

Mining the ChEMBL database: An efficient chemoinformatics workflow for assembling an ion channel-focused screening library

N. Yi Mok and Ruth Brenk

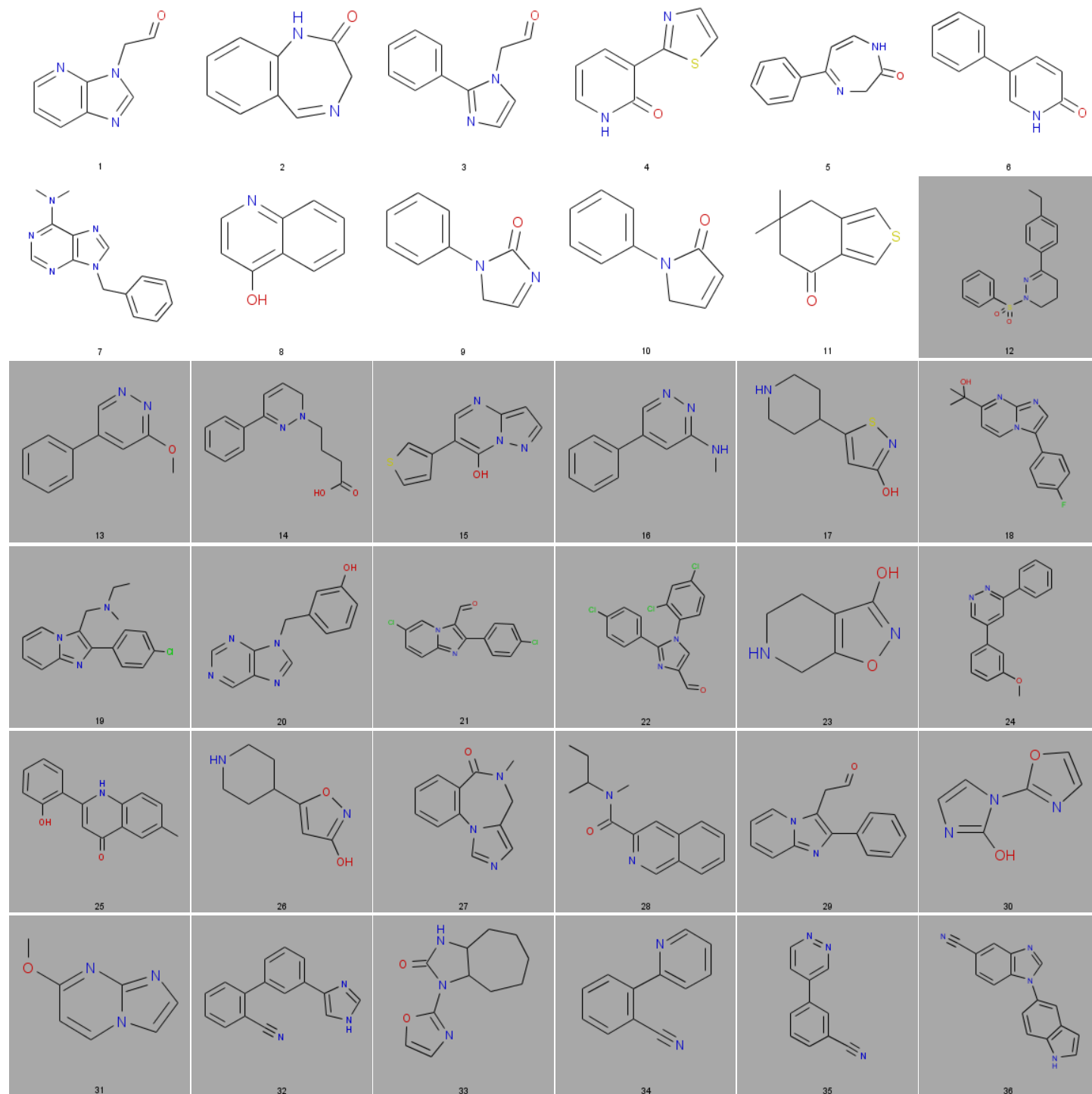
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DD1 5EH, UK

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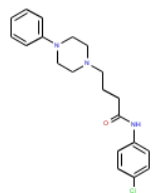
Table S1	Structures of shortlisted bioactive templates	S2
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Table S1. Structures of bioactive templates shortlisted for commercial availability search within each ion channel category. Structures shown represent the substructures used for mapping. Templates which did not retrieve any commercially available compounds are shaded in grey.

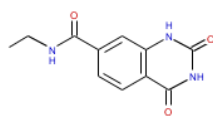
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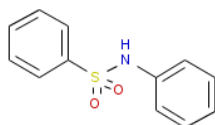
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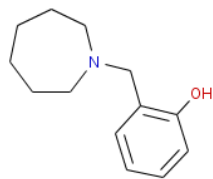
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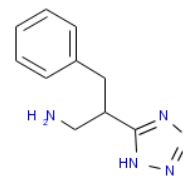
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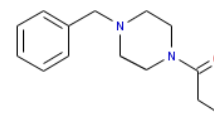
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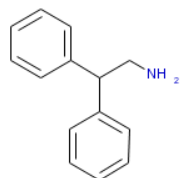
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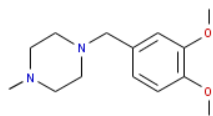
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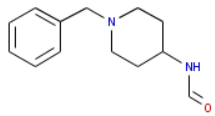
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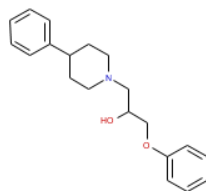
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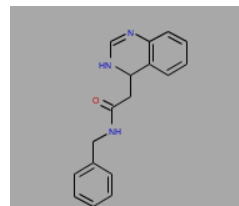
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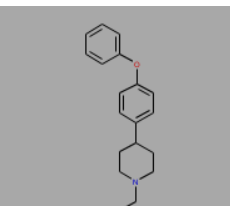
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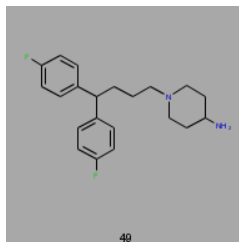
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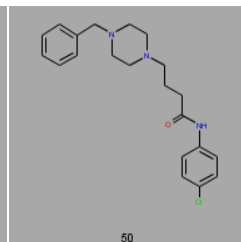
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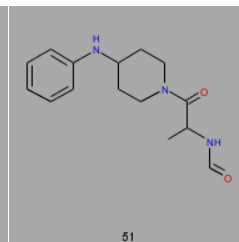
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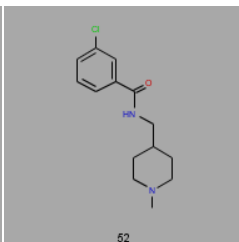
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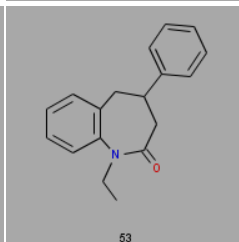
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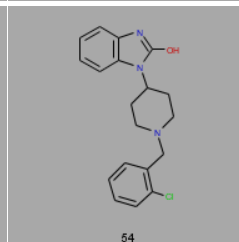
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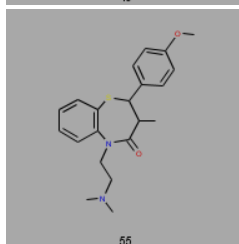
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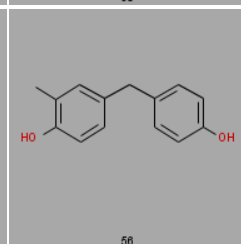
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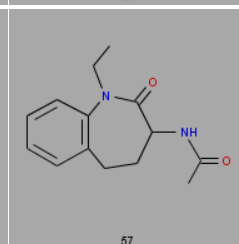
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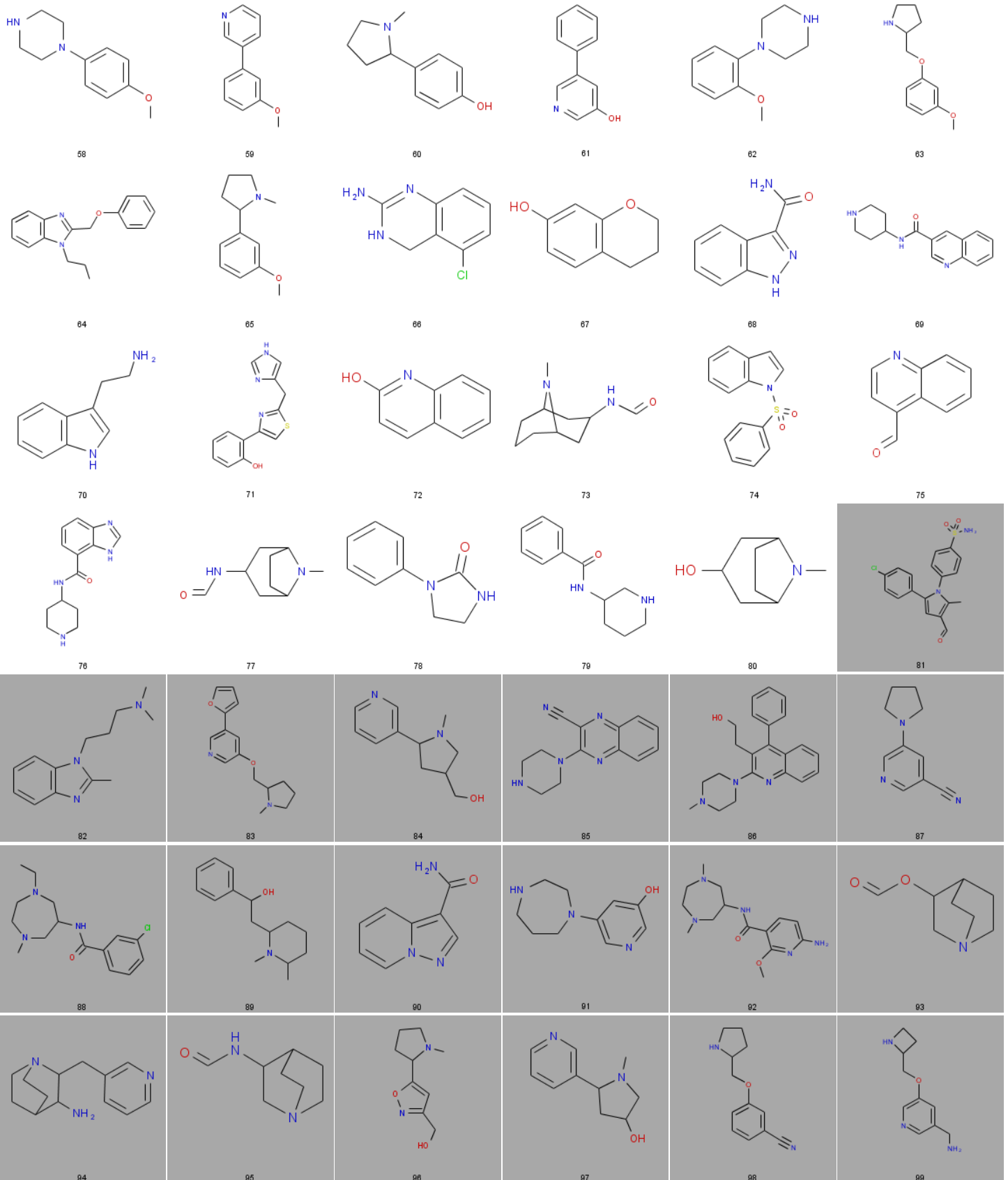


