Supporting Information

Design and Computational Screening of High-Energy, Low-Sensitivity Bistetrazole-Based Energetic Molecuvles

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1. Table S1. Side substituents and bridging groups for combining with bis-tetrazolium rings.

Chemical group number	Structures
side_substituent_1	$-NO_2$
side_substituent_2	$-CO_3$
side_substituent_3	$-NH_2$
side_substituent_4	$-NHNO_2$
side_substituent_5	$-NHC(NO_2)_3$
side_substituent_6	-CH2ONO_2
side_substituent_7	$-Ph(NO_2)_3$
side_substituent_8	$-NHCH_2C(NO_2)_3$
side_substituent_9	$-N(=O)NH_2$
side_substituent_10	-N=NH
side_substituent_11	-CN
side_substituent_12	$-NHC(=NH)NH_2$
side_substituent_13	-C(=NH)NHNHCH=NH
side_substituent_14	-OH
side_substituent_15	-C(=NH)N=NCH=NH
side_substituent_16	$-N(NO_2)CH_2CH_2NHNO_2$
side_substituent_17	$-NHCH(NO_2)_2$
side_substituent_18	$-NHCH_2CH(NO_2)_2$
side_substituent_19	$-ONO_2$
side_substituent_20	$-CH_2C{\equiv}CH$
side_substituent_21	$-CH_2CH=CH_2$
side_substituent_22	$-CH_2CH_2OCH_3$
side_substituent_23	$-N(CH_2NO_2)_2$
side_substituent_24	$-NHNO_2$
side_substituent_25	$-CH_2CN$
side_substituent_26	-NHCN
side_substituent_27	$-CH_2C(=O)CH_3$
side_substituent_28	$-CH(NO_2)_2$
side_substituent_29	$-C(NO_2)_3$
bridgehead_1	-NH-
bridgehead_2	$-CH_2-$
bridgehead_3	$-N(NO_2)-$
bridgehead_4	-O-
bridgehead_5	-N=N-
bridgehead_6	-NHC(=O)NH-
bridgehead_7	-C(=NH)N=NC(=NH)-
bridgehead_8	$-N(NO_2)CH_2CH_2N(NO_2)-$
bridgehead_9	$-NHCH_2C(NO_2)_2-$
bridgehead_10	$-NHC(NO_2)_2-$
bridgehead_11	$-CH_2O-$
bridgehead_12	-Ph-

bridgehead_13	-C(=O)NH-
bridgehead_14	-C(=NH)NHNHC(=NH)-
bridgehead_15	-CH_2C≡C-
bridgehead_16	-CH_2CH=CH-
bridgehead_17	-$CH_2CH_2OCH_2$-
bridgehead_18	-N(CH_2NO_2)-
bridgehead_19	-NHNH-
bridgehead_20	-CH_2C(=O)CH_2-
bridgehead_21	None

2. Principles and methods for predicting various properties of molecules.

SYBA(SYnthetic Bayesian Accessibility):

The evaluation of synthesis difficulty relies on the trained SYBA model, which is available for download on GitHub. The model distinguishes the synthesis difficulty of molecules primarily based on the relative positions and quantities of functional groups within the molecule. The results for organic molecule synthesis difficulty are generally reliable. The model assigns a score to the molecule based on its prediction, which can be either positive or negative. The higher the score, the lower the synthesis difficulty. According to the model's creators, molecules with a score greater than 0 are categorized as "easily synthesizable," meaning they are less difficult to synthesize. Molecules with a score less than 0 are categorized as "difficult to synthesize," meaning they are challenging. During our selection process, we excluded molecules with SYBA scores less than 0, meaning the molecules we selected all have a positive score, indicating that they are easier to synthesize. Therefore, the molecules we have left after screening are more likely to be easily synthesized, not those that are difficult to synthesize.

Oxygen balance index：

$$OB = \frac{1600 \times [c - 2a - \frac{b}{2}]}{M} \quad (1)$$

In the formula, OB represents the oxygen balance index, where a, b, and c are the numbers of carbon, hydrogen, and oxygen atoms in the energetic molecule, respectively, and M is the molar mass of the molecule.

SYBAscores: The score is a model that Milan Voršilák et al. trained on a machine learning approach to discriminate between synthesized difficulties quickly[1].

Solid density: The method used for this part of the calculation is the equation corrected by Politzer et al.'s introduction of electrostatic potential at the molecular surface. Considering the interactions between the molecules in the lattice, the corrected solid density is given by[2-4] equation 2.

$$\rho = \alpha\left(\frac{M}{V(0.001)}\right) + \beta(\upsilon\sigma_{Tot}^2) + \gamma \quad (2)$$

Electrostatic equilibrium parameter: The electrostatic equilibrium parameter υ in the general interaction properties function (GIPF) descriptor compares energy-containing molecules' stability. The closer υ is to 0.25, the more stable the molecule's structure is. The calculation formula is:

$$\upsilon = \frac{\sigma_+^2 \sigma_-^2}{\left[\sigma_{Tot}^2\right]} \quad (3)$$

For Equations 2 and 3, α=1.0462, β=0.0021, and γ=-0.1586 are

empirical parameters, M is molecular molar mass, and V is molecular volume. σ_{Tot}^{2} denotes the variance of the total surface electrostatic potential, υ denotes the equilibrium [5]constant of positive and negative electrostatic potentials at the surface of the molecule, and $\sigma_{+}^{2}\sigma_{-}^{2}$ denotes the product of the squares of the positive surface potential and the negative surface potential.

Enthalpy of generation: the molecular enthalpy of generation is calculated sequentially using the atomic energy and the isobond reaction methods.

Atomization Energy Method: Predicts the heat of generation of the gas phase of the desired molecule by calculating the enthalpy change of the atomization energy reaction in conjunction with the known heat of generation of isolated atoms. The formula is given below.[6]

$$\Delta_f H^0(A_xB_y,0K) = x\Delta_f H^0(A,0K) + y\Delta_f H^0(B,0K) - \Sigma D_0 \qquad \text{(S4)}$$

where $\Delta_f H^0(A,0K)$ and $\Delta_f H^0(B,0K)$ denote the heat of generation at 0K for atoms A and B, respectively, and ΣD0 denotes the difference between the sum of the molecular and atomic energies.

Isobonding method: Using Hess's law, construct a suitable isobonding reaction, calculate the energy change of the reaction, and predict the heat of gas phase generation of the target molecule in combination with the known heat of gas phase generation of the molecule in the reaction. The standard enthalpy change during the reaction is calculated as follows[7]:

$$\Delta H_{Reaction}^{0} = \Delta_f H^0(Products) + \Delta_f H^0(Reactants) \qquad \text{(S5)}$$

Where $\Delta_f H^0(Products)$ and $\Delta_f H^0(Reactants)$ denote the heat of generation of the products and reactants, respectively.

The enthalpy of generation of the gas phase was calculated based on the two methods, according to:

$$\Delta H(Solid) = \Delta H(Gas) - \Delta H(Sublimation) \quad \text{(S6)}$$

The enthalpy of sublimation is added to the enthalpy of formation of the gas phase to obtain the enthalpy of formation of the solid. The enthalpy of sublimation is calculated by the empirical formula:

$$\Delta H(Sublimation) = a(SA)^2 + b\sqrt{\sigma_{Tot}^2 \upsilon} + c \quad \text{(S7)}$$

(6,7) where $\Delta H(Solid)$ and $\Delta H(Gas)$ denote the heat of generation in the solid and gas phases, respectively, SA denotes the molecular surface area, i.e., the area of the 0.001e·bohr^{-3} isoelectronic density surface used in the calculation of the electrostatic potential, in Å^2, σ_{Tot}^2 denotes the variance of the electrostatic potential of the total surface, in (kcal·mol^{-1})2, and υ denotes the positive and negative molecular surface electrostatic potential equilibrium constants, a, b, and c are three empirical parameters, and the relevant parameters are given as a = 0.000267, b = 1.650087, and c = 2.966087 by Rice et al.

The heat of burst, burst pressure, and burst velocity are collectively known as the detonation properties of the molecule, which are calculated using the following equations.

Heat of Explosion: Calculated directly from the equation for the

enthalpy change of heat produced by an explosion in an ideal state:

$$Q_{det} \cong -\Delta H_0 = -\frac{[\Delta H_f(detonationproducts) - \Delta H_f(explosive)]}{M_r} \quad \text{(S8)}$$

Burst pressure: The formula is calculated by the K-J empirical equation proposed by Kamlet and Jacobs:

$$p = K\rho_0\Phi,\ \Phi = N\bar{M}^{1/2}Q^{1/2} \quad \text{(S9)}$$

The burst velocity D is calculated from the K-J empirical equation:

$$D = A\Phi^{1/2}(1 + B\rho_0) \quad \text{(S10)}$$

(8-10) where $\Delta H_f(detonationproducts)$ and $\Delta H_f(explosive)$ represent the standard enthalpy of generation of the explosion products and explosives, respectively, Mr is the total molar mass of explosives in g·mol^{-1}, Q_{det} is the heat of detonation Q in kJ·g^{-1}, and p denotes the detonation pressure in GPa; K is a coefficient with a value of 1.558; ρ_0 is the explosive charge density, using the previous calculation of the theoretical density instead, the unit g·cm^{-3}; N is the total number of moles of gas produced per gram of explosives, $\bar{M}$ is the average molecular weight of the products of the explosion reaction, the unit of g·mol^{-1}; Q is the heat of detonation calculated earlier, here the unit is cal·g^{-1}; D is the detonation velocity, the unit of km·s^{-1}; [8]A, B are coefficients, the value is respectively 1.01, 1.3.

