

Supplementary molecular list-1

Generated 426 molecules in SMILES and calculated molecular density and PBF.

No.	SMILES	Molecular density	PBF
1	<chem>O=[N+](O)c1c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.22	0.45
2	<chem>Nc1c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.20	0.40
3	<chem>[N-]=[N+]=Nc1c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.19	0.46
4	<chem>Nc1c(N)c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.16	0.35
5	<chem>[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.16	0.35
6	<chem>[N-]=[N+]=Nc1c(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.15	0.53
7	<chem>Nc1c([N+](=O)[O-])c(N)c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.16	0.35
8	<chem>[N-]=[N+]=Nc1c([N+](=O)[O-])c(N)c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.16	0.41
9	<chem>[N-]=[N+]=Nc1c([N+](=O)[O-])c(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.15	0.46
10	<chem>Nc1c(N)c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1N</chem>	1.13	0.30
11	<chem>[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.12	0.27
12	<chem>[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1N</chem>	1.12	0.28
13	<chem>[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]</chem>	1.12	0.30
14	<chem>[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.12	0.27
15	<chem>[N-]=[N+]=Nc1c(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]</chem>	1.11	0.49
16	<chem>Nc1c([N+](=O)[O-])c([N+](=O)[O-])c(N)c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.17	0.34
17	<chem>[N-]=[N+]=Nc1c([N+](=O)[O-])c([N+](=O)[O-])c(N)c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.16	0.42
18	<chem>[N-]=[N+]=Nc1c([N+](=O)[O-])c([N+](=O)[O-])c(N=[N+]=[N-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.15	0.48
19	<chem>Nc1c(N)c([N+](=O)[O-])c([N+](=O)[O-])c(N)c1[N+](=O)[O-]</chem>	1.13	0.30
20	<chem>[N-]=[N+]=Nc1c([N+](=O)[O-])c(N)c(N)c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.12	0.37
21	<chem>[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N)c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.12	0.28
22	<chem>[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.12	0.38
23	<chem>[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c([N+](=O)[O-])c(N)c1[N+](=O)[O-]</chem>	1.12	0.28

24	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.12	0.35
25	$[N-]=[N+]=Nc1c(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c(N)c1[N+](=O)[O-]$	1.12	0.48
26	$[N-]=[N+]=Nc1c(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.11	0.50
27	$Nc1c(N)c(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N$	1.08	0.22
28	$[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c1[N+](=O)[O-]$	1.08	0.22
29	$[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N$	1.08	0.21
30	$[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]$	1.08	0.20
31	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1N$	1.08	0.21
32	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c([N+](=O)[O-])c(N)c1N=[N+]=[N-]$	1.08	0.47
33	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]$	1.08	0.45
34	$[N-]=[N+]=Nc1c(N)c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c1[N+](=O)[O-]$	1.08	0.19
35	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]$	1.08	0.45
36	$[N-]=[N+]=Nc1c(N=[N+]=[N-])c(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]$	1.08	0.60
37	$Nc1c([N+](=O)[O-])c(N)c([N+](=O)[O-])c(N)c1[N+](=O)[O-]$	1.13	0.26
38	$[N-]=[N+]=Nc1c([N+](=O)[O-])c(N)c([N+](=O)[O-])c(N)c1[N+](=O)[O-]$	1.12	0.35
39	$[N-]=[N+]=Nc1c([N+](=O)[O-])c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.12	0.40
40	$[N-]=[N+]=Nc1c([N+](=O)[O-])c(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.11	0.49
41	$Nc1c(N)c([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N$	1.08	0.19
42	$[N-]=[N+]=Nc1c([N+](=O)[O-])c(N)c(N)c(N)c1[N+](=O)[O-]$	1.08	0.40
43	$[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c(N)c1[N+](=O)[O-]$	1.09	0.20
44	$[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.08	0.38
45	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N$	1.08	0.20
46	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N$	1.08	0.31
47	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N=[N+]=[N-]$	1.08	0.44
48	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N=[N+]=[N-]$	1.08	0.51
49	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c(N)c1[N+](=O)[O-]$	1.08	0.18
50	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.08	0.28
51	$[N-]=[N+]=Nc1c(N=[N+]=[N-])c([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N=[N+]=[N-]$	1.08	0.44
52	$[N-]=[N+]=Nc1c(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N=[N+]=[N-]$	1.08	0.51
53	$Nc1c(N)c([N+](=O)[O-])c(N)c(N)c1[N+](=O)[O-]$	1.08	0.22
54	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N)c(N)c1[N+](=O)[O-]$	1.08	0.21

