Supporting Information

Very thermostable energetic materials based on a fused-triazole: 3,6-Diamino-1*H*-[1,2,4]triazolo[4,3-*b*][1,2,4]triazole

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Crystal Structure Analysis

Table S1. Crystal data and structure refinement for **1.**

Compound	**1**
Formula	$C_3H_5N_7$
CCDC	2036395
$D_{calc.}$/ g cm^{-3}	1.766
μ/mm^{-1}	1.134
Formula Weight	139.14
Colour	colourless
Shape	needle
Size/mm^3	0.13×0.13×0.10
T/K	99.9(3)
Crystal System	monoclinic
Space Group	$P2_1/n$
a/Å	10.5503(4)
b/Å	3.56337(11)
c/Å	14.3130(5)
α/°	90
β/°	103.468(4)
γ/°	90
V/Å^3	523.29(3)
Z	4
Z'	1
Wavelength/Å	1.54184
Radiation type	Cu K_α
Θ_{min}/°	4.721
Θ_{max}/°	76.646
Measured Refl's.	4889
Indep't Refl's	1079
Refl's I≥2 (I)	1009
R_{int}	0.0360
Parameters	112
Restraints	0
Largest Peak	0.233
Deepest Hole	-0.203
GooF	1.092
wR_2 (all data)	0.0876
wR_2	0.0863
R_1 (all data)	0.0348
R_1	0.0334

Table S2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^3 x\ 10^3$) for **1**. U (eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	Ueq
N1	4227.6(11)	7427(3)	5884.0(8)	15.8(3)
N2	3588.8(10)	8884(3)	6563.0(8)	15.2(3)
N3	2181.9(10)	7619(3)	5210.7(7)	13.1(3)
N4	1208.7(10)	6851(3)	4396.2(7)	14.0(3)
N5	3253.2(10)	5202(3)	4193.1(7)	14.3(3)
N6	1330.6(10)	9974(3)	6505.8(8)	16.4(3)
N7	1389.3(11)	4508(3)	2886.0(8)	16.2(3)
C1	3353.2(12)	6628(4)	5074.2(9)	13.7(3)
C2	2336.4(12)	8962(4)	6127.5(9)	13.5(3)
C3	1927.7(12)	5438(3)	3825.6(9)	13.2(3)

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2\ [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

Atom	U11	U22	U33	U23	U13	U12
N1	11.1(5)	21.8(6)	14.1(5)	-2.0(4)	2.4(4)	2.6(4)
N2	14.3(5)	17.9(5)	13.8(5)	-1.3(4)	4.2(4)	2.1(4)
N3	10.3(5)	16.0(5)	12.7(5)	0.2(4)	2.0(4)	0.9(4)
N4	11.9(5)	16.9(5)	12.2(5)	-1.0(4)	0.6(4)	-0.2(4)
N5	12.3(5)	16.6(5)	13.9(5)	-0.5(4)	2.7(4)	0.6(4)
N6	13.5(6)	21.7(6)	13.7(5)	-2.3(4)	2.8(4)	3.5(4)
N7	15.2(6)	19.1(6)	14.0(5)	-2.2(4)	2.9(4)	0.8(4)
C1	12.1(6)	14.0(6)	15.1(6)	2.0(5)	3.3(5)	1.4(5)
C2	14.7(6)	12.9(6)	12.4(6)	1.2(4)	2.4(5)	0.3(5)
C3	13.6(6)	11.6(6)	14.2(6)	1.2(4)	3.0(5)	-0.6(4)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

Atom	x	y	z	U*eq*
H7A	1825(17)	2630(50)	2652(13)	26(4)
H6A	1503(16)	11090(50)	7085(13)	22(4)
H1	5069(19)	6920(60)	6033(13)	35(5)
H7B	497(18)	4240(50)	2751(12)	23(4)
H6B	584(19)	10760(60)	6092(13)	31(5)

Table S5. Bond lengths [Å] and angles [°] for **1.**

Atom	Atom	Length/Å	Atom	Atom	Atom	Angle/°
N1	N2	1.4047(14)	C1	N1	N2	109.51(10)
N1	C1	1.3332(17)	C2	N2	N1	105.62(10)
N2	C2	1.3234(16)	C1	N3	N4	110.57(10)
N3	N4	1.3896(14)	C1	N3	C2	108.84(11)
N3	C1	1.3426(16)	C2	N3	N4	140.55(10)
N3	C2	1.3703(16)	C3	N4	N3	99.98(9)
N4	C3	1.3357(16)	C1	N5	C3	100.76(10)
N5	C1	1.3407(16)	N1	C1	N3	106.94(11)
N5	C3	1.3772(16)	N1	C1	N5	141.78(12)
N6	C2	1.3480(16)	N5	C1	N3	111.29(11)
N7	C3	1.3731(16)	N2	C2	N3	109.07(11)
			N2	C2	N6	127.55(11)
			N6	C2	N3	123.29(11)
			N4	C3	N5	117.40(11)
			N4	C3	N7	121.70(11)
			N7	C3	N5	120.73(11)

Table S6. Torsion angles [°] for **1.**

Atom	Atom	Atom	Atom	Angle/°
N1	N2	C2	N3	-0.08(13)
N1	N2	C2	N6	176.55(12)
N2	N1	C1	N3	1.46(14)
N2	N1	C1	N5	-178.44(16)
N3	N4	C3	N5	0.45(14)
N3	N4	C3	N7	-174.85(11)
N4	N3	C1	N1	-179.62(10)
N4	N3	C1	N5	0.32(15)
N4	N3	C2	N2	178.21(14)
N4	N3	C2	N6	1.4(2)
C1	N1	N2	C2	-0.86(14)
C1	N3	N4	C3	-0.44(13)
C1	N3	C2	N2	0.99(14)
C1	N3	C2	N6	-175.82(12)
C1	N5	C3	N4	-0.28(14)
C1	N5	C3	N7	175.07(12)
C2	N3	N4	C3	-177.63(15)
C2	N3	C1	N1	-1.50(14)
C2	N3	C1	N5	178.44(10)
C3	N5	C1	N1	179.87(17)
C3	N5	C1	N3	-0.04(13)

Table S7. Hydrogen bonds for **1** [Å and °].

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N6	H6A	N21	0.900(18)	2.198(18)	3.0788(16)	166.2(15)
N1	H1	N52	0.88(2)	2.02(2)	2.8444(15)	155.3(17)
N6	H6B	N43	0.91(2)	2.04(2)	2.9177(15)	160.1(17)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z+1 #2 -x+3/2,y+1/2,-z+1/2 #3 -x+1,-y+1,-z+1
#4 -x+3/2,y-1/2,-z+3/2 #5 x+1/2,-y+3/2,z+1/2

Table S8. Crystal data and structure refinement for **4·H_2O.**

Compound	**4·H_2O**
Formula	$C_6H_8N_{12}O_7$
CCDC	2036394
$D_{calc.}$/ g cm^{-3}	1.794
μ/mm^{-1}	1.424
Formula Weight	360.24
Colour	yellow
Shape	needle
Size/mm^3	0.33×0.05×0.02
T/K	100.00(10)
Crystal System	monoclinic
Space Group	$P2_1/n$
a/Å	13.6133(4)
b/Å	4.83877(10)
c/Å	20.4591(5)
α/°	90
β/°	98.220(3)
γ/°	90
V/Å^3	1333.83(6)
Z	4
Z'	1
Wavelength/Å	1.54184
Radiation type	Cu K_α
Θ_{min}/°	3.671
Θ_{max}/°	77.645
Measured Refl's.	29865
Indep't Refl's	2788
Refl's I≥2 (I)	2020
R_{int}	0.1288
Parameters	253
Restraints	0
Largest Peak	0.338
Deepest Hole	-0.352
GooF	1.129
wR_2 (all data)	0.1345
wR_2	0.1012
R_1 (all data)	0.0748
R_1	0.0435

