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3-Amino-1,2,4(4*H*)-oxadiazol-5-one (AOD) and its Nitrogen-Rich Salts: A Class of Insensitive Energetic Materials

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SUPPORTING INFORMATION

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General Experimental

All solvents used were purchased from Merck and were distilled and dried with molecular sieves prior to usage. Sodium dicyanamide (purity 96%), hydroxylamine hydrochloride (purity 99%), sodium hydroxide pellets (purity 99%) were purchased from Alfa Aesar, and hydroxylamine solution (50 wt. % in H_2O), hydrazine solution (purity 99%) were purchased from Sigma Aldrich and was used as received. FT-IR spectra were recorded using pressed KBr pellets on a Shimadzu IR Prestige-21 spectrometer. FT-Raman spectra were recorded using a Bruker FT Raman 1064 nm Nd:YAG laser. ^{1}H and ^{13}C NMR spectra were recorded with a 300 MHz Bruker Avance Nuclear magnetic resonance spectrometer operating at 300.13 and 75.48 MHz respectively, using DMSO-d_6 as the solvent and TMS as the internal standard. The chemical shifts in ppm are reported relative to TMS. Single-crystal X-ray data were collected at 100 K on Bruker SMART APEX3 CCD single-crystal diffractometer by using graphite-monochromated Mo Kα radiation (0.71073 Å). Thermogravimetric analysis (TGA) data was obtained by subjecting the sample and reference to a temperature scanning program from 50–500 ^{o}C at 10 ^{o}C min^{-1}. DTA measurements were recorded using Shimadzu, DTG 50H. Bomb calorimetry measurements were performed on a Parr 6200 bomb calorimeter using an 1108P oxygen bomb. The sample was burned inside the oxygen bomb pressurized to 3.2 MPa with pure oxygen. Sensitivity measurements were made using standard BAM Fall hammer with 2 kg drop weight and BAM friction tester. Kinetic analysis of the compounds was done by the method of Kissinger and Ozawa, using differential heating rate method, as per the ASTM standard.[1] Energy of activation was calculated from the peak values of exothermic decomposition peaks from DTA thermogram. Experiments were carried out from 50–500 ^{o}C at different heating rates of β=2, 4, 6, and 8 ^{o}C. The rate constant for the solid state decomposition was assumed to follow the Arrhenius rate law, and the first stage exothermic decomposition reaction is used to calculate the kinetic parameters, considering it as a single step. In the present study activation energies were computed using the logarithmic relations coined by Kissinger.[2] The calculated activation energy from Ozawa relation was refined as per the ASTM procedure. The simplified form of Ozawa (refined form) and Kissinger relations used for activation energy calculation are given in Equation (4) and (5).

$$E_a = -2.303\ R/D\ [d \log_{10} \beta/d\ (1/T)] \qquad (4)$$

$$E_a = -\ R\ [d \ln (\beta/Tp^2)/d\ (1/T)] \qquad (5)$$

Experimental Procedures:

General procedure for the preparation of AOD (3): Hydroxylamine hydrochloride (14 g, 0.20 mol) and sodium hydroxide (8 g, 0.20 mol) were dissolved in 50 ml of water. The reaction was heated at 40 ^{o}C, and sodium dicyanamide (9 g, 0.10 mol) in 50 mL of water was added drop-wise and the reaction was allowed to stir for another 4 h at 70 ^{o}C. Finally, the reaction mixture was cooled and acidified with concentrated hydrochloric acid (37%) till pH=1 and the white precipitate was filtered off. The precipitate was washed with cold water to obtain crude AOD (**3**) and recrystallized from hot methanol to produce white solid (6.20 g) in 60% yield.

General procedure for the preparation of salts 5 and 6 from AOD: A solution of 1 equiv. of hydroxylamine, (0.654 g, 0.01 mol), or hydrazine (0.316 g, 0.01 mol) was slowly added drop wise to a solution of AOD (1.0 g, 0.01 mol) in 10 mL of methanol/ethanol (2:1) at room temperature respectively. After stirring for 30 min at room temperature, the suspended AOD reaction mixture turned to a clear solution and re-precipitated as the respective salt and was filtered off, and dried to obtain the desired products **5** and **6**.

3-amino-1,2,4(4*H*)- oxadiazol-5-one (3): Yield: white solid, 6.20 g (60 %); FTIR (KBr) = 3356, 3204, 3076, 2880, 2720, 1796, 1686, 1533, 1466, 1385, 1261, 1124, 1070, 989, 906, 739 cm^{-1}; Raman (300 mW, 25 °C, cm^{-1}): ν = 3471, 3209, 2722, 1745, 1660, 1629, 1539, 1453, 1264, 1125, 1070, 988, 905, 769, 668, 589, 370 cm^{-1}; ^{1}H NMR (DMSO-d_6, ppm): δ = 6.19 (s, 2H); ^{13}C NMR (DMSO-d_6, ppm): δ = 159.1, 157.5; Δ_{comb} U: –2073.9 cal g^{-1}.

Hydroxylammonium-3-amino-5-oxo-1,2,4-oxadiazol-4-ide (5): Yield: white solid, 1.20 g (91 %); FTIR (KBr) = 3458, 3358, 3205, 2962, 2881, 2721, 2358, 1797, 1757, 1683, 1662, 1533, 1471, 1274, 1244, 1103, 1070, 989, 972, 939, 783. 680, 590 cm^{-1}; Raman (300 mW, 25 °C, cm^{-1}): ν = 3355, 1622, 1573, 1452, 1251, 1117, 1009, 975, 939, 797, 681, 589 cm^{-1}; ^{1}H NMR (DMSO-d_6, ppm): δ = 7.11 (br), 6.11 (br); ^{13}C NMR (DMSO-d_6, ppm): δ = 160.6, 159.7; Δ_{comb} U: –1682.5 cal g^{-1}.

Hydrazinium-3-amino-5-oxo-1,2,4-oxadiazol-4-ide (6): Yield: white solid, 0.465 g (70 %); FTIR (KBr) = 3387, 3323, 1674, 1620, 1556, 1467, 1236, 1176, 1118, 1091, 968, 898, 796, 785, 678 cm^{-1}; Raman (300 mW, 25 °C, cm^{-1}): ν = 3327, 3201, 3152, 1689, 1653, 1630, 1537, 1483, 1238, 1101, 978, 898, 777, 681 cm^{-1}; ^{1}H NMR (DMSO-d_6, ppm): δ = 7.47 (br), 5.46 (br); ^{13}C NMR (DMSO-d_6, ppm): δ = 170.9, 166.9; Δ_{comb} U: –2484.5 cal g^{-1}.