55	$[N-]=[N+]=Nc1c(N=[N+]=[N-])c([N+](=O)[O-])c(N)c(N)c1[N+](=O)[O-]$	1.08	0.43
56	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c(N)c1[N+](=O)[O-]$	1.08	0.20
57	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N)c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.08	0.21
58	$[N-]=[N+]=Nc1c(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c(N)c1[N+](=O)[O-]$	1.08	0.35
59	$[N-]=[N+]=Nc1c(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.08	0.57
60	$Nc1c(N)c(N)c([N+](=O)[O-])c(N)c1N$	1.03	0.13
61	$[N-]=[N+]=Nc1c(N)c(N)c(N)c(N)c1[N+](=O)[O-]$	1.04	0.12
62	$[N-]=[N+]=Nc1c(N)c(N)c(N)c([N+](=O)[O-])c1N$	1.04	0.12
63	$[N-]=[N+]=Nc1c(N)c(N)c(N)c([N+](=O)[O-])c1N=[N+]=[N-]$	1.04	0.12
64	$[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c(N)c1N$	1.04	0.12
65	$[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c1N$	1.04	0.11
66	$[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c(N)c1N=[N+]=[N-]$	1.04	0.11
67	$[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]$	1.04	0.20
68	$[N-]=[N+]=Nc1c(N)c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c1N$	1.04	0.10
69	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c(N)c([N+](=O)[O-])c1N$	1.04	0.10
70	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N$	1.04	0.17
71	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c(N)c1N=[N+]=[N-]$	1.04	0.39
72	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N)c(N=[N+]=[N-])c1N=[N+]=[N-]$	1.04	0.40
73	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]$	1.04	0.40
74	$[N-]=[N+]=Nc1c(N)c(N)c(N)c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.04	0.11
75	$[N-]=[N+]=Nc1c(N)c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c1N=[N+]=[N-]$	1.04	0.40
76	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N$	1.04	0.11
77	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]$	1.04	0.39
78	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N=[N+]=[N-]$	1.04	0.43
79	$[N-]=[N+]=Nc1c(N=[N+]=[N-])c(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]$	1.05	0.41
80	$Nc1c(N)c(N)c(N)c1N$	0.96	0.00
81	$[N-]=[N+]=Nc1c(N)c(N)c(N)c(N)c1N$	0.98	0.00
82	$[N-]=[N+]=Nc1c(N)c(N)c(N)c(N)c1N=[N+]=[N-]$	0.98	0.43
83	$[N-]=[N+]=Nc1c(N)c(N)c(N)c(N=[N+]=[N-])c1N$	0.99	0.00
84	$[N-]=[N+]=Nc1c(N)c(N)c(N)c(N=[N+]=[N-])c1N=[N+]=[N-]$	1.00	0.38
85	$[N-]=[N+]=Nc1c(N)c(N)c(N=[N+]=[N-])c(N)c1N$	0.99	0.00
86	$[N-]=[N+]=Nc1c(N)c(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c1N$	1.00	0.38
87	$[N-]=[N+]=Nc1c(N)c(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]$	1.00	0.37
88	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c(N)c(N=[N+]=[N-])c1N$	1.00	0.00
89	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1N$	1.00	0.36
90	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c(N)c1N=[N+]=[N-]$	1.00	0.37
91	$[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]$	1.01	0.57

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92	[N-]=[N+]=Nc1c(N=[N+]=[N-])c(N=[N+]=[N-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.02	0.35
93	O=[N+](=[O-])c1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.21	0.37
94	Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.18	0.34
95	[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.16	0.31
96	Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.14	0.30
97	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.13	0.27
98	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.12	0.26
99	Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.18	0.26
100	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.17	0.37
101	Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])c1[N+](=O)[O-]	0.99	0.23
102	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.13	0.21
103	[N-]=[N+]=Nc1c([N+](=O)[O-])nc(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.13	0.39
104	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.12	0.37
105	Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1N	1.14	0.28
106	[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1N	1.13	0.25
107	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.13	0.25
108	[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.12	0.23
109	Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N	1.09	0.24
110	[N-]=[N+]=Nc1nc(N)c(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.09	0.21
111	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N	1.09	0.21
112	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1N	1.08	0.19
113	[N-]=[N+]=Nc1c(N)nc(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.09	0.22
114	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.09	0.19
115	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.08	0.20
116	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.08	0.17
