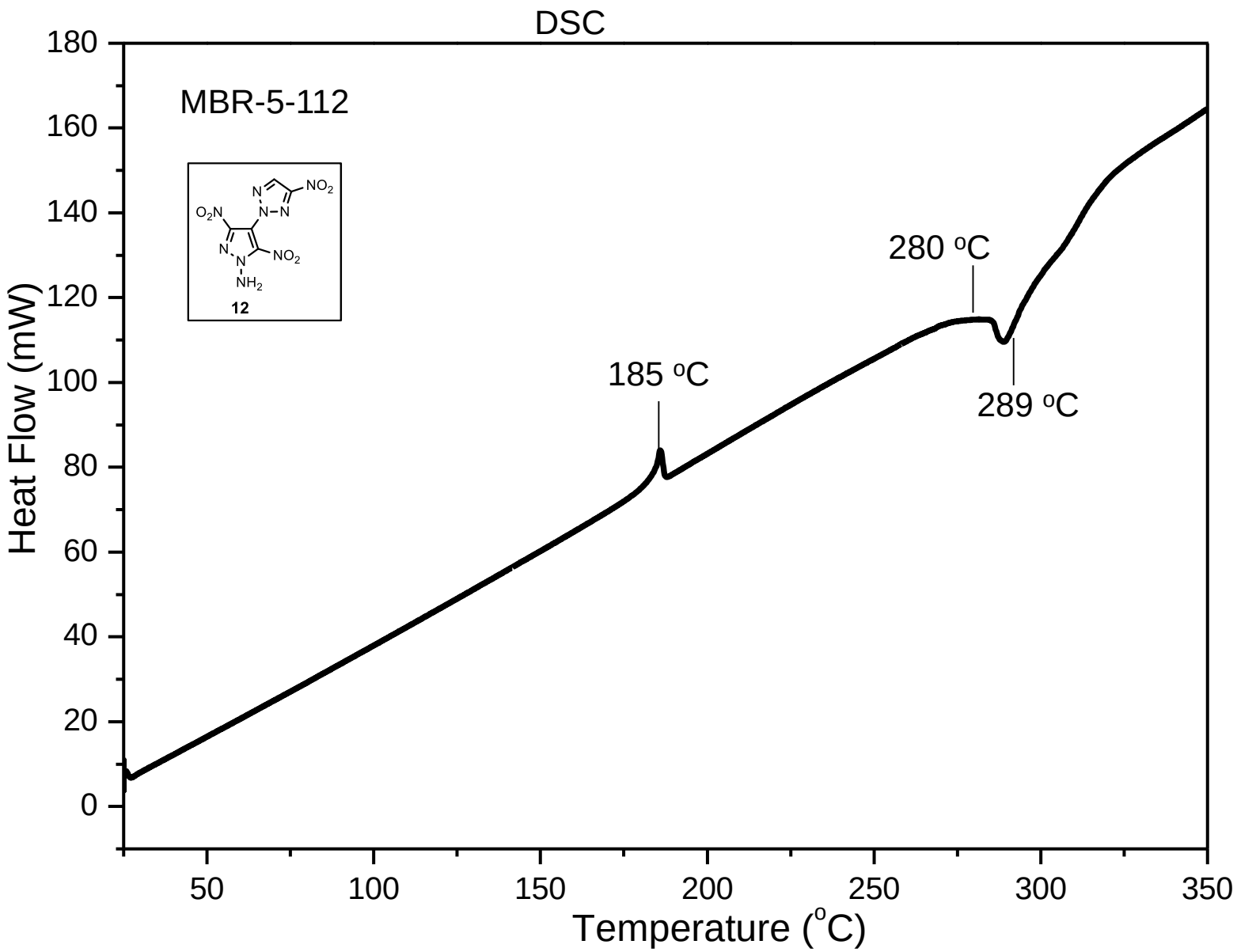

DSC
MBR-1-141
7
20
10
0
Heat Flow
135 °C
177 °C
180 °C
100
150
200
Temperature (°C)

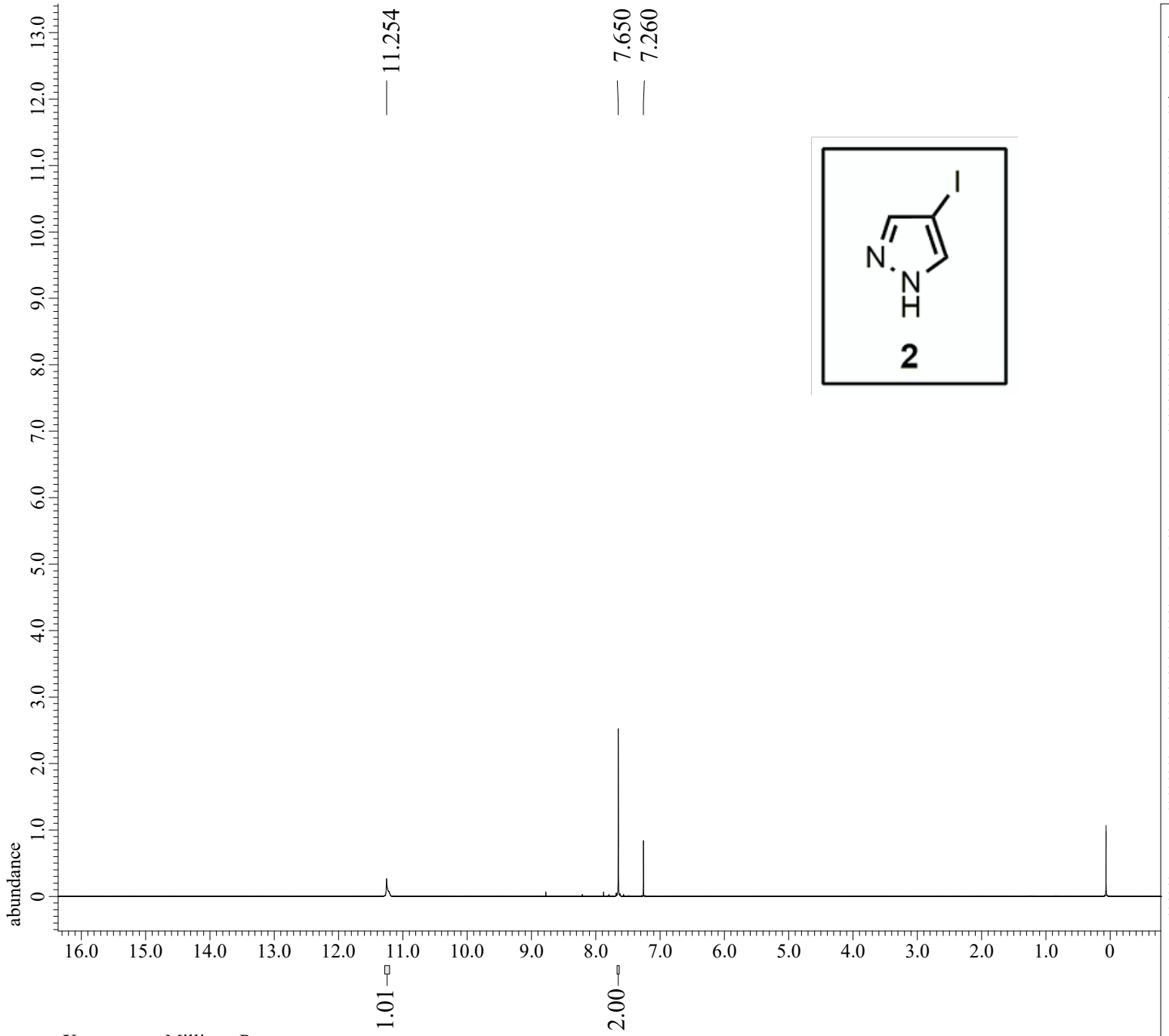

DSC-TGA
MBR-5-115
8
Weight (%)
Heat Flow (mW)
Temperature (°C)
134 °C
230 °C
288 °C
100
90
80
70
60
50
40
30
20
10
0
0
-20
-40
-60
-80
100
200
300
400


DSC
VS-8-18b
9
204 °C
261 °C
274 °C
Heat Flow (mW)
Temperature (°C)
0
20
40
60
80
100
120
140
160
50
100
150
200
250
300


DSC
MBR-5-108
290 °C
310 °C
Heat Flow (mW)
Temperature (°C)
100
80
60
40
20
0
-20
50
100
150
200
250
300
350
10


DSC
MBR-5-110
268 °C
282 °C
11
Heat Flow (mW)
Temperature (°C)
120
100
80
60
40
20
0
-20
50
100
150
200
250
300


DSC
MBR-5-112
12
280 °C
185 °C
289 °C
Heat Flow (mW)
Temperature (°C)
0
20
40
60
80
100
120
140
160
180
50
100
150
200
250
300
350

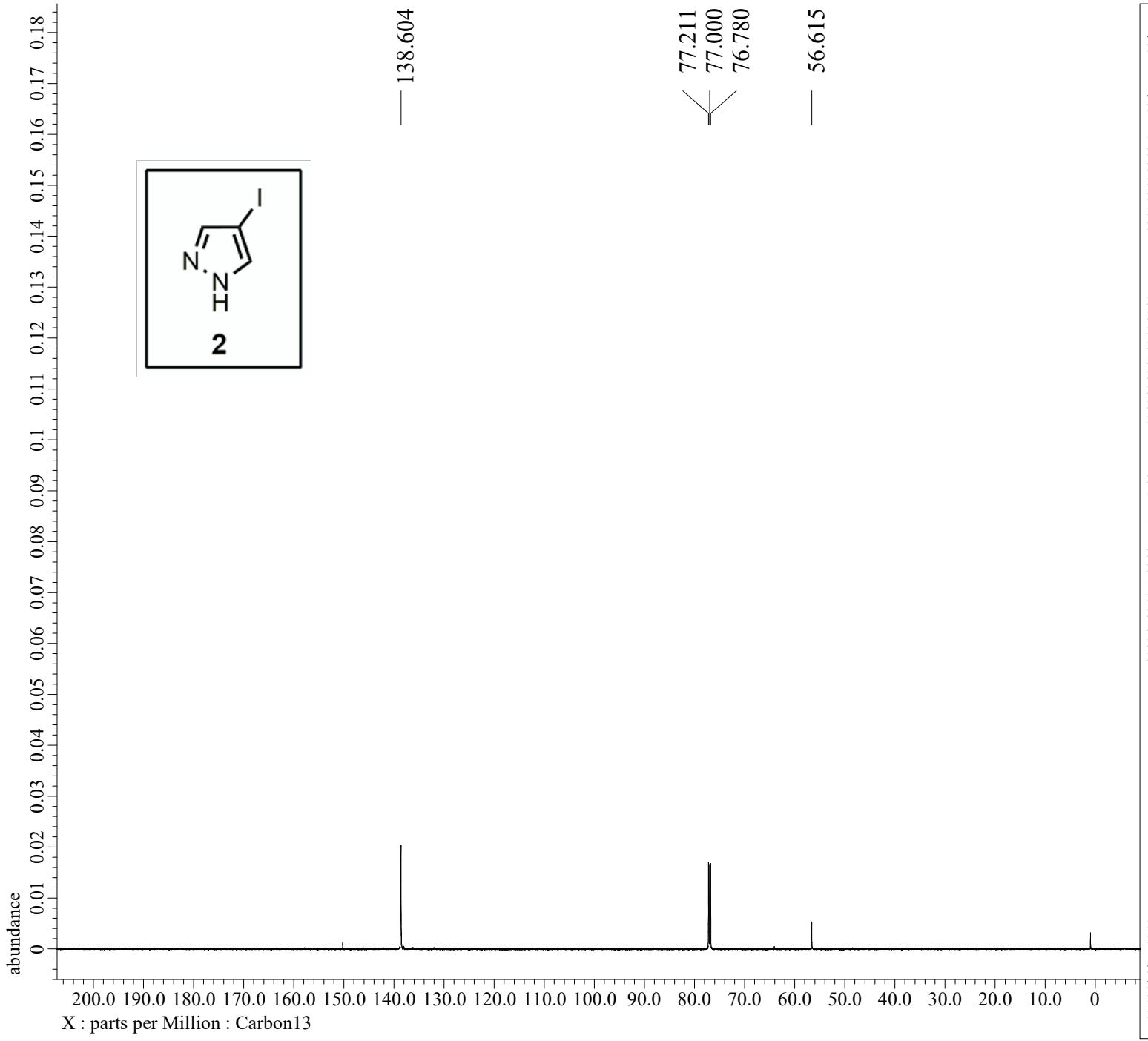



```
Filename               = MBR-5-17_proton-1-3.j
Author                 = delta
Experiment             = proton_auto.jxp
Sample_Id              = MBR-5-17
Solvent                = CHLOROFORM-D
Actual_Start_Time      =  3-JAN-2023 11:20:11
Revision_Time          =  3-JAN-2023 17:30:03

Comment                = single_pulse
Data_Format            = 1D COMPLEX
Dim_Size               = 52429
X_Domain               = Proton
Dim_Title              = Proton
Dim_Units              = [ppm]
Dimensions             = X
Site                   = ACRHEM_UOH
Spectrometer           = JNM-ECZ600R/M1

Field_Strength         = 14.09636928[T] (600[M
X_Acq_Duration         = 1.09051904[s]
X_Domain               = Proton
X_Freq                 = 600.1723046[MHz]
X_Offset               = 7.0[ppm]
X_Points               = 16384
X_Prescans             = 1
X_Resolution           = 0.91699454[Hz]
X_Sweep                = 15.02403846[kHz]
X_Sweep_Clipped        = 12.01923077[kHz]
Irr_Domain             = Proton
Irr_Freq               = 600.1723046[MHz]
Irr_Offset             = 5[ppm]
Tri_Domain             = Proton
Tri_Freq               = 600.1723046[MHz]
Tri_Offset             = 5[ppm]
Blanking               = 2[us]
Clipped                = FALSE
Scans                  = 8
Total_Scans            = 8

Relaxation_Delay       = 5[s]
Recvr_Gain             = 56
Temp_Get               = 20.1[dC]
X_90_Width             = 6.89[us]
X_Acq_Time             = 1.09051904[s]
X_Angle                = 45[deg]
X_Atn                  = 12.6[dB]
X_Pulse                = 3.445[us]
Irr_Mode               = Off
Tri_Mode               = Off
Dante_Loop             = 500
Dante_Presat           = FALSE
Decimation_Rate        = 0
Experiment_Path        = C:\Users\delta\Docume
Initial_Wait           = 1[s]
Phase                  = {0, 90, 270, 180, 180
Presat_Time            = 5[s]
Presat_Time_Flag       = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time        = 6.09051904[s]
```

