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Electronic Supplementary Information

Bipyrrole Scaffold as an Emerging Frontier in Robust Design of High Energy Materials

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1. General Information

i) General experimental information

Pyrrole, dichloromethane (DCM), and N,N′-dimethylformamide (DMF) were dried over calcium hydride and distilled before use, while acetic anhydride was dried over P_2O_5 and subsequently distilled. Potassium hydroxide pellets were ground into powder and further dried in a vacuum oven. Bromotrimethylsilane (TMSBr), bis(trifluoroacetoxy)iodobenzene (PIFA), $(CuNO_3)_2.3H_2O$, KNO_3, NO_2BF_4, and H_2SO_4 were obtained from Finar and Sigma-Aldrich and used as received unless otherwise specified. All reactions were carried out in oven-dried round-bottom flasks. Reaction progress was monitored by thin-layer chromatography (TLC) on silica gel GF254 plates, with visualization under UV light (254 nm) and/or iodine staining. Purification was achieved by column chromatography on silica gel (100–200 mesh) using hexane/ethyl acetate mixtures as eluents.

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 **3, 4, 6, 7** and **HNDMBP** in this paper have been deposited in the Cambridge Crystallographic Data Centre as supplementary publication numbers **2503546-2503550**, respectively. 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 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 1:

In a two-neck round-bottom flask, DCM (1100 mL) was cooled to -78 °C and pyrrole (5 g) was added and stirred for 30 min. PIFA (10.65 g) and TMSBr (6.51 mL) were then added simultaneously, and the mixture was warmed to -40 °C and stirred for 2 h. The reaction was quenched with $NaHCO_3$ solution, extracted with DCM, and purified by flash chromatography followed by Kugelrohr distillation.

General procedure for the synthesis of compounds 2- 7 and HNDMBP

Synthesis of Compounds 2 and 3 using NO_2BF_4:

In an oven-dried 50 mL two-necked round-bottom flask, **1** (0.500 g) was dissolved in acetonitrile (10 mL) and cooled to - 30 °C. To this solution, NO_2BF_4 (1.0 equiv.) was added gradually, in small portions over 15 min. The reaction mixture was then slowly warmed to -30 °C and stirred at this temperature for 1 h. Upon completion, the mixture was quenched by pouring onto crushed ice and extracted with ethyl acetate. The crude product was purified by column chromatography using hexane/ethyl acetate (90:10) as the eluent, affording compounds **2** and **3**.

Compound 2: **Orange solid;** Yield: 0.2943 mg, 35%; ^{1}H NMR (600 MHz, DMSO-d_6) δ 6.81 (d, J = 1.73 Hz, 2H), 7.99 (d, J = 1.10 Hz, 2H), 12.84 (s, 2H) ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 136.9, 122.1, 106.0, 100.9 ppm. HRMS (ESI) m/z $(M+NH_4)^+$ calculated for $C_8H_6N_4O+NH_4$ 240.0732, found 240.0732. FTIR (cm^{-1}) ῡ 3273, 3129, 2919, 2850, 2350, 2111, 1558, 1515, 1476, 1390, 1260, 1086, 977, 875, 785, 742.

Compound 3: **White solid;** Yield: 0.1093 mg, 13%; ^{1}H NMR (500.19 MHz, DMSO-d_6) δ 6.76 (d, J = 4.52 Hz, 1H), 6.84 (d, J = 3.18 Hz, 1H), 7.08 (d, J = 3.71 Hz, 1H), 7.28 (d, J = 4.62 Hz, 1H), 12.46 (s, 1H), 13.25 (s, 1H) ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 138.2, 133.9, 126.9, 122.3, 120.7, 113.1, 112.5, 107.6 ppm. HRMS (ESI) m/z $(M+NH_4)^+$ calculated for $C_8H_6N_4O_4+NH_4$ 240.0732, found 240.0732. FTIR (cm^{-1}) ῡ 3274, 2918, 2850, 1558, 1515, 1476, 1419, 1389, 1311, 1259, 1207, 1086, 1058, 976, 876, 785, 715.

Synthesis of Compounds 2 and 3 using $Cu(NO_3)_2$:

Compound **1** was dissolved in acetic anhydride (15 mL) and cooled to - 30 °C. Finely powdered, dried $Cu(NO_3)_2.3H_2O$ (1.0 equiv.) was then added slowly, in small portions over 30 min. The reaction mixture was gradually warmed to -30 °C and stirred at this temperature for 2 h. After completion, the mixture was poured onto crushed ice and extracted with ethyl acetate. The product mixture was purified by column chromatography using hexane/ethyl acetate (90:10) as the eluent, providing compounds **2** and **3**.

Compound 2: **Orange solid;** Yield: 0.1850 mg, 22%.

Compound 3: **White solid;** Yield: 0.0925 mg, 11%.

Synthesis of Compounds 4 and 5

5,5′-Dinitro-2,2′-bipyrrole **2** or 3,4′-dinitro-2,2′-bipyrrole **3** (0.200 g) was dissolved in H_2O (3 mL), and KOH (1.0 equiv., 21.5 mmol) was added. The mixture was stirred at room temperature for 3 h. After completion, the water was removed under reduced pressure, and the resulting residue was dissolved in DMF (5 mL). The solution was stirred for 10 min, followed by the addition of iodomethane (2.0 equiv.). The reaction mixture was stirred at room temperature overnight, poured into crushed ice, and the precipitate formed was collected by filtration.

Compound 4: **Yellow solid;** Yield: 0.1260 mg, 56%; ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.40 (d, J = 4.39 Hz, 2H), 6.60 (d, J = 4.29 Hz, 2H), 3.79 (s, 3H) ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 139.6, 130.2, 113.9, 113.0, 29.48 ppm. HRMS (ESI) m/z $(M+H)^+$ calculated for $C_9H_5N_7O_{10}$+H 251.0780, found 251.0782. FTIR (cm^{-1}) ῡ 3131, 2346, 1519, 1505, 1490, 1444, 1409, 1320, 1291, 1269, 1131, 1014, 978, 817, 738.

Compound 5: **Yellow solid;** Yield: 0.1170 mg, 52%; ^{1}H NMR (500.19 MHz, DMSO-d_6) δ 7.39 (d, J = 4.39 Hz, 1H), 7.22 (d, J = 3.38 Hz, 1H), 6.92 (d, J = 3.08 Hz, 1H), 6.59 (d, J = 4.53 Hz, 1H), 3.64 (s, 3H), 3.52 (s, 3H) ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 139.2, 136.1, 128.7,

125.6, 122.0, 113.7, 112.8, 105.9, 35.8, 35.3 ppm. HRMS (ESI) m/z $(M+H)^+$ calculated for $C_9H_6N_6O_8$+H 251.0780, found 251.0780. FTIR (cm^{-1}) ῡ 3131, 2662, 2346, 1519, 1505, 1490, 1444, 1409, 1291, 1269, 1203, 1131, 978, 817, 738.

Synthesis of Compounds 6 and 7

1,1′-Dimethyl-5,5′-dinitro-2,2′-bipyrrole **4** or 1,1′-dimethyl-3,4′-dinitro-2,2′-bipyrrole **5** (0.100 g) was placed in a round-bottom flask and dissolved in concentrated H_2SO_4 (10 mL) at -15 °C. Finely powdered KNO_3 (8.0 equiv.) was added in small portions over 30 min. The reaction mixture was stirred at -15 °C for 30 min, then the temperature was increased to 0 °C and stirred for an additional 1 h. After completion, the mixture was poured onto crushed ice, and the precipitated product was collected and purified by column chromatography using hexane/ethyl acetate (70:30) as the eluent.

Compound 6: **White solid;** Yield: 0.0408 mg, 30%; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.11 (s, 2H), 3.82 (s, 3H) ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 138.6, 134.6, 122.0, 108.7, 36.62 ppm. HRMS (ESI) m/z $(M+H)^+$ calculated for $C_9H_6N_6O_8$+H 341.0481, found 341.0481. FTIR (cm^{-1}) ῡ 3129, 2924, 1510, 1490, 1442, 1302, 1268, 1203, 1185, 1130, 1015, 976, 843, 870, 815, 785.

Compound 7: **White solid;** Yield: 0.0263 mg, 17%; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.13 (s, 1H), 3. 88 (s, 3H), 3. 86 (s, 3H) ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 139.0, 135.1, 130.4, 127.0, 126.1, 120.1, 119.4, 108.7, 37.1, 36.9. HRMS (ESI) m/z $(M+H)^+$ calculated for $C_9H_6N_6O_8{}^+$H 385.0254, found 385.0254. FTIR (cm^{-1}) ῡ 2922, 1679, 1557, 1515, 1469, 1389, 1310, 1200, 907, 852, 837, 795.

Synthesis of compound HNDMBP from 7

1,1'-dimethyl-3,3',4,5,5'-pentanitro-2,2'-bipyrrole **7** (0.200 g) was placed in a round-bottom flask and dissolved in concentrated H_2SO_4 (15 mL) at -15 °C. Finely powdered KNO_3 (4 equiv.) was added in small portions over 30 min. The reaction mixture was stirred at -15 °C for 30 min, then temperature was increased to RT and stirred for an additional 6 h. After completion, the mixture was poured onto crushed ice, and the precipitated product was filtered.

Compound HNDMBP: White solid; Yield: 0.0316 mg, 28%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 3.94 ppm. ^{13}C NMR (39.5 MHz, DMSO-d_6) δ 130.8, 126.9, 126.7, 117.6, 37.5 ppm. ^{15}N 81 MHz, DMSO-d_6) δ -225.03 (N1), -35.31 (N2), -31.39 (N3), -30.02 (N4) ppm. HRMS (ESI) m/z

$(M+Na)^+$ calculated for $C_9H_9N_3O_2$+ Na 453.0002, found 453.0002. FTIR (cm^{-1}) ῡ 3128, 2922, 1504, 1489, 1442, 1408, 1302, 1268, 1203, 1130, 1049, 975, 843, 815, 784.

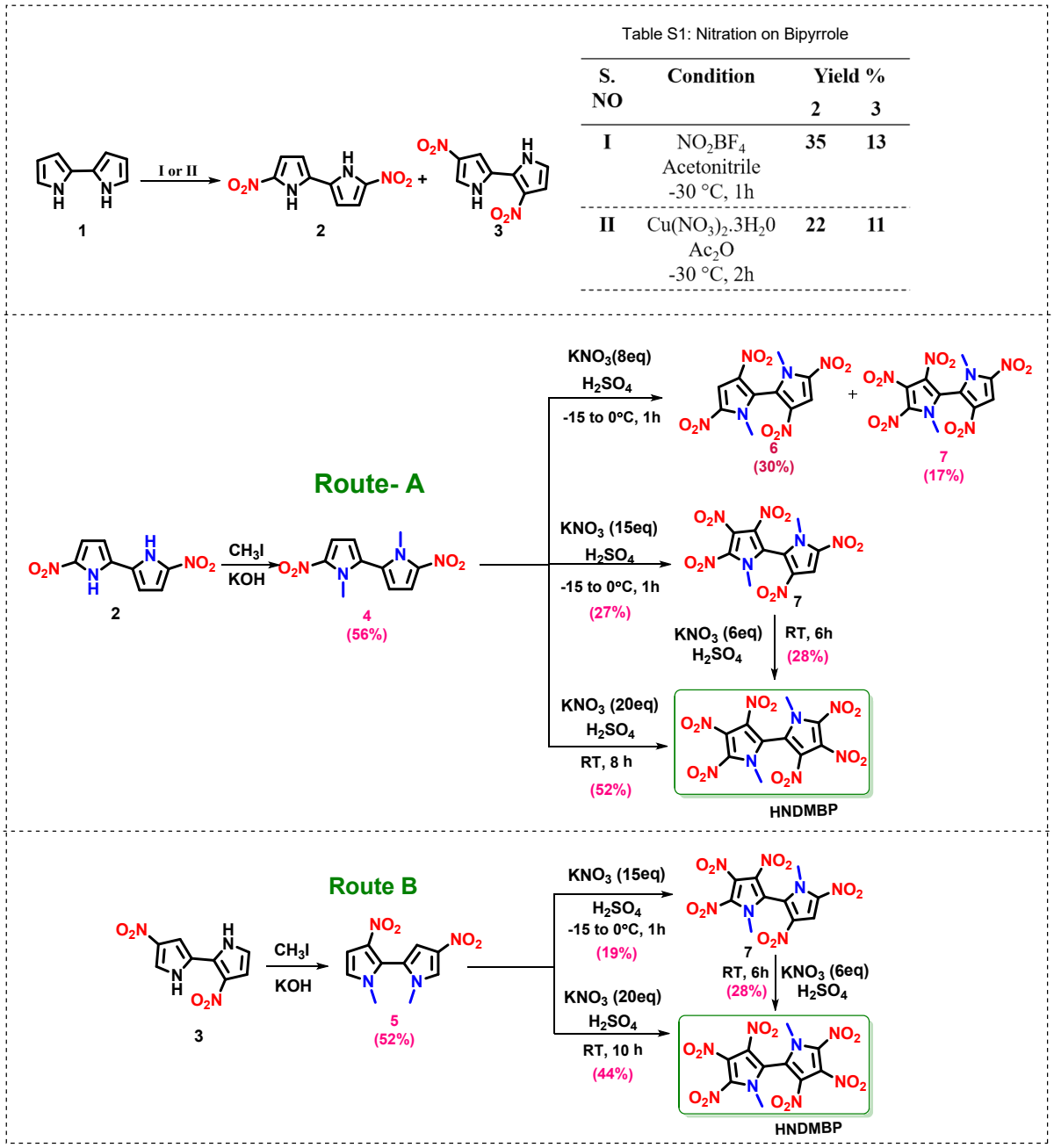
Synthesis of compound HNDMBP from 4 and 5

1,1′-Dimethyl-5,5′-dinitro-2,2′-bipyrrole **4** or 1,1′-dimethyl-3,4′-dinitro-2,2′-bipyrrole **5** (0.200 g) was placed in a round-bottom flask and dissolved in concentrated H_2SO_4 (10 mL) at -15 °C. Finely powdered KNO_3 (4 equiv.) was added in small portions over 10 minutes. The reaction mixture was stirred at -15 °C for 30 min, then the temperature was increased to RT and stirred for an additional 10 h. After completion, the mixture was poured onto crushed ice, and the precipitated product was filtered.

Yield of compound 8 from 4: 0.1790 mg, 52%

Yield of compound 8 from 5: 0.1514 mg, 44%

Yield of compound 8 from (4 + 5): 0.1617 mg, 47%

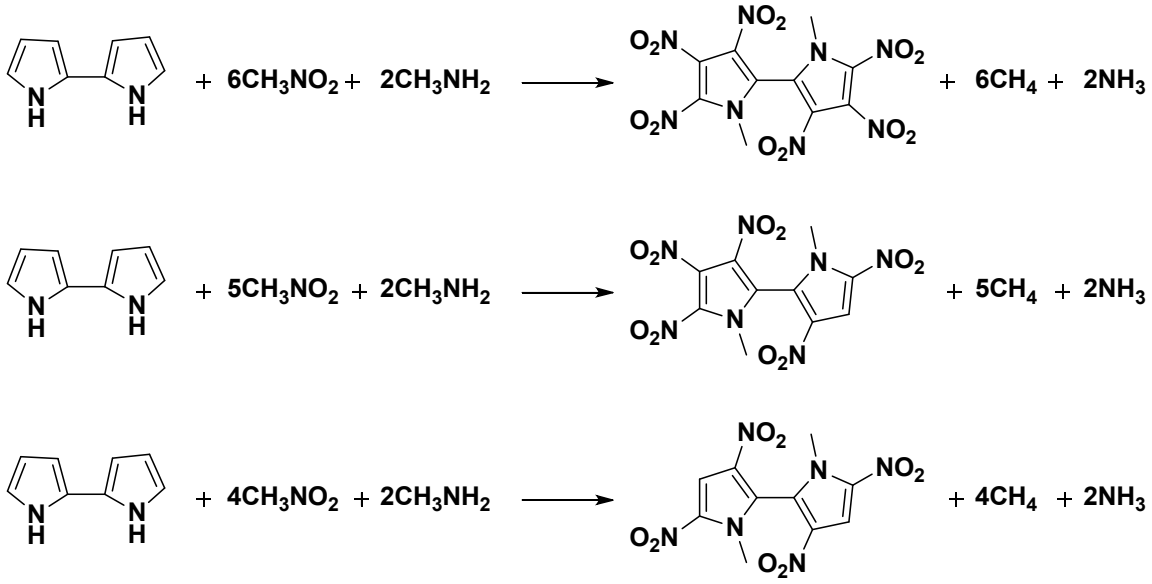


Scheme S1: Detailed stepwise synthesis of **HNDMBP** via compounds **2 & 3**.

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 compound were calculated with the EXPLO5 (v6.03) by using crystal densities.[S3]

Isodesmic reaction



Scheme S2: Isodesmic reactions for compound **HNDMBP.**

Table S1: Heat of formation of compounds **6, 7, HNDMBP.**

Comp	ZPE	H_{corr}	Scaled ZPE	ΔH_T	Mp-6-311++G**	Corrected	ΔH_r	ΔH_r (kJ/mol)	ΔH_f (kJ/mol)
compound-6	0.212039	0.234165	0.203557	0.022126	-1312.839666	-1312.613982	0.05449486	143.0762412	118.7172588
compound-7	0.200014	0.225243	0.19201344	0.025229	-1516.918032	-1516.70079	0.04877378	128.0555471	133.7379529
HNDMBP	0.216037	0.243785	0.20739552	0.027748	-1721.009917	-1720.774774	0.03022922	79.3668094	183.0266905

Table S2: Physicochemical and energetic properties of compounds **6** and **7**

Compound. No	[a]ρ g cm^{-3}	[b]D_v m s^{-1}	[c]P GPa	[d]ΔH_f kJmol^{-1}	[e]OB %
6	1.63	7.04	20.67	118	-75.29
7	1.73	7.62	25.11	133	-56.10
TNT	1.65	7.30	21.3	-59.4	-74

[a] crystal density, [b] Detonation velocity, [c] Detonation pressure (calculated with Explo5 version 6.02), [d] Heat of formation (By Isodesmic reactions), [e] Oxygen balance (%).

Activation energy:

Table S3. Non-isothermal reaction kinetics parameters of **HNDMBP** using Kissinger's method.

B[a] (° C min^{-1})	T_m [b] (° C)	T_m (K)	$1/T_m$ (K^{-1})	$-\ln(\beta/T_m^2)$	R^2 [c] (R_K)	E_a [d] (kJ mol^{-1})	$\ln A_K$[e]
5	295	568.15	0.001760	11.0753			
10	299	572.15	0.001748	10.3962	**0.939**	**278.7**	**48.06**
15	303	576.15	0.001736	10.0047			
20	308	581.15	0.001721	9.7343			

[a] Heating rate; [b] decomposition temperature (peak); [c] linear correlation coefficient; [d] activation energy; [e] pre-exponential constant.

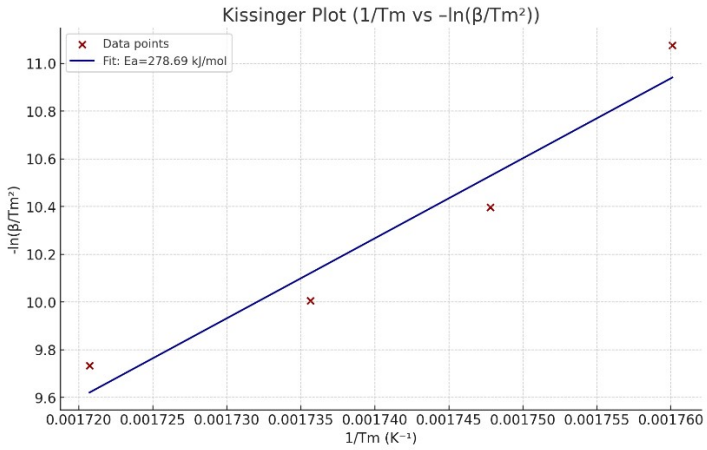


Figure S1. A plot of $1/T_m$ vs -ln (β/T_m^2) (Kissinger method) for **HNDMBP**.

Table S4. Non-isothermal reaction kinetics parameters of **HNDMBP** using Ozawa Doyle's method.

B[a] (° C min^{-1})	**Tm [b]** (° C)	**T_m** (K)	**$1/T_m$** (K^{-1})	**ln(β)**	**R_0 [c]** (R_k)	**E_0 [d]** (kJ mol^{-1})
5	295	568.15	0.001760	1.609		
10	299	572.15	0.001748	2.303	**0.943**	**274.0**
15	303	576.15	0.001736	2.708		
20	308	581.15	0.001721	2.996		

[a] Heating rate; [b] decomposition temperature (peak); [c] linear correlation coefficient; [d] activation energy.

