Supporting Information

Insights into Triazole-Based Energetic Material Design from Decomposition Pathways of Triazole Derivatives

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1. Materials and methods

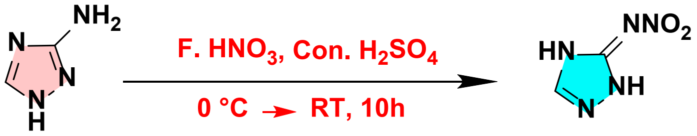
1.1 Materials

The required reagents and solvents were purchased from Sigma Aldrich, Avra, Isochem, or Qualigens-Thermo Fisher Scientific, and used without further purification.

NMR spectra were recorded on a JEOL 500 MHz NMR Spectrometer with dimethyl sulfoxide (DMSO-d_6) as the solvent. Chemical shift values are reported in δ units (parts per million) relative to tetramethylsilane (TMS) as an internal standard.

1.2 Synthesis

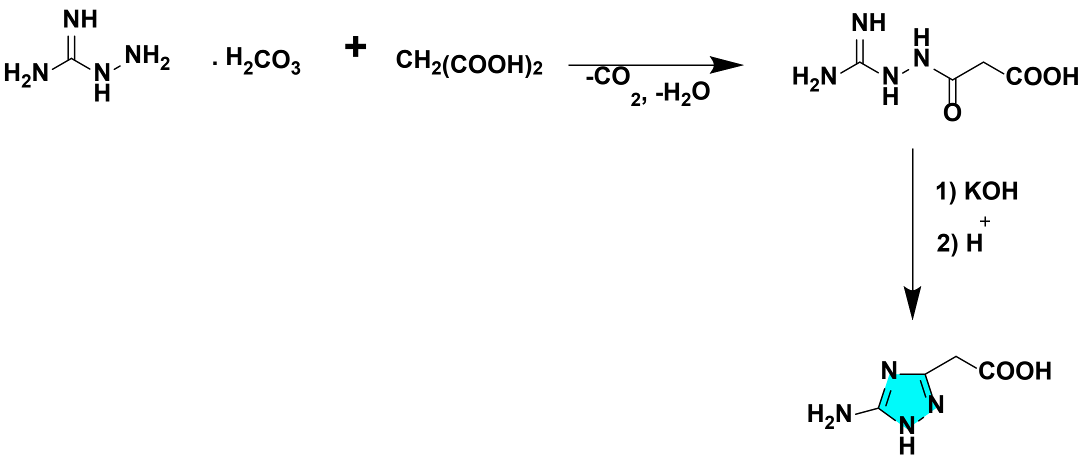
*1.2.1 Synthesis of 2,4-Dihydro-3H-1,2,4-triazol-3-ylidene-nitramide (Compound **2**):*[1]



Scheme. S1 Synthesis scheme of compound **2**

To a cold mixture of fuming nitric acid (2.5 mL) and concentrated sulphuric acid (3 mL), 3-amino-1,2,4-triazole (0.5g, 5.9 mmol) was added portion-wise. The resulting reaction mixture was stirred at room temperature for 10 hours and poured into ice-cold water. The precipitate formed was filtered off and dried under vacuum to obtain 2,4-Dihydro-3H-1,2,4-triazol-3-ylidene-nitramide as a white solid (0.69g, 91%). ^{1}H NMR (500 MHz, DMSO-d_6) δ: 14.18 (br. s, 2H), 8.45 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ: 152.72, 139.52; HRMS (ESI-TOF): calculated for $C_2H_2N_5O_2^-$ $[M-H]^-$:128.0214, found: 128.0211.

*1.2.2 Synthesis of 5-amino-1,2,4-triazole-3-yl-acetic acid (Compound **3**):*[2]



Scheme. S2 Synthesis scheme of compound **3**

Aminoguanidine hydrogen carbonate (3.4g, 25 mmol) was added gradually to a hot solution (60-70 °C) of malonic acid (2.6g, 25 mmol) in water (7.5 mL). Then the mixture was heated in a water bath for 4 hours and then cooled to room temperature. Potassium hydroxide (2.5g, 44.5 mmol) was added to it and the resulting mixture was heated at 100 °C for 2 hours. The mixture was then cooled and acidified with concentrated hydrochloric acid to pH 3-4. The precipitate formed was filtered off and dried to obtain 5-amino-1,2,4-triazol-3-yl-acetic acid as a white solid (2.3g, 65%). ^{1}H NMR (500 MHz, DMSO-d_6) δ: 5.74 (br. s, 2H), 3.322 (s, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ: 171.07, 157.93, 153.98, 34.56; HRMS (ESI-TOF): calculated for $C_4H_5N_4O_2^-$ $[M-H]^-$:141.0418, found: 141.0418.

1.3 HRMS analysis

The source temperature applied was 120 °C, and the desolvation gas flow was maintained at 900 L/h with a desolvation temperature of 400 °C. The capillary voltage was at 2.8 kV, and a cone voltage of 35 V was used. All the tandem mass spectra (MS/MS) were recorded using argon as the collision gas with a collision energy of 20 V. The obtained mass fragments were fitted to the possible molecular formulas using the i-Fit software available with the instrument.

1.4 Kinetics analysis

In Vyazovkin's method[3], for a set of 'n' experiments are conducted at different heating rates, the apparent activation energy can be determined at any given value of α by identifying the value of E_α for which the given function, Eq. (2), is a minimum. Here, β represents the heating rate, i and j are the set of experiments performed under different heating rates, and n is the total number of experiments performed. The third-degree approximation shown in Eq. (4) [4] was used to calculate the integral in Eq. (3). MATLAB R2020a was used to perform the kinetic computations.

$$\sum_{i}^{n}\sum_{j\neq i}^{n}[I\,(E_{\alpha},T_{\alpha,\mathrm{i}})\beta_j]/[\,I\,(E_{\alpha},T_{\alpha,\mathrm{j}})\beta_i] = min \ldots\ldots\ldots (2)$$

$$\text{Where, } I\,(E,T) = \int_0^T e^{-(\frac{E}{RT})}\,dT \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

$$f(x) = \frac{e^{-x}}{x} \times \frac{x^2+10x+18}{x^3+12x^2+36x+24} \ldots\ldots\ldots\ldots\ldots\ldots (4)$$

$$\text{Where, } x = \frac{E}{RT} \quad \text{and } I(E,T) = \frac{E}{R} f(x) \ldots\ldots\ldots\ldots\ldots (5)$$