117	Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N)c1[N+](=O)[O-]	1.14	0.13
118	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N)c1[N+](=O)[O-]	1.13	0.27
119	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]	1.13	0.36
120	Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N	1.10	0.14
121	[N-]=[N+]=Nc1c([N+](=O)[O-])nc(N)c(N)c1[N+](=O)[O-]	1.09	0.34
122	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N	1.09	0.12
123	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N	1.08	0.31
124	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c(N)c1[N+](=O)[O-]	1.09	0.12
125	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]	1.09	0.26
126	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N=[N+]=[N-]	1.09	0.12
127	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.08	0.29
128	Nc1nc(N)c(N)c([N+](=O)[O-])c1N	1.04	0.14
129	[N-]=[N+]=Nc1c(N)nc(N)c(N)c1[N+](=O)[O-]	1.04	0.12

130	$[N-]=[N+]=Nc1nc(N)c(N)c([N+](=O)[O-])c1N$	1.03	0.12
131	$[N-]=[N+]=Nc1nc(N)c(N)c([N+](=O)[O-])c1N=[N+]=[N-]$	1.04	0.11
132	$[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c([N+](=O)[O-])c1N$	1.04	0.11
133	$[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N)c([N+](=O)[O-])c1N$	1.04	0.10
134	$[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N$	1.04	0.10
135	$[N-]=[N+]=Nc1c(N)nc(N)c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.05	0.11
136	$[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c([N+](=O)[O-])c1N=[N+]=[N-]$	1.05	0.10
137	$[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N=[N+]=[N-]$	1.04	0.09
138	$Nc1c([N+](=O)[O-])c([N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]$	1.18	0.31
139	$[N-]=[N+]=Nc1c([N+](=O)[O-])c([N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]$	1.17	0.35
140	$Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N)c1[N+](=O)[O-]$	1.14	0.26
141	$[N-]=[N+]=Nc1c([N+](=O)[O-])c(N)nc([N+](=O)[O-])c1[N+](=O)[O-]$	1.13	0.34
142	$[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N)c1[N+](=O)[O-]$	1.13	0.24
143	$[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.12	0.32
144	$Nc1nc(N)c([N+](=O)[O-])c(N)c1[N+](=O)[O-]$	1.09	0.22
145	$[N-]=[N+]=Nc1c([N+](=O)[O-])c(N)nc(N)c1[N+](=O)[O-]$	1.09	0.39
146	$[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N)c1[N+](=O)[O-]$	1.09	0.19
147	$[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.08	0.38
148	$[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N)c1[N+](=O)[O-]$	1.08	0.15
149	$[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.08	0.36
150	$Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c([N+](=O)[O-])c1N$	1.14	0.17
151	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]$	1.13	0.18
152	$[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c([N+](=O)[O-])c1N$	1.13	0.21
153	$[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]$	1.13	0.43
154	$Nc1nc([N+](=O)[O-])c(N)c(N)c1[N+](=O)[O-]$	1.09	0.12
155	$[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N)c1[N+](=O)[O-]$	1.09	0.10
156	$[N-]=[N+]=Nc1c([N+](=O)[O-])nc(N)c([N+](=O)[O-])c1N$	1.09	0.14
157	$[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c(N)c1[N+](=O)[O-]$	1.09	0.13
158	$[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])nc(N)c1[N+](=O)[O-]$	1.09	0.13
159	$[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.09	0.12
160	$[N-]=[N+]=Nc1c([N+](=O)[O-])nc(N)c([N+](=O)[O-])c1N=[N+]=[N-]$	1.09	0.41
161	$[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1[N+](=O)[O-]$	1.08	0.38
162	$Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N)c1N$	1.09	0.20
163	$[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N)c1N$	1.08	0.18
164	$[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c([N+](=O)[O-])c1N$	1.09	0.18
165	$[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N)c1N=[N+]=[N-]$	1.08	0.16
166	$[N-]=[N+]=Nc1c(N)c(N)nc([N+](=O)[O-])c1[N+](=O)[O-]$	1.09	0.18
167	$[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N$	1.08	0.16
168	$[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]$	1.09	0.17
169	$[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]$	1.09	0.17
170	$Nc1nc(N)c([N+](=O)[O-])c(N)c1N$	1.04	0.14
171	$[N-]=[N+]=Nc1nc(N)c(N)c(N)c1[N+](=O)[O-]$	1.04	0.11

172	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N)c1N	1.04	0.12
173	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N)c1N	1.04	0.10
174	[N-]=[N+]=Nc1c(N)nc(N)c([N+](=O)[O-])c1N	1.04	0.12
175	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c(N)c1[N+](=O)[O-]	1.04	0.10
176	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N)c1N=[N+]=[N-]	1.04	0.11
177	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N)c1N=[N+]=[N-]	1.04	0.09
178	[N-]=[N+]=Nc1c(N)c(N)nc(N)c1[N+](=O)[O-]	1.04	0.12
179	[N-]=[N+]=Nc1nc(N)c(N)c(N=[N+]=[N-])c1[N+](=O)[O-]	1.04	0.11
