

Supporting Information

Molecular and Crystal Features of Thermostable Energetic Materials – Guidelines for Architecture of “Bridged” Compounds

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1. Experimental Section

General Methods.

All chemical reagents and solvents used in this work were of analytical grade and were used as supplied, without additional purification. ^1H and ^{13}C NMR spectra were recorded on a Bruker Avance III 400 MHz spectrometer at 25 °C. Infrared spectra were measured on a Bruker Tensor 27 FTIR spectrometer equipped with a diamond ATR unit. Melting and decomposition temperatures were measured by a Differential Scanning Calorimetry at a scan rate of 5 °C·min⁻¹. Densities were determined at room temperature on a Micromeritics AccuPyc 1330 gas pycnometer. The impact sensitivity of compounds was tested according to STANAG 4489 protocols, using a BAM drop-hammer. The friction sensitivity was tested according STANAG 4487 protocols, using a BAM friction tester.

Safety Instructions.

Caution! Energetic compounds could be sensitive to mechanical impact, friction and electrostatic discharge. Therefore, the work and storage of these materials requires mandatory safety precautions. Protective equipment including antistatic shoes, protective coat, suitable gloves, goggles and facial protection are obligatory for the synthesis, handling and experimenting with energetic materials.

1-(Ethoxymethyl)-4-methyl-3,5-dinitropyrazole (HL1). A mixture of 4-methyl-3,5-dinitropyrazole (3.44 g, 0.02 mol), chloromethylethyl ether (2.1 g, 0.02 mol) and K_2CO_3 (3.31 g, 0.022 mol) was reacted in CH_3CN (30 mL) at ambient temperature for overnight. After that time, H_2O (30 mL) was added to the reaction mixture and the resulted solution was extracted with ethyl acetate (3×20 mL). The combined organic fractions were washed with brine, dried over MgSO_4 and evaporated to afford pure 1-(ethoxymethyl)-4-methyl-3,5-dinitropyrazole as a white solid (4.35 g, 93.5%). ^1H NMR (400 MHz, CDCl_3): δ 5.93 (s, 2H), 3.60 (q, 2H), 2.69 (s, 3H), 1.17 (t, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ 151.4, 142.9, 115.4, 82.9, 65.9, 14.2, 9.5. IR (ATR, cm^{-1}): 2982, 2930, 1587, 1519, 1446, 1382, 1329, 1301, 1254, 1108, 1031, 866, 772. MS (ES^-): 171.0 [$\text{M}-\text{C}_3\text{H}_7\text{O}$]⁻. Elemental analysis calcd. (%) for $\text{C}_7\text{H}_{10}\text{N}_4\text{O}_5$: C 36.53, H 4.38, N 24.34; found: C 35.99, H 4.33, N 24.03.

1,2-Bis(1-(ethoxymethyl)-3,5-dinitropyrazol)ethane (HL2). To a solution of 1-(ethoxymethyl)-4-methyl-3,5-dinitropyrazole (3.0 g, 0.013 mol) in THF (45 mL) powder of potassium tert-butoxide (1.68 g, 0.015 mol) was added in portions at 4 °C. Then, Br_2 (0.9 mL, 0.017 mol) was added dropwise to the reaction mixture. After 30 min., the resulted mixture was poured into ice-water mixture (100 mL) containing Na_2CO_3 (1.5 g). Formed precipitate was filtered, washed with water and vacuum dried to afford pure 1,2-bis(1-(ethoxymethyl)-3,5-dinitropyrazol)ethane as a light yellow solid (2.6 g, 94.1%). ^1H NMR (400 MHz, CDCl_3): δ 5.90 (s, 4H), 3.62 (s, 4H), 3.51 (q, 4H), 1.17(t, 6H). ^{13}C NMR (100 MHz, CDCl_3): δ 151.3, 143.2, 116.8, 83.6, 66.3, 22.3, 14.4. IR (ATR, cm^{-1}): 2986, 1580, 1516, 1446, 1335, 1298, 1248, 1109, 1040, 864, 779, 699. MS (ES^-): 399.2 [$\text{M}-\text{C}_3\text{H}_7\text{O}$]⁻. Elemental analysis calcd. (%) for $\text{C}_{14}\text{H}_{18}\text{N}_8\text{O}_{10}$: C 36.69, H 3.96, N 24.45; found: C 36.57, H 4.01, N 23.84.

1,2-Bis(3,5-dinitropyrazol)ethane (HL3). To a solution of 1,2-bis(1-(ethoxymethyl)-3,5-dinitropyrazol)ethane (2.8 g, 0.006 mol) in CH_2Cl_2 (30 mL), trifluoroacetic acid (10 mL) was added and the resulted solution was stirred at RT for overnight. After that time, the resulted precipitate was filtered, washed with CH_2Cl_2 and vacuum dried to afford pure 1,2-bis(3,5-dinitropyrazol)ethane (1.83 g, 87.6%). ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 3.48 (s, 4H). ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 149.3, 113.9, 21.3. IR (ATR, cm^{-1}): 3152, 2953, 1585, 1543, 1491, 1447, 1426, 1338, 1235, 1166, 1003, 845, 773. MS (ES^-): 341.2 [$\text{M}-1$]⁻. Elemental analysis calcd. (%) for $\text{C}_8\text{H}_6\text{N}_8\text{O}_8$: C 28.08, H 1.77, N 32.75; found: C 27.94, H 1.83, N 31.94.

3,5-Dinitropyrazole-4-carboxylic acid (HL4). To a solution of 4-methyl-3,5-dinitropyrazole (5.16 g, 0.03 mol) in concentrated H_2SO_4 (98%, 90 mL) powder of $\text{Na}_2\text{Cr}_2\text{O}_7 \cdot \text{H}_2\text{O}$ (17.88 g, 0.06 mol) was added in small portions at 4 °C. At the end the addition, the reaction mixture was allowed to warm up to RT and stirred for 24 hrs. Then, the reaction mixture was poured into ice-water mixture (500 mL) and extracted with ethyl acetate (5×150 mL).

The combined organic fractions were washed with brine, dried over MgSO_4 and evaporated to afford 3,5-dinitro-pyrazole-4-carboxylic acid as a white solid (4.08 g, 67.3%). ^1H NMR (400 MHz, DMSO-d_6): δ 11.67 (br, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 161.2, 148.9, 108.6. IR (ATR, cm^{-1}): 3166, 2961, 1737, 1546, 1488, 1432, 1333, 1294, 1257, 1210, 1120, 1029, 849, 826, 743. MS (ES^-): 201.0 $[\text{M}-1]^-$. Elemental analysis calcd. (%) for $\text{C}_4\text{H}_2\text{N}_4\text{O}_6$: C 23.77, H 1.00, N 27.73; found: C 23.79, H 1.13, N 26.78.

3,5-Dinitropyrazole-4-carbohydrazide (HL5). To a solution of 1*H*-benzo[d][1,2,3]triazole (7.05 g, 0.06 mol) in CH_2Cl_2 (100 mL) thionyl chloride (1.6 mL, 22.5 mmol) was added dropwise at 4 °C and reaction mixture was stirred for 30 min. Then, to the resulted solution a powder of 3,5-dinitropyrazole-4-carboxylic acid (3.0 g, 0.015 mol) was added in portions and the resulted suspension was allowed to warm up to RT and stirred for 6 hrs. After that time, obtained white precipitate of (1*H*-benzo[d][1,2,3]triazol-1-yl)(3,5-dinitro-1*H*-pyrazol-4-yl)methanone was filtered and washed with CH_2Cl_2 and water. Subsequently, the precipitate was re-dissolved in a mixture of THF (50 mL) and water (50 mL), and hydrazine monohydrate (3 mL, 0.06 mol) was added dropwise. The resulted mixture was stirred at room temperature for overnight and after that time, aqueous HCl (10%) solution was added dropwise to adjust the pH to 3. Then, vacuum evaporation of all volatiles resulted in yellow solid residue that was washed with ethyl acetate (to remove residual benzotriazole) and then with water, to give 3,5-dinitropyrazole-4-carbohydrazide as a white solid (2.4 g, 74.1%). ^1H NMR (400 MHz, DMSO-d_6): δ 10.29 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 161.4, 153.3, 107.7. IR (ATR, cm^{-1}): 3453, 3358, 2980, 1686, 1597, 1498, 1416, 1402, 1355, 1305, 1277, 1183, 1118, 953, 849. MS (ES^-): 215.1 $[\text{M}-1]^-$.

***N*′, *N*′-bis(3,5-dinitro-1*H*-pyrazole-4-carbonyl)oxalohydrazide (HL6).** To a suspension of 3,5-dinitropyrazole-4-carbohydrazide (216 mg, 1 mmol) and NaHCO_3 (84 mg, 1 mmol) in dry THF (5 mL), oxalyl chloride (0.043 mL, 0.5 mmol) was added dropwise at 4 °C and the resulted reaction mixture was allowed to warm up to RT and stirred for overnight. Then, solvent was evaporated and water (15 mL) was added. A white precipitate of *N*′, *N*′-bis(3,5-dinitro-1*H*-pyrazole-4-carbonyl)oxalohydrazide (182 mg, 75.0%) was filtered and vacuum dried. The material was sufficiently pure to be used without further purification. ^1H NMR (400 MHz, DMSO-d_6): δ 11.16 (s, 1H), 10.72 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 157.8, 156.8, 149.3, 107.9. IR (ATR, cm^{-1}): 3227, 2924, 1673, 1540, 1427, 1345, 1314, 1230, 1126, 1012, 840, 769. MS (ES^-): 485.0 $[\text{M}-1]^-$.

5,5′-Bis(3,5-dinitropyrazol)-2,2′-bi(1,3,4-oxadiazole) (HL7). *N*′, *N*′-bis(3,5-dinitropyrazole-4-carbonyl)oxalohydrazide (157 mg, 0.32 mmol) was added to oleum (20%, 3 mL) at RT. The resulted dark mixture was stirred for 24 hrs and then poured onto crushed ice. Formed precipitate was filtered, washed with water and vacuum dried to afford 5,5′-bis(3,5-dinitropyrazol)-2,2′-bi(1,3,4-oxadiazole) as light yellow solid (120 mg, 83.3%). ^{13}C NMR (100 MHz, DMSO-d_6): δ 158.7, 154.5, 153.5, 93.7. IR (ATR, cm^{-1}): 3367, 1550, 1474, 1422, 1338, 1194, 1155, 1076, 1012, 961, 840. MS (ES^-): 449.1 $[\text{M}-1]^-$. Elemental analysis calcd. (%) for $\text{C}_{10}\text{H}_2\text{N}_{12}\text{O}_{10}$: C 26.68, H 0.45, N 37.34; found: C 26.54, H 0.54, N 36.44.

4,4′-Dipyrazolylmethane (HL8). 1,1′-Dipyrazolylmethane was converted to its hydrobromide salt by dissolving in aqueous HBr (48%, 5 mL). After evaporation, the obtained hydrobromide salt was transferred into a sealed glass tube and heated to 200 °C for 2 hrs. The resulted brown solid was dissolved in water (5 mL) and aqueous NaOH solution (50%) was added dropwise until the pH of the solution reached 12. Formed gray precipitate of 4,4′-dipyrazolylmethane (0.56 g, 56.0%) was filtered and vacuum dried. The material was sufficiently pure to be used without further purification. ^1H NMR (400 MHz, DMSO-d_6): δ 7.41 (s, 4H), 3.61 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 132.4, 119.8, 18.7. IR (ATR, cm^{-1}): 3133, 3053, 2936, 1505, 1392, 1348, 1131, 1045, 998, 955, 867, 812, 739. MS (ES^+): 149.1 $[\text{M}+1]^+$. Elemental analysis calcd. (%) for $\text{C}_7\text{H}_8\text{N}_4$: C 56.74, H 5.44, N 37.81; found: C 55.48, H 5.40, N 36.75.

4,4′-(3,5-Dinitropyrazolyl)methane (HL9). Powder of 4,4′-dipyrazolylmethane (0.4 g, 2.7 mmol) was added portion wise to fuming H_2SO_4 (10 mL) at 4 °C. To the obtained solution, fuming HNO_3 (0.7 mL) was added dropwise and at the end of the addition, the mixture was heated to 100 °C for 6 hrs. After cooling down to room

temperature, the reaction mixture was poured onto crushed ice. Formed white precipitate was filtered, washed with water till neutral pH and vacuum dried to give pure 4,4'-(3,5-dinitropyrazolyl)methane (0.45 g, 51.1%). ^1H NMR (400 MHz, DMSO- d_6): δ 4.92 (s, 2H). ^{13}C NMR (100 MHz, DMSO- d_6): δ 149.6, 110.2, 16.6. IR (ATR, cm^{-1}): 3219, 2873, 1586, 1522, 1423, 1338, 897, 833. MS (ES^-): 327.0 $[\text{M}-1]^-$. Elemental analysis calcd. (%) for $\text{C}_7\text{H}_4\text{N}_8\text{O}_8$: C 25.62, H 1.23, N 34.15; found: C 24.28, H 1.98, N 30.51.

2. ^1H NMR, ^{13}C NMR, MS Spectra and DSC Thermograms

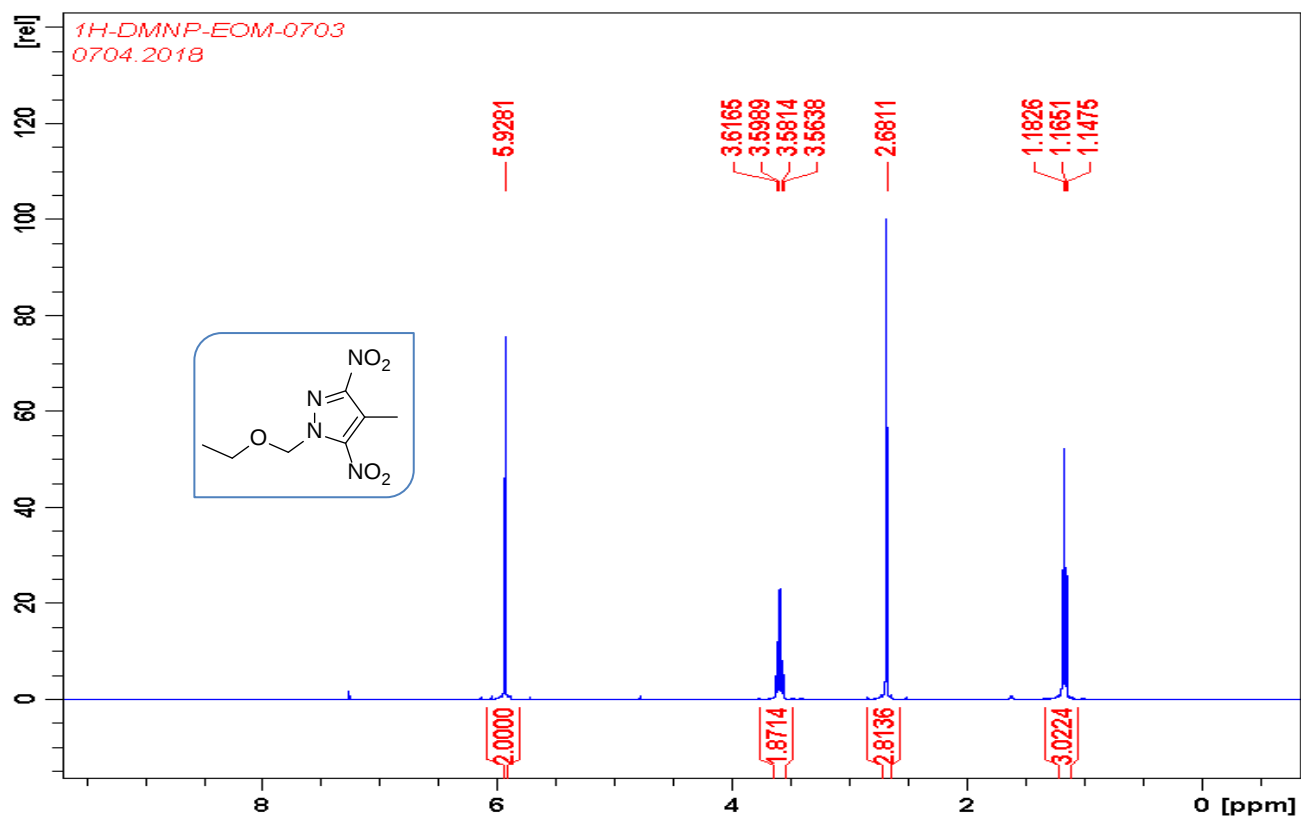


Figure S1. ^1H NMR spectrum of HL1.

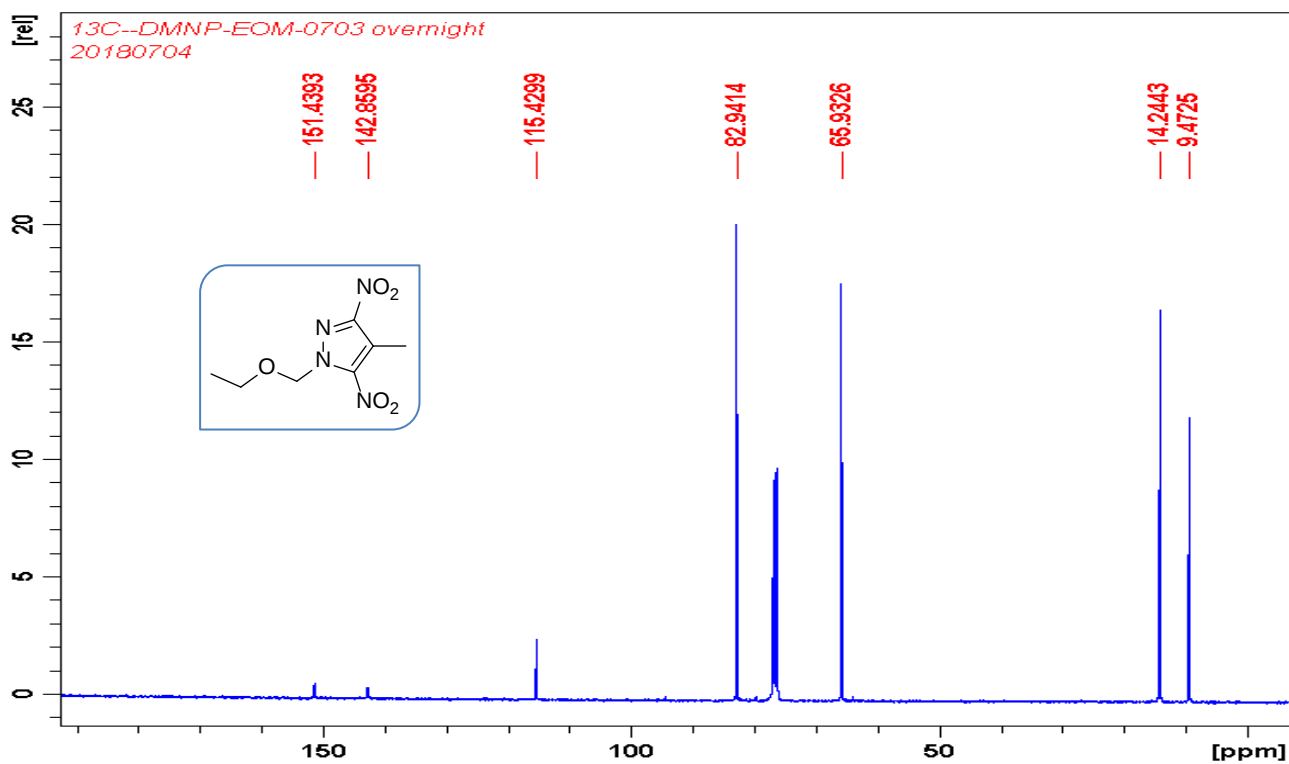


Figure S2. ^{13}C NMR spectrum of HL1.

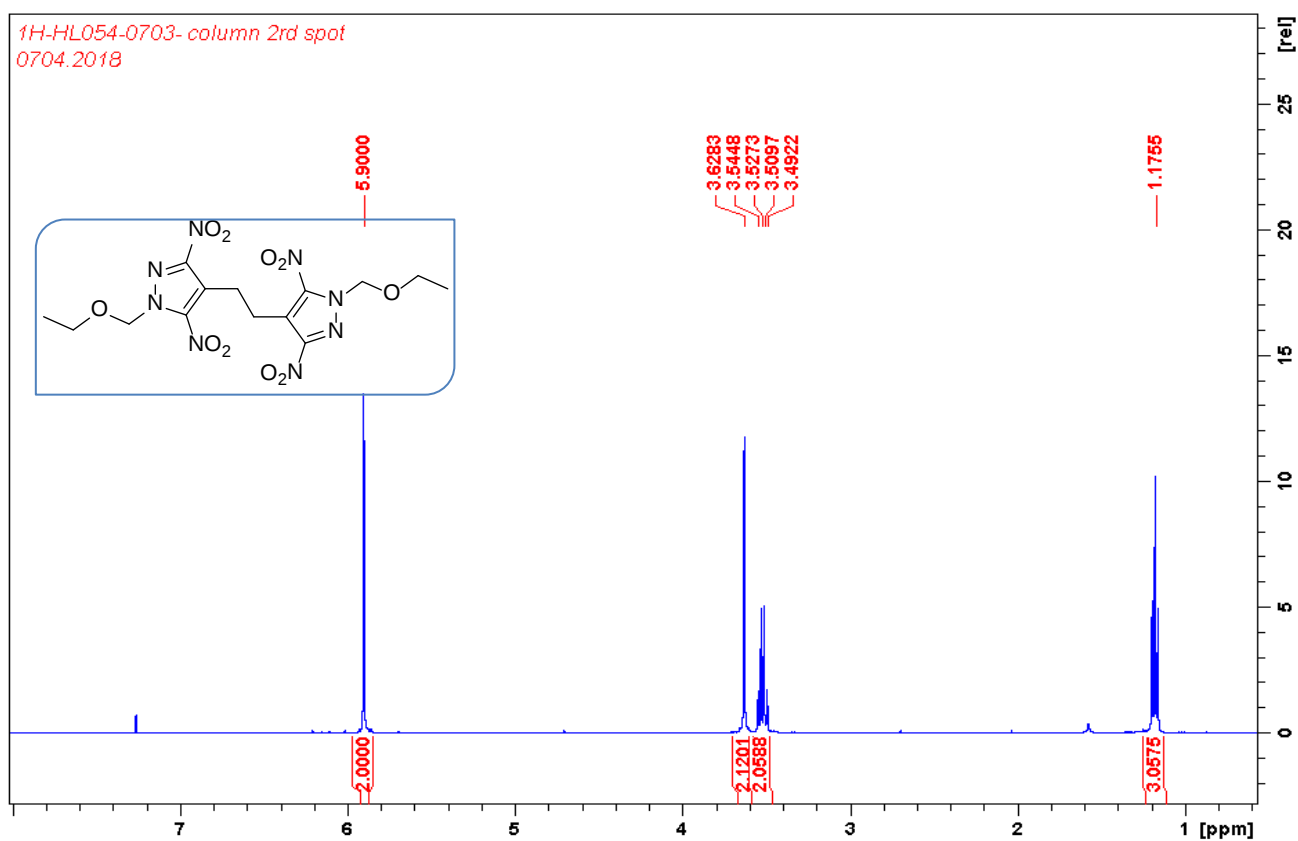


Figure S3. ^1H NMR spectrum of HL2.

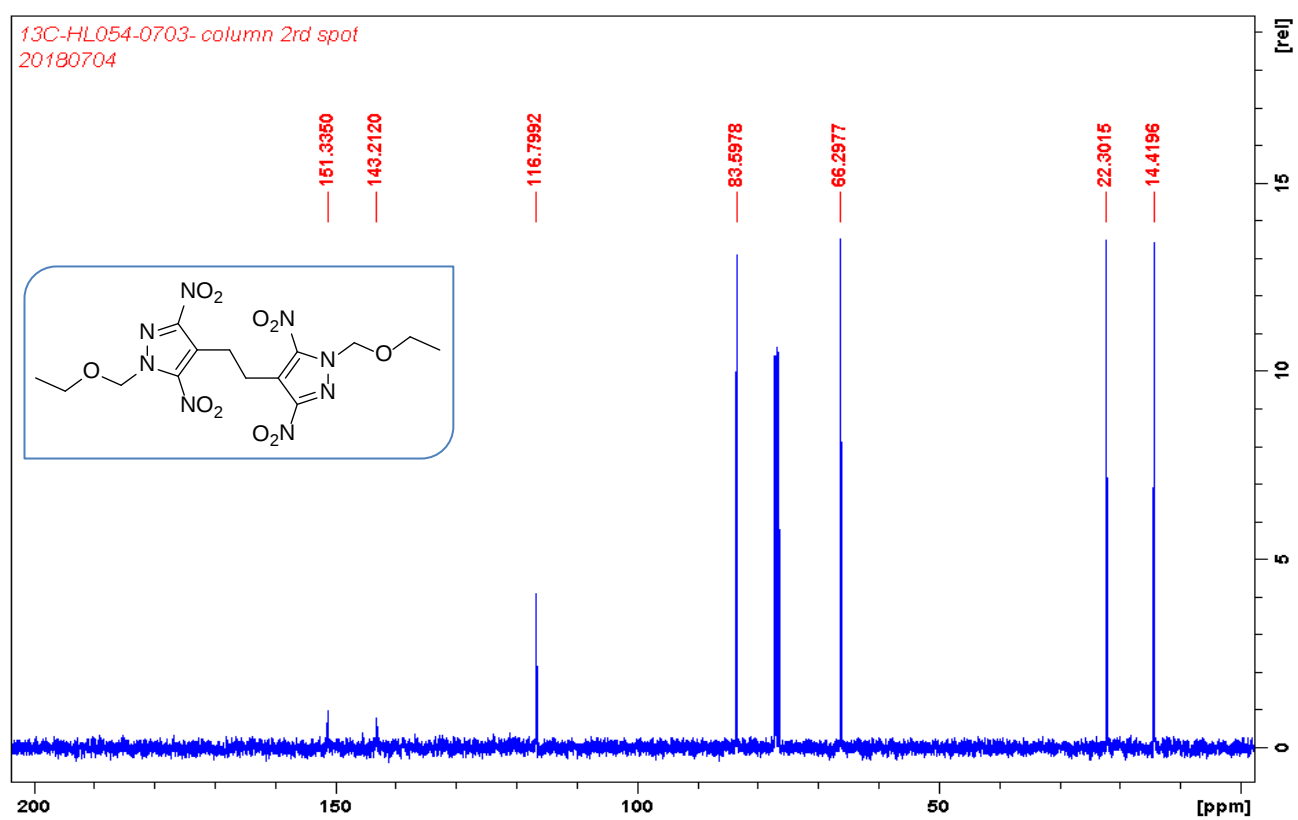


Figure S4. ^{13}C NMR spectrum of HL2

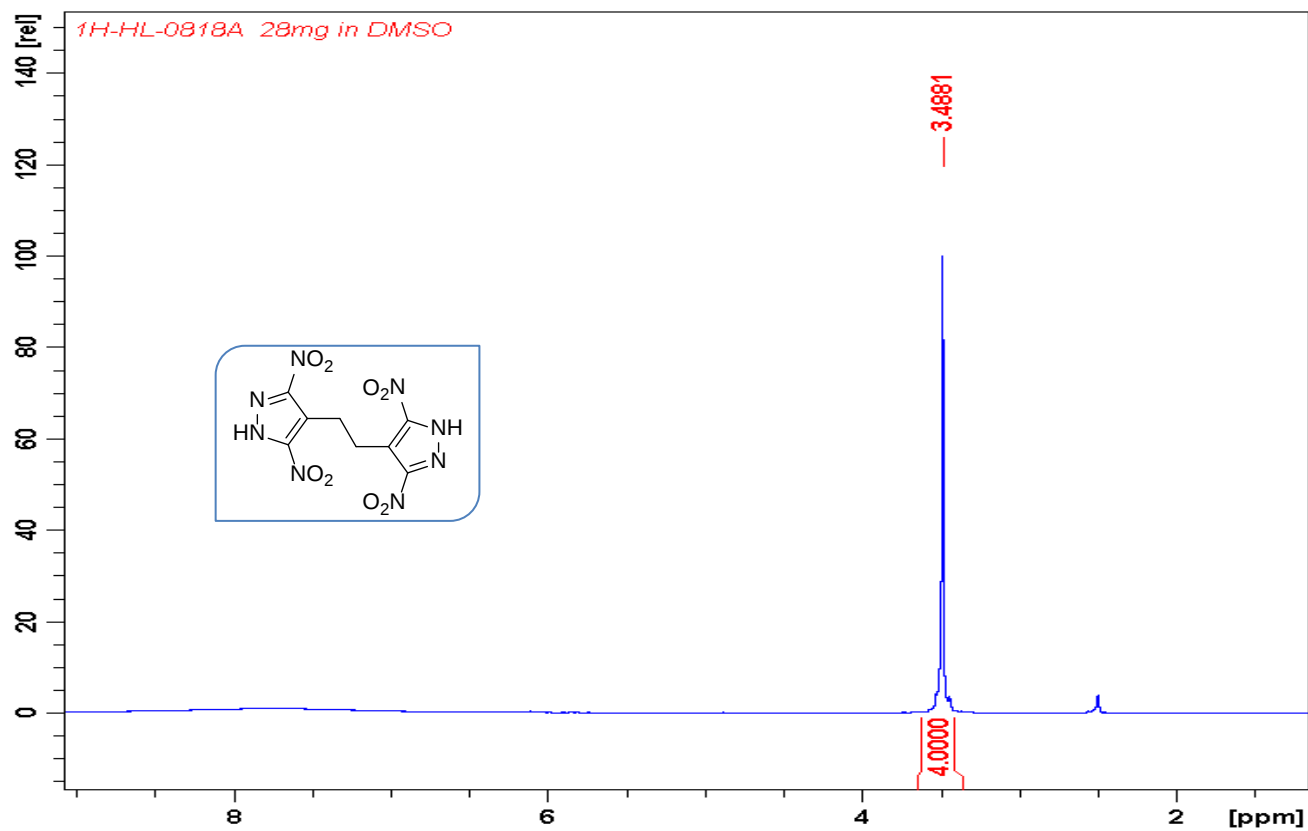


Figure S5. ¹H NMR spectrum of HL3.

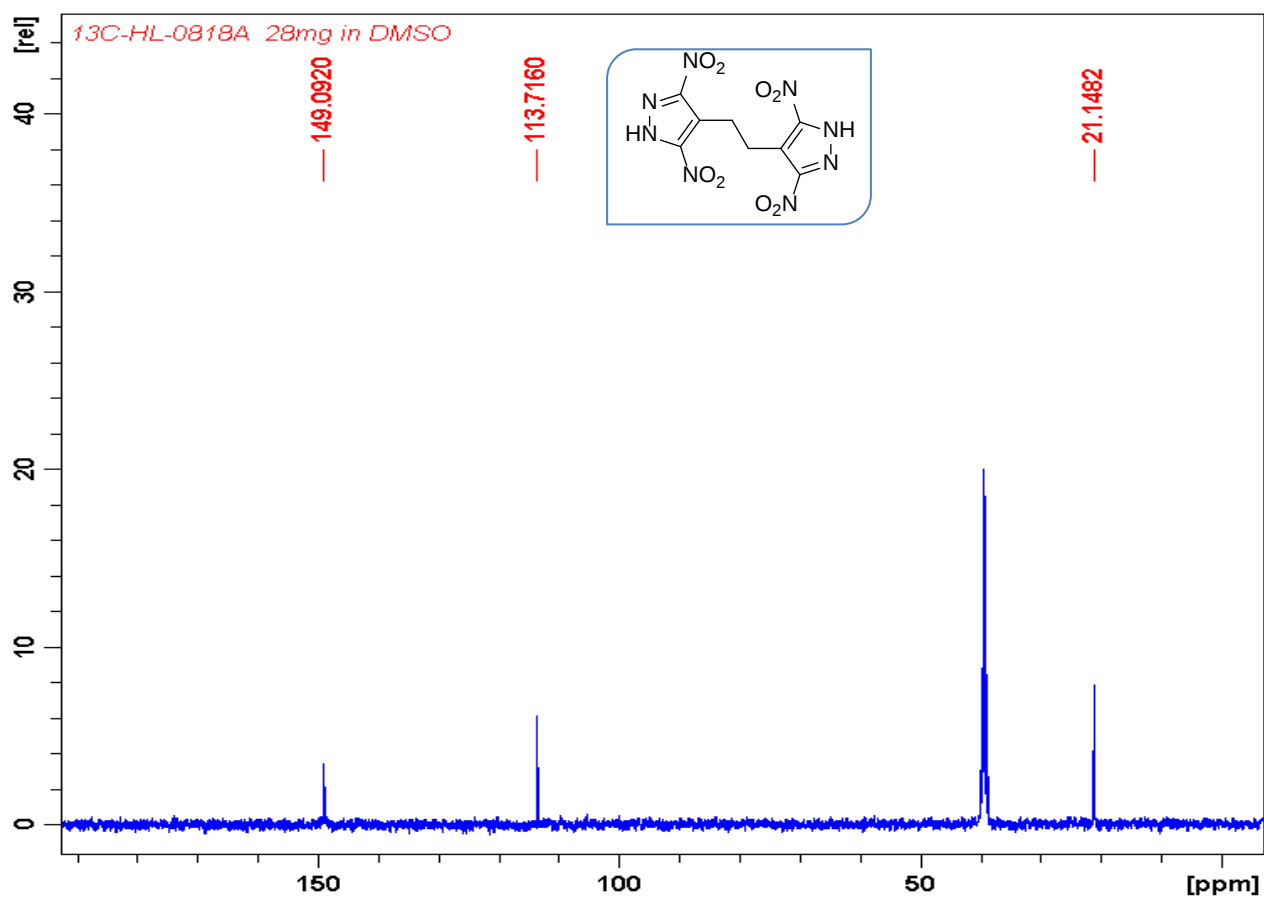
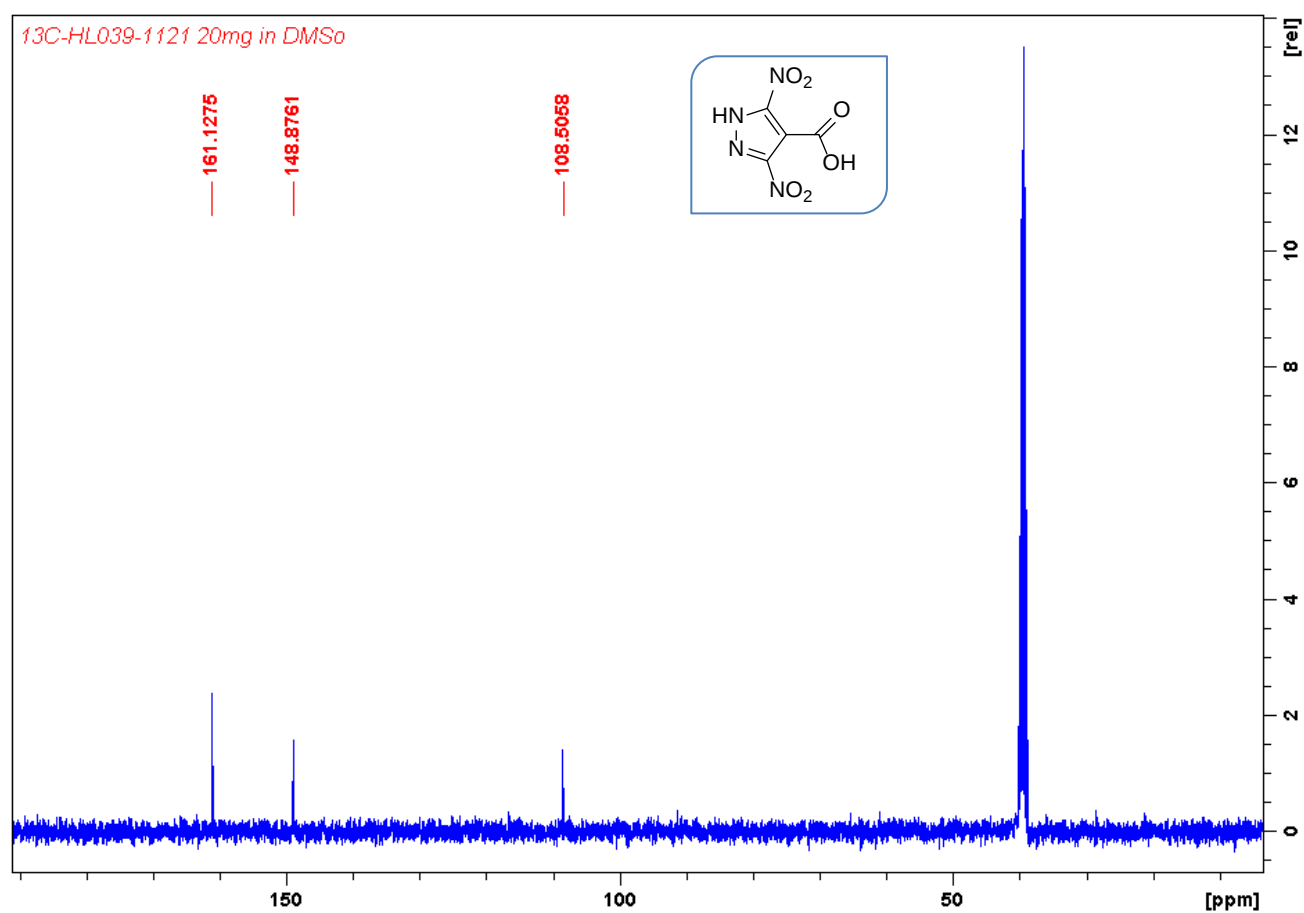
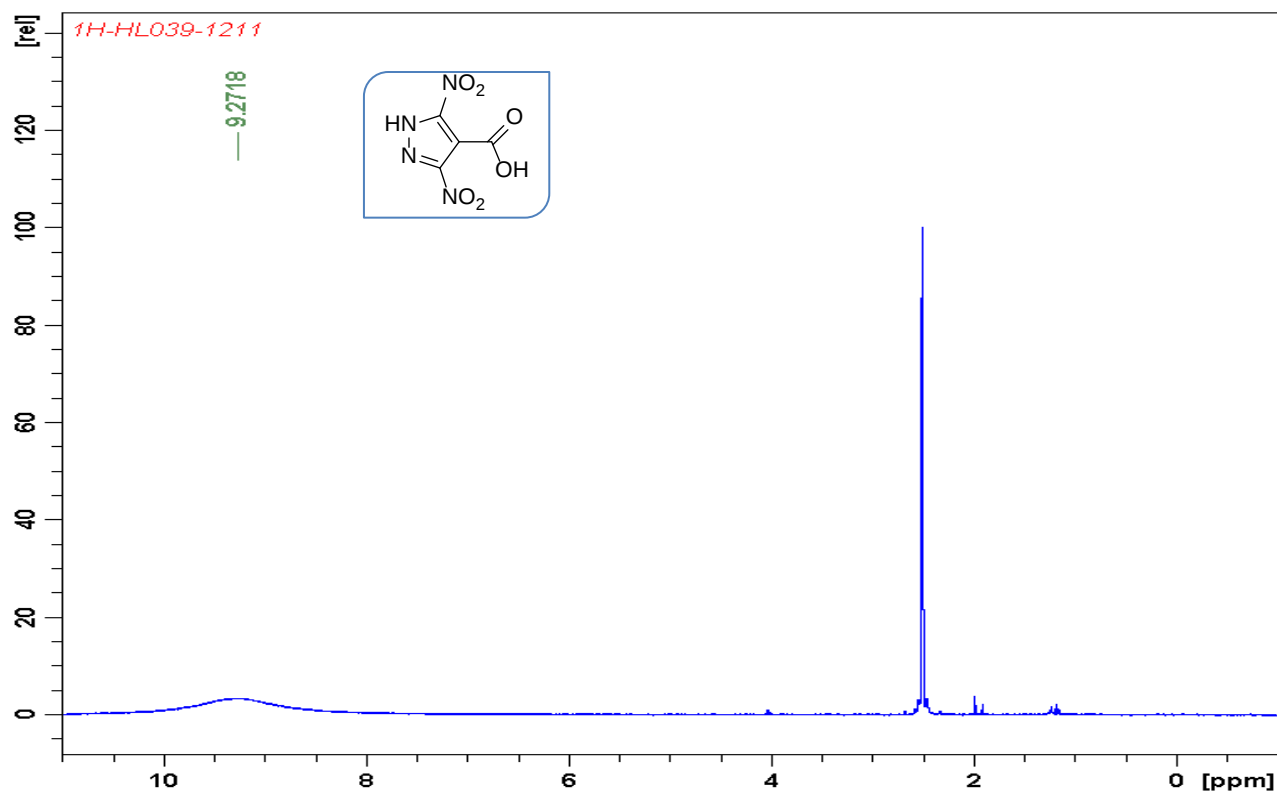
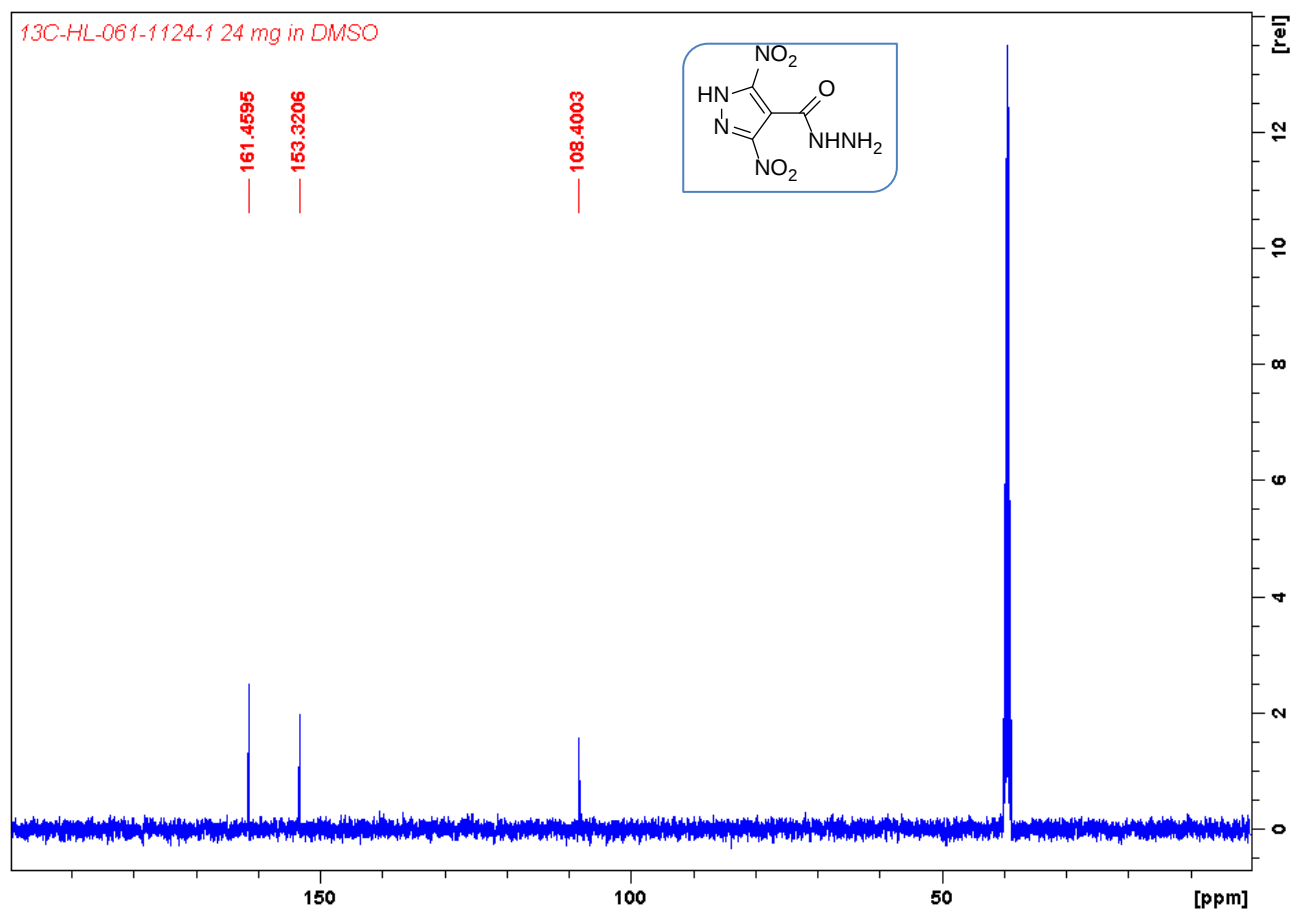
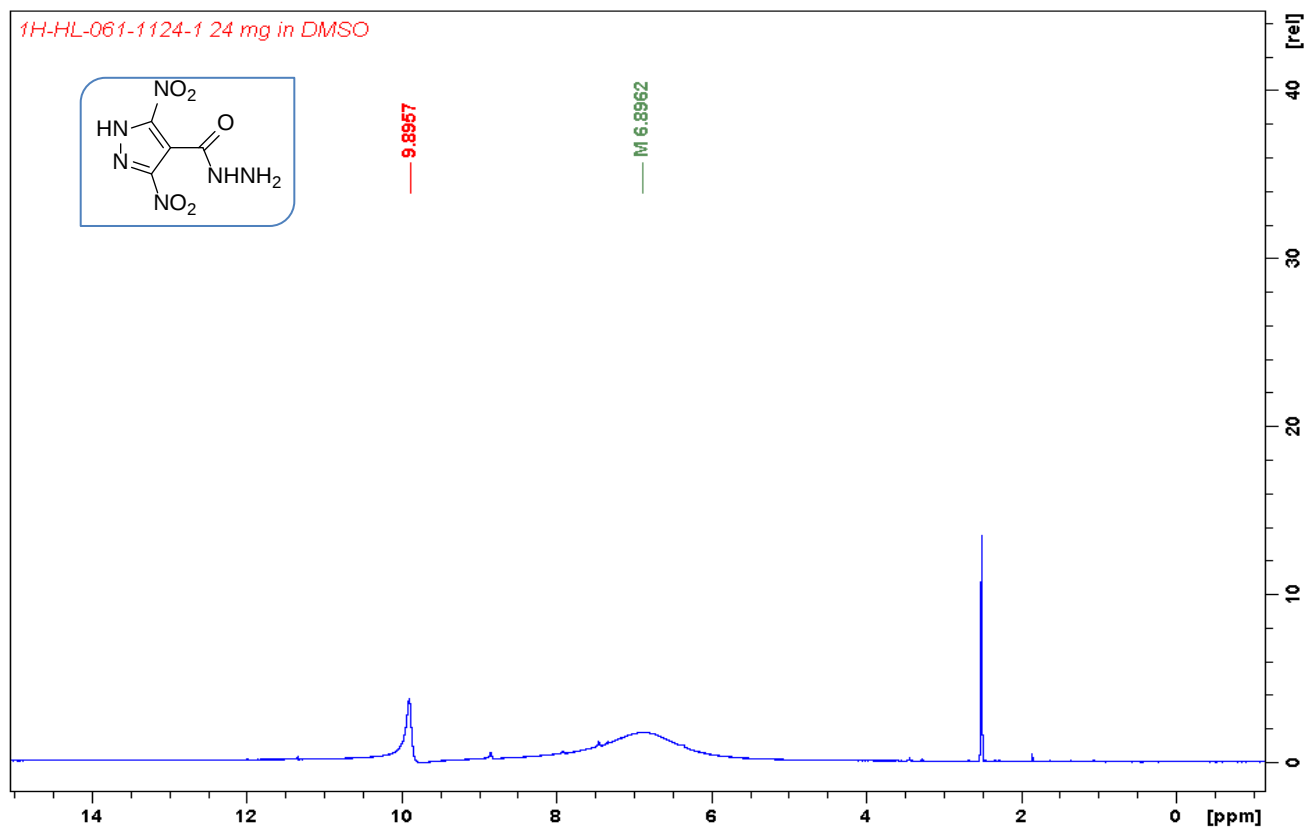


