Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

5-amino-4H-1,2,4-triazole-3-carbohydrazide and its applications in synthesis of energetic salts: a new strategy for constructing nitrogen-rich cation based on the energetic moieties combination

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Table S1. Crystal data and structure refinement details for **ATCH(1)**, **DH-ATCH(2)**, **DN-ATCH(3)**, **DPC ATCH(4)**, **TNPG-ATCH(7)**, and **SP-ATCH(8)**.

	1	**2**	**3**	**4**	**7**	**8**
Formula	$C_3H_6N_6O$	$C_3H_8Cl_2N_6O$	$C_6H_{19}N_{16}O_{15.5}$	$C_3H_{14}Cl_2N_6O_{12}$	$C_9H_9N_9O_{10}$	$C_3H_8N_6O_5S$
M_w[g mol^{-1}]	142.14	215.05	563.37	397.10	403.25	240.21
T [K]	296(2)	173(2)	296(2)	100(2)	293(2)	173(2)
Crystal size [mm^3]	0.18×0.15×0.10	0.19×0.16×0.11	0.20x0.16x0.05	0.18×0.15×0.11	0.28×0.15×0.12	0.10×0.07×0.04
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic	Triclinic	Monoclinic
Space group	*P2$_1$/n*	*P*2$_1$/*c*	*P*-1	*P*2$_1$/*n*	*P*-1	*P*2$_1$/*c*
a [Å]	5.2108(2)	12.0906(3)	8.1276(2)	14.953(4)	7.251(2)	5.6170(2)
b [Å]	8.5731(3)	4.70700(10)	11.7571(3)	4.8569(12)	8.401(2)	18.6083(6)
c [Å]	13.2997(4)	14.6257(4)	12.4802(3)	19.280(5)	12.141(4)	8.1288(3)
α [˚]	90	90	68.1870(10)	90	96.687(16)	90
β [˚]	98.5020(10)	91.7100(10)	73.4280(10)	93.743(6)	98.3178(19)	91.1320(10)
γ [˚]	90	90	85.5050(10)	90	93.39(3)	90
V [Å^3]	587.60(4)	831.98(4)	1060.68(5)	1397.2(6)	724.6(4)	849.48(5)
Z	4	4	2	4	2	4
ρ_{calc} [g cm^{-3}]	1.607	1.717	1.764	1.888	1.848	1.878
μ [mm^{-1}]	0.128	0.743	0.169	0.546	0.169	0.401
λ [Å]	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
F (000)	296	440	582	816	412	496
2*ϑ* range [˚]	6.194-51.986	6.428-52.000	3.658-54.988	3.344-52.714	3.418-51	4.378-51.982
Reflections collected	9651 / 1144	12363 / 1597	45515 / 4859	8214 / 2769	5609 / 2656	12166 / 1658
Index ranges	-6≤*h*≤6 -10≤*k*≤10 -16≤*l*≤16	-14≤*h*≤14 -5≤*k*≤5 -18≤*l*≤18	-10≤*h*≤10 -15≤*k*≤15 -16≤*l*≤16	-18≤*h*≤15 -6≤*k*≤6 -24≤*l*≤24	-8≤*h*≤8 -10≤*k*≤10 -14≤*l*≤14	-6≤*h*≤6 -22≤*k*≤22 -10≤*l*≤10
R_{int}	0.0461	0.0476	0.0750	0.0712	0.0300	0.0449
Data / restraints / parameters	1144 / 0 / 115	1597 / 1 /141	4859 / 18 / 370	2769 / 8 / 219	2656 / 2 / 263	1658 / 0 / 169
Final R index [*I* > 2*σ*(*I*)]	R_1=0.0364, wR_2=0.1055	R_1=0.0250, wR_2=0.0652	R_1=0.0532, wR_2=0.1506	R_1=0.0528, wR_2=0.1320	R_1=0.0473, wR_2=0.1305	R_1=0.0341, wR_2=0.0822
Final R index [all data]	R_1=0.0381, wR_2=0.1081	R_1=0.0256, wR_2=0.0658	R_1=0.0662, wR_2=0.1645	R_1=0.0744, wR_2=0.1450	R_1=0.0615, wR_2=0.1404	R_1=0.0398, wR_2=0.0873
GOF on F^2	1.065	1.098	1.012	1.029	1.016	1.098
CCDC	1831245	1831246	1831247	1831248	1831250	1831249

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **ATCH(1)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	7066(2)	4427.8(12)	3911.3(8)	28.3(1)
N(2)	3725(2)	4011.0(13)	2731.0(9)	33.5(3)
N(3)	3397(2)	5497.3(12)	3051.2(8)	34.2(3)
N(4)	7884(2)	7283.8(13)	5011.5(9)	31.7(3)
N(5)	8431(2)	8691.8(14)	5555.9(10)	37.1(3)
N(6)	6666(3)	1930.7(14)	3093.8(12)	52.7(3)
O(1)	4369(2)	8302.8(12)	4071.1(8)	48.6(3)
C(1)	5890(2)	3394.7(15)	3245.1(9)	29.8(3)
C(2)	5441(2)	5677.5(14)	3752.9(9)	26.5(3)
C(3)	5852(2)	7191.4(14)	4288.2(9)	29.8(3)

Table S3. Bond lengths [Å] and angles [°] for **ATCH(1)**.

N(1)-C(1)	1.3360(15)
N(1)-C(2)	1.3626(16)
N(2)-C(1)	1.3385(17)
N(2)-N(3)	1.3622(16)
N(2)-H(2)	0.872(19)
N(3)-C(2)	1.3175(16)
N(4)-C(3)	1.3230(17)
N(4)-N(5)	1.4148(15)
N(4)-H(4)	0.864(19)
N(5)-H(5C)	0.86(3)
N(5)-H(5B)	0.90(5)
N(6)-C(1)	1.3429(18)
N(6)-H(6A)	0.85(2)
N(6)-H(6B)	0.94(2)
O(1)-C(3)	1.2341(16)
C(2)-C(3)	1.4806(17)
C(1)-N(1)-C(2)	101.82(10)
C(1)-N(2)-N(3)	110.17(10)

C(1)-N(2)-H(2)	127.7(11)
N(3)-N(2)-H(2)	121.9(11)
C(2)-N(3)-N(2)	101.86(10)
C(3)-N(4)-N(5)	120.15(11)
C(3)-N(4)-H(4)	122.15(11)
N(5)-N(4)-H(4)	117.5(11)
N(4)-N(5)-H(5C)	111(2)
N(4)-N(5)-H(5B)	108(2)
H(5C)-N(5)-H(5B)	99(3)
C(1)-N(6)-H(6A)	118.3(13)
C(1)-N(6)-H(6B)	121.0(13)
H(6A)-N(6)-H(6B)	120.5(18)
N(1)-C(1)-N(2)	110.28(11)
N(1)-C(1)-N(6)	126.88(12)
N(2)-C(1)-N(6)	122.83(12)
N(3)-C(2)-N(1)	115.87(11)
N(3)-C(2)-C(3)	119.20(11)
N(1)-C(2)-C(3)	124.91(11)
O(1)-C(3)-N(4)	122.00(12)
O(1)-C(3)-C(2)	121.55(12)
N(4)-C(3)-C(2)	116.45(11)

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **ATCH(1)**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	27.8(5)	26.8(6)	27.5(5)	-3.7(4)	-5.3(4)	0.6(4)
N(2)	35.4(6)	29.0(6)	30.6(6)	-5.7(4)	-13.2(5)	-0.4(4)
N(3)	36.1(6)	28.0(6)	33.3(6)	-0.7(4)	-11.9(5)	2.1(4)
N(4)	31.9(6)	22.7(5)	36.0(6)	-6.2(4)	-9.3(4)	3.9(4)
N(5)	39.5(7)	26.0(6)	40.9(7)	-9.1(5)	-10.5(5)	0.8(5)
N(6)	44.7(7)	37.8(7)	65.9(9)	-24.2(7)	-24.0(7)	11.3(6)
O(1)	57.5(7)	31.0(5)	47.1(6)	-7.0(4)	-25.9(5)	15.4(4)
C(1)	29.7(6)	29.0(6)	28.0(6)	-4.5(5)	-5.1(5)	-0.6(5)
C(2)	28.7(6)	24.8(6)	23.6(6)	1.6(4)	-3.9(5)	0.3(4)
C(3)	34.7(7)	24.5(6)	27.2(6)	1.3(5)	-5.1(5)	2.4(5)

Table S5. Hydrogen coordinates (Å x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **ATCH(1)**.

	x	y	z	U(eq)
H(2)	2700(30)	3600(20)	2220(14)	40(4)
H(4)	8980(30)	6530(20)	5136(12)	40(4)
H(6A)	5690(40)	1360(20)	2681(16)	56(5)
H(6B)	8170(40)	1520(20)	3485(16)	60(5)
H(5C)	8100(60)	9490(40)	5170(30)	109(10)
H(5B)	7210(80)	8830(40)	5970(30)	143(13)

Table S6. Torsion angles [°] for **ATCH(1)**.

C(1)-N(2)-N(3)-C(2)	0.06(14)
C(2)-N(1)-C(1)-N(2)	0.20(14)
C(2)-N(1)-C(1)-N(6)	-178.90(15)
N(3)-N(2)-C(1)-N(1)	-0.18(15)
N(3)-N(2)-C(1)-N(6)	178.97(14)
N(2)-N(3)-C(2)-N(1)	0.08(14)
N(2)-N(3)-C(2)-C(3)	178.73(11)
C(1)-N(1)-C(2)-N(3)	-0.19(14)
C(1)-N(1)-C(2)-C(3)	-178.75(12)
N(5)-N(4)-C(3)-O(1)	-0.7(2)
N(5)-N(4)-C(3)-C(2)	179.51(12)
N(3)-C(2)-C(3)-O(1)	-2.2(2)
N(1)-C(2)-C(3)-O(1)	176.28(12)
N(3)-C(2)-C(3)-N(4)	177.52(11)
N(1)-C(2)-C(3)-N(4)	-3.96(19)

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **DH-ATCH(2)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	3500.4(3)	135.0(7)	4197.2(2)	17.56(13)
Cl(2)	1053.4(3)	7905.8(7)	5825.3(2)	15.71(13)
N(1)	2794.0(10)	1139(3)	1679.9(8)	12.7(2)
N(2)	4367.3(10)	3209(3)	1800.1(8)	15.4(3)
N(3)	3680.9(10)	4724(3)	2355.9(8)	14.8(3)
N(4)	1736.9(10)	6300(3)	3286.4(8)	13.8(3)
N(5)	760.5(10)	6952(3)	3757.7(8)	13.5(3)
N(6)	4261.4(12)	-791(3)	816.9(9)	18.4(3)
O(1)	915.2(8)	2408(2)	2657.9(7)	14.3(2)
C(1)	3834.9(11)	1064(3)	1384.9(9)	13.0(3)
C(2)	2745.3(11)	3393(3)	2265.6(9)	11.7(3)
C(3)	1713.8(11)	3980(3)	2757.1(9)	11.5(3)

Table S8. Bond lengths [Å] and angles [°] for **DH-ATCH(2)**.

N(1)-C(1)	1.3430(18)
N(1)-C(2)	1.3659(18)
N(1)-H(1)	0.82(2)
N(2)-C(1)	1.3339(19)
N(2)-N(3)	1.3777(17)
N(2)-H(2)	0.803(14)
N(3)-C(2)	1.2963(18)
N(4)-C(3)	1.3382(18)
N(4)-N(5)	1.4182(16)
N(4)-H(4)	0.80(2)
N(5)-H(5C)	0.91(2)
N(5)-H(5B)	0.88(2)
N(5)-H(5A)	0.88(2)
N(6)-C(1)	1.3206(19)
N(6)-H(6B)	0.82(2)
N(6)-H(6A)	0.82(2)
O(1)-C(3)	1.2217(17)

C(2)-C(3)	1.4840(19)
C(1)-N(1)-C(2)	106.28(12)
C(1)-N(1)-H(1)	124.8(13)
C(2)-N(1)-H(1)	128.9(13)
C(1)-N(2)-N(3)	111.68(12)
C(1)-N(2)-H(2)	124.1(13)
N(3)-N(2)-H(2)	122.8(13)
C(2)-N(3)-N(2)	103.24(11)
C(3)-N(4)-N(5)	117.03(12)
C(3)-N(4)-H(4)	125.7(13)
N(5)-N(4)-H(4)	116.1(13)
N(4)-N(5)-H(5C)	110.8(12)
N(4)-N(5)-H(5B)	110.1(11)
H(5C)-N(5)-H(5B)	108.9(16)
N(4)-N(5)-H(5A)	110.6(13)
H(5C)-N(5)-H(5A)	106.0(17)
H(5B)-N(5)-H(5A)	110.3(17)
C(1)-N(6)-H(6B)	122.0(13)
C(1)-N(6)-H(6A)	117.7(15)
H(6B)-N(6)-H(6A)	120(2)
N(6)-C(1)-N(2)	126.49(14)
N(6)-C(1)-N(1)	127.36(14)
N(2)-C(1)-N(1)	106.13(12)
N(3)-C(2)-N(1)	112.66(12)
N(3)-C(2)-C(3)	127.17(13)
N(1)-C(2)-C(3)	120.07(12)
O(1)-C(3)-N(4)	124.45(13)
O(1)-C(3)-C(2)	120.15(12)
N(4)-C(3)-C(2)	115.39(12)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **DH-ATCH(2)**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

Cl(1)	14.3(2)	19.7(2)	18.6(2)	-1.91(13)	0.54(13)	-3.57(13)
Cl(2)	16.1(2)	18.2(2)	12.83(19)	-0.48(12)	-0.23(13)	2.47(12)
N(1)	10.9(6)	12.1(6)	15.0(6)	-1.5(5)	1.4(4)	-0.4(5)
N(2)	9.1(6)	17.7(6)	19.6(6)	-1.0(5)	4.4(5)	-0.5(5)
N(3)	11.4(6)	16.1(6)	17.1(6)	-1.4(5)	2.4(5)	0.7(4)
N(4)	8.7(6)	15.8(6)	17.0(6)	-4.4(5)	2.2(4)	-1.3(5)
N(5)	11.8(6)	16.1(6)	12.7(6)	-2.5(5)	1.5(4)	1.5(5)
N(6)	17.9(7)	18.5(6)	19.1(6)	-1.8(5)	5.7(5)	3.8(5)
O(1)	11.9(5)	15.1(5)	16.1(5)	-1.8(4)	1.5(4)	-2.7(4)
C(1)	13.0(6)	13.3(6)	12.6(6)	3.5(5)	1.1(5)	2.5(5)
C(2)	12.0(6)	11.5(6)	11.6(6)	0.8(5)	-0.(5)	1.2(5)
C(3)	11.8(6)	12.6(6)	10.1(6)	2.2(5)	-0.5(5)	1.3(5)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **DH-ATCH(2)**.

	x	y	z	U(eq)
H(5C)	922(16)	7280(40)	4364(15)	29(5)
H(6B)	3879(17)	-1930(40)	532(14)	25(5)
H(4)	2293(17)	7210(40)	3434(13)	24(5)
H(5B)	434(16)	8460(50)	3525(13)	26(5)
H(1)	2282(17)	50(40)	1510(13)	24(5)
H(5A)	301(19)	5530(50)	3739(15)	35(6)
H(2)	4966(13)	3790(40)	1656(12)	23(5)
H(6A)	4930(20)	-860(50)	795(15)	37(6)

Table S11. Torsion angles [°] for **DH-ATCH(2)**.

