Supporting Information

Combination furoxan and 1,2,4-oxadiazole for the generation of high-performance energetic materials.

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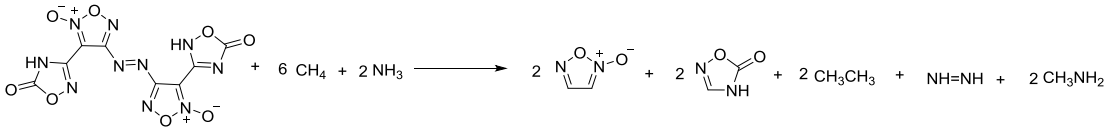
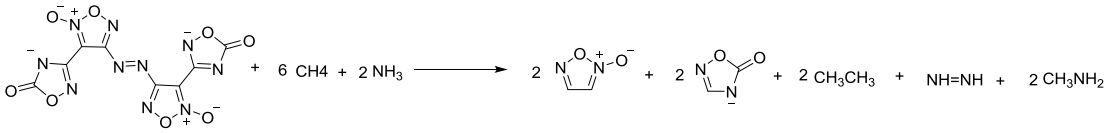
1. Computational details

Computations were performed by using the Gaussian09 suite of programs.[1] The elementary geometric optimization and the frequency analysis were performed at the level of the Becke three parameter, Lee-Yan-Parr (B3LYP) functional with the 6-311+G** basis set.[2-4] All of the optimized structures were characterized to be local energy minima on the potential surface without any imaginary frequencies. Atomization energies were calculated by the CBS-4M.[5] All the optimized structures were characterized to be true local energy minima on the potential-energy surface without imaginary frequencies.

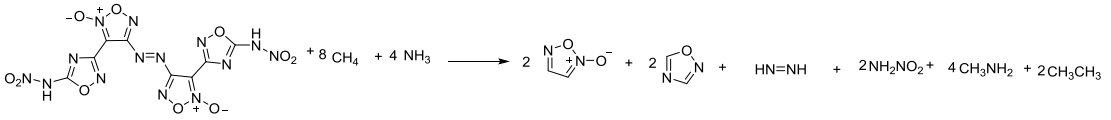
The predictions of heats of formation (HOF) of compounds used the hybrid DFTB3LYP methods with the 6-311+G** basis set through designed isodesmic reactions. The isodesmic reaction processes, that is, the number of each kind of formal bond is conserved, were used with the application of the bond separation reaction (BSR) rules. The molecule was broken down into a set of two heavy-atom molecules containing the same component bonds. The isodesmic reactions used to derive the HOF shown in Scheme S1-S4.



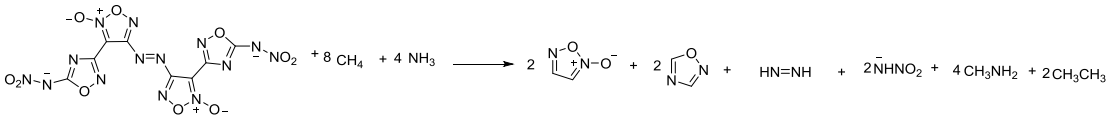
Scheme 1. The isodesmic reactions for calculating heat of formation for **3**.



Scheme 2. The isodesmic reactions for calculating heat of formation for the anion of **3**.



Scheme 3. The isodesmic reactions for calculating heat of formation for **4**



Scheme 4. The isodesmic reactions for calculating heat of formation for anion of **3**.

The change of enthalpy for the reactions at 298K can be expressed by Equation (1):

$$\Delta H_{298} = \Sigma\Delta_f H_P - \Sigma\Delta_f H_R \qquad (1)$$

Where $\Sigma\Delta_f H_P$ and $\Sigma\Delta_f H_R$ are the HOF of t,e reactants and products at 298 K, respectively, and ΔH_{298} can be calculated from the following expression in Equation (2):

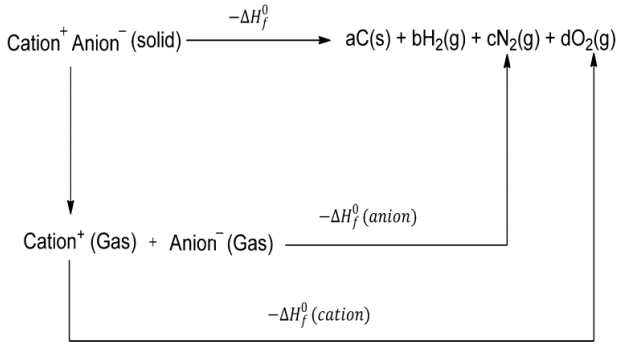
$$\Delta H_{298} = \Delta E_{298} + \Delta(PV) = \Delta E_0 + \Delta ZPE + \Delta H_T + \Delta nRT \qquad (2)$$

where ΔE_0 is the change in total energy between the products and the reactants at 0 K; ΔZPE is the difference between the zero-point energies (*ZPE*) of the products and the reactants at 0 K; ΔH_T is the thermal correction from 0 to 298 K. The $\Delta(PV)$ value in Equation(2) is the *PV* work term. It equals ΔnRT for the reactions of an ideal gas. For the isodesmic reactions $\Delta n = 0$, so $\Delta(PV) = 0$. On the left side of Equation (2), apart from target compound all the others are called reference

compounds. The HOF of reference compounds are available either from experiments or from the high level computing such as CBS-4M.

Based on a Born-Haber energy cycle (Scheme S5), the heat of formation of a salt can be simplified by Equation (3):

$$\Delta H_f°(\text{ionic salt, 298 K}) = \Delta H_f°(\text{cation, 298 K}) + \Delta H_f°(\text{anion, 298 K}) - \Delta H_L \quad (3)$$



Scheme S5 Born–Haber cycle for the formation of energetic salts

where ΔH_L is the lattice energy of the salt which could be predicted by the formula suggested by Jenkins et al.[4] as given in Equation (4):

$$\Delta H_L = U_{POT} + [p(nM/2-2) + q(nX/2-2)]RT \quad (4)$$

where n_M and n_X depend on the nature of the ions Mp^+ and Xq^-, respectively, and are equal to 3 for monatomic ions, 5 for linear polyatomic ions, and 6 for nonlinear polyatomic ions. The equation for lattice potential energy U_{POT} takes the form of equation (5):

$$U_{POT}(\text{kJ mol}^{-1}) = \gamma(\rho_m/M_m)^{1/3} + \delta \quad (5)$$

where ρ_m is the density (g cm^{-3}), M_m is the chemical formula mass of the ionic material and the coefficients γ (kJ mol^{-1}cm) and δ (kJ mol^{-1}) are 8375.6 and -178.8, respectively.

Table S1. Calculated zero-point energy (ZPE), thermal correction to enthalpy (H_T), total energy (E_0) and heats of formation (HOF)

Compound	E_0 / a.u.	*ZPE* / kJ mol^{-1}	ΔH_T / kJ mol^{-1}	HOF/kJ mol^{-1}
3	-1455.301011	380.05	57.53	633.44
4	-1824.554989	451.4	73.23	1241.14
CH_4	-40.5339263	112.26	10.04	-74.60
NH_3	-56.5826356	86.27	10.05	-45.9
furoxan	-337.3042877	124.09	14.34	224.73
1,2,4- oxadiazole	-262.1529348	116.9	11.67	99.8
NH_2NO_2	-261.1248168	98.79	12.39	-3.9
CH_3NO_2	-245.0915559	124.93	11.60	-80.80
CH_3CH_3	-79.8565413	187.31	11.79	-84.01
NH^-NO_2	-260.5730748	65.76	11.37	-120.22
NHNH	-110.679524	70.35	10.03	194.97
CH_3NH_2	-95.8938402	160.78	11.64	-22.5
1,2,4-oxadiazol-5(4H)-one	-337.4295337	128.36	14.48	-128.96
1,2,4-oxadiazol-5-one anion	-336.894443	95.94	13.5	-285.12

2. Crystallographic data

Table S2 Crystallographic data for compounds 3 and 4a

Empirical formula	$C_8H_2N_{10}O_8 \cdot CH_3COCH_3$	$C_8H_8N_{16}O_{10} \cdot 2H_2O$
Formula weight	424.27	524.34
Temperature/K	100	173
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	C2/c
a/Å	14.572(3)	29.577(3)
b/Å	11.493(2)	5.0295(4)
c/Å	9.5435(18)	14.2565(12)
α/°	90	90
β/°	98.872(7)	92.983(3)
γ/°	90	90
Volume/$Å^3$	1579.1(5)	2117.9(3)
Z	4	4
$\rho_{calc}mg/mm^3$	1.785	1.644
m/mm^{-1}	0.157	0.152
F(000)	864.0	1072.0
Crystal size/mm^3	0.12 × 0.08 × 0.05	0.14 x 0.08 x 0.05
2Θ range for data collection	4.534 to 52.894	3.111 to 25.020
Index ranges	$-18 \le h \le 17$, $-12 \le k \le 14$, $-11 \le l \le 11$	-33<=h<=34,-5<=k<=5, -16<=l<=16
Reflections collected	9208	6910
Independent reflections	3204 [R_{int} = 0.0538, R_{sigma} = 0.0614]	1836 [R_{int} = 0.0624]
Data/restraints/parameters	3204/0/273	1836 / 22 / 181
Goodness-of-fit on F^2	0.953	1.169
Final R indexes [I>=2σ (I)]	0.0465，0.1190	0.0691, 0.1790
Final R indexes [all data]	0.0777， 0.1532	0.1134, 0.2079
CCDC	1936651	1825381

Table S3 Selected bond lengths [Å] and angles [°] for **3**

O1-N3	1.454(3)	O8-N7	1.346(3)
O1-N4	1.359(3)	O8-N8	1.481(3)
O2-N3	1.219(3)	O9-C10	1.231(3)
O3-N1	1.418(3)	N1-C2	1.302(3)
O3-C1	1.370(3)	N2-C2	1.359(3)
O4-C1	1.201(3)	N2-C1	1.365(3)
O5-C8	1.197(3)	N3-C3	1.326(3)
O6-N9	1.421(3)	N4-C4	1.311(3)
O6-C8	1.363(3)	N5-C4	1.422(3)
O7-N8	1.211(3)	N5-N6	1.254(3)
N6 -C5	1.396(3)	C5 -C6	1.431(4)

N7 -C5	1.311(3)	C6 -C7	1.444(4)
N8 -C6	1.329(3)	C9 -C10	1.491(4)
N9 -C7	1.300(3)	C10-C11	1.489(4)
N10-C7	1.362(3)	C9 -H9A	0.9800
N10-C8	1.372(3)	C9 -H9B	0.9800
N2 -H2	0.8800	C9 -H9C	0.9800
N10-H10	0.8800	C11-H11A	0.9800
C2 -C3	1.440(3)	C11-H11B	0.9800
C3 -C4	1.412(3)	C11-H11C	0.9800
N3-O1 -N4	108.33(16)	N3 -C3 -C4	106.60(19)
N1-O3 -C1	109.28(18)	C2 -C3 -C4	131.8(2)
N9-O6 -C8	109.80(19)	N3 -C3 -C2	121.6(2)
N7-O8 -N8	107.62(17)	N5 -C4 -C3	124.5(2)
O3-N1 -C2	104.36(19)	N4 -C4 -N5	123.5(2)
C1-N2 -C2	107.3(2)	N4 -C4 -C3	112.0(2)
O1-N3 -O2	117.98(19)	N6 -C5 -C6	136.1(2)
O1-N3 -C3	106.44(18)	N7 -C5 -C6	112.0(2)
O2-N3 -C3	135.6(2)	N6 -C5 -N7	111.9(2)
O1-N4 -C4	106.65(19)	N8 -C6 -C5	105.8(2)
N6-N5 -C4	111.0(2)	N8 -C6 -C7	117.9(2)
N5-N6 -C5	116.1(2)	C5 -C6 -C7	136.3(2)
O8-N7 -C5	107.9(2)	N9 -C7 -N10	112.4(2)
O7-N8 -O8	117.14(19)	N9 -C7 -C6	121.6(2)
O7-N8 -C6	136.0(2)	N10-C7 -C6	125.9(2)
O8-N8 -C6	106.8(2)	O5 -C8 -N10	130.6(2)
O6-N9 -C7	104.5(2)	O6 -C8 -N10	105.6(2)
C7-N10-C8	107.7(2)	O5 -C8 -O6	123.8(2)
C2-N2 -H2	126.00	O9 -C10-C9	121.9(3)
C1-N2 -H2	126.00	O9 -C10-C11	120.1(2)
C7-N10-H10	126.00	C9 -C10-C11	118.0(2)
C8-N10-H10	126.00	C10-C9 -H9A	109.00
O3-C1 -O4	123.1(2)	C10-C9 -H9B	109.00
O3-C1 -N2	106.2(2)	C10-C9 -H9C	109.00
O4-C1 -N2	130.7(2)	H9A-C9 -H9B	109.00
N1-C2 -N2	113.0(2)	H9A-C9 -H9C	110.00
N1-C2 -C3	121.2(2)	H9B-C9 -H9C	110.00
N2-C2 -C3	125.8(2)	C10-C11-H11A	109.00
C10-C11-H11B	110.00	H11A-C11-H11C	109.00
C10-C11-H11C	109.00	H11B-C11-H11C	109.00
H11A-C11-H11B	109.00		

