Supporting Information

Molecular Design of Fused 1,2,3,4-Tetrazine-Based High Performance Energetic Material with Zero Oxygen Balance

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S1. Experimental Sections

1.1 Safety Precaution

In this work, all new compounds are potential energetic materials that tend to explode under certain external stimuli. Therefore, the whole experimental process should be carried out by using proper safety equipment, such as safety shields, eye protection, and leather gloves.

1.2 General methods

^{1}H NMR and ^{13}C NMR spectra were recorded at 25 ºC on a Bruker 400 MHz spectrometer and 125 MHz spectrometer, respectively. Chemical shifts were reported in parts per million (ppm). The onset decomposition temperature was measured using a TA Instruments DSC25 differential scanning calorimeter at a heating rate of 5 °C min^{-1} under a dry nitrogen atmosphere. Infrared spectra (IR) were obtained on a PerkinElmer Spectrum BX FT-IR instrument equipped with an ATR unit at 25 °C. Impact and friction sensitivities were tested by a BAM fallhammer and friction tester. Densities were determined by conducting X-ray diffractions of all single crystals were carried out at room temperature on a Bruker D8 VENTURE diffractometer using Mo-Kα radiation (λ = 0.71073 Å). Integration and scaling of intensity data were performed using the SAINT program. Data were corrected for the effects of absorption using SADABS. The structures were solved by direct method and refined with full-matrix least-squares technique using SHELX-2014 software. Non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms were placed in calculated positions and refined with a riding model. The crystal structures were produced employing Mercury 2021.1.0 software.

1.3 Synthetic Procedures

5,5'-Bis(trinitromethyl)-2H,2'H-[3,3'-bi(1,2,4-triazole)]-2,2'-diamine (TBTD)

According to the literature, 5,5'-bis(trinitromethyl)-2*H*,2'*H*-3,3'-bi(1,2,4-triazole) was obtained.[1] Compound 5,5'-bis(trinitromethyl)-2*H*,2'*H*-3,3'-bi(1,2,4-triazole) (1.0 g, 2.3 mmol) was treated with 25% tetraethylammonium hydroxide in water (1.15 g, 2.0 eq). The mixture was stirred for 30 minutes at room temperature, and the water was removed by rotary evaporation and dissolved in acetonitrile (10 mL). Toluenesulfonyl-O-hydroxylamine (1.08 g, 2.5 eq) was added to dichloromethane (10 mL) at -5°C and added to the reaction mixture portionwise over 5min. The system continued to react for 24 hours, remained at this temperature. TLC monitoring and after the reaction, the solvent was evaporated. Collecting the crude products, the crude amide was purified by column chromatography on silica gel eluting with dichloromethane, which gave the title compounds TBTD in 58% isolated yield (0.62 g). **^{1}H NMR** (400 MHz, CD_3CN) δ 6.58 (s, 2H). **^{13}C NMR** (100 MHz, CD_3CN) δ 145.2, 142.2. **^{15}N NMR** (50.68 MHz, CD_3CN) δ -32.95, -64.68, -120.84, -136.42, -292.89. **Elem. Anal. Calc** for $C_6H_4N_{14}O_{12}$: N%: 42.25, C%: 15.53, H%: 0.87; found: N%: 42.13, C%: 15.67, H%: 0.91.

2,9-Bis(trinitromethyl)bis([1,2,4]triazolo)[1,5-d:5',1'-f][1,2,3,4]tetrazine (TNF)

TBTD (0.2 g, 0.43 mmol) was dissolved in acetonitrile (10 mL) at -5°C, and treated dropwise with

tert-butyl hypochlorite (0.12 g, 2.5 eq). TLC monitoring and after the reaction, the solvent was evaporated. Collecting the crude products, the crude amide was purified by column chromatography on silica gel eluting with dichloromethane, which gave the title compounds TNF in 78% isolated yield (0.15 g). **^{13}C NMR** (100 MHz, CD_3CN) δ 171.6, 151.9, 139.6. **^{15}N NMR** (50.68 MHz, CD_3CN) δ -21.40, -37.10, -79.22, -84.22, -111.61, -134.14, -130.48, -137.59. **Elem. Anal. Calc** for $C_4N_{14}O_{12}$: N%: 42.62, C%: 15.66; found: N%: 42.46, C%: 15.57.

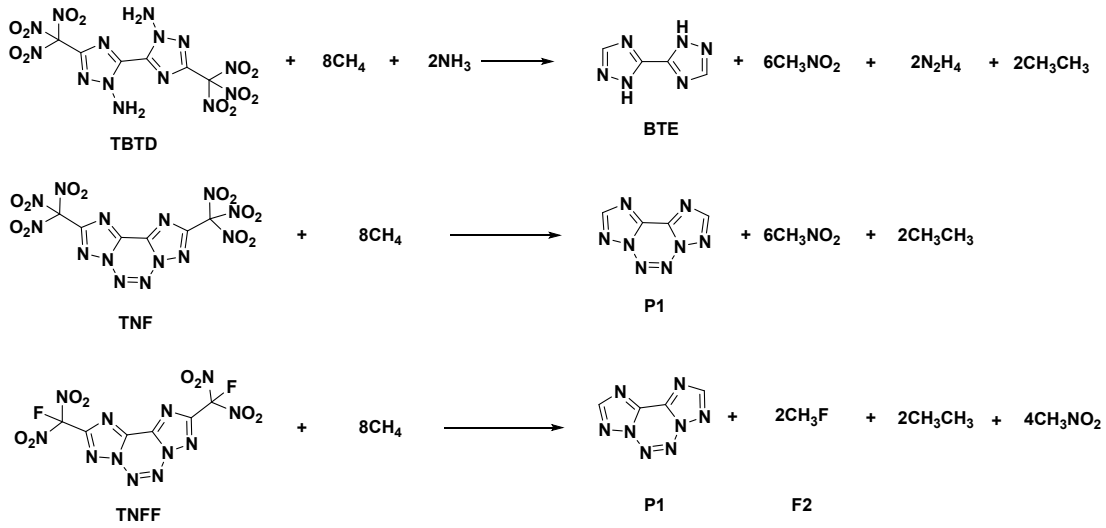
2,9-Bis(fluorodinitromethyl)bis([1,2,4]triazolo)[1,5-d:5',1'-f][1,2,3,4]tetrazine (TNFF)

At -5 °C, TNF (0.5 g, 1.0 mmol) was added to the mixture of acetonitrile and methanol. After the system's stable temperature, potassium iodide (4.5 eq, 0.81g) was slowly added in batches, and the reaction temperature was maintained for 3 hours. The system was filtered, and the filter cake was washed with methanol and dried to obtain potassium salt compounds. Add 0.2 g of potassium salt compounds to acetonitrile at room temperature. Weigh the selective fluorine reagent (selectfluor, 1.0 eq, 0.15g) and add it slowly (*The addition of reagents too fast will lead to low yield*). After an overnight reaction at room temperature, TLC monitoring and filtration column chromatography obtained the target compound TNFF (0.13 g, 73%). **^{19}F NMR** (377 MHz, CD_3CN) δ -99.73. **^{13}C NMR** (100 MHz, CD_3CN) δ 153.09, 152.83, 139.43. **^{15}N NMR** (50.68 MHz, CD_3CN) δ -22.37, -27.76, -28.15, -83.39, -111.93, -136.42, -138.37.

