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Electronic Supplementary Information

Bionic Inspired Multifunctional Modular Energetic Materials: an Exploration of New Generation of Application Oriented Energetic Materials

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Methods

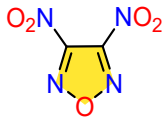
General. Caution! The prepared compounds as well as their precursors and intermediates are energetic materials and may explode under certain conditions even the target products (**1**, **2** and **3**) show the surprisingly low sensitivities to external mechanical stimuli (such as impact and friction), the precursors Caro's acid, intermediates 3,4-dinitrofurazan and 3-hydroxy-4-nitrofurazan are extremely active and dangerous. Laboratories and personnel must be properly grounded, and appropriate safety precautions (including protective gloves, coats, face shield and explosion-proof baffle) are recommended.

Materials. 3,4-Diaminofurzan (99%), sulfuric acid (98%), hydrogen peroxide (50%), ammonium persulfate (99%), sodium carbonate decahydrate (99%), potassium carbonate (99%), acetonitrile (99.8%), dichloromethane (99.8%) and dimethyl formanmide (99.5%) were all purchased from commercial sources and used without further purification.

Product characterization. ^{1}H NMR spectra were measured at 600 MHz (Bruker AVANCE 600) with DMSO-d_6 as the solvent. ^{13}C NMR spectra were measured at 125 MHz (Bruker AVANCE 600) with DMSO-d_6 as the solvent. FT-IR spectra were recorded on an FT-IR spectrometer (Bruker Tensor 27 instrument). High resolution mass spectra were performed on a micrOTOF-Q II 10280 mass spectrometer using electrospray ionization (ESI). The DSC curves under the condition of flowingnitrogen gas were obtained by a NETZSCH DSC200 F3 apparatus. The TG–FTIR–MS experiment was performed with a 449C thermal analyzer (NETZSCH, Germany), a QMS-403C mass spectrometer (NETZSCH, Germany) and a 5700 infrared spectrometer (Nicolet, USA) under an argon atmosphere at a flow rate of 75 mL min^{-1}. The heating rate was 10^{o}C min^{-1} from ambient temperature to 500^{o}C. Mass spectra measurements were performed with a model HP5989B mass

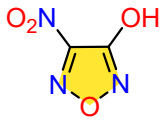
spectrometer (HP, USA). Impact and friction sensitivity measurements were made using a standard BAM Fall hammer and a BAM friction tester.

Synthesis of 3,4-Dinitrofurazan



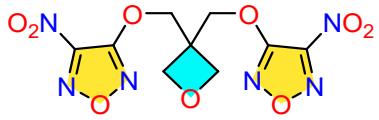
3,4-Diaminofurazan (DAF, 10.00 g, 0.1 mol) was added to a Caro's acid oxidation system (consists of $NH_4S_2O_8$ 22.80 g, 98% H_2SO_4 400.00 g and 50% H_2O_2 340.00 g), and the mixture was heated to 35°C. After reacting for 3.5 h, the solution was extracted by CH_2Cl_2, washed with water, and was evaporated by reduced pressure distillation. The crude brownish-yellow liquid of DNF was obtained (12.00 g, 68.3%). ^{13}C NMR (125 MHz, DMSO-d_6) δ 152.57, 152.73, 152.90 ppm.

Synthesis of 3-Hydroxy-4-nitrofurazan



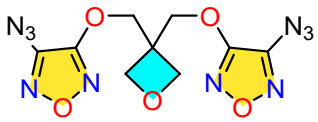
3,4-Dinitrofurazan (DNF, 10.00 g, 0.0625 mol) was added to a solution of sodium carbonate decahydrate ($Na_2CO_3 \cdot 10H_2O$) in 10 mL of acetonitrile (MeCN), and the mixture was heated to 80°C. After refluxing for 1 h, the solution was extracted by absolute ether, washed with water, and was evaporated by reduced pressure distillation. The crude yellow liquid of 3-Hydroxy-4-nitrofurazan was obtained (7.80 g, 95%). ^{13}C NMR (125MHz, DMSO-*d*6) δ 151.49, 151.64, 151.78, 156.94 ppm.

Synthesis of 4,4'-((oxetane-3,3-diylbis(methylene))bis(oxy))bis(3-nitrofurazan)



3-Hydroxy-4-nitrofurazan (10.00 g, 0.076 mol) and 3,3-bis(bromomethyl)oxetane (BBMO, 7.50 g, 0.031 mol) was added to a solution of potassium carbonate (K_2CO_3, 13.80 g, 0.1 mol) in 100 mL N,N-dimethylformamide (DMF), and the mixture was heated to 80°C. After reacting for 2.5 h, the solution was diluted by saturated salt solution, extracted by CH_2Cl_2 and washed with saturated salt solution. Then it was evaporated by reduced pressure distillation. Finally the crude yellow solid of 4,4'-((oxetane-3,3-diylbis(methylene))bis(oxy))bis(3-nitrofurazan) was purify by recrystallization (8.00 g, 61.6%). **1** crystal suitable for X-ray diffraction studies were obtained by crystallization from methyl alcohol. T_m (onset) 102.27°C T_d (onset) 220.80°C. ^{13}C NMR (125 MHz, DMSO-d_6) δ 158.75, 152.63, 73.40, 73.31, 42.66 ppm. ^{1}H NMR (600 MHz, DMSO-d_6) δ 4.80, 4.64 ppm. ESI-HRMS: *m*/*z* calcd for $[M+Na]^+$: 367.0250, found: 367.0249. IR (KBr) $\tilde{\nu}$= 2971, 2888, 1605, 989 cm^{-1}. (The images of ^{1}H NMR, ^{13}C NMR, FTIR spectra and ESI-HRMS spectra are provided in **Supplementary Fig. 1, 2, 3, 4** respectively, the single-crystal structure result is provided in **Supplementary Table. 2, 3**)

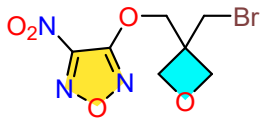
Synthesis of 4,4'-((oxetane-3,3-diylbis(methylene))bis(oxy))bis(3-azidofurazan)



4,4'-((Oxetane-3,3-diylbis(methylene))bis(oxy))bis(3-nitrofurazan) (10.00 g, 0.029 mol) was added to a solution of NaN_3 (4.55 g, 0.07 mol) in 100 mL DMF, and the mixture was react in room temperature for 0.5 h, the solution was diluted by saturated salt solution, extracted by ethyl

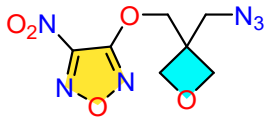
acetate and washed with saturated salt solution. Then it was evaporated by reduced pressure distillation. Finally the crude yellow solid of 4,4'-((oxetane-3,3-diylbis(methylene))bis(oxy))bis(3-azidofurazan) was purify by recrystallization (9.26 g, 95%). **2** crystal suitable for X-ray diffraction studies were obtained by crystallization from methyl alcohol. T_m (onset) 79.88°C T_d (onset) 180.53°C. ^{13}C NMR (125 MHz, DMSO-d_6) δ 159.28, 145.25, 73.44, 72.79, 42.48 ppm. ^{1}H NMR (600 MHz, DMSO-d_6) δ 4.67, 4.58 ppm. ESI-HRMS: *m*/*z* calcd for $[M+H]^+$: 337.0757, found: 337.0862 .IR (KBr) $\tilde{\nu}$= 2961, 2886, 2145, 1588, 1544, 1306, 1168, 993 cm^{-1}. (The images of ^{1}H NMR, ^{13}C NMR, FTIR spectra and ESI-HRMS spectra are provided in **Supplementary Fig. 1, 2, 3, 5** respectively, the single-crystal structure result is provided in **Supplementary Table. 4, 5**).

Synthesis of 3-((3-(bromomethyl)oxetan-3-yl)methoxy)-4-nitrofurazan



3-Hydroxy-4-nitrofurazan (10.00 g, 0.076 mol) and 3,3-bis(bromomethyl)oxetane (BBMO, 7.50 g, 0.031 mol) was added to a solution of potassium carbonate (K_2CO_3, 13.80 g, 0.1 mol) in 100 mL DMF, and the mixture was heated to 65°C. After reacting for 2 h, the solution was diluted by saturated salt solution, extracted by CH_2Cl_2 and washed with saturated salt solution. Then it was evaporated by reduced pressure distillation. Finally the crude white solid of 3-((3-(bromomethyl)oxetan-3-yl)methoxy)-4-nitrofurazan was purified by recrystallization (15.00 g, 67.0%). T_m (onset) 82.26°C, T_d (onset) 218.38 °C. ^{13}C NMR (125 MHz, DMSO-d_6) δ 158.79、152.65、74.94、74.15,、43.37、36.44 ppm. ^{1}H NMR (600 MHz, DMSO-d_6) δ 4.73、4.56、4.55、4.44、4.43、3.99 ppm. IR (KBr) $\tilde{\nu}$= 2970、2883、1608、980 cm^{-1}. (The images of ^{1}H NMR, ^{13}C NMR, FTIR spectra are provided in Supplementary **Fig. 1, 2, 3** respectively)

Synthesis of 3-((3-(azidomethyl)oxetan-3-yl)methoxy)-4-nitrofurazan



Since the reactivity of the nitro group of the furazan is much higher than the bromine-methyl group of the oxetane during azidation, 3-((3-(azidomethyl)oxetan-3-yl)methoxy)-4-nitrofurazan cannot be synthesized by the azidation of 3-((3-(bromomethyl)oxetan-3-yl)methoxy) -4-nitrofurazan.

3,3-Bis(bromomethyl)oxetane (10.00 g, 0.041 mol) was added to a solution of sodium azide (NaN_3, 3.33 g, 0.005 mol) in 100 mL DMF, and the mixture was heated to 65°C. After reacting for 1.5 h, the solution was diluted by saturated salt solution, extracted by ethyl acetate and washed with saturated salt solution. Then it was evaporated by reduced pressure distillation. The intermediate product 3-azidomethyl-3-bromomethyloxetane was synthesized in this way.

