Electronic Supplementary Information

Taming of 4-Azido-3,5-dinitropyrazole Based Energetic Materials

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1. Crystal structure data

Table 1: Crystal data and structure refinement for Compound 4.

Identification code	cu_PKP_28092022_TVK_DNAP_AM_OXD_cu2_0m_a (2)
Empirical formula	$C_6H_4N_{10}O_5$
Formula weight	296.19
Temperature/K	295(2)
Crystal system	orthorhombic
Space group	$Pca2_1$
a/Å	14.708(3)
b/Å	5.921(2)
c/Å	25.458(5)
α/°	90.00(3)
β/°	90.00(3)
γ/°	90.00(3)
Volume/Å^3	2216.9(10)
Z	8
ρ_{calc}g/cm^3	1.775
μ/mm^{-1}	1.368
F(000)	1200.0
Crystal size/mm^3	0.263 × 0.108 × 0.102
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.944 to 120.058
Index ranges	$-16 \leq h \leq 16$, $-6 \leq k \leq 6$, $-28 \leq l \leq 28$
Reflections collected	26328
Independent reflections	3239 [R_{int} = 0.0359, R_{sigma} = 0.0218]
Data/restraints/parameters	3239/1/395
Goodness-of-fit on F^2	1.133
Final R indexes [I>=2σ (I)]	R_1 = 0.0423, wR_2 = 0.1161
Final R indexes [all data]	R_1 = 0.0427, wR_2 = 0.1167
Largest diff. peak/hole / e Å^{-3}	0.32/-0.23
Flack parameter	0.23(6)
CCDC number	2287540

Table 2: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O_1	7128(3)	16070(7)	6612.6(18)	79.1(13)
O_2	6339(3)	14717(7)	5984(2)	79.5(13)

O_3	8311(3)	6908(5)	5429.0(14)	58.8(9)
O_4	9678(3)	7878(7)	5660.0(19)	79.8(13)
O_5	9370.2(17)	6276(5)	7263.8(12)	40.2(7)
N_1	6996(2)	14721(6)	6260.0(16)	45.2(8)
N_2	8838(3)	8199(6)	5639.5(15)	43.7(9)
N_3	6840(2)	10595(7)	5546.5(14)	50.2(10)
N_4	6879(2)	9218(6)	5177.5(14)	43.0(8)
N_5	6766(3)	8095(7)	4825.8(19)	61.9(11)
N_6	8970(2)	11453(6)	6220.7(13)	35.3(7)
N_7	8485(2)	13190(6)	6403.8(13)	37.9(8)
N_8	10616(2)	8228(6)	7057.4(15)	41.4(8)
N_9	9103(2)	8021(6)	6908.2(13)	39.1(8)
N_{10}	10685(3)	5039(7)	7631.2(16)	46.3(10)
C_1	7683(3)	13006(6)	6165.2(16)	35.7(9)
C_2	7619(3)	11143(6)	5823.7(15)	35.3(8)
C_3	8482(2)	10177(7)	5879.9(14)	33.6(8)
C_4	9889(3)	11084(8)	6450.5(15)	37.4(9)
C_5	9859(2)	9054(7)	6811.1(14)	30.5(8)
C_6	10276(3)	6512(7)	7327.6(15)	34.1(8)

Table 3: Anisotropic Displacement Parameters ($Å^2×10^3$) for 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O_1	59(2)	73(2)	106(3)	-50(2)	-3(2)	14.2(18)
O_2	59(2)	76(3)	103(3)	-25(2)	-33(2)	29.8(19)
O_3	53(2)	53.8(19)	70(2)	-22.6(17)	-9.7(18)	4.3(15)
O_4	51(2)	87(3)	101(3)	-41(3)	-5(2)	21.7(19)
O_5	27.6(14)	46.4(15)	46.5(14)	7.7(13)	-4.4(11)	-3.8(11)
N_1	39.5(19)	38.6(19)	58(2)	-1.4(16)	-3.7(17)	3.5(16)
N_2	39(2)	48(2)	44.3(18)	-5.6(16)	-3.2(16)	9.2(15)
N_3	35(2)	64(2)	52(2)	-22(2)	-9.3(15)	5.3(18)
N_4	35.4(19)	49(2)	44(2)	0.3(19)	-5.1(15)	-3.1(15)
N_5	59(3)	64(3)	62(3)	-15(2)	-10(2)	-0.5(19)
N_6	28.6(18)	38.9(18)	38.4(17)	-0.8(13)	-5.3(14)	-2.0(13)
N_7	36.1(19)	33.0(17)	44.4(19)	0.3(13)	-3.1(14)	-0.1(14)
N_8	28.9(17)	51(2)	44.0(18)	6.7(15)	-7.5(15)	-3.5(14)
N_9	26.5(17)	41.9(19)	49(2)	5.7(15)	-7.6(13)	2.5(13)
N_{10}	26(2)	60(3)	53(2)	16.2(18)	-9.1(17)	-7.6(17)
C_1	33(2)	35.2(19)	39(2)	-0.8(17)	2.4(17)	2.9(15)
C_2	37(2)	34(2)	34.6(19)	2.7(15)	-3.4(16)	-0.8(16)
C_3	30.2(18)	38(2)	32.8(17)	-1.1(15)	-1.1(15)	1.8(15)
C_4	30(2)	42(2)	41(2)	1.9(17)	-8.0(16)	-0.9(15)
C_5	23.1(18)	35(2)	33.3(17)	-3.8(16)	-4.2(14)	0.6(14)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C_6	31(2)	38.8(19)	33.0(19)	-1.9(16)	-1.1(15)	-6.9(15)
O_{1_1}	65(2)	69(3)	98(3)	-42(2)	-4(2)	15.6(18)
O_{2_1}	50(2)	51.5(19)	77(2)	2.8(16)	-11.0(18)	13.6(15)
O_{3_1}	53(2)	44.3(17)	61.1(19)	-16.0(14)	-7.3(16)	-1.7(13)
O_{4_1}	45(2)	86(3)	94(3)	-46(3)	-13(2)	22.0(18)
O_{5_1}	29.9(14)	52.5(17)	42.6(15)	4.7(13)	6.5(12)	11.5(12)
N_{1_1}	35.2(19)	38.7(18)	59(2)	-1.5(16)	4.9(17)	1.2(14)
N_{2_1}	35.3(19)	45.6(19)	37.9(17)	-5.4(15)	-4.3(15)	3.0(13)
N_{3_1}	36(2)	58(2)	52(2)	-8.9(19)	-6.0(15)	5.1(16)
N_{4_1}	39.1(19)	46(2)	44(2)	3(2)	0.0(15)	-4.7(15)
N_{5_1}	55(2)	62(3)	54(2)	-10(2)	-11.6(19)	-7.0(18)
N_{6_1}	33.3(17)	33.5(16)	34.9(16)	-0.3(12)	2.5(13)	0.1(13)
N_{7_1}	38(2)	33.5(18)	38.3(17)	0.5(13)	0.6(15)	-2.0(12)
N_{8_1}	26.4(17)	45.7(18)	43.5(18)	4.4(14)	-1.4(14)	-0.1(13)
N_{9_1}	30.5(18)	49.0(19)	39.0(17)	2.5(14)	0.8(14)	2.6(14)
N_{10_1}	28.5(18)	57(2)	52(2)	16.8(17)	1.8(15)	3.6(15)
C_{1_1}	38(2)	32(2)	40(2)	5.0(16)	1.8(18)	-0.7(15)
C_{2_1}	27.3(19)	38.0(19)	33(2)	1.8(15)	1.6(15)	-2.0(15)
C_{3_1}	31.0(19)	31.7(18)	31.8(17)	3.1(15)	-1.1(15)	-1.8(15)
C_{4_1}	27.0(19)	45(2)	45(2)	-0.5(18)	-3.6(16)	-3.5(15)
C_{5_1}	24.3(17)	37(2)	32.8(17)	-10.6(16)	-0.3(14)	-1.4(14)
C_{6_1}	22.5(19)	50(2)	39(2)	-2.3(17)	-0.4(16)	-2.0(15)

Table 4: Bond Lengths for 4.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O_1	N_1	1.217(5)	O_{1_1}	N_{1_1}	1.211(5)
O_2	N_1	1.196(5)	O_{2_1}	N_{1_1}	1.211(5)
O_3	N_2	1.214(5)	O_{3_1}	N_{2_1}	1.239(5)
O_4	N_2	1.251(5)	O_{4_1}	N_{2_1}	1.200(5)
O_5	N_9	1.429(4)	O_{5_1}	N_{9_1}	1.434(4)
O_5	C_6	1.349(5)	O_{5_1}	C_{6_1}	1.340(5)
N_3	N_4	1.245(5)	N_{3_1}	N_{4_1}	1.253(6)
N_4	N_5	1.127(6)	N_{4_1}	N_{5_1}	1.109(5)
N_6	N_7	1.336(5)	N_{6_1}	N_{7_1}	1.333(5)
N_6	C_3	1.357(5)	N_{6_1}	C_{3_1}	1.380(5)
N_8	C_5	1.368(5)	N_{6_1}	C_{4_1}	1.463(5)
C_1	N_1	1.452(5)	N_{7_1}	C_{1_1}	1.333(6)
C_1	N_7	1.332(5)	N_{8_1}	C_{5_1}	1.357(5)
C_1	C_2	1.408(6)	N_{8_1}	C_{6_1}	1.316(6)
C_2	N_3	1.383(5)	N_{9_1}	C_{5_1}	1.299(5)
C_2	C_3	1.399(6)	N_{10_1}	C_{6_1}	1.324(6)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C_3	N_2	1.422(5)	C_{1_1}	N_{1_1}	1.449(6)
C_4	N_6	1.489(5)	C_{2_1}	N_{3_1}	1.390(6)
C_5	N_9	1.294(5)	C_{2_1}	C_{1_1}	1.393(6)
C_5	C_4	1.513(5)	C_{3_1}	N_{2_1}	1.420(5)
C_6	N_8	1.325(5)	C_{3_1}	C_{2_1}	1.397(5)
C_6	N_{10}	1.312(6)	C_{4_1}	C_{5_1}	1.487(6)

Table 5: Bond Angles for 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C_6	O_5	N_9	105.9(3)	C_{6_1}	O_{5_1}	N_{9_1}	106.1(3)
O_1	N_1	C_1	118.1(4)	O_{1_1}	N_{1_1}	O_{2_1}	124.4(4)
O_2	N_1	O_1	124.3(4)	O_{1_1}	N_{1_1}	C_{1_1}	118.2(4)
O_2	N_1	C_1	117.6(4)	O_{2_1}	N_{1_1}	C_{1_1}	117.4(4)
O_3	N_2	O_4	123.6(4)	O_{3_1}	N_{2_1}	C_{3_1}	117.4(3)
O_3	N_2	C_3	118.2(4)	O_{4_1}	N_{2_1}	O_{3_1}	122.8(3)
O_4	N_2	C_3	118.2(4)	O_{4_1}	N_{2_1}	C_{3_1}	119.7(3)
N_4	N_3	C_2	120.0(4)	N_{4_1}	N_{3_1}	C_{2_1}	121.2(3)
N_5	N_4	N_3	168.1(4)	N_{5_1}	N_{4_1}	N_{3_1}	168.3(4)
N_7	N_6	C_3	111.6(3)	N_{7_1}	N_{6_1}	C_{3_1}	110.1(3)
N_7	N_6	C_4	117.5(3)	N_{7_1}	N_{6_1}	C_{4_1}	119.2(3)
C_3	N_6	C_4	130.6(3)	C_{3_1}	N_{6_1}	C_{4_1}	130.7(3)
C_1	N_7	N_6	104.6(3)	N_{6_1}	N_{7_1}	C_{1_1}	105.6(3)
C_6	N_8	C_5	101.8(3)	C_{6_1}	N_{8_1}	C_{5_1}	103.2(3)
C_5	N_9	O_5	103.0(3)	C_{5_1}	N_{9_1}	O_{5_1}	102.8(3)
N_7	C_1	N_1	118.9(4)	N_{7_1}	C_{1_1}	N_{1_1}	117.8(4)
N_7	C_1	C_2	113.9(3)	N_{7_1}	C_{1_1}	C_{2_1}	113.9(3)
C_2	C_1	N_1	127.2(4)	C_{2_1}	C_{1_1}	N_{1_1}	128.1(4)
N_3	C_2	C_1	123.6(4)	N_{3_1}	C_{2_1}	C_{1_1}	123.2(4)
N_3	C_2	C_3	135.0(4)	N_{3_1}	C_{2_1}	C_{3_1}	134.9(4)
C_3	C_2	C_1	101.3(3)	C_{1_1}	C_{2_1}	C_{3_1}	101.8(3)
N_6	C_3	N_2	122.6(3)	N_{6_1}	C_{3_1}	N_{2_1}	121.6(3)
N_6	C_3	C_2	108.6(3)	N_{6_1}	C_{3_1}	C_{2_1}	108.6(3)
C_2	C_3	N_2	128.8(4)	C_{2_1}	C_{3_1}	N_{2_1}	129.7(3)
N_6	C_4	C_5	109.2(3)	N_{6_1}	C_{4_1}	C_{5_1}	111.2(3)
N_8	C_5	C_4	122.6(3)	N_{8_1}	C_{5_1}	C_{4_1}	123.5(3)
N_9	C_5	N_8	116.3(4)	N_{9_1}	C_{5_1}	N_{8_1}	115.4(4)
N_9	C_5	C_4	121.1(3)	N_{9_1}	C_{5_1}	C_{4_1}	121.0(3)
N_8	C_6	O_5	113.0(3)	N_{8_1}	C_{6_1}	O_{5_1}	112.4(3)
N_{10}	C_6	O_5	117.1(4)	N_{8_1}	C_{6_1}	N_{10_1}	129.4(4)
N_{10}	C_6	N_8	130.0(4)	N_{10_1}	C_{6_1}	O_{5_1}	118.2(4)

Table 6: Crystal data and structure refinement for Compound 7.

Identification code	AZ_AMS_Rt_Cu
Empirical formula	$C_6H_6N_{12}O_7$
Formula weight	358.23
Temperature/K	298.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.3320(8)
b/Å	7.5876(3)
c/Å	14.6125(8)
α/°	90
β/°	116.909(7)
γ/°	90
Volume/Å^3	1318.12(14)
Z	4
ρ_{calc}g/cm^3	1.805
μ/mm^{-1}	1.441
F(000)	728.0
Crystal size/mm^3	0.123 × 0.112 × 0.095
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.46 to 137.928
Index ranges	$-16 \leq h \leq 15$, $-9 \leq k \leq 7$, $-17 \leq l \leq 17$
Reflections collected	7678
Independent reflections	2424 [R_{int} = 0.0306, R_{sigma} = 0.0241]
Data/restraints/parameters	2424/0/242
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0351, wR_2 = 0.0861
Final R indexes [all data]	R_1 = 0.0448, wR_2 = 0.0935
Largest diff. peak/hole / e Å^{-3}	0.19/-0.18
CCDC number	2287541

Table 7: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 7. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O_1	8829.0(14)	-3323(2)	6857.5(11)	59.6(4)
O_2	10227.0(13)	-3613(2)	6505.6(13)	63.2(5)
O_3	8791.9(13)	67(2)	2825.2(12)	58.1(4)
O_4	7205.1(12)	1202(2)	2593.7(11)	55.1(4)
O_5	7050.7(10)	5133.4(17)	4621.4(11)	45.9(4)
O_6	3738.6(11)	5619.8(19)	3484.5(12)	52.6(4)

O_7	4030.9(13)	8333.9(18)	3950.4(12)	53.3(4)
N_1	9307.1(13)	-3029(2)	6331.1(12)	39.8(4)
N_2	8030.5(13)	281(2)	3064.3(12)	37.3(4)
N_3	10001.6(13)	-2345(2)	4662.9(12)	44.0(4)
N_4	10178.7(12)	-2388(2)	3900.5(12)	39.8(4)
N_5	10529.8(16)	-2576(3)	3342.8(14)	62.5(6)
N_6	7443.3(12)	-304.1(18)	4396.8(11)	30.7(3)
N_7	7803.0(12)	-1139.1(18)	5297.9(11)	32.5(3)
N_8	5506.1(11)	3517.3(17)	3946.9(10)	28.5(3)
N_9	7396.7(13)	3374(2)	4586.5(14)	43.4(4)
N_{10}	5504.0(13)	6718.1(19)	4263.1(12)	38.6(4)
N_{11}	4401.6(14)	6849(2)	3883.1(12)	38.3(4)
C_1	8744.8(14)	-1934(2)	5433.8(13)	31.4(4)
C_2	9028.3(14)	-1660(2)	4631.2(13)	31.5(4)
C_3	8160.2(14)	-580(2)	3978.0(13)	31.1(4)
C_4	6354.8(14)	590(2)	4005.9(14)	32.2(4)
C_5	6458.6(13)	2531(2)	4191.8(13)	29.8(4)
C_6	5919.1(14)	5101(2)	4230.8(13)	31.3(4)
N_{12}	3342.8(15)	11843(2)	3234.3(16)	40.4(4)

Table 8: Anisotropic Displacement Parameters ($Å^2×10^3$) for 7. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O_1	67.1(10)	72.8(11)	47.8(8)	18.7(8)	33.7(8)	24.5(9)
O_2	46.4(9)	72.5(11)	68.0(10)	28.0(9)	23.5(8)	29.8(8)
O_3	61.4(10)	62.6(10)	66.2(10)	18.8(8)	42.7(9)	17.9(8)
O_4	47.6(9)	58.5(10)	54.1(8)	21.4(7)	18.4(7)	19.3(7)
O_5	29.5(7)	27.1(7)	71.9(9)	-9.3(6)	14.9(7)	-4.1(5)
O_6	33.2(7)	38.6(8)	73.3(10)	1.4(7)	13.0(7)	5.9(6)
O_7	74.8(10)	31.5(8)	68.9(9)	12.5(7)	45.9(9)	25.4(7)
N_1	37.3(9)	37.1(9)	39.5(8)	2.5(7)	12.4(7)	7.9(7)
N_2	38.2(9)	31.1(8)	41.7(8)	1.6(6)	17.3(7)	1.9(7)
N_3	36.1(9)	54.2(11)	45.3(9)	5.8(8)	21.7(8)	14.8(8)
N_4	29.5(8)	41.9(10)	42.8(9)	-3.6(7)	11.9(7)	6.1(7)
N_5	55.3(12)	85.5(16)	50.8(11)	4.7(10)	27.6(10)	22.9(11)
N_6	27.0(7)	24.4(7)	37.2(7)	0.2(6)	11.5(6)	3.6(6)
N_7	32.9(8)	25.4(8)	36.5(7)	0.3(6)	13.3(7)	3.6(6)
N_8	25.9(7)	22.2(7)	35.7(7)	0.7(5)	12.3(6)	1.8(5)
N_9	28.8(8)	29.6(9)	65.2(11)	-6.3(7)	15.5(8)	1.6(6)
N_{10}	39.0(9)	24.5(8)	51.3(9)	-2.7(6)	19.5(7)	2.4(6)
N_{11}	46.8(9)	28.4(8)	43.4(8)	8.3(6)	23.7(8)	11.0(7)
C_1	28.8(9)	24.6(8)	35.2(8)	-0.2(7)	9.5(7)	3.5(7)
C_2	26.4(9)	25.0(9)	39.6(9)	-4.2(7)	11.9(7)	0.6(7)

C_3	29.7(9)	25.3(8)	35.8(8)	-2.2(7)	12.8(7)	0.7(7)
C_4	24.0(8)	25.4(9)	43.8(9)	0.8(7)	12.3(7)	4.6(7)
C_5	24.9(8)	26.4(9)	35.3(8)	0.0(7)	11.2(7)	1.6(7)
C_6	28.9(9)	25.5(9)	36.6(9)	-1.7(7)	12.4(8)	-0.1(7)
N_{12}	31.1(9)	33.3(9)	54.4(11)	1.0(8)	17.2(9)	-1.0(7)

Table 9: Bond Lengths for 7.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O_1	N_1	1.221(2)	N_6	N_7	1.339(2)
O_3	N_2	1.225(2)	N_6	C_3	1.364(2)
O_4	N_2	1.220(2)	N_6	C_4	1.463(2)
O_5	N_9	1.4206(19)	N_7	C_1	1.324(2)
O_5	C_6	1.350(2)	N_8	C_5	1.375(2)
O_6	N_{11}	1.235(2)	N_8	C_6	1.308(2)
O_7	N_{11}	1.2517(19)	N_9	C_5	1.286(2)
N_1	O_2	1.218(2)	N_{10}	C_6	1.356(2)
N_1	C_1	1.443(2)	N_{11}	N_{10}	1.319(2)
N_2	C_3	1.425(2)	C_2	C_1	1.401(2)
N_3	C_2	1.379(2)	C_2	C_3	1.387(2)
N_4	N_3	1.239(2)	C_5	C_4	1.493(2)
N_4	N_5	1.117(2)			

Table 10: Bond Angles for 7.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C_6	O_5	N_9	106.63(13)	O_7	N_{11}	N_{10}	116.05(17)
O_1	N_1	C_1	118.23(15)	N_7	C_1	N_1	117.77(16)
O_2	N_1	O_1	124.38(17)	N_7	C_1	C_2	113.80(15)
O_2	N_1	C_1	117.38(16)	C_2	C_1	N_1	128.33(16)
O_3	N_2	C_3	116.24(15)	N_3	C_2	C_1	121.49(16)
O_4	N_2	O_3	124.59(16)	N_3	C_2	C_3	136.51(17)
O_4	N_2	C_3	119.14(16)	C_3	C_2	C_1	101.92(15)
N_4	N_3	C_2	122.62(16)	N_6	C_3	N_2	122.52(15)
N_5	N_4	N_3	166.41(19)	N_6	C_3	C_2	108.53(15)
N_7	N_6	C_3	110.90(13)	C_2	C_3	N_2	128.71(16)
N_7	N_6	C_4	116.97(14)	N_6	C_4	C_5	113.10(14)
C_3	N_6	C_4	131.93(14)	N_8	C_5	C_4	119.43(14)
C_1	N_7	N_6	104.84(14)	N_9	C_5	N_8	116.24(15)
C_6	N_8	C_5	102.17(14)	N_9	C_5	C_4	124.33(15)
C_5	N_9	O_5	102.60(13)	O_5	C_6	N_{10}	111.36(15)
N_{11}	N_{10}	C_6	116.63(15)	N_8	C_6	O_5	112.36(15)
O_6	N_{11}	O_7	119.55(16)	N_8	C_6	N_{10}	136.25(16)
O_6	N_{11}	N_{10}	124.40(15)				

Table 11: Crystal data and structure refinement for Compound 9.

