Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting information

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Experimental section

N,N',N'',N'''-(4H,4'H-[3,3'-bi(1,2,4-triazole)]-4,4',5,5'-tetrayl)tetraacetamide (2)

Compound **1** (2.5 g, 0.013 mol) was added slowly to acetic anhydride (70 ml) and heated to 100 ℃. After refluxing 4 h and cooling to the room temperature, the precipitate was filtered to get the white compound **2** (4.2 g, 88.7% yield). ^{1}H NMR ([D6] DMSO, 500 MHz): d=1.29 ppm (s, 3H, CH_3); d=3.69 ppm (s, 1H, NH); d=8.49 ppm (s,1H, NH).

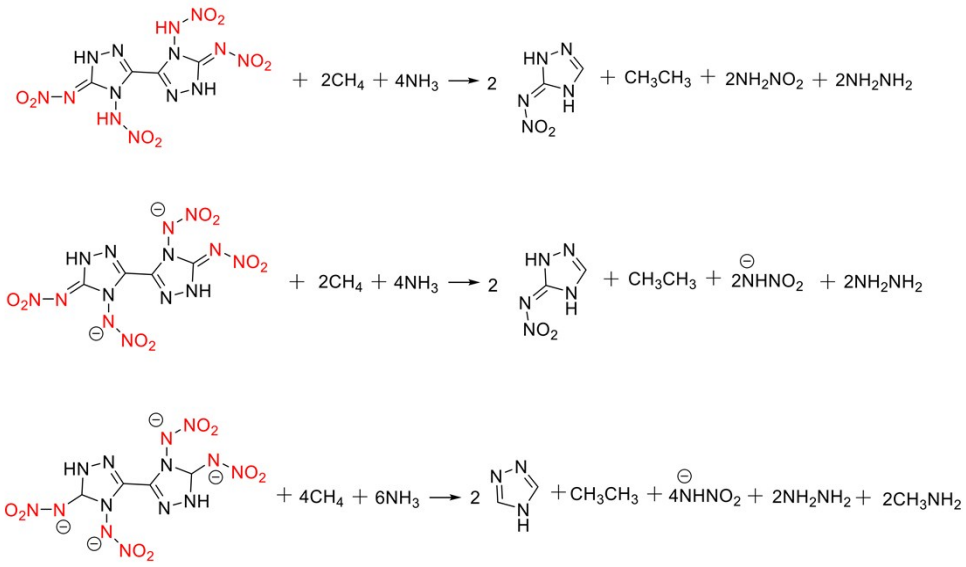
N,N',N'',N'''-(4H,4'H-[3,3'-bi(1,2,4-triazole)]-4,4',5,5'-tetrayl)tetrakis(N-nitroacetamide) (3)

Compound **2** (0.5 g, 1.37 mmol) was added slowly in 95% HNO_3 (3 ml) at -5 ℃. After stirring at room temperature for 6 hours, several solid was generated. The mixture was poured into trifluoroacetic acid (30 ml) and filtered to get compound 3 (0.15 g, 20.1% yield). 1H NMR ([D6] DMSO, 500 MHz): d=1.32 ppm (s, 3H, CH_3).

Computational Details

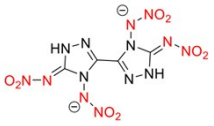
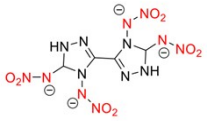
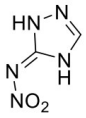
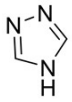
Computations were performed by using the *Gaussian 09* suite of programs.[1] The elementary geometric optimization and the frequency analysis were performed at the level of the Becke three parameter, Lee-Yan-Parr (B3LYP)[2] functional with the 6-311++G** basis set.[3] All of the optimized structures 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. The isodesmic reaction processes, that is, the number of each kind of formal bond is conserved, were used with the application of the bond separation reaction (BSR) rules. The molecule was broken down into a set of two heavy-atom molecules containing the same component bonds. The isodesmic reaction used to derive the HOF of compound **NT-00**, **T1-T5** and **D1-D5** is shown in Scheme S1.



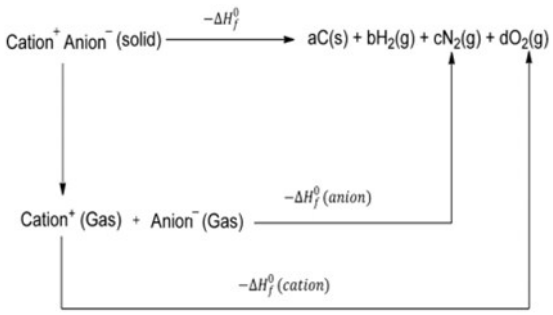
Scheme S1. Isodesmic reaction for calculating heat of formation for **NT-00**, **T1-T5** and **D1-D5**.

Table S1. Calculated zero-point energy (ZPE), thermal correction to enthalpy (HT), total energy (E0) and gas phase heats of formation (HOF)

Compd.	ZPE/au	H_T/au	E_0/au	HOF/kJ mol^{-1}
NT-00	0.171247	0.023533	-1522.633	707.1
	0.145085	0.022826	-1521.557	678.4
	0.117838	0.021583	-1520.049	1794.1
CH_4	0.043894	0.003821	-40.52616	-74.6
NH_3	0.033694	0.003825	-56.56711	-45.9
CH_3CH_3	0.073092	0.004484	-79.84168	-84
$NHNO_2$ anion	0.025624	0.004336	-260.5046	-6.74
NH_2NH_2	0.051515	0.003928	-111.8769	95.35
	0.07755	0.008047	-502.117	210.9
	0.057813	0.004688	-242.2577	193.7
CH_3NH_2	0.062724	0.004419	-95.871	-23
NH_2NO_2	0.037485	0.004404	-261.0369	-6.11

M	HOF/ kJ mol^{-1}
Ammonium ion	626.4
Hydroxylammonium ion	699.5
Hydrazinium ion	770.0
Potassium ion	501.1
Sodium ion	363.7

For energetic salts, the solid-phase heat of formation is calculated on the basis of a Born-Haber energy cycle (Scheme S2). The number is simplified by equation 1:



Scheme S2. Born-Haber energy cycle

ΔH_f (salt, 298K) = ΔH_f (cation, 298K) + ΔH_f (anion, 298K) – ΔH_L (1)

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

$\Delta H_L = U_{pot} + [p (nM /2 – 2) + q (nX /2 – 2)] RT$ (2)

In this equation, nM and nX depend on the nature of the ions Mp^+ and Xq^-, respectively.

The equation for lattice potential energy U_{pot} (equation 3) has the form:

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

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. By using the measured room temperature densities, all the newly prepared compounds are listed in Table S2.

Table S2. Densities, calculated lattice energies, and calculated heats of formation of **T1-T5, D1-D5**.

compound	**d [g cm^{-3}]**	**$\Delta_f H_{Lat}$ [kJ mol^{-1}]**	**$\Delta_f H$ [kJ mol^{-1}/kJ g^{-1}]**
T1	1.75	4246.80	34.78/ 0.078
T2	1.80	4145.18	729.8/ 1.45
T3	1.82	4148.93	444.1/ 0.87
T4	2.01	4207.31	-408.81/ -0.77
T5	1.98	4349.2	-1145.24/ -2.17
D1	1.82	1205.11	726.09/ 1.77
D2	1.86	1182.87	1035.53/ 2.35
D3	1.89	1188.06	889.34/ 2.01
D4	2.13	1198.50	482.1/ 1.07
D5	2.05	1241.93	163.85/ 0.39