3-Hydroxy-4-nitrofurazan (10.00 g, 0.076 mol) and 3-azidomethyl-3-bromomethyloxetane (16.51 g, 0.08 mol) was added to a solution of potassium carbonate (K_2CO_3, 13.80 g, 0.1 mol) in 100 mL DMF, and the mixture was heated to 85°C. After reacting for 2.5 h, the solution was diluted by saturated salt solution, extracted by CH_2Cl_2 and washed with saturated salt solution. Then it was evaporated by reduced pressure distillation. Finally the crude yellow liquid of 3-((3-(azidomethyl)oxetan-3-yl)methoxy)-4-azidofurazan was purify by HPLC (high performance liquid chromatography) (8.47 g, 43.5%). T_d (onset) 243.36°C. ^{13}C NMR (125 MHz, DMSO-d_6) δ 158.80, 152.64, 74.28, 74.14, 52.65, 42.76 ppm. ^{1}H NMR (600 MHz, DMSO-d_6) δ 4.65, 4.52, 4.43, 3.88 ppm. ESI-HRMS: *m/z* calcd for $[M+H]^+$: 257.0634, found: 257.0673 IR (KBr) $\tilde{\nu}$=2962, 2883, 2108, 1604, 1502, 1366, 1283, 1207, 1035, 986 cm^{-1}. (The images of ^{1}H NMR, ^{13}C NMR, FTIR

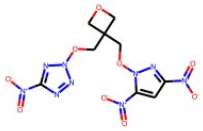
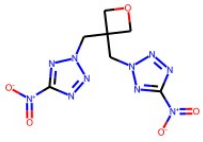
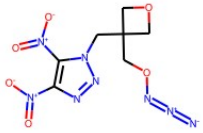
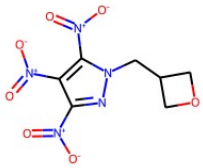
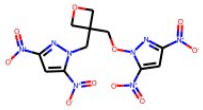
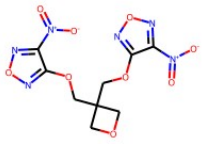
spectra and ESI-HRMS spectra are provided in **Supplementary Fig. 1, 2, 3, 6** respectively)

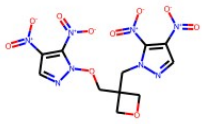
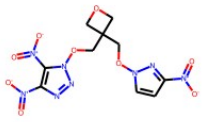
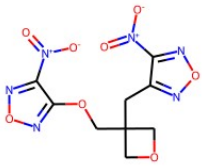
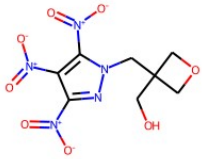
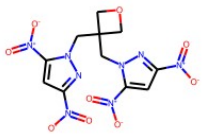
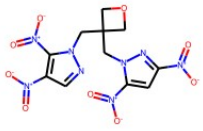
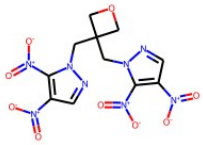
Polymerization of 4,4'-((oxetane-3,3-diylbis(methylene))bis(oxy))bis(3-nitrofurazan)

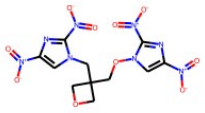
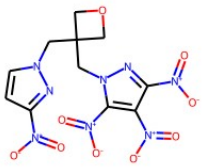
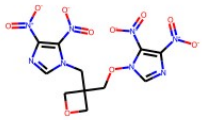
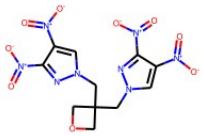
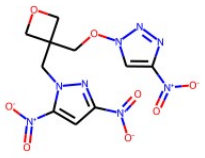
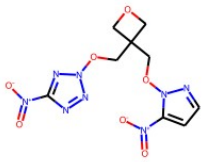
$BF_3 \cdot OEt_2$ (2.84 g ,0.02 mol) and BDO (0.90 g ,0.01 mol) was added to100 mL CH_2Cl_2 ($H_2O \leq$ 0.004%). The mixture reacted for 1 hour. After the full activation of the initiating system, the 4,4'-((oxetane-3,3-diylbis(methylene))bis(oxy))bis(3-nitrofurazan) monomers (20.64 g, 0.06 mol) are intensive dried and dissolve in the dichloromethane.

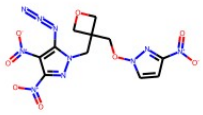
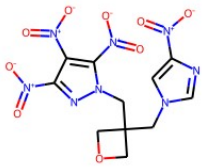
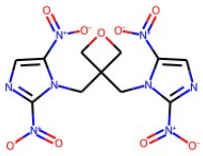
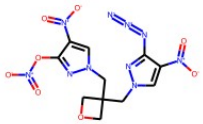
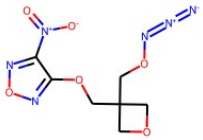
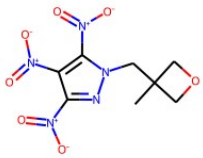
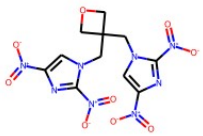
After reacting for 72 h, the initiating system was inactivated by saturated $NaHCO_3$ solution, sedimented in cold CH_2OH. Then it was drying by reduced pressure oven. Finally the crude yellow solid of poly(**1**) was obtained (*M*n=2000, PDI=1.45). ^{1}H NMR (600 MHz, DMSO-d_6) δ 3.61, 4.56 ppm. IR (KBr) $\tilde{\nu}$= 2971, 2888, 1752, 1605 cm^{-1}. (The images of GPC, FTIR, ^{1}H NMR spectra are provided in **Supplementary Fig. 7, 8, 9**).

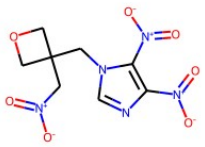
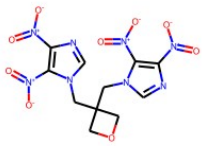
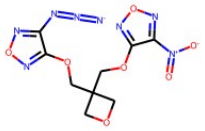
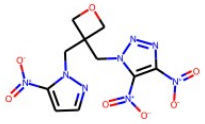
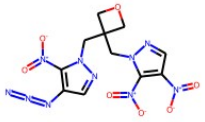
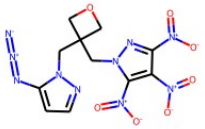
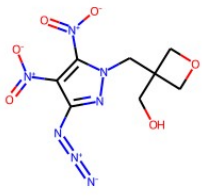
Table S1 73 candidates after high-throughput screen

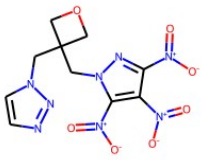
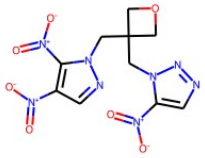
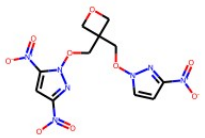
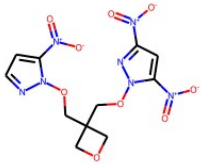
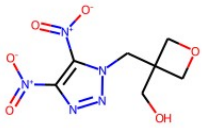
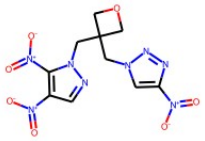
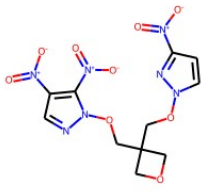
ID	Smiles	D (km·s^{-1})	P (GPa)	SYBA score	Density (g·cm^{-3})	SAS core	SCS core	Molecule
0	[H]c1c([N+](=O)[O-])nn(OC([H])([H])C2(C([H])([H])On3nnc([N+](=O)[O-])n3)C([H])([H])OC2([H])[H])c1[N+](=O)[O-]	7.53	24.36	19.43	1.71	4.23	2.98	
1	[H]C1([H])OC([H])([H])C1(C([H])([H])n1nnc([N+](=O)[O-])n1)C([H])([H])n1nnc([N+](=O)[O-])n1	7.40	23.45	25.85	1.70	3.78	2.79	
2	[H]C([H])(ON=[N+]=[N-])C1(C([H])([H])n2nnc([N+](=O)[O-])c2[N+](=O)[O-])C([H])([H])OC1([H])[H]	7.32	22.59	22.37	1.66	4.12	2.99	
3	[H]C1([H])OC([H])([H])C1([H])C([H])([H])n1nc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	7.31	22.73	22.01	1.68	3.29	2.61	
4	[H]c1c([N+](=O)[O-])nn(OC([H])([H])C2(C([H])([H])n3nc([N+](=O)[O-])c([H])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c1[N+](=O)[O-]	7.23	22.41	21.77	1.70	3.95	2.92	
5	[H]C([H])(Oc1nonc1[N+](=O)[O-])C1(C([H])([H])Oc2nonc2[N+](=O)[O-])C([H])([H])OC1([H])[H]	7.20	22.24	20.58	1.70	3.77	2.03	

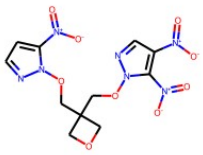
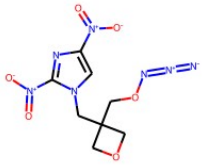
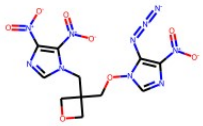
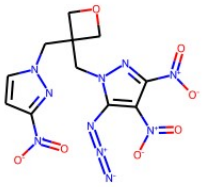
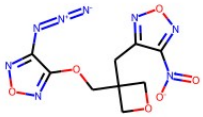
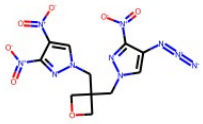
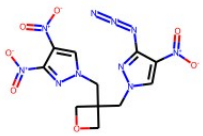
6	[H]c1nn(OC([H])([H])C2(C([H])([H])n3nc([H])c([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[N+](=O)[O-]	7.20	22.12	19.59	1.69	3.88	2.82	
7	[H]c1c([N+](=O)[O-])nn(OC([H])([H])C2(C([H])([H])On3nnc([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c1[H]	7.18	21.86	20.11	1.68	4.10	2.86	
8	[H]C([H])(Oc1nonc1[N+](=O)[O-])C1(C([H])([H])c2nonc2[N+](=O)[O-])C([H])([H])OC1([H])[H]	7.14	21.78	21.33	1.69	3.79	2.80	
9	[H]OC([H])([H])C1(C([H])([H])n2nc([N+](=O)[O-])c([N+](=O)[O-])c2[N+](=O)[O-])C([H])([H])OC1([H])[H]	7.12	21.47	27.99	1.67	3.47	2.75	
10	[H]c1c([N+](=O)[O-])nn(C([H])([H])C2(C([H])([H])n3nc([N+](=O)[O-])c([H])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c1[N+](=O)[O-]	7.09	21.52	25.41	1.70	3.70	2.47	
11	[H]c1nn(C([H])([H])C2(C([H])([H])n3nc([N+](=O)[O-])c([H])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[N+](=O)[O-]	7.07	21.39	33.15	1.69	3.68	2.97	
12	[H]c1nn(C([H])([H])C2(C([H])([H])n3nc([H])c([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[N+](=O)[O-]	7.07	21.37	24.69	1.69	3.65	2.33	

