

Supporting Information (SI)

Synthesis and characterization of a new family of energetic salts based on guanidinium cation containing picryl moiety

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1. Computational Details

Method of calculated densities

One of the most important physical properties of an energetic material is its density. The theoretical detonation parameters were calculated with the density from theoretical calculation. For an ionic crystal with formula unit M_pX_q , their volumes are simply the sum of the volumes of the ions contained in the formula unit:^[1]

$$V = pV_{M^+} + qV_{X^-} \quad (1)$$

where M denotes the cation and X denotes the anion. Because the volumes of individual ions are able to be evaluated using the DFT procedure, equation (1) was used to calculate formula unit volumes for ionic crystal. For those salts that contain hydrogen atoms, a “correct” molecular volume using a molecular structure optimized at the DFT level can be calculated using:

$$V_{(\text{corrected})\text{Opt}} = V_{(\text{uncorrected})\text{Opt}} - [0.6763 + 0.9418 \times (\text{no. of hydrogen atoms in the ion})] \quad (2)$$

$$\rho \text{ (g} \cdot \text{cm}^{-3}\text{)} = M_m / V_{(\text{corrected})\text{Opt}} \quad (3)$$

Heat of formation

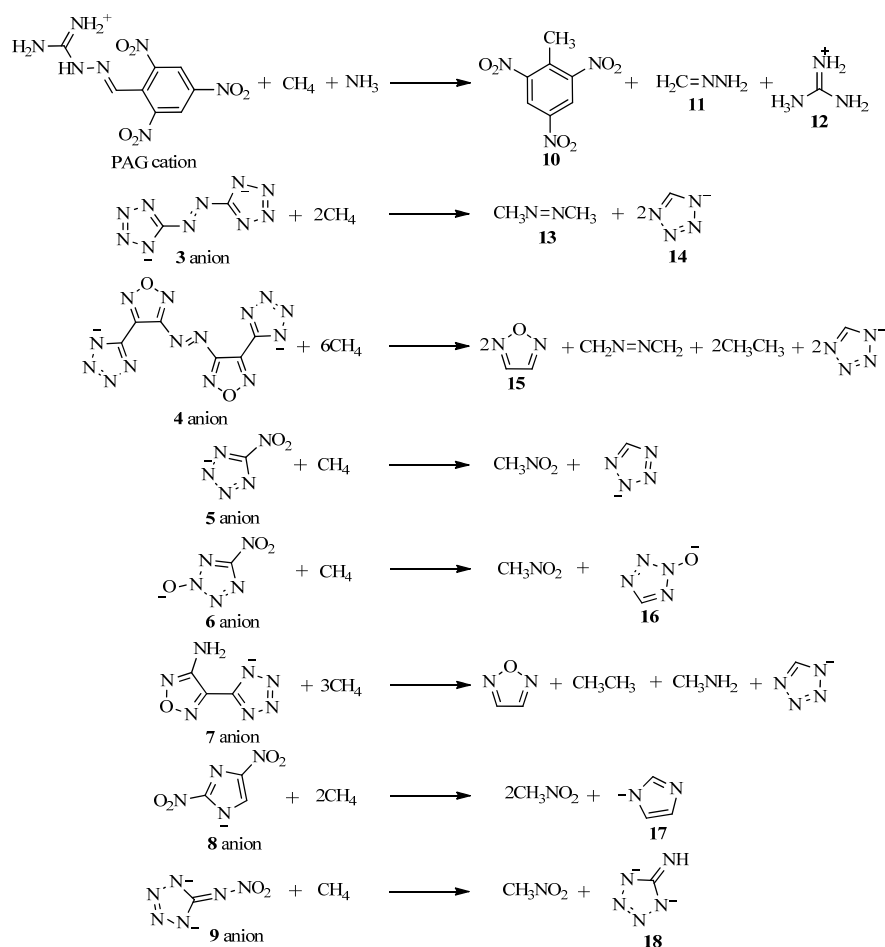
Calculations were performed by using the Gaussian 09 suite of programs. The geometric optimization of all the structures and frequency analyses for calculation of heats of formation was carried out by using B3-LYP functional^[1] with 6-311+G** basis set,^[2] All of the optimized structures were characterized to be local energy minima on the potential surface without any imaginary frequencies. The heats of formation (HOF) of the guanidinium cation containing picryl moiety (PAG cation) and anions were computed through appropriate isodesmic reactions (Scheme S1). 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

$$\Delta H_{298} = \sum \Delta_f H_P - \sum \Delta_f H_R \quad (1)$$

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

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

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 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 reactions for the furoxanyl functionalized guanidinium cation (FAG cation) and anions.

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 M_p^+ and X_q^- , respectively, and are equal to 3 for monatomic ions, 5 for linear polyatomic ions, and 6 for nonlinear polyatomic ions. 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 mol^{-1}) is the chemical formula mass of the ionic material and the coefficients γ ($\text{kJ mol}^{-1} \text{cm}$) and δ (kJ mol^{-1}) are assigned literature values.^[6]

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

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

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

Table S1 Total energy and heat of formation for the title compounds at B3LYP/6-311+G** level^a

	$E_0/\text{a.u.}$	ZPE/ $\text{kJ} \cdot \text{mol}^{-1}$	$\Delta H_T/\text{kJ mol}^{-1}$	HOF/ kJ mol^{-1}
CH ₄	-40.5339263	112.26	10.04	-74.60 ^b
NH ₃	-56.5826356	86.27	10.05	-45.90 ^b
H ₂ N-NH ₂	-111.9105763	134.28	11.16	95.40 ^b

CH ₃ NO ₂	-245.0915559	124.93	11.60	-80.80 ^b
CH ₃ CH ₃	-79.8565413	187.31	11.79	-84.00 ^b
CH ₃ NH ₂	-95.8938402	160.78	11.64	-22.50 ^b
PAG cation	-1144.038686	492.56	56.04	866.06
3 anion	-623.787668	144.11	25.27	788.47
4 anion	-1145.654207	273.34	45.46	1200.14
5 anion	-462.3675686	90.67	17.74	112.01
6 anion	-537.5669458	101.24	19.85	57.84
7 anion	-574.1182105	191.70	22.33	331.55
8 anion	-634.8962488	157.74	25.06	-129.87
9 anion	-517.0464687	100.91	19.95	402.04
10	-885.3022741	338.50	39.86	24.10 ^b
11	-150.0115259	140.79	11.57	174.76 ^c
12	-205.8352863	220.21	15.56	565.59 ^d
13	-189.3337358	211.85	16.32	147.85 ^c
14	-257.7887821	84.91	11.26	175.75 ^d
15	-262.1183629	114.62	11.84	215.72 ^c
16	-332.9899087	96.05	13.15	117.33 ^d
17	-225.7140337	144.06	12.04	60.08 ^d
18	-312.4067394	93.18	13.81	617.14 ^d

^a E₀ in a.u. ZPE (vibrational zero-point energy), ΔH_T (thermal correction to enthalpy) and HOF are in kJ mol⁻¹. ^b Data are from Ref. [D. R. Lide, ed., CRC Handbook of Chemistry and Physics, 88th Edition (Internet Version 2008), CRC Press/Taylor and Francis, Boca Raton, FL.]. ^c Data obtained from CBS-4M calculation in combination with the atomization reaction of the corresponding compound. ^d Data are calculated by protonation reactions, such as, guanidine + H⁺ → guanidinium.

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2. Table S2-S7 Selected bond lengths [Å], angles [°] and hydrogen bonds details of salts 1 and 5.

Table S2 Selected bond distances for salt 1

Parameter	bond length(Å)	Parameter	bond length(Å)
C(1)-C(6)	1.384(4)	C(15)-N(9)	1.275(3)
C(1)-C(2)	1.404(4)	C(16)-N(12)	1.308(3)
C(1)-N(1)	1.480(3)	C(16)-N(11)	1.320(3)
C(2)-C(3)	1.397(4)	C(16)-N(10)	1.351(3)
C(2)-C(7)	1.469(4)	N(1)-O(1)	1.220(3)
C(3)-C(4)	1.379(4)	N(1)-O(2)	1.227(3)
C(3)-N(6)	1.476(3)	N(2)-N(3)	1.359(3)
C(4)-C(5)	1.380(3)	N(6)-O(4)	1.217(3)
C(5)-C(6)	1.367(4)	N(6)-O(3)	1.222(3)
C(5)-N(7)	1.475(4)	N(7)-O(5)	1.221(3)
C(7)-N(2)	1.277(3)	N(7)-O(6)	1.228(3)
C(8)-N(4)	1.310(3)	N(8)-O(8)	1.218(3)
C(8)-N(5)	1.314(3)	N(8)-O(7)	1.229(3)
C(8)-N(3)	1.351(3)	N(9)-N(10)	1.363(3)
C(9)-C(14)	1.382(4)	N(13)-O(10)	1.213(3)
C(9)-C(10)	1.404(4)	N(13)-O(9)	1.217(3)
C(9)-N(8)	1.478(3)	N(14)-O(11)	1.217(3)
C(10)-C(11)	1.401(4)	N(14)-O(12)	1.221(3)
C(10)-C(15)	1.467(4)	N(15)-O(14)	1.235(3)
C(11)-C(12)	1.381(4)	N(15)-O(15)	1.243(3)

C(11)-N(13)	1.480(3)	N(15)-O(13)	1.247(3)
C(12)-C(13)	1.371(4)	N(16)-O(18)	1.244(3)
C(13)-C(14)	1.374(4)	N(16)-O(17)	1.246(3)
C(13)-N(14)	1.483(4)	N(16)-O(16)	1.250(3)

Table S3 Selected bond angles of **1** (°)

