

Supplementary molecular list-2

273 molecules after first screening in SMILES and their calculated molecular density and PBF

No.	SMILES	Molecular Density	PBF
1	<chem>[N-]=[N+]=Nc1nc(N)nc([N+](=O)[O-])n1</chem>	1.05	0.00
2	<chem>[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N=[N+]=[N-])c1N</chem>	1.04	0.00
3	<chem>[N-]=[N+]=Nc1nnnc([N+](=O)[O-])n1</chem>	1.06	0.00
4	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])nn1</chem>	1.06	0.00
5	<chem>[N-]=[N+]=Nc1nnnc(N=[N+]=[N-])c1N=[N+]=[N-]</chem>	1.00	0.00
6	<chem>[N-]=[N+]=Nc1nnnnc1N=[N+]=[N-]</chem>	1.00	0.00
7	<chem>Nc1nnc([N+](=O)[O-])nc1[N+](=O)[O-]</chem>	1.12	0.00
8	<chem>[N-]=[N+]=Nc1nnnc([N+](=O)[O-])c1N</chem>	1.06	0.00
9	<chem>Nc1nnnc([N+](=O)[O-])n1</chem>	1.07	0.00
10	<chem>Nc1nnc([N+](=O)[O-])nn1</chem>	1.07	0.00
11	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N=[N+]=[N-])n1</chem>	1.05	0.00
12	<chem>[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])nc1N</chem>	1.04	0.00
13	<chem>[N-]=[N+]=Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])n1</chem>	1.10	0.00
14	<chem>O=[N+](O-)[c1nnc([N+](=O)[O-])nn1</chem>	1.13	0.00
15	<chem>[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])n1</chem>	1.10	0.00
16	<chem>[N-]=[N+]=Nc1nc(N)nc([N+](=O)[O-])c1N</chem>	1.04	0.00
17	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])nc1[N+](=O)[O-]</chem>	1.10	0.00
18	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N)c1N=[N+]=[N-]</chem>	1.05	0.00
19	<chem>[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N)c1N</chem>	1.04	0.00
20	<chem>Nc1nnc(N)c([N+](=O)[O-])n1</chem>	1.05	0.00
21	<chem>[N-]=[N+]=Nc1nc(N)c(N)nc1[N+](=O)[O-]</chem>	1.04	0.00
22	<chem>Nc1nc([N+](=O)[O-])nc(N)c1N</chem>	1.04	0.00
23	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])nc1N=[N+]=[N-]</chem>	1.05	0.00
24	<chem>[N-]=[N+]=Nc1nnnnc1[N+](=O)[O-]</chem>	1.07	0.00
25	<chem>[N-]=[N+]=Nc1nnc(N)c([N+](=O)[O-])n1</chem>	1.05	0.00
26	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N)c1N</chem>	1.04	0.00
27	<chem>[N-]=[N+]=Nc1nc(N=[N+]=[N-])nc([N+](=O)[O-])n1</chem>	1.05	0.00
28	<chem>[N-]=[N+]=Nc1nc([N+](=O)[O-])nnnc1N</chem>	1.05	0.00
29	<chem>[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])nc1N=[N+]=[N-]</chem>	1.04	0.00
30	<chem>Nc1nnc([N+](=O)[O-])c(N)n1</chem>	1.05	0.00
31	<chem>[N-]=[N+]=Nc1nc(N)nnc1[N+](=O)[O-]</chem>	1.05	0.00
32	<chem>Nc1nc([N+](=O)[O-])nnc1[N+](=O)[O-]</chem>	1.11	0.00
33	<chem>Nc1nnnnc1[N+](=O)[O-]</chem>	1.07	0.00
34	<chem>[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])nc1N=[N+]=[N-]</chem>	1.04	0.00
35	<chem>[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N=[N+]=[N-])c1N</chem>	1.05	0.00

36	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])nc1N	1.04	0.00
37	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)nc1[N+](=O)[O-]	1.10	0.00
38	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)nc1N	1.04	0.00
39	Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])n1	1.11	0.00
40	Nc1nc(N)nc([N+](=O)[O-])n1	1.05	0.00
41	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N=[N+]=[N-])c1N=[N+]=[N-]	1.04	0.00
42	[N-]=[N+]=Nc1c([N+](=O)[O-])nnc(N)c1N	1.05	0.00