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4·H₂O**. U(*eq*) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U*eq*
O1	6690.6(15)	-147(4)	6721.8(10)	30.6(5)
O2	8134.7(15)	-1207(4)	7268.4(10)	30.7(5)
O3	10246.3(16)	-771(4)	6822.6(10)	31.9(5)
O4	10187.9(15)	2810(4)	7447.2(9)	29.7(5)
O5	10755.5(14)	4726(4)	6034.7(9)	25.9(4)
O6	9846.2(15)	7617(4)	5396.8(9)	26.9(4)
N8	7532.7(17)	3780(5)	6042.4(11)	23.4(5)
N9	8169.3(17)	5343(4)	5753.6(11)	23.2(5)
N10	7591.8(17)	133(4)	6850.9(11)	24.4(5)
N11	9897.1(16)	1442(4)	6954.2(11)	21.8(5)
N12	9951.3(17)	5725(4)	5803.4(11)	21.8(5)
C4	8073(2)	2126(5)	6484.0(12)	21.3(5)
C5	9074.0(19)	2576(5)	6503.2(12)	20.2(5)
C6	9086.4(19)	4600(5)	6027.1(12)	20.3(5)
O1W	12652.2(16)	2941(4)	7133.4(10)	32.0(5)
N1	6328.4(17)	601(5)	4736.2(11)	22.1(5)
N2	7030.9(17)	3454(5)	4047.9(11)	24.1(5)
N3	6020.6(16)	3975(4)	4044.8(10)	20.8(5)
N4	4493.3(17)	4988(5)	4002.8(11)	22.7(5)
N5	4654.3(17)	2795(4)	4453.5(11)	22.6(5)
N6	8029.3(19)	93(5)	4655.6(13)	28.5(5)
N7	5437.2(19)	7723(4)	3328.5(11)	23.1(5)
C1	7173(2)	1394(5)	4478.8(13)	22.9(6)
C2	5305(2)	5691(5)	3750.8(12)	21.3(5)
C3	5592.9(19)	2304(5)	4455.1(12)	20.7(5)

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4·H_2O**. The anisotropic displacement factor exponent takes the form: $-2^2\ [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

Atom	U11	U22	U33	U23	U13	U12
O1	27.0(11)	26.4(10)	38.3(12)	-5.2(9)	4.6(8)	-4.4(8)
O2	34.8(11)	23.8(10)	32.9(11)	9.0(8)	3.2(9)	2.4(8)
O3	40.5(12)	19.9(10)	32.7(11)	-5.8(8)	-3.9(9)	11.0(8)
O4	40.7(12)	20.6(10)	24.4(10)	-6.8(8)	-6.6(8)	2.2(8)
O5	23.5(10)	24.2(10)	29.6(10)	0.9(8)	2.0(8)	3.5(8)
O6	34.8(11)	19.7(9)	25.7(10)	6.8(7)	2.7(8)	0.7(8)
N8	24.8(12)	19.6(11)	25.2(11)	0.3(9)	2.1(9)	-0.1(9)
N9	25.7(12)	19.1(11)	24.1(11)	0.2(9)	1.2(9)	0.8(9)
N10	28.0(13)	16.7(11)	28.7(12)	-2.4(9)	5.0(9)	-1.9(9)
N11	26.0(12)	16.1(10)	22.6(11)	-0.5(8)	1.3(9)	0.5(9)
N12	26.4(12)	17.7(11)	20.7(11)	-1.4(8)	1.4(9)	1.1(9)
C4	25.0(13)	17.7(12)	20.9(12)	-0.4(10)	2.5(10)	-0.8(10)
C5	23.3(13)	13.4(11)	22.7(12)	-1.8(9)	-0.4(10)	2.3(10)
C6	21.9(13)	16.6(12)	21.5(12)	-2.2(10)	-0.3(10)	0.5(10)
O1W	35.5(12)	30.1(11)	30.0(11)	0.9(9)	3.5(9)	-0.3(9)
N1	25.5(12)	17.1(11)	23.1(11)	3.5(9)	0.9(9)	0.5(9)
N2	24.0(12)	18.3(11)	29.0(12)	4.3(9)	0.5(9)	1.2(9)
N3	23.1(12)	16.3(10)	22.6(11)	1.4(8)	1.9(8)	0.3(8)
N4	24.2(12)	18.5(10)	24.5(11)	3.8(9)	0.4(9)	1.9(9)
N5	26.4(12)	16.5(10)	24.3(11)	3.6(8)	1.3(9)	0.6(9)
N6	23.8(13)	23.3(12)	38.0(14)	8.1(11)	2.3(10)	3.1(10)
N7	28.0(13)	17.1(11)	24.1(11)	3.4(9)	2.8(9)	0.8(9)
C1	24.7(14)	18.0(12)	24.9(13)	0.5(10)	-0.2(10)	0.4(10)
C2	25.9(14)	16.2(12)	20.6(12)	-3.2(9)	-0.6(10)	-0.5(10)
C3	24.3(13)	15.9(12)	21.2(12)	0.4(9)	0.9(10)	-1.3(10)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **4·H_2O**.

Atom	x	y	z	U*eq*
H1WA	12637.86	4262.88	7405.19	48
H1WB	12408.28	3479.83	6748.71	48
H1	6230(30)	-590(80)	5028(19)	46(11)
H4	3820(20)	5740(70)	3925(15)	30(8)
H6A	8540(30)	710(80)	4533(19)	44(11)
H6B	8050(30)	-1240(80)	4919(18)	41(10)
H7A	6020(30)	7550(70)	3121(17)	35(9)
H7B	4820(30)	8400(80)	3121(18)	45(10)

Table S12. Bond lengths [Å] and angles [°] for **4·H_2O**.

Atom	Atom	Length/Å	Atom	Atom	Atom	Angle/°
O1	N10	1.225(3)	C4	N8	N9	107.7(2)
O2	N10	1.231(3)	C6	N9	N8	106.5(2)
O3	N11	1.217(3)	O1	N10	O2	125.1(2)
O4	N11	1.224(3)	O1	N10	C4	118.6(2)
O5	N12	1.228(3)	O2	N10	C4	116.3(2)
O6	N12	1.231(3)	O3	N11	O4	124.6(2)
N8	N9	1.349(3)	O3	N11	C5	118.8(2)
N8	C4	1.344(3)	O4	N11	C5	116.6(2)
N9	C6	1.342(3)	O5	N12	O6	124.4(2)
N10	C4	1.436(3)	O5	N12	C6	117.1(2)
N11	C5	1.453(3)	O6	N12	C6	118.5(2)
N12	C6	1.431(3)	N8	C4	N10	120.3(2)
C4	C5	1.376(4)	N8	C4	C5	111.7(2)
C5	C6	1.383(4)	C5	C4	N10	128.0(2)
N1	C1	1.386(3)	C4	C5	N11	129.0(2)
N1	C3	1.359(3)	C4	C5	C6	101.8(2)
N2	N3	1.397(3)	C6	C5	N11	128.9(2)
N2	C1	1.327(3)	N9	C6	N12	121.6(2)
N3	C2	1.354(3)	N9	C6	C5	112.3(2)
N3	C3	1.356(3)	C5	C6	N12	126.0(2)
N4	N5	1.403(3)	C3	N1	C1	105.8(2)
N4	C2	1.328(3)	C1	N2	N3	100.9(2)
N5	C3	1.299(3)	C2	N3	N2	139.3(2)
N6	C1	1.328(4)	C2	N3	C3	107.2(2)
N7	C2	1.338(3)	C3	N3	N2	113.5(2)
			C2	N4	N5	112.9(2)
			C3	N5	N4	101.6(2)
			N2	C1	N1	114.2(2)
			N2	C1	N6	125.2(3)
			N6	C1	N1	120.6(2)
			N4	C2	N3	104.9(2)
			N4	C2	N7	129.4(2)
			N7	C2	N3	125.6(2)
			N3	C3	N1	105.5(2)
			N5	C3	N1	140.9(2)
			N5	C3	N3	113.5(2)

Table S13. Torsion angles [°] for **4·H$_2$O**.

