Supporting Information (SI)

Amino-nitramino functionalized triazolotriazines: a good balance between high energy and low sensitivity

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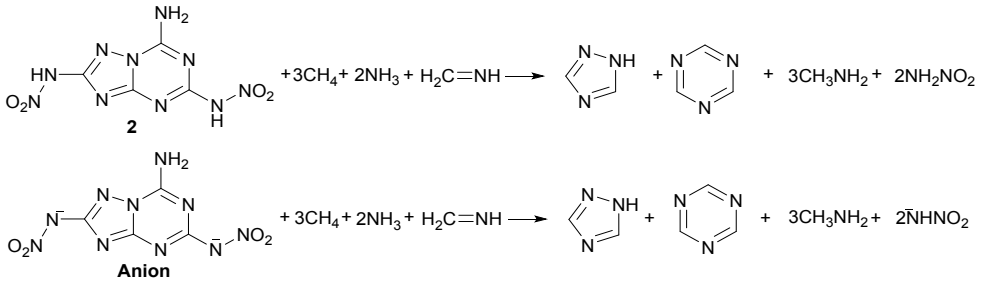
Table of Contents

1. Computational data

All computations were carried out using the Gaussian09 program package.[1] The elementary geometric optimization and the frequency analysis were performed at the level of the Becke three parameter, Lee-Yan-Parr (B3LYP)[2] functional with the 6-311+G** basis set.[3] 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.[4] 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 (Scheme S1).



Scheme S1. Isodesmic and tautomeric reactions to compute the HOF.

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

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

$\Delta_f H_R$ and $\Delta_f H_P$ are the HOF of the reactants and products at 298 K, respectively, and ΔH_{298} can be calculated from the following expression, see Equation (2).

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

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 (1), apart from target compound, all the others are called reference compounds. The HOF of reference compounds are available either from experiments[5] or from the high-level computing such as CBS-4M.

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

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

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

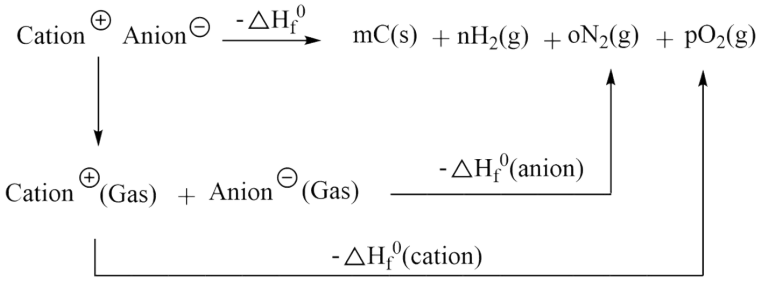


Fig. S1 Born−Haber Cycle for the Formation of Energetic Salts.

Based on Born-Haber energy cycles, the heat of formation of a salt can be simplified and expressed as Equation (3), in which ΔH_L is the lattice energy of the salt. This quantity could be predicted by the formula suggested by Jenkins et al (Equation (4)), in which n_M and n_X depend on the nature of the ions Mp^+ and Xq^-, respectively. The equation for the lattice potential energy, U_{POT}, takes the form of equation (5), where ρ_m (g cm^{-3}) is the density, M_m (g) is the chemical formula mass of the ionic material and the coefficients γ (kJ mol^{-1} cm) and δ (kJ mol^{-1}) are assigned literature values.

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]
2	-1003.27	347.17	42.35	544.93
CH_4	-40.53	112.26	10.04	-74.6[e]
NH_3	-56.58	86.27	10.05	-45.9[e]
CNH_3	-94.66	100.29	10.19	69.0[f]
CH_3NH_2	-95.89	160.78	11.64	-22.5[e]
NH_2NO_2	-261.12	98.79	12.39	-3.9[e]
$NHNO_2^-$	-260.57	65.76	11.37	-120.22[g]
	-242.32	150.39	12.06	192.7[g]
	-280.44	164.06	13.6	224.7[g]

[a] Total energy calculated by B3LYP/6-311+G** method (a.u=2625.5 kJ mol^{-1}); [b] zero-point correction (kJ mol^{-1}); [c] thermal correction to enthalpy (kJ mol^{-1}); [d] heat of formation (kJ mol^{-1}); [e] D. R. Lide, CRC Handbook of Chemistry and Physics, 84th Edition (2003-2004), CRC Press/Taylor and Francis, Boca Raton, FL; [f] Ref. 5; [g] calculated by CBS-4 Enthalpy.

Table S2 Natural Population Analysis of **1**

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.55647	1.99946	3.40740	0.03667	5.44353
N	2	-0.57060	1.99939	5.55359	0.01762	7.57060
N	3	-0.29034	1.99919	5.26132	0.02982	7.29034
N	4	-0.42164	1.99941	5.39917	0.02306	7.42164
C	5	0.59800	1.99929	3.36762	0.03509	5.40200
N	6	-0.58253	1.99929	5.56495	0.01829	7.58253
C	7	0.65529	1.99933	3.31578	0.02959	5.34471
N	8	-0.62517	1.99933	5.60753	0.01831	7.62517
C	9	0.61524	1.99936	3.34815	0.03725	5.38476
N	10	-0.77209	1.99939	5.75619	0.01651	7.77209
N	11	-0.79096	1.99938	5.77348	0.01810	7.79096
N	12	-0.76889	1.99940	5.75502	0.01448	7.76889
H	13	0.39955	0.00000	0.59819	0.00226	0.60045
H	14	0.39549	0.00000	0.60227	0.00225	0.60451
H	15	0.39445	0.00000	0.60315	0.00239	0.60555
H	16	0.38825	0.00000	0.60936	0.00238	0.61175
H	17	0.40739	0.00000	0.59036	0.00225	0.59261
H	18	0.41208	0.00000	0.58586	0.00206	0.58792

Table S3 Natural Population Analysis of **2**

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.52384	1.99930	3.43773	0.03913	5.47616
N	2	-0.53304	1.99932	5.51489	0.01883	7.53304
N	3	-0.27063	1.99910	5.24218	0.02935	7.27063
N	4	-0.34957	1.99937	5.32748	0.02272	7.34957
C	5	0.58942	1.99923	3.37495	0.03641	5.41058
N	6	-0.53876	1.99924	5.52042	0.01911	7.53876
C	7	0.65409	1.99927	3.31611	0.03053	5.34591
N	8	-0.55140	1.99923	5.53290	0.01927	7.55140
C	9	0.59591	1.99922	3.36674	0.03814	5.40409
N	10	-0.43406	1.99924	5.41087	0.02395	7.43406
N	11	-0.42930	1.99922	5.40710	0.02297	7.42930
N	12	-0.74034	1.99937	5.72764	0.01333	7.74034

N	13	0.62256	1.99962	4.32033	0.05750	6.37744
O	14	-0.38903	1.99979	6.37381	0.01543	8.38903
O	15	-0.35245	1.99978	6.33740	0.01527	8.35245
N	16	0.62333	1.99962	4.31910	0.05795	6.37667
O	17	-0.34267	1.99978	6.32725	0.01565	8.34267
O	18	-0.38704	1.99979	6.37166	0.01558	8.38704
H	19	0.42814	0.00000	0.56910	0.00276	0.57186
H	20	0.43066	0.00000	0.56666	0.00267	0.56934
H	21	0.42911	0.00000	0.56880	0.00209	0.57089
H	22	0.42125	0.00000	0.57654	0.00220	0.57875

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2. Crystallographic data and refinement parameters of 2•2H_2O and 4•3H_2O

Table S4 Crystallographic data and refinement parameters

	2·2H_2O	**4**·3H_2O
CCDC number	1584074	1580294
Formula	$C_4H_8N_{10}O_6$	$C_4H_{16}N_{12}O_7$
weight [g mol^{-1}]	292.20	344.29
Temperature [K]	173	173
Crystal system	Orthorhombic	Monoclinic
Space group	*Pca*2$_1$	*P*2$_1$/*c*
Crystal size [mm]	0.330 x 0.160 x 0.020	0.310 x 0.140 x 0.080
a [Å]	8.9661(7)	8.8384(9)
b [Å]	6.7936(6)	20.599(2)
c [Å]	18.1976(17)	7.5457(8)
α [°]	90	90
β [°]	90	90.749(4)
γ [°]	90	90
Cell volume [Å^3]	1108.45(17)	1373.7(3)
Z	4	4
ρ_{calc} [g cm^{-3}]	1.751	1.665
μ [mm^{-1}]	0.159	0.151
F (000)	600	720
θ range [°]	3.743-25.490	2.875-25.367
index ranges	-10<=h<=10 -8<=k<=7 -22<=l<=22	-8<=h<=10 -24<=k<=24 -9<=l<=8
Reflns collected	9606	7267
indep ref./ R_{int}	2045/ 0.0971	2492/ 0.0769
Goodness-of-fit on F^2	1.096	1.034
Final *R* indices [I>2sigma(I)]	R_1 = 0.0707, wR_2 = 0.1648	R_1 = 0.0551, wR_2 = 0.1106
R indices (all data)	R_1 = 0.1092, wR_2 = 0.1894	R_1 = 0.1104, wR_2 = 0.1321
largest diff. peak / hole [e Å^3]	0.377/ -0.396	0.301/ -0.300

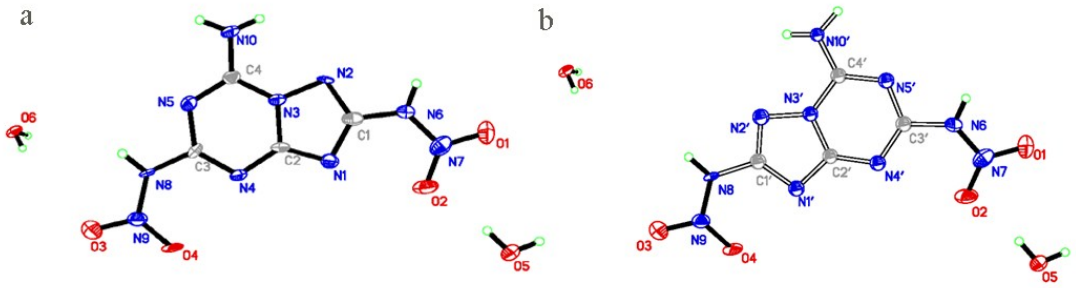

Fig. S2 Single-crystal X-ray structure of **2**·2H_2O (ellipsoids are set at 50% probability) (a) The part of the 2-fold disordered atoms with higher occupancy (0.78); (b) The part of the 2-fold disordered atoms with lower occupancy (0.22)

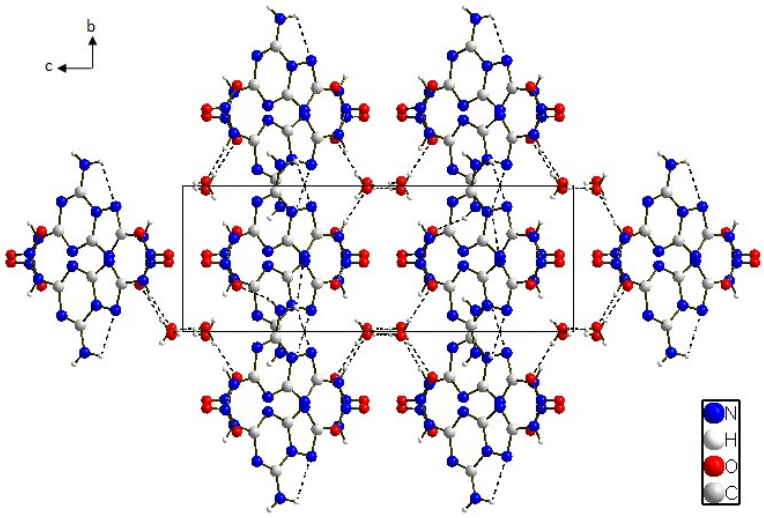

Fig. S3 Packing diagram of **2**·2H_2O (with lower occupancy (0.22)) viewed down the a-axis. Unit cell indicated and dashed lines represent hydrogen bonding.

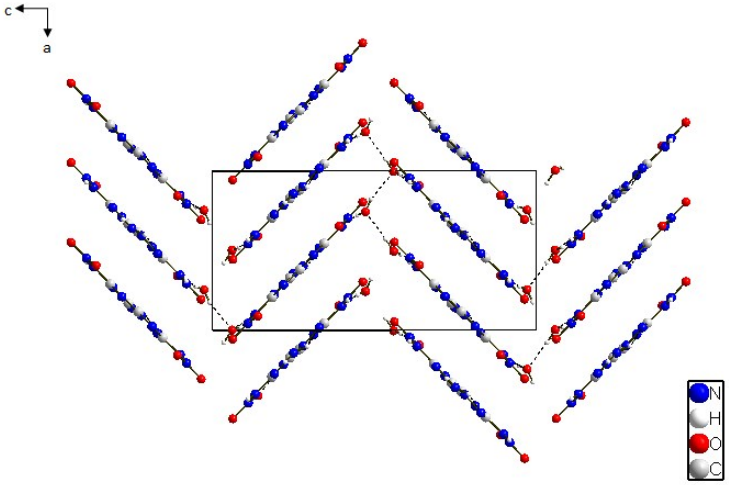

Fig. S4 Packing diagram of **2**·2H_2O (with lower occupancy (0.22)) viewed down the b-axis. Unit cell indicated and dashed lines represent hydrogen bonding.