Table S4 Selected torsion angles for [°] **3**

N4-O1-N3-O2	-178.23(19)	N5-N6 -C5-C6	-2.3(4)
N4-O1-N3-C3	0.8(2)	O8-N7 -C5-N6	177.47(19)

N3-O1-N4-C4	-0.5(2)	O8-N7 -C5-C6	-0.9(3)
C1-O3-N1-C2	0.4(2)	O7-N8 -C6-C5	178.6(3)
N1-O3-C1-O4	177.1(2)	O7-N8 -C6-C7	0.9(4)
N1-O3-C1-N2	-0.5(2)	O8-N8 -C6-C5	-0.5(3)
C8-O6-N9-C7	0.8(3)	O8-N8 -C6-C7	-178.2(2)
N9-O6-C8-O5	178.9(2)	O6-N9 -C7-N10	-1.0(3)
N9-O6-C8-N10	-0.3(3)	O6-N9 -C7-C6	-179.1(2)
N8-O8-N7-C5	0.6(3)	C8-N10-C7-N9	0.9(3)
N7-O8-N8-O7	-179.3(2)	C8-N10-C7-C6	178.9(2)
N7-O8-N8-C6	0.0(2)	C7-N10-C8-O5	-179.5(3)
O3-N1-C2-N2	-0.1(3)	C7-N10-C8-O6	-0.3(3)
O3-N1-C2-C3	-178.4(2)	N1-C2 -C3-N3	177.9(2)
C2-N2-C1-O3	0.4(3)	N1-C2 -C3-C4	-1.8(4)
C2-N2-C1-O4	-176.9(3)	N2-C2 -C3-N3	-0.2(4)
C1-N2-C2-N1	-0.2(3)	N2-C2 -C3-C4	-179.8(2)
C1-N2-C2-C3	178.0(2)	N3-C3 -C4-N4	0.6(3)
O1-N3-C3-C2	179.5(2)	N3-C3 -C4-N5	-178.5(2)
O1-N3-C3-C4	-0.8(2)	C2-C3 -C4-N4	-179.7(2)
O2-N3-C3-C2	-1.7(4)	C2-C3 -C4-N5	1.2(4)
O2-N3-C3-C4	178.0(3)	N6-C5 -C6-N8	-176.9(3)
O1-N4-C4-N5	179.0(2)	N6-C5 -C6-C7	0.1(5)
O1-N4-C4-C3	0.0(3)	N7-C5 -C6-N8	0.9(3)
C4-N5-N6-C5	179.1(2)	N7-C5 -C6-C7	177.9(3)
N6-N5-C4-N4	3.9(3)	N8-C6 -C7-N9	1.1(4)
N6-N5-C4-C3	-177.2(2)	N8-C6 -C7-N10	-176.7(2)
N5-N6-C5-N7	179.8(2)	C5-C6 -C7-N9	-175.7(3)
C5-C6-C7-N10	6.5(5)		

Table S5 Hydrogen bonds for [Å and ゜] **3**

D—H ···A	d(D-H)/ Å	d(H...A)/ Å	d(D...A)/ Å	<(DHA)/ °
N2-H2 ···O2	0.8800	2.4200	2.924(3)	117.00
N2 -H2 ···O9^{i}	0.8800	1.8900	2.709(3)	154.00
N10-H10 ···N1	0.8800	2.2600	2.969(3)	138.00
N10-H10 ···N5	0.8800	2.2400	2.927(3)	135.00
C11-H11A ···N9^{iii}	0.9800	2.6100	3.505(4)	153.00

Symmetry Code: i: 1-x,1-y,1-z, ii: 2-x,1/2+y,3/2-z

Table S6 Selected bond lengths [Å] and angles [゜] for **4a·2H$_2$O**

O1-N2	1.455(5)	N6 -C4	1.359(5)
O1-N3	1.367(5)	N8 -H8A_b	0.97(5)
O2-N2	1.212(6)	N8 -H8A	0.97(5)
O3-N4	1.408(5)	N8 -H8D	0.96(5)
O3-C4	1.348(5)	N8 -H8C_b	0.97(5)
O4-N7	1.249(4)	N8 -H8D_b	0.96(6)

O5-N7	1.248(5)	N8 -H8B_b	0.97(5)
O6-H6A	0.8500	N8 -H8C	0.97(5)
O6-H6B	0.8500	N8 -H8B	0.97(5)
O6-H6'B	0.8500	N9 -H9C	0.9000
O6-H6'A	0.8500	N9 -H9B	0.9000
N1-N1_a	1.255(5)	N9 -H9A	0.9000
N1-C2	1.407(6)	N9 -H9D	0.9000
N2-C1	1.339(6)	C1 -C2	1.410(6)
N3-C2	1.311(5)	C1 -C3	1.454(6)
N4-C3	1.304(6)	N9'-H9'A	0.9000
N5-C3	1.368(5)	N9'-H9'B	0.9000
N5-C4	1.315(5)	N9'-H9'C	0.9000
N6-N7	1.332(6)	N9'-H9'D	0.9000
N2 -O1 -N3	108.1(3)	H8A -N8-H8D	110(5)
N4 -O3 -C4	107.0(3)	H8A -N8-H8A_b	81(4)
H6A-O6 -H6B	110.00	H8A -N8-H8B_b	158(5)
H6'A -O6'-H6'B	108.00	H8A -N8-H8C_b	49(5)
N1_a -N1 -C2	111.7(3)	H8A -N8-H8D_b	84(4)
O1 -N2 -C1	107.1(4)	H8B -N8-H8C	109(5)
O1 -N2 -O2	117.2(4)	H8B -N8-H8D	109(4)
O2 -N2 -C1	135.7(4)	H8A_b-N8-H8B	158(5)
O1 -N3 -C2	106.2(4)	H8B -N8-H8B_b	68(4)
O3 -N4 -C3	102.2(4)	H8B -N8-H8C_b	92(5)
C3 -N5 -C4	101.5(3)	H8B -N8-H8D_b	55(4)
N7 -N6 -C4	117.4(4)	H8C -N8-H8C_b	155(5)
O4 -N7 -N6	115.7(4)	H8A_b-N8-H8C	49(5)
O5 -N7 -N6	123.5(3)	H8B_b-N8-H8C	92(5)
O4 -N7 -O5	120.9(4)	H8C -N8-H8D_b	74(5)
H8B_b-N8 -H8D	55(4)	H9A -N9-H9B	107.00
H8A_b-N8 -H8D	84(4)	H9B -N9-H9D	111.00
H8A_b-N8 -H8B_b	110(4)	H9C -N9-H9D	109.00
H8C_b-N8 -H8D	74(5)	H9A -N9-H9C	110.00
H8A_b-N8 -H8D_b	110(5)	H9A -N9-H9D	110.00
H8B_b-N8 -H8C_b	109(5)	H9B -N9-H9C	111.00
H8B_b-N8 -H8D_b	109(4)	C2 -C1-C3	133.3(4)
H8C_b-N8 -H8D_b	110(5)	N2 -C1-C3	121.3(4)
H8D -N8 -H8D_b	163(4)	N2 -C1-C2	105.4(4)
H8C -N8 -H8D	110(5)	N1 -C2-C1	125.2(3)
H8A_b-N8 -H8C_b	109(5)	N1 -C2-N3	121.5(4)
H8A -N8 -H8B	110(4)	N3 -C2-C1	113.2(4)
H8A -N8 -H8C	109(5)	N4 -C3-N5	116.6(4)
N4 -C3- C1	121.1(4)	H9'A-N9'-H9'C	110.00
N5 -C3- C1	122.3(4)	H9'A-N9'-H9'D	110.00
O3 -C4- N6	110.1(4)	H9'B-N9'-H9'C	110.00

N5	-C4- N6	137.1(4)	H9'B-N9'-H9'D		110.00
O3	-C4- N5	112.8(4)	H9'C-N9'-H9'D		108.00
H9'A-N9-'H9'B		108.00			

Table S7 Selected torsion angles for [ ] **4a·2H$_2$O**

N2	-O1-N3	-C2	-0.2(4)	O1	-N2-C1	-C3	177.4(3)
N3	-O1-N2	-O2	179.7(3)	O2	-N2-C1	-C3	-0.8(7)
N3	-O1-N2	-C1	1.1(4)	O1	-N3-C2	-C1	-0.8(4)
N4	-O3-C4	-N6	-179.1(3)	O1	-N3-C2	-N1	-178.5(3)
C4	-O3-N4	-C3	-0.4(4)	O3	-N4-C3	-C1	-177.3(4)
N4	-O3-C4	-N5	0.6(5)	O3	-N4-C3	-N5	0.1(5)
C2	-N1-N1_a	-C2_a	-180.0(3)	C4	-N5-C3	-C1	177.5(4)
N1_a	-N1-C2	-N3	-32.5(5)	C3	-N5-C4	-O3	-0.5(4)
N1_a	-N1-C2	-C1	150.1(4)	C4	-N5-C3	-N4	0.2(5)
O2	-N2-C1	-C2	-179.7(5)	C3	-N5-C4	-N6	179.0(5)
O1	-N2-C1	-C2	-1.5(4)	C4	-N6-N7	-O4	-178.6(3)
C4	-N6-N7	-O5	0.4(5)	C3-C1-C2-N1			0.4(7)
N7	-N6-C4	-O3	177.3(3)	C3-C1-C2-N3			-177.2(4)
N7	-N6-C4	-N5	-2.2(7)	N2-C1-C3-N4			-0.6(6)
C2	-C1-C3	-N5	0.7(7)	N2-C1-C3-N5			-177.8(4)
N2	-C1-C2	-N1	179.1(3)	C2-C1-C3-N4			177.9(4)
N2	-C1-C2	-N3	1.5(5)				

Table S8 Hydrogen bonds for [Å and] **4a·2H$_2$O**

D—H ··A	d(D-H)/ Å	d(H...A)/ Å	d(D...A)/ Å	<(DHA)/ °
O6-H6B...N6	0.8500^{i}	2.0100	2.858(10)	177.00
N8-H8C...N1	0.97(5) ^{ii}	2.55(5)	3.308(3)	135(4)
N8-H8C...N5	0.97(5) ^{iii}	2.55(6)	3.247(4)	129(4)

