Electronic Supplementary Information
For

Design and Synthesis of Phenylene-Bridged Isoxazole and Tetrazole-1-ol Based Energetic Materials of Low Sensitivity

Sohan Lal[a], Richard J. Staples[b], Jean'ne M. Shreeve[a]*

[a]Department of Chemistry, University of Idaho, Moscow, Idaho 83844-2343

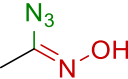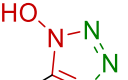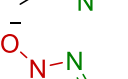[b]Department of Chemistry, Michigan State University, East Lansing, Michigan 48824
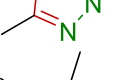
To whom correspondence should be addressed. E-mail: jshreeve@uidaho.edu. Fax: +1-208-885-6173

Table S1. Calculated Total Energy (E_0), Zero-point Energy (ZPE), values of Thermal Correction (H_T) and Enthalpy of Formation ($\Delta H_f°(g)$) of the compounds using B3LYP/6-31+G**//MP2/6-311++G** level of theory (Isodesmic)[1]

Compounds	E_0 [Hartree/Particle]	ZPE [Hartree/Particle]	H_T [Hartree/Particle]	$\Delta H_f°$ (g) kJ/mol
CH_4	-40.3796224	0.044793	0.003812	-74.60[a]
CH_3ONO_2	-319.509055	0.054251	0.005933	-137.28
CH_3N_3	-203.607680	0.050250	0.00543	296.54
(structure)	-231.5842377	0.100451	0.005346	82.90[b]
(structure)	-371.870596	0.076242	0.008229	301.80[b]
(structure)	-371.8748474	0.077582	0.007588	280.72[b]
(structure)	-371.3480753	0.065401	0.006759	108.09[b]
(structure)	-363.0455559	0.140777	0.009666	-41.26[b]

[a] Data are from Ref. [D. R. Lide ed., CRC Handbook of Chemistry and Physics, 88th Edition (Internet Version **2008**), CRC Press/Taylor and Francis, Boca Raton, FL.] [b]Obtained at G2 level. [c]Calculated according to the isodesmic equations as shown in Figure 1.

The gas phase enthalpies of formation $\Delta H_f°(g)$ were predicted using isodesmic equations as shown in Figure 1. Subsequently, their solid phase enthalpy of formation $\Delta H_f°$ (s) were calculated by using equations 6-7.[2-4]
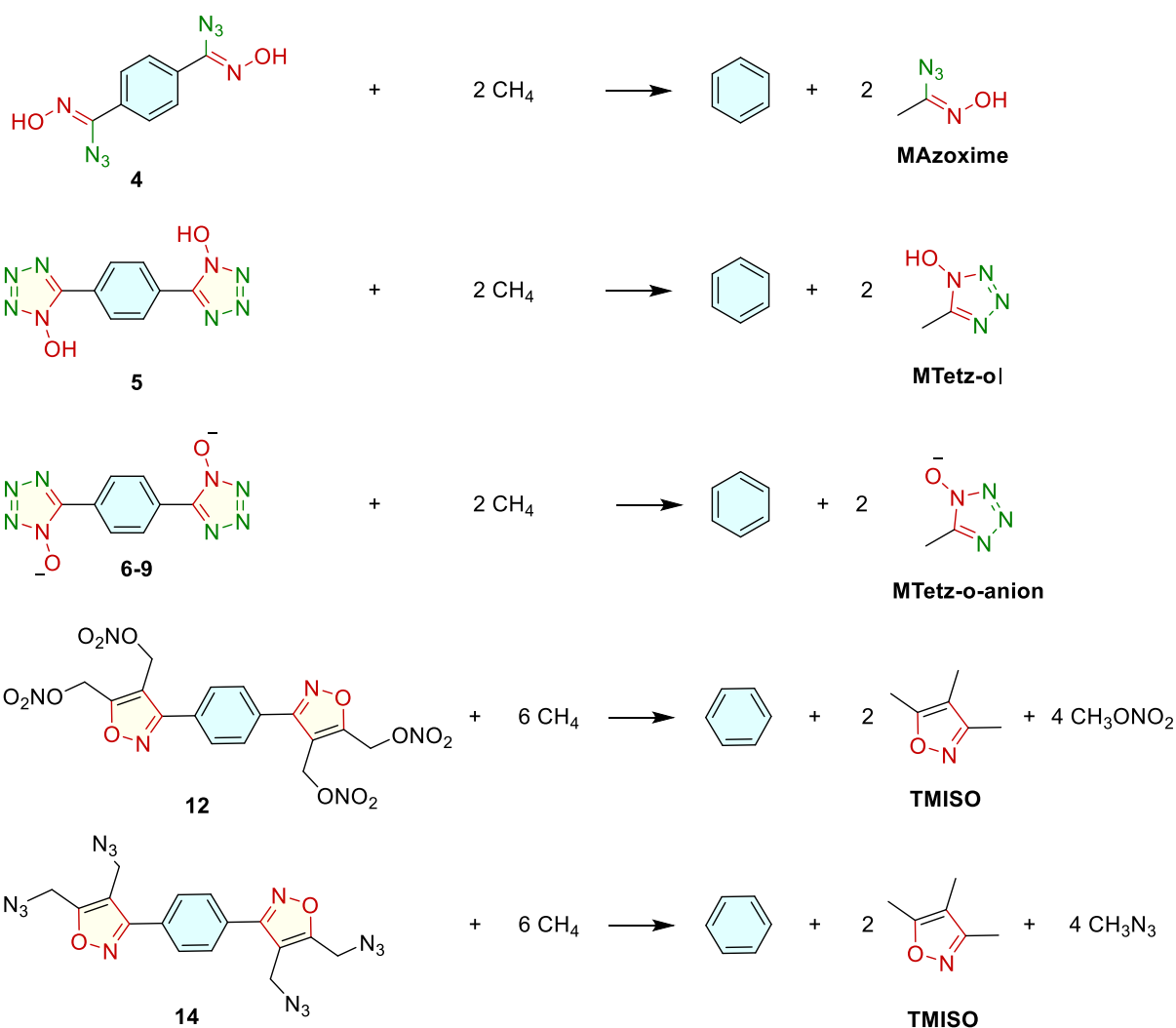
Figure 1: Isodesmic reactions for the title compounds **4, 5, 6-9, 12,** and **14**.

$\Delta H_f^\circ(g)_{\text{Compound 4}} = \Delta H_f^\circ(g)_{\text{Benzene}} + 2\Delta H_f^\circ(g)_{\text{MAzoxime}} - 2\Delta H_f^\circ(g)_{\text{Methane}}$ (1)

$\Delta H_f^\circ(g)_{\text{Compound 5}} = \Delta H_f^\circ(g)_{\text{Benzene}} + 2\Delta H_f^\circ(g)_{\text{MTetz-ol}} - 2\Delta H_f^\circ(g)_{\text{Methane}}$ (2)

$\Delta H_f^\circ(g)_{\text{Compound 6-9}} = \Delta H_f^\circ(g)_{\text{Benzene}} + 2\Delta H_f^\circ(g)_{\text{MTetz-o-anion}} - 2\Delta H_f^\circ(g)_{\text{Methane}}$ (3)

$\Delta H_f^\circ(g)_{\text{Compound 12}} = \Delta H_f^\circ(g)_{\text{Benzene}} + 2\Delta H_f^\circ(g)_{\text{TMISO}} + 4\Delta H_f^\circ(g)_{\text{Methylazide}} - 6\Delta H_f^\circ(g)_{\text{Methane}}$ (4)

$\Delta H_f^\circ(g)_{\text{Compound14}} = \Delta H_f^\circ(g)_{\text{Benzene}} + 2\Delta H_f^\circ(g)_{\text{TMISO}} + 4\Delta H_f^\circ(g)_{\text{Methylnitrate}} - 6\Delta H_f^\circ(g)_{\text{Methane}}$ (5)

$\Delta H_f^\circ(s) = \Delta H_f^\circ(g) - \Delta H_{\text{sub}}$ (6)

Where $\Delta H_f^\circ(s)$ is the solid phase enthalpy of formation, $\Delta H_f^\circ(g)$ is the gas phase enthalpy of formation and ΔH_{sub} is the enthalpy of sublimation.

The enthalpy of sublimation was calculated based on Trouton's rule according to equation 2.[3]

$\Delta H_{\text{sub}} = T \times 188/\text{Jmol}^{-1}\text{K}^{-1}$ (7)

Where, T, represents either the melting point or the decomposition temperature when no melting occurs before decomposition.

For salts, the solid-state enthalpy of formation is obtained using a Born-Haber energy cycle.[4]

Table S2. The standard enthalpies of combustion $\Delta H_{f(combust)}$ for the title compounds were calculated by following equation

$$\Delta H_{f(combust)} = \Sigma\Delta H_{f\,(products)} - \Sigma\Delta H_{f\,(reactants)} \tag{8}$$

RDX $\quad = \quad C_3H_6N_6O_6\,(s) \quad + \quad 1.5\,O_2\,(g) \quad\longrightarrow\quad 3CO_2\,(g) \; + \; 3H_2O\,(g) \; + \; 3N_2\,(g)$

TNT $\quad = \quad C_7H_5N_3O_6\,(s) \; + \; 5.25\,O_2\,(g) \quad\longrightarrow\quad 7CO_2\,(g) \; + \; 2.5H_2O\,(g) \; + \; 1.5N_2\,(g)$

HNS $\quad = \quad C_{14}H_6N_6O_{12}\,(s) \; + \; 9.5\,O_2\,(g) \quad\longrightarrow\quad 14CO_2\,(g) \; + \; 3H_2O\,(g) \; + \; 3N_2\,(g)$

4 $\quad = \quad C_8H_6N_8O_2\,(s) \; + \; 8.5\,O_2\,(g) \quad\longrightarrow\quad 8CO_2\,(g) \; + \; 3H_2O\,(g) \; + \; 4N_2\,(g)$

5 $\quad = \quad C_8H_6N_8O_2\,(s) \; + \; 8.5\,O_2\,(g) \quad\longrightarrow\quad 8CO_2\,(g) \; + \; 3H_2O\,(g) \; + \; 4N_2\,(g)$

6 $\quad = \quad C_8H_{12}N_{10}O_4\,(s) \; + \; 9\,O_2\,(g) \quad\longrightarrow\quad 8CO_2\,(g) \; + \; 6H_2O\,(g) \; + \; 5N_2\,(g)$

7 $\quad = \quad C_8H_{12}N_{10}O_2\,(s) \; + \; 10\,O_2\,(g) \quad\longrightarrow\quad 8CO_2\,(g) \; + \; 6H_2O\,(g) \; + \; 5N_2\,(g)$

8 $\quad = \quad C_8H_{14}N_{12}O_2\,(s) \; + \; 10.5\,O_2\,(g) \quad\longrightarrow\quad 8CO_2\,(g) \; + \; 7H_2O\,(g) \; + \; 6N_2\,(g)$

9 $\quad = \quad C_8H_4K_2N_8O_2\,(s) \; + \; 8\,O_2\,(g) \quad\longrightarrow\quad 8CO_2\,(g) \; + \; 2H_2O\,(g) \; + \; 4N_2\,(g)$

12 $\quad = \quad C_{16}H_{12}N_6O_{14}\,(s) \; + \; 12\,O_2\,(g) \quad\longrightarrow\quad 16CO_2\,(g) \; + \; 6H_2O\,(g) \; + \; 3N_2\,(g)$

14 $\quad = \quad C_{16}H_{12}N_{14}O_2\,(s) \; + \; 18\,O_2\,(g) \quad\longrightarrow\quad 16CO_2\,(g) \; + \; 6H_2O\,(g) \; + \; 7N_2\,(g)$

The standard enthalpy of formation for CO_2 ($\Delta H_{f\,(CO2)}$ = -393.51 kJmol^{-1}); H_2O ($\Delta H_{f\,(H2O)}$ = -243.015 kJmol^{-1}).

Table S3. Computed electrostatic potential (ESP) of RDX and TNT
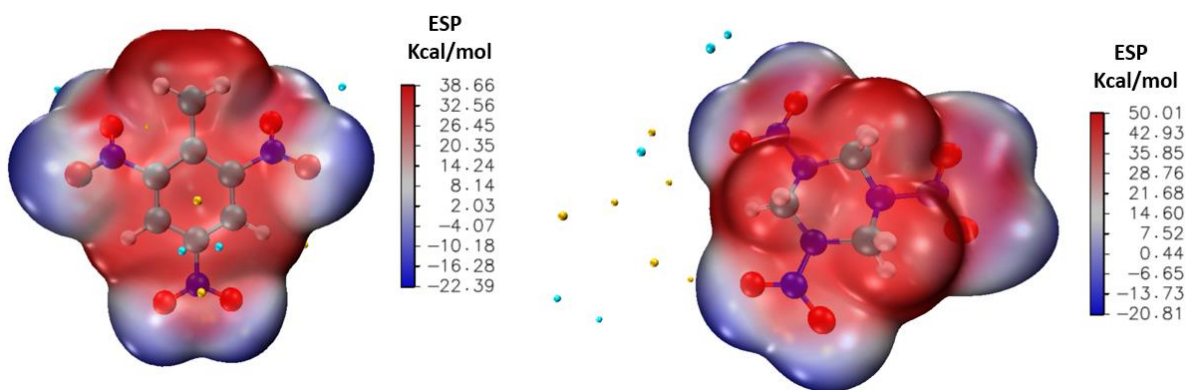
Computed electrostatic potential (ESP) maps of (a) TNT, (b) RDX. Color ranges in kcal/mol: Red, more positive; Blue, more negative and Greyer, in between positive and negative.

Table S4: Crystal data and structure refinement[5-11] for compound **12**

O_2NO ... ONO_2

12
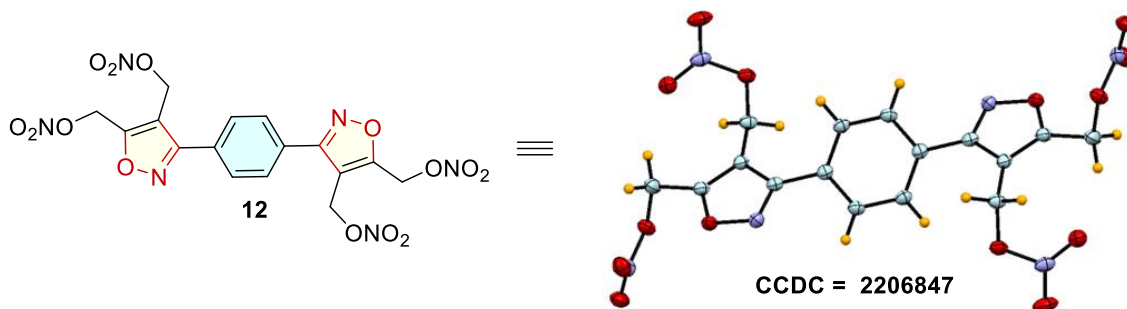
CCDC = 2206847

Compound	**12**
CCDC Number	2206847
Formula	$C_{16}H_{12}N_6O_{14}$
$D_{calc.}$/ g cm^{-3}	1.697
m/mm^{-1}	1.345
Formula Weight	512.32
Color	yellow
Shape	plate-shaped
Size/mm^3	0.23×0.13×0.02
T/K	100.00(10)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	7.58035(14)
b/Å	13.1249(3)
c/Å	10.13126(18)
a/°	90
b/°	95.9409(16)
g/°	90
V/Å^3	1002.56(3)
Z	2
Z'	0.5
Wavelength/Å	1.54184
Radiation type	Cu K$_a$
Q_{min}/°	5.535
Q_{max}/°	76.070
Measured Refl's.	11142
Indep't Refl's	2018
Refl's I≥2 s(I)	1831
R_{int}	0.0332
Parameters	194
Restraints	6
Largest Peak	0.333
Deepest Hole	-0.231
GooF	1.064
wR_2 (all data)	0.0955
wR_2	0.0924
R_1 (all data)	0.0382
R_1	0.0347

Table S5: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for **12**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
O1	6021.0(12)	5989.9(7)	1888.0(10)	22.9(2)
O2	4463.9(13)	2686.9(7)	1297.4(9)	24.0(2)
O3	7398.2(14)	2808.1(8)	1853.2(10)	30.1(3)
O4	6302.2(17)	1703.8(8)	397.8(11)	38.0(3)
O5	8004(3)	5287.2(19)	4485(2)	24.7(6)
O5B	8900(2)	5639.4(14)	3696.8(19)	25.7(6)
O6	9180(3)	6595.9(17)	3430(2)	31.3(6)
O6B	6917(3)	5450.7(16)	5165(2)	34.3(6)
O7	8970(70)	6660(30)	5540(30)	33.6(5)
O7B	8930(60)	6620(30)	5450(30)	33.6(5)
N1	4327.1(15)	6097.4(9)	1196.0(11)	21.9(3)
N2	6212.2(17)	2384.0(9)	1185.4(11)	26.0(3)
N3	8786(4)	6268(2)	4462(3)	25.3(7)
N3B	8172(4)	5923(2)	4869(3)	25.5(6)
C1	3554.1(17)	5205.7(10)	1271.6(12)	19.5(3)
C2	4697.2(17)	4487.7(10)	2007.7(13)	20.1(3)
C3	6192.4(18)	5031.3(10)	2364.1(13)	21.4(3)
C4	4296.5(18)	3415.2(10)	2372.1(13)	22.1(3)
C5	7933(2)	4773.7(11)	3116.1(15)	28.2(3)
C6	1724.6(17)	5086.4(10)	636.6(12)	19.7(3)
C7	603.2(18)	5936.9(10)	508.8(13)	21.3(3)
C8	-1101.8(18)	5850.7(10)	-122.0(13)	20.9(3)

Table S6: Anisotropic Displacement Parameters ($\times 10^4$) for **12**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	22.5(5)	16.9(5)	28.4(5)	-1.5(4)	-2.0(4)	0.0(3)
O2	29.8(5)	17.1(5)	24.1(5)	-0.5(4)	-1.4(4)	1.5(4)
O3	29.5(5)	26.4(5)	33.9(6)	-3.5(4)	1.3(4)	2.1(4)
O4	59.1(8)	24.6(6)	28.8(6)	-7.7(4)	-2.6(5)	14.7(5)
O5	29.1(12)	19.6(13)	24.8(11)	-0.5(9)	-0.9(9)	-4.6(9)
O5B	23.2(10)	26.2(11)	27.4(10)	-6.6(8)	2.0(7)	-4.2(7)
O6	30.5(12)	30.2(13)	33.2(12)	4.8(9)	2.7(9)	-6.6(9)
O6B	44.5(13)	28.6(11)	31.4(11)	-3.4(8)	12.1(9)	-6.5(9)
O7	36.6(19)	25(2)	36(2)	-9.4(12)	-9(2)	0.4(12)
O7B	36.6(19)	25(2)	36(2)	-9.4(12)	-9(2)	0.4(12)
N1	20.7(6)	19.2(6)	25.2(6)	-0.3(4)	-0.9(4)	2.0(4)
N2	36.1(7)	18.8(6)	23.0(6)	1.9(4)	2.0(5)	5.9(5)
N3	20.6(14)	24.8(16)	29.5(16)	-0.9(13)	-2.3(11)	0.0(11)
N3B	28.0(14)	21.4(16)	25.7(14)	-2.1(12)	-4.0(11)	4.4(11)
C1	23.1(7)	16.8(6)	19.0(6)	-1.3(5)	3.4(5)	2.0(5)
C2	22.4(6)	18.3(7)	19.4(6)	-1.7(5)	1.2(5)	2.5(5)
C3	26.0(7)	16.3(6)	21.2(6)	-2.0(5)	-0.1(5)	2.4(5)
C4	27.2(7)	18.4(7)	20.3(6)	0.5(5)	1.3(5)	1.1(5)
C5	28.3(7)	21.1(7)	32.9(8)	-4.7(6)	-8.5(6)	2.2(5)
C6	22.0(6)	18.8(6)	18.1(6)	1.8(5)	2.3(5)	1.0(5)
C7	25.4(7)	15.6(6)	22.8(6)	-0.1(5)	2.1(5)	0.4(5)
C8	23.5(6)	17.1(6)	21.9(6)	1.7(5)	1.8(5)	3.5(5)

Table S7: Bond Angles in for **compound 12**.

Atom	Atom	Atom	Angle/°
C3	O1	N1	108.74(10)
N2	O2	C4	113.67(10)
N3	O5	C5	111.01(19)
N3B	O5B	C5	108.9(2)
C1	N1	O1	105.75(10)
O3	N2	O2	118.77(11)
O4	N2	O2	112.55(12)
O4	N2	O3	128.68(13)
O6	N3	O5	118.9(2)
O6	N3	O7	128.3(18)
O7	N3	O5	112.8(18)
O6B	N3B	O5B	117.6(3)
O7B	N3B	O5B	114.0(17)
O7B	N3B	O6B	128.4(17)
N1	C1	C2	111.46(12)
N1	C1	C6	118.27(11)
C2	C1	C6	130.26(12)
C1	C2	C4	128.27(12)
C3	C2	C1	103.64(12)
C3	C2	C4	127.98(12)
O1	C3	C2	110.40(12)
O1	C3	C5	116.18(12)
C2	C3	C5	133.39(13)
O2	C4	C2	113.32(10)
O5B	C5	C3	114.49(13)
C3	C5	O5	107.92(13)
C7	C6	C1	119.32(12)
C81	C6	C1	121.44(12)
C81	C6	C7	119.21(12)
C8	C7	C6	120.36(13)
C7	C8	C61	120.42(12)

Table S8: Bond Lengths in Å for compound **12**.

Atom	Atom	Length/Å
O1	N1	1.4050(14)
O1	C3	1.3488(16)
O2	N2	1.3994(16)
O2	C4	1.4642(16)
O3	N2	1.2042(16)
O4	N2	1.2039(16)
O5	N3	1.419(4)
O5	C5	1.538(3)
O5B	N3B	1.410(3)
O5B	C5	1.444(2)

Atom	Atom	Length/Å
O6	N3	1.197(4)
O6B	N3B	1.200(4)
O7	N3	1.199(16)
O7B	N3B	1.199(15)
N1	C1	1.3146(18)
C1	C2	1.4357(18)
C1	C6	1.4755(18)
C2	C3	1.3562(19)
C2	C4	1.4945(18)
C3	C5	1.4923(19)
C6	C7	1.4010(19)
C6	C8[1]	1.3987(19)
C7	C8	1.3860(19)

Table S9: Torsion Angles in ° for **compound 12**.

Atom	Atom	Atom	Atom	Angle/°
O1	N1	C1	C2	0.03(14)
O1	N1	C1	C6	179.43(10)
O1	C3	C5	O5	74.45(17)
O1	C3	C5	O5B	24.18(19)
N1	O1	C3	C2	0.78(14)
N1	O1	C3	C5	179.16(11)
N1	C1	C2	C3	0.42(15)
N1	C1	C2	C4	176.88(12)
N1	C1	C6	C7	-28.19(18)
N1	C1	C6	C8[1]	149.78(12)
N2	O2	C4	C2	81.13(13)
N3	O5	C5	C3	-91.6(2)
N3B	O5B	C5	C3	78.8(2)
C1	C2	C3	O1	-0.72(14)
C1	C2	C3	C5	-178.72(15)
C1	C2	C4	O2	81.32(16)
C1	C6	C7	C8	177.92(11)
C2	C1	C6	C7	151.07(13)
C2	C1	C6	C8[1]	-30.9(2)
C2	C3	C5	O5	-107.64(18)
C2	C3	C5	O5B	-157.91(16)
C3	O1	N1	C1	-0.48(13)
C3	C2	C4	O2	-103.05(15)
C4	O2	N2	O3	-7.62(16)
C4	O2	N2	O4	172.26(11)
C4	C2	C3	O1	-177.19(12)
C4	C2	C3	C5	4.8(2)
C5	O5	N3	O6	4.3(3)
C5	O5	N3	O7	-175(3)
C5	O5B	N3B	O6B	-1.8(3)
C5	O5B	N3B	O7B	178(3)
C6	C1	C2	C3	-178.88(13)

Atom	Atom	Atom	Atom	Angle/°
C6	C1	C2	C4	-2.4(2)
C6	C7	C8	C6[1]	0.1(2)
C8[1]	C6	C7	C8	-0.1(2)

Table S10: Hydrogen Fractional Atomic Coordinates ($\times10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2\times10^3$) for **compound 12**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	Z	U_{eq}
H4A	5114.13	3212.6	3153.54	26
H4B	3072.68	3383.79	2629.07	26
H5AA	8917.03	5023.07	2632.16	34
H5AB	8050.15	4026	3220.12	34
H5BC	7723.38	4289.38	3832.7	34
H5BD	8678.22	4423.49	2509.64	34
H7	1013.81	6576.32	856.54	26
H8	-1852.36	6431.75	-205.52	25

Table S11: Atomic Occupancies for all atoms that are not fully occupied in **compound 12**.