Table S5 Bond lengths [Å] and angles [°] of compound **2**·2H_2O

N(6)-N(7)	1.347(15)	C(2)-N(4)	1.35(2)
N(6)-C(1)	1.395(15)	N(4)-C(3)	1.335(19)
N(6)-C(3')	1.40(2)	C(3)-N(5)	1.364(19)
N(6)-H(6A)	0.85(3)	N(5)-C(4)	1.343(18)
N(7)-O(1)	1.236(16)	C(4)-N(10)	1.311(15)
N(7)-O(2)	1.240(14)	N(10)-H(10A)	0.86(3)
N(8)-N(9)	1.337(13)	N(10)-H(10B)	0.86(3)
N(8)-C(1')	1.39(2)	N(1')-C(2')	1.34(4)
N(8)-C(3)	1.396(14)	N(1')-C(1')	1.35(3)
N(8)-H(8A)	0.85(3)	C(1')-N(2')	1.31(3)
N(9)-O(3)	1.223(15)	C(1')-C(2')	2.03(4)
N(9)-O(4)	1.229(12)	N(2')-N(3')	1.38(3)
O(5)-H(5C)	0.8501	N(3')-C(4')	1.36(2)
O(5)-H(5D)	0.8499	N(3')-C(2')	1.37(2)
O(6)-H(6C)	0.82(3)	C(2')-N(4')	1.35(4)
O(6)-H(6D)	0.82(3)	N(4')-C(3')	1.35(3)
N(1)-C(2)	1.34(2)	C(3')-N(5')	1.37(3)
N(1)-C(1)	1.349(19)	N(5')-C(4')	1.34(3)
C(1)-N(2)	1.318(17)	C(4')-N(10')	1.32(3)
N(2)-N(3)	1.379(16)	N(10')-H(10C)	0.86(3)
N(3)-C(4)	1.353(13)	N(10')-H(10D)	0.87(3)
N(3)-C(2)	1.365(13)		
N(7)-N(6)-C(1)	125.0(11)	N(10)-C(4)-N(5)	122.5(12)
N(7)-N(6)-C(3')	132(2)	N(10)-C(4)-N(3)	119.8(11)
N(7)-N(6)-H(6A)	118(8)	N(5)-C(4)-N(3)	117.8(11)
C(1)-N(6)-H(6A)	117(8)	C(4)-N(10)-H(10A)	114(6)
C(3')-N(6)-H(6A)	110(8)	C(4)-N(10)-H(10B)	115(6)
O(1)-N(7)-O(2)	126.3(12)	H(10A)-N(10)-H(10B)	131(10)
O(1)-N(7)-N(6)	115.2(11)	C(2')-N(1')-C(1')	98(2)
O(2)-N(7)-N(6)	118.5(12)	N(2')-C(1')-N(1')	124(3)
N(9)-N(8)-C(1')	122(3)	N(2')-C(1')-N(8)	112(4)
N(9)-N(8)-C(3)	127.8(11)	N(1')-C(1')-N(8)	124(4)
N(9)-N(8)-H(8A)	120(8)	N(2')-C(1')-C(2')	82.7(18)
C(1')-N(8)-H(8A)	118(8)	N(1')-C(1')-C(2')	40.8(15)
C(3)-N(8)-H(8A)	112(8)	N(8)-C(1')-C(2')	165(4)
O(3)-N(9)-O(4)	123.4(10)	C(1')-N(2')-N(3')	96(2)

O(3)-N(9)-N(8)	115.7(10)	C(4')-N(3')-C(2')	121(3)
O(4)-N(9)-N(8)	120.9(11)	C(4')-N(3')-N(2')	127(3)
H(5C)-O(5)-H(5D)	108.6	C(2')-N(3')-N(2')	111(2)
H(6C)-O(6)-H(6D)	101(10)	N(1')-C(2')-N(4')	127(3)
C(2)-N(1)-C(1)	99.2(12)	N(1')-C(2')-N(3')	111(3)
N(2)-C(1)-N(1)	121.7(12)	N(4')-C(2')-N(3')	123(3)
N(2)-C(1)-N(6)	113.9(12)	N(1')-C(2')-C(1')	41.3(16)
N(1)-C(1)-N(6)	124.5(13)	N(4')-C(2')-C(1')	167(4)
C(1)-N(2)-N(3)	97.5(9)	N(3')-C(2')-C(1')	69.4(18)
C(4)-N(3)-C(2)	121.8(12)	C(3')-N(4')-C(2')	114(3)
C(4)-N(3)-N(2)	127.1(10)	N(4')-C(3')-N(5')	126(3)
C(2)-N(3)-N(2)	111.1(12)	N(4')-C(3')-N(6)	121(3)
N(1)-C(2)-N(4)	126.9(11)	N(5')-C(3')-N(6)	113(3)
N(1)-C(2)-N(3)	110.5(16)	C(4')-N(5')-C(3')	119(3)
N(4)-C(2)-N(3)	122.6(15)	N(10')-C(4')-N(5')	123(3)
C(3)-N(4)-C(2)	112.4(12)	N(10')-C(4')-N(3')	119(2)
N(4)-C(3)-N(5)	128.2(12)	N(5')-C(4')-N(3')	118(2)
N(4)-C(3)-N(8)	121.5(14)	C(4')-N(10')-H(10C)	113(7)
N(5)-C(3)-N(8)	110.3(12)	C(4')-N(10')-H(10D)	113(7)
C(4)-N(5)-C(3)	117.1(11)	H(10C)-N(10')-H(10D)	129(10)

Table S6 Hydrogen bonds of compound **2**·2H_2O [Å and °]

D-H···A	d(D-H)/ Å	d(H•••A)/ Å	d(D•••A)/ Å	<(DHA)/ °	comment
O(5)-H(5C)···O(6)^{iv}	0.85	1.89	2.734(15)	172	Inter
O(5)-H(5D)···O(2)	0.85	2.01	2.854(12)	171	Inter
N(6)-H(6A)···O(5)^{iii}	0.85(10)	1.89(9)	2.736(13)	179(14)	Inter
O(6)-H(6C)···O(5)^{v}	0.83(7)	1.99(8)	2.781(15)	161(9)	Inter
O(6)-H(6D)···O(4)^{i}	0.82(8)	2.06(8)	2.880(11)	175(12)	Inter
N(8)-H(8A)···O(6)^{ii}	0.85(8)	1.89(9)	2.735(12)	170(9)	Inter
N(10)-H(10A)···O(4)^{iii}	0.86(9)	2.49(11)	3.300(17)	158(9)	Inter
N(10)-H(10A)···N(4)^{iii}	0.86(9)	2.25(7)	2.901(18)	133(8)'	Inter
N(10)-H(10B)···N(1)^{iii}	0.86(14)	2.48(9)	2.962(19)	117(8)	Inter
N(10)-H(10B)···N(2)	0.86(14)	2.46(10)	2.836(18)	107(7)'	Intra

i: -x,1-y,-1/2+z; *ii*: -x,2-y,1/2+z; *iii*: x,1+y,z; *iv*: 1/2+x,1-y,1+z; *v*: x,1+y,-1+z

Table S7 Bond lengths [Å] and angles [°] of compound **4**·3H_2O

C(1)-N(2)	1.331(4)	N(9)-O(4)	1.260(3)
C(1)-N(6)	1.380(4)	N(10)-H(10A)	0.86(3)

C(1)-N(1)	1.380(4)	N(10)-H(10B)	0.85(4)
C(2)-N(1)	1.326(4)	N(11)-H(11A)	0.902(19)
C(2)-N(4)	1.344(4)	N(11)-H(11B)	0.893(19)
C(2)-N(3)	1.373(4)	N(11)-H(11C)	0.902(19)
C(3)-N(4)	1.343(4)	N(11)-H(11D)	0.898(19)
C(3)-N(5)	1.359(4)	N(12)-H(12A)	0.96(4)
C(3)-N(8)	1.384(4)	N(12)-H(12B)	0.99(4)
C(4)-N(10)	1.318(4)	N(12)-H(12C)	0.86(4)
C(4)-N(5)	1.334(4)	N(12)-H(12D)	0.98(5)
C(4)-N(3)	1.358(4)	O(5)-H(5E)	0.837(18)
N(2)-N(3)	1.385(4)	O(5)-H(5F)	0.827(18)
N(6)-N(7)	1.318(3)	O(6)-H(6E)	0.84(2)
N(7)-O(1)	1.257(3)	O(6)-H(6F)	0.868(19)
N(7)-O(2)	1.257(3)	O(7)-H(7E)	0.816(18)
N(8)-N(9)	1.324(4)	O(7)-H(7F)	0.827(18)
N(9)-O(3)	1.244(3)		
N(2)-C(1)-N(6)	130.0(3)	N(9)-N(8)-C(3)	121.5(3)
N(2)-C(1)-N(1)	116.1(3)	O(3)-N(9)-O(4)	119.3(3)
N(6)-C(1)-N(1)	113.9(3)	O(3)-N(9)-N(8)	124.7(3)
N(1)-C(2)-N(4)	128.8(3)	O(4)-N(9)-N(8)	115.9(3)
N(1)-C(2)-N(3)	107.8(3)	C(4)-N(10)-H(10A)	120(2)
N(4)-C(2)-N(3)	123.4(3)	C(4)-N(10)-H(10B)	118(3)
N(4)-C(3)-N(5)	126.1(3)	H(10A)-N(10)-H(10B)	123(4)
N(4)-C(3)-N(8)	124.9(3)	H(11A)-N(11)-H(11B)	110.2(17)
N(5)-C(3)-N(8)	108.9(3)	H(11A)-N(11)-H(11C)	108.3(16)
N(10)-C(4)-N(5)	124.3(3)	H(11B)-N(11)-H(11C)	109.6(17)
N(10)-C(4)-N(3)	118.5(3)	H(11A)-N(11)-H(11D)	109.7(17)
N(5)-C(4)-N(3)	117.2(3)	H(11B)-N(11)-H(11D)	110.3(17)
C(2)-N(1)-C(1)	104.0(3)	H(11C)-N(11)-H(11D)	108.7(17)
C(1)-N(2)-N(3)	99.9(2)	H(12A)-N(12)-H(12B)	105(3)
C(4)-N(3)-C(2)	120.7(3)	H(12A)-N(12)-H(12C)	109(4)
C(4)-N(3)-N(2)	126.9(3)	H(12B)-N(12)-H(12C)	110(4)
C(2)-N(3)-N(2)	112.2(3)	H(12A)-N(12)-H(12D)	111(3)
C(3)-N(4)-C(2)	112.9(3)	H(12B)-N(12)-H(12D)	117(3)
C(4)-N(5)-C(3)	119.4(3)	H(12C)-N(12)-H(12D)	105(4)
N(7)-N(6)-C(1)	118.0(2)	H(5E)-O(5)-H(5F)	102(3)

O(1)-N(7)-O(2)	119.6(3)	H(6E)-O(6)-H(6F)	98(3)
O(1)-N(7)-N(6)	116.0(3)	H(7E)-O(7)-H(7F)	107(3)
O(2)-N(7)-N(6)	124.4(3)		

Table S8 Hydrogen bonds of compound **4**·3H_2O [Å and °]

D-H···A	d(D-H)/ Å	d(H•••A)/ Å	d(D•••A)/ Å	<(DHA)/ °	comment
O(5)-H(5E)···O(7)	0.84(3)	2.06(3)	2.814(4)	150(4)	Inter
O(5)-H(5F)···N(1)^{iii}	0.83(3)	2.00(3)	2.821(4)	173(3)	Inter
O(6)-H(6E)···O(4)^{iii}	0.84(3)	2.43(5)	2.949(4)	121(5)	Inter
O(6)-H(6E)···O(1)^{v}	0.84(3)	2.27(5)	2.965(4)	141(5)'	Inter
O(6)-H(6F)···O(7)^{iv}	0.87(3)	2.46(3)	3.271(4)	156(3)	Inter
O(7)-H(7E)···N(5)^{vi}	0.82(3)	2.01(3)	2.814(4)	169(4)	Inter
O(7)-H(7F)···O(5)^{vii}	0.82(3)	2.12(3)	2.932(4)	167(3)	Inter
N(10)-H(10A)···O(6)^{i}	0.86(4)	2.01(4)	2.861(5)	167(3)	Inter
N(10)-H(10B)···N(2)	0.85(4)	2.47(4)	2.821(4)	106(3)	Intra
N(10)-H(10B)···O(2)^{i}	0.85(4)	2.10(4)	2.922(4)	163(3)'	Inter
N(11)-H(11A)···O(5)^{i}	0.90(2)	2.06(2)	2.936(4)	164(2)	Inter
N(11)-H(11B)···O(3)^{viii}	0.89(3)	2.22(2)	2.841(4)	127(2)	Inter
N(11)-H(11B)···N(4)^{viii}	0.89(3)	2.14(3)	2.973(4)	157(2)'	Inter
N(11)-H(11C)···O(2)	0.90(2)	2.33(2)	2.972(4)	128(2)	Inter
N(11)-H(11C)···O(2)^{i}	0.90(2)	2.21(3)	2.918(4)	135(2)'	Inter
N(11)-H(11C)···N(2)^{i}	0.90(2)	2.57(2)	3.215(4)	129(2)''	Inter
N(11)-H(11D)···O(3)^{ii}	0.90(3)	2.03(3)	2.921(4)	174(3)	Inter
N(11)-H(11D)···O(4)^{ii}	0.90(3)	2.51(3)	3.167(4)	131(2)'	Inter
N(11)-H(11D)···N(9)^{ii}	0.90(3)	2.61(3)	3.462(4)	158(2)''	Inter
N(12)-H(12A)···N(8)^{ix}	0.96(4)	2.00(4)	2.944(4)	168(3)	Inter
N(12)-H(12B)···O(7)^{iii}	0.99(4)	1.84(4)	2.821(4)	172(3)	Inter
N(12)-H(12C)···N(6)	0.86(4)	2.10(4)	2.923(4)	162(4)	Inter
N(12)-H(12D)···O(4)^{ii}	0.98(4)	2.18(4)	2.975(4)	138(3)	Inter
N(12)-H(12D)···O(1)^{x}	0.98(4)	2.34(4)	2.865(4)	113(3)'	Inter

i: 1-x, 1-y, 1-z; *ii*: -x, 1-y, -z; *iii*: -x, 1-y, 1-z; *iv*: 1-x, 1-y, 2-z; *v*: x, 3/2-y, 1/2+z; *vi*: x, y, 1+z; *vii*: x, 1/2-y, 1/2+z; *viii*: 1+x, y, z; *ix*: -x, 1/2+y, 1/2-z; *x*: x,3/2-y,-1/2+z