X-ray crystallography

X-ray reflections for compounds **3**, **4c**, **5** and **6** were collected on a Bruker diffractometer that was equipped with a graphite monochromator and a Mo Kα fine-focus sealed tube (λ = 0.71073 Å). Data integration was done by using SAINT.[3] The intensities of the absorption were corrected by using SADABS.[4] Structure solution and refinement were carried out by using Bruker SHELX-TL.[5] All non-hydrogen atoms were refined anisotropically and the C-H hydrogen atoms were placed at fixed positions. CCDC-1407655 (**3**), CCDC-1561177 (**4c**), CCDC-1560543 (**5**), and CCDC-1561922 (**6**) 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.

The complete list of hydrogen-bond geometry, bond lengths, bond angles, atom coordinates, refinements and thermal displacement parameters are detailed in Table S1-S17.

Table S1. Hydrogen-bond geometry (Å, o) for **5**.

D–H···A	*D*–H	H···A	*D*···A	<*D*–H···A
N4–H4B···N2	0.91	1.90	2.76	158
N4–H4A···O2	0.91	1.85	2.74	168
O3–H3···N1	0.84	1.82	2.65	171

Symmetry elements: (i) -x,1/2+y,1/2-z; (ii) x,1/2-y,1/2+z

Table S2. Hydrogen-bond geometry (Å, o) for **6**.

D–H···A	*D*–H	H···A	*D*···A	<*D*–H···A
N3–N3H···O2	0.88	2.20	3.02	154
N5–N1H···O2	0.88	2.52	2.96	111
N5–N2H···O2	0.90	2.09	2.97	163
N4–H4B···N1	0.91	1.90	2.76	155
N4–H4C···N5	0.91	2.01	2.90	165

Symmetry elements: (i) -x, -y, 1/2+z; (ii) 1/2-x, 1/2+y, 1/2+z

Table S3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for **3**. U(eq) is defined as one third of the trace of the orthogonalzed U_{ij} tensor.

	x/a	**y/b**	**z/c**	**U(eq)**
C1	0.1133(2)	0.9611(6)	0.98696(19)	0.0107(4)
C2	0.2131(2)	0.7070(6)	0.16092(19)	0.0109(4)
N1	0.0865(2)	0.8782(5)	0.08729(17)	0.0108(4)
N2	0.2215(2)	0.5783(6)	0.26671(17)	0.0142(4)
N3	0.3182(2)	0.6661(5)	0.11256(16)	0.0140(4)
O1	0.03366(17)	0.1251(4)	0.90006(14)	0.0145(4)
O2	0.25253(15)	0.8311(4)	0.99774(12)	0.0130(4)

Table S4. Bond lengths (Å) for **3**.

C1-O1	1.222(3)	C1-O2	1.350(3)
C1-N1	1.356(3)	C2-N3	1.311(3)
C2-N2	1.342(3)	C2-N1	1.372(3)
N3-O2	1.451(2)		

Table S5. Bond angles (°) for **3**.

O1-C1-O2	123.0(2)	O1-C1-N1	129.7(2)
O2-C1-N1	107.35(19)	N3-C2-N2	125.1(2)
N3-C2-N1	111.99(19)	N2-C2-N1	122.7(2)
C1-N1-C2	107.8(2)	C2-N3-O2	103.98(15)
C1-O2-N3	108.85(15)		

Table S6. Anisotropic atomic displacement parameters ($Å^2$) for **3**. The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}]$

	U_{11}	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
C1	0.0079(8)	0.0118(9)	0.0122(9)	-0.0020(8)	0.0032(7)	-0.0019(7)
C2	0.0096(8)	0.0114(9)	0.0108(9)	-0.0005(8)	0.0021(7)	0.0012(7)
N1	0.0071(8)	0.0147(8)	0.0105(8)	0.0009(7)	0.0028(7)	0.0021(6)
N2	0.0121(9)	0.0189(9)	0.0118(9)	0.0007(7)	0.0044(7)	0.0037(7)
N3	0.0105(8)	0.0204(10)	0.0101(9)	0.0022(7)	0.0022(7)	0.0042(7)
O1	0.0096(8)	0.0190(8)	0.0135(8)	0.0033(6)	0.0018(6)	0.0007(6)
O2	0.0098(8)	0.0188(8)	0.0110(7)	0.0024(6)	0.0042(6)	0.0024(6)

Table S7. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for **3**.

	x/a	**y/b**	**z/c**	**U(eq)**
H1	0.0028	0.9257	0.1025	0.016
H1N	0.306(3)	0.494(8)	0.314(2)	0.021
H2N	0.163(4)	0.677(9)	0.300(2)	0.021

Table S8. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for **5**. U(eq) is defined as one third of the trace of the orthogonalzed U_{ij} tensor.

	x/a	**y/b**	**z/c**	**U(eq)**
C1	0.67957(15)	0.23522(16)	0.55496(9)	0.0095(2)
C2	0.41578(15)	0.28413(17)	0.60291(9)	0.0106(2)
N1	0.35150(13)	0.26858(15)	0.49318(8)	0.01143(19)
N2	0.61388(13)	0.26397(15)	0.64558(8)	0.01084(19)
N3	0.29387(15)	0.30778(18)	0.67022(9)	0.0160(2)
N4	0.90604(13)	0.35396(15)	0.83931(8)	0.01038(19)
O1	0.52772(11)	0.23311(13)	0.45906(6)	0.01102(17)
O2	0.85080(11)	0.21185(13)	0.54821(7)	0.01210(18)
O3	0.02612(11)	0.17328(14)	0.82915(7)	0.01426(18)

Table S9. Bond lengths (Å) for **5**.

C1-O2	1.2430(13)	C1-N2	1.3371(14)
C1-O1	1.3691(13)	C2-N1	1.3152(14)
C2-N3	1.3584(14)	C2-N2	1.3616(13)
N1-O1	1.4350(12)	N4-O3	1.4188(12)

Table S10. Bond angles (°) for **5**.

