High-Throughput Design of Energetic Molecules

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Supplementary Information

Table S1 Hyper-parameters of D-MPNN.

Hyper-parameter	Value
activation	ReLU
batch size	32
D-MPNN depth	5
D-MPNN nodes	128
Dropout	0.0
global features	rdkit 2D
FFN nodes	128
FFN layers	3
initial learning rate	0.001
initial learning rate	0.0001
number of folds	10
split sizes	train : valid : test = 8 : 1 : 1
total epochs	100

Table S2 Test scores of 10-fold cross-validations.

Score	Fold	BDE_{R-NO_2} (kJ/mol)	ρ_{cryst} (g/cm^3)	$\Delta_f H_s^{\ominus}$ (kJ/mol)	D (km/s)	P (GPa)	Q (kJ/g)	T (K×10^3)	V (L/kg)
R^2	0	0.874	0.932	0.970	0.988	0.983	0.976	0.977	0.993
	1	0.898	0.929	0.979	0.989	0.984	0.985	0.982	0.995
	2	0.905	0.941	0.976	0.985	0.972	0.963	0.965	0.990
	3	0.907	0.951	0.975	0.990	0.986	0.986	0.985	0.995
	4	0.889	0.928	0.984	0.985	0.977	0.984	0.982	0.989
	5	0.873	0.924	0.976	0.988	0.980	0.983	0.984	0.992
	6	0.900	0.924	0.977	0.988	0.983	0.966	0.969	0.993
	7	0.883	0.926	0.966	0.985	0.981	0.978	0.976	0.990
	8	0.928	0.948	0.979	0.988	0.986	0.986	0.983	0.993
	9	0.890	0.955	0.981	0.991	0.987	0.983	0.990	0.991
RMSE	0	22	0.038	51	0.14	0.9	0.21	0.14	10
	1	15	0.040	40	0.13	0.9	0.15	0.11	8
	2	17	0.035	43	0.15	1.1	0.24	0.15	11
	3	18	0.035	43	0.13	0.9	0.16	0.11	8
	4	20	0.040	36	0.15	1.1	0.16	0.11	11
	5	21	0.038	45	0.13	0.9	0.16	0.11	10
	6	18	0.040	39	0.14	0.9	0.23	0.15	9
	7	17	0.045	57	0.16	1.1	0.19	0.13	11
	8	15	0.032	38	0.13	0.8	0.15	0.10	10
	9	18	0.035	42	0.13	0.9	0.18	0.09	10
MAE	0	13	0.028	32	0.10	0.6	0.13	0.08	6
	1	11	0.029	27	0.10	0.6	0.10	0.08	6
	2	11	0.027	30	0.10	0.6	0.13	0.08	7
	3	12	0.026	29	0.10	0.6	0.11	0.08	6
	4	13	0.031	24	0.11	0.7	0.10	0.07	8
	5	12	0.030	32	0.10	0.7	0.11	0.07	7
	6	11	0.030	27	0.09	0.6	0.15	0.09	7
	7	12	0.030	31	0.11	0.7	0.11	0.08	6
	8	10	0.026	26	0.10	0.6	0.10	0.07	7
	9	13	0.029	25	0.10	0.6	0.13	0.07	7

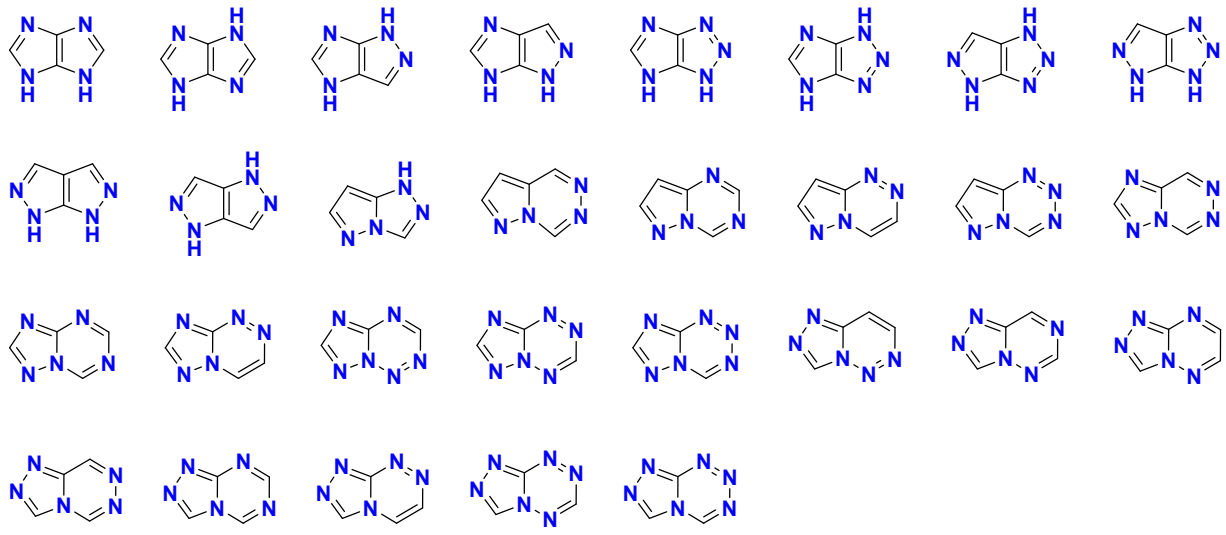

Figure S1. Molecular skeletons used for HTC aided energetic molecules screening.

Table S3 Result of HTC-aided energetic molecules screening.

SMILES	Density g/cm^3	HOF kJ/mol	D km/s	P GPa	BDE kJ/mol	Source
O=[N+]([O-])c1nn([N+](=O)[O-])c2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.943	506	9.37	41.5	140.4	ref[1]
Nc1c([N+](=O)[O-])nnc2c([N+](=O)[O-])c([N+](=O)[O-])nn12	1.909	378	8.55	34.2	248.4	ref[2]
Nn1nc([N+](=O)[O-])c2c1c([N+](=O)[O-])nn2N	1.857	475	8.48	33.1	300.2	ref[1]
Nc1c([N+](=O)[O-])nnc2nc([N+](=O)[O-])nn12	1.893	466	8.45	33.3	259.3	ref[3]
O=[N+]([O-])c1nn([N+](=O)[O-])c2c1c([N+](=O)[O-])nn2[N+](=O)[O-]	1.945	527	9.4	41.8	166.9	
O=[N+]([O-])c1nn([N+](=O)[O-])c2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.95	492	9.38	41.6	181.7	
O=[N+]([O-])c1nc2nc([N+](=O)[O-])n([N+](=O)[O-])c2n1[N+](=O)[O-]	1.963	458	9.38	41.9	181	
O=[N+]([O-])c1nn([N+](=O)[O-])c2nc([N+](=O)[O-])n([N+](=O)[O-])c12	1.947	494	9.37	41.5	174.4	
O=[N+]([O-])c1nc2c(nnn2[N+](=O)[O-])n1[N+](=O)[O-]	1.914	591	9.36	41	170.7	
O=[N+]([O-])c1nc2c(nc([N+](=O)[O-])n2[N+](=O)[O-])n1[N+](=O)[O-]	1.958	438	9.34	41.4	191.3	
O=[N+]([O-])c1nn2c([N+](=O)[O-])nn([N+](=O)[O-])c2c1[N+](=O)[O-]	1.932	477	9.3	40.7	224.3	
O=[N+]([O-])c1nc2nn[nH]c2n1[N+](=O)[O-]	1.938	533	9.1	39.1	231.9	
O=[N+]([O-])c1nnnc2nnc([N+](=O)[O-])n12	1.884	754	9.09	38.4	213.2	
O=[N+]([O-])c1nnc2nnc([N+](=O)[O-])n2c1[N+](=O)[O-]	1.921	616	9.08	38.7	240.3	
O=[N+]([O-])c1nnc([N+](=O)[O-])n2c([N+](=O)[O-])nnc12	1.918	619	9.07	38.6	203.8	
O=[N+]([O-])c1nn2c([N+](=O)[O-])n[nH]c2c1[N+](=O)[O-]	1.966	377	9.06	39	260.3	
O=[N+]([O-])c1n[nH]c2nc([N+](=O)[O-])n([N+](=O)[O-])c12	1.953	406	9.06	38.9	184.5	
O=[N+]([O-])c1nn([N+](=O)[O-])c2c([N+](=O)[O-])n[nH]c12	1.954	398	9.05	38.8	187.8	
O=[N+]([O-])c1nn([N+](=O)[O-])c2[nH]nnc12	1.922	527	9.04	38.4	217.4	
O=[N+]([O-])c1nn([N+](=O)[O-])c2nn[nH]c12	1.92	528	9.03	38.3	214.5	
Nc1nn2c([N+](=O)[O-])nn([N+](=O)[O-])c2c1[N+](=O)[O-]	1.933	442	9.02	38.3	255.1	
Nc1c([N+](=O)[O-])nn2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.942	423	9.02	38.5	233.6	
O=[N+]([O-])c1nc([N+](=O)[O-])c2nnc([N+](=O)[O-])n2n1	1.925	559	9.02	38.3	233.2	
O=[N+]([O-])c1n[nH]c2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.95	388	9.02	38.5	229.9	
O=[N+]([O-])c1n[nH]c2c1c([N+](=O)[O-])nn2[N+](=O)[O-]	1.942	398	9.01	38.3	176.8	
O=[N+]([O-])c1nc2nnc([N+](=O)[O-])c([N+](=O)[O-])n2n1	1.924	549	9	38.1	248.5	
O=[N+]([O-])c1nc([N+](=O)[O-])n2c([N+](=O)[O-])nnc2n1	1.918	558	9	38	186	
Nc1nn([N+](=O)[O-])c2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.924	451	9	38.1	139.1	
O=[N+]([O-])c1nc2c([N+](=O)[O-])nnc([N+](=O)[O-])n2n1	1.923	544	8.99	38	215	
O=[N+]([O-])c1nc2nnc([N+](=O)[O-])n2nc1[N+](=O)[O-]	1.919	544	8.98	37.9	247.6	
O=[N+]([O-])c1nn2c([N+](=O)[O-])nnnc2c1[N+](=O)[O-]	1.904	576	8.97	37.6	258.3	
Nn1nc([N+](=O)[O-])c2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.916	451	8.97	37.8	224.5	

O=[N+]([O-])c1nc2[nH]nnc2n1[N+](=O)[O-]	1.918	494	8.97	37.8	209.8
O=[N+]([O-])c1nn2c([N+](=O)[O-])nnc([N+](=O)[O-])c2c1[N+](=O)[O-]	1.909	494	8.96	37.6	230.6
Nn1nc([N+](=O)[O-])c2c1c([N+](=O)[O-])nn2[N+](=O)[O-]	1.9	484	8.96	37.5	206
Nc1nn([N+](=O)[O-])c2c1c([N+](=O)[O-])nn2[N+](=O)[O-]	1.916	436	8.95	37.6	158.3
Nn1nc([N+](=O)[O-])c2nc([N+](=O)[O-])n([N+](=O)[O-])c21	1.913	433	8.94	37.4	240.1
O=[N+]([O-])c1nc2nnnc([N+](=O)[O-])n2n1	1.891	643	8.94	37.2	239
O=[N+]([O-])c1nc2nc([N+](=O)[O-])n([N+](=O)[O-])c2[nH]1	1.95	328	8.93	37.8	225.7
O=[N+]([O-])c1n[nH]c2nnn([N+](=O)[O-])c12	1.905	495	8.93	37.3	137.4
O=[N+]([O-])c1nn([N+](=O)[O-])c2cnn([N+](=O)[O-])c12	1.897	453	8.93	37.2	120.8
Nn1nc([N+](=O)[O-])n2nc([N+](=O)[O-])c([N+](=O)[O-])c12	1.899	456	8.92	37.1	278.5
O=[N+]([O-])c1nnc2c([N+](=O)[O-])c([N+](=O)[O-])nn2n1	1.902	543	8.92	37.2	248.1
O=[N+]([O-])c1nc2c(nc([N+](=O)[O-])n2[N+](=O)[O-])[nH]1	1.949	323	8.92	37.7	218.3
O=[N+]([O-])c1nc([N+](=O)[O-])n2nc([N+](=O)[O-])nc2n1	1.925	486	8.92	37.4	208.9
Nn1nc([N+](=O)[O-])c2c([N+](=O)[O-])nn([N+](=O)[O-])c21	1.893	472	8.92	37.1	199.2
Nc1nn([N+](=O)[O-])c2nc([N+](=O)[O-])n([N+](=O)[O-])c12	1.92	405	8.92	37.4	177.4
Nc1nn([N+](=O)[O-])c2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.918	408	8.92	37.4	169.5
O=[N+]([O-])c1nc2ncn([N+](=O)[O-])c2n1[N+](=O)[O-]	1.906	423	8.92	37.2	141.6
Nc1nn([N+](=O)[O-])c2c([N+](=O)[O-])c([N+](=O)[O-])nn12	1.912	413	8.91	37.2	224.8
O=[N+]([O-])c1n[nH]c2c1nnn2[N+](=O)[O-]	1.912	471	8.91	37.2	199.4
O=[N+]([O-])c1nn2c([N+](=O)[O-])c([N+](=O)[O-])nnc2c1[N+](=O)[O-]	1.897	472	8.9	36.9	237.8
O=[N+]([O-])c1nc([N+](=O)[O-])n2nc([N+](=O)[O-])c([N+](=O)[O-])c2n1	1.914	416	8.89	37	235.7
Nn1c([N+](=O)[O-])nc2nc([N+](=O)[O-])n([N+](=O)[O-])c21	1.909	400	8.88	36.9	242.4
Nn1c([N+](=O)[O-])nc2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.904	403	8.87	36.8	249.3
Nn1c([N+](=O)[O-])nc2c([N+](=O)[O-])nn([N+](=O)[O-])c21	1.875	474	8.87	36.4	236.9
O=[N+]([O-])c1cc2n([N+](=O)[O-])nc([N+](=O)[O-])n2n1	1.891	423	8.87	36.6	219.8
O=[N+]([O-])c1nc2c([N+](=O)[O-])nn([N+](=O)[O-])c2[nH]1	1.915	367	8.87	36.9	219.5
O=[N+]([O-])c1nc2c(ncn2[N+](=O)[O-])n1[N+](=O)[O-]	1.899	404	8.87	36.7	160
O=[N+]([O-])c1cnn2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.873	460	8.86	36.4	224.4
O=[N+]([O-])c1nc2nnn([N+](=O)[O-])c2[nH]1	1.907	451	8.86	36.7	223.7
O=[N+]([O-])c1nn([N+](=O)[O-])c2c1cnn2[N+](=O)[O-]	1.872	461	8.86	36.3	148.9
O=[N+]([O-])c1nn([N+](=O)[O-])c2c1ncn2[N+](=O)[O-]	1.88	434	8.85	36.3	146.6
Nn1c([N+](=O)[O-])nc2c1c([N+](=O)[O-])nn2[N+](=O)[O-]	1.876	441	8.83	36.1	225.1
Nc1nc2nc([N+](=O)[O-])n([N+](=O)[O-])c2n1[N+](=O)[O-]	1.919	337	8.83	36.6	191.8
Nc1nc2nnn([N+](=O)[O-])c2n1[N+](=O)[O-]	1.886	492	8.83	36.2	154.8
O=[N+]([O-])c1nc2c(nnn2[N+](=O)[O-])[nH]1	1.899	442	8.82	36.3	202.9
Nc1nc2c(c([N+](=O)[O-])nn2[N+](=O)[O-])n1[N+](=O)[O-]	1.901	378	8.82	36.4	180.2
Nc1nn([N+](=O)[O-])c2nnn([N+](=O)[O-])c12	1.874	505	8.81	35.9	136.7
Nc1nn([N+](=O)[O-])c2c1nnn2[N+](=O)[O-]	1.874	506	8.81	35.9	128.3

