Supporting Information

Design, synthesis and characterization of a carbonyl-containing high-density-pyrazolotriazine-based energetic compound

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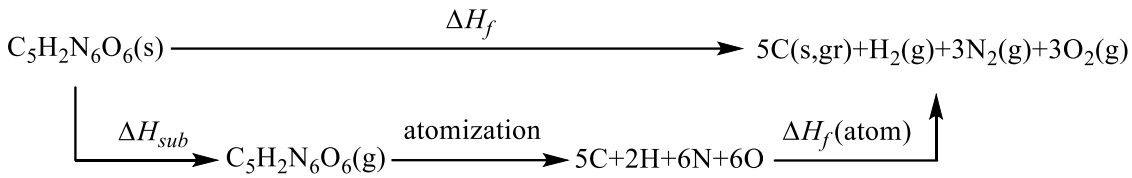
Table of contents

1 Computational Details

Structure optimizations and energy calculations were accomplished with Gaussian 09 Rev. D.01 suite of package [1]. The initial configuration of **4** were taken from its corresponding single-crystal structure coordinates. High-precision molecular energy was calculated with G2 method. Gas-phase heats of formation were determined based on an atomization method (Scheme S1). Experimental atomic heats of formation were taken from NIST Chemistry WebBook [2]. Sublimation heat was estimated with Trouton's rule (Eqs. 1–2) [3–4]. ^{13}C NMR chemical shifts were predicted with a literature method [5]. The geometry was optimized at B3LYP/6-31+G(d,p) level of theory in gas phase. Isotropic magnetic shielding constants were calculated at mPW1PW91/6-311+G(2d,p) level of theory with GIAO method in gas phase.



Scheme S1. Atomization method for the calculation of heat of formation.

$$\Delta H_f\,(\text{solid}) = \Delta H_f\,(\text{gas}) - \Delta H_{sub} \quad (1)$$

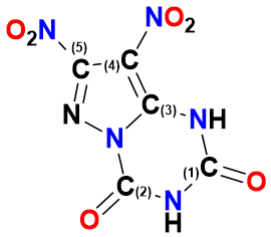
$$\Delta H_{sub} = 0.188\ \text{J mol}^{-1}\ \text{K}^{-1} * T \quad (2)$$

(T = decomposition temperature [K])

Table S1. Calculated enthalpies of **4** and atoms and heat of formation of **4**.

Species	G2 Enthalpy	ΔH_f (gas) kJ mol^{-1}	ΔH_{sub} kJ mol^{-1}	ΔH_f (solid) kJ mol^{-1}
C	−37.78194	716.67		
H	−0.497639	218		
N	−54.515599	472.68		
O	−74.979669	249.18		
4	−970.104702	−115.839	90.804	−206.643

Table S2. Calculated ^{13}C NMR chemical shifts for **4**.



$\delta = (\text{intercept} - \sigma_{isot}) / (-k)$ (3)

(intercept = 182.2853, $k = -1.0267$)

Item	C(1)	C(2)	C(3)	C(4)	C(5)
σ_{isot}	41.83	39.03	42.40	72.21	30.77
Calculated δ_C	139.7	143.2	139.4	111.6	152.1
Measured δ_C	142.7	148.4	142.1	109.5	150.4

2 Crystallographic Data

Table S3 Crystallographic data and structure refinement for **4** $\mathbf{H_2O}$.

CCDC	**2465473**
Empirical formula	$C_5H_4N_6O_7$
Formula weight	260.14
Temperature/K	185.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.5513(16)
b/Å	5.3556(8)
c/Å	20.766(4)
α/°	90
β/°	100.797(6)
γ/°	90
Volume/Å^3	934.2(3)
Z	4
ρ_{calc} g/cm^3	1.850
μ/mm^{-1}	0.173
F(000)	528.0
Crystal size/mm^3	0.19 × 0.18 × 0.16

Radiation	MoKα (λ = 0.71073 Å)
2Θ range for data collection/°	3.994 to 52.846
Index ranges	$-9 \le h \le 10, -6 \le k \le 6, -26 \le l \le 18$
Reflections collected	4990
Independent reflections	1872 [R_{int} = 0.0920, R_{sigma} = 0.1233]
Data/restraints/parameters	1872/54/198
Goodness–of–fit on F^2	1.067
Final R indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0680, wR_2 = 0.1416
Final R indexes [all data]	R_1 = 0.1518, wR_2 = 0.1847
Largest diff. peak/hole / e Å^{-3}	0.30/−0.31

Table S4 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **4 H_2O**.