O2-C1-N2	129.50(10)	O2-C1-O1	119.31(9)
N2-C1-O1	111.19(9)	N1-C2-N3	122.87(10)
N1-C2-N2	115.26(10)	N3-C2-N2	121.79(10)
C2-N1-O1	103.32(8)	C1-N2-C2	103.84(9)
C1-O1-N1	106.37(8)		

Table S11. Anisotropic atomic displacement parameters (Å^2) for **5**. The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}]$

	U_{11}	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
C1	0.0106(4)	0.0079(4)	0.0090(4)	0.0000(3)	0.0007(4)	-0.0002(3)
C2	0.0090(4)	0.0097(5)	0.0127(5)	0.0004(4)	0.0023(4)	-0.0003(3)
N1	0.0084(4)	0.0129(4)	0.0126(4)	0.0002(3)	0.0021(3)	0.0012(3)
N2	0.0083(4)	0.0141(4)	0.0098(4)	-0.0004(3)	0.0017(3)	0.0005(3)
N3	0.0101(4)	0.0240(5)	0.0144(5)	-0.0011(4)	0.0044(3)	0.0005(4)
N4	0.0098(4)	0.0117(4)	0.0097(4)	-0.0003(3)	0.0028(3)	0.0007(3)
O1	0.0090(3)	0.0137(4)	0.0093(3)	-0.0004(3)	0.0007(3)	0.0008(3)
O2	0.0099(3)	0.0151(4)	0.0115(4)	-0.0006(3)	0.0032(3)	0.0009(3)
O3	0.0103(3)	0.0168(4)	0.0134(4)	-0.0041(3)	-0.0006(3)	0.0045(3)

Table S12. Hydrogen atomic coordinates & isotropic atomic displacement parameters (Å^2) for **5**.

	x/a	**y/b**	**z/c**	**U(eq)**
H1N	0.178(2)	0.357(3)	0.6391(14)	0.024
H2N	0.352(2)	0.363(3)	0.7361(12)	0.024
H4A	0.8740	0.3450	0.9056	0.016
H4B	0.7944	0.3522	0.7817	0.016
H4C	0.9727	0.4806	0.8372	0.016
H3	1.1313	0.1779	0.8808	0.021

Table S13. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	**y/b**	**z/c**	**U(eq)**
C1	0.22679(14)	0.93941(17)	0.0350(5)	0.0115(4)
C2	0.35079(14)	0.03785(17)	0.2523(6)	0.0103(4)
N1	0.25605(12)	0.05307(14)	0.1257(5)	0.0117(4)
N2	0.38562(13)	0.92384(15)	0.2439(5)	0.0126(4)
N3	0.40764(12)	0.13302(15)	0.3684(6)	0.0139(4)
N4	0.08925(12)	0.20312(14)	0.1513(5)	0.0106(3)
N5	0.03124(12)	0.13804(15)	0.8812(5)	0.0123(4)
O1	0.30137(10)	0.85605(12)	0.0962(4)	0.0128(3)
O2	0.14548(10)	0.90308(13)	0.9126(5)	0.0150(3)

Table S14. Bond lengths (Å) for **6**.

C1-O2	1.242(2)	C1-N1	1.339(2)
C1-O1	1.366(2)	C2-N2	1.325(2)
C2-N3	1.354(3)	C2-N1	1.360(3)
N2-O1	1.452(2)	N4-N5	1.450(2)

Table S15. Bond angles (°) for **6**.

O2-C1-N1	129.84(18)	O2-C1-O1	119.19(17)
N1-C1-O1	110.97(16)	N2-C2-N3	121.73(17)
N2-C2-N1	115.64(17)	N3-C2-N1	122.60(17)
C1-N1-C2	104.24(15)	C2-N2-O1	102.22(15)
C1-O1-N2	106.92(13)		

Table S16. Anisotropic atomic displacement parameters (Å^2) for **6**. The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}]$

	U_{11}	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
C1	0.0126(9)	0.0107(8)	0.0113(9)	0.0000(7)	0.0015(8)	0.0012(7)
C2	0.0102(8)	0.0106(9)	0.0101(8)	0.0012(8)	0.0023(7)	0.0001(7)
N1	0.0107(8)	0.0099(7)	0.0145(7)	-0.0009(7)	0.0004(7)	0.0006(6)
N2	0.0109(7)	0.0104(7)	0.0166(8)	-0.0014(7)	-0.0018(7)	-0.0004(6)
N3	0.0123(8)	0.0098(8)	0.0195(9)	-0.0011(7)	-0.0025(8)	-0.0001(6)
N4	0.0115(7)	0.0105(7)	0.0099(8)	-0.0008(7)	-0.0013(6)	-0.0001(6)
N5	0.0126(7)	0.0120(8)	0.0122(8)	-0.0014(7)	-0.0025(7)	-0.0025(6)
O1	0.0120(6)	0.0099(6)	0.0166(8)	-0.0010(6)	-0.0013(6)	-0.0001(5)
O2	0.0126(6)	0.0129(7)	0.0195(7)	-0.0018(6)	-0.0016(6)	-0.0025(5)

Table S17. Hydrogen atomic coordinates & isotropic atomic displacement parameters (Å^2) for **6**.

	x/a	**y/b**	**z/c**	**U(eq)**
H3N	0.3742(18)	0.202(2)	0.410(9)	0.021
H4N	0.4596(17)	0.116(2)	0.515(7)	0.021
H4A	0.0892	0.2850	0.1001	0.016
H4B	0.1533	0.1745	0.1504	0.016
H4C	0.0617	0.1907	0.3729	0.016
H1N	-0.0329(15)	0.145(2)	-0.059(8)	0.018
H2N	0.0539(18)	0.0597(19)	-0.103(8)	0.018

Figure S1. Kissinger and Ozawa plot for **3**.