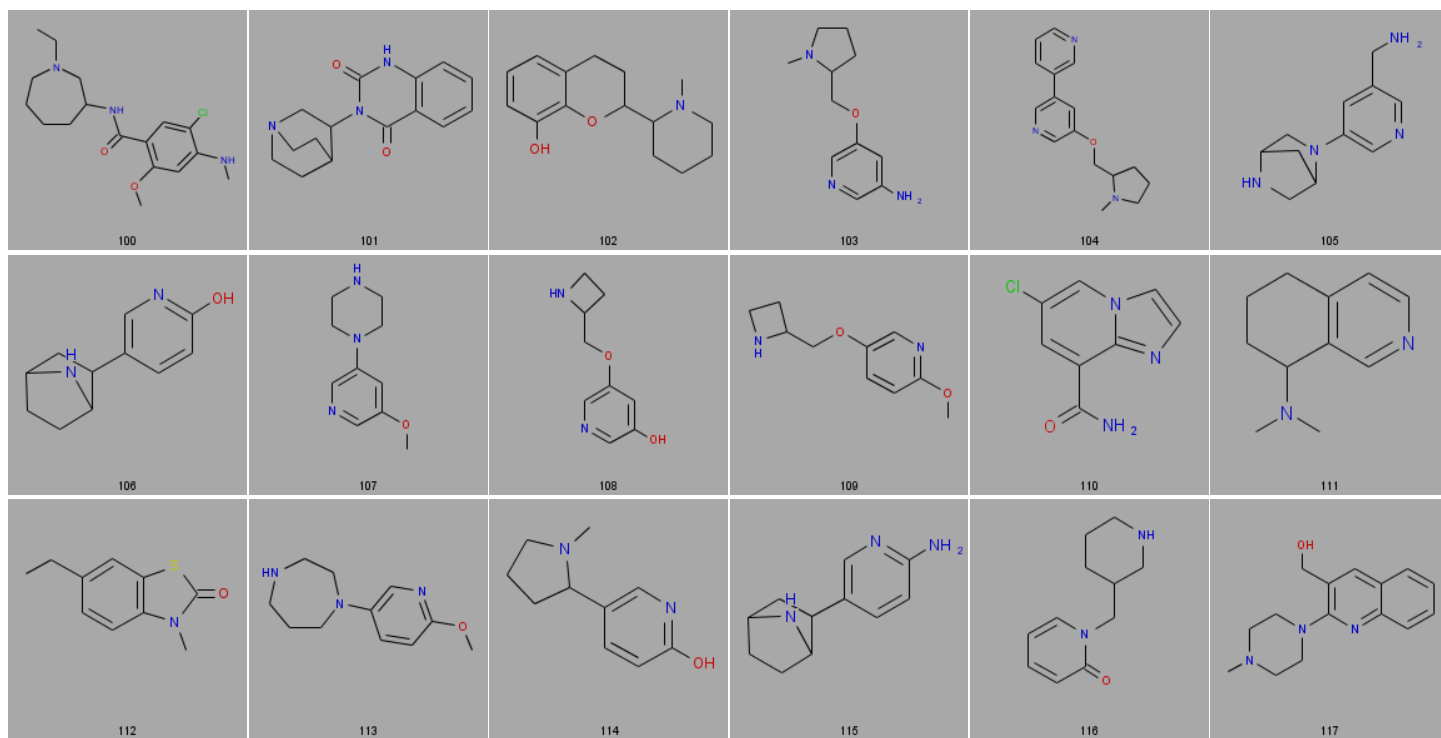
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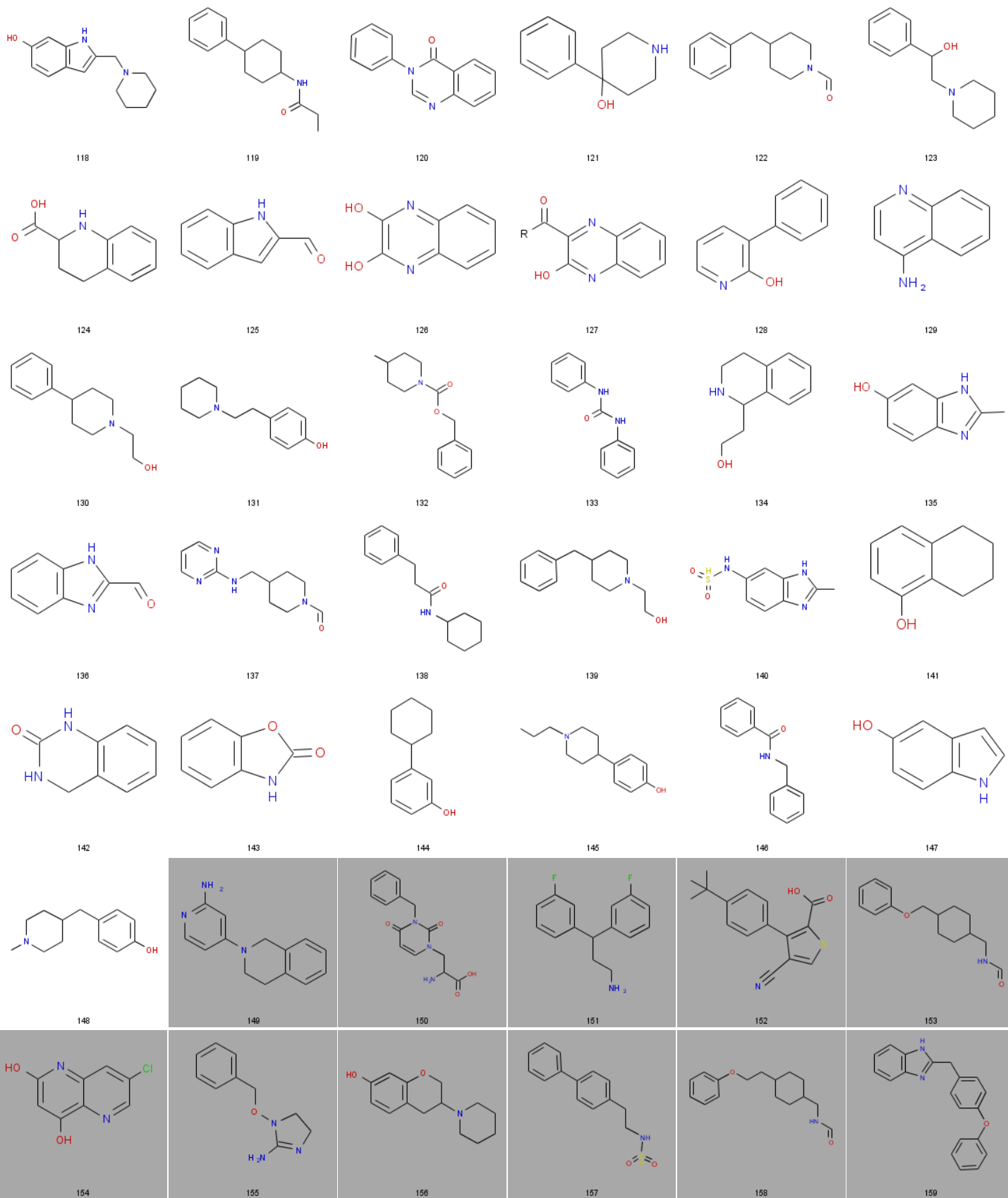
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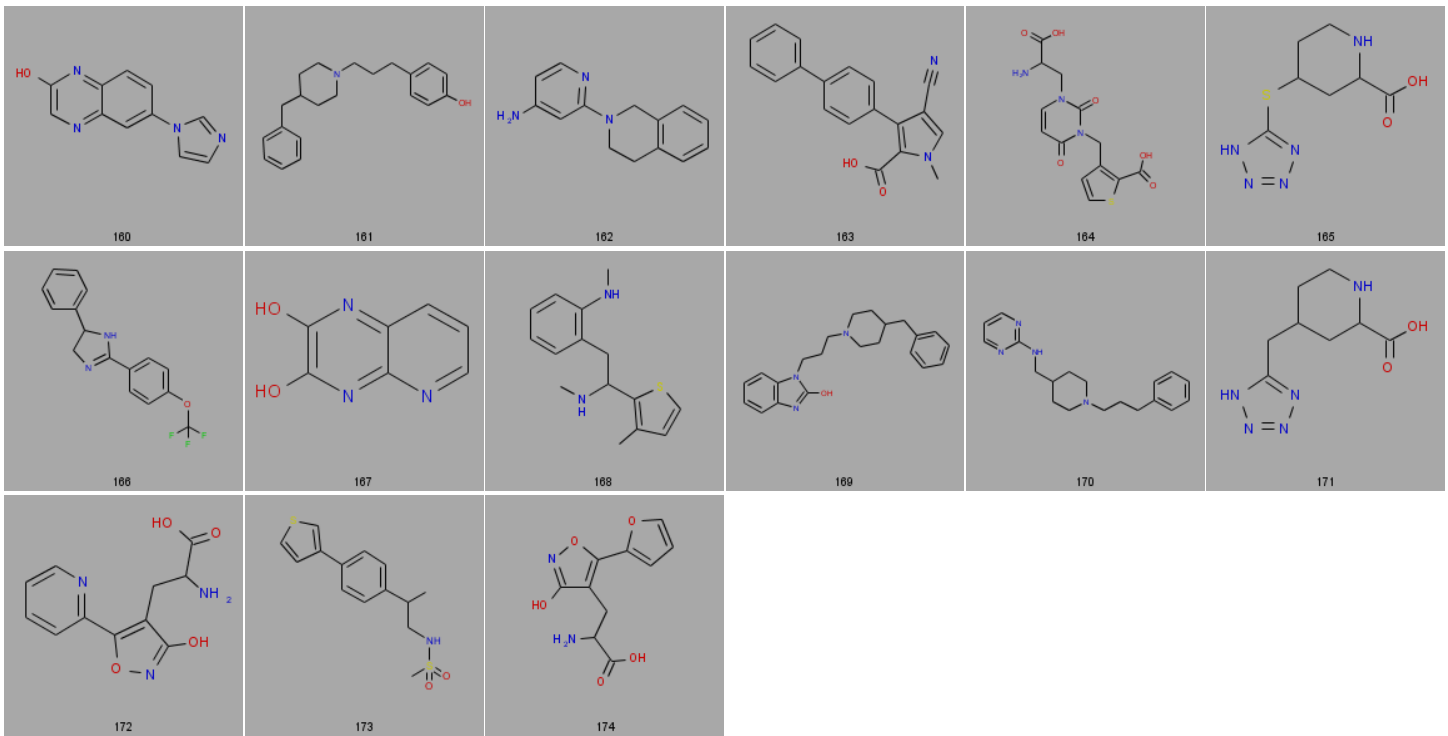
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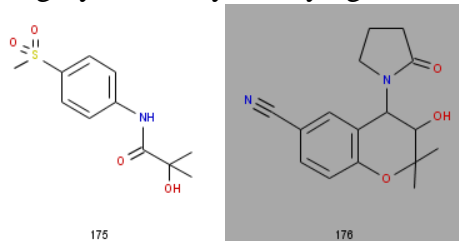