Nc1nc2c([N+](=O)[O-])nn([N+](=O)[O-])c2n1[N+](=O)[O-]	1.9	365	8.8	36.2	189.6
O=[N+]([O-])c1nc2c([nH]1)c([N+](=O)[O-])nn2[N+](=O)[O-]	1.906	327	8.79	36.1	209.9
Nc1nc2c(nc([N+](=O)[O-])n2[N+](=O)[O-])n1[N+](=O)[O-]	1.92	310	8.79	36.3	201
Nn1nc([N+](=O)[O-])c2c1nnn2[N+](=O)[O-]	1.846	551	8.79	35.5	168.3
O=[N+]([O-])c1nc2cnn([N+](=O)[O-])c2n1[N+](=O)[O-]	1.876	402	8.79	35.8	143
O=[N+]([O-])c1nc2c(cnn2[N+](=O)[O-])n1[N+](=O)[O-]	1.877	390	8.78	35.7	151.9
Nc1nc2c(nnn2[N+](=O)[O-])n1[N+](=O)[O-]	1.88	469	8.77	35.7	178.8
Nn1c([N+](=O)[O-])nc2c1nnn2[N+](=O)[O-]	1.843	530	8.75	35.1	238.8
Nn1c([N+](=O)[O-])nc2nnn([N+](=O)[O-])c21	1.843	531	8.75	35.1	234.9
Nn1nc([N+](=O)[O-])c2nnn([N+](=O)[O-])c21	1.843	536	8.75	35.1	207.4
O=[N+]([O-])c1nn2cnn([N+](=O)[O-])c2c1[N+](=O)[O-]	1.853	411	8.73	35.1	190.4
Nc1nnc2nnc([N+](=O)[O-])n2c1[N+](=O)[O-]	1.903	608	8.71	35.4	272.9
Nc1nn2c([N+](=O)[O-])nnc([N+](=O)[O-])c2c1[N+](=O)[O-]	1.911	431	8.63	34.9	266.2
Nc1nnc([N+](=O)[O-])c2nnc([N+](=O)[O-])n12	1.889	580	8.62	34.6	250.3
Nc1c([N+](=O)[O-])nn2c([N+](=O)[O-])nnc([N+](=O)[O-])c12	1.92	400	8.62	34.9	225.7
Nc1nnc2nnc([N+](=O)[O-])c([N+](=O)[O-])n12	1.883	585	8.61	34.4	261.2
Nc1c([N+](=O)[O-])nn2c([N+](=O)[O-])c([N+](=O)[O-])nnc12	1.922	387	8.61	34.8	248.1
Nc1nnc([N+](=O)[O-])n2nc([N+](=O)[O-])c([N+](=O)[O-])c12	1.92	392	8.61	34.8	245.2
Nc1c([N+](=O)[O-])nn2c([N+](=O)[O-])nc([N+](=O)[O-])nc12	1.932	362	8.61	34.9	239
Nc1nnc([N+](=O)[O-])c2c([N+](=O)[O-])c([N+](=O)[O-])nn12	1.908	414	8.6	34.6	239.7
Nc1nnc2c([N+](=O)[O-])c([N+](=O)[O-])nn2c1[N+](=O)[O-]	1.908	409	8.59	34.5	265.6
Nc1nnc([N+](=O)[O-])n2c([N+](=O)[O-])nnc12	1.888	558	8.58	34.3	215.9
Nc1nn2c([N+](=O)[O-])c([N+](=O)[O-])nnc2c1[N+](=O)[O-]	1.909	393	8.57	34.4	256.9
O=[N+]([O-])c1n[nH]c2c([N+](=O)[O-])n[nH]c12	1.941	346	8.56	34.6	290.3
Nn1nc([N+](=O)[O-])c2[nH]nc([N+](=O)[O-])c21	1.905	410	8.55	34.2	290.9
Nc1nnc2nc([N+](=O)[O-])nn2c1[N+](=O)[O-]	1.901	512	8.55	34.1	272.4
O=[N+]([O-])c1cnnc2nnc([N+](=O)[O-])n12	1.849	611	8.55	33.5	244.1
O=[N+]([O-])c1cnn2c([N+](=O)[O-])nnc([N+](=O)[O-])c12	1.865	481	8.55	33.7	237.2
O=[N+]([O-])c1n[nH]c2[nH]nc([N+](=O)[O-])c12	1.927	367	8.55	34.4	217.3
Nc1nc([N+](=O)[O-])c2nnc([N+](=O)[O-])n2n1	1.896	515	8.54	34	252.5
Nc1c([N+](=O)[O-])nnc2nnc([N+](=O)[O-])n12	1.885	536	8.54	33.9	250.9
Nn1nc([N+](=O)[O-])c2c([N+](=O)[O-])n[nH]c21	1.9	416	8.54	34.1	241.1
Nc1nc([N+](=O)[O-])n2c([N+](=O)[O-])nnc2n1	1.894	517	8.54	34	211.5
Nc1nn2c([N+](=O)[O-])nc([N+](=O)[O-])nc2c1[N+](=O)[O-]	1.913	352	8.53	34.1	257.6
Nc1nc([N+](=O)[O-])n2nc([N+](=O)[O-])c([N+](=O)[O-])c2n1	1.919	334	8.53	34.1	247.9
O=[N+]([O-])c1nnc([N+](=O)[O-])n2cnnc12	1.861	570	8.52	33.5	239.6
O=[N+]([O-])c1ncnc2nnc([N+](=O)[O-])n12	1.868	554	8.52	33.5	199.2
Nc1nn2c([N+](=O)[O-])nnnc2c1[N+](=O)[O-]	1.876	534	8.51	33.5	286.8
O=[N+]([O-])c1nnc2nncn2c1[N+](=O)[O-]	1.852	578	8.51	33.3	268.8
O=[N+]([O-])c1nncn2c([N+](=O)[O-])nnc12	1.854	577	8.51	33.3	252.1

O=[N+]([O-])c1cc2nnc([N+](=O)[O-])c([N+](=O)[O-])n2n1	1.875	428	8.51	33.6	246.5
Nc1nnc2c([N+](=O)[O-])nnc([N+](=O)[O-])n12	1.877	532	8.51	33.5	225.7
O=[N+]([O-])c1nn2c([N+](=O)[O-])cnnc2c1[N+](=O)[O-]	1.858	464	8.5	33.3	270.2
Nc1c([N+](=O)[O-])nn2c([N+](=O)[O-])nnnc12	1.894	493	8.5	33.7	258.4
Nc1nc([N+](=O)[O-])nc2c([N+](=O)[O-])c([N+](=O)[O-])nn12	1.909	335	8.5	33.8	253.3
Nc1nn2c([N+](=O)[O-])n[nH]c2c1[N+](=O)[O-]	1.93	331	8.49	34	302.3
Nc1nnc([N+](=O)[O-])n2nc([N+](=O)[O-])nc12	1.893	483	8.48	33.5	252.5
O=[N+]([O-])c1cc2c([N+](=O)[O-])nnc([N+](=O)[O-])n2n1	1.874	402	8.48	33.3	205.1
Nc1nn2nc([N+](=O)[O-])nnc2c1[N+](=O)[O-]	1.883	499	8.47	33.3	272.4
O=[N+]([O-])c1nn2c([N+](=O)[O-])ncnc2c1[N+](=O)[O-]	1.865	414	8.46	33.1	246.9
O=[N+]([O-])c1cc2nc([N+](=O)[O-])nc([N+](=O)[O-])n2n1	1.883	369	8.46	33.2	227.9
O=[N+]([O-])c1nncc2nnc([N+](=O)[O-])n12	1.836	581	8.46	32.7	187
Nc1nc2nnc([N+](=O)[O-])n2nc1[N+](=O)[O-]	1.891	465	8.45	33.2	266.5
O=[N+]([O-])c1nnc2c([N+](=O)[O-])cnn2c1[N+](=O)[O-]	1.85	443	8.45	32.8	252.6
O=[N+]([O-])c1cn2c([N+](=O)[O-])nnc2nn1	1.845	556	8.45	32.8	252.6
Nc1nn2c([N+](=O)[O-])nnc2nc1[N+](=O)[O-]	1.891	469	8.45	33.2	248.2
O=[N+]([O-])c1nn2c([N+](=O)[O-])nncc2c1[N+](=O)[O-]	1.861	414	8.45	32.9	238
Nc1nnc2c([N+](=O)[O-])nc([N+](=O)[O-])nn12	1.889	472	8.45	33.2	232.8
Nc1n[nH]c2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.916	334	8.45	33.5	222.3
Nn1nc([N+](=O)[O-])c2c([N+](=O)[O-])nn(N)c21	1.857	447	8.44	32.8	268.8
Nc1c([N+](=O)[O-])nn2c([N+](=O)[O-])nn(N)c12	1.887	383	8.43	33	302.5
Nn1nc([N+](=O)[O-])c2nn[nH]c21	1.852	556	8.43	32.6	301.2
Nc1nn2c([N+](=O)[O-])nn([N+](=O)[O-])c2c1N	1.89	375	8.43	33	250.5
O=[N+]([O-])c1nc([N+](=O)[O-])n2ncc([N+](=O)[O-])c2n1	1.867	386	8.43	32.8	246
Nc1nc([N+](=O)[O-])nc2nnc([N+](=O)[O-])n12	1.886	467	8.43	33	223.5
Nc1n[nH]c2c1c([N+](=O)[O-])nn2[N+](=O)[O-]	1.908	334	8.43	33.2	220.1
Nc1nnc2c([N+](=O)[O-])c([N+](=O)[O-])nn2n1	1.873	483	8.42	32.8	248.1
Nc1nc2nnc([N+](=O)[O-])c([N+](=O)[O-])n2n1	1.887	458	8.42	33	247.3
O=[N+]([O-])c1cn2nc([N+](=O)[O-])c([N+](=O)[O-])c2nn1	1.847	425	8.42	32.5	237.9
O=[N+]([O-])c1nc2nncc([N+](=O)[O-])n2n1	1.852	516	8.41	32.5	268.3
O=[N+]([O-])c1cnc2nnc([N+](=O)[O-])n2n1	1.859	504	8.41	32.6	260
Nc1nnc([N+](=O)[O-])c2nc([N+](=O)[O-])nn12	1.887	454	8.41	32.9	236.5
Nc1nn(N)c2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.871	405	8.41	32.8	221.3
O=[N+]([O-])c1nn2cnnc([N+](=O)[O-])c2c1[N+](=O)[O-]	1.838	438	8.41	32.3	195.4
O=[N+]([O-])n1ncc2c1cnn2[N+](=O)[O-]	1.842	443	8.41	32.4	135.5
Nc1nn2c([N+](=O)[O-])nn(N)c2c1[N+](=O)[O-]	1.87	397	8.4	32.6	315.1
O=[N+]([O-])c1n[nH]c2nn[nH]c12	1.867	512	8.4	32.6	306.2
O=[N+]([O-])c1cnn2c([N+](=O)[O-])nnnc12	1.825	566	8.4	32.2	268.4
Nc1nnnc2c([N+](=O)[O-])c([N+](=O)[O-])nn12	1.863	491	8.4	32.5	262.5
O=[N+]([O-])c1ncn2nc([N+](=O)[O-])c([N+](=O)[O-])c2n1	1.865	370	8.4	32.6	251.6

Nc1nnc2nc([N+](=O)[O-])c([N+](=O)[O-])nn12	1.88	456	8.4	32.7	249.7
Nc1nc([N+](=O)[O-])n2nc([N+](=O)[O-])nc2n1	1.9	420	8.4	32.9	238.1
O=[N+]([O-])c1nnc([N+](=O)[O-])n2ncnc12	1.85	517	8.4	32.5	214.3
Nc1nnc2nc([N+](=O)[O-])nc([N+](=O)[O-])n12	1.88	460	8.4	32.7	193.1
Nc1n[nH]c2c([N+](=O)[O-])c([N+](=O)[O-])nn12	1.911	309	8.39	33	267.9
Nc1nc([N+](=O)[O-])nn2c([N+](=O)[O-])nnc12	1.881	450	8.39	32.7	242.5
Nc1nc2c([N+](=O)[O-])nn([N+](=O)[O-])c2[nH]1	1.924	288	8.39	33.1	235.5
Nc1nn([N+](=O)[O-])c2c(N)nn([N+](=O)[O-])c12	1.883	367	8.39	32.7	157.6
O=[N+]([O-])n1cnc2nn[nH]c21	1.85	528	8.38	32.3	242.2
O=[N+]([O-])c1nnc2ncnn2c1[N+](=O)[O-]	1.843	513	8.38	32.2	236.5
O=[N+]([O-])c1ncnn2c([N+](=O)[O-])nnc12	1.849	503	8.38	32.2	225.6
Nc1nn([N+](=O)[O-])c2c([N+](=O)[O-])nn(N)c12	1.866	396	8.38	32.5	217.5
Nc1c([N+](=O)[O-])nn2c([N+](=O)[O-])n[nH]c12	1.914	294	8.37	32.9	277.6
O=[N+]([O-])c1ncn2c([N+](=O)[O-])nnc2n1	1.862	473	8.37	32.3	237.1
O=[N+]([O-])c1cnn2c([N+](=O)[O-])n[nH]c12	1.88	340	8.36	32.4	286.4
Nc1nn2c(N)nn([N+](=O)[O-])c2c1[N+](=O)[O-]	1.882	354	8.36	32.5	263.3
O=[N+]([O-])c1nnnc2nncn12	1.788	712	8.36	31.5	256.9
Nc1nn([N+](=O)[O-])c2nc([N+](=O)[O-])[nH]c12	1.911	290	8.36	32.7	232.2
O=[N+]([O-])c1cnn2c([N+](=O)[O-])nnc2n1	1.842	504	8.36	32	228.8
Nn1nc([N+](=O)[O-])c2nc([N+](=O)[O-])n(N)c21	1.843	421	8.35	32	298.9
O=[N+]([O-])c1nnc2nnncn12	1.794	696	8.35	31.5	258
Nc1nn([N+](=O)[O-])c2c1c([N+](=O)[O-])nn2N	1.86	388	8.35	32.2	217.3
Nc1nn([N+](=O)[O-])c2[nH]nc([N+](=O)[O-])c12	1.891	321	8.35	32.5	202.6
O=[N+]([O-])c1nc([N+](=O)[O-])n2cnnc2n1	1.847	491	8.35	32	202
Nc1nn([N+](=O)[O-])c2c([N+](=O)[O-])n[nH]c12	1.892	316	8.35	32.4	169.1
O=[N+]([O-])c1nn2ncnnc2c1[N+](=O)[O-]	1.821	535	8.34	31.7	252.8
O=[N+]([O-])c1cn2nc([N+](=O)[O-])nc2nn1	1.848	478	8.34	31.9	248.6
O=[N+]([O-])c1nc2nncn2nc1[N+](=O)[O-]	1.832	514	8.34	31.8	244
Nc1nc([N+](=O)[O-])nc2nc([N+](=O)[O-])nn12	1.896	395	8.34	32.5	241
O=[N+]([O-])c1nc2ncnc([N+](=O)[O-])n2n1	1.867	446	8.34	32.2	232
Nc1nc2c([N+](=O)[O-])nnc([N+](=O)[O-])n2n1	1.872	439	8.34	32.2	226
Nc1nc2[nH]nc([N+](=O)[O-])c2n1[N+](=O)[O-]	1.901	295	8.34	32.4	212.6
O=[N+]([O-])c1nc2c([N+](=O)[O-])nncn2n1	1.84	496	8.34	31.8	208.1
O=[N+]([O-])c1nnc2c([N+](=O)[O-])cnn2n1	1.829	515	8.33	31.7	254
Nc1c([N+](=O)[O-])nn2nc([N+](=O)[O-])nnc12	1.873	427	8.33	32.1	242.7
O=[N+]([O-])c1cc2nnnc([N+](=O)[O-])n2n1	1.84	489	8.33	31.8	240.4
O=[N+]([O-])c1nc2cn[nH]c2n1[N+](=O)[O-]	1.873	339	8.33	32.1	225.1
O=[N+]([O-])c1nn([N+](=O)[O-])c2[nH]ncc12	1.871	342	8.33	32.1	223.2
Nc1cnn2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.843	395	8.33	31.8	211.4
O=[N+]([O-])n1ncc2nn[nH]c21	1.83	534	8.33	31.7	199.9

O=[N+]([O-])c1n[nH]c2[nH]nnc12	1.833	528	8.32	31.7	282.9
Nc1nnc2nnnc([N+](=O)[O-])n12	1.806	670	8.32	31.4	236.1
O=[N+]([O-])c1n[nH]c2c1ncn2[N+](=O)[O-]	1.881	319	8.32	32.1	234.5
O=[N+]([O-])c1nc2cnnc([N+](=O)[O-])n2n1	1.84	485	8.32	31.7	232.4
O=[N+]([O-])c1nn([N+](=O)[O-])c2cn[nH]c12	1.861	352	8.32	31.9	217
Nn1nc([N+](=O)[O-])c2c1nc([N+](=O)[O-])n2N	1.842	396	8.31	31.6	282.5
Nc1nn(N)c2c([N+](=O)[O-])c([N+](=O)[O-])nn12	1.86	365	8.31	31.9	277.1
Nn1c([N+](=O)[O-])nc2[nH]nc([N+](=O)[O-])c21	1.87	333	8.31	31.9	274.6
O=[N+]([O-])c1ncc2nnc([N+](=O)[O-])n2n1	1.834	489	8.31	31.6	224.3
Nc1nn(N)c2c1c([N+](=O)[O-])nn2[N+](=O)[O-]	1.851	379	8.31	31.7	204.9
Nc1nn([N+](=O)[O-])c2c1c(N)nn2[N+](=O)[O-]	1.865	352	8.31	31.9	180.2
Nn1nc([N+](=O)[O-])c2[nH]nnc21	1.839	518	8.3	31.6	308.1
Nc1nc2c([N+](=O)[O-])n[nH]c2n1[N+](=O)[O-]	1.905	269	8.3	32.2	259.9
O=[N+]([O-])c1ncn2nc([N+](=O)[O-])nc2n1	1.864	424	8.3	31.8	239.3
Nc1nnnc2nnc([N+](=O)[O-])n12	1.807	655	8.3	31.2	238.7
Nn1c([N+](=O)[O-])nc2c([N+](=O)[O-])n[nH]c21	1.864	335	8.29	31.7	280.6
Nc1nn([N+](=O)[O-])c2nc([N+](=O)[O-])n(N)c12	1.847	375	8.29	31.5	243.9
Nc1nc2c(c([N+](=O)[O-])nn2N)n1[N+](=O)[O-]	1.869	334	8.29	31.8	241.5
Nc1nn([N+](=O)[O-])c2[nH]c([N+](=O)[O-])nc12	1.889	290	8.29	32	237.8
Nc1n[nH]c2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.896	281	8.29	32.1	235.9
Nc1nc2nc([N+](=O)[O-])nc([N+](=O)[O-])n2n1	1.888	380	8.29	32	208.5
Nc1n[nH]c2nc([N+](=O)[O-])n([N+](=O)[O-])c12	1.897	279	8.29	32.1	191.7
O=[N+]([O-])c1nc([N+](=O)[O-])c2nncn2n1	1.835	478	8.29	31.5	191.7
Nn1nc([N+](=O)[O-])n2ncc([N+](=O)[O-])c12	1.817	417	8.28	31.2	295.4
Nn1nc([N+](=O)[O-])c2[nH]c([N+](=O)[O-])nc21	1.88	300	8.28	31.8	284.6
O=[N+]([O-])c1cc2[nH]nc([N+](=O)[O-])n2n1	1.886	287	8.28	31.9	265.3
Nc1nn([N+](=O)[O-])c2c1nc([N+](=O)[O-])n2N	1.845	374	8.28	31.5	235.4
Nc1n[nH]c2nnn([N+](=O)[O-])c12	1.834	515	8.28	31.4	194.1
O=[N+]([O-])c1n[nH]c2cnn([N+](=O)[O-])c12	1.861	328	8.28	31.6	128.1
Nn1ncc2c1c([N+](=O)[O-])nn2[N+](=O)[O-]	1.82	403	8.27	31.1	219.6
Nc1nc2c([nH]1)c([N+](=O)[O-])nn2[N+](=O)[O-]	1.891	276	8.27	31.8	216.1
Nc1nn(N)c2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.858	341	8.27	31.5	215.9
Nn1ncc2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.841	367	8.27	31.4	213.7
O=[N+]([O-])c1nc([N+](=O)[O-])n2ncnc2n1	1.847	438	8.27	31.4	185.3
O=[N+]([O-])n1ncc2cnn([N+](=O)[O-])c21	1.815	410	8.27	31.1	121.6
Nn1c([N+](=O)[O-])nc2c1nc([N+](=O)[O-])n2N	1.841	366	8.26	31.2	304.3
Nn1nc([N+](=O)[O-])c2nc([N+](=O)[O-])[nH]c21	1.869	309	8.26	31.5	272.8
Nc1nc2c(nc([N+](=O)[O-])n2[N+](=O)[O-])n1N	1.887	284	8.26	31.7	248.2
Nc1nc2c([N+](=O)[O-])nn([N+](=O)[O-])c2n1N	1.865	326	8.26	31.5	234.5
O=[N+]([O-])c1nn([N+](=O)[O-])c2[nH]cnc12	1.877	290	8.26	31.6	214.1