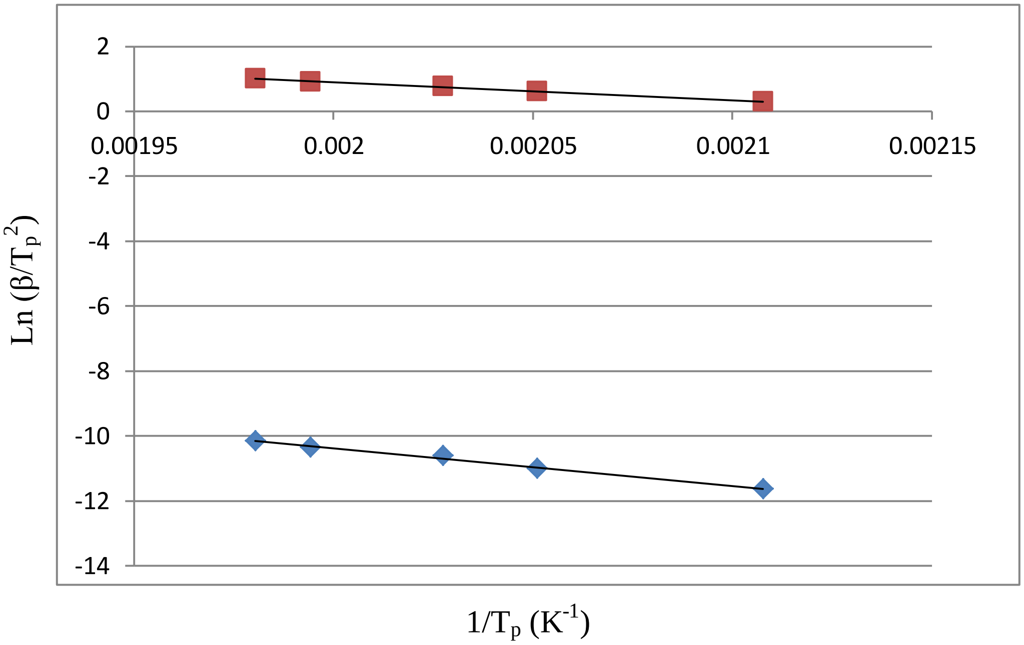


Figure S2. Kissinger and Ozawa plot for **5**.

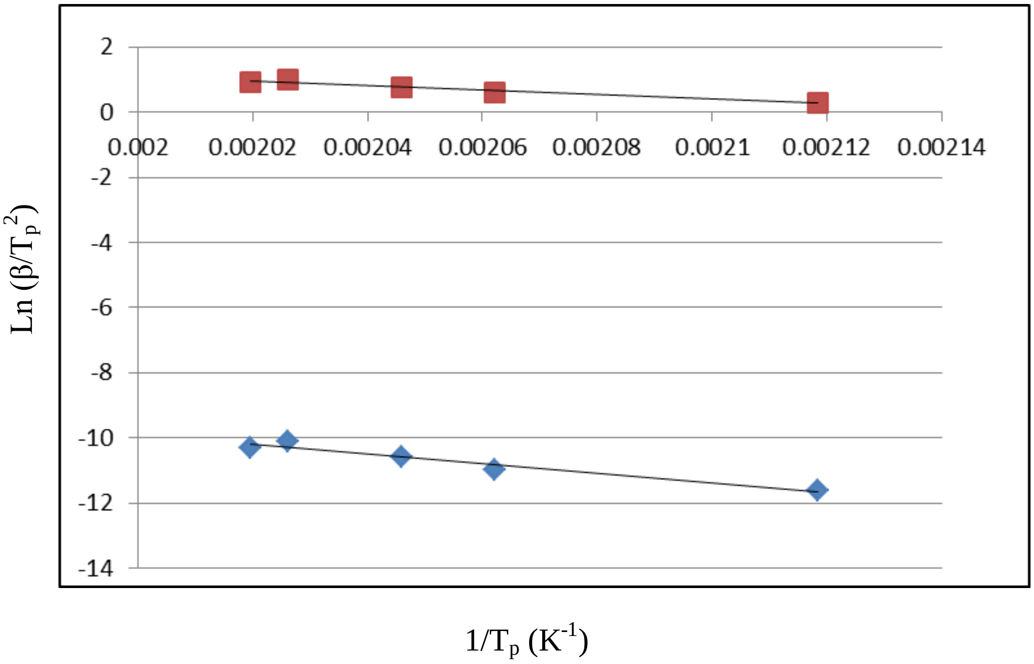
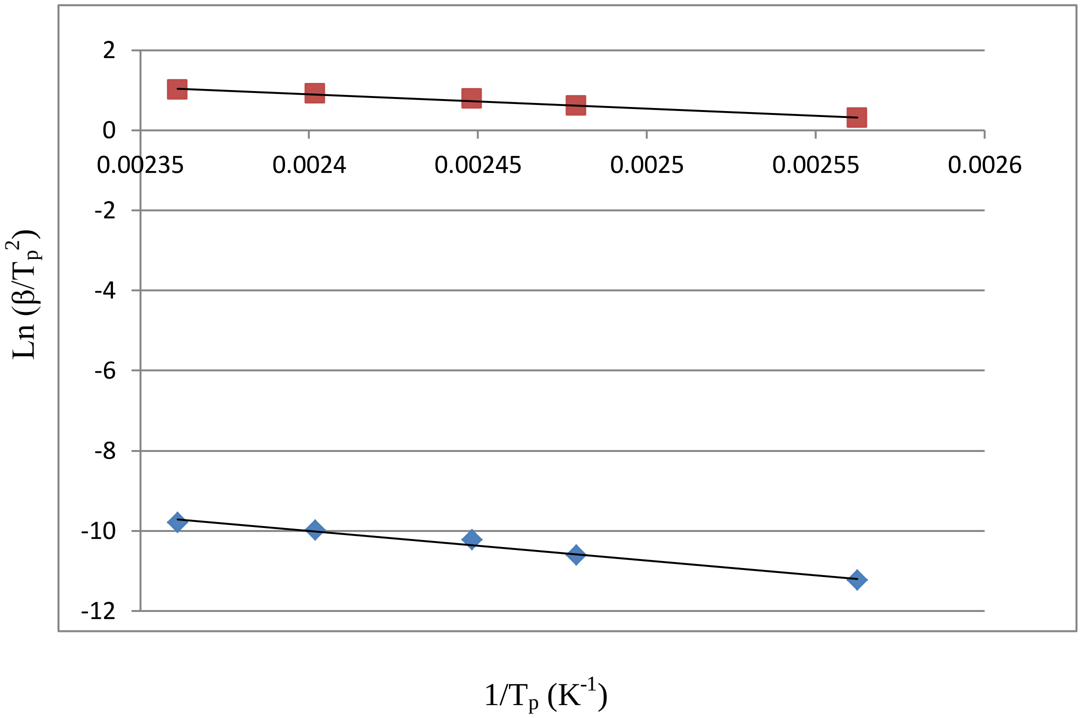


Figure S3. Kissinger and Ozawa plot for **6**.