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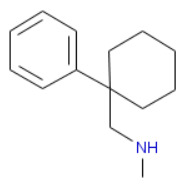




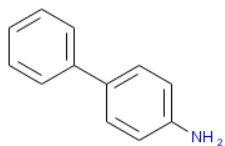
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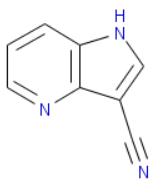
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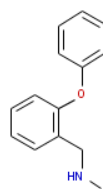
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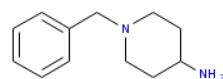
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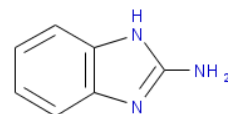
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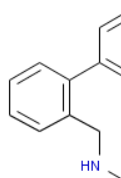
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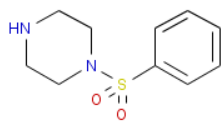
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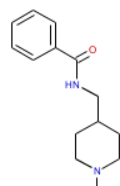
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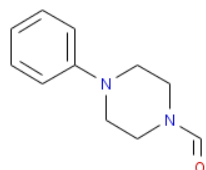
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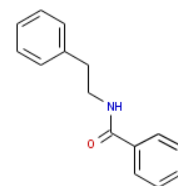
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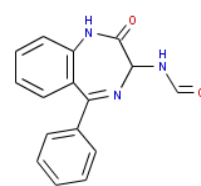
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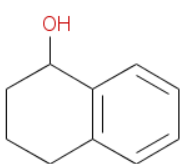
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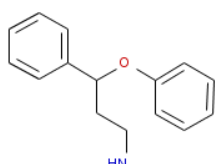
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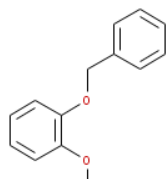
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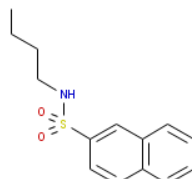
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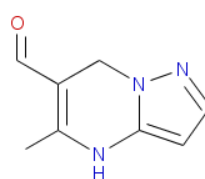
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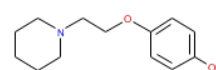
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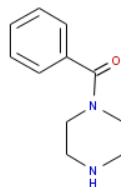
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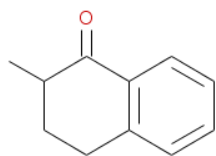
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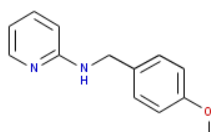
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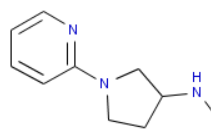
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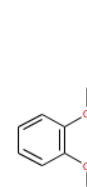
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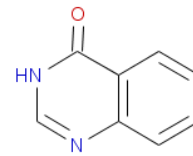
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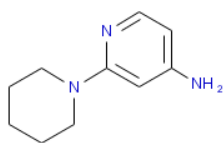
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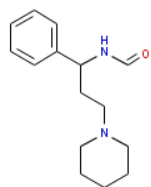
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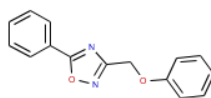
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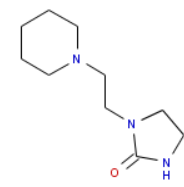
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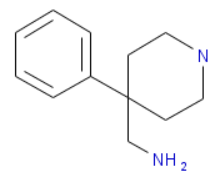
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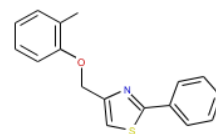
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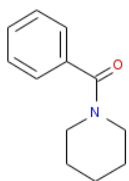
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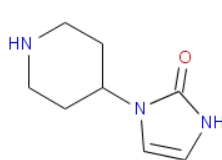
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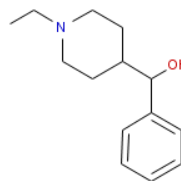
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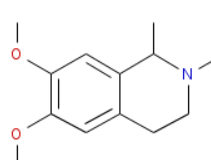
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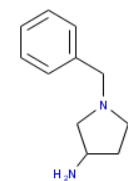
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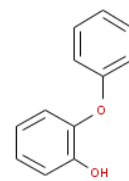
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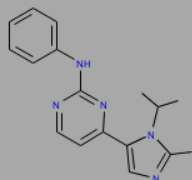
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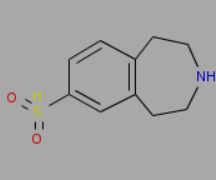
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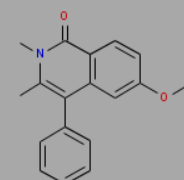
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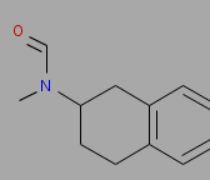
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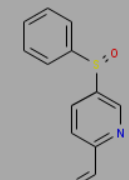
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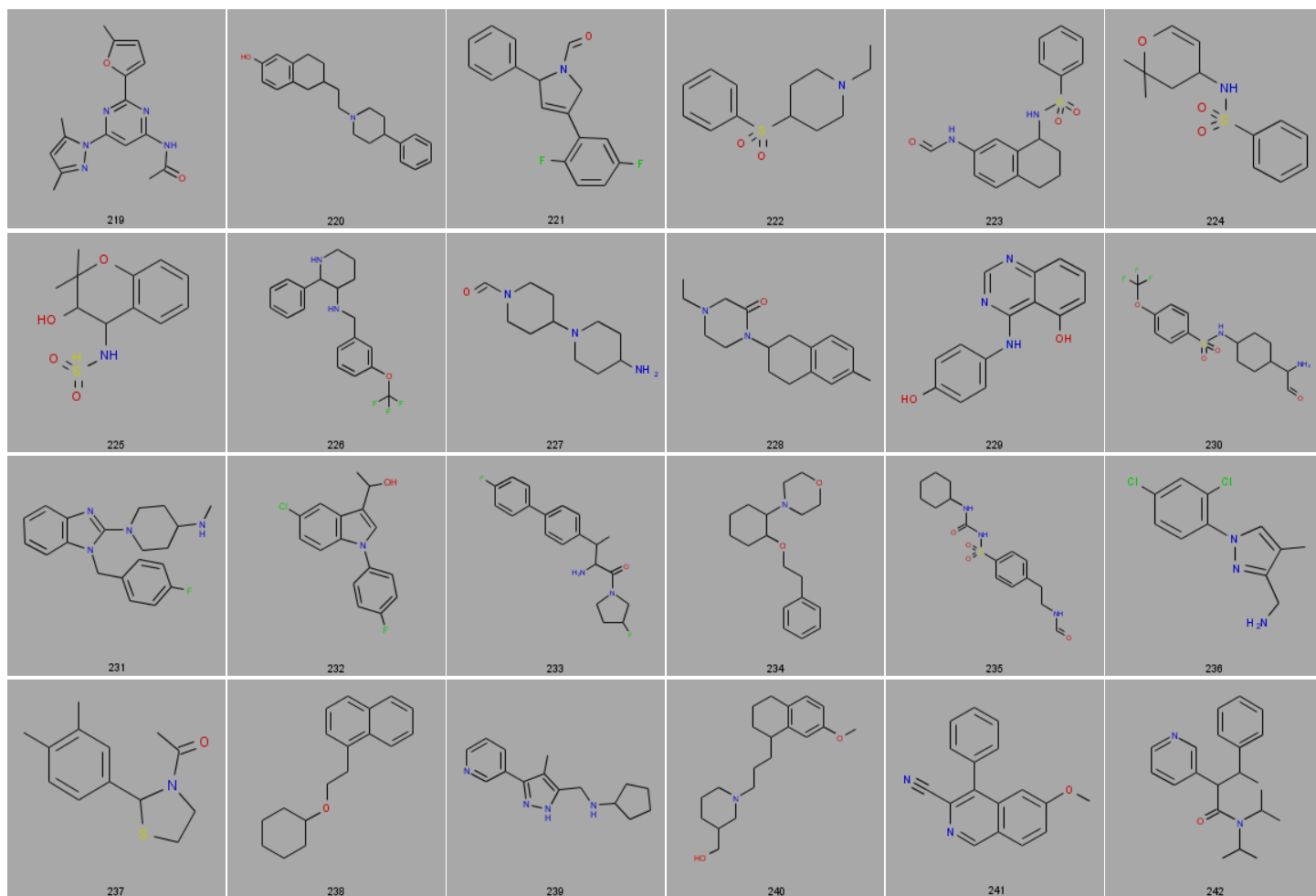
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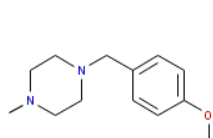
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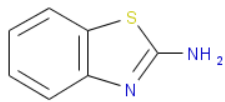
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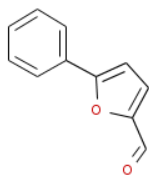
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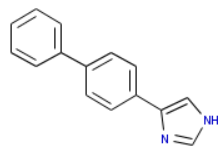
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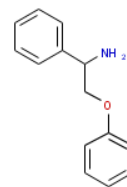
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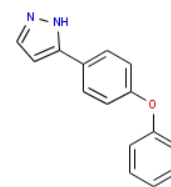
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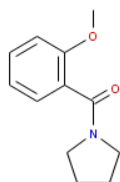
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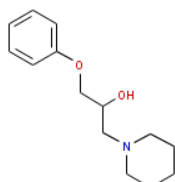
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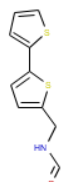
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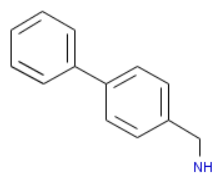
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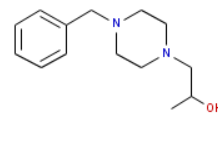
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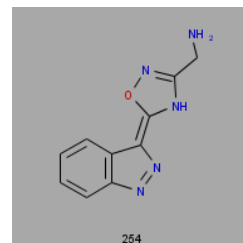
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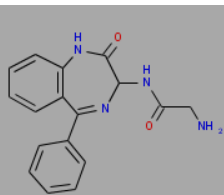
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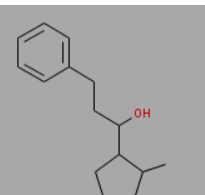
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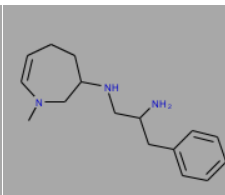
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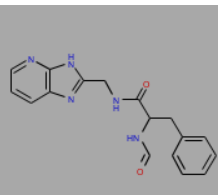
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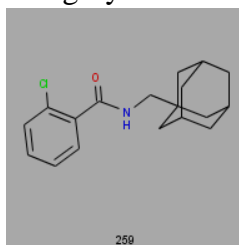


