Electronic Supplementary Information

Single-step nitration of N,N′-Bispyrrolylmethane: Polynitro Derivatives as Insensitive Energetic Materials

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1. General Information

i) General experimental information

All the reactions were performed in an oven-dried round-bottomed flask. Commercial-grade solvents were distilled before use. Column chromatography was performed using silica gel (100-200 Mesh) with a hexane and ethyl acetate mixture. Thin-layer chromatography (TLC) was performed on silica gel GF254 plates. The spots on the TLC plate were visualized with UV light (254 nm) and/or staining over I_2 chamber.

ii) Materials

Pyrrole, dichloromethane (DCM), and *N,N′*-dimethylformamide (DMF) were dried over calcium hydride and distilled before use. Potassium hydroxide pellets were used as powder by grinding and drying properly in a vacuum oven. Commercially available potassium nitrate and H_2SO_4 were used for nitration.

iii) Product characterization

^{1}H NMR, ^{13}C NMR, and ^{15}N NMR spectra were recorded on a JEOL JNM-ECZ-600R/M1 (600.17 MHz) FT NMR spectrometer at 600.17, 150.9, and 60.81 MHz, as well as with a 500 MHz (Bruker Advance) NMR spectrometer operating at 500.19, 125.78, and 36.14 MHz. Chemical shifts in the ^{1}H and ^{13}C NMR spectra are reported relative to Me_4Si as an internal standard, by using solvent (^{1}H NMR, DMSO-d_6 at 2.52 ppm; ^{13}C NMR, DMSO-d_6 at 39.52 ppm, and ^{15}N NMR spectra to nitromethane as an external standard. The chemical shift values (ppm) are expressed relative to the chemical shift of [D]solvent, and abbreviations for multiplicities and descriptors are: s = singlet, br = broad signal, m = multiplet, and q = quartet. High-resolution mass spectral determinations were carried out by Bruker-maXis by HR-ESI-MS techniques. Decomposition temperature was determined by DSC-TGA on a Perkin Elmer simultaneous thermal analyser STA- 6000 instrument. Infra-red spectra were recorded on an FT-IR spectrometer (Nicolet Is5IR). Crystallographic data (collected at 297 K) on a Bruker APEX-III CCD Mo-Kα radiation (0.71073 Å). Data reduction was performed using Bruker APEX-3 software. The structures were solved using SHELXT-97 and OLEX 2-1.2, and the data were refined using the program SHELXL-2018/7. [S1]

Crystallographic data (including the structure factor files) for structures **1, 2, 3, 4, 5, 6, 7, 8,** and **9** in this paper have been deposited in the Cambridge Crystallographic Data Centre as

supplementary publication numbers 2476735-2476743, respectively. For compound **5** (2476739), the data quality was poor; it was added for additional confirmation regarding the regiochemistry of the nitro group. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44(0)-1223-336033 or e-mail: deposit@ccdc.cam.ac.uk).

2. Experimental Section

***Caution*.** All the compounds prepared are energetic materials and are insensitive towards external stimuli. While we have not encountered any issues in the handling of these compounds, proper protective measures (face shield, eye protection, apron, and leather gloves) should be taken at all times. In addition, all of the energetic compounds were prepared only on a small scale and handled using a PTFE spatula.

Synthesis of compound I: BPM was prepared according to the literature procedure.

General procedure for the synthesis of compounds 1, 2, 3, and 4.

Synthetic procedure by using KNO_3. In an oven-dried 50 mL two-neck round-bottomed flask, BPM was taken and dissolved in conc. H_2SO_4 (10 mL) at -15 °C to which KNO_3 (4 eq) was added pinch-wise. The reaction mixture was stirred at this temperature for 15 min. After completion, the reaction mixture was poured onto crushed ice, resulting precipitate was collected by filtration and then purified by column chromatography using Hexane-ethyl acetate (90:10) as eluent.

Synthetic procedure by using $Cu(NO_3)_2.3H_2O$. BPM was taken and dissolved in acetic anhydride (15 mL) at 0 °C, to then $Cu(NO_3)_2.3H_2O$ (4 eq) was added pinch-wise. The reaction mixture was stirred at this temperature for 15 min, then allowed to warm to room temperature, where it was stirred continuously for 5. After completion, the reaction mixture was poured onto crushed ice, and the resulting precipitate was collected by filtration and purified by column chromatography using Hexane-ethyl acetate (90:10) as eluent.

Compound 1: **White solid;** Yield: 11%; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.74 (s, 1H), 8.57 (d, 1H), 7.91 (d, 1H), 6.97 (s, 2H) ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 137.2, 135.0, 129.9, 128.8, 127.4, 127.2, 126.3, 109.7, 61.7 ppm. ^{15}N NMR (60.81 MHz, DMSO-d_6) δ -231.96 (N1), -220.15 (N2), -30.12 (N3), -27.59 (N4), -27.12 (N5), -24.66 (N6), -19. 78 (N7) ppm. FTIR (cm^{-1}) ῡ 3154, 3131, 1526, 1549, 1510, 1437, 1367, 1315, 1294, 1274, 1199, 1135, 991, 870, 861,

805, 763, 622, 479. HRMS (ESI) m/z $(M+H)^+$ calculated for $C_9H_5N_7O_{10}^+$ 372.0176, found 372.0168.

Compound 2: **White solid;** Yield: 9%; ^{1}H NMR (500.19 MHz, DMSO-d_6) δ 8.55 (d, 1H), 8.01 (d, 1H), 7.56 (s, 2H), 7.04 (s, 2H) ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 140.6, 136.1, 134.5, 126.3, 113.5, 108.8, 60.0 ppm. ^{15}N NMR (60.81 MHz, DMSO-d_6) δ -244.01 (N1), -219.06 (N2), -29.04 (N3), -27.98 (N4), -22.07 (N5) ppm. FTIR (cm^{-1}) ῡ 3154, 3131, 1526, 1549, 1510, 1474, 1437, 1395, 1361, 1315, 1274, 1199, 1135, 976, 870, 861, 805, 740, 621, 481. HRMS (ESI) m/z $(M+NH_4)^+$ calculated for $C_9H_6N_6O_8^+$ 344.0590, found 344.0589.

Compound 3: **White solid;** Yield: 14%; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.48 (s, 2H), 7.90 (s, 2H), 6.94 (s, 2H) ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 137.3, 135.5, 128.8, 109.5, 60.9 ppm. ^{15}N NMR (60.81 MHz, DMSO-d_6) δ -223.89 (N1), -28.27 (N2), -21.57 (N3) ppm. FTIR (cm^{-1}) ῡ 3151, 3130, 2921, 1549, 1512, 1474, 1394, 1314, 1273, 1198, 1134, 1085, 974,859, 836, 803,762, 739, 621, 594, 512. HRMS (ESI) m/z $(M+NH_4)^+$ calculated for $C_9H_6N_6O_8^+$ 344.0590, found 344.0586.

Compound 4: **White solid;** Yield: 8%; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.72 (d, 1H), 8.31 (s, 2H), 7.91 (d, 1H), 6.54 (s, 2H) ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 136.3, 134.7, 129.5, 126.1, 126.0, 109.6, 62.0 ppm. ^{15}N 81 MHz, DMSO-d_6) δ -223.93 (N1), -211.79 (N2), -28.24 (N3), -25.83 (N4), -21.83 (N5) ppm. NMR (60.FTIR (cm^{-1}) ῡ 3381, 3153, 3131, 1550, 1511, 1475, 1437,1395, 1315,1294,1199,1087,976,842,870,805,763,621,596. HRMS (ESI) m/z $(M+NH_4)^+$ calculated for $C_9H_6N_6O_8^+$ 344.0590, found 344.0590.

Synthetic procedure for compounds 5, 6, 7, 8, and 9.

BPM was taken and dissolved in acetic anhydride (10 mL) at -15 °C, to then $Cu(NO_3)_2.3H_2O$ (0.5 eq) was added pinch-wise. The reaction mixture temperature was decreased to 0 °C, where it was stirred continuously for 1 h and 30 min. After completion, the reaction mixture was poured onto crushed ice, the resulting precipitate was collected by filtration, then purified by column chromatography using silica gel and hexane-ethyl acetate (95:5) as eluent.

5: **White solid;** Yield: 16%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.49 (s, 1H), 7.31 (d, 1H), 6.99 (s, 2H), 6.45 (s, 2H), 6.34 (s, 1H), 6.07 (s, 2H), ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 136.5, 131.3, 121.2, 116.3, 110.3, 109.6, 60.3 ppm. HRMS (ESI) m/z $(M+K)^+$ calculated for $C_9H_9N_3O_2^+$ 230.0331, found 230.0331.

6: **White solid;** Yield: 7%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.19 (t, 1H), 7.15 (t, 1H), 7.09 (t, 2H), 6.68 (t, 1H), 6.07 (, 4H), ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 136.8, 123.0, 122.8, 121.3, 109.7, 105.5, 61.2 ppm. HRMS (ESI) m/z $(M+Na)^+$ calculated for $C_9H_9N_3O_2^+$ 214.0592, found 214.0592.

7: **White solid;** Yield: 8%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.36 (t, 2H), 7.27 (t, 2H), 6.38 (s, 2H), 6.37 (q, 2H), ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 137.3, 130.4, 116.2, 110.4, 60.4 ppm. HRMS (ESI) m/z $(M+NH_4)^+$ calculated for $C_9H_8N_4O_4^+$ 254.0889, found 254.0889.

8: **White solid;** Yield: 5%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.11 (s, 1H), 7.70 (s, 1H), 7.36 (t, 1H), 7.09 (s, 1H), 6.72 (s, 1H), 6.52 (s, 2H), 6.41 (d, 1H) ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 137.0, 136.6, 132.1, 122.7, 116.7, 110.4, 105.8, 60.7 ppm. HRMS (ESI) m/z $(M+K)^+$ calculated for $C_9H_8N_4O_4^+$ 275.0182, found 275.0182.

9: **White solid;** Yield: 2%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.23 (t, 1H), 7.89 (d, 1H), 7.07 (s, 2H), 6.51 (s, 2H), 6.13 (d, 2H), ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 135.8, 134.5, 127.4, 121.7, 110.7, 110.3, 109.2, 61.7 ppm. HRMS (ESI) m/z $(M+K)^+$ calculated for $C_9H_5N_7O_{10}^+$ 275.0182, found 275.0182.

Table S1: Nitration of bis(2,4-dinitro-1H-pyrrol-1-yl)methane **3** under different conditions.

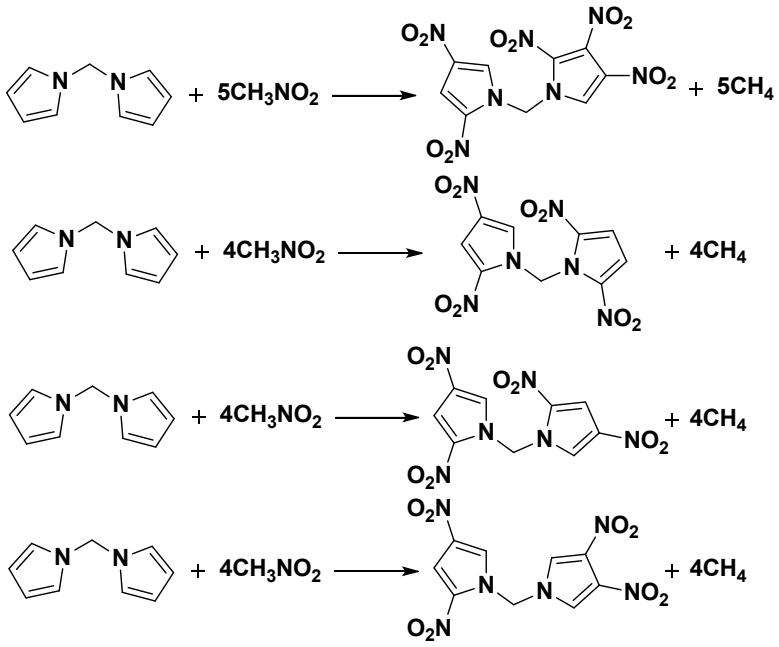
S. No.	Nitrate salt	Equivalence	Solvent	Temperature	Time	Yield		
						I	II	III
1	NO_2BF_4	10	CH_3CN (10 mL)	-30 °C - 15 °C	3 h	-	9	4
2	NO_2BF_4	4	CH_3CN (5 mL)	-15 °C - RT	3 h	12	6	-
3	Cu $(NO_3)_2.3H_2O$	10	Ac_2O (15mL)	0 °C	48 h	-	3	5
4	Cu $(NO_3)_2.3H_2O$	4	Ac_2O (15 mL)	0 °C - 50 °C	30 min	10	7	
5	KNO_3	8	H_2SO_4 (10 mL)	-15 °C	24 h	-	7	9
6	KNO_3	3	H_2SO_4 (10 mL)	-15 °C - 0 °C	24 h	-	4	6

Bis(2,4-dinitro-1H-pyrrol-1-yl)methane **3** - 0.100 (0.306 mol) [a] Entry 1 & 2 – procedure: compound was taken in RB flask dissolved in H_2SO_4 to which KNO_3 was added. [b] Entry 3 & 4 – procedure: compound was taken in RB flask, dissolved in acetic anhydride, to then $Cu(NO_3)_2$ $3H_2O$ was added. [c] Entry 5 & 6 – procedure: compound was taken in RB flask, dissolved in acetonitrile, to then NO_2BF_4 was added. **Remark:** Along with product I- 2,4-dinitro-1H-pyrrole , II- 2,3,4-trinitro-1H-pyrrole, III- 2,3,5-trinitro-1H-pyrrole were also formed.

3. Theoretical Study and Isodesmic Reactions

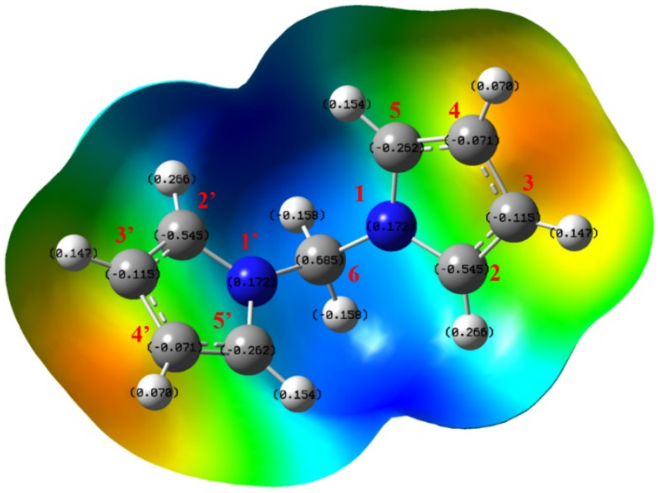
Theoretical calculation was performed using the Gaussian 09 program provided by CMSD facility of University of Hyderabad.[S2] The geometric optimization and frequency analyses were performed using the B3LYP functional with the 6-31G basis set, based on the single crystal structure. The optimized geometry was a minimum on the potential-energy surface, and no imaginary frequencies were found. The method of isodesmic reaction has been employed to calculate HOF from total energies obtained from DFT calculations. The detonation parameters for the compound were calculated with the EXPLO5 (v6.03) [S3] by using crystal densities.

Isodesmic reaction



1. ESP charge calculations.

In this study, **computational charge analysis** and **electrostatic potential (ESP) mapping** were employed to visualize and predict the **regioselectivity of electrophilic aromatic substitution (EAS)** reactions on *di(1H-pyrrol-1-yl)methane* (BPM). The **ESP charges** were calculated using the **B3LYP/6-31G** level of theory to identify electron-rich sites that are likely to undergo electrophilic attack. [S4] As shown in **Figure S1**, the ESP charge distribution provides a clear rationale for the experimentally observed nitration pattern. The relative reactivity toward nitration follows the trend: **C-2, C-2' > C-5, C-5' > C-3, C-3' > C-4, C-4'**. This hierarchy of electron density correlates strongly with the experimental data [5–9], confirming that ESP mapping is a reliable tool for predicting regioselectivity in substituted pyrrole systems.



C-2	-0.545
C-3	-0. 115
C-4	-0.071
C-5	- 0.262
C-2’	0.545
C-3’	-0.115
C-4’	0.071
C-5’	-0.262
C-10	0.585

Figure S1: a. ESP-mapped surface and b. ESP charge densities of BPM.

During the nitration of BPM, we observed the formation of several mono- and di- nitrated products, including: **1-((1H-pyrrol-1-yl)methyl)-2-nitro-1H-pyrrole (Compound 5)**, **1-((1H-pyrrol-1-yl)methyl)-3-nitro-1H-pyrrole (Compound 6)**, **bis(2-nitro-1H-pyrrol-1-yl)methane (Compound 7)**, **2-nitro-1-((3-nitro-1H-pyrrol-1-yl)methyl)-1H-pyrrole (Compound 8)**, **1-((1H-pyrrol-1-yl)methyl)-2,4-dinitro-1H-pyrrole (Compound 9)**.

2. Bond Dissociation Energy (BDE) analysis

Experimentally, multiple deprotected products were identified from nitration reactions, including compound-**I**, compound-**II**, compound-**III**, and compound-**IV.** Notably, the deprotection of highly nitrated bis(pyrrolyl)methane frameworks has been consistently observed via homolytic cleavage of the central **N–C–N** bond, highlighting its critical role in the decomposition pathway. All quantum chemical calculations were performed using the **B3LYP** exchange–correlation functional in conjunction with the **6-31+G(d,p)** basis set. [S5-S6] BDEs were evaluated with zero-point energy (ZPE) corrections to improve thermochemical accuracy. The strength of the N–C–N bond was determined through isodesmic reaction analysis (Equation 1), which allows reliable comparison of bond stabilities across structurally related systems. The calculated BDE values for the N–C–N linkage serve as a key metric for assessing molecular stability. Compounds exhibiting higher BDEs demonstrate greater resistance to homolytic cleavage and are therefore more thermodynamically stable. In contrast, lower BDEs correspond to enhanced susceptibility to bond rupture. Upon N–C–N bond cleavage, the system undergoes fragmentation into two free radical species, as

illustrated in the dissociation pathways (BDE-BPM to BDE-9) and (BDE-I to BDE-K). These findings underscore the mechanistic importance of the N–C–N bond in governing the stability and reactivity of nitrated BPM derivatives and provide valuable insight into their decomposition behaviour under energetic conditions.

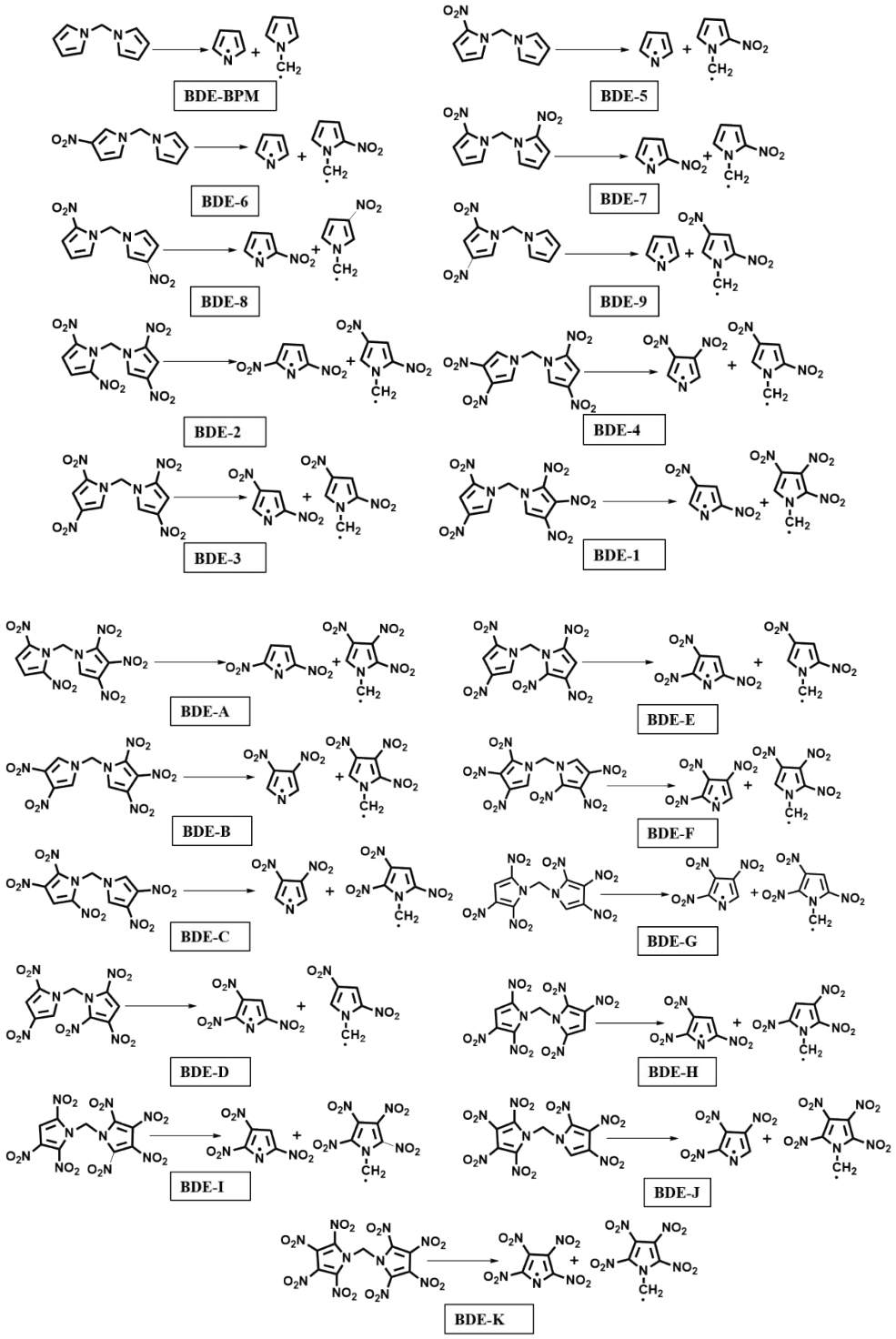


Figure S2: Deprotection and bond dissociation analysis of N–C–N linkage in highly nitrated BPM derivatives.

During the reaction, BDE can be calculated according to equation (1):

$$D_0(\text{R-N-CH}_2\text{-N-R}) = E_0(\text{R-N}\cdot) + E_0(\cdot\text{CH2-N-R}) - E_0(\text{R-N-CH}_2\text{-N-R})$$

Where $D_0(\text{R-N-CH}_2\text{-N-R})$ represents the molar enthalpy of reaction for the compound and is defined as the bond dissociation energy. $E_0(\text{R-N}\cdot)$, $E_0(\cdot\text{CH2-N-R})$, and $E_0(\text{R-N-CH}_2\text{-N-R})$ represent the enthalpies of formation for the free radicals and the studied compound, respectively. Fig. S5 and Table S10 present the N-C-N BDE values for all the EMs investigated.

Table S2: Trend in BDE in KJ mol^{-1}.

S.NO	BDE
BPM	285.7
5	334.9
6	286.8
7	237.9
8	302.8
9	288.9
3	300.1
2	356.1
4	303.0
1	298.01

S.NO	BDE
A	129.0
B	37.0
C	-726.7
D	-199.5
E	-566.0
F	26.1
G	-1166.4
H	-1189.0
I	-2348.5
J	18.2
K	-3347.4

A clear inverse correlation was observed between the degree of nitro substitution and the bond dissociation energy (BDE) of the N–C–N linkage, as summarized in Table S10. As the number of nitro groups increases, the BDE values systematically decrease, reflecting a weakening of the N–C–N bond. This computational trend is in excellent agreement with experimental observations. Specifically, compounds synthesized in this study (**BPM, 1–9**) consistently exhibited high and positive BDE values, indicating robust N–C–N bonds and enhanced thermodynamic stability. In contrast, compounds designated A–K displayed markedly lower, and in some cases negative, BDE values, suggesting significant instability. The absence of A–K derivatives among the isolated products, even under mild nitration conditions, is thus rationalized by their unfavourable energetic profiles. Among the dinitro-substituted

derivatives, Compounds **7, 8**, and **9**, Compound **7** stands out with the lowest BDE of **237.9 kJ mol^{-1}**, strongly implying a predisposition toward homolytic N–C–N bond cleavage. This is consistent with experimental findings, where Compound **7** underwent facile deprotection during further nitration. For the tetranitro-substituted series (Compounds **2, 3,** and **4**), Compound **3** exhibited a comparatively lower BDE of **300.1 kJ mol^{-1}**, which explains its susceptibility to deprotection despite the higher overall substitution. The alignment between computational BDE data and experimental outcomes underscores the predictive value of bond dissociation energy as a stability descriptor in this class of energetic heterocyclic systems.

Natural bonding orbital (NBO) analysis of Oligonitro bispyrrolylmethanes

A comprehensive natural bond orbital (NBO) analysis was employed to elucidate the electronic structure and stability of oligonitro bispyrrolylmethane compounds. The molecular geometries were first optimized using the B3LYP functional with the 3-21G basis set, followed by frequency calculations to confirm the absence of imaginary modes, thereby ensuring that all structures represent true minima on the potential energy surface. Single-point energy calculations were subsequently performed at the MP2(full)/6-311++G(d,p) level. The NBO calculations, conducted using version 3.1 integrated within the Gaussian 04 suite, provided detailed insights into bonding interactions and hybridization patterns in the optimized systems. [S7, S8] Nitro groups are among the most potent electron-withdrawing substituents, and their electron-accepting capacity can be effectively quantified by evaluating the net atomic charges within the nitro moiety. A higher (i.e., more negative) net charge on the nitro group generally signifies reduced electron affinity and is indicative of greater molecular stability. To systematically assess this behaviour, the Nitro Group Charge Method (NGCM) was recently developed and successfully applied to predict key properties of nitro-containing compounds, including their chemical stability and impact sensitivity. Within this framework, the stability of a given molecule is correlated with the nitro group charge, denoted as (Q_{nitro}), which is calculated as the algebraic sum of the partial charges on the nitrogen and both oxygen atoms in each nitro group (Equation 1). When multiple nitro groups are present, an average (Q_{nitro}), value is determined using Equation 2. More negative (Q_{nitro}), values are typically associated with enhanced molecular stability and reduced sensitivity, offering a valuable predictive descriptor for the design and evaluation of energetic materials.

$$Q_{nitro} = Q_N + Q_{O1} + Q_{O2} \quad (2)$$

$$\bar{Q}_{nitro} = \frac{1}{n}\sum_{i=1}^{n} Q_{nitro} \quad (3)$$

Natural bond orbital analysis provides an efficient method for investigating charge distribution in molecular systems. The charge distribution data calculated by the NBO method for optimized geometries of **K**, **J**, **F**, **1** and **3** are given in Figures S1-S4. Their calculations of $\bar{Q}_{nitro}$ are listed in Table 1.

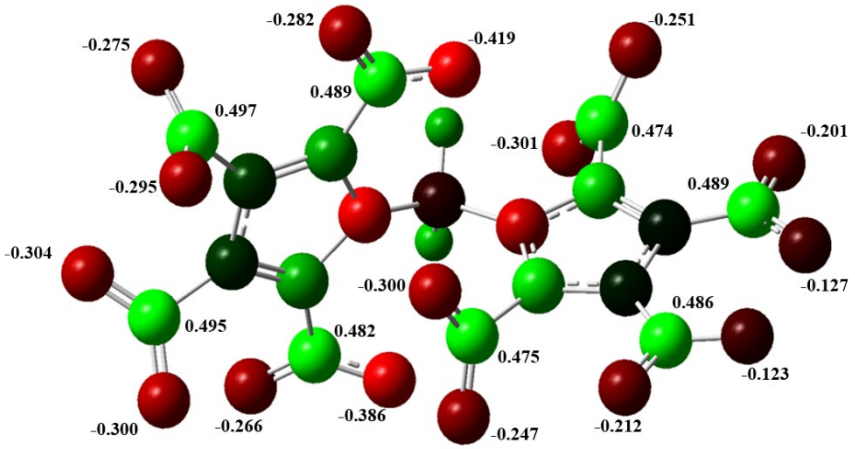


Figure S3: NBO analysis of compound **K**.

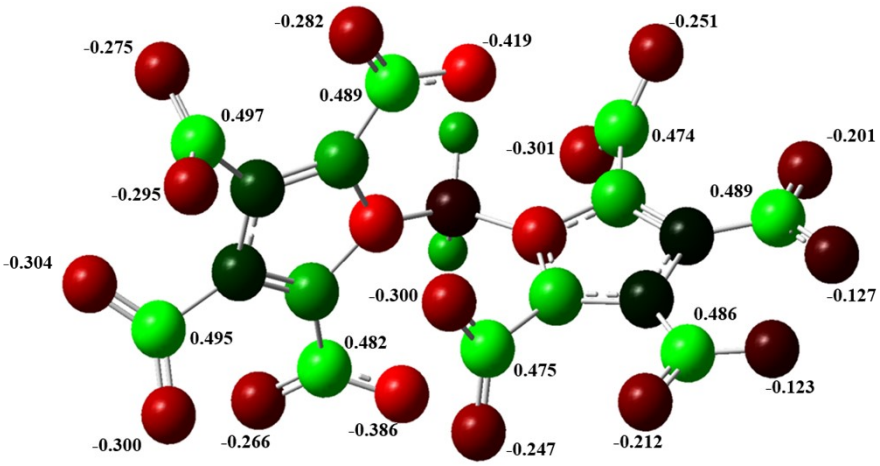


Figure S4: NBO analysis of compound **J**.

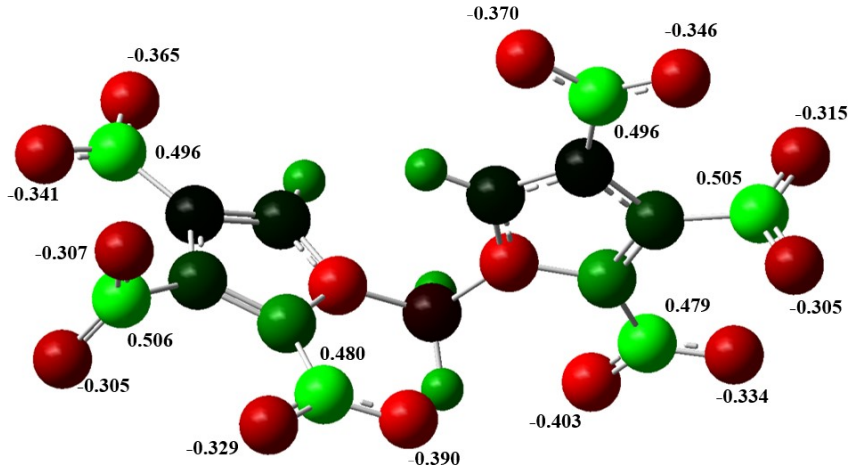


Figure S5: NBO analysis of compound **F**.