Atom	x	y	z	U(eq)
O1	7287(5)	2(6)	5819.8(19)	39.7(9)
O2	9153(3)	3288(6)	6893.0(16)	38.0(9)
O3	6911(4)	10221(6)	7619.5(18)	42.8(9)
O4	4220(4)	2779(6)	5326.2(17)	41.9(9)
O5	2126(4)	5154(6)	5051.5(18)	54.0(11)
O6B	1220(20)	10080(40)	5449(12)	60(3)
O7A	558(5)	7513(10)	6000(3)	61.9(16)
N1	8058(5)	6775(7)	7246(2)	32.1(10)
N2	6649(4)	4354(7)	6399.4(19)	28.7(9)
N3	5493(4)	7862(6)	6790.7(18)	28.2(9)
N4	4139(4)	9292(6)	6701(2)	33.8(10)
N5	1588(5)	9076(7)	6027(2)	43.6(11)
N6	3365(5)	4596(7)	5418(2)	36.4(10)
C1	8044(5)	4719(8)	6856(2)	29.9(11)
C2	6855(5)	8451(8)	7264(2)	30.5(11)
C3	5405(5)	5916(7)	6368(2)	27.0(10)
C4	3922(5)	6077(8)	5974(2)	30.4(11)
C5	3221(5)	8192(8)	6211(3)	32.2(11)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Table S5 Anisotropic Displacement Parameters (Å^2×10^3) for **4 H_2O**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	32(2)	38.0(19)	47(3)	−5.8(17)	1.4(18)	2.8(15)
O2	29.2(17)	40.6(18)	41(2)	1.3(15)	−1.8(15)	6.5(14)
O3	40(2)	39.7(19)	48(2)	−16.9(17)	6.4(17)	−2.8(15)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O4	39.0(19)	37.4(18)	46(2)	−11.3(16)	−0.4(16)	2.9(15)
O5	46(2)	62(2)	44(3)	−1.2(19)	−17.0(19)	9.9(17)
O6B	37(5)	63(6)	79(5)	22(5)	8(5)	6(5)
O7A	33(2)	61(3)	87(4)	7(3)	–1(3)	−5(2)
N1	27(2)	32(2)	33(3)	–2.9(18)	–2.6(19)	–3.5(17)
N2	25(2)	29(2)	31(2)	−2.9(18)	–0.5(17)	4.0(16)
N3	24.7(19)	29(2)	30(2)	−3.0(17)	4.2(16)	−0.4(15)
N4	29(2)	30(2)	44(3)	1.0(19)	9.8(19)	3.7(16)
N5	30(2)	39(2)	62(3)	5(2)	10(2)	4.3(17)
N6	33(2)	42(2)	32(3)	−0.9(19)	1.0(19)	2.0(18)
C1	24(2)	33(2)	31(3)	–1(2)	1(2)	−0.4(19)
C2	31(2)	32(2)	29(3)	1(2)	8(2)	−4(2)
C3	24(2)	24(2)	31(3)	−1.2(19)	1(2)	–3.0(18)
C4	27(2)	33(2)	29(3)	4(2)	0(2)	1.5(19)
C5	24(2)	32(2)	41(3)	3(2)	5(2)	0.6(19)

The Anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S6 Bond Lengths for **4 H_2O**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O2	C1	1.211(5)	N2	C3	1.345(5)
O3	C2	1.196(5)	N3	N4	1.372(5)
O4	N6	1.253(5)	N3	C2	1.412(6)
O5	N6	1.220(5)	N3	C3	1.355(5)
O6B	N5	1.30(2)	N4	C5	1.303(6)
O7A	N5	1.209(6)	N5	C5	1.456(6)
N1	C1	1.365(6)	N6	C4	1.409(6)
N1	C2	1.371(6)	C3	C4	1.377(6)
N2	C1	1.392(6)	C4	C5	1.412(6)

Table S7 Bond Angles for **4 H_2O**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C2	128.4(4)	N1	C1	N2	115.4(4)
C3	N2	C1	121.0(4)	O3	C2	N1	126.3(4)
N4	N3	C2	122.3(4)	O3	C2	N3	122.6(4)
C3	N3	N4	113.5(3)	N1	C2	N3	111.0(4)
C3	N3	C2	124.1(3)	N2	C3	N3	120.0(4)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C5	N4	N3	102.9(3)	N2	C3	C4	134.4(4)
O6B	N5	C5	115.7(9)	N3	C3	C4	105.7(4)
O7A	N5	C5	116.2(4)	N6	C4	C5	129.6(4)
O4	N6	C4	116.4(4)	C3	C4	N6	125.8(4)
O5	N6	O4	124.0(4)	C3	C4	C5	104.3(4)
O5	N6	C4	119.6(4)	N4	C5	N5	117.7(4)
O2	C1	N1	123.6(4)	N4	C5	C4	113.7(4)
O2	C1	N2	121.0(4)	C4	C5	N5	128.1(4)

Table S8 Torsion Angles for **4 H_2O**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O4	N6	C4	C3	9.6(7)	N6	C4	C5	N4	−172.8(4)
O4	N6	C4	C5	−178.8(4)	N6	C4	C5	N5	14.8(8)
O5	N6	C4	C3	−169.0(5)	C1	N1	C2	O3	179.1(5)
O5	N6	C4	C5	2.6(7)	C1	N1	C2	N3	−2.0(6)
O6B	N5	C5	N4	115.3(12)	C1	N2	C3	N3	−0.8(6)
O6B	N5	C5	C4	−72.5(12)	C1	N2	C3	C4	178.4(5)
O7A	N5	C5	N4	−126.4(6)	C2	N1	C1	O2	−177.0(4)
O7A	N5	C5	C4	45.9(8)	C2	N1	C1	N2	3.3(7)
N2	C3	C4	N6	−6.4(8)	C2	N3	N4	C5	177.3(4)
N2	C3	C4	C5	−179.7(5)	C2	N3	C3	N2	2.3(6)
N3	N4	C5	N5	173.4(4)	C2	N3	C3	C4	−177.1(4)
N3	N4	C5	C4	0.1(5)	C3	N2	C1	O2	178.6(4)
N3	C3	C4	N6	172.9(4)	C3	N2	C1	N1	−1.7(6)
N3	C3	C4	C5	−0.4(5)	C3	N3	N4	C5	−0.4(5)
N4	N3	C2	O3	0.5(7)	C3	N3	C2	O3	178.0(4)
N4	N3	C2	N1	−178.5(4)	C3	N3	C2	N1	−1.0(6)
N4	N3	C3	N2	180.0(4)	C3	C4	C5	N4	0.2(5)
N4	N3	C3	C4	0.5(5)	C3	C4	C5	N5	−172.3(5)

Table S9 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **4 H_2O**.

Atom	*x*	*y*	*z*	U(eq)
H1A	6830(90)	−820(140)	5420(40)	130(30)
H1B	8250(70)	−20(100)	5900(30)	70(20)
H1	8810(60)	7100(90)	7510(30)	48(17)
H2	6730(60)	3040(100)	6130(30)	69(19)

Table S10 Atomic Occupancy for **4 H_2O**.

Atom	Occupancy	Atom	Occupancy
O6B	0.203(7)	O7A	0.797(7)

Table S11 Crystallographic data and structure refinement for **IM-3b H_2O HCl**.