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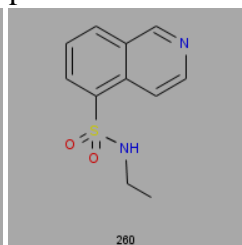


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Category: Purinoceptors

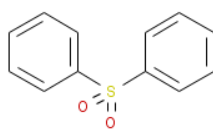


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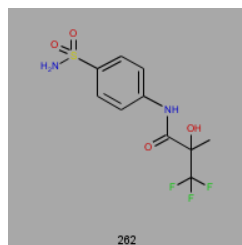


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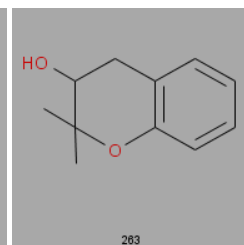
Category: Sulfonylurea



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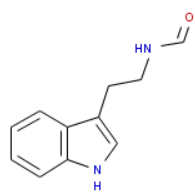


262

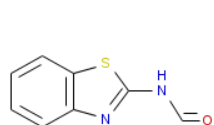


263

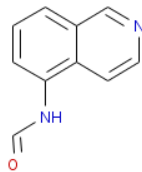
Category: Transient receptor potential



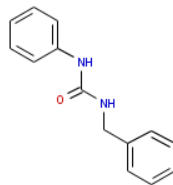
264



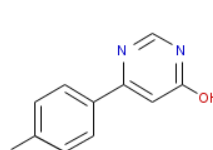
265



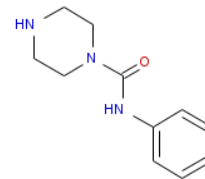
266



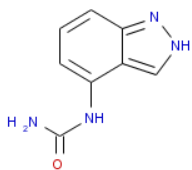
267



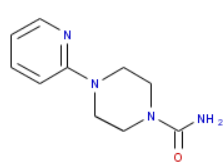
268



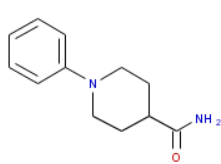
269



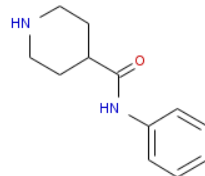
270



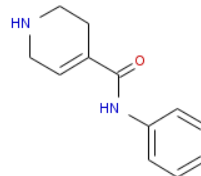
271



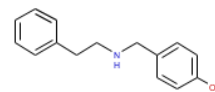
272



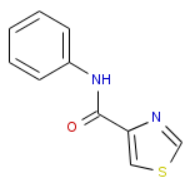
273



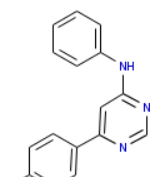
274



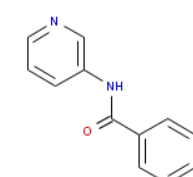
275



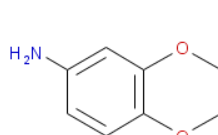
276



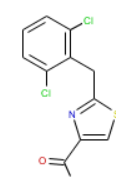
277



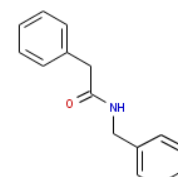
278



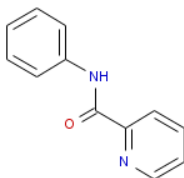
279



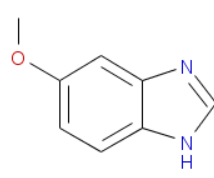
280



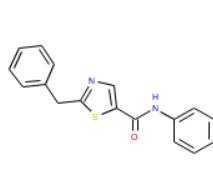
281



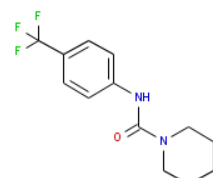
282



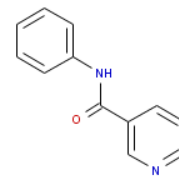
283



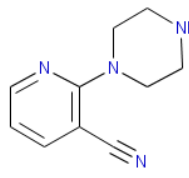
284



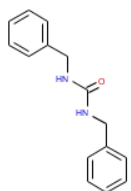
285



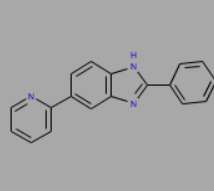
286



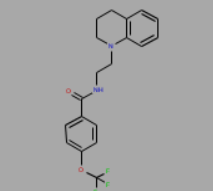
287



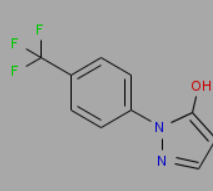
288



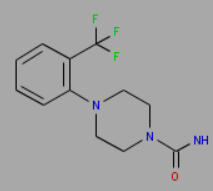
289



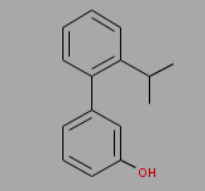
290



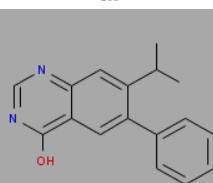
291



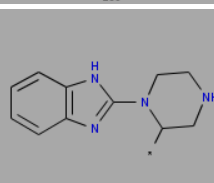
292



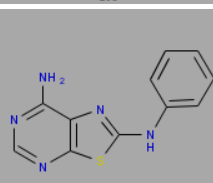
293



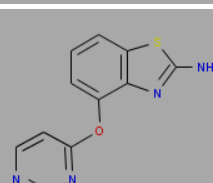
294



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296



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Table S2. SMARTS strings of bioactive templates shortlisted.

Category: AnionicCysLoop

Template_ID	TEMPLATE_SMARTS
1	[O;R0]=[C;R0][C;R0][n;R]1:[c;R]:[n;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[n;R]:[c;R]:1:2
2	[O;R0]=[C;R]1[C;R][N;R]=[C;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[N;R]1
3	[O;R0]=[C;R0][C;R0][n;R]1:[c;R]:[c;R]:[n;R]:[c;R]:1-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
4	[O;R0]=[C;R]1[N;R][C;R]=[C;R][C;R]=[C;R]1[c;R]2:[n;R]:[c;R]:[c;R]:[s;R]:2
5	[O;R0]=[C;R]1[C;R][N;R]=[C;R]([c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2)[c;R]:[c;R][N;R]1
6	[O;R0]=[C;R]1[N;R][C;R]=[C;R]([c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2)[C;R]=[C;R]1
7	[N;R0]([c;R]1:[c;R]2:[n;R]:[c;R]:[n;R]([C;R0][c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:3):[c;R]2:[n;R]:[c;R]:[n;R]1)([C;R0])[C;R0]
8	[O;R0][c;R]1:[c;R]:[c;R]:[n;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:1:2
9	[O;R0]=[C;R]1[N;R]=[C;R][C;R][N;R]1[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
10	[O;R0]=[C;R]1[C;R]=[C;R][C;R][N;R]1[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
11	[O;R0]=[C;R]1[C;R][C;R]([C;R][c;R]2:[c;R]:[s;R]:[c;R]:[c;R]1:2)([C;R0])[C;R0]
12	[O;R0]=[S;R0]([N;R]1[N;R]=[C;R]([c;R]2:[c;R]:[c;R]:[c;R]([C;R0][C;R0]):[c;R]:[c;R]:2)[C;R][C;R][C;R]1)(=[O;R0])[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:3
13	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R](:[c;R]:[n;R]:[n;R]:1)-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
14	[O;R0][C;R0]([C;R0][C;R0][C;R0][N;R]1[N;R]=[C;R]([C;R]=[C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2)=[O;R0]
15	[O;R0][C;R]1=[C;R]([C;R]=[N;R][c;R]2:[c;R]:[c;R]:[n;R]:[n;R]1:2)[c;R]3:[c;R]:[c;R]:[s;R]:[c;R]:3
16	[N;R0]([C;R0])[c;R]1:[c;R]:[c;R](:[c;R]:[n;R]:[n;R]:1)-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
17	[O;R0][c;R]1:[c;R]:[c;R](:[s;R]:[n;R]:1)[C;R]2[C;R][C;R][N;R][C;R][C;R]2
18	[O;R0][C;R0]([C;R0])([C;R0])[C;R]1[C;R]=[C;R][n;R]2:[c;R](:[c;R]:[n;R]:[c;R]:2[N;R]=1)-[c;R]3:[c;R]:[c;R]:[c;R]([F;R0]):[c;R]:[c;R]:3
19	[N;R0]([C;R0][C;R0])([C;R0])[C;R0][c;R]1:[c;R](:[n;R]:[c;R]2[C;R]=[C;R][C;R]=[C;R][n;R]:1:2)-[c;R]3:[c;R]:[c;R]:[c;R]([Cl;R0]):[c;R]:[c;R]:3
20	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]([C;R0][n;R]2:[c;R]:[n;R]:[c;R]3:[c;R]:[n;R]:[c;R]:[n;R]:[c;R]:2:3):[c;R]:1
21	[O;R0]=[C;R0][c;R]1:[c;R](:[n;R]:[c;R]2[C;R]=[C;R][C;R]([Cl;R0]=[C;R][n;R]:1:2)-[c;R]3:[c;R]:[c;R]:[c;R]([Cl;R0]):[c;R]:[c;R]:3
22	[O;R0]=[C;R0][c;R]1:[c;R]:[n;R](-[c;R]2:[c;R]:[c;R]:[c;R]([Cl;R0]):[c;R]:[c;R]:2[Cl;R0]):[c;R](:[n;R]:1)-[c;R]3:[c;R]:[c;R]:[c;R]([Cl;R0]):[c;R]:[c;R]:3
23	[O;R0][c;R]1:[n;R]:[o;R]:[c;R]2[C;R][N;R][C;R][C;R][c;R]:1:2