Atom	Atom	Atom	Atom	Angle/°
O1	N10	C4	N8	4.7(4)
O1	N10	C4	C5	-173.0(2)
O2	N10	C4	N8	-176.6(2)
O2	N10	C4	C5	5.7(4)
O3	N11	C5	C4	87.3(3)
O3	N11	C5	C6	-100.2(3)
O4	N11	C5	C4	-92.4(3)
O4	N11	C5	C6	80.1(3)
O5	N12	C6	N9	-172.8(2)
O5	N12	C6	C5	3.2(4)
O6	N12	C6	N9	7.3(3)
O6	N12	C6	C5	-176.6(2)
N8	N9	C6	N12	175.8(2)
N8	N9	C6	C5	-0.7(3)
N8	C4	C5	N11	173.0(2)
N8	C4	C5	C6	-1.1(3)
N9	N8	C4	N10	-177.4(2)
N9	N8	C4	C5	0.7(3)
N10	C4	C5	N11	-9.1(4)
N10	C4	C5	C6	176.8(2)
N11	C5	C6	N9	-173.0(2)
N11	C5	C6	N12	10.7(4)
C4	N8	N9	C6	0.0(3)
C4	C5	C6	N9	1.1(3)
C4	C5	C6	N12	-175.2(2)
N2	N3	C2	N4	-179.2(3)
N2	N3	C2	N7	-2.5(5)
N2	N3	C3	N1	-0.6(3)
N2	N3	C3	N5	179.8(2)
N3	N2	C1	N1	0.4(3)
N3	N2	C1	N6	179.1(3)
N4	N5	C3	N1	-179.8(3)
N4	N5	C3	N3	-0.4(3)
N5	N4	C2	N3	-1.0(3)
N5	N4	C2	N7	-177.5(2)
C1	N1	C3	N3	0.8(3)
C1	N1	C3	N5	-179.8(3)
C1	N2	N3	C2	-180.0(3)
C1	N2	N3	C3	0.1(3)
C2	N3	C3	N1	179.5(2)
C2	N3	C3	N5	-0.1(3)
C2	N4	N5	C3	0.9(3)

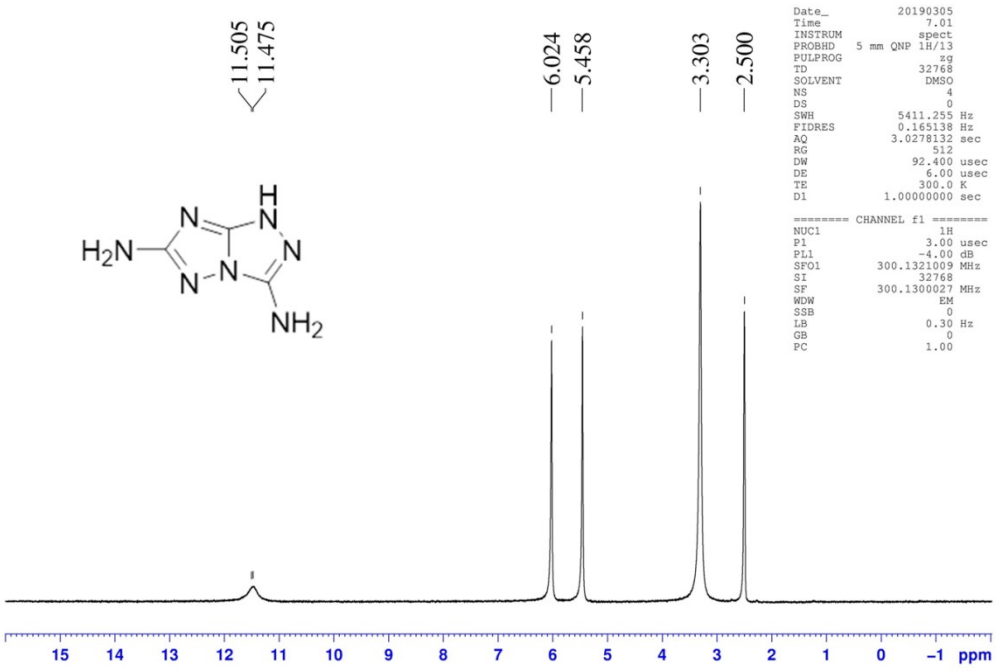
Atom	Atom	Atom	Atom	Angle/°
C3	N1	C1	N2	-0.8(3)
C3	N1	C1	N6	-179.5(2)
C3	N3	C2	N4	0.7(3)
C3	N3	C2	N7	177.4(2)

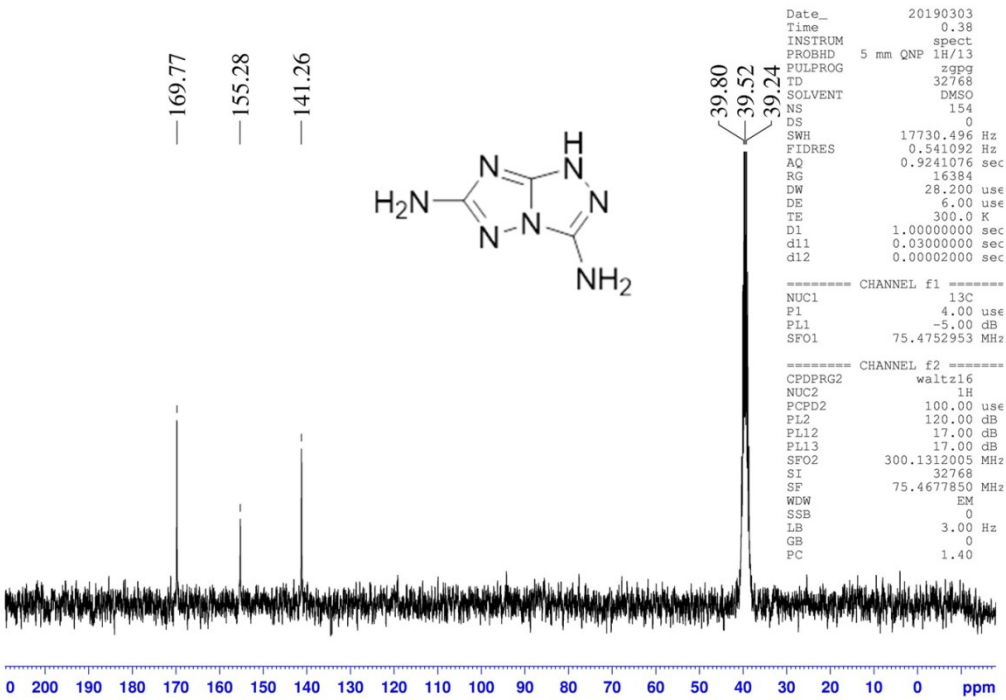
Table S14. Hydrogen bonds for **4·H_2O** [Å and °].