3. Table S2. The molecules obtained after the initial screening correspond to SMILES, OB and SYBA score.

Index	SMILES	OB(%)	SYBA
1	O=[N+]([O-])n1nnc(C(Nc2nnn(O)n2)([N+](=O)[O-	0.00	10.21

	])[N+](=O)[O-])n1		
2	O=[N+]([O-])C(Nn1nnc(NC(c2nnn([N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	1.90	12.20
3	O=[N+]([O-])OCn1nnc(NC(c2nnn([N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-2.12	19.06
4	O=[N+]([O-])n1nnc(C(Nc2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	0.00	16.00
5	O=[N+]([O-])n1nnc(OCc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	17.00
6	O=C(Nc1nnn([N+](=O)[O-])n1)c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	0.00	23.31
7	O=[N+]([O-])CN(c1nnn(O[N+](=O)[O-])n1)c1nnn([N+](=O)[O-])n1	0.00	6.62
8	O=[N+]([O-])CN(c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn([N+](=O)[O-])n1	1.90	5.69
9	O=[N+]([O-])On1nnc(NNc2nnn([N+](=O)[O-])n2)n1	0.00	11.74
10	O=[N+]([O-])n1nnc(NNc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.12	9.32
11	O=[N+]([O-])OCn1nnc(N(c2nnn([N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	10.82
12	O=[N+]([O-])N(c1nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn([N+](=O)[O-])n1	1.90	11.15
13	O=[N+]([O-])C(Nn1nnc(Oc2nnn([N+](=O)[O-])n2)n1)[N+](=O)[O-]	0.00	7.94
14	O=[N+]([O-])n1nnc(Oc2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	11.73
15	O=[N+]([O-])n1nnc(N=Nc2nnn([N+](=O)[O-])n2)n1	0.00	10.37
16	O=[N+]([O-])N(CCN(c1nnn([N+](=O)[O-])n1)[N+](=O)[O-])c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.62	6.03
17	O=[N+]([O-])On1nnc(NCC(c2nnn([N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-2.12	19.99
18	O=[N+]([O-])n1nnc(C(CNc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	0.00	18.28
19	N#Cn1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	-2.07	5.33
20	O=[N+]([O-])C(Nn1nnc(Nc2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	-2.40	8.04
21	O=[N+]([O-])n1nnc(NC(c2nnn(O)n2)([N+](=O)[O-])[N+](=O)[O-])n1	0.00	10.21
22	O=[N+]([O-])Nn1nnc(NC(c2nnn(O)n2)([N+](=O)[O-])[N+](=O)[O-])n1	-2.40	9.17
23	O=[N+]([O-])C(Nn1nnc(N(c2nnn(O)n2)[N+](=O)[O-	-2.40	3.89

	])n1)[N+](=O)[O-]		
24	O=[N+]([O-])Nn1nnc(N(c2nnn(O)n2)[N+](=O)[O-])n1	0.00	5.02
25	O=[N+]([O-])C(Nn1nnc(N=Nc2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	2.11
26	O=[N+]([O-])On1nnc(Nc2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.40	12.46
27	O=[N+]([O-])C(Nn1nnc(Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	0.00	12.34
28	O=[N+]([O-])C(Nn1nnc(C(Nc2nnn([N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	1.90	11.51
29	O=[N+]([O-])C(Nn1nnc(NC(c2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-1.62	15.17
30	O=[N+]([O-])Nn1nnc(NC(c2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	0.00	12.77
31	O=[N+]([O-])CN(c1nnn(NC([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.62	5.81
32	O=[N+]([O-])C(Nn1nnc(NNc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	-1.77	10.14
33	O=[N+]([O-])C(Nn1nnc(N(c2nnn(O)n2)[N+](=O)[O-])n1)[N+](=O)[O-]	-2.40	3.89
34	O=[N+]([O-])C(Nn1nnc(N(c2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	0.00	10.33
35	O=[N+]([O-])Nn1nnc(N(c2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	2.12	8.62
36	O=[N+]([O-])C(Nn1nnc(N(c2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	-1.62	11.27
37	O=[N+]([O-])C(Nn1nnc(Oc2nnn([N+](=O)[O-])n2)n1)[N+](=O)[O-]	0.00	7.94
38	O=[N+]([O-])Nn1nnc(Oc2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.40	9.20
39	O=[N+]([O-])On1nnc(N=Nc2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	5.83
40	O=[N+]([O-])C(Nn1nnc(N=Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	1.78	5.71
41	O=[N+]([O-])C(CNn1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	-1.62	9.04
42	O=[N+]([O-])On1nnc(Nc2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.40	12.46
43	O=[N+]([O-])Nn1nnc(Nc2nnn(O[N+](=O)[O-])n2)n1	0.00	12.90
44	Nn1nnc(NC(c2nnn(O[N+](=O)[O-])n2)([N+](=O)[O-	-2.40	12.77

	])[N+](=O)[O-])n1		
45	O=[N+]([O-])OCn1nnc(NC(c2nnn(O[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	2.04	20.23
46	O=[N+]([O-])On1nnc(COc2nnn(O[N+](=O)[O-])n2)n1	0.00	20.33
47	O=[N+]([O-])On1nnc(OCc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.04	15.55
48	O=[N+]([O-])CN(c1nnn(O[N+](=O)[O-])n1)c1nnn([N+](=O)[O-])n1	0.00	6.62
49	O=[N+]([O-])CN(c1nnn(N[N+](=O)[O-])n1)c1nnn(O[N+](=O)[O-])n1	-2.40	7.07
50	O=[N+]([O-])On1nnc(NNc2nnn([N+](=O)[O-])n2)n1	0.00	11.74
51	O=[N+]([O-])On1nnc(Cc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	13.40
52	Nn1nnc(N(c2nnn(O[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	7.14
53	O=[N+]([O-])OCn1nnc(Oc2nnn(O[N+](=O)[O-])n2)n1	0.00	12.70
54	O=[N+]([O-])On1nnc(Oc2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.04	10.28
55	O=[N+]([O-])On1nnc(N=Nc2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	5.83
56	O=[N+]([O-])On1nnc(N=Nc2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-1.98	9.62
57	O=[N+]([O-])On1nnc(N(CCN(c2nnn(O[N+](=O)[O-])n2)[N+](=O)[O-])[N+](=O)[O-])n1	0.00	9.93
58	O=[N+]([O-])On1nnc(N(CCN(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])[N+](=O)[O-])n1	1.57	5.14
59	O=[N+]([O-])On1nnc(C(CNc2nnn([N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-2.12	19.99
60	O=[N+]([O-])On1nnc(NCC(c2nnn(O[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	2.04	22.95
61	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	-1.62	4.31
62	NNn1nnc(C(Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.77	6.81
63	NNn1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	1.96
64	Nn1nnc(C(Nc2nnn(O[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-2.40	12.77
65	Nn1nnc(C(Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	0.00	11.06
66	Nn1nnc(N(c2nnn(O[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	7.14
67	Nn1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	2.12	6.20

68	Nn1nnc(Oc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.40	6.78
69	O=[N+]([O-])Nn1nnc(Nc2nnn(O[N+](=O)[O-])n2)n1	0.00	12.90
70	O=[N+]([O-])Nn1nnc(Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.12	12.78
71	O=[N+]([O-])Nn1nnc(C(Nc2nnn(O)n2)([N+](=O)[O-])[N+](=O)[O-])n1	-2.40	9.17
72	O=[N+]([O-])Nn1nnc(C(Nc2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	0.00	13.46
73	O=[N+]([O-])Nn1nnc(NC(c2nnn(N[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	2.12	15.61
74	O=[N+]([O-])Nn1nnc(C(Nc2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.62	17.26
75	O=C(Nc1nnn(N[N+](=O)[O-])n1)c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.98	25.96
76	O=[N+]([O-])CN(c1nnn(N[N+](=O)[O-])n1)c1nnn(O[N+](=O)[O-])n1	-2.40	7.07
77	O=[N+]([O-])CN(c1nnn(N[N+](=O)[O-])n1)c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	0.00	6.95
78	O=[N+]([O-])Nn1nnc(NNc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	10.58
79	O=[N+]([O-])Nn1nnc(N(c2nnn(O)n2)[N+](=O)[O-])n1	0.00	5.02
80	O=[N+]([O-])Nn1nnc(N(c2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	2.12	8.62
81	O=[N+]([O-])Nn1nnc(N(c2nnn(CO[N+](=O)[O-])n2)[N+](=O)[O-])n1	-2.40	11.26
82	O=[N+]([O-])Nn1nnc(N(c2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	12.41
83	O=[N+]([O-])Nn1nnc(Oc2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.40	9.20
84	O=[N+]([O-])Nn1nnc(Oc2nnn(N[N+](=O)[O-])n2)n1	0.00	12.04
85	O=[N+]([O-])Nn1nnc(C(CNc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.62	19.53
86	O=[N+]([O-])C(Nn1nnc(Nc2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	-2.40	8.04
87	O=[N+]([O-])C(Nn1nnc(Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	0.00	12.34
88	O=[N+]([O-])Nn1nnc(Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.12	12.78
89	O=[N+]([O-])C(CNn1nnc(Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-	-1.62	16.14

	])[N+](=O)[O-]		
90	NNn1nnc(NC(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.77	6.12
91	Nn1nnc(NC(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	0.00	10.36
92	O=[N+]([O-])n1nnc(COc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	17.00
93	O=[N+]([O-])On1nnc(COc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.04	15.55
94	O=C(Nc1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn([N+](=O)[O-])n1	0.00	24.70
95	O=C(Nc1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(N[N+](=O)[O-])n1	-1.98	25.96
96	O=[N+]([O-])CN(c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn([N+](=O)[O-])n1	1.90	5.69
97	O=[N+]([O-])CN(c1nnn(NC([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.62	5.81
98	O=[N+]([O-])CN(c1nnn(N[N+](=O)[O-])n1)c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	0.00	6.95
99	O=[N+]([O-])n1nnc(NNc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.12	9.32
100	O=[N+]([O-])C(Nn1nnc(NNc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	-1.77	10.14
101	O=[N+]([O-])Nn1nnc(NNc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	10.58
102	O=[N+]([O-])On1nnc(Cc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	13.40
103	O=[N+]([O-])C(Nn1nnc(Cc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	17.25
104	N#Cn1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	-2.07	5.33
105	O=[N+]([O-])C(CNn1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	-1.62	9.04
106	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	-1.62	4.31
107	NNn1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	1.96
108	Nn1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	2.12	6.20

