

# **Reverse design of high-detonation-velocity organic energetic compounds based on an accurate BPNN with wide applicability**

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# Qiong Wu and Guan-chen Dong contributed equally to this paper;

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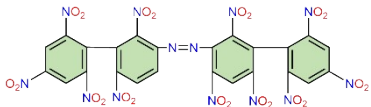




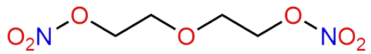
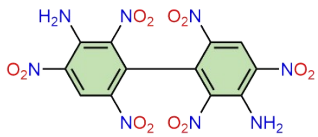
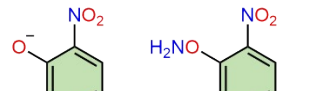
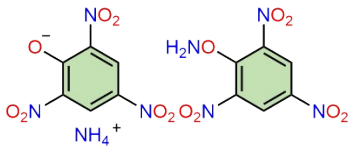
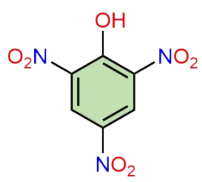

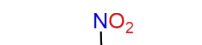

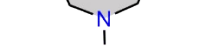

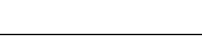
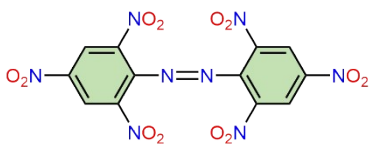
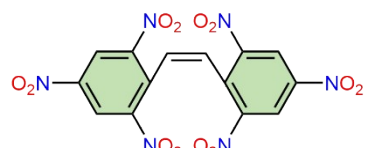
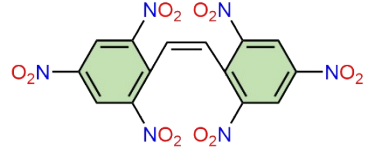
Email address: tanlh@njust.edu.cn (Ling-hua Tan) and lvjing9487@163.com (Jing Lv)

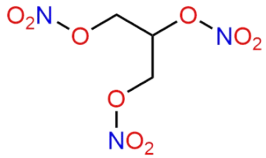
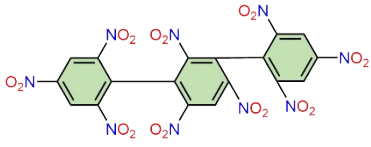
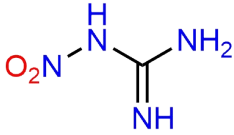
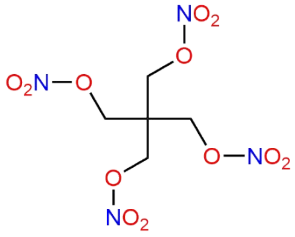
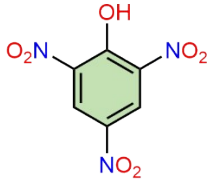
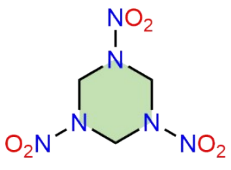
## Supplementary Information

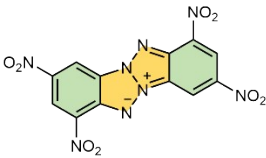

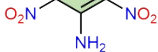
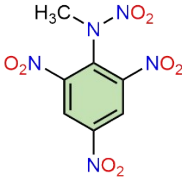
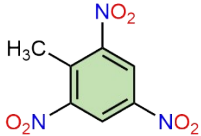
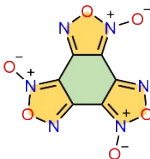
Table S1: The initial dataset for the ML; Table S2: The Pearson's correlation coefficients of descriptors for detonation velocity ( $D$ ); Table S3: The setting of the RF model; Table S4: The setting of the SVR model;

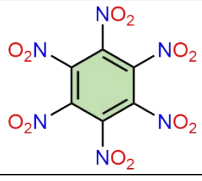
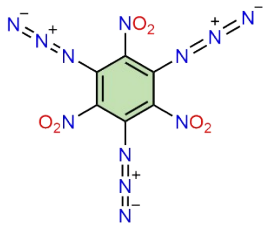
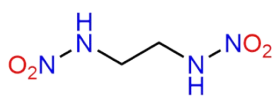
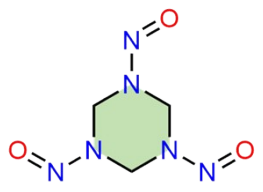
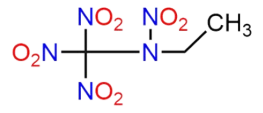
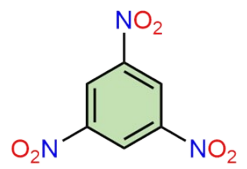
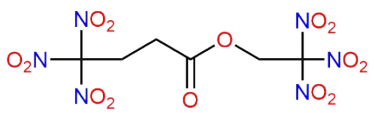
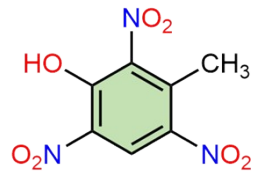
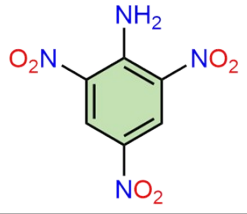
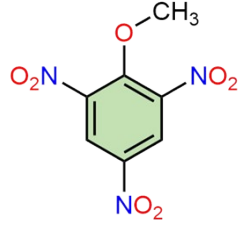
Table S5: The setting of the MLP model; Table S6: The setting of the BPNN model; Table S7: The predicted  $D$  values of compounds in the test set; Table S8: The dataset of new test set 1; Table S9: The new dataset of new modified ML model; Table S10: The dataset of new energetic compounds; Table S11: The predicted  $D$  values of isomers; Figure S1: The loss function of ML models; Figure S2: The relationships between  $nC/V_m$ ,  $nH/V_m$ ,  $V_m$ ,  $M$ ,  $OB$ ,  $F$  and experimental  $D$ ; Figure S3: The scatter graph of the training/test set; Figure S4: The predicted residual plot of models for the  $D$ ; Figure S5: The Williams plot of models for the test set of the  $D$ .

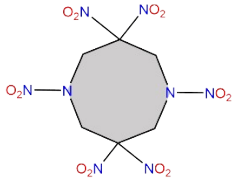
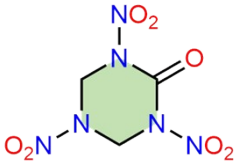
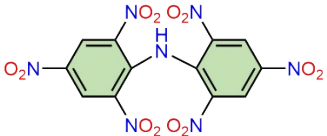
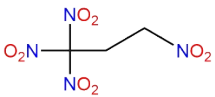
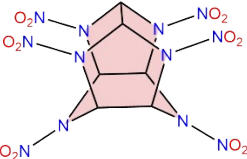

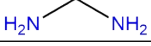
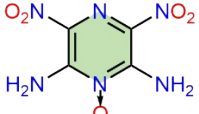
**Table S1.** The initial dataset for the ML.<sup>1</sup>

NO.	Structure	$\rho$	$nO/V_m$	$nN/V_m$	$nC/V_m$	$nH/V_m$	$V_m$	$M$	OB	$F$
<b>Training set</b>										
1		1.64	0.045	0.026	0.045	0.011	532.90	874.0	-0.494	5.47
2		1.78	0.049	0.029	0.049	0.012	490.99	874.0	-0.494	5.47
3		1.80	0.044	0.037	0.044	0.037	135.02	243.0	-0.560	4.83
4		1.43	0.035	0.029	0.035	0.029	170.32	243.0	-0.560	4.83
5		1.38	0.034	0.028	0.034	0.028	176.37	243.0	-0.560	4.83
6		1.38	0.049	0.014	0.028	0.056	142.05	196.0	-0.408	5.86
7		1.76	0.047	0.031	0.047	0.023	257.97	454.0	-0.529	5.22
8		1.55	0.044	0.025	0.038	0.038	158.73	246.0	-0.520	5.15
9		1.48	0.042	0.024	0.036	0.036	166.24	246.0	-0.520	5.15
10		1.63	0.046	0.027	0.040	0.040	150.94	246.0	-0.520	5.15
11		1.89	0.051	0.051	0.026	0.051	156.66	296.1	-0.216	6.08
12		1.60	0.043	0.043	0.022	0.043	185.05	296.1	-0.216	6.08
13		1.40	0.038	0.038	0.019	0.038	211.49	296.1	-0.216	6.08
14		1.20	0.032	0.032	0.016	0.032	246.73	296.1	-0.216	6.08
15		1.00	0.027	0.027	0.014	0.027	296.08	296.1	-0.216	6.08
16		0.75	0.020	0.020	0.010	0.020	394.77	296.1	-0.216	6.08
17		1.60	0.042	0.028	0.042	0.014	282.50	452.0	-0.496	5.27
18		1.60	0.043	0.021	0.050	0.021	281.25	450.0	-0.676	5.21
19		1.70	0.045	0.023	0.053	0.023	264.71	450.0	-0.676	5.21