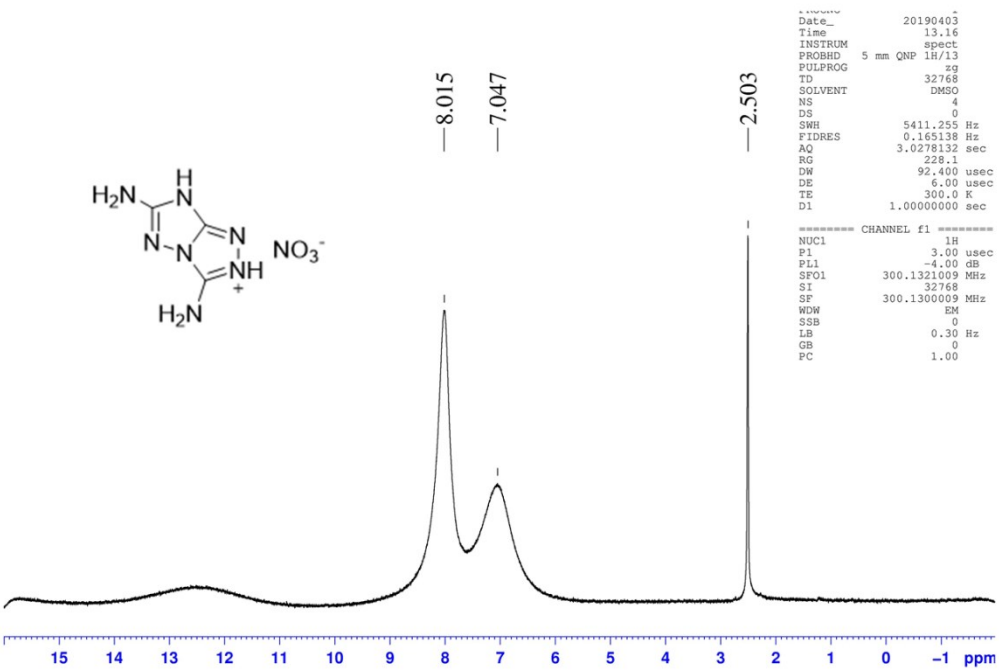
D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O1W	H1WA	O1W1	0.85	2.08	2.907(2)	164.9
O1W	H1WB	N22	0.85	2.41	3.061(3)	134.1
N1	H1	N53	0.86(4)	2.02(4)	2.806(3)	153(4)
N4	H4	N84	0.98(3)	1.87(3)	2.810(3)	161(3)
N6	H6B	O65	0.84(4)	2.57(4)	2.963(3)	110(3)
N7	H7A	O1W2	0.95(3)	1.97(4)	2.909(3)	169(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z+1 #2 -x+3/2,y+1/2,-z+1/2 #3 -x+1,-y+1,-z+1
#4 -x+3/2,y-1/2,-z+3/2 #5 x+1/2,-y+3/2,z+1/2