109	NC(=O)n1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	-1.98	6.67
110	Nn1nnc(Oc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.40	6.78
111	O=[N+]([O-])OCn1nnc(Oc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.04	9.71
112	O=[N+]([O-])C(Nn1nnc(N=Nc2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	2.11
113	O=[N+]([O-])C(Nn1nnc(N=Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	1.78	5.71
114	O=[N+]([O-])OCn1nnc(N=Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-1.98	9.05
115	O=[N+]([O-])C(CNn1nnc(N=Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	10.21
116	N=C(Nc1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)Nc1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.53	7.27
117	O=[N+]([O-])N(CCN(c1nnn([N+](=O)[O-])n1)[N+](=O)[O-])c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.62	6.03
118	O=[N+]([O-])On1nnc(N(CCN(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])[N+](=O)[O-])n1	1.57	5.14
119	O=[N+]([O-])n1nnc(NCC(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	0.00	17.58
120	O=[N+]([O-])Nn1nnc(NCC(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.62	18.84
121	O=[N+]([O-])OCn1nnc(C(Nc2nnn([N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-2.12	17.15
122	O=[N+]([O-])OCn1nnc(C(Nc2nnn(O[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	2.04	18.32
123	O=[N+]([O-])OCn1nnc(N(c2nnn([N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	10.82
124	O=[N+]([O-])Nn1nnc(N(c2nnn(CO[N+](=O)[O-])n2)[N+](=O)[O-])n1	-2.40	11.26
125	O=[N+]([O-])OCn1nnc(Oc2nnn(O[N+](=O)[O-])n2)n1	0.00	12.70
126	O=[N+]([O-])OCn1nnc(Oc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.04	9.71
127	O=[N+]([O-])OCn1nnc(N=Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-1.98	9.05
128	O=[N+]([O-])C(CNn1nnc(Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-	-1.62	16.14

	])[N+](=O)[O-]		
129	O=[N+]([O-])n1nnc(NC(c2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	0.00	16.00
130	O=[N+]([O-])Nn1nnc(NC(c2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.62	17.26
131	O=[N+]([O-])N(c1nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn([N+](=O)[O-])n1	1.90	11.15
132	O=[N+]([O-])C(Nn1nnc(N(c2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	-1.62	11.27
133	O=[N+]([O-])Nn1nnc(N(c2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	12.41
134	O=[N+]([O-])n1nnc(Oc2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	11.73
135	O=[N+]([O-])On1nnc(Oc2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.04	10.28
136	O=[N+]([O-])On1nnc(N=Nc2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-1.98	9.62
137	O=[N+]([O-])C(CNn1nnc(N=Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	10.21
138	NC(=O)n1nnc(N(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	-1.98	6.67
139	O=[N+]([O-])n1nnnc1C(Nc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	0.00	5.93
140	O=[N+]([O-])C(Nn1nnnc1NC(c1nnnn1[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.90	11.68
141	O=[N+]([O-])OCn1nnnc1NC(c1nnnn1[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	18.28
142	O=[N+]([O-])n1nnnc1C(Nc1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	16.17
143	O=[N+]([O-])n1nnnc1OCc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	16.33
144	O=C(Nc1nnnn1[N+](=O)[O-])c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	17.24
145	O=[N+]([O-])CN(c1nnnn1O[N+](=O)[O-])c1nnnn1[N+](=O)[O-]	0.00	4.08
146	O=[N+]([O-])CN(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1[N+](=O)[O-]	1.90	3.60
147	O=[N+]([O-])On1nnnc1NNc1nnnn1[N+](=O)[O-]	0.00	10.19
148	O=[N+]([O-])n1nnnc1NNc1nnnn1NC([N+](=O)[O-	2.12	8.90

	])([N+](=O)[O-])[N+](=O)[O-]		
149	O=[N+]([O-])OCn1nnnc1N(c1nnnn1[N+](=O)[O-])[N+](=O)[O-]	0.00	9.80
150	O=[N+]([O-])N(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1[N+](=O)[O-]	1.90	9.05
151	O=[N+]([O-])C(Nn1nnnc1Oc1nnnn1[N+](=O)[O-])[N+](=O)[O-]	0.00	7.59
152	O=[N+]([O-])n1nnnc1Oc1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	11.37
153	O=[N+]([O-])n1nnnc1N=Nc1nnnn1[N+](=O)[O-]	0.00	9.69
154	O=[N+]([O-])N(CCN(c1nnnn1[N+](=O)[O-])[N+](=O)[O-])c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.62	1.30
155	O=[N+]([O-])On1nnnc1NCC(c1nnnn1[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	16.85
156	O=[N+]([O-])n1nnnc1C(CNc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	16.27
157	N=Nn1nnnc1C(Nc1nnnn1O[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	0.80
158	N=Nn1nnnc1C(Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.78	0.23
159	N#Cn1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-2.07	0.93
160	O=[N+]([O-])C(Nn1nnnc1Nc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	-2.40	6.07
161	O=[N+]([O-])n1nnnc1NC(c1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	0.00	5.93
162	O=[N+]([O-])Nn1nnnc1NC(c1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	-2.40	6.39
163	O=[N+]([O-])C(Nn1nnnc1N(c1nnnn1O)[N+](=O)[O-])[N+](=O)[O-]	-2.40	0.64
164	O=[N+]([O-])Nn1nnnc1N(c1nnnn1O)[N+](=O)[O-]	0.00	1.77
165	O=[N+]([O-])C(Nn1nnnc1N=Nc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	0.00	0.68
166	O=[N+]([O-])On1nnnc1Nc1nnnn1NC([N+](=O)[O-])[N+](=O)[O-]	-2.40	13.10
167	O=[N+]([O-])C(Nn1nnnc1Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	13.02
168	O=[N+]([O-])C(Nn1nnnc1C(Nc1nnnn1[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.90	10.98
169	O=[N+]([O-])C(Nn1nnnc1NC(c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.62	16.83
170	O=[N+]([O-])Nn1nnnc1NC(c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	13.34

171	O=[N+]([O-])CN(c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-])c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.62	5.91
172	O=[N+]([O-])C(Nn1nnnc1NNc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.77	11.22
173	O=[N+]([O-])C(Nn1nnnc1N(c1nnnn1O)[N+](=O)[O-])[N+](=O)[O-]	-2.40	0.64
174	O=[N+]([O-])C(Nn1nnnc1N(c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	10.43
175	O=[N+]([O-])Nn1nnnc1N(c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	2.12	8.72
176	O=[N+]([O-])C(Nn1nnnc1N(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.62	11.37
177	O=[N+]([O-])C(Nn1nnnc1Oc1nnnn1[N+](=O)[O-])[N+](=O)[O-]	0.00	7.59
178	O=[N+]([O-])Nn1nnnc1Oc1nnnn1NC([N+](=O)[O-])[N+](=O)[O-]	-2.40	11.04
179	O=[N+]([O-])On1nnnc1N=Nc1nnnn1NC([N+](=O)[O-])[N+](=O)[O-]	0.00	7.71
180	O=[N+]([O-])C(Nn1nnnc1N=Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.78	7.63
181	O=[N+]([O-])C(CNn1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.62	9.15
182	O=[N+]([O-])On1nnnc1Nc1nnnn1NC([N+](=O)[O-])[N+](=O)[O-]	-2.40	13.10
183	O=[N+]([O-])Nn1nnnc1Nc1nnnn1O[N+](=O)[O-]	0.00	13.54
184	N=Nn1nnnc1NC(c1nnnn1O[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	2.75
185	Nn1nnnc1NC(c1nnnn1O[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.40	10.54
186	O=[N+]([O-])OCn1nnnc1NC(c1nnnn1O[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.04	21.61
187	O=[N+]([O-])On1nnnc1COc1nnnn1O[N+](=O)[O-]	0.00	19.34
188	O=[N+]([O-])On1nnnc1OCc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.04	17.04
189	O=[N+]([O-])CN(c1nnnn1O[N+](=O)[O-])c1nnnn1[N+](=O)[O-]	0.00	4.08
190	O=[N+]([O-])CN(c1nnnn1N[N+](=O)[O-])c1nnnn1O[N+](=O)[O-]	-2.40	7.13
191	O=[N+]([O-])On1nnnc1NNc1nnnn1[N+](=O)[O-]	0.00	10.19
192	O=[N+]([O-])On1nnnc1Cc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	11.32
193	Nn1nnnc1N(c1nnnn1O[N+](=O)[O-])[N+](=O)[O-]	0.00	3.34
194	O=[N+]([O-])OCn1nnnc1Oc1nnnn1O[N+](=O)[O-]	0.00	10.05
195	O=[N+]([O-])On1nnnc1Oc1nnnn1NCC([N+](=O)[O-	2.04	12.08

	])([N+](=O)[O-])[N+](=O)[O-]		
196	O=[N+]([O-])On1nnnc1N=Nc1nnnn1NC([N+](=O)[O-])[N+](=O)[O-]	0.00	7.71
197	O=[N+]([O-])On1nnnc1N=Nc1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.98	11.50
198	O=[N+]([O-])On1nnnc1N(CCN(c1nnnn1O[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	9.58
199	O=[N+]([O-])On1nnnc1N(CCN(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.57	2.57
200	O=[N+]([O-])On1nnnc1C(CNc1nnnn1[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	16.85
201	O=[N+]([O-])On1nnnc1NCC(c1nnnn1O[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.04	22.01
202	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.62	3.03
203	NNn1nnnc1C(Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.77	8.48
204	NNn1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	1.37
205	Nn1nnnc1C(Nc1nnnn1O[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.40	10.54
206	Nn1nnnc1C(Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	9.97
207	Nn1nnnc1N(c1nnnn1O[N+](=O)[O-])[N+](=O)[O-]	0.00	3.34
208	Nn1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	2.12	2.85
209	Nn1nnnc1Oc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.40	5.17
210	O=[N+]([O-])Nn1nnnc1Nc1nnnn1O[N+](=O)[O-]	0.00	13.54
211	O=[N+]([O-])Nn1nnnc1Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.12	13.46
212	O=[N+]([O-])Nn1nnnc1C(Nc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	-2.40	7.49
213	O=[N+]([O-])Nn1nnnc1C(Nc1nnnn1NC([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	15.13
214	O=[N+]([O-])Nn1nnnc1NC(c1nnnn1N[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.12	16.18
215	O=[N+]([O-])Nn1nnnc1C(Nc1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.62	19.62
216	O=C(Nc1nnnn1N[N+](=O)[O-])c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.98	20.70
217	O=[N+]([O-])CN(c1nnnn1N[N+](=O)[O-	-2.40	7.13