Figure S6. ¹³C NMR spectrum of HL3





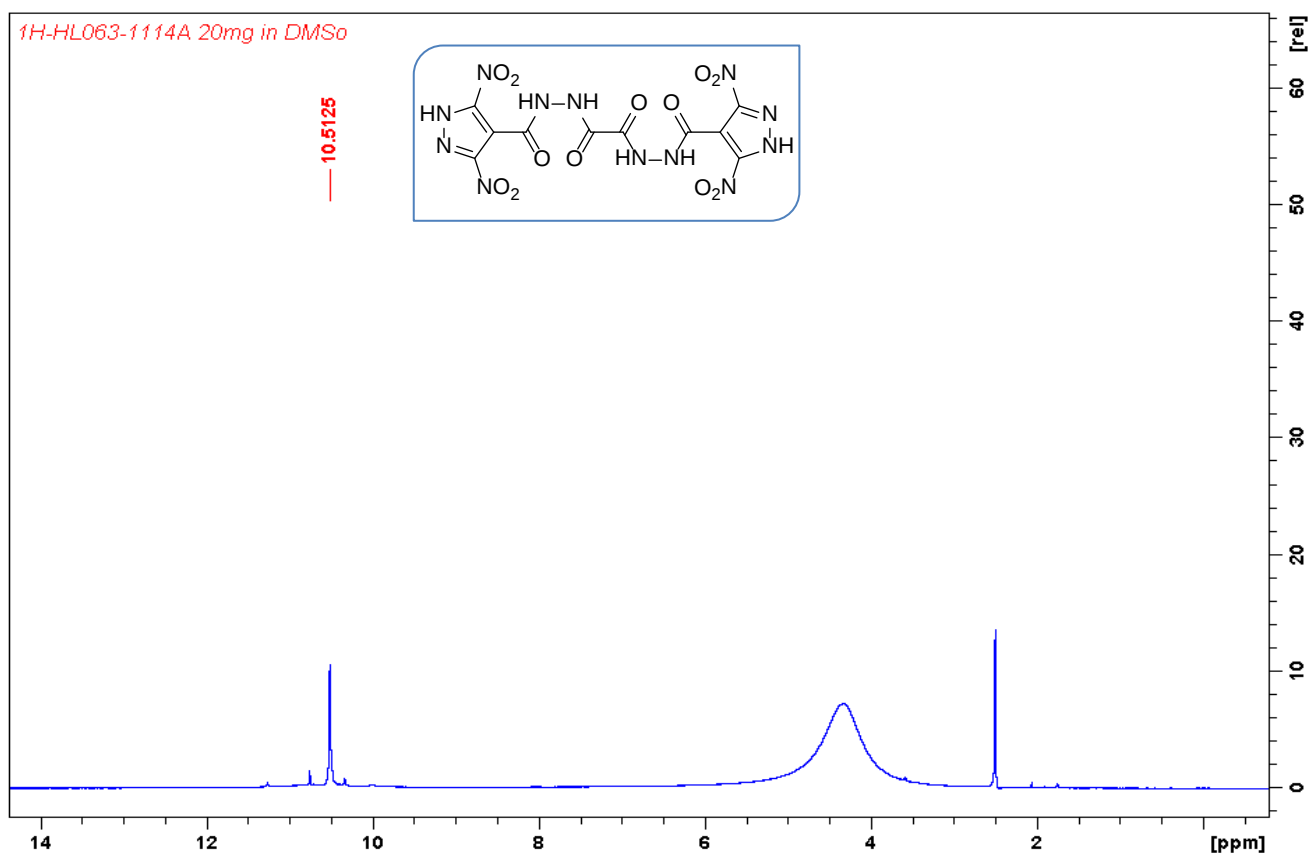


Figure S11. ¹H NMR spectrum of HL6.

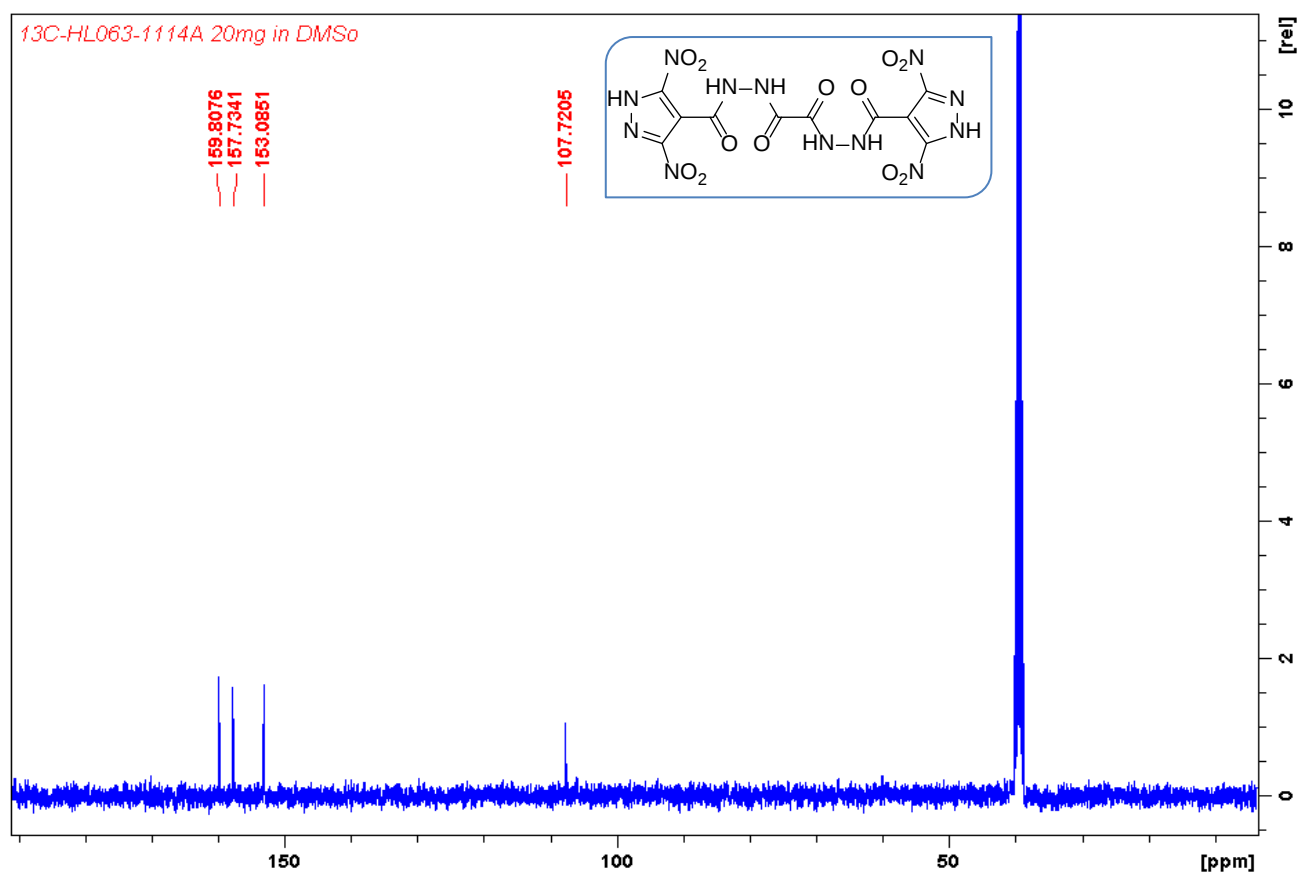


Figure S12. ¹³C NMR spectrum of HL6.

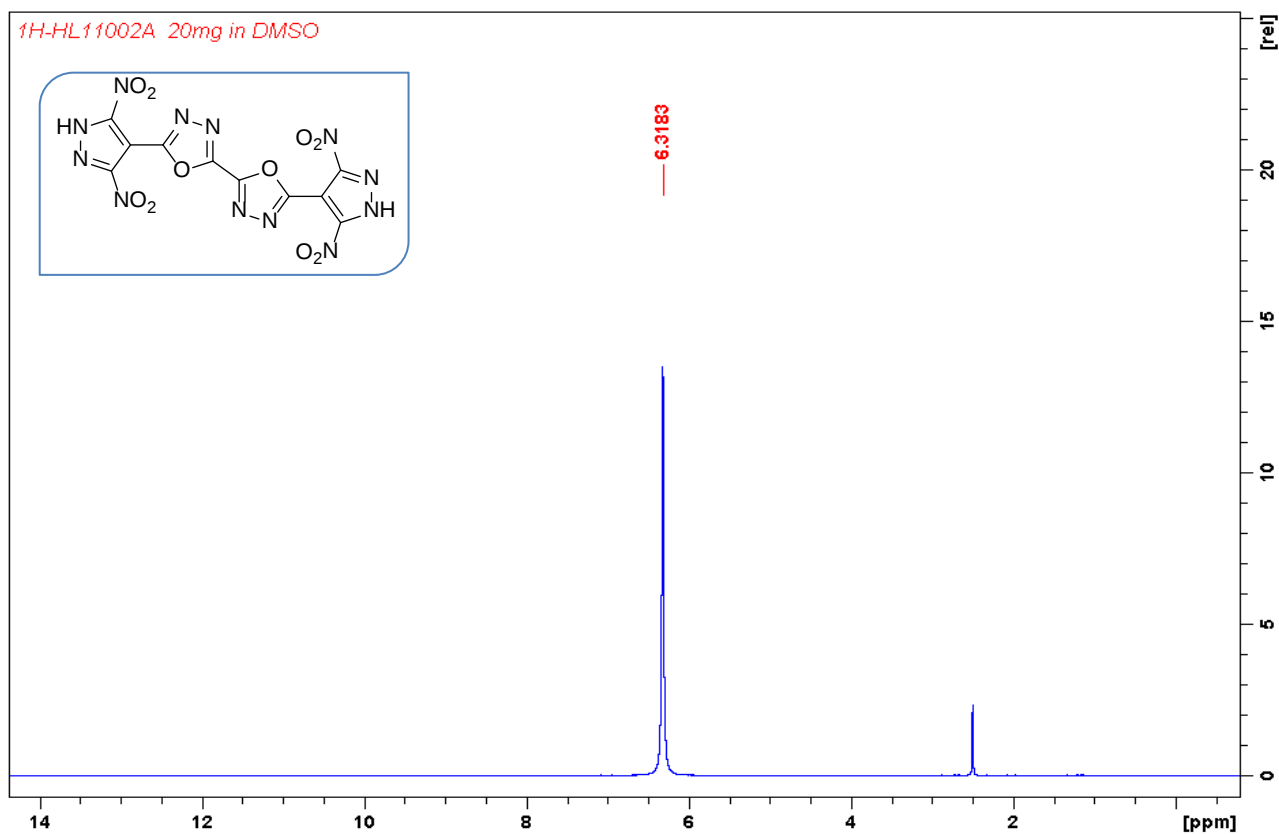


Figure S13. ^1H NMR spectrum of HL7.

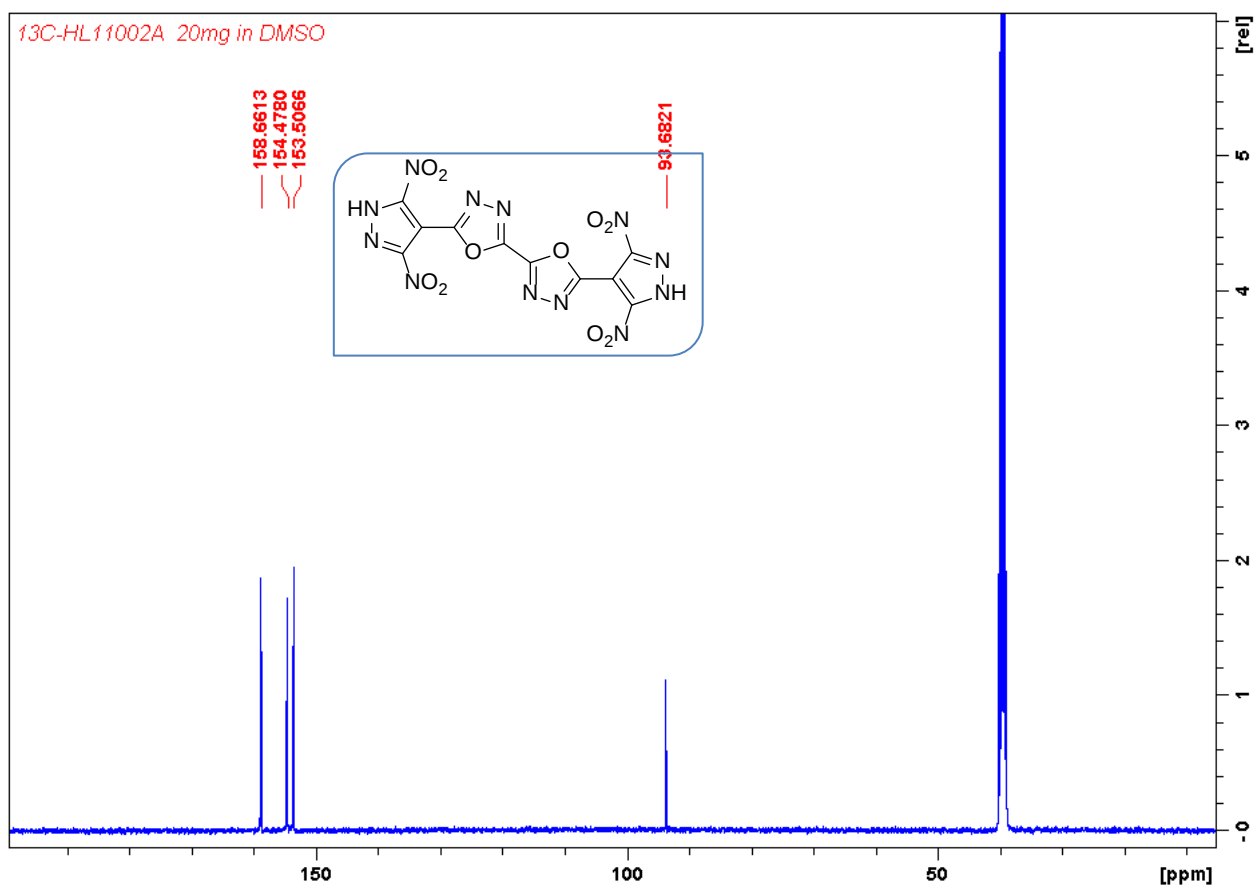


Figure S14a. ^{13}C NMR spectrum of HL7.

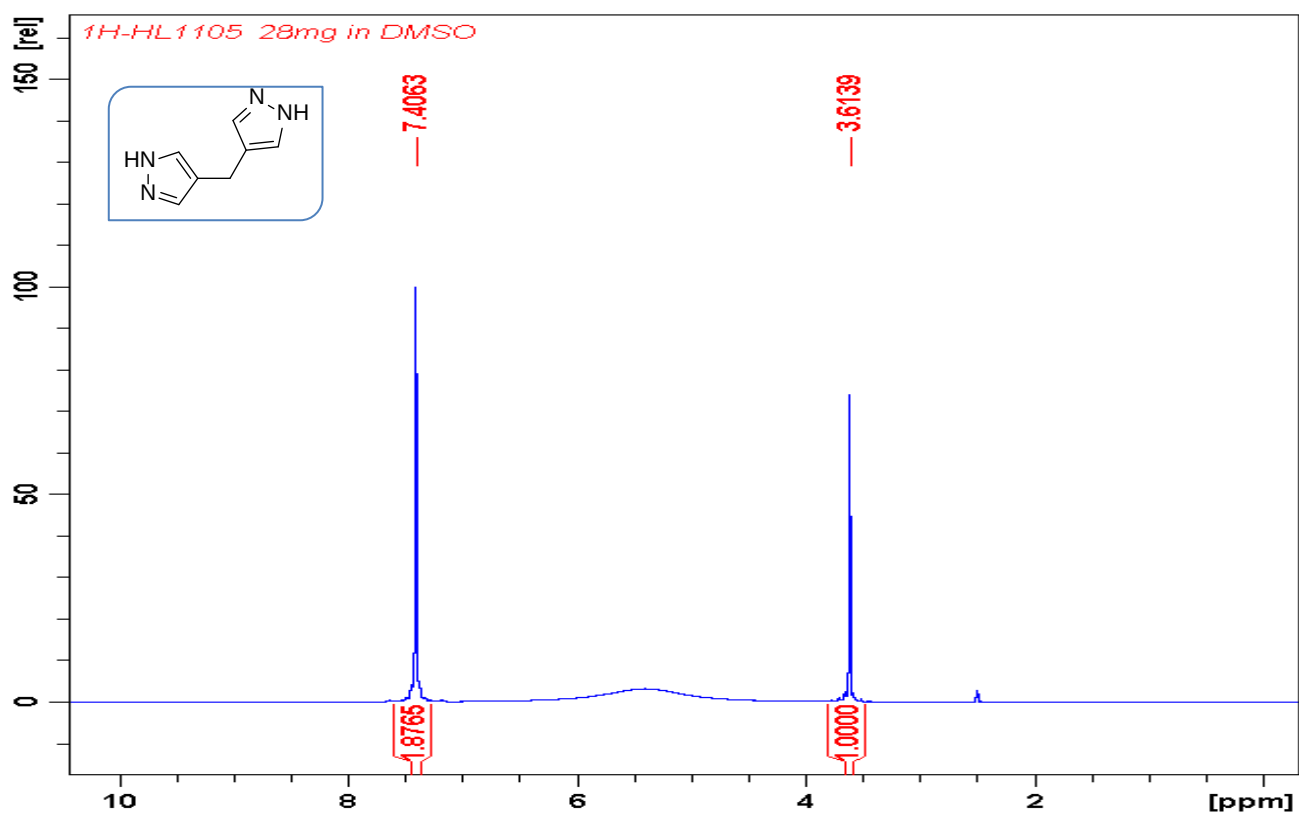


Figure S14b. ¹H NMR spectrum of HL8.

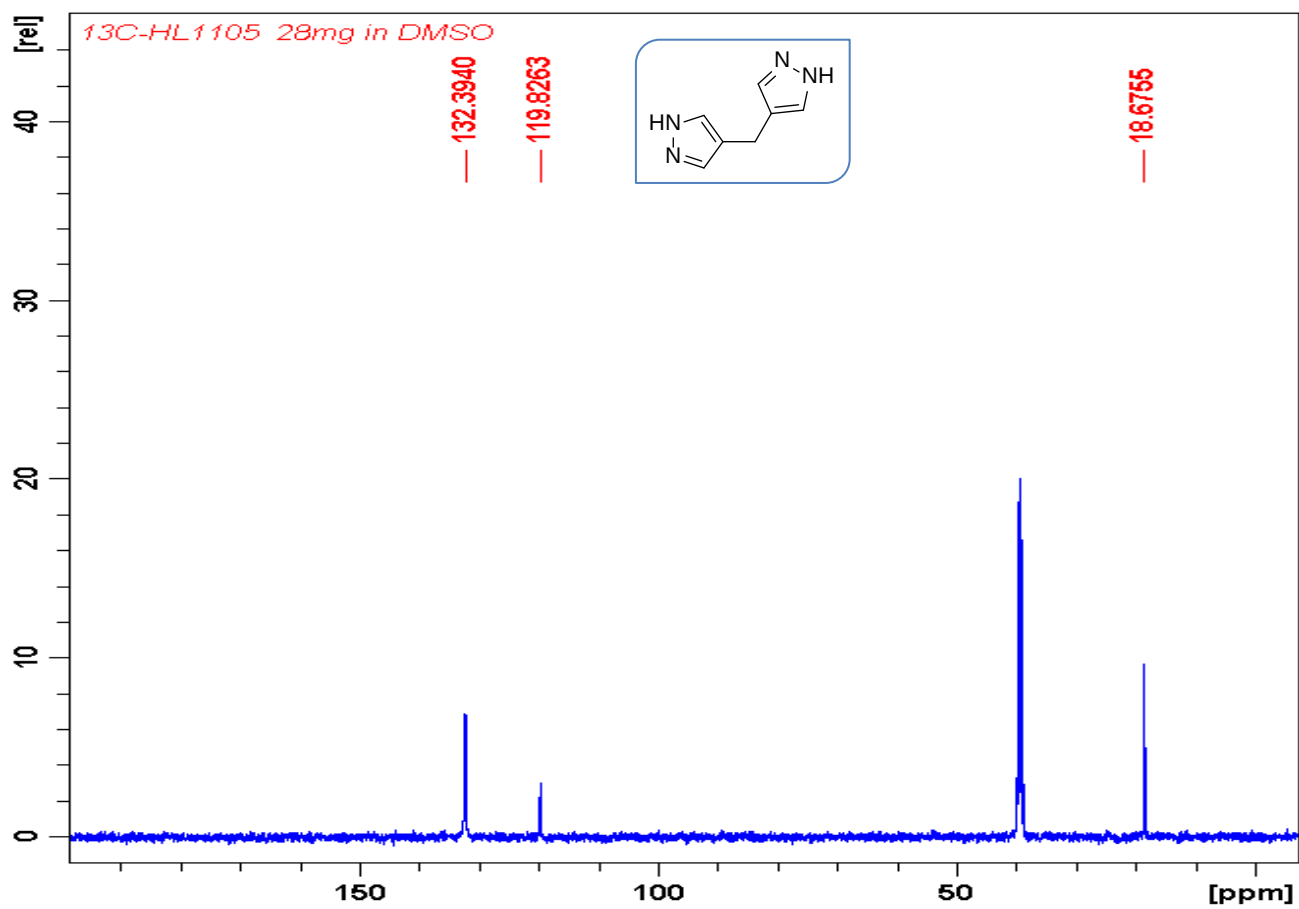


Figure S15. ¹³C NMR spectrum of HL8.

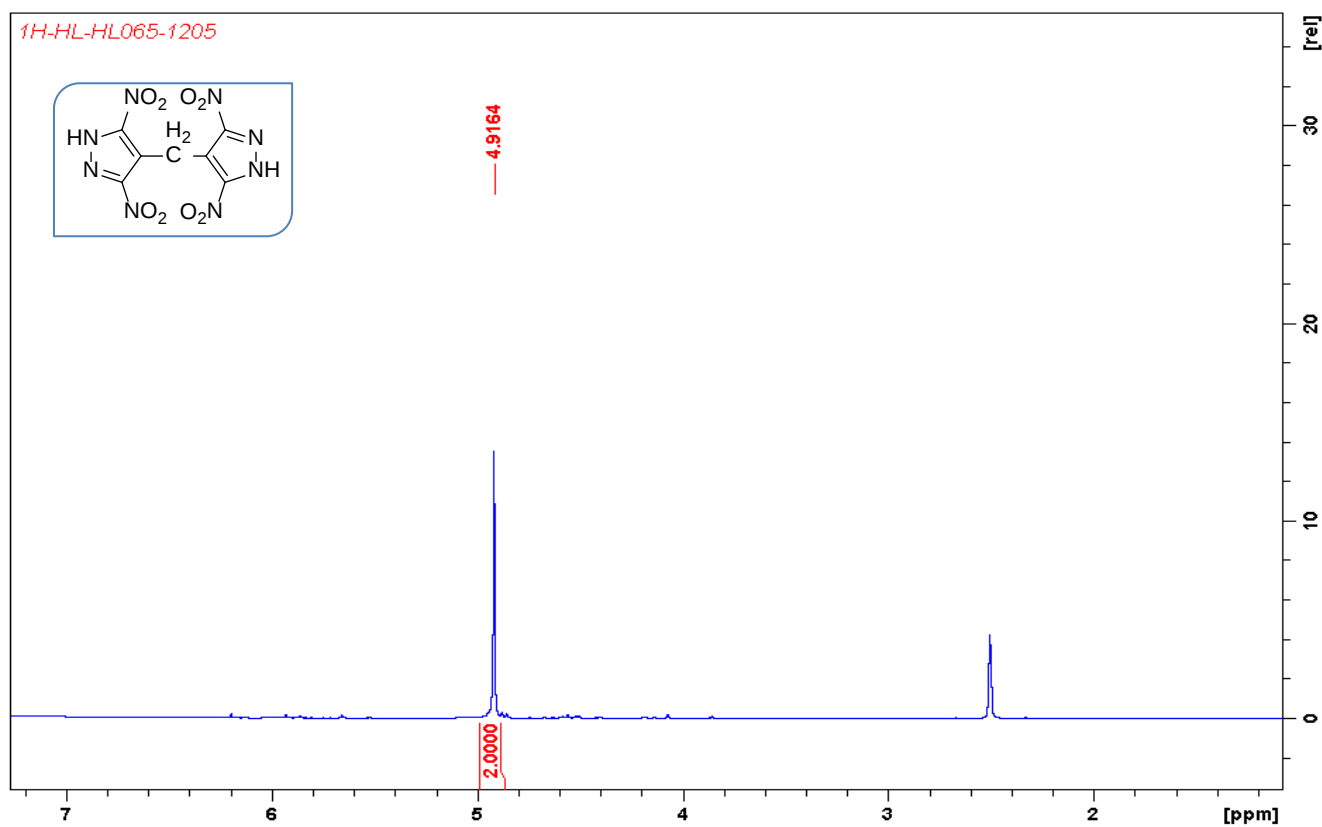


Figure S16. ^1H NMR spectrum of HL9.

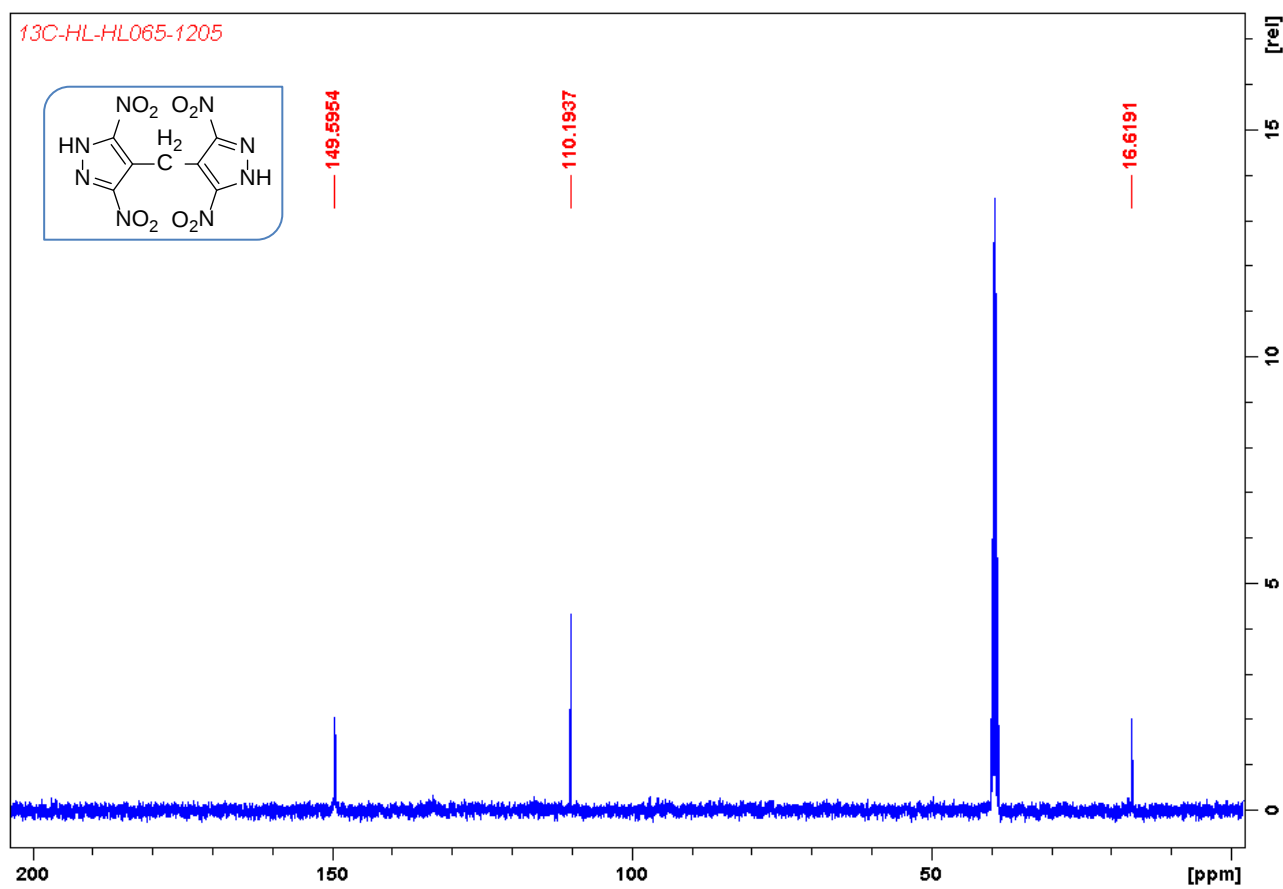


Figure S17. ^{13}C NMR spectrum of HL9.

HL-DMNP_EOM

HL

06-Nov-2018
Coll energy 3
2: MS2 ES-
2.97e7

Gozin_HL-DMNP_EOM 14 (0.243) Cm (7:20)

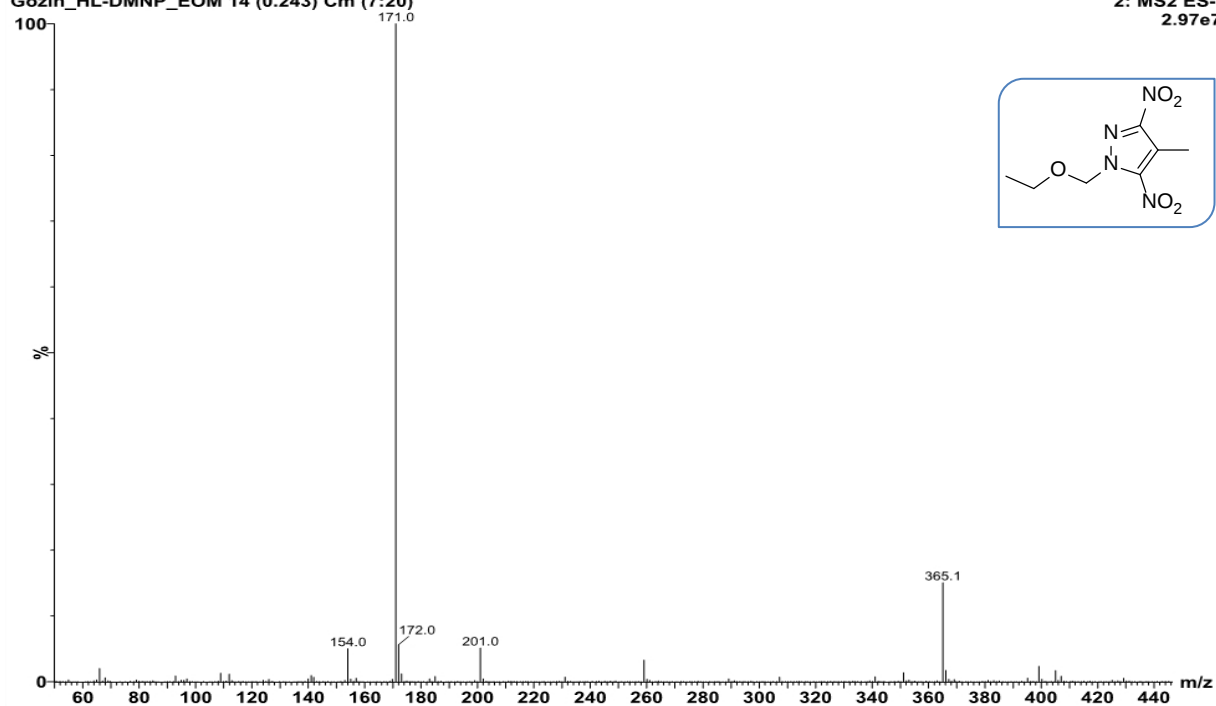


Figure S18. MS spectrum of HL1.