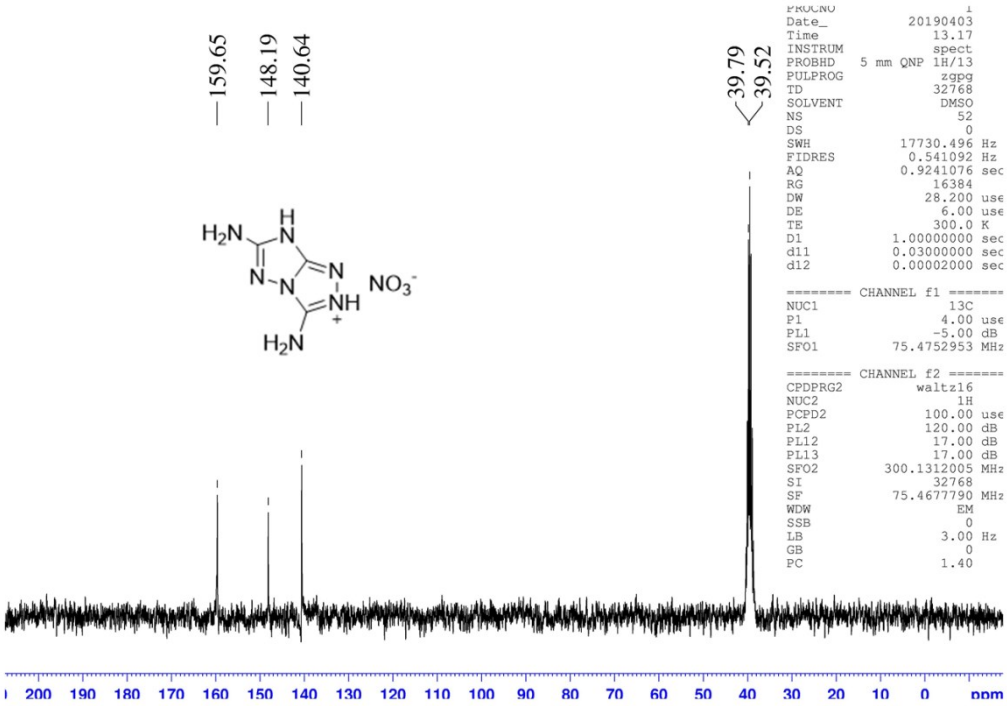
^{1}H and ^{13}C NMR Spectra



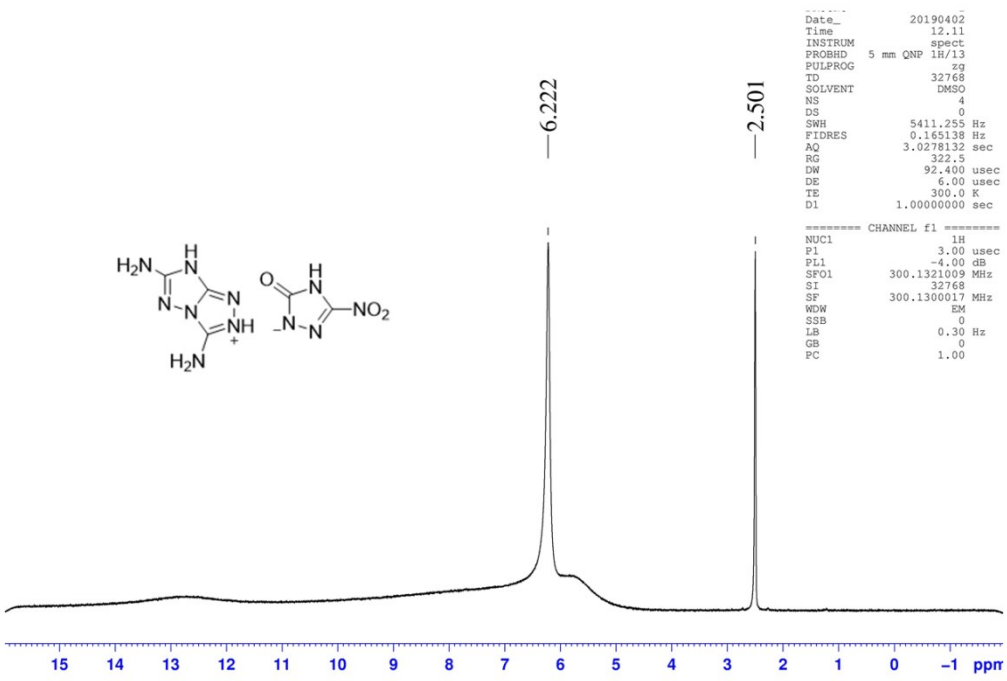


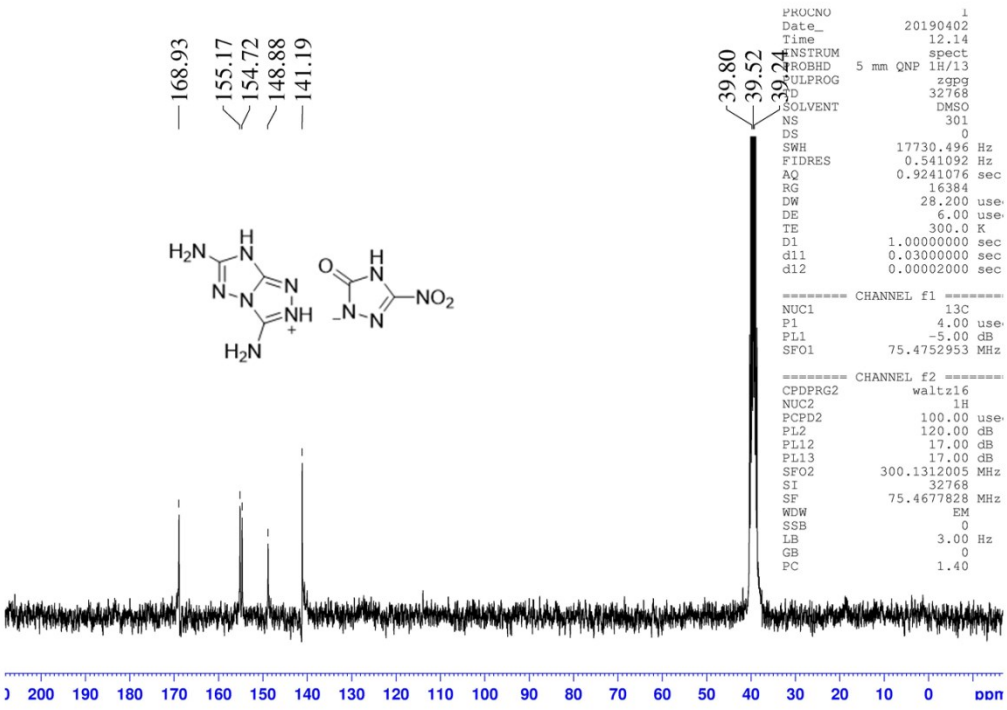


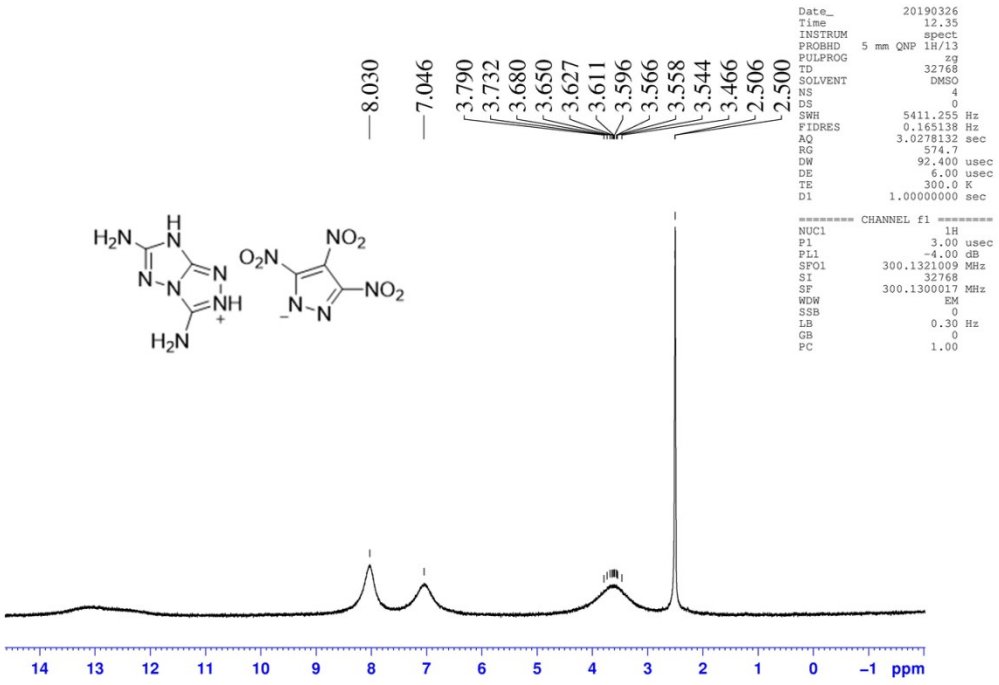

```
Date_           20190403
Time               13.16
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG              zg
TD                32768
SOLVENT            DMSO
NS                    4
DS                    0
SWH            5411.255 Hz
FIDRES        0.165138 Hz
AQ            3.0278132 sec
RG                228.1
DW               92.400 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        300.1321009 MHz
SI                32768
SF          300.1300009 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                 1.00
```

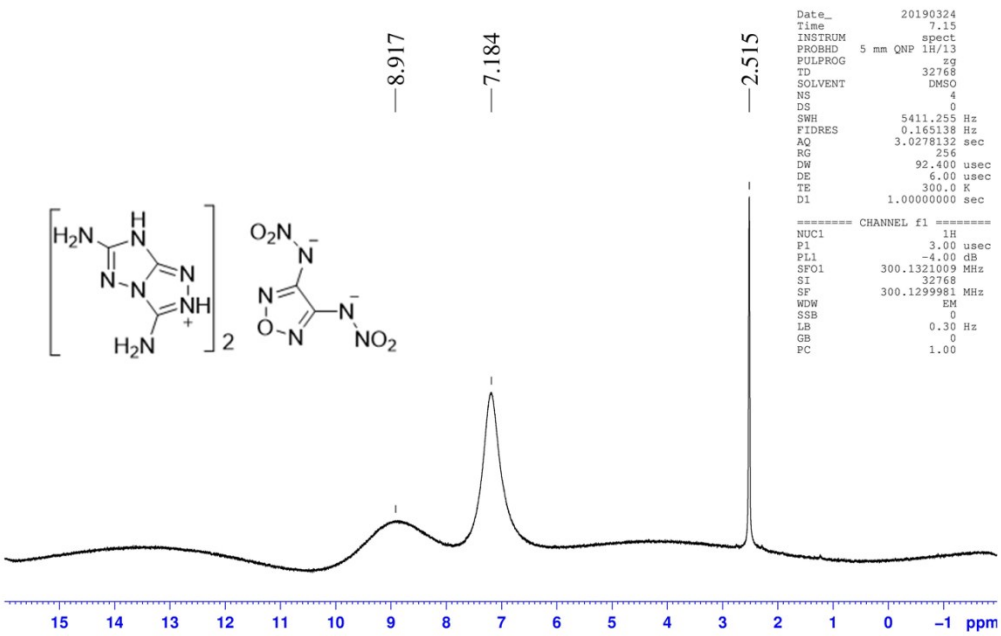


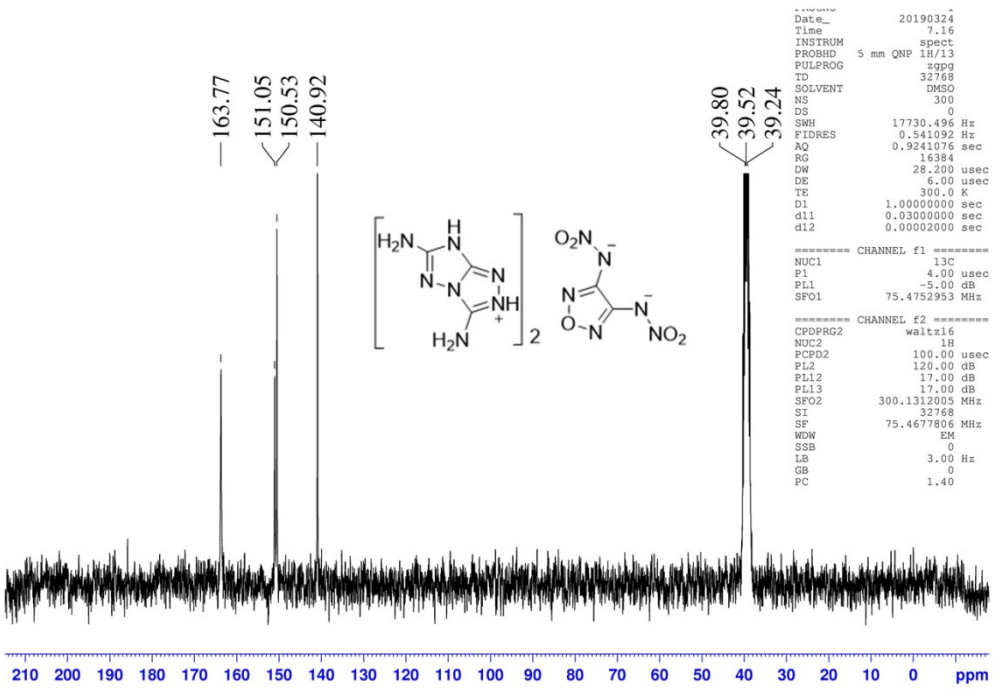

```
PROCNO                1
Date_          20190403
Time              13.17
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg
TD               32768
SOLVENT           DMSO
NS                  52
DS                   0
SWH          17730.496 Hz
FIDRES        0.541092 Hz
AQ            0.9241076 sec
RG                16384
DW               28.200 use
DE                6.00 use
TE               300.0 K
D1            1.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1               4.00 use
PL1              -5.00 dB
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2          100.00 use
PL2            120.00 dB
PL12            17.00 dB
PL13            17.00 dB
SFO2        300.1312005 MHz
SI               32768
SF          75.4677790 MHz
WDW                 EM
SSB                  0
LB               3.00 Hz
GB                   0
PC                1.40
```