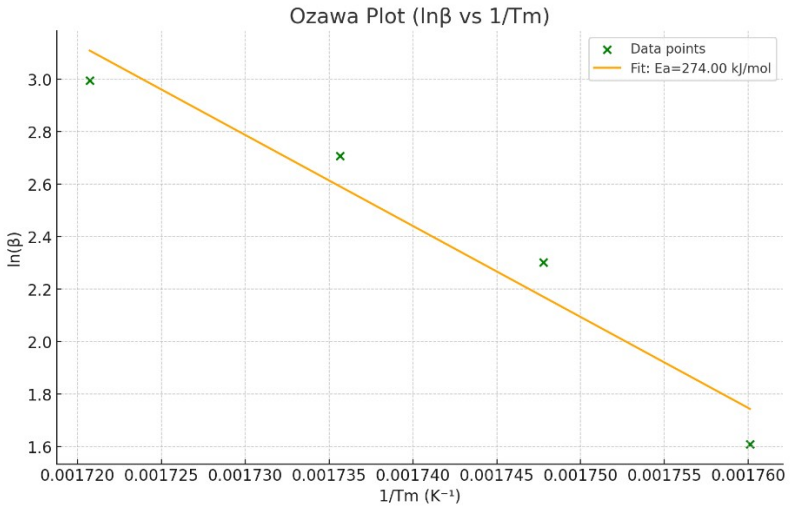


Figure S2. A plot of $1/T_m$ vs – ln(β) (Ozawa Doyle's method) for **HNDMBP**.

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

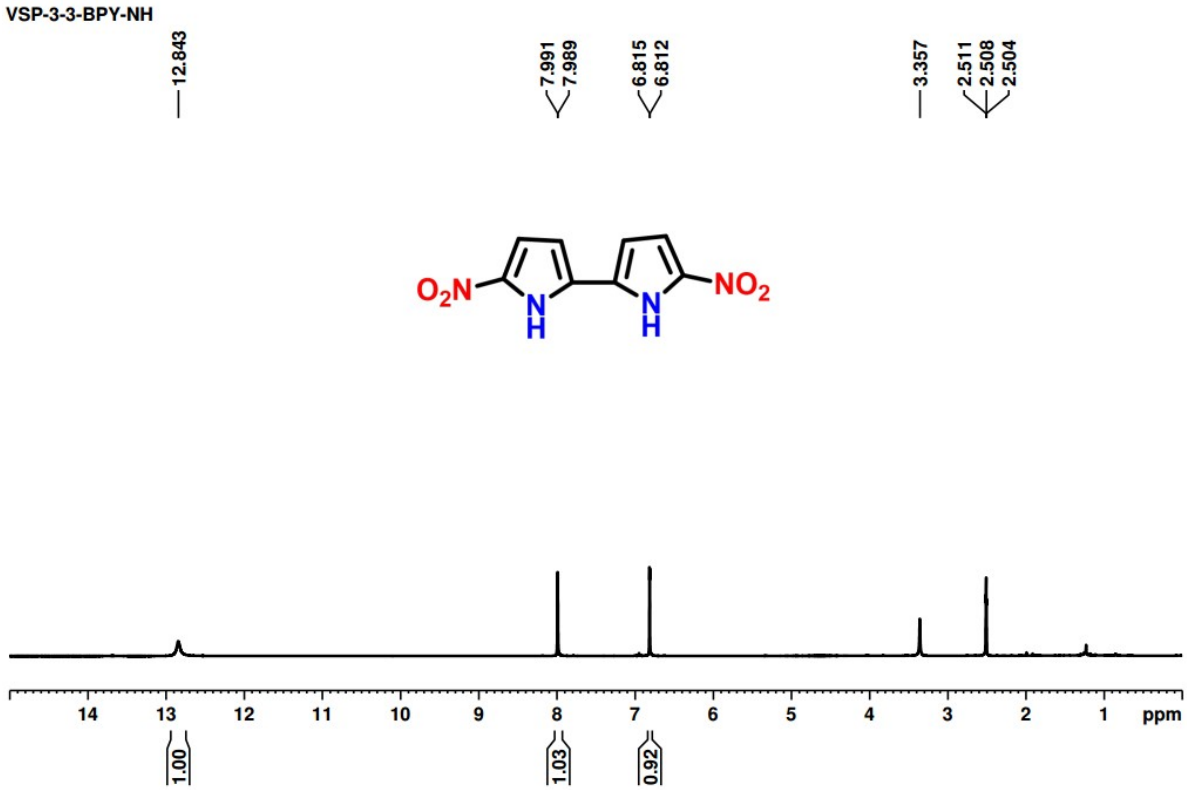


Figure S3: ^{1}H NMR spectrum of compound **2** in dimethyl sulfoxide-d_6.

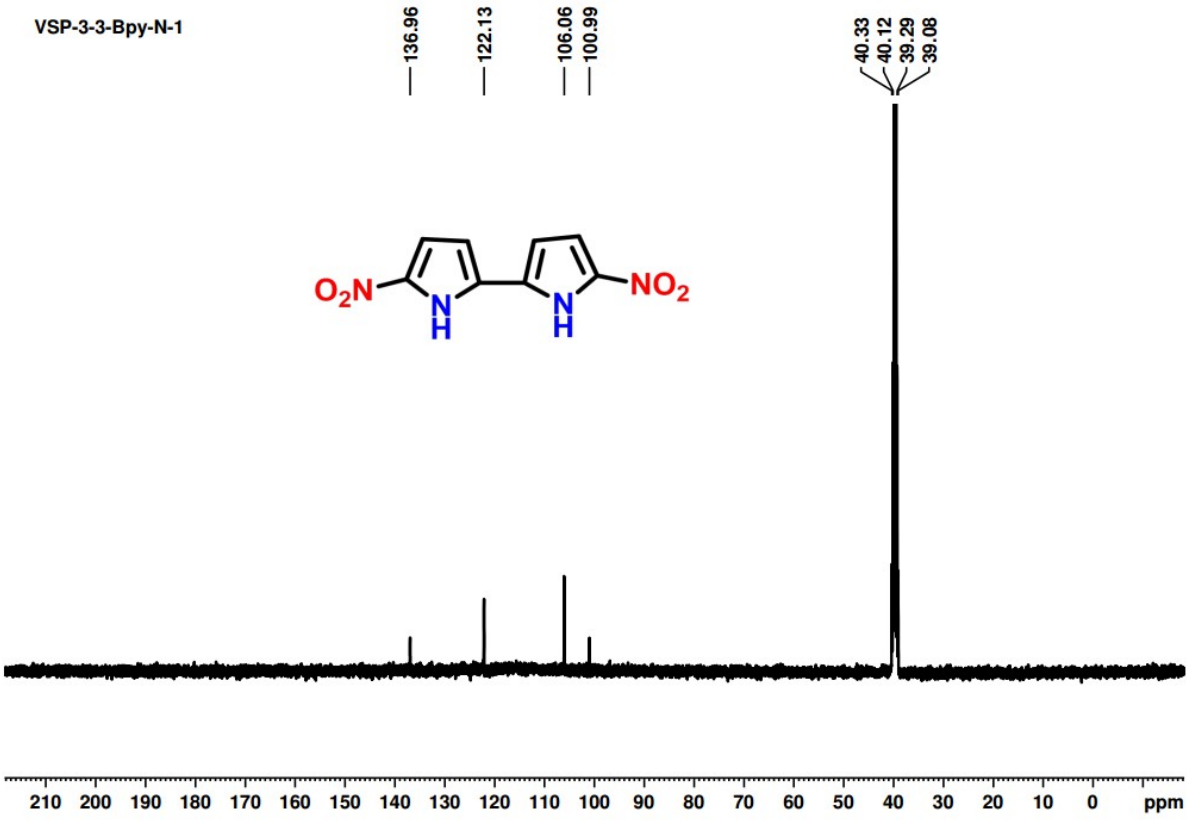


Figure S4: ^{13}C NMR spectrum of compound **2** in dimethyl sulfoxide-d_6.

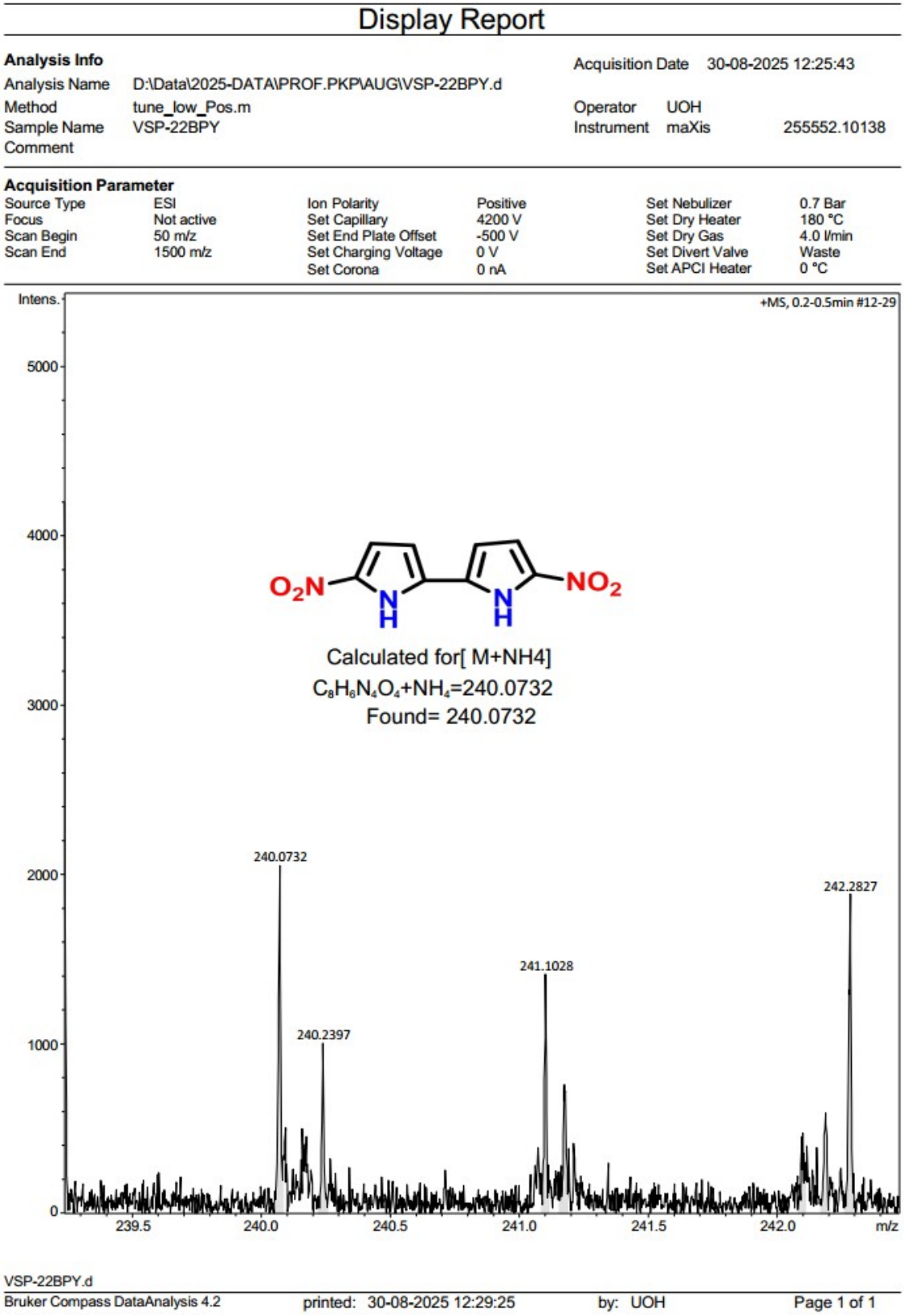


Figure S5: HRMS spectrum of compound **2**.

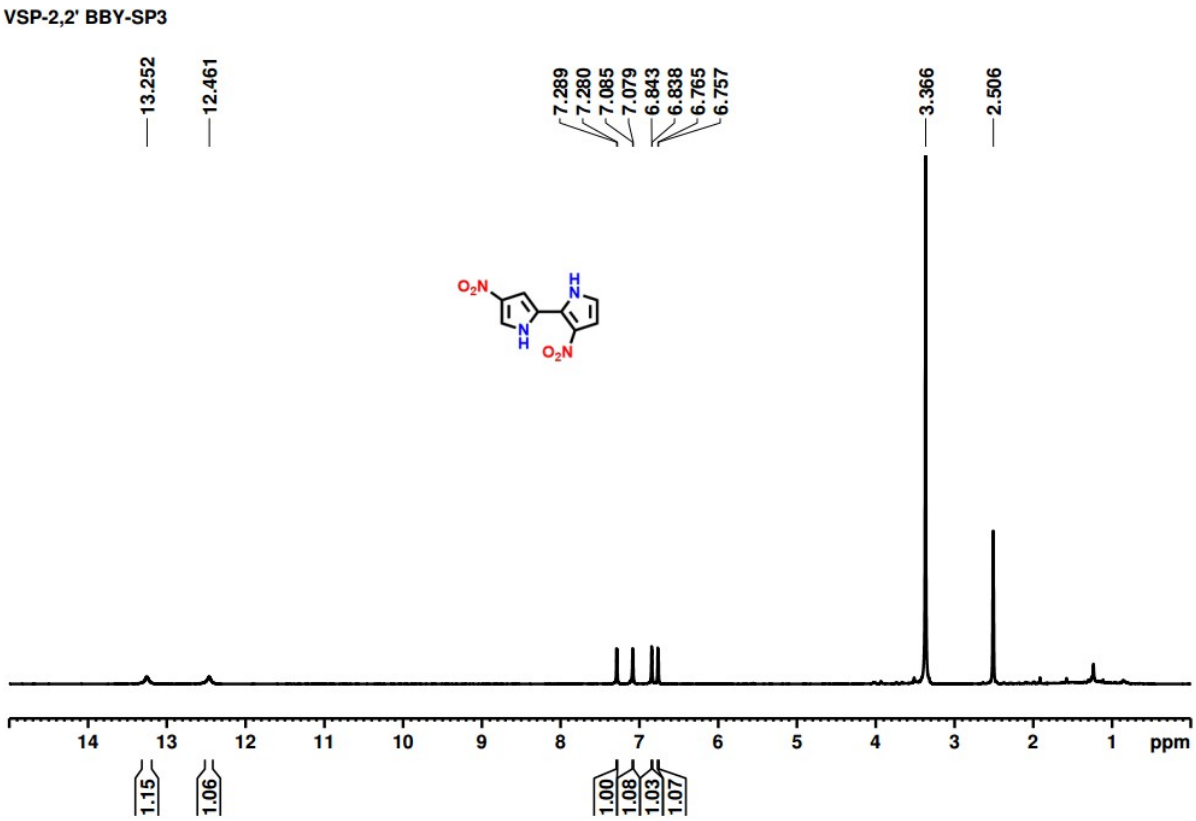


Figure S6: ^{1}H NMR spectrum of compound **3** in dimethyl sulfoxide-d_6.

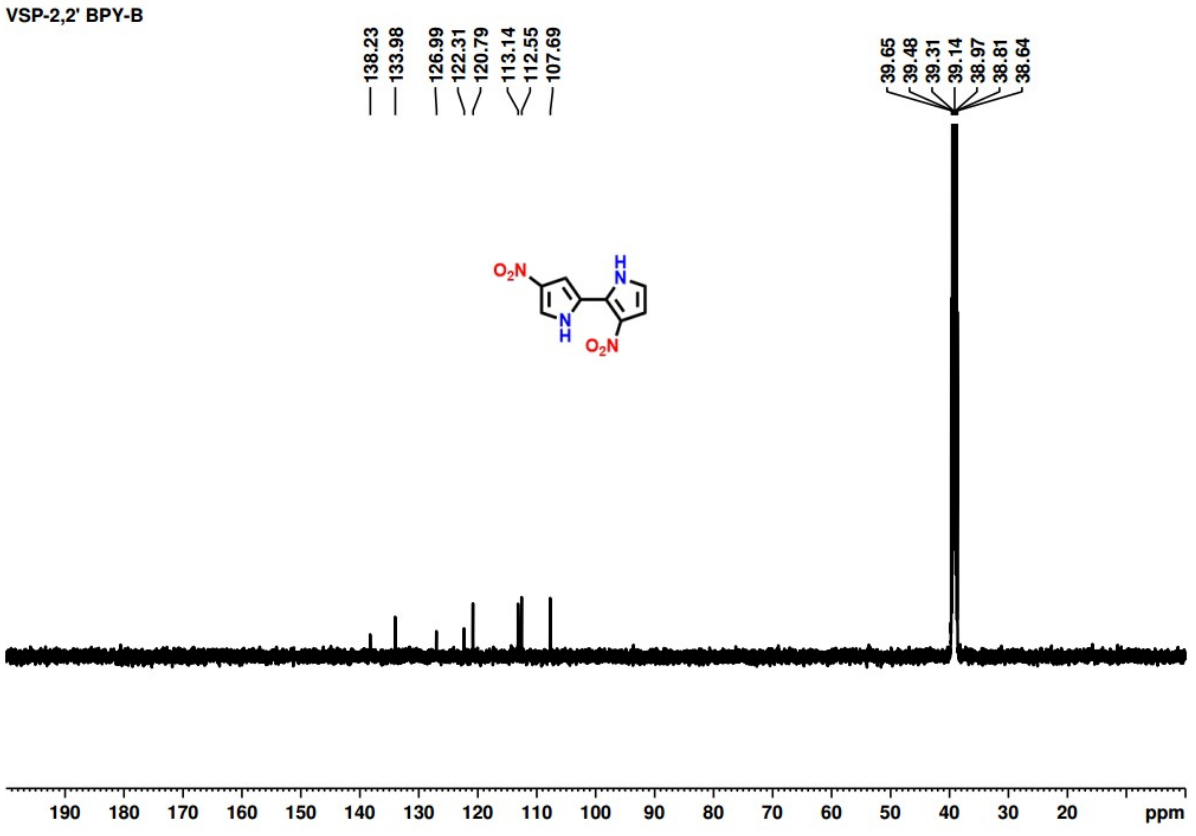


Figure S7: ^{13}C NMR spectrum of compound **3** in dimethyl sulfoxide-d_6.

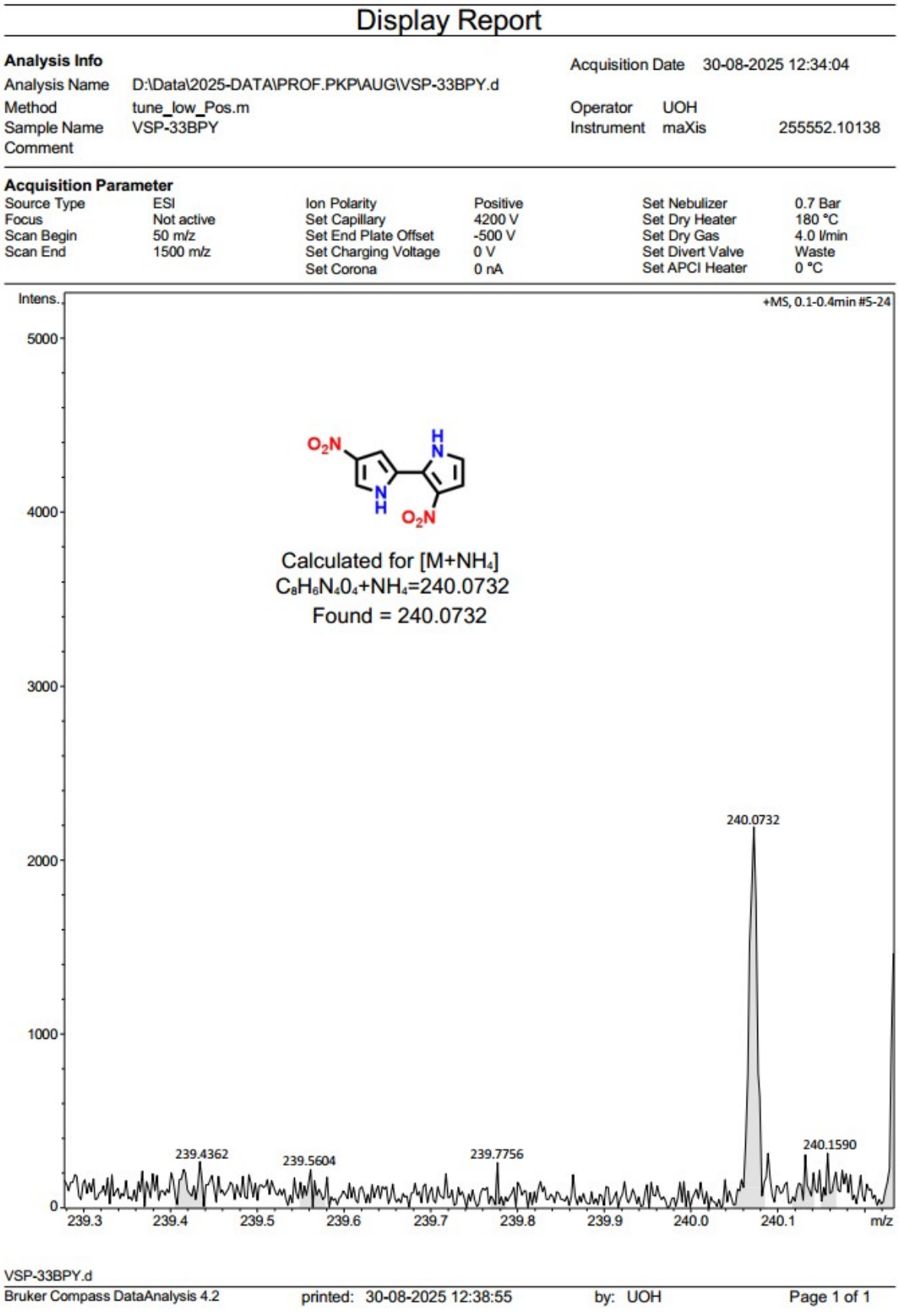


Figure S8: HRMS spectrum of compound **3**.