Atom	Occupancy
O5	0.475(3)
O5B	0.525(3)
O6	0.475(3)
O6B	0.525(3)
O7	0.475(3)
O7B	0.525(3)
N3	0.475(3)
N3B	0.525(3)
H5AA	0.475(3)
H5AB	0.475(3)
H5BC	0.525(3)
H5BD	0.525(3)

Figure S2. FTIR-Spectrum of Compound **2**

Figure S3. ^{1}H NMR Spectrum of Compound **2**

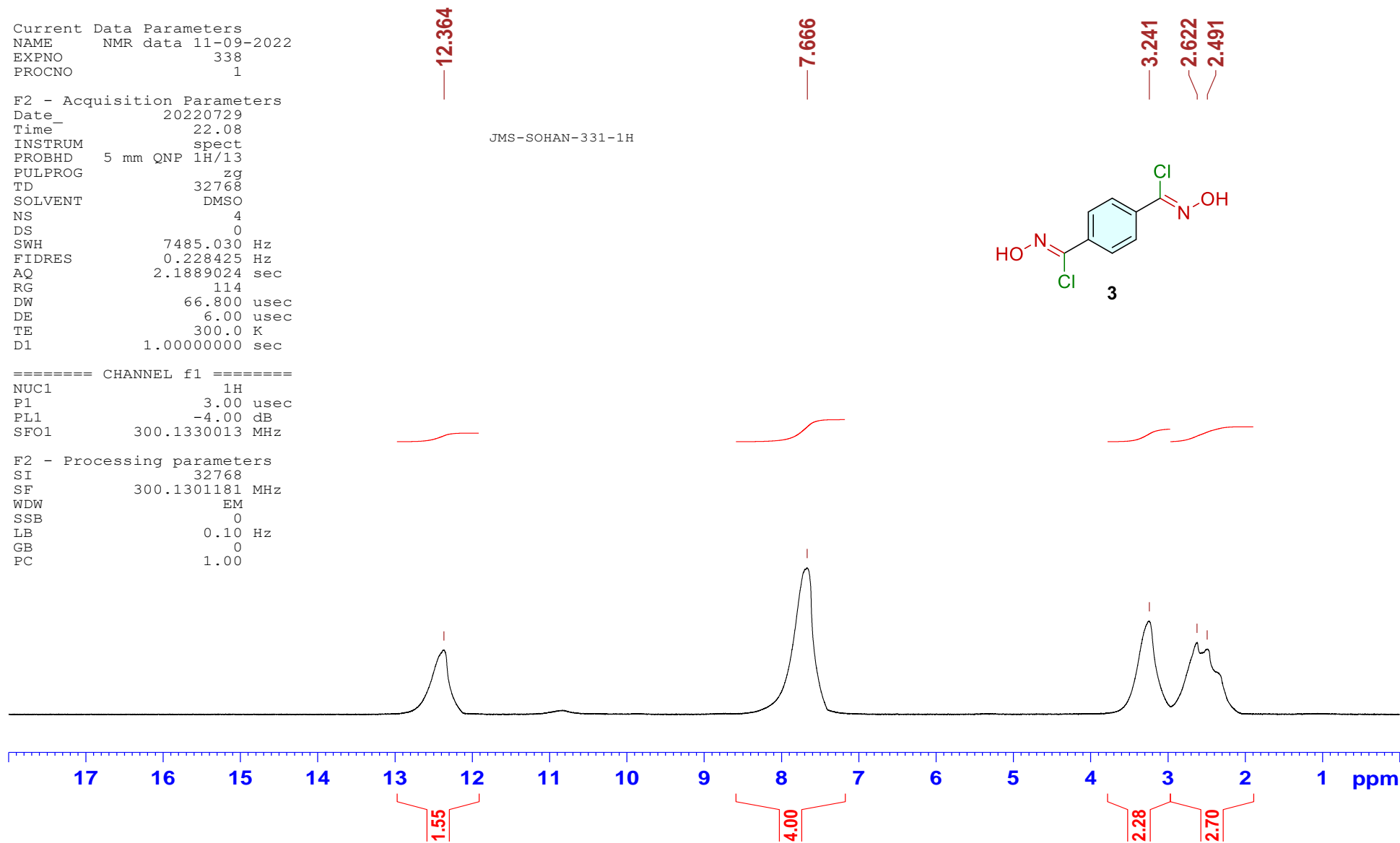**Figure S4.** ^{13}C NMR Spectrum of Compound **2**

Current Data Parameters
NAME   DEPT135
EXPNO   94
PROCNO   1

F2 - Acquisition Parameters
Date_   20220727
Time   16.45
INSTRUM   spect
PROBHD   5 mm QNP 1H/13
PULPROG   dept135
TD   32768
SOLVENT   DMSO
NS   8
DS   16
SWH   19960.080 Hz
FIDRES   0.609133 Hz
AQ   0.8208384 sec
RG   18390.4
DW   25.050 usec
DE   6.00 usec
TE   300.0 K
CNST2   140.0000000
D1   2.00000000 sec
d2   0.00357143 sec
d12   0.00002000 sec
DELTA   0.00000891 sec

======== CHANNEL f1 ========
NUC1   13C
P1   7.00 usec
p2   14.00 usec
PL1   -5.00 dB
SFO1   75.4760505 MHz

======== CHANNEL f2 ========
CPDPRG[2   waltz16
NUC2   1H
P3   6.10 usec
p4   12.20 usec
PCPD2   100.00 usec
PL2   -6.00 dB
PL12   18.54 dB
SFO2   300.1312005 MHz

F2 - Processing parameters
SI   32768
SF   75.4677765 MHz
WDW   EM
SSB   0
LB   1.00 Hz
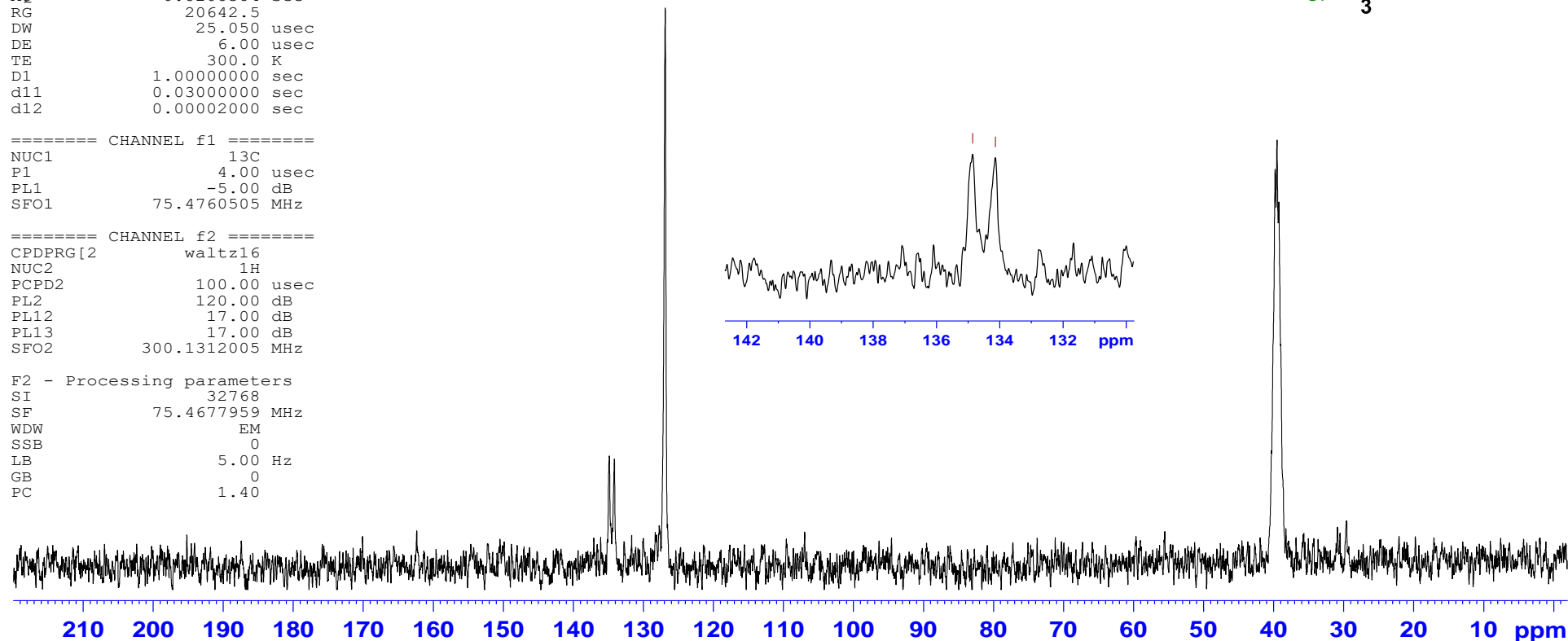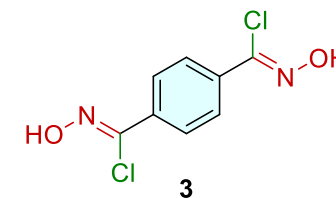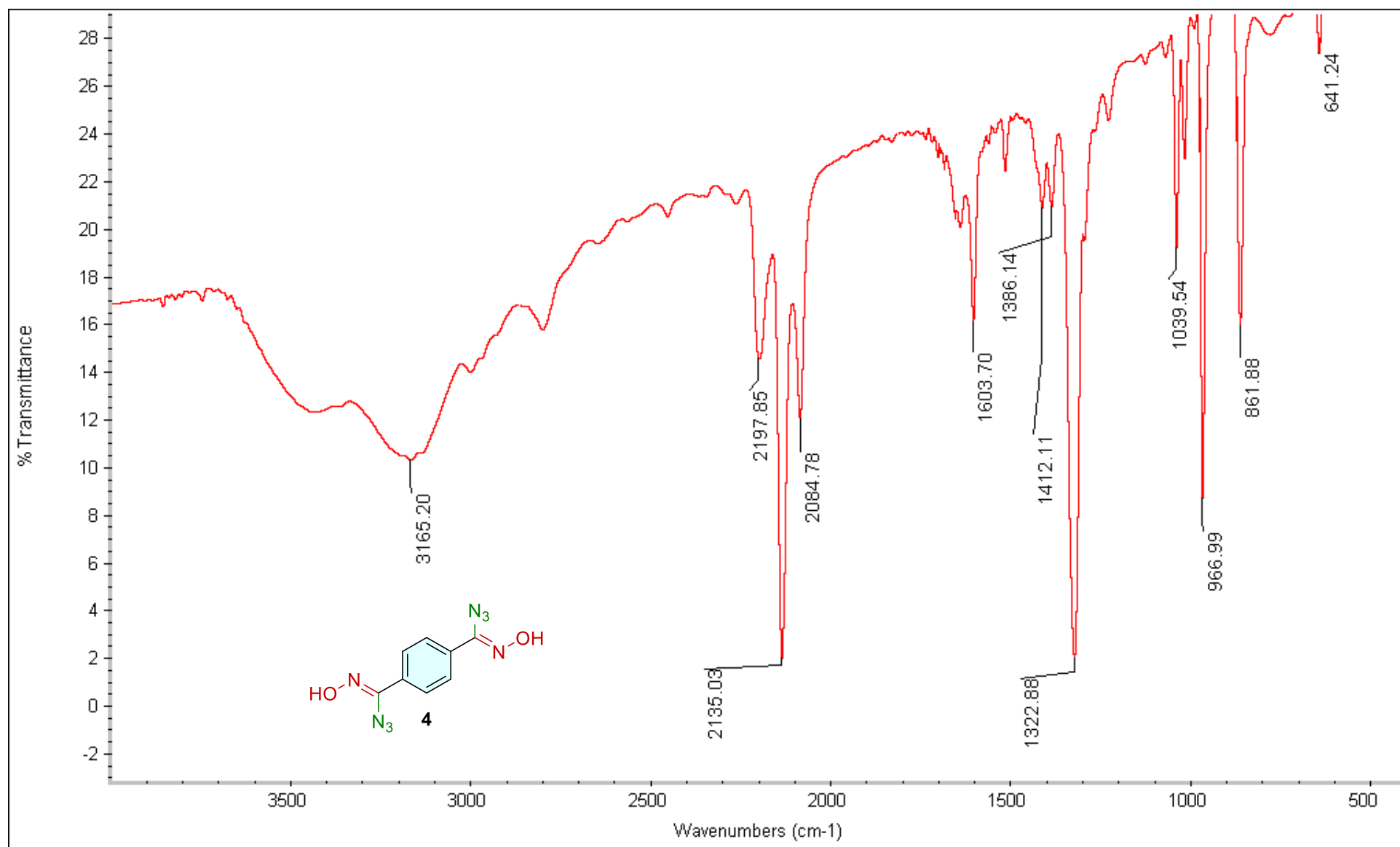GB   0
PC   1.40

147.90

126.80

JMS-SOHAN-326R-DEPT135

2

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
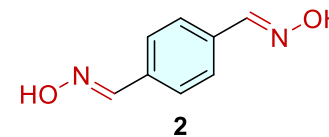
Figure S5. ^{13}C-DEPT135 NMR Spectrum of Compound **2**

Figure S6. DSC of compound **2** at 5 °C min^{-1}

Figure S7. FTIR-Spectrum of Compound **3**

Figure S8. ^{1}H NMR Spectrum of Compound **3**

Figure S9. ^{13}C NMR Spectrum of Compound **3**

Figure S10. FTIR-Spectrum of Compound **4**

Figure S11. ^{1}H NMR Spectrum of Compound **4**

Figure S12. ^{13}C NMR Spectrum of Compound **4**

Sample: SOHAN-336 at 5°C
Size: 0.1000 mg
Method: Ramp
Comment: Cell constant calibration

DSC

File: C:...\DSC\SOHAN\SOHAN-336 at 5°C.001
Operator: SOHAN
Run Date: 11-Aug-2022 16:15
Instrument: DSC Q2000 V24.11 Build 124

167.07°C

249614J/g

4

Exo Up

Universal V4.5A TA Instruments

Figure S13. DSC of compound **4** at 5 °C min^{-1}

Figure S14. TGA of compound **4** at 5 °C min^{-1}

Figure S15. FTIR-Spectrum of Compound **5**

Figure S16. ^{1}H NMR Spectrum of Compound **5**

Figure S17. ^{13}C NMR Spectrum of Compound **5**

Figure S18. ^{13}C-DEPT135 NMR Spectrum of Compound **5**

Sample: SOHAN-341 at 5°C
Size: 0.1000 mg
Method: Ramp
Comment: Cell constant calibration

DSC

File: C:...\DSC\SOHAN\SOHAN-341 at 5°C.001
Operator: SOHAN
Run Date: 21-Aug-2022 20:21
Instrument: DSC Q2000 V24.11 Build 124

Figure S19. DSC of compound **5** at 5 °C min^{-1}

Figure S20. TGA of compound **5** at 5 °C min^{-1}

Figure S21. FTIR-Spectrum of Compound **6**

Figure S22. ^{1}H NMR Spectrum of Compound **6**

Figure S23. ^{13}C NMR Spectrum of Compound **6**
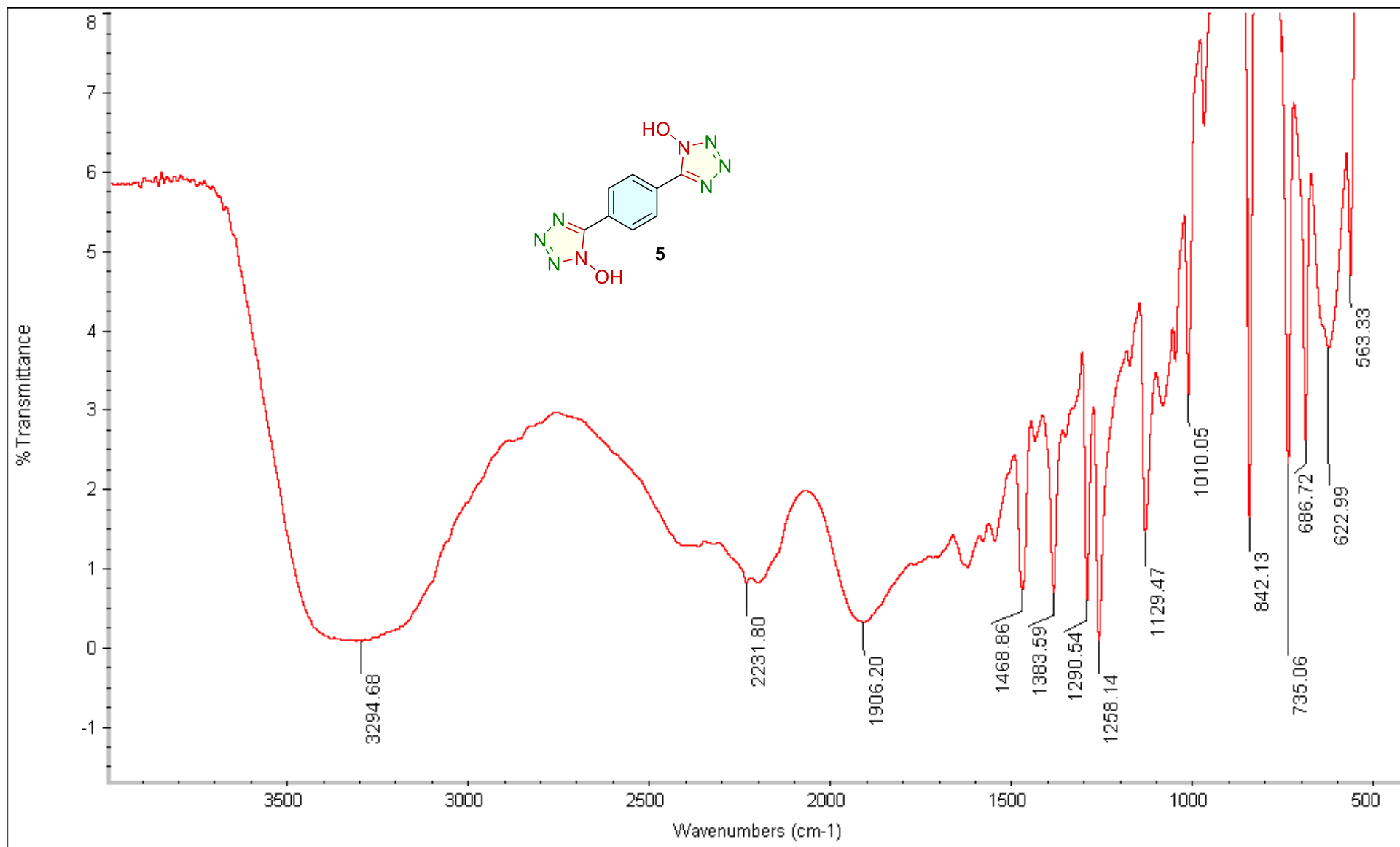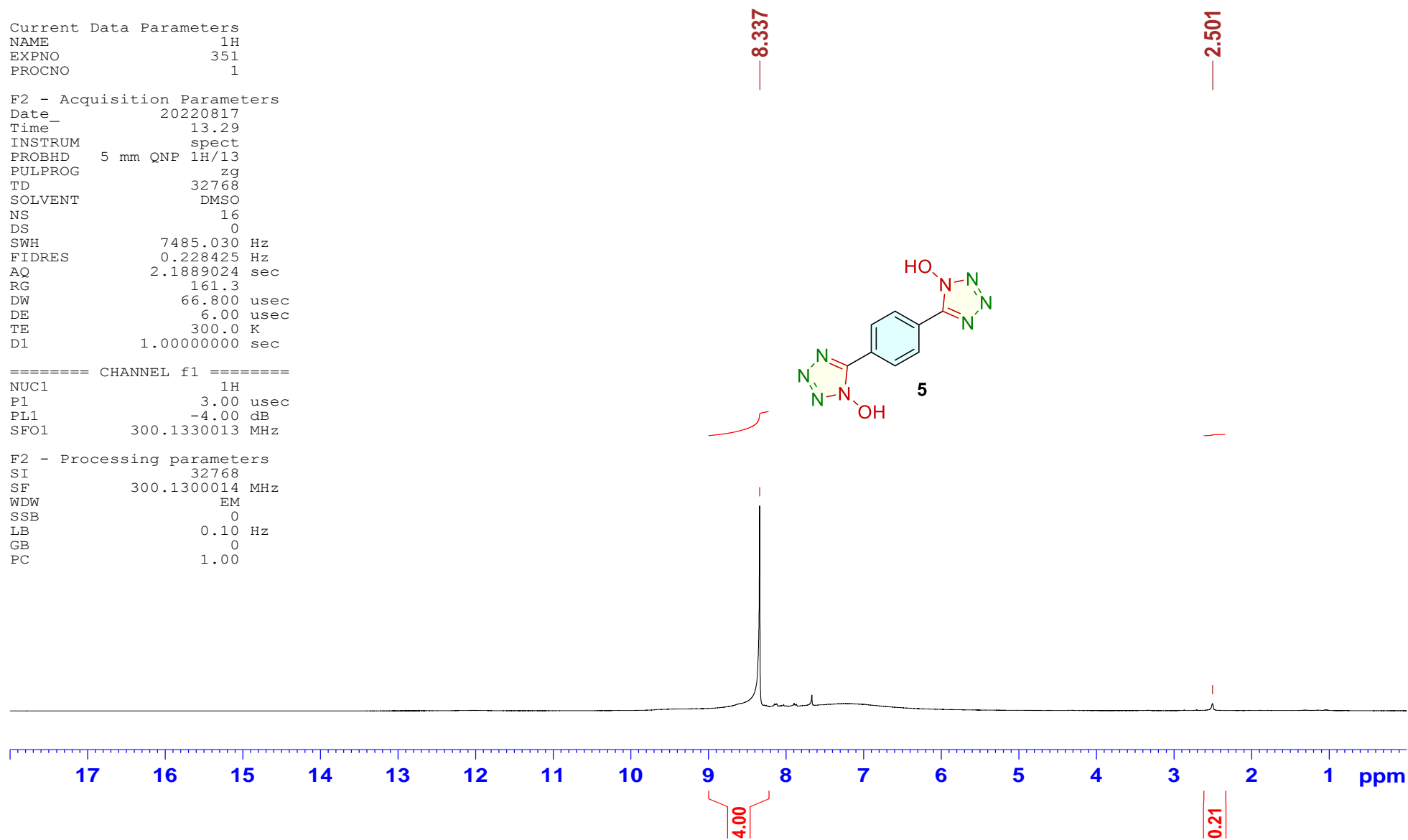
Current Data Parameters
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EXPNO   105
PROCNO   1

F2 - Acquisition Parameters
Date_   20220820
Time   11.52
INSTRUM   spect
PROBHD   5 mm QNP 1H/13
PULPROG   dept135
TD   32768
SOLVENT   DMSO
NS   36
DS   16
SWH   19960.080 Hz
FIDRES   0.609133 Hz
AQ   0.8208384 sec
RG   18390.4
DW   25.050 usec
DE   6.00 usec
TE   300.0 K
CNST2   140.0000000
D1   2.00000000 sec
d2   0.00357143 sec
d12   0.00002000 sec
DELTA   0.00000891 sec

======== CHANNEL f1 ========
NUC1   13C
P1   7.00 usec
p3   14.00 usec

======== CHANNEL f2 ========
CPDPRG[2   waltz16
NUC2   1H
P3   6.10 usec
p4   12.20 usec
PCPD2   100.00 usec
PL2   -6.00 dB
PL12   18.54 dB
SFO2   300.1312005 MHz