3. Mass spectra of compound 2

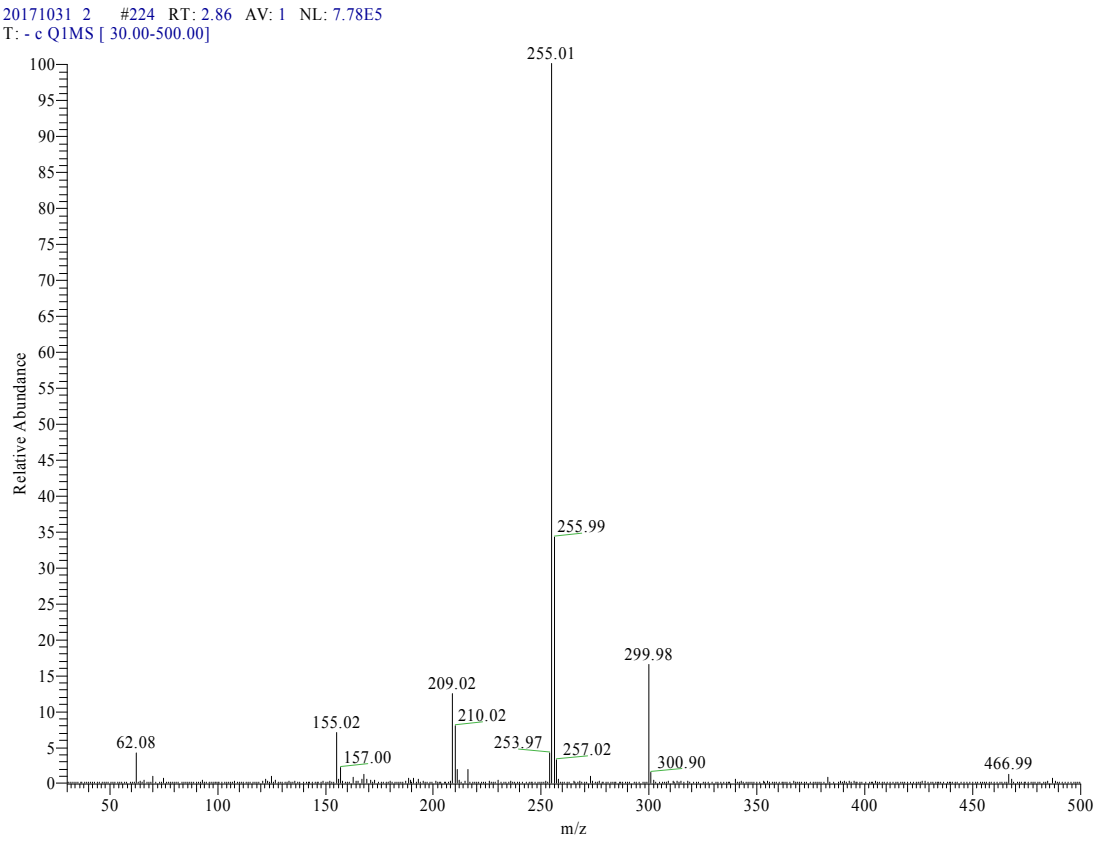

Fig. S5 Mass spectrum of **2**

4. ^{1}H NMR and ^{13}C NMR spectra

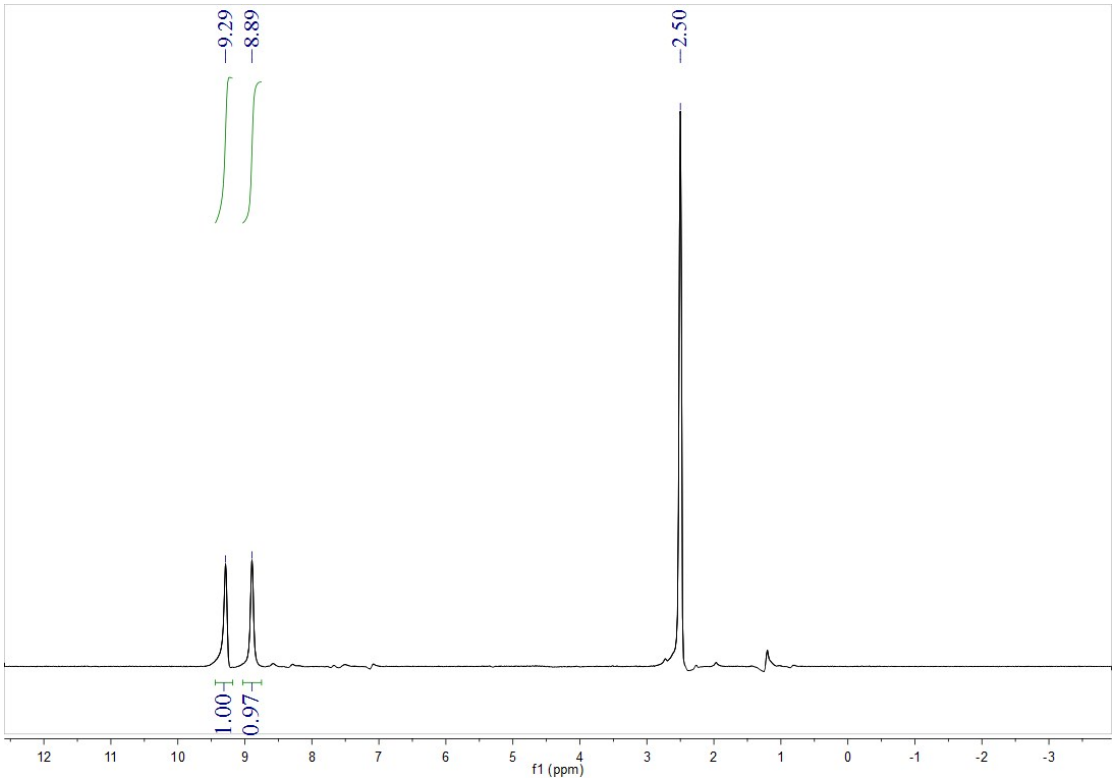

Fig. S6 ^{1}H-NMR spectra (300 MHz) of **2** in DMSO-d_6 at 25°C

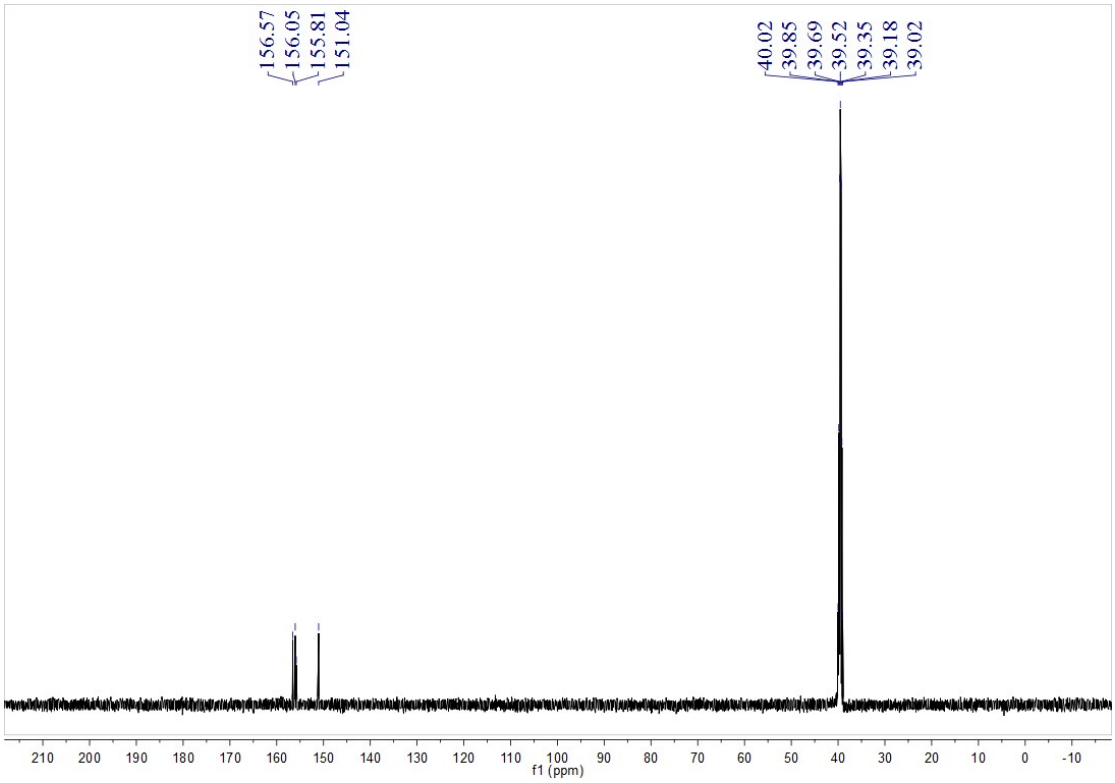

Fig. S7 ^{13}C-NMR spectra (126 MHz) of **2** in DMSO-d_6 at 25°C

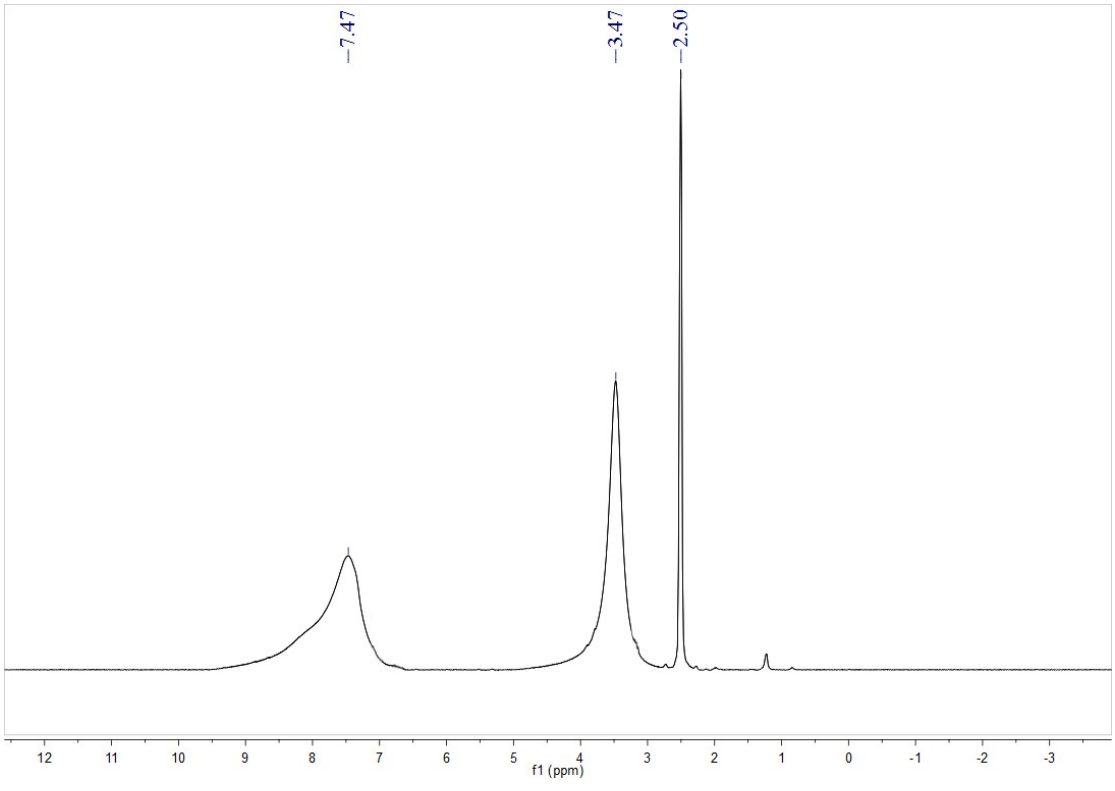

Fig. S8 ^{1}H-NMR spectra (300 MHz) of **4** in DMSO-d_6 at 25°C

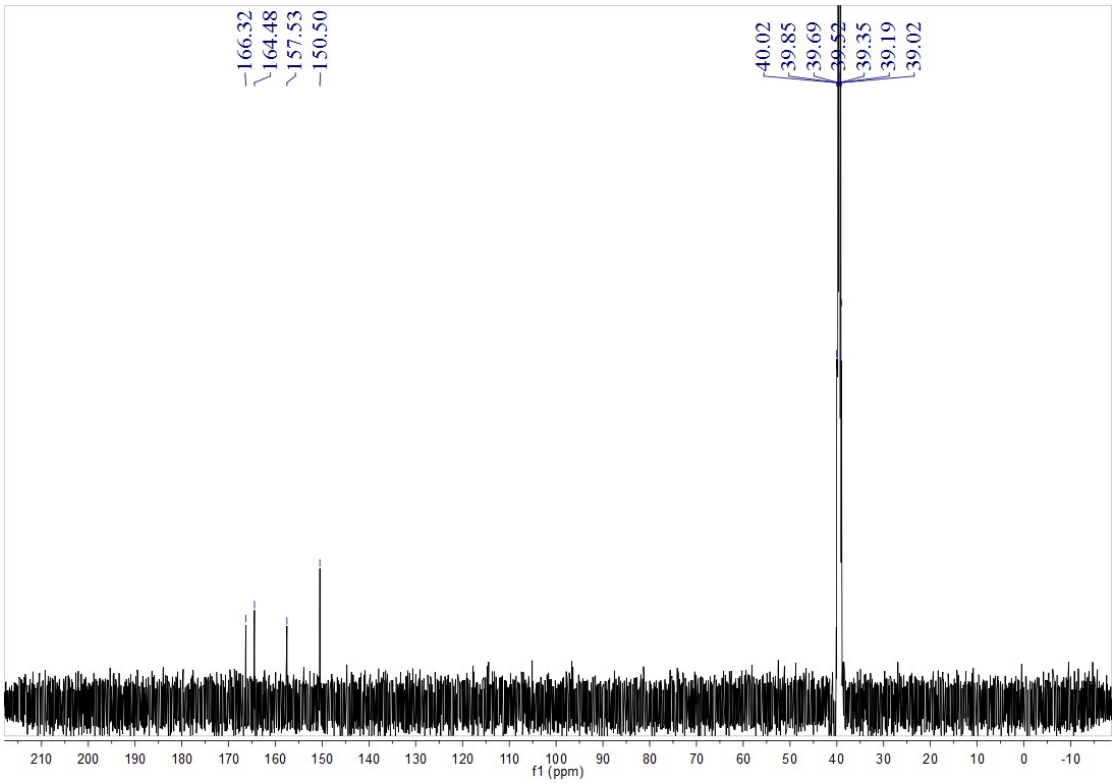

Fig. S9 ^{13}C-NMR spectra (126 MHz) of **4** in DMSO-d_6 at 25°C