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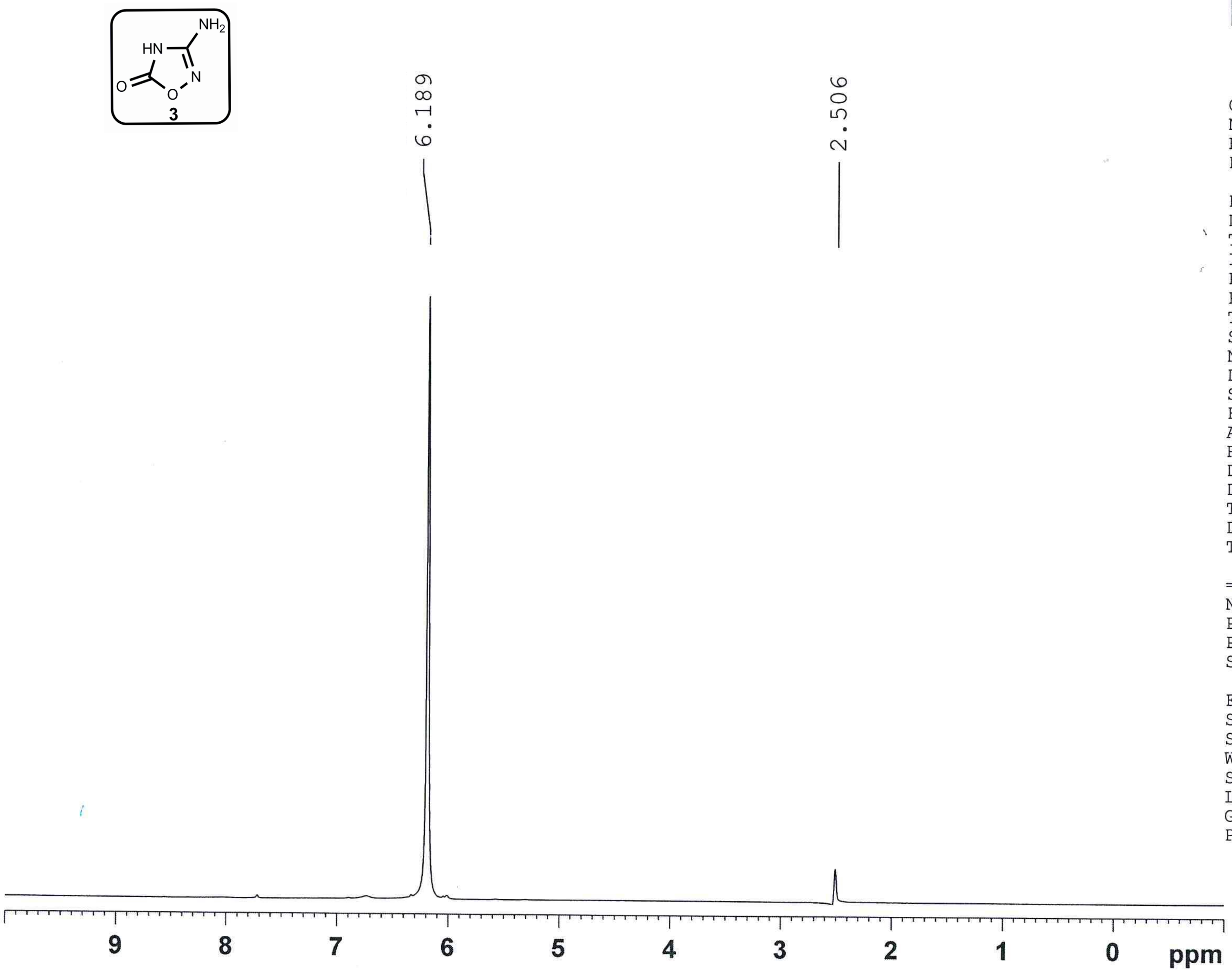
Proton NMR



