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Supporting information

Performance Enhancement through a Positional Isomerism Modification Strategy

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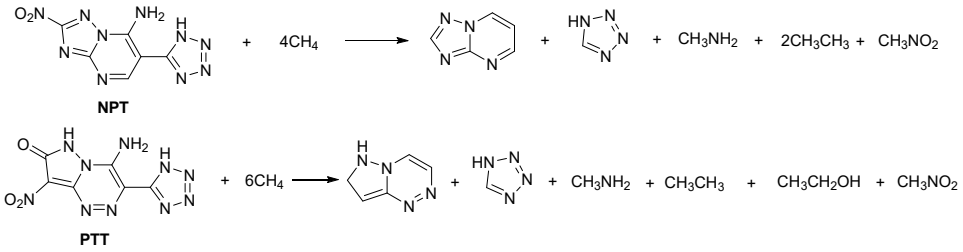
Computational Details

Computations were performed by using the Gaussian09 suite of programs.[1] The geometric optimization and frequency analyses of the structures were calculated using B3LYP/6-31+G** level and single energy points were calculated at the MP2/6-311++G** level.[2-4] The gas phase heats of formation (HOF) for compounds **NPT** and **PTT** were calculated through designed isodesmic reactions (**Scheme S2**).



Scheme S1 Isodesmic reactions for calculating heats of formation for **NPT** and **PTT**

The solid-state enthalpy of formation for neutral compound can be estimated by subtracting the heat of sublimation from gas-phase heat of formation.[5] The heat of sublimation can be estimated with Trouton's rule according to supplementary equation 1:

$$\Delta H_{sub} = \frac{188}{J \cdot mol^{-1} K^{-1}} \times T \quad \text{(supplementary equation 1)}$$

where T represents either the melting point or the decomposition temperature when no melting occurs prior to decomposition.

X-ray crystallographic Data

Table S1. Crystal parameters for compounds **2**, **NPT**, **TPTO** and **PTT**

Compound	**2·CH_3OH**	**NPT·DMF**	**TPTO·$NHMe_2$·H_2O**	**PTT·$Mg_{0.5}$·$9H_2O$**
formula	$C_7H_7N_7O_3$	$C_9H_{11}N_{11}O_3$	$C_{16}H_{23}N_{18}O_{10}$	$C_6H_{17}Mg_{0.5}N_{10}O_{10}$
Temperature [K]	298(2)	298(2)	298(2)	113.90(14)
Crystal system	orthorhombic	monoclinic	monoclinic	monoclinic
Space group	*Pnma(62)*	$P2_1/c$	$P2_1/m$	$P2_1/c$
A [Å]	12.8331(13)	6.9809(7)	9.1828(9)	9.323(2)
B [Å]	6.4142(7)	6.8761(7)	6.5037(8)	26.924(6)
C [Å]	12.1223(14)	28.243(3)	11.7685(13)	6.725(4)
α [°]	90.00	90.00	90.00	90.00
β [°]	90.00	92.736(2)	95.504(3)	108.46(4)
γ [°]	90.00	90.00	90.00	90.00
V [$Å^3$]	997.84(19)	1354.2(2)	699.60(13)	1601.2(11)
Z	4	4	1	4
ρ [$g \cdot cm^{-3}$]	1.57884	1.576	1.492	1.665
F(000)	488.0	664.0	326.0	836
Crystal size [mm^3]	0.36 × 0.20 × 0.16	0.36 × 0.30 × 0.08	0.32 × 0.27 × 0.05	0.29 × 0.12 × 0.08

2Θ [°]	4.62 to 50.04	5.78 to 50.02	4.46 to 50.04	6.06 to 49.98
Index ranges	-15 ≤ h ≤ 15, -5 ≤ k ≤ 7, -14 ≤ l ≤ 14	-6 ≤ h ≤ 8, -6 ≤ k ≤ 8, -33 ≤ l ≤ 33	-10 ≤ h ≤ 8, -7 ≤ k ≤ 7, -14 ≤ l ≤ 12	-11 ≤ h ≤ 7, -32 ≤ k ≤ 29, -5 ≤ l ≤ 7
Reflections collected	4706	6274	3498	6285
Independent reflections	962	2371	1335	2796
Goodness-of-fit on F^2	1.081	1.098	1.081	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0528, wR_2 = 0.1412	R_1 = 0.0861, wR_2 = 0.2121	R_1 = 0.0629, wR_2 = 0.1302	R_1 = 0.0973, wR_2 = 0.2214
Final R indexes [all data]	R_1 = 0.0722, wR_2 = 0.1560	R_1 = 0.1203, wR_2 = 0.2279	R_1 = 0.1194, wR_2 = 0.1478	R_1 = 0.1533, wR_2 = 0.2571
CCDC	**2168315**	**2168314**	**2168316**	**2133016**

Crystal structure plots and tables

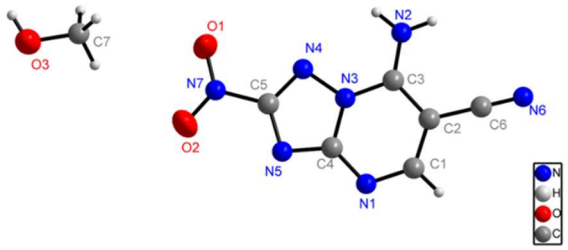


Figure S1 The crystal structure of **2·MeOH**

Table S1 Bond Lengths for **2·MeOH**

Atom 1	Atom 2	Length/Å	Atom 1	Atom 2	Length/Å
N1	C1	1.320(5)	N6	C6	1.136(5)
N1	C4	1.329(4)	N7	O1	1.203(4)
N2	C3	1.300(4)	N7	O2	1.206(4)
N3	C3	1.353(4)	N7	C5	1.444(5)
N3	N4	1.365(3)	O3	C7	1.393(6)
N3	C4	1.373(4)	C1	C2	1.380(5)
N4	C5	1.300(4)	C2	C6	1.408(5)
N5	C4	1.320(5)	C2	C3	1.411(4)