Symmetry Code: i: x,-1+y,z ii : 1/2+x,-1/2+y,z, iii: 1/2+x,-3/2+y,z

3. ^{1}H NMR and ^{13}C NMR of compounds 2-4,3a-d and 4a-c

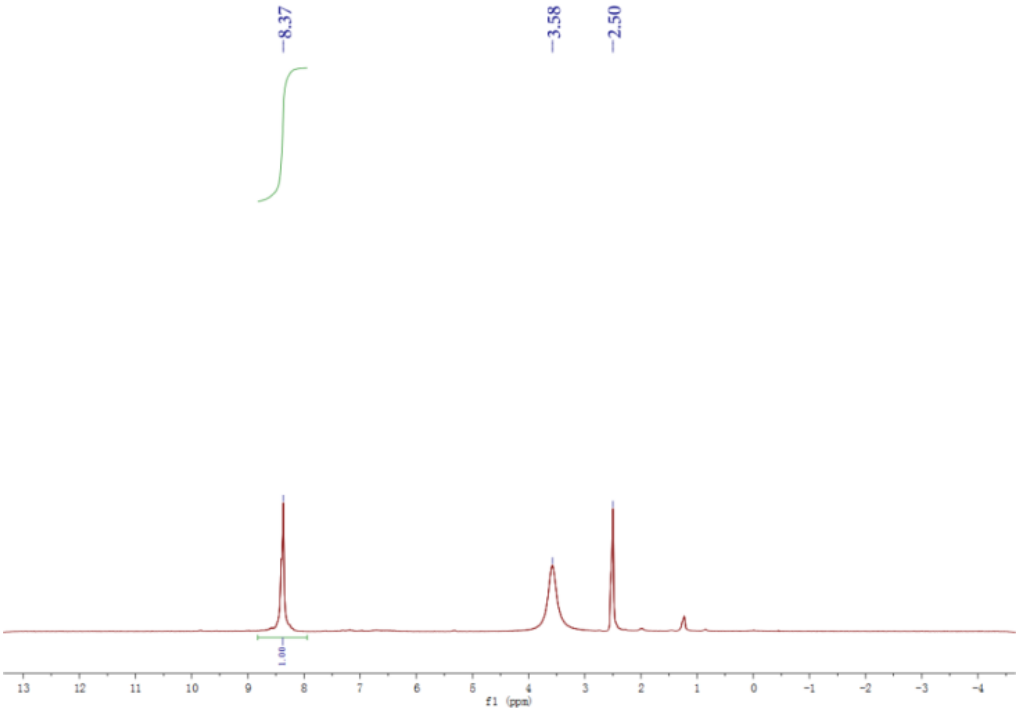


Figure S1. ^{1}H NMR spectra in DMSO-d_6 for compound **2.**

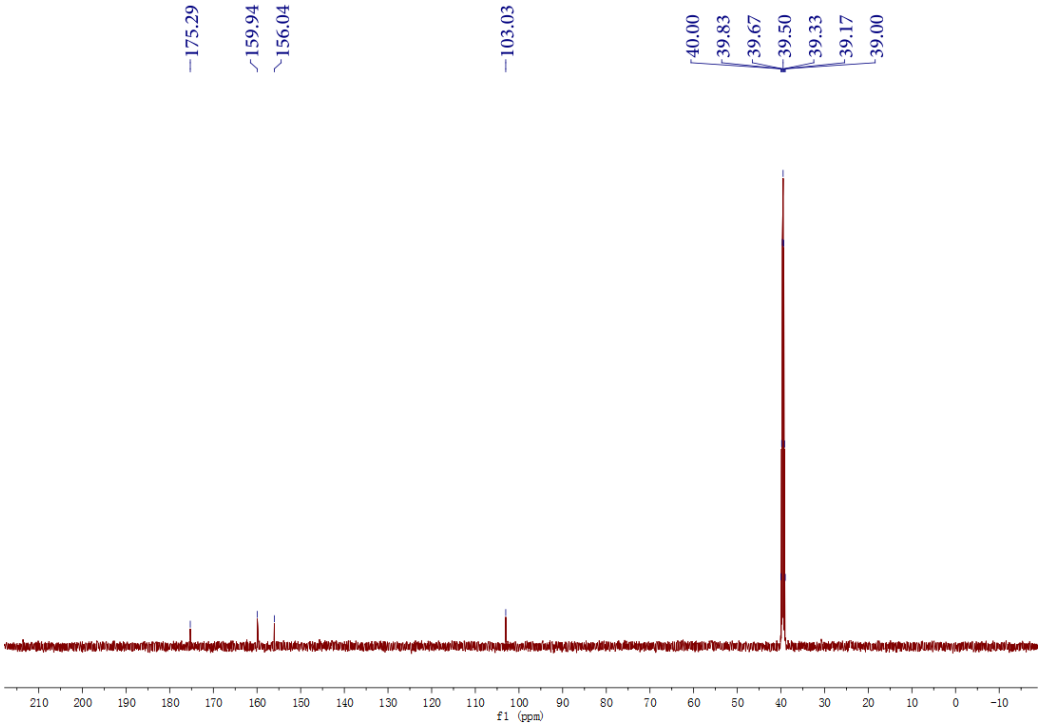


Figure S2. ^{13}C NMR spectra in DMSO-d_6 for compound **2.**

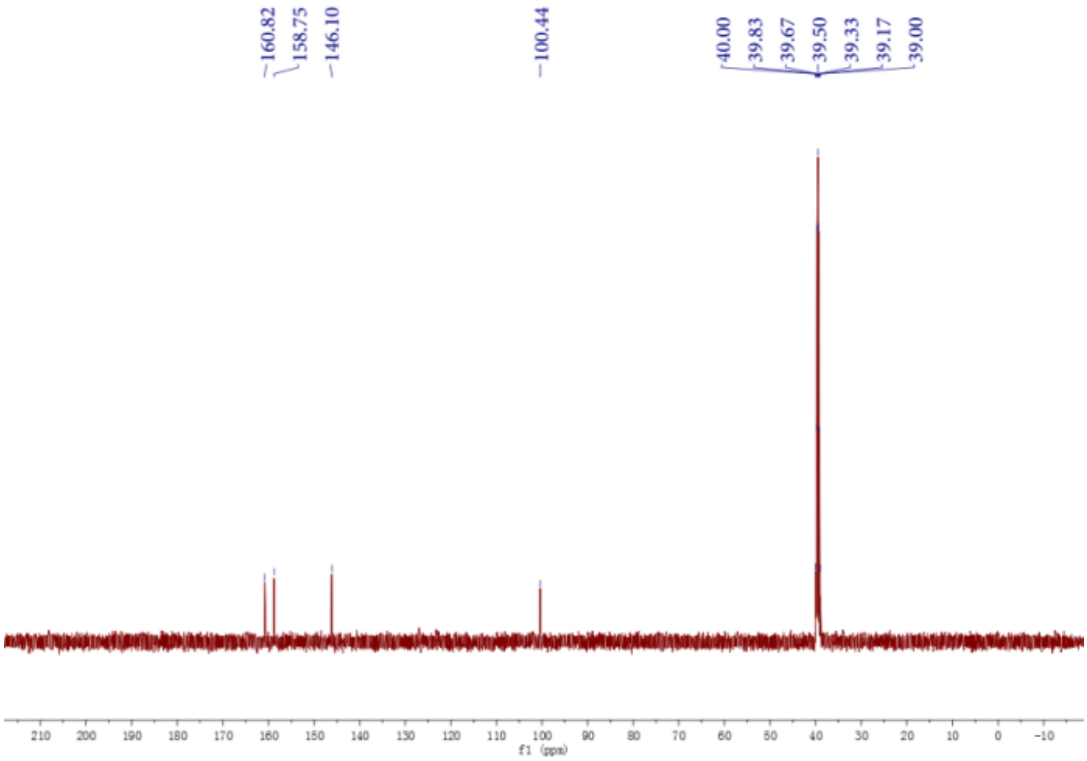


Figure S3. ^{13}C NMR spectra in DMSO-d_6 for compound **3**

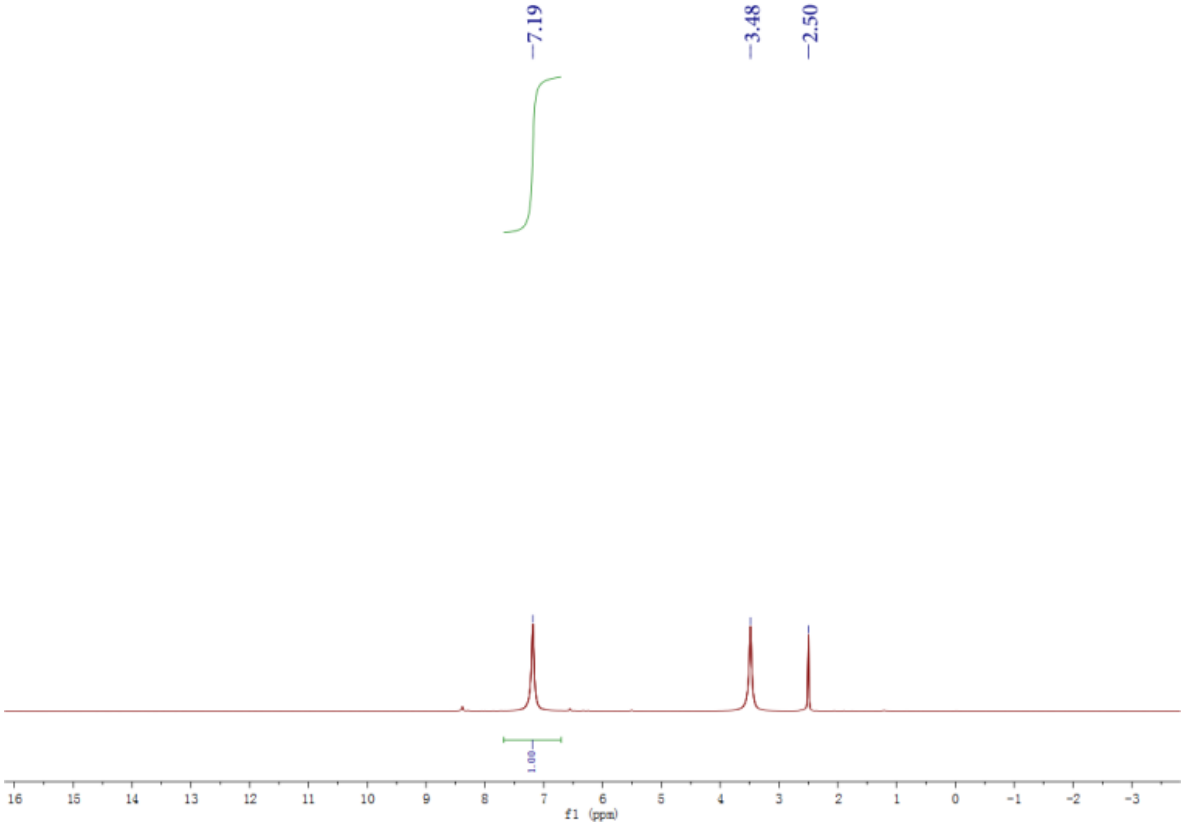


Figure S4. ^{1}H NMR spectra in DMSO-d_6 for compound **3a**

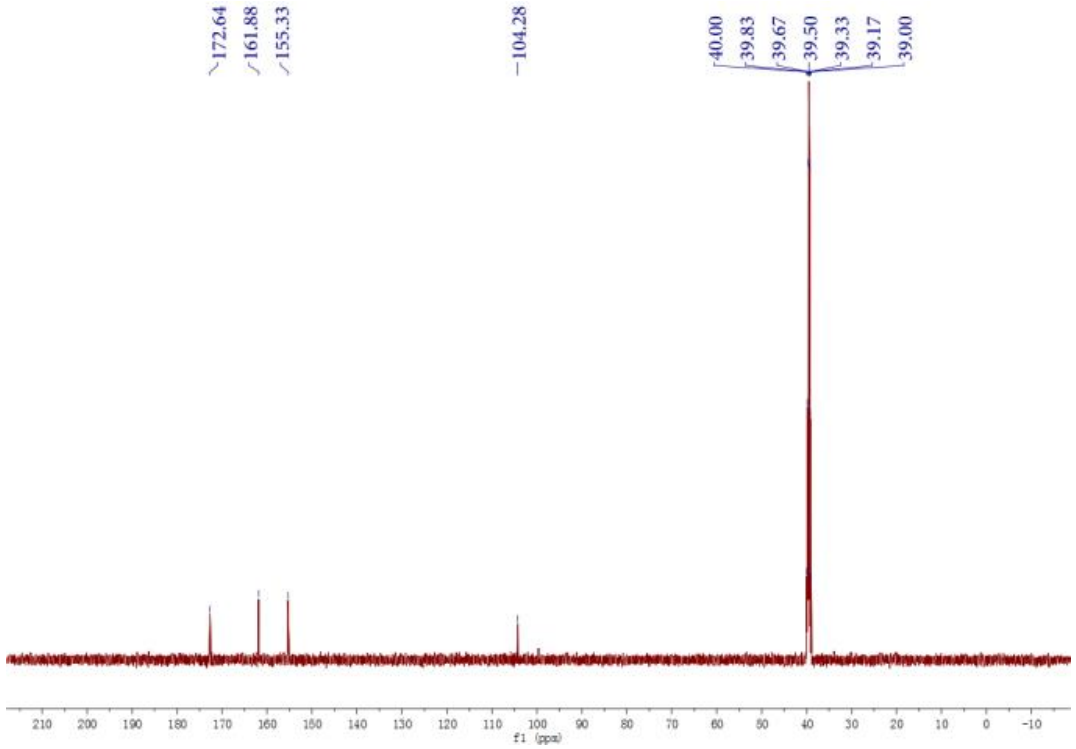