C(1)-N(2)-N(3)-C(2)	0.89(15)
N(3)-N(2)-C(1)-N(6)	-179.38(13)
N(3)-N(2)-C(1)-N(1)	-0.91(15)
C(2)-N(1)-C(1)-N(6)	179.01(14)
C(2)-N(1)-C(1)-N(2)	0.56(15)
N(2)-N(3)-C(2)-N(1)	-0.51(15)
N(2)-N(3)-C(2)-C(3)	175.77(13)

C(1)-N(1)-C(2)-N(3)	-0.01(16)
C(1)-N(1)-C(2)-C(3)	-176.59(12)
N(5)-N(4)-C(3)-O(1)	-0.2(2)
N(5)-N(4)-C(3)-C(2)	179.17(11)
N(3)-C(2)-C(3)-O(1)	-174.13(13)
N(1)-C(2)-C(3)-O(1)	1.9 (2)
N(3)-C(2)-C(3)-N(4)	6.5(2)
N(1)-C(2)-C(3)-N(4)	-177.47(11)

Symmetry transformations used to generate equivalent atoms:

Table S12. Hydrogen bonds for **DH-ATCH(2)** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(6A)...Cl(1)#1	0.82(2)	2.67(2)	3.3171(14)	137.0(2)
N(2)-H(2)...Cl(1)#2	0.808(15)	2.352(15)	3.1338(13)	163.0(17)
N(5)-H(5A)...Cl(2)#3	0.87(2)	2.40(2)	3.2387(13)	161.9(19)
N(1)-H(1)...Cl(2)#4	0.84(2)	2.25(2)	3.0756(15)	170.3(18)
N(5)-H(5B)...O(1)#5	0.88(2)	2.390(2)	2.8613(16)	113.6(16)
N(5)-H(5B)...O(1)#6	0.88(2)	2.33(2)	3.0392(17)	137.8(16)
N(5)-H(5B)...Cl(2)#7	0.88(2)	2.68 (2)	3.3348(13)	132.8(16)
N(4)-H(4)...Cl(1)#6	0.82(2)	2.28(2)	3.0676(13)	162.5(18)
N(6)-H(6B)...Cl(1)#8	0.82(2)	2.50(2)	3.2418(15)	152.3(18)
N(5)-H(5C)...Cl(2)	0.91(2)	2.16(2)	3.0671(13)	171.6(17)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z+1/2 #2 -x+1,y+1/2,-z+1/2 #3 -x,-y+1,-z+1

#4 x,-y+1/2,z-1/2 #5 -x,y+1/2,-z+1/2 #6 x,y+1,z

#7 -x,-y+2,-z+1 #8 x,-y-1/2,z-1/2

Table S13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **DN-ATCH(3)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	2991(2)	-141.3(15)	3322.1(14)	32.4(4)
N(2)	4155(2)	1210.1(16)	3762.8(15)	37.7(4)

N(3)	3024(2)	423.5(16)	4762.6(15)	37.2(4)
N(4)	1204(3)	-1282.7(17)	5257.2(16)	45.8(5)
N(5)	6161(2)	2304(16)	1369.9(15)	38.3(4)
N(6)	7172(2)	2835.9(17)	165.1 (15)	42(4)
N(7)	6541(2)	4401(15)	6386.6(15)	34.2(4)
N(8)	5435(2)	3026.4(16)	5938.7(15)	36.8(4)
N(9)	6517(2)	3839.6(16)	4938.5(15)	37.4(4)
N(10)	8293(3)	5576.3(17)	4451.6(17)	45.4(5)
N(11)	3500(2)	1863.3(16)	8322.6(15)	35.2(4)
N(12)	2591(2)	1246.4(16)	9535.9(15)	37.9(4)
N(13)	7664(2)	4511.3(16)	1974.6(16)	41.3(4)
N(14)	8804(2)	2059.1(17)	7594.7(16)	40.3(4)
N(15)	8345(3)	6390.7(19)	7153.8(19)	50.7(5)
N(16)	1300(2)	9838.3(15)	7804.8(14)	33.2(4)
O(1)	5052(2)	873(14)	937.6(13)	41.1(4)
O(2)	4720.5(19)	3186.9(14)	8822.5(13)	40.4(4)
O(3)	7965(3)	4676.316)	899.7(15)	58.3(5)
O(4)	6834(3)	3557.3(16)	2755(15)	58.5(5)
O(5)	8129(3)	5280.4(16)	2287.1(16)	62.2(5)
O(6)	9288(2)	2250.8(18)	6509(15)	55.9(5)
O(7)	7632(2)	1272.7(18)	8239.4(17)	65(5)
O(8)	9438(3)	2648(2)	8014.5(18)	74.6(6)
O(9)	7330(3)	5504(2)	7774(2)	90.6(8)
O(10)	8978(3)	6572(2)	6087.8(19)	79(7)
O(11)	8720(3)	7081(2)	7594.6(19)	71.4(6)
O(12)	467(2)	9280.2(16)	7460.4(15)	54(5)
O(13)	926(2)	9706(15)	8890.9(13)	44.1(4)
O(14)	2549(2)	10538.8(14)	7070.9(13)	42.1(4)
O(15)	9434(2)	7079.1(15)	9729.6(16)	44.9(4)
O(16)	5000	5000	0	129.6(17)
C(1)	4094(2)	841.4(18)	2917.1(17)	31.9(4)
C(2)	2320(2)	-400.3(18)	4508.1(17)	33.1(4)
C(3)	5126(2)	1346.2(18)	1649.7(17)	32.2(4)
C(4)	5475(2)	3394.5(17)	6792(17)	32.4(4)
C(5)	7209(3)	4673.8(2)	5196(18)	34.3(4)
C(6)	4532(2)	2814.7(17)	8074.8(17)	31.2(4)

Table S14. Bond lengths [Å] and angles [°] for **DN-ATCH(3)**.

N(1)-C(2)	1.346(2)
N(1)-C(1)	1.365(2)
N(1)-H(1)	0.80(3)
N(2)-C(1)	1.295(3)
N(2)-N(3)	1.370(2)
N(3)-C(2)	1.336(2)
N(3)-H(3)	0.82(3)
N(4)-C(2)	1.310(3)
N(4)-H(1A)	0.78(3)
N(4)-H(4B)	0.90(3)
N(5)-C(3)	1.336(2)
N(5)-N(6)	1.416(2)
N(5)-H(5)	0.83(3)
N(6)-H(6A)	0.98(3)
N(6)-H(6B)	0.88(3)
N(6)-H(6C)	0.82(4)
N(7)-C(5)	1.349(3)
N(7)-C(4)	1.368(2)
N(7)-H(7)	0.79(3)
N(8)-C(4)	1.299(3)
N(8)-N(9)	1.365(2)
N(9)-C(5)	1.343(3)
N(9)-H(9)	0.83(3)
N(10)-C(5)	1.309(3)
N(10)-H(10A)	0.78(3)
N(10)-H(10B)	0.86(3)
N(11)-C(6)	1.339(2)
N(11)-N(12)	1.412(2)
N(11)-H(11)	0.75(3)
N(12)-H(12A)	0.88(3)
N(12)-H(12B)	0.98(3)
N(12)-H(12C)	0.81(3)
N(13)-O(5)	1.230(2)
N(13)-O(3)	1.235(2)
N(13)-O(4)	1.262(2)
N(14)-O(8)	1.225(2)

N(14)-O(6)	1.235(2)
N(14)-O(7)	1.246(2)
N(15)-O(10)	1.223(3)
N(15)-O(11)	1.233(2)
N(15)-O(9)	1.240(3)
N(16)-O(12)	1.232(2)
N(16)-O(13)	1.253(2)
N(16)-O(14)	1.260(2)
O(1)-C(3)	1.227(2)
O(2)-C(6)	1.217(2)
O(15)-H(15C)	0.826(19)
O(15)-H(15D)	0.818(19)
O(16)-H(16A)	0.9789
C(1)-C(3)	1.477(3)
C(4)-C(6)	1.479(3)

C(2)-N(1)-C(1)	106.12(16)
C(2)-N(1)-H(1)	122.4(19)
C(1)-N(1)-H(1)	131.2(19)
C(1)-N(2)-N(3)	103.52(16)
C(2)-N(3)-N(2)	111.67(16)
C(2)-N(3)-H(3)	127.0(19)
N(2)-N(3)-H(3)	121.2(19)
C(2)-N(4)-H(1A)	119(2)
C(2)-N(4)-H(4B)	118.7(18)
H(1A)-N(4)-H(4B)	122(3)
C(3)-N(5)-N(6)	117.77(16)
C(3)-N(5)-H(5)	124.3(19)
N(6)-N(5)-H(5)	117.7(19)
N(5)-N(6)-H(6A)	107.0(17)
N(5)-N(6)-H(6B)	114(2)
H(6A)-N(6)-H(6B)	104(3)
N(5)-N(6)-H(6C)	117(2)
H(6A)-N(6)-H(6C)	103(3)
H(6B)-N(6)-H(6C)	110(3)
C(5)-N(7)-C(4)	106.19(16)
C(5)-N(7)-H(7)	125(2)
C(4)-N(7)-H(7)	129(2)

C(4)-N(8)-N(9)	103.74(16)
C(5)-N(9)-N(8)	111.78(17)
C(5)-N(9)-H(9)	130(2)
N(8)-N(9)-H(9)	118(2)
C(5)-N(10)-H(10A)	118(2)
C(5)-N(10)-H(10B)	121.4(18)
H(10A)-N(10)-H(10B)	121(3)
C(6)-N(11)-N(12)	117.44(16)
C(6)-N(11)-H(11)	125(2)
N(12)-N(11)-H(11)	118(2)
N(11)-N(12)-H(12A)	105.6(17)
N(11)-N(12)-H(12B)	111.2(16)
H(12A)-N(12)-H(12B)	107(2)
N(11)-N(12)-H(12C)	111(2)
H(12A)-N(12)-H(12C)	110(3)
H(12B)-N(12)-H(12C)	111(3)
O(5)-N(13)-O(3)	120.59(19)
O(5)-N(13)-O(4)	119.97(19)
O(3)-N(13)-O(4)	119.41(18)
O(8)-N(14)-O(6)	120.4(2)
O(8)-N(14)-O(7)	121.4(2)
O(6)-N(14)-O(7)	118.18(19)
O(10)-N(15)-O(11)	120.1(2)
O(10)-N(15)-O(9)	118.7(2)
O(11)-N(15)-O(9)	121.2(2)
O(12)-N(16)-O(13)	120.46(17)
O(12)-N(16)-O(14)	120.36(16)
O(13)-N(16)-O(14)	119.23(16)
H(15C)-O(15)-H(15D)	101(4)
N(2)-C(1)-N(1)	112.66(17)
N(2)-C(1)-C(3)	126.27(18)
N(1)-C(1)-C(3)	121.02(17)
N(4)-C(2)-N(3)	127.18(19)
N(4)-C(2)-N(1)	126.79(18)
N(3)-C(2)-N(1)	106.03(17)
O(1)-C(3)-N(5)	123.94(18)
O(1)-C(3)-C(1)	120.90(18)
N(5)-C(3)-C(1)	115.11(17)

N(8)-C(4)-N(7)	112.48(17)
N(8)-C(4)-C(6)	125.92(17)
N(7)-C(4)-C(6)	121.59(17)
N(10)-C(5)-N(9)	127.58(19)
N(10)-C(5)-N(7)	126.61(19)
N(9)-C(5)-N(7)	105.81(17)
O(2)-C(6)-N(11)	124.33(18)
O(2)-C(6)-C(4)	121.25(17)
N(11)-C(6)-C(4)	114.42(16)

Symmetry transformations used to generate equivalent atoms:

Table S15. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **DN-ATCH(3)**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	35.1(8)	34.3(8)	28.9(8)	-12.1(7)	-8.2(6)	-5.7(7)
N(2)	37.4(9)	42.4(9)	33.2(8)	-15.2(7)	-5.1(7)	-9.5(7)
N(3)	40.4(9)	43.4(10)	28.6(8)	-14.8(7)	-5.2(7)	-11.1(7)
N(4)	54.0(11)	45.3(10)	34.5(9)	-14.5(8)	-1.8(8)	-17.5(9)
N(5)	41.9(9)	40.0(9)	31.2(8)	-14.2(7)	-1.6(7)	-14.2(7)
N(6)	44.7(10)	45.4(10)	31.1(8)	-9.3(7)	-5.7(7)	-14.5(8)
N(7)	37.1(8)	32.8(8)	35.0(8)	-14.2(7)	-8.7(7)	-6.9(7)
N(8)	40.6(9)	35.2(09)	34.6(8)	-11.4(7)	-9.7(7)	-7.9(7)
N(9)	44.2(9)	37.2(9)	30.9(8)	-11.8(7)	-8.6(7)	-9.1(7)
N(10)	51.2(11)	44.0(10)	38.8(9)	-12.2(8)	-8.4(8)	-17.6(8)
N(11)	37.8(9)	39.1(9)	31.9(8)	-17.3(7)	-5.4(7)	-10.6(7)
N(12)	38.0(9)	37.6(9)	37.8(9)	-15.9(7)	-3.6(7)	-11.7(7)
N(13)	47.3(10)	37.1(9)	40.1(9)	-15.5(8)	-9.8(8)	-3.1(8)
N(14)	39.0(9)	41.5(10)	41.9(10)	-17.5(8)	-9.4(7)	-2.7(7)
N(15)	51.2(11)	54.7(12)	55.6(12)	-30.5(10)	-8.7(9)	-14.9(9)
N(16)	37.2(8)	31.9(8)	33.7(8)	-15.1(7)	-9.1(7)	-4.8(7)
O(1)	50.1(9)	43.6(1)	31.7(7)	-13.3(6)	-11.5(6)	-11.9(7)
O(2)	46.1(8)	41.6(8)	38.8(8)	-18.7(6)	-10.8(6)	-11.9(6)
O(3)	80.3(13)	50.3(10)	40.5(9)	-21.1(8)	-0.4(8)	-14.7(9)
O(4)	82.3(13)	49.4(10)	39.3(9)	-12.6(7)	-7.3(8)	-27.6(9)
O(5)	95.2(15)	45.9(10)	54.3(10)	-17.5(8)	-29.4(10)	-19.3(9)

O(6)	66.3(11)	67.2(11)	41.6(9)	-29.0(8)	-10.1(8)	-11.4(9)
O(7)	48.3(10)	63.4(12)	62.3(11)	-3.6(9)	-6.0(9)	-13.5(9)
O(8)	92.5(15)	91.1(15)	58.2(12)	-46.4(11)	-14.8(11)	-25.0(12)
O(9)	102.4(18)	97.5(17)	70.4(14)	-41.6(13)	9.6(12)	-58.8(15)
O(10)	98.5(16)	88.2(15)	56.0(12)	-41.8(11)	3.6(11)	-45.1(13)
O(11)	92.4(15)	75.1(13)	64.2(12)	-41.3(11)	-19.6(11)	-24.6(11)
O(12)	65.7(11)	58.5(10)	47.7(9)	-24.0(8)	-17.4(8)	-24.0(8)
O(13)	48.7(9)	52.7(9)	32.7(7)	-21.1(7)	-1.8(6)	-16.8(7)
O(14)	44.5(8)	47.6(9)	34.4(7)	-17.0(6)	-4.0(6)	-14.3(7)
O(15)	47.6(9)	39.9(8)	41.7(8)	-13.4(7)	-3.4(7)	-9.1(7)
O(16)	177(5)	141(4)	107(3)	-67(3)	-73(3)	37(3)
C(1)	30.7(9)	32.3(9)	31.9(9)	-10.2(8)	-8.0(7)	-4.1(7)
C(2)	33.3(9)	34.3(10)	31.7(9)	-11.6(8)	-8.9(7)	-2.1(8)
C(3)	33.6(9)	33.2(9)	29.4(9)	-9.2(7)	-10.0(7)	-3.1(7)
C(4)	32.3(9)	30.8(9)	34.8(10)	-11.9(8)	-10.1(8)	-3.7(7)
C(5)	35.4(10)	32.5(10)	36.3(10)	-11.6(8)	-12.1(8)	-2.1(8)
C(6)	30.6(9)	30.5(9)	34.4(9)	-13.5(8)	-8.6(67)	-2.5(7)

Table S16. Hydrogen coordinates (Å x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **DN-ATCH(3)**.

	x	y	z	U(eq)
H(1)	2770.65	-518.81	2903.89	39
H(3)	2795.59	456.1	5466.95	45
H(4A)	849.18	-1376.72	6004.16	55
H(4B)	826.56	-1768.15	5001.95	55
H(5)	6210.43	2587.77	1903.73	46
H(6A)	8142(9)	2960(30)	320(30)	50
H(6B)	7200(60)	2259(10)	-153(7)	50
H(6C)	6650(30)	3554(15)	-63(10)	50
H(6D)	7640(30)	3587(10)	-73(7)	50
H(6E)	8205(5)	2521(8)	-44(3)	50
H(6F)	6662(9)	2879(17)	-401(9)	50
H(7)	6743.68	4783.03	6806.65	41
H(9)	6730.26	3820.08	4229.97	45
H(10A)	8640.74	5684.52	3701.04	54

H(10B)	8658.55	6061.18	4713.1	54
H(11)	3394.13	1636.58	7764.32	42
H(12A)	3331.3	970.81	9974.53	57
H(12B)	1982.21	618.13	9594.91	57
H(12C)	1887.2	1761.6	9802.8657	
H(15A)	9130(40)	6340(30)	10170(30)	54
H(15B)	9430(40)	7060(30)	9060(30)	54
H(16A)	4510(20)	4870(70)	782(17)	155
H(16B)	5780(20)	5060(20)	360(30)	155

Table S17. Torsion angles [°] for **DN-ATCH(3)**.