F2 - Processing parameters
SI   32768
SF   75.4677790 MHz
WDW   EM
SSB   0
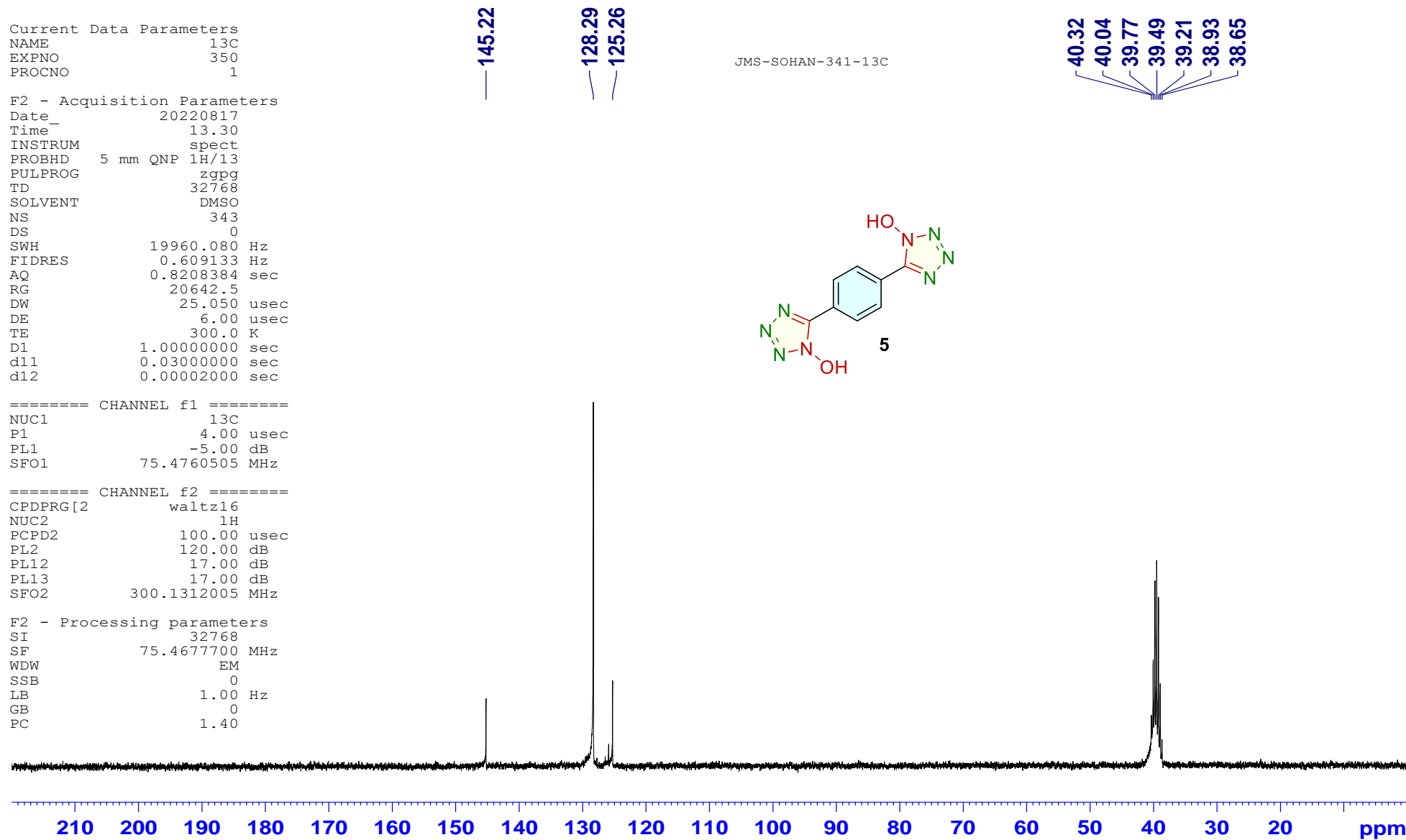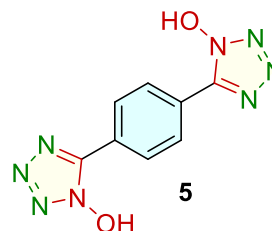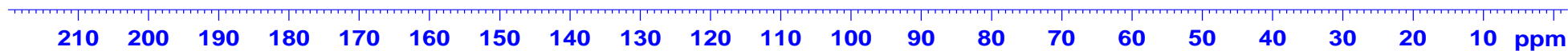LB   1.00 Hz
GB   0
PC   1.40

125.79

JMS-SOHAN-349-DEPT135
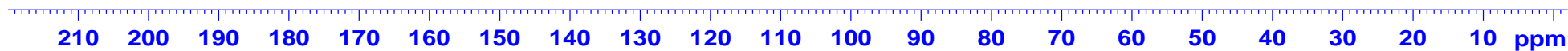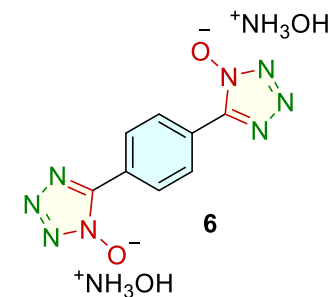
Figure S24. ^{13}C-DEPT135 NMR Spectrum of Compound **6**

Figure S25. ^{15}N NMR Spectrum of Compound **6** in DMSO-d$_6$ (at 50.70 MHz)

Figure S26. DSC of compound **6** at 5 °C min^{-1}

Figure S27. TGA of compound **6** at 5 °C min^{-1}

Figure S28. FTIR-Spectrum of Compound **7**

Figure S29. ^{1}H NMR Spectrum of Compound **7**

Figure S30. ^{13}C NMR Spectrum of Compound **7**

Figure S31. DSC of compound 7 at 5 °C min^{-1}

Figure S32. TGA of compound **7** at 5 °C min^{-1}

Figure S33. FTIR-Spectrum of Compound **8**

Figure S34. ^{1}H NMR Spectrum of Compound **8**

Figure S35. ^{13}C NMR Spectrum of Compound **8**

Figure S36. ^{13}C-DEPT135 NMR Spectrum of Compound **8**

15N{1H}_5865   Sohan 352

Current Data Parameters
NAME   New folder
EXPNO   5865
PROCNO   1

F2 - Acquisition Parameters
Date_   20220922
Time   10.16
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgig
TD   16248
SOLVENT   DMSO
NS   635
DS   0
SWH   34722.223 Hz
FIDRES   2.137015 Hz
AQ   0.2339712 sec
RG   27.83
DW   14.400 usec
DE   8.00 usec
TE   303.2 K
D1   10.00000000 sec
D11   0.03000000 sec
TD0   10240

======= CHANNEL f1 ========
SFO1   50.6963210 MHz
NUC1   15N
P1   12.00 usec
PLW1   155.00000000 W

======= CHANNEL f2 ========
SFO2   500.1920008 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   80.00 usec
PLW2   26.00000000 W
PLW12   0.27649999 W

F2 - Processing parameters
SI   32768
SF   50.7031345 MHz
WDW   EM
SSB   0
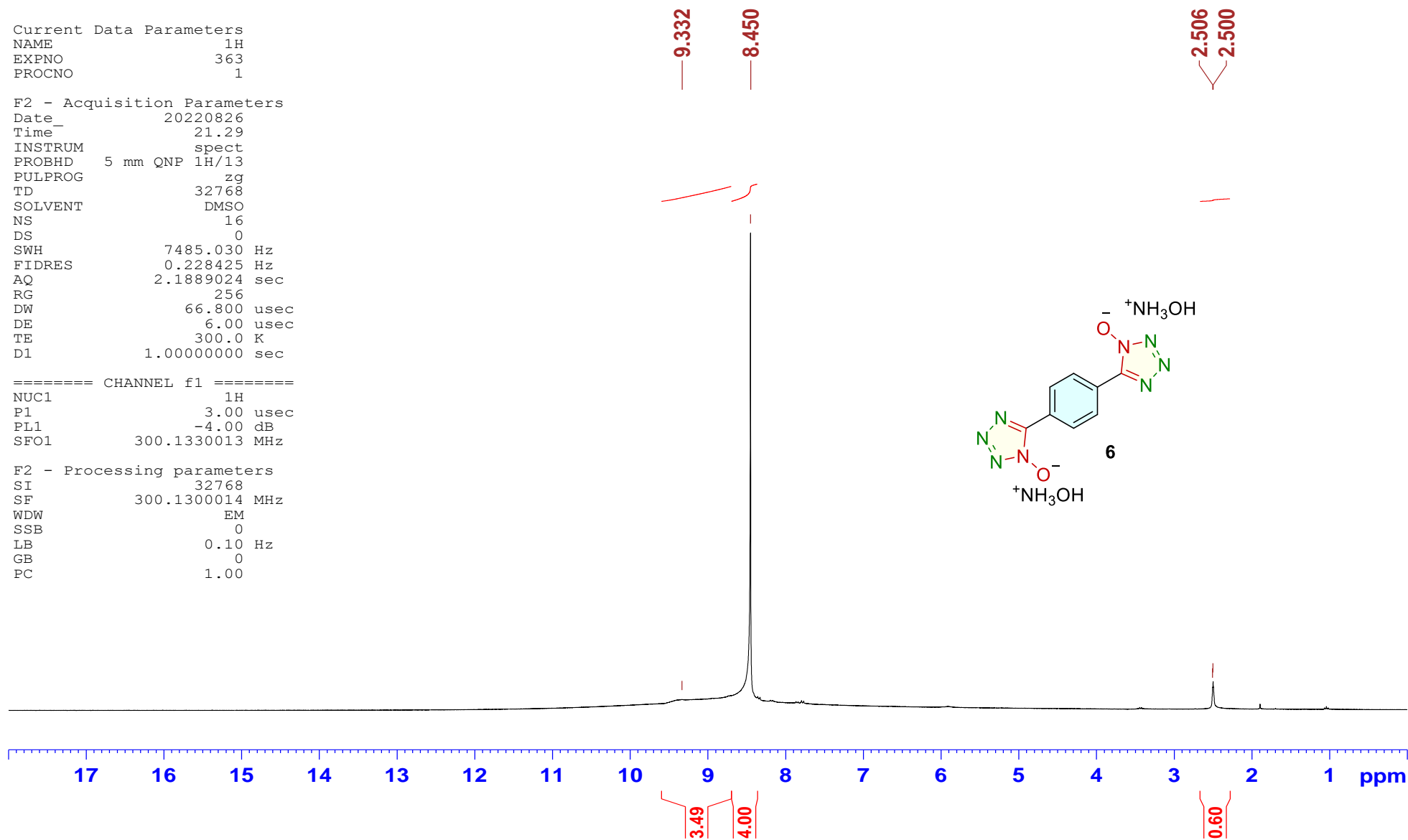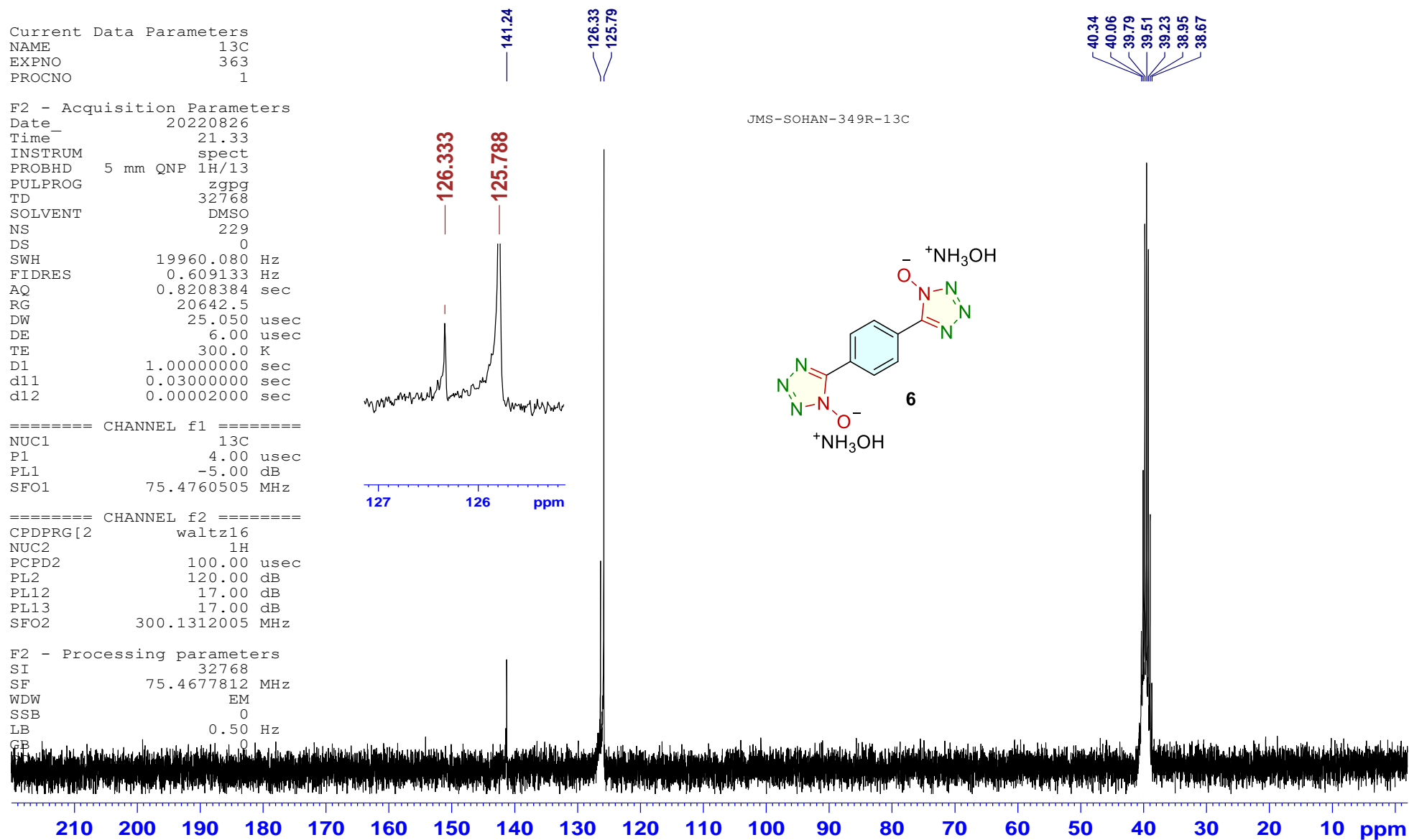LB   5.00 Hz
GB   0
PC   0.20

−14.91
−15.50
−60.41
−84.56
−108.29
−331.07

−14.907
−15.495

−15   ppm

150   100   50   0   −50   −100   −150   −200   −250   −300   −350   −400   ppm
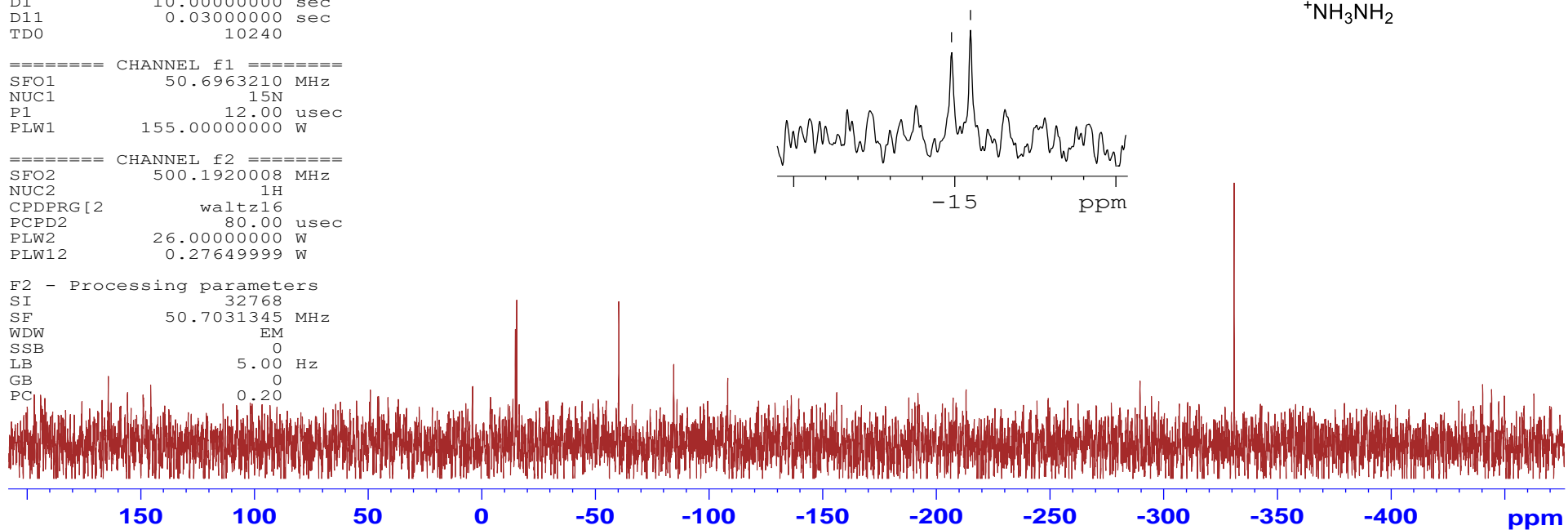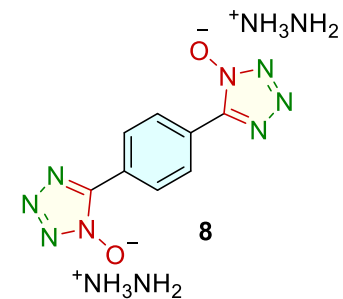
Figure S37. ^{15}N NMR Spectrum of Compound **8** in DMSO-d_6 (at 50.70 MHz)
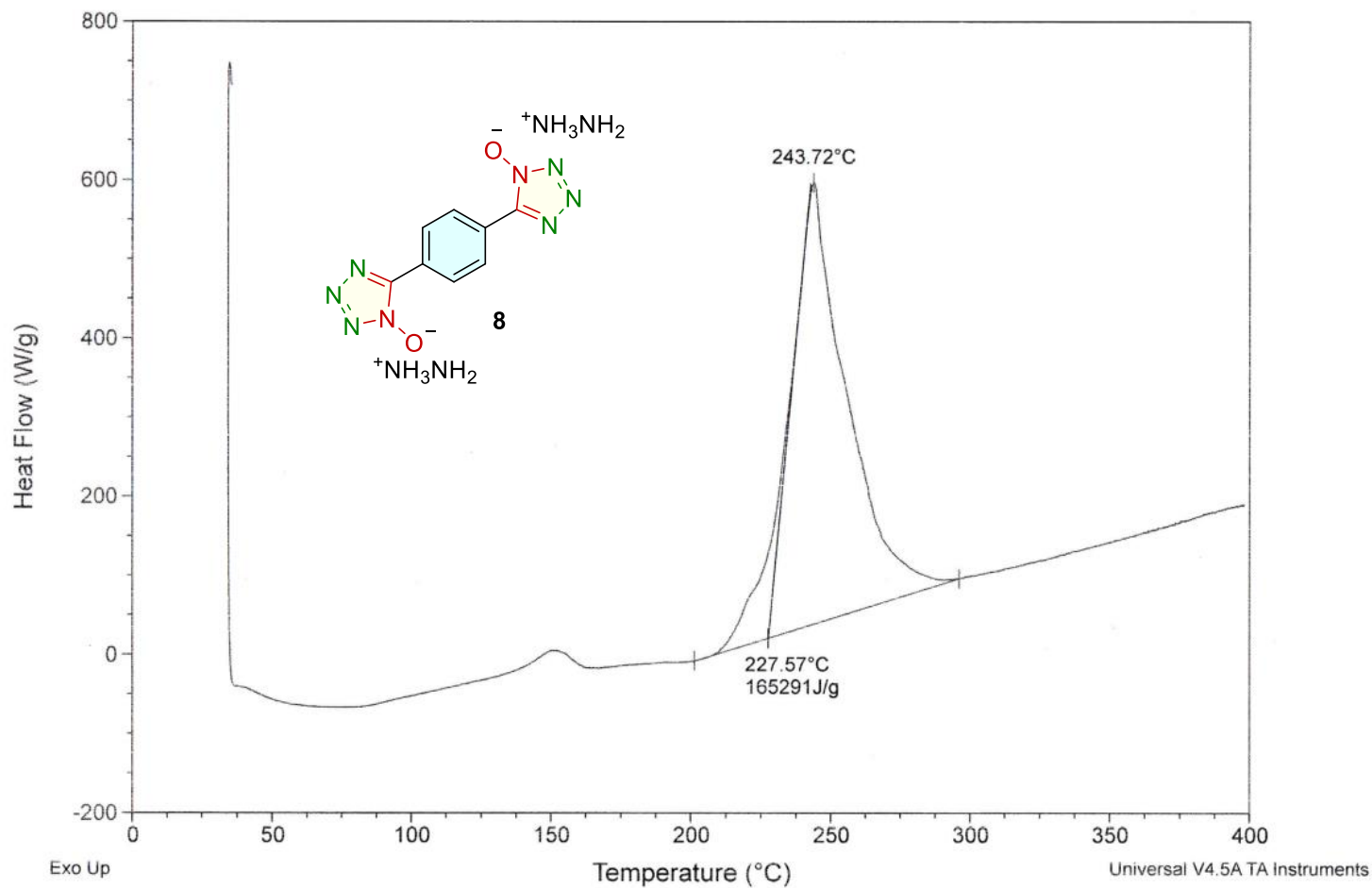
Figure S38. DSC of compound **8** at 5 °C min^{-1}
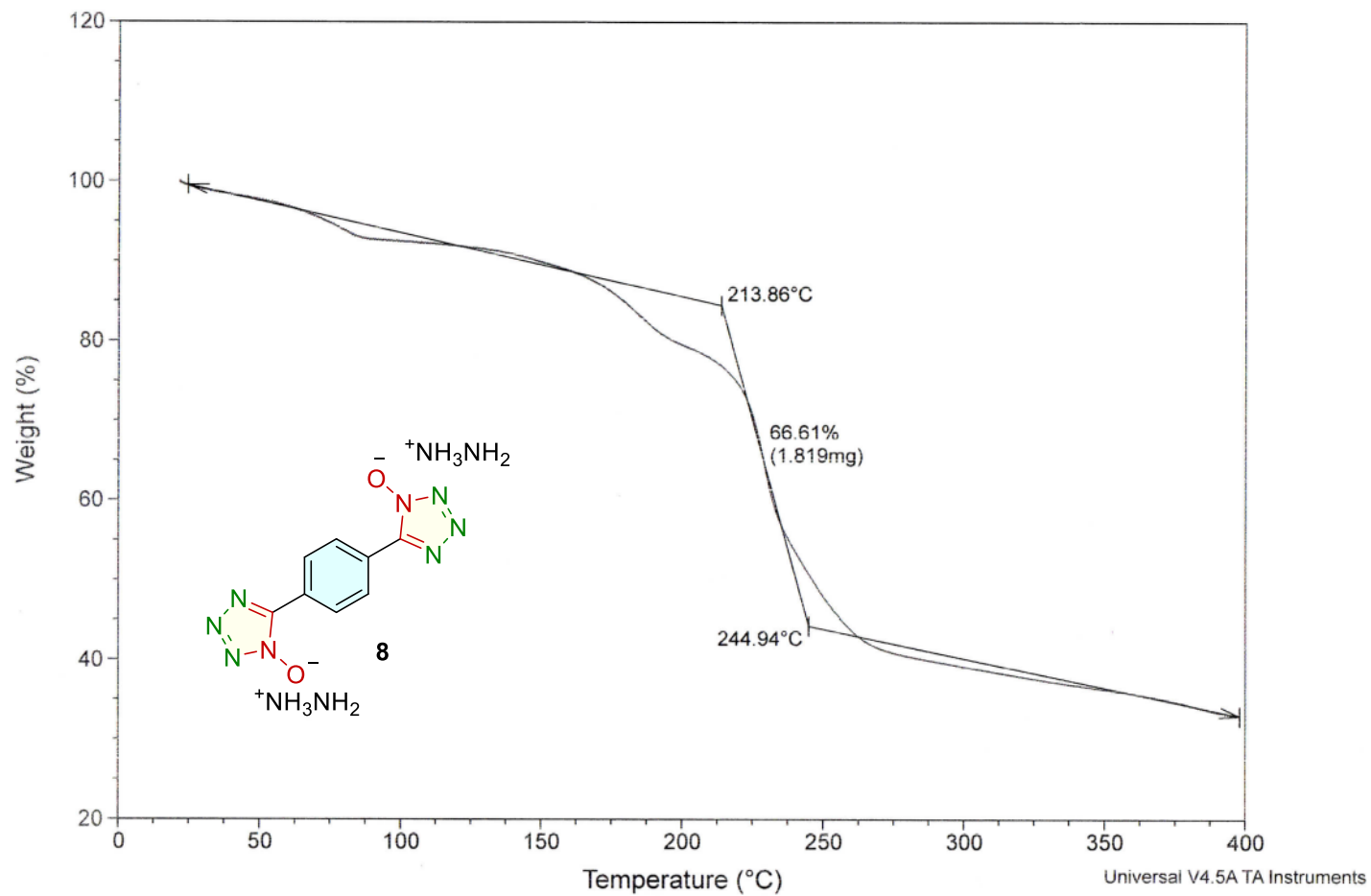
Figure S39. TGA of compound **8** at 5 °C min^{-1}
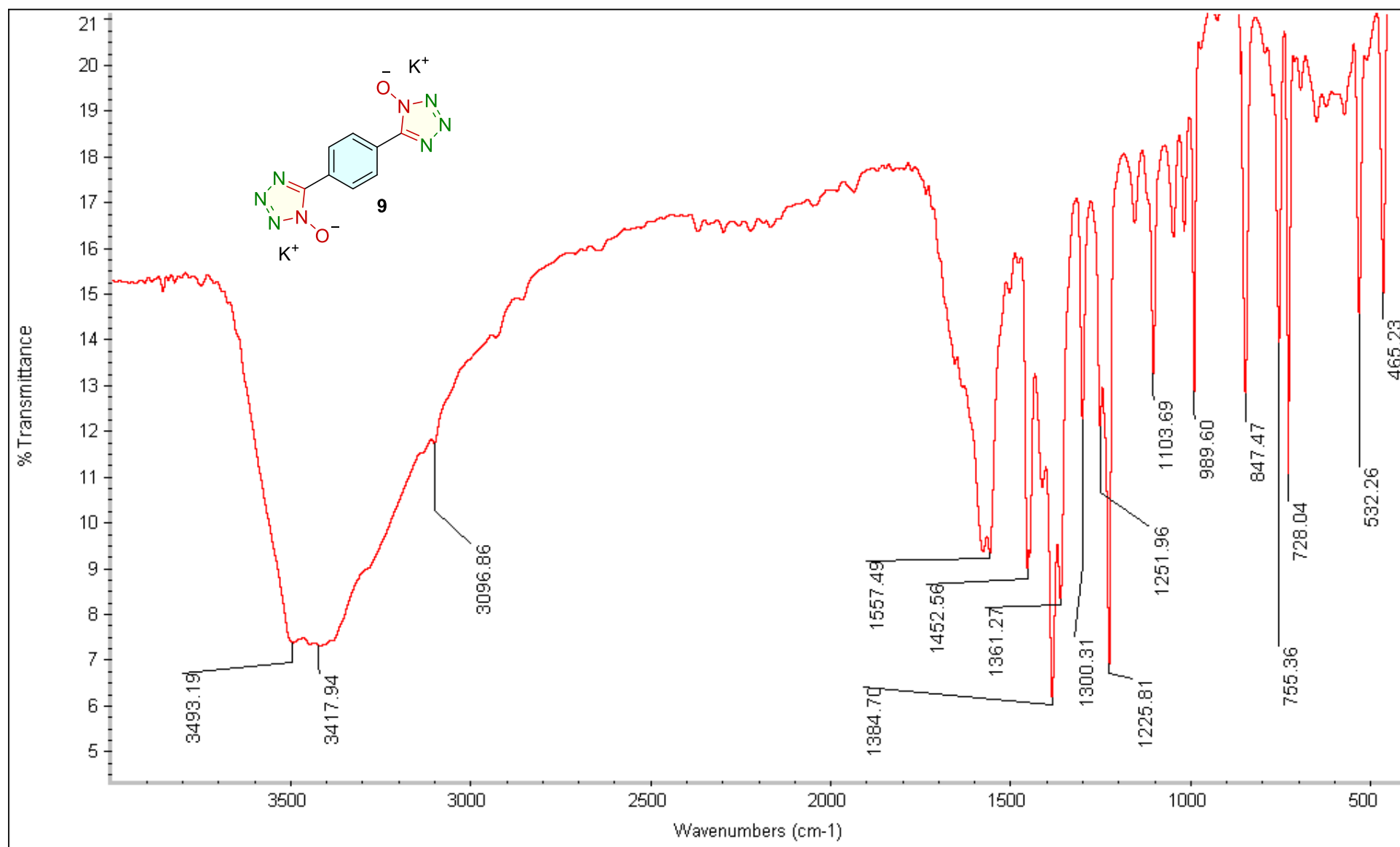
Figure S40. FTIR-Spectrum of Compound **9**