43	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])nc1[N+](=O)[O-]	1.09	0.00
44	[N-]=[N+]=Nc1nnc(N)nc1[N+](=O)[O-]	1.05	0.00
45	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])nc1N	1.04	0.00
46	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])nc1[N+](=O)[O-]	1.09	0.00
47	[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c([N+](=O)[O-])n1	1.05	0.00
48	[N-]=[N+]=Nc1nc(N)c(N)c([N+](=O)[O-])n1	1.04	0.00
49	Nc1nc(N)c([N+](=O)[O-])nc1[N+](=O)[O-]	1.10	0.00
50	Nc1nc(N)c(N)c([N+](=O)[O-])n1	1.04	0.00
51	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])nc1[N+](=O)[O-]	1.09	0.00
52	O=[N+](O)c1nc([N+](=O)[O-])nc([N+](=O)[O-])n1	1.16	0.00
53	Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N)c1N	1.09	0.00
54	Nc1c([N+](=O)[O-])nnc([N+](=O)[O-])c1N	1.11	0.00
55	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c(N)c1N	1.04	0.00
56	Nc1nnnc([N+](=O)[O-])c1N	1.06	0.00
57	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N=[N+]=[N-])c1N	1.04	0.00
58	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N)n1	1.06	0.00
59	[N-]=[N+]=Nc1c(N)c(N)nc([N+](=O)[O-])c1N	1.04	0.00
60	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])nc1N	1.04	0.00
61	Nc1c([N+](=O)[O-])nc([N+](=O)[O-])nc1[N+](=O)[O-]	1.15	0.00
62	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N)c1N=[N+]=[N-]	1.04	0.00
63	[N-]=[N+]=Nc1nc([N+](=O)[O-])nnc1[N+](=O)[O-]	1.10	0.00
64	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.01	0.00
65	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N)c([N+](=O)[O-])n1	1.04	0.00
66	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N)c1N=[N+]=[N-]	1.04	0.00
67	Nc1nc([N+](=O)[O-])c(N)c(N)c1N	1.03	0.00
68	Nc1nnc([N+](=O)[O-])nc1N	1.05	0.00
69	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])nc1[N+](=O)[O-]	1.10	0.00
70	Nc1nc(N)c([N+](=O)[O-])nc1N	1.04	0.00
71	[N-]=[N+]=Nc1nnc(N)c(N=[N+]=[N-])c1N=[N+]=[N-]	1.00	0.00
72	[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])nc([N+](=O)[O-])c1N	1.09	0.00
73	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1N	1.00	0.00
74	[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.01	0.00
75	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N)c1N	1.03	0.00
76	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])c1N	1.09	0.00
77	O=[N+](O)c1nnnc([N+](=O)[O-])n1	1.13	0.00
78	[N-]=[N+]=Nc1c(N)nnc([N+](=O)[O-])c1N	1.05	0.00

79	[N-]=[N+]=Nc1nnnc([N+](=O)[O-])c1N=[N+]=[N-]	1.06	0.00
80	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c([N+](=O)[O-])n1	1.05	0.00
81	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N=[N+]=[N-])c1N=[N+]=[N-]	1.04	0.00
82	Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])c1N	1.10	0.00
83	Nc1nc([N+](=O)[O-])c(N)nc1[N+](=O)[O-]	1.10	0.00
84	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c(N)c1N	1.04	0.00
85	Nc1nnc([N+](=O)[O-])c(N)c1N	1.05	0.00
86	Nc1c([N+](=O)[O-])nnnc1[N+](=O)[O-]	1.12	0.00
87	[N-]=[N+]=Nc1nnc([N+](=O)[O-])nc1N	1.05	0.00
88	Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])n1	1.10	0.00
89	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N)c1N	1.09	0.00
90	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c(N)c1N=[N+]=[N-]	1.05	0.01
91	[N-]=[N+]=Nc1c(N)nnnc1[N+](=O)[O-]	1.06	0.02