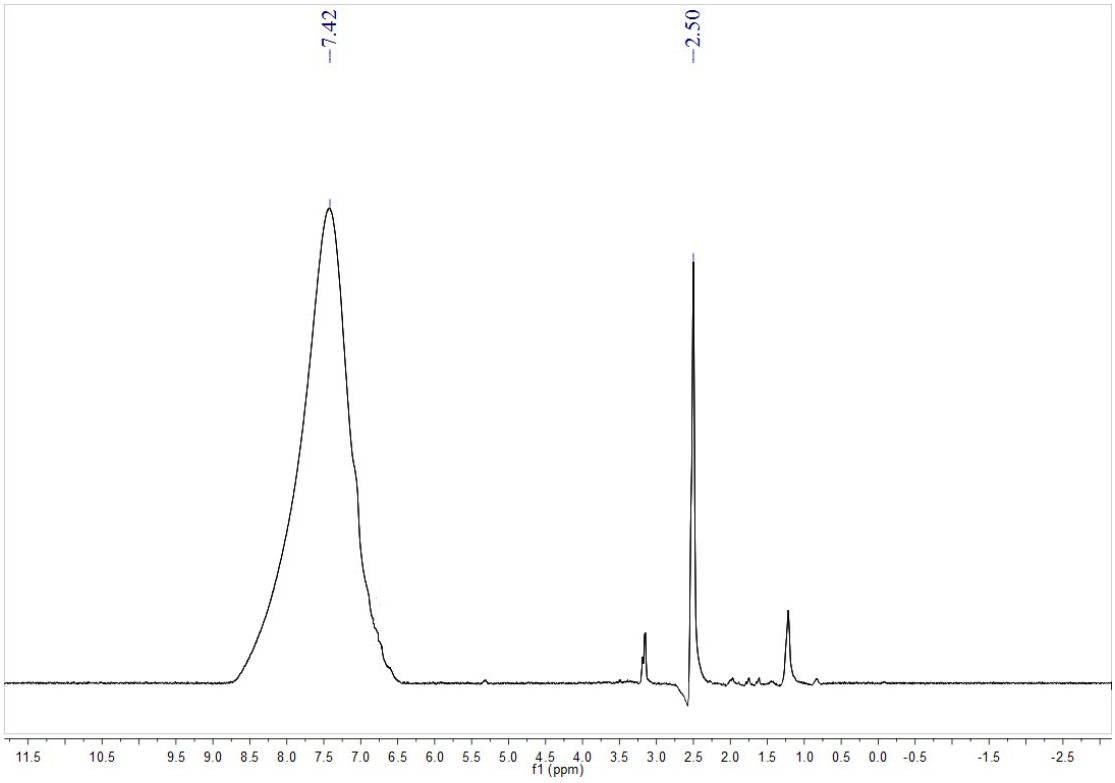

Fig. S10 ^{1}H-NMR spectra (300 MHz) of **5** in DMSO-d_6 at 25°C

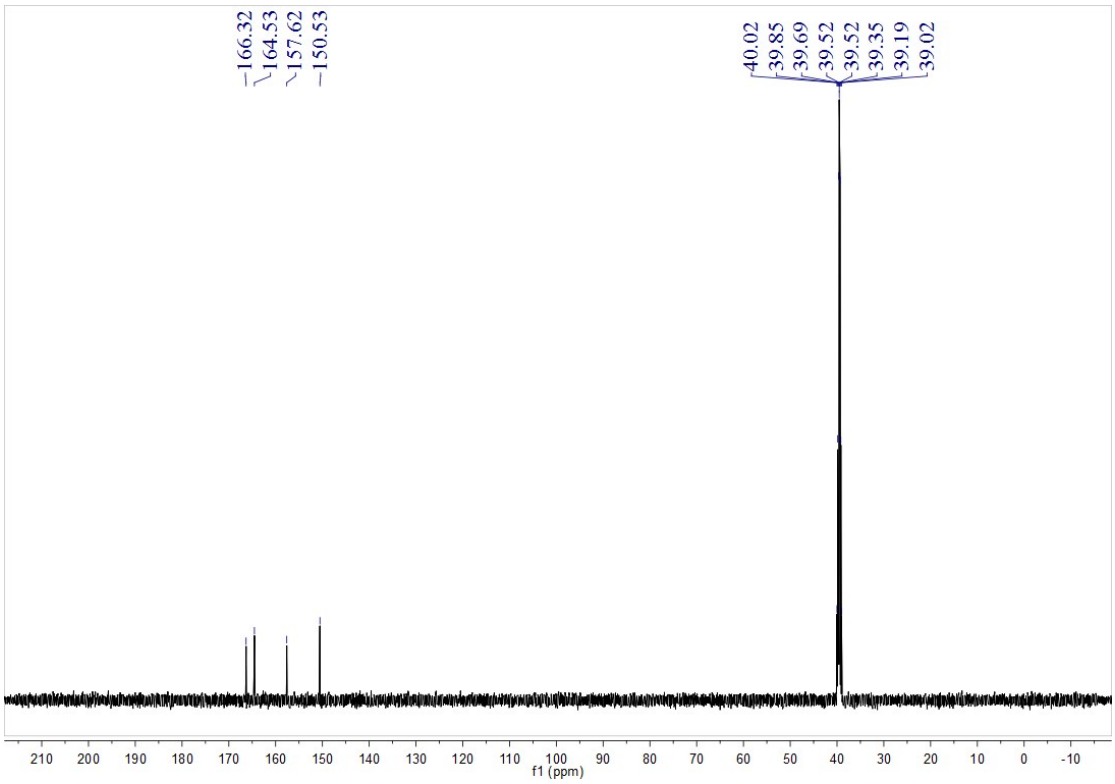

Fig. S11 ^{13}C-NMR spectra (126 MHz) of **5** in DMSO-d_6 at 25°C

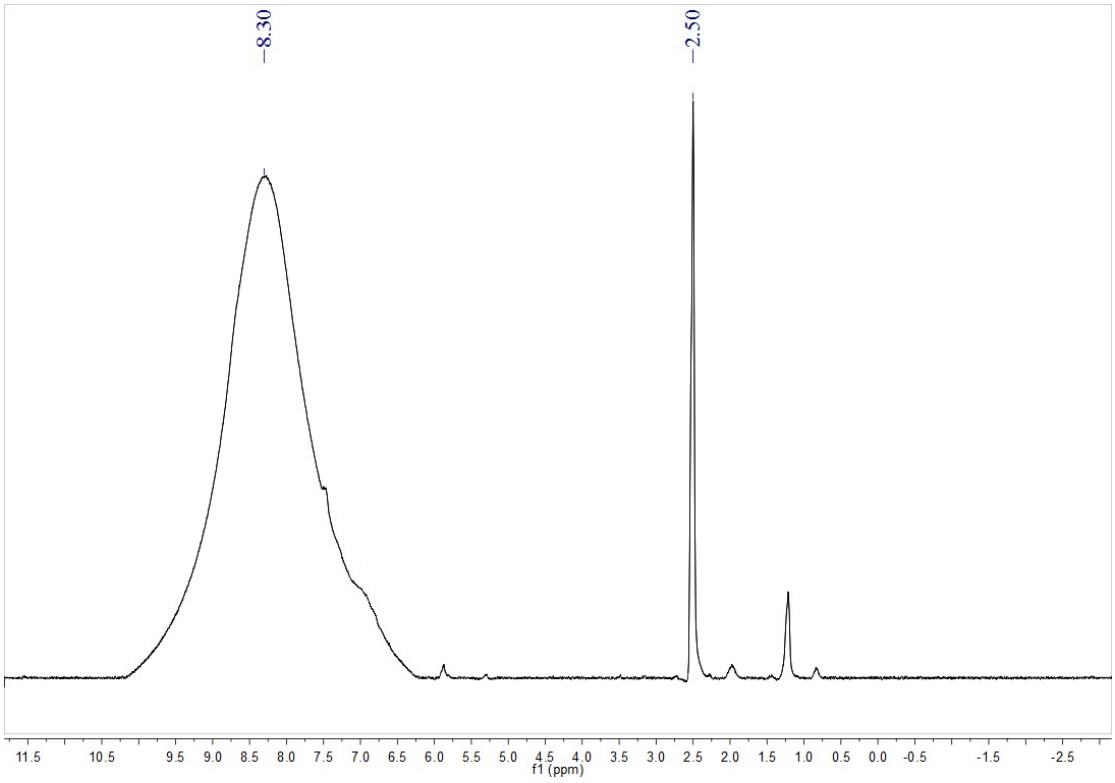

Fig. S12 ^{1}H-NMR spectra (300 MHz) of **6** in DMSO-d_6 at 25°C

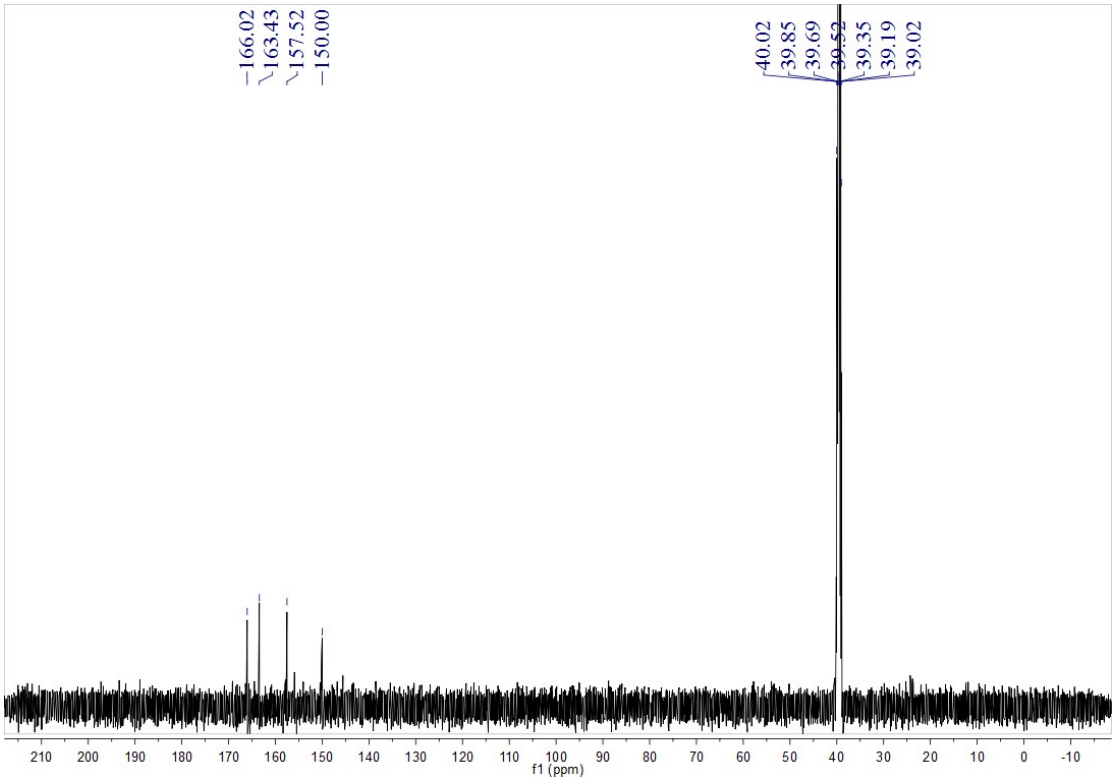

Fig. S13 ^{13}C-NMR spectra (126 MHz) of **6** in DMSO-d_6 at 25°C

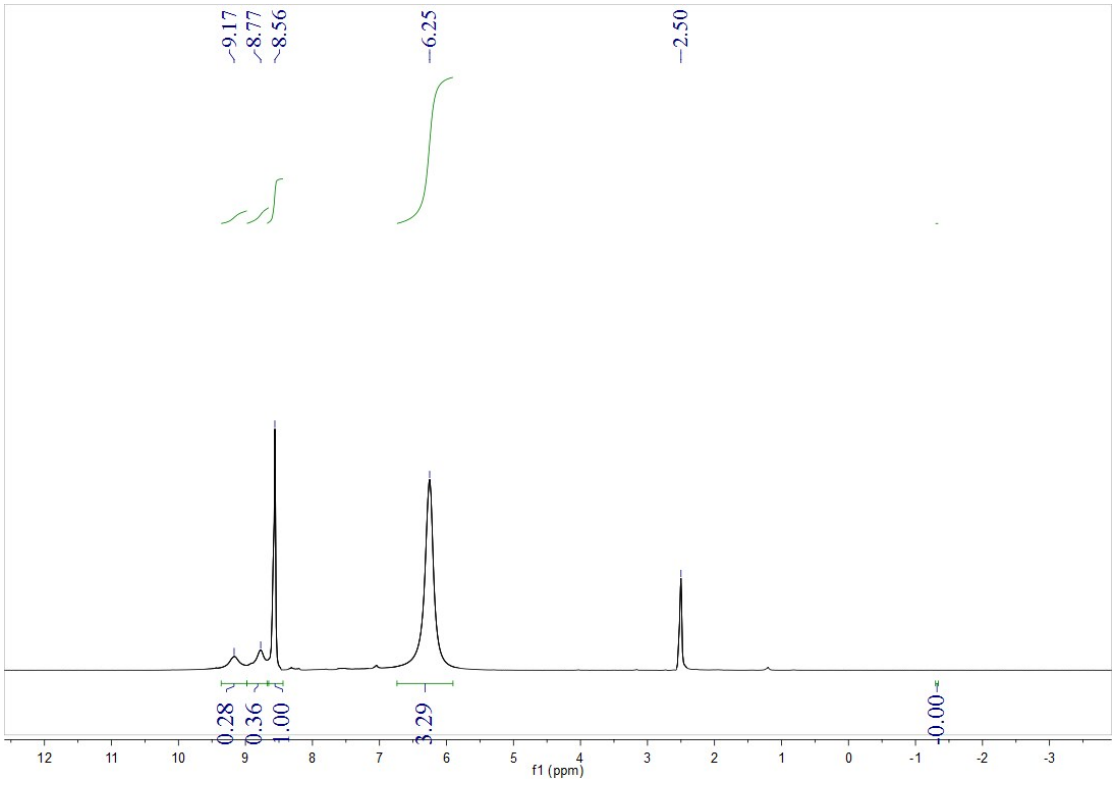

Fig. S14 ^{1}H-NMR spectra (300 MHz) of **7** in DMSO-d_6 at 25°C

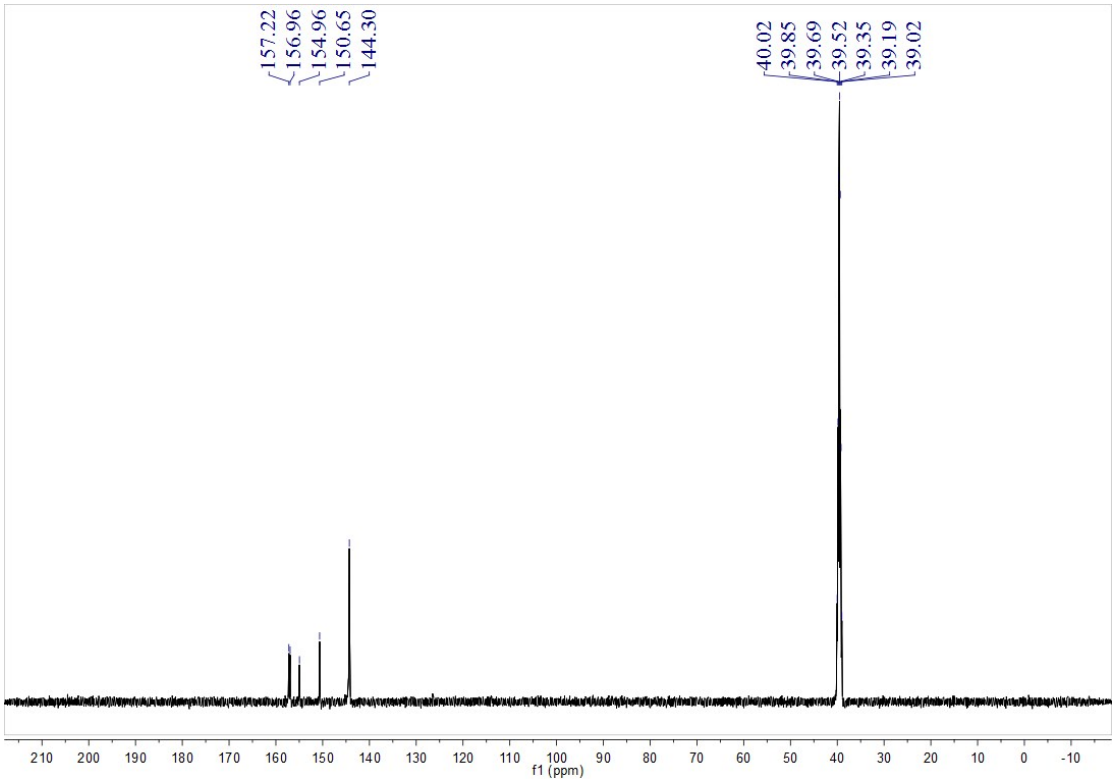