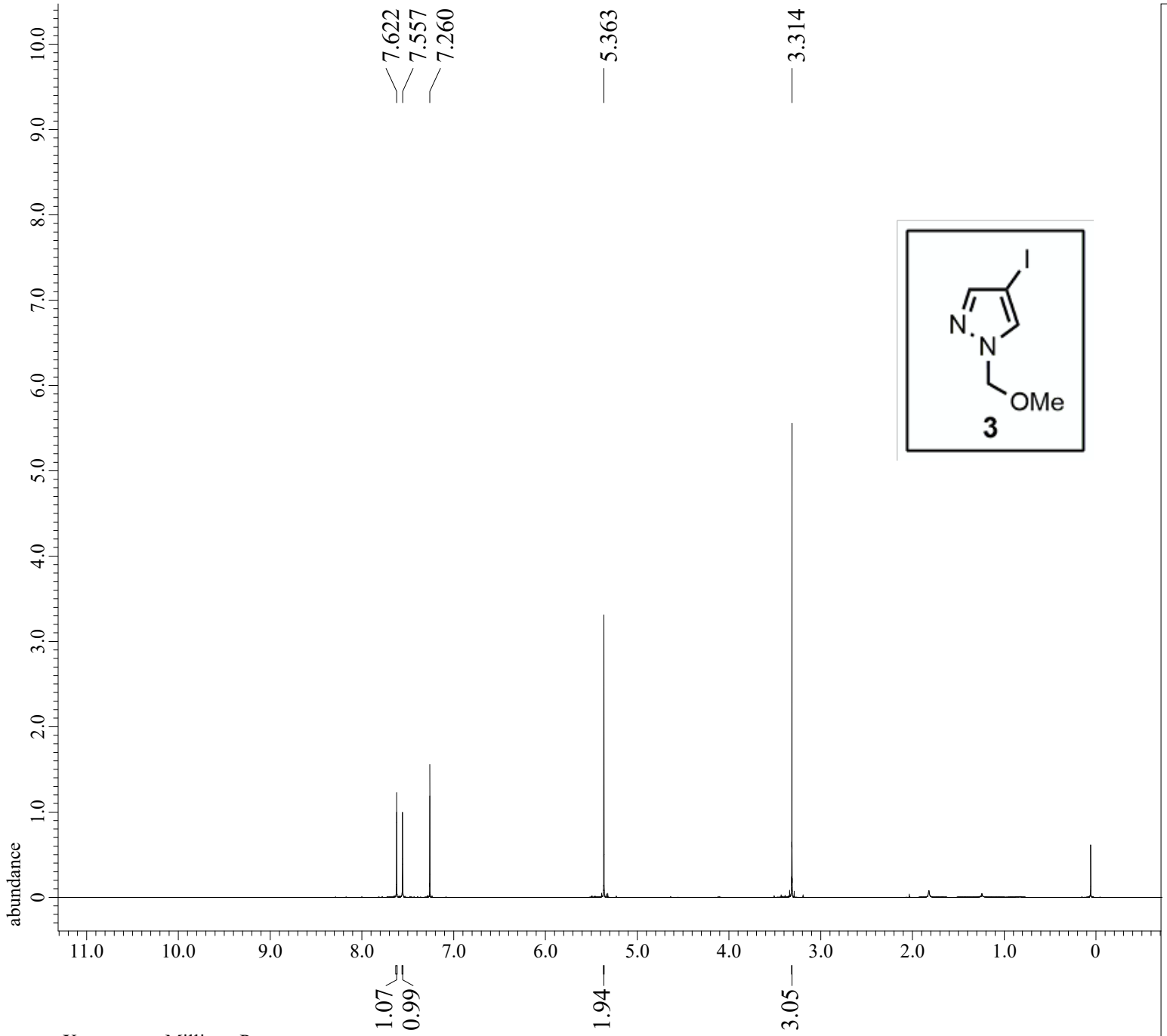



```
Filename                    = MBR-5-17_Carbon-1-
Author                      = delta
Experiment                  = carbon_auto.jxp
Sample_Id                   = MBR-5-17
Solvent                     = CHLOROFORM-D
Actual_Start_Time           =  3-JAN-2023 11:21:
Revision_Time               = 22-JAN-2023 23:42:

Comment                     = single pulse decou
Data_Format                 = 1D COMPLEX
Dim_Size                    = 26214
X_Domain                    = Carbon13
Dim_Title                   = Carbon13
Dim_Units                   = [ppm]
Dimensions                  = X
Site                        = ACRHEM_UOH
Spectrometer                = JNM-ECZ600R/M1

Field_Strength              = 14.09636928[T] (60
X_Acq_Duration              = 0.34603008[s]
X_Domain                    = Carbon13
X_Freq                      = 150.91343039[MHz]
X_Offset                    = 100[ppm]
X_Points                    = 16384
X_Prescans                  = 4
X_Resolution                = 2.88992217[Hz]
X_Sweep                     = 47.34848485[kHz]
X_Sweep_Clipped             = 37.87878788[kHz]
Irr_Domain                  = Proton
Irr_Freq                    = 600.1723046[MHz]
Irr_Offset                  = 5[ppm]
Blanking                    = 2[us]
Clipped                     = FALSE
Scans                       = 1024
Total_Scans                 = 1024

Relaxation_Delay            = 1[s]
Recvr_Gain                  = 56
Temp_Get                    = 20.3[dC]
X_90_Width                  = 11[us]
X_Acq_Time                  = 0.34603008[s]
X_Angle                     = 30[deg]
X_Atn                       = 10.3[dB]
X_Pulse                     = 3.66666667[us]
Irr_Atn_Dec                 = 33.452[dB]
Irr_Atn_Dec_Calc            = 33.452[dB]
Irr_Atn_Dec_Default_Calc    = 33.452[dB]
Irr_Atn_Noe                 = 33.452[dB]
Irr_Dec_Bandwidth_Hz        = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm       = 12.05794078[ppm]
Irr_Dec_Freq                = 600.1723046[MHz]
Irr_Dec_Merit_Factor        = 2.2
Irr_Decoupling              = TRUE
Irr_Noe                     = TRUE
Irr_Noise                   = WALTZ
Irr_Offset_Default          = 5[ppm]
Irr_Pwidth                  = 76[us]
Irr_Pwidth_Default          = 76[us]
Irr_Pwidth_Default_Calc     = 76[us]
Irr_Pwidth_Temp1            = 76[us]
Irr_Wurst                   = FALSE
Decimation_Rate             = 0
Experiment_Path             = c:\Program Files\J
Initial_Wait                = 1[s]
Noe_Time                    = 1[s]
Noe_Time_Flag               = FALSE
Relaxation_Delay_Calc       = 0[s]
Relaxation_Delay_Temp       = 1[s]
```




```
Filename                = ASW-B-MOM_proton-1-2.
Author                  = delta
Experiment              = proton_auto.jxp
Sample_Id               = ASW-B-MOM
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 27-DEC-2022 17:15:20
Revision_Time           = 28-DEC-2022 16:09:06

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 52429
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = ACRHEM_UOH
Spectrometer            = JNM-ECZ600R/M1

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 1.09051904[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 7.0[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.91699454[Hz]
X_Sweep                 = 15.02403846[kHz]
X_Sweep_Clipped         = 12.01923077[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 19.4[dC]
X_90_Width              = 6.89[us]
X_Acq_Time              = 1.09051904[s]
X_Angle                 = 45[deg]
X_Atn                   = 12.6[dB]
X_Pulse                 = 3.445[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = C:\Users\delta\Docume
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 5[s]
Repetition_Time         = 6.09051904[s]
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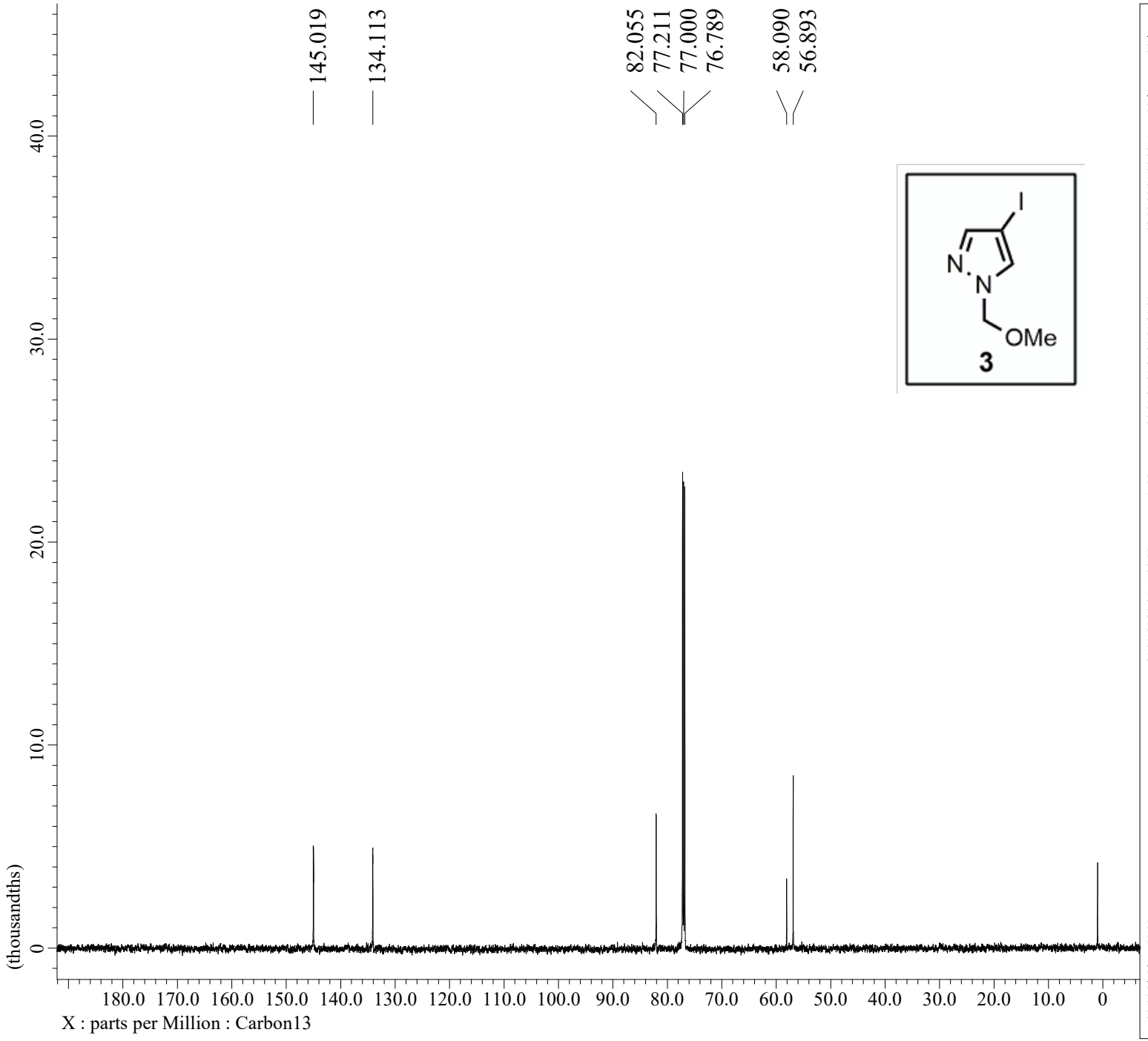
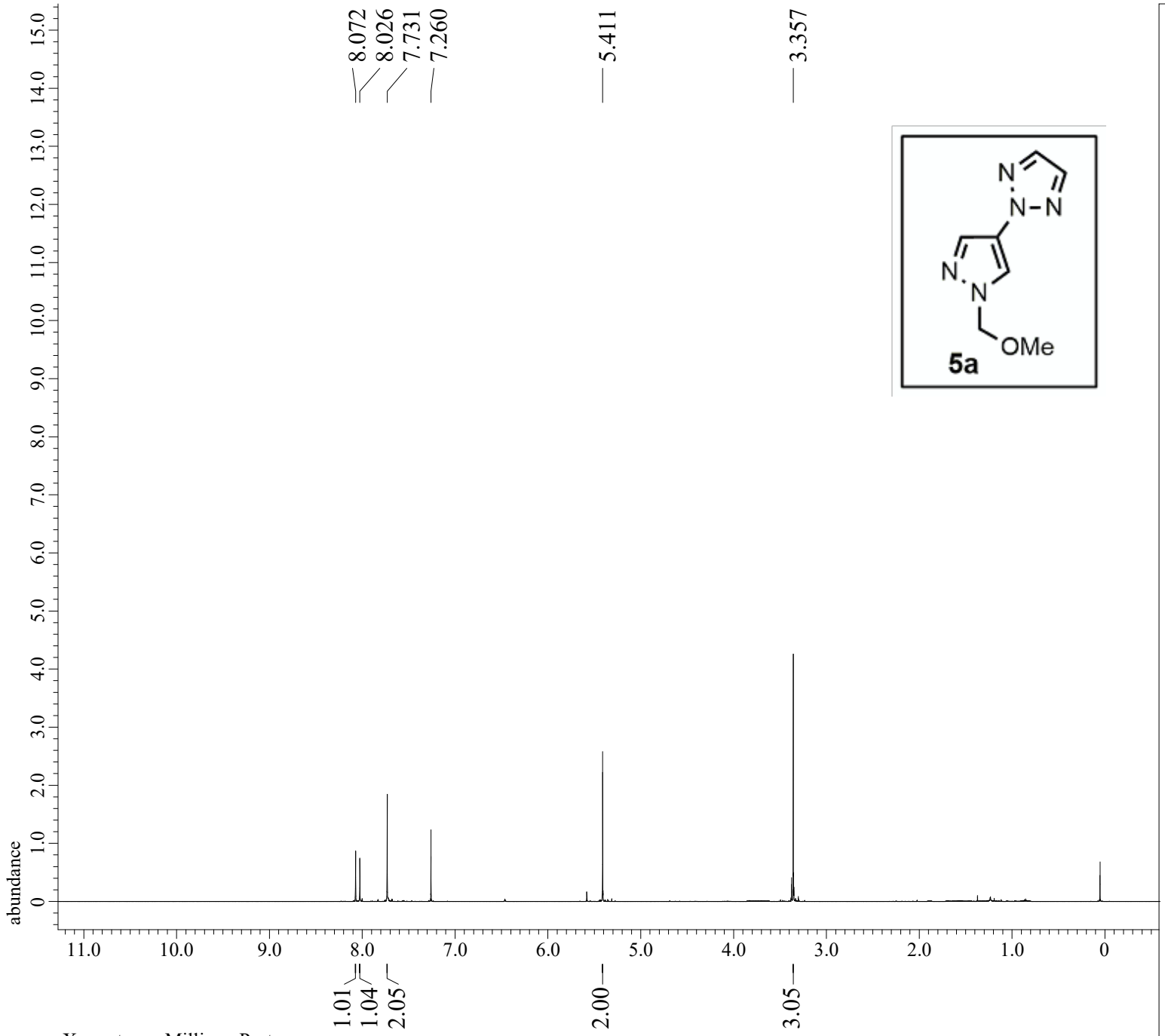


Filename	= ASW-MOM-1_Carbon-1
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= ASW-MOM-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-DEC-2022 15:56:
Revision_Time	= 31-DEC-2022 16:39:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 512
Total_Scans	= 512
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.4[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]



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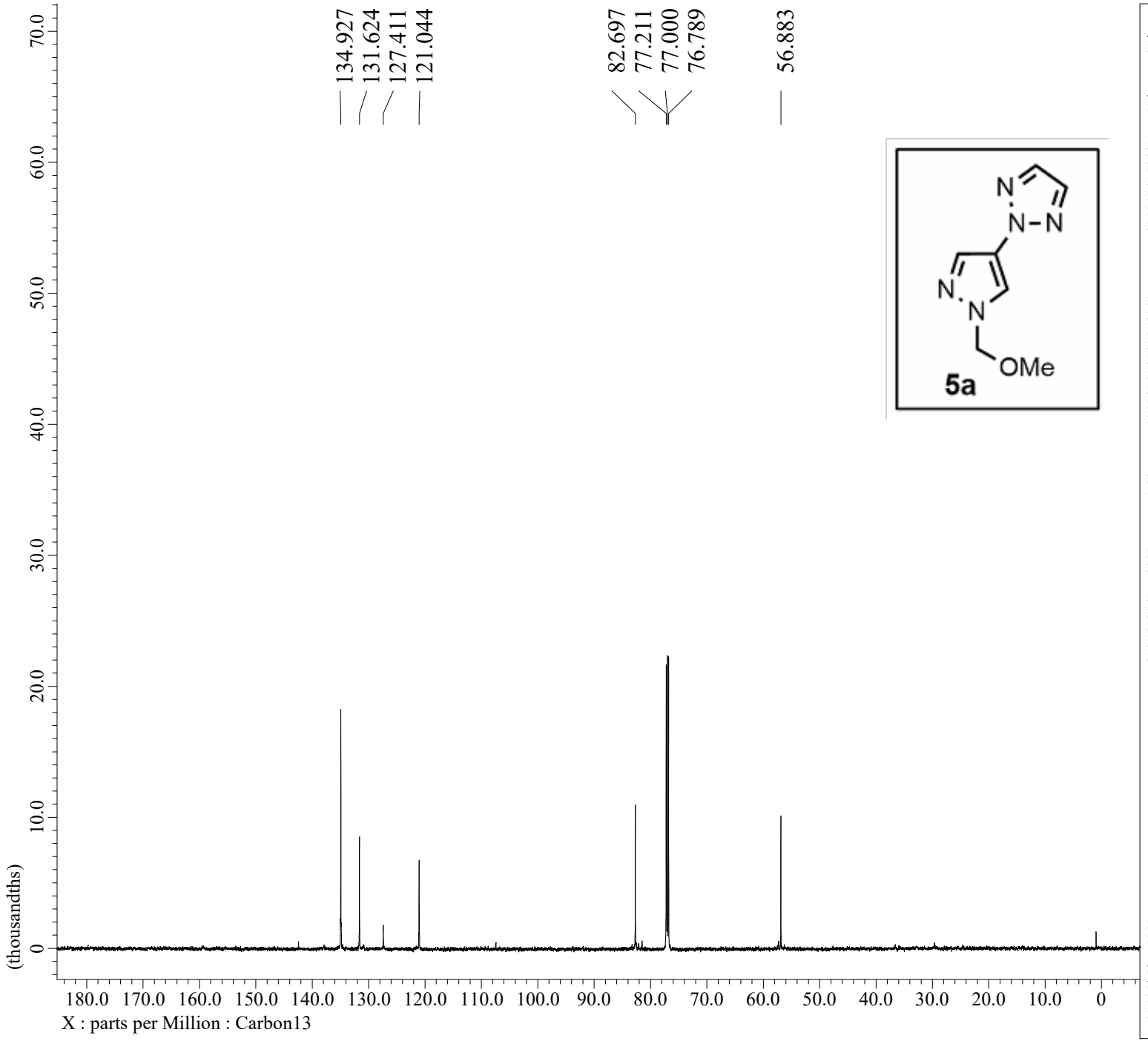
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= MBR-5-29-1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JAN-2023 16:56:07
Revision_Time	= 4-JAN-2023 15:58:40
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 1.09051904[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 7.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.91699454[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 20.5[dC]
X_90_Width	= 6.89[us]
X_Acq_Time	= 1.09051904[s]
X_Angle	= 45[deg]
X_Atn	= 12.6[dB]
X_Pulse	= 3.445[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Users\delta\Docume
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 6.09051904[s]

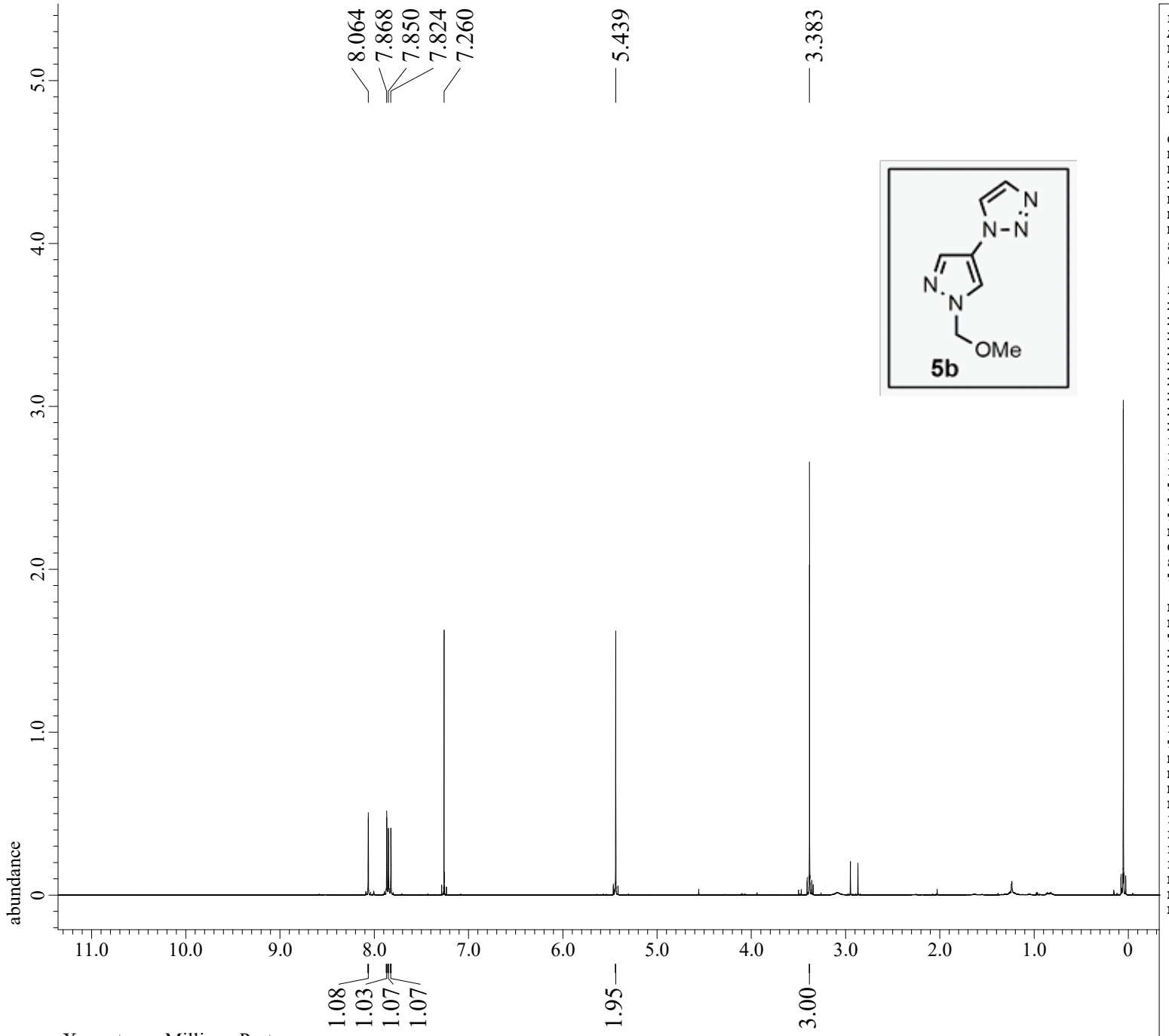



```
Filename                    = MBR-5-29-1_Carbon-
Author                      = delta
Experiment                  = carbon_auto.jxp
Sample_Id                   = MBR-5-29-1
Solvent                     = CHLOROFORM-D
Actual_Start_Time           =  3-JAN-2023 16:57:
Revision_Time               =  4-JAN-2023 16:02:

Comment                     = single pulse decou
Data_Format                 = 1D COMPLEX
Dim_Size                    = 26214
X_Domain                    = Carbon13
Dim_Title                   = Carbon13
Dim_Units                   = [ppm]
Dimensions                  = X
Site                        = ACRHEM_UOH
Spectrometer                = JNM-ECZ600R/M1

Field_Strength              = 14.09636928[T] (60
X_Acq_Duration              = 0.34603008[s]
X_Domain                    = Carbon13
X_Freq                      = 150.91343039[MHz]
X_Offset                    = 100[ppm]
X_Points                    = 16384
X_Prescans                  = 4
X_Resolution                = 2.88992217[Hz]
X_Sweep                     = 47.34848485[kHz]
X_Sweep_Clipped             = 37.87878788[kHz]
Irr_Domain                  = Proton
Irr_Freq                    = 600.1723046[MHz]
Irr_Offset                  = 5[ppm]
Blanking                    = 2[us]
Clipped                     = FALSE
Scans                       = 1024
Total_Scans                 = 1024

Relaxation_Delay            = 1[s]
Recvr_Gain                  = 56
Temp_Get                    = 20.3[dC]
X_90_Width                  = 11[us]
X_Acq_Time                  = 0.34603008[s]
X_Angle                     = 30[deg]
X_Atn                       = 10.3[dB]
X_Pulse                     = 3.66666667[us]
Irr_Atn_Dec                 = 33.452[dB]
Irr_Atn_Dec_Calc            = 33.452[dB]
Irr_Atn_Dec_Default_Calc    = 33.452[dB]
Irr_Atn_Noe                 = 33.452[dB]
Irr_Dec_Bandwidth_Hz        = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm       = 12.05794078[ppm]
Irr_Dec_Freq                = 600.1723046[MHz]
Irr_Dec_Merit_Factor        = 2.2
Irr_Decoupling              = TRUE
Irr_Noe                     = TRUE
Irr_Noise                   = WALTZ
Irr_Offset_Default          = 5[ppm]
Irr_Pwidth                  = 76[us]
Irr_Pwidth_Default          = 76[us]
Irr_Pwidth_Default_Calc     = 76[us]
Irr_Pwidth_Temp1            = 76[us]
Irr_Wurst                   = FALSE
Decimation_Rate             = 0
Experiment_Path             = c:\Program Files\J
Initial_Wait                = 1[s]
Noe_Time                    = 1[s]
Noe_Time_Flag               = FALSE
Relaxation_Delay_Calc       = 0[s]
Relaxation_Delay_Temp       = 1[s]
```

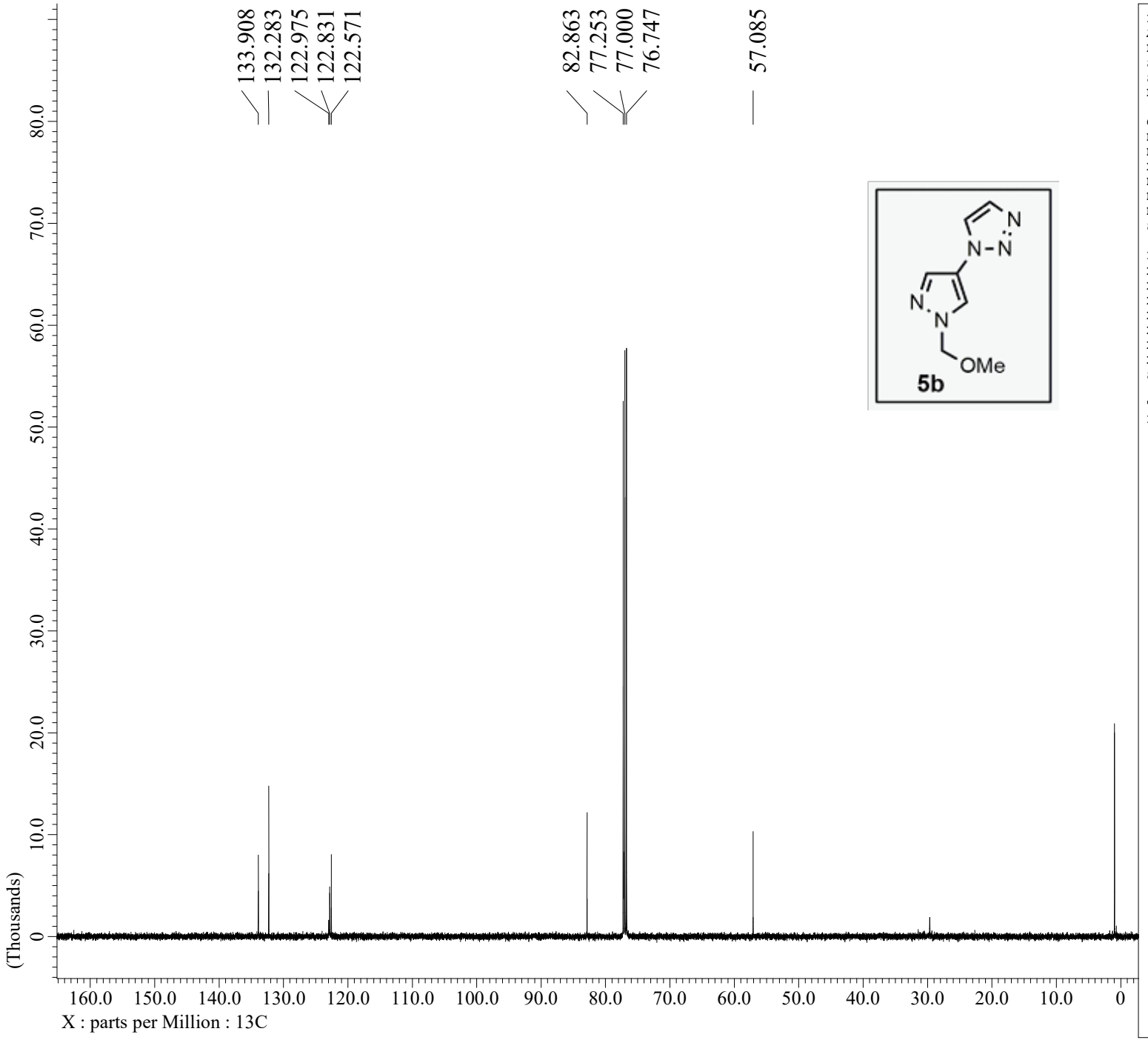