HL054

HL

06-Nov-2018
Coll energy 3
2: MS2 ES-
2.92e7

Gozin_HL054 11 (0.191) Cm (8:16)

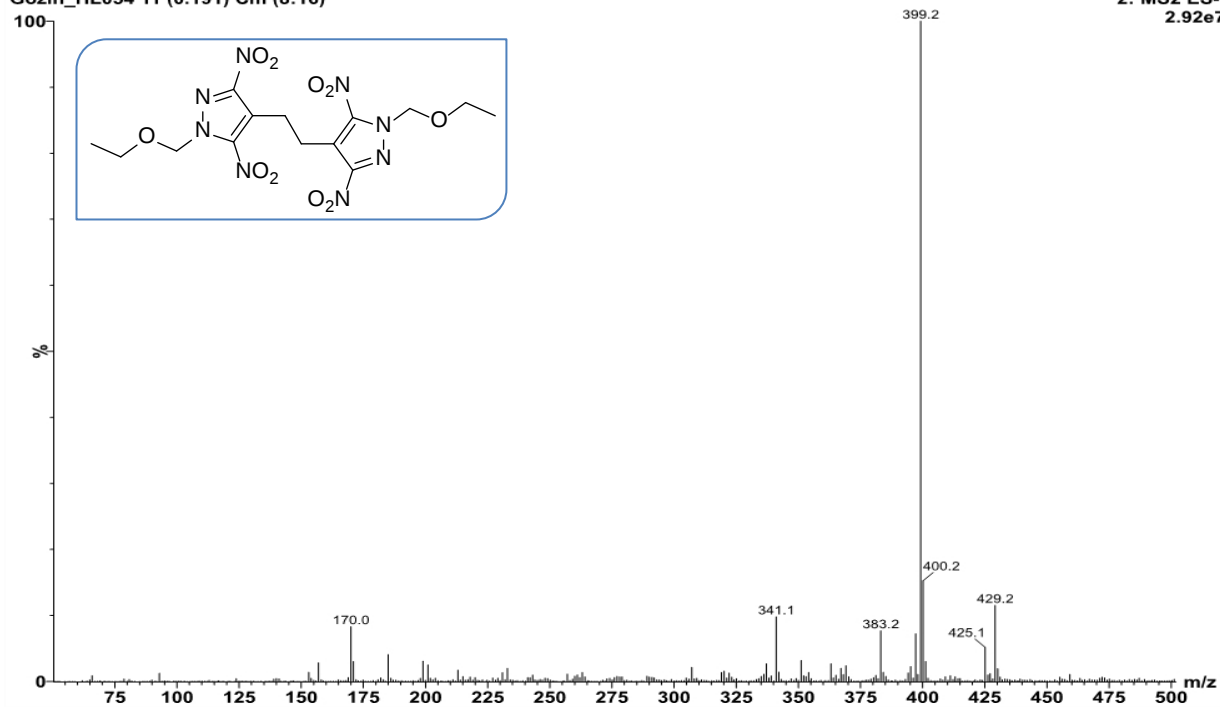


Figure S19. MS spectrum of HL2.

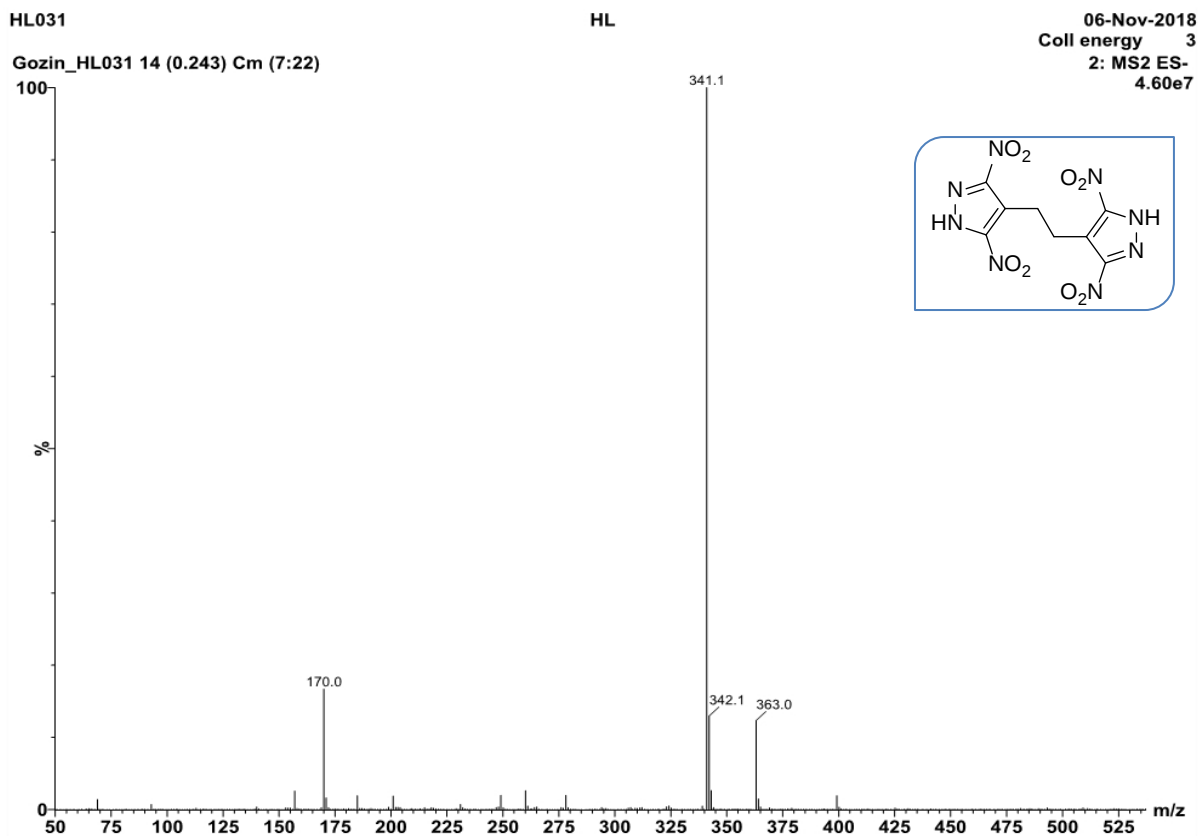


Figure S20. MS spectrum of HL3.

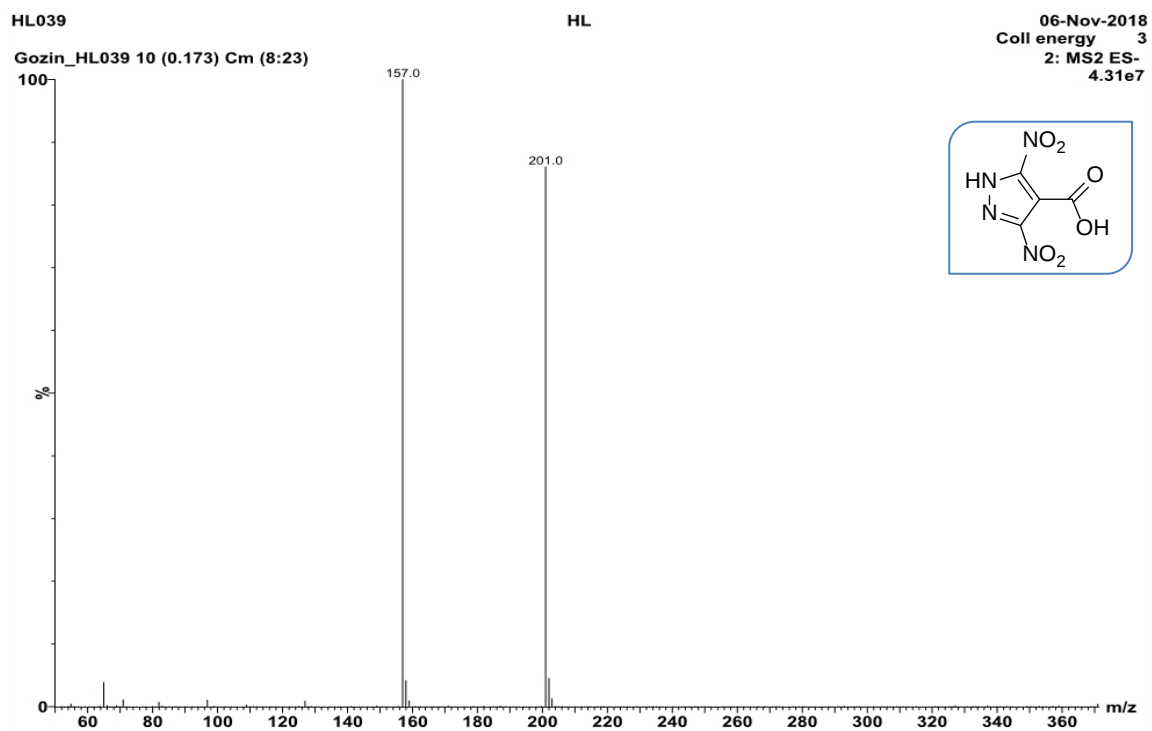


Figure S21. MS spectrum of HL4.

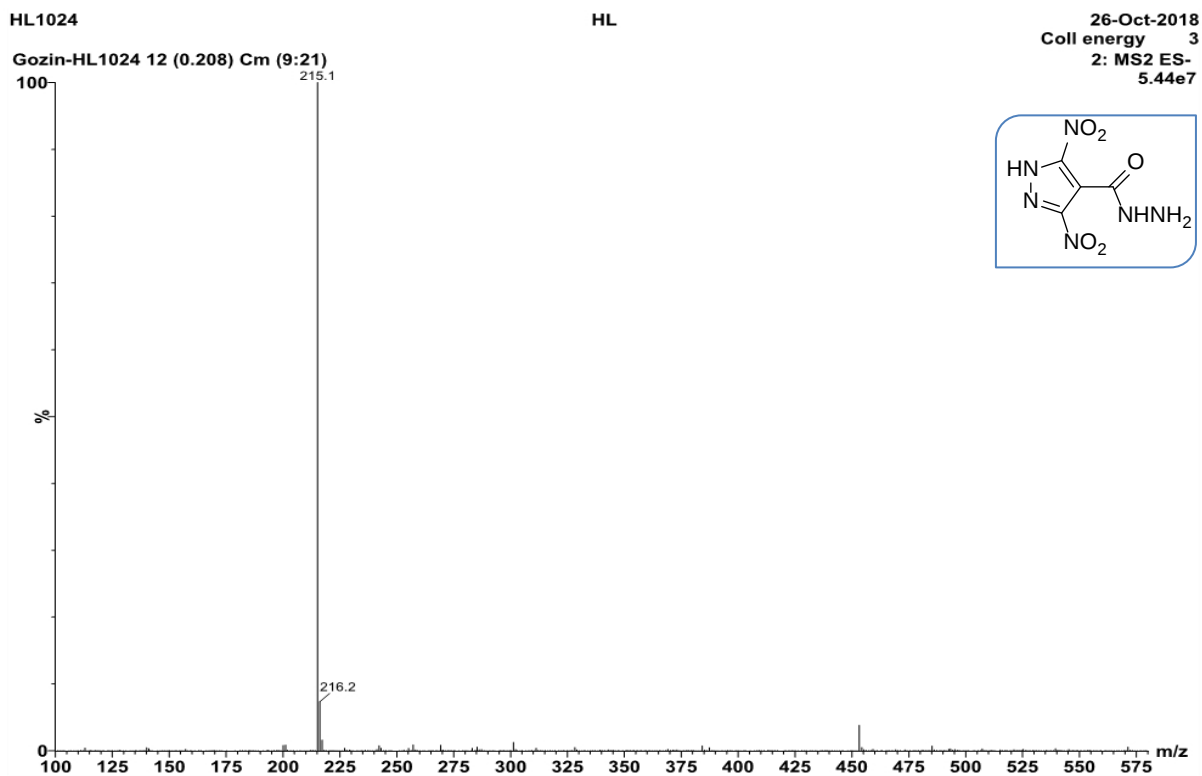


Figure S22. MS spectrum of HL5.

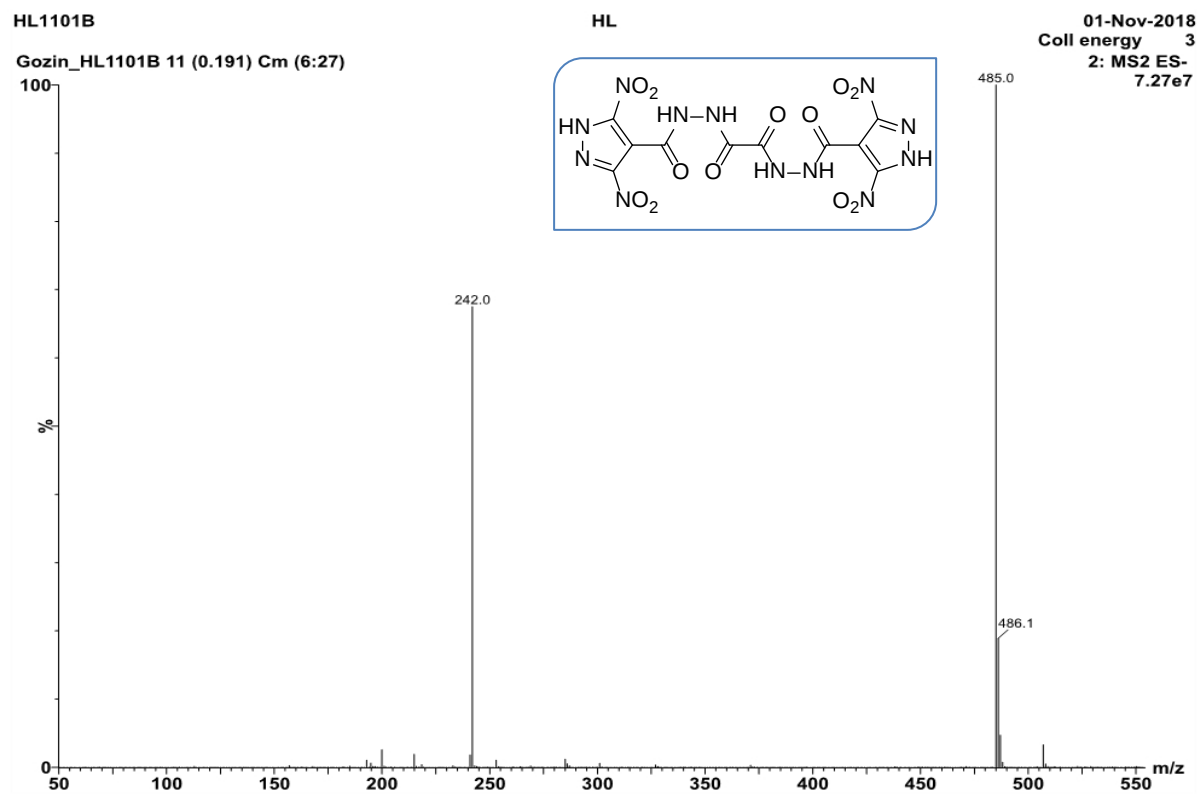


Figure S23. MS spectrum of HL6.

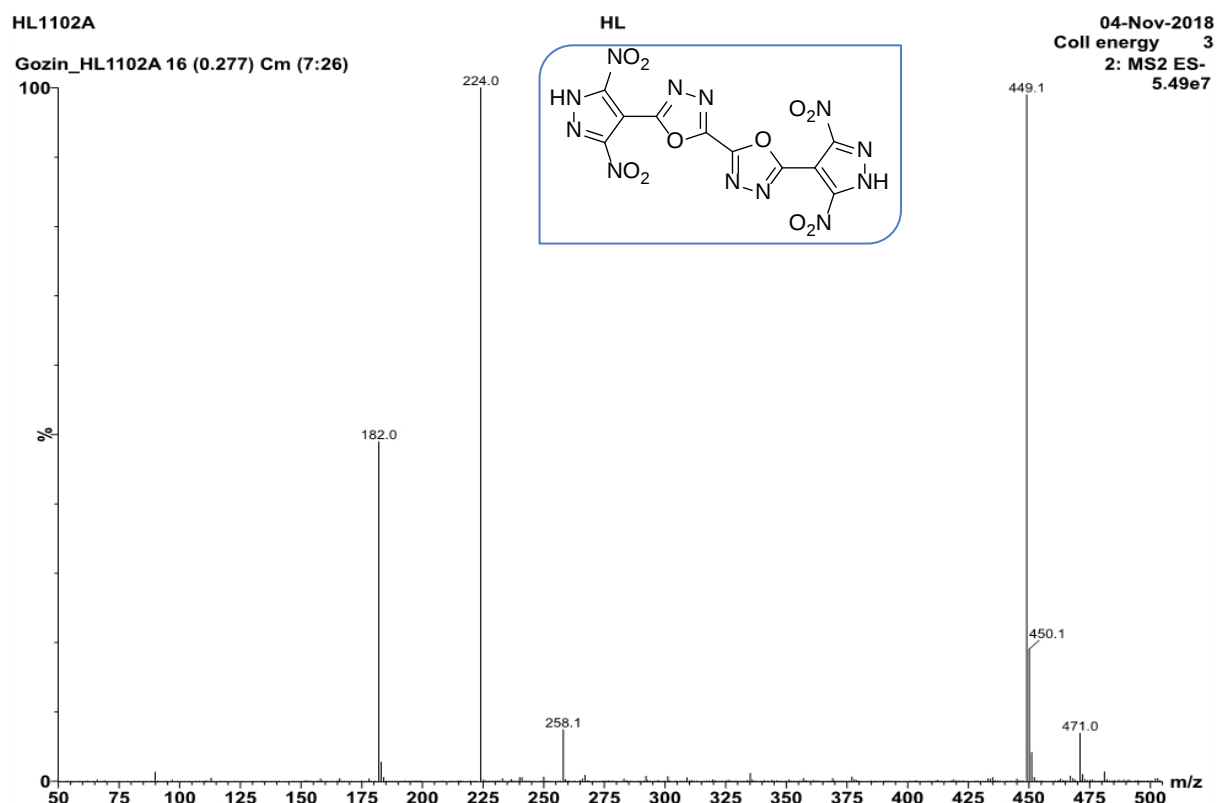


Figure S24. MS spectrum of HL7.

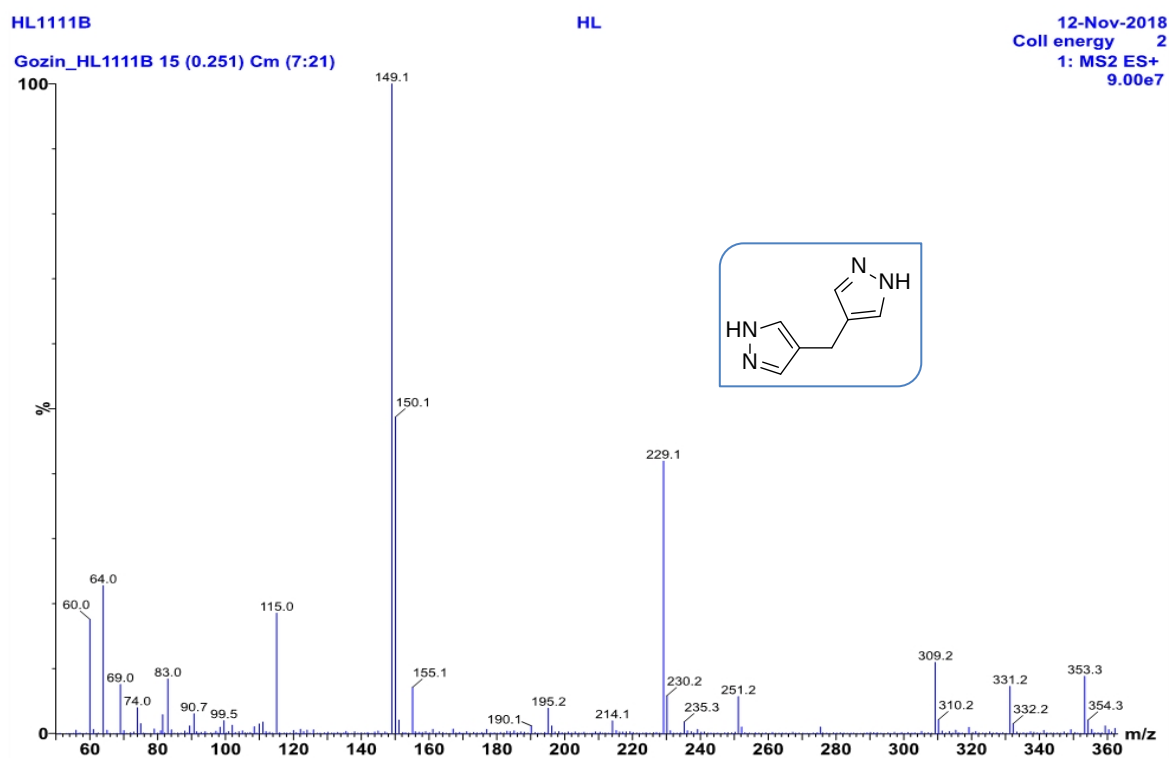


Figure S25. MS spectrum of HL8.

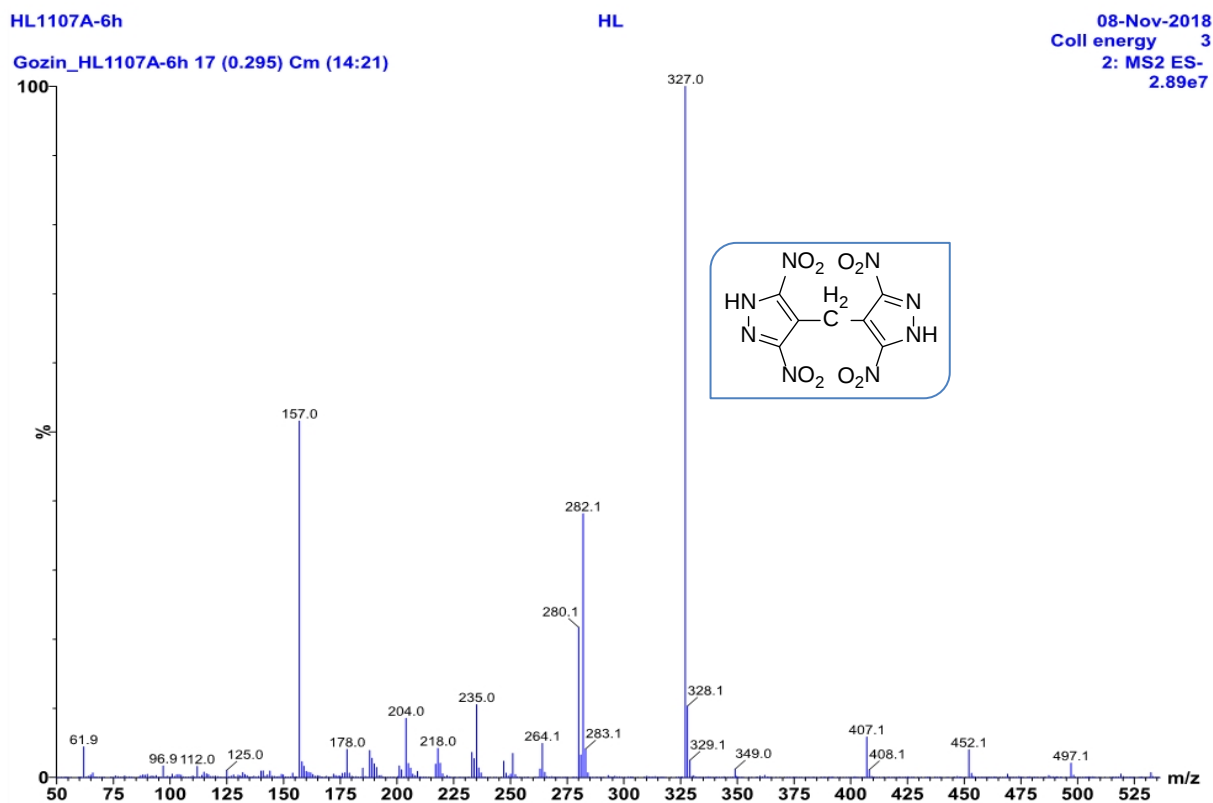


Figure S26. MS spectrum of HL9.

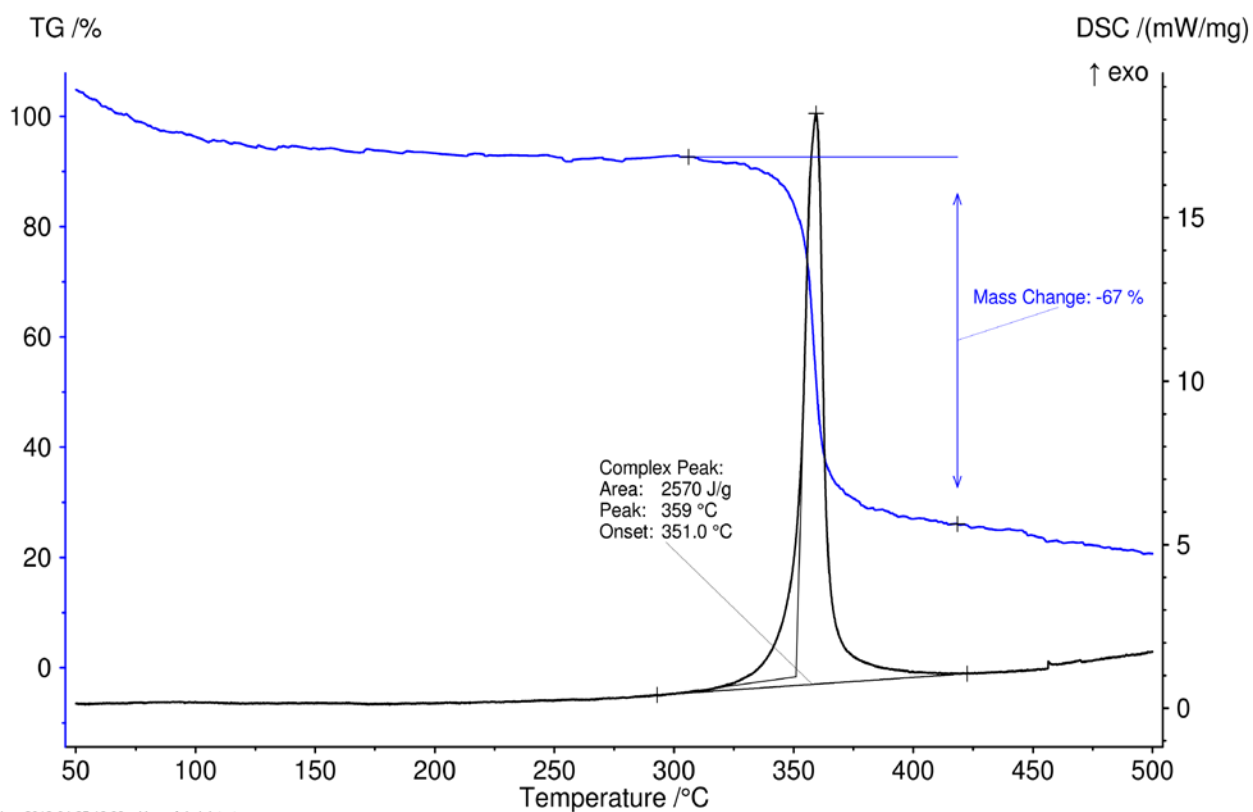


Figure S27. DSC and TG thermograms of HL3.

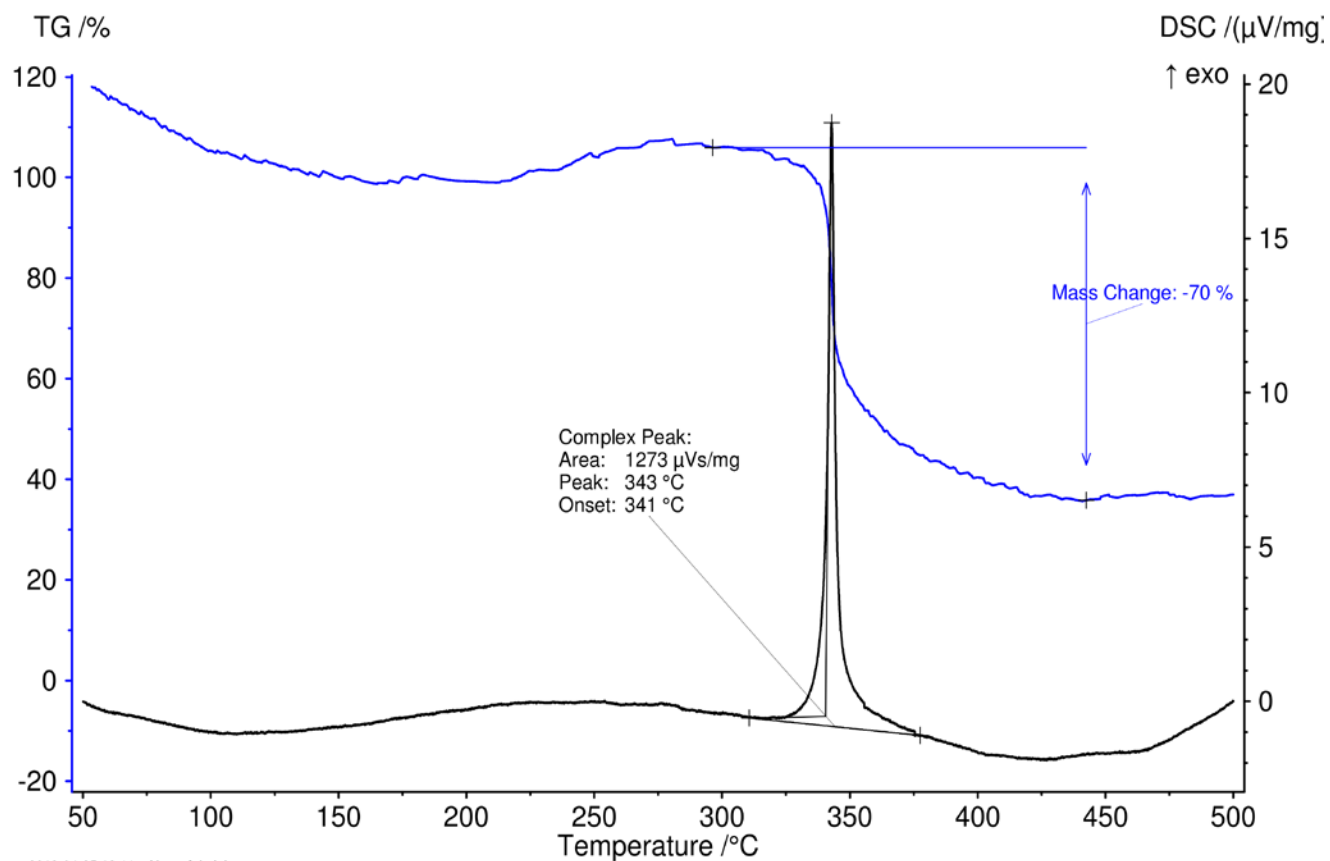


Figure S28. DSC and TG thermograms of **HL7**.

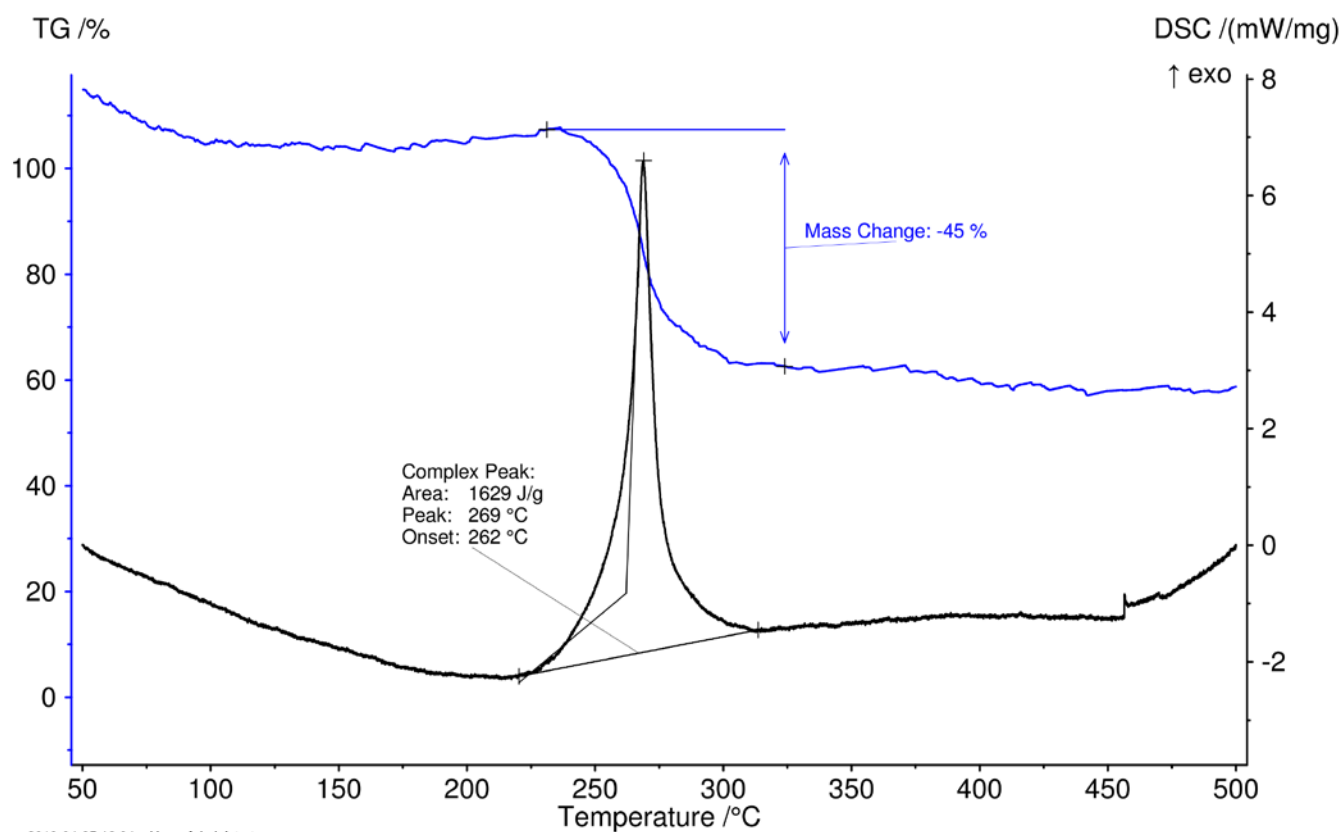


Figure S29. DSC and TG thermograms of **HL9**.

3. X-ray Crystallography

Table S1. X-ray Crystallography data for synthesized compounds

Compound	4-MDNP	HL3	HL7	HL9
Formula	C4H4N4O4	C8H6N8O8	C10H6 N12 O12	C7 H4 N8 O8
<i>Mr</i>	172.11	342.21	486.27	328.18
<i>T</i> /K	173	173	173	173
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P2 ₁ /c	P2 ₁ /c	<i>Cc</i>	P2 ₁ /c
<i>a</i> /Å	11.648(5)	11.325(10)	17.626(5)	10.141(3)
<i>b</i> /Å	6.027(3)	5.811(5)	14.273(4)	9.516(2)
<i>c</i> /Å	9.805(4)	10.418(9)	7.2055(19)	12.412(3)
<i>a</i> /°	90	90	90	90
<i>b</i> /°	97.078(9)	113.593(19)	106.048(7)	91.173(7)
<i>g</i> /°	90	90	90	90
Volume	683.1(5)	628.2(9)	1742.1(8)	1197.5(5)
<i>Z</i>	4	2	4	4
ρ /g·cm ⁻³	1.674	1.809	1.854	1.820
Mu/mm ⁻¹	0.150	0.160	0.171	0.167
F(000)	352.0	348.0	984.0	664.0
θ /°	3.525 to 25.561	3.920 to 19.203	1.866 to 25.007	2.009 to 26.478
index range	-14 ≤ <i>h</i> ≤ 14 -6 ≤ <i>k</i> ≤ 7 -11 ≤ <i>l</i> ≤ 12	-14 ≤ <i>h</i> ≤ 13 -7 ≤ <i>k</i> ≤ 7 -13 ≤ <i>l</i> ≤ 13	-20 ≤ <i>h</i> ≤ 20 -14 ≤ <i>k</i> ≤ 16 -6 ≤ <i>k</i> ≤ 8	-11 ≤ <i>h</i> ≤ 12 -11 ≤ <i>h</i> ≤ 11 -15 ≤ <i>h</i> ≤ 15
reflections collected	4328	4306	4146	8300
Independent reflections	1383 [R _{int} = 0.0523]	1476 [R _{int} = 0.0659]	2559 [R _{int} = 0.0681]	2464 [R _{int} = 0.0766]
data/restraints/parameters	1383/ 0 / 110	4306/ 0 /113	2559/ 16 / 319	2446/ 0 / 216
GOF on F ²	1.006	1.005	1.016	0.863
<i>R</i> ₁ [<i>I</i> > 2σ(<i>I</i>)]	0.0479	0.0598	0.0630	0.0520
<i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.1288	0.1551	0.1305	0.1329
<i>R</i> ₁ (all data)	0.0753	0.1161	0.0865	0.0970
<i>wR</i> ₂ (all data)	0.1462	0.1890	0.1455	0.1688
largest diff. peak and hole [e Å ⁻³]	0.229/ -0.228	0.283/ -0.343	0.286/ -0.333	0.230/ -0.276
CCDC	1910475	1910476	1910477	1910478

4. Performance Prediction

The heat of formation of **HL3**, **HL7** and **HL9** molecules were calculated on the basis of the isodesmic reaction by using the Gaussian 09 package. The geometric optimization and frequency analyses were performed at the B3LYP/6-31+G** level and the single energy points were calculated at the MP2/6-311++G** level. The isodesmic reactions of **HL3**, **HL7** and **HL9** are



and



respectively. The enthalpies of the building-block molecules were obtained by using the atomization method (Please refer to the supporting information for the detailed energetics.) By such a way, the heat of formation of **HL3**, **HL7** and **HL9** molecules were calculated to be 301.7 kJ/mol, 561.9 kJ/mol and 324.7 kJ/mol, respectively. The detailed parameters and results are shown in Table S2.

Table S2. Parameters and results of the isodesmic reactions of the HL3, HL7 and HL9 molecules.

	$\Delta fH^\circ_{\text{gas}}$ (kJ/mol)	E0 (Hartree)	ZPE (Hartree/particle)	ΔHT (Hartree/particle)
HL3	301.70	-1347.45	0.19	0.02
CH ₄	-74.87	-40.48	0.04	0.00
CH ₃ NO ₂	-81.00	-244.95	0.05	0.01
C ₄ H ₁₀	-125.60	-158.34	0.13	0.01
C ₃ H ₄ N ₂	179.40	-226.10	0.07	0.00
HL7	561.90	-1790.51	0.18	0.03
CH ₄	-74.87	-40.48	0.04	0.00
CH ₃ NO ₂	-81.00	-244.95	0.05	0.01
C ₂ H ₆	-84.00	-79.77	0.07	0.00
C ₃ H ₄ N ₂	179.40	-226.10	0.07	0.00
C ₂ H ₂ N ₂ O	63.24	-262.01	0.05	0.00
HL9	324.70	-1308.16	0.16	0.02
CH ₄	-74.87	-40.48	0.04	0.00
CH ₃ NO ₂	-81.00	-244.95	0.05	0.01
C ₃ H ₈	-104.70	-119.06	0.10	0.01
C ₃ H ₄ N ₂	179.40	-226.10	0.07	0.00

Table S3. Detonation performance of **HL3**, **HL7**, **HL9** and HNS EMs calculated by HASEM, for a comparison with the EXPLO 5 results.