Fig. S15 ^{13}C-NMR spectra (126 MHz) of **7** in DMSO-d_6 at 25°C

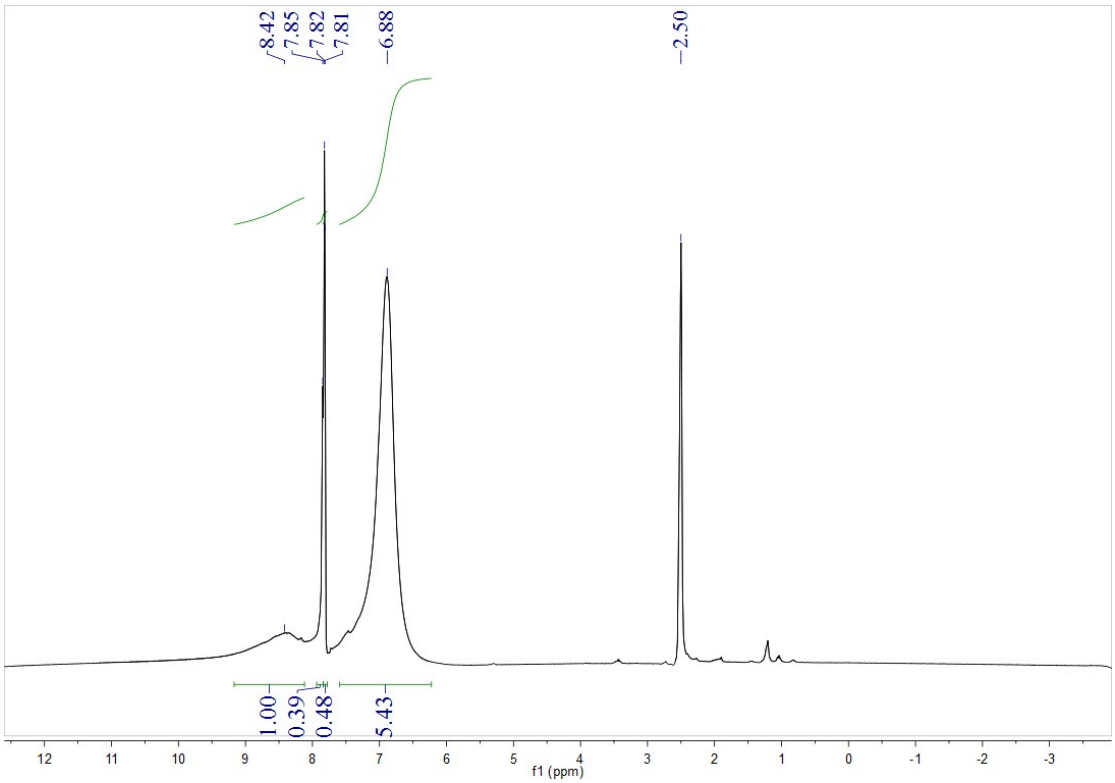

Fig. S16 ^{1}H-NMR spectra (300 MHz) of **8** in DMSO-d_6 at 25°C

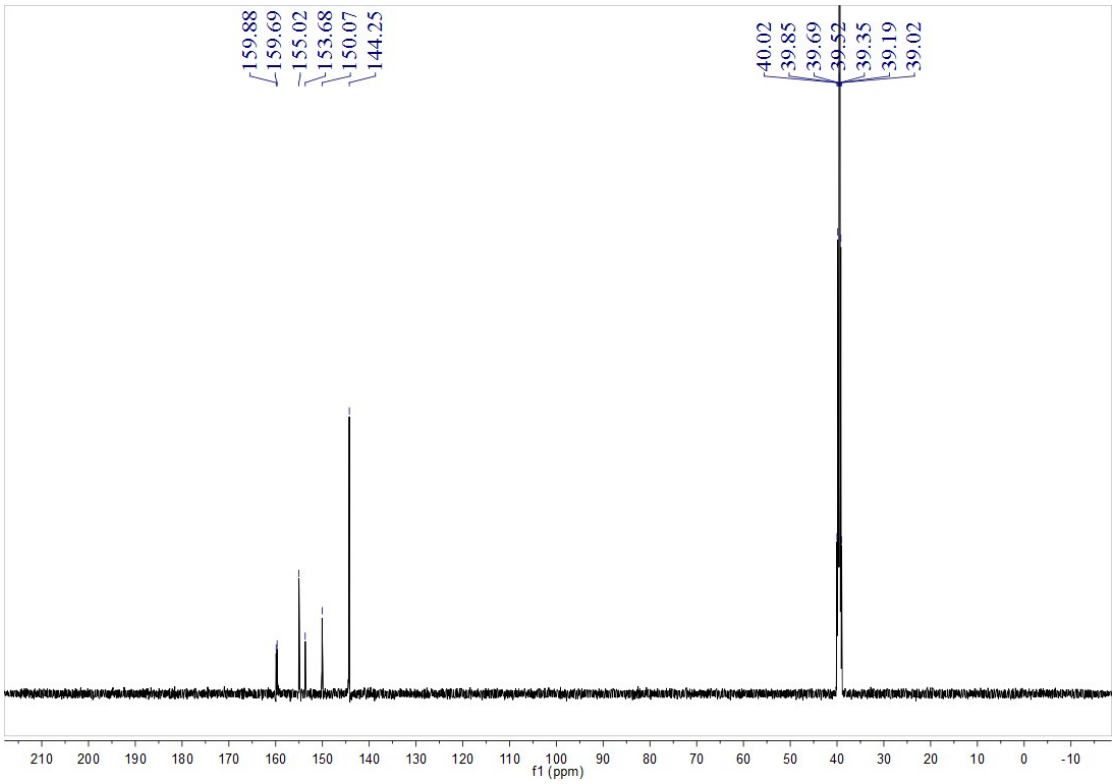

Fig. S17 ^{13}C-NMR spectra (126 MHz) of **8** in DMSO-d_6 at 25°C

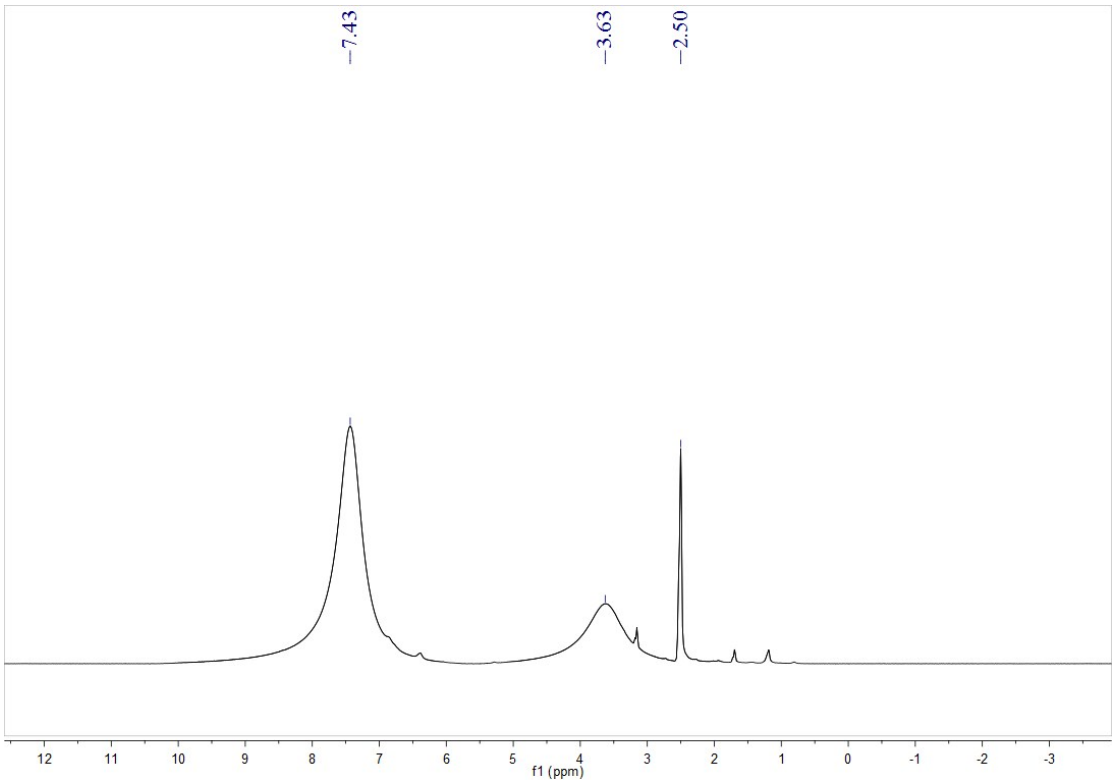

Fig. S18 ^{1}H-NMR spectra (300 MHz) of **9** in DMSO-d_6 at 25°C

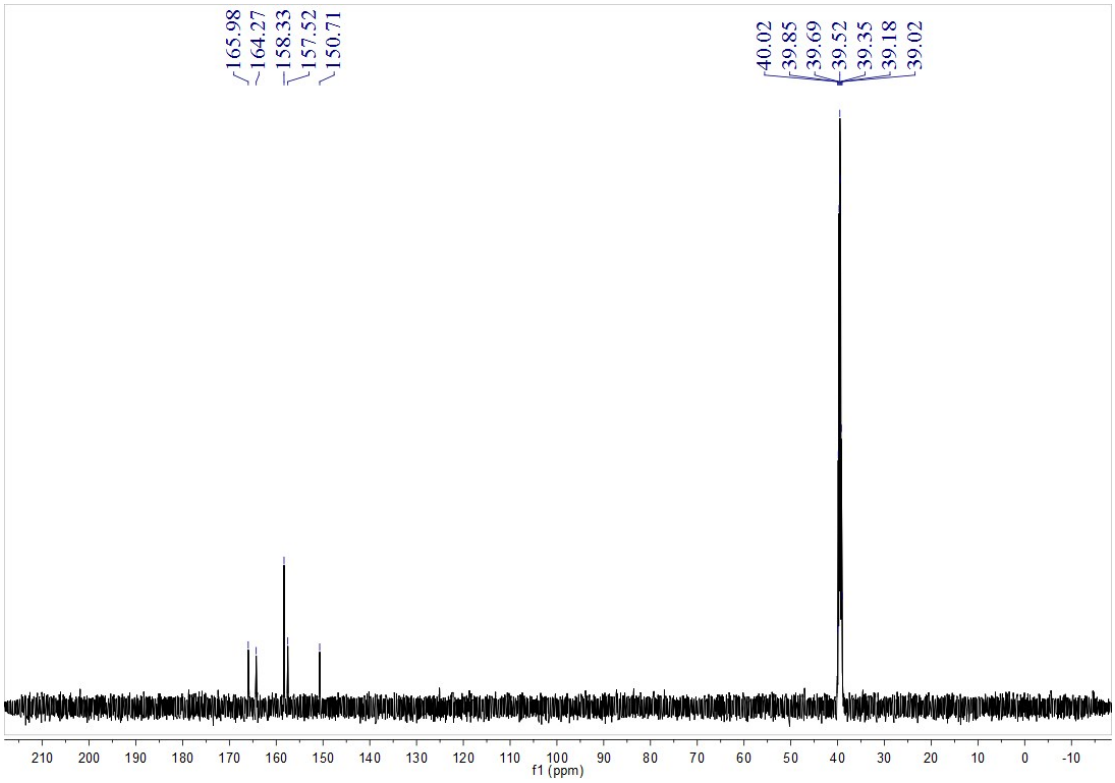

Fig. S19 ^{13}C-NMR spectra (126 MHz) of **9** in DMSO-d_6 at 25°C

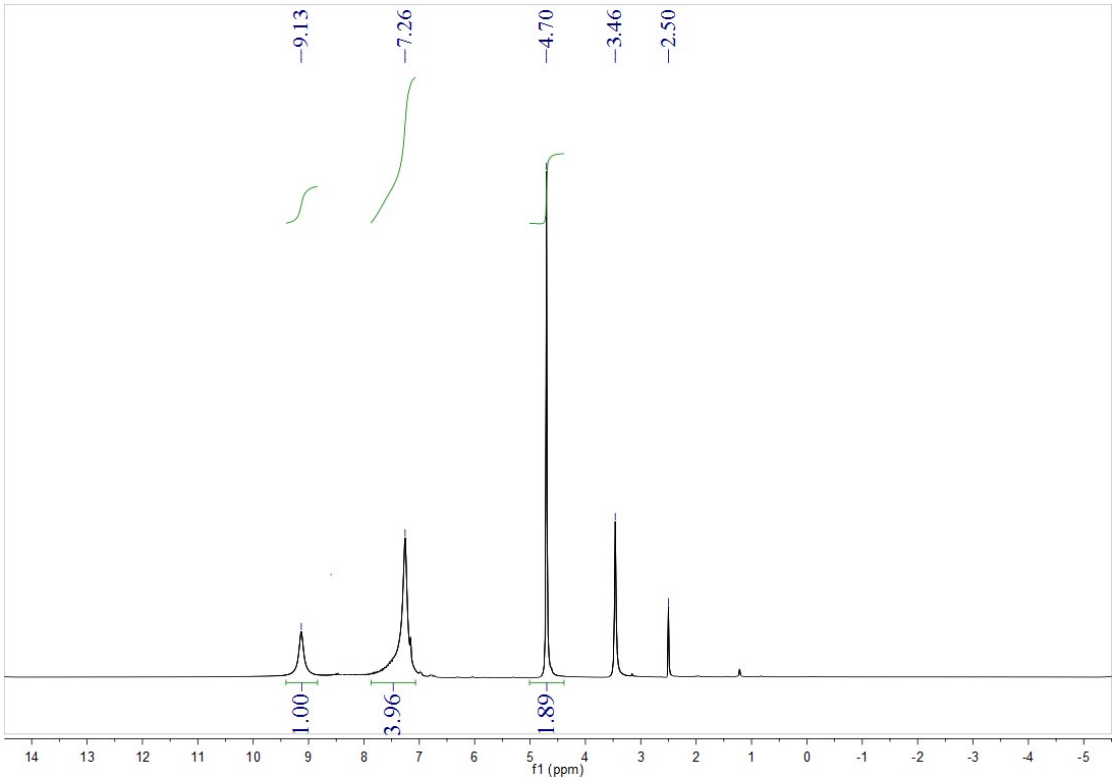