180	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N=[N+]=[N-])c1N	1.04	0.11
181	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N	1.04	0.09
182	[N-]=[N+]=Nc1c(N)nc(N)c([N+](=O)[O-])c1N=[N+]=[N-]	1.05	0.11
183	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c1[N+](=O)[O-]	1.05	0.10
184	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.05	0.10
185	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.05	0.09
186	Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N)c1N	1.09	0.00
187	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N)c1N	1.09	0.00
188	[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])nc([N+](=O)[O-])c1N	1.09	0.00
189	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N)c1N=[N+]=[N-]	1.09	0.10
190	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N=[N+]=[N-])c1N	1.09	0.08
191	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.09	0.37
192	Nc1nc([N+](=O)[O-])c(N)c(N)c1N	1.03	0.00
193	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N)c1N	1.03	0.00
194	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c(N)c1N	1.04	0.00
195	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N)c1N=[N+]=[N-]	1.04	0.00
196	[N-]=[N+]=Nc1c(N)c(N)nc([N+](=O)[O-])c1N	1.04	0.00
197	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N=[N+]=[N-])c1N	1.04	0.00
198	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c(N)c1N=[N+]=[N-]	1.04	0.40
199	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N=[N+]=[N-])c1N=[N+]=[N-]	1.04	0.00
200	[N-]=[N+]=Nc1c([N+](=O)[O-])nc(N)c(N)c1N	1.04	0.05
201	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c(N)c1N	1.04	0.00
202	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c(N=[N+]=[N-])c1N	1.05	0.05
203	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c(N)c1N=[N+]=[N-]	1.05	0.01
204	[N-]=[N+]=Nc1c([N+](=O)[O-])nc(N)c(N)c1N=[N+]=[N-]	1.05	0.07
205	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1N	1.04	0.36
206	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.05	0.15
207	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.05	0.13
208	Nc1nc(N)c(N)c(N)c1N	0.97	0.00
209	[N-]=[N+]=Nc1nc(N)c(N)c(N)c1N	0.98	0.00
210	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N)c(N)c1N	0.98	0.00
211	[N-]=[N+]=Nc1c(N)nc(N)c(N)c1N	0.98	0.00
212	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c(N)c1N	0.99	0.00
213	[N-]=[N+]=Nc1nc(N)c(N)c(N)c1N=[N+]=[N-]	0.99	0.00
214	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c(N)c1N	0.99	0.00

215	[N-]=[N+]=Nc1c(N)nc(N)c(N=[N+]=[N-])c1N	0.99	0.00
216	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c(N)c1N=[N+]=[N-]	1.00	0.00
217	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c(N)c1N=[N+]=[N-]	1.00	0.00
218	[N-]=[N+]=Nc1c(N)c(N)nc(N)c1N	0.98	0.00
219	[N-]=[N+]=Nc1nc(N)c(N)c(N=[N+]=[N-])c1N	0.99	0.00
220	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N)c(N=[N+]=[N-])c1N	0.99	0.00
221	[N-]=[N+]=Nc1c(N)nc(N)c(N)c1N=[N+]=[N-]	0.99	0.44
222	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c1N	1.00	0.00
223	[N-]=[N+]=Nc1nc(N)c(N)c(N=[N+]=[N-])c1N=[N+]=[N-]	1.00	0.00
224	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1N	1.00	0.00
225	[N-]=[N+]=Nc1c(N)nc(N)c(N=[N+]=[N-])c1N=[N+]=[N-]	1.00	0.05
226	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.01	0.06
227	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.01	0.00
228	O=[N+](=[O-])c1nc([N+](=O)[O-])c([N+](=O)[O-])nc1[N+](=O)[O-]	1.19	0.29
229	Nc1nc([N+](=O)[O-])c([N+](=O)[O-])nc1[N+](=O)[O-]	1.15	0.17
230	[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])nc1[N+](=O)[O-]	1.14	0.16
231	Nc1nc([N+](=O)[O-])c([N+](=O)[O-])nc1N	1.10	0.19
232	[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])nc1N	1.09	0.17
233	[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])nc1N=[N+]=[N-]	1.09	0.16
234	Nc1nc([N+](=O)[O-])c(N)nc1[N+](=O)[O-]	1.10	0.00
235	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)nc1[N+](=O)[O-]	1.10	0.00
236	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])nc1[N+](=O)[O-]	1.09	0.00
237	Nc1nc(N)c([N+](=O)[O-])nc1[N+](=O)[O-]	1.10	0.00
238	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])nc1[N+](=O)[O-]	1.09	0.00
239	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])nc1[N+](=O)[O-]	1.09	0.00
240	Nc1nc(N)c([N+](=O)[O-])nc1N	1.04	0.00
241	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)nc1N	1.04	0.00
242	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])nc1N	1.04	0.00
243	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])nc1N=[N+]=[N-]	1.04	0.00
244	[N-]=[N+]=Nc1nc(N)c(N)nc1[N+](=O)[O-]	1.04	0.00
245	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])nc1N	1.04	0.00
246	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])nc1N	1.04	0.00
247	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])nc1N=[N+]=[N-]	1.04	0.00