```
Filename                = MBR-1-29-2_proton-1-3
Author                  = delta
Experiment              = proton_auto.jxp
Sample_Id               = MBR-1-29-2
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 23-JAN-2023 15:02:18
Revision_Time           = 23-JAN-2023 20:49:15

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 52429
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = ACRHEM_UOH
Spectrometer            = JNM-ECZ600R/M1

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 1.09051904[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 7.0[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.91699454[Hz]
X_Sweep                 = 15.02403846[kHz]
X_Sweep_Clipped         = 12.01923077[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 19.7[dC]
X_90_Width              = 6.89[us]
X_Acq_Time              = 1.09051904[s]
X_Angle                 = 45[deg]
X_Atn                   = 12.6[dB]
X_Pulse                 = 3.445[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = C:\Users\delta\Docume
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 5[s]
Repetition_Time         = 6.09051904[s]
```

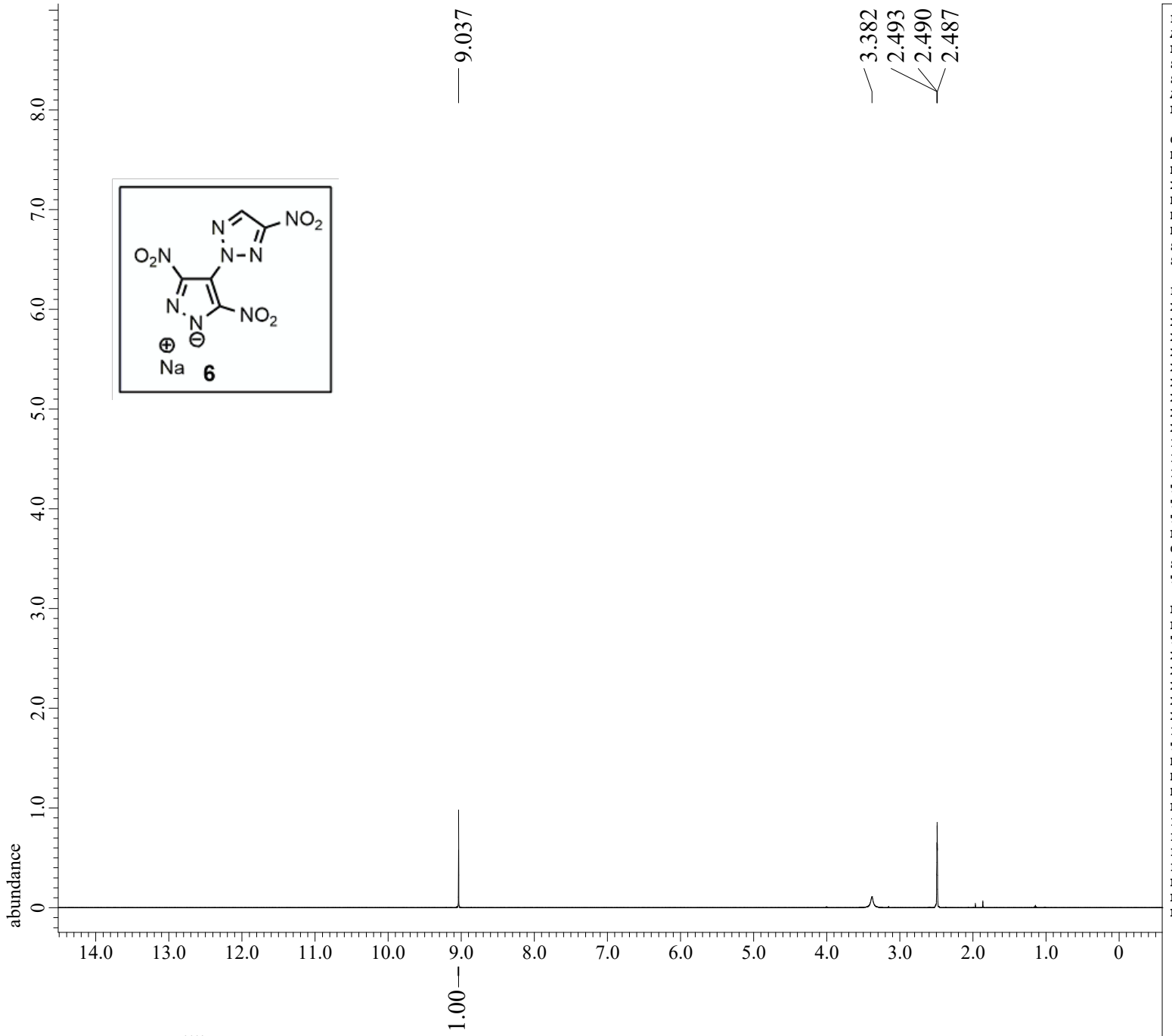



```
Filename        = MBR-5-29-2-2.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = MBR-5-29(2)
Solvent         = CHLOROFORM-D
Revision_Time   = 13-FEB-2023 20:05:25

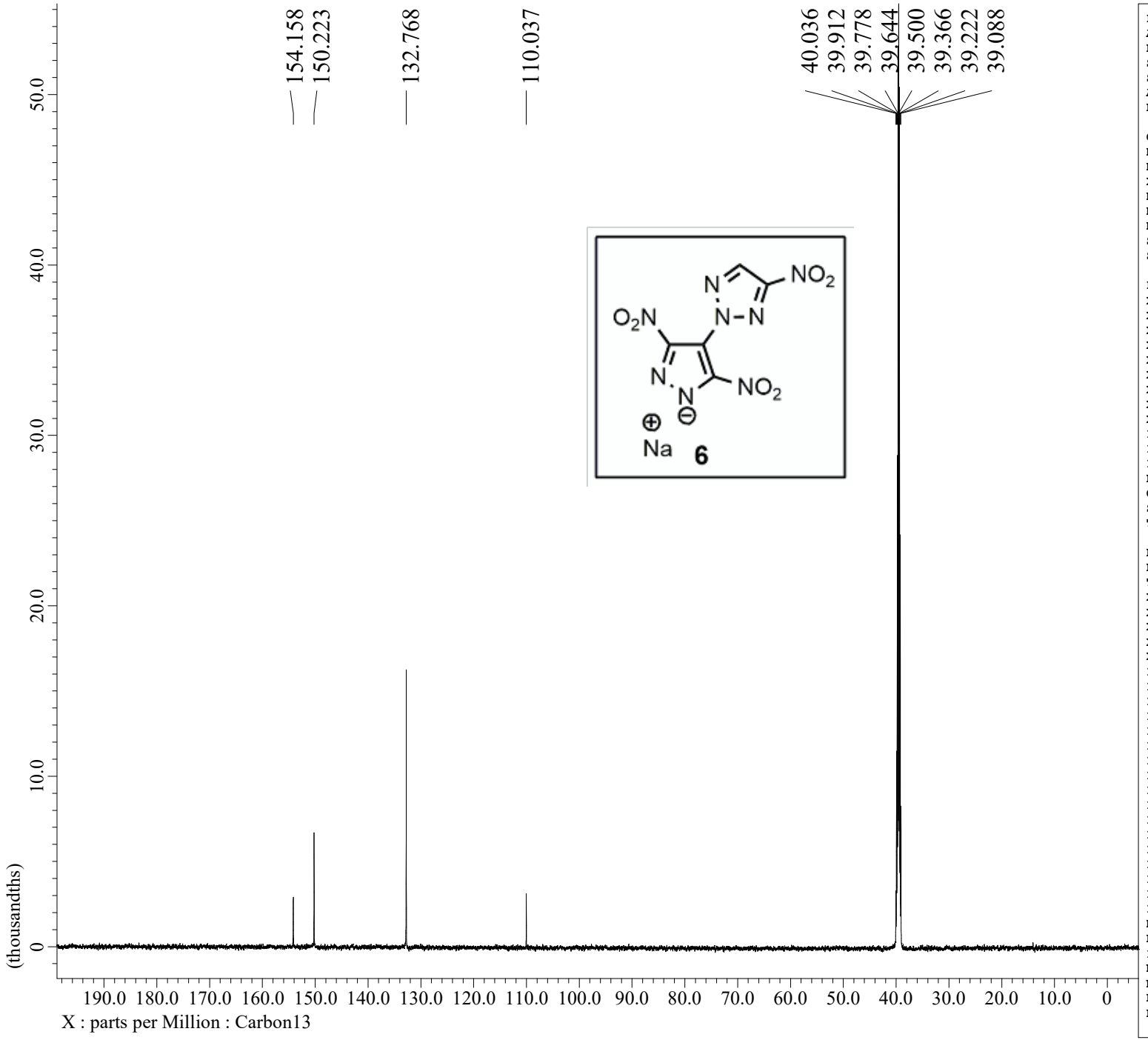
Comment         = MBR-5-29(2)
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
X_Domain        = 13C
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 11.74782964[T] (500[MHz])
X_Domain        = 13C
X_Freq          = 125.77036104[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 12.577036[kHz]
X_Points        = 32768
X_Prescans      = 4
X_Sweep         = 29.75892887[kHz]
Scans           = 378

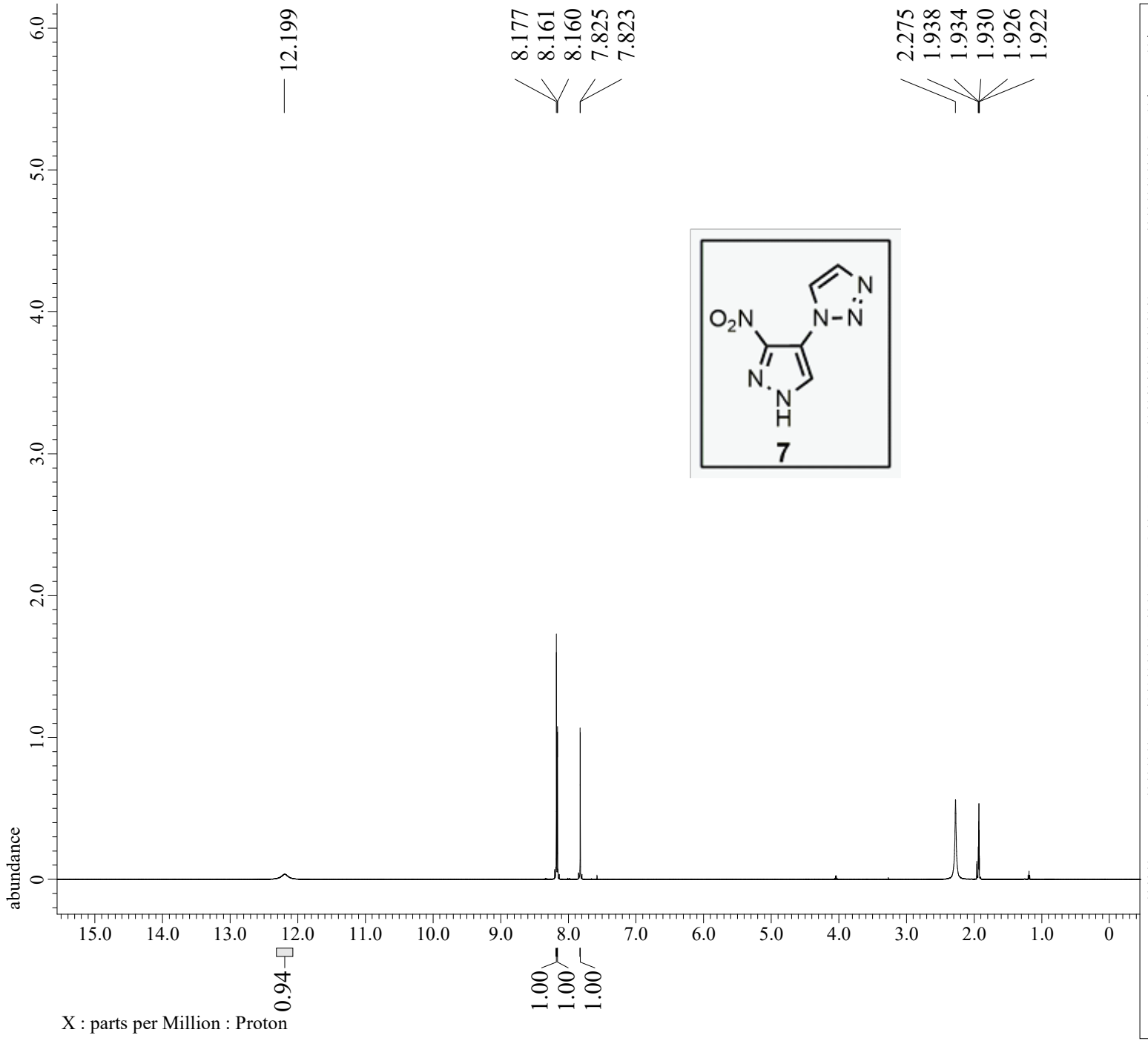
Temp_Get        = 295.76[K]
Filter_Factor   = 672
```



Filename	= MBR-5-36N_proton-1-2.
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= MBR-5-36N
Solvent	= DMSO-D6
Actual_Start_Time	= 3-JAN-2023 11:55:32
Revision_Time	= 3-JAN-2023 18:00:47
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 1.09051904[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 7.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.91699454[Hz]
X_Sweep	= 15.02403846[kHz]
X_Sweep_Clipped	= 12.01923077[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 20.2[dC]
X_90_Width	= 6.89[us]
X_Acq_Time	= 1.09051904[s]
X_Angle	= 45[deg]
X_Atn	= 12.6[dB]
X_Pulse	= 3.445[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Users\delta\Docume
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 6.09051904[s]



Filename	= MBR-5-36N_Carbon-1
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= MBR-5-36N
Solvent	= DMSO-D6
Actual_Start_Time	= 3-JAN-2023 11:56:
Revision_Time	= 3-JAN-2023 18:04:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 20.3[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]

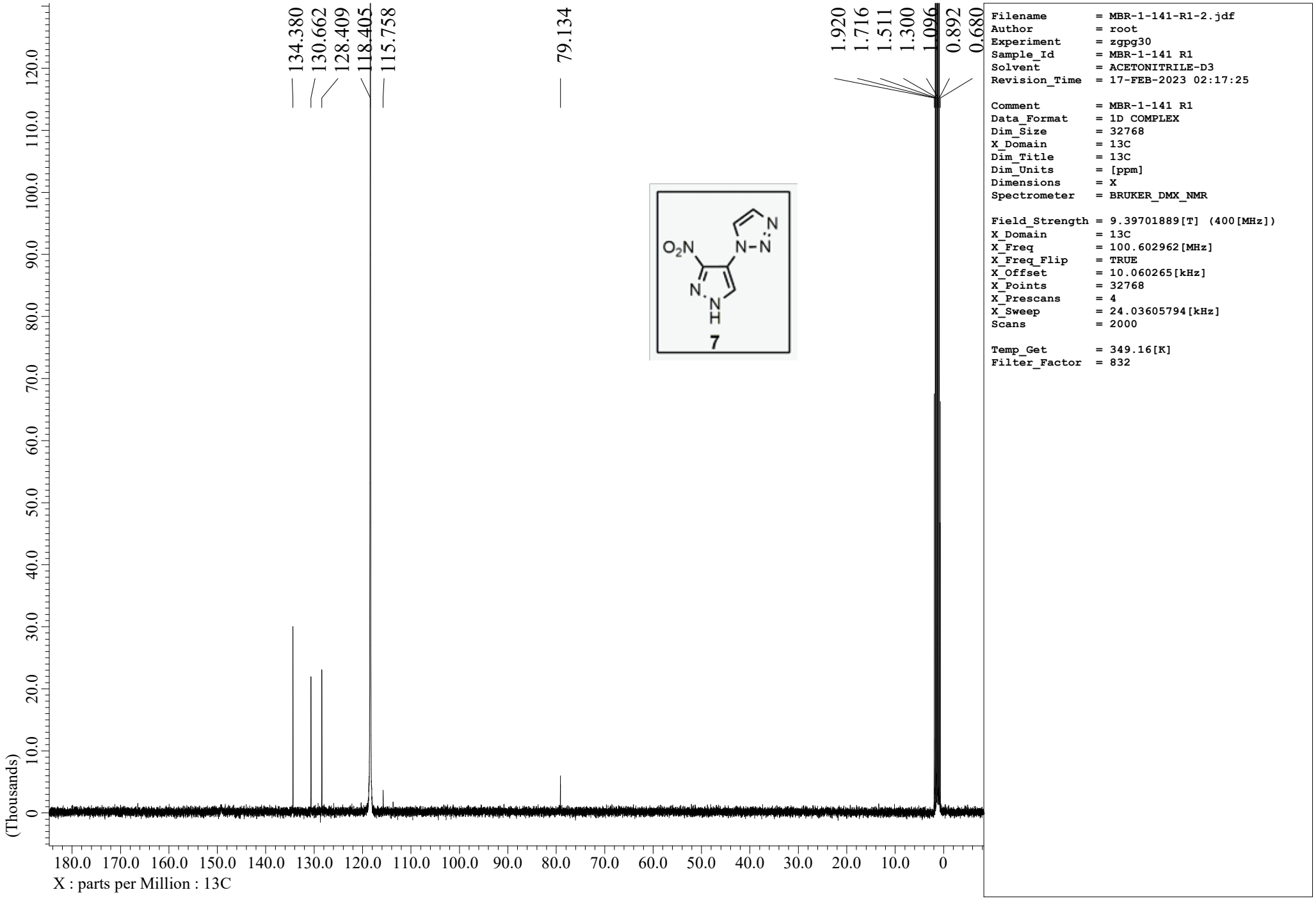



```
Filename                = MBR-1-141-1_proton-1-
Author                  = delta
Experiment              = proton_auto.jxp
Sample_Id               = MBR-1-141-1
Solvent                 = ACETONITRILE-D3
Actual_Start_Time       = 23-JAN-2023 10:28:16
Revision_Time           = 23-JAN-2023 22:19:34

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 52429
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = ACRHEM_UOH
Spectrometer            = JNM-ECZ600R/M1