Fig. S20 ^{1}H-NMR spectra (300 MHz) of **11** in DMSO-d_6 at 25°C

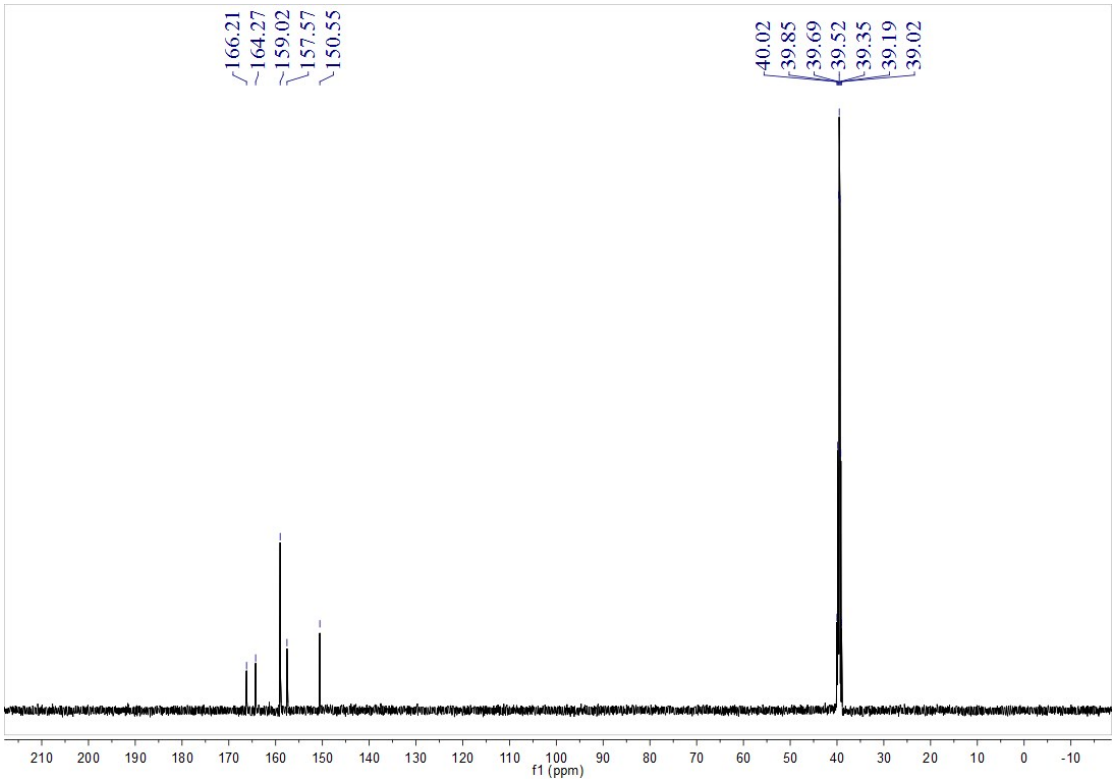

Fig. S21 ^{13}C-NMR spectra (126 MHz) of **11** in DMSO-d_6 at 25°C

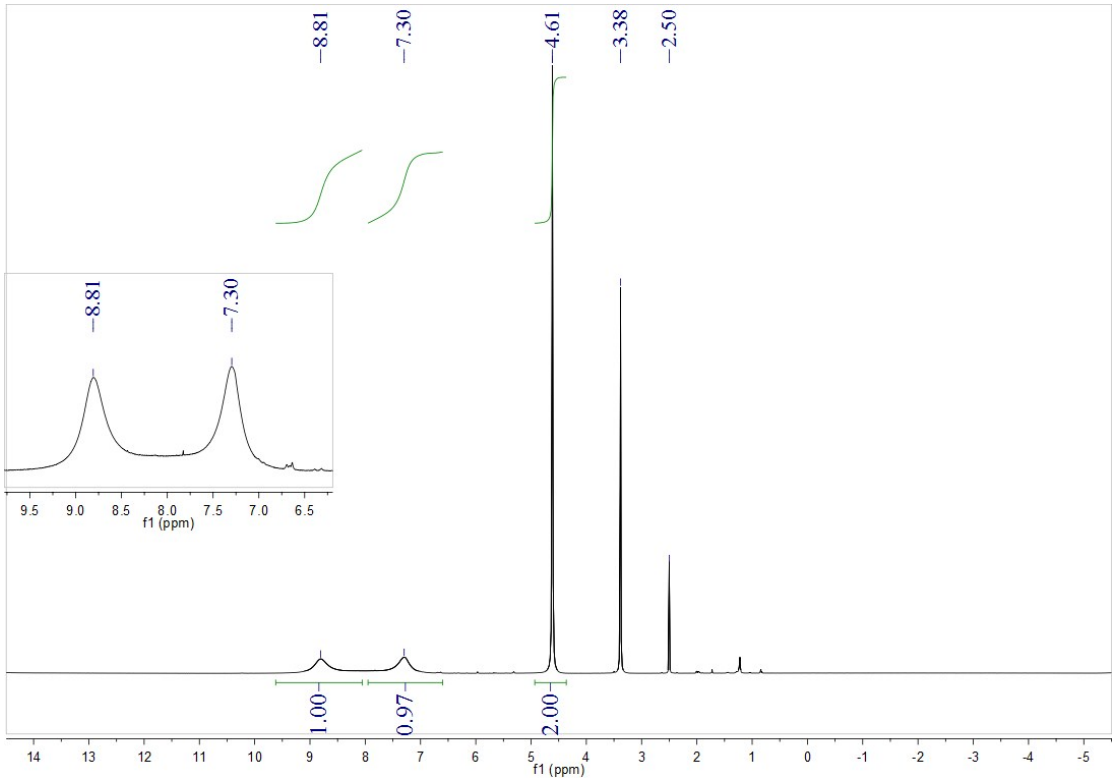

Fig. S22 ^{1}H-NMR spectra (300 MHz) of **12** in DMSO-d_6 at 25°C

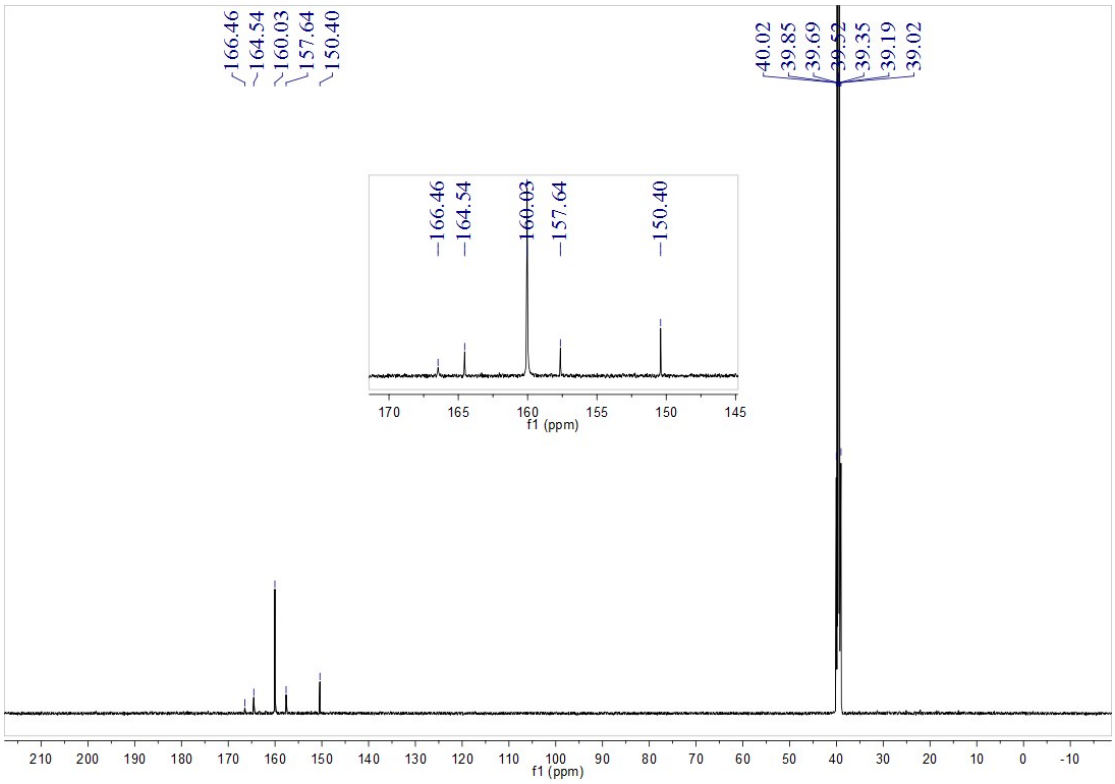

Fig. S23 ^{13}C-NMR spectra (126 MHz) of **12** in DMSO-d_6 at 25°C

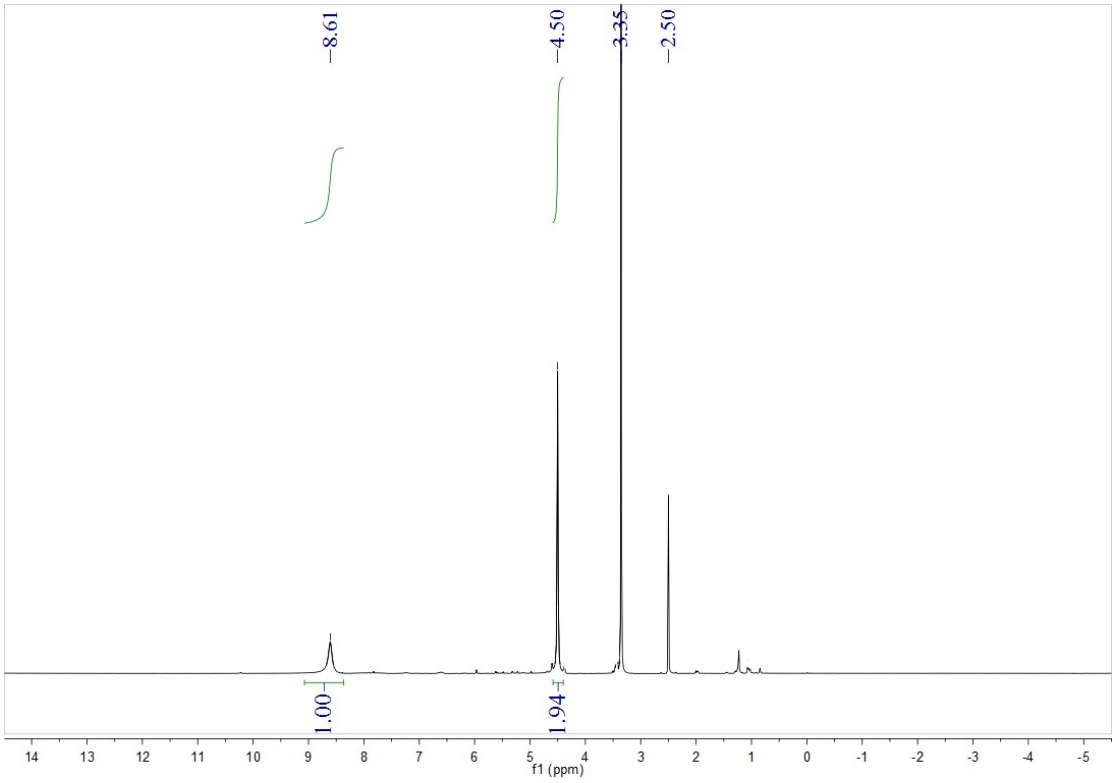

Fig. S24 ^{1}H-NMR spectra (300 MHz) of **13** in DMSO-d_6 at 25°C

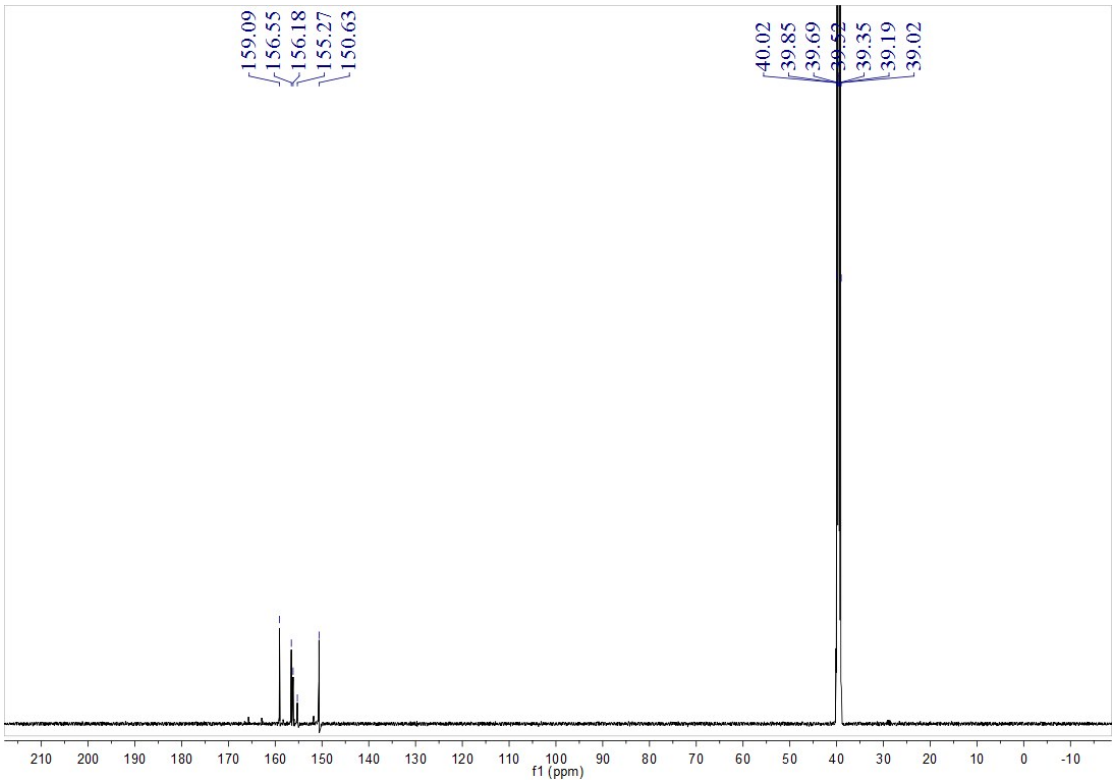

Fig. S25 ^{13}C-NMR spectra (126 MHz) of **13** in DMSO-d_6 at 25°C