Table S2 Bond Angles for **2·MeOH**

Atom 1	Atom 2	Atom 3	Angle/°	Atom 1	Atom 2	Atom 3	Angle/°
C1	N1	C4	114.4(3)	C6	C2	C3	119.4(3)
C3	N3	N4	124.5(2)	N2	C3	N3	119.8(3)
C3	N3	C4	124.8(3)	N2	C3	C2	128.1(3)
N4	N3	C4	110.6(3)	N3	C3	C2	112.1(3)
C5	N4	N3	99.4(2)	N5	C4	N1	128.5(3)
C4	N5	C5	101.8(3)	N5	C4	N3	108.7(3)

O1	N7	C5	117.8(3)	N4	C5	N5	119.5(3)
N1	C1	C2	125.7(3)	N5	C5	N7	120.9(3)
C1	C2	C6	120.4(3)	N6	C6	C2	179.8(3)

Table S3 Torsion Angles for **2·MeOH**

Atom 1	Atom 2	Atom 3	Atom 4	Angle/°	Atom 1	Atom 2	Atom 3	Atom 4	Angle/°
C3	N3	N4	C5	180	C1	N1	C4	N3	0
C4	N3	N4	C5	0	C3	N3	C4	N5	180
C4	N1	C1	C2	0.000(1)	N4	N3	C4	N5	0
N1	C1	C2	C6	180	C3	N3	C4	N1	0
N1	C1	C2	C3	0.000(1)	N4	N3	C4	N1	180
N4	N3	C3	N2	0	N3	N4	C5	N5	0
C4	N3	C3	N2	180	N3	N4	C5	N7	180
N4	N3	C3	C2	180	C4	N5	C5	N4	0
C4	N3	C3	C2	0	C4	N5	C5	N7	180
C1	C2	C3	N2	180	O1	N7	C5	N4	0

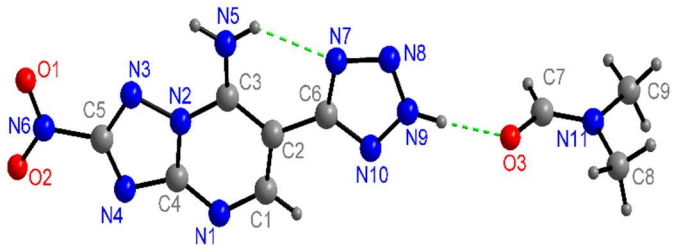


Figure S2 The crystal structure of **NPT·DMF**

Table S4 Bond Lengths for **NPT·DMF**

Atom 1	Atom 2	Length/Å	Atom 1	Atom 2	Length/Å
N1	C1	1.317(5)	N7	C6	1.311(6)
N1	C4	1.324(5)	N7	N8	1.331(5)
N2	N3	1.348(4)	N8	N9	1.283(5)
N2	C3	1.354(5)	N9	N10	1.316(5)
N2	C4	1.364(6)	N10	C6	1.315(5)
N3	C5	1.312(5)	N11	C7	1.277(6)
N4	C5	1.307(5)	N11	C8	1.449(6)
N4	C4	1.340(5)	N11	C9	1.453(6)
N5	C3	1.318(5)	O3	C7	1.243(6)
N6	O2	1.188(5)	C1	C2	1.386(6)
N6	O1	1.199(5)	C2	C3	1.395(5)
N6	C5	1.461(5)	C2	C6	1.458(5)

Table S5 Bond Angles for **NPT·DMF**

Atom 1	Atom 2	Atom 3	Angle/°	Atom 1	Atom 2	Atom 3	Angle/°
C1	N1	C4	114.4(4)	C1	C2	C3	119.2(4)
N3	N2	C3	125.6(3)	C1	C2	C6	120.1(4)

N3	N2	C4	110.6(3)	C3	C2	C6	120.7(4)
C3	N2	C4	123.8(3)	N5	C3	N2	118.1(3)
C5	N3	N2	99.2(3)	N5	C3	C2	128.3(4)
C5	N4	C4	100.6(4)	N2	C3	C2	113.6(4)
O2	N6	O1	124.4(4)	N1	C4	N4	127.8(4)
O2	N6	C5	117.8(4)	N1	C4	N2	123.1(4)
O1	N6	C5	117.9(4)	N4	C4	N2	109.0(3)
C6	N7	N8	106.8(3)	N4	C5	N3	120.6(4)
N9	N8	N7	104.8(4)	N4	C5	N6	121.7(4)
N8	N9	N10	114.8(3)	N3	C5	N6	117.7(4)
C6	N10	N9	101.5(4)	N7	C6	N10	112.1(4)
C7	N11	C8	120.7(4)	N7	C6	C2	123.7(4)
C7	N11	C9	122.6(4)	N10	C6	C2	124.2(4)
C8	N11	C9	116.7(4)	O3	C7	N11	124.8(5)
N1	C1	C2	125.8(4)				