20		1.60	0.063	0.021	0.021	0.035	141.87	227.0	0.035	7.29
21		1.70	0.048	0.024	0.048	0.013	373.51	635.0	-0.517	5.64
22		1.78	0.034	0.068	0.017	0.068	58.46	104.1	-0.308	4.20
23		1.62	0.031	0.062	0.016	0.062	64.23	104.1	-0.308	4.20
24		1.55	0.030	0.060	0.015	0.060	67.14	874.0	-0.308	4.20
25		1.55	0.030	0.060	0.015	0.060	67.14	874.0	-0.308	4.20
26		1.76	0.067	0.022	0.028	0.045	179.55	243.0	-0.101	6.92
27		1.70	0.065	0.022	0.027	0.043	185.88	243.0	-0.101	6.92
28		1.67	0.063	0.021	0.026	0.042	189.22	243.0	-0.101	6.92
29		1.60	0.061	0.020	0.025	0.041	197.50	104.1	-0.101	6.92
30		1.45	0.055	0.018	0.023	0.037	217.93	104.1	-0.101	6.92
31		1.23	0.047	0.016	0.019	0.031	256.91	316.0	-0.101	6.92
32		0.99	0.038	0.013	0.016	0.025	319.19	316.0	-0.101	6.92
33		0.88	0.033	0.011	0.014	0.022	359.09	316.0	-0.101	6.92
34		0.50	0.019	0.006	0.008	0.013	632.00	316.0	-0.101	6.92
35		0.48	0.018	0.006	0.008	0.012	658.33	316.0	-0.101	6.92
36		0.30	0.011	0.004	0.005	0.008	1053.33	316.0	-0.101	6.92
37		0.25	0.009	0.003	0.004	0.006	1264.00	316.0	-0.101	6.92
38		1.76	0.054	0.023	0.046	0.023	130.11	316.0	-0.454	5.61
39		1.71	0.052	0.022	0.045	0.022	133.91	316.0	-0.454	5.61
40		1.60	0.049	0.021	0.042	0.021	143.12	316.0	-0.454	5.61
41		1.70	0.052	0.022	0.045	0.022	134.70	316.0	-0.454	5.61
42		1.80	0.049	0.049	0.024	0.049	123.37	316.0	-0.216	6.08
43		1.77	0.048	0.048	0.024	0.048	125.46	229.0	-0.216	6.08
44		1.77	0.048	0.048	0.024	0.048	125.81	229.0	-0.216	6.08
45		1.72	0.046	0.046	0.023	0.046	129.10	229.0	-0.216	6.08
46		1.70	0.046	0.046	0.023	0.046	130.62	229.0	-0.216	6.08

47		1.66	0.045	0.045	0.022	0.045	133.77	222.1	-0.216	6.08
48		1.60	0.043	0.043	0.022	0.043	138.79	222.1	-0.216	6.08
49		1.46	0.039	0.039	0.020	0.039	152.10	222.1	-0.216	6.08
50		1.40	0.038	0.038	0.019	0.038	158.61	222.1	-0.216	6.08
51		1.29	0.035	0.035	0.017	0.035	172.14	222.1	-0.216	6.08
52		1.20	0.032	0.032	0.016	0.032	185.05	222.1	-0.216	6.08
53		1.10	0.030	0.030	0.015	0.030	201.87	222.1	-0.216	6.08
54		1.00	0.027	0.027	0.014	0.027	222.06	222.1	-0.216	6.08
55		0.95	0.026	0.026	0.013	0.026	233.75	222.1	-0.216	6.08
56		0.70	0.019	0.019	0.009	0.019	317.23	222.1	-0.216	6.08
57		0.56	0.015	0.015	0.008	0.015	396.54	222.1	-0.216	6.08
58		1.85	0.038	0.038	0.057	0.019	209.75	388.0	-0.742	4.08
59		1.88	0.044	0.044	0.044	0.044	137.27	258.1	-0.558	4.52
60		1.85	0.043	0.043	0.043	0.043	139.49	258.1	-0.558	4.52
61		1.73	0.048	0.030	0.042	0.030	165.91	287.0	-0.474	5.70
62		1.71	0.048	0.030	0.042	0.030	167.85	287.0	-0.474	5.70
63		1.68	0.047	0.029	0.041	0.029	170.85	287.0	-0.474	5.70
64		1.61	0.045	0.028	0.039	0.028	178.27	287.0	-0.474	5.70
65		1.36	0.038	0.024	0.033	0.024	211.04	287.0	-0.474	5.70
66		1.20	0.033	0.021	0.029	0.021	239.18	287.0	-0.474	5.70
67		1.64	0.043	0.022	0.051	0.036	138.43	227.0	-0.740	5.11
68		1.45	0.038	0.019	0.045	0.032	156.57	227.0	-0.740	5.11
69		1.36	0.036	0.018	0.042	0.030	166.93	227.0	-0.740	5.11
70		1.00	0.026	0.013	0.031	0.022	227.02	227.0	-0.740	5.11
71		0.80	0.021	0.011	0.025	0.018	283.78	227.0	-0.740	5.11
72		0.73	0.019	0.010	0.023	0.016	310.14	227.0	-0.740	5.11
73		1.86	0.044	0.044	0.044	0.000	135.48	252.0	-0.381	-0.30
74		1.76	0.042	0.042	0.042	0.000	143.18	252.0	-0.381	-0.30

75		1.97	0.068	0.034	0.034	0.000	176.62	347.9	0.000	6.91
76		1.74	0.031	0.062	0.031	0.000	193.14	336.1	-0.286	3.58
77		1.62	0.043	0.043	0.022	0.065	92.63	150.1	-0.320	5.91
78		1.51	0.026	0.052	0.026	0.052	115.06	174.1	-0.551	-0.43
79		1.79	0.060	0.037	0.022	0.037	133.75	239.0	-0.033	6.72
80		1.66	0.047	0.023	0.047	0.023	128.16	213.0	-0.563	5.57
<b>Test set</b>										
1		1.77	0.064	0.028	0.028	0.028	217.58	386.0	-0.041	6.25
2		1.68	0.048	0.021	0.048	0.035	144.65	243.0	-0.625	5.19
3		1.72	0.045	0.030	0.045	0.030	132.57	228.0	-0.561	5.17
4		1.57	0.045	0.019	0.045	0.032	154.78	243.0	-0.625	5.19

5		1.85	0.058	0.038	0.029	0.038	208.15	384.0	-0.167	6.31
6		1.85	0.055	0.047	0.023	0.031	127.93	236.0	-0.068	6.19
7		1.59	0.043	0.025	0.043	0.018	276.10	439.0	-0.528	5.42
8		1.68	0.060	0.030	0.022	0.030	133.49	224.0	0.000	6.86
9		1.93	0.053	0.053	0.026	0.026	226.97	438.1	-0.110	6.25
10		1.86	0.051	0.051	0.025	0.025	235.52	438.1	-0.110	6.25
11		1.33	0.036	0.036	0.018	0.018	330.11	438.1	-0.110	6.25
12		1.88	0.051	0.051	0.025	0.051	78.74	148.0	-0.216	5.07
13		1.78	0.048	0.048	0.024	0.048	83.17	148.0	-0.216	5.07
14	$\text{H}_3\text{C}-\text{NO}_2$	1.13	0.037	0.018	0.018	0.055	54.10	61.0	-0.393	6.04
15		1.91	0.044	0.053	0.035	0.035	112.94	216.1	-0.370	3.36

**Table S2.** The calculated Pearson's correlation coefficients of nine descriptors for the ML of *D*.

Parament	$\rho$	nO/ $V_m$	nN/ $V_m$	nC/ $V_m$	nH/ $V_m$	$V_m$	$M$	OB	$F$
PCC- <i>D</i>	0.9381	0.7756	0.7605	0.3410	0.4220	-0.6937	-0.0011	0.1437	-0.2027



**Table S3.** The setting of the RF model.

NO.	Parameter Name	Parameter settings
1	bootstrap	True
2	ccp_alpha	0.0
3	criterion	mse
4	max_depth	None
5	max_features	auto
6	max_leaf_nodes	None
7	max_samples	None
8	min_impurity_decrease	0.0
9	min_samples_leaf	1
10	n_estimators	200

**Table S4.** The setting of the SVR model.

NO.	Parameter Name	Parameter settings
1	C	1.0
2	cache_size	200M
3	coef0	0
4	degree	10
5	epsilon	0.1
6	gamma	Scale
7	kernel	rbf
8	max_iter	-1

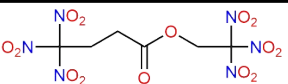
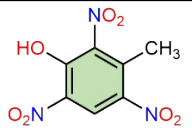
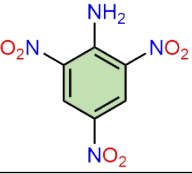
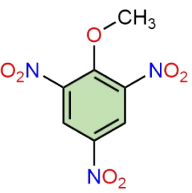
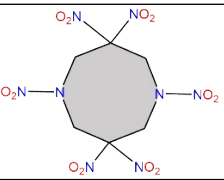
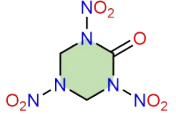
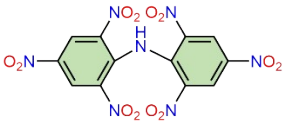
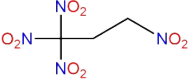
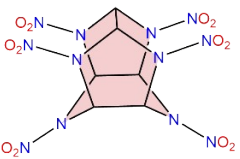
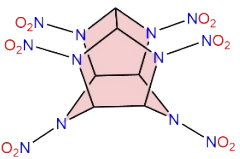
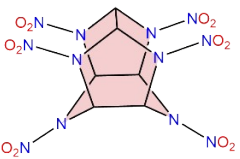
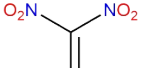
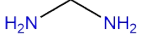
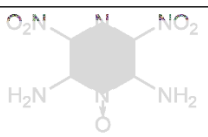
**Table S5.** The setting of the MLP model.