2. Characterization data:

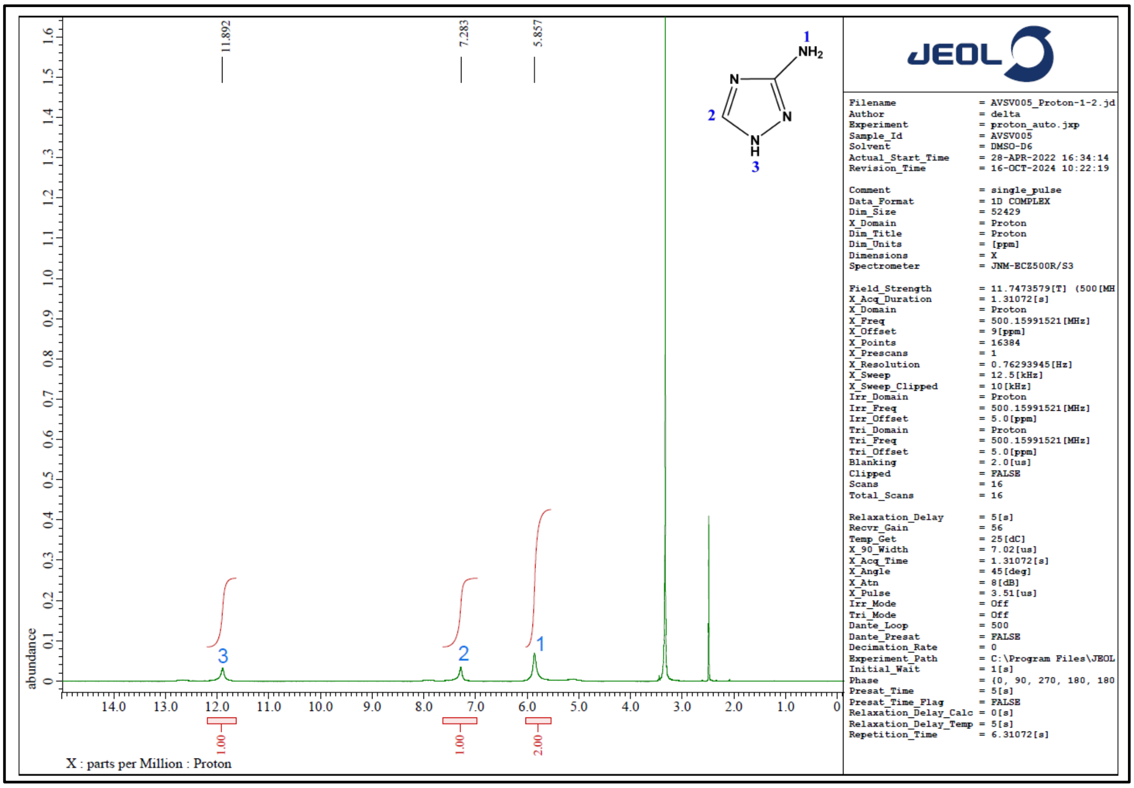


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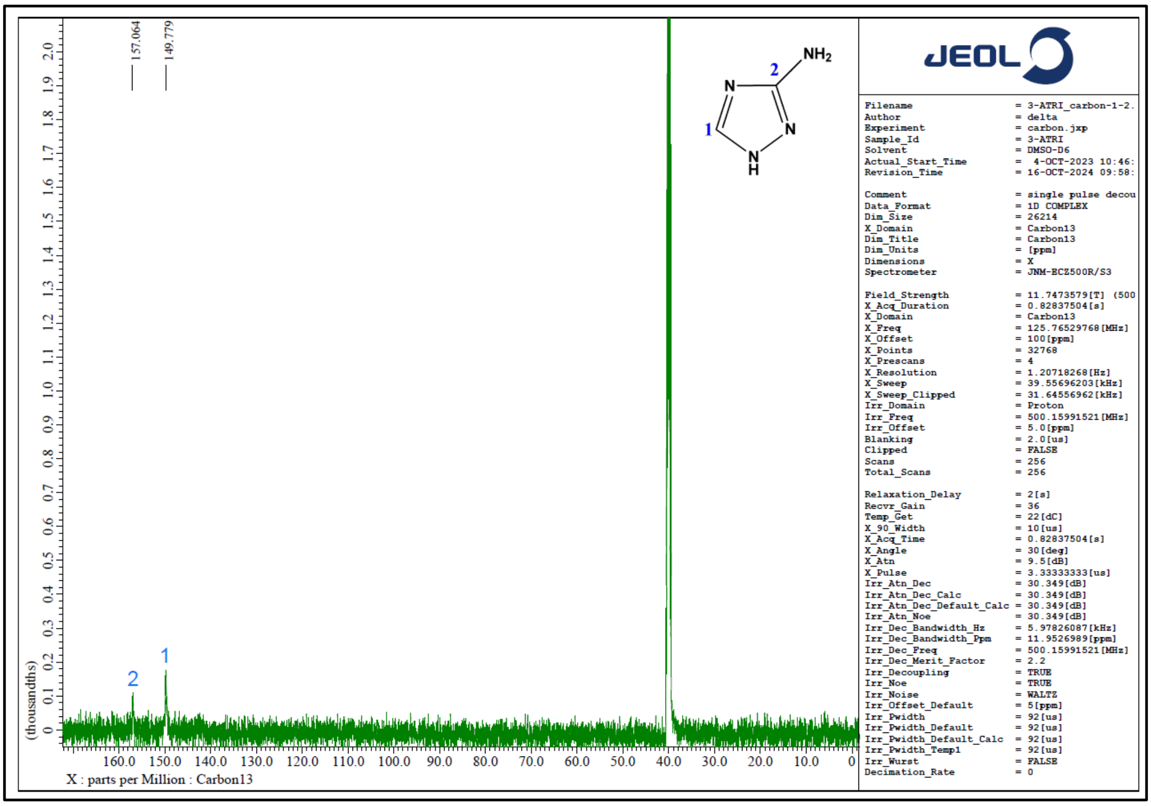
Fig. S1 ^{1}H NMR spectrum of compound **1** in DMSO-d$_6$



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X_Sweep_Clipped             = 31.64556962[kHz]
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Irr_Noe                     = TRUE
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Fig. S2 ^{13}C NMR spectrum of compound **1** in DMSO-d$_6$

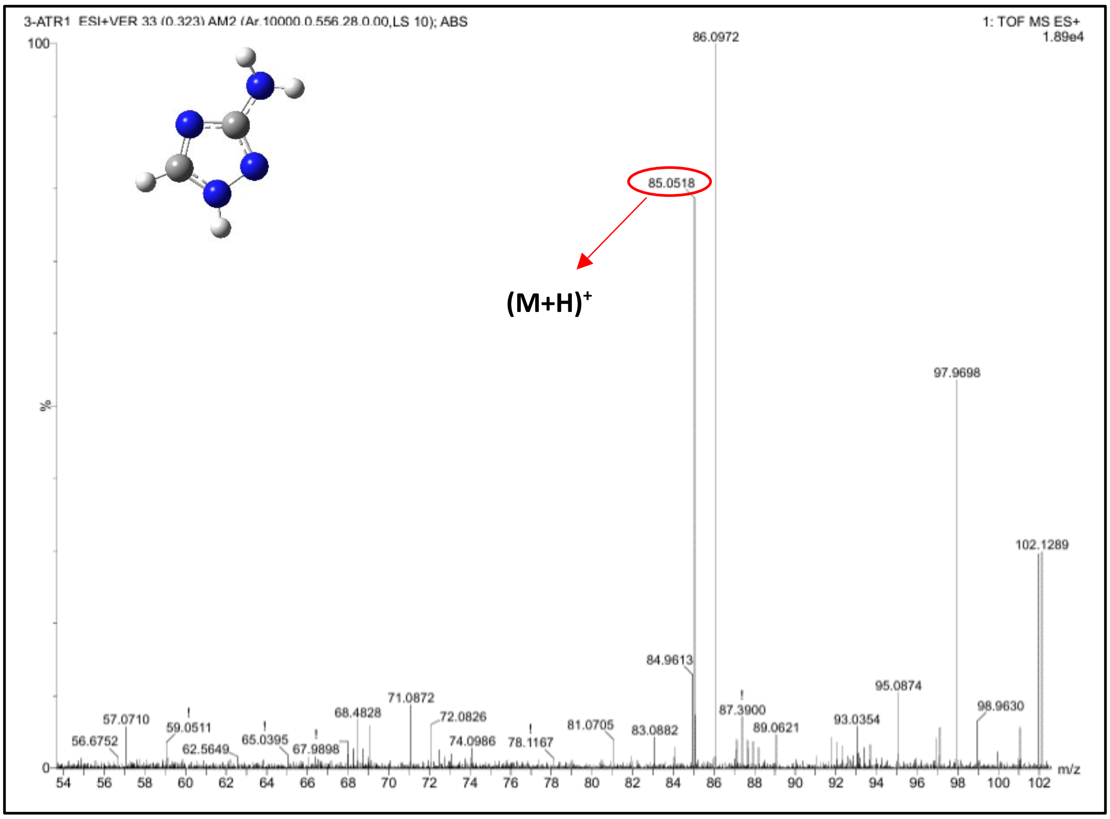
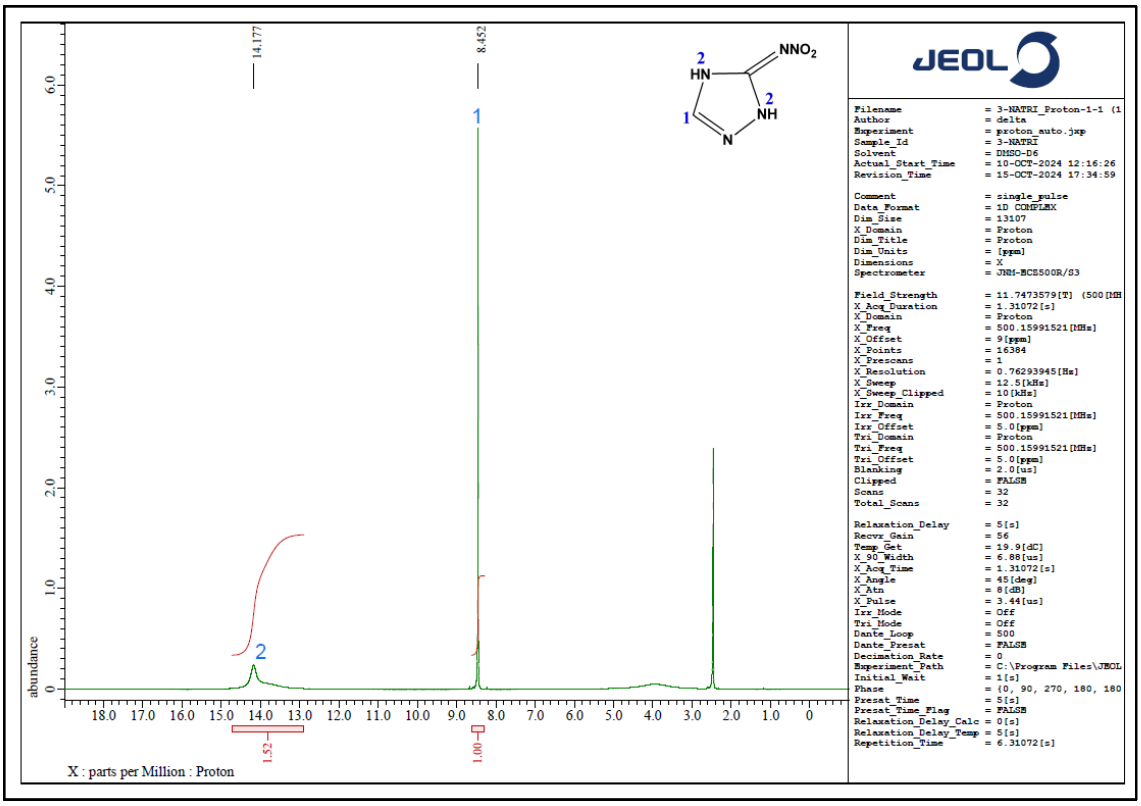


