Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information(SI)

Synthesis of high-performance insensitive energetic materials based on the nitropyrazole and 1,2,4-triazole

Minxian Xu,[a] Guangbin Cheng,[a] Hualin Xiong,[a] Bohan Wang[a] Xuhai Ju,[a] and Hongwei Yang,*[a]

[a]*School of Chemical Engineering,Nanjing University of Science and Technology,Nanjing, 210094, China. Email: hyang@mail.njust.edu.cn*

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1. Computation data

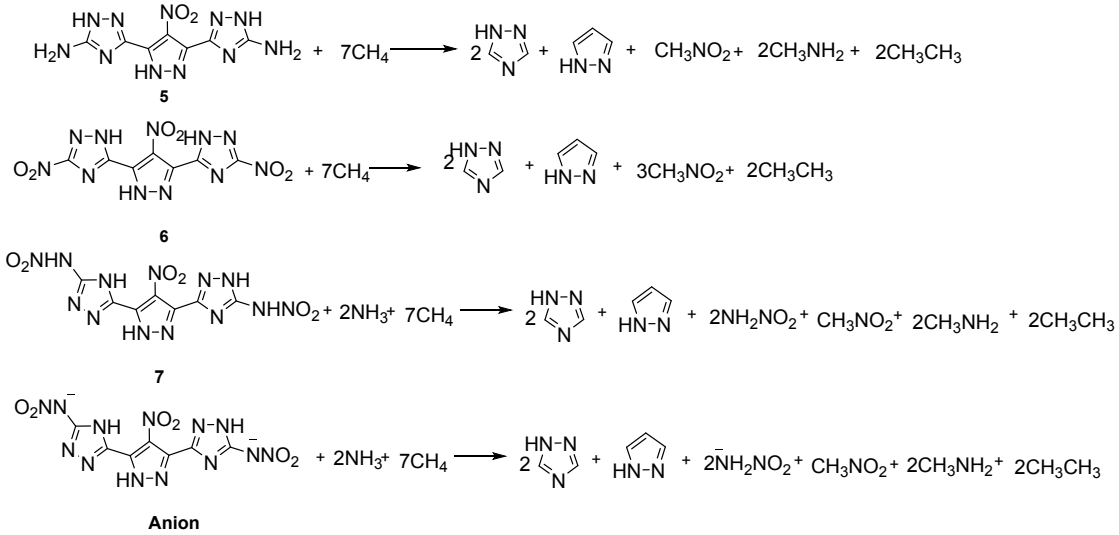
Calculations were performed by using the Gaussian 09 suite of programs. The geometric optimization of all the structures and frequency analyses for calculation of heats of formation was carried out by using B3-LYP functional[1] with 6-311+G** basis set,[2] All of the optimized structures were characterized to be local energy minima on the potential surface without any imaginary frequencies. The heats of formation (HOF) of the title compounds were computed through appropriate isodesmic reactions (Scheme S1 and S2). The isodesmic reaction processes, i.e., the number of each kind of formal bond is conserved, are used with application of the bond separation reaction (BSR) rules. The molecule is broken down into a set of two heavy-atom molecules containing the same component bonds. The isodesmic reactions used to derive the HOF of the title compounds are in Scheme S1. The change of enthalpy for the reactions at 298 K can be expressed as

$$\Delta H_{298K} = \sum \Delta_f H_P - \sum \Delta_f H_P \qquad (1)$$

where $\Delta_f H_R$ and $\Delta_f H_P$ are the HOF of reactants and products at 298 K, respectively, and ΔH_{298K} can be calculated using the following expression:

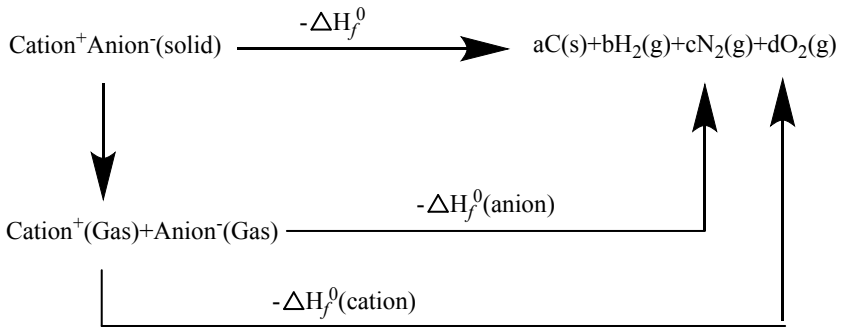
$$\Delta H_{298} = \Delta E_{298} + \Delta(PV) = \Delta E_0 + \Delta ZPE + \Delta H_T + \Delta nRT \qquad (2)$$

where E_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; ΔHT is thermal correction from 0 to 298 K. The $\Delta(PV)$ value in eq (2) is the *PV* work term. It equals ΔnRT for the reactions of ideal gas. For the isodesmic reactions, $\Delta n = 0$, so $\Delta(PV) = 0$. On the left side of Eq. (1), apart from target compound, all the others are called reference compounds. The HOF of reference compounds are available either from the experiments [3-5]or from the high level computing like CBS-4M.



Scheme S1. Isodesmic and tautomeric reactions for 1-4 to calculate the HOF.

For energetic salts, the solid-phase heat of formation is calculated on the basis of a Born-Haber energy cycle [6](Scheme S3). The number is simplified by equation 3:



Scheme S2. Born−Haber Cycle for the Formation of energetic salts

$$\Delta H_f^{\,0}(salt, 298K) = \Delta H_f^{\,0}(cation, 298K) + \Delta H_f^{\,0}(anion, 298K) - \Delta H_L \qquad (3)$$

in which ΔH_L can be predicted by using the formula suggested by Jenkins, et al.(equation 4)

$$\Delta H_L = U_{POT} + [p(n_M/2-2) + q(n_X/2-2)]RT \qquad (4)$$

In this equation, n_M and n_X depend on the nature of the ions Mp+ and Xq-, respectively. The equation for lattice potential energy U_{pot}(equation 5) has the form:[6]

$$U_{POT}[kJ.mol^{-1}] = \gamma(\rho_m / M_m)^{1/3} + \delta \qquad (5)$$

where ρ_m [g cm^{-3}] is the density of the salt, M_m is the chemical formula mass of the ionic material, and values for g and the coefficients γ (kJ mol^{-1} cm) and δ (kJ mol^{-1}) are assigned literature values.[7]

Table S1 Ab initio computational values of small molecules used in isodesmic and tautomeric reactions

Compound	E_0[a]	ZPE[b]	H_T[c]	HOF[d]
5	-1023.797084	472.12	47.78	555.0
6	-0.03116268	45.38	-25.36	737.6
7	-1432.862745	486.27	59.11	791.8
Anion	-1431.702776	413.66	59.39	699.37[e]
NH_2NO_2	-261.1248168	98.79	12.39	-3.9
CH_3NO_2	-245.0915559	124.93	11.6	-80.8
CH_3NH_2	-95.8938402	160.78	11.64	-22.5
$^-NHNO_2$	-259.936099	65.95	11.23	-84.0
	-242.3203873	150.39	12.06	192.7
	-226.2603313	179.2	12.57	177.4

[a]Total energy calculated by B3LYP/6-311+G**method (a.u);[b]zero-point correction (kJ mol^{-1}); [c] thermal correction to enthalpy (kJ mol^{-1}); [d] heat of formation (kJ mol^{-1}). [e]HOF(s) = HOF(g) (543.2)+ ΔH_L(156.17)

2. References

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3. Crystallographic data for compounds 6·2H_2O and 7·H_2O

Table S2.Crystallographic data for the compounds **6**·2H_2O and **7**·H_2O

Empirical formula	$C_7H_7N_{11}O_8$	$C_7H_7N_{13}O_7$
Formula weight	373.24	385.26
Temperature [K]	173	173
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	*P*-1(2)
a[Å]	5.0463(5)	8.6518(13)
b[Å]	14.9379(12)	8.7863(13)
c[Å]	18.6918(18)	9.9600(14)

α[°]	90	83.380(5)
β[°]	93.903(9)	66.139(5)
γ[°]	90	76.502(5)
Volum[A^3]	1405.7	673.11
Z	4	2
ρ_{cal}($g.cm^{-3}$)	1.764	1.901
μ(mm^{-1})	0.159	0.169
F(000)	424.0	392.0
Crystal size [mm^3]	0.210×0.110×0.090	0.090×0.070×0.050
Radiation	MoKα(λ=0.71073)	MoKα(λ=0.71073)
2Θ range for data collection/°	4.368 to 53.992	6.334 to 50.042
Index ranges	-10≤h≤10, -10≤k≤11, -12≤l≤12	-10≤h≤10, -10≤k≤10, -11≤l≤11
Reflections collected	11323	5838
Goodness-of-fit on F^2	1.053	1.048
Final R indexes [I>=2σ (I)]	R_1°=0.0486,wR_2°= 0.1127	R_1°=0.0721,wR_2°= 0.1423
Final R indexes [all data]	R_1°=0.0806,wR_2°= 0.1280	R_1°=0.1343,wR_2°= 0.1730
CCDC	1877695	1854906

4. X-ray Diffraction

Table S3. Selected bond lengths [Å] for compound **6**·2H_2O

Parameter	Bond length(Å)	Parameter	Bond length(Å)
O1-N6	1.215(3)	N5-C5	1.332(3)
O2-N6	1.212(3)	N6-C4	1.451(3)
O3-N7	1.227(3)	N7-C2	1.419(3)
O4-N7	1.221(3)	N8-C7	1.341(3)
O5-N11	1.215(3)	N8-N9	1.346(3)
O6-N11	1.213(3)	N9-C6	1.308(3)
O7-H7A	0.85(3)	N10-C7	1.330(3)
O7-H7B	0.83(3)	N10-C6	1.333(3)
O8-H8A	0.81(2)	N11-C6	1.456(3)
O8-H8B	0.80(2)	N1-H1	0.88(2)
N1-N2	1.342(3)	N3-H3	0.86(2)
N1-C3	1.339(3)	N8-H8	0.86(2)
N2-C1	1.333(3)	C1-C2	1.411(3)
N3-N4	1.352(3)	C1-C5	1.462(3)
N3-C5	1.333(3)	C2-C3	1.394(3)
N4-C4	1.306(3)	C3-C7	1.460(3)
N5-C4	1.332(3)		

Table S4 Selected bond angles [°] for compound **6**·2H_2O

Parameter	Bond Angles(°)	Parameter	Bond Angles(°)
H7A-O7-H7B	105(3)	N9-N8-H8	118.0(17)
H8A-O8-H8B	104(4)	C7-N8-H8	132.1(17)
N2-N1-C3	113.89(18)	N2-C1-C5	115.98(18)
N1-N2-C1	105.63(18)	C2-C1-C5	134.45(19)
N4-N3-C5	111.02(19)	N2-C1-C2	109.44(18)
N3-N4-C4	100.14(19)	N7-C2-C3	125.8(2)
C4-N5-C5	101.30(19)	C1-C2-C3	106.29(18)
O1-N6-O2	125.6(2)	N7-C2-C1	127.95(19)
O2-N6-C4	117.7(2)	N1-C3-C2	104.73(18)
O1-N6-C4	116.7(2)	N1-C3-C7	117.61(18)
O3-N7-C2	119.68(19)	C2-C3-C7	137.6(2)
O3-N7-O4	123.1(2)	N4-C4-N5	118.1(2)
O4-N7-C2	117.24(19)	N4-C4-N6	120.1(2)
N9-N8-C7	109.95(19)	N5-C4-N6	121.8(2)
N8-N9-C6	101.26(19)	N3-C5-N5	109.48(19)
C6-N10-C7	101.29(19)	N5-C5-C1	121.99(19)
O6-N11-C6	117.7(2)	N3-C5-C1	128.5(2)
O5-N11-O6	124.5(2)	N9-C6-N11	121.2(2)
O5-N11-C6	117.9(2)	N10-C6-N11	121.4(2)
N2-N1-H1	118.0(15)	N9-C6-N10	117.4(2)
C3-N1-H1	128.1(15)	N8-C7-C3	129.9(2)
N4-N3-H3	120.6(17)	N10-C7-C3	120.00(19)
C5-N3-H3	128.2(17)	N8-C7-N10	110.07(19)

Table S5. Selected torsion angles [°] for compound **6**·2H_2O

Parameter	Torsion Angles(°)	Parameter	Torsion Angles(°)
C3-N1-N2-C1	1.0(2)	N8-N9-C6-N10	0.1(3)
N2-N1-C3-C7	175.35(18)	C7-N10-C6-N9	0.1(3)
N2-N1-C3-C2	-1.6(2)	C6-N10-C7-C3	-178.4(2)
N1-N2-C1-C5	-176.41(18)	C7-N10-C6-N11	-179.5(2)
N1-N2-C1-C2	0.2(2)	C6-N10-C7-N8	-0.2(2)
N4-N3-C5-C1	-176.6(2)	O5-N11-C6-N10	171.2(2)
C5-N3-N4-C4	-0.3(2)	O6-N11-C6-N10	-8.8(3)
N4-N3-C5-N5	0.6(3)	O6-N11-C6-N9	171.7(2)
N3-N4-C4-N6	176.8(2)	O5-N11-C6-N9	-8.4(3)
N3-N4-C4-N5	-0.2(3)	C2-C1-C5-N3	-1.5(4)
C5-N5-C4-N6	-176.4(2)	N2-C1-C2-N7	178.0(2)
C5-N5-C4-N4	0.5(3)	C5-C1-C2-N7	-6.3(4)
C4-N5-C5-C1	176.8(2)	C5-C1-C2-C3	174.6(2)
C4-N5-C5-N3	-0.6(2)	N2-C1-C5-N3	174.0(2)
O2-N6-C4-N4	153.2(2)	N2-C1-C5-N5	-2.9(3)