NO.	Parameter Name	Parameter settings
1	Input Layer Nodes	9
2	Hidden Layer Nodes	30
3	Output Layer Nodes	1
4	Activation function	tanh
5	Learning rate	0.001
6	Error	$0.65 \times 10^{-3}$
7	Epochs	2000
8	Optimization solver	Sgd
9	Loss function	MSE

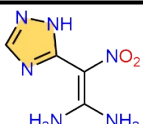
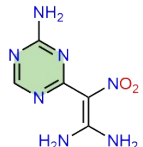
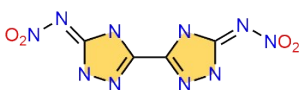
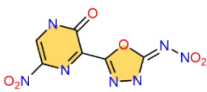
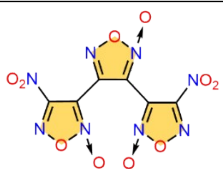
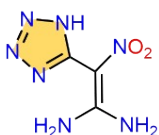
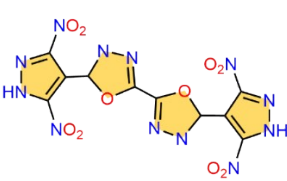
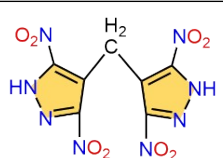
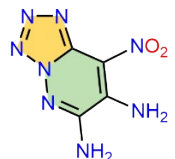
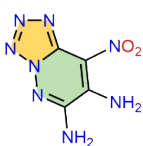
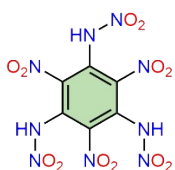
**Table S6.** The setting of the BPNN model.

NO.	Parameter Name	Parameter settings
1	Input Layer Nodes	9
2	Hidden Layer Nodes	40
3	Output Layer Nodes	1
4	Activation function	tanh
5	Training function	trainIm
6	Learning rate	0.001
7	Error	$0.65 \cdot 10^{-3}$
8	Epochs	4000
9	Optimization solver	RMSprop
10	Loss function	MSE

**Table S7.** The predicted  $D$  ( $\text{km}\cdot\text{s}^{-1}$ ) values of fifteen compounds in the test set.

NO.	Structure	Exp.	BPNN	MLP	RF
1		8.326	8.206	7.997	8.337
2		6.850	7.105	7.467	7.157
3		7.300	7.474	7.633	7.482
4		6.800	6.812	7.209	6.912
5		8.800	8.778	8.305	8.622
6		9.180	9.199	8.293	8.721
7		6.993	7.105	7.322	7.128
8		8.302	8.215	7.708	7.928
9		9.560	9.443	8.615	8.913
10		9.102	9.171	8.434	8.832
11		7.000	7.131	6.914	6.845
12		8.792	8.935	8.533	8.850
13		8.430	8.547	8.268	8.695
14	$\text{H}_3\text{C}-\text{NO}_2$	6.290	6.191	6.372	6.719
15		8.500	8.383	8.563	8.525

**Table S8.** The dataset of new test set 1.<sup>2-14</sup>

NO.	Structure	$\rho$	nO/ $V_m$	nN/ $V_m$	nC/ $V_m$	nH/ $V_m$	$V_m$	$M$	OB	$F$
1(P1)		1.71	0.020	0.060	0.040	0.060	99.47	170.1	-0.847	1.84
2(P2)		1.70	0.017	0.060	0.043	0.060	115.95	197.1	-0.933	1.49
3(P3)		1.80	0.028	0.070	0.028	0.028	142.28	256.1	-0.375	3.42
4(P4)		1.77	0.041	0.048	0.034	0.021	145.22	257.0	-0.342	3.48
5		1.91	0.056	0.044	0.033	0.000	180.09	344.0	-0.093	2.11
6		1.83	0.021	0.075	0.032	0.053	93.50	171.1	-0.608	1.94
7		1.87	0.041	0.050	0.041	0.008	241.05	450.0	-0.391	3.25
8		1.81	0.044	0.044	0.039	0.022	181.24	328.0	-0.390	4.53
9		1.82	0.016	0.082	0.033	0.016	122.03	222.1	-0.504	1.52
10		1.80	0.018	0.073	0.037	0.037	108.94	196.1	-0.653	1.66
1		1.800	0.048	0.043	0.034	0.014	207.23	373.0	-0.236	5.28

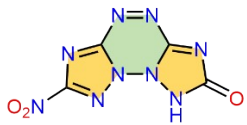
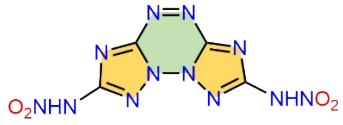
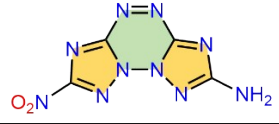
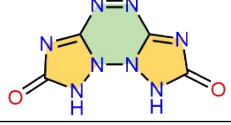
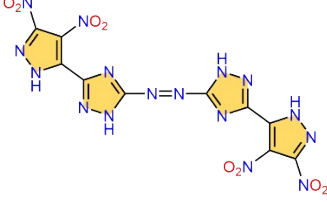
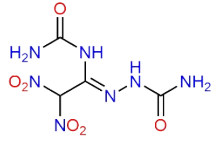
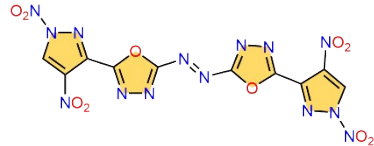
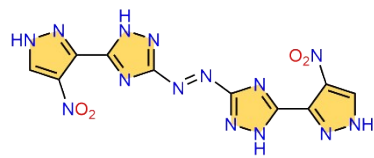
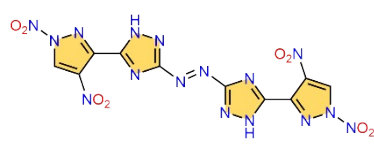
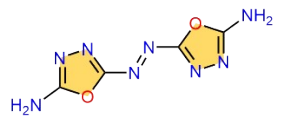
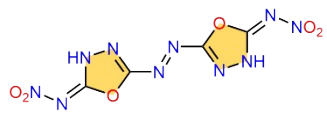
12		1.82	0.052	0.044	0.030	0.009	229.67	418.0	-0.115	5.68
13		1.91	0.041	0.059	0.035	0.012	170.71	326.1	-0.294	2.65
14		1.92	0.042	0.052	0.042	0.010	190.65	366.0	-0.393	2.29
15		1.21	0.047	0.016	0.016	0.047	63.64	77.0	-0.104	7.06
16		1.82	0.028	0.071	0.028	0.042	70.91	129.1	-0.434	2.76
17		1.75	0.018	0.080	0.027	0.027	112.63	197.1	-0.446	1.74
18		1.77	0.014	0.078	0.036	0.021	140.75	249.1	-0.610	1.28
19		1.81	0.020	0.070	0.040	0.040	100.60	182.1	-0.703	1.78
20		1.83	0.039	0.068	0.019	0.029	103.31	189.1	-0.127	4.79
21		1.88	0.031	0.070	0.031	0.023	128.23	241.1	-0.365	3.34
22		1.88	0.022	0.078	0.034	0.022	178.80	336.1	-0.476	2.53
23		1.92	0.032	0.070	0.032	0.027	184.96	355.1	-0.383	3.50
24		1.80	0.033	0.065	0.027	0.033	183.40	330.1	-0.339	3.79

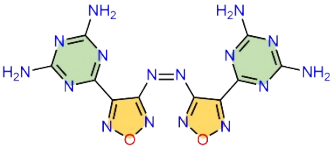
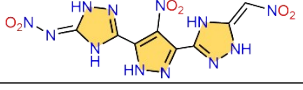
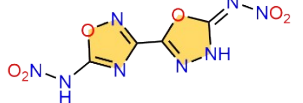
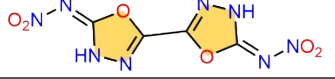
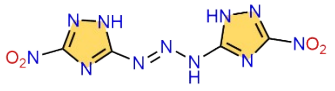
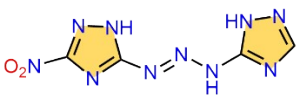
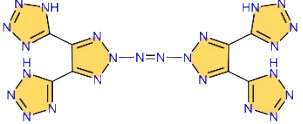
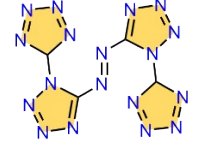
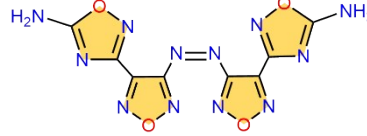
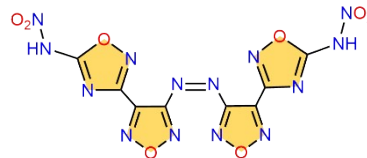
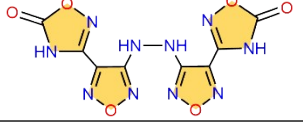
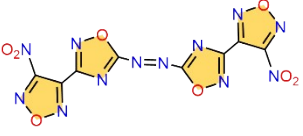
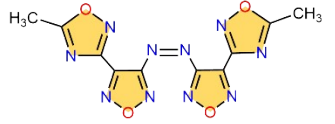
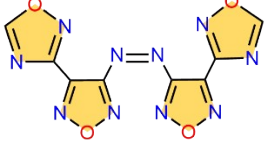
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26		1.88	0.039	0.065	0.026	0.039	77.15	145.1	-0.276	2.97
27		1.86	0.043	0.058	0.029	0.014	138.73	258.0	-0.186	1.60
28		1.90	0.039	0.055	0.039	0.024	126.87	241.1	-0.431	3.29
29		1.76	0.025	0.058	0.042	0.042	120.21	211.1	-0.720	1.45
30		1.73	0.033	0.049	0.041	0.033	122.72	212.1	-0.604	1.47
31		1.82	0.042	0.049	0.035	0.021	141.62	257.0	-0.342	1.24
32		1.89	0.039	0.056	0.039	0.011	178.86	338.1	-0.379	3.25
33		1.88	0.039	0.054	0.039	0.015	202.69	381.1	-0.399	3.89
34		1.88	0.033	0.061	0.039	0.017	179.30	337.1	-0.451	3.24
35		1.76	0.030	0.059	0.037	0.015	135.26	238.1	-0.470	1.37
36		1.83	0.041	0.055	0.034	0.000	146.46	268.0	-0.239	2.75