Fig. S3 HRMS spectrum of compound **1**



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X_Sweep_Clipped       = 10[kHz]
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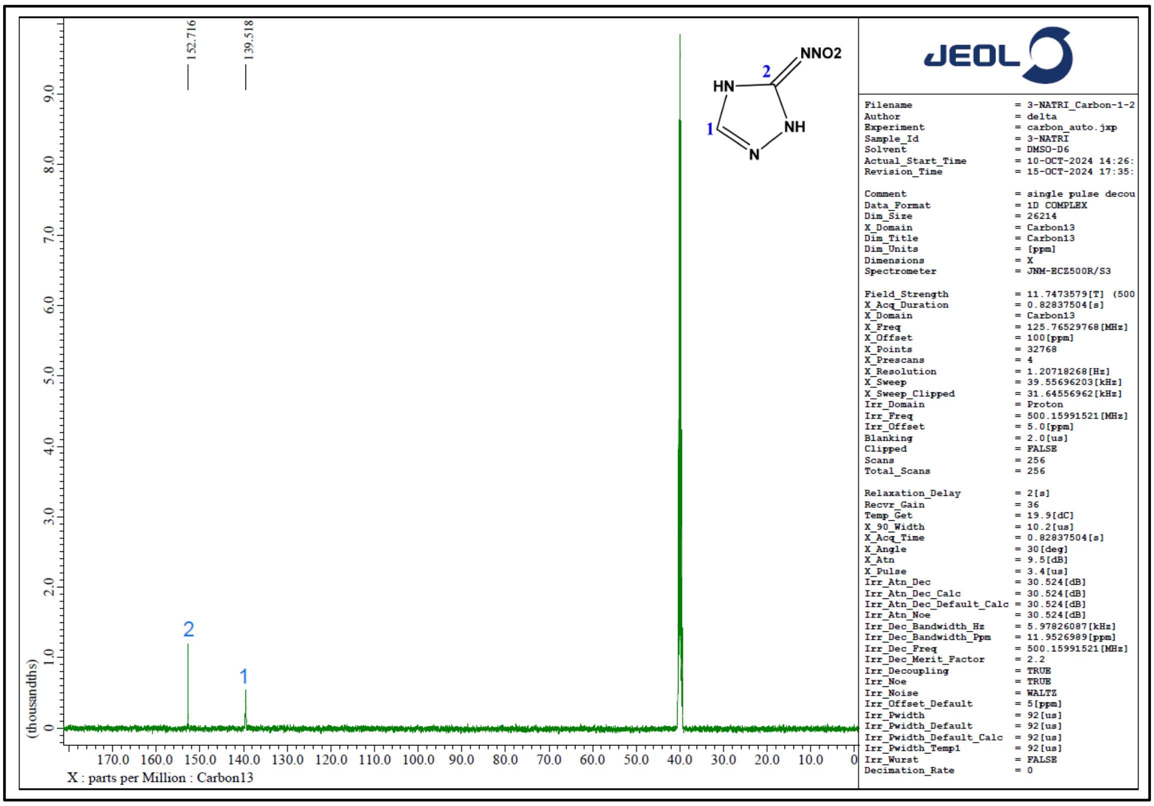
Fig. S4 ^{1}H NMR spectrum of compound **2** in DMSO-d_6



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Dimensions                    = X
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Fig. S5 ^{13}C NMR spectrum of compound **2** in DMSO-d_6