CCDC	2465568
Empirical formula	$C_{12}H_{24}Cl_2N_{18}O$
Formula weight	507.39
Temperature/K	273(2)
Crystal system	monoclinic
Space group	$C2/c$
a/Å	16.7890(2)
b/Å	10.83470(10)
c/Å	15.9281(2)
α/°	90
β/°	118.1790(10)
γ/°	90
Volume/Å^3	2553.97(5)
Z	4
ρ_{calc} g/cm^3	1.320
μ/mm^{-1}	2.661
F(000)	1056.0
Crystal size/mm^3	0.12 × 0.1 × 0.08
Radiation	CuKα (λ = 1.54178 Å)
2Θ range for data collection/°	10.118 to 144.354
Index ranges	$-20 \le h \le 17$, $-11 \le k \le 13$, $-19 \le l \le 19$
Reflections collected	8528
Independent reflections	2434 [R_{int} = 0.0694, R_{sigma} = 0.0571]
Data/restraints/parameters	2434/0/155
Goodness-of-fit on F^2	1.103
Final R indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0711, wR_2 = 0.2130
Final R indexes [all data]	R_1 = 0.0726, wR_2 = 0.2141
Largest diff. peak/hole / e Å^{-3}	1.00/−0.59

Table S12 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **IM-3b H_2O HCl**.

Atom	*x*	*y*	*z*	U(eq)
C2	4742.0(17)	6229(2)	6282.5(19)	28.8(6)
C5	6180.8(17)	3895(2)	6160.6(18)	27.2(6)
C3	4894.6(16)	4980(2)	6217.4(18)	27.6(5)
C1	5501.9(16)	6854(2)	6315.3(18)	27.4(5)
C6	6291.8(17)	1770(2)	6206.4(19)	30.1(6)
C4	3975.4(18)	6796(3)	6255(2)	34.6(6)
Cl1	7558.7(5)	8834.5(6)	6373.1(6)	43.5(3)
N1	5611.9(16)	8116(2)	6345.2(18)	34.6(5)
N3	6085.6(15)	6094.8(19)	6263.2(17)	28.8(5)
N4	5704.2(13)	4925(2)	6192.5(15)	27.3(5)
N5	4396.7(17)	4004(2)	6169(2)	43.1(7)
N6	6946.7(15)	4135(2)	6141.8(18)	33.9(5)
N7	5813.6(15)	2821(2)	6117.1(18)	33.9(5)
N8	7033.7(16)	1530(2)	7002.9(19)	39.6(6)
N9	5960.2(19)	976(2)	5506(2)	44.8(7)
N2	3368(2)	7316(3)	6228(2)	55.1(8)
O1	8 069(5)	6123(4)	5885(4)	57.1(15)

Ueq is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Table S13 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **IM-3b H_2O HCl**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C2	21.4(13)	30.1(14)	41.2(13)	1.6(10)	20.1(11)	6.2(9)
C5	17.8(12)	28.5(13)	37.9(13)	0.3(9)	15.3(10)	5.2(9)
C3	19.4(11)	29.9(13)	39.8(13)	2.5(10)	19.1(10)	4.4(9)
C1	21.6(12)	27.3(12)	37.6(12)	2.5(10)	17.4(10)	5.3(9)
C6	25.1(12)	24.6(12)	47.8(14)	3.4(10)	23.2(11)	1.4(10)
C4	27.5(13)	35.1(14)	50.9(15)	1.9(11)	26.5(12)	6.4(11)
Cl1	37.6(5)	35.1(5)	73.3(6)	4.5(3)	39.0(4)	3.5(3)
N1	30.5(11)	25.3(11)	53.6(13)	0.5(9)	24.5(10)	5.5(9)
N3	21.3(11)	23.5(11)	47.3(12)	1.0(8)	20.8(10)	2.3(8)
N4	19.0(10)	22.4(11)	46.8(12)	0.6(8)	20.6(9)	3.7(7)
N5	29.9(13)	33.5(13)	81.7(19)	0.0(12)	39.3(13)	–0.1(10)
N6	25.7(11)	27.0(11)	59.4(14)	1.1(10)	28.7(11)	5.3(9)
N7	21.9(10)	25.3(11)	58.7(14)	–0.1(10)	22.4(10)	2.8(9)
N8	28.1(12)	34.8(13)	53.9(14)	1.6(10)	17.7(10)	7.6(10)
N9	43.0(15)	29.0(12)	57.9(15)	–2.1(11)	20.0(12)	7.6(10)
N2	42.4(15)	50.5(17)	91(2)	7.1(15)	46.6(16)	18.6(13)
O1	120(5)	20.5(19)	63(3)	3.2(17)	70(3)	8(2)

The Anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S14 Bond Lengths for **IM-3b H_2O HCl**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C2	C3	1.390(4)	C1	N1	1.377(4)
C2	C1	1.424(4)	C1	N3	1.312(3)
C2	C4	1.408(3)	C6	N7	1.362(3)
C5	N4	1.388(3)	C6	N8	1.318(4)
C5	N6	1.326(3)	C6	N9	1.306(4)
C5	N7	1.303(3)	C4	N2	1.148(4)
C3	N4	1.380(3)	N3	N4	1.400(3)
C3	N5	1.327(4)			

Table S15 Bond Angles for **IM-3b H_2O HCl**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C3	C2	C1	105.8(2)	N3	C1	N1	122.2(2)
C3	C2	C4	128.4(3)	N8	C6	N7	120.5(3)
C4	C2	C1	125.7(2)	N9	C6	N7	118.0(2)
N6	C5	N4	115.2(2)	N9	C6	N8	121.3(3)
N7	C5	N4	117.0(2)	N2	C4	C2	176.5(3)
N7	C5	N6	127.8(2)	C1	N3	N4	104.2(2)
N4	C3	C2	105.2(2)	C5	N4	N3	118.7(2)
N5	C3	C2	130.3(2)	C3	N4	C5	128.9(2)
N5	C3	N4	124.5(2)	C3	N4	N3	112.2(2)
N1	C1	C2	125.3(2)	C5	N7	C6	120.0(2)
N3	C1	C2	112.5(2)				