O1-N6-C4-N5	148.2(2)	N2-C1-C2-C3	-1.1(2)
O2-N6-C4-N5	-30.1(3)	C2-C1-C5-N5	-178.3(2)
O1-N6-C4-N4	-28.6(3)	C1-C2-C3-C7	-174.4(2)
O4-N7-C2-C3	2.7(3)	N7-C2-C3-N1	-177.6(2)
O3-N7-C2-C3	-178.7(2)	N7-C2-C3-C7	6.4(4)
O4-N7-C2-C1	-176.3(2)	C1-C2-C3-N1	1.6(2)
O3-N7-C2-C1	2.3(3)	N1-C3-C7-N8	-176.1(2)
C7-N8-N9-C6	-0.2(2)	C2-C3-C7-N10	177.4(2)
N9-N8-C7-C3	178.3(2)	N1-C3-C7-N10	1.7(3)
N9-N8-C7-N10	0.3(3)	C2-C3-C7-N8	-0.5(4)
N8-N9-C6-N11	179.7(2)		

Table S6. Hydrogen bonds present in compound **6**·2H_2O

D-H···A	d(D···H)/Å	H···A/Å	D-H···A/Å	<DHA/°	comment
N1-H1···O7	0.88(2)	1.81(2)	2.693(3)	176(2)	inter
N3-H3···O3	0.86(2)	2.04(2)	2.690(3)	132(2)	intra
N3-H3···O6	0.86(2)	2.44(3)	3.156(3)	141(2)	inter
O7-H7A···N5	0.85(3)	2.01(3)	2.850(3)	168(3)	inter
O7-H7B···N10	0.83(3)	2.45(3)	2.883(3)	114(2)	inter
N8-H8···O4	0.86(2)	2.15(2)	2.706(3)	123(2)	intra
N8-H8···O8	0.86(2)	1.92(2)	2.722(3)	154(2)	inter
O8-H8A···N4	0.81(2)	2.33(2)	3.121(3)	167(4)	inter
O8-H8B···N9	0.80(2)	2.14(3)	2.928(3)	172(3)	inter

Table S7. Selected bond lengths [Å] for compound **7**·H_2O

Parameter	Bond length(Å)	Parameter	Bond length(Å)
O1-N7	1.234(6)	N8-C2	1.431(8)
O2-N7	1.255(6)	N9-N10	1.385(6)
O3-N8	1.244(6)	N9-C7	1.305(7)
O4-N8	1.226(6)	N10-C6	1.330(6)
O5-N13	1.245(6)	N11-C7	1.371(6)
O6-N13	1.238(6)	N11-C6	1.353(7)
O7-H7B	0.83(5)	N12-N13	1.349(6)
O7-H7A	0.83(5)	N12-C6	1.346(6)
N1-C3	1.341(7)	N1-H1	0.90(5)
N1-N2	1.356(6)	N4-H4	0.89(3)
N2-C1	1.333(7)	N5-H5	0.90(4)
N3-C5	1.300(7)	N10-H10	0.90(4)
N3-N4	1.369(5)	N11-H11	0.90(4)
N4-C4	1.333(6)	C1-C2	1.419(8)
N5-C5	1.353(6)	C1-C5	1.462(7)
N5-C4	1.358(6)	C2-C3	1.381(7)
N6-N7	1.341(6)	C3-C7	1.454(7)
N6-C4	1.337(6)		

Table S8. Selected bond angles [°] for compound **7**·H_2O

Parameter	Bond Angles(°)	Parameter	Bond Angles(°)
H7A-O7-H7B	96(5)	N9-N10-H10	121(3)
N2-N1-C3	113.5(5)	C6-N10-H10	127(4)
N1-N2-C1	105.0(4)	C7-N11-H11	131(3)
N4-N3-C5	103.5(4)	C6-N11-H11	122(3)
N3-N4-C4	112.3(4)	C2-C1-C5	132.6(5)
C4-N5-C5	107.0(4)	N2-C1-C5	117.4(5)
N7-N6-C4	116.7(4)	N2-C1-C2	110.0(4)
O1-N7-N6	116.6(4)	N8-C2-C3	128.2(5)
O2-N7-N6	121.4(4)	C1-C2-C3	105.9(5)
O1-N7-O2	122.0(4)	N8-C2-C1	125.6(5)
O3-N8-C2	117.5(4)	C2-C3-C7	133.8(5)
O4-N8-C2	118.6(4)	N1-C3-C2	105.7(5)
O3-N8-O4	123.8(5)	N1-C3-C7	120.5(5)
N10-N9-C7	103.7(4)	N4-C4-N5	104.9(4)
N9-N10-C6	111.7(4)	N4-C4-N6	135.0(4)
C6-N11-C7	106.9(4)	N5-C4-N6	120.1(4)
N13-N12-C6	115.2(4)	N3-C5-N5	112.2(4)
O5-N13-N12	116.1(4)	N3-C5-C1	122.3(4)
O6-N13-N12	121.8(4)	N5-C5-C1	125.4(5)
O5-N13-O6	122.2(4)	N11-C6-N12	119.5(4)
C3-N1-H1	134(4)	N10-C6-N11	106.0(4)
N2-N1-H1	112(4)	N10-C6-N12	134.5(5)
C4-N4-H4	126(4)	N9-C7-C3	125.0(4)
N3-N4-H4	121(4)	N11-C7-C3	123.1(4)
C4-N5-H5	124(3)	N9-C7-N11	111.7(4)
C5-N5-H5	128(3)		

Table S9 Selected torsion angles [°] for compound **7**·H_2O

Parameter	Torsion Angles(°)	Parameter	Torsion Angles(°)
C3-N1-N2-C1	0.8(7)	N9-N10-C6-N11	1.4(7)
N2-N1-C3-C7	178.0(5)	C6-N11-C7-C3	-175.2(6)
N2-N1-C3-C2	-1.0(7)	C6-N11-C7-N9	0.9(8)
N1-N2-C1-C5	179.1(5)	C7-N11-C6-N12	177.9(6)
N1-N2-C1-C2	-0.2(6)	C7-N11-C6-N10	-1.3(7)
N4-N3-C5-C1	176.9(6)	N13-N12-C6-N11	-169.3(6)
C5-N3-N4-C4	-0.8(7)	C6-N12-N13-O6	-1.2(9)
N4-N3-C5-N5	0.7(7)	N13-N12-C6-N10	9.6(11)
N3-N4-C4-N6	-179.4(7)	C6-N12-N13-O5	176.4(6)
N3-N4-C4-N5	0.6(7)	N2-C1-C5-N5	130.8(6)
C5-N5-C4-N4	-0.1(7)	N2-C1-C5-N3	-44.8(9)
C4-N5-C5-C1	-176.5(6)	N2-C1-C2-N8	173.1(5)
C4-N5-C5-N3	-0.4(8)	C5-C1-C2-N8	-6.0(10)
C5-N5-C4-N6	179.9(6)	C2-C1-C5-N3	134.2(7)

N7-N6-C4-N5	179.3(6)	C2-C1-C5-N5	-50.1(11)
C4-N6-N7-O2	-0.2(9)	C5-C1-C2-C3	-179.5(6)
N7-N6-C4-N4	-0.7(11)	N2-C1-C2-C3	-0.4(7)
C4-N6-N7-O1	-178.9(6)	N8-C2-C3-C7	8.7(11)
O4-N8-C2-C3	173.6(5)	N8-C2-C3-N1	-172.4(5)
O4-N8-C2-C1	1.6(8)	C1-C2-C3-N1	0.8(6)
O3-N8-C2-C3	-4.3(8)	C1-C2-C3-C7	-178.0(6)
O3-N8-C2-C1	-176.3(5)	C2-C3-C7-N9	47.3(11)
N10-N9-C7-C3	175.9(6)	C2-C3-C7-N11	-137.2(7)
C7-N9-N10-C6	-0.9(7)	N1-C3-C7-N9	-131.4(7)
N10-N9-C7-N11	0.0(7)	N1-C3-C7-N11	44.1(9)
N9-N10-C6-N12	-177.6(7)		

Table S10. Hydrogen bonds present in compound **7**·H_2O

D-H···A	d(D···H)/Å	d(H···A)/Å	d(D-H···A)/Å	<DHA(°)	comment
N1-H1···O7	0.90(5)	1.82(5)	2.694(7)	164(4)	inter
N4-H4···O2	0.89(3)	2.15(5)	2.584(5)	109(4)	intra
N4-H4···O3	0.89(3)	1.98(4)	2.803(5)	153(5)	inter
N5-H5···N6	0.90(4)	1.92(5)	2.809(6)	170(4)	Inter
O7-H7A···O2	0.83(5)	2.07(5)	2.884(6)	171(5)	inter
O7-H7B···O6	0.83(5)	2.39(5)	2.803(6)	112(4)	inter
N10-H10···O6	0.90(4)	2.13(5)	2.553(6)	108(4)	intra
N10-H10···N2	0.90(4)	2.46(4)	3.339(6)	165(6)	inter
N11-H11···N12	0.90(4)	2.01(4)	2.894(6)	166(4)	inter