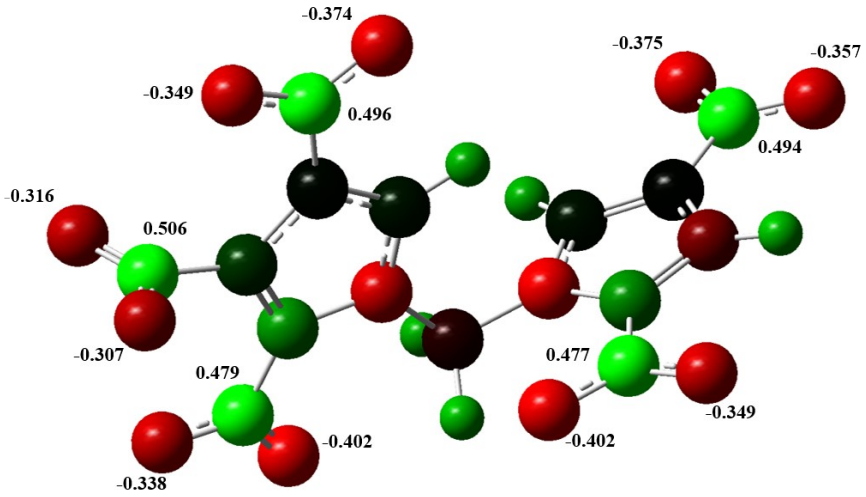


Figure S6: NBO analysis of compound **1**.

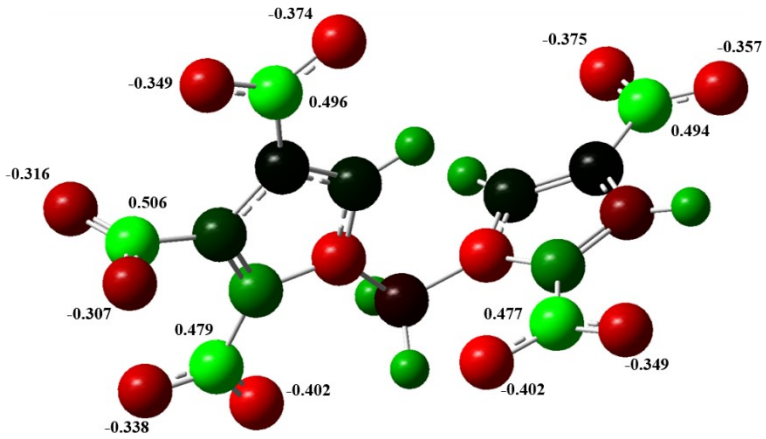


Figure S7: NBO analysis of compound **3**.

Table S3: Q_{Nitro} and the average Q_{Nitro} of compounds **K, J, F, 1** and **3**.

S.NO	Qnitro (e)	Qnitro (e)	Qnitro (e)	Qnitro (e)	Qnitro (e)	Qnitro(e)	Qnitro(e)	Qnitro(e)	$\bar{Q}$nitro (e)
K	- .073	- 0.109	- 0.17	- 0.072	0.151	0.161	- 0.078	- 0.212	- 0.0502
J	- 0.148	- 0.176	- 0.1	- 0.219	- 0.239	- 0.116	-0.217		- 0.1735
F	-0.22	-0.115	- 0.264	- 0.247	- 0.106	- 0.21			- 0.1936
1	-0. 228	-0. 117	-0.261	-0.271	-0.238				-0.223
3	- 0.256	- 0.291	- 0.275	- 0.246					- 0.2662

4. NMR spectra (^{1}H, ^{13}C), HRMS, and IR spectra of compounds

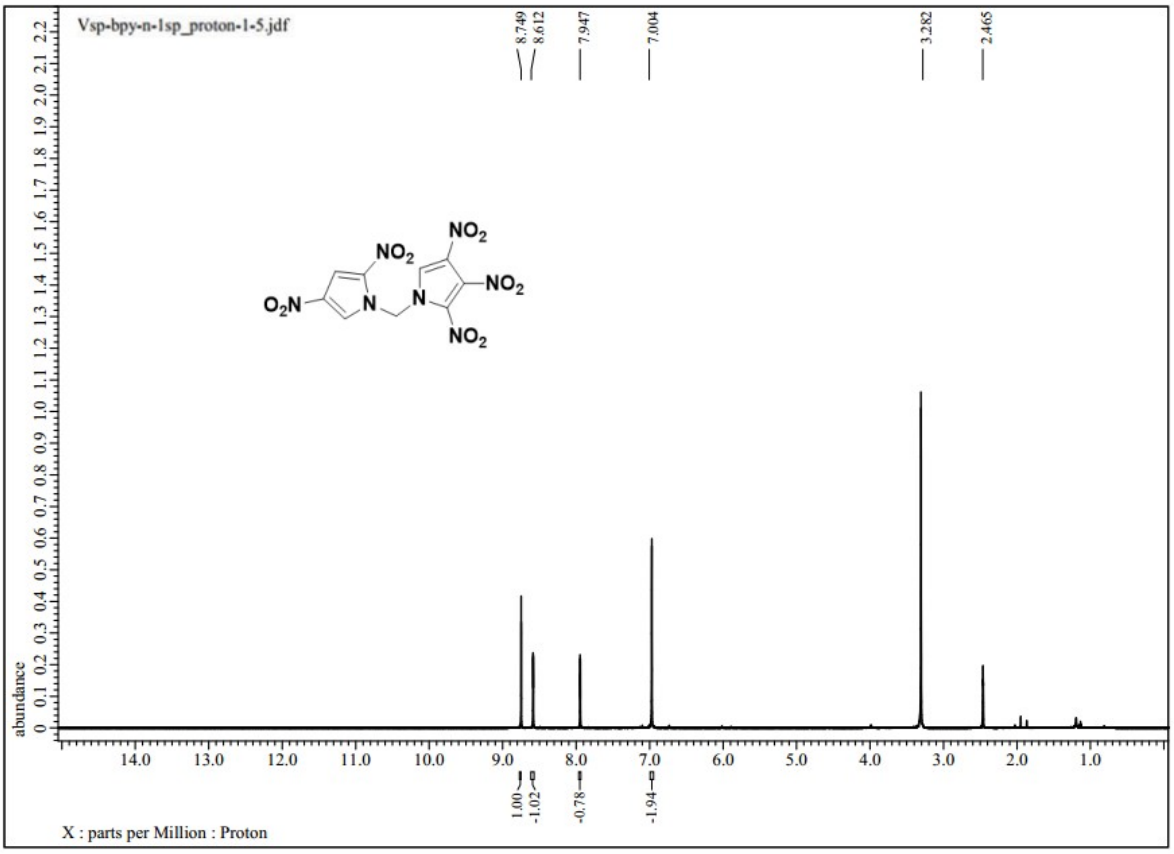


Figure S8: ^{1}H NMR spectrum of compound **1** in dimethyl sulfoxide-d_6.

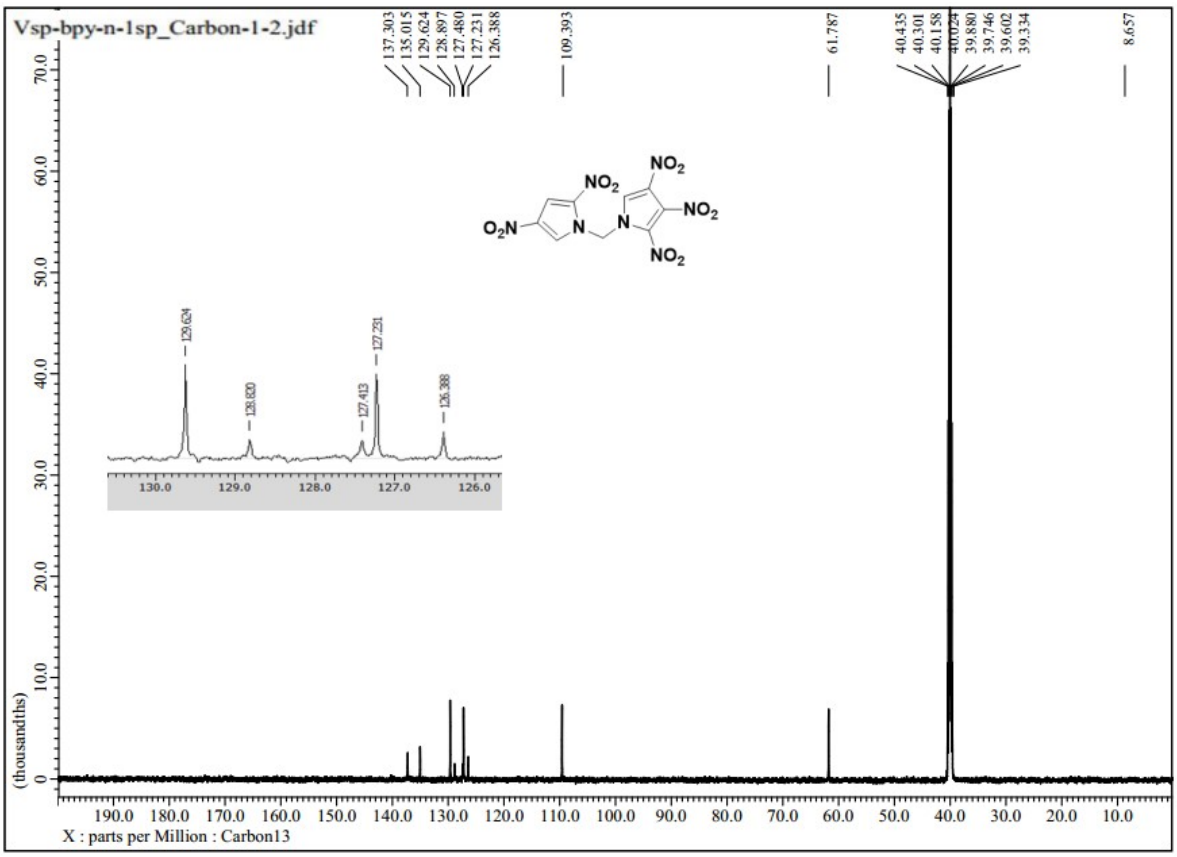


Figure S9: ^{13}C NMR spectrum of compound **1** in dimethyl sulfoxide-d_6.

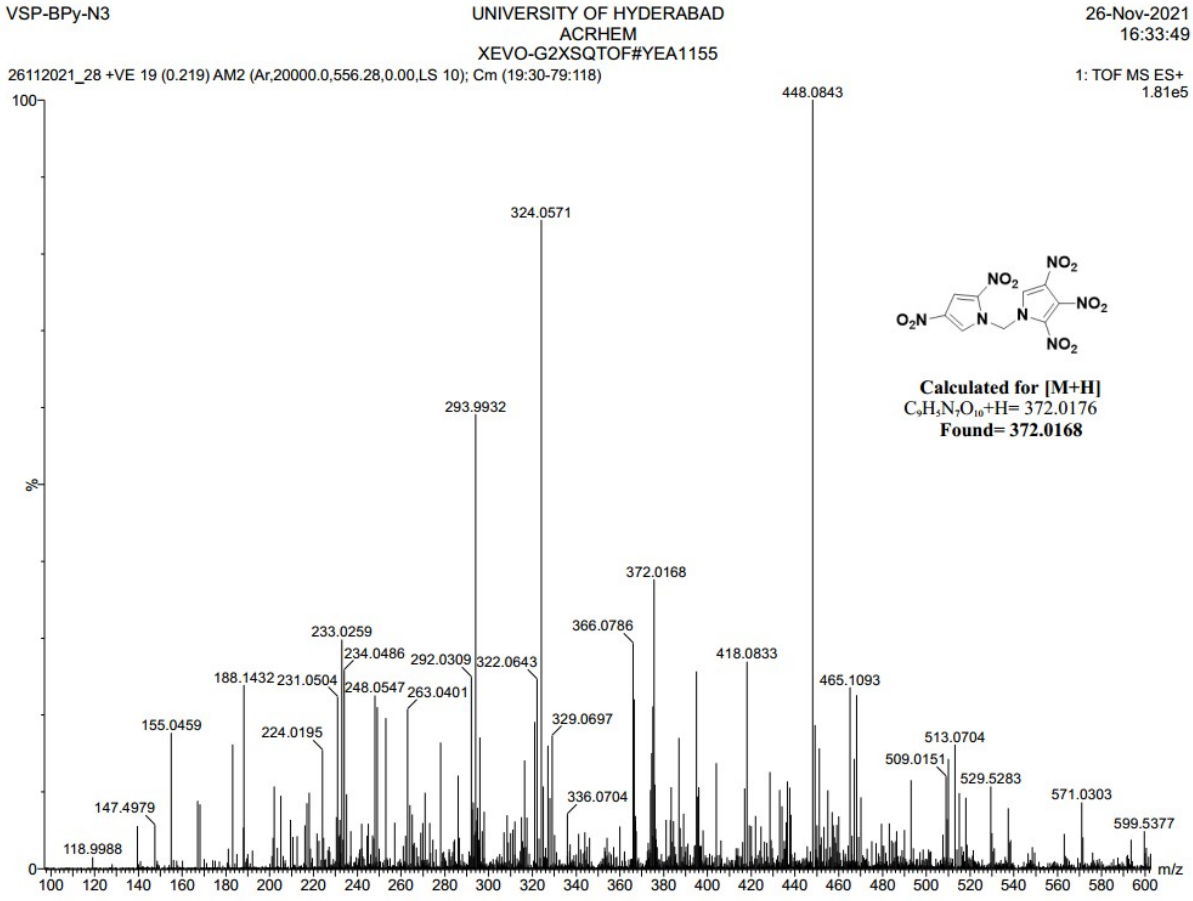


Figure S10: HRMS spectrum of compound **1**.

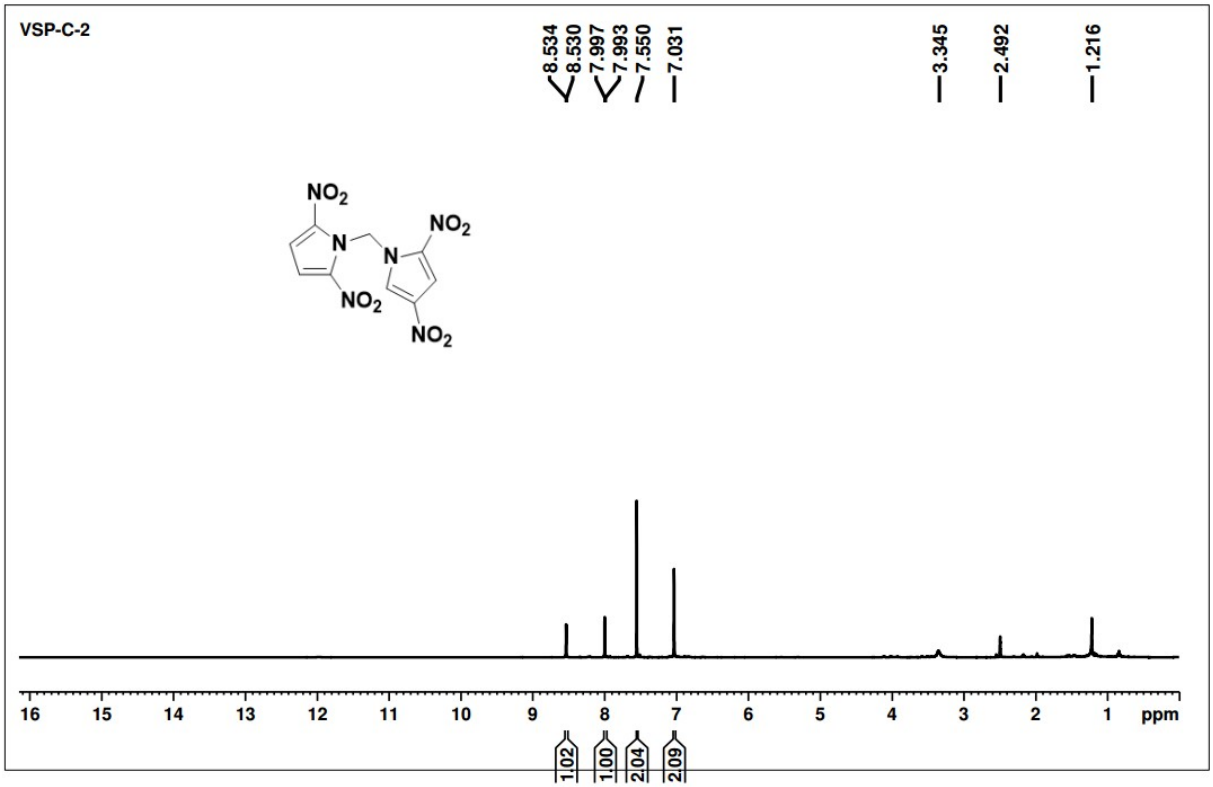


Figure S11: ^{1}H NMR spectrum of compound **2** in dimethyl sulfoxide-d_6.

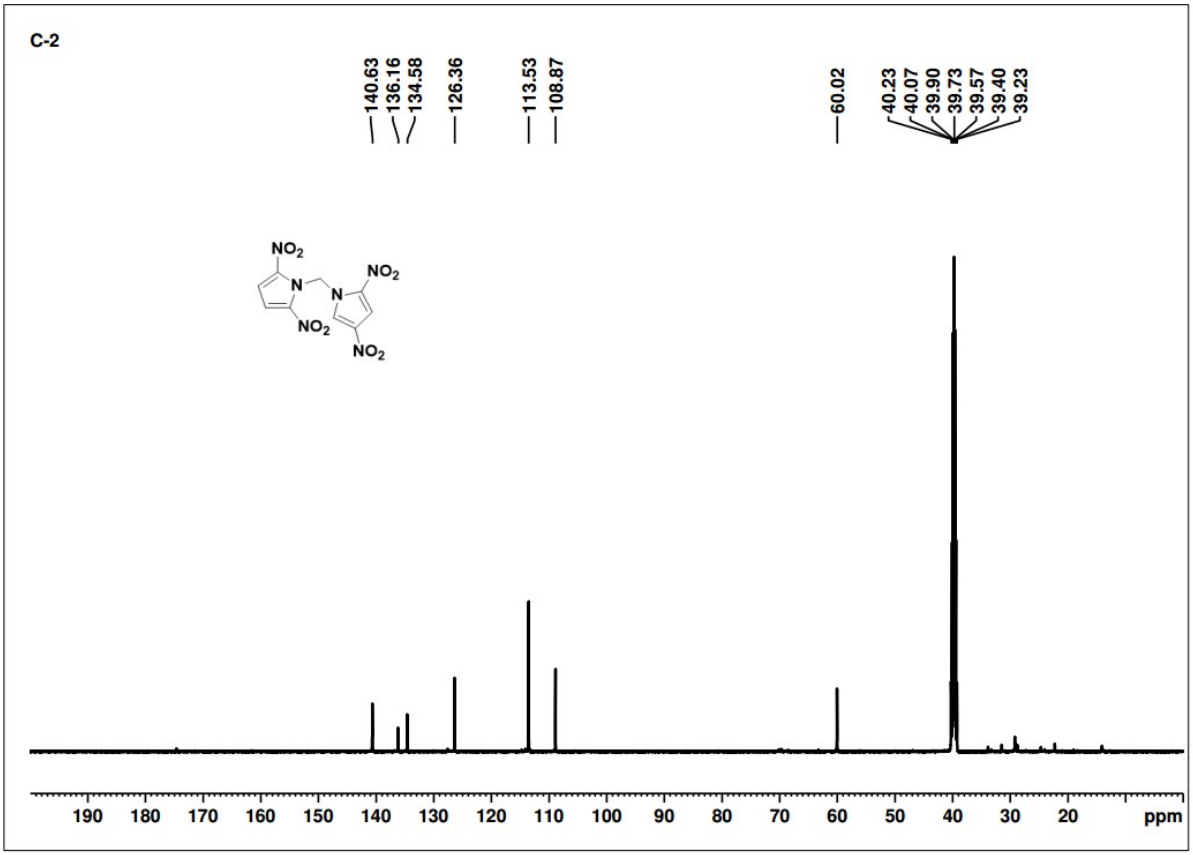


Figure S12: ^{13}C NMR spectrum of compound **2** in dimethyl sulfoxide-d_6.

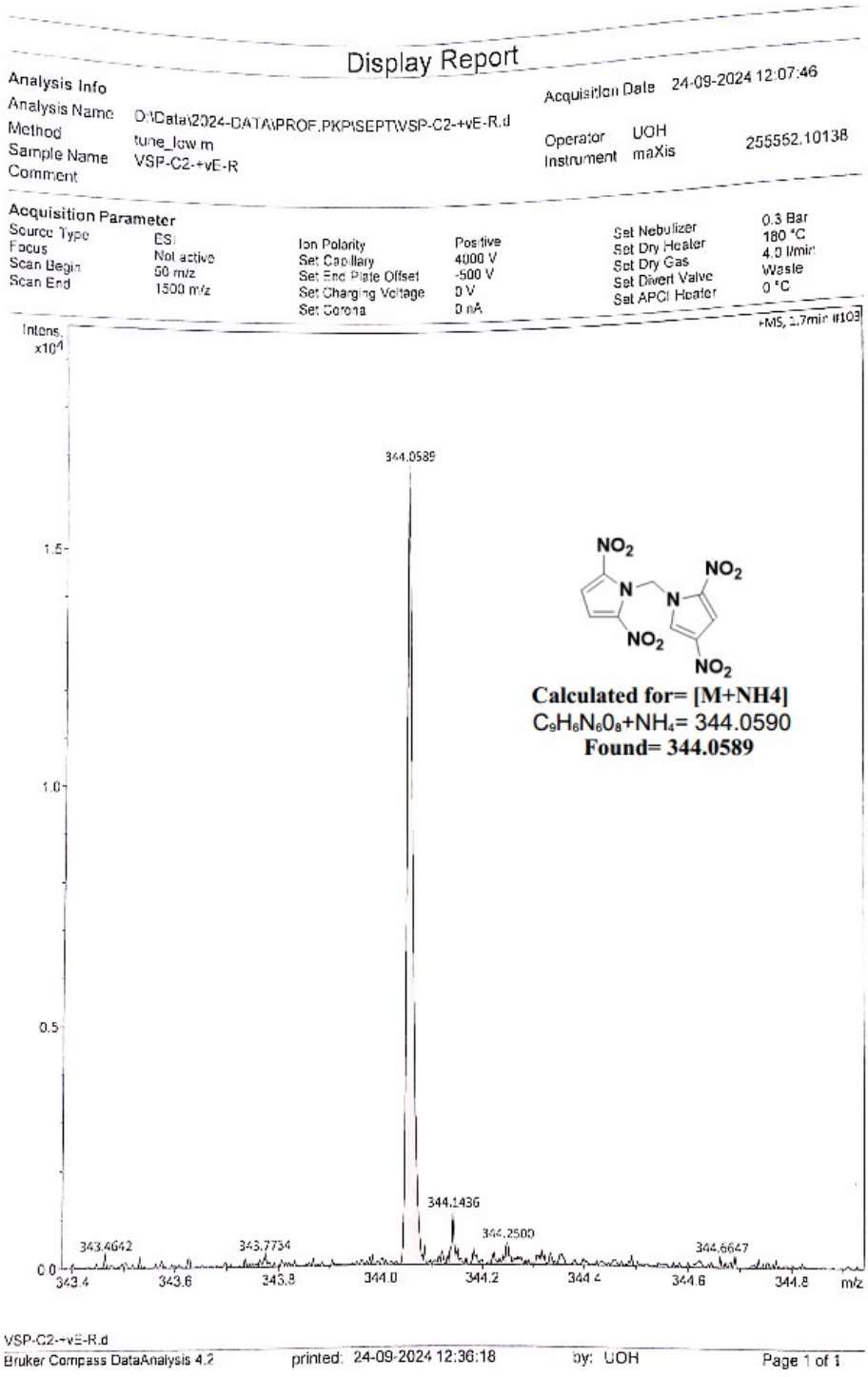


Figure S13: HRMS spectrum of compound **2**.

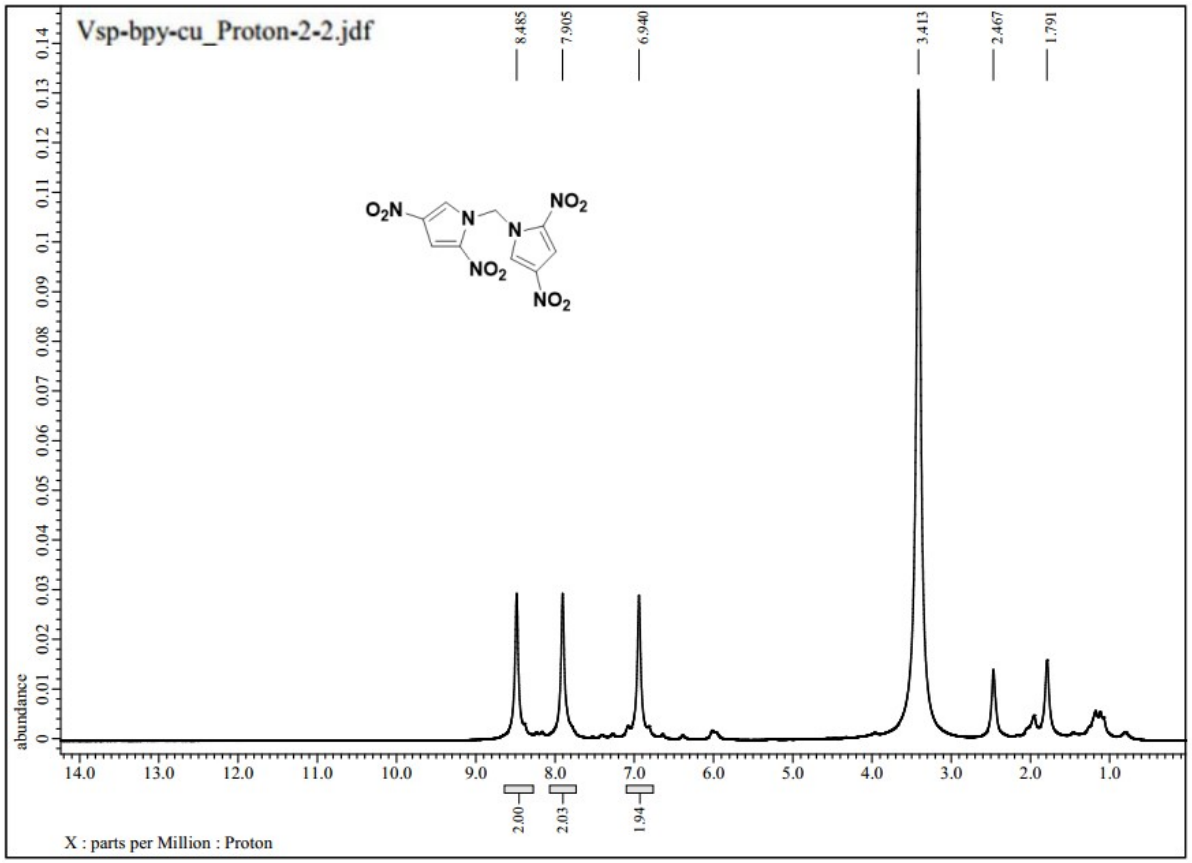


Figure S14: ^{1}H NMR spectrum of compound **3** in dimethyl sulfoxide-d_6.

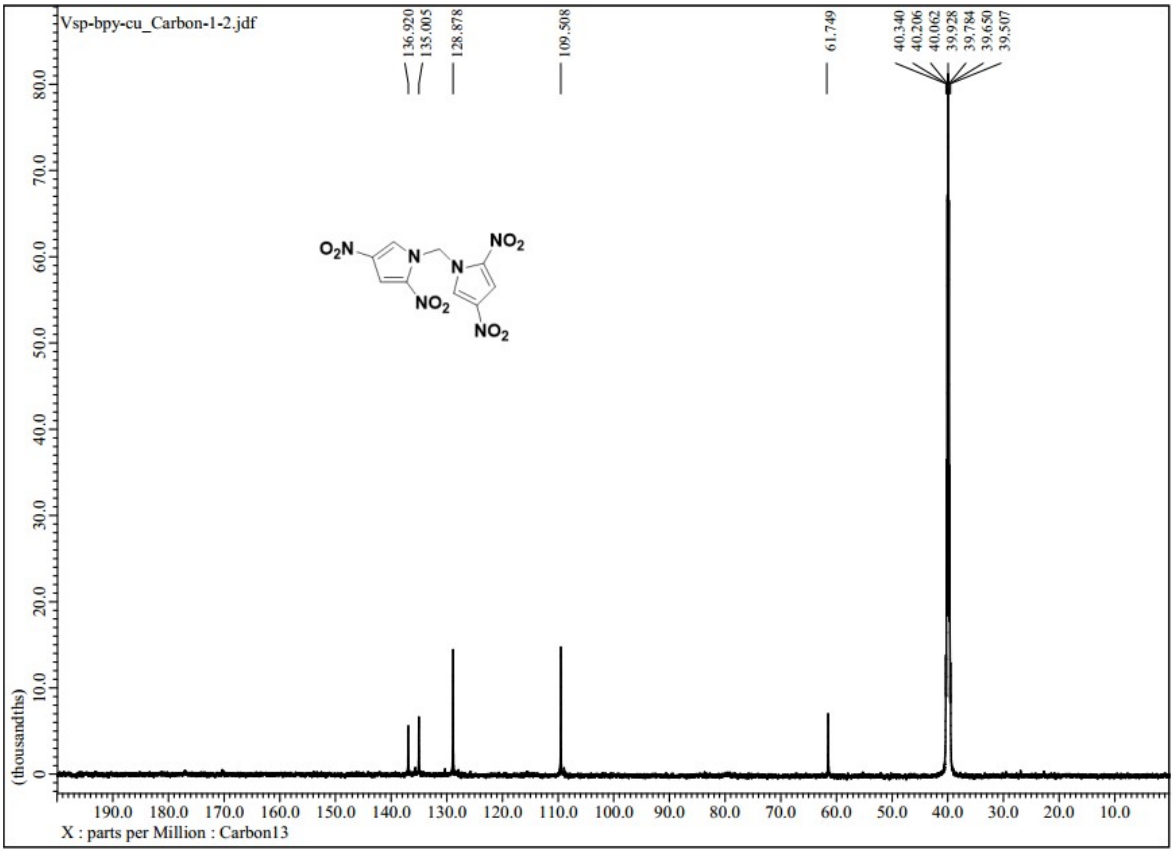


Figure S15: ^{13}C NMR spectrum of compound **3** in dimethyl sulfoxide-d_6.

