

Supporting information (SI)

Synthesis of C-C bonded Trifluoromethyl based High Energy Density

Materials via ANRORC Mechanism

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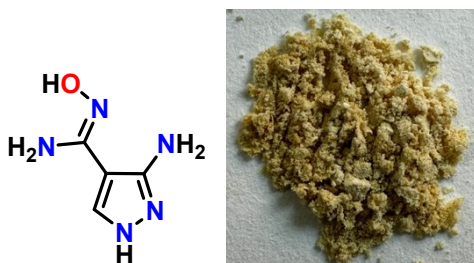
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Caution! All the compounds investigated are potentially explosive, energetic materials. Although we have experienced no difficulties in syntheses and characterization of these compounds, manipulations must be carried out by using appropriate standard safety precautions. Eye protection and leather gloves must be always worn.

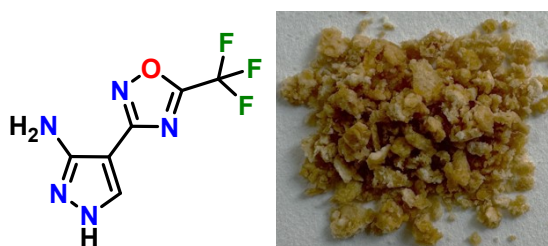
General Methods

Reagents were purchased from Ak Scientifics, Acros Organics or Aldrich as analytical grade and were used as received. ^1H NMR, ^{13}C NMR spectra were recorded using JEOL DELTA (ECS) 500 (^1H , 500 MHz; ^{13}C , 126 MHz; ^{19}F , 471 MHz) and JEOL DELTA (ECS) 400 (^1H , 400 MHz; ^{13}C , 101 MHz; ^{19}F , 373 MHz) nuclear magnetic resonance spectrometer. DMSO- d_6 was employed as the solvent and locking solvent. Chemical shifts are given relative to $(\text{CH}_3)_4\text{Si}$ for ^1H and ^{13}C spectra and CFCl_3 for ^{19}F . Decomposition temperatures (onset) were recorded using a dry nitrogen gas purge and at heating rate of $5\text{ }^\circ\text{C min}^{-1}$ on a differential scanning calorimeter (SDT650). IR spectra were recorded using Zn-Se pellets with ECO-ATR spectrometer (Bruker Alpha II). HRMS was recorded on a Quadrupole Time-of-Flight (TOF) Mass Spectrometry. Density was determined at room temperature by employing Anton Par Ultra5000 gas pycnometer in helium atmosphere. Impact and friction-sensitivity measurements were tested by employing a standard BAM Fall hammer and a BAM friction tester. The single-crystal X-ray data collection was carried out using Bruker APEX-II CCD diffractometer. The crystal was kept at 100 K during data collection.

Experimental Section



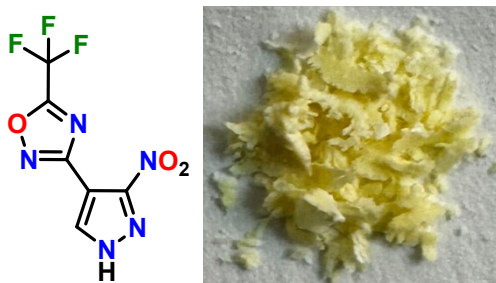
Synthesis of 3-amino-*N'*-hydroxy-1*H*-pyrazole-4-carboximidamide (2)^[2]: 3-amino-1*H*-pyrazole-4-carbonitrile (**1**) (150 mg, 1.38 mmol) was suspended in ethanol (3 ml) in round-bottom flask and 50 % hydroxyl amine hydrate (0.05 mL, 2.08 mmol) was added dropwise at room temperature. The reaction mixture was refluxed for 12 hours, and the newly formed precipitate was filtered off, washed with cold ethanol, and dried in air to give compound **2** in 92 % yield (180 mg, 1.27 mmol).



Synthesis of 4-(5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl)-1*H*-pyrazol-3-amine (3): 3-amino-*N'*-hydroxy-1*H*-pyrazole-4-carboximidamide (**2**) (100 mg; 0.70 mmol) was added in

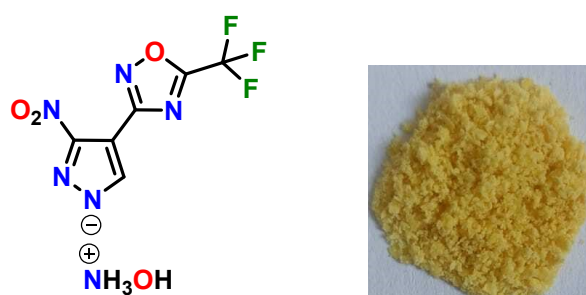
trifluoroacetic anhydride (1 ml) at 0 °C in ice bath for 30 min with continuous stirring and then allowed to stir at room temperature for 30 min and refluxed for 12 hours. Mixture was cooled down to the room temperature and the pH of the solution was adjusted to 9 using saturated sodium bicarbonate solution and extracted using ethyl acetate (3×10 ml). The organic layers were washed with brine and dried over sodium sulfate and evaporated to dryness under reduced pressure to give compound **3** in 80 % yield (124 mg, 0.56 mmol). T_d (onset): 203 °C.

^1H NMR (400MHz, DMSO- d_6): δ (ppm) = 13.72 (1H, br, s), 11.66 (2H, s), 8.63 (1H, s). ^{13}C NMR (101MHz, DMSO- d_6): δ (ppm) = 165.64, 163.61, 142.19, 135.26 (q, $\underline{\text{C}}\text{-CF}_3$, $J_{\text{C-F}}=43$ Hz), 116.53 (q, $\text{C}\text{-}\underline{\text{C}}\text{F}_3$, $J_{\text{C-F}}=280.4$ Hz), 102.71. ^{19}F NMR (471MHz, DMSO- d_6): δ -64.50 ppm. HRMS (ESI-QTOF) m/z : calculated for $[\text{M}+\text{H}] = 220.0441$; Found $[\text{M}+\text{H}] = 220.0449$; IR (ATR, ZnSe, cm^{-1}): ν 3428, 3266, 2926, 1724, 1544, 1415, 1375, 1326, 1148, 994, 912, 817, 761, 652. Elemental analysis: (%) calculated for $\text{C}_6\text{H}_4\text{F}_3\text{N}_5\text{O}\cdot 0.93\text{CF}_3\text{COOH}$ (313.65): C, 29.03; H, 1.53; N, 21.53; found C, 29.34; H, 1.10; N, 21.91.



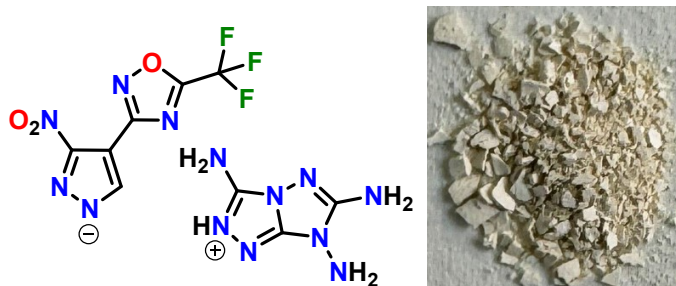
Synthesis of 3-(3-nitro-1H-pyrazol-4-yl)-5-(trifluoromethyl)-1,2,4-oxadiazole (4): To the ice-cooled solution of 30% H_2O_2 (2 mL), con. H_2SO_4 (2 mL, 98 %) was taken in round bottom flask and slowly added to compound **3** (100 mg, 0.45 mmol) for 30 mins with uniform stirring. The homogenous reaction mixture was further stirred at room temperature for 2 hours and subsequently heated to 45 °C for another 9 hours to get compound **4** in 63 % yield (72 mg, 0.27 mmol). T_d (onset): 177.6 °C.

^1H NMR (400MHz, DMSO- d_6): δ (ppm) = 14.69 (1H, br, s), 8.73 (1H, s) ppm. ^{13}C NMR (101MHz, DMSO- d_6): δ (ppm) = 164.77 (q, $\underline{\text{C}}\text{-CF}_3$, $J_{\text{C-F}}= 43.7$ Hz), 161.83, 152.85, 135.37, 115.71 (q, $\text{C}\text{-}\underline{\text{C}}\text{F}_3$, $J_{\text{C-F}}= 273.4$ Hz), 101.18. ^{19}F NMR (373MHz, DMSO- d_6): δ = -64.63 ppm. HRMS (ESI-QTOF) m/z : calculated for $[\text{M}+\text{H}] = 247.0111$; Found $[\text{M}+\text{H}] = 247.0188$; IR (ATR, ZnSe, cm^{-1}): ν 3147, 2922, 1613, 1544, 1381, 1333, 1144, 994, 954, 894, 818, 757, 719, 642 cm^{-1} . Elemental analysis: (%) calculated for $\text{C}_6\text{H}_2\text{F}_3\text{N}_5\text{O}_3\cdot 0.41\text{H}_2\text{O}$ (256.49): C, 28.10; H, 1.11; N, 27.30; found C, 28.31; H, 1.47; N, 27.31.



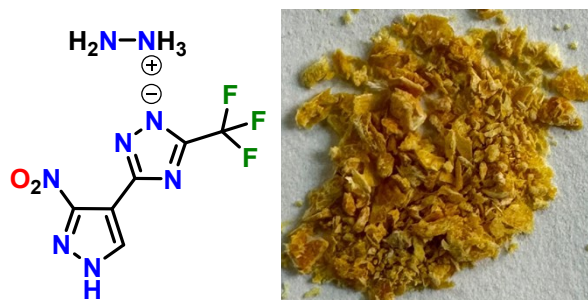
Synthesis of hydroxylammonium-3-(3-nitro-1H-pyrazol-4-yl)-5-(trifluoromethyl)-1,2,4-oxadiazole (5): A solution of 50% aqueous hydroxylamine (0.4 ml, 14.65 mmol) was added dropwise to suspension of **4** (100 mg, 0.4 mmol) in 2 mL of methanol and acetonitrile at room temperature and stirred for 12 hours at same temperature. The newly formed precipitate was collected by filtration and washed with methanol to get compound **5** in 70 % yield (120 mg, 0.28 mmol). T_d (onset): 170.8 °C.

^1H NMR (400MHz, DMSO- d_6): δ (ppm) = 8.83 (s), 7.40 (3H, br, s), 5.51 (1H, br, s). ^{13}C NMR (101MHz, DMSO- d_6): δ (ppm) = 172.15, 160.61 (q, $\underline{\text{C}}\text{-CF}_3$, $J_{\text{C-F}} = 48.8$), 153.30, 138.21, 118.05 (q, $\text{C-}\underline{\text{C}}\text{F}_3$, $J_{\text{C-F}} = 271.7$ Hz), 99.16. ^{19}F NMR (471MHz, DMSO- d_6): $\delta = -64.43$ ppm. IR (ATR, ZnSe, cm^{-1}): ν 3290, 3015, 2854, 1681, 1630, 1617, 1551, 1392, 1342, 1202, 1153, 1061, 989, 925, 828, 753, 718, 660, 615 cm^{-1} . Elemental analysis: (%) calculated for $\text{C}_6\text{H}_5\text{F}_3\text{N}_6\text{O}_4 \cdot 0.8 \text{CH}_3\text{CN} \cdot \text{NH}_3$ (302.95): C, 27.49; H, 3.16; N, 32.91; found C, 27.86; H, 3.43; N, 31.97.



Synthesis of 3,6,7-triamino-7H- [1,2,4] triazolo[4,3-b] [1,2,4] triazol-2-ium 3-(3-nitro-1H-pyrazol-4-yl)-5-(trifluoromethyl)-1,2,4-oxadiazole (6): 7H- [1,2,4] triazolo[4,3-b] [1,2,4] triazole-3,6,7-triamine (60 mg, 0.4 mmol) was taken in methanol: acetonitrile (4 mL, 1:1) and was added dropwise at room temperature to a stirred suspension of **4** (100 mg, 0.4 mmol) in methanol and the reaction was stirred at room temperature for 12 hours. The formed precipitate was collected by filtration and dried to give compound **6** in 82 % yield (132 mg, 0.32 mmol). T_d (onset): 224.4 °C.

^1H NMR (400MHz, DMSO- d_6): δ (ppm) = 8.31 (1H, s), 6.60 (2H, s), 6.23 (2H, s), 5.64 (2H, s). ^{13}C NMR (101MHz, DMSO- d_6): δ (ppm) = 164.66, 161.57, 160.15, 155.03, 149.05, 143.47, 133.73, 114.00, 100.22. ^{19}F NMR (373MHz, DMSO- d_6): $\delta = -64.62$ ppm. IR (ATR, ZnSe, cm^{-1}): ν 3452, 3414, 3305, 3144, 2711, 1688, 1565, 1526, 1410, 1384, 1337, 1201, 1154, 1099, 1033, 968, 845, 795, 707, 668 cm^{-1} . Elemental analysis: (%) calculated for $\text{C}_9\text{H}_8\text{F}_3\text{N}_{13}\text{O}_3 \cdot 2\text{H}_2\text{O}$ (403.0825): C, 24.61; H, 2.75; N, 41.45; found C, 24.64; H, 3.23; N, 42.72.



Synthesis of hydrazinium 3-(3-nitro-1H-pyrazol-4-yl)-5-(trifluoromethyl)-1,2,4-triazol-1-ide (7): Hydrazine monohydrate (80 %) (0.4 ml, 12.48 mmol) was added to a solution of **4** (100 mg, 0.4 mmol) in methanol: acetonitrile solution (4 ml, ratio 1: 1) at room temperature and continued for 12 hours. The formed precipitate was collected by filtration and dried in air to give compound **7** in 89 % yield (100 mg, 0.35 mmol). The obtained compound possesses low solubility and get precipitates out. T_d (onset): 202.58 °C.

^1H NMR (400MHz, DMSO- d_6): δ (ppm) = 7.91 (1H, s), 7.51 (3H, br, s). ^{19}F NMR (373MHz, DMSO- d_6): δ = -64.21 ppm. IR (ATR, ZnSe, cm^{-1}): ν 3334, 3273, 3069, 2973, 2911, 2872, 2736, 2609, 1649, 1384, 1602, 1498, 1398, 1199, 1093, 925, 846, 768 cm^{-1} . Elemental analysis: (%) calculated for $\text{C}_6\text{H}_7\text{F}_3\text{N}_8\text{O}_2 \cdot 0.8\text{CH}_3\text{OH}$ (305.80): C, 26.71; H, 3.36; N, 36.64; found C, 26.51; H, 3.39; N, 35.25.

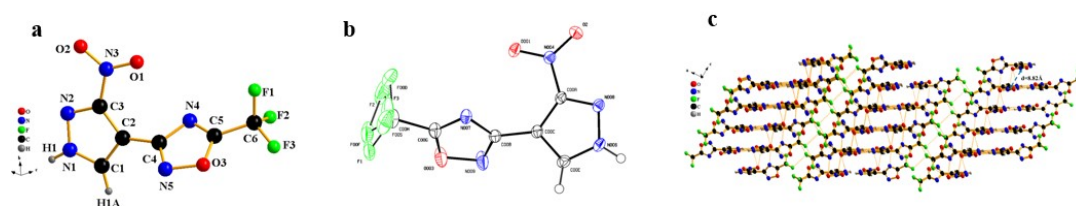
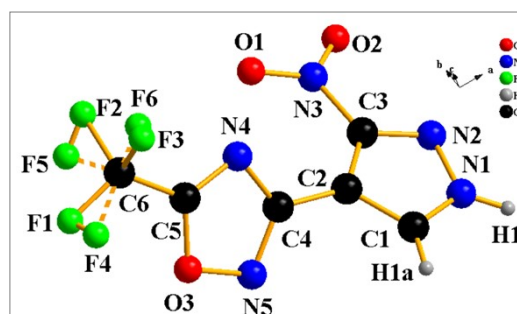
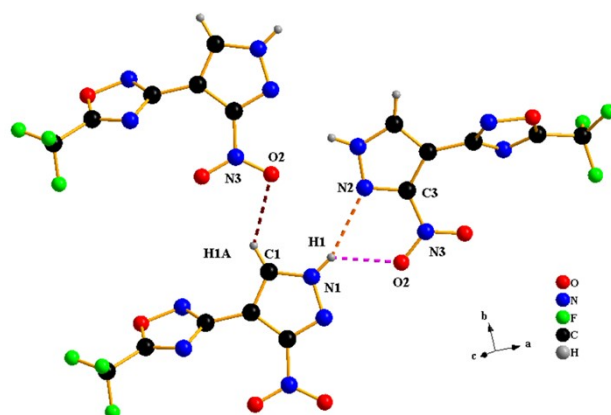


Figure S1. Crystal structure and packing of compound **4**.





S. No.	(H \cdots A)-bond	d (H \cdots A) (Å)
1	N1-H1 \cdots N2	2.42 (1)
2	N1-H1 \cdots O2	2.20 (2)
3	C1-H1A \cdots O2	2.47 (2)

Figure S2. Asymmetrical unit showing disorder and hydrogen bond distances of compound **4**. (Ball-and-stick diagram)

Table S1. Crystal data and structure refinement for **4**.