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 1.09051904[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 7.0[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.91699454[Hz]
X_Sweep                 = 15.02403846[kHz]
X_Sweep_Clipped         = 12.01923077[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 19.2[dC]
X_90_Width              = 6.89[us]
X_Acq_Time              = 1.09051904[s]
X_Angle                 = 45[deg]
X_Atn                   = 12.6[dB]
X_Pulse                 = 3.445[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = C:\Users\delta\Docume
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time         = 6.09051904[s]
```

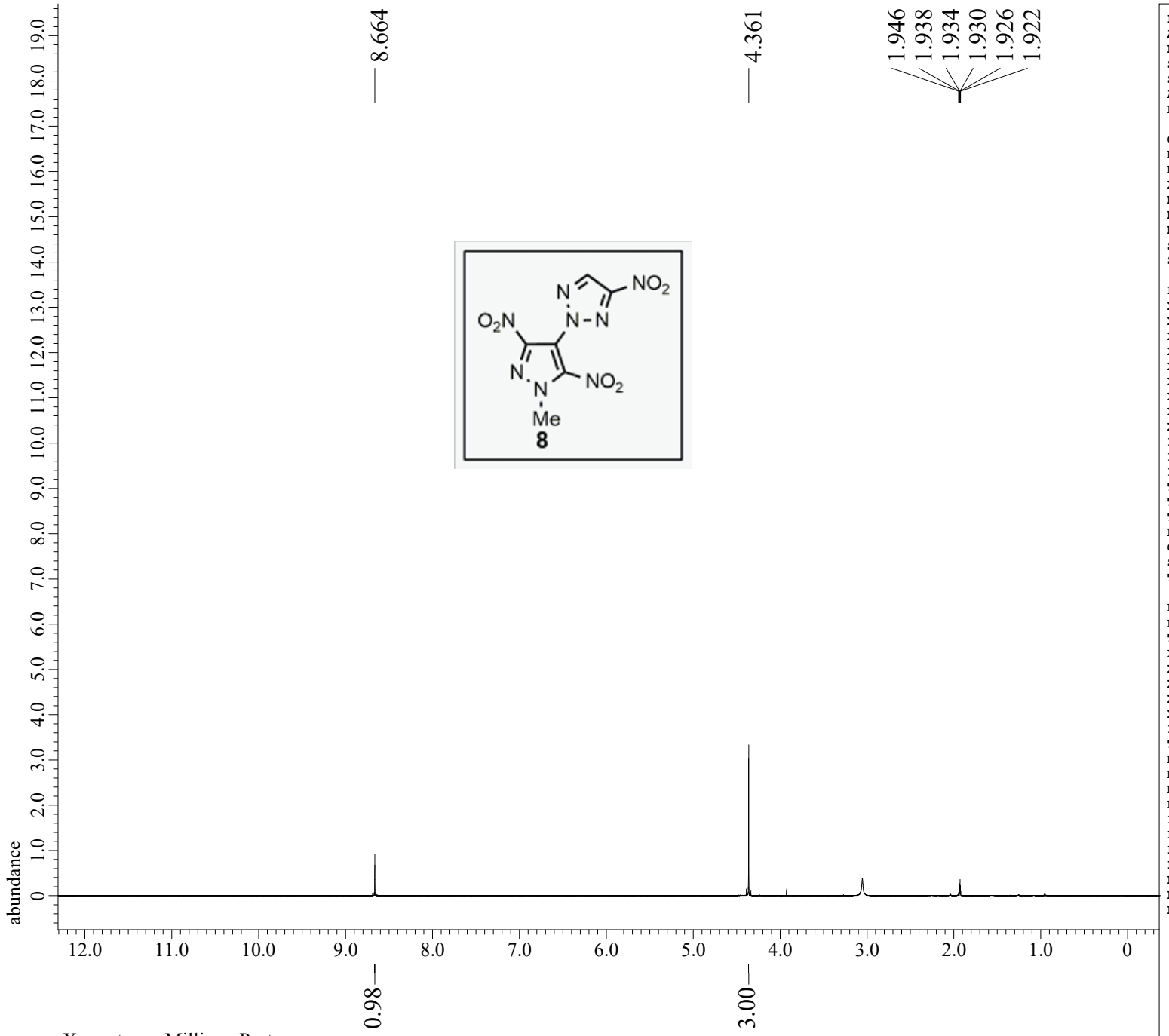



```
Filename        = MBR-1-141-R1-2.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = MBR-1-141 R1
Solvent         = ACETONITRILE-D3
Revision_Time   = 17-FEB-2023 02:17:25

Comment         = MBR-1-141 R1
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
X_Domain        = 13C
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39701889[T] (400[MHz])
X_Domain        = 13C
X_Freq          = 100.602962[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 10.060265[kHz]
X_Points        = 32768
X_Prescans      = 4
X_Sweep         = 24.03605794[kHz]
Scans           = 2000

Temp_Get        = 349.16[K]
Filter_Factor   = 832
```

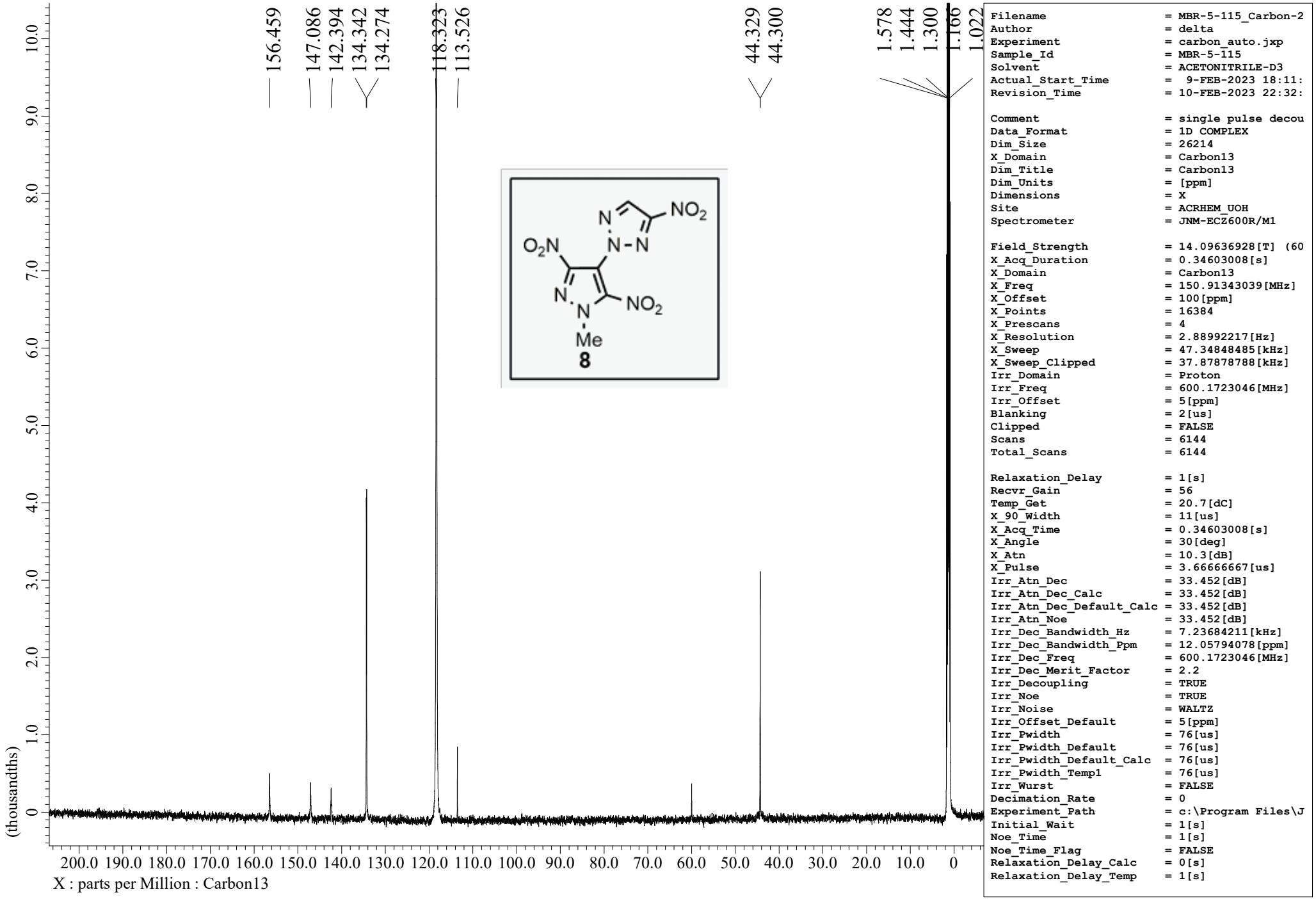


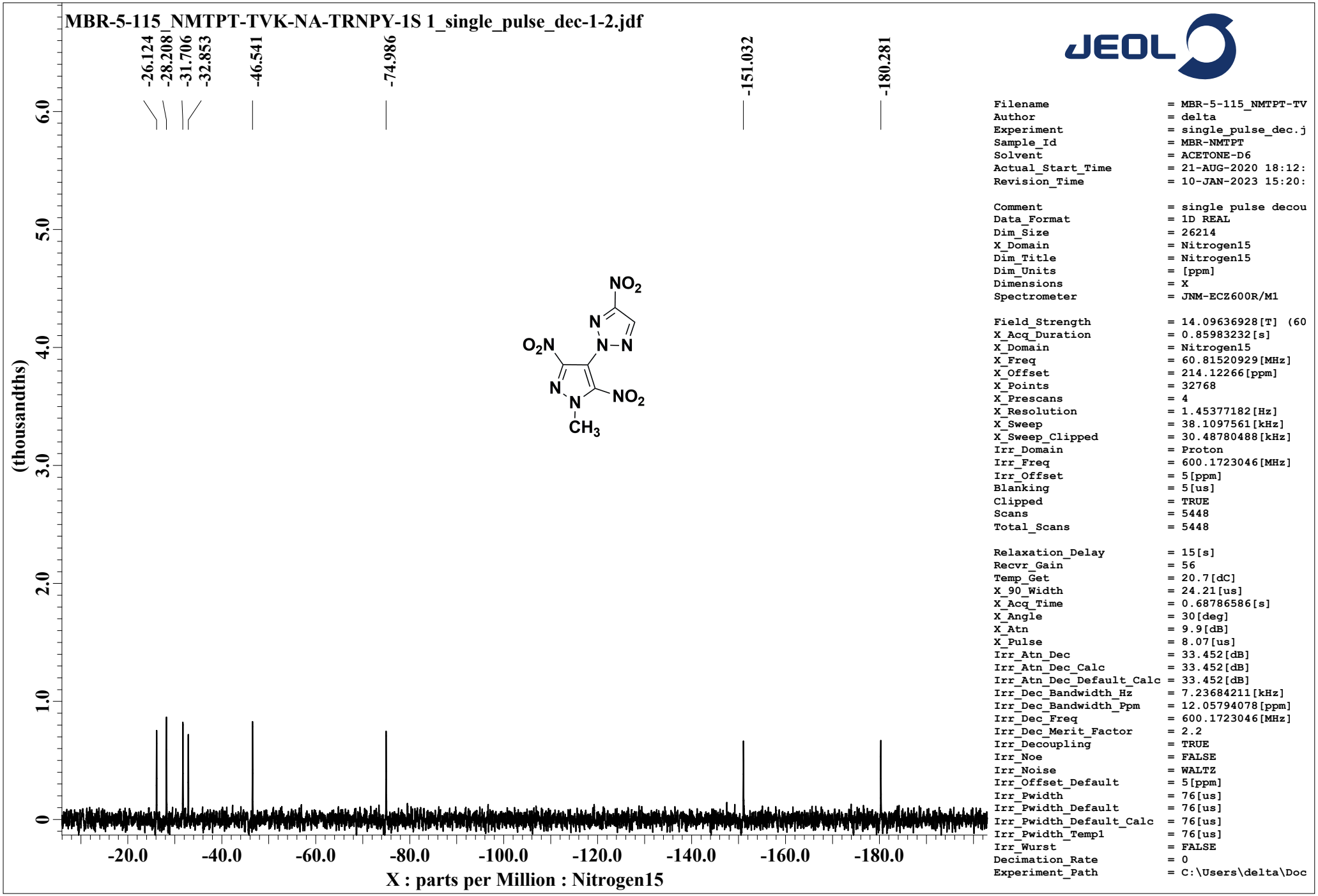

```
Filename                = MBR-5-115 1_proton-1-
Author                  = delta
Experiment              = proton_auto.jxp
Sample_Id               = MBR-5-115 1
Solvent                 = ACETONITRILE-D3
Actual_Start_Time       =  8-FEB-2023 14:55:49
Revision_Time           =  9-FEB-2023 12:46:25

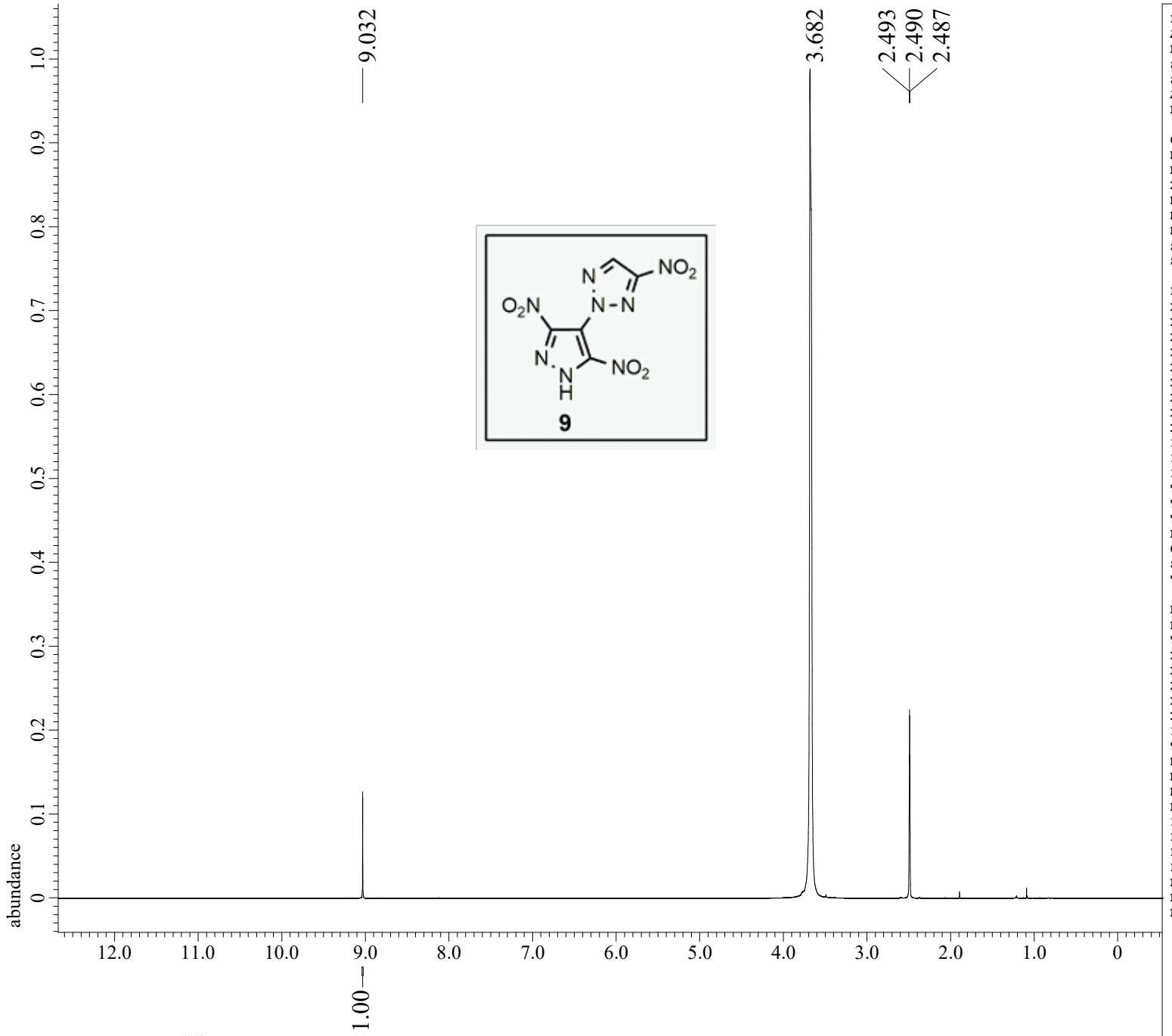
Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 52429
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = ACRHEM_UOH
Spectrometer            = JNM-ECZ600R/M1

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 1.09051904[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 7.0[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.91699454[Hz]
X_Sweep                 = 15.02403846[kHz]
X_Sweep_Clipped         = 12.01923077[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 21[dC]
X_90_Width              = 6.89[us]
X_Acq_Time              = 1.09051904[s]
X_Angle                 = 45[deg]
X_Atn                   = 12.6[dB]
X_Pulse                 = 3.445[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = C:\Users\delta\Docume
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 5[s]
Repetition_Time         = 6.09051904[s]
```


156.459
147.086
142.394
134.342
134.274
118.323
113.526
44.329
44.300
1.578
1.444
1.300
1.166
1.022
(thousandths)
X : parts per Million : Carbon13
Filename = MBR-5-115_Carbon-2
Author = delta
Experiment = carbon_auto.jxp
Sample_Id = MBR-5-115
Solvent = ACETONITRILE-D3
Actual_Start_Time = 9-FEB-2023 18:11:
Revision_Time = 10-FEB-2023 22:32:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ACRHEM_UOH
Spectrometer = JNM-ECZ600R/M1
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0.34603008[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 2.88992217[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 6144
Total_Scans = 6144
Relaxation_Delay = 1[s]
Recvr_Gain = 56
Temp_Get = 20.7[dC]
X_90_Width = 11[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 30[deg]
X_Atn = 10.3[dB]
X_Pulse = 3.66666667[us]
Irr_Atn_Dec = 33.452[dB]
Irr_Atn_Dec_Calc = 33.452[dB]
Irr_Atn_Dec_Default_Calc = 33.452[dB]
Irr_Atn_Noe = 33.452[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\J
Initial_Wait = 1[s]
Noe_Time = 1[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 1[s]


MBR-5-115_NMTPT-TVK-NA-TRNPY-1S 1_single_pulse_dec-1-2.jdf
-26.124
-28.208
-31.706
-32.853
-46.541
-74.986
-151.032
-180.281
(thousandths)
6.0
5.0
4.0
3.0
2.0
1.0
0
-20.0
-40.0
-60.0
-80.0
-100.0
-120.0
-140.0
-160.0
-180.0
X : parts per Million : Nitrogen15
NO2
N
O2N
N-N
N
N
NO2
CH3
Filename = MBR-5-115_NMTPT-TV
Author = delta
Experiment = single_pulse_dec.j
Sample_Id = MBR-NMTPT
Solvent = ACETONE-D6
Actual_Start_Time = 21-AUG-2020 18:12:
Revision_Time = 10-JAN-2023 15:20:
Comment = single pulse decou
Data_Format = 1D REAL
Dim_Size = 26214
X_Domain = Nitrogen15
Dim_Title = Nitrogen15
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/M1
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0.85983232[s]
X_Domain = Nitrogen15
X_Freq = 60.81520929[MHz]
X_Offset = 214.12266[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.45377182[Hz]
X_Sweep = 38.1097561[kHz]
X_Sweep_Clipped = 30.48780488[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 5448
Total_Scans = 5448
Relaxation_Delay = 15[s]
Recvr_Gain = 56
Temp_Get = 20.7[dC]
X_90_Width = 24.21[us]
X_Acq_Time = 0.68786586[s]
X_Angle = 30[deg]
X_Atn = 9.9[dB]
X_Pulse = 8.07[us]
Irr_Atn_Dec = 33.452[dB]
Irr_Atn_Dec_Calc = 33.452[dB]
Irr_Atn_Dec_Default_Calc = 33.452[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = FALSE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Experiment_Path = C:\Users\delta\Doc

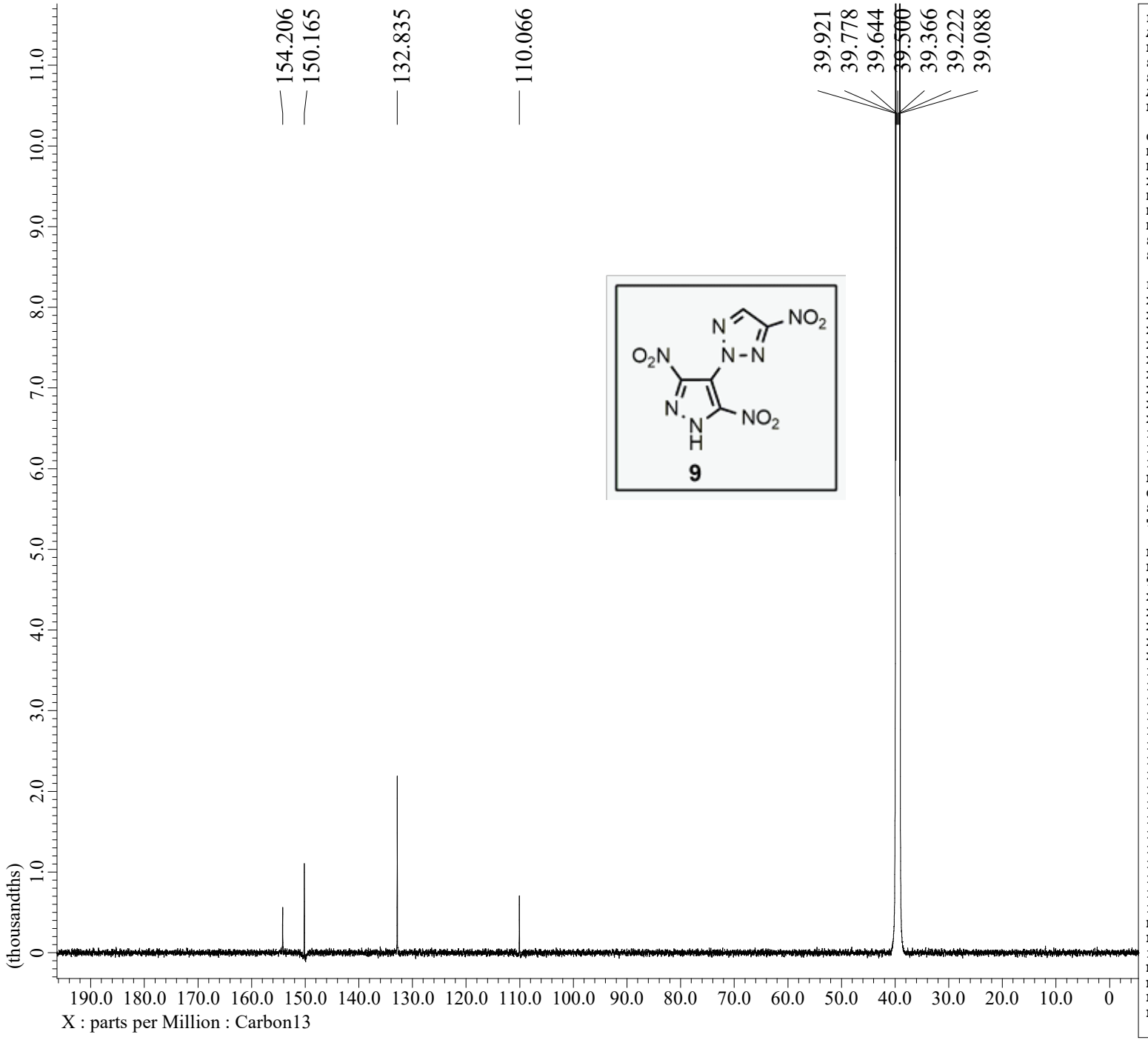