92	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c([N+](=O)[O-])n1	1.05	0.03
93	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])c1N=[N+]=[N-]	1.09	0.03
94	[N-]=[N+]=Nc1c(N)nc(N)nc1[N+](=O)[O-]	1.05	0.03
95	[N-]=[N+]=Nc1nc(N)nc([N+](=O)[O-])c1N=[N+]=[N-]	1.05	0.03
96	[N-]=[N+]=Nc1c(N)nnc([N+](=O)[O-])c1N=[N+]=[N-]	1.05	0.03
97	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.05	0.04
98	[N-]=[N+]=Nc1c([N+](=O)[O-])nc(N)c(N)c1N	1.04	0.05
99	[N-]=[N+]=Nc1c(N)nc(N)c(N=[N+]=[N-])c1N=[N+]=[N-]	1.00	0.05
100	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c(N=[N+]=[N-])c1N	1.05	0.05
101	[N-]=[N+]=Nc1c([N+](=O)[O-])nnnc([N+](=O)[O-])c1N	1.10	0.06
102	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.01	0.06
103	[N-]=[N+]=Nc1c([N+](=O)[O-])nc(N)c(N)c1N=[N+]=[N-]	1.05	0.07
104	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N=[N+]=[N-])c1N	1.09	0.08
105	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N=[N+]=[N-])c1[N+](=O)[O-]	1.09	0.09
106	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])n1	1.04	0.09
107	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N)c1N=[N+]=[N-]	1.04	0.09
108	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.04	0.09
109	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N	1.04	0.09
110	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.05	0.09
111	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N)c1N=[N+]=[N-]	1.09	0.10
112	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c(N)c1[N+](=O)[O-]	1.04	0.10
113	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N	1.04	0.10
114	[N-]=[N+]=Nc1nc(N)nc(N=[N+]=[N-])c1[N+](=O)[O-]	1.04	0.10
115	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N)c1N	1.04	0.10
116	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N=[N+]=[N-])n1	1.04	0.10
117	[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.05	0.10
118	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.05	0.10
119	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c1[N+](=O)[O-]	1.05	0.10
120	[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c([N+](=O)[O-])c1N	1.05	0.10
121	[N-]=[N+]=Nc1nc([N+](=O)[O-])nc(N)c1[N+](=O)[O-]	1.09	0.10

122	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N)c1[N+](=O)[O-]	1.09	0.10
123	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.05	0.10
124	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c(N)c([N+](=O)[O-])c1N	1.04	0.10
125	[N-]=[N+]=Nc1c(N)c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c1N	1.04	0.10
126	[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c(N)c([N+](=O)[O-])c1N	1.04	0.10
127	[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c1N	1.04	0.11
128	[N-]=[N+]=Nc1nc(N)c(N=[N+]=[N-])c([N+](=O)[O-])c1N	1.04	0.11
129	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N)c1N=[N+]=[N-]	1.04	0.11
130	[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c(N)c1N=[N+]=[N-]	1.04	0.11
131	[N-]=[N+]=Nc1nc(N)c(N)c(N=[N+]=[N-])c1[N+](=O)[O-]	1.04	0.11
132	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N=[N+]=[N-])c1N	1.04	0.11
133	[N-]=[N+]=Nc1nnc(N)c(N=[N+]=[N-])c1[N+](=O)[O-]	1.05	0.11
134	[N-]=[N+]=Nc1nc(N)c(N)c([N+](=O)[O-])c1N=[N+]=[N-]	1.04	0.11