5. Copies of Spectra

5.1 ^{1}H and ^{13}C NMR spectra of the compounds 5-16

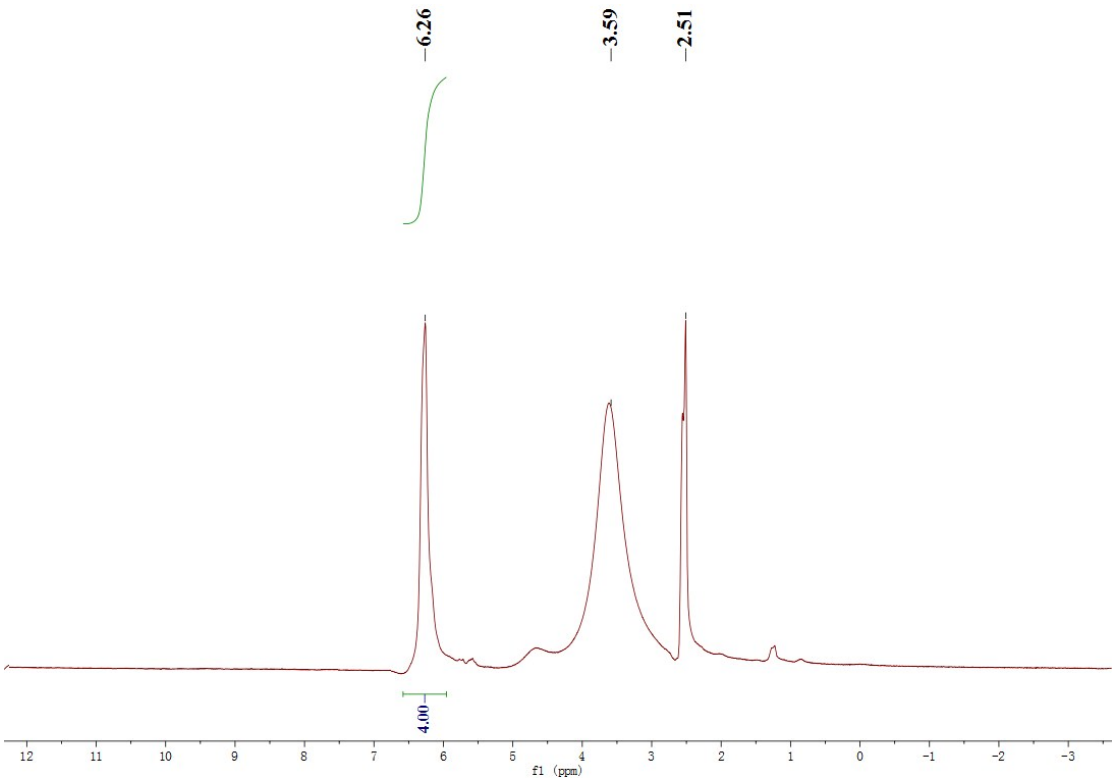

Figure S1 ^{1}H NMR spectra (300 MHz) of **5** in DMSO-d_6 at 25 ℃

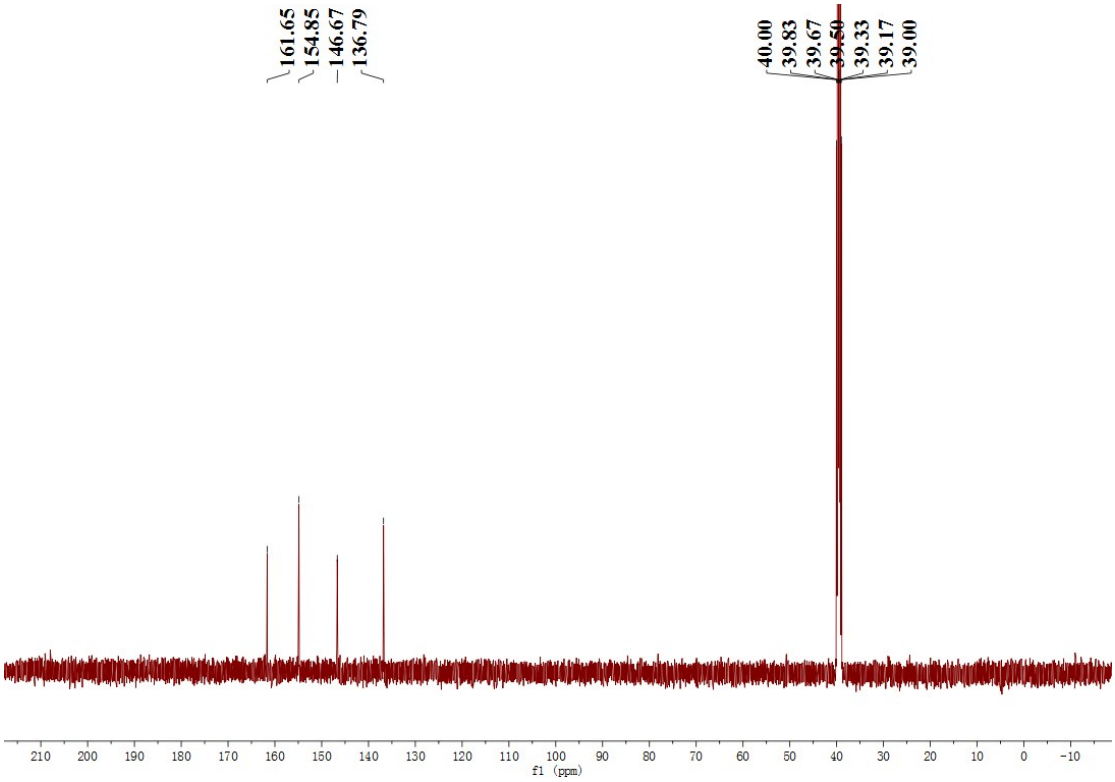

Figure S2 ^{13}C spectra (125 MHz) of **5** in DMSO-d_6 at 25 ℃

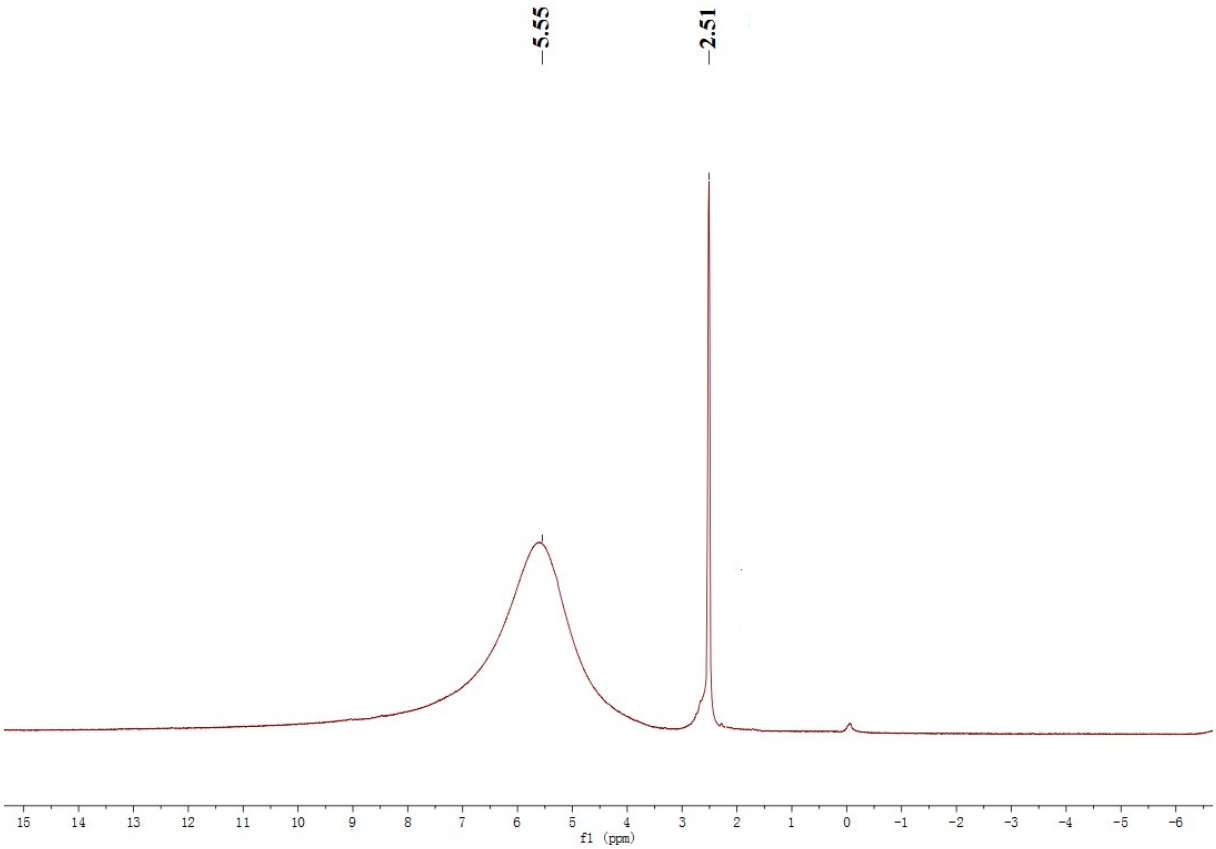

Figure S3 ^{1}H NMR spectra (300 MHz) of **6** in DMSO-d_6 at 25 ℃

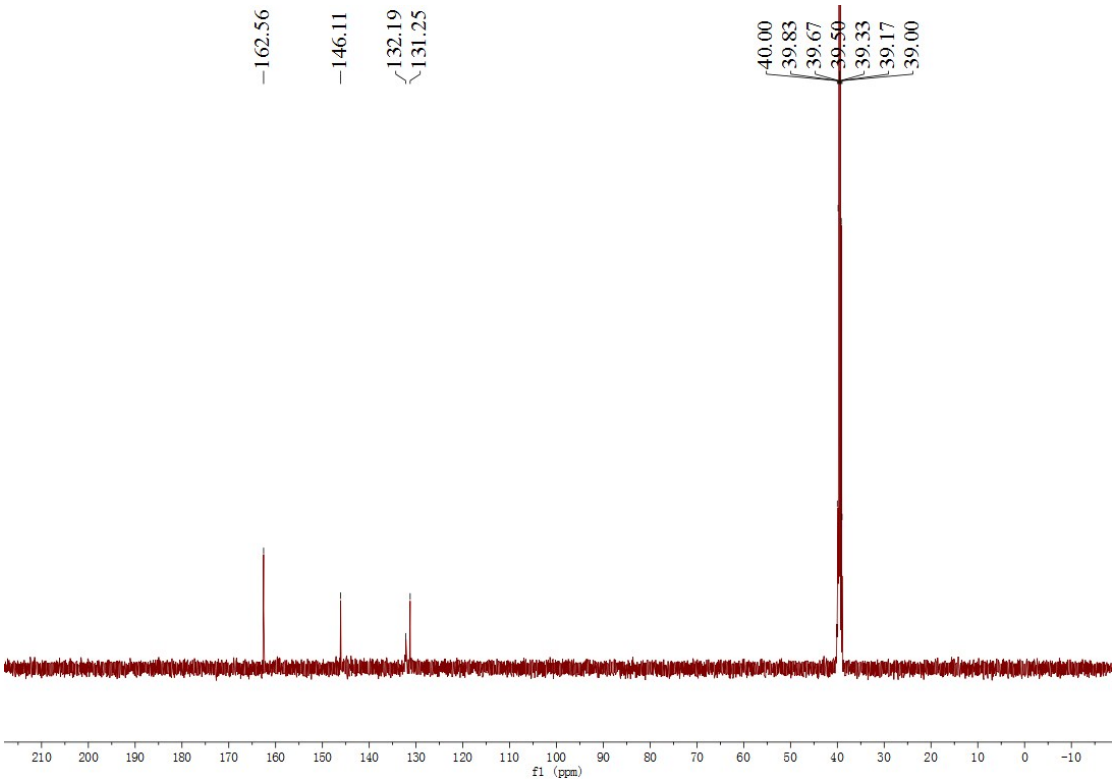

Figure S4 ^{13}C spectra (125 MHz) of **6** in DMSO-d_6 at 25 ℃

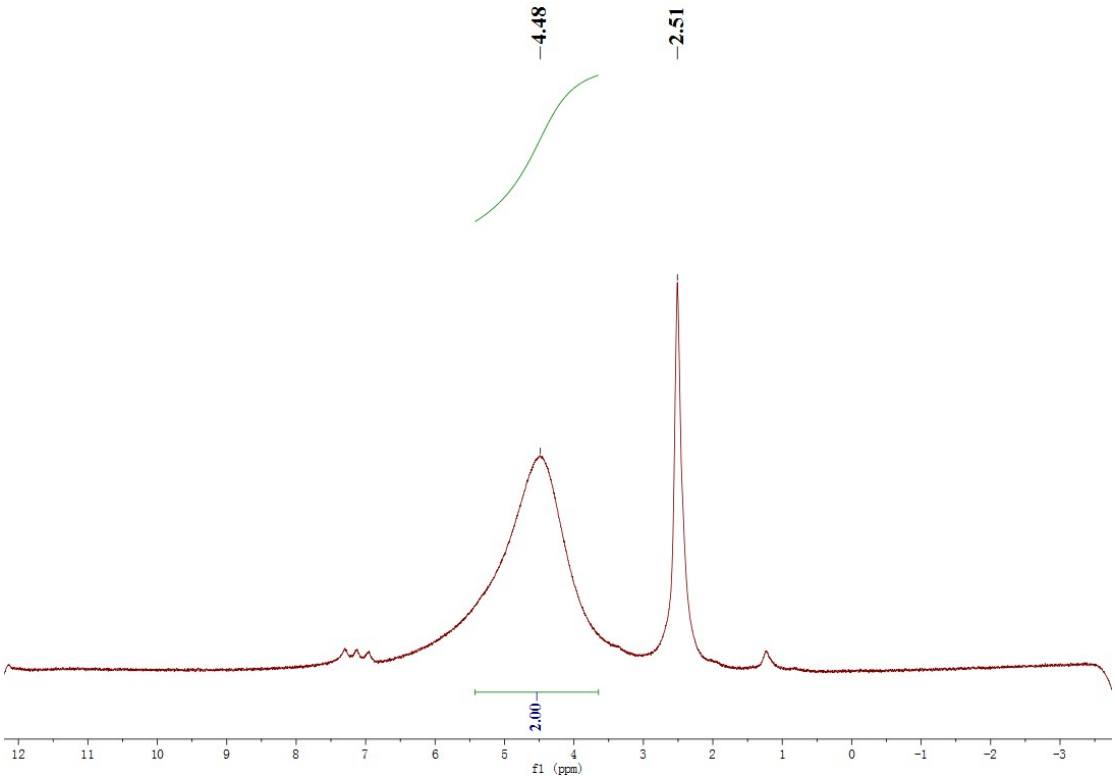

Figure S5 ^{1}H NMR spectra (300 MHz) of **7** in DMSO-d_6 at 25 ℃