N(3)-N(2)-C(1)-C(3)	-177.45(18)
C(2)-N(1)-C(1)-N(2)	0.0(2)
C(2)-N(1)-C(1)-C(3)	177.34(17)
N(2)-N(3)C-(2)-N(4)	179.5(2)
N(2)-N(3)-C(2)-N(1)	-0.5(2)
C(1)-N(1)-C(2)-N(4)	-179.6(2)
C(1)-N(1)-C(2)-N(3)	0.3(2)
N(6)-N(5)-C(3)-O(1)	3.0(3)
N(6)-N(5)-C(3)-C(1)	-179.42(17)
N(2)-C(1)-C(3)-O(1)	175.0(2)
N(1)-C(1)-C(3)-O(1)	-2.0(3)
N(2)-C(1)-C(3)-N(5)	-2.7(3)
N(1)-C(1)-C(3)-N(5)	179.68(17)
N(9)-N(8)-C(4)-N(7)	-0.4(2)
N(9)-N(8)-C(4)-C(6)	-179.25(18)
C(5)-N(7)-C(4)-N(8)	-0.1(2)
C(5)-N(7)-C(4)-C(6)	178.87(17)
N(8)-N(9)-C(5)-N(10)	179.9(2)
N(8)-N(9)-C(5)-N(7)	-0.7(2)
C(4)-N(7)-C(5)-N(10)	179.8(2)
C(4)-N(7)-C(5)-N(9)	0.5(2)
N(12)-N(11)-C(6)-O(2)	-0.8(3)
N(12-)N(11)-C(6)-C(4)	178.46(16)
N(8)-C(4)-C(6)-O(2)	176.03(19)

N(7)-C(4)-C(6)-O(2)	-2.8(3)
N(8)-C(4)-C(6)-N(11)	-3.3(3)
N(7)-C(4)-C(6)-N(11)	177.93(17)

Table S19. Hydrogen bonds for **DN-ATCH(3)** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(15)-H(15D)...O(11)	0.818(19)	2.10(3)	2.881(3)	158(5)
O(15)-H(15C)...O(5)#1	0.826(19)	2.38(3)	3.030(2)	137(4)
O(15)-H(15C)...O(3)#1	0.826(19)	2.04(2)	2.828(2)	160(4)
O(15)-H(15C)...N(13)#1	0.826(19)	2.54(2)	3.335(2)	162(4)
N(12)-H(12C)...O(1)#1	0.81(3)	2.16(3)	2.926(3)	159(3)
N(6)-H(6C)...O(16)#2	0.82(4)	2.29(4)	2.962(2)	139(3)
N(12)-H(12B)...O(15)#3	0.98(3)	1.75(3)	2.718(3)	172(2)
N(10)-H(10B)...O(8)#4	0.86(3)	2.50(3)	3.136(3)	131(2)
N(10)-H(10B)...O(5)	0.86(3)	2.15(3)	2.887(3)	143(2)
N(6)-H(6B)...O(8)#2	0.88(3)	2.30(3)	2.862(3)	121(3)
N(6)-H(6B)...O(7)#2	0.88(3)	2.58(4)	3.456(3)	172(3)
N(4)-H(4B)...O(12)#5	0.90(3)	2.12(3)	2.948(3)	154(2)
N(4)-H(4B)...O(11)#6	0.90(3)	2.46(3)	3.059(3)	124(2)
N(12)-H(12A)...O(13)#7	0.88(3)	2.55(3)	2.991(2)	112(2)
N(12)-H(12A)...O(13)#5	0.88(3)	1.96(3)	2.800(2)	159(2)
N(10)-H(10A)...O(10)	0.78(3)	2.17(3)	2.896(3)	155(3)
N(10)-H(10A)...O(6)#4	0.78(3)	2.49(3)	3.001(3)	124(3)
N(6)-H(6A)...O(15)#4	0.98(3)	1.83(3)	2.808(3)	177(3)
N(4)-H(1A)...O(10)#6	0.78(3)	2.35(3)	2.902(3)	129(3)
N(4)-H(1A)...O(6)#8	0.78(3)	2.26(3)	2.962(3)	151(3)
N(11)-H(11)...O(14)#5	0.75(3)	2.13(3)	2.857(2)	161(3)
N(9)-H(9)...O(5)	0.83(3)	2.48(3)	3.042(3)	126(2)
N(9)-H(9)...O(4)	0.83(3)	1.98(3)	2.806(2)	177(3)
N(9)-H(9)...N(13)	0.83(3)	2.57(3)	3.340(3)	154(3)
N(7)-H(7)...O(10)	0.79(3)	2.63(3)	3.201(3)	131(2)
N(7)-H(7)...O(9)	0.79(3)	1.96(3)	2.745(3)	176(3)
N(7)-H(7)...N(15)	0.79(3)	2.66(3)	3.399(2)	158(3)
N(5)-H(5)...O(4)	0.83(3)	2.01(3)	2.832(2)	167(3)
N(5)-H(5)...O(3)	0.83(3)	2.58(3)	3.038(2)	115(2)

N(5)-H(5)...N(13)	0.83(3)	2.66(3)	3.360(3)	142(2)
N(3)-H(3)...O(14)#5	0.82(3)	2.03(3)	2.851(2)	176(3)
N(1)-H(1)...O(7)#8	0.80(3)	2.12(3)	2.905(3)	168(3)
N(1)-H(1)...O(6)#8	0.80(3)	2.49(3)	3.121(2)	137(2)
N(1)-H(1)...N(14)#8	0.80(3)	2.68(3)	3.453(2)	165(2)
O(16)-H(16A)...O(3)#9	0.98	2.22	2.883(2)	123.6
O(16)-H(16A)...O(2)	0.98	2.31	3.0587(14)	132.2

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1 #2 x,y,z-1 #3 -x+1,-y+1,-z+2 #4 -x+2,-y+1,-z+1

#5 x,y-1,z #6 x-1,y-1,z #7 -x,-y+1,-z+2 #8 -x+1,-y,-z+1

#9 -x+1,-y+1,-z+1

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **DPC-ATCH(4)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(2)	475.0(6)	5259.0(18)	3649.9(4)	11.1(2)
Cl(1)	5655.9(6)	8621.0(19)	3398.5(4)	14.1(2)
O(5)	2701.6(17)	8920(5)	3075.7(12)	12.7(6)
O(1W)	2378.3(18)	5883(5)	6654.6(12)	13.8(6)
O(9)	436.4(17)	7954(5)	3334.0(12)	13.1(6)
O(6)	1222.1(17)	3737(5)	3380.8(12)	14.9(6)
O(4)	4800.0(18)	9759(5)	3139.2(13)	16.5(6)
O(2W)	3461.2(18)	5859(5)	8104.9(14)	16.3(6)
O(7)	648.0(19)	5561(5)	4391.6(12)	18.5(6)
O(8)	-343.3(18)	3817(6)	3498.8(14)	20.4(6)
O(2)	5611.4(19)	5667(6)	3323.9(15)	22.3(7)
O(3)	6360.4(19)	9690(6)	3017.5(15)	22.2(7)
O(1)	5809.5(19)	9331(6)	4125.4(13)	22.0(7)
N(4)	2060(2)	10051(6)	4390.4(14)	12.1(7)
N(5)	3480(2)	5237(6)	3520.3(14)	12.2(7)
N(2)	2357(2)	7723(6)	5324.3(14)	12.8(7)
N(6)	3782(2)	4747(6)	2845.6(14)	10.7(7)
N(3)	2842(2)	6473(6)	4827.9(14)	12.9(7)
N(1)	1331(2)	11427(7)	5400.2(15)	16.7(7)
C(1)	2948(2)	7423(7)	3572.3(17)	10.2(8)

C(2)	2631(3)	7940(7)	4269.0(17)	11.4(8)
C(3)	1874(3)	9845(7)	5064.4(17)	12.5(8)
O(W2A)	4235(3)	2050(11)	4474(2)	20.9(10)
O(W2B)	4654(4)	3700(11)	4600(3)	20.9(10)

Table S21. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **DPC-ATCH(4)**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(2)	11.0(5)	10.2(5)	12.2(4)	0.8(3)	2.2(3)	0.1(4)
Cl(1)	10.3(5)	11.2(5)	20.7(5)	-0.8(3)	0.1(3)	-0.3(4)
O(5)	10.9(14)	15.3(14)	12.0(12)	2.7(10)	1.5(10)	2.9(12)
O(1W)	13.4(15)	13.8(14)	14.1(13)	2.7(10)	-0.2(11)	-2.0(12)
O(9)	16.7(15)	7.9(13)	15.0(12)	5.6(9)	3.5(10)	0.3(11)
O(6)	10.8(15)	15.4(15)	18.8(13)	1.3(10)	4.1(10)	7.5(12)
O(4)	13.4(15)	13.1(14)	22.4(14)	1.6(10)	-3.0(11)	4.3(12)
O(2W)	12.7(15)	12.9(14)	23.8(14)	-1.8(11)	4.0(11)	-1.2(12)
O(7)	25.8(17)	22.7(16)	7.3(12)	1.6(10)	3.1(11)	-0.2(13)
O(8)	9.0(15)	17.6(16)	34.3(16)	2.7(12)	-1.8(11)	-5.1(12)
O(2)	16.2(16)	7.0(14)	43.3(18)	-3.2(11)	-2.2(13)	0.9(12)
O(3)	12.9(16)	21.7(16)	33.1(16)	-3.0(12)	9.3(12)	-6.3(13)
O(1)	22.5(17)	22.2(16)	20.3(15)	-2.6(11)	-6.7(12)	1.3(13)
N(4)	14.8(18)	12.7(17)	9.2(15)	1.3(11)	3.6(12)	0.9(14)
N(5)	17.8(19)	10.9(17)	8.4(14)	0.9(11)	4.3(12)	1.4(14)
N(2)	16.8(18)	15.7(17)	6.2(13)	0.2(11)	4.3(12)	2.9(14)
N(6)	10.5(17)	11.8(16)	10.2(14)	-0.8(11)	3.2(12)	3.1(13)
N(3)	13.5(18)	15.8(18)	10.0(14)	-2.9(12)	5.0(12)	0.5(14)
N(10)	23(2)	17.5(18)	9.9(15)	1.6(12)	6.5(13)	8.3(15)
C(1)	8(2)	10.3(19)	11.9(17)	-2.5(13)	1.4(13)	-3.2(16)
C(2)	12(2)	8.7(18)	13.7(17)	0.2(13)	1.1(14)	-0.4(16)
C(3)	13(2)	13(2)	11.0(17)	0.0(14)	0.6(14)	-2.4(16)
O(W2A)	24(3)	27(3)	11.5(18)	0.8(18)	2.4(17)	11.0(19)
O(W2B)	24(3)	27(3)	11.5(18)	0.8(18)	2.4(17)	11.0(19)

Table S22. Bond Lengths [Å] and angles [°] for **DPC-**

ATCH(4).

Cl(2)-O(9)	1.443(3)
Cl(2)-O(6)	1.463(3)
Cl(2)-O(7)	1.444(3)
Cl(2)-O(8)	1.423(3)
Cl(1)-O(4)	1.452(3)
Cl(1)-O(2)	1.443(3)
Cl(1)-O(3)	1.421(3)
Cl(1)-O(1)	1.447(3)
O(5)-C(1)	1.239 (4)
N(4)-C(2)	1.364(5)
N(4)-C(3)	1.350(4)
N(5)-N(6)	1.424(4)
N(5)-C(1)	1.334(5)
N(2)-N(3)	1.379(4)
N(2)-C(3)	1.337(5)
N(3)-C(2)	1.313(5)
N(1)-C(3)	1.319(5)
C(1)-C(2)	1.475(5)

O(9)-Cl(2)-O(6)	108.62(15)
O(9)-Cl(2)-O(7)	108.99(15)
O(7)-Cl(2)-O(6)	108.13(16)
O(8)-Cl(2)-O(9)	110.46(16)
O(8)-Cl(2)-O(6)	110.18(16)
O(8)-Cl(2)-O(7)	110.40(16)
O(2)-Cl(1)-O(4)	108.07(16)
O(3)-Cl(1)-O(4)	110.45(17)
O(3)-Cl(1)-O(2)	110.04(17)
O(3)-Cl(1)-O(1)	109.70(17)
O(1)-Cl(1)-O(4)	108.86(16)
C(3)-N(4)-C(2)	106.3(3)
C(1)-N(5)-N(6)	115.3(3)
C(3)-N(2)-N(3)	112.0(3)
C(2)-N(3)-N(2)	102.8(3)
O(5)-C(1)-N(5)	123.9(3)
O(5)-C(1)-C(2)	120.5(3)
N(5)-C(1)-C(2)	115.6(3)
N(4)-C(2)-C(1)	121.7(3)

N(3)-C(2)-N(4)	112.8(3)
N(3)-C(2)-C(1)	125.5(3)
N(2)-C(3)-N(4)	106.1(3)
N(1)-C(3)-N(4)	127.0(3)
N(1)-C(3)-N(2)	126.9(3)

Table S23. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **DPC-ATCH(4)**.

	x	y	z	U(eq)
H(1WA)	2190.5	4219.23	6727.53	21
H(1WB)	2936.82	5871.72	6812.32	21
H(2WA)	4012.87	5852.7	7987.01	25
H(2WB)	3280.36	4170.22	8040.85	25
H(4)	1854.85	11297.8	4089.56	15
H(5)	3633.76	4172.85	3877.81	15
H(2)	2364.76	7187.04	5760.65	15
H(6A)	4219.38	3442.4	2872.79	16
H(6B)	4003.46	6335.5	2674.84	16
H(6C)	3314.78	4149.29	2558.25	16
H(1A)	1257.44	11128	5843.12	20
H(1B)	1040.75	12780.71	5181.35	20
H(2A1)	4075.05	1849.78	4903.72	31
H(2A2)	4741.94	1103.16	4468.65	31
H(2B1)	4380.45	3067.75	4969.95	31
H(2B2)	5048.32	2094.46	4551.87	31

Table S24. Atomic Occupancy for **DPC-ATCH(4)**.