Table S6 Torsion Angles for **NPT·DMF**

Atom 1	**Atom 2**	**Atom 3**	**Atom 4**	**Angle/°**	**Atom 1**	**Atom 2**	**Atom 3**	**Atom 4**	**Angle/°**
C3	N2	N3	C5	-177.9(4)	C3	N2	C4	N1	-2.4(6)
C4	N2	N3	C5	0.5(4)	N3	N2	C4	N4	0.2(4)
C6	N7	N8	N9	-0.1(5)	C3	N2	C4	N4	178.7(3)
N7	N8	N9	N10	0.1(5)	C4	N4	C5	N3	1.4(5)
N8	N9	N10	C6	-0.1(5)	C4	N4	C5	N6	178.4(3)
C4	N1	C1	C2	0.3(6)	N2	N3	C5	N4	-1.2(5)
N1	C1	C2	C3	-0.6(7)	N2	N3	C5	N6	-178.4(3)
N1	C1	C2	C6	179.6(4)	O2	N6	C5	N4	1.8(6)
N3	N2	C3	N5	1.0(6)	O1	N6	C5	N4	-178.9(4)
C4	N2	C3	N5	-177.2(4)	O2	N6	C5	N3	178.9(4)
N3	N2	C3	C2	-179.9(3)	O1	N6	C5	N3	-1.7(6)
C4	N2	C3	C2	1.9(5)	N8	N7	C6	N10	0.1(5)
C1	C2	C3	N5	178.5(4)	N8	N7	C6	C2	179.8(4)
C6	C2	C3	N5	-1.7(6)	N9	N10	C6	N7	0.0(5)
C1	C2	C3	N2	-0.5(5)	N9	N10	C6	C2	-179.8(4)
C6	C2	C3	N2	179.3(3)	C1	C2	C6	N7	177.5(4)
C1	N1	C4	N4	179.9(4)	C3	C2	C6	N7	-2.3(6)
C1	N1	C4	N2	1.1(6)	C1	C2	C6	N10	-2.7(6)
C5	N4	C4	N1	-179.7(4)	C3	C2	C6	N10	177.5(4)
C5	N4	C4	N2	-0.9(4)	C8	N11	C7	O3	1.6(7)
N3	N2	C4	N1	179.2(4)	C9	N11	C7	O3	-179.5(5)

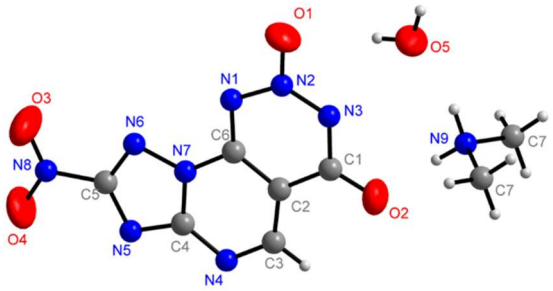


Figure S3 The crystal structure of **TPTO·NHMe$_2$·H$_2$O**

Table S7 Bond Lengths for **TPTO·NHMe$_2$·H$_2$O**

Atom 1	Atom 2	Length/Å	Atom 1	Atom 2	Length/Å
O1	N2	1.259(4)	N5	C4	1.354(4)
O2	C1	1.260(4)	N6	C5	1.312(4)
O3	N8	1.216(4)	N6	N7	1.383(4)
N1	C6	1.345(4)	N7	C6	1.396(4)
N1	N2	1.372(4)	N8	C5	1.489(5)
N2	N3	1.344(4)	C1	C2	1.452(5)
N3	C1	1.390(5)	C2	C6	1.403(5)
N4	C3	1.336(4)	C2	C3	1.413(5)
N5	C5	1.350(5)	N9	C7	1.473(4)

Table S8 Bond Angles for **TPTO·NHMe$_2$·H$_2$O**

Atom 1	Atom 2	Atom 3	Angle/°	Atom 1	Atom 2	Atom 3	Angle/°
C6	N1	N2	111.5(3)	N3	C1	C2	118.5(3)
O1	N2	N3	116.7(3)	C6	C2	C3	120.0(3)
O1	N2	N1	115.0(3)	C6	C2	C1	114.8(3)
N3	N2	N1	128.3(3)	C3	C2	C1	125.2(4)
N2	N3	C1	118.4(3)	N4	C3	C2	125.0(4)
C3	N4	C4	114.7(3)	N5	C4	N4	127.8(4)
C5	N5	C4	101.6(3)	N5	C4	N7	108.3(3)
C5	N6	N7	99.8(3)	N4	C4	N7	123.9(3)
C4	N7	N6	110.7(3)	N6	C5	N5	119.5(3)
C4	N7	C6	122.3(3)	N6	C5	N8	119.5(4)
N6	N7	C6	127.0(3)	N5	C5	N8	121.0(3)
O3	N8	O4	125.0(4)	N1	C6	N7	117.4(3)
O3	N8	C5	118.1(3)	N1	C6	C2	128.4(3)
O4	N8	C5	117.0(4)	N7	C6	C2	114.2(3)
O2	C1	N3	117.9(4)	C71	N9	C7	111.6(4)

Table S9 Torsion Angles for **TPTO·NHMe$_2$·H$_2$O**

Atom 1	Atom 2	Atom 3	Atom 4	Angle/°	Atom 1	Atom 2	Atom 3	Atom 4	Angle/°
C6	N1	N2	O1	180	N6	N7	C4	N4	180
C6	N1	N2	N3	0	C6	N7	C4	N4	0
O1	N2	N3	C1	180	N7	N6	C5	N5	0

N1	N2	N3	C1	0	N7	N6	C5	N8	180
C5	N6	N7	C4	0	C4	N5	C5	N6	0
C5	N6	N7	C6	180	C4	N5	C5	N8	180
N2	N3	C1	O2	180	O3	N8	C5	N6	0
N2	N3	C1	C2	0	O4	N8	C5	N6	180
O2	C1	C2	C6	180	O3	N8	C5	N5	180
N3	C1	C2	C6	0	O4	N8	C5	N5	0
O2	C1	C2	C3	0	N2	N1	C6	N7	180
N3	C1	C2	C3	180	N2	N1	C6	C2	0
C4	N4	C3	C2	0	C4	N7	C6	N1	180
C6	C2	C3	N4	0	N6	N7	C6	N1	0
C1	C2	C3	N4	180	C4	N7	C6	C2	0
C5	N5	C4	N4	180	N6	N7	C6	C2	180
C5	N5	C4	N7	0	C3	C2	C6	N1	180
C3	N4	C4	N5	180	C1	C2	C6	N1	0
C3	N4	C4	N7	0	C3	C2	C6	N7	0
N6	N7	C4	N5	0	C1	C2	C6	N7	180
C6	N7	C4	N5	180					