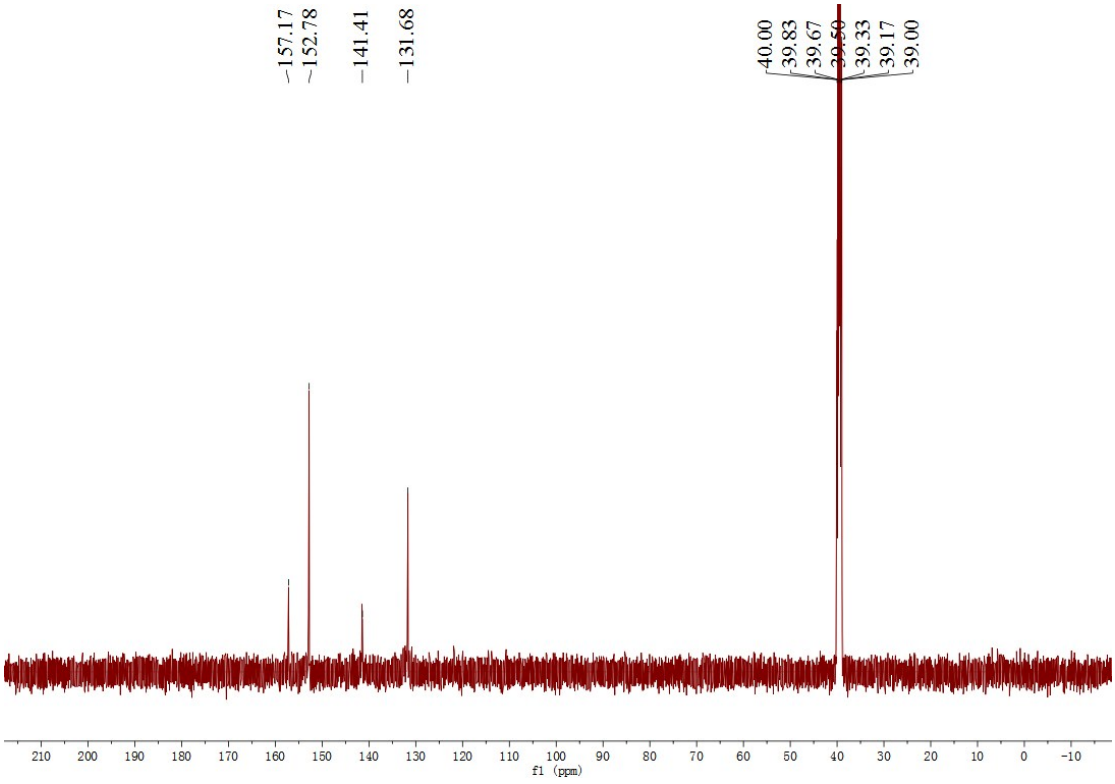

Figure S6 ^{13}C NMR spectra (300 MHz) of **7** in DMSO-d_6 at 25 ℃

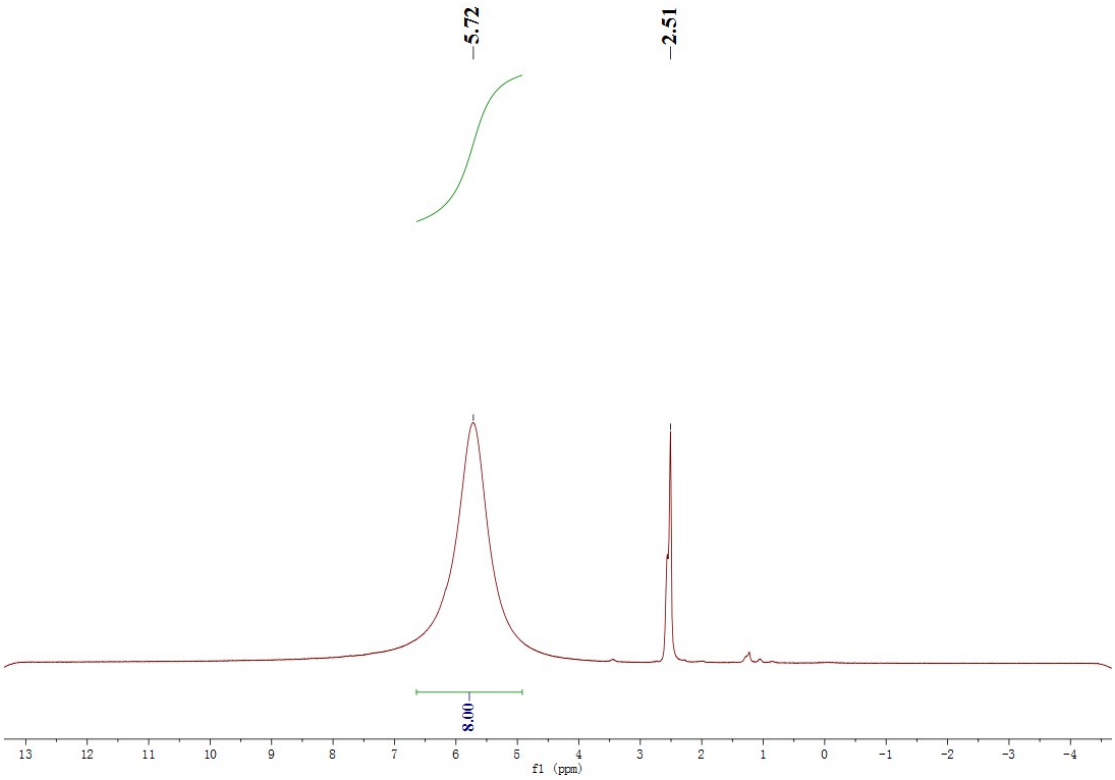

Figure S7 ^{1}H NMR spectra (300 MHz) of **8** in DMSO-d_6 at 25 ℃

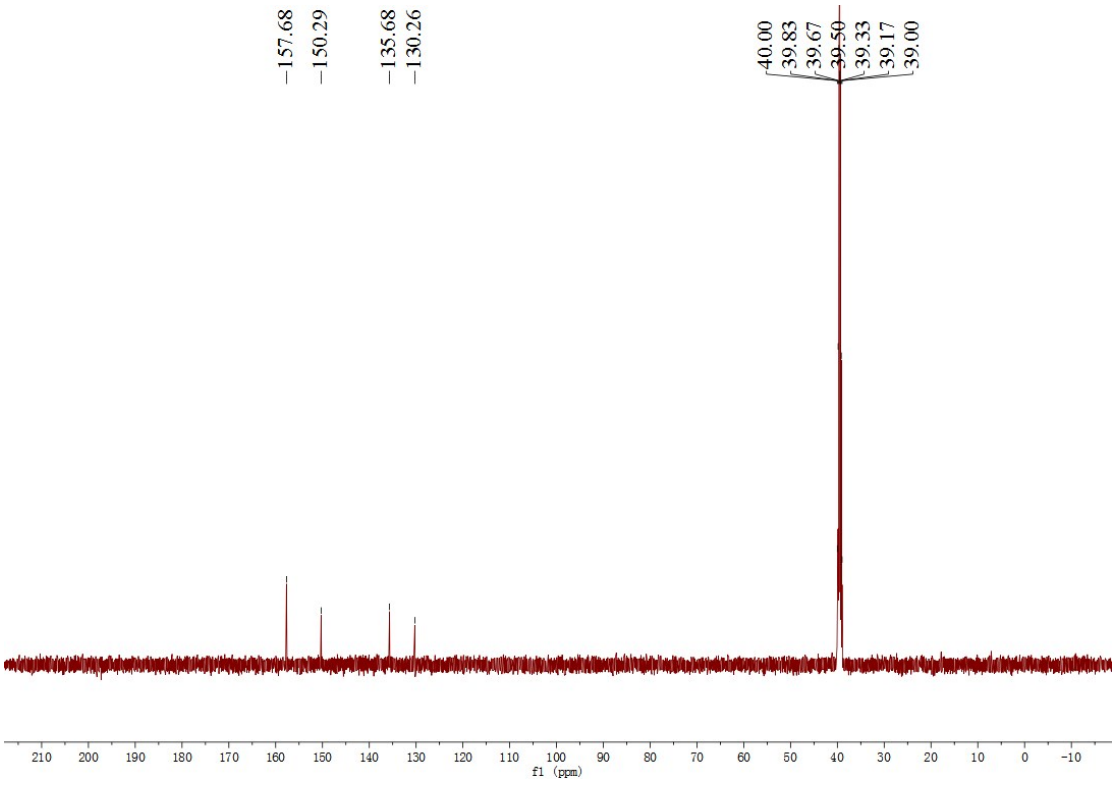

Figure S8 ^{13}C spectra (125 MHz) of **8** in DMSO-d_6 at 25 ℃

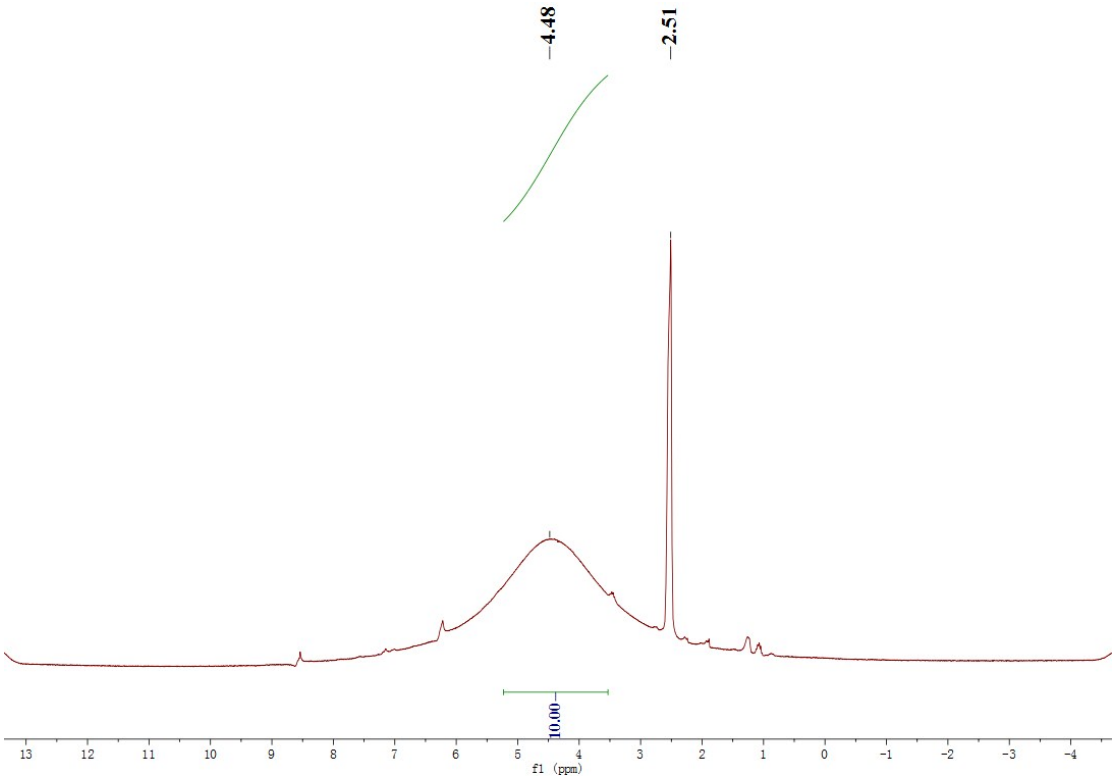

Figure S9 ^{1}H NMR spectra (300 MHz) of **9** in DMSO-d_6 at 25 ℃

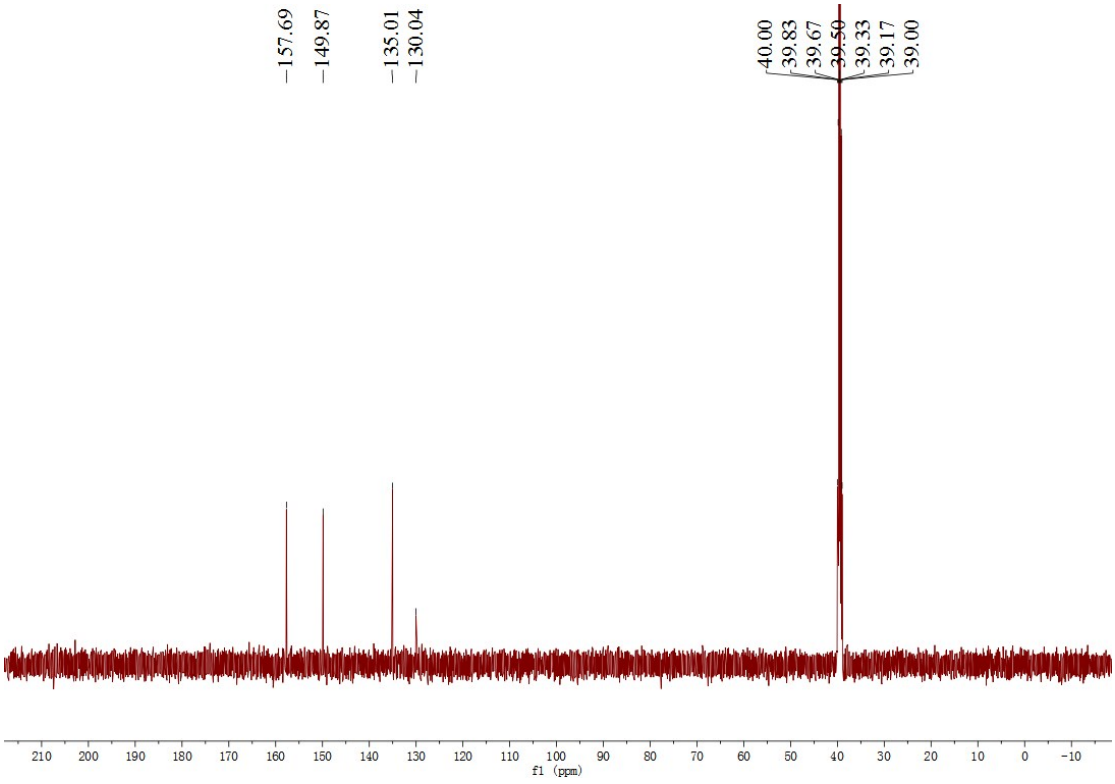

Figure S10 ^{13}C spectra (125 MHz) of **9** in DMSO-d_6 at 25 ℃

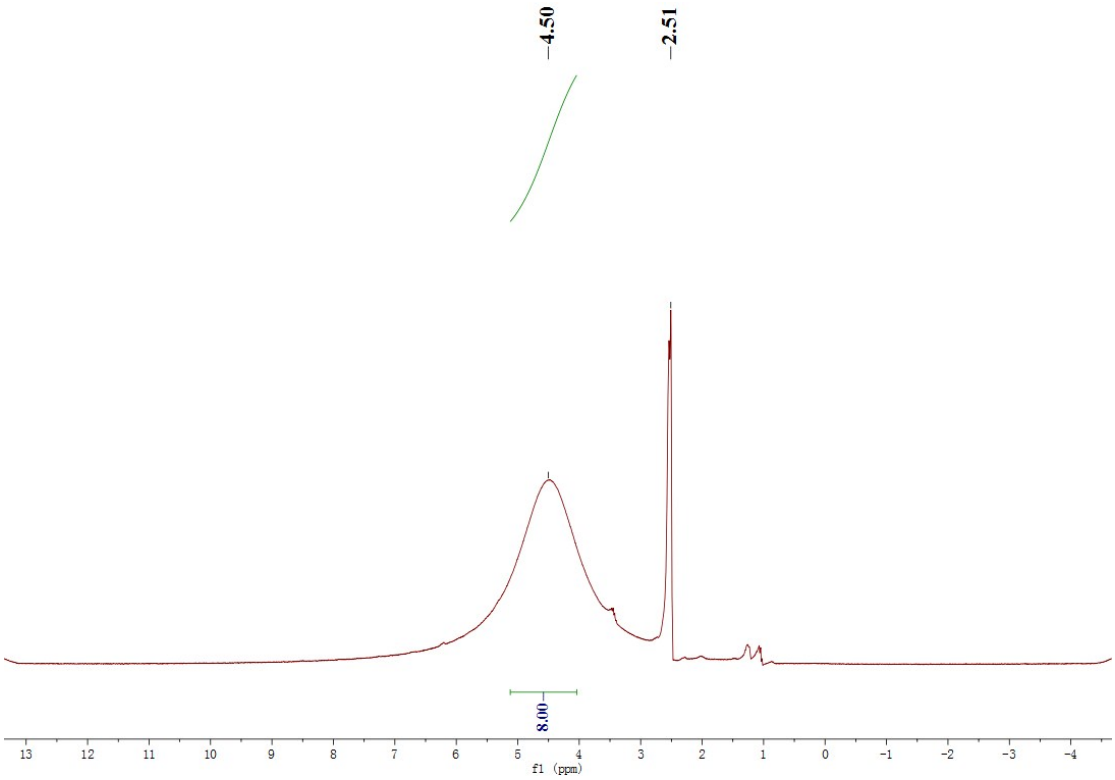