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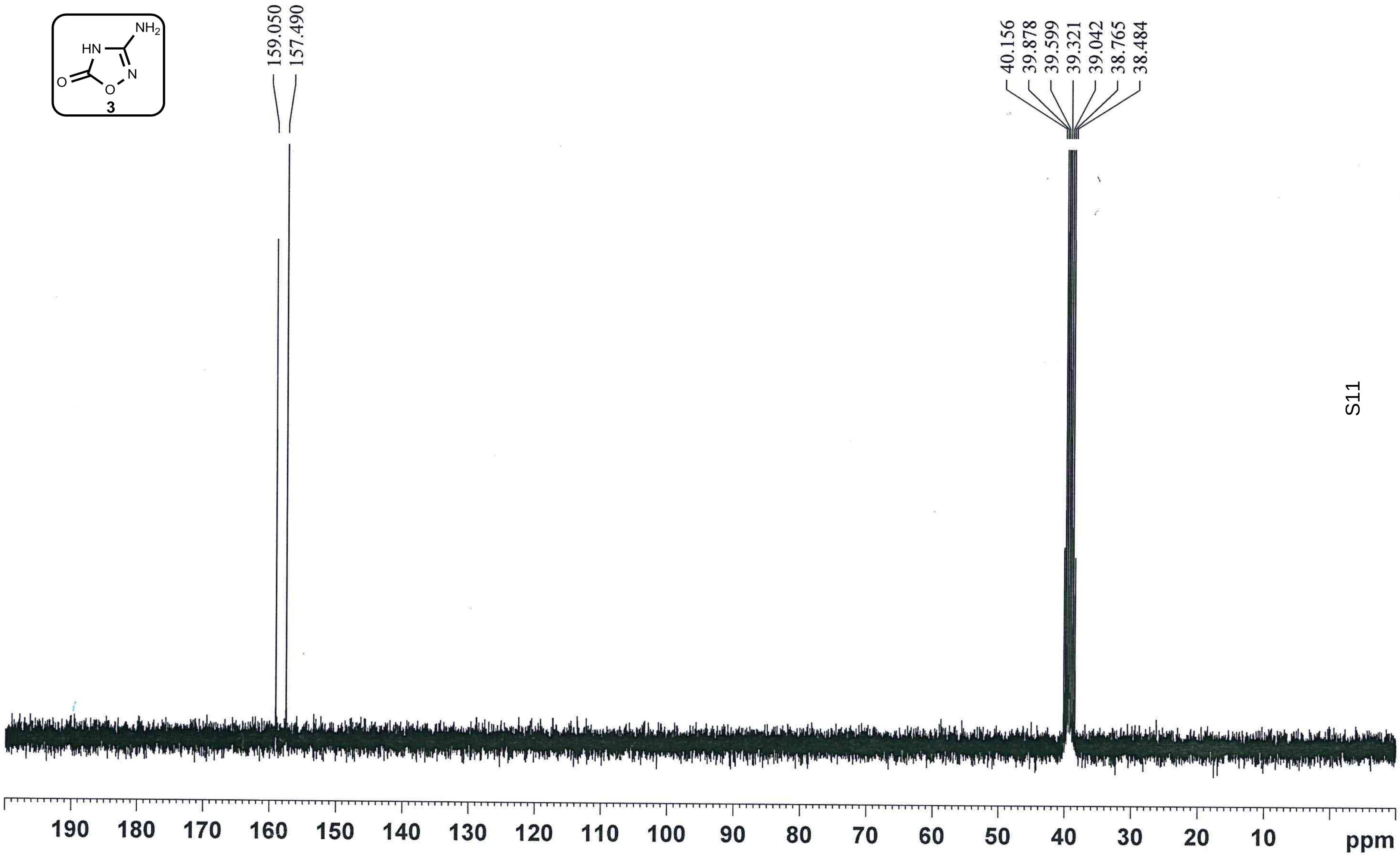
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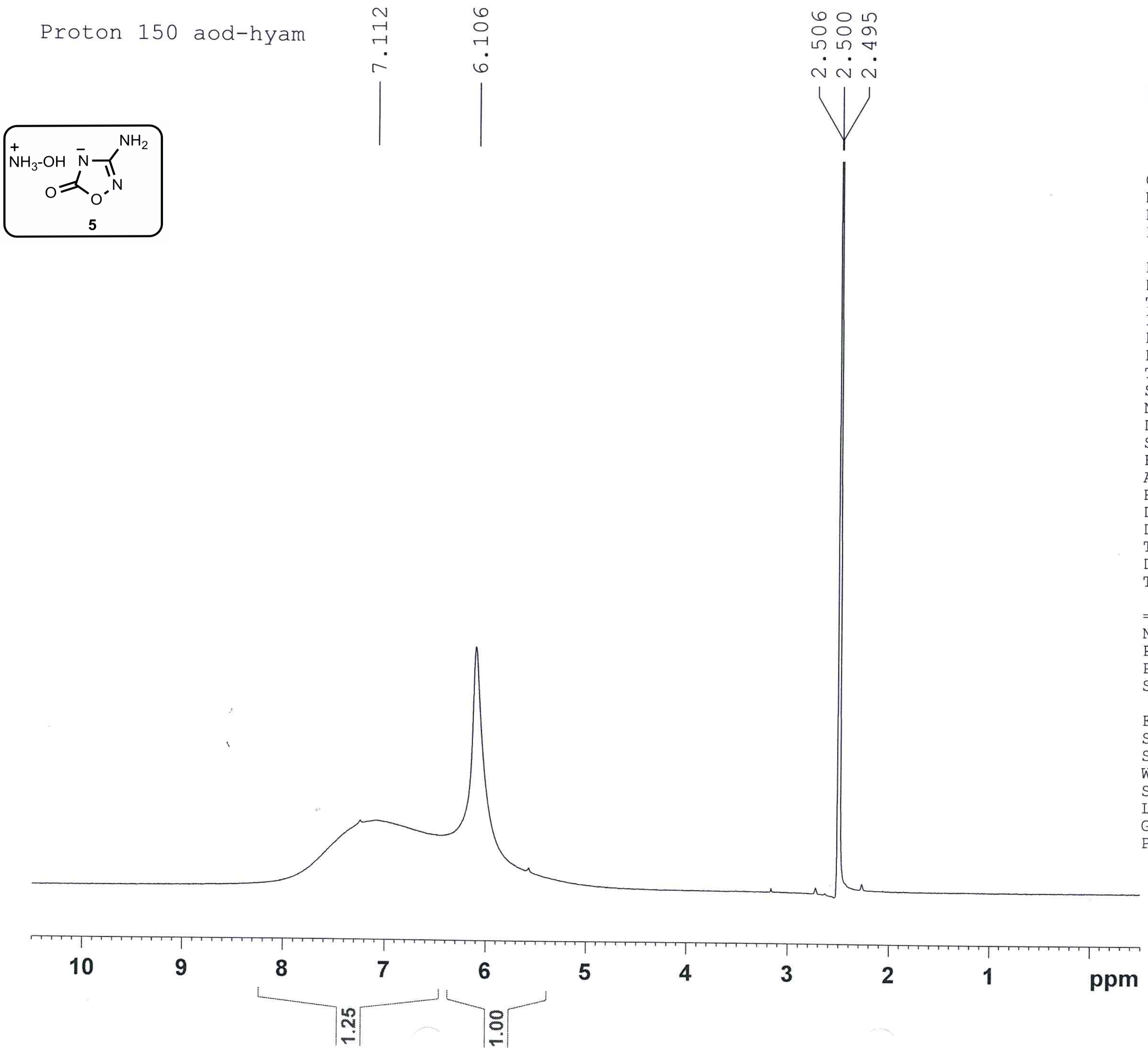