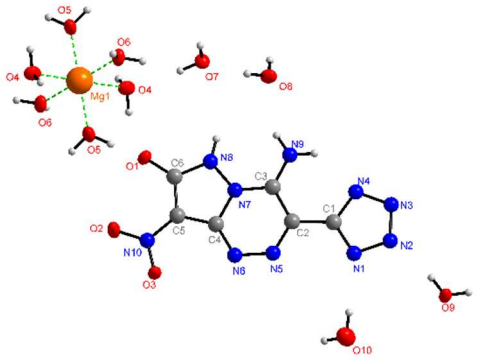


Figure S4 The asymmetric structure of **TPTO·NHMe$_2$·H$_2$O**

Table S10 Bond Lengths for **PTT·Mg$_{0.5}$·9H$_2$O**

Atom 1	Atom 2	Length/Å	Atom 1	Atom 2	Length/Å
Mg1	O6	2.127(5)	N3	N4	1.341(7)
Mg1	O4	2.156(5)	N10	O2	1.242(7)
Mg1	O5	2.055(5)	N10	C5	1.393(8)
N9	C3	1.311(8)	N1	C1	1.350(8)
N7	N8	1.376(7)	N4	C1	1.336(8)
N7	C3	1.331(8)	N5	C2	1.334(8)
N7	C4	1.404(7)	C2	C3	1.444(9)
O1	C6	1.274(7)	C2	C1	1.463(8)
N8	C6	1.368(8)	C4	C5	1.398(8)
N6	N5	1.345(7)	C5	C6	1.445(9)
N6	C4	1.327(8)			

Table S11 Bond Angles for **PTT·$Mg_{0.5}$·$9H_2O$**

Atom 1	Atom 2	Atom 3	Angle/°	Atom 1	Atom 2	Atom 3	Angle/°
O6	Mg1	O4	91.47(17)	C1	N4	N3	104.2(5)
N8	N7	C4	112.9(4)	C3	C2	C1	120.5(5)
C3	N7	N8	124.8(5)	N9	C3	N7	121.4(6)
C3	N7	C4	122.3(5)	N7	C3	C2	113.9(5)
C6	N8	N7	106.0(5)	N6	C4	N7	122.0(5)
C4	N6	N5	117.4(5)	N6	C4	C5	133.5(5)
N2	N3	N4	109.8(5)	C5	C4	N7	104.4(5)
O3	N10	O2	122.2(5)	N1	C1	C2	124.4(5)
O3	N10	C5	118.1(5)	N4	C1	N1	112.3(5)
O1	C6	N8	122.5(6)	N4	C1	C2	123.3(5)
O1	C6	C5	128.6(6)	N10	C5	C4	125.6(6)
N8	C6	C5	108.9(5)	N10	C5	C6	126.6(6)
C4	C5	C6	107.8(5)				

Table S12 Torsion Angles for **PTT·$Mg_{0.5}$·$9H_2O$**

Atom 1	Atom 2	Atom 3	Atom 4	Angle/°	Atom 1	Atom 2	Atom 3	Atom 4	Angle/°
N7	N8	C6	O1	-178.9(6)	C4	N7	N8	C6	0.4(7)
N7	N8	C6	C5	0.0(7)	C4	N7	C3	N9	-178.8(6)
N7	C4	C5	N10	-178.9(6)	C4	N7	C3	C2	0.8(8)
N7	C4	C5	C6	0.6(7)	C4	N6	N5	C2	-0.8(9)
N8	N7	C3	N9	0.6(9)	C4	C5	C6	O1	178.4(7)
N8	N7	C3	C2	-179.8(5)	C4	C5	C6	N8	-0.4(7)
N8	N7	C4	N6	179.2(6)	O2	N10	C5	C4	-178.0(6)
N8	N7	C4	C5	-0.6(7)	O2	N10	C5	C6	2.6(10)
N6	N5	C2	C3	0.3(9)	C1	N1	N2	N3	-1.0(7)
N6	N5	C2	C1	179.6(5)	C1	C2	C3	N9	0.0(10)
N6	C4	C5	N10	1.3(12)	C1	C2	C3	N7	-179.6(6)
N6	C4	C5	C6	-179.2(7)	N5	C2	C3	N9	179.3(6)
O3	N10	C5	C4	0.8(10)	N5	C2	C3	N7	-0.3(9)
O3	N10	C5	C6	-178.6(6)	N5	C2	C1	N1	3.3(10)
N3	N4	C1	N1	-0.6(7)	N5	C2	C1	N4	-176.9(6)
N3	N4	C1	C2	179.5(6)	N2	N3	N4	C1	0.0(7)
N10	C5	C6	O1	-2.1(11)	N2	N1	C1	N4	1.0(7)
N10	C5	C6	N8	179.1(6)	N2	N1	C1	C2	-179.2(6)
N4	N3	N2	N1	0.7(8)	C3	N7	N8	C6	-179.1(6)
N5	N6	C4	N7	1.2(9)	C3	N7	C4	N6	-1.3(9)