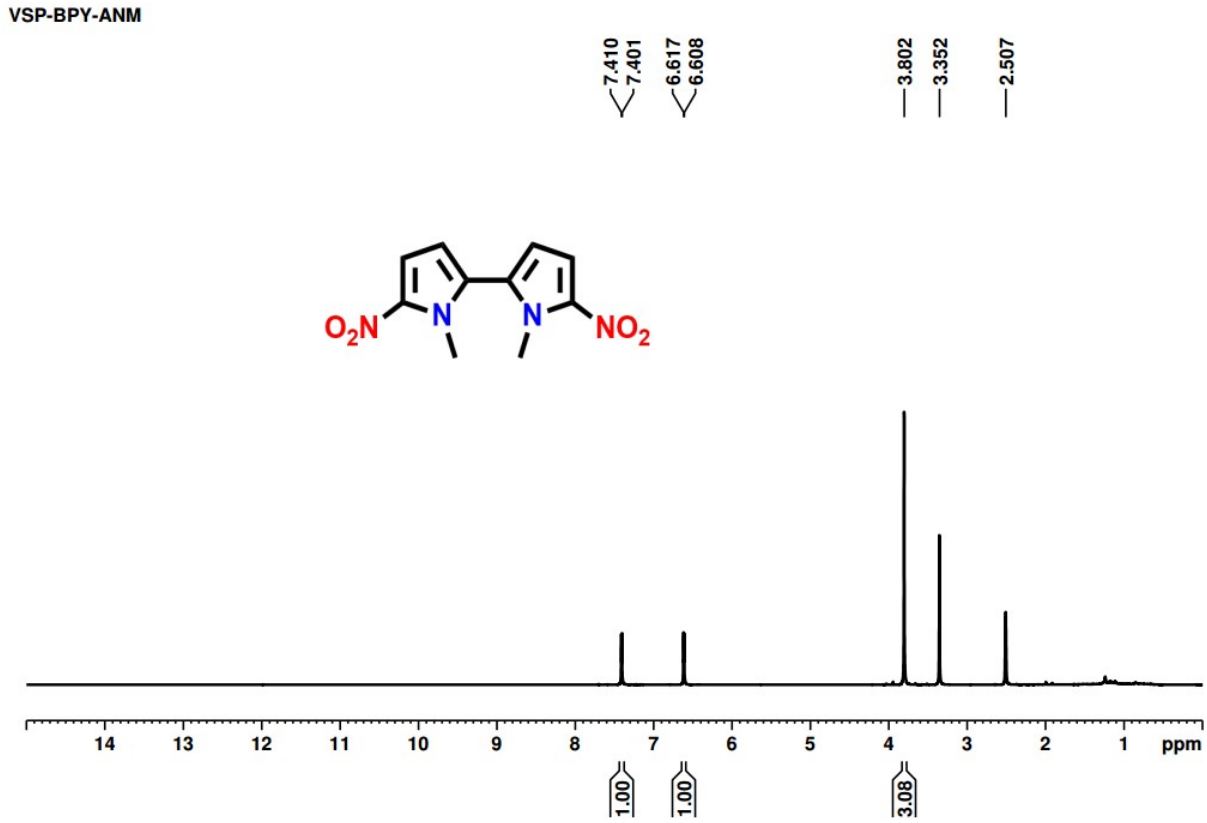


Figure S9: [1]H NMR spectrum of compound **4** in dimethyl sulfoxide-d_6.

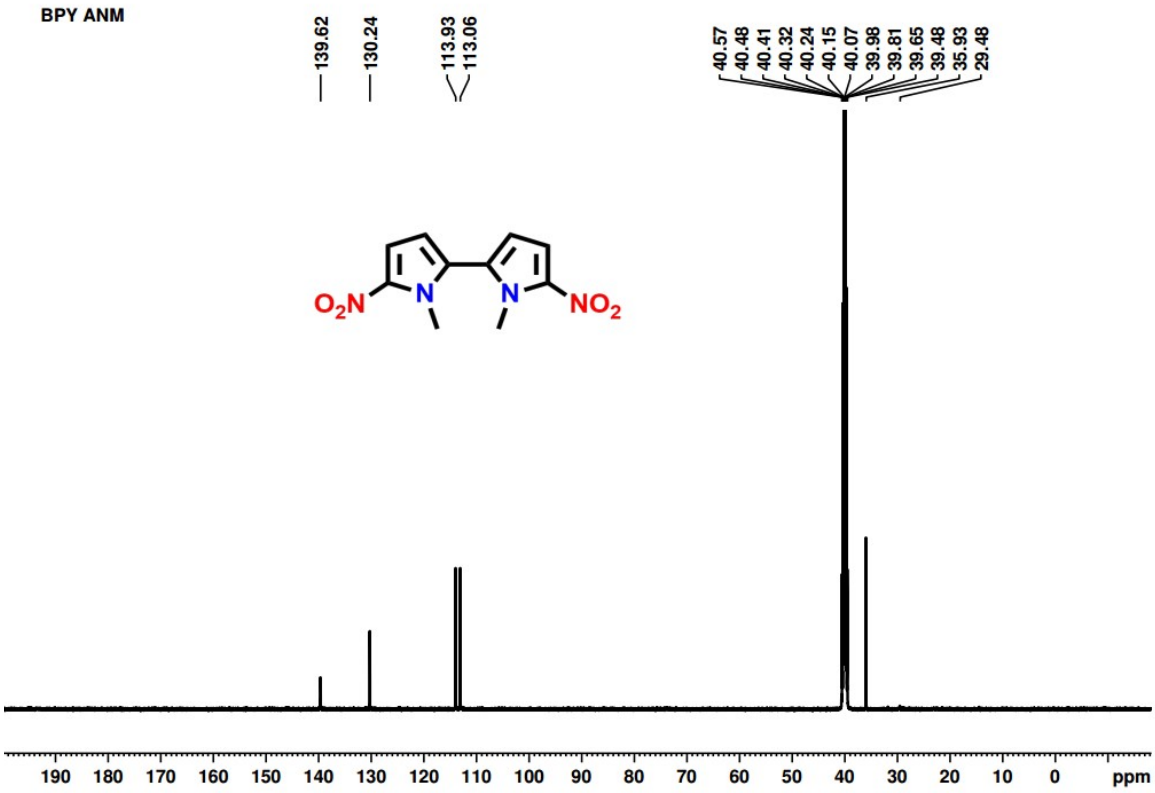


Figure S10: [13]C NMR spectrum of compound **4** in dimethyl sulfoxide-d_6.

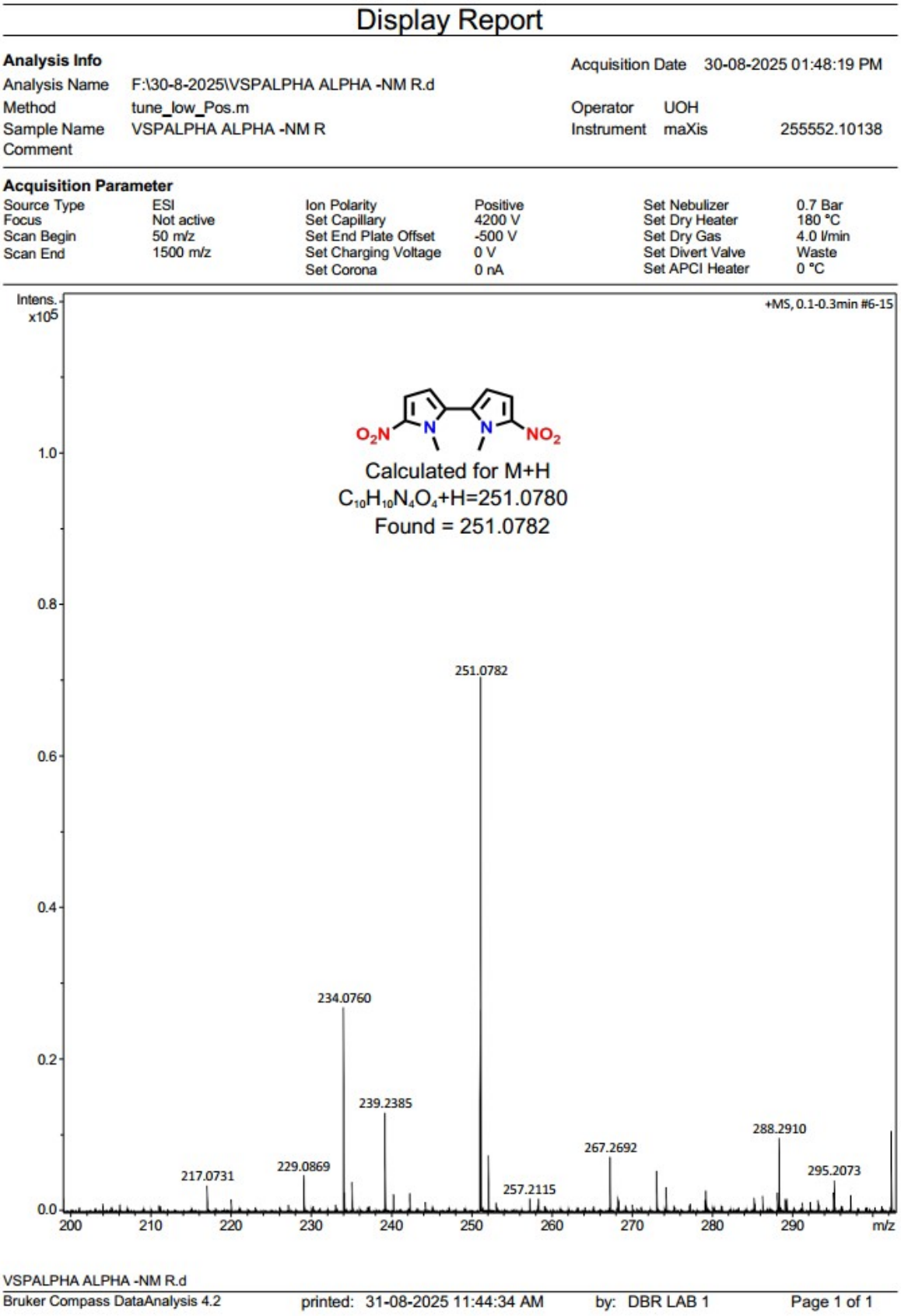


Figure S11: HRMS spectrum of compound **4**.

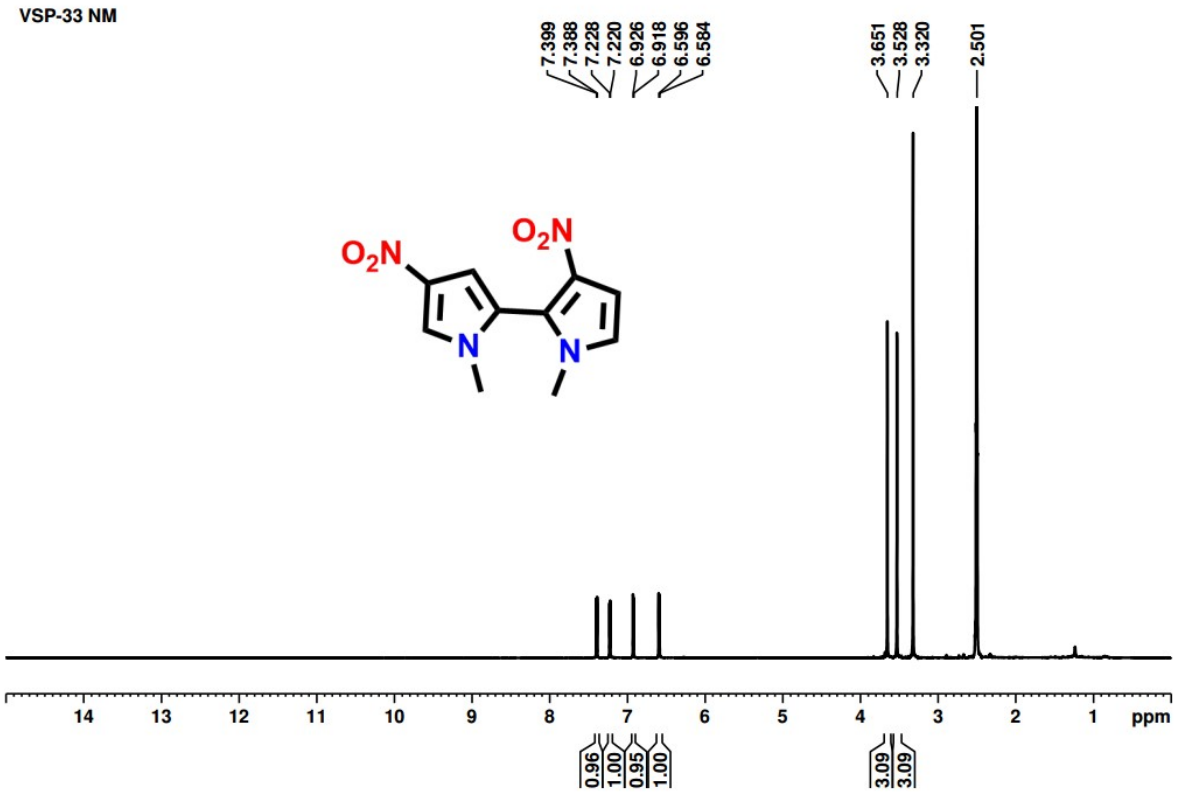


Figure S12: [1]H NMR spectrum of compound **5** in dimethyl sulfoxide-d_6.

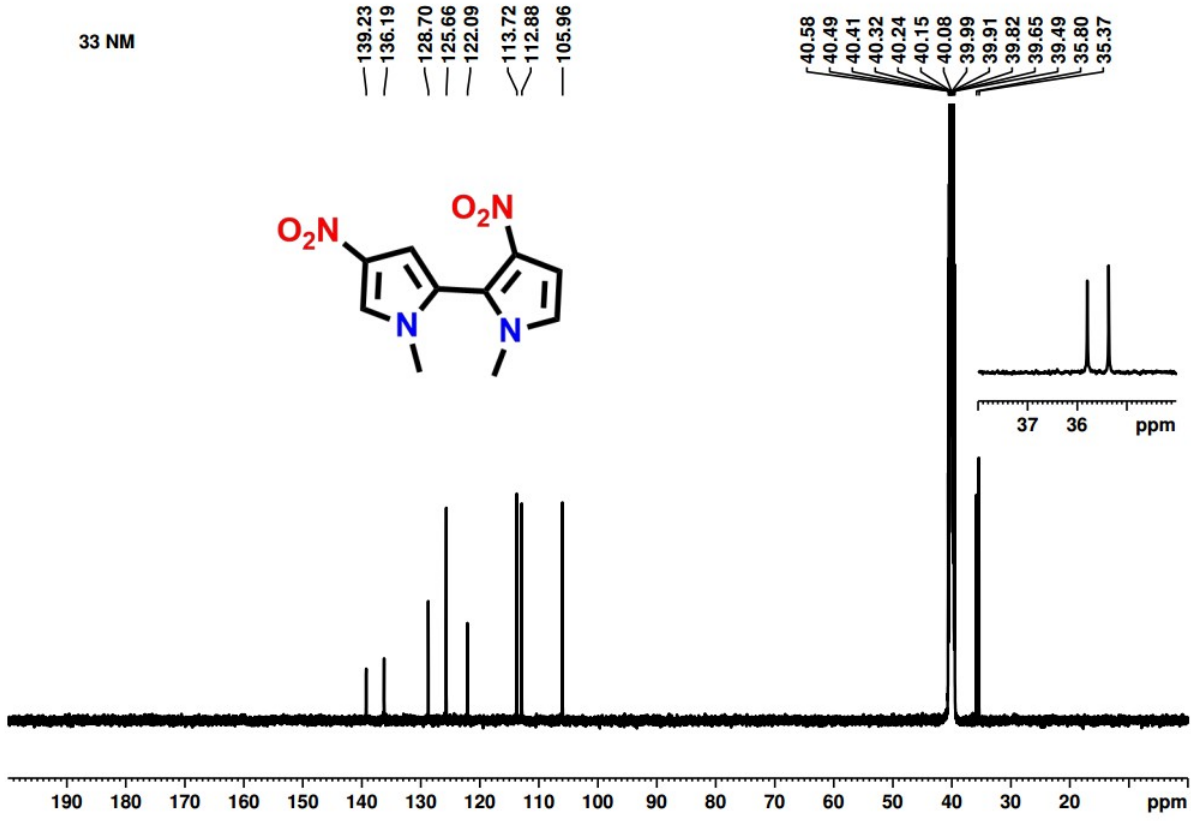


Figure S13: [13]C NMR spectrum of compound **5** in dimethyl sulfoxide-d_6.

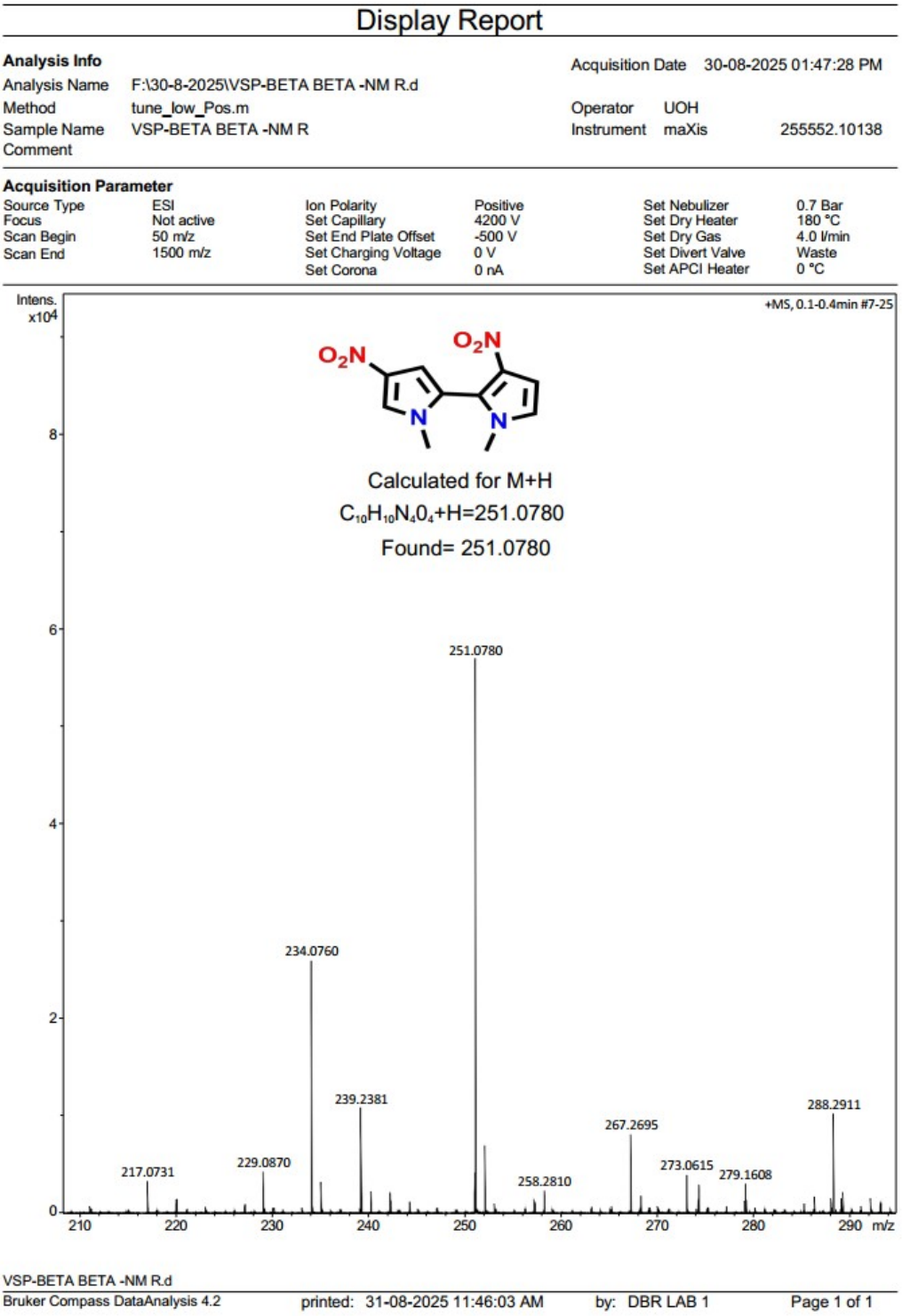


Figure S14: HRMS spectrum of compound **5**.