Figure S11 ^{1}H NMR spectra (300 MHz) of **10** in DMSO-d_6 at 25 ℃

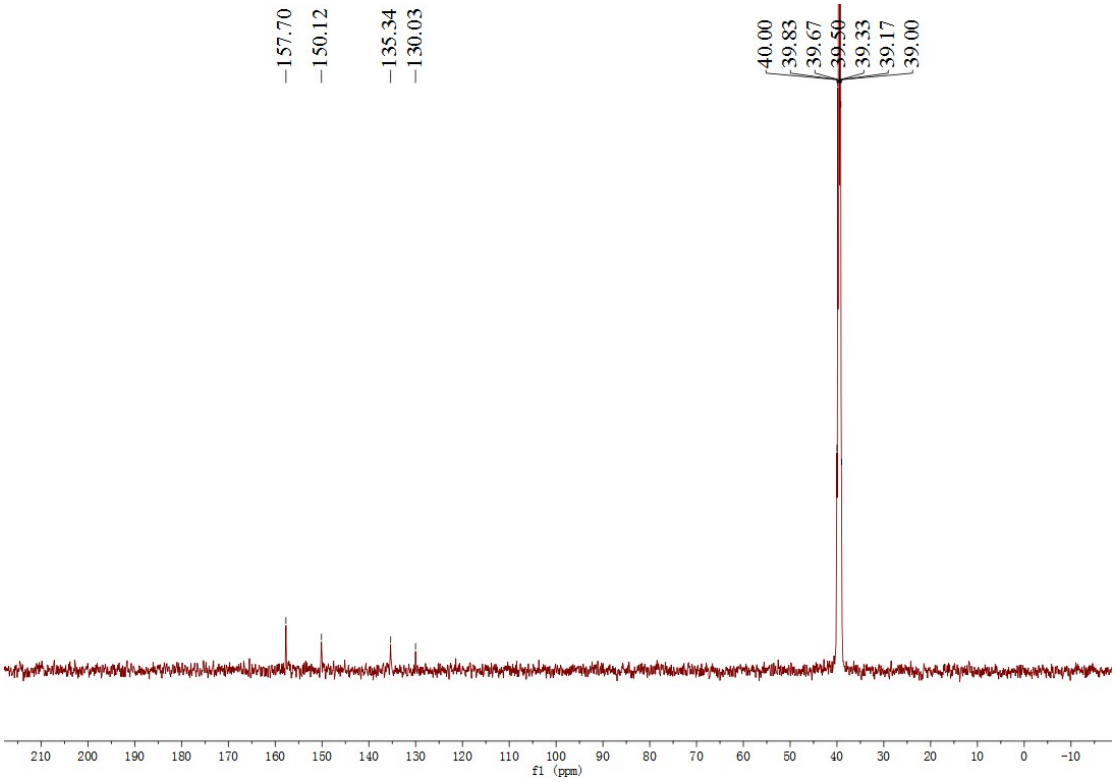

Figure S12 ^{13}C spectra (125 MHz) of **10** in DMSO-d_6 at 25 ℃

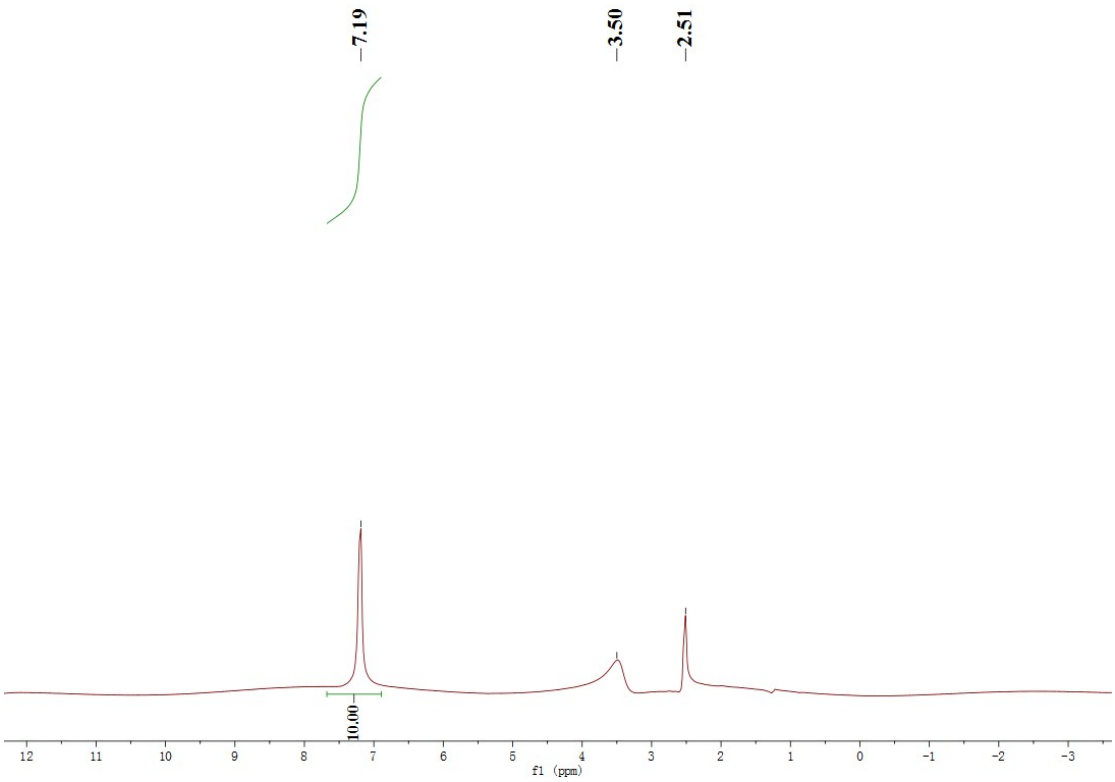

Figure S13 ^{1}H NMR spectra (300 MHz) of **11** in DMSO-d_6 at 25 ℃

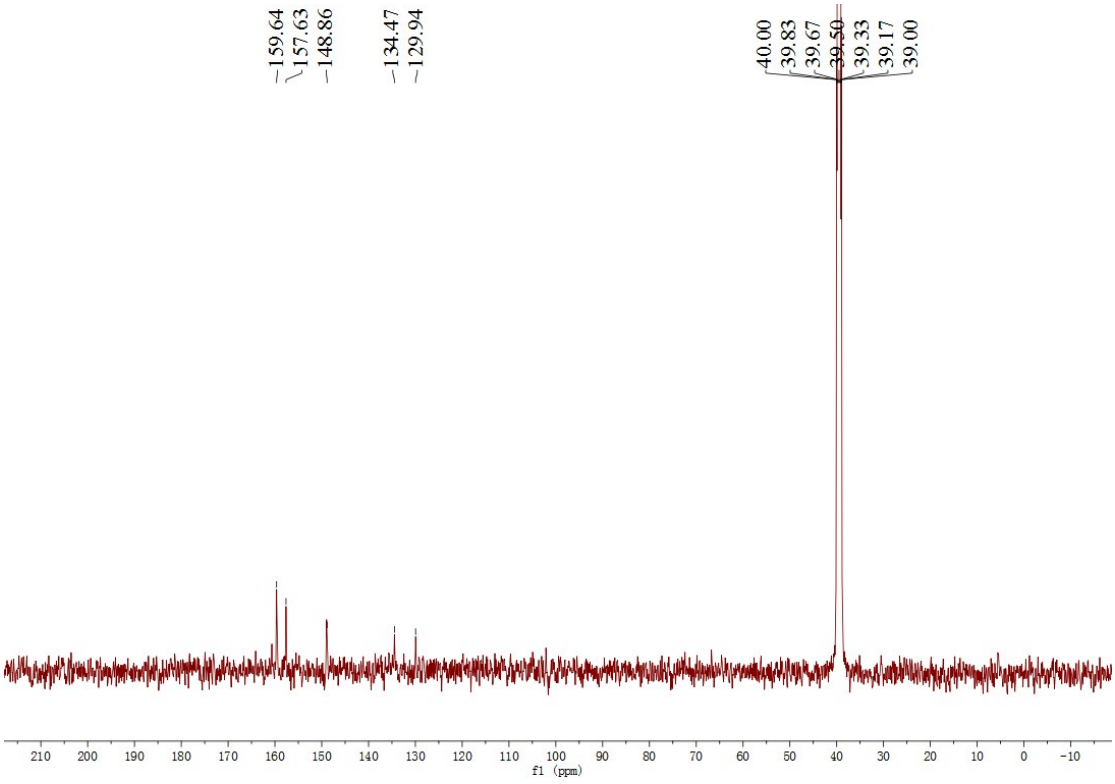

Figure S14 ^{13}C spectra (125 MHz) of **11** in DMSO-d_6 at 25 ℃

Figure S15 ^{1}H NMR spectra (300 MHz) of **12** in DMSO-d_6 at 25℃

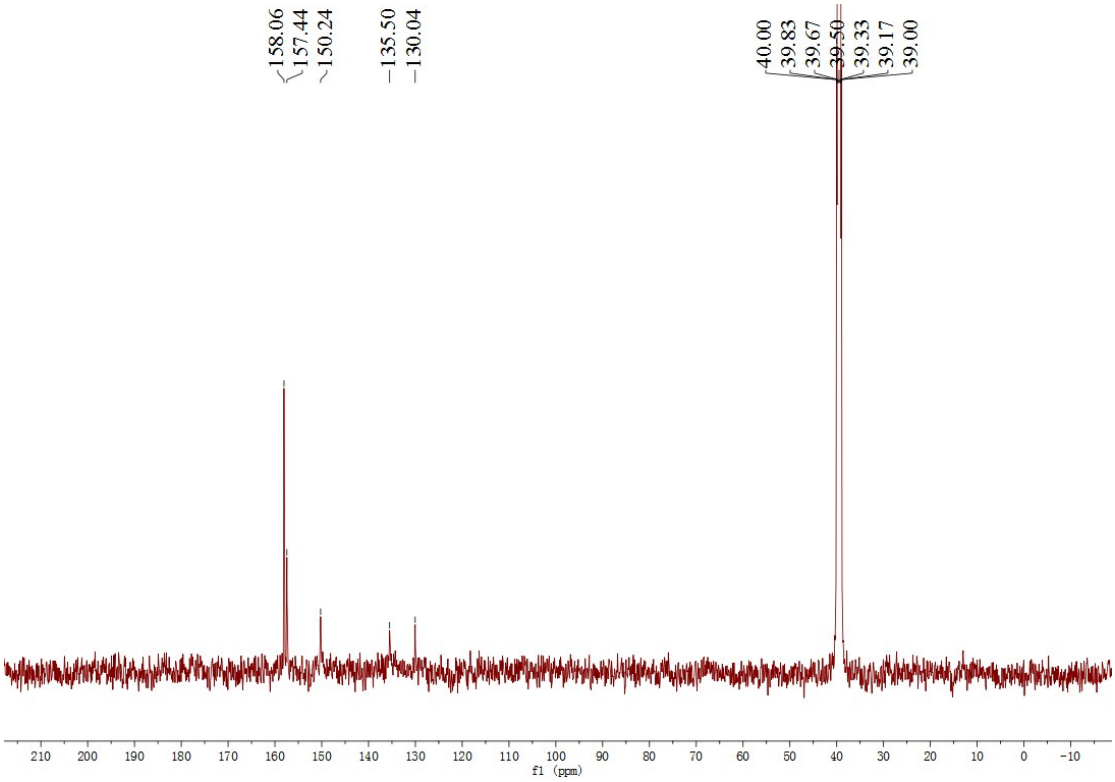

Figure S16 ^{13}C spectra (125 MHz) of **12** in DMSO-d_6 at 25 ℃

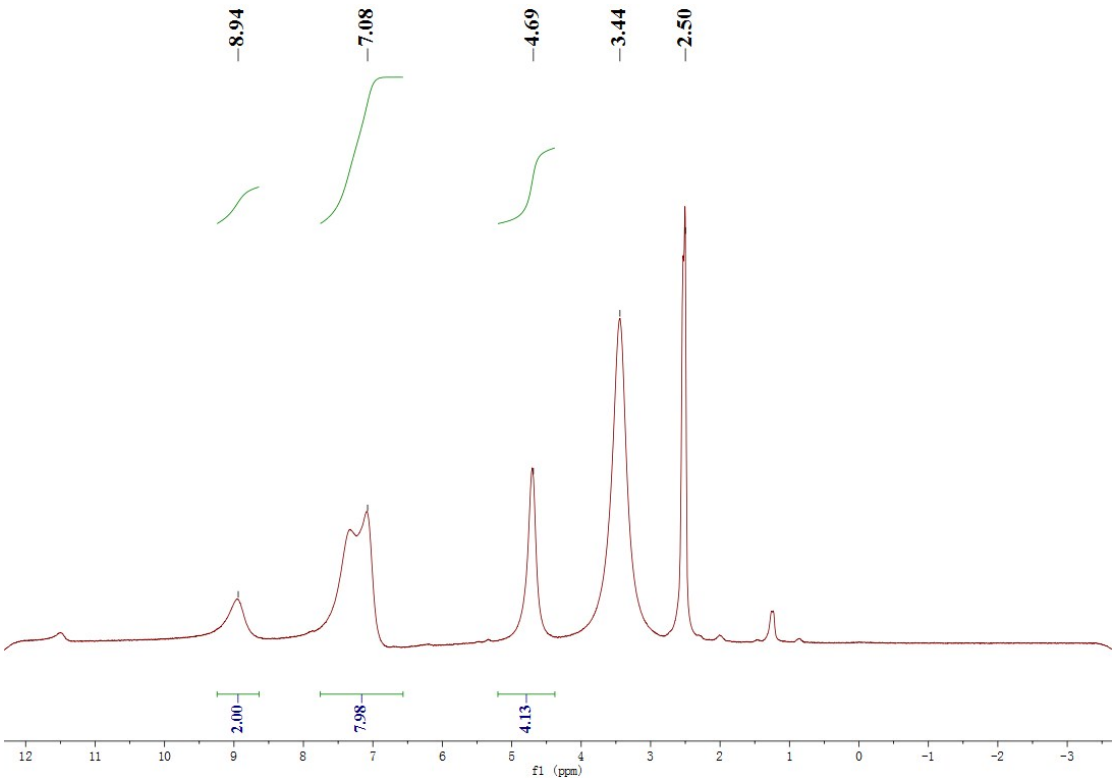