NMR spectra

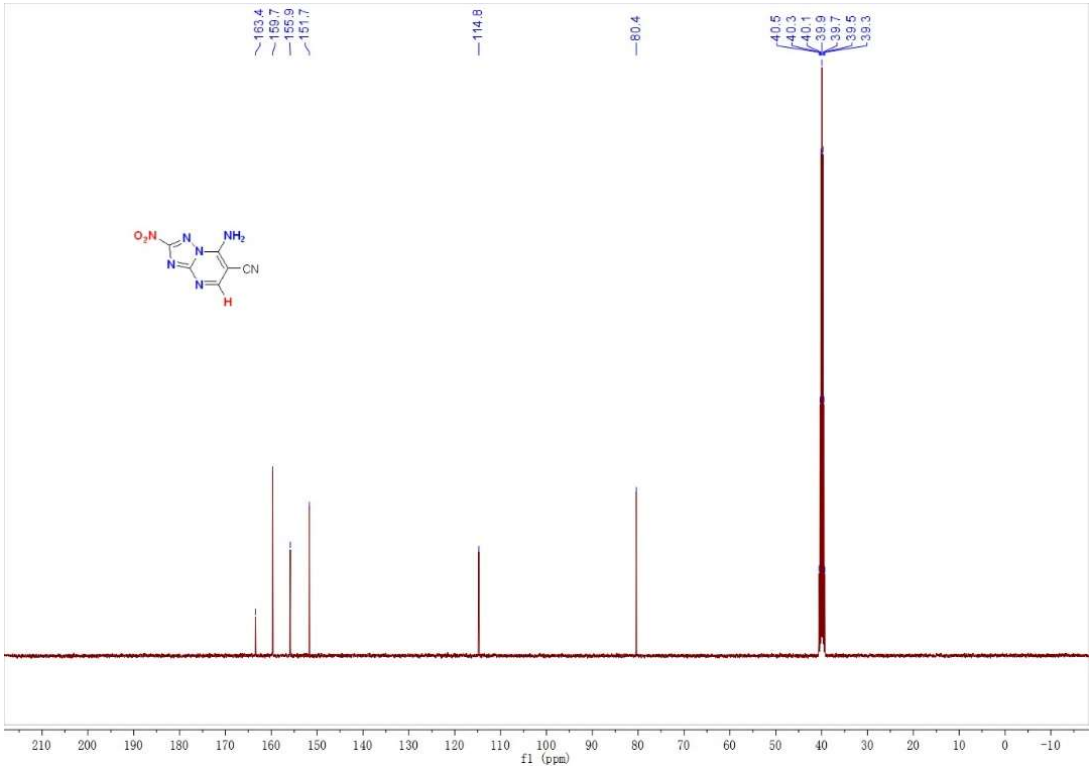


Figure S5 ^{13}C NMR spectra in DMSO-d_6 for compound **2**.