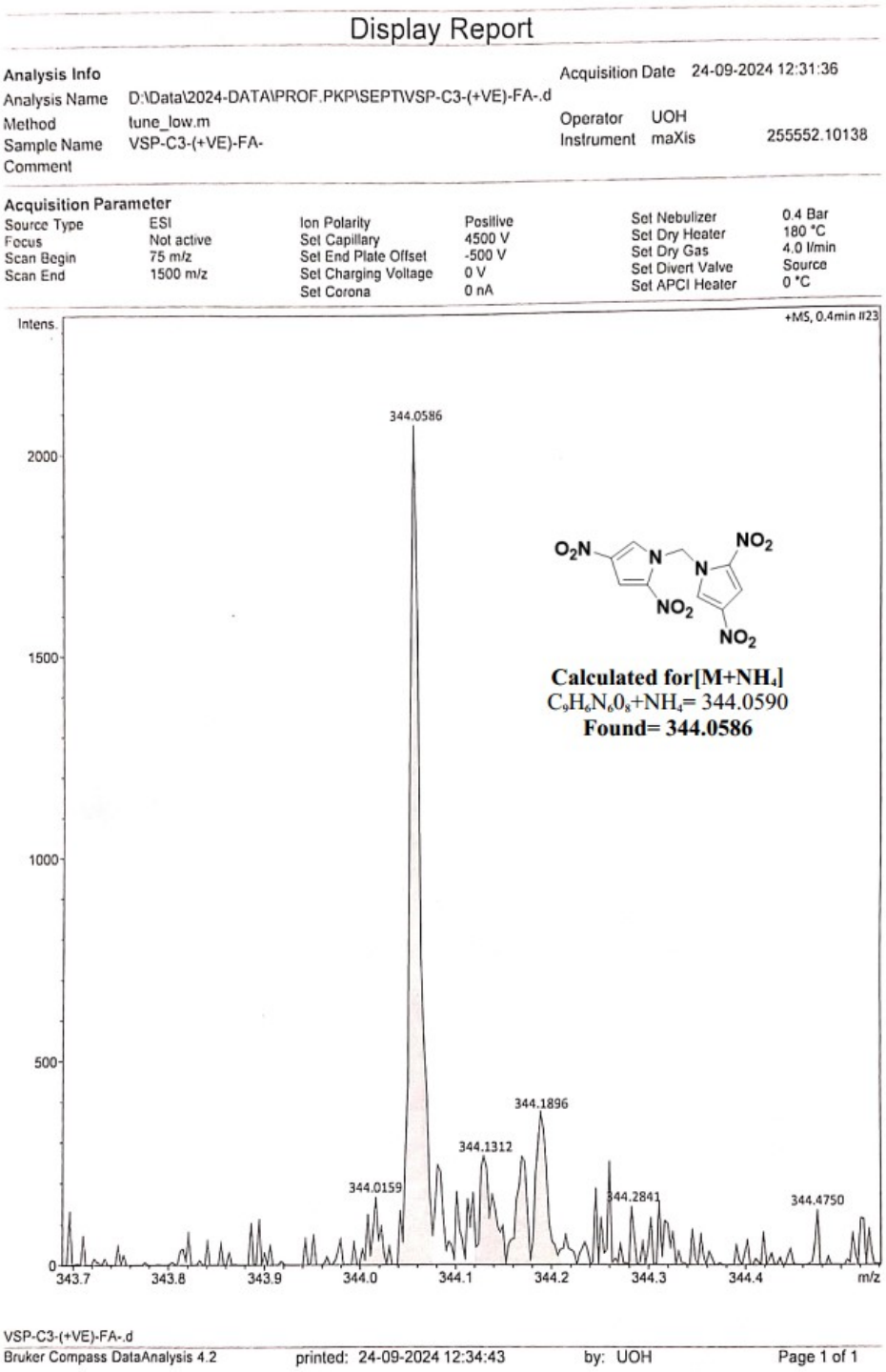


Figure S16: HRMS spectrum of compound **3**.

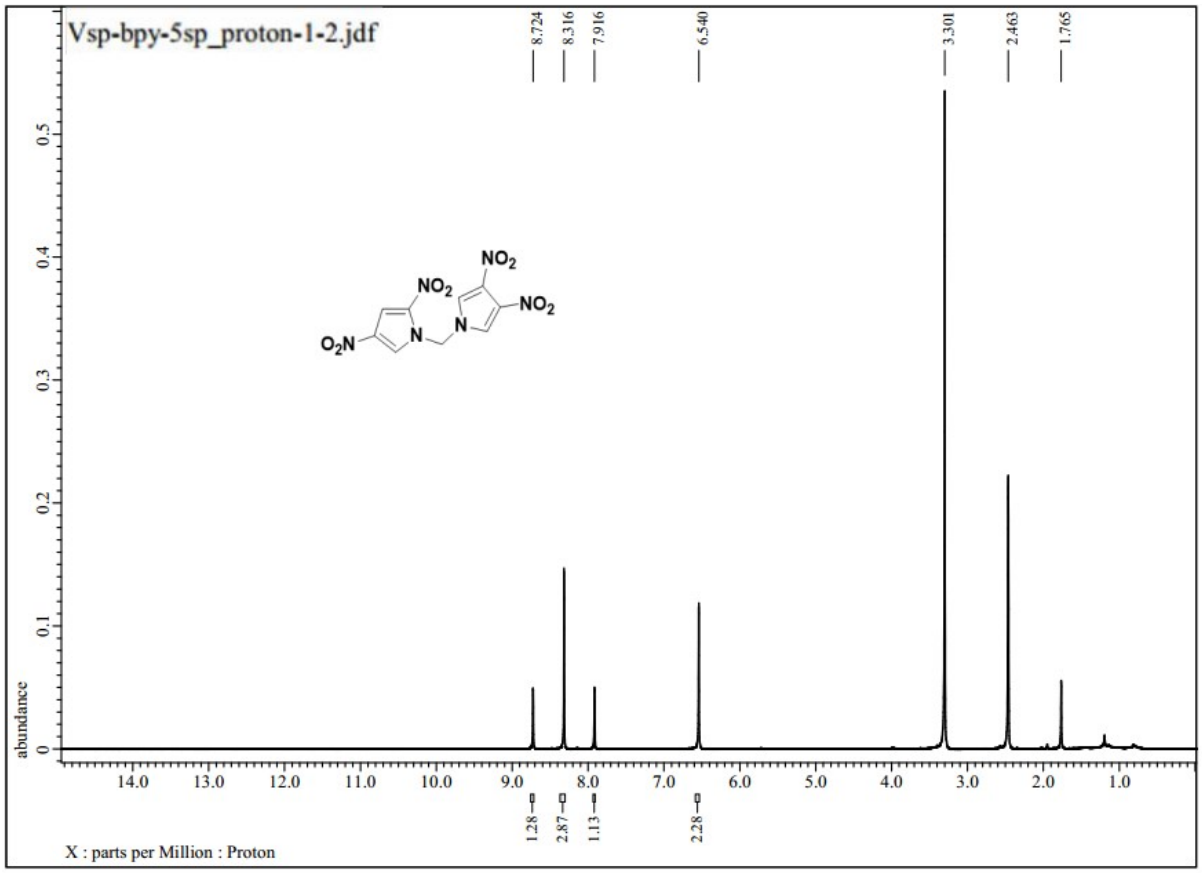


Figure S17: ^{1}H NMR spectrum of compound **4** in dimethyl sulfoxide-d_6.

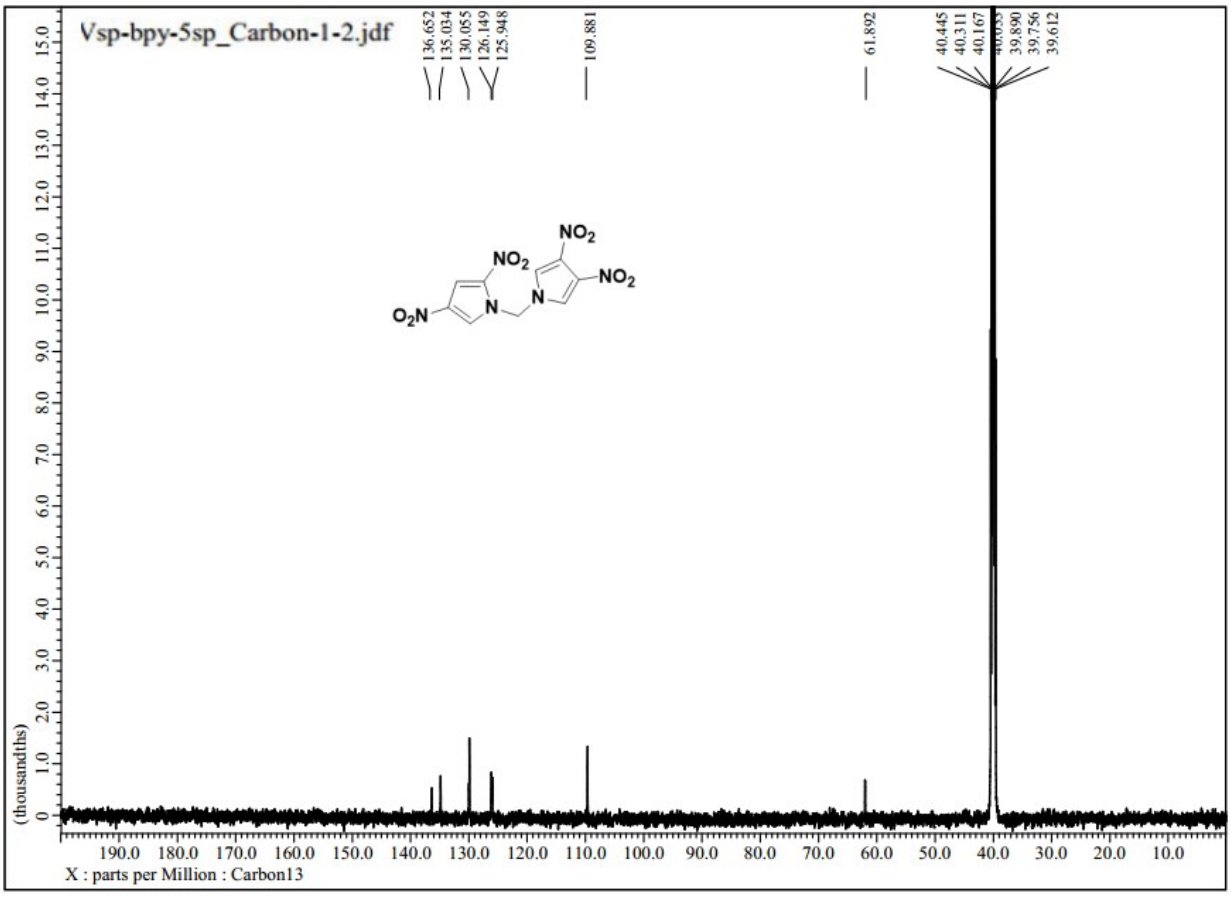


Figure S18: ^{13}C NMR spectrum of compound **4** in dimethyl sulfoxide-d_6.

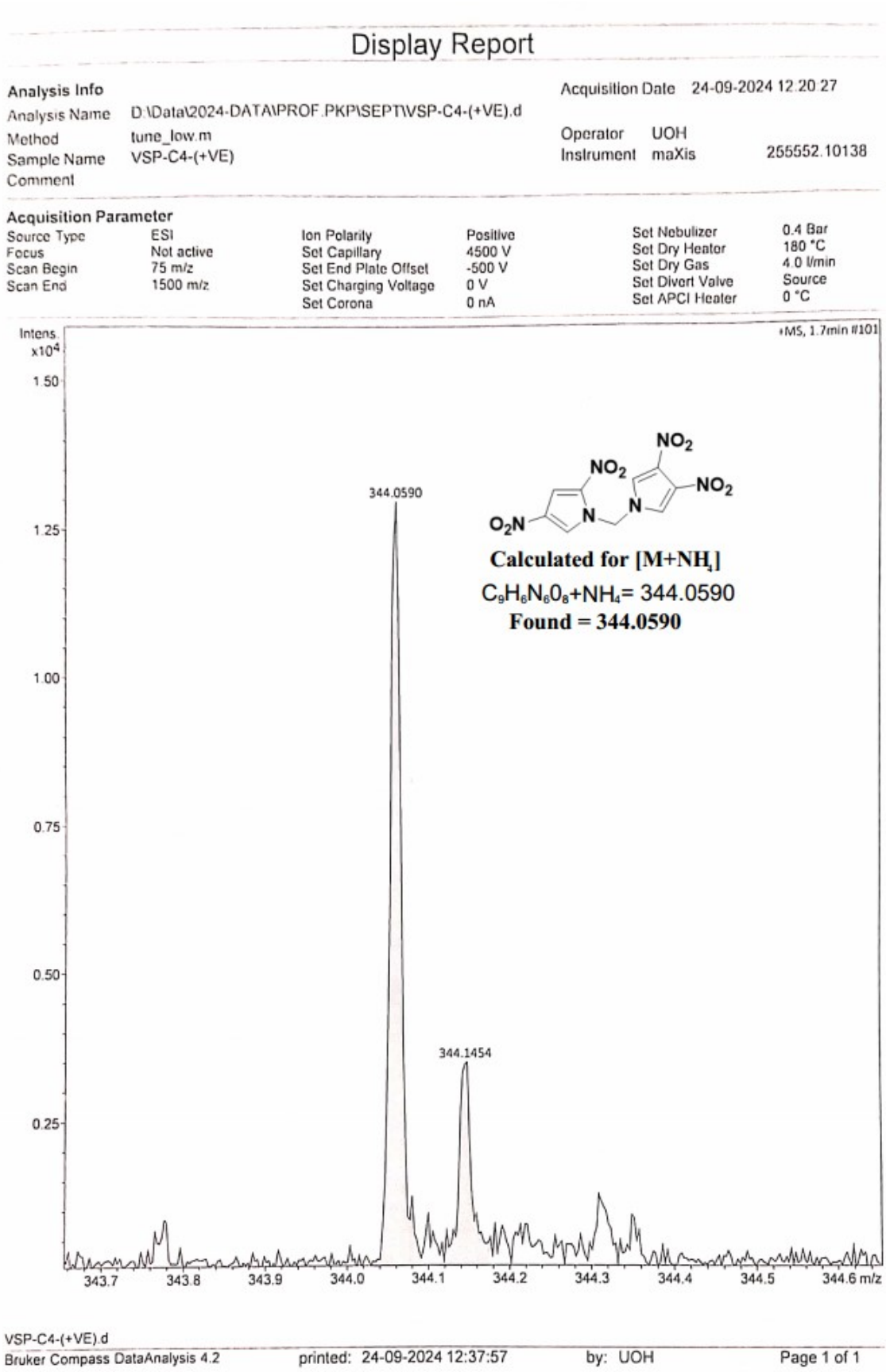


Figure S19: HRMS spectrum of compound **4**.

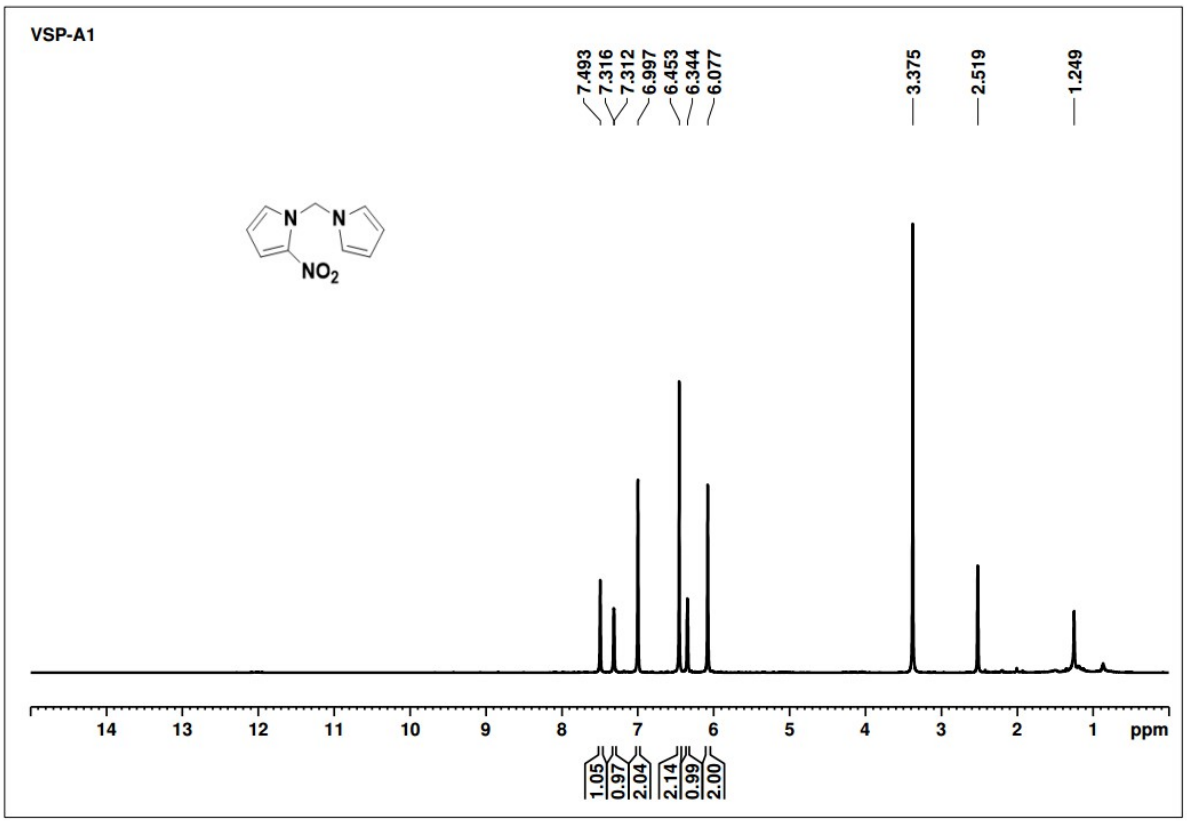


Figure S20: ^{1}H NMR spectrum of compound **5** in dimethyl sulfoxide-d_6.

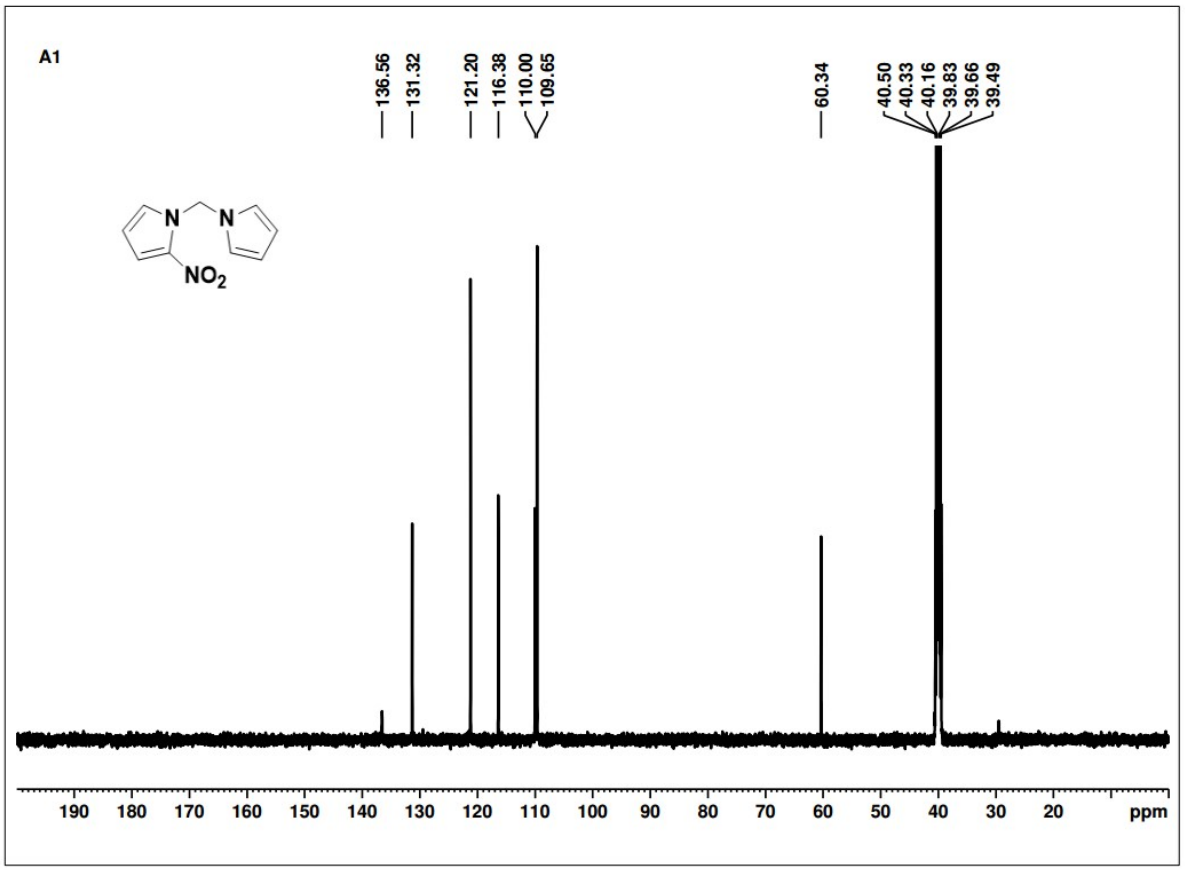


Figure S21: ^{13}C NMR spectrum of compound **5** in dimethyl sulfoxide-d_6.

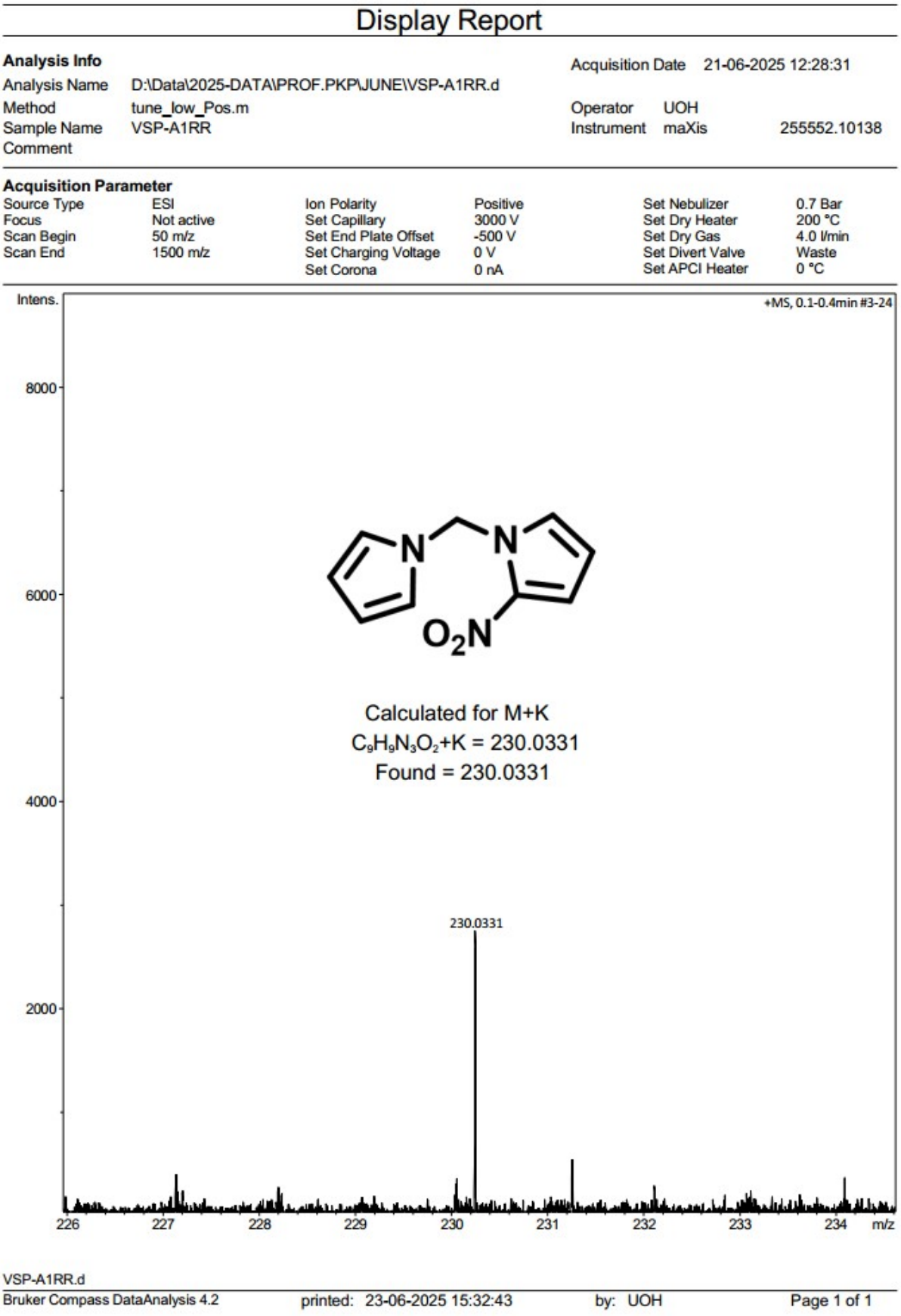


Figure S22: HRMS spectrum of compound **5**.

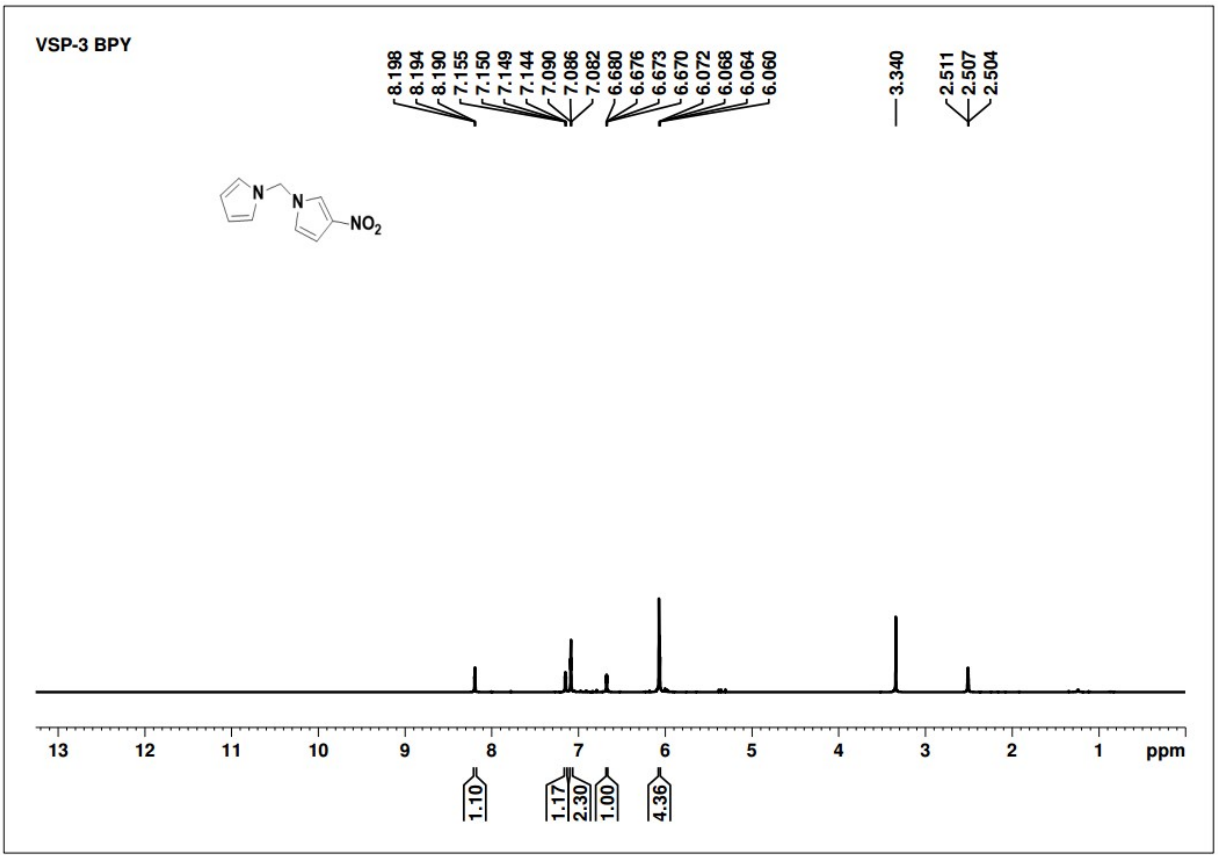


Figure S23: ^{1}H NMR spectrum of compound **6** in dimethyl sulfoxide-d_6.

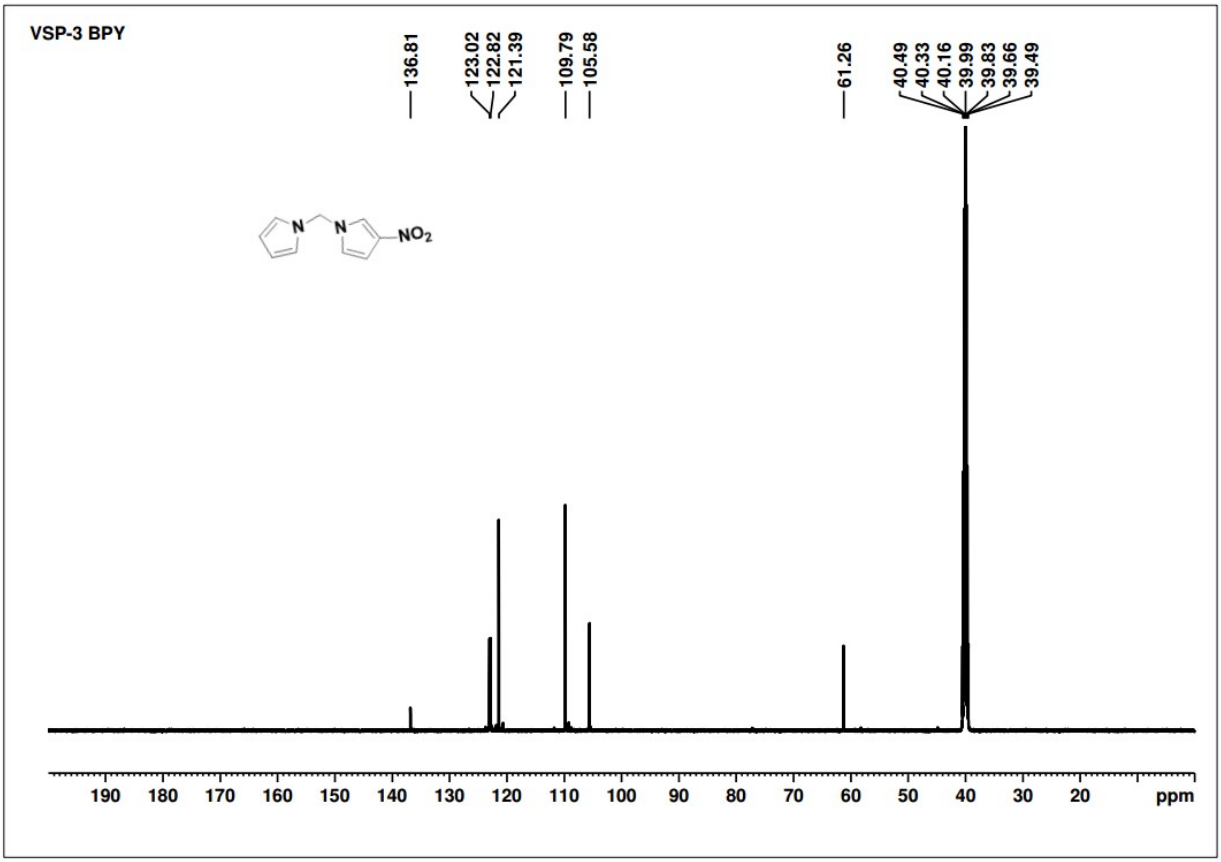


Figure S24: ^{13}C NMR spectrum of compound **6** in dimethyl sulfoxide-d_6.