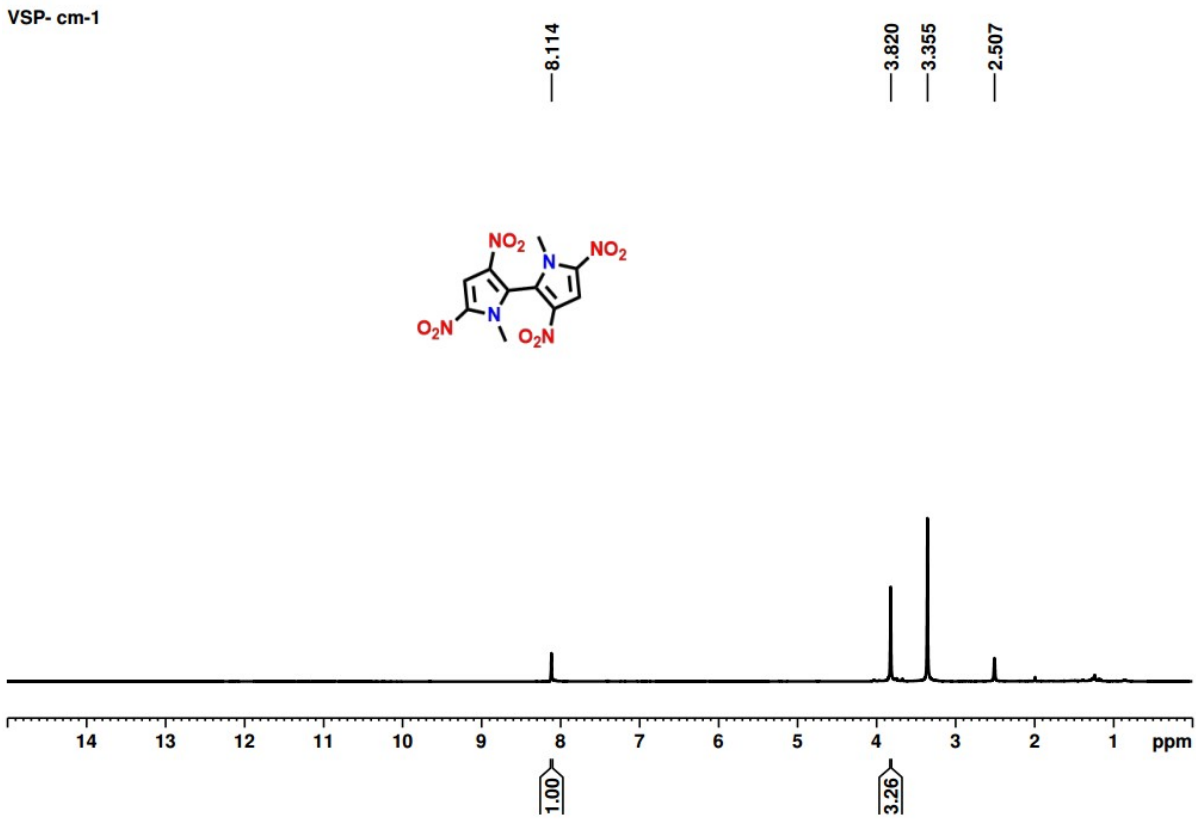


Figure S15: ^{1}H NMR spectrum of compound **6** in dimethyl sulfoxide-d_6.

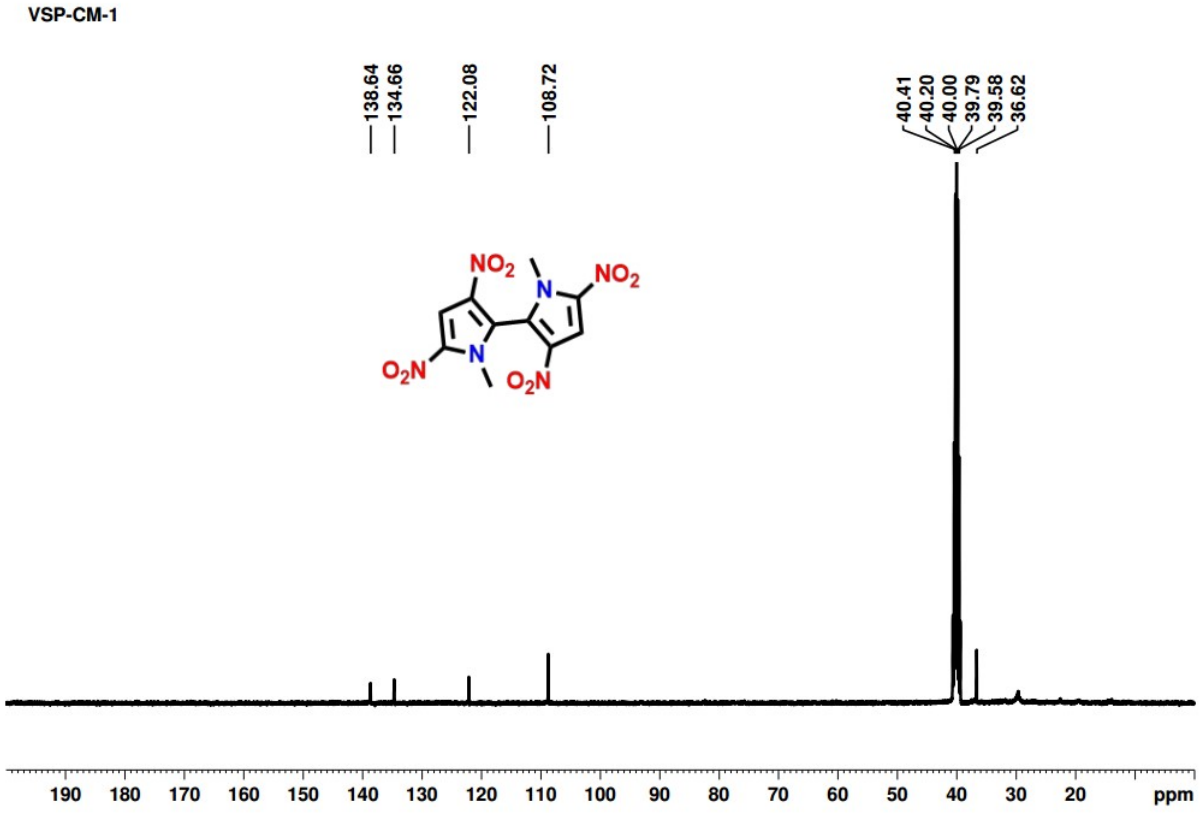


Figure S16: ^{13}C NMR spectrum of compound **6** in dimethyl sulfoxide-d_6.

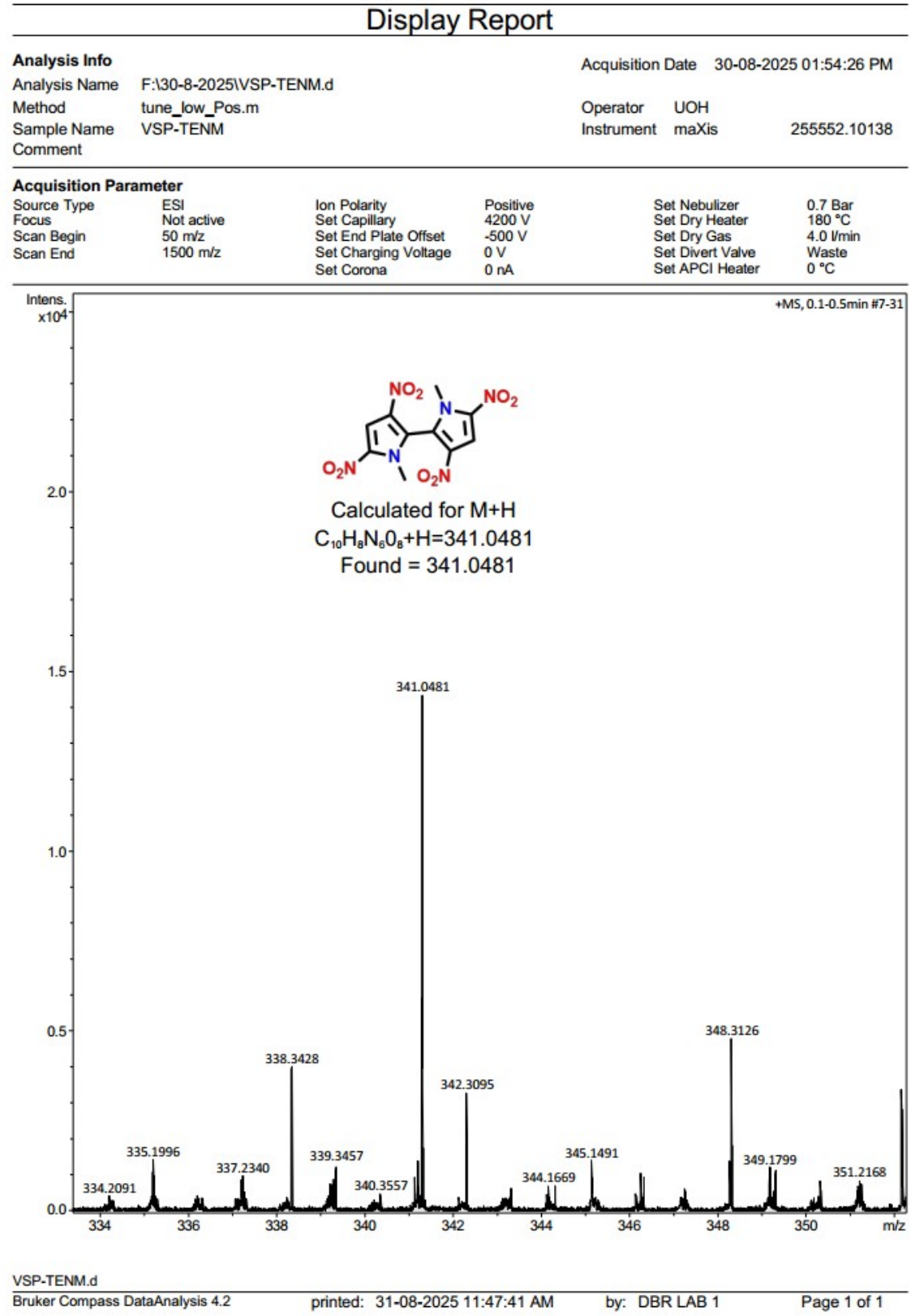


Figure S17: HRMS spectrum of compound **6**.

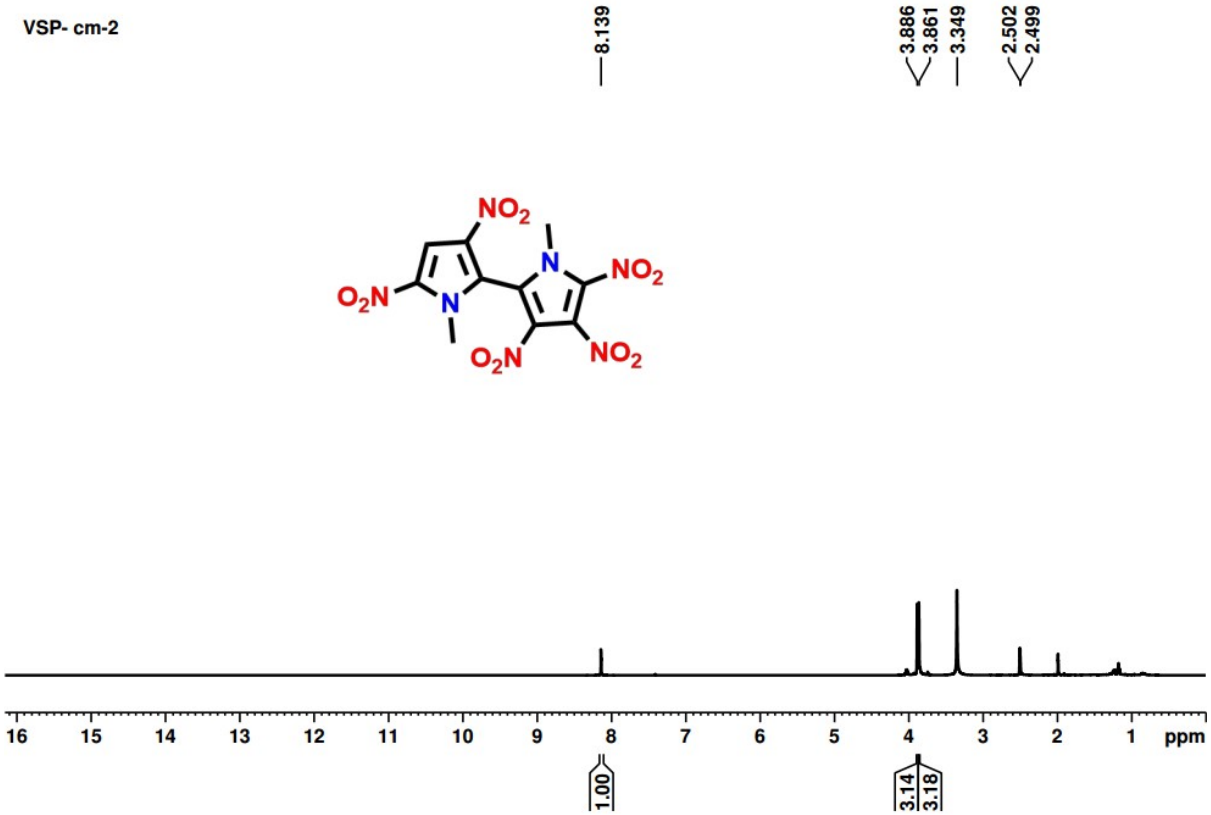


Figure S18: [1]H NMR spectrum of compound **7** in dimethyl sulfoxide-d_6.

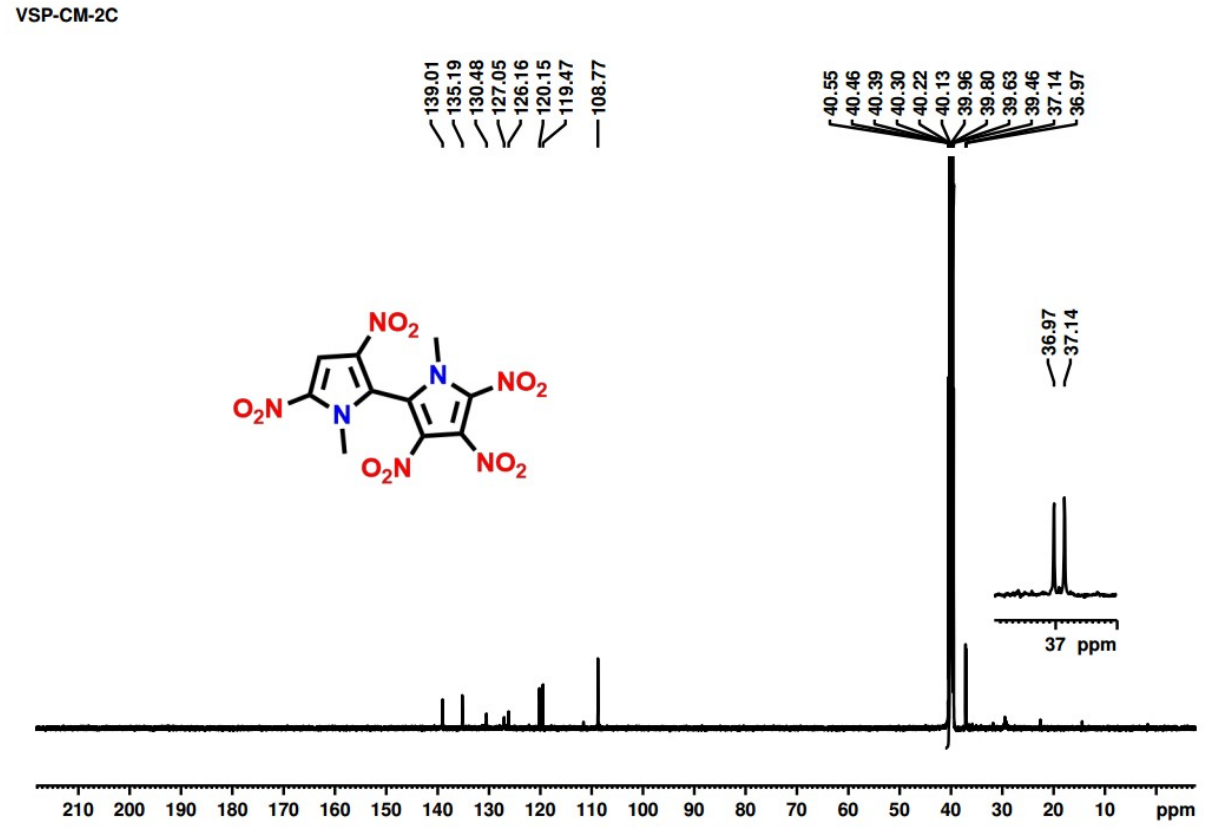


Figure S19: [13]C NMR spectrum of compound **7** in dimethyl sulfoxide-d_6.

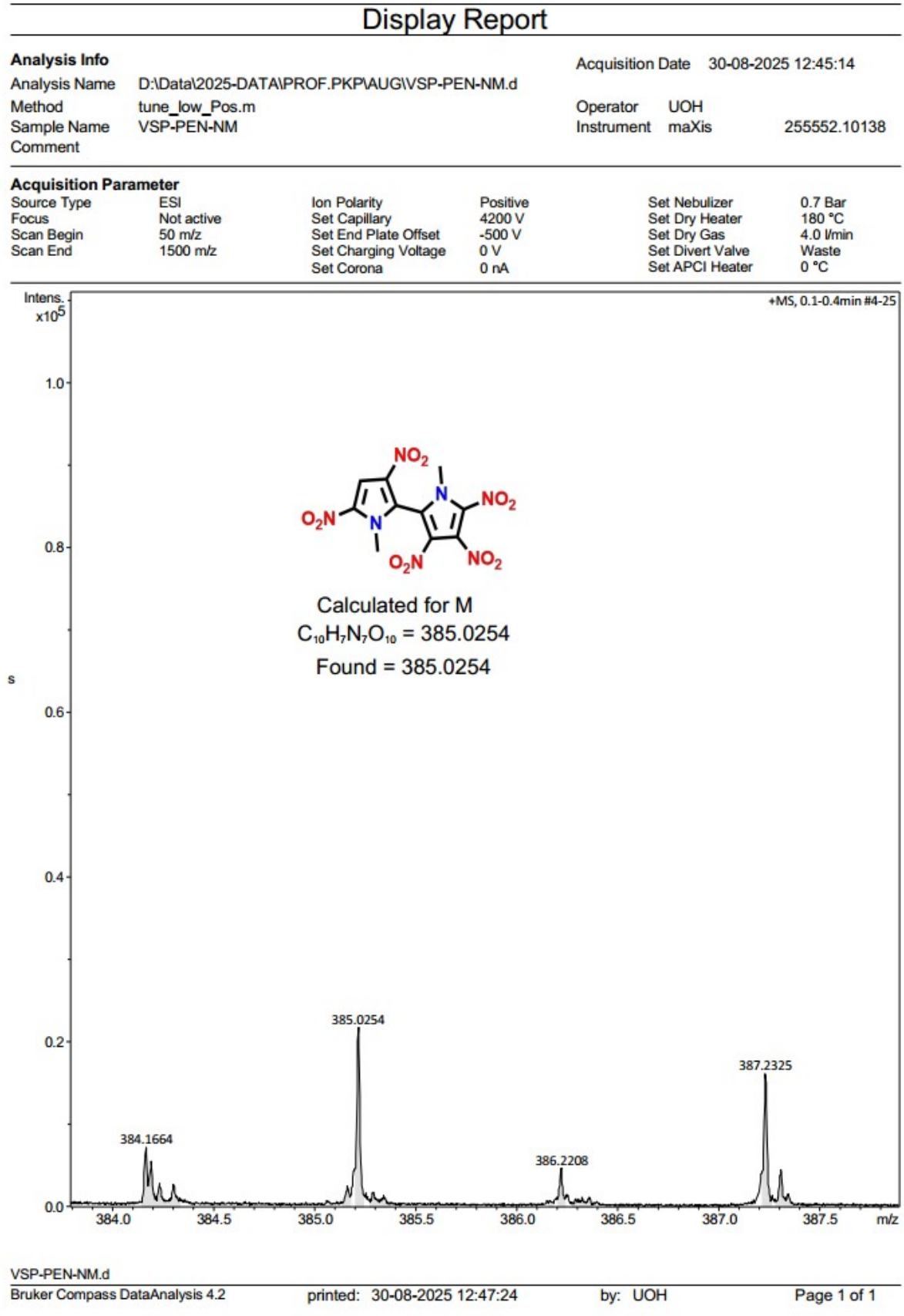


Figure S20: HRMS spectrum of compound **7**.

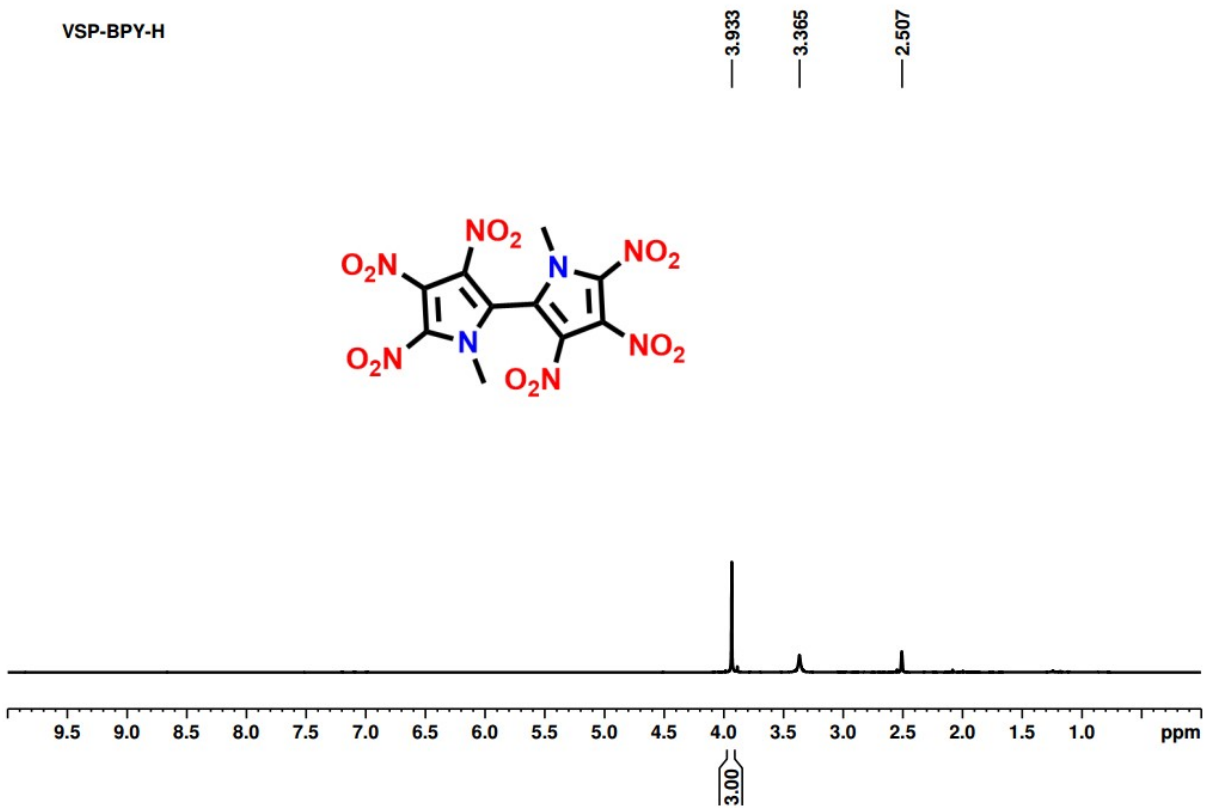


Figure S21: [1]H NMR spectrum of compound **HNDMBP** in dimethyl sulfoxide-d_6.