135	[N-]=[N+]=Nc1c(N)c(N)c(N)c(N=[N+]=[N-])c1[N+](=O)[O-]	1.04	0.11
136	[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N	1.04	0.11
137	[N-]=[N+]=Nc1nc(N)c(N)c(N)c1[N+](=O)[O-]	1.04	0.11
138	[N-]=[N+]=Nc1c(N)nc(N)c([N+](=O)[O-])c1N=[N+]=[N-]	1.05	0.11
139	[N-]=[N+]=Nc1c(N)nc(N)c(N=[N+]=[N-])c1[N+](=O)[O-]	1.05	0.11
140	[N-]=[N+]=Nc1nc(N)nc(N)c1[N+](=O)[O-]	1.04	0.11
141	[N-]=[N+]=Nc1nnc(N)c([N+](=O)[O-])c1N=[N+]=[N-]	1.05	0.11
142	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N)c1N	1.04	0.12
143	[N-]=[N+]=Nc1nnc(N)c(N)c1[N+](=O)[O-]	1.05	0.12
144	[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c(N)c1N	1.04	0.12
145	[N-]=[N+]=Nc1c(N)c(N)c(N)c1[N+](=O)[O-]	1.04	0.12
146	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c(N=[N+]=[N-])c1[N+](=O)[O-]	1.09	0.12
147	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N=[N+]=[N-]	1.09	0.12
148	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c(N)n1	1.05	0.12
149	Nc1nc([N+](=O)[O-])c(N)c(N)c1[N+](=O)[O-]	1.09	0.12
150	Nc1nc([N+](=O)[O-])nc(N)c1[N+](=O)[O-]	1.10	0.12
151	[N-]=[N+]=Nc1nc(N)c(N)c([N+](=O)[O-])c1N	1.03	0.12
152	[N-]=[N+]=Nc1c(N)c(N)c(N)c([N+](=O)[O-])c1N=[N+]=[N-]	1.04	0.12
153	[N-]=[N+]=Nc1c(N)c(N)c(N)c([N+](=O)[O-])c1N	1.04	0.12
154	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c(N)c1[N+](=O)[O-]	1.09	0.12
155	[N-]=[N+]=Nc1c(N)nc(N)c([N+](=O)[O-])c1N	1.04	0.12
156	[N-]=[N+]=Nc1c(N)c(N)nc(N)c1[N+](=O)[O-]	1.04	0.12
157	[N-]=[N+]=Nc1nnnc(N)c1[N+](=O)[O-]	1.06	0.12
158	[N-]=[N+]=Nc1c(N)nc(N)c(N)c1[N+](=O)[O-]	1.04	0.12
159	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c(N)c1[N+](=O)[O-]	1.10	0.12
160	[N-]=[N+]=Nc1nnc(N)c([N+](=O)[O-])c1N	1.05	0.12
161	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N	1.09	0.12
162	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.05	0.13
163	[N-]=[N+]=Nc1c(N)nnc(N)c1[N+](=O)[O-]	1.05	0.13
164	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N=[N+]=[N-])c(N)c1[N+](=O)[O-]	1.09	0.13

165	$\text{Nc1c(N)c(N)c([N+](=O)[O-])c(N)c1N}$	1.03	0.13
166	$[\text{N-}]=[\text{N+}]=\text{Nc1c(N)c([N+](=O)[O-])nc(N)c1[N+](=O)[O-]}$	1.09	0.13
167	$\text{Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c(N)c1[N+](=O)[O-]}$	1.14	0.13
168	$[\text{N-}]=[\text{N+}]=\text{Nc1c([N+](=O)[O-])nc(N)c([N+](=O)[O-])c1N}$	1.09	0.14
169	$\text{Nc1nc(N)c([N+](=O)[O-])c(N)n1}$	1.05	0.14
170	$\text{Nc1nc(N)c(N)c([N+](=O)[O-])c1N}$	1.04	0.14
171	$\text{Nc1nc(N)c([N+](=O)[O-])c(N)c1N}$	1.04	0.14
172	$\text{Nc1nnc([N+](=O)[O-])c(N)c1[N+](=O)[O-]}$	1.11	0.14
173	$\text{Nc1nnc(N)c([N+](=O)[O-])c1N}$	1.05	0.14
174	$\text{Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N}$	1.10	0.14
175	$\text{Nc1nnnc(N)c1[N+](=O)[O-]}$	1.06	0.15
176	$[\text{N-}]=[\text{N+}]=\text{Nc1c(N)nc([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]}$	1.05	0.15
177	$[\text{N-}]=[\text{N+}]=\text{Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c(N)c1[N+](=O)[O-]}$	1.08	0.15
178	$[\text{N-}]=[\text{N+}]=\text{Nc1nc([N+](=O)[O-])c([N+](=O)[O-])nc1[N+](=O)[O-]}$	1.14	0.16
179	$[\text{N-}]=[\text{N+}]=\text{Nc1nc([N+](=O)[O-])c([N+](=O)[O-])nc1N=[N+]=[N-]}$	1.09	0.16
180	$[\text{N-}]=[\text{N+}]=\text{Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N)c1N=[N+]=[N-]}$	1.08	0.16