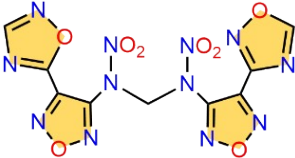
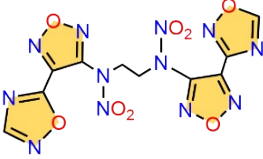
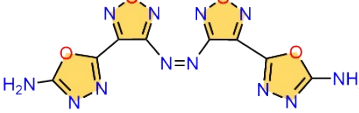
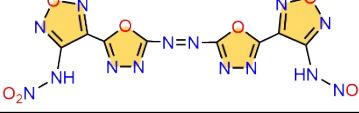
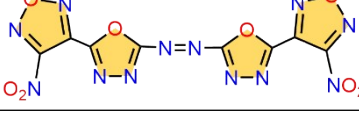
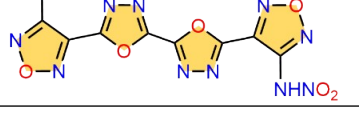
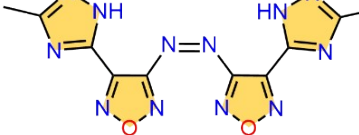
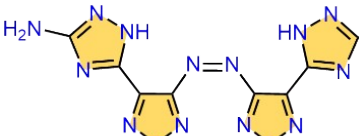
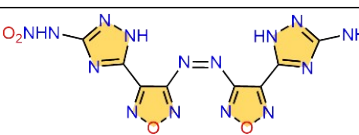
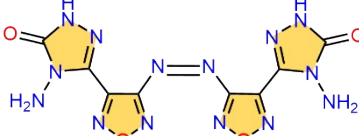
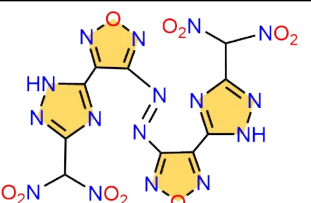
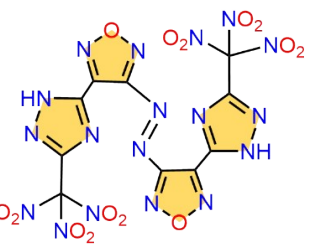


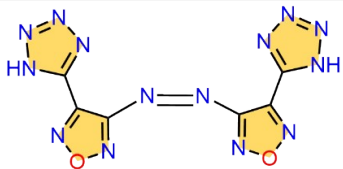
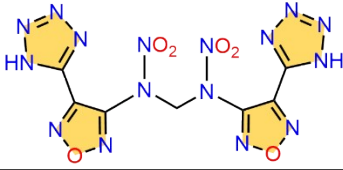
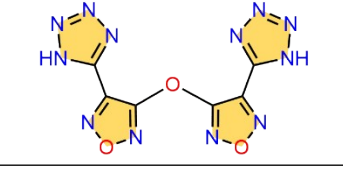
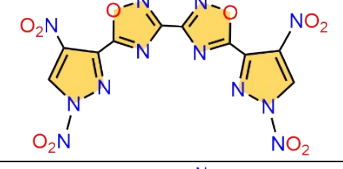
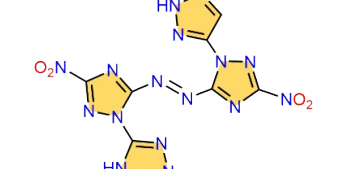
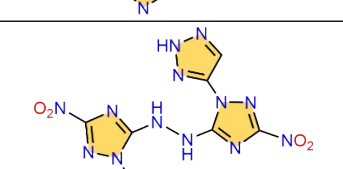
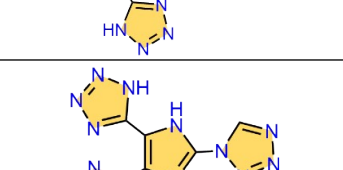
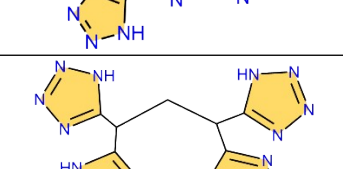
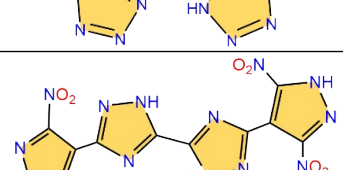
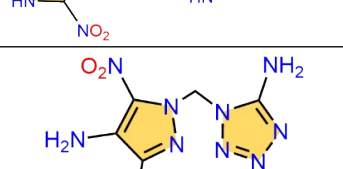
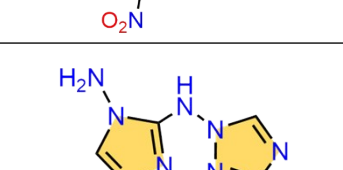


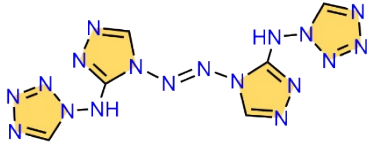
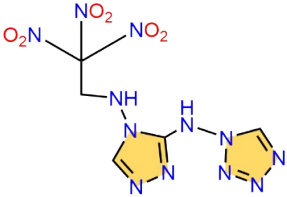
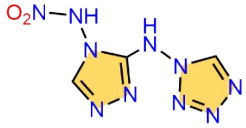
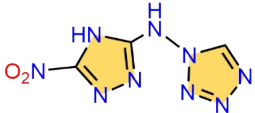
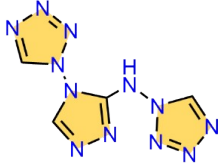
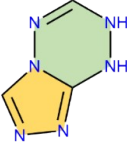
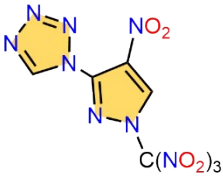
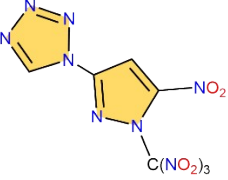
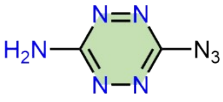
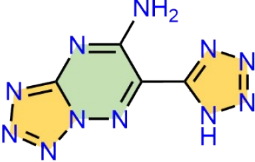
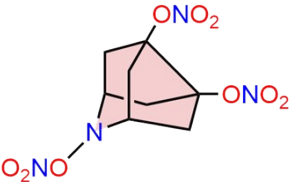
**Table S9.** The new dataset of new modified ML model.<sup>15-27</sup>

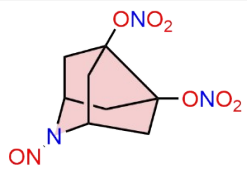
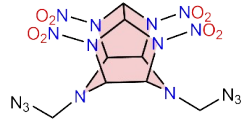
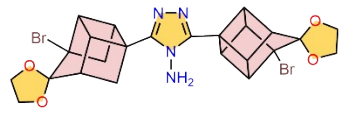
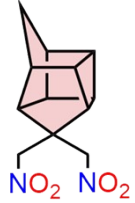
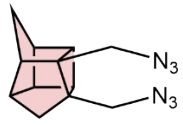
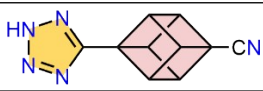
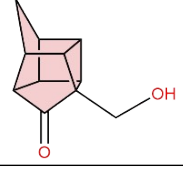
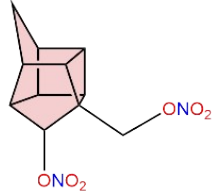
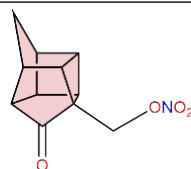
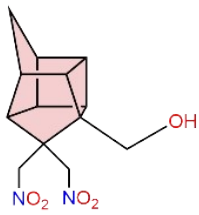
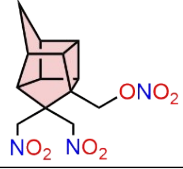
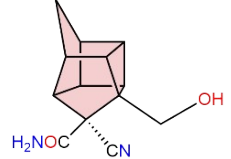
NO.	Structure	$\rho$	$nO/V_m$	$nN/V_m$	$nC/V_m$	$nH/V_m$	$V_m$	$M$	OB	$F$
<b>New training set</b>										
1		1.973	0.039	0.052	0.052	0.013	77.56	153.0	-0.575	2.90
2		1.998	0.028	0.085	0.028	0.014	141.19	282.1	-0.284	3.15
3		1.892	0.017	0.085	0.034	0.017	117.39	222.1	-0.504	0.62
4		1.903	0.020	0.078	0.039	0.020	101.99	194.1	-0.577	0.71
5		1.855	0.031	0.062	0.039	0.016	256.67	476.1	-0.470	3.05
6		1.700	0.041	0.048	0.027	0.041	145.92	248.1	-0.322	3.68
7		1.890	0.040	0.055	0.040	0.008	252.94	478.1	-0.368	3.37
8		1.800	0.019	0.065	0.047	0.028	214.53	386.2	-0.787	1.65
9		1.900	0.032	0.064	0.040	0.016	250.59	476.1	-0.470	3.36
10		1.760	0.018	0.072	0.036	0.036	111.42	196.1	-0.653	3.70
11		1.970	0.041	0.069	0.028	0.014	145.21	286.1	-0.168	3.10