	])c1nnnn1O[N+](=O)[O-]		
218	O=[N+]([O-])CN(c1nnnn1N[N+](=O)[O-])c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	7.05
219	O=[N+]([O-])Nn1nnnc1NNc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	11.66
220	O=[N+]([O-])Nn1nnnc1N(c1nnnn1O)[N+](=O)[O-]	0.00	1.77
221	O=[N+]([O-])Nn1nnnc1N(c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	2.12	8.72
222	O=[N+]([O-])Nn1nnnc1N(c1nnnn1CO[N+](=O)[O-])[N+](=O)[O-]	-2.40	12.84
223	O=[N+]([O-])Nn1nnnc1N(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	12.51
224	O=[N+]([O-])Nn1nnnc1Oc1nnnn1NC([N+](=O)[O-])[N+](=O)[O-]	-2.40	11.04
225	O=[N+]([O-])Nn1nnnc1Oc1nnnn1N[N+](=O)[O-]	0.00	13.88
226	O=[N+]([O-])Nn1nnnc1C(CNc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.62	19.73
227	O=[N+]([O-])C(Nn1nnnc1Nc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	-2.40	6.07
228	O=[N+]([O-])C(Nn1nnnc1Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	13.02
229	O=[N+]([O-])Nn1nnnc1Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.12	13.46
230	O=[N+]([O-])C(CNn1nnnc1Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.62	17.51
231	N=Nn1nnnc1NC(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.78	1.48
232	NNn1nnnc1NC(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.77	8.48
233	Nn1nnnc1NC(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	9.28
234	O=[N+]([O-])n1nnnc1COc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	16.33
235	O=[N+]([O-])On1nnnc1COc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.04	14.96
236	O=C(Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1[N+](=O)[O-]	0.00	17.94
237	O=C(Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1N[N+](=O)[O-]	-1.98	21.39
238	O=[N+]([O-])CN(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1[N+](=O)[O-]	1.90	3.60
239	O=[N+]([O-])CN(c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-	-1.62	5.91

	])c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]		
240	O=[N+]([O-])CN(c1nnnn1N[N+](=O)[O-])c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	7.05
241	O=[N+]([O-])n1nnnc1NNc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.12	8.90
242	O=[N+]([O-])C(Nn1nnnc1NNc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.77	11.22
243	O=[N+]([O-])Nn1nnnc1NNc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	11.66
244	O=[N+]([O-])On1nnnc1Cc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	11.32
245	O=[N+]([O-])C(Nn1nnnc1Cc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	15.90
246	N#Cn1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-2.07	0.93
247	O=[N+]([O-])C(CNn1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.62	9.15
248	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.62	3.03
249	NNn1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	1.37
250	Nn1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	2.12	2.85
251	NC(=O)n1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.98	12.16
252	Nn1nnnc1Oc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.40	5.17
253	O=[N+]([O-])OCn1nnnc1Oc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.04	7.50
254	O=[N+]([O-])C(Nn1nnnc1N=Nc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	0.00	0.68
255	O=[N+]([O-])C(Nn1nnnc1N=Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.78	7.63
256	O=[N+]([O-])OCn1nnnc1N=Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.98	12.16
257	O=[N+]([O-])C(CNn1nnnc1N=Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	12.13
258	N=C(Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.53	7.69
259	O=[N+]([O-])N(CCN(c1nnnn1[N+](=O)[O-])[N+](=O)[O-	-1.62	1.30

	])c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]		
260	O=[N+]([O-])On1nnnc1N(CCN(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.57	2.57
261	O=[N+]([O-])n1nnnc1NCC(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	15.58
262	O=[N+]([O-])Nn1nnnc1NCC(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.62	19.03
263	O=[N+]([O-])OCn1nnnc1C(Nc1nnnn1[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	17.69
264	O=[N+]([O-])OCn1nnnc1C(Nc1nnnn1O[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.04	21.02
265	O=[N+]([O-])OCn1nnnc1N(c1nnnn1[N+](=O)[O-])[N+](=O)[O-]	0.00	9.80
266	O=[N+]([O-])Nn1nnnc1N(c1nnnn1CO[N+](=O)[O-])[N+](=O)[O-]	-2.40	12.84
267	O=[N+]([O-])OCn1nnnc1Oc1nnnn1O[N+](=O)[O-]	0.00	10.05
268	O=[N+]([O-])OCn1nnnc1Oc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.04	7.50
269	O=[N+]([O-])OCn1nnnc1N=Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.98	12.16
270	O=[N+]([O-])C(CNn1nnnc1Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.62	17.51
271	O=[N+]([O-])n1nnnc1NC(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	15.48
272	O=[N+]([O-])Nn1nnnc1NC(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.62	17.83
273	O=[N+]([O-])N(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1[N+](=O)[O-]	1.90	9.05
274	O=[N+]([O-])C(Nn1nnnc1N(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.62	11.37
275	O=[N+]([O-])Nn1nnnc1N(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	12.51
276	O=[N+]([O-])n1nnnc1Oc1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	11.37
277	O=[N+]([O-])On1nnnc1Oc1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.04	12.08
278	O=[N+]([O-])On1nnnc1N=Nc1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.98	11.50
279	O=[N+]([O-])C(CNn1nnnc1N=Nc1nnnn1NC([N+](=O)[O-	0.00	12.13

	])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]		
280	NC(=O)n1nnnc1N(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.98	12.16
281	O=[N+]([O-])n1nnc(OCc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	21.07
282	O=C(Nc1nnn([N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	2.13	28.87
283	O=[N+]([O-])n1nnc(-c2nnn([N+](=O)[O-])n2)n1	0.00	12.40
284	O=[N+]([O-])N(CCN(c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-])c1nnn([N+](=O)[O-])n1	0.00	10.10
285	O=[N+]([O-])n1nnc(C(CNc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	1.72	23.14
286	N#Cn1nnc(C(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.86	15.05
287	N#Cn1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	9.40
288	O=[N+]([O-])C(n1nnc(Nc2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	12.91
289	O=[N+]([O-])C(n1nnc(NC(c2nnn(O)n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-2.12	15.38
290	O=[N+]([O-])CN(c1nnn(O)n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-2.12	6.28
291	O=[N+]([O-])C(n1nnc(NNc2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	-2.40	10.71
292	O=[N+]([O-])C(Nn1nnc(-c2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	4.14
293	O=[N+]([O-])C(n1nnc(N(c2nnn(O)n2)[N+](=O)[O-])n1)[N+](=O)[O-]	0.00	9.75
294	O=[N+]([O-])C(n1nnc(N=Nc2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	2.42	8.38
295	O=[N+]([O-])NCCN(n1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	-1.62	13.05
296	O=[N+]([O-])C(Nn1nnc(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	1.90	14.90
297	O=[N+]([O-])C(Nn1nnc(C(Nc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	0.00	18.07
298	O=C(Nc1nnn(NC([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.78	28.77
299	O=[N+]([O-])CN(c1nnn(NC([N+](=O)[O-])[N+](=O)[O-	0.00	9.07

	])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1		
300	O=[N+]([O-])C(Nn1nnc(NNc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	0.00	12.70
301	O=[N+]([O-])On1nnc(-c2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	7.86
302	O=[N+]([O-])C(Nn1nnc(-c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	1.90	8.43
303	O=[N+]([O-])C(Nn1nnc(N(c2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	1.90	13.92
304	O=[N+]([O-])C(Nn1nnc(Oc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	-2.12	14.50
305	O=[N+]([O-])C(Nn1nnc(C(CNc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-1.48	20.96
306	O=[N+]([O-])C(CNn1nnc(C(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-1.48	16.46
307	O=[N+]([O-])C(CNn1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	0.00	12.30
308	O=[N+]([O-])On1nnc(Nc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	19.11
309	O=[N+]([O-])CN(c1nnn(O[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])[N+](=O)[O-])n1	-2.12	11.79
310	O=[N+]([O-])On1nnc(NNc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.40	16.91
311	O=[N+]([O-])On1nnc(Cc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	17.48
312	O=[N+]([O-])On1nnc(-c2nnn(NC([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	7.86
313	O=[N+]([O-])On1nnc(-c2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	10.95
314	O=[N+]([O-])On1nnc(N=Nc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.42	11.69
315	N=C(Nc1nnn(O[N+](=O)[O-])n1)Nc1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.98	8.29
316	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnc(C(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.48	14.88
317	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	8.38
318	NNn1nnc(C(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-	0.00	9.38

	])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1		
319	NNn1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	2.12	5.22
320	NNn1nnc(Oc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.40	5.80
321	N#CNn1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	-2.07	6.59
322	O=[N+]([O-])On1nnc(Nc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	19.11
323	O=[N+]([O-])C(n1nnc(Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	1.90	16.69
324	O=[N+]([O-])C(n1nnc(C(Nc2nnn(O)n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-2.12	15.38
325	O=[N+]([O-])C(Nn1nnc(NC(c2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	0.00	18.76
326	O=[N+]([O-])C(n1nnc(NC(c2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	1.72	21.82
327	O=[N+]([O-])Nn1nnc(NC(c2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	1.90	17.81
328	O=[N+]([O-])C(n1nnc(C(Nc2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-1.48	21.17
329	O=[N+]([O-])C(n1nnc(OCc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	-1.90	26.24
330	O=C(Nc1nnn(C([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	0.00	35.43
331	O=C(Nc1nnn(C([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.78	29.87
332	O=[N+]([O-])CN(c1nnn(O[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])[N+](=O)[O-])n1	-2.12	11.79
333	O=[N+]([O-])CN(c1nnn(C([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	1.72	14.93
334	O=[N+]([O-])CN(c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])[N+](=O)[O-])n1	0.00	10.86
335	O=[N+]([O-])On1nnc(NNc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.40	16.91
336	O=[N+]([O-])C(n1nnc(NNc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	1.90	19.36
337	O=[N+]([O-])C(n1nnc(NNc2nnn(NC([N+](=O)[O-	0.00	14.49