181	$[\text{N-}]=[\text{N+}]=\text{Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]}$	1.14	0.16
182	$[\text{N-}]=[\text{N+}]=\text{Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N}$	1.08	0.16
183	$[\text{N-}]=[\text{N+}]=\text{Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])n1}$	1.09	0.16
184	$[\text{N-}]=[\text{N+}]=\text{Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]}$	1.09	0.17
185	$[\text{N-}]=[\text{N+}]=\text{Nc1c(N)c(N=[N+]=[N-])c(N=[N+]=[N-])c([N+](=O)[O-])c1N}$	1.04	0.17
186	$[\text{N-}]=[\text{N+}]=\text{Nc1nc([N+](=O)[O-])c([N+](=O)[O-])nc1N}$	1.09	0.17
187	$[\text{N-}]=[\text{N+}]=\text{Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]}$	1.09	0.17
188	$[\text{N-}]=[\text{N+}]=\text{Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]}$	1.08	0.17
189	$\text{Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c([N+](=O)[O-])c1N}$	1.14	0.17
190	$[\text{N-}]=[\text{N+}]=\text{Nc1c(N)nc([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]}$	1.09	0.17
191	$\text{Nc1nc([N+](=O)[O-])c([N+](=O)[O-])nc1[N+](=O)[O-]}$	1.15	0.17
192	$[\text{N-}]=[\text{N+}]=\text{Nc1c(N)c([N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]}$	1.13	0.18
193	$\text{O}=[\text{N+}]([\text{O-}])\text{c1nnc([N+](=O)[O-])c([N+](=O)[O-])n1}$	1.17	0.18
194	$[\text{N-}]=[\text{N+}]=\text{Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N)c1N}$	1.08	0.18
195	$[\text{N-}]=[\text{N+}]=\text{Nc1c(N)nc([N+](=O)[O-])c([N+](=O)[O-])c1N}$	1.09	0.18
196	$[\text{N-}]=[\text{N+}]=\text{Nc1c(N)c(N)nc([N+](=O)[O-])c1[N+](=O)[O-]}$	1.09	0.18
197	$[\text{N-}]=[\text{N+}]=\text{Nc1nc(N)nc([N+](=O)[O-])c1[N+](=O)[O-]}$	1.10	0.18
198	$\text{Nc1nc([N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]}$	1.15	0.18
199	$[\text{N-}]=[\text{N+}]=\text{Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])n1}$	1.10	0.18
200	$[\text{N-}]=[\text{N+}]=\text{Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])n1}$	1.11	0.18
201	$[\text{N-}]=[\text{N+}]=\text{Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])c1N}$	1.10	0.18
202	$[\text{N-}]=[\text{N+}]=\text{Nc1c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c(N)c1[N+](=O)[O-]}$	1.08	0.18
203	$[\text{N-}]=[\text{N+}]=\text{Nc1c(N)c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c1[N+](=O)[O-]}$	1.08	0.19
204	$[\text{N-}]=[\text{N+}]=\text{Nc1nc(N)c(N=[N+]=[N-])c([N+](=O)[O-])c1[N+](=O)[O-]}$	1.09	0.19
205	$[\text{N-}]=[\text{N+}]=\text{Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1N}$	1.08	0.19
206	$[\text{N-}]=[\text{N+}]=\text{Nc1nc(N)c([N+](=O)[O-])c(N)c1[N+](=O)[O-]}$	1.09	0.19
207	$[\text{N-}]=[\text{N+}]=\text{Nc1nnnc([N+](=O)[O-])c1[N+](=O)[O-]}$	1.11	0.19

208	[N-]=[N+]=Nc1nnc(N=[N+]=[N-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.09	0.19
209	[N-]=[N+]=Nc1c(N)nnc([N+](=O)[O-])c1[N+](=O)[O-]	1.10	0.19
210	Nc1c(N)c([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N	1.08	0.19
211	Nc1nc([N+](=O)[O-])c([N+](=O)[O-])nc1N	1.10	0.19
212	Nc1c([N+](=O)[O-])nnc([N+](=O)[O-])c1[N+](=O)[O-]	1.15	0.19
213	Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])n1	1.12	0.20