Figure S41. ^{1}H NMR Spectrum of Compound **9**

JMS-SOHAN-353-13C

140.00

126.73
124.79

40.34
40.07
39.79
39.51
39.23
38.96
38.68

Figure S42. ^{13}C NMR Spectrum of Compound **9**
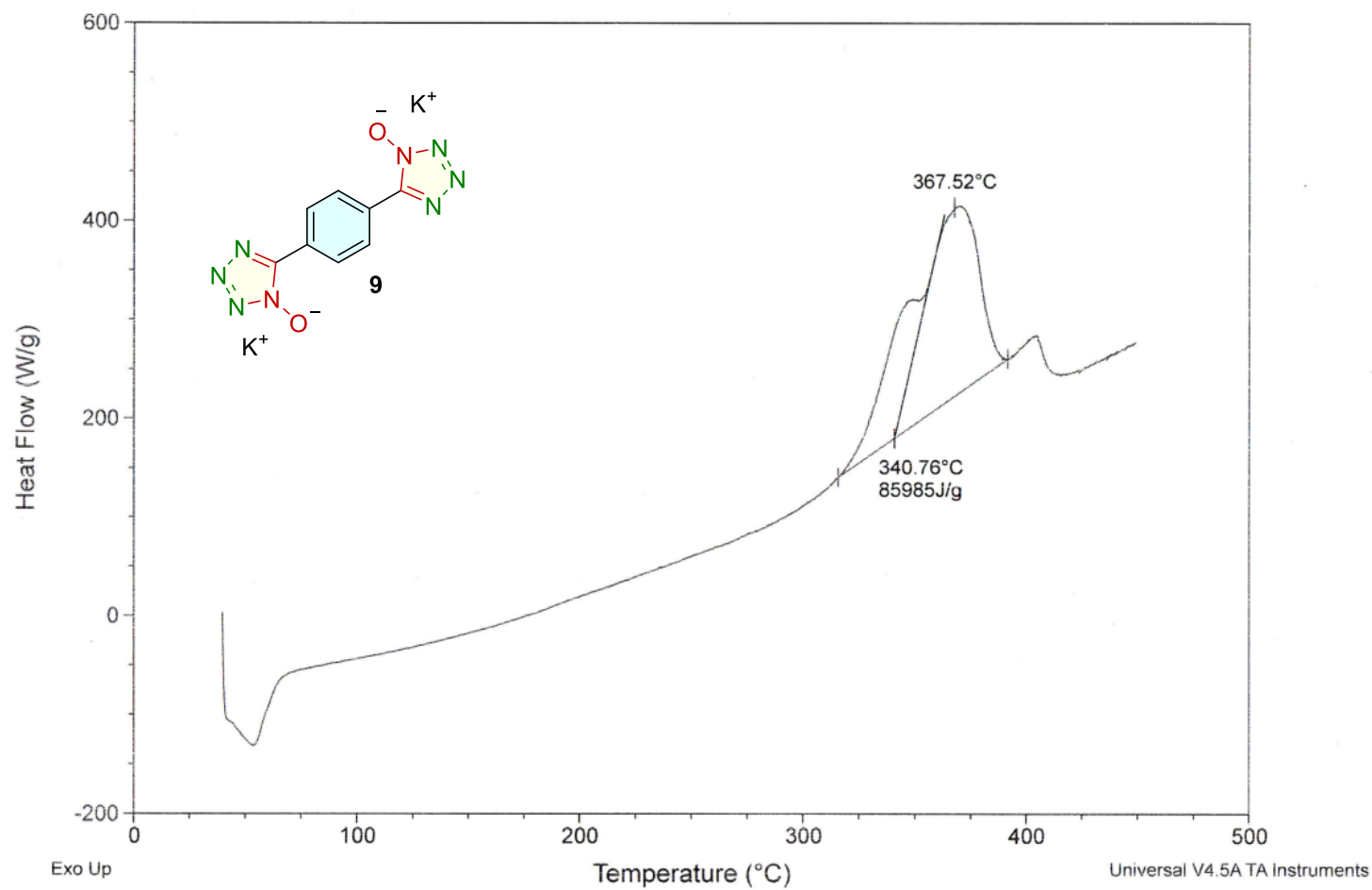
Figure S43. DSC of compound **9** at 5 °C min^{-1}
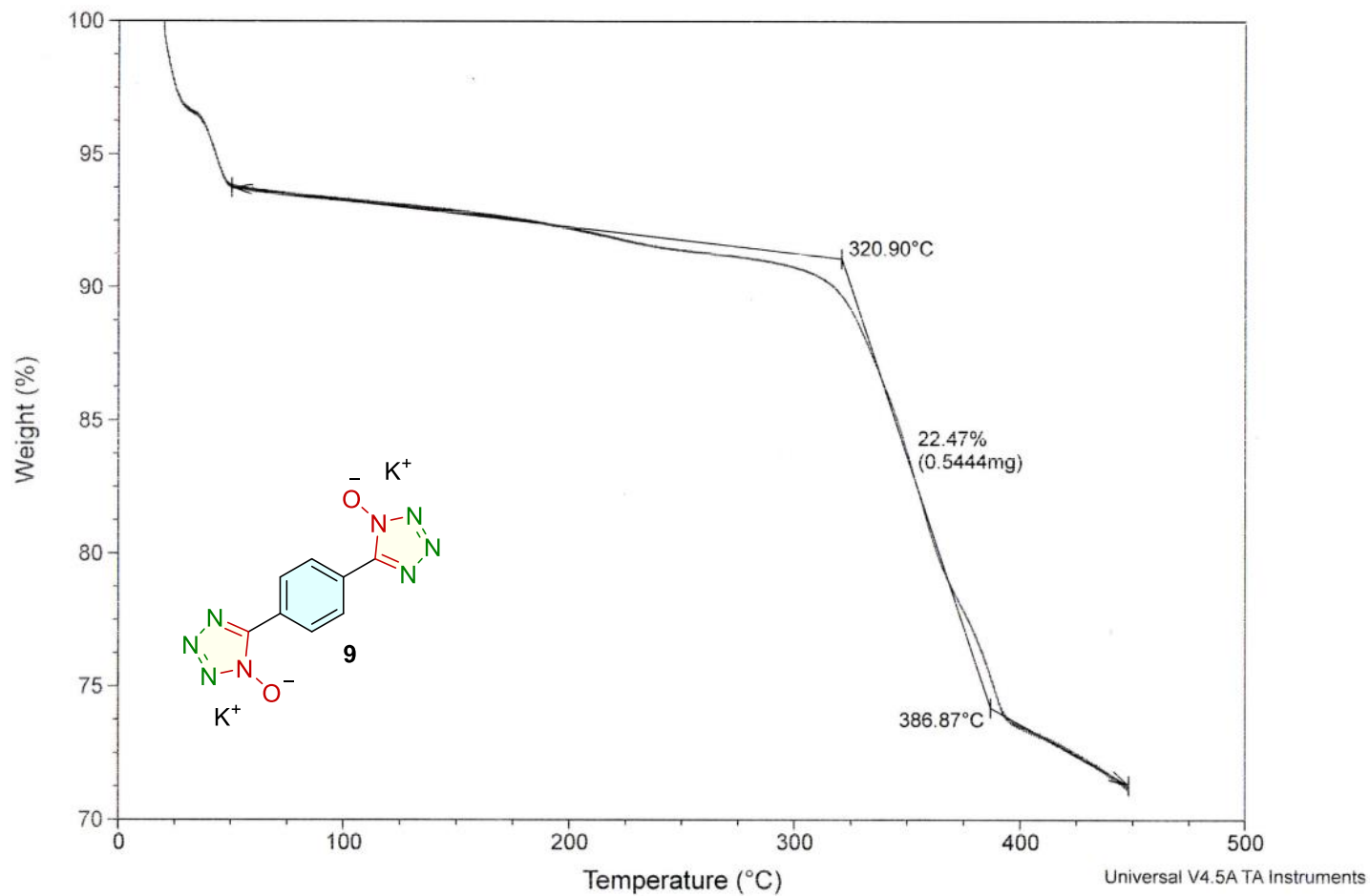
Figure S44. TGA of compound **9** at 5 °C min⁻¹
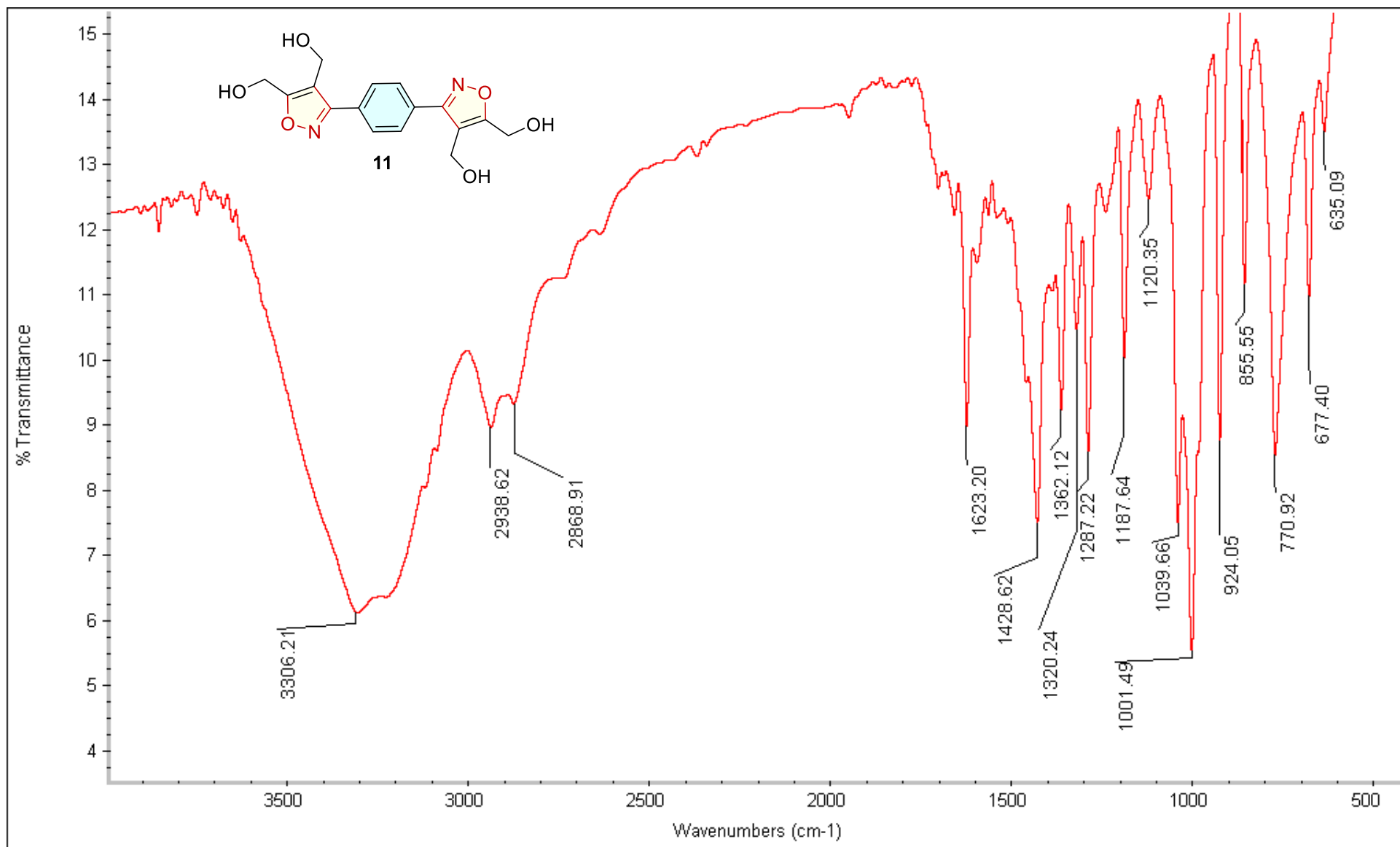
Figure S45. FTIR-Spectrum of Compound **11**

Figure S46. ^{1}H NMR Spectrum of Compound **11**

Figure S47. ^{13}C NMR Spectrum of Compound **11**

Figure S48. ^{13}C-DEPT135 NMR Spectrum of Compound **11**

Figure S49. DSC of compound **11** at 5 °C min^{-1}

Figure S50. TGA of compound **11** at 5 °C min^{-1}

Figure S51. FTIR-Spectrum of Compound **12**

Figure S52. ^{1}H NMR Spectrum of Compound **12**

Figure S53. ^{13}C NMR Spectrum of Compound **12**

15N{1H}_5894 Sohan 343

Current Data Parameters
NAME   New folder
EXPNO   5894
PROCNO   1

F2 - Acquisition Parameters
Date_   20220926
Time   18.07
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgig
TD   16248
SOLVENT   DMSO
NS   5626
DS   0
SWH   40760.871 Hz
FIDRES   2.508670 Hz
AQ   0.1993088 sec
RG   27.83
DW   12.267 usec
DE   8.00 usec
TE   303.2 K
D1   10.00000000 sec
D11   0.03000000 sec
TD0   10240

======== CHANNEL f1 ========
SFO1   50.6963210 MHz
NUC1   15N
P1   12.00 usec
PLW1   155.00000000 W

======== CHANNEL f2 ========
SFO2   500.1920008 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   80.00 usec
PLW2   26.00000000 W
PLW12   0.27649999 W