```
Filename                = Vs-8-16B_proton-1-3.j
Author                  = delta
Experiment              = proton_auto.jxp
Sample_Id               = Vs-8-16B
Solvent                 = DMSO-D6
Actual_Start_Time       = 11-JUL-2022 16:35:47
Revision_Time           = 11-FEB-2023 19:44:17

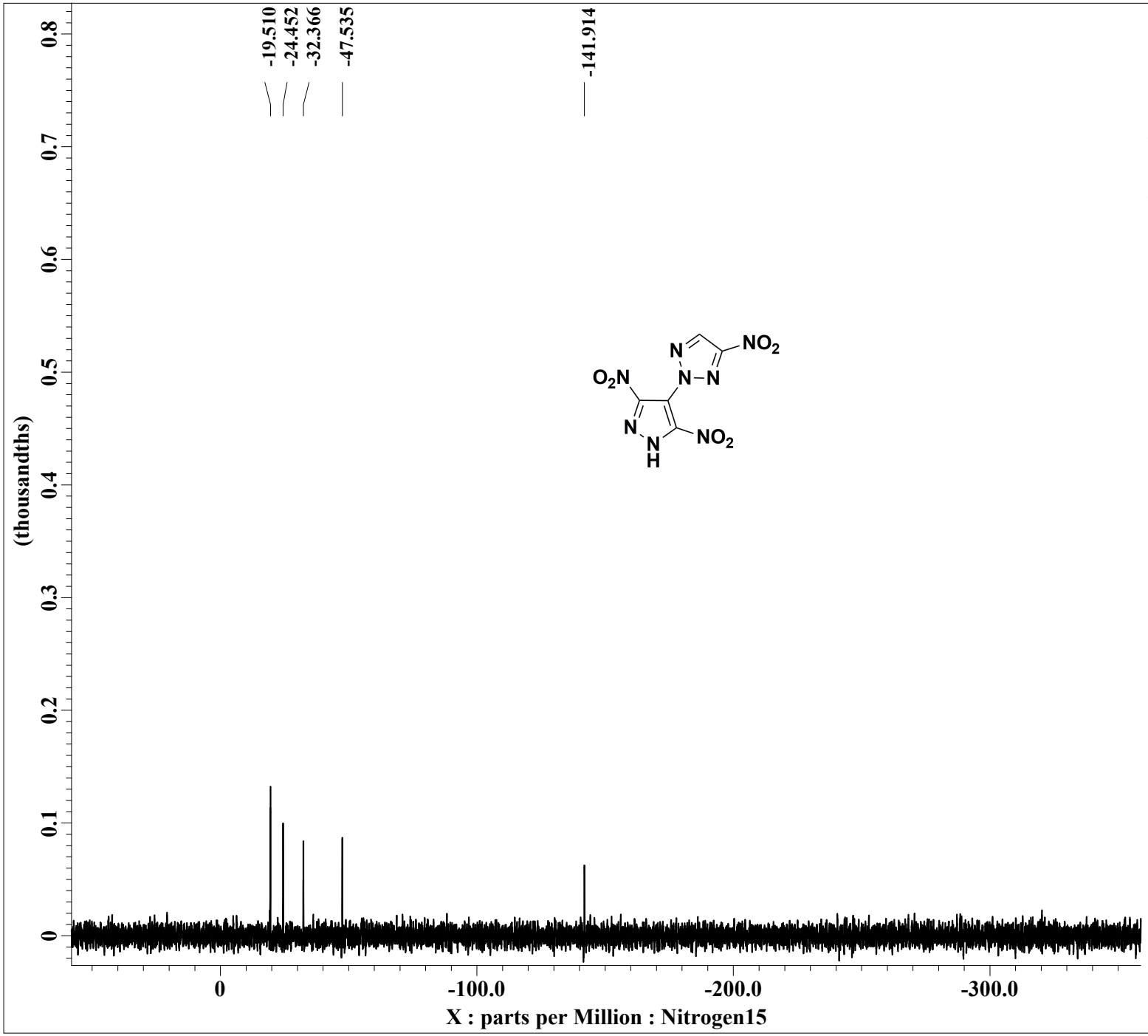
Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 52429
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = ACRHEM_UOH
Spectrometer            = JNM-ECZ600R/M1

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 1.09051904[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 7.0[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.91699454[Hz]
X_Sweep                 = 15.02403846[kHz]
X_Sweep_Clipped         = 12.01923077[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 46
Temp_Get                = 20.4[dC]
X_90_Width              = 6.89[us]
X_Acq_Time              = 1.09051904[s]
X_Angle                 = 45[deg]
X_Atn                   = 12.6[dB]
X_Pulse                 = 3.445[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = C:\Users\delta\Docume
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time         = 6.09051904[s]
```



Filename	= Vs-8-16B_Carbon-1-
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= Vs-8-16B
Solvent	= DMSO-D6
Actual_Start_Time	= 11-JUL-2022 16:41:
Revision_Time	= 12-JUL-2022 15:58:
Comment	= single pulse decou
Data_Format	= 1D REAL
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 10240
Total_Scans	= 10240
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 18.4[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]

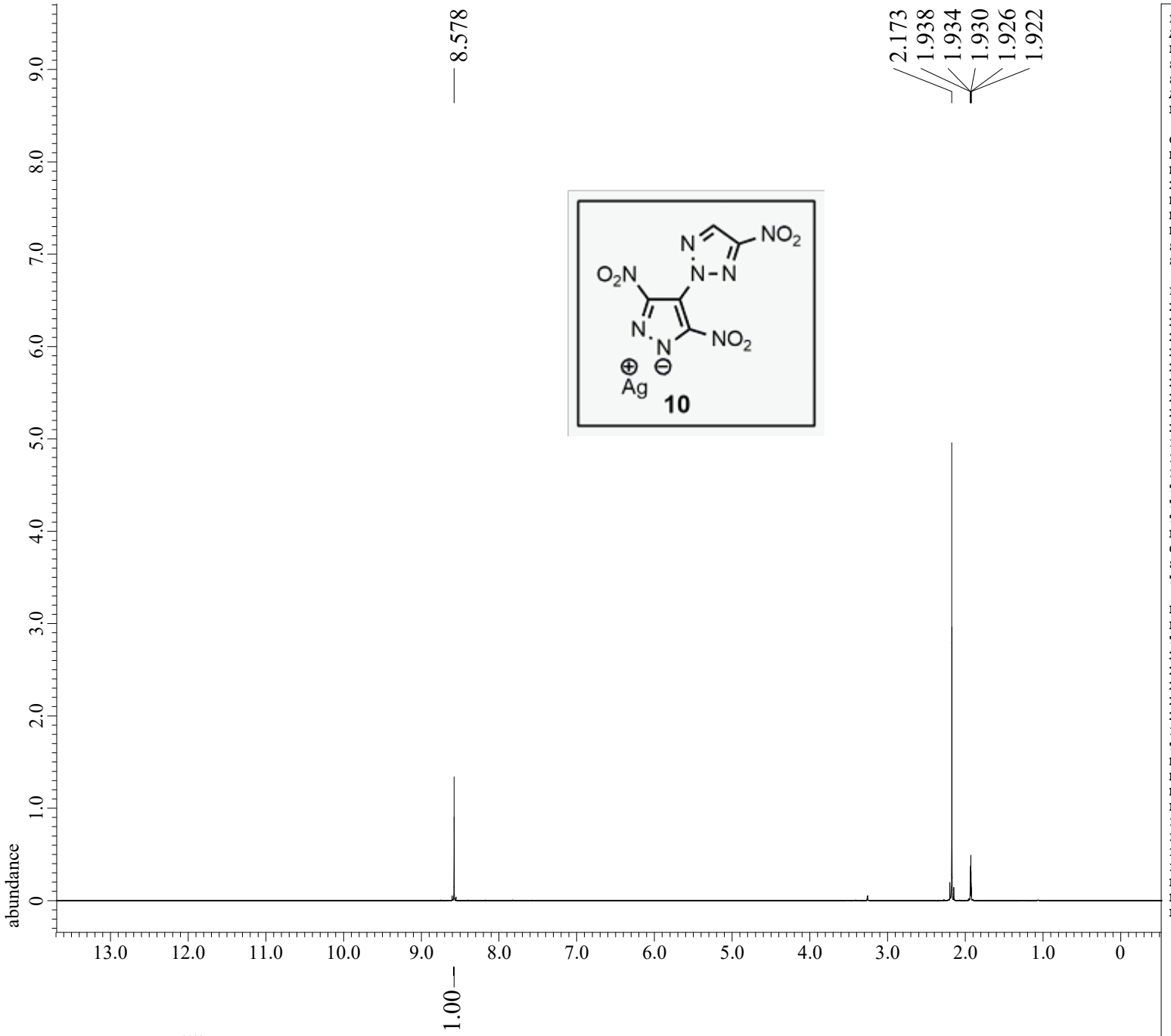



```
Filename                  = Vs-8-16b 1_1d_15N-
Author                    = delta
Experiment                = single_pulse_dec.j
Sample_Id                 = Vs-8-16b 1
Solvent                   = DMSO-D6
Actual_Start_Time         = 15-JUL-2022 18:18:
Revision_Time             = 19-JUL-2022 15:13:

Comment                   = single pulse decou
Data_Format               = 1D REAL
Dim_Size                  = 52429
X_Domain                  = Nitrogen15
Dim_Title                 = Nitrogen15
Dim_Units                 = [ppm]
Dimensions                = X
Site                      = ACRHEM_UOH
Spectrometer              = JNM-ECZ600R/M1

Field_Strength            = 14.09636928[T] (60
X_Acq_Duration            = 0.85983232[s]
X_Domain                  = Nitrogen15
X_Freq                    = 60.81520929[MHz]
X_Offset                  = 214.12266[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 1.45377182[Hz]
X_Sweep                   = 38.1097561[kHz]
X_Sweep_Clipped           = 30.48780488[kHz]
Irr_Domain                = Proton
Irr_Freq                  = 600.1723046[MHz]
Irr_Offset                = 5[ppm]
Blanking                  = 5[us]
Clipped                   = TRUE
Scans                     = 18000
Total_Scans               = 18000

Relaxation_Delay          = 15[s]
Recvr_Gain                = 52
Temp_Get                  = 20.3[dC]
X_90_Width                = 24.21[us]
X_Acq_Time                = 0.68786586[s]
X_Angle                   = 30[deg]
X_Atn                     = 9.9[dB]
X_Pulse                   = 8.07[us]
Irr_Atn_Dec               = 33.452[dB]
Irr_Atn_Dec_Calc          = 33.452[dB]
Irr_Atn_Dec_Default_Calc  = 33.452[dB]
Irr_Dec_Bandwidth_Hz      = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm     = 12.05794078[ppm]
Irr_Dec_Freq              = 600.1723046[MHz]
Irr_Dec_Merit_Factor      = 2.2
Irr_Decoupling            = TRUE
Irr_Noe                   = FALSE
Irr_Noise                 = WALTZ
Irr_Offset_Default        = 5[ppm]
Irr_Pwidth                = 76[us]
Irr_Pwidth_Default        = 76[us]
Irr_Pwidth_Default_Calc   = 76[us]
Irr_Pwidth_Temp1          = 76[us]
Irr_Wurst                 = FALSE
Decimation_Rate           = 0
```

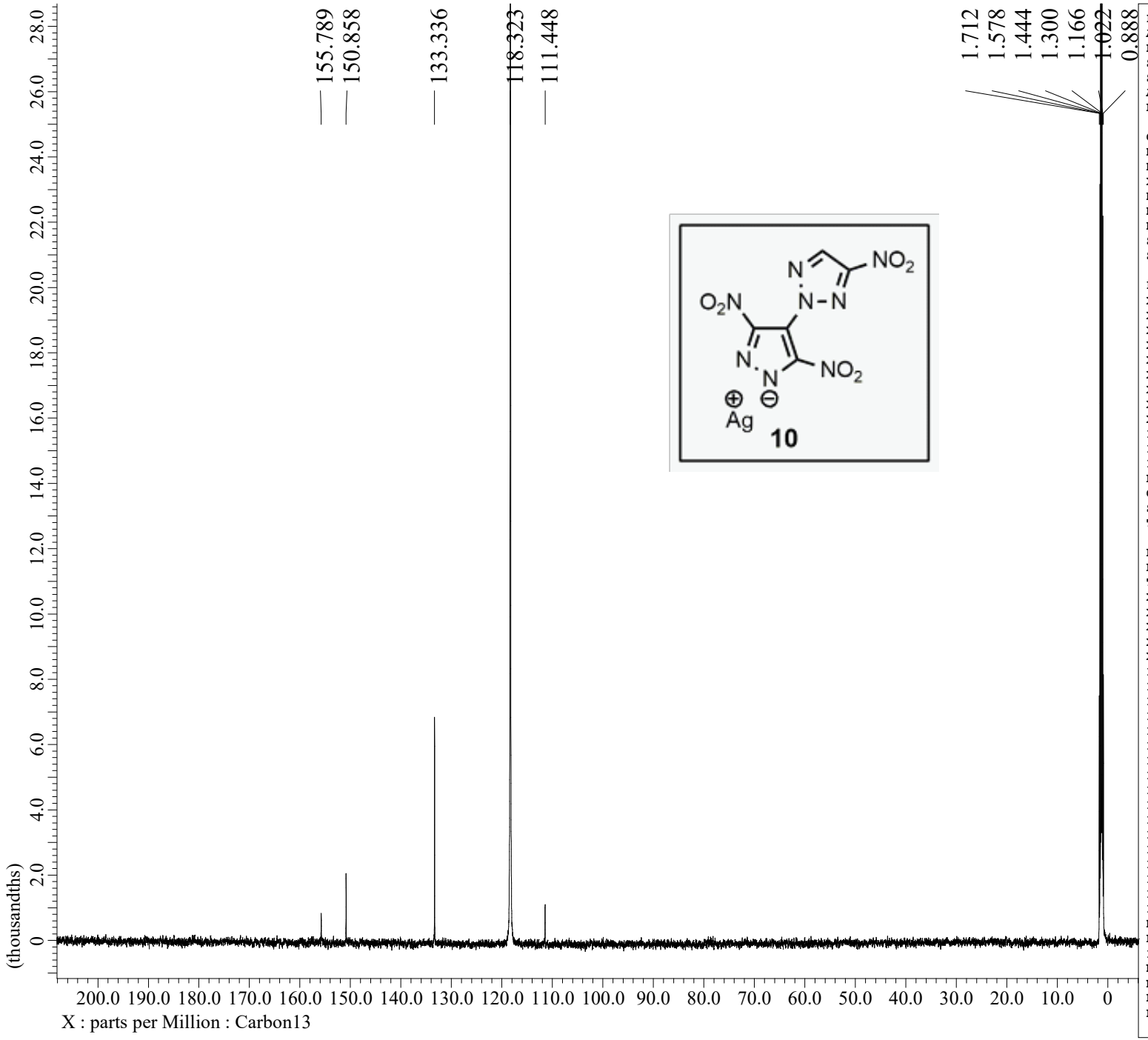



```
Filename                = MBR-5-108_proton-1-3.
Author                  = delta
Experiment              = proton_auto.jxp
Sample_Id               = MBR-5-108
Solvent                 = ACETONITRILE-D3
Actual_Start_Time       = 23-JAN-2023 15:54:25
Revision_Time           = 23-JAN-2023 22:24:57

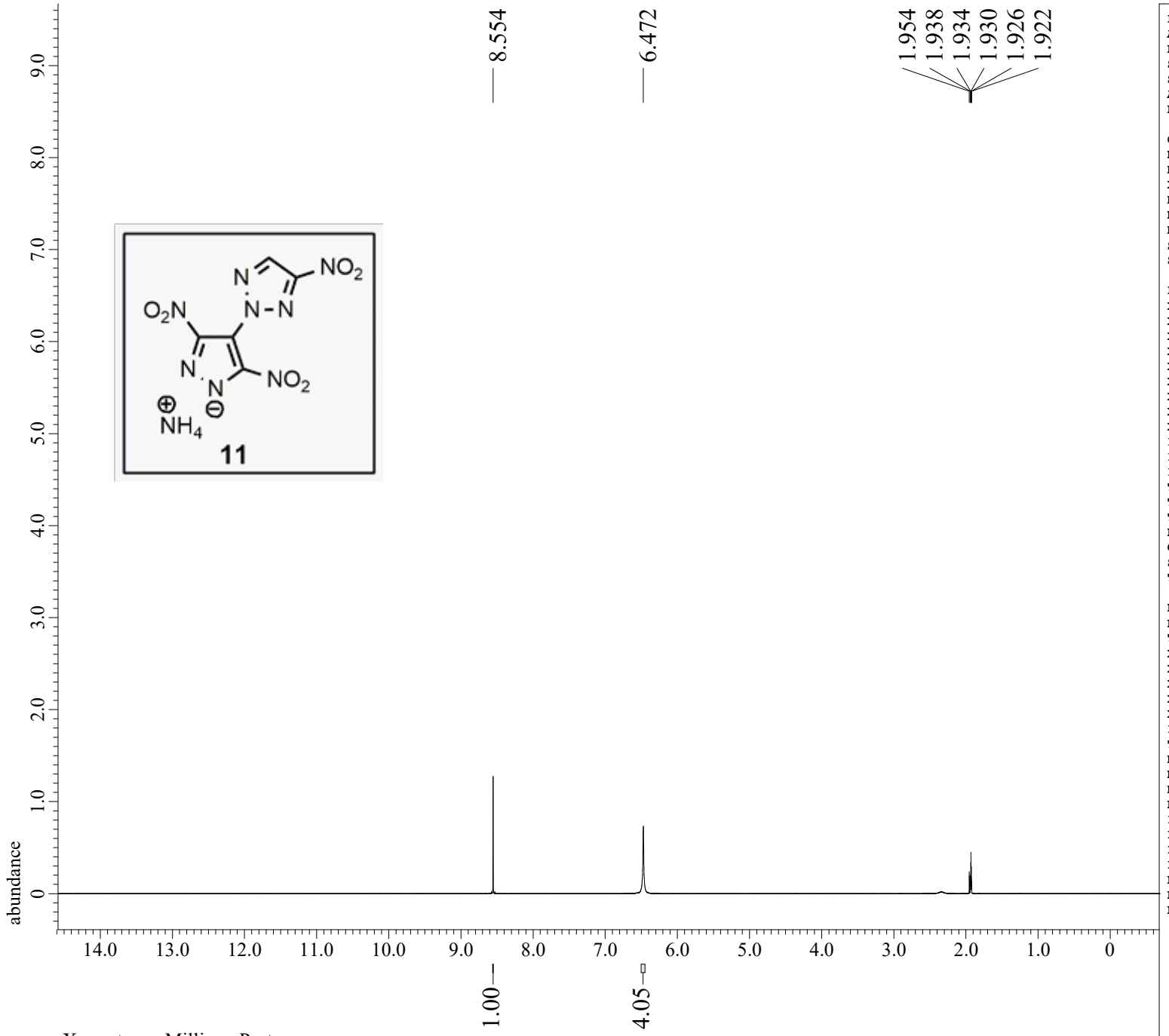
Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 52429
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = ACRHEM_UOH
Spectrometer            = JNM-ECZ600R/M1