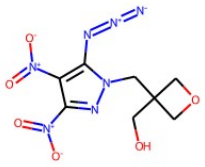
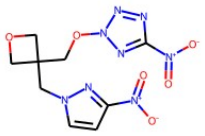
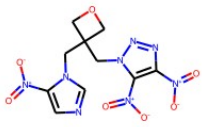
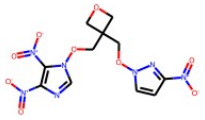
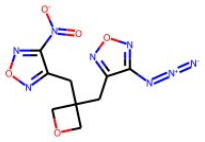
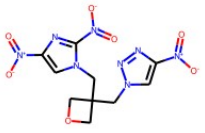
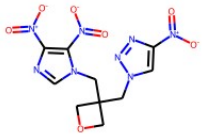
13	[H]c1c([N+](=O)[O-])nc([N+](=O)[O-])n1OC([H])([H])C1(C([H])([H])n2c([N+](=O)[O-])nc([N+](=O)[O-])c2[H])C([H])([H])OC1([H])[H]	7.07	21.30	22.19	1.69	4.02	2.99	
14	[H]c1c([N+](=O)[O-])nn(C([H])([H])C2(C([H])([H])n3nc([N+](=O)[O-])c([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c1[H]	7.07	21.27	45.12	1.69	3.64	2.86	
15	[H]c1nc([N+](=O)[O-])c([N+](=O)[O-])n1OC([H])([H])C1(C([H])([H])n2c([H])nc([N+](=O)[O-])c2[N+](=O)[O-])C([H])([H])OC1([H])[H]	7.06	21.25	23.19	1.69	3.92	2.80	
16	[H]c1c([N+](=O)[O-])c([N+](=O)[O-])nn1C([H])([H])C1(C([H])([H])n2nc([N+](=O)[O-])c([N+](=O)[O-])c2[H])C([H])([H])OC1([H])[H]	7.04	21.08	24.41	1.68	3.64	2.57	
17	[H]c1c([N+](=O)[O-])nn(C([H])([H])C2(C([H])([H])On3nnc([N+](=O)[O-])c3[H])C([H])([H])OC2([H])[H])c1[N+](=O)[O-]	7.04	21.03	19.55	1.68	4.03	2.92	
18	[H]c1nn(OC([H])([H])C2(C([H])([H])On3nnc([N+](=O)[O-])n3)C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[H]	7.02	20.78	20.49	1.65	4.20	2.98	

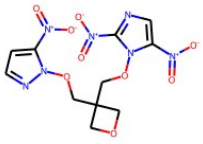
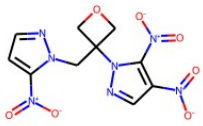
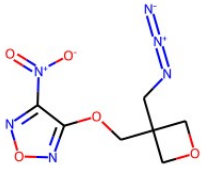
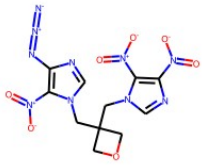
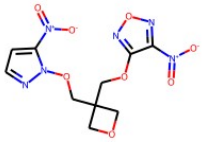
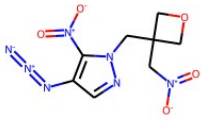
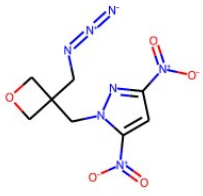
19	[H]c1c([N+](=O)[O-])nn(OC([H])([H])C2(C([H])([H])n3nc([N+](=O)[O-])c([N+](=O)[O-])c3N=[N+]=[N-])C([H])([H])OC2([H])[H])c1[H]	7.01	20.78	23.82	1.66	4.17	2.98	
20	[H]c1nc([N+](=O)[O-])c([H])n1C([H])([H])C1(C([H])([H])n2nc([N+](=O)[O-])c([N+](=O)[O-])c2[N+](=O)[O-])C([H])([H])OC1([H])[H]	7.01	20.93	44.36	1.68	3.70	2.94	
21	[H]c1nc([N+](=O)[O-])n(C([H])([H])C2(C([H])([H])n3c([N+](=O)[O-])nc([H])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c1[N+](=O)[O-]	7.00	21.06	27.13	1.71	3.72	2.88	
22	[H]c1c([N+](=O)[O-])c(N=[N+]=[N-])nn1C([H])([H])C1(C([H])([H])n2nc(O[N+](=O)[O-])c([N+](=O)[O-])c2[H])C([H])([H])OC1([H])[H]	7.00	20.67	18.90	1.66	4.06	2.93	
23	[H]C([H])(ON=[N+]=[N-])C1(C([H])([H])Oc2nonc2[N+](=O)[O-])C([H])([H])OC1([H])[H]	7.00	20.35	22.10	1.62	4.09	2.66	
24	[H]C([H])([H])C1(C([H])([H])n2nc([N+](=O)[O-])c([N+](=O)[O-])c2[N+](=O)[O-])C([H])([H])OC1([H])[H]	6.98	20.34	18.42	1.63	3.44	2.32	
25	[H]c1c([N+](=O)[O-])nc([N+](=O)[O-])n1C([H])([H])C1(C([H])([H])n2c([N+](=O)[O-])nc([N+](=O)[O-])c2[H])C([H])([H])OC1([H]	6.98	20.78	26.15	1.69	3.80	2.48	

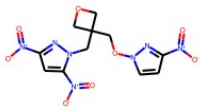
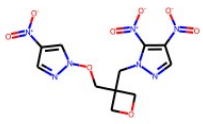
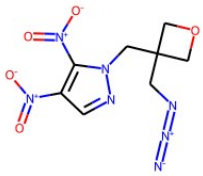
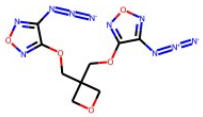
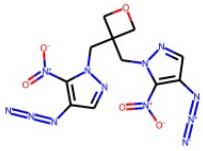
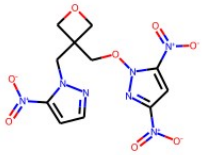
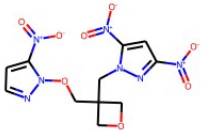
	])[H]							
26	[H]c1nc([N+](=O)[O-])c([N+](=O)[O-])n1C([H])([H])C1(C([H])([H])[N+](=O)[O-])C([H])([H])OC1([H])[H]	6.97	20.51	20.50	1.66	3.57	2.76	
27	[H]c1nc([N+](=O)[O-])c([N+](=O)[O-])n1C([H])([H])C1(C([H])([H])n2c([H])nc([N+](=O)[O-])c2[N+](=O)[O-])C([H])([H])OC1([H])[H]	6.96	20.63	28.94	1.69	3.69	2.44	
28	[H]C([H])(Oc1nonc1N=[N+]=[N-])C1(C([H])([H])Oc2nonc2[N+](=O)[O-])C([H])([H])OC1([H])[H]	6.95	20.45	22.37	1.67	4.01	2.28	
29	[H]c1nn(C([H])([H])C2(C([H])([H])n3nnc([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[H]	6.88	20.06	35.35	1.67	3.70	2.96	
30	[H]c1nn(C([H])([H])C2(C([H])([H])n3nc([H])c([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1N=[N+]=[N-]	6.88	19.99	29.64	1.66	3.92	2.92	
31	[H]c1nn(C([H])([H])C2(C([H])([H])n3nc([N+](=O)[O-])c([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c(N=[N+]=[N-])c1[H]	6.88	19.94	31.80	1.65	3.98	2.94	
32	[H]OC([H])([H])C1(C([H])([H])n2nc(N=[N+]=[N-])c([N+](=O)[O-])c2[N+](=O)[O-])C([H])([H])OC1([H])[H]	6.88	19.76	23.96	1.63	3.87	2.89	

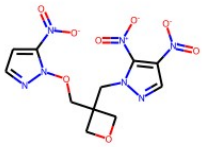
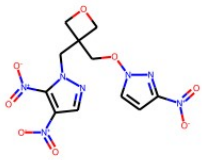
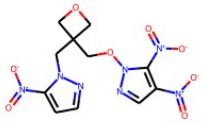
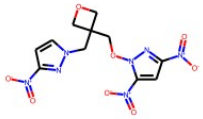
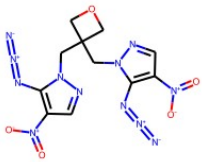
33	[H]c1nnn(C([H])([H])C2(C([H])([H])n3nc([N+](=O)[O-])c([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c1[H]	6.88	20.00	39.64	1.66	3.64	2.96	
34	[H]c1nn(C([H])([H])C2(C([H])([H])n3nnc([H])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[N+](=O)[O-]	6.88	20.04	25.63	1.67	3.74	3.00	
35	[H]c1c([N+](=O)[O-])nn(OC([H])([H])C2(C([H])([H])On3nc([N+](=O)[O-])c([H])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c1[H]	6.87	19.87	18.25	1.65	4.09	2.63	
36	[H]c1nn(OC([H])([H])C2(C([H])([H])On3nc([N+](=O)[O-])c([H])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[H]	6.87	19.82	21.51	1.65	4.12	2.88	
37	[H]OC([H])([H])C1(C([H])([H])n2nnc([N+](=O)[O-])c2[N+](=O)[O-])C([H])([H])OC1([H])[H]	6.87	19.74	25.89	1.64	3.50	2.58	
38	[H]c1nn(C([H])([H])C2(C([H])([H])n3nnc([N+](=O)[O-])c3[H])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[N+](=O)[O-]	6.87	19.93	32.82	1.66	3.71	2.83	
39	[H]c1nn(OC([H])([H])C2(C([H])([H])On3nc([N+](=O)[O-])c([H])c3[H])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[N+](=O)[O-]	6.87	19.79	18.85	1.65	4.03	2.85	