F2 - Processing parameters
SI   32768
SF   50.7031345 MHz
WDW   EM
SSB   0
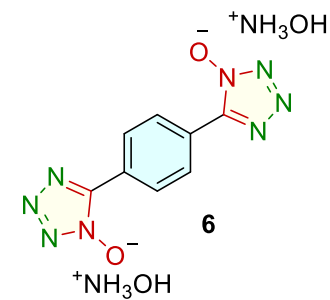LB   1.00 Hz
GB   0
PC   0.20
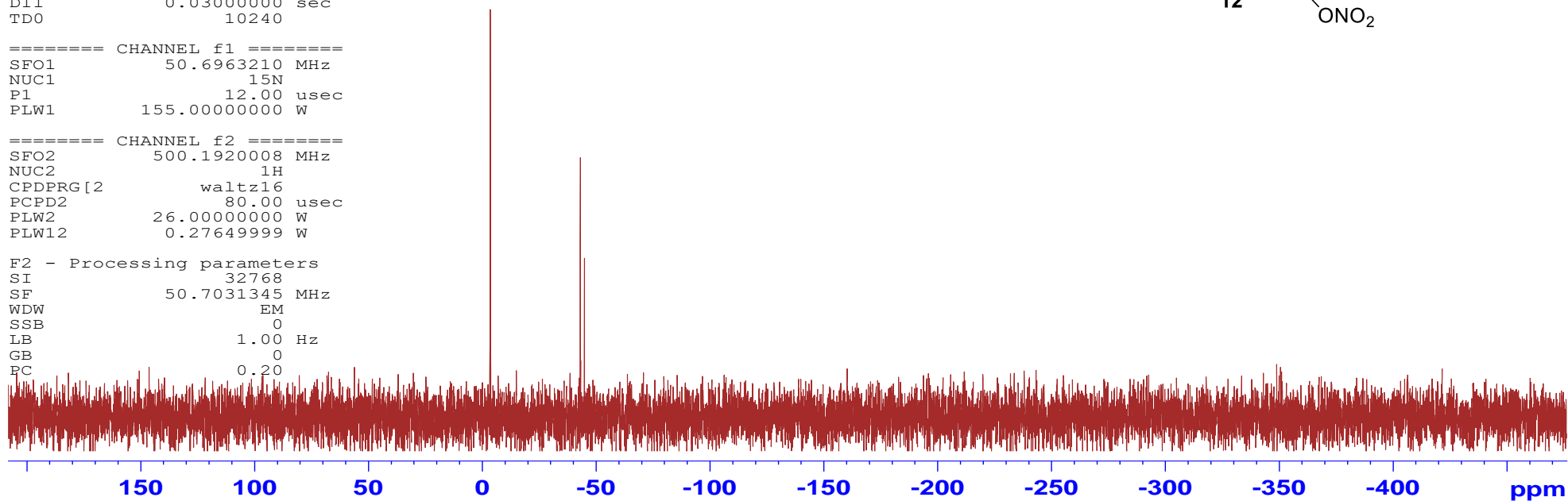
Figure S54. ^{15}N NMR Spectrum of Compound **12** in DMSO-d_6 (at 50.70 MHz)
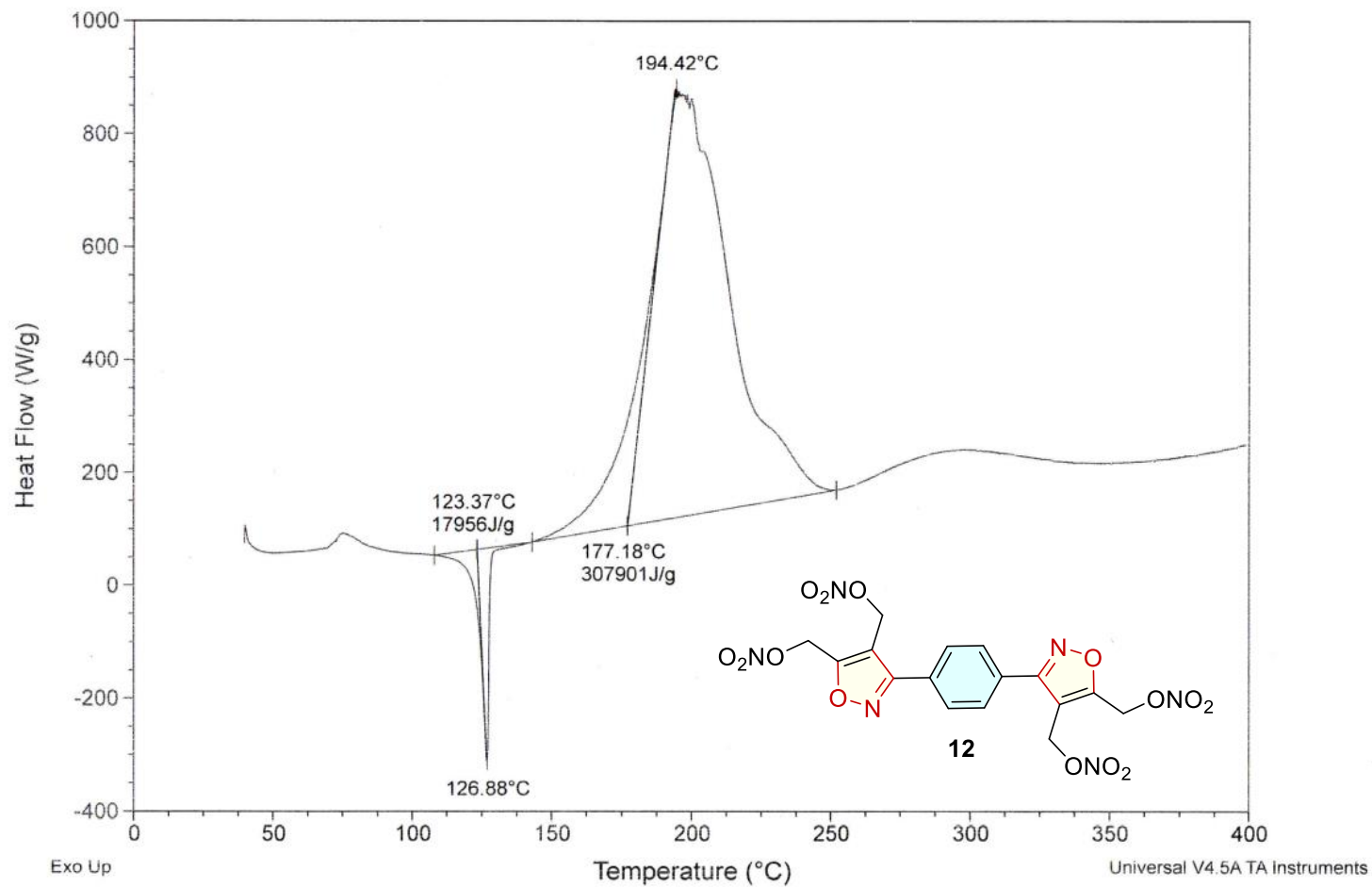
Figure S55. DSC of compound **12** at 5 °C min^{-1}
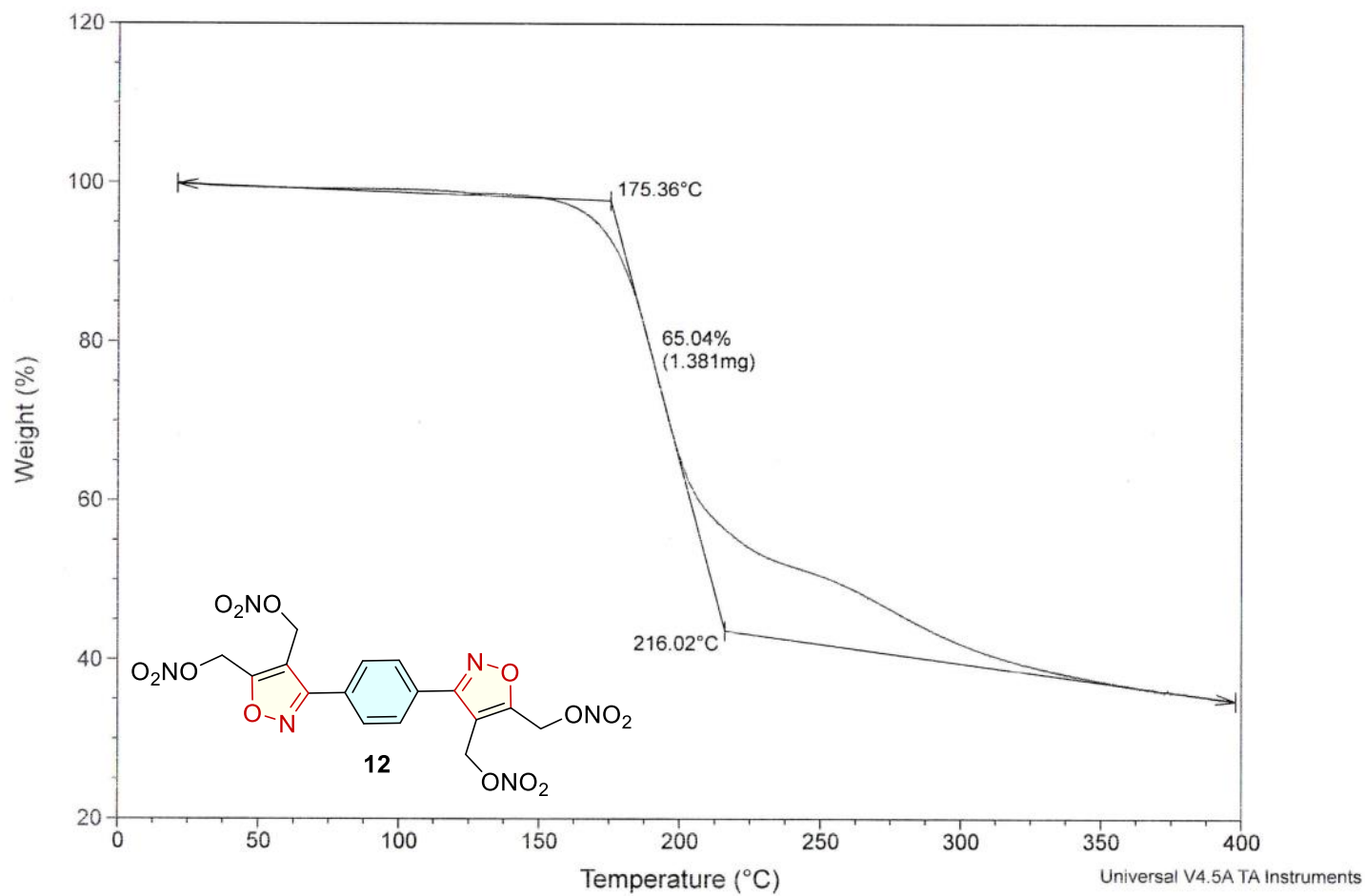
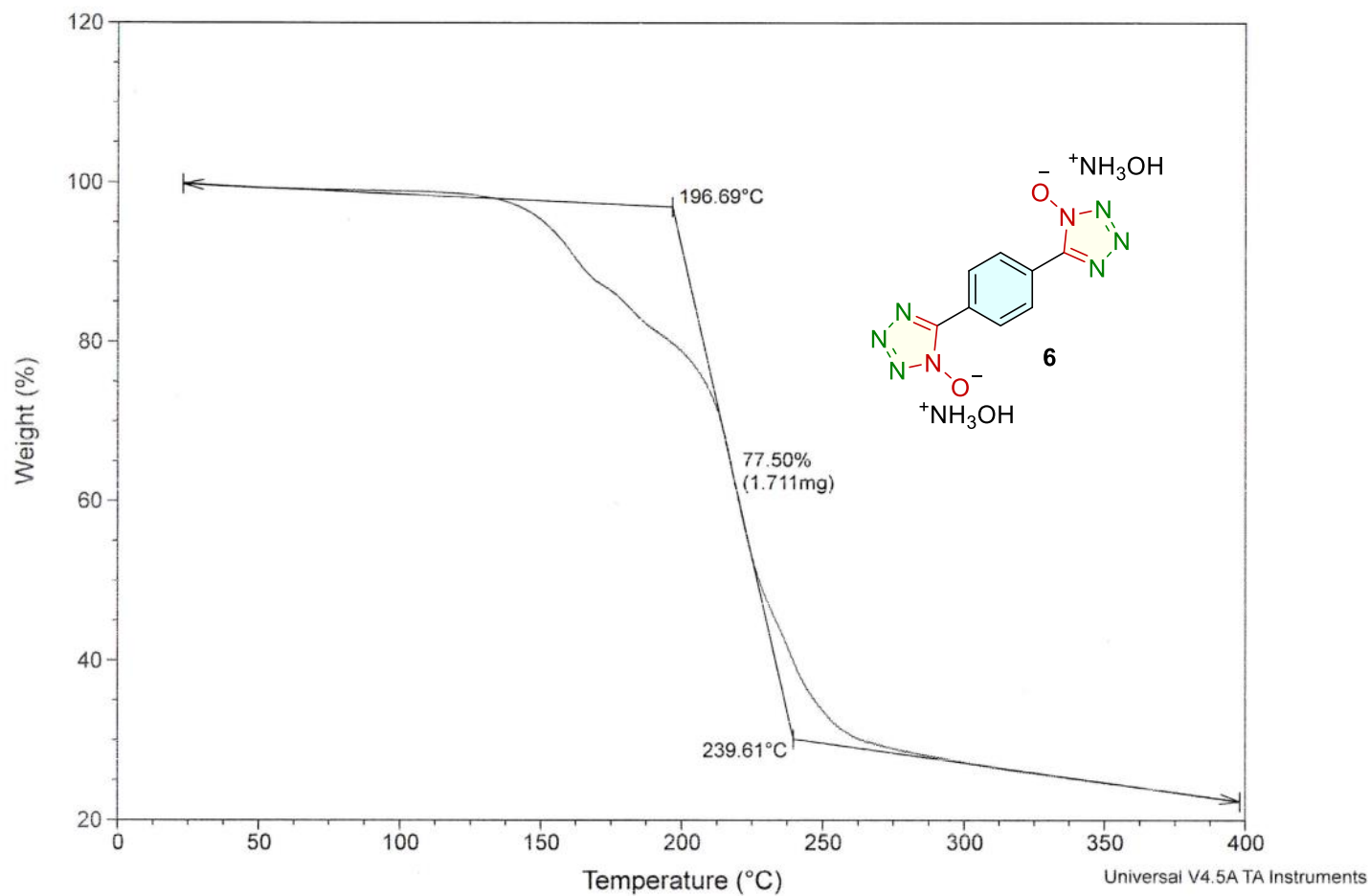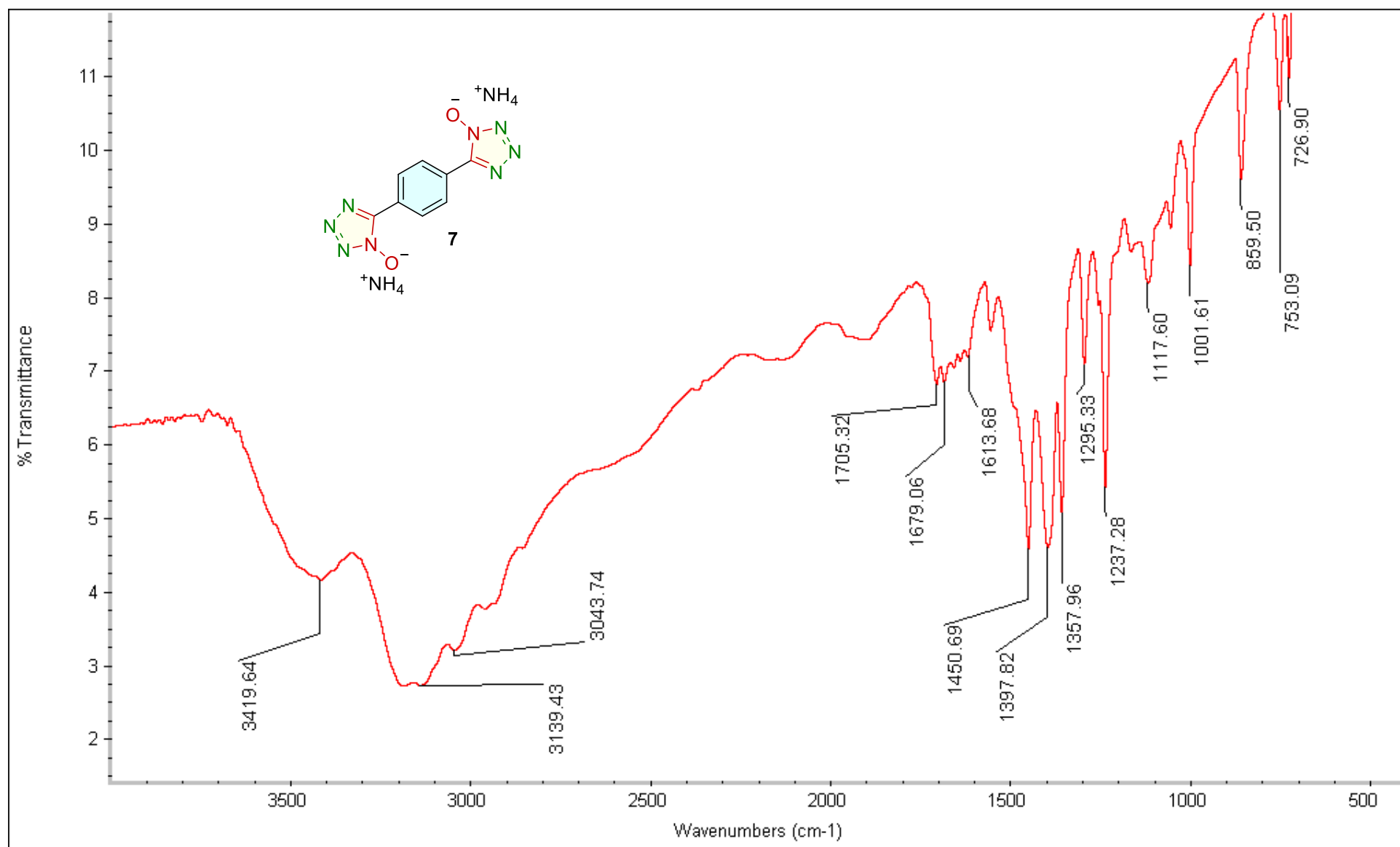**Figure S56**. TGA of compound **12** at 5 °C min^{-1}
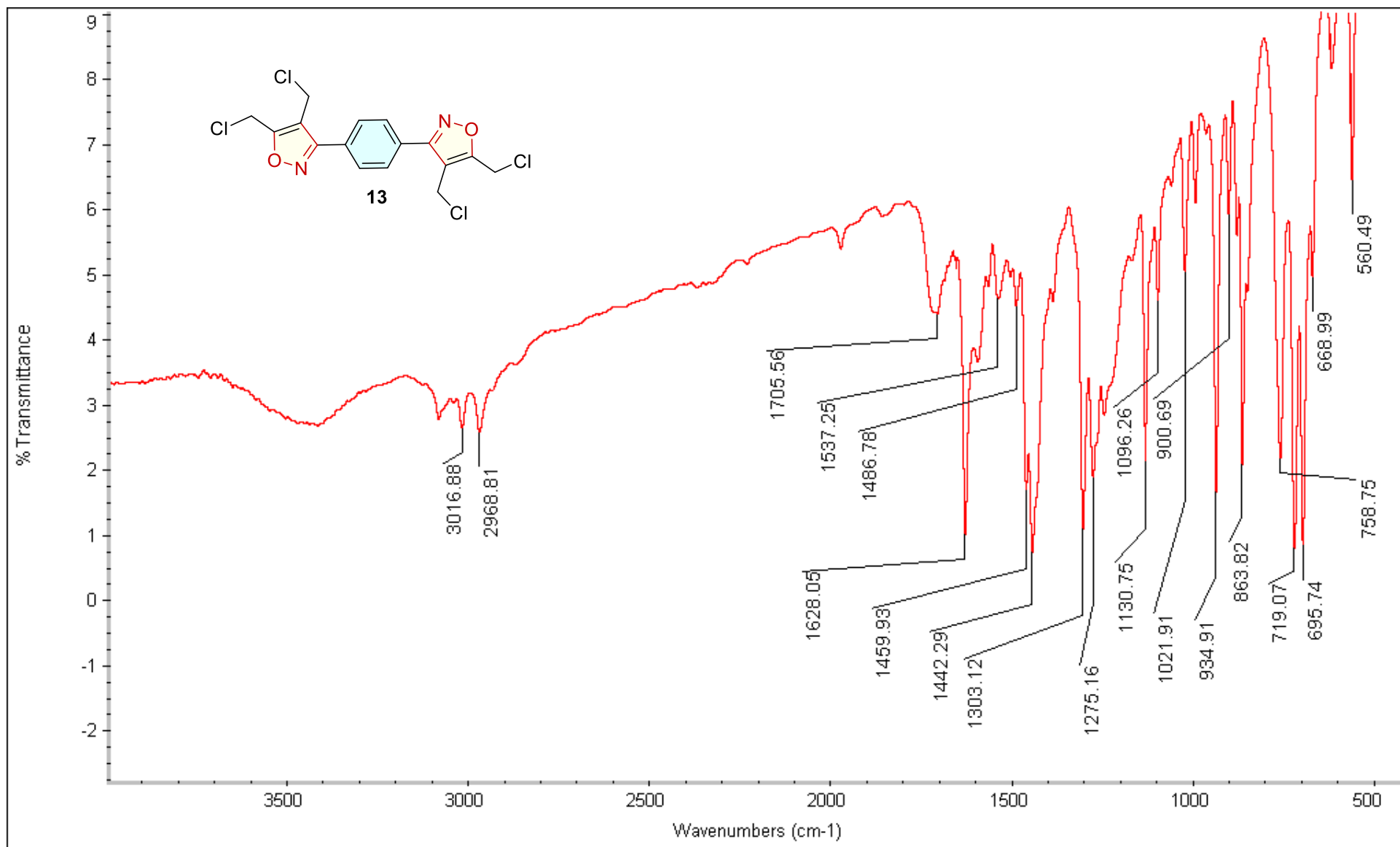
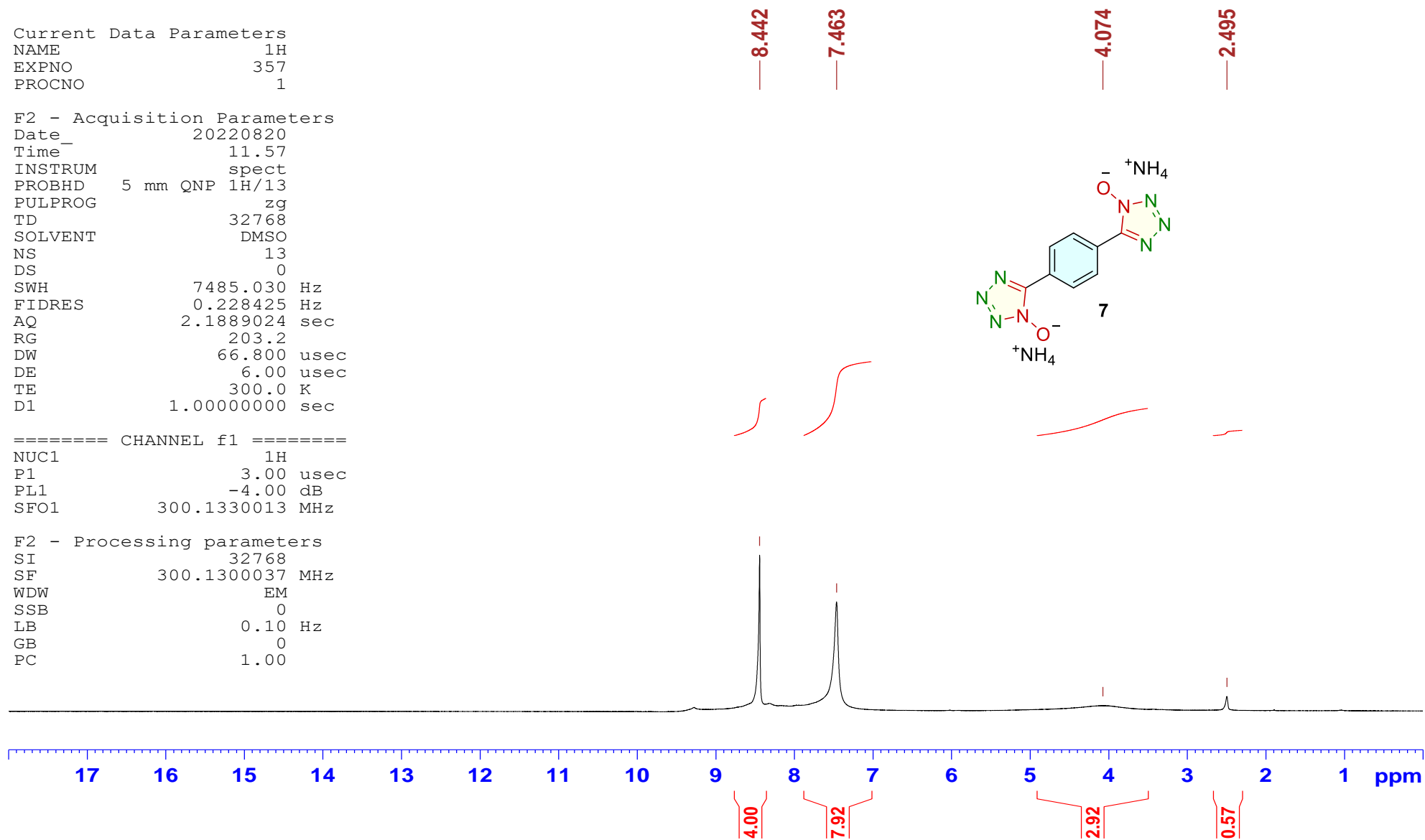**Figure S57.** FTIR-Spectrum of Compound **13**

Current Data Parameters
NAME   1H
EXPNO   349
PROCNO   1

F2 - Acquisition Parameters
Date_   20220817
Time   12.15
INSTRUM   spect
PROBHD   5 mm QNP 1H/13
PULPROG   zg
TD   32768
SOLVENT   DMSO
NS   8
DS   0
SWH   7485.030 Hz
FIDRES   0.228425 Hz
AQ   2.1889024 sec
RG   128
DW   66.800 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec

======== CHANNEL f1 ========
NUC1   1H
P1   3.00 usec
PL1   -4.00 dB
SFO1   300.1330013 MHz