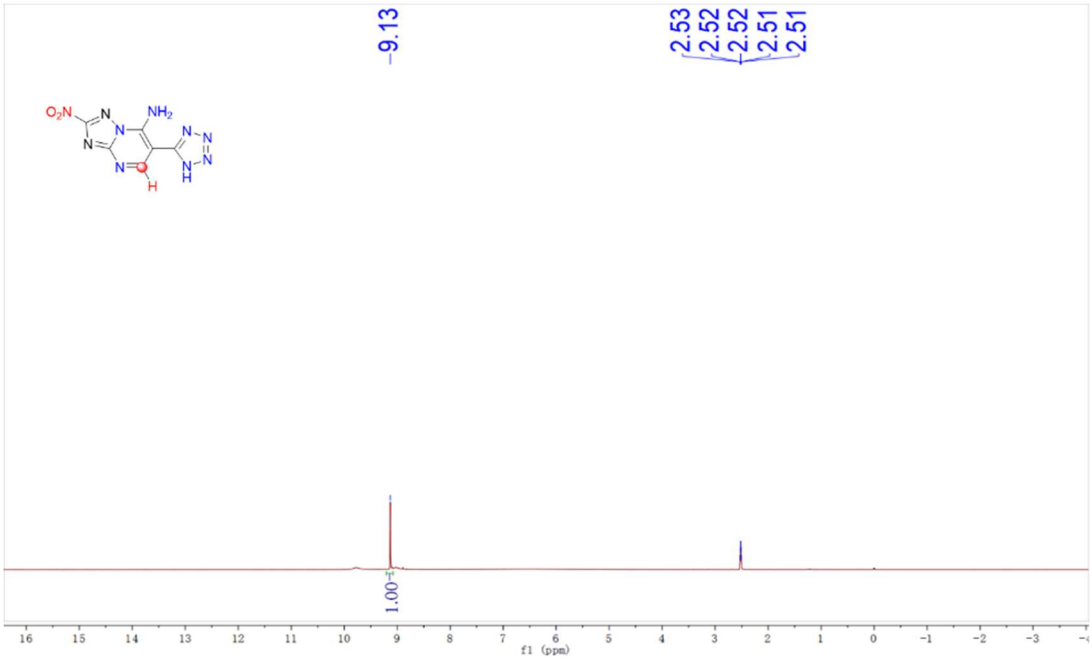


Figure S6 ^{1}H NMR spectra in DMSO-d_6 for compound **NPT**

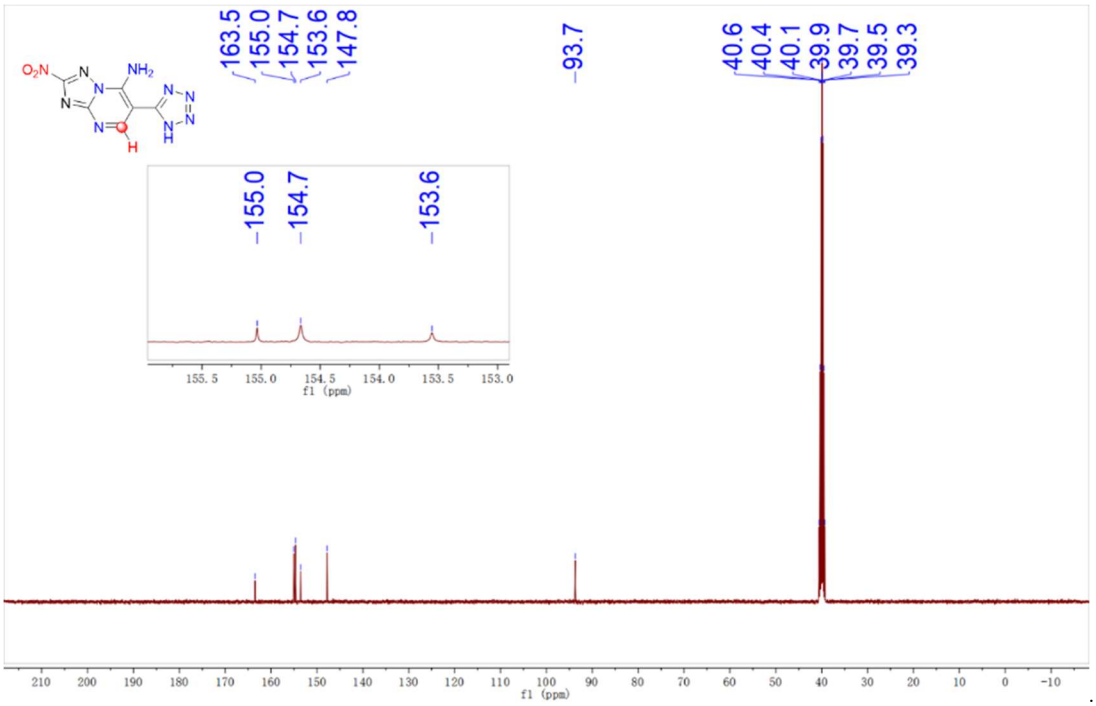


Figure S7 ^{13}C NMR spectra in DMSO-d_6 for compound **NPT**.

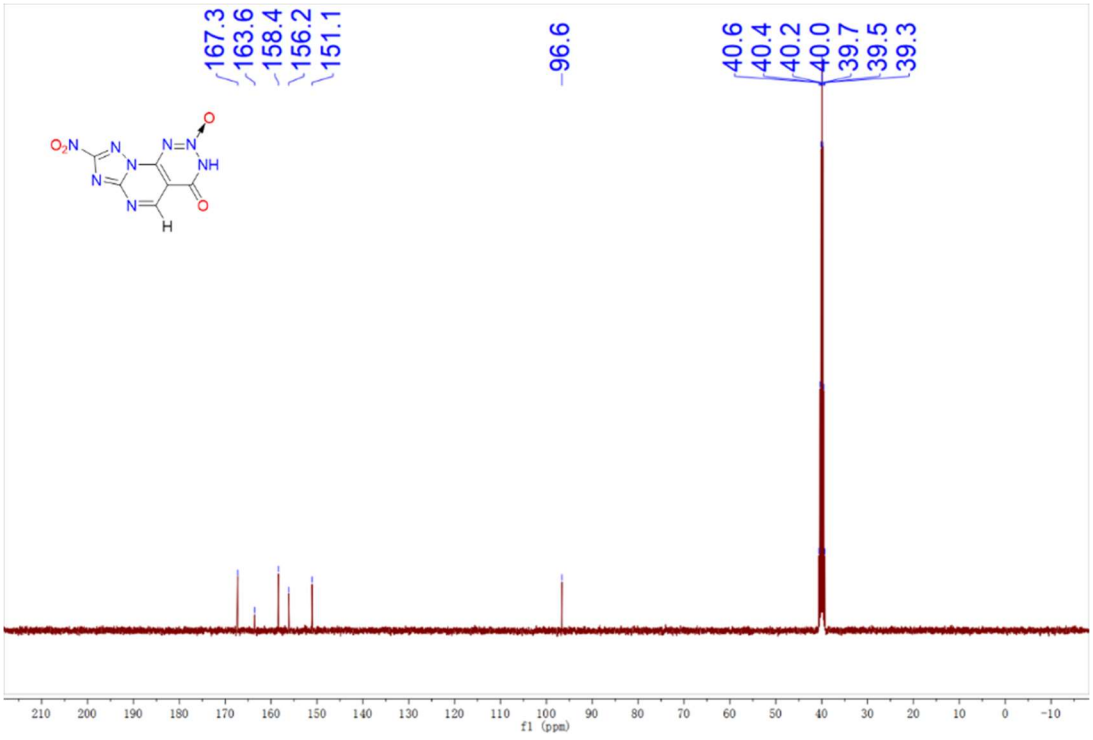


Figure S8 ^{13}C NMR spectra in DMSO-d_6 for compound **TPTO**.