Figure S5. ^{13}C NMR spectra in DMSO-d_6 for compound **3a**

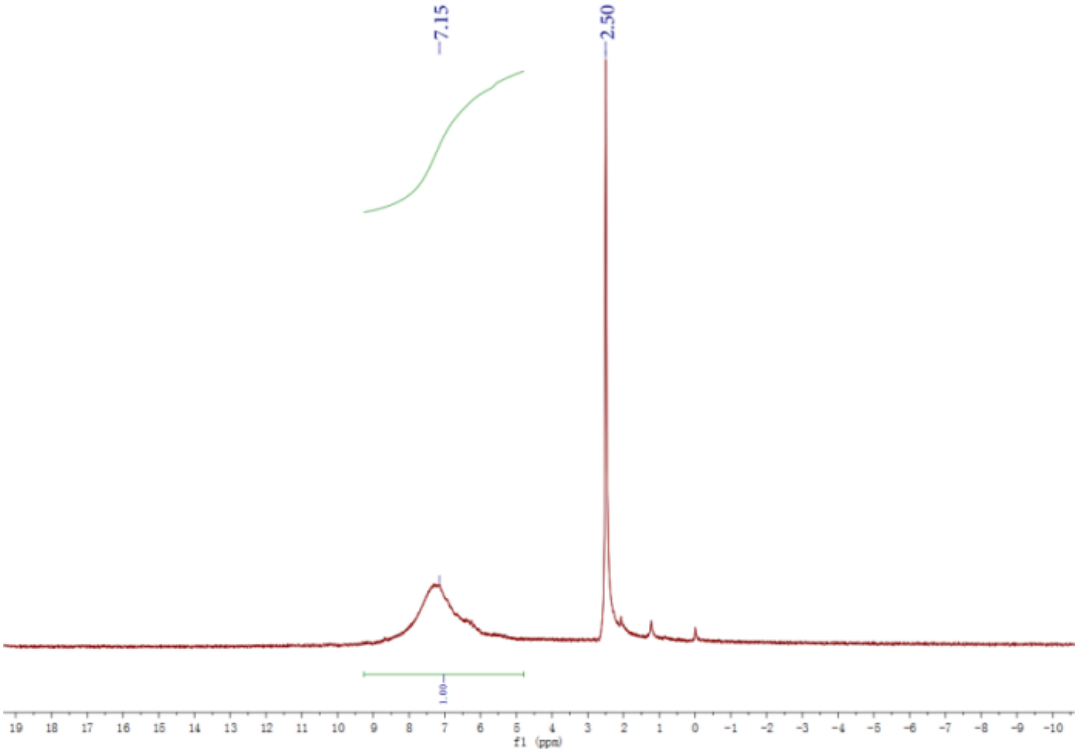


Figure S6. ^{1}H NMR spectra in DMSO-d_6 for compound **3b**

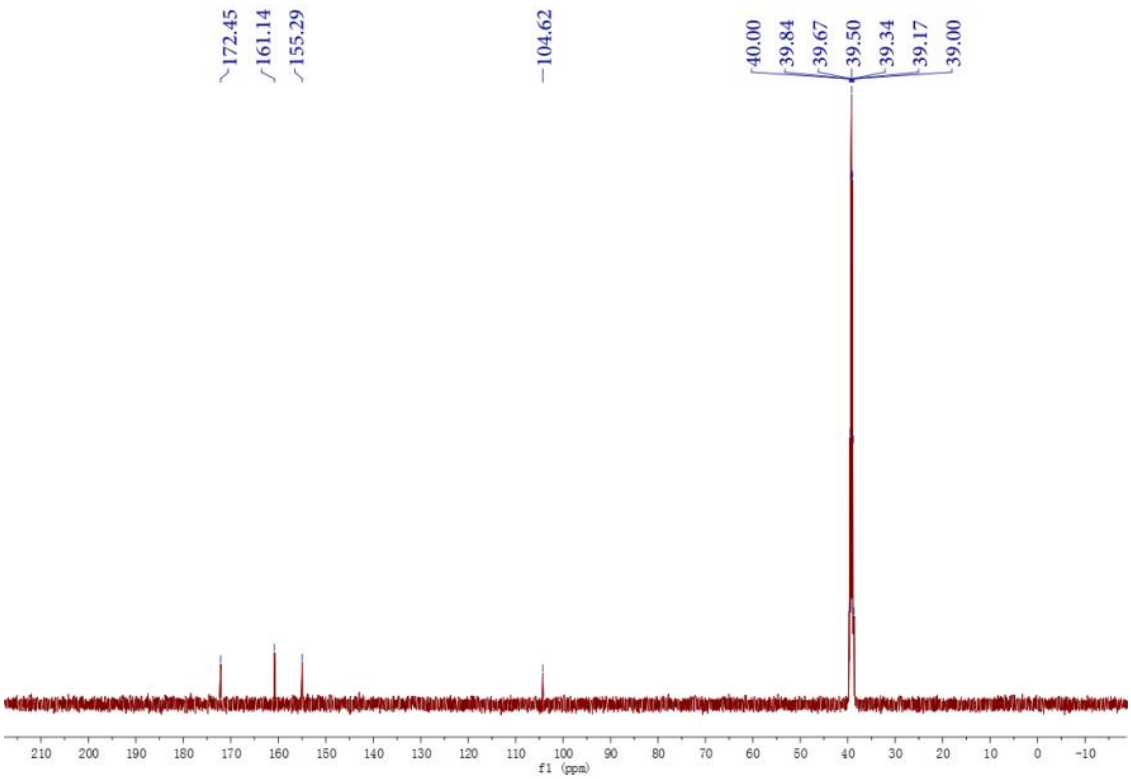


Figure S7. ^{13}C NMR spectra in DMSO-d_6 for compound **3b**

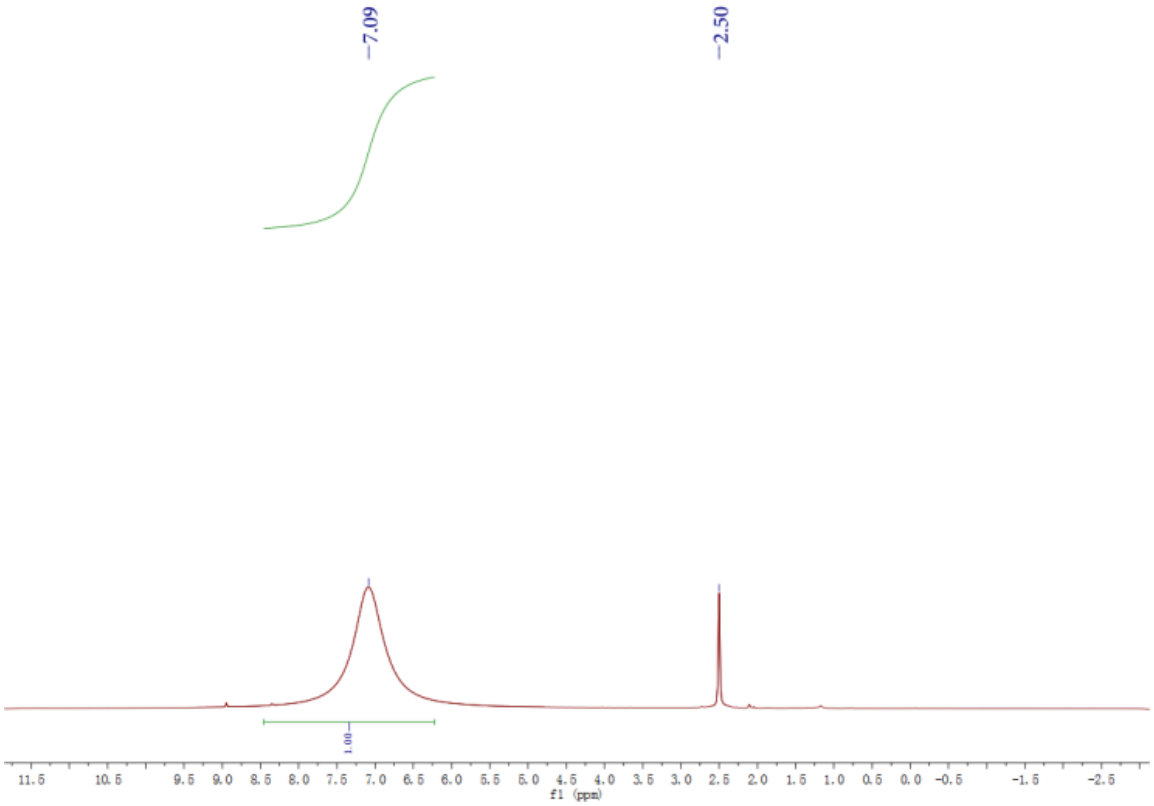


Figure S8. ^{1}H NMR spectra in DMSO-d_6 for compound **3c**

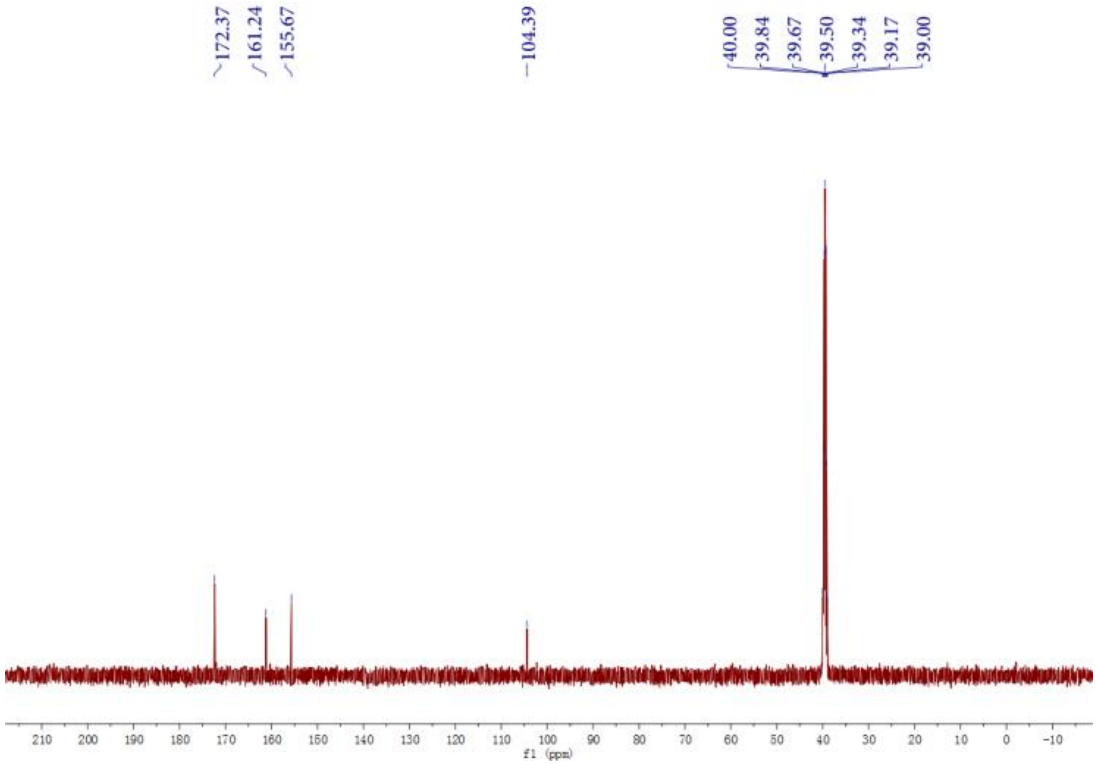


Figure S9. ^{13}C NMR spectra in DMSO-d_6 for compound **3c**

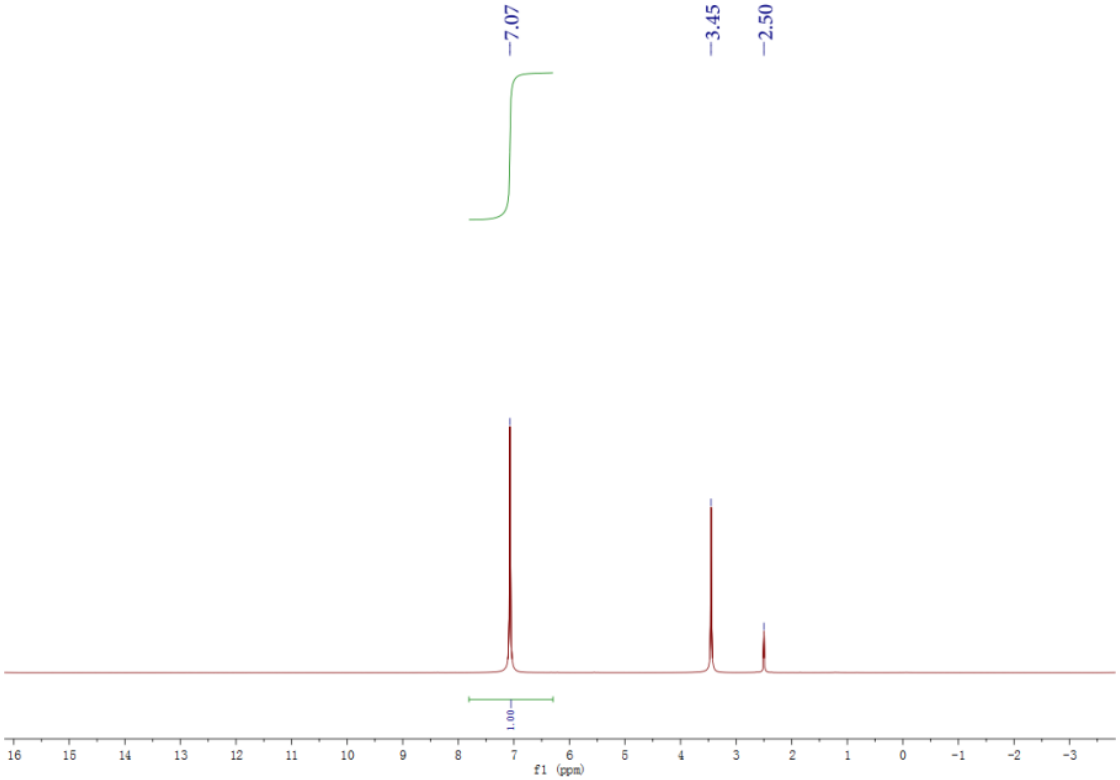


Figure S10. ^{1}H NMR spectra in DMSO-d_6 for compound **3d**