Identification code	Comp. 4 .
CCDC Number	2371546
Empirical formula	C ₆ H ₂ F ₃ N ₅ O ₃
Formula weight	249.110
Temperature/K	100
Crystal system	Monoclinic
Space group	<i>P2₁/c</i>
$a/\text{Å}$	15.7760(15)
$b/\text{Å}$	7.3324(6)
$c/\text{Å}$	7.5674(8)
$\alpha/^\circ$	90
$\beta/^\circ$	95.769(3)
$\gamma/^\circ$	90
Volume/Å ³	870.93(14)
Z	4
$\rho_{\text{calc}}/\text{g/cm}^3$	1.900
μ/mm^{-1}	0.193
$F(000)$	496.4
Crystal size/mm ³	0.21 \times 0.12 \times 0.1
Radiation	Mo K α ($\lambda = 0.71073$)
2 Θ range for data collection/ $^\circ$	5.2 to 56.8
Index ranges	-21 $\leq h \leq$ 20, -9 $\leq k \leq$ 9, -10 $\leq l \leq$ 10
Reflections collected	13853
Independent reflections	2177 [$R_{\text{int}} = 0.0294$, $R_{\text{sigma}} = 0.0192$]
Data/restraints/parameters	2177/0/185

Goodness-of-fit on F^2	1.106
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0352$, $wR_2 = 0.0831$
Final R indexes [all data]	$R_1 = 0.0423$, $wR_2 = 0.0888$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.32/-0.30

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **4**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
O1	8111.0(6)	8406.7(13)	5248.0(11)	20.5(2)
O2	9212.9(6)	8991.7(13)	3845.1(14)	26.7(2)
O3	6104.0(7)	4079.4(18)	5470.9(14)	36.1(3)
N3	8693.4(6)	7936.5(14)	4403.3(13)	17.5(2)
F3	6329(4)	4960(7)	9904(7)	46.8(13)
N1	9321.8(7)	3696.8(15)	3021.3(14)	19.7(2)
N4	7285.4(7)	5331.2(16)	6740.8(14)	20.6(2)
N2	9446.0(7)	5497.1(15)	3230.4(13)	18.0(2)
N5	6729.2(8)	3831(2)	4284.0(17)	34.4(3)
C3	8777.4(8)	6023.1(17)	4025.9(15)	16.0(2)
C4	7403.0(8)	4595.9(18)	5101.6(16)	19.0(3)
C2	8214.0(8)	4594.3(17)	4329.2(15)	17.5(2)
F2	6042.1(15)	7440(4)	8554(4)	35.6(6)
C1	8601.4(8)	3098.9(18)	3644.1(17)	20.3(3)
F1	5195.0(17)	5220(4)	8071(4)	47.7(8)
C5	6495.6(8)	4972(2)	6846.5(18)	23.6(3)
C6	5976.5(10)	5535(2)	8331(2)	32.3(3)
F5	5627(3)	7040(5)	7945(6)	98.4(16)
F6	6387(3)	5383(9)	9825(6)	68.1(18)
F4	5315.5(17)	4262(4)	8357(4)	38.3(6)

Table S3. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **4**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2U_{11}+2hka*b*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	23.8(4)	22.6(5)	16.0(4)	4.2(4)	5.9(3)	-1.2(3)
O2	28.7(5)	18.5(5)	34.9(6)	-3.3(4)	12.6(4)	2.0(4)
O3	24.3(5)	59.3(8)	26.4(5)	-12.2(5)	9.9(4)	-10.6(5)
N3	20.0(5)	18.3(5)	14.3(5)	0.9(4)	2.7(4)	0.9(4)
F3	66(3)	52.7(17)	25.7(18)	25.2(18)	23.3(17)	17.5(14)
N1	23.2(5)	20.7(6)	15.7(5)	3.6(4)	4.7(4)	-3.7(4)
N4	21.8(5)	25.6(6)	15.3(5)	0.8(4)	5.6(4)	-0.3(4)
N2	21.2(5)	20.2(5)	12.8(5)	2.0(4)	3.1(4)	-0.4(4)
N5	28.1(6)	52.9(9)	24.2(6)	-13.2(6)	12.1(5)	-11.4(6)
C3	19.7(5)	17.3(6)	11.2(5)	1.9(4)	2.7(4)	0.2(4)
C4	23.3(6)	19.0(6)	15.3(5)	-0.8(5)	4.5(4)	0.6(5)

Table S3. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **4**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C2	21.2(6)	19.6(6)	12.1(5)	0.1(5)	3.6(4)	-0.0(4)
F2	39.3(12)	34.5(13)	34.4(11)	10.2(10)	11.0(9)	-7.6(9)
C1	26.2(6)	18.3(6)	16.6(5)	0.4(5)	3.3(5)	-1.8(5)
F1	25.0(11)	75(2)	46.2(15)	-14.9(14)	17.3(10)	-30.4(16)
C5	22.5(6)	29.3(7)	19.6(6)	0.0(5)	5.8(5)	-0.2(5)
C6	27.0(7)	41.7(9)	30.2(8)	3.3(6)	13.5(6)	-0.9(6)
F5	131(4)	47(2)	135(4)	46(2)	103(3)	26(2)
F6	27.2(17)	150(5)	29(2)	-24(2)	10.9(14)	-48(2)
F4	26.5(11)	52.6(16)	38.9(12)	-12.6(12)	18.2(9)	-14.7(13)

Table S4. Bond Lengths for **4**.

Atom	Atom	Length/ \AA	Atom	Atom	Length/ \AA
O1	N3	1.2205(13)	C3	C2	1.4076(17)
O2	N3	1.2322(14)	C4	C2	1.4591(17)
O3	N5	1.4110(15)	C2	C1	1.3814(18)
O3	C5	1.3282(17)	F2	C6	1.409(3)
N3	C3	1.4405(16)	F2	F5	0.816(5)
F3	C6	1.331(5)	F1	C6	1.250(3)
F3	F6	0.330(10)	F1	F5	1.506(5)
N1	N2	1.3416(16)	F1	F4	0.754(3)
N1	C1	1.3467(17)	C5	C6	1.5126(19)
N4	C4	1.3820(16)	C6	F5	1.254(4)
N4	C5	1.2839(17)	C6	F6	1.250(5)
N2	C3	1.3234(15)	C6	F4	1.401(3)
N5	C4	1.3019(18)			

Table S5. Bond Angles for **4**.

Atom	Atom	Atom	Angle/ $^\circ$	Atom	Atom	Atom	Angle/ $^\circ$
C5	O3	N5	105.23(10)	F2	C6	F3	100.8(3)
O2	N3	O1	124.32(11)	F1	C6	F3	113.6(3)
C3	N3	O1	117.91(10)	F1	C6	F2	105.1(2)
C3	N3	O2	117.77(10)	C5	C6	F3	111.6(3)
F6	F3	C6	68.8(15)	C5	C6	F2	108.71(16)
C1	N1	N2	113.42(11)	C5	C6	F1	115.57(18)
C5	N4	C4	101.22(11)	F5	C6	F3	128.4(4)
C3	N2	N1	103.10(10)	F5	C6	F2	35.1(2)
C4	N5	O3	103.38(11)	F5	C6	F1	73.9(3)
N2	C3	N3	117.87(11)	F5	C6	C5	109.0(2)

Table S5. Bond Angles for **4**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C3	N3	128.35(11)	F6	C6	F3	14.2(5)
C2	C3	N2	113.73(11)	F6	C6	F2	87.4(3)
N5	C4	N4	114.69(12)	F6	C6	F1	122.6(3)
C2	C4	N4	124.20(11)	F6	C6	C5	112.2(3)
C2	C4	N5	121.08(11)	F6	C6	F5	117.7(4)
C4	C2	C3	131.16(12)	F4	C6	F3	91.2(3)
C1	C2	C3	102.66(11)	F4	C6	F2	134.77(19)
C1	C2	C4	126.15(12)	F4	C6	F1	32.41(15)
F5	F2	C6	62.0(4)	F4	C6	C5	106.74(16)
C2	C1	N1	107.08(12)	F4	C6	F5	106.2(3)
F5	F1	C6	53.2(2)	F4	C6	F6	104.2(3)
F4	F1	C6	84.9(4)	F1	F5	F2	128.7(6)
F4	F1	F5	137.8(5)	C6	F5	F2	82.9(5)
N4	C5	O3	115.48(12)	C6	F5	F1	52.9(2)
C6	C5	O3	118.20(12)	C6	F6	F3	96.9(16)
C6	C5	N4	126.27(13)	C6	F4	F1	62.7(3)

Table S6. Torsion Angles for **4**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	N3	C3	N2	-174.91(10)	N1	C1	C2	C3	0.04(11)
O1	N3	C3	C2	7.94(13)	N1	C1	C2	C4	178.17(9)
O2	N3	C3	N2	5.37(12)	N4	C4	C2	C3	-53.54(16)
O2	N3	C3	C2	-171.78(11)	N4	C4	C2	C1	128.89(13)
O3	N5	C4	N4	0.25(14)	N4	C5	C6	F2	54.30(18)
O3	N5	C4	C2	178.32(10)	N4	C5	C6	F1	172.2(2)
O3	C5	N4	C4	0.63(14)	N4	C5	C6	F5	91.4(3)
O3	C5	C6	F3	126.8(3)	N4	C5	C6	F6	-40.7(3)
O3	C5	C6	F2	-122.90(17)	N4	C5	C6	F4	-154.3(2)
O3	C5	C6	F1	-5.0(2)	N2	C3	C2	C4	-177.74(10)
O3	C5	C6	F5	-85.8(3)	N2	C3	C2	C1	0.25(11)
O3	C5	C6	F6	142.1(3)	N5	C4	C2	C3	128.58(14)
O3	C5	C6	F4	28.53(18)	N5	C4	C2	C1	-48.99(16)
N3	C3	N2	N1	-177.99(11)	F2	C6	F1	F5	16.1(3)
N3	C3	C2	C4	-0.49(16)	F2	C6	F1	F4	-159.2(5)
N3	C3	C2	C1	177.50(14)	F2	C6	F5	F1	-152.2(3)
F3	C6	F2	F5	-145.9(6)	F2	C6	F4	F1	28.8(4)
F3	C6	F1	F5	125.4(5)	F2	F5	F1	C6	-36.4(5)
F3	C6	F1	F4	-50.0(5)	F2	F5	F1	F4	-29.5(8)
F3	C6	C5	N4	-56.0(3)	F2	F5	C6	F1	152.2(5)
F3	C6	F5	F2	44.6(5)	F2	F5	C6	C5	-95.8(4)
F3	C6	F5	F1	-107.6(5)	F2	F5	C6	F6	33.4(5)

Table S6. Torsion Angles for **4**.

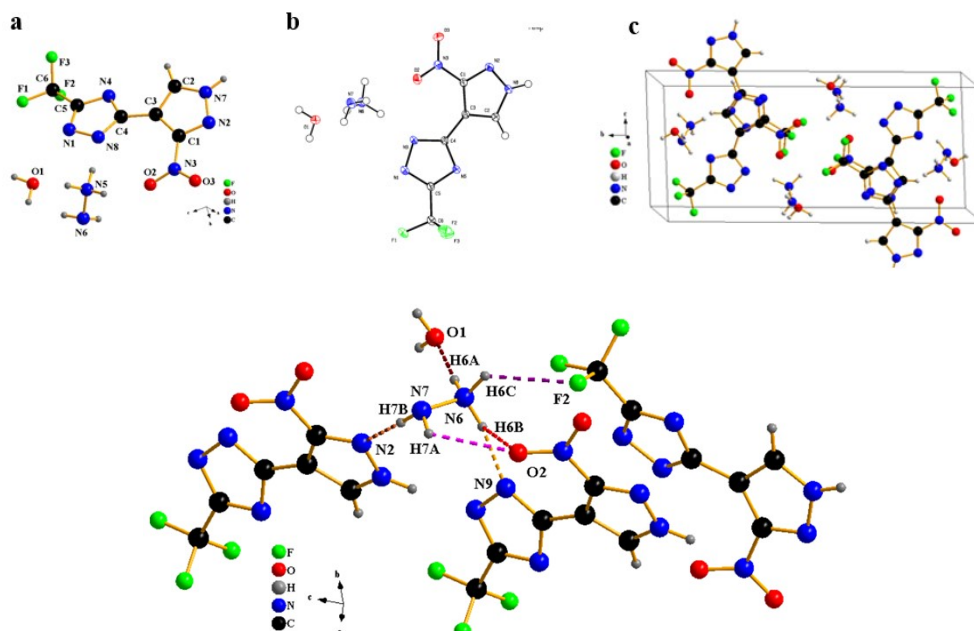
A	B	C	D	Angle/°	A	B	C	D	Angle/°
F3	C6	F4	F1	135.4(6)	F2	F5	C6	F4	149.6(4)
F3	F6	C6	F2	160(2)	F1	F5	C6	C5	112.07(17)
F3	F6	C6	F1	54(2)	F1	F5	C6	F6	-118.8(3)
F3	F6	C6	C5	-91(2)	F1	F5	C6	F4	-2.6(2)
F3	F6	C6	F5	142(2)	F1	F4	C6	C5	-111.5(4)
F3	F6	C6	F4	24(2)	F1	F4	C6	F5	4.6(5)
N1	N2	C3	C2	-0.42(10)	F1	F4	C6	F6	129.6(5)

Table S7. Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **4**.

Atom	x	y	z	U(eq)
H1	9676.3(7)	2977.0(15)	2525.5(14)	23.6(3)
H1A	8426(11)	1870(30)	3610(20)	30(4)

Table S8. Atomic Occupancy for **4**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
F3	0.500000	F2	0.500000	F1	0.500000
F5	0.500000	F6	0.500000	F4	0.500000



Sr. No.	(H \cdots A)-bond	d (H \cdots A) (\AA)
1	N2- H7B \cdots N7	2.21 (2)
2	O2- H7A \cdots N7	2.53 (2)

3	O2- H6B...N6	2.51 (3)
4	N9- H6B...N6	1.85 (2)
5	O1- H6A...N6	1.78 (3)
6	N6- H6C...F2	2.52 (2)

Figure S3. Crystal Structure, unit cell packing and hydrogen bonding of compound 7.

Table S9. Crystal data and structure refinement for 7.

Identification code	Comp. 7
CCDC Number	2371545
Empirical formula	C ₆ H ₉ F ₃ N ₈ O ₃
Formula weight	298.21
Temperature/K	100
Crystal system	Monoclinic
Space group	<i>P2₁/n</i>
<i>a</i> /Å	7.408(3)
<i>b</i> /Å	19.158(6)
<i>c</i> /Å	8.467(3)
α /°	90
β /°	111.839(11)
γ /°	90
Volume/Å ³	1115.5(6)
<i>Z</i>	4
ρ_{calc} /cm ³	1.776
μ /mm ⁻¹	0.173
<i>F</i> (000)	608.0
Crystal size/mm ³	0.2 × 0.15 × 0.1
Radiation	MoK α (λ = 0.71073)
2 Θ range for data collection/°	4.252 to 56.77
Index ranges	-9 ≤ <i>h</i> ≤ 9, -25 ≤ <i>k</i> ≤ 25, -11 ≤ <i>l</i> ≤ 11
Reflections collected	18291
Independent reflections	2775 [<i>R</i> _{int} = 0.0694, <i>R</i> _{sigma} = 0.0436]
Data/restraints/parameters	2775/0/204
Goodness-of-fit on <i>F</i> ²	1.046
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0452, <i>wR</i> ₂ = 0.1022
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0641, <i>wR</i> ₂ = 0.1129
Largest diff. peak/hole / e Å ⁻³	0.33/-0.31

Table S10. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 7. *U*_{eq} is defined as 1/3 of the trace of the orthogonalised *U*_{ij} tensor.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
F2	8399.1(17)	809.2(7)	9029.1(16)	24.8(3)
F1	6277(2)	1174.2(7)	9999.6(15)	25.8(3)
F3	5390.0(19)	589.7(6)	7652.4(16)	25.1(3)

Table S10. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **7**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	$U(\text{eq})$
O1	2542(2)	4282.7(7)	9209.4(19)	21.8(3)
O2	7675(2)	4041.2(8)	5902.9(18)	20.7(3)
O3	6895(2)	4573.8(7)	3468.3(19)	22.4(3)
N3	7109(2)	4042.0(9)	4336(2)	15.8(3)
N5	6564(2)	1772.4(8)	6063.9(19)	13.6(3)
N8	6193(2)	2687.7(9)	1427(2)	14.8(3)
N2	6584(2)	3358.1(8)	1869(2)	15.1(3)
N6	5409(3)	4169.5(9)	7969(2)	18.1(4)
N9	5991(2)	2831.7(8)	6919.4(19)	14.3(3)
N1	6065(2)	2358.5(8)	8171(2)	15.4(3)
N7	7241(3)	4355.1(10)	9296(2)	20.4(4)
C4	6306(3)	2462.2(10)	5706(2)	12.3(4)
C1	6673(3)	3376.8(10)	3474(2)	13.0(4)
C3	6349(3)	2720.9(10)	4089(2)	12.8(4)
C6	6606(3)	1083.2(10)	8565(2)	15.8(4)
C2	6035(3)	2294.9(10)	2684(2)	14.8(4)
C5	6405(3)	1749.1(10)	7596(2)	13.3(4)