Identification code	tatotdk_0m_a
Empirical formula	$C_9H_9N_{19}O_7$
Formula weight	495.35
Temperature/K	310(2)
Crystal system	triclinic
Space group	P-1
a/Å	5.9663(7)
b/Å	12.5080(15)
c/Å	13.4585(17)
α/°	75.226(4)
β/°	80.633(4)
γ/°	77.189(4)
Volume/Å^3	941.0(2)
Z	2
ρ_{calc}g/cm^3	1.748
μ/mm^{-1}	0.151
F(000)	504.0
Crystal size/mm^3	0.16 × 0.14 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.43 to 51.384
Index ranges	-7 ≤ h ≤ 7, -15 ≤ k ≤ 15, -16 ≤ l ≤ 16
Reflections collected	27517
Independent reflections	3580 [R_{int} = 0.0661, R_{sigma} = 0.0379]
Data/restraints/parameters	3580/0/316
Goodness-of-fit on F^2	0.877
Final R indexes [I>=2σ (I)]	R_1 = 0.0532, wR_2 = 0.1429
Final R indexes [all data]	R_1 = 0.0954, wR_2 = 0.1784
Largest diff. peak/hole / e Å^{-3}	0.26/-0.31
CCDC number	2287542

Table 12: Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement Parameters (Å2×103) for Compound 9. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

Atom	*x*	*y*	*z*	U(eq)
O5	1121(4)	7454.3(18)	2508.7(17)	68.4(6)
N15	6526(4)	2266.1(19)	984.9(19)	55.5(6)

N6	637(4)	3867(2)	3858.2(19)	57.3(7)
N11	6345(5)	6818(2)	1068.9(19)	58.2(7)
O7	7864(5)	7351(2)	578(2)	86.4(8)
O6	6637(4)	5798.7(18)	1117(2)	84.8(8)
N7	2202(4)	4036(2)	4376(2)	59.3(7)
N13	4597(4)	3751(2)	1406.5(19)	58.5(7)
N8	2550(5)	5759(2)	2219.4(19)	58.3(7)
O1	5493(5)	3730(2)	5611(2)	89.7(8)
N19	7947(5)	1310(2)	686(2)	62.8(7)
O4	-2627(6)	2953(3)	3246(2)	93.6(9)
N10	4531(5)	7387(2)	1518(2)	64.8(7)
N1	5005(5)	2895(3)	5466(2)	66.7(7)
N16	4402(5)	1007(2)	1442(2)	70.6(8)
N14	3133(5)	2956(2)	1767(2)	64.6(7)
N12	8379(5)	3841(2)	510(2)	71.6(8)
N2	-919(6)	2319(3)	3576(2)	75.3(8)
N9	-469(5)	6768(2)	3037(2)	71.5(8)
O2	6058(5)	1938(2)	5755(2)	97.4(9)
N3	2575(7)	961(3)	5058(3)	86.2(10)
C1	3118(5)	3016(3)	4879(2)	55.2(7)
C6	2875(6)	6798(2)	2051(2)	56.3(8)
O3	-377(6)	1322(3)	3557(3)	112.9(11)
C7	6639(5)	3339(2)	938(2)	53.2(7)
C2	2173(6)	2161(3)	4700(2)	60.5(8)
C3	581(6)	2757(3)	4033(2)	58.4(8)
N18	7037(6)	-476(2)	895(3)	94.7(11)
C8	4432(6)	2088(3)	1465(3)	60.0(8)
C5	480(6)	5796(3)	2836(2)	61.0(8)
N17	2640(6)	384(3)	1812(3)	100.1(12)
C9	6551(6)	581(3)	985(3)	66.1(9)
C4	-729(6)	4828(3)	3202(3)	71.4(9)
N4	2948(8)	643(3)	5880(4)	106.7(13)
N5	3368(14)	131(5)	6710(4)	187(3)

Table 13: Anisotropic Displacement Parameters ($Å^2×10^3$) for 9. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O5	72.5(16)	52.2(13)	72.5(15)	5.4(11)	6.9(12)	-23.7(11)
N15	53.6(16)	44.6(14)	67.6(17)	1.4(11)	-3.6(13)	-22.5(12)
N6	54.8(16)	56.9(16)	60.8(16)	-9.6(13)	2.2(13)	-20.3(13)
N11	75.1(19)	42.0(14)	54.6(15)	-2.9(13)	2.1(14)	-18.0(12)
O7	101(2)	54.3(14)	94.5(19)	-14.2(14)	32.8(16)	-27.8(13)

O6	87.3(18)	45.6(14)	119(2)	-8.6(12)	23.7(16)	-38.7(13)
N7	57.4(16)	55.8(16)	68.3(17)	-10.2(13)	-4.2(14)	-22.5(13)
N13	60.2(16)	50.2(15)	65.3(16)	2.7(13)	-3.2(13)	-26.2(12)
N8	63.8(17)	49.7(15)	58.7(15)	-0.4(12)	-3.7(13)	-17.8(12)
O1	89(2)	78.4(18)	115(2)	-28.3(15)	-30.4(17)	-22.6(16)
N19	57.3(16)	46.5(14)	83.2(19)	2.8(12)	-0.5(14)	-27.0(13)
O4	84(2)	122(3)	86(2)	-39.0(19)	-15.0(16)	-23.1(17)
N10	77.9(19)	42.9(14)	66.5(17)	1.4(14)	9.2(15)	-20.7(13)
N1	59.3(18)	64.8(19)	73.8(19)	-10.0(15)	-3.6(15)	-15.2(15)
N16	57.4(18)	55.7(17)	100(2)	-5.9(14)	0.3(16)	-29.5(15)
N14	56.5(16)	63.5(17)	78.4(19)	-3.5(14)	-3.5(14)	-33.0(14)
N12	68.2(19)	49.7(16)	94(2)	-4.9(14)	13.6(16)	-30.1(14)
N2	81(2)	90(3)	66.5(19)	-35(2)	4.8(17)	-30.7(17)
N9	67.4(19)	63.6(18)	74.6(19)	2.0(15)	3.9(15)	-18.9(15)
O2	90(2)	77(2)	120(2)	0.0(16)	-35.0(18)	-12.8(17)
N3	122(3)	57(2)	85(2)	-16.7(19)	-20(2)	-20.7(18)
C1	53.1(18)	53.2(19)	59.3(18)	-9.5(15)	2.8(15)	-18.7(14)
C6	67(2)	46.8(18)	51.1(17)	6.8(15)	-3.9(15)	-20.4(14)
O3	144(3)	95(2)	126(3)	-50(2)	-7(2)	-54(2)
C7	56.7(19)	45.8(17)	56.2(18)	2.4(14)	-6.1(15)	-20.0(14)
C2	68(2)	54.6(19)	59.4(19)	-14.0(16)	8.0(17)	-20.6(15)
C3	62(2)	62(2)	56.9(19)	-19.2(16)	4.9(16)	-24.8(15)
N18	77(2)	50.5(17)	157(3)	-7.1(15)	10(2)	-44.0(19)
C8	53.9(19)	53.3(19)	74(2)	-0.7(15)	-3.3(16)	-26.6(16)
C5	61(2)	57(2)	60(2)	2.8(16)	-7.2(16)	-15.9(15)
N17	68(2)	74(2)	170(4)	-22.1(18)	17(2)	-55(2)
C9	59(2)	47.0(18)	92(3)	-0.9(16)	-6.4(18)	-24.4(17)
C4	63(2)	68(2)	81(2)	-6.0(18)	-10.7(18)	-16.3(18)
N4	150(4)	65(2)	112(3)	-43(2)	-21(3)	-8(2)
N5	300(9)	147(5)	129(5)	-111(5)	-78(5)	33(4)

Table 14: Table containing bond lengths of 9.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O5	C6	1.347(3)	N10	C6	1.362(4)
O5	N9	1.404(4)	N1	O2	1.220(4)
N15	C7	1.344(4)	N1	C1	1.438(4)
N15	C8	1.347(4)	N16	C8	1.365(4)
N15	N19	1.413(3)	N16	C9	1.383(4)
N6	N7	1.333(4)	N16	N17	1.398(4)
N6	C3	1.354(4)	N14	C8	1.302(4)
N6	C4	1.465(4)	N12	C7	1.309(4)
N11	O6	1.233(3)	N2	O3	1.223(4)
N11	O7	1.245(3)	N2	C3	1.430(4)

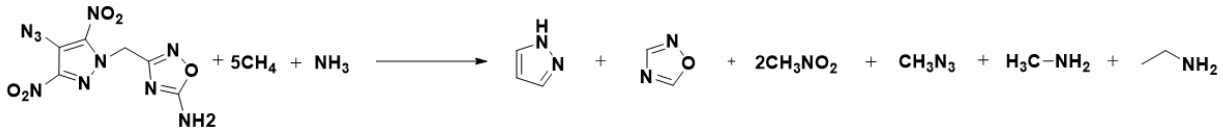
N11	N10	1.307(3)	N9	C5	1.298(4)
N7	C1	1.325(4)	N3	N4	1.118(5)
N13	C7	1.336(4)	N3	C2	1.433(4)
N13	N14	1.410(4)	C1	C2	1.401(4)
N8	C6	1.313(4)	C2	C3	1.373(5)
N8	C5	1.370(4)	N18	C9	1.322(4)
O1	N1	1.212(4)	C5	C4	1.482(5)
N19	C9	1.314(4)	N4	N5	1.173(6)
O4	N2	1.214(4)			

Table 15: Table containing bond angles of compound 9.

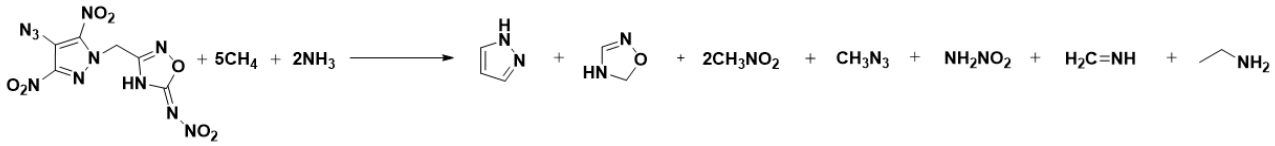
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C6	O5	N9	106.9(2)	N7	C1	C2	113.2(3)
C7	N15	C8	107.8(2)	N7	C1	N1	118.8(3)
C7	N15	N19	138.4(3)	C2	C1	N1	127.8(3)
C8	N15	N19	113.7(2)	N8	C6	O5	112.4(3)
N7	N6	C3	111.2(3)	N8	C6	N10	136.1(3)
N7	N6	C4	119.8(3)	O5	C6	N10	111.6(3)
C3	N6	C4	129.0(3)	N12	C7	N13	129.4(3)
O6	N11	O7	119.2(3)	N12	C7	N15	126.3(3)
O6	N11	N10	124.0(3)	N13	C7	N15	104.3(3)
O7	N11	N10	116.8(2)	C3	C2	C1	102.2(3)
C1	N7	N6	104.7(2)	C3	C2	N3	123.9(3)
C7	N13	N14	113.3(2)	C1	C2	N3	133.9(3)
C6	N8	C5	102.1(2)	N6	C3	C2	108.7(3)
C9	N19	N15	100.9(2)	N6	C3	N2	123.9(3)
N11	N10	C6	116.4(2)	C2	C3	N2	127.5(3)
O1	N1	O2	124.6(3)	N14	C8	N15	114.2(3)
O1	N1	C1	119.2(3)	N14	C8	N16	141.2(3)
O2	N1	C1	116.1(3)	N15	C8	N16	104.6(3)
C8	N16	C9	106.8(3)	N9	C5	N8	115.7(3)
C8	N16	N17	129.5(3)	N9	C5	C4	120.7(3)
C9	N16	N17	123.7(3)	N8	C5	C4	123.5(3)
C8	N14	N13	100.4(2)	N19	C9	N18	126.3(3)
O4	N2	O3	125.0(3)	N19	C9	N16	113.9(3)
O4	N2	C3	118.2(3)	N18	C9	N16	119.8(3)
O3	N2	C3	116.8(4)	N6	C4	C5	112.0(3)
C5	N9	O5	103.0(2)	N3	N4	N5	168.5(5)
N4	N3	C2	115.0(3)				

Isodesmic reactions:

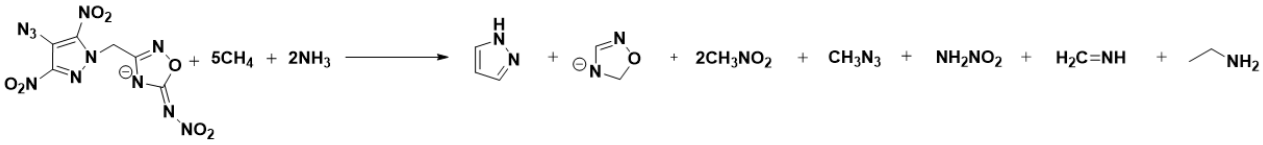
Compound 4:



Compound 6:



Compound 7-17:



NMR Spectra:

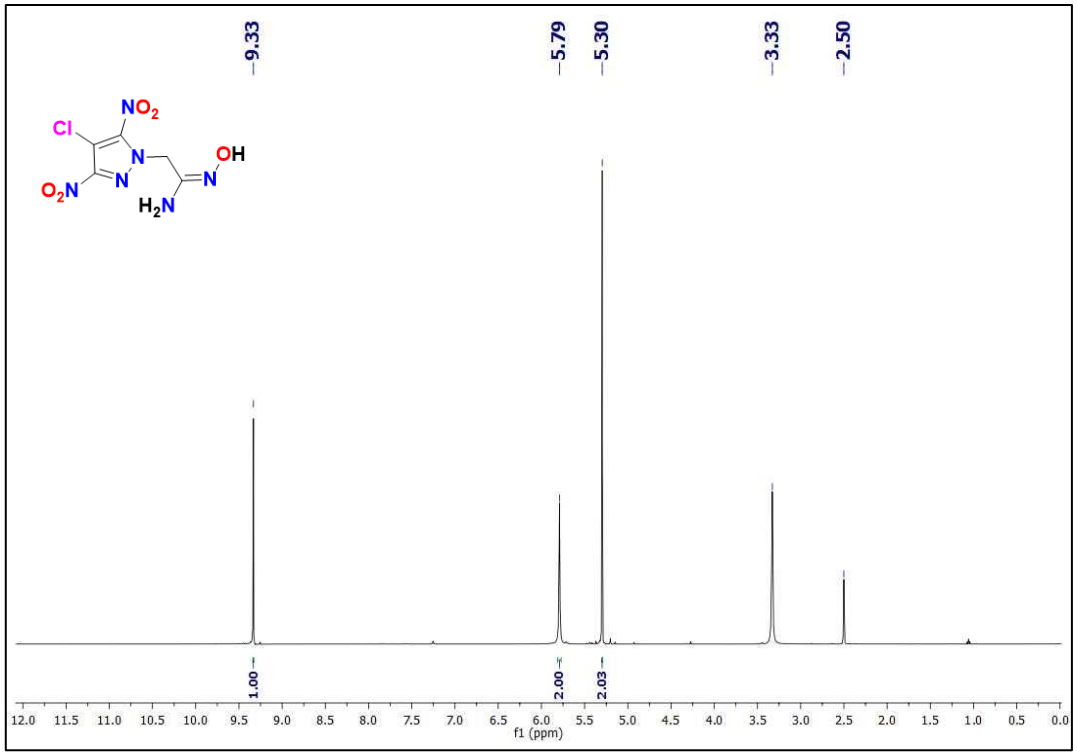


Fig.S1: ^{1}H NMR Spectra of compound **2**

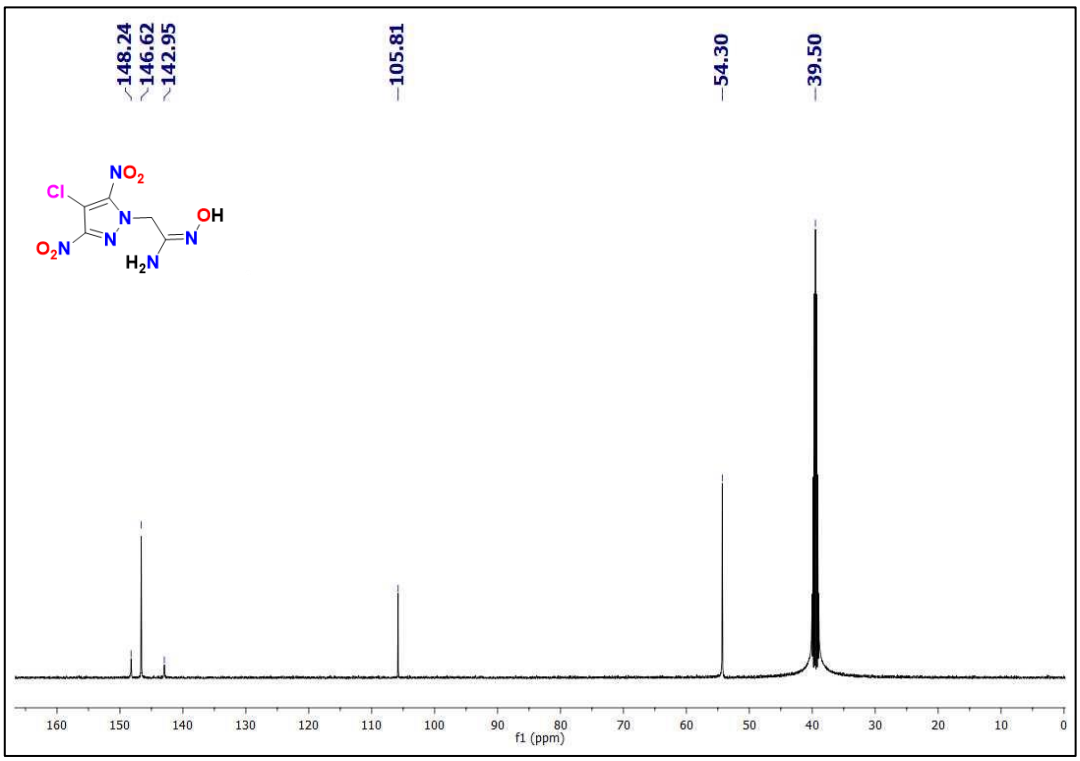


Fig.S2: ^{13}C{^{1}H}NMR Spectra of compound **2**

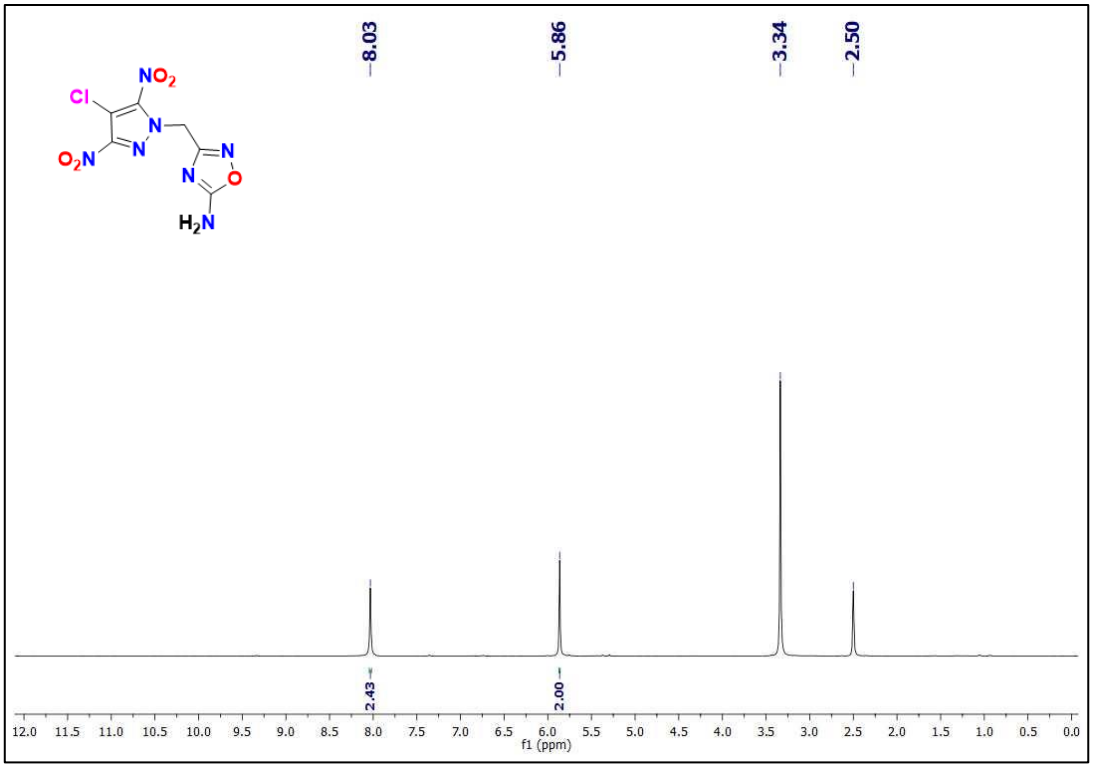


Fig.S3: ^{1}H NMR Spectra of compound **3**

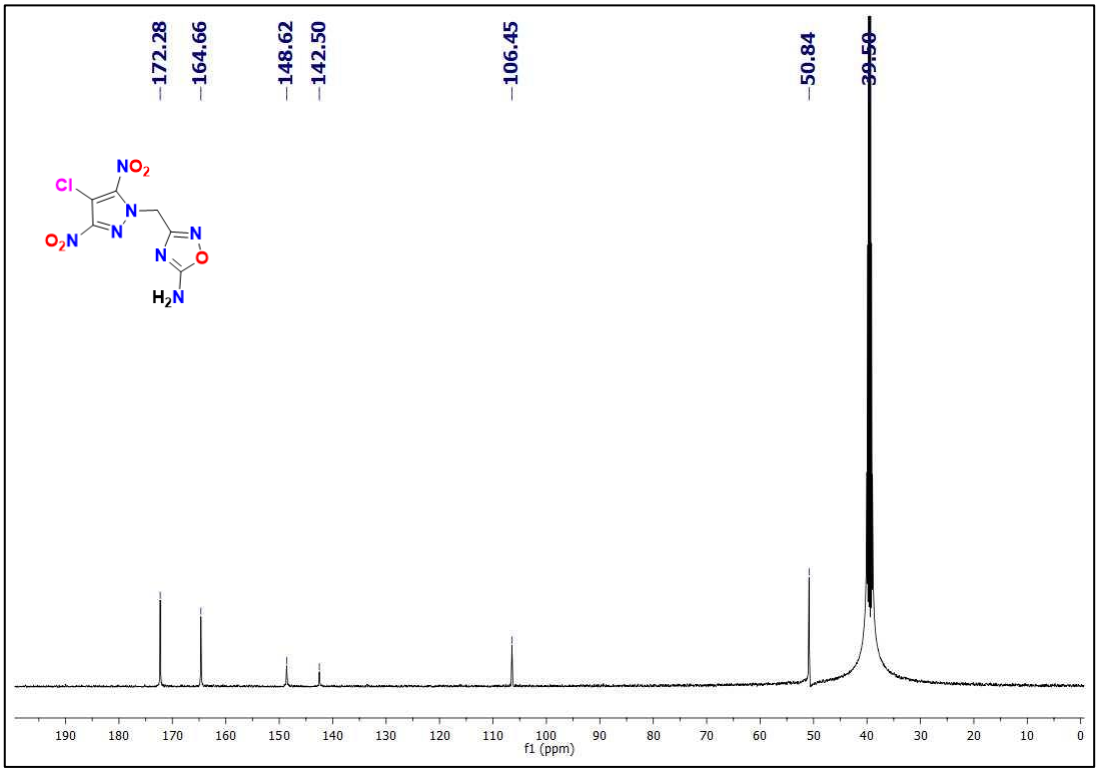


Fig.S4: ^{13}C{^{1}H}NMR Spectra of compound **3**

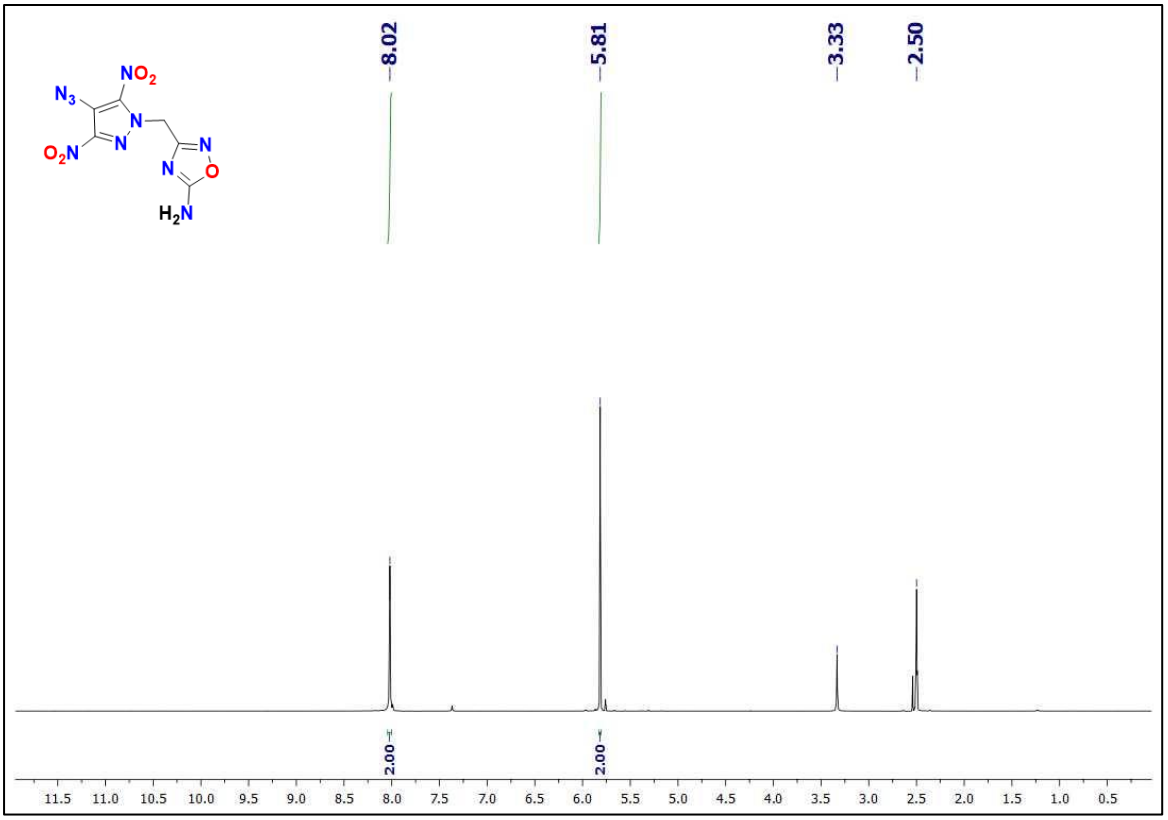


Fig.S5: ^{1}H NMR Spectra of compound **4**

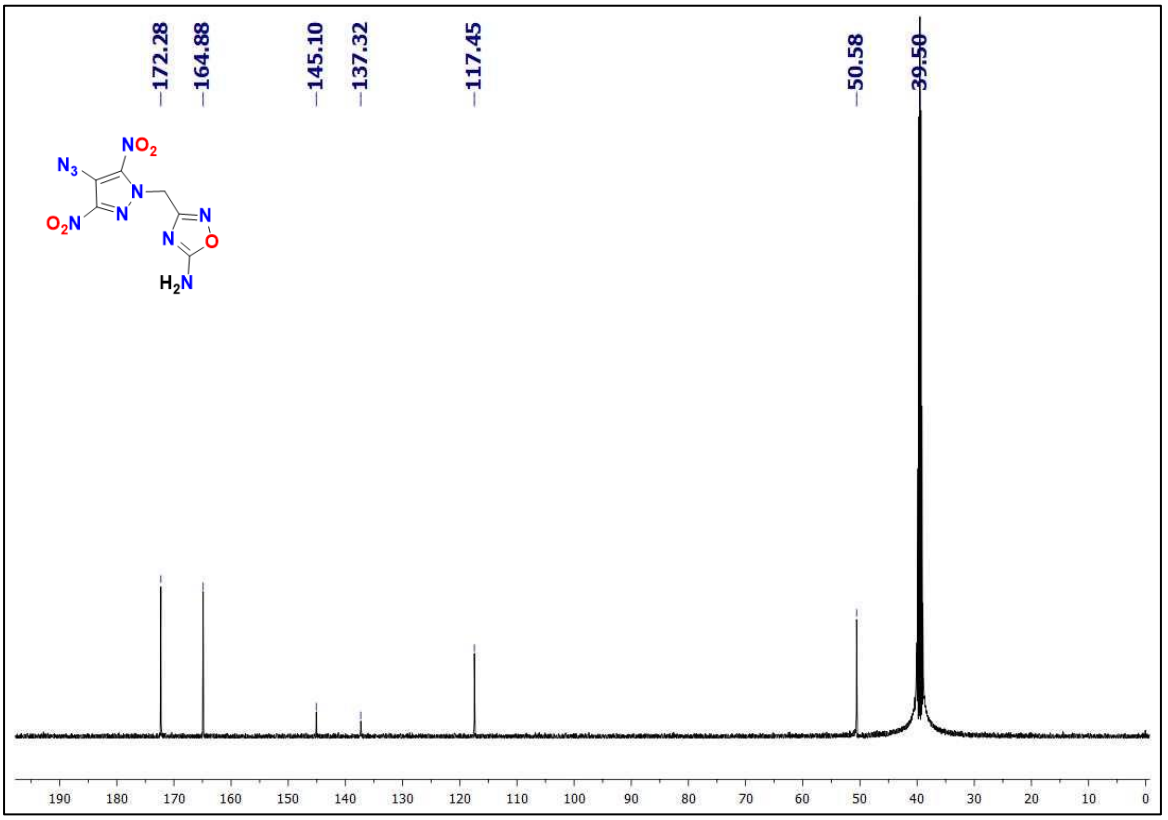


Fig.S6: ^{13}C{^{1}H} NMR Spectra of compound **4**

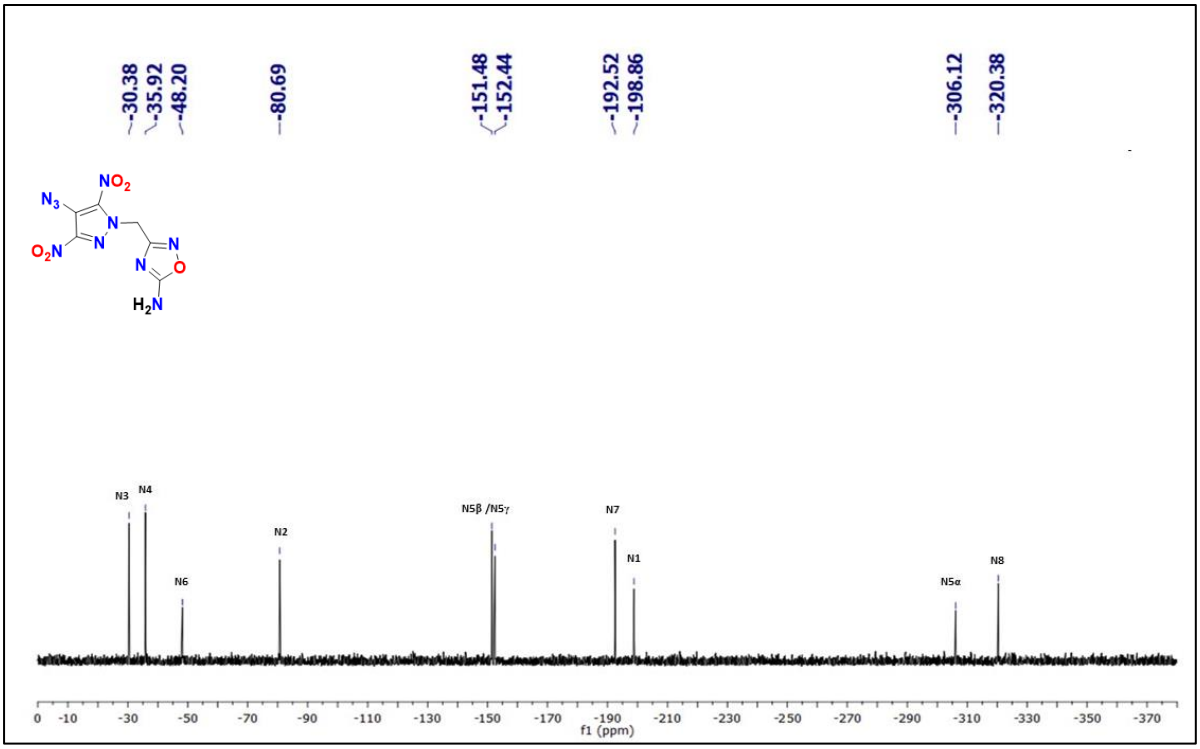


Fig.S7: ^{15}N NMR Spectra of compound **4**

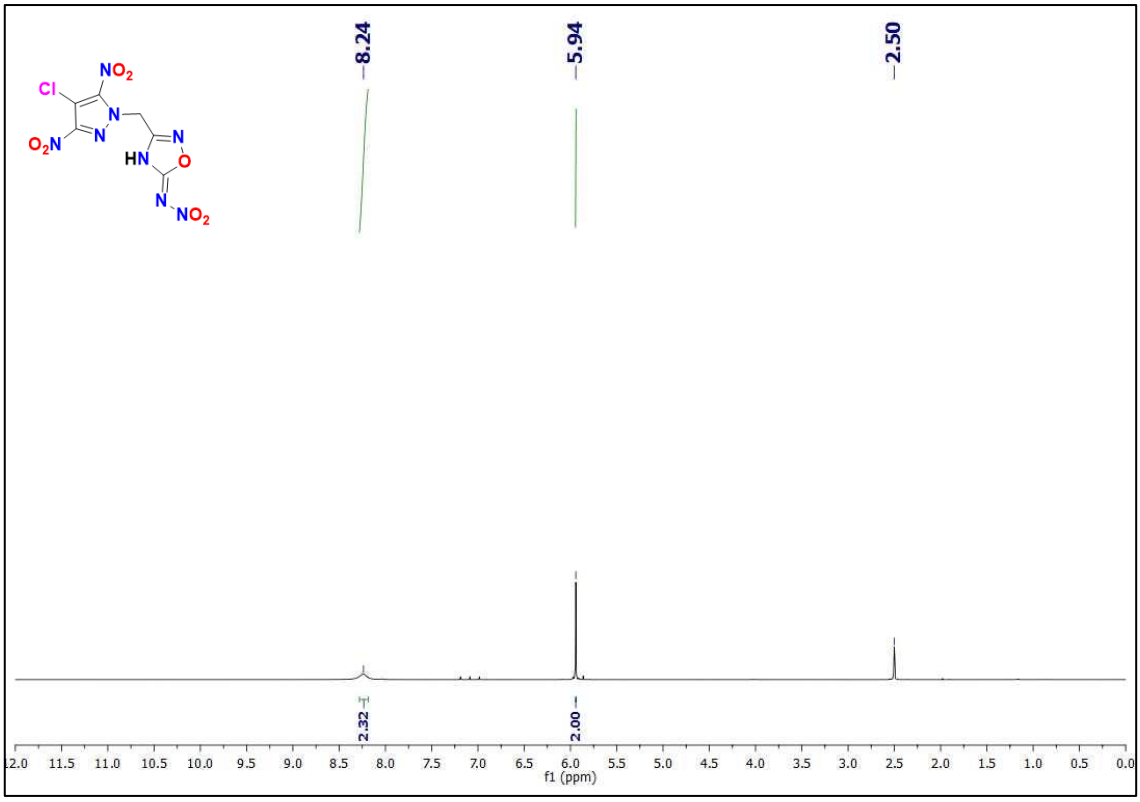


Fig.S8: ^{1}H NMR Spectra of compound **5**

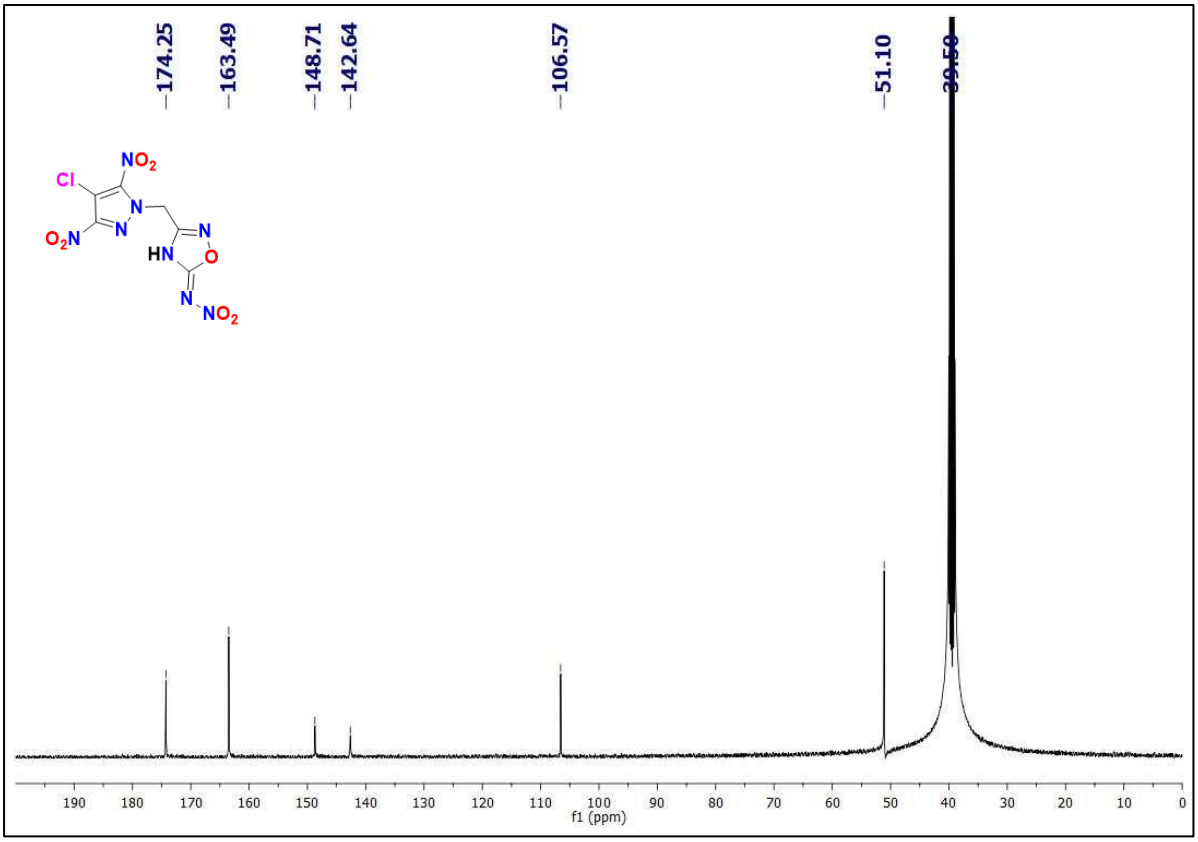


Fig.S9: $^{13}C\{^{1}H\}$ NMR Spectra of compound **5**