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 1.09051904[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 7.0[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.91699454[Hz]
X_Sweep                 = 15.02403846[kHz]
X_Sweep_Clipped         = 12.01923077[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 20.1[dC]
X_90_Width              = 6.89[us]
X_Acq_Time              = 1.09051904[s]
X_Angle                 = 45[deg]
X_Atn                   = 12.6[dB]
X_Pulse                 = 3.445[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = C:\Users\delta\Docume
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 5[s]
Repetition_Time         = 6.09051904[s]
```



Filename	= MBR-5-108_Carbon-2
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= MBR-5-108
Solvent	= ACETONITRILE-D3
Actual_Start_Time	= 24-JAN-2023 12:47:
Revision_Time	= 24-JAN-2023 15:12:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 1[s]
Recvr_Gain	= 56
Temp_Get	= 19.7[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 1[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 1[s]

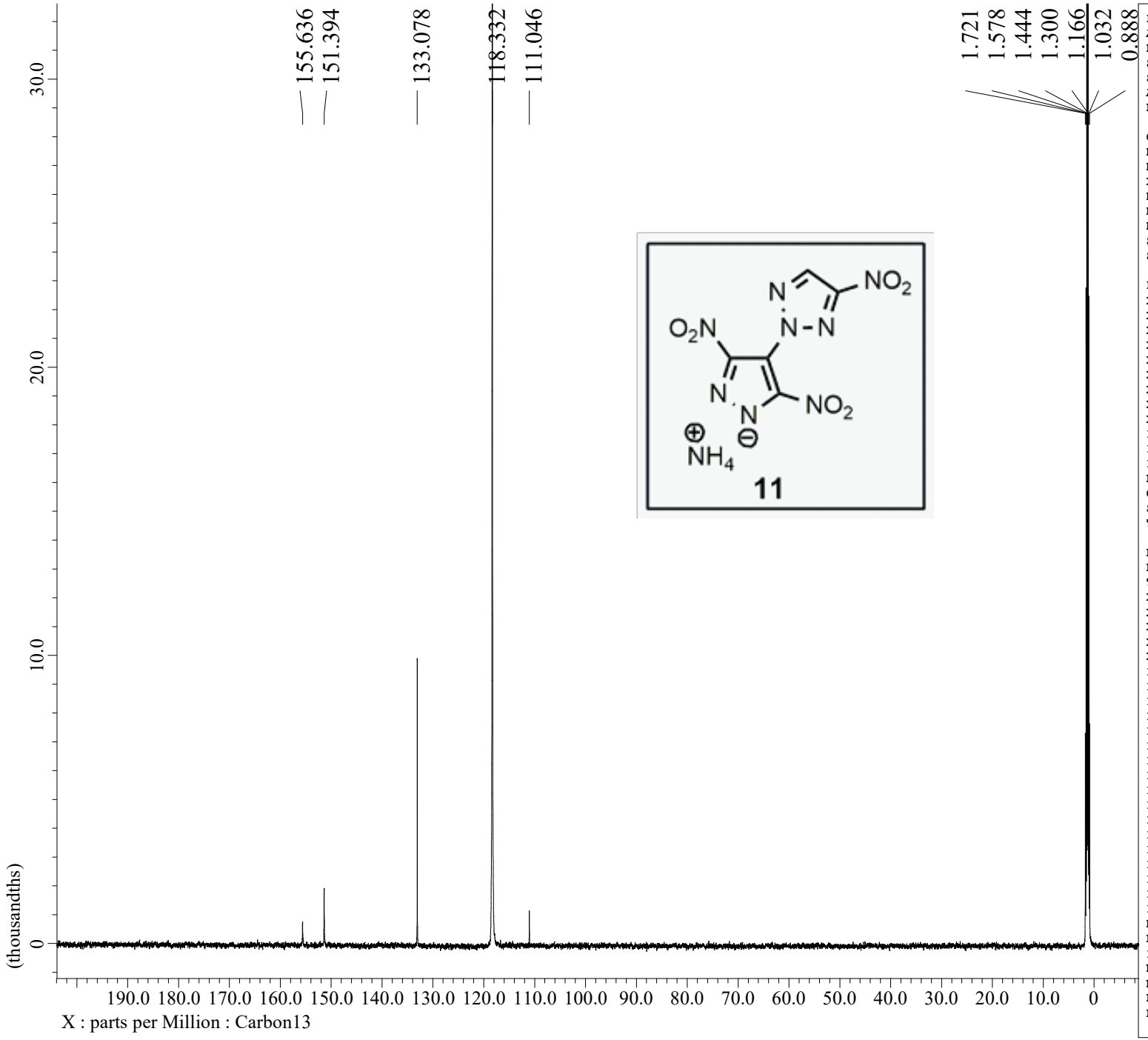



```
Filename                = MBR-5-110-N_proton-1-
Author                  = delta
Experiment              = proton_auto.jxp
Sample_Id               = MBR-5-110-N
Solvent                 = ACETONITRILE-D3
Actual_Start_Time       =  2-JAN-2023 17:13:48
Revision_Time           =  3-JAN-2023 21:39:47

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 52429
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = ACRHEM_UOH
Spectrometer            = JNM-ECZ600R/M1

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 1.09051904[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 7.0[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.91699454[Hz]
X_Sweep                 = 15.02403846[kHz]
X_Sweep_Clipped         = 12.01923077[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 21.3[dC]
X_90_Width              = 6.89[us]
X_Acq_Time              = 1.09051904[s]
X_Angle                 = 45[deg]
X_Atn                   = 12.6[dB]
X_Pulse                 = 3.445[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = C:\Users\delta\Docume
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time         = 6.09051904[s]
```

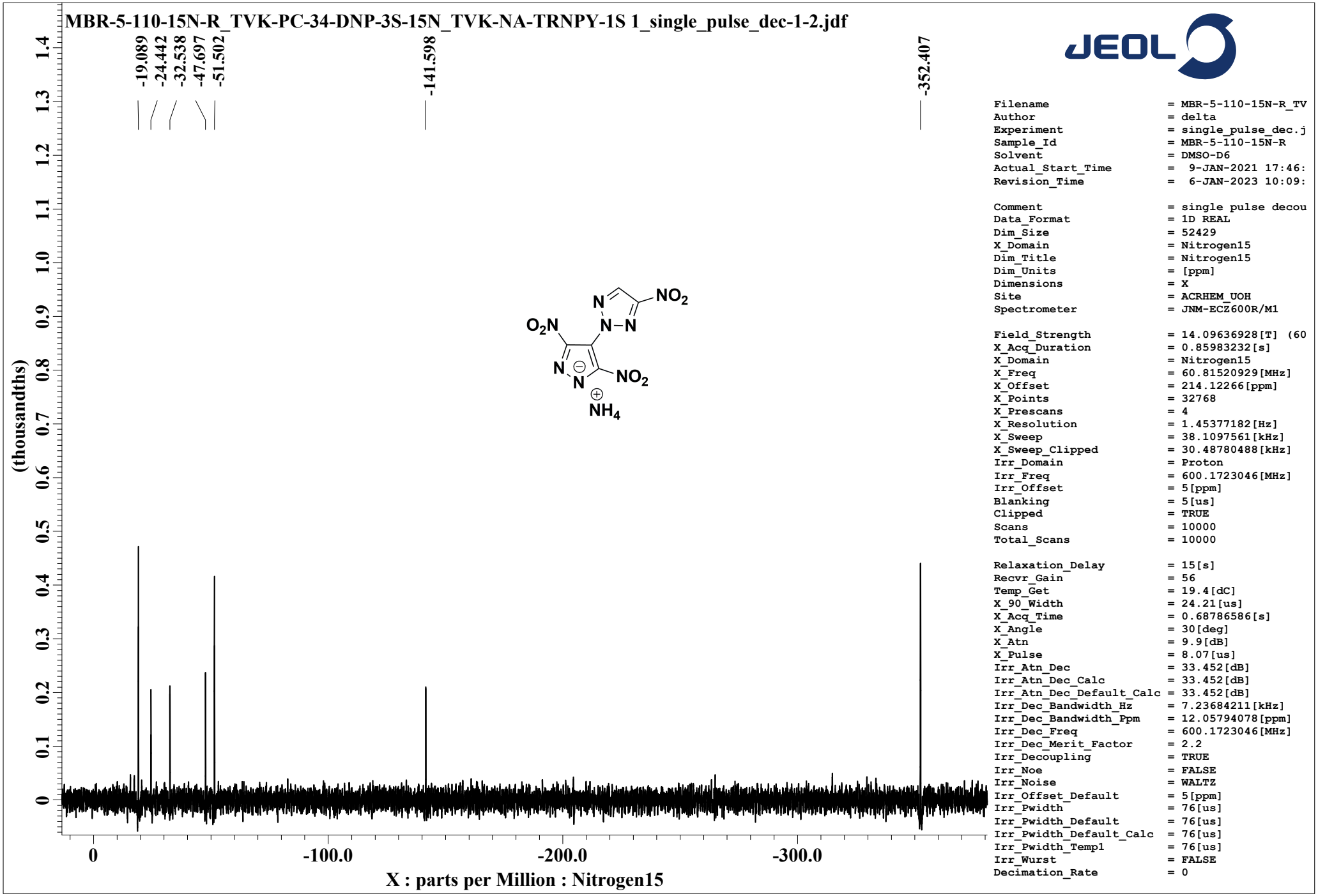


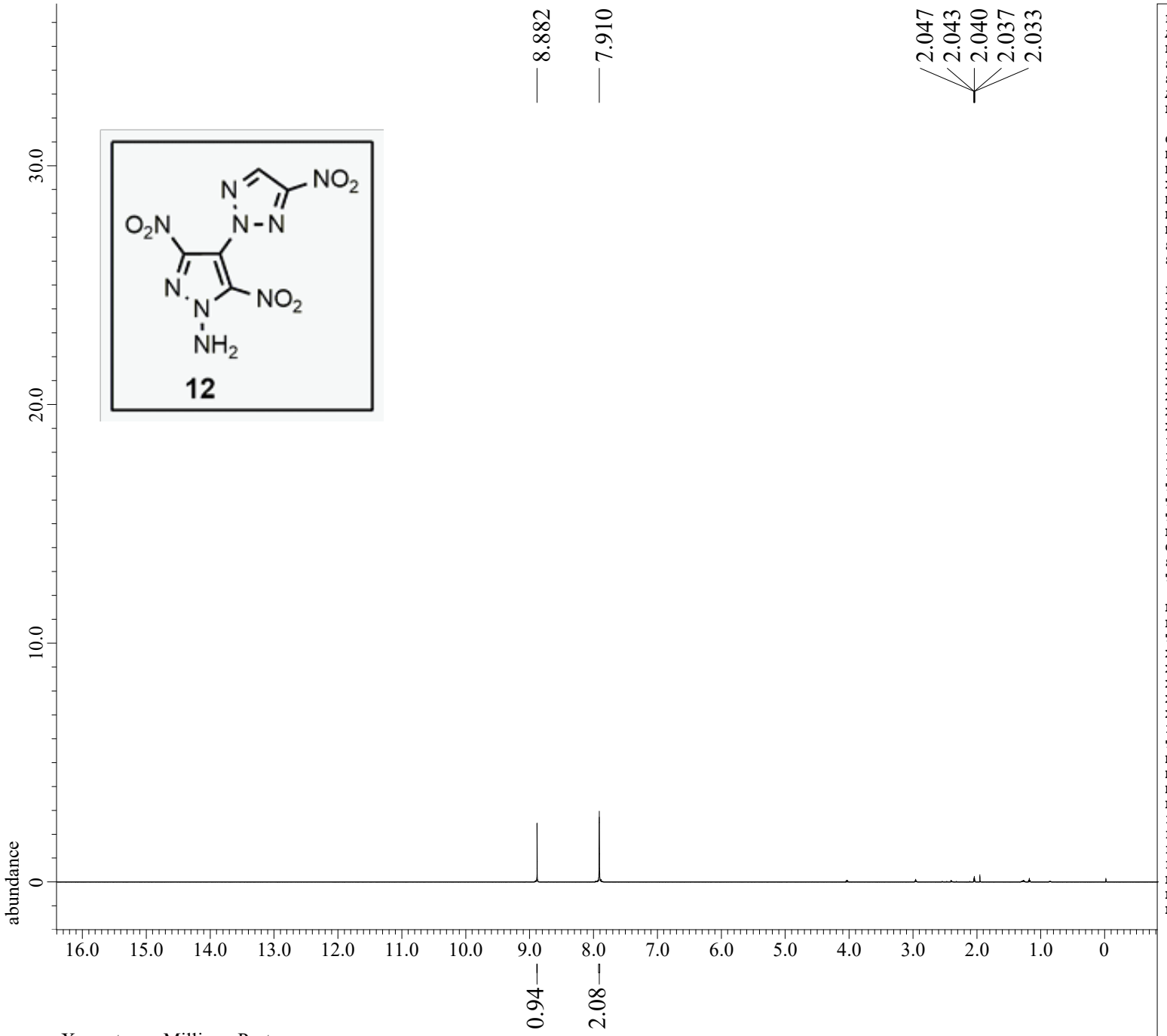

```
Filename                    = MBR-5-110-N_Carbon
Author                      = delta
Experiment                  = carbon_auto.jxp
Sample_Id                   = MBR-5-110-N
Solvent                     = ACETONITRILE-D3
Actual_Start_Time           =  4-JAN-2023 13:13:
Revision_Time               =  4-JAN-2023 16:24:

Comment                     = single pulse decou
Data_Format                 = 1D COMPLEX
Dim_Size                    = 26214
X_Domain                    = Carbon13
Dim_Title                   = Carbon13
Dim_Units                   = [ppm]
Dimensions                  = X
Site                        = ACRHEM_UOH
Spectrometer                = JNM-ECZ600R/M1

Field_Strength              = 14.09636928[T] (60
X_Acq_Duration              = 0.34603008[s]
X_Domain                    = Carbon13
X_Freq                      = 150.91343039[MHz]
X_Offset                    = 100[ppm]
X_Points                    = 16384
X_Prescans                  = 4
X_Resolution                = 2.88992217[Hz]
X_Sweep                     = 47.34848485[kHz]
X_Sweep_Clipped             = 37.87878788[kHz]
Irr_Domain                  = Proton
Irr_Freq                    = 600.1723046[MHz]
Irr_Offset                  = 5[ppm]
Blanking                    = 2[us]
Clipped                     = FALSE
Scans                       = 2048
Total_Scans                 = 2048

Relaxation_Delay            = 1[s]
Recvr_Gain                  = 56
Temp_Get                    = 20.3[dC]
X_90_Width                  = 11[us]
X_Acq_Time                  = 0.34603008[s]
X_Angle                     = 30[deg]
X_Atn                       = 10.3[dB]
X_Pulse                     = 3.66666667[us]
Irr_Atn_Dec                 = 33.452[dB]
Irr_Atn_Dec_Calc            = 33.452[dB]
Irr_Atn_Dec_Default_Calc    = 33.452[dB]
Irr_Atn_Noe                 = 33.452[dB]
Irr_Dec_Bandwidth_Hz        = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm       = 12.05794078[ppm]
Irr_Dec_Freq                = 600.1723046[MHz]
Irr_Dec_Merit_Factor        = 2.2
Irr_Decoupling              = TRUE
Irr_Noe                     = TRUE
Irr_Noise                   = WALTZ
Irr_Offset_Default          = 5[ppm]
Irr_Pwidth                  = 76[us]
Irr_Pwidth_Default          = 76[us]
Irr_Pwidth_Default_Calc     = 76[us]
Irr_Pwidth_Temp1            = 76[us]
Irr_Wurst                   = FALSE
Decimation_Rate             = 0
Experiment_Path             = c:\Program Files\J
Initial_Wait                = 1[s]
Noe_Time                    = 1[s]
Noe_Time_Flag               = FALSE
Relaxation_Delay_Calc       = 0[s]
Relaxation_Delay_Temp       = 1[s]
```


MBR-5-110-15N-R_TVK-PC-34-DNP-3S-15N_TVK-NA-TRNPY-1S 1_single_pulse_dec-1-2.jdf
-19.089
-24.442
-32.538
-47.697
-51.502
-141.598
-352.407
(thousandths)
X : parts per Million : Nitrogen15
0
-100.0
-200.0
-300.0
Filename = MBR-5-110-15N-R_TV
Author = delta
Experiment = single_pulse_dec.j
Sample_Id = MBR-5-110-15N-R
Solvent = DMSO-D6
Actual_Start_Time = 9-JAN-2021 17:46:
Revision_Time = 6-JAN-2023 10:09:
Comment = single pulse decou
Data_Format = 1D REAL
Dim_Size = 52429
X_Domain = Nitrogen15
Dim_Title = Nitrogen15
Dim_Units = [ppm]
Dimensions = X
Site = ACRHEM_UOH
Spectrometer = JNM-ECZ600R/M1
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0.85983232[s]
X_Domain = Nitrogen15
X_Freq = 60.81520929[MHz]
X_Offset = 214.12266[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.45377182[Hz]
X_Sweep = 38.1097561[kHz]
X_Sweep_Clipped = 30.48780488[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 10000
Total_Scans = 10000
Relaxation_Delay = 15[s]
Recvr_Gain = 56
Temp_Get = 19.4[dC]
X_90_Width = 24.21[us]
X_Acq_Time = 0.68786586[s]
X_Angle = 30[deg]
X_Atn = 9.9[dB]
X_Pulse = 8.07[us]
Irr_Atn_Dec = 33.452[dB]
Irr_Atn_Dec_Calc = 33.452[dB]
Irr_Atn_Dec_Default_Calc = 33.452[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = FALSE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0

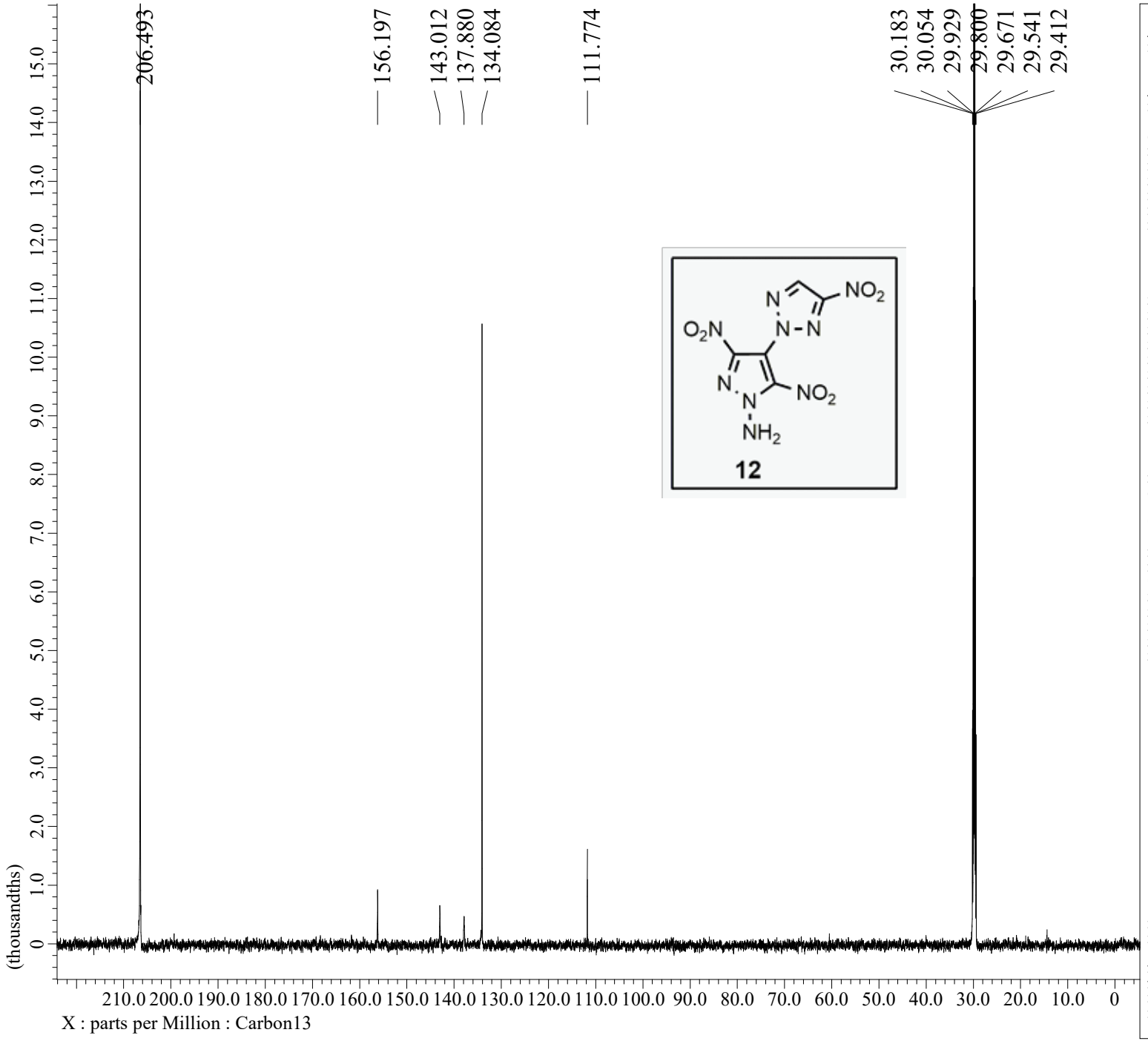



```
Filename                = MBR-5-112 proton-1-3.
Author                  = delta
Experiment              = proton_auto.jxp
Sample_Id               = MBR-6-124-13C
Solvent                 = ACETONE-D6
Actual_Start_Time       =  1-JAN-2021 15:30:02
Revision_Time           = 10-JAN-2023 17:54:33