Table S11. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **7**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F2	18.0(6)	27.0(7)	30.4(7)	13.2(5)	10.3(5)	5.1(5)
F1	39.9(8)	25.6(7)	18.9(6)	5.6(5)	19.1(6)	3.0(6)
F3	27.4(7)	18.1(6)	23.8(6)	3.2(5)	2.6(5)	-6.5(5)
O1	34.2(9)	14.6(7)	20.5(7)	0.8(6)	14.7(7)	-1.0(6)
O2	28.4(8)	19.8(7)	15.9(7)	-3.5(6)	10.8(6)	-2.9(6)
O3	31.6(9)	13.6(7)	26.4(8)	4.0(6)	16.0(7)	2.4(6)
N3	17.6(8)	15.3(8)	17.4(8)	0.8(6)	10.0(7)	0.4(6)
N5	18.2(8)	13.7(8)	10.2(7)	0.7(6)	6.7(6)	0.2(6)
N8	20.0(8)	15.6(8)	9.9(7)	0.5(6)	6.9(7)	0.4(6)
N2	17.7(8)	15.3(8)	13.0(7)	2.4(6)	6.6(6)	1.7(6)
N6	23.6(9)	17.2(9)	13.6(8)	0.8(7)	7.1(7)	3.6(7)
N9	19.4(8)	15.2(8)	9.8(7)	1.3(6)	7.3(6)	1.2(6)
N1	18.9(8)	16.9(8)	11.0(7)	0.8(6)	6.4(6)	0.4(6)
N7	25.1(10)	22.1(9)	13.2(8)	-1.0(7)	6.4(7)	-1.0(7)
C4	13.6(9)	13.7(9)	9.3(8)	-0.6(7)	3.7(7)	0.7(7)
C1	15.1(9)	13.2(9)	11.5(8)	0.2(7)	5.8(7)	1.6(7)
C3	13.6(9)	13.6(9)	10.9(8)	0.1(7)	4.3(7)	1.8(7)
C6	15.3(9)	19.5(10)	13.7(9)	1.1(7)	6.6(7)	-0.2(7)
C2	18.7(10)	14.2(9)	11.9(9)	0.3(7)	6.2(7)	0.3(7)
C5	14.9(9)	14.4(9)	12.0(8)	-0.4(7)	6.7(7)	-0.5(7)

Table S12. Bond Lengths for 7.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F2	C6	1.344(2)	N2	C1	1.336(2)
F1	C6	1.336(2)	N6	N7	1.448(3)
F3	C6	1.336(2)	N9	N1	1.380(2)
O2	N3	1.234(2)	N9	C4	1.338(2)
O3	N3	1.231(2)	N1	C5	1.325(2)
N3	C1	1.444(2)	C4	C3	1.467(2)
N5	C4	1.354(2)	C1	C3	1.415(3)
N5	C5	1.346(2)	C3	C2	1.389(3)
N8	N2	1.339(2)	C6	C5	1.494(3)
N8	C2	1.344(2)			

Table S13. Bond Angles for 7.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	N3	C1	117.70(16)	C1	C3	C4	135.16(17)
O3	N3	O2	124.02(17)	C2	C3	C4	123.08(17)
O3	N3	C1	118.28(16)	C2	C3	C1	101.76(16)
C5	N5	C4	101.09(15)	F2	C6	C5	112.32(16)
N2	N8	C2	112.89(16)	F1	C6	F2	106.26(16)
C1	N2	N8	103.53(15)	F1	C6	C5	111.93(16)
C4	N9	N1	105.90(15)	F3	C6	F2	105.85(16)
C5	N1	N9	104.77(15)	F3	C6	F1	107.86(16)
N5	C4	C3	119.23(16)	F3	C6	C5	112.23(16)
N9	C4	N5	113.27(16)	N8	C2	C3	108.26(17)
N9	C4	C3	127.48(17)	N5	C5	C6	122.08(17)
N2	C1	N3	117.05(16)	N1	C5	N5	114.97(17)
N2	C1	C3	113.56(16)	N1	C5	C6	122.95(16)
C3	C1	N3	129.39(16)				

Table S14. Torsion Angles for 7.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
F2	C6	C5	N5	64.4(2)	N2	C1	C3	C4	179.4(2)
F2	C6	C5	N1	-115.3(2)	N2	C1	C3	C2	-0.4(2)
F1	C6	C5	N5	-176.18(17)	N9	N1	C5	N5	0.0(2)
F1	C6	C5	N1	4.1(3)	N9	N1	C5	C6	179.74(17)
F3	C6	C5	N5	-54.7(2)	N9	C4	C3	C1	22.5(3)

Table S14. Torsion Angles for 7.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
F3	C6	C5	N1	125.5(2)	N9	C4	C3	C2	-157.67(19)
O2	N3	C1	N2	-162.16(17)	N1	N9	C4	N5	0.6(2)
O2	N3	C1	C3	16.6(3)	N1	N9	C4	C3	179.20(17)
O3	N3	C1	N2	17.8(3)	C4	N5	C5	N1	0.4(2)
O3	N3	C1	C3	-163.41(19)	C4	N5	C5	C6	-179.38(17)
N3	C1	C3	C4	0.6(4)	C4	N9	N1	C5	-0.4(2)
N3	C1	C3	C2	-179.23(19)	C4	C3	C2	N8	-179.35(17)
N5	C4	C3	C1	-159.0(2)	C1	C3	C2	N8	0.5(2)
N5	C4	C3	C2	20.8(3)	C2	N8	N2	C1	0.1(2)
N8	N2	C1	N3	179.15(16)	C5	N5	C4	N9	-0.6(2)
N8	N2	C1	C3	0.2(2)	C5	N5	C4	C3	-179.30(17)
N2	N8	C2	C3	-0.4(2)					

Table S15. Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 7.

Atom	x	y	z	U(eq)
H1A	2365.78	3987.69	9888.07	33
H1B	2588.33	4674.79	9693.8	33
H6A	4420(40)	4155(12)	8400(30)	22
H6B	5500(40)	3727(13)	7480(30)	22
H7A	7290(40)	4083(13)	10140(30)	24
H7B	8200(40)	4256(13)	9000(30)	24
H2	5755.31	1809.48	2622.01	18
H8	6130(40)	2549(14)	380(40)	35(7)
H6C	5060(40)	4525(13)	7120(30)	25(6)

NMR Spectra, IR Spectrum & DSC plots for compounds 3 to 7.

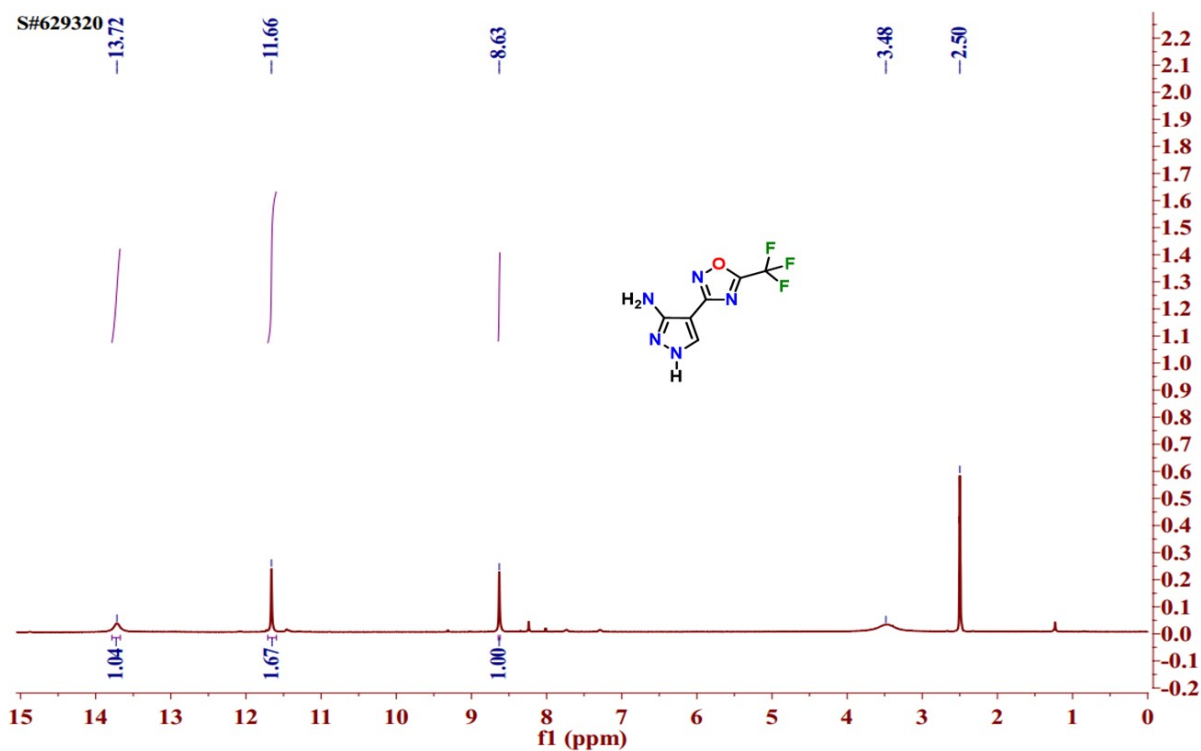


Figure S4. $^1\text{H-NMR}$ for compound of 3 in $\text{DMSO-}d_6$.

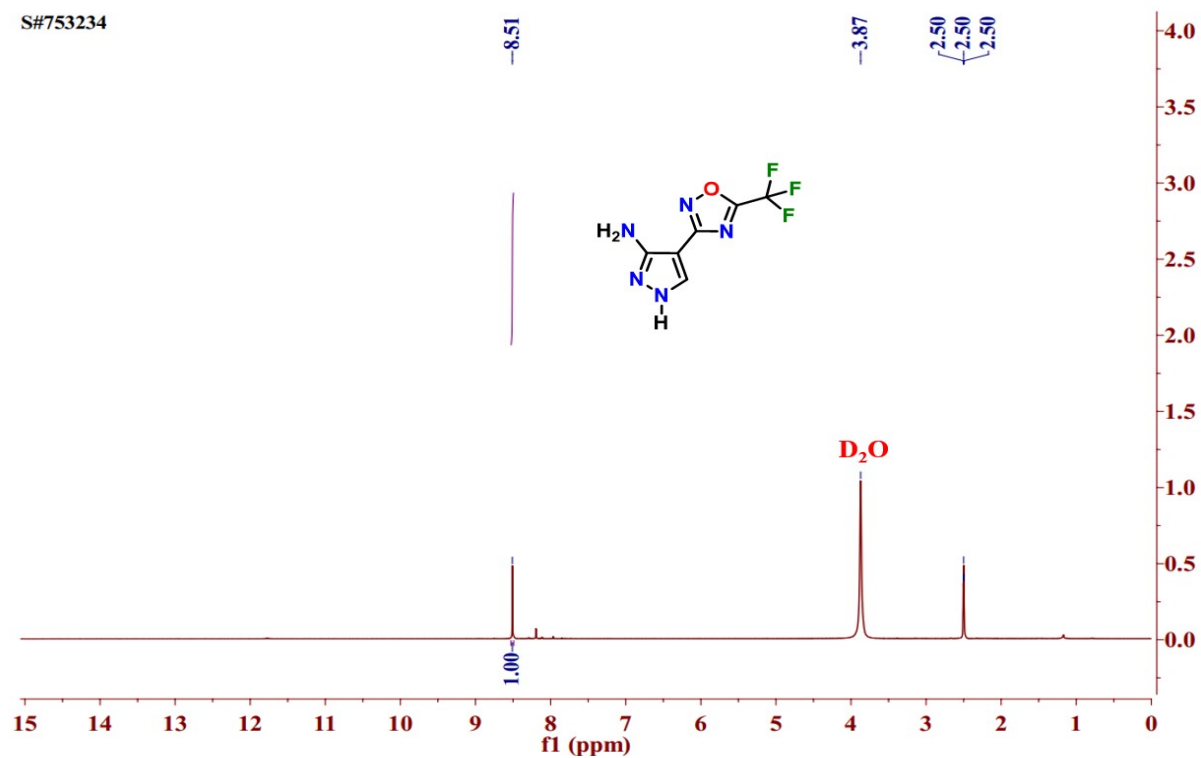


Figure S5. $^1\text{H-NMR}$ for compound of 3 in $\text{DMSO-}d_6 + \text{D}_2\text{O}$.

S#256975

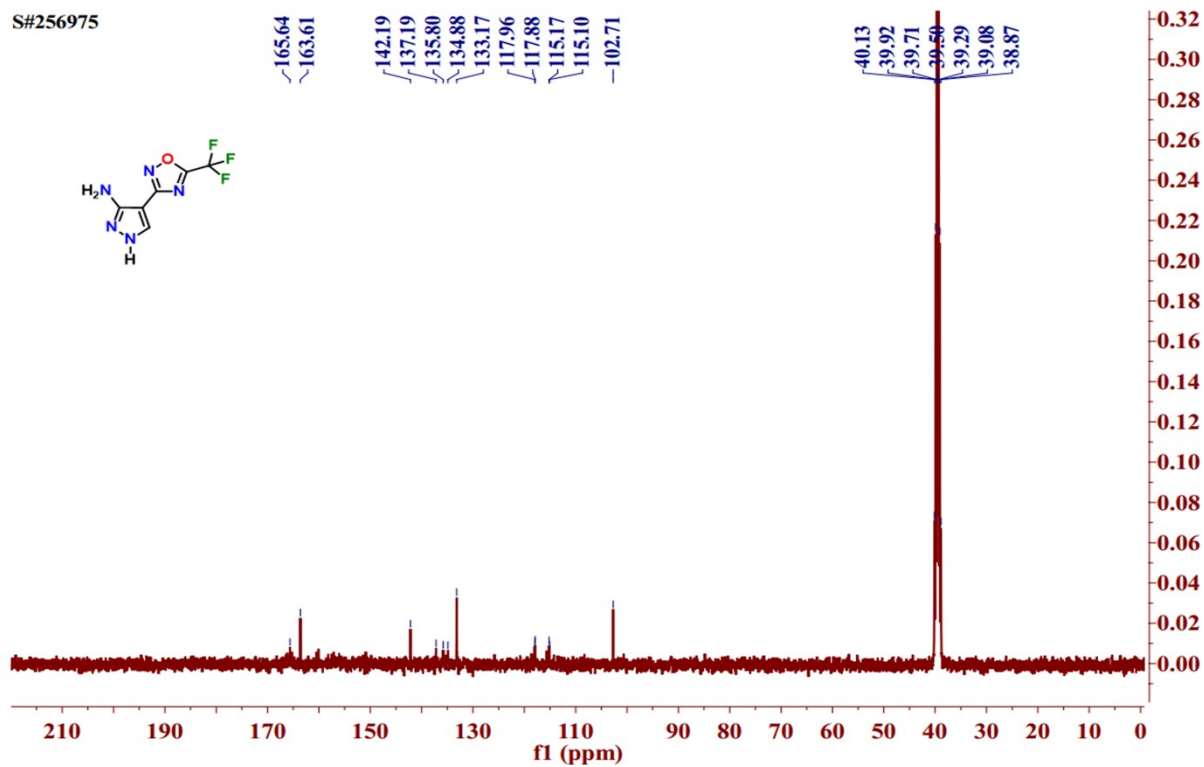


Figure S6. ¹³C-NMR for compound 3 in DMSO-*d*₆.