S2. Computational Details

Theoretical calculations were performed by using the Gaussian 09 suite of programs.[2, 3] Gas phase heats of formation of the title compounds were computed based on an isodesmic reaction (Scheme S1). The enthalpy of reaction was carried out by combining the M062X/6-311++G** energy difference for the reactions, the scaled zero-point energies (ZPE), values of thermal correction (HT), and other thermal factors. The solid-state heats of formation were obtained by employing Trouton's rule according to equation 1 (T represents either melting point or decomposition temperature when no melting occurs prior to decomposition).[4]

$$\Delta H_{sub} = 188/J\ mol^{-1}\ K^{-1} \times T \quad (1)$$



Scheme S1. Isodesmic reactions for **TBTD, TNF** and **TNFF**.

Species	ZPE	H_{corr}	E_0	Corrected E_0	ΔH_f (kJ/mol)
Tetra	0.086661	0.094693	-591.5231	-591.4319	816.48574
BTE	0.100371	0.108321	-483.3296	-483.2253	382.25163
CH_3CH_3	0.074397	0.078825	-79.80667	-79.73082	-86.07562
N_2H_4	0.053277	0.057483	-111.8626	-111.8072	99.122171
CH_3F	0.039006	0.042862	-139.7207	-139.6794	-234.3
CH_3NO_2	0.049673	0.054999	-245.0103	-244.9573	-88.06903
NH_3	0.034305	0.038114	-56.55195	-56.51521	-45.09579
CH_4	0.044599	0.048412	-40.50181	-40.45518	-74.6
TBTD	0.200425	0.229912	-1899.554	-1899.332	676.5034367
TNF	0.153087	0.180152	-1897.088	-1896.914	929.2759303
TNFF	0.134116	0.157461	-1686.62	-1686.468	348.23843

Table S1. The scaled zero point energies (***ZPE***), values of thermal correction (***H_{corr}***), total energy (***E_0***) and heats of formation (***HOF***)

S3. Crystallographic data for TBTD, TNF and TNFF.

CCDC No.	2252071	2257694	2322374
Empirical formula	$C_6H_4N_{14}O_{12}$	$C_6N_{14}O_{12}$	$C_6F_2N_{12}O_8$
Formula weight	464.23	460.2	406.18
Temperature/K	296.15	296(2)	296
Crystal system	monoclinic	triclinic	triclinic
Space group	$P2_1/n$	P-1	P-1
a/Å	11.453(3)	5.859(5)	5.7826(2)
b/Å	10.262(2)	11.684(10)	10.8042(3)
c/Å	14.329(3)	12.127(10)	12.2660(4)
α/°	90	100.143(9)	108.876(3)
β/°	97.651(6)	98.783(9)	90.143(3)
γ/°	90	100.825(9)	105.181(3)
Volume/Å^3	1669.2(6)	787.8(11)	696.62(4)
Z	4	2	2
ρ_{calc}g/cm^3	1.847	1.94	1.936
μ/mm^{-1}	0.176	0.186	1.735
F(000)	936	460	404
Crystal size/mm^3	0.2 × 0.2 × 0.2	0.19 × 0.16 × 0.15	0.29 × 0.19 × 0.17
Goodness-of-fit on F^2	1.057	1.005	1.071
Final R indexes	R_1 = 0.1054, wR_2 =	R_1 = 0.0647, wR_2 =	R_1 = 0.0513, wR_2 =

[I>=2σ (I)]	0.2838	0.1647	0.1554
Final R indexes [all data]	R_1 = 0.1726, wR_2 = 0.3267	R_1 = 0.1142, wR_2 = 0.1998	R_1 = 0.0569, wR_2 = 0.1633

S4. TG-DSC data of new compounds.

The decomposition temperature was investigated using TG-DSC at a heating rate of 5 °C·min^{-1} under dry nitrogen atmosphere (50 mL·min^{-1}).