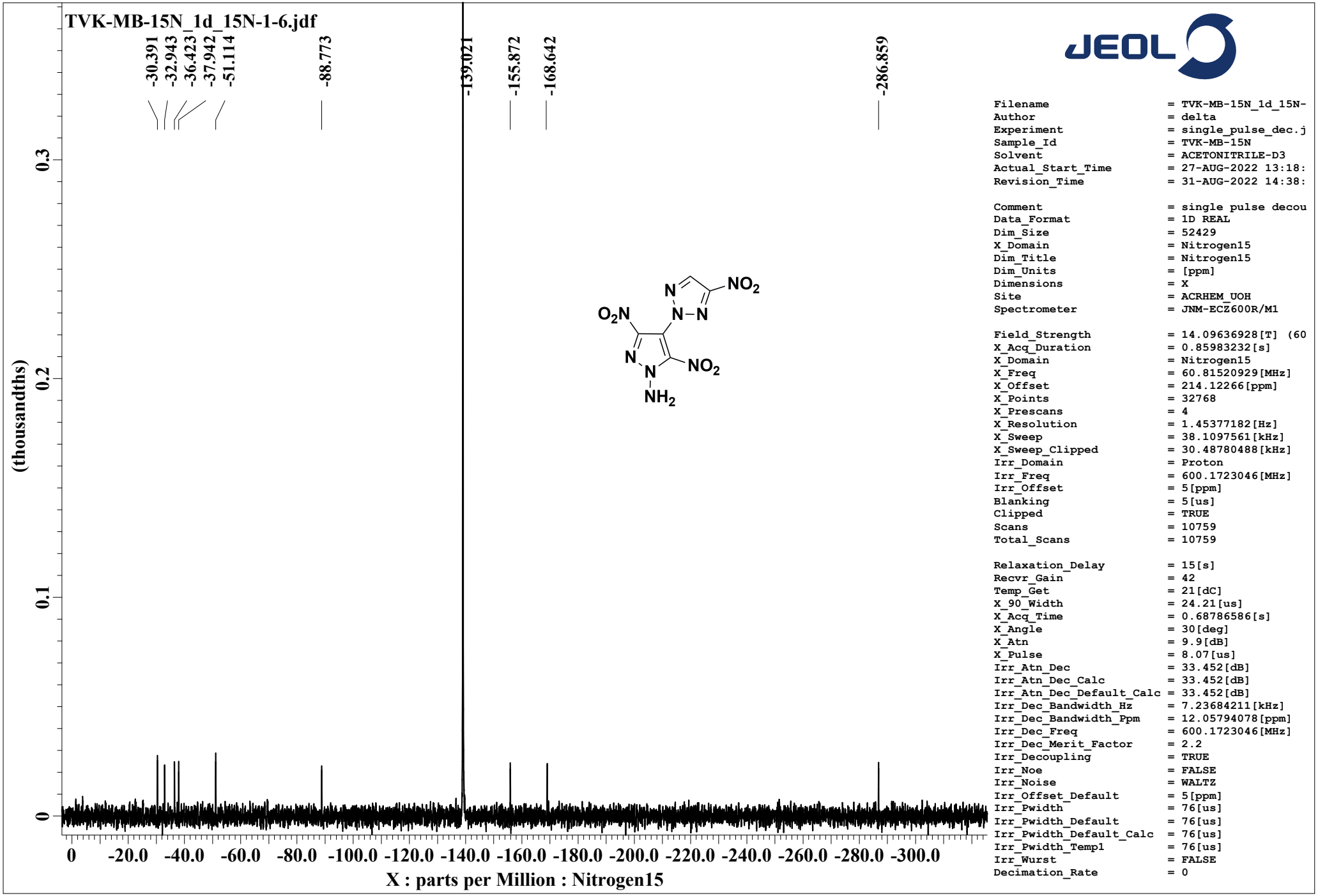
Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 52429
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = ACRHEM_UOH
Spectrometer            = JNM-ECZ600R/M1

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 0.72876032[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 6.5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 1.37219326[Hz]
X_Sweep                 = 22.48201439[kHz]
X_Sweep_Clipped         = 17.98561151[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 2
Total_Scans             = 2