Nc1nn(N)c2nc([N+](=O)[O-])n([N+](=O)[O-])c12	1.862	327	8.26	31.4	199
Nn1c([N+](=O)[O-])nc2nc([N+](=O)[O-])n(N)c21	1.837	368	8.25	31.1	304.8
Nc1nc2nc([N+](=O)[O-])n([N+](=O)[O-])c2n1N	1.889	275	8.25	31.7	239.6
Nc1nn([N+](=O)[O-])c2c([N+](=O)[O-])cnn12	1.84	358	8.25	31.2	211.4
Nn1nc([N+](=O)[O-])n2nc([N+](=O)[O-])cc12	1.825	380	8.24	31	279.7
Nc1nn([N+](=O)[O-])c2[nH]nnc12	1.84	487	8.24	31.1	240.4
Nc1nc2c(c([N+](=O)[O-])nn2[N+](=O)[O-])n1N	1.857	327	8.24	31.3	228.9
O=[N+]([O-])c1nn2cnnnc2c1[N+](=O)[O-]	1.802	512	8.24	30.7	226.9
O=[N+]([O-])c1nc2[nH]ncc2n1[N+](=O)[O-]	1.867	299	8.24	31.4	198
O=[N+]([O-])c1n[nH]c2ncn([N+](=O)[O-])c12	1.857	313	8.24	31.2	145.8
Nn1c([N+](=O)[O-])nc2nn[nH]c21	1.824	507	8.23	30.9	304.8
Nn1c([N+](=O)[O-])nc2[nH]c([N+](=O)[O-])nc21	1.879	275	8.23	31.4	292.6
Nn1c([N+](=O)[O-])nc2nc([N+](=O)[O-])[nH]c21	1.879	276	8.23	31.4	291
Nc1nc2nn[nH]c2n1[N+](=O)[O-]	1.84	484	8.23	31.1	272.7
Nc1nc2c([N+](=O)[O-])nn(N)c2n1[N+](=O)[O-]	1.858	319	8.23	31.2	260.1
Nc1c([N+](=O)[O-])nn2c(N)nn([N+](=O)[O-])c12	1.866	306	8.23	31.3	225
Nn1ncc2nc([N+](=O)[O-])n([N+](=O)[O-])c21	1.824	376	8.23	30.9	212.1
O=[N+]([O-])c1nc2c(cnn2[N+](=O)[O-])[nH]1	1.875	277	8.23	31.3	209
Nc1cc2n([N+](=O)[O-])nc([N+](=O)[O-])n2n1	1.835	351	8.23	31	191.8
O=[N+]([O-])c1cc2nnc([N+](=O)[O-])nn2n1	1.828	445	8.22	30.8	230.5
Nn1ncc2c([N+](=O)[O-])nn([N+](=O)[O-])c21	1.82	375	8.22	30.8	209.9
Nc1nn([N+](=O)[O-])c2c1nc(N)n2[N+](=O)[O-]	1.872	288	8.22	31.3	199.8
O=[N+]([O-])c1n[nH]c2c1cnn2[N+](=O)[O-]	1.853	310	8.22	31.1	198.3
O=[N+]([O-])n1cnc2ncn([N+](=O)[O-])c21	1.836	342	8.22	30.9	123.3
Nn1c([N+](=O)[O-])nc2[nH]nnc21	1.823	500	8.21	30.7	303
Nn1nc([N+](=O)[O-])c2c1nnn2N	1.796	554	8.21	30.4	287.4
O=[N+]([O-])c1nn2cn[nH]c2c1[N+](=O)[O-]	1.838	333	8.21	30.9	252.6
Nc1nc2nc([N+](=O)[O-])n([N+](=O)[O-])c2[nH]1	1.912	211	8.21	31.6	227.6
Nc1nc2c(nc([N+](=O)[O-])n2[N+](=O)[O-])[nH]1	1.907	216	8.21	31.5	221
Nn1cnc2c1c([N+](=O)[O-])nn2[N+](=O)[O-]	1.826	356	8.21	30.7	204
Nc1nn([N+](=O)[O-])c2c1cnn2[N+](=O)[O-]	1.828	356	8.21	30.8	133.8
O=[N+]([O-])c1nc2nc([N+](=O)[O-])[nH]c2[nH]1	1.9	223	8.2	31.4	272.9
Nc1nn2cnn([N+](=O)[O-])c2c1[N+](=O)[O-]	1.835	338	8.2	30.8	213.5
Nn1cnc2c([N+](=O)[O-])nn([N+](=O)[O-])c21	1.826	352	8.2	30.7	205.7
O=[N+]([O-])n1cnc2[nH]nnc21	1.814	498	8.2	30.5	180.2
Nc1nc2nc([N+](=O)[O-])[nH]c2n1[N+](=O)[O-]	1.906	208	8.19	31.4	263.9
Nc1nc2[nH]nnc2n1[N+](=O)[O-]	1.829	478	8.19	30.6	249.6
Nc1nc2nc(N)n([N+](=O)[O-])c2n1[N+](=O)[O-]	1.888	245	8.19	31.2	237.8
O=[N+]([O-])c1nnnc2ncnn12	1.784	631	8.19	30.2	233.3
Nc1nn([N+](=O)[O-])c2cc([N+](=O)[O-])nn12	1.838	325	8.19	30.7	218

O=[N+]([O-])c1nc2c([N+](=O)[O-])n[nH]c2[nH]1	1.877	248	8.18	31	253.3
Nc1nn([N+](=O)[O-])c2nc(N)n([N+](=O)[O-])c12	1.862	283	8.18	30.9	187.3
Nc1c([N+](=O)[O-])nn2cnn([N+](=O)[O-])c12	1.835	325	8.18	30.6	181.8
Nn1nc([N+](=O)[O-])c2c1cnn2[N+](=O)[O-]	1.801	385	8.18	30.2	161.6
O=[N+]([O-])c1nc2[nH]nc([N+](=O)[O-])c2[nH]1	1.88	240	8.17	31	272.3
Nc1nc2nc([N+](=O)[O-])n(N)c2n1[N+](=O)[O-]	1.863	277	8.17	30.8	257.5
Nc1nc2c(nc([N+](=O)[O-])n2N)n1[N+](=O)[O-]	1.862	276	8.17	30.8	255.3
Nn1nc([N+](=O)[O-])c2c1ncn2[N+](=O)[O-]	1.818	347	8.17	30.3	181.4
Nc1nc2cnn([N+](=O)[O-])c2n1[N+](=O)[O-]	1.836	315	8.17	30.5	155.4
O=[N+]([O-])c1nc2[nH]c([N+](=O)[O-])nc2[nH]1	1.895	210	8.16	31	274.7
O=[N+]([O-])c1nc2nnncn2n1	1.783	614	8.16	29.9	252.8
Nn1c([N+](=O)[O-])nc2c1cnn2[N+](=O)[O-]	1.8	375	8.16	30.1	232.6
Nc1nn([N+](=O)[O-])c2nn[nH]c12	1.818	480	8.16	30.3	203.7
Nn1nc([N+](=O)[O-])c2cnn([N+](=O)[O-])c21	1.799	378	8.16	30.1	196.3
O=[N+]([O-])n1cnc2c1ncn2[N+](=O)[O-]	1.834	311	8.16	30.4	139.1
Nc1nc2[nH]c([N+](=O)[O-])nc2n1[N+](=O)[O-]	1.897	202	8.15	31	249
Nc1nc2c(nc(N)n2[N+](=O)[O-])n1[N+](=O)[O-]	1.877	239	8.15	30.8	242.1
O=[N+]([O-])c1cnn2cnn([N+](=O)[O-])c12	1.8	367	8.15	30	178.3
Nc1nn([N+](=O)[O-])c2ncn([N+](=O)[O-])c12	1.839	300	8.15	30.4	128.2
Nn1c([N+](=O)[O-])nc2cnn([N+](=O)[O-])c21	1.794	374	8.14	29.9	216.8
O=[N+]([O-])c1nc2cnn([N+](=O)[O-])c2[nH]1	1.854	265	8.14	30.5	216
Nn1nc([N+](=O)[O-])c2ncn([N+](=O)[O-])c21	1.817	334	8.14	30.1	215.7
Nn1cnc2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.836	299	8.14	30.3	213.7
Nn1cnc2nc([N+](=O)[O-])n([N+](=O)[O-])c21	1.838	298	8.14	30.4	201.6
Nc1nc2c(cnn2[N+](=O)[O-])n1[N+](=O)[O-]	1.833	307	8.14	30.3	160.7
Nc1nc2ncn([N+](=O)[O-])c2n1[N+](=O)[O-]	1.845	276	8.13	30.3	152.5
Nc1nn([N+](=O)[O-])c2c1ncn2[N+](=O)[O-]	1.831	301	8.13	30.2	129.5
Nn1ncn2nc([N+](=O)[O-])c([N+](=O)[O-])c12	1.794	365	8.12	29.8	250
Nc1n[nH]c2c1nnn2[N+](=O)[O-]	1.823	458	8.12	30.1	220.5
O=[N+]([O-])c1nc2nc[nH]c2n1[N+](=O)[O-]	1.86	246	8.12	30.4	203.4
O=[N+]([O-])c1nn([N+](=O)[O-])c2ccnn12	1.787	376	8.12	29.7	165.9
Nc1nnnc2nc([N+](=O)[O-])nn12	1.813	553	8.11	29.9	258.7
O=[N+]([O-])n1ncc2[nH]nnc21	1.782	503	8.11	29.5	163.9
O=[N+]([O-])c1nc2ncn([N+](=O)[O-])c2[nH]1	1.859	235	8.1	30.2	228.9
Nc1nc2nnnc([N+](=O)[O-])n2n1	1.806	553	8.09	29.7	250.5
Nn1c([N+](=O)[O-])nc2ncn([N+](=O)[O-])c21	1.812	312	8.09	29.7	219.4
Nc1nn([N+](=O)[O-])c2c1nnn2N	1.795	498	8.09	29.6	217.7
O=[N+]([O-])c1cc2n([N+](=O)[O-])ncn2n1	1.796	342	8.09	29.6	191.6
Nc1nn(N)c2nnn([N+](=O)[O-])c12	1.785	512	8.09	29.5	188.9
O=[N+]([O-])c1nn([N+](=O)[O-])c2nc[nH]c12	1.834	270	8.09	29.9	181.2

Nc1nc2c(ncn2[N+](=O)[O-])n1[N+](=O)[O-]	1.844	258	8.09	30	163.2
Nc1nn([N+](=O)[O-])c2nnn(N)c12	1.786	506	8.08	29.4	235.9
Nn1c([N+](=O)[O-])nc2c1ncn2[N+](=O)[O-]	1.812	307	8.08	29.6	219.7
O=[N+]([O-])c1nc2[nH]cnc2n1[N+](=O)[O-]	1.847	245	8.08	30	195.2
Nc1nc2nnn(N)c2n1[N+](=O)[O-]	1.803	472	8.07	29.4	247.7
O=[N+]([O-])c1nc2c(ncn2[N+](=O)[O-])[nH]1	1.85	229	8.06	29.8	204.7
Nc1nn(N)c2c1nnn2[N+](=O)[O-]	1.781	501	8.06	29.2	201.9
Nc1nc2c(nnn2N)n1[N+](=O)[O-]	1.805	463	8.05	29.4	257.9
Nc1nc2nnn([N+](=O)[O-])c2[nH]1	1.823	427	8.05	29.6	219.7
Nc1nnc([N+](=O)[O-])n2nc([N+](=O)[O-])c(N)c12	1.884	341	8.03	30	290.4
O=[N+]([O-])c1nc2nn[nH]c2[nH]1	1.831	388	8	29.2	305.2
Nc1nn2c([N+](=O)[O-])nnc(N)c2c1[N+](=O)[O-]	1.873	344	8	29.7	296.1
Nc1nn2c([N+](=O)[O-])nnc([N+](=O)[O-])c2c1N	1.867	351	8	29.6	261.8

Table S4 Result of AI-aided energetic molecules screening.

SMILES	Density g/cm^3	HOF kJ/mol	D km/s	P GPa	BDE kJ/mol	Novel	Source
Nc1nc([N+](=O)[O-])nn1N	1.781	174.2	8.11	29.6	282.6	1	ref[5]
Nn1cnc([N+](=O)[O-])c1[N+](=O)[O-]	1.785	142.2	8.24	30.3	266.7	1	ref[6]
Nn1nc([N+](=O)[O-])nc1[N+](=O)[O-]	1.851	236	8.92	36.6	267.9		ref[7]
Nc1c([N+](=O)[O-])nc([N+](=O)[O-])n1N	1.835	123.2	8.35	32.1	290.8	1	ref[8]
O=[N+]([O-])c1nn([N+](=O)[O-])c2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.943	506.2	9.41	41.4	140.4		ref[1]
NN=c1n([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1[N+](=O)[O-]	1.917	274	9.53	41.9	128.9		
N=c1n([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1[N+](=O)[O-]	1.947	153	9.43	42	158.9		
Nn1c([N+](=O)[O-])c([N+](=O)[O-])n([N+](=O)[O-])c1=NN[N+](=O)[O-]	1.893	281.5	9.32	39.5	130.9		
O=[N+]([O-])c1nn([N+](=O)[O-])c2nnn([N+](=O)[O-])c12	1.898	593.3	9.31	40.2	123.4	1	
O=[N+]([O-])c1nn([N+](=O)[O-])c2nnnn12	1.92	693.4	9.29	40.9	213.9	1	
NN=c1n(N[N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1N[N+](=O)[O-]	1.882	348.5	9.29	37.4	136.6		
O=[N+]([O-])c1nc2n([N+](=O)[O-])nc([N+](=O)[O-])n2n1	1.924	535.5	9.28	39.8	211.9		
O=[N+]([O-])c1nn2c([N+](=O)[O-])nn([N+](=O)[O-])c2c1[N+](=O)[O-]	1.932	476.9	9.24	39.4	224.3		
Nc1c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1[N+](=O)[O-]	1.919	65.4	9.23	39.5	210	1	
O=[N+]([O-])NN=c1c2nc([N+](=O)[O-])n([N+](=O)[O-])c2nc([N+](=O)[O-])n1[N+](=O)[O-]	1.968	576.2	9.2	38.7	128.5	1	
Nc1c([N+](=O)[O-])c([N+](=O)[O-])n([N+](=O)[O-])c1[N+](=O)[O-]	1.925	17.9	9.15	38.7	199.9	1	
O=[N+]([O-])c1nc([N+](=O)[O-])c2c([N+](=O)[O-])nn([N+](=O)[O-])c2n1	1.946	494.8	9.15	38.3	170.8		
O=[N+]([O-])C1=NC(=C([N+](=O)[O-])[N+](=O)[O-])NN1[N+](=O)[O-]	1.895	163.1	9.15	38.4	140	1	
NN1N=C([N+](=O)[O-])[N-][N+](=O)N=C1[N+](=O)[O-]	1.882	311.8	9.13	37.9	144.9	1	
Nc1c([N+](=O)[O-])nc([N+](=O)[O-])n1[N+](=O)[O-]	1.914	138.8	9.12	38.3	222	1	
NN1NC([N+](=O)[O-])=NC1=C([N+](=O)[O-])[N+](=O)[O-]	1.878	184.4	9.12	36.4	152.9		
Nc1noc(=N[N+](=O)[O-])n1[N+](=O)[O-]	1.894	166.9	9.12	37.5	128.8	1	
NN=c1[nH]nc(N[N+](=O)[O-])n1[N+](=O)[O-]	1.906	327.2	9.12	37.6	125	1	
Nc1nc([N+](=O)[O-])n([N+](=O)[O-])c1[N+](=O)[O-]	1.904	117.3	9.1	38.8	172.2	1	
NC1=NN([N+](=O)[O-])C([N+](=O)[O-])=C([N+](=O)[O-])N1N	1.912	137.4	9.1	37.7	136.1	1	
NC(N)=C1N=C([N+](=O)[O-])N([N+](=O)[O-])C([N+](=O)[O-])=C([N+](=O)[O-])N1[N+](=O)[O-]	1.935	69.4	9.09	38.4	131.3	1	
Nc1c([N+](=O)[O-])n[n+](=O)nc([N+](=O)[O-])c1[N+](=O)[O-]	1.937	133.1	9.08	39.4	241.9	1	
Nn1nc([N+](=O)[O-])c2c1c([N+](=O)[O-])nn2[N+](=O)[O-]	1.9	484.1	9.08	36.9	206		