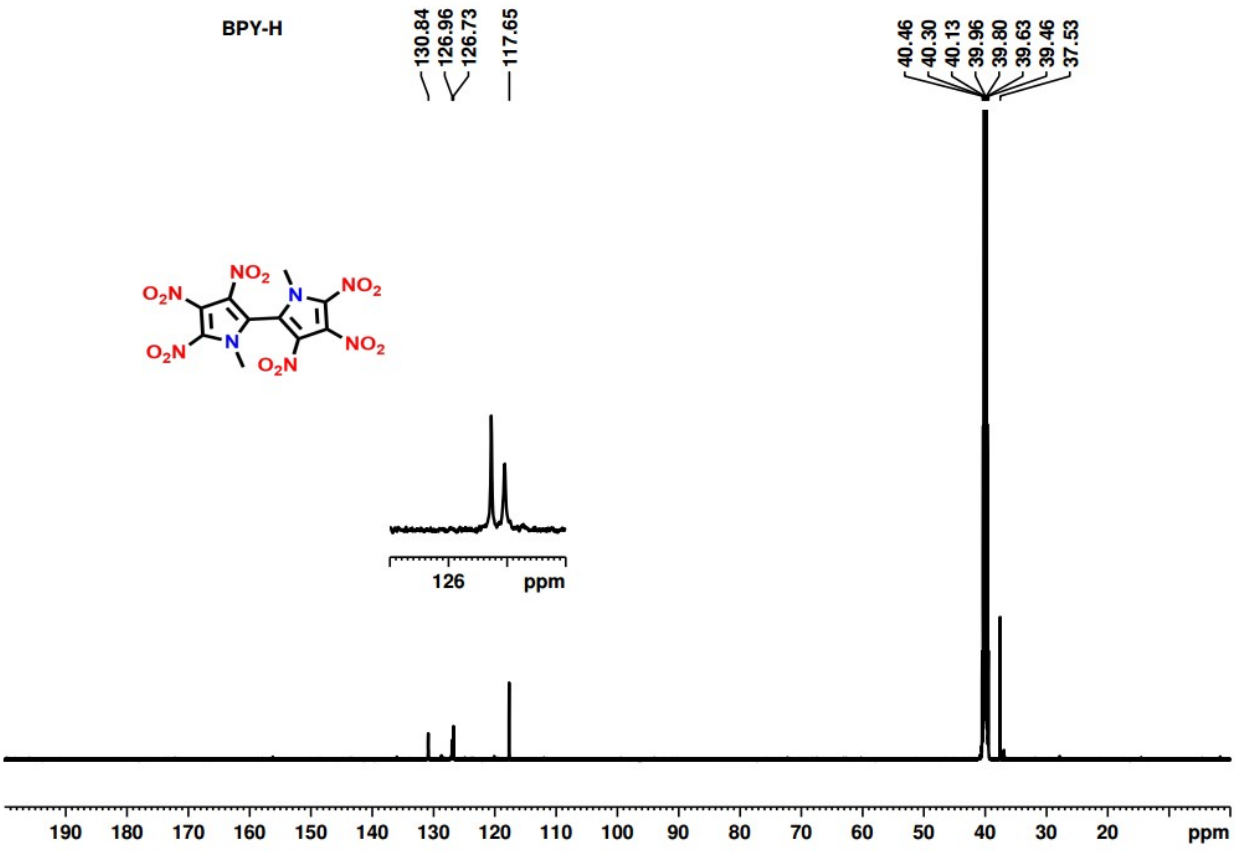


Figure S22: [13]C NMR spectrum of compound **HNDMBP** in dimethyl sulfoxide-d_6.

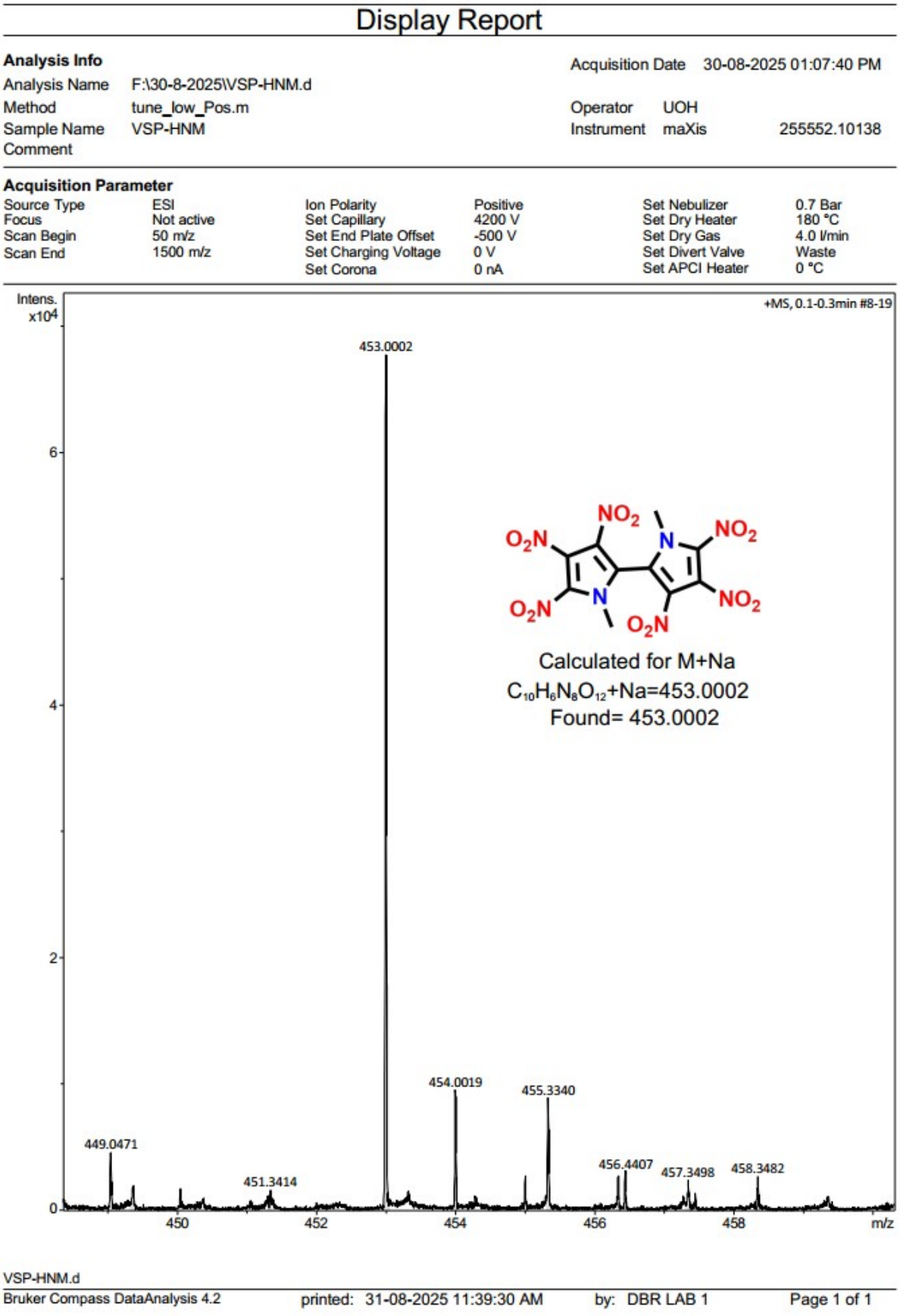


Figure S23: HRMS spectrum of compound **HNDMBP**.

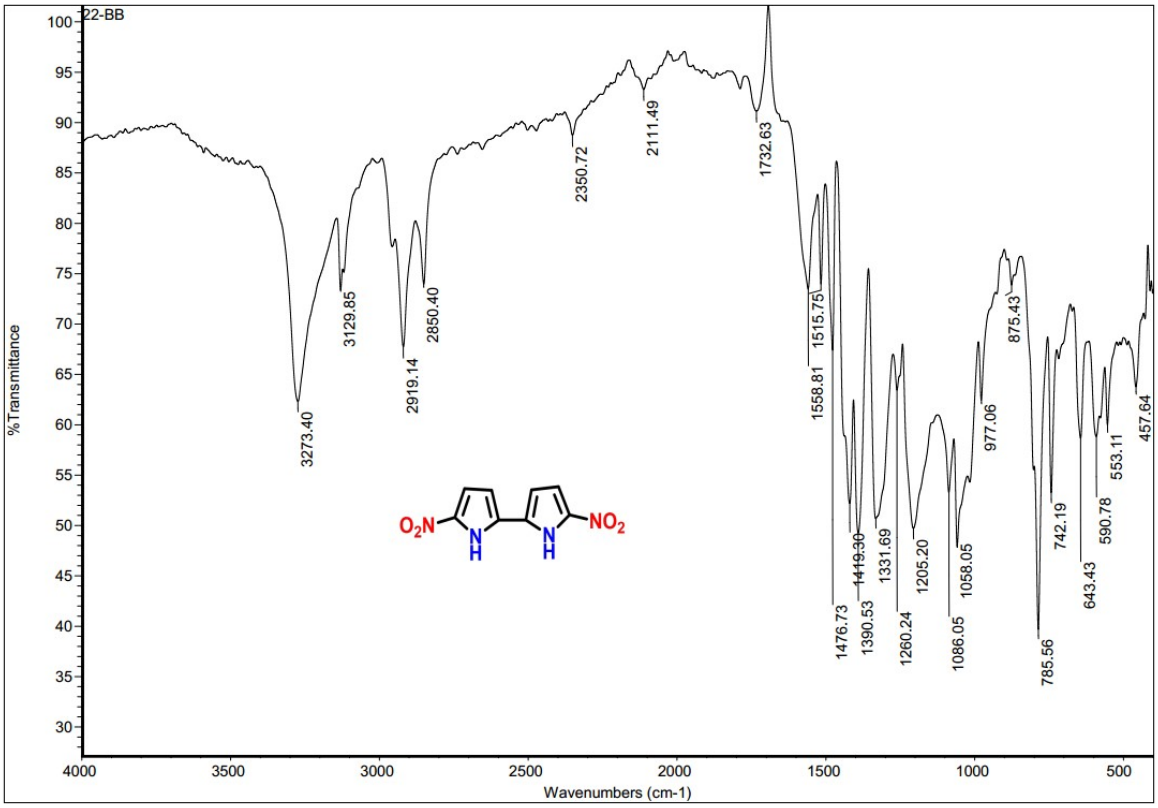


Figure S24: IR spectrum of compound **2**.

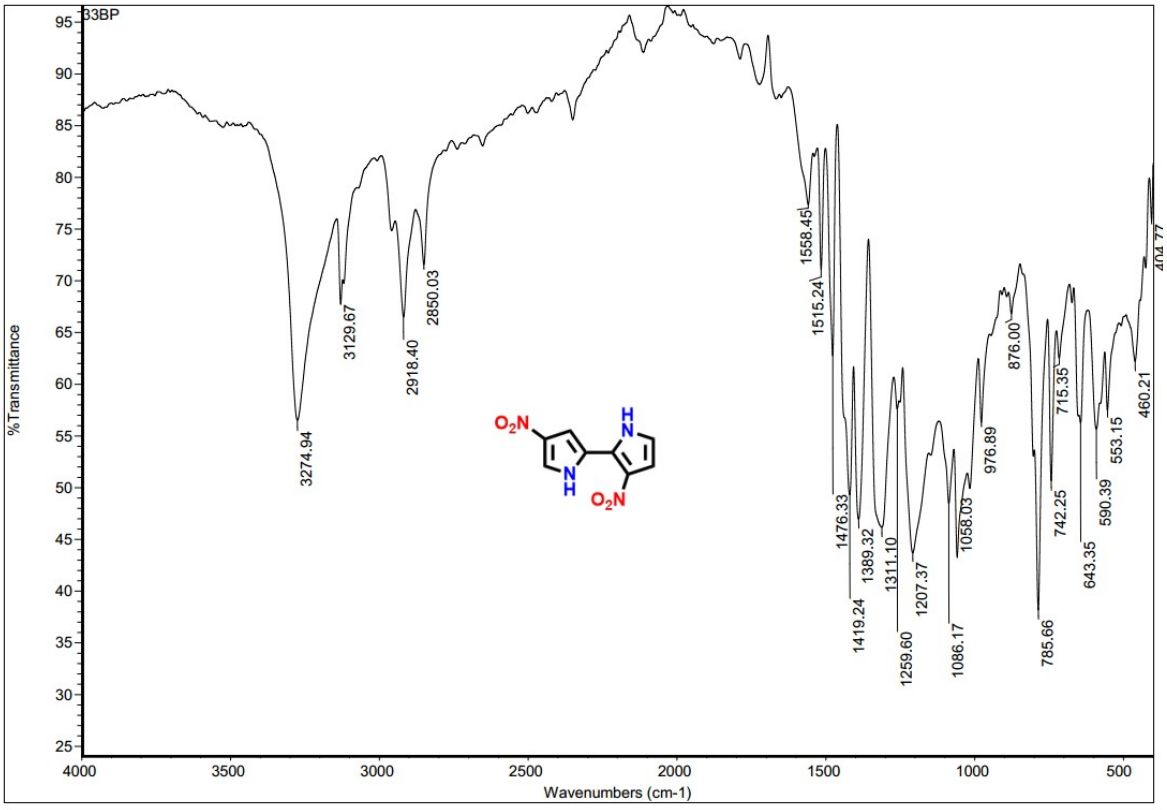


Figure S25: IR spectrum of compound **3**.

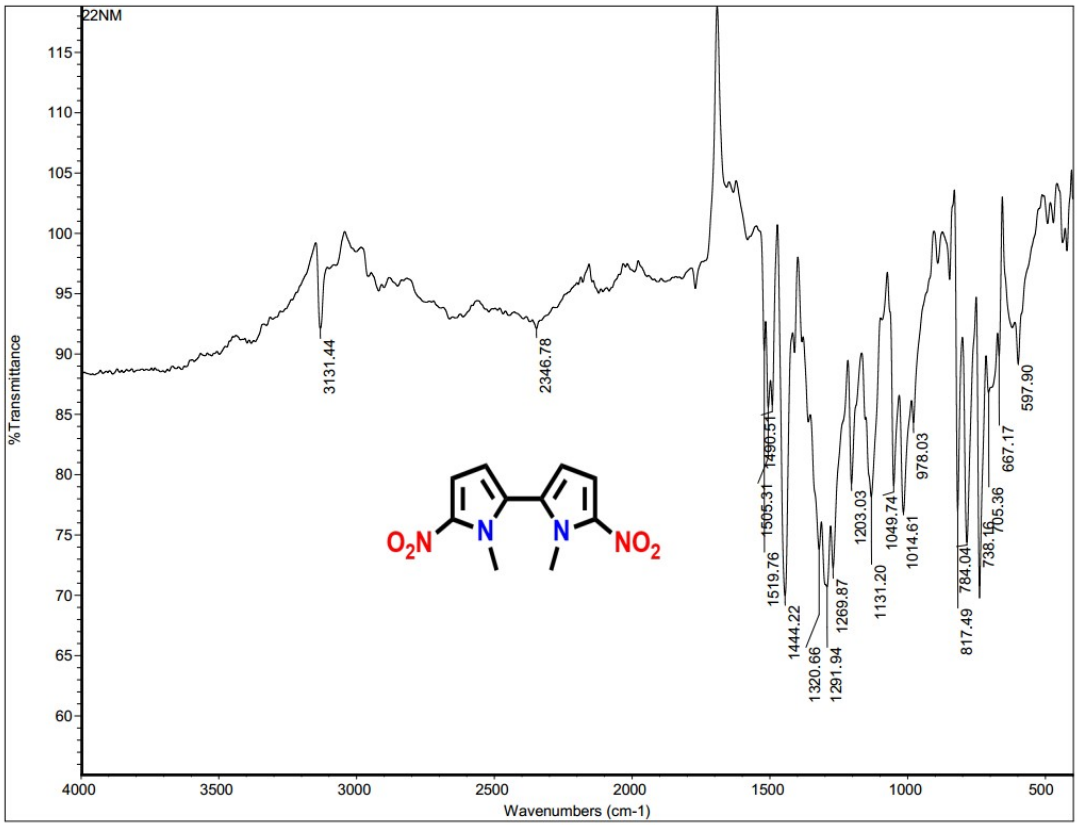


Figure S26: IR spectrum of compound **4**.

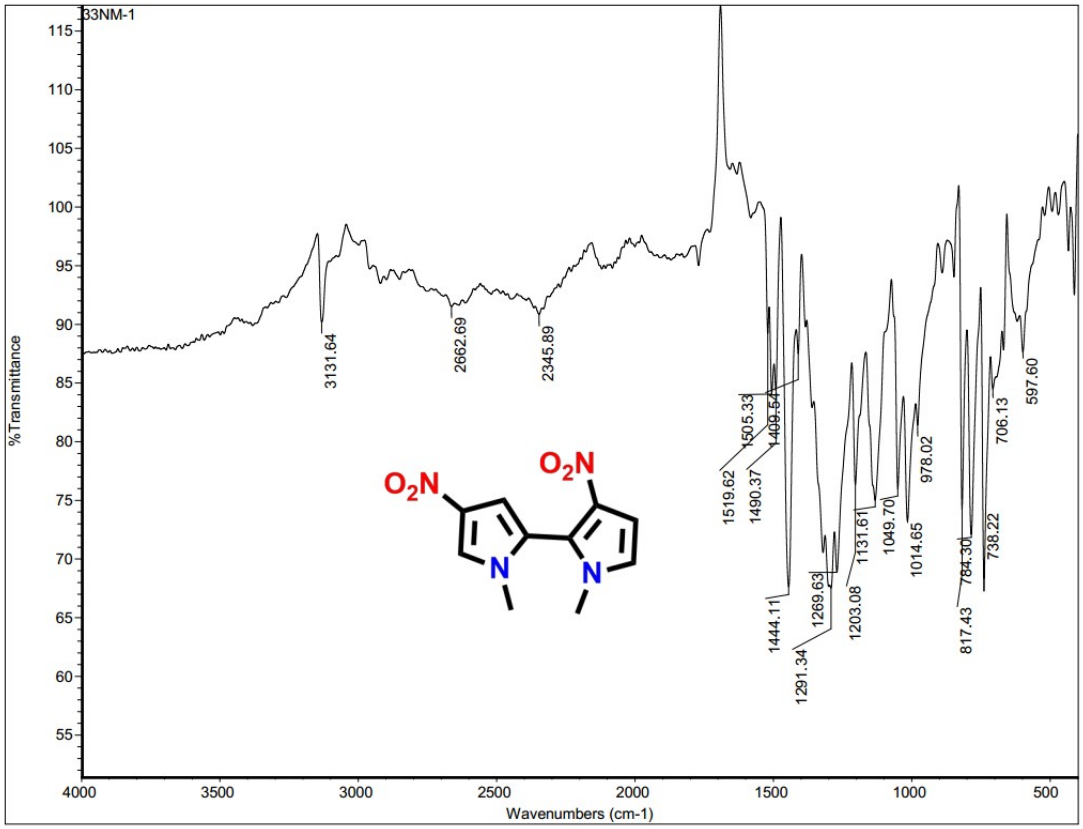


Figure S27: IR spectrum of compound **5**.