248	Nc1nc(N)c(N)nc1N	0.97	0.00
249	[N-]=[N+]=Nc1nc(N)c(N)nc1N	0.98	0.00
250	[N-]=[N+]=Nc1nc(N)c(N)nc1N=[N+]=[N-]	0.99	0.00
251	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])nc1N	0.98	0.00
252	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N)nc1N	0.85	0.00
253	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])nc1N	0.99	0.00
254	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])nc1N=[N+]=[N-]	1.00	0.00
255	O=[N+](=[O-])c1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1	1.19	0.22
256	Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1	1.15	0.25
257	[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1	1.14	0.22

258	Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]	1.15	0.18
259	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]	1.14	0.16
260	Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])n1	1.10	0.21
261	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])n1	1.10	0.18
262	[N-]=[N+]=Nc1nc(N)nc([N+](=O)[O-])c1[N+](=O)[O-]	1.10	0.18
263	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])n1	1.09	0.16
264	Nc1nc([N+](=O)[O-])nc(N)c1[N+](=O)[O-]	1.10	0.12
265	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N)c1[N+](=O)[O-]	1.09	0.10
266	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N=[N+]=[N-])c1[N+](=O)[O-]	1.09	0.09
267	Nc1nc(N)c([N+](=O)[O-])c(N)n1	1.05	0.14
268	[N-]=[N+]=Nc1nc(N)nc(N)c1[N+](=O)[O-]	1.04	0.11
269	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N)n1	1.05	0.12
270	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N=[N+]=[N-])n1	1.04	0.10
271	[N-]=[N+]=Nc1nc(N)nc(N=[N+]=[N-])c1[N+](=O)[O-]	1.04	0.10
272	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])n1	1.04	0.09
273	Nc1c([N+](=O)[O-])nc([N+](=O)[O-])nc1[N+](=O)[O-]	1.15	0.00
274	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])nc1[N+](=O)[O-]	1.14	0.28
275	Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])n1	1.10	0.00
276	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])n1	1.10	0.00
277	[N-]=[N+]=Nc1c([N+](=O)[O-])nc(N)nc1[N+](=O)[O-]	1.10	0.31
278	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c([N+](=O)[O-])n1	1.09	0.28
279	Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])c1N	1.10	0.00
280	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])c1N	1.09	0.00
281	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])nc1[N+](=O)[O-]	1.10	0.00
282	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])c1N=[N+]=[N-]	1.09	0.03
283	Nc1nc(N)c(N)c([N+](=O)[O-])n1	1.04	0.00
284	[N-]=[N+]=Nc1nc(N)c(N)c([N+](=O)[O-])n1	1.04	0.00
285	[N-]=[N+]=Nc1nc(N)nc([N+](=O)[O-])c1N	1.04	0.00
286	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N)c([N+](=O)[O-])n1	1.04	0.00
287	[N-]=[N+]=Nc1c(N)nc(N)nc1[N+](=O)[O-]	1.05	0.03
288	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c([N+](=O)[O-])n1	1.05	0.03
289	[N-]=[N+]=Nc1nc(N)nc([N+](=O)[O-])c1N=[N+]=[N-]	1.05	0.03
290	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c([N+](=O)[O-])n1	1.05	0.00
291	Nc1nc([N+](=O)[O-])nc(N)c1N	1.04	0.00
292	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N)c1N	1.04	0.00
293	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])nc1N	1.04	0.00
294	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N)c1N=[N+]=[N-]	1.04	0.00
295	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N=[N+]=[N-])c1N	1.04	0.00
296	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N=[N+]=[N-])c1N=[N+]=[N-]	1.04	0.00
297	Nc1nc(N)c(N)c(N)n1	0.97	0.00
298	[N-]=[N+]=Nc1nc(N)c(N)c(N)n1	0.98	0.00
299	[N-]=[N+]=Nc1nc(N)nc(N)c1N	0.98	0.00
300	[N-]=[N+]=Nc1nc(N)c(N)c(N=[N+]=[N-])n1	0.98	0.00

301	[N-]=[N+]=Nc1nc(N)nc(N=[N+]=[N-])c1N	0.99	0.00
302	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N)c(N=[N+]=[N-])n1	0.99	0.00
303	[N-]=[N+]=Nc1c(N)nc(N)nc1N	0.98	0.00
304	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c(N)n1	0.99	0.00
305	[N-]=[N+]=Nc1nc(N)nc(N)c1N=[N+]=[N-]	0.99	0.00
306	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c(N=[N+]=[N-])n1	1.00	0.00
307	[N-]=[N+]=Nc1nc(N)nc(N=[N+]=[N-])c1N=[N+]=[N-]	1.00	0.00
308	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c(N=[N+]=[N-])n1	1.00	0.00
309	O=[N+](=[O-])c1nnc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.19	0.32
310	Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.15	0.28
311	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.14	0.25
312	Nc1nnc(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.11	0.24
313	[N-]=[N+]=Nc1nnc(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.10	0.22
314	[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.09	0.19
315	Nc1c([N+](=O)[O-])nnc([N+](=O)[O-])c1[N+](=O)[O-]	1.15	0.19
316	[N-]=[N+]=Nc1c([N+](=O)[O-])nnc([N+](=O)[O-])c1[N+](=O)[O-]	1.14	0.32
317	Nc1nnc([N+](=O)[O-])c(N)c1[N+](=O)[O-]	1.11	0.14