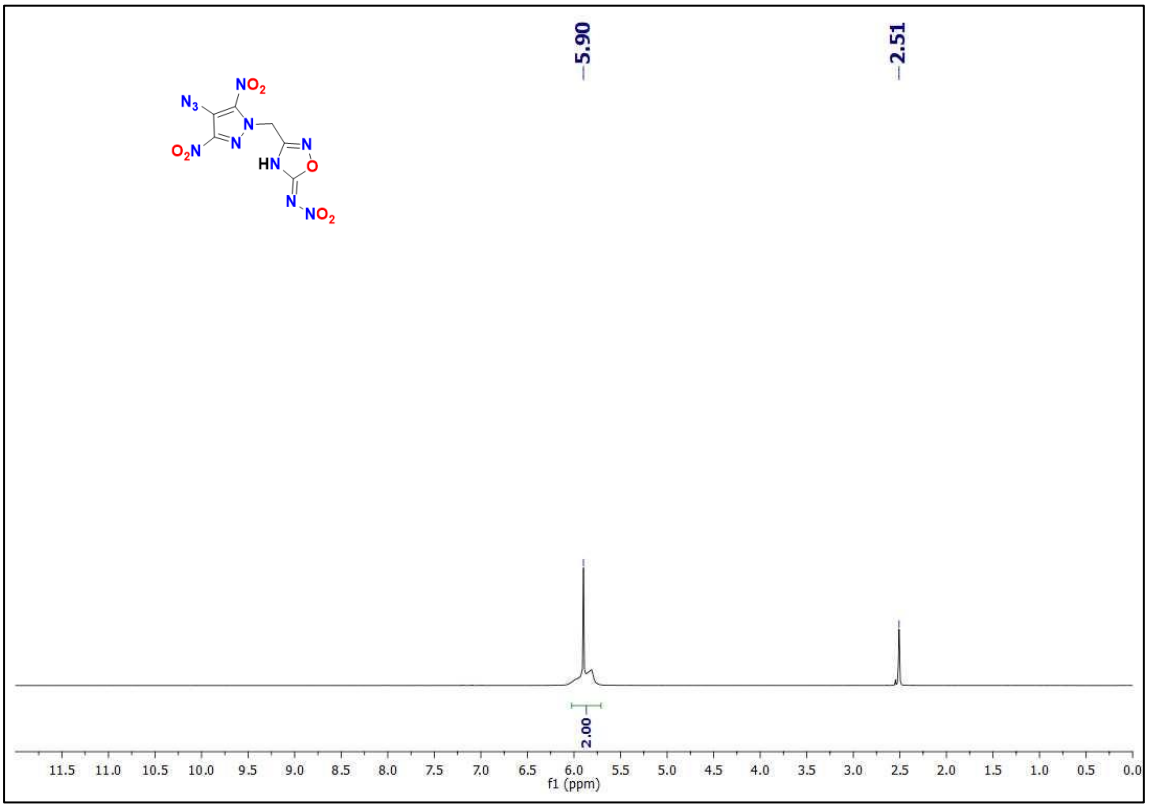


Fig.S10: ^{1}H NMR Spectra of compound **6**

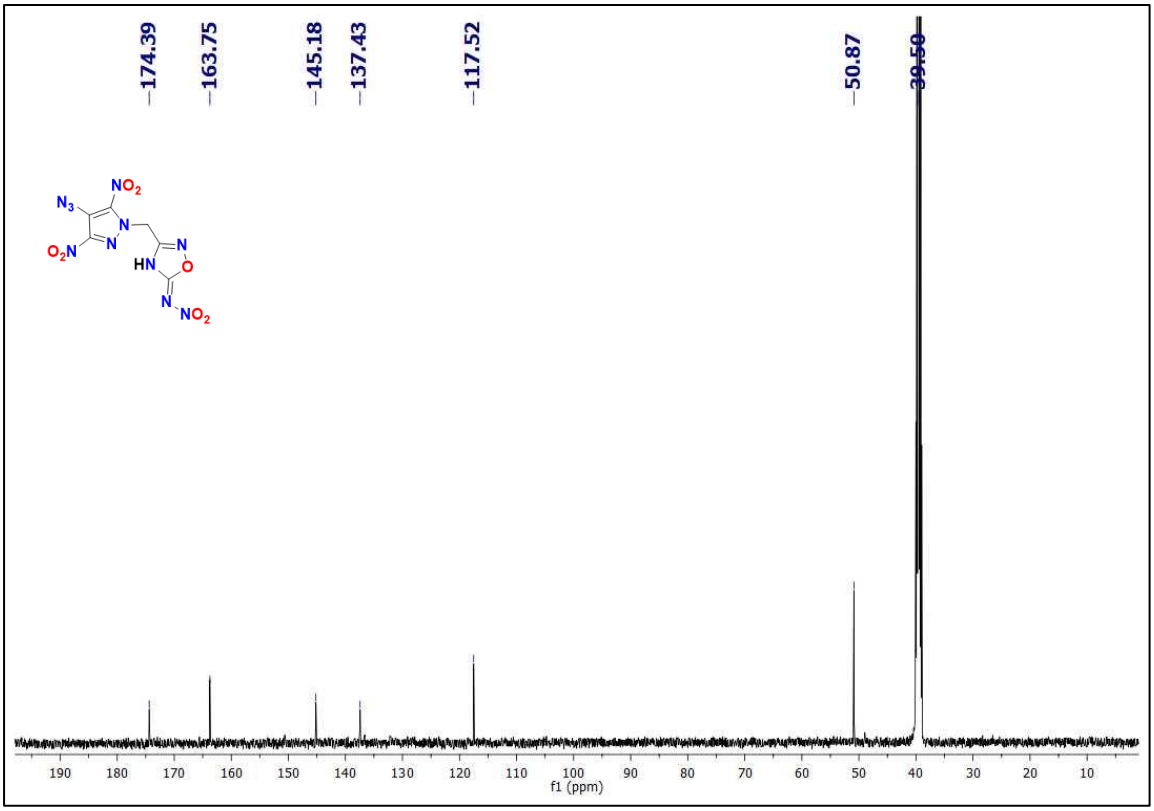


Fig.S11: $^{13}C\{^{1}H\}$NMR Spectra of compound **6**

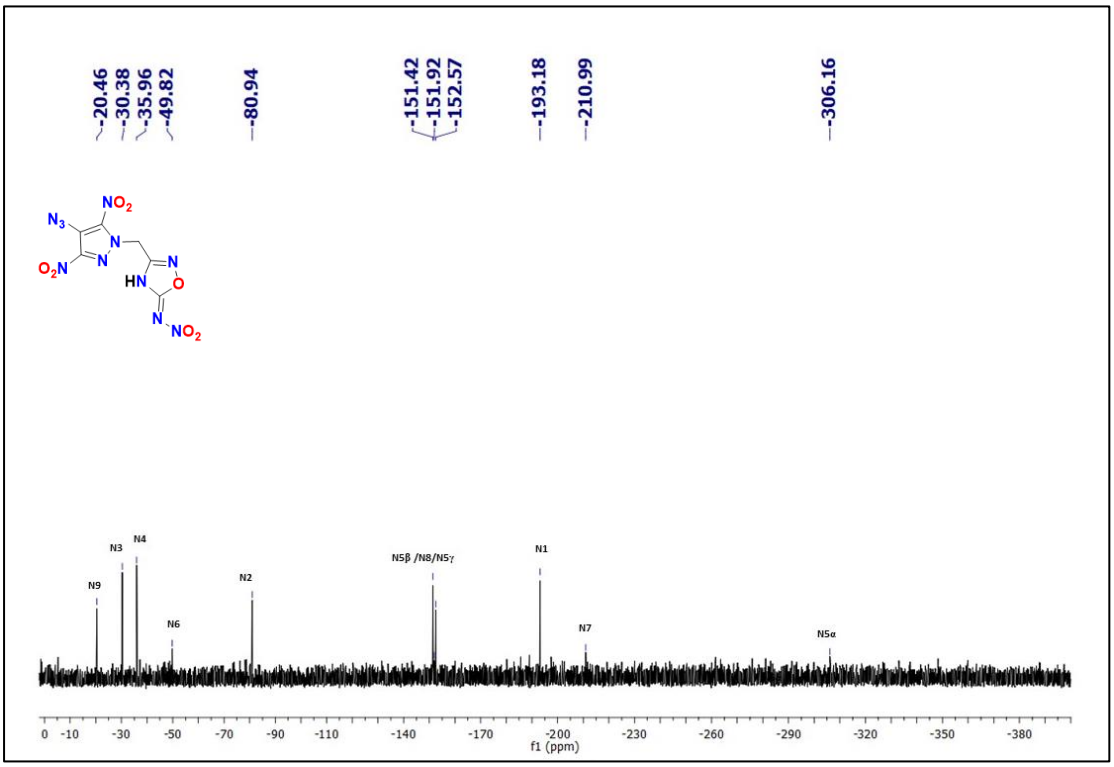


Fig.S12: ^{15}N NMR Spectra of compound **6**

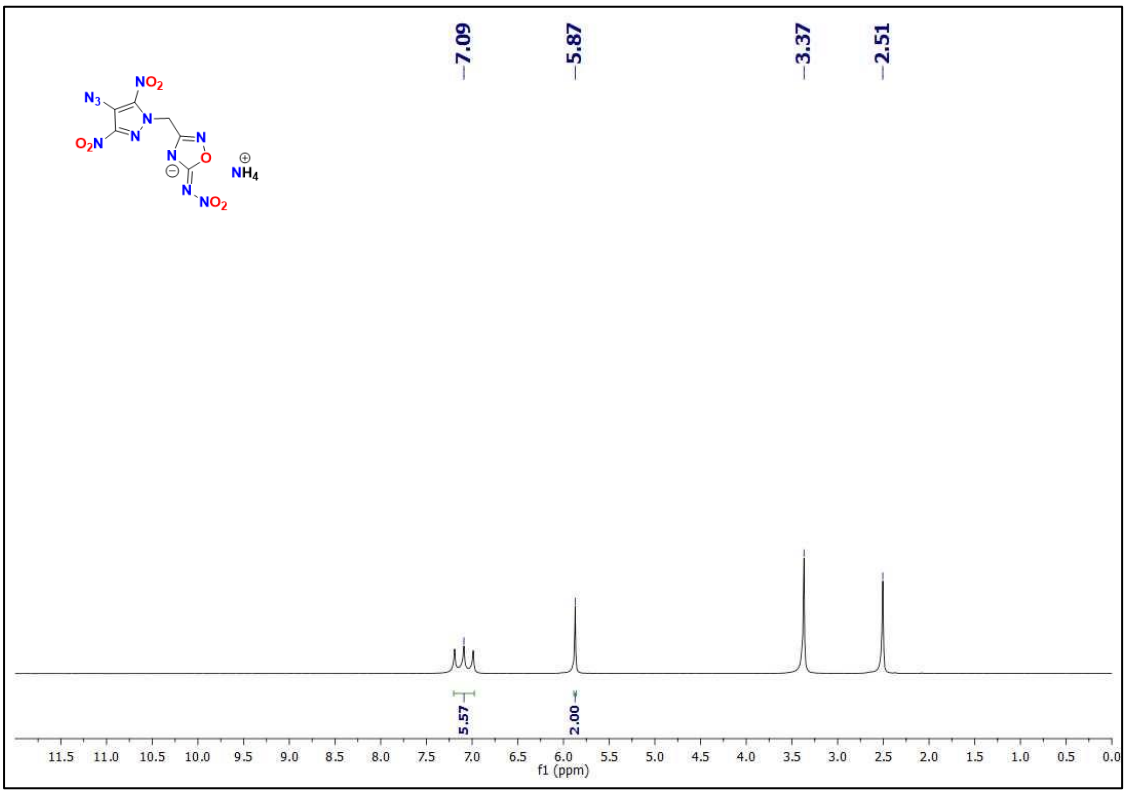


Fig.S13: ^{1}H NMR Spectra of compound **7**

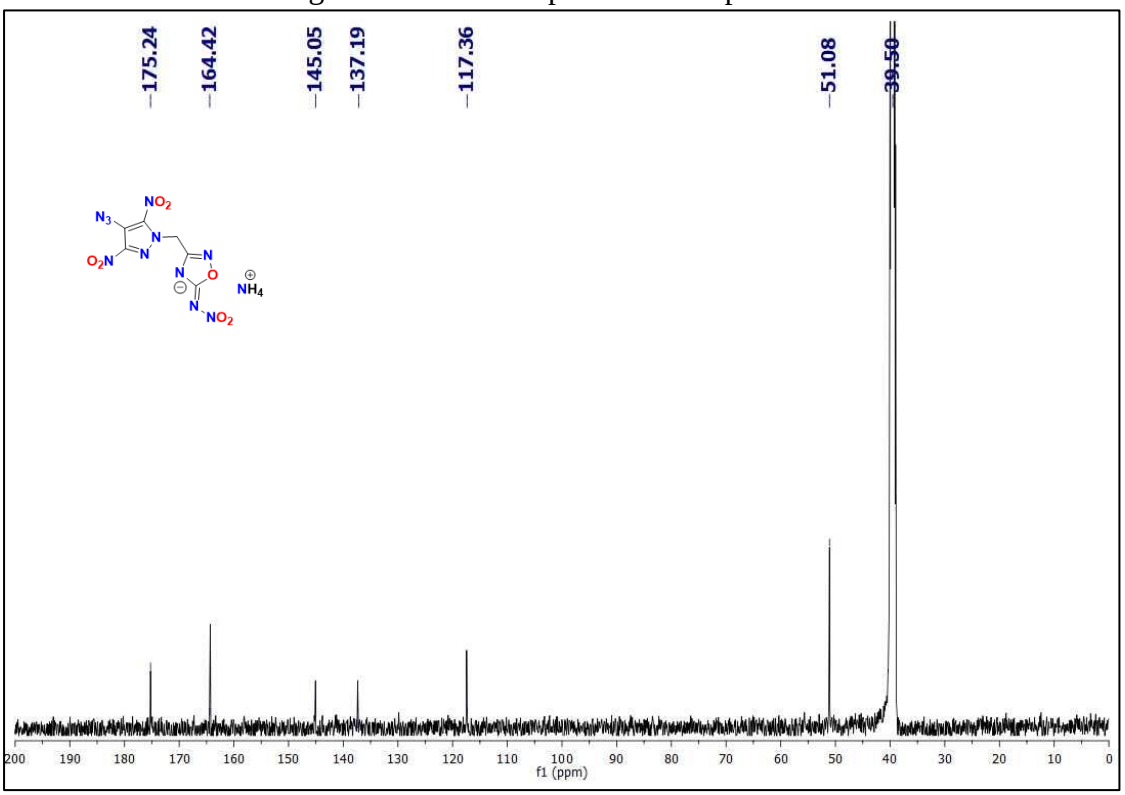


Fig.S14: ^{13}C{^{1}H}NMR Spectra of compound **7**

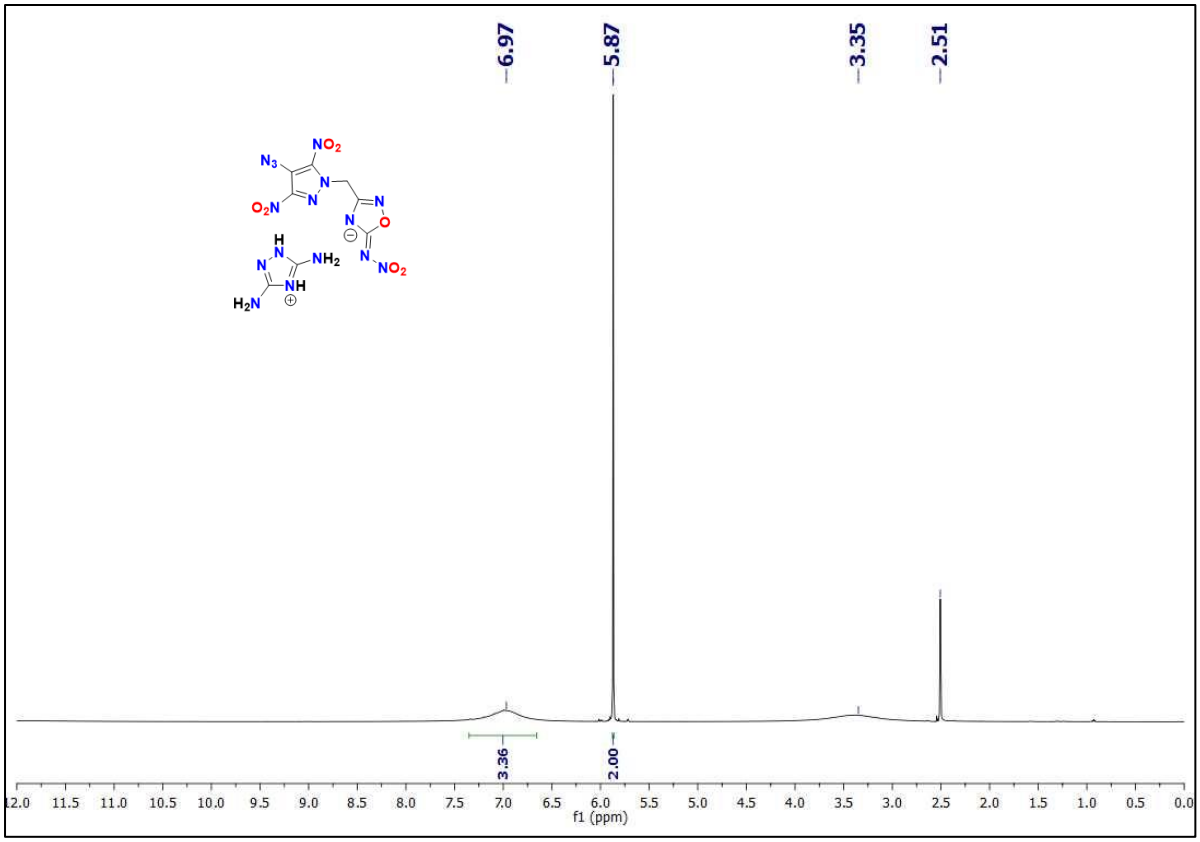


Fig.S15: ^{1}H NMR Spectra of compound **8**

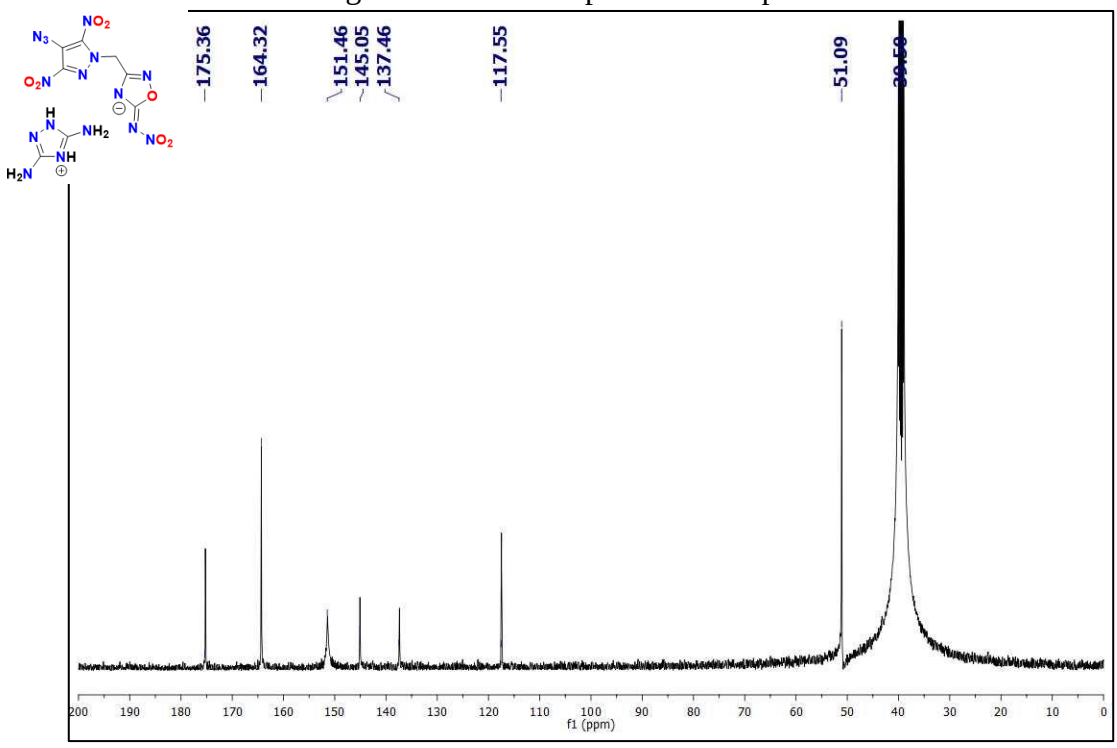


Fig.S16: ^{13}C{^{1}H}NMR Spectra of compound **8**

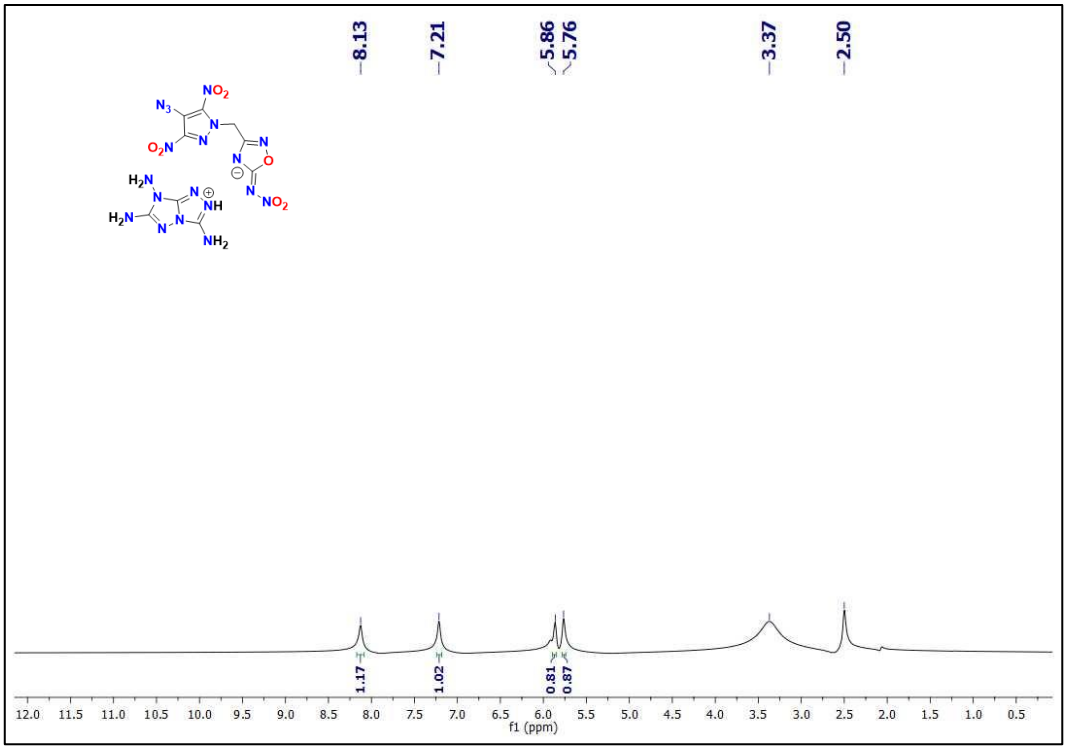


Fig.S17: ^{1}H NMR Spectra of compound **9**

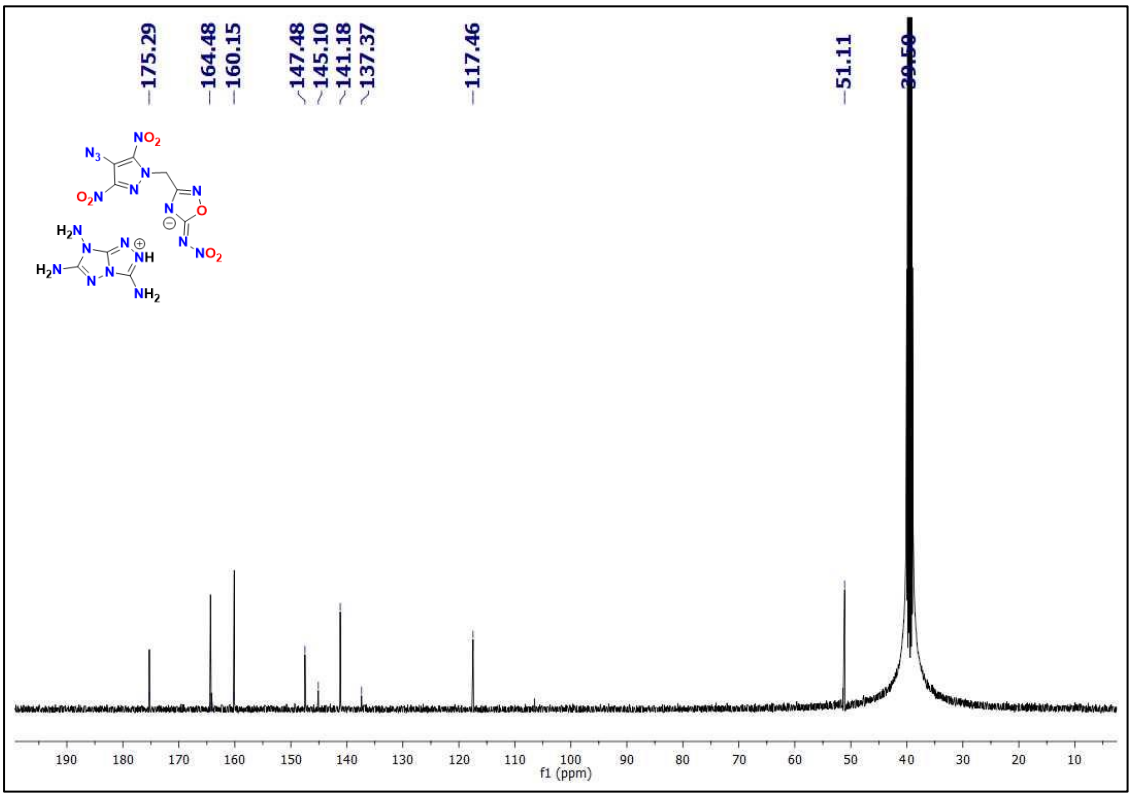