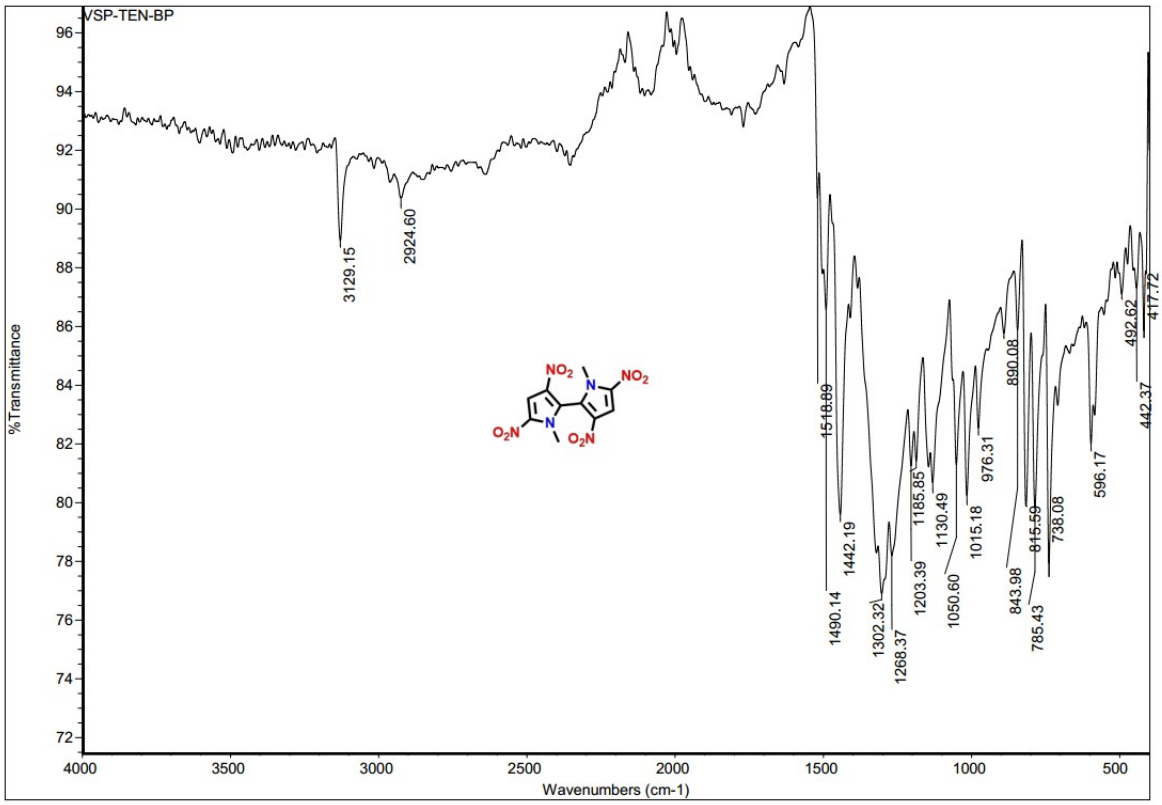


Figure S28: IR spectrum of compound **6**.

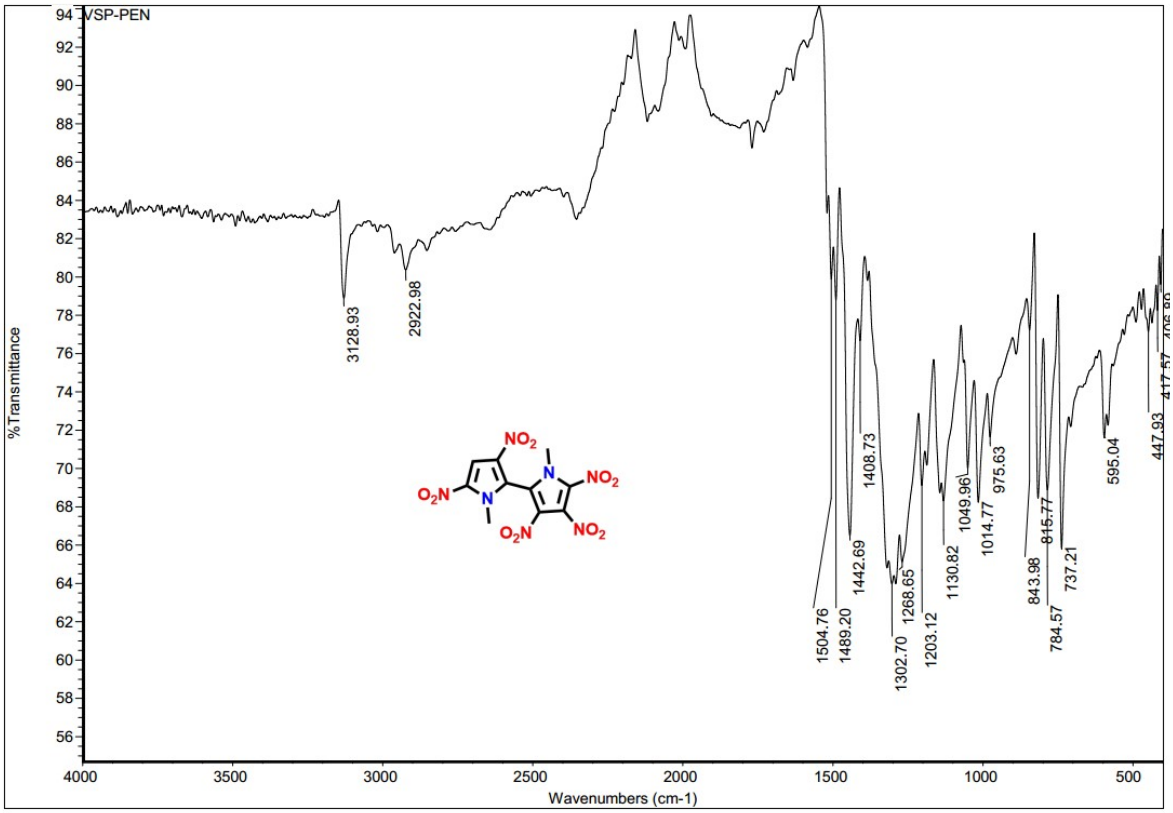


Figure S29: IR spectrum of compound **7**.

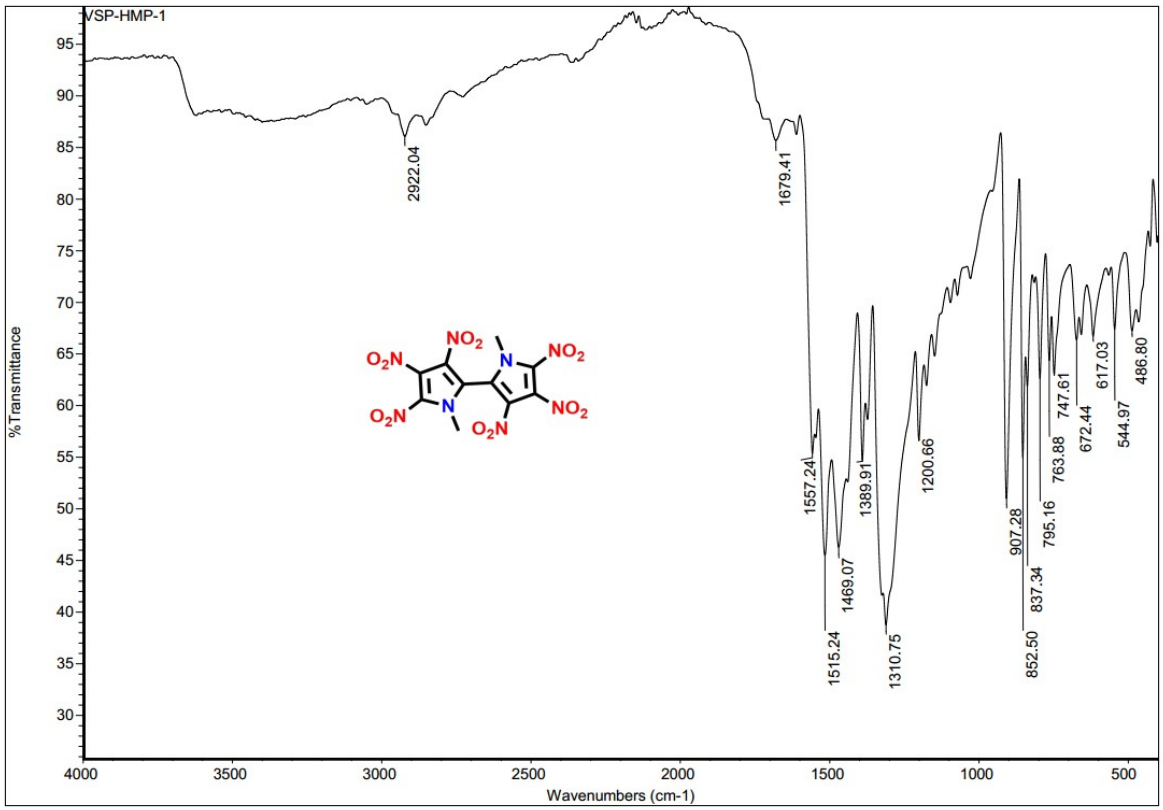


Figure S30: IR spectrum of compound **HNDMBP**.

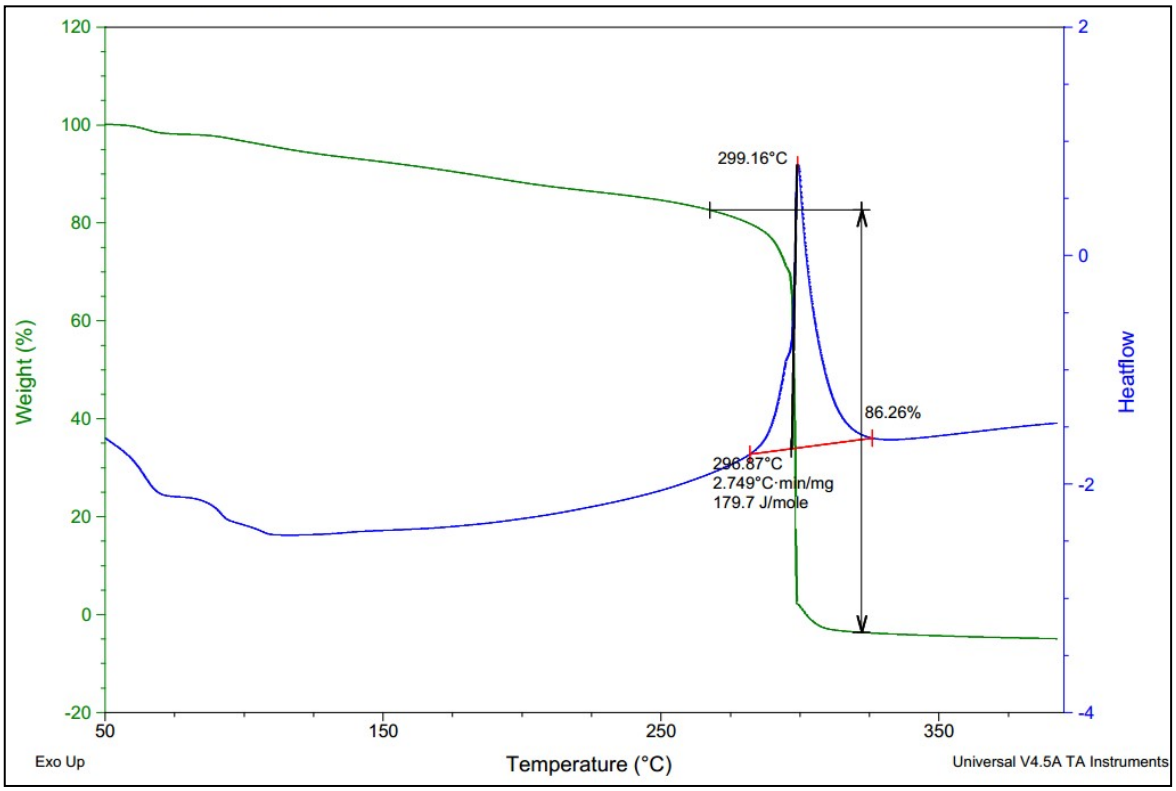


Figure S31: TG - DSC data of compound **HNDMBP**.

Crystal structures:

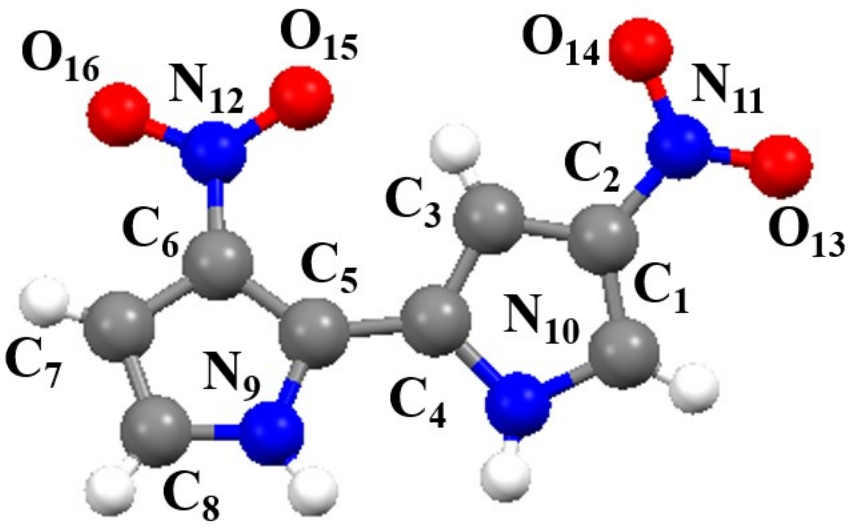


Figure S32: Single-crystal XRD of compound **3**.

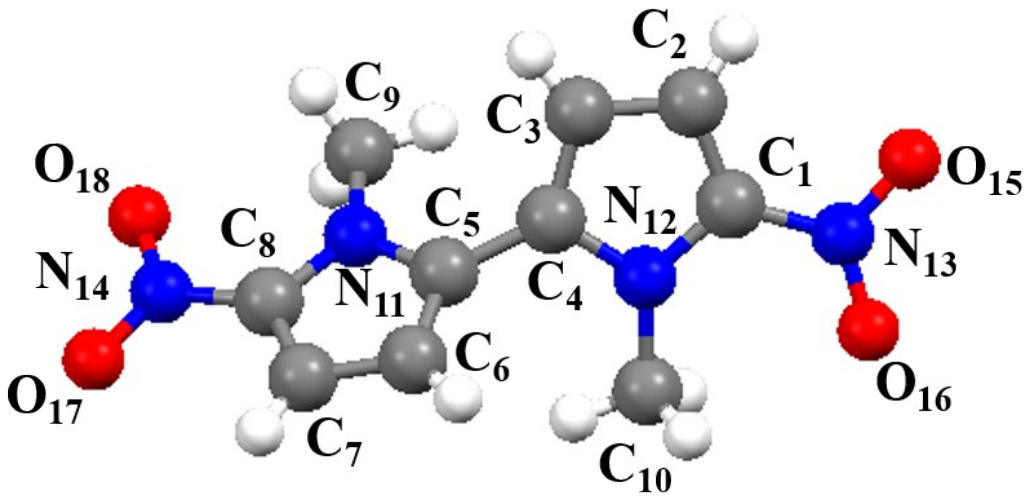


Figure S33: Single-crystal XRD of compound **4**.

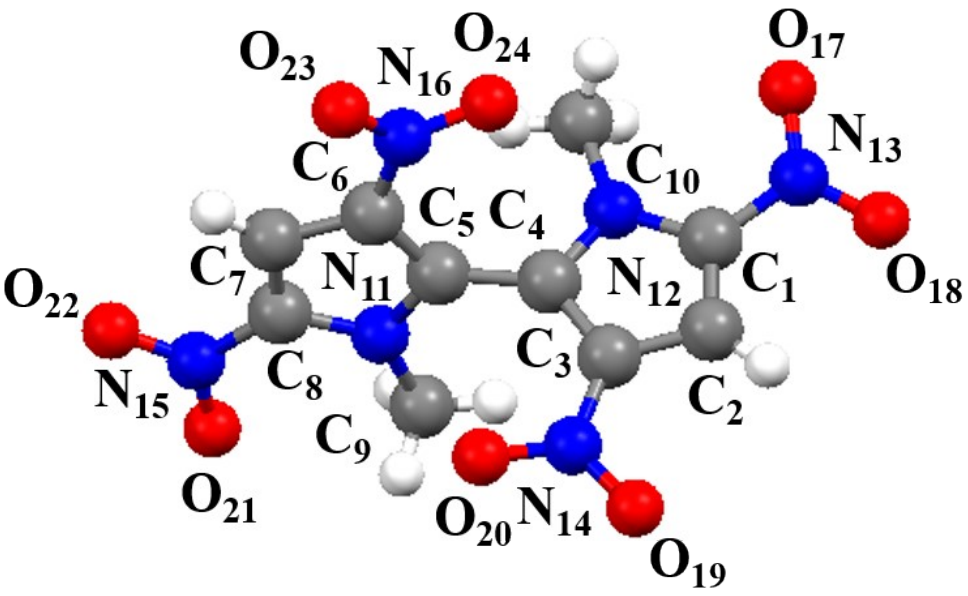


Figure S34: Single-crystal XRD of compound **6**.

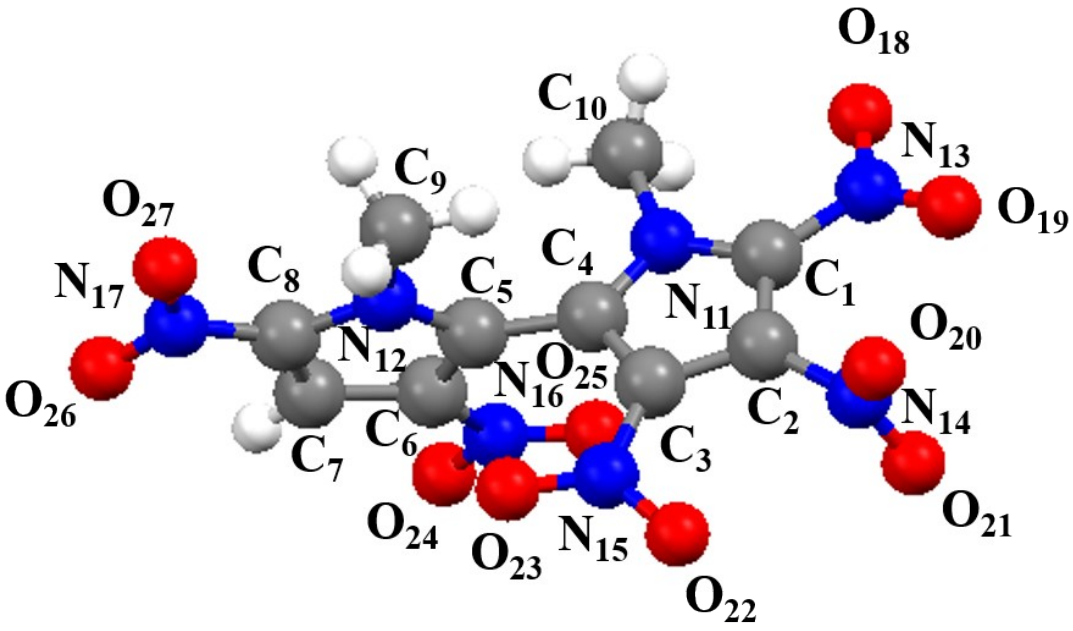


Figure S35: Single-crystal XRD of compound **7**.

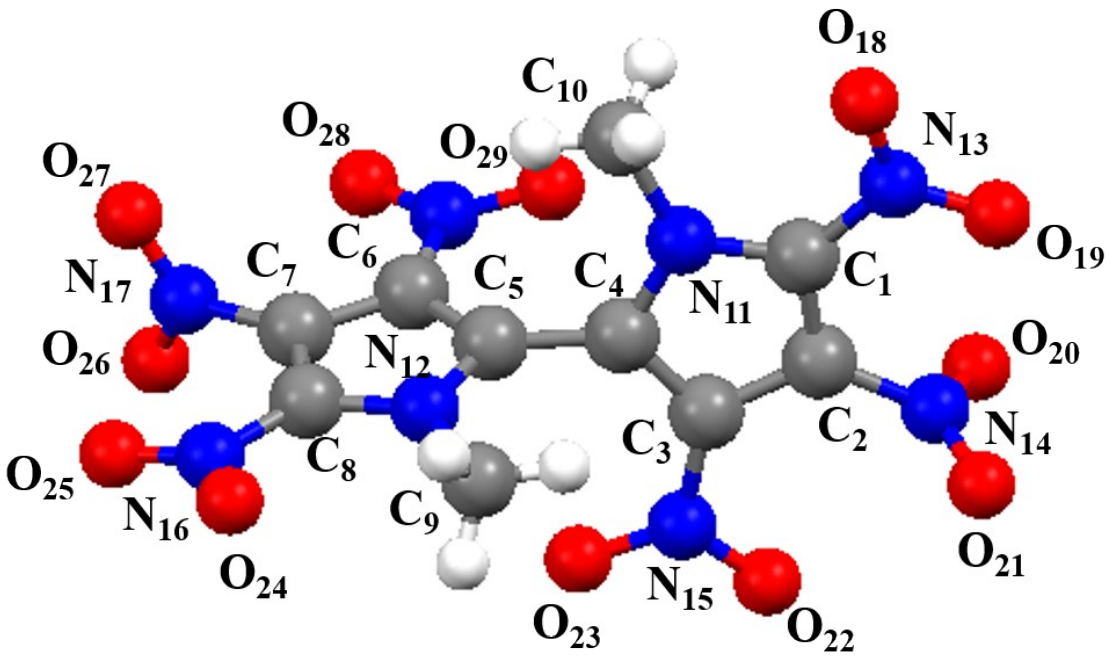


Figure S36: Single-crystal XRD of compound **HNDMBP**.

Compound 3

Table S5 Crystal data and structure refinement for compound 3.