	])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]		
338	O=[N+]([O-])C(n1nnc(N(c2nnn(O)n2)[N+](=O)[O-])n1)[N+](=O)[O-]	0.00	9.75
339	O=[N+]([O-])C(Nn1nnc(N(c2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	1.90	13.92
340	O=[N+]([O-])OCn1nnc(N(c2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	-2.12	15.99
341	O=[N+]([O-])C(n1nnc(N(c2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	0.00	16.32
342	O=[N+]([O-])C(Nn1nnc(Oc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	-2.12	14.50
343	O=[N+]([O-])C(n1nnc(Oc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	0.00	16.77
344	O=[N+]([O-])Nn1nnc(Oc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	14.25
345	O=[N+]([O-])On1nnc(N=Nc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.42	11.69
346	O=[N+]([O-])C(n1nnc(N(CCN(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-1.48	15.27
347	O=[N+]([O-])C(n1nnc(C(CNc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	0.00	28.31
348	O=[N+]([O-])C(n1nnc(C(CNc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-1.48	23.44
349	O=[N+]([O-])C(n1nnc(Nc2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	12.91
350	O=[N+]([O-])C(Nn1nnc(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	1.90	14.90
351	O=[N+]([O-])OCn1nnc(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	21.76
352	O=[N+]([O-])C(CNn1nnc(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	18.70
353	N#Cn1nnc(NC(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.86	13.44
354	O=[N+]([O-])C(CNn1nnc(NC(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-1.48	14.85
355	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnc(NC(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.48	13.27

356	NNn1nnc(NC(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	0.00	7.77
357	Nn1nnc(NC(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	1.90	14.31
358	NC(=O)n1nnc(NC(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.78	14.78
359	O=[N+]([O-])n1nnc(COc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	21.07
360	O=[N+]([O-])C(n1nnc(COc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	-1.90	26.24
361	O=[N+]([O-])Nn1nnc(COc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	21.51
362	O=C(Nc1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn([N+](=O)[O-])n1	2.13	29.57
363	O=C(Nc1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(NC([N+](=O)[O-])[N+](=O)[O-])n1	-1.78	27.38
364	O=C(Nc1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])[N+](=O)[O-])n1	0.00	34.04
365	O=C(Nc1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(N[N+](=O)[O-])n1	0.00	28.52
366	O=[N+]([O-])CN(c1nnn(O)n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-2.12	6.28
367	O=[N+]([O-])CN(c1nnn(NC([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	0.00	9.07
368	O=[N+]([O-])CN(c1nnn(C([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	1.72	14.93
369	O=[N+]([O-])CN(c1nnn(N[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	1.90	10.21
370	O=[N+]([O-])CN(c1nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.48	12.26
371	O=[N+]([O-])C(n1nnc(NNc2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	-2.40	10.71
372	O=[N+]([O-])C(Nn1nnc(NNc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	0.00	12.70
373	O=[N+]([O-])C(n1nnc(NNc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	1.90	19.36
374	O=[N+]([O-])Nn1nnc(NNc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.12	13.14
375	O=[N+]([O-])C(CNn1nnc(NNc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-	-1.62	16.50

	])[N+](=O)[O-]		
376	O=[N+]([O-])On1nnc(Cc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	17.48
377	O=[N+]([O-])C(Nn1nnc(Cc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	1.72	17.25
378	O=[N+]([O-])OCn1nnc(-c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	17.32
379	O=[N+]([O-])C(CNn1nnc(-c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	1.72	15.49
380	N#Cn1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	9.40
381	O=[N+]([O-])NCCN(n1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	-1.62	13.05
382	O=[N+]([O-])C(CNn1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	0.00	12.30
383	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	8.38
384	NNn1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	2.12	5.22
385	N#CNn1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	-2.07	6.59
386	NC(=O)n1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	10.74
387	NNn1nnc(Oc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.40	5.80
388	Nn1nnc(Oc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	10.86
389	O=[N+]([O-])C(n1nnc(N=Nc2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	2.42	8.38
390	O=[N+]([O-])OCn1nnc(N=Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	15.32
391	O=[N+]([O-])C(CNn1nnc(N=Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	1.62	15.66
392	N=C(Nc1nnn(O[N+](=O)[O-])n1)Nc1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.98	8.29
393	N=C(Nc1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)Nc1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	1.62	12.14

394	N=C(Nc1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)Nc1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	0.00	6.58
395	O=[N+]([O-])N(CCN(c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-])c1nnn([N+](=O)[O-])n1	0.00	10.10
396	O=[N+]([O-])C(n1nnc(N(CCN(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-1.48	15.27
397	O=[N+]([O-])Nn1nnc(N(CCN(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])[N+](=O)[O-])n1	-1.62	10.55
398	O=[N+]([O-])n1nnc(NCC(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	1.72	23.14
399	O=[N+]([O-])C(Nn1nnc(NCC(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-1.48	21.66
400	O=[N+]([O-])C(n1nnc(NCC(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	0.00	28.31
401	O=[N+]([O-])Nn1nnc(NCC(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	0.00	22.10
402	Nn1nnc(C(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	1.90	15.92
403	Nn1nnc(Oc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	10.86
404	O=[N+]([O-])Nn1nnc(C(Nc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	1.90	17.81
405	O=[N+]([O-])Nn1nnc(OCc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	21.51
406	O=C(Nc1nnn(N[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	0.00	29.21
407	O=[N+]([O-])CN(c1nnn(N[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	1.90	10.21
408	O=[N+]([O-])Nn1nnc(NNc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	2.12	13.14
409	O=[N+]([O-])Nn1nnc(Oc2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	14.25
410	O=[N+]([O-])Nn1nnc(N(CCN(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])[N+](=O)[O-])n1	-1.62	10.55
411	O=[N+]([O-])Nn1nnc(C(CNc2nnn(C([N+](=O)[O-	0.00	22.10

	])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1		
412	O=[N+]([O-])C(n1nnc(Nc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	1.90	16.69
413	O=C(Nc1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])[N+](=O)[O-])n1	-1.78	29.17
414	O=[N+]([O-])CN(c1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])[N+](=O)[O-])n1	0.00	10.86
415	O=[N+]([O-])C(n1nnc(NNc2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	0.00	14.49
416	O=[N+]([O-])C(Nn1nnc(Cc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	1.72	17.25
417	O=[N+]([O-])C(Nn1nnc(-c2nnn(O)n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	4.14
418	O=[N+]([O-])C(Nn1nnc(-c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)[N+](=O)[O-]	1.90	8.43
419	O=[N+]([O-])OCn1nnc(-c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	13.25
420	O=[N+]([O-])C(CNn1nnc(-c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	12.23
421	N=C(Nc1nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)Nc1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	0.00	6.58
422	O=[N+]([O-])C(n1nnc(NCC(c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-1.48	22.75
423	O=[N+]([O-])OCn1nnc(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	21.76
424	O=[N+]([O-])OCn1nnc(-c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	17.32
425	O=[N+]([O-])OCn1nnc(-c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	13.25
426	O=[N+]([O-])OCn1nnc(N(c2nnn(C([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	-2.12	15.99
427	O=[N+]([O-])OCn1nnc(N=Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	0.00	15.32
428	O=[N+]([O-])C(CNn1nnc(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	18.70
429	O=[N+]([O-])C(n1nnc(NC(c2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1)[N+](=O)[O-]	-1.48	21.17

430	O=[N+]([O-])CN(c1nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1)c1nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n1	-1.48	12.26
431	O=[N+]([O-])C(CNn1nnc(NNc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	-1.62	16.50
432	O=[N+]([O-])On1nnc(-c2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1	-2.12	10.95
433	O=[N+]([O-])C(CNn1nnc(-c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	1.72	15.49
434	O=[N+]([O-])C(CNn1nnc(-c2nnn(NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	0.00	12.23
435	O=[N+]([O-])C(n1nnc(N(c2nnn(NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1)[N+](=O)[O-]	0.00	16.32
436	O=[N+]([O-])C(CNn1nnc(N=Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)n1)([N+](=O)[O-])[N+](=O)[O-]	1.62	15.66
437	NC(=O)n1nnc(C(Nc2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)([N+](=O)[O-])[N+](=O)[O-])n1	-1.78	16.39
438	NC(=O)n1nnc(N(c2nnn(C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])n2)[N+](=O)[O-])n1	0.00	10.74
439	O=[N+]([O-])n1nnnc1OCc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	26.19
440	O=C(Nc1nnnn1[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.13	25.41
441	O=[N+]([O-])n1nnnc1-c1nnnn1[N+](=O)[O-]	0.00	9.69
442	O=[N+]([O-])N(CCN(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])c1nnnn1[N+](=O)[O-]	0.00	10.61
443	O=[N+]([O-])n1nnnc1C(CNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.72	23.74
444	N=Nn1nnnc1Oc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.42	2.11
445	N=Nn1nnnc1N=Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.33	1.76
446	N#Cn1nnnc1C(Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.86	15.51
447	N#Cn1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	7.60
448	O=[N+]([O-])C(n1nnnc1Nc1nnnn1O)([N+](=O)[O-	0.00	12.15

	])[N+](=O)[O-]		
449	O=[N+]([O-])C(n1nnnc1NC(c1nnnn1O)([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-2.12	11.41
450	O=[N+]([O-])CN(c1nnnn1O)c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	5.64
451	O=[N+]([O-])C(n1nnnc1NNc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	-2.40	11.74
452	O=[N+]([O-])C(Nn1nnnc1-c1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	0.00	0.69
453	O=[N+]([O-])C(n1nnnc1N(c1nnnn1O)[N+](=O)[O-])[N+](=O)[O-]	0.00	5.30
454	O=[N+]([O-])C(n1nnnc1N=Nc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	2.42	7.36
455	O=[N+]([O-])NCCN(n1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.62	14.37
456	O=[N+]([O-])C(Nn1nnnc1Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.90	19.29
457	O=[N+]([O-])C(Nn1nnnc1C(Nc1nnnn1C([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	17.86
458	O=C(Nc1nnnn1NC([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.78	26.52
459	O=[N+]([O-])CN(c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	12.18
460	O=[N+]([O-])C(Nn1nnnc1NNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	17.49
461	O=[N+]([O-])On1nnnc1-c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-]	0.00	7.72
462	O=[N+]([O-])C(Nn1nnnc1-c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.90	7.64
463	O=[N+]([O-])C(Nn1nnnc1N(c1nnnn1C([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.90	13.24
464	O=[N+]([O-])C(Nn1nnnc1Oc1nnnn1C([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-2.12	15.56
465	O=[N+]([O-])C(Nn1nnnc1C(CNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.48	24.16
466	O=[N+]([O-])C(CNn1nnnc1C(Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.48	21.83
467	O=[N+]([O-])C(CNn1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	15.41
468	O=[N+]([O-])On1nnnc1Nc1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	0.00	16.08
469	O=[N+]([O-])CN(c1nnnn1O[N+](=O)[O-	-2.12	10.66