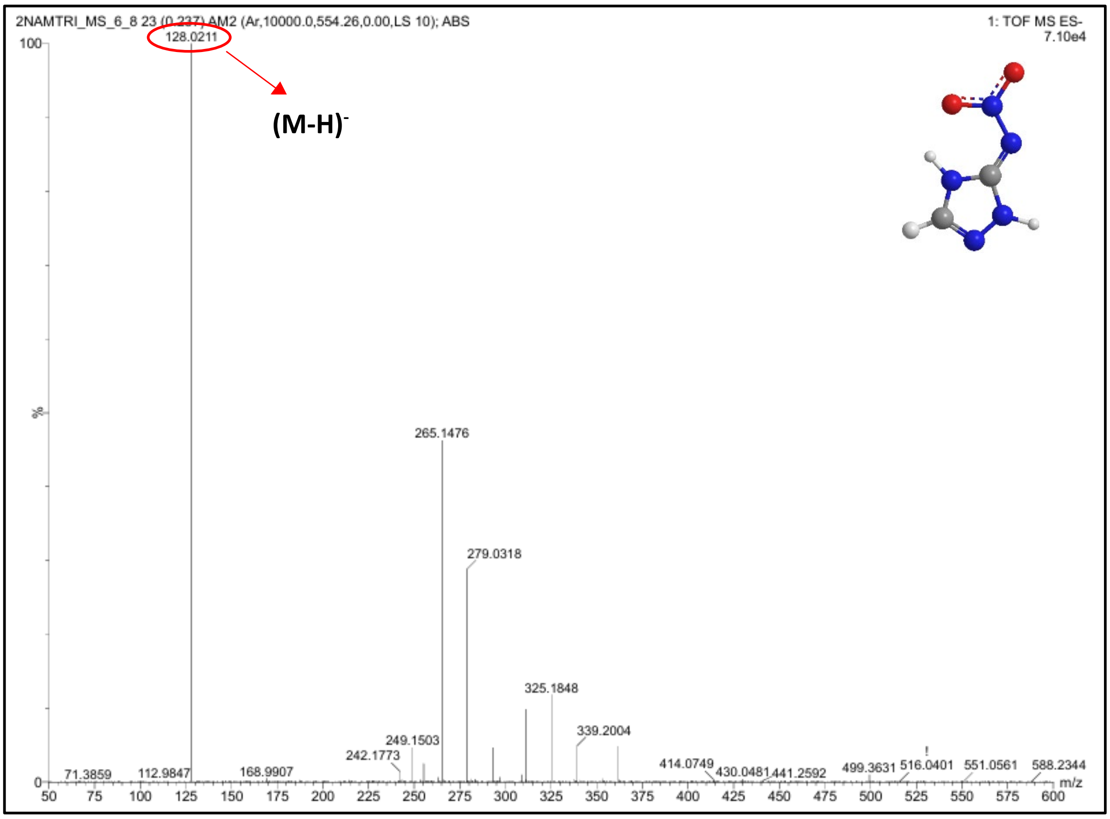

Fig. S6 HRMS spectrum of compound **2**

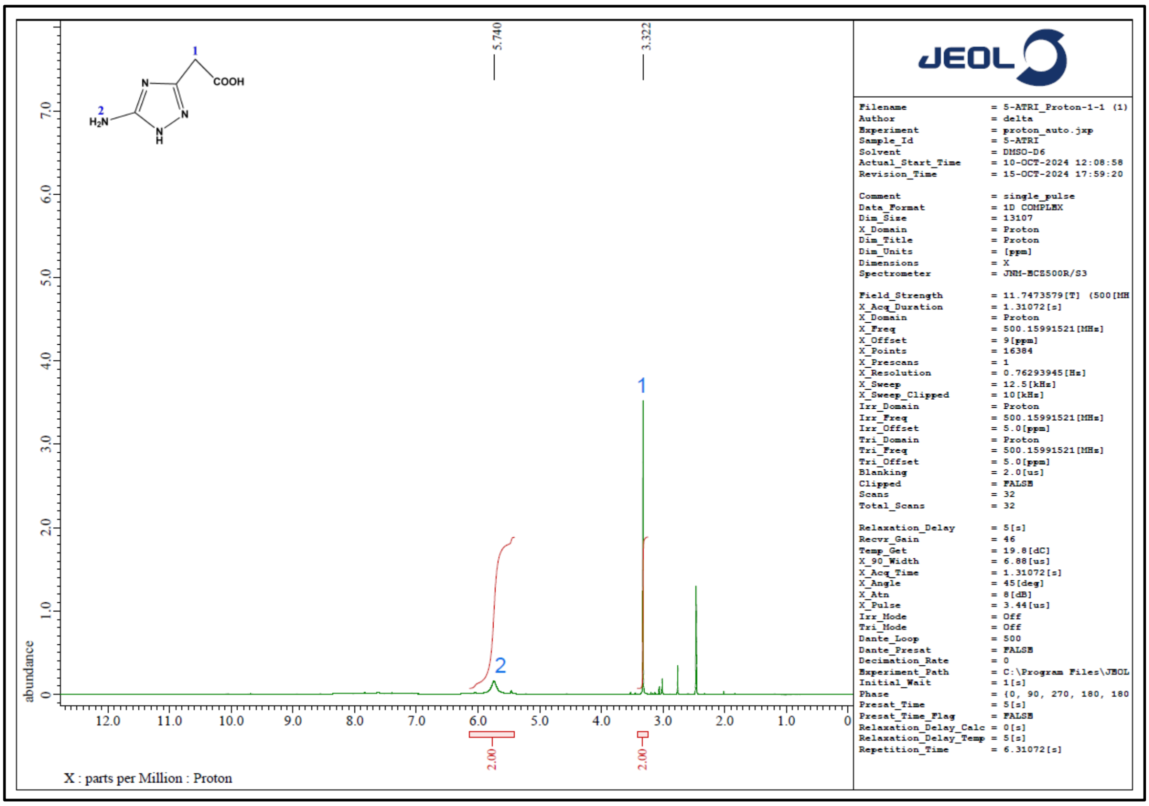

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Fig. S7 ^{1}H NMR spectrum of compound **3** in DMSO-d_6

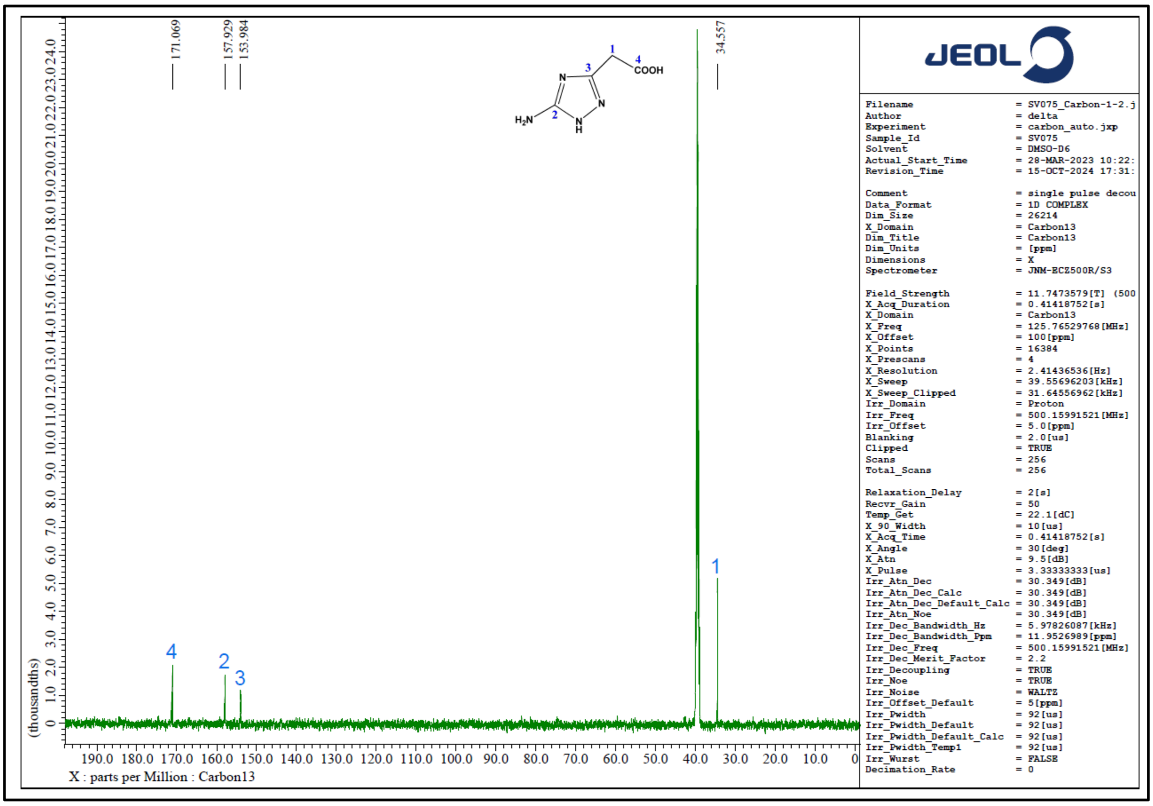

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Fig. S8 ^{13}C NMR spectrum of compound **3** in DMSO-d_6

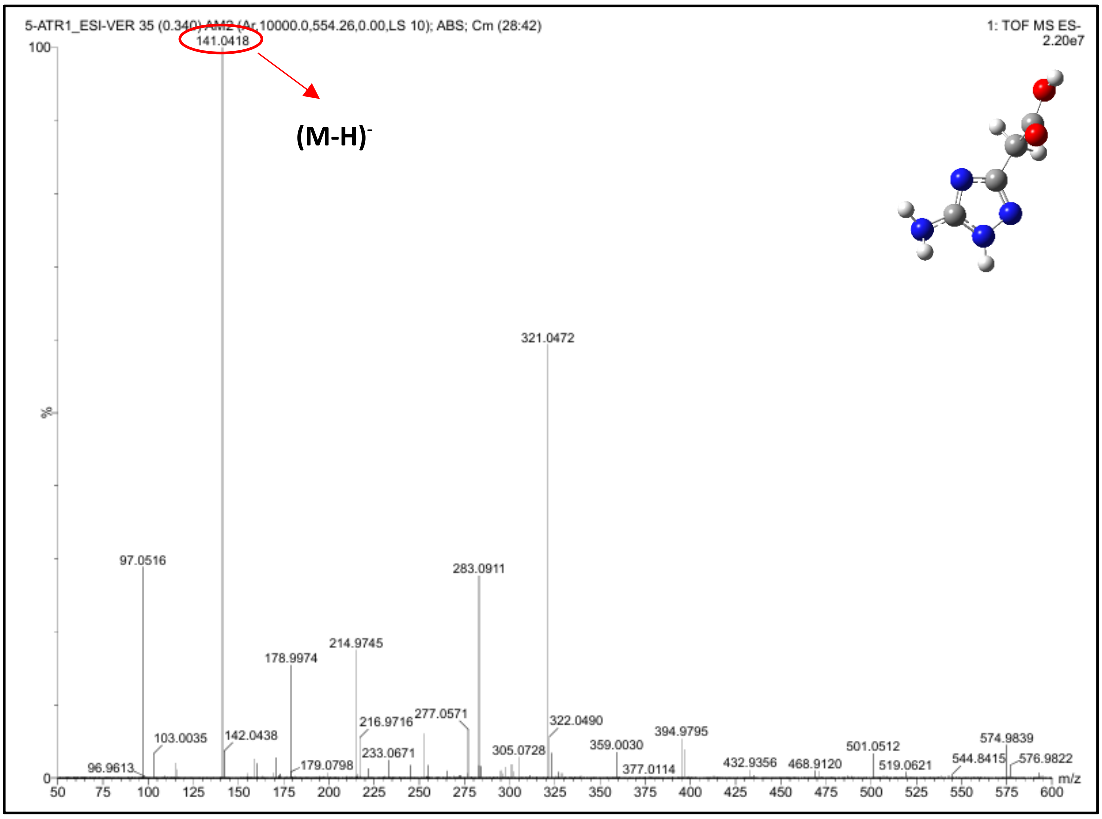


Fig. S9 HRMS spectrum of compound **3**

3. Thermal analysis data:

Compound	Melting point (°C) (DSC)	Decomposition					
		Onset temperature (°C)		Peak temperature (°C)		End temperature (°C)	
		TG (DTG)	DSC	TG (DTG)	DSC	TG (DTG)	DSC
Compound **1**	156	168	174	223	224	234	231
Compound **2**	-	164	153	209	209	232	233
Compound **3**	184	166	168	188	184	198	193
		198	230	212	257	232	276