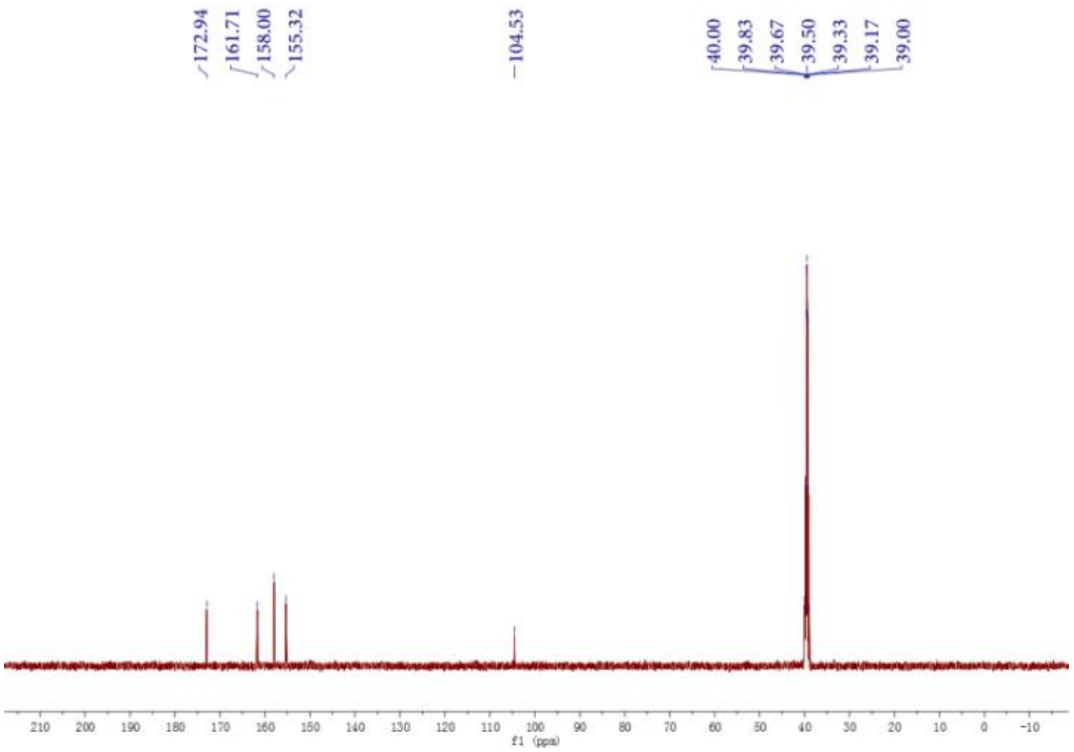


Figure S11. ^{13}C NMR spectra in DMSO-d_6 for compound **3d**

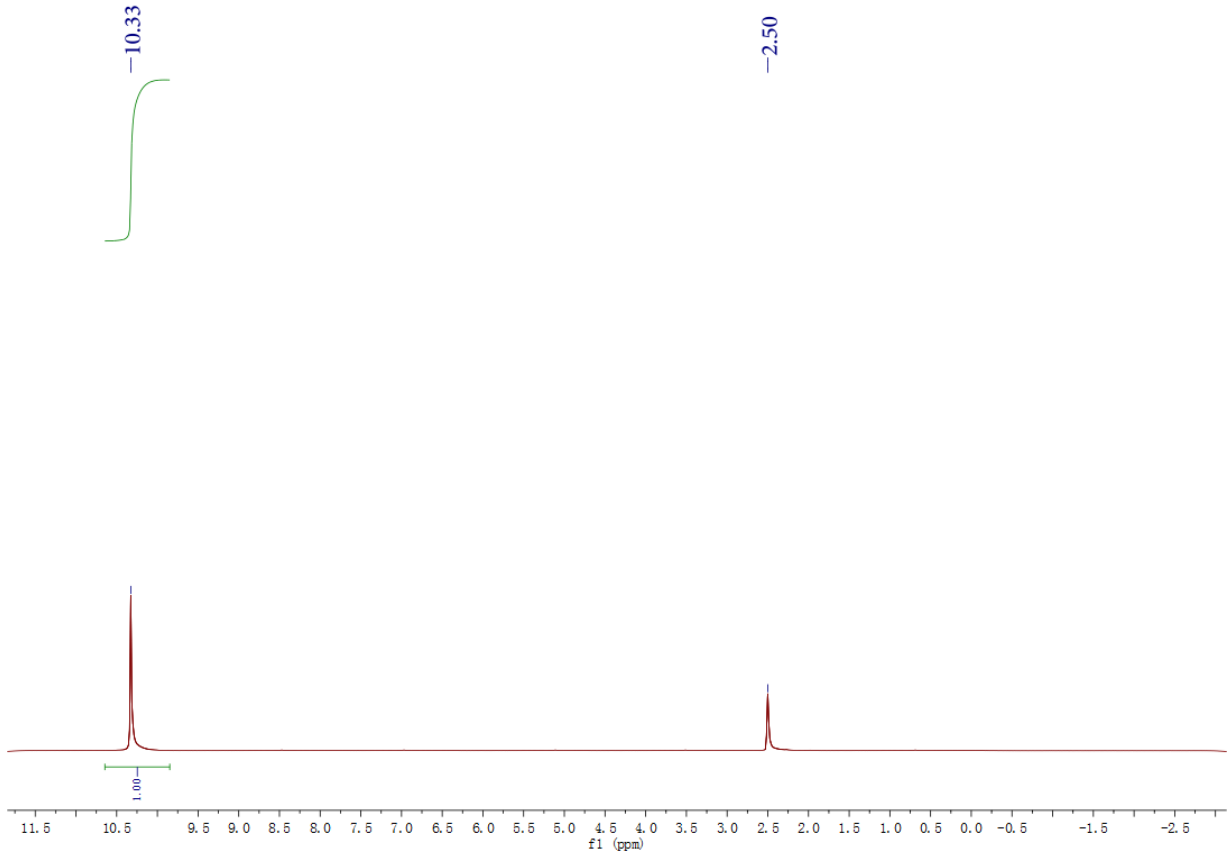


Figure S12. ^{1}H NMR spectra in DMSO-d_6 for compound **4**

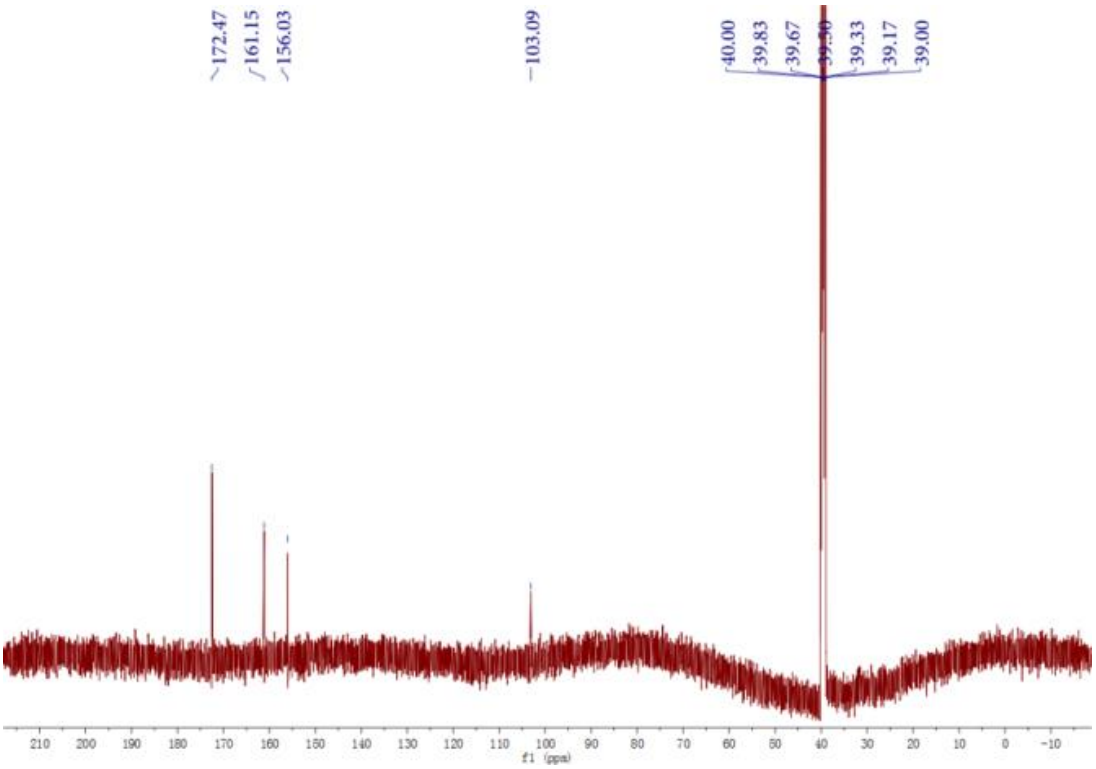


Figure S13. ^{13}C NMR spectra in DMSO-d_6 for compound **4**

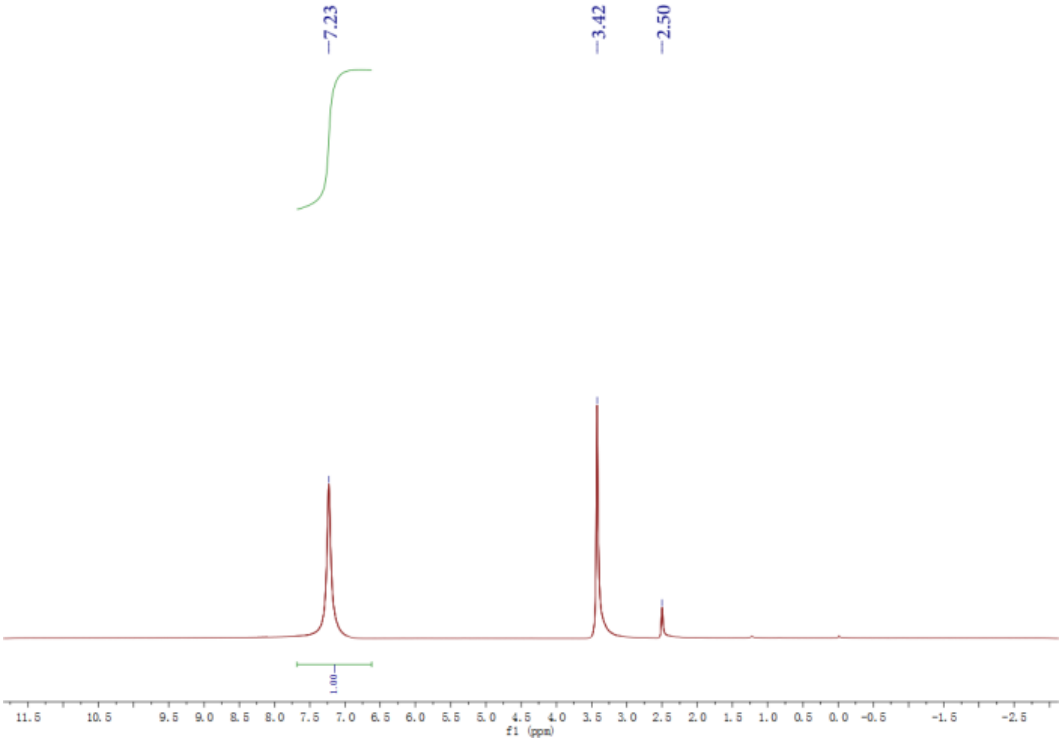


Figure S14. ^{1}H NMR spectra in DMSO-d_6 for compound **4a**

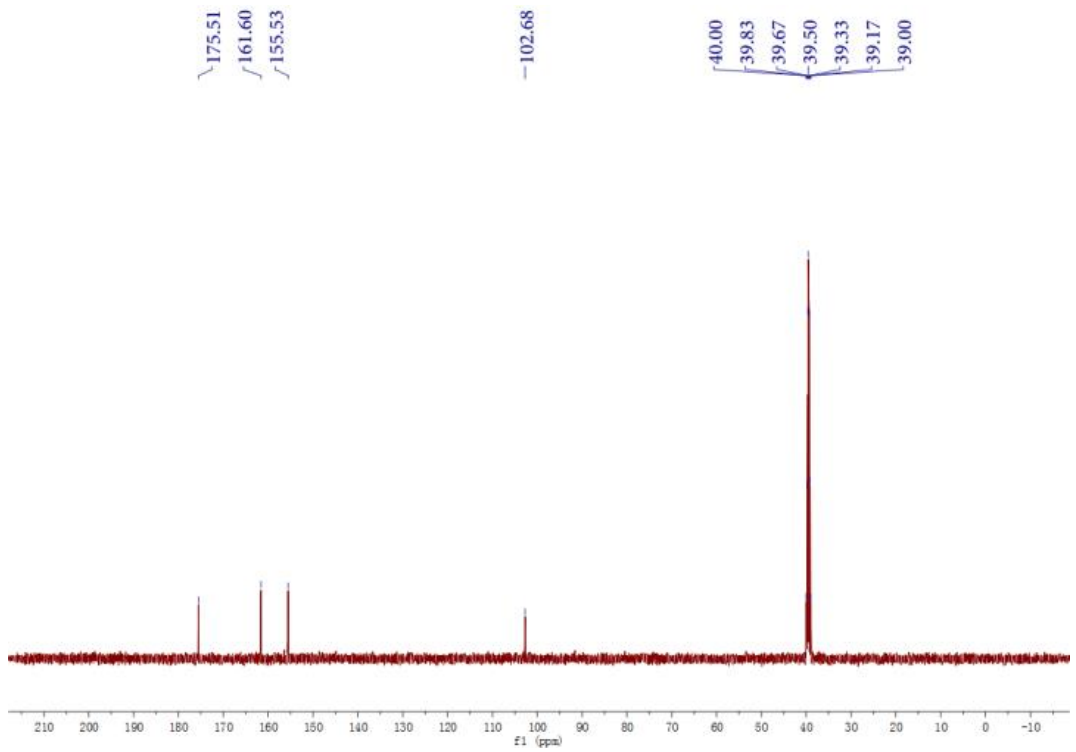


Figure S15. ^{13}C NMR spectra in DMSO-d_6 for compound **4a**

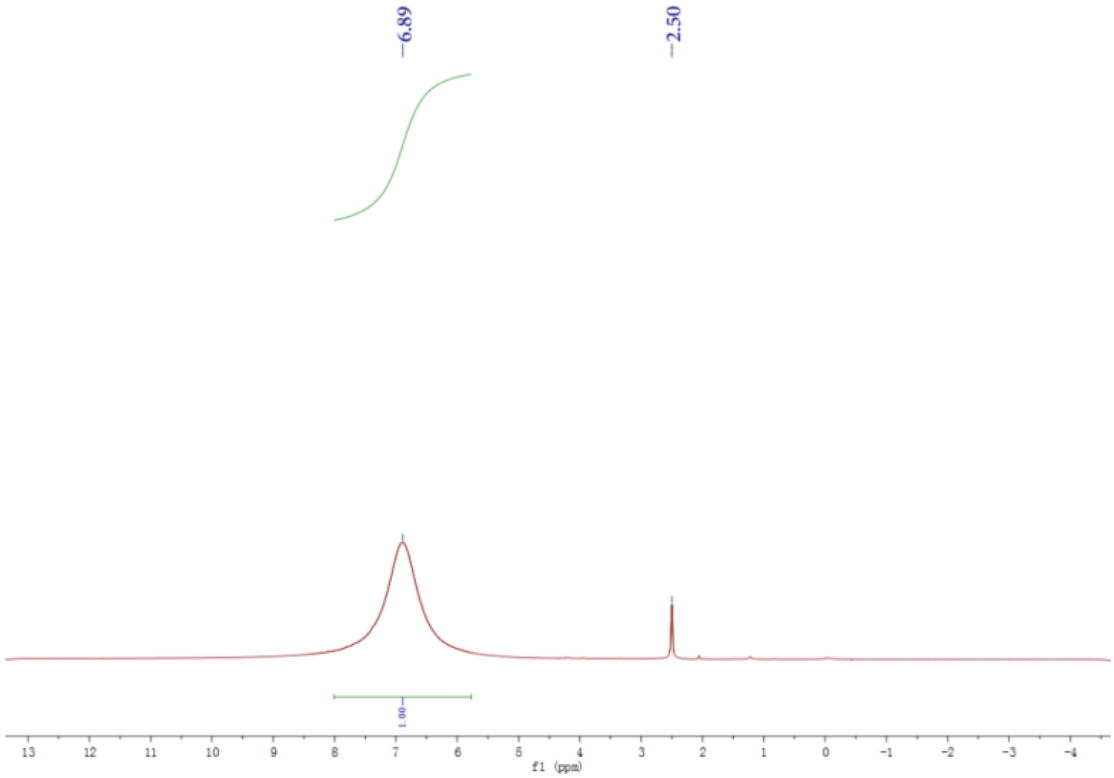


Figure S16. ^{1}H NMR spectra in DMSO-d_6 for compound **4b**