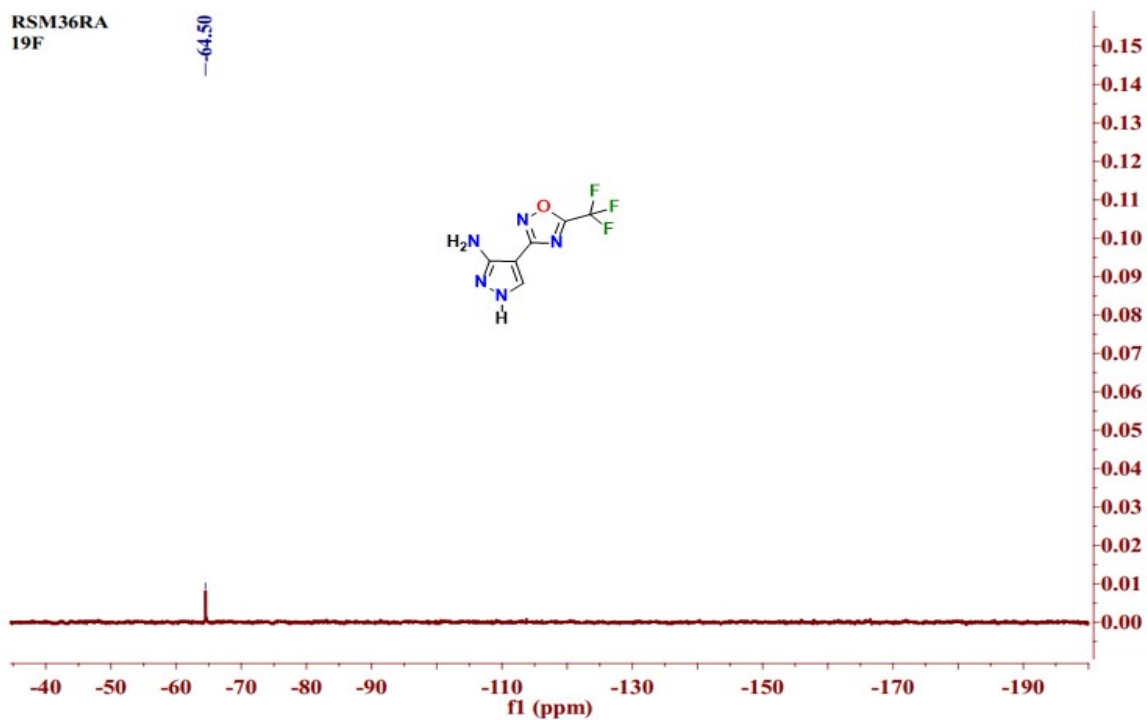


Figure S7. ¹⁹F-NMR for compound 3 in DMSO-*d*₆.

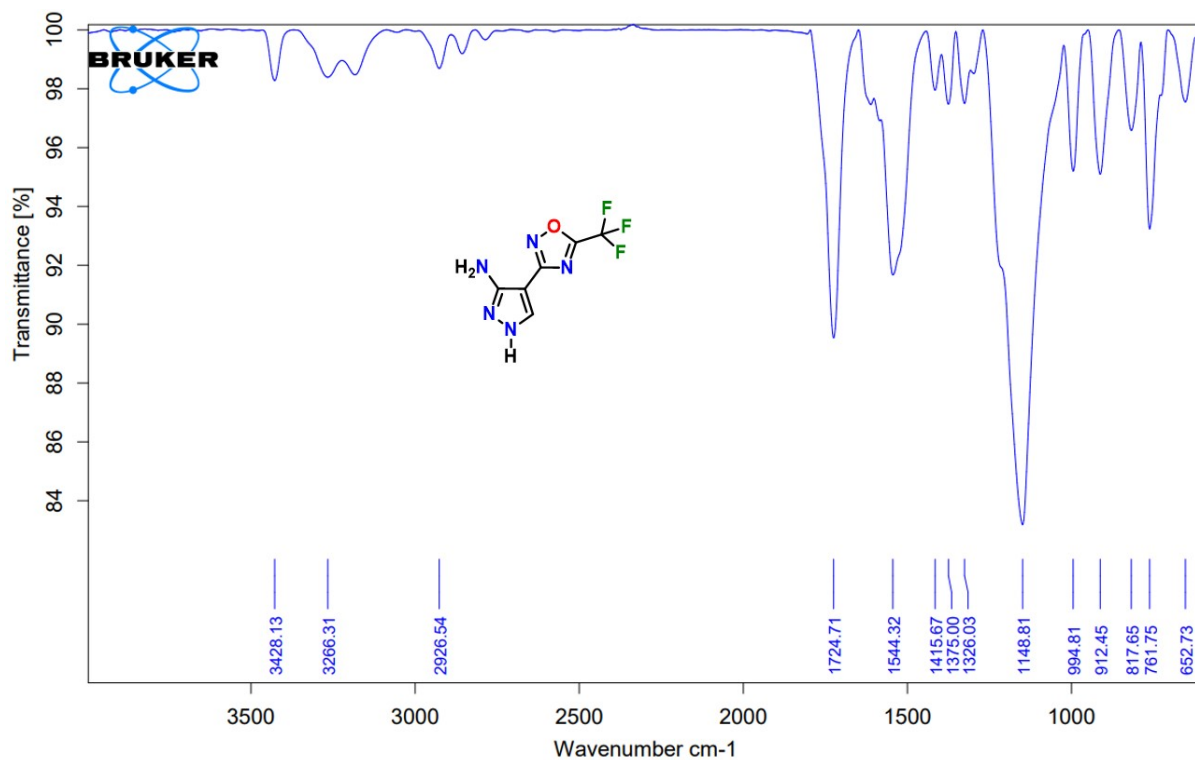


Figure S8. IR spectra for compound 3.

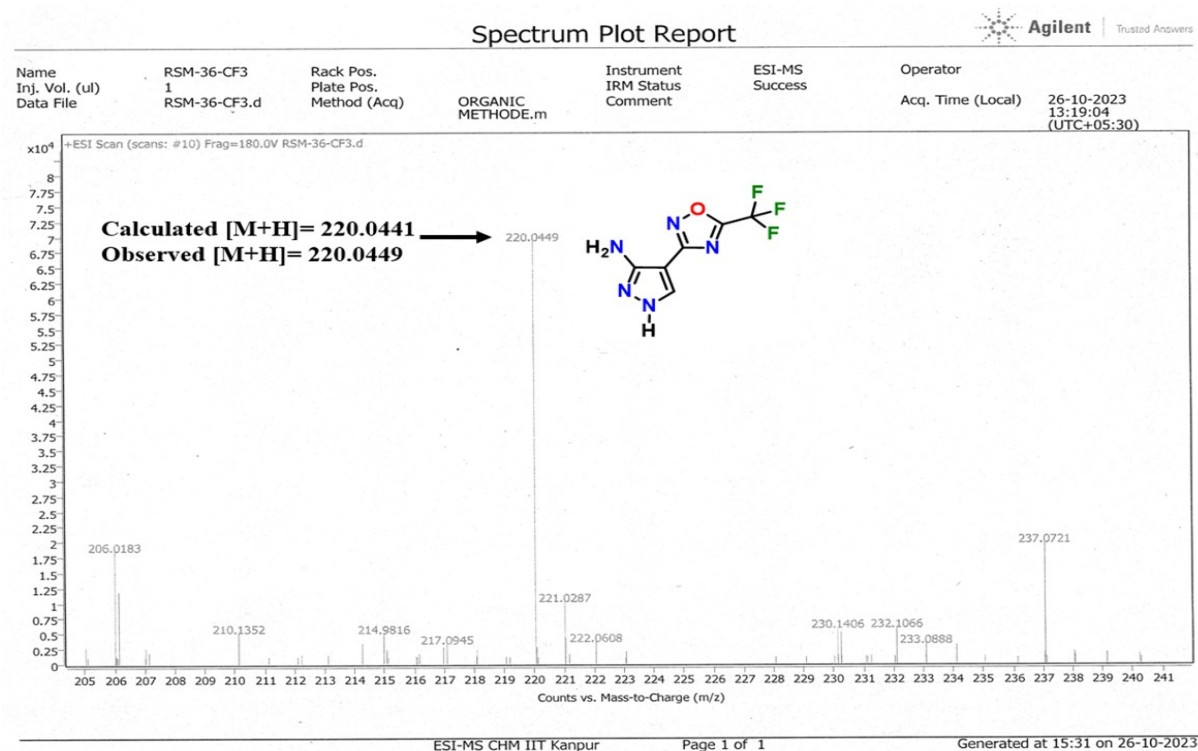


Figure S9. Mass spectra for compound 3.

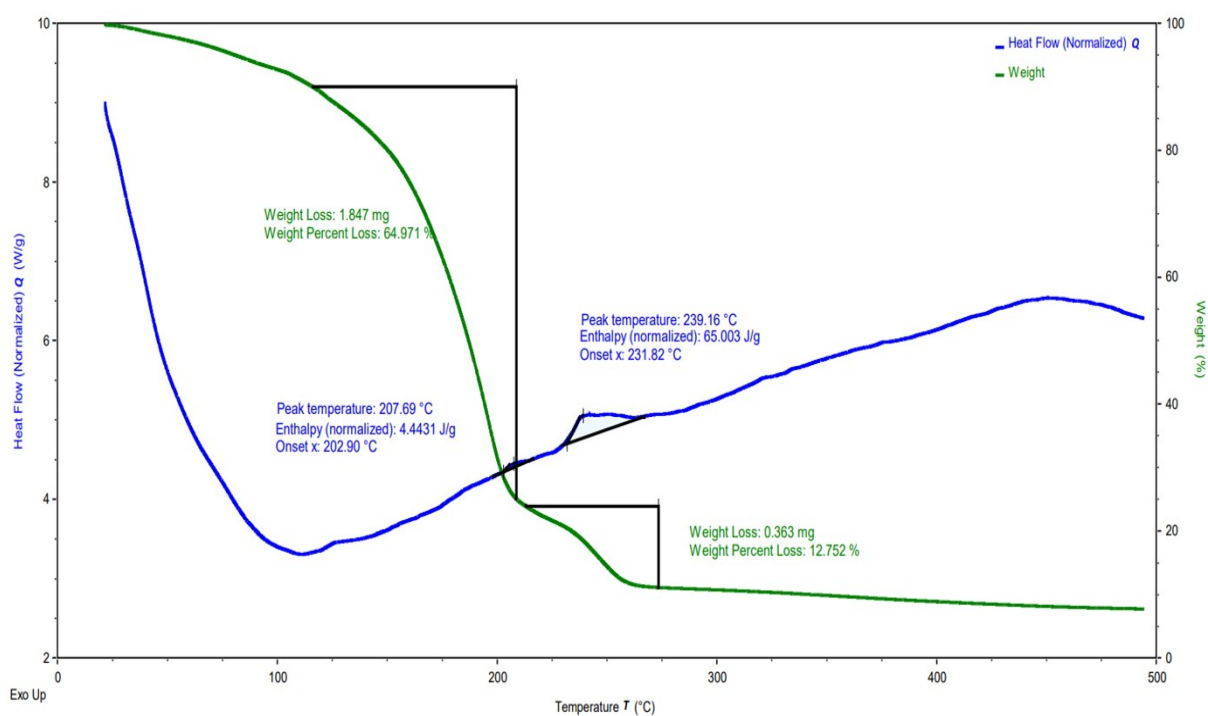


Figure S10. TGA-DSC for compound 3 at heating rate 5 °C min⁻¹.

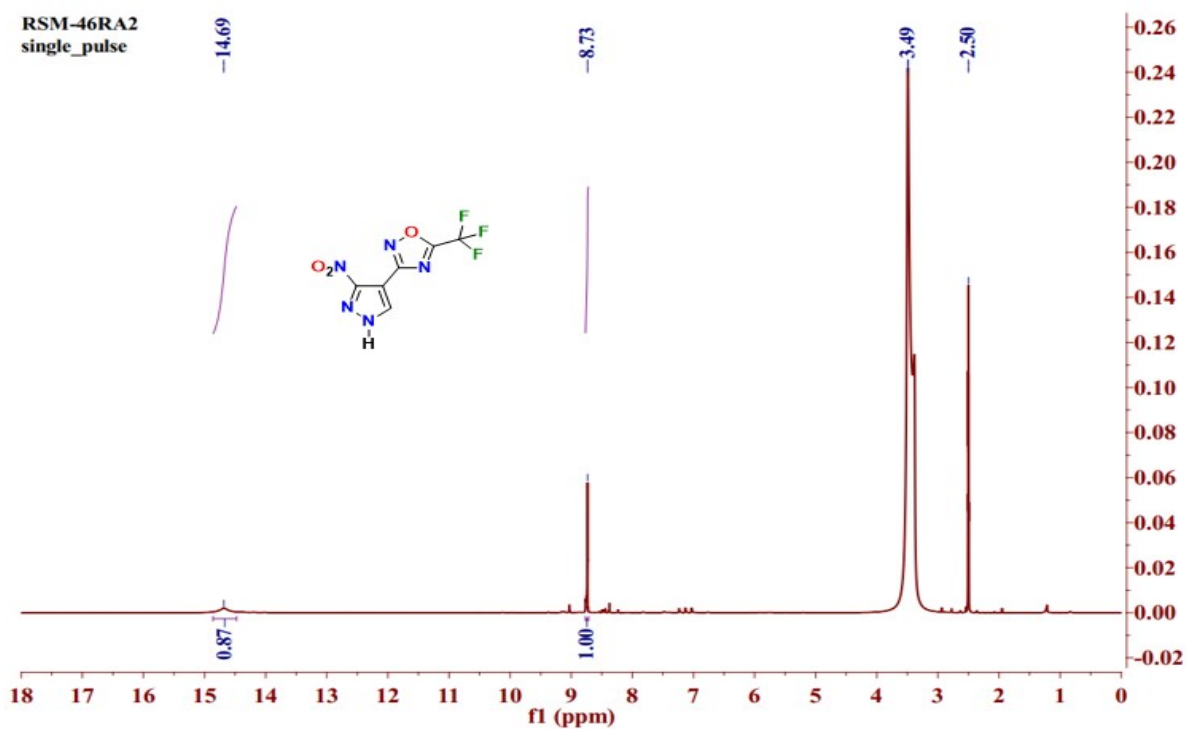


Figure S11. ¹H-NMR for compound 4 in DMSO-d₆.

S#275283

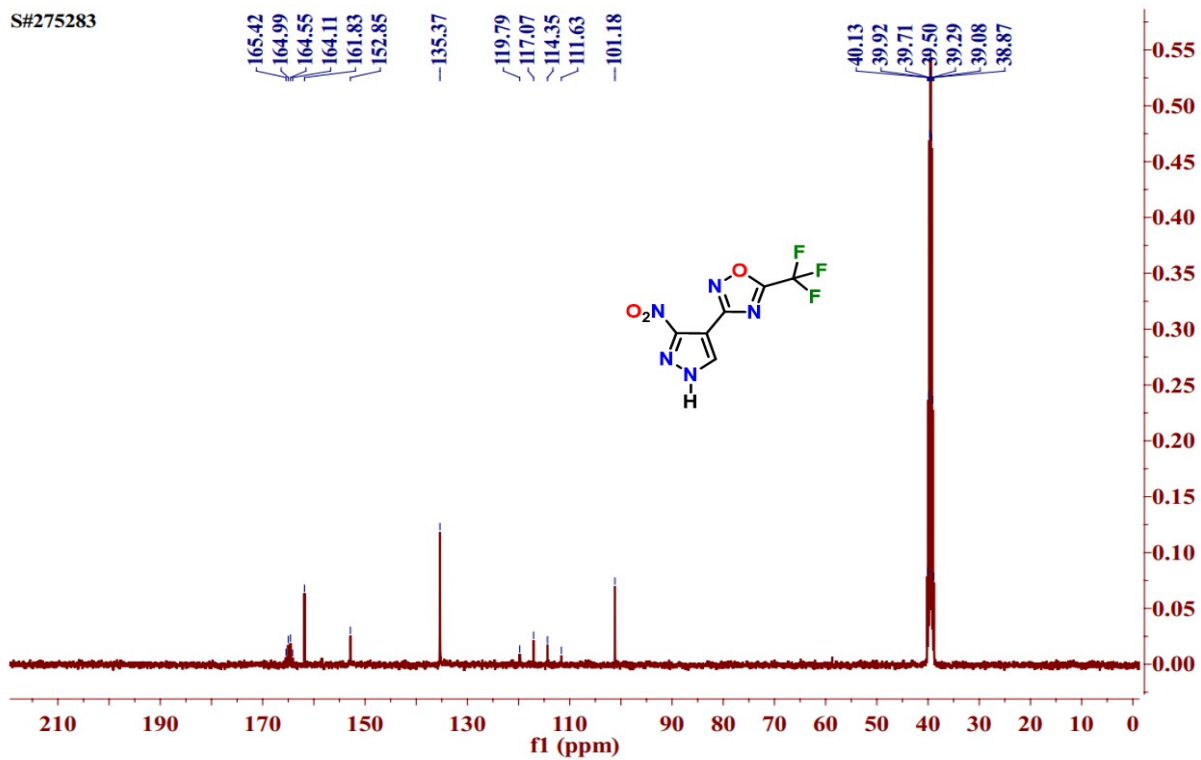


Figure S12. ^{13}C -NMR for compound 4 in $\text{DMSO-}d_6$.