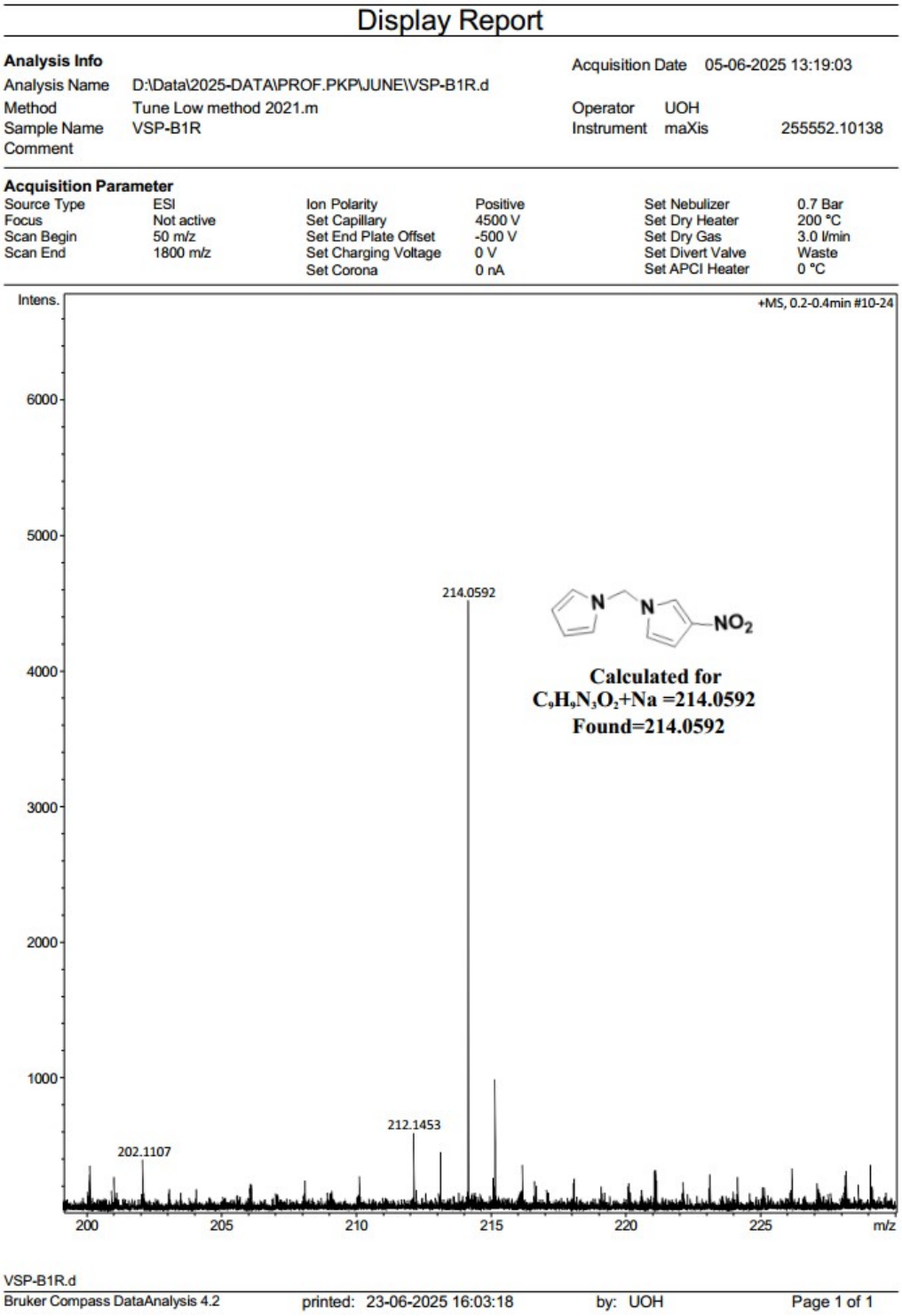


Figure S25: HRMS spectrum of compound **6**.

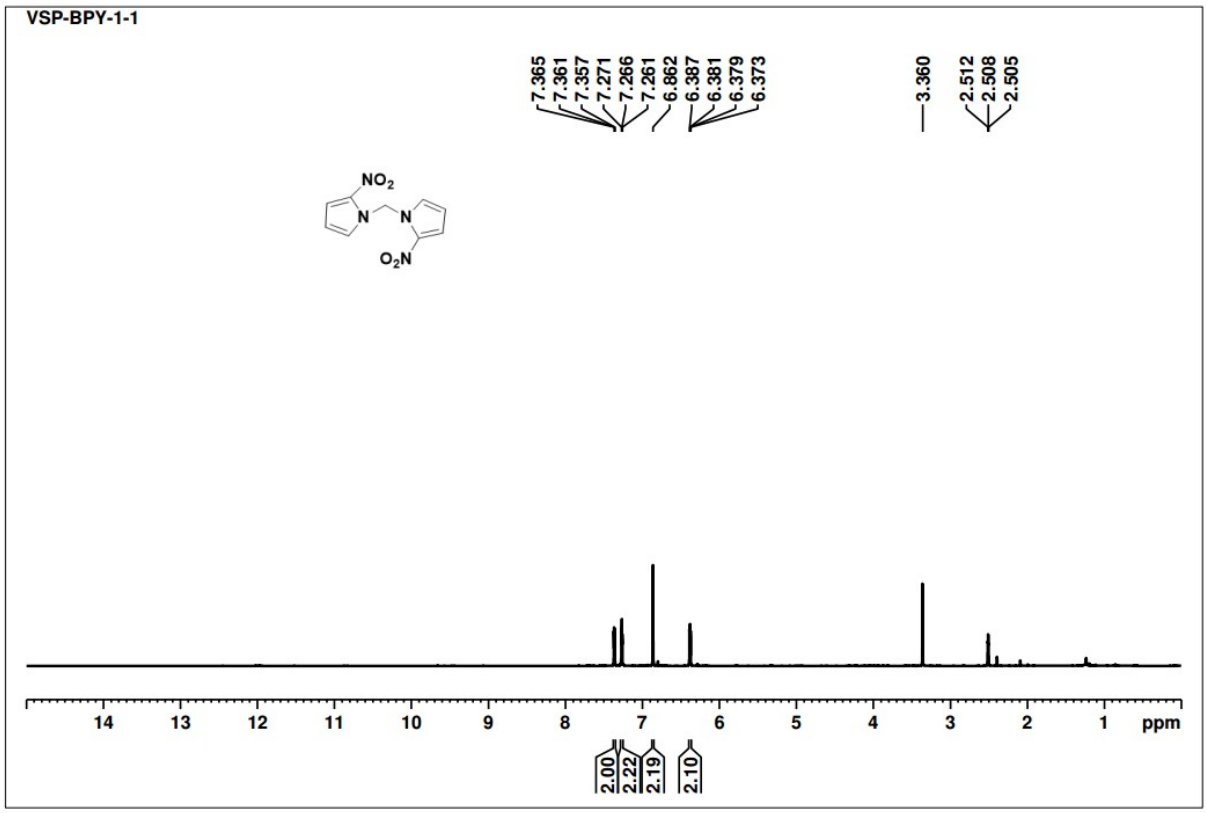


Figure S26: ^{1}H NMR spectrum of compound **7** in dimethyl sulfoxide-d_6.

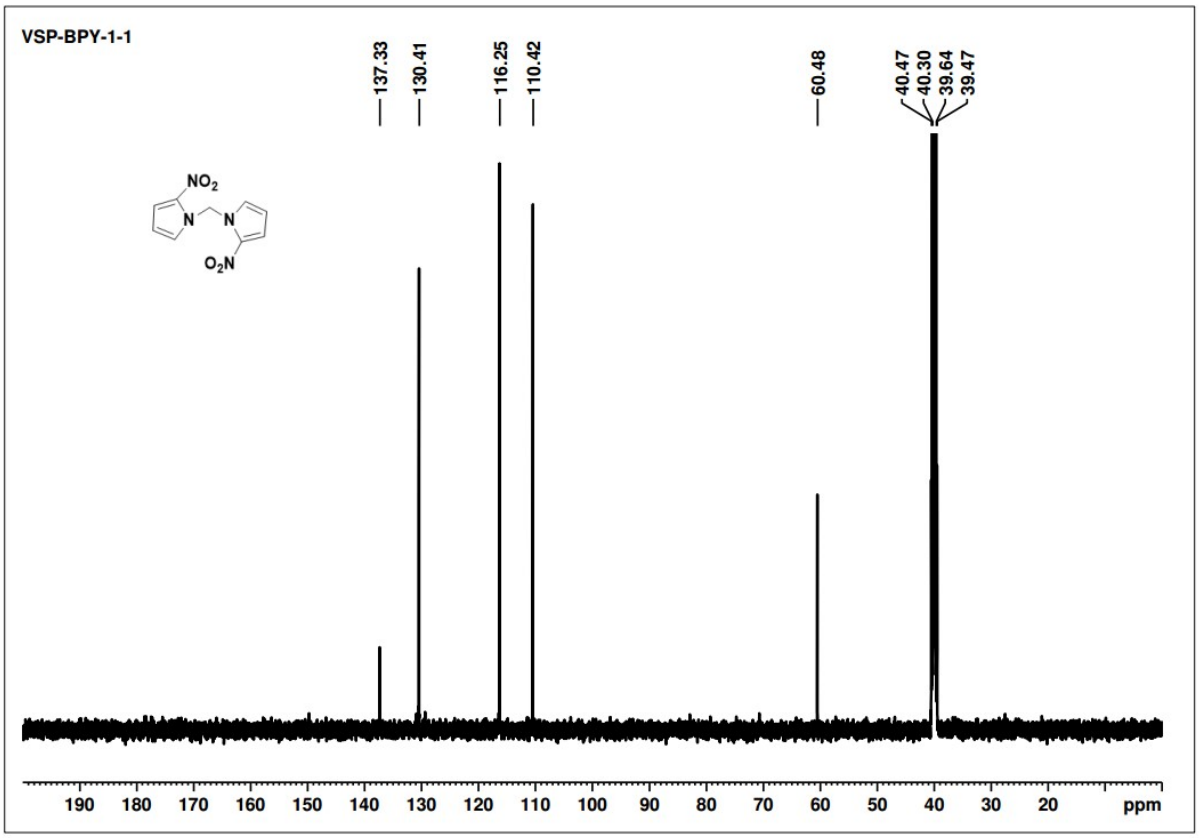


Figure S27: ^{13}C NMR spectrum of compound **7** in dimethyl sulfoxide-d_6.

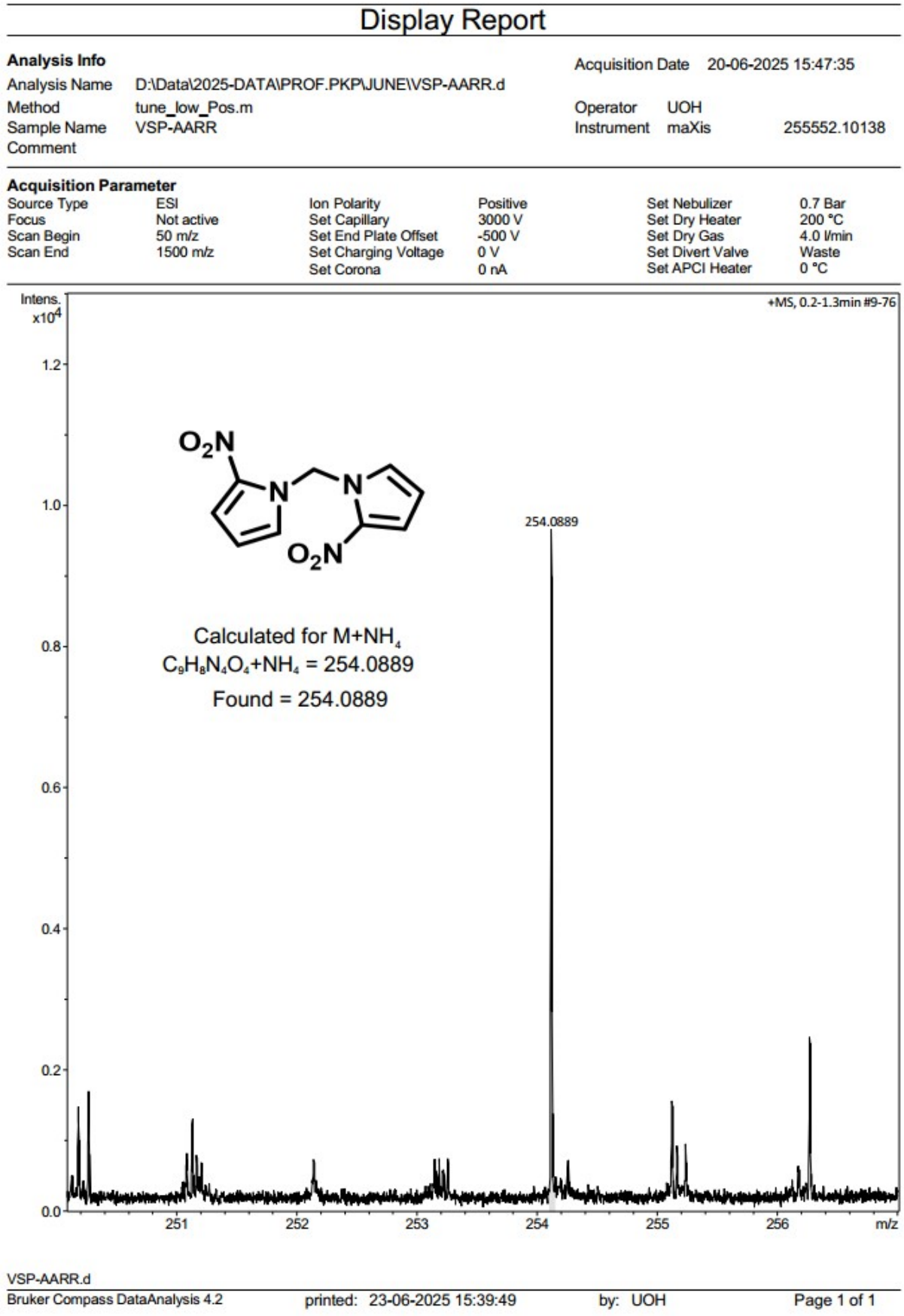


Figure S28: HRMS spectrum of compound **7**.

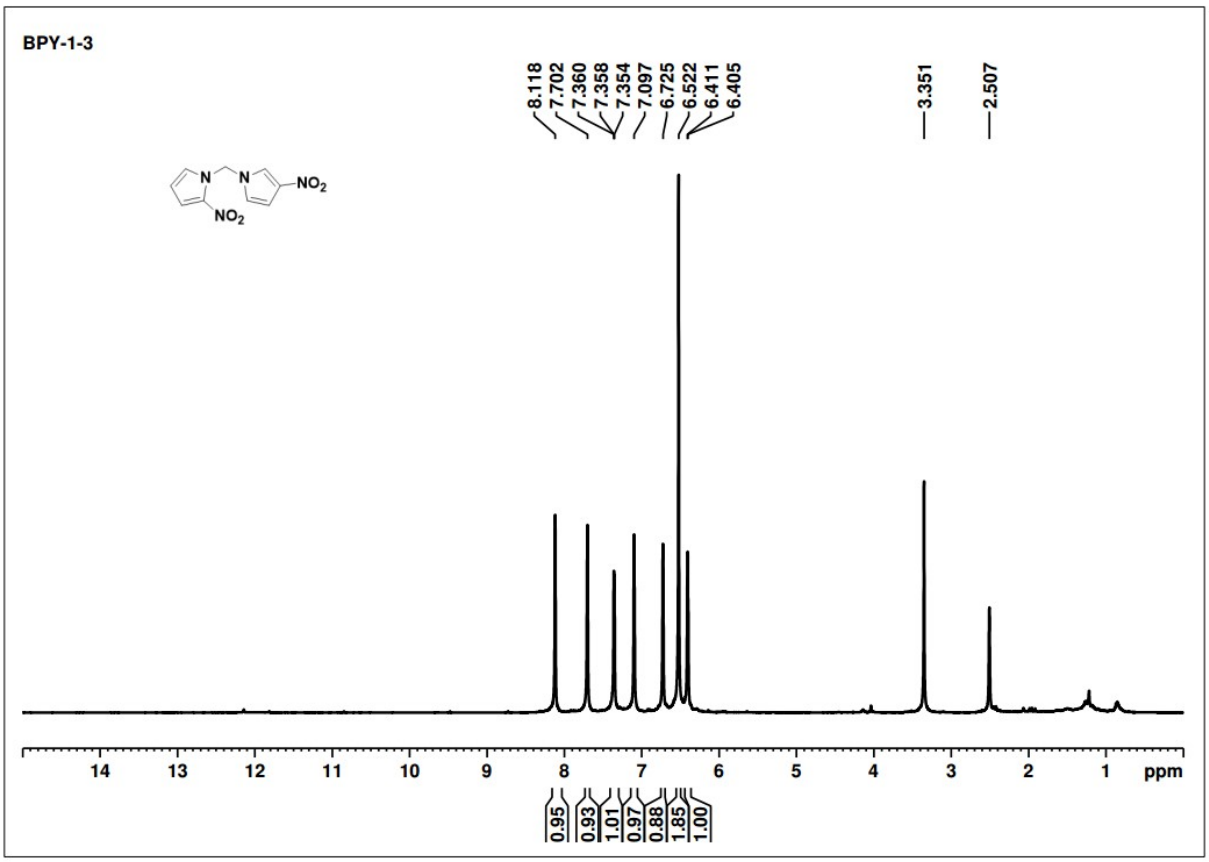


Figure S29: ^{1}H NMR spectrum of compound **8** in dimethyl sulfoxide-d_6.

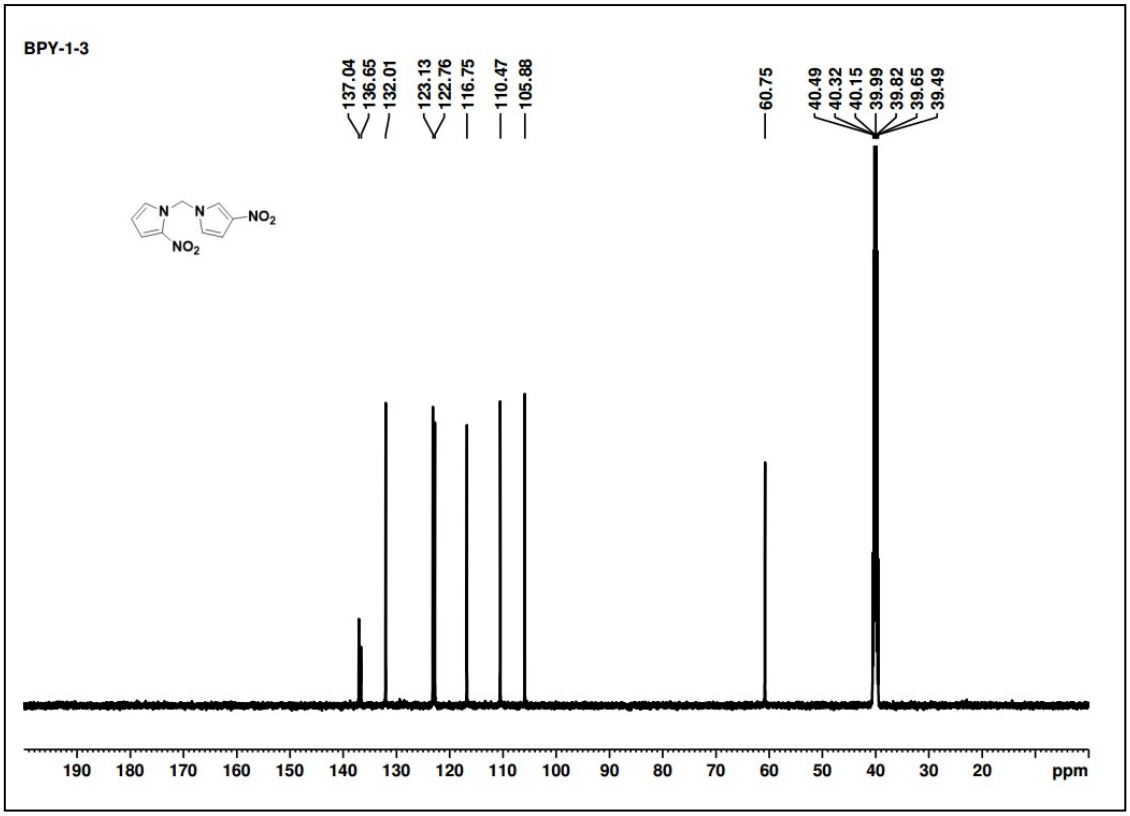


Figure S30: ^{13}C NMR spectrum of compound **8** in dimethyl sulfoxide-d_6.

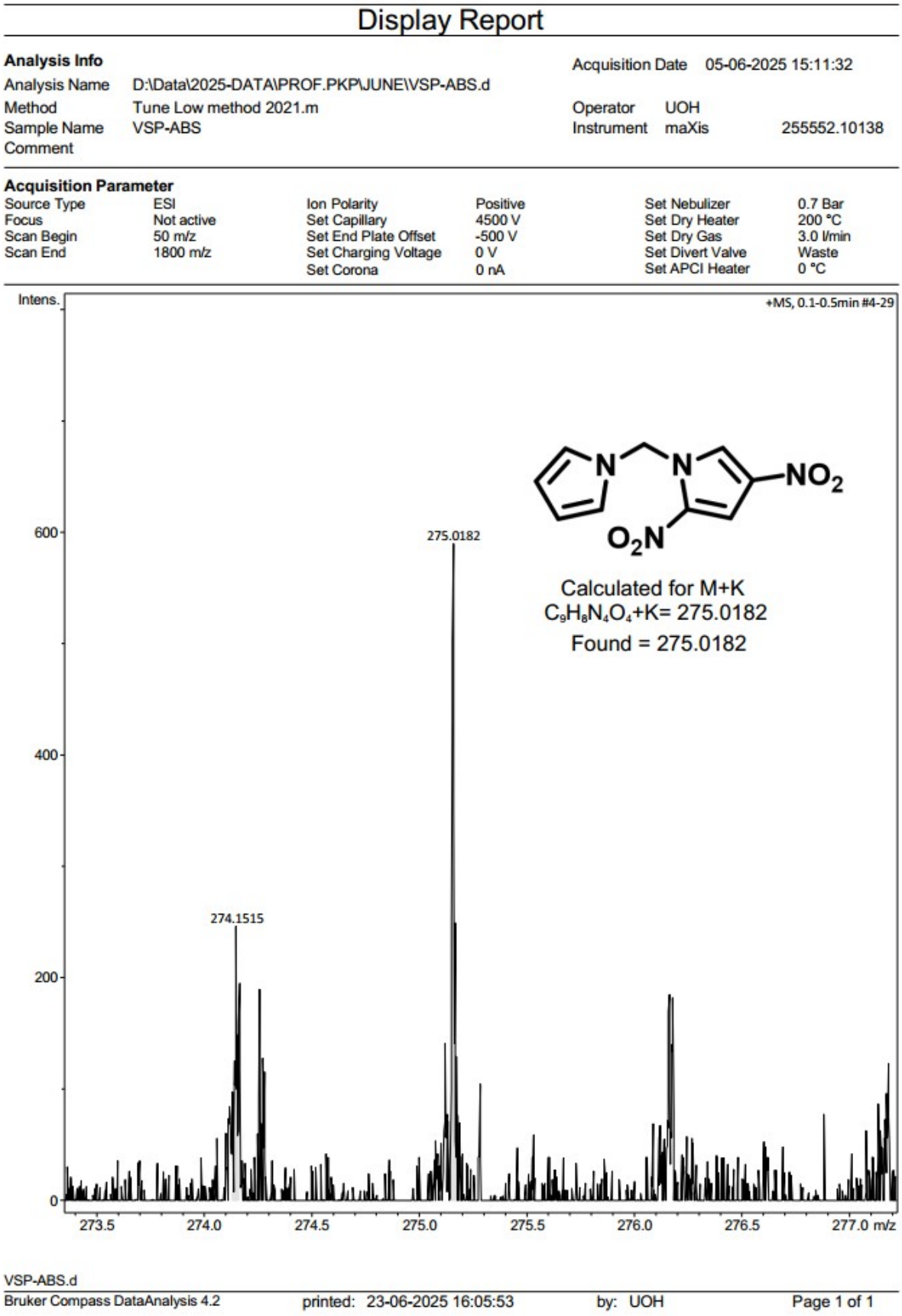


Figure S31: HRMS spectrum of compound **8**.

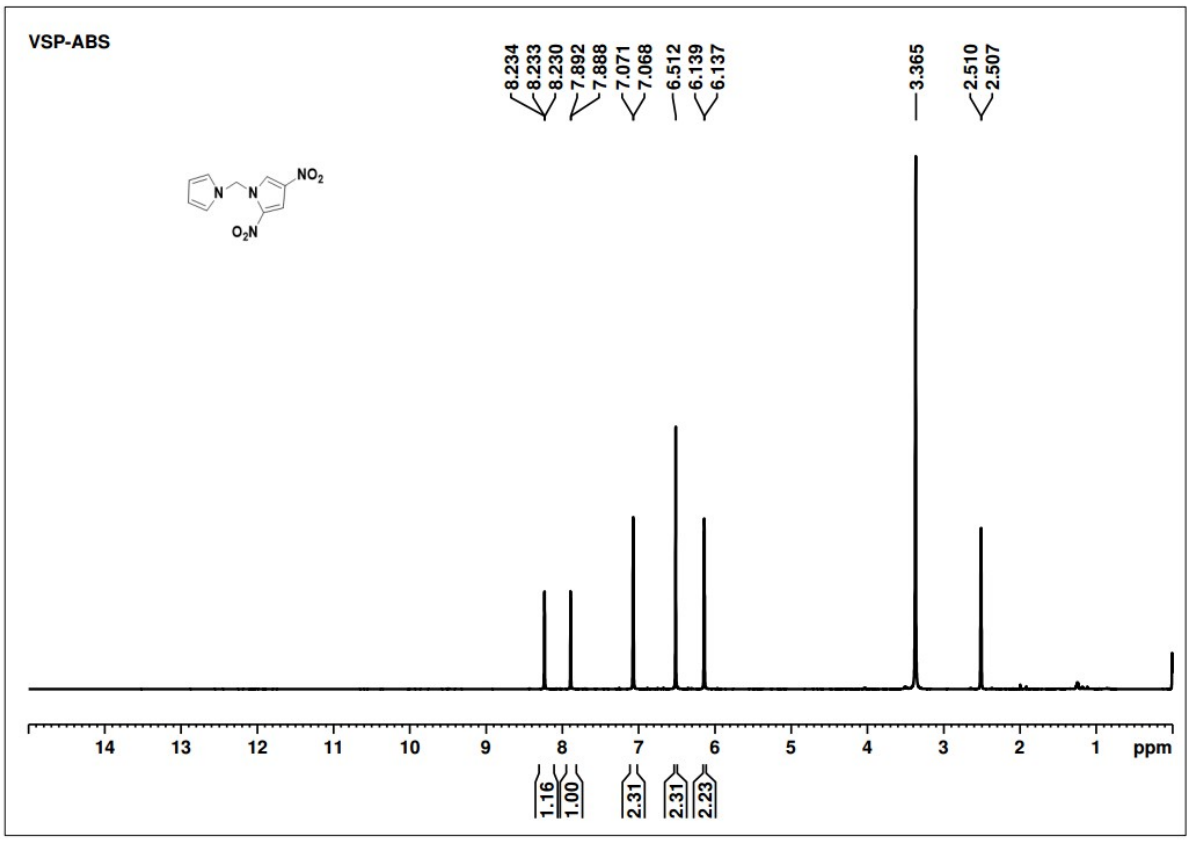


Figure S32: ^{1}H NMR spectrum of compound **9** in dimethyl sulfoxide-d_6.

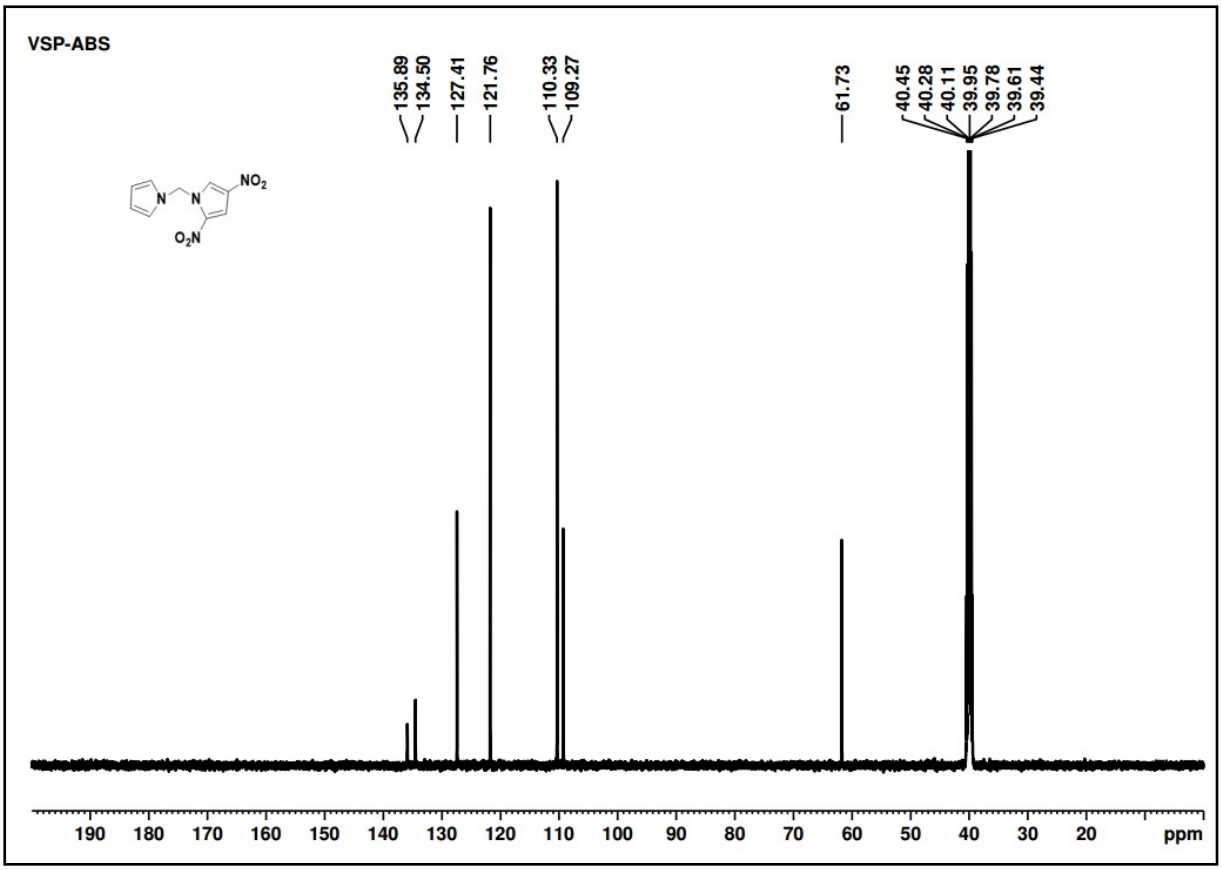


Figure S33: ^{13}C NMR spectrum of compound **9** in dimethyl sulfoxide-d_6.