	])c1nnnn1C([N+](=O)[O-])[N+](=O)[O-]		
470	O=[N+]([O-])On1nnnc1NNc1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	-2.40	15.67
471	O=[N+]([O-])On1nnnc1Cc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	22.56
472	O=[N+]([O-])On1nnnc1-c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-]	0.00	7.72
473	O=[N+]([O-])On1nnnc1-c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	11.50
474	O=[N+]([O-])On1nnnc1N=Nc1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	2.42	12.38
475	N=C(Nc1nnnn1O[N+](=O)[O-])Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.98	11.28
476	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnnc1C(Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.48	18.46
477	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	9.70
478	NNn1nnnc1C(Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	14.06
479	NNn1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	2.12	7.63
480	NNn1nnnc1Oc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.40	9.95
481	N#CNn1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-2.07	10.40
482	O=[N+]([O-])On1nnnc1Nc1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	0.00	16.08
483	O=[N+]([O-])C(n1nnnc1Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.90	16.18
484	O=[N+]([O-])C(n1nnnc1C(Nc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-2.12	13.42
485	O=[N+]([O-])C(Nn1nnnc1NC(c1nnnn1C([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	20.56
486	O=[N+]([O-])C(n1nnnc1NC(c1nnnn1C([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.72	22.12
487	O=[N+]([O-])Nn1nnnc1NC(c1nnnn1C([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.90	18.52
488	O=[N+]([O-])C(n1nnnc1C(Nc1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.48	23.67
489	O=[N+]([O-])C(n1nnnc1OCc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.90	32.76

490	O=C(Nc1nnnn1C([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	30.89
491	O=C(Nc1nnnn1C([N+](=O)[O-])[N+](=O)[O-])c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.78	22.73
492	O=[N+]([O-])CN(c1nnnn1O[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	-2.12	10.66
493	O=[N+]([O-])CN(c1nnnn1C([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.72	16.85
494	O=[N+]([O-])CN(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	0.00	10.18
495	O=[N+]([O-])On1nnnc1NNc1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	-2.40	15.67
496	O=[N+]([O-])C(n1nnnc1NNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.90	21.85
497	O=[N+]([O-])C(n1nnnc1NNc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	14.38
498	O=[N+]([O-])C(n1nnnc1N(c1nnnn1O)[N+](=O)[O-])[N+](=O)[O-]	0.00	5.30
499	O=[N+]([O-])C(Nn1nnnc1N(c1nnnn1C([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.90	13.24
500	O=[N+]([O-])OCn1nnnc1N(c1nnnn1C([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-2.12	16.38
501	O=[N+]([O-])C(n1nnnc1N(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	15.63
502	O=[N+]([O-])C(Nn1nnnc1Oc1nnnn1C([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-2.12	15.56
503	O=[N+]([O-])C(n1nnnc1Oc1nnnn1C([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	17.42
504	O=[N+]([O-])Nn1nnnc1Oc1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	0.00	15.30
505	O=[N+]([O-])On1nnnc1N=Nc1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	2.42	12.38
506	O=[N+]([O-])C(n1nnnc1N(CCN(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.48	17.19
507	O=[N+]([O-])C(n1nnnc1C(CNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	31.24
508	O=[N+]([O-])C(n1nnnc1C(CNc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.48	23.77
509	O=[N+]([O-])C(n1nnnc1Nc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	0.00	12.15
510	O=[N+]([O-])C(Nn1nnnc1Nc1nnnn1C([N+](=O)[O-	1.90	19.29

	])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]		
511	O=[N+]([O-])OCn1nnnc1Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	24.50
512	O=[N+]([O-])C(CNn1nnnc1Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	23.78
513	N#Cn1nnnc1NC(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.86	14.82
514	O=[N+]([O-])C(CNn1nnnc1NC(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.48	21.83
515	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnnc1NC(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.48	17.76
516	NNn1nnnc1NC(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	14.06
517	Nn1nnnc1NC(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.90	16.74
518	NC(=O)n1nnnc1NC(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.78	25.36
519	O=[N+]([O-])n1nnnc1COc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	23.01
520	O=[N+]([O-])C(n1nnnc1COc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.90	38.59
521	O=[N+]([O-])Nn1nnnc1COc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	26.05
522	O=C(Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1[N+](=O)[O-]	2.13	25.41
523	O=C(Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-]	-1.78	25.83
524	O=C(Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	0.00	32.39
525	O=C(Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1N[N+](=O)[O-]	0.00	26.97
526	O=[N+]([O-])CN(c1nnnn1O)c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	5.64
527	O=[N+]([O-])CN(c1nnnn1NC([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	12.18
528	O=[N+]([O-])CN(c1nnnn1C([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.72	16.85
529	O=[N+]([O-])CN(c1nnnn1N[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.90	13.32
530	O=[N+]([O-])CN(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-	-1.48	15.37

	])[N+](=O)[O-]		
531	O=[N+]([O-])C(n1nnnc1NNc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	-2.40	11.74
532	O=[N+]([O-])C(Nn1nnnc1NNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	17.49
533	O=[N+]([O-])C(n1nnnc1NNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.90	21.85
534	O=[N+]([O-])Nn1nnnc1NNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.12	17.93
535	O=[N+]([O-])C(CNn1nnnc1NNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.62	21.98
536	O=[N+]([O-])On1nnnc1Cc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	22.56
537	O=[N+]([O-])C(Nn1nnnc1Cc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.72	23.47
538	O=[N+]([O-])OCn1nnnc1-c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	20.81
539	O=[N+]([O-])C(CNn1nnnc1-c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.72	20.48
540	N#Cn1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	7.60
541	O=[N+]([O-])NCCN(n1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.62	14.37
542	O=[N+]([O-])C(CNn1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	15.41
543	O=[N+]([O-])CN(C[N+](=O)[O-])n1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	9.70
544	NNn1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	2.12	7.63
545	N#CNn1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-2.07	10.40
546	NC(=O)n1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	18.84
547	N=Nn1nnnc1Oc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.42	2.11
548	NNn1nnnc1Oc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.40	9.95
549	Nn1nnnc1Oc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	11.85
550	N=Nn1nnnc1N=Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-	-2.33	1.76

	])[N+](=O)[O-]		
551	O=[N+]([O-])C(n1nnnc1N=Nc1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	2.42	7.36
552	O=[N+]([O-])OCn1nnnc1N=Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	18.83
553	O=[N+]([O-])C(CNn1nnnc1N=Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.62	18.39
554	N=C(Nc1nnnn1O[N+](=O)[O-])Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.98	11.28
555	N=C(Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.62	15.16
556	N=C(Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	10.70
557	O=[N+]([O-])N(CCN(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])c1nnnn1[N+](=O)[O-]	0.00	10.61
558	O=[N+]([O-])C(n1nnnc1N(CCN(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.48	17.19
559	O=[N+]([O-])Nn1nnnc1N(CCN(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.62	13.66
560	O=[N+]([O-])n1nnnc1NCC(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.72	23.05
561	O=[N+]([O-])C(Nn1nnnc1NCC(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.48	24.16
562	O=[N+]([O-])C(n1nnnc1NCC(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	27.14
563	O=[N+]([O-])Nn1nnnc1NCC(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	24.61
564	Nn1nnnc1C(Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.90	17.44
565	Nn1nnnc1Oc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	11.85
566	O=[N+]([O-])Nn1nnnc1C(Nc1nnnn1C([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.90	17.60
567	O=[N+]([O-])Nn1nnnc1OCc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	29.23

568	O=C(Nc1nnnn1N[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	26.97
569	O=[N+]([O-])CN(c1nnnn1N[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.90	13.32
570	O=[N+]([O-])Nn1nnnc1NNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	2.12	17.93
571	O=[N+]([O-])Nn1nnnc1Oc1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	0.00	15.30
572	O=[N+]([O-])Nn1nnnc1N(CCN(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.62	13.66
573	O=[N+]([O-])Nn1nnnc1C(CNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	25.30
574	O=[N+]([O-])C(n1nnnc1Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.90	16.18
575	O=C(Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	-1.78	24.92
576	O=[N+]([O-])CN(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])[N+](=O)[O-]	0.00	10.18
577	O=[N+]([O-])C(n1nnnc1NNc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	14.38
578	O=[N+]([O-])C(Nn1nnnc1Cc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.72	23.47
579	O=[N+]([O-])C(Nn1nnnc1-c1nnnn1O)([N+](=O)[O-])[N+](=O)[O-]	0.00	0.69
580	O=[N+]([O-])C(Nn1nnnc1-c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	1.90	7.64
581	O=[N+]([O-])OCn1nnnc1-c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	12.05
582	O=[N+]([O-])C(CNn1nnnc1-c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	10.75
583	N=C(Nc1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	10.70
584	O=[N+]([O-])C(n1nnnc1NCC(c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.48	19.67
585	O=[N+]([O-])OCn1nnnc1Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	24.50
586	O=[N+]([O-])OCn1nnnc1-c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	20.81
587	O=[N+]([O-])OCn1nnnc1-c1nnnn1NC([N+](=O)[O-	-2.12	12.05

	])([N+](=O)[O-])[N+](=O)[O-]		
588	O=[N+]([O-])OCn1nnnc1N(c1nnnn1C([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-2.12	16.38
589	O=[N+]([O-])OCn1nnnc1N=Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	18.83
590	O=[N+]([O-])C(CNn1nnnc1Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	23.78
591	O=[N+]([O-])C(n1nnnc1NC(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	-1.48	20.96
592	O=[N+]([O-])CN(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.48	15.37
593	O=[N+]([O-])C(CNn1nnnc1NNc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.62	21.98
594	O=[N+]([O-])On1nnnc1-c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-2.12	11.50
595	O=[N+]([O-])C(CNn1nnnc1-c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.72	20.48
596	O=[N+]([O-])C(CNn1nnnc1-c1nnnn1NC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	0.00	10.75
597	O=[N+]([O-])C(n1nnnc1N(c1nnnn1NCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	15.63
598	O=[N+]([O-])C(CNn1nnnc1N=Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	1.62	18.39
599	NC(=O)n1nnnc1C(Nc1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	-1.78	26.74
600	NC(=O)n1nnnc1N(c1nnnn1C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.00	18.84