F2 - Processing parameters
SI   32768
SF   300.1300021 MHz
WDW   EM
SSB   0
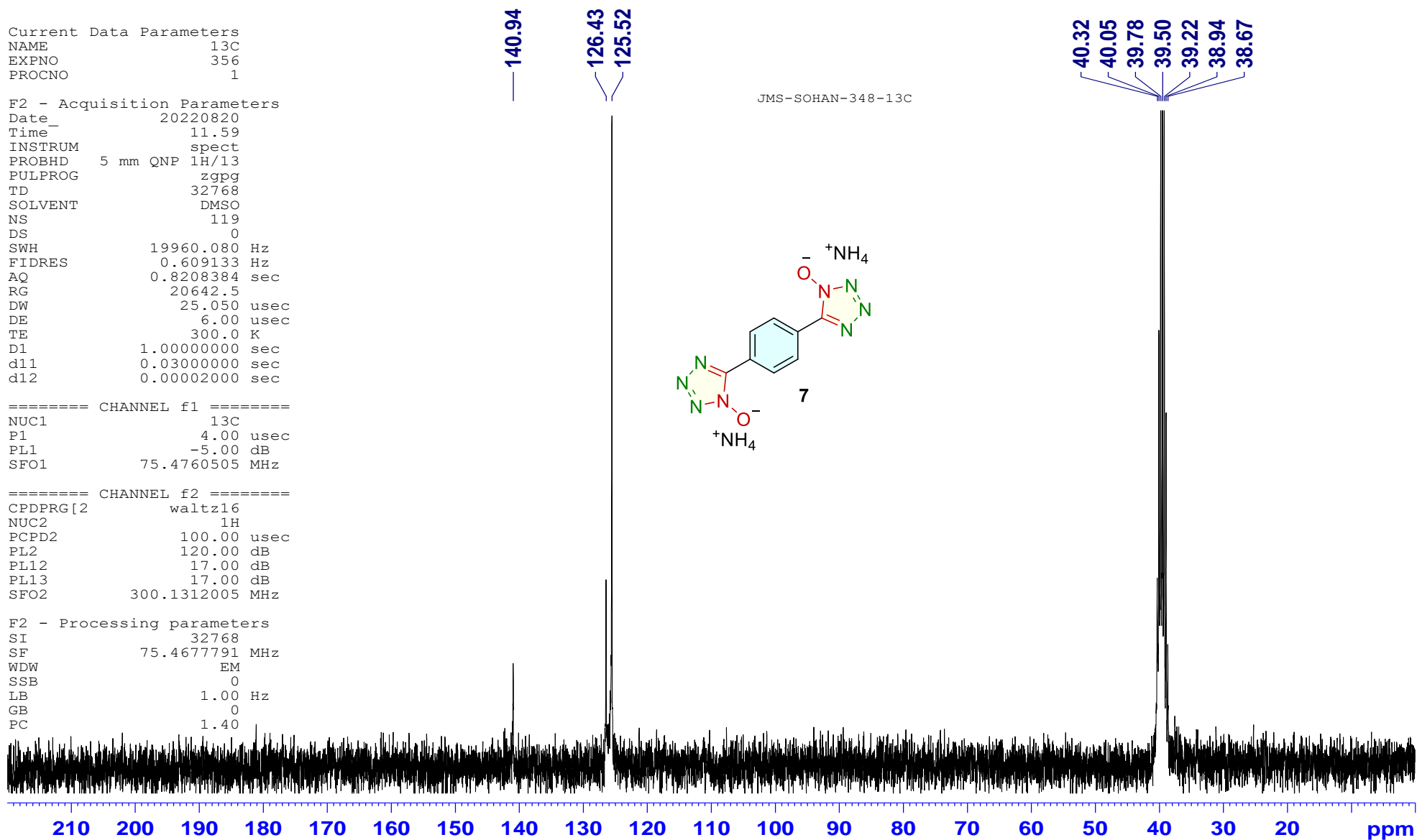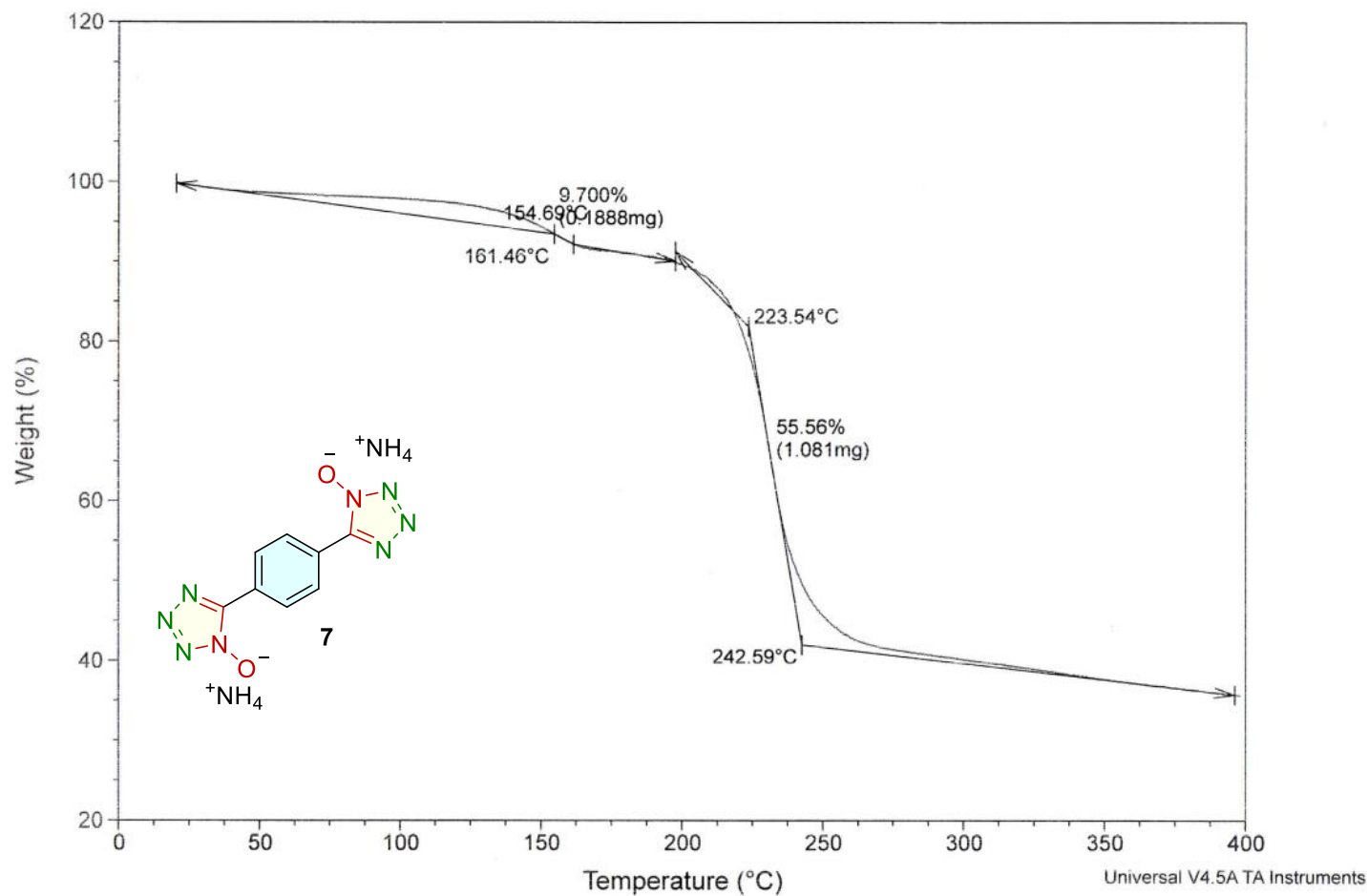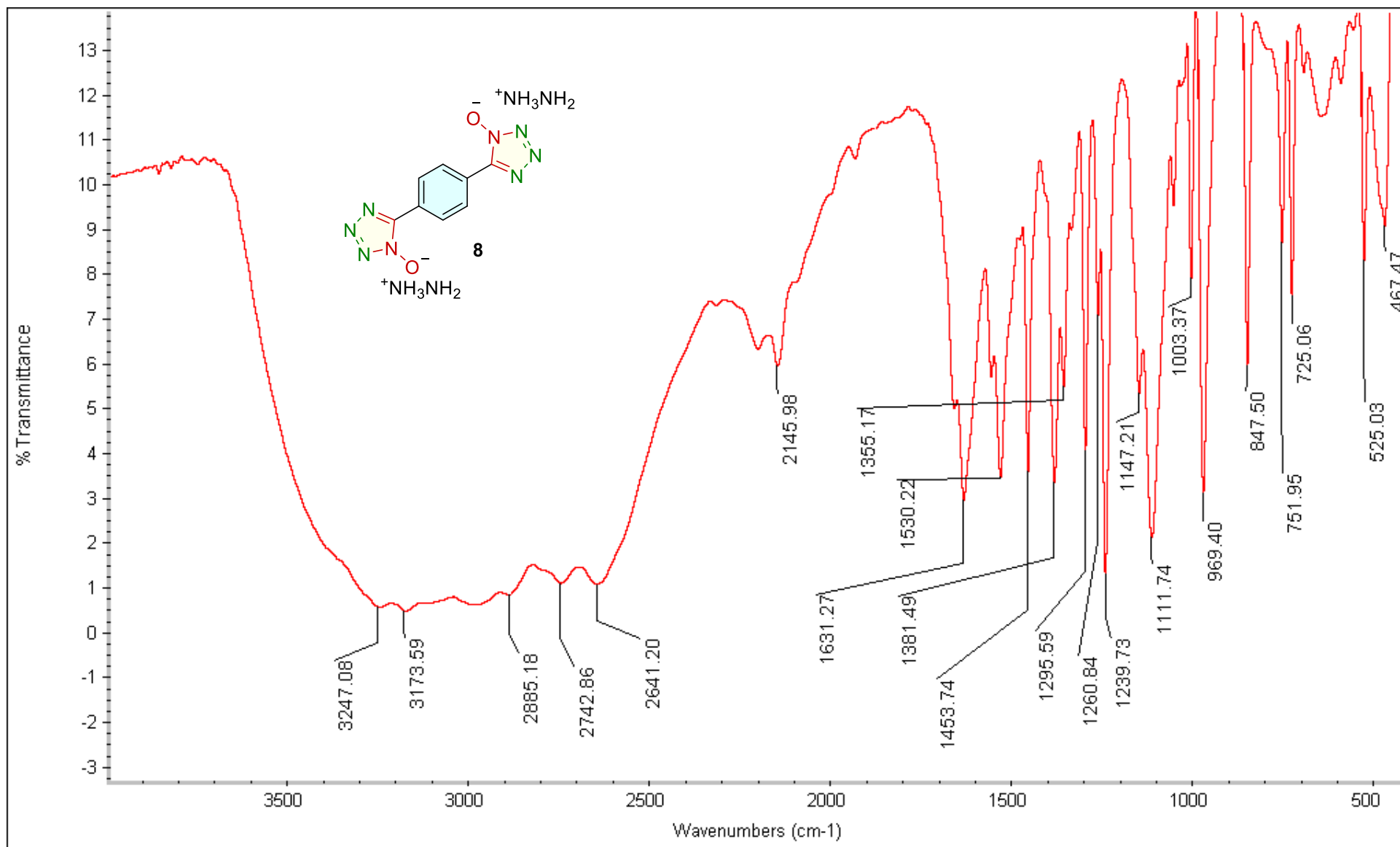LB   0.10 Hz
GB   0
PC   1.00

7.997
5.195
4.987
3.581
2.500

13

4.00   4.35 4.43   1.63   0.48
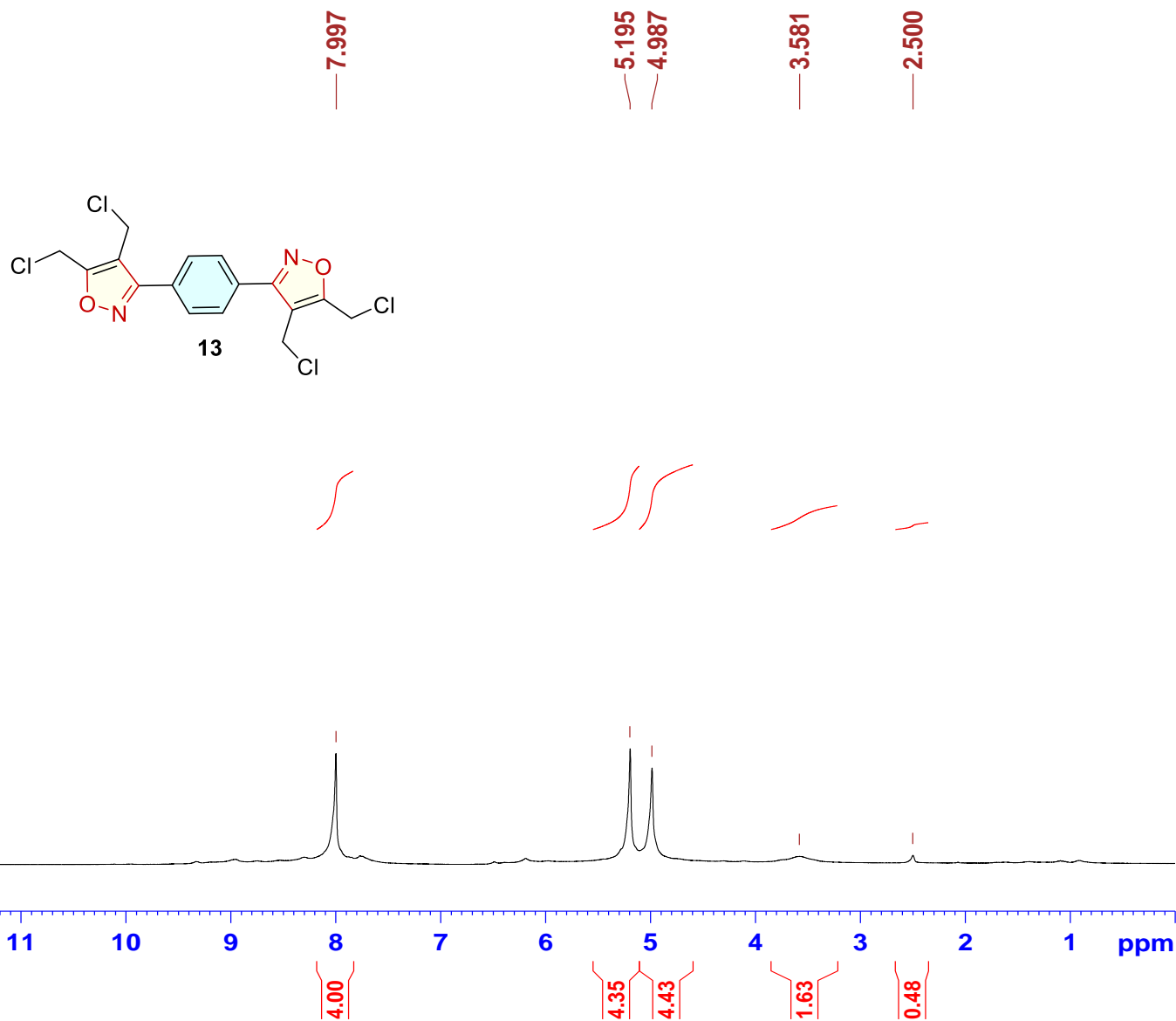
Figure S58. ^{1}H NMR Spectrum of Compound **13**

Figure S59. ^{13}C NMR Spectrum of Compound **13**

Figure S60. ^{13}C-DEPT135 NMR Spectrum of Compound **13**

Figure S61. FTIR-Spectrum of Compound **14**

Figure S62. ¹H NMR Spectrum of Compound **14**

Figure S63. ^{13}C NMR Spectrum of Compound **14**

JMS-SOHAN-345-DEPT135

128.65

42.91
41.65

14

Figure S64. ^{13}C-DEPT135 NMR Spectrum of Compound **14**

15N{1H}_5880   Sohan 345

Current Data Parameters
NAME   New folder
EXPNO   5880
PROCNO   1

F2 - Acquisition Parameters
Date_   20220922
Time   17.51
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgig
TD   32632
SOLVENT   DMSO
NS   4611
DS   0
SWH   40760.871 Hz
FIDRES   1.249107 Hz
AQ   0.4002859 sec
RG   27.83
DW   12.267 usec
DE   8.00 usec
TE   303.2 K
D1   12.00000000 sec
D11   0.03000000 sec
TD0   10240

======== CHANNEL f1 ========
SFO1   50.6963210 MHz
NUC1   15N
P1   12.00 usec
PLW1   155.00000000 W

======== CHANNEL f2 ========
SFO2   500.1920008 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   80.00 usec
PLW2   26.00000000 W
PLW12   0.27649999 W

F2 - Processing parameters
SI   32768
SF   50.7031345 MHz
WDW   EM
SSB   0
LB   5.00 Hz
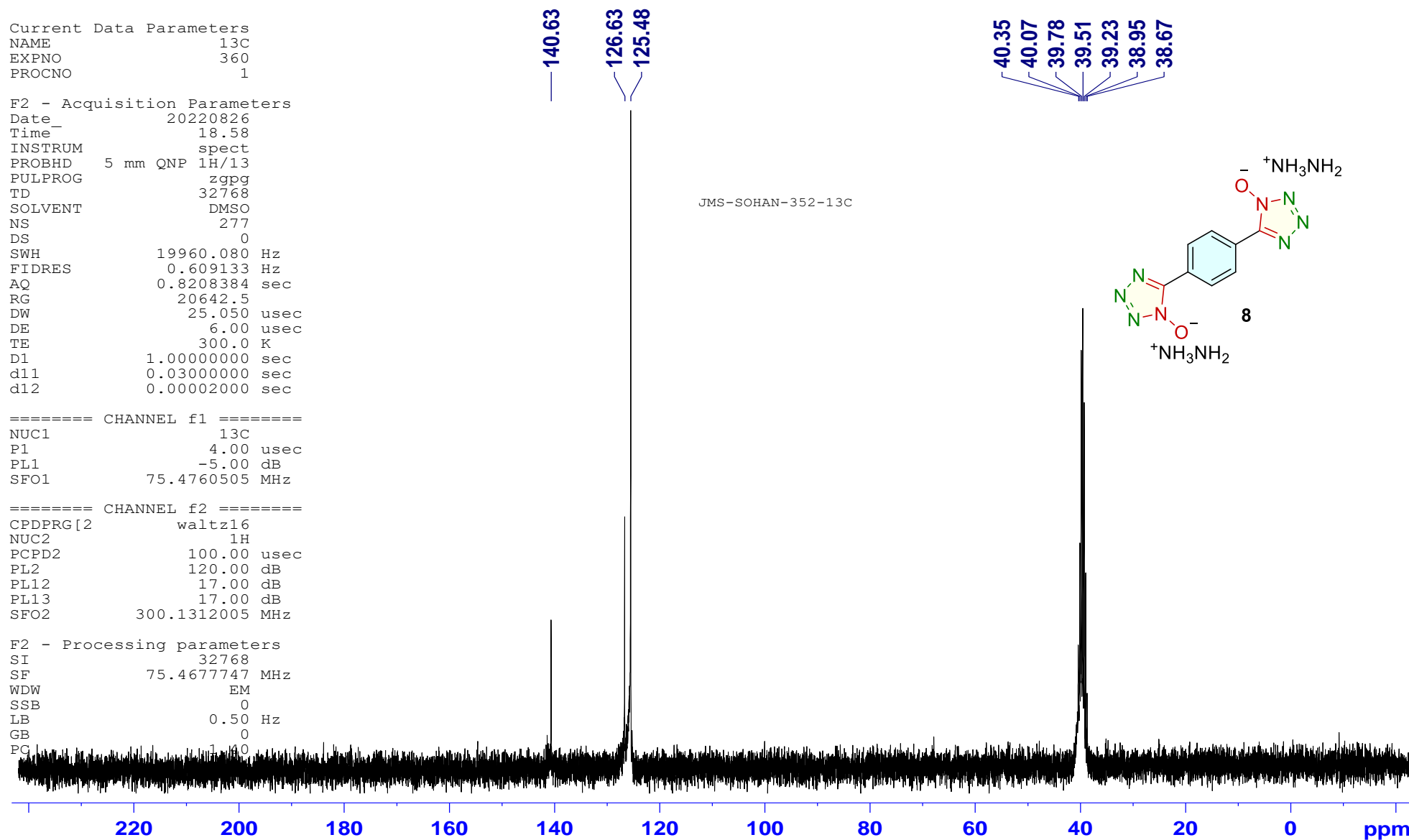GB   0
PC   0.20

-5.69

-133.16

-165.62
-166.43

-305.71
-309.65

-165.618
-166.427

-160   -170   ppm

150   100   50   0   -50   -100   -150   -200   -250   -300   -350   -400   ppm
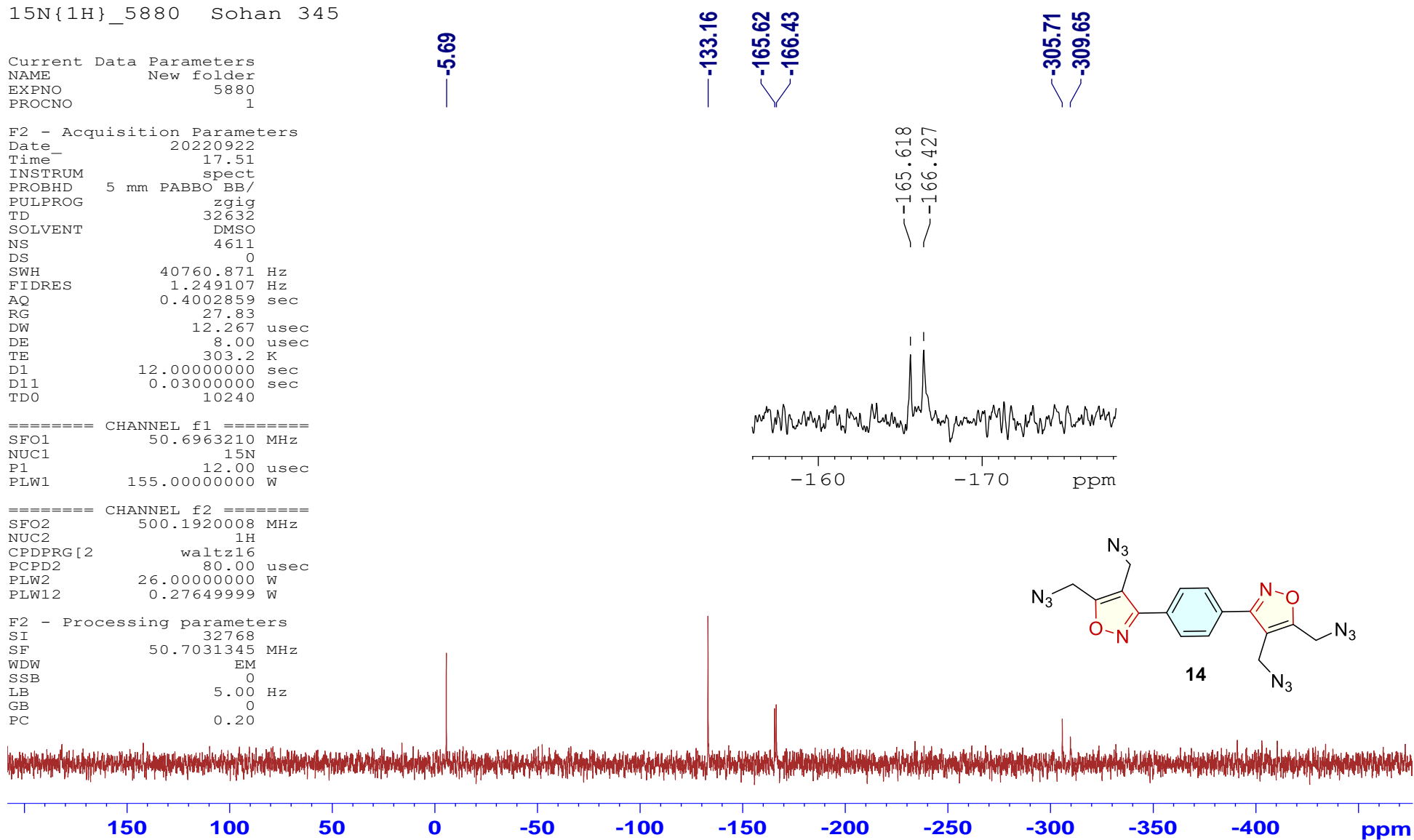
Figure S65. ^{15}N NMR Spectrum of Compound **14** in DMSO-d_6 (at 50.70 MHz)
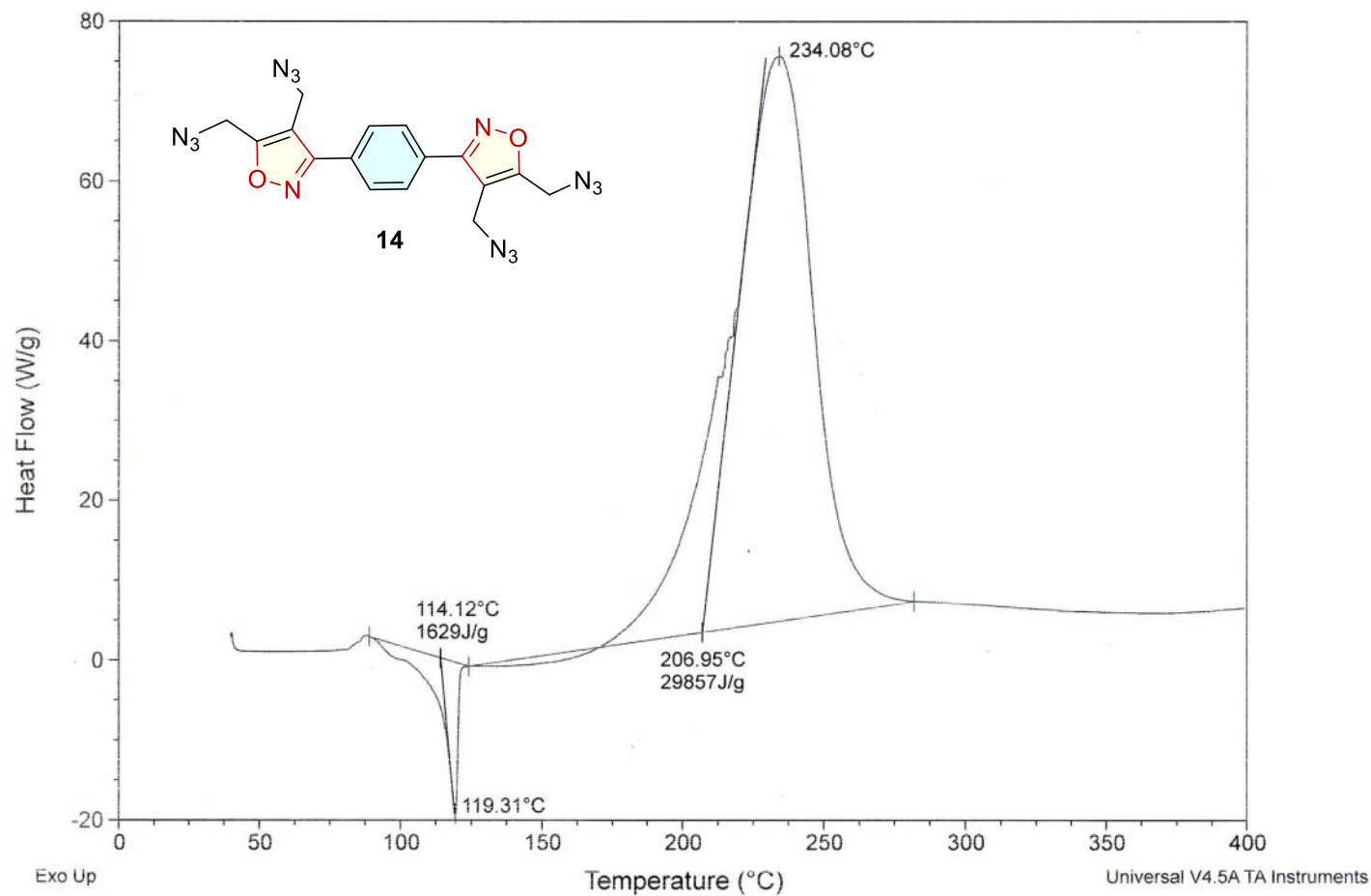
Figure S66. DSC of compound **14** at 5 °C min^{-1}
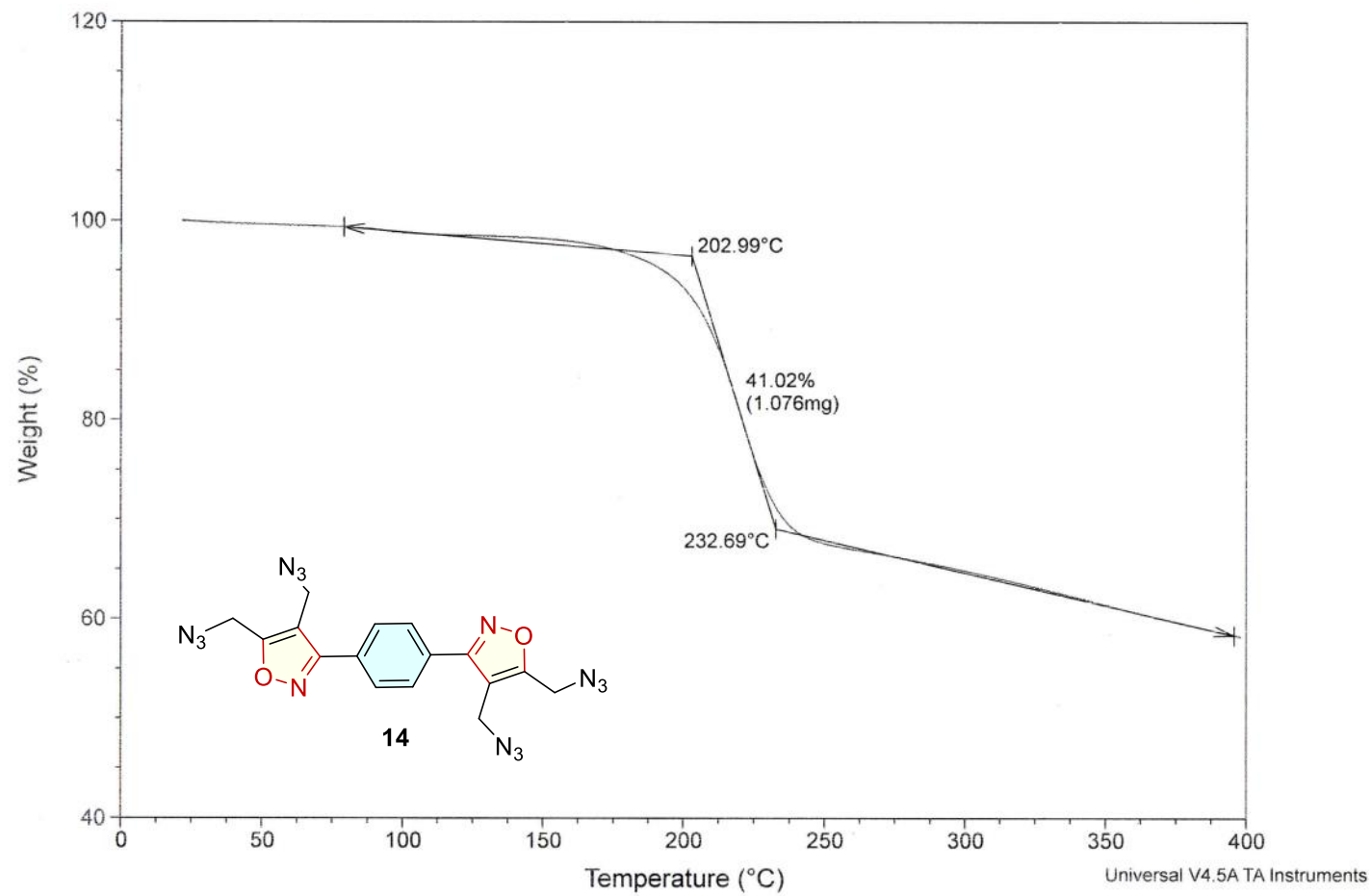
Figure S67. TGA of compound **14** at 5 °C min^{-1}