NN1C([N+](=O)[O-])=NC([N+](=O)[O-])=NC1=C([N+](=O)[O-])[N+](=O)[O-]	1.908	146.1	9.08	36.3	155.1	
NN1N=C([N+](=O)[O-])N2C(N[N+](=O)[O-])=NN([N+](=O)[O-])C2=C1[N+](=O)[O-]	1.956	442.1	9.08	37.9	128	1
O=[N+]([O-])c1nc([N+](=O)[O-])c2nnnn2c1[N+](=O)[O-]	1.925	573.8	9.07	39.2	253.2	1
NNN1C([N+](=O)[O-])=C1[N+](=O)[O-]	1.89	180.6	9.07	37.7	202.7	1
Nc1c([N+](=O)[O-])n[n+](=O)[n-]c1[N+](=O)[O-]	1.895	136.3	9.07	38.3	196.8	
O=[N+]([O-])c1nc([N+](=O)[O-])c2nnc([N+](=O)[O-])n2c1[N+](=O)[O-]	1.917	514.7	9.06	36.9	233.1	1
NC1=C([N+](=O)[O-])ON=C([N+](=O)[O-])N1[N+](=O)[O-]	1.923	17	9.06	37.8	150.1	1
NN=c1[nH]c([N+](=O)[O-])c([N+](=O)[O-])n1N[N+](=O)[O-]	1.892	227.5	9.04	35.3	167.1	
O=[N+]([O-])c1nc2n(c1[N+](=O)[O-])N([N+](=O)[O-])C=NO2	1.927	347.3	9.03	38.2	145.7	1
O=[N+]([O-])c1nc2onc([N+](=O)[O-])n2c1[N+](=O)[O-]	1.93	403.1	9.02	38.6	224.8	
Nc1nnn2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.906	560.3	9.02	37.3	222.6	1
O=[N+]([O-])c1nn([N+](=O)[O-])c2c([N+](=O)[O-])onc12	1.913	404.2	9.02	38	196.2	1
O=[N+]([O-])c1nn([N+](=O)[O-])c2nonc12	1.889	495.8	9.02	37.7	190.2	1
O=[N+]([O-])NN1O[N-]C=C1[N+](=O)[O-]	1.879	200.7	9.02	36	134.5	1
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])N([N+](=O)[O-])N1	1.877	183.1	9.01	34.8	122.7	1
Nc1nnn([N+](=O)[O-])c1[N+](=O)[O-]	1.856	213.4	9	36.8	139.5	
NN1C(=N[N+](=O)[O-])NC([N+](=O)[O-])=NC([N+](=O)[O-])=C1[N+](=O)[O-]	1.91	184.5	9	35.7	139	1
O=[N+]([O-])c1nnc2nnnn2c1[N+](=O)[O-]	1.891	686.6	8.99	38.8	252.9	1
O=[N+]([O-])c1nc([N+](=O)[O-])c2nc([N+](=O)[O-])n([N+](=O)[O-])c2n1	1.938	447.3	8.99	37.4	196.3	
Nc1nc([N+](=O)[O-])c([N+](=O)[O-])[n-][n+]1=O	1.885	128.9	8.98	37.8	204.9	
O=[N+]([O-])C1=NC(=C([N+](=O)[O-])[N+](=O)[O-])NN1	1.898	122.6	8.98	36.2	165.5	
N=c1n(N)c([N+](=O)[O-])c(N[N+](=O)[O-])n1[N+](=O)[O-]	1.867	222.6	8.98	36.2	130.7	1
O=[N+]([O-])c1nc([N+](=O)[O-])n2nc([N+](=O)[O-])nc2n1	1.925	486.3	8.97	37.4	208.9	
N=c1[nH]nc(N[N+](=O)[O-])n1[N+](=O)[O-]	1.897	160.5	8.97	36.6	128.2	1
Nn1nc([N+](=O)[O-])nc2n(c([N+](=O)[O-])c1[N+](=O)[O-])N=C2[N+](=O)[O-]	1.928	405.3	8.96	36.2	248.5	1
Nc1c([N+](=O)[O-])[nH]n1[N+](=O)[O-]	1.903	40.2	8.96	35.3	247.6	1
Nn1nc([N+](=O)[O-])n2nc([N+](=O)[O-])c([N+](=O)[O-])c12	1.899	456.1	8.95	37.1	278.5	
Nn1c(N[N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]	1.861	159.9	8.95	36.2	131.5	1
O=[N+]([O-])Nc1[nH]c([N+](=O)[O-])nc1[N+](=O)[O-]	1.915	122.4	8.95	37.4	130.8	1
O=[N+]([O-])c1nn[nH]c1[N+](=O)[O-]	1.877	244.9	8.94	37	272.4	
O=[N+]([O-])c1nc([N+](=O)[O-])n2ncn2c1[N+](=O)[O-]	1.894	392.4	8.94	36.9	235.1	1
O=[N+]([O-])c1nc2c([N+](=O)[O-])c([N+](=O)[O-])nc([N+](=O)[O-])n2n1	1.916	426.6	8.94	36.5	233.2	

O=[N+]([O-])c1nn([N+](=O)[O-])c2c([N+](=O)[O-])n[nH]c12	1.954	398.1	8.94	37	187.8	
Nn1[nH]c([N+](=O)[O-])nc1=N[N+](=O)[O-]	1.876	197.3	8.94	36.1	173.7	1
NN1O[N-]N=C1[N+](=O)[O-]	1.821	321	8.94	34.6	162.6	1
O=[N+]([O-])c1nc([N+](=O)[O-])c2nnn([N+](=O)[O-])c2n1	1.887	517	8.94	36.7	153.8	1
Nc1[n-][n+](=O)oc1[N+](=O)[O-]	1.864	86	8.93	37	232.7	1
O=[N+]([O-])c1nc2nnnc-2n([N+](=O)[O-])n1	1.891	617.7	8.93	36.6	204.9	1
NN=c1n(N)c([N+](=O)[O-])c(N[N+](=O)[O-])n1[N+](=O)[O-]	1.854	309.4	8.93	36.2	121.6	
Nn1nc([N+](=O)[O-])n2onc2nnc([N+](=O)[O-])c1[N+](=O)[O-]	1.896	562.6	8.92	36.6	252.4	1
Nc1nc([N+](=O)[O-])nn1[N+](=O)[O-]	1.87	196.8	8.92	37	238.1	
NN=c1c2nc([N+](=O)[O-])n([N+](=O)[O-])c2nc([N+](=O)[O-])n1[N+](=O)[O-]	1.942	463.9	8.92	37.2	177	
O=[N+]([O-])C(=C1N=C[N+]([O-])ON([N+](=O)[O-])N1)[N+](=O)[O-]	1.866	132.6	8.92	35.5	127.7	1
O=[N+]([O-])c1nc2onc([N+](=O)[O-])n2n1	1.921	425.7	8.91	37	229.2	1
Nc1nc2n([N+](=O)[O-])nc([N+](=O)[O-])n2c1[N+](=O)[O-]	1.929	413.4	8.9	37	236.9	1
O=[N+]([O-])c1nc([N+](=O)[O-])n2c([N+](=O)[O-])nc([N+](=O)[O-])c2n1	1.908	472.8	8.9	36.4	191.5	1
NC1=C([N+](=O)[O-])N([N+](=O)[O-])C([N+](=O)[O-])=Nc2nnc([N+](=O)[O-])n21	1.935	418.2	8.89	37	146.6	1
O=[N+]([O-])C1=Nn2c([N+](=O)[O-])nc([N+](=O)[O-])c21	1.923	422.4	8.88	37.6	215.8	1
Nn1nc([N+](=O)[O-])[nH]c1=N[N+](=O)[O-]	1.88	215.7	8.88	35.3	210.6	1
NN1NC(=C(N[N+](=O)[O-])[N+](=O)[O-])N=C1[N+](=O)[O-]	1.868	132.2	8.88	34.3	145.9	
N=c1[nH]c([N+](=O)[O-])c([N+](=O)[O-])n1[N+](=O)[O-]	1.934	14.6	8.87	37.2	240.6	
N=c1n([N+](=O)[O-])cc([N+](=O)[O-])n1[N+](=O)[O-]	1.881	131.5	8.87	36.6	161.6	
NN=c1n(C=N[N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1[N+](=O)[O-]	1.856	280.3	8.87	35.8	132	
NN=c1n(N)c([N+](=O)[O-])c([N+](=O)[O-])n1N[N+](=O)[O-]	1.845	288.5	8.86	34.7	214.4	
Nc1[n-][n+](=O)c([N+](=O)[O-])nc1[N+](=O)[O-]	1.906	142.3	8.86	37.6	209.6	
Nc1[n-][n+](=O)[n-]c1[N+](=O)[O-]	1.866	249.7	8.86	36.5	203	1
O=[N+]([O-])N=Cc1[n-][n+](=O)c([N+](=O)[O-])nc1[N+](=O)[O-]	1.873	257.4	8.86	37.2	128.2	
NC1=NNC([N+](=O)[O-])=NN1C(=NC(=C([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.892	244.7	8.85	34.5	207.1	1
N=c1[nH]c([N+](=O)[O-])c([N+](=O)[O-])n1N[N+](=O)[O-]	1.906	65.4	8.85	35.1	132.1	
Nn1nc([N+](=O)[O-])n2nc([N+](=O)[O-])nc12	1.884	514.6	8.84	35.9	277.4	
Nc1nnc([N+](=O)[O-])n2c([N+](=O)[O-])nn([N+](=O)[O-])c3nnc1n3-2	1.941	795.3	8.84	37.1	237.5	1
Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1	1.875	124.9	8.84	36.6	204.9	1
Nn1nc([N+](=O)[O-])n2c(N[N+](=O)[O-])nn([N+](=O)[O-])c3nnc1n3-2	1.913	770.6	8.84	37	152.8	

NN=c1n(N)c([N+](=O)[O-])c([N+](=O)[O-])n1[N+](=O)[O-]	1.861	219.3	8.83	36.1	232.3	
O=[N+]([O-])C1=NC([N+](=O)[O-])=NC(=C([N+](=O)[O-])[N+](=O)[O-])C([N+](=O)[O-])=N1	1.882	83.3	8.83	34.8	165.1	1
NC1=C([N+](=O)[O-])C([N+](=O)[O-])=Nc2c([N+](=O)[O-])nnn2N1[N+](=O)[O-]	1.901	408.3	8.83	35.7	146.8	1
Nc1noc([N+](=O)[O-])nc1=N[N+](=O)[O-]	1.871	125.3	8.83	34.8	130.8	1
Nc1nc([N+](=O)[O-])c2c([N+](=O)[O-])nnn2c1[N+](=O)[O-]	1.919	452.9	8.82	36.1	247.3	1
N=c1n(N)c([N+](=O)[O-])c([N+](=O)[O-])n1N[N+](=O)[O-]	1.855	172.6	8.82	34.7	170.6	
N=c1c2nc([N+](=O)[O-])n([N+](=O)[O-])c2nc([N+](=O)[O-])n1[N+](=O)[O-]	1.94	358.9	8.81	36.8	195.5	
NC1=Nc2c([N+](=O)[O-])nn([N+](=O)[O-])c2N=C([N+](=O)[O-])N1[N+](=O)[O-]	1.928	388.4	8.81	35.3	155.9	1
NC1=C(N[N+](=O)[O-])C(=C(N[N+](=O)[O-])[N+](=O)[O-])N=C([N+](=O)[O-])N1N[N+](=O)[O-]	1.869	144.7	8.81	33.3	121.3	1
Nc1c2nc([N+](=O)[O-])n([N+](=O)[O-])c2nn1[N+](=O)[O-]	1.924	374.1	8.8	35.9	203.9	1
O=[N+]([O-])C1=Nc2c([N+](=O)[O-])nn([N+](=O)[O-])c21	1.891	357.9	8.8	35.9	153.1	1
O=[N+]([O-])N=Cc1c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1[N+](=O)[O-]	1.856	189.6	8.8	36.2	145.5	1
O=[N+]([O-])c1nn[nH]c2nc([N+](=O)[O-])c([N+](=O)[O-])c1-2	1.94	389.7	8.79	35.1	225.6	1
O=[N+]([O-])c1nn([N+](=O)[O-])c2nn[nH]c12	1.92	528.5	8.79	36.1	214.5	1
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])NN1[N+](=O)[O-]	1.868	195.7	8.79	33.9	144.8	1
Nn1c([N+](=O)[O-])c([N+](=O)[O-])n(C=N[N+](=O)[O-])c1=N[N+](=O)[O-]	1.845	211.3	8.79	34.8	136.2	
Nc1nnc2n(N[N+](=O)[O-])c([N+](=O)[O-])nn12	1.884	512	8.79	36.3	130.5	1
O=[N+]([O-])N=CC(=C1N=C([N+](=O)[O-])N(C=N[N+](=O)[O-])N1[N+](=O)[O-])[N+](=O)[O-]	1.853	269.4	8.79	33.3	121.1	1
N=c1n([N+](=O)[O-])nc([N+](=O)[O-])n1N	1.864	193.9	8.78	35.5	254.3	1
NN1N=C([N+](=O)[O-])n2nc([N+](=O)[O-])c3nnc1n32	1.886	755.9	8.78	36.1	172.1	1
Nn1cc([N+](=O)[O-])n(N[N+](=O)[O-])c1=NN[N+](=O)[O-]	1.823	274.7	8.78	33.8	159.6	
Nn1c([N+](=O)[O-])nc2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.904	402.9	8.77	35.6	249.3	1
O=[N+]([O-])c1nn2c([N+](=O)[O-])nc([N+](=O)[O-])c([N+](=O)[O-])c2c2nnnc1-2	1.946	620.1	8.77	35.5	246.6	1
O=[N+]([O-])N=c1c2nc([N+](=O)[O-])[nH]c2nc([N+](=O)[O-])n1[N+](=O)[O-]	1.938	364.9	8.77	36.3	131.9	
NN1N=C([N+](=O)[O-])c2c(nc([N+](=O)[O-])nc2[N+](=O)[O-])O1	1.916	360.7	8.77	35.3	122	1
Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c2nnc([N+](=O)[O-])n12	1.918	427	8.76	36.2	236.7	1
Nc1nc2n([N+](=O)[O-])nc([N+](=O)[O-])n2n1	1.891	452	8.76	36.6	205	
Nn1c(N[N+](=O)[O-])nnc2c([N+](=O)[O-])nc([N+](=O)[O-])c1-2	1.929	398	8.76	34.9	157.3	1
N=c1n(NC=N[N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-	1.84	200.3	8.76	35	150.4	1

])n1[N+](=O)[O-]						
O=[N+]([O-])NN1C([N+](=O)[O-])=NC=NC1=C([N+](=O)[O-])[N+](=O)[O-]	1.846	224	8.76	33.2	128.7	1
NN=c1c2nc([N+](=O)[O-])nc([N+](=O)[O-])c2nc([N+](=O)[O-])n1[N+](=O)[O-]	1.936	465.4	8.75	35.4	171.4	
N[N+]([O-])N=CN=c1[nH]nnn1[N+](=O)[O-]	1.825	474.5	8.75	33.4	149.3	1
O=[N+]([O-])c1nc2n([N+](=O)[O-])ncn2c1[N+](=O)[O-]	1.879	422.1	8.74	35.3	227.5	1
NN1N=C([N+](=O)[O-])c2nnn([N+](=O)[O-])c2N=C1[N+](=O)[O-]	1.863	563.6	8.74	34.8	133.7	1
O=[N+]([O-])c1cnc([N+](=O)[O-])[n+](=O)[n-]1	1.867	148.4	8.73	35	169.3	
Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(=N[N+](=O)[O-])n1N	1.857	144.4	8.73	34	150.6	
N=c1n(C=N[N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1[N+](=O)[O-]	1.866	195.3	8.73	36.2	137.6	
O=[N+]([O-])c1nc2n(n1)c1nnc([N+](=O)[O-])n12	1.893	695.5	8.72	34.3	260.1	1
O=[N+]([O-])c1nc([N+](=O)[O-])c2nncn2c1[N+](=O)[O-]	1.889	465	8.72	34.3	259.3	1
Nc1c([N+](=O)[O-])n[nH]c(=NN[N+](=O)[O-])c1[N+](=O)[O-]	1.892	218.7	8.72	34.8	200.6	1
Nc1nc([N+](=O)[O-])nc2c1c([N+](=O)[O-])nn2[N+](=O)[O-]	1.911	395.8	8.72	34.5	198.6	
NNC(=C1N=NN=C1[N+](=O)[O-])[N+](=O)[O-]	1.838	319.4	8.72	33.8	177.3	1
NC1=NN(N)C([N+](=O)[O-])N(N)C([N+](=O)[O-])=C([N+](=O)[O-])N1[N+](=O)[O-]	1.88	116.2	8.72	35.6	133.1	1
O=[N+]([O-])N=Cn1c([N+](=O)[O-])nc2c(nc([N+](=O)[O-])n2[N+](=O)[O-])c1=N[N+](=O)[O-]	1.91	547.3	8.72	35.4	127.2	1
Nc1nc([N+](=O)[O-])c2nc([N+](=O)[O-])nn2c1[N+](=O)[O-]	1.934	392.4	8.71	35.9	256.2	1
N=c1[nH]nnn1[N+](=O)[O-]	1.89	277.7	8.71	33.8	243.3	
O=[N+]([O-])c1nn2cnn([N+](=O)[O-])c2c1[N+](=O)[O-]	1.853	410.6	8.71	35.6	190.4	
Nn1c([N+](=O)[O-])c(N[N+](=O)[O-])[nH]c1=NN[N+](=O)[O-]	1.852	228	8.71	34.6	144.8	
O=[N+]([O-])C1=NC(=C([N+](=O)[O-])[N+](=O)[O-])N1	1.881	90.3	8.7	34.3	202.8	1
O=[N+]([O-])N=CN1C([N+](=O)[O-])=NC1=C([N+](=O)[O-])[N+](=O)[O-]	1.854	164.7	8.7	33.7	141.2	1
Nn1nc([N+](=O)[O-])nc2c([N+](=O)[O-])nc([N+](=O)[O-])c-2c1=NN[N+](=O)[O-]	1.898	491.8	8.69	34.1	193.6	1
Nn1nc([N+](=O)[O-])n2onc([N+](=O)[O-])c3nnc1n3-2	1.88	720.1	8.68	34.7	251.3	1
O=[N+]([O-])c1nc2n([N+](=O)[O-])ncn2n1	1.861	432.9	8.68	34.9	170.1	
NN=c1c2nc([N+](=O)[O-])n(N[N+](=O)[O-])c2c([N+](=O)[O-])c([N+](=O)[O-])n1N[N+](=O)[O-]	1.885	485.2	8.68	33.6	155.3	1
NC(N)=C1N=C([N+](=O)[O-])N=C([N+](=O)[O-])N1[N+](=O)[O-]	1.88	72.7	8.68	34.2	132.8	1
NC1=Nc2nnn([N+](=O)[O-])c2N=C([N+](=O)[O-])N1[N+](=O)[O-]	1.887	444.9	8.68	34.2	122.2	1
Nc1nnnn1[N+](=O)[O-]	1.819	384.1	8.67	34.4	227.5	
Nc1nn2n3c(nnc13)N([N+](=O)[O-])N=C2[N+](=O)[O-]	1.901	726.7	8.67	34.5	175.8	1