Identification code	compound 3
Empirical formula	$C_8H_6N_4O_4$
Formula weight	222.17
Temperature/K	295.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.5856(7)
b/Å	20.0958(19)
c/Å	6.9138(7)
α/°	90
β/°	96.051(3)
γ/°	90
Volume/Å^3	909.89(16)
Z	4
ρ_{calc}g/cm^3	1.622

μ/mm^{-1}	0.134
F(000)	456.0
Crystal size/mm^3	0.1× 0.2 × 0.3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.222 to 55.044
Index ranges	-8 ≤ h ≤ 8, -26 ≤ k ≤ 26, -8 ≤ l ≤ 8
Reflections collected	16463
Independent reflections	2078 [R_{int} = 0.0534, R_{sigma} = 0.0296]
Data/restraints/parameters	2078/0/145
Goodness-of-fit on F^2	1.156
Final R indexes [I>=2σ (I)]	R_1 = 0.1085, wR_2 = 0.3201
Final R indexes [all data]	R_1 = 0.1192, wR_2 = 0.3268
Largest diff. peak/hole / e Å^{-3}	0.96/-0.76

Table S6 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for compound 3. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O001	3937(4)	1993.6(16)	4974(5)	46.9(9)
O002	4108(4)	3043.2(15)	5599(5)	45.9(9)
N003	4867(5)	2483.7(16)	5701(5)	32.5(8)
N004	10002(5)	2500.9(16)	7908(5)	32.3(8)
C005	6770(5)	3979.8(17)	7194(6)	29.1(8)
C006	8328(5)	2857.7(19)	7256(5)	28.1(8)
O1	4156(6)	4994(2)	7236(9)	90.7(18)
C008	6859(5)	2378.5(19)	6614(5)	29.7(8)
C009	8430(5)	3578.1(19)	7309(5)	31.3(9)
N1	5981(6)	5141(2)	7370(8)	64.1(14)
O00B	6591(7)	5712.8(19)	7470(10)	96(2)
C00C	7708(6)	1737(2)	6944(6)	35.8(9)
C00D	9655(6)	1832(2)	7737(6)	35.9(9)
C00E	7414(6)	4619(2)	7385(8)	44.7(11)
N2	10144(6)	3983(2)	7576(8)	60.6(13)
C00G	9496(7)	4641(2)	7620(8)	49.7(12)

Table S7 Anisotropic Displacement Parameters (Å^2×10^3) for compound 3. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U$_{11}$+2hka*b*U$_{12}$+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

O001	30.9(15)	44.3(17)	62(2)	-6.0(14)	-12.6(13)	-7.5(12)
O002	26.0(14)	41.2(16)	67(2)	-2.3(14)	-10.6(13)	4.5(12)
N003	21.5(15)	38.8(18)	36.3(17)	1.7(13)	-0.6(12)	-3.1(12)
N004	18.6(14)	37.0(18)	39.8(17)	-0.1(13)	-2.8(12)	1.2(11)
C005	15.7(15)	24.1(16)	47(2)	-1.5(14)	0.4(13)	-0.6(12)
C006	19.7(15)	36.3(19)	27.8(17)	1.3(13)	1.0(13)	2.5(13)
O1	29.3(18)	49(2)	194(6)	-6(3)	9(2)	4.2(15)
C008	21.8(17)	36.4(19)	30.2(17)	2.7(14)	0.0(13)	0.8(13)
C009	22.5(17)	37(2)	34.0(19)	-1.1(14)	0.8(14)	1.9(14)
N1	33(2)	35(2)	123(4)	-6(2)	5(2)	3.6(16)
O00B	57(3)	30.6(19)	201(6)	-12(2)	13(3)	-2.4(16)
C00C	34(2)	34(2)	39(2)	-1.2(15)	-1.7(16)	-1.2(15)
C00D	30.4(19)	36(2)	40(2)	0.8(16)	0.3(15)	7.6(15)
C00E	31(2)	33(2)	69(3)	-2.3(19)	1.8(19)	-1.9(16)
N2	34(2)	57(3)	91(4)	-7(2)	3(2)	-2.5(18)
C00G	30(2)	38(2)	80(4)	-7(2)	3(2)	-7.9(17)

Table S8 Bond Lengths for compound 3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O001	N003	1.238(4)	O1	N1	1.232(6)
O002	N003	1.229(4)	C008	C00C	1.414(5)
N003	C008	1.410(5)	C009	N2	1.388(6)
N004	C006	1.352(4)	N1	O00B	1.217(6)
N004	C00D	1.366(5)	N1	C00E	1.410(6)
C005	C009	1.354(5)	C00C	C00D	1.354(6)
C005	C00E	1.354(5)	C00E	C00G	1.365(6)
C006	C008	1.404(5)	N2	C00G	1.390(7)
C006	C009	1.450(5)			

Table S9 Bond Angles for compound 3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O001	N003	C008	117.4(3)	C005	C009	N2	107.4(4)
O002	N003	O001	121.6(3)	N2	C009	C006	128.6(4)
O002	N003	C008	121.1(3)	O1	N1	C00E	118.0(4)
C006	N004	C00D	111.7(3)	O00B	N1	O1	123.0(4)
C009	C005	C00E	108.5(3)	O00B	N1	C00E	119.0(4)
N004	C006	C008	104.6(3)	C00D	C00C	C008	106.2(3)
N004	C006	C009	119.2(3)	C00C	C00D	N004	108.4(3)
C008	C006	C009	136.2(3)	C005	C00E	N1	120.2(4)
N003	C008	C00C	122.8(3)	C005	C00E	C00G	110.0(4)
C006	C008	N003	128.0(3)	C00G	C00E	N1	129.8(4)
C006	C008	C00C	109.1(3)	C009	N2	C00G	108.2(4)
C005	C009	C006	124.0(3)	C00E	C00G	N2	105.9(4)

Table S10 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for compound 3.

Atom	*x*	*y*	*z*	U(eq)
H004	11144.88	2673.77	8372.62	39
H005	5417.04	3840.37	7015.48	35
H00C	7059.73	1331.84	6671.63	43
H00D	10596.55	1498.49	8104.17	43
H2	11392.47	3849.71	7694.02	73
H00G	10314.35	5018.11	7776.65	60

Compound-4

Table S11 Crystal data and structure refinement for compound 4.

Identification code	VSP-22-NM
Empirical formula	$C_{10}H_{10}N_4O_4$
Formula weight	250.22
Temperature/K	296.0
Crystal system	monoclinic
Space group	C2/c
a/Å	20.286(7)
b/Å	8.192(3)
c/Å	13.640(5)
α/°	90
β/°	100.804(14)
γ/°	90
Volume/Å^3	2226.5(13)
Z	8
ρ_{calc}g/cm^3	1.493
μ/mm^{-1}	0.118
F(000)	1040.0
Crystal size/mm^3	0.2× 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.376 to 55.754
Index ranges	$-26 \le h \le 26$, $-10 \le k \le 10$, $-17 \le l \le 17$
Reflections collected	25615
Independent reflections	2607 [R_{int} = 0.0597, R_{sigma} = 0.0306]
Data/restraints/parameters	2607/0/165
Goodness-of-fit on F^2	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.0555, wR_2 = 0.1578
Final R indexes [all data]	R_1 = 0.0722, wR_2 = 0.1675

Largest diff. peak/hole / e $Å^{-3}$ 0.33/-0.28

Table S12 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 4. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N001	5615.5(7)	1366.6(17)	6165.3(10)	48.3(4)
N002	6508.1(7)	5138.4(16)	6552.5(11)	49.9(4)
O003	5110.2(10)	-1807.7(19)	6235.1(12)	86.4(6)
N1	4737.1(10)	-653(2)	6278.5(11)	64.6(5)
O1	4152.8(10)	-812(2)	6365.2(14)	93.6(6)
C006	5634.5(9)	3036(2)	6078.6(12)	48.1(4)
N2	7476.7(9)	6959(2)	6625(2)	86.5(7)
C008	4966.6(9)	983(2)	6209.9(12)	51.7(4)
C009	6240.6(9)	3885(2)	5948.7(12)	49.8(4)
O00A	7340.5(11)	7730(3)	7329(2)	134.6(10)
C00B	5005.6(9)	3660(2)	6069.9(14)	57.5(5)
C00C	4585.0(10)	2361(2)	6151.7(14)	59.4(5)
C00D	7055.8(9)	5676(2)	6202.8(16)	61.0(5)
O2	7969.0(10)	7253(3)	6270(2)	129.2(9)
C00F	6286.6(10)	5624(2)	7463.7(15)	63.4(5)
C00G	6620.2(11)	3652(3)	5221.5(16)	68.9(6)
C00H	6198.1(10)	297(3)	6321.1(16)	66.1(5)
C00I	7130.1(11)	4777(3)	5383.1(18)	77.2(7)

Table S13 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N001	58.6(9)	43.5(7)	43.1(7)	2.0(6)	10.1(6)	-8.0(6)
N002	48.8(8)	38.6(7)	59.3(9)	1.5(6)	2.7(6)	-1.8(6)
O003	118.9(15)	49.9(8)	85.9(11)	4.0(7)	7.5(10)	-18.5(9)
N1	91.1(13)	59.3(10)	43.7(8)	-1.3(7)	13.2(8)	-31.3(10)
O1	102.7(13)	91.4(12)	94.2(12)	-8.2(9)	38.1(10)	-53.9(10)
C006	56.5(10)	44.8(9)	44.0(8)	-0.2(6)	12.2(7)	-8.8(7)
N2	51.7(11)	57.0(11)	141(2)	6.4(12)	-7.3(11)	-9.3(8)
C008	63.7(10)	51.4(9)	40.9(8)	-1.5(7)	12.3(7)	-20.0(8)
C009	54.6(10)	43.5(8)	52.1(9)	0.1(7)	12.1(7)	-7.7(7)

O00A	81.3(14)	98.0(15)	218(3)	-76.9(17)	11.1(15)	-23.6(11)
C00B	60.5(11)	50.7(10)	64.3(11)	-1.1(8)	19.4(8)	-5.5(8)
C00C	56.3(11)	66.6(12)	58.1(10)	-5.3(9)	18.1(8)	-12.4(9)
C00D	47.1(9)	48.5(10)	84.7(14)	10.8(9)	5.1(9)	-9.2(7)
O2	70.3(12)	112.5(16)	203(2)	12.9(15)	21.6(13)	-43.8(11)
C00F	70.9(12)	54.9(10)	62.8(11)	-14.1(8)	8.1(9)	3.9(9)
C00G	78.5(13)	72.5(13)	61.9(11)	-9.6(10)	29.0(10)	-20.2(11)
C00H	70.8(13)	56.1(11)	69.5(12)	4.4(9)	8.5(9)	0.4(9)
C00I	70.8(14)	82.9(15)	85.2(15)	7.6(12)	33.5(12)	-19.1(11)

Table S14 Bond Lengths for compound 4.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N001	C006	1.374(2)	C006	C00B	1.372(3)
N001	C008	1.366(2)	N2	O00A	1.223(3)
N001	C00H	1.455(2)	N2	C00D	1.408(3)
N002	C009	1.364(2)	N2	O2	1.213(3)
N002	C00D	1.362(2)	C008	C00C	1.362(3)
N002	C00F	1.454(2)	C009	C00G	1.378(3)
O003	N1	1.219(2)	C00B	C00C	1.382(3)
N1	O1	1.220(2)	C00D	C00I	1.370(3)
N1	C008	1.428(2)	C00G	C00I	1.372(3)
C006	C009	1.452(2)			

Table S15 Bond Angles for compound 4.

Table 5 Bond Angles for compound 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C006	N001	C00H	125.26(15)	O2	N2	C00D	117.8(3)
C008	N001	C006	105.99(14)	N001	C008	N1	123.19(18)
C008	N001	C00H	128.21(15)	C00C	C008	N001	110.42(15)
C009	N002	C00F	124.80(15)	C00C	C008	N1	126.37(18)
C00D	N002	C009	106.87(15)	N002	C009	C006	122.48(15)
C00D	N002	C00F	127.87(16)	N002	C009	C00G	109.03(16)
O003	N1	O1	123.05(18)	C00G	C009	C006	128.45(16)
O003	N1	C008	120.80(18)	C006	C00B	C00C	107.44(17)
O1	N1	C008	116.1(2)	C008	C00C	C00B	106.86(17)
N001	C006	C009	121.67(15)	N002	C00D	N2	124.8(2)
C00B	C006	N001	109.29(15)	N002	C00D	C00I	109.50(17)
C00B	C006	C009	128.89(16)	C00I	C00D	N2	125.7(2)
O00A	N2	C00D	119.9(2)	C00I	C00G	C009	107.32(19)

O2	N2	O00A	122.3(2)	C00D C00I	C00G 107.29(18)

Table S16 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for compound 4.

Atom	*x*	*y*	*z*	U(eq)
H00B	4884.73	4756.18	6018.46	69
H00C	4128.77	2416.08	6164.48	71
H00A	5928.83	4921.69	7573.81	95
H00D	6129.99	6732.22	7401.38	95
H00E	6654.8	5540.2	8017.41	95
H00G	6544.57	2876.73	4714.87	83
H00F	6597.91	937.44	6354.37	99
H00H	6161.16	-461.81	5776.93	99
H00I	6219.84	-292.24	6934.89	99
H00J	7464.14	4905.61	5006.42	93

Compound 6

Table S17 Crystal data and structure refinement for compound 6.

Identification code	Compound 6
Empirical formula	$C_{10}H_8N_6O_8$
Formula weight	340.22
Temperature/K	295.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.5493(18)
b/Å	13.507(3)
c/Å	12.111(3)
α/°	90
β/°	97.395(7)
γ/°	90
Volume/Å^3	1386.9(5)
Z	4
ρ_{calc}g/cm^3	1.629
μ/mm^{-1}	0.144
F(000)	696.0
Crystal size/mm^3	0.2× 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.804 to 46.828
Index ranges	-9 ≤ h ≤ 9, -15 ≤ k ≤ 15, -13 ≤ l ≤ 13

Reflections collected	15650
Independent reflections	1987 [R_{int} = 0.0747, R_{sigma} = 0.0509]
Data/restraints/parameters	1987/0/219
Goodness-of-fit on F^2	1.084
Final R indexes [I>=2σ (I)]	R_1 = 0.0773, wR_2 = 0.1899
Final R indexes [all data]	R_1 = 0.0856, wR_2 = 0.1991
Largest diff. peak/hole / e $Å^{-3}$	0.51/-0.43

Table S18 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for compound 6. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O11	10684(3)	7311.3(17)	4336(2)	59.1(7)
N6	10061(3)	8079.7(19)	4588(2)	46.3(7)
N9	8347(3)	5855.7(18)	3340.7(19)	40.2(7)
N11	6437(3)	5915(2)	5805(2)	45.4(7)
N7	5888(3)	7851.6(18)	3749(2)	40.3(7)
N8	4802(4)	9548(2)	3659(2)	51.2(8)
O15	6093(3)	5228.2(19)	6383(2)	68.7(8)
O13	5142(4)	10428.1(19)	3753(2)	71.6(8)
O10	10788(3)	8755(2)	5084(3)	76.3(9)
O14	6138(4)	6774.8(19)	5997(2)	72.9(9)
N10	9289(4)	4143(2)	3150(2)	60.0(9)
O12	3469(3)	9245(2)	3407(3)	76.7(9)
C9	7342(3)	7435(2)	4006(2)	37.1(7)
C17	7599(3)	6365(2)	4075(2)	35.4(7)
O17	8993(5)	3280(2)	3350(3)	94.8(11)
O16	10229(4)	4394(3)	2559(3)	96.6(11)
C16	7223(3)	5693(2)	4874(2)	37.0(7)
C11	7599(4)	9096(2)	4218(2)	43.7(8)
C10	8405(3)	8198(2)	4290(2)	38.3(7)
C14	8451(4)	4886(2)	3685(2)	41.4(8)
C15	7761(4)	4757(2)	4616(3)	42.2(8)
C12	6075(4)	8861(2)	3882(2)	40.3(8)
C18	8821(5)	6282(3)	2319(3)	59.5(10)
C13	4448(4)	7292(3)	3368(3)	61.3(10)

Table S19 Anisotropic Displacement Parameters (Å^2×10^3) for compound 6. 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}
O11	51.1(14)	48.2(15)	75.7(17)	-4.9(12)	-0.1(12)	6.8(11)
N6	49.6(16)	36.5(16)	51.9(15)	-0.4(12)	3.7(12)	-8.2(13)
N9	43.7(14)	39.0(15)	38.8(13)	-4.7(11)	8.3(11)	-4.2(11)
N11	51.8(16)	41.6(16)	44.1(15)	1.3(12)	10.7(12)	-3.7(12)
N7	44.8(15)	32.2(14)	43.8(14)	1.4(10)	4.7(11)	-1.7(11)
N8	66(2)	45.3(19)	42.8(15)	3.9(12)	9.8(13)	10.6(14)
O15	96(2)	58.9(16)	56.7(15)	10.8(12)	33.0(14)	-15.9(14)
O13	96(2)	36.0(16)	84.2(19)	2.3(12)	17.0(16)	16.6(13)
O10	60.4(16)	57.3(17)	106(2)	-20.8(15)	-7.4(15)	-18.6(13)
O14	111(2)	47.3(16)	69.6(16)	-0.8(12)	45.9(16)	12.6(14)
N10	68(2)	58(2)	52.8(17)	-13.4(14)	2.4(15)	16.3(15)
O12	60.2(18)	65.8(18)	99(2)	5.5(15)	-8.5(15)	15.6(14)
C9	45.5(17)	30.6(15)	35.6(15)	0.5(11)	7.0(13)	-2.0(13)
C17	37.7(15)	31.4(15)	36.9(15)	-3.1(12)	4.1(12)	-4.2(12)
O17	156(3)	43.5(18)	87(2)	-4.2(14)	23(2)	38.6(18)
O16	91(2)	94(2)	116(3)	-29(2)	56(2)	7.4(18)
C16	41.1(16)	32.4(15)	37.4(15)	0.4(12)	4.1(12)	-2.8(12)
C11	60(2)	29.7(16)	42.4(16)	-2.1(12)	10.4(15)	-6.2(14)
C10	44.3(17)	31.2(16)	39.8(16)	-0.1(12)	6.9(13)	-4.0(13)
C14	45.6(17)	31.6(16)	46.0(17)	-7.5(12)	1.5(14)	6.4(13)
C15	51.3(18)	28.8(16)	45.1(17)	2.2(12)	0.4(14)	2.9(13)
C12	53.4(19)	31.0(16)	37.1(16)	2.5(12)	8.5(13)	5.9(14)
C18	75(2)	66(2)	40.9(18)	-3.6(16)	18.5(17)	-10.5(19)
C13	49(2)	46(2)	86(3)	2.9(17)	-1.7(18)	-6.6(16)

Table S20 Bond Lengths for compound 6.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O11	N6	1.223(3)	N8	O12	1.213(4)
N6	O10	1.218(3)	N8	C12	1.430(4)
N6	C10	1.425(4)	N10	O17	1.222(4)
N9	C17	1.349(4)	N10	O16	1.192(4)
N9	C14	1.374(4)	N10	C14	1.435(4)
N9	C18	1.468(4)	C9	C17	1.463(4)
N11	O15	1.221(3)	C9	C10	1.388(4)
N11	O14	1.217(4)	C17	C16	1.394(4)
N11	C16	1.417(4)	C16	C15	1.395(4)

N7	C9	1.363(4)	C11	C10	1.392(4)
N7	C12	1.379(4)	C11	C12	1.352(4)
N7	C13	1.468(4)	C14	C15	1.349(4)
N8	O13	1.225(4)			

Table S21 Bond Angles for compound 6.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O11	N6	C10	118.9(2)	N7	C9	C10	107.4(3)
O10	N6	O11	123.2(3)	C10	C9	C17	129.1(3)
O10	N6	C10	118.0(3)	N9	C17	C9	123.1(2)
C17	N9	C14	107.7(2)	N9	C17	C16	107.3(3)
C17	N9	C18	124.2(3)	C16	C17	C9	129.5(3)
C14	N9	C18	128.0(3)	C17	C16	N11	126.2(3)
O15	N11	C16	118.0(3)	C17	C16	C15	108.8(3)
O14	N11	O15	122.9(3)	C15	C16	N11	125.0(3)
O14	N11	C16	119.1(2)	C12	C11	C10	105.3(3)
C9	N7	C12	107.0(2)	C9	C10	N6	125.3(3)
C9	N7	C13	124.2(3)	C9	C10	C11	109.2(3)
C12	N7	C13	128.7(3)	C11	C10	N6	125.5(3)
O13	N8	C12	116.5(3)	N9	C14	N10	123.1(3)
O12	N8	O13	123.7(3)	C15	C14	N9	111.0(3)
O12	N8	C12	119.7(3)	C15	C14	N10	125.8(3)
O17	N10	C14	116.7(3)	C14	C15	C16	105.2(3)
O16	N10	O17	124.3(3)	N7	C12	N8	123.1(3)
O16	N10	C14	119.1(3)	C11	C12	N7	111.1(3)
N7	C9	C17	123.1(2)	C11	C12	N8	125.8(3)

Table S22 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for compound 6.

Atom	*x*	*y*	*z*	U(eq)
H11	8019.3	9723.67	4369.14	52
H15	7664.35	4169.53	5002.12	51
H18A	8425.5	5875.84	1693.96	89
H18B	9950.96	6309.83	2381.06	89
H18C	8396.38	6937.78	2213.2	89
H13A	4018.52	7515.41	2639.28	92
H13B	3688.21	7394.54	3875.7	92
H13C	4694.8	599.81	3339.97	92

Compound-7

Table S23 Crystal data and structure refinement for compound-7.