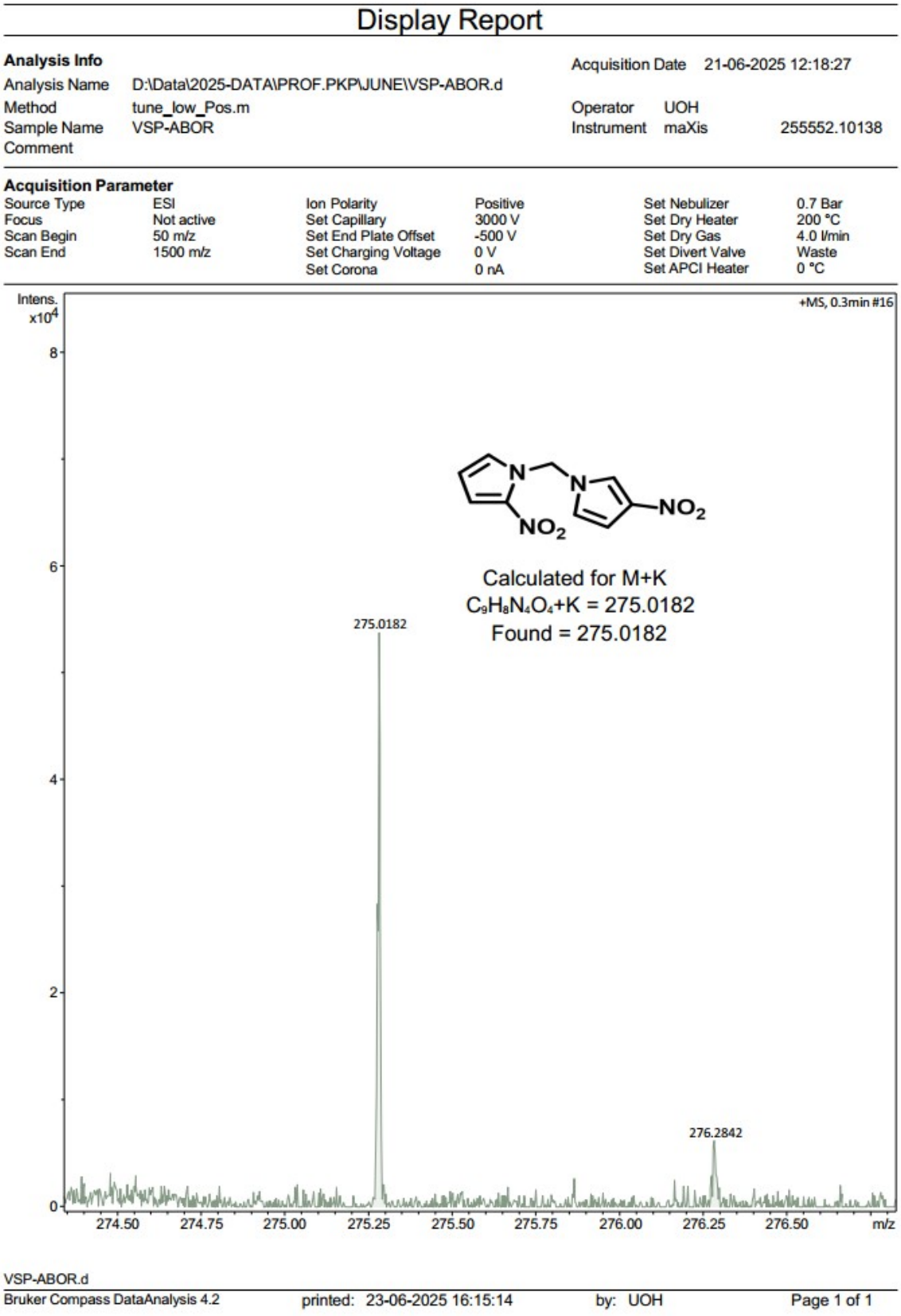


Figure S34: HRMS spectrum of compound **9**.

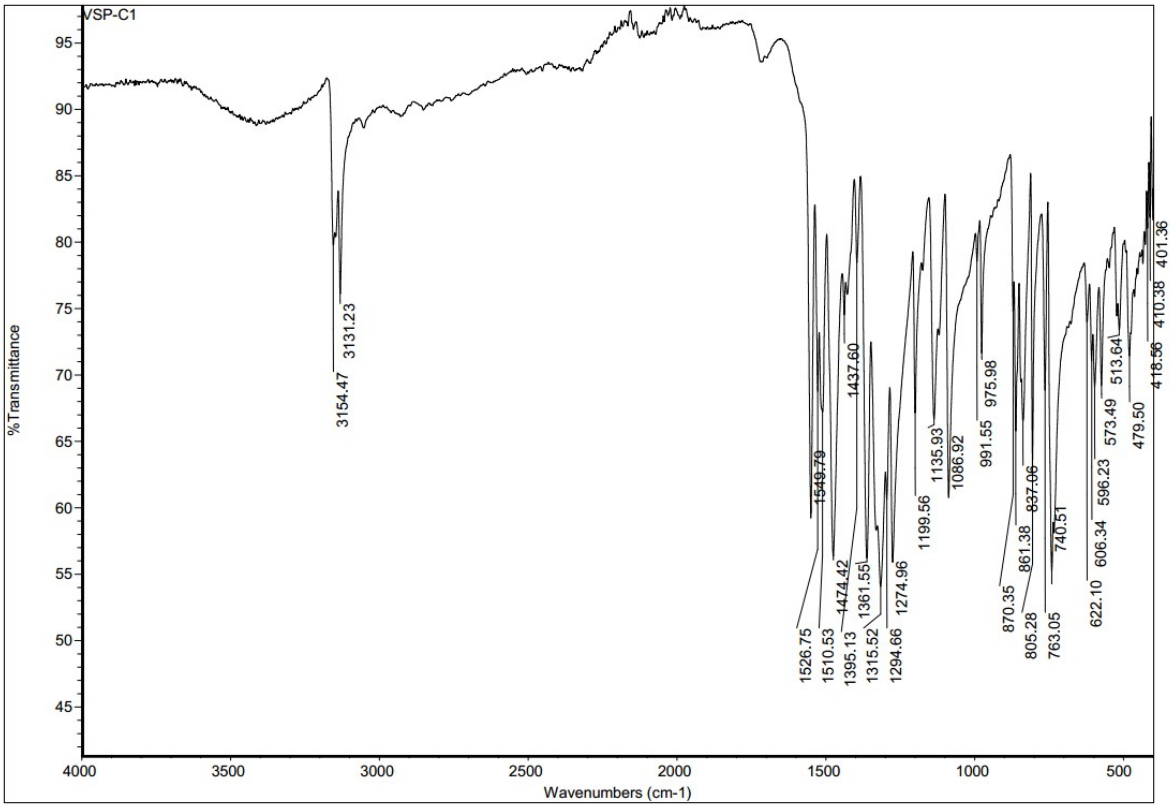


Figure S35: IR spectrum of compound **1**.

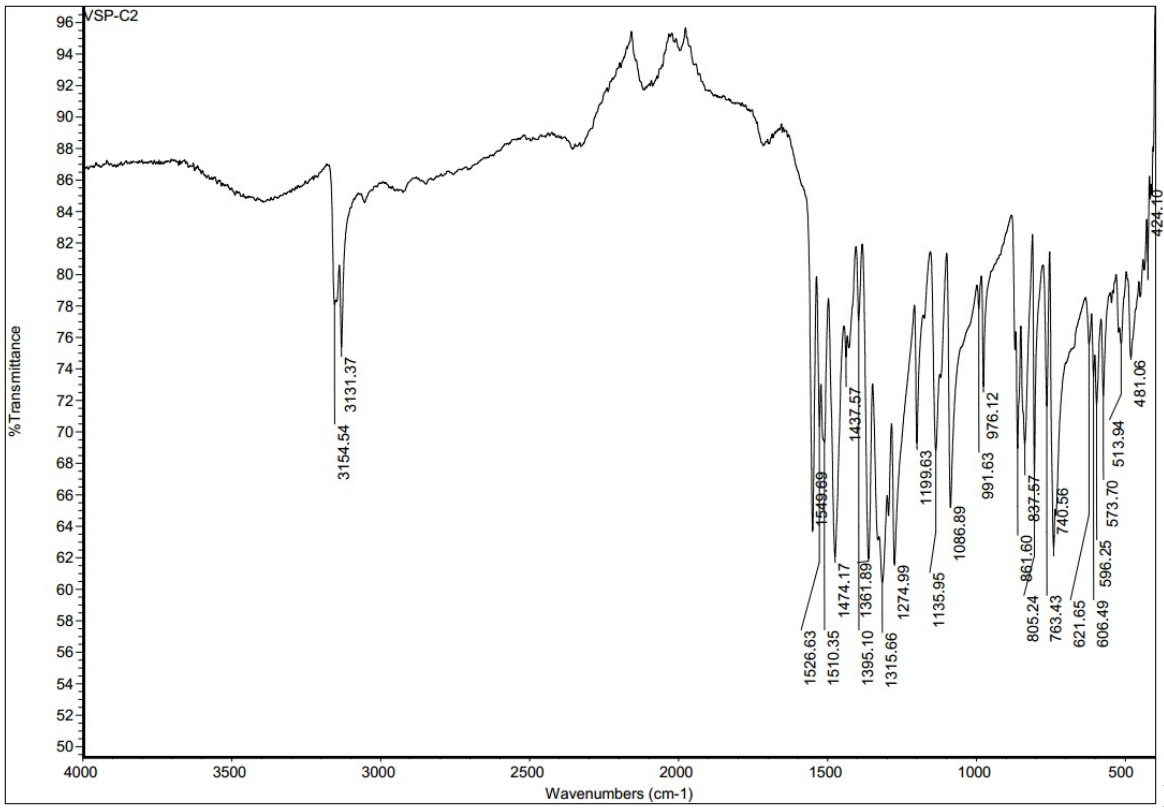


Figure S36: IR spectrum of compound **2**.

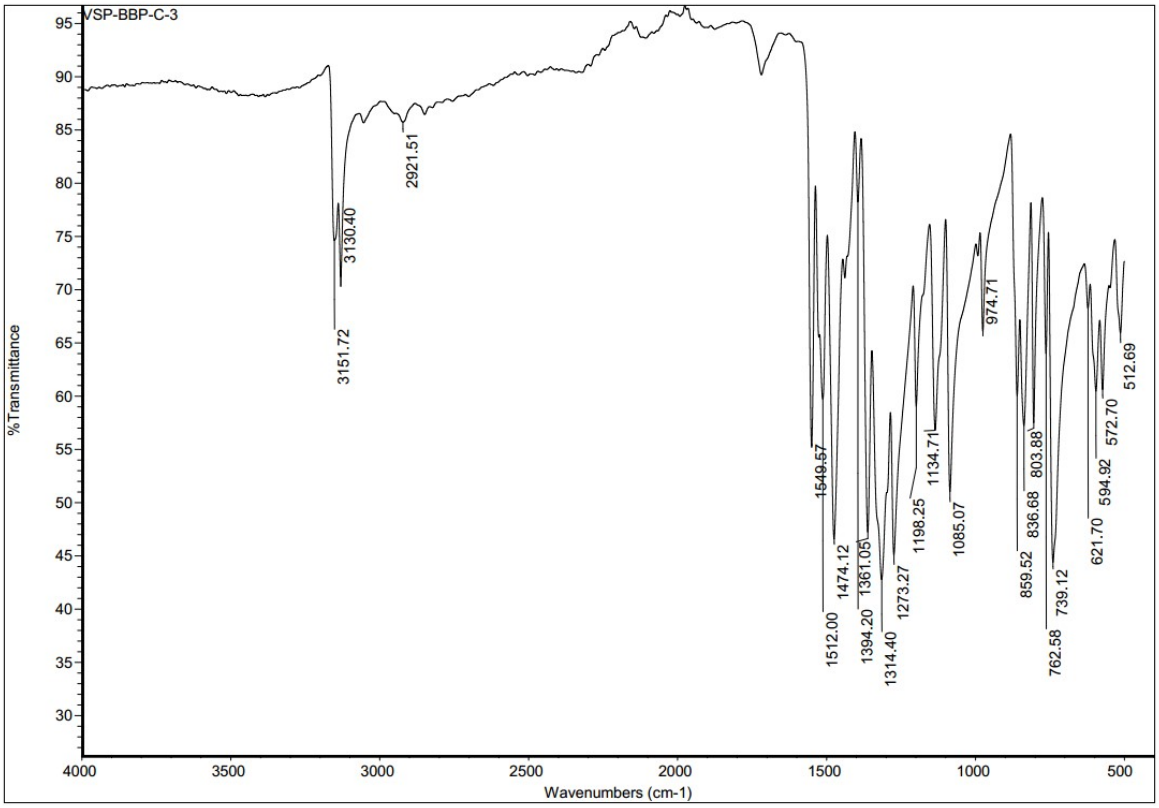


Figure S37: IR spectrum of compound **3**.

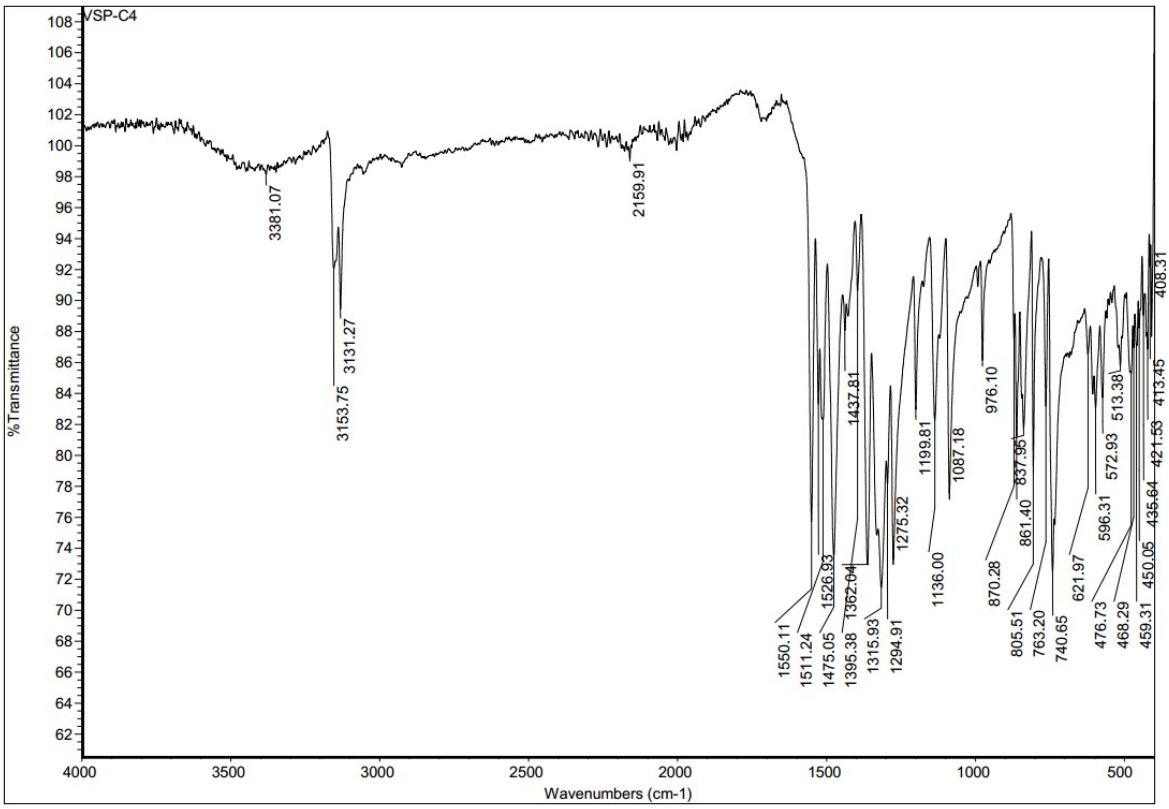


Figure S38: IR spectrum of compound **4**.

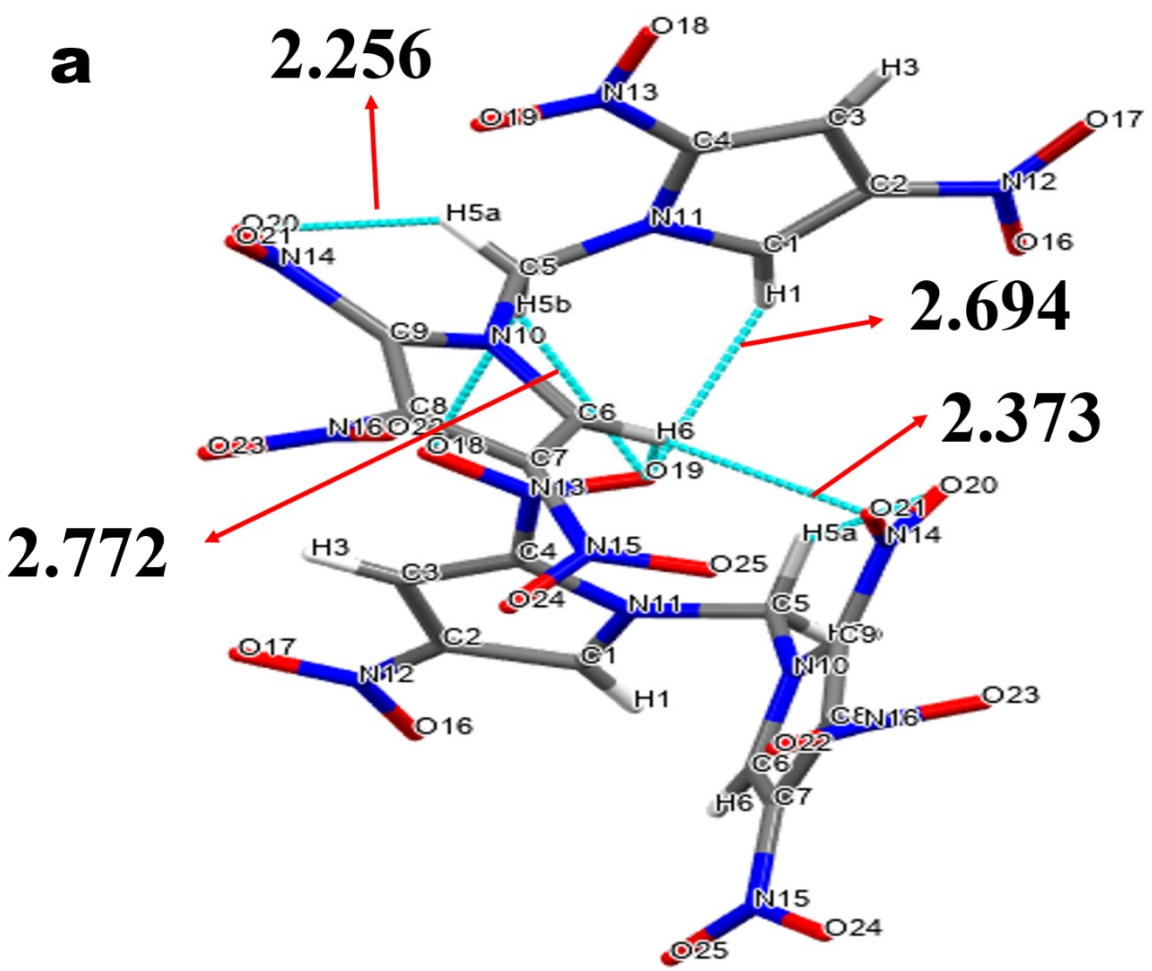


Figure S39: Representation of the hydrogen-bonding network in compound **1**.

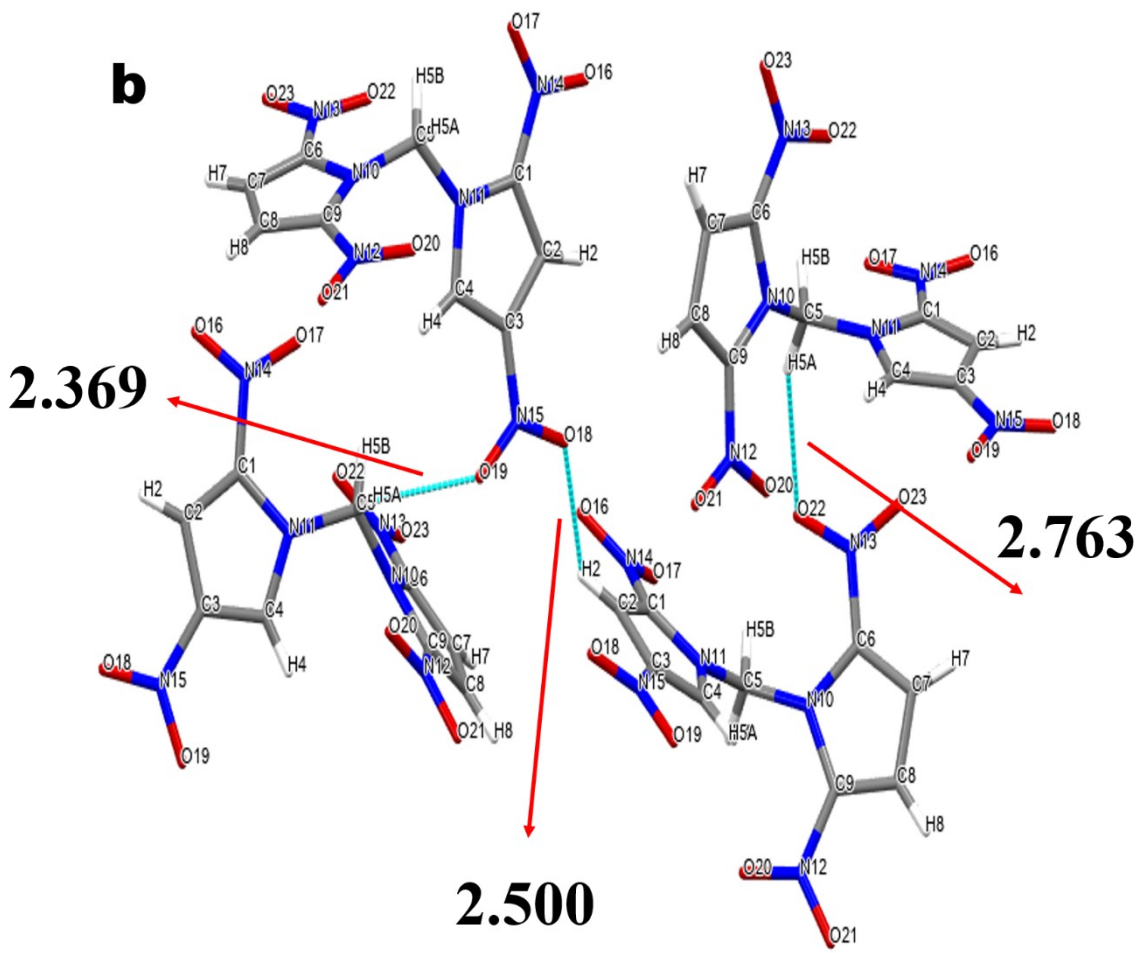


Figure S40: Representation of the hydrogen-bonding network in compound **2**.

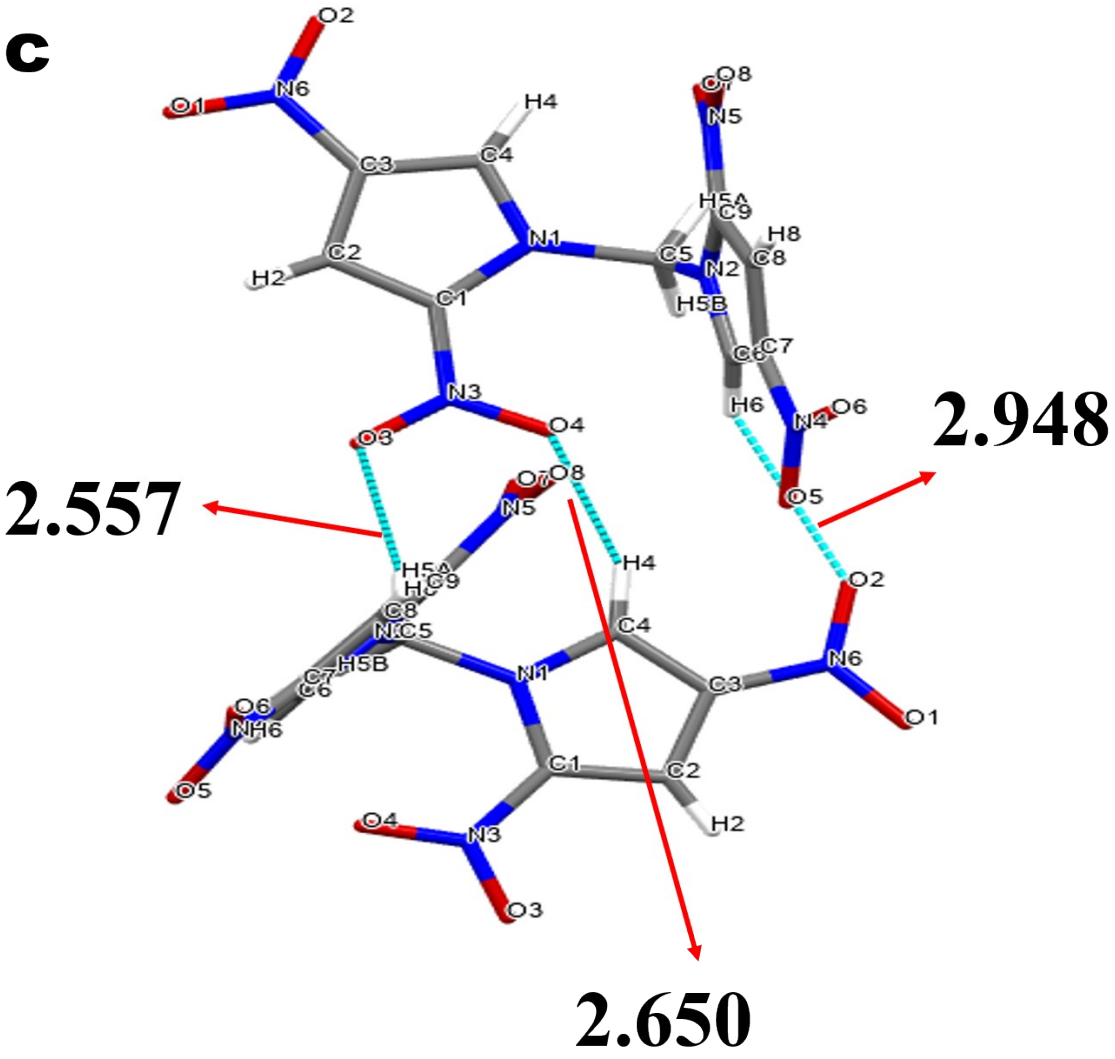


Figure S41: Representation of the hydrogen-bonding network in compound **3**.

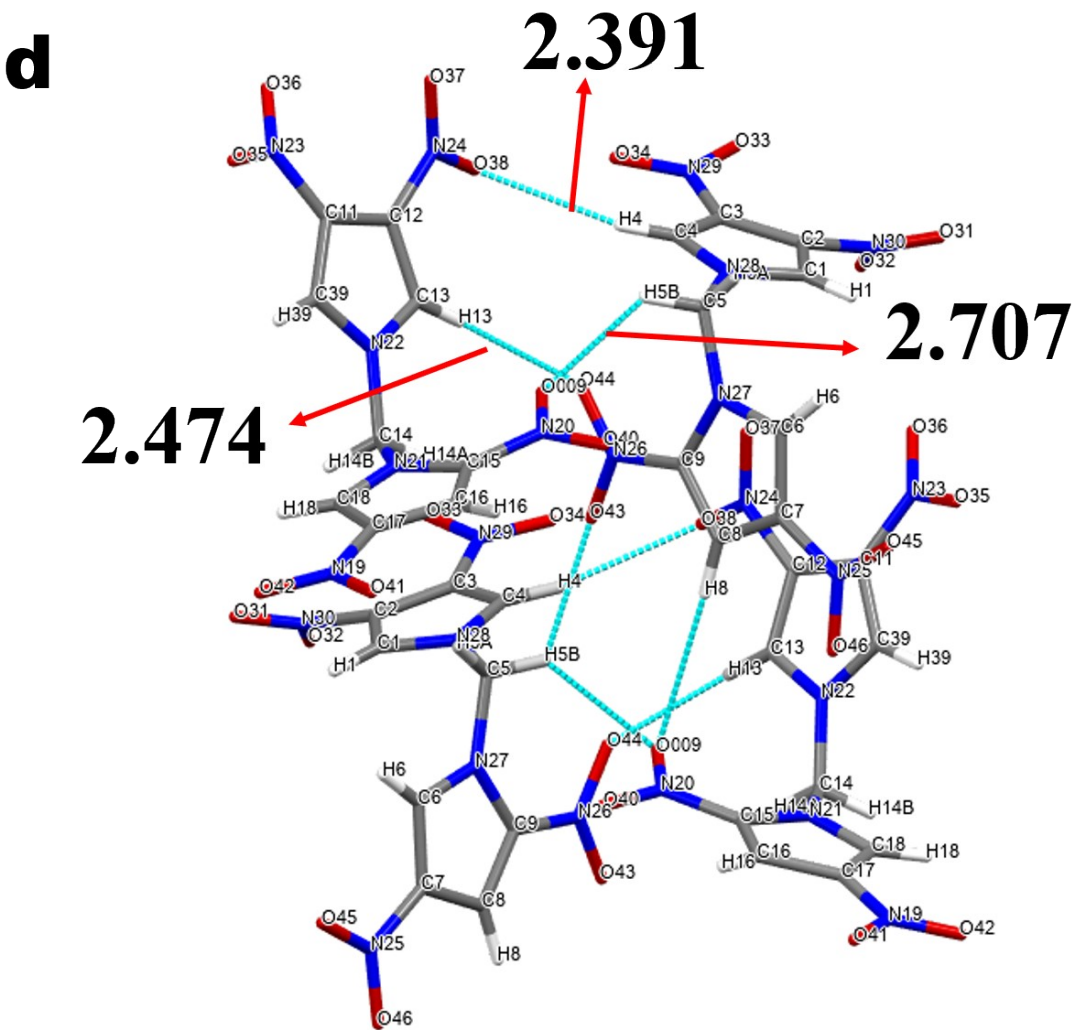


Figure S42: Representation of the hydrogen-bonding network in compound **4**.

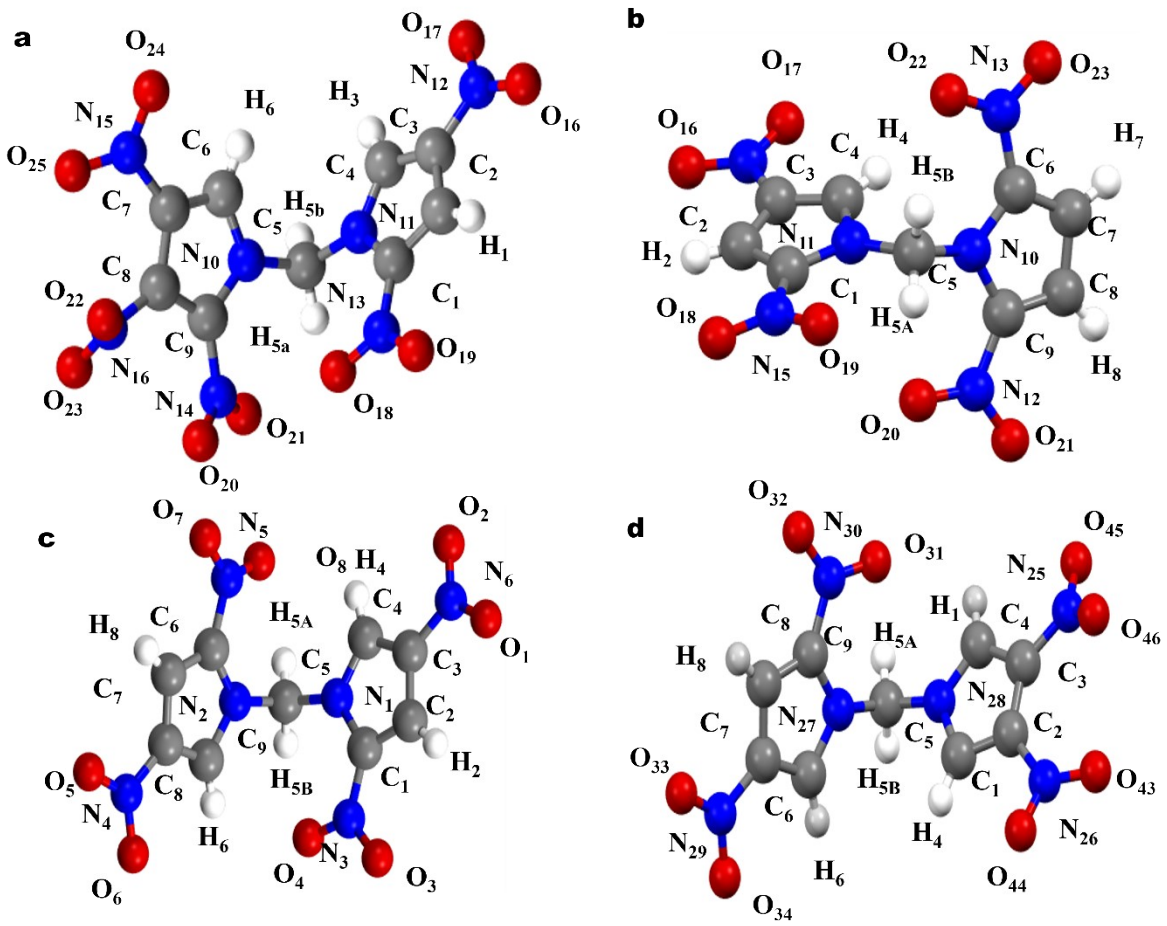


Figure S43: Molecular structure with atom labelling of Compound **1, 2, 3,** and **4**.