Table S12. Cartesian coordinates (in Å) for the optimized structure of compound **4** obtained using the B3LYP/6-311++G(d,p) level of theory
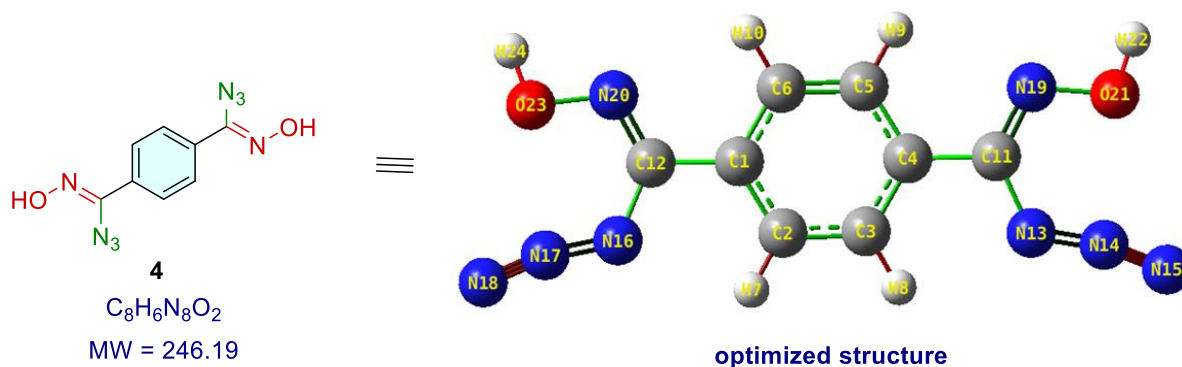
Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.719694	3.543572	-0.265989
2	C	3.093502	3.299594	-0.186882
3	C	3.995430	4.352361	-0.060970
4	C	3.545175	5.674430	-0.011194
5	C	2.163550	5.919163	-0.090135
6	C	1.267406	4.873097	-0.215286
7	H	3.459905	2.282452	-0.224399
8	H	5.055446	4.144887	-0.001218
9	H	1.803747	6.938652	-0.051728
10	H	0.206005	5.073278	-0.275367
11	C	4.501516	6.799017	0.121988
12	C	0.755662	2.425841	-0.401359
13	N	5.842076	6.391216	0.187347
14	N	6.800185	7.169294	0.301698
15	N	7.803309	7.675461	0.402485
16	N	1.362589	1.161461	-0.429865
17	N	0.741208	0.094811	-0.542144
18	N	0.394876	-0.974965	-0.632989
19	N	4.031562	7.996691	0.163168
20	N	-0.497936	2.708238	-0.477161
21	O	5.036581	8.960175	0.289485
22	H	4.548300	9.790057	0.306718
23	O	-1.295044	1.566544	-0.601177
24	H	-2.188585	1.922802	-0.646742

E_0 = -896.756502 Hartree/particle; ZPE = 0.157956 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S13. Cartesian coordinates (in Å) for the optimized structure of compound **4A** obtained using the B3LYP/6-311++G(d,p) level of theory
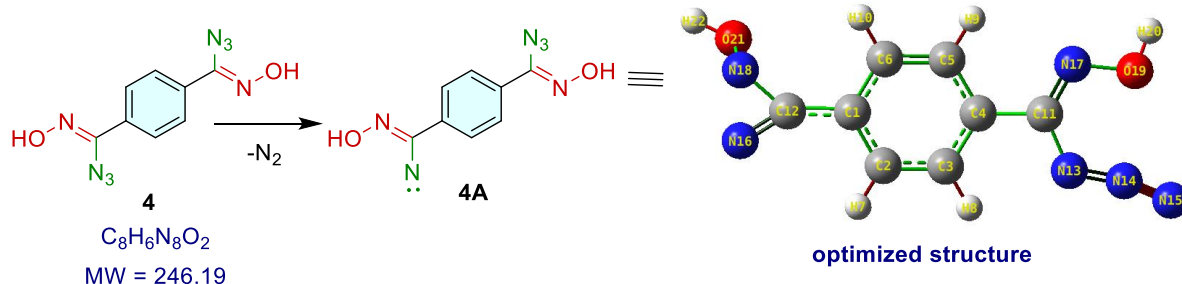
Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.761341	3.499892	-0.038856
2	C	3.141568	3.267616	-0.060069
3	C	4.024944	4.336864	-0.016846
4	C	3.544879	5.653233	0.046139
5	C	2.159712	5.879256	0.065373
6	C	1.275650	4.813447	0.023946
7	H	3.515265	2.251652	-0.109653
8	H	5.091480	4.158107	-0.032092
9	H	1.789291	6.894256	0.111385
10	H	0.206405	4.986896	0.034357
11	C	4.489486	6.796957	0.091235
12	C	0.835439	2.393127	-0.072419
13	N	5.836307	6.413795	0.050901
14	N	6.784356	7.213856	0.077932
15	N	7.780194	7.742157	0.089978
16	N	0.699296	1.151112	-0.153522
17	N	3.997103	7.984013	0.161102
18	N	-0.551965	2.164738	-0.059610
19	O	4.983668	8.968910	0.196925
20	H	4.481315	9.789359	0.247955
21	O	-1.035011	2.432808	-1.387280
22	H	-1.902625	2.008835	-1.385235

E_0 = -787.214664 Hartree/particle; ZPE = 0.146786 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S14. Cartesian coordinates (in Å) for the optimized structure of compound **5** obtained using the B3LYP/6-311++G(d,p) level of theory
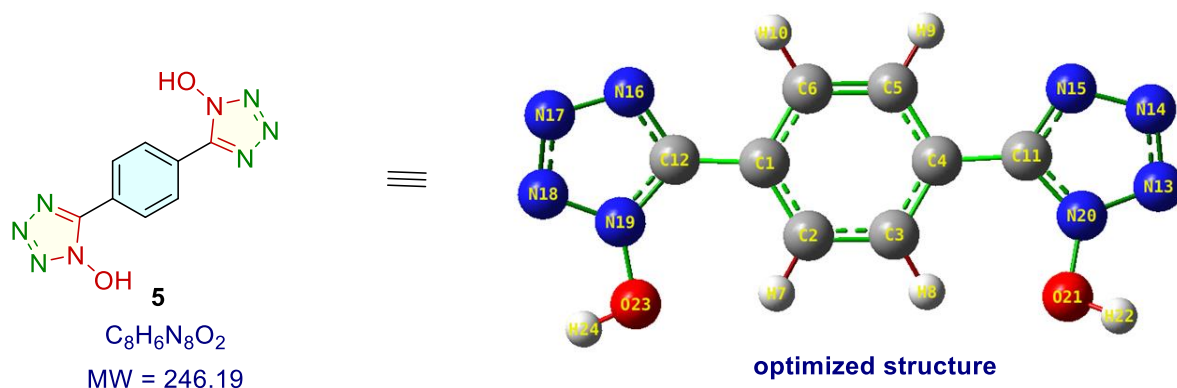
Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.262547	4.405405	-0.547907
2	C	2.385756	3.582238	-0.398174
3	C	3.587806	4.109076	0.060529
4	C	3.689234	5.468631	0.381189
5	C	2.562072	6.293799	0.229181
6	C	1.365896	5.769545	-0.226916
7	H	2.330875	2.530077	-0.638841
8	H	4.442019	3.455457	0.165964
9	H	2.641763	7.344808	0.474793
10	H	0.497190	6.404739	-0.341556
11	C	4.923851	6.082732	0.864221
12	C	-0.028710	3.912623	-1.021825
13	N	6.988424	6.394798	1.593025
14	N	6.373128	7.537160	1.530780
15	N	5.115635	7.383548	1.083648
16	N	-1.149762	4.627764	-1.119015
17	N	-2.106157	3.817513	-1.601407
18	N	-1.643899	2.620355	-1.803921
19	N	-0.357121	2.675212	-1.452643
20	N	6.093874	5.490097	1.188074
21	O	6.424622	4.163134	1.119559
22	H	7.215238	4.090929	1.679418
23	O	0.435473	1.561308	-1.530985
24	H	-0.071356	0.955451	-2.096675

E_0 = -896.758882 Hartree/particle; ZPE = 0.160846 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S15. Cartesian coordinates (in Å) for the optimized structure of compound **5A** obtained using the B3LYP/6-311++G(d,p) level of theory

optimized structure
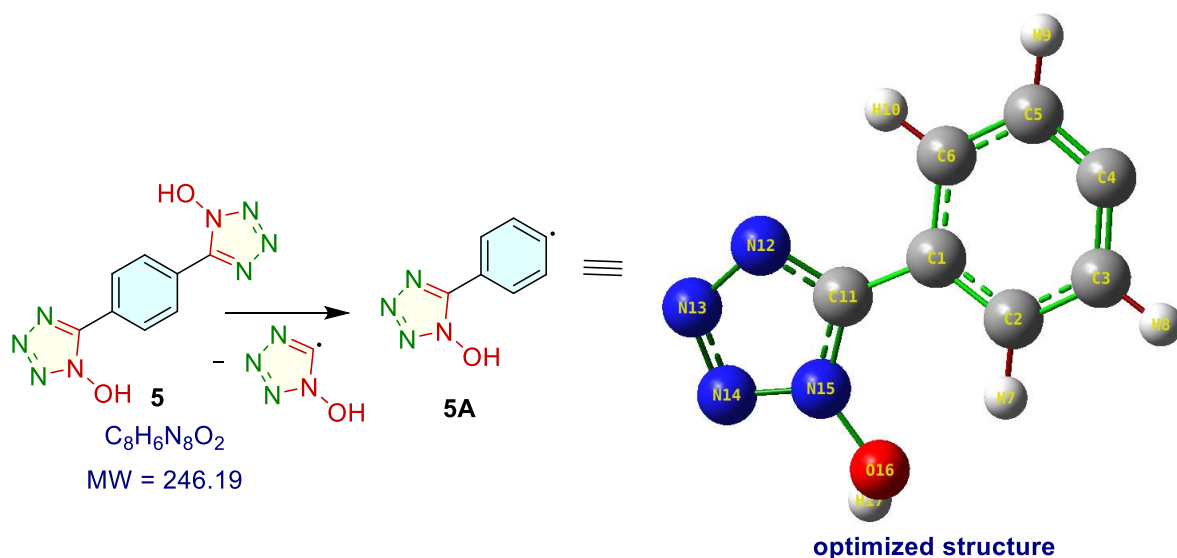
Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.240868	4.425749	-0.524535
2	C	2.295552	3.593036	-0.119649
3	C	3.492937	4.151683	0.342708
4	C	3.567141	5.522514	0.376643
5	C	2.569696	6.391967	0.000948
6	C	1.379993	5.822839	-0.457801
7	H	2.189796	2.517164	-0.155025
8	H	4.311437	3.516118	0.660477
9	H	2.684832	7.468507	0.052043
10	H	0.553211	6.451017	-0.766409
11	C	-0.037805	3.899608	-1.003829
12	N	-1.161128	4.594956	-1.149094
13	N	-2.097672	3.750727	-1.631851
14	N	-1.622159	2.556297	-1.777388
15	N	-0.336456	2.641149	-1.404391
16	O	0.467851	1.534032	-1.396521
17	H	0.332588	1.119476	-2.263010

E$_0$ = -563.806523 Hartree/particle; ZPE = 0.117484 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S16. Cartesian coordinates (in Å) for the optimized structure of compound **5B** obtained using the B3LYP/6-311++G(d,p) level of theory

optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-0.018166	3.874794	-1.367008
2	N	-0.950452	4.632538	-1.805932
3	N	-2.028407	3.770184	-2.021024
4	N	-1.722465	2.555702	-1.700268
5	N	-0.437162	2.601093	-1.302496
6	O	0.210800	1.528291	-0.769410
7	H	0.369430	0.921107	-1.508677

E_0 = -332.757968 Hartree/particle; ZPE = 0.036750 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S14. Cartesian coordinates (in Å) for the optimized structure of compound **5C** obtained using the B3LYP/6-311++G(d,p) level of theory

optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.201957	4.365221	-0.571996
2	C	2.226602	3.468572	-0.239403
3	C	3.447823	3.942087	0.226732
4	C	3.667724	5.315209	0.368924
5	C	2.642891	6.211866	0.038541

		X	Y	Z
6	C	1.423924	5.744061	-0.425310
7	H	2.076340	2.402755	-0.337828
8	H	4.232982	3.243033	0.482585
9	H	2.808623	7.277240	0.141092
10	H	0.632359	6.435399	-0.683855
11	C	4.970501	5.835861	0.883071
12	C	-0.104386	3.934386	-1.065743
13	N	5.064921	7.010813	1.407190
14	N	-1.142508	4.729391	-1.326663
15	N	-2.146122	3.953101	-1.768512
16	N	-1.794343	2.703064	-1.788220
17	N	-0.529031	2.686449	-1.360849
18	N	6.034046	4.969365	0.755642
19	O	7.167561	5.517470	1.275153
20	H	7.838438	4.838214	1.124199
21	O	0.151607	1.503741	-1.244292
22	H	-0.361992	0.885676	-1.789987

$E_0 = -787.209997$ Hartree/particle; ZPE = 0.147372 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S17. Cartesian coordinates (in Å) for the optimized structure of compound **12** obtained using the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.826055	4.118684	-0.465678
2	C	2.989533	3.337694	-0.481338
3	C	4.222433	3.906135	-0.186997
4	C	4.319926	5.267005	0.130300
5	C	3.156663	6.048358	0.144352
6	C	1.923849	5.479880	-0.150273
7	H	2.927645	2.276245	-0.687645
8	H	5.116608	3.295531	-0.189877
9	H	3.218788	7.109847	0.349803
10	H	1.030011	6.090940	-0.149621
11	C	5.638648	5.857312	0.425281
12	C	0.506878	3.528051	-0.756514

13	N	-0.549310	3.933635	-0.086259
14	N	6.696459	5.455619	-0.243957
15	C	-1.201972	2.402628	-1.567711
16	C	-2.233522	1.572988	-2.245273
17	H	-1.828733	0.608152	-2.553472
18	H	-3.086688	1.414593	-1.585251
19	C	0.144777	2.536840	-1.732915
20	C	5.998672	6.839314	1.412529
21	C	5.141430	7.508627	2.427087
22	H	4.359885	6.843062	2.797709
23	H	5.726904	7.868876	3.273386
24	C	7.347051	6.972448	1.253854
25	C	8.378350	7.800267	1.932932
26	H	8.110041	7.993286	2.972749
27	H	9.349797	7.306219	1.895004
28	O	-1.630109	3.226262	-0.598986
29	O	7.776222	6.157580	0.277837
30	O	-2.642222	2.330471	-3.415973
31	O	4.516619	8.647212	1.762834
32	O	8.430198	9.052016	1.200259
33	N	3.696996	9.442235	2.627006
34	O	3.657991	9.127487	3.791688
35	O	3.152930	10.336465	2.048201
36	N	9.415410	9.966929	1.702116
37	O	10.053800	9.610536	2.662455
38	O	9.456726	10.982632	1.075299
39	N	-3.701599	1.709097	-4.161402
40	O	-4.020170	2.348193	-5.119132
41	O	-4.119533	0.657518	-3.744192
42	C	0.993483	1.860570	-2.750565
43	H	1.783705	2.517237	-3.117437
44	H	0.405012	1.512729	-3.599482
45	O	1.600289	0.710146	-2.084817
46	N	2.439875	-0.077576	-2.937240
47	O	2.951780	-0.991397	-2.358077
48	O	2.524145	0.260628	-4.092007

E_0 = -1998.131739 Hartree/particle; ZPE = 0.316338 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S18. Cartesian coordinates (in Å) for the optimized structure of compound **12A** obtained using the B3LYP/6-311++G(d,p) level of theory
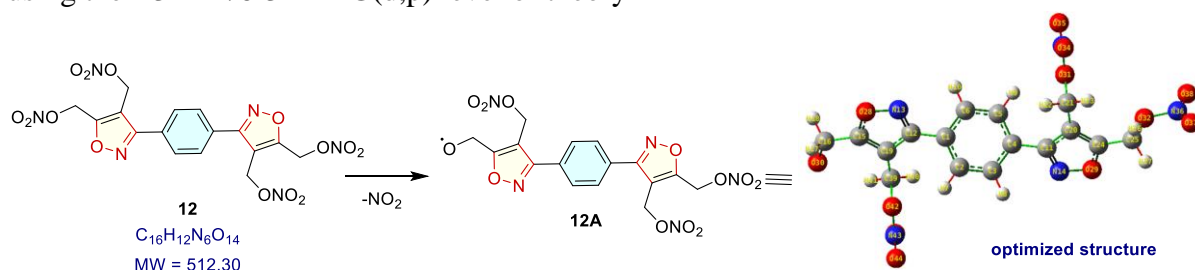
Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.735682	4.217984	-0.417912
2	C	2.894456	3.439957	-0.543627
3	C	4.143671	3.991258	-0.287683
4	C	4.263279	5.331611	0.101159
5	C	3.104824	6.110161	0.226043
6	C	1.855820	5.558745	-0.030706
7	H	2.817986	2.392297	-0.807258
8	H	5.034267	3.381856	-0.376785
9	H	3.180930	7.158155	0.488486
10	H	0.965172	6.168185	0.056837
11	C	5.598152	5.903989	0.355612
12	C	0.399717	3.643722	-0.666176
13	N	-0.607037	3.998997	0.098076
14	N	6.615676	5.545811	-0.395713
15	C	-1.353430	2.570057	-1.451620
16	C	-2.461412	1.774950	-2.085333
17	H	-2.807659	0.985456	-1.385083
18	H	-3.366117	2.404559	-2.196392
19	C	-0.018840	2.722100	-1.691362
20	C	6.016036	6.822458	1.380716
21	C	5.218714	7.424814	2.482136
22	H	4.455273	6.737328	2.850343
23	H	5.850910	7.728442	3.317003
24	C	7.353808	6.965859	1.155668
25	C	8.423639	7.749242	1.827392
26	H	8.204564	7.891356	2.886757
27	H	9.387358	7.250231	1.720062
28	O	-1.721131	3.318726	-0.401200
29	O	7.725468	6.214209	0.108151
30	O	-2.180135	1.178463	-3.269063
31	O	4.563970	8.605430	1.928747
32	O	8.455726	9.036482	1.157241
33	N	3.792343	9.340258	2.884202
34	O	3.813335	8.950256	4.026457
35	O	3.220255	10.269857	2.394498
36	N	9.475282	9.914132	1.655306
37	O	10.154919	9.503206	2.564308
38	O	9.499787	10.959897	1.078750
39	C	0.791285	2.121782	-2.786471
40	H	1.581154	2.796714	-3.119291
41	H	0.169808	1.834817	-3.630774
42	O	1.408831	0.918746	-2.222732
43	N	2.186601	0.174006	-3.157621
44	O	2.684230	-0.801057	-2.669147
45	O	2.252529	0.597078	-4.285855

E_0 = -1792.955713 Hartree/particle; ZPE = 0.299583 Hartree/particle.