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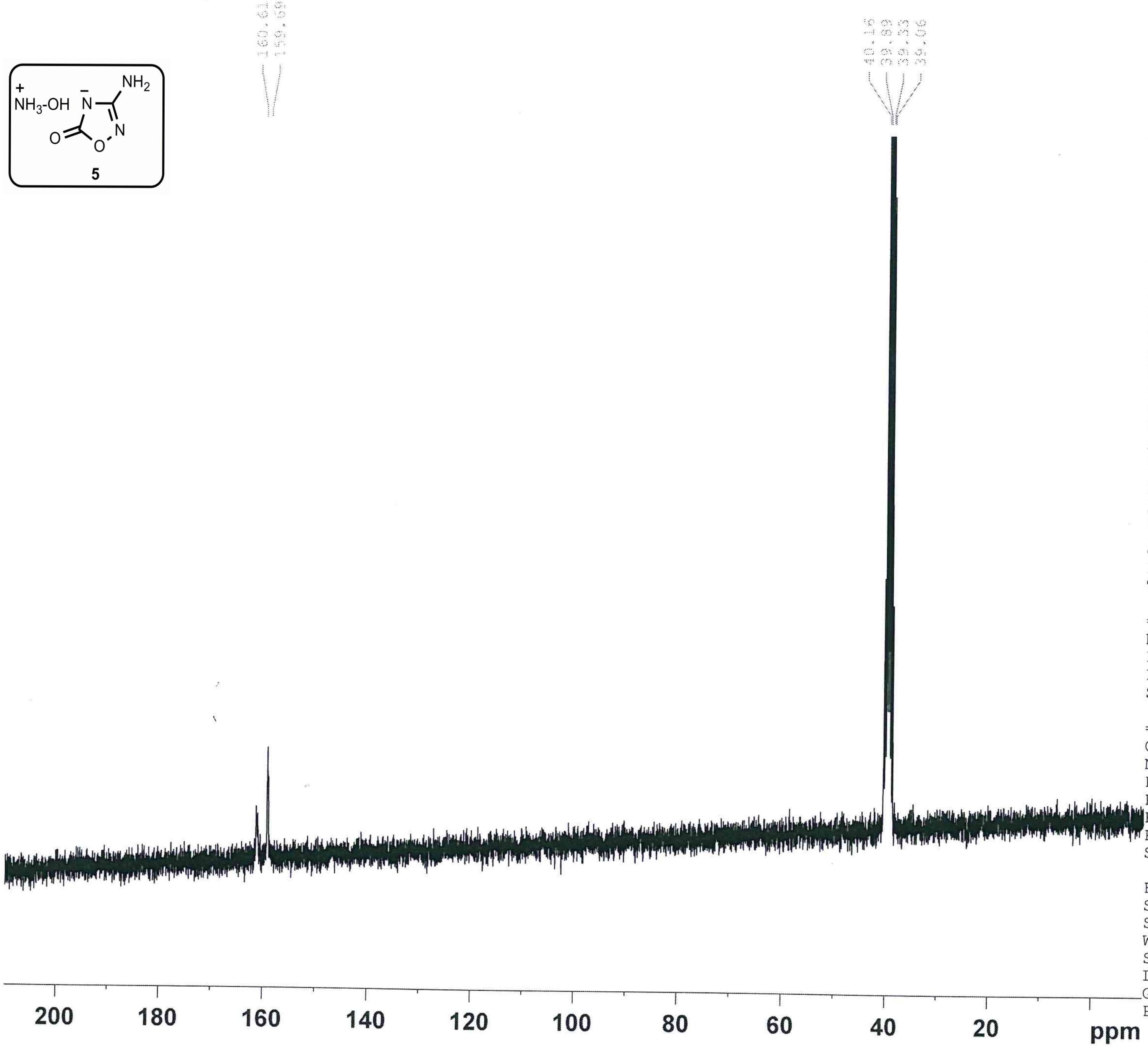
P1                     8.80 usec
PL1                   -3.00 dB
SFO1            300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF              300.1300019 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                    10.00
```

C13 137 aod-hyam



```
Current Data Parameters
NAME                carbon
EXPNO                  137
PROCNO                   1

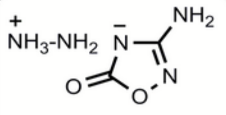
F2 - Acquisition Parameters
Date_             20170720
Time                 10.46
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                   65536
SOLVENT               DMSO
NS                     504
DS                       0
SWH              17985.611 Hz
FIDRES            0.274439 Hz
AQ               1.8219508 sec
RG                  1149.4
DW                  27.800 usec
DE                    6.00 usec
TE                   296.8 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