Table S16 Torsion Angles for **IM-3b H_2O HCl**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C2	C3	N4	C5	177.7(2)	C4	C2	C1	N3	−175.1(3)
C2	C3	N4	N3	1.5(3)	N1	C1	N3	N4	−176.7(2)
C2	C1	N3	N4	0.1(3)	N4	C5	N7	C6	−171.6(2)
C3	C2	C1	N1	177.4(3)	N5	C3	N4	C5	−3.3(5)
C3	C2	C1	N3	0.8(3)	N5	C3	N4	N3	−179.5(3)
C1	C2	C3	N4	−1.3(3)	N6	C5	N4	C3	180.0(3)
C1	C2	C3	N5	179.8(3)	N6	C5	N4	N3	−4.0(3)

Table S16 Torsion Angles for **IM-3b H_2O HCl**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	N3	N4	C5	−177.6(2)	N6	C5	N7	C6	11.2(4)
C1	N3	N4	C3	−1.0(3)	N7	C5	N4	C3	2.4(4)
C4	C2	C3	N4	174.5(3)	N7	C5	N4	N3	178.5(2)
C4	C2	C3	N5	−4.4(5)	N8	C6	N7	C5	63.0(4)
C4	C2	C1	N1	1.5(4)	N9	C6	N7	C5	−121.4(3)

Table S17 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **IM-3b H_2O HCl**.

Atom	*x*	*y*	*z*	U(eq)
H1A	6185	8293	6511	52
H1B	5469	8436	6771	52
H1C	5253	8433	5773	52
H5A	4574	3276	6119	52
H5B	3897	4100	6189	52
H6A	7263	3540	6096	41
H6B	7127	4885	6175	41
H8A	7310	840	7069	48
H8B	7242	2064	7456	48
H9A	5560	496	5566	54
H9B	6406	514	5523	54
H1D	8021	6630	6267	86
H1E	7783	6463	5342	86

Table S18 Atomic Occupancy for **IM-3b H_2O HCl**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
O1	0.5	H1D	0.5	H1E	0.5

2 NMR Spectra

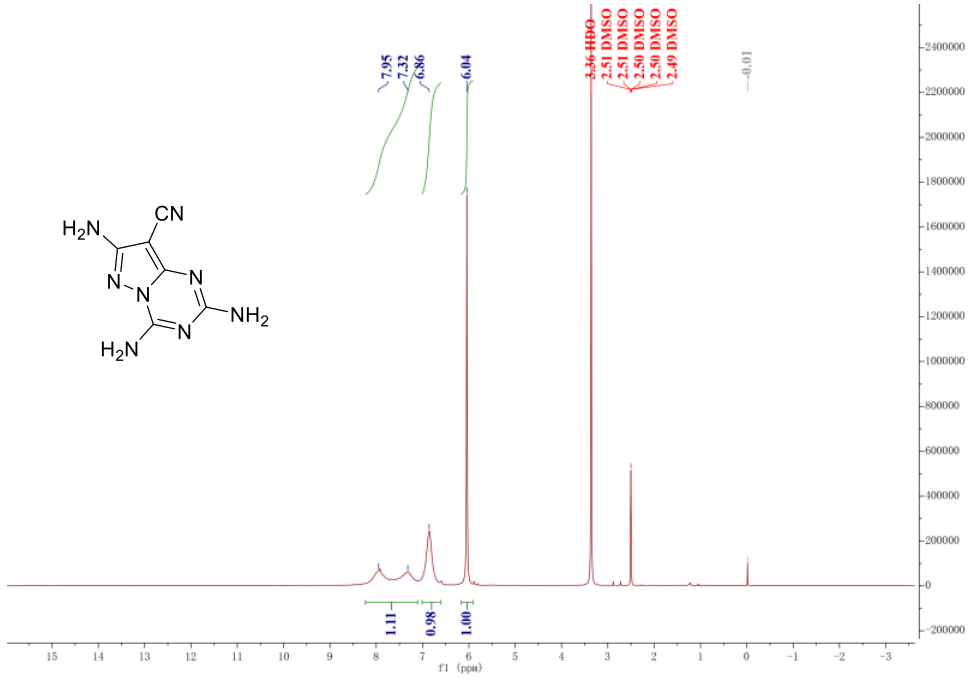


Figure S1. ^{1}H NMR spectrum of **2** in DMSO-d_6 at 300.13 MHz.

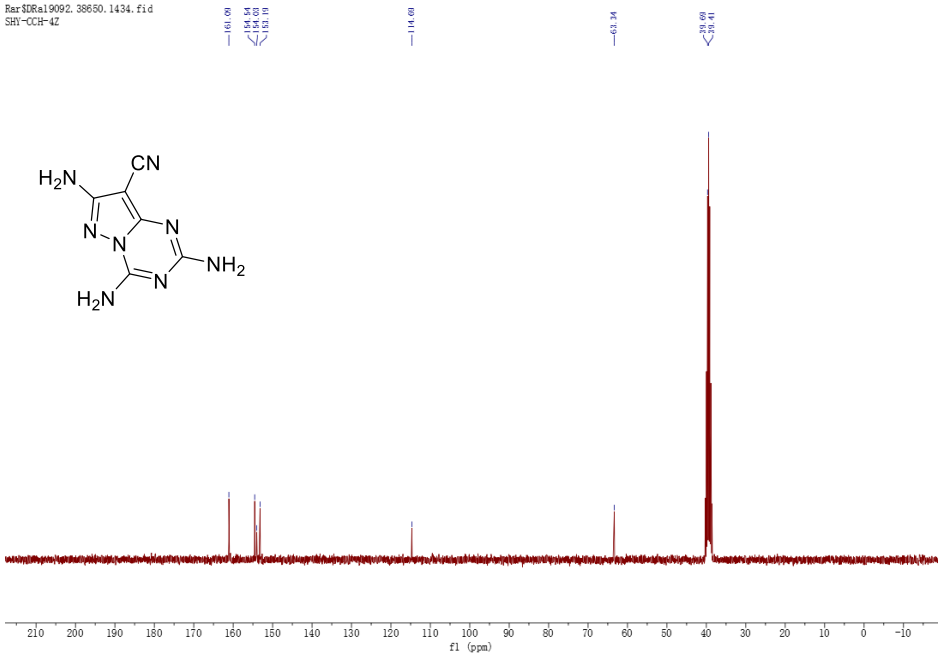


Figure S2. ^{13}C{^{1}H} NMR spectrum of **2** in DMSO-d_6 at 75.47 MHz.