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S19. Cartesian coordinates (in Å) for the optimized structure of compound **14** obtained using the B3LYP/6-311++G(d,p) level of theory


12

$C_{16}H_{12}N_{14}O_2$

MW = 432.37

optimized structure
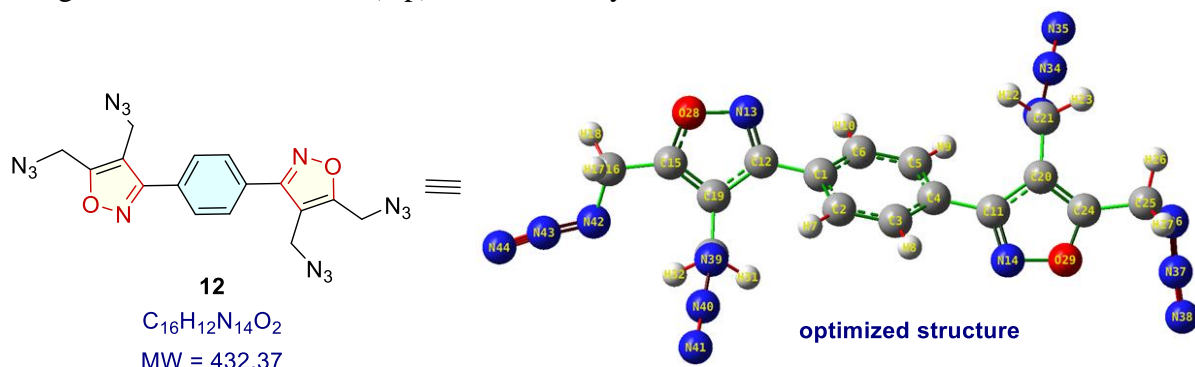
Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.765621	4.329901	-0.442053
2	C	2.907838	3.517601	-0.461767
3	C	4.153665	4.047849	-0.154124
4	C	4.289719	5.401251	0.181468
5	C	3.147643	6.213434	0.200982
6	C	1.901712	5.682778	-0.106520
7	H	2.815514	2.461253	-0.685186
8	H	5.032075	3.415059	-0.163021
9	H	3.239763	7.269859	0.423172
10	H	1.023350	6.315681	-0.098619
11	C	5.624089	5.949635	0.487129
12	C	0.432597	3.778434	-0.746717
13	N	-0.619273	4.231642	-0.100689
14	N	6.676982	5.475847	-0.141785
15	C	-1.289147	2.691737	-1.570386
16	C	-2.352293	1.850577	-2.198082
17	H	-2.287123	0.825374	-1.812736
18	H	-3.326014	2.261068	-1.912103
19	C	0.062364	2.780304	-1.712720
20	C	6.001166	6.953906	1.445814
21	C	5.142195	7.712558	2.401862
22	H	4.341889	7.066481	2.778884
23	H	5.738723	8.039439	3.259864
24	C	7.355958	7.023522	1.317762
25	C	8.414140	7.854849	1.966507
26	H	8.070577	8.192540	2.942754
27	H	9.313545	7.247403	2.110767
28	O	-1.711544	3.547384	-0.624056
29	O	7.774440	6.151538	0.382192
30	C	0.924139	2.046640	-2.686507
31	H	1.755195	2.684700	-3.004467
32	H	0.334541	1.785069	-3.568280
33	N	4.543705	8.899461	1.726809
34	N	3.976584	9.695037	2.477875
35	N	3.437737	10.499368	3.068443

36	N	8.727785	9.094989	1.215783
37	N	9.402729	8.947197	0.192036
38	N	10.018913	8.958789	-0.758161
39	N	1.465427	0.807195	-2.050531
40	N	2.060969	0.046335	-2.815490
41	N	2.621649	-0.730965	-3.422150
42	N	-2.183913	1.856890	-3.668981
43	N	-2.969731	1.138097	-4.290346
44	N	-3.633428	0.521832	-4.971190

E_0 = -1533.563301 Hartree/particle; ZPE = 0.303009 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S20. Cartesian coordinates (in Å) for the optimized structure of compound **14** obtained using the B3LYP/6-311++G(d,p) level of theory
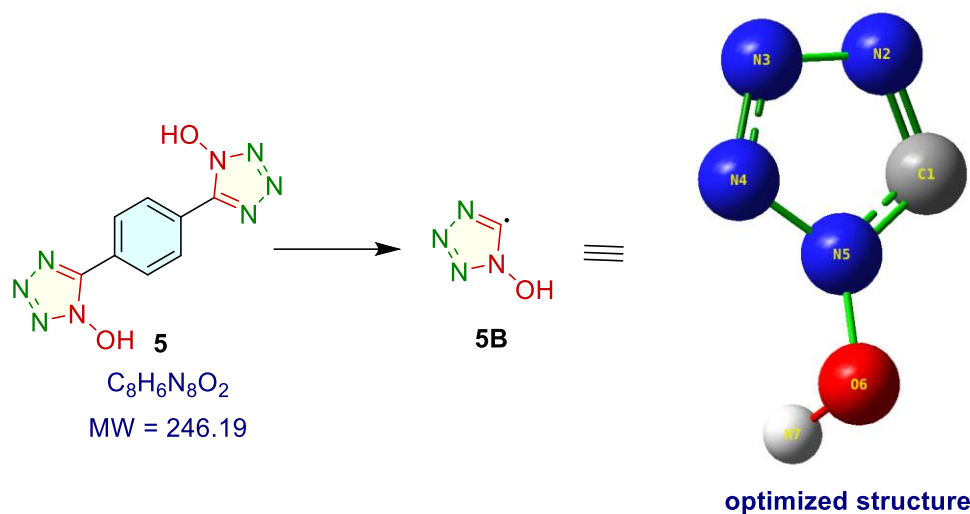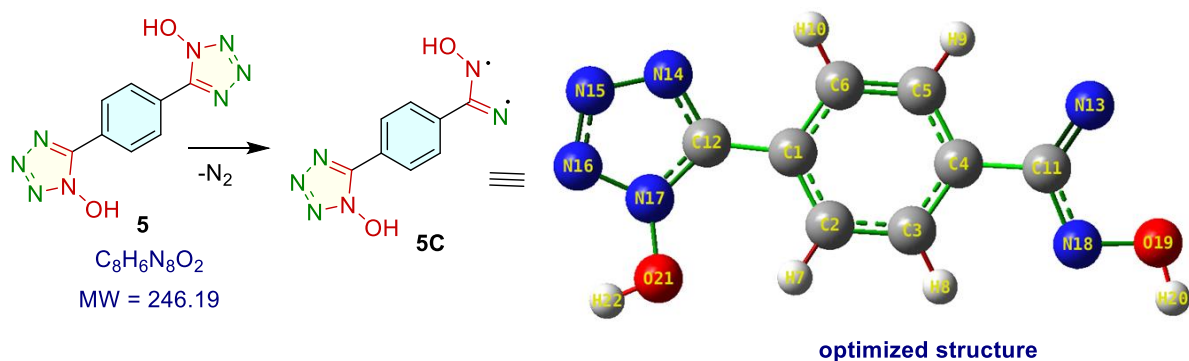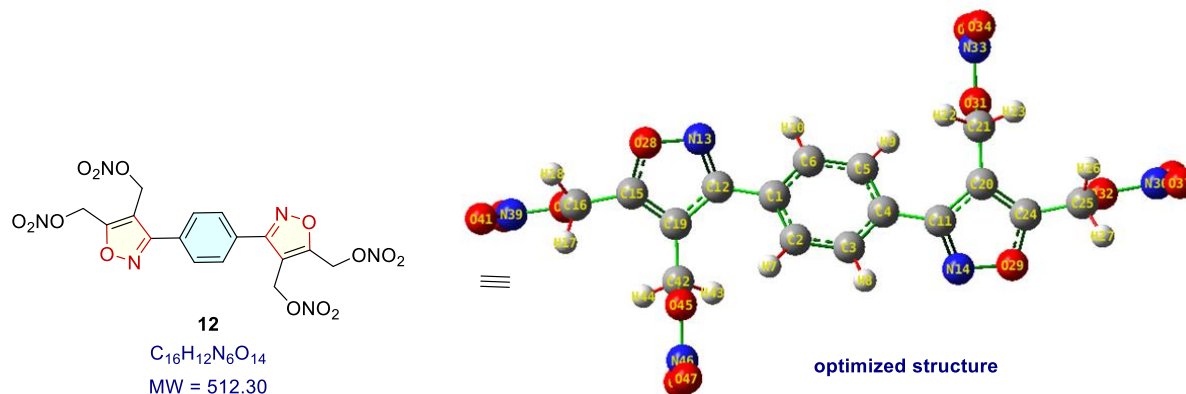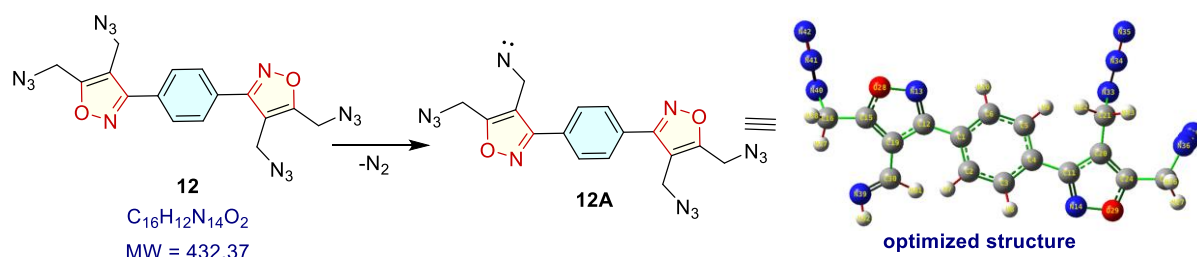

Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.980601	4.161155	-0.647610
2	C	3.079640	3.321163	-0.421886
3	C	4.302162	3.847134	-0.027906
4	C	4.457684	5.228260	0.150824
5	C	3.359730	6.069109	-0.074336
6	C	2.136171	5.540508	-0.466202
7	H	2.970314	2.247611	-0.519744
8	H	5.145219	3.192747	0.153611
9	H	3.472440	7.142081	0.024763
10	H	1.292368	6.194876	-0.644813
11	C	5.768888	5.770872	0.552415
12	C	0.669024	3.612928	-1.041532
13	N	-0.423175	4.120338	-0.519364
14	N	6.866175	5.178244	0.136194
15	C	-1.003694	2.484648	-1.932479
16	C	-1.999740	1.635575	-2.655254
17	H	-1.452808	1.004201	-3.351711
18	H	-2.519948	0.989040	-1.938323
19	C	0.365484	2.550204	-1.965010
20	C	6.070473	6.889079	1.405772
21	C	5.137661	7.794901	2.141583
22	H	4.265979	7.229149	2.488110
23	H	5.642461	8.217705	3.013574
24	C	7.432517	6.898216	1.441961

25	C	8.452385	7.752197	2.138206
26	H	8.588341	7.413720	3.166987
27	H	9.412395	7.633591	1.624796
28	O	-1.481665	3.403895	-1.084707
29	O	7.922086	5.893568	0.695212
30	C	1.285673	1.794793	-2.813881
31	H	2.295509	2.212687	-2.884365
32	H	1.687188	0.376667	-4.004378
33	N	4.687254	8.899357	1.244851
34	N	4.061656	9.801744	1.805734
35	N	3.484335	10.689247	2.211137
36	N	8.058467	9.170280	2.247124
37	N	8.103573	9.819558	1.195292
38	N	8.108681	10.527447	0.312925
39	N	0.923284	0.741890	-3.435966
40	N	-2.961785	2.433552	-3.446476
41	N	-3.932675	2.885446	-2.833718
42	N	-4.874719	3.346275	-2.404751

E_0 = -1424.100658 Hartree/particle; ZPE = 0.293828 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S21. Cartesian coordinates (in Å) for the optimized structure of compound **TNT** obtained using the B3LYP/6-311++G(d,p) level of theory


optimized structure
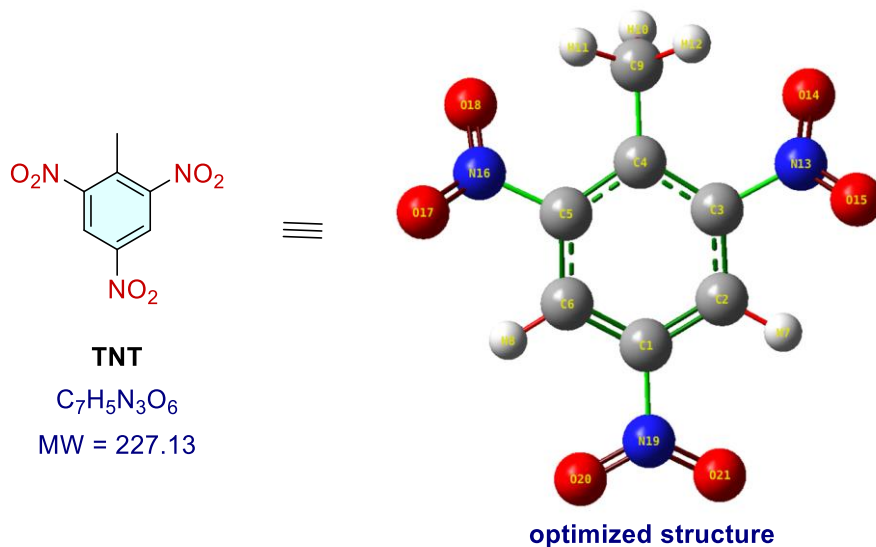
Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.597261	4.608254	-0.850586
2	C	2.657772	3.781366	-0.520382
3	C	3.551130	4.220788	0.445588
4	C	3.437258	5.444490	1.129105
5	C	2.329845	6.217375	0.737487
6	C	1.406789	5.826941	-0.221553
7	H	2.783498	2.820556	-0.999509
8	H	0.561655	6.454127	-0.468170
9	C	4.373170	5.854860	2.235370

10	H	5.209381	6.429721	1.831596
11	H	3.865132	6.482326	2.964868
12	H	4.786447	4.984463	2.740763
13	N	4.682632	3.301131	0.729155
14	O	5.787103	3.800233	0.881851
15	O	4.429510	2.106955	0.762326
16	N	2.083680	7.547550	1.350937
17	O	0.923199	7.835382	1.599371
18	O	3.052508	8.267559	1.538711
19	N	0.637246	4.174154	-1.893531
20	O	-0.285036	4.931852	-2.152145
21	O	0.837781	3.090177	-2.419191

E_0 = -885.154386 Hartree/particle; ZPE = 0.134371 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S22. Cartesian coordinates (in Å) for the optimized structure of compound **TNT-A** obtained using the B3LYP/6-311++G(d,p) level of theory


TNT

$C_7H_5N_3O_6$

MW = 227.13

TNT-A

optimized structure
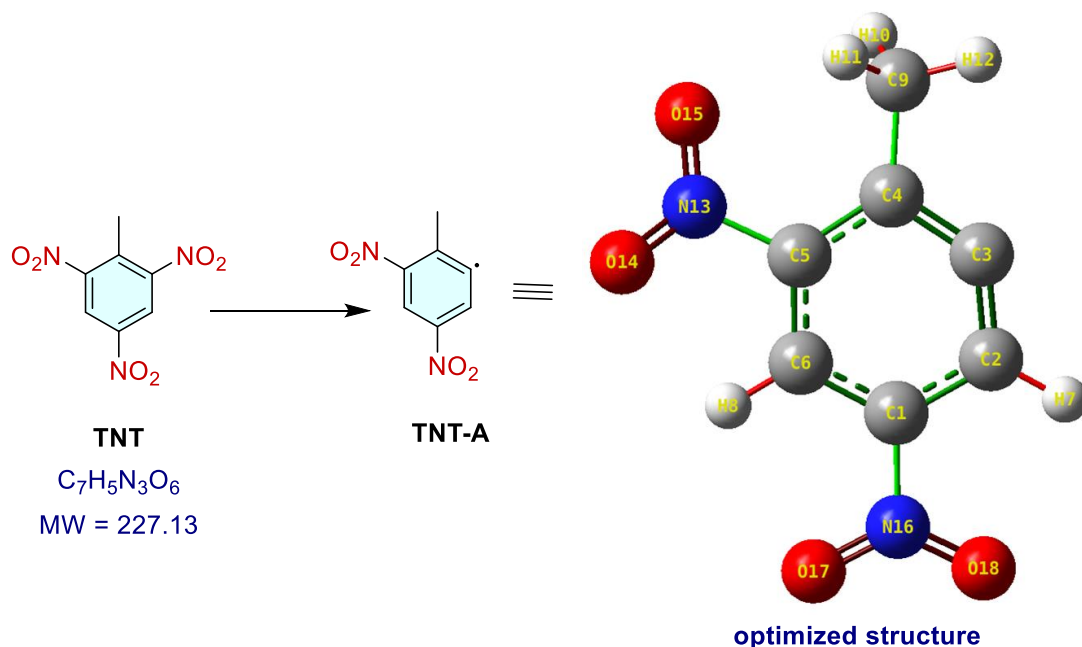
Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.591948	4.601005	-0.833609
2	C	2.651918	3.762255	-0.475255
3	C	3.475031	4.257161	0.498263
4	C	3.404740	5.468670	1.158326
5	C	2.309046	6.254927	0.738237
6	C	1.404086	5.835931	-0.232521
7	H	2.782896	2.798284	-0.950078
8	H	0.569865	6.463293	-0.510171
9	C	4.413441	5.826863	2.218565
10	H	5.086213	6.608208	1.859756
11	H	3.931608	6.214226	3.117486
12	H	4.997731	4.943298	2.474969

13	N	2.058124	7.595392	1.326884
14	O	0.908768	8.009485	1.311081
15	O	3.018951	8.201511	1.780986
16	N	0.640651	4.157094	-1.880540
17	O	-0.269412	4.917460	-2.174936
18	O	0.833111	3.056879	-2.378711

E_0 = -679.935543 Hartree/particle; ZPE = 0.119143 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S23. Cartesian coordinates (in Å) for the optimized structure of compound **RDX** obtained using the B3LYP/6-311++G(d,p) level of theory


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.816365	-0.180319	0.408278
2	C	-0.138655	0.573606	1.753153
3	C	1.642655	2.196997	1.126967
4	H	2.423146	-0.515542	1.265272
5	H	2.233384	2.081240	2.050319
6	H	0.287267	0.308304	2.734482
7	H	2.055562	-0.778842	-0.461929
8	H	-1.217239	0.483652	1.789297
9	H	1.764945	3.201517	0.741427
10	N	2.055917	1.229800	0.114034
11	N	3.255253	1.519777	-0.555184
12	O	3.636600	2.676666	-0.513734
13	O	3.787506	0.595563	-1.145094
14	N	0.389907	-0.288735	0.700205
15	N	0.226962	1.935438	1.372693
16	N	-0.151688	-1.581794	0.637646
17	O	0.485893	-2.410137	0.010757
18	O	-1.226661	-1.749848	1.187054
19	N	-0.480820	2.961172	2.018260

20	O	-1.543401	2.652274	2.529283
21	O	0.015144	4.073872	1.979381

E_0 = -897.516473 Hartree/particle; ZPE = 0.141466 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S24. Cartesian coordinates (in Å) for the optimized structure of compound **RDX-A** obtained using the B3LYP/6-311++G(d,p) level of theory
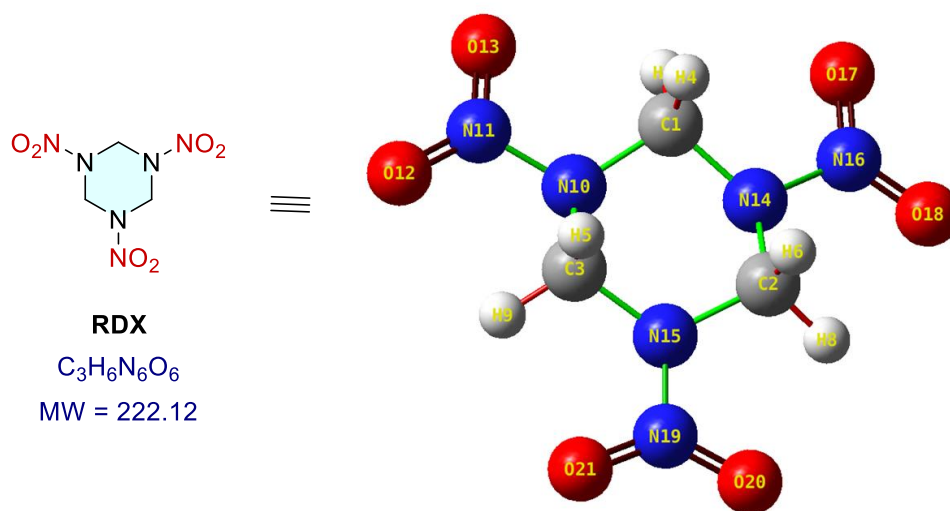

RDX
$C_3H_6N_6O_6$
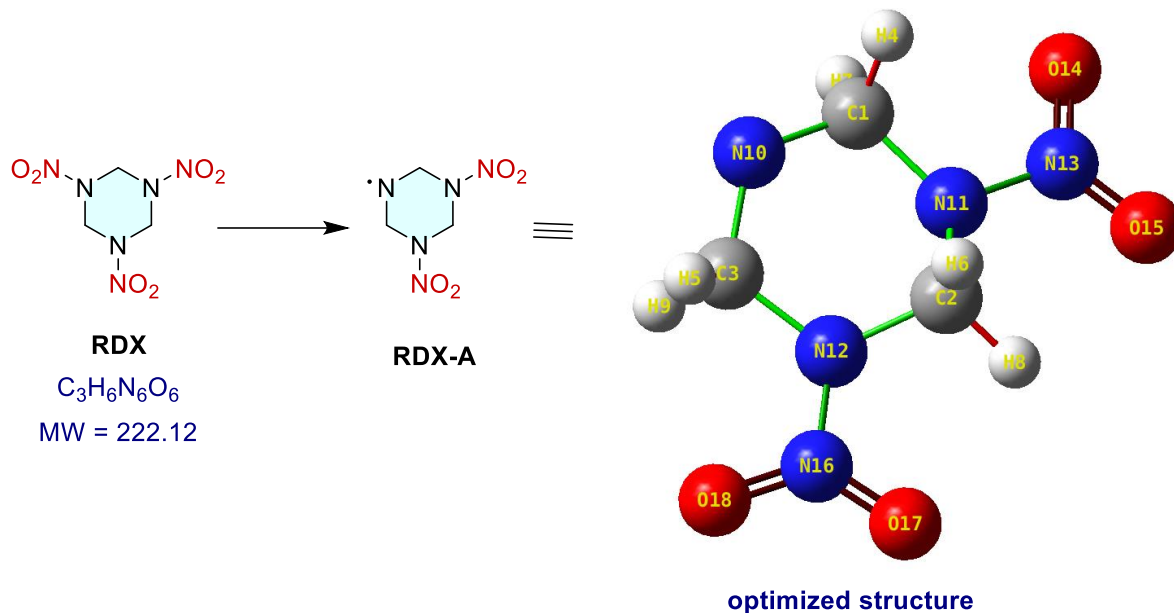MW = 222.12

RDX-A

optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.729397	-0.135230	0.242168
2	C	-0.066072	0.531506	1.851363
3	6	1.586271	2.223979	1.032743
4	H	2.363649	-0.921563	0.678771
5	H	2.148909	2.657285	1.873329
6	H	0.492004	0.257247	2.760821
7	H	1.751433	-0.300874	-0.842540
8	H	-1.128030	0.407489	2.029541
9	H	1.546393	3.006872	0.264488
10	N	2.330636	1.125004	0.518705
11	N	0.339334	-0.278807	0.714634
12	N	0.208514	1.902285	1.452293
13	N	-0.218467	-1.545026	0.605552
14	O	0.340579	-2.307974	-0.171027
15	O	-1.222981	-1.778803	1.260573
16	N	-0.480986	2.906993	2.116230
17	O	-1.475949	2.586889	2.749105
18	O	-0.036682	4.038882	1.977731

E_0 = -692.338611 Hartree/particle; ZPE = 0.124580 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

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