40	[H]c1nn(OC([H])([H])C2(C([H])([H])On3nc([H])c([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[H]	6.87	19.77	20.65	1.64	4.06	2.88	
41	[H]c1c([N+](=O)[O-])nc([N+](=O)[O-])n1C([H])([H])C1(C([H])([H])ON=[N+]=[N-])C([H])([H])OC1([H])[H]	6.87	19.64	26.02	1.63	4.08	2.98	
42	[H]c1nc([N+](=O)[O-])c(N=[N+]=[N-])n1OC([H])([H])C1(C([H])([H])n2c([H])nc([N+](=O)[O-])c2[N+](=O)[O-])C([H])([H])OC1([H])[H]	6.86	19.84	22.81	1.66	4.15	2.82	
43	[H]c1c([N+](=O)[O-])nn(C([H])([H])C2(C([H])([H])n3nc([N+](=O)[O-])c([N+](=O)[O-])c3N=[N+]=[N-])C([H])([H])OC2([H])[H])c1[H]	6.86	19.77	43.13	1.65	3.89	2.93	
44	[H]C([H])(Oc1nonc1N=[N+]=[N-])C1(C([H])([H])c2nonc2[N+](=O)[O-])C([H])([H])OC1([H])[H]	6.86	19.75	23.12	1.65	4.04	2.93	
45	[H]c1c(N=[N+]=[N-])c([N+](=O)[O-])nn1C([H])([H])C1(C([H])([H])n2nc([N+](=O)[O-])c([N+](=O)[O-])c2[H])C([H])([H])OC1([H])[H]	6.86	19.73	29.14	1.65	3.92	2.94	
46	[H]c1c([N+](=O)[O-])c(N=[N+]=[N-])nn1C([H])([H])C1(C([H])([H])n2nc([N+](=O)[O-])c([N+](=O)[O-])c2[H])C([H])([H])OC1([H]	6.85	19.72	25.51	1.65	3.92	2.75	

	])[H]							
47	[H]OC([H])([H])C1(C([H])([H])n2nc([N+](=O)[O-])c([N+](=O)[O-])c2N=[N+]=[N-])C([H])([H])OC1([H])[H]	6.85	19.51	26.00	1.62	3.81	2.82	
48	[H]c1c([N+](=O)[O-])nn(C([H])([H])C2(C([H])([H])On3nnc([N+](=O)[O-])n3)C([H])([H])OC2([H])[H])c1[H]	6.84	19.61	33.08	1.64	3.88	2.88	
49	[H]c1nc([H])n(C([H])([H])C2(C([H])([H])n3nnc([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c1[N+](=O)[O-]	6.82	19.68	29.27	1.67	3.72	2.99	
50	[H]c1c([N+](=O)[O-])nn(OC([H])([H])C2(C([H])([H])On3c([H])nc([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c1[H]	6.81	19.49	18.05	1.65	4.05	2.82	
51	[H]C1([H])OC([H])([H])C1(C([H])([H])c1nonc1N=[N+]=[N-])C([H])([H])c1nonc1[N+](=O)[O-]	6.80	19.33	18.67	1.63	4.02	2.95	
52	[H]c1c([N+](=O)[O-])nnn1C([H])([H])C1(C([H])([H])n2c([N+](=O)[O-])nc([N+](=O)[O-])c2[H])C([H])([H])OC1([H])[H]	6.80	19.50	31.81	1.66	3.79	2.88	
53	[H]c1c([N+](=O)[O-])nnn1C([H])([H])C1(C([H])([H])n2c([H])nc([N+](=O)[O-])c2[N+](=O)[O-])C([H])([H])OC1([H])[H]	6.79	19.46	37.07	1.66	3.73	2.94	

54	[H]c1nn(OC([H])([H])C2(C([H])([H])On3c([N+](=O)[O-])nc([H])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[H]	6.79	19.33	20.30	1.64	4.11	2.95	
55	[H]c1nn(C([H])([H])C2(n3nc([H])c([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[H]	6.79	19.52	19.69	1.67	3.68	2.92	
56	[H]C([H])(N=[N+]=[N-])C1(C([H])([H])Oc2nonc2[N+](=O)[O-])C([H])([H])OC1([H])[H]	6.76	18.89	18.65	1.61	3.92	2.83	
57	[H]c1nc(N=[N+]=[N-])c([N+](=O)[O-])n1C([H])([H])C1(C([H])([H])n2c([H])nc([N+](=O)[O-])c2[N+](=O)[O-])C([H])([H])OC1([H])[H]	6.76	19.25	30.32	1.65	3.97	2.97	
58	[H]c1nn(OC([H])([H])C2(C([H])([H])Oc3nonc3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[H]	6.75	19.15	26.05	1.65	3.92	2.99	
59	[H]c1nn(C([H])([H])C2(C([H])([H])[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1N=[N+]=[N-]	6.74	18.88	18.96	1.62	3.93	2.78	
60	[H]c1c([N+](=O)[O-])nn(C([H])([H])C2(C([H])([H])N=[N+]=[N-])C([H])([H])OC2([H])[H])c1[N+](=O)[O-]	6.73	18.73	23.48	1.61	3.80	2.97	

61	[H]c1c([N+](=O)[O-])nn(OC([H])([H])C2(C([H])([H])n3nc([N+](=O)[O-])c([H])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c1[H]	6.72	19.00	23.79	1.65	3.86	2.74	
62	[H]c1nn(OC([H])([H])C2(C([H])([H])n3nc([H])c([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([H])c1[N+](=O)[O-]	6.72	19.00	19.67	1.65	3.74	2.97	
63	[H]c1nn(C([H])([H])C2(C([H])([H])N=[N+]=[N-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[N+](=O)[O-]	6.72	18.70	22.76	1.61	3.77	2.85	
64	[H]C([H])(Oc1nonc1N=[N+]=[N-])C1(C([H])([H])Oc2nonc2N=[N+]=[N-])C([H])([H])OC1([H])[H]	6.72	18.82	18.08	1.63	4.24	2.26	
65	[H]c1nn(C([H])([H])C2(C([H])([H])n3nc([H])c(N=[N+]=[N-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1N=[N+]=[N-]	6.72	18.79	27.40	1.63	4.19	2.52	
66	[H]c1nn(C([H])([H])C2(C([H])([H])On3nc([N+](=O)[O-])c([H])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[H]	6.72	18.93	29.66	1.65	3.88	2.74	
67	[H]c1nn(OC([H])([H])C2(C([H])([H])n3nc([N+](=O)[O-])c([H])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[H]	6.71	18.88	26.82	1.64	3.89	2.87	

68	[H]c1nn(OC([H])([H])C2(C([H])([H])n3nc([H])c([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[H]	6.71	18.87	26.98	1.64	3.87	2.91	
69	[H]c1nn(C([H])([H])C2(C([H])([H])On3nc([N+](=O)[O-])c([H])c3[H])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[N+](=O)[O-]	6.71	18.89	25.40	1.65	3.83	2.93	
70	[H]c1nn(C([H])([H])C2(C([H])([H])On3nc([H])c([N+](=O)[O-])c3[N+](=O)[O-])C([H])([H])OC2([H])[H])c([N+](=O)[O-])c1[H]	6.71	18.85	28.80	1.64	3.82	2.88	
71	[H]c1c([N+](=O)[O-])nn(OC([H])([H])C2(C([H])([H])n3nc([N+](=O)[O-])c([H])c3[H])C([H])([H])OC2([H])[H])c1[N+](=O)[O-]	6.71	18.82	33.97	1.64	3.82	2.82	
72	[H]c1nn(C([H])([H])C2(C([H])([H])n3nc([H])c([N+](=O)[O-])c3N=[N+]=[N-])C([H])([H])OC2([H])[H])c(N=[N+]=[N-])c1[N+](=O)[O-]	6.71	18.71	23.40	1.62	4.14	2.97	