4. X-Ray Crystallographic Data

4.1 Crystallographic data for compound **1**.

Table S4: Crystal data and structure refinement for VSP-C1

Identification code	VSP-C1
Empirical formula	$C_9H_5N_7O_{10}$
Formula weight	371.20
Temperature/K	295.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.7945(4)
b/Å	8.7209(3)
c/Å	12.6951(3)
α/°	90

β/°	108.9810(10)
γ/°	90
Volume/Å^3	1339.49(7)
Z	4
ρ_{calc}g/cm^3	1.841
μ/mm^{-1}	0.170
F(000)	752.0
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.774 to 55.016
Index ranges	-16 ≤ h ≤ 16, -11 ≤ k ≤ 11, -16 ≤ l ≤ 16
Reflections collected	29401
Independent reflections	3028 [R_{int} = 0.0349, R_{sigma} = 0.0170]
Data/restraints/parameters	3028/0/235
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0384, wR_2 = 0.0936
Final R indexes [all data]	R_1 = 0.0457, wR_2 = 0.0997
Largest diff. peak/hole / e Å^{-3}	0.21/-0.23

Table S5: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) forVSP-C1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*y*	*z*	U(eq)
O001	2034.8(10)	7347.5(13)	6969.9(9)	49.1(3)
N002	3028.1(10)	8149.2(14)	5218.5(9)	35.8(3)
N003	1580.0(9)	6260.0(13)	4802.8(9)	34.1(3)
O004	1733.4(12)	5107.6(14)	7524.1(9)	56.5(3)
O005	500.9(11)	2855.7(16)	2499.9(10)	61.5(4)
O006	3598.8(12)	10175.7(16)	7714.9(10)	60.7(4)
O007	6615.2(11)	8282.2(18)	5679.4(12)	65.5(4)
O008	2162.0(11)	10509.7(15)	6248.3(12)	64.4(4)
N009	1795.2(10)	5982.0(14)	6800.4(9)	36.5(3)
O00A	5838.4(12)	6215.4(17)	4839.5(12)	66.5(4)
N00B	3070.2(12)	9983.6(14)	6730.0(11)	43.6(3)
O00C	432.6(13)	1456.4(16)	3887.3(12)	70.1(4)
O00D	6250.0(12)	8819(2)	7803.1(11)	76.7(5)
N00E	651.7(11)	2645.2(16)	3494.3(12)	46.3(3)
C00F	1560.4(11)	5380.5(16)	5707.2(11)	33.1(3)
N00G	5829.5(12)	7408.7(17)	5328.9(11)	46.6(3)
C00H	3592.0(12)	9054.9(16)	6107.5(11)	36.0(3)
N00I	5577.5(12)	9642.4(19)	7162.1(11)	51.1(4)
O00J	5579.5(14)	11040.3(18)	7167.5(14)	80.3(5)
C00K	1277.4(11)	5332.0(18)	3896.1(11)	37.9(3)
C00L	1252.2(11)	3913.6(17)	5383.5(12)	37.0(3)
C00M	1073.8(11)	3906.5(17)	4237.8(12)	36.9(3)

C00N	4695.6(12)	8896.7(17)	6294.8(11)	37.5(3)
C00O	4814.4(12)	7855.0(17)	5503.8(12)	38.7(3)
C00P	3782.1(13)	7412.7(18)	4854.7(12)	40.3(3)
C00Q	1832.3(12)	7880.1(17)	4745.3(12)	38.0(3)

Table S6: Anisotropic Displacement Parameters ($Å^2×10^3$) forVSP-C1. 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}
O001	66.4(7)	41.8(6)	40.7(6)	-5.1(5)	19.5(5)	-5.4(5)
N002	39.2(6)	36.9(6)	30.3(5)	-0.1(5)	9.9(5)	-3.0(5)
N003	33.0(6)	37.7(6)	28.7(5)	1.8(5)	6.1(4)	-0.2(5)
O004	84.8(9)	52.4(7)	39.2(6)	4.6(5)	29.8(6)	-7.0(6)
O005	68.6(8)	65.4(8)	43.2(6)	-16.1(6)	8.4(6)	3.0(6)
O006	75.6(9)	65.5(8)	43.7(6)	-16.4(6)	23.2(6)	-6.3(7)
O007	46.1(7)	80.0(10)	74.8(9)	-7.7(7)	25.8(6)	-13.4(7)
O008	62.2(8)	49.7(7)	78.3(9)	-8.5(6)	18.7(7)	16.4(6)
N009	35.9(6)	41.3(7)	33.0(6)	0.8(5)	12.3(5)	1.9(5)
O00A	69.6(9)	66.5(9)	74.2(9)	-15.6(7)	38.0(7)	3.2(7)
N00B	52.6(8)	34.6(6)	47.0(7)	-4.2(5)	20.9(6)	-2.2(6)
O00C	83.0(10)	52.4(8)	72.7(9)	-12.5(7)	22.1(7)	-21.2(7)
O00D	54.3(8)	114.4(13)	47.6(7)	4.1(8)	-2.6(6)	-12.1(8)
N00E	38.2(7)	47.0(7)	49.0(8)	-11.9(6)	7.8(6)	1.2(6)
C00F	29.6(6)	38.6(7)	30.0(6)	2.3(5)	8.0(5)	2.1(5)
N00G	46.9(7)	54.2(8)	42.3(7)	3.4(6)	19.6(6)	-0.3(6)
C00H	43.4(7)	32.4(7)	31.9(7)	-0.3(5)	12.0(6)	-2.3(6)
N00I	46.7(7)	66.9(10)	41.8(7)	-12.8(7)	17.3(6)	-19.5(7)
O00J	85.0(11)	64.8(9)	94.6(11)	-33.6(8)	34.0(9)	-34.2(8)
C00K	33.3(7)	47.5(8)	29.6(6)	-2.2(6)	5.7(5)	1.1(6)
C00L	32.7(7)	38.6(7)	38.8(7)	1.5(6)	10.4(5)	2.1(5)
C00M	27.9(6)	41.1(7)	38.4(7)	-5.0(6)	6.3(5)	2.1(5)
C00N	42.1(7)	37.8(7)	31.6(7)	0.2(5)	10.8(6)	-6.6(6)
C00O	42.1(8)	40.8(8)	35.4(7)	1.0(6)	15.6(6)	-2.6(6)
C00P	47.1(8)	41.8(8)	34.0(7)	-4.3(6)	15.9(6)	-4.4(6)
C00Q	38.5(7)	38.7(7)	32.3(7)	5.3(6)	5.2(5)	0.8(6)

Table S7: Bond Lengths for VSP-C1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O001	N009	1.2311(16)	N00B	C00H	1.4386(19)
N002	C00H	1.3742(18)	O00C	N00E	1.2220(19)
N002	C00P	1.3588(19)	O00D	N00I	1.210(2)
N002	C00Q	1.4694(18)	N00E	C00M	1.4356(19)
N003	C00F	1.3878(17)	C00F	C00L	1.362(2)

N003	C00K	1.3564(18)	N00G	C00O	1.441(2)
N003	C00Q	1.4564(18)	C00H	C00N	1.360(2)
O004	N009	1.2162(16)	N00I	O00J	1.219(2)
O005	N00E	1.2273(19)	N00I	C00N	1.4492(19)
O006	N00B	1.2242(17)	C00K	C00M	1.369(2)
O007	N00G	1.2239(19)	C00L	C00M	1.397(2)
O008	N00B	1.2135(19)	C00N	C00O	1.399(2)
N009	C00F	1.4214(17)	C00O	C00P	1.365(2)

Table S8: Bond Angles for VSP-C1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C00H	N002	C00Q	128.78(12)	O00A	N00G	C00O	118.00(14)
C00P	N002	C00H	108.05(12)	N002	C00H	N00B	124.14(13)
C00P	N002	C00Q	123.06(12)	C00N	C00H	N002	108.85(12)
C00F	N003	C00Q	129.91(11)	C00N	C00H	N00B	127.00(13)
C00K	N003	C00F	107.18(12)	O00D	N00I	O00J	126.18(16)
C00K	N003	C00Q	122.89(12)	O00D	N00I	C00N	116.89(15)
O001	N009	C00F	119.29(12)	O00J	N00I	C00N	116.91(16)
O004	N009	O001	123.24(12)	N003	C00K	C00M	107.70(12)
O004	N009	C00F	117.46(12)	C00F	C00L	C00M	104.57(13)
O006	N00B	C00H	115.92(13)	C00K	C00M	N00E	123.84(13)
O008	N00B	O006	125.69(14)	C00K	C00M	C00L	110.02(13)
O008	N00B	C00H	118.39(13)	C00L	C00M	N00E	125.95(14)
O005	N00E	C00M	117.48(14)	C00H	C00N	N00I	126.49(14)
O00C	N00E	O005	124.51(14)	C00H	C00N	C00O	106.82(12)
O00C	N00E	C00M	117.96(14)	C00O	C00N	N00I	126.68(14)
N003	C00F	N009	123.29(12)	C00N	C00O	N00G	126.88(14)
C00L	C00F	N003	110.53(12)	C00P	C00O	N00G	125.05(14)
C00L	C00F	N009	126.14(13)	C00P	C00O	C00N	107.89(13)
O007	N00G	C00O	116.80(14)	N002	C00P	C00O	108.40(13)
O00A	N00G	O007	125.19(15)	N003	C00Q	N002	110.65(11)

Table S9: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for VSP-C1.

Atom	*X*	*y*	*z*	U(eq)
H00K	1218.65	5613.35	3172.42	45
H00L	1177.37	3098.87	5826.19	44
H00P	3622.14	6724.26	4263.91	48
H00A	1450.83	8475.17	5153.7	46
H00B	1572.28	8215.43	3975	46

4.2 Crystallographic data for compound **2**.

Table S10: Crystal data and structure refinement for -VSP-C2

Identification code	VSP-C2
Empirical formula	$C_9H_6N_6O_8$
Formula weight	326.20
Temperature/K	296.0
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	18.645(11)
b/Å	10.520(5)
c/Å	6.239(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1223.7(11)
Z	4
ρ_{calc}g/cm^3	1.771
μ/mm^{-1}	0.158
F(000)	664.0
Crystal size/mm^3	0.201 × 0.14 × 0.039
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.446 to 40.268
Index ranges	-17 ≤ h ≤ 18, -10 ≤ k ≤ 10, -6 ≤ l ≤ 6
Reflections collected	1130
Independent reflections	1130 [R_{int} = ?, R_{sigma} = 0.0264]
Data/restraints/parameters	1130/1/209
Goodness-of-fit on F^2	1.076
Final R indexes [I>=2σ (I)]	R_1 = 0.0209, wR_2 = 0.0506
Final R indexes [all data]	R_1 = 0.0220, wR_2 = 0.0516
Largest diff. peak/hole / e Å^{-3}	0.08/-0.09
Flack parameter	0.7(7)

Table S11: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for VSP-C-2. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*y*	*z*	U(eq)
C1	3600(2)	2603(3)	6833(6)	32.8(9)
C2	4112.0(19)	3260(3)	5774(7)	37.7(10)
C3	3773.5(19)	3715(3)	3950(6)	32.7(9)
C4	3071(2)	3356(3)	3951(6)	36.4(10)
C5	2272.4(17)	2032(3)	6294(6)	39.2(11)

C6	1255(2)	3641(3)	6627(6)	36.2(10)
C7	637(2)	3918(4)	5584(8)	45.6(11)
C8	632(2)	3203(4)	3714(7)	46.5(12)
C9	1248(2)	2517(3)	3708(6)	35.6(10)
N10	1657.1(14)	2760(3)	5497(5)	33.0(7)
N11	2953.4(13)	2662(3)	5733(5)	33.1(7)
N12	1470(2)	1692(3)	1999(6)	48.1(9)
N13	1493(2)	4230(3)	8579(5)	49.2(9)
N14	3707(2)	1881(3)	8733(6)	47.4(9)
N15	4103(2)	4466(3)	2302(6)	42.8(8)
O16	4298.8(18)	1965(3)	9594(5)	67.3(9)
O17	3226.5(16)	1196(3)	9408(5)	76.5(10)
O18	4742.3(16)	4716(3)	2501(5)	65.7(9)
O19	3736.0(15)	4797(2)	775(5)	57.0(8)
O20	2039.6(18)	1126(3)	2122(6)	71.1(9)
O21	1068.0(18)	1631(3)	446(5)	68.1(9)
O22	2091.4(17)	3968(3)	9292(5)	62.4(9)
O23	1069.0(18)	4962(3)	9444(5)	72.7(9)

Table S12: Anisotropic Displacement Parameters ($Å^2×10^3$) for VSP-C2. 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}
C1	35(2)	34(2)	29(2)	3(2)	-4(2)	2.4(19)
C2	30(2)	38.8(19)	45(3)	-10(2)	-1(2)	-1.3(18)
C3	32(2)	31.8(18)	34(3)	1(2)	8(2)	-5.7(19)
C4	38(3)	39(2)	32(3)	5(2)	0.9(19)	-0.2(17)
C5	35(2)	39(2)	43(3)	7.7(19)	0.3(19)	-1.4(19)
C6	37(2)	35(2)	37(3)	1(2)	2(2)	-3.4(19)
C7	40(3)	42(2)	55(3)	6(3)	5(2)	4.8(19)
C8	39(3)	50(2)	51(3)	6(3)	-8(2)	-7(2)
C9	39(3)	32(2)	35(3)	4(2)	4(2)	-6(2)
N10	29.3(17)	37.4(17)	32.3(19)	0.5(16)	0.3(19)	-3.2(15)
N11	27.0(19)	37.5(16)	34.7(19)	6.1(17)	0.0(17)	-4.8(14)
N12	56(3)	48(2)	40(3)	0(2)	4(2)	-15(2)
N13	58(3)	46(2)	43(2)	0(2)	3(2)	-10.9(19)
N14	43(2)	54(2)	45(2)	2(2)	-1(2)	7.5(19)
N15	40(2)	40.5(19)	48(2)	-2(2)	9(2)	0.9(18)
O16	62(2)	76(2)	64(2)	8.7(17)	-28.9(19)	3.6(17)
O17	48.7(19)	104(2)	77(2)	53(2)	6.6(18)	6.7(19)
O18	49(2)	81(2)	68(2)	7.0(19)	8.2(19)	-22.6(16)
O19	54(2)	59.4(17)	58(2)	24.5(17)	8(2)	9.2(14)
O20	64(2)	88(2)	61(2)	-17(2)	16(2)	12.5(19)
O21	90(2)	68.8(18)	46(2)	-8.6(16)	-12(2)	-20.5(16)
O22	55(2)	79(2)	53(2)	-11.4(18)	-10.4(18)	-12.3(17)
O23	92(2)	64.9(19)	61(2)	-24(2)	12(2)	15.7(19)

Table S13: Bond Lengths for VSP-C2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.352(5)	C7	C8	1.388(6)
C1	N11	1.388(4)	C8	C9	1.356(5)
C1	N14	1.423(5)	C9	N10	1.375(5)
C2	C3	1.386(5)	C9	N12	1.436(5)
C3	C4	1.363(5)	N12	O20	1.220(4)
C3	N15	1.435(5)	N12	O21	1.227(4)
C4	N11	1.348(5)	N13	O22	1.233(4)
C5	N10	1.466(4)	N13	O23	1.228(4)
C5	N11	1.474(4)	N14	O16	1.229(4)
C6	C7	1.356(5)	N14	O17	1.225(4)
C6	N10	1.385(5)	N15	O18	1.227(4)
C6	N13	1.436(5)	N15	O19	1.224(4)

Table S14: Bond Angles VSP-C2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	N11	110.4(3)	C9	N10	C5	127.7(3)
C2	C1	N14	125.5(4)	C9	N10	C6	103.7(3)
N11	C1	N14	123.9(3)	C1	N11	C5	127.6(3)
C1	C2	C3	104.8(3)	C4	N11	C1	106.9(3)
C2	C3	N15	125.7(3)	C4	N11	C5	125.4(3)
C4	C3	C2	110.0(3)	O20	N12	C9	119.9(4)
C4	C3	N15	124.4(4)	O20	N12	O21	123.8(4)
N11	C4	C3	107.9(3)	O21	N12	C9	116.3(4)
N10	C5	N11	111.0(3)	O22	N13	C6	119.2(4)
C7	C6	N10	111.1(3)	O23	N13	C6	116.4(4)
C7	C6	N13	125.2(4)	O23	N13	O22	124.4(3)
N10	C6	N13	123.6(4)	O16	N14	C1	116.9(3)
C6	C7	C8	106.9(3)	O17	N14	C1	119.8(3)
C9	C8	C7	106.6(4)	O17	N14	O16	123.3(3)
C8	C9	N10	111.6(3)	O18	N15	C3	117.5(4)
C8	C9	N12	124.6(4)	O19	N15	C3	118.4(3)
N10	C9	N12	123.7(4)	O19	N15	O18	124.1(3)

Table S15: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for VSP-C2.

Atom	*X*	*y*	*z*	U(eq)
H2	4587.11	3380.83	6179.15	45
H4	2732.85	3553.76	2906.76	44

H5A	2264.13	1185.51	5678.39	47
H5B	2238.23	1949.07	7838.84	47
H7	282.44	4480.57	6035.53	55
H8	276.88	3196.23	2668.29	56

4.3 Crystallographic data for compound **3**.

Table S16: Crystal data and structure refinement for VSP-C3

Identification code	VSP-C3
Empirical formula	$C_9H_6N_6O_8$
Formula weight	326.20
Temperature/K	297(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.5972(10)
b/Å	8.9758(8)
c/Å	13.1358(11)
α/°	90
β/°	93.377(3)
γ/°	90
Volume/Å^3	1247.29(19)
Z	4
ρ_{calc}g/cm^3	1.737
μ/mm^{-1}	0.153
F(000)	664.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	8.772 to 56.63
Index ranges	$-14 \le h \le 14$, $-11 \le k \le 11$, $-17 \le l \le 17$
Reflections collected	21994
Independent reflections	3027 [R_{int} = 0.0299, R_{sigma} = 0.0212]
Data/restraints/parameters	3027/0/208
Goodness-of-fit on F^2	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0448, wR_2 = 0.1170
Final R indexes [all data]	R_1 = 0.0480, wR_2 = 0.1198
Largest diff. peak/hole / e Å^{-3}	0.30/-0.27

Table S17: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for VSP-C3. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*y*	*z*	U(eq)
N1	1576.0(10)	6601.8(12)	5627.2(8)	32.9(2)
O1	1474.2(17)	1695.7(15)	5050.5(15)	88.8(5)
C1	1273.1(12)	5772.1(15)	6468.1(10)	37.8(3)
N2	3012.8(10)	8695.3(12)	5947.6(8)	34.7(2)
O2	1695.9(15)	3023.9(17)	3694.5(12)	76.8(4)
C2	1250.3(14)	4289.0(16)	6236.1(12)	45.7(3)
O3	734(2)	5534(2)	8100.3(11)	106.2(7)
N3	999.0(13)	6391.9(16)	7423.6(9)	51.8(3)
C3	1537.7(12)	4216.1(15)	5219.2(12)	41.0(3)
O4	1025.2(12)	7738.2(14)	7536.4(9)	58.1(3)
N4	4949.9(12)	10207.5(14)	8023.9(10)	45.9(3)
C4	1734.3(12)	5625.6(15)	4856.8(10)	39.4(3)
C5	1773.8(13)	8215.6(14)	5515.0(10)	37.0(3)
N5	4453.0(14)	7872.7(14)	4632.0(10)	49.2(3)
O5	4232.7(13)	10533.6(15)	8679.2(9)	61.6(3)
O6	6084.9(12)	10424.6(17)	8097.9(11)	69.3(4)
N6	1582.0(12)	2884.9(15)	4610.0(14)	56.5(4)
C6	3162.7(12)	9372.5(14)	6870.6(10)	36.3(3)
O7	3555.6(14)	7729.4(15)	4000.9(9)	65.4(4)
C7	4432.8(13)	9525.1(14)	7103.8(10)	38.1(3)
C8	5113.0(13)	8941.4(15)	6320.0(11)	41.4(3)
O8	5559.5(14)	7622.6(16)	4456.3(11)	67.9(4)
C9	4215.6(13)	8440.5(14)	5615.8(10)	38.5(3)

Table S18: Anisotropic Displacement Parameters ($Å^2×10^3$) for VSP-C3. 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}
N1	33.0(5)	32.3(5)	32.7(5)	-1.6(4)	-3.1(4)	-1.5(4)
O1	102.5(12)	35.7(6)	127.9(14)	-13.4(7)	4.9(10)	-8.8(7)
C1	36.6(6)	39.5(7)	36.7(6)	0.9(5)	-1.9(5)	-4.4(5)
N2	38.8(5)	30.1(5)	35.0(5)	-0.5(4)	0.5(4)	-3.1(4)
O2	77.8(9)	73.6(9)	80.5(10)	-39.0(8)	17.2(7)	-12.5(7)
C2	45.0(7)	37.8(7)	53.7(8)	4.8(6)	-3.0(6)	-7.5(5)
O3	194(2)	84.0(11)	43.0(7)	3.8(7)	26.3(10)	-43.8(12)
N3	60.9(8)	57.3(8)	37.4(6)	-4.3(5)	3.5(5)	-16.0(6)
C3	31.0(6)	35.0(6)	56.6(8)	-9.0(5)	-0.7(5)	-2.9(5)
O4	64.8(7)	59.5(7)	51.4(6)	-17.0(5)	15.3(5)	-10.5(5)
N4	44.6(6)	40.2(6)	51.8(7)	-3.1(5)	-6.3(5)	-9.5(5)
C4	38.1(6)	40.7(7)	39.3(6)	-8.2(5)	1.3(5)	-5.0(5)
C5	41.3(6)	31.3(6)	37.3(6)	1.5(5)	-7.8(5)	0.1(5)
N5	67.2(8)	36.3(6)	46.1(7)	-1.2(5)	18.9(6)	-8.0(5)
O5	65.3(7)	64.5(8)	55.1(7)	-22.0(6)	4.9(6)	-13.7(6)
O6	43.8(6)	83.2(9)	79.1(9)	-14.0(7)	-13.3(6)	-15.5(6)
N6	39.7(6)	43.0(7)	86.5(11)	-21.9(7)	2.7(6)	-5.5(5)

C6	39.0(6)	32.4(6)	37.5(6)	-3.2(5)	1.3(5)	-3.9(5)
O7	83.5(9)	71.3(8)	42.3(6)	-12.1(5)	12.3(6)	-20.6(7)
C7	38.9(6)	32.2(6)	42.7(7)	-0.2(5)	-1.0(5)	-6.1(5)
C8	38.5(6)	33.8(6)	52.3(7)	2.0(5)	5.7(5)	-3.8(5)
O8	74.1(8)	63.3(8)	70.0(8)	-2.3(6)	34.5(7)	4.2(6)
C9	45.6(7)	29.2(6)	41.4(7)	0.8(5)	9.4(5)	-3.0(5)

Table S19: Bond Lengths for VSP-C3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.3854(16)	N3	O4	1.2175(19)
N1	C4	1.3565(16)	C3	C4	1.3720(19)
N1	C5	1.4722(16)	C3	N6	1.4403(18)
O1	N6	1.223(2)	N4	O5	1.2172(18)
C1	C2	1.3656(19)	N4	O6	1.2167(17)
C1	N3	1.4186(18)	N4	C7	1.4346(18)
N2	C5	1.4644(16)	N5	O7	1.231(2)
N2	C6	1.3573(16)	N5	O8	1.2290(19)
N2	C9	1.3901(17)	N5	C9	1.4253(18)
O2	N6	1.222(2)	C6	C7	1.3696(18)
C2	C3	1.389(2)	C7	C8	1.393(2)
O3	N3	1.2211(19)	C8	C9	1.363(2)

Table S20: Bond Angles for VSP-C3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C5	130.52(11)	O6	N4	C7	117.54(14)
C4	N1	C1	106.99(11)	N1	C4	C3	107.99(12)
C4	N1	C5	122.43(11)	N2	C5	N1	112.34(10)
N1	C1	N3	124.31(12)	O7	N5	C9	118.51(13)
C2	C1	N1	110.37(12)	O8	N5	O7	124.22(14)
C2	C1	N3	125.30(13)	O8	N5	C9	117.19(15)
C6	N2	C5	122.23(11)	O1	N6	C3	117.01(17)
C6	N2	C9	107.01(11)	O2	N6	O1	124.91(16)
C9	N2	C5	130.37(11)	O2	N6	C3	118.06(15)
C1	C2	C3	104.98(12)	N2	C6	C7	107.84(11)
O3	N3	C1	117.70(15)	C6	C7	N4	123.55(13)
O4	N3	C1	119.50(13)	C6	C7	C8	109.97(12)
O4	N3	O3	122.79(15)	C8	C7	N4	126.48(13)
C2	C3	N6	126.13(14)	C9	C8	C7	104.76(12)
C4	C3	C2	109.67(12)	N2	C9	N5	123.86(13)

C4	C3	N6	124.17(14)	C8	C9	N2	110.42(12)
O5	N4	C7	118.37(12)	C8	C9	N5	125.44(13)

Table S21: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for VSP-C3.

Atom	*X*	*y*	*z*	U(eq)
H2	1079.58	3499.58	6665.45	55
H4	1939.92	5869.04	4198.6	47
H5A	1698.61	8473.06	4796.8	44
H5B	1118.9	8746.54	5851.94	44
H6	2517.58	9678.55	7273.13	44
H8	5986.33	8902.07	6285.03	50

4.4 Crystallographic data for compound **4**.

Table S22: Crystal data and structure refinement for VSP-C4.