Fig.S18: ^{13}C{^{1}H}NMR Spectra of compound **9**

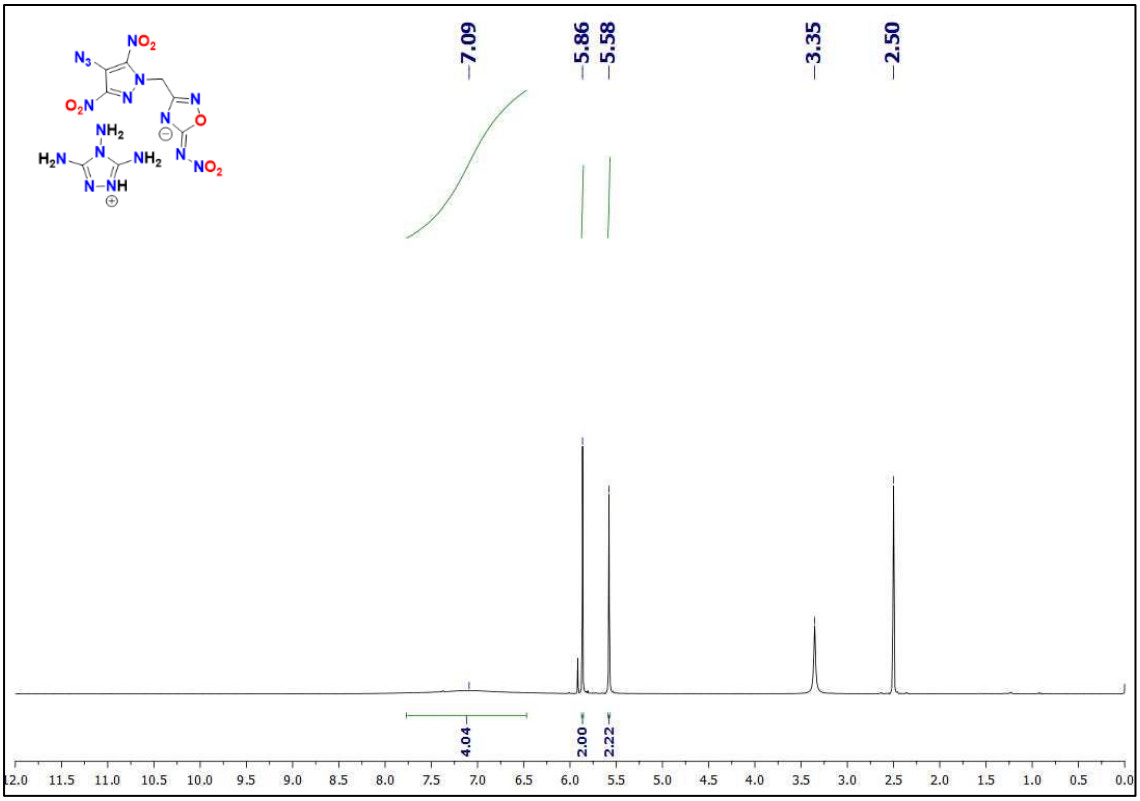


Fig.S19: ^{1}H NMR Spectra of compound **10**

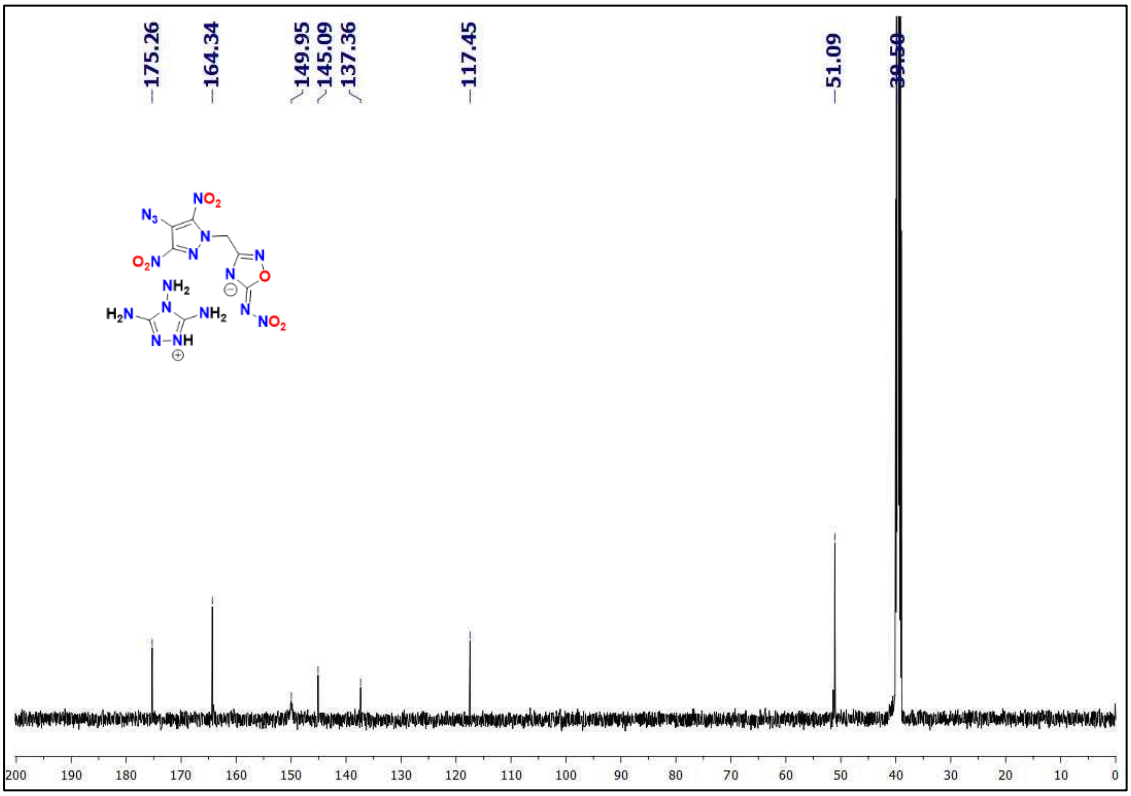


Fig.S20: ^{13}C{^{1}H}NMR Spectra of compound **10**

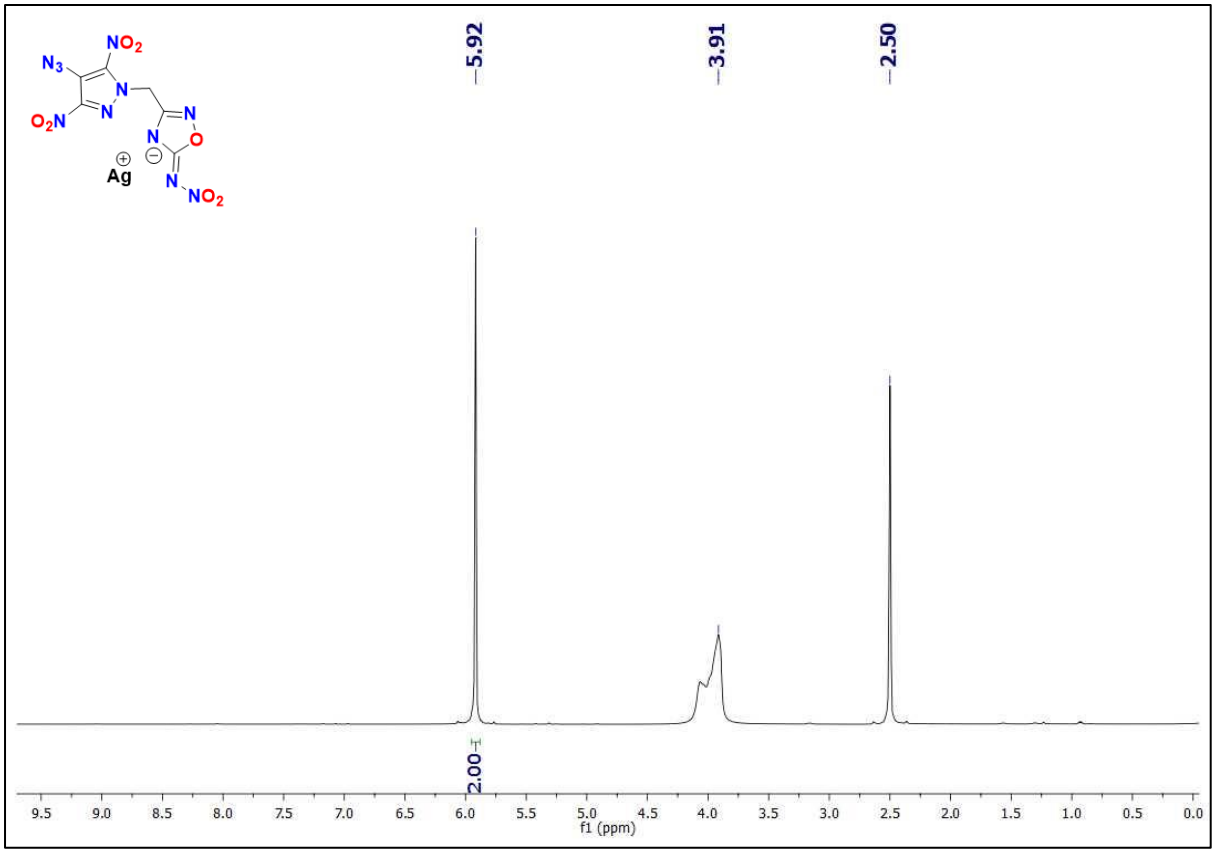


Fig.S21: ^{1}H NMR Spectra of compound **11**

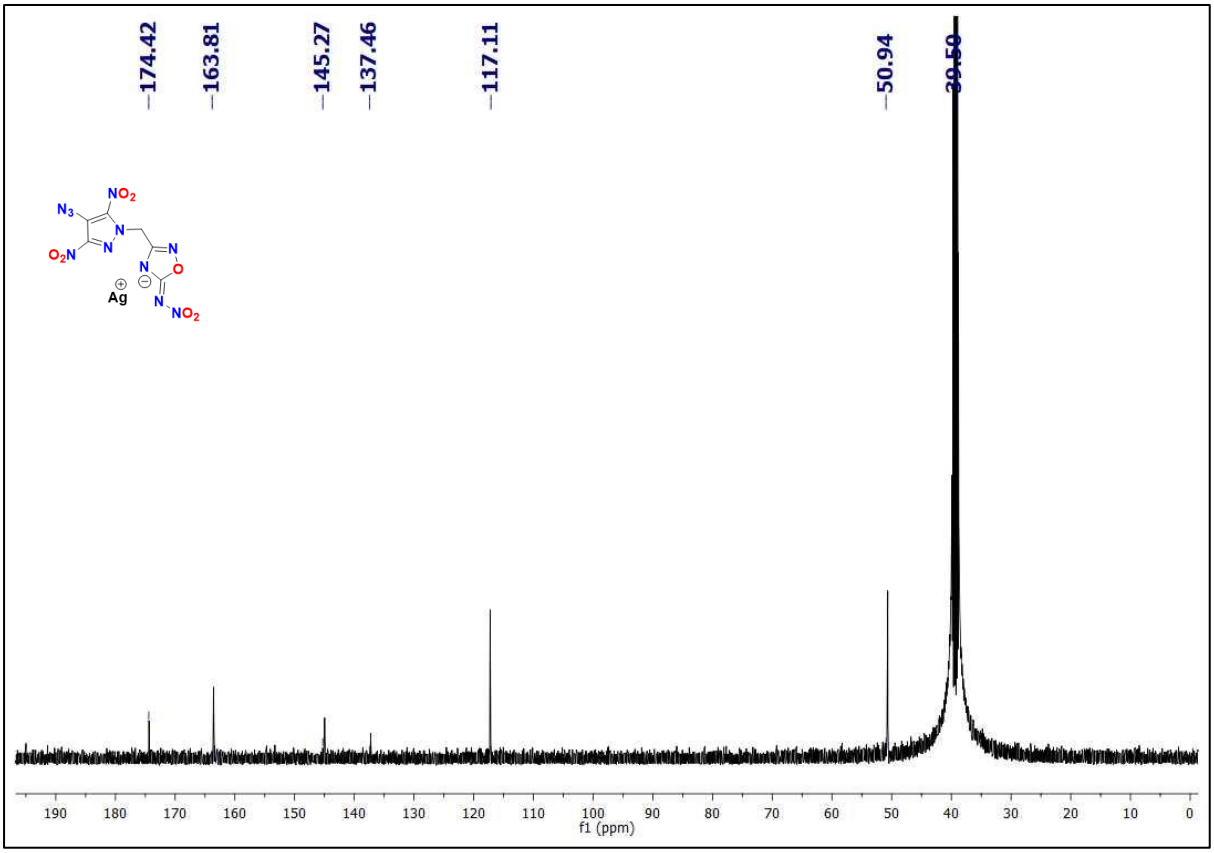


Fig.S22: ^{13}C{^{1}H}NMR Spectra of compound **11**

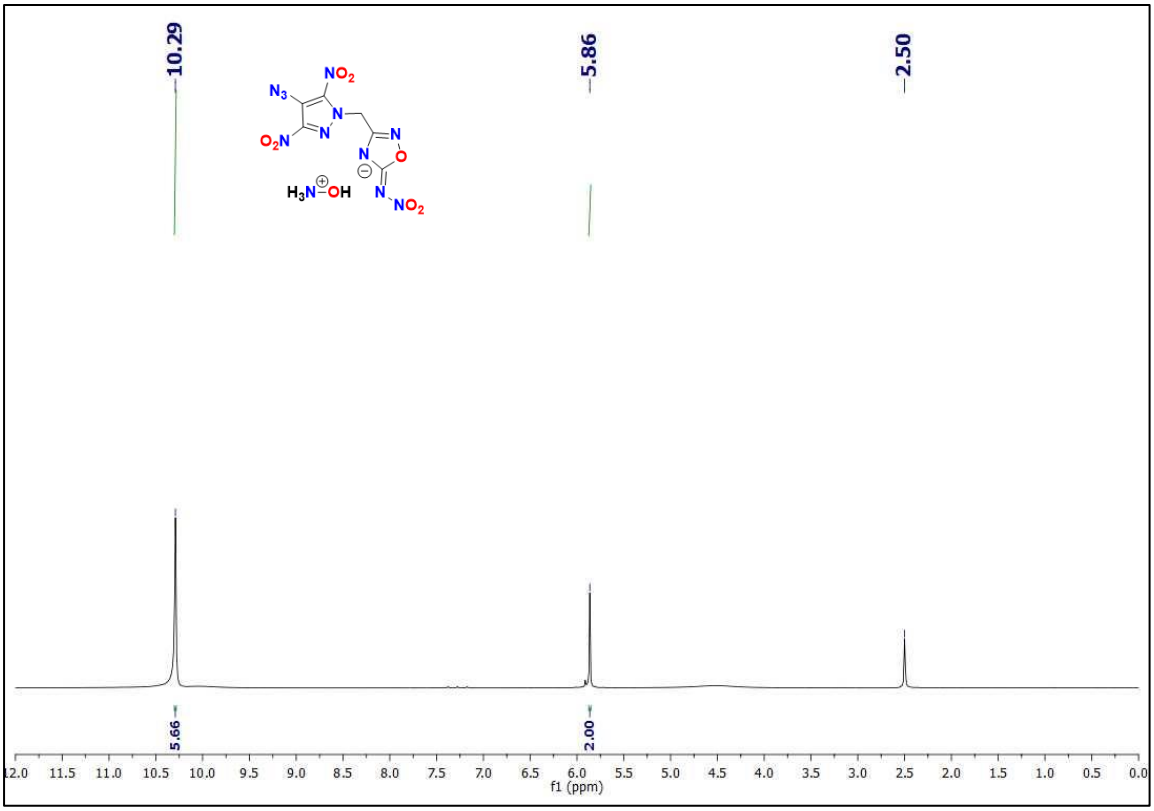


Fig.S23: ^{1}H NMR Spectra of compound **12**

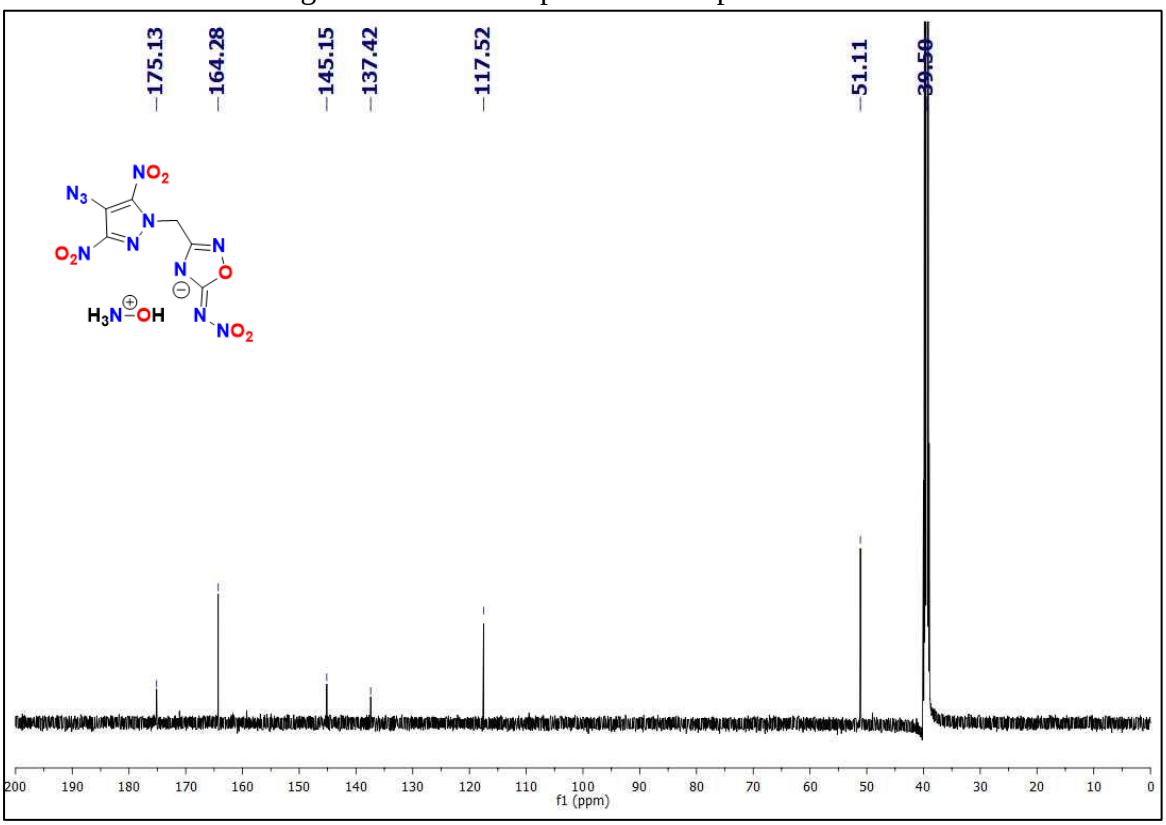


Fig.S24: ^{13}C{^{1}H}NMR Spectra of compound **12**

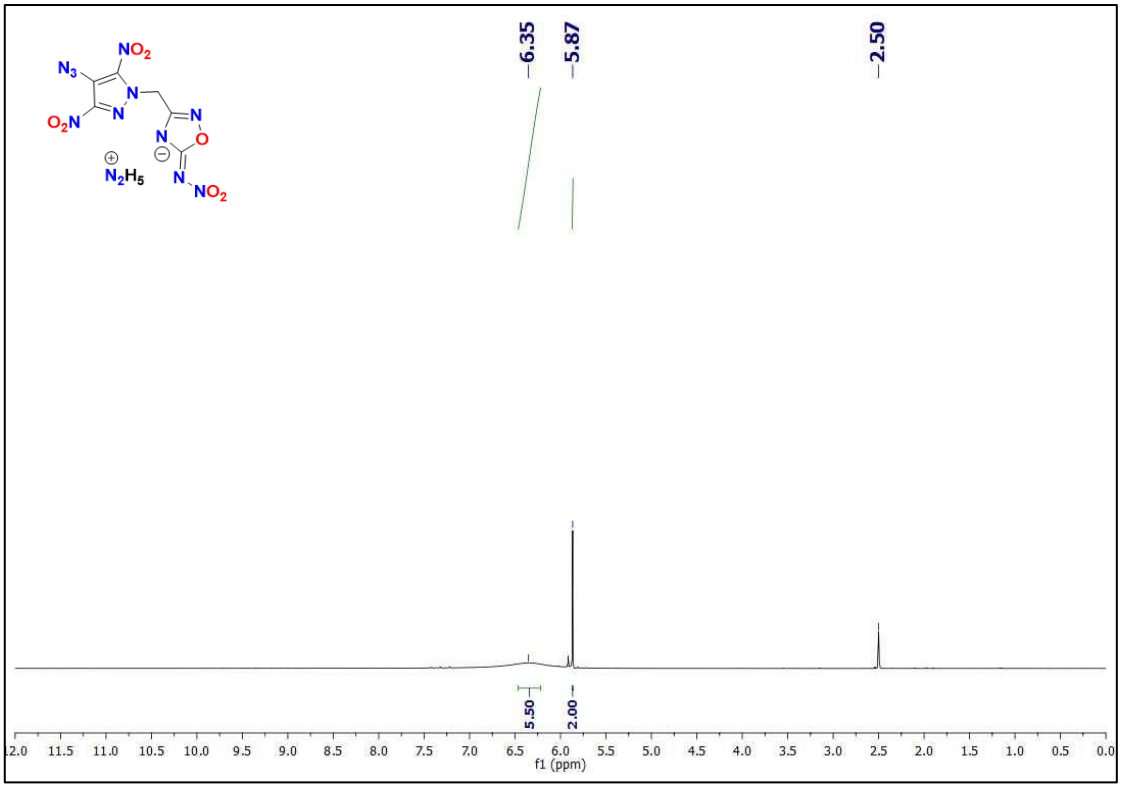


Fig.S25: ^{1}H NMR Spectra of compound **13**

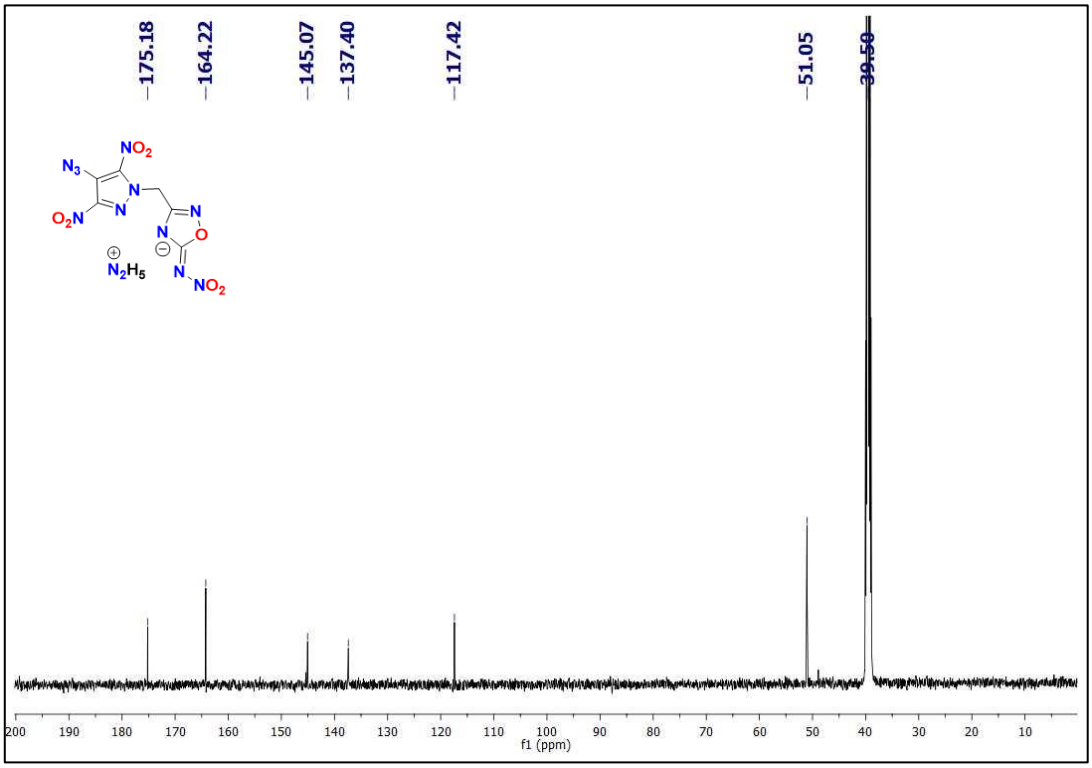


Fig.S26: ^{13}C{^{1}H}NMR Spectra of compound **13**

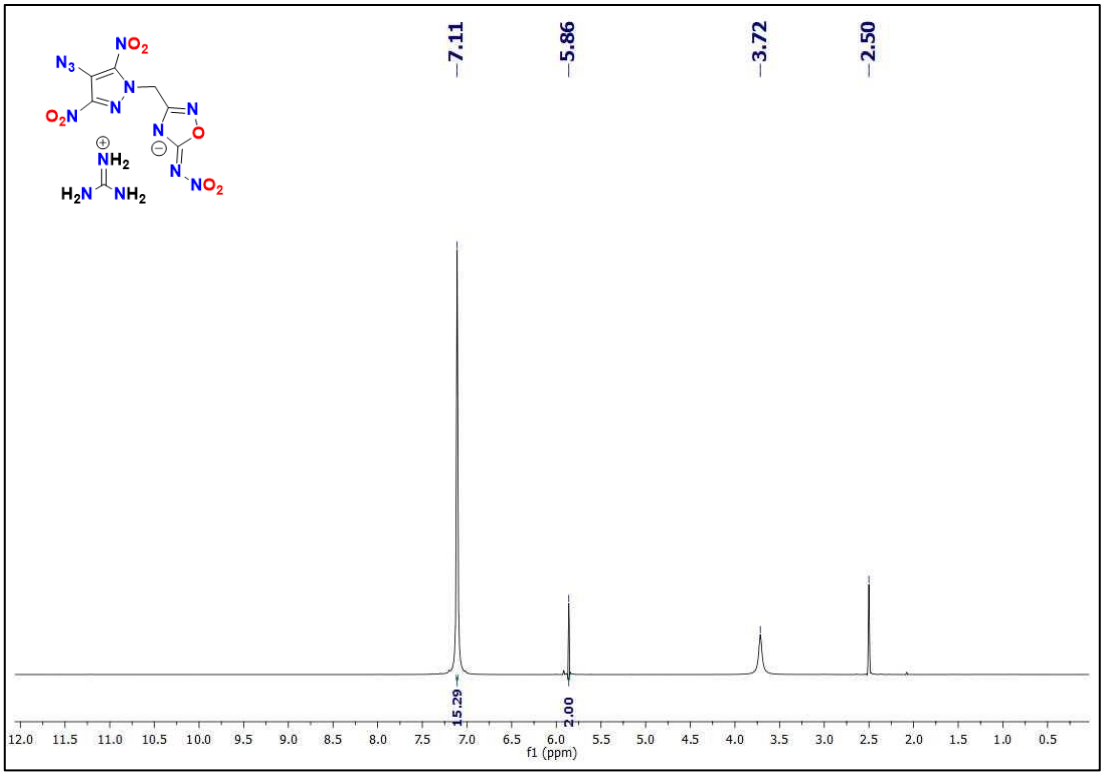