Crystallographic data for NT-00, T2, T4, D1, D4, D5

Table S3. Crystallographic data of **NT-00, T2, T4, D1, D4, D5**

Compd.	**NT-00**	**T2**	**T4**	**D1**	**D4**	**D5**
CCDC number	1980541	1980542	1980543	1980544	1980545	1980546
formula	$C_4H_{14.5}N_{14}O_{13.25}$	$C_4H_{24}N_{22}O_{10}$	$C_4H_8N_{14}O_{12}K_4$	$C_4H_{10}N_{16}O_8$	$C_4H_{10}N_{14}O_{12}K_2$	$C_4H_6N_{14}O_{10}Na_2$
Mw	470.8	540.45	600.64	410.28	524.46	456.21
crystal system	monoclinic	monoclinic	triclinic	monoclinic	triclinic	triclinic
space group	C 2/c	P 21/c	P -1	P 21/n	P -1	C c
a [Å]	8.9398(7)	a=7.2053(4)	7.197(2)	7.3769(14)	7.1556(18)	9.5313(9)
b [Å]	20.6711(17)	17.3968(11)	8.971(3)	13.894(3)	9.681(3)	11.5462(12)
c [Å]	10.4206(7)	8.5866(5)	9.188(2)	7.3845(13)	14.024(4)	14.4382(14)
α [°]	90	90	61.707(7)	90	100.925(8)	90
β [°]	102.471(3)	105.620(2)	72.877(8)	99.407(6)	95.155(8)	104.885(3)
γ [°]	90	90	81.944(9)	90	104.206(8)	90
V [Å^3]	1880.2(2)	1036.57(11)	499.2(2)	746.7(3)	915.2(5)	1535.6(3)
Z	4	2	2	2	2	4
T [K]	296(2)	296	296	296	296	296
λ [Å]	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
ρ_{calcd} [g cm^{-3}]	1.663	1.732	1.998	1.825	1.903	1.973
μ [mm^{-1}]	0.162	0.158	0.985	0.168	0.616	0.230
F (000)	970.0	564	302.0	420.0	532.0	920.0
θ range [°]	2.53-26.02	2.34-27.49	2.58-27.30	3.16-27.48	2.22-27.42	2.83-27.62
Data/restraints/parameter	0.995/0/150	0.968/0/163	0.970/0/154	0.984/0/127	0.987/0/294	0.83/2/274
S	1.035	1.011	1.072	1.051	1.037	1.038
R_1 [$I > 2\sigma(I)$]	0.0585	0.393	0.0480	0.1512	0.0424	0.0325
wR_2 [$I > 2\sigma(I)$]	0.1739	0.1130	0.1223	0.1414	0.1129	0.0876

Table S4. Selected bond lengths [Å] and angles [°] for compound **NT-00**

C(1)-N(2)	1.290(3)	N(2)-C(1)-N(1)	111.1(2)
C(1)-N(1)	1.380(3)	N(2)-C(1)-C(1)#1	125.1(3)
C(1)-C(1)#1	1.451(5)	N(1)-C(1)-C(1)#1	123.8(3)
C(2)-N(6)	1.323(3)	N(6)-C(2)-N(3)	136.7(2)
C(2)-N(3)	1.333(3)	N(6)-C(2)-N(1)	118.7(2)
C(2)-N(1)	1.370(3)	N(3)-C(2)-N(1)	104.58(19)
N(1)-N(4)	1.367(3)	N(4)-N(1)-C(2)	122.40(19)
N(2)-N(3)	1.382(3)	N(4)-N(1)-C(1)	129.80(19)
N(3)-H(3)	0.8701	C(2)-N(1)-C(1)	107.31(18)
N(4)-N(5)	1.385(3)	C(1)-N(2)-N(3)	104.75(19)
N(4)-H(4)	0.8600	C(2)-N(3)-N(2)	112.27(19)
N(5)-O(2)	1.204(3)	C(2)-N(3)-H(3)	128.3
N(5)-O(1)	1.214(3)	N(2)-N(3)-H(3)	118.7
N(6)-N(7)	1.354(3)	N(1)-N(4)-N(5)	114.13(19)
N(7)-O(4)	1.224(3)	N(1)-N(4)-H(4)	122.9
N(7)-O(3)	1.226(3)	N(5)-N(4)-H(4)	122.9
O(5)-H(5A)	0.8500	O(2)-N(5)-O(1)	127.0(2)
O(5)-H(5B)	0.8500	O(2)-N(5)-N(4)	114.9(2)
O(6)-H(6A)	0.8500	O(1)-N(5)-N(4)	118.1(2)
O(6)-H(6B)	1.0011	C(2)-N(6)-N(7)	115.9(2)
O(7)-H(7A)	0.8367	O(4)-N(7)-O(3)	123.4(3)
O(7)-H(7B)	0.8608	O(4)-N(7)-N(6)	121.7(2)
O(7)-H(7A)#2	0.8367	O(3)-N(7)-N(6)	114.9(2)
O(7)-H(7B)#2	0.8608	H(5A)-O(5)-H(5B)	109.5
O(8)-O(8)#2	0.54(3)	H(6A)-O(6)-H(6B)	113.7
O(8)-H(8A)	0.8398	H(7A)-O(7)-H(7B)	104.7
O(8)-H(8B)	0.8682	H(7A)-O(7)-H(7A)#2	144.8
O(8)-H(8B)#2	0.54(7)	H(7B)-O(7)-H(7A)#2	48.5
O(8)#2-O(8)-H(8A)	115.1	H(7A)-O(7)-H(7B)#2	48.5
O(8)#2-O(8)-H(8B)	37.0	H(7B)-O(7)-H(7B)#2	94.9
H(8A)-O(8)-H(8B)	103.8	H(7A)#2-O(7)-H(7B)#2	104.7
O(8)#2-O(8)-H(8B)#2	107(10)	H(8B)-O(8)-H(8B)#2	121.7
H(8A)-O(8)-H(8B)#2	39.8	H(8A)-O(8)-H(8B)#2	39.8
		H(8B)-O(8)-H(8B)#2	121.7

Table S5. Selected bond lengths [Å] and angles [°] for compound **T2**

C(1)-N(2)	1.3093(19)	N(2)-C(1)-N(1)	109.87(13)
C(1)-N(1)	1.366(2)	N(2)-C(1)-C(1)#1	126.50(17)
C(1)-C(1)#1	1.449(3)	N(1)-C(1)-C(1)#1	123.62(16)
C(2)-N(3)	1.3249(19)	N(3)-C(2)-N(1)	109.25(13)
C(2)-N(1)	1.3661(19)	N(3)-C(2)-N(6)	134.62(14)
C(2)-N(6)	1.367(2)	N(1)-C(2)-N(6)	116.10(13)
N(1)-N(4)	1.3986(17)	C(1)-N(1)-C(2)	106.03(12)
N(2)-N(3)	1.3934(19)	C(1)-N(1)-N(4)	128.28(12)
N(4)-N(5)	1.3067(19)	C(2)-N(1)-N(4)	124.72(12)
N(5)-O(1)	1.2388(18)	C(1)-N(2)-N(3)	107.55(12)
N(5)-O(2)	1.2671(16)	C(2)-N(3)-N(2)	107.30(12)
N(6)-N(7)	1.3165(18)	N(5)-N(4)-N(1)	109.50(12)
N(7)-O(4)	1.2447(17)	O(1)-N(5)-O(2)	121.25(13)
N(7)-O(3)	1.2550(18)	O(1)-N(5)-N(4)	124.69(13)
N(8)-N(9)	1.432(2)	O(2)-N(5)-N(4)	114.05(12)
N(8)-H(8A)	0.8900	N(7)-N(6)-C(2)	117.20(13)
N(8)-H(8B)	0.8900	O(4)-N(7)-O(3)	120.80(13)
N(8)-H(8C)	0.9217	O(4)-N(7)-N(6)	124.26(13)
N(9)-H(9A)	0.8900	O(3)-N(7)-N(6)	114.93(13)
N(9)-H(9B)	0.8900	N(9)-N(8)-H(8A)	109.2
N(10)-N(11)	1.425(2)	N(9)-N(8)-H(8B)	109.2
N(10)-H(10A)	0.8900	H(8A)-N(8)-H(8B)	109.5
N(10)-H(10B)	0.8900	N(9)-N(8)-H(8C)	112.1
N(10)-H(10C)	0.9272	H(8A)-N(8)-H(8C)	108.2
N(11)-H(11A)	0.8900	H(8B)-N(8)-H(8C)	108.6
N(11)-H(11B)	0.8900	N(8)-N(9)-H(9A)	109.3
O(5)-H(5A)	0.9028	N(8)-N(9)-H(9B)	109.2
O(5)-H(5B)	0.8568	H(9A)-N(9)-H(9B)	109.5
N(10)-N(11)-H(11A)	109.4	N(11)-N(10)-H(10A)	109.6
N(10)-N(11)-H(11B)	109.3	N(11)-N(10)-H(10B)	109.6
H(11A)-N(11)-H(11B)	109.5	H(10A)-N(10)-H(10B)	109.5
H(5A)-O(5)-H(5B)	99.1	N(11)-N(10)-H(10C)	111.0
H(10B)-N(10)-H(10C)	110.0	H(10A)-N(10)-H(10C)	107.2