Table. S1 Thermal analysis data of compound **1**, **2**, and **3**

4. TG-FTIR analysis

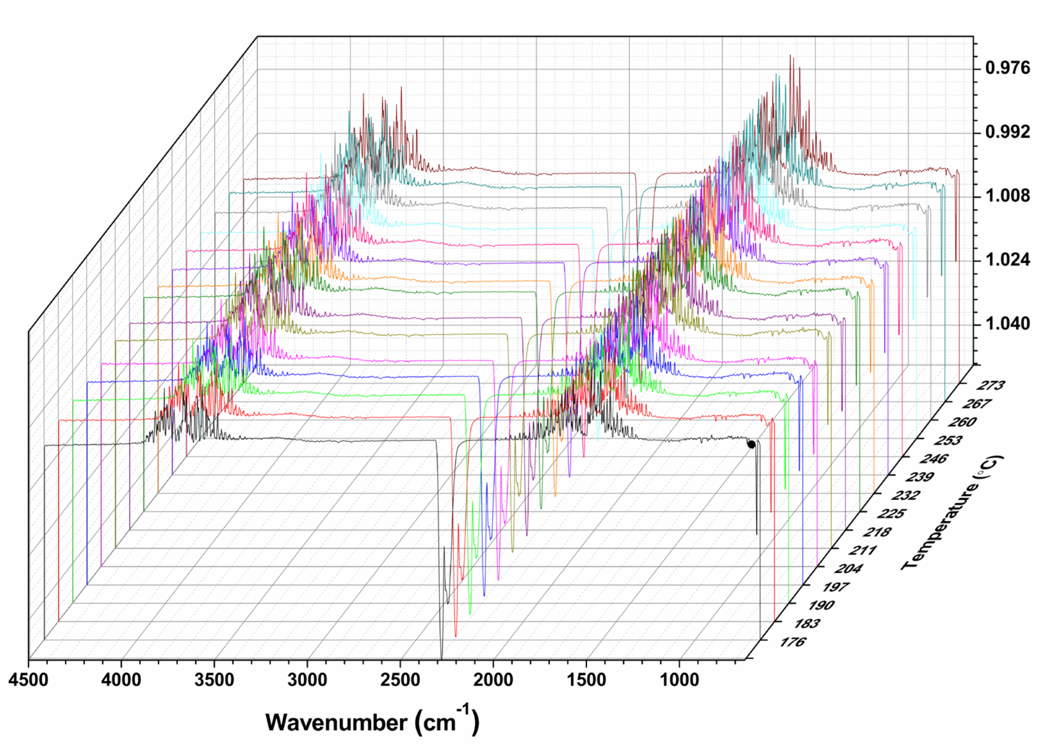


Fig. S10 TG-FTIR of compound **1**

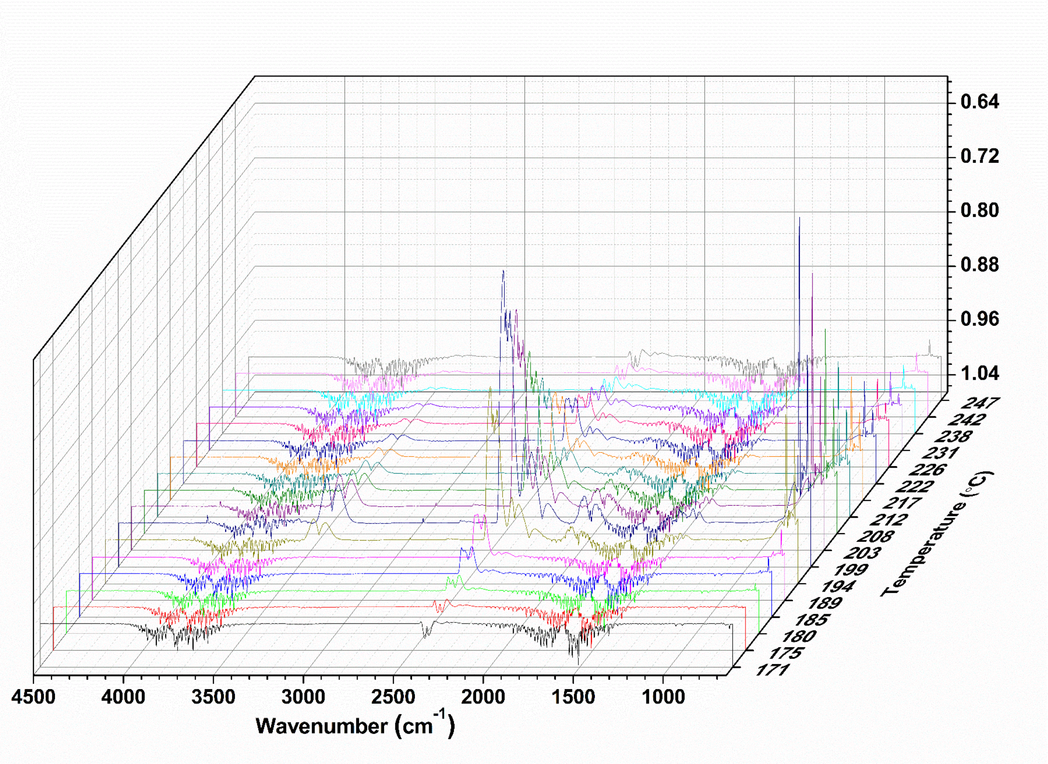


Fig. S11 TG-FTIR of compound **2**

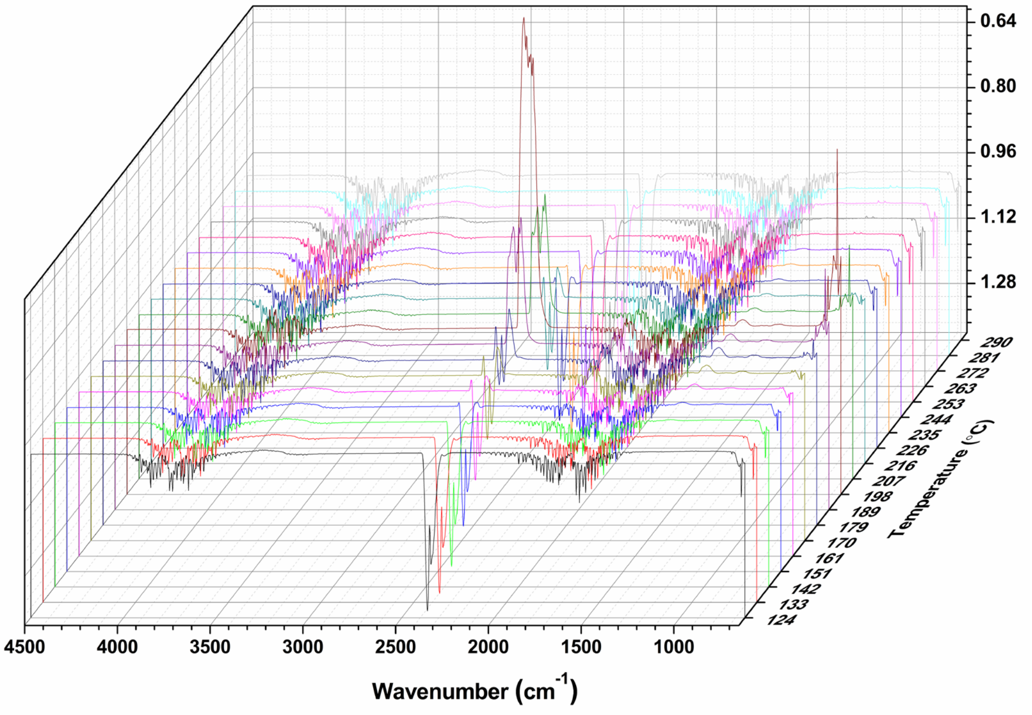


Fig. S12 TG-FTIR of compound **3**

5. GC-MS and MS/MS analysis data:

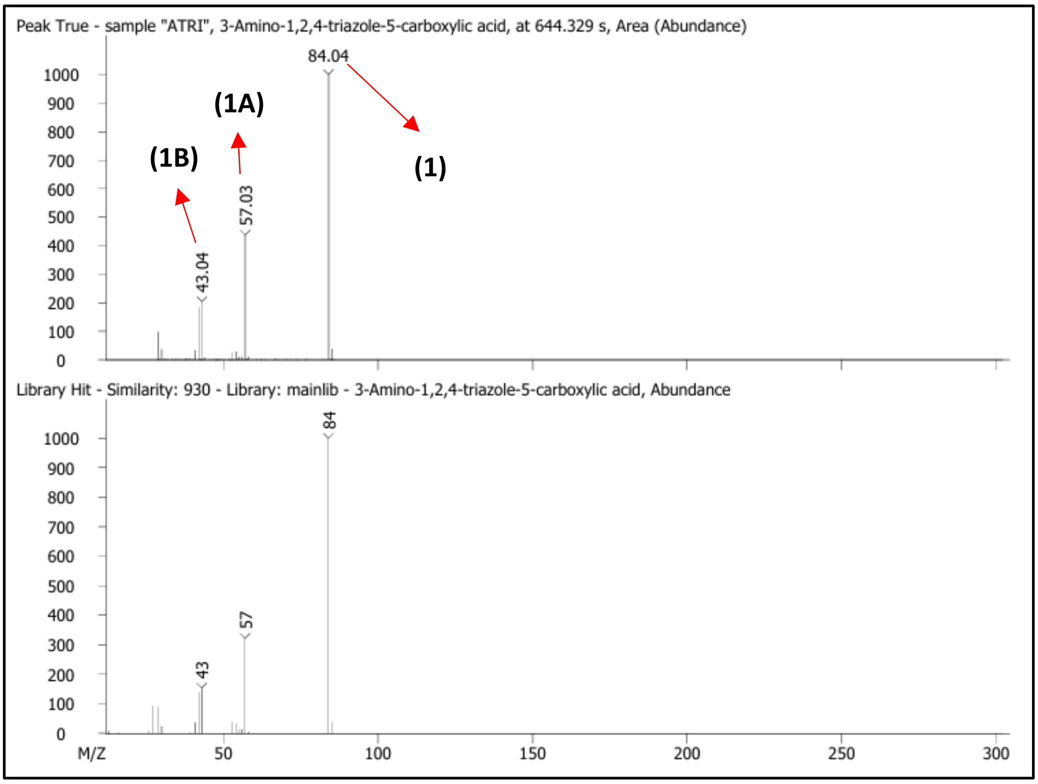