Fig.S27: ^{1}H NMR Spectra of compound **14**

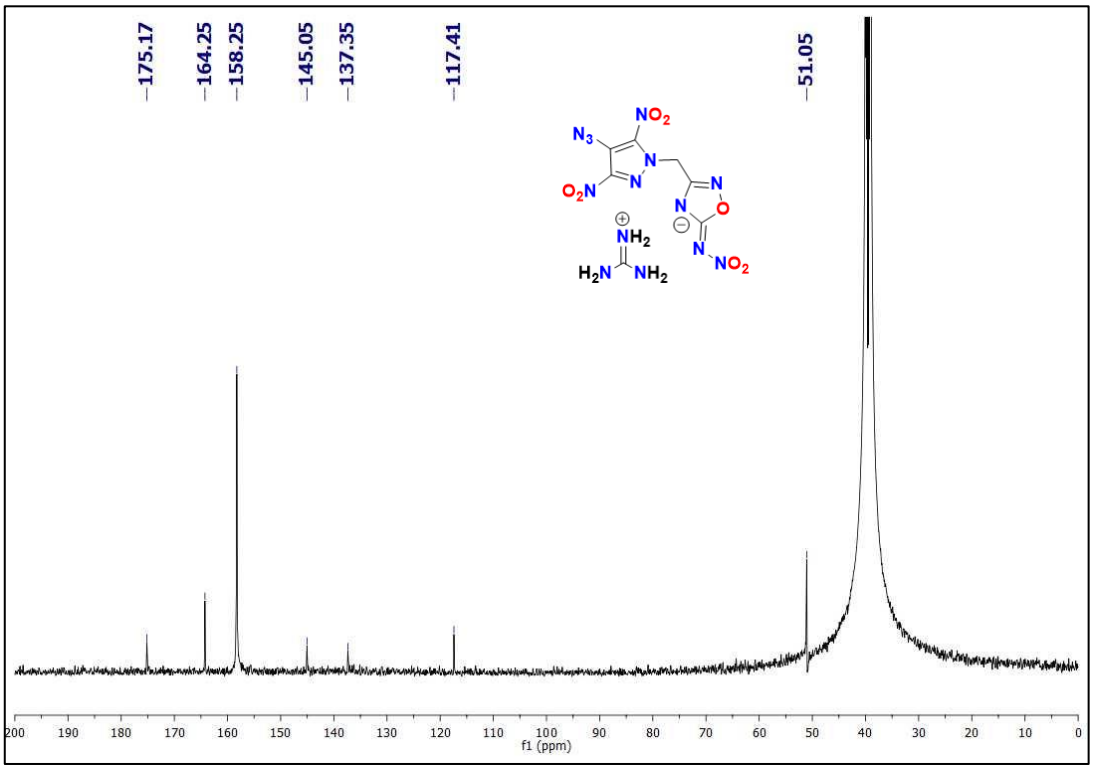


Fig.S28: ^{13}C{^{1}H}NMR Spectra of compound **14**

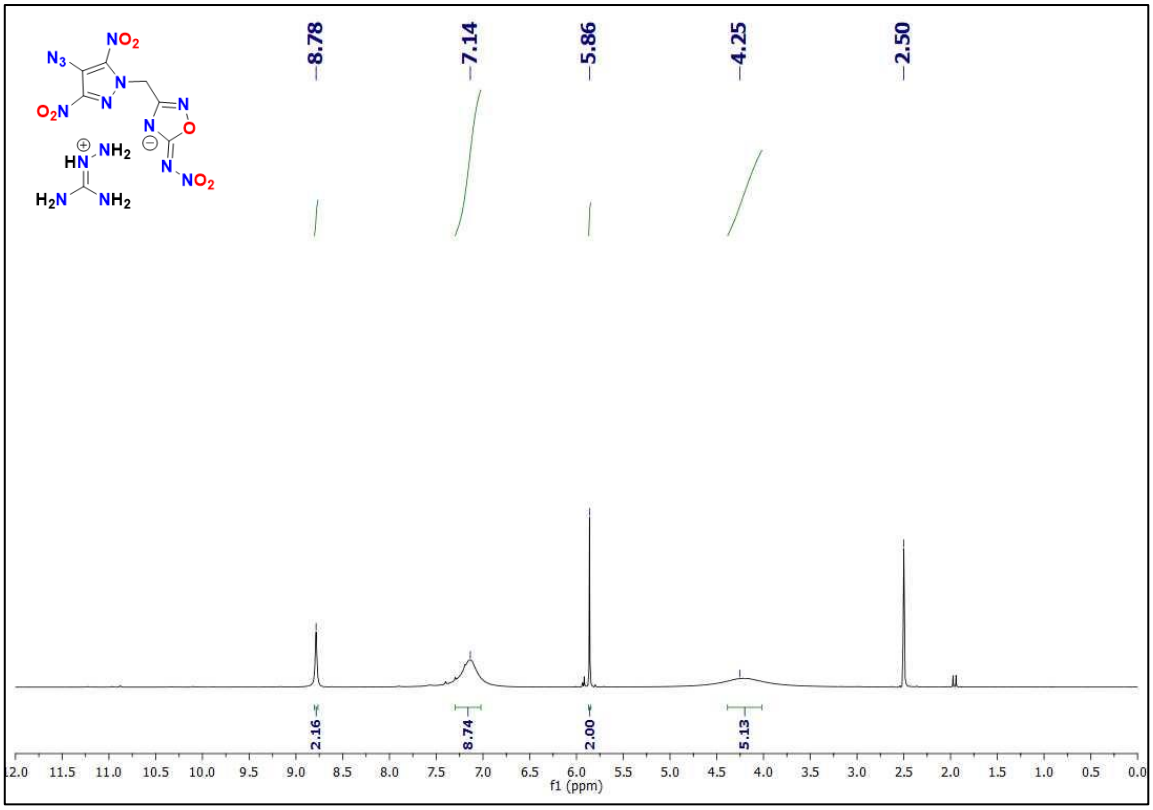


Fig.S29: ^{1}H NMR Spectra of compound **15**

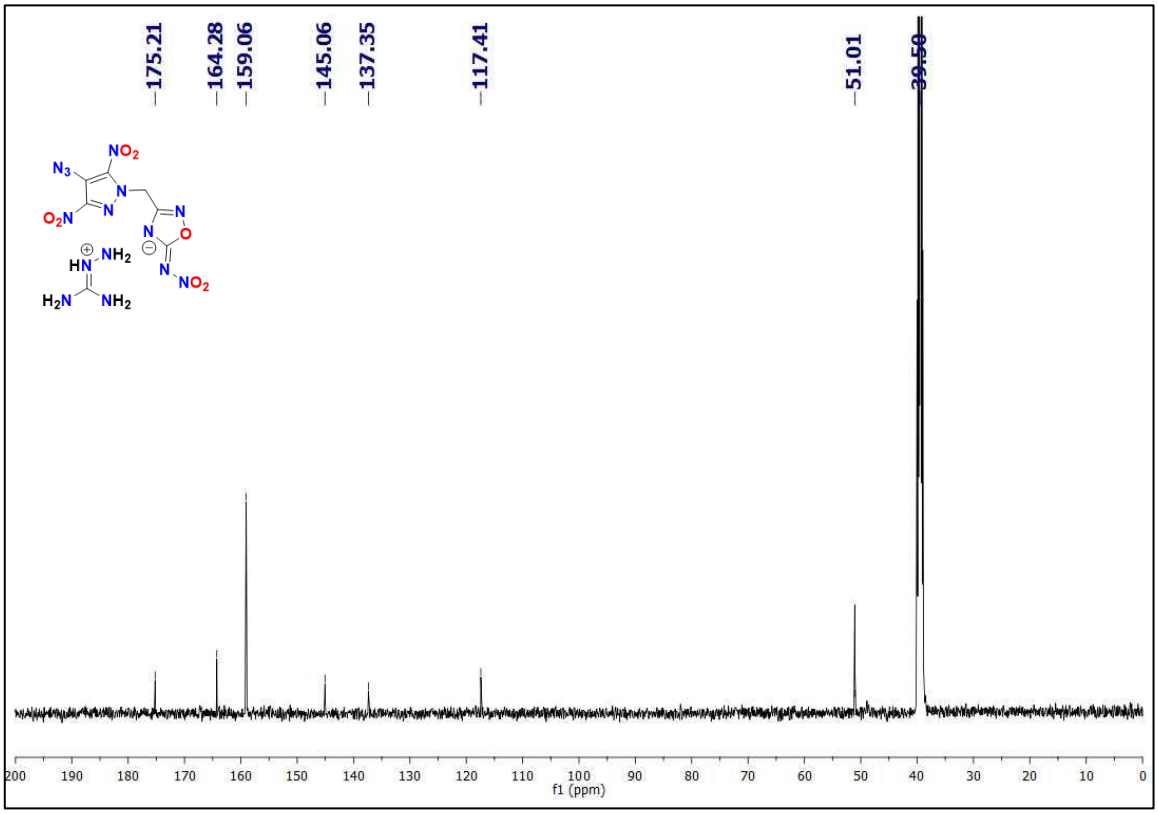


Fig.S30: ^{13}C{^{1}H}NMR Spectra of compound **15**

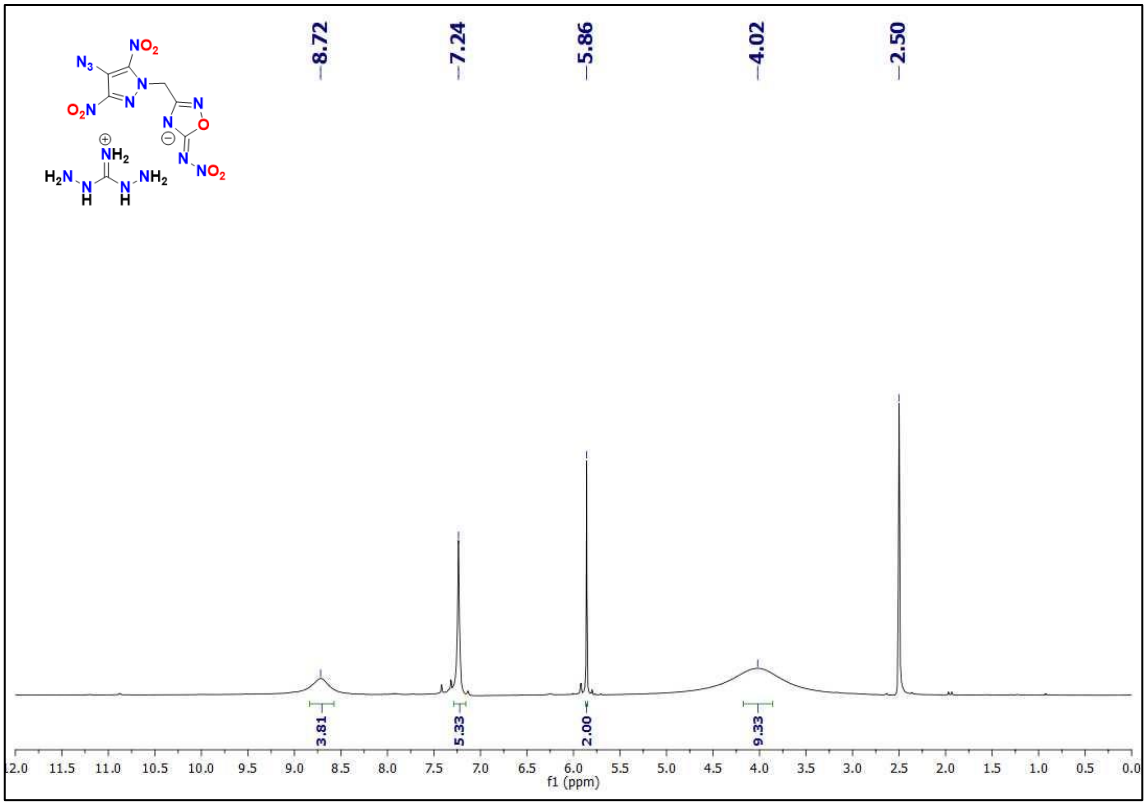


Fig.S31: ^{1}H NMR Spectra of compound **16**

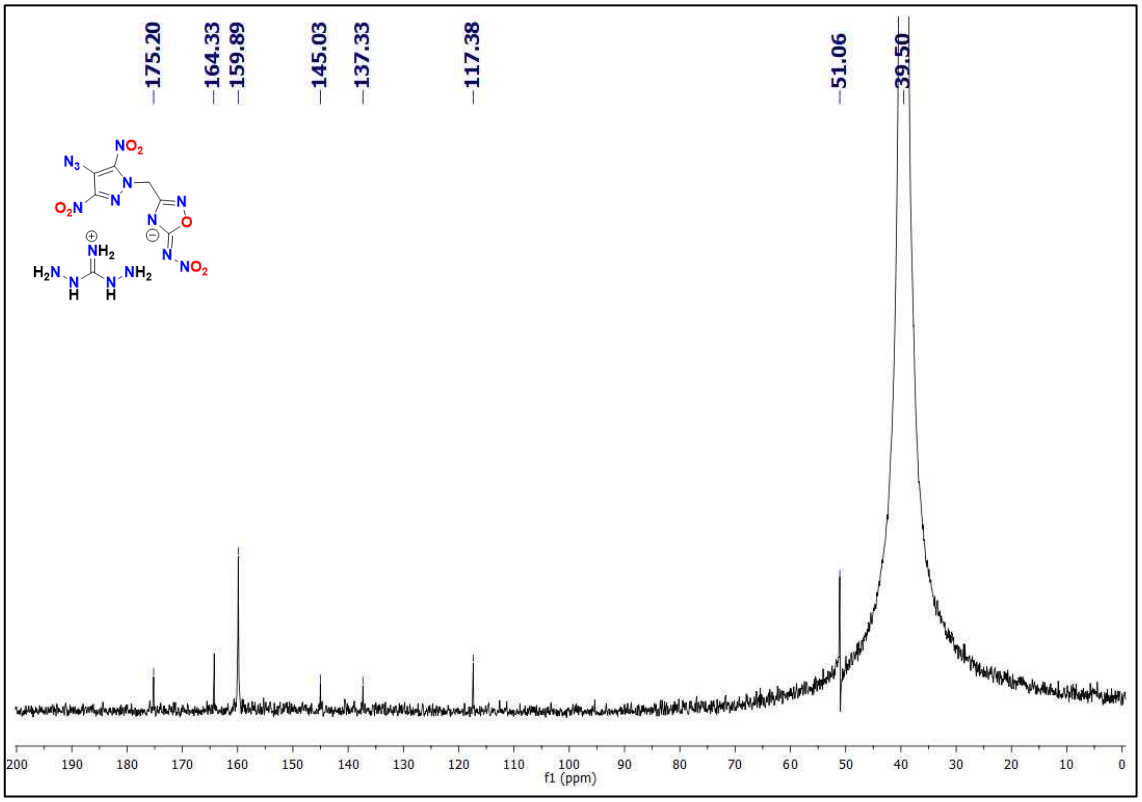


Fig.S32: ^{13}C{^{1}H}NMR Spectra of compound **16**

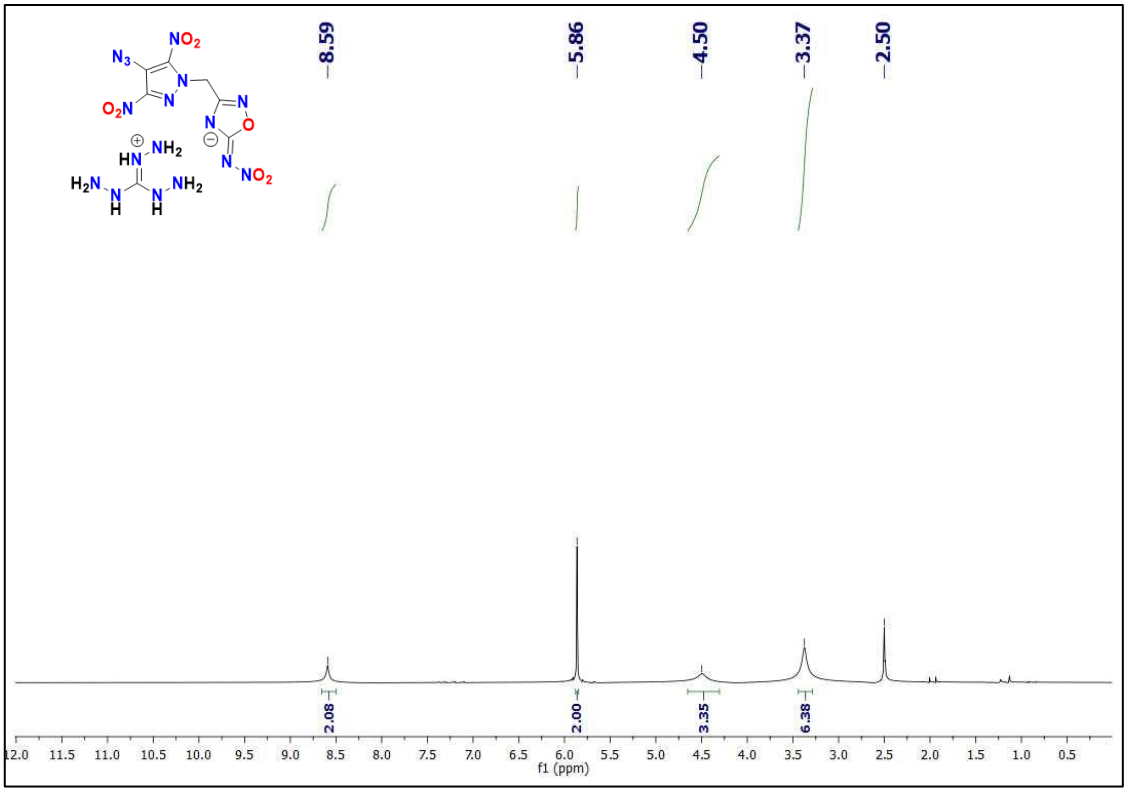


Fig.S33: ^{1}H NMR Spectra of compound **17**

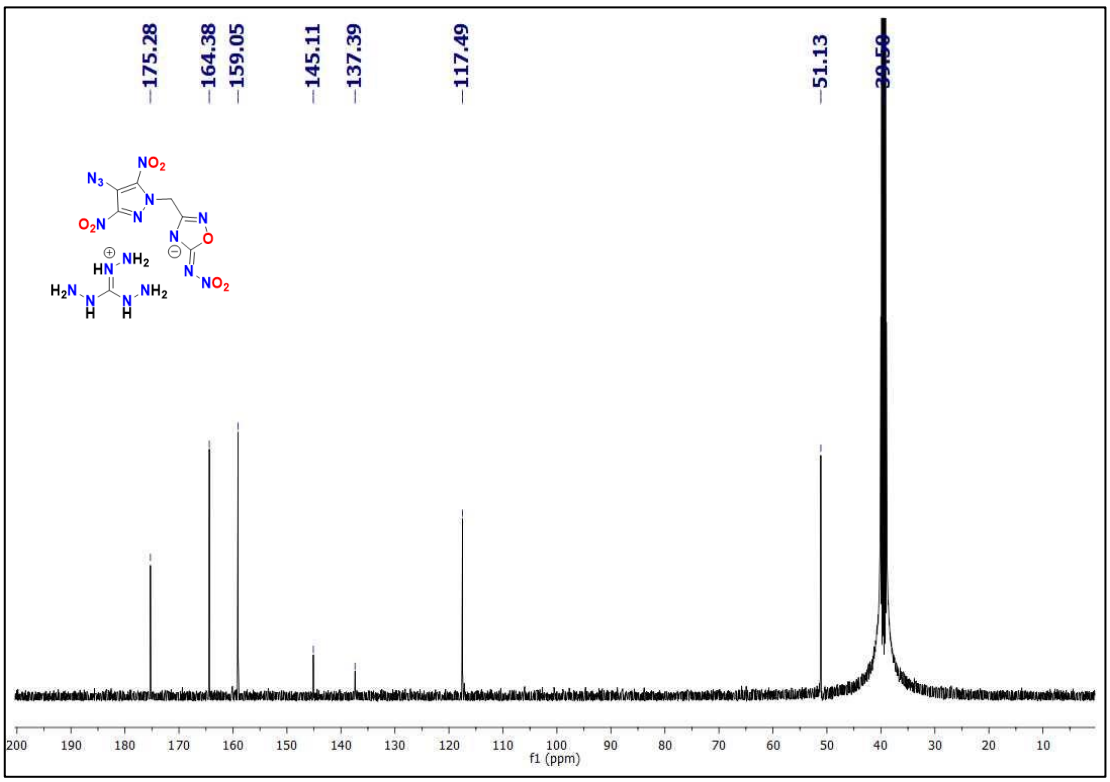


Fig.S34: ^{13}C{^{1}H}NMR Spectra of compound **17**

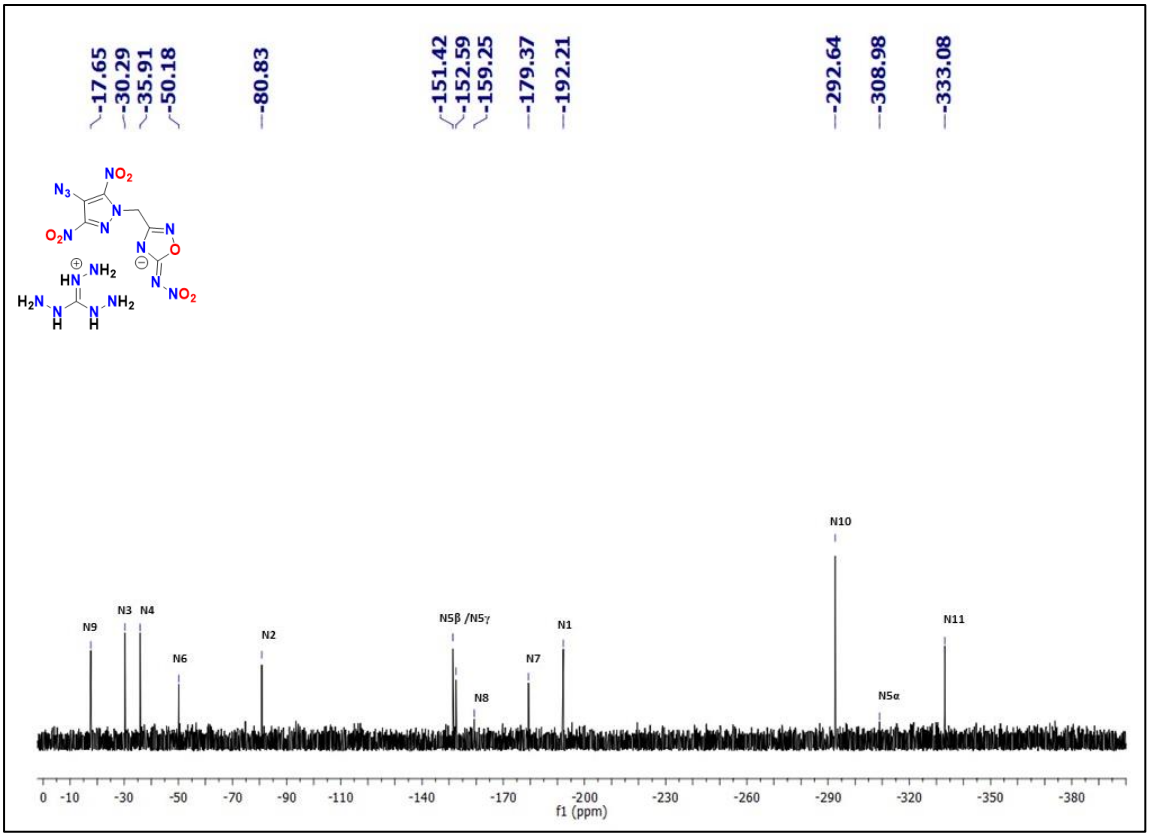


Fig.S35: ^{15}N NMR Spectra of compound **17**

IR Spectra:

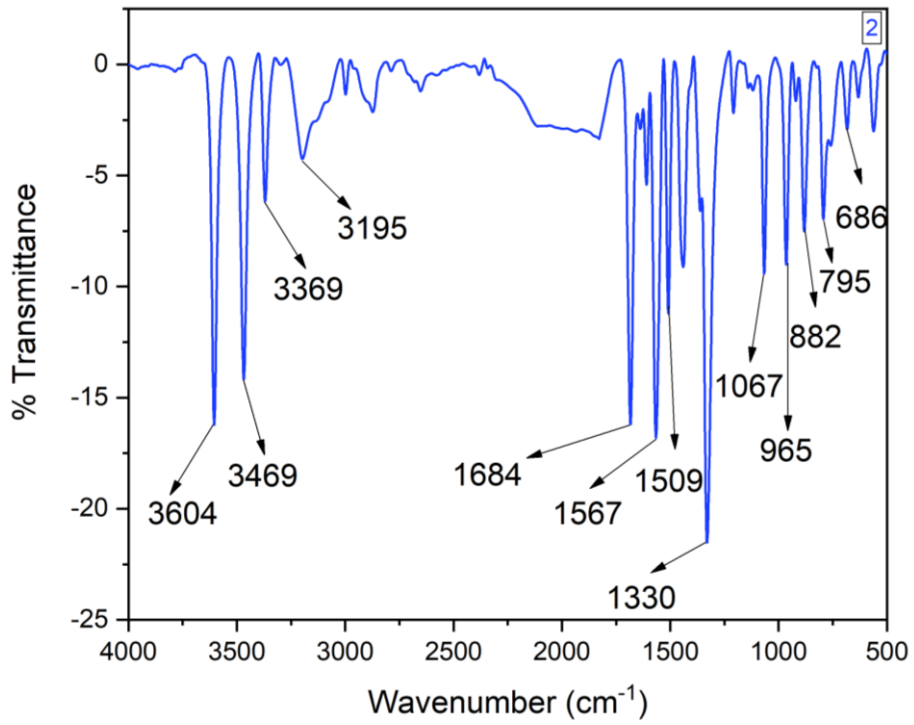


Fig.S36: FTIR Spectra of compound **2**

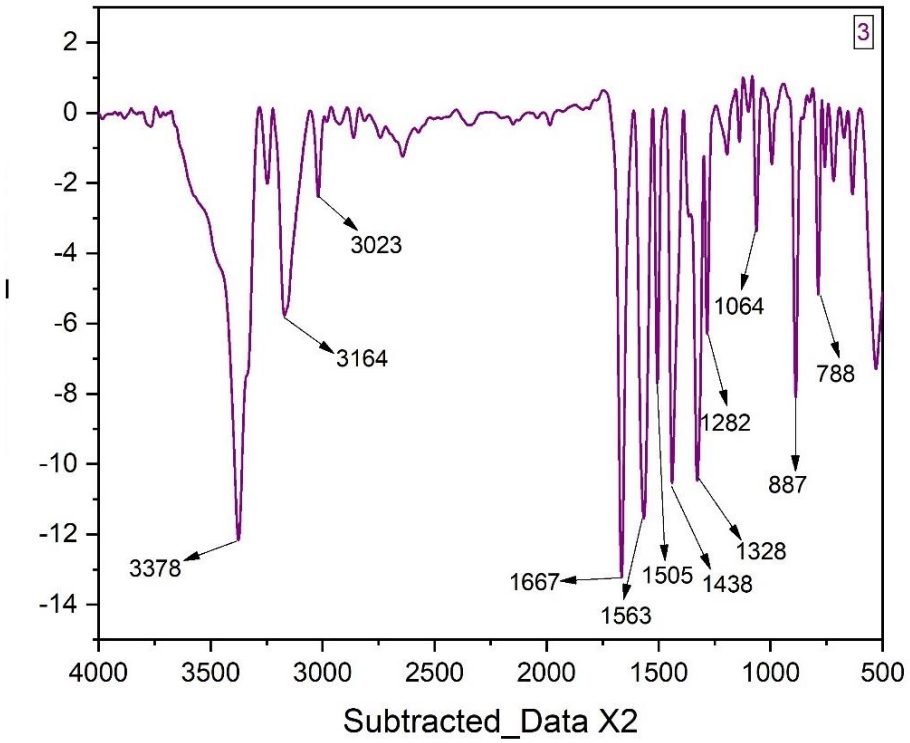


Fig.S37: FTIR Spectra of compound **3**

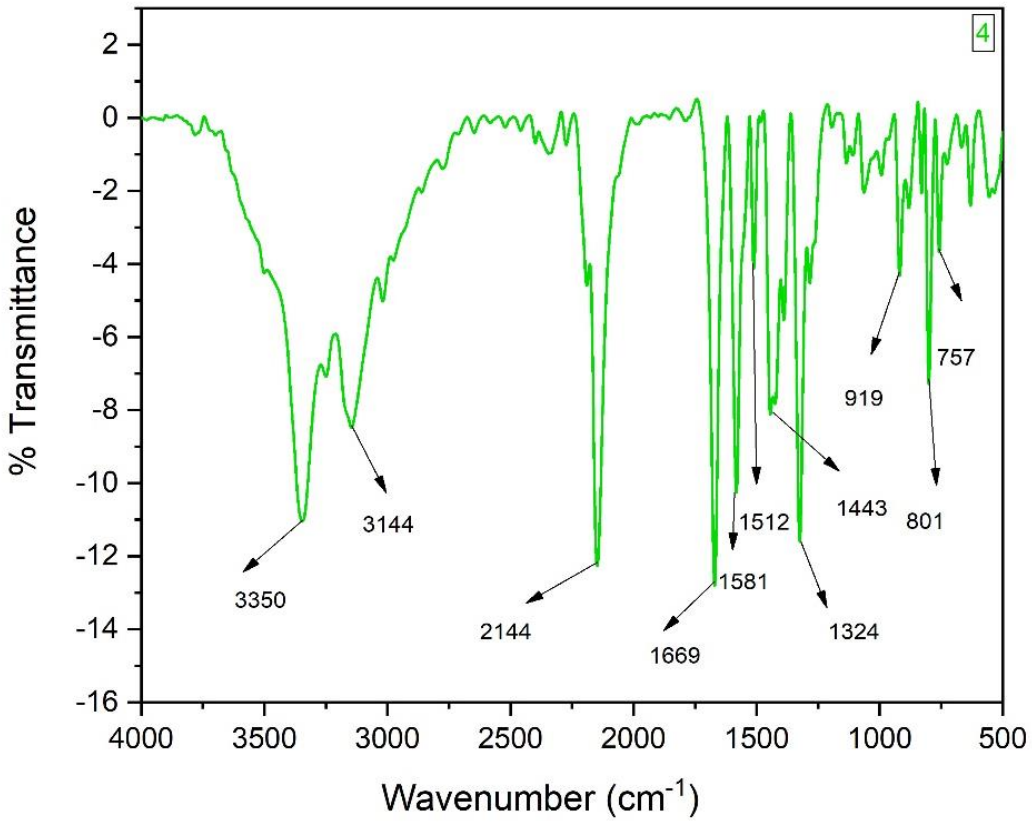


Fig.S38: FTIR Spectra of compound **4**

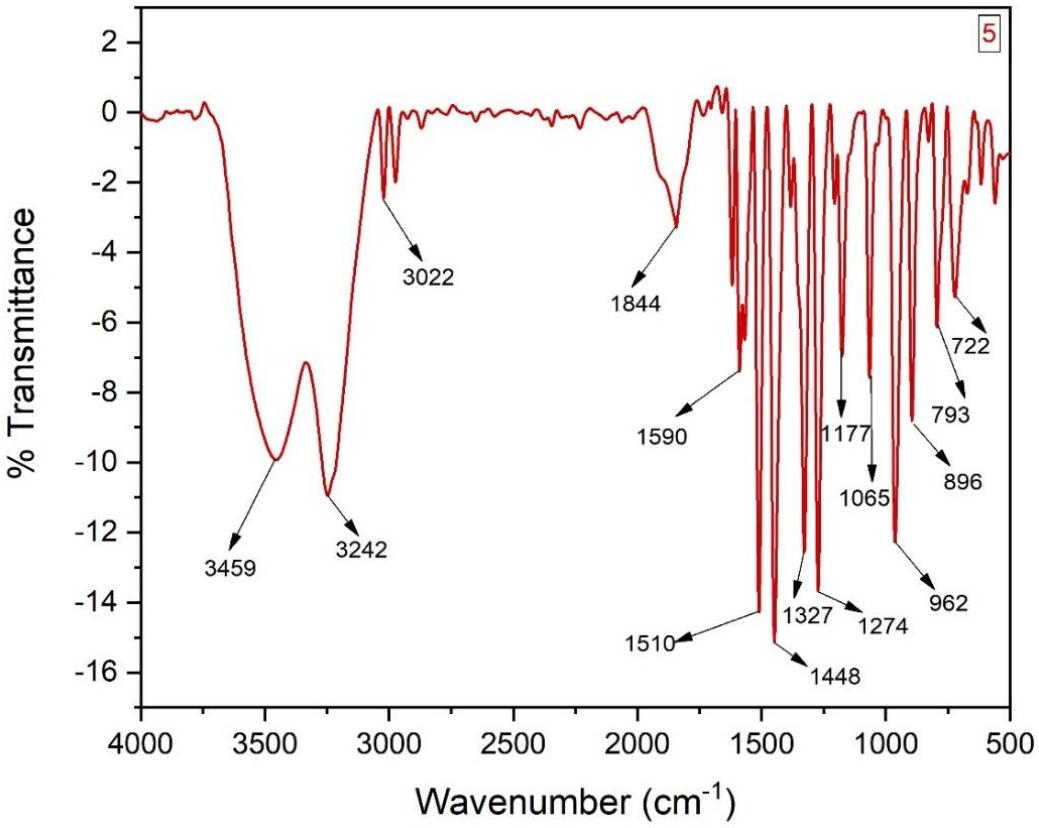


Fig.S39: FTIR Spectra of compound **5**

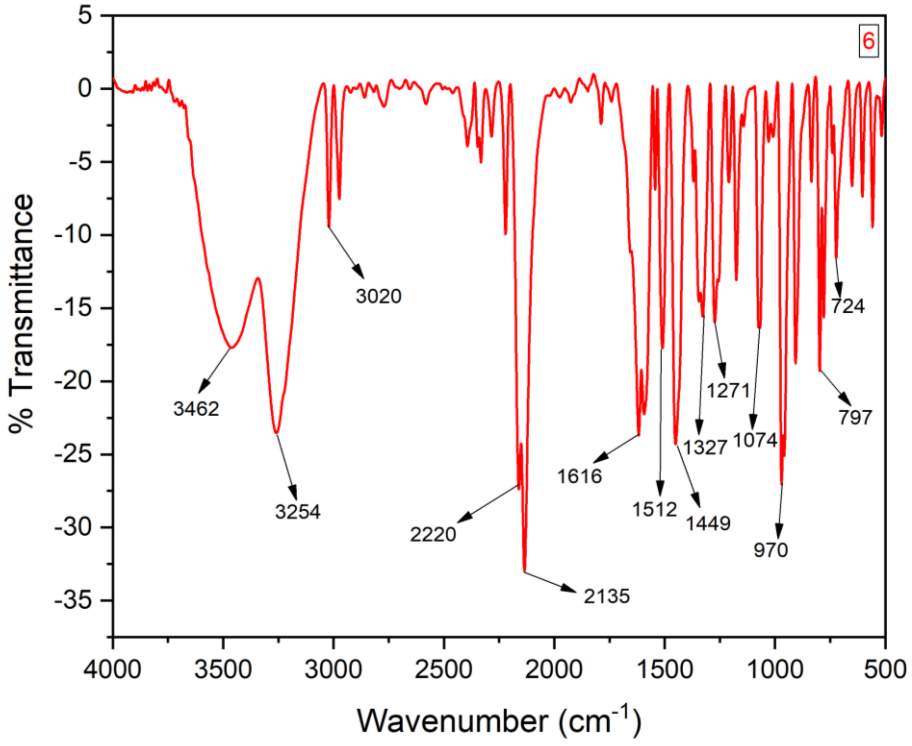


Fig.S40: FTIR Spectra of compound **6**

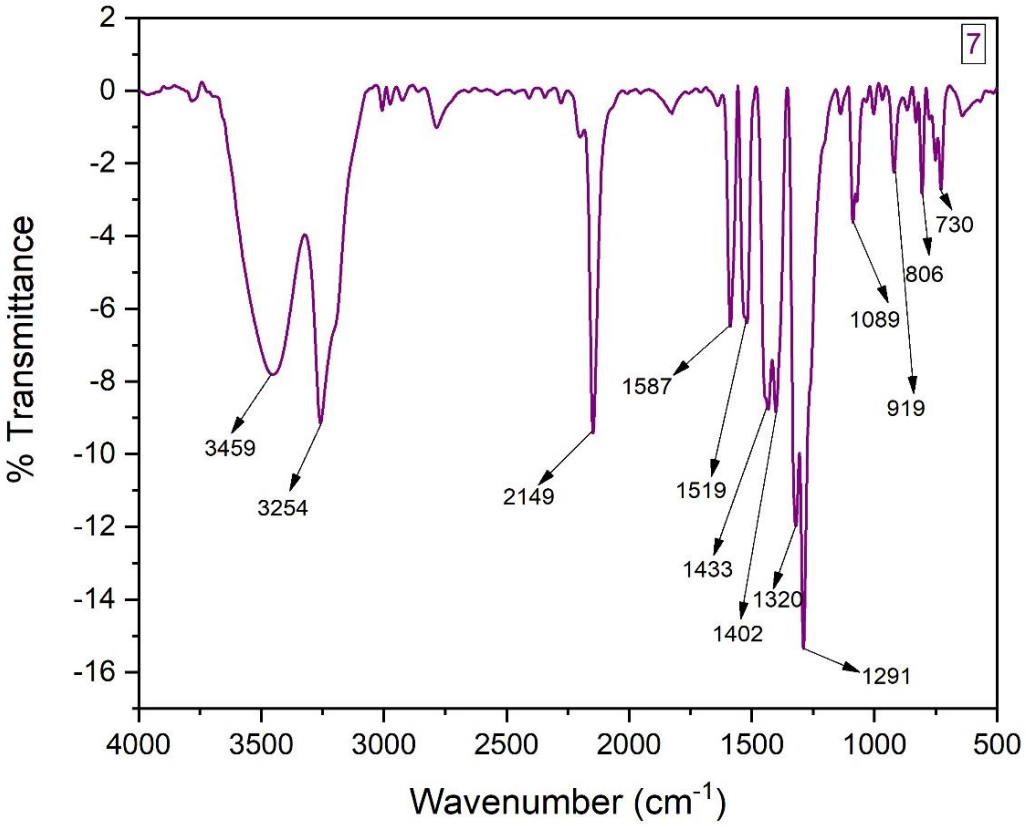


Fig.S41: FTIR Spectra of compound **7**

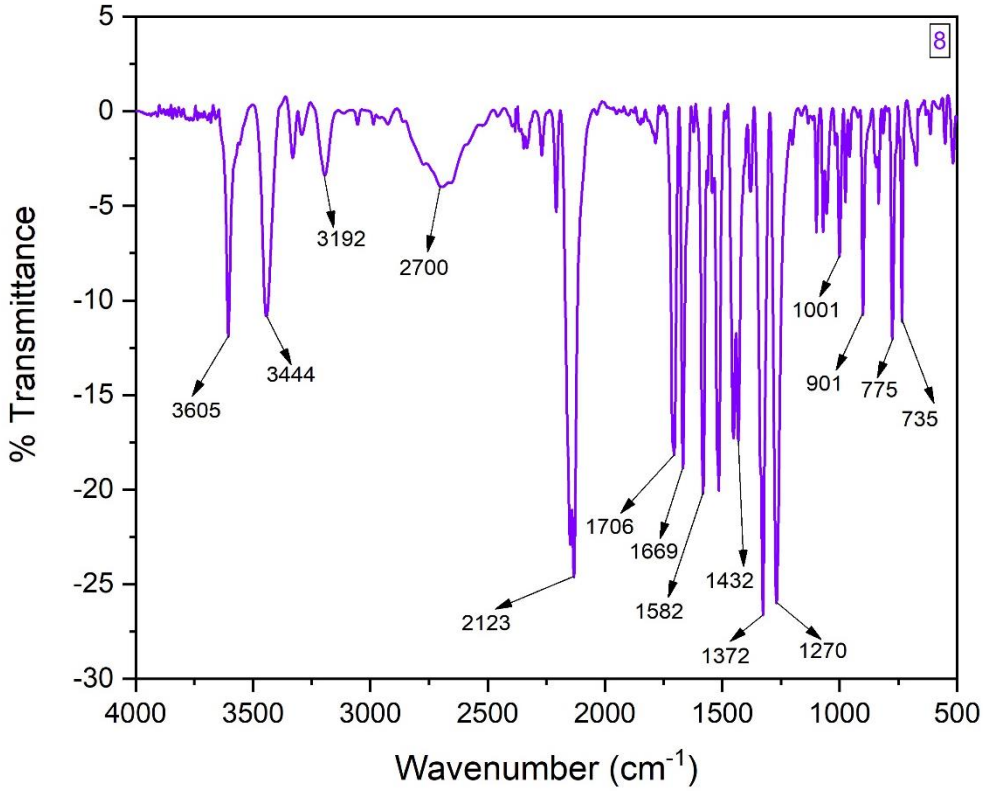


Fig.S42: FTIR Spectra of compound **8**

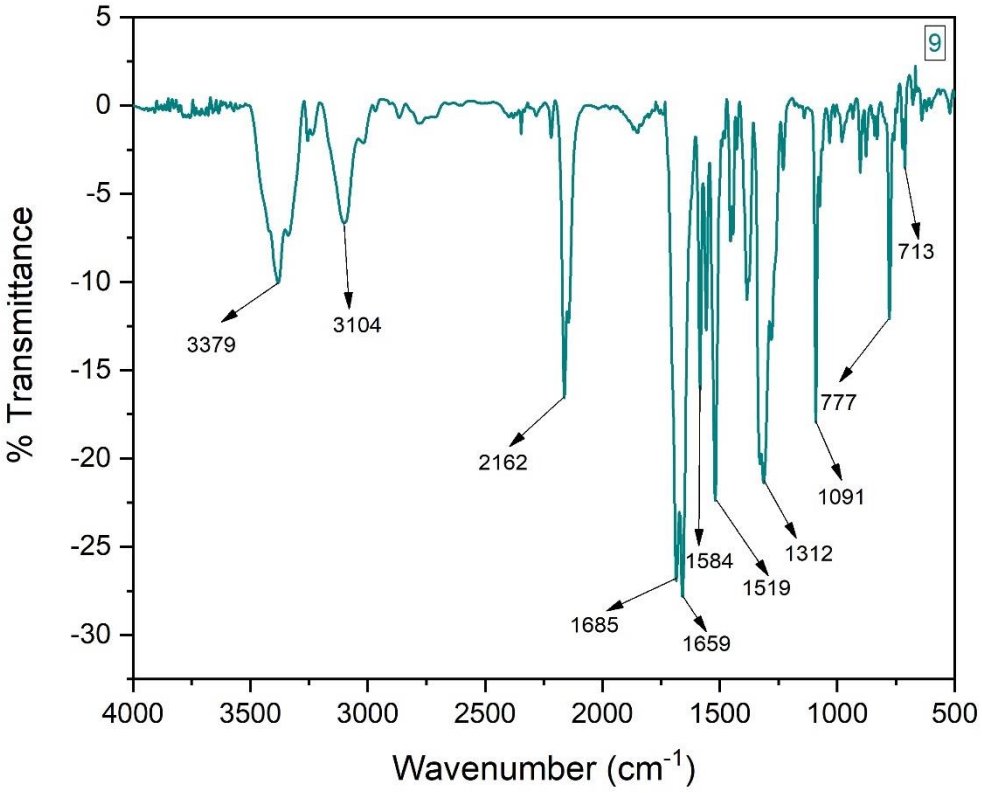


Fig.S43: FTIR Spectra of compound **9**

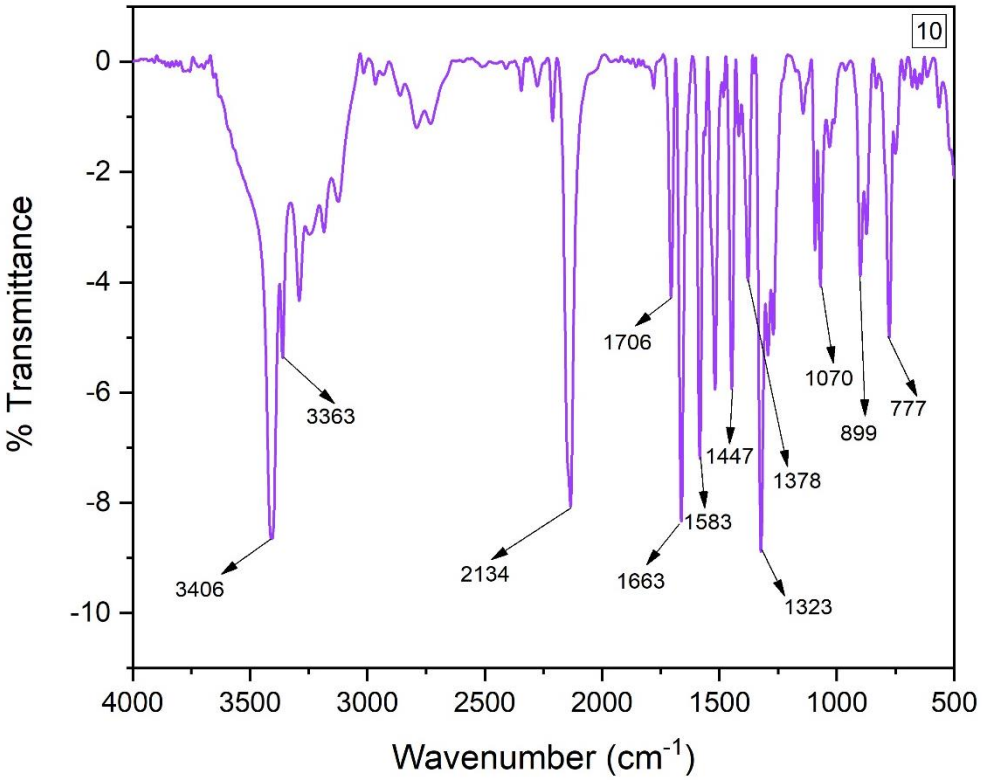


Fig.S44: FTIR Spectra of compound **10**

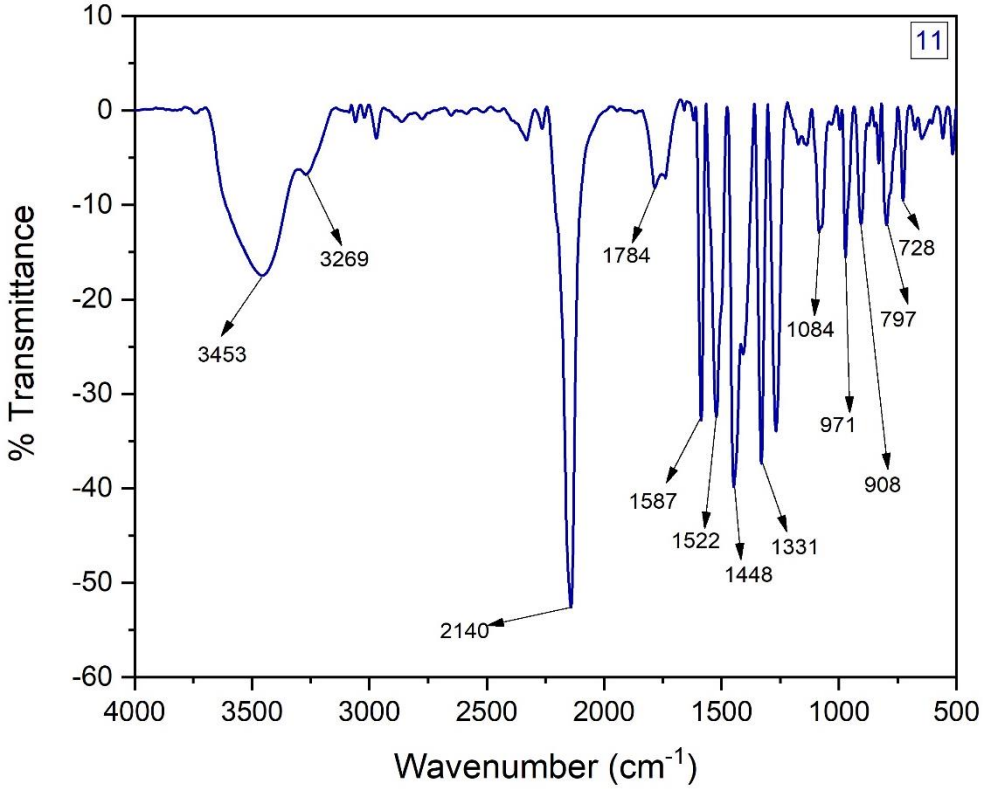


Fig.S45: FTIR Spectra of compound **11**

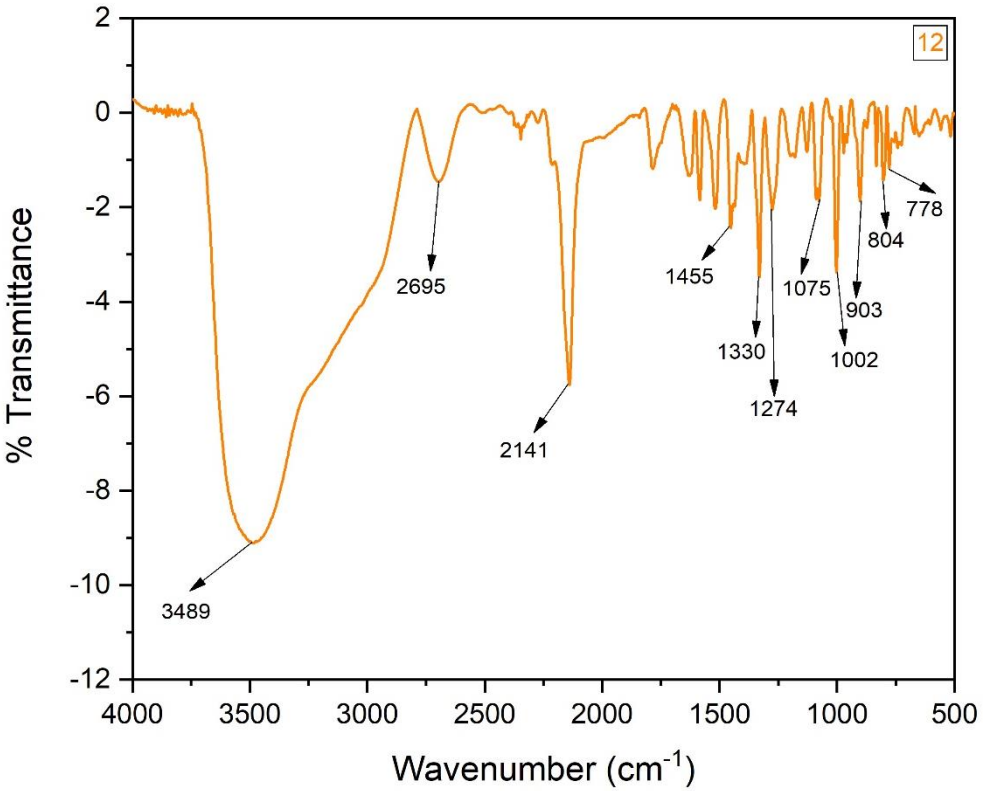


Fig.S46: FTIR Spectra of compound **12**

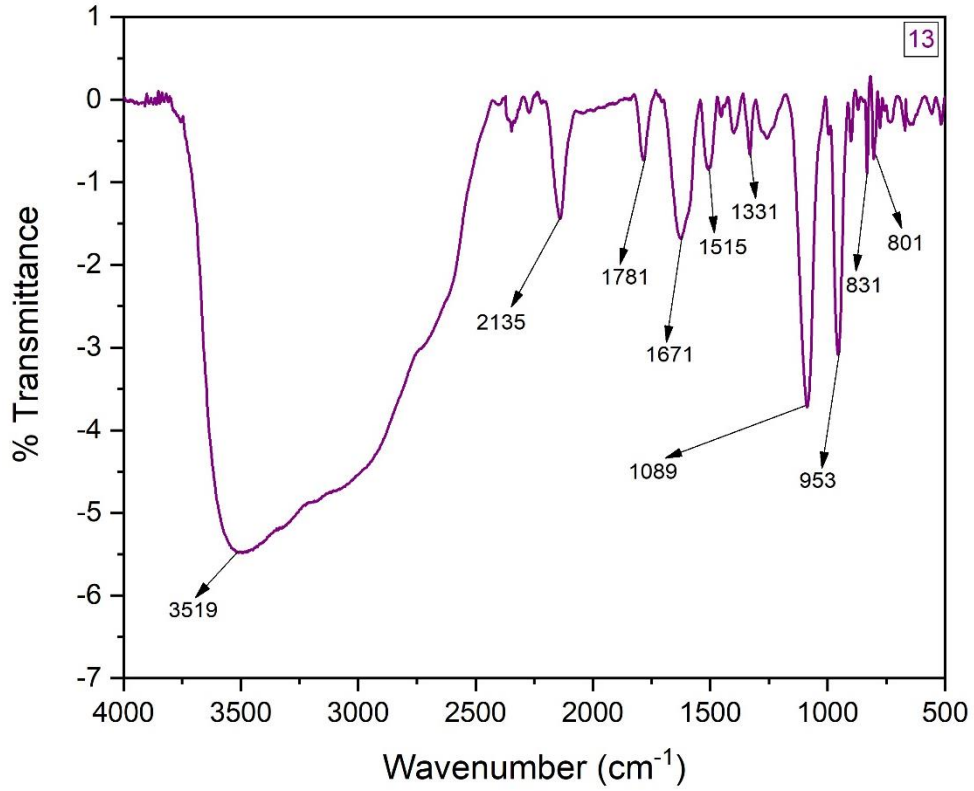


Fig.S47: FTIR Spectra of compound **13**

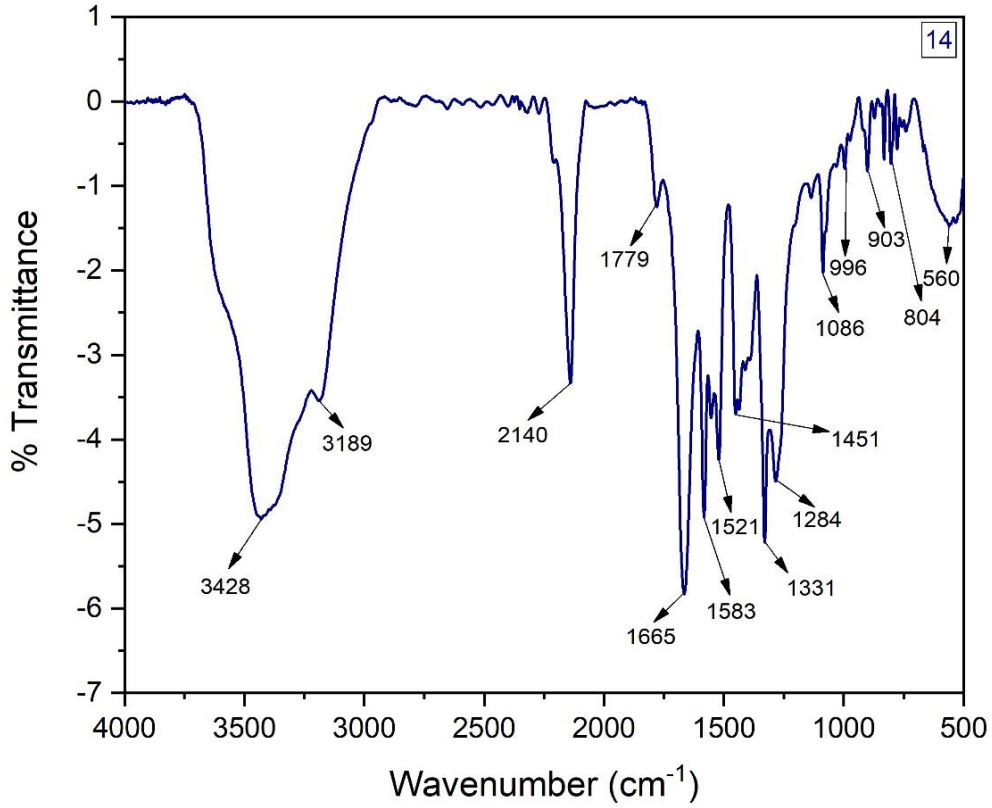


Fig.S48: FTIR Spectra of compound **14**

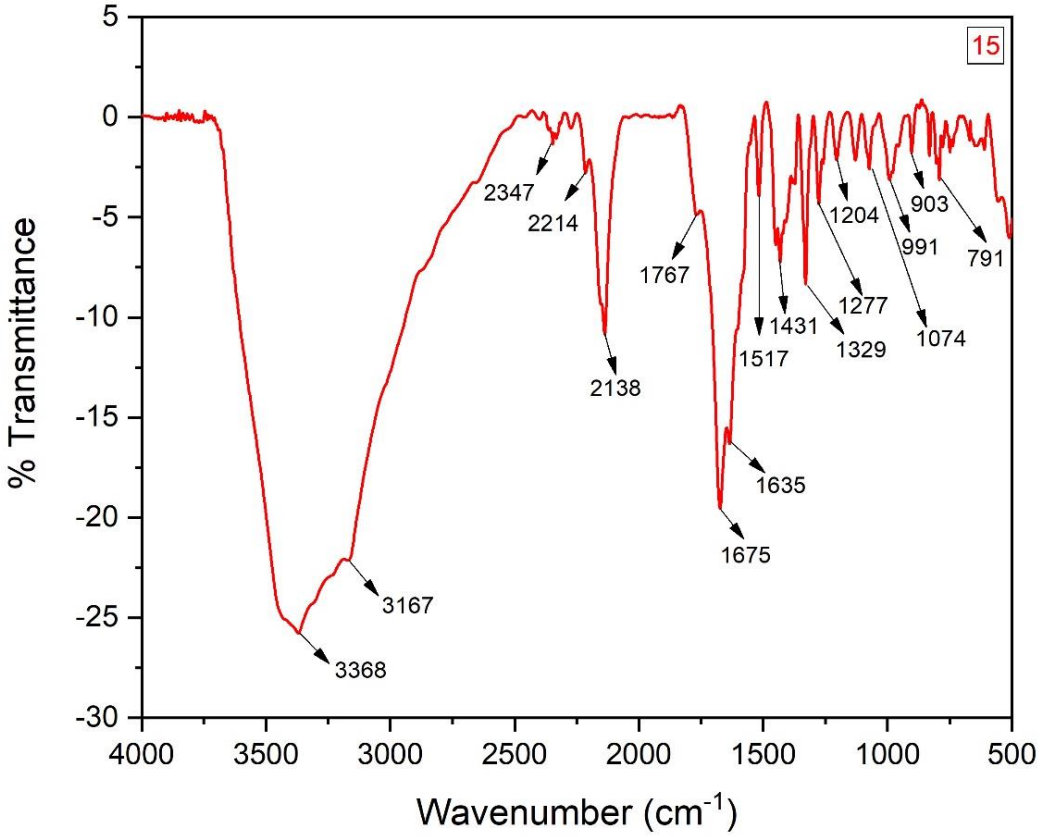


Fig.S49: FTIR Spectra of compound **15**

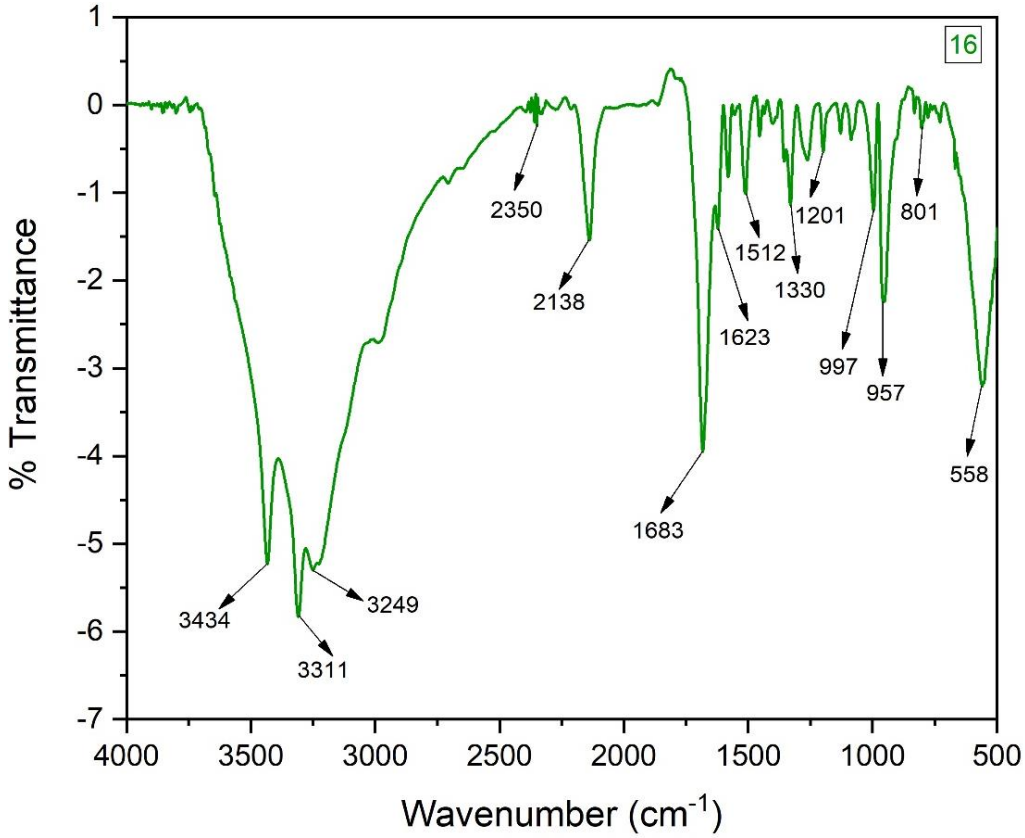


Fig.S50: FTIR Spectra of compound **16**

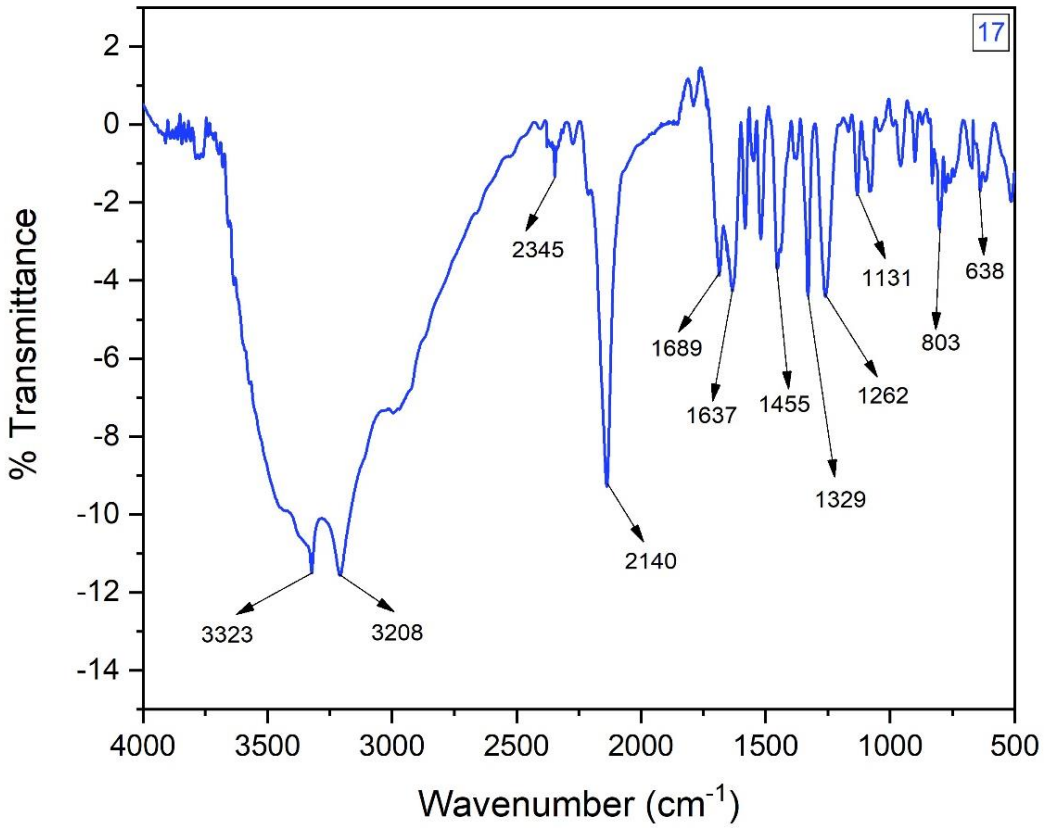


Fig.S51: FTIR Spectra of compound **17**

Mass Spectra:

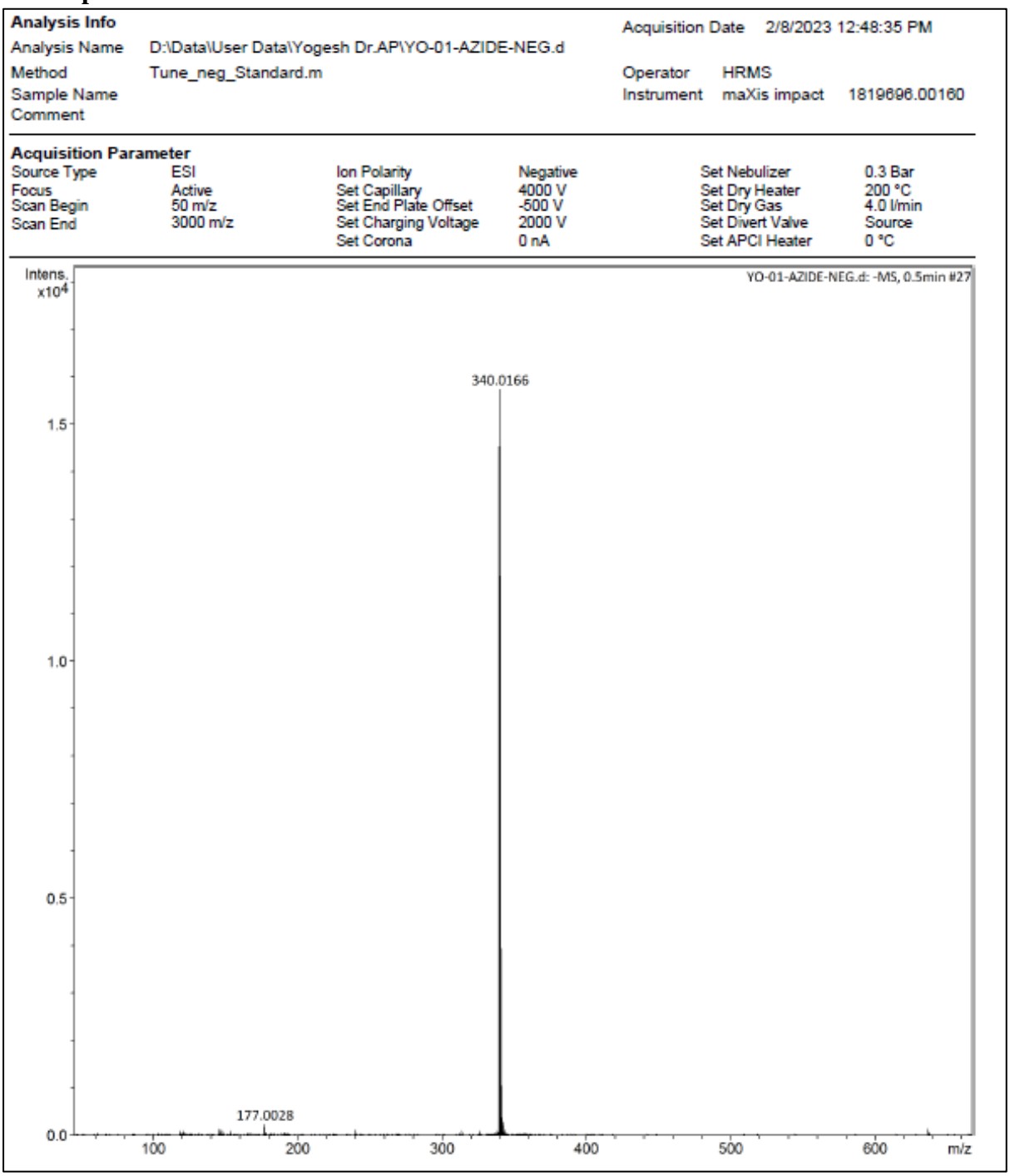


Fig.S52: Mass spectrum of compound **6**

Thermal Analysis

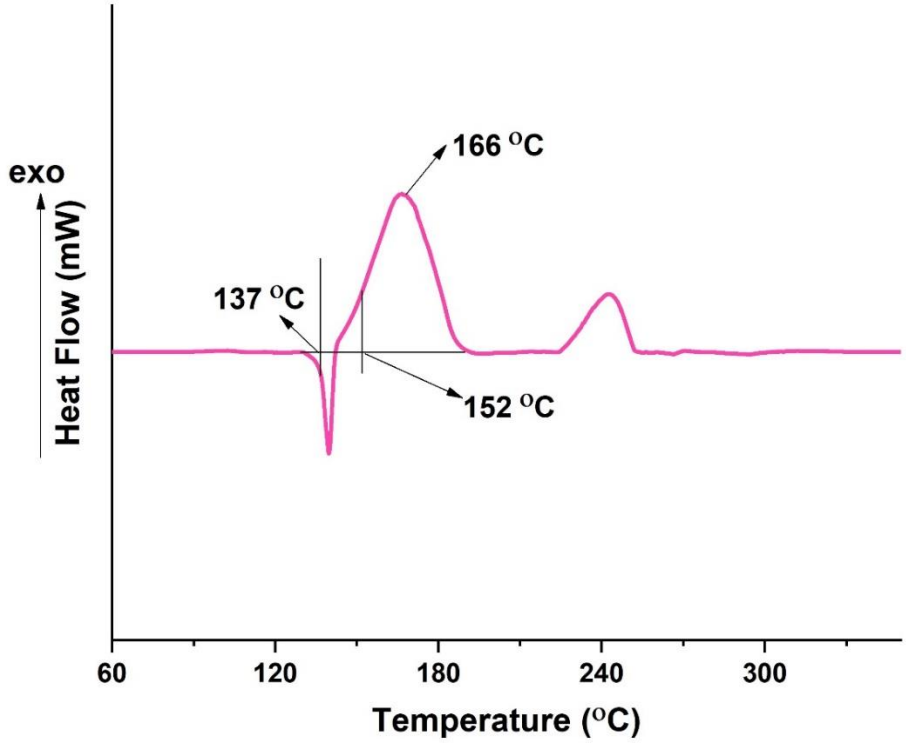


Fig.S53: DSC curve of compound **4**

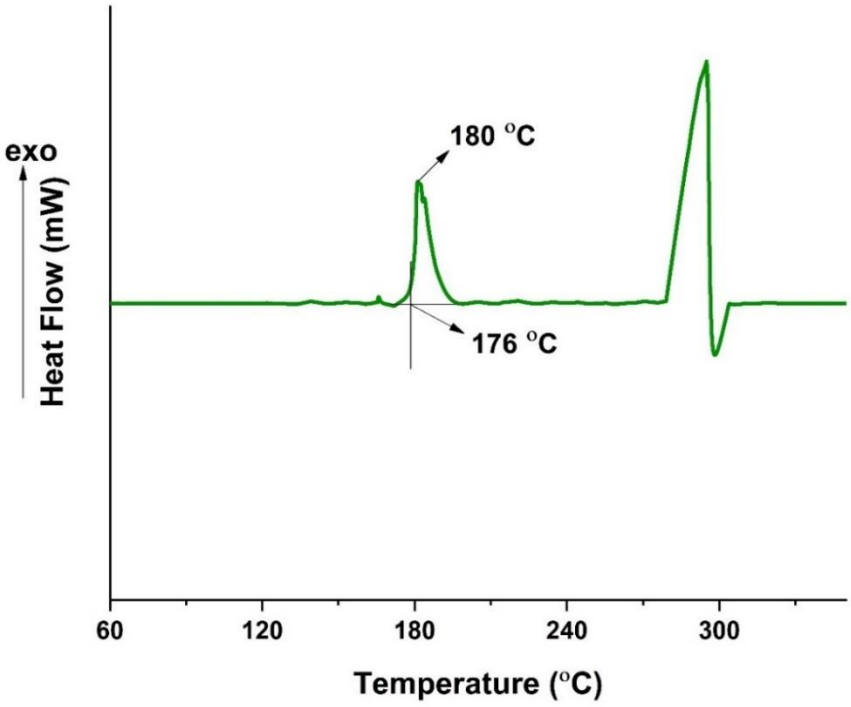


Fig.S54: DSC curve of compound **5**

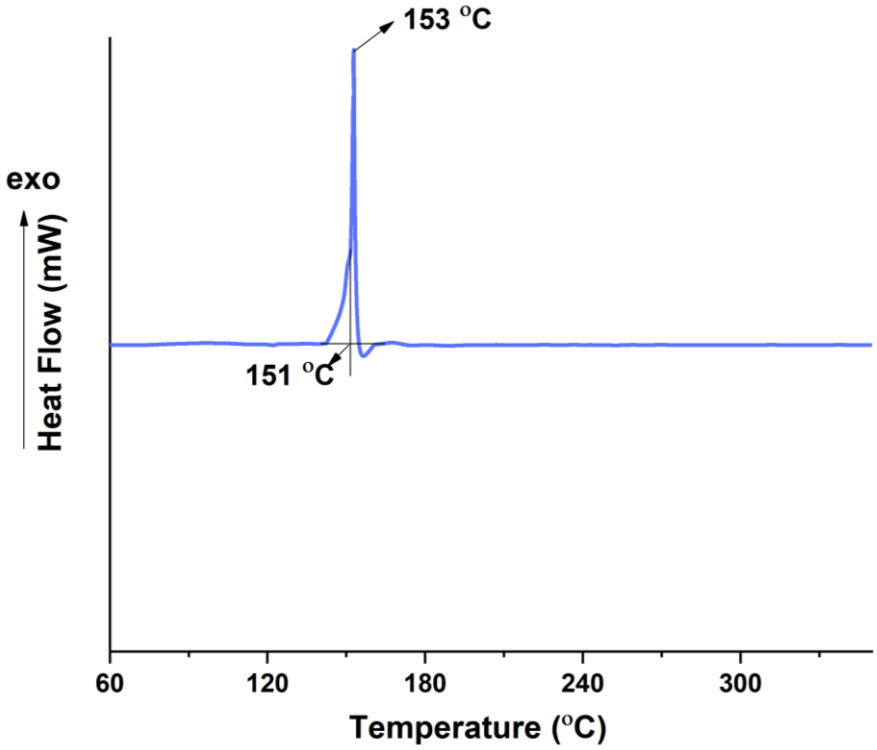


Fig.S55: DSC curve of compound **6**

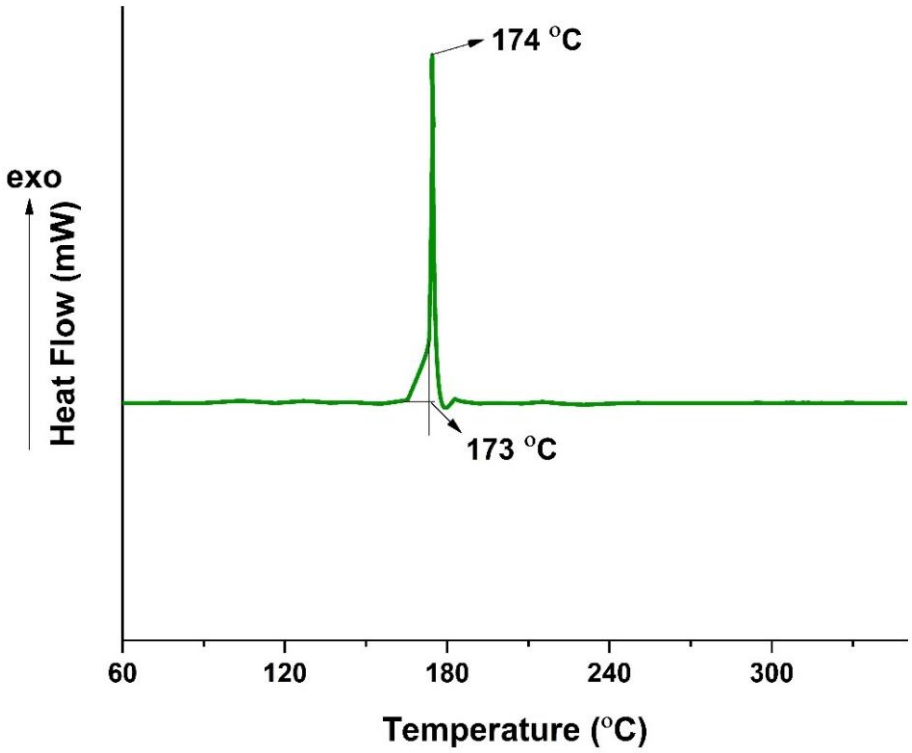


Fig.S56: DSC curve of compound **7**

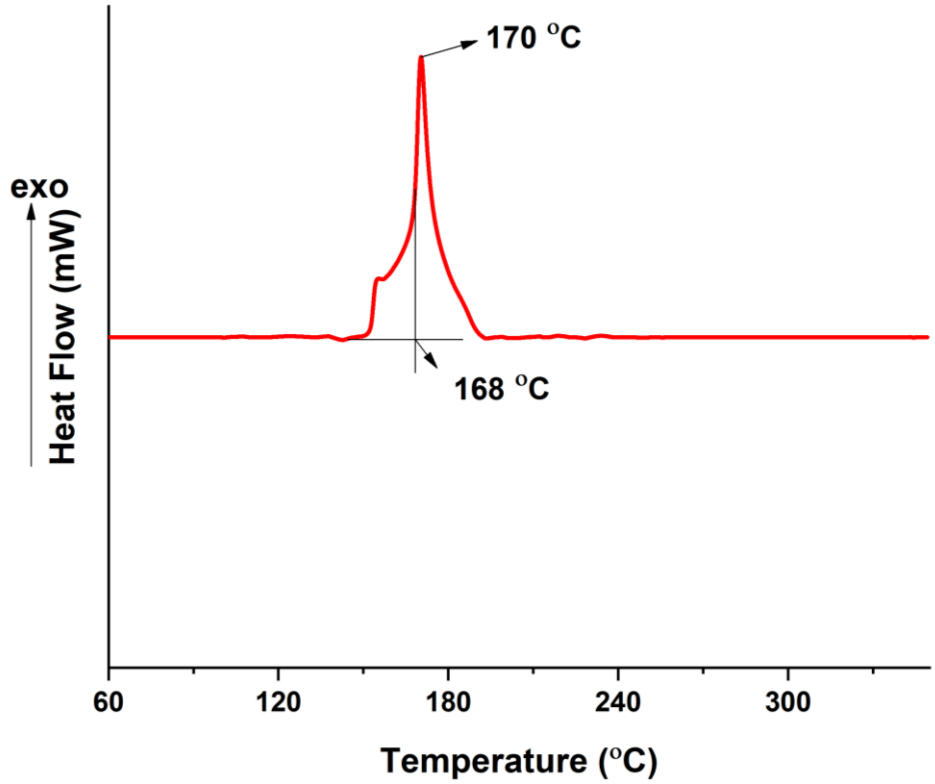


Fig.S57: DSC curve of compound **8**

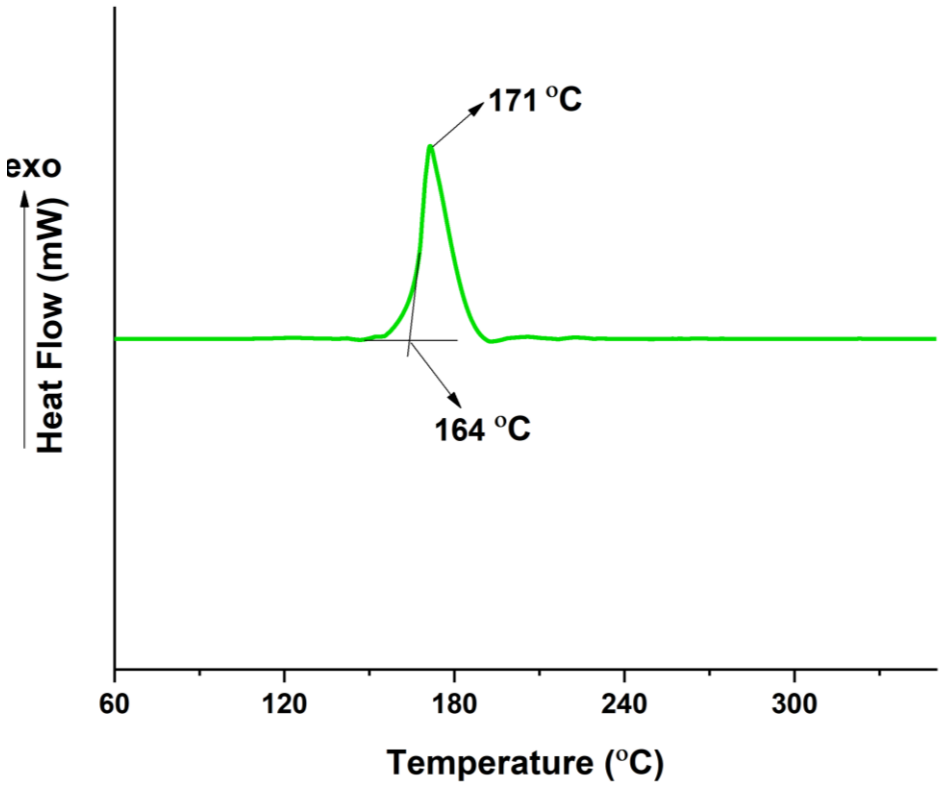


Fig.S58: DSC curve of compound **9**

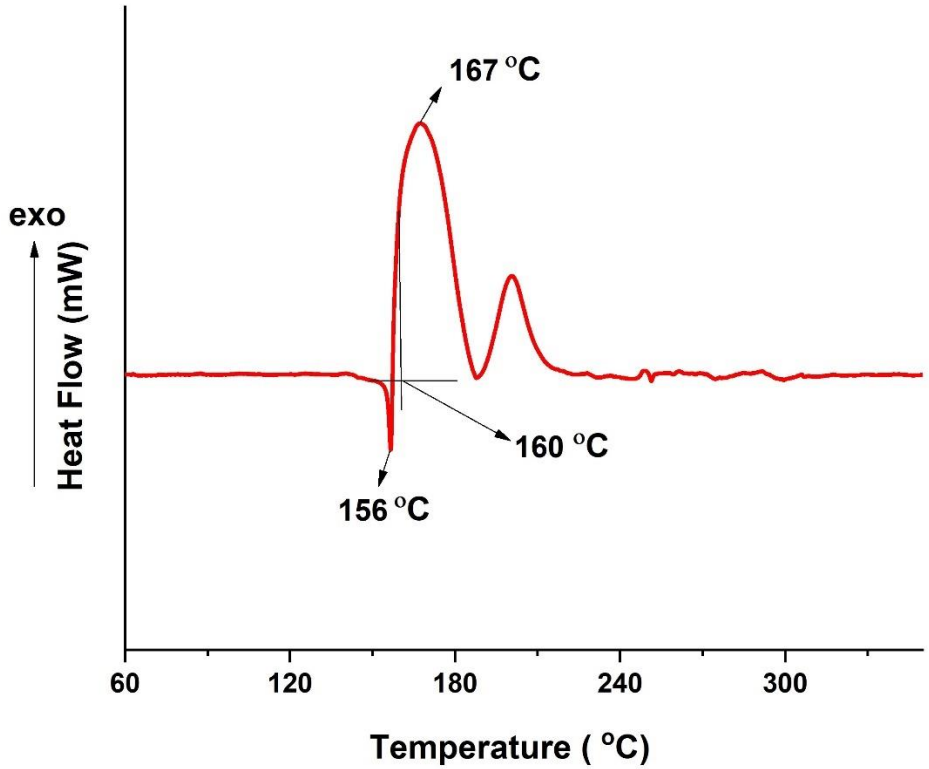


Fig.S59: DSC curve of compound **10**

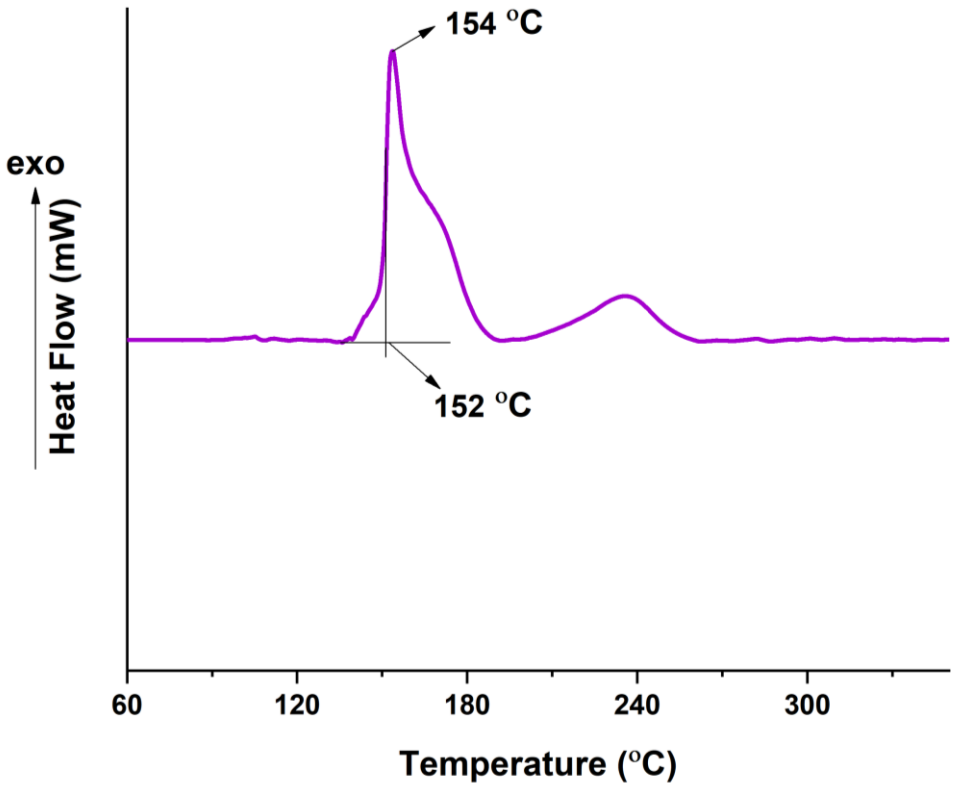


Fig.S60: DSC curve of compound **12**

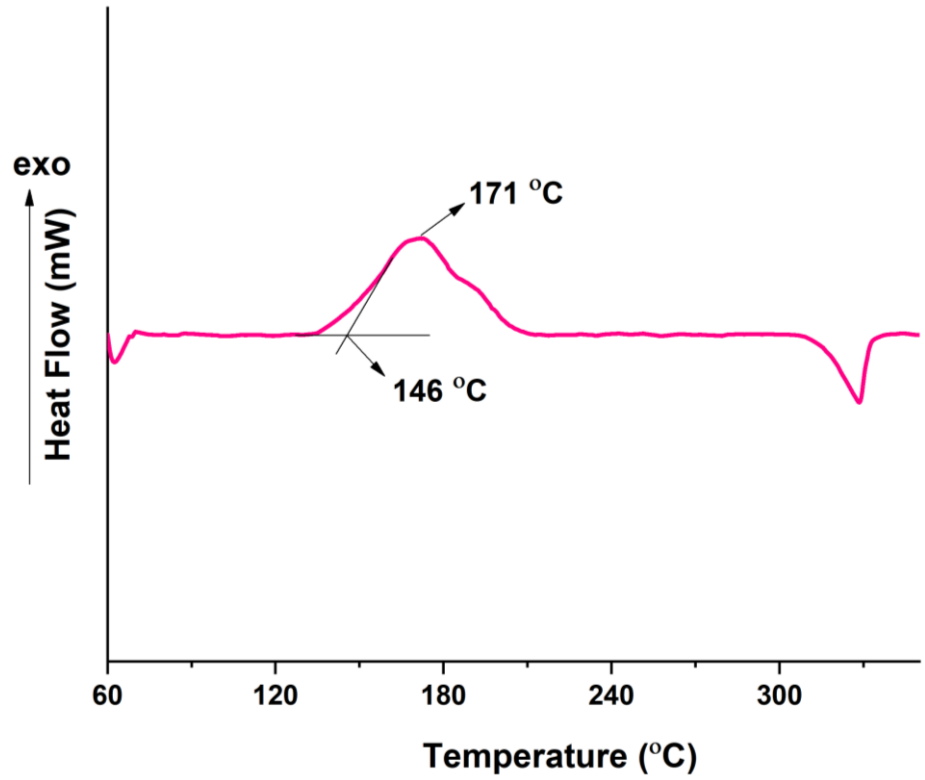


Fig.S61: DSC curve of compound **13**

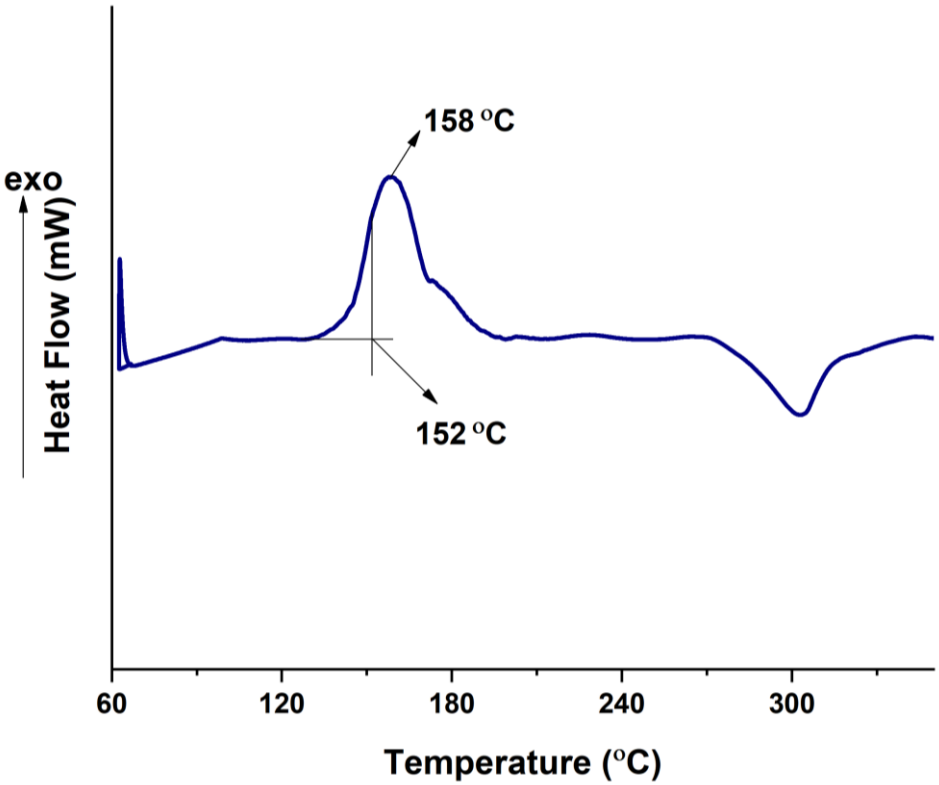


Fig.S63: DSC curve of compound **15**

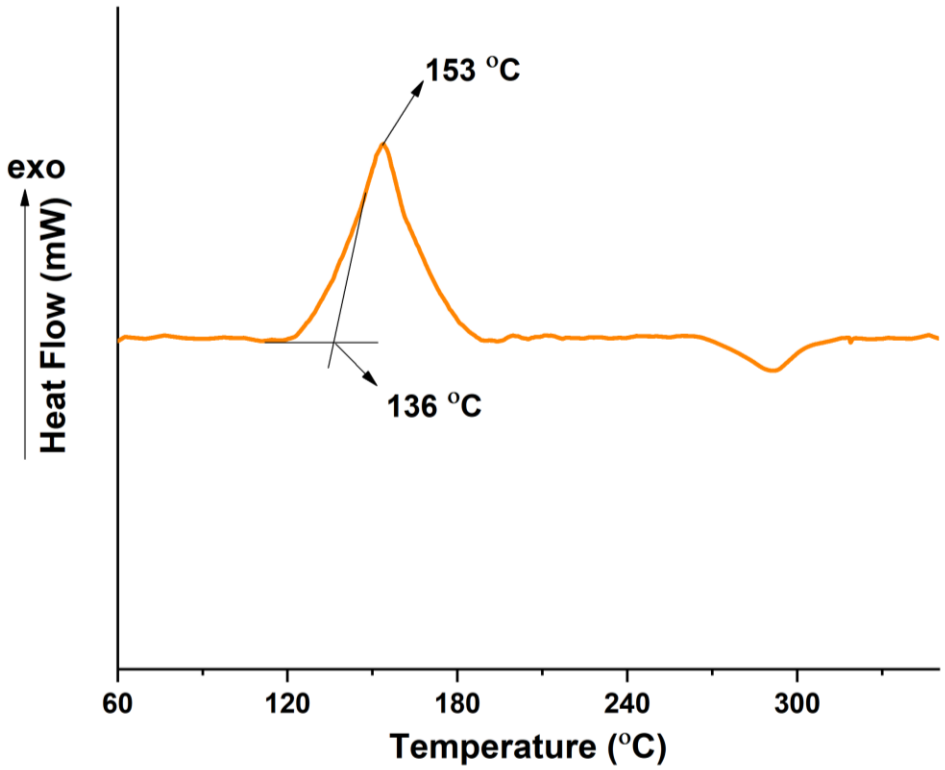


Fig.S64: DSC curve of compound **16**

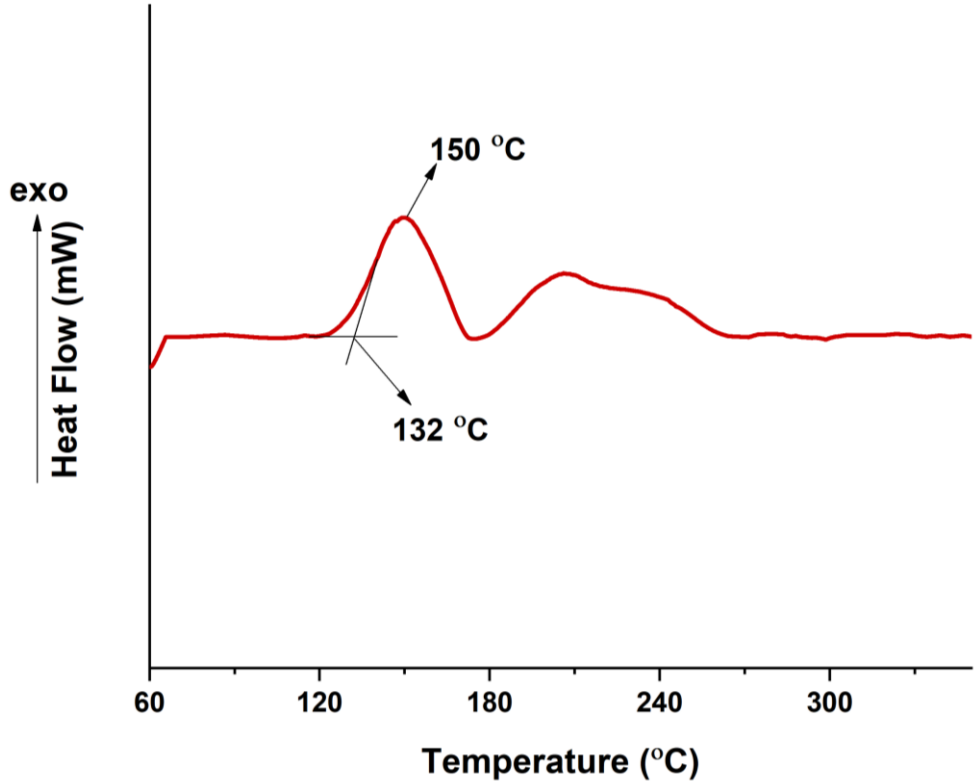


Fig.S65: DSC curve of compound **17**