Table S6. Selected bond lengths [Å] and angles [°] for compound **T4**

C(1)-N(2)	1.313(4)	N(2)-C(1)-N(6)	134.8(3)
C(1)-N(6)	1.372(5)	N(2)-C(1)-N(3)	109.8(3)
C(1)-N(3)	1.379(4)	N(6)-C(1)-N(3)	115.4(3)
C(2)-N(1)	1.313(4)	N(1)-C(2)-N(3)	109.1(3)
C(2)-N(3)	1.372(5)	N(1)-C(2)-C(2)#1	126.1(4)
C(2)-C(2)#1	1.441(7)	N(3)-C(2)-C(2)#1	124.8(4)
N(1)-N(2)	1.395(4)	C(2)-N(1)-N(2)	108.4(3)
N(1)-K(2)#2	3.118(4)	C(2)-N(1)-K(2)#2	107.4(2)
N(2)-K(1)	2.939(3)	N(2)-N(1)-K(2)#2	94.1(2)
N(3)-N(4)	1.441(4)	C(1)-N(2)-N(1)	107.0(3)
N(4)-N(5)	1.287(5)	C(1)-N(2)-K(1)	122.1(2)
N(4)-K(1)#2	3.083(4)	N(1)-N(2)-K(1)	127.7(2)
N(5)-O(2)	1.233(4)	C(2)-N(3)-C(1)	105.7(3)
N(5)-O(1)	1.267(5)	C(2)-N(3)-N(4)	129.2(3)
N(5)-K(2)#3	3.416(4)	C(1)-N(3)-N(4)	123.5(3)
N(6)-N(7)	1.306(4)	N(5)-N(4)-N(3)	108.0(3)
N(6)-K(2)	2.957(3)	N(5)-N(4)-K(1)#2	105.7(2)
N(7)-O(4)	1.255(4)	N(3)-N(4)-K(1)#2	146.2(2)
N(7)-O(3)	1.257(4)	O(2)-N(5)-O(1)	117.6(4)
O(1)-K(2)#3	2.744(4)	O(2)-N(5)-N(4)	119.0(4)
O(2)-K(2)#4	2.778(3)	O(1)-N(5)-N(4)	123.4(3)
O(2)-K(1)#5	2.787(3)	O(2)-N(5)-K(2)#3	94.0(3)
O(2)-K(1)#2	3.313(4)	O(1)-N(5)-K(2)#3	48.4(2)
O(3)-K(2)	2.857(3)	N(4)-N(5)-K(2)#3	124.9(2)
O(4)-K(1)	2.710(3)	N(7)-N(6)-C(1)	117.5(3)
O(4)-K(1)#6	2.893(3)	N(7)-N(6)-K(2)	96.8(2)
K(1)-O(5)	2.734(3)	C(1)-N(6)-K(2)	145.5(2)
K(1)-O(7)	2.824(3)	K(2)-O(7)#5	2.799(4)
K(1)-K(2)#7	3.9354(15)	K(2)-K(2)#8	4.666(2)
K(1)-K(1)#6	4.031(2)	K(2)-H(5A)#5	2.124(4)
K(1)-K(2)#2	4.1757(18)	O(5)-H(5A)	0.8500
K(2)-O(5)#5	2.774(3)	O(5)-H(5B)	0.8500
K(2)-O(7)#5	2.799(4)	O(7)-H(6A)	0.8705
		O(7)-H(6B)	0.8586

Table S7. Selected bond lengths [Å] and angles [°] for compound **D1**

C(1)-N(3)	1.328(3)	N(3)-C(1)-N(6)	135.86(19)
C(1)-N(6)	1.340(3)	N(3)-C(1)-N(1)	104.64(17)
C(1)-N(1)	1.359(3)	N(6)-C(1)-N(1)	119.40(18)
C(2)-N(2)	1.302(3)	N(2)-C(2)-N(1)	110.81(18)
C(2)-N(1)	1.369(3)	N(2)-C(2)-C(2)#1	125.5(2)
C(2)-C(2)#1	1.446(4)	N(1)-C(2)-C(2)#1	123.7(2)
N(1)-N(4)	1.395(2)	C(1)-N(1)-C(2)	107.60(16)
N(2)-N(3)	1.368(3)	C(1)-N(1)-N(4)	123.98(16)
N(3)-H(3)	0.8337	C(2)-N(1)-N(4)	128.29(17)
N(4)-N(5)	1.320(3)	C(2)-N(2)-N(3)	104.28(16)
N(5)-O(2)	1.235(3)	C(1)-N(3)-N(2)	112.66(16)
N(5)-O(1)	1.253(2)	C(1)-N(3)-H(3)	122.4
N(6)-N(7)	1.355(3)	N(2)-N(3)-H(3)	122.0
N(7)-O(3)	1.226(3)	N(5)-N(4)-N(1)	108.33(16)
N(7)-O(4)	1.244(3)	O(2)-N(5)-O(1)	122.0(2)
N(8)-H(8A)	0.9432	O(2)-N(5)-N(4)	124.50(17)
N(8)-H(8B)	0.9293	O(1)-N(5)-N(4)	113.5(2)
N(8)-H(8C)	0.9380	C(1)-N(6)-N(7)	114.46(19)
N(8)-H(8D)	0.9129	O(3)-N(7)-O(4)	122.5(2)
H(8B)-N(8)-H(8C)	84.6	O(3)-N(7)-N(6)	115.6(2)
H(8A)-N(8)-H(8D)	127.3	O(4)-N(7)-N(6)	121.93(19)
H(8B)-N(8)-H(8D)	145.4	H(8A)-N(8)-H(8B)	70.7
H(8C)-N(8)-H(8D)	122.0	H(8A)-N(8)-H(8C)	86.5