Nc1nn([N+](=O)[O-])c2c(N[N+](=O)[O-])nnc-2c1[N+](=O)[O-]	1.921	436.6	8.67	33.7	139.5	1
Nc1nc([N+](=O)[O-])c2nnnn2c1[N+](=O)[O-]	1.897	529.7	8.66	36	285.2	1
NC1=C([N+](=O)[O-])OO[N+](=O)[N-]1	1.894	37.3	8.66	34.2	237.6	1
Nc1nnc([N+](=O)[O-])n(N)c1=N[N+](=O)[O-]	1.841	273.7	8.66	33.2	172.9	1
O=[N+]([O-])N=Cc1c([N+](=O)[O-])nc2n([N+](=O)[O-])nc([N+](=O)[O-])n12	1.873	558.7	8.66	35	155.6	1
NC1=C([N+](=O)[O-])C([N+](=O)[O-])=C(N[N+](=O)[O-])NN1	1.886	160.7	8.66	34.9	138.6	1
Nn1c([N+](=O)[O-])c([N+](=O)[O-])nc(C=N[N+](=O)[O-])c1=N[N+](=O)[O-]	1.835	204.9	8.66	33.2	125.8	1
O=[N+]([O-])c1nc2[nH]c([N+](=O)[O-])nc([N+](=O)[O-])c-2n1	1.949	324.6	8.65	34.5	233.6	
O=[N+]([O-])N=Cn1nc([N+](=O)[O-])[nH]1	1.833	226.4	8.65	33.9	150.5	1
Nc1c([N+](=O)[O-])c([N+](=O)[O-])nc2nnc([N+](=O)[O-])n12	1.906	392.8	8.64	35.4	224	
NN1C([N+](=O)[O-])=CC(=C([N+](=O)[O-])[N+](=O)[O-])N=C1[N+](=O)[O-]	1.847	99.4	8.64	32.7	183	1
Nc1c(N[N+](=O)[O-])nc([N+](=O)[O-])c2nnc([N+](=O)[O-])n12	1.907	411.6	8.64	34.8	132.3	1
Nc1nnc([N+](=O)[O-])nc1[N+](=O)[O-]	1.865	223.9	8.63	35.2	236.4	
O=[N+]([O-])NN=c1[nH]c([N+](=O)[O-])cnc1[N+](=O)[O-]	1.868	159.1	8.63	32.7	178.4	1
Nc1nc([N+](=O)[O-])c2nnnc-2c([N+](=O)[O-])c1[N+](=O)[O-]	1.921	497.6	8.62	34.1	269.1	1
Nc1nc([N+](=O)[O-])c2n(nc([N+](=O)[O-])n1C=N[N+](=O)[O-])C([N+](=O)[O-])=N2	1.926	494.1	8.62	33.4	201.5	1
O=[N+]([O-])N=Cc1c([N+](=O)[O-])nc([N+](=O)[O-])[nH]c1=N[N+](=O)[O-]	1.867	156	8.62	33.7	124.2	
Nc1c([N+](=O)[O-])c([N+](=O)[O-])nc2c([N+](=O)[O-])nc([N+](=O)[O-])n12	1.909	292.7	8.61	35.4	218.9	1
Nc1c([N+](=O)[O-])[n-]oc1=NN[N+](=O)[O-]	1.832	205.2	8.61	34	154.4	1
N=c1c2nc([N+](=O)[O-])n(N[N+](=O)[O-])c2nc([N+](=O)[O-])n1[N+](=O)[O-]	1.915	368.1	8.61	34.5	145.2	
O=[N+]([O-])N=Cc1c([N+](=O)[O-])noc1[N+](=O)[O-]	1.816	220.2	8.61	33.5	139.3	1
O=[N+]([O-])N=Cn1[nH]c([N+](=O)[O-])c1N=C([N+](=O)[O-])[N+](=O)[O-]	1.835	196.1	8.61	33.3	137.4	1
O=[N+]([O-])C=C1NN=NN1[N+](=O)[O-]	1.833	318.9	8.61	33.1	125.2	1
Nc1nc([N+](=O)[O-])n([N+](=O)[O-])c2nc([N+](=O)[O-])nc1-2	1.935	324.3	8.6	34.6	222.8	
O=[N+]([O-])c1cc([N+](=O)[O-])nc([N+](=O)[O-])n1	1.847	154.5	8.6	34.7	196	1
NC1=NN(C=N[N+](=O)[O-])N2NN=C([N+](=O)[O-])N12	1.893	491.5	8.6	32.9	168.9	1
NN1C([N+](=O)[O-])=NC=NC1=C([N+](=O)[O-])[N+](=O)[O-]	1.807	194	8.6	31.9	146.1	
NC1=NC(C=N[N+](=O)[O-])=C([N+](=O)[O-])N=C([N+](=O)[O-])N1[N+](=O)[O-]	1.863	163.8	8.6	32.6	125.8	1
N=C1N(C=N[N+](=O)[O-])C(C=N[N+](=O)[O-])=C([N+](=O)[O-])N=C([N+](=O)[O-])N1[N+](=O)[O-]	1.848	252.6	8.6	31.7	125.5	1

NN=c1n(N[N+](=O)[O-])c([N+](=O)[O-])c(C=N[N+](=O)[O-])c2nnnn12	1.87	665.8	8.6	32.4	125.3	1
Nc1nn2c([N+](=O)[O-])n[nH]c3c(n2n1[N+](=O)[O-])=NN=3	1.964	653.3	8.59	35.6	305	1
Nc1c([N+](=O)[O-])nnc2c([N+](=O)[O-])nc([N+](=O)[O-])c-2c1[N+](=O)[O-]	1.949	357.6	8.59	33.7	251.7	1
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])N(N)N1	1.821	184.5	8.59	31.5	185.5	
O=[N+]([O-])N=Cc1c([N+](=O)[O-])nc([N+](=O)[O-])c2nnc([N+](=O)[O-])n12	1.902	565.3	8.59	34.2	183.8	1
Nc1nc([N+](=O)[O-])c2c([N+](=O)[O-])nn([N+](=O)[O-])c2n1	1.903	373.4	8.59	34.3	155.6	
Nn1c([N+](=O)[O-])nc(C=N[N+](=O)[O-])c([N+](=O)[O-])c1=N[N+](=O)[O-]	1.828	291.5	8.59	33	146.3	1
Nc1nc([N+](=O)[O-])oc1[N+](=O)[O-]	1.869	-27.9	8.58	34.1	276	1
O=[N+]([O-])c1nc2cnnn2c([N+](=O)[O-])c1[N+](=O)[O-]	1.858	439.7	8.58	33.5	237.2	1
NC1=NN([N+](=O)[O-])C(N)=NN1[N+](=O)[O-]	1.872	193.9	8.58	34.7	158.4	1
NN1C=NC([N+](=O)[O-])=NC(=C([N+](=O)[O-])[N+](=O)[O-])N1	1.812	179.6	8.58	31.2	157.5	1
NC1=C([N+](=O)[O-])N=C([N+](=O)[O-])N2C(N[N+](=O)[O-])=NC([N+](=O)[O-])=NN12	1.927	341.3	8.58	34	146.6	1
NC(C=N[N+](=O)[O-])=C1N=C([N+](=O)[O-])N=C(N[N+](=O)[O-])N1[N+](=O)[O-]	1.835	246.7	8.58	31.7	124	1
NC1=C(N[N+](=O)[O-])N(N)NC([N+](=O)[O-])=C1[N+](=O)[O-]	1.869	156.1	8.58	34.3	123	1
NN1N=C1N[N+](=O)[O-]	1.779	339.6	8.58	31.8	121.2	1
Nn1nc([N+](=O)[O-])nc2c([N+](=O)[O-])nnc1-2	1.87	484.1	8.57	33.4	274.5	1
Nn1nc([N+](=O)[O-])o1	1.799	128.4	8.57	32.6	232.5	1
NC1NC([N+](=O)[O-])=NC(=C([N+](=O)[O-])[N+](=O)[O-])N1	1.839	25.8	8.57	32.4	214.5	1
Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c2c1nnn2[N+](=O)[O-]	1.889	363.6	8.57	34	191.5	
NC1=NC([N+](=O)[O-])=C([N+](=O)[O-])C([N+](=O)[O-])=Nc2c1nnn2N[N+](=O)[O-]	1.879	420.2	8.57	33.1	140.8	1
O=[N+]([O-])c1cc([N+](=O)[O-])n2c([N+](=O)[O-])nc([N+](=O)[O-])c2n1	1.887	356.9	8.56	33.6	220.8	1
Nc1c([N+](=O)[O-])nnc2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.91	403.1	8.56	34	214.6	1
Nn1c([N+](=O)[O-])nc2c1nnn2N[N+](=O)[O-]	1.837	543.2	8.56	34.2	183.7	1
NC1=NNC(=C([N+](=O)[O-])[N+](=O)[O-])N(N)N1	1.836	280.3	8.56	32.6	168.8	1
O=[N+]([O-])NN=c1o[nH]c2c([N+](=O)[O-])nc([N+](=O)[O-])nc12	1.938	269	8.56	34.8	158.1	1
NN1C([N+](=O)[O-])=NC=NC1=C(N[N+](=O)[O-])[N+](=O)[O-]	1.819	144.5	8.56	30.6	130.8	
O=[N+]([O-])N=CC(C=N[N+](=O)[O-])=C1N=C([N+](=O)[O-])N=C([N+](=O)[O-])N1N[N+](=O)[O-]	1.829	325.2	8.56	31	129.3	1
Nn1c([N+](=O)[O-])c(N[N+](=O)[O-])c2c1nc([N+](=O)[O-])n2N[N+](=O)[O-]	1.894	307.1	8.56	34.5	120.9	1

NN=c1c(=N[N+](=O)[O-])[nH]c([N+](=O)[O-])c([N+](=O)[O-])n1N	1.881	180.7	8.55	33.2	242.1	1
Nc1c2nc([N+](=O)[O-])c([N+](=O)[O-])nc([N+](=O)[O-])c-2nc1[N+](=O)[O-]	1.94	256.1	8.55	34.1	231.3	1
Nn1nc(C=N[N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.797	234.9	8.55	32.4	214.9	1
NC1=Nc2c(nc([N+](=O)[O-])n2[N+](=O)[O-])C([N+](=O)[O-])=NN(N)C1=N[N+](=O)[O-]	1.898	481.1	8.55	32	138.1	1
N=c1c(C=N[N+](=O)[O-])c([N+](=O)[O-])nc([N+](=O)[O-])n1[N+](=O)[O-]	1.856	178.4	8.55	34	131.7	
N=c1oc(C=N[N+](=O)[O-])c([N+](=O)[O-])n1[N+](=O)[O-]	1.855	36.3	8.55	33.3	129.6	1
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])NNC1[N+](=O)[O-]	1.843	117.8	8.55	32.5	129.5	1
Nc1c(N[N+](=O)[O-])nc([N+](=O)[O-])c2nc([N+](=O)[O-])nn12	1.913	344.7	8.55	34.4	123.5	1
NN1C(C=N[N+](=O)[O-])=C([N+](=O)[O-])N=C([N+](=O)[O-])N1C=N[N+](=O)[O-]	1.818	212.1	8.55	31.5	123.3	1
O=[N+]([O-])N=CC1=C([N+](=O)[O-])N=C([N+](=O)[O-])N[N+](=O)[N-]1	1.847	252.5	8.55	33.7	120.2	1
Nc1nc([N+](=O)[O-])n2nc([N+](=O)[O-])nc2n1	1.9	419.9	8.54	34.2	238.1	
Nc1nc2c([N+](=O)[O-])c([N+](=O)[O-])nc([N+](=O)[O-])n2n1	1.901	318.3	8.54	35.2	231	
Nc1nc([N+](=O)[O-])c2nnn([N+](=O)[O-])c2c1[N+](=O)[O-]	1.89	380.1	8.54	33.8	224.6	
NC(C=N[N+](=O)[O-])=C1N=C([N+](=O)[O-])N=C([N+](=O)[O-])N1NC1N=C([N+](=O)[O-])N=C([N+](=O)[O-])N1N[N+](=O)[O-]	1.816	537.8	8.54	28.5	146.9	1
N=c1onc(C=N[N+](=O)[O-])n1[N+](=O)[O-]	1.842	198	8.54	33.5	122.6	1
Nn1nc([N+](=O)[O-])c2nnc([N+](=O)[O-])nc21	1.855	489.4	8.53	32.9	245.6	1
Nc1nc([N+](=O)[O-])n2onc([N+](=O)[O-])c12	1.891	334.9	8.53	33.9	243.2	1
NC(N)=c1nc([N+](=O)[O-])nnc1=C([N+](=O)[O-])[N+](=O)[O-]	1.885	255.8	8.53	32.9	236.1	1
Nc1nc([N+](=O)[O-])nc2c1nnn2[N+](=O)[O-]	1.875	426.3	8.53	33.3	209.2	1
Nc1nc([N+](=O)[O-])[nH]c(=NN[N+](=O)[O-])c1[N+](=O)[O-]	1.883	170.4	8.53	33.5	193.2	
N[N+]([O-])c1cn2onc([N+](=O)[O-])n12	1.83	450.4	8.53	31.9	190	1
Nn1c([N+](=O)[O-])ncc([N+](=O)[O-])c1=N[N+](=O)[O-]	1.808	188	8.53	32.6	163.1	
O=[N+]([O-])N=Cc1c([N+](=O)[O-])nc([N+](=O)[O-])c2nnn([N+](=O)[O-])c12	1.882	573.9	8.53	32.9	156.3	
NC(NC(=N[N+](=O)[O-])[N+](=O)[O-])=c1nc(N[N+](=O)[O-])[nH]n([N+](=O)[O-])c(=C([N+](=O)[O-])[N+](=O)[O-])nc1N	1.86	367.8	8.53	32.1	129.4	1
Nc1nc([N+](=O)[O+])c([N+](=O)[O-])c2nnnn12	1.873	427.9	8.52	34.4	252.2	1
Nc1oc([N+](=O)[O-])nc1[N+](=O)[O-]	1.876	-40.3	8.52	34.4	244.8	1
Nc1nc([N+](=O)[O-])nc2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.91	331.7	8.52	34.2	203.8	
N=c1c([N+](=O)[O-])nc(C=N[N+](=O)[O-])c([N+](=O)[O-])n1[N+](=O)[O-]	1.844	181.8	8.52	33.7	141.3	1

NC=C1N=C([N+](=O)[O-])N=C([N+](=O)[O-])N1N[N+](=O)[O-]	1.841	150.8	8.52	32.4	134.1	
Nc1c([N+](=O)[O-])c([N+](=O)[O-])nc2nc(N[N+](=O)[O-])nn12	1.906	295.2	8.52	34.3	131.2	
Nc1nc2onc([N+](=O)[O-])n2c1[N+](=O)[O-]	1.915	314.5	8.51	34.6	266.6	
NC1=C([N+](=O)[O-])Nc2nc([N+](=O)[O-])nn2C([N+](=O)[O-])=N1	1.936	333.4	8.51	34.2	256.3	1
Nc1nc([N+](=O)[O-])c2onc([N+](=O)[O-])n12	1.902	319.7	8.51	34.4	243.7	1
O=[N+]([O-])c1cn2ncn([N+](=O)[O-])n12	1.847	363.3	8.51	32.5	199.5	1
NC1=c2nc([N+](=O)[O-])nc([N+](=O)[O-])c2=NC(N[N+](=O)[O-])=C([N+](=O)[O-])N1	1.945	309.5	8.51	32.4	156.2	1
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])NN1C(N)N[N+](=O)[O-]	1.802	169.8	8.51	30.5	152.9	1
NN1C=NN2C(=N1)N([N+](=O)[O-])N=C2[N+](=O)[O-]	1.852	493	8.51	31.9	133.1	1
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])NN1	1.847	155.5	8.5	31.8	203.9	
Nc1nc([N+](=O)[O-])c2c(nnn2[N+](=O)[O-])c1[N+](=O)[O-]	1.892	373.1	8.5	33.7	202.6	
NN=c1[nH]c([N+](=O)[O-])nc2c([N+](=O)[O-])nc([N+](=O)[O-])nc2c1=NN[N+](=O)[O-]	1.899	537.4	8.5	32.5	166.9	1
O=[N+]([O-])N=C1Nc2c([N+](=O)[O-])nc([N+](=O)[O-])n21	1.911	365.4	8.5	34.9	150.8	1
NN=CN1C([N+](=O)[O-])=C([N+](=O)[O-])N=C(N[N+](=O)[O-])N1N	1.831	229.1	8.5	31.6	142	1
O=[N+]([O-])N=Cc1nc([N+](=O)[O-])n(C=N[N+](=O)[O-])c(=N[N+](=O)[O-])c1[N+](=O)[O-]	1.856	383.5	8.5	33.6	130.8	1
Nc1c(C=N[N+](=O)[O-])nc([N+](=O)[O-])n1[N+](=O)[O-]	1.81	197.1	8.5	32.2	129.7	1
Nc1nnnc2c([N+](=O)[O-])nnc-2c1[N+](=O)[O-]	1.898	589	8.49	32.5	295.6	1
O=[N+]([O-])N=Cc1nnc2c([N+](=O)[O-])c([N+](=O)[O-])nc([N+](=O)[O-])n12	1.876	510.7	8.49	33.5	163.5	
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])N(C=N[N+](=O)[O-])N=N1	1.8	293.1	8.49	30.4	143	1
NC(C=N[N+](=O)[O-])=C1N=C([N+](=O)[O-])N=C([N+](=O)[O-])N1N[N+](=O)[O-]	1.826	244.7	8.49	30.9	132.3	1
Nc1nc([N+](=O)[O-])nc2nc([N+](=O)[O-])nn12	1.896	394.7	8.48	34.1	241	
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])NN1N	1.818	160.1	8.48	30.8	197	
NC1=C([N+](=O)[O-])N=NC1Nc1c([N+](=O)[O-])n(C=N[N+](=O)[O-])n1[N+](=O)[O-]	1.838	363.8	8.48	30.9	169.6	1
Nc1c([N+](=O)[O-])nn2onc(N[N+](=O)[O-])n3nnnc3c12	1.912	630	8.48	33.8	157.9	1
N=c1n(C=N[N+](=O)[O-])c(C=N[N+](=O)[O-])c([N+](=O)[O-])n1[N+](=O)[O-]	1.823	256.9	8.48	32.2	129.8	
NC1=C([N+](=O)[O-])N=C([N+](=O)[O-])C1=NN[N+](=O)[O-]	1.872	131.5	8.48	32.5	126.8	1
Nc1c([N+](=O)[O-])cc(N[N+](=O)[O-])n1[N+](=O)[O-]	1.823	93.8	8.48	31.3	125.7	1
Nn1nc([N+](=O)[O-])c2[nH]nc([N+](=O)[O-])c21	1.905	410.4	8.47	31.8	290.9	
N=c1n(C=N[N+](=O)[O-])c(N)c([N+](=O)[O-])n1[N+](=O)[O-]	1.836	180.8	8.47	32.2	161.6	
Nc1nc([N+](=O)[O-])n2nc(N[N+](=O)[O-])c([N+](=O)[O-	1.894	344.2	8.47	33.8	132.1	1