4. Error plots comparing theoretically calculated and experimental values for four reference molecules.

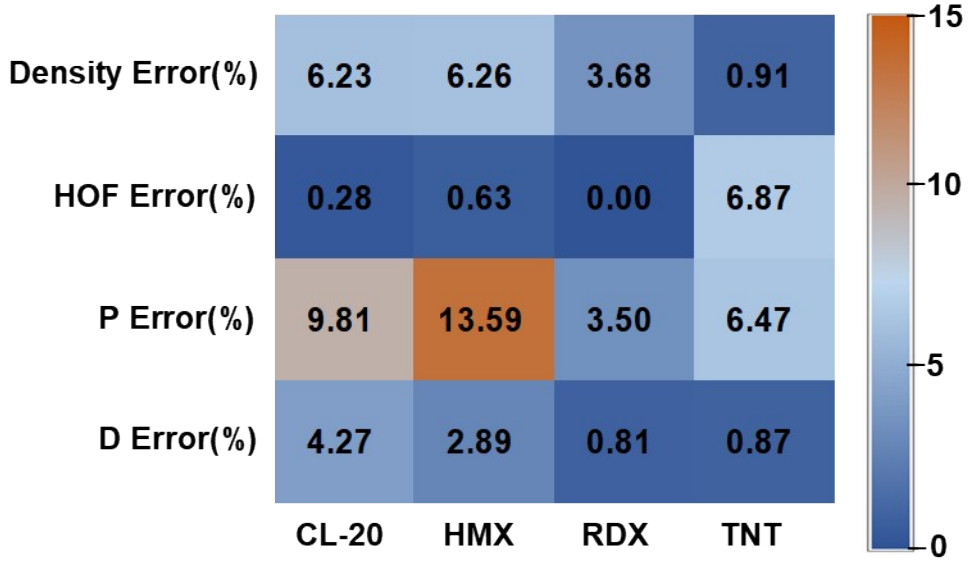

Fig.S1 Error plots(%) comparing theoretically calculated and experimental values for four reference molecules.

Table S3. Comparison of experimental and predicted performance of reference molecule parts

Reference molecule	CL-20	HMX	RDX	TNT
Molecular formula	$C_6H_6N_{12}O_{12}$	$C_4H_8N_8O_8$	$C_3H_6N_6O_6$	$C_7H_5N_3O_6$
ρ ($g\cdot cm^{-3}$)[a]	2.04	1.90	1.82	1.65
ρ ($g\cdot cm^{-3}$)[b]	1.913	1.781	1.753	1.635
HOF ($kJ\cdot mol^{-1}$)[a]	377.4	104.8	92.6	-63.2
HOF ($kJ\cdot mol^{-1}$)[b]	378.45	105.46	92.60	-67.54
P (GPa)[a]	43	39	34	19
P (GPa)[b]	38.78	33.70	32.81	20.23
D_v ($km\cdot s^{-1}$)[a]	9.6	9.0	8.6	6.9
D_v ($km\cdot s^{-1}$)[b]	9.19	8.74	8.67	6.96

1) a：Experimentally measured values(Data from NIST Research Library). b：Calculate the predicted value.

5. Table S4. Molecules obtained after secondary screening and corresponding selection properties(#1-4 are reference molecules, Molecules labelled '/' were deleted.)

Index	New Index	υ	Density($g\cdot cm^{-3}$)
46	#5	0.24373	1.90953
48	#6	0.201055	1.90913
57	#7	0.246242	1.92621
75	#8	0.206789	1.97055

94	#9	0.221644	1.98165
95	#10	0.211175	1.98088
118	#11	0.214043	1.95237
136	#12	0.206531	1.90806
160	/	0.214523	2.06556
166	#13	0.231615	2.03493
167	#14	0.195685	2.03648
182	/	0.197128	2.06289
187	#15	0.215586	1.90425
193	#16	0.222691	1.91862
197	#17	0.204639	1.91561
198	#18	0.202182	1.90449
227	#19	0.212963	2.02499
228	/	0.15775	2.05674
229	#20	0.215066	2.05328
236	#21	0.199638	2.03285
258	#22	0.2235	2.06789
267	#23	0.202178	1.91593
277	#24	0.230878	2.02442
2	#25	0.225296	1.97586
18	#26	0.200248	1.94081
33	#27	0.211778	1.92726
51	#28	0.203252	1.98253
78	#29	0.236507	1.97774
91	#30	0.20681	1.92319
126	#31	0.209859	1.95403
168	#32	0.235005	2.00063
188	#33	0.22836	2.00228
199	#34	0.218784	1.94637
200	#35	0.233278	1.94834
230	#36	0.196183	2.00719
231	#37	0.200182	1.93431
251	#38	0.232284	2.03145
256	#39	0.214158	1.95831
274	#40	0.232107	2.03222
281	#41	0.195583	2.01816
310	#42	0.205374	2.00201

6 Table S5 The properties of each candidate molecule were calculated with high precision.

INDEX	υ	Density	Q	D	P	SYBA
#1	0.0592	1.9127	6.5605	9.1857	38.7846	1.2634
#2	0.1357	1.7807	6.2797	8.7449	33.7034	2.0766
#3	0.1723	1.7526	6.3405	8.6695	32.8065	2.0766
#4	0.2021	1.6352	5.3963	6.9565	20.2276	34.5318
#5	0.2379	1.8272	6.8759	9.1097	37.1422	20.3318
#6	0.1852	1.8346	6.7988	9.1400	37.4790	6.6249
#7	0.2411	1.8844	7.0145	9.4187	40.4285	9.9256
#8	0.2043	1.9173	6.1977	9.1990	38.9508	25.9560
#9	0.2171	1.9385	6.2771	9.2660	39.7686	24.6989
#10	0.2106	1.9289	6.2042	9.2412	39.4446	25.9560
#11	0.1987	1.8951	6.6880	9.3399	39.8847	5.1439
#12	0.1970	1.8479	6.8884	9.2011	38.1436	9.6166
#13	0.2228	1.9724	6.5427	9.5716	42.8523	13.0989
#14	0.1799	1.9697	6.4761	9.5475	42.6042	13.0186
#15	0.2048	1.8261	6.8904	9.1104	37.1341	19.3394
#16	0.2174	1.8690	6.8284	9.3722	39.8394	3.3419
#17	0.1968	1.8670	6.9416	9.2862	39.0879	11.4981
#18	0.1810	1.8478	7.0150	9.2888	38.8732	9.5819
#19	0.2055	1.9647	6.3466	9.4723	41.8763	6.0668
#20	0.2038	1.9885	6.3348	9.5885	43.2003	13.4614
#21	0.1861	1.9782	6.3850	9.4423	41.7718	17.9381
#22	0.2129	1.9990	6.3617	9.5858	43.3028	7.6927
#23	0.1963	1.8698	6.5483	9.1466	37.9541	10.0473
#24	0.2228	1.9645	6.4634	9.4544	41.7163	12.0844
#25	0.2210	1.9335	6.0764	9.1165	38.4402	28.8733
#26	0.1928	1.8900	6.1684	9.0337	37.2550	28.7713
#27	0.2043	1.8781	6.7824	9.2467	38.8890	10.9500
#28	0.1977	1.9266	6.1170	9.1389	38.5500	29.8656
#29	0.2361	1.9209	5.9032	9.0390	37.6489	14.7801
#30	0.2036	1.8675	6.6128	9.2300	38.6219	10.7092
#31	0.2082	1.9047	6.2642	9.1458	38.3556	29.2141
#32	0.2305	1.9469	6.4201	9.3985	41.0155	12.1492
#33	0.2213	1.9443	6.5514	9.4370	41.3206	16.0772
#34	0.1950	1.9052	6.6670	9.4186	40.6842	7.6349
#35	0.2232	1.8931	6.5671	9.3034	39.5504	9.9529
#36	0.1821	1.9427	6.3003	9.3418	40.4716	19.2851
#37	0.1922	1.8873	6.3539	9.1287	38.0105	24.5013
#38	0.2281	1.9757	6.5044	9.5692	42.8719	11.7382
#39	0.2175	1.9192	6.8800	9.3842	40.5581	22.5581
#40	0.2291	1.9718	6.4137	9.4663	41.9083	11.2753
#41	0.1728	1.9598	6.5798	9.4589	41.6981	24.1645
#42	0.1894	1.9339	6.5199	9.3748	40.6532	23.7788

7. Table S6. Comparison of the thermal stability of reference and pre-selected molecules

	CL-20	HMX	RDX	TNT	#7	#22	#33
T_d(℃)	230	280	200	240	80	89	169
NGCM (e)	-0.125	-0.165	-0.153	-0.148	0.0345	-0.137	-0.0646
BDE ($kJ·mol^{-1}$)	165.79	190.59	171.25	259.96	55.74	53.03	122.81

8. Table S7. Comparison of mechanical stability of reference and pre-selected molecules

	CL-20	HMX	RDX	TNT	#7	#22	#33
υ	0.059	0.136	0.172	0.202	0.241	0.213	0.221
ESP_Max ($kJ·mol^{-1}·e^{-1}$)	266.14	235.14	206.35	163.85	169.83	286.06	258.74
Friction Sensibility (N)	54	120	120	353	/	/	/
Impact Sensitivity (N·m)	228	287	230	300	/	/	/

9.The positive and negative ESP area and their distribution

```
Volume:  2420.13911 Bohr^3  ( 358.62762 Angstrom^3)
Estimated density according to mass and volume (M/V):    1.8899 g/cm^3
Minimal value:    -33.36489 kcal/mol   Maximal value:     40.59190 kcal/mol
Overall surface area:        1118.38260 Bohr^2  ( 313.17903 Angstrom^2)
Positive surface area:        641.82847 Bohr^2  ( 179.73028 Angstrom^2)
Negative surface area:        476.55413 Bohr^2  ( 133.44875 Angstrom^2)
Overall average value:    0.00507631 a.u.  (      3.18543 kcal/mol)
Positive average value:   0.02230950 a.u.  (     13.99943 kcal/mol)
Negative average value:  -0.01813355 a.u.  (    -11.37898 kcal/mol)
Overall variance (sigma^2_tot):  0.00039356 a.u.^2 (   154.97315 (kcal/mol)^2)
Positive variance:        0.00023382 a.u.^2 (     92.07067 (kcal/mol)^2)
Negative variance:        0.00015974 a.u.^2 (     62.90248 (kcal/mol)^2)
Balance of charges (nu):   0.24114383
Product of sigma^2_tot and nu:   0.00009491 a.u.^2 (   37.37082 (kcal/mol)^2)
Internal charge separation (Pi):   0.02015538 a.u.  (     12.64771 kcal/mol)
Molecular polarity index (MPI):   0.55865202 eV (     12.88283 kcal/mol)
Nonpolar surface area (|ESP| <= 10 kcal/mol):    140.99 Angstrom^2  ( 45.02 %)
Polar surface area (|ESP| > 10 kcal/mol):        172.19 Angstrom^2  ( 54.98 %)

Surface analysis finished!
Total wall clock time passed during this task:   107 s
Note: Previous orbital information has been restored
Citation of molecular polarity index (MPI): Carbon, 171, 514 (2021) DOI: 10.1016/j.carbon.2020.09.048
```

Fig.S2 Quantitative analysis of molecular surface for #7.