S#572548

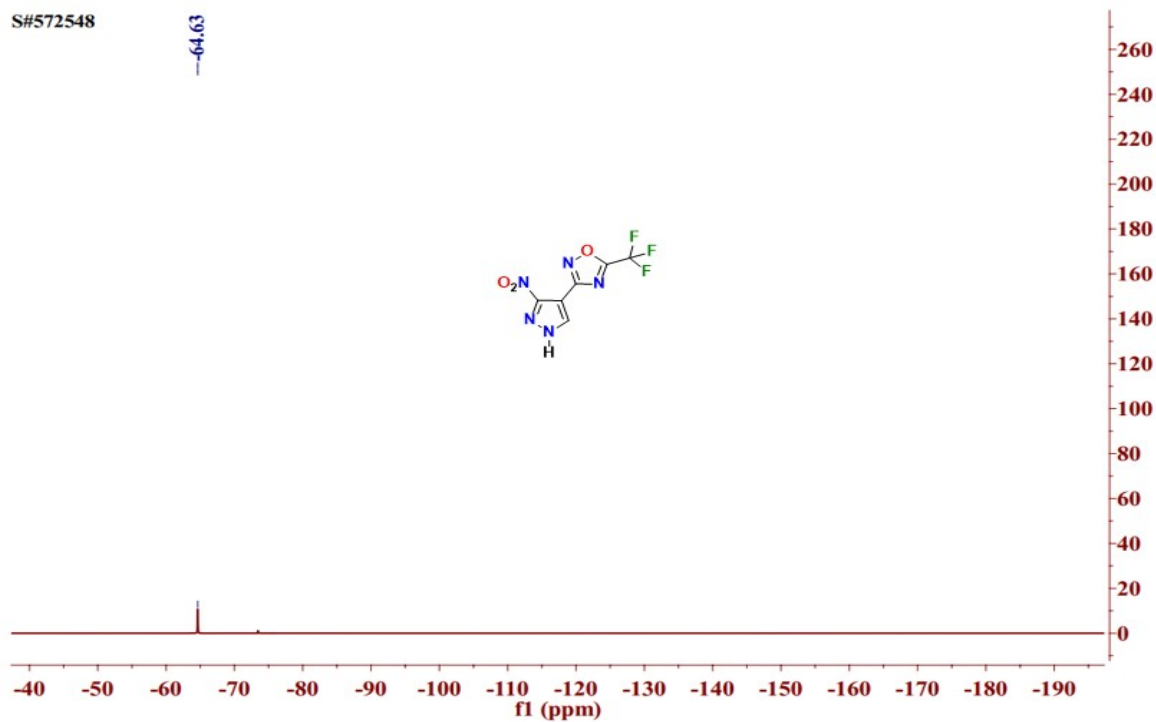


Figure S13. ^{19}F -NMR for compound 4 in $\text{DMSO-}d_6$.

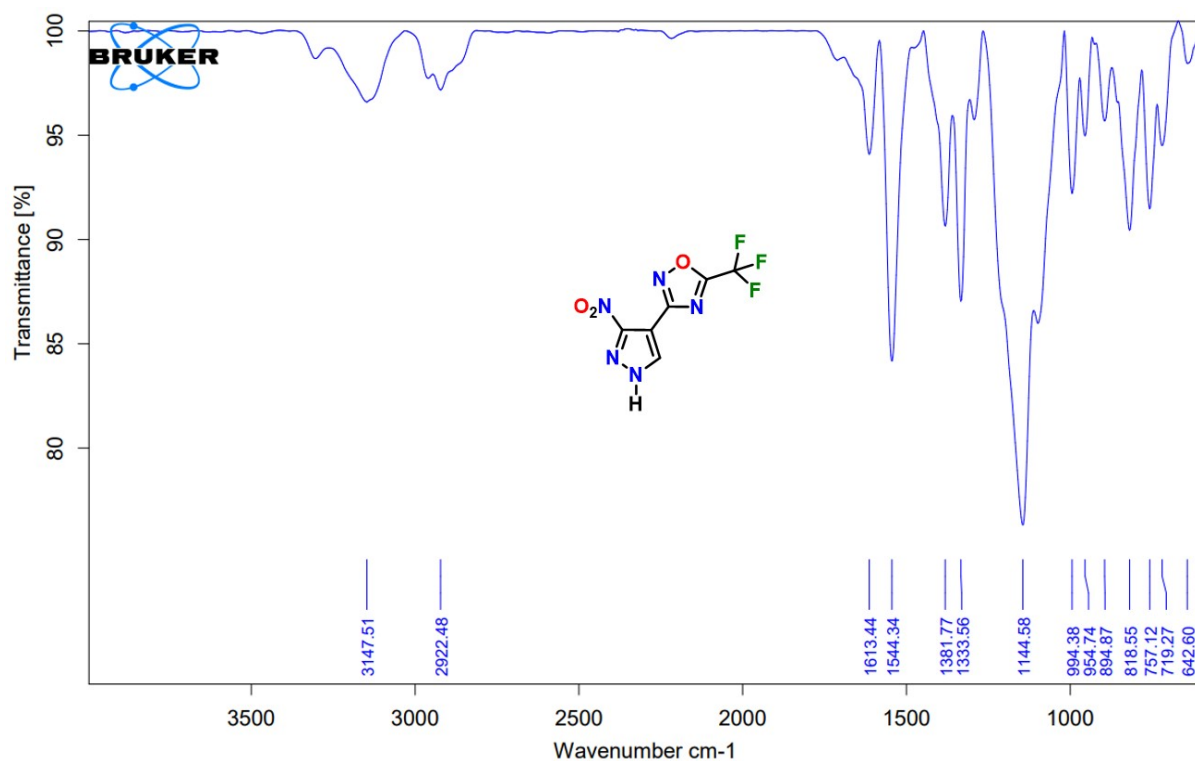


Figure S14. IR spectra for compound 4.

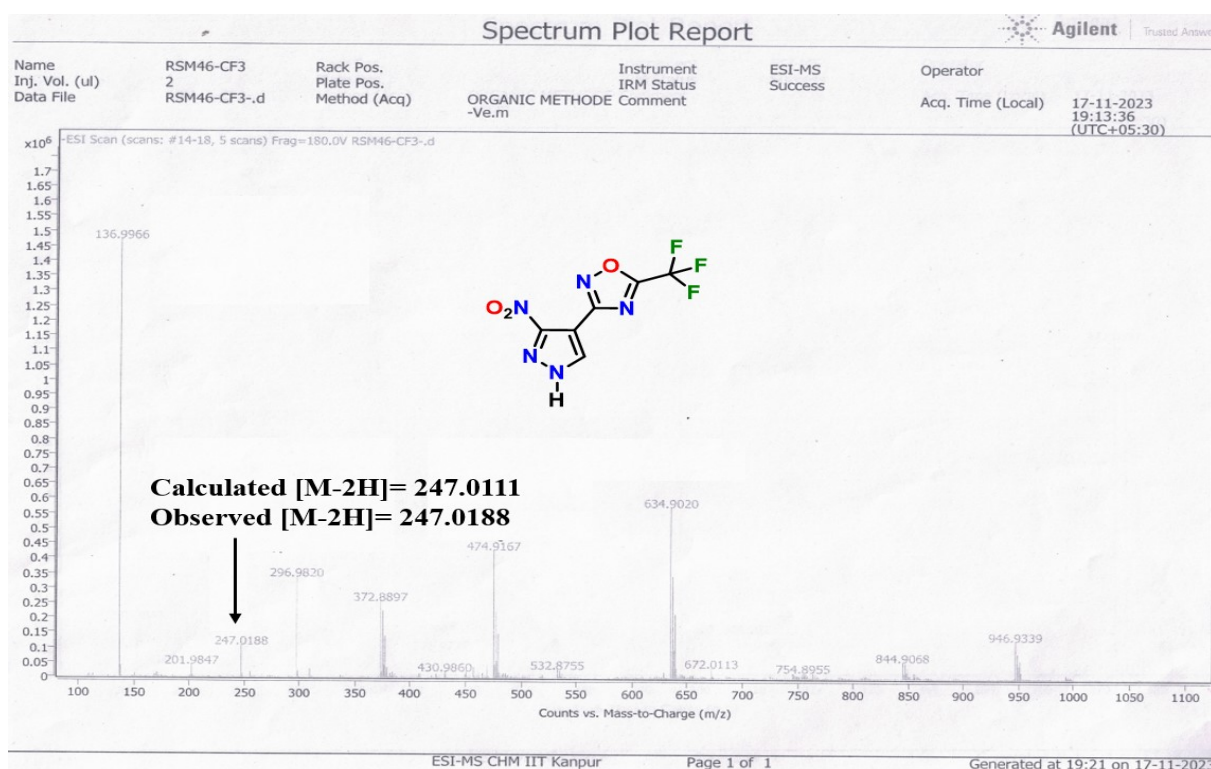


Figure S15. Mass spectra for compound 4.

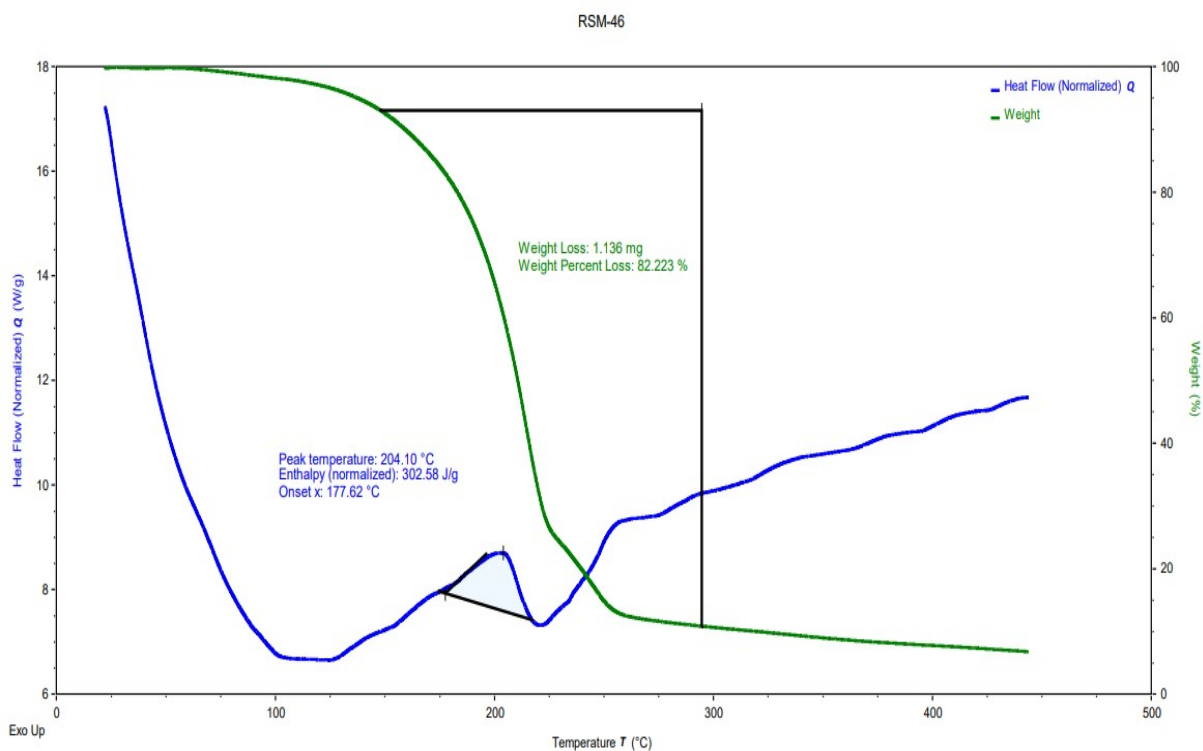


Figure S16. TGA-DSC for compound **4** at heating rate 5 °C min⁻¹.

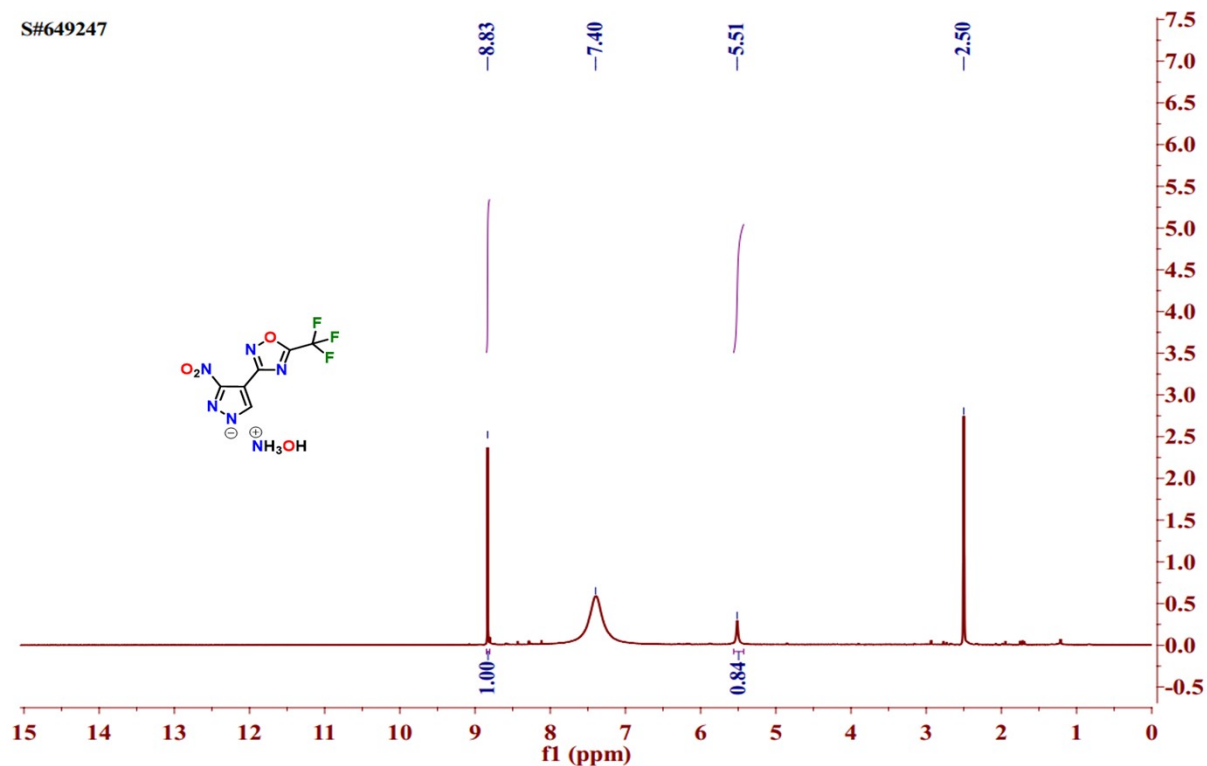


Figure S17. ¹H-NMR for compound **5** in DMSO-*d*₆.

RSM-86AD
single_pulse

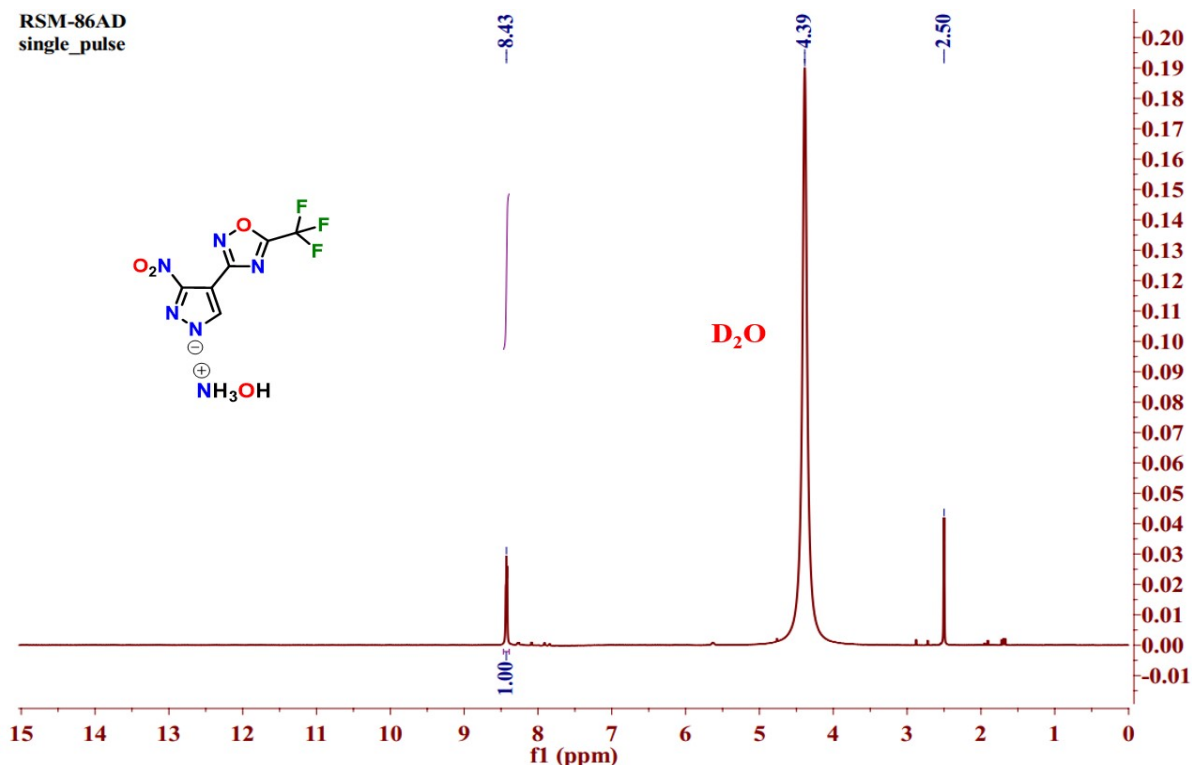


Figure S18. ^1H -NMR for compound 5 in $\text{DMSO-}d_6 + \text{D}_2\text{O}$.