Identification code	compound-7
Empirical formula	$C_{40}H_{28}N_{28}O_{40}$
Formula weight	1540.90
Temperature/K	273.15
Crystal system	triclinic
Space group	P1
a/Å	10.309(4)
b/Å	11.351(5)
c/Å	12.680(5)
α/°	89.771(13)
β/°	89.807(13)
γ/°	89.955(14)
Volume/Å^3	1483.8(10)
Z	1
ρ_{calc}g/cm^3	1.724
μ/mm^{-1}	0.157
F(000)	784.0
Crystal size/mm^3	0.1 × 0.02 × 0.01
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.588 to 49.416
Index ranges	-12 ≤ h ≤ 12, -10 ≤ k ≤ 13, -14 ≤ l ≤ 14
Reflections collected	15551
Independent reflections	7818 [R_{int} = 0.0995, R_{sigma} = 0.2457]
Data/restraints/parameters	7818/3/983
Goodness-of-fit on F^2	0.949
Final R indexes [I>=2σ (I)]	R_1 = 0.0855, wR_2 = 0.1869
Final R indexes [all data]	R_1 = 0.1884, wR_2 = 0.2310
Largest diff. peak/hole / e Å^{-3}	0.25/-0.27
Flack parameter	-0.9(10)

Table S24 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for compound-7. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N14	-3363(11)	-8661(9)	-4424(11)	48(3)
O002	-2025(11)	-7098(8)	-6183(11)	70(3)
N11	-4854(13)	-6292(9)	-3783(11)	52(3)
N13	-3153(14)	-10612(10)	-4734(12)	62(4)

N10	-2161(12)	-6217(10)	-5764(12)	54(4)
O9	-6312(12)	-6903(9)	-5956(12)	84(4)
O14	-2244(13)	-10648(8)	-4088(11)	77(4)
O15	-1412(12)	-5490(9)	-6047(13)	84(4)
N15	-5285(17)	-10192(11)	-6513(15)	78(5)
O7	-6159(15)	-4729(12)	-2534(14)	97(4)
N12	-5991(13)	-7793(10)	-6275(13)	63(4)
N9	-5284(15)	-4436(11)	-3172(13)	68(4)
O11	-6302(14)	-10573(10)	-6222(13)	90(4)
C00E	-3997(14)	-6760(10)	-4533(13)	42(3)
O12	-4838(15)	-10284(12)	-7462(14)	95(4)
O00G	-3700(15)	-11336(12)	-5196(14)	102(5)
C00H	-4714(12)	-9385(10)	-5738(12)	36(3)
O10	-6563(15)	-8280(11)	-7067(15)	102(5)
C00J	-4507(13)	-5222(11)	-3819(13)	41(4)
C00K	-4981(14)	-8336(11)	-5647(13)	43(3)
C00L	-3186(15)	-6024(11)	-5007(14)	48(4)
C00M	-4164(14)	-7902(10)	-4861(13)	43(4)
C00N	-3536(15)	-5039(13)	-4527(15)	55(4)
C00O	-5818(16)	-6800(13)	-3100(15)	59(4)
C00P	-2318(18)	-8470(12)	-3625(17)	65(5)
C00Q	-3721(14)	-9595(11)	-4962(13)	48(4)
O8	-4984(17)	-3533(13)	-3365(17)	119(6)

Table S25 Bond Lengths for compound-7.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N14	C00M	1.362(17)	N15	O12	1.175(18)
N14	C00P	1.43(2)	N15	C00H	1.47(2)
N14	C00Q	1.381(18)	O7	N9	1.215(19)
O002	N10	1.222(14)	N12	O10	1.238(19)
N11	C00E	1.362(18)	N12	C00K	1.437(18)
N11	C00J	1.403(18)	N9	C00J	1.474(19)
N11	C00O	1.414(19)	N9	O8	1.205(18)
N13	O14	1.190(16)	C00E	C00L	1.36(2)
N13	O00G	1.198(18)	C00E	C00M	1.503(18)
N13	C00Q	1.440(19)	C00H	C00K	1.361(18)
N10	O15	1.244(15)	C00H	C00Q	1.38(2)
N10	C00L	1.38(2)	C00J	C00N	1.30(2)
O9	N12	1.229(16)	C00K	C00M	1.34(2)
N15	O11	1.201(18)	C00L	C00N	1.41(2)

Table S26 Bond Angles for compound-7.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C00M	N14	C00P	124.7(12)	N11	C00E	C00M	119.9(12)
C00M	N14	C00Q	106.4(12)	C00L	C00E	C00M	129.2(14)
C00Q	N14	C00P	128.8(12)	C00K	C00H	N15	130.0(13)
C00E	N11	C00J	103.7(12)	C00K	C00H	C00Q	107.0(12)
C00E	N11	C00O	126.8(12)	C00Q	C00H	N15	123.0(13)
C00J	N11	C00O	129.4(13)	N11	C00J	N9	120.0(12)
O14	N13	O00G	127.7(16)	C00N	C00J	N11	112.7(13)
O14	N13	C00Q	117.8(14)	C00N	C00J	N9	127.1(13)
O00G	N13	C00Q	114.5(15)	C00H	C00K	N12	125.3(13)
O002	N10	O15	120.4(13)	C00M	C00K	N12	125.9(13)
O002	N10	C00L	119.3(13)	C00M	C00K	C00H	108.8(13)
O15	N10	C00L	120.3(13)	N10	C00L	C00N	126.3(14)
O11	N15	C00H	117.8(16)	C00E	C00L	N10	126.3(13)
O12	N15	O11	123.6(19)	C00E	C00L	C00N	107.3(14)
O12	N15	C00H	117.2(16)	N14	C00M	C00E	121.4(13)
O9	N12	O10	122.8(14)	C00K	C00M	N14	109.4(12)
O9	N12	C00K	119.3(14)	C00K	C00M	C00E	129.1(13)
O10	N12	C00K	117.7(13)	C00J	C00N	C00L	106.0(14)
O7	N9	C00J	119.6(15)	N14	C00Q	N13	125.4(13)
O8	N9	O7	126.1(17)	C00H	C00Q	N14	108.3(12)
O8	N9	C00J	114.3(15)	C00H	C00Q	N13	126.3(13)
N11	C00E	C00L	110.2(12)				

Table S27 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for compound-7.

Atom	*x*	*y*	*z*	U(eq)
H00N	-3153.06	-4389.61	-4682.91	66
H00A	-6659.43	-6604.2	-3387.95	89
H00B	-5734.99	-6588.93	-2288.86	89

H00C	-5713.66	-7550.77	-3159.96	89
H00D	-1511.36	-8501.31	-4046.82	98
H00E	-2323.05	-8996.13	-3015.26	98
H00F	-2416.38	-7783.6	-3277.32	98

Compound HNDMBP

Table S28 Crystal data and structure refinement for compound HNDMBP.

Identification code	Compound **HNDMBP**
Empirical formula	$C_{10}H_6N_8O_{12}$
Formula weight	430.23
Temperature/K	273.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.1882(13)
b/Å	9.3309(9)
c/Å	14.4003(14)
α/°	90
β/°	99.528(4)
γ/°	90
Volume/Å^3	1615.1(3)
Z	4
ρ_{calc}g/cm^3	1.769
μ/mm^{-1}	0.165
F(000)	872.0
Crystal size/mm^3	0.2 × 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.388 to 51.384
Index ranges	$-14 \leq h \leq 14$, $-9 \leq k \leq 11$, $-17 \leq l \leq 16$
Reflections collected	19545
Independent reflections	3059 [R_{int} = 0.0367, R_{sigma} = 0.0258]
Data/restraints/parameters	3059/0/273
Goodness-of-fit on F^2	1.206
Final R indexes [I>=2σ (I)]	R_1 = 0.0636, wR_2 = 0.1533
Final R indexes [all data]	R_1 = 0.0679, wR_2 = 0.1611
Largest diff. peak/hole / e Å^{-3}	0.54/-0.59

Table S29 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for compound HNDMBP. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N001	8176.3(13)	5184.6(18)	6289.9(11)	32.0(4)
O002	5592.6(15)	4843.3(17)	5908.7(13)	52.2(4)
N003	7305.7(13)	8661.0(18)	5972.6(11)	34.0(4)

O004	4205.1(14)	6182(2)	6134.3(15)	63.2(5)
O005	9692.7(18)	3134(3)	7136.3(15)	76.7(7)
O006	7420.9(18)	11586(2)	6407.4(18)	74.2(6)
O007	3742.7(15)	9390(2)	5733.9(14)	66.4(6)
N008	5170.2(14)	6005(2)	6028.8(12)	39.9(4)
O009	7573.1(18)	5752(3)	3163.4(11)	68.8(6)
O00A	9561.3(17)	3875(3)	3818.3(17)	78.4(7)
N00B	4458.7(16)	9145(2)	6397.7(13)	45.1(5)
N00C	9455.0(16)	3123(2)	6286.8(17)	50.1(5)
C00D	8411.9(16)	4382(2)	4876.5(15)	36.0(5)
O00E	8228(2)	2436(3)	3921(2)	90.9(9)
C00F	7771.3(16)	5624(2)	4754.3(13)	33.0(4)
N00G	7362.5(16)	6317(2)	3875.2(12)	45.0(5)
O00H	6851(2)	7426(2)	3892.8(13)	72.8(6)
C00I	7620.5(15)	6094(2)	5637.5(13)	30.7(4)
N00J	8758.5(16)	3492(2)	4140.5(15)	48.7(5)
C00K	8663.3(16)	4144(2)	5825.8(15)	35.5(4)
C00L	5850.0(16)	7262(2)	6043.3(13)	32.3(4)
O00M	9860(2)	2316(2)	5769.8(18)	81.4(7)
N00N	6527.5(18)	11014(2)	6319.9(16)	51.8(5)
C00O	6941.9(16)	7281(2)	5889.7(13)	30.8(4)
C00P	5539.7(16)	8662(2)	6207.7(13)	34.0(4)
O00Q	4348(2)	9247(4)	7199.3(15)	96.8(9)
C00R	6447.8(17)	9491(2)	6164.6(14)	35.8(5)
C00S	8187(2)	5317(3)	7312.3(15)	47.3(5)
O00T	5658(2)	11616(2)	6359(3)	105.1(10)
C00U	8417.8(19)	9121(3)	5817(2)	53.4(6)

Table S30 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for compound HNDMBP. 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	30.5(8)	31.3(8)	34.8(8)	3.4(6)	7.3(6)	-1.3(6)
O002	58.7(10)	33.8(9)	65.5(11)	-1.8(7)	14.6(8)	-5.4(7)
N003	33.2(8)	31.0(9)	37.8(9)	-0.8(7)	5.7(7)	-2.2(6)
O004	39.8(9)	59.8(11)	93.6(14)	-7.1(10)	21.6(9)	-11.8(8)
O005	73.4(13)	87.4(16)	68.4(13)	30.6(11)	9.0(10)	31.3(12)
O006	72.6(13)	39.6(10)	113.1(18)	-11.4(10)	23.1(12)	-18.5(9)
O007	44.7(10)	84.3(14)	68.5(12)	19.2(10)	4.7(9)	18.2(9)
N008	38.4(9)	41.2(10)	41.3(9)	-0.8(7)	9.8(7)	-8.0(8)
O009	81.2(13)	93.8(15)	32.7(9)	-7.7(9)	12.8(8)	-0.1(12)
O00A	61.4(12)	86.7(15)	99.9(16)	-43.3(13)	50.6(11)	-29.2(11)
N00B	43.0(10)	47.9(11)	46.5(10)	-1.1(8)	13.5(8)	8.1(8)
N00C	39.0(10)	38.9(10)	74.8(15)	11.7(10)	16.0(9)	5.7(8)
C00D	31.2(9)	33.2(10)	45.4(11)	-9.8(8)	12.1(8)	-7.0(8)

O00E	86.6(15)	72.6(15)	126(2)	-63.3(14)	54.7(14)	-40.8(12)
C00F	32.3(9)	35.0(10)	31.9(9)	-2.4(8)	6.1(7)	-4.1(8)
N00G	46.0(10)	55.4(12)	33.3(9)	1.7(8)	5.6(7)	-5.0(9)
O00H	98.5(16)	68.3(13)	50.2(10)	15.2(9)	8.5(10)	30.4(12)
C00I	29.4(9)	28.6(9)	34.4(9)	0.2(7)	6.3(7)	-2.8(7)
N00J	39.5(10)	46.6(11)	64.0(12)	-21.6(9)	19.8(9)	-9.3(8)
C00K	29.7(9)	26.7(9)	51.2(12)	1.8(8)	9.4(8)	-0.6(7)
C00L	33.7(10)	32.7(10)	31.0(9)	-0.5(7)	6.6(7)	-2.0(8)
O00M	81.2(14)	64.8(13)	101.1(17)	0.6(12)	23.7(12)	40.3(11)
N00N	59.1(13)	31.6(10)	65.0(13)	-4.7(9)	10.8(10)	-0.2(9)
C00O	33.1(9)	29.2(9)	30.0(9)	0.6(7)	5.4(7)	-0.3(7)
C00P	34.0(10)	37.1(10)	31.3(9)	-0.3(8)	6.3(7)	4.6(8)
O00Q	77.8(14)	164(3)	54.8(12)	-16.7(14)	28.4(11)	30.9(16)
C00R	41.7(11)	28.4(10)	36.6(10)	-0.9(8)	4.0(8)	3.3(8)
C00S	51.8(13)	56.6(14)	33.5(11)	5.9(9)	7.2(9)	6.0(11)
O00T	74.4(15)	42.6(12)	203(3)	-26.9(15)	36.9(17)	12.1(10)
C00U	36.5(11)	43.6(13)	81.8(17)	-1.4(12)	14.4(11)	-8.1(10)

Table S31 Bond Lengths for compound HNDMBP.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N001	C00I	1.360(2)	N00C	C00K	1.438(3)
N001	C00K	1.369(3)	N00C	O00M	1.219(3)
N001	C00S	1.475(3)	C00D	C00F	1.392(3)
O002	N008	1.224(3)	C00D	N00J	1.463(3)
N003	C00O	1.360(3)	C00D	C00K	1.369(3)
N003	C00R	1.366(3)	O00E	N00J	1.192(3)
N003	C00U	1.474(3)	C00F	N00G	1.436(3)
O004	N008	1.222(2)	C00F	C00I	1.386(3)
O005	N00C	1.210(3)	N00G	O00H	1.210(3)
O006	N00N	1.200(3)	C00I	C00O	1.464(3)
O007	N00B	1.205(3)	C00L	C00O	1.385(3)
N008	C00L	1.434(3)	C00L	C00P	1.391(3)
O009	N00G	1.217(3)	N00N	C00R	1.439(3)
O00A	N00J	1.204(3)	N00N	O00T	1.209(3)
N00B	C00P	1.461(3)	C00P	C00R	1.361(3)
N00B	O00Q	1.188(3)			

Table S32 Bond Angles for compound HNDMBP.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C00I	N001	C00K	108.16(16)	N001	C00I	C00F	108.07(17)
C00I	N001	C00S	123.94(17)	N001	C00I	C00O	122.53(16)
C00K	N001	C00S	127.86(18)	C00F	C00I	C00O	129.29(17)

C00O	N003	C00R	107.78(16)	O00A	N00J	C00D	117.46(18)
C00O	N003	C00U	123.84(18)	O00E	N00J	O00A	125.6(2)
C00R	N003	C00U	128.29(18)	O00E	N00J	C00D	116.89(19)
O002	N008	C00L	118.06(17)	N001	C00K	N00C	123.8(2)
O004	N008	O002	124.99(19)	N001	C00K	C00D	109.23(17)
O004	N008	C00L	116.95(19)	C00D	C00K	N00C	126.2(2)
O007	N00B	C00P	117.86(18)	C00O	C00L	N008	125.22(18)
O00Q	N00B	O007	124.9(2)	C00O	C00L	C00P	108.07(17)
O00Q	N00B	C00P	117.2(2)	C00P	C00L	N008	126.71(18)
O005	N00C	C00K	119.4(2)	O006	N00N	C00R	119.5(2)
O005	N00C	O00M	124.7(2)	O006	N00N	O00T	125.1(2)
O00M	N00C	C00K	115.8(2)	O00T	N00N	C00R	115.4(2)
C00F	C00D	N00J	127.2(2)	N003	C00O	C00I	123.29(17)
C00K	C00D	C00F	106.81(17)	N003	C00O	C00L	107.84(17)
C00K	C00D	N00J	126.0(2)	C00L	C00O	C00I	128.81(17)
C00D	C00F	N00G	126.32(18)	C00L	C00P	N00B	126.93(19)
C00I	C00F	C00D	107.70(17)	C00R	C00P	N00B	126.78(19)
C00I	C00F	N00G	125.95(19)	C00R	C00P	C00L	106.29(17)
O009	N00G	C00F	117.2(2)	N003	C00R	N00N	123.87(19)
O00H	N00G	O009	124.7(2)	C00P	C00R	N003	110.01(18)
O00H	N00G	C00F	118.15(19)	C00P	C00R	N00N	126.1(2)

Table S33 Torsion Angles for compound HNDMBP.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N001	C00I	C00O	N003	99.5(2)	N00J	C00D	C00F	N00G	-3.0(3)
N001	C00I	C00O	C00L	-83.5(3)	N00J	C00D	C00F	C00I	178.44(18)
O002	N008	C00L	C00O	3.1(3)	N00J	C00D	C00K	N001	-178.79(17)
O002	N008	C00L	C00P	-177.2(2)	N00J	C00D	C00K	N00C	10.8(3)
O004	N008	C00L	C00O	-176.61(19)	C00K	N001	C00I	C00F	-0.6(2)
O004	N008	C00L	C00P	3.1(3)	C00K	N001	C00I	C00O	175.87(17)
O005	N00C	C00K	N001	2.4(3)	C00K	C00D	C00F	N00G	176.87(18)
O005	N00C	C00K	C00D	171.5(2)	C00K	C00D	C00F	C00I	-1.7(2)
O006	N00N	C00R	N003	-9.9(3)	C00K	C00D	N00J	O00A	-98.0(3)
O006	N00N	C00R	C00P	168.4(2)	C00K	C00D	N00J	O00E	81.0(3)
O007	N00B	C00P	C00L	-85.5(3)	C00L	C00P	C00R	N003	0.5(2)
O007	N00B	C00P	C00R	95.2(3)	C00L	C00P	C00R	N00N	-178.0(2)
N008	C00L	C00O	N003	-179.25(17)	O00M	N00C	C00K	N001	-176.0(2)
N008	C00L	C00O	C00I	3.4(3)	O00M	N00C	C00K	C00D	-6.9(3)
N008	C00L	C00P	N00B	-0.1(3)	C00O	N003	C00R	N00N	178.61(19)
N008	C00L	C00P	C00R	179.35(18)	C00O	N003	C00R	C00P	0.1(2)
N00B	C00P	C00R	N003	179.95(18)	C00O	C00L	C00P	N00B	179.65(18)
N00B	C00P	C00R	N00N	1.5(3)	C00O	C00L	C00P	C00R	-0.9(2)
C00D	C00F	N00G	O009	1.7(3)	C00P	C00L	C00O	N003	1.0(2)

C00D	C00F	N00G	O00H	-177.2(2)	C00P	C00L	C00O	C00I	-176.35(18)
C00D	C00F	C00I	N001	1.4(2)	O00Q	N00B	C00P	C00L	93.5(3)
C00D	C00F	C00I	C00O	-174.75(18)	O00Q	N00B	C00P	C00R	-85.9(3)
C00F	C00D	N00J	O00A	81.9(3)	C00R	N003	C00O	C00I	176.82(17)
C00F	C00D	N00J	O00E	-99.2(3)	C00R	N003	C00O	C00L	-0.7(2)
C00F	C00D	C00K	N001	1.3(2)	C00S	N001	C00I	C00F	-178.46(18)
C00F	C00D	C00K	N00C	-169.13(19)	C00S	N001	C00I	C00O	-2.0(3)
C00F	C00I	C00O	N003	-84.8(3)	C00S	N001	C00K	N00C	-12.0(3)
C00F	C00I	C00O	C00L	92.1(3)	C00S	N001	C00K	C00D	177.28(19)
N00G	C00F	C00I	N001	-177.14(17)	O00T	N00N	C00R	N003	170.7(3)
N00G	C00F	C00I	C00O	6.7(3)	O00T	N00N	C00R	C00P	-11.0(4)
C00I	N001	C00K	N00C	170.27(18)	C00U	N003	C00O	C00I	0.2(3)
C00I	N001	C00K	C00D	-0.5(2)	C00U	N003	C00O	C00L	-177.34(19)
C00I	C00F	N00G	O009	-180.0(2)	C00U	N003	C00R	N00N	-4.9(3)
C00I	C00F	N00G	O00H	1.1(3)	C00U	N003	C00R	C00P	176.6(2)

Table S34 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for compound HNDMBP.

Atom	*x*	*y*	*z*	U(eq)
H00A	8921.92	5570	7618.91	71
H00B	7975.14	4419.54	7556.07	71
H00C	7671.79	6048.09	7427.07	71
H00D	8847.79	8295.92	5704.94	80
H00E	8785.86	9620.5	6363.95	80
H00F	8344.16	9746.58	5281.02	80

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