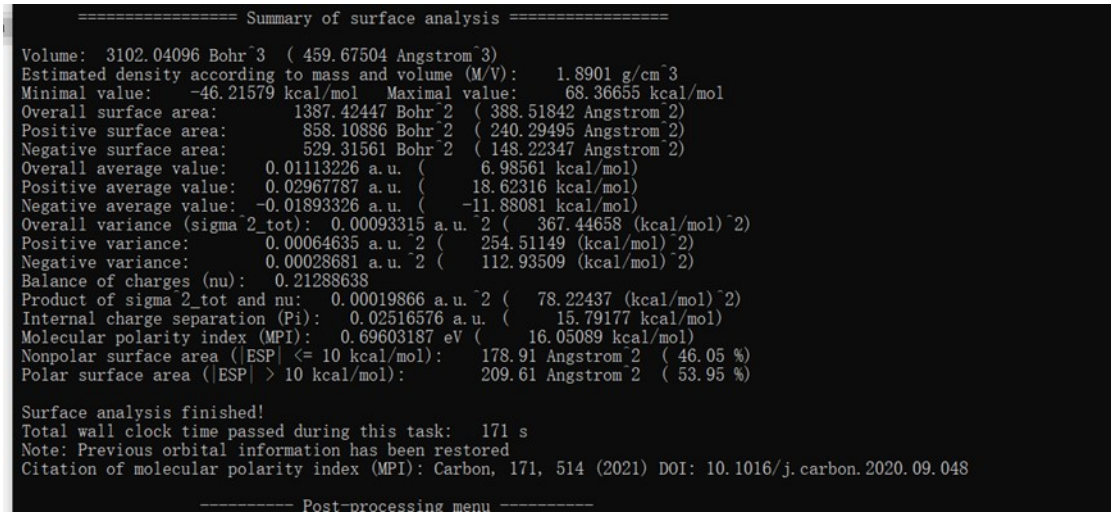

Fig.S3 Quantitative analysis of molecular surface for #22.

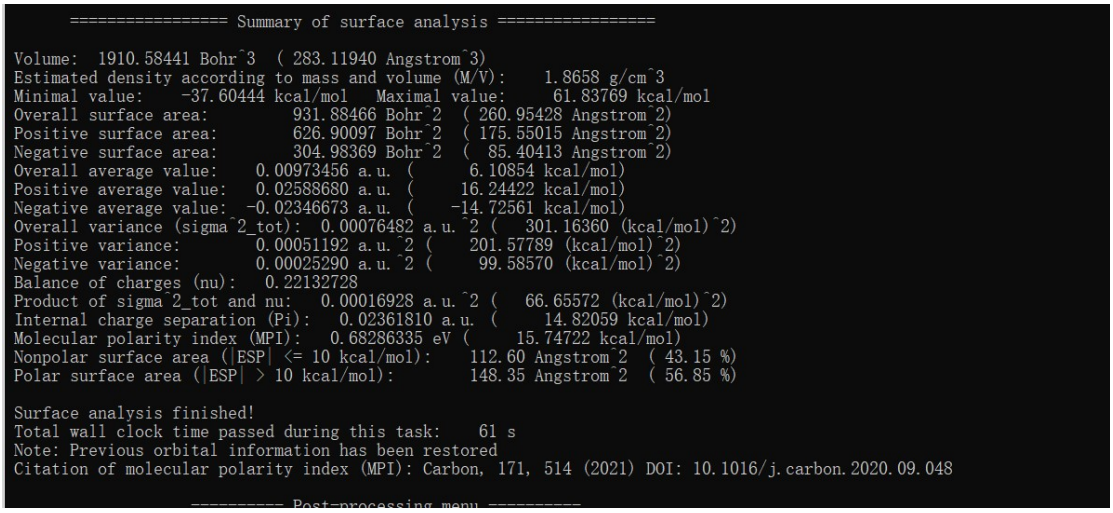

Fig.S4 Quantitative analysis of molecular surface for #33.

10. The optimized Cartesian coordinates of screened molecules

#7

0 1

O	-0.53917900	2.25655300	-0.90910400
N	-0.01602000	3.21476800	-0.46119400
O	-0.34280400	4.25346600	-0.02713900
O	1.65445200	3.09682100	-0.42854200
N	1.99403300	1.89321100	-0.80559400
N	2.30383100	1.57656800	-2.07293800
N	2.53786800	0.30210600	-2.06863400
C	2.30215900	-0.13005900	-0.79014300
N	2.44987900	-1.42362100	-0.30916800
C	2.49307400	-1.65552500	1.13831900

C	1.13341900	-1.85944800	1.81963200
N	0.22314800	-0.70770000	1.79317900
C	-0.72776700	-0.58509000	0.79090700
N	-0.55671600	-1.21530900	-0.41218800
N	-1.61088300	-0.96299700	-1.12113100
N	-2.36592800	-0.17386200	-0.34689900
O	-3.51786700	0.30064500	-0.74876100
N	-4.72007300	-0.76696000	-0.32422300
O	-5.75880900	-0.32682000	-0.64899200
O	-4.31648200	-1.74005000	0.20531900
N	-1.87321700	0.06417500	0.87325700
N	0.61090500	0.44308800	2.51895900
O	1.53421700	0.27360500	3.29396600
O	-0.00687500	1.46521000	2.32225400
N	2.03448900	-2.51883300	-1.11807900
O	1.98202000	-3.58891100	-0.53435100
O	1.80887900	-2.30133700	-2.28074700
N	1.96041100	0.84925100	0.02647200
H	3.01268100	-0.80458500	1.57146700
H	3.08937500	-2.54991200	1.30896300
H	0.59837300	-2.68115600	1.34981400
H	1.31174900	-2.11424900	2.86351100

#22

0 1

N	0.12833300	3.99700900	-0.10386100
C	0.18058700	2.82033900	-0.52779500
N	-0.88330600	1.91884300	-0.81570800
C	-2.18759600	2.20424000	-0.57937800
N	-2.76428200	3.33986000	-0.26603000
N	-4.10701200	3.05512300	-0.13469000
N	-4.37132800	1.83119900	-0.34622800
N	-3.15256000	1.24010900	-0.63324800
N	-2.95087900	-0.07084600	-0.98302900
C	-3.09931800	-1.03499000	0.02323800
N	-2.55008500	-0.47869800	1.34917600
O	-3.32755100	-0.33069000	2.25491500
O	-1.36625700	-0.20632100	1.30976600
N	-2.31314800	-2.30765400	-0.36857900
O	-1.80378600	-2.94027100	0.51890600
O	-2.34095300	-2.54706500	-1.56052700
N	-4.57346800	-1.57173300	0.22698800
O	-5.39422100	-1.09353000	-0.51977400

O	-4.70564100	-2.43574200	1.05936300
N	1.39099700	2.15829700	-0.82110500
C	2.55521000	2.28088600	-0.12960500
N	3.00942200	3.20793400	0.67799700
N	4.24787200	2.77122300	1.08838700
N	4.56891800	1.64707600	0.58519600
N	3.49855400	1.29256600	-0.20710400
N	3.43978700	0.12414600	-0.92212400
C	3.08314500	-1.05256400	-0.26447500
N	1.52258500	-1.28310400	-0.19641500
O	1.12409200	-2.02856200	0.65427200
O	0.86822700	-0.71211200	-1.05587800
N	3.64623500	-2.26139800	-1.07479600
O	3.14229900	-3.32947800	-0.84494100
O	4.54805800	-1.99984600	-1.84272800
N	3.59376900	-1.16319900	1.20003400
O	2.99123800	-0.47929500	1.99254000
O	4.57104900	-1.85315600	1.36527500
H	-0.82458900	4.29551700	0.09920400
H	-0.66367600	0.92858500	-0.81383500
H	-3.36808600	-0.33835000	-1.86894600
H	1.33686000	1.33893700	-1.41026900
H	4.21208400	-0.01089900	-1.57159600

#33

0 1

O	2.27848300	-2.99908600	-0.04766000
N	2.27748100	-1.87709000	0.29553000
O	2.18989800	-1.27317500	1.30461400
O	2.43400400	-0.86620100	-1.05754400
N	2.51729100	0.37663600	-0.64600500
N	3.68798300	0.99836800	-0.28841400
N	3.34243000	2.14961500	0.13018600
N	1.96809400	2.34417800	0.09061300
C	1.48335400	1.23221800	-0.37852100
N	0.19624100	0.81369800	-0.58998700
C	-0.93034100	1.51234800	-0.24612600
N	-1.12324700	2.79736800	-0.12510100
N	-2.42719700	2.94225100	0.27794200
N	-3.02787400	1.83077200	0.39852000
N	-2.09539400	0.85956200	0.06632100
C	-2.36384400	-0.49244200	0.30301800
N	-1.25843900	-1.11668100	1.21720700

O	-0.74678200	-2.14907100	0.83756100
O	-1.03854300	-0.49364100	2.22568600
N	-2.39614400	-1.33661900	-0.97592200
O	-3.24314400	-2.19491800	-1.01975500
O	-1.56218700	-1.06900000	-1.82680200
H	0.06043700	-0.01453200	-1.16271100
H	-3.31786500	-0.61189600	0.80744200

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