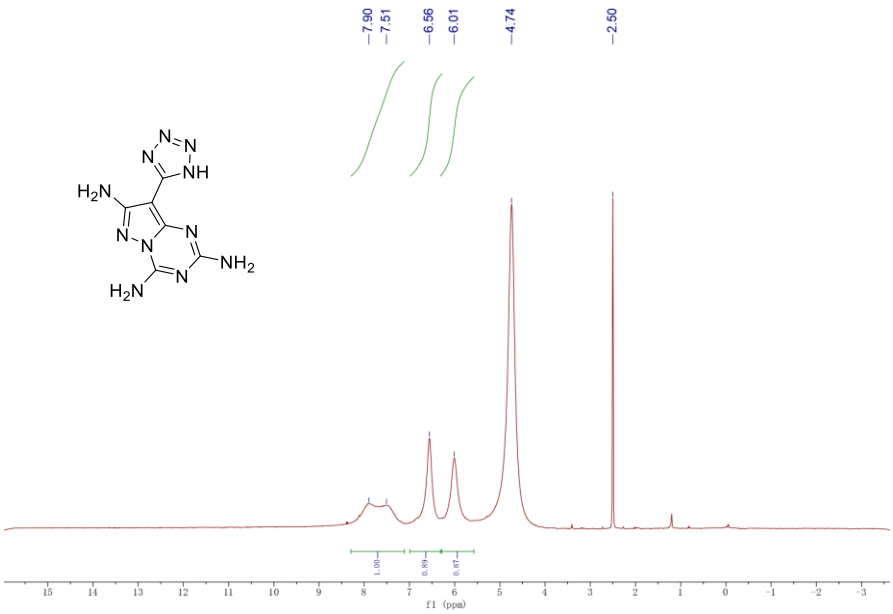


Figure S3. ^{1}H NMR spectrum of **3** in DMSO-d_6 at 300.13 MHz.

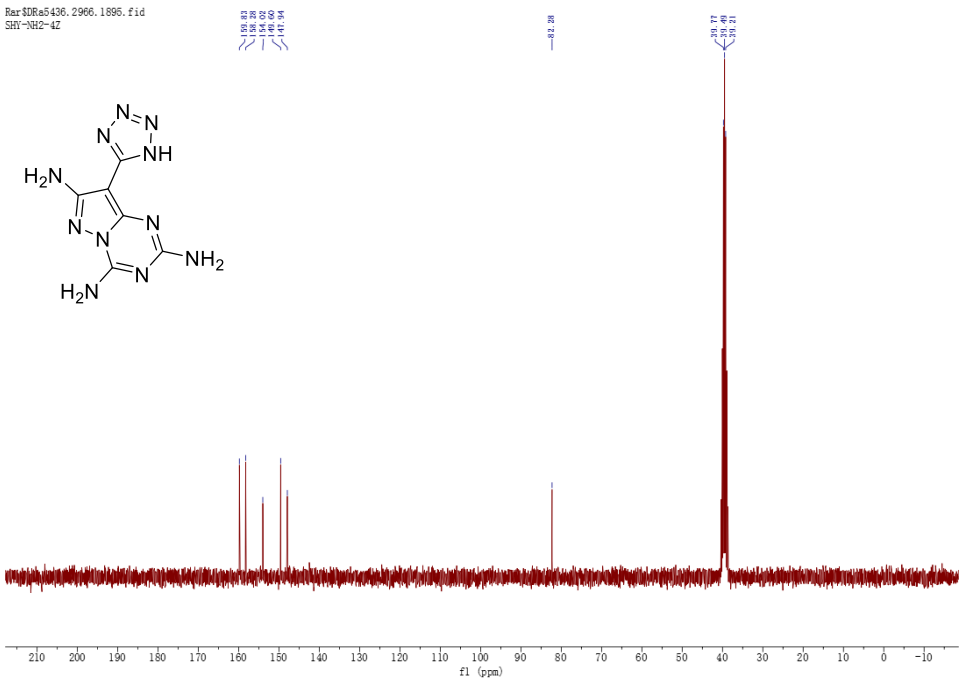


Figure S4. ^{13}C{^{1}H} NMR spectrum of **3** in DMSO-d_6 at 75.47 MHz.

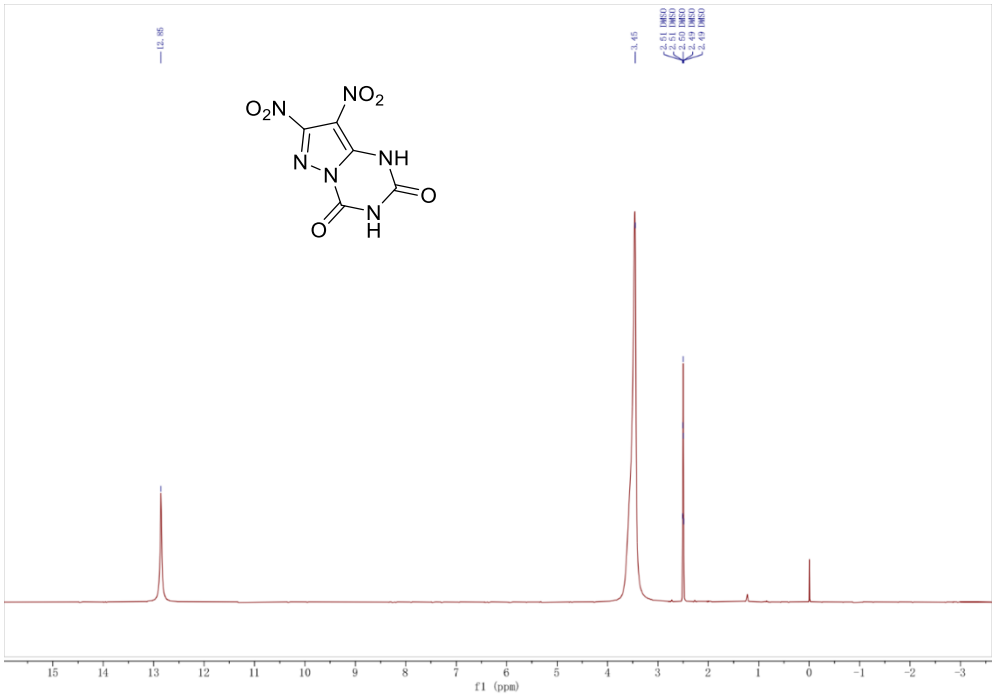


Figure S5. ^{1}H NMR spectrum of **4** in DMSO-d_6 at 300.13 MHz.