Table S8. Selected bond lengths [Å] and angles [°] for compound **D4**

C(1)-N(3)	1.333(3)	N(3)-C(1)-N(6)	135.77(19)
C(1)-N(6)	1.343(3)	N(3)-C(1)-N(1)	105.03(17)
C(1)-N(1)	1.357(3)	N(6)-C(1)-N(1)	119.20(18)
C(2)-N(2)	1.302(3)	N(2)-C(2)-N(1)	110.99(17)
C(2)-N(1)	1.368(3)	N(2)-C(2)-C(2)#1	125.4(2)
C(2)-C(2)#1	1.453(4)	N(1)-C(2)-C(2)#1	123.6(2)
C(3)-N(8)	1.298(3)	N(8)-C(3)-N(10)	111.12(17)
C(3)-N(10)	1.370(3)	N(8)-C(3)-C(3)#2	125.1(2)
C(3)-C(3)#2	1.453(4)	N(10)-C(3)-C(3)#2	123.7(2)
C(4)-N(9)	1.330(3)	N(9)-C(4)-N(11)	135.4(2)
C(4)-N(11)	1.347(3)	N(9)-C(4)-N(10)	105.29(17)
C(4)-N(10)	1.356(3)	N(11)-C(4)-N(10)	119.26(19)
K(1)-O(2)	2.7436(19)	O(2)-K(1)-O(9)	82.62(9)
K(1)-O(9)	2.745(3)	O(2)-K(1)-O(5)	76.86(6)
K(1)-O(5)	2.7832(19)	O(9)-K(1)-O(5)	157.32(8)
K(1)-O(6)#3	2.825(2)	O(2)-K(1)-O(6)#3	77.59(6)
K(1)-O(7)#4	2.850(2)	O(9)-K(1)-O(6)#3	89.58(9)
K(1)-N(4)#5	2.9555(19)	O(5)-K(1)-O(6)#3	95.27(6)
K(1)-O(1)#5	3.053(2)	O(2)-K(1)-O(7)#4	76.96(6)
K(1)-N(2)#3	3.141(2)	O(9)-K(1)-O(7)#4	79.54(7)
K(1)-N(5)#5	3.386(2)	O(5)-K(1)-O(7)#4	86.47(6)
K(1)-K(2)#6	4.8917(13)	O(6)#3-K(1)-O(7)#4	153.37(6)
K(2)-O(8)	2.7836(18)	O(2)-K(1)-N(4)#5	142.67(6)
K(2)-O(1)#7	2.8044(19)	O(9)-K(1)-N(4)#5	128.01(10)
K(2)-O(10)	2.901(3)	O(5)-K(1)-N(4)#5	68.39(5)
K(2)-O(4)	2.9108(18)	O(6)#3-K(1)-N(4)#5	117.92(6)
K(2)-O(7)#8	3.022(2)	O(7)#4-K(1)-N(4)#5	87.46(5)
K(2)-N(8)#9	3.055(2)	O(2)-K(1)-O(1)#5	143.29(6)
K(2)-O(11)	3.062(2)	O(9)-K(1)-O(1)#5	87.33(10)
K(2)-O(3)#9	3.069(2)	O(5)-K(1)-O(1)#5	103.42(5)
K(2)-N(13)#8	3.093(2)	O(6)#3-K(1)-O(1)#5	137.74(6)
K(2)-O(3)	3.191(2)	O(7)#4-K(1)-O(1)#5	66.50(5)
K(2)-N(14)#8	3.381(2)	N(4)#5-K(1)-O(1)#5	42.12(5)
N(1)-N(4)	1.404(2)	O(2)-K(1)-N(2)#3	148.20(6)
N(2)-N(3)	1.370(2)	O(9)-K(1)-N(2)#3	100.99(8)
N(3)-H(3)	0.8600	O(5)-K(1)-N(2)#3	101.53(5)
N(4)-N(5)	1.325(3)	O(6)#3-K(1)-N(2)#3	70.90(6)

Table S9. Selected bond lengths [Å] and angles [°] for compound **D5**

Na(2)-O(10)	2.300(4)	N(3)-C(1)-N(1)	110.8(3)
Na(2)-O(2)#1	2.336(3)	N(3)-C(1)-C(3)	124.6(3)
Na(2)-O(6)	2.355(3)	N(1)-C(1)-C(3)	124.6(2)
Na(2)-O(9)#2	2.389(3)	N(2)-C(2)-N(6)	135.4(3)
Na(2)-O(3)#3	2.546(3)	N(2)-C(2)-N(1)	105.1(2)
Na(2)-N(11)	2.773(3)	N(6)-C(2)-N(1)	119.5(3)
Na(2)-N(12)	2.998(3)	N(10)-C(3)-N(8)	111.4(3)
Na(2)-Na(1)#2	3.959(2)	N(10)-C(3)-C(1)	125.4(3)
Na(2)-H(10B)	2.6763	N(8)-C(3)-C(1)	123.2(2)
C(1)-N(3)	1.304(4)	N(9)-C(4)-N(13)	135.8(3)
C(1)-N(1)	1.373(4)	N(9)-C(4)-N(8)	104.9(2)
C(1)-C(3)	1.451(3)	N(13)-C(4)-N(8)	119.1(2)
C(2)-N(2)	1.331(4)	C(2)-N(1)-C(1)	107.2(2)
C(2)-N(6)	1.351(4)	C(2)-N(1)-N(4)	124.0(2)
C(2)-N(1)	1.359(4)	C(1)-N(1)-N(4)	128.7(2)
C(3)-N(10)	1.301(4)	C(2)-N(2)-N(3)	112.3(2)
C(3)-N(8)	1.373(4)	C(2)-N(2)-H(2)	123.8
C(4)-N(9)	1.333(4)	N(3)-N(2)-H(2)	123.8
C(4)-N(13)	1.341(4)	C(1)-N(3)-N(2)	104.6(3)
C(4)-N(8)	1.367(4)	O(4)-N(7)-Na(1)#4	58.49(16)
N(1)-N(4)	1.407(3)	O(3)-N(7)-Na(1)#4	63.90(18)
N(2)-N(3)	1.363(4)	N(6)-N(7)-Na(1)#4	164.5(2)
N(2)-H(2)	0.8600	C(4)-N(8)-C(3)	107.0(2)
N(3)-Na(1)#2	2.965(3)	C(4)-N(8)-N(11)	123.3(2)
N(4)-N(5)	1.330(4)	C(3)-N(8)-N(11)	129.7(2)
N(5)-O(2)	1.243(4)	C(4)-N(9)-N(10)	112.4(3)
N(5)-O(1)	1.251(3)	C(4)-N(9)-H(9)	123.8
N(6)-N(7)	1.328(4)	N(10)-N(9)-H(9)	123.8
N(7)-O(4)	1.246(4)	C(3)-N(10)-N(9)	104.2(3)
N(7)-O(3)	1.248(4)	N(12)-N(11)-N(8)	108.2(2)
N(7)-Na(1)#4	2.987(3)	N(12)-N(11)-Na(2)	86.51(16)
N(8)-N(11)	1.392(3)	N(8)-N(11)-Na(2)	158.94(19)
N(9)-N(10)	1.374(4)	O(5)-N(12)-O(6)	121.8(3)

Table S10. Hydrogen bonds present in compound **T2**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(8)-H(8A)...N(4)#2	0.89	2.48	3.124(2)	130.2
N(8)-H(8A)...O(2)#2	0.89	2.11	2.917(2)	150.1
N(8)-H(8B)...N(3)#3	0.89	2.07	2.904(2)	155.4
N(8)-H(8B)...O(4)#3	0.89	2.36	3.005(2)	129.6
N(8)-H(8C)...O(2)	0.92	2.04	2.7948(18)	137.9
N(9)-H(9B)...N(3)#5	0.89	2.26	3.143(2)	168.9
N(10)-H(10A)...N(6)#2	0.89	2.28	3.035(2)	143.2
N(10)-H(10A)...N(7)#2	0.89	2.68	3.485(2)	151.3
N(10)-H(10A)...O(3)#2	0.89	2.26	2.997(2)	140.2
N(10)-H(10B)...O(1)#4	0.89	2.32	3.015(2)	134.9
N(10)-H(10B)...O(3)#6	0.89	2.31	2.974(2)	130.8
N(10)-H(10C)...N(9)	0.93	1.99	2.914(2)	173.7
N(11)-H(11B)...N(6)#2	0.89	2.69	3.250(2)	122.0
N(11)-H(11B)...O(1)#7	0.89	2.43	3.076(2)	129.8

Table S11. Hydrogen bonds present in compound **D1**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3)...O(1)#2	0.83	2.04	2.774(3)	146.5
N(3)-H(3)...O(4)	0.83	2.11	2.562(2)	113.4
N(8)-H(8B)...O(2)	0.93	2.30	2.891(3)	120.9
N(8)-H(8C)...N(6)#3	0.94	2.30	3.219(3)	165.9
N(8)-H(8C)...O(1)#4	0.94	2.52	3.049(3)	115.8
N(8)-H(8D)...N(2)#5	0.91	2.68	3.340(4)	129.7
N(8)-H(8D)...N(4)#4	0.91	2.41	3.065(3)	129.0
N(8)-H(8D)...O(4)#6	0.91	2.45	2.910(3)	111.5