Template_ID	TEMPLATE_SMARTS
24	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:([c;R]:1)-[c;R]2:[c;R]:[n;R]:[n;R]:[c;R]:[c;R]:([c;R]:2)-[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3
25	[O;R0]=[C;R]1[C;R]=[C;R]([N;R][c;R]2:[c;R]:[c;R]:[c;R]([C;R0]):[c;R]:[c;R]1:2)[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3[O;R0]
26	[O;R0][c;R]1:[c;R]:[c;R]:([o;R]:[n;R]:1)[C;R]2[C;R][C;R][N;R][C;R][C;R]2
27	[O;R0]=[C;R]1[N;R]([C;R][c;R]2:[n;R]:[c;R]:[n;R]:[c;R]:2)-[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]1:3[C;R0]
28	[N;R0]([C;R0]([C;R0][C;R0])[C;R0])([C;R0][C;R0]=[O;R0])[c;R]1:[c;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:[c;R]:[n;R]:1
29	[O;R0]=[C;R0][C;R0][c;R]1:[c;R]:([n;R]:[c;R]2[C;R]=[C;R][C;R]=[C;R][n;R]:1:2)-[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3
30	[O;R0][c;R]1:[n;R]:[c;R]:[c;R]:[n;R]:1-[c;R]2:[o;R]:[c;R]:[c;R]:[n;R]:2
31	[O;R0]([C;R]1=[N;R][c;R]2:[n;R]:[c;R]:[c;R]:[n;R]:2[C;R]=[C;R]1)[C;R0]
32	[N;R0]#[C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R](-[c;R]3:[n;R]:[c;R]:[n;R]:[c;R]:3):[c;R]:2
33	[O;R0]=[C;R]1[N;R][C;R]2[C;R][C;R][C;R][C;R][C;R]2[N;R]1[c;R]3:[o;R]:[c;R]:[c;R]:[n;R]:3
34	[N;R0]#[C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1-[c;R]2:[n;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
35	[N;R0]#[C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R](-[c;R]2:[c;R]:[c;R]:[n;R]:[n;R]:[c;R]:2):[c;R]:1
36	[N;R0]#[C;R0][c;R]1:[c;R]:[c;R]:[c;R]2:[c;R]:([c;R]:1):[n;R]:[c;R]:[n;R]:2-[c;R]3:[c;R]:[c;R]:[c;R]4:[n;R]:[c;R]:[c;R]:[c;R]:4:[c;R]:3

Category: Ca²⁺

Template_ID	TEMPLATE_SMARTS
37	[N;R0]([c;R]1:[c;R]:[c;R]:[c;R]([C;R0]):[c;R]:[c;R]:1)[C;R0]=[O;R0][C;R0][C;R0][C;R0][N;R]2[C;R][C;R][N;R]([C;R][C;R]2)[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:3
38	[O;R0]=[C;R0]([N;R0][C;R0][C;R0])[c;R]1:[c;R]:[c;R]:[c;R]2[C;R]=[O;R0][N;R][C;R]([=O;R0][N;R][c;R]:2:[c;R]:1
39	[O;R0]=[S;R0]([N;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)=[O;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
40	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1[C;R0][N;R]2[C;R][C;R][C;R][C;R][C;R]2
41	[N;R0][C;R0][C;R0]([C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[c;R]2:[n;R]:[n;R]:[n;R]:[n;R]:2
42	[O;R0]=[C;R0]([N;R]1[C;R][C;R][N;R]([C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2)[C;R][C;R]1)[C;R0][C;R0]
43	[N;R0][C;R0][C;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
44	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]([C;R0][N;R]2[C;R][C;R][N;R]([C;R][C;R]2)[C;R0]):[c;R]:[c;R]:1[O;R0][C;R0]
45	[O;R0]=[C;R0][N;R0][C;R]1[C;R][C;R][N;R]([C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2)[C;R][C;R]1
46	[O;R0][C;R0]([C;R0][O;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[C;R0][N;R]2[C;R][C;R][C;R]([C;R][C;R]2)[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3
47	[O;R0]=[C;R0]([C;R0][C;R]1[N;R][C;R]=[N;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1:2)[N;R0][C;R0][c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3

Template_ID	TEMPLATE_SMARTS
48	[O;R0]([c;R]1:[c;R]:[c;R]:[c;R]([C;R]2[C;R][C;R][N;R]([C;R0][C;R0])[C;R][C;R]2):[c;R]:[c;R]:1)[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3
49	[N;R0][C;R]1[C;R][C;R][N;R]([C;R][C;R]1)[C;R0][C;R0][C;R0][C;R0]([C;R]2:[c;R]:[c;R]:[c;R]([F;R0]):[c;R]:[c;R]:2)[c;R]3:[c;R]:[c;R]:[c;R]([F;R0]):[c;R]:[c;R]:3
50	[N;R0]([c;R]1:[c;R]:[c;R]:[c;R]([Cl;R0]):[c;R]:[c;R]:1)[C;R0](=[O;R0])[C;R0][C;R0][C;R0][N;R]2[C;R][C;R][N;R]([C;R0][c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3)[C;R][C;R]2
51	[O;R0]=[C;R0][N;R0][C;R0]([C;R0]([N;R]1[C;R][C;R][C;R]([N;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2)[C;R][C;R]1)=O;R0)[C;R0]
52	[O;R0]=[C;R0]([N;R0][C;R0][C;R]1[C;R][C;R][N;R]([C;R0])[C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]([Cl;R0]):[c;R]:2
53	[O;R0]=[C;R]1[N;R]([c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[C;R][C;R]([c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3)[C;R]1)[C;R0][C;R0]
54	[O;R0][c;R]1:[n;R]([C;R]2[C;R][C;R][N;R]([C;R0][c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3[Cl;R0])[C;R][C;R]2):[c;R]4:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1
55	[N;R0]([C;R0][C;R0][N;R]1[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[S;R][C;R]([c;R]3:[c;R]:[c;R]:[c;R]([O;R0][C;R0]):[c;R]:[c;R]:3)[C;R]([C;R]1=[O;R0])[C;R0]([C;R0])[C;R0]
56	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]([C;R0][c;R]2:[c;R]:[c;R]:[c;R]([O;R0]):[c;R]([C;R0]):[c;R]:2):[c;R]:[c;R]:1
57	[O;R0]=[C;R0]([N;R0][C;R]1[C;R]([N;R]([c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[C;R][C;R]1)[C;R0][C;R0])=O;R0)[C;R0]

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58	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R](:[c;R]:[c;R]:1)[N;R]2[C;R][C;R][N;R][C;R][C;R]2
59	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]:[c;R](:[c;R]:1)-[c;R]2:[c;R]:[n;R]:[c;R]:[c;R]:[c;R]:2
60	[O;R0][c;R]1:[c;R]:[c;R]:[c;R](:[c;R]:[c;R]:1)[C;R]2[C;R][C;R][N;R]2[C;R0]
61	[O;R0][c;R]1:[c;R]:[n;R]:[c;R]:[c;R](:[c;R]:1)-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
62	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1[N;R]2[C;R][C;R][N;R][C;R][C;R]2
63	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]:[c;R]([O;R0][C;R0][C;R]2[C;R][C;R][C;R][N;R]2):[c;R]:1
64	[O;R0]([C;R0][c;R]1:[n;R]([C;R0][C;R0][C;R0]):[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2:[n;R]:1)[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3
65	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]:[c;R](:[c;R]:1)[C;R]2[C;R][C;R][C;R][N;R]2[C;R0]
66	[N;R0][C;R]1=[N;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]([Cl;R0]):[c;R]:2[C;R][N;R]1
67	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]2[C;R][C;R][C;R][O;R][c;R]:2:[c;R]:1
68	[N;R0][C;R0](=[O;R0])[c;R]1:[n;R]:[n;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1:2
69	[O;R0]=[C;R0]([N;R0][C;R]1[C;R][C;R][N;R][C;R][C;R]1)[c;R]2:[c;R]:[n;R]:[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3:c;R:2
70	[N;R0][C;R0][C;R0][c;R]1:[c;R]:[n;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1:2