Fig. S13 GC-MS spectrum of compound **1**

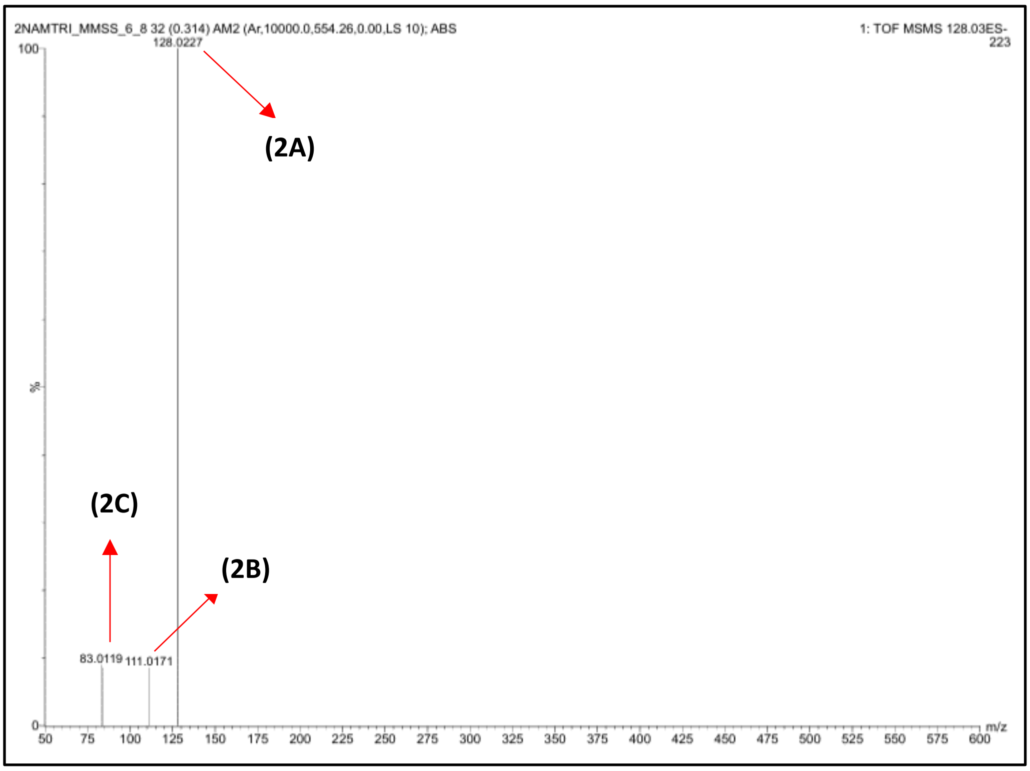


Fig. S14 MS/MS spectrum of compound **2** at m/z 128.03

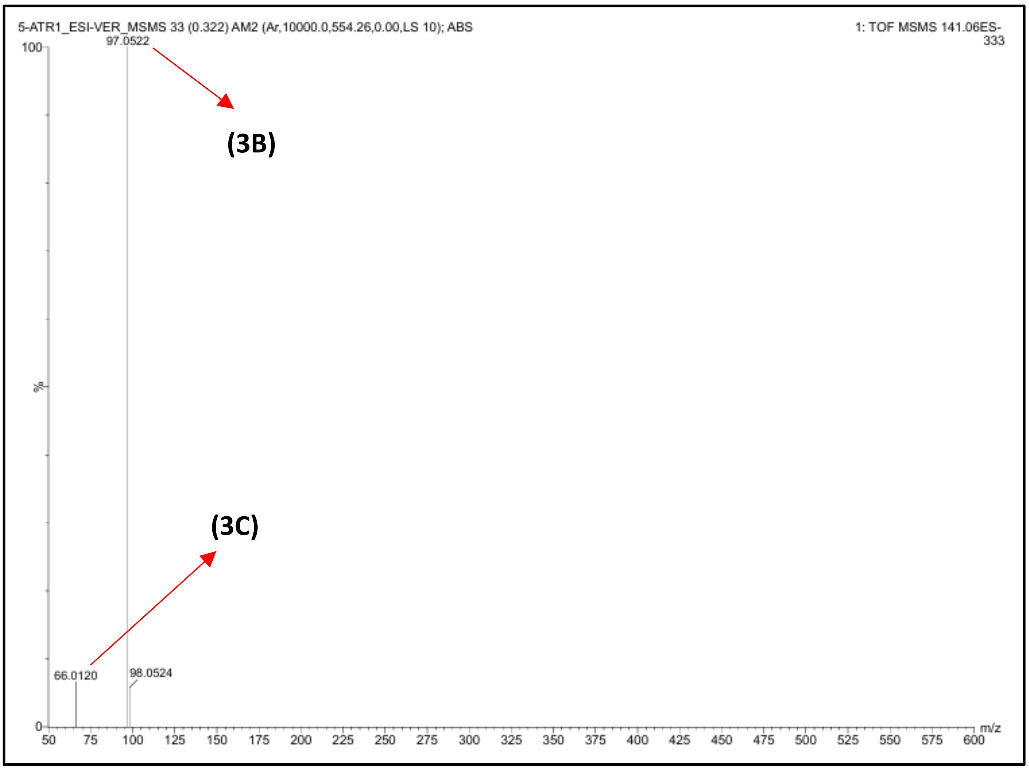


Fig. S15 MS/MS spectrum of compound **3** at m/z 141.06

6. Computational Studies:

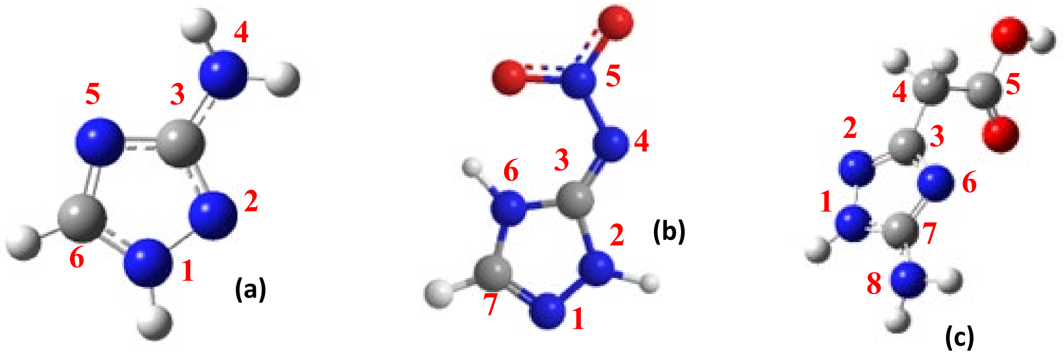


Fig. S16 Optimized molecular structures of compounds **1** (a), **2** (b), and **3**(c)