Figure S17 ^{1}H NMR spectra (300 MHz) of **13** in DMSO-d_6 at 25 ℃

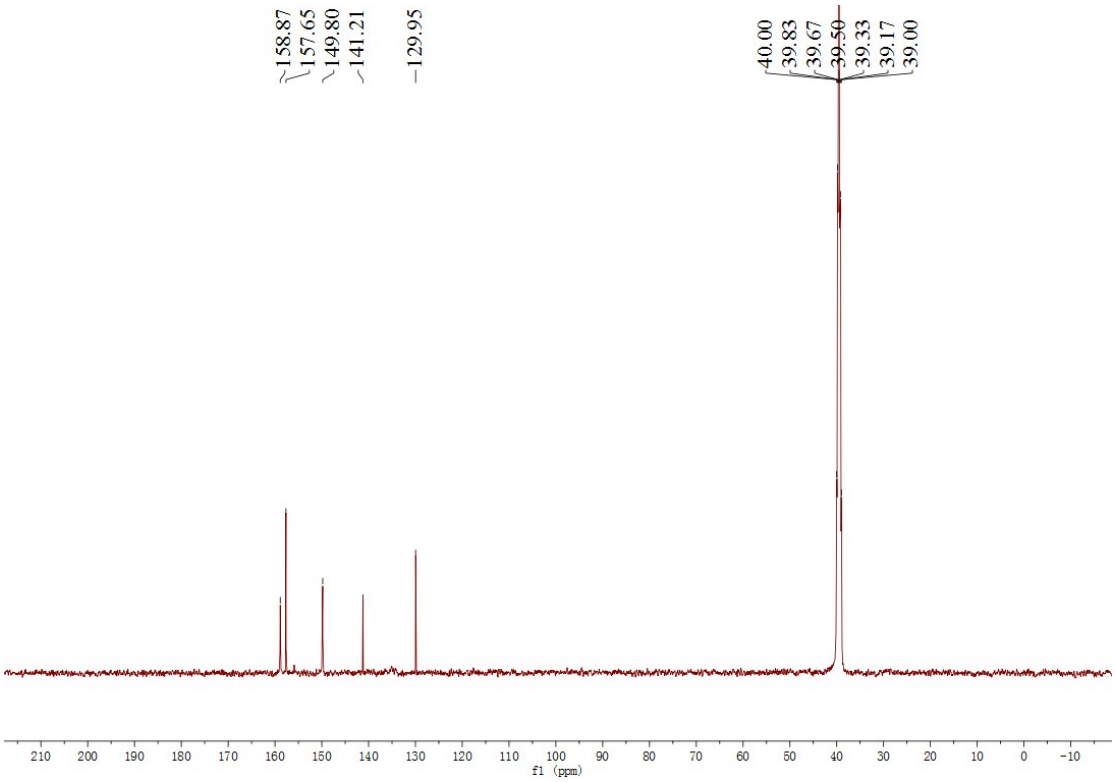

Figure S18 ^{13}C spectra (125 MHz) of **13** in DMSO-d_6 at 25 ℃

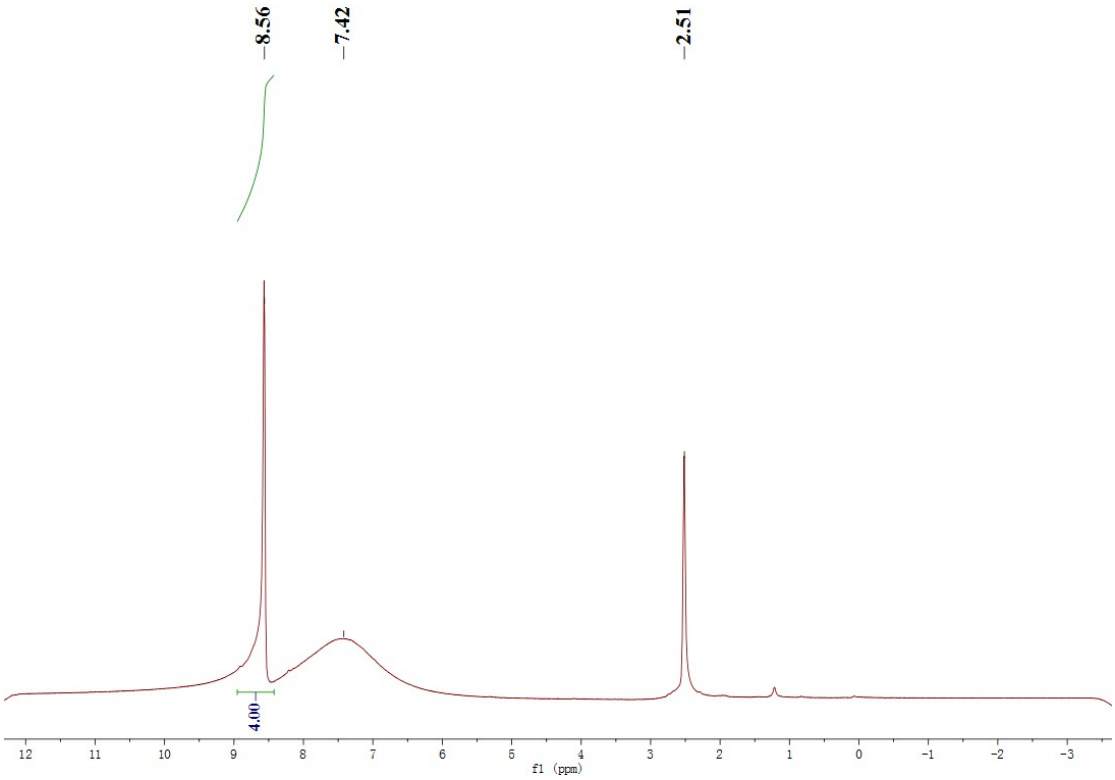

Figure S19 ^{1}H NMR spectra (300 MHz) of **14** in DMSO-d_6 at 25 ℃

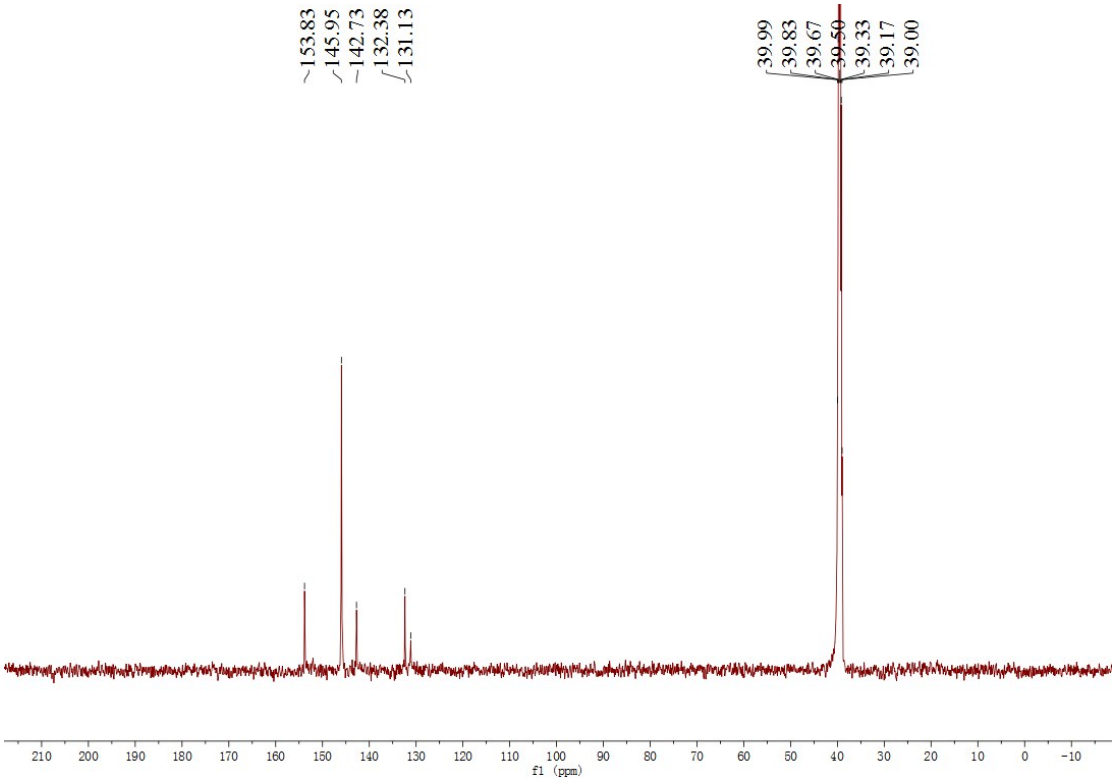

Figure S20 ^{13}C spectra (125 MHz) of **14** in DMSO-d_6 at 25 ℃

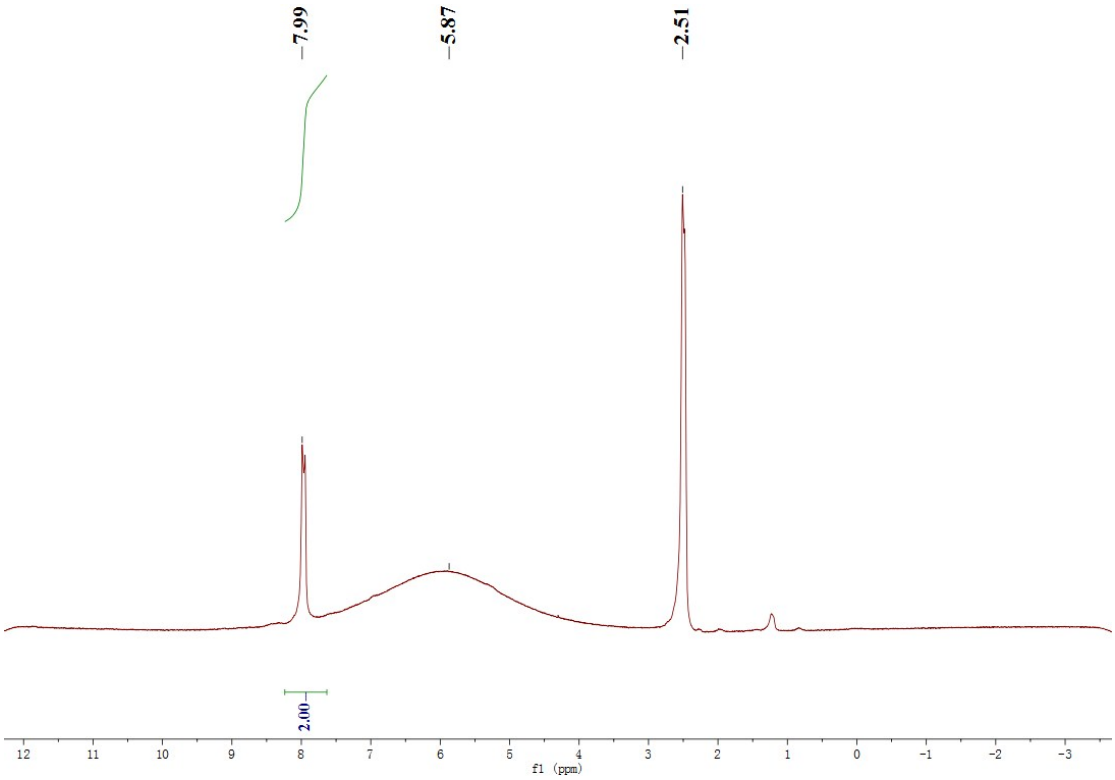

Figure S21 ^{1}H NMR spectra (300 MHz) of **15** in DMSO-d_6 at 25℃

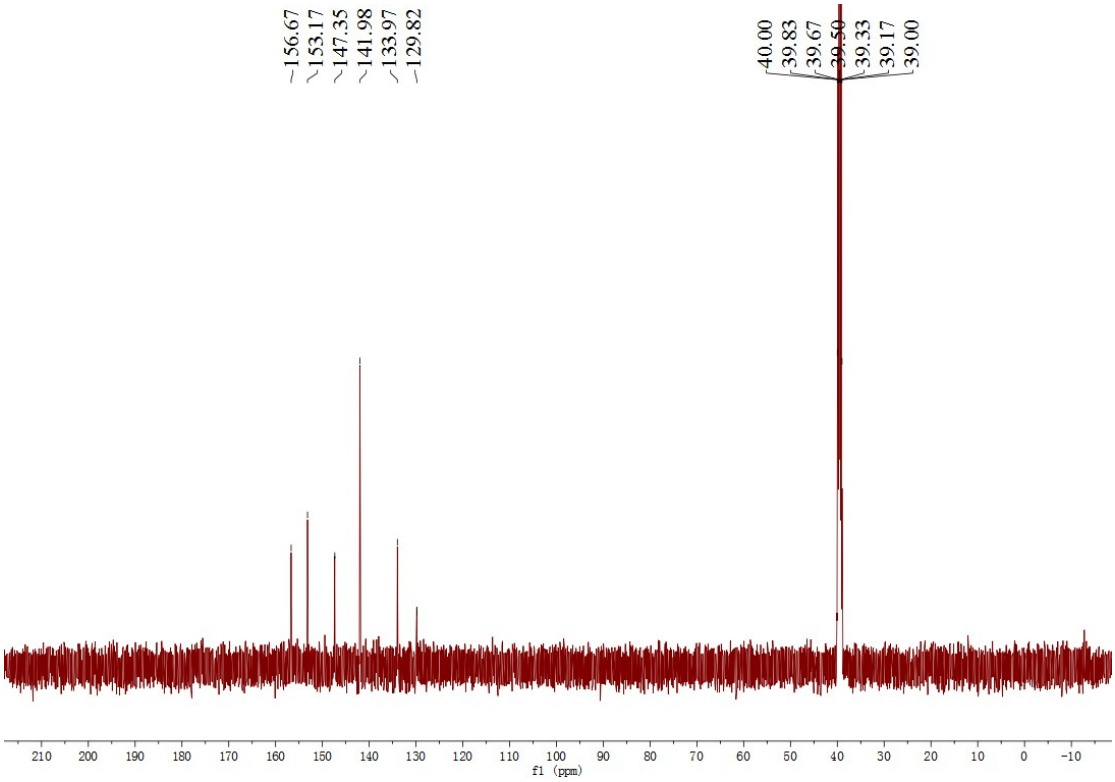

Figure S22 ^{13}C spectra (125 MHz) of **15** in DMSO-d_6 at 25 ℃