O(W2A)	0.525(5)
O(W2B)	0.475(5)
H(2A1)	0.525(5)
H(2B1)	0.475(5)
H(2A2)	0.525(5)
H(2B2)	0.475(5)

Table S25. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) **TNPG-ATCH(7)**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

	x	y	z	U(eq)
O(1)	9405(3)	3670(2)	4064.0(16)	31.1(5)
O(2)	8880(2)	1779(2)	2667.8(15)	29.0(5)
O(3)	7272(3)	3981(2)	5503.9(15)	29.5(5)
O(4)	5350(3)	2836(2)	7101.5(15)	31.6(5)
O(5)	2630(3)	3528(2)	6402.8(16)	35.9(5)
O(6)	1657(2)	765(2)	4925.0(16)	27.2(4)
O(7)	790(2)	-1065(2)	3146.4(16)	31.5(5)
O(8)	2003(3)	-628(3)	1680.8(16)	39.9(6)
O(9)	5465(2)	523(2)	2019.6(15)	25.9(4)
N(8)	8333(3)	2550(2)	3466.4(18)	21.2(5)
N(7)	2037(3)	-367(3)	2703.3(18)	24.6(5)
N(9)	4134(3)	2959(2)	6304.5(17)	21.3(5)
C(1)	6527(3)	2195(3)	3753(2)	18.2(5)
C(2)	6140(3)	2880(3)	4815(2)	19.7(5)
C(3)	4470(3)	2374(3)	5169(2)	19.9(5)
C(4)	3141(3)	1262(3)	4488(2)	17.8(5)
C(5)	3430(3)	704(3)	3391(2)	18.9(5)
C(6)	5176(3)	1096(3)	2965(2)	17.2(5)
O(10)	9362(2)	2865(2)	250.3(15)	27.4(4)
N(1)	10911(3)	5244(3)	1897.6(19)	24.9(5)
N(2)	8959(3)	4894(2)	1593.6(17)	20.7(5)
N(4)	5128(3)	4027(2)	1166.0(17)	20.9(5)
N(5)	3391(3)	3293(2)	699.2(17)	21.1(5)
N(3)	5384(3)	2114(2)	-216.9(18)	18.0(5)
N(6)	2168(3)	1182(3)	-768.4(18)	27.1(5)
C(7)	8355(3)	3664(3)	800.7(19)	18.4(5)
C(14)	6290(3)	3293(3)	602.3(19)	16.7(5)
C(8)	3541(3)	2131(3)	-142(2)	18.8(5)

Table S26. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **TNPG-ATCH(7)**. The Anisotropic

displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\cdots]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	23.7(10)	33.2(10)	32.4(11)	-6.1(8)	4.9(8)	-11.7(8)
O(2)	23.8(10)	34.5(11)	28.9(11)	-5.0(8)	13.1(8)	-0.4(8)
O(3)	29.4(11)	33.4(11)	22.2(10)	-6.8(8)	6.9(8)	-14.0(8)
O(4)	37.6(12)	37.8(11)	17.5(10)	-1.4(8)	0.3(9)	5.8(9)
O(5)	30.2(12)	48.3(13)	28.1(11)	-9.6(9)	9.0(9)	12.2(9)
O(6)	21.8(10)	31.6(11)	27.1(11)	-5.8(8)	11.3(8)	-7.2(8)
O(7)	22.9(10)	31.4(10)	36.8(11)	-9.0(8)	8.0(8)	-9.2(8)
O(8)	22.0(11)	69.6(15)	20.2(11)	-22.1(9)	2.3(8)	-4.2(9)
O(9)	25.9(10)	28.5(10)	22.3(10)	-5.3(8)	9.0(8)	-1.9(7)
N(8)	18.5(11)	23.1(11)	22.4(11)	3.0(9)	4.2(9)	1.2(8)
N(7)	17.0(11)	27.3(12)	27.5(13)	-7.5(9)	5.3(9)	1.3(9)
N(9)	26.3(12)	19.9(11)	16.8(11)	-4.6(8)	6.4(9)	-1.3(9)
C(1)	17.0(13)	18.8(12)	18.7(13)	1.7(10)	3.4(10)	1.0(9)
C(2)	21.9(13)	18.2(12)	17.5(13)	-0.6(10)	1.1(10)	-0.2(10)
C(3)	24.1(14)	20.6(12)	13.6(12)	-4(1)	4(1)	0.2(10)
C(4)	15.2(12)	18.8(12)	20.0(13)	1.3(10)	4.9(10)	1.6(9)
C(5)	16.0(13)	20.2(12)	18.6(13)	-4.3(10)	2.4(10)	0.8(9)
C(6)	18.0(13)	17.0(12)	16.9(13)	0.4(9)	3.6(10)	4.0(9)
O(10)	17(1)	33.4(10)	28.7(10)	-11.3(8)	5.4(8)	0.9(7)
N(1)	14.2(11)	29.3(12)	27.4(12)	-8.9(9)	1.4(9)	-0.8(9)
N(2)	13.8(11)	23.4(11)	23.0(11)	-7.8(9)	4.7(8)	1.6(8)
N(4)	13.4(11)	22.0(11)	24.7(12)	-5.0(9)	1.3(9)	0.2(8)
N(5)	13.8(11)	22.6(11)	24.2(12)	-4.7(9)	0.7(8)	-0.7(8)
N(3)	14.3(11)	19.6(11)	19.3(11)	-5.1(9)	4.8(8)	3.4(8)
N(6)	14.7(11)	32.5(12)	30.0(13)	-14(1)	4.8(9)	-0.7(9)
C(7)	15.8(13)	22.3(12)	16.7(12)	0.5(10)	3(1)	0.9(10)
C(14)	16.9(12)	17.1(11)	15.3(12)	-1.4(9)	3.1(9)	0.5(9)
C(8)	15.3(13)	21.2(12)	19.0(13)	-2.2(10)	3.8(10)	1.6(9)

Table S27. Bond Lengths [Å] and angles [°] for **TNPG-ATCH(7)**.

O(1)-N(8)	1.268(3)
O(2)-N(8)	1.230(3)
O(3)-C(2)	1.327(3)

O(4)-N(9)	1.229(3)
O(5)-N(9)	1.232(3)
O(6)-C(4)	1.333(3)
O(7)-N(7)	1.265(3)
O(8)-N(7)	1.232(3)
O(9)-C(6)	1.244(3)
N(8)-C(1)	1.426(3)
N(7)-C(5)	1.414(3)
N(9)-C(3)	1.468(3)
C(1)-C(2)	1.422(3)
C(1)-C(6)	1.465(3)
C(2)-C(3)	1.402(3)
C(3)-C(4)	1.403(3)
C(4)-C(5)	1.409(3)
C(5)-C(6)	1.469(3)
O(10)-C(7)	1.235(3)
N(1)-N(2)	1.415(3)
N(2)-C(7)	1.334(3)
N(4)-N(5)	1.381(3)
N(4)-C(8)	1.299(3)
N(5)-C(15)	1.349(3)
N(3)-C(8)	1.381(3)
N(3)-C(14)	1.353(3)
N(6)-C(8)	1.323(3)
N(6)-C(15)	1.323(3)
C(7)-C(14)	1.490(3)

O(1)-N(8)-C(1)	118.9(2)
O(2)-N(8)-O(1)	119.5(2)
O(2)-N(8)-C(1)	121.6(2)
O(7)-N(7)-C(5)	119.4(2)
O(8)-N(7)-O(7)	119.2(2)
O(8)-N(7)-C(5)	121.4(2)
O(4)-N(9)-O(5)	123.8(2)
O(4)-N(9)-C(3)	118.5(2)
O(5)-N(9)-C(3)	117.7(2)
N(8)-C(1)-C(6)	118.9(2)
C(2)-C(1)-N(8)	118.4(2)

C(2)-C(1)-C(6) 122.7(2)
O(3)-C(2)-C(1) 123.9(2)
O(3)-C(2)-C(3) 117.2(2)
C(3)-C(2)-C(1) 118.9(2)
C(2)-C(3)-N(9) 119.4(2)
C(2)-C(3)-C(4) 121.9(2)
C(4)-C(3)-N(9) 118.7(2)
O(6)-C(4)-C(3) 117.7(2)
O(6)-C(4)-C(5) 122.9(2)
C(3)-C(4)-C(5) 119.4(2)
N(7)-C(5)-C(6) 118.8(2)
C(4)-C(5)-N(7) 118.5(2)
C(4)-C(5)-C(6) 122.5(2)
O(9)-C(6)-C(1) 123.7(2)
O(9)-C(6)-C(5) 122.2(2)
C(1)-C(6)-C(5) 114.1(2)
C(7)-N(2)-N(1) 118.0(2)
C(14)-N(4)-N(5) 104.66(19)
C(8)-N(5)-N(4) 110.74(19)
C(8)-N(3)-C(14) 106.29(19)
O(10)-C(7)-N(2) 125.1(2)
O(10)-C(7)-C(14) 120.4(2)
N(2)-C(7)-C(14) 114.4(2)
N(4)-C(14)-N(3) 111.9(2)
N(4)-C(14)-C(7) 124.8(2)
N(3)-C(14)-C(7) 123.3(2)
N(5)-C(8)-N(3) 106.4(2)
N(6)-C(8)-N(5) 127.2(2)
N(6)-C(8)-N(3) 126.4(2)

Table S28. Hydrogen Bonds for **TNPG-ATCH(7)** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3)…O(1)	0.82	1.78	2.498(3)	144.8
N(6)-H(6A)…O(10^{1})	0.86	2.17	2.886(3)	140.7
N(6)-H(6B)…O(9^{2})	0.86	2.06	2.800(3)	144.1

O(6)-H(6)…O(7)	0.842(19)	1.70(3)	2.478(3)	153(4)

Symmetry transformations used to generate equivalent atoms:

[1]-1+X,+Y,+Z; [2]1-X,-Y,-Z

Table S29.Torsion Angles [°] for **TNPG-ATCH(7)**.

O(1)-N(8)-C(1)-C(2)	-12.4(3)
O(1)-N(8)-C(1)-C(6)	169.9(2)
O(2)-N(8)-C(1)-C(2)	166.4(2)
O(2)-N(8)-C(1)-C(6)	-11.3(3)
O(3)-C(2)- C(3)-N(9)	-5.5(3)
O(3)-C(2)- C(3)-C(4)	177.5(2)
O(4)-N(9)-C(3)-C(2)	-51.1(3)
O(4)-N(9)-C(3)-C(4)	125.9(2)
O(5)-N(9)-C(3)-C(2)	129.7(2)
O(5)-N(9)-C(3)-C(4)	-53.2(3)
O(6)-C(4)- C(5)-N(7)	3.4(4)
O(6)-C(4)- C(5)-C(6)	-172.0(2)
O(7)-N(7)-C(5)-C(4)	-15.2(3)
O(7)-N(7)-C(5)-C(6)	160.3(2)
O(8)-N(7)-C(5)-C(4)	164.3(2)
O(8)-N(7)-C(5)-C(6)	-20.2(4)
N(8)-C(1)- C(2)-O(3)	8.3(4)
N(8)-C(1)-C(2)-C(3)	-171.6(2)
N(8)-C(1)- C(6)-O(9)	-4.7(3)
N(8)-C(1)-C(6)-C(5)	174.7(2)
N(7)-C(5)-C(6)-O(9)	0.3(4)
N(7)-C(5)-C(6)-C(1)	-179.1(2)
N(9)-C(3)-C(4)-O(6)	-1.6(3)
N(9)-C(3)-C(4)-C(5)	179.2(2)
C(1)-C(2)- C(3)-N(9)	174.4(2)
C(1)-C(2)-C(3)-C(4)	-2.6(4)
C(2)-C(1)-C(6)-O(9)	177.7(2)
C(2)-C(1)-C(6)-C(5)	-2.9(3)
C(2)-C(3)-C(4)-O(6)	175.4(2)
C(2)-C(3)-C(4)-C(5)	-3.8(4)
C(3)-C(4)-C(5)-N(7)	-177.5(2)

C(3)-C(4)-C(5)-C(6)	7.1(4)
C(4)-C(5)-C(6)-O(9)	175.7(2)
C(4)-C(5)-C(6)-C(1)	-3.8(3)
C(6)-C(1)-C(2)-O(3)	-174.1(2)
C(6)-C(1)-C(2)-C(3)	6.0(4)
O(10)-C(7)-C(14)-N(4)	177.4(2)
O(10)-C(7)-C(14)-N(3)	-2.8(4)
N(1)-N(2)-C(7)-O(10)	-5.3(4)
N(1)-N(2)-C(7)-C(14)	175.0(2)
N(2)-C(7)-C(14)-N(4)	-2.9(3)
N(2)-C(7)-C(14)-N(3)	176.9(2)
N(4)-N(5)-C(8)-N(3)	0.1(3)
N(4)-N(5)-C(8)-N(6)	179.6(2)
N(5)-N(4)-C(14)-N(3)	0.2(3)
N(5)-N(4)-C(14)-C(7)	-179.9(2)
C(14)-N(4)-N(5)-C(8)	-0.2(3)
C(14)-N(3)-C(8)-N(5)	0.0(3)
C(14)-N(3)-C(8)-N(6)	-179.5(2)
C(8)-N(3)-C(14)-N(4)	-0.2(3)
C(15)-N(3)-C(14)-C(13)	179.9(2)

Table S30. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **TNPG-ATCH(7)**.

	x	y	z	U(eq)
H(3)	8201.33	4192.64	5219.8	44
H(1A)	11216.27	6245.61	1780.98	37
H(1B)	11506.51	4562.62	1483.1	37
H(1C)	11238.91	5143.07	2619.89	37
H(2)	8183.85	5458.34	1910.36	25
H(6A)	1032.82	1273.13	-656.43	33
H(6B)	2411.67	473.77	-1287.51	33
H(6)	1090(50)	50(40)	4430(30)	74(14)
H(3A)	5770(40)	1470(30)	-640(20)	30(8)

Table S31. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **SP-ATCH(8)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	7507.1(9)	5976.0(3)	1631.5(7)	13.49(19)
N(1)	5165(3)	2698.2(10)	4629(2)	17.0(4)
N(2)	8136(4)	3104.9(10)	6056(3)	18.1(4)
N(3)	7040(3)	3701.2(10)	5365(2)	19.5(4)
N(4)	3958(4)	4516.2(10)	3233(2)	17.6(4)
N(5)	2285(4)	4906.2(11)	2267(2)	14.3(4)
N(6)	7547(4)	1840.4(11)	6060(3)	18.6(4)
O(1)	1640(3)	3520.5(9)	3082(2)	25.8(4)
O(2)	7778(3)	5509.5(9)	3089.2(19)	18.1(4)
O(3)	5132(3)	5873.0(8)	856(2)	19.4(4)
O(4)	7745(3)	6741.9(8)	2134(2)	20.8(4)
O(5)	9350(3)	5800.6(9)	450.4(19)	19.3(4)
C(1)	7023(4)	2503.5(13)	5606(3)	16.6(5)
C(2)	5267(4)	3433.3(12)	4528(3)	16.9(5)
C(3)	3444(4)	3827.3(12)	3549(3)	17.6(5)

Table S32. Bond lengths [Å] and angles [°] for **SP-ATCH(8)**.