Spectrogram

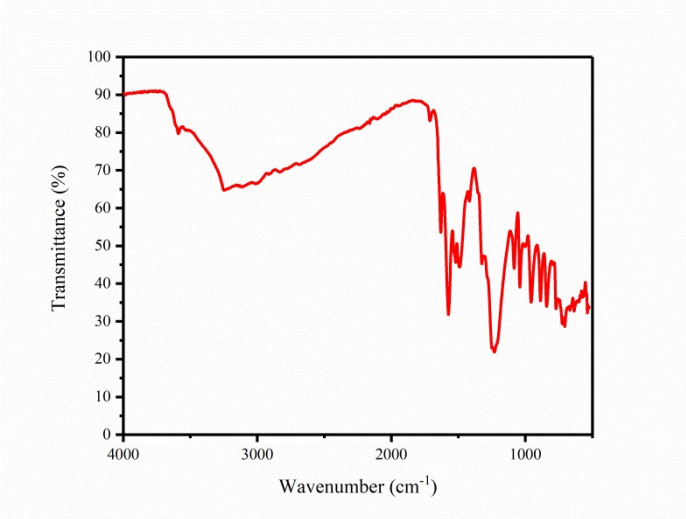


Figure S1. IR spectra for **NT-00.**

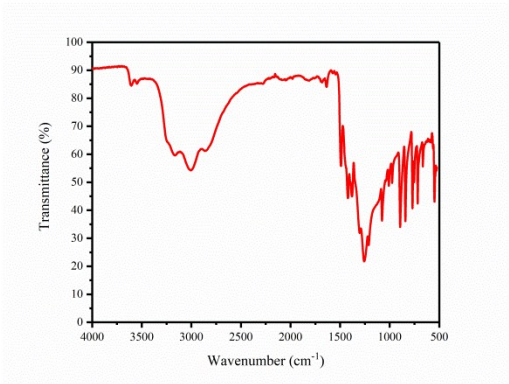


Figure S2. IR spectra for **T1.**

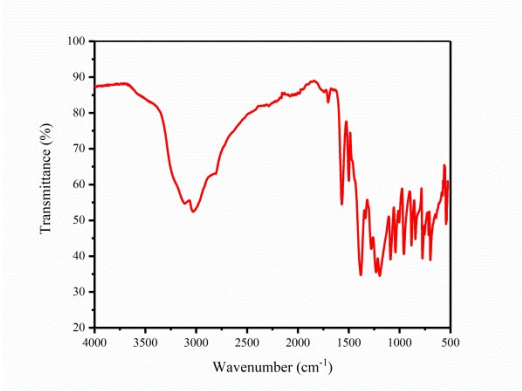


Figure S3. IR spectra for **D1.**

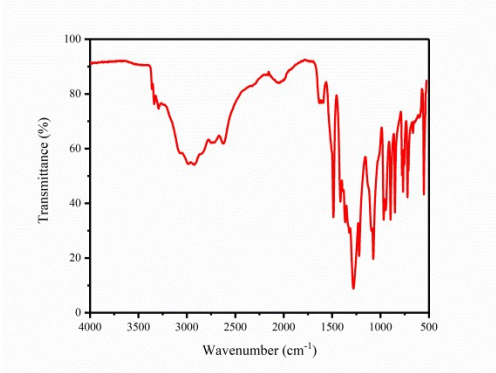


Figure S4. IR spectra for **T2.**

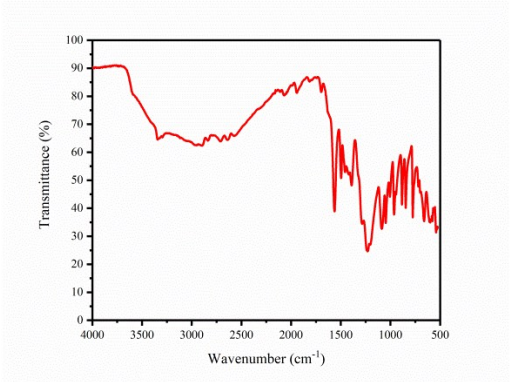


Figure S5. IR spectra for **D2.**

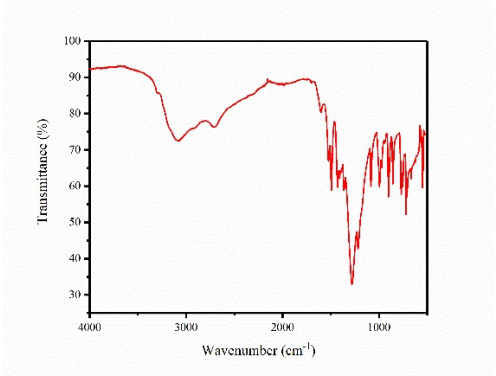


Figure S6. IR spectra for **T3.**

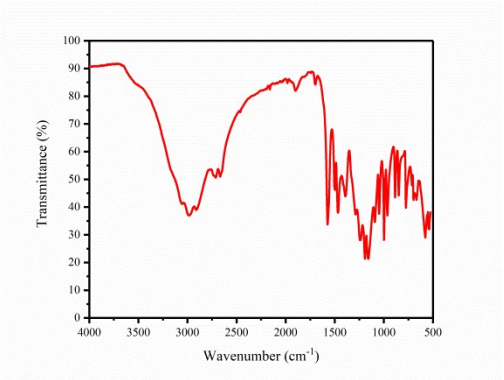


Figure S7. IR spectra for **D3.**

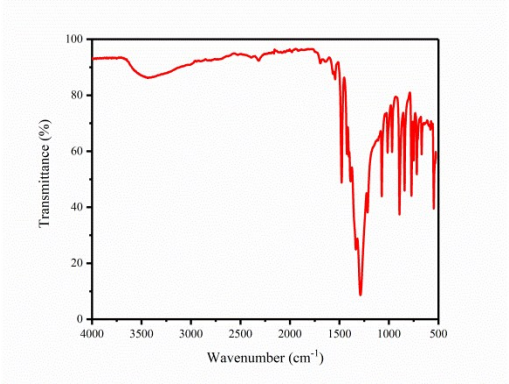


Figure S8. IR spectra for **T4.**

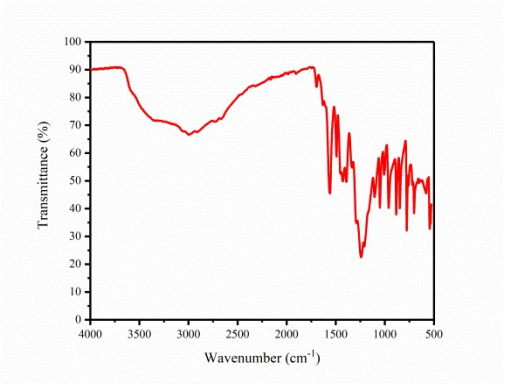


Figure S9. IR spectra for **D4.**

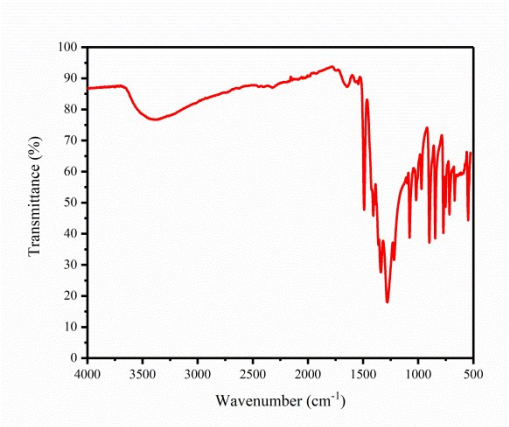


Figure S10. IR spectra for **T5.**

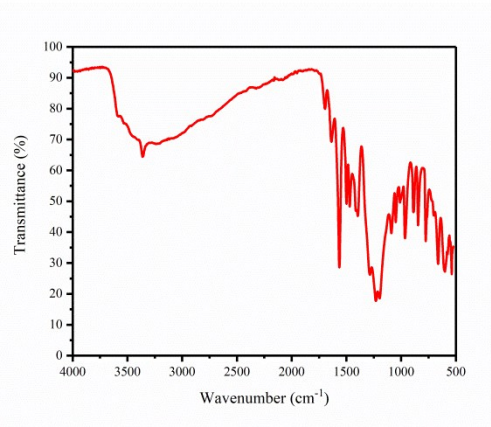


Figure S11. IR spectra for **D5.**

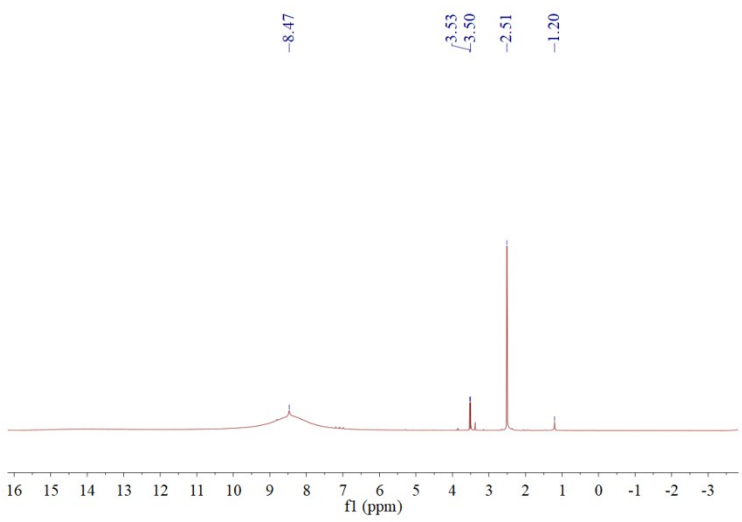


Figure S12. ^{1}H NMR spectra in DMSO-d_6 for **NT-00**.