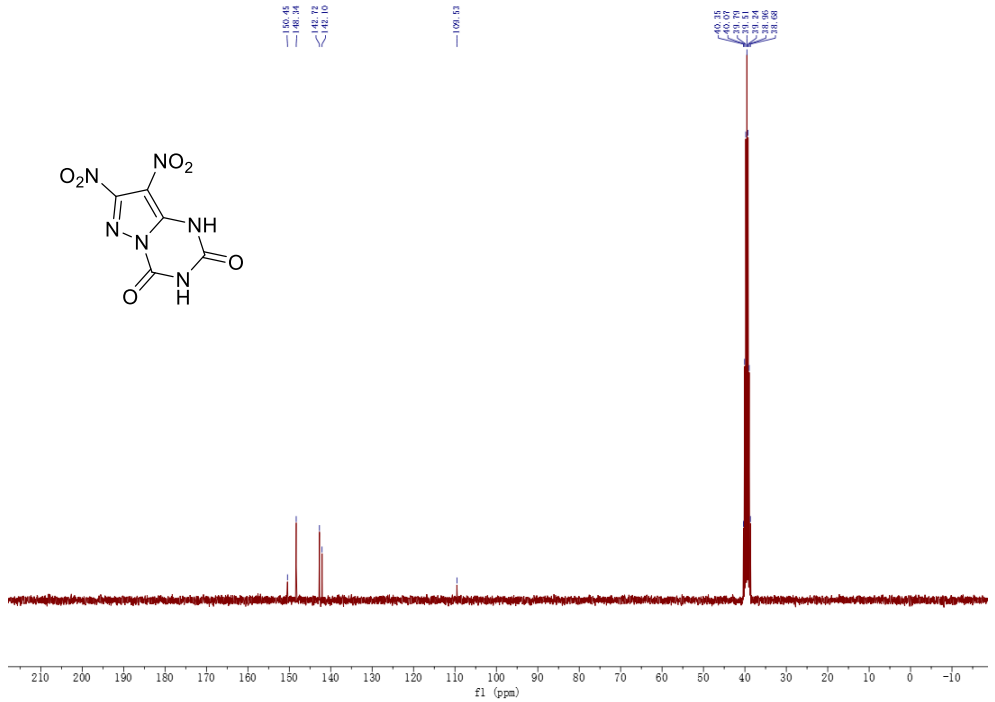


Figure S6. ^{13}C{^{1}H} NMR spectrum of **4** in DMSO-d_6 at 75.47 MHz.

3 HRMS Spectra

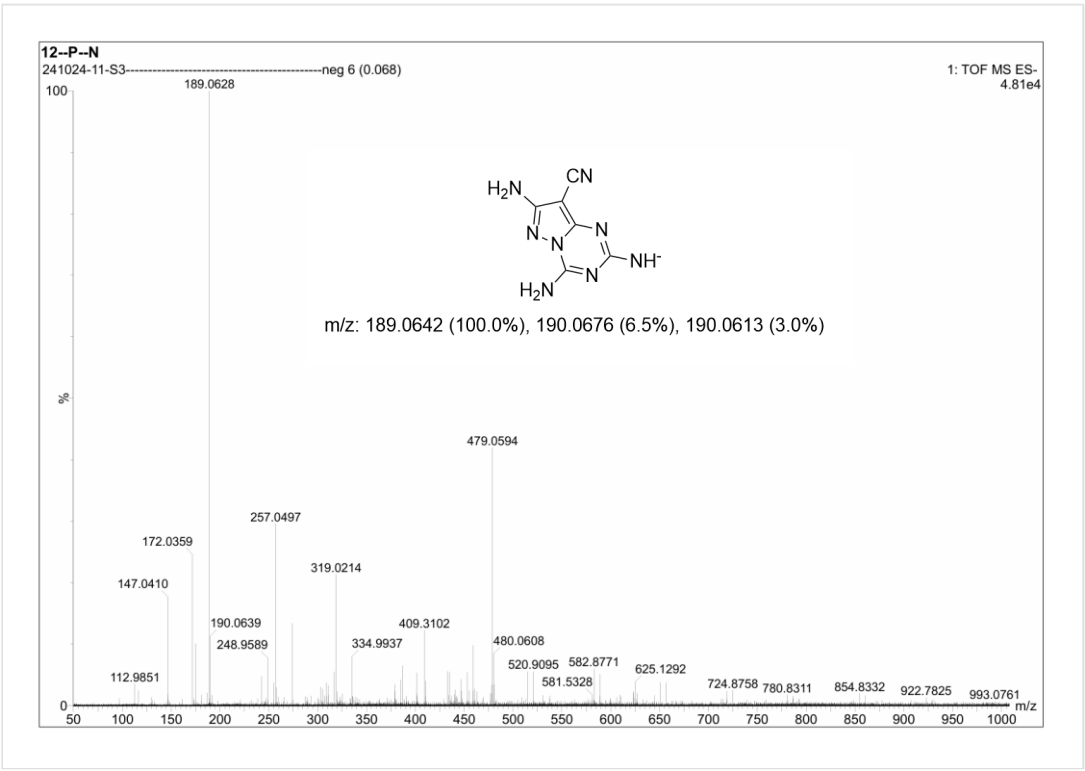


Figure S7. HRMS (ESI–) spectrum of **2**.