S(1)-O(5)	1.4626(17)
S(1)-O(2)	1.4743(16)
S(1)-O(3)	1.4764(16)
S(1)-O(4)	1.4879(16)
N(1)-C(1)	1.348(3)
N(1)-C(2)	1.372(3)
N(1)-H(1)	1.01(4)
N(2)-C(1)	1.330(3)
N(2)-N(3)	1.383(3)
N(2)-H(2)	0.81(3)
N(3)-C(2)	1.295(3)
N(4)-C(3)	1.340(3)
N(4)-N(5)	1.413(3)
N(4)-H(4)	0.87(3)

N(5)-H(5A)	0.88(3)
N(5)-H(5B)	0.86(3)
N(5)-H(5C)	0.97(3)
N(6)-C(1)	1.319(3)
N(6)-H(6B)	0.80(3)
N(6)-H(6A)	0.77(3)
O(1)-C(3)	1.217(3)
C(2)-C(3)	1.479(3)

O(5)-S(1)-O(2)	109.45(9)
O(5)-S(1)-O(3)	109.64(10)
O(2)-S(1)-O(3)	110.15(9)
O(5)-S(1)-O(4)	109.46(10)
O(2)-S(1)-O(4)	109.64(10)
O(3)-S(1)-O(4)	108.47(9)
C(1)-N(1)-C(2)	105.71(19)
C(1)-N(1)-H(1)	127(2)
C(2)-N(1)-H(1)	128(2)
C(1)-N(2)-N(3)	111.13(19)
C(1)-N(2)-H(2)	123.8(19)
N(3)-N(2)-H(2)	124.9(19)
C(2)-N(3)-N(2)	103.66(19)
C(3)-N(4)-N(5)	117.0(2)
C(3)-N(4)-H(4)	126.1(19)
N(5)-N(4)-H(4)	116.2(19)
N(4)-N(5)-H(5A)	107.7(19)
N(4)-N(5)-H(5B)	113.4(19)
H(5A)-N(5)-H(5B)	110(3)
N(4)-N(5)-H(5C)	105.2(19)
H(5A)-N(5)-H(5C)	112(3)
H(5B)-N(5)-H(5C)	108(3)
C(1)-N(6)-H(6B)	117(2)
C(1)-N(6)-H(6A)	114(2)
H(6B)-N(6)-H(6A)	120(3)
N(6)-C(1)-N(2)	127.5(2)
N(6)-C(1)-N(1)	125.6(2)
N(2)-C(1)-N(1)	106.9(2)
N(3)-C(2)-N(1)	112.6(2)

N(3)-C(2)-C(3)	127.5(2)
N(1)-C(2)-C(3)	119.8(2)
O(1)-C(3)-N(4)	124.7(2)
O(1)-C(3)-C(2)	119.9(2)
N(4)-C(3)-C(2)	115.3(2)

Table S33. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **SP-ATCH(8)**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
S1	12.2(3)	11.0(3)	17.1(3)	-0.8(2)	-4.0(2)	-0.10(19)
N1	16.4(10)	15.5(10)	19.0(10)	0.2(8)	-3.9(8)	0.2(8)
N2	14.3(10)	15.6(10)	24.0(10)	-1.5(8)	-8.5(8)	0.0(8)
N3	18.3(10)	16.9(10)	23.1(10)	0.7(8)	-4.0(8)	1.1(8)
N4	14.8(10)	15.3(9)	22.3(10)	3.6(8)	-5.8(8)	-1.5(8)
N5	13.4(10)	13.1(10)	16.1(10)	0.9(8)	-3.3(8)	1.7(8)
N6	16.7(11)	14.1(10)	24.5(11)	-2.0(9)	-8.2(9)	2.5(8)
O1	20.9(9)	23.2(9)	32.7(10)	6.0(8)	-11.9(7)	-5.6(7)
O2	16.5(8)	20.0(8)	17.6(8)	2.6(7)	-2.7(6)	0.6(6)
O3	14.4(8)	17.9(8)	25.6(9)	2.7(7)	-7.8(7)	-2.2(6)
O4	20.7(9)	12.4(8)	28.8(9)	-4.1(7)	-10.5(7)	1.6(6)
O5	17.7(8)	20.1(9)	20.0(8)	-0.6(7)	1.5(6)	0.5(7)
C1	15.3(11)	18.9(11)	15.6(11)	-1.1(9)	-2.0(8)	0.8(9)
C2	17.7(12)	15.6(11)	17.6(11)	0.1(9)	-0.8(9)	0.0(9)
C3	17.4(12)	18.2(11)	17.1(11)	0.2(9)	-0.8(9)	-0.6(9)

Table S34. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for **SP-ATCH(8)**.

	x	y	z	U(eq)
H(2)	9350(50)	3114(14)	6600(30)	17(7)
H(6B)	8810(60)	1774(15)	6500(40)	26(8)
H(4)	5310(60)	4730(15)	3440(30)	26(7)

H(5A)	1780(50)	4623(16)	1470(40)	28(8)
H(5B)	1090(50)	5060(15)	2820(30)	21(7)
H(5C)	3160(60)	5319(18)	1860(40)	40(9)
H(6A)	6970(60)	1548(17)	5510(40)	27(8)
H(1)	3970(60)	2367(19)	4090(40)	49(10)

Table S35. Torsion angles [°] for **SP-ATCH(8)**.

C(1)-N(2)-N(3)-C(2)	0.7(3)
N(3)-N(2)-C(1)-N(6)	-178.4(2)
N(3)-N(2)-C(1)-N(1)	-0.7(3)
C(2)-N(1)-C(1)-N(6)	178.2(2)
C(2)-N(1)-C(1)-N(2)	0.4(2)
N(2)-N(3)-C(2)-N(1)	-0.4(3)
N(2)-N(3)-C(2)-C(3)	178.9(2)
C(1)-N(1)-C(2)-N(3)	0.0(3)
C(1)-N(1)-C(2)-C(3)	-179.3(2)
N(5)-N(4)-C(3)-O(1)	-0.9(3)
N(5)-N(4)-C(3)-C(2)	178.51(19)
N(3)-C(2)-C(3)-O(1)	-166.2(2)
N(1)-C(2)-C(3)-O(1)	13.0(3)
N(3)-C(2)-C(3)-N(4)	14.3(3)
N(1)-C(2)-C(3)-N(4)	-166.4(2)

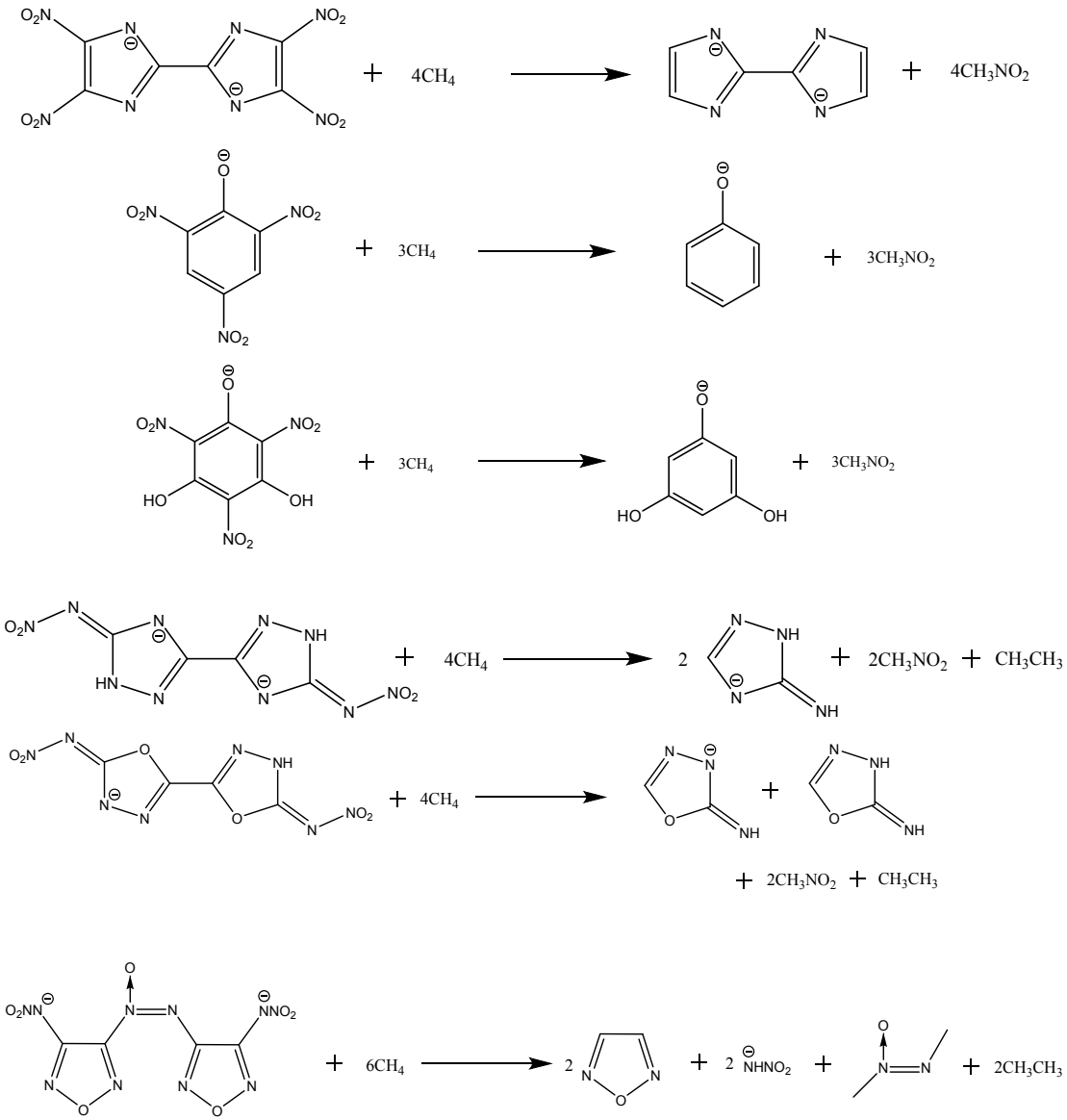

Fig. S1. Isodesmic reactions for cations in **3–11**.

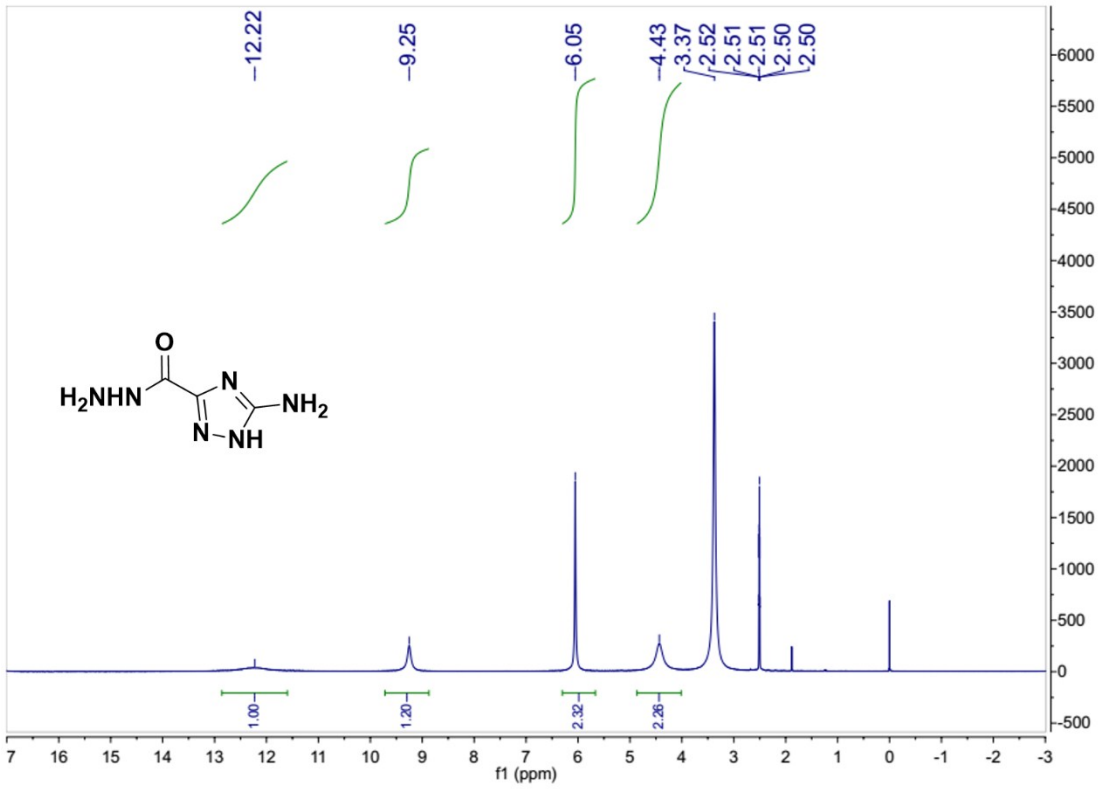

Fig. S2.[1]H NMR for **1**.

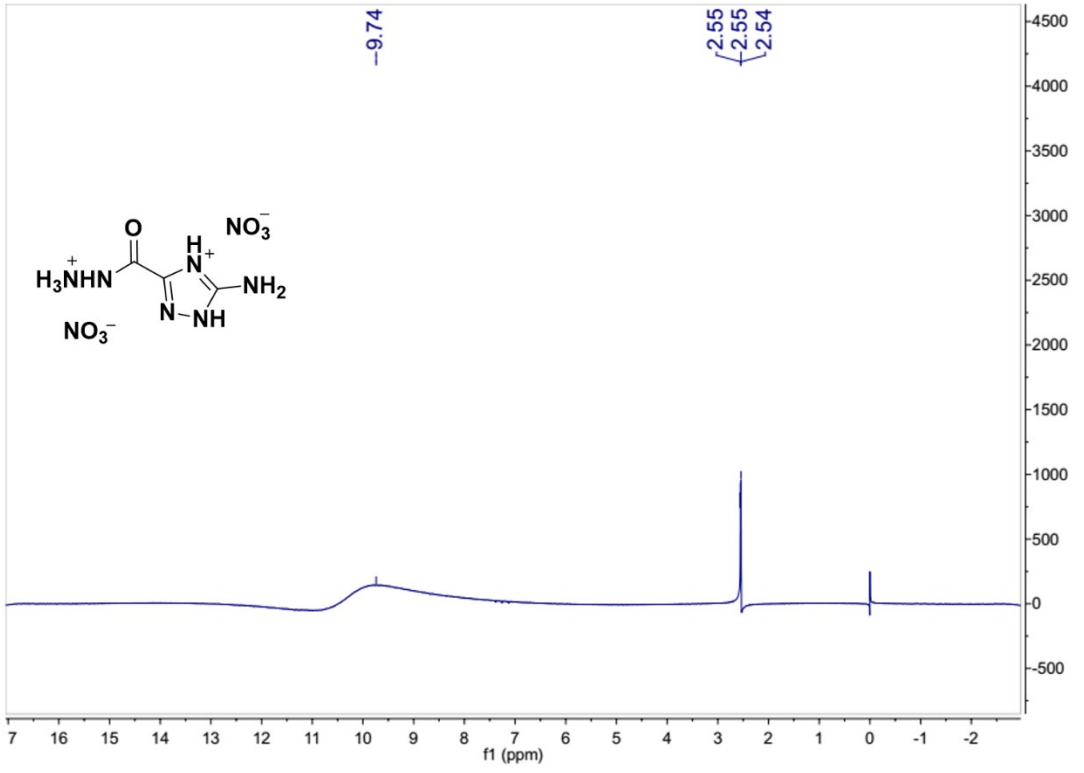

Fig. S3.[1]H NMR for **3**.