Compounds		Detonation Velocity (km/s)	Detonation Pressure (GPa)	Heat of Explosion (kcal/kg)	Explosion Temp. (K)
HL3	HASEM	7.83	28.19	1188.35	3696
	EXPLO 5	7.92	26.18	-	-
HL7	HASEM (with solvent)	7.66	26.91	1027.94	3570
	EXPLO 5 (without solvent)	8.27	28.99	-	-
HL9	HASEM	7.96	28.98	1247.07	4090
	EXPLO 5	8.15	28.24	-	-
HNS	HASEM	7.34	24.12	1359.29	4053
	EXPLO 5	7.61	24.30	-	-
	Exp.	7.0-7.13 ^[1, 2]	26.20 ^[1]	1360 ^[1]	4150 (other cal.) ^[3]

5. Field Detonation Experiments

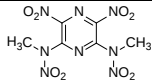
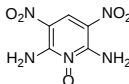
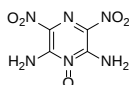
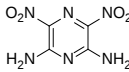
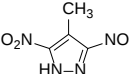
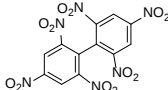
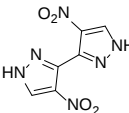
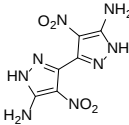
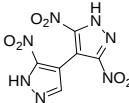
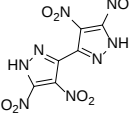
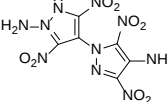
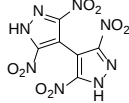
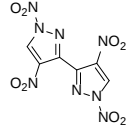
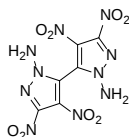
Table S4. Detonation Experiments Frame Cuts from High-speed Videos

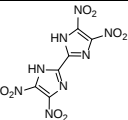
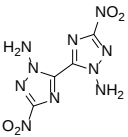
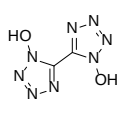
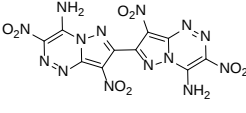
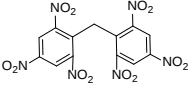
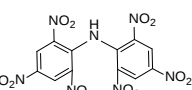
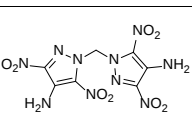
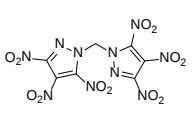
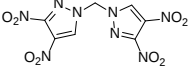
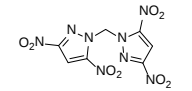
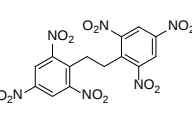
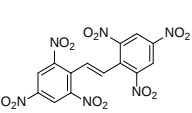
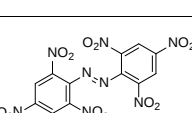
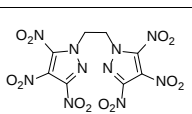
	Sample	Before Detonation	Moment of Fuse Detonation	Charge Detonation	Detonation Propagation	Maximum Size Fire Cloud
1.	H ₂ O (reference, fuse only)					
2.	HNS (#1; reference)					
3.	HNS (#2; reference)					
4.	HL3 (#1)					
5.	HL3 (#2)					
6.	HL7					

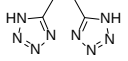
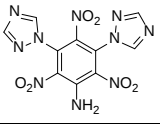
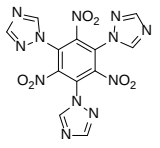
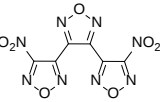
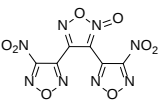
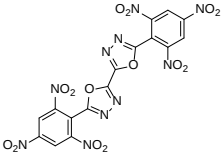
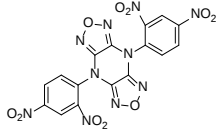
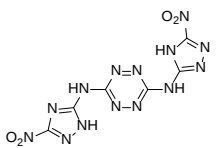
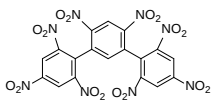
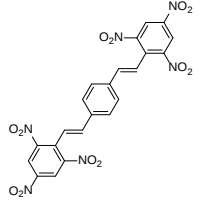
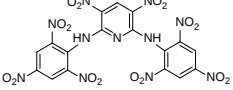
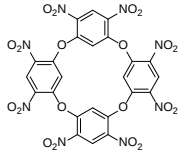
6. Computational and Additional Experimental Data

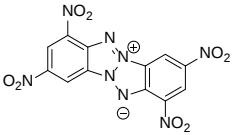
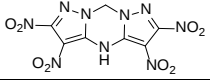
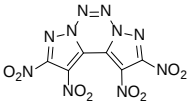
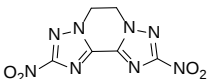
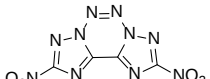
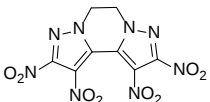
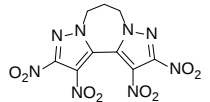
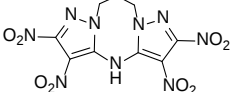
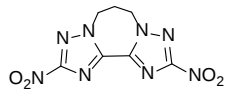
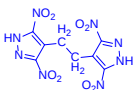
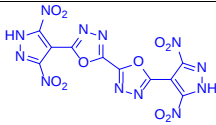
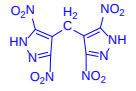
Table S5. Reported melting and decomposition temperatures that were determined by DSC and DTA techniques, at various heating rates, for all 63 EMs that were mentioned in this study.

Comp. Label	CAS No.	Structures	Measured Thermal Properties			
			T _m (°C)	DSC peak (°C); heating rate (°C·min ⁻¹)	DSC onset (°C); heating rate (°C·min ⁻¹)	DTA onset (°C); heating rate (°C·min ⁻¹)
A1	99-35-4		122.7 ^[4]			
A2	489-98-5		192.0 ^[5]			
A3	1630-08-6		286.0 ^[6]			
A4	3058-38-6			366.4 (5) ^[7]		
A5	56140-58-0		no melting			275.0 ^[8]
A6	97217-74-8		240.0 ^[9]			
A7	118-96-7		78.6 ^[10]	303.4 (5) ^[10]		
A8	134282-42-1		no melting		232.0 (5) ^[11]	
A9	39771-28-3		no melting	321.6 (10) ^[12]		
A10	78013-51-1		162.0 (6) ^[13]			
A11	25242-76-6		no melting			170.0 (6) ^[13]

A12	436848-40-7		no melting	160.0 ^[14]		
A13	132683-64-8		no melting	350.7 (10) ^[15]		
A14	194486-77-6		no melting ¹⁶	345.3 (5) ^[16]		
A15	52173-59-8		no melting		357.0 (10)	
A16	1246853-06-4		211.0 ^[17]			
B1	4433-16-3		242.0 ^[18]			
B2	131394-28-0		305.0 ^[19]		365.0 (5) ^[19]	
B3	2243211-28-9		no melting		228.0 (5) ^[20]	
B4	1262155-57-6		306.0 ^[21]			314.0 (5) ^[21]
B5	152678-74-5		209.0 ^[19]		243.0 (5) ^[19]	
B6	1573131-04-0		377.0 ^[21]			382.0 (5) ^[21]
B7	131394-26-8		292.0 ²²			298.0 (5) ²²
B8	1006545-77-2		no melting		205.5 (5) ^[19]	
B9	2215034-55-0		209.0 ^[22]		253.2 (5) ^[22]	

B10	131394-26-8		no melting ^[23]]		290.0 (5) ^[23]	
B11	1605347-16-7		241.0 ^[24]			
B12	134293-22-4				214.0 (5) ^[25]	
B13	2243696-54-8		no melting		315.1(5) ^[20]	
C1	32255-27-9		231.0 ^[26]			
C2	131-73-7		254.0 ^[27]	275.0 (10) ^[27]		
C3	2072820-21-2		no melting		310.0 (5) ^[28]	
C4	2072820-20-1		no melting		205.0 (5) ^[28]	
C5	NA		156.0 ^[29]		319.0 (5) ^[29]	
C6	NA		191.0 ^[29]		330.0 (5) ^[29]	
C7	5180-53-0		222.0 ^[30]	332.6 ^[30]		
C8	20062-22-0		318.0 ^[31]		318.0 (5) ^[31]	
C9	19159-68-3		219.7 ^[32]		348.1 (10) ^[32]	
C10	1644578-17-5		203.6 ^[33]		249.9 (5) ^[33]	

C11	26670-16-6		250.0 ^[34]	266.0 (5) ^[34]		
D1	1198599-46-0		no melting		293.9 (10) ^[35]	
D2	1198599-36-8		no melting		223.5 (10) ^[35]	
D3	782438-60-2		82.6 ^[36]	186.0 (10) ^[36]		
D4	371951-09-6		109.0 ^[10]	272.0 (5) ^[10]		
D5	2095393-79-4		no melting		335.0 (5) ^[31]	
D6	1819967-31-1				354.0 (10) ^[37]	
D7	1801269-93-1		no melting		302.0 (5) ^[38]	
D8	33491-88-2			362.0 ^[39]		
D9	133502-79-1		no melting ^[40]		299.0 (5) ^[40]	
D10	38082-89-2		no melting	360.0 (5) ^[41]		
D11	55148-03-3		no melting		369.5 (10) ^[42]	

E1	25243-36-1		342.0 ^[43]	394.0 (5) ^[43]		
E2	2134229-83-5		no melting		261.2 (5) ^[44]	
E3	2195346-95-1		205.5 ^[22]		233.1 (5) ^[22]	
E4	293324-58-0		304.0 ^[45]		307.0 (5) ^[45]	
E5	1809272-88-5		no melting ²⁶	138.0 ²⁶		
E6	NA		233.0 ^[45]		261.0 (5) ^[45]	
E7	NA		278.0 ^[45]		280.0 (5) ^[45]	
E8	2134229-85-7		no melting		307.2 (5) ^[45]	
E9	NA		325.0 ^[45]		328.0 (5) ^[45]	
HL3			no melting		351.0 (5)	
HL7			no melting		340.8 (5)	
HL9			no melting		261.9 (5)	

7. Correlations between various molecular and crystal level parameters with thermostability of all 63 (including 60 reported and 3 newly synthesized) EMs that were mentioned in this study.

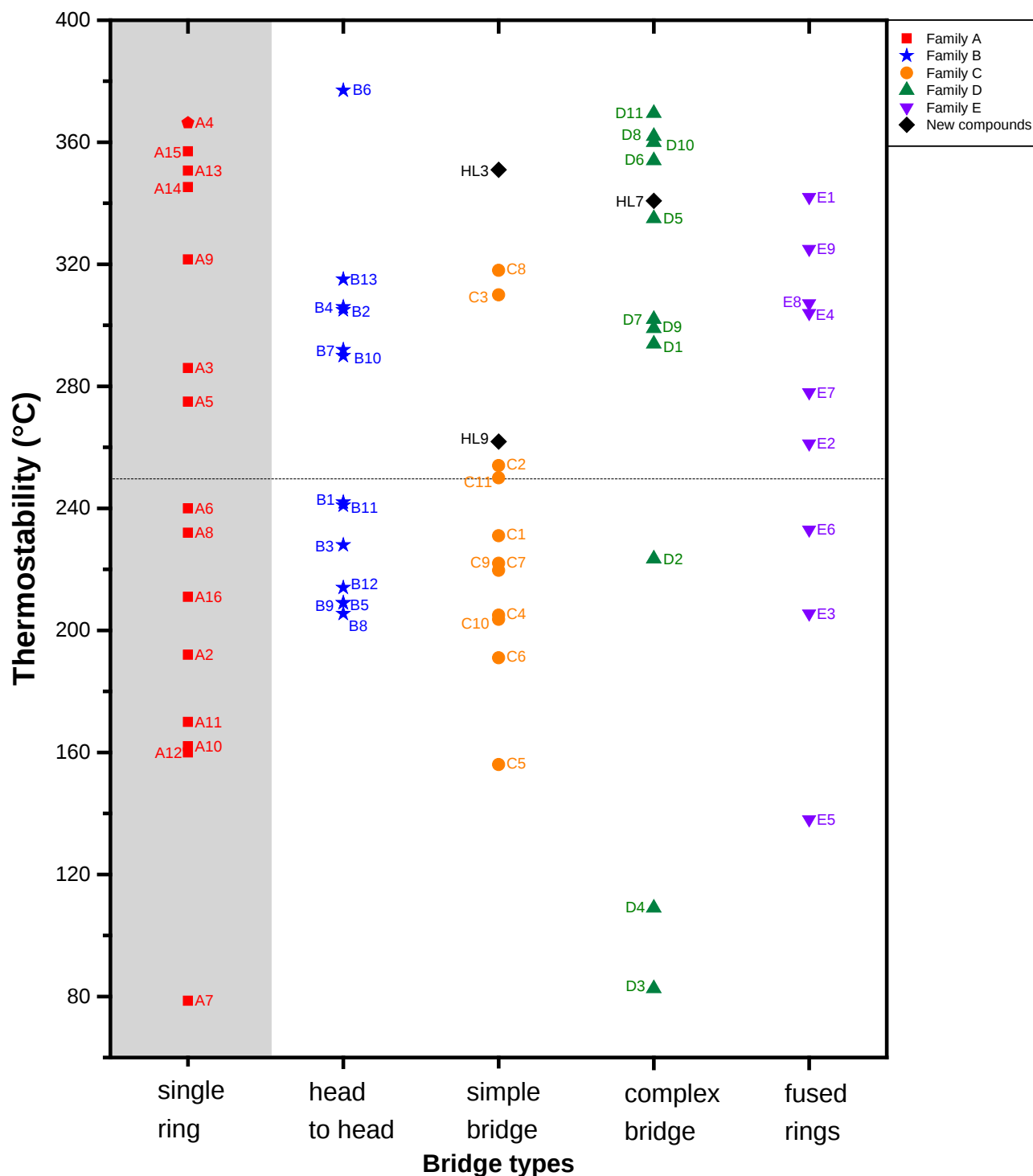
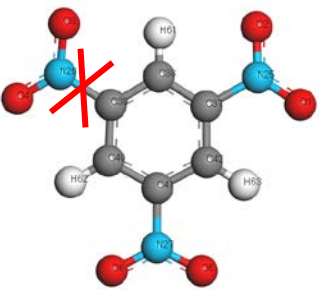
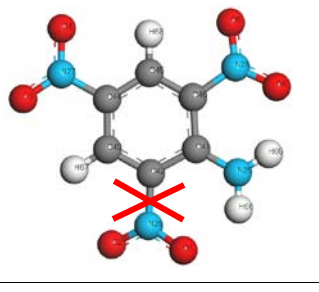


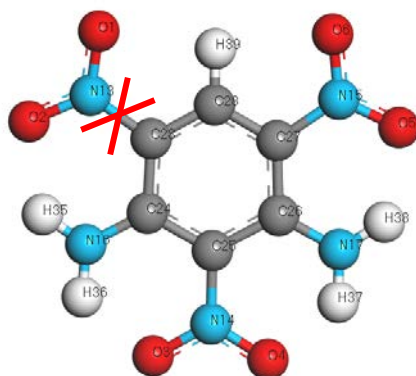
Figure S30. Full temperature range correlation between a bridge type and thermostability of all 63 EMs that were mentioned in this study.

Table S6. List of calculated length (Å) and strength (kcal·mol⁻¹) of each chemical bond found in all 63 EMs mentioned in this study. The 1st and 2nd weakest bonds in each compound are marked by red and blue colors (red and blue crosses in molecular structures and red and blue text in corresponding data tables).

A1								
								
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-25	1.27	133.84	25-37	1.48	104.43	37-38	1.40	133.46
2-25	1.27	135.29	26-39	1.49	99.15	38-39	1.39	134.06
3-26	1.27	129.75	27-41	1.49	99.30	39-40	1.39	132.12
4-26	1.26	135.15				40-41	1.39	132.36
5-27	1.27	132.13				41-42	1.39	133.99
6-27	1.26	133.34				42-37	1.40	132.83

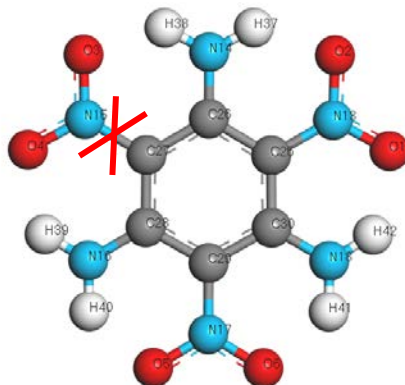
A2								
								
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-26	1.28	127.52	25-41	1.34	132.69	41-42	1.44	133.58
2-26	1.27	133.75	26-42	1.46	108.00	42-43	1.39	134.30
3-27	1.27	132.21	27-44	1.46	108.22	43-44	1.40	130.51
4-27	1.27	130.80	28-46	1.46	108.96	44-45	1.39	129.98
5-28	1.27	136.70				45-46	1.39	132.59
6-28	1.29	125.00				46-41	1.44	133.78

A3



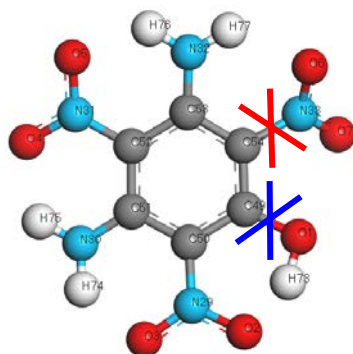
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-13	1.27	135.36	23-13	1.45	115.68	23-24	1.44	130.60
2-13	1.29	126.72	24-16	1.33	133.54	24-25	1.45	131.55
3-14	1.28	130.12	25-14	1.43	120.77	25-26	1.45	132.81
4-14	1.29	127.00	26-17	1.33	132.34	26-27	1.44	131.31
5-15	1.29	126.07	27-15	1.44	117.50	27-28	1.39	133.20
6-15	1.28	133.42				28-23	1.38	134.08

A4



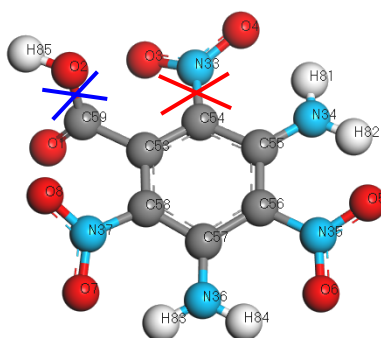
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-13	1.29	129.55	25-13	1.43	125.92	25-26	1.45	130.88
2-13	1.30	126.52	26-14	1.33	133.53	26-27	1.45	130.72
3-15	1.29	128.47	27-15	1.43	124.08	27-28	1.45	130.84
4-15	1.29	127.41	28-16	1.33	133.92	28-29	1.45	130.44
5-17	1.29	129.31	29-17	1.43	125.85	29-30	1.45	130.65
6-17	1.30	127.17	30-18	1.33	134.21	30-25	1.45	130.97

A5



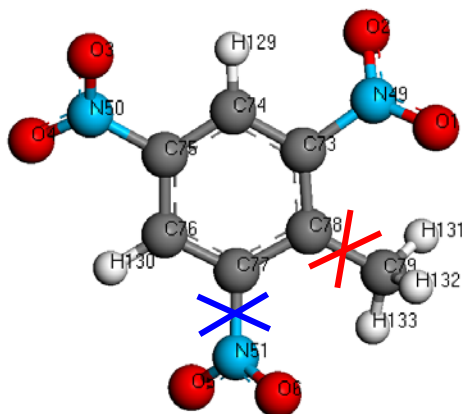
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
2-29	1.31	121.29	50-29	1.41	128.57	49-50	1.43	137.33
3-29	1.28	130.80	51-30	1.33	133.87	50-51	1.45	130.27
4-31	1.29	126.89	52-31	1.42	123.79	51-52	1.44	132.62
5-31	1.29	128.76	53-32	1.33	133.71	52-53	1.45	131.14
6-33	1.28	124.68	54-33	1.45	109.43	53-54	1.43	133.89
7-33	1.27	134.16	O-C (2 nd weakest)			54-49	1.40	140.97
			1-49	1.34	110.05			

A6



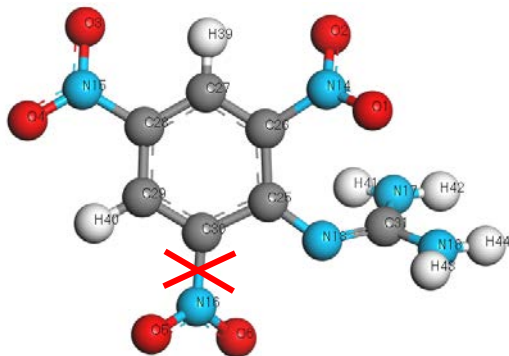
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
3-33	1.28	131.94	54-33	1.45	112.23	53-54	1.40	136.76
4-33	1.28	126.76	55-34	1.33	134.66	54-55	1.45	131.00
5-35	1.28	132.91	56-35	1.44	119.45	55-56	1.44	133.63
6-35	1.29	125.69	57-36	1.34	134.37	56-57	1.44	133.45
7-37	1.28	130.09	58-37	1.45	115.15	57-58	1.44	132.11
8-37	1.28	132.45	O-C (2 nd weakest)			58-53	1.40	136.11
			59-1	1.27	148.99	53-59	1.52	119.23
			59-2	1.33	113.46			

A7



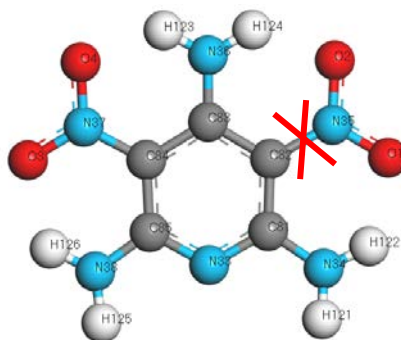
O-N			N-C (2 nd weakest)			C-C (1 st weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-49	1.27	131.74	49-73	1.48	100.58	78-73	1.41	136.23
2-49	1.27	133.73	50-75	1.47	101.71	73-74	1.39	133.14
3-50	1.27	130.48	51-77	1.49	96.37	74-75	1.39	134.07
4-50	1.27	131.94				75-76	1.39	133.70
6-51	1.27	133.96				76-77	1.39	134.55
5-51	1.27	131.38				77-78	1.41	136.60
						78-79	1.49	93.08

A8



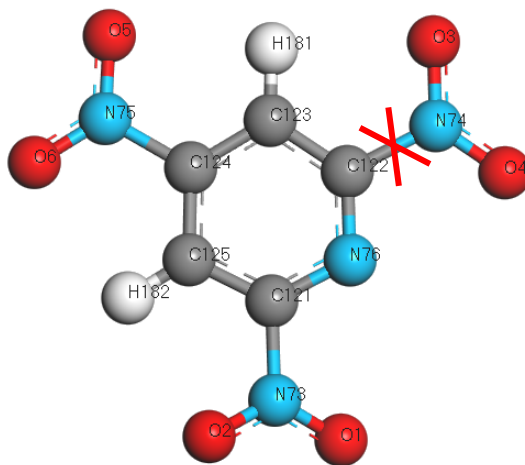
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-14	1.28	130.25	14-26	1.45	108.36	25-26	1.45	131.25
2-14	1.28	132.91	15-28	1.44	113.15	26-27	1.39	134.91
3-15	1.28	126.54	16-30	1.47	104.52	27-28	1.40	130.94
4-15	1.27	132.97	31-17	1.35	134.03	28-29	1.40	129.48
5-16	1.27	129.17	31-18	1.34	131.24	29-30	1.38	135.45
6-16	1.26	132.34	13-31	1.35	152.69	30-25	1.45	127.59
			25-13	1.32	157.35			

A9



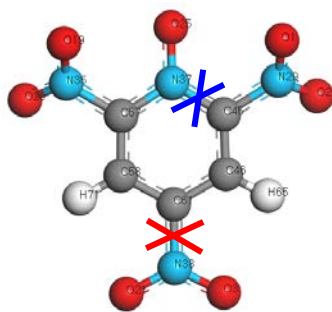
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-35	1.29	127.33	81-34	1.34	131.91	81-82	1.44	131.44
2-35	1.29	126.01	82-35	1.42	122.26	82-83	1.44	131.28
3-37	1.30	126.24	83-36	1.34	131.05	83-84	1.45	130.30
4-37	1.29	126.77	84-37	1.42	124.09	84-85	1.45	131.28
			85-38	1.34	134.69			
			85-33	1.36	143.66			
			81-33	1.36	142.97			

A10



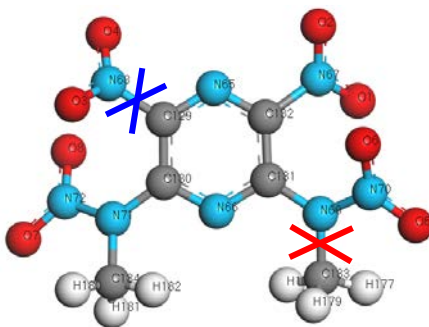
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-73	1.26	134.15	73-121	1.50	94.95	121-125	1.39	139.88
2-73	1.26	133.61	74-122	1.50	94.50	125-124	1.39	135.27
3-74	1.26	131.93	75-124	1.49	99.62	124-123	1.39	133.96
4-74	1.26	134.70	76-122	1.34	153.90	123-122	1.40	138.72
5-75	1.27	132.55	76-121	1.33	156.40			
6-75	1.26	136.94						

A11



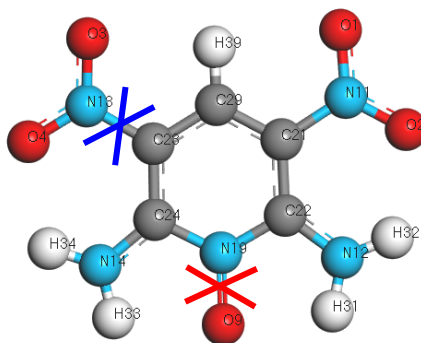
O-N			N-C (1 st and 2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-29	1.26	134.42	29-45	1.48	104.96	57-58	1.38	142.73
2-29	1.27	135.27	38-61	1.47	103.13	58-61	1.40	132.09
3-38	1.27	133.58	35-57	1.48	104.96	61-46	1.39	132.09
21-38	1.27	133.58	37-45	1.40	129.07	46-45	1.38	142.73
19-35	1.26	134.41	37-57	1.40	129.08			
20-35	1.27	135.31						
25-37	1.30	131.37						

A12



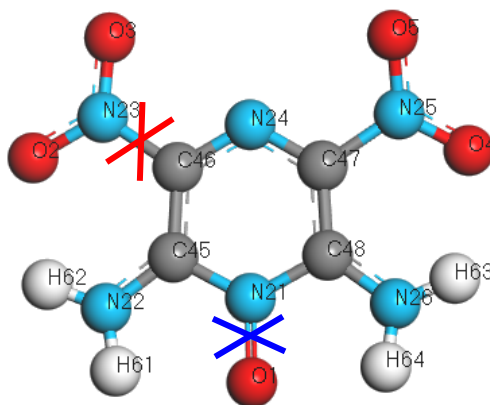
O-N			N-C (1 st and 2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
67-132	1.49	98.66	67-132	1.49	98.66	129-130	1.42	147.49
68-129	1.49	97.53	68-129	1.49	97.53	131-132	1.42	145.36
71-134	1.47	91.41	71-134	1.47	91.41	N-N		
69-133	1.47	90.77	69-133	1.47	90.77	71-72	1.44	110.25
66-130	1.35	156.09	66-130	1.35	156.09	69-70	1.44	109.92
66-131	1.35	157.12	66-131	1.35	157.12			
65-129	1.33	159.78	65-129	1.33	159.78			
65-132	1.32	161.01	65-132	1.32	161.01			
			71-130	1.40	122.06			
			69-131	1.40	122.53			

A13



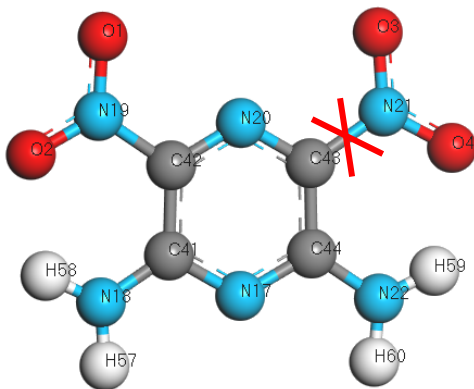
O-N (1 st weakest)			N-C (2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-11	1.27	133.97	11-21	1.44	114.85	24-23	1.43	135.24
2-11	1.28	128.21	13-23	1.44	114.85	23-29	1.39	131.52
3-13	1.27	133.97	12-22	1.34	137.17	29-21	1.39	131.52
4-13	1.28	128.21	14-24	1.34	137.17	21-22	1.43	135.24
9-19	1.35	110.67	19-22	1.39	134.99			
			19-24	1.39	134.99			

A14



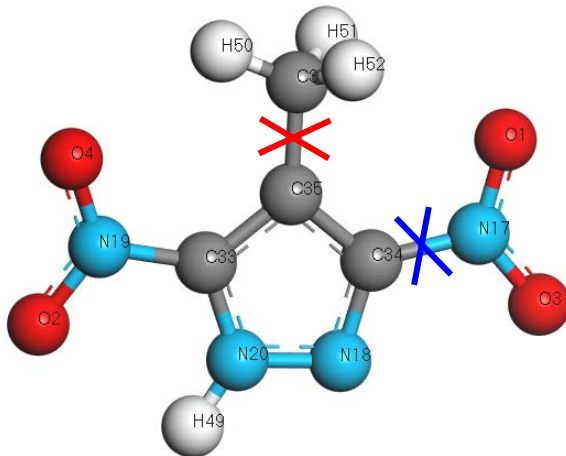
O-N (2 nd weakest)			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-21	1.34	112.89	23-46	1.46	106.28	45-46	1.43	139.31
2-23	1.28	127.46	25-47	1.46	107.47	47-48	1.42	139.52
3-23	1.27	134.77	22-45	1.33	137.42			
4-25	1.27	132.09	26-48	1.33	139.29			
5-25	1.27	130.26	21-45	1.40	132.16			
			21-48	1.40	131.77			
			24-46	1.33	156.49			
			24-47	1.32	158.15			

A15



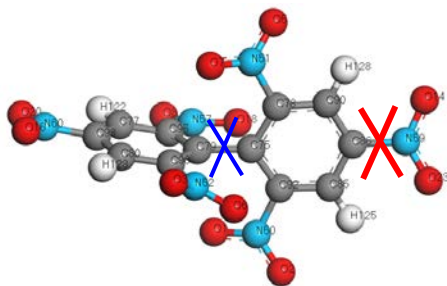
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-19	1.27	133.58	19-42	1.46	111.38	41-42	1.45	134.86
2-19	1.28	127.98	21-43	1.46	107.85	43-44	1.45	135.33
3-21	1.28	130.95	18-41	1.34	132.11			
4-21	1.28	130.32	22-44	1.34	128.63			
			17-41	1.35	152.16			
			17-44	1.36	150.63			
			20-42	1.33	154.04			
			20-43	1.33	155.30			

A16



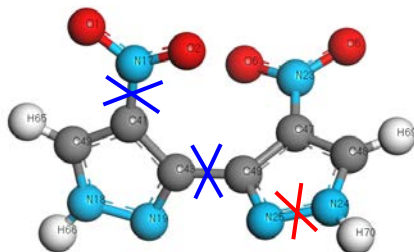
O-N			N-C (2 nd weakest)			C-C (1 st weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-17	1.27	131.66	17-34	1.44	114.28	33-35	1.40	142.12
3-17	1.27	131.83	19-33	1.43	118.96	35-34	1.42	135.52
2-19	1.28	129.10	33-20	1.38	123.20	35-36	1.48	96.27
4-19	1.27	132.80	18-34	1.37	135.32	N-N		
						18-20	1.35	126.68

B1



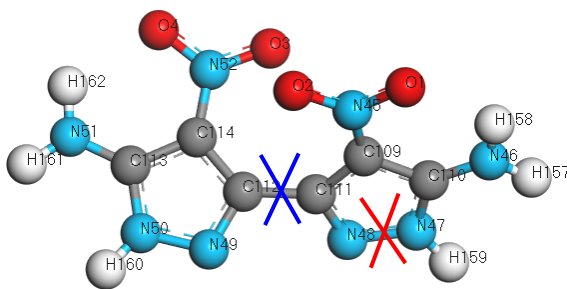
O-N			N-C (1 st weakest)			C-C (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-50	1.27	131.10	78-51	1.49	101.41	75-78	1.41	138.70
2-50	1.26	135.41	86-59	1.48	100.01	78-90	1.39	134.47
3-52	1.27	132.76	92-50	1.48	100.55	90-86	1.39	135.62
6-52	1.27	132.19	93-60	1.48	101.44	86-85	1.39	133.97
5-51	1.27	133.62	95-57	1.48	102.28	85-92	1.39	134.94
7-51	1.27	131.98	96-52	1.48	103.64	92-75	1.41	139.29
8-57	1.27	131.75				77-95	1.39	134.23
18-57	1.26	133.46				95-79	1.41	137.60
14-59	1.27	132.43				79-96	1.41	138.59
23-59	1.27	133.01				96-80	1.39	134.22
16-60	1.27	133.42				80-93	1.39	133.90
20-60	1.27	131.57				93-77	1.39	133.85
						75-79	1.50	112.46

B2



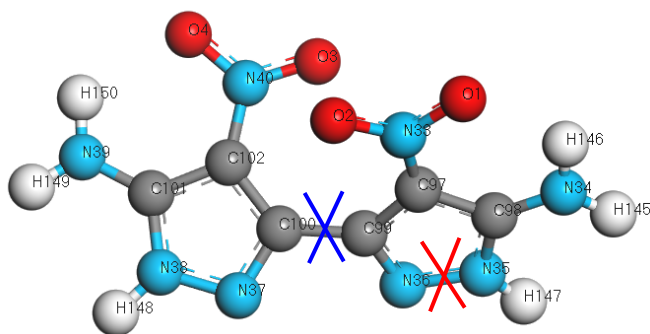
O-N			N-C (2 nd weakest)			C-C (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-17	1.27	131.55	17-41	1.42	112.79	42-41	1.40	136.35
2-17	1.27	130.84	23-47	1.42	112.79	41-43	1.43	132.49
5-23	1.27	131.55	18-42	1.35	127.77	48-47	1.40	136.36
6-23	1.27	130.82	19-43	1.36	141.82	47-49	1.43	132.49
N-N (1 st weakest)			24-48	1.35	127.76	43-49	1.47	114.94
18-19	1.40	105.20	25-49	1.36	141.81			
25-24	1.40	105.19						

B3



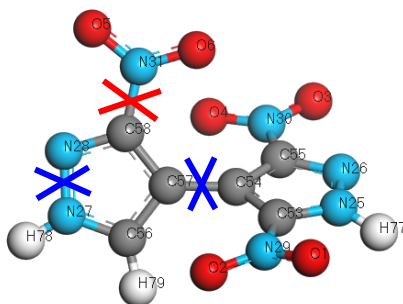
O-N			N-C			C-C (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-45	1.31	118.75	45-109	1.38	128.99	113-114	1.44	137.22
2-45	1.28	135.37	52-114	1.39	126.60	114-112	1.43	129.08
3-52	1.29	128.57	46-110	1.33	134.64	111-109	1.43	126.79
4-52	1.29	126.18	51-113	1.34	133.60	109-110	1.43	139.40
N-N (1st weakest)			50-113	1.37	125.58	111-112	1.45	116.56
49-50	1.40	110.59	49-112	1.34	140.19			
48-47	1.41	107.94	47-110	1.37	124.58			
			48-111	1.34	146.36			

B3-solvent free



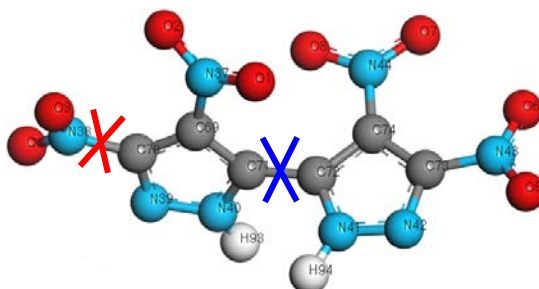
O-N			N-C			C-C (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-33	1.31	119.79	33-97	1.38	128.43	101-102	1.43	137.55
2-33	1.27	135.92	40-102	1.40	123.63	102-100	1.44	126.11
3-40	1.29	125.53	34-98	1.33	132.63	97-99	1.43	126.11
4-40	1.29	125.44	39-101	1.35	129.26	97-98	1.43	140.01
N-N (1st weakest)			38-101	1.36	127.07	100-99	1.46	114.36
37-38	1.41	111.01	37-100	1.35	144.07			
36-35	1.41	106.75	35-98	1.37	122.16			
			36-99	1.35	147.44			

B4

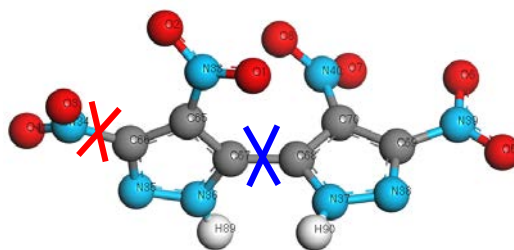


O-N			N-C (1 st weakest)			C-C (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-29	1.27	130.67	29-53	1.44	114.49	55-54	1.42	133.19
2-29	1.27	133.00	30-55	1.44	112.35	54-53	1.40	143.91
3-30	1.28	128.20	31-58	1.44	111.95	56-57	1.40	136.45
4-30	1.27	135.38	53-25	1.38	122.06	57-58	1.42	132.08
5-31	1.27	130.55	55-26	1.36	142.33	54-57	1.45	118.32
6-31	1.27	133.05	56-27	1.36	121.79	N-N (2 nd weakest)		
			58-28	1.35	139.82	25-26	1.35	125.74
						27-28	1.37	116.97

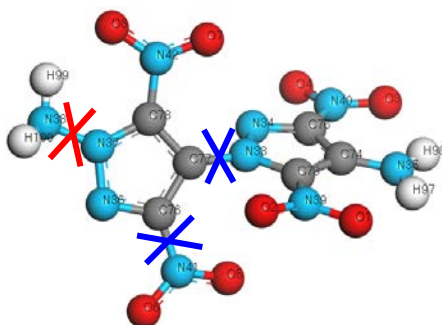
B5



O-N			N-C (1 st weakest)			C-C (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-37	1.27	135.55	37-69	1.44	109.31	70-69	1.41	135.68
2-37	1.27	131.00	38-70	1.46	106.50	69-71	1.40	145.91
3-38	1.26	133.58	43-73	1.46	110.67	72-74	1.41	144.95
4-38	1.26	134.57	44-74	1.44	108.75	74-73	1.43	132.69
5-43	1.28	127.73	70-39	1.35	146.23	71-72	1.46	121.31
6-43	1.26	139.74	71-40	1.37	122.36	N-N		
7-44	1.27	134.13	72-41	1.36	123.17	39-40	1.37	121.56
8-44	1.28	130.98	73-42	1.35	142.71	41-42	1.36	121.22