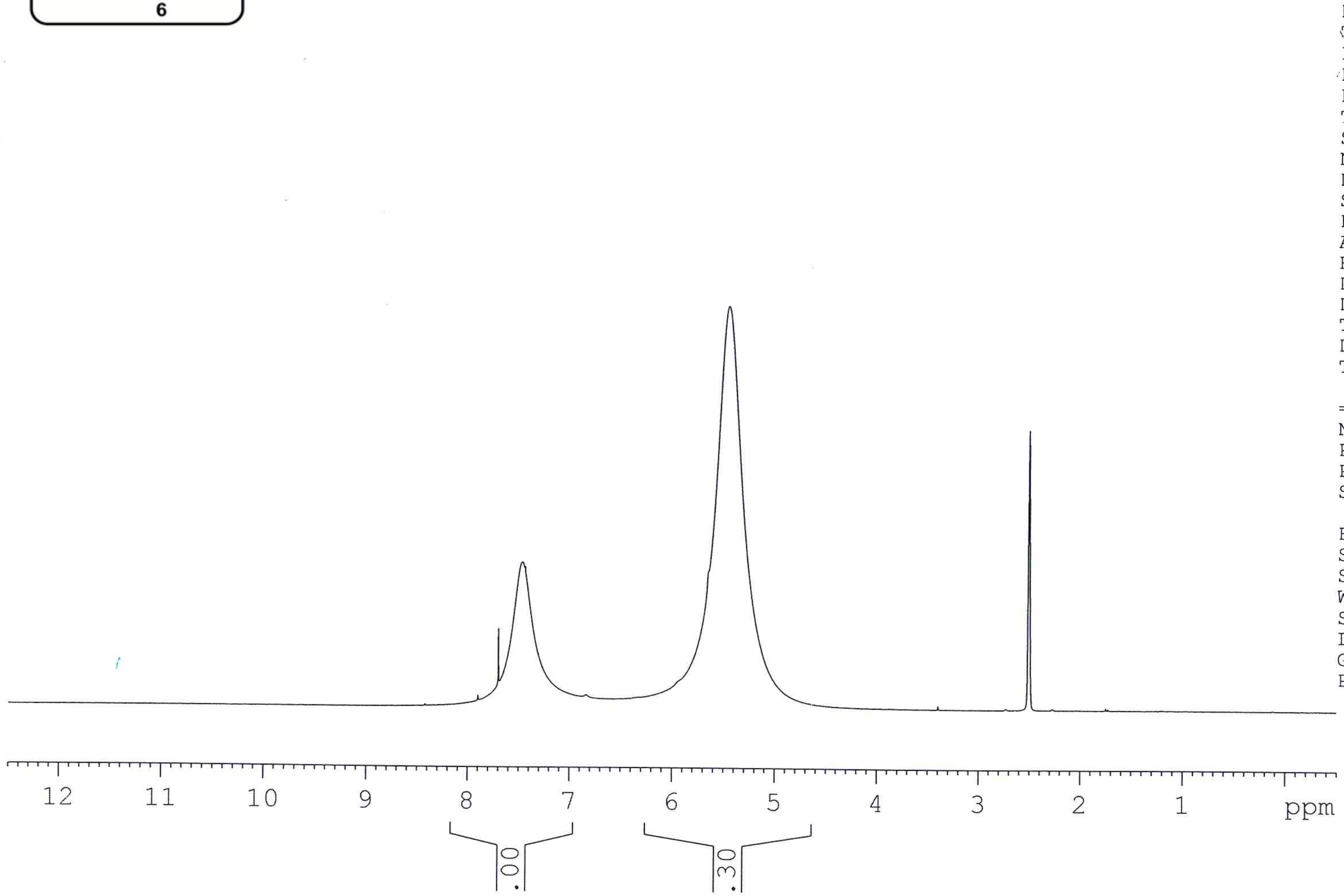
======== CHANNEL f1 ========
NUC1                   13C
P1                    9.50 usec
PL1                  -2.00 dB
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -3.00 dB
PL12                 16.17 dB
PL13                 18.00 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                   32768
SF              75.4677736 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    5.00
```

Proton 153 aod-hy


6

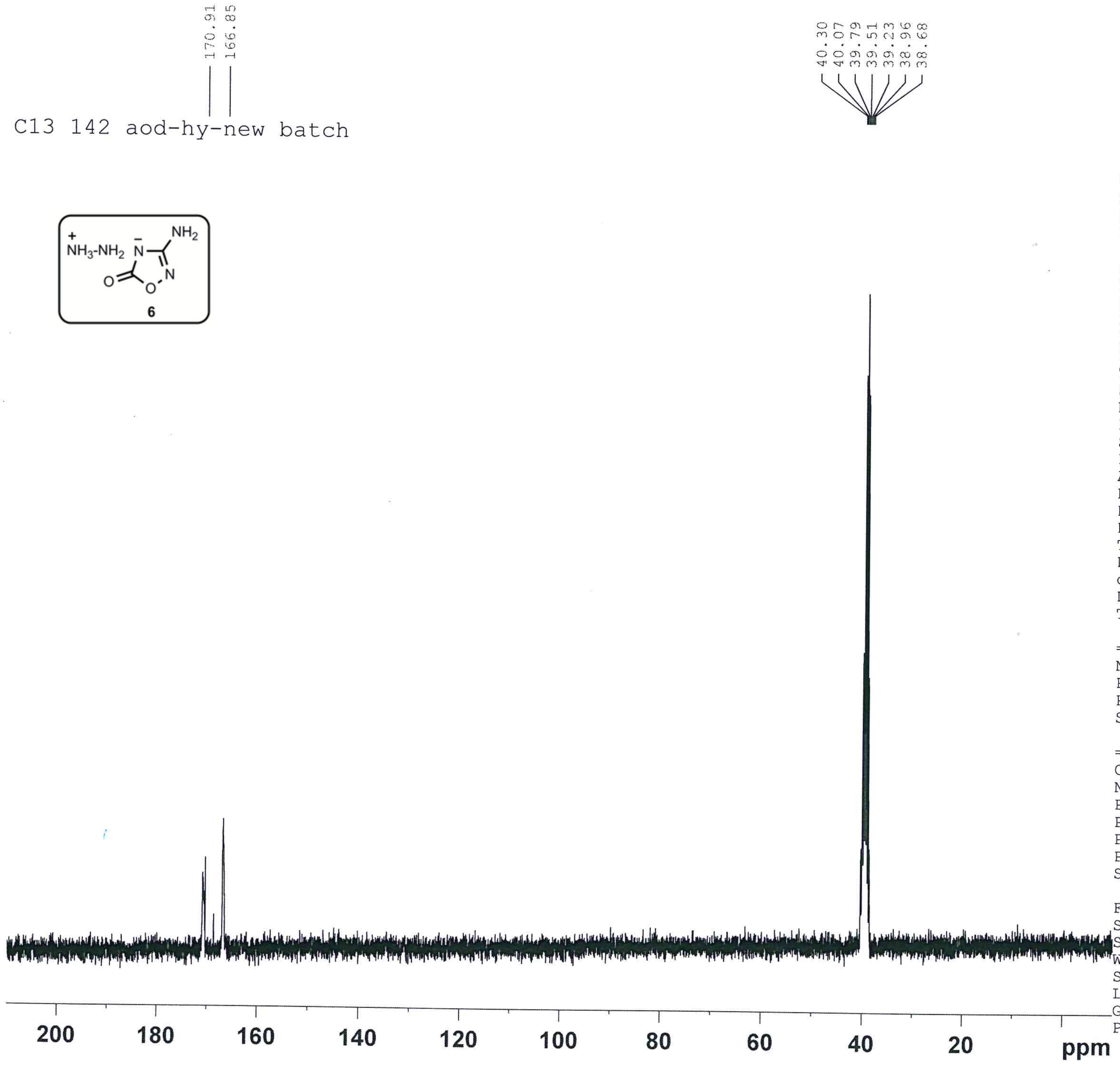


```
Current Data Parameters
NAME                 proton
EXPNO                   153
PROCNO                    1

F2 - Acquisition Parameters
Date_              20170803
Time                  12.32
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        8
DS                        0
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                5.3084660 sec
RG                     71.8
DW                   81.000 usec
DE                     6.00 usec
TE                    296.2 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                     8.80 usec
PL1                   -3.00 dB
SFO1            300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF              300.1300022 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                    10.00
```



```
Current Data Parameters
NAME                  carbon
EXPNO                    142
PROCNO                     1

F2 - Acquisition Parameters
Date_               20170818
Time                   12.10
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                 DMSO
NS                       204
DS                         0
SWH                17985.611 Hz
FIDRES              0.274439 Hz
AQ                 1.8219508 sec
RG                      3251
DW                    27.800 usec
DE                      6.00 usec
TE                     296.5 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      9.50 usec
PL1                    -2.00 dB
SFO1              75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -3.00 dB
PL12                   16.17 dB
PL13                   18.00 dB
SFO2             300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF                75.4677656 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.50
```