214	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.08	0.20
215	[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c1N=[N+]=[N-]	1.04	0.20
216	[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c(N)c1[N+](=O)[O-]	1.09	0.20
217	Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N)c1N	1.09	0.20
218	[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N=[N+]=[N-])c(N)c1[N+](=O)[O-]	1.08	0.20
219	[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N)c([N+](=O)[O-])c1N	1.08	0.20
220	[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.08	0.20
221	[N-]=[N+]=Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N	1.09	0.21
222	[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N)c(N=[N+]=[N-])c1[N+](=O)[O-]	1.08	0.21
223	Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])c1N	1.10	0.21
224	[N-]=[N+]=Nc1nc([N+](=O)[O-])c(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.13	0.21
225	[N-]=[N+]=Nc1c(N)c(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N	1.08	0.21
226	[N-]=[N+]=Nc1c([N+](=O)[O-])nc([N+](=O)[O-])c([N+](=O)[O-])c1N	1.13	0.21
227	[N-]=[N+]=Nc1c(N)c(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1N	1.08	0.21
228	Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])n1	1.10	0.21
229	[N-]=[N+]=Nc1c(N)c([N+](=O)[O-])c(N)c(N)c1[N+](=O)[O-]	1.08	0.21
230	[N-]=[N+]=Nc1nc(N)c(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.09	0.21
231	[N-]=[N+]=Nc1c(N)c(N)c(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.08	0.22
232	O=[N+](O)c1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1	1.19	0.22
233	[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1	1.14	0.22
234	Nc1nnnc([N+](=O)[O-])c1[N+](=O)[O-]	1.12	0.22
235	[N-]=[N+]=Nc1c(N)nc(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.09	0.22
236	Nc1nc(N)c([N+](=O)[O-])c(N)c1[N+](=O)[O-]	1.09	0.22
237	Nc1c(N)c(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N	1.08	0.22
238	Nc1c(N)c([N+](=O)[O-])c(N)c(N)c1[N+](=O)[O-]	1.08	0.22
239	[N-]=[N+]=Nc1nnc(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.10	0.22
240	O=[N+](O)c1nnnnc1[N+](=O)[O-]	1.14	0.22
241	[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1N=[N+]=[N-]	1.12	0.23
242	Nc1nc(N)c([N+](=O)[O-])c([N+](=O)[O-])c1N	1.09	0.24
243	[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c(N)c1[N+](=O)[O-]	1.13	0.24
244	Nc1nnc(N)c([N+](=O)[O-])c1[N+](=O)[O-]	1.11	0.24
245	[N-]=[N+]=Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1N	1.13	0.25
246	[N-]=[N+]=Nc1c(N)nc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.13	0.25
247	Nc1nc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])n1	1.15	0.25
248	[N-]=[N+]=Nc1nnc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.14	0.25
249	[N-]=[N+]=Nc1nc(N=[N+]=[N-])c([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	1.12	0.26

	]		
250	$\text{Nc1c}([N+](=O)[O-])\text{nc}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c1}[N+](=O)[O-]$	1.18	0.26
251	$[N-]=[N+]=\text{Nc1nnnc}(N=[N+]=[N-])\text{c1}[N+](=O)[O-]$	1.06	0.26
252	$\text{Nc1c}([N+](=O)[O-])\text{c}(N)\text{c}([N+](=O)[O-])\text{c}(N)\text{c1}[N+](=O)[O-]$	1.13	0.26
253	$[N-]=[N+]=\text{Nc1c}(N)\text{nc}([N+](=O)[O-])\text{c}(N=[N+]=[N-])\text{c1}[N+](=O)[O-]$	1.09	0.26