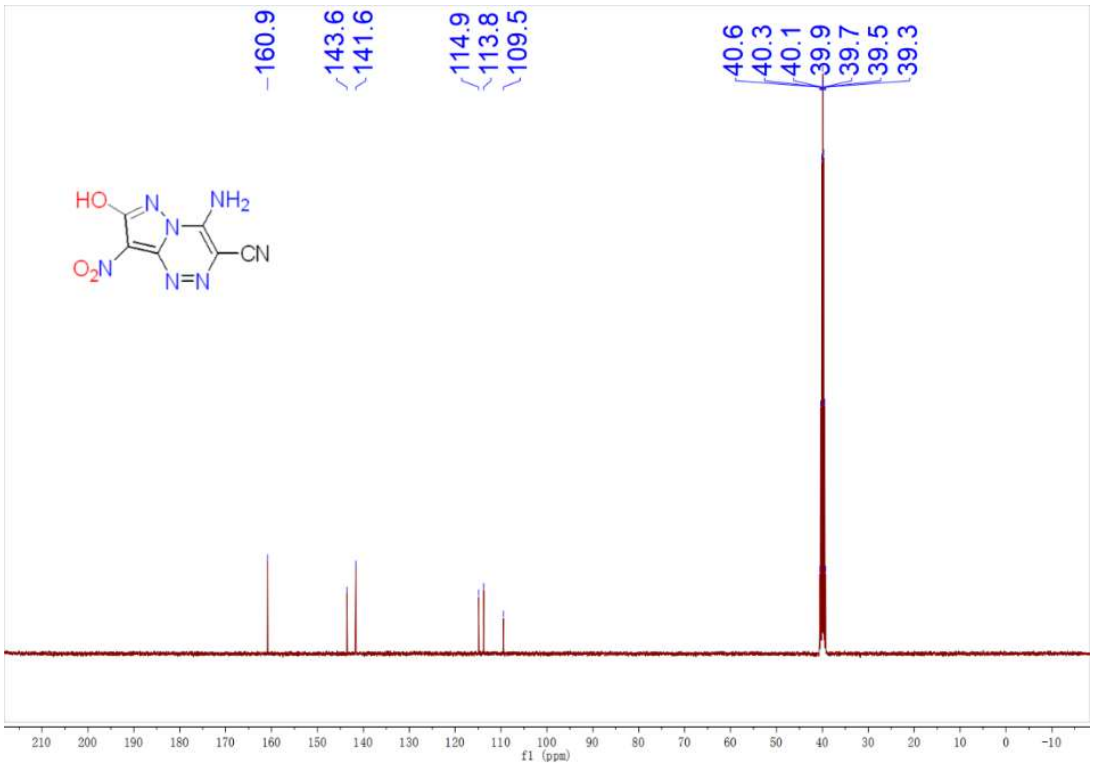


Figure S9 ^{13}C NMR spectra in DMSO-d_6 for compound **4**.

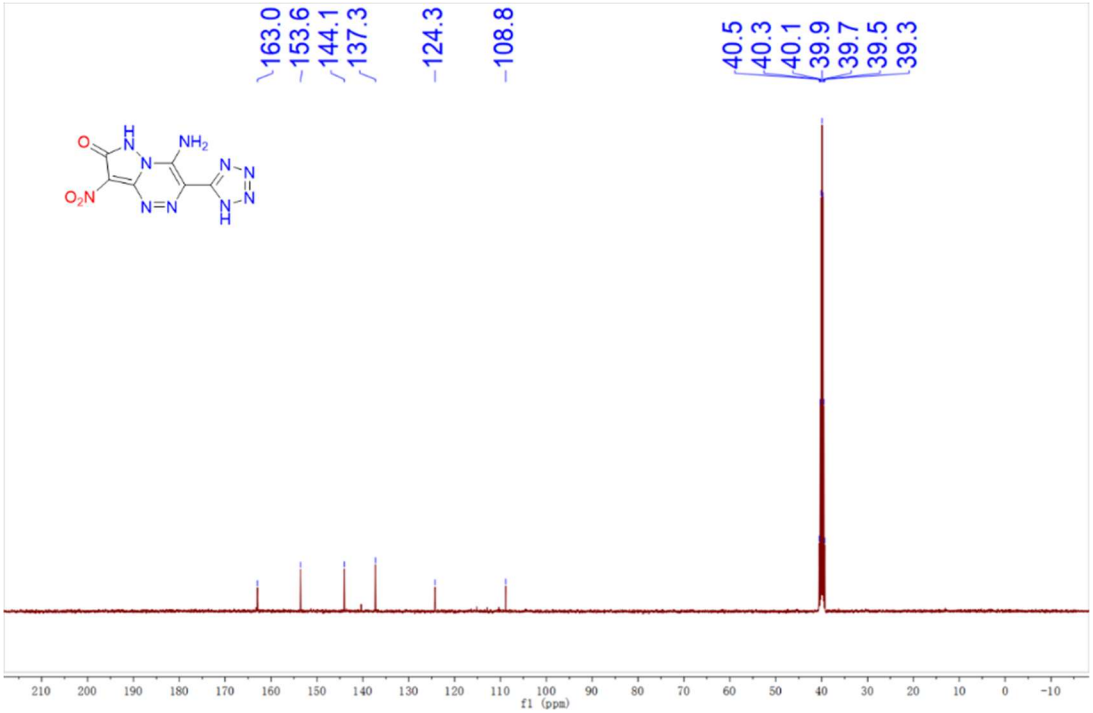


Figure S10 ^{13}C NMR spectra in DMSO-d_6 for compound **PTT**.