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71	[O;R0][c;R]1:[c;R];[c;R];[c;R];[c;R];[c;R];[c;R];1-[c;R]2:[n;R];[c;R]([C;R0][c;R]3:[n;R];[c;R];[n;R];[c;R];3):[s;R];[c;R];2
72	[O;R0][c;R]1:[c;R];[c;R];[c;R]2:[c;R];[c;R];[c;R];[c;R];[c;R];[c;R];2:[n;R];1
73	[O;R0]=[C;R0][N;R0][C;R]1[C;R][C;R]2[C;R][C;R][C;R][C;R]([N;R]2[C;R0])[C;R]1
74	[O;R0]=[S;R0]([n;R]1:[c;R];[c;R];[c;R]2:[c;R];1:[c;R];[c;R];[c;R];[c;R];2)(=[O;R0])[c;R]3:[c;R];[c;R];[c;R];[c;R];[c;R];3
75	[O;R0]=[C;R0][c;R]1:[c;R];[c;R];[n;R];[c;R]2:[c;R];[c;R];[c;R];[c;R];[c;R];1:2
76	[N;R]1[C;R][C;R][C;R]([N;R0][C;R0](=[O;R0])[c;R]2:[c;R];[c;R];[c;R];[c;R]3:[n;R];[c;R];[n;R];[c;R];3:2)[C;R][C;R]1
77	[O;R0]=[C;R0][N;R0][C;R]1[C;R][C;R]2[C;R][C;R][C;R]([N;R]2[C;R0])[C;R]1
78	[O;R0]=[C;R]1[N;R][C;R][C;R][N;R]1[c;R]2:[c;R];[c;R];[c;R];[c;R];[c;R];2
79	[O;R0]=[C;R0]([N;R0][C;R]1[C;R][N;R][C;R][C;R][C;R]1)[c;R]2:[c;R];[c;R];[c;R];[c;R];[c;R];2
80	[O;R0][C;R]1[C;R][C;R]2[C;R][C;R][C;R]([N;R]2[C;R0])[C;R]1
81	[O;R0]=[C;R0][c;R]1:[c;R]([C;R0]);[n;R](:[c;R](:[c;R]:1)-[c;R]2:[c;R];[c;R];[c;R]([C;R0]);[c;R];[c;R];2)-[c;R]3:[c;R];[c;R];[c;R](:[c;R];[c;R];3)[S;R0](=[O;R0])(=[O;R0])[N;R0]
82	[N;R0]([C;R0])([C;R0])[C;R0][C;R0][C;R0][n;R]1:[c;R]([C;R0]);[n;R];[c;R]2:[c;R];[c;R];[c;R];[c;R];[c;R];1:2
83	[O;R0]([C;R0][C;R]1[C;R][C;R][C;R][N;R]1[C;R0])[c;R]2:[c;R];[n;R];[c;R];[c;R](:[c;R]:2)-[c;R]3:[o;R];[c;R];[c;R];[c;R];3
84	[O;R0][C;R0][C;R]1[C;R][N;R]([C;R0])[C;R]([C;R]1)[c;R]2:[c;R];[c;R];[c;R];[n;R];[c;R];2
85	[N;R0]#[C;R0][c;R]1:[n;R];[c;R]2:[c;R];[c;R];[c;R];[c;R];[c;R];2:[n;R];[c;R];1[N;R]3[C;R][C;R][N;R][C;R][C;R]3
86	[O;R0][C;R0][C;R0][c;R]1:[c;R](:[c;R]2:[c;R];[c;R];[c;R];[c;R];[c;R];2:[n;R];[c;R];1[N;R]3[C;R][C;R][N;R]([C;R0])[C;R][C;R]3)-[c;R]4:[c;R];[c;R];[c;R];[c;R];[c;R];4
87	[N;R0]#[C;R0][c;R]1:[c;R];[n;R];[c;R];[c;R](:[c;R]:1)[N;R]2[C;R][C;R][C;R][C;R]2
88	[O;R0]=[C;R0]([N;R0][C;R]1[C;R][N;R]([C;R][C;R][N;R]([C;R0][C;R0])[C;R]1)[C;R0])[c;R]2:[c;R];[c;R]([C;R0]);[c;R];[c;R];[c;R];2
89	[O;R0][C;R0]([C;R0][C;R]1[C;R][C;R][C;R][C;R]([N;R]1[C;R0])[C;R0])[c;R]2:[c;R];[c;R];[c;R];[c;R];[c;R];2
90	[N;R0][C;R0](=[O;R0])[c;R]1:[c;R];[n;R];[n;R]2[C;R]=[C;R][C;R]=[C;R][c;R];1:2
91	[O;R0][c;R]1:[c;R];[n;R];[c;R];[c;R](:[c;R]:1)[N;R]2[C;R][C;R][C;R][N;R][C;R][C;R]2
92	[N;R0][c;R]1:[n;R];[c;R]([O;R0][C;R0]);[c;R](:[c;R];[c;R];1)[C;R0](=[O;R0])[N;R0][C;R]2[C;R][N;R]([C;R0])[C;R][C;R][N;R]([C;R0])[C;R]2
93	[O;R0]=[C;R0][O;R0][C;R]1[C;R][N;R]2[C;R][C;R][C;R]1[C;R][C;R]2
94	[N;R0][C;R]1[C;R]2[C;R][C;R][N;R]([C;R][C;R]2)[C;R]1[C;R0][c;R]3:[c;R];[c;R];[c;R];[n;R];[c;R];3
95	[O;R0]=[C;R0][N;R0][C;R]1[C;R][N;R]2[C;R][C;R][C;R]1[C;R][C;R]2
96	[O;R0][C;R0][c;R]1:[n;R];[o;R];[c;R]([C;R]2[C;R][C;R][C;R][N;R]2[C;R0]);[c;R];1
97	[O;R0][C;R]1[C;R][N;R]([C;R0])[C;R]([C;R]1)[c;R]2:[c;R];[c;R];[c;R];[n;R];[c;R];2

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98	[N;R0]#[C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]([O;R0][C;R0][C;R]2[C;R][C;R][C;R][N;R]2):[c;R]:1
99	[N;R0][C;R0][c;R]1:[c;R]:[n;R]:[c;R]:[c;R]([O;R0][C;R0][C;R]2[C;R][C;R][N;R]2):[c;R]:1
100	[N;R0]([c;R]1:[c;R]:[c;R]:[c;R]([C;R0]([N;R0][C;R]2[C;R][C;R][C;R][C;R][N;R]([C;R0][C;R0])[C;R]2)=([O;R0]):[c;R]:[c;R]1)[O;R0][C;R0][C;R0])
101	[O;R0]=[C;R]1[N;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[C;R]([=O;R0])[N;R]1[C;R]3[C;R][N;R]4[C;R][C;R][C;R]3[C;R][C;R]4
102	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]2[C;R][C;R][C;R]([C;R]3[C;R][C;R][C;R][C;R][N;R]3[C;R0])[O;R][c;R]:1:2
103	[N;R0][c;R]1:[c;R]:[n;R]:[c;R]:[c;R]([O;R0][C;R0][C;R]2[C;R][C;R][C;R][N;R]2[C;R0]):[c;R]:1
104	[O;R0]([C;R0][C;R]1[C;R][C;R][C;R][N;R]1[C;R0])[c;R]2:[c;R]:[n;R]:[c;R]:[c;R](:[c;R]:2)-[c;R]3:[c;R]:[c;R]:[n;R]:[c;R]:3
105	[N;R0][C;R0][c;R]1:[c;R]:[n;R]:[c;R]:[c;R](:[c;R]:1)[N;R]2[C;R][C;R]3[C;R][C;R]2[C;R][N;R]3
106	[O;R0][c;R]1:[c;R]:[c;R]:[c;R](:[c;R]:[n;R]:1)[C;R]2[C;R][C;R]3[C;R][C;R][C;R]2[N;R]3
107	[O;R0]([C;R0])[c;R]1:[c;R]:[n;R]:[c;R]:[c;R](:[c;R]:1)[N;R]2[C;R][C;R][N;R][C;R][C;R]2
108	[O;R0][c;R]1:[c;R]:[n;R]:[c;R]:[c;R]([O;R0][C;R0][C;R]2[C;R][C;R][N;R]2):[c;R]:1
109	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]([O;R0][C;R0][C;R]2[C;R][C;R][N;R]2):[c;R]:[n;R]:1
110	[N;R0][C;R0]([C;R]1=[C;R][C;R]([C;R0])=[C;R][n;R]2:[c;R]:[c;R]:[n;R]:[c;R]1:2)=([O;R0])
111	[N;R0]([C;R0])([C;R0])[C;R]1[C;R][C;R][C;R][c;R]2:[c;R]:[c;R]:[n;R]:[c;R]:[c;R]1:2
112	[O;R0]=[C;R]1[N;R]([C;R0])[c;R]2:[c;R]:[c;R]:[c;R](:[c;R]:[c;R]:2[S;R]1)[C;R0][C;R0]
113	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R](:[c;R]:[n;R]:1)[N;R]2[C;R][C;R][C;R][N;R][C;R][C;R]2
114	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]([C;R]2[C;R][C;R][C;R][N;R]2[C;R0]):[c;R]:[n;R]:1
115	[N;R0][c;R]1:[c;R]:[c;R]:[c;R](:[c;R]:[n;R]:1)[C;R]2[C;R][C;R]3[C;R][C;R][C;R]2[N;R]3
116	[O;R0]=[C;R]1[C;R]=[C;R][C;R]=[C;R][N;R]1[C;R0][C;R]2[C;R][C;R][C;R][N;R][C;R]2
117	[O;R0][C;R0][c;R]1:[c;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:[n;R]:[c;R]:1[N;R]3[C;R][C;R][N;R]([C;R0])[C;R][C;R]3

Category: Glutamate

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118	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]2:[c;R]:[c;R]([C;R0][N;R]3[C;R][C;R][C;R][C;R]3):[n;R]:[c;R]:2:[c;R]:1
119	[O;R0]=[C;R0]([N;R0][C;R]1[C;R][C;R][C;R]([C;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2)[C;R][C;R]1)[C;R0][C;R0]
120	[O;R0]=[C;R]1[C;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[N;R]=[C;R][N;R]1[C;R]3:[c;R]:[c;R]:[c;R]:[c;R]:3
121	[O;R0][C;R]1([C;R][C;R][N;R][C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
122	[O;R0]=[C;R0][N;R]1[C;R][C;R][C;R]([C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2)[C;R][C;R]1

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123	[O;R0][C;R0]([C;R0][N;R]1[C;R][C;R][C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
124	[O;R0][C;R0](=[O;R0])[C;R]1[C;R][C;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[N;R]1
125	[O;R0]=[C;R0][c;R]1:[c;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:[n;R]:1
126	[O;R0][c;R]1:[n;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:[n;R]:[c;R]:1[O;R0]
127	[C;R0](=[O;R0])[c;R]1:[n;R][c;R]2:[c;R][c;R][c;R][c;R]2[n;R][c;R]:1[O;R0]
128	[O;R0][c;R]1:[n;R]:[c;R]:[c;R]:[c;R]:[c;R]:1-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
129	[N;R0][c;R]1:[c;R]:[c;R]:[n;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1:2
130	[O;R0][C;R0][C;R0][N;R]1[C;R][C;R][C;R]([C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
131	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]([C;R0][C;R0][N;R]2[C;R][C;R][C;R][C;R]2):[c;R]:[c;R]:1
132	[O;R0]=[C;R0]([O;R0][C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[N;R]2[C;R][C;R]([C;R0][C;R][C;R]2
133	[O;R0]=[C;R0]([N;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[N;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
134	[O;R0][C;R0][C;R0][C;R]1[N;R][C;R][C;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]1:2
135	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]2:[n;R]:[c;R]([C;R0]):[n;R]:[c;R]:2:[c;R]:1
136	[O;R0]=[C;R0][c;R]1:[n;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:[n;R]:1
137	[O;R0]=[C;R0][N;R]1[C;R][C;R][C;R]([C;R0][N;R0][c;R]2:[n;R]:[c;R]:[c;R]:[c;R]:[n;R]:2)[C;R][C;R]1
138	[O;R0]=[C;R0]([N;R0][C;R]1[C;R][C;R][C;R][C;R]1)[C;R0][C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
139	[O;R0][C;R0][C;R0][N;R]1[C;R][C;R][C;R]([C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2)[C;R][C;R]1
140	[O;R0]=[S;R0](=[O;R0])[N;R0][c;R]1:[c;R]:[c;R]:[c;R]2:[n;R]:[c;R]([C;R0]):[n;R]:[c;R]:2:[c;R]:1
141	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]2[C;R][C;R][C;R][C;R]:1:2
142	[O;R0]=[C;R]1[N;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[C;R][N;R]1
143	[O;R0]=[C;R]1[N;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[O;R]1
144	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]([C;R]2[C;R][C;R][C;R][C;R]2):[c;R]:1
145	[O;R0][c;R]1:[c;R]:[c;R]:[c;R](:[c;R]:[c;R]:1)[C;R]2[C;R][C;R][N;R]([C;R0][C;R0][C;R0])[C;R][C;R]2
146	[O;R0]=[C;R0]([N;R0][C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
147	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]2:[n;R]:[c;R]:[c;R]:[c;R]:2:[c;R]:1
148	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]([C;R0][C;R]2[C;R][C;R][N;R]([C;R0])[C;R][C;R]2):[c;R]:[c;R]:1
149	[N;R0][c;R]1:[c;R]:[c;R](:[c;R]:[c;R]:[n;R]:1)[N;R]2[C;R][C;R][c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3[C;R]2
150	[O;R0][C;R0]([C;R0]([N;R0])[C;R0][N;R]1[C;R]=[C;R][C;R](=[O;R0])[N;R]([C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2)[C;R]1=[O;R0])=[O;