5. Differential scanning calorimetry (DSC) curves

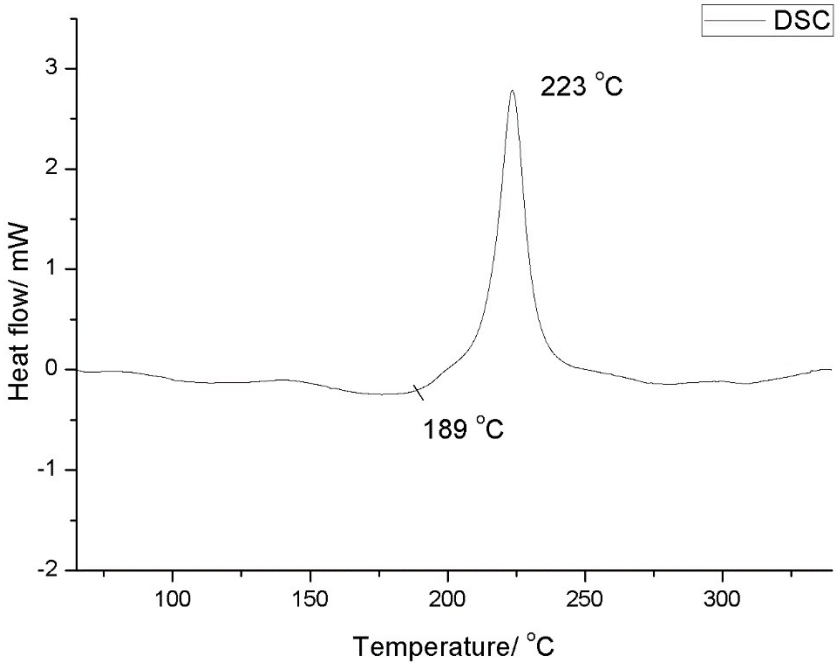

Fig. S26 DSC curves of **2** under nitrogen with a heating rate of 5 °C min^{-1}.

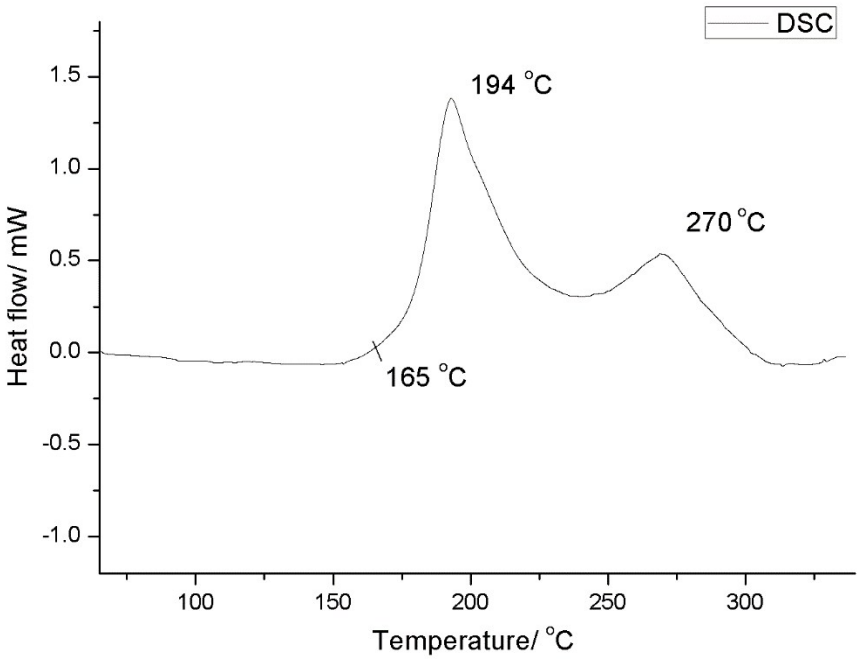

Fig. S27 DSC curves of **4** under nitrogen with a heating rate of 5 ˚C min^{-1}.

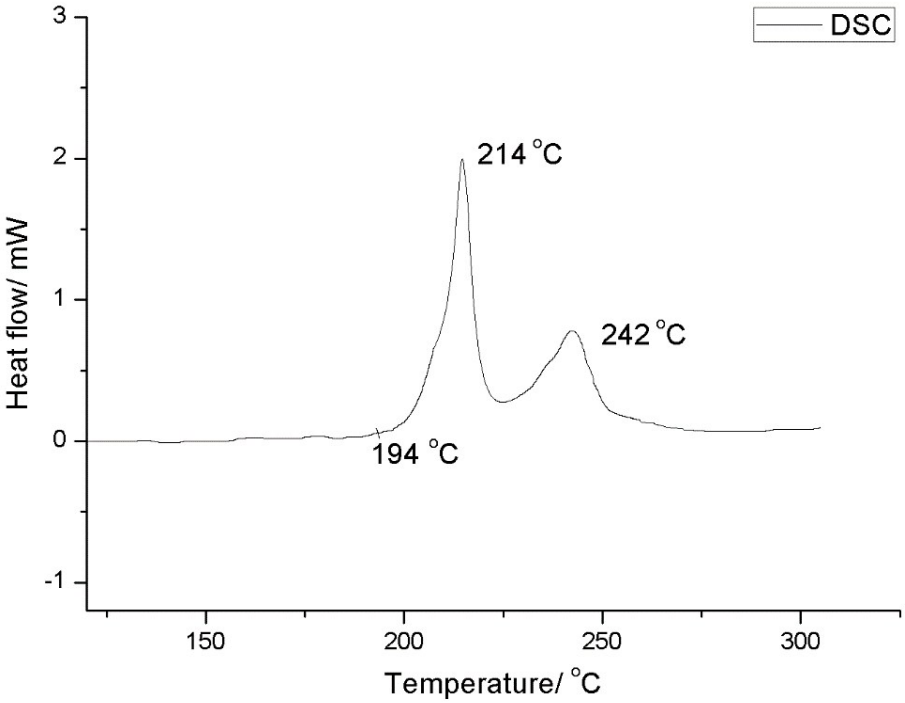

Fig. S28 DSC curves of **5** under nitrogen with a heating rate of 5 ˚C min^{-1}.

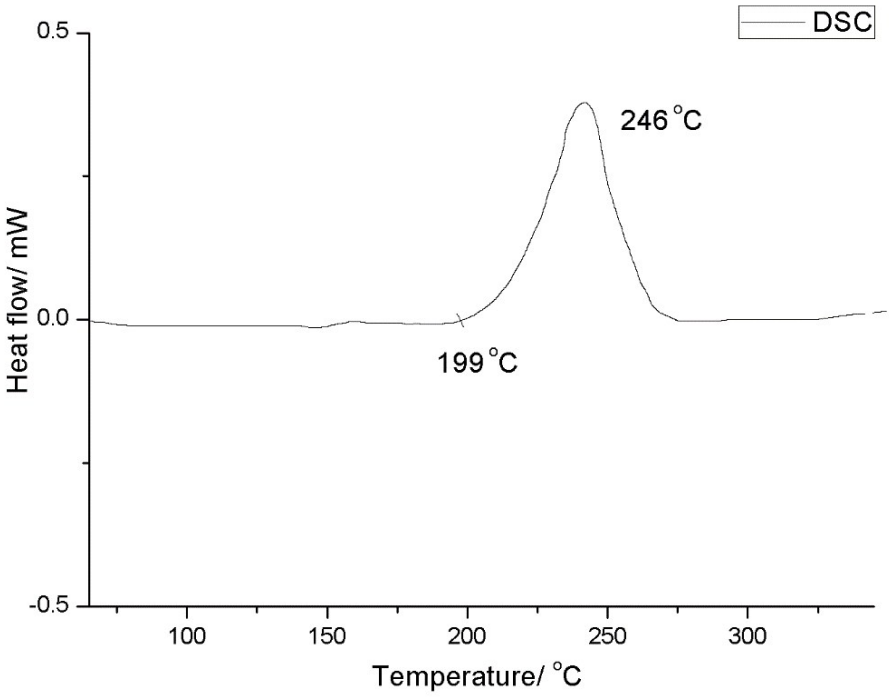

Fig. S29 DSC curves of **6** under nitrogen with a heating rate of 5 °C min^{-1}.