318	[N-]=[N+]=Nc1c([N+](=O)[O-])nnc(N)c1[N+](=O)[O-]	1.10	0.34
319	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N)c1[N+](=O)[O-]	1.10	0.12
320	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N=[N+]=[N-])c1[N+](=O)[O-]	1.09	0.33
321	Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])c1N	1.10	0.21
322	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])c1N	1.10	0.18
323	[N-]=[N+]=Nc1c(N)nnc([N+](=O)[O-])c1[N+](=O)[O-]	1.10	0.19
324	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.09	0.17
325	Nc1nnc(N)c([N+](=O)[O-])c1N	1.05	0.14
326	[N-]=[N+]=Nc1nnc(N)c(N)c1[N+](=O)[O-]	1.05	0.12
327	[N-]=[N+]=Nc1nnc(N)c([N+](=O)[O-])c1N	1.05	0.12
328	[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c([N+](=O)[O-])c1N	1.05	0.10
329	[N-]=[N+]=Nc1c(N)nnc([N+](=O)[O-])c1[N+](=O)[O-]	1.05	0.13
330	[N-]=[N+]=Nc1nnc(N)c(N=[N+]=[N-])c1[N+](=O)[O-]	1.05	0.11
331	[N-]=[N+]=Nc1nnc(N)c([N+](=O)[O-])c1N=[N+]=[N-]	1.05	0.11
332	[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.05	0.10
333	Nc1c([N+](=O)[O-])nnc([N+](=O)[O-])c1N	1.11	0.00
334	[N-]=[N+]=Nc1c([N+](=O)[O-])nnc([N+](=O)[O-])c1N	1.10	0.06
335	[N-]=[N+]=Nc1c([N+](=O)[O-])nnc([N+](=O)[O-])c1N=[N+]=[N-]	1.10	0.30
336	Nc1nnc([N+](=O)[O-])c(N)c1N	1.05	0.00
337	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N)c1N	1.04	0.00
338	[N-]=[N+]=Nc1c(N)nnc([N+](=O)[O-])c1N	1.05	0.00
339	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N)c1N=[N+]=[N-]	1.05	0.00
340	[N-]=[N+]=Nc1c([N+](=O)[O-])nnc(N)c1N	1.05	0.00
341	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N=[N+]=[N-])c1N	1.05	0.00
342	[N-]=[N+]=Nc1c(N)nnc([N+](=O)[O-])c1N=[N+]=[N-]	1.05	0.03
343	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.05	0.04

344	<chem>Nc1nnc(N)c(N)c1N</chem>	0.97	0.00
345	<chem>[N-]=[N+]=Nc1nnc(N)c(N)c1N</chem>	0.98	0.00
346	<chem>[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c(N)c1N</chem>	0.99	0.00
347	<chem>[N-]=[N+]=Nc1c(N)nnc(N)c1N</chem>	0.98	0.00
348	<chem>[N-]=[N+]=Nc1nnc(N)c(N=[N+]=[N-])c1N</chem>	0.99	0.00
349	<chem>[N-]=[N+]=Nc1nnc(N)c(N)c1N=[N+]=[N-]</chem>	0.99	0.00
350	<chem>[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c(N=[N+]=[N-])c1N</chem>	1.00	0.00
351	<chem>[N-]=[N+]=Nc1c(N)nnc(N)c1N=[N+]=[N-]</chem>	0.99	0.46
352	<chem>[N-]=[N+]=Nc1nnc(N)c(N=[N+]=[N-])c1N=[N+]=[N-]</chem>	1.00	0.00
353	<chem>[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]</chem>	1.01	0.00
354	<chem>O=[N+](=[O-])c1nnc([N+](=O)[O-])c([N+](=O)[O-])n1</chem>	1.17	0.18
355	<chem>Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])n1</chem>	1.12	0.20
356	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])n1</chem>	1.11	0.18
357	<chem>Nc1nnc([N+](=O)[O-])nc1[N+](=O)[O-]</chem>	1.12	0.00
358	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])nc1[N+](=O)[O-]</chem>	1.10	0.00
359	<chem>Nc1nnc(N)c([N+](=O)[O-])n1</chem>	1.05	0.00
360	<chem>[N-]=[N+]=Nc1nnc(N)c([N+](=O)[O-])n1</chem>	1.05	0.00
361	<chem>[N-]=[N+]=Nc1nnc(N)nc1[N+](=O)[O-]</chem>	1.05	0.00
362	<chem>[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c([N+](=O)[O-])n1</chem>	1.05	0.00
363	<chem>Nc1nc([N+](=O)[O-])nnc1[N+](=O)[O-]</chem>	1.11	0.00
364	<chem>[N-]=[N+]=Nc1nc([N+](=O)[O-])nnc1[N+](=O)[O-]</chem>	1.10	0.00
365	<chem>Nc1nnc([N+](=O)[O-])c(N)n1</chem>	1.05	0.00
366	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N)n1</chem>	1.06	0.00
367	<chem>[N-]=[N+]=Nc1nc(N)nnc1[N+](=O)[O-]</chem>	1.05	0.00
368	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N=[N+]=[N-])n1</chem>	1.05	0.00
369	<chem>Nc1nnc([N+](=O)[O-])nc1N</chem>	1.05	0.00
370	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])nc1N</chem>	1.05	0.00
371	<chem>[N-]=[N+]=Nc1nc([N+](=O)[O-])nnc1N</chem>	1.05	0.00
372	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])nc1N=[N+]=[N-]</chem>	1.05	0.00
373	<chem>Nc1nnc(N)c(N)n1</chem>	0.97	0.00
374	<chem>[N-]=[N+]=Nc1nnc(N)c(N)n1</chem>	0.98	0.00
375	<chem>[N-]=[N+]=Nc1nnc(N)nc1N</chem>	0.98	0.00
376	<chem>[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c(N)n1</chem>	0.99	0.00
377	<chem>[N-]=[N+]=Nc1nc(N)nnc1N</chem>	0.98	0.00
378	<chem>[N-]=[N+]=Nc1nnc(N)c(N=[N+]=[N-])n1</chem>	0.99	0.00
379	<chem>[N-]=[N+]=Nc1nnc(N)nc1N=[N+]=[N-]</chem>	0.99	0.00
380	<chem>[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c(N=[N+]=[N-])n1</chem>	1.00	0.00
381	<chem>O=[N+](=[O-])c1nnnc([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.17	0.27
382	<chem>Nc1nnnc([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.12	0.22
383	<chem>[N-]=[N+]=Nc1nnnc([N+](=O)[O-])c1[N+](=O)[O-]</chem>	1.11	0.19
384	<chem>Nc1nnnc(N)c1[N+](=O)[O-]</chem>	1.06	0.15
385	<chem>[N-]=[N+]=Nc1nnnc(N)c1[N+](=O)[O-]</chem>	1.06	0.12
386	<chem>[N-]=[N+]=Nc1nnnc(N=[N+]=[N-])c1[N+](=O)[O-]</chem>	1.06	0.26