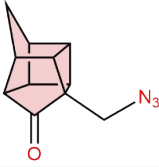
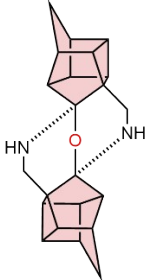
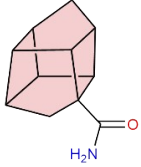
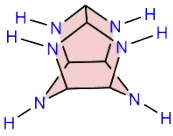
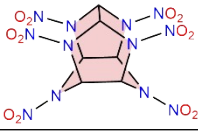
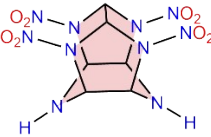
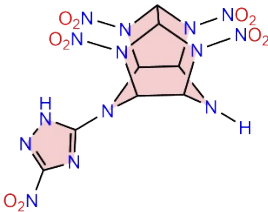
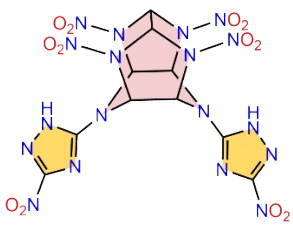
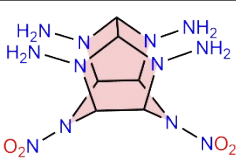
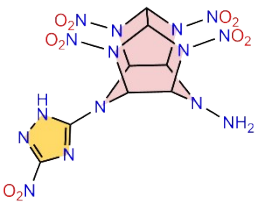
12		1.712	0.009	0.071	0.045	0.036	224.43	384.2	-0.916	-0.46
13		1.920	0.031	0.068	0.037	0.026	191.21	367.1	-0.458	2.26
14		1.860	0.043	0.057	0.028	0.036	140.36	261.1	-0.276	3.33
15		1.990	0.046	0.062	0.031	0.015	129.67	258.0	-0.186	3.44
16		1.862	0.072	0.026	0.026	0.020	151.97	283.0	0.085	2.58
17		1.679	0.070	0.014	0.028	0.028	142.92	240.0	0.000	6.36
18		1.820	0.015	0.087	0.029	0.015	274.86	500.2	-0.448	-0.25
19		1.820	0.011	0.098	0.022	0.011	183.62	334.2	-0.335	-0.19
20		1.85	0.030	0.045	0.060	0.030	134.09	248.1	-0.903	2.72
21		2.12	0.040	0.070	0.040	0.010	199.09	422.1	-0.341	1.98
22		1.86	0.033	0.055	0.044	0.022	180.69	336.1	-0.571	0.22
23		1.92	0.038	0.057	0.038	0.057	210.50	404.2	-0.554	1.55
24		1.75	0.021	0.053	0.053	0.032	188.64	330.1	-0.921	-0.49
25		1.68	0.022	0.056	0.044	0.011	179.81	302.1	-0.689	-0.37

26		1.77	0.036	0.054	0.036	0.009	222.63	394.1	-0.365	2.13
27		1.75	0.033	0.050	0.041	0.025	241.20	422.1	-0.569	1.87
28		1.77	0.021	0.064	0.043	0.021	187.64	332.1	-0.674	-0.38
29		1.83	0.035	0.061	0.035	0.009	230.64	422.1	-0.341	1.98
30		1.79	0.036	0.054	0.036	0.036	223.53	400.1	-0.480	1.62
31		1.92	0.039	0.058	0.039	0.010	205.24	394.1	-0.365	2.13
32		1.810	0.012	0.060	0.060	0.048	165.83	300.2	-1.173	-0.58
33		1.790	0.011	0.076	0.043	0.033	184.46	330.2	-0.824	-0.42
34		1.870	0.027	0.071	0.036	0.018	224.67	420.1	-0.457	1.96
35		1.680	0.019	0.065	0.037	0.028	215.57	362.2	-0.663	0.17
36		1.760	0.035	0.055	0.035	0.014	288.69	508.1	-0.378	2.85
37		1.900	0.044	0.057	0.032	0.006	314.77	598.1	-0.187	3.78

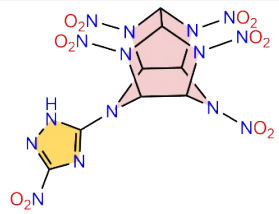
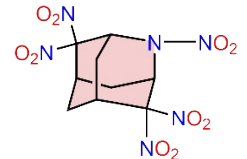
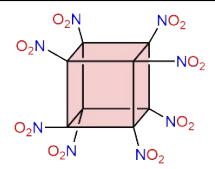
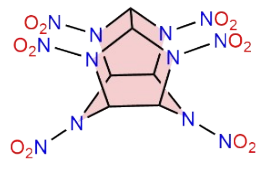
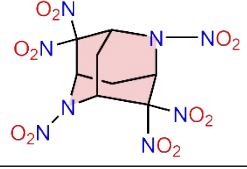
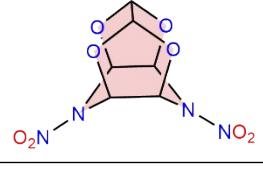
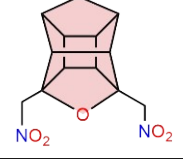
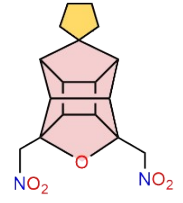
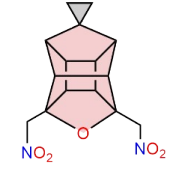
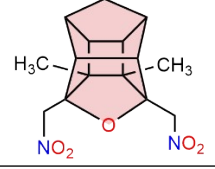
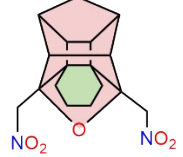
38		1.690	0.011	0.078	0.034	0.011	178.78	302.1	-0.583	-0.29
39		1.830	0.027	0.072	0.032	0.009	221.92	406.1	-0.355	1.72
40		1.740	0.018	0.072	0.036	0.012	166.73	290.1	-0.552	-0.30
41		1.830	0.041	0.049	0.041	0.008	245.92	450.0	-0.391	3.25
42		1.820	0.019	0.084	0.028	0.019	215.48	392.2	-0.408	1.78
43		1.760	0.018	0.081	0.027	0.009	221.68	390.2	-0.369	1.83
44		1.650	0.020	0.069	0.029	0.020	203.72	336.1	-0.476	-0.30
45		1.640	0.030	0.059	0.026	0.030	270.83	444.2	-0.360	-0.31
46		1.870	0.033	0.058	0.042	0.017	239.63	448.1	-0.500	3.24
47		1.806	0.027	0.067	0.033	0.040	149.57	270.1	-0.533	2.59
48		1.650	0.033	0.060	0.020	0.033	149.75	247.1	-0.227	-0.28

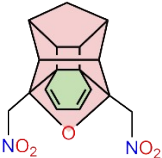
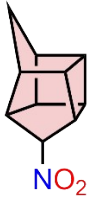
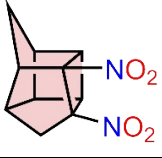
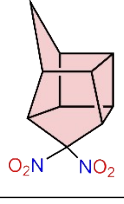
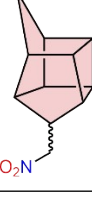
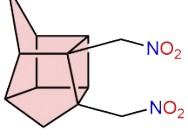
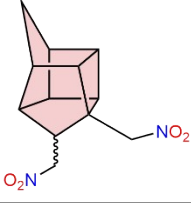
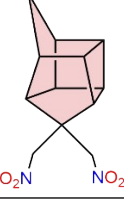
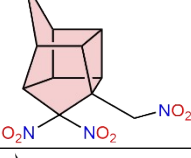
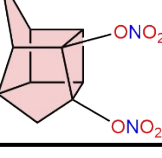
49		1.680	0.024	0.071	0.024	0.024	253.68	426.2	-0.338	-0.26
50		1.770	0.032	0.064	0.027	0.032	186.51	330.1	-0.339	3.33
51		1.780	0.017	0.084	0.025	0.034	119.17	212.1	-0.453	1.94
52		1.740	0.024	0.073	0.024	0.024	122.47	213.1	-0.338	1.61
53		1.710	0.019	0.077	0.026	0.019	156.21	267.1	-0.389	-0.26
54		1.680	0.022	0.065	0.033	0.022	91.70	154.1	-0.519	-0.32
55		1.794	0.045	0.056	0.023	0.011	177.28	318.0	-0.050	4.83
56		1.757	0.043	0.053	0.027	0.011	187.84	330.0	-0.145	4.62
57		1.680	0.020	0.079	0.020	0.020	101.24	170.1	-0.282	-0.22
58		1.795	0.021	0.078	0.028	0.021	141.01	253.1	-0.411	-0.27
59		1.678	0.046	0.023	0.046	0.058	172.86	290.1	-0.717	5.042