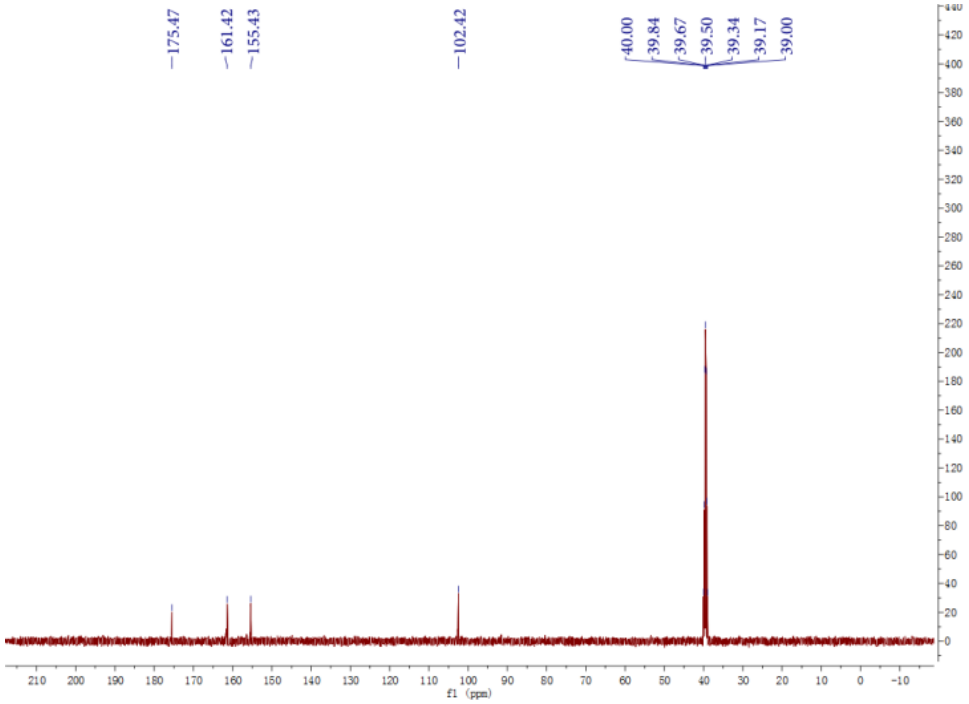


Figure S17. ^{13}C NMR spectra in DMSO-d_6 for compound **4b**

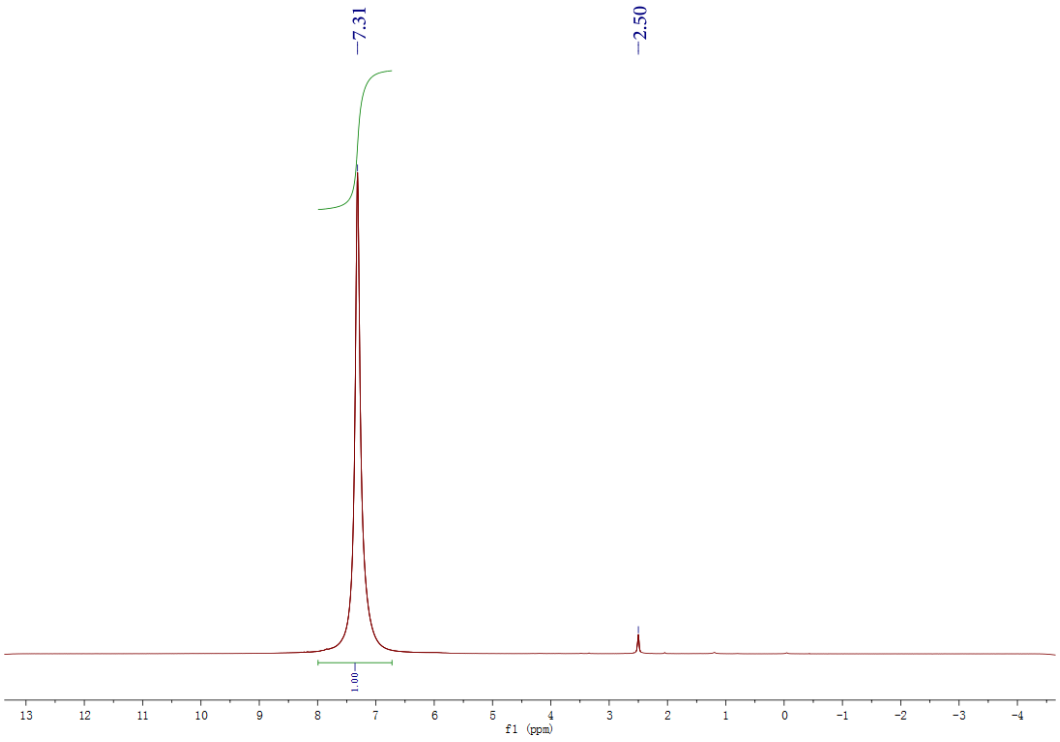


Figure S18. ^{1}H NMR spectra in DMSO-d_6 for compound **4c**

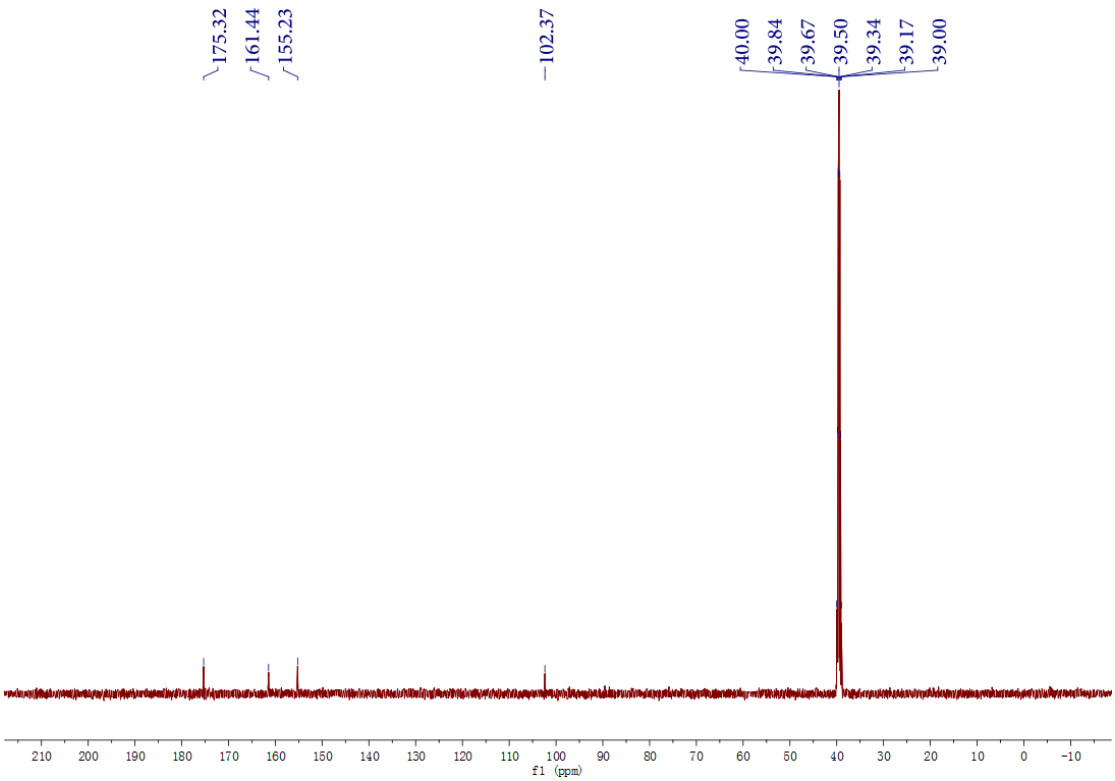


Figure S19. ^{13}C NMR spectra in DMSO-d_6 for compound **4c**

4. The DSC plots of compounds 3, 4, 3a-d, 4a-c, RDX, HMX and CL-20.

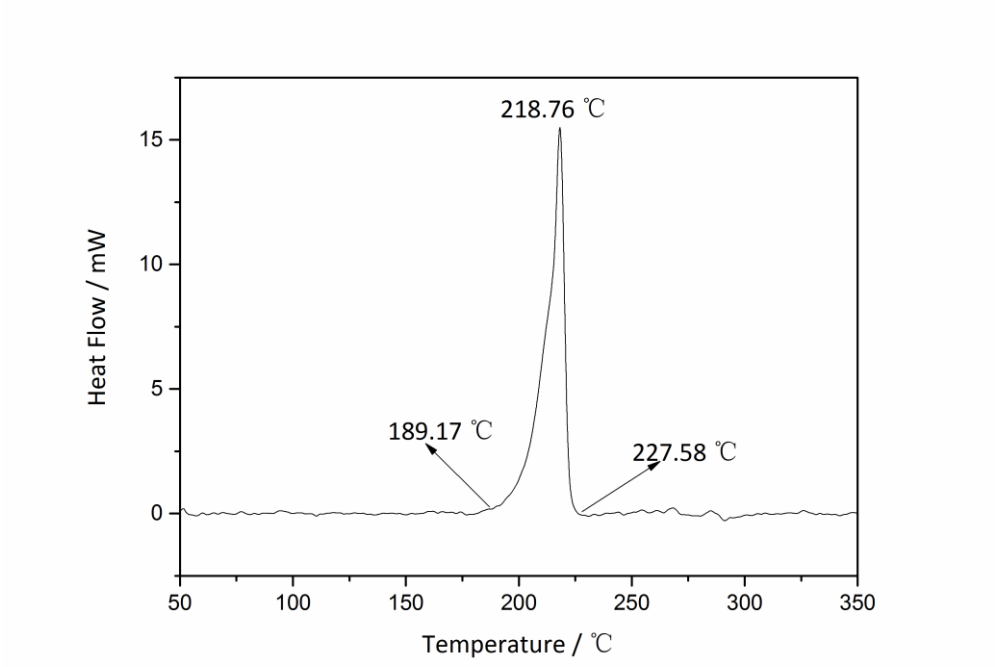


Figure S20. The DSC plot of compound **3**

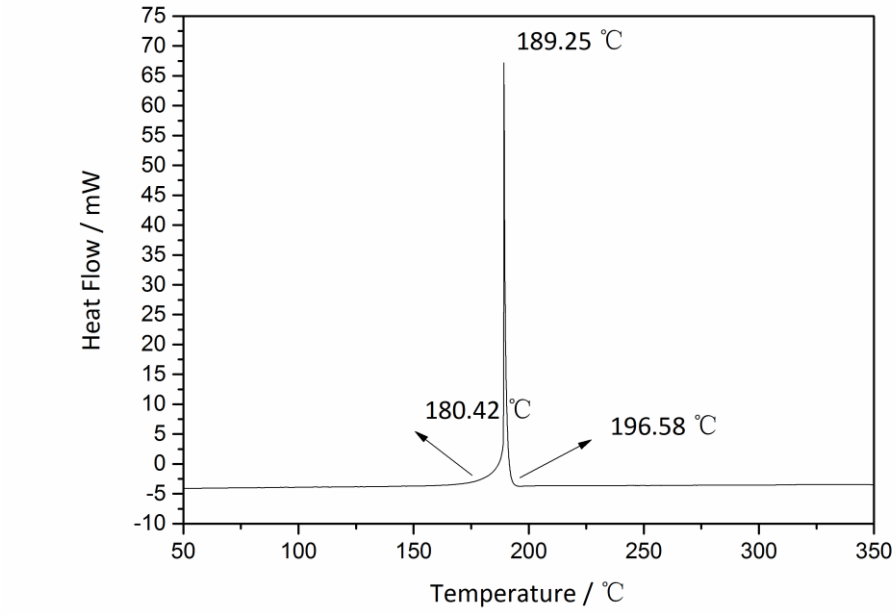


Figure S21. The DSC plot of compound **3a**