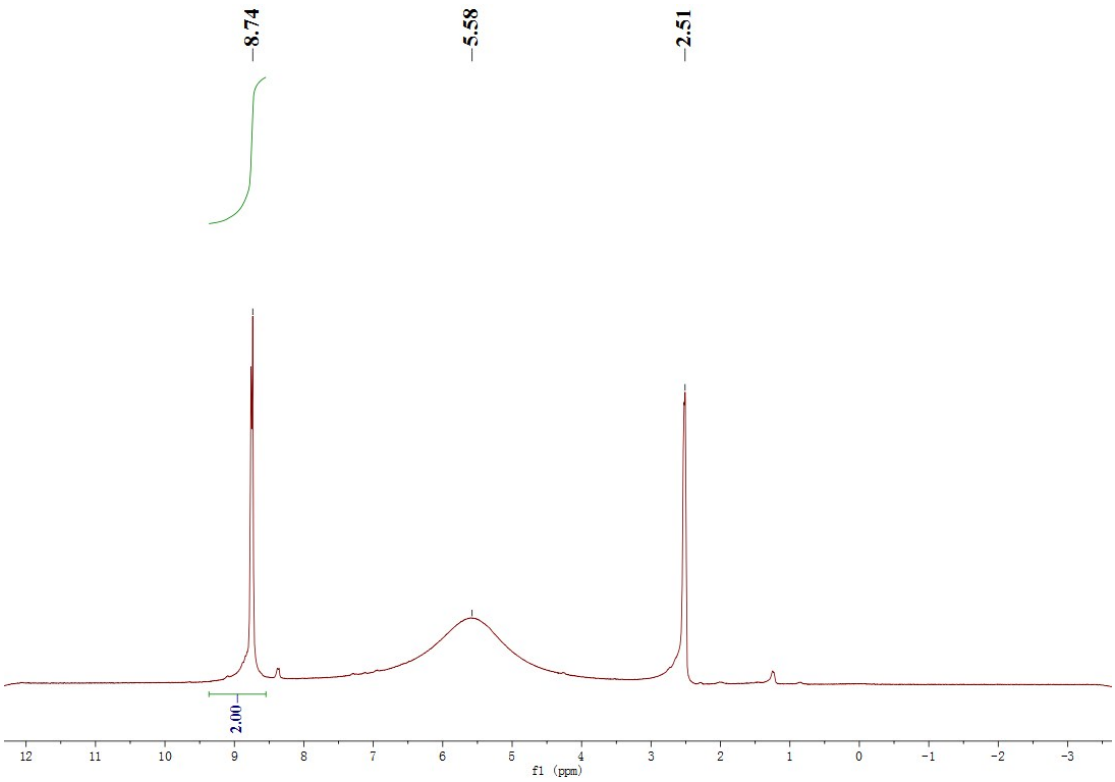

Figure S23 ^{1}H NMR spectra (300 MHz) of **16** in DMSO-d_6 at 25 ℃

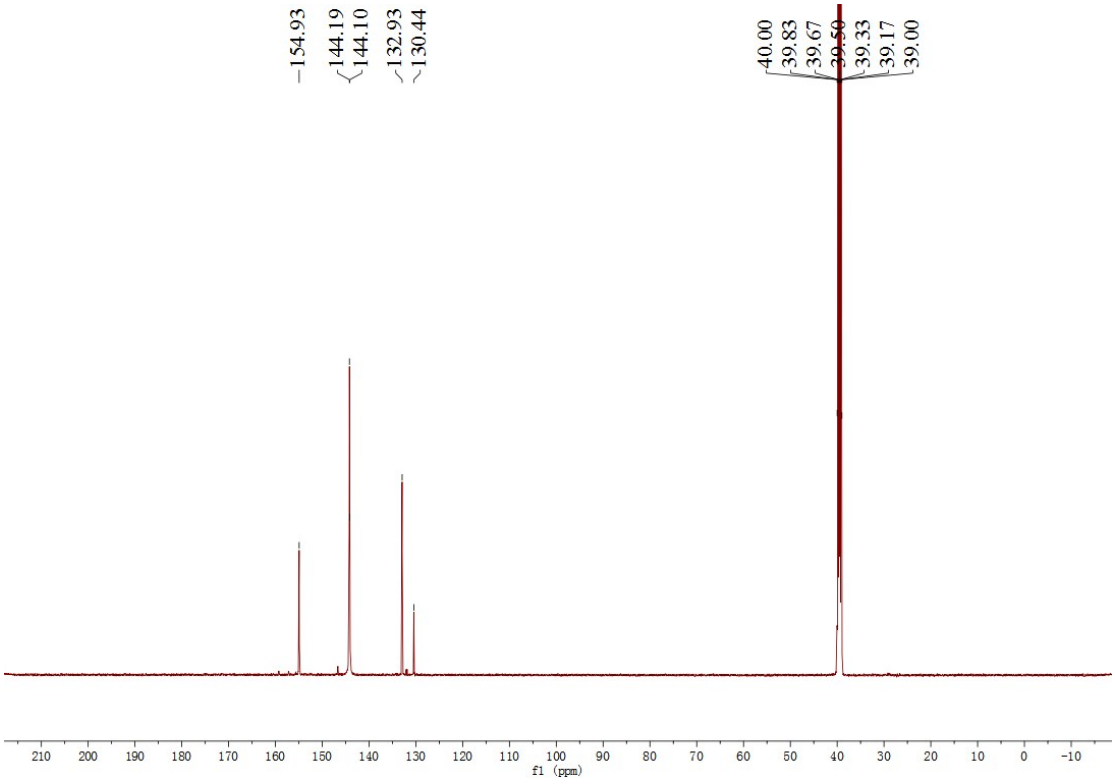

Figure S24 ^{13}C spectra (125 MHz) of **16** in DMSO-d_6 at 25 ℃

5.2 DSC curves of the compounds 5-16

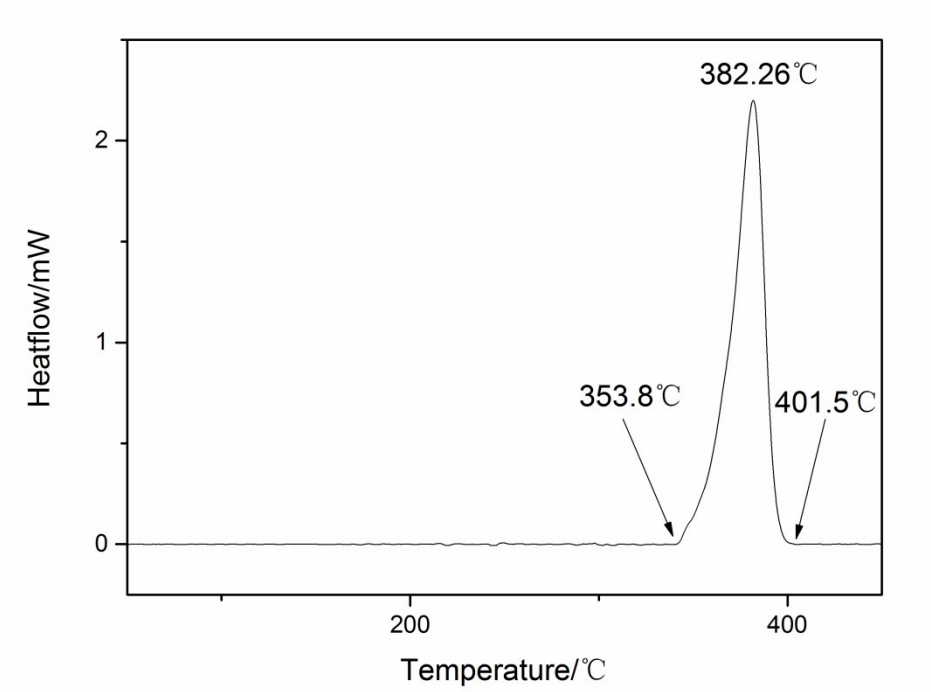

Figure S25 DSC curve of parent compound **5**

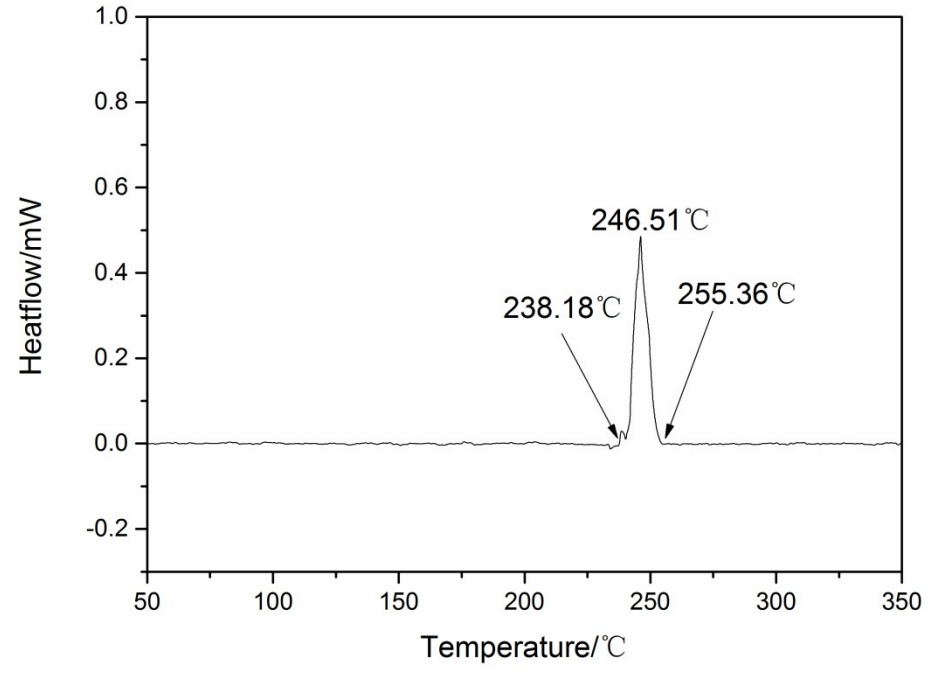

Figure S26 DSC curve of parent compound **6**

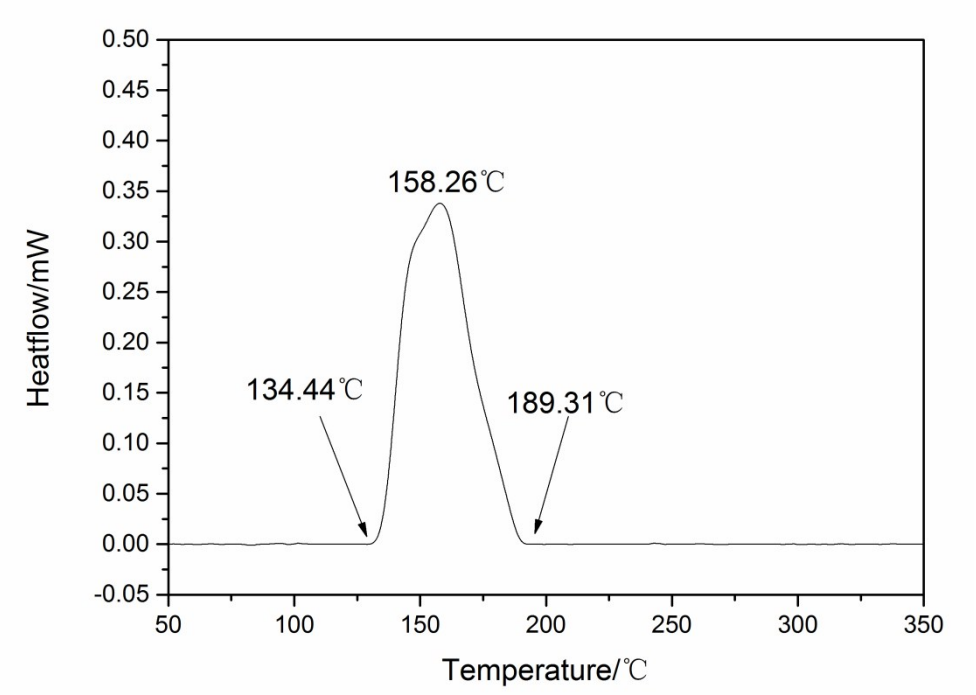

Figure S27 DSC curve of **7**

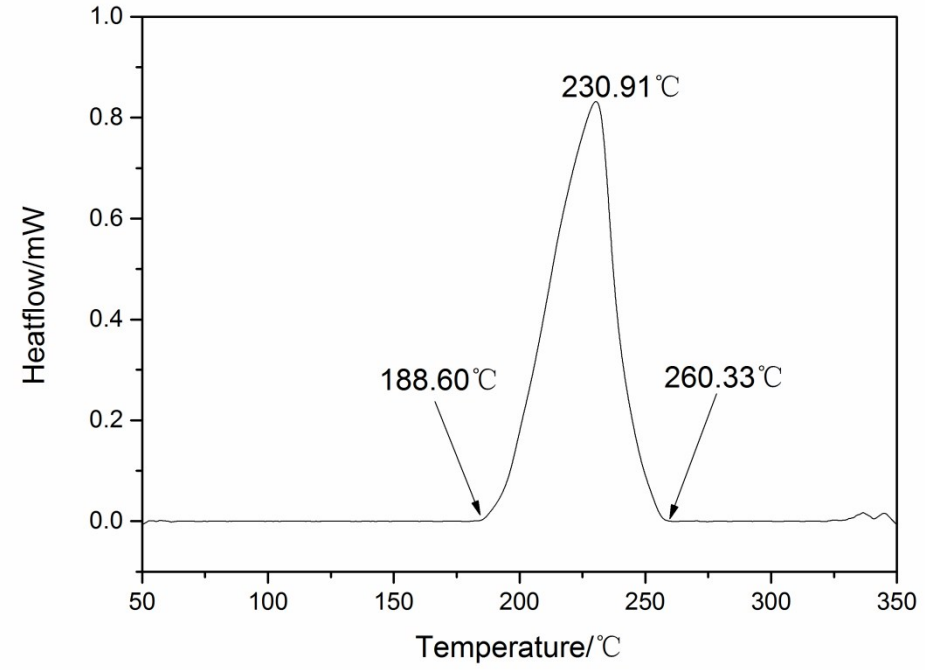

Figure S28 DSC curve of salt **8**