Bond	Compound 1	Compound 2	Compound 3
1,2	1.37	1.37	1.37
2,3	1.33	1.36	1.32
3,4	1.38	1.32	1.49
4,5	-	1.38	1.52
5,6	1.32	-	-
3,5	1.37	-	-
3,6	-	1.37	1.37
6,7	-	1.37	1.32
7,8	-	-	1.38
1,6	1.34	-	-
1,7	-	1.3	1.35

Table. S2 Bond lengths (Å) of different bonds in compounds **1**, **2**, and **3**

7. Kinetic analysis data:

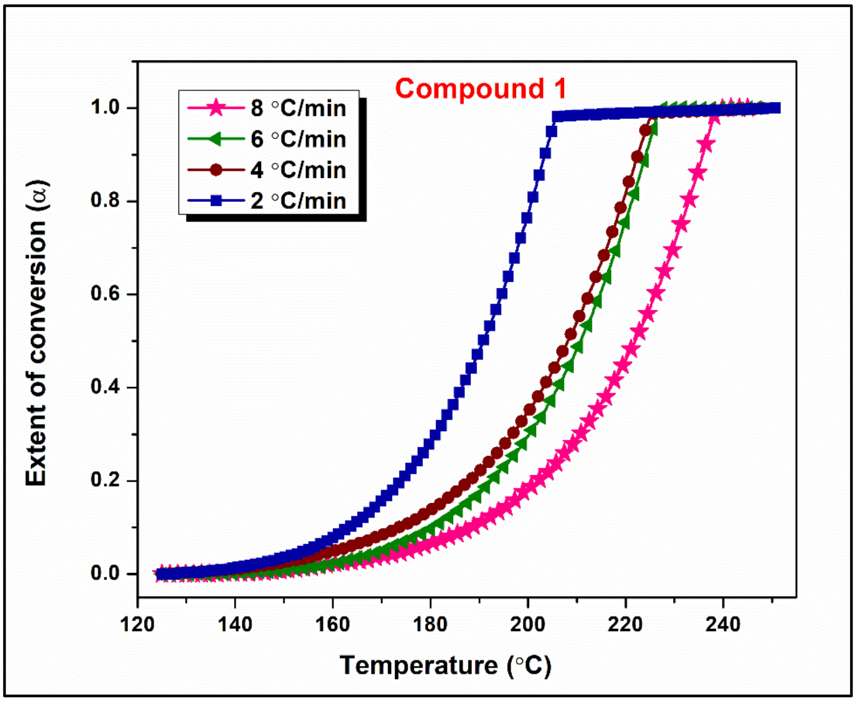


Fig. S17 α-T curve of compound **1**

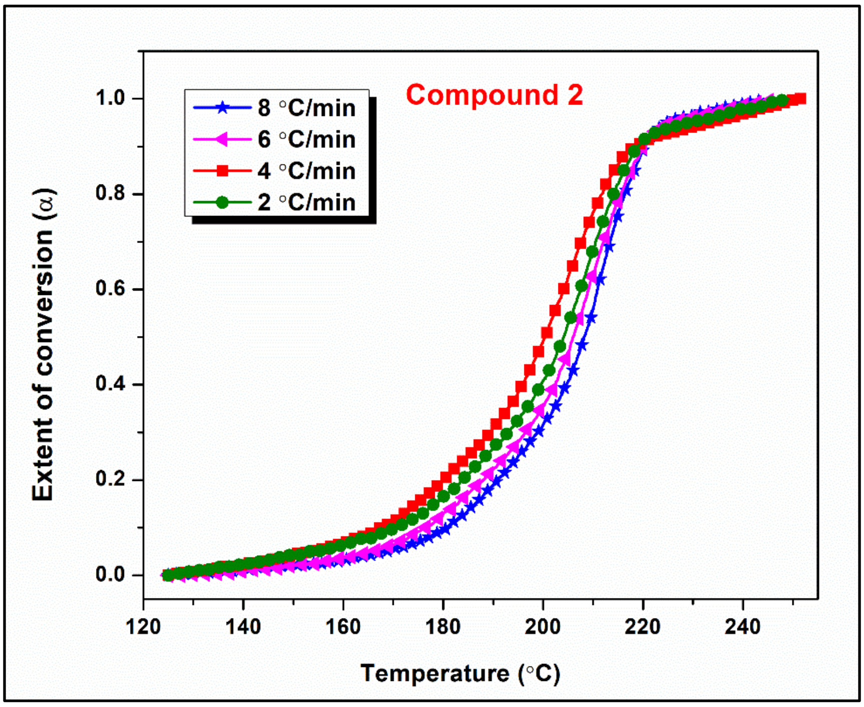


Fig. S18 α-T curve of compound **2**

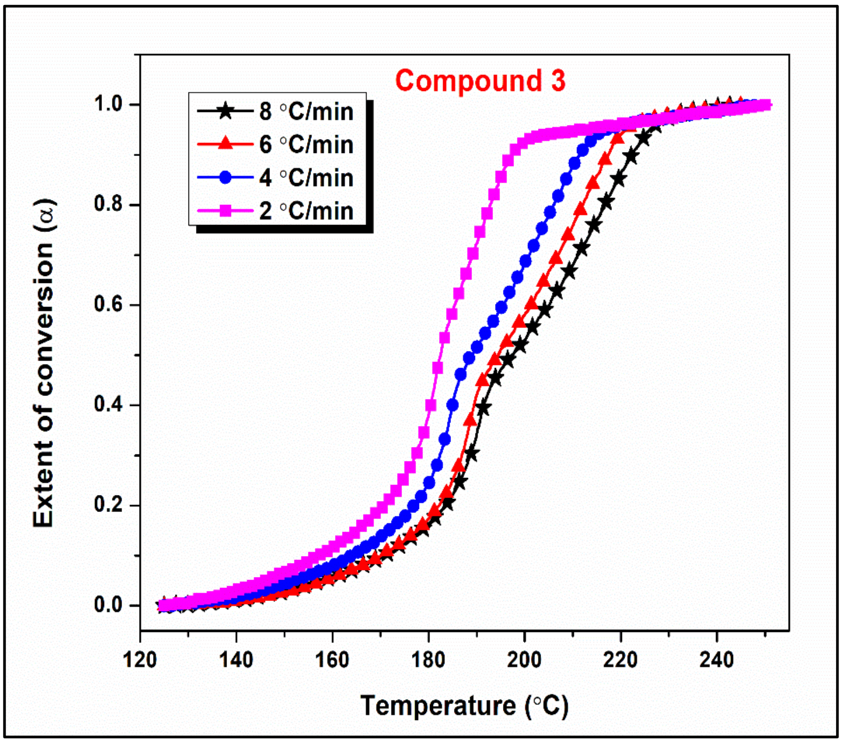


Fig. S19 α-T curve of compound **3**

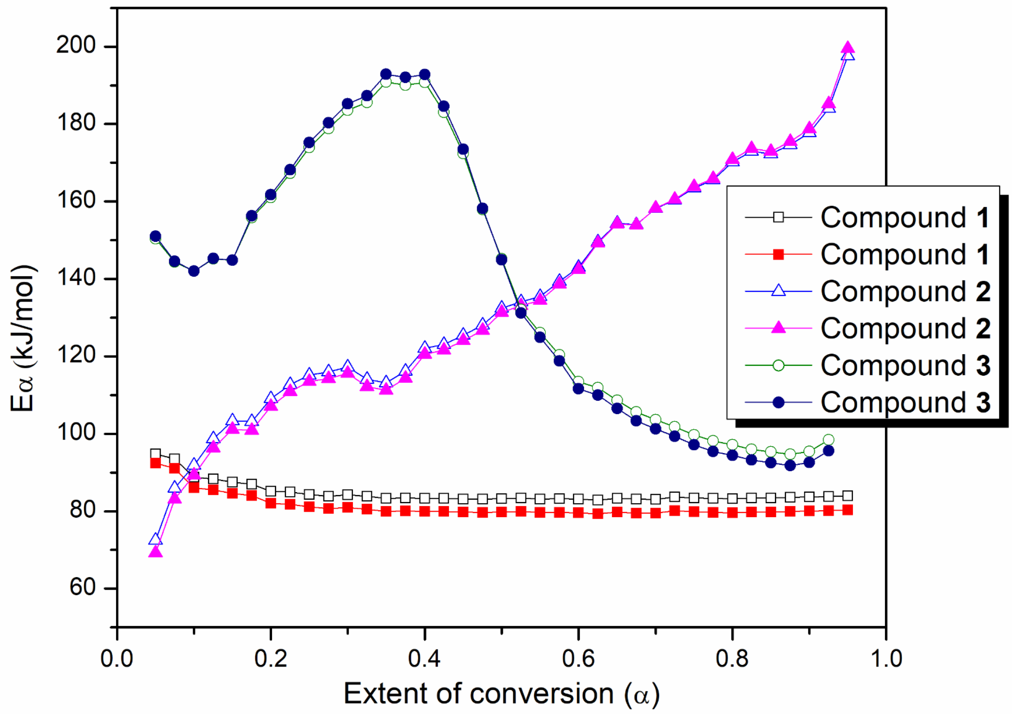
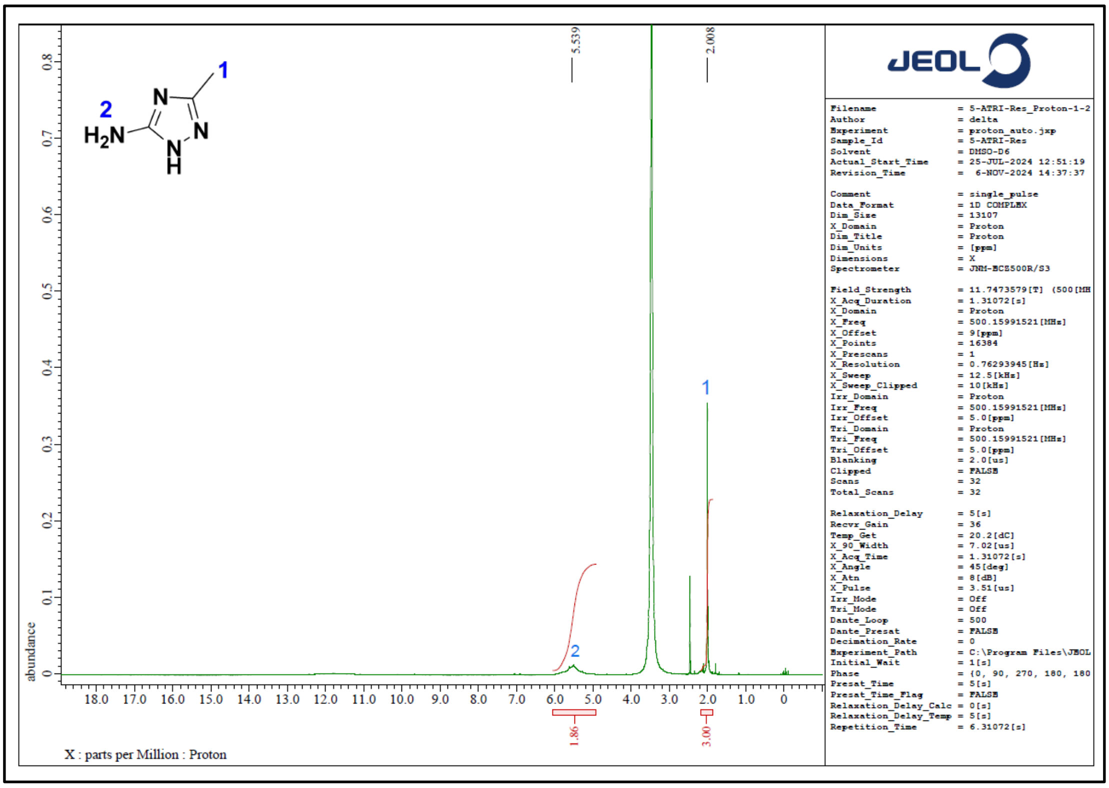


Fig. S20 E_α – α curve of compounds obtained by Vyazovkin's non linear integral method and Flynn-Wall-Ozawa Method. The open symbols (□) represents E_α obtained using Flynn-Wall-Ozawa Method[5, 6] and filled symbols (■) represents E_α obtained using Vyazovkin's non linear integral method

8. Residue Analysis



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Author                  = delta
Experiment              = proton_auto.jxp
Sample_Id               = 5-ATRI-Res
Solvent                 = DMSO-D6
Actual_Start_Time       = 25-JUL-2024 12:51:19
Revision_Time           =  6-NOV-2024 14:37:37

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ500R/S3

Field_Strength          = 11.7473579[T] (500[MH