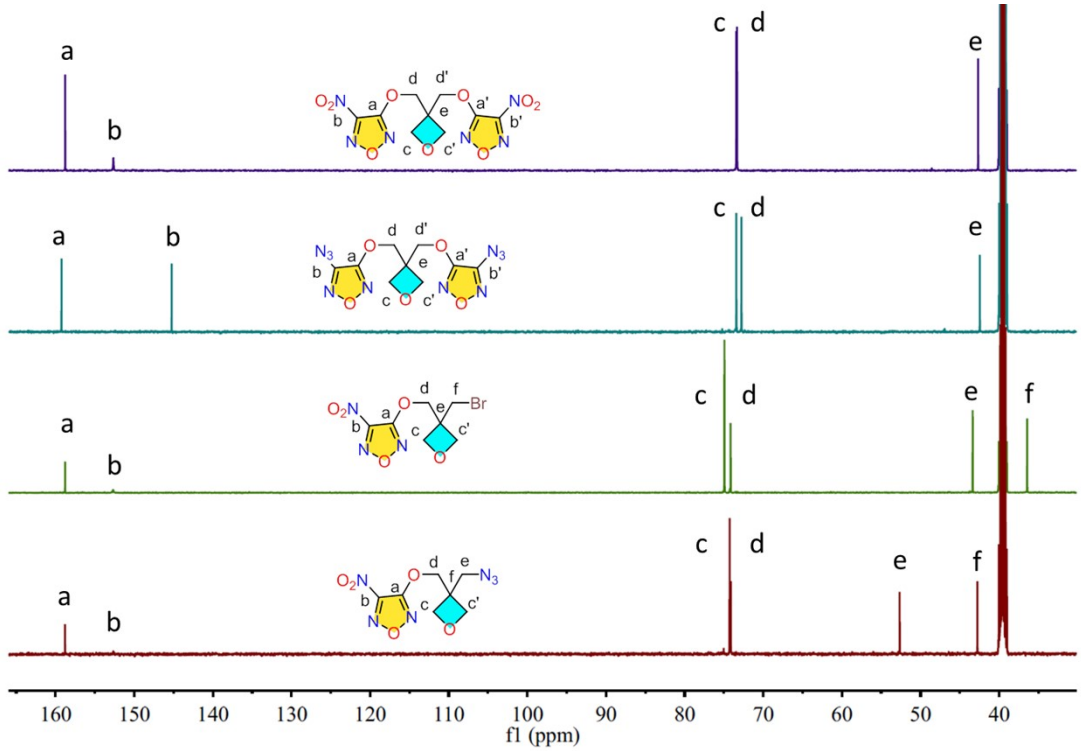


Fig. S1 ^{13}C NMR spectrogram of **1, 2, BrFNO$_2$** and **3**

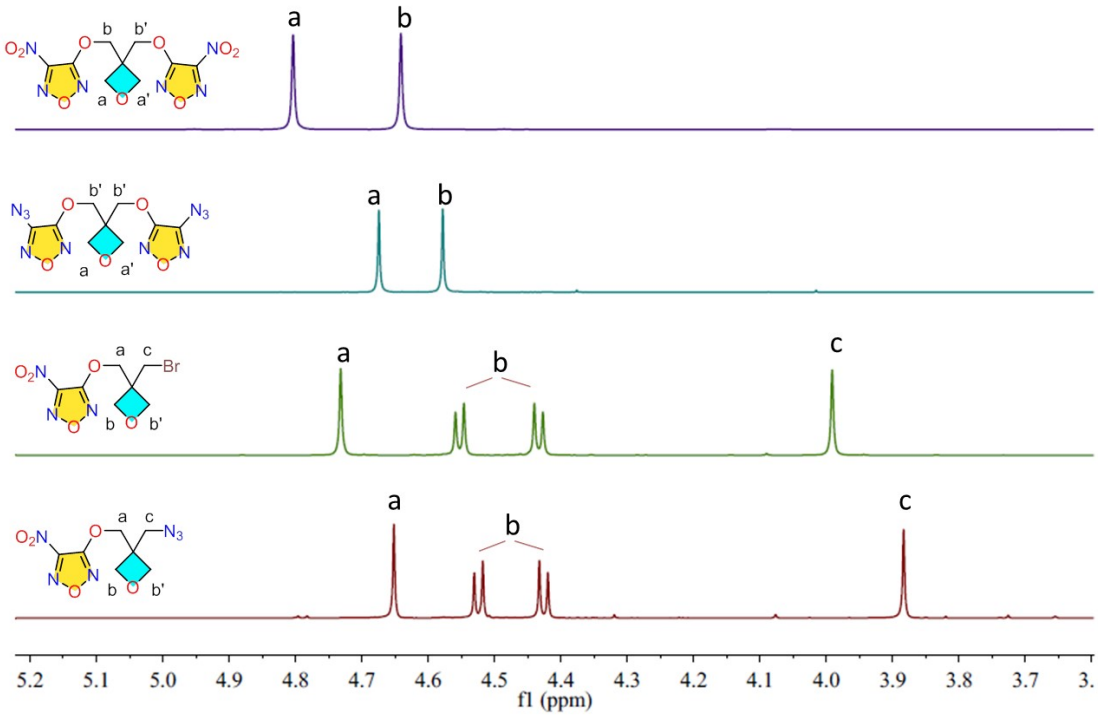


Fig. S2 ^{1}H NMR spectrogram of **1, 2, BrFNO$_2$** and **3**

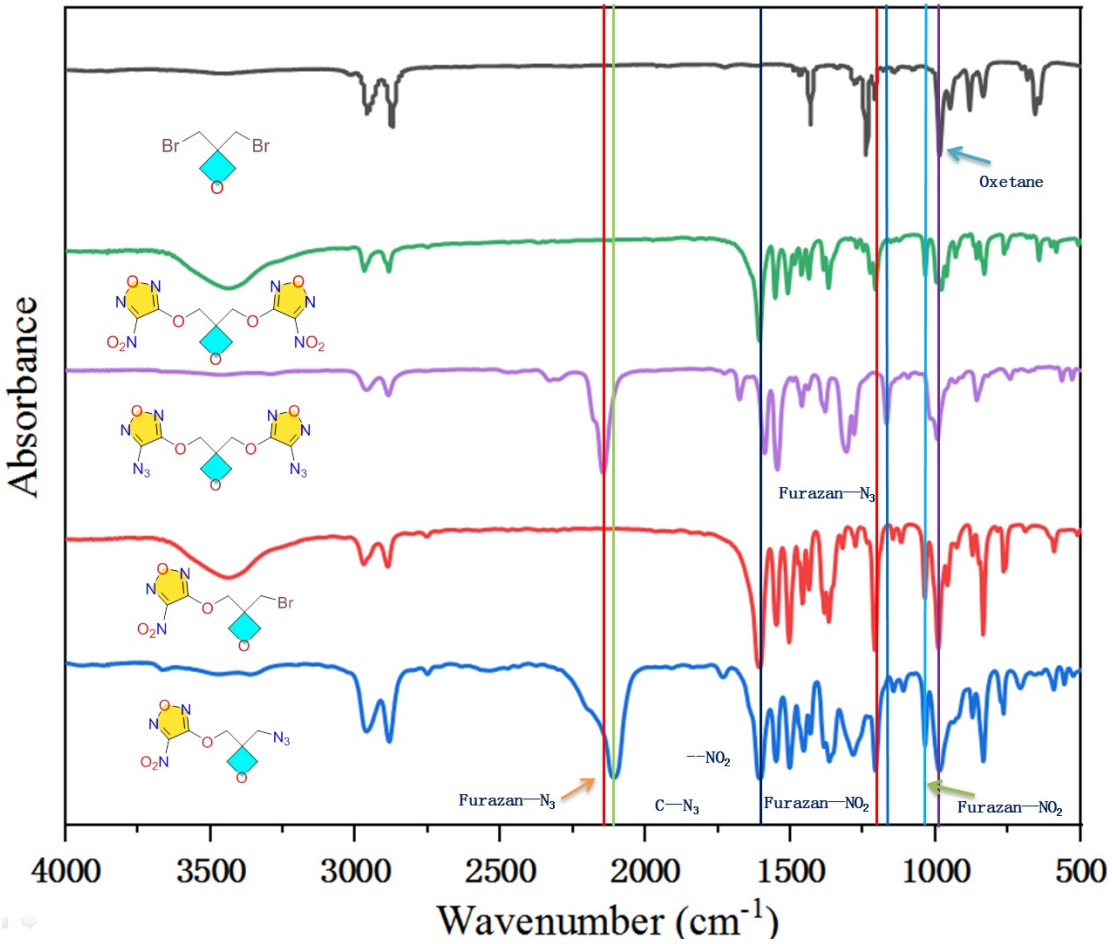


Fig. S3 FTIR spectrogram of **BBMO**, **1**, **2**, **BrFNO$_2$** and **3**

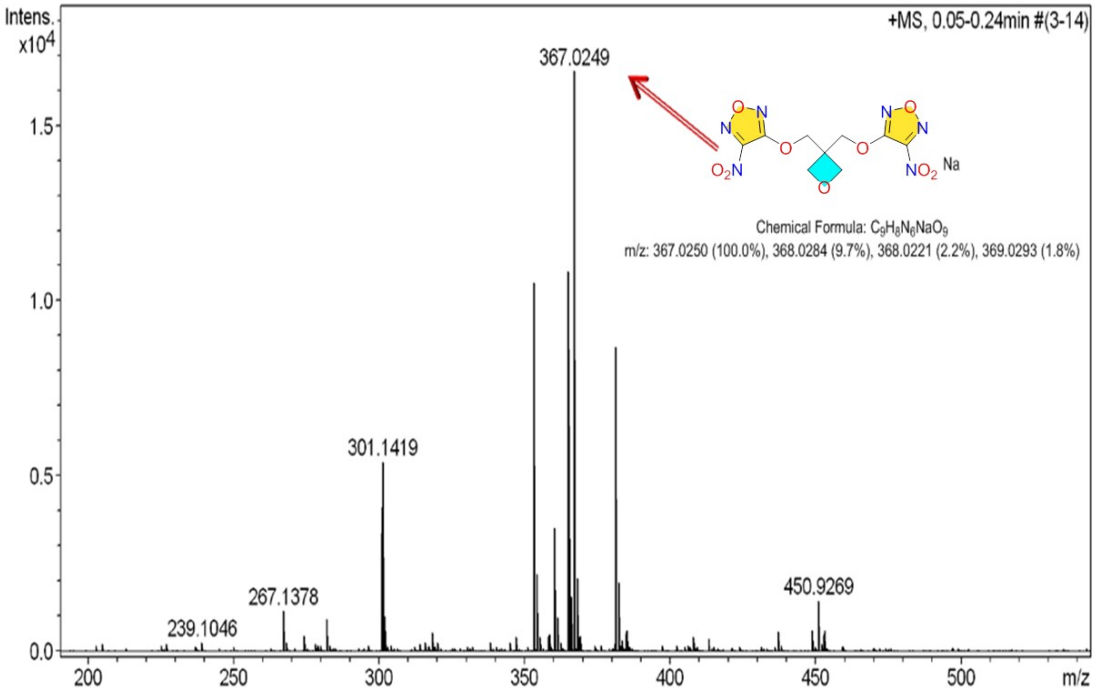


Fig. S4 ESI-HRMS spectrogram of **1**

Table. S2 Single-crystal structure result of **1**

Empirical formula	$C_9H_8N_6O_9$
Formula weight	344.21
Temperature/K	273.15
Crystal system	triclinic
Space group	$P\bar{1}$（No.2）
Unit cell dimensions/Å, °	a=8.960（9）, α=88.615（16） b=9.401（10）, β=88.119（19） c=18.73（2）, γ=63.780（16）
Cell volume/Å^3	1415（3）
Z	4
ρcal/g cm^{-3}	1.616
F（000）	704
Crystal size/mm	0.3*0.2*0.15
Goodness-of-fit on F^2	1.021
Final R indices [I ≥ 2σ]	R_1=0.0437, wR_2=0.1065
R indices [all data]	R_1=0.0774, wR_2=0.1256

Table. S3 Bond length, bond angel and torsion angle of **1**

Bond	Length/nm	Bond	Angel/(°)	Bond	Torsion angle/(°)
O3 C7	1.316(5)	C7 O3 C4	114.8(3)	O3 C7 C8 N6	-0.1(6)
O3 C4	1.451(5)	C6 O2 C5	115.1(3)	O3 C7 C8 N5	-178.6(4)
O2 C6	1.327(5)	C1 O1 C2	91.9(3)	O2 C6 C9 N3	-0.4(7)
O2 C5	1.457(5)	N2 O4 N1	111.1(3)	O2 C6 C9 N2	179.7(4)
O1 C1	1.429(6)	N5 O5 N4	111.8(3)	O4 N1 C6 O2	-179.9(4)
O1 C2	1.437(6)	O9 N6 C8	118.4(4)	O4 N1 C6 C9	0.9(5)
O4 N1	1.398(5)	O8 N6 O9	124.7(5)	O4 N2 C9 N3	-179.1(4)
O4 N2	1.347(6)	O8 N6 C8	116.9(4)	O4 N2 C9 C6	0.7(5)
O5 N4	1.395(5)	O6 N3 O7	124.9(5)	O5 N4 C7 O3	179.3(4)
O5 N5	1.360(6)	O6 N3 C9	118.3(4)	O5 N4 C7 C8	1.0(5)
O9 N6	1.220(5)	O7 N3 C9	116.8(4)	O5 N5 C8 N6	-179.1(4)
O8 N6	1.195(5)	C6 N1 O4	104.7(4)	O5 N5 C8 C7	-0.5(5)
O6 N3	1.204(5)	C9 N2 O4	105.6(4)	O9 N6 C8 N5	11.1(6)
O7 N3	1.205(6)	C7 N4 O5	104.7(4)	O9 N6 C8 C7	-167.2(4)
N6 C8	1.433(6)	C8 N5 O5	104.4(4)	O8 N6 C8 N5	-169.7(4)
N3 C9	1.437(7)	O2 C6 C9	125.6(4)	O8 N6 C8 C7	12.0(6)
N1 C6	1.285(6)	N1 C6 O2	125.6(4)	O6 N3 C9 N2	11.6(7)
N2 C9	1.284(6)	N1 C6 C9	108.8(4)	O6 N3 C9 C6	-168.2(4)
N4 C7	1.295(6)	O3 C7 C8	126.4(4)	O7 N3 C9 N2	-166.4(5)
N5 C8	1.278(5)	N4 C7 O3	125.7(4)	O7 N3 C9 C6	13.8(7)
C6 C9	1.415(6)	N4 C7 C8	107.8(4)	N1 O4 N2 C9	-0.2(5)
C7 C8	1.421(6)	C5 C3 C4	112.2(3)	N1 C6 C9 N3	178.7(4)
C3 C5	1.497(6)	C5 C3 C1	111.8(4)	N1 C6 C9 N2	-1.1(5)

C3 C4	1.499(6)	C5 C3 C2	114.0(3)	N2 O4 N1 C6	-0.5(5)
C3 C1	1.549(6)	C4 C3 C1	117.1(3)	N4 O5 N5 C8	1.2(5)
C3 C2	1.535(6)	C4 C3 C2	115.2(4)	N4 C7 C8 N6	178.1(4)
N1 O2	1.197(6)	C2 C3 C1	83.9(3)	N4 C7 C8 N5	-0.3(5)
N1 O5	1.185(6)	N5 C8 N6	120.0(4)	N5 O5 N4 C7	-1.4(5)
O1 N3	1.195(6)	N5 C8 C7	111.3(4)	C6 O2 C5 C3	175.3(3)
N3 O4	1.218(7)	C7 C8 N6	128.7(3)	C7 O3 C4 C3	174.8(3)
		O2 C5 C3	106.6(3)	C5 O2 C6 N1	-2.2(6)
		N2 C9 N3	121.1(4)	C5 O2 C6 C9	176.8(4)
		N2 C9 C6	109.8(5)	C5 C3 C4 O3	-63.8(4)
		C6 C9 N3	129.1(4)	C5 C3 C1 O1	-105.6(4)
		O3 C4 C3	106.4(3)	C5 C3 C2 O1	103.4(4)
		O1 C1 C3	91.4(3)	C4 O3 C7 N4	-6.7(5)
		O1 C2 C3	91.7(3)	C4 O3 C7 C8	171.3(4)
		O5 N1 O2	123.3(5)	C4 C3 C5 O2	-67.5(4)
		O1 N3 O4	124.0(5)	C4 C3 C1 O1	123.0(4)
				C4 C3 C2 O1	-124.9(4)
				C1 O1 C2 C3	8.4(4)
				C1 C3 C5 O2	158.7(3)
				C1 C3 C4 O3	67.4(4)
				C1 C3 C2 O1	-7.8(4)
				C2 O1 C1 C3	-8.3(4)
				C2 C3 C5 O2	65.7(4)
				C2 C3 C4 O3	163.6(3)
				C2 C3 C1 O1	7.8(4)

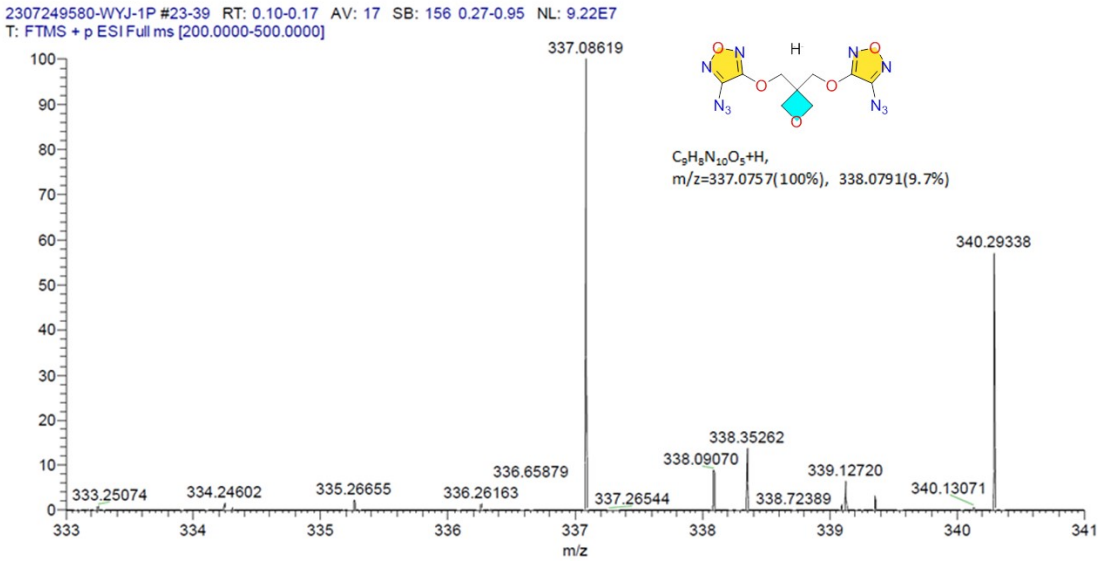


Fig. S5 ESI-HRMS spectrogram of **2**

Table S4 Single-crystal structure result of **2**

Empirical formula	$C_9H_8N_{10}O_5$
Formula weight	336.25
Temperature/K	273.15
Crystal system	triclinic
Space group	$P2_1/c(No.14)$
Unit cell dimensions/Å, °	a=14.2832（19）, α=90 b=7.5634（9）, β=105.893（6） c=13.8345（18）, γ=90
Cell volume/Å^3	1437.4（3）
Z	4
ρcal/g cm^{-3}	1.554
F（000）	688
Crystal size/mm	0.5*0.4*0.3
Goodness-of-fit on F^2	0.997
Final R indices [$I \geq 2\sigma$]	R_1=0.0487, wR_2=0.0996
R indices [all data]	R_1=0.1434, wR_2=0.1358

Table. S5 Bond length, bond angel and torsion angle of **2**

Bond	Length/nm	Bond	Angel/(°)	Bond	Torsion angle/(°)
O3 C7	1.3321(15)	C7 O3 C4	115.33(10)	O3 C7 C9 N4	-178.72(12)
O3 C4	1.4508(15)	C6 O2 C5	116.27(10)	O3 C7 C9 N8	1.0(2)
O2 C6	1.3300(16)	C2 O1 C1	90.79(9)	O3 C4 C3 C5	64.94(13)
O2 C5	1.4493(16)	N4 O5 N3	111.02(10)	O3 C4 C3 C1	-66.32(14)
O1 C1	1.4431(17)	N2 O4 N1	111.01(10)	O3 C4 C3 C2	-162.90(11)
O1 C2	1.4420(19)	N7 N6 N5	171.15(17)	O2 C6 C8 N5	0.1(2)
O5 N3	1.3981(17)	C7 N3 O5	104.44(12)	O2 C6 C8 N2	179.22(13)
O5 N4	1.3851(19)	C9 N4 O5	105.14(11)	O5 N3 C7 O3	178.64(12)
O4 N1	1.4002(17)	C6 N1 O4	104.33(12)	O5 N3 C7 C9	-0.64(16)
O4 N2	1.3884(18)	N6 N5 C8	115.43(13)	O5 N4 C9 C7	-0.21(15)
N6 N5	1.2485(18)	C8 N2 O4	104.69(12)	O5 N4 C9 N8	-179.93(12)
N6 N7	1.1125(19)	O3 C7 C9	123.95(12)	O4 N1 C6 O2	-179.39(13)
N3 C7	1.2885(17)	N3 C7 O3	125.98(12)	O4 N1 C6 C8	-0.34(16)
N4 C9	1.2912(18)	N3 C7 C9	110.07(12)	O4 N2 C8 N5	179.19(14)
N1 C6	1.2889(18)	O3 C4 C3	106.64(10)	O4 N2 C8 C6	0.14(16)
N5 C8	1.3892(19)	C4 C3 C5	113.34(11)	N6 N5 C8 N2	0.4(2)
N2 C8	1.2893(17)	C4 C3 C1	116.79(11)	N6 N5 C8 C6	179.32(14)
C7 C9	1.4246(19)	C4 C3 C2	115.89(11)	N3 O5 N4 C9	-0.18(16)
C4 C3	1.5059(18)	C5 C3 C1	111.22(10)	N3 C7 C9 N4	0.57(17)
C3 C5	1.5100(17)	C5 C3 C2	112.42(11)	N3 C7 C9 N8	-179.75(15)
C3 C1	1.5343(18)	C1 C3 C2	83.99(10)	N4 O5 N3 C7	0.53(16)
C3 C2	1.5359(18)	O2 C6 C8	123.29(12)	N4 C9 N8 N9	-172.57(14)

C6 C8	1.417(2)	N1 C6 O2	126.69(13)	N1 O4 N2 C8	-0.36(17)
C9 N8	1.3807(19)	N1 C6 C8	110.01(12)	N1 C6 C8 N5	-178.97(14)
N9 N8	1.2473(19)	N4 C9 C7	109.33(13)	N1 C6 C8 N2	0.14(18)
N9 N10	1.1094(19)	N4 C9 N8	118.84(13)	N2 O4 N1 C6	0.44(17)
O3 C7	1.3321(15)	N8 C9 C7	131.83(12)	C7 O3 C4 C3	178.67(10)
O3 C4	1.4508(15)	N5 C8 C6	122.73(12)	C7 C9 N8 N9	7.8(2)
O2 C6	1.3300(16)	N2 C8 N5	127.31(14)	C4 O3 C7 N3	16.42(19)
O2 C5	1.4493(16)	N2 C8 C6	109.95(13)	C4 O3 C7 C9	-164.41(12)
		O2 C5 C3	107.01(10)	C4 C3 C5 O2	59.79(14)
		O1 C1 C3	91.59(10)	C4 C3 C1 O1	-126.58(11)
		O1 C2 C3	91.56(10)	C4 C3 C2 O1	127.48(11)
		N10 N9 N8	169.83(17)	C6 O2 C5 C3	169.17(11)
		N9 N8 C9	116.47(12)	C5 O2 C6 N1	2.5(2)
				C5 O2 C6 C8	-176.45(13)
				C5 C3 C1 O1	101.19(11)
				C5 C3 C2 O1	-99.94(11)
				C1 O1 C2 C3	-11.18(10)
				C1 C3 C5 O2	-166.25(11)
				C1 C3 C2 O1	10.56(9)
				C2 O1 C1 C3	11.19(10)
				C2 C3 C5 O2	-74.04(14)
				C2 C3 C1 O1	-10.56(9)

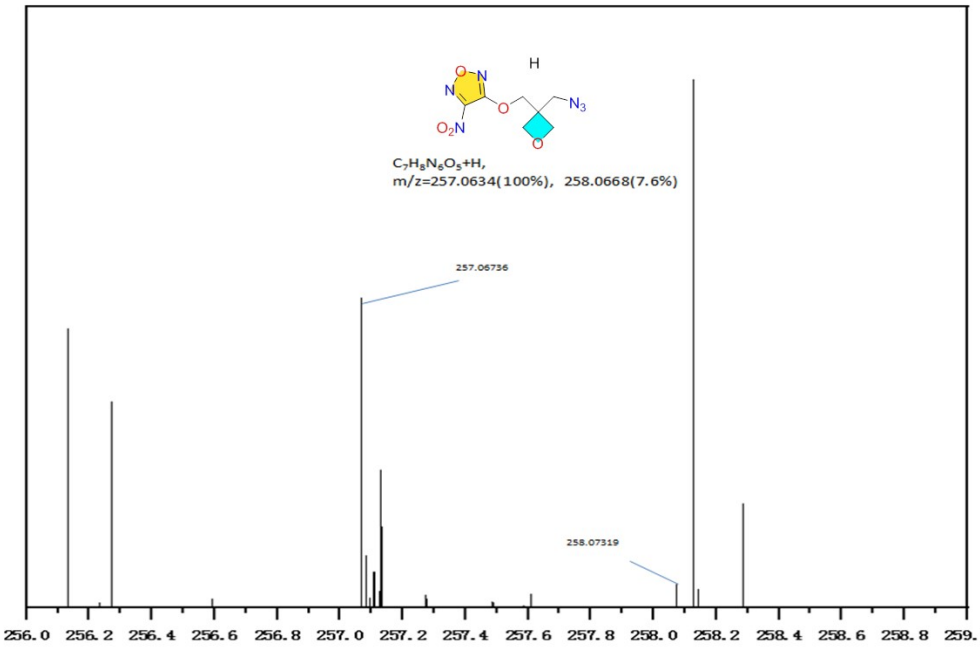


Fig. S6 ESI-HRMS spectrogram of **3**

Table. S6 Properties comparisons of MEMMs with traditional energetic materials

	T_m[a] (°C)	T_d[b] (°C)	D[c] (g cm^{-3})	$\Delta_f H$[d] (kJ mol^{-1})	v_D[e] (m s^{-1})	P[f] (GPa)	Q_v[g] (kJ kg^{-1}).	IS[h] (J)	FS[i] (N)	Ref.
TNT	81	295	1.65	-67.0	6.90	20.00	5223	15	360	[1]
BAMO	-	160	1.20	446.9	5.85	11.70	4199	25	60	[2]
TMETN	-3	182	1.49	-442.4	7.47	22.40	6100	12	0	[3]
1	102	222	1.67	-108.8	7.33	23.24	5439	>60	>360	
2	80	186	1.62	-132.3	6.10	15.80	3127	>60	>360	
3	-	252	1.55	190.2	6.87	19.45	5364	>60	>360	

[a] Molting temperature, [b] Decomposition temperature, [c] Density measured by gas pycnometry, [d] Formation heat, [e] Detonation velocity, [f] Detonation pressure , [g] Heat of detonation [kJ kg^{-1}], [h] Impact sensitivity, [i] Friction sensitivity.

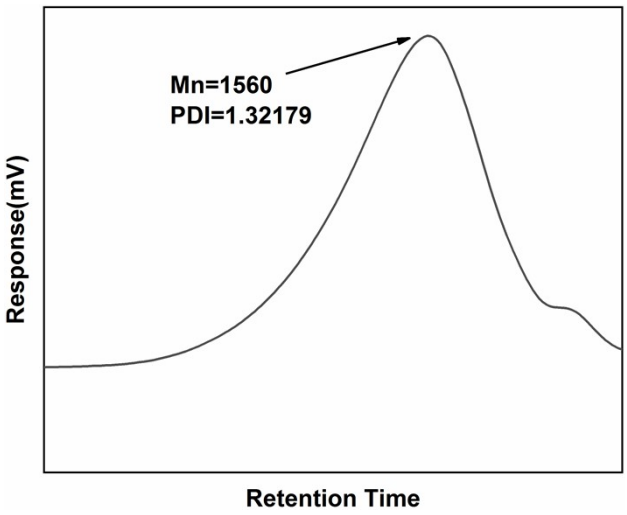


Fig. S7 GPC plot of **Poly 1**

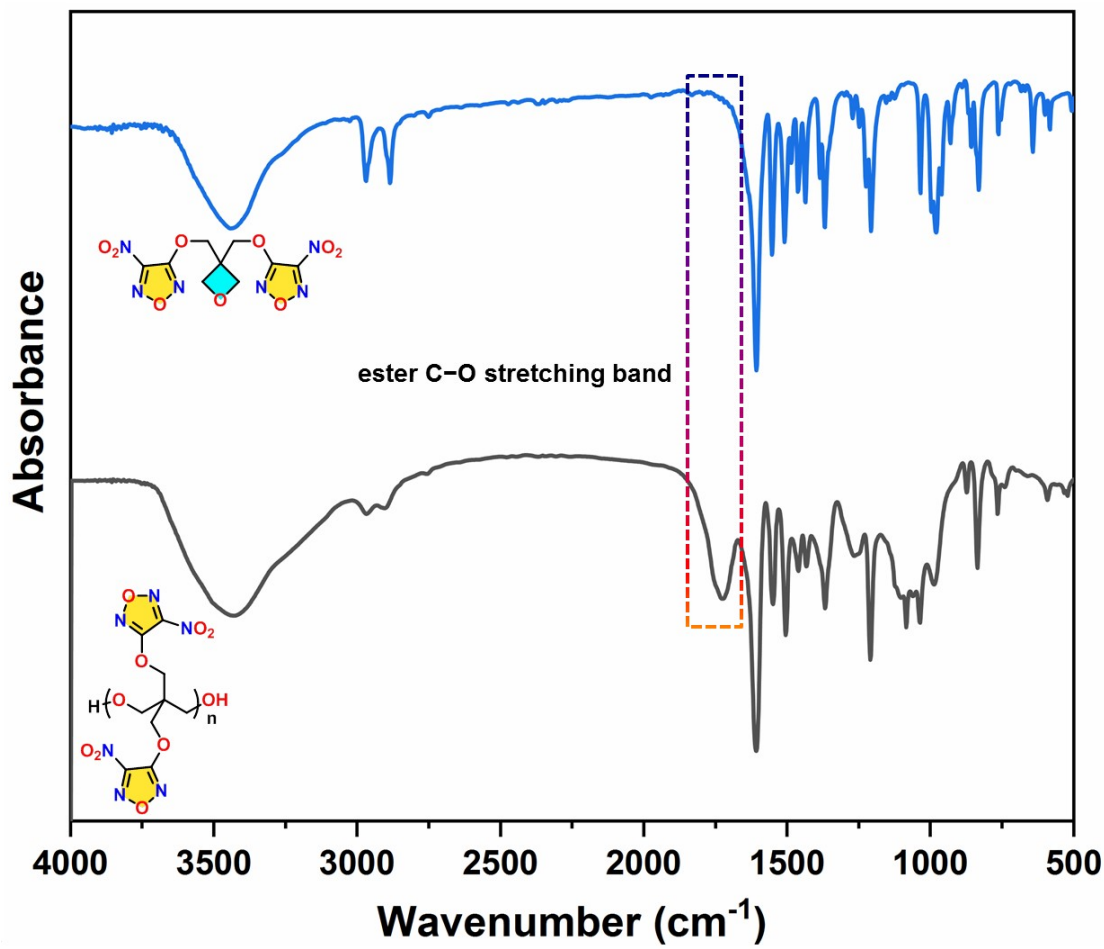


Fig. S8 FTIR spectrogram of **1** and **Poly 1**

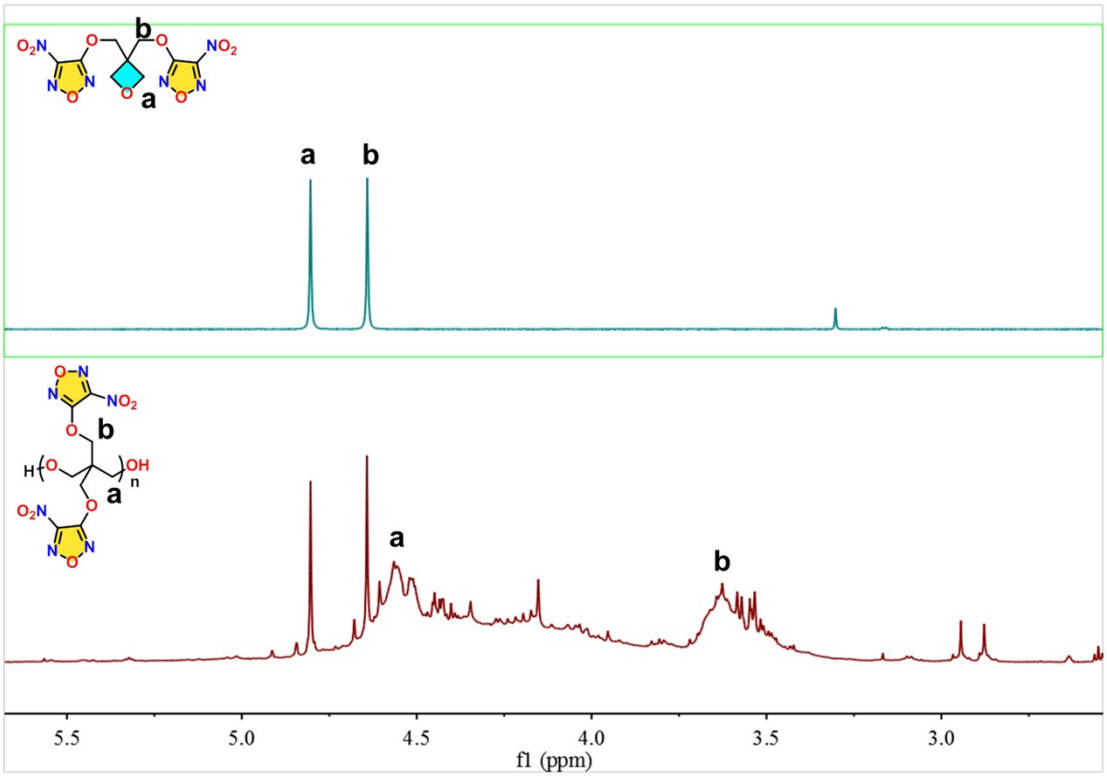


Fig. S9 ^{1}H NMR spectrogram of **1** and **Poly 1**

Table. S7 Comparison and Connection between Stem Cells and MMEMs

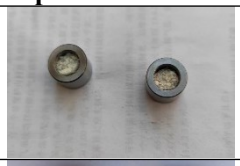
Comparison and Connection between Stem Cells and MMEMs				
		Stem cells	**MMEMs**	**Explanation**
Prolife-ration	Maintena-nce quantity	**Ability of indefinitely proliferate**	**Ability of large-scale production**	Taking the difficulty of synthesis as one of the key factors to consider whether the designed structure can be used as MMEMs, pursuing the overall optimum rather than just the optimal energy characteristics.
	Standby mode	**Cease division and stably exist in the form of stem cells**	**Without polymerization and stably exist in the form of energetic monomers**	The stability of the monomer (friction sensitivity, impact sensitivity, thermal decomposition temperature, chemical stability) is also considered as one of the key factors in determining whether the designed structure can be used as MMEMs.
Differentiation		**Differentiate into cells with different functions if necessity**	**Modularly assembled to create energetic materials with different functions if necessity**	The introducing of oxetane groups with polymerization ability will inevitably bring up the problem of energy reduction, but this is acceptable. The impact of the functional groups on energy can be minimized through high-throughput screening based on machine learning.
Specific function		**Red blood cells: Transport oxygen to the organs of the body**	**Oxidizer: Provide oxygen for the release of energy in the formulation.**	**Implementation method:** The monomer can be directly added as an oxidizer to the formulation, or it can be polymerized to obtain polymer energetic materials, which can be used in situations that require higher stability. (When used as an oxidizer, targeted molecular structure design should be carried out to provide high oxygen balance groups)
		Osteocyte：Provide support and shaping functions for the organism	**Binder: Provides support and shaping functions for the formulation**	**Implementation method:** Use cationic ring-opening polymerization to produce energetic polymers that can be used as energetic binders.
		Neurocyte：Balance the basic life activities of the organism	**Plasticizer: Balance the mold ability and process ability of the formulation.**	**Implementation method:** Utilize the flexible ether bonds to connect the furazan ether structures, which are commonly used as energetic plasticizers, to achieve the plasticizing effect through intramolecular plasticization channels.
		Adipocyte：Provide a source of energy for the organism	**Fuel: Provide a source of energy for the formulation**	**Implementation method:** The monomer can be directly added as fuel to the formula, or it can be polymerized to obtain polymer energetic materials, which can be used in situations that require higher stability.
Significance		**Maintain the body's diverse cell renewal requirements at the lowest energy cost**	**Maintain the national ammunition reserve demand at the lowest economic cost**	Applying bionic patterns to energetic materials. Pursuing standardization and generalization; Pursuing optimizing overall performance rather than local performance.

In conclusion, similar to the stem cells, MMEMs rely on scale-up production capacity to support sufficient quantities, followed by multi-functional differentiation to achieve the balance between cost and versatility. Moreover, both of stem cells and MMEMs are capable of targeted differentiation to fulfill specific requirements (such as oxygen supply, structural support, energy provision, etc.) and can meet as much as possible demands at minimal possible costs. They share significant correlation and application prospects.

To validate its energetic characteristics from multiple perspectives, we conducted verification experiments: 1) Extreme impact sensitivity testing; 2) Laser ignition experiment. The results are as follows:

1) Extreme impact sensitivity testing: Conventional impact sensitivity tests typically classify a material as "insensitive energetic" once the impact energy reaches 60 J, without further increasing the impact energy to test its extreme sensitivity. To verify whether it has energetic properties, we progressively increased the impact energy until it exploded and ultimately measured an extreme impact sensitivity of 75 J (Table. 1). The material exhibits insensitivity to impacts but not complete non-sensitivity. This result proves its energetic characteristics as an energetic material.

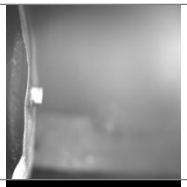
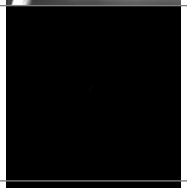
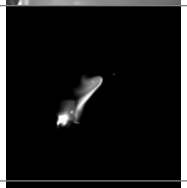
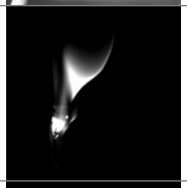
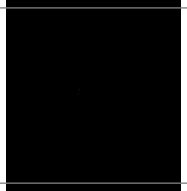
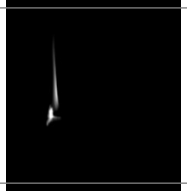
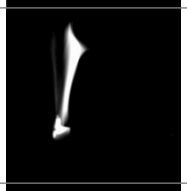
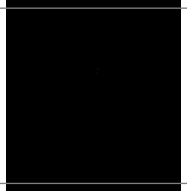
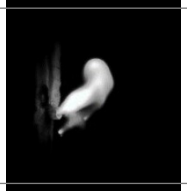
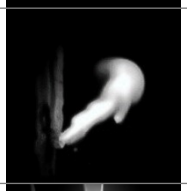
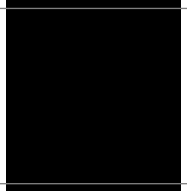
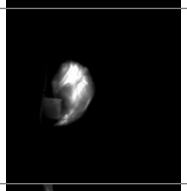
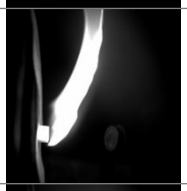
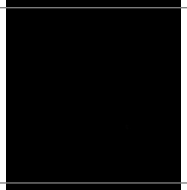
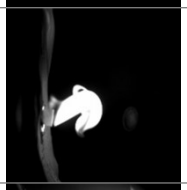
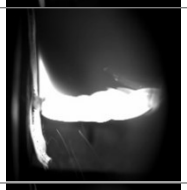
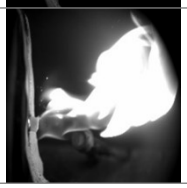
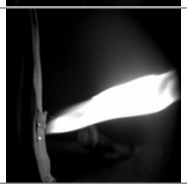
Table. 1 Extreme impact sensitivity testing of compound **1**

Experiment condition	Experimental result	Experimental analysis
0 J		Sample preparation
60 J		Repeat the experiment six times, Undecomposed, unexploded, increasing the impact energy, IS > 60 J
70 J		Repeat the experiment six times, Undecomposed, unexploded increasing the impact energy IS > 70 J
80 J		Exploded decreasing the impact energy 80 J > IS > 70 J
75 J		Exploded decreasing the impact energy 75 J > IS > 70 J
73 J		Repeat the experiment six times, Undecomposed, unexploded 75 J > IS > 73 J

2) Laser ignition experiment：To qualitatively assess its energetic properties, we observed combustion flames during laser ignition experiments (Table. 2). Comparing the combustion flames of compound **1** with non-energetic monomer 3,4-Diaminofurazan (DAF, which has the similar structure of furazan), lower-energy density energetic binder monomers (AMMO, BAMO), energetically similar materials such as trinitrotoluene (TNT), and higher-energy density energetic materials like octogen (HMX) and cyclonite (RDX). The results showed that different from non-energetic monomers (DAF) which only emitted smoke and melted without burning, and low-energy density energetic binder monomers (AMMO, BAMO) burned steadily

at a slow pace while high-energy monomers (RDX, HMX) exhibited intense jet-like flames. The flame intensity of compound **1** was moderate with slight splattering and had similar burning characteristics to TNT, which can also prove its energetic characteristics as an energetic material.

Table. 2 Laser ignition experiment of compound **1**

Sample	I	II	III	Experimental analysis
DAF				Emitted smoke and melted without burning
AMMO				Burned steadily at a slow pace
BAMO				Burned steadily at a slow pace
TNT				Flame intensity is moderate with slight splattering
Compound 1				Flame intensity is moderate with slight splattering
RDX				Exhibited intense jet-like flames
HMX				Exhibited intense jet-like flames

Reference

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[3] Lisa, M.; Edwards, J.; Johnson, E.; Sabatini, J.; Baran, P. Impact of Stereo- and Regiochemistry on energetic materials. *J Am Chem Soc* **2019**, *141*(32), 12531-12535. https://doi.org/10.1021/jacs.9b06961.