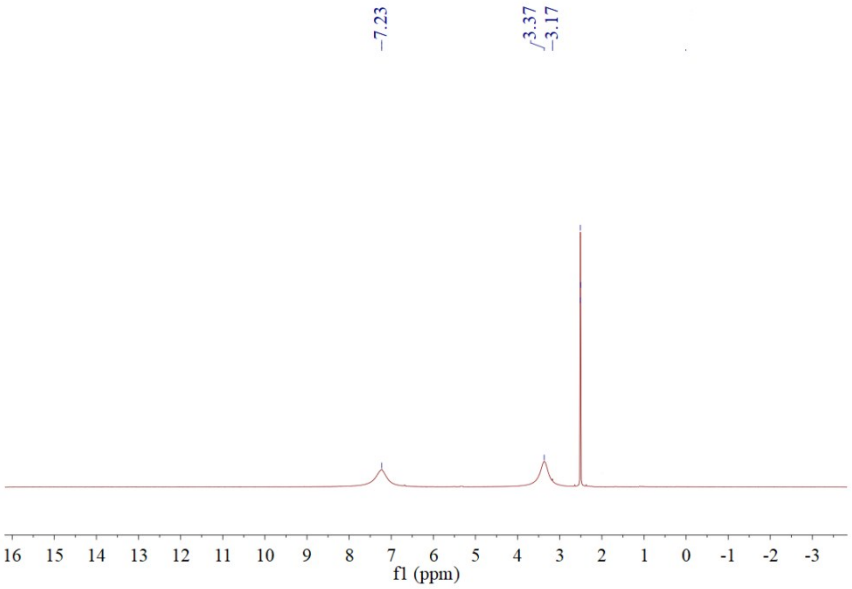


Figure S12. ^{1}H NMR spectra in DMSO-d_6 for **T1**.

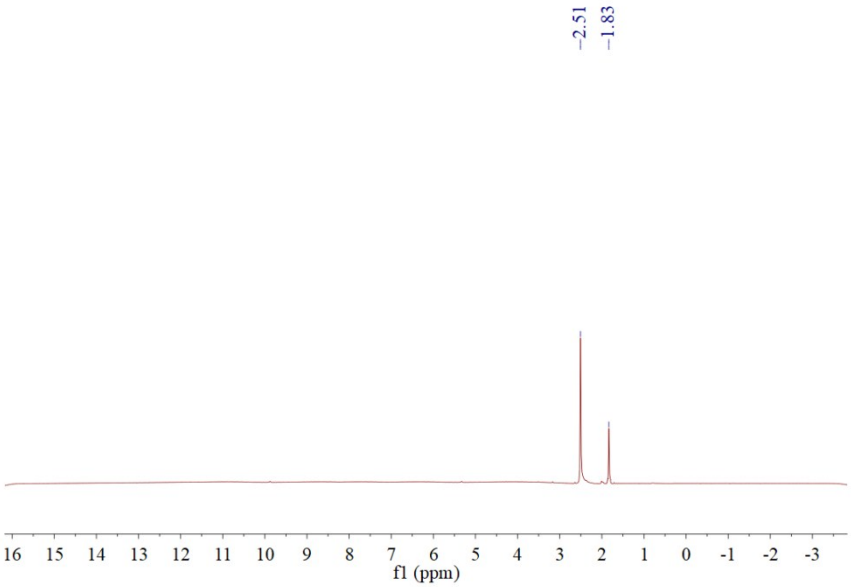


Figure S12. ^{1}H NMR spectra in DMSO-d_6 for **T2**.

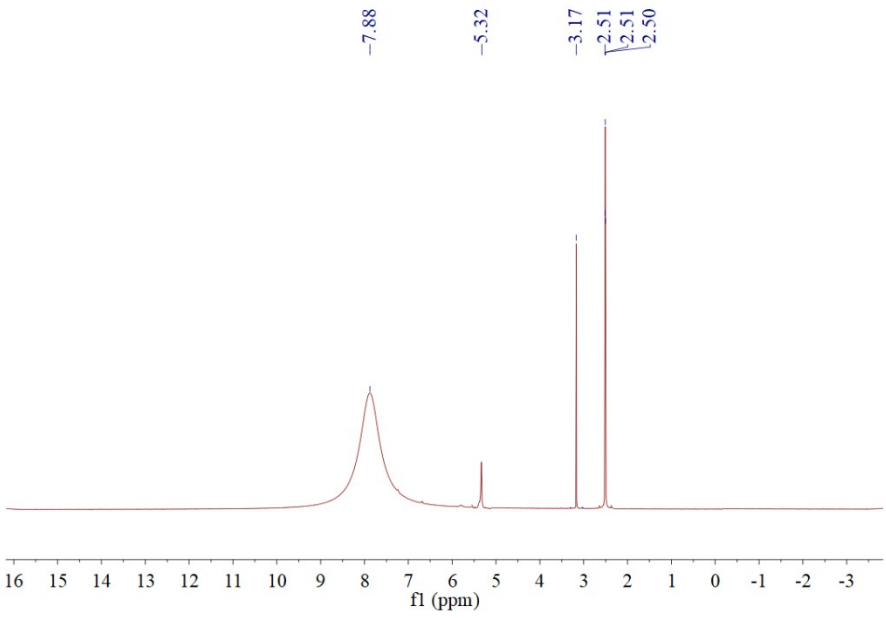


Figure S12. ^{1}H NMR spectra in DMSO-d_6 for **T3**.

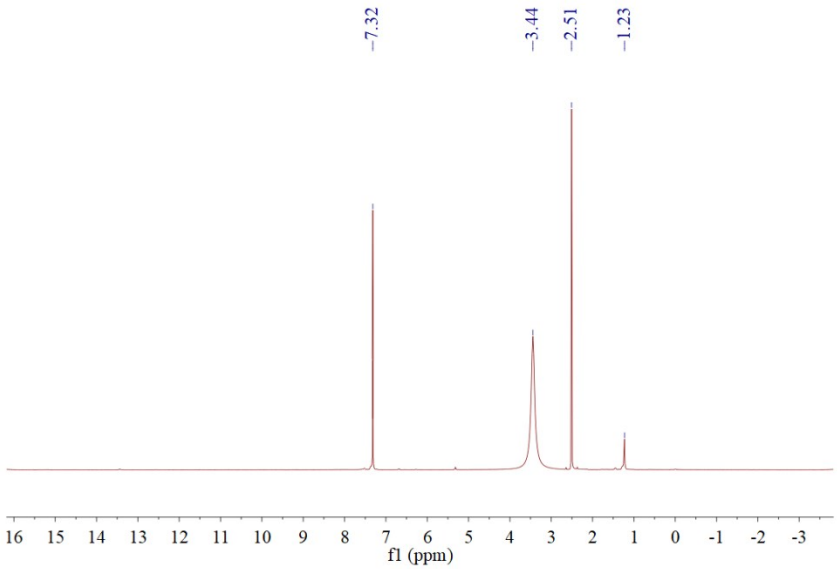


Figure S12. ^{1}H NMR spectra in DMSO-d_6 for**D1**.