Identification code	VSP-C4
Empirical formula	$C_9H_6N_6O_8$
Formula weight	326.20
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.6057(4)
b/Å	23.5270(9)
c/Å	12.9863(6)
α/°	90
β/°	107.6950(10)
γ/°	90
Volume/Å^3	2504.89(19)
Z	8
ρ_{calc}g/cm^3	1.730
μ/mm^{-1}	0.155
F(000)	1328.0
Crystal size/mm^3	0.1 × 0.08 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.778 to 50
Index ranges	$-10 \le h \le 10$, $-27 \le k \le 27$, $-15 \le l \le 15$
Reflections collected	41866
Independent reflections	4368 [R_{int} = 0.0417, R_{sigma} = 0.0222]
Data/restraints/parameters	4368/0/415
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0411, wR_2 = 0.0962

Final R indexes [all data]	R_1 = 0.0526, wR_2 = 0.1044
Largest diff. peak/hole / e Å^{-3}	0.25/-0.21

Table S23: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for VSP-C4. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*y*	*z*	U(eq)
O1	5859(2)	5274.9(7)	6954.1(13)	63.3(5)
O2	3336(3)	5009.2(9)	6332.8(16)	88.5(7)
O5	1873(2)	7113.6(7)	3215.5(16)	65.8(5)
O6	-485(3)	7516.3(8)	2810(2)	95.9(7)
O7	-3620(2)	5084.8(8)	1345.2(14)	65.3(5)
O8	-4965(2)	5839.4(9)	1508.7(17)	76.3(6)
O15	6603(2)	6418.3(8)	6885.2(13)	65.4(5)
O16	7348(2)	6726.0(8)	5531.5(15)	69.0(5)
N00P	379(2)	7099.0(7)	2880.5(16)	51.4(5)
N1	436.3(18)	6075.2(6)	2462.8(12)	34.4(4)
N2	3173.5(19)	5952.8(6)	3692.5(12)	34.9(4)
N3	6486(2)	6433.8(8)	5923.9(15)	47.8(4)
N4	4501(3)	5295.1(8)	6287.8(14)	48.1(5)
N5	-3696(2)	5582.8(9)	1597.6(15)	48.8(5)
C1	-689(2)	5659.1(8)	2118.4(15)	37.1(4)
C2	-2196(2)	5888.8(9)	2000.6(15)	38.1(4)
C3	-2035(2)	6463.4(9)	2269.3(17)	42.2(5)
C4	-406(2)	6568.1(8)	2548.5(16)	38.1(4)
C5	2159(2)	5986.7(9)	2571.0(15)	37.9(4)
C6	3013(2)	5563.3(8)	4429.8(15)	36.5(4)
C7	4243(2)	5659.0(8)	5365.3(15)	36.2(4)
C8	5197(2)	6116.7(8)	5176.4(15)	37.0(4)
C9	4505(2)	6287.0(8)	4138.4(16)	39.1(5)
O3	-491(2)	5526.9(8)	6284.8(15)	73.7(5)
O4	-223(2)	5911.2(9)	4831.1(14)	69.5(5)
O9	5059.5(19)	7581.3(6)	7834.7(13)	53.3(4)
O10	4379(2)	7522.5(8)	6086.7(14)	67.9(5)
O11	11104(2)	6418.5(9)	10205.9(15)	73.2(5)
O12	10185(3)	7263.1(10)	10229(2)	110.3(9)
O13	9702(2)	5577.1(8)	8701.9(16)	73.1(5)
O14	8152(2)	5046.0(7)	9301.8(14)	60.1(4)
N6	4277(2)	7366.8(7)	6965.9(15)	43.0(4)
N7	3088.2(18)	6642.8(7)	7889.8(12)	34.6(4)
N8	5682.2(18)	6550.6(7)	9257.3(12)	35.2(4)
N9	9988(2)	6763.1(9)	10034.6(16)	54.1(5)
N10	8625(2)	5509.5(8)	9109.4(13)	43.8(4)
N11	129(2)	5868.6(9)	5812.1(16)	50.9(5)
C10	1941(2)	6231.1(9)	7570.6(16)	39.9(5)

C11	1357(2)	6242.8(8)	6464.3(16)	38.8(4)
C12	2145(2)	6669.5(8)	6070.3(16)	39.8(5)
C13	3207(2)	6907.9(8)	6966.5(15)	34.7(4)
C14	3999(2)	6739.4(9)	9025.5(15)	38.9(5)
C15	7026(2)	6888.9(9)	9582.1(16)	40.1(5)
C16	8347(2)	6562.1(9)	9619.8(15)	37.9(4)
C17	7783(2)	6003.7(8)	9327.1(14)	34.8(4)
C18	6142(2)	6006.3(8)	9112.9(14)	35.4(4)

Table S24: Anisotropic Displacement Parameters ($Å^2×10^3$) for VSP-C4. 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}
O1	75.8(12)	58.9(10)	44.8(9)	6.9(8)	2.9(9)	19.2(9)
O2	99.4(16)	94.1(15)	67.3(12)	31.3(11)	18.2(11)	-32.4(13)
O5	45.4(10)	43.8(9)	96.6(14)	-4.0(9)	4.4(9)	-8.4(7)
O6	74.7(13)	39.5(10)	155(2)	-17.2(11)	7.4(13)	15.1(9)
O7	64.5(11)	63.0(12)	70.7(11)	-13.8(9)	23.8(9)	-26.3(9)
O8	35.5(9)	86.4(14)	103.5(15)	13.3(11)	16.1(9)	-3.0(9)
O15	74.0(12)	67.0(11)	41.8(9)	-6.3(8)	-2.4(8)	-2.9(9)
O16	52.5(10)	68.4(12)	79.5(12)	0.3(9)	10.1(9)	-19.5(9)
N00P	50.2(12)	34.9(10)	62.9(12)	-0.3(8)	7.9(9)	0.6(8)
N1	33.3(8)	33.3(8)	35.4(8)	1.1(7)	8.6(7)	1.4(7)
N2	33.2(8)	33.0(8)	35.8(8)	1.7(7)	6.6(7)	0.5(7)
N3	41.0(10)	44.2(10)	51.4(12)	0.3(8)	3.9(8)	2.7(8)
N4	66.1(13)	40.7(10)	37.0(10)	2.9(8)	14.8(9)	6.9(9)
N5	40.4(11)	58.0(13)	47.3(11)	7.6(9)	12.2(8)	-10.8(9)
C1	41.7(11)	31.9(10)	36.2(10)	0.5(8)	9.8(8)	-3.1(8)
C2	35.5(11)	42.2(11)	36.6(10)	4.9(8)	10.8(8)	-4.0(8)
C3	37.2(11)	42.8(12)	47.0(12)	4.9(9)	13.2(9)	6.9(9)
C4	39.2(11)	30.8(10)	42.1(11)	2.1(8)	9.2(8)	2.0(8)
C5	32.2(10)	45.2(11)	35.1(10)	1.5(8)	8.4(8)	4.0(8)
C6	40.9(11)	30.1(10)	39.9(11)	1.1(8)	14.2(9)	-0.8(8)
C7	42.5(11)	32.3(10)	34.6(10)	1.9(8)	12.9(8)	7.1(8)
C8	33.0(10)	34.7(10)	39.3(10)	-1.2(8)	5.0(8)	3.4(8)
C9	35.1(10)	36.1(11)	44.9(11)	4.8(8)	10.7(9)	-0.8(8)
O3	69.8(12)	76.3(13)	73.4(12)	-9.4(10)	19.5(10)	-35.9(10)
O4	59.0(11)	95.8(14)	47.1(10)	-15.5(9)	6.4(8)	-13.3(10)
O9	59.3(10)	39.8(8)	62.5(10)	-11.0(7)	21.1(8)	-10.4(7)
O10	81.1(13)	65.4(11)	57.9(10)	20.6(9)	22.1(9)	-16.1(9)
O11	37.8(9)	98.1(15)	78.0(13)	18.5(11)	9.2(8)	4.1(10)
O12	65.5(13)	79.2(16)	181(3)	-50.5(16)	29.1(15)	-35.1(12)

O13	81.1(13)	68.9(12)	90.1(14)	10.8(10)	57.1(11)	19.5(10)
O14	61.6(10)	39.2(9)	76.0(12)	0.1(8)	15.6(9)	3.6(8)
N6	43.6(10)	33.9(9)	52.3(11)	4.8(8)	15.8(8)	0.7(8)
N7	31.9(8)	36.5(9)	36.3(8)	-1.4(7)	11.9(7)	0.8(7)
N8	32.7(8)	36.7(9)	36.1(8)	-3.7(7)	10.4(7)	-1.4(7)
N9	42.5(11)	65.7(14)	53.8(11)	-5.3(10)	13.9(9)	-14.4(10)
N10	44.4(10)	46.2(11)	39.9(9)	4.9(8)	11.6(8)	9.6(8)
N11	40.9(10)	56.9(12)	53.3(12)	-9.3(9)	12.0(9)	-5.6(9)
C10	35.7(10)	39.9(11)	45.8(11)	2.3(9)	14.7(9)	-4.3(9)
C11	31.6(10)	39.1(11)	44.6(11)	-5.0(9)	9.7(8)	-1.6(8)
C12	39.9(11)	39.9(11)	38.1(10)	3.9(9)	9.8(9)	6.7(9)
C13	36.5(10)	28.1(9)	41.0(10)	2.1(8)	14.1(8)	2.8(8)
C14	35.3(10)	47.9(12)	35.6(10)	-4.3(9)	13.8(8)	2.9(9)
C15	44.2(11)	33.7(10)	41.3(11)	-6.6(8)	11.4(9)	-6.8(9)
C16	32.7(10)	45.4(11)	34.5(10)	-0.1(8)	8.6(8)	-5.2(9)
C17	39.2(11)	36.1(10)	29.0(9)	2.2(8)	10.3(8)	3.1(8)
C18	39.6(11)	32.7(10)	33.0(10)	-1.0(8)	9.6(8)	-3.2(8)

Table S25: Bond Lengths for VSP-C4.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	N4	1.225(2)	O3	N11	1.227(3)
O2	N4	1.224(3)	O4	N11	1.221(2)
O5	N00P	1.226(2)	O9	N6	1.232(2)
O6	N00P	1.218(2)	O10	N6	1.227(2)
O7	N5	1.224(3)	O11	N9	1.225(3)
O8	N5	1.222(3)	O12	N9	1.204(3)
O15	N3	1.222(2)	O13	N10	1.210(2)
O16	N3	1.230(2)	O14	N10	1.216(2)
N00P	C4	1.423(3)	N6	C13	1.420(3)
N1	C1	1.354(2)	N7	C10	1.355(2)
N1	C4	1.390(2)	N7	C13	1.382(2)
N1	C5	1.461(2)	N7	C14	1.462(2)
N2	C5	1.455(2)	N8	C14	1.456(2)
N2	C6	1.362(2)	N8	C15	1.361(2)
N2	C9	1.365(2)	N8	C18	1.370(2)
N3	C8	1.440(3)	N9	C16	1.430(3)
N4	C7	1.434(3)	N10	C17	1.442(3)
N5	C2	1.431(3)	N11	C11	1.437(3)
C1	C2	1.370(3)	C10	C11	1.371(3)
C2	C3	1.393(3)	C11	C12	1.393(3)
C3	C4	1.359(3)	C12	C13	1.363(3)
C6	C7	1.365(3)	C15	C16	1.361(3)
C7	C8	1.420(3)	C16	C17	1.412(3)
C8	C9	1.358(3)	C17	C18	1.354(3)

Table S26: Bond Angles for VSP-C4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O5	N00P	C4	118.82(17)	O9	N6	C13	119.02(17)
O6	N00P	O5	123.66(19)	O10	N6	O9	123.77(18)
O6	N00P	C4	117.51(19)	O10	N6	C13	117.21(18)
C1	N1	C4	106.96(15)	C10	N7	C13	107.22(16)
C1	N1	C5	122.12(16)	C10	N7	C14	122.47(16)
C4	N1	C5	130.55(16)	C13	N7	C14	130.27(16)
C6	N2	C5	125.62(16)	C15	N8	C14	125.70(17)
C6	N2	C9	109.90(16)	C15	N8	C18	109.60(16)
C9	N2	C5	124.34(16)	C18	N8	C14	124.57(16)
O15	N3	O16	124.6(2)	O11	N9	C16	118.7(2)
O15	N3	C8	118.72(19)	O12	N9	O11	123.7(2)
O16	N3	C8	116.63(19)	O12	N9	C16	117.5(2)
O1	N4	C7	119.1(2)	O13	N10	O14	123.84(19)
O2	N4	O1	124.36(19)	O13	N10	C17	118.49(18)
O2	N4	C7	116.54(19)	O14	N10	C17	117.58(17)
O7	N5	C2	117.64(19)	O3	N11	C11	117.38(19)
O8	N5	O7	124.5(2)	O4	N11	O3	124.6(2)
O8	N5	C2	117.8(2)	O4	N11	C11	118.00(19)
N1	C1	C2	108.02(17)	N7	C10	C11	107.88(17)
C1	C2	N5	124.09(19)	C10	C11	N11	125.11(19)
C1	C2	C3	109.64(18)	C10	C11	C12	109.59(17)
C3	C2	N5	126.17(19)	C12	C11	N11	125.30(19)
C4	C3	C2	105.01(18)	C13	C12	C11	104.94(18)
N1	C4	N00P	123.05(17)	N7	C13	N6	124.23(17)
C3	C4	N00P	126.57(18)	C12	C13	N6	125.41(18)
C3	C4	N1	110.37(17)	C12	C13	N7	110.36(17)
N2	C5	N1	112.75(15)	N8	C14	N7	110.83(15)
N2	C6	C7	107.34(17)	N8	C15	C16	107.61(17)
C6	C7	N4	121.77(19)	C15	C16	N9	123.03(19)
C6	C7	C8	107.68(17)	C15	C16	C17	107.50(17)
C8	C7	N4	130.24(18)	C17	C16	N9	128.93(19)
C7	C8	N3	130.06(18)	C16	C17	N10	130.59(18)
C9	C8	N3	122.12(18)	C18	C17	N10	121.19(18)
C9	C8	C7	107.04(17)	C18	C17	C16	107.63(17)
C8	C9	N2	108.03(17)	C17	C18	N8	107.62(17)

Table S27: Torsion Angles for VSP-C4.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	N4	C7	C6	156.34(19)	O3	N11	C11	C10	3.1(3)
O1	N4	C7	C8	-16.5(3)	O3	N11	C11	C12	-177.5(2)
O2	N4	C7	C6	-21.4(3)	O4	N11	C11	C10	-176.8(2)
O2	N4	C7	C8	165.7(2)	O4	N11	C11	C12	2.6(3)

O5	N00P	C4	N1	-7.9(3)	O9	N6	C13	N7	-6.6(3)
O5	N00P	C4	C3	172.4(2)	O9	N6	C13	C12	172.73(19)
O6	N00P	C4	N1	171.8(2)	O10	N6	C13	N7	172.63(18)
O6	N00P	C4	C3	-7.9(3)	O10	N6	C13	C12	-8.1(3)
O7	N5	C2	C1	0.1(3)	O11	N9	C16	C15	168.0(2)
O7	N5	C2	C3	176.0(2)	O11	N9	C16	C17	-2.5(3)
O8	N5	C2	C1	-178.4(2)	O12	N9	C16	C15	-9.5(3)
O8	N5	C2	C3	-2.5(3)	O12	N9	C16	C17	179.9(2)
O15	N3	C8	C7	-18.7(3)	O13	N10	C17	C16	-32.7(3)
O15	N3	C8	C9	149.9(2)	O13	N10	C17	C18	137.3(2)
O16	N3	C8	C7	164.8(2)	O14	N10	C17	C16	150.7(2)
O16	N3	C8	C9	-26.6(3)	O14	N10	C17	C18	-39.3(3)
N1	C1	C2	N5	176.81(17)	N7	C10	C11	N11	179.51(18)
N1	C1	C2	C3	0.3(2)	N7	C10	C11	C12	0.0(2)
N2	C6	C7	N4	-175.40(17)	N8	C15	C16	N9	-173.45(18)
N2	C6	C7	C8	-1.1(2)	N8	C15	C16	C17	-1.1(2)
N3	C8	C9	N2	-170.76(17)	N9	C16	C17	N10	-16.8(3)
N4	C7	C8	N3	-15.9(3)	N9	C16	C17	C18	172.11(19)
N4	C7	C8	C9	174.27(19)	N10	C17	C18	N8	-171.62(16)
N5	C2	C3	C4	-176.48(18)	N11	C11	C12	C13	-179.39(19)
C1	N1	C4	N00P	-179.33(18)	C10	N7	C13	N6	179.60(18)
C1	N1	C4	C3	0.4(2)	C10	N7	C13	C12	0.2(2)
C1	N1	C5	N2	-107.7(2)	C10	N7	C14	N8	107.8(2)
C1	C2	C3	C4	-0.1(2)	C10	C11	C12	C13	0.1(2)
C2	C3	C4	N00P	179.50(19)	C11	C12	C13	N6	-179.59(18)
C2	C3	C4	N1	-0.2(2)	C11	C12	C13	N7	-0.2(2)
C4	N1	C1	C2	-0.4(2)	C13	N7	C10	C11	-0.1(2)
C4	N1	C5	N2	80.4(2)	C13	N7	C14	N8	-70.0(2)
C5	N1	C1	C2	-174.02(16)	C14	N7	C10	C11	-178.33(16)
C5	N1	C4	N00P	-6.4(3)	C14	N7	C13	N6	-2.4(3)
C5	N1	C4	C3	173.27(18)	C14	N7	C13	C12	178.23(18)
C5	N2	C6	C7	177.07(17)	C14	N8	C15	C16	-174.72(17)
C5	N2	C9	C8	-176.72(17)	C14	N8	C18	C17	175.04(16)
C6	N2	C5	N1	59.7(2)	C15	N8	C14	N7	116.7(2)
C6	N2	C9	C8	-0.8(2)	C15	N8	C18	C17	-1.2(2)
C6	C7	C8	N3	170.52(19)	C15	C16	C17	N10	171.51(19)
C6	C7	C8	C9	0.7(2)	C15	C16	C17	C18	0.4(2)
C7	C8	C9	N2	0.1(2)	C16	C17	C18	N8	0.5(2)
C9	N2	C5	N1	-125.02(19)	C18	N8	C14	N7	-59.0(2)
C9	N2	C6	C7	1.2(2)	C18	N8	C15	C16	1.5(2)

Table S28: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for VSP-C4.

Atom	*X*	*y*	*z*	U(eq)
H1	-476.17	5283.18	1985.2	44

H3	-2861.44	6719.81	2259.82	51
H5A	2274.62	5637.66	2203.41	45
H5B	2540.78	6297.14	2219.56	45
H6	2214.64	5283.91	4316.93	44
H9	4873.52	6580.02	3792.11	47
H10	1608.27	5984.27	8022.27	48
H12	1981.53	6769.78	5352.43	48
H14A	3980.82	7141.13	9189.64	47
H14B	3482.7	6534.16	9481.28	47
H15	7038.87	7273.71	9748.2	48
H18	5452.04	5694.85	8905.38	42

4.5 Crystallographic data for compound **5**.

Table S29: Crystal data and structure refinement for VSP-C5.

Identification code	VSP-C5
Empirical formula	$C_9H_9N_3O_2$
Formula weight	191.06
Temperature/K	273.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.976(6)
b/Å	17.567(10)
c/Å	7.562(4)
α/°	90
β/°	96.90(3)
γ/°	90
Volume/Å^3	920.0(10)
Z	4
ρ_{calc}g/cm^3	1.286
Mμ/mm^{-1}	0.092
F(000)	356.0
Crystal size/mm^3	0.1 × 0.2 ×
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.882 to 49.11
Index ranges	$-8 \leq h \leq 7$, $-20 \leq k \leq 20$, $-8 \leq l \leq 7$
Reflections collected	5925

Independent reflections	1455 [R_{int} = 0.7058, R_{sigma} = 0.6102]
Data/restraints/parameters	1455/0/127
Goodness-of-fit on F^2	0.98
Final R indexes [I>=2σ (I)]	R_1 = 0.2430, wR_2 = 0.4633
Final R indexes [all data]	R_1 = 0.4888, wR_2 = 0.6054
Largest diff. peak/hole / e Å^{-3}	0.30/-0.36

Table S30: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for VSP-C5 U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C001	4830(20)	6586(8)	7890(20)	56(4)
C002	7990(30)	6563(12)	9300(30)	105(6)
O003	2370(19)	5843(10)	1871(19)	144(6)
N004	2500(19)	5722(8)	6520(20)	89(5)
C005	2460(30)	6084(14)	3350(20)	89(6)
C006	7860(30)	7078(10)	7750(30)	93(6)
O	2320(30)	6731(10)	3667(19)	146(6)
C008	5960(40)	7059(10)	7000(30)	99(7)
C009	2490(20)	5526(12)	4780(30)	104(7)
C00A	2790(30)	6453(10)	7460(20)	104(6)
C00B	6090(30)	6279(10)	9330(20)	100(7)
C00C	2450(20)	4748(10)	4540(20)	99(6)
C00D	2450(30)	5037(12)	7500(30)	107(7)
C00E	2440(30)	4433(12)	6230(30)	101(7)

Table S31: Anisotropic Displacement Parameters (Å^2×10^3) for VSP-C5. 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}
C001	60(10)	37(9)	70(10)	8(8)	-1(9)	11(9)
C002	122(18)	85(15)	114(16)	-1(12)	37(13)	0(13)
O003	177(15)	155(16)	97(11)	26(10)	10(9)	-2(10)
N004	135(13)	70(11)	59(9)	-26(8)	-7(8)	18(8)
C005	134(16)	102(18)	23(10)	-15(12)	-20(9)	-3(14)
C006	119(17)	66(13)	97(14)	-9(10)	23(12)	-6(11)
O	248(18)	77(11)	109(11)	9(9)	10(9)	6(12)
C008	139(19)	52(12)	106(15)	-37(10)	6(14)	12(12)
C009	117(17)	94(18)	92(16)	23(14)	-28(11)	10(12)
C00A	145(18)	65(14)	98(13)	-38(10)	1(12)	22(11)
C00B	128(17)	69(13)	92(13)	-8(10)	-35(12)	44(12)
C00C	135(18)	46(13)	109(16)	-5(11)	-10(11)	8(11)

C00D	125(16)	57(13)	138(17)	42(14)	15(12)	-3(11)
C00E	131(17)	86(15)	80(13)	19(13)	-21(11)	1(12)

Table S32: Bond Lengths for VSP-C5.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C001	C008	1.38(2)	N004	C00D	1.42(2)
C001	C00A	1.44(2)	C005	O	1.17(2)
C001	C00B	1.420(19)	C005	C009	1.46(2)
C002	C006	1.48(2)	C006	C008	1.38(2)
C002	C00B	1.42(2)	C009	C00C	1.38(2)
O003	C005	1.191(17)	C00C	C00E	1.39(2)
N004	C009	1.36(2)	C00D	C00E	1.43(3)
N004	C00A	1.47(2)			

Table S33: Bond Angles for VSP-C5.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C008	C001	C00A	126.7(17)	C008	C006	C002	105.9(16)
C008	C001	C00B	105.4(17)	C001	C008	C006	113.2(18)
C00B	C001	C00A	127.9(19)	N004	C009	C005	123.0(19)
C00B	C002	C006	105.1(17)	N004	C009	C00C	112.0(17)
C009	N004	C00A	132.6(17)	C00C	C009	C005	125(2)
C009	N004	C00D	107.2(16)	C001	C00A	N004	108.8(14)
C00D	N004	C00A	119.7(16)	C001	C00B	C002	110.4(19)
O003	C005	C009	117(2)	C009	C00C	C00E	106.1(17)
O	C005	O003	123(2)	N004	C00D	C00E	106.0(16)
O	C005	C009	119.9(18)	C00C	C00E	C00D	108.7(17)

Table S34: Torsion Angles for VSP-C5.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C002	C006	C008	C001	-0.2(19)	C009	C00C	C00E	C00D	1(2)
O003	C005	C009	N004	-176.7(17)	C00A	C001	C008	C006	178.9(14)
O003	C005	C009	C00C	1(3)	C00A	C001	C00B	C002	-178.8(14)
N004	C009	C00C	C00E	0(2)	C00A	N004	C009	C005	-11(3)
N004	C00D	C00E	C00C	-1(2)	C00A	N004	C009	C00C	170.9(17)
C005	C009	C00C	C00E	-178.1(16)	C00A	N004	C00D	C00E	-171.7(15)
C006	C002	C00B	C001	0.2(19)	C00B	C001	C008	C006	0.4(18)
O	C005	C009	N004	-5(3)	C00B	C001	C00A	N004	-81(2)
O	C005	C009	C00C	173(2)	C00B	C002	C006	C008	0.0(18)
C008	C001	C00A	N004	101.2(18)	C00D	N004	C009	C005	177.5(15)
C008	C001	C00B	C002	-0.4(18)	C00D	N004	C009	C00C	0(2)

C009	N004	C00A	C001	-84(2)	C00D	N004	C00A	C001	86(2)
C009	N004	C00D	C00E	1(2)					

Table S35: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for VSP-C5.

Atom	*x*	*y*	*z*	U(eq)
H002	8963.1	6477.96	10008.49	125
H006	8823.6	7328.1	7313.11	101
H008	5487.14	7367.72	6074.91	109
H00A	2198.25	6847.89	6745.77	105
H00B	2248.38	6396.35	8539.16	105
H00C	5651.93	5957.73	10156.38	121
H00D	2454.49	4499.86	3503.11	104
H00E	2310(190)	5260(90)	8800(200)	101
H00F	2393.16	3959.03	6430.36	100

4.6 Crystallographic data for compound **6**.

Table S36: Crystal data and structure refinement for VSP-C6.

Identification code	VSP-C6
Empirical formula	$C_{18}H_{22}N_6O_4$
Formula weight	193.21
Temperature/K	273.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	20.760(3)
b/Å	10.7770(15)
c/Å	8.4910(11)
α/°	90
β/°	101.119(5)
γ/°	90
Volume/Å^3	1864.0(4)
Z	8
ρ_{calc}g/cm^3	1.377
μ/mm^{-1}	0.100
F(000)	816.0
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2 to 52.872
Index ranges	-25 ≤ h ≤ 26, -13 ≤ k ≤ 13, -8 ≤ l ≤ 10
Reflections collected	29713
Independent reflections	3828 [R_{int} = 0.0846, R_{sigma} = 0.0941]
Data/restraints/parameters	3828/0/253

Goodness-of-fit on F^2	1.116
Final R indexes [I>=2σ (I)]	R_1 = 0.0938, wR_2 = 0.2618
Final R indexes [all data]	R_1 = 0.1479, wR_2 = 0.2813
Largest diff. peak/hole / e $Å^{-3}$	0.29/-0.38

Table S37: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for VSP-C6. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*		*z*	U(eq)
N001	5454.2(17)	8766(3)	6043(4)	54.3(10)
N002	8480.1(16)	2843(3)	4448(4)	51.4(9)
N003	9508.7(16)	3815(3)	5541(4)	52.0(9)
N004	6510.1(18)	7884(4)	5972(4)	59.1(10)
O005	6740.3(19)	1496(4)	6260(5)	89.1(12)
N006	8014(2)	7585(4)	8753(6)	67.6(11)
N007	6985(2)	2418(4)	5808(6)	66.6(11)
O008	8182.4(18)	8630(4)	9204(6)	98.0(14)
O009	8339(2)	6678(4)	9215(6)	108.9(16)
C00A	7588.6(19)	2324(4)	5270(5)	48.4(10)
C00B	7415.0(19)	7442(4)	7623(5)	51.0(11)
O00C	6731(2)	3445(4)	5791(7)	113.8(17)
C00D	7018(2)	8396(4)	6980(6)	55.9(12)
C00E	7923(2)	1219(4)	5079(6)	59.7(12)
C00F	7939(2)	3315(4)	4882(6)	53.5(11)
C00G	5443(2)	9710(4)	7117(6)	61.9(13)
C00H	4923(2)	8025(5)	6064(6)	61.3(12)
C00I	8468(2)	1571(4)	4570(6)	62.3(13)
C00J	7139(2)	6327(4)	6997(6)	62.9(13)
C00K	4919(3)	9540(5)	7786(6)	72.4(15)
C00L	9475(3)	4759(4)	6589(6)	64.0(13)
C00M	6574(2)	6626(5)	5988(6)	65.6(13)
C00N	9030(2)	3567(5)	4118(6)	60.5(12)
C00O	10051(2)	3116(5)	6103(6)	61.8(13)
C00P	4586(2)	8478(5)	7119(6)	68.2(14)
C00Q	9995(3)	4641(6)	7805(6)	76.1(16)
C00R	5947(2)	8583(5)	5104(6)	70.7(15)
C00S	10362(3)	3604(6)	7497(7)	80.2(17)

Table S38: Anisotropic Displacement Parameters (Å²×10³) for VSP-C6. 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}
N001	48(2)	60(2)	52(2)	10.5(18)	2.4(17)	4.3(17)
N002	44.1(19)	53(2)	56(2)	0.8(17)	7.6(16)	-5.1(16)
N003	46(2)	58(2)	52(2)	5.1(18)	11.3(17)	-8.4(17)
N004	51(2)	73(3)	53(2)	8.9(19)	7.1(18)	4.7(19)
O005	72(2)	73(2)	127(3)	10(2)	32(2)	-25.4(19)
N006	54(2)	54(2)	91(3)	-1(2)	4(2)	-9(2)
N007	56(2)	48(2)	97(3)	-6(2)	19(2)	-7.9(19)
O008	59(2)	67(2)	156(4)	-28(2)	-11(2)	-13.2(18)
O009	75(3)	71(3)	156(4)	19(3)	-39(3)	4(2)
C00A	41(2)	38(2)	66(3)	-1.1(19)	9(2)	-2.0(17)
C00B	41(2)	44(2)	67(3)	-2(2)	7(2)	-2.6(18)
O00C	73(3)	64(3)	223(5)	-18(3)	76(3)	-3(2)
C00D	50(2)	45(2)	75(3)	6(2)	16(2)	2.4(19)
C00E	59(3)	41(2)	77(3)	-5(2)	9(2)	0(2)
C00F	48(2)	35(2)	77(3)	-3(2)	11(2)	-1.6(18)
C00G	61(3)	46(3)	72(3)	2(2)	-2(3)	5(2)
C00H	58(3)	61(3)	64(3)	3(2)	8(2)	-4(2)
C00I	53(3)	56(3)	78(3)	-10(2)	11(2)	7(2)
C00J	60(3)	47(3)	79(3)	-5(2)	7(3)	3(2)
C00K	84(4)	77(4)	55(3)	3(3)	10(3)	32(3)
C00L	73(3)	53(3)	70(3)	1(2)	24(3)	-5(2)
C00M	57(3)	66(3)	72(3)	-12(3)	8(2)	-9(2)
C00N	49(2)	77(3)	56(3)	9(2)	12(2)	-11(2)
C00O	47(2)	67(3)	72(3)	7(3)	11(2)	5(2)
C00P	55(3)	82(4)	67(3)	18(3)	12(3)	0(3)
C00Q	93(4)	83(4)	55(3)	0(3)	20(3)	-34(3)
C00R	59(3)	97(4)	57(3)	22(3)	13(2)	15(3)
C00S	63(3)	100(5)	73(4)	31(3)	3(3)	-13(3)

Table S39: Bond Lengths for VSP-C6

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N001	C00G	1.369(6)	N006	C00B	1.425(6)
N001	C00H	1.365(6)	N007	C00A	1.418(6)
N001	C00R	1.427(6)	N007	O00C	1.224(5)
N002	C00F	1.347(5)	C00A	C00E	1.404(6)
N002	C00I	1.376(6)	C00A	C00F	1.368(6)

N002	C00N	1.454(5)	C00B	C00D	1.364(6)
N003	C00L	1.363(6)	C00B	C00J	1.393(6)
N003	C00N	1.433(6)	C00E	C00I	1.340(7)
N003	C00O	1.362(6)	C00G	C00K	1.333(7)
N004	C00D	1.342(6)	C00H	C00P	1.331(7)
N004	C00M	1.362(6)	C00J	C00M	1.351(7)
N004	C00R	1.465(6)	C00K	C00P	1.400(8)
O005	N007	1.212(5)	C00L	C00Q	1.348(8)
N006	O008	1.218(5)	C00O	C00S	1.342(7)
N006	O009	1.209(5)	C00Q	C00S	1.406(8)

Table S40: Bond Angles for VSP-C6.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C00G	N001	C00R	125.5(4)	C00F	C00A	C00E	109.7(4)
C00H	N001	C00G	107.9(4)	C00D	C00B	N006	124.7(4)
C00H	N001	C00R	126.5(4)	C00D	C00B	C00J	109.0(4)
C00F	N002	C00I	109.1(4)	C00J	C00B	N006	126.3(4)
C00F	N002	C00N	125.3(4)	N004	C00D	C00B	106.6(4)
C00I	N002	C00N	125.1(4)	C00I	C00E	C00A	105.3(4)
C00L	N003	C00N	125.1(4)	N002	C00F	C00A	106.3(4)
C00O	N003	C00L	109.1(4)	C00K	C00G	N001	107.6(4)
C00O	N003	C00N	125.7(4)	C00P	C00H	N001	109.0(5)
C00D	N004	C00M	109.9(4)	C00E	C00I	N002	109.6(4)
C00D	N004	C00R	124.2(4)	C00M	C00J	C00B	106.2(4)
C00M	N004	C00R	125.7(4)	C00G	C00K	C00P	108.6(5)
O008	N006	C00B	118.1(4)	C00Q	C00L	N003	107.1(5)
O009	N006	O008	122.5(4)	C00J	C00M	N004	108.4(4)
O009	N006	C00B	119.4(4)	N003	C00N	N002	112.3(3)
O005	N007	C00A	119.6(4)	C00S	C00O	N003	108.5(5)
O005	N007	O00C	122.6(4)	C00H	C00P	C00K	106.8(5)
O00C	N007	C00A	117.8(4)	C00L	C00Q	C00S	108.4(5)
C00E	C00A	N007	125.8(4)	N001	C00R	N004	112.2(4)
C00F	C00A	N007	124.5(4)	C00O	C00S	C00Q	106.8(5)

Table S41: Torsion Angles for VSP-C6.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N001	C00G	C00K	C00P	-0.5(5)	C00F	C00A	C00E	C00I	-0.4(5)

N001	C00H	C00P	C00K	-0.1(5)	C00G	N001	C00H	C00P	-0.3(5)
N003	C00L	C00Q	C00S	0.3(5)	C00G	N001	C00R	N004	85.6(6)
N003	C00O	C00S	C00Q	0.1(6)	C00G	C00K	C00P	C00H	0.4(6)
O005	N007	C00A	C00E	5.4(7)	C00H	N001	C00G	C00K	0.5(5)
O005	N007	C00A	C00F	-173.4(5)	C00H	N001	C00R	N004	-92.8(6)
N006	C00B	C00D	N004	179.6(4)	C00I	N002	C00F	C00A	-0.2(5)
N006	C00B	C00J	C00M	179.6(4)	C00I	N002	C00N	N003	-84.2(6)
N007	C00A	C00E	C00I	-179.3(4)	C00J	C00B	C00D	N004	-0.3(5)
N007	C00A	C00F	N002	179.3(4)	C00L	N003	C00N	N002	-83.5(5)
O008	N006	C00B	C00D	1.4(7)	C00L	N003	C00O	C00S	0.1(5)
O008	N006	C00B	C00J	-178.7(5)	C00L	C00Q	C00S	C00O	-0.3(6)
O009	N006	C00B	C00D	-178.0(5)	C00M	N004	C00D	C00B	0.9(5)
O009	N006	C00B	C00J	2.0(8)	C00M	N004	C00R	N001	89.3(6)
C00A	C00E	C00I	N002	0.2(5)	C00N	N002	C00F	C00A	-172.5(4)
C00B	C00J	C00M	N004	0.9(6)	C00N	N002	C00I	C00E	172.3(4)
O00C	N007	C00A	C00E	-174.4(5)	C00N	N003	C00L	C00Q	176.8(4)
O00C	N007	C00A	C00F	6.8(7)	C00N	N003	C00O	C00S	-177.0(4)
C00D	N004	C00M	C00J	-1.2(6)	C00O	N003	C00L	C00Q	-0.2(5)
C00D	N004	C00R	N001	-85.1(6)	C00O	N003	C00N	N002	93.1(5)
C00D	C00B	C00J	C00M	-0.4(6)	C00R	N001	C00G	C00K	-178.1(4)
C00E	C00A	C00F	N002	0.3(5)	C00R	N001	C00H	C00P	178.3(4)
C00F	N002	C00I	C00E	0.0(5)	C00R	N004	C00D	C00B	176.1(4)
C00F	N002	C00N	N003	86.9(5)	C00R	N004	C00M	C00J	-176.2(4)

Table S42: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for VSP-C6.