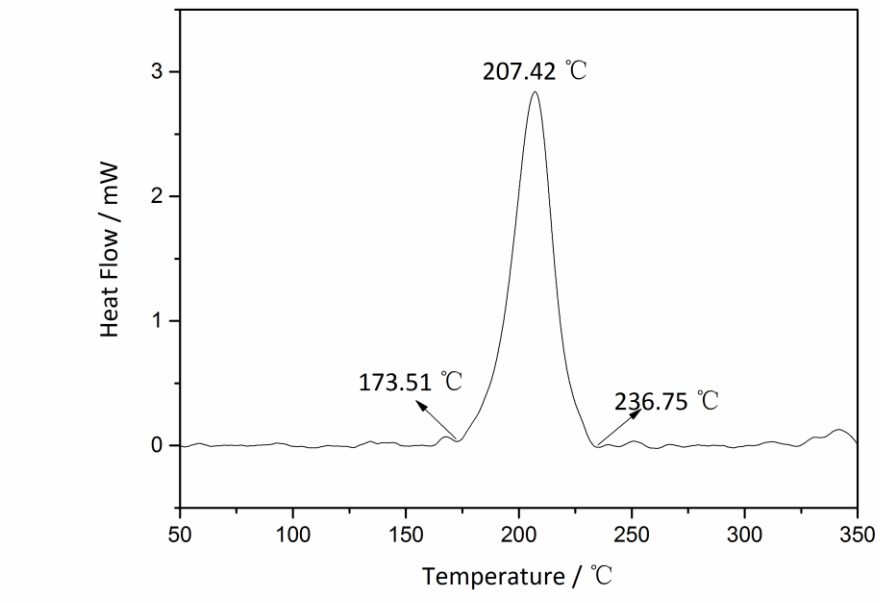


Figure S22. The DSC plot of compound **3b**

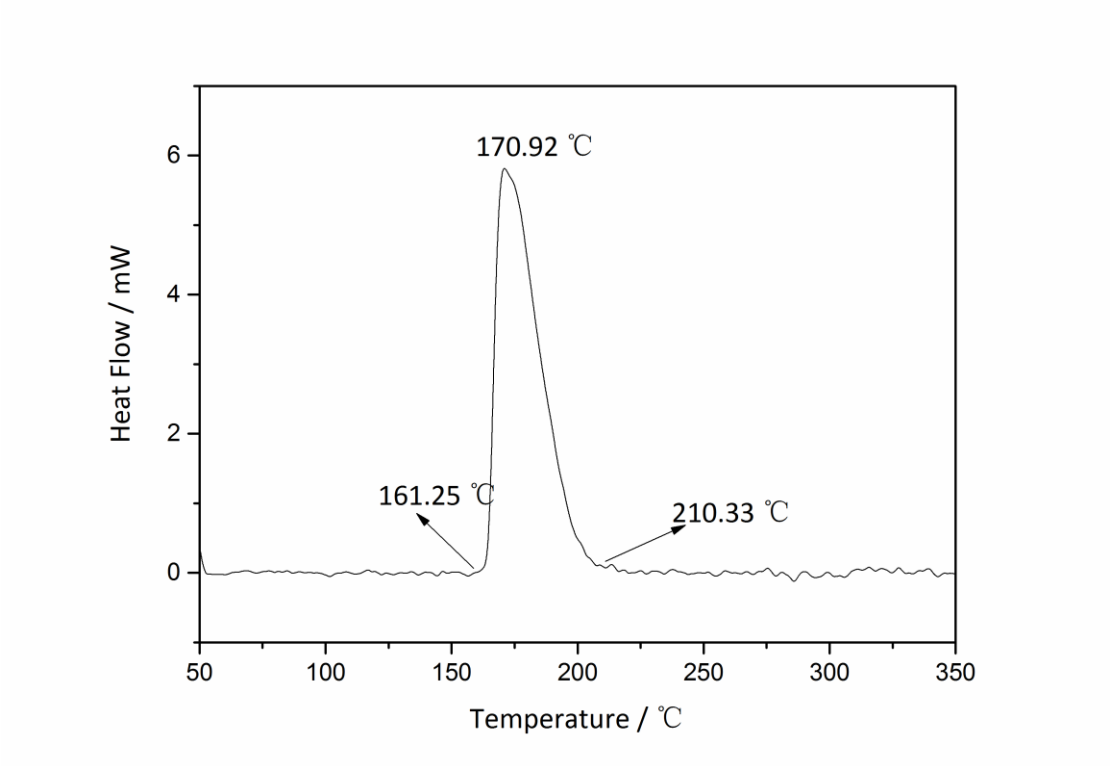


Figure S23. The DSC plot of compound **3c**

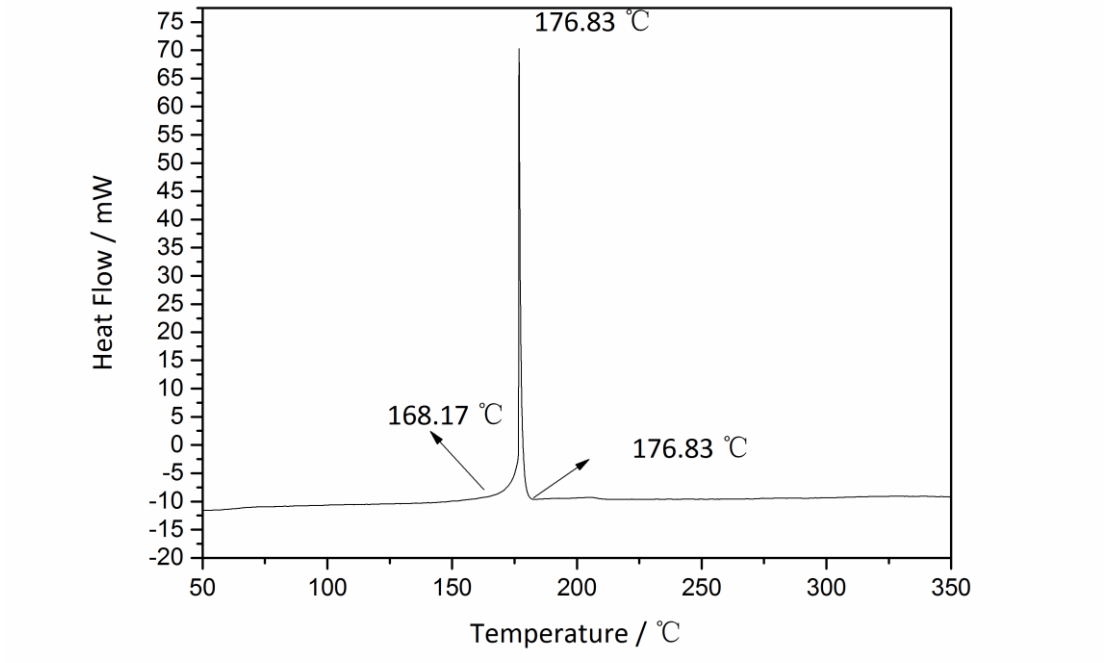


Figure S24. The DSC plot of compound **3d**

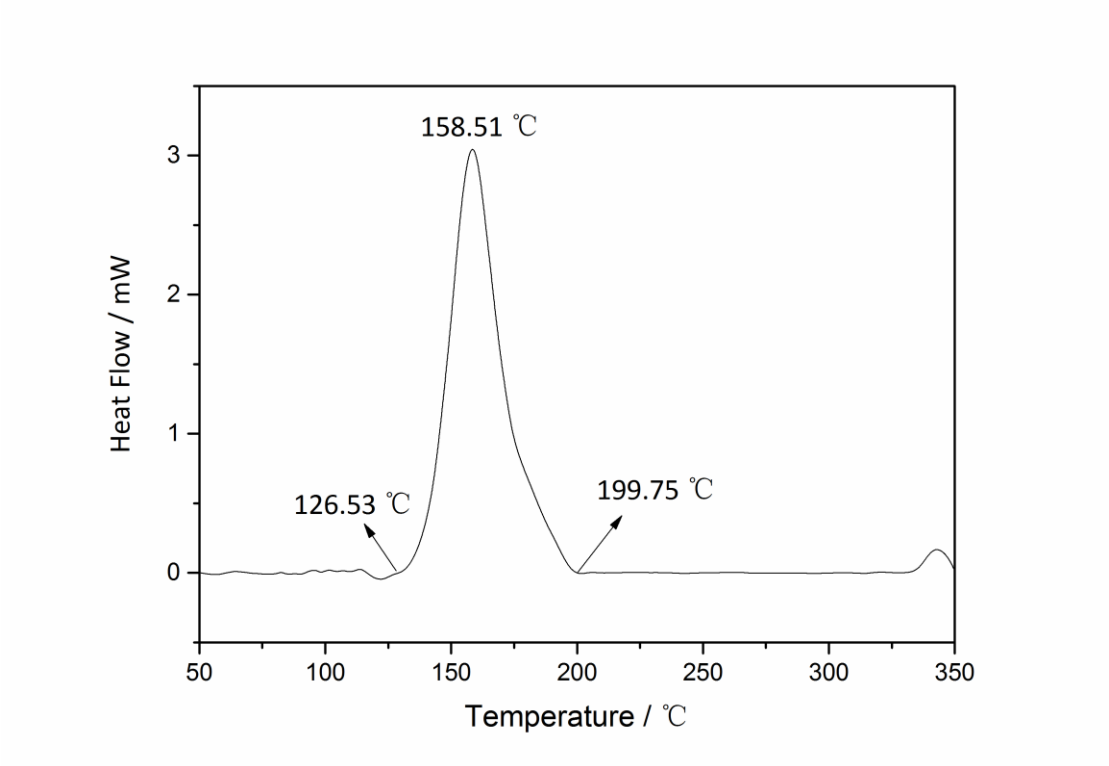


Figure S25. The DSC plot of compound **4**

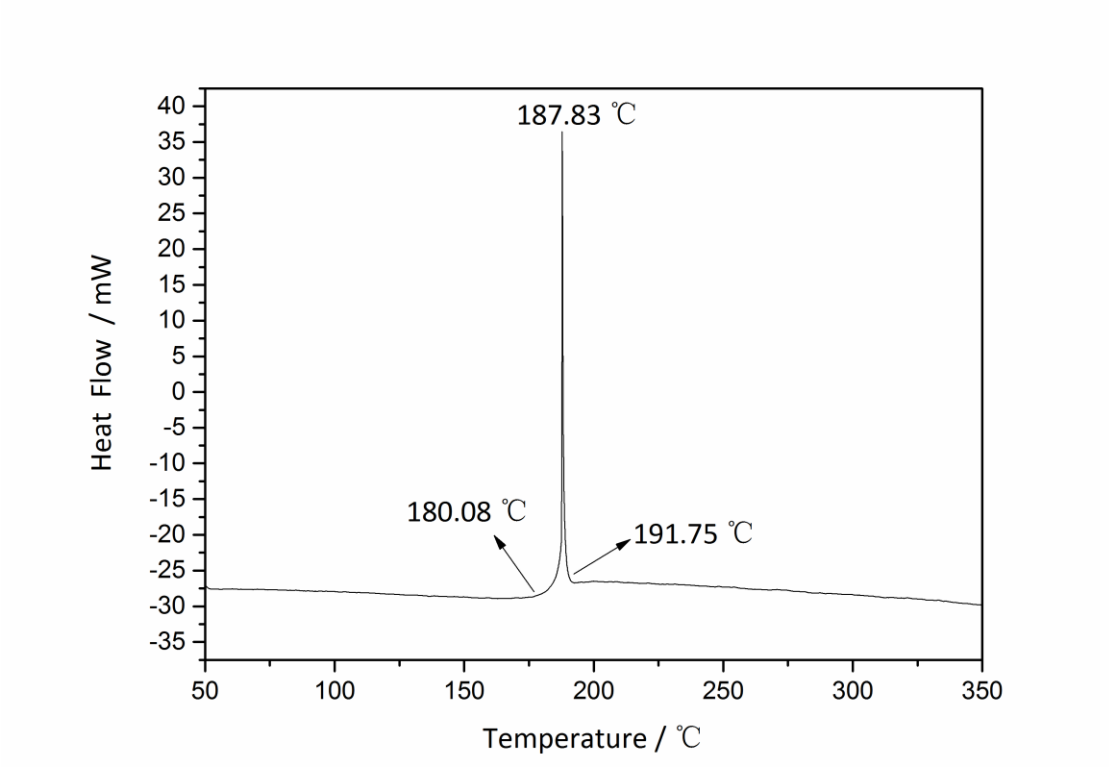


Figure S26. The DSC plot of compound **4a**

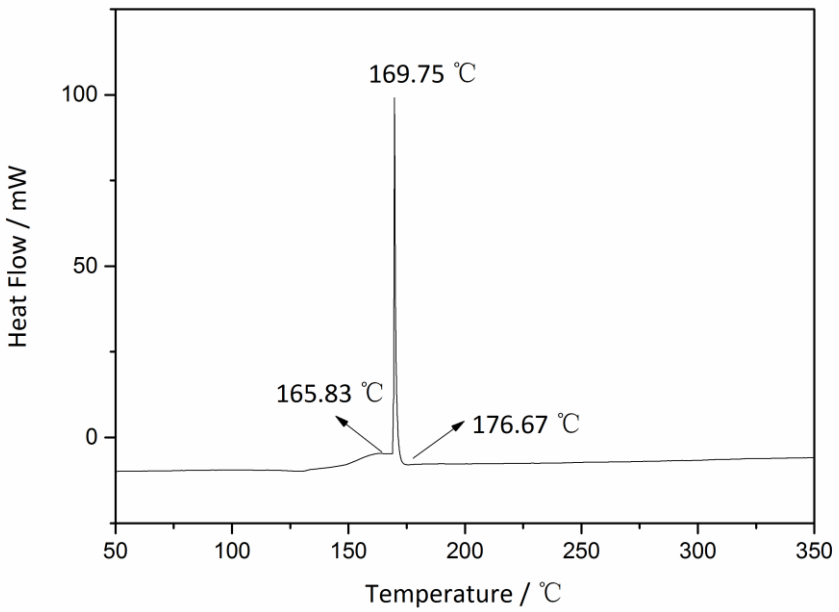


Figure S27. The DSC plot of compound **4b**

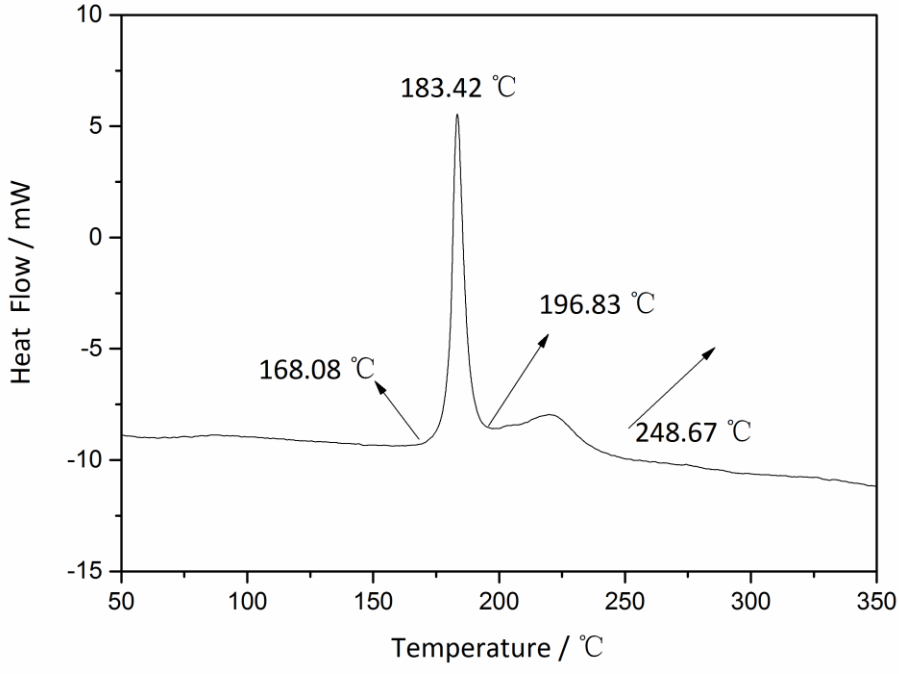


Figure S28. The DSC plot of compound **4c**