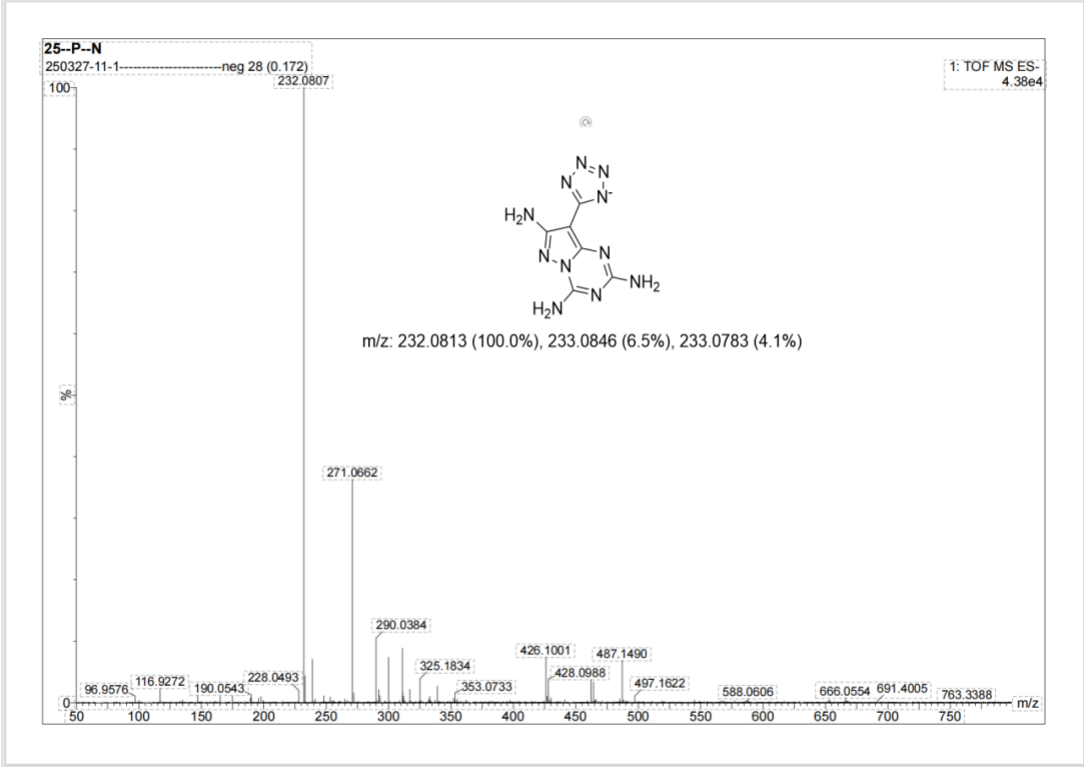


Figure S8. HRMS (ESI–) spectrum of **3**.

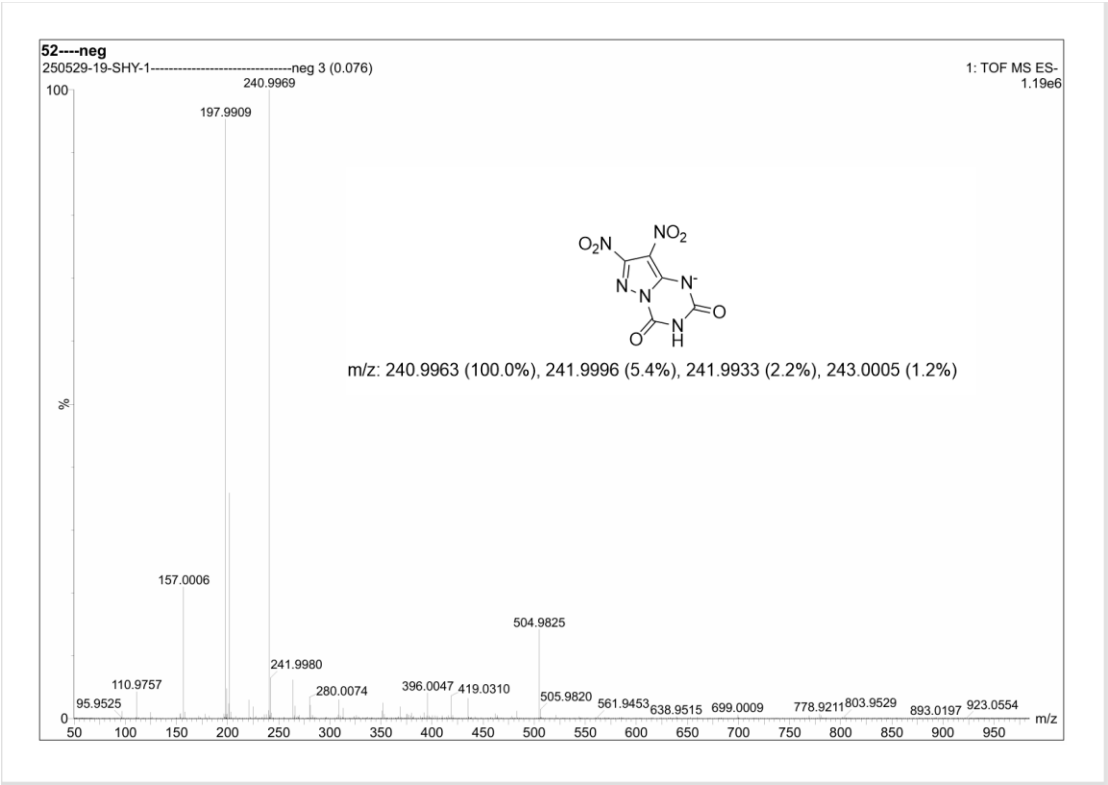


Figure S9. HRMS (ESI–) spectrum of **4**.