254	$\text{Nc1nc}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c}(N)\text{c1}[N+](=O)[O-]$	1.14	0.26
255	$[N-]=[N+]=\text{Nc1c}(N)\text{c}(N=[N+]=[N-])\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c1}[N+](=O)[O-]$	1.12	0.27
256	$O=[N+](\text{[O-]})\text{c1nnnc}([N+](=O)[O-])\text{c1}[N+](=O)[O-]$	1.17	0.27
257	$[N-]=[N+]=\text{Nc1c}([N+](=O)[O-])\text{nc}([N+](=O)[O-])\text{c}(N)\text{c1}[N+](=O)[O-]$	1.13	0.27
258	$[N-]=[N+]=\text{Nc1c}(N)\text{c}(N)\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c1}[N+](=O)[O-]$	1.12	0.27
259	$[N-]=[N+]=\text{Nc1nc}(N)\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c1}[N+](=O)[O-]$	1.13	0.27
260	$\text{Nc1nc}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c1}N$	1.14	0.28
261	$[N-]=[N+]=\text{Nc1c}([N+](=O)[O-])\text{nc}([N+](=O)[O-])\text{nc1}[N+](=O)[O-]$	1.14	0.28
262	$[N-]=[N+]=\text{Nc1c}(N)\text{c}([N+](=O)[O-])\text{c}(N)\text{c}([N+](=O)[O-])\text{c1}[N+](=O)[O-]$	1.12	0.28
263	$[N-]=[N+]=\text{Nc1nc}([N+](=O)[O-])\text{c}(N=[N+]=[N-])\text{c}([N+](=O)[O-])\text{n1}$	1.09	0.28
264	$[N-]=[N+]=\text{Nc1c}(N)\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c1}N$	1.12	0.28
265	$[N-]=[N+]=\text{Nc1c}(N)\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c}(N)\text{c1}[N+](=O)[O-]$	1.12	0.28
266	$\text{Nc1nnc}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c1}[N+](=O)[O-]$	1.15	0.28
267	$[N-]=[N+]=\text{Nc1c}(N)\text{c}(N=[N+]=[N-])\text{c}([N+](=O)[O-])\text{c}(N=[N+]=[N-])\text{c1}[N+](=O)[O-]$	1.08	0.28
268	$O=[N+](\text{[O-]})\text{c1nc}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{nc1}[N+](=O)[O-]$	1.19	0.29
269	$[N-]=[N+]=\text{Nc1nc}([N+](=O)[O-])\text{c}(N=[N+]=[N-])\text{c}([N+](=O)[O-])\text{c1}N=[N+]=[N-]$	1.08	0.29
270	$\text{Nc1c}(N)\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c}(N)\text{c1}[N+](=O)[O-]$	1.13	0.30
271	$[N-]=[N+]=\text{Nc1c}([N+](=O)[O-])\text{nnc}([N+](=O)[O-])\text{c1}N=[N+]=[N-]$	1.10	0.30
272	$\text{Nc1c}(N)\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c1}N$	1.13	0.30
273	$[N-]=[N+]=\text{Nc1c}(N)\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c}([N+](=O)[O-])\text{c1}N=[N+]=[N-]$	1.12	0.30

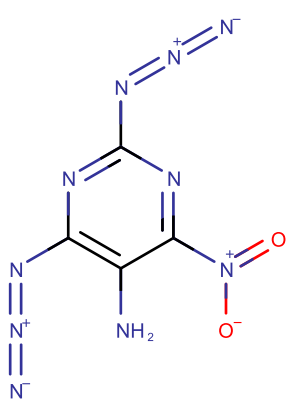
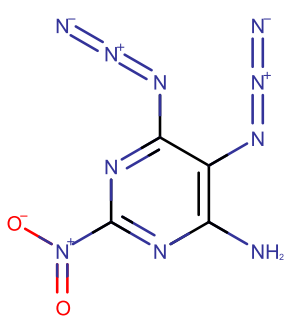
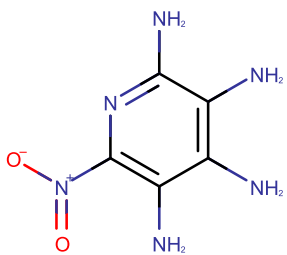
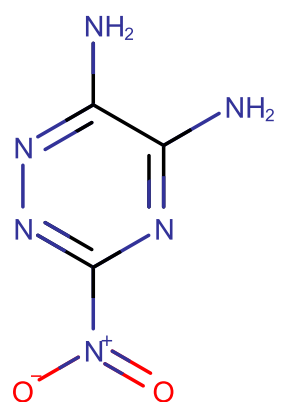
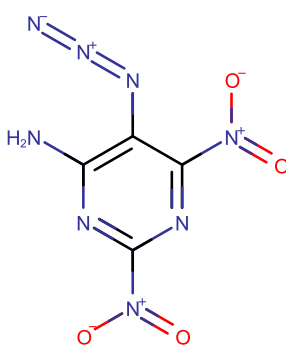
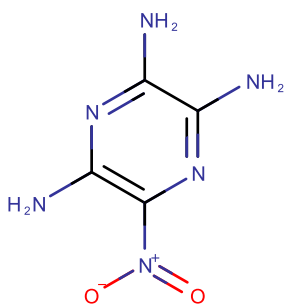
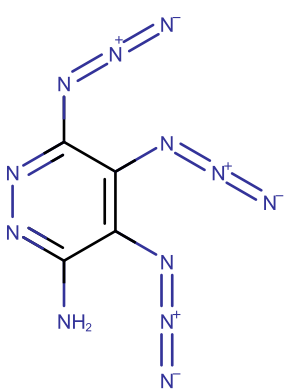
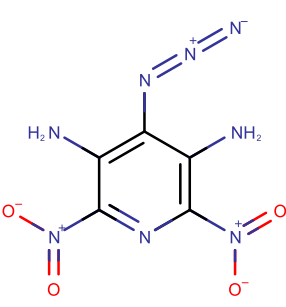
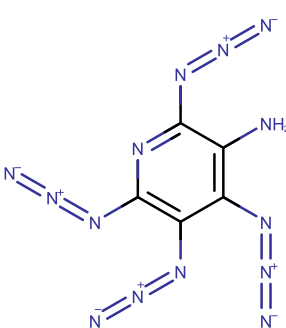
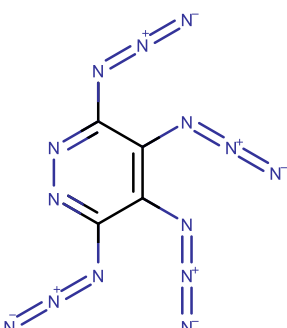
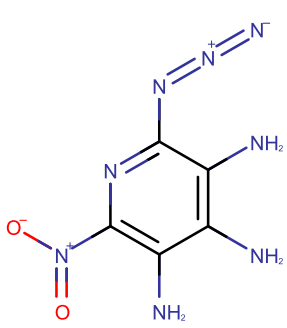
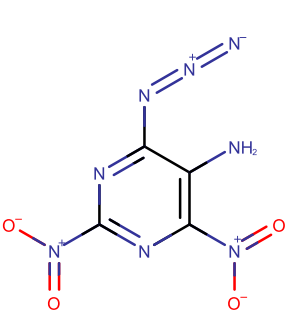
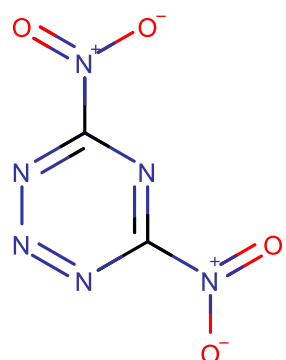
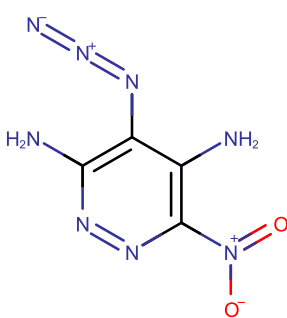
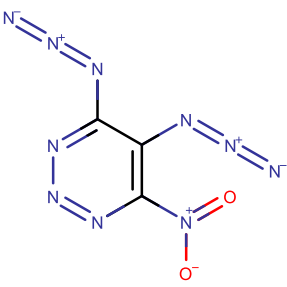
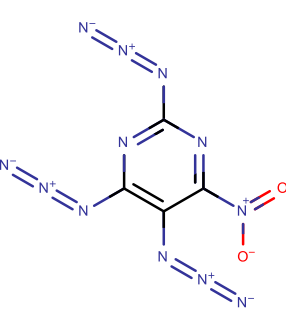
273 Molecular structures after first screening

1	2	3	4
5	6	7	8
9	10	11	12
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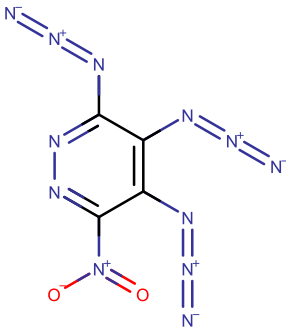
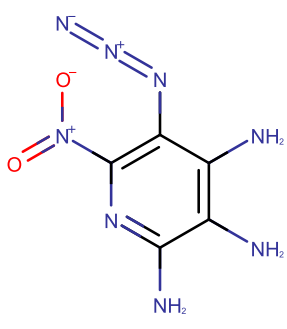
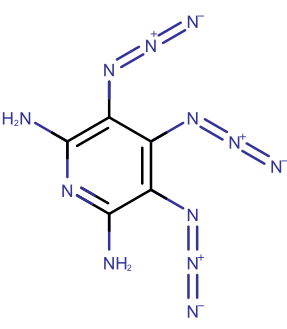
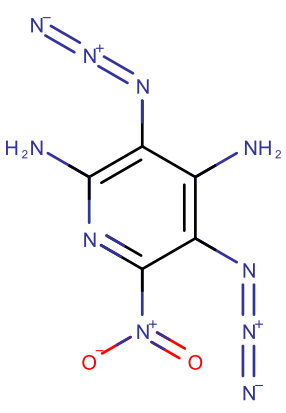
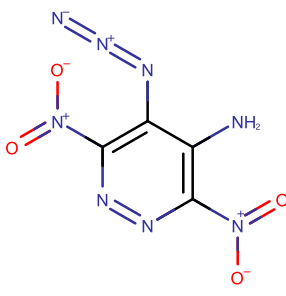