387	$\text{Nc1c}([\text{N}^+](=\text{O})[\text{O}^-])\text{nnnc1}[\text{N}^+](=\text{O})[\text{O}^-]$	1.12	0.00
388	$[\text{N}^-]=[\text{N}^+]=\text{Nc1c}([\text{N}^+](=\text{O})[\text{O}^-])\text{nnnc1}[\text{N}^+](=\text{O})[\text{O}^-]$	1.11	0.32
389	$\text{Nc1nnnc}([\text{N}^+](=\text{O})[\text{O}^-])\text{c1N}$	1.06	0.00
390	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}([\text{N}^+](=\text{O})[\text{O}^-])\text{c1N}$	1.06	0.00
391	$[\text{N}^-]=[\text{N}^+]=\text{Nc1c}(\text{N})\text{nnnc1}[\text{N}^+](=\text{O})[\text{O}^-]$	1.06	0.02
392	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}([\text{N}^+](=\text{O})[\text{O}^-])\text{c1N}=[\text{N}^+]=[\text{N}^-]$	1.06	0.00
393	$\text{Nc1nnnc}(\text{N})\text{c1N}$	0.98	0.00
394	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}(\text{N})\text{c1N}$	0.98	0.00
395	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}(\text{N}=[\text{N}^+]=[\text{N}^-])\text{c1N}$	0.99	0.00
396	$[\text{N}^-]=[\text{N}^+]=\text{Nc1c}(\text{N})\text{nnnc1N}$	0.99	0.00
397	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}(\text{N})\text{c1N}=[\text{N}^+]=[\text{N}^-]$	1.00	0.00
398	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}(\text{N}=[\text{N}^+]=[\text{N}^-])\text{c1N}=[\text{N}^+]=[\text{N}^-]$	1.00	0.00
399	$\text{O}=[\text{N}^+](\text{O}^-)\text{c1nnnnnc1}[\text{N}^+](=\text{O})[\text{O}^-]$	1.14	0.22
400	$\text{Nc1nnnnnc1}[\text{N}^+](=\text{O})[\text{O}^-]$	1.07	0.00
401	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnnnc1}[\text{N}^+](=\text{O})[\text{O}^-]$	1.07	0.00
402	Nc1nnnnnc1N	0.98	0.00
403	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnnnc1N}$	0.99	0.00
404	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnnnc1N}=[\text{N}^+]=[\text{N}^-]$	1.00	0.00
405	$\text{O}=[\text{N}^+](\text{O}^-)\text{c1nc}([\text{N}^+](=\text{O})[\text{O}^-])\text{nc}([\text{N}^+](=\text{O})[\text{O}^-])\text{n1}$	1.16	0.00
406	$\text{Nc1nc}([\text{N}^+](=\text{O})[\text{O}^-])\text{nc}([\text{N}^+](=\text{O})[\text{O}^-])\text{n1}$	1.11	0.00
407	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nc}([\text{N}^+](=\text{O})[\text{O}^-])\text{nc}([\text{N}^+](=\text{O})[\text{O}^-])\text{n1}$	1.10	0.00
408	$\text{Nc1nc}(\text{N})\text{nc}([\text{N}^+](=\text{O})[\text{O}^-])\text{n1}$	1.05	0.00
409	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nc}(\text{N})\text{nc}([\text{N}^+](=\text{O})[\text{O}^-])\text{n1}$	1.05	0.00
410	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nc}(\text{N}=[\text{N}^+]=[\text{N}^-])\text{nc}([\text{N}^+](=\text{O})[\text{O}^-])\text{n1}$	1.05	0.00
411	$\text{Nc1nc}(\text{N})\text{nc}(\text{N})\text{n1}$	0.97	0.00
412	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nc}(\text{N})\text{nc}(\text{N})\text{n1}$	0.98	0.00
413	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nc}(\text{N})\text{nc}(\text{N}=[\text{N}^+]=[\text{N}^-])\text{n1}$	0.99	0.00
414	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nc}(\text{N}=[\text{N}^+]=[\text{N}^-])\text{nc}(\text{N}=[\text{N}^+]=[\text{N}^-])\text{n1}$	1.00	0.00
415	$\text{O}=[\text{N}^+](\text{O}^-)\text{c1nnnc}([\text{N}^+](=\text{O})[\text{O}^-])\text{nn1}$	1.13	0.00
416	$\text{Nc1nnnc}([\text{N}^+](=\text{O})[\text{O}^-])\text{nn1}$	1.07	0.00
417	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}([\text{N}^+](=\text{O})[\text{O}^-])\text{nn1}$	1.06	0.00
418	$\text{Nc1nnnc}(\text{N})\text{nn1}$	0.98	0.00
419	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}(\text{N})\text{nn1}$	0.99	0.00
420	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}(\text{N}=[\text{N}^+]=[\text{N}^-])\text{nn1}$	1.00	0.00
421	$\text{O}=[\text{N}^+](\text{O}^-)\text{c1nnnnnc}([\text{N}^+](=\text{O})[\text{O}^-])\text{n1}$	1.13	0.00
422	$\text{Nc1nnnc}([\text{N}^+](=\text{O})[\text{O}^-])\text{n1}$	1.07	0.00
423	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}([\text{N}^+](=\text{O})[\text{O}^-])\text{n1}$	1.06	0.00
424	$\text{Nc1nnnc}(\text{N})\text{n1}$	0.98	0.00
425	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}(\text{N})\text{n1}$	0.99	0.00
426	$[\text{N}^-]=[\text{N}^+]=\text{Nc1nnnc}(\text{N}=[\text{N}^+]=[\text{N}^-])\text{n1}$	1.00	0.00

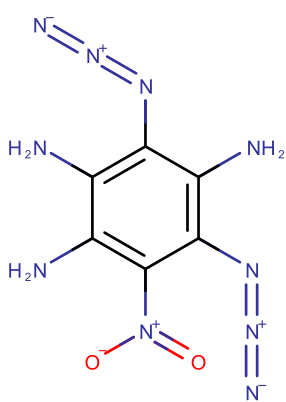
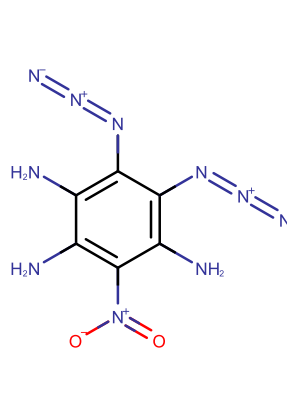
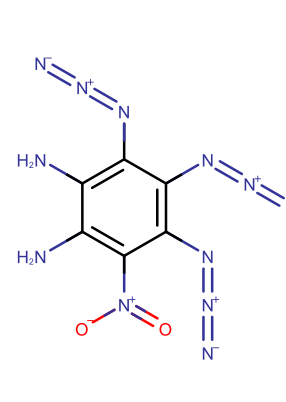
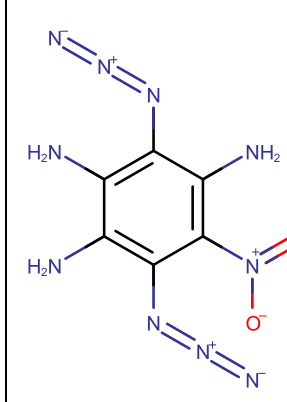
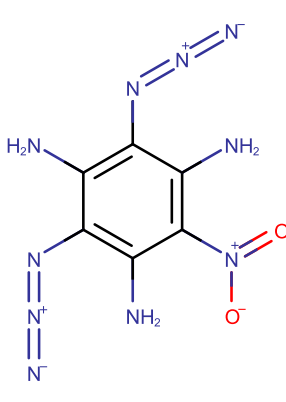
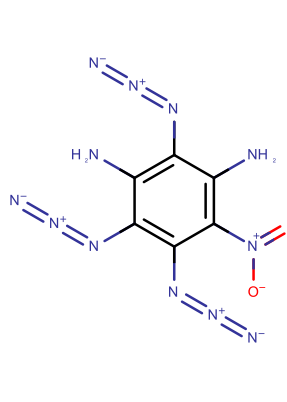
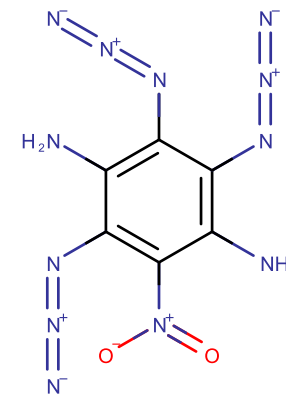
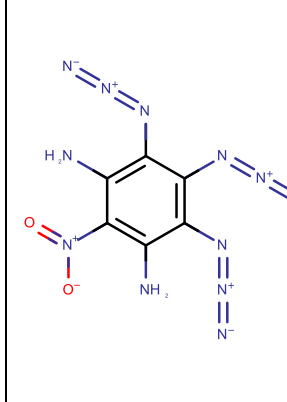
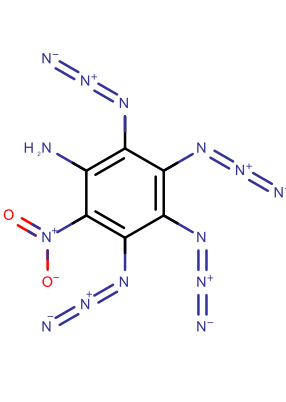
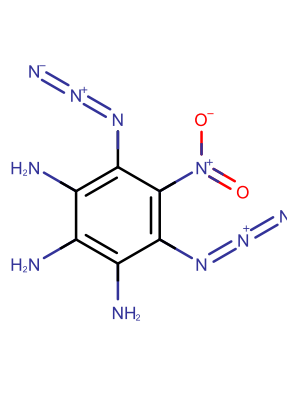
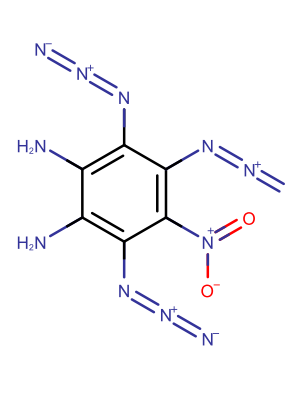
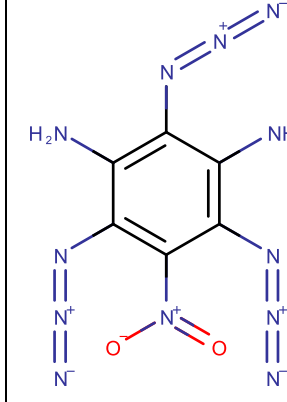
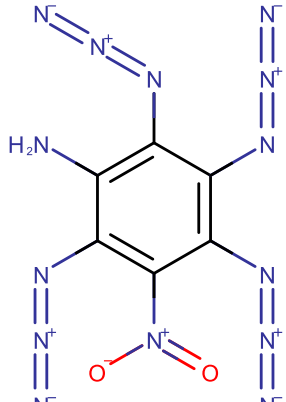
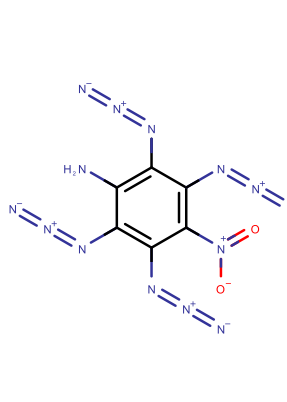
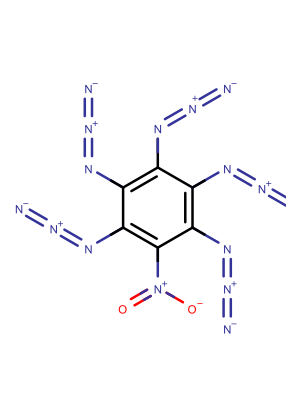