Atom	*x*	*y*	*z*	U(eq)
H00A	8573.59	8751.51	9932.1	118
H00B	7919.59	9305.08	8821.5	118
H00F	6334.02	3538.38	6133.74	137
H00I	6933.95	4130.35	5435.28	137
H00D	7086.47	9237.02	7196.63	67
H00L	7794.76	414.33	5266.32	72
H00N	7826.29	4148.97	4911.28	64
H00G	5745.72	10352.19	7339.25	74
H00H	4813.52	7318.21	5441.32	74

H00O	8788.27	1036.58	4335.04	75
H00J	7308.76	5534.73	7227.02	75
H00K	4795.13	10044.47	8565.31	87
H00Q	9152.77	5370.49	6486.1	77
H00M	6279.49	6068.7	5402.64	79
H00R	9238	3119.47	3359.22	73
H00S	8867.99	4347.24	3625.7	73
H00T	10183.22	2418.98	5603.75	74
H00P	4202.64	8150.61	7366.05	82
H00U	10093.85	5158.69	8695.04	91
H00C	6096.27	9384.55	4796.74	85
H00E	5757.85	8139.96	4130.47	85
H00V	10746.12	3311.2	8138	96

4.7 Crystallographic data for compound **7**.

Table S43 Crystal data and structure refinement for VSP-C7.

Identification code	VSP-C7
Empirical formula	$C_9H_8N_4O_4$
Formula weight	236.19
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	7.4622(8)
b/Å	10.6054(12)
c/Å	13.7873(16)
α/°	71.770(4)
β/°	76.216(4)
γ/°	79.495(3)
Volume/Å^3	999.6(2)
Z	4
ρ_{calc}g/cm^3	1.569
μ/mm^{-1}	0.127
F(000)	488.0
Crystal size/mm^3	0.09 × 0.07 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.072 to 49.994
Index ranges	$-7 \leq h \leq 8$, $-12 \leq k \leq 12$, $-16 \leq l \leq 16$
Reflections collected	22093
Independent reflections	3513 [R_{int} = 0.0594, R_{sigma} = 0.0411]
Data/restraints/parameters	3513/0/307
Goodness-of-fit on F^2	1.087
Final R indexes [I>=2σ (I)]	R_1 = 0.0566, wR_2 = 0.1374
Final R indexes [all data]	R_1 = 0.0688, wR_2 = 0.1456

Largest diff. peak/hole / e Å^{-3} 0.38/-0.35

Table S44 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for VSP-C7. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	9672(3)	6884.1(18)	1064.9(16)	82.4(6)
O4	3071(2)	1542.0(19)	4111.4(15)	83.2(6)
O5	3421(2)	6762.4(16)	3824.6(14)	64.5(5)
O7	-3366(2)	9226.0(18)	2767.7(16)	72.9(5)
N1	6306(2)	4791.4(16)	1262.6(12)	41.9(4)
N2	7247(2)	2624.4(16)	2434.0(12)	41.5(4)
O2	10138(2)	4795.7(18)	1116.1(13)	66.6(5)
O3	3514(2)	2494.5(17)	2456.9(14)	65.9(5)
N6	476(2)	9059.8(16)	2683.8(13)	43.4(4)
N5	-321(2)	6836.6(16)	3730.1(12)	41.4(4)
O6	3995(2)	4765.5(17)	3648.2(13)	64.8(5)
C3	4228(3)	6614(2)	1104.1(16)	53.0(6)
C4	4503(3)	5274(2)	1210.0(15)	47.9(5)
C5	7029(3)	3389(2)	1376.2(15)	45.0(5)
C9	5947(3)	2076.1(19)	3291.1(16)	44.6(5)
C8	6810(3)	1460(2)	4121.3(17)	54.0(6)
N3	9094(3)	5839(2)	1123.9(14)	54.6(5)
C1	7181(3)	5874(2)	1184.5(15)	45.4(5)
C7	8674(3)	1612(2)	3769.8(18)	53.9(6)
C6	8913(3)	2324(2)	2749.4(17)	47.9(5)
N4	4083(2)	2041.1(18)	3275.9(16)	54.4(5)
C2	5914(3)	6993(2)	1094.4(17)	54.0(6)
O9	-2983(3)	10315(2)	1134.1(15)	81.7(6)
N8	-2363(3)	9726.3(18)	1937.2(17)	54.8(5)
C18	-452(3)	9690(2)	1869.8(16)	45.4(5)
C14	-189(3)	8197(2)	3717.7(16)	47.0(5)
C10	1054(3)	5780(2)	3672.8(14)	41.2(5)
C11	267(3)	4709(2)	3675.5(16)	46.8(5)
N7	2927(2)	5776.6(18)	3713.5(13)	47.5(4)
C17	749(3)	10388(2)	1040.2(18)	54.3(6)
C16	2446(3)	10193(2)	1344.4(19)	59.3(6)
C15	2237(3)	9388(2)	2342.4(18)	52.3(6)
C13	-1947(3)	6389(2)	3773.8(15)	46.5(5)
C12	-1618(3)	5098(2)	3739.1(16)	49.0(5)

Table S45 Anisotropic Displacement Parameters (Å^2×10^3) for VSP-C7. 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}

O1	70.6(12)	69.1(12)	105.4(15)	0.1(10)	-27.3(10)	-33.3(10)
O4	55.5(10)	85.9(13)	77.2(13)	8.0(10)	8.5(9)	-13.9(9)
O5	51.9(9)	59.6(10)	85.7(12)	-15.3(9)	-23.9(8)	-11.5(8)
O7	46.8(9)	69.6(11)	90.5(13)	-8.1(10)	-11.2(9)	-6.1(8)
N1	38.5(9)	49.9(10)	36.6(9)	-11.6(7)	-7.1(7)	-4.9(7)
N2	40.3(9)	42.0(9)	43.9(9)	-17.2(7)	-8.0(7)	-0.4(7)
O2	42.9(9)	76.2(12)	73.6(11)	-13.3(9)	-8.9(8)	-6.6(8)
O3	51.7(9)	72.7(11)	71.2(11)	-10.7(9)	-17.0(8)	-12.5(8)
N6	40.5(9)	39.8(9)	53.0(10)	-17.8(8)	-9.1(7)	-3.5(7)
N5	38.6(9)	43.5(9)	40.8(9)	-11.5(7)	-6.1(7)	-4.2(7)
O6	44.7(9)	68.3(11)	77.9(11)	-25.3(9)	-11.7(8)	9.9(8)
C3	48.3(12)	56.8(14)	49.2(13)	-10.1(10)	-13.2(10)	1.7(10)
C4	41.1(11)	61.3(14)	41.0(11)	-11.5(10)	-10.1(9)	-7.7(10)
C5	45.0(11)	53.5(12)	39.5(11)	-19.7(9)	-5.4(8)	-5.5(9)
C9	43.8(11)	37.8(11)	50.3(12)	-14.1(9)	-5.2(9)	-2.1(9)
C8	67.1(15)	41.8(12)	49.9(13)	-10.6(10)	-11.8(11)	-1.7(10)
N3	48.9(11)	63.7(13)	45.7(11)	0.2(9)	-10.8(8)	-18.4(10)
C1	44.9(11)	51.9(12)	37.3(11)	-5.3(9)	-6.9(8)	-14.7(9)
C7	62.4(14)	42.3(12)	64.8(15)	-18.8(11)	-28.3(11)	2.4(10)
C6	43.0(11)	45.4(12)	61.1(14)	-23.8(10)	-13.3(10)	0.3(9)
N4	46.4(10)	44.0(10)	64.4(13)	-8.5(9)	-5.2(9)	-3.2(8)
C2	59.8(14)	47.9(13)	50.9(13)	-6.1(10)	-13.2(10)	-8.6(11)
O9	68.1(11)	96.7(14)	85.3(13)	-21.5(11)	-38.9(10)	2.4(10)
N8	50.8(11)	44.8(11)	75.0(14)	-22.8(10)	-21.2(10)	1.3(9)
C18	46.8(11)	39.8(11)	56.5(13)	-23.0(10)	-13.9(10)	-0.7(9)
C14	46.9(11)	50.4(12)	47.8(12)	-22.4(10)	-7.2(9)	-3.3(9)
C10	38.0(10)	48.5(12)	34.5(10)	-10.1(8)	-6.0(8)	-2.6(9)
C11	49.8(12)	45.1(12)	45.1(11)	-14.7(9)	-7.7(9)	-3.2(9)
N7	39.7(9)	54.3(11)	43.9(10)	-8.5(8)	-7.9(7)	-3.8(9)
C17	62.3(14)	45.2(12)	54.1(13)	-14.8(10)	-8.9(11)	-5.0(10)
C16	50.4(13)	51.8(14)	70.9(16)	-13.7(12)	-3.2(11)	-11.9(10)
C15	43.2(12)	46.6(12)	70.1(15)	-17.9(11)	-14.4(10)	-5.7(9)
C13	34.9(10)	53.0(13)	46.9(12)	-7.8(9)	-7.2(8)	-5.7(9)
C12	47.3(12)	50.3(13)	49.1(12)	-8.9(10)	-10.3(9)	-12.9(10)

Table S46 Bond Lengths for VSP-C7.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	N3	1.234(2)	O6	N7	1.228(2)
O4	N4	1.236(2)	C3	C4	1.364(3)
O5	N7	1.233(2)	C3	C2	1.385(3)
O7	N8	1.228(2)	C9	C8	1.372(3)
N1	C4	1.360(3)	C9	N4	1.404(3)
N1	C5	1.459(3)	C8	C7	1.381(3)

N1	C1	1.385(3)	N3	C1	1.404(3)
N2	C5	1.462(3)	C1	C2	1.368(3)
N2	C9	1.380(3)	C7	C6	1.359(3)
N2	C6	1.364(3)	O9	N8	1.239(3)
O2	N3	1.232(2)	N8	C18	1.401(3)
O3	N4	1.225(2)	C18	C17	1.372(3)
N6	C18	1.385(3)	C10	C11	1.369(3)
N6	C14	1.459(3)	C10	N7	1.411(3)
N6	C15	1.356(3)	C11	C12	1.382(3)
N5	C14	1.458(3)	C17	C16	1.387(3)
N5	C10	1.383(2)	C16	C15	1.363(3)
N5	C13	1.363(3)	C13	C12	1.360(3)

Table S47 Bond Angles for VSP-C7.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C4	N1	C5	123.08(17)	C6	C7	C8	107.9(2)
C4	N1	C1	106.14(17)	C7	C6	N2	109.73(19)
C1	N1	C5	130.78(16)	O4	N4	C9	117.4(2)
C9	N2	C5	130.35(17)	O3	N4	O4	122.5(2)
C6	N2	C5	123.32(17)	O3	N4	C9	120.16(18)
C6	N2	C9	106.33(16)	C1	C2	C3	107.2(2)
C18	N6	C14	129.89(17)	O7	N8	O9	122.3(2)
C15	N6	C18	106.31(17)	O7	N8	C18	120.7(2)
C15	N6	C14	123.79(18)	O9	N8	C18	116.9(2)
C10	N5	C14	130.17(17)	N6	C18	N8	124.62(19)
C13	N5	C14	123.47(17)	C17	C18	N6	109.13(19)
C13	N5	C10	106.33(16)	C17	C18	N8	125.9(2)
C4	C3	C2	107.23(19)	N5	C14	N6	113.76(15)
N1	C4	C3	110.19(19)	N5	C10	N7	124.84(18)
N1	C5	N2	114.18(15)	C11	C10	N5	109.01(17)
N2	C9	N4	124.73(18)	C11	C10	N7	125.86(18)
C8	C9	N2	109.17(19)	C10	C11	C12	107.23(18)
C8	C9	N4	125.79(19)	O5	N7	C10	119.64(17)
C9	C8	C7	106.9(2)	O6	N7	O5	122.81(18)
O1	N3	C1	117.6(2)	O6	N7	C10	117.55(18)
O2	N3	O1	122.21(19)	C18	C17	C16	107.0(2)
O2	N3	C1	120.21(19)	C15	C16	C17	107.3(2)
N1	C1	N3	124.92(19)	N6	C15	C16	110.3(2)
C2	C1	N1	109.19(18)	C12	C13	N5	109.84(18)
C2	C1	N3	125.7(2)	C13	C12	C11	107.59(19)

Table S48 Torsion Angles for VSP-C7.

A	B	C	D	Angle/°	A	B	C	D	Angle/°

O1	N3	C1	N1	-179.46(19)	C1	N1	C4	C3	-0.1(2)
O1	N3	C1	C2	6.0(3)	C1	N1	C5	N2	78.8(2)
O7	N8	C18	N6	3.1(3)	C6	N2	C5	N1	-100.6(2)
O7	N8	C18	C17	-169.0(2)	C6	N2	C9	C8	0.6(2)
N1	C1	C2	C3	-0.7(2)	C6	N2	C9	N4	-173.34(18)
N2	C9	C8	C7	-0.9(2)	N4	C9	C8	C7	172.98(19)
N2	C9	N4	O4	-178.45(19)	C2	C3	C4	N1	-0.3(2)
N2	C9	N4	O3	1.5(3)	O9	N8	C18	N6	-178.98(18)
O2	N3	C1	N1	1.5(3)	O9	N8	C18	C17	9.0(3)
O2	N3	C1	C2	-173.0(2)	N8	C18	C17	C16	172.86(19)
N6	C18	C17	C16	-0.2(2)	C18	N6	C14	N5	77.4(2)
N5	C10	C11	C12	-0.2(2)	C18	N6	C15	C16	-0.3(2)
N5	C10	N7	O5	1.2(3)	C18	C17	C16	C15	0.1(2)
N5	C10	N7	O6	-179.67(17)	C14	N6	C18	N8	7.5(3)
N5	C13	C12	C11	0.2(2)	C14	N6	C18	C17	-179.26(18)
C4	N1	C5	N2	-101.4(2)	C14	N6	C15	C16	179.32(18)
C4	N1	C1	N3	-174.84(18)	C14	N5	C10	C11	-177.80(18)
C4	N1	C1	C2	0.5(2)	C14	N5	C10	N7	8.1(3)
C4	C3	C2	C1	0.6(2)	C14	N5	C13	C12	177.95(17)
C5	N1	C4	C3	-179.94(17)	C10	N5	C14	N6	77.3(2)
C5	N1	C1	N3	5.0(3)	C10	N5	C13	C12	-0.4(2)
C5	N1	C1	C2	-179.70(17)	C10	C11	C12	C13	0.0(2)
C5	N2	C9	C8	-179.21(18)	C11	C10	N7	O5	-171.85(19)
C5	N2	C9	N4	6.9(3)	C11	C10	N7	O6	7.3(3)
C5	N2	C6	C7	179.74(17)	N7	C10	C11	C12	173.76(18)
C9	N2	C5	N1	79.1(2)	C17	C16	C15	N6	0.2(3)
C9	N2	C6	C7	-0.1(2)	C15	N6	C18	N8	-172.87(19)
C9	C8	C7	C6	0.8(2)	C15	N6	C18	C17	0.3(2)
C8	C9	N4	O4	8.6(3)	C15	N6	C14	N5	-102.2(2)
C8	C9	N4	O3	-171.4(2)	C13	N5	C14	N6	-100.5(2)
C8	C7	C6	N2	-0.5(2)	C13	N5	C10	C11	0.4(2)
N3	C1	C2	C3	174.61(19)	C13	N5	C10	N7	-173.71(18)

Table S49 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement

Parameters ($Å^2×10^3$) for VSP-C7.

Atom	*x*	*y*	*z*	U(eq)
H3	3116.41	7169.03	1048.8	64
H4	3589.07	4764.06	1241.66	57
H5A	8225.98	3342.61	912.45	54
H5B	6195.46	2974.05	1159.06	54
H8	6247.75	1023.36	4792.55	65
H7	9601.52	1285.81	4161.97	65
H6	10040.89	2568.95	2329.38	57
H2	6142.95	7849.54	1037.25	65
H14A	643.66	8163.31	4170.6	56
H14B	-1405.75	8587.5	3998.08	56
H11	886.34	3875.12	3640.96	56
H17	477.63	10894.79	396.65	65
H16	3525.52	10546.75	941.85	71
H15	3168.39	9103.85	2733.14	63
H13	-3107.71	6891.11	3820.37	56
H12	-2501.2	4572.89	3755.26	59

4.8 Crystallographic data for compound **8**.

Table S50: Crystal data and structure refinement for VSP-C8.

Identification code	VSP-C8
Empirical formula	$C_9H_8N_4O_4$
Formula weight	236.19
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.3802(6)
b/Å	8.4707(4)
c/Å	10.1162(5)
α/°	90
β/°	105.237(2)
γ/°	90
Volume/$Å^3$	1023.58(9)

Z	4
ρ_{calc}g/cm^3	1.533
μ/mm^{-1}	0.124
F(000)	488.0
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.41 to 55.738
Index ranges	-16 ≤ h ≤ 16, -9 ≤ k ≤ 11, -13 ≤ l ≤ 11
Reflections collected	17895
Independent reflections	2436 [R_{int} = 0.0604, R_{sigma} = 0.0336]
Data/restraints/parameters	2436/0/154
Goodness-of-fit on F^2	1.056
Final R indexes [I>=2σ (I)]	R_1 = 0.0633, wR_2 = 0.1687
Final R indexes [all data]	R_1 = 0.0922, wR_2 = 0.1997
Largest diff. peak/hole / e Å^{-3}	0.51/-0.64

Table S51: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for VSP-C8. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N001	7635.9(11)	5813.2(18)	5783.6(13)	34.8(4)
N002	7527.3(12)	5779.6(18)	8134.8(13)	36.2(4)
O003	6037.4(16)	2827(2)	10829.7(15)	64.9(5)
O004	4932.1(13)	3241(3)	8822.3(19)	70.2(6)
N005	5830.6(14)	3432(2)	9687.0(16)	44.7(4)
O006	9953.4(15)	3358(3)	5849(2)	76.7(6)
N007	9392.0(14)	4310(3)	6302.9(18)	53.4(5)
C008	6719.6(15)	5923(2)	4692.3(17)	40.5(4)
O009	9717.3(16)	4912(4)	7429.1(19)	98.1(9)
C00A	8257.2(16)	5570(2)	9413.2(17)	42.8(4)
C00B	6548.1(14)	5054(2)	8083.0(16)	37.2(4)
C00C	6838.4(17)	4920(3)	3681.6(17)	46.4(5)
C00D	6663.2(14)	4364(2)	9339.7(16)	36.3(4)
C00E	7749.3(15)	6730(2)	7033.4(16)	39.8(4)

C00F	7868.2(18)	4160(2)	4149.0(18)	45.0(5)
C00G	8338.4(14)	4724(2)	5440.3(16)	37.8(4)
C00H	7737.5(16)	4693(2)	10186.3(17)	43.2(4)

Table S52: Anisotropic Displacement Parameters ($Å^2×10^3$) for VSP-C8. 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}
N001	30.6(7)	41.0(8)	33.1(6)	0.9(5)	9.1(5)	1.9(6)
N002	36.1(7)	40.1(8)	33.0(7)	-3.9(5)	9.9(5)	-4.4(6)
O003	87.7(12)	65.8(11)	46.7(8)	8.5(7)	27.3(7)	-15.2(9)
O004	42.2(8)	87.9(14)	78.1(11)	22.6(9)	11.2(7)	-16.7(8)
N005	46.9(9)	44.7(9)	46.8(8)	0.8(6)	20.3(6)	-3.3(7)
O006	56.9(10)	80.7(14)	94.6(13)	12.8(10)	23.6(9)	33.8(9)
N007	36.0(8)	73.4(13)	51.3(9)	12.9(8)	12.5(7)	13.7(8)
C008	36.1(8)	46.3(11)	38.0(8)	8.9(6)	7.6(6)	4.0(7)
O009	52.6(11)	175(3)	55.1(10)	-18.2(12)	-7.2(8)	34.3(13)
C00A	39.8(9)	47.8(11)	37.2(8)	-5.3(7)	3.7(7)	-6.8(7)
C00B	34.2(8)	41.8(10)	35.1(8)	-0.7(6)	8.0(6)	-4.5(7)
C00C	49.6(10)	55.0(12)	31.9(8)	3.6(7)	5.6(7)	-3.3(8)
C00D	38.2(8)	36.4(9)	36.1(8)	-2.0(6)	12.9(6)	0.5(7)
C00E	45.6(9)	39.3(10)	36.9(8)	-3.1(6)	15.0(6)	-6.8(7)
C00F	54.8(11)	44.4(11)	40.2(8)	0.6(7)	20.0(7)	2.4(8)
C00G	34.6(8)	42.8(10)	37.8(8)	6.9(6)	12.9(6)	5.2(7)
C00H	49.6(10)	44.9(10)	31.7(8)	-2.3(6)	4.8(7)	-3.9(8)

Table S53: Bond Lengths for VSP-C8.

Atom	Atom	Length/Å	Atom		Length/Å
N001	C008	1.362(2)	N007		1.230(3)
N001	C00E	1.459(2)	O009		1.216(3)
N001	C00G	1.374(2)	C00G		1.410(2)
N002	C00A	1.381(2)	C008	C00C	1.366(3)
N002	C00B	1.348(2)	C00A	C00H	1.357(3)
N002	C00E	1.458(2)	C00B	C00D	1.372(2)

O003	N005	1.228(2)	C00C	C00F	1.395(3)
O004	N005	1.232(2)	C00D	C00H	1.408(2)
N005	C00D	1.414(2)	C00F	C00G	1.369(3)

Table S54: Bond Angles for VSP-C8.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C008	N001	C00E	122.41(15)	C00H	C00A	N002	108.51(16)
C008	N001	C00G	106.77(14)	N002	C00B	C00D	106.55(14)
C00G	N001	C00E	130.81(14)	C008	C00C	C00F	107.57(16)
C00A	N002	C00E	125.33(15)	C00B	C00D	N005	124.26(16)
C00B	N002	C00A	109.77(15)	C00B	C00D	C00H	109.32(16)
C00B	N002	C00E	124.77(14)	C00H	C00D	N005	126.39(16)
O003	N005	O004	122.65(17)	N002	C00E	N001	111.95(14)
O003	N005	C00D	118.78(17)	C00G	C00F	C00C	106.47(17)
O004	N005	C00D	118.56(16)	N001	C00G	N007	123.70(16)
O006	N007	C00G	116.98(19)	C00F	C00G	N001	109.70(15)
O009	N007	O006	122.97(19)	C00F	C00G	N007	126.58(18)
O009	N007	C00G	120.03(19)	C00A	C00H	C00D	105.85(15)
N001	C008	C00C	109.49(16)				

Table S55: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for VSP-C8.

Atom	*x*	*y*	*z*	U(eq)
H008	6107.83	6578.66	4642.88	49
H00A	8982.84	5963.26	9696.79	51
H00B	5917.95	5026.07	7340.87	45
H00C	6325.93	4771.97	2835.93	56
H00D	8502.12	7154.87	7327.62	48
H00E	7231.04	7611.19	6842.62	48
H00F	8174.66	3415.88	3676.38	54

H00H	8030.81	4375.19	11089.49

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4.9 Crystallographic data for compound **9**.

Table S56: Crystal data and structure refinement for VSP-C9.

Identification code	VSP-C9
Empirical formula	$C_9H_8N_4O_4$
Formula weight	236.19
Temperature/K	273
Crystal system	orthorhombic
Space group	$Pca2_1$
a/Å	10.2722(5)
b/Å	8.8323(4)
c/Å	11.4857(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1042.06(8)
Z	4
ρ_{calc}g/cm^3	1.5054
μ/mm^{-1}	0.122
F(000)	488.3
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.62 to 51.38
Index ranges	$-12 \leq h \leq 12$, $-10 \leq k \leq 9$, $-11 \leq l \leq 14$
Reflections collected	8480
Independent reflections	1799 [R_{int} = 0.0364, R_{sigma} = 0.0326]
Data/restraints/parameters	1799/1/155
Goodness-of-fit on F^2	1.056
Final R indexes [I>=2σ (I)]	R_1 = 0.0487, wR_2 = 0.1109
Final R indexes [all data]	R_1 = 0.0504, wR_2 = 0.1128
Largest diff. peak/hole / e Å^{-3}	0.35/-0.33
Flack parameter	-0.1(12)

Table S57: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for VSP-C9. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O001	8037.4(16)	2221(2)	6818.9(17)	67.2(5)
N002	2770.5(15)	1454.9(16)	5556.2(14)	40.8(4)
N003	4934.0(13)	2494.6(15)	5501.7(14)	36.9(4)
N004	5898.2(17)	4910(2)	3166.7(19)	56.0(5)
N005	6855.0(15)	2068(2)	6743.1(16)	47.7(4)
O006	6959.0(18)	5483(2)	2964.1(17)	74.3(6)
O007	6207.8(19)	1378(3)	7445.9(16)	80.6(6)
C008	4663.2(17)	3264.1(19)	4525.5(17)	39.9(4)
O009	4949.0(19)	5081(3)	2554(2)	86.1(7)
C00A	5790.6(17)	3976(2)	4173.9(18)	43.0(4)
C00B	3979.8(17)	1535(2)	6157.5(19)	42.7(4)
C00C	2504(2)	506(2)	4649.5(18)	44.6(5)
C00D	6234.7(17)	2716.9(18)	5759.8(18)	37.3(4)
C00E	6786.3(17)	3637(2)	4944.5(17)	42.6(4)
C00F	1693(2)	2330(2)	5781(2)	51.9(5)
C00G	759(2)	1914(3)	5009(3)	62.5(6)
C00H	1263(2)	769(3)	4293(2)	56.5(5)

Table S58: Anisotropic Displacement Parameters ($Å^2×10^3$) for VSP-C9. 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}
O001	45.8(8)	88.5(12)	67.2(12)	4.3(7)	-15.3(8)	2.0(9)
N002	38.2(8)	42.7(7)	41.6(9)	-2.8(6)	6.2(6)	-1.6(7)
N003	35.1(7)	37.3(7)	38.2(9)	1.8(6)	1.1(6)	-1.3(6)
N004	50.5(10)	54.5(10)	63.1(12)	-3.8(8)	2.2(9)	20.7(9)
N005	43.6(9)	56.0(10)	43.5(10)	5.6(7)	-6.9(8)	-1.0(8)
O006	60.2(10)	82.2(12)	80.4(13)	-19.8(8)	7.6(9)	32.0(10)
O007	60.3(10)	120.5(17)	61.2(12)	-3.5(9)	-12.3(8)	42.2(12)
C008	35.7(8)	41.4(8)	42.7(10)	1.7(7)	-1.8(7)	5.7(7)
O009	66.1(10)	106.0(13)	86.1(16)	-9.8(9)	-14.9(10)	54.9(13)
C00A	42.3(9)	39.5(9)	47.2(10)	-0.0(7)	1.7(8)	4.6(8)
C00B	43.4(10)	46.9(10)	37.9(10)	-3.4(7)	3.1(7)	3.3(8)
C00C	49.8(10)	43.2(8)	40.8(10)	-5.5(7)	4.0(8)	-0.4(8)
C00D	34.1(8)	39.1(8)	38.7(10)	5.0(7)	-2.4(7)	-3.8(7)
C00E	35.4(8)	40.0(9)	52.4(11)	-1.0(7)	1.2(8)	0.4(8)
C00F	44.5(11)	48.5(10)	62.8(14)	2.2(7)	10.3(10)	-2.7(9)
C00G	40.5(9)	62.5(13)	84.3(18)	-0.3(9)	-2.5(11)	12.6(13)
C00H	57.7(13)	60.5(11)	51.5(13)	-16.5(10)	-8.7(10)	10.3(10)

Table S59: Bond Lengths for VSP-C9.

Atom Atom Length/Å Atom Atom Length/Å

O001	N005	1.225(2)	N004	C00A	1.425(3)
N002	C00B	1.423(3)	N005	O007	1.210(3)
N002	C00C	1.364(2)	N005	C00D	1.418(3)
N002	C00F	1.374(3)	C008	C00A	1.378(3)
N003	C008	1.340(2)	C00A	C00E	1.385(3)
N003	C00B	1.499(2)	C00C	C00H	1.358(3)
N003	C00D	1.383(2)	C00D	C00E	1.363(3)
N004	O006	1.224(3)	C00F	C00G	1.357(4)
N004	O009	1.212(3)	C00G	C00H	1.403(4)

Table S60: Bond Angles for VSP-C9.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C00C	N002	C00B	125.19(16)	C008	C00A	N004	124.55(18)
C00F	N002	C00B	125.70(17)	C00E	C00A	N004	125.90(17)
C00F	N002	C00C	109.09(18)	C00E	C00A	C008	109.55(17)
C00B	N003	C008	124.85(15)	N003	C00B	N002	110.81(16)
C00D	N003	C008	107.93(15)	C00H	C00C	N002	108.26(18)
C00D	N003	C00B	127.20(16)	N005	C00D	N003	123.21(18)
O009	N004	O006	123.67(19)	C00E	C00D	N003	109.82(16)
C00A	N004	O006	117.58(19)	C00E	C00D	N005	126.97(17)
C00A	N004	O009	118.75(17)	C00D	C00E	C00A	105.12(15)
O007	N005	O001	123.5(2)	C00G	C00F	N002	107.1(2)
C00D	N005	O001	117.24(19)	C00H	C00G	C00F	108.4(2)
C00D	N005	O007	119.20(16)	C00G	C00H	C00C	107.1(2)
C00A	C008	N003	107.58(16)				

Table S61: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for VSP-C9.

Atom	*x*	*y*	*z*	U(eq)
H008	3860.4(17)	3309.3(19)	4152.9(17)	47.9(5)
H00a	3841.9(17)	1961(2)	6926.0(19)	51.3(5)
H00b	4331.5(17)	524(2)	6252.0(19)	51.3(5)
H00C	3073(2)	-199(2)	4330.2(18)	53.5(5)
H00E	7645.5(17)	3967(2)	4912.5(17)	51.1(5)
H00F	1619(2)	3069(2)	6354(2)	62.3(6)
H00G	-75(2)	2320(3)	4963(3)	75.0(8)
H00H	830(2)	281(3)	3689(2)	67.9(7)

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