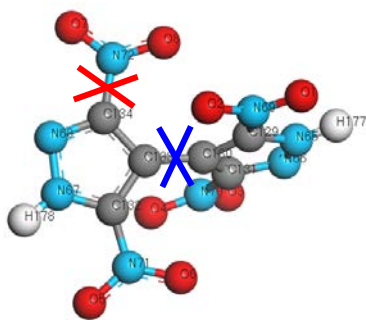
B5-solvent free

O-N			N-C (1 st weakest)			C-C (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-33	1.27	135.93	33-65	1.43	111.37	66-65	1.42	135.32
2-33	1.27	130.28	34-66	1.46	101.89	65-67	1.40	145.97
3-34	1.27	132.79	39-69	1.45	108.81	68-70	1.40	148.20
4-34	1.26	133.32	40-70	1.44	105.91	70-69	1.42	135.07
5-39	1.26	137.42	66-35	1.35	149.09	67-68	1.45	121.41
6-39	1.28	129.26	67-36	1.37	122.77	N-N		
7-40	1.27	131.41	68-37	1.37	120.08	35-36	1.37	122.24
8-40	1.27	134.55	69-38	1.35	143.77	37-38	1.36	120.05

B6

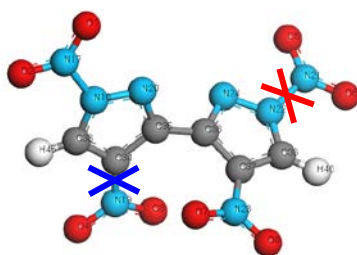
O-N			N-C (2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-39	1.29	125.02	35-74	1.34	126.77	73-74	1.42	143.63
2-39	1.28	129.72	39-73	1.40	125.08	74-75	1.44	133.77
3-40	1.28	131.37	40-75	1.42	114.98	76-77	1.40	140.22
4-40	1.27	131.06	41-76	1.43	112.10	77-78	1.41	143.92
5-41	1.27	128.85	42-78	1.42	122.07	N-N (1 st weakest)		
6-41	1.27	132.79	33-73	1.40	119.91	37-38	1.37	109.61
7-42	1.27	135.86	34-75	1.35	144.85	33-34	1.37	121.72
8-42	1.28	128.89	37-78	1.40	122.07	36-37	1.35	128.69
			36-76	1.36	143.67			
			33-77	1.41	119.18			

B7



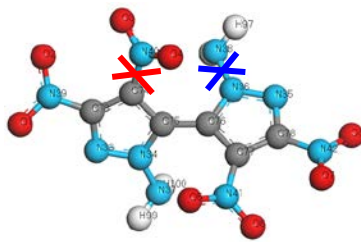
O-N			N-C (1 st weakest)			C-C (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-69	1.27	129.94	69-129	1.44	113.15	129-130	1.40	144.74
2-69	1.27	134.29	70-131	1.44	111.06	130-131	1.42	134.57
3-70	1.28	128.73	71-132	1.43	115.52	132-133	1.40	145.21
4-70	1.26	135.79	72-134	1.44	109.76	133-134	1.42	135.48
5-71	1.27	129.75	129-65	1.37	122.83	130-133	1.45	120.10
6-71	1.27	134.25	131-66	1.36	143.14	N-N		
7-72	1.26	140.39	132-67	1.37	120.57	66-65	1.35	123.92
-72	1.28	127.98	134-68	1.36	143.27	67-68	1.35	128.23

B8



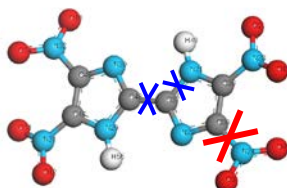
O-N			N-C (2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-17	1.24	157.16	19-34	1.43	108.28	33-34	1.39	139.63
2-17	1.25	153.98	23-37	1.43	108.28	34-35	1.43	131.58
3-19	1.27	127.52	18-33	1.37	119.79	36-37	1.39	139.63
4-19	1.27	135.15	20-35	1.35	144.56	37-38	1.43	131.58
5-21	1.24	157.16	24-38	1.35	144.56	35-38	1.46	116.20
6-21	1.25	153.98	22-36	1.37	119.79	N-N (1 st and 2 nd weakest)		
7-23	1.27	127.52				20-18	1.39	102.27
8-23	1.27	135.16				22-24	1.39	102.27
						17-18	1.51	89.57
						21-22	1.51	89.57

B9

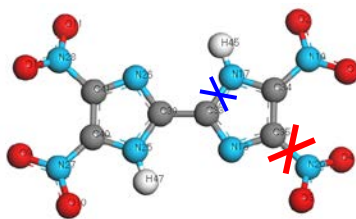


O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-39	1.27	132.24	39-73	1.45	111.40	78-77	1.41	133.82
2-39	1.26	137.53	40-74	1.46	104.19	77-76	1.40	144.79
3-40	1.26	135.58	41-77	1.44	108.90	75-74	1.40	144.91
4-40	1.27	131.44	42-78	1.46	107.67	74-73	1.41	136.00
5-41	1.27	132.53	78-35	1.35	143.69	76-75	1.44	125.60
6-41	1.27	134.36	76-36	1.38	127.00	N-N (2 nd weakest)		
7-42	1.26	135.08	73-33	1.35	141.47	36-38	1.39	107.73
8-42	1.27	130.78	75-34	1.38	126.74	34-37	1.40	108.79
						35-36	1.38	116.24
						34-33	1.38	116.19

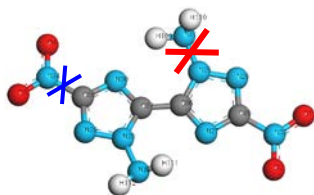
B10



O-N			N-C (1 st and 2 nd weakest)			C-C (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-23	1.27	134.51	23-38	1.43	120.57	38-39	1.40	141.65
2-23	1.28	132.04	24-39	1.45	104.35	44-45	1.40	141.65
3-24	1.27	129.44	31-44	1.43	120.57	37-43	1.43	128.43
4-24	1.27	133.85	32-45	1.45	104.35			
11-31	1.27	134.51	38-21	1.37	134.46			
12-31	1.28	132.04	21-37	1.37	126.41			
13-32	1.27	129.44	37-22	1.36	148.77			
14-32	1.27	133.85	22-39	1.36	143.18			
			45-30	1.36	143.18			
			30-43	1.36	148.77			
			43-29	1.37	126.41			
			29-44	1.37	134.46			

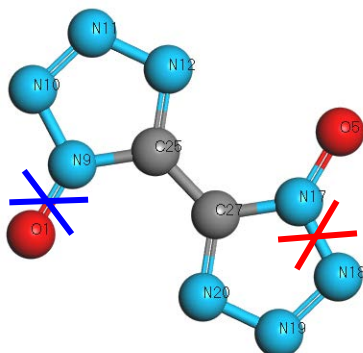
B10-solvent free

O-N			N-C (1 st and 2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-19	1.28	129.75	19-34	1.43	121.93	34-35	1.41	142.90
2-19	1.27	136.31	20-35	1.46	100.20	40-41	1.41	142.91
3-20	1.26	133.59	27-40	1.43	121.94	33-39	1.43	129.70
4-20	1.27	132.11	28-41	1.46	100.22			
9-27	1.28	129.70	34-17	1.38	133.46			
10-27	1.27	136.12	17-33	1.38	125.33			
11-28	1.26	133.62	33-18	1.36	152.11			
12-28	1.27	132.26	18-35	1.36	144.42			
			25-40	1.38	133.37			
			25-39	1.38	125.33			
			39-26	1.36	152.12			
			26-41	1.36	144.34			

B11

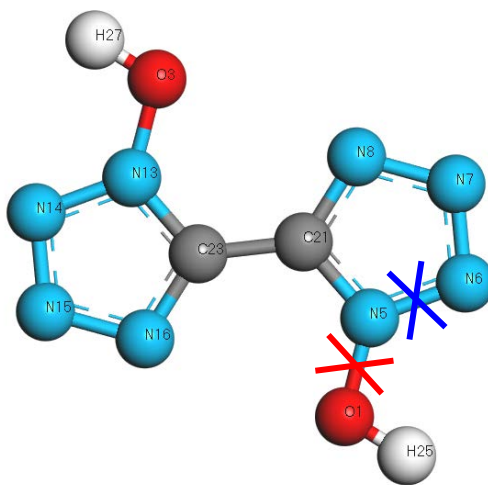
O-N			N-C (2 nd weakest)			N-N (1 st weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-32	1.27	132.24	32-85	1.44	111.42	25-31	1.40	103.25
2-32	1.27	131.35	34-88	1.45	108.13	28-33	1.39	109.80
3-34	1.27	135.07	25-86	1.39	120.98	25-26	1.37	127.58
4-34	1.27	131.69	27-86	1.35	153.78	28-29	1.37	125.80
			27-85	1.36	140.16	C-C bridge		
			85-26	1.35	144.50	86-87	1.43	130.60
			29-88	1.36	143.08			
			88-30	1.36	144.61			
			30-87	1.35	153.57			
			87-28	1.39	118.31			

B12



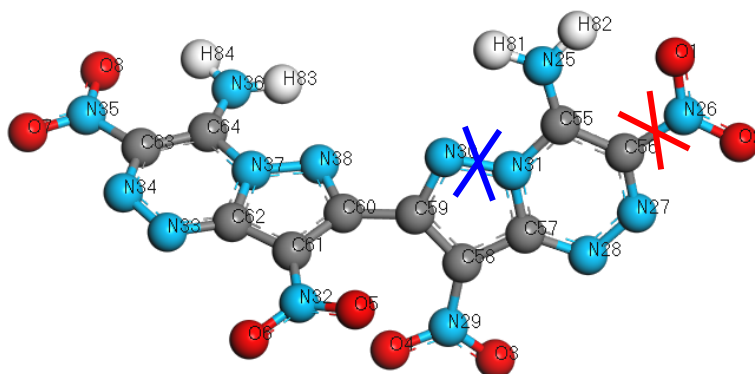
O-N (2 nd weakest)			N-C			N-N (1 st weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-9	1.33	115.50	9-25	1.38	130.23	9-10	1.39	106.13
5-17	1.33	115.50	12-25	1.36	144.19	10-11	1.34	117.72
			17-27	1.38	130.23	11-12	1.38	109.03
			20-27	1.36	144.19	17-18	1.39	106.13
			C-C bridge			18-19	1.34	117.72
			25-27	1.43	125.48	19-20	1.38	109.03

B12-solvent free



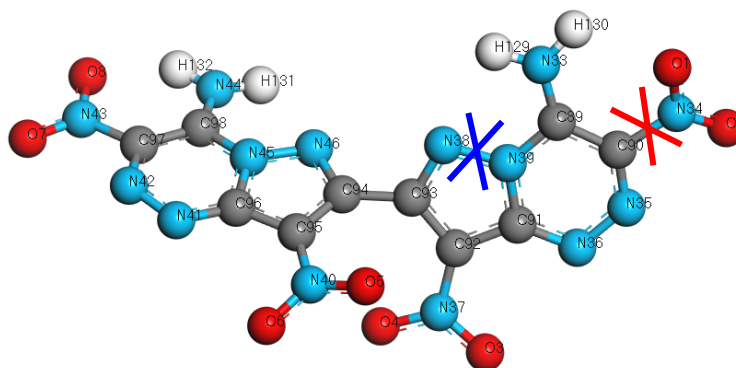
O-N (1 st weakest)			N-C			N-N (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-5	1.38	93.01	5-21	1.37	133.93	5-6	1.38	98.96
3-13	1.38	93.01	21-8	1.36	147.51	6-7	1.35	118.16
			13-23	1.37	133.93	7-8	1.40	104.63
			23-16	1.36	147.51	13-14	1.38	98.96
			C-C bridge			14-15	1.35	118.17
			21-23	1.44	123.76	15-16	1.40	104.63

B13



O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-26	1.28	128.83	26-56	1.47	108.14	63-64	1.43	142.48
2-26	1.26	135.92	29-58	1.42	120.99	62-61	1.41	140.97
3-29	1.28	128.69	32-61	1.42	113.48	61-60	1.42	133.57
4-29	1.27	136.86	35-63	1.46	110.85	55-56	1.43	141.67
5-32	1.28	132.80	25-55	1.31	147.74	58-57	1.41	140.90
6-32	1.28	130.67	36-64	1.31	145.04	58-59	1.42	132.95
7-35	1.26	136.08	56-27	1.34	142.29	60-59	1.46	118.04
8-35	1.28	127.48	57-28	1.37	139.90	N-N (2 nd weakest)		
			57-31	1.40	118.25	33-34	1.34	138.38
			31-55	1.39	128.82	37-38	1.39	110.33
			30-59	1.36	145.08	30-31	1.40	108.57
			63-34	1.34	144.16	27-28	1.35	127.18
			33-62	1.37	139.18			
			62-37	1.40	120.21			
			37-64	1.39	131.50			
			38-60	1.36	144.40			

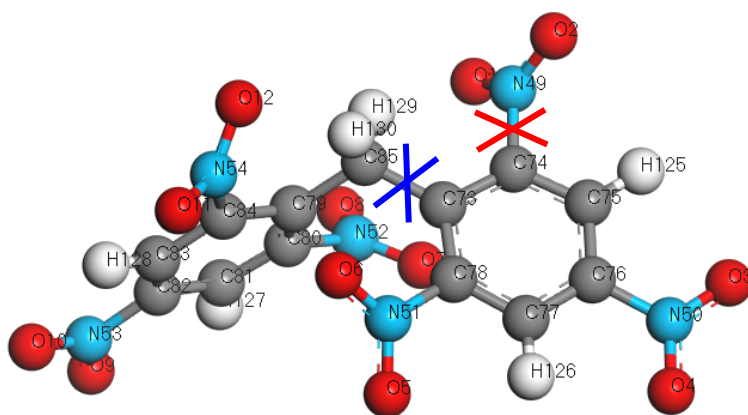
B13-solvent free



O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-34	1.27	128.00	34-90	1.48	100.68	89-90	1.43	142.52
2-34	1.26	136.97	37-92	1.43	114.25	91-92	1.42	138.89
3-37	1.28	127.39	40-95	1.42	114.21	92-93	1.43	134.00
4-37	1.28	132.00	43-97	1.45	110.15	97-98	1.42	143.98
5-40	1.28	131.20	33-89	1.32	143.41	96-95	1.40	140.53
6-40	1.27	134.83	44-98	1.33	136.81	95-94	1.42	134.54
7-43	1.27	135.49	90-35	1.34	143.84	93-94	1.46	115.27
8-43	1.29	126.70	36-91	1.36	139.45	N-N (2 nd weakest)		
			91-39	1.40	118.63	41-42	1.33	138.38
			39-89	1.38	129.97	45-46	1.40	110.33
			93-38	1.36	144.56	38-39	1.40	108.57
			97-42	1.36	135.93	35-36	1.36	127.18
			41-96	1.36	140.81			
			96-45	1.40	117.25			
			45-98	1.38	133.91			
			46-94	1.36	144.73			

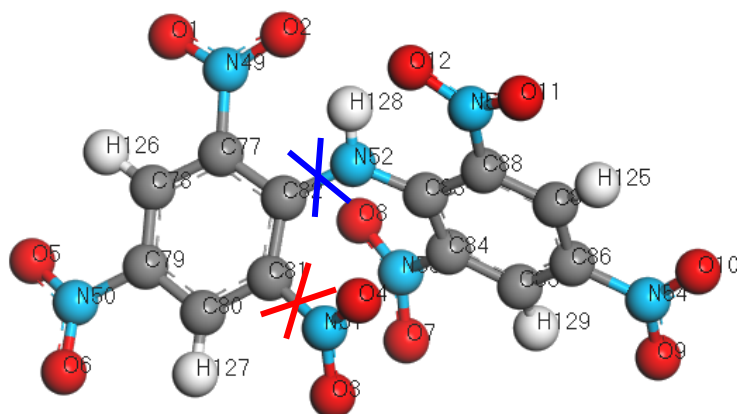
C1

ORTEP diagram of the molecular structure of compound 1, showing a complex polycyclic system with multiple nitro groups. The structure is drawn with thermal ellipsoids at the 50% probability level. Displacement ellipsoid for N49 is shown as a red cross. Hydrogen atoms are shown as small spheres of arbitrary radii. The molecule features a central benzene ring substituted with various functional groups, including nitro groups and a complex side chain.



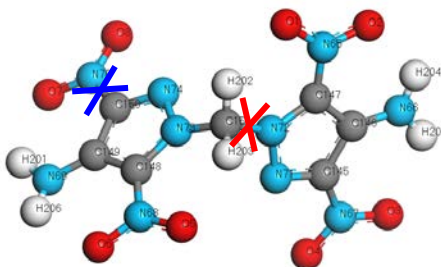
O-N			N-C (1 st weakest)			C-C (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-49	1.27	132.02	49-74	1.49	93.99	73-74	1.41	139.03
2-49	1.26	134.44	50-76	1.48	99.82	74-75	1.39	133.44
3-50	1.27	131.27	51-78	1.48	101.17	75-76	1.39	133.02
4-50	1.26	131.70	52-80	1.49	94.28	76-77	1.39	133.18
5-51	1.27	134.32	53-82	1.48	102.47	77-78	1.39	131.79
6-51	1.27	129.93	54-84	1.48	98.42	78-73	1.41	138.28
7-52	1.27	131.39				79-80	1.41	140.15
8-52	1.26	135.29				80-81	1.39	132.53
9-53	1.27	130.23				81-82	1.39	134.00
10-53	1.26	135.06				82-83	1.39	132.95
11-54	1.26	137.83				83-84	1.39	132.68
12-54	1.27	128.56				84-79	1.42	139.03
						73-85	1.51	96.71
						85-79	1.52	97.47

C2



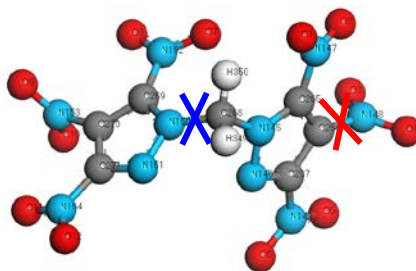
O-N			N-C (1 st and 2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-49	1.27	135.04	49-77	1.48	106.38	77-78	1.39	132.51
2-49	1.27	129.30	51-81	1.48	100.12	78-79	1.39	133.16
3-51	1.27	134.90	50-79	1.47	101.61	79-80	1.39	132.12
4-51	1.27	133.05	53-84	1.48	101.21	80-81	1.39	133.84
5-50	1.27	130.47	54-86	1.47	104.45	81-82	1.42	138.62
6-50	1.26	133.45	55-88	1.48	107.19	82-77	1.43	137.90
7-53	1.27	133.66	83-52	1.38	128.69	83-84	1.42	138.02
8-53	1.27	134.32	52-82	1.38	128.23	84-85	1.39	133.63
9-54	1.27	131.94				85-86	1.39	131.85
10-54	1.27	133.43				86-87	1.39	133.31
11-55	1.26	137.80				87-88	1.39	134.30
12-55	1.28	125.99				88-83	1.43	137.38

C3



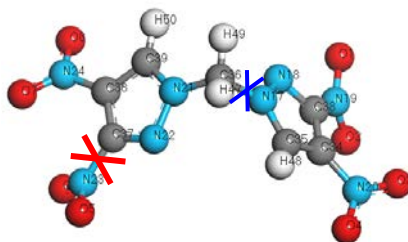
O-N			N-C (1 st and 2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-65	1.28	130.36	65-147	1.40	127.27	145-146	1.43	134.32
2-65	1.29	125.39	67-145	1.42	116.99	146-147	1.42	142.47
3-67	1.28	126.97	68-148	1.40	124.59	148-149	1.42	142.69
4-67	1.27	129.86	70-150	1.42	115.39	149-150	1.43	134.88
5-68	1.28	130.13	66-146	1.33	131.04	N-N		
6-68	1.29	126.22	69-149	1.34	129.37	71-72	1.36	125.27
7-70	1.28	128.46	147-72	1.40	122.56	73-74	1.35	125.87
8-70	1.27	130.34	145-71	1.36	142.19			
			148-73	1.40	123.42			
			150-74	1.35	141.63			
			151-72	1.47	102.33			
			151-73	1.46	103.90			

C4



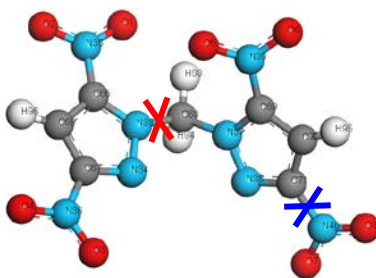
O-N			N-C (1 st and 2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-147	1.27	130.37	147-265	1.44	113.70	265-266	1.39	149.33
2-147	1.27	136.13	148-266	1.48	95.84	266-267	1.41	138.33
3-148	1.26	133.06	149-267	1.45	108.01	269-270	1.39	149.52
4-148	1.26	137.78	152-269	1.44	113.98	270-271	1.41	140.70
5-149	1.27	130.34	153-270	1.48	97.48	N-N		
6-149	1.26	135.66	154-271	1.45	105.10	145-146	1.37	122.87
7-152	1.27	131.66	145-265	1.39	125.50	150-151	1.37	126.61
8-152	1.26	137.11	146-267	1.35	146.07			
9-153	1.26	138.13	150-269	1.39	125.13			
10-153	1.26	135.67	151-271	1.35	144.54			
11-154	1.27	131.27	145-268	1.48	105.00			
12-154	1.26	135.01	150-268	1.46	103.66			

C5



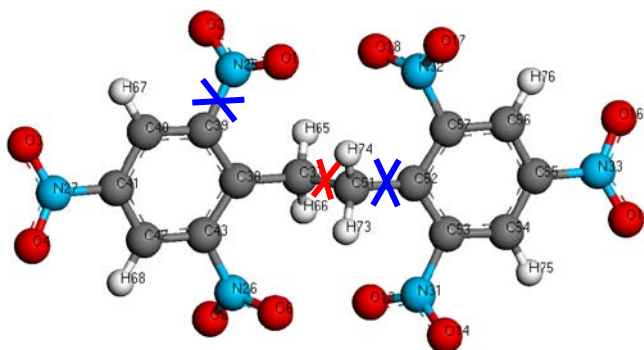
O-N			N-C (1 st and 2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-19	1.27	132.81	19-33	1.46	106.58	37-38	1.42	133.42
2-19	1.27	134.24	20-34	1.44	108.77	38-39	1.39	139.56
3-20	1.27	131.89	23-37	1.45	105.79	33-34	1.42	132.61
4-20	1.27	132.14	24-38	1.44	107.73	34-35	1.39	138.91
5-23	1.26	132.95	33-18	1.35	148.07	N-N		
6-23	1.26	135.51	35-17	1.37	128.08	17-18	1.39	116.47
7-24	1.27	132.20	37-22	1.34	147.16	21-22	1.39	116.23
8-24	1.27	132.92	39-21	1.37	128.37			
			17-36	1.46	105.93			
			36-21	1.46	108.59			

C6



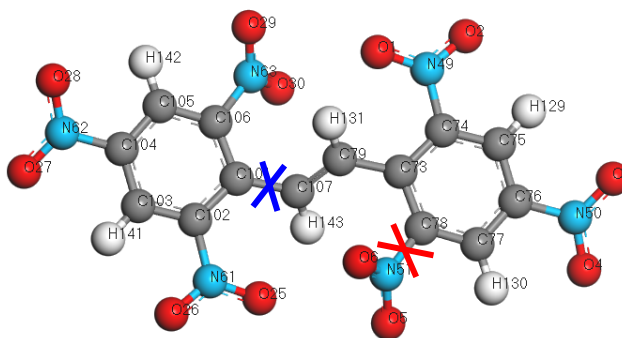
O-N			N-C (1 st and 2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-35	1.27	130.18	35-65	1.45	110.32	65-66	1.39	142.18
2-35	1.26	136.39	36-67	1.45	107.10	66-67	1.41	131.91
3-36	1.27	133.13	39-69	1.44	114.80	69-70	1.39	143.35
4-36	1.27	129.06	40-71	1.45	106.57	70-71	1.41	131.74
5-39	1.27	132.76	33-68	1.47	100.51	N-N		
6-39	1.27	135.19	68-37	1.45	103.78	33-34	1.37	124.21
7-40	1.26	133.41				37-38	1.37	124.63
8-40	1.27	132.75						

C7



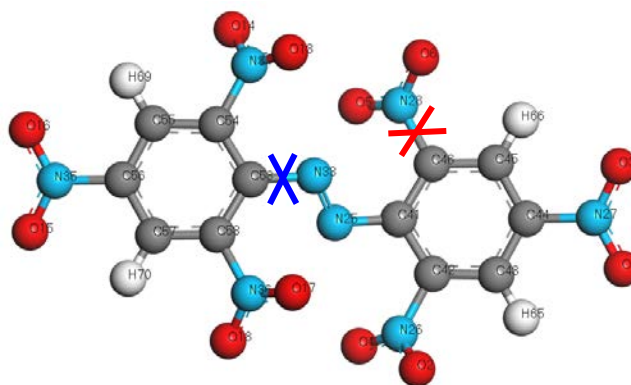
O-N			N-C (2 nd weakest)			C-C (1 st and 2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-25	1.26	134.08	25-39	1.49	95.78	38-39	1.41	137.88
2-25	1.27	132.51	26-43	1.49	96.93	39-40	1.39	133.40
3-27	1.26	134.27	27-41	1.48	101.80	40-41	1.39	133.06
4-27	1.27	130.51	31-53	1.49	95.78	41-42	1.39	133.57
5-26	1.27	132.45	32-57	1.49	96.93	42-43	1.39	134.11
6-26	1.27	135.43	33-55	1.48	101.80	43-38	1.41	137.88
13-31	1.26	134.08				52-53	1.41	137.88
14-31	1.27	132.51				53-54	1.39	133.40
15-33	1.26	134.27				54-55	1.39	133.06
16-33	1.27	130.51				55-56	1.39	133.57
17-32	1.27	132.45				56-57	1.39	134.11
18-32	1.27	135.43				57-52	1.41	137.88
						38-37	1.51	93.46
						37-51	1.56	75.76
						51-52	1.51	93.46

C8



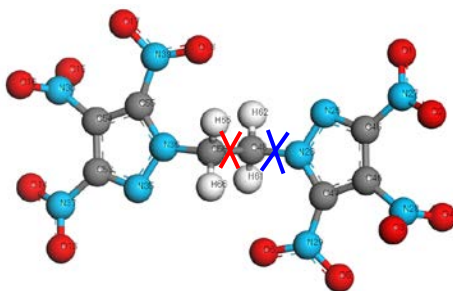
O-N			N-C (1 st weakest)			C-C (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-49	1.27	132.05	49-74	1.48	102.69	73-74	1.42	133.88
2-49	1.27	133.76	50-76	1.47	102.28	74-75	1.40	132.49
3-50	1.27	133.73	51-78	1.49	96.85	75-76	1.39	132.30
4-50	1.27	129.40	61-102	1.48	102.75	76-77	1.39	133.52
5-51	1.27	132.36	62-104	1.47	102.31	77-78	1.39	135.04
6-51	1.26	136.33	63-106	1.49	96.97	78-73	1.42	134.90
25-61	1.27	131.92				101-102	1.42	133.93
26-61	1.27	133.89				102-103	1.40	132.48
27-62	1.27	133.84				103-104	1.39	132.33
28-62	1.27	129.46				104-105	1.39	133.66
29-63	1.27	132.37				105-106	1.39	135.03
30-63	1.26	136.18				106-101	1.41	135.00
						101-107	1.46	112.81
						107-79	1.36	142.08
						79-73	1.46	112.85

C9



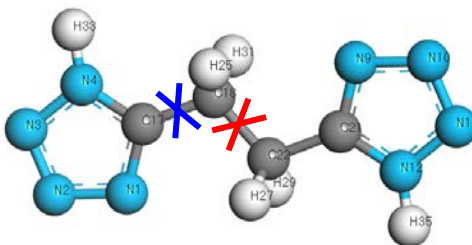
O-N			N-C (1 st and 2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-26	1.26	135.31	26-42	1.49	99.77	41-42	1.41	138.78
2-26	1.26	133.64	27-44	1.48	100.25	42-43	1.39	135.42
3-27	1.27	134.34	28-46	1.49	98.85	43-44	1.39	134.07
4-27	1.27	132.79	34-54	1.49	99.82	44-45	1.40	132.28
5-28	1.26	137.34	35-56	1.48	100.23	45-46	1.39	135.25
6-28	1.27	131.96	36-58	1.49	98.88	46-41	1.41	137.02
13-34	1.26	135.33	53-33	1.41	126.29	53-54	1.41	138.70
14-34	1.27	133.53	41-25	1.41	126.32	54-55	1.39	135.41
15-35	1.27	134.33				55-56	1.39	134.04
16-35	1.27	132.79				56-57	1.40	132.26
17-36	1.26	137.41				57-58	1.39	135.21
18-36	1.27	132.03				58-53	1.41	137.05
N-N								
25-33	1.29	133.02						

C10



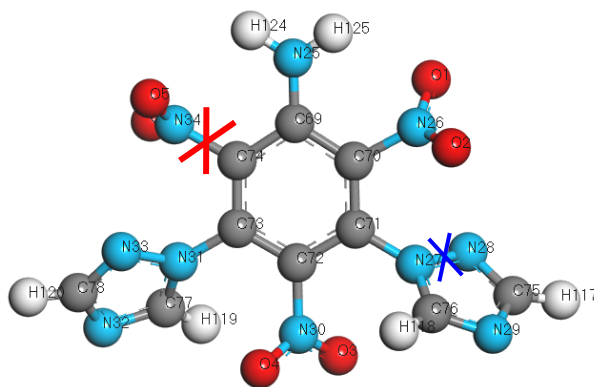
O-N			N-C (2 nd weakest)			C-C (1 st weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-27	1.26	132.70	27-45	1.45	102.76	45-46	1.40	140.03
2-27	1.27	130.89	28-46	1.46	98.67	46-47	1.39	148.35
3-28	1.26	133.96	29-47	1.43	115.72	53-54	1.40	140.03
4-28	1.26	136.38	37-53	1.45	102.76	54-55	1.39	148.35
5-29	1.27	135.05	38-54	1.46	98.67	48-56	1.54	75.75
6-29	1.27	132.23	39-55	1.43	115.72	N-N bridge		
13-37	1.26	132.70	25-45	1.36	145.09	25-26	1.37	125.37
14-37	1.27	130.89	26-47	1.38	126.65	35-36	1.37	125.37
15-38	1.26	133.96	35-53	1.36	145.09			
16-38	1.26	136.38	36-55	1.38	126.65			
17-39	1.27	135.06	26-48	1.47	93.31			
18-39	1.27	132.23	36-56	1.47	93.31			

C11



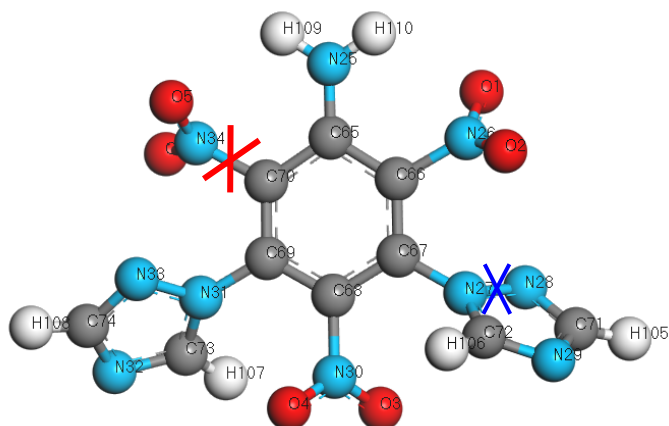
N-C			C-C bridge (1 st and 2 nd weakest)			N-N		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
21-9	1.35	153.32	17-18	1.49	99.12	1-2	1.40	103.14
21-12	1.37	130.40	18-22	1.53	81.65	2-3	1.33	120.87
17-1	1.35	153.32	22-21	1.49	99.12	3-4	1.38	111.55
17-4	1.37	130.40				9-10	1.40	103.14
						10-11	1.33	120.87
						11-12	1.38	111.55

D1



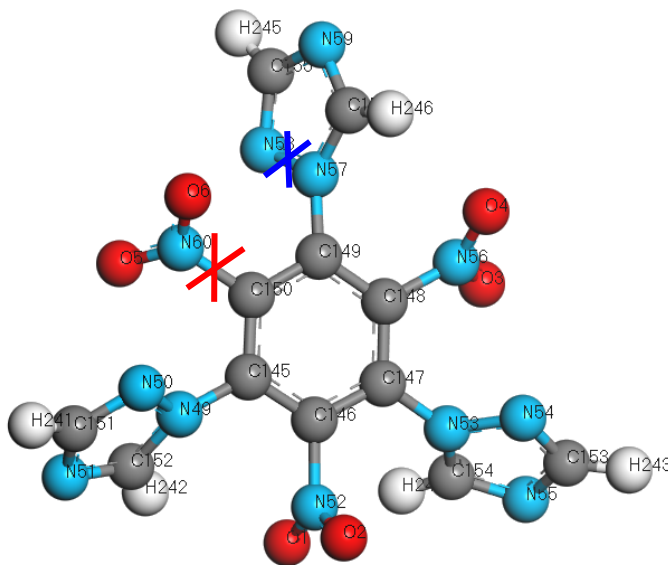
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-26	1.27	130.56	26-70	1.48	101.94	69-70	1.43	135.99
2-26	1.26	135.96	30-72	1.47	102.93	70-71	1.39	143.35
3-30	1.27	133.98	34-74	1.48	100.14	71-72	1.40	140.65
4-30	1.27	134.51	28-75	1.34	145.69	72-73	1.41	140.25
5-34	1.27	134.38	29-75	1.39	125.55	73-74	1.39	144.86
6-34	1.26	136.51	29-76	1.34	151.18	74-69	1.43	135.80
N-N (2 nd weakest)			27-76	1.37	128.25			
27-28	1.41	106.66	31-77	1.38	127.15			
31-33	1.42	106.70	32-77	1.34	151.57			
			32-78	1.39	126.13			
			33-78	1.34	145.49			
			71-27	1.42	115.32			
			73-31	1.42	115.41			

D1-solvent free



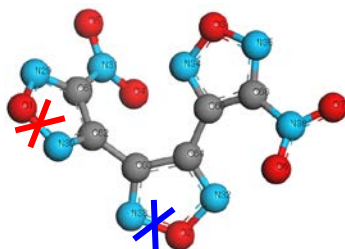
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-26	1.27	130.87	26-66	1.48	100.08	65-66	1.43	134.84
2-26	1.26	135.76	30-68	1.47	101.56	66-67	1.39	142.79
3-30	1.27	133.63	34-70	1.48	98.97	67-68	1.40	139.33
4-30	1.27	132.61	31-73	1.38	127.22	68-69	1.41	139.08
5-34	1.27	131.34	73-32	1.34	150.93	69-70	1.39	143.75
6-34	1.27	136.27	32-74	1.39	125.76	70-65	1.43	134.95
N-N (2 nd weakest)			74-33	1.34	143.65			
31-33	1.42	108.36	27-72	1.37	128.45			
27-28	1.41	107.80	72-29	1.34	150.77			
			29-71	1.39	124.92			
			71-28	1.34	143.84			
			69-31	1.42	114.34			
			67-27	1.42	114.21			

D2



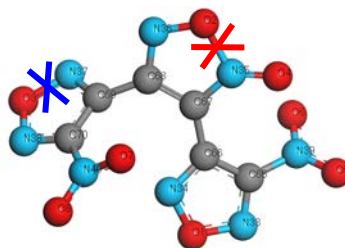
O-N			N-C (1 st weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-52	1.27	130.14	52-146	1.49	98.61	145-146	1.40	143.59
2-52	1.25	141.13	56-148	1.48	100.55	146-147	1.40	144.33
3-56	1.26	136.88	60-150	1.49	98.23	147-148	1.40	143.28
4-56	1.26	134.73	57-156	1.38	119.62	148-149	1.40	142.66
5-60	1.26	137.13	156-59	1.34	155.88	149-150	1.40	144.01
6-60	1.26	136.80	59-155	1.39	132.54	150-145	1.40	144.03
N-N (2 nd weakest)			155-58	1.34	139.32			
49-50	1.42	110.11	49-152	1.38	117.84			
53-54	1.41	110.84	152-51	1.33	159.60			
57-58	1.42	106.90	51-151	1.39	132.86			
			151-50	1.34	142.04			
			154-53	1.39	119.05			
			154-55	1.34	155.98			
			55-153	1.39	129.46			
			153-54	1.34	141.25			
			49-145	1.42	116.48			
			53-147	1.42	117.07			
			57-149	1.42	116.60			

D3



O-N (1 st weakest)			N-C			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
4-31	1.26	134.83	31-61	1.46	107.07	61-62	1.43	139.67
5-31	1.26	137.30	36-66	1.47	100.28	65-66	1.43	137.88
6-36	1.26	133.67	29-61	1.33	147.39	Complex bridge (2 nd weakest)		
7-36	1.26	135.96	30-62	1.34	148.50	62-63	1.46	116.53
1-29	1.41	67.43	34-65	1.34	149.86	64-65	1.45	121.55
1-30	1.42	63.46	35-66	1.32	152.45	63-64	1.44	134.06
3-34	1.41	64.04				32-64	1.33	147.53
3-35	1.40	68.41				33-63	1.33	149.86
						2-32	1.41	65.35
						2-33	1.42	64.46

D4



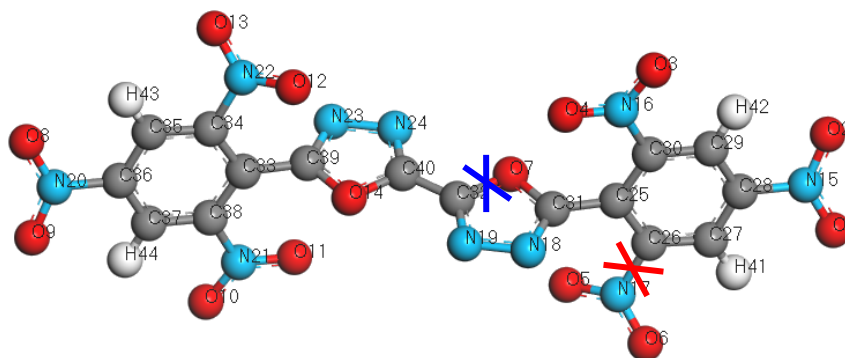
O-N (2 nd weakest)			N-C			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
5-39	1.26	137.49	39-65	1.47	95.72	65-66	1.43	139.23
6-39	1.26	134.42	40-70	1.45	106.60	67-68	1.42	141.62
7-40	1.27	134.02	33-65	1.32	156.27	69-70	1.43	139.04
8-40	1.27	135.21	34-66	1.34	148.69	Complex bridge (1 st weakest)		
1-33	1.41	67.36	37-69	1.33	148.33	66-67	1.44	127.32
1-34	1.41	65.03	38-70	1.33	146.78	68-69	1.46	117.68
3-37	1.42	62.97				35-67	1.35	140.31
3-38	1.41	67.07				36-68	1.34	147.88
						2-35	1.55	50.69
						2-36	1.38	76.88
						4-35	1.24	146.30

D5

ORTEP diagram of the crystal structure of compound 5, showing the molecular structure with thermal ellipsoids at the 50% probability level. The structure is a complex organic molecule with multiple nitrogen and oxygen atoms. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as small spheres of arbitrary radii. The molecule is shown in a perspective view, with atoms labeled with their respective element symbols and numbers.