Relaxation_Delay        = 5[s]
Recvr_Gain              = 46
Temp_Get                = 20[dC]
X_90_Width              = 6.89[us]
X_Acq_Time              = 0.72876032[s]
X_Angle                 = 45[deg]
X_Atn                   = 12.6[dB]
X_Pulse                 = 3.445[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = C:\Users\delta\Docume
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time         = 5.72876032[s]
```



Filename	= MBR-5-112 Carbon-1
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= MBR-6-124-13C
Solvent	= ACETONE-D6
Actual_Start_Time	= 1-JAN-2021 15:30:
Revision_Time	= 10-JAN-2023 17:59:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.1[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]


TVK-MB-15N_1d_15N-1-6.jdf
-30.391
-32.943
-36.423
-37.942
-51.114
-88.773
-139.021
-155.872
-168.642
-286.859
(thousandths)
0.3
0.2
0.1
0
0 -20.0 -40.0 -60.0 -80.0 -100.0 -120.0 -140.0 -160.0 -180.0 -200.0 -220.0 -240.0 -260.0 -280.0 -300.0
X : parts per Million : Nitrogen15
Filename = TVK-MB-15N_1d_15N-
Author = delta
Experiment = single_pulse_dec.j
Sample_Id = TVK-MB-15N
Solvent = ACETONITRILE-D3
Actual_Start_Time = 27-AUG-2022 13:18:
Revision_Time = 31-AUG-2022 14:38:
Comment = single pulse decou
Data_Format = 1D REAL
Dim_Size = 52429
X_Domain = Nitrogen15
Dim_Title = Nitrogen15
Dim_Units = [ppm]
Dimensions = X
Site = ACRHEM_UOH
Spectrometer = JNM-ECZ600R/M1
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0.85983232[s]
X_Domain = Nitrogen15
X_Freq = 60.81520929[MHz]
X_Offset = 214.12266[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.45377182[Hz]
X_Sweep = 38.1097561[kHz]
X_Sweep_Clipped = 30.48780488[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 10759
Total_Scans = 10759
Relaxation_Delay = 15[s]
Recvr_Gain = 42
Temp_Get = 21[dC]
X_90_Width = 24.21[us]
X_Acq_Time = 0.68786586[s]
X_Angle = 30[deg]
X_Atn = 9.9[dB]
X_Pulse = 8.07[us]
Irr_Atn_Dec = 33.452[dB]
Irr_Atn_Dec_Calc = 33.452[dB]
Irr_Atn_Dec_Default_Calc = 33.452[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = FALSE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0

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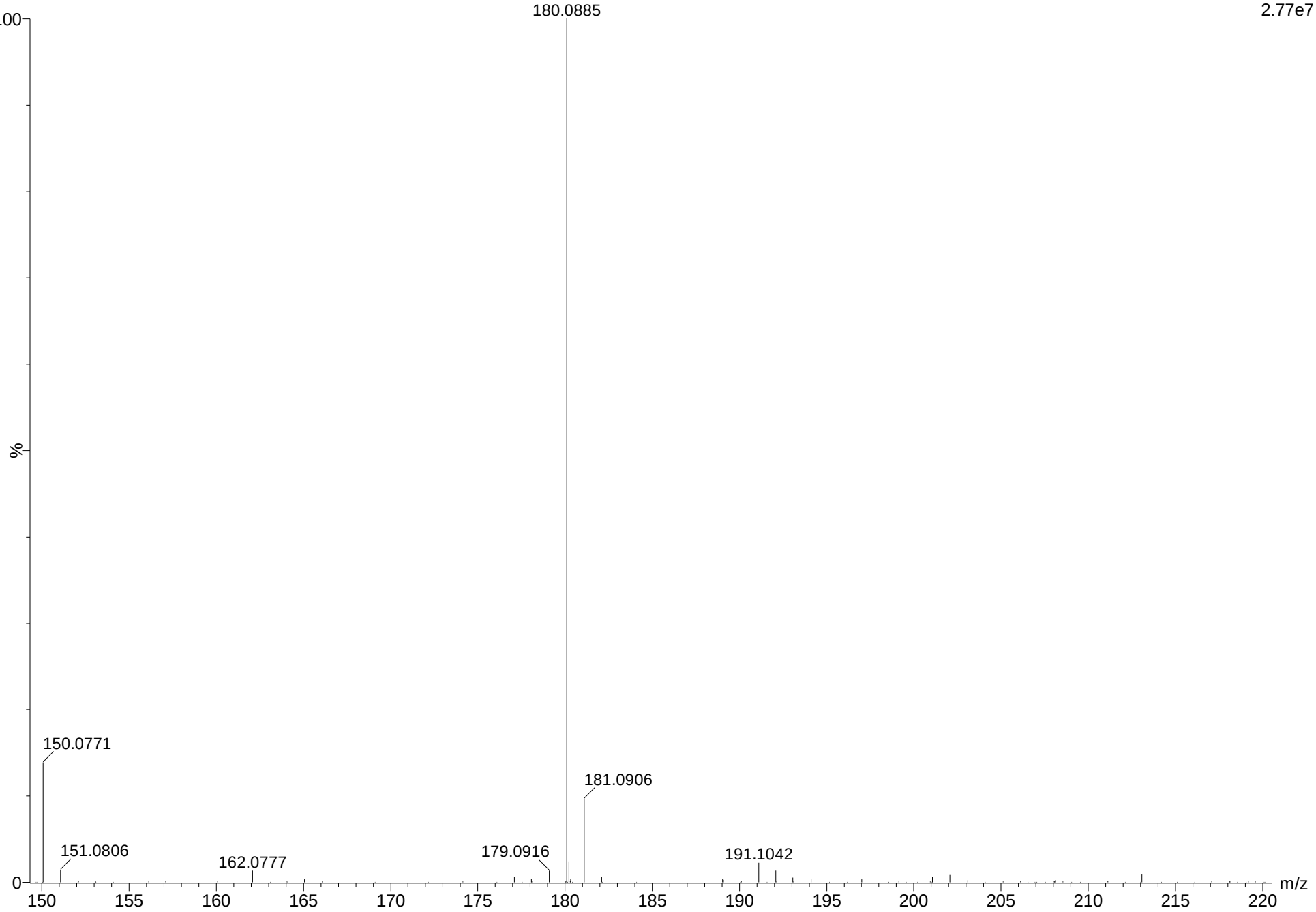
ACRHEM
XEVO-G2XSQTOF#YEA1155

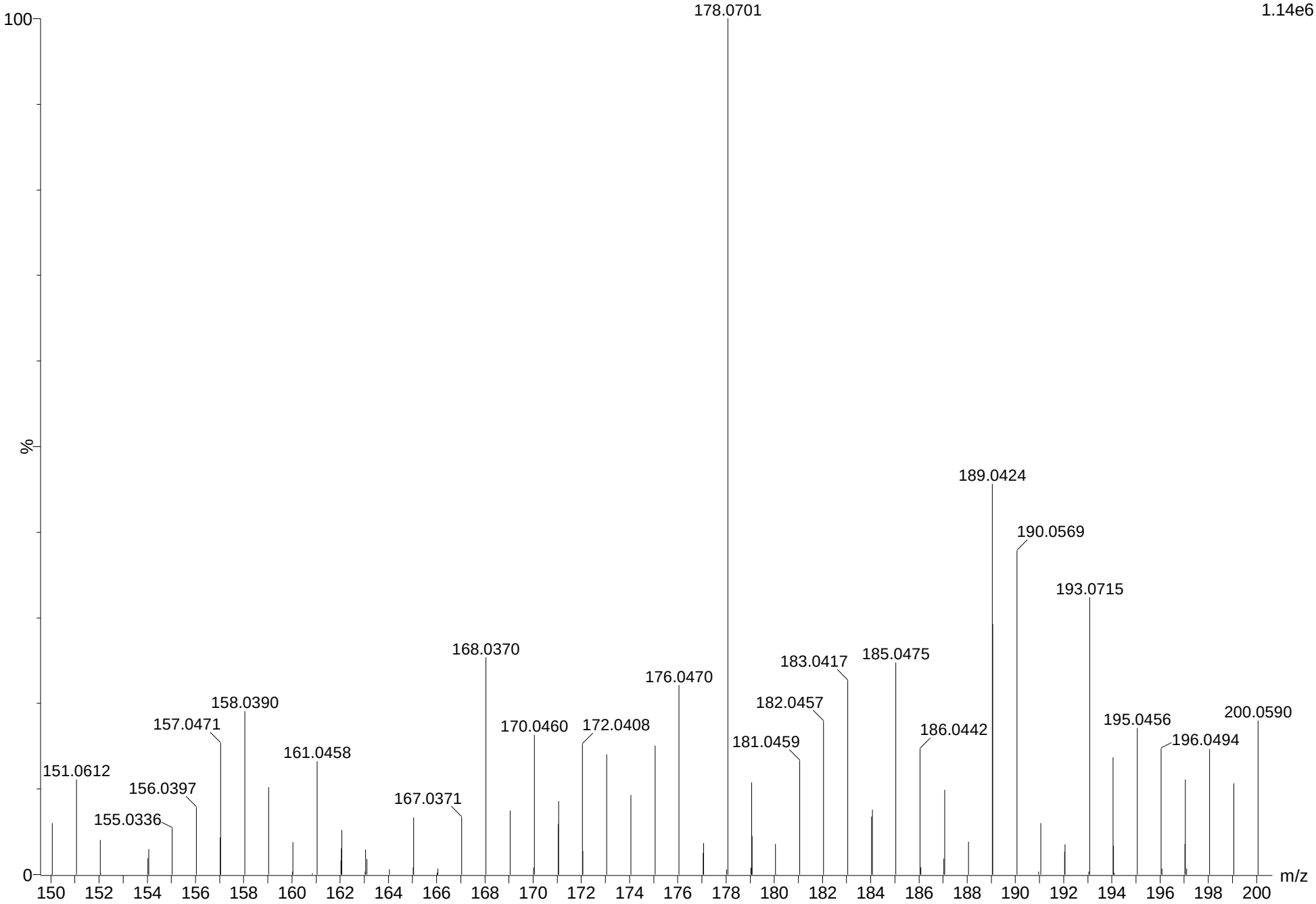
17012019_09 +ve 19 (0.219) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (19:28-112:144)

1: TOF MS ES+
2.77e7

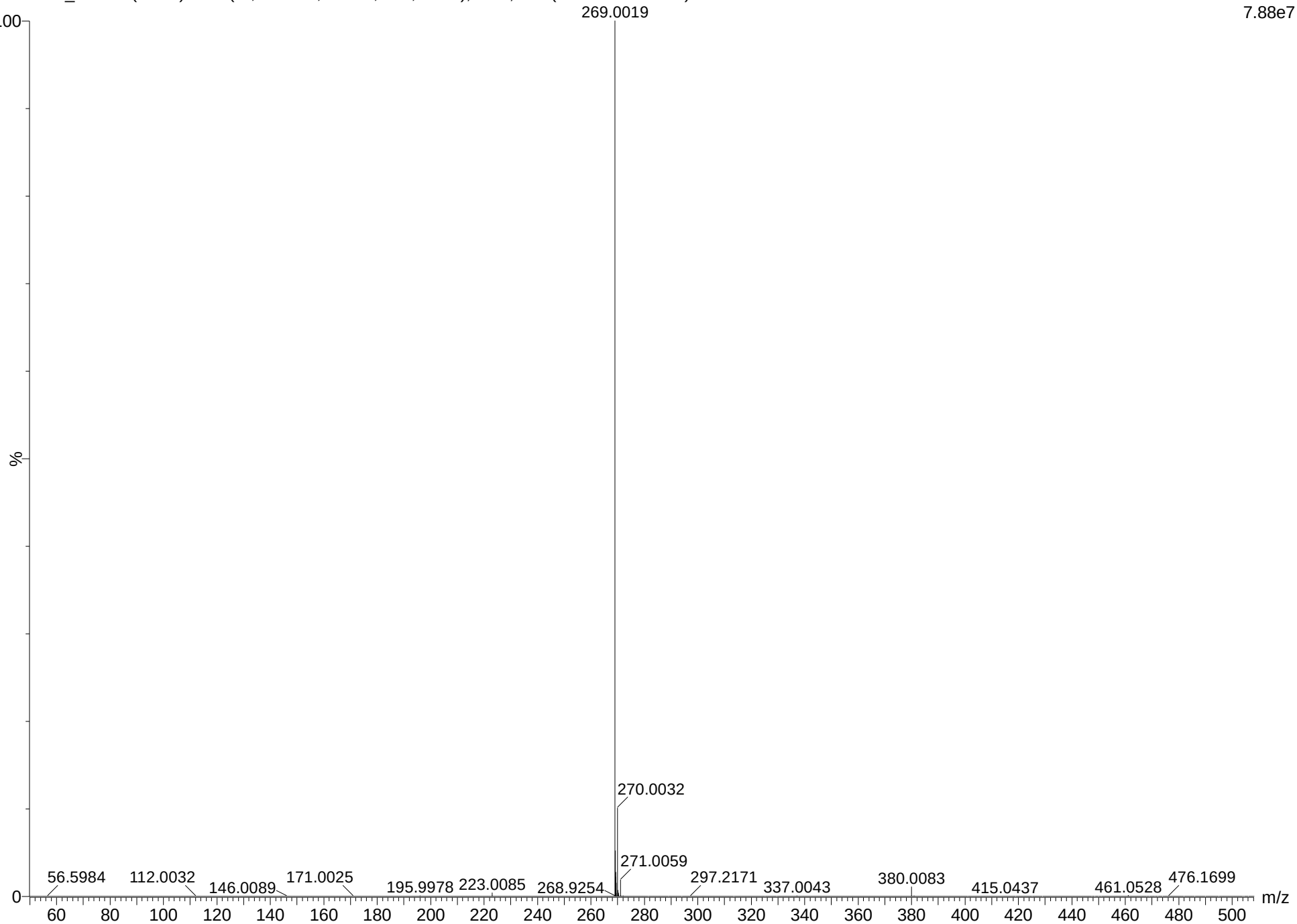


17012019_22 -ve 16 (0.194) AM2 (Ar,22000.0,554.26,0.00,LS 10); Cm (16:23-114:161)

1: TOF MS ES-
1.14e6



19092018_03 536 (5.206) AM2 (Ar,22000.0,554.26,0.00,LS 10); ABS; Cm (536:545-580:594) 1: TOF MS ES-
7.88e7



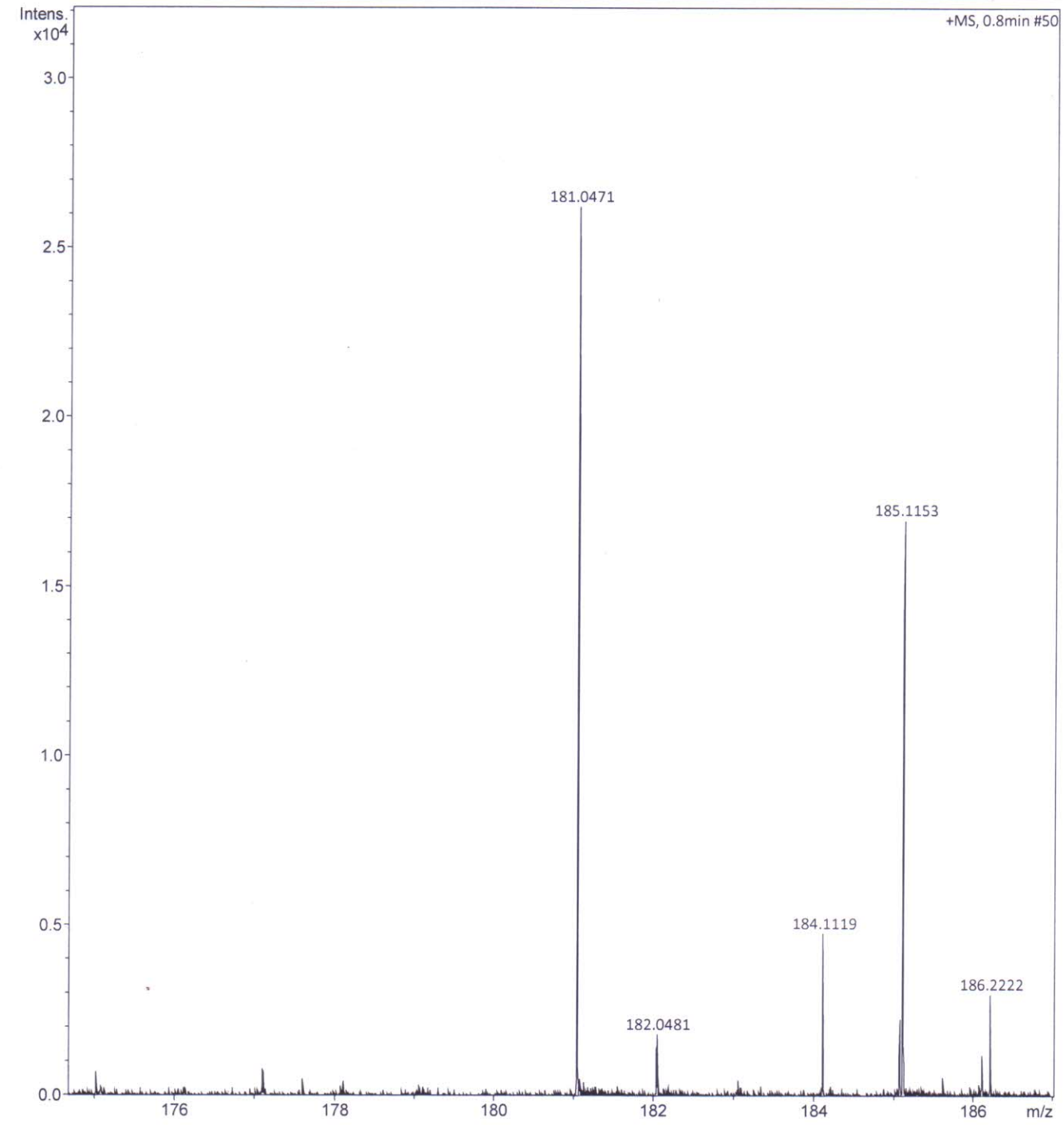
Display Report

Analysis Info

Analysis Name	D:\Data\2023-DATA\PROF. AKS\JAN\MBR-1-141 +VE.d	Acquisition Date	21-01-2023 12:22:24
Method	tune_low.m	Operator	UOH
Sample Name	MBR-1-141 +VE	Instrument	maXis 255552.10138
Comment			

Acquisition Parameter

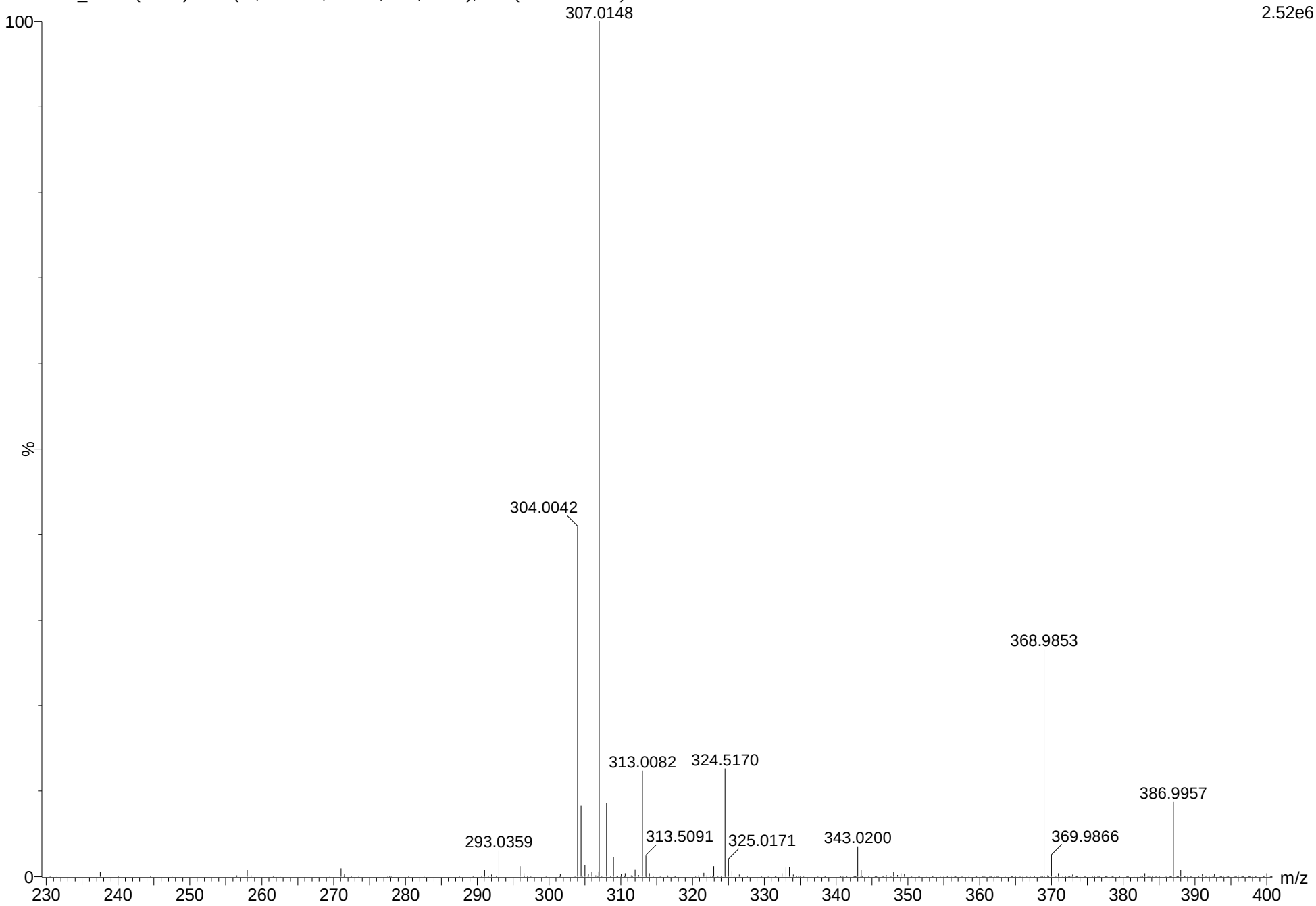
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



MBR-1-141 +VE.d

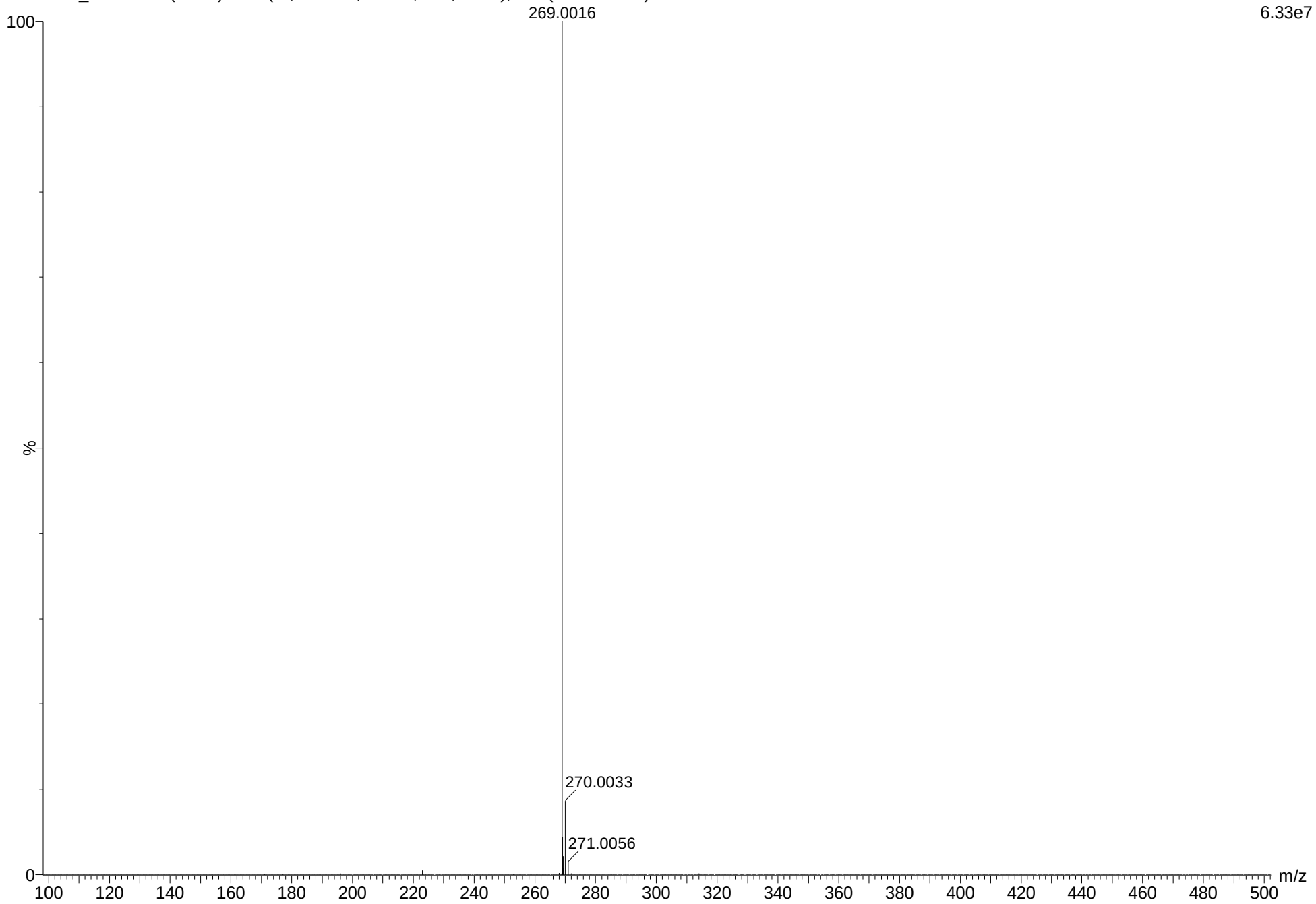
21012019_02 19 (0.219) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (19:28-69:108)

1: TOF MS ES+
2.52e6



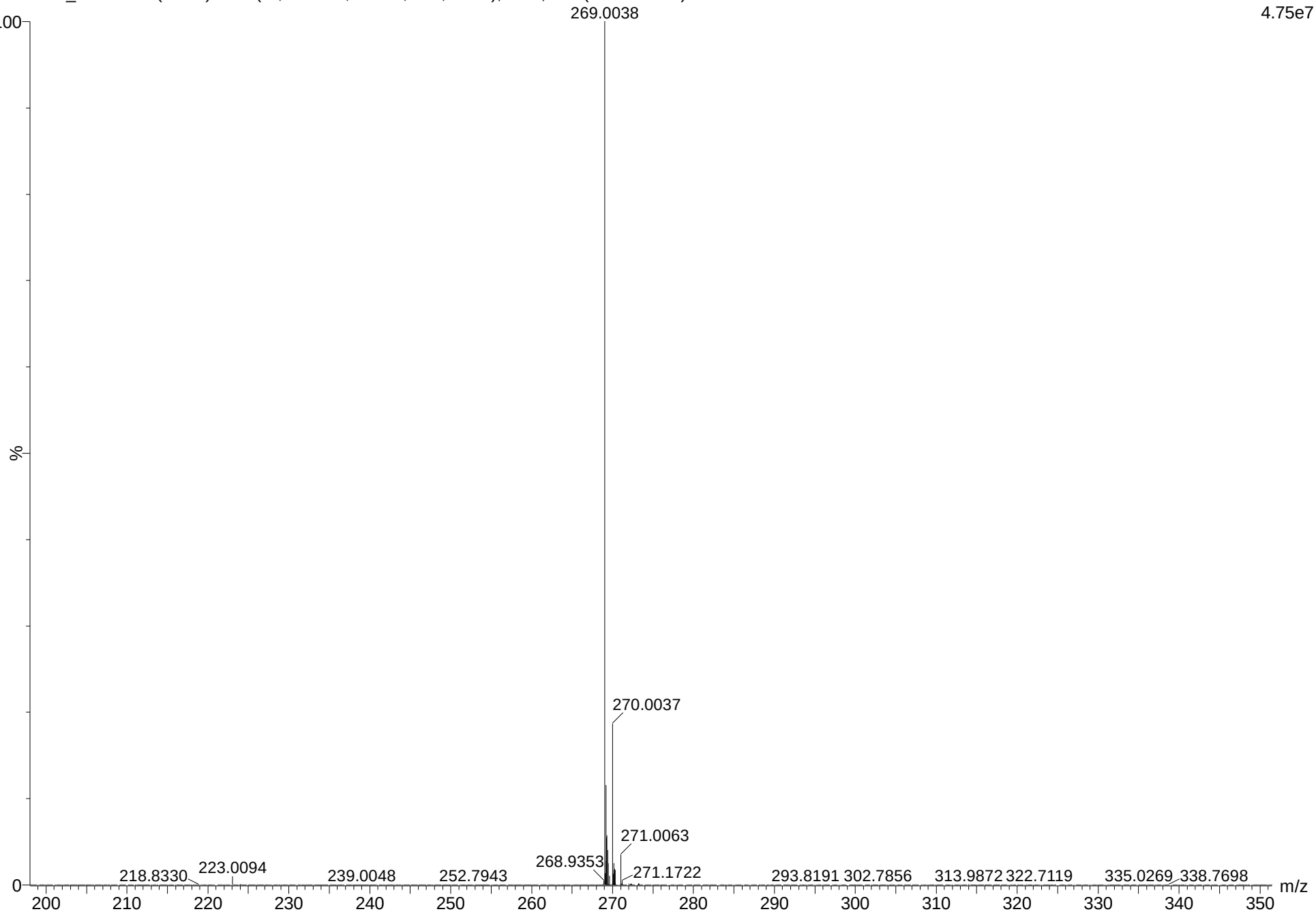
12072022_05 -VE 39 (0.450) AM2 (Ar,22000.0,554.26,0.00,LS 10); Cm (39:48-73:89)

1: TOF MS ES-
6.33e7



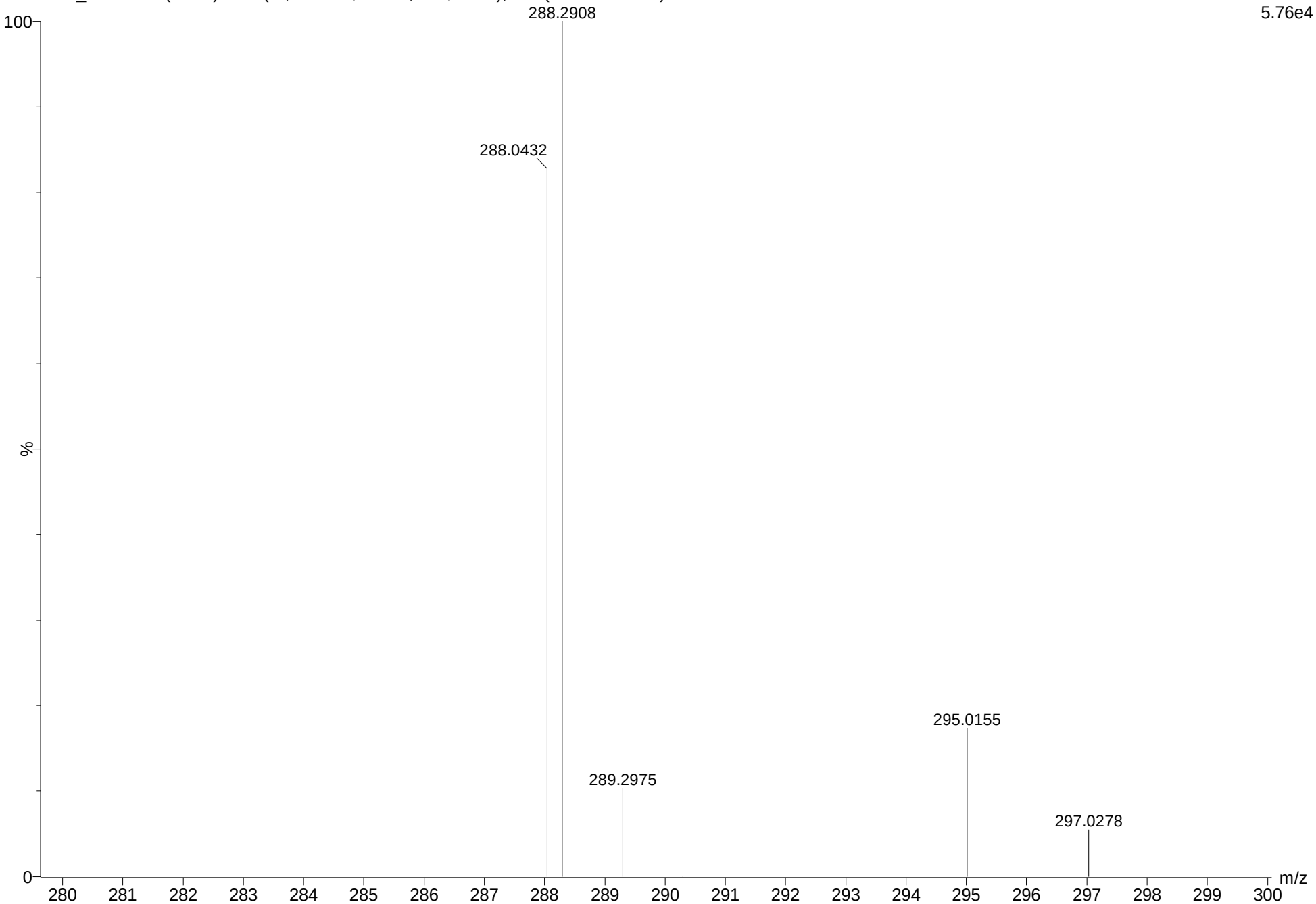
26042019_11 -VE 19 (0.239) AM2 (Ar,22000.0,554.26,0.00,LS 10); ABS; Cm (19:23-49:56)

1: TOF MS ES-
4.75e7



17012019_11 +ve 14 (0.157) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (14:18-124:160)

1: TOF MS ES+
5.76e4



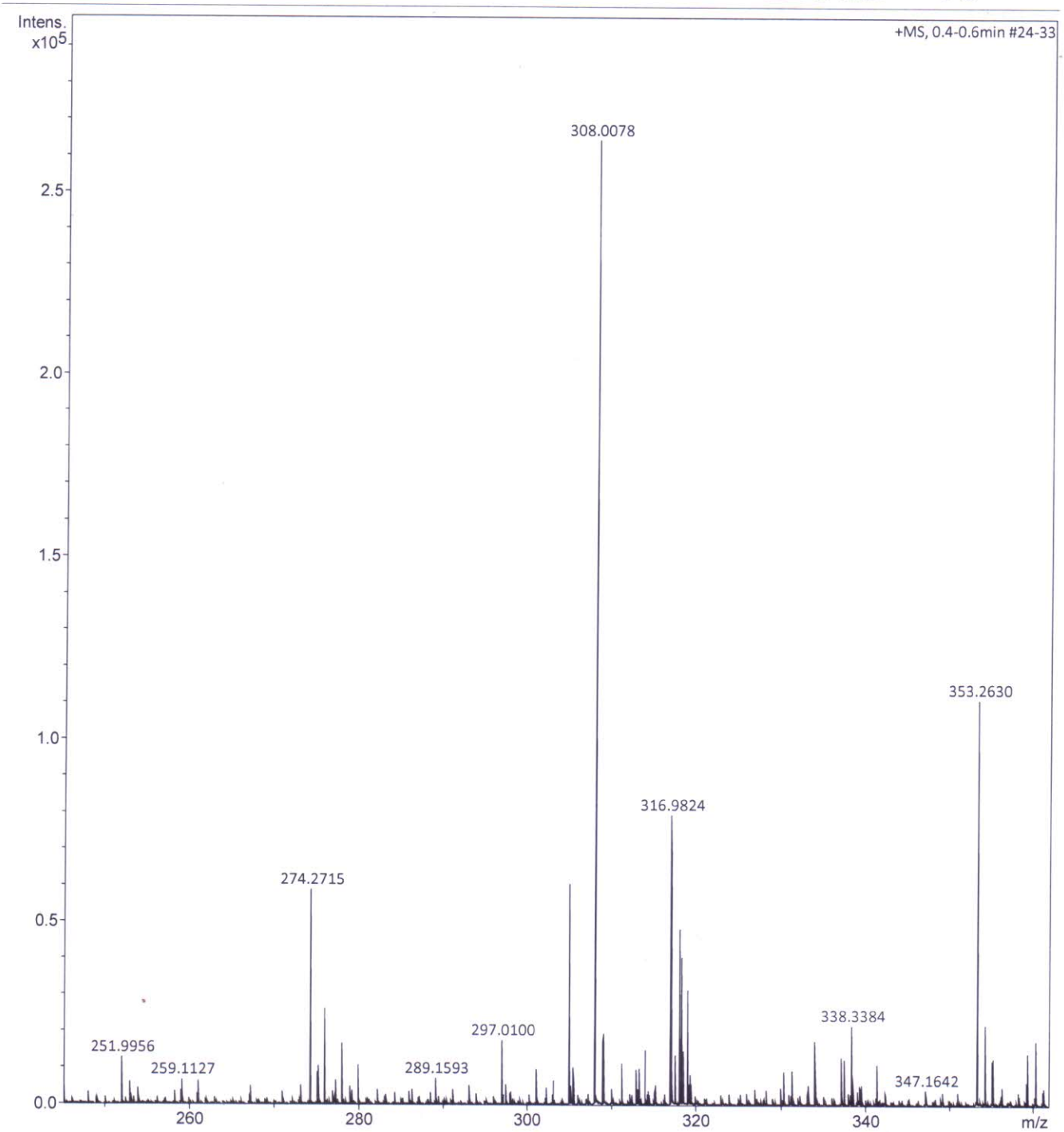
Display Report

Analysis Info

Analysis Name	D:\Data\2023-DATA\PROF. AKS\JAN\MPG-112.d	Acquisition Date	09-01-2023 16:28:33
Method	TL-P.m	Operator	UOH
Sample Name	MPG-112	Instrument	maXis 255552.10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



MPG-112.d

Bruker Compass DataAnalysis 4.2 printed: 09-01-2023 16:35:01 by: UOH Page 1 of 1