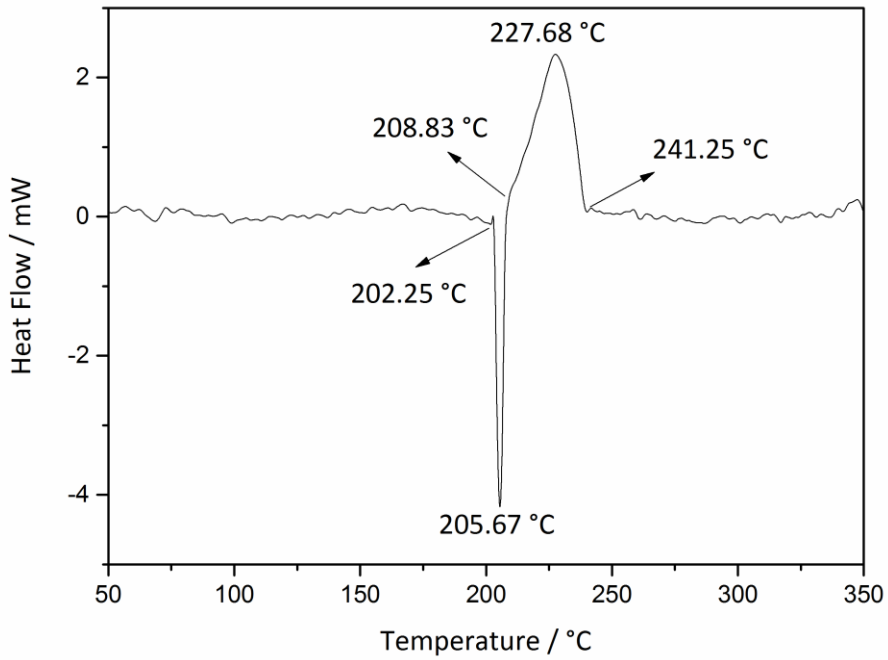


Figure S29. The DSC plot of compound RDX

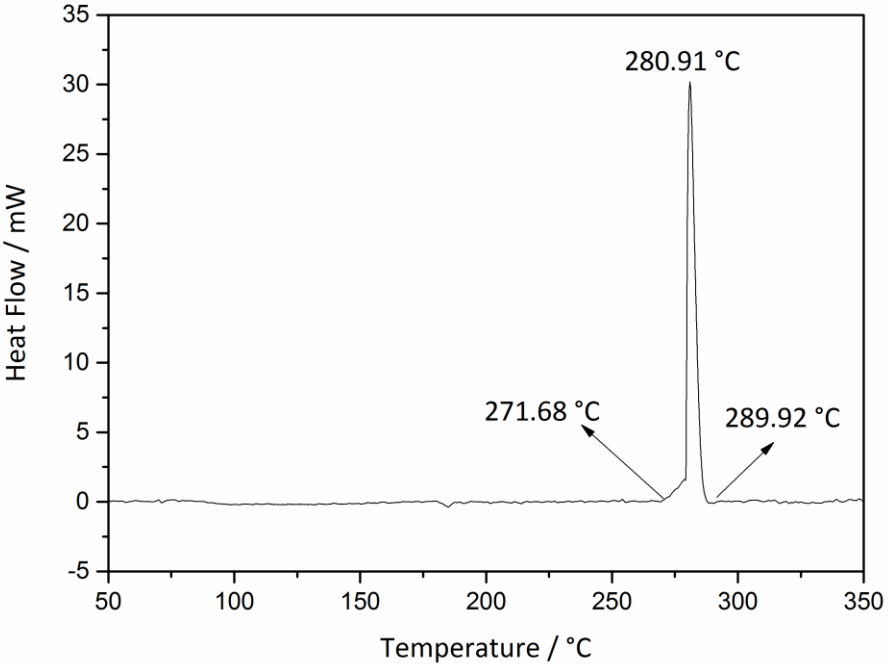


Figure S30. The DSC plot of compound HMX

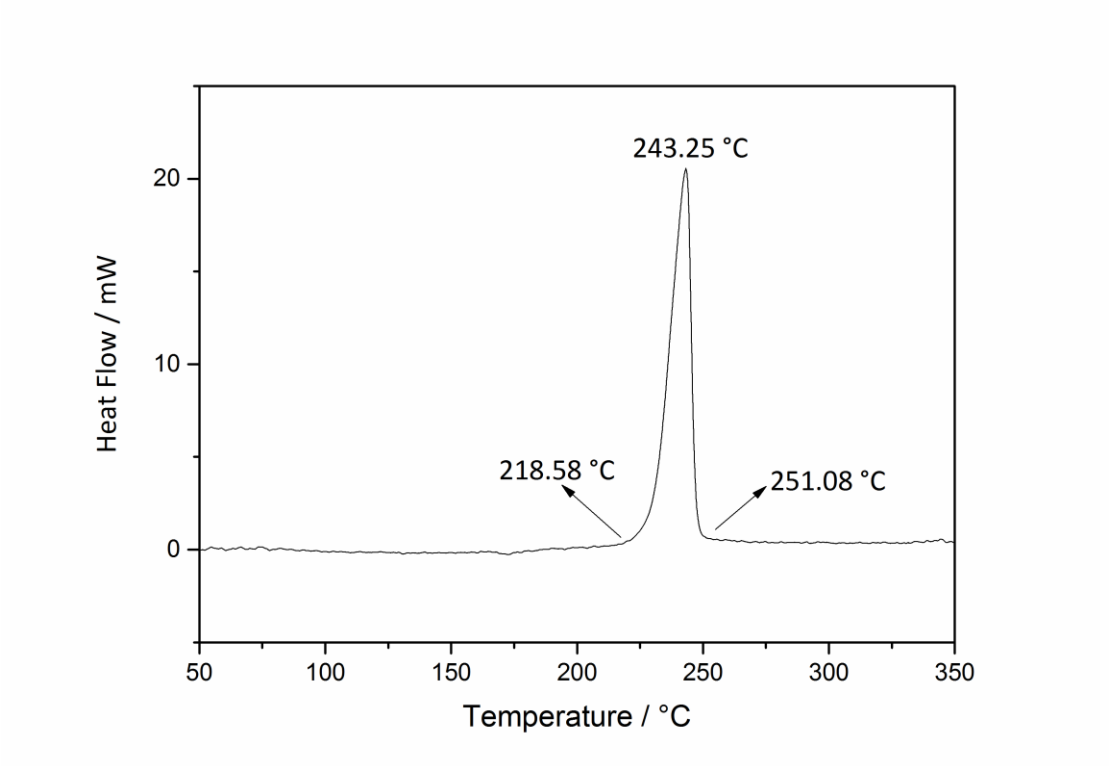


Figure S31. The DSC plot of compound CL-20

5. Reference

[1] M. J. Frisch, et al. Gaussian 09, Revision D. 01 (Gaussian Inc., 2009).

[2] A. D. Becke, *J. Chem. Phys*. 1993, **98**, 5648-5652

[3] P. J. Stephens; F. J. Devlin; C. F. Chabalowski; M. J. Frisch. *J. Phys. Chem*. 1994, **98**, 11623-11627.

[4] P. C. Hariharan; J. A. Pople, *Theor. Chim. Acta*. 1973, **28**, 213-222.