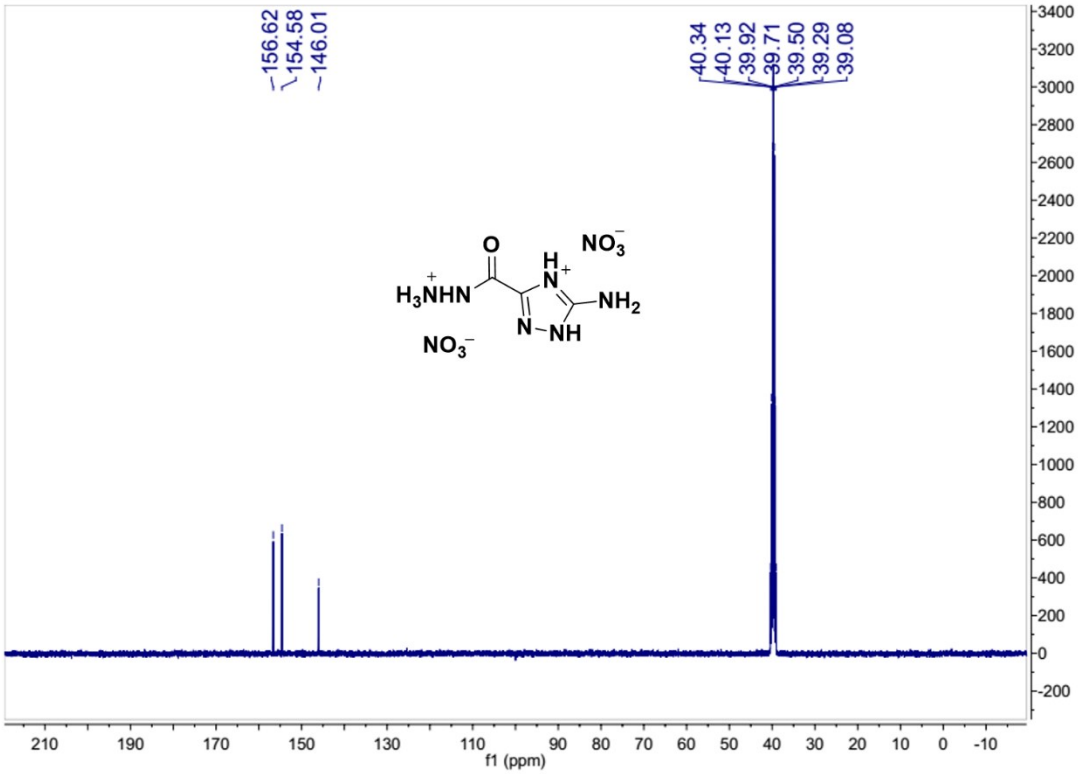

Fig. S4.[13]C NMR for **3**.

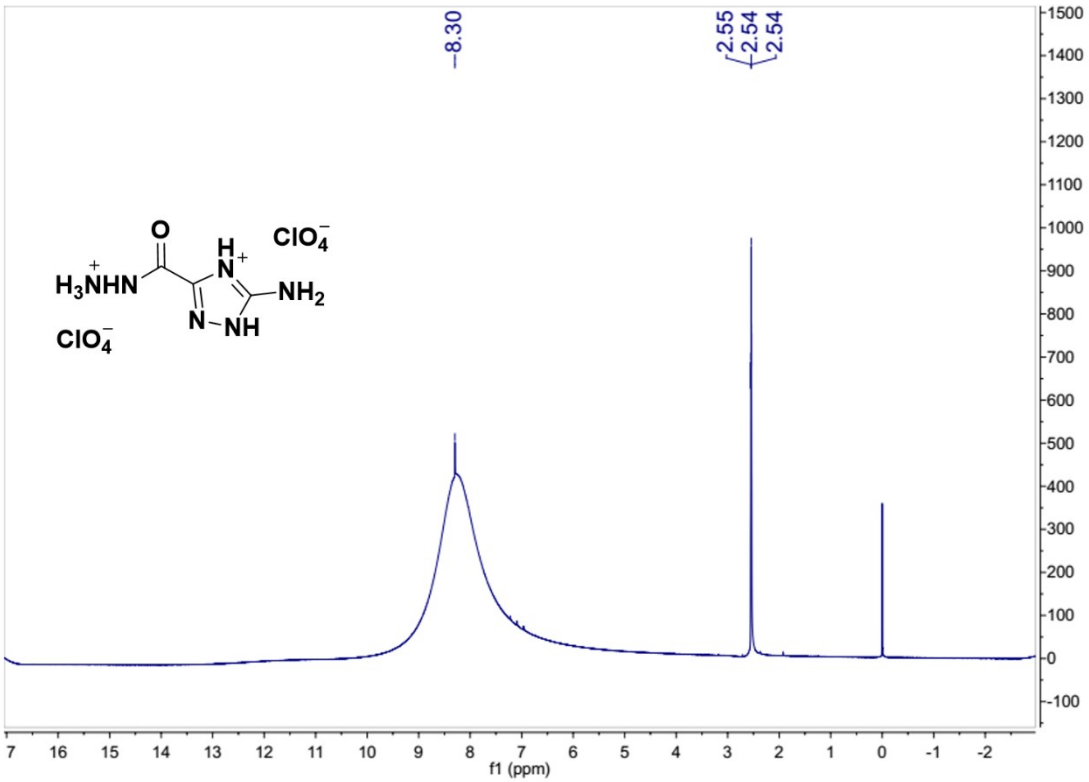

Fig. S5.[1]H NMR for **4**.

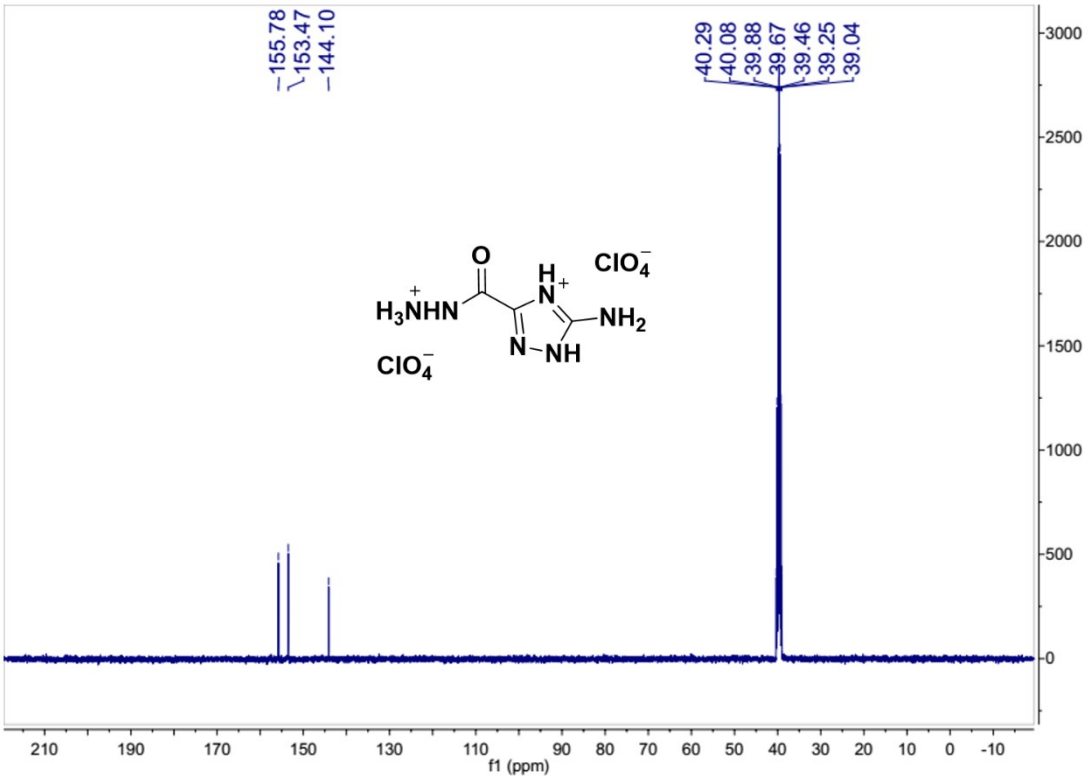

Fig. S6.^{13}C NMR for **4**.

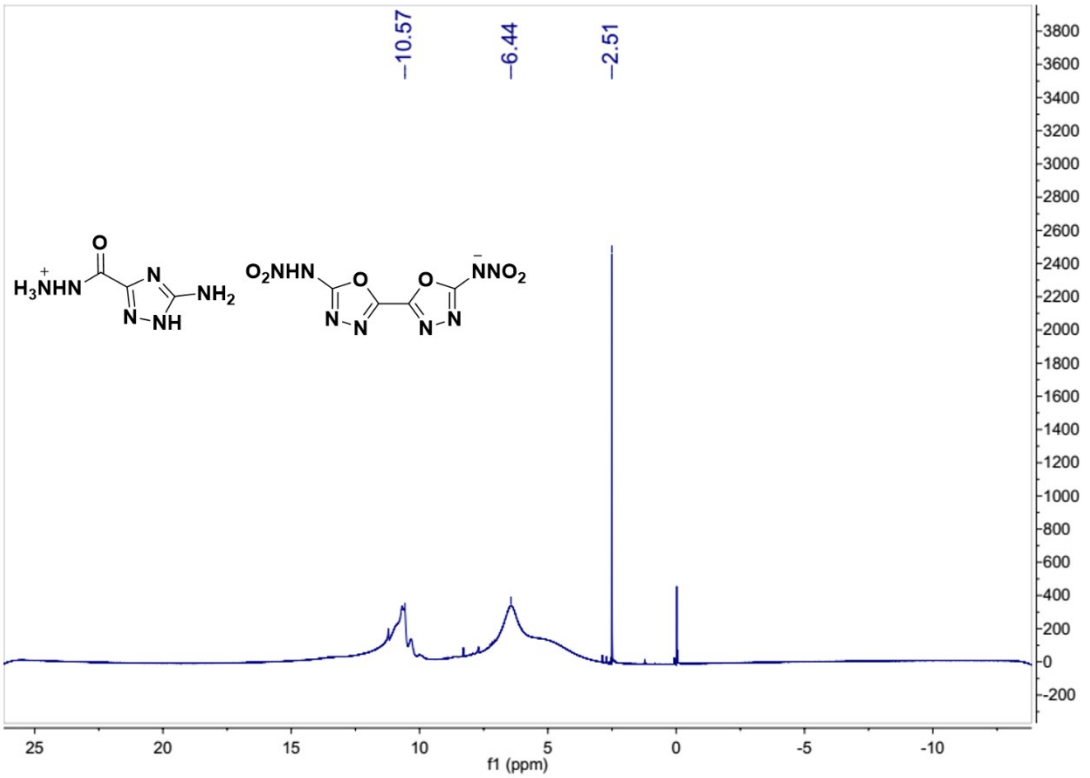

Fig. S7.^{1}H NMR for **5**.

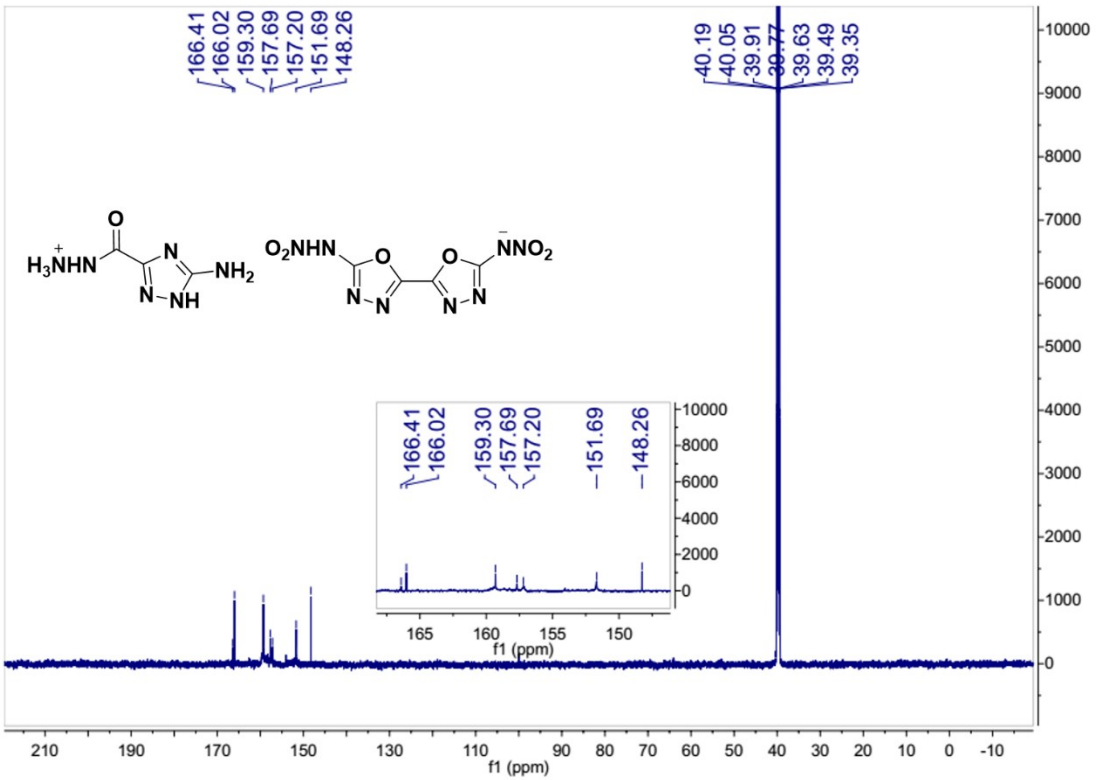

Fig. S8.^{13}C NMR for **5**.

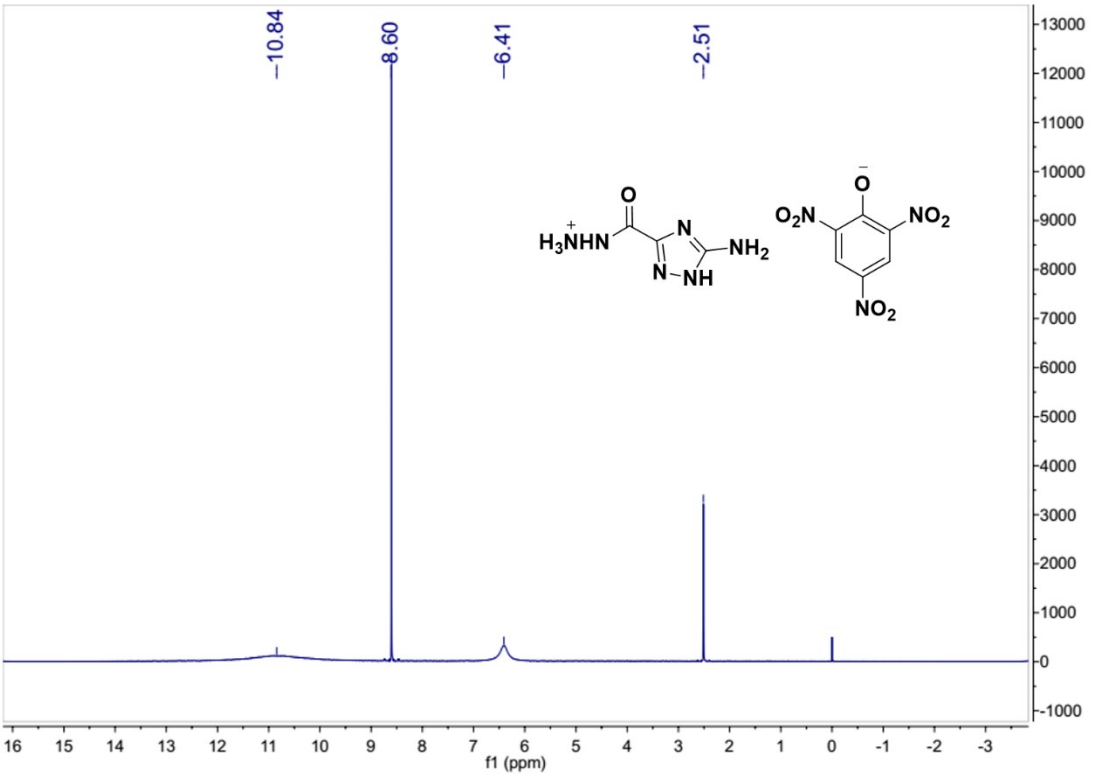

Fig. S9.^{1}H NMR for **6**.