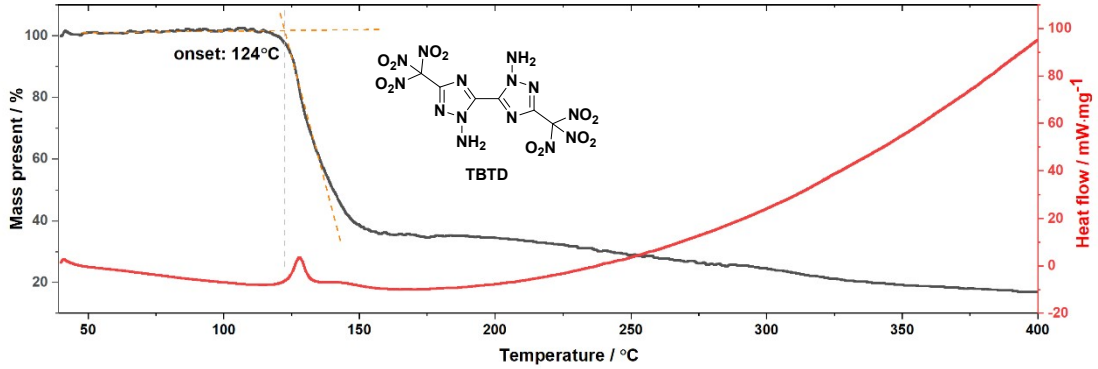


Figure S1. TG-DSC curves of TBTD

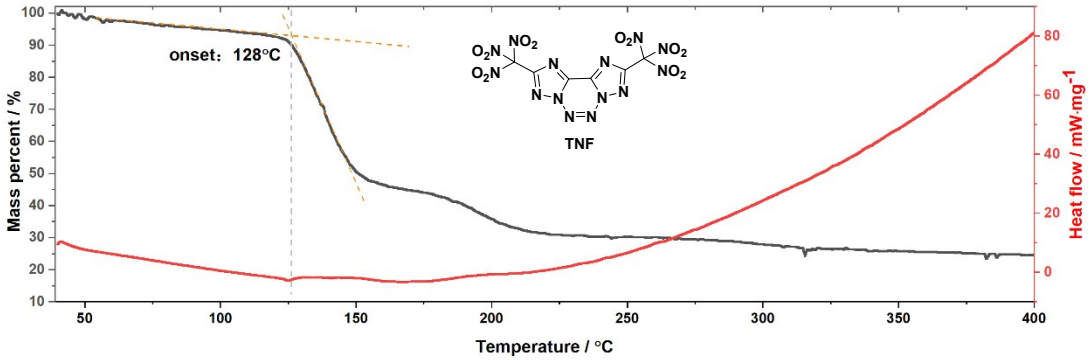


Figure S2. TG-DSC curves of TNF

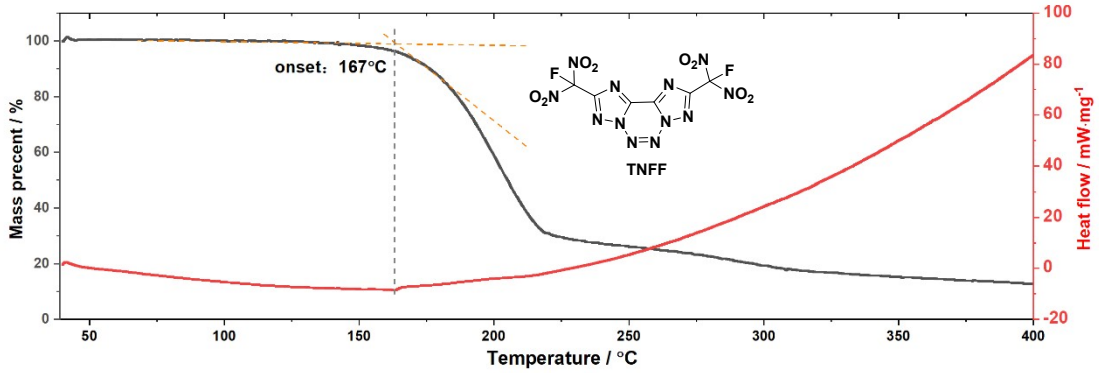


Figure S3. TG-DSC curves of TNFF

S5. NMR spectra for all new compounds.