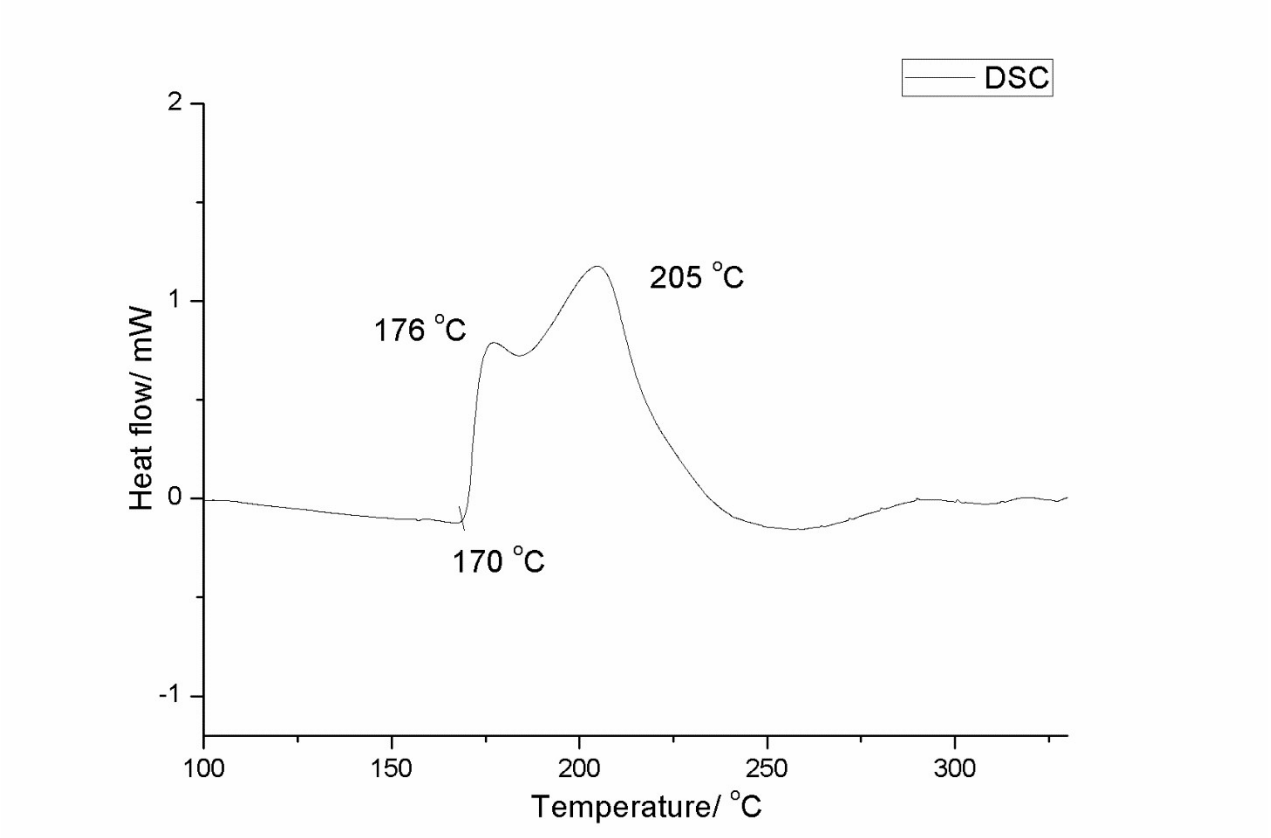

Fig. S30 DSC curves of **7** under nitrogen with a heating rate of 5 °C min^{-1}.

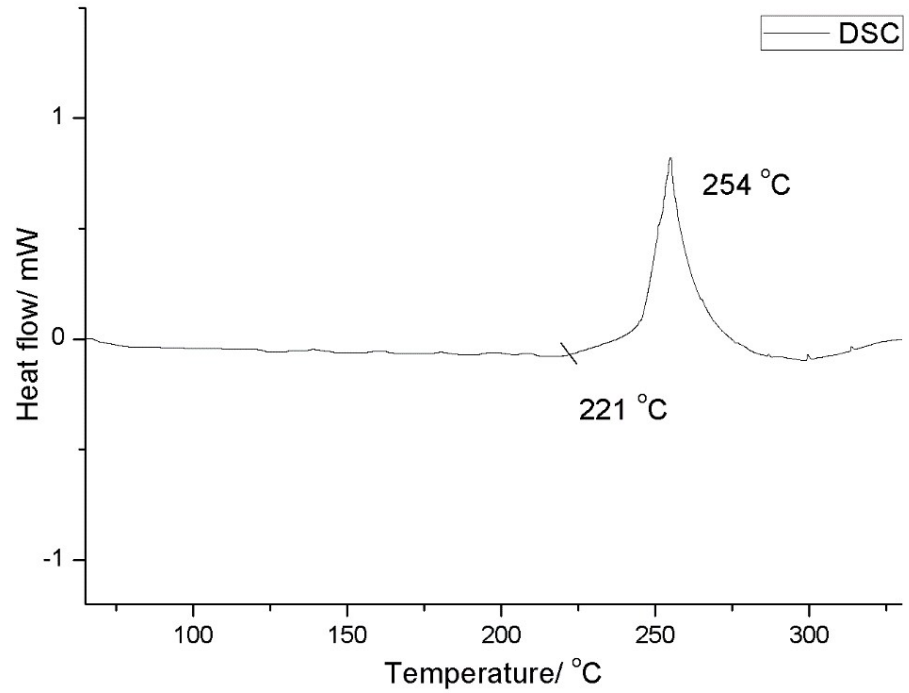

Fig. S31 DSC curves of **8** under nitrogen with a heating rate of 5 °C min^{-1}.

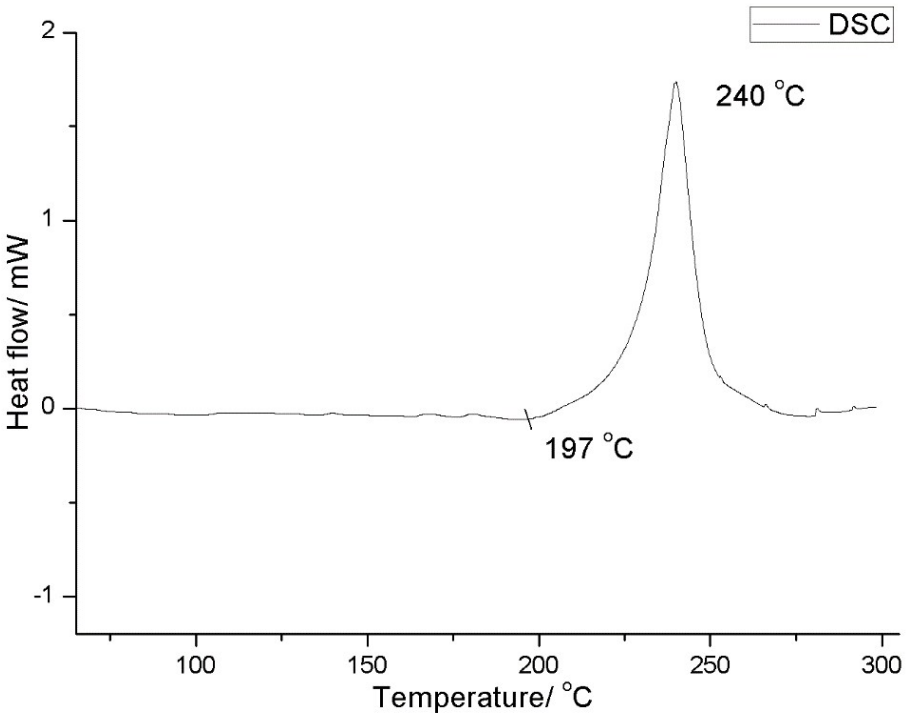

Fig. S32 DSC curves of **9** under nitrogen with a heating rate of 5 °C min^{-1}.

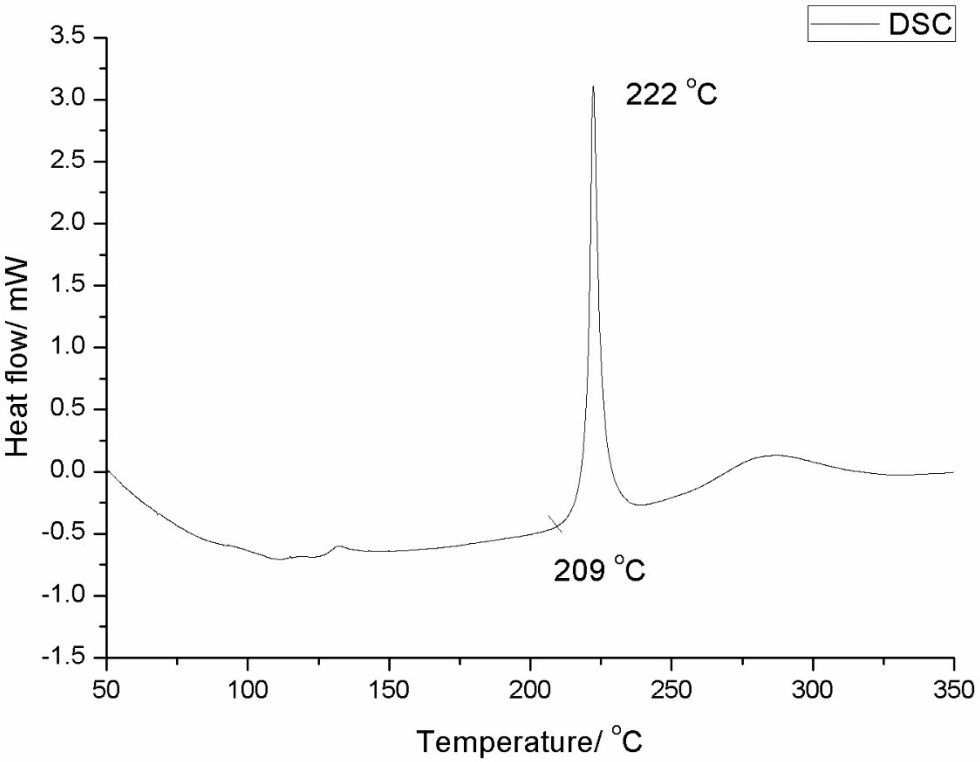

Fig. S33 DSC curves of **11** under nitrogen with a heating rate of 5 °C min^{-1}.

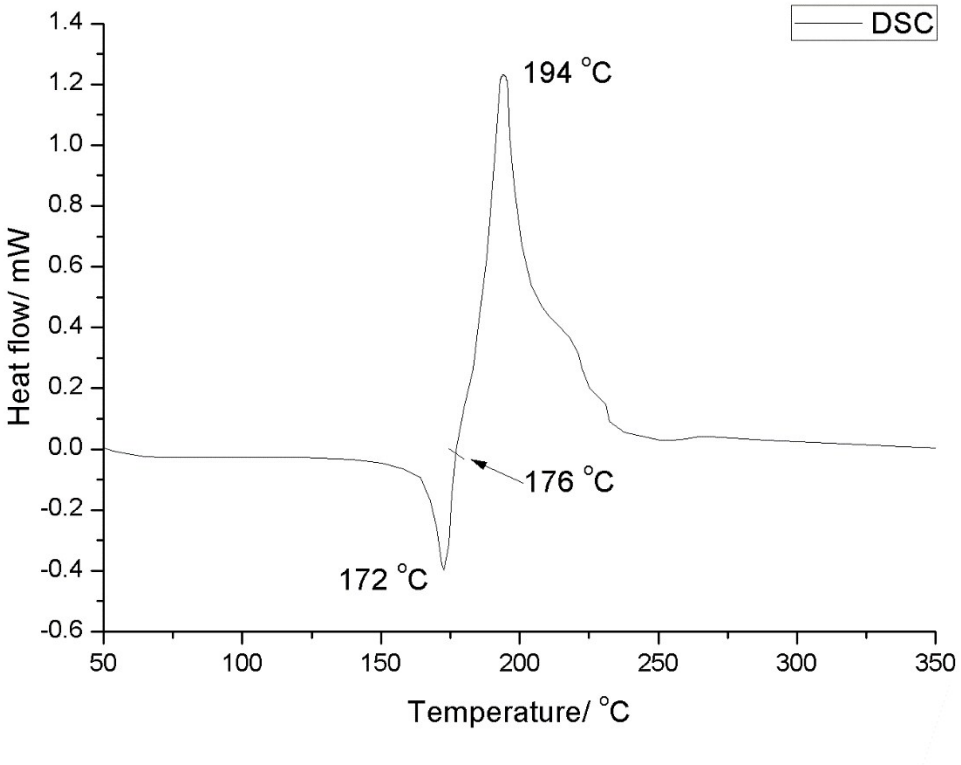

Fig. S34 DSC curves of **12** under nitrogen with a heating rate of 5 °C min^{-1}.

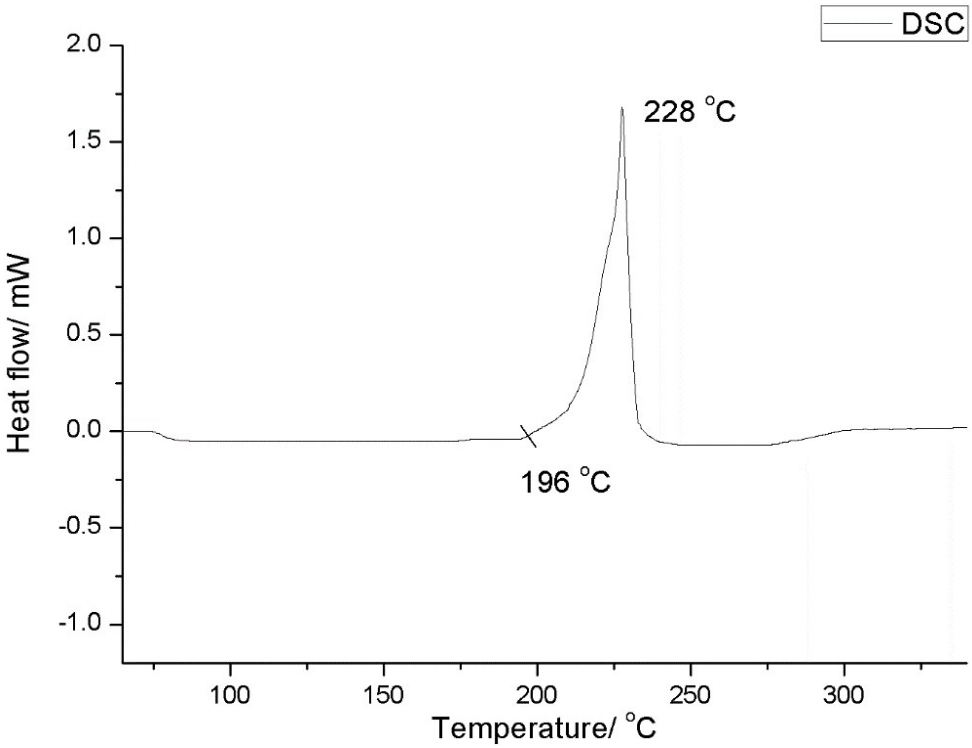

Fig. S35 DSC curves of **13** under nitrogen with a heating rate of 5 °C min^{-1}.