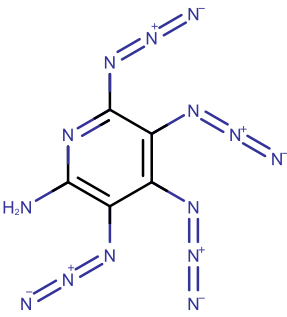
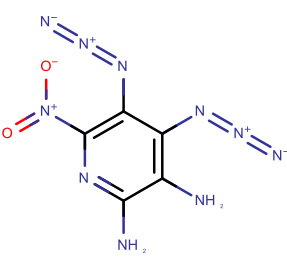
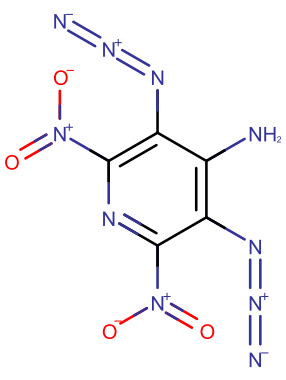
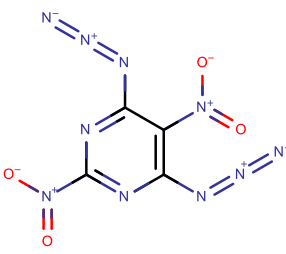
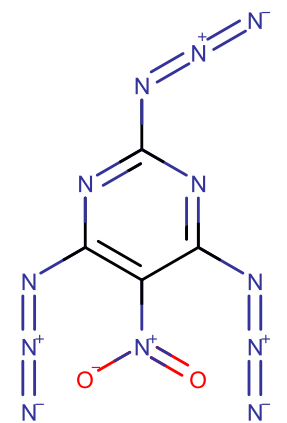
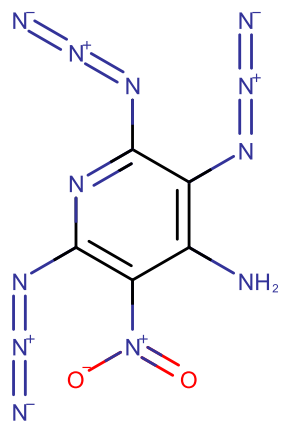
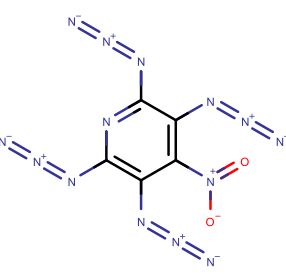
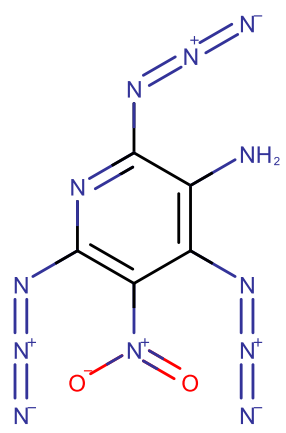
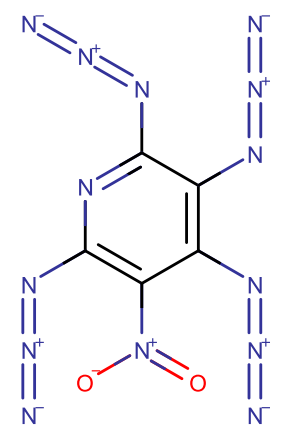
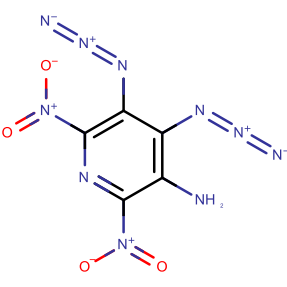
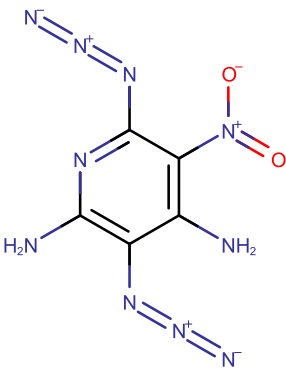
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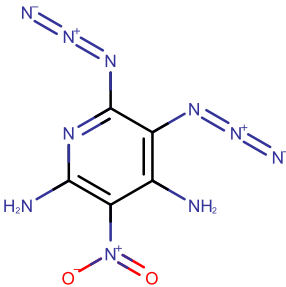
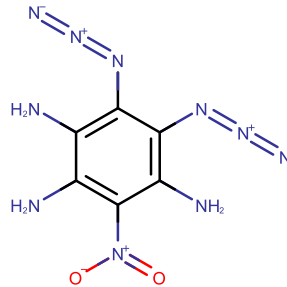
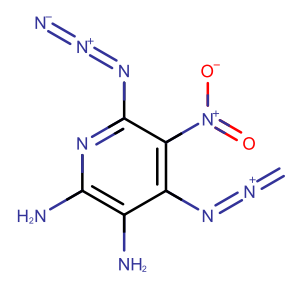
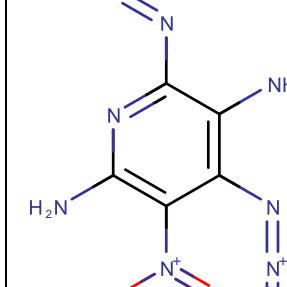
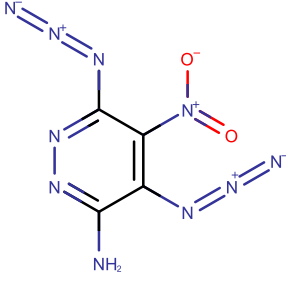
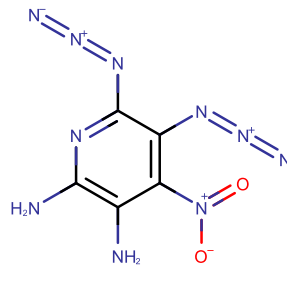
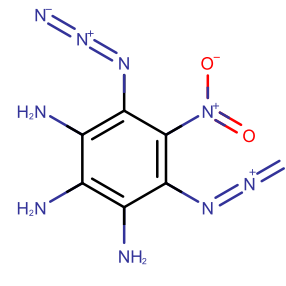
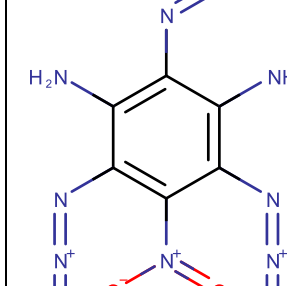
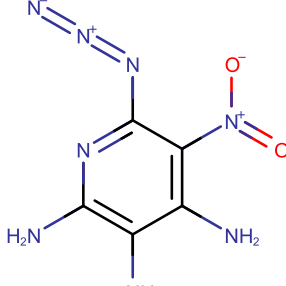
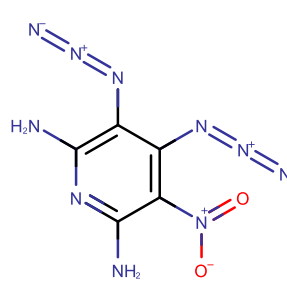
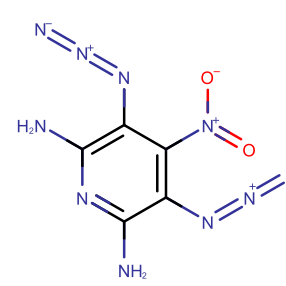
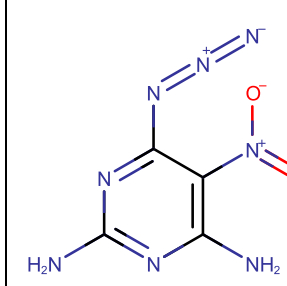
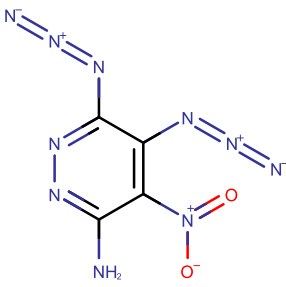
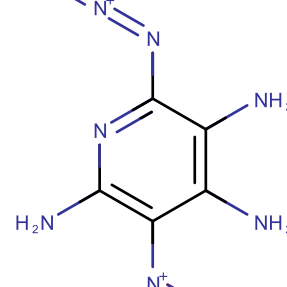
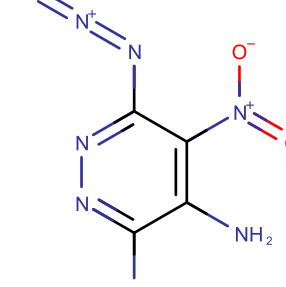
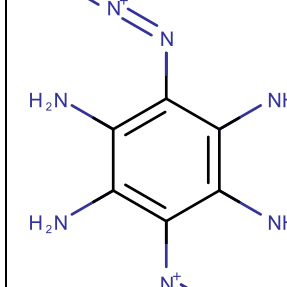
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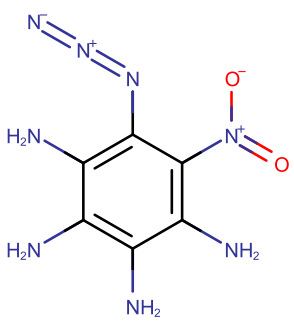
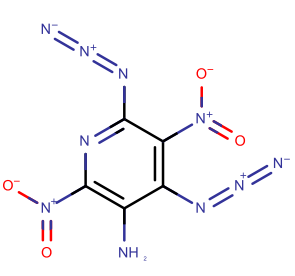
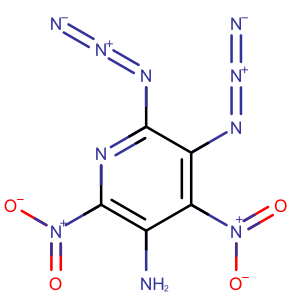
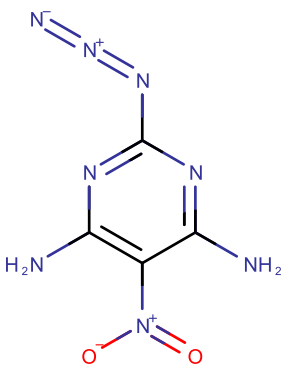
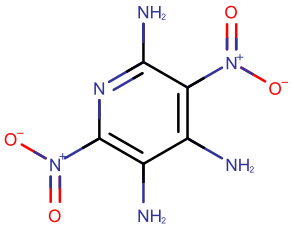
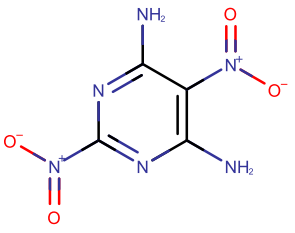
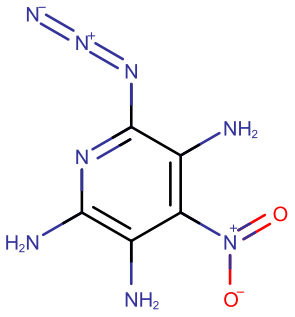
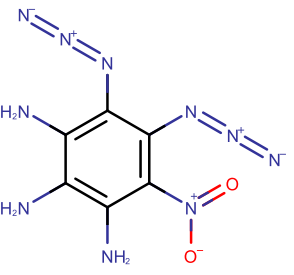
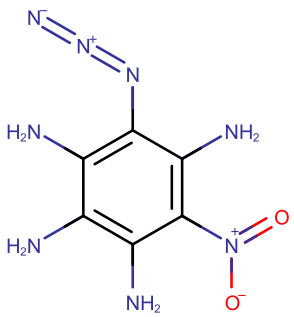
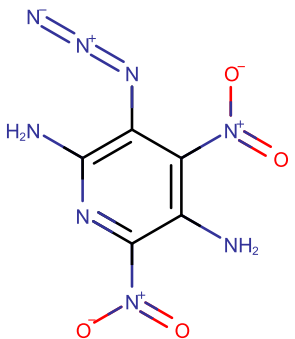
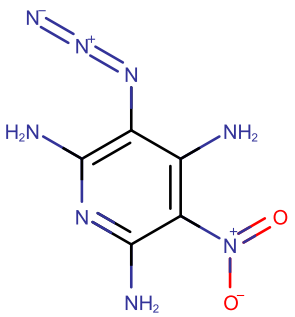
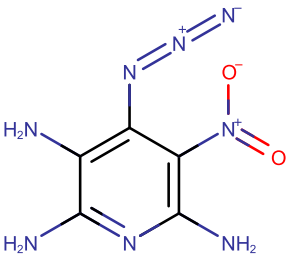
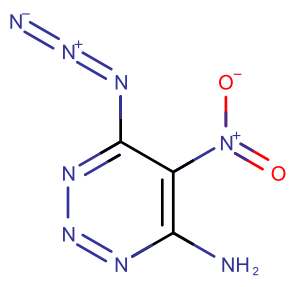
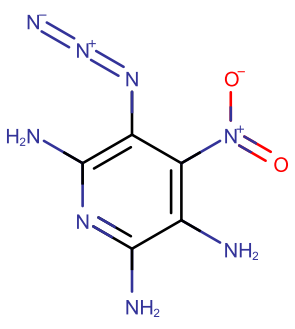
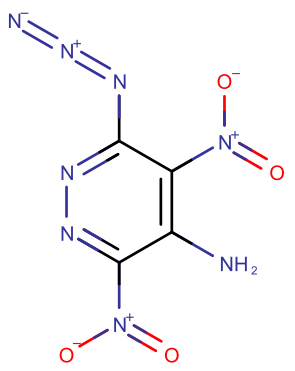
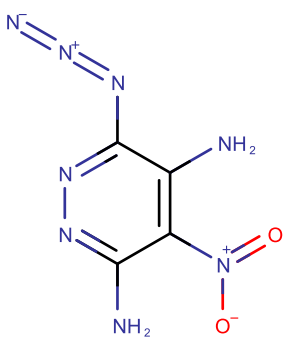
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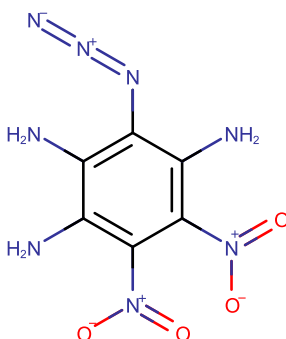
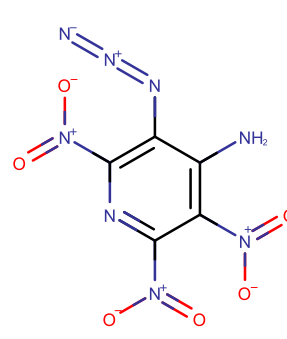
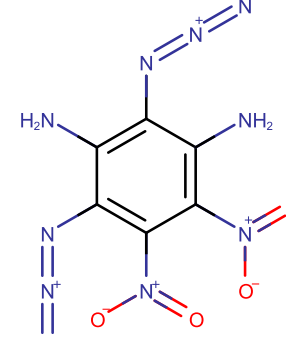
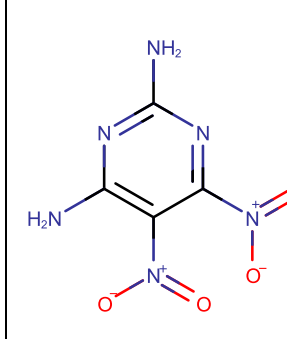
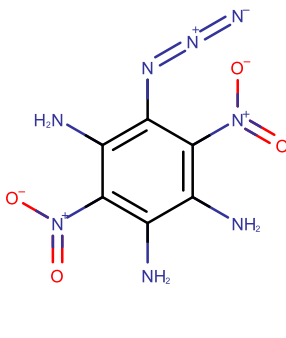
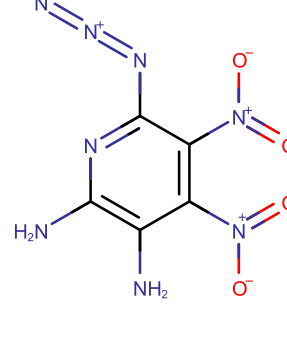
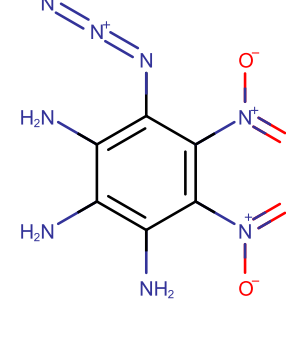
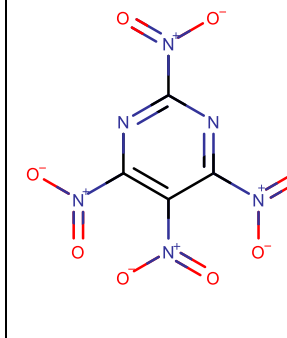
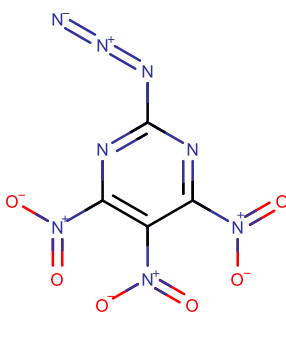
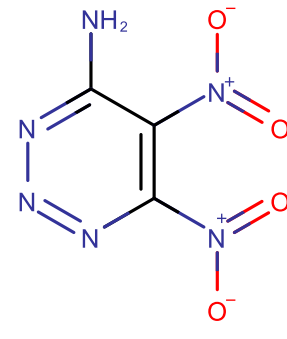
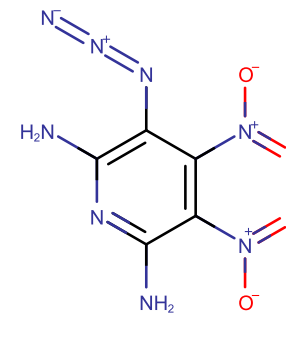
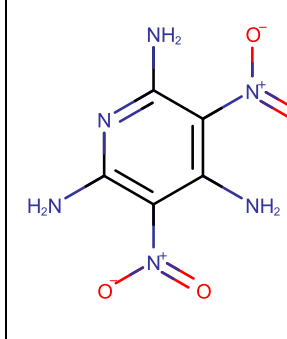
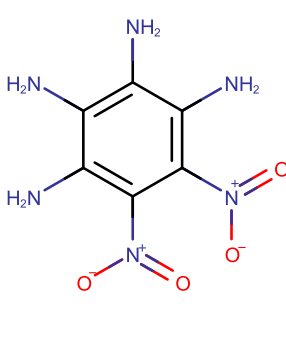
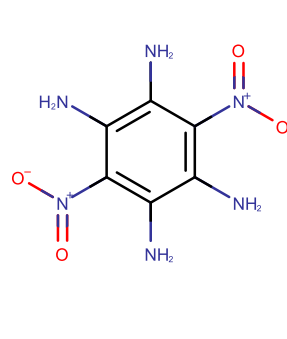
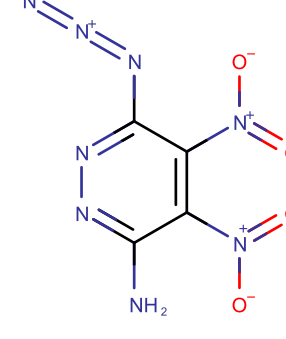
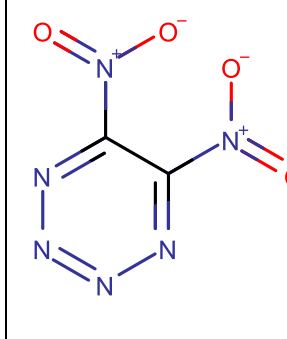
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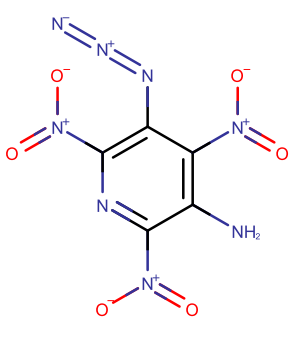
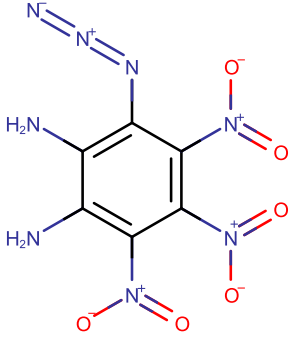
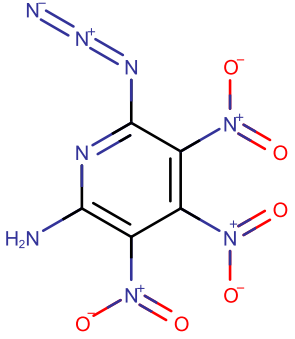
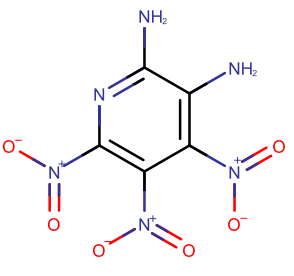
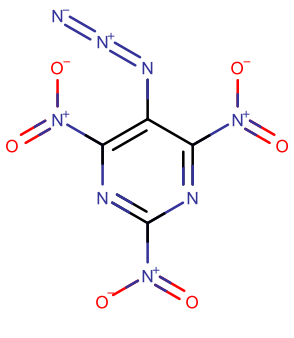
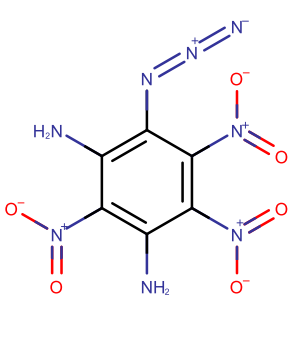
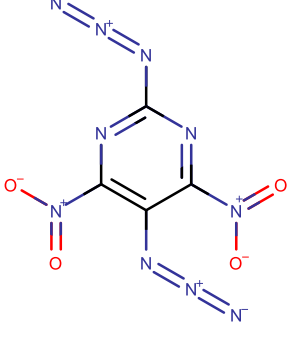
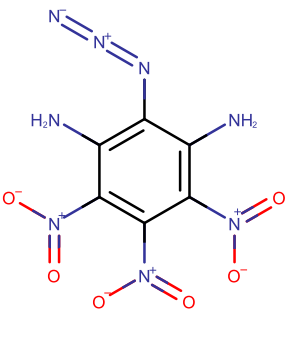
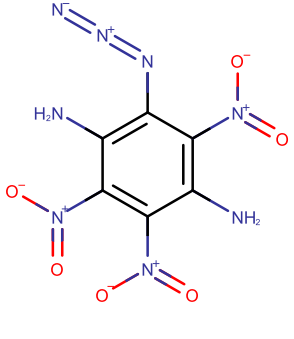
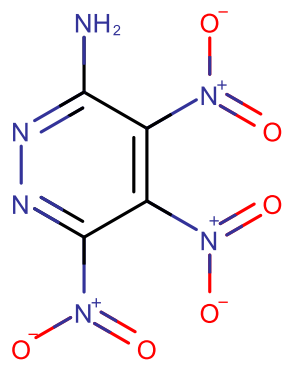
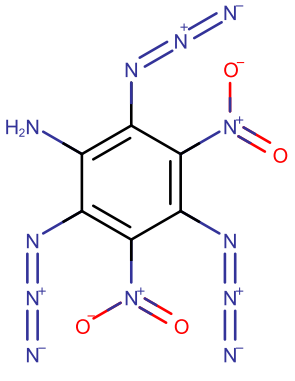
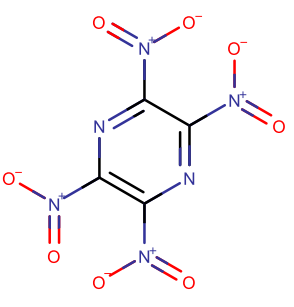
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