S#109826

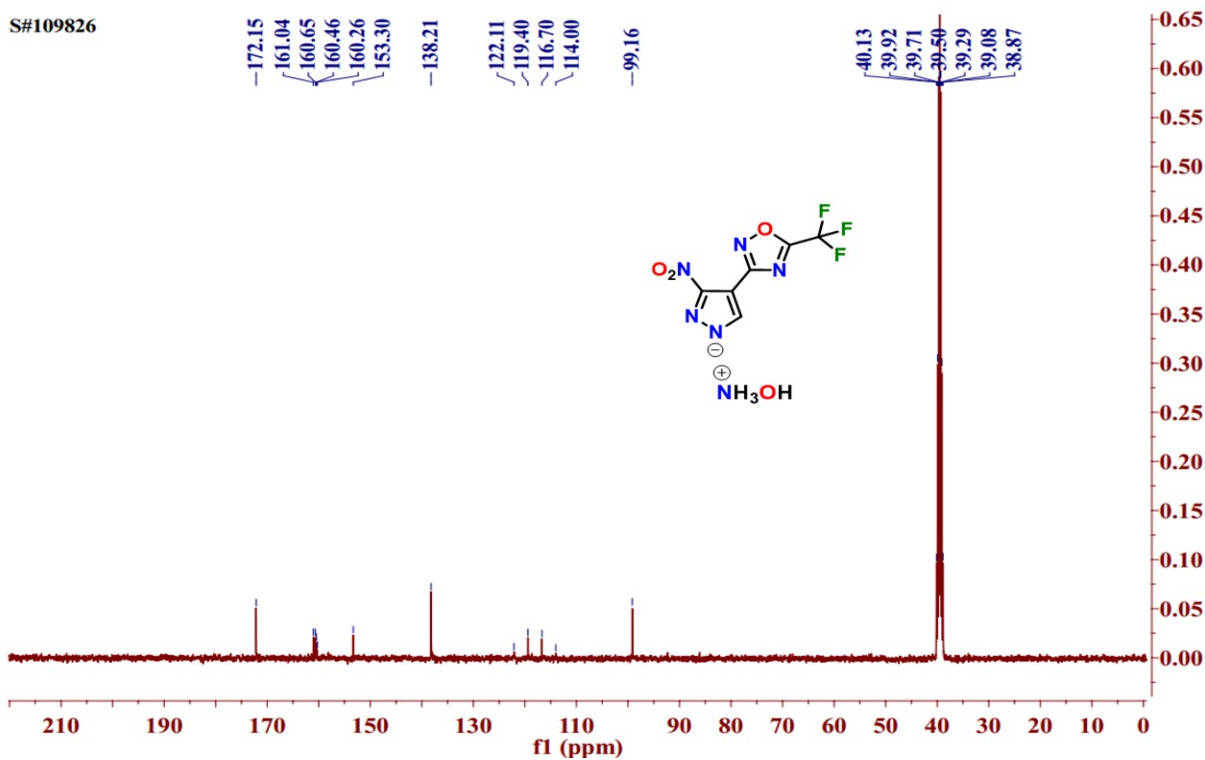


Figure S19. ^{13}C -NMR for compound 5 in $\text{DMSO-}d_6$.

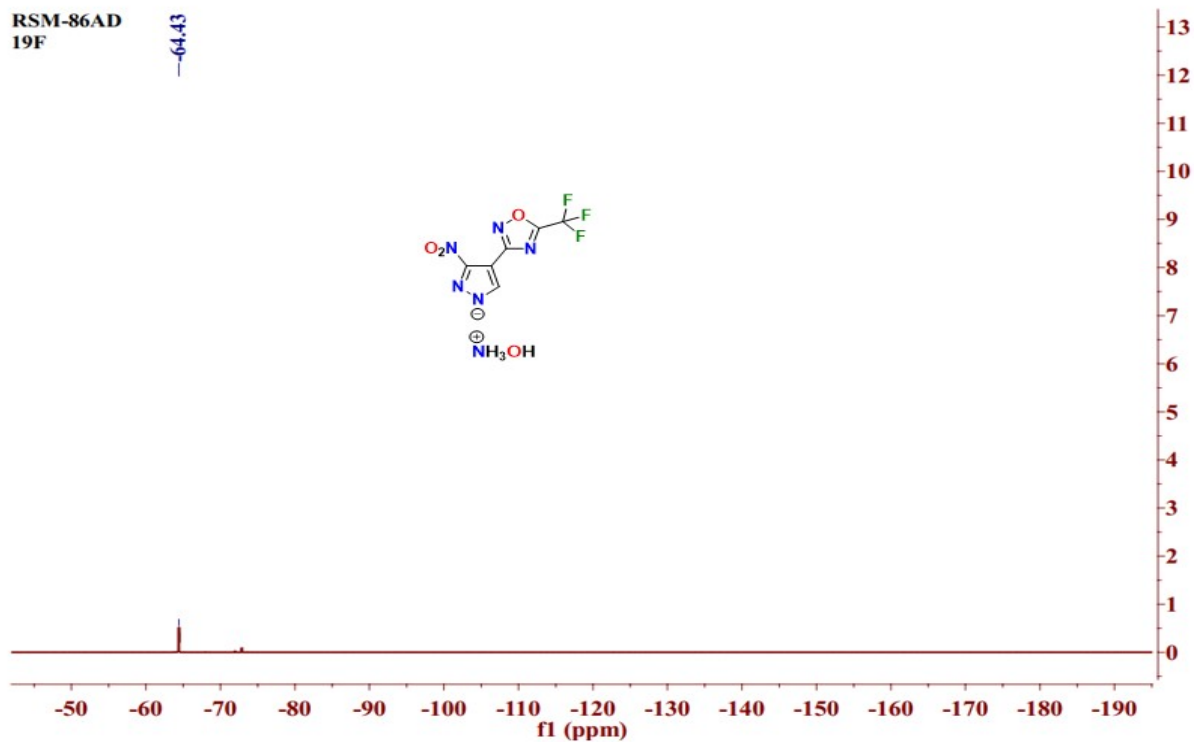


Figure S20. ^{19}F -NMR for compound 5 in $\text{DMSO-}d_6$.

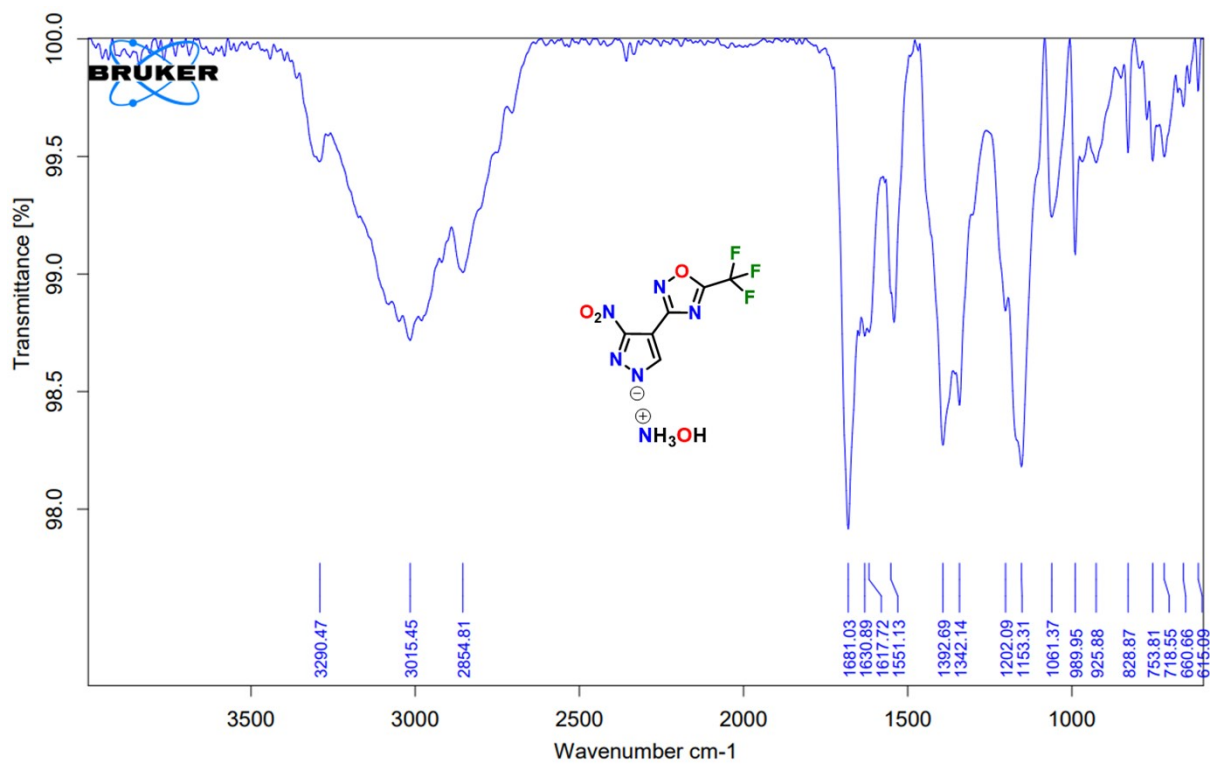


Figure S21. IR spectra for compound 5.

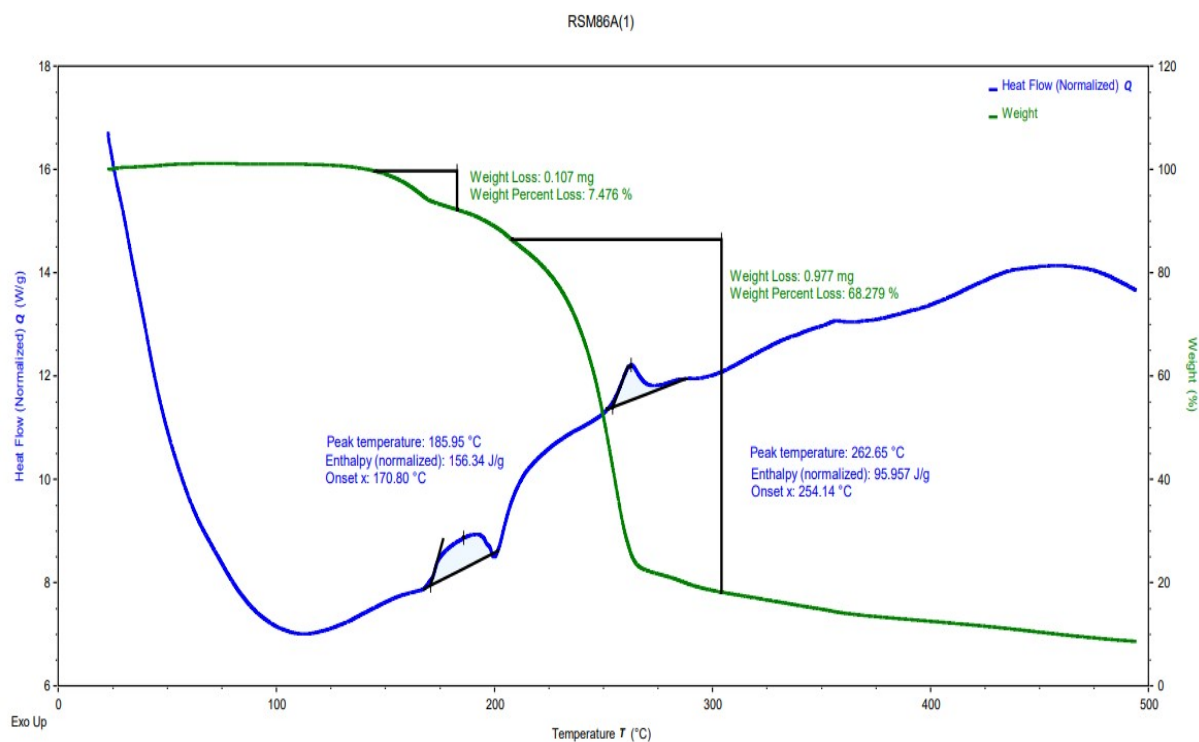


Figure S22. TGA-DSC for compound **5** at heating rate 5 $^{\circ}\text{C min}^{-1}$.

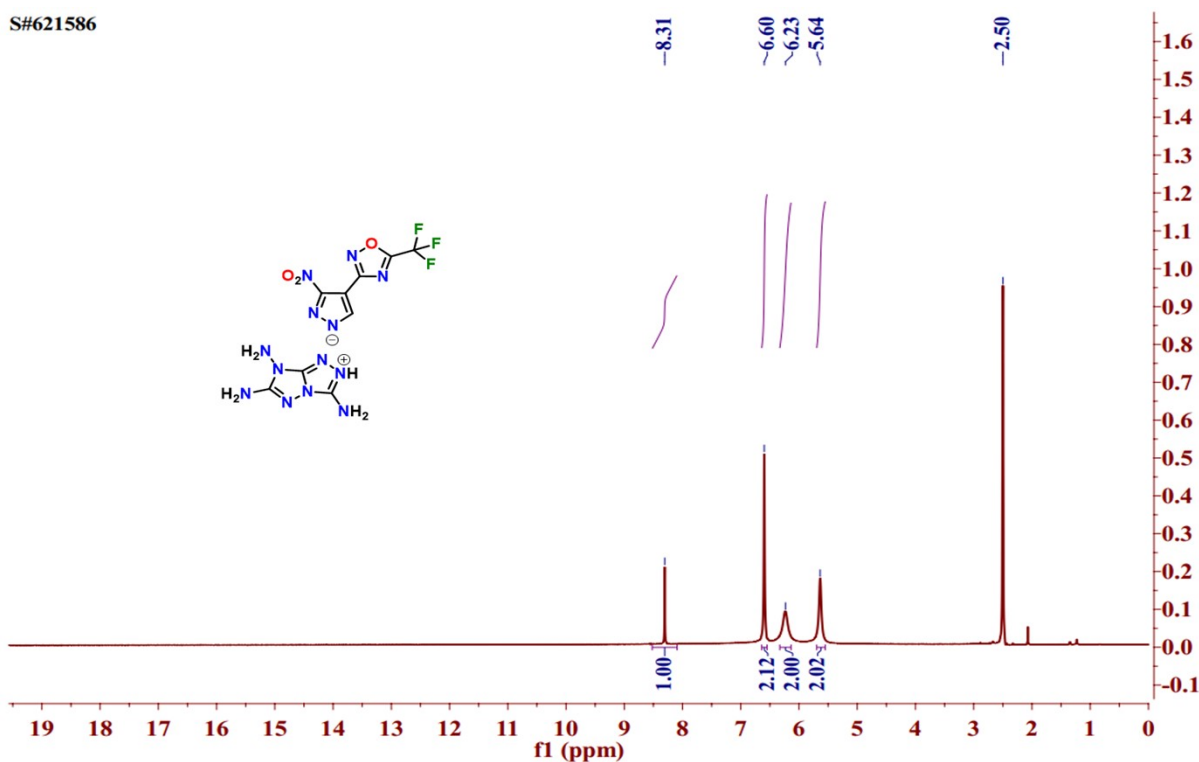


Figure S23. $^1\text{H-NMR}$ for compound **6** in $\text{DMSO-}d_6$.

S#664603

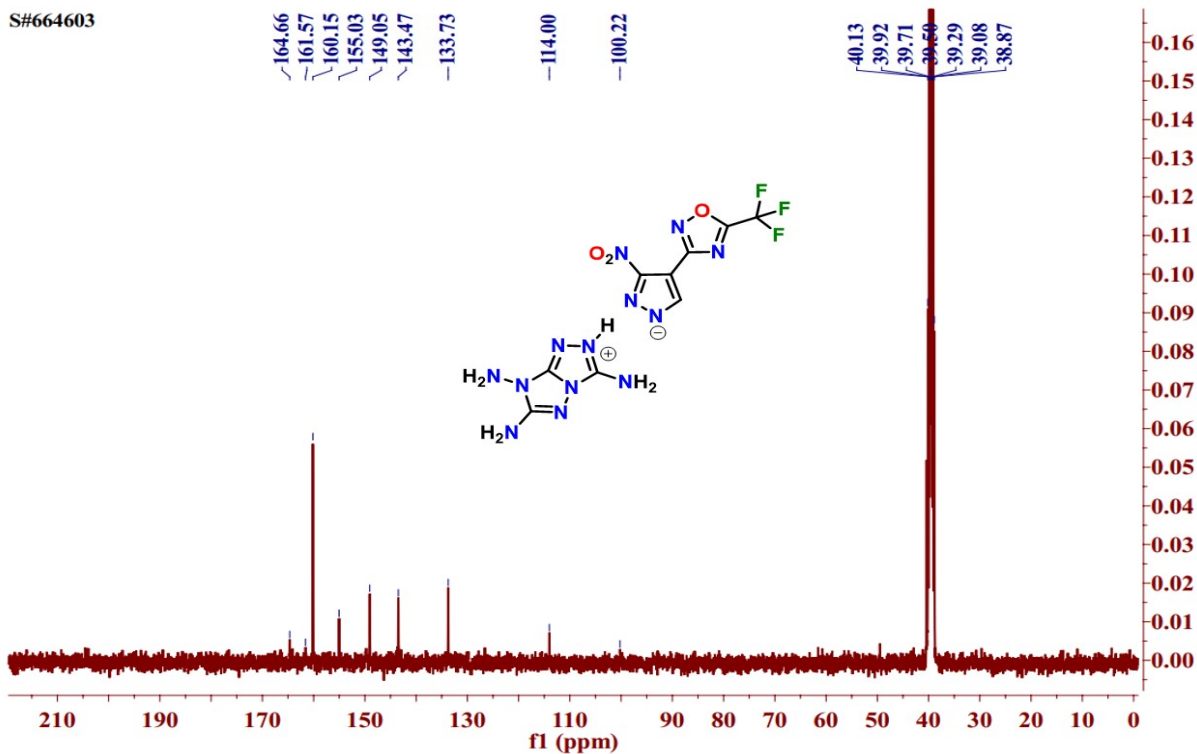


Figure S24. ^{13}C -NMR for compound 6 in $\text{DMSO-}d_6$.