Parameter	bond angle (°)	Parameter	bond angle (°)
C(6)-C(1)-C(2)	123.9(3)	N(9)-C(15)-C(10)	118.9(3)
C(6)-C(1)-N(1)	116.0(2)	N(12)-C(16)-N(11)	122.3(3)
C(2)-C(1)-N(1)	119.9(3)	N(12)-C(16)-N(10)	120.1(3)
C(3)-C(2)-C(1)	113.9(2)	N(11)-C(16)-N(10)	117.6(3)
C(3)-C(2)-C(7)	123.2(2)	O(1)-N(1)-O(2)	125.6(3)
C(1)-C(2)-C(7)	122.9(2)	O(1)-N(1)-C(1)	117.5(3)
C(4)-C(3)-C(2)	124.5(3)	O(2)-N(1)-C(1)	116.8(2)
C(4)-C(3)-N(6)	114.3(2)	C(7)-N(2)-N(3)	118.0(2)
C(2)-C(3)-N(6)	121.1(2)	C(8)-N(3)-N(2)	117.5(2)
C(3)-C(4)-C(5)	117.6(3)	O(4)-N(6)-O(3)	125.3(2)
C(6)-C(5)-C(4)	122.1(3)	O(4)-N(6)-C(3)	118.4(2)
C(6)-C(5)-N(7)	119.7(3)	O(3)-N(6)-C(3)	116.3(2)
C(4)-C(5)-N(7)	118.2(3)	O(5)-N(7)-O(6)	125.2(3)
C(5)-C(6)-C(1)	118.0(3)	O(5)-N(7)-C(5)	117.3(3)
N(2)-C(7)-C(2)	117.7(2)	O(6)-N(7)-C(5)	117.5(3)
N(4)-C(8)-N(5)	121.5(3)	O(8)-N(8)-O(7)	125.2(2)
N(4)-C(8)-N(3)	120.5(3)	O(8)-N(8)-C(9)	117.7(3)

N(5)-C(8)-N(3)	118.0(3)	O(7)-N(8)-C(9)	117.1(2)
C(14)-C(9)-C(10)	124.0(3)	C(15)-N(9)-N(10)	116.6(2)
C(14)-C(9)-N(8)	115.6(2)	C(16)-N(10)-N(9)	118.1(2)
C(10)-C(9)-N(8)	120.3(2)	O(10)-N(13)-O(9)	124.7(2)
C(11)-C(10)-C(9)	113.9(3)	O(10)-N(13)-C(11)	116.5(2)
C(11)-C(10)-C(15)	123.3(3)	O(9)-N(13)-C(11)	118.8(2)
C(9)-C(10)-C(15)	122.8(2)	O(11)-N(14)-O(12)	125.4(3)
C(12)-C(11)-C(10)	124.4(3)	O(11)-N(14)-C(13)	117.2(3)
C(12)-C(11)-N(13)	114.5(2)	O(12)-N(14)-C(13)	117.4(3)
C(10)-C(11)-N(13)	121.1(2)	O(14)-N(15)-O(15)	118.8(2)
C(13)-C(12)-C(11)	117.6(3)	O(14)-N(15)-O(13)	121.4(2)
C(12)-C(13)-C(14)	122.3(3)	O(15)-N(15)-O(13)	119.8(2)
C(12)-C(13)-N(14)	118.2(3)	O(18)-N(16)-O(17)	120.5(2)
C(14)-C(13)-N(14)	119.5(3)	O(18)-N(16)-O(16)	119.7(2)
C(13)-C(14)-C(9)	117.8(3)	O(17)-N(16)-O(16)	119.8(2)

Table S4 Hydrogen bonds presented in salt **1**

D—H...A	d(D-H)/ Å	d(H...A)/ Å	d(D...A)/ Å	<(DHA)/ °	comment
N(3)—H(3) ...O(16) ⁱ	0.88	2.02	2.844(3)	156	inter
N(3)—H(3) ...O(17) ⁱ	0.88	2.47	3.144(3)	134	inter
N(4)—H(4A) ...O(17) ⁱⁱ	0.88	2.06	2.930(3)	170	inter
N(4)—H(4B) ...O(4)	0.88	2.59	3.417(3)	157	intra
N(4)—H(4B) ...N(2)	0.88	2.32	2.646(3)	102	intra
N(5)—H(5A) ...O(18) ⁱⁱ	0.88	2.03	2.888(3)	165	inter
N(5)—H(5A) ...O(14) ⁱ	0.88	2.38	2.925(3)	120	inter

N(5)—H(5B) •••O(13) ⁱ	0.88	2.30	2.984(4)	135	inter
N(5)—H(5B) •••O(16) ⁱ	0.88	2.42	3.154(3)	141	inter
N(10)—H(10) •••O(13) ⁱⁱⁱ	0.88	2.26	3.035(3)	146	inter
N(10)—H(10) •••O(15) ⁱⁱⁱ	0.88	2.15	2.976(3)	155	inter
N(11)—H(11A) •••O(18) ⁱⁱⁱ	0.88	2.35	2.974(3)	128	inter
N(11)—H(11A) •••O(14) ^{iv}	0.88	2.18	3.000(3)	156	inter
N(11)—H(11B) •••O(13) ⁱⁱⁱ	0.88	2.24	3.027(3)	149	inter
N(12)—H(12A) •••O(14) ^{iv}	0.88	2.56	3.288(3)	140	inter
N(12)—H(12A) •••O(15) ^{iv}	0.88	2.07	2.932(3)	165	inter
N(12)—H(12B) •••N(9)	0.88	2.32	2.650(3)	102	intra
C(7)—H(7) •••O(2)	0.95	2.28	2.807(3)	114	intra
C(7)—H(7) •••O(17) ⁱ	0.95	2.51	3.230(4)	132	inter
C(12)—H(12) •••O(4) ⁱ	0.95	2.51	3.349(4)	147	inter
C(15)—H(15) •••O(7)	0.95	2.31	2.786(3)	110	intra
C(15)—H(15) •••O(15) ⁱⁱⁱ	0.95	2.42	3.205(4)	140	intra

i: 1-x, 1-y, 1-z ; ii: 1-x, 1/2+y, 3/2-z ; iii: 1+x, y, z ; iv: 1+x, 1/2-y, 1/2+z

Table S5 Selected bond distances for salt **5**

Parameter	bond length(Å)	Parameter	bond length(Å)
C(1)-N(1)	1.323(3)	C(9)-N(9)	1.314(3)
C(1)-N(4)	1.324(3)	C(9)-N(8)	1.349(3)
C(1)-N(5)	1.440(3)	N(1)-N(2)	1.345(3)
C(2)-C(7)	1.380(3)	N(2)-N(3)	1.331(3)
C(2)-C(3)	1.394(3)	N(3)-N(4)	1.343(2)
C(2)-N(6)	1.476(3)	N(5)-O(1)	1.222(2)
C(3)-C(4)	1.403(3)	N(5)-O(2)	1.223(3)

C(3)-C(8)	1.475(3)	N(6)-O(3)	1.221(2)
C(4)-C(5)	1.372(3)	N(6)-O(4)	1.229(2)
C(4)-N(11)	1.476(3)	N(7)-N(8)	1.365(2)
C(5)-C(6)	1.371(3)	N(11)-O(6)	1.216(3)
C(6)-C(7)	1.384(3)	N(11)-O(5)	1.229(2)
C(6)-N(12)	1.473(3)	N(12)-O(8)	1.226(2)
C(8)-N(7)	1.277(3)	N(12)-O(7)	1.229(2)
C(9)-N(10)	1.310(3)		

Table S6 Selected bond angles of **5** (°)

Parameter	bond angle (°)	Parameter	bond angle (°)
N(1)-C(1)-N(4)	115.2(2)	N(9)-C(9)-N(8)	117.3(2)
N(1)-C(1)-N(5)	123.6(2)	C(1)-N(1)-N(2)	102.43(19)
N(4)-C(1)-N(5)	121.2(2)	N(3)-N(2)-N(1)	110.17(19)
C(7)-C(2)-C(3)	125.0(2)	N(2)-N(3)-N(4)	109.07(18)
C(7)-C(2)-N(6)	115.3(2)	C(1)-N(4)-N(3)	103.18(18)
C(3)-C(2)-N(6)	119.7(2)	O(1)-N(5)-O(2)	124.7(2)
C(2)-C(3)-C(4)	114.2(2)	O(1)-N(5)-C(1)	117.6(2)
C(2)-C(3)-C(8)	121.3(2)	O(2)-N(5)-C(1)	117.6(2)
C(4)-C(3)-C(8)	124.3(2)	O(3)-N(6)-O(4)	125.0(2)
C(5)-C(4)-C(3)	123.9(2)	O(3)-N(6)-C(2)	117.9(2)
C(5)-C(4)-N(11)	116.4(2)	O(4)-N(6)-C(2)	117.01(19)
C(3)-C(4)-N(11)	119.8(2)	C(8)-N(7)-N(8)	116.19(19)
C(6)-C(5)-C(4)	117.7(2)	C(9)-N(8)-N(7)	118.27(19)

C(5)-C(6)-C(7)	123.0(2)	O(6)-N(11)-O(5)	125.3(2)
C(5)-C(6)-N(12)	118.9(2)	O(6)-N(11)-C(4)	117.4(2)
C(7)-C(6)-N(12)	118.1(2)	O(5)-N(11)-C(4)	117.2(2)
C(2)-C(7)-C(6)	116.2(2)	O(8)-N(12)-O(7)	124.7(2)
N(7)-C(8)-C(3)	116.0(2)	O(8)-N(12)-C(6)	117.9(2)
N(10)-C(9)-N(9)	122.4(2)	O(7)-N(12)-C(6)	117.4(2)
N(10)-C(9)-N(8)	120.3(2)		

Table S7 Hydrogen bonds presented in salt **5**

D—H...A	d(D-H)/ Å	d(H...A)/ Å	d(D...A)/ Å	<(DHA)/ °	comment
N(8)—H(8A) ...N(2) ⁱ	0.88	2.0	2.862(3)	165	inter
N(9)—H(9A) ...N(4) ⁱⁱ	0.88	2.07	2.916(3)	160	inter
N(9)—H(9B) ...O(5) ⁱ	0.88	2.52	2.916(3)	108	inter
N(10)—H(10A) ...N(3) ⁱⁱ	0.88	2.20	3.068(3)	168	inter
N(10)—H(10A) ...N(4) ⁱⁱ	0.88	2.60	3.308(3)	138	inter
N(10)—H(10B) ...N(7)	0.88	2.33	2.658(3)	102	intra
N(10)—H(10B) ...O(7) ⁱⁱⁱ	0.88	2.18	3.038(3)	164	inter
C(5)—H(5) ...O(4) ^{iv}	0.95	2.47	3.380(3)	161	inter
C(7)—H(7) ...O(1) ⁱⁱⁱ	0.95	2.57	3.507(3)	169	inter
C(8)—H(8) ...O(5)	0.95	2.41	2.757(4)	102	intra

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

3. Figure S1-S20 ^1H and ^{13}C NMR spectra of salts 1-9

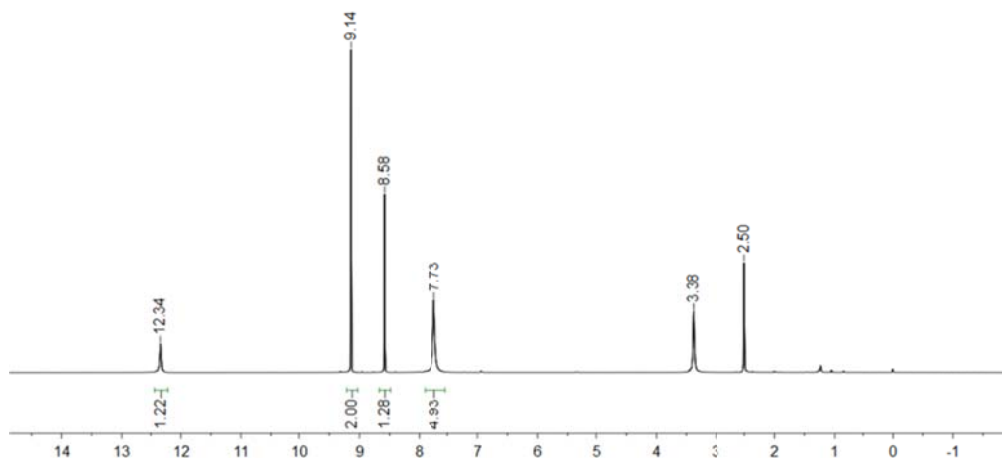


Figure S1 ^1H NMR spectra (300 MHz) of **1** in $[\text{D}_6]\text{DMSO}$ at 25 $^\circ\text{C}$

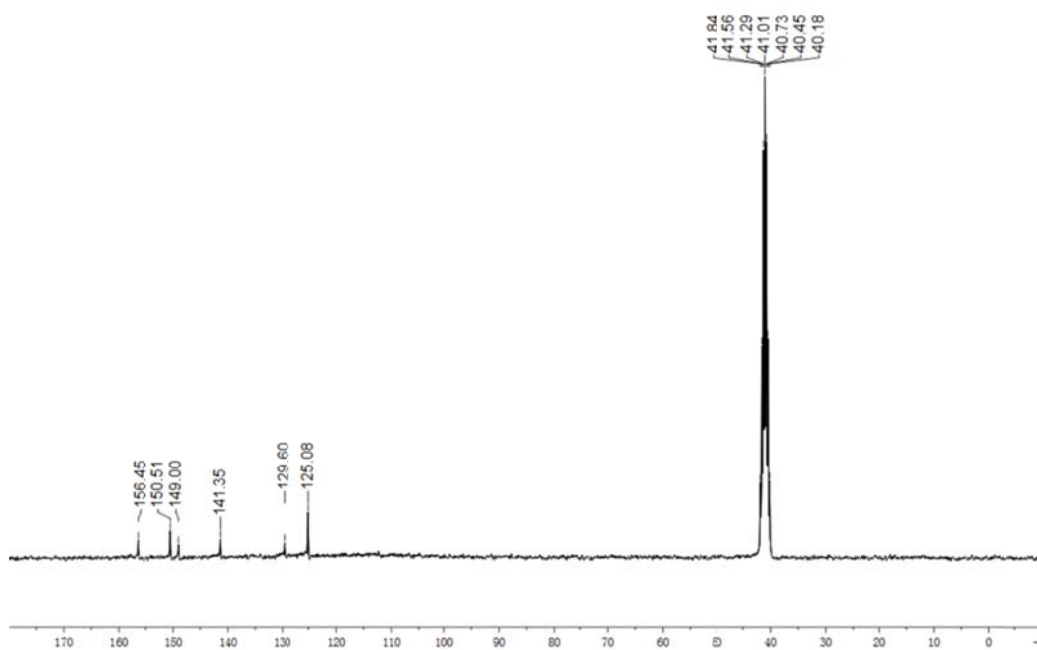


Figure S2 ^{13}C NMR spectra (75 MHz) of **1** in $[\text{D}_6]\text{DMSO}$ at 25 $^\circ\text{C}$

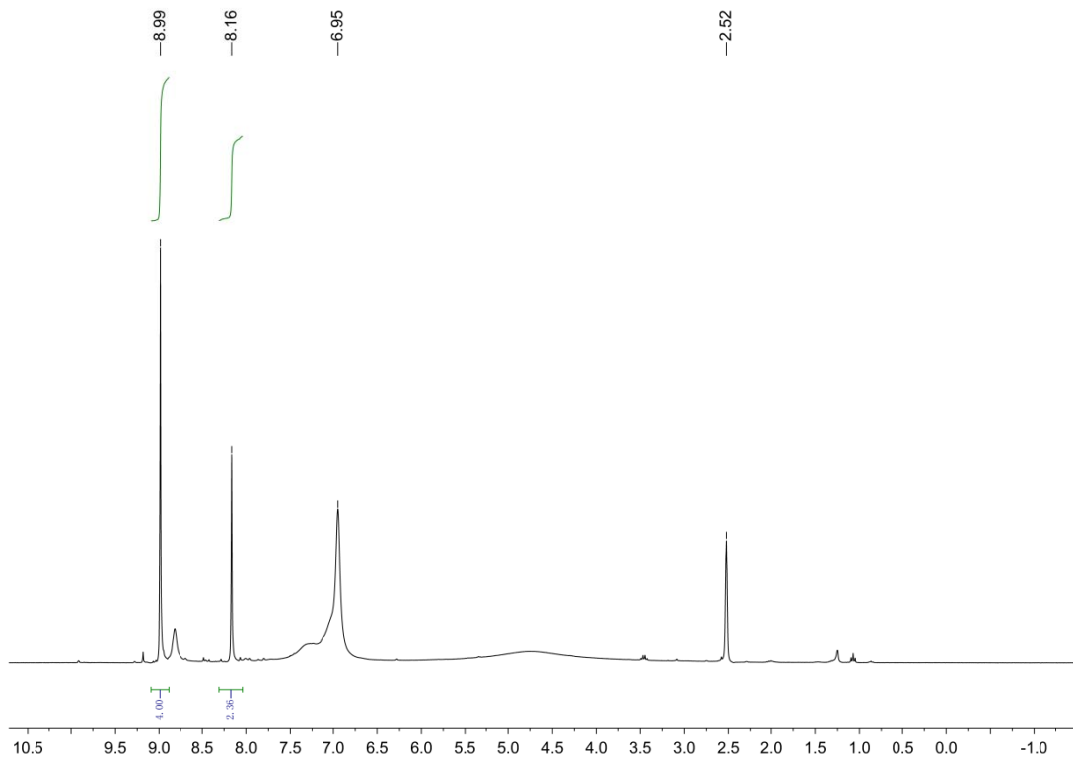


Figure S3 ^1H NMR spectra (300 MHz) of **2** in $[\text{D}_6]\text{DMSO}$ at 25 °C

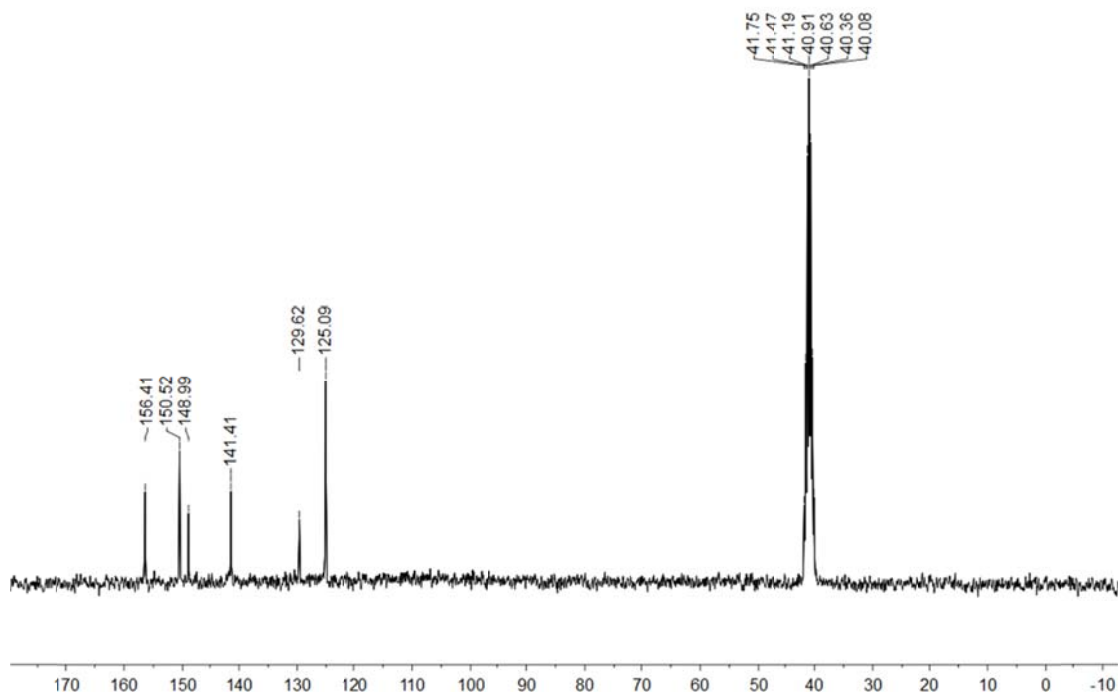


Figure S4 ^{13}C NMR spectra (75 MHz) of **2** in $[\text{D}_6]\text{DMSO}$ at 25 °C

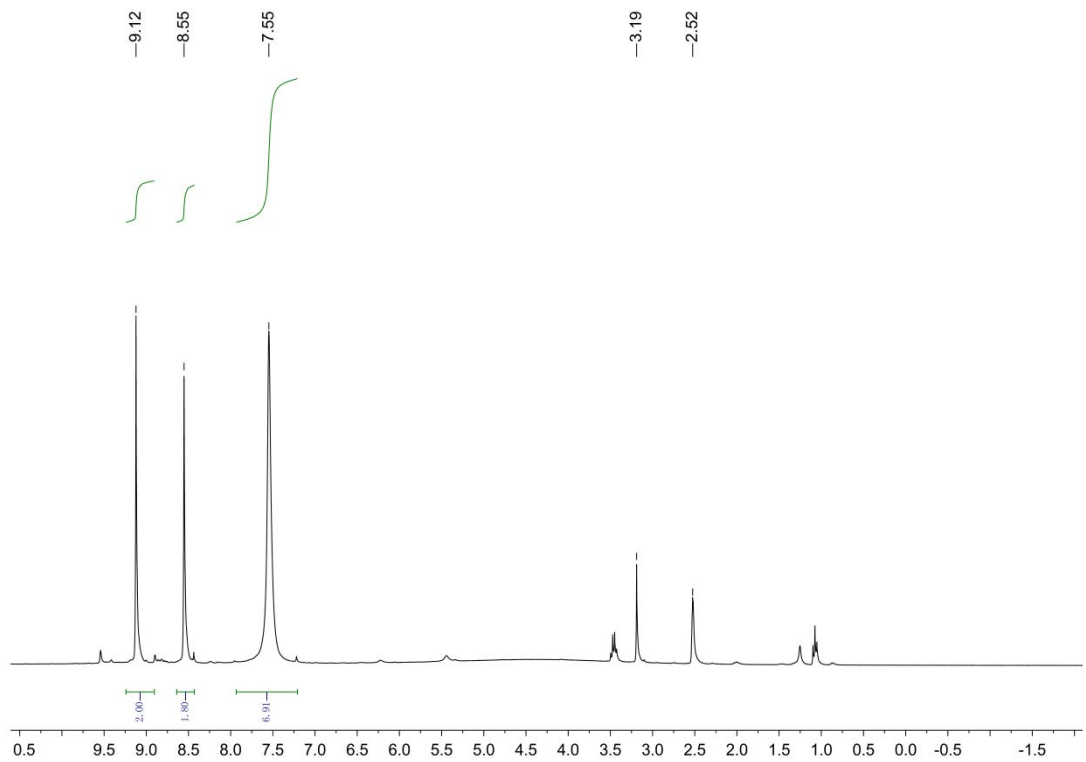


Figure S5 ^1H NMR spectra (300 MHz) of **3** in $[\text{D}_6]\text{DMSO}$ at $25\text{ }^\circ\text{C}$

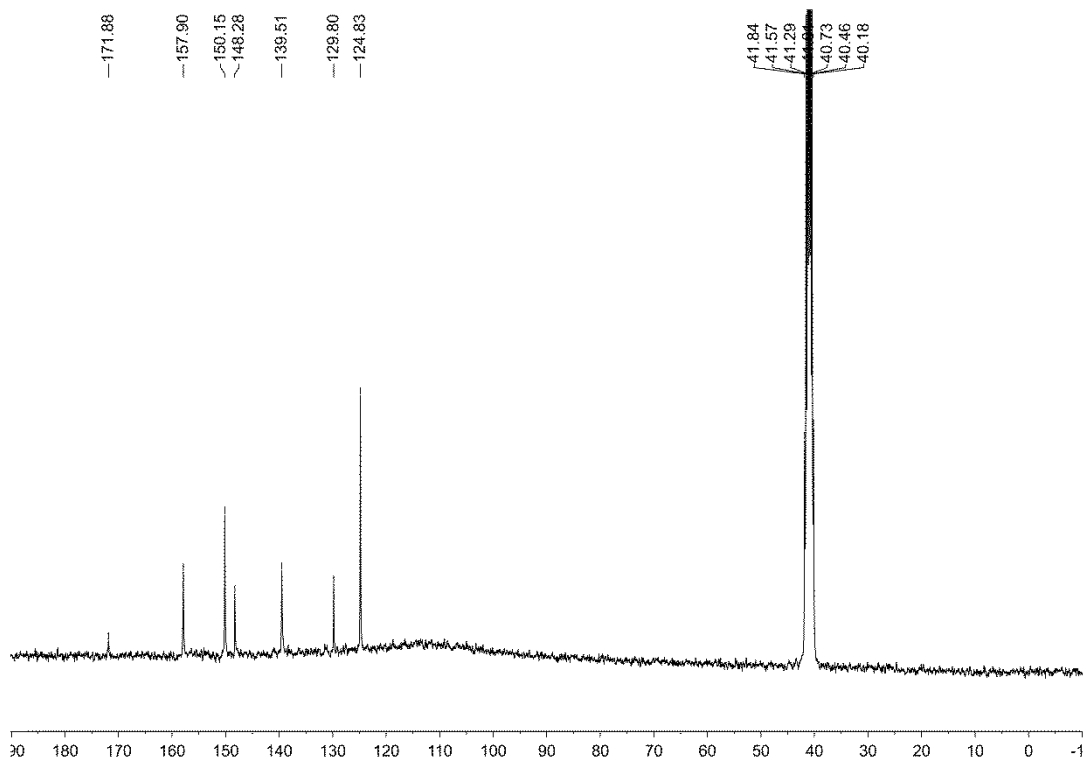


Figure S6 ^{13}C NMR spectra (75 MHz) of **3** in $[\text{D}_6]\text{DMSO}$ at $25\text{ }^\circ\text{C}$

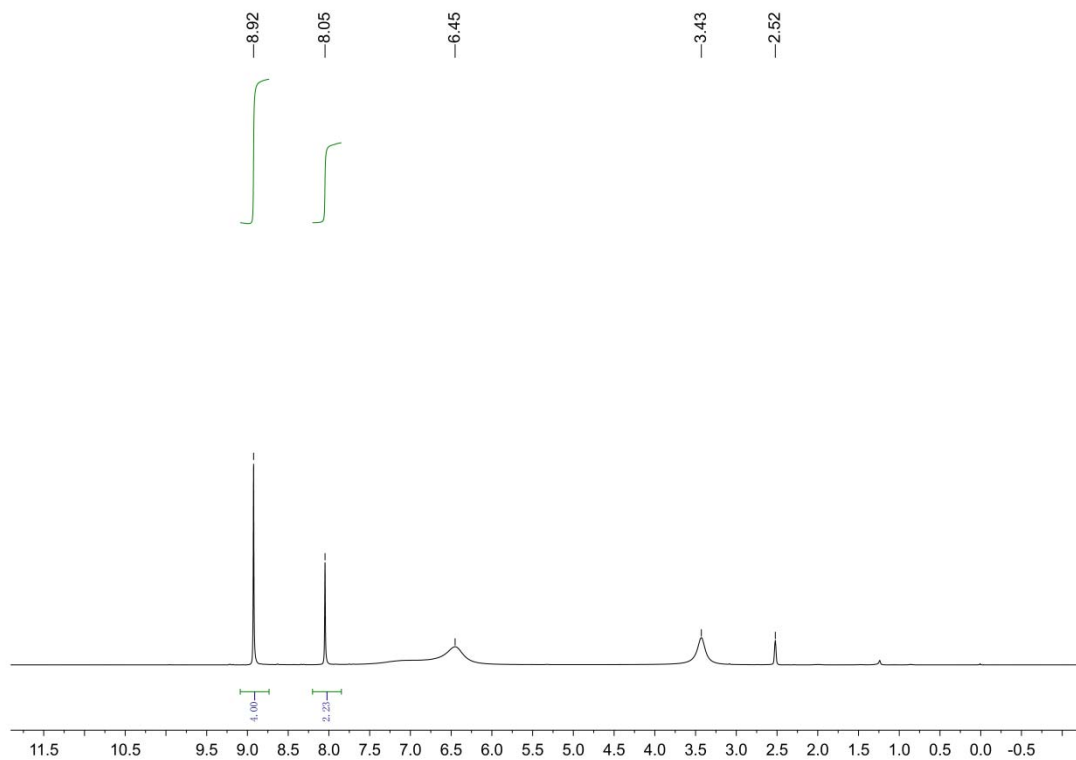


Figure S7 ^1H NMR spectra (300 MHz) of **4** in $[\text{D}_6]\text{DMSO}$ at 25 °C

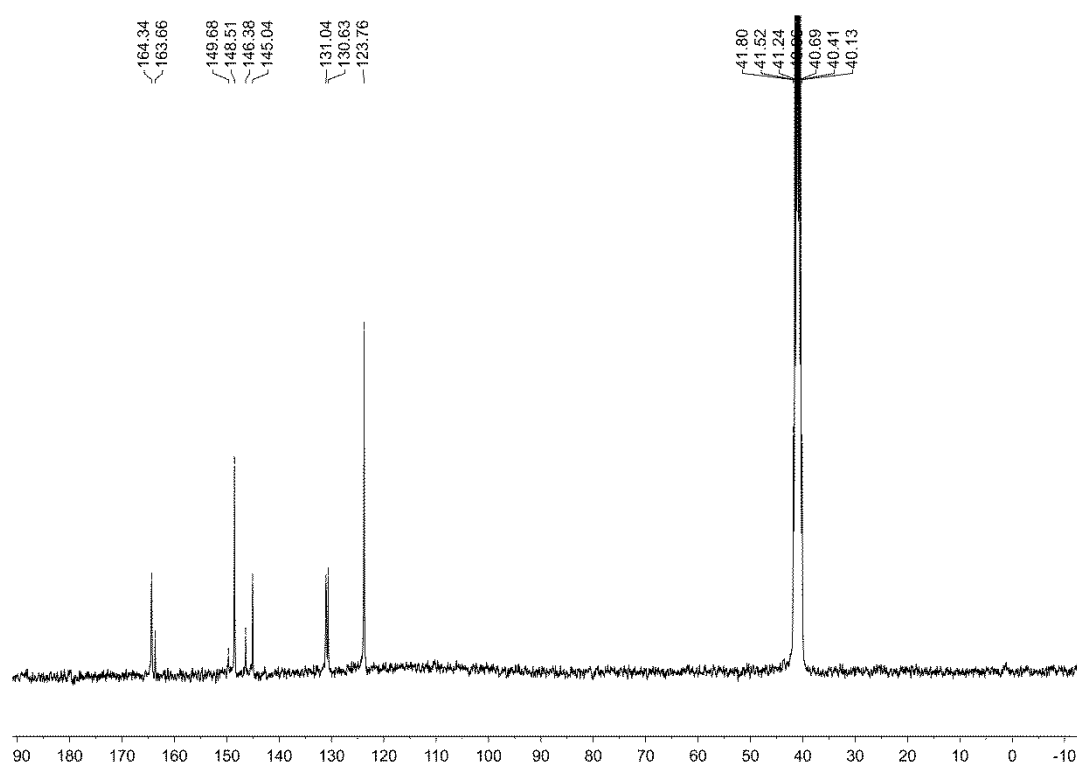


Figure S8 ^{13}C NMR spectra (75 MHz) of **4** in $[\text{D}_6]\text{DMSO}$ at 25 °C

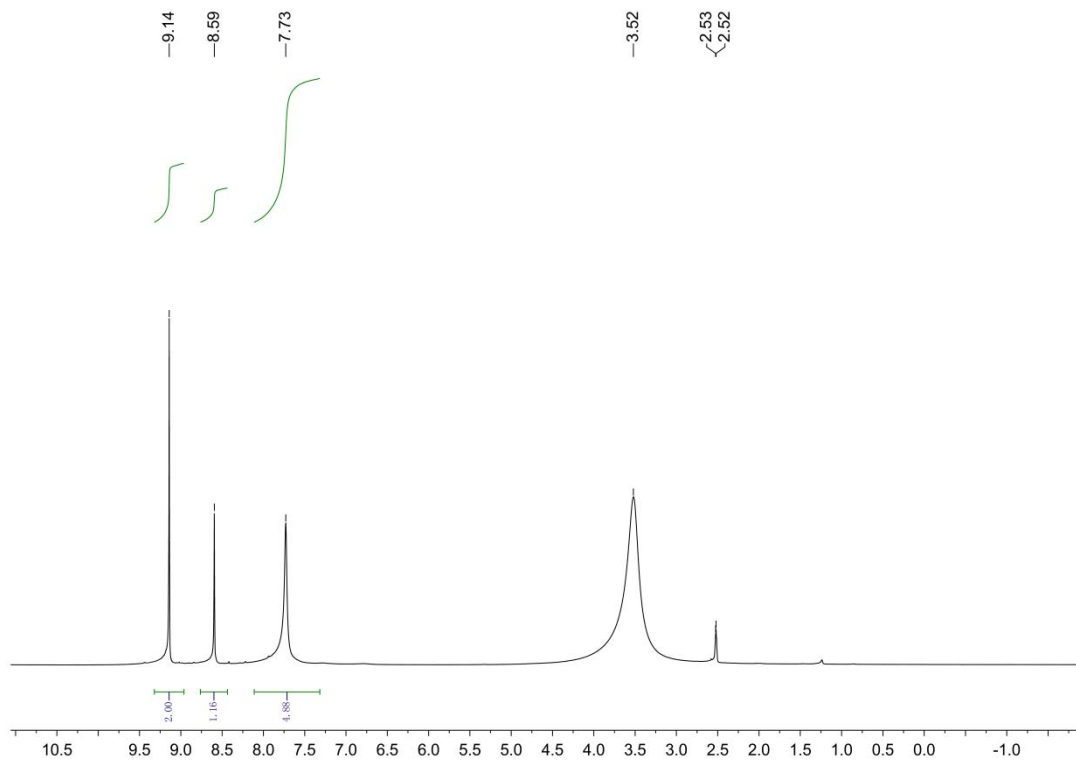


Figure S9 ^1H NMR spectra (300 MHz) of **5** in $[\text{D}_6]\text{DMSO}$ at 25 °C

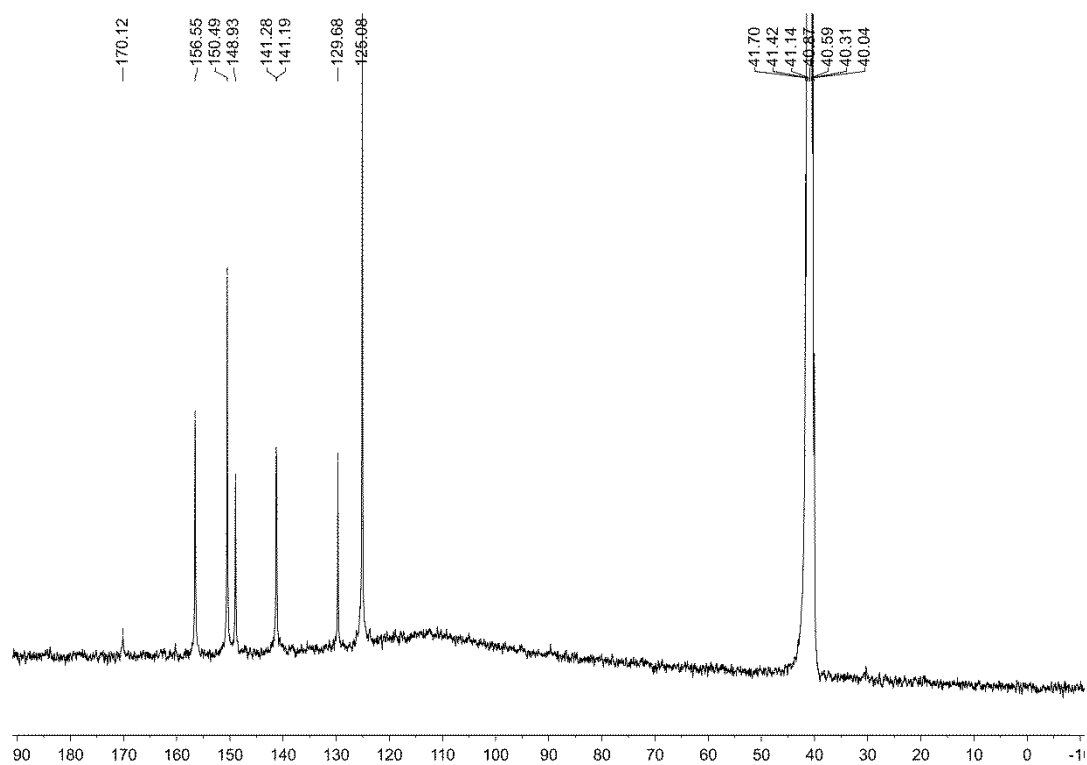


Figure S10 ^{13}C NMR spectra (75 MHz) of **5** in $[\text{D}_6]\text{DMSO}$ at 25 °C

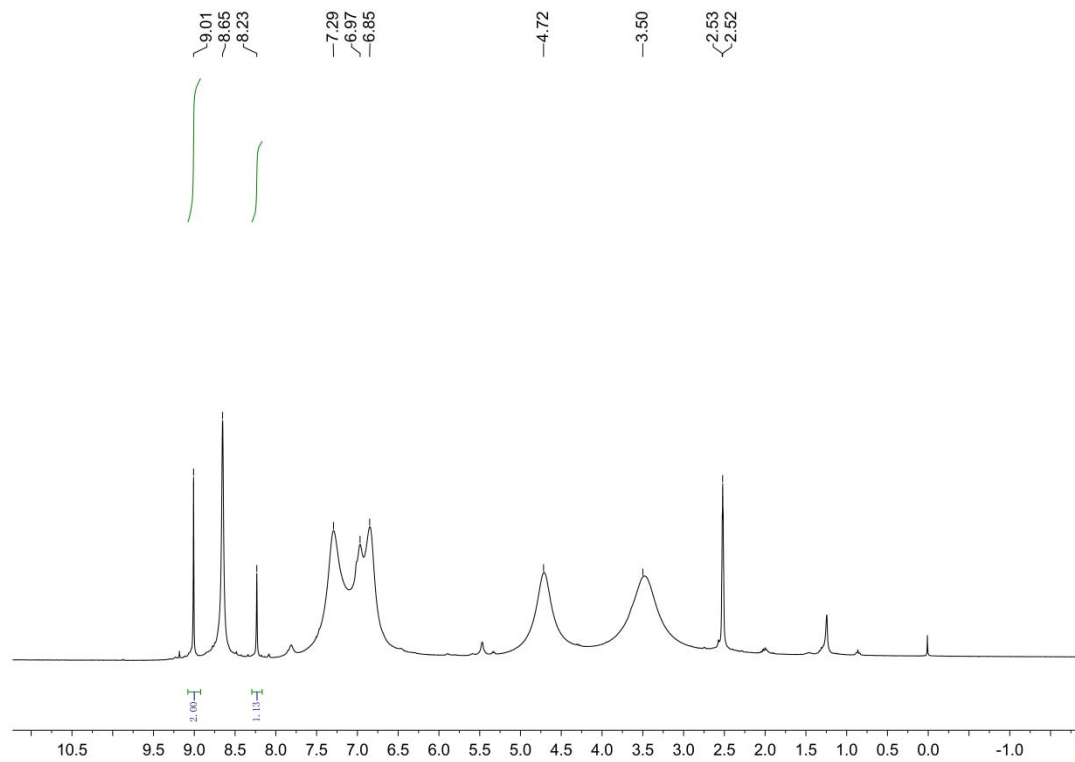


Figure S11 ^1H NMR spectra (300 MHz) of **6** in $[\text{D}_6]\text{DMSO}$ at 25 $^\circ\text{C}$

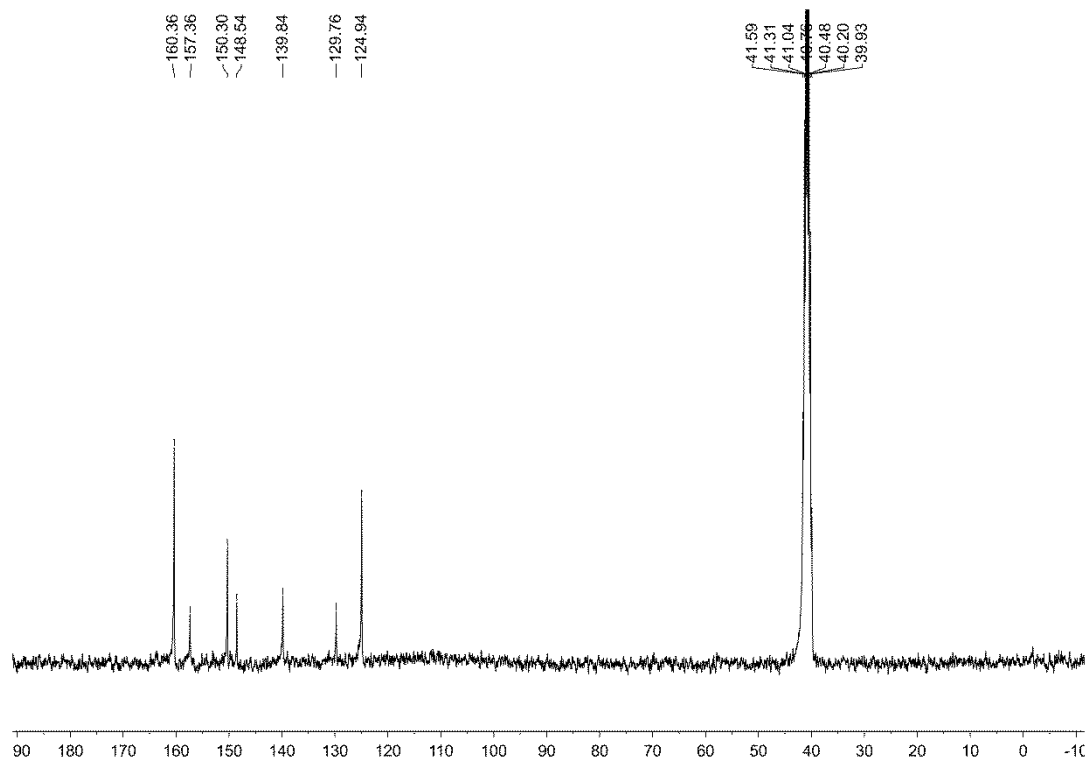


Figure S12 ^{13}C NMR spectra (75 MHz) of **6** in $[\text{D}_6]\text{DMSO}$ at 25 $^\circ\text{C}$

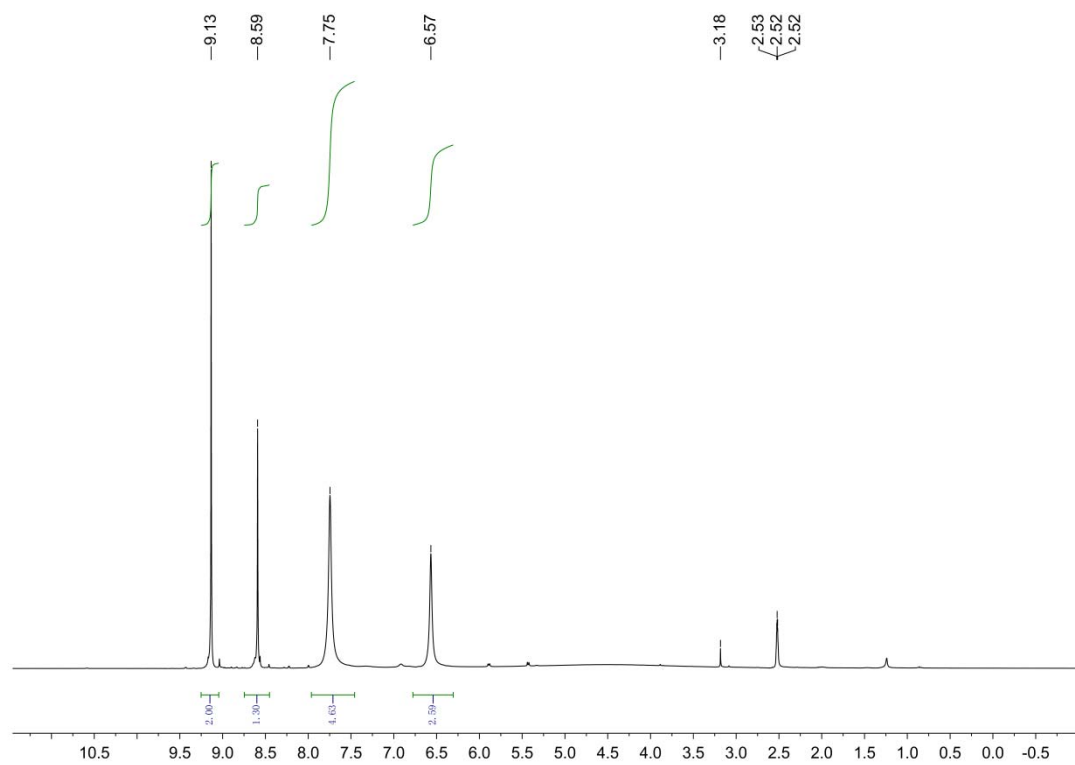


Figure S13 ^1H NMR spectra (300 MHz) of **7** in $[\text{D}_6]\text{DMSO}$ at 25 $^\circ\text{C}$

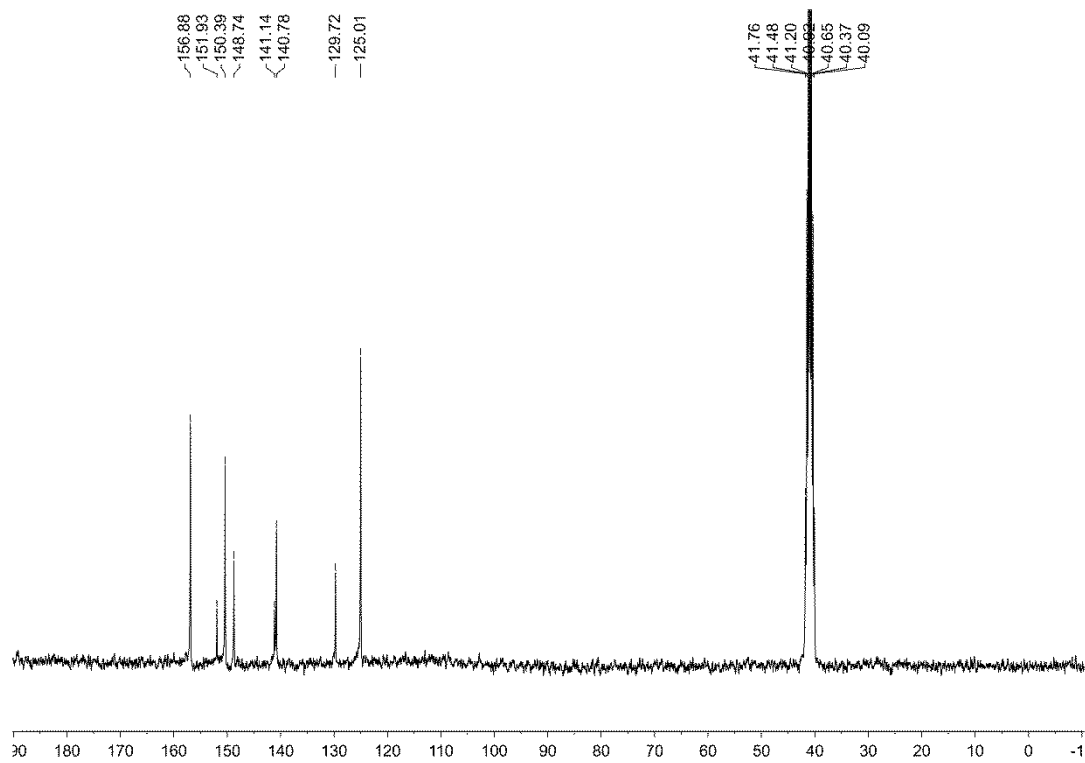


Figure S14 ^{13}C NMR spectra (75 MHz) of **7** in $[\text{D}_6]\text{DMSO}$ at 25 $^\circ\text{C}$

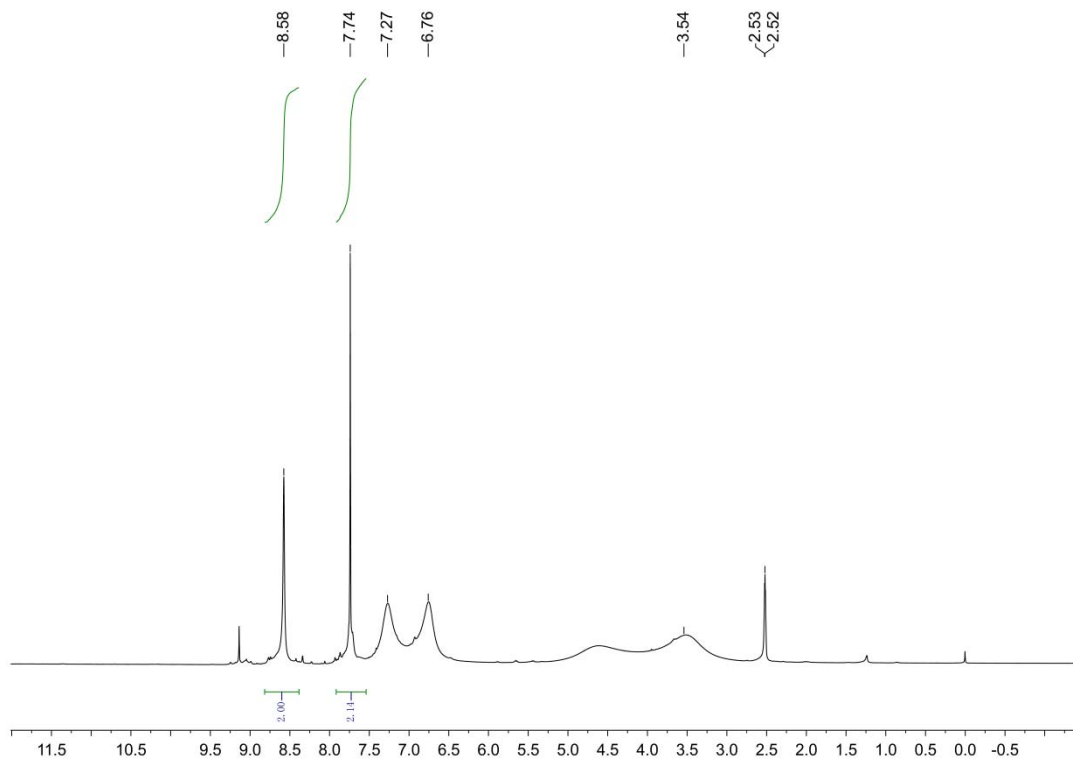


Figure S15 ^1H NMR spectra (300 MHz) of **8** in $[\text{D}_6]\text{DMSO}$ at $25\text{ }^\circ\text{C}$

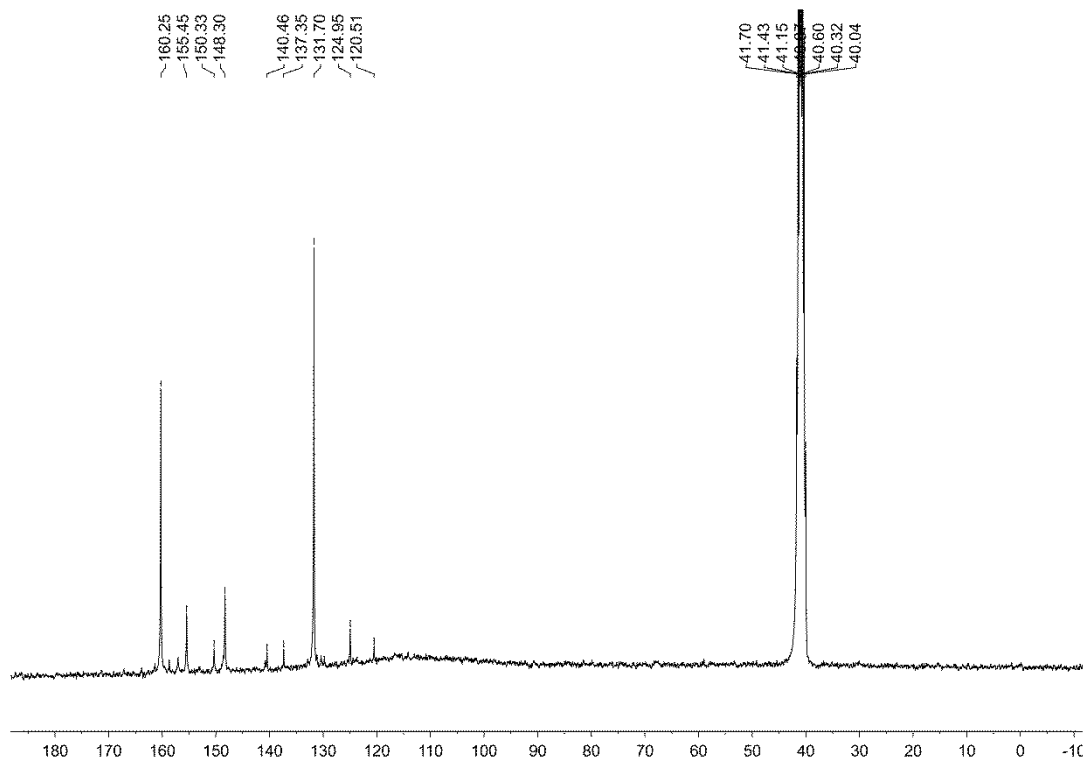


Figure S16 ^{13}C NMR spectra (75 MHz) of **8** in $[\text{D}_6]\text{DMSO}$ at $25\text{ }^\circ\text{C}$

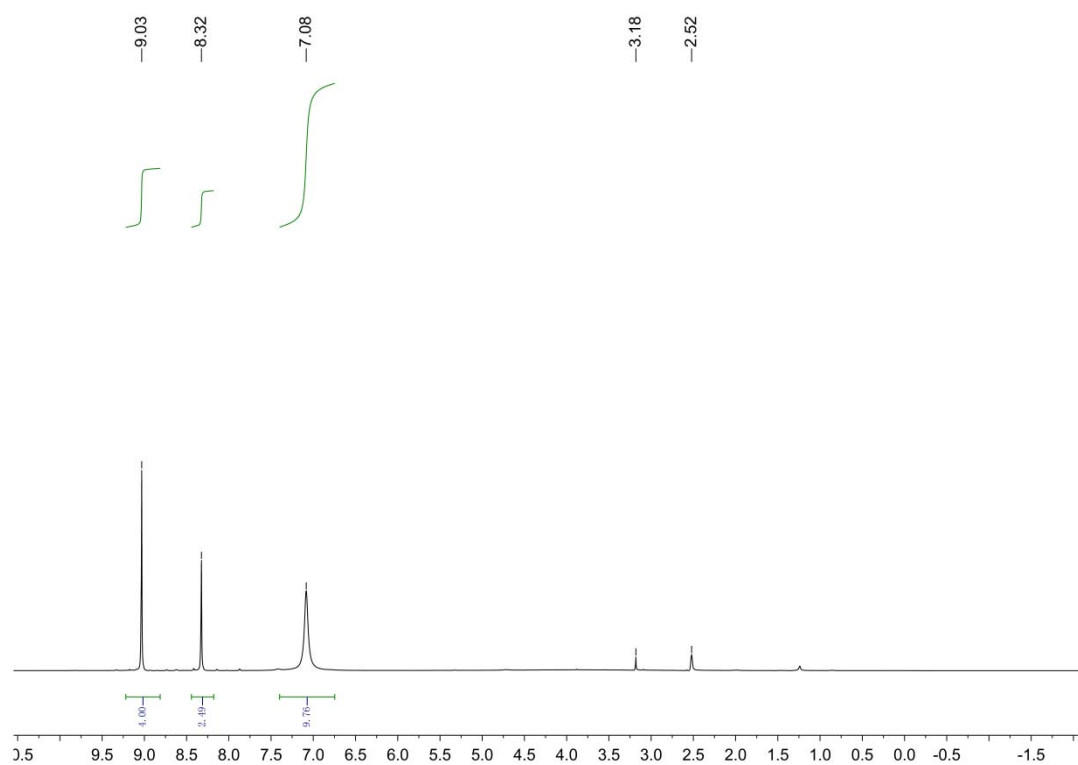


Figure S17 ^1H NMR spectra (300 MHz) of **9** in $[\text{D}_6]\text{DMSO}$ at 25 $^\circ\text{C}$

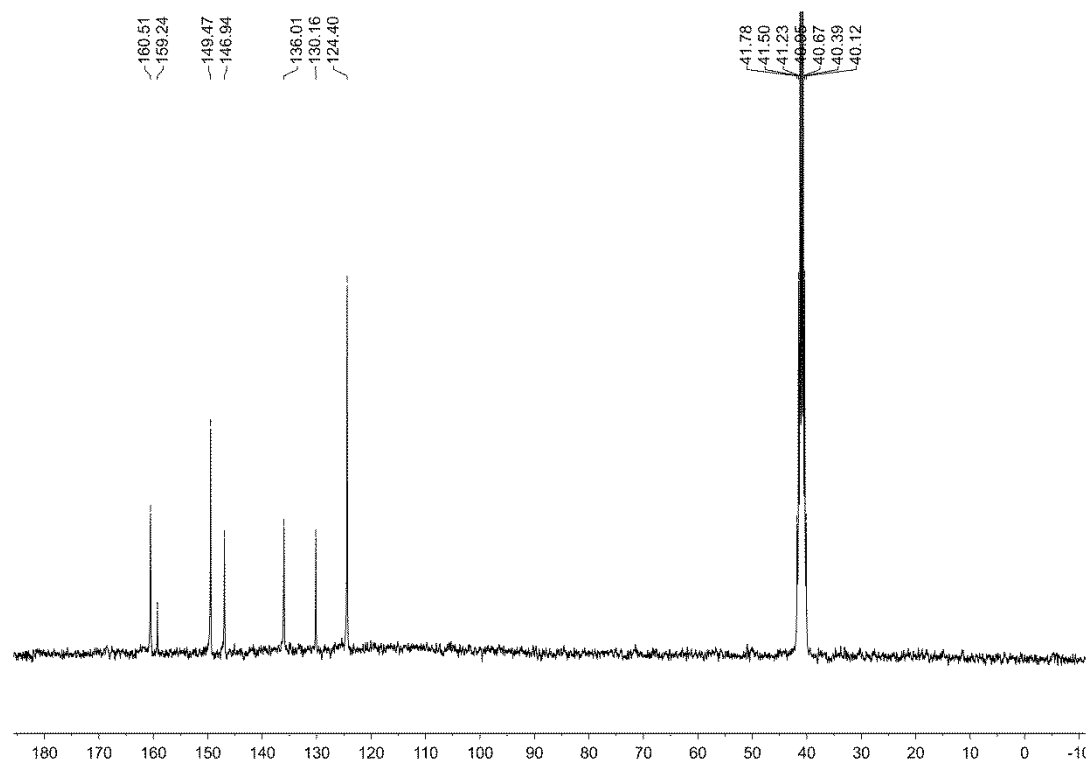


Figure S18 ^{13}C NMR spectra (75 MHz) of **9** in $[\text{D}_6]\text{DMSO}$ at 25 $^\circ\text{C}$

4. Figure S19-S26 DSC and TG plots of compounds 1 and 3-9

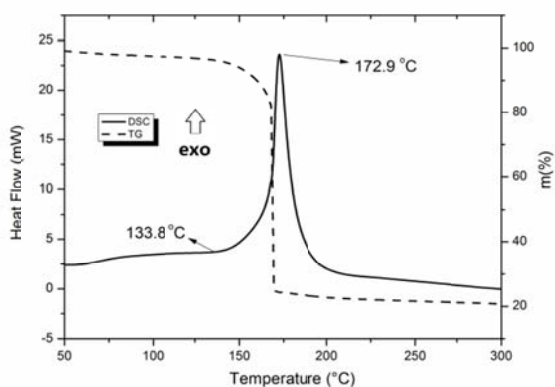


Figure S19 The DSC and TG plots of 1

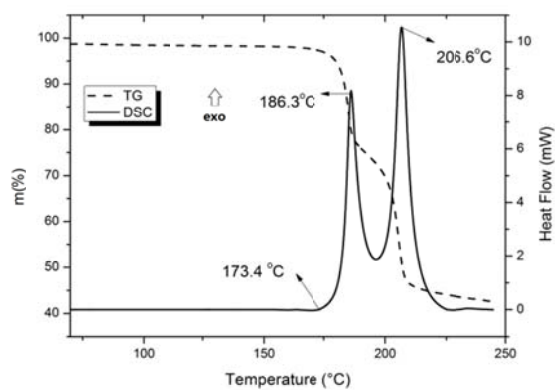


Figure S20 The DSC and TG plots of 3

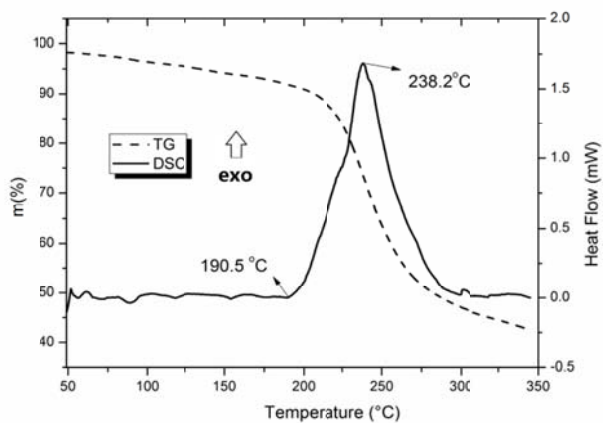


Figure S21 The DSC and TG plots of 4

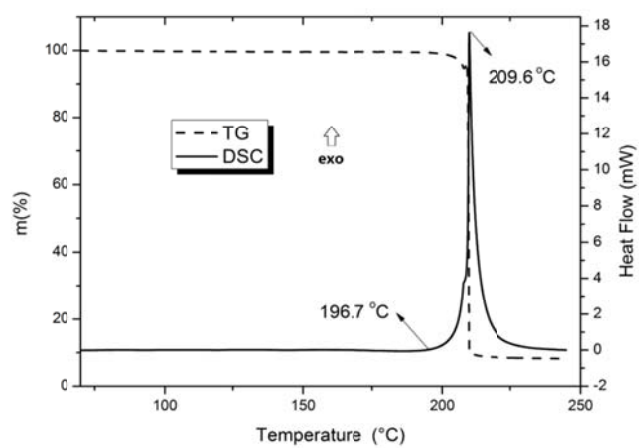


Figure S22 The DSC and TG plots of 5

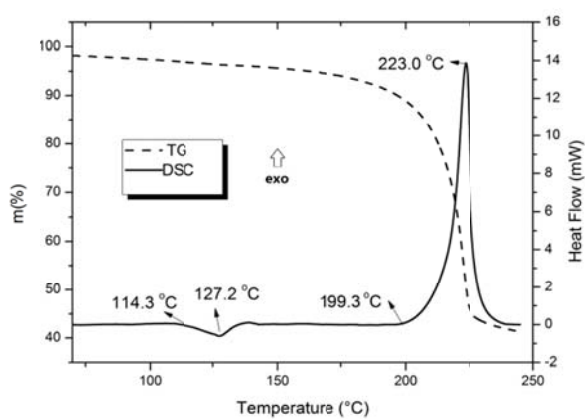


Figure S23 The DSC and TG plots of 6

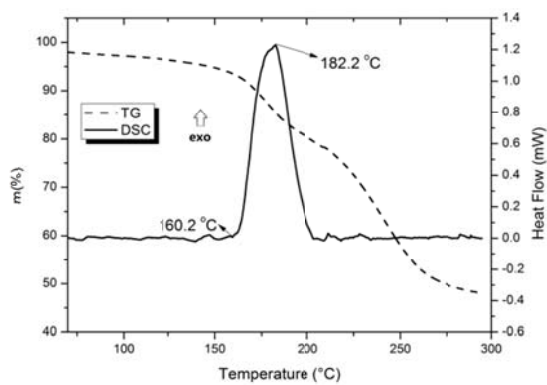


Figure S24 The DSC and TG plots of 7

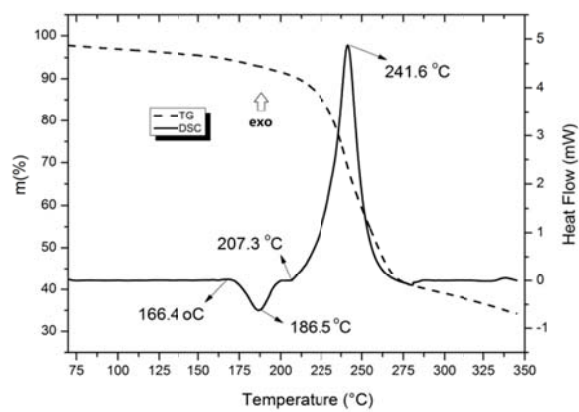


Figure S25 The DSC and TG plots of **8**

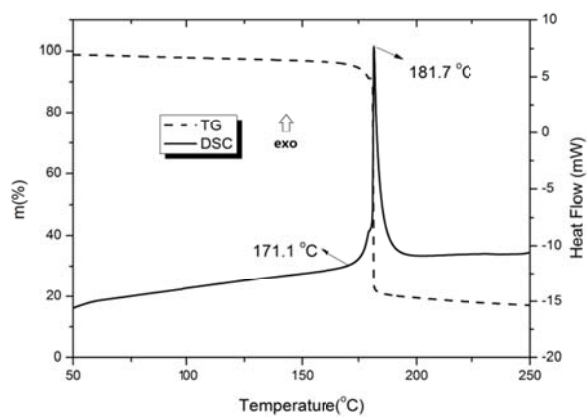


Figure S26 The DSC and TG plots of **9**