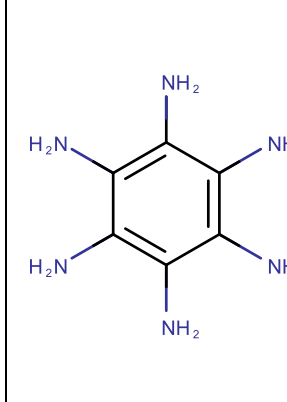
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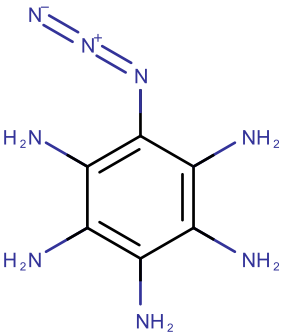
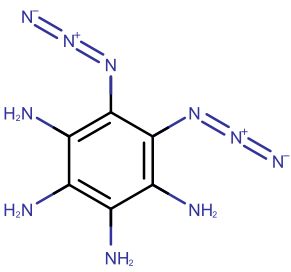
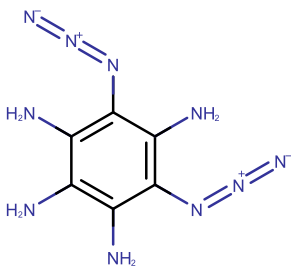
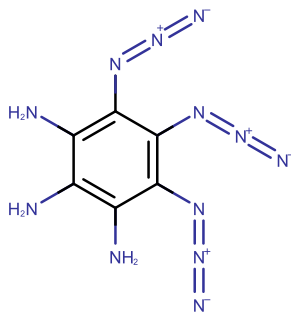
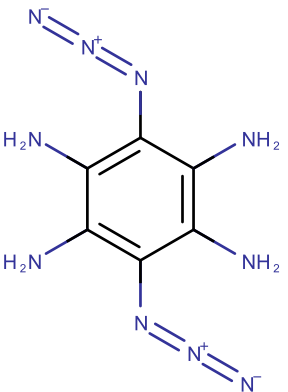
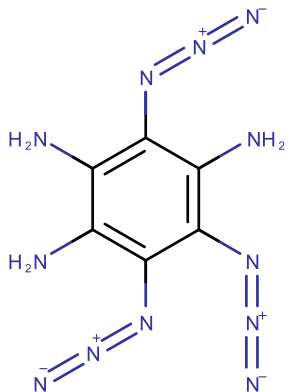
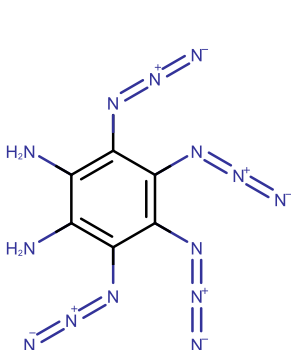
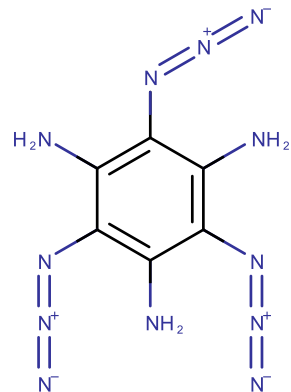
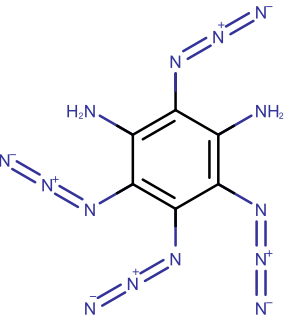
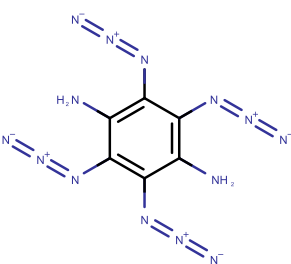
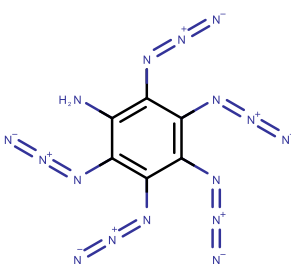
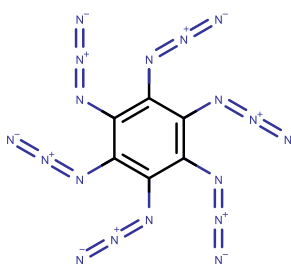
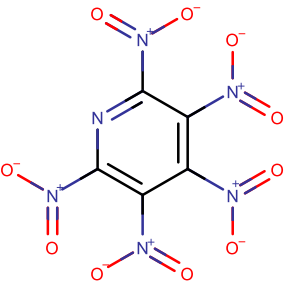
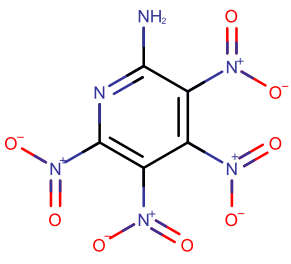
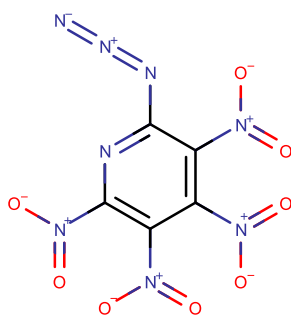
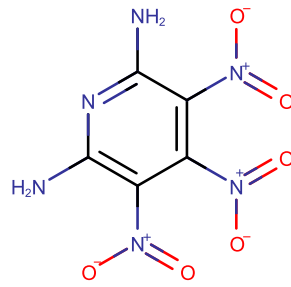
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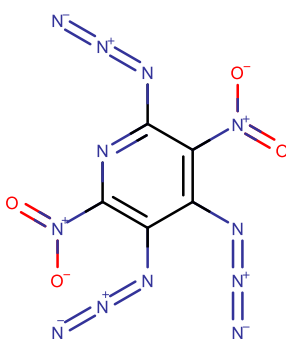
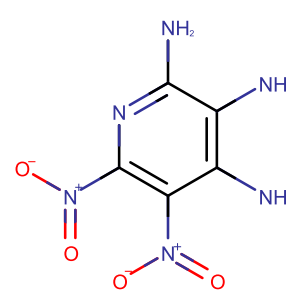
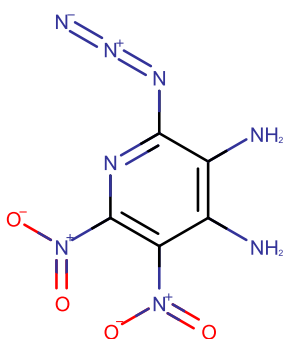
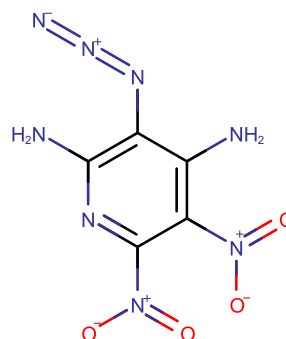
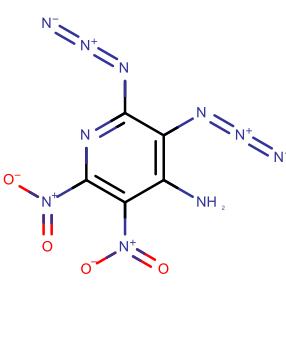
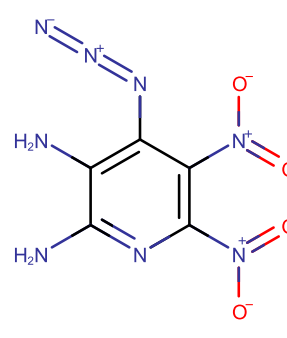
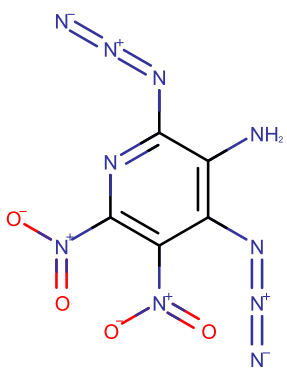
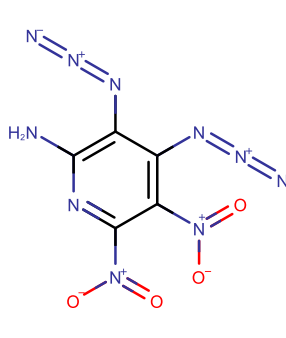
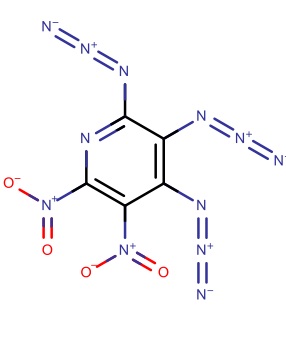
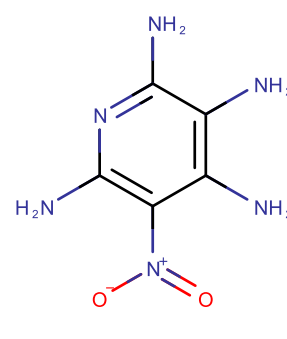
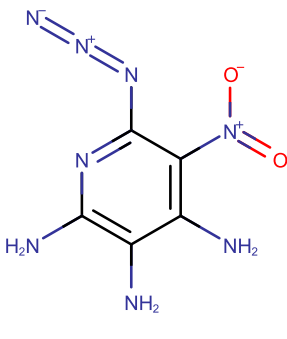
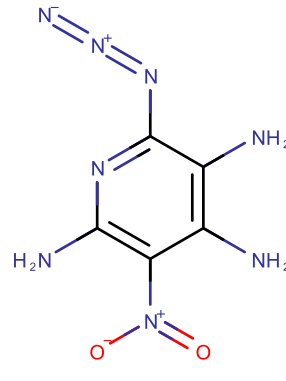
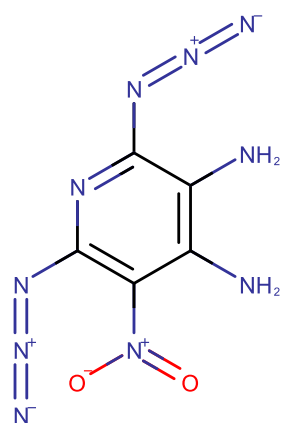
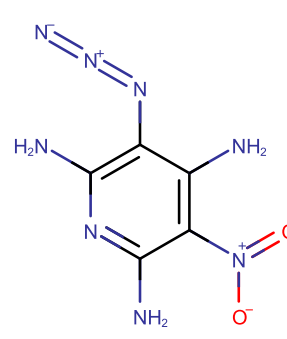
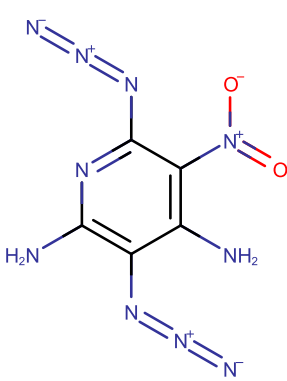
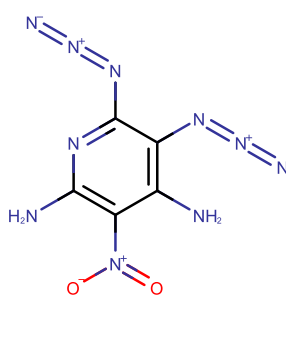
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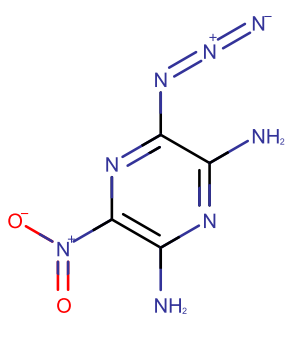
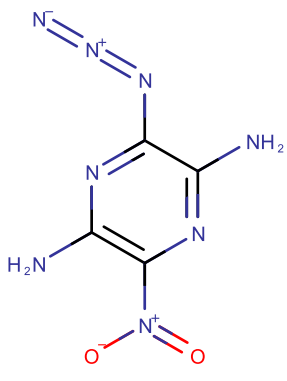
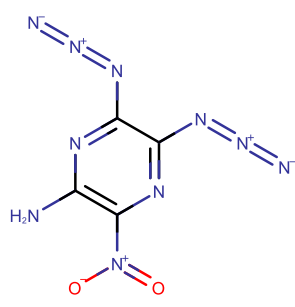
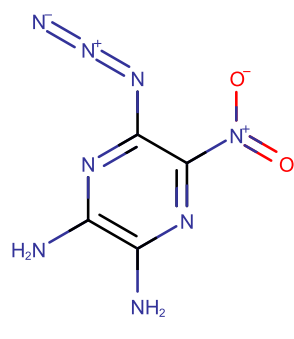
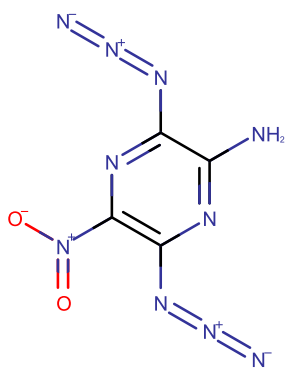
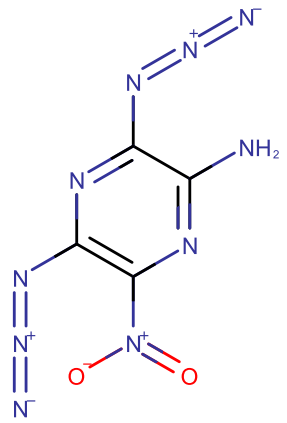
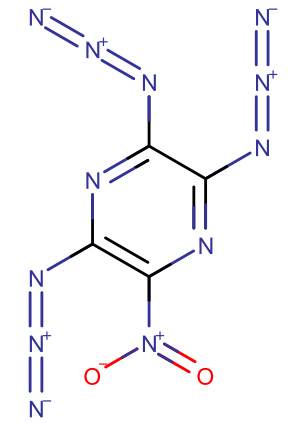
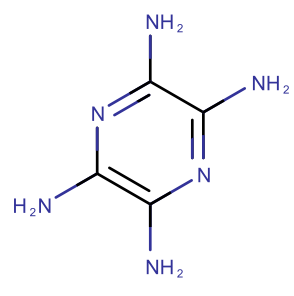
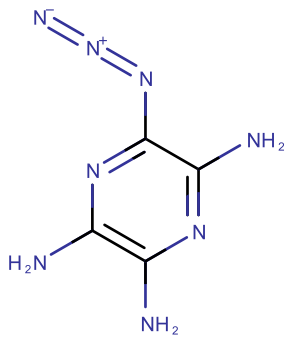
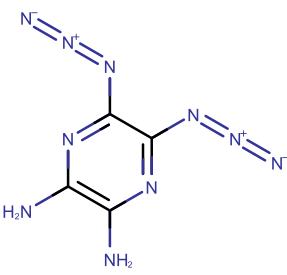
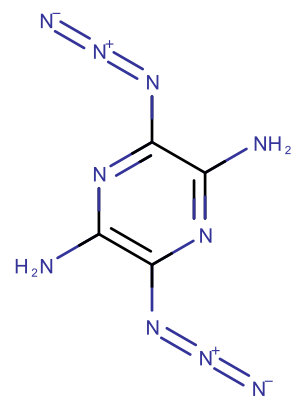
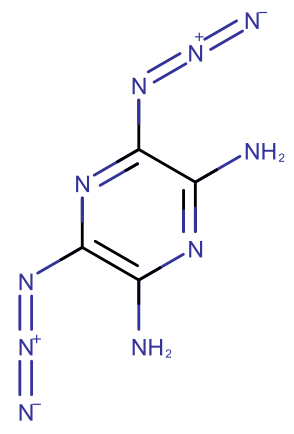
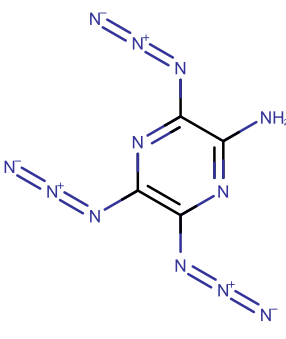
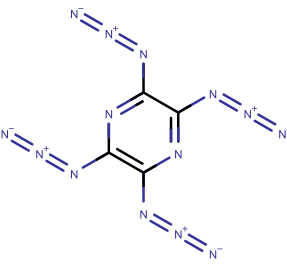
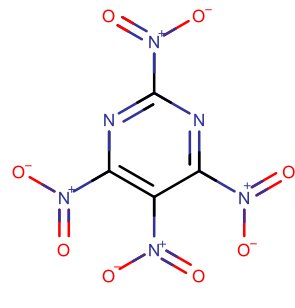
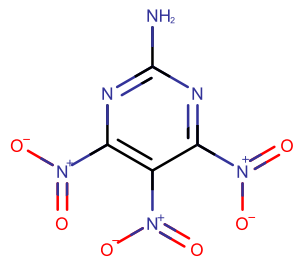
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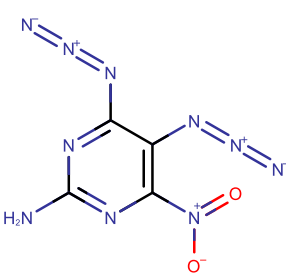
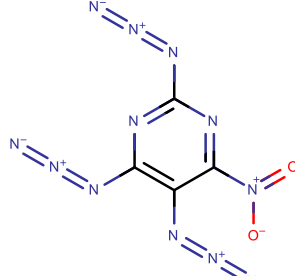
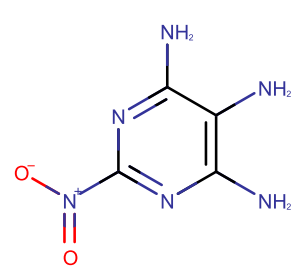
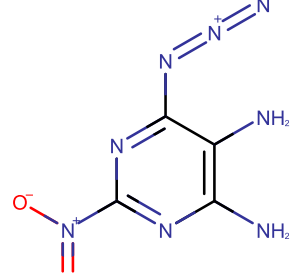
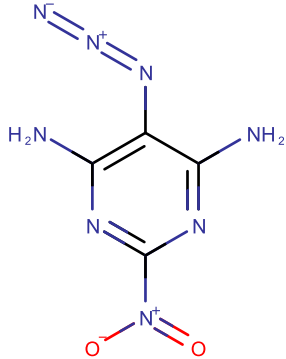
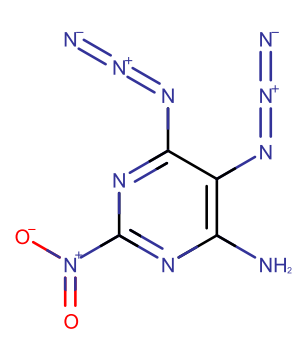
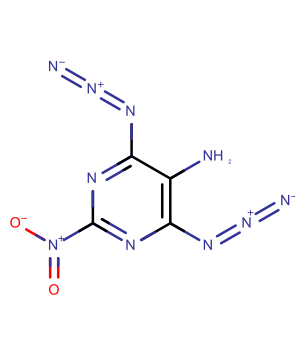
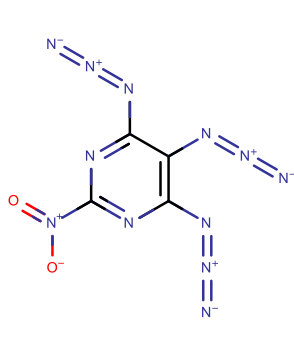
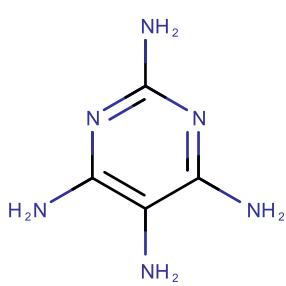
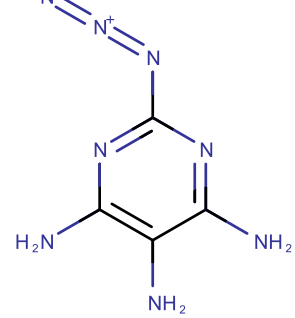
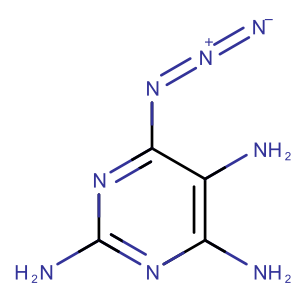
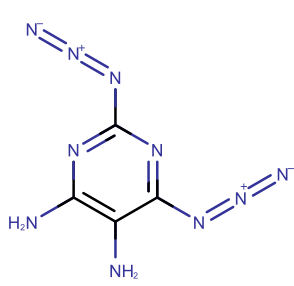
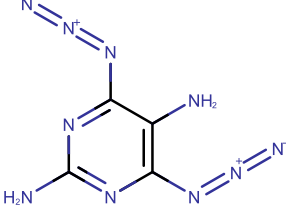
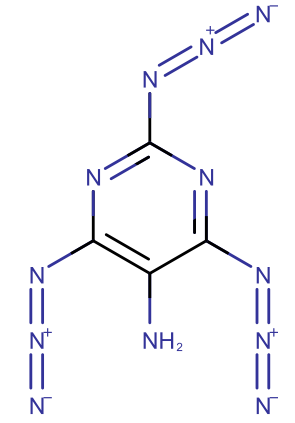
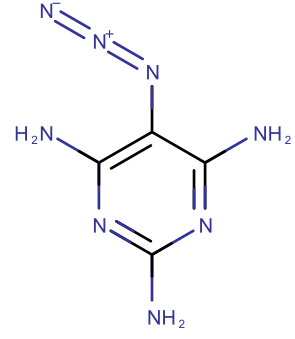
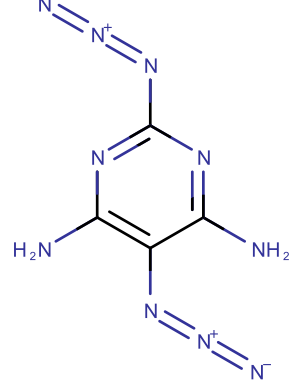
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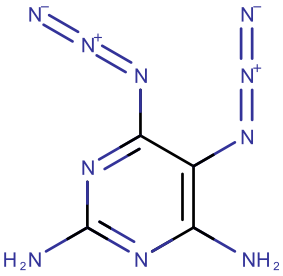
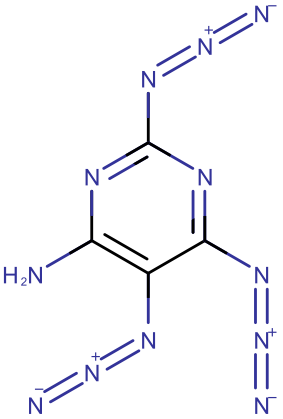
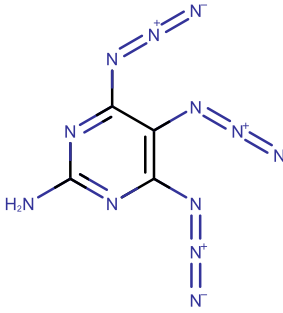
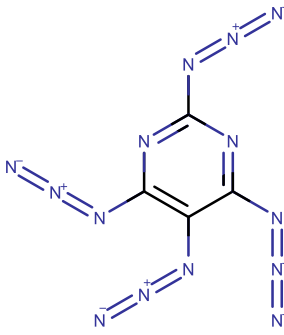
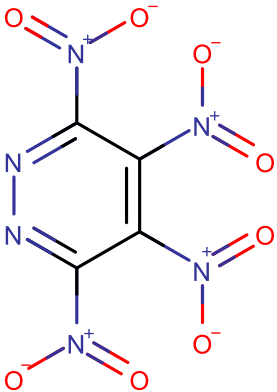
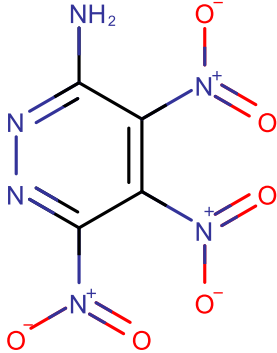
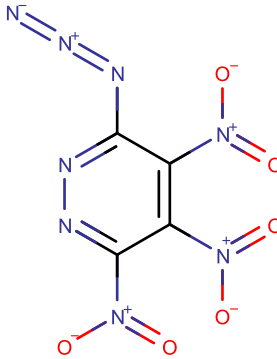
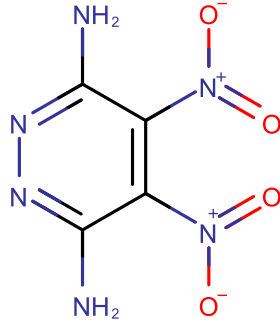
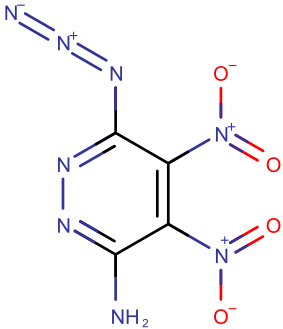
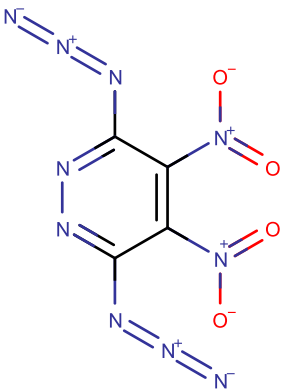
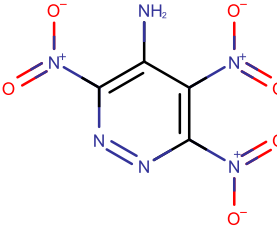
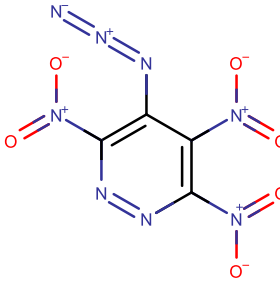
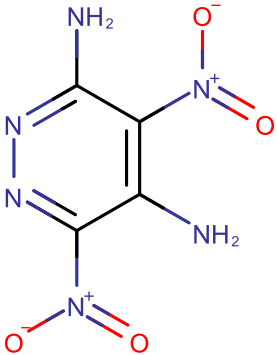
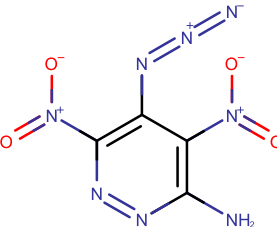
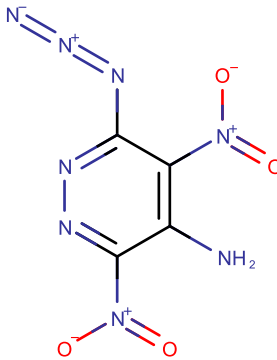
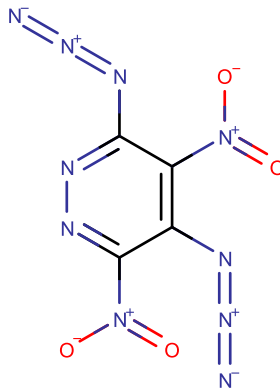
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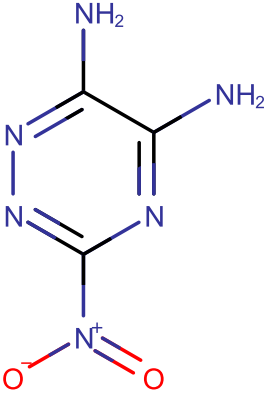
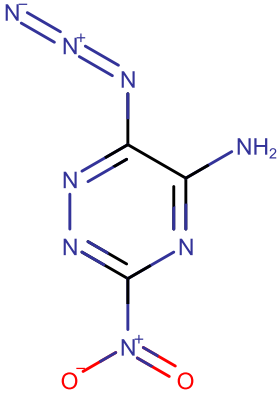
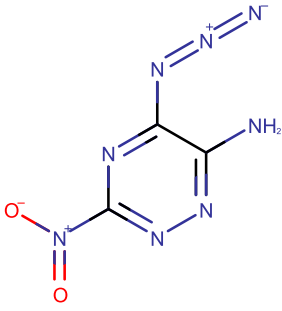
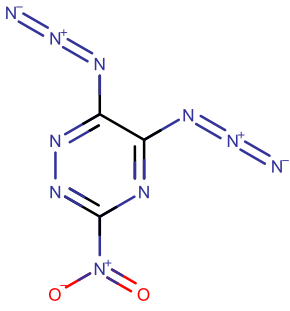
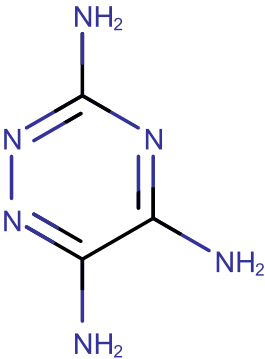
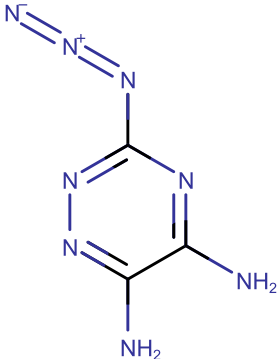
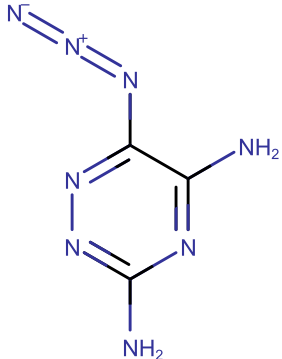
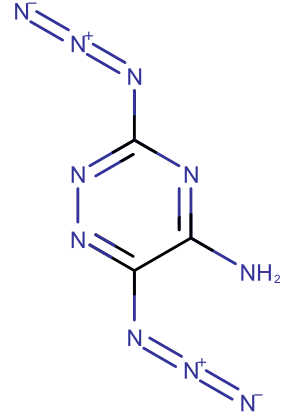
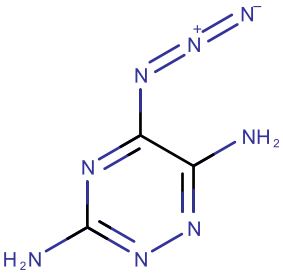
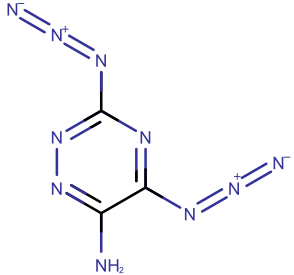
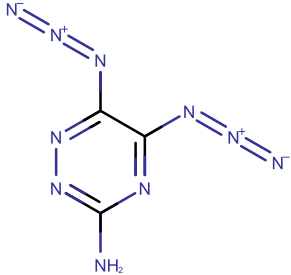
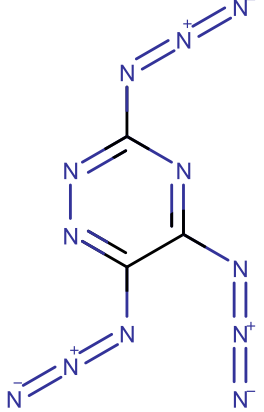
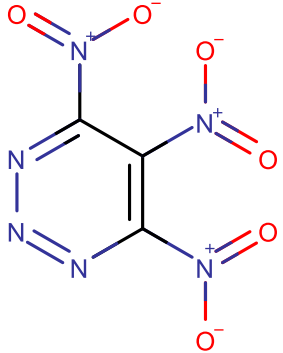
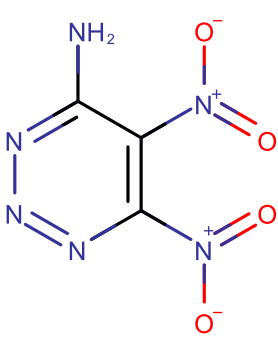
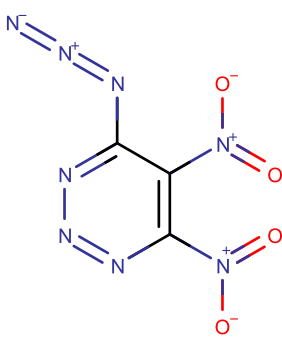
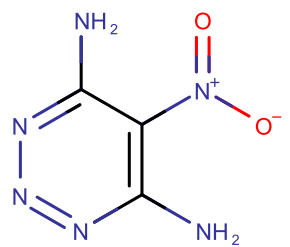
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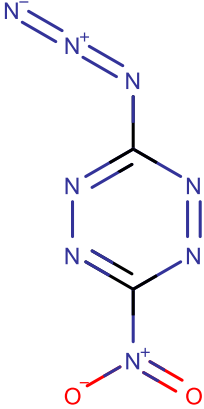
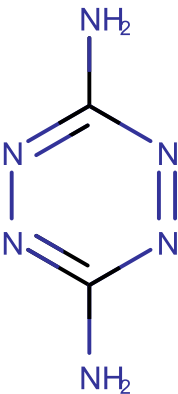
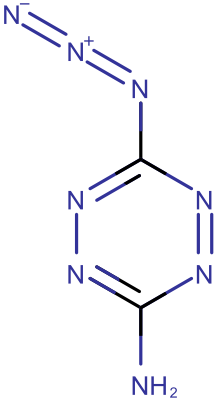
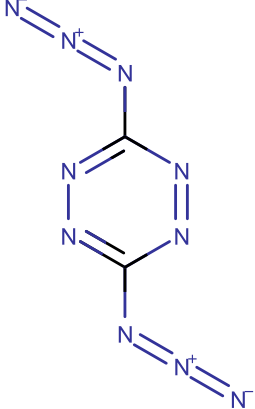
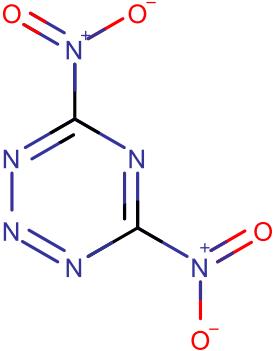
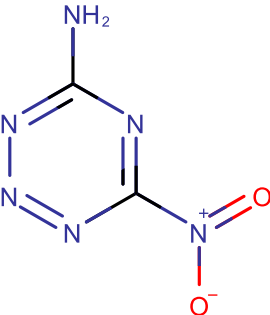
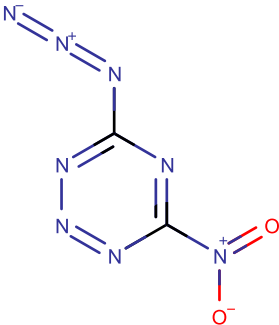
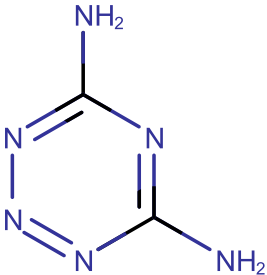
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