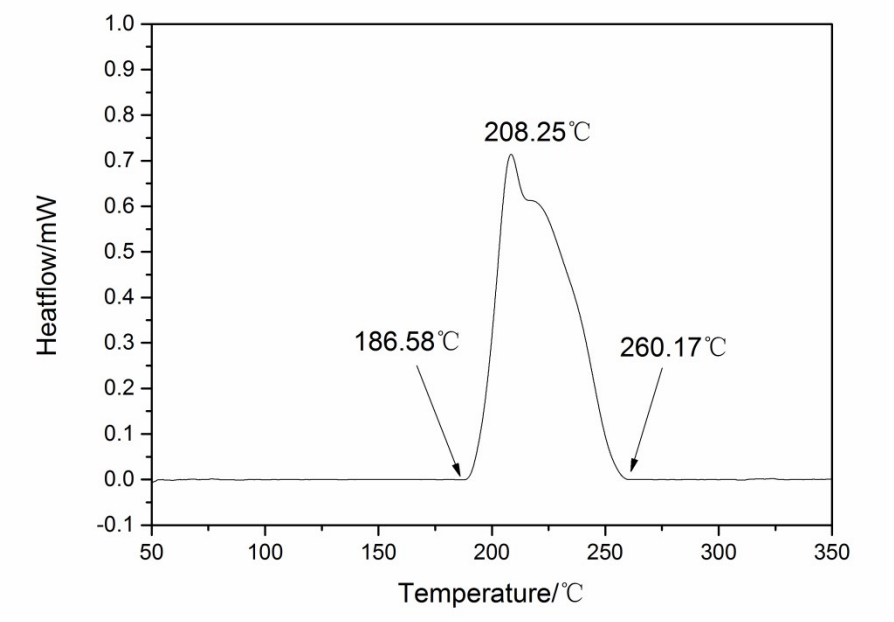

Figure S29 DSC curve of salt **9**

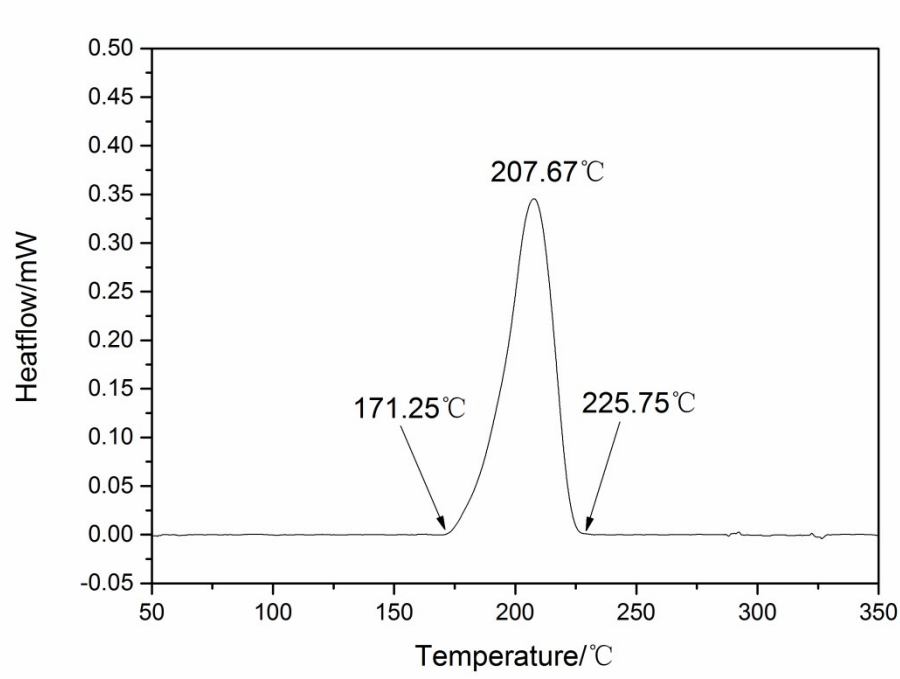

Figure S30 DSC curve of salt **10**

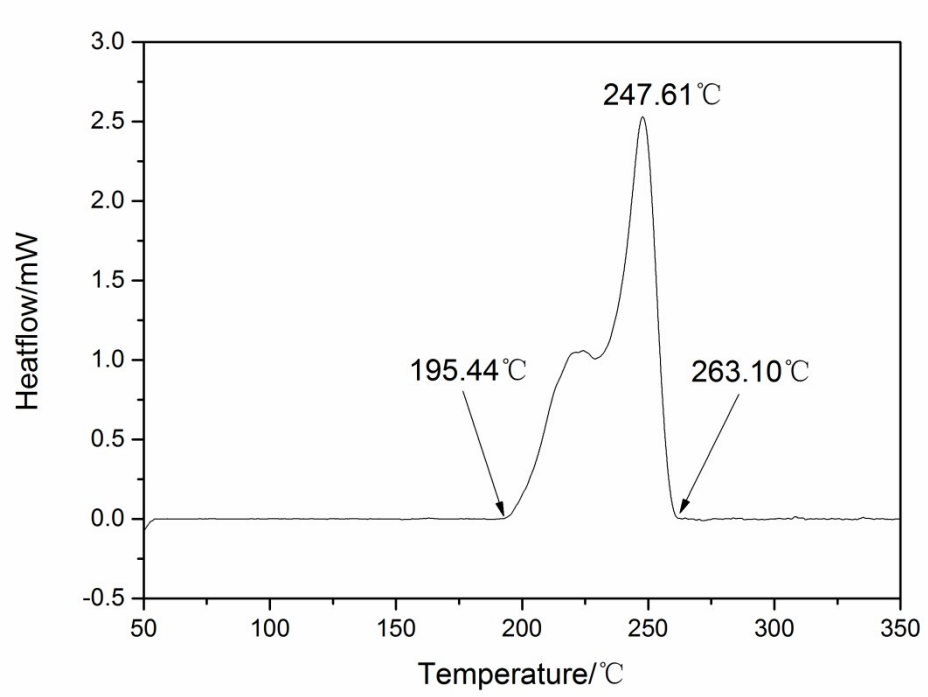

Figure S31 DSC curve of salt **11**

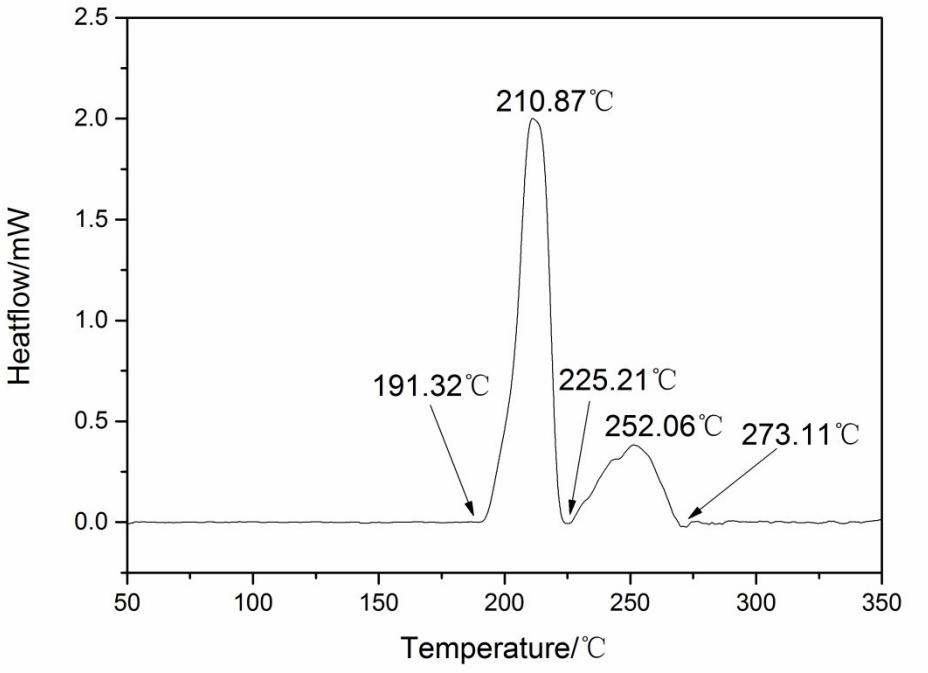

Figure S32 DSC curve of salt **12**

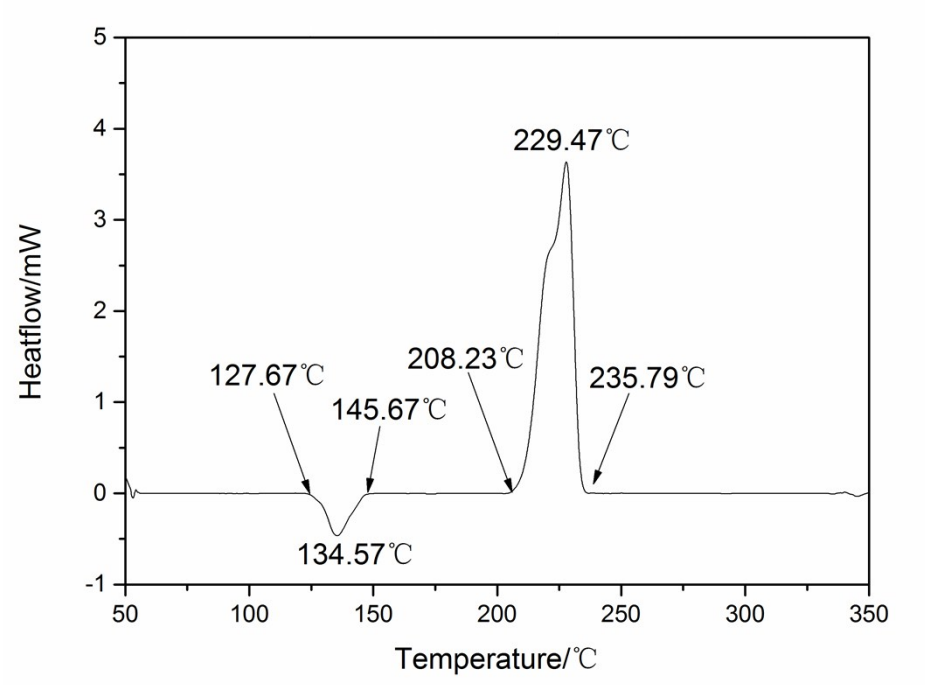

Figure 33 DSC curve of salt **13**

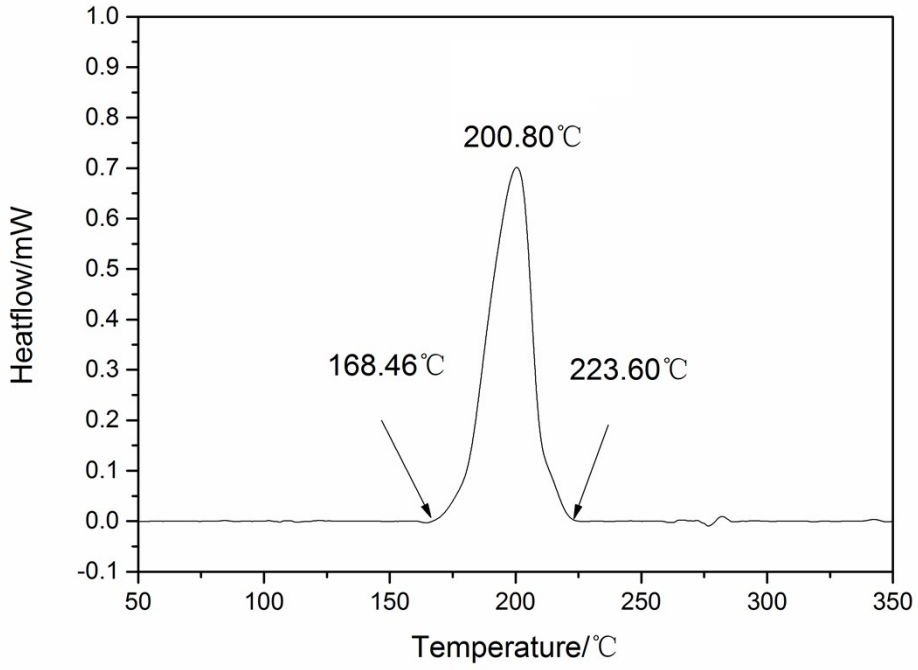

Figure S34 DSC curve of salt **14**

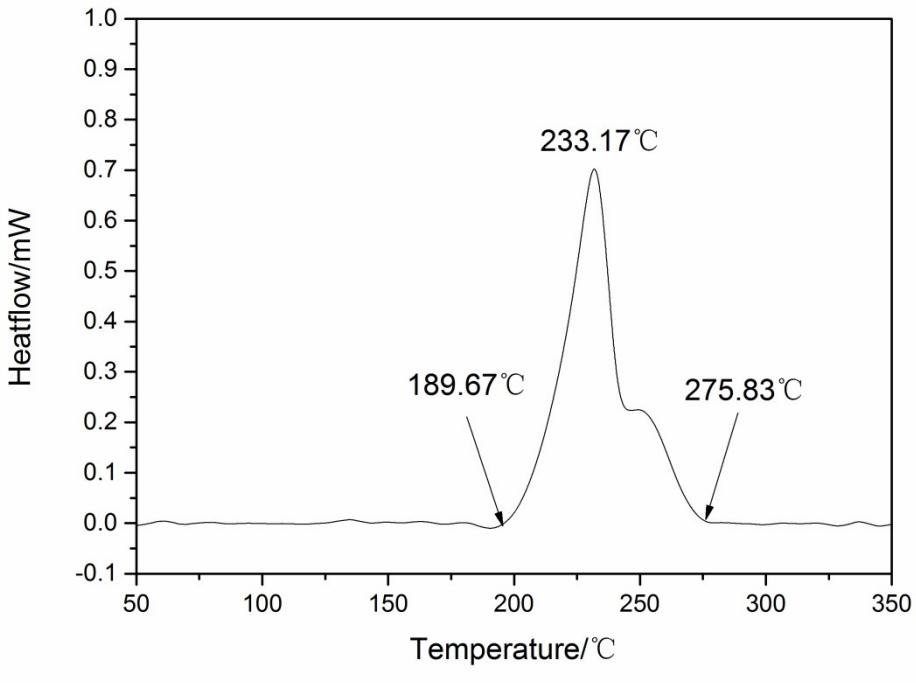

Figure S35 DSC curve of salt **15**

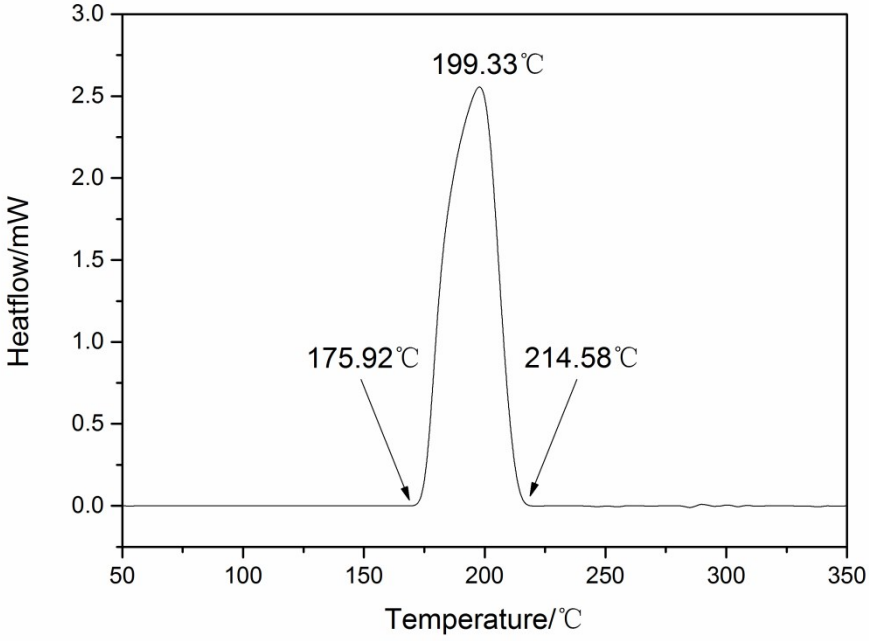

Figure S36 DSC curve of salt **16**