O-N			N-C (2 nd weakest)			Complex bridge (1 st and 2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-21	1.26	134.20	21-34	1.48	103.64	45-51	1.47	123.02
2-21	1.27	133.29	22-36	1.49	106.99	52-38	1.43	137.49
3-22	1.26	139.91	23-32	1.49	100.78	37-31	1.47	123.02
4-22	1.27	135.40	26-48	1.48	103.64	17-51	1.39	100.29
5-23	1.27	131.64	27-50	1.49	106.99	17-52	1.39	98.72
6-23	1.26	135.28	28-46	1.49	100.78	7-37	1.39	100.29
11-26	1.26	134.20	C-C			7-38	1.39	98.72
12-26	1.27	133.29	45-46	1.41	139.75	29-30	1.44	109.53
13-27	1.26	139.91	46-47	1.39	135.62	24-25	1.44	109.53
14-27	1.27	135.40	47-48	1.40	135.70	24-37	1.32	154.94
15-28	1.27	131.64	48-49	1.39	136.00	25-38	1.32	150.13
16-28	1.26	135.28	49-50	1.39	136.94	29-51	1.32	154.94
			50-45	1.41	138.93	30-52	1.32	150.13
			31-32	1.41	139.75			
			32-33	1.39	135.62			
			33-34	1.40	135.70			
			34-35	1.39	136.00			
			35-36	1.39	136.94			
			36-31	1.41	138.94			

D5-solvent free



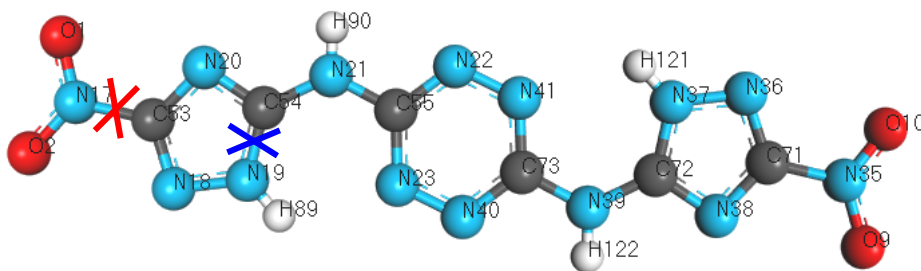
O-N			N-C (1 st weakest)			Complex bridge (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-15	1.26	134.09	15-28	1.49	98.61	33-39	1.47	121.32
2-15	1.27	131.78	16-30	1.48	103.88	40-32	1.44	134.10
3-16	1.27	136.66	17-26	1.49	96.94	31-25	1.47	121.32
4-16	1.27	133.96	20-36	1.49	98.61	14-39	1.39	100.78
5-17	1.27	132.89	21-38	1.48	103.88	14-40	1.40	99.29
6-17	1.26	135.84	22-34	1.49	96.94	7-31	1.39	100.78
8-20	1.26	134.09	C-C			7-32	1.40	99.29
9-20	1.27	131.78	25-26	1.41	138.75	23-24	1.43	107.35
10-21	1.27	136.66	26-27	1.39	134.22	18-19	1.43	107.35
11-21	1.27	133.96	27-28	1.39	134.46	18-31	1.32	153.38
12-22	1.27	132.89	28-29	1.39	134.80	19-32	1.32	149.43
13-22	1.26	135.84	29-30	1.39	134.75	23-39	1.32	153.38
			30-25	1.41	138.33	24-40	1.32	149.43
			33-34	1.41	138.75			
			34-35	1.39	134.22			
			35-36	1.39	134.46			
			36-37	1.39	134.80			
			37-38	1.39	134.75			
			38-33	1.41	138.33			

D6

ORTEP diagram of the crystal structure of compound 6, showing the molecular structure with thermal ellipsoids at the 50% probability level. The structure is a complex organic molecule with multiple nitrogen and oxygen atoms. A red 'X' is drawn over the N25-O5 bond, and a blue 'X' is drawn over the N21-O4 bond.

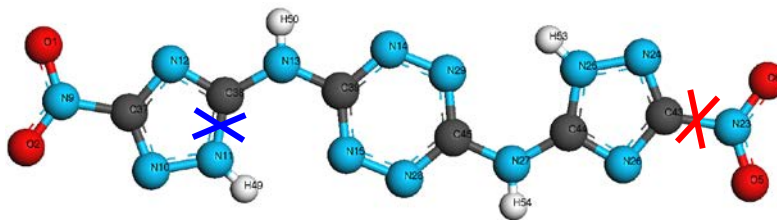
O-N			N-C (2 nd weakest)			Complex bridge (1 st weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-21	1.27	131.18	21-43	1.47	101.45	46-23	1.43	115.60
2-21	1.27	132.04	22-45	1.47	104.14	62-33	1.43	115.58
3-22	1.27	135.27	31-59	1.47	101.46	5-24	1.43	68.48
4-22	1.27	133.60	32-61	1.47	104.17	5-25	1.43	67.17
11-31	1.27	131.13	C-C			15-34	1.43	68.35
12-31	1.27	132.00	41-42	1.39	129.41	15-35	1.43	67.29
13-32	1.27	135.38	42-43	1.40	132.59	23-48	1.40	129.45
14-32	1.27	133.53	43-44	1.39	133.61	23-47	1.40	131.23
			44-45	1.39	133.34	24-63	1.30	154.14
			45-46	1.41	139.23	25-48	1.32	153.88
			46-41	1.40	134.53	33-63	1.40	131.21
			57-58	1.39	129.43	33-64	1.40	129.46
			58-59	1.40	132.60	47-34	1.30	154.11
			59-60	1.39	133.64	64-35	1.32	153.90
			60-61	1.39	133.36			
			61-62	1.41	139.25			
			62-57	1.40	134.54			
			48-63	5.43	139.40			
			47-64	5.43	139.45			

D7



O-N			N-C (1 st and 2 nd weakest)			Complex bridge		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-17	1.27	131.13	17-53	1.45	109.97	54-21	1.37	127.02
2-17	1.27	132.02	53-18	1.35	138.95	21-55	1.37	131.44
9-35	1.27	131.13	53-20	1.36	139.87	72-39	1.37	127.02
10-35	1.27	132.02	20-54	1.36	158.15	39-73	1.37	131.43
N-N			54-19	1.38	120.99	55-22	1.37	138.81
18-19	1.38	121.42	35-71	1.45	109.97	55-23	1.37	137.97
36-37	1.38	121.42	71-36	1.35	138.95	22-41	1.35	130.53
			71-38	1.36	139.87	23-40	1.35	130.53
			38-72	1.36	158.15	73-40	1.37	138.81
			72-37	1.38	120.99	73-41	1.37	137.97

D7-solvent free

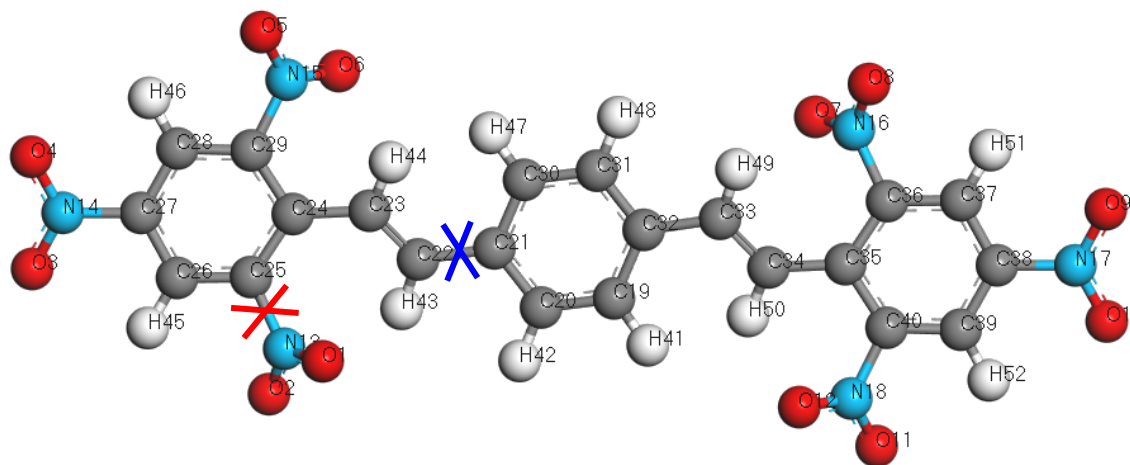


O-N			N-C (1 st and 2 nd weakest)			Complex bridge		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-9	1.26	131.94	9-37	1.46	107.49	13-39	1.39	129.64
2-9	1.27	133.10	23-43	1.46	107.42	38-13	1.37	130.39
5-23	1.26	131.79	10-37	1.34	145.20	44-27	1.37	130.38
6-23	1.27	133.19	37-12	1.36	141.05	27-45	1.39	129.59
N-N			12-38	1.36	158.02	15-28	1.35	132.52
11-10	1.39	120.78	38-11	1.37	127.99	14-29	1.35	132.59
24-25	1.39	120.71	26-43	1.36	141.03	39-14	1.37	139.79
			43-24	1.34	145.11	39-15	1.37	138.09
			25-44	1.37	127.99	45-29	1.37	138.07
			44-26	1.36	157.95	45-28	1.37	139.70

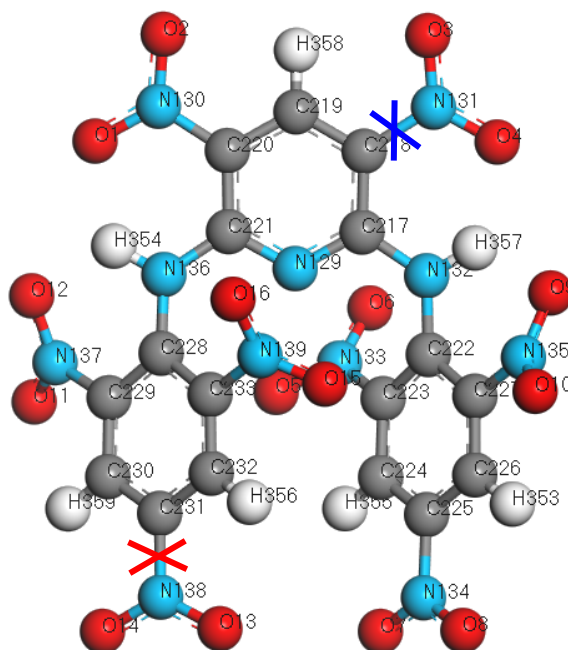
D8

ORTEP diagram of the crystal structure of 2,2'-(1,3-phenylene)bis(4-nitrophenol) (D8). The molecule is shown as a single unit with thermal ellipsoids at the 50% probability level. Atoms are labeled: C1-C14 for the carbon framework, N1-N4 for the nitro groups, and O1-O8 for the oxygen atoms. Hydrogen atoms are labeled H1-H14. The structure features a central biphenyl core with nitro groups at the 2 and 2' positions. A red cross is drawn over the C11-C12 bond, and a blue cross is drawn over the C13-C14 bond.

O-N			N-C (1 st weakest)			Complex bridge (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
3-68	1.27	130.91	65-108	1.49	101.54	102-103	1.49	110.95
4-67	1.27	131.24	66-97	1.48	101.37	105-101	1.49	110.82
5-66	1.27	131.11	67-111	1.49	100.30	13-71	1.27	131.95
6-65	1.27	132.06	68-100	1.48	100.39	14-72	1.27	132.96
7-67	1.26	134.87	69-107	1.48	102.57	1-71	1.27	131.25
8-68	1.26	133.99	70-112	1.48	103.12	2-72	1.27	130.39
9-70	1.27	133.54	C-C			98-103	1.40	130.18
10-69	1.27	132.45	97-101	1.41	137.14	105-98	1.40	129.92
11-65	1.26	136.04	109-97	1.39	134.28	106-113	1.39	133.76
12-66	1.26	135.21	107-109	1.39	132.69	110-106	1.39	133.84
15-69	1.27	133.62	114-107	1.39	133.39	113-105	1.40	139.38
16-70	1.26	133.42	100-114	1.39	134.44	103-110	1.40	139.74
			101-100	1.41	137.40	71-113	1.48	101.31
			111-102	1.41	137.63	72-110	1.48	101.61
			102-108	1.41	137.25			
			108-99	1.39	134.28			
			99-112	1.39	133.02			
			112-104	1.39	133.50			
			104-111	1.39	134.44			

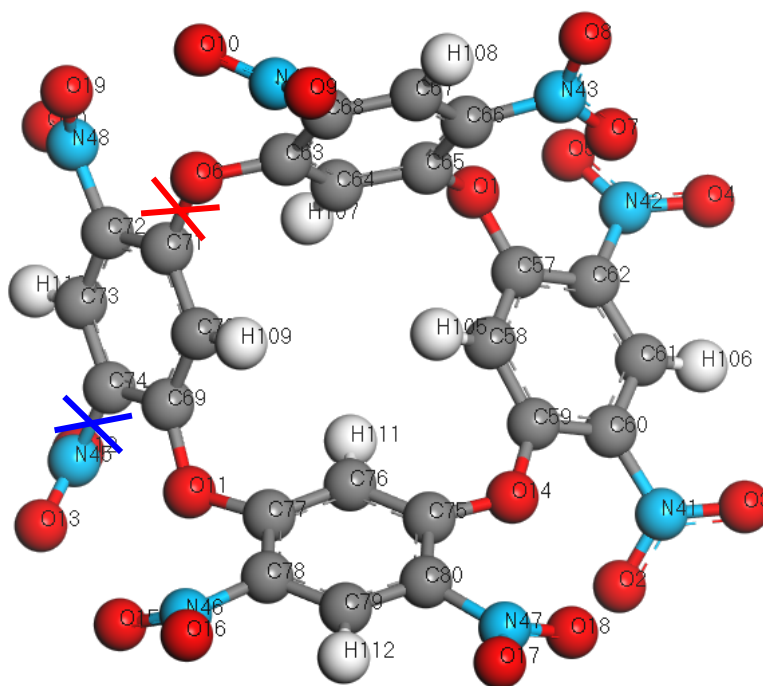
D9


O-N			N-C (1 st weakest)			Complex bridge (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-13	1.27	135.81	13-25	1.49	99.04	24-23	1.45	117.38
2-13	1.26	136.94	14-27	1.47	102.59	23-22	1.36	136.88
3-14	1.27	131.49	15-29	1.48	101.39	22-21	1.46	111.43
4-14	1.27	131.83	16-36	1.49	99.04	32-33	1.46	111.43
5-15	1.26	136.97	17-38	1.47	102.59	33-34	1.36	136.88
6-15	1.27	131.72	18-40	1.48	101.39	34-35	1.45	117.38
7-16	1.27	135.81	C-C			32-19	17.93	123.83
8-16	1.26	136.94	24-25	1.42	135.53	19-20	1.39	126.08
9-17	1.27	131.49	25-26	1.39	135.26	30-31	1.39	126.08
10-17	1.27	131.83	26-27	1.40	133.45	31-32	1.41	122.06
11-18	1.26	136.97	27-28	1.39	133.62	20-21	1.41	122.06
12-18	1.27	131.72	28-29	1.39	133.90	21-30	17.93	123.83
			29-24	1.42	133.92			
			35-36	1.42	135.53			
			36-37	1.39	135.26			
			37-38	1.40	133.45			
			38-39	1.39	133.62			
			39-40	1.39	133.90			
			40-35	1.42	133.92			

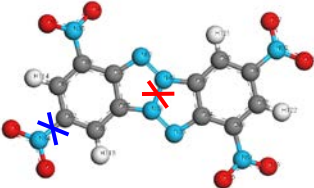
D10


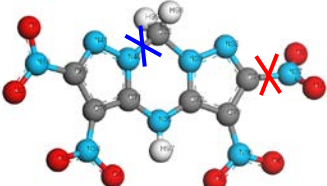
O-N			N-C (1 st weakest)			Complex bridge (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
5-133	1.27	135.92	133-223	1.48	100.60	132-217	1.38	131.41
6-133	1.27	135.37	134-225	1.47	102.54	132-222	1.39	122.40
7-134	1.27	131.08	135-227	1.47	106.53	136-221	1.37	132.44
8-134	1.27	132.25	137-229	1.47	103.32	136-228	1.40	120.50
9-135	1.27	129.60	138-231	1.48	100.17	1-130	1.28	128.22
10-135	1.27	133.20	139-233	1.48	102.03	2-130	1.27	132.51
11-137	1.27	133.73	C-C			3-131	1.27	132.34
12-137	1.27	127.55	222-223	1.42	139.29	4-131	1.28	127.79
13-138	1.27	132.25	223-224	1.39	134.67	217-218	1.43	138.28
14-138	1.27	129.38	224-225	1.40	132.71	218-219	1.39	133.54
15-139	1.26	137.38	225-226	1.39	134.51	219-220	1.39	134.67
16-139	1.26	134.84	226-227	1.39	134.48	220-221	1.43	137.43
			227-222	1.42	140.10	129-217	1.34	156.42
			228-229	1.42	139.15	129-221	1.35	155.56
			229-230	1.39	133.27	130-220	1.45	111.47
			230-231	1.39	134.65	131-218	1.45	110.18
			231-232	1.39	131.82			
			232-233	1.39	134.27			
			233-228	1.42	139.11			

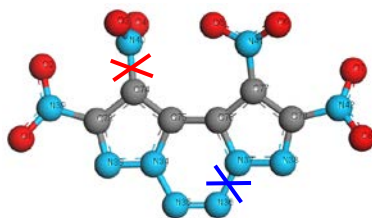
D11



O-N			N-C (2 nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
2-41	1.27	133.76	41-60	1.47	99.98	57-58	1.40	139.59
3-41	1.27	131.51	42-62	1.46	104.22	58-59	1.39	140.23
4-42	1.27	131.42	43-66	1.46	107.13	59-60	1.41	142.58
5-42	1.27	133.81	44-68	1.48	98.98	60-61	1.39	134.43
7-43	1.27	129.54	45-74	1.48	96.63	61-62	1.39	133.40
8-43	1.27	134.75	46-78	1.47	102.57	62-57	1.41	142.64
9-44	1.26	132.88	47-80	1.47	103.95	63-64	1.40	137.37
10-44	1.26	133.75	48-72	1.46	105.08	64-65	1.39	143.03
12-45	1.27	132.42	Complex bridge (1 st weakest)			65-66	1.41	142.51
13-45	1.27	130.54	1-57	1.39	94.41	66-67	1.40	132.37
15-46	1.27	132.78	1-65	1.40	92.87	67-68	1.39	135.01
16-46	1.27	132.75	6-63	1.38	95.90	68-63	1.41	143.90
17-47	1.26	134.37	6-71	1.40	90.79	69-70	1.40	138.14
18-47	1.27	130.78	11-69	1.39	94.72	70-71	1.40	141.26
19-48	1.28	129.08	11-77	1.40	93.07	71-72	1.41	143.97
20-48	1.27	136.79	14-59	1.39	93.88	72-73	1.39	131.98
			14-75	1.38	95.64	73-74	1.39	134.62
						74-69	1.41	143.90

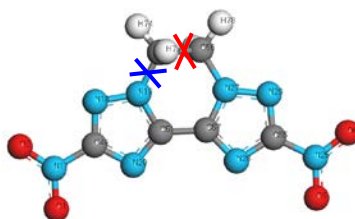
E1								
								
O-N			N-C (2nd weakest)			C-C		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-34	1.27	132.61	34-67	1.47	104.64	65-66	1.39	133.29
2-34	1.27	131.76	35-69	1.46	106.32	66-67	1.39	134.51
3-35	1.27	134.30	50-91	1.47	104.64	67-68	1.40	130.70
4-35	1.27	132.02	51-93	1.46	106.32	68-69	1.38	136.59
17-50	1.27	132.61	Complex bridge (1st weakest)			69-70	1.42	133.26
18-50	1.27	131.76	52-49	1.37	120.76	70-65	1.44	133.89
19-51	1.27	134.30	49-33	1.41	86.40	89-90	1.39	133.29
20-51	1.27	132.02	33-36	1.37	120.76	90-91	1.39	134.51
			70-52	1.38	141.46	91-92	1.40	130.70
			65-33	1.38	129.00	92-93	1.38	136.59
			89-49	1.38	129.00	93-94	1.42	133.26
			94-36	1.38	141.46	94-89	1.44	133.89

E2								
								
O-N			N-C (1st weakest)			Complex bridge (2nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-33	1.26	134.39	33-69	1.47	103.15	75-40	1.48	100.59
2-33	1.26	131.43	34-70	1.43	116.04	39-75	1.47	100.88
3-34	1.26	137.55	36-73	1.41	118.49	71-35	1.36	134.08
4-34	1.29	124.13	37-74	1.46	98.35	35-72	1.36	132.14
5-36	1.28	128.54	69-41	1.34	149.08	C-C		
6-36	1.27	133.45	71-40	1.37	132.10	69-70	1.43	131.28
7-37	1.26	135.04	72-39	1.37	133.17	70-71	1.41	145.32
8-37	1.26	131.09	38-74	1.34	155.06	72-73	1.40	144.93
			N-N			73-74	1.42	134.88
			38-39	1.40	119.36			
			40-41	1.39	117.84			
E3								



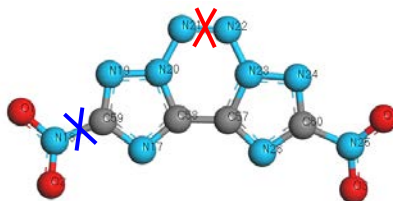
O-N			N-C (1 st weakest)			Complex bridge (2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-39	1.26	133.54	39-73	1.46	103.73	75-76	1.43	139.75
2-39	1.26	133.07	40-74	1.48	93.12	34-35	1.39	100.39
3-40	1.26	134.69	41-77	1.44	109.07	35-36	1.28	169.71
4-40	1.26	136.16	42-78	1.47	102.75	36-37	1.40	98.44
5-41	1.27	133.72	73-33	1.34	149.36	C-C		
6-41	1.26	133.42	75-34	1.42	110.46	73-74	1.41	140.07
7-42	1.26	139.87	78-38	1.34	153.57	74-75	1.40	147.11
8-42	1.26	136.45	76-37	1.40	114.06	76-77	1.40	146.87
			N-N			77-78	1.43	134.87
			34-33	1.37	120.94			
			37-38	1.37	119.52			

E4



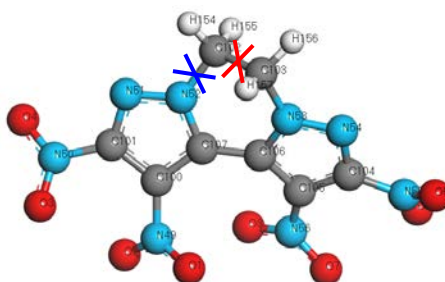
O-N			N-C			Complex bridge (1 st and 2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-17	1.27	133.68	17-49	1.45	107.78	51-57	1.43	129.45
2-17	1.27	132.46	25-55	1.45	107.78	50-56	1.53	82.73
5-25	1.27	133.68	18-49	1.36	144.28	27-56	1.48	96.09
6-25	1.27	132.45	49-20	1.37	141.54	19-50	1.48	96.09
N-N			20-51	1.35	157.61			
18-19	1.37	128.66	51-19	1.38	121.37			
26-27	1.37	128.66	26-55	1.36	144.28			
			55-28	1.37	141.54			
			28-57	1.35	157.61			
			57-27	1.38	121.37			

E5



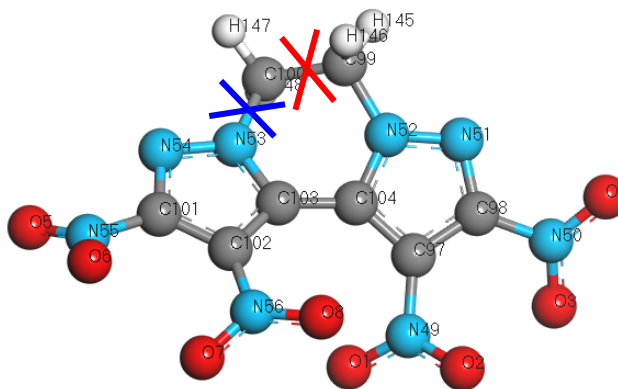
O-N			N-C (2 nd weakest)			Complex bridge (1 st weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-18	1.26	135.15	18-59	1.47	102.53	57-58	1.42	135.42
2-18	1.26	137.15	25-60	1.47	102.81	20-21	1.40	95.14
3-25	1.26	134.73	59-19	1.35	146.78	21-22	1.29	166.94
4-25	1.26	135.78	59-17	1.37	143.48	22-23	1.40	96.71
N-N			17-58	1.33	162.03			
19-20	1.38	122.94	58-20	1.42	107.19			
23-24	1.38	122.63	24-60	1.35	147.79			
			60-26	1.37	143.37			
			26-57	1.33	161.96			
			57-23	1.42	107.19			

E6



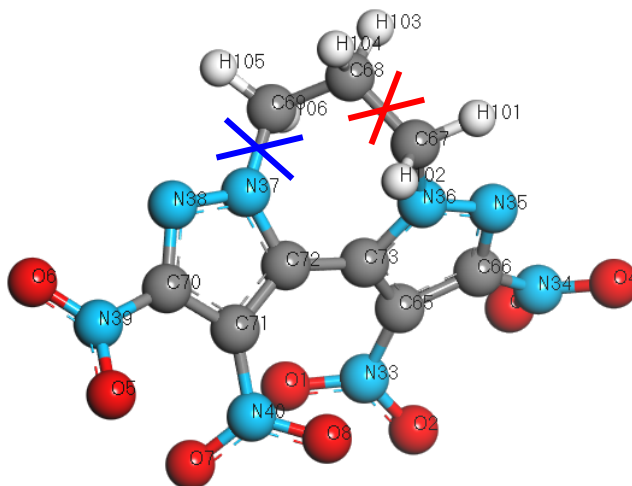
O-N			N-C			Complex bridge (1 st and 2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-49	1.27	134.74	49-100	1.44	108.86	106-107	1.43	132.75
2-49	1.27	135.96	50-101	1.45	105.39	102-103	1.53	80.48
3-50	1.26	133.03	55-104	1.45	103.83	52-102	1.48	94.83
4-50	1.26	134.79	56-105	1.43	113.46	53-103	1.48	96.30
5-55	1.27	133.62	51-101	1.35	147.45	C-C		
6-55	1.26	132.60	52-107	1.38	125.29	101-100	1.42	137.10
7-56	1.27	133.32	53-106	1.38	126.25	100-107	1.40	144.60
8-56	1.27	134.05	54-104	1.35	149.11	104-105	1.42	134.83
N-N						105-106	1.41	143.21
51-52	1.37	125.10						
53-54	1.37	123.99						

E6-solvent free



O-N			N-C			Complex bridge (1 st and 2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-49	1.27	135.19	49-97	1.45	108.15	102-101	1.42	135.54
2-49	1.27	135.26	50-98	1.45	105.75	99-100	1.53	80.50
3-50	1.26	132.80	55-101	1.46	101.88	52-99	1.48	94.84
4-50	1.26	134.14	56-102	1.44	111.90	53-100	1.48	94.81
5-55	1.26	134.97	98-51	1.35	146.83	C-C		
6-55	1.26	132.06	104-52	1.38	125.25	98-97	1.41	136.87
7-56	1.27	134.39	101-54	1.35	149.92	97-104	1.40	144.44
8-56	1.27	133.61	103-53	1.38	123.76	104-103	1.43	132.40
N-N						103-102	1.40	144.04
51-52	1.37	125.20						
53-54	1.38	122.90						

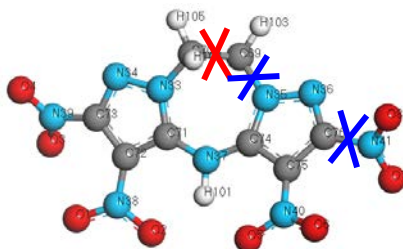
E7



O-N			N-C			Complex bridge (1 st and 2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-33	1.28	133.00	33-65	1.43	114.83	67-68	1.54	77.83
2-33	1.27	136.59	34-66	1.45	105.98	68-69	1.53	78.59
3-34	1.27	135.71	39-70	1.46	105.01	73-72	1.44	128.84
4-34	1.26	133.74	40-71	1.45	106.38	67-36	1.48	92.35
5-39	1.27	132.53	66-35	1.35	148.98	69-37	1.48	92.05
6-39	1.26	134.40	73-36	1.38	124.78	C-C		
7-40	1.26	135.41	72-37	1.38	123.69	66-65	1.41	135.92
8-40	1.27	130.90	70-38	1.35	147.00	65-73	1.40	144.36
N-N						72-71	1.40	144.81
35-36	1.38	124.18				71-70	1.41	135.91
37-38	1.37	124.43						

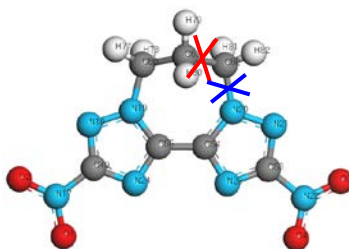
E8

ORTEP diagram of the 3D structure of compound 10, showing the molecular structure with thermal ellipsoids at the 50% probability level. The structure is a complex organic molecule with a central ring system and various substituents. A red 'X' is placed over the C1-C2 bond, and a blue 'X' is placed over the C2-C3 bond.

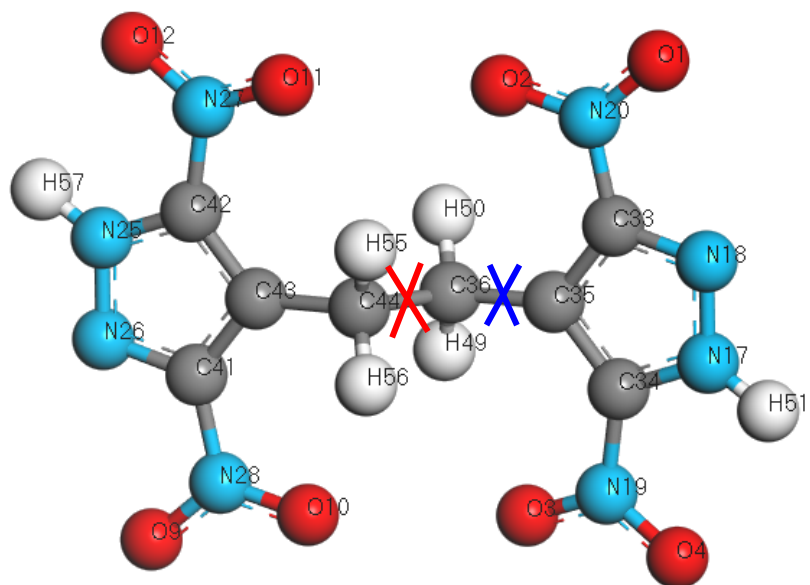


E9

A 3D ball-and-stick model of a chemical structure, likely a substituted benzene derivative. The structure features a central benzene ring with two nitro groups (NO₂) attached at the para positions. The atoms are color-coded: carbon (grey), hydrogen (white), nitrogen (blue), and oxygen (red). A red 'X' is drawn over a C-H bond, and a blue 'X' is drawn over a C-C bond, indicating specific points of interest or modification.

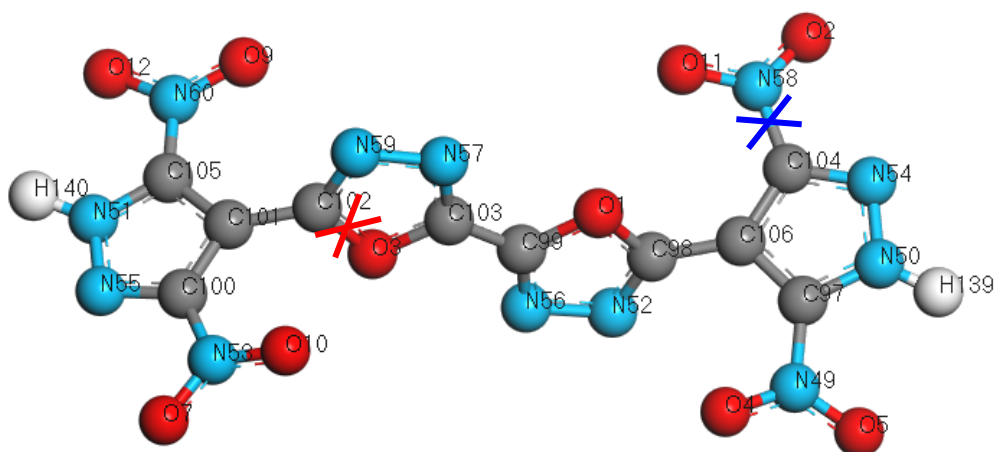


HL3



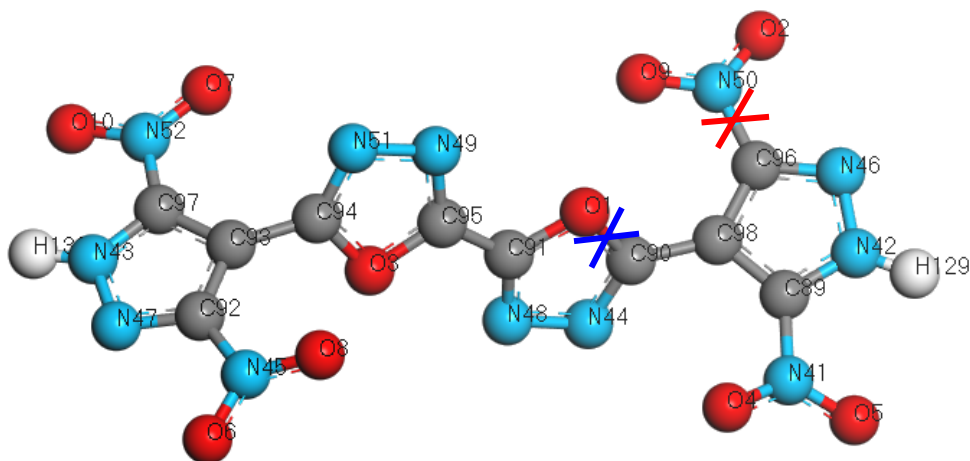
O-N			N-C			C-C (1 st and 2 nd weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-20	1.27	131.37	19-34	1.43	118.74	33-35	1.42	134.78
2-20	1.27	131.14	20-33	1.44	114.07	35-34	1.40	142.97
3-19	1.27	133.17	27-42	1.43	118.79	41-43	1.42	134.76
4-19	1.28	130.11	28-41	1.44	114.13	43-42	1.40	142.95
9-28	1.27	131.45	17-34	1.38	123.26	35-36	1.49	97.23
10-28	1.27	131.08	18-33	1.37	135.89	36-44	1.56	71.63
11-27	1.27	133.16	25-42	1.38	123.24	44-43	1.49	97.26
12-27	1.28	130.01	26-41	1.37	135.93	N-N		
						17-18	1.35	125.52
						25-26	1.35	125.56

HL7



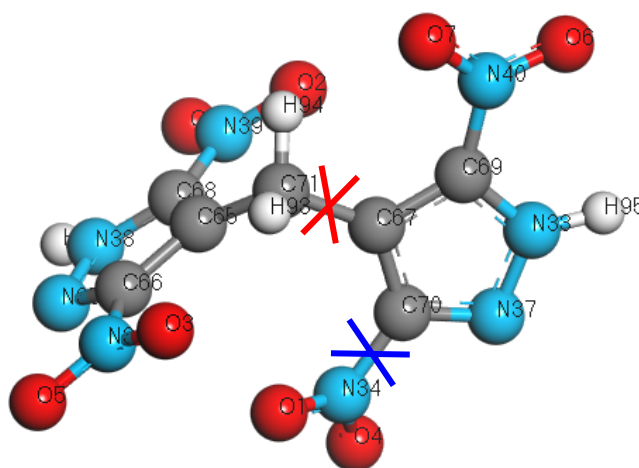
O-N			N-C (2 nd weakest)			Complex bridge (1 st weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
2-58	1.26	133.43	58-104	1.45	106.92	98-106	1.45	124.89
11-58	1.27	132.93	49-97	1.44	115.36	99-103	1.43	133.84
4-49	1.26	136.67	53-100	1.45	106.27	101-102	1.45	123.87
5-49	1.27	132.18	60-105	1.43	116.33	1-98	1.40	97.90
7-53	1.27	132.86	51-105	1.37	124.83	1-99	1.39	99.52
10-53	1.27	132.03	55-100	1.36	142.69	3-102	1.40	96.84
12-60	1.28	128.84	50-97	1.37	124.93	3-103	1.39	101.03
9-60	1.27	135.35	54-104	1.36	142.36	57-59	1.44	105.42
N-N			C-C			52-56	1.43	108.23
51-55	1.36	124.34	105-101	1.40	144.21	52-98	1.32	152.07
50-54	1.36	124.84	101-100	1.41	136.27	56-99	1.32	148.79
			97-106	1.40	144.68	59-102	1.32	152.36
			104-106	1.42	136.27	57-103	1.32	147.95

HL7-solvent free



O-N			N-C (2 nd weakest)			Complex bridge (1 st weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
2-50	1.27	131.21	50-96	1.45	104.98	90-98	1.45	124.08
9-50	1.26	133.46	41-89	1.44	114.56	91-95	1.43	132.67
4-41	1.26	134.98	45-92	1.45	107.63	93-94	1.45	124.99
5-41	1.27	133.26	52-97	1.44	117.28	1-90	1.40	97.31
6-45	1.27	133.01	43-97	1.37	124.61	1-91	1.39	99.63
8-45	1.26	134.15	47-92	1.36	145.84	3-94	1.40	98.81
7-52	1.26	137.69	42-89	1.36	122.16	3-95	1.39	99.48
10-52	1.28	129.65	46-96	1.36	143.30	44-48	1.43	108.16
C-C			N-N			49-51	1.44	106.87
96-98	1.42	134.94	42-46	1.37	121.62	44-90	1.32	150.59
89-98	1.40	143.40	43-47	1.36	120.94	48-91	1.32	147.50
92-93	1.42	136.93				49-95	1.32	149.04
93-97	1.40	146.88				51-94	1.31	151.87

HL9



O-N			N-C (2 nd weakest)			C-C (1 st weakest)		
Label	Length	Strength	Label	Length	Strength	Label	Length	Strength
1-34	1.27	131.35	34-70	1.44	103.64	69-67	1.40	144.22
4-34	1.26	133.17	39-68	1.42	119.67	67-70	1.42	136.59
2-39	1.28	130.08	36-66	1.45	110.76	66-65	1.42	137.05
8-39	1.27	136.58	40-69	1.43	116.11	65-68	1.40	145.19
3-36	1.27	132.65	33-69	1.37	119.19	67-71	1.50	95.91
5-36	1.27	130.71	37-70	1.37	142.30	65-71	1.50	96.52
7-40	1.27	132.41	35-66	1.36	136.80	N-N		
6-40	1.27	130.56	38-68	1.38	121.56	33-37	1.35	126.17
						35-38	1.36	122.65

Molecular Level Correlations

Table S7. Summary of parameters including Molecular Weight (MW, Da), Oxygen Balance (OB_{CO2}, %) and the calculated length (*L*, Å) and strength (*S*, kcal·mol⁻¹) for all 63 EMs mentioned in this study. Data for crystals that contained solvent molecules and solvent-free crystals are presented in separate entries. The bond length and strength parameters are presented for all EMs in their optimized crystal form. The bonds strength was determined by the integration of the crystal orbital Hamilton population (COHP) below the Fermi energy level. Due to the anisotropic distribution of the electron density surrounding each molecule, and due to the different polarization extent for different functional groups, the same type of covalent bonds in different energetic molecules may have different lengths and strengths.