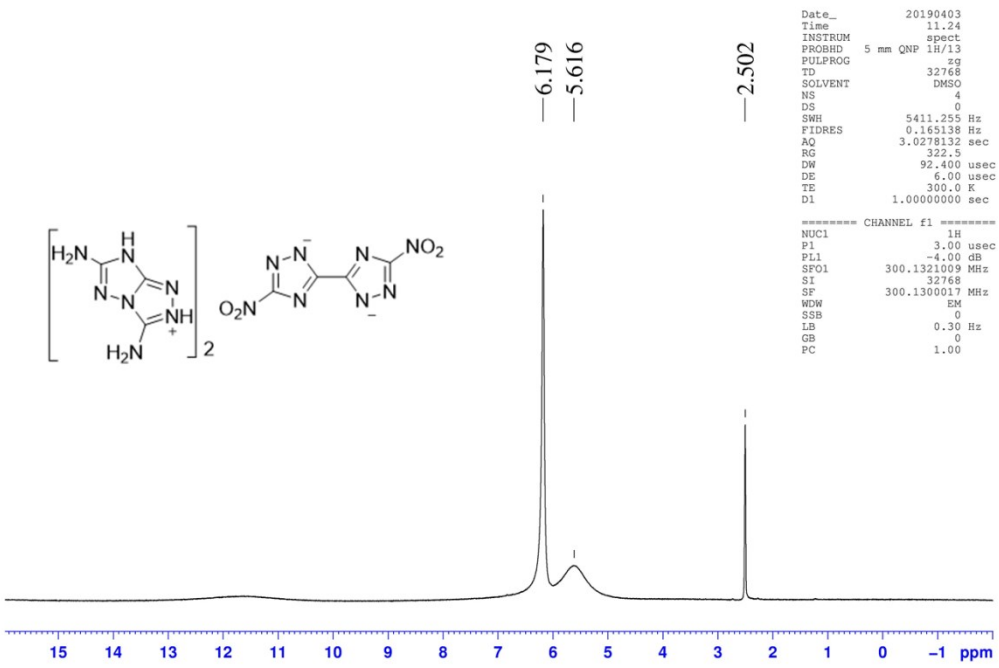

6.222
2.501
Date_ 20190402
Time 12.11
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT DMSO
NS 4
DS 0
SWH 5411.255 Hz
FIDRES 0.165138 Hz
AQ 3.0278132 sec
RG 322.5
DW 92.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1321009 MHz
SI 32768
SF 300.1300017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm

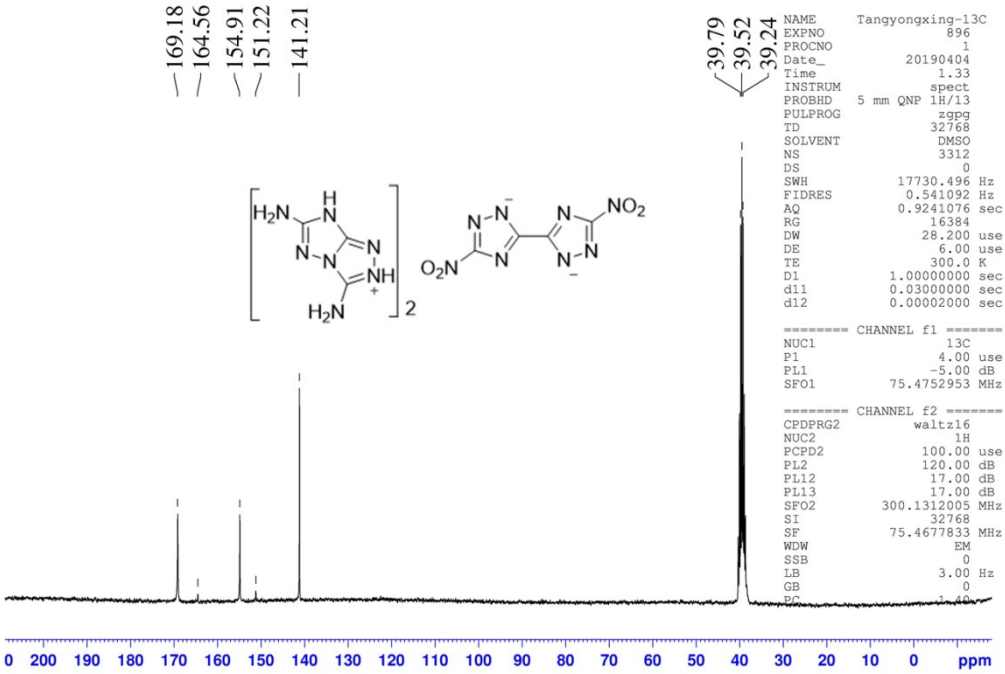

168.93
155.17
154.72
148.88
141.19
39.80
39.52
39.24
PROCNO 1
Date_ 20190402
Time 12.14
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 301
DS 0
SWH 17730.496 Hz
FIDRES 0.541092 Hz
AQ 0.9241076 sec
RG 16384
DW 28.200 use
DE 6.00 use
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
CHANNEL f1
NUC1 13C
P1 4.00 use
PL1 -5.00 dB
SFO1 75.4752953 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 use
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677828 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