S#617929

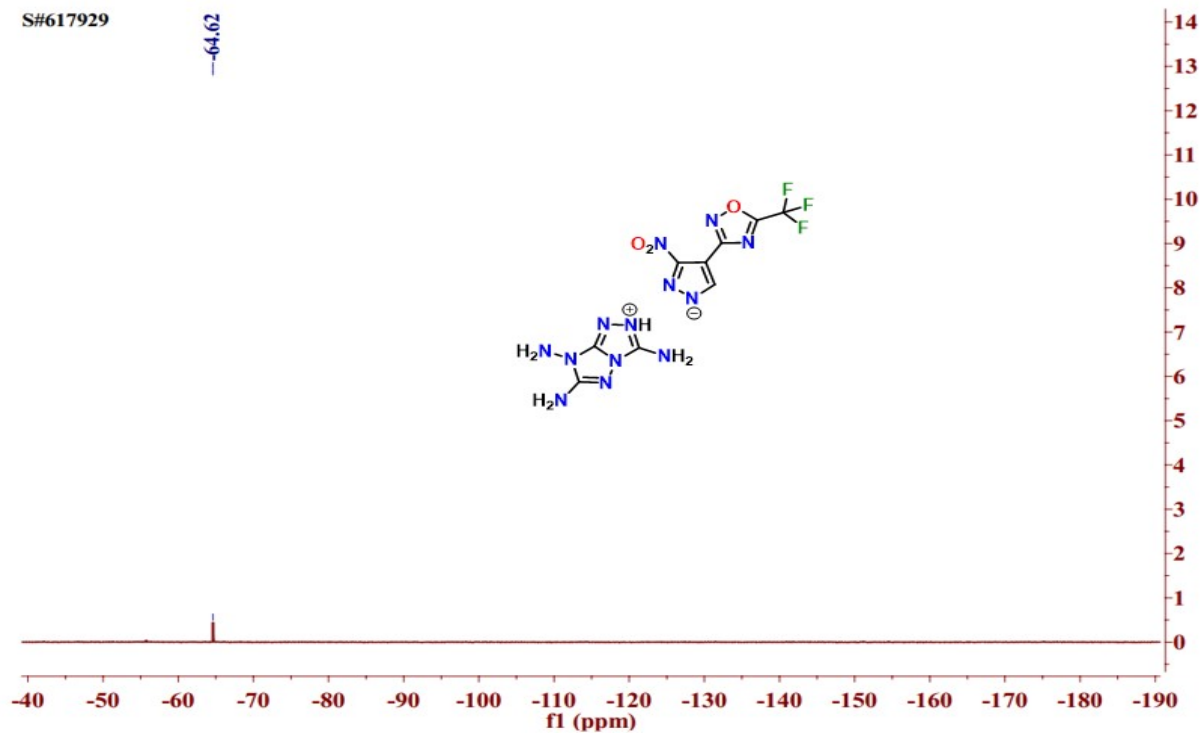


Figure S25. ^{19}F -NMR for compound 6 in $\text{DMSO-}d_6$.

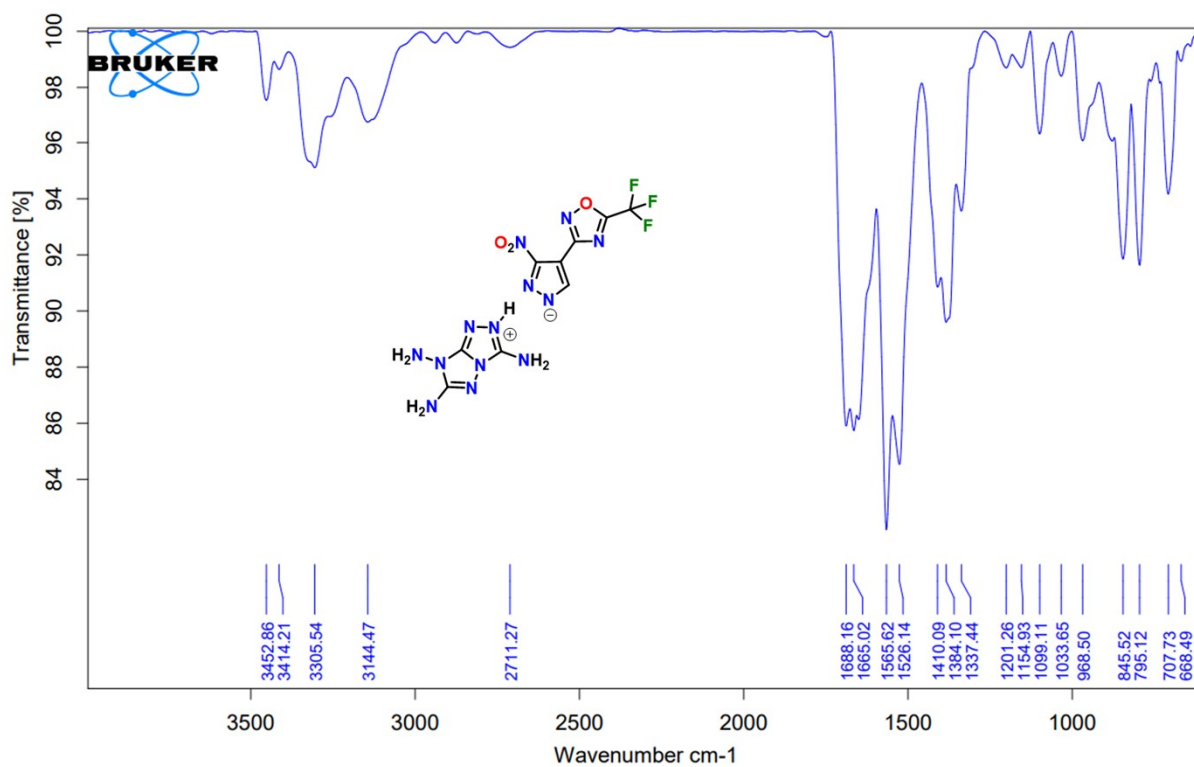


Figure S26. IR spectra for compound 6.

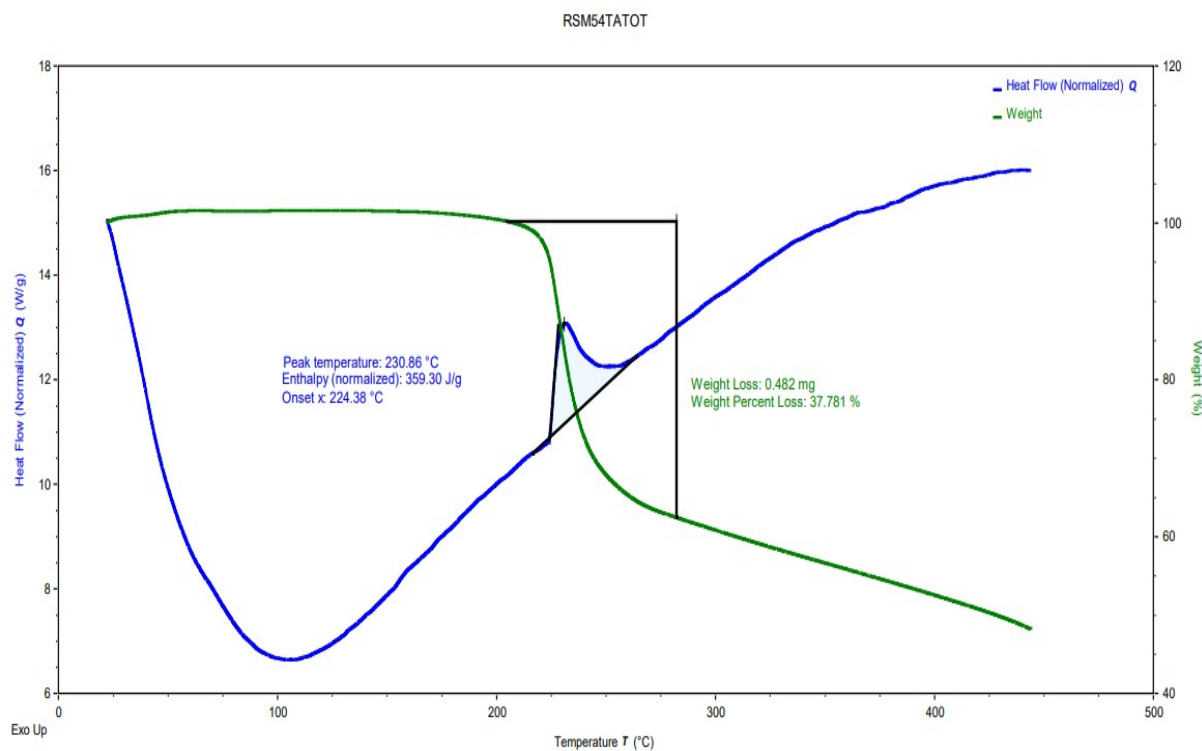


Figure S27. TGA-DSC for compound 6 at heating rate 5 °C min⁻¹.

S#617423

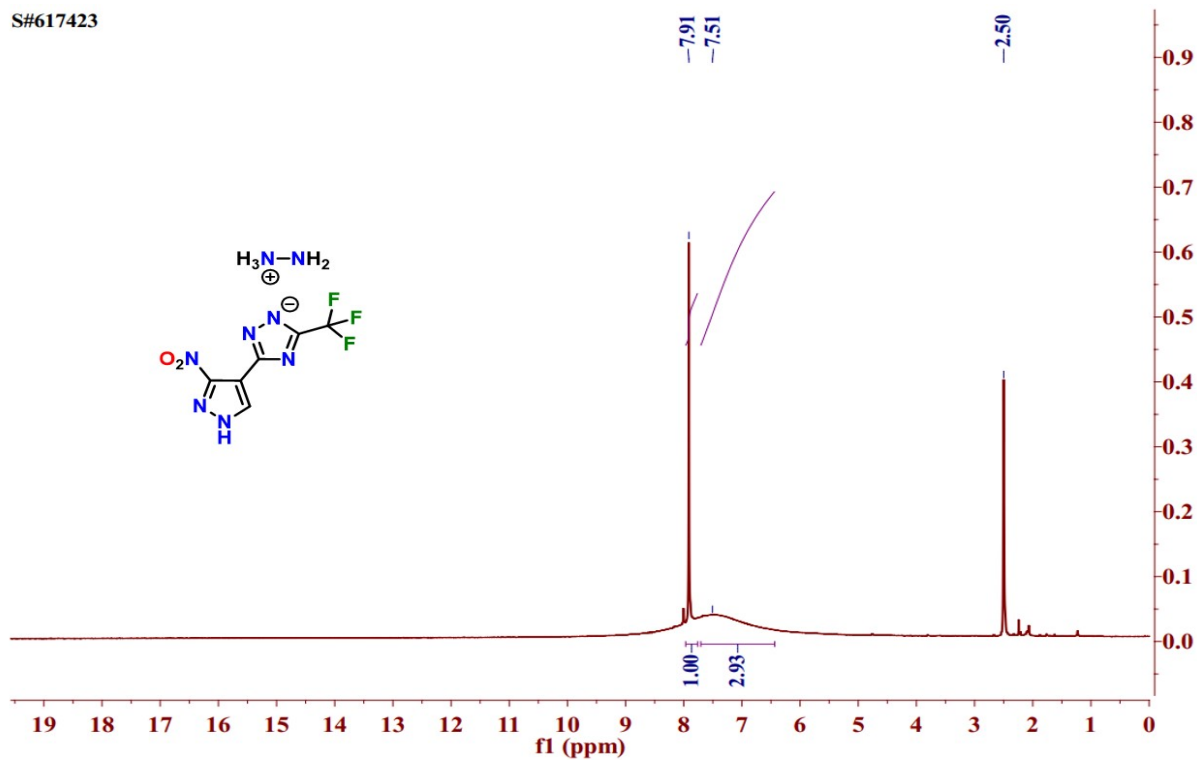


Figure S28. $^1\text{H-NMR}$ for compound 7 in $\text{DMSO-}d_6$.

S#613833

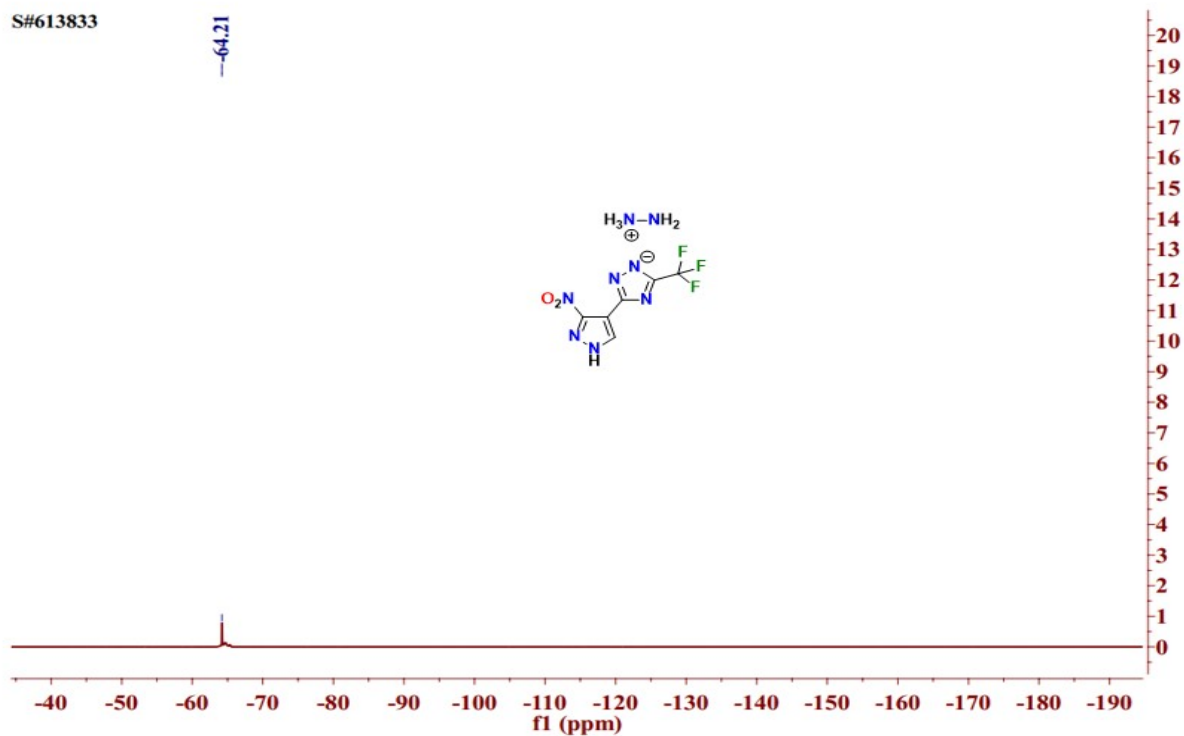


Figure S29. $^{19}\text{F-NMR}$ for compound 7 in $\text{DMSO-}d_6$.