Comp. Label	MW (Da)	OB _{CO2} (%)	1 st weakest bond			2 nd weakest bond		
			<i>L</i> (Å)	<i>S</i> (kcal/mol)	Type	<i>L</i> (Å)	<i>S</i> (kcal/mol)	Type
A1	213.12	-56.31	1.49	99.15	C-NO ₂			
A2	228.14	-56.11	1.46	108.00	C-NO ₂			
A3	243.16	-55.93	1.45	115.68	C-NO ₂			
A4	258.18	-55.78	1.43	124.08	C-NO ₂			
A5	259.16	-46.30	1.45	109.43	C-NO ₂	1.34	110.05	C-OH
A6	287.17	-47.36	1.45	112.23	C-NO ₂	1.33	113.46	C-OH
A7	227.15	-73.96	1.49	93.08	C-CH ₃	1.49	96.37	C-NO ₂
A8	270.19	-65.14	1.47	104.52	C-NO ₂			
A9	214.17	-67.24	1.42	122.26	C-NO ₂			
A10	214.11	-37.36	1.5	94.50	C-NO ₂			
A11	230.11	-27.81	1.47	103.13	C-NO ₂	1.40	129.07	C-N in 6-hetero-cycle
A12	318.2	-35.20	1.47	90.77	N-CH ₃	1.49	97.53	C-NO ₂
A13	215.15	-55.78	1.35	110.67	N=O	1.44	114.85	C-NO ₂
A14	216.14	-37.01	1.46	106.28	C-NO ₂	1.34	112.89	N=O
A15	200.14	-47.97	1.46	107.85	C-NO ₂			
A16	172.12	-55.78	1.48	96.27	C-CH ₃	1.44	114.28	C-NO ₂
B1	424.22	-52.80	1.48	100.01	C-NO ₂	1.50	112.46	C-C bridge
B2	224.16	-71.38	1.4	105.19	N-N in 5-hetero-cycle	1.42	112.79	C-NO ₂
B3	281.23	-62.58	1.41	107.94	N-N in 5-hetero-cycle	1.45	116.56	C-C bridge
B3-solvent free	254.2	-69.24	1.41	106.75	N-N in 5-hetero-cycle	1.46	114.36	C-C bridge

B4	269.16	-44.58	1.44	111.95	C-NO ₂	1.37	116.9 7	N-N in 5-hetero- cycle
B5	332.18	-24.08	1.46	106.50	C-NO ₂	1.46	121.3 1	C-C bridge
B5-solvent free	314.16	-25.46	1.46	101.89	C-NO ₂	1.45	121.4 1	C-C bridge
B6	344.2	-27.89	1.37	109.61	N-NH ₂	1.43	112.1 0	C-NO ₂
B7	314.16	-25.46	1.44	109.76	C-NO ₂	1.45	120.1 0	C-C bridge
B8	314.16	-25.46	1.51	89.57	N-NO ₂	1.43	108.2 8	C-NO ₂
B9	344.2	-27.89	1.46	104.19	C-NO ₂	1.39	107.7 3	N-NH ₂
B10	350.2	-22.84	1.45	104.35	C-NO ₂	1.43	128.4 3	C-N in 5-hetero- cycle
B10-solvent free	314.16	-25.46	1.46	100.20	C-NO ₂	1.38	125.3 3	C-C bridge
B11	256.18	-37.47	1.4	103.25	N-NH ₂	1.45	108.1 3	C-NO ₂
B12	206.16	-23.28	1.39	106.13	N-N in 5-hetero- cycle	1.33	115.5 0	N=O
B12-solvent free	170.12	-28.22	1.38	93.01	N-OH	1.38	98.96	N-N in 5-hetero- cycle
B13	573.43	-59.99	1.47	108.14	C-NO ₂	1.40	108.5 7	N-N in 5-hetero- cycle
B13-solvent free	448.28	-49.97	1.48	100.68	C-NO ₂	1.40	108.5 7	N-N in 5-hetero- cycle
C1	438.25	-62.07	1.49	93.99	C-NO ₂	1.51	96.71	C-C bridge
C2	439.24	-52.82	1.48	100.12	C-NO ₂	1.38	128.2 3	C-N bridge
C3	358.23	-40.20	1.47	102.33	C-N bridge	1.42	115.3 9	C-NO ₂
C4	418.19	-11.48	1.48	95.84	C-NO ₂	1.46	103.6 6	C-N bridge
C5	328.19	-39.00	1.45	105.79	C-NO ₂	1.46	105.9 3	C-N bridge
C6	328.19	-39.00	1.47	100.51	C-N bridge	1.45	106.5 7	C-NO ₂
C7	452.28	-70.75	1.56	75.76	C-C bridge	1.51	93.46	C-C bridge
C8	450.26	-67.52	1.49	96.85	C-NO ₂	1.46	112.8 1	C-C bridge
C9	452.24	-49.53	1.49	98.85	C-NO ₂	1.41	126.2 9	C-N bridge
C10	432.22	-22.21	1.54	75.75	C-C bridge	1.47	93.31	C-N bridge

C11	166.18	-105.91	1.53	81.65	C-C bridge	1.49	99.12	C-C bridge
D1	403.32	-89.26	1.48	100.14	C-NO ₂	1.41	106.66	N-N in 5-hetero-cycle
D1-solvent free	362.26	-75.08	1.48	98.97	C-NO ₂	1.41	107.80	N-N in 5-hetero-cycle
D2	414.3	-81.10	1.49	98.23	C-NO ₂	1.42	106.90	N-N in 5-hetero-cycle
D3	296.14	-27.01	1.42	63.46	N-O in 5-hetero-cycle	1.42	64.46	N-O in 5-hetero-cycle bridge
D4	312.14	-20.50	1.55	50.69	N-O in 5-hetero-cycle bridge	1.42	62.97	N-O in 5-hetero-cycle
D5	824.66	-97.01	1.39	98.72	C-O in 5-hetero-cycle bridge	1.39	100.29	C-O in 5-hetero-cycle bridge
D5-solvent free	560.3	-57.11	1.49	96.94	C-NO ₂	1.40	99.29	C-O in 5-hetero-cycle bridge
D6	498.32	-80.27	1.43	67.17	N-O in 5-hetero-cycle bridge	1.47	101.45	C-NO ₂
D7	628.68	-111.98	1.45	109.97	C-NO ₂	1.38	120.99	C-N in 5-heterocycle
D7-solvent free	336.24	-47.59	1.46	107.42	C-NO ₂	1.37	127.99	C-N in 5-hetero-cycle
D8	590.32	-62.34	1.49	100.30	C-NO ₂	1.48	101.31	C-NO ₂ in complex bridge
D9	552.4	-110.07	1.49	99.04	C-NO ₂	1.46	111.43	C-C bridge
D10	621.35	-55.36	1.48	100.17	C-NO ₂	1.45	110.18	C-NO ₂ in complex bridge
D11	728.4	-70.29	1.4	90.79	O-C bridge	1.48	96.63	C-NO ₂
E1	388.24	-74.18	1.41	86.40	N-N in 5-hetero-cycle bridge	1.47	104.64	C-NO ₂
E2	341.19	-35.17	1.46	98.35	C-NO ₂	1.48	100.59	C-N in 6-hetero-cycle bridge
E3	340.16	-18.81	1.48	93.12	C-NO ₂	1.40	98.44	N-N in 6-hetero-cycle bridge
E4	252.18	-63.45	1.53	82.73	C-C in 6-hetero-cycle bridge	1.48	96.09	C-N in 6-hetero-cycle bridge
E5	252.14	-25.38	1.40	95.14	N-N in 6-hetero-cycle bridge	1.47	102.53	C-NO ₂
E6	360.73	-56.55	1.53	80.48	C-C bridge	1.48	94.83	C-N bridge
E6-solvent free	340.2	-47.03	1.53	80.50	C-C bridge	1.48	94.81	C-N bridge
E7	354.23	-58.72	1.54	77.83	C-C bridge	1.48	92.05	C-N bridge
E8	355.22	-47.29	1.53	81.64	C-C bridge	1.46	97.85	C-NO ₂
E9	266.21	-78.13	1.52	80.27	C-C bridge	1.48	95.46	C-N bridge
HL3	342.22	-51.43	1.56	71.63	C-C bridge	1.49	97.23	C-C bridge

HL7	486.28	-36.19	1.40	96.84	C-O in 5-hetero-cycle bridge	1.39	99.52	C-O in 5-hetero-cycle bridge
HL7-solvent free	450.24	-39.09	1.40	98.81	C-O in 5-hetero-cycle bridge	1.39	99.63	C-O in 5-hetero-cycle bridge
HL9	328.19	-39.00s	1.50	95.91	C-C bridge	1.44	103.64	C-NO2

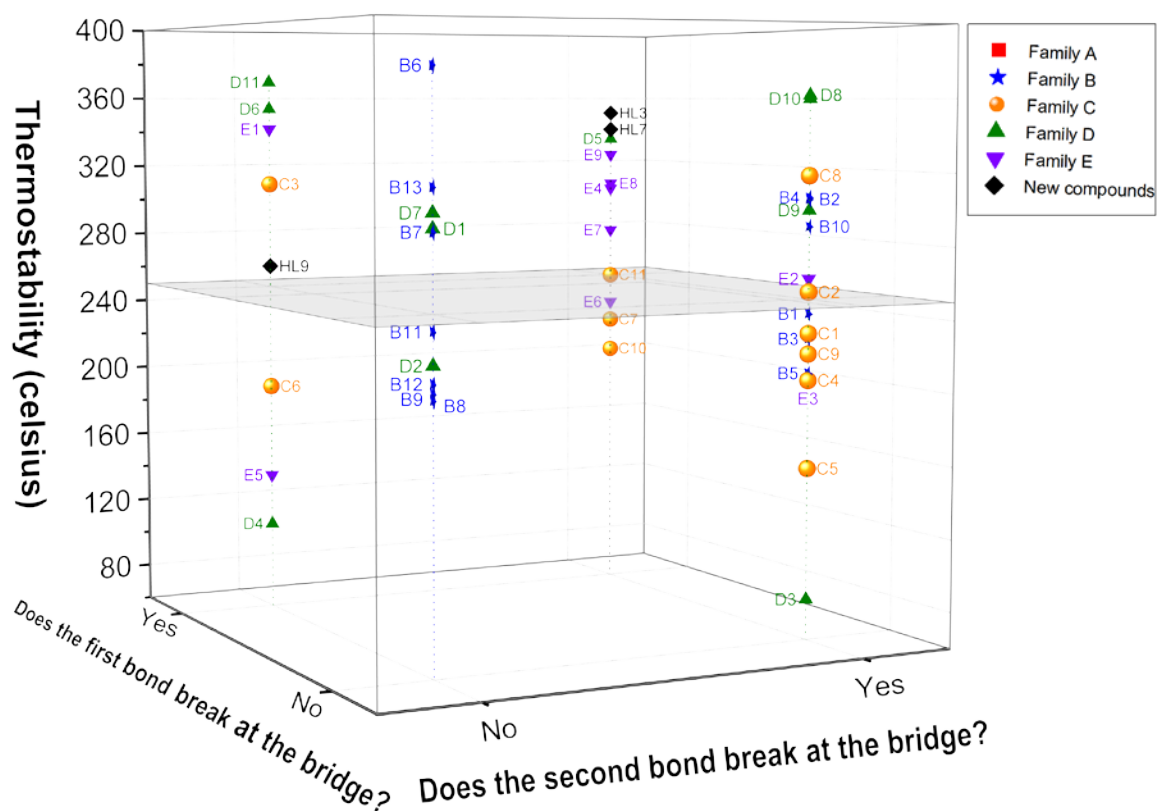


Figure S31. Full temperature range correlation between the bridge bonds reactivity and the thermostability of all bridged EMs that were mentioned in this study.

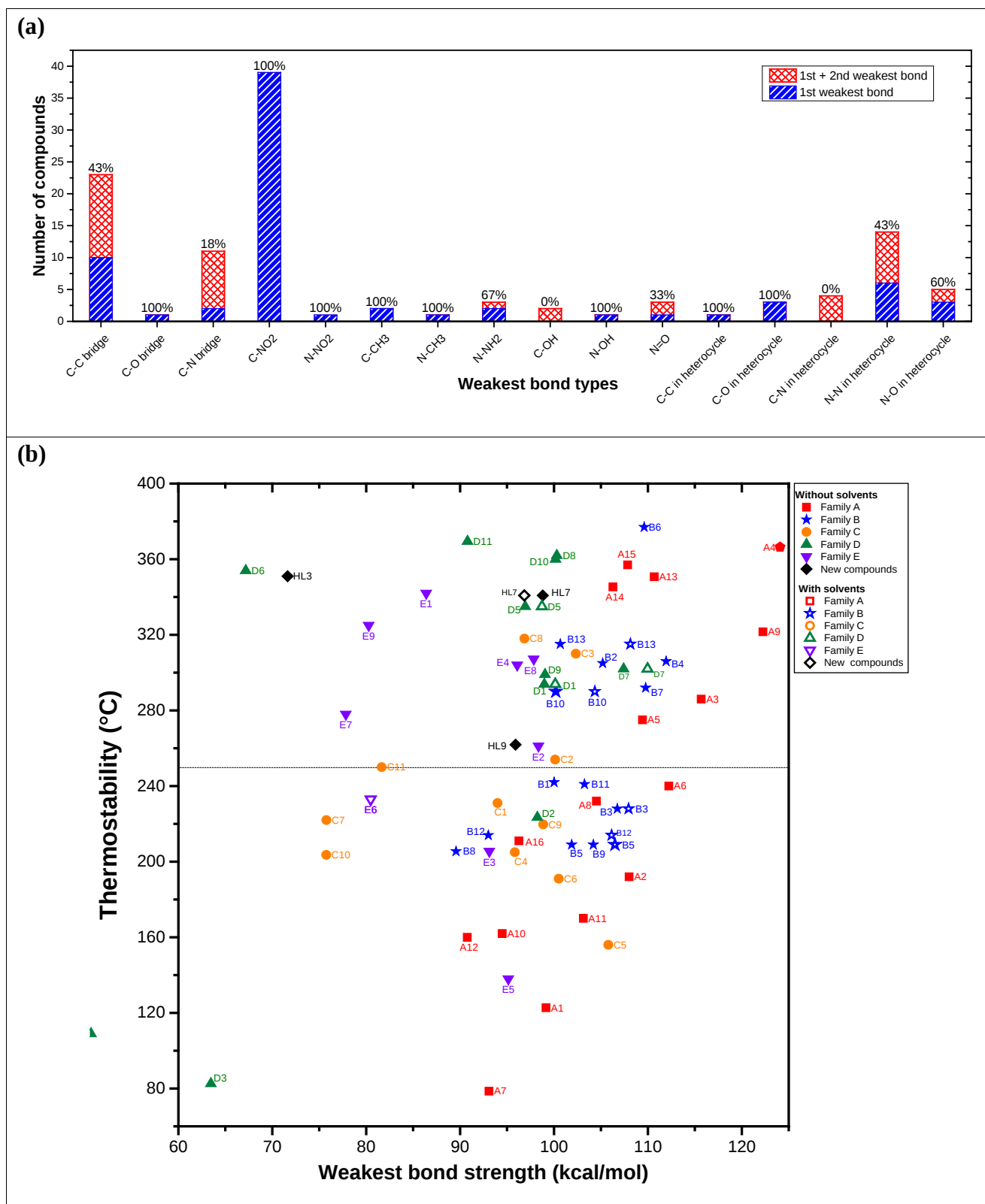


Figure S32. (a) Distribution of the 1st and the 2nd weakest bonds among various types of covalent bonds in all 63 EMs mentioned in this study; (b) full temperature range correlation between the strength of 1st weakest bond and compound's thermostability in all 63 EMs mentioned in this study.

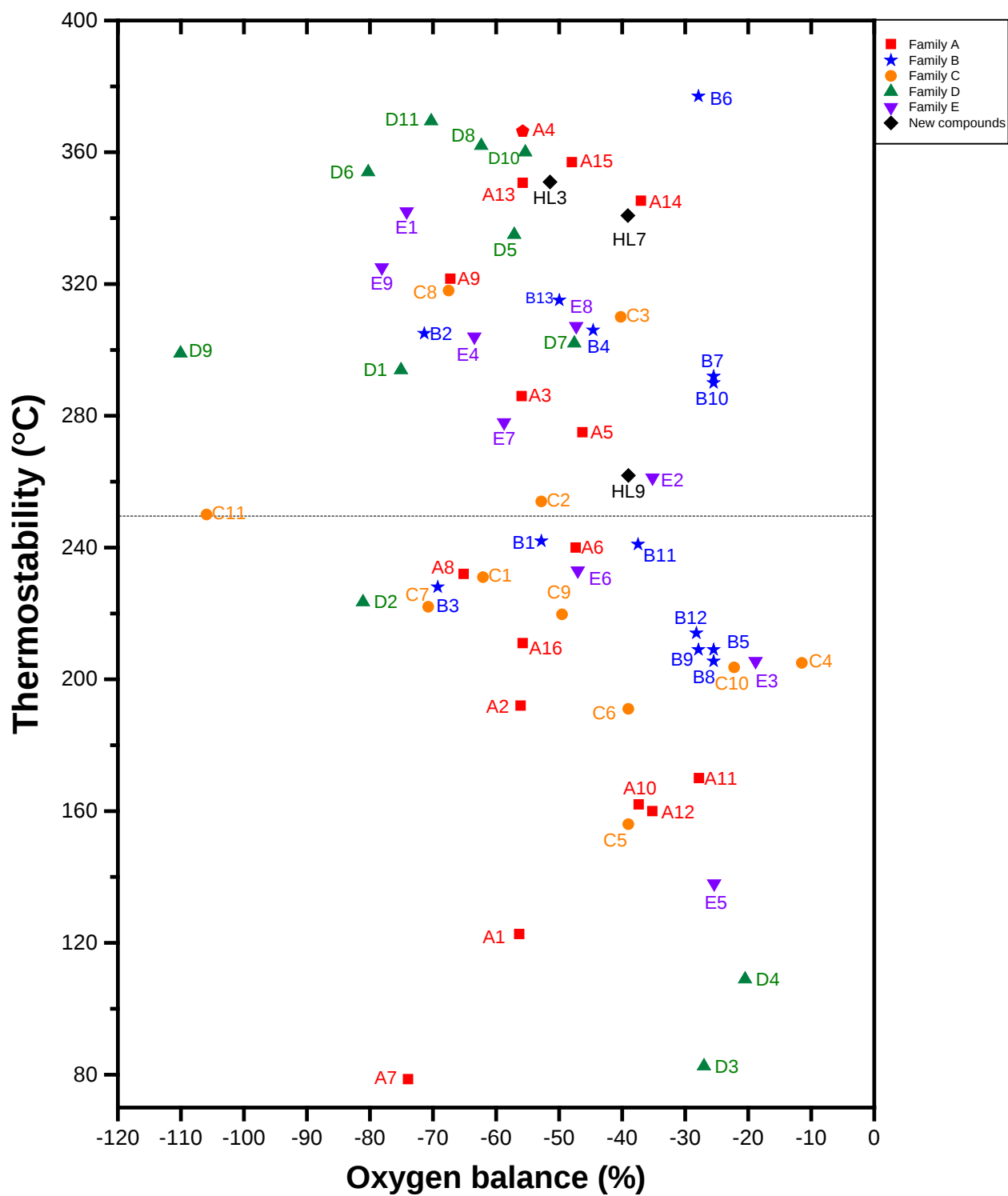


Figure S33. Full temperature range correlation between the Oxygen Balance (OB, %) values and thermostability in all 63 EMs mentioned in this study.

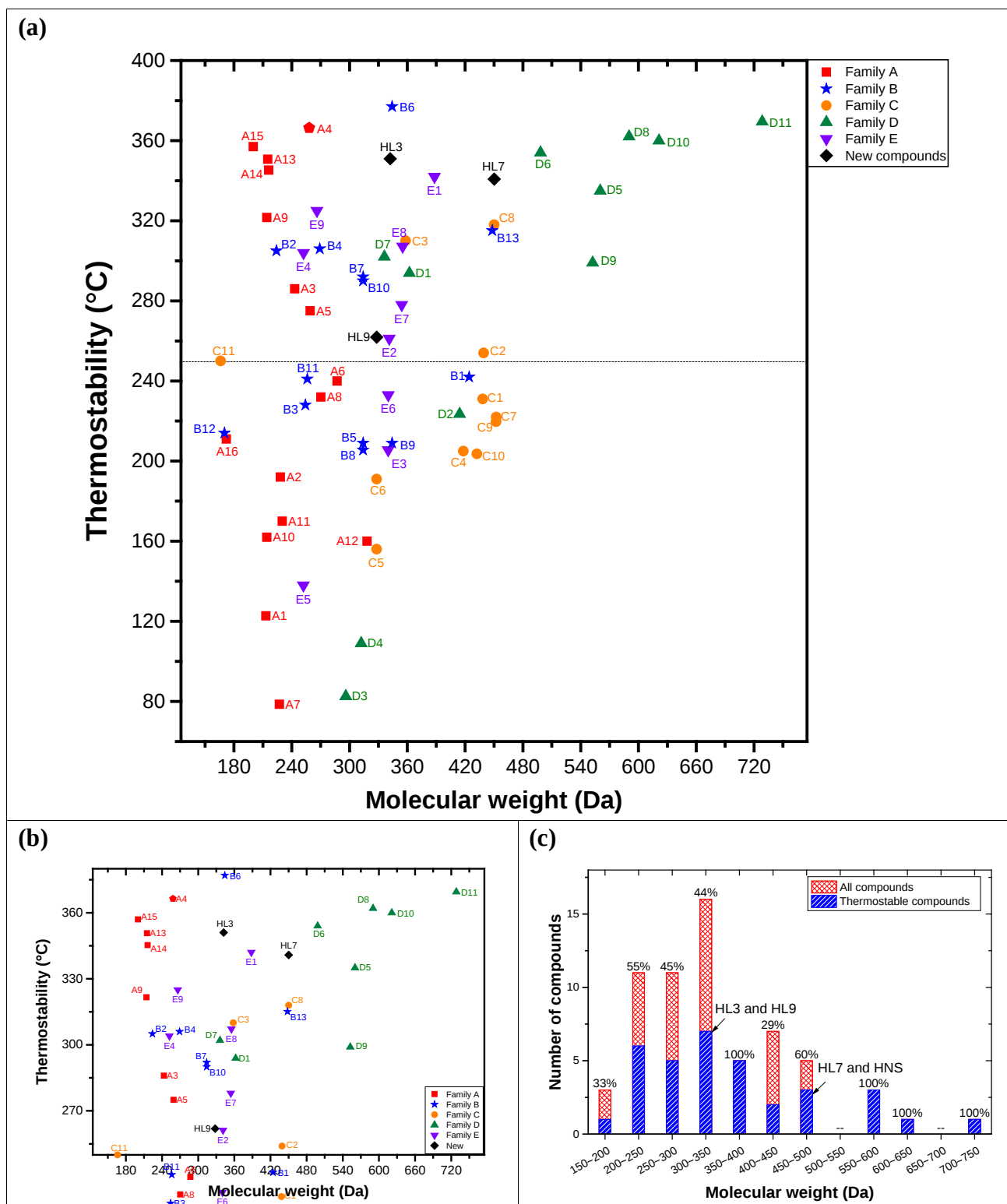


Figure S34. (a) Full temperature range correlation between the Molecular Weight (MW, Da) and the thermostability of all 63 EMs mentioned in this study; (b) focused temperature range (>250 °C) correlation between MW and EMs' thermostability; (c) distribution of thermostable EMs with respect to their MW, among all 63 EMs.

Crystal Level Correlations

Table S8. Summary of DFT-optimized crystal structure parameters of all EMs in this study. The parameters include crystal volume (V , Å³), three lattice lengths (a , b and c , Å), three lattice angles (α , β and γ , degrees), crystal density (ρ , g·cm⁻³), crystal packing coefficient (PC, %), crystal symmetry (space group number), number of molecules located in each primitive cell (n_{Mol}) and the binding energy (BE, kcal·mol⁻¹). Comparison of these calculated parameters to the x-ray crystallography for the same compounds showed very small discrepancies between the computational and experimental results, validating the reliability and precision of the used DFT method. For the solvent-containing crystals, the corresponding calculated solvent-free structures were obtained by simple removal of the solvent molecules, followed by re-optimization on the basis of the Conjugate Gradient method.

Label	Methods	V (Å ³)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	α (°)	β (°)	γ (°)	ρ (g/cm ³)	PC (%)	Space group	Space Group	n_{Mol}	BE (kcal·mol ⁻¹)
A1	Exp.	824.53	12.90	5.72	11.29	90.00	98.19	90.00	1.72	72.97	P21/c	14	4	19.23
	DFT	809.98	12.87	5.93	10.79	90.00	100.36	90.00	1.75					
	Error	-1.76	-0.16	3.61	-4.43	0.00	2.21	0.00	1.79					
A2	Exp.	827.87	5.97	9.18	15.29	90.00	99.07	90.00	1.77	74.79	P21/c	14	4	22.26
	DFT	840.99	6.01	9.33	15.16	90.00	98.54	90.00	1.79					
	Error	-1.19	-0.06	-0.60	-0.73	0.01	-0.68	0.00	1.20					
A3	Exp.	435.79	7.31	5.17	11.58	90.00	95.22	90.00	1.85	76.37	Pc	7	2	26.19
	DFT	432.94	7.21	5.32	11.30	90.00	92.69	90.00	1.87					
	Error	-0.65	-1.37	2.91	-2.43	0.00	-2.66	0.00	0.66					
A4	Exp.	442.52	9.01	9.03	6.81	119.97	91.82	108.58	1.94	78.36	P-1	2	2	30.29
	DFT	431.65	9.09	9.11	6.47	119.89	91.77	107.73	1.99					
	Error	-2.46	0.93	0.85	-4.97	-0.06	-0.05	-0.78	2.52					
A5	Exp.	910.48	4.97	8.90	20.61	90.00	90.00	90.00	1.89	76.77	P212121	19	4	25.5
	DFT	916.59	5.03	8.89	20.50	90.00	90.00	90.00	1.88					
	Error	0.67	1.31	-0.12	-0.51	0.00	0.00	0.00	-0.67					
A6	Exp.	1023.79	7.25	10.31	13.96	90.00	101.02	90.00	1.86	74.45	P21/c	14	4	32.58
	DFT	1028.89	7.33	10.21	14.04	90.00	101.91	90.00	1.85					
	Error	0.50	1.19	-0.96	0.59	0.00	0.87	0.00	-0.50					
A7	Exp.	1770.58	14.91	6.03	19.68	90.00	90.00	90.00	1.70	76.01	Pca21	29	8	21.3

	DFT	1773.45	15.21	5.96	19.55	90.00	90.00	90.00	1.70					
	Error	0.16	2.04	-1.21	-0.64	0.00	0.00	0.00	-0.16					
A8	Exp.	500.08	7.66	7.73	9.04	103.12	95.00	104.05	1.79	77.81	P-1	2	2	41.86
	DFT	507.91	7.66	7.78	9.05	101.75	96.17	102.98	1.77					
	Error	1.56	0.02	0.65	0.08	-1.33	1.23	-1.03	-1.54					
A9	Exp.	1563.72	16.96	8.93	10.35	90.00	94.30	90.00	1.82	76.34	P21/c	14	8	30.22
	DFT	1524.81	16.71	9.00	10.20	89.96	96.26	90.01	1.87					
	Error	-2.49	-1.43	0.71	-1.46	-0.05	2.08	0.01	2.55					
A10	Exp.	2436.82	28.57	9.74	8.76	90.00	90.00	90.00	1.75	72.60	Pbcn	60	12	20.23
	DFT	2392.29	28.09	9.77	8.72	90.00	90.00	90.00	1.78					
	Error	-1.83	-1.70	0.29	-0.41	0.00	0.00	0.00	1.86					
A11	Exp.	815.30	9.63	14.13	5.99	90.00	90.00	90.00	1.87	78.63	Pnma	62	4	23.87
	DFT	800.95	9.79	14.03	5.83	90.00	90.00	90.00	1.91					
	Error	-1.76	1.74	-0.68	-2.78	0.00	0.00	0.00	1.79					
A12	Exp.	2454.09	11.07	13.97	15.87	90.00	90.00	90.00	1.72	70.87	Pbca	61	8	31.14
	DFT	2436.25	11.23	13.52	16.05	90.00	90.00	90.00	1.74					
	Error	-0.73	1.45	-3.23	1.12	0.00	0.00	0.00	0.73					
A13	Exp.	378.43	8.22	8.22	7.57	52.64	109.27	109.27	1.89	80.03	C2/C	15	2	29.28
	DFT	378.43	8.05	8.05	7.58	55.21	107.72	107.72	1.89					
	Error	0.00	-2.13	-2.13	0.03	4.87	-1.42	-1.42	0.00					
A14	Exp.	748.16	5.72	15.85	8.41	90.00	101.04	90.00	1.92	76.10	P21/n	14	4	28.93
	DFT	750.37	5.69	15.91	8.45	90.00	101.29	90.00	1.91					
	Error	0.30	-0.43	0.35	0.47	0.00	0.25	0.00	-0.29					
A15	Exp.	733.72	9.01	12.96	6.39	90.00	100.77	90.00	1.81	74.82	P21/c	14	4	32.67
	DFT	733.72	9.12	12.96	6.41	90.00	104.67	90.00	1.81					
	Error	0.00	1.20	0.01	0.33	0.00	3.87	0.00	0.00					
A16	Exp.	683.09	11.65	6.03	9.80	90.00	97.08	90.00	1.67	71.92	P21/c	14	4	25.22
	DFT	658.50	11.50	5.97	9.64	89.95	95.79	90.00	1.74					
	Error	-3.60	-1.25	-0.96	-1.69	-0.06	-1.33	0.00	3.73					

B1	Exp.	1532.05	8.19	12.14	16.20	104.69	93.10	98.73	1.84	73.91	P-1	2	4	24.73
	DFT	1554.03	8.20	12.18	16.40	105.21	92.58	99.30	1.81					
	Error	1.44	0.17	0.39	1.23	0.50	-0.55	0.58	-1.41					
B2	Exp.	800.47	11.80	5.74	11.83	90.00	92.21	90.00	1.86	79.13	C2/c	15	4	37.54
	DFT	800.53	11.58	5.95	11.66	90.00	95.11	90.00	1.86					
	Error	0.01	-1.86	3.71	-1.42	0.00	3.15	0.00	-0.01					
B3	Exp.	2217.31	10.85	14.22	14.38	90.00	90.00	90.00	1.68	71.07	Pbcn	60	8	77.51
	DFT	2221.68	10.95	13.89	14.60	89.03	89.42	89.96	1.68					
	Error	0.20	0.95	-2.28	1.59	-1.08	-0.65	-0.04	-0.20					
B3-solvent free	DFT	2179.27	10.61	13.82	14.86	90.00	90.00	90.00	1.55	66.37	Pbcn	60	8	42.8
B4	Exp.	950.81	8.61	11.96	10.12	90.00	114.15	90.00	1.88	75.13	P21/c	14	4	37.77
	DFT	943.27	8.63	11.68	10.24	90.00	114.05	90.00	1.90					
	Error	-0.79	0.27	-2.35	1.23	0.00	-0.09	0.00	0.80					
B5	Exp.	1192.17	6.85	14.12	12.39	90.00	96.01	90.00	1.85	73.92	P21/c	14	4	60
	DFT	1172.43	6.80	14.33	12.08	90.00	95.36	90.00	1.88					
	Error	-1.66	-0.72	1.53	-2.54	0.00	-0.68	-0.01	1.68					
B5-solvent free	DFT	1161.21	6.60	13.94	12.75	89.99	97.76	90.00	1.80	71.43	P21/c	14	4	39.65
B6	Exp.	1219.68	10.65	10.16	11.34	90.00	96.26	90.00	1.87	74.05	P21/n	14	4	33.75
	DFT	1219.48	10.71	9.99	11.46	90.00	96.41	90.00	1.87					
	Error	-0.02	0.56	-1.61	1.09	0.00	0.15	0.00	0.02					
B7	Exp.	2259.05	16.43	16.43	8.37	90.00	90.00	90.00	1.85	71.88	P42/n	86	8	31.96
	DFT	2277.36	16.76	16.76	8.11	90.00	90.00	90.00	1.83					
	Error	0.81	2.01	2.01	-3.12	0.00	0.00	0.00	-0.80					
B8	Exp.	554.02	8.70	10.69	5.95	90.00	90.00	90.00	1.88	75.89	P21212	18	2	25.08
	DFT	557.93	8.71	10.75	5.96	90.00	90.00	90.00	1.87					
	Error	0.71	0.04	0.58	0.09	0.00	0.00	0.00	-0.70					
B9	Exp.	1262.39	7.81	10.11	16.09	90.00	96.01	90.00	1.81	71.63	P21/c	14	4	36.25
	DFT	1258.93	7.79	9.96	16.33	90.00	96.43	90.00	1.82					

	Error	-0.27	-0.18	-1.50	1.50	0.00	0.44	0.00	0.27					
B10	Exp.	650.09	5.03	8.48	15.36	90.00	97.18	90.00	1.79	73.43	P21/n	14	2	74.93
	DFT	650.09	4.96	8.41	15.72	90.00	97.77	90.00	1.79					
	Error	0.00	-1.33	-0.84	2.34	0.00	0.61	0.00	0.00					
B10-solvent free	DFT	562.46	15.51	8.49	13.22	90.02	161.14	89.98	1.85	74.22	P21/n	14	2	32.56
B11	Exp.	1374.63	7.97	13.00	13.59	90.00	102.34	90.00	1.86	74.96	P21/n	14	6	42.67
	DFT	1361.99	7.90	13.05	13.46	90.00	101.18	90.00	1.87					
	Error	-0.92	-0.81	0.40	-0.93	0.00	-1.13	0.00	0.93					
B12	Exp.	378.06	7.74	6.25	8.70	90.00	116.05	90.00	1.81	73.88	C2/m	12	2	87.5
	DFT	378.06	7.77	6.18	8.85	90.00	117.24	90.00	1.81					
	Error	0.00	0.31	-1.03	1.78	0.00	1.02	0.00	0.00					
B12-solvent free	DFT	328.88	6.22	6.00	9.09	90.00	104.32	90.00	1.72	69.66	C2/m	12	2	22.47
B13	Exp.	2305.45	8.84	18.93	16.38	90.00	122.72	90.00	1.65	70.49	Cc	9	2	106.18
	DFT	2255.85	8.75	18.62	16.44	90.00	122.56	90.00	1.69					
	Error	-2.15%	-1.07%	-1.65%	0.36%	0.00%	-0.12%	0.00%	2.20					
B13-solvent free	DFT	1948.19	8.16	17.80	14.91	90.00	115.93	90.00	1.53	61.23	Cc	9	4	40.05
C1	Exp.	1670.35	10.67	12.84	12.30	90.00	97.74	90.00	1.74	72.42	P21/n	14	4	30.26
	DFT	1633.81	10.16	13.06	12.43	90.00	98.13	90.00	1.78					
	Error	-2.19	-4.74	1.70	1.06	0.00	0.40	0.00	2.24					
C2	Exp.	1604.70	7.36	11.64	18.73	90.00	90.00	90.00	1.82	74.18	P212121	19	4	27.75
	DFT	1645.91	7.34	11.76	19.08	90.00	90.00	90.00	1.77					
	Error	2.57	-0.31	1.01	1.86	0.00	0.00	0.00	-2.50					
C3	Exp.	2592.06	12.21	9.60	22.11	90.00	90.00	90.00	1.84	73.85	Pbca	61	8	39.36
	DFT	2592.71	12.35	9.49	22.11	90.00	90.00	90.00	1.84					
	Error	0.03	1.17	-1.11	-0.02	0.00	0.00	0.00	-0.03					
C4	Exp.	4229.59	8.61	16.57	29.79	90.00	95.94	90.00	1.97	75.80	P21/n	14	12	29.35
	DFT	4328.61	8.69	16.72	29.92	90.00	95.78	90.00	1.93					

	Error	2.34	0.95	0.91	0.44	0.00	-0.16	0.00	-2.29					
C5	Exp.	605.74	8.34	8.34	10.33	97.86	110.12	110.12	1.80	72.58	Cc	9	2	38.55
	DFT	606.22	8.37	8.37	10.19	97.38	109.92	109.92	1.80					
	Error	0.08	0.39	0.39	-1.32	-0.49	-0.18	-0.18	-0.08					
C6	Exp.	1241.52	8.64	9.85	14.59	90.00	90.00	90.00	1.76	70.41	P212121	19	4	28.69
	DFT	1263.55	8.69	9.84	14.77	90.00	90.00	90.00	1.73					
	Error	1.77	0.55	-0.02	1.24	0.00	0.00	0.00	-1.74					
C7	Exp.	847.38	5.85	8.13	17.98	90.00	97.15	90.00	1.77	75.70	P21/c	14	2	37.61
	DFT	850.10	5.83	8.03	18.32	90.00	97.93	90.00	1.77					
	Error	0.32	-0.22	-1.19	1.94	0.00	0.80	0.00	-0.32					
C8	Exp.	1713.68	22.33	5.57	14.67	90.00	110.04	90.00	1.75	74.36	P21/c	14	4	33.54
	DFT	1692.34	22.12	5.53	14.82	90.00	111.19	89.98	1.77					
	Error	-1.25	-0.91	-0.64	1.06	0.01	1.04	-0.02	1.26					
C9	Exp.	836.41	10.15	8.26	10.05	90.00	97.29	90.00	1.80	74.01	P21/c	14	2	31.89
	DFT	843.31	10.07	8.42	10.02	90.00	96.67	90.00	1.78					
	Error	0.83	-0.81	1.86	-0.34	0.00	-0.64	0.00	-0.82					
C10	Exp.	770.58	6.72	8.15	14.44	90.00	102.92	90.00	1.86	73.50	P21/n	14	2	32.04
	DFT	788.46	6.66	8.38	14.51	90.00	103.22	90.00	1.82					
	Error	2.32	-0.90	2.89	0.48	0.00	0.30	0.00	-2.27					
C11	Exp.	335.58	10.95	6.68	5.03	90.00	114.25	90.00	1.64	77.55	C2/m	12	2	47.04
	DFT	335.58	11.12	6.53	5.04	90.00	113.52	90.00	1.64					
	Error	0.00	1.51	-2.27	0.24	0.00	-0.64	0.00	0.00					
D1	Exp.	1725.95	9.67	9.46	19.04	90.00	97.70	90.00	1.55	68.00	P21/c	14	4	50.11
	DFT	1739.93	9.69	9.47	19.14	90.00	97.88	90.00	1.54					
	Error	0.81	0.20	0.13	0.53	0.00	0.19	0.00	-0.80					
D1-solvent free	DFT	1702.53	9.67	9.31	19.03	90.00	96.74	90.00	1.41	59.48	P21/c	14	4	31.23
D2	Exp.	3149.54	12.26	10.71	24.01	90.00	92.25	90.00	1.75	74.09	P21/c	14	8	29.91
	DFT	3212.84	12.34	10.77	24.20	90.00	92.56	90.00	1.70					