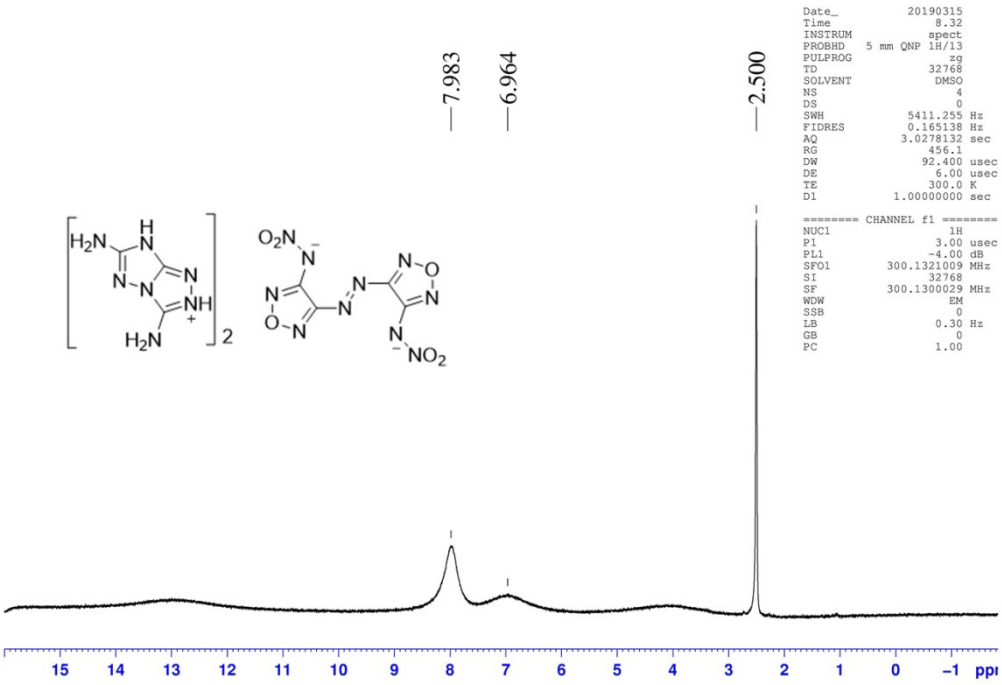

8.030
7.046
3.790
3.732
3.680
3.650
3.627
3.611
3.596
3.566
3.558
3.544
3.466
2.506
2.500
Date_ 20190326
Time 12.35
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT DMSO
NS 4
DS 0
SWH 5411.255 Hz
FIDRES 0.165138 Hz
AQ 3.0278132 sec
RG 574.7
DW 92.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1321009 MHz
SI 32768
SF 300.1300017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm

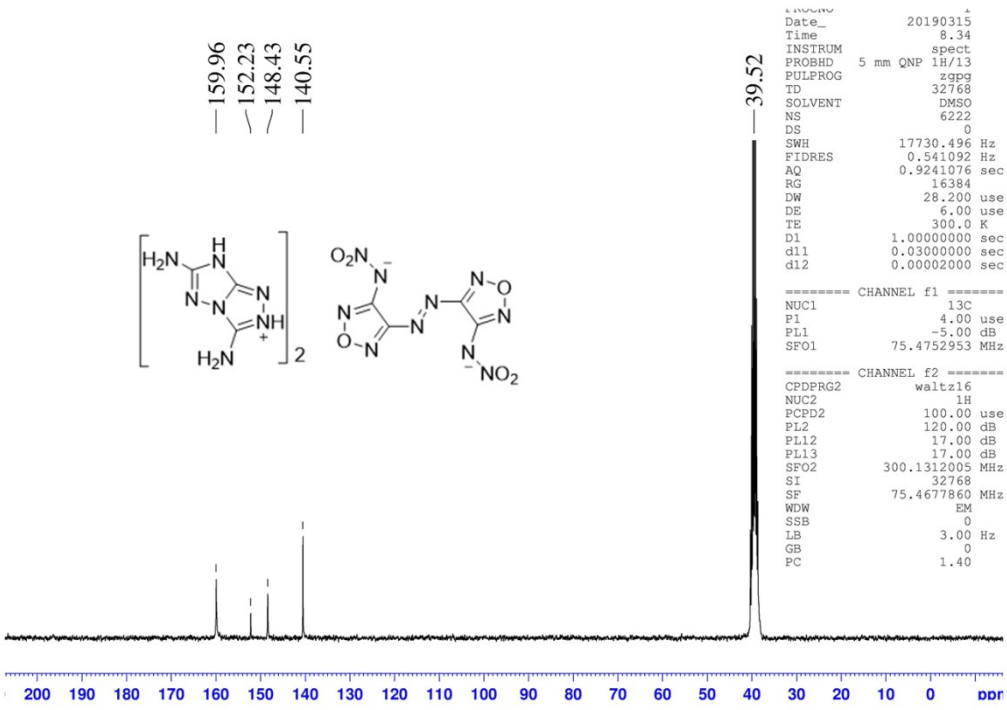

8.917
7.184
2.515
Date_ 20190324
Time 7.15
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT DMSO
NS 4
DS 0
SWH 5411.255 Hz
FIDRES 0.165138 Hz
AQ 3.0278132 sec
RG 256
DW 92.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1321009 MHz
SI 32768
SF 300.1299981 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm

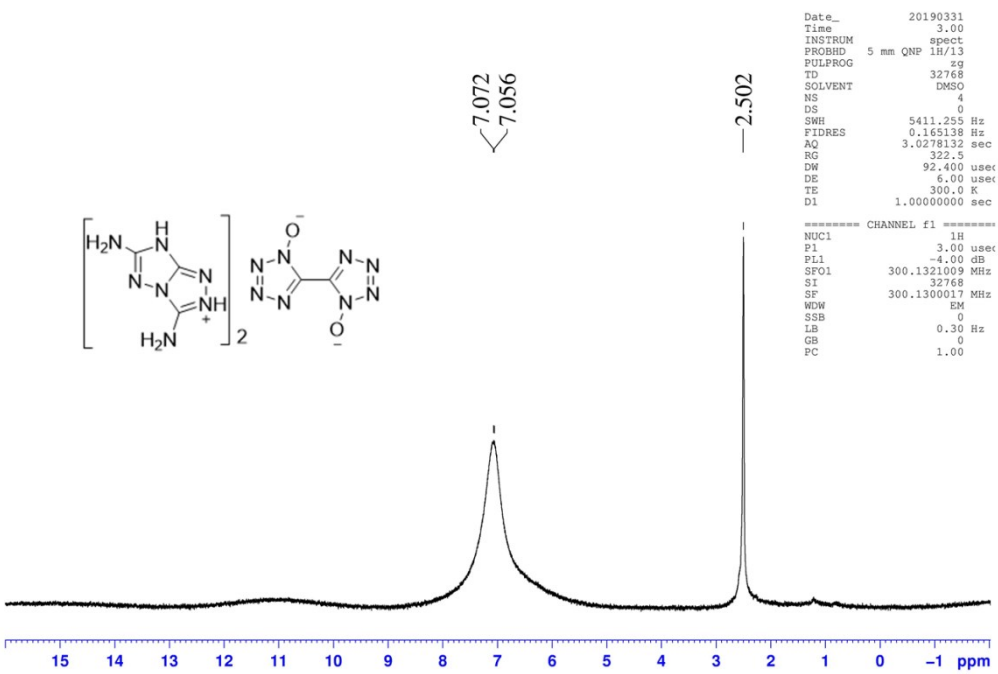

163.77
151.05
150.53
140.92
39.80
39.52
39.24
Date_ 20190324
Time 7.16
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 300
DS 0
SWH 17730.496 Hz
FIDRES 0.541092 Hz
AQ 0.9241076 sec
RG 16384
DW 28.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677806 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