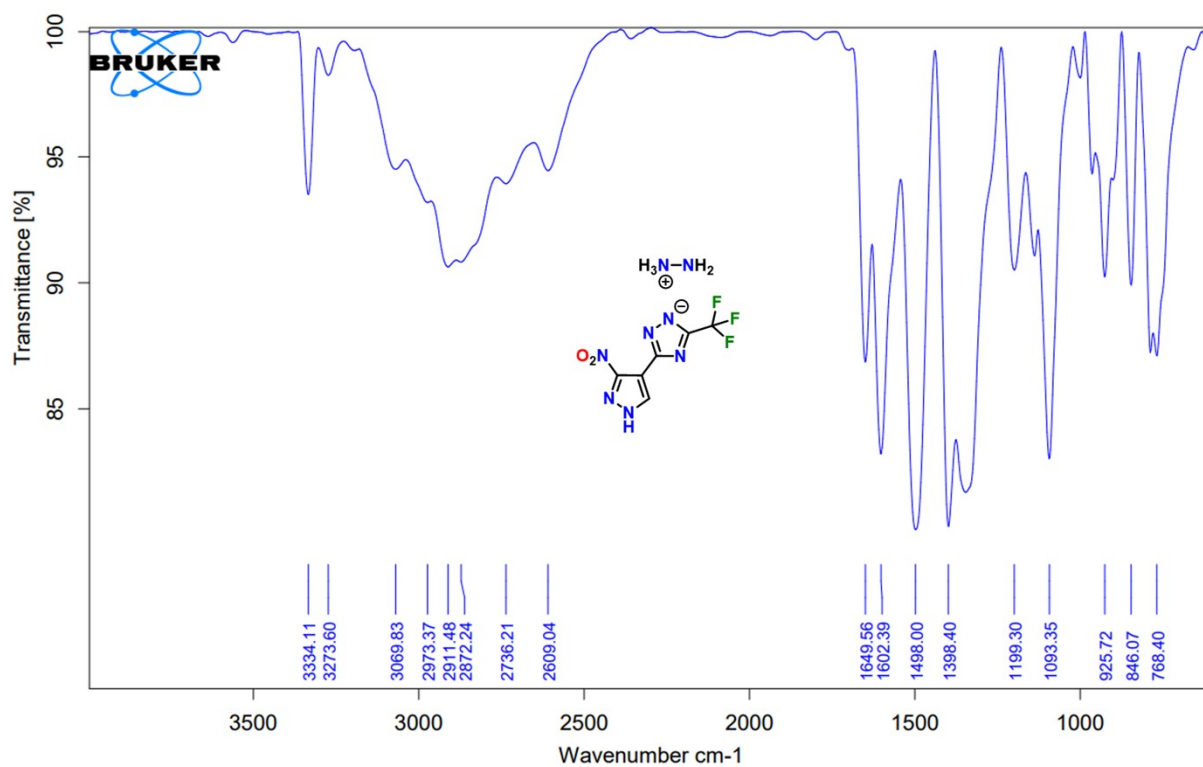


Figure S30. IR spectra for compound 7.

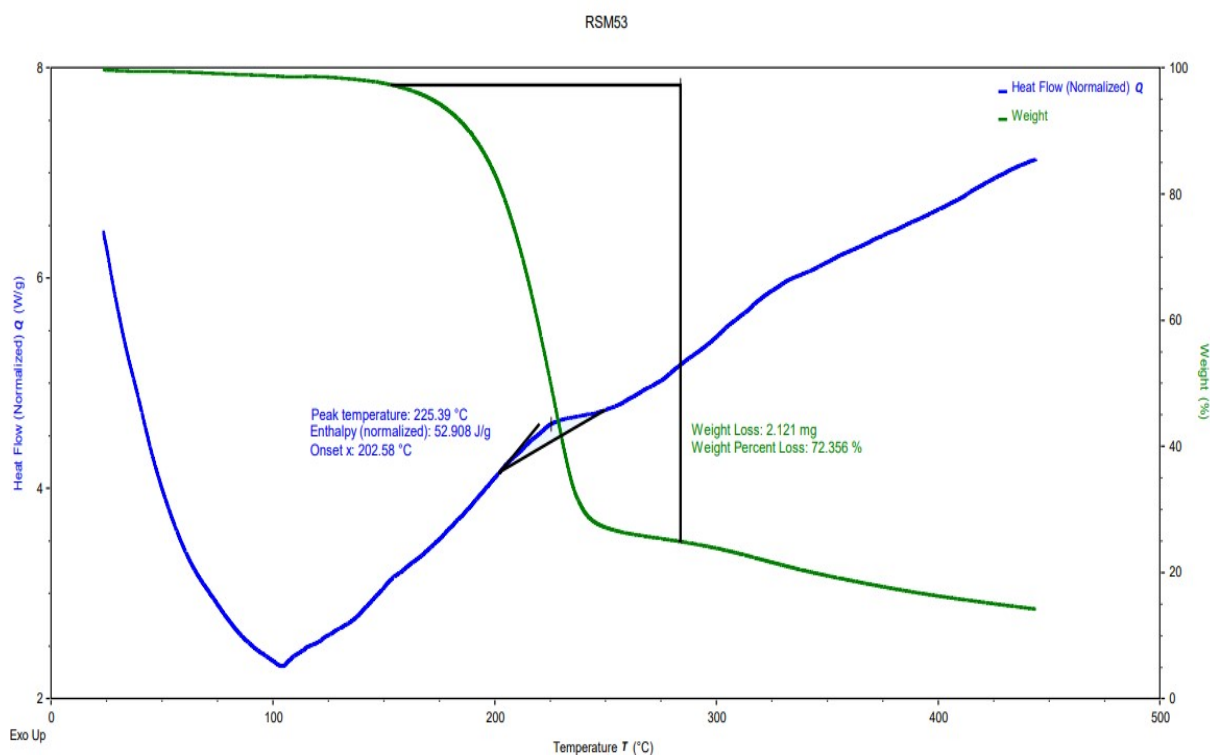


Figure S31. TGA-DSC for compound 7 at heating rate 5 $^{\circ}\text{C min}^{-1}$.

Computational details:

Computations were carried out using the Gaussian 09 program suite.⁸ The structure optimizations are performed with M06-2X/def2-TZVPP level of theory and characterized to be true local energy minima on the potential energy surface and no imaginary frequencies were

found. Isodesmic reactions have been designed to predict the gas phase HOF (HOF_{gas}) and are shown in Figure S32. The total energies (E_0), zero-point correction (ZPE), thermal corrections (H_T), and the experimental/calculated HOF values of the reference compounds used in isodesmic reactions and other derivatives are given in Tables S16 and S17. The usage of HOF_{gas} in the calculation of detonation properties slightly overestimates the values of detonation velocity and detonation pressure, and hence, the solid phase HOF ($\text{HOF}_{\text{solid}}$) can effectively reduce the errors. The $\text{HOF}_{\text{solid}}$ is calculated as the difference between HOF_{gas} and heat of sublimation (HOF_{sub}) as,

$$\text{HOF}_{\text{solid}} = \text{HOF}_{\text{gas}} - \text{HOF}_{\text{sub}} \quad (1)$$

HOF_{sub} depend on the molecular surface properties and calculated using equation (2) proposed by Politzer et al.,⁹

$$\text{HOF}_{\text{sub}} = 4.4307 \times 10^{-4} A^2 + 2.0599 (\nu \sigma_{\text{tot}}^2)^{0.5} - 2.4825 \quad (2)$$

where A represent the surface area of the 0.001 electrons/bohr³ isosurface of electronic density, ν denotes the degree of balance between the positive and negative surface potentials, and σ_{tot}^2 is the electrostatic potential variance. The molecular surface properties (see Table S18) were obtained using the Multiwfn program.¹⁰ The HOF of energetic salts were predicted using Born–Haber cycle (Figure S33) and can be simplified by the equation (3),

$$\text{HOF}(\text{salt}, 298 \text{ K}) = \text{HOF}(\text{cation}, 298 \text{ K}) + \text{HOF}(\text{anion}, 298 \text{ K}) - H_L \quad (3)$$

in above equation, H_L is the lattice energy of the salts (see Table S19), which can be predicted by using the formula proposed by Jenkins et al.¹¹

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

The nature of the cation M_p^+ and anion X_q^- decide n_M and n_X values, respectively and are equal to three for monoatomic ions, five for linear polyatomic ions, and six for nonlinear polyatomic ions. U_{POT} is the lattice potential energy, calculated using the density (ρ in g/cm³) and the chemical formula mass (M in g/mol) of the ionic salt.

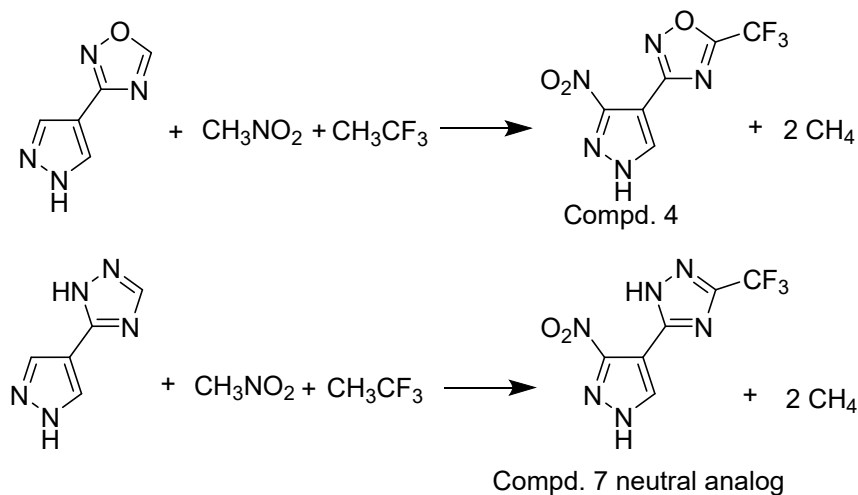


Figure S32. Designed isodesmic reactions for the prediction of HOF_{gas} of compounds **2** and **5**.

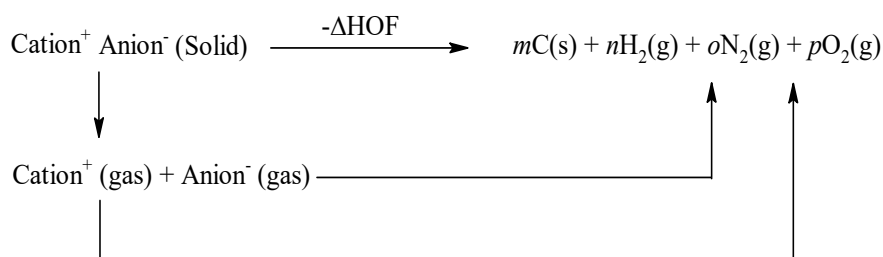
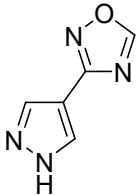


Figure S33. Born-Haber cycle for the formation of energetic salts.

Table S16. Calculated total energies at 298K (E_0), zero-point energies (ZPE), and thermal corrections (H_T) and experimental HOF_{gas} of reference compounds used isodesmic reaction at the M06-2X/def2-TZVPP level.

Compd.	E_0 (a.u.)	ZPE (au)	H_T (au)	HOF_{gas} (kJ/mol)
	-487.000649	0.1004	0.0080	274.6

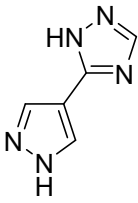
	-467.149286	0.1135	0.0081	375.8
CH ₄	-40.453065	0.0449	0.0038	-74.8
CH ₃ CF ₃	-377.53801	0.0530	0.0057	-748.7
CH ₃ NO ₂	-244.955044	0.0506	0.0053	-81

Table S17. Calculated total energies at 298K (E_0), zero-point energies (ZPE), and thermal corrections (H_T) and experimental HOF_{gas} of target compounds at the M06-2X/def2-TZVPP level.

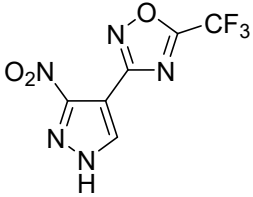
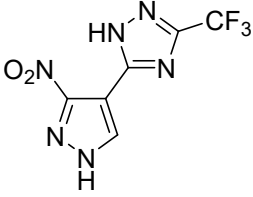
Compd.	E_0 (a.u.)	ZPE (au)	H_T (au)
	-1028.564079	0.1082	0.0141
	-1008.72661	0.1214	0.0142

Table S18. Calculated molecular surface properties and heat of sublimation of target compounds.

Compd.	Surface area (\AA^2)	Volume (\AA^3)	σ_{tot}^2 (kcal/mol) ²	ν	$\text{HOF}_{\text{Sublimation}}$ (kJ/mol)

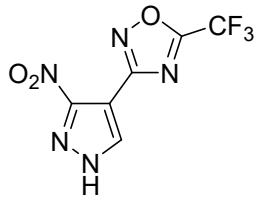
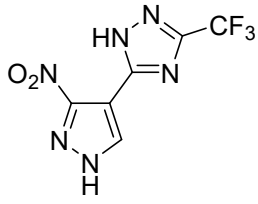
	220.0	217.40	358.52	0.1822	122.34
	226.11	222.65	330.04	0.1478	117.80

Table S19. Energy content of salts **6-8**.

Salt	HOF _c ^a	HOF _a ^b	U _{Pot} ^c	H _L ^d	HOF _{salt} ^e
5	675.6	-585.6	465.72	470.67	-380.67
6	1112.0	-585.6	423.85	428.81	97.59
7	769.5	-555.8	470.05	475.01	-261.31

^aHeat of formation of cation (kJ mol⁻¹). ^bHeat of formation of anion (kJ mol⁻¹). ^cLattice potential energy (kJ mol⁻¹). ^dLattice energy (kJ mol⁻¹). ^eHeat of formation of salt (kJ mol⁻¹).

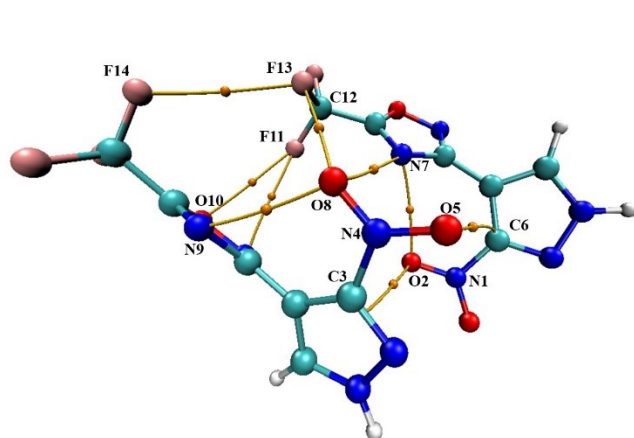
Oxygen balance (OB) is one of the methods of quantifying how well an explosive provides its own oxidant.¹² Most of the energy released comes from oxidation (reaction with oxygen), the amount of oxygen available is a critical factor. For an explosive which contains only some or all of the atoms: aluminium, boron, carbon, calcium, chlorine, fluorine, hydrogen, potassium, nitrogen, sodium and oxygen (with the formula Al_{al}, B_b, C_c, Ca_{ca}, Cl_{cl}, F_f, H_h, K_k, N_n, Na_{na}, O_o), the oxygen balance will be;

$$OB (\%) = - \frac{32 \left(\frac{3}{4}al + \frac{3}{4}b + 1c + \frac{1}{2}ca - \frac{1}{4}cl - \frac{1}{4}f + \frac{1}{4}h + \frac{1}{4}k + 0n + \frac{1}{4}na - \frac{1}{2}o \right)}{\text{Molecular weight of explosive}} \times 100$$

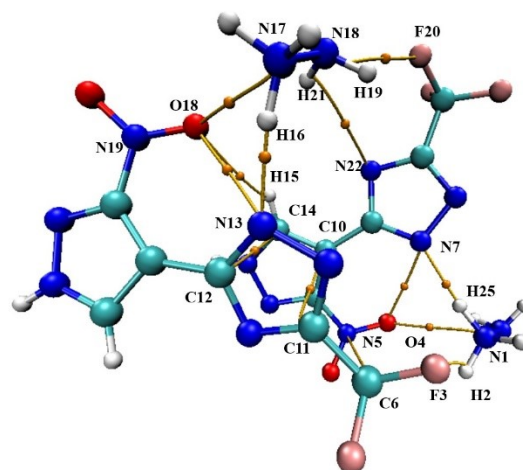
Table S20. Computed stabilizing interactions and hydrogen bond energy (E_H) using the QTAIM topological parameters at the (3,-1) bond critical point for compounds **4** and **7**.

Compd.	Interaction	Bond Length (Å)	E _H (kJ/mol)	Total E _H (kJ/mol)
4	N1-O2...C3	2.975	-7.86	-48.78

	C4-N5...O6	2.984	-9.52	
	N7-O8...C	2.975	-1.46	
	N4-O8...N7	2.890	-7.20	
	C12-F11...N9	3.186	-3.07	
	C12-F11...O15	3.108	-5.35	
	C12-F11...O10	2.901	-3.17	
	N4-O8...N7	2.890	-9.67	
	C12-F13...F14	3.341	-1.48	
7	N1-H2...F3	2.562	-6.14	-155.13
	N1-H25...N7	3.153	-1.73	
	N5-O4...N1	2.850	-10.05	
	C14-H15...O18	2.742	-3.53	
	N5-O4...N7	2.909	-10.00	
	N17-H16...N13	1.844	-45.69	
	C10-H23...C11	3.306	-4.36	
	N18-H21...N22	1.844	-45.51	
	N19-O18...N13	2.909	-9.95	
	N5-C6...C24	3.889	-2.95	
	N19-O18...N17	2.520	-10.09	
	N18-H19...F20	3.010	-5.14	



4



7

Figure S34. Molecular structures of compounds **4** and **7** and their corresponding intramolecular hydrogen-bonding interactions.

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