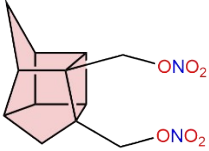
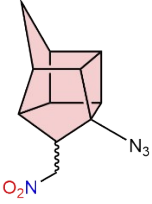
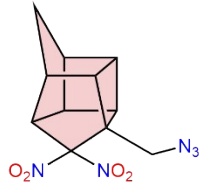
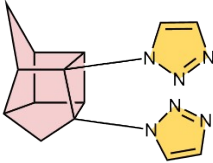
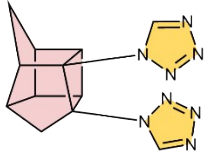
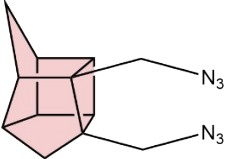
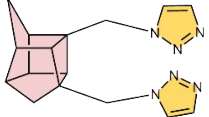
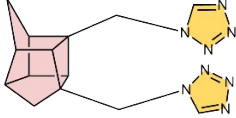
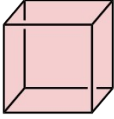
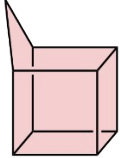
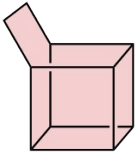
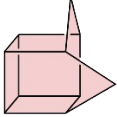
60		1.645	0.042	0.024	0.048	0.060	166.61	274.1	-0.817	5.336
61		1.850	0.032	0.065	0.032	0.040	247.66	458.2	-0.454	3.792
62		2.050	0.019	0.019	0.114	0.105	209.86	430.2	-2.045	-1.017
63		1.580	0.025	0.013	0.076	0.088	158.30	250.1	-1.727	2.249
64		1.440	0.000	0.036	0.071	0.083	168.19	242.2	-2.048	-0.981
65		1.560	0.000	0.038	0.077	0.100	130.24	203.2	-2.087	-1.015
66		1.360	0.016	0.000	0.085	0.085	128.74	175.1	-2.330	-0.607
67		1.520	0.034	0.011	0.063	0.052	174.38	265.1	-1.238	3.608
68		1.590	0.029	0.007	0.079	0.079	139.04	221.1	-1.701	2.120
69		1.400	0.025	0.010	0.065	0.080	200.09	280.1	-1.656	1.919
70		1.480	0.032	0.014	0.059	0.068	219.67	325.1	-1.304	3.441
71		1.500	0.013	0.013	0.085	0.091	153.43	230.1	-2.155	-0.543

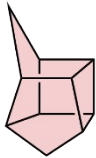
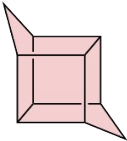
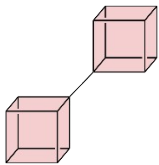
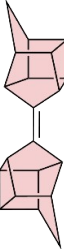
72		1.350	0.007	0.020	0.074	0.067	148.24	200.1	-2.079	-0.500
73		1.300	0.004	0.008	0.087	0.087	254.02	330.2	-2.616	-1.249
74		1.370	0.008	0.008	0.086	0.102	127.83	175.1	-2.512	-0.678
75		1.570	0.000	0.056	0.056	0.112	107.12	168.2	-1.712	-0.892
76		1.970	0.054	0.054	0.027	0.027	222.37	438.1	-0.110	6.249
77		1.870	0.043	0.054	0.032	0.043	186.15	348.1	-0.368	5.099
78		1.870	0.041	0.057	0.033	0.033	246.05	460.1	-0.348	4.673
79		1.840	0.038	0.058	0.032	0.032	312.04	574.2	-0.362	4.376
80		1.720	0.022	0.065	0.032	0.076	185.01	318.2	-0.754	2.475
81		1.840	0.039	0.058	0.031	0.035	258.23	475.1	-0.354	4.512



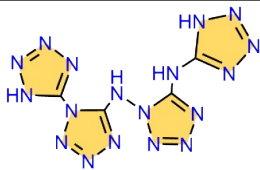
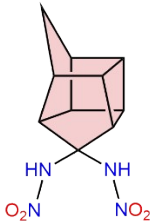
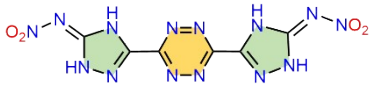
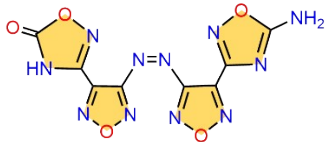
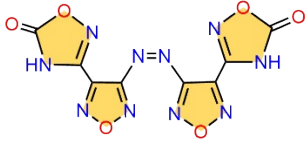
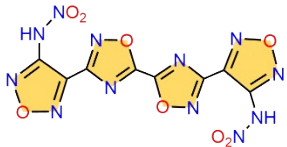
82		1.900	0.045	0.056	0.030	0.026	265.84	505.1	-0.238	5.209
83		1.813	0.050	0.030	0.045	0.040	198.59	360.0	-0.533	3.993
84		1.979	0.068	0.034	0.034	0.000	234.42	463.9	0.000	6.682
85		2.040	0.076	0.040	0.020	0.020	300.96	614.0	0.208	4.459
86		1.960	0.058	0.038	0.038	0.038	208.18	408.0	-0.314	5.882
87		1.990	0.061	0.030	0.046	0.046	131.67	262.0	-0.427	3.196
88		1.600	0.012	0.029	0.076	0.082	170.11	272.2	-1.822	2.021
89		1.590	0.010	0.024	0.083	0.097	205.18	326.2	-2.060	1.418
90		1.510	0.010	0.025	0.076	0.081	197.48	298.2	-1.932	1.719
91		1.370	0.009	0.023	0.068	0.082	219.13	300.2	-1.972	1.666
92		1.460	0.009	0.022	0.076	0.090	223.45	326.2	-2.060	1.418

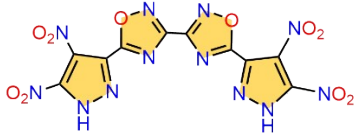
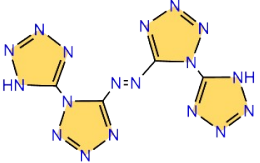
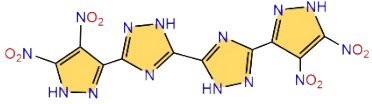
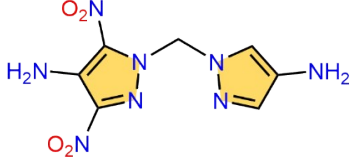
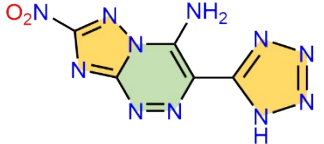
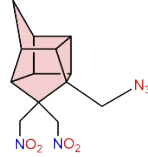
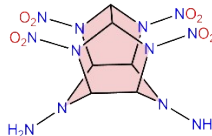
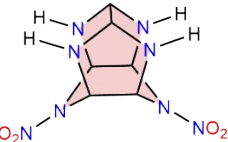
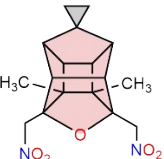
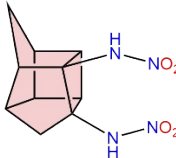
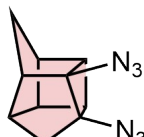
93		1.410	0.009	0.022	0.074	0.070	228.50	322.2	-1.986	1.513
94		1.460	0.048	0.009	0.044	0.048	229.47	335.0	-0.692	0.616
95		1.490	0.014	0.027	0.068	0.068	146.39	218.1	-1.687	2.808
96		1.650	0.015	0.030	0.076	0.076	132.19	218.1	-1.687	2.808
97		1.390	0.047	0.007	0.040	0.047	274.12	381.0	-0.651	1.526
98		1.540	0.013	0.025	0.075	0.088	159.84	246.2	-1.885	2.285
99		1.500	0.012	0.024	0.073	0.085	164.11	246.2	-1.885	2.285
100		1.580	0.013	0.026	0.077	0.090	155.80	246.2	-1.885	2.285
101		1.580	0.017	0.034	0.063	0.063	174.14	275.1	-1.425	3.612
102		1.580	0.013	0.039	0.064	0.064	155.78	246.1	-1.495	3.910

103		1.590	0.012	0.035	0.070	0.081	172.44	274.2	-1.692	3.328
104		1.550	0.025	0.012	0.074	0.087	161.37	250.1	-1.727	0.650
105		1.660	0.030	0.024	0.065	0.065	168.13	279.1	-1.290	2.127
106		1.370	0.039	0.017	0.039	0.039	357.71	490.1	-0.686	-0.536
107		1.570	0.041	0.027	0.041	0.041	293.04	460.1	-0.626	-0.489
108		1.440	0.043	0.019	0.037	0.043	323.65	466.1	-0.584	-0.510
109		1.520	0.047	0.016	0.042	0.047	382.93	582.1	-0.632	-0.537
110		1.530	0.044	0.022	0.039	0.044	360.84	552.1	-0.580	-0.498
111		1.290	0.030	0.030	0.030	0.030	266.73	344.1	-0.558	-0.436
112		1.340	0.030	0.033	0.030	0.033	300.08	402.1	-0.557	-0.435
113		1.190	0.026	0.031	0.026	0.031	386.67	460.1	-0.556	-0.435
114		1.520	0.033	0.040	0.033	0.040	302.72	460.1	-0.556	-0.435

115		1.070	0.023	0.028	0.023	0.028	430.04	460.1	-0.556	-0.435
116		1.370	0.030	0.036	0.030	0.036	335.87	460.1	-0.556	-0.435
117		1.450	0.035	0.031	0.035	0.031	453.88	658.1	-0.559	-0.437
118		1.340	0.031	0.031	0.031	0.031	641.94	860.2	-0.558	-0.436

### New test set 2

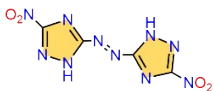
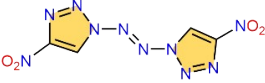
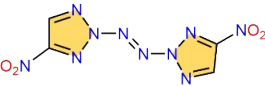
1(P5)		1.790	0.024	0.078	0.024	0.024	166.55	298.1	-0.322	-0.25
2(P6)		1.570	0.025	0.025	0.062	0.075	160.59	252.1	-1.396	2.975
3		1.880	0.022	0.078	0.034	0.022	178.80	336.1	-0.476	2.53
4		1.8	0.027	0.059	0.043	0.016	185.05	333.1	-0.600	-0.36
5		1.89	0.034	0.057	0.045	0.011	176.75	334.1	-0.527	0.26
6		1.85	0.038	0.056	0.038	0.009	213.01	394.1	-0.365	2.13