	Error	2.01	0.63	0.58	0.81	0.00	0.33	0.00	-2.77					
D3	Exp.	1070.84	7.15	9.80	15.28	90.00	90.00	90.00	1.84	71.29	P212121	19	4	14.61
	DFT	1059.69	7.16	9.76	15.16	90.00	90.00	90.00	1.86					
	Error	-1.04	0.11	-0.37	-0.78	0.00	0.00	0.00	1.05					
D4	Exp.	1070.23	10.75	15.10	6.60	90.00	90.00	90.00	1.94	74.67	P212121	19	4	15.72
	DFT	1097.22	10.91	15.07	6.68	90.00	90.00	90.00	1.89					
	Error	2.52	1.51	-0.21	1.21	0.00	0.00	0.00	-2.46					
D5	Exp.	842.46	6.70	7.77	16.65	91.64	99.92	98.63	1.63	74.36	P-1	2	1	104.03
	DFT	826.95	6.66	7.71	16.55	92.00	98.55	99.44	1.66					
	Error	-1.84	-0.59	-0.79	-0.61	0.40	-1.38	0.83	1.87					
D5-solvent free	DFT	817.26	6.39	7.77	16.62	91.93	94.65	96.33	1.14	47.31	P-1	2	1	23.9
D6	Exp.	954.30	5.88	8.92	18.38	90.00	98.19	90.00	1.73	73.16	P21/n	14	2	34.92
	DFT	953.81	5.80	9.12	18.10	90.00	94.85	90.00	1.74					
	Error	-0.05	-1.35	2.21	-1.53	0.00	-3.41	0.00	0.05					
D7	Exp.	1546.76	3.83	17.65	22.91	90.00	93.49	90.00	1.35	65.76	P21/c	14	2	137.35
	DFT	1527.86	3.79	17.53	23.06	90.00	93.61	90.00	1.37					
	Error	-1.22	-1.14	-0.71	0.65	0.00	0.13	0.00	1.24					
D7-solvent free	DFT	632.60	5.04	9.69	12.95	90.09	87.86	89.98	1.77	71.46	P21/c	14	2	44.76
D8	Exp.	2138.38	11.41	11.41	16.42	90.00	90.00	90.00	1.83	74.10	P212121	19	4	37.46
	DFT	2153.34	11.25	11.31	16.93	90.00	90.00	90.00	1.82					
	Error	0.70	-1.42	-0.94	3.12	0.00	0.00	0.00	-0.69					
D9	Exp.	562.54	8.23	8.63	9.59	117.00	109.35	90.23	1.63	73.02	P-1	2	1	44.07
	DFT	559.24	8.15	8.68	9.54	116.84	109.10	90.43	1.64					
	Error	-0.59	-1.02	0.60	-0.45	-0.14	-0.23	0.22	0.59					
D10	Exp.	4697.26	14.52	17.66	18.32	90.00	90.00	90.00	1.76	71.14	P212121	19	8	33.48
	DFT	4735.89	14.30	17.94	18.46	90.00	90.00	89.99	1.74					
	Error	0.82	-1.47	1.56	0.76	0.00	0.00	-0.01	-0.82					
D11	Exp.	1379.91	11.47	11.47	11.69	63.87	92.26	92.26	1.75	71.23	Cc	9	2	51.01

	DFT	1399.93	11.58	11.58	11.59	64.38	91.19	91.19	1.73					
	Error	1.45	0.93	0.93	-0.92	0.78	-1.16	-1.16	-1.43					
E1	Exp.	1409.22	8.59	11.45	14.33	90.00	90.00	90.00	1.83	75.65	Pbca	61	4	34.15
	DFT	1403.80	8.62	11.52	14.13	90.00	90.00	90.00	1.84					
	Error	-0.38	0.39	0.61	-1.37	0.00	0.00	0.00	0.39					
E2	Exp.	1169.95	10.48	13.15	8.49	90.00	90.00	90.00	1.94	76.12	Pna21	33	4	31.77
	DFT	1155.74	10.30	13.18	8.51	90.00	90.00	90.00	1.96					
	Error	-1.21	-1.68	0.23	0.24	0.00	0.00	0.00	1.23					
E3	Exp.	1123.86	7.89	11.95	11.93	90.00	90.00	90.00	2.01	75.11	Pca21	29	4	22.83
	DFT	1131.77	7.87	12.04	11.95	90.00	90.00	90.00	2.00					
	Error	0.70	-0.26	0.79	0.18	0.00	0.00	0.00	-0.70					
E4	Exp.	966.26	12.33	6.68	12.13	90.00	104.52	90.00	1.73	71.53	C2/c	15	4	37.22
	DFT	966.26	12.33	6.68	12.13	90.00	104.52	90.00	1.82					
	Error	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.73					
E5	Exp.	857.55	6.00	6.89	20.73	90.00	90.00	90.00	1.95	74.26	P212121	19	4	25.45
	DFT	864.86	6.00	6.84	21.09	90.00	90.00	90.00	1.94					
	Error	0.85	-0.06	-0.81	1.74	0.00	0.00	0.00	-0.85					
E6	Exp.	2096.61	8.44	8.44	33.96	120.00	90.00	90.00	1.71	70.61	P3221	154	6	42.98
	DFT	2046.74	8.31	8.30	34.24	120.01	90.03	90.14	1.76					
	Error	-2.38	-1.55	-1.63	0.82	0.01	0.03	0.16	2.44					
E6-solvent free	DFT	2016.94	8.26	8.26	34.08	119.87	90.21	89.79	1.68	69.08	P3221	154	6	32.52
E7	Exp.	1411.03	9.44	11.56	12.94	90.00	92.31	90.00	1.67	68.85	P21/n	14	4	35.37
	DFT	1401.22	9.20	11.91	12.80	90.00	92.37	90.00	1.68					
	Error	-0.70	-2.51	2.98	-1.08	0.00	0.07	0.00	0.70					
E8	Exp.	1295.24	8.40	9.40	16.42	90.00	90.00	90.00	1.82	73.37	P212121	19	4	34.9
	DFT	1319.39	8.51	9.48	16.34	90.00	90.00	90.00	1.79					
	Error	1.86	1.38	0.93	-0.45	0.00	0.00	0.00	-1.83					
E9	Exp.	1081.87	9.60	11.59	9.79	90.00	96.84	90.00	1.63	68.42	P21/n	14	4	39.96

	DFT	1056.04	9.24	11.71	9.82	90.00	96.50	90.00	1.67					
	Error	-2.39	-3.72	1.05	0.27	0.00	-0.35	0.00	2.45					
HL3	Exp.	628.30	11.33	5.81	10.42	90.00	113.59	90.00	1.81	76.25	P21/c	14	2	46.68
	DFT	612.70	11.04	5.73	10.35	90.00	110.61	90.00	1.85					
	Error	-2.48	-2.55	-1.34	-0.70	0.00	-2.63	0.00	2.55					
HL7	Exp.	1742.09	17.63	14.27	7.21	90.00	106.05	90.00	1.85	74.87	Cc	9	4	85.90
	DFT	1748.12	17.80	13.97	7.33	90.00	106.36	90.00	1.85					
	Error	0.35	0.98	-2.13	1.70	0.00	0.30	0.00	-0.35					
HL7-solvent free	DFT	1763.15	17.51	14.37	7.25	90.00	104.84	90.00	1.70	67.64	Cc	9	4	37.13
HL9	Exp.	1197.53	10.14	9.52	12.41	90.00	91.17	90.00	1.82	73.43	P21/c	14	4	35.67
	DFT	1185.85	10.38	9.49	12.05	90.00	92.35	90.00	1.84					
	Error	-0.98	2.39	-0.32	-2.91	0.00	1.30	0.00	0.99					

Table S9. Summary of DFT-optimized crystal structure parameters and intermolecular interactions in all 63 EMs mentioned in this study. The parameters and interactions include enclosed volume into a Hirshfeld surface (V , Å³), an area of a Hirshfeld surface (A , Å²), a globularity and an asphericity of a Hirshfeld surface, as well as a relative population (%) and absolute areas (Å²) of Hirshfeld surface for the hydrogen bonding interactions. For the solvent-containing crystals, the corresponding calculated solvent-free structures were obtained by simple removal of the solvent molecules, followed by re-optimization on the basis of the Conjugate Gradient method.

Label	V (Å ³)	A (Å ²)	Globularity	Asphericity	Hydrogen bonding	
					Population (%)	Area (Å ²)
A1	201.6	206.38	0.81	0.11	36.30	74.92
A2	209.23	209.20	0.82	0.11	46.20	96.65
A3	213.54	213.75	0.81	0.12	48.60	103.88
A4	217.04	215.13	0.81	0.12	60.40	129.94
A5	223.24	220.10	0.81	0.10	50.10	110.27
A6	251.27	235.90	0.82	0.10	45.90	108.28
A7	217.23	218.67	0.80	0.09	48.50	106.05

A8	245.07	245.16	0.77	0.13	61.30	150.28
A9	191.6	195.06	0.82	0.13	56.90	110.99
A10	195.9	203.39	0.80	0.10	28.60	58.17
A11	199.39	208.34	0.79	0.09	28.80	60.00
A12	301.28	282.82	0.77	0.10	50.60	143.11
A13	185.13	191.46	0.82	0.13	69.50	133.06
A14	182.81	191.47	0.81	0.12	53.60	102.63
A15	179.04	189.06	0.81	0.13	57.40	108.52
A16	166.68	177.64	0.83	0.12	41.80	74.25
B1	378.08	330.52	0.77	0.13	27.90	92.22
B2	195.34	201.77	0.81	0.09	50.70	102.30
B3	232.99	230.35	0.80	0.17	69.60	160.32
B3-solvent free	266.6	261.10	0.77	0.16	67.80	177.03
B4	232.9	230.06	0.80	0.05	42.00	96.63
B5	265.92	259.52	0.77	0.21	37.00	96.02
B5-solvent free	284.77	273.85	0.76	0.20	27.10	74.21
B6	299.47	286.45	0.76	0.09	39.50	113.15
B7	277.35	260.50	0.79	0.01	25.50	66.43
B8	271.28	270.06	0.75	0.11	23.90	64.54
B9	310.12	285.57	0.78	0.14	44.00	125.65
B10	267.97	272.51	0.74	0.27	43.40	118.27
B10-solvent free	301.14	335.39	0.65	0.24	17.80	59.70
B11	224.82	243.61	0.73	0.25	47.30	115.23
B12	139.75	158.95	0.82	0.13	73.80	117.31
B12-solvent free	160.13	176.11	0.81	0.18	41.80	73.61
B13	386.65	362.73	0.71	0.27	47.30	171.57
B13-solvent free	486.44	423.64	0.71	0.30	22.80	96.59
C1	411.68	353.34	0.76	0.14	39.60	139.92
C2	395.37	339.71	0.77	0.16	35.90	121.96

C3	318.16	305.38	0.74	0.11	48.00	146.58
C4	351.5	328.13	0.73	0.12	16.00	52.50
C5	296.94	294.31	0.73	0.16	37.20	109.48
C6	304.38	295.16	0.74	0.12	36.10	106.55
C7	416.95	375.02	0.72	0.26	46.30	173.63
C8	423.06	374.23	0.73	0.27	41.40	154.93
C9	411.79	366.03	0.73	0.25	33.20	121.52
C10	379.19	354.70	0.71	0.29	27.20	96.48
C11	163.49	176.70	0.82	0.27	57.60	101.78
D1	356.26	313.84	0.77	0.12	54.40	170.73
D1-solvent free	419.09	364.33	0.74	0.15	44.60	162.49
D2	389.75	348.33	0.74	0.08	40.70	141.77
D3	262.83	251.59	0.79	0.10	0.00	0.00
D4	262.78	251.97	0.79	0.10	0.00	0.00
D5	487.06	447.76	0.67	0.45	63.60	284.78
D5-solvent free	918.96	704.45	0.65	0.48	10.70	75.38
D6	469.72	415.47	0.70	0.34	32.90	136.69
D7	297.06	311.13	0.69	0.67	64.30	200.06
D7-solvent free	308.97	321.91	0.69	0.62	38.70	124.58
D8	527.38	450.36	0.70	0.09	32.10	144.57
D9	553.83	505.78	0.65	0.54	56.30	284.75
D10	580.57	450.27	0.75	0.08	29.90	134.63
D11	681.62	549.88	0.68	0.03	34.50	189.71
E1	345.77	334.15	0.71	0.27	29.90	99.91
E2	287.12	282.60	0.75	0.27	32.00	90.43
E3	275.86	267.93	0.77	0.20	0.00	0.00
E4	236.31	243.86	0.76	0.23	52.50	128.03
E5	209.36	223.03	0.77	0.31	0.00	0.00
E6	309.81	288.83	0.77	0.15	47.80	138.06

E6-solvent free	330.9	301.72	0.77	0.14	40.20	121.29
E7	347	310.21	0.77	0.10	51.50	159.76
E8	318.11	300.24	0.75	0.24	38.70	116.19
E9	264.97	260.53	0.77	0.15	61.90	161.27
HL3	308.37	292.94	0.75	0.15	46.60	136.51
HL7	376.84	370.33	0.68	0.33	25.00	92.58
HL7-solvent free	432.57	422.42	0.66	0.35	19.30	81.53
HL9	294.28	269.50	0.79	0.06	36.10	97.29

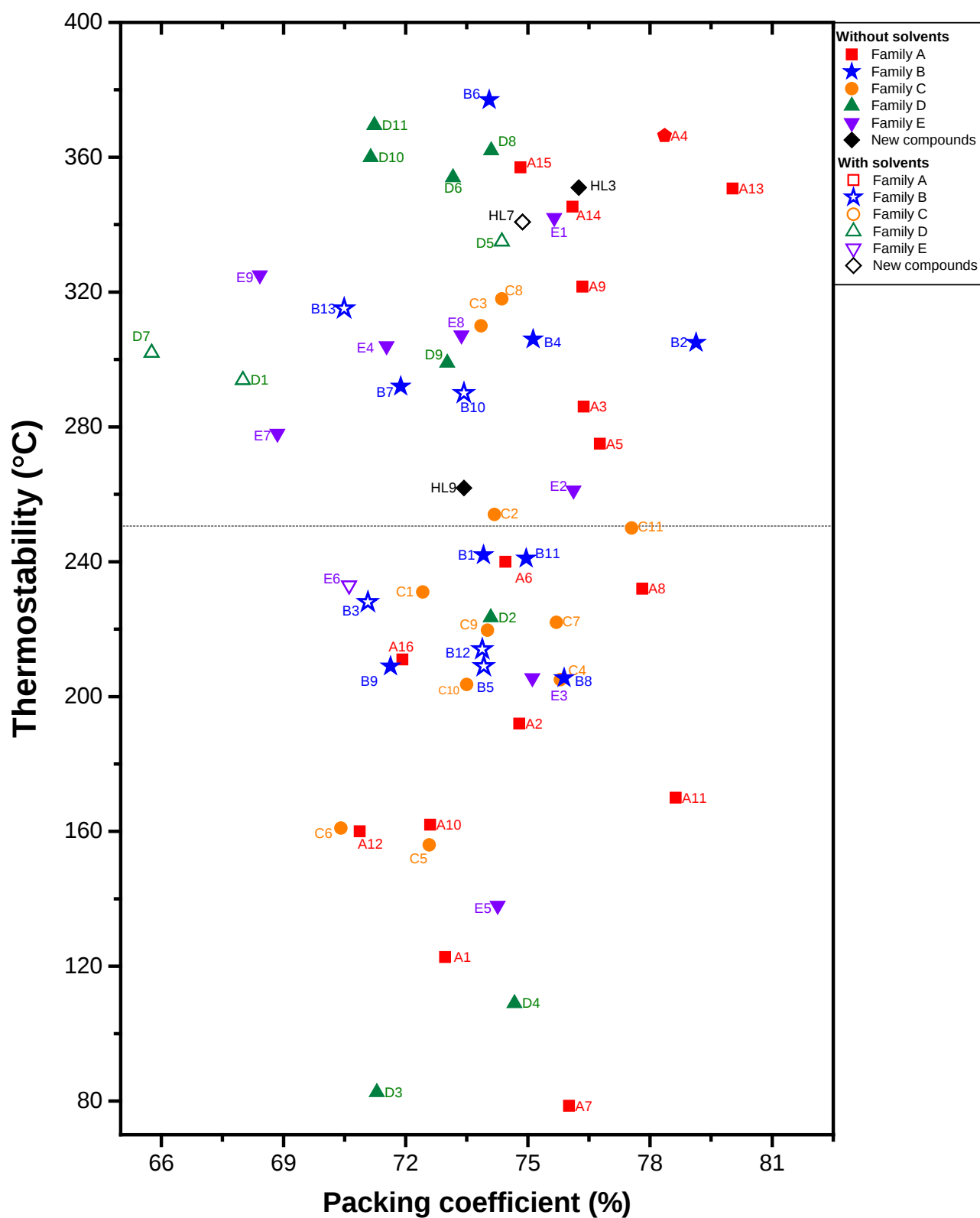


Figure S35. Full temperature range correlations between the EM crystals Packing Coefficient values and the thermostability of all 63 EMs mentioned in this study.

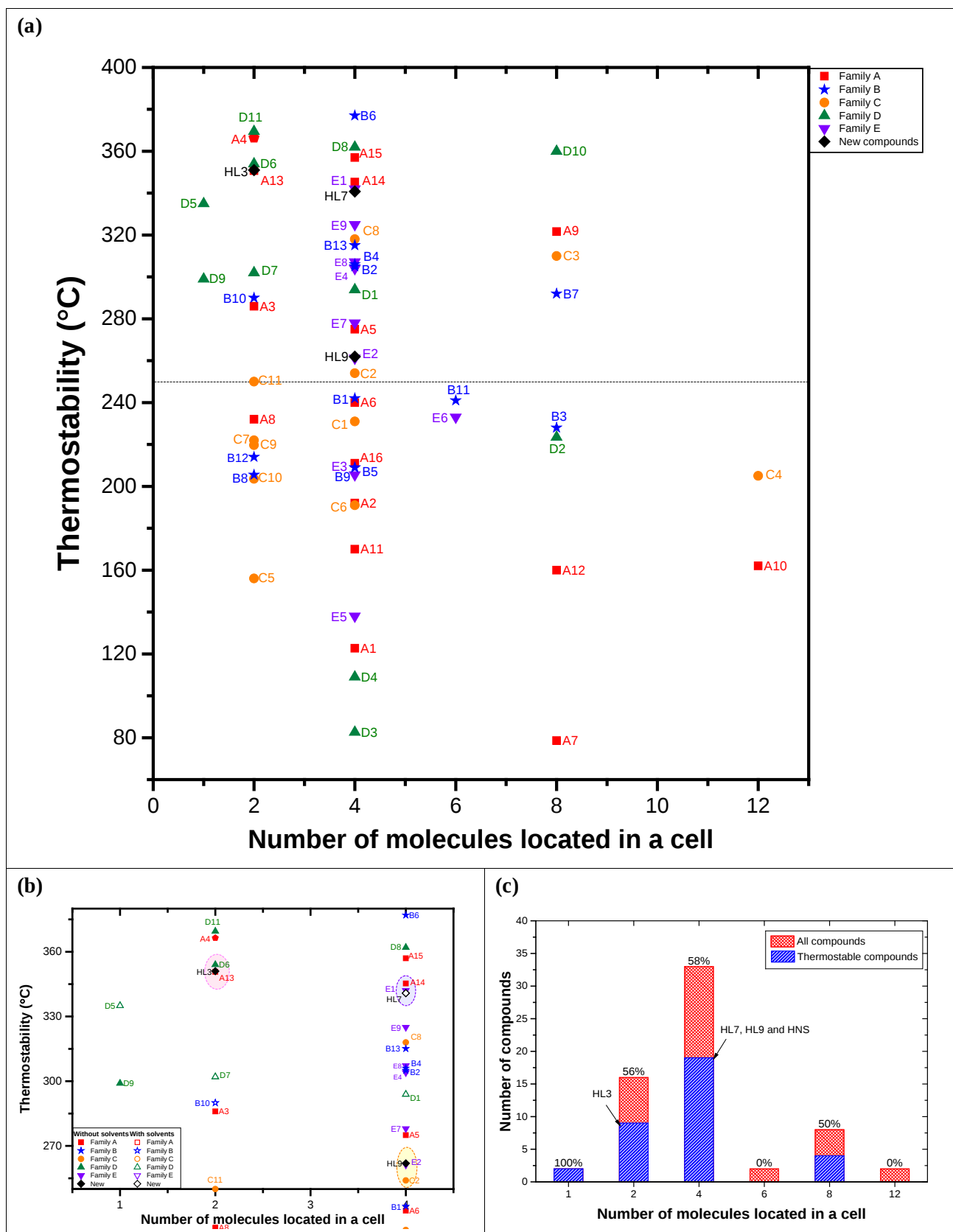


Figure S36. (a) Full temperature range correlation between the number of molecules located in a crystal cell and the thermostability of all 63 EMs mentioned in this study; (b) focused temperature range (>250 °C) correlation between the number of molecules located in a crystal cell and EMs' thermostability; (c) distribution of thermostable EMs with respect to the number of molecules located in their primitive cell, among all 63 EMs.

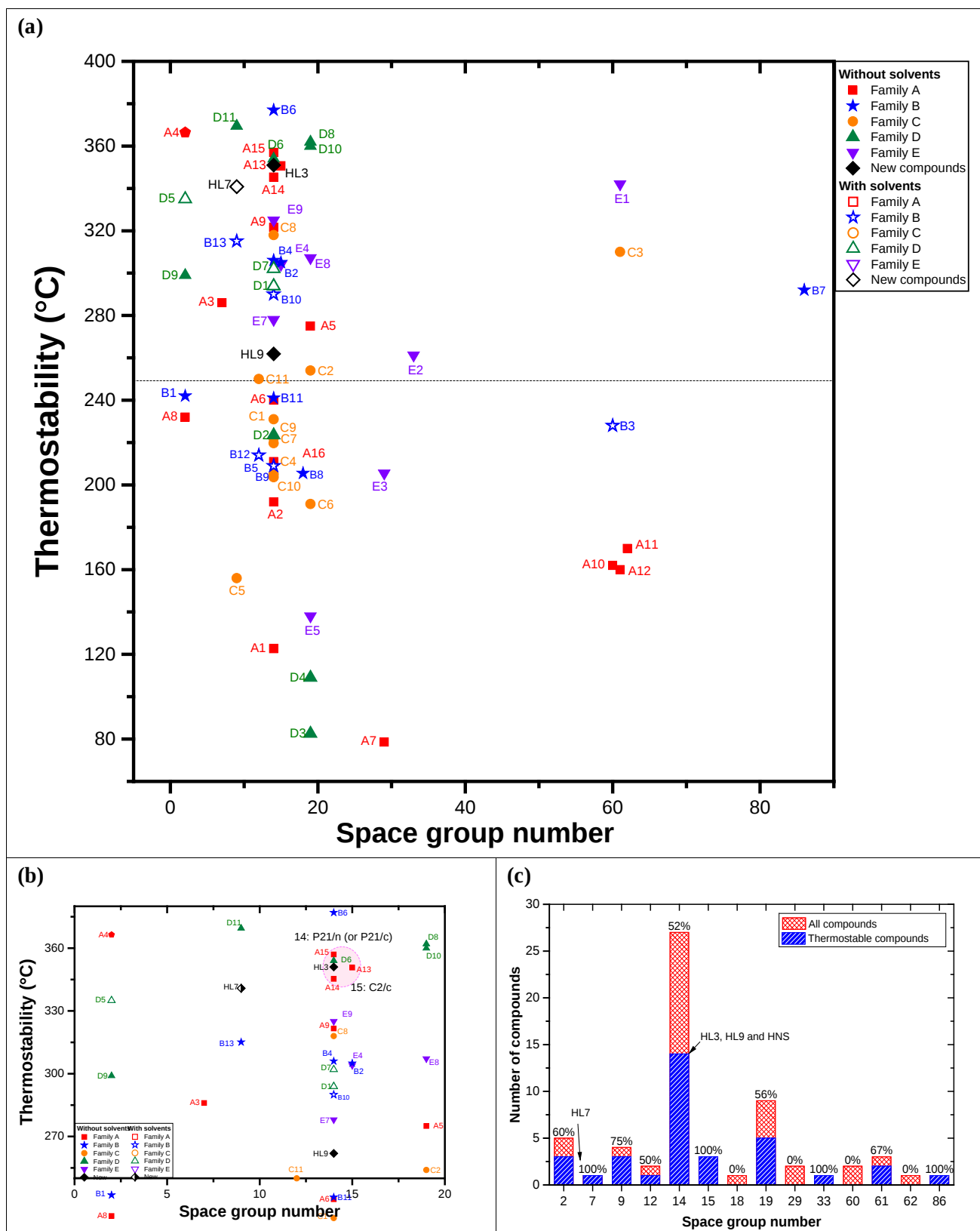


Figure S37. (a) Full temperature range correlation between the crystals' symmetry (represented by space group number) and the thermostability of all 63 EMs mentioned in this study; (b) focused temperature range (>250 °C) correlation between the crystals' symmetry and EMs' thermostability; (c) distribution of thermostable EMs with respect to their crystals' symmetry, among all 63 EMs.

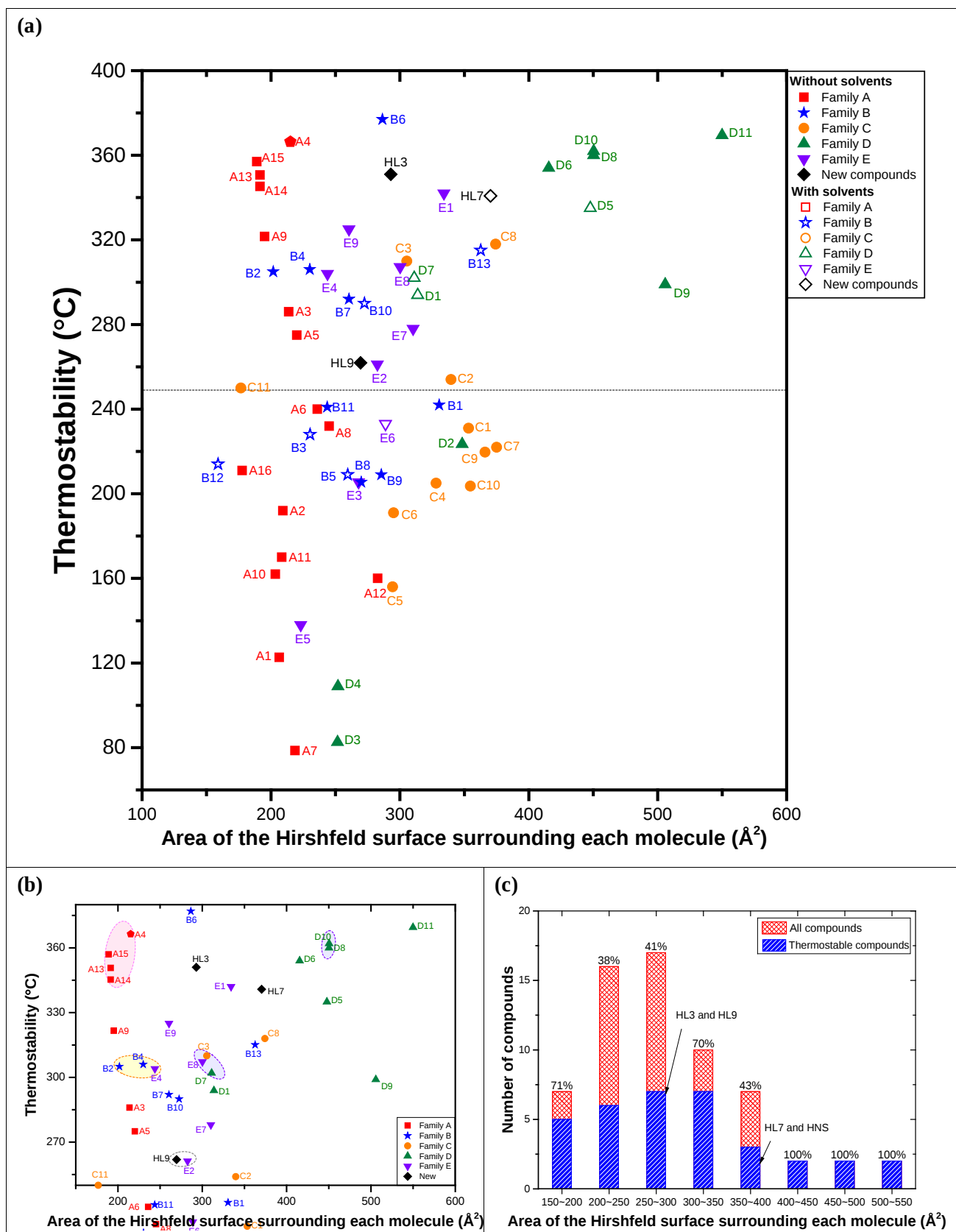


Figure S38. (a) Full temperature range correlation between the Hirshfeld surface area of each molecule in a crystal and the thermostability of all 63 EMs mentioned in this study; (b) focused temperature range (>250 °C) correlation between the Hirshfeld surface area of each molecule and EMs' thermostability; (c) distribution of the thermostable EMs, with respect to their Hirshfeld surface area surrounding each molecule, among all 63 EMs.

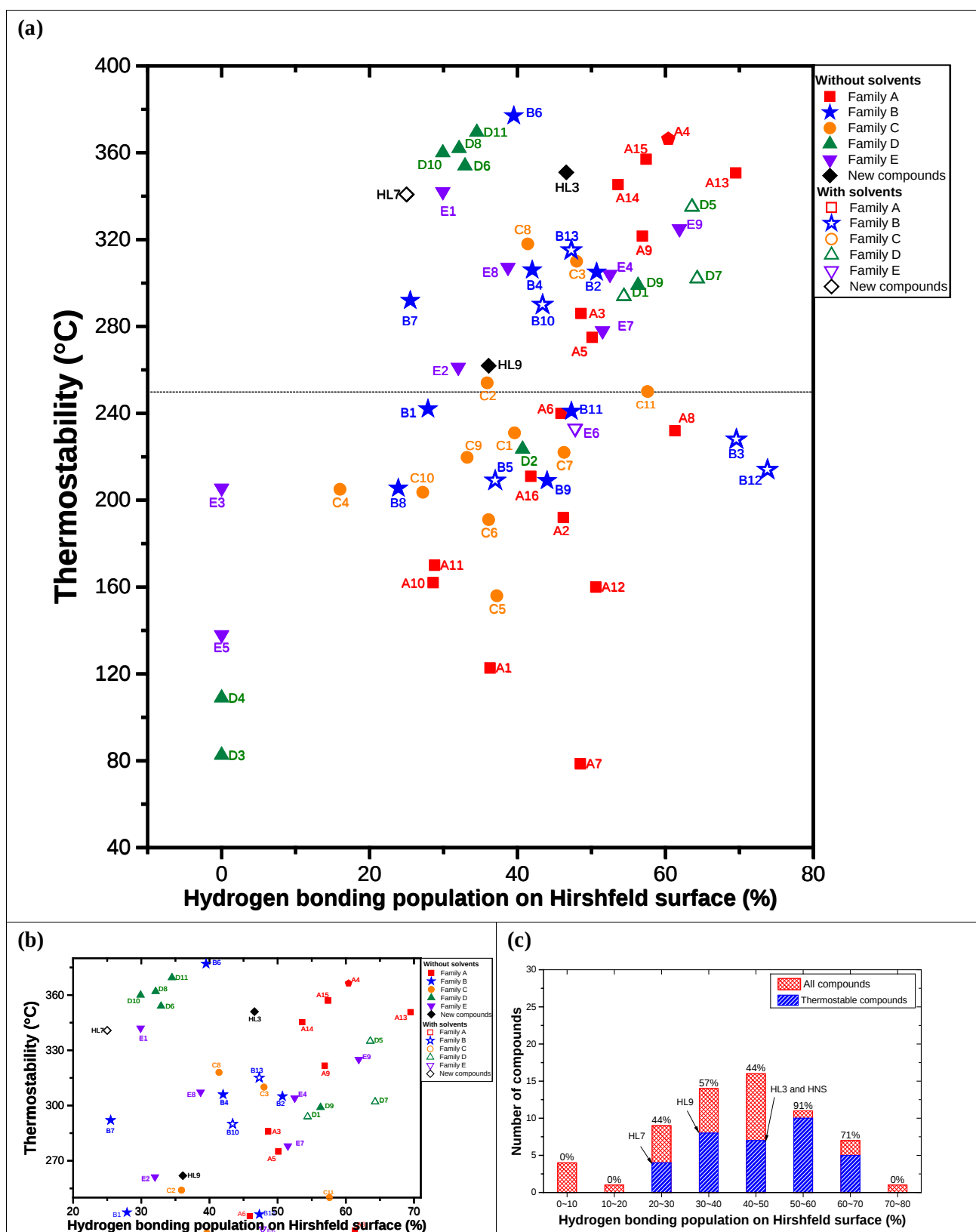


Figure S39. (a) Full temperature range correlation between the hydrogen bonding population on a Hirshfeld surface of a molecule and the thermostability of all 63 EMs mentioned in this study; (b) focused temperature range (>250 °C) correlation between the hydrogen bonding population on a Hirshfeld surface and EMs' thermostability; (c) distribution of the thermostable EMs, with respect to their hydrogen bonding population on a Hirshfeld surface area, among all 63 EMs.

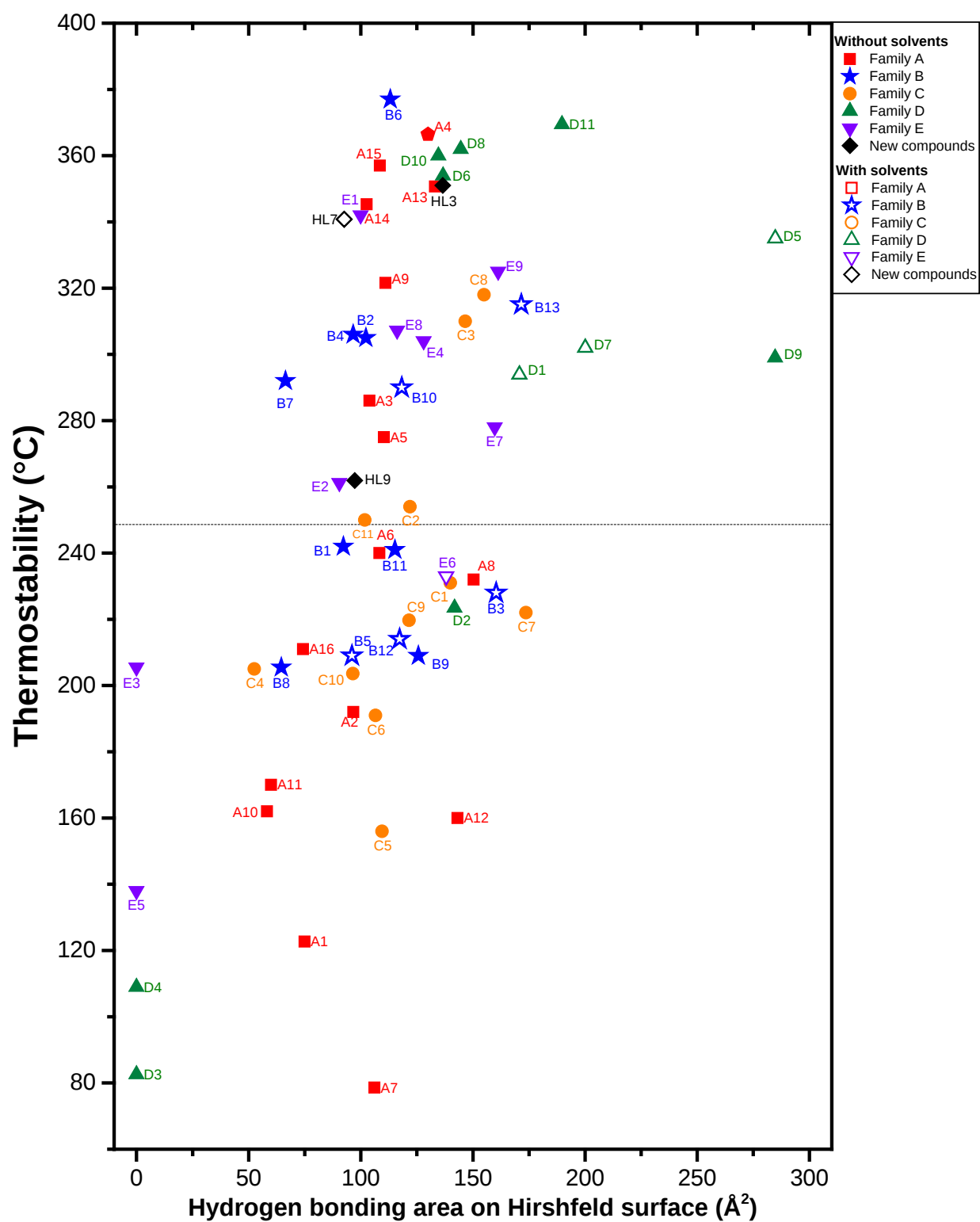


Figure S40. Full temperature range correlation between the hydrogen bonding area on a Hirshfeld surface of all 63 EMs mentioned in this study and their thermostability.

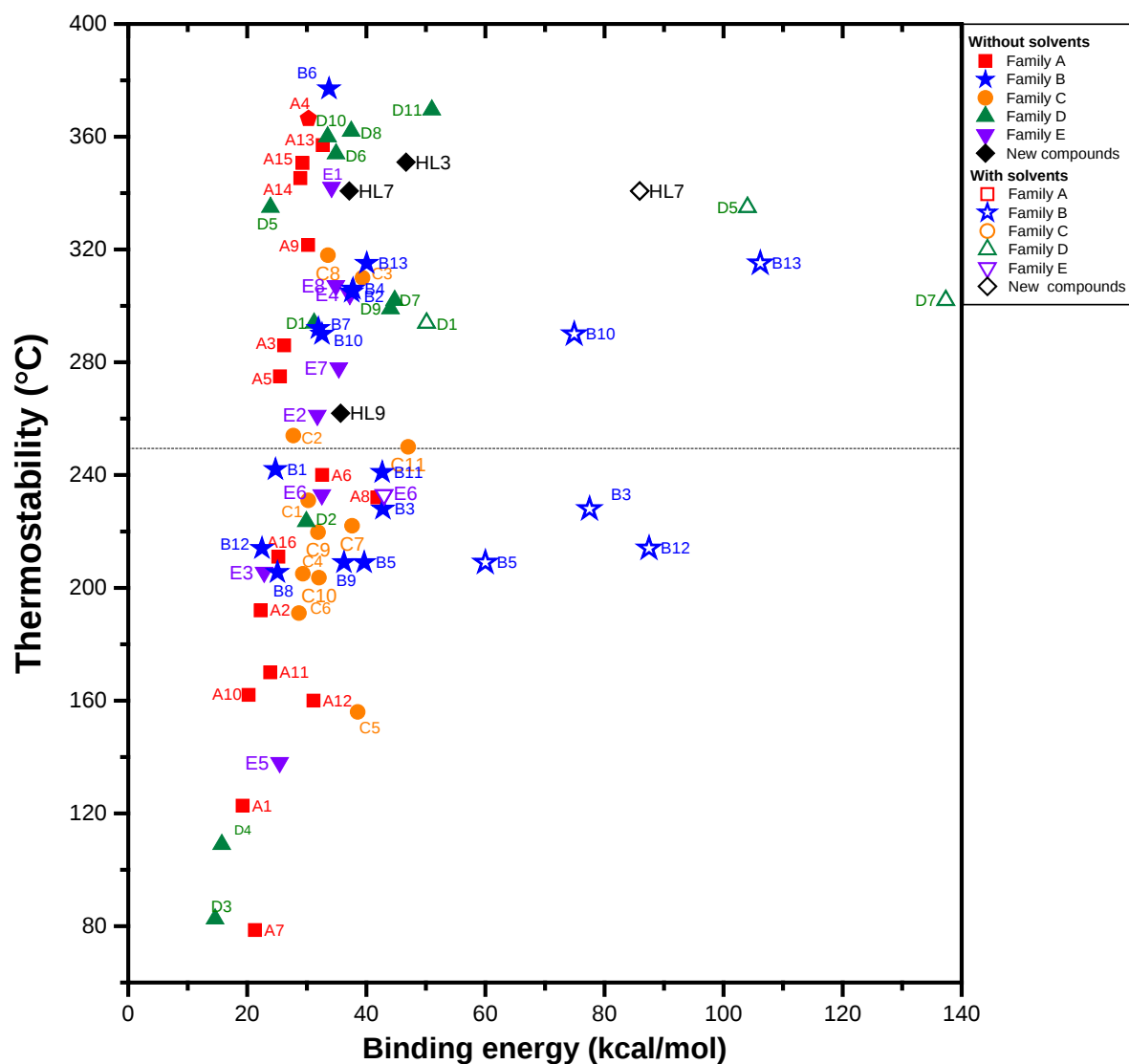


Figure S41. Full temperature range correlation between the crystal binding energy for each EM mentioned in this study and these EMs thermostability.

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