X_Acq_Duration          = 1.31072[s]
X_Domain                = Proton
X_Freq                  = 500.15991521[MHz]
X_Offset                = 9[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.76293945[Hz]
X_Sweep                 = 12.5[kHz]
X_Sweep_Clipped         = 10[kHz]
Irr_Domain              = Proton
Irr_Freq                = 500.15991521[MHz]
Irr_Offset              = 5.0[ppm]
Tri_Domain              = Proton
Tri_Freq                = 500.15991521[MHz]
Tri_Offset              = 5.0[ppm]
Blanking                = 2.0[us]
Clipped                 = FALSE
Scans                   = 32
Total_Scans             = 32

Relaxation_Delay        = 5[s]
Recvr_Gain              = 36
Temp_Get                = 20.2[dC]
X_90_Width              = 7.02[us]
X_Acq_Time              = 1.31072[s]
X_Angle                 = 45[deg]
X_Atn                   = 8[dB]
X_Pulse                 = 3.51[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = C:\Program Files\JEOL
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time         = 6.31072[s]
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Fig. S21 ^{1}H NMR spectrum of Compound 3-Residue in DMSO-d_6

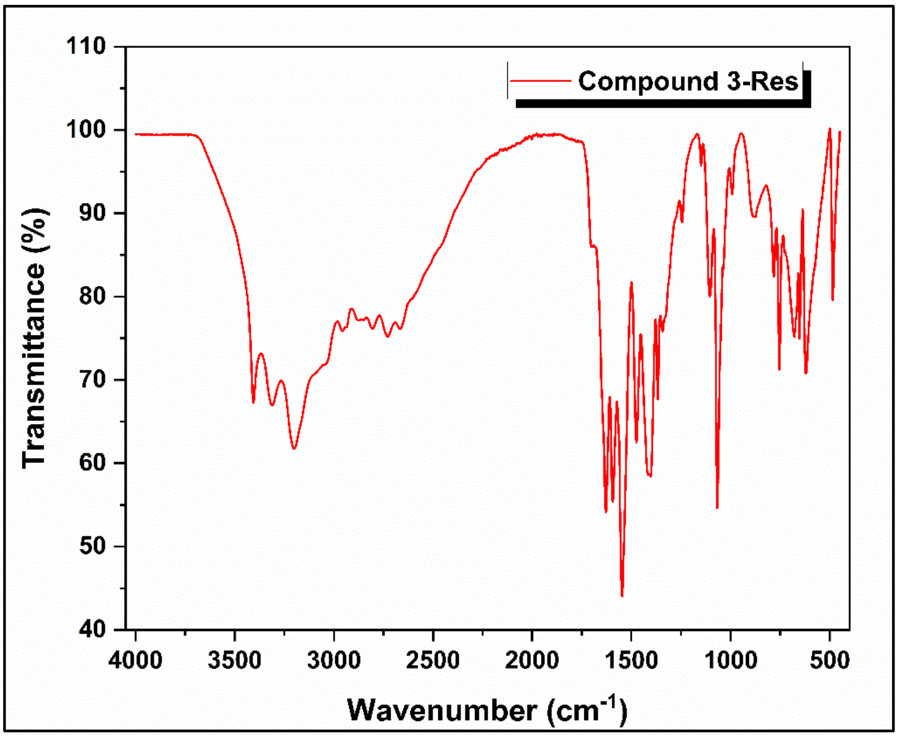

Fig. S22 FTIR spectrum of Compound 3-Residue (3-methyl-1,2,4-triazol-5-amine)

Reference:

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