7		1.860	0.041	0.050	0.041	0.008	241.96	450.0	-0.391	3.25
8		1.820	0.014	0.090	0.028	0.014	145.13	264.1	-0.424	-0.24
9		1.880	0.034	0.059	0.042	0.017	238.35	448.1	-0.500	3.24
10		1.770	0.026	0.066	0.033	0.039	152.61	270.1	-0.533	2.59
11		1.873	0.015	0.083	0.038	0.023	133.01	249.1	-0.610	1.28
12		1.490	0.020	0.024	0.063	0.073	204.81	305.2	-1.547	1.782
13		1.960	0.041	0.062	0.031	0.052	192.93	378.1	-0.381	4.661
14		1.790	0.028	0.055	0.042	0.069	144.21	258.1	-0.806	3.148
15		1.440	0.009	0.022	0.075	0.088	226.55	326.2	-2.060	1.418
16		1.390	0.022	0.022	0.055	0.066	181.38	252.1	-1.396	2.975
17		1.480	0.040	0.024	0.040	0.040	252.74	374.1	-0.642	-0.501

**Table S10.** The dataset of new energetic compounds.

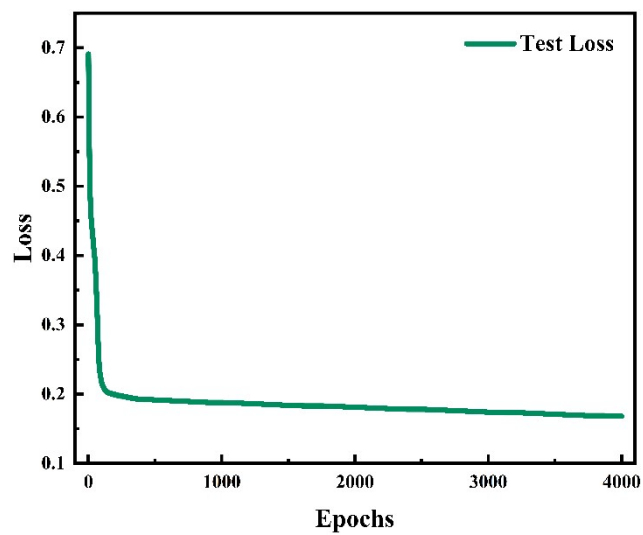
NO.	Name	$\rho$	nO/ $V_m$	nN/ $V_m$	nC/ $V_m$	nH/ $V_m$	$V_m$	$M$	OB	$F$
1	NEC1	1.80	0.054	0.039	0.031	0.047	128.93	232.1	-0.414	3.07
2	NEC2	1.81	0.050	0.044	0.031	0.044	160.82	291.1	-0.357	3.76
3	NEC3	1.79	0.063	0.031	0.031	0.031	127.42	228.1	-0.421	3.18
4	NEC4	1.77	0.053	0.035	0.035	0.041	170.11	301.1	-0.505	3.59
5	NEC5	1.89	0.077	0.031	0.026	0.015	195.30	369.1	-0.238	3.44
6	NEC6	1.88	0.078	0.029	0.024	0.020	204.33	384.1	-0.250	3.29
7	NEC7	1.94	0.055	0.049	0.031	0.006	162.38	315.0	-0.127	4.15
8	NEC8	1.91	0.052	0.046	0.035	0.017	172.27	329.0	-0.267	3.89
9	NEC9	1.91	0.073	0.034	0.021	0.009	233.47	445.9	0.215	4.09
10	NEC10	1.92	0.076	0.032	0.020	0.016	249.96	479.9	0.233	3.15
11	NEC11	1.92	0.035	0.056	0.045	0.042	287.59	552.2	-0.637	5.64
12	NEC12	1.94	0.036	0.061	0.040	0.030	328.96	638.2	-0.476	6.15

**Table S11.** The  $D$  prediction results of three isomers

NO.	Structure <sup>a)</sup>	$\rho/\text{g}\cdot\text{cm}^{-3}$	$D/\text{km}\cdot\text{s}^{-1}$	Predicted $D$ $/\text{km}\cdot\text{s}^{-1}$	Relative error $/\%$
I1		1.800	8.574 <sup>b)</sup>	8.941	4.280
		1.880	8.952	8.998	0.514
I2		1.800	8.990 <sup>b)</sup>	8.941	-0.545
		1.777	8.916	8.922	0.067
I3		1.800	8.935 <sup>b)</sup>	8.941	0.067
		1.795	8.917	8.937	0.224

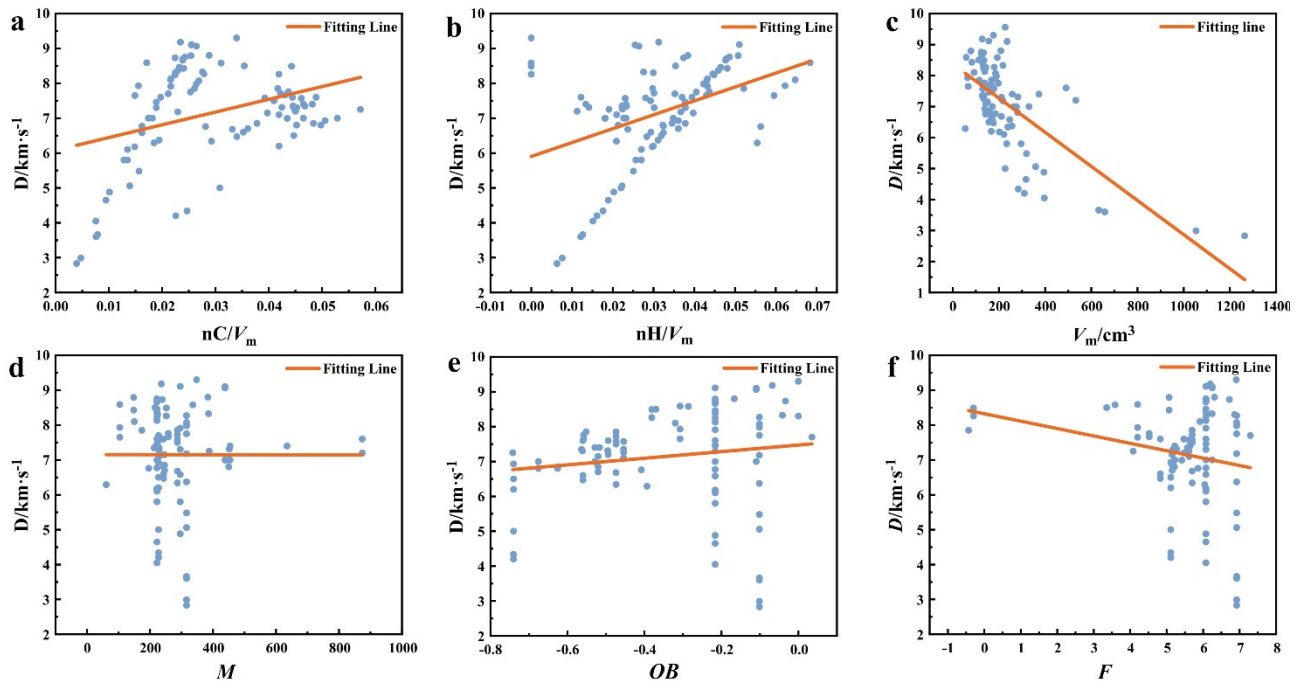
a) I1 is 3 from Yu's work (Z. Anorg. Allg. Chem. 2020); I2 and I3 is N8L and N8B from Lai's work (Chem. Eng. J. 2021).

b) These data were computed by EXPLO5.