])c2n1						
O=[N+]([O-])N=c1[nH]cnc2c([N+](=O)[O-])nc([N+](=O)[O-])nc2c1=N[N+](=O)[O-]	1.934	400	8.47	33	124.1	1
N=c1[nH]c([N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]	1.9	-34	8.46	34.1	245.2	
NC1=NNC([N+](=O)[O-])=C([N+](=O)[O-])N1N	1.862	153.9	8.46	32.6	221.4	1
Nn1nc([N+](=O)[O-])n2nc([N+](=O)[O-])cc2c1=NN[N+](=O)[O-]	1.848	478.3	8.46	32.2	216	1
O=[N+]([O-])c1nc([N+](=O)[O-])c2[nH]c([N+](=O)[O-])nc2n1	1.925	297.4	8.46	34.9	215.9	
Nc1nc([N+](=O)[O-])n(C=N[N+](=O)[O-])c1[N+](=O)[O-]	1.843	185.3	8.46	33.1	186.1	1
N=[N+]([O-])NC(=C1N=C(N)N1[N+](=O)[O-])[N+](=O)[O-]	1.871	178.9	8.46	31.9	165.2	1
NC1=NN=C([N+](=O)[O-])C([N+](=O)[O-])=C(N)N1[N+](=O)[O-]	1.866	71.9	8.46	33.3	151.1	1
Nc1nn(C=N[N+](=O)[O-])c2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.871	470.4	8.46	31.2	144.5	
Nc1nc([N+](=O)[O-])c2nnon(N[N+](=O)[O-])c3nnc1n23	1.844	605.7	8.46	32.1	143.1	1
O=[N+]([O-])c1nc2nnncn2c1[N+](=O)[O-]	1.843	549.5	8.45	32.4	253.1	1
N[N+]([O-])c1cn2nnnc2c([N+](=O)[O-])c1[N+](=O)[O-]	1.864	537.6	8.45	34.3	207.1	1
N[N+]([O-])C1=NC2=C([N+](=O)[O-])N2N=C1[N+](=O)[O-]	1.91	325.6	8.45	32.7	188	1
NC1=NN2C([N+](=O)[O-])=NC([N+](=O)[O-])=NC([N+](=O)[O-])=C2C([N+](=O)[O-])=N1	1.914	293.1	8.45	31.7	187.7	1
N=C1C([N+](=O)[O-])=C([N+](=O)[O-])N1N	1.843	109.3	8.45	32.1	177.6	1
NC1=c2nc([N+](=O)[O-])n([N+](=O)[O-])c2=NN=C([N+](=O)[O-])N1C=N[N+](=O)[O-]	1.899	417.1	8.45	32.6	171.5	1
O=[N+]([O-])N=Cc1[nH]nc([N+](=O)[O-])c1[N+](=O)[O-]	1.832	196.6	8.45	32.4	167.6	1
Nn1nc([N+](=O)[O-])n2c(C=N[N+](=O)[O-])c([N+](=O)[O-])nc2c1=NN[N+](=O)[O-]	1.85	610.4	8.45	31.8	160.4	1
Nc1nc2c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])nn2c1[N+](=O)[O-]	1.902	271.2	8.44	34.7	251.1	1
NN=c1[nH]c([N+](=O)[O-])nc2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.923	380.1	8.44	33.4	232.5	
O=[N+]([O-])c1cnn2c([N+](=O)[O-])nc([N+](=O)[O-])c2n1	1.859	429.7	8.44	33	228.5	1
Nn1nc([N+](=O)[O-])n2c(C=N[N+](=O)[O-])nn([N+](=O)[O-])c3nnc1n3-2	1.86	845	8.44	33.9	209.6	
Nc1nc([N+](=O)[O-])nc2c([N+](=O)[O-])c([N+](=O)[O-])nc-2c(=N[N+](=O)[O-])c1[N+](=O)[O-]	1.932	302.3	8.44	33.7	190.8	1
NC1=C([N+](=O)[O-])C(=C(N[N+](=O)[O-])[N+](=O)[O-])N1	1.887	35.6	8.44	31.7	180.7	1
Nc1c([N+](=O)[O-])c([N+](=O)[O-])n(C=N[N+](=O)[O-])c1[N+](=O)[O-]	1.845	67.9	8.44	31.8	175.2	1
Nc1[nH]c(=N[N+](=O)[O-])n(C=N[N+](=O)[O-])c1[N+](=O)[O-]	1.85	118.5	8.44	30.9	165.6	
NN1NC1[N+](=O)[O-]	1.708	110.6	8.44	31.4	145.4	1
O=[N+]([O-])Nc1[nH]c2nc([N+](=O)[O-])n3nnnc3c2c1[N+](=O)[O-]	1.962	535.8	8.44	33.5	131.1	

Nc1nc([N+](=O)[O-])c2c([N+](=O)[O-])nnoc1-2	1.905	310.2	8.43	32.4	237.9	1
Nc1c(C=N[N+](=O)[O-])c([N+](=O)[O-])nc([N+](=O)[O-])n2[nH]nc(N)n2c1[N+](=O)[O-]	1.941	508	8.43	32.3	231.3	1
N=C1N=NC([N+](=O)[O-])=C1[N+](=O)[O-]	1.829	173.9	8.43	32.4	205.7	
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])N([N+](=O)[O-])C(N)=N1	1.854	109.2	8.43	31.5	168.9	1
Nc1nc([N+](=O)[O-])c2nnn([N+](=O)[O-])c2n1	1.858	434.7	8.43	33.6	156	1
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])N(C=N[N+](=O)[O-])N=C1[N+](=O)[O-]	1.831	167.4	8.43	30.2	154.4	1
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])NN1C=N[N+](=O)[O-]	1.813	221.2	8.43	30.2	123.9	1
Nc1nn(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.843	112.9	8.42	32.2	294.5	1
Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c2nnnn12	1.88	492.2	8.42	34.3	248.6	1
O=[N+]([O-])N=C1NC=NN2C(=C1[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])=C2[N+](=O)[O-]	1.904	616.8	8.42	32.1	171.1	1
NC1=NC(=C(N[N+](=O)[O-])[N+](=O)[O-])N=C1[N+](=O)[O-]	1.873	51.1	8.42	31.3	136.2	1
Nc1[nH]c([N+](=O)[O-])nc1[N+](=O)[O-]	1.879	37.8	8.41	32	294	1
NN=C1N=C([N+](=O)[O-])C([N+](=O)[O-])=N1	1.821	217.4	8.41	31.3	179.5	1
NN=c1ncn([N+](=O)[O-])nc1[N+](=O)[O-]	1.793	263.8	8.41	31.4	158.9	1
O=[N+]([O-])N=Cc1[nH]c(=N[N+](=O)[O-])n(C=N[N+](=O)[O-])c1[N+](=O)[O-]	1.822	234.7	8.41	31.3	132.6	
Nn1nc(C=N[N+](=O)[O-])[nH]c1=N[N+](=O)[O-]	1.825	259.9	8.41	31.5	130.4	1
NC1=C([N+](=O)[O-])N2C(N)=C([N+](=O)[O-])NN2C([N+](=O)[O-])=N1	1.931	240.8	8.4	33.5	285	1
O=[N+]([O-])c1cc2onc([N+](=O)[O-])n2c1[N+](=O)[O-]	1.88	226.1	8.4	32.9	236.5	1
NN=c1[nH]c([N+](=O)[O-])nc2c1nnn2N[N+](=O)[O-]	1.891	516.1	8.4	31.6	180.1	1
Nc1cn(N)c(=N[N+](=O)[O-])n1[N+](=O)[O-]	1.808	150.4	8.4	30.4	148.7	1
Nn1nc([N+](=O)[O-])nc1C=N[N+](=O)[O-]	1.771	242.2	8.4	31.4	145.8	
NC1=C(C=N[N+](=O)[O-])[N-][N+](=O)C(=N[N+](=O)[O-])c2nc([N+](=O)[O-])nc([N+](=O)[O-])c2C([N+](=O)[O-])=N1	1.873	551.5	8.4	33.4	140.9	1
N=c1n(C=N[N+](=O)[O-])c([N+](=O)[O-])c(C=N[N+](=O)[O-])n1[N+](=O)[O-]	1.817	259.9	8.4	32.2	126.3	
NN=c1[nH]c([N+](=O)[O-])c([N+](=O)[O-])n1N	1.853	178	8.39	31.1	328.1	
Nn1nc(C=N[N+](=O)[O-])n2c([N+](=O)[O-])nn([N+](=O)[O-])c3nnc1n3-2	1.846	796.5	8.39	33.5	200	
NC1=NC(=C(N[N+](=O)[O-])[N+](=O)[O-])N=C([N+](=O)[O-])N1	1.845	86.3	8.39	30.3	142	1
Nn1cnn2c([N+](=O)[O-])nn([N+](=O)[O-])c3nnc1n3-2	1.828	703.5	8.38	33.4	235	1
Nc1nc([N+](=O)[O-])n2oc([N+](=O)[O-])nc12	1.9	227	8.38	33.6	234.7	1
Nn1c([N+](=O)[O-])nc(C=N[N+](=O)[O-])c1[N+](=O)[O-]	1.794	201.1	8.38	31.6	196.9	1
Nc1nnc2nc([N+](=O)[O-])nc([N+](=O)[O-])nc-2c1=NN[N+](=O)[O-]	1.89	512.3	8.38	33.3	174.8	1
NN=c1[nH]c([N+](=O)[O-])nc2c1nc([N+](=O)[O-])n2N[N+](=O)[O-]	1.904	400.1	8.38	33.7	170.4	

Nn1c([N+](=O)[O-])nc2c(nc(C=N[N+](=O)[O-])n2[N+](=O)[O-])c1=N[N+](=O)[O-]	1.865	509.2	8.38	31.7	162.3	
O=[N+]([O-])N=Cc1c([N+](=O)[O-])nn2c([N+](=O)[O-])cc(=N[N+](=O)[O-])c([N+](=O)[O-])nc12	1.905	453.2	8.38	32.3	158	1
O=[N+]([O-])NC1=C([N+](=O)[O-])N(N[N+](=O)[O-])C([N+](=O)[O-])=CC1=C1N=NN=N1	1.85	450.4	8.38	30.7	142.1	1
NC1=C([N+](=O)[O-])C(=N[N+](=O)[O-])N1C=N[N+](=O)[O-]	1.823	165.8	8.38	30.4	120.2	1
NC(=C1N=C([N+](=O)[O-])N(N)N1)[N+](=O)[O-]	1.832	142.2	8.37	30.9	239.6	
Nc1nc([N+](=O)[O-])n([N+](=O)[O-])c1N	1.849	59.7	8.37	31.6	227.9	1
O=[N+]([O-])c1cc2nnnn2c([N+](=O)[O-])n1	1.841	486.2	8.37	32.9	212.3	1
NN=c1n(N)c([N+](=O)[O-])c(C=N[N+](=O)[O-])n1[N+](=O)[O-]	1.809	278.2	8.37	30.2	209.2	
NN=c1c(=NN[N+](=O)[O-])c2nc([N+](=O)[O-])nn12	1.862	461.7	8.37	32	185.9	1
O=[N+]([O-])N=Cc1[nH]c(=N[N+](=O)[O-])[nH]c1[N+](=O)[O-]	1.858	160.6	8.37	30.6	170.1	
NC1=NC(N[N+](=O)[O-])=C([N+](=O)[O-])C([N+](=O)[O-])=Nc2c1nnn2[N+](=O)[O-]	1.871	430.7	8.37	31.4	132.1	1
NN=c1n(C=N[N+](=O)[O-])c(N)c([N+](=O)[O-])n1N[N+](=O)[O-]	1.811	271.4	8.37	30.8	129.7	
NC1=NC(N[N+](=O)[O-])=C([N+](=O)[O-])C(C=N[N+](=O)[O-])=C([N+](=O)[O-])N1[N+](=O)[O-]	1.84	193.3	8.37	30	126.2	1
Nc1n[nH]c2c([N+](=O)[O-])nc([N+](=O)[O-])n12	1.914	331.4	8.36	33.4	252.3	1
N=c1c([N+](=O)[O-])nc([N+](=O)[O-])c2n1C([N+](=O)[O-])=N2	1.92	323.2	8.36	34.4	252.1	1
O=[N+]([O-])c1cc2n([N+](=O)[O-])c1N=NN2	1.848	414.5	8.36	30.2	214.6	1
NN1C=NC(=C([N+](=O)[O-])[N+](=O)[O-])NC(N[N+](=O)[O-])=C1N=C(N=C(n1cnnn1)[N+](=O)[O-])[N+](=O)[O-]	1.795	564.7	8.36	27.4	160.2	1
N=c1oc([N+](=O)[O-])nc2c1nnn2N[N+](=O)[O-]	1.889	307.3	8.36	33	144.5	1
Nc1nc([N+](=O)[O-])c(N[N+](=O)[O-])[nH]1	1.856	68.9	8.36	32.1	143.8	1
NN1N=C([N+](=O)[O-])N2C(N[N+](=O)[O-])=NC([N+](=O)[O-])=NC2=C1C=N[N+](=O)[O-]	1.871	430.3	8.36	30.6	132.7	1
O=[N+]([O-])N=c1[nH]cnc2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.901	381.2	8.36	32.1	132	1
Nn1ccn([N+](=O)[O-])c1=NN[N+](=O)[O-]	1.763	235.4	8.36	29.9	120	
Nc1c([N+](=O)[O-])ncn2c([N+](=O)[O-])nn12	1.872	312.1	8.35	32.3	260.8	1
Nc1nc2nc([N+](=O)[O-])c([N+](=O)[O-])nc([N+](=O)[O-])c-2n1	1.925	315.1	8.35	33.5	250.9	1
NN=c1c2nc([N+](=O)[O-])nc([N+](=O)[O-])c2nc([N+](=O)[O-])n1C=N[N+](=O)[O-]	1.893	468.4	8.35	32.1	166.8	
NC(N)=C1N=C([N+](=O)[O-])NN1[N+](=O)[O-]	1.843	104	8.35	31.3	158.6	
NC1=C(C=N[N+](=O)[O-])C=C([N+](=O)[O-])N=C([N+](=O)[O-])N1[N+](=O)[O-]	1.807	105.9	8.35	30	125.8	1
O=[N+]([O-])N=Cc1nc([N+](=O)[O-])[nH]c(=NN[N+](=O)[O-])c1[N+](=O)[O-]	1.829	225.2	8.35	31.2	124.5	
N=c1[nH]c([N+](=O)[O-])nc2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.932	241.9	8.34	32.8	241.9	