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	R0]
151	[N;R0][C;R0][C;R0][C;R0]([c;R]1:[c;R];[c;R];[c;R];[c;R]([F;R0]):[c;R]:1)[c;R]2:[c;R];[c;R];[c;R];[c;R]([F;R0]):[c;R]:2
152	[N;R0]#[C;R0][c;R]1:[c;R](:[c;R](:[s;R]:[c;R]:1)[C;R0](=[O;R0])[O;R0]-[c;R]2:[c;R];[c;R];[c;R](:[c;R]:[c;R]:2)[C;R0]([C;R0])([C;R0])[C;R0]
153	[O;R0]=[C;R0][N;R0][C;R0][C;R]1[C;R][C;R][C;R]([C;R0][O;R0][c;R]2:[c;R];[c;R];[c;R];[c;R]:[c;R]:2)[C;R][C;R]1
154	[O;R0][c;R]1:[n;R];[c;R]2:[c;R];[c;R]([Cl;R0]):[c;R]:[n;R];[c;R]:2:[c;R]([O;R0]):[c;R]:1
155	[N;R0][C;R]1=[N;R][C;R][C;R][N;R]1[O;R0][C;R0][c;R]2:[c;R];[c;R];[c;R];[c;R];[c;R]:2
156	[O;R0][c;R]1:[c;R];[c;R];[c;R]2[C;R][C;R]([C;R][O;R][c;R]:2:[c;R]:1)[N;R]3[C;R][C;R][C;R][C;R]3
157	[O;R0]=[S;R0](=[O;R0])[N;R0][C;R0][C;R0][c;R]1:[c;R];[c;R];[c;R](:[c;R]:[c;R]:1)-[c;R]2:[c;R];[c;R];[c;R];[c;R]:2
158	[O;R0]=[C;R0][N;R0][C;R0][C;R]1[C;R][C;R][C;R]([C;R0][C;R0][O;R0][c;R]2:[c;R];[c;R];[c;R];[c;R]:[c;R]:2)[C;R][C;R]1
159	[O;R0]([c;R]1:[c;R];[c;R];[c;R]([C;R0][c;R]2:[n;R];[c;R]3:[c;R];[c;R];[c;R];[c;R];[c;R]:3:[n;R]:2):[c;R];[c;R]:1)[c;R]4:[c;R];[c;R];[c;R];[c;R];[c;R]:4
160	[O;R0][c;R]1:[n;R];[c;R]2:[c;R];[c;R];[c;R](:[c;R]:[c;R]:2:[n;R];[c;R]:1)-[n;R]3:[c;R];[c;R];[n;R];[c;R]:3
161	[O;R0][c;R]1:[c;R];[c;R];[c;R]([C;R0][C;R0][C;R0][N;R]2[C;R][C;R][C;R]([C;R0][c;R]3:[c;R];[c;R];[c;R];[c;R]:3)[C;R][C;R]2):[c;R];[c;R]:1
162	[N;R0][c;R]1:[c;R];[c;R];[n;R];[c;R](:[c;R]:1)[N;R]2[C;R][C;R][c;R]3:[c;R];[c;R];[c;R];[c;R]:3[C;R]2
163	[N;R0]#[C;R0][c;R]1:[c;R];[n;R](:[c;R](:[c;R]:1-[c;R]2:[c;R];[c;R];[c;R](:[c;R]:[c;R]:2)-[c;R]3:[c;R];[c;R];[c;R];[c;R]:3)[C;R0](=[O;R0])[O;R0][C;R0]
164	[O;R0][C;R0]([c;R]1:[s;R];[c;R];[c;R];[c;R]:1[C;R0][N;R]2[C;R]([C;R]=[C;R][N;R]([C;R0][C;R0]([N;R0])[C;R0](=[O;R0])[O;R0])[C;R]2=[O;R0])=[O;R0])=[O;R0]
165	[O;R0][C;R0](=[O;R0])[C;R]1[C;R][C;R]([C;R][C;R][N;R]1)[S;R0][c;R]2:[n;R];[n;R];[n;R]:2
166	[O;R0]([C;R0]([F;R0])([F;R0])[F;R0])[c;R]1:[c;R];[c;R];[c;R](:[c;R]:[c;R]:1)[C;R]2=[N;R][C;R][C;R]([N;R]2)[c;R]3:[c;R];[c;R];[c;R];[c;R]:3
167	[O;R0][c;R]1:[n;R];[c;R]2:[c;R];[c;R];[c;R];[n;R];[c;R]:2:[n;R];[c;R]:1[O;R0]
168	[N;R0]([C;R0])[C;R0]([C;R0][c;R]1:[c;R];[c;R];[c;R];[c;R]:1[N;R0][C;R0])[c;R]2:[s;R];[c;R];[c;R];[c;R]:2[C;R0]
169	[O;R0][c;R]1:[n;R];[c;R]2:[c;R];[c;R];[c;R];[c;R]:2:[n;R]:1[C;R0][C;R0][C;R0][N;R]3[C;R][C;R][C;R]([C;R0][c;R]4:[c;R];[c;R];[c;R];[c;R]:4)[C;R][C;R]3
170	[N;R0]([C;R0][C;R]1[C;R][C;R][N;R]([C;R0][C;R0][C;R0][c;R]2:[c;R];[c;R];[c;R];[c;R]:2)[C;R][C;R]1)[c;R]3:[n;R];[c;R];[c;R];[c;R]:[n;R]:3
171	[O;R0][C;R0](=[O;R0])[C;R]1[C;R][C;R]([C;R0][c;R]2:[n;R];[n;R];[n;R]:2)[C;R][C;R][N;R]1
172	[O;R0][C;R0]([C;R0]([N;R0])[C;R0][c;R]1:[c;R]([O;R0]):[n;R];[o;R]:[c;R]:1-[c;R]2:[c;R];[c;R];[c;R];[c;R]:[n;R]:2)=[O;R0]
173	[O;R0]=[S;R0]([N;R0][C;R0][C;R0]([C;R0])[c;R]1:[c;R];[c;R];[c;R](:[c;R]:[c;R]:1)-[c;R]2:[c;R];[c;R];[s;R]:[c;R]:2)=[O;R0][C;R0]
174	[O;R0][C;R0]([C;R0]([N;R0])[C;R0][c;R]1:[c;R]([O;R0]):[n;R];[o;R]:[c;R]:1-[c;R]2:[o;R];[c;R];[c;R];[c;R]:2)=[O;R0]

Category: InwardlyRectifyingK⁺

Template_ID	TEMPLATE_SMARTS
175	[C;R0][C;R0]([O;R0])([C;R0](=[O;R0])[N;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[S;R0](=[O;R0])(=[O;R0])[N,C,R,R0][C;R0]
176	[N;R0]#[C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]2[O;R][C;R]([C;R0])([C;R0])[C;R]([C;R]([c;R]:2:[c;R]:1)[N;R]3[C;R][C;R][C;R]3=[O;R0])[O;R0]

Category: K⁺

Template_ID	TEMPLATE_SMARTS
177	[N;R0]([C;R0])[C;R0][C;R]1([C;R][C;R][C;R][C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
178	[N;R0][c;R]1:[c;R]:[c;R]:[c;R]([c;R]:[c;R]:1)-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
179	[N;R0]#[C;R0][c;R]1:[c;R]2:[n;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:[n;R]:[c;R]:1
180	[N;R0]([C;R0])[C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1[O;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
181	[N;R0][C;R]1[C;R][C;R][N;R]([C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2)[C;R][C;R]1
182	[N;R0][c;R]1:[n;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:[n;R]:1
183	[N;R0]([C;R0])[C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
184	[O;R0]=[S;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:1)(=[O;R0])[N;R]2[C;R][C;R][N;R][C;R][C;R]2
185	[O;R0]=[C;R0]([N;R0][C;R0][C;R]1[C;R][C;R][N;R]([C;R0])[C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
186	[O;R0]=[C;R0][N;R]1[C;R][C;R][N;R]([C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
187	[O;R0]=[C;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:1)[N;R0][C;R0][C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
188	[O;R0]=[C;R0][N;R0][C;R]1[C;R]([N;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2[C;R](=[N;R]1)[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:3)=[O;R0]
189	[O;R0][C;R]1[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[C;R][C;R][C;R]1
190	[N;R0]([C;R0])[C;R0][C;R0][C;R0]([O;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
191	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1[O;R0][C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
192	[N;R0]([C;R0][C;R0][C;R0][C;R0])[S;R0](=[O;R0])(=[O;R0])[c;R]1:[c;R]:[c;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:[c;R]:1
193	[O;R0]=[C;R0][C;R]1=[C;R]([C;R0])[N;R][c;R]2:[c;R]:[c;R]:[n;R]:[n;R]:2[C;R]1
194	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]([O;R0][C;R0][C;R0][N;R]2[C;R][C;R][C;R][C;R]2):[c;R]:[c;R]:1
195	[O;R0]=[C;R0]([N;R]1[C;R][C;R][N;R][C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
196	[O;R0]=[C;R]1[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[C;R][C;R][C;R]1[C;R0]
197	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]([C;R0][N;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[n;R]:2):[c;R]:[c;R]:1