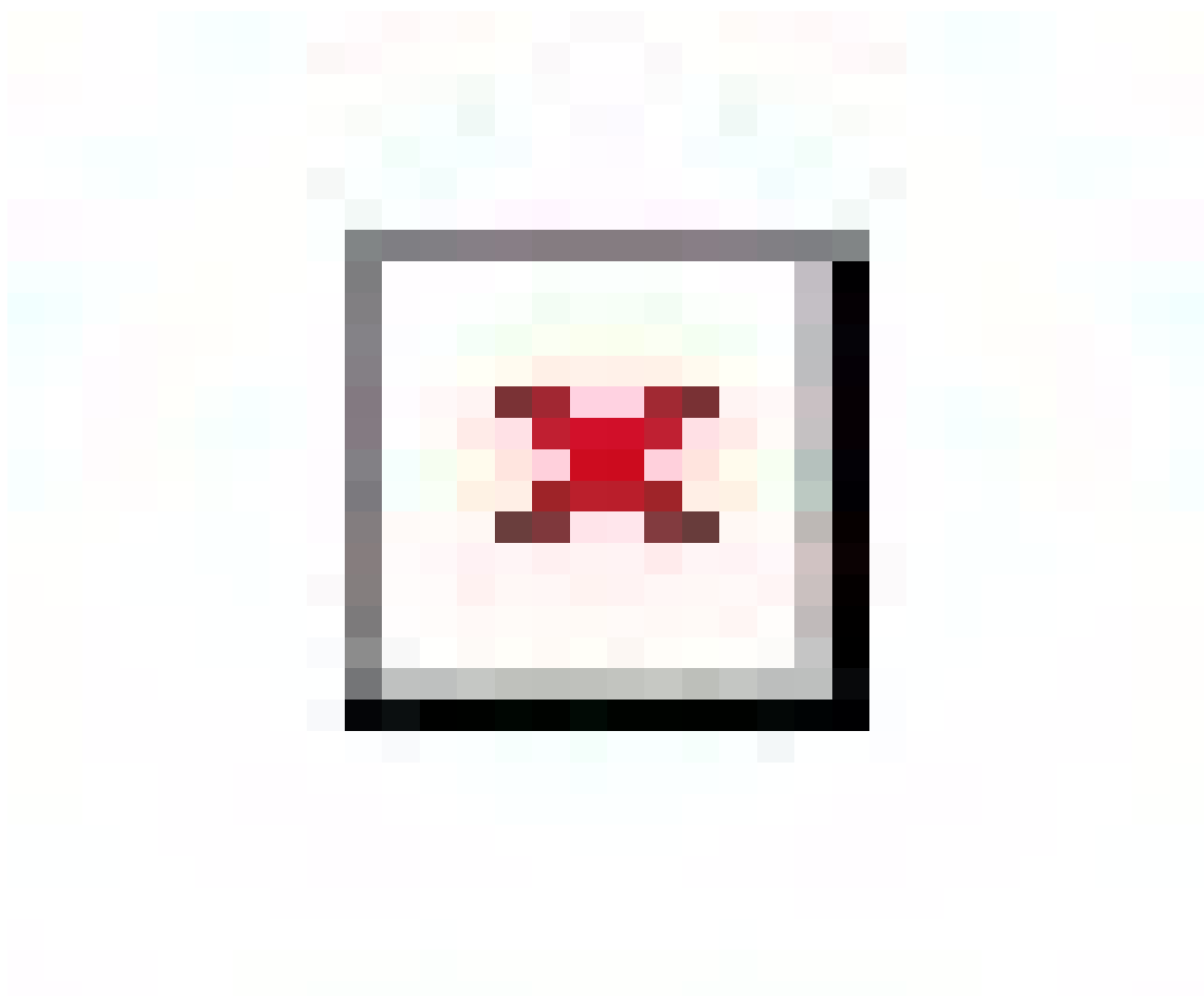


**Figure S1.** The loss function of ML models



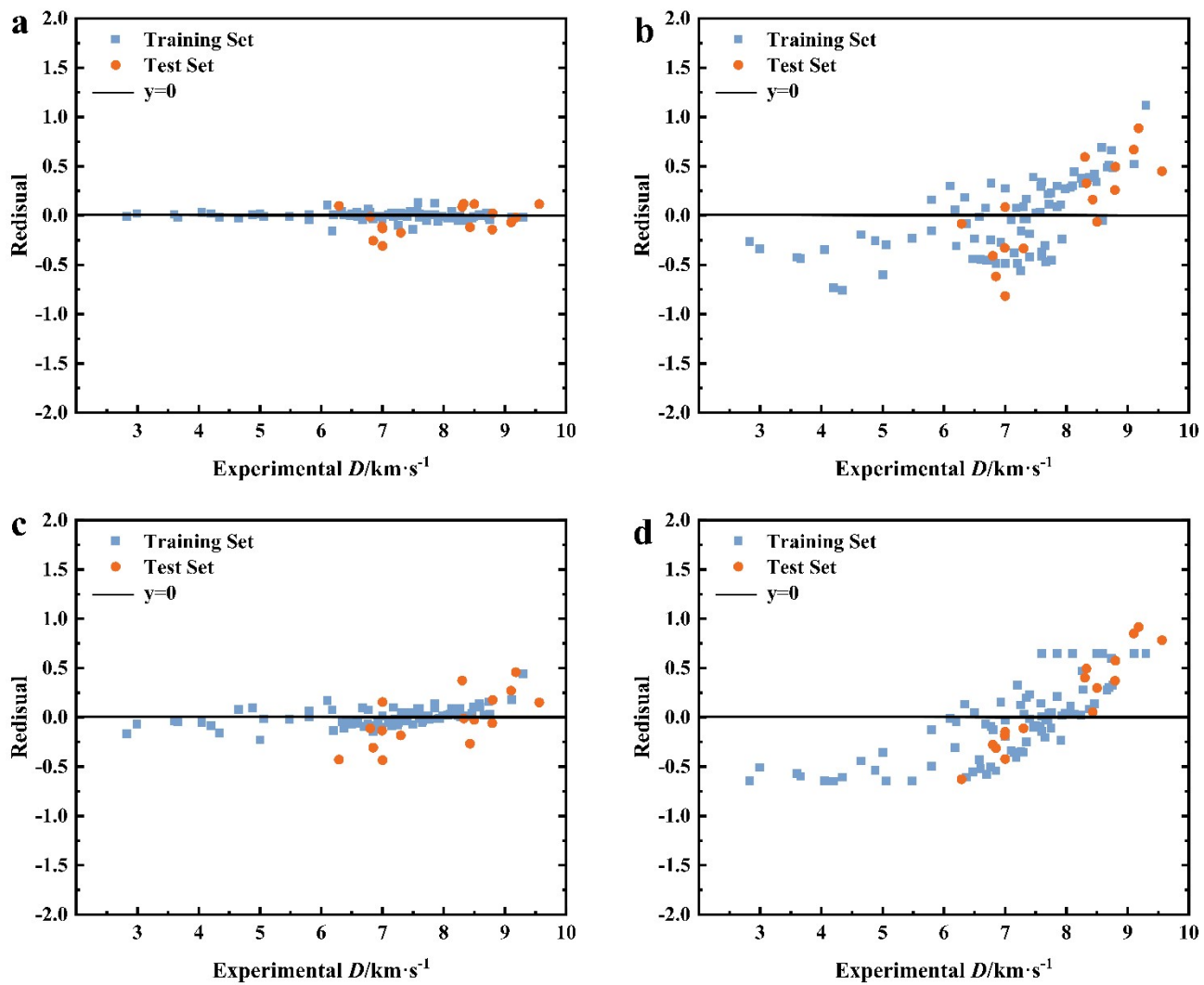


**Figure S2.** The relationships between  $nC/V_m$ ,  $nH/V_m$ ,  $V_m$ ,  $M$ ,  $OB$ ,  $F$  and experimental  $D$  results

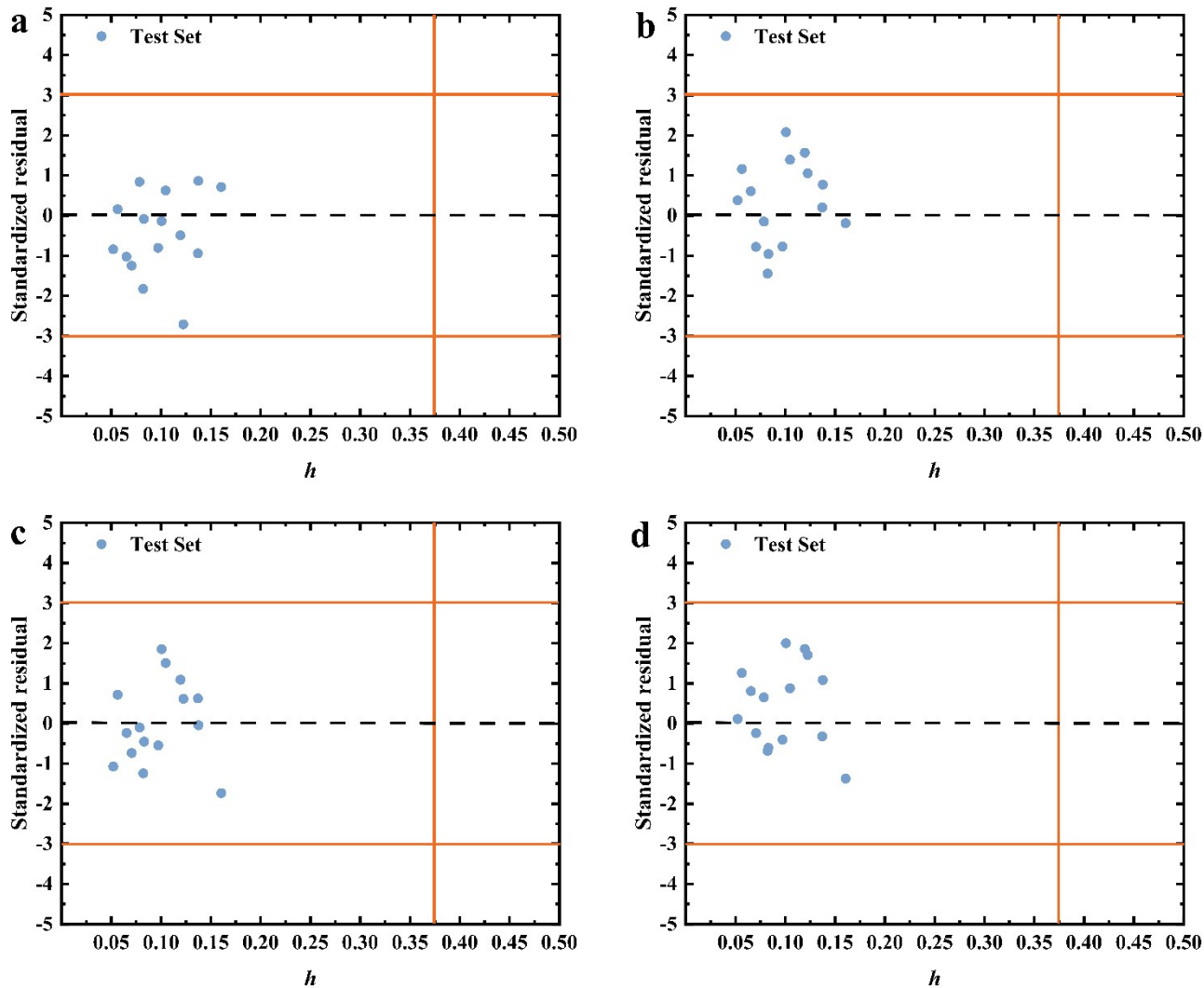


**Figure S3.** The scatter graph of the training/test set showing the  $D$  predicted vs experimental values:

(a)BPNN, (b)MLP, (c)RF and (d)SVR models



**Figure S4.** The predicted residual plot of (a)BPNN, (b)MLP, (c)RF and (d)SVR models for the  $D$



**Figure S5.** The Williams plot of (a)BPNN, (b)MLP, (c)RF and (d)SVR models for the test set of the  $D$

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