4 DSC Plots

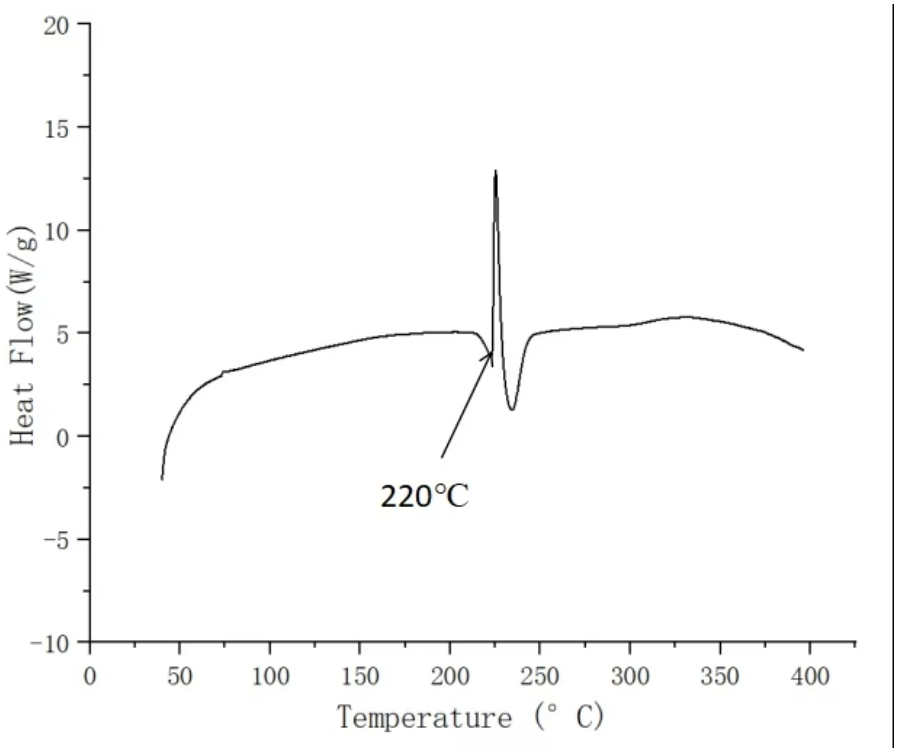


Figure S10.DSC Plot of **2**.

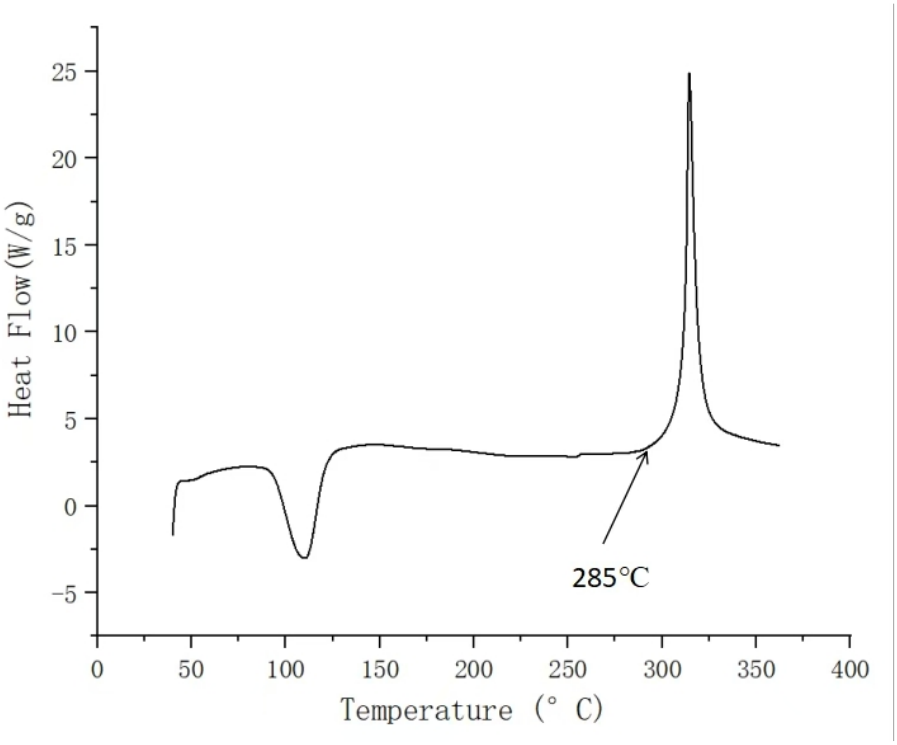


Figure S11.DSC Plot of **3**.

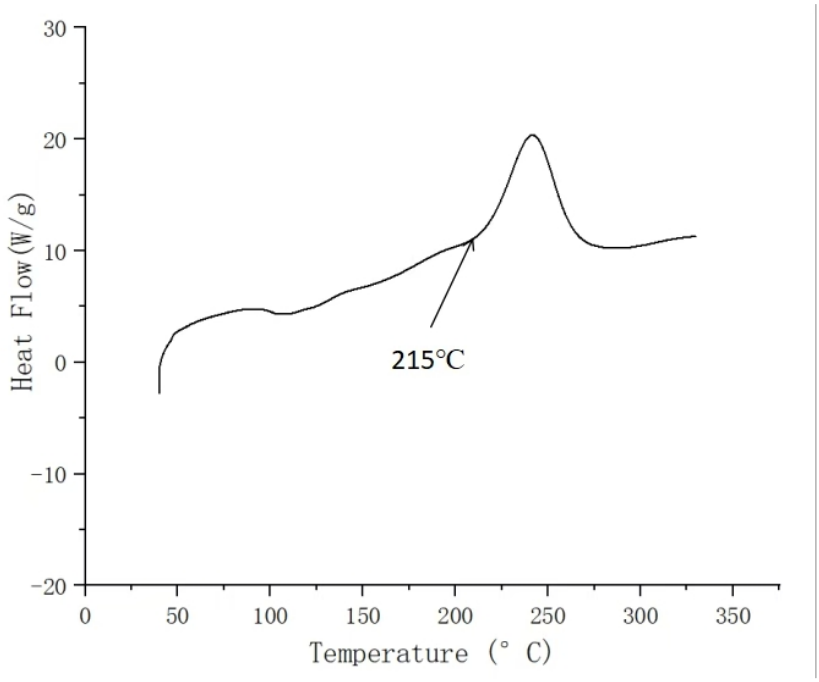


Figure S12.DSC Plot of **4**.

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