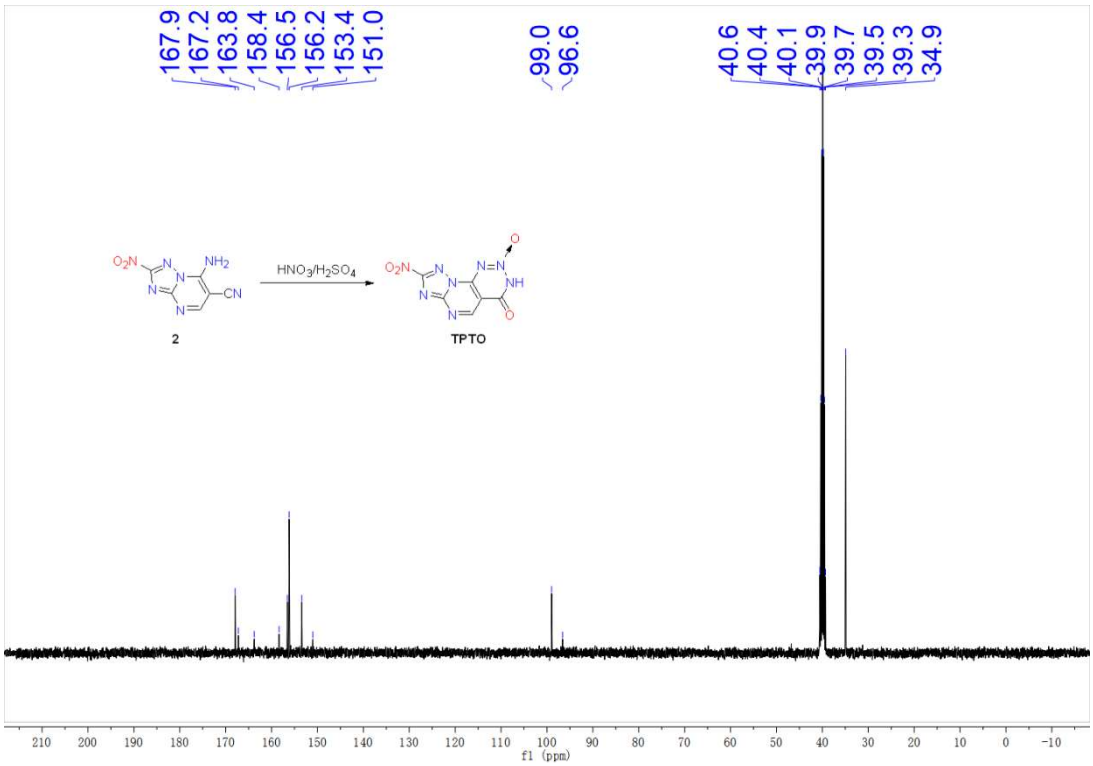


Figure S11 ^{13}C NMR spectra in DMSO-d_6 for nitration compound obtained from compound **2**.

DSC curves

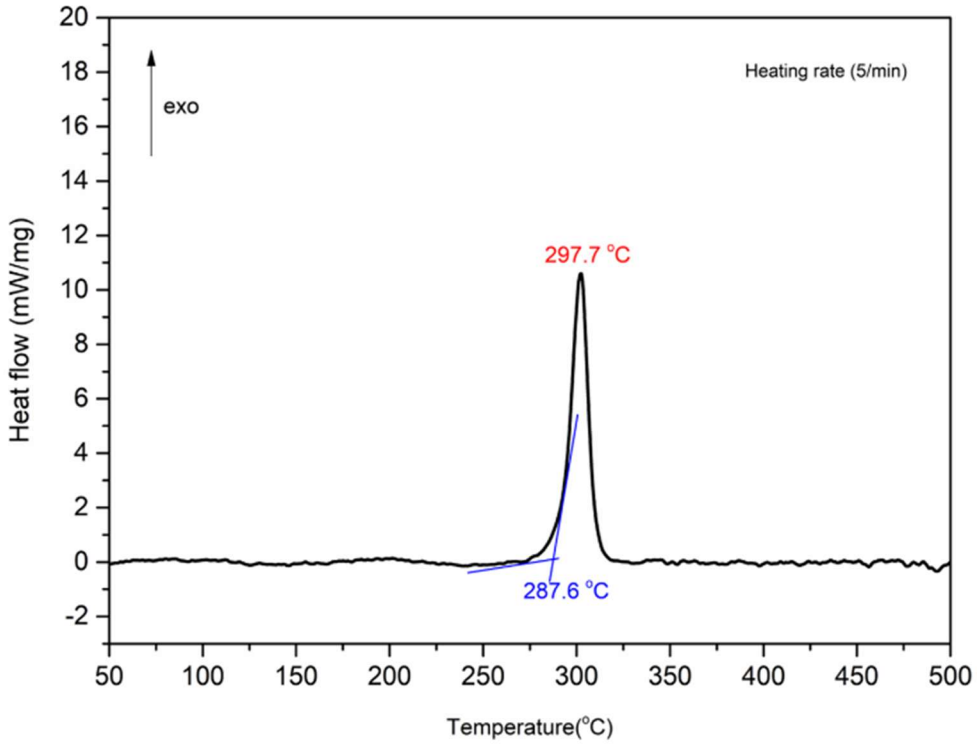


Figure S12 DSC curve of **NPT** measured at a heating rate of 5 °C·min^{-1} (exo up).

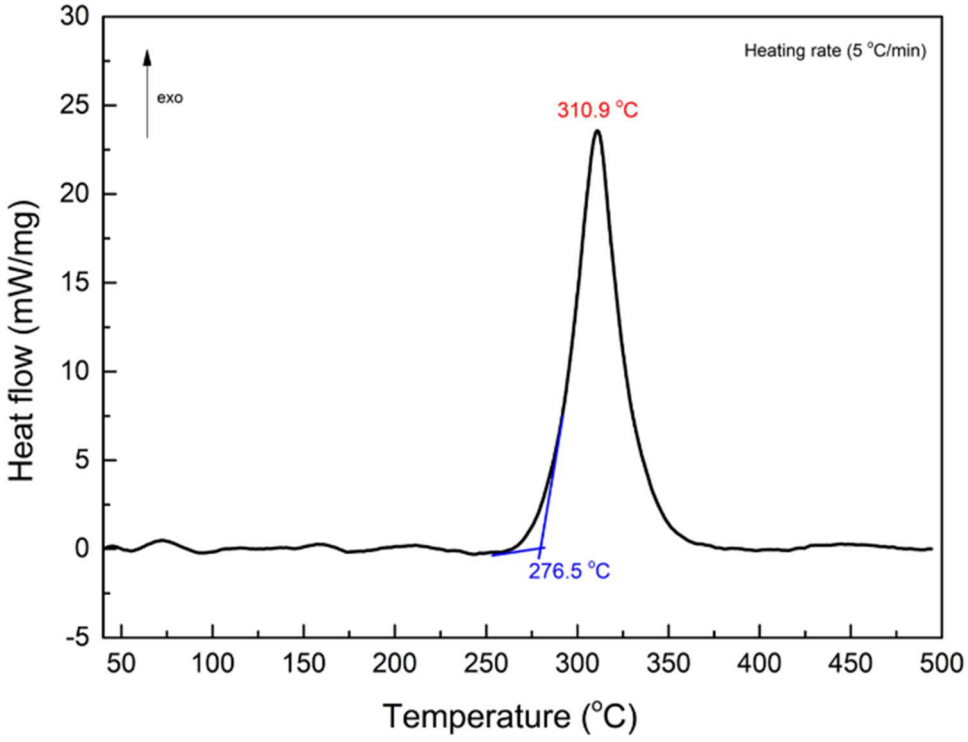


Figure S13 DSC curve of **PTT** measured at a heating rate of 5 °C·min^{-1} (exo up).

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