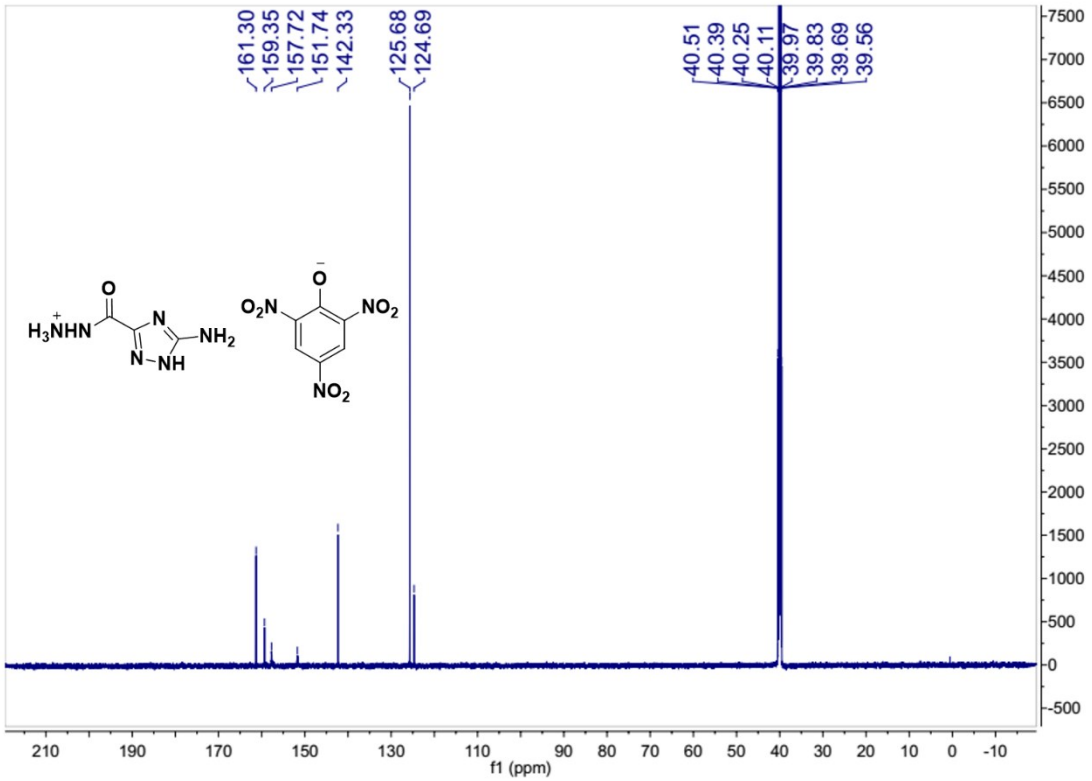

Fig. S10.[13]C NMR for **6**.

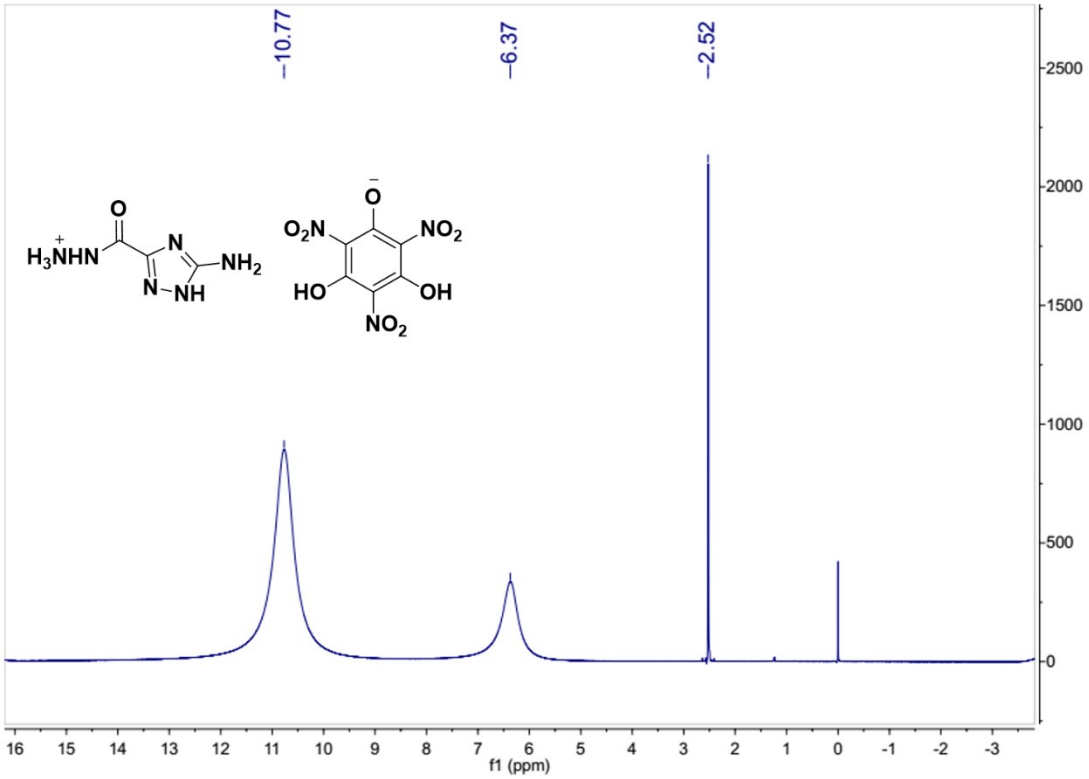

Fig. S11.[1]H NMR for **7**.

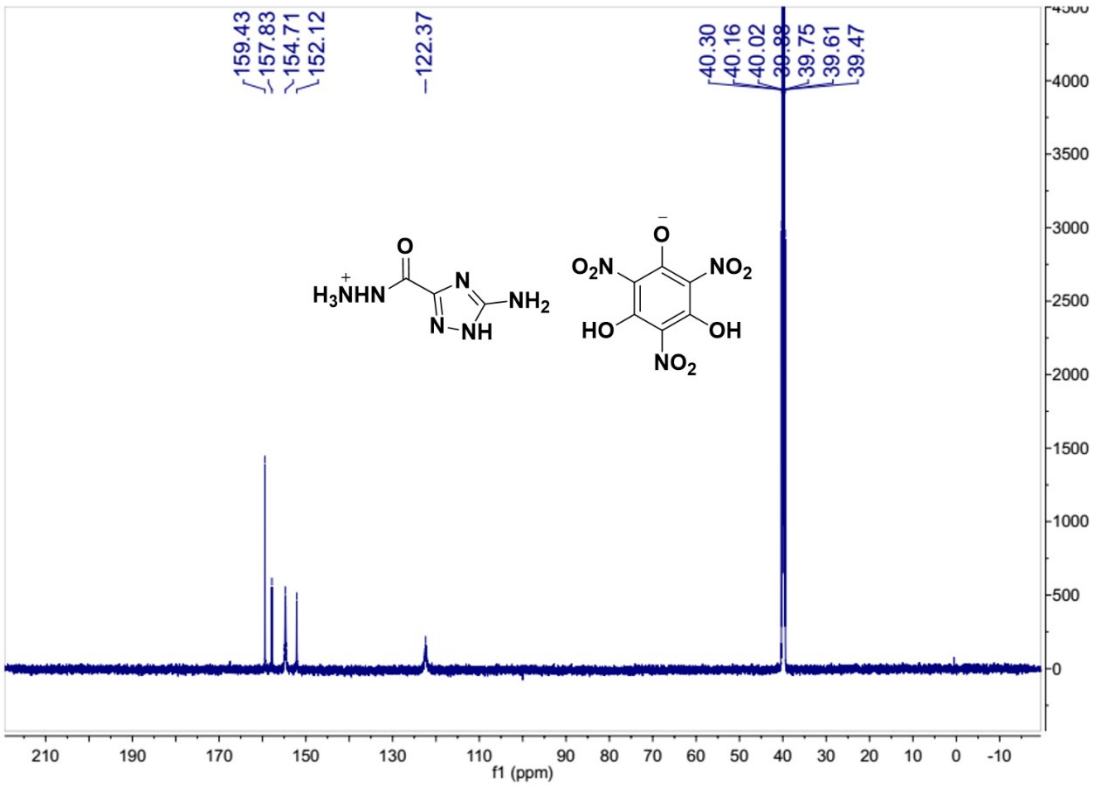

Fig. S12.[13]C NMR for **7**.

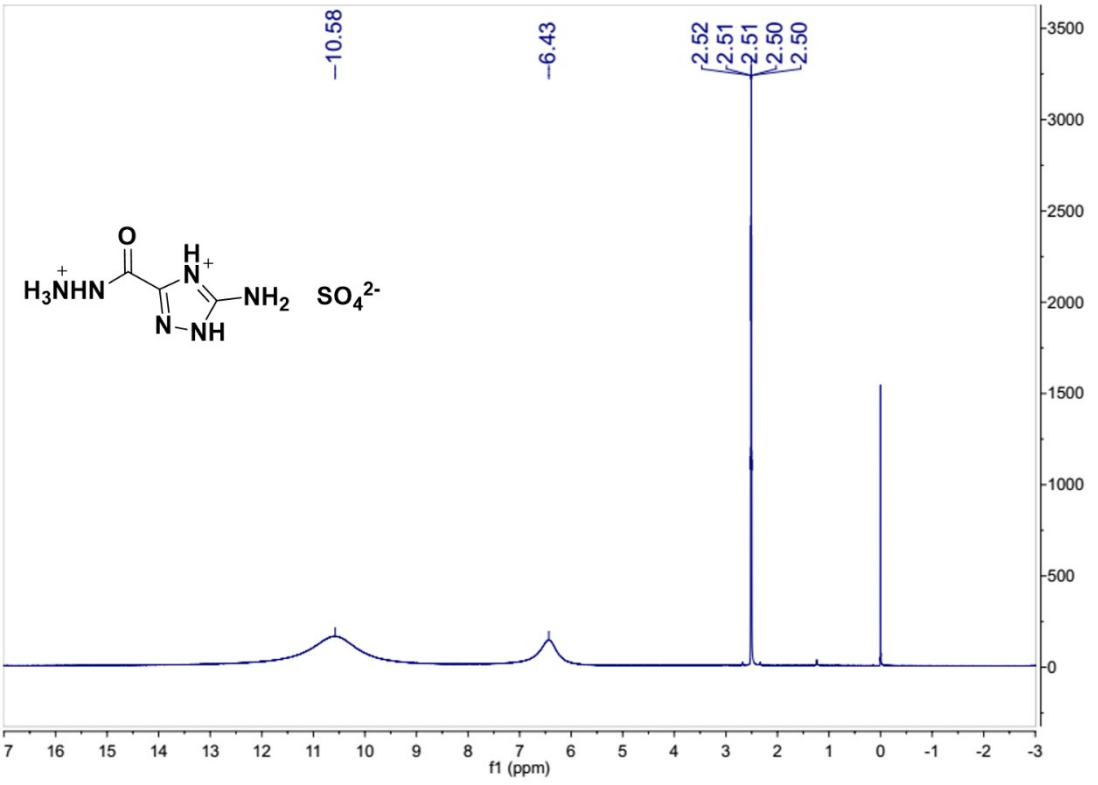

Fig. S13.[1]H NMR for **8**.

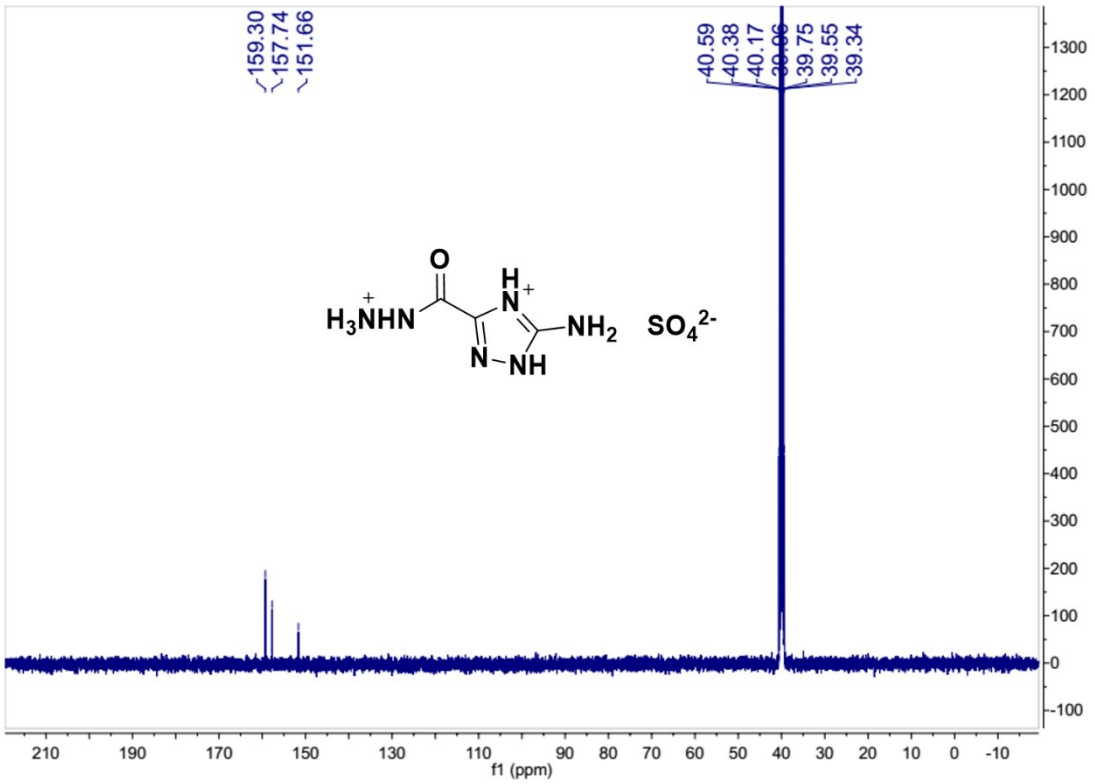

Fig. S14.[13]C NMR for **8**.