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198	[N;R0]([C;R0])[C;R]1[C;R][C;R][N;R]([C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[n;R]:2
199	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1[O;R0][C;R0][C;R0][N;R]2[C;R][C;R][C;R][C;R]2
200	[O;R0]=[C;R]1[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[N;R]=[C;R][N;R]1
201	[N;R0][c;R]1:[c;R]:[c;R]([N;R]2[C;R][C;R][C;R][C;R][C;R]2):[n;R]:[c;R]:[c;R]:1
202	[O;R0]=[C;R0][N;R0][C;R0]([C;R0][C;R0][N;R]1[C;R][C;R][C;R][C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
203	[O;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[C;R0][c;R]2:[n;R]:[o;R]:[c;R](:[n;R]:2)-[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3
204	[O;R0]=[C;R]1[N;R][C;R][C;R][N;R]1[C;R0][C;R0][N;R]2[C;R][C;R][C;R][C;R][C;R]2
205	[N;R0][C;R0][C;R]1([C;R][C;R][N;R][C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
206	[O;R0]([C;R0][c;R]1:[n;R]:[c;R](-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2):[s;R]:[c;R]:1)[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3[C;R0]
207	[O;R0]=[C;R0]([N;R]1[C;R][C;R][C;R][C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
208	[O;R0]=[C;R]1[N;R]([C;R]2[C;R][C;R][N;R][C;R][C;R]2)[c;R]:[c;R][N;R]1
209	[O;R0][C;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[C;R]2[C;R][C;R][N;R]([C;R0][C;R0])[C;R][C;R]2
210	[O;R0]([c;R]1:[c;R]:[c;R]2[C;R]([N;R]([C;R][C;R][c;R]:2:[c;R]:[c;R]:1[O;R0][C;R0])[C;R0])[C;R0])[C;R0]
211	[N;R0][C;R]1[C;R][N;R]([C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2)[C;R][C;R]1
212	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1[O;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
213	[N;R0]([c;R]1:[n;R]:[c;R]:[c;R]:[c;R](-[c;R]2:[c;R]:[n;R]:[c;R](:[n;R]:2[C;R0]([C;R0])[C;R0]):[n;R]:1)[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3
214	[O;R0]=[S;R0](=[O;R0])[c;R]1:[c;R]:[c;R]:[c;R]2[C;R][C;R][N;R][C;R][C;R]:2:[c;R]:1
215	[N;R0]([C;R0])[C;R0](=[O;R0])[c;R]1:[c;R]([N;R0][C;R0]):[n;R]:[c;R](:[n;R]:[c;R]:1[O;R0][C;R0][C;R]2[C;R][C;R][N;R][C;R][C;R]2)[C;R0]#[N;R0]
216	[O;R0]=[C;R]1[c;R]2:[c;R]:[c;R]:[c;R]([O;R0][C;R0]):[c;R]:[c;R]:2[C;R](=[C;R]([N;R]1[C;R0])[C;R0])[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3
217	[O;R0]=[C;R0][N;R0]([C;R]1[C;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[C;R][C;R]1)[C;R0]
218	[O;R0]=[S;R0]([c;R]1:[c;R]:[c;R]:[c;R]([C;R0]=[C;R0]):[n;R]:[c;R]:1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
219	[O;R0]=[C;R0]([C;R0][N;R0][c;R]1:[c;R]:[c;R](:[n;R]:[c;R](:[n;R]:1)-[c;R]2:[o;R]:[c;R]([C;R0]):[c;R]:[c;R]:2)-[n;R]3:[n;R]:[c;R]([C;R0]):[c;R]:[c;R]:3[C;R0])
220	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]2[C;R][C;R]([C;R0][C;R0][N;R]3[C;R][C;R][C;R]([C;R][C;R]3)[c;R]4:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:4)[C;R][C;R][c;R]:2:[c;R]:1
221	[O;R0]=[C;R0][N;R]1[C;R][C;R](=[C;R][C;R]1[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2)[c;R]3:[c;R]:[c;R]([F;R0]):[c;R]:[c;R]:[c;R]:3[F;R0]
222	[O;R0]=[S;R0](=[O;R0])([C;R]1[C;R][C;R][N;R]([C;R0][C;R0])[C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
223	[O;R0]=[C;R0][N;R0][c;R]1:[c;R]:[c;R]:[c;R]2[C;R][C;R][C;R][C;R]([N;R0][S;R0]([c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3)(=[O;R0]=[O;R0])[c;R]:2:[c;R]:1

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224	[O;R0]=[S;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)(=[O;R0])[N;R0][C;R]2[C;R][C;R]([C;R0])([C;R0])[O;R][c;R]:[c;R]2
225	[O;R0]=[S;R0]([N;R0][C;R]1[C;R]([O;R0])[C;R]([C;R0])([C;R0])[O;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]1:2)=[O;R0]
226	[O;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[C;R0][N;R0][C;R]2[C;R][C;R][C;R][N;R][C;R]2[C;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]3)[C;R0]([F;R0])([F;R0])[F;R0]
227	[N;R0][C;R]1[C;R][C;R][N;R]([C;R]2[C;R][C;R][N;R]([C;R0]=[O;R0])[C;R][C;R]2)[C;R][C;R]1
228	[O;R0]=[C;R]1[C;R][N;R]([C;R][C;R][N;R]1[C;R]2[C;R][c;R]3:[c;R]:[c;R]:[c;R]([C;R0]):[c;R]:[c;R]:3[C;R][C;R]2)[C;R0][C;R0]
229	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]([N;R0][c;R]2:[n;R]:[c;R]:[n;R]:[c;R]3:[c;R]:[c;R]:[c;R]([O;R0]):[c;R]:2:3):[c;R]:[c;R]:1
230	[O;R0]=[C;R0][C;R0]([N;R0])[C;R]1[C;R][C;R][C;R]([C;R][C;R]1)[N;R0][S;R0]([O;R0])(=[O;R0])[c;R]2:[c;R]:[c;R]:[c;R]([O;R0][C;R0]([F;R0])([F;R0])[F;R0]):[c;R]:[c;R]:2
231	[N;R0]([C;R0])[C;R]1[C;R][C;R][N;R]([C;R][C;R]1)[c;R]2:[n;R]:[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3:[n;R]:2[C;R0][c;R]4:[c;R]:[c;R]:[c;R]([F;R0]):[c;R]:[c;R]:4
232	[O;R0][C;R0]([C;R0])[c;R]1:[c;R]:[n;R](-[c;R]2:[c;R]:[c;R]:[c;R]([F;R0]):[c;R]:[c;R]:2):[c;R]3:[c;R]:[c;R]:[c;R]([Cl;R0]):[c;R]:[c;R]:1:3
233	[N;R0][C;R0]([C;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)-[c;R]2:[c;R]:[c;R]:[c;R]([F;R0]):[c;R]:[c;R]:2)[C;R0]([O;R0])[N;R]3[C;R][C;R]([F;R0])[C;R]3
234	[O;R0]([C;R0][C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:1)[C;R]2[C;R][C;R][C;R][C;R]2[N;R]3[C;R][C;R][O;R][C;R][C;R]3
235	[O;R0]=[C;R0][N;R0][C;R0][C;R0][c;R]1:[c;R]:[c;R]:[c;R]([c;R]:[c;R]:1)[S;R0]([O;R0])(=[O;R0])[N;R0][C;R0]([O;R0])[N;R0][C;R]2[C;R][C;R][C;R][C;R]2
236	[N;R0][C;R0][c;R]1:[n;R]:[n;R]([c;R]:[c;R]:1[C;R0])-[c;R]2:[c;R]:[c;R]:[c;R]([Cl;R0]):[c;R]:[c;R]:2[Cl;R0]
237	[O;R0]=[C;R0]([N;R]1[C;R][C;R][S;R][C;R]1[c;R]2:[c;R]:[c;R]:[c;R]([C;R0]):[c;R]([c;R]:2)[C;R0])[C;R0]
238	[O;R0]([C;R]1[C;R][C;R][C;R][C;R]1)[C;R0][C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:3
239	[N;R0]([C;R0][c;R]1:[c;R]([c;R](-[c;R]2:[c;R]:[n;R]:[c;R]:[c;R]:[c;R]:2):[n;R]:[n;R]:1)[C;R0])[C;R]3[C;R][C;R][C;R]3
240	[O;R0][C;R0][C;R]1[C;R][C;R][C;R][N;R]([C;R0][C;R0][C;R0][C;R]2[C;R][C;R][C;R]3:[c;R]:[c;R]:[c;R]([O;R0][C;R0]):[c;R]:[c;R]2:3)[C;R]1
241	[N;R0][C;R0][c;R]1:[n;R]:[c;R]:[c;R]2:[c;R]:[c;R]:[c;R]([O;R0][C;R0]):[c;R]:[c;R]:2:[c;R]:1-[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:3
242	[N;R0]([C;R0]([C;R0]([C;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[c;R]2:[c;R]:[c;R]:[c;R]:[n;R]:[c;R]:2)=[O;R0])([C;R0]([C;R0])[C;R0][C;R0]([C;R0])[C;R0]

Category: Na⁺

Template_ID	TEMPLATE_SMARTS
243	[O;R0]([C;R0])[c;R]1:[c;R]:[c;R]:[c;R]([C;R0][N;R]2[C;R][C;R][N;R]([C;R][C;R]2)[C;R0]):[c;R]:[c;R]:1
244	[N;R0][c;R]1:[n;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:[s;R]:1
245	[O;R0]=[C;R0][c;R]1:[o;R]:[c;R](-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2):[c;R]:[c;R]:1

Template_ID	TEMPLATE_SMARTS
246	[c;R]1:[n;R]:[c;R]:([c;R]:[n;R]:1)-[c;R]2:[c;R]:[c;R]:[c;R]:([c;R]:[c;R]:2)-[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3
247	[N;R0][C;R0]([C;R0][O;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
248	[O;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[c;R]2:[c;R]:[c;R]:[c;R]:([c;R]:[c;R]:2)-[c;R]3:[c;R]:[c;R]:[n;R]:[n;R]:3
249	[O;R0]=[C;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1[O;R0][C;R0])[N;R]2[C;R][C;R][C;R]2
250	[O;R0][C;R0]([C;R0][N;R]1[C;R][C;R][C;R][C;R]1)[C;R0][O;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
251	[O;R0]=[C;R0][N;R0][C;R0][c;R]1:[c;R]:[c;R]:[c;R]:([s;R]:1)-[c;R]2:[c;R]:[c;R]:[c;R]:[s;R]:2
252	[N;R0][C;R0][c;R]1:[c;R]:[c;R]:[c;R]:([c;R]:[c;R]:1)-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
253	[O;R0][C;R0]([C;R0][N;R]1[C;R][C;R][N;R]([C;R][C;R]1)[C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2)[C;R0]
254	[N;R0][C;R0][c;R]1:[n;R]:[o;R]:[c;R]:([n;R]:1)-[c;R]2:[n;R]:[n;R]:[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:3
255	[N;R]1