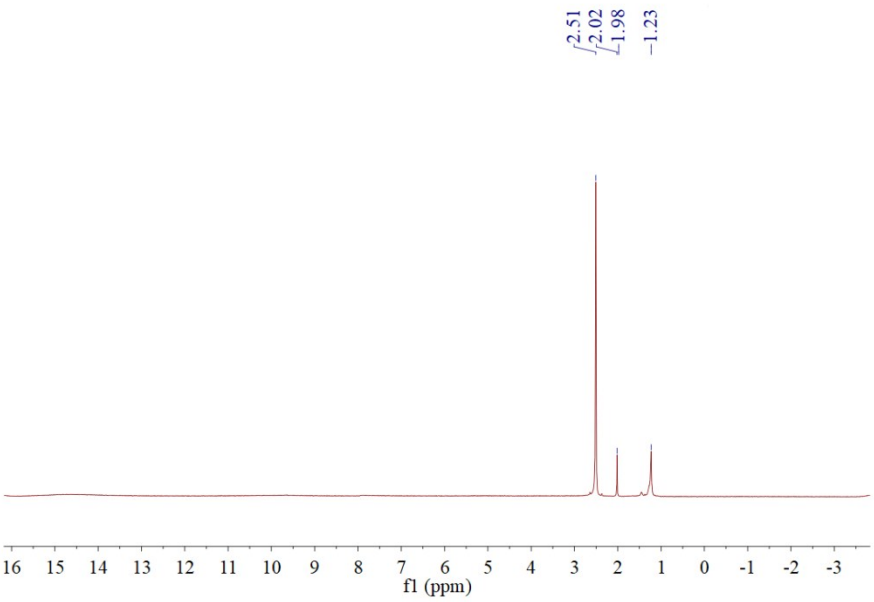


Figure S12. ^{1}H NMR spectra in DMSO-d_6 for **D2**.

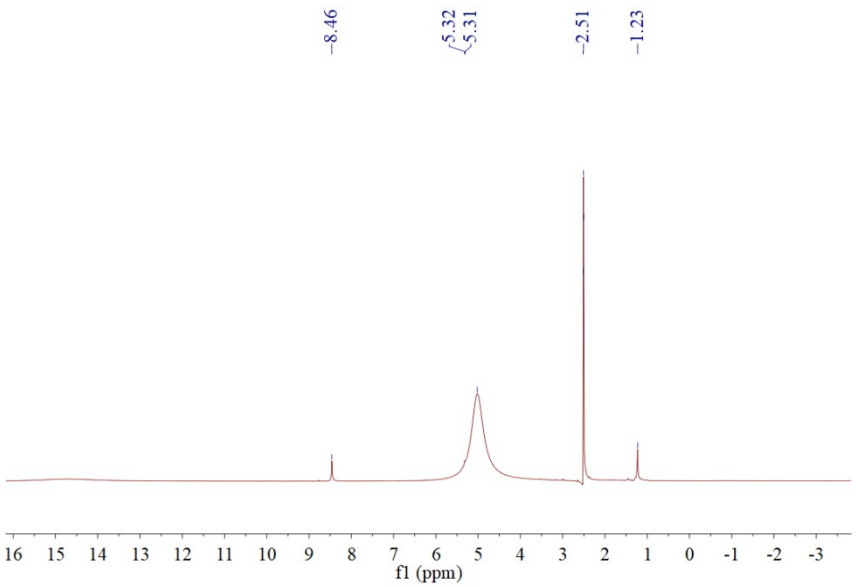


Figure S12. [1]H NMR spectra in DMSO-d_6 for **D3**.