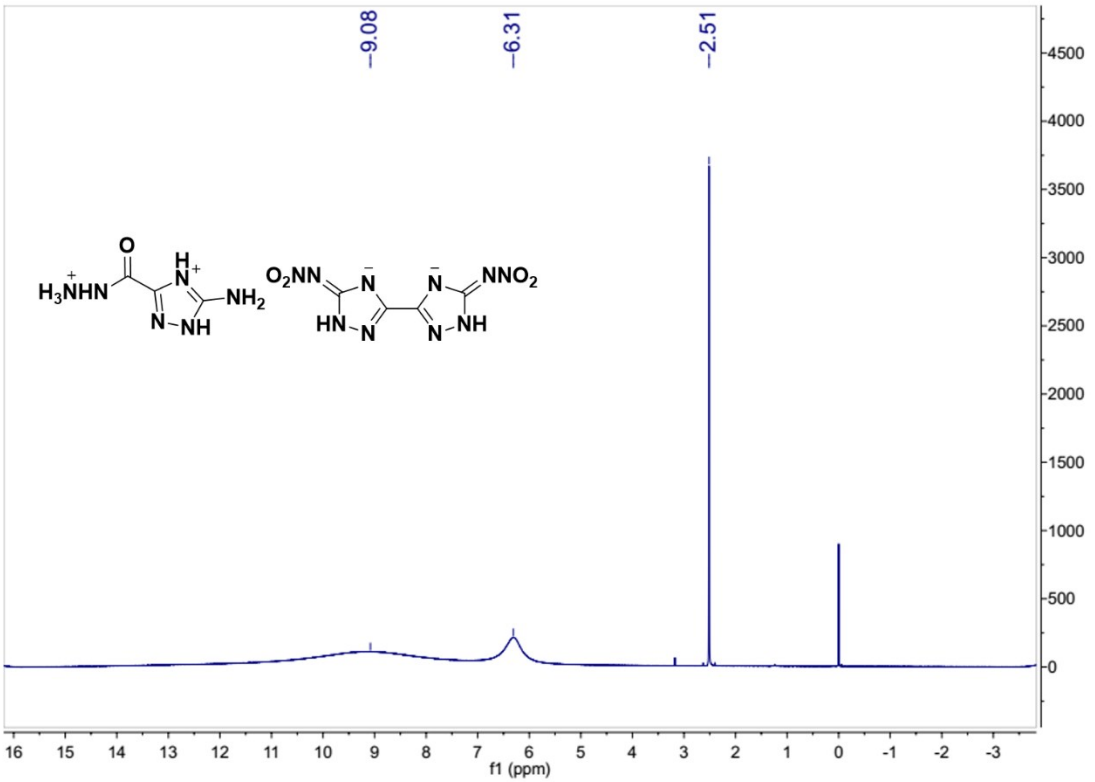

Fig. S15.[1]H NMR for **9**.

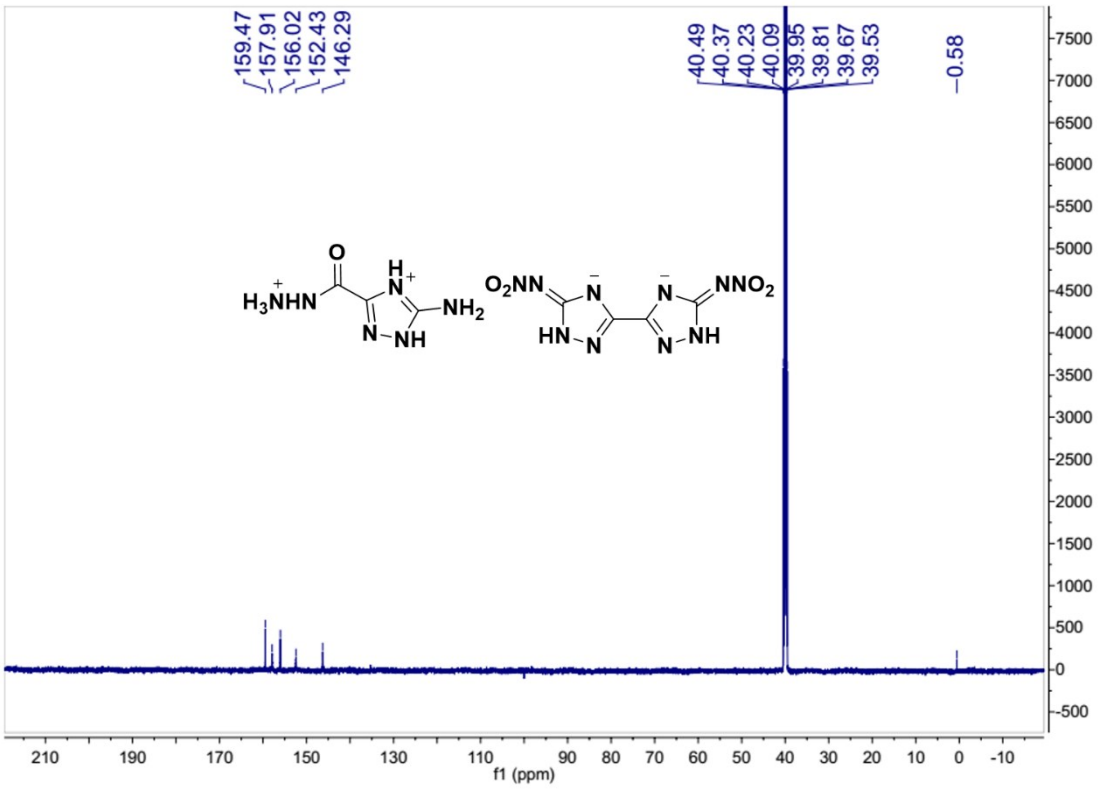

Fig. S16.[13]C NMR for **9**.

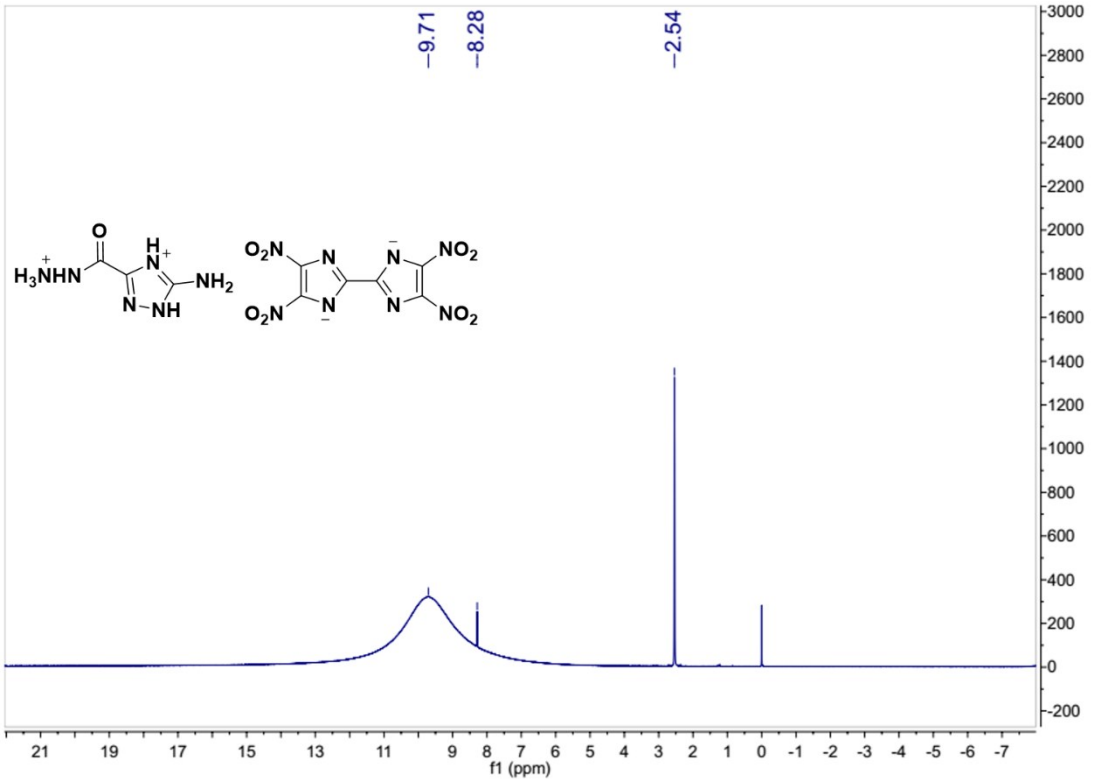

Fig. S17.[1]H NMR for **10**.

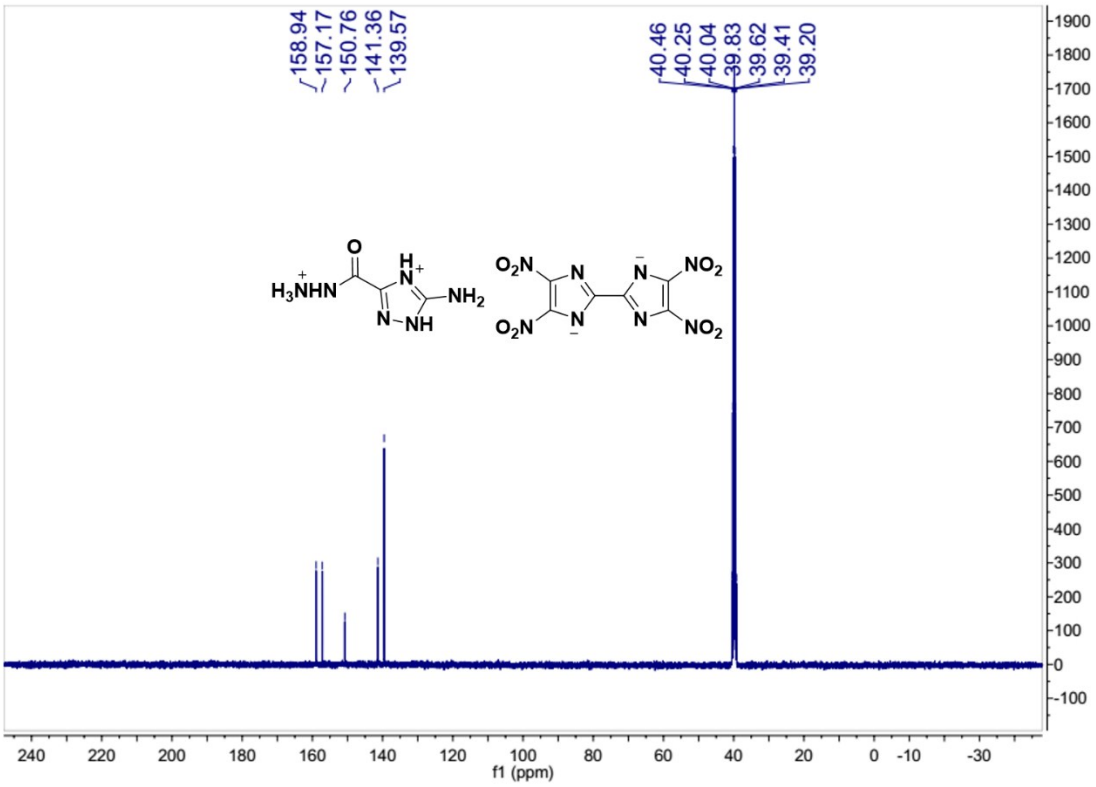

Fig. S18.^{13}C NMR for **10**.

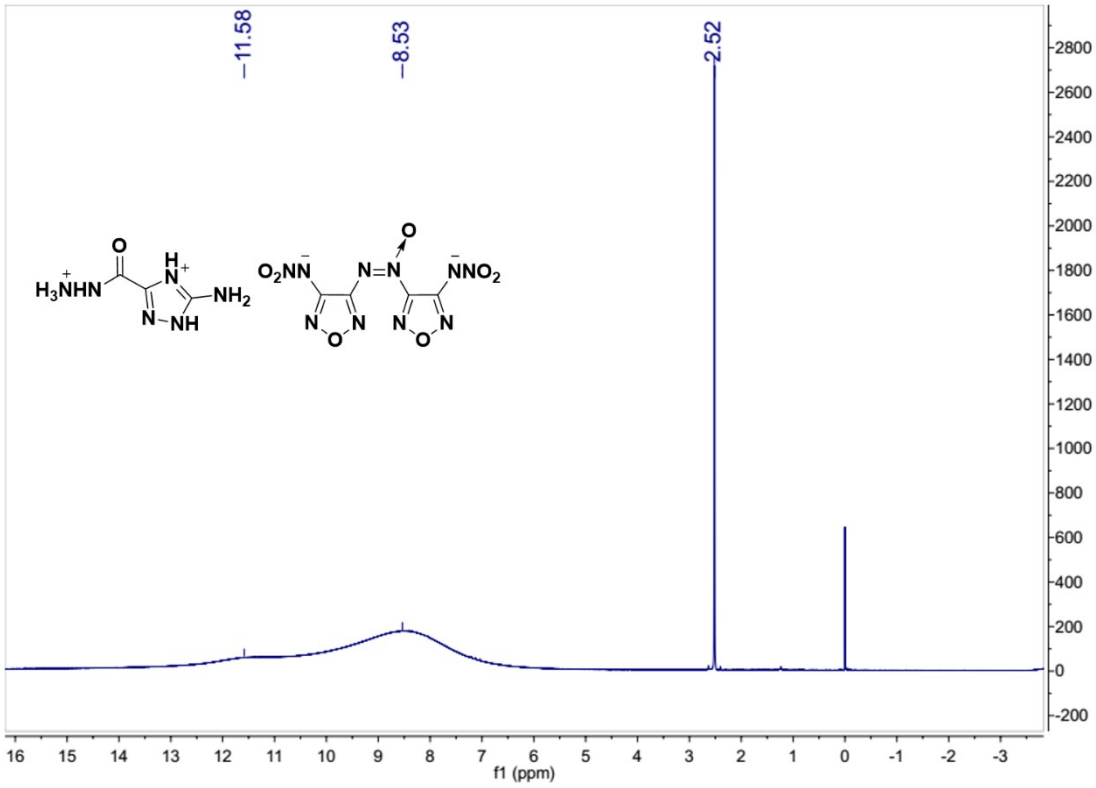

Fig. S19.[1]H NMR for **11**.

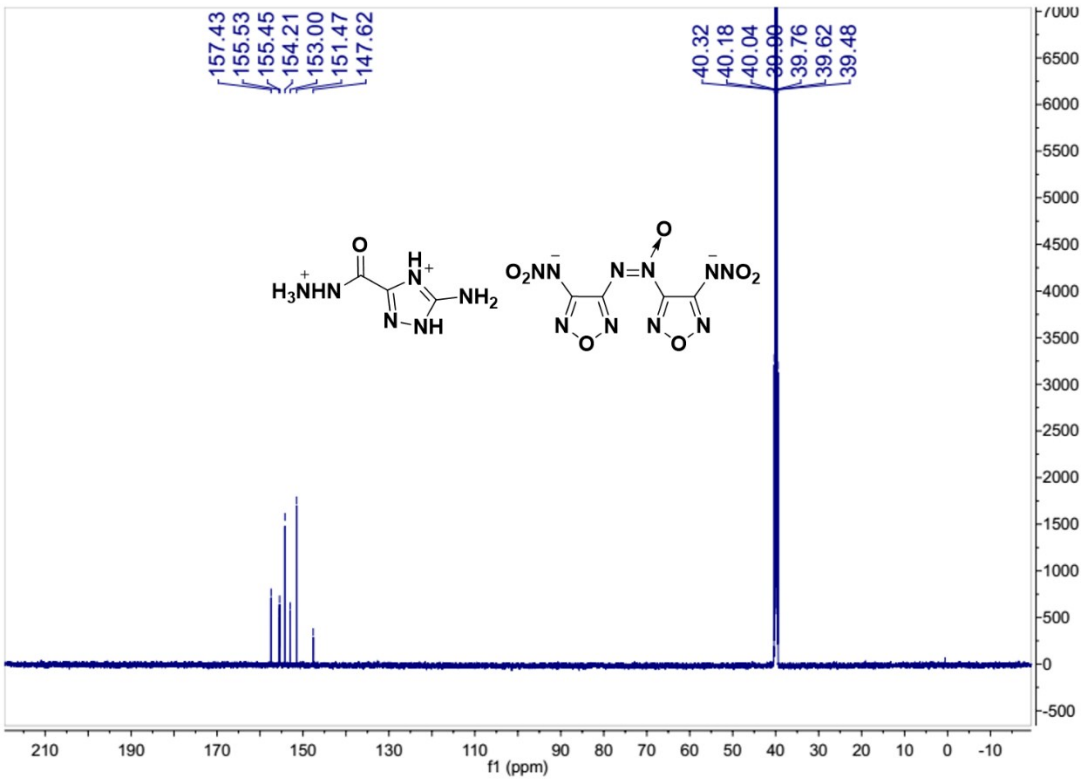

Fig. S20.[13]C NMR for **11**.