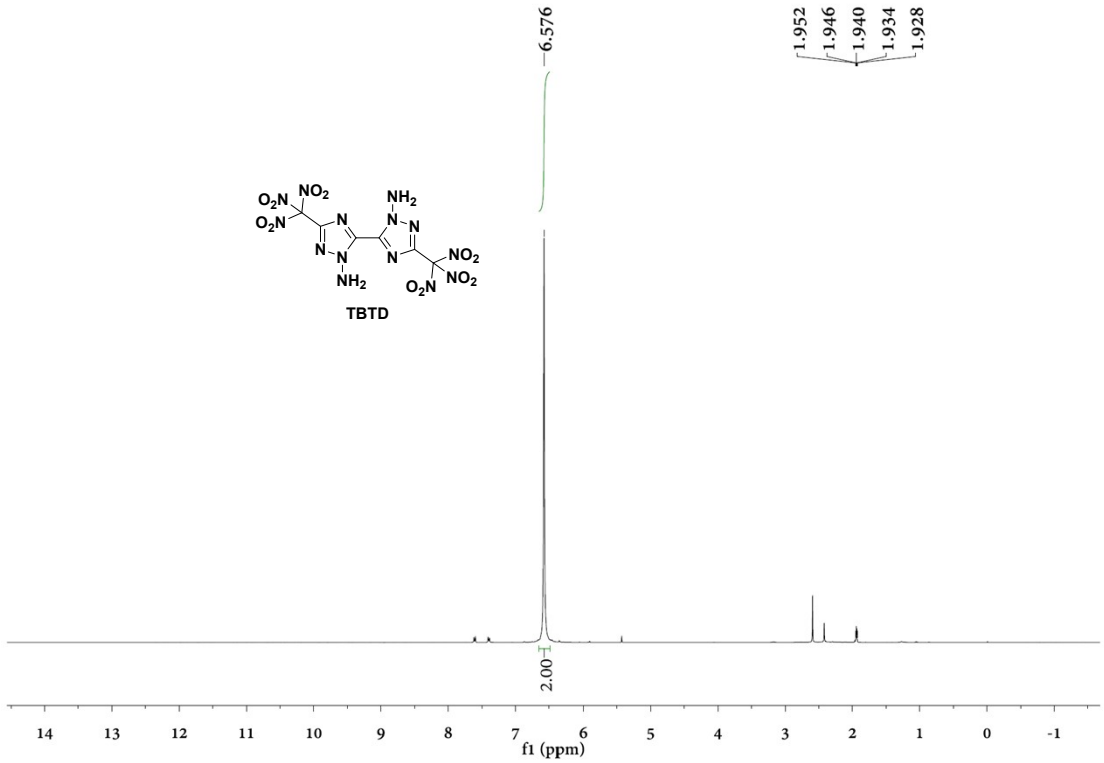


Figure S4. TBTD-^{1}HNMR

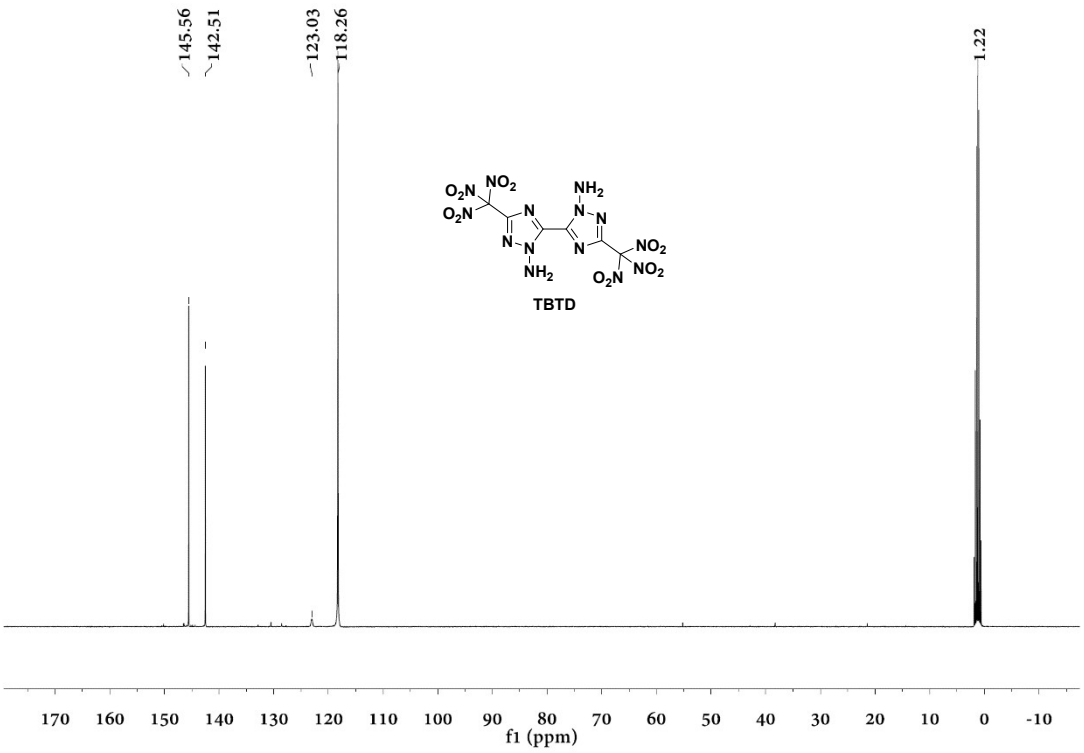


Figure S5. TBTD-^{13}CNMR

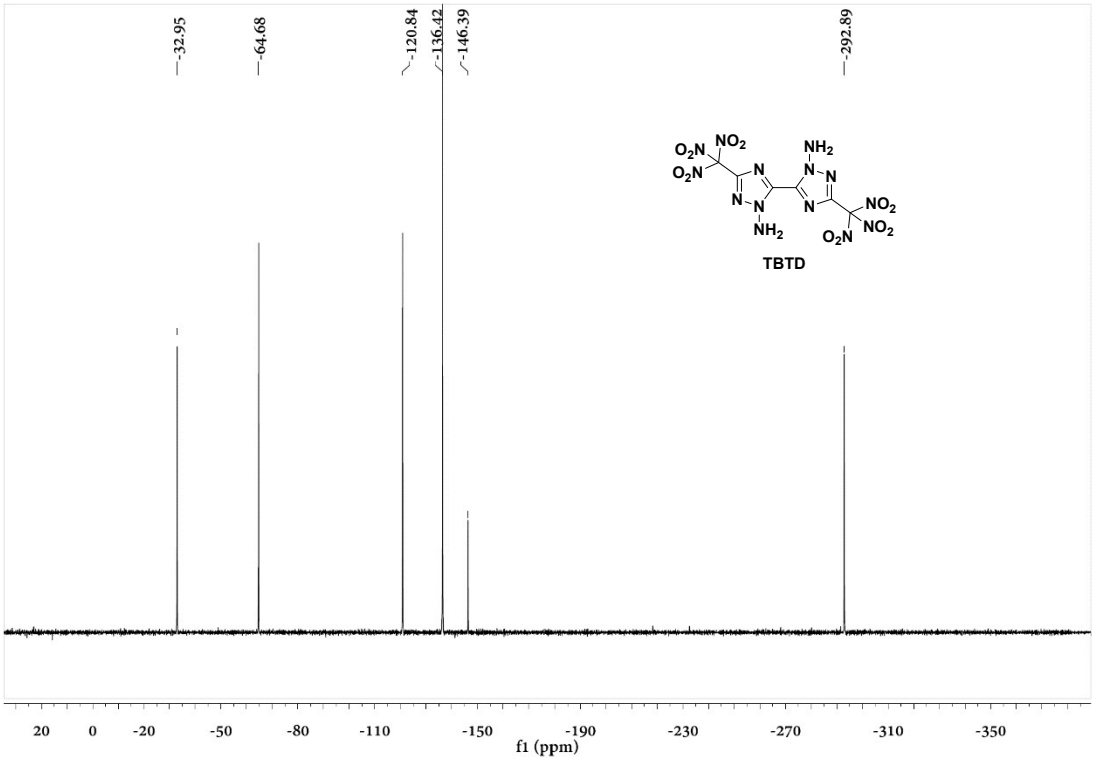


Figure S6. TBTD-^{15}NNMR

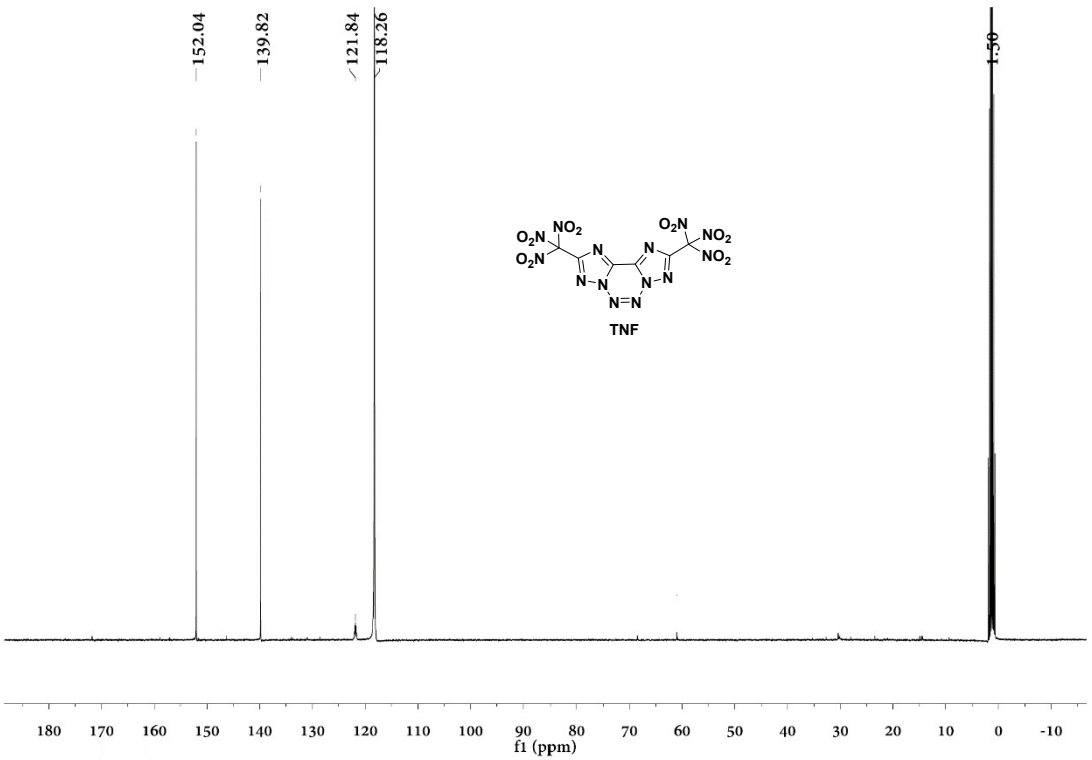


Figure S7. TNF-^{13}CNMR

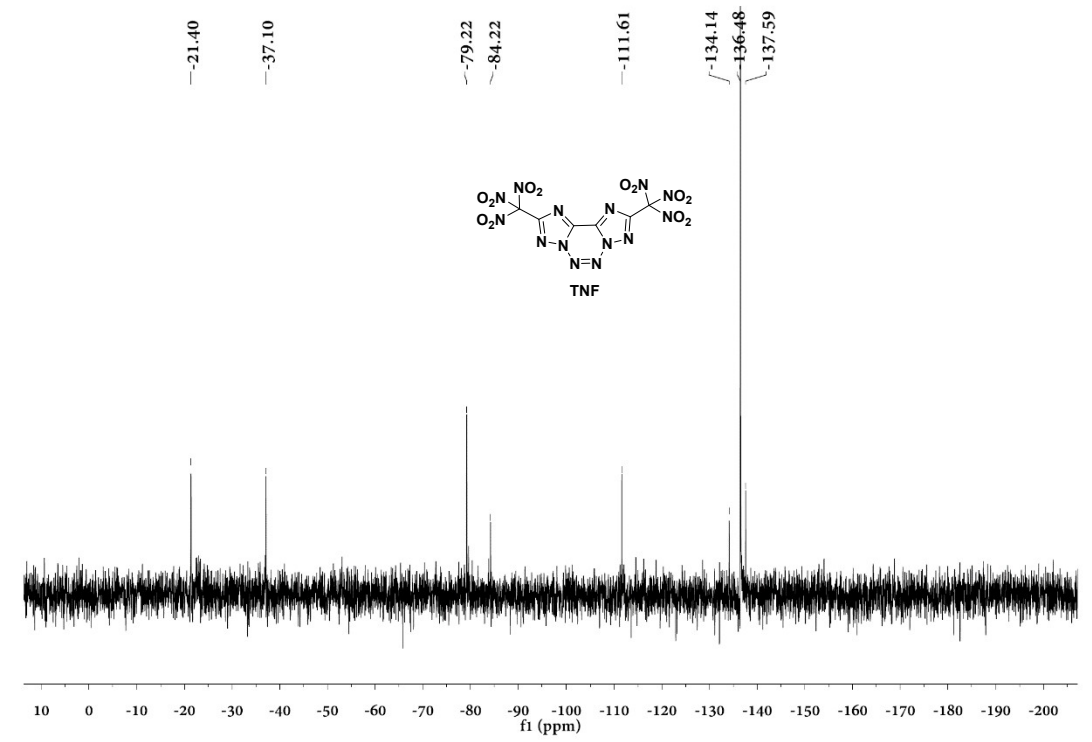


Figure S8. TNF-^{15}NNMR

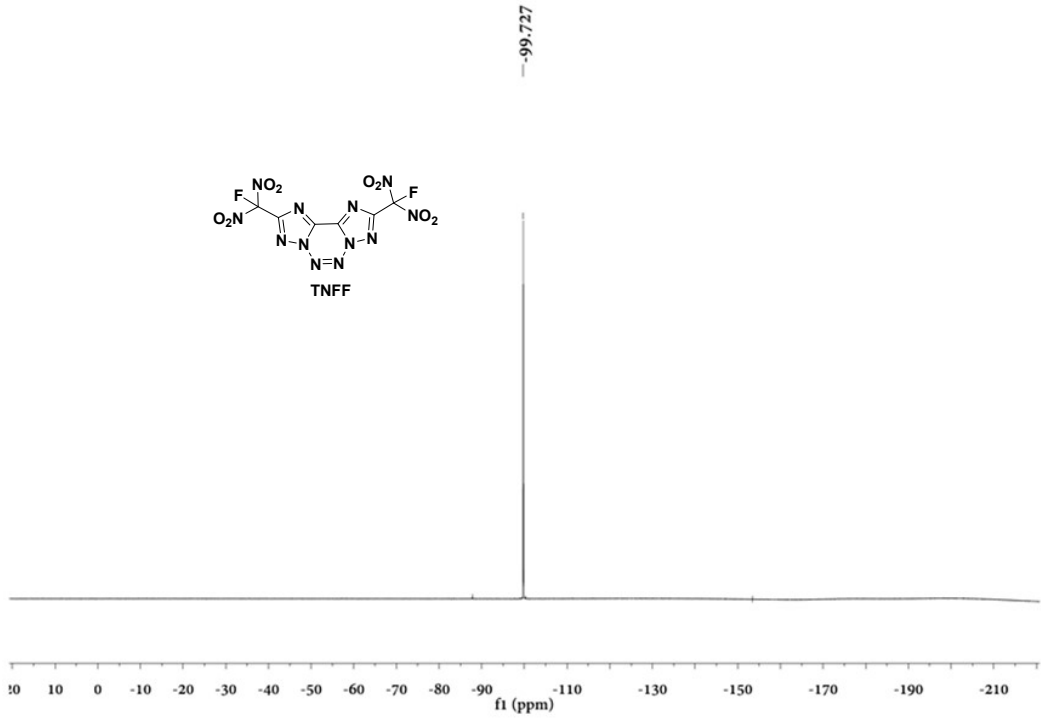


Figure S9. TNFF-^{19}FNMR

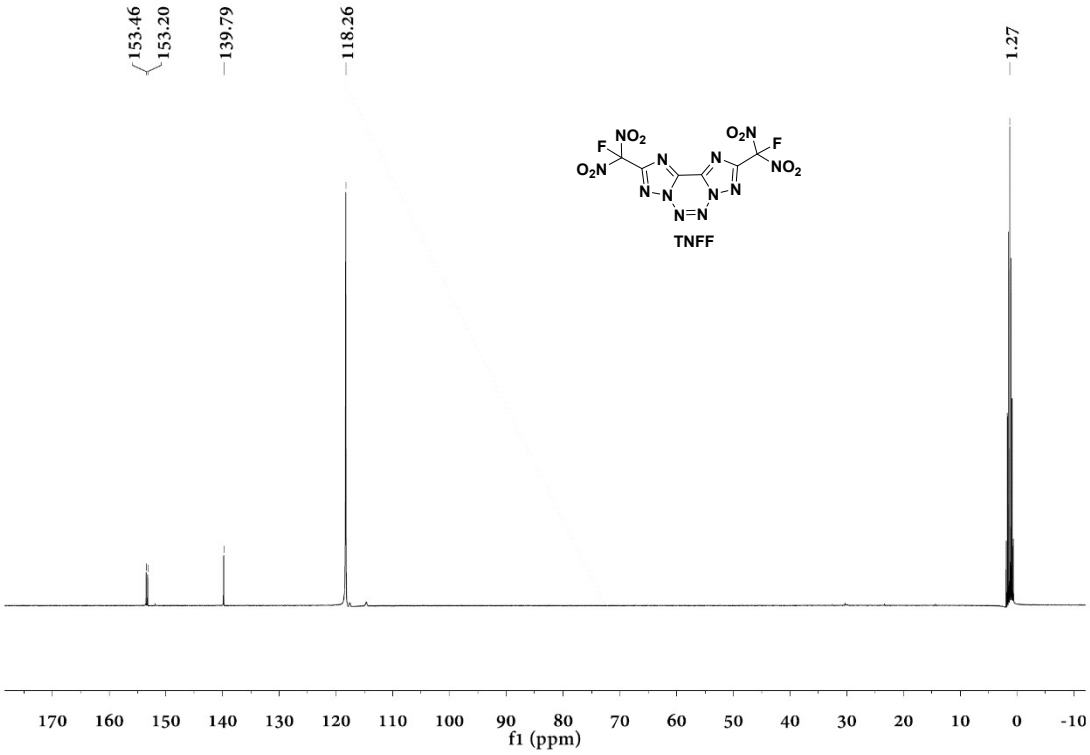


Figure S10. TNFF-^{13}CNMR

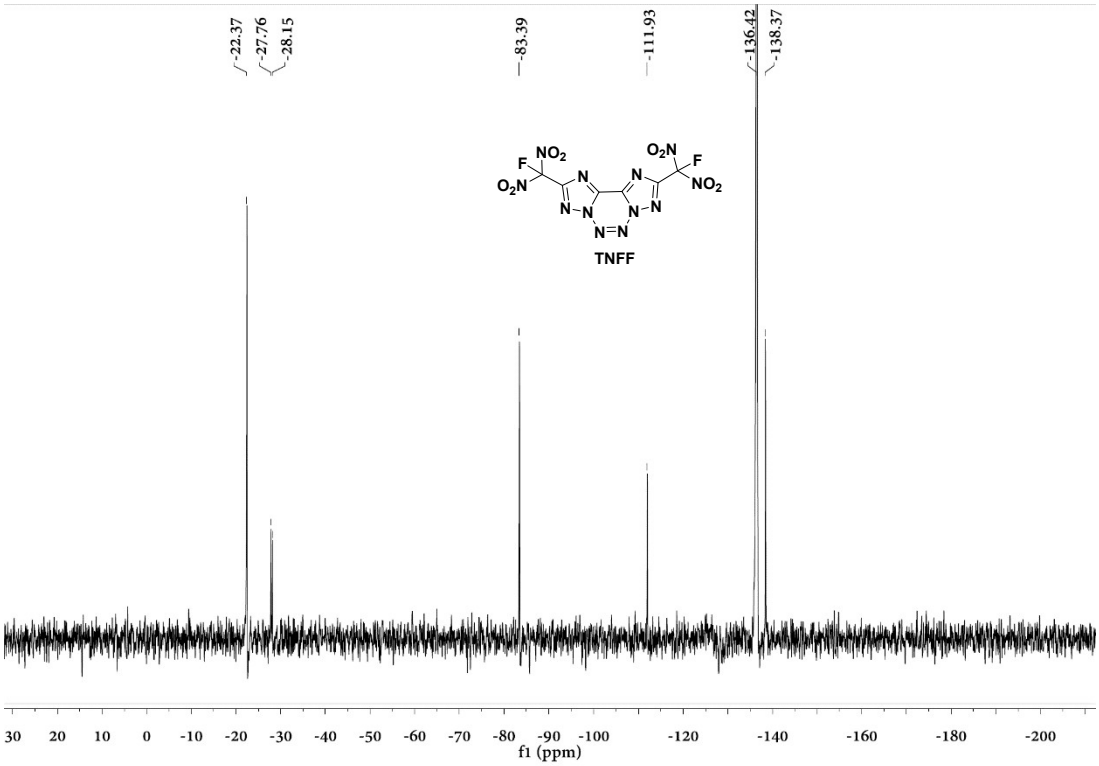


Figure S11. TNFF-^{15}NNMR

S6. IR spectra.

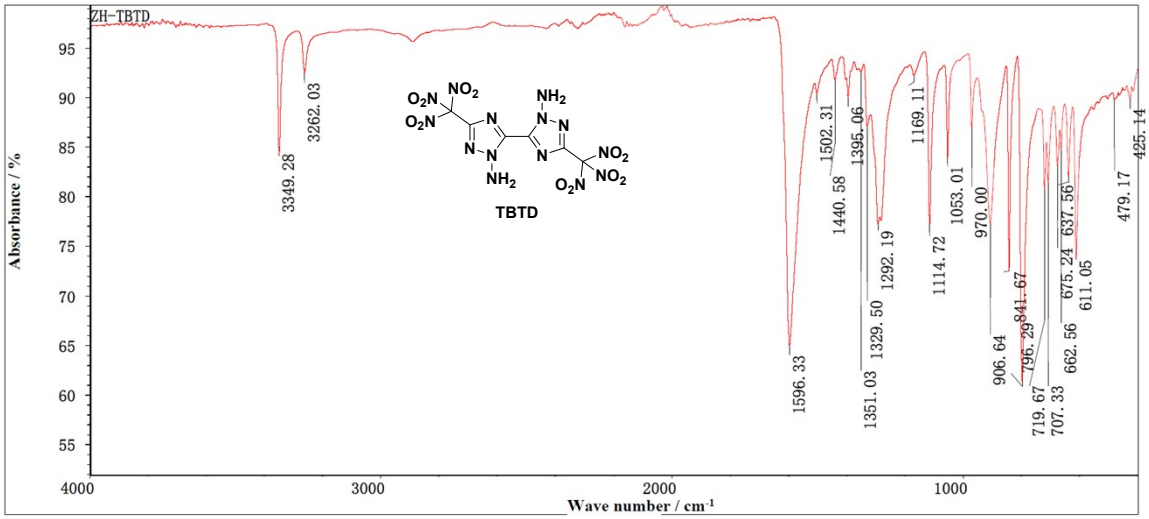


Figure S12. FT-IR curves of TBTD

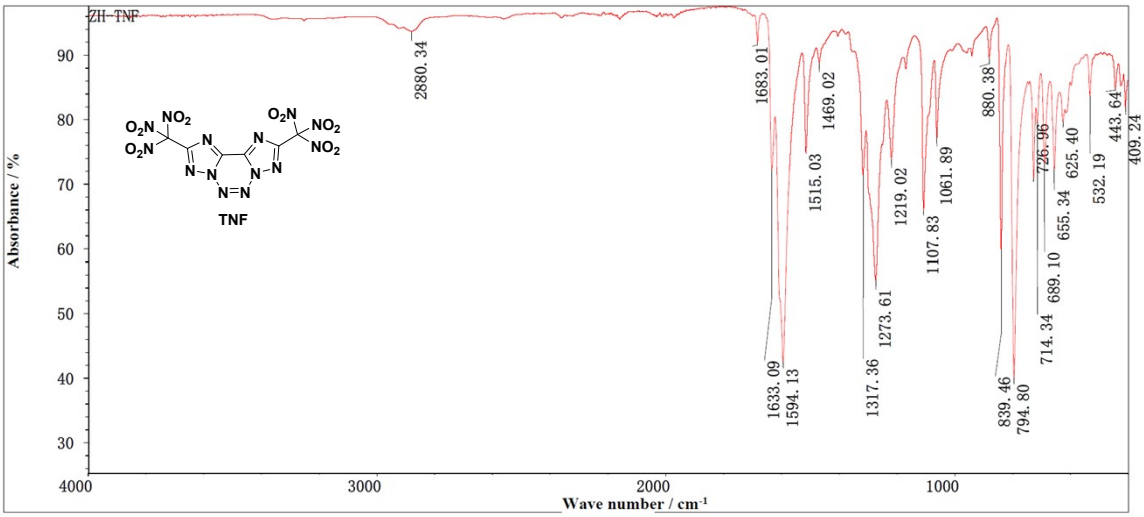


Figure S13. FT-IR curves of TNF

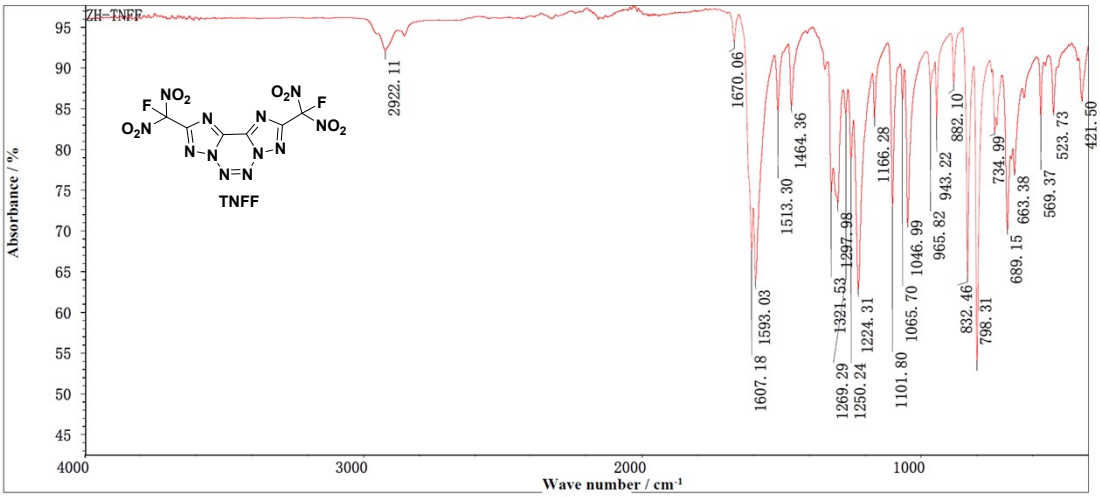
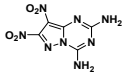
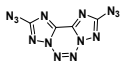
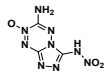
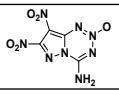
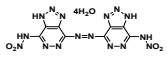
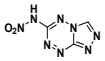
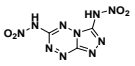
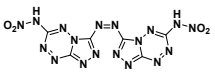
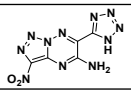
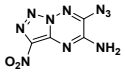
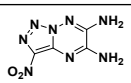
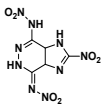
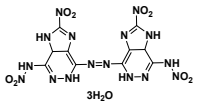
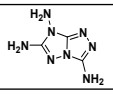
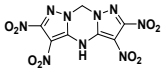
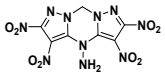
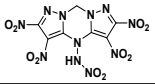


Figure S14. FT-IR curves of TNFF

S7. Oxygen balance and detonation properties of reported fused-ring energetic compounds.

Number	Structure	Oxygen balance	Detonation velocity	Detonation pressure	Reference
1		-53.30	8422	29.8	5
2		-84.14	8421	26.0	6

3		-52.43	8773	31.1	7
4		-33.78	9047	35.1	8
5		-26.43	9317	39.3	8
6		-26.43	9317	39.3	9
7		-42.77	8875	34.5	10
8		-65.26	-	-	10
9		-43.93	8621	30.4	11
10		-19.83	9301	38.3	11
11		-36.90	9500	39.8	11
12		-61.01	8423	27.3	12
13		-50.42	8912	32.2	12
14		-65.26	8623	28.4	12
15		-36.22	8568	31.5	13
16		-53.30	8263	28.6	13
17		-93.42	8580	25.9	14
18		-35.17	8792	34.3	15
19		-35.94	8356	29.6	15
20		-21.94	9226	38.8	15
21		-47.97	8250	27.4	16
22		-5.52	9460	40.9	16

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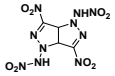
24		-9.99	9507	41.8	16
25		-39.44	9120	35.1	17
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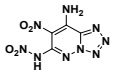
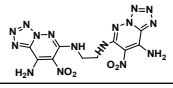
27		-52.76	8528	29.4	19
28		-71.99	8102	25.0	19
29		-36.50	8926	33.7	20
30		-80.33	8809	29.3	20
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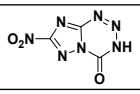
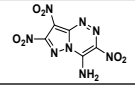
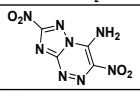
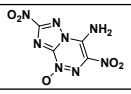
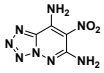
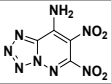
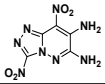
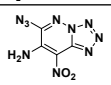
32		-30.59	-	-	22
33		-29.62	8998	36.04	23
34		-35.38	8700	32	24
35		-26.43	8970	35.4	24
36		-65.26	8899	30.3	25
37		-35.38	9021	34.8	25
38		-26.65	8994	34.1	26
39		-42.08	8819	32.4	26
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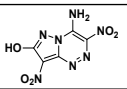
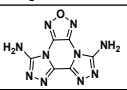
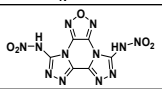
42		-43.13	8538	30.4	28
43		-89.59	7980	23.7	29
44		-37.25	9241	37.8	29

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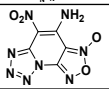
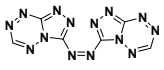
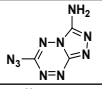
48		-47.03	8838	36.01	33
49		-76.99	9200	34.8	34
50		-62.88	8581	28.5	34
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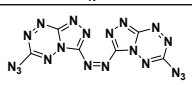
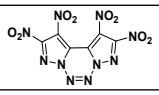
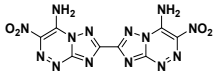
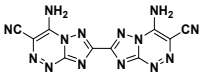
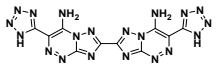
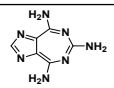
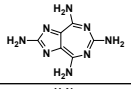
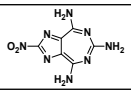
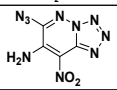
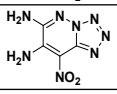
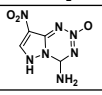
52		-54.51	9149	34.3	34
53		-18.82	9631	44	35
54		-62.19	8837	32.9	36
55		-109.92	7769	21.9	36
56		-90.57	8501	27.5	36
57		-139.98	6747	14.1	37
58		-133.20	7000	18.5	37
59		-93.63	7600	19.9	37
60		-50.42	8746	31.5	38
61		-57.11	8434	27.7	38
62		-60.26	8935	34.5	39
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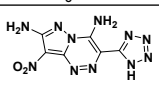
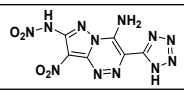
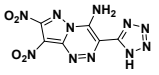
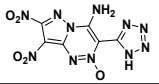
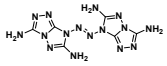
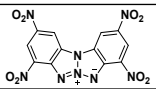
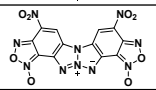
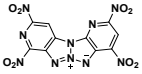
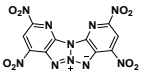
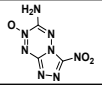
64		-75.97	7853	24.5	40
65		-76.58	8657	27.82	41
66		-51.92	8990	33.45	41

67		-51.85	8755	31.67	41
68		-43.99	8851	32.89	41
69		-84.14	-	-	42
70		-74.20	7060	20.2	43
71		-65.67	7520	24.5	43
72		-53.31	8010	29.2	43
73		-53.31	8010	29.2	43
74		-32.31	9384	39.1	44
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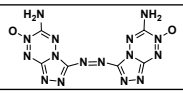
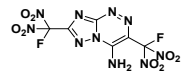
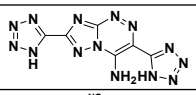
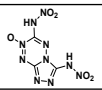
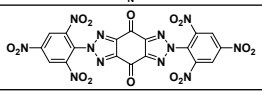
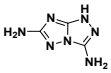
76		-57.80	9008	28.8	44
77		-21.04	8883	34.8	45
78		-82.29	7658	19.8	45
79		-12.40	9503	41	46
80		-62.71	7800	29	47
81		-97.76	7891	21	48
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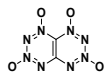
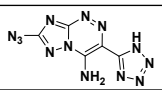
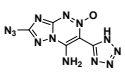
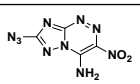
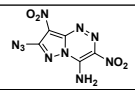
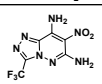
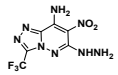
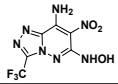
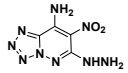
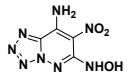
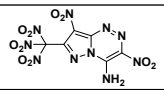
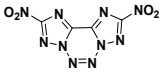
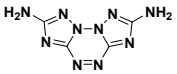
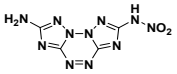
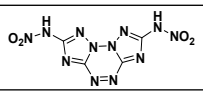
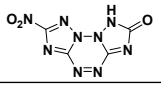
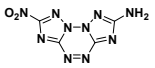
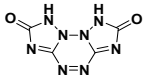
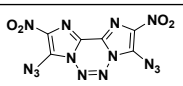
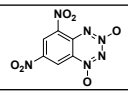
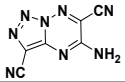
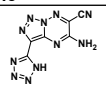
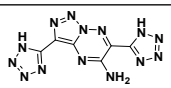
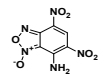
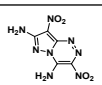
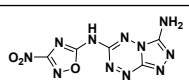
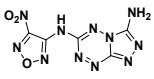
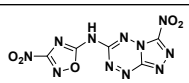
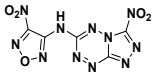
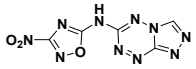
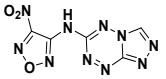
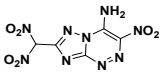
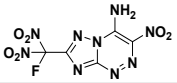
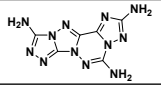
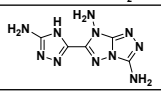
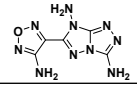
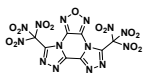
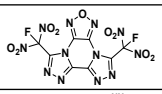
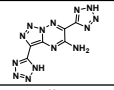
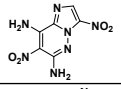
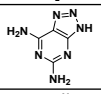
83		-8.00	9710	43.2	50
84		-75.05	8338	26.9	51
85		-64.33	8926	32.1	51
86		-50.42	9029	34.3	51
87		-42.08	8807	32.9	51
88		-72.97	6865	17.9	52

89		-71.90	7420	21.1	[52]
90		-63.05	7480	23.8	[52]
91		-64.41	8833	29.1	[52]
92		-52.80	8797	31.3	[52]
93		-12.83	9492	41	[53]
94		-25.39	9400	38	[54]
95		-83.27	8340	29.2	[55]
96		-50.60	8940	38	[55]
97		-28.35	9370	45.9	[55]
98		-39.44	8855	38.7	[55]
99		-50.42	8930	38.1	[55]
100		-57.70	8360	31.8	[55]
101		-38.54	9256	36.7	[56]
102		-44.07	8411	33	[57]
103		-111.75	6648	16.27	[58]
104		-94.25	7005	16.91	[58]
105		-82.33	7723	31.03	[58]
106			-	-	[59]
107		-53.30	8727	32.6	[60]
108		-51.29	8555	30	[61]
109		-51.29	8755	32.1	[61]
110		-29.82	8976	34.6	[61]

111		-29.82	9182	36.7	61
112		-51.17	8069	25.7	61
113		-51.17	8532	29.9	61
114		-30.86	8597	31.9	62
115		-26.39	8547	32.5	62
116		-97.48	8262	24.6	63
117		-97.65	8273	24.3	64
118		-32.41	8530	27.3	64
119		-9.60	9010	35	65
120		-25.10	8590	33	65
121		-82.33	8196	24.2	66
123		-70.25	8336	27.3	67
124		-111.16	7426	18.16	68
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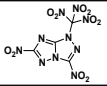
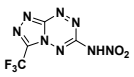
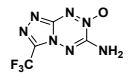
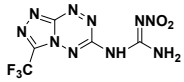
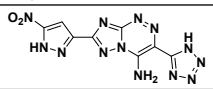
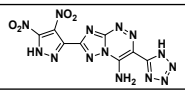
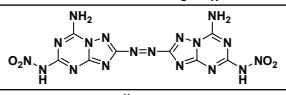
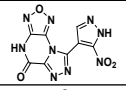
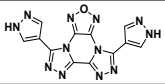
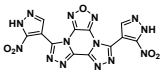
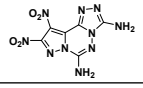
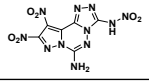
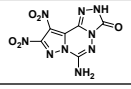
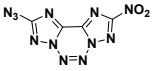
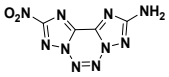
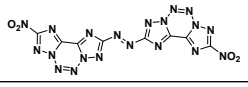
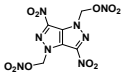
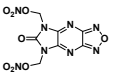
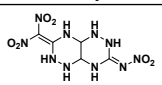
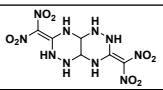
126		9.19	9199	37.1	69
127		-41.58	7179	20.76	70
128		-57.91	6925	18.81	70
129		-52.03	7877	26.8	70
130		-83.75	8322	26.7	71
131		-62.16	8710	31.5	71
132		-57.38	8084	24.9	72
133		-115.14	7080	17.42	73

134		-104.84	6919	16.98	[73]
135		-74.70	8047	23.61	[73]
136		-124.45	7384	19.37	[73]
137		-79.20	8004	24.18	[73]
138		-108.38	7160	19.41	[74]
139		-28.56	8376	31.2	[74]
141		-62.07	8644	30.9	[75]
142		-78.71	8817	32	[75]
143		-57.11	8855	33.6	[76]
144		-36.91	9202	35.5	[76]
145		-48.37	8841	34.2	[76]
146		-38.69	8855	31.7	
147		-50.42	8544	29.1	
148		-43.61	9197	35.6	
149		-18.38	8674	33.1	[77]
150		-30.37	8669	33.4	[77]
151		-39.01	8057	27.3	[77]
152		-51.92	8292	27.6	[77]
153		-69.52	8323	27.8	[77]
154		-42.08	8492	29.4	[78]
155		-36.76	8862	35.2	[78]
156		12.90	9182	37.8	[79]

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