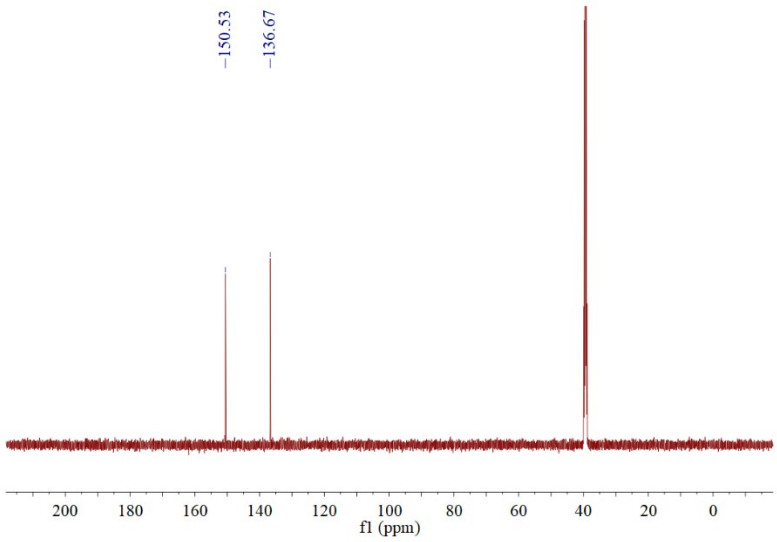


Figure S13. [13]C NMR spectra in DMSO-d_6 for **NT-00.**

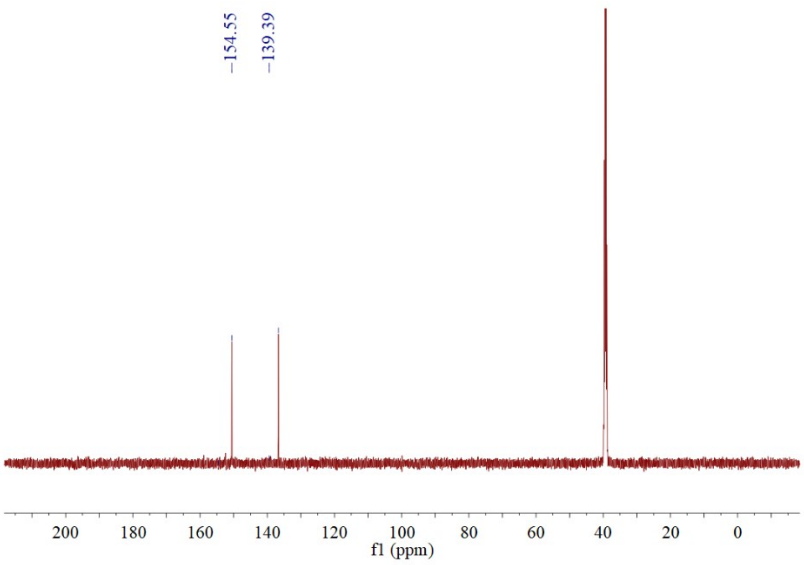


Figure S14. ^{13}C NMR spectra in DMSO-d_6 for **T1.**

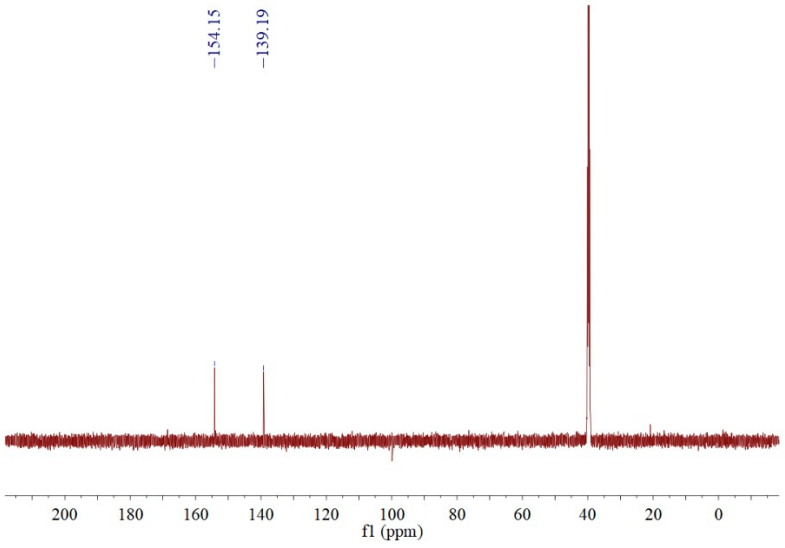


Figure S15. ^{13}C NMR spectra in DMSO-d_6 for **T2.**

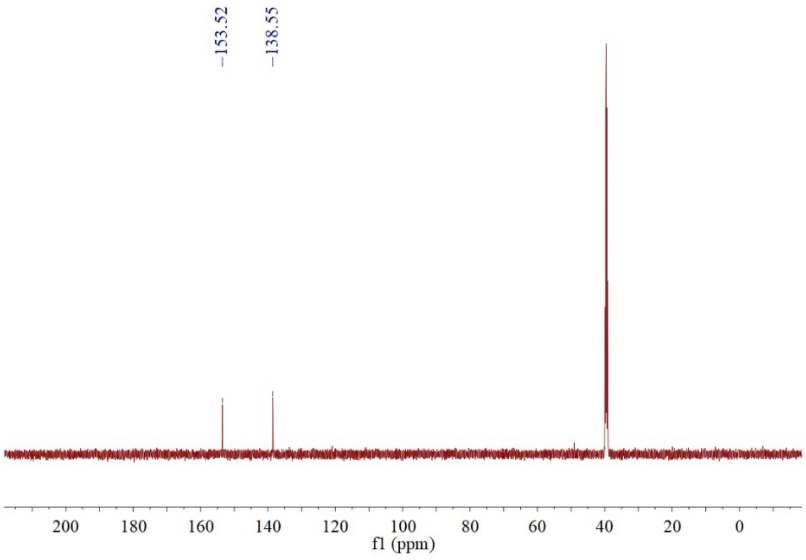


Figure S16. ^{13}C NMR spectra in DMSO-d_6 for **T3.**

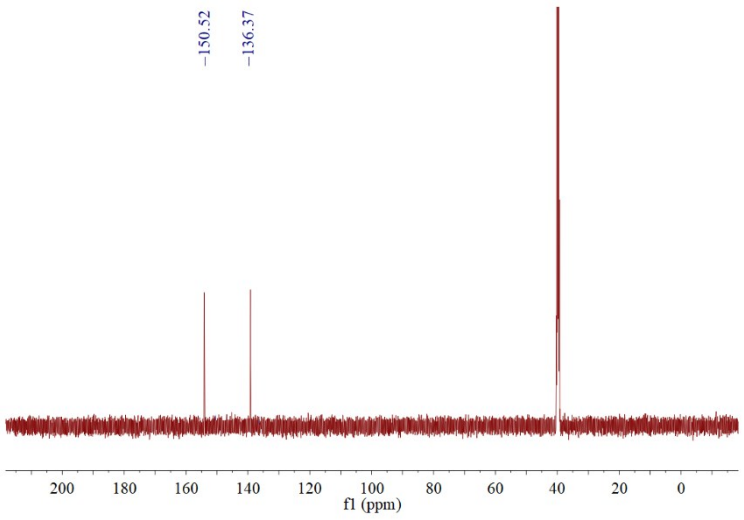


Figure S17. ^{13}C NMR spectra in DMSO-d_6 for **D1.**

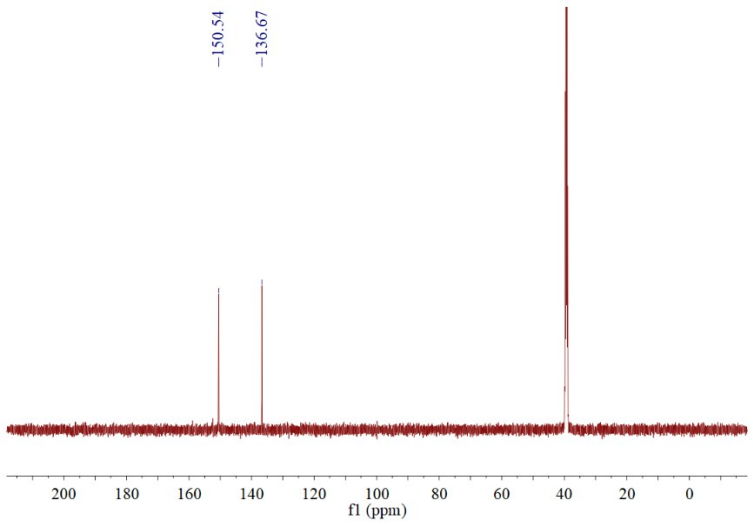


Figure S18. ^{13}C NMR spectra in DMSO-d_6 for **D2.**

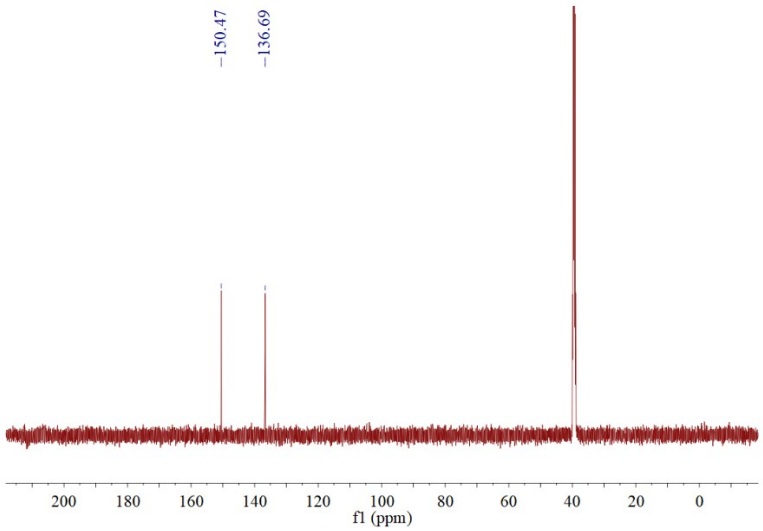


Figure S19. ^{13}C NMR spectra in DMSO-d_6 for **D3.**

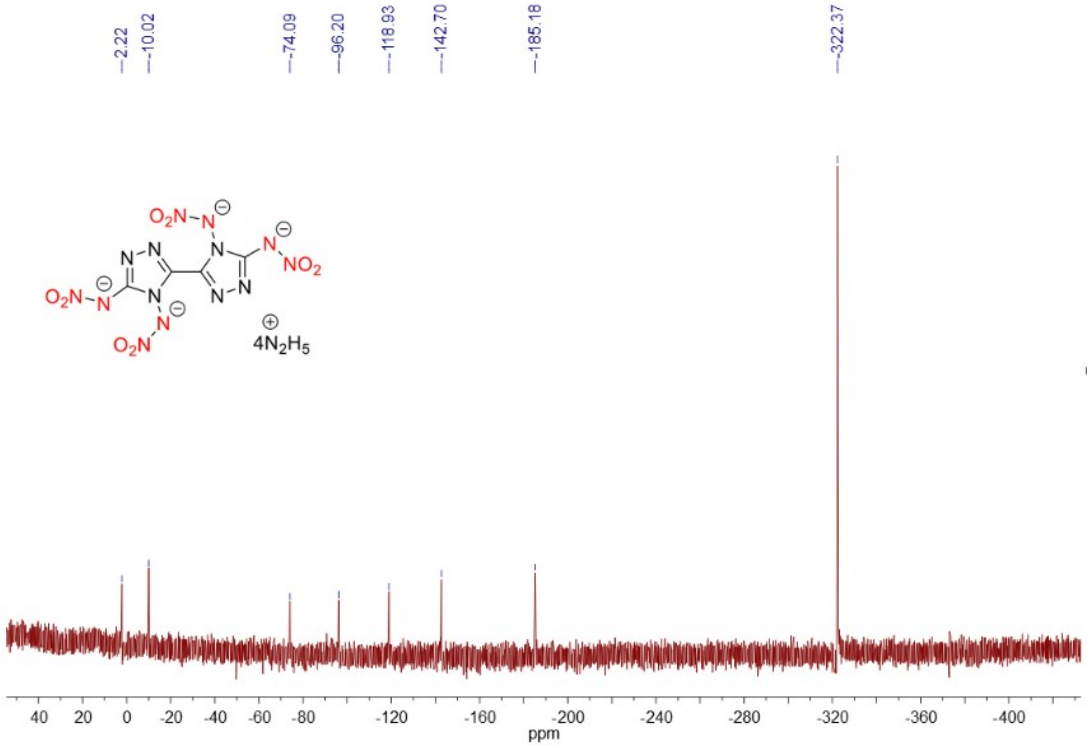


Figure S20. ^{15}N NMR spectra in DMSO-d_6 for **T2**.

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