N=c1n(N)cc([N+](=O)[O-])n1[N+](=O)[O-]	1.801	75.5	8.34	30	239.8	
Nc1c(N=C([N+](=O)[O-])[N+](=O)[O-])[nH]n1C=N[N+](=O)[O-]	1.827	170.3	8.34	30.3	163.7	1
NC1=NC(=C(N[N+](=O)[O-])[N+](=O)[O-])N(N)N1	1.799	161.7	8.34	29.6	162.9	
Nc1c([N+](=O)[O-])ncn1N[N+](=O)[O-]	1.824	127.3	8.34	31.2	132.9	1
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])NNC(N)=C([N+](=O)[O-])C1=N[N+](=O)[O-]	1.863	207.8	8.34	31.4	130	1
NC1=NC(=C(N[N+](=O)[O-])[N+](=O)[O-])N([N+](=O)[O-])C(N)=N1	1.858	96.4	8.34	29.9	126.6	1
Nc1nc([N+](=O)[O-])c[nH]c([N+](=O)[O-])nc2nnc([N+](=O)[O-])n12	1.904	439.5	8.33	32.5	240.5	1
N=c1n(C=N[N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1C=N[N+](=O)[O-]	1.817	203.9	8.33	31.8	144	
Nc1nnc2nnc([N+](=O)[O-])nn12	1.818	607.3	8.32	31.5	257.5	
NN=C1NN=NC(N[N+](=O)[O-])=Nc2nnnn21	1.803	742.1	8.32	29.7	142.2	1
NC1=NC(NC(=N[N+](=O)[O-])[N+](=O)[O-])N=C1[N+](=O)[O-]	1.83	11.2	8.32	31	135.6	1
NC1=NON=CN1C1=C([N+](=O)[O-])N1[N+](=O)[O-]	1.846	230.1	8.32	31.4	126.2	1
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])NC1=N[N+](=O)[O-]	1.861	122.6	8.32	30.7	122.6	1
NN1C(=C[N+](=O)[O-])N=C([N+](=O)[O-])N1C=N[N+](=O)[O-]	1.773	209.4	8.32	29.5	121.6	
NC1=C([N+](=O)[O-])N=NNC([N+](=O)[O-])=N1	1.851	150.6	8.31	32	268.1	1
NN=c1n(N)cc([N+](=O)[O-])n1[N+](=O)[O-]	1.795	179.9	8.31	30.3	237.6	
NN1C(=C[N+](=O)[O-])N=C1[N+](=O)[O-]	1.77	136.6	8.31	28.6	189.1	1
NN=c1[nH]c([N+](=O)[O-])nc([N+](=O)[O-])c1C=N[N+](=O)[O-]	1.859	231.4	8.31	30.4	179.1	
Nc1nc([N+](=O)[O-])n2[nH]c([N+](=O)[O-])c(N[N+](=O)[O-])n3nnnc3c12	1.91	603.7	8.31	32.7	166.3	1
O=[N+]([O-])N=Cn1c([N+](=O)[O-])cnc1[N+](=O)[O-]	1.79	217.2	8.31	30.9	145.5	1
Nc1c([N+](=O)[O-])n(C=N[N+](=O)[O-])c(=N[N+](=O)[O-])n1N	1.814	155.6	8.31	30.5	140.5	
O=[N+]([O-])N=Cc1[nH]c(=NN[N+](=O)[O-])[nH]c1[N+](=O)[O-]	1.838	223.4	8.31	30.8	138.5	
N=c1c(C=N[N+](=O)[O-])nc([N+](=O)[O-])c(C=N[N+](=O)[O-])n1[N+](=O)[O-]	1.833	280.2	8.31	30.8	135.4	1
O=[N+]([O-])C1=NC2=C([N+](=O)[O-])NC([N+](=O)[O-])=NC([N+](=O)[O-])=C([N+](=O)[O-])C2=N1	1.881	165.2	8.3	31.4	208.5	1
NN=c1c2c(nnn2N)c([N+](=O)[O-])c([N+](=O)[O-])n1N[N+](=O)[O-]	1.847	492.5	8.3	32	190.4	1
N=c1[nH]c([N+](=O)[O-])nc2c1nc([N+](=O)[O-])n2N[N+](=O)[O-]	1.922	255.7	8.3	32.4	182.7	
NC1=NC(=C(N[N+](=O)[O-])[N+](=O)[O-])NN1	1.825	111	8.3	29.5	174.7	1
N=c1c(C=N[N+](=O)[O-])c([N+](=O)[O-])n2nnnc2n1[N+](=O)[O-]	1.867	613.9	8.3	31.6	172.5	1
Nc1c([N+](=O)[O-])nc([N+](=O)[O-])n1C=N[N+](=O)[O-]	1.814	158.9	8.3	31.3	164.7	1
NN1NC(=C[N+](=O)[O-])N=C1N[N+](=O)[O-]	1.763	226.8	8.3	28.1	131.9	

Nc1nc([N+](=O)[O-])n2c(C=N[N+](=O)[O-])nn([N+](=O)[O-])c12	1.828	435.8	8.3	32.1	121.1	1
NN=c1n(N)c([N+](=O)[O-])c([N+](=O)[O-])n1N	1.814	269	8.29	30.9	328.4	
Nn1c([N+](=O)[O-])n[nH]c1=NC=N[N+](=O)[O-]	1.822	278.2	8.29	31	238.1	1
O=[N+]([O-])c1nc([N+](=O)[O-])n2ncnnc12	1.826	553.3	8.29	31.5	226.8	1
NN=c1n(N)c(N)c([N+](=O)[O-])n1N[N+](=O)[O-]	1.805	267	8.29	30.3	226.4	
NN1NC(=C[N+](=O)[O-])N=C1[N+](=O)[O-]	1.784	196.8	8.29	30	223.7	
Nc1nc2n([N+](=O)[O-])nc([N+](=O)[O-])n2c1C=N[N+](=O)[O-]	1.843	475	8.29	31.1	164.7	1
NC1=Nc2c([N+](=O)[O-])nn([N+](=O)[O-])c2N=C([N+](=O)[O-])N1C=N[N+](=O)[O-]	1.869	415.8	8.29	30.9	161.2	1
N=C1NC(=N[N+](=O)[O-])N1C=N[N+](=O)[O-]	1.802	232.1	8.29	28.6	140.1	1
Nn1cnn(C=N[N+](=O)[O-])nc([N+](=O)[O-])n1C=N[N+](=O)[O-]	1.757	364.4	8.29	30.3	136.6	1
N=c1[nH]c([N+](=O)[O-])c([N+](=O)[O-])[nH]1	1.89	-71.7	8.28	31	274.6	
Nc1noc([N+](=O)[O-])n1	1.792	71.5	8.28	31	258.9	
N=c1[nH]c(N[N+](=O)[O-])c([N+](=O)[O-])n1N	1.833	132.9	8.28	31	188.9	
O=[N+]([O-])N=Cc1nc2oc([N+](=O)[O-])nn2c1[N+](=O)[O-]	1.86	330.8	8.28	32.4	178.9	1
O=[N+]([O-])N=CC1=C([N+](=O)[O-])N=C([N+](=O)[O-])NC([N+](=O)[O-])=N1	1.838	102.4	8.28	31.5	153.6	1
NC1=NC(=C(N[N+](=O)[O-])[N+](=O)[O-])N(N)C([N+](=O)[O-])=C([N+](=O)[O-])C1=C1N=NN=N1	1.853	484.4	8.28	28.6	145.6	1
Nc1c(N[N+](=O)[O-])nn2c([N+](=O)[O-])nn(N)c12	1.855	365	8.28	31	141.6	
NC1=NC([N+](=O)[O-])=NC(=C2NN([N+](=O)[O-])C(=C(N[N+](=O)[O-])[N+](=O)[O-])N=C2N)N=C1[N+](=O)[O-]	1.849	387.6	8.28	27.8	141.1	1
NN1N=C([N+](=O)[O-])N2NC(C=N[N+](=O)[O-])=NN=C12	1.838	519.7	8.28	29.5	131.3	1
O=[N+]([O-])N=CN=c1[nH]c([N+](=O)[O-])nc2c1nc([N+](=O)[O-])n2N[N+](=O)[O-]	1.876	422.4	8.28	30.8	126.9	
O=[N+]([O-])N=c1[nH]ccn1[N+](=O)[O-]	1.805	139.1	8.28	30.2	124.2	
Nn1nc([N+](=O)[O-])n2nc([N+](=O)[O-])cc12	1.825	379.8	8.27	30.1	279.7	
N=c1n(N)c(N)c([N+](=O)[O-])n1[N+](=O)[O-]	1.852	77.4	8.27	31.2	261.5	
NN=c1n(N)c(N)c([N+](=O)[O-])n1[N+](=O)[O-]	1.824	195.3	8.27	30.2	241	
NC1=C([N+](=O)[O-])C([N+](=O)[O-])=Nc2c([N+](=O)[O-])nc([N+](=O)[O-])c3nnc1n23	1.872	446	8.27	31.9	219.9	1
Nn1nc([N+](=O)[O-])c2[nH]nc(N[N+](=O)[O-])c21	1.889	364.8	8.27	31.5	159.9	
N=c1n(N)c([N+](=O)[O-])c([N+](=O)[O-])n1N	1.836	135.2	8.26	31.1	312.5	
O=[N+]([O-])c1cn2nnc3c(c([N+](=O)[O-])nn3[N+](=O)[O-])c2n1	1.84	661.9	8.26	31.6	203.5	
N=c1c(C=N[N+](=O)[O-])c2nnnc-2c([N+](=O)[O-])nn1[N+](=O)[O-]	1.884	617.5	8.26	30.9	202.9	1
Nn1nc([N+](=O)[O-])n2c(C=N[N+](=O)[O-])nnc12	1.804	563.6	8.26	30.5	185.7	1
N=c1c2nc([N+](=O)[O-])n(C=N[N+](=O)[O-])c2nc([N+](=O)[O-])n1[N+](=O)[O-]	1.879	404.3	8.26	32.8	174.4	

O=[N+]([O-])C1=Cc2nn[nH]c2N=C([N+](=O)[O-])N1[N+](=O)[O-]	1.88	330	8.26	32.8	133.2	1
O=[N+]([O-])C1=Cn2nnc([N+](=O)[O-])c21	1.839	387.6	8.25	29.2	253.1	1
NN=c1c([N+](=O)[O-])c(C=N[N+](=O)[O-])nc([N+](=O)[O-])n1C=N[N+](=O)[O-]	1.818	322.2	8.25	29.8	156.2	
NC1=C(C=N[N+](=O)[O-])N=C([N+](=O)[O-])N=C([N+](=O)[O-])N1C=N[N+](=O)[O-]	1.825	185.9	8.25	28.7	147.7	1
N[N+]([O-])c1cn2c([N+](=O)[O-])nc([N+](=O)[O-])nc2n1	1.856	452.3	8.25	31.7	147.5	1
NC(C=N[N+](=O)[O-])=C1N=C([N+](=O)[O-])N=C([N+](=O)[O-])N1C=N[N+](=O)[O-]	1.83	200.7	8.25	29.4	141.7	
NN=c1[nH]nc([N+](=O)[O-])o1	1.853	121.5	8.24	31.4	301.6	
Nn1ncc2c([N+](=O)[O-])nn([N+](=O)[O-])c21	1.82	375.5	8.24	30.4	209.9	
Nc1nnnc([N+](=O)[O-])c1C=N[N+](=O)[O-]	1.771	344	8.24	29.7	177.6	
Nc1nc([N+](=O)[O-])nc2c(nc(C=N[N+](=O)[O-])n2[N+](=O)[O-])c1=N[N+](=O)[O-]	1.887	482.5	8.24	30.9	132.9	1
NC1=C([N+](=O)[O-])N=C(C=N[N+](=O)[O-])C1=N[N+](=O)[O-]	1.839	142.7	8.24	29.3	132.9	1
O=[N+]([O-])N=CC(=C1N=C([N+](=O)[O-])N1C=N[N+](=O)[O-])[N+](=O)[O-]	1.797	163.3	8.24	29.9	131.4	1
Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c2nonc12	1.904	308.1	8.23	31.5	265.9	1
N=c1c([N+](=O)[O-])ncc2c([N+](=O)[O-])nn([N+](=O)[O-])c2c1[N+](=O)[O-]	1.886	324.7	8.23	31.6	200.3	1
NC1=CN2N=C([N+](=O)[O-])C([N+](=O)[O-])=NC([N+](=O)[O-])=C2C([N+](=O)[O-])=N1	1.905	249.7	8.23	31.4	185.6	1
NN=c1[nH]c(N[N+](=O)[O-])c([N+](=O)[O-])n1N	1.829	213	8.23	31.9	184.7	
NC1=C(C=N[N+](=O)[O-])N(C=N[N+](=O)[O-])C([N+](=O)[O-])=NC([N+](=O)[O-])=N1	1.828	177.1	8.23	28.8	151.8	1
O=[N+]([O-])N=Cc1ncc([N+](=O)[O-])n1[N+](=O)[O-]	1.751	212.5	8.23	30.5	120.6	1
Nc1nc2nnnc-2c([N+](=O)[O-])nc1[N+](=O)[O-]	1.887	484.7	8.22	31.5	271.7	1
N=C1NC([N+](=O)[O-])=C1[N+](=O)[O-]	1.865	-7.4	8.22	31.1	220.9	1
Nc1nc2nnn([N+](=O)[O-])c2nc1[N+](=O)[O-]	1.855	400.4	8.22	32.5	204.1	1
Nc1nc2[nH]c([N+](=O)[O-])c([N+](=O)[O-])n(C=N[N+](=O)[O-])c=2c1=NN[N+](=O)[O-]	1.907	320.8	8.22	29.6	179.2	1
Nn1nc([N+](=O)[O-])c2c1nc(C=N[N+](=O)[O-])n2[N+](=O)[O-]	1.819	450.8	8.22	30.6	165	1
Nc1c(C=N[N+](=O)[O-])nnc2c([N+](=O)[O-])nn([N+](=O)[O-])c12	1.853	503.8	8.22	29.4	161.9	1
NC1=C([N+](=O)[O-])N=c2c([N+](=O)[O-])ncnc2=NN1[N+](=O)[O-]	1.892	335.3	8.22	31.5	161.8	1
NC1=C([N+](=O)[O-])C([N+](=O)[O-])N(N)C=NC(=C(N[N+](=O)[O-])[N+](=O)[O-])N1	1.796	66.8	8.22	28.3	156.9	1
Nc1nc(C=N[N+](=O)[O-])c([N+](=O)[O-])c(=N[N+](=O)[O-])n1N	1.8	197	8.22	29	144.6	1
Nc1c([N+](=O)[O-])nc(N[N+](=O)[O-])c2nonc12	1.901	273.9	8.22	30.7	144.4	1
Nc1[nH]c(=NN[N+](=O)[O-])[nH]c1[N+](=O)[O-]	1.86	115.8	8.21	30.9	235.7	
O=[N+]([O-])c1nc([N+](=O)[O-])n2ncoc12	1.853	264.2	8.21	31.6	232.7	

N=c1nc([N+](=O)[O-])c(C=N[N+](=O)[O-])c([N+](=O)[O-])n1N	1.823	226.9	8.21	30.2	210.2	1
Nc1c([N+](=O)[O-])nn2c([N+](=O)[O-])c([N+](=O)[O-])nc2c1C=N[N+](=O)[O-]	1.884	398	8.21	31.6	204.9	1
N=c1n(N)c(N[N+](=O)[O-])c([N+](=O)[O-])n1N	1.801	203.4	8.21	30.3	184	
O=[N+]([O-])N=c1[nH]cnc2c([N+](=O)[O-])nc([N+](=O)[O-])n12	1.879	334	8.21	32.6	149.3	1
NC1=Nc2c(nc([N+](=O)[O-])n2[N+](=O)[O-])C1=NN[N+](=O)[O-]	1.846	367.6	8.21	29.5	135.8	1
O=[N+]([O-])N=c1[nH]cnc2c([N+](=O)[O-])nc([N+](=O)[O-])nc12	1.897	282.8	8.21	31.4	131.3	
NC1=NN(N)C([N+](=O)[O-])=NN1C(N1C([N+](=O)[O-])N=C([N+](=O)[O-])N1C=N[N+](=O)[O-])[N+](=O)[O-]	1.813	299.3	8.21	29.4	125.9	1
NC1C([N+](=O)[O-])=NC=NC1=C(N[N+](=O)[O-])[N+](=O)[O-]	1.794	-8.7	8.21	29.2	123.7	1
NC1=C(N[N+](=O)[O-])C([N+](=O)[O-])=NN2C1=C2[N+](=O)[O-]	1.92	213.8	8.21	30.7	120.9	1
O=[N+]([O-])C1=CNN=NC([N+](=O)[O-])=N1	1.818	149.3	8.2	30.9	218.4	1
Nn1nc(C=N[N+](=O)[O-])n2c([N+](=O)[O-])nn(C=N[N+](=O)[O-])c3nnc1n3-2	1.838	793.4	8.2	31.1	186.6	1
N=c1c(C=N[N+](=O)[O-])c([N+](=O)[O-])nc([N+](=O)[O-])n1C=N[N+](=O)[O-]	1.831	249.2	8.2	29.9	147.7	1
NN1C([N+](=O)[O-])=CC(=C2N=NN=N2)C(N[N+](=O)[O-])=C([N+](=O)[O-])N1C=N[N+](=O)[O-]	1.802	577.2	8.2	27.7	147	1
Nc1nc([N+](=O)[O-])n(N)c(=N[N+](=O)[O-])c1C=N[N+](=O)[O-]	1.815	204.3	8.2	29.4	144	1
Nc1c([N+](=O)[O-])c([N+](=O)[O-])nc2nc(N)n-2c1[N+](=O)[O-]	1.93	213.8	8.19	31.6	272.3	1
O=[N+]([O-])C1=Nc2n[nH]c([N+](=O)[O-])c21	1.879	282.2	8.19	30	220.1	1
NC1=Nc2c([N+](=O)[O-])nn([N+](=O)[O-])c21	1.869	263.5	8.19	29.1	215.4	1
Nc1nc([N+](=O)[O-])nc(C=N[N+](=O)[O-])c2nc([N+](=O)[O-])n1-2	1.888	359.7	8.19	30.2	183.4	1
N=c1c([N+](=O)[O-])nc(N[N+](=O)[O-])c2nn[nH]c2c1[N+](=O)[O-]	1.929	416.8	8.19	32.2	146.2	1
Nn1cnn2nc(N[N+](=O)[O-])c([N+](=O)[O-])c12	1.827	364.1	8.19	30.9	128.1	1
NC1=C([N+](=O)[O-])c2c(nc([N+](=O)[O-])n3nnnc23)NN=C1[N+](=O)[O-]	1.909	660.1	8.18	31.1	226.3	1
NC1=C(N)n2nc([N+](=O)[O-])c([N+](=O)[O-])c2N=NC(N[N+](=O)[O-])=N1	1.833	389.3	8.18	29.9	174.9	1
O=[N+]([O-])N=CN1C([N+](=O)[O-])=C[N-]N=C1[N+](=O)[O-]	1.788	190.1	8.18	30.9	125	1
Nc1nnc([N+](=O)[O-])nc1C=N[N+](=O)[O-]	1.78	270.5	8.17	29.1	159	
Nc1nc(C=N[N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1	1.804	175	8.17	30.1	154.4	1
Nc1c([N+](=O)[O-])nc2nnc(N)n2c1[N+](=O)[O-]	1.89	349	8.16	31.2	277	
Nc1nnc2n(N)nc([N+](=O)[O-])n12	1.802	513.1	8.16	29.5	272	1
O=[N+]([O-])C1=NN=NC1=NNc1c([N+](=O)[O-])nc2[nH]nnc([N+](=O)[O-])c1-2	1.893	726.3	8.16	29.8	219	1