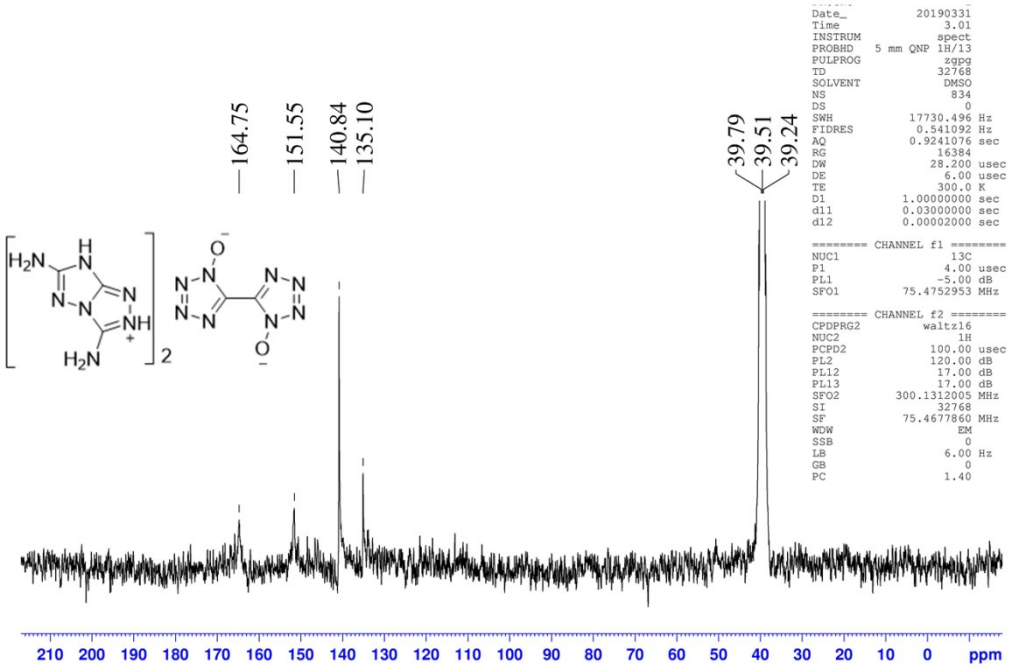

6.179
5.616
2.502
Date_ 20190403
Time 11.24
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT DMSO
NS 4
DS 0
SWH 5411.255 Hz
FIDRES 0.165138 Hz
AQ 3.0278132 sec
RG 322.5
DW 92.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1321009 MHz
SI 32768
SF 300.1300017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm

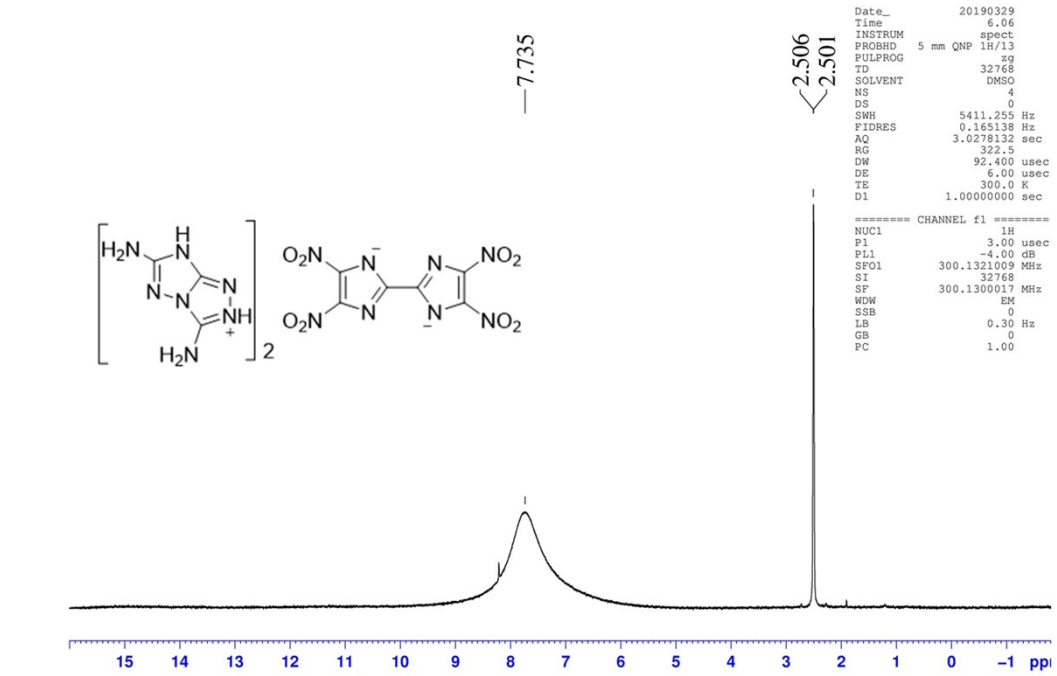

169.18
164.56
154.91
151.22
141.21
39.79
39.52
39.24
NAME Tangyongxing-13C
EXPNO 896
PROCNO 1
Date_ 20190404
Time 1.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 3312
DS 0
SWH 17730.496 Hz
FIDRES 0.541092 Hz
AQ 0.9241076 sec
RG 16384
DW 28.200 use
DE 6.00 use
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
CHANNEL f1
NUC1 13C
P1 4.00 use
PL1 -5.00 dB
SFO1 75.4752953 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 use
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677833 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
0 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

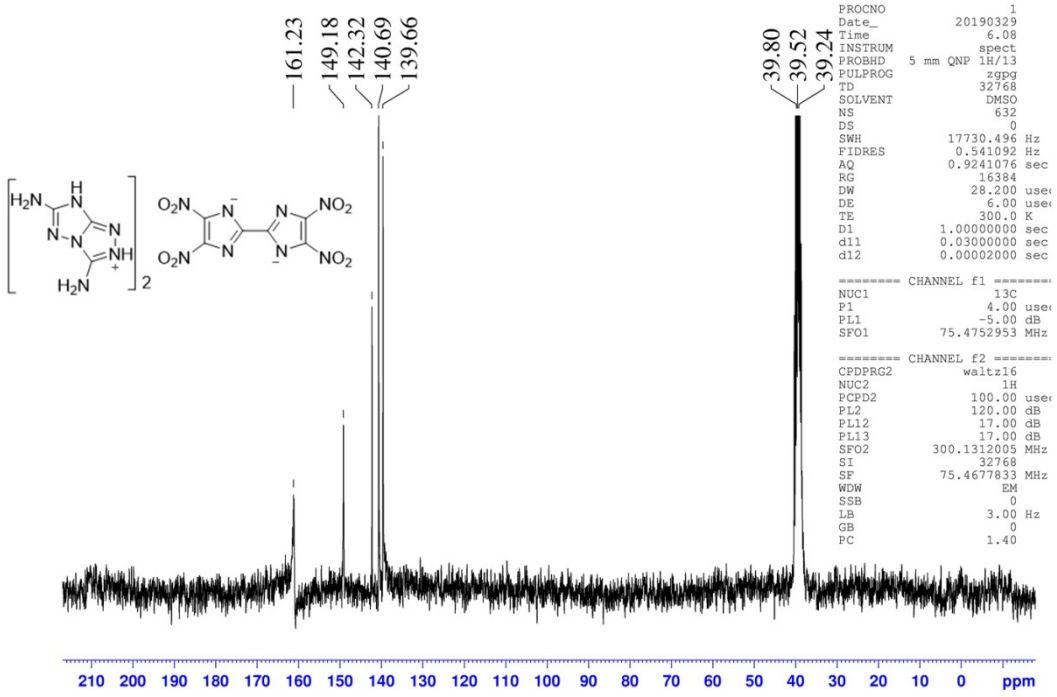

7.983
6.964
2.500
Date_ 20190315
Time 8.32
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT DMSO
NS 4
DS 0
SWH 5411.255 Hz
FIDRES 0.165138 Hz
AQ 3.0278132 sec
RG 456.1
DW 92.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1321009 MHz
SI 32768
SF 300.1300029 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm


159.96
152.23
148.43
140.55
39.52
Date_ 20190315
Time 8.34
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 6222
DS 0
SWH 17730.496 Hz
FIDRES 0.541092 Hz
AQ 0.9241076 sec
RG 16384
DW 28.200 use
DE 6.00 use
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 use
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 use
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677860 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.072
7.056
2.502
Date_ 20190331
Time 3.00
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT DMSO
NS 4
DS 0
SWH 5411.255 Hz
FIDRES 0.165138 Hz
AQ 3.0278132 sec
RG 322.5
DW 92.400 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 300.1321009 MHz
SI 32768
SF 300.1300017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm


164.75
151.55
140.84
135.10
39.79
39.51
39.24
Date_ 20190331
Time 3.01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 834
DS 0
SWH 17730.496 Hz
FIDRES 0.541092 Hz
AQ 0.9241076 sec
RG 16384
DW 28.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677860 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.735
2.506
2.501
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm


161.23
149.18
142.32
140.69
139.66
39.80
39.52
39.24
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm