Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information (SI)

Synthesis of nitrogen-rich and thermostable energetic materials based on hetarenecarboxylic acids

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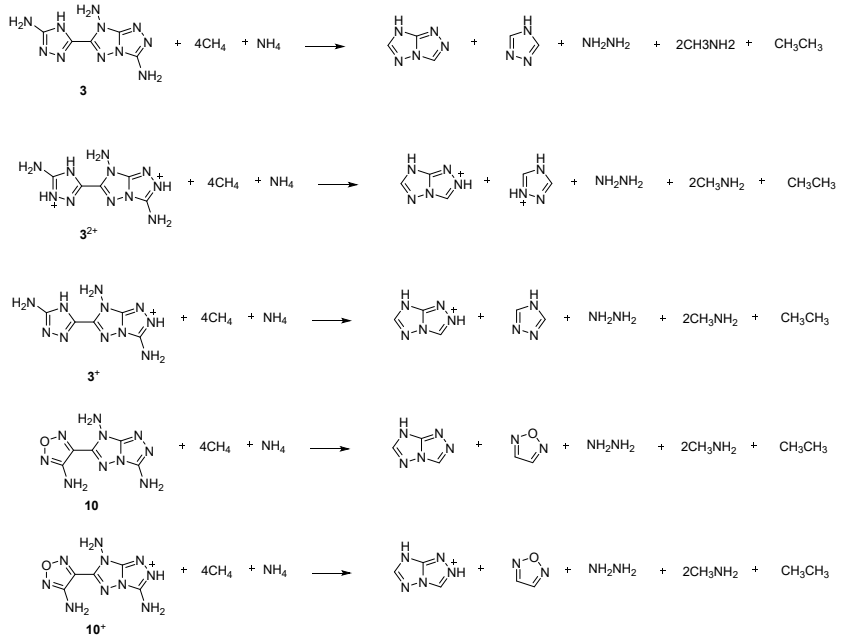
Table of Content

1. Computational details

The calculation was performed by using the Gaussian 09 program package[1]. The geometric optimization of all the structures and frequency analyses for calculation of heats of formation was carried out by using B3-LYP functional[2] with 6-311+G** basis set[3,4] . 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 these compounds were computed through appropriate isodesmic reactions (Scheme S1). Atomization energies were calculated by the CBS-4M[5]. Total energy and heat of formation for the reference compounds are summarized in Table S11. All the optimized structures were characterized to be true local energy minima on the potential-energy surface without imaginary frequencies.



Scheme S1 Isodesmic and tautomeric reactions to compute the HOF.

Table S1 Total energy and heat of formation for the reference compounds

	E_0[a]/a.u.	ZPE [b] / kJ·mol^{-1}	ΔH_T [c] / kJ mol^{-1}	HOF [d] / kJ mol^{-1}
3	-797.1001102	419.07	38.61	769.5
3 cation^{+}	-797.5007581	448.33	41.61	1283.2
3 cation^{2+}	-798.5648624	478.65	40.23	2112.1
10	-816.9084255	384.06	39	820.3
10 cation^{+}	-817.2945799	415.46	40.62	1372.8
CH_3NH_2	-95.89384	160.78	11.64	-22.5
NH_2NH_2	-111.9105763	134.28	11.16	95.4
CH_3CH_3	-79.8565413	187.31	11.79	-84.0

[a] E_0 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 from Ref. [N. Fischer, T. M. Klapötke and J. Stierstorfer, Z. Anorg. Allg. Chem., 2009, 635, 271.]

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2. The crystallographic data

Experimental section

Caution! Although we experienced no explosion in handling these energetic materials, the use of small scale and best safety practices (leather gloves, face shield) are strongly encouraged **!**

General methods

^{1}H and ^{13}C NMR spectra are recorded on a 500 MHz (Bruker AVANCE 500) NMR spectrometer operating at 500 and 125 MHz, respectively. The decomposition points are obtained on a differential scanning calorimeter at a heating rate of 5°C min^{-1}. IR spectra are recorded on a FT-IR spectrometer (Thermo Nicolet AVATAR 370) as thin films by using KBr plates. Densities are determined at 25 °C by employing a Micromeritics AccuPyc II 1340 gas pycnometer. Elemental analyses were carried out by using a Vario Micro cube Elementar Analyser. Impact and friction sensitivity measurements are made by using a standard BAM Fall hammer and a BAM friction tester. Detonation velocity and detonation pressure data are calculated by program package EXPLO5 (version 6.02).

X-ray crystallography

The data for **4**•H_2O, **7** and **11**•H_2O were collected with a Bruker SMART APEX II CCD diffractometer with graphite-monochromated Mo-Ka radiation (λ=0.071073 nm) at 160 K or 170 K. The data collection and the initial unit cell refinement are performed by using APEX2 (v2010.3-0). Data Reduction is performed by using SAINT (v7.68A) and XPREP (v2008/2). Empirical absorption corrections are applied by using the SADABS (v2008/1) program. The structures are solved by direct methods and refined by the full matrix least-squares based on F2 using SHELXTL--2014/7 (Sheldrick, 2014) programme package. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms attached to ligands are included using a riding model. The crystallographic data and CCDC numbers for these compounds are summarized in Table S2

Table S2 Crystallographic Data for **4**•H_2O, **7** and **11**•H_2O

	4•H_2O	**7**	**11**•H_2O
Empirical formula	$C_5H_{11}N_{13}O_7$	$C_5H_6N_{10}O$	$C_5H_9N_{11}O_5$
Formula weight	365.27	220.20	303.23
Temperature/K	160	170.0	160
Crystal system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	$P2_1/c$
a/Å	6.5824(11)	6.8113(9)	7.0384(3)
b/Å	9.6308(11)	8.2072(10)	13.0429(6)
c/Å	11.1986(16)	8.5119(12)	12.7579(6)
α/°	77.516(4)	108.619(5)	90
β/°	75.288(4)	109.314(5)	104.682(2)
γ/°	89.243(3)	92.750(5)	90
Volume/Å^3	669.76(17)	419.23(10)	1132.95(9)
Z	2	2	4
ρ_{calc} g/cm^3	1.811	1.760	1.778
μ/mm^{-1}	0.163	0.138	0.156
F(000)	376	228.0	624.0
Crystal size/mm^3	0.04 x0.09 x0.16	0.15 × 0.08 × 0.05	0.17 × 0.11 × 0.06
Radiation	MoKα (λ=0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.854 to52.89	5.316 to 52.842	4.544 to 55.078
Index ranges	-8≤h≤8, -12≤k≤12, -14≤l≤ 13	-8≤ h ≤ 8, -10 ≤ k ≤ 10, -10 ≤ l ≤ 10	-9 ≤ h ≤ 8, -16 ≤ k ≤ 16, -16 ≤ l ≤ 16
Reflections collected	7581	4856	12695
Independent reflections	2733 [R_{int} = 0.0576, R_{sigma} = 0.0762]	1710 [R_{int} = 0.0468, R_{sigma} = 0.0580]	2580 [Rint = 0.0401, Rsigma = 0.0321]
Data/restraints/parameters	2733/1/241	1710/0/155	2580/0/218
Goodness-of-fit on F^2	1.049	1.031	1.019
Final R indexes [I>=2σ (I)]	R_1 = 0.0720, wR_2 = 0.1770	R1 = 0.0461, wR2 =0.1013	R1 = 0.0411, wR2 = 0.1000
Final R indexes [all data]	R_1 = 0.11151, wR_2 = 0.2144	R1 = 0.0782, wR2 = 0.1219	R1 = 0.0549, wR2 = 0.1110
Largest diff. peak/hole / e Å^{-3}	0.61/-0.36	0.25/-0.25	0.35/-0.27
CCDC	2078516	2078515	2078514

Table S3 Bond distance of compound **4**•H_2O

parameter	Å	parameter	Å
O2-N13	1.268(5)	N6 -C2	1.370(5)
O3-N13	1.246(5)	N8-C4	1.376(5)

O4 -N13	1.239(5)	N8-C5	1.361(5)
O5-N12	1.251(5)	N9-N10	1.375(4)
O6-N12	1.246(5)	N9 -C4	1.296(5)
O7 -N12	1.262(4)	N10-C5	1.327(4)
O1-H1B	0.8700	N11-C5	1.313(5)
O1 -H1A	0.8700	N2-H2	0.95(5)
N1-C2	1.285(5)	N3 -H3A	0.8800
N1-N2	1.407(5)	N3 -H3B	0.8800
N2-C1	1.332(5)	N7-H7A	0.89(4)
N3-C1	1.305(5)	N7-H7B	0.90(5)
N4-C1	1.370(5)	N8-H8	0.8800
N4-C2	1.364(5)	N10 -H10	0.8800
N4-N5	1.392(4)	N11-H11B	0.8800
N5-C3	1.323(5)	N11-H11A	0.8800
N6-N7	1.400(5)	C3-C4	1.444(6)
N6-C3	1.377(5)		

Table S4 Bond angle of compound **4**•H_2O

parameter	°	parameter	°
H1A-O1-H1B	104.00	C5-N11-H11A	120.00
N2-N1-C2	100.5(3)	H11A-N11-H11B	120.00
N1 -N2 -C1	114.7(3)	C5-N11-H11B	120.00
N5-N4 -C2	114.3(3)	O2-N13-O4	120.2(4)
C1-N4-C2	107.1(3)	O3-N13-O4	120.7(3)
N5-N4-C1	138.3(3)	O2-N13 -O3	119.0(3)
N4-N5-C3	100.8(3)	O5-N12-O7	119.6(3)
N7-N6-C2	129.2(3)	O6 -N12-O7	119.9(4)
C2-N6-C3	106.5(3)	O5-N12-O6	120.4(3)
N7-N6-C3	124.1(3)	N2-C1 -N3	130.0(4)
C4-N8-C5	106.2(3)	N2 -C1-N4	103.1(3)
N10-N9-C4	104.7(3)	N3-C1-N4	126.9(4)
N9-N10-C5	111.5(3)	N4 -C2-N6	104.1(3)
N1-N2-H2	121(3)	N1-C2-N6	141.2(3)
C1-N2-H2	124(3)	N1-C2-N4	114.7(3)
C1-N3-H3B	120.00	N5-C3-C4	122.5(3)
H3A-N3-H3B	120.00	N5-C3 -N6	114.4(3)
C1-N3-H3A	120.00	N6-C3-C4	123.1(3)
N6-N7-H7B	106(3)	N8-C4 -N9	111.5(3)
H7A-N7-H7B	116(4)	N8-C4-C3	125.4(3)
N6-N7-H7A	111(3)	N9 -C4-C3	123.0(3)
C4-N8-H8	127.00	N8-C5-N10	106.1(3)
C5-N8-H8	127.00	N8-C5-N11	125.3(3)
C5-N10-H10	124.00	N10-C5-N11	128.6(4)
N9-N10-H10	124.00		

Table S5 Torsion angles of compound **4**•H_2O

parameter	°	parameter	°
C2-N1-N2-C1	-0.5(4)	C4 -N8-C5 -N11	179.8(4)
N2 -N1-C2 -N4	1.4(4)	C4-N9-N10 -C5	0.0(4)
N2 -N1 -C2-N6	-174.9(5)	N10-N9 -C4-N8	-0.3(4)
N1-N2-C1 -N3	178.7(4)	N10-N9-C4-C3	-177.6(4)
N1 -N2-C1 -N4	-0.5(4)	N9-N10-C5-N8	0.2(4)
C1-N4-N5 -C3	-172.7(5)	N9 -N10-C5-N11	-179.9(4)
C2-N4-N5-C3	-1.1(4)	N5-C3-C4-N8	-165.6(4)
N5-N4-C1-N2	173.2(4)	N5-C3-C4 -N9	11.3(6)
N5-N4-C1-N3	-6.0(8)	N6-C3-C4-N8	13.3(6)
C2-N4-C1-N2	1.3(4)	N6C3-C4-N9	-169.8(4)
C2-N4-C1-N3	-178.0(4)	N7 -N6-C3 -N5	176.1(4)
N5 -N4-C2 -N1	-176.0(3)	N7-N6 -C3 -C4	-3.0(6)
N5-N4-C2 -N6	1.7(4)	C2-N6-C3 -N5	0.9(5)
C1 -N4-C2 -N1	-1.8(5)	C2-N6-C3-C4	-178.1(4)
C1-N4-C2-N6	175.8(3)	C5-N8-C4-N9	0.4(5)
N4-N5-C3 -N6	0.1(4)	C5-N8-C4 -C3	177.6(4)
N4-N5-C3-C4	179.1(4)	C4 -N8-C5-N10	-0.3(4)
N7 -N6 -C2 -N1	0.2(8)	C3-N6-C2 -N1	175.1(5)
N7-N6-C2 -N4	-176.3(4)	C3-N6 -C2 -N4	-1.5(4)

Table S6 Hydrogen bonds of compound **4**•H_2O

D-H···A	d(D-H)/Å	d(H···A)/ Å	d(D···A)/ Å	<(DHA)/ °
O1-H1A··· N9	0.8700	2.0700	2.914(5)	165.00
O1- H1B··· O2	0.8700	1.9000	2.769(4)	173.00
O1-H1B···O3	0.8700	2.5700	3.095(4)	119.00
N2- H2···O6	0.95(5)	2.50(4)	3.063(5)	118(3)
N2-H2···O7	0.95(5)	1.94(5)	2.884(5)	174(3)
N3-H3A···O5	0.8800	2.4000	2.947(5)	121.00
N3-H3A···O7	0.8800	2.1700	3.043(5)	174.00
N3-H3B···O2	0.8800	2.0300	2.905(5)	173.00
N7-H7A···N1	0.89(4)	2.30(4)	3.038(5)	141(3)
N7-H7B···O3	0.90(5)	2.60(5)	3.285(5)	134(4)
N7- H7B··· O3	0.90(5)	2.24(5)	2.960(5)	137(4)
N8-H8···O6	0.8800	2.0700	2.904(5)	158.00

N8 - H8···N7	0.8800	2.2800	2.809(5)	119.00
N10-H10···O1	0.8800	1.7600	2.619(4)	164.00
N11-H11A··· O3	0.8800	2.1500	3.000(4)	163.00
N11- H11A···O4	0.8800	2.5300	2.835(4)	101.00
N11-H11B···O5	0.8800	1.9800	2.858(4)	177.00
N11-H11B···O4	0.8800	2.5200	2.835(4)	102.00

Table S7 Bond distances of compound **7**

parameter	Å	parameter	Å
O1-N1	1.404(3)	N7-N8	1.431(3)
O1-N3	1.363(3)	N7-C4	1.303(3)
N1-C1	1.309(3)	N8-C5	1.320(3)
N2-C1	1.361(3)	N9-C5	1.373(3)
N3-C2	1.306(3)	N2-H2B	0.89(3)
N4-N5	1.388(2)	N2-H2A	0.90(3)
N4-C3	1.316(3)	N9-H9A	0.8800
N5-C4	1.350(3)	N9-H9B	0.8800
N5-C5	1.376(3)	N10 -H10B	0.8800
N6-N10	1.398(3)	N10-H10A	0.8800
N6-C3	1.386(3)	C1-C2	1.433(3)
N6-C4	1.370(3)	C2-C3	1.454(3)

Table S8 Bond angles of compound **7**

parameter	°	parameter	°
N1-O1-N3	111.09(19)	N6-N10-H10A	109.00
O1-N1-C1	105.3(2)	N6-N10-H10B	109.00
O1-N3-C2	105.8(2)	H10A-N10-H10B	109.00
N5 -N4 -C3	101.96(19)	N1-C1-C2	108.3(2)
N4-N5 -C4	113.41(19)	N2-C1-C2	128.0(2)
N4-N5-C5	141.0(2)	N1 -C1-N2	123.6(2)
C4-N5-C5	105.57(18)	N3-C2 -C1	109.6(2)
N10-N6-C3	131.50(19)	C1-C2 -C3	127.0(2)
N10-N6-C4	122.64(19)	N3-C2-C3	123.4(2)
C3-N6-C4	105.73(19)	N4-C3-N6	113.7(2)
N8-N7-C4	102.98(18)	N6-C3-C2	124.5(2)
N7-N8-C5	109.78(17)	N4-C3 -C2	121.8(2)
C1-N2-H2A	114.6(19)	N5-C4-N7	113.9(2)
C1 -N2-H2B	114.7(19)	N6-C4-N7	140.8(2)
H2A-N2-H2B	115(3)	N5-C4-N6	105.25(19)
C5-N9-H9A	109.00	N8 -C5 -N9	128.1(2)
C5-N9-H9B	110.00	N5-C5 -N8	107.76(19)

H9A-N9-H9B	109.00	N5-C5-N9	123.9(2)

Table S9 Torsion angles of compound **7**

parameter	Å	parameter	Å
N3-O1-N1-C1	0.5(3)	N8-N7-C4-N6	177.6(3)
N1-O1-N3-C2	-0.4(2)	N7-N8-C5-N5	0.1(2)
O1-N1-C1-N2	-177.3(2)	N7-N8-C5-N9	-174.0(2)
O1-N1-C1-C2	-0.4(3)	N1-C1-C2 -N3	0.2(3)
O1-N3-C2-C1	0.2(3)	N1-C1-C2-C3	-178.9(2)
O1-N3-C2-C3	179.3(2)	N2 -C1-C2 -N3	176.9(2)
C3-N4-N5-C4	0.4(2)	N2-C1-C2-C3	-2.2(4)
C3-N4 -N5 -C5	177.9(3)	N3-C2-C3-N4	-175.1(2)
N5-N4-C3 -N6	-0.3(2)	N3 -C2 -C3-N6	4.9(4)
N5-N4-C3-C2	179.6(2)	C1-C2-C3 -N4	3.9(4)
N4-N5-C4-N6	-0.4(2)	C1-C2-C3-N6	-176.2(2)
N4-N5-C4-N7	177.57(18)	C4-N6 -C3-C2	-179.8(2)
C5-N5-C4-N6	-178.71(18)	N10-N6 -C4-N5	176.39(19)
C5-N5-C4-N7	-0.8(3)	N10-N6-C4 -N7	-0.6(4)
N4 -N5 -C5 -N8	-177.2(2)	C3-N6-C4-N5	0.1(2)
N4-N5 -C5-N9	-2.9(4)	C3-N6-C4 -N7	-176.9(3)
C4-N5-C5-N8	0.4(2)	C4-N7-N8 -C5	-0.5(2)
C4-N5-C5-N9	174.7(2)	N8-N7-C4-N5	0.8(2)
N10-N6-C3 -N4	-175.7(2)	C4-N6-C3-N4	0.1(3)
N10-N6-C3 -C2	4.5(4)		

Table S10 Hydrogen bonds of compound **7**

D-H···A	d(D-H)/Å	d(H···A)/ Å	d(D···A)/ Å	<(DHA)/ °
N2-H2A···N7	0.90(3)	2.12(3)	2.988(3)	163(2)
N2-H2B···N4	0.89(3)	2.38(3)	2.980(3)	125(2)
N9-H9A···N10	0.8800	2.4100	3.230(3)	155.00
N9-H9B···N8	0.8800	2.2100	3.063(2)	163.00
N10-H10A···N3	0.8800	2.4900	3.219(3)	141.00
N10-H10B···N9	0.8800	2.5800	3.298(3)	139.00

Table S11 Bond distance of compound **11**·H_2O

parameter	Å	parameter	Å
O5-N8	1.3592(18)	N6-N7	1.404(2)
O5-N9	1.400(2)	N6-C2	1.363(2)
O2 -N11	1.2551(19)	N6-C3	1.388(2)
O3-N11	1.250(2)	N8-C4	1.306(2)

O4-N11	1.2288(19)	N9-C5	1.311(2)
O1-H1A	0.8700	N10 -C5	1.352(2)
O1-H1B	0.83(3)	N1-H1	0.93(2)
N1-N2	1.409(2)	N4-H4A	0.90(2)
N1 -C1	1.334(2)	N4-H4B	0.88(2)
N2-C2	1.2985(19)	N7-H7B	0.92(2)
N3-N5	1.3871(17)	N7-H7A	0.88(2)
N3-C2	1.358(2)	N10-H10B	0.8800
N3-C1	1.3640(19)	N10 -H10A	0.8800
N4 -C1	1.318(2)	C3-C4	1.453(2)
N5 -C3	1.313(2)	C4 -C5	1.440(2)

Table S12 Bond angle of compound **11**·H_2O

parameter	°	parameter	°
N8-O5-N9	111.28(12)	C5-N10-H10B	109.00
H1A-O1-H1B	109.00	H10A-N10 -H10B	109.00
N2-N1-C1	114.74(12)	C5-N10-H10A	109.00
N1-N2-C2	100.01(12)	O2-N11-O4	120.54(16)
N5-N3-C2	113.42(12)	O3 -N11-O4	122.30(16)
C1-N3-C2	107.35(12)	O2 -N11-O3	117.13(14)
N5-N3-C1	139.22(14)	N1 -C1-N3	103.26(13)
N3-N5 -C3	101.74(12)	N1-C1-N4	129.85(14)
N7 -N6 -C3	131.47(13)	N3 -C1-N4	126.82(14)
C2-N6 -C3	105.84(13)	N2-C2-N3	114.64(13)
N7-N6-C2	122.69(13)	N2-C2-N6	140.29(14)
O5-N8-C4	105.73(13)	N3-C2 -N6	105.06(12)
O5-N9-C5	105.63(12)	N5-C3-N6	113.93(13)
C1-N1-H1	129.3(14)	N5-C3 -C4	122.28(13)
N2-N1-H1	116.0(14)	N6-C3 -C4	123.79(13)
C1 -N4-H4A	117.7(14)	N8-C4-C3	121.71(13)
C1-N4-H4B	119.7(15)	N8-C4-C5	109.71(13)
H4A-N4 -H4B	122(2)	C3-C4-C5	128.58(13)
N6-N7-H7A	108.5(15)	N9-C5-N10	124.12(15)
N6-N7-H7B	107.8(14)	N9-C5-C4	107.65(13)
H7A-N7-H7B	109(2)	N10 -C5-C4	128.14(14)

Table S13 Torsion Angles compound **11**·H_2O

parameter	°	parameter	°
N9-O5-N8-C4	-0.20(18)	O5-N8 -C4 -C5	0.21(18)
N8-O5-N9-C5	0.11(17)	O5-N9-C5-N10	176.86(15)
C1-N1-N2 -C2	-0.03(18)	O5 -N9 -C5-C4	0.03(17)
N2 -N1-C1 -N3	-0.36(17)	N5 -C3-C4-N8	-177.10(15)
N2-N1-C1-N4	-177.51(15)	N5-C3-C4-C5	3.7(3)

N1-N2 -C -N3	0.42(17)	N6-C3 -C4-N8	3.8(2)
N1-N2-C2 -N6	-177.9(2)	N6-C3-C4-C5	-175.40(15)
C1-N3-N5-C3	-178.21(18)	N8-C4-C5-N9	-0.16(19)
C2-N3 -N5-C3	0.69(17)	N8 -C4-C5-N10	-176.82(17)
N5-N3-C1-N1	179.53(17)	C3-C4-C5-N9	179.13(16)
N5-N3-C1 -N4	-3.2(3)	C3-C4-C5 -N10	2.5(3)
C2-N3-C1-N1	0.58(16)	C2 -N6 -C3 -N5	-0.59(18)
C2-N3-C1-N4	177.85(15)	C2-N6-C3-C4	178.57(14)
N5-N3-C2 -N2	-179.92(14)	O5 -N8 -C4 -C3	-179.13(14)
N5-N3-C2 -N6	-1.06(17)	N7 -N6 -C2 -N3	179.90(15)
C1-N3-C2-N2	-0.67(18)	C3-N6-C2 -N2	179.3(2)
C1-N3-C2-N6	178.19(12)	C3-N6 -C2 -N3	0.95(16)
N3-N5-C3-N6	-0.04(17)	N7-N6-C3 -N5	-179.41(16)
N3-N5-C3 -C4	-179.22(14)	N7-N6-C3-C4	-0.3(3)
N7 -N6-C2-N2	-1.7(3)		

Table S14 Hydrogen bonds compound **11**·H_2O

D-H···A	d(D-H)/Å	d(H···A)/ Å	d(D···A)/ Å	<(DHA)/ °
N1-H1···O1	0.93(2)	1.95(2)	2.746(19)	143.8(19)
N1- H1···O3	0.93(2)	2.18(2)	2.847(2)	128.5(18)
O1-H1A···O2	0.8700	1.8900	2.729(2)	162.00
O1-H1B···N9	0.83(3)	2.12(3)	2.924(19)	164(2)
N4- H4A···O2	0.90(2)	2.01(2)	2.895(19)	169.1(18)
N4-H4A···O3	0.90(2)	2.42(2)	3.101(2)	132.7(18)
N4- H4B···N7	0.88(2)	2.08(2)	2.962(2)	175.5(19)
N7-H7A···O3	0.88(2)	2.00(2)	2.863(2)	166(2)
N7-H7B···O1	0.92(2)	2.07(2)	2.964(2)	161.9(19)
N10-H10A··· O4	0.8800	2.2600	3.124(2)	167.00
N10- H10B ···N5	0.8800	2.5500	3.051(19)	117.00
N10-H10B···O3	0.8800	2.5500	3.398(2)	163.00

3. ^{1}H and ^{13}C NMR spectra of new compounds

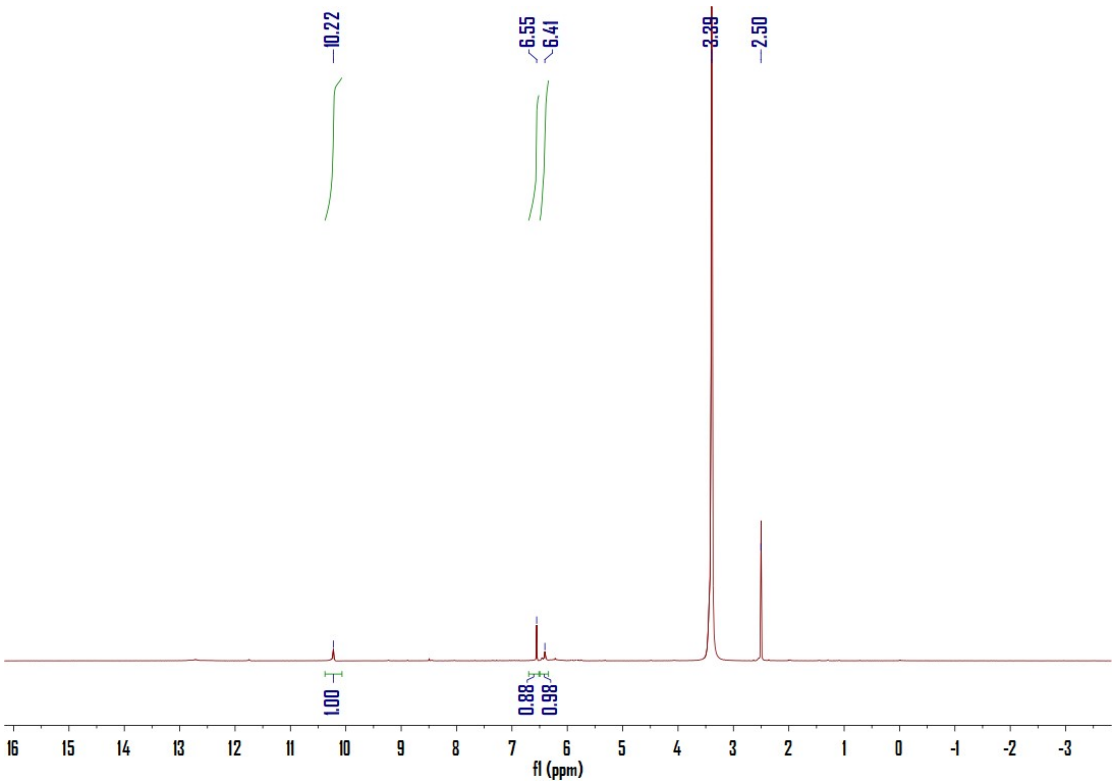

Figure S1^{1}H NMR spectra (500MHz) of **2** in [D_6] DMSO at 25 ^{o}C.

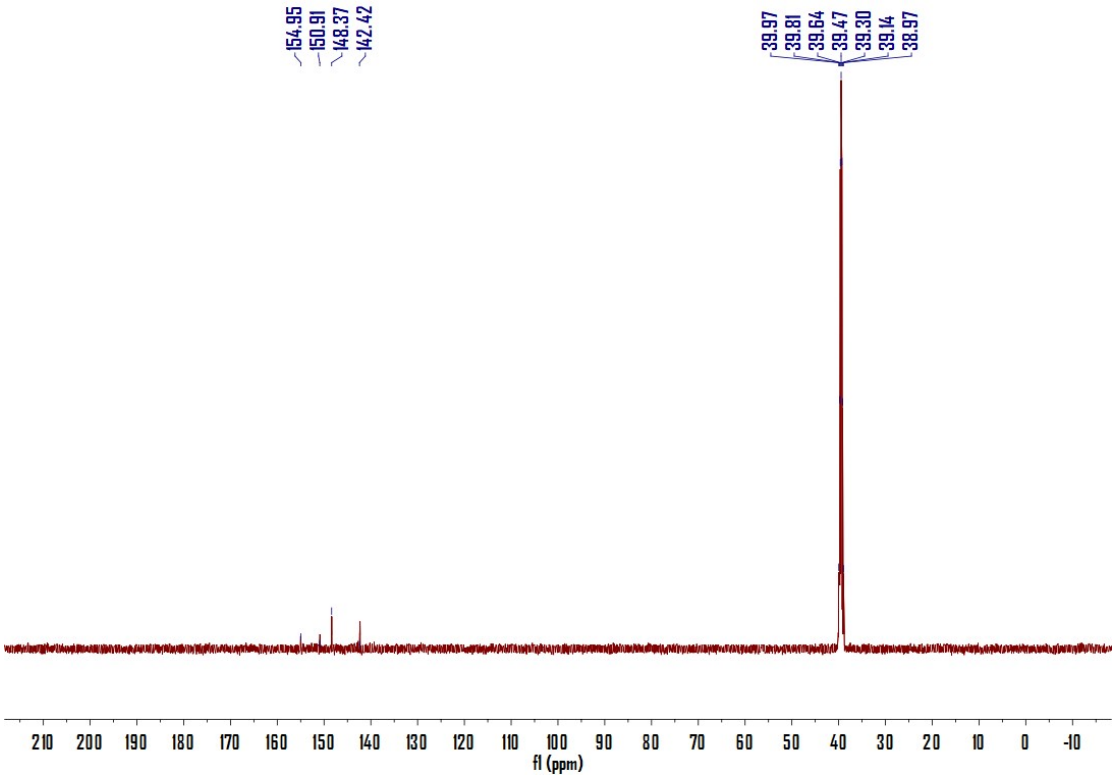

Figure S2 ^{13}C NMR spectra (125 MHz) of **2** in [D6] DMSO at 25 ^{o}C.

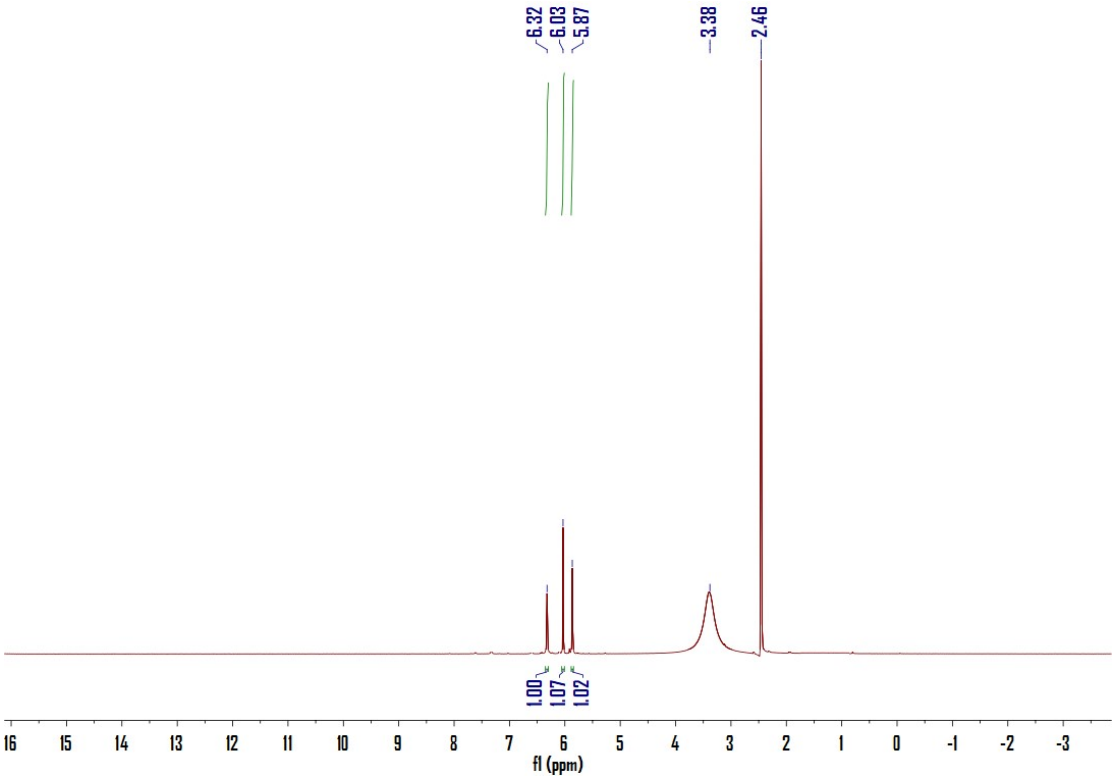

Figure S3[1]H NMR spectra (500MHz) of **3** in [D_6] DMSO at 25 °C.

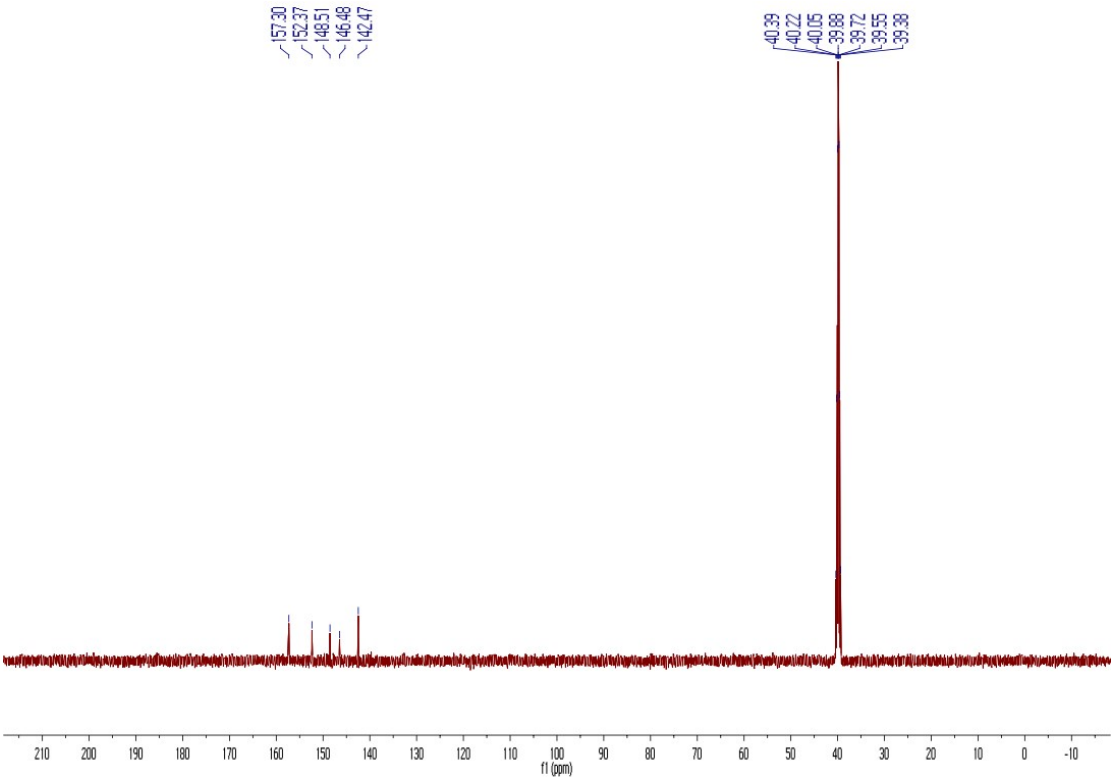

Figure S4 [13]C NMR spectra (125 MHz) of **3** in [D6] DMSO at 25 °C.

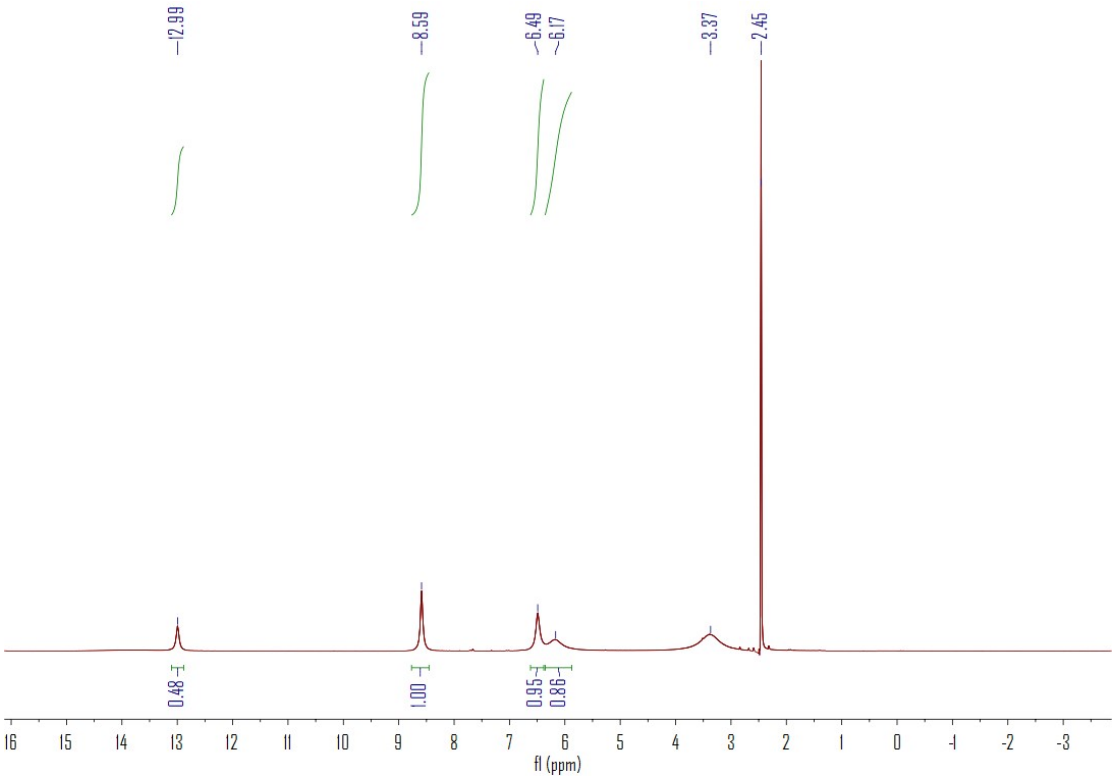

Figure S5 ^{1}H NMR spectra (500MHz) of **4** in [D_6] DMSO at 25 ^{o}C.

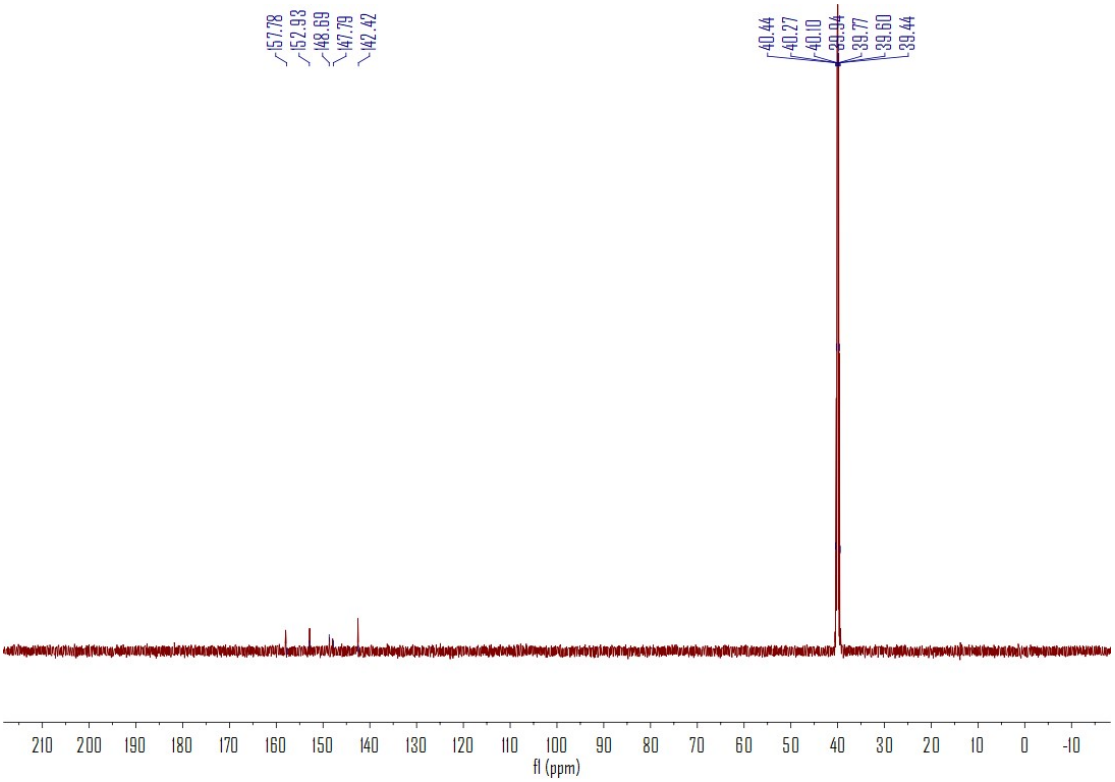

Figure S6 ^{13}C NMR spectra (125 MHz) of **4** in [D6] DMSO at 25 ^{o}C.

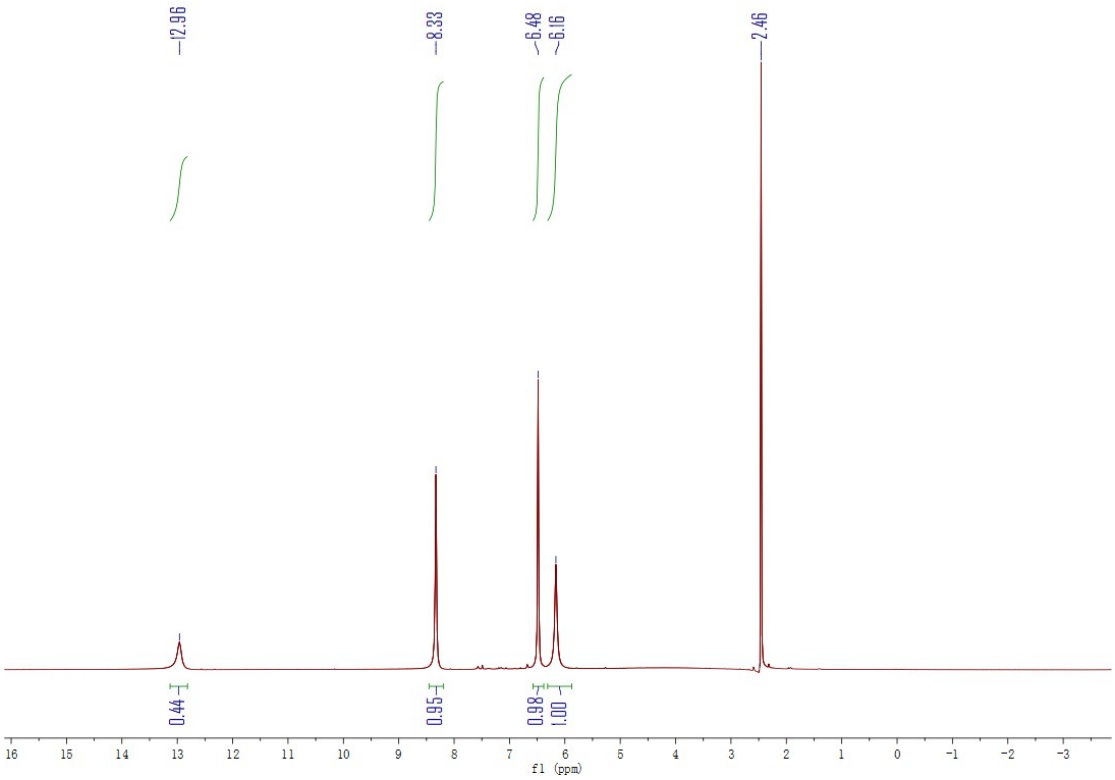

Figure S7 ^{1}H NMR spectra (500MHz) of **5** in [D_6] DMSO at 25 ^{o}C.

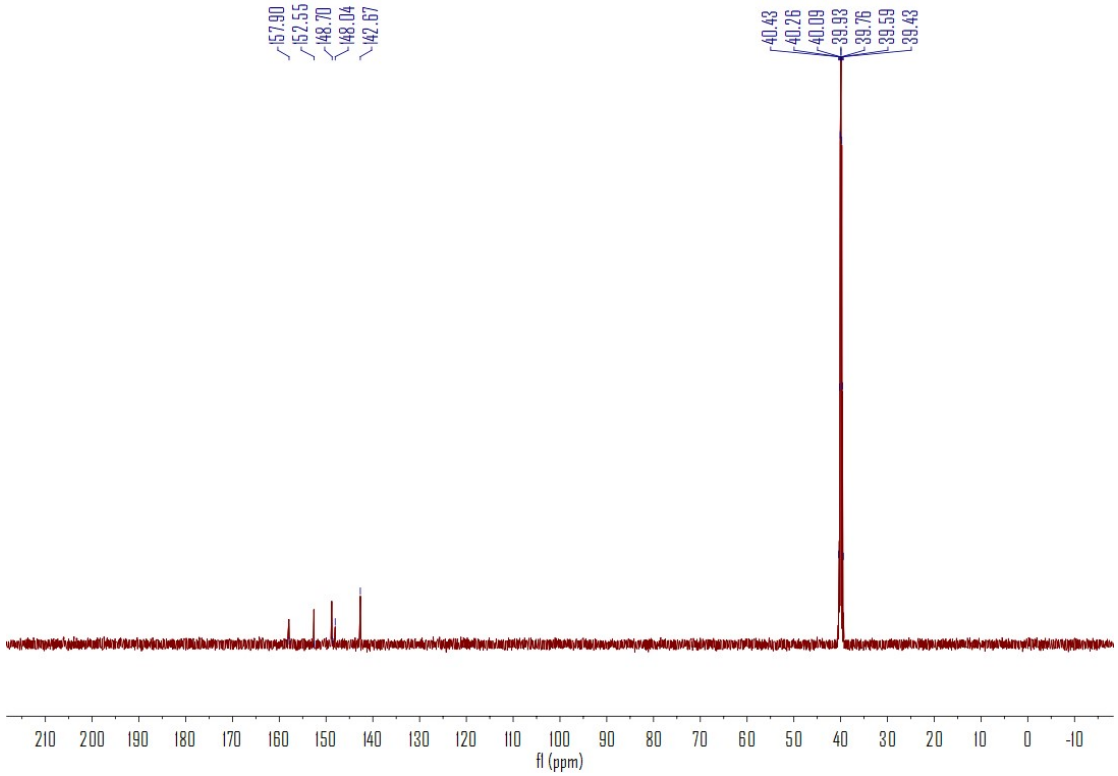

Figure S8 ^{13}C NMR spectra (125 MHz) of **5** in [D6] DMSO at 25 ^{o}C.

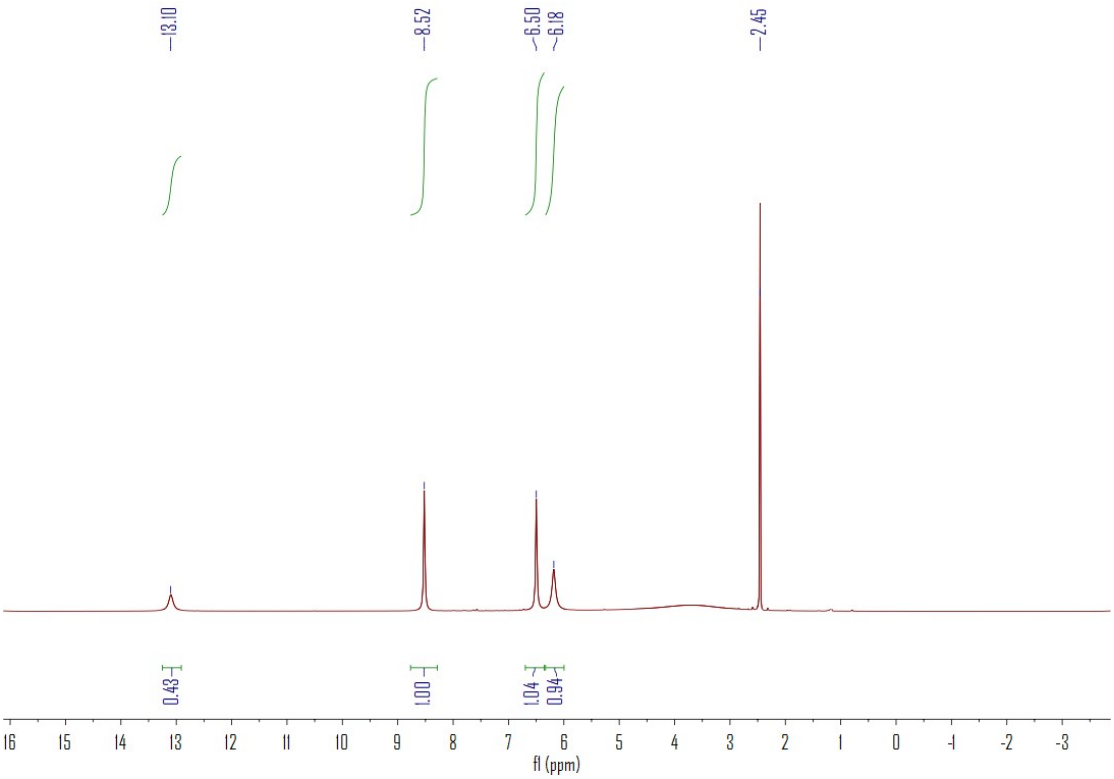

Figure S9[1]H NMR spectra (500MHz) of **6** in [D_6] DMSO at 25 °C.

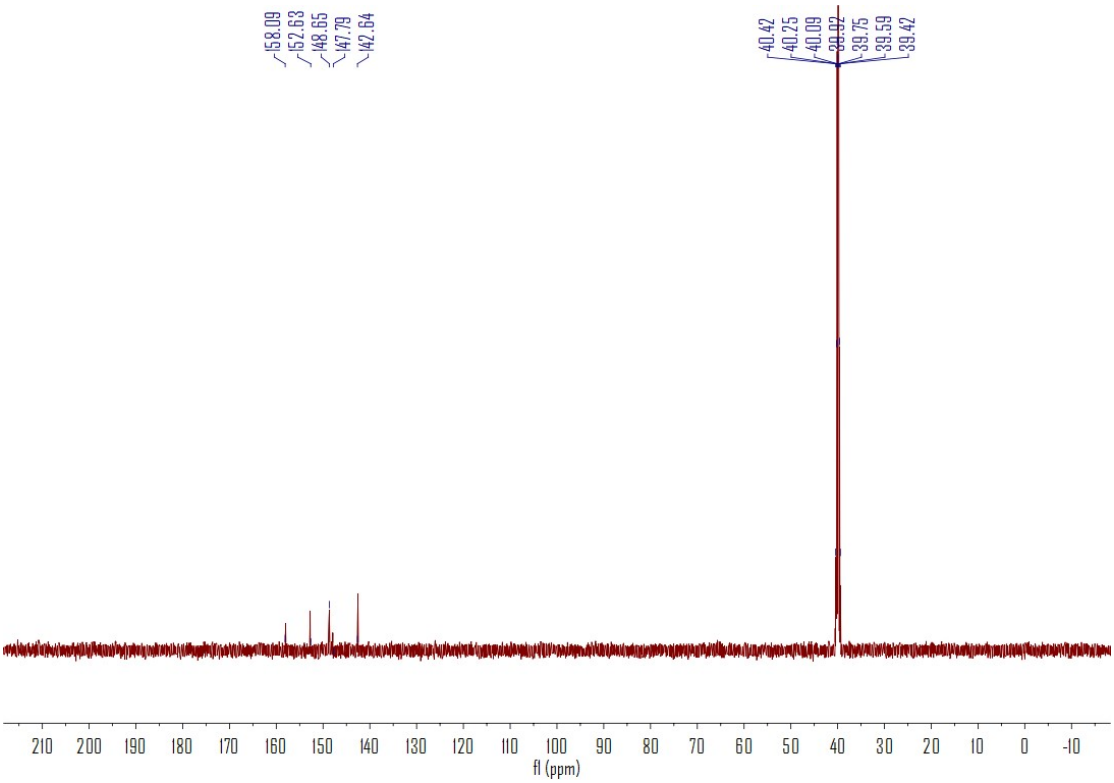

Figure S10 [13]C NMR spectra (125 MHz) of **6** in [D6] DMSO at 25 °C.

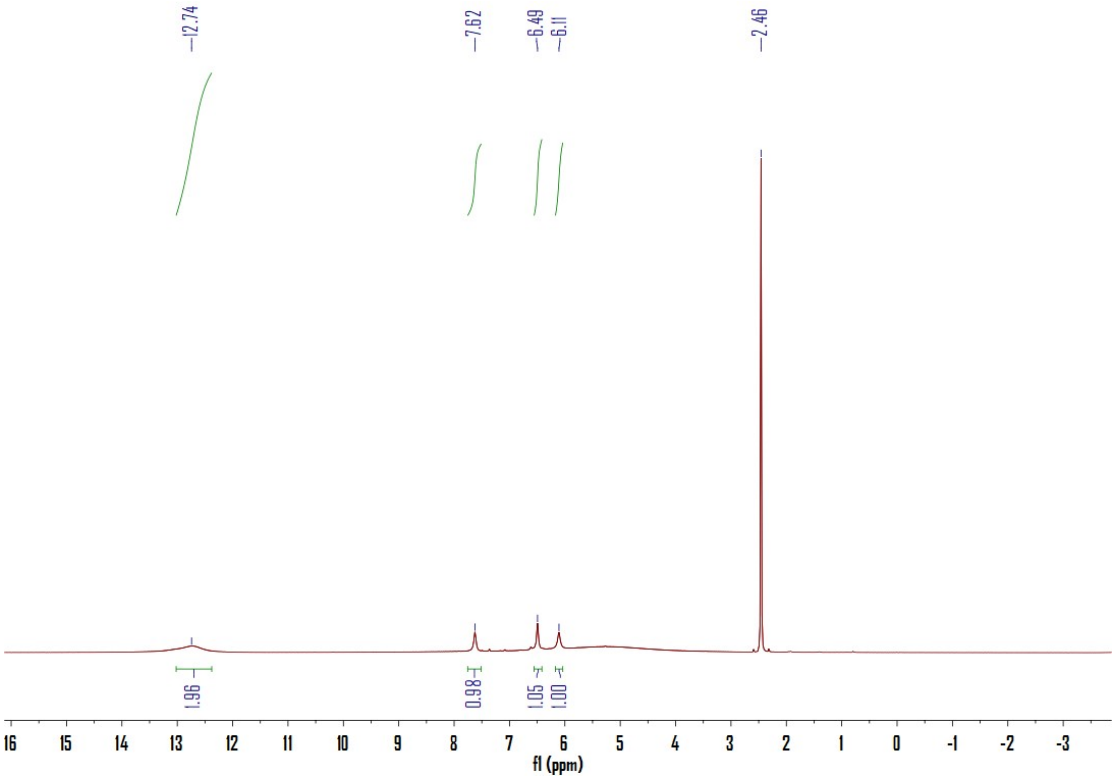

Figure S11[1]H NMR spectra (500MHz) of **7** in [D_6] DMSO at 25 °C.

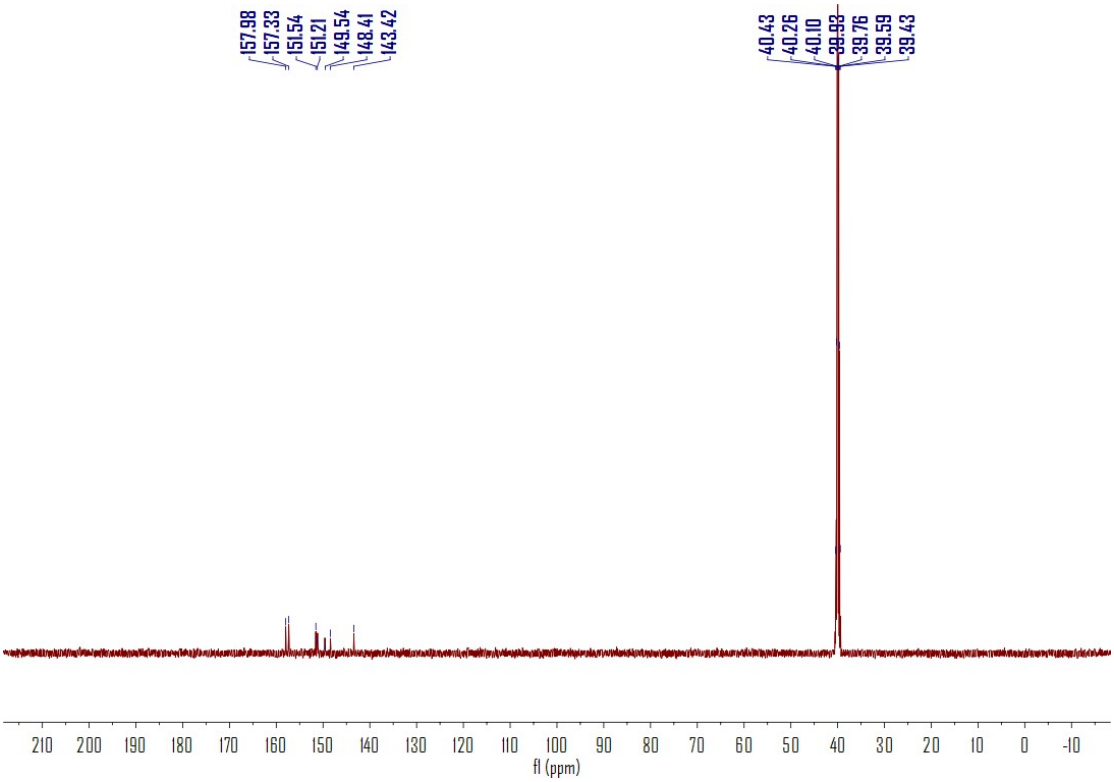

Figure S12[13]C NMR spectra (125 MHz) of **7** in [D6] DMSO at 25 °C.

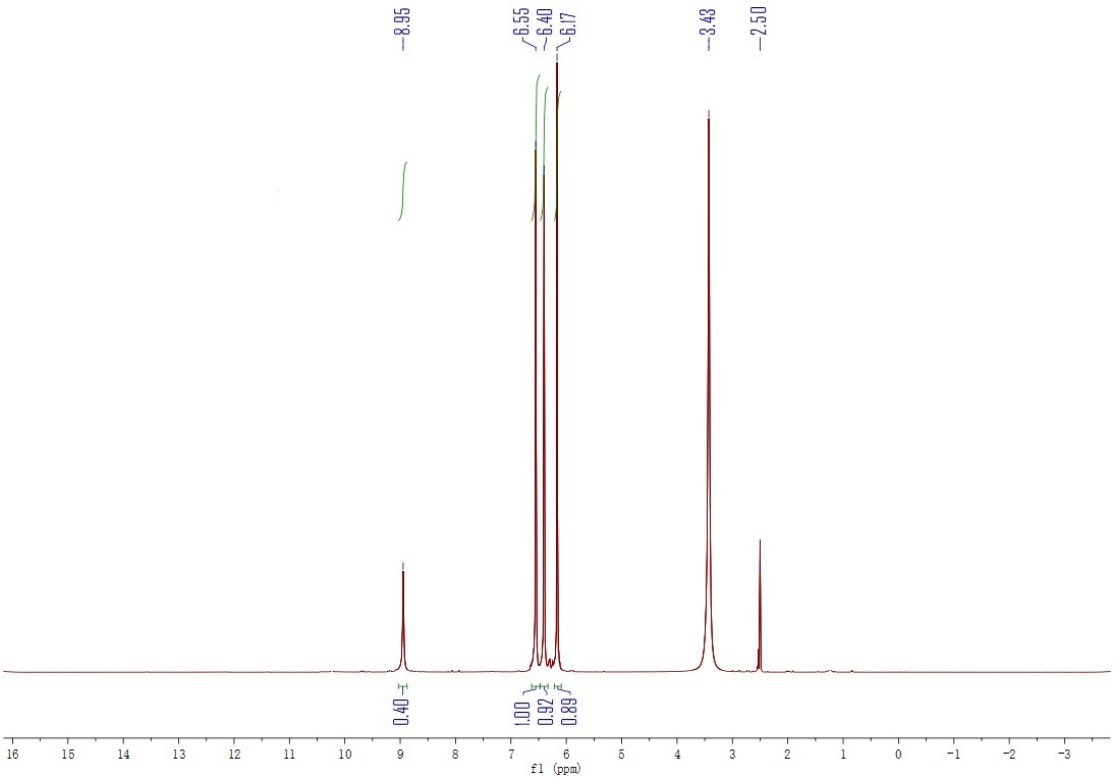

Figure S13[1]H NMR spectra (500MHz) of **9** in [D_6] DMSO at 25 °C.

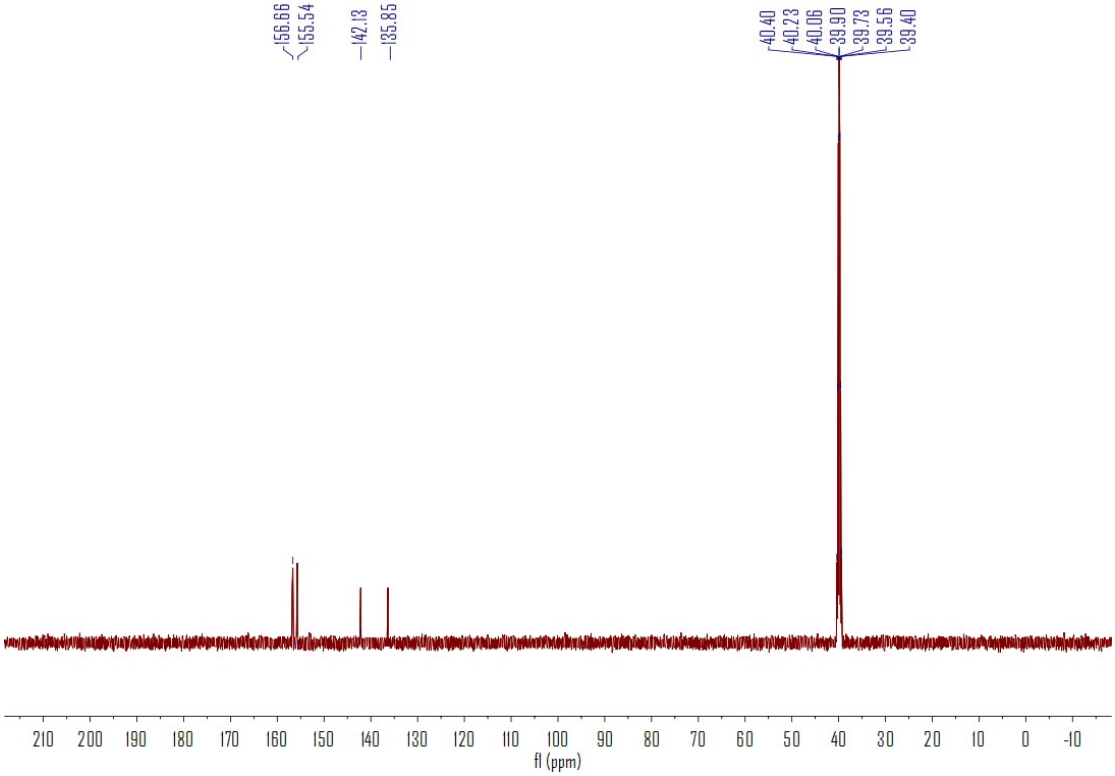

Figure S14[13]C NMR spectra (125 MHz) of **9** in [D6] DMSO at 25 °C.

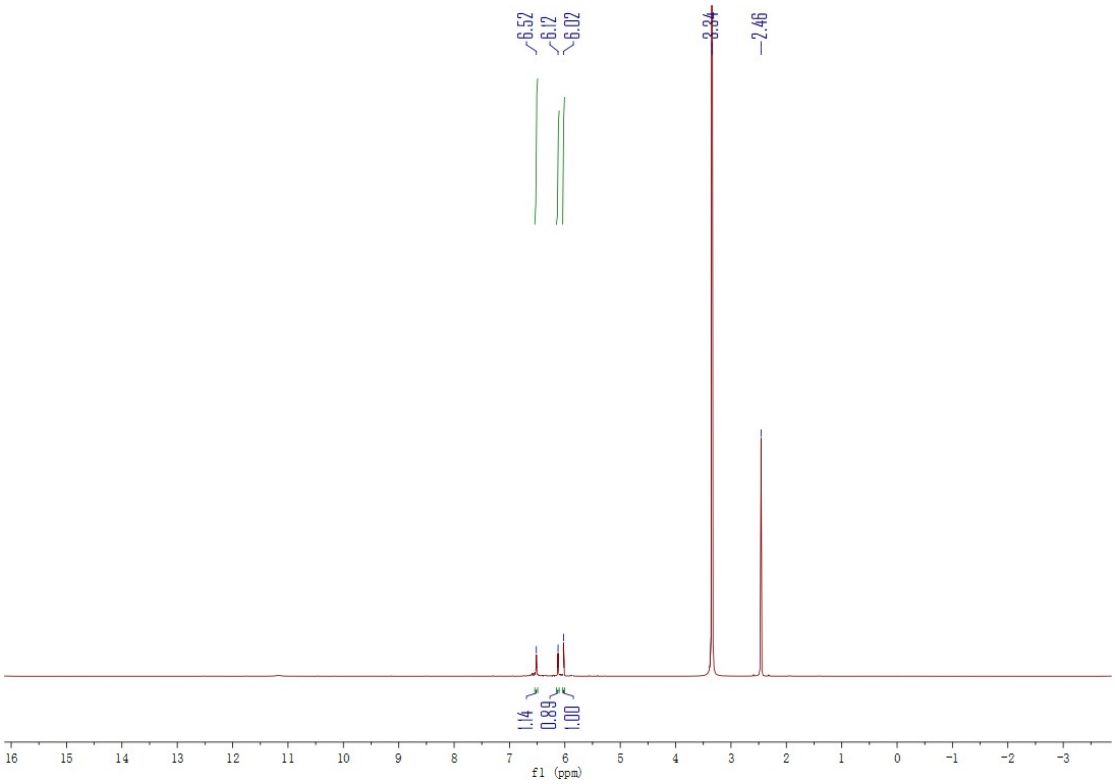

Figure S15 ^{1}H NMR spectra (500MHz) of **10** in [D_6] DMSO at 25 ^{o}C.

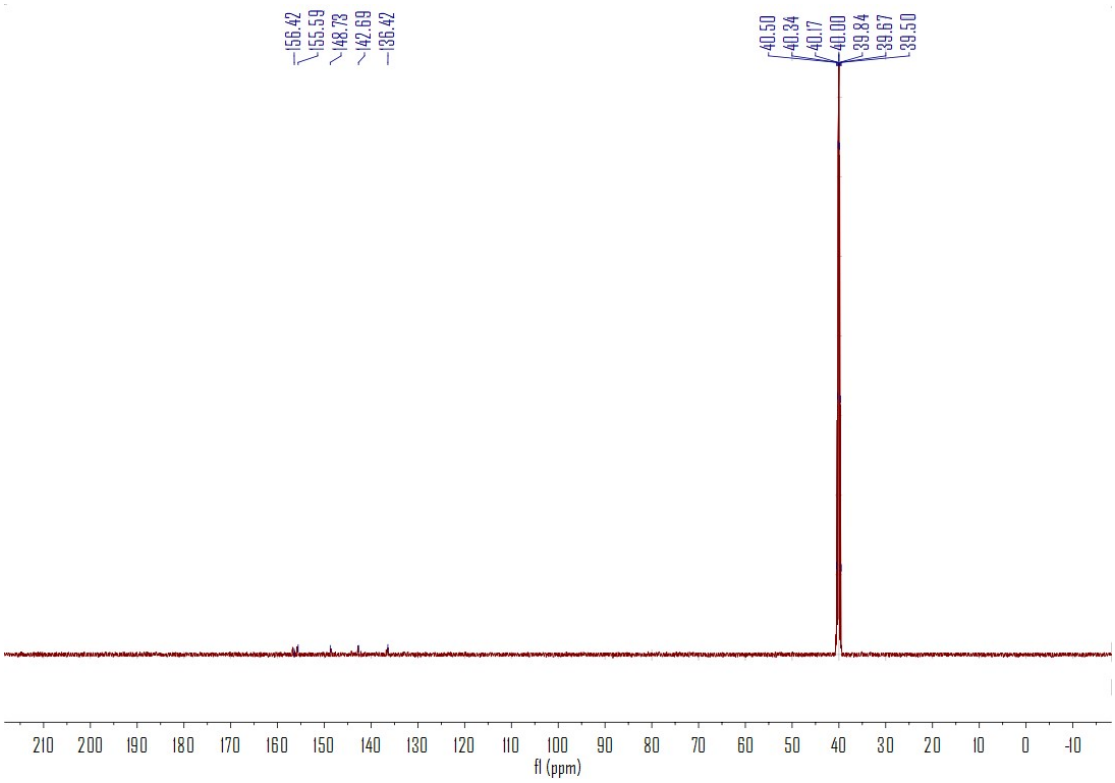

Figure S16 ^{13}C NMR spectra (125 MHz) of **10** in [D6] DMSO at 25 ^{o}C.

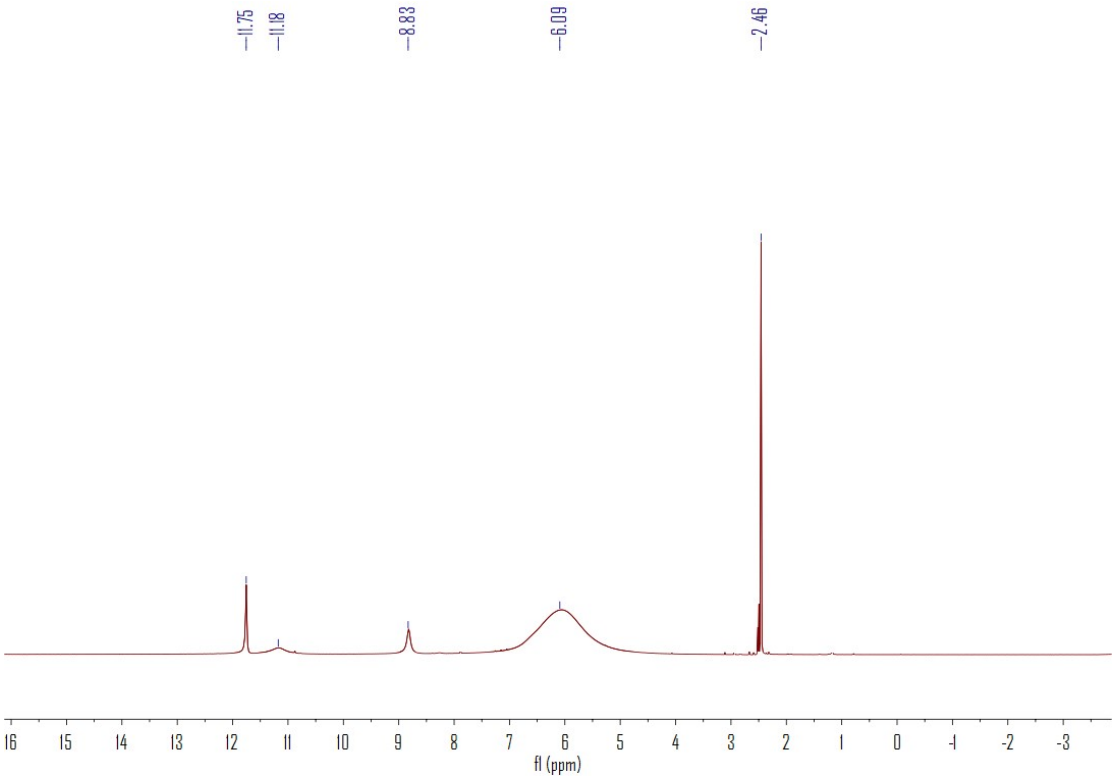

Figure S17 ^{1}H NMR spectra (500MHz) of **11** in [D_6] DMSO at 25 ^{o}C.

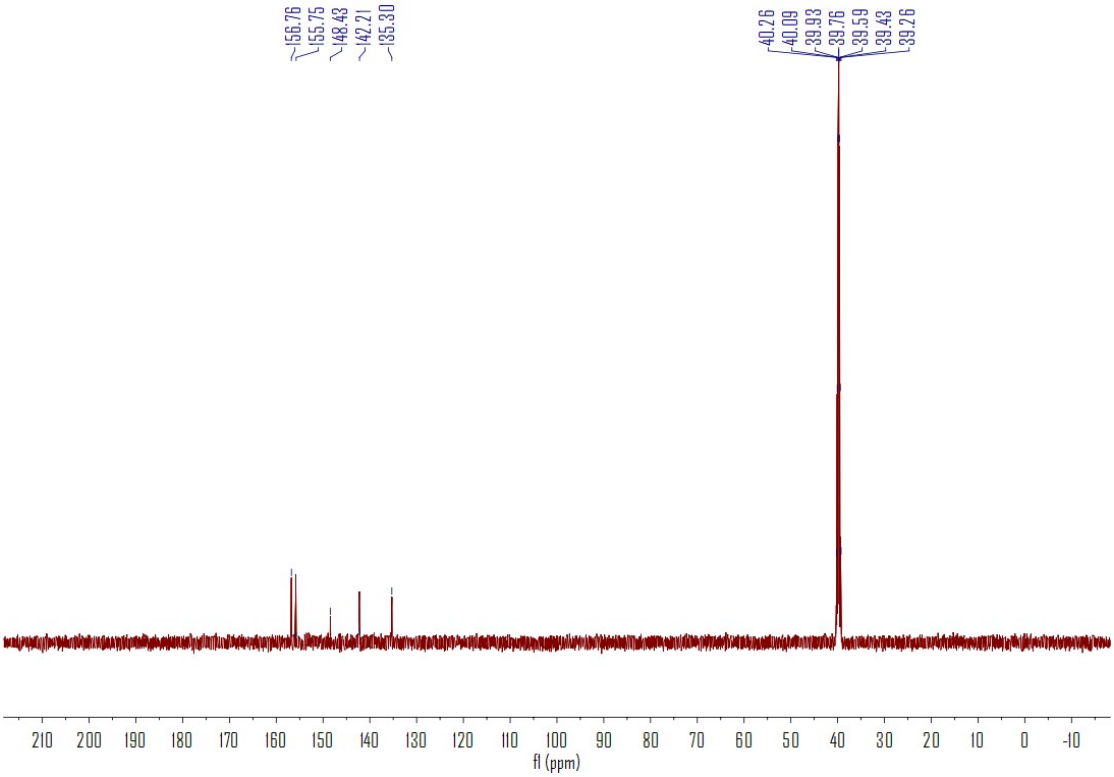

Figure S18 ^{13}C NMR spectra (125 MHz) of **11** in [D6] DMSO at 25 ^{o}C.

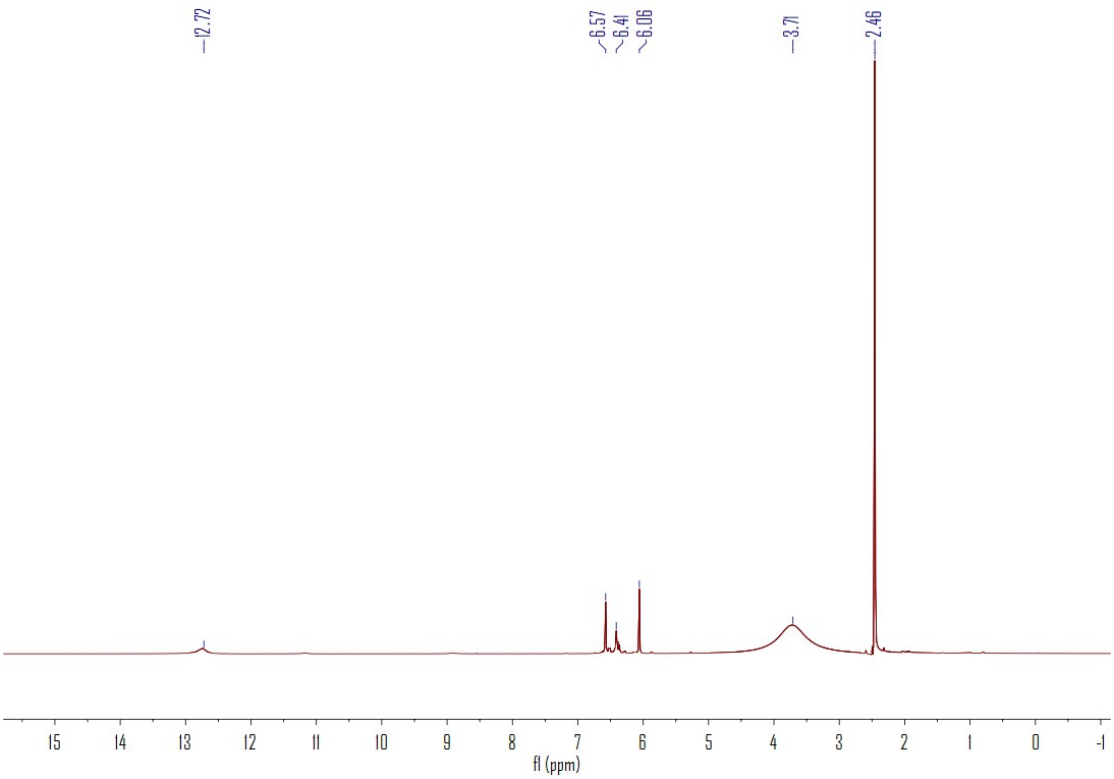

Figure S19[1]H NMR spectra (500MHz) of **11** in [D_6] DMSO at 25 °C.

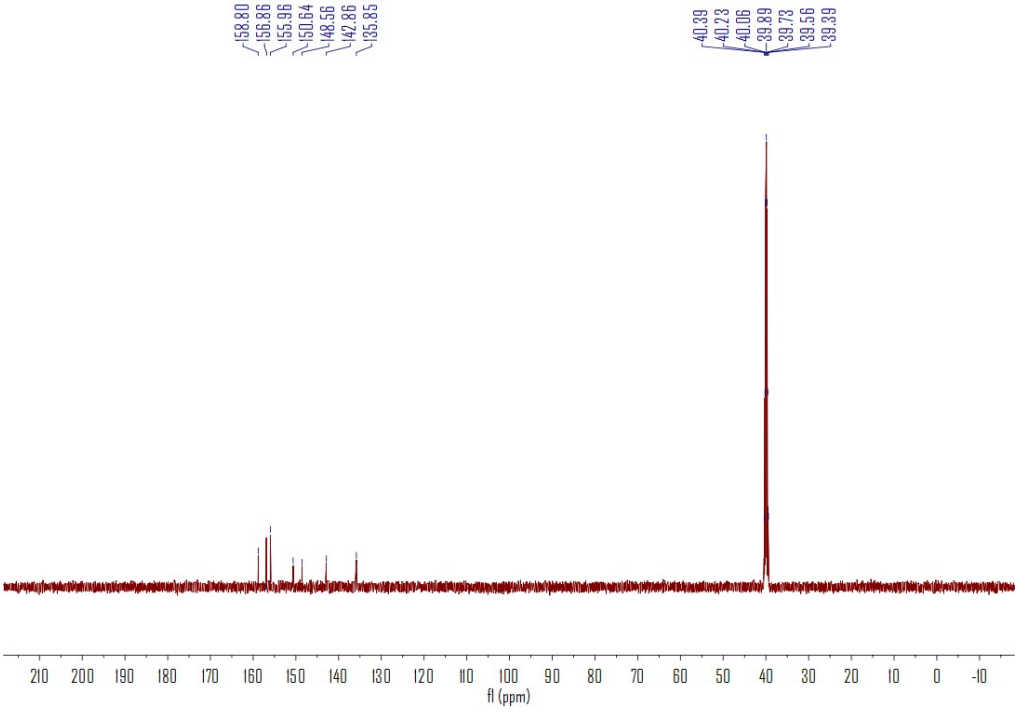

Figure S20 [13]C NMR spectra (125 MHz) of **11** in [D6] DMSO at 25 °C.