N=c1c2nc([N+](=O)[O-])nc([N+](=O)[O-])c2nc([N+](=O)[O-])n1C=N[N+](=O)[O-]	1.888	392.5	8.16	31.6	183.8	
NC1=NC([N+](=O)[O-])=c2nc([N+](=O)[O-])n(N[N+](=O)[O-])c2=C(N)N1N	1.845	333.4	8.16	29.5	162.5	1
Nc1nc2n([N+](=O)[O-])nc(C=N[N+](=O)[O-])n2n1	1.836	447	8.16	30	137.1	1
NC1=NC([N+](=O)[O-])=C([N+](=O)[O-])C(C=N[N+](=O)[O-])=NN1N	1.801	180.2	8.16	29	130	1
N=C1C(=N[N+](=O)[O-])NC([N+](=O)[O-])=C1C=N[N+](=O)[O-]	1.836	154.1	8.16	28.8	129	1
NC1=Nc2nnn(N[N+](=O)[O-])c2C(C=N[N+](=O)[O-])=C([N+](=O)[O-])NC1=N[N+](=O)[O-]	1.84	607	8.16	27.5	121	1
Nn1cnn2c([N+](=O)[O-])c([N+](=O)[O-])nc12	1.81	362.3	8.15	29.8	278.6	1
Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c2nnoc12	1.889	301.3	8.15	31.2	260	1
Nc1nc([N+](=O)[O-])n([N+](=O)[O-])c2c(N)c-2nc1[N+](=O)[O-]	1.928	206.6	8.15	29.9	254.5	1
Nn1cnc([N+](=O)[O-])c1N=C(N=C(n1cnnn1)[N+](=O)[O-])[N+](=O)[O-]	1.774	614.7	8.15	28.6	230.3	1
NC1=NC([N+](=O)[O-])=C([N+](=O)[O-])C([N+](=O)[O-])=Nc2nnc(N)n21	1.886	364.9	8.15	30.5	224.4	1
Nc1nc([N+](=O)[O-])c2[nH]c([N+](=O)[O-])nc2nnc([N+](=O)[O-])n1C=N[N+](=O)[O-]	1.882	506.6	8.15	30.8	209.2	1
Nc1nnnc(C=N[N+](=O)[O-])c1[N+](=O)[O-]	1.762	341.5	8.15	29.2	207.8	
O=[N+]([O-])N=Cc1nc([N+](=O)[O-])n2c(C=N[N+](=O)[O-])nnc2c1[N+](=O)[O-]	1.845	552.3	8.15	31.1	151.2	
NN1C=NC([N+](=O)[O-])=NC1=C(C=N[N+](=O)[O-])[N+](=O)[O-]	1.762	173.7	8.15	28	138.6	1
NN1C([N+](=O)[O-])=CC(=C2N=NN=N2)C(N[N+](=O)[O-])N1C=N[N+](=O)[O-]	1.77	533.1	8.15	27.2	130.1	1
Nc1c([N+](=O)[O-])n(C=N[N+](=O)[O-])n1N	1.782	148.4	8.14	28.8	220.7	1
N=c1c2nc([N+](=O)[O-])n(N[N+](=O)[O-])c2c([N+](=O)[O-])c([N+](=O)[O-])n1N	1.855	279.7	8.14	31.2	209.8	1
NC1=C(C=N[N+](=O)[O-])NC([N+](=O)[O-])=Nc2c1nc([N+](=O)[O-])n2[N+](=O)[O-]	1.854	337.4	8.14	29.4	189.1	1
Nc1nc([N+](=O)[O-])c2nnn([N+](=O)[O-])c2c1C=N[N+](=O)[O-]	1.867	458.4	8.14	29	165.6	
NC1=C([N+](=O)[O-])C(=N[N+](=O)[O-])C(C=N[N+](=O)[O-])=N1	1.82	172.2	8.14	28.7	153	1
Nc1c(C=N[N+](=O)[O-])c([N+](=O)[O-])n(C=N[N+](=O)[O-])c1[N+](=O)[O-]	1.817	144.3	8.14	29.2	150.8	1
NN=c1onc(C=N[N+](=O)[O-])n1C=N[N+](=O)[O-]	1.763	255.3	8.14	28.5	122.8	1
O=[N+]([O-])N=CN=C1C([N+](=O)[O-])=NC([N+](=O)[O-])=C1C=N[N+](=O)[O-]	1.807	193.3	8.14	28.6	120.4	1
O=[N+]([O-])c1nnc2n1c1nncn1c1nnc([N+](=O)[O-])n12	1.842	891.9	8.13	30.7	264.4	1
Nc1nc(C=N[N+](=O)[O-])c([N+](=O)[O-])c(=NN[N+](=O)[O-])[nH]1	1.823	214.4	8.13	28.6	149	
Nc1nc([N+](=O)[O-])n(N)c(=NN[N+](=O)[O-])c1C=N[N+](=O)[O-]	1.78	281.9	8.13	28.4	144.2	
NC1=C(C=N[N+](=O)[O-])NC([N+](=O)[O-])=C([N+](=O)[O-])C([N+](=O)[O-])=N1	1.837	27	8.13	30.3	136.6	1

Nn1c(N[N+](=O)[O-])nc([N+](=O)[O-])c2nc(C=N[N+](=O)[O-])nc1-2	1.877	400.5	8.13	29.3	126.9	1
O=[N+]([O-])N=CN=C1C(N[N+](=O)[O-])=C(N[N+](=O)[O-])c2c1ncn2[N+](=O)[O-]	1.836	567.6	8.13	28.6	120.3	1
N=c1c([N+](=O)[O-])c2nc(C=N[N+](=O)[O-])n([N+](=O)[O-])c2nn1[N+](=O)[O-]	1.836	456.6	8.12	30.6	173.8	1
Nc1nc([N+](=O)[O-])nnc1C=N[N+](=O)[O-]	1.78	261.2	8.12	29	163.6	1
O=[N+]([O-])N=Cc1n[nH]c2nc([N+](=O)[O-])nc([N+](=O)[O-])c12	1.894	411.9	8.12	30.2	151.5	1
NC1=C(N[N+](=O)[O-])N(N)C([N+](=O)[O-])=C([N+](=O)[O-])C1=C1N=NN=N1	1.809	417.8	8.12	28.3	145.8	
NC1=NN(N)C([N+](=O)[O-])=NC1=C(C=N[N+](=O)[O-])[N+](=O)[O-]	1.757	167.4	8.12	28	126.1	1
NN=C1NC(N[N+](=O)[O-])=C1[N+](=O)[O-]	1.815	205.5	8.12	28.7	122.3	1
Nc1noc(=NN[N+](=O)[O-])n1N	1.765	224.4	8.11	29.4	198.9	
N=c1[nH]c([N+](=O)[O-])nc([N+](=O)[O-])c1C=N[N+](=O)[O-]	1.854	91.1	8.11	29.4	191.3	
Nc1c([N+](=O)[O-])c([N+](=O)[O-])nn2c([N+](=O)[O-])c(C=N[N+](=O)[O-])nc2c1=NN[N+](=O)[O-]	1.87	541.2	8.11	30.3	176.1	1
NN=c1[nH]nc(N[N+](=O)[O-])n1N	1.779	270.6	8.11	29	146.8	1
N=c1[nH]c([N+](=O)[O-])nc([N+](=O)[O-])c1N	1.884	-26.9	8.1	29.2	268.9	
NC1=NN(N)C([N+](=O)[O-])=NN1N	1.768	298.3	8.1	29.3	243.8	
Nc1c(C=N[N+](=O)[O-])nnc2c([N+](=O)[O-])c([N+](=O)[O-])nn12	1.831	439.2	8.1	30.9	189.4	
O=[N+]([O-])N=Cc1c2c([N+](=O)[O-])nnc-2c1=NN[N+](=O)[O-]	1.872	467.9	8.1	28.1	160	1
N=c1[nH]nc(N[N+](=O)[O-])n1N	1.798	155.1	8.1	28.6	147.7	1
NC1=C(N)n2nc([N+](=O)[O-])c(N[N+](=O)[O-])c2NN=N1	1.89	397.8	8.1	29.2	140.8	1
Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c2nn[nH]c12	1.9	383.1	8.09	29.3	287.2	1
NC1=C([N+](=O)[O-])c2c(nc([N+](=O)[O-])n3nnnc23)NN=N1	1.895	673.3	8.09	30.3	261.6	1
Nc1nc2nc(N[N+](=O)[O-])c([N+](=O)[O-])[nH]c(=NN[N+](=O)[O-])c-2n1	1.895	261.3	8.09	30.1	166.3	1
NN1NC1C=N[N+](=O)[O-]	1.627	190.7	8.09	26.6	150.2	1
Nc1noc(=N[N+](=O)[O-])n1N	1.783	100.7	8.09	29.1	137.6	1
O=[N+]([O-])N=Cc1[nH]c(=N[N+](=O)[O-])n(C=N[N+](=O)[O-])c1C=N[N+](=O)[O-]	1.777	272.2	8.09	27.7	124.5	
NN1C=NC([N+](=O)[O-])N1C(C=NC(=C1N=C([N+](=O)[O-])N(C=N[N+](=O)[O-])N1[N+](=O)[O-])[N+](=O)[O-])N[N+](=O)[O-]	1.775	375.1	8.09	26.9	121	1
Nc1nc([N+](=O)[O-])n([N+](=O)[O-])c2nc(C=N[N+](=O)[O-])nc1-2	1.881	356.9	8.08	29.8	202.2	1
Nc1c(C=N[N+](=O)[O-])c([N+](=O)[O-])nc2c1nc([N+](=O)[O-])n2N[N+](=O)[O-]	1.869	402.1	8.08	30.1	129.4	1
NC(C=N[N+](=O)[O-])=C1N=NN=C1[N+](=O)[O-]	1.758	276	8.08	27.7	126.9	
Nc1c([N+](=O)[O-])nn2c(N)nnc2c1[N+](=O)[O-]	1.864	328	8.07	30.3	292.6	1
NN1C=C([N+](=O)[O-])N=C([N+](=O)[O-])c2nnn(N)c21	1.823	373.2	8.07	27.8	229.8	1

Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c2nnn-2c1C=N[N+](=O)[O-]	1.838	473.3	8.07	30	197.5	1
Nc1nc2c(c([N+](=O)[O-])n1)C([N+](=O)[O-])=NNC([N+](=O)[O-])=N2	1.869	351.2	8.07	30.3	183.3	1
NC1=C([N+](=O)[O-])N=CN(N)N1C=N[N+](=O)[O-]	1.788	154	8.07	26.5	166.8	1
O=[N+]([O-])N=Cn1nc([N+](=O)[O-])n2cnnc12	1.79	563.7	8.07	28.4	166.6	1
NN1C=NC1=C(C=N[N+](=O)[O-])[N+](=O)[O-]	1.742	201.9	8.07	26.5	142.9	1
NC1N=C([N+](=O)[O-])N1C=N[N+](=O)[O-]	1.718	99.5	8.07	26.8	135.3	1
O=[N+]([O-])N=CC1=Nc2nc([N+](=O)[O-])c([N+](=O)[O-])nc2C1=NN[N+](=O)[O-]	1.84	464.9	8.07	29.6	133.9	1
Nc1nc([N+](=O)[O-])c2nc([N+](=O)[O-])n(N[N+](=O)[O-])c2c1C=N[N+](=O)[O-]	1.865	413.9	8.07	29.5	124.4	1
O=[N+]([O-])N=CN1C([N+](=O)[O-])=CC(=C2N=NN=N2)C(N[N+](=O)[O-])=C1[N+](=O)[O-]	1.814	450.1	8.07	27.9	122.5	1
NC1=NC(=C([N+](=O)[O-])[N+](=O)[O-])N1	1.827	91.1	8.06	28.3	241.5	1
NC1=c2nnc3n2N(N=C([N+](=O)[O-])N=3)C([N+](=O)[O-])=N1	1.857	609.3	8.06	30.9	230	1
Nc1c([N+](=O)[O-])c([N+](=O)[O-])nc2c([N+](=O)[O-])nn(C=N[N+](=O)[O-])c12	1.881	313.3	8.06	30.1	204.5	1
Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c2nnn(C=N[N+](=O)[O-])c12	1.867	483.1	8.06	29.6	202.4	1
Nn1c([N+](=O)[O-])nc2c1nc(C=N[N+](=O)[O-])n2[N+](=O)[O-]	1.83	412.4	8.06	30.8	185.1	1
NN=c1[nH]c([N+](=O)[O-])c(C=N[N+](=O)[O-])n1C=N[N+](=O)[O-]	1.805	272.2	8.06	28.4	181.2	1
N=c1c([N+](=O)[O-])c([N+](=O)[O-])nc(N)n1C=N[N+](=O)[O-]	1.82	146.6	8.05	29.1	206.6	1
Nc1nc([N+](=O)[O-])c2c(nnn2[N+](=O)[O-])c1N	1.863	326.7	8.05	30.4	197.2	1
NC(=C1N=CN=C([N+](=O)[O-])N1N)[N+](=O)[O-]	1.773	124.6	8.05	27.3	183.8	
NC1=C([N+](=O)[O-])N=C2C([N+](=O)[O-])=NC([N+](=O)[O-])=C2C1=NN[N+](=O)[O-]	1.887	286.9	8.05	29.8	154.6	1
Nc1c(C=N[N+](=O)[O-])nc([N+](=O)[O-])c2c1nnn2[N+](=O)[O-]	1.847	421	8.05	28.6	128	1
NC(C=N[N+](=O)[O-])=C1N=C([N+](=O)[O-])N(C=N[N+](=O)[O-])N1	1.774	223.5	8.05	28	120.8	1
O=[N+]([O-])N=CN=C1NN=C1[N+](=O)[O-]	1.78	232.6	8.05	29.1	120.7	1
C=[N+]([O-])c1c([N+](=O)[O-])[nH]c(=N[N+](=O)[O-])c(=N)n1N	1.826	142.6	8.04	28.3	285.1	1
NC(N)=C1N=C([N+](=O)[O-])N=C([N+](=O)[O-])N1	1.85	74.2	8.04	29.3	238	1
Nn1nc([N+](=O)[O-])c2nc([N+](=O)[O-])c([N+](=O)[O-])c(C=N[N+](=O)[O-])c21	1.852	367.5	8.04	30	233.6	1
O=[N+]([O-])N=CC1=Nn2c(nc([N+](=O)[O-])c2C=N[N+](=O)[O-])C1=NN[N+](=O)[O-]	1.809	553.6	8.04	27.7	147.1	1
Nc1c(N[N+](=O)[O-])nc([N+](=O)[O-])c2nnn(N)c12	1.857	419.1	8.04	28.4	146.8	1
Nc1nn(C=N[N+](=O)[O-])c([N+](=O)[O-])c1C=N[N+](=O)[O-]	1.765	229	8.04	28.1	140.5	1
O=[N+]([O-])c1cn2n3c(nnc13)N([N+](=O)[O-])C=N2	1.807	593.5	8.04	28.6	138.3	1

O=[N+]([O-])N=Cn1c([N+](=O)[O-])nn1C(C1=NC=C1[N+](=O)[O-])[N+](=O)[O-]	1.785	323.2	8.04	30.5	137.3	1
Nc1nc(C=N[N+](=O)[O-])c([N+](=O)[O-])cc([N+](=O)[O-])c1=N[N+](=O)[O-]	1.794	187.7	8.04	28.5	122.8	1
Nc1ncc([N+](=O)[O-])[n-][n+]1=O	1.769	107.9	8.03	29	270.4	1
Nc1nc([N+](=O)[O-])c2nnn(C=N[N+](=O)[O-])c2c1[N+](=O)[O-]	1.85	470.7	8.03	29.3	216.8	1
N=C1N=NC([N+](=O)[O-])=N1	1.751	208.3	8.03	28.3	203.7	1
O=[N+]([O-])N=C1OC([N+](=O)[O-])=C1O	1.858	-205.1	8.03	28.7	173.8	1
Nc1c([N+](=O)[O-])c(C=N[N+](=O)[O-])c2n(C=N[N+](=O)[O-])nc-2c(=N[N+](=O)[O-])n1C=N[N+](=O)[O-]	1.876	537.8	8.02	27.6	167.3	1
N=C1c2nc([N+](=O)[O-])n(N[N+](=O)[O-])c2N=C(C=N[N+](=O)[O-])N=C([N+](=O)[O-])N1C=N[N+](=O)[O-]	1.789	498.6	8.02	26.6	127.5	1
N=C1OC(=NN[N+](=O)[O-])N1N	1.796	25.6	8.02	28.8	122.6	1
Nc1nc2nc([N+](=O)[O-])nc(N)n2c1[N+](=O)[O-]	1.88	274.9	8.01	30.7	279.3	1
Nc1nc(N)n([N+](=O)[O-])c1[N+](=O)[O-]	1.834	42.1	8.01	30	258	1
NN=C1N=NC([N+](=O)[O-])=N1	1.74	320	8.01	27.6	216.6	1
NC1=C([N+](=O)[O-])NC1[N+](=O)[O-]	1.823	-53.3	8.01	27.8	210.5	1
Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])ncc(C=N[N+](=O)[O-])n1C=N[N+](=O)[O-]	1.773	356	8.01	29.3	152.8	1
NC1=NN([N+](=O)[O-])C2=NN12	1.81	489.1	8.01	28.9	145	1
N=c1c(C=N[N+](=O)[O-])nc([N+](=O)[O-])cn1[N+](=O)[O-]	1.778	149	8.01	27.9	140.4	1
O=[N+]([O-])C1=Cn2nc([N+](=O)[O-])nc21	1.835	314.9	8	28.5	249.6	1
NC(N)=C1N=C([N+](=O)[O-])N=C1[N+](=O)[O-]	1.826	36.7	8	29.5	214.6	1
Nc1nc(C=N[N+](=O)[O-])c([N+](=O)[O-])c2c([N+](=O)[O-])nc([N+](=O)[O-])nc12	1.881	344.4	8	29.1	189.7	1
Nc1c([N+](=O)[O-])nc(N[N+](=O)[O-])c2nnn(N)c12	1.866	392.9	8	29	146.9	1
N=c1c(C=N[N+](=O)[O-])c2nc(C=N[N+](=O)[O-])n([N+](=O)[O-])c2nn1[N+](=O)[O-]	1.829	500.9	8	28.2	137.7	1
NN=c1c(C=N[N+](=O)[O-])c(C=N[N+](=O)[O-])nc([N+](=O)[O-])n1C=N[N+](=O)[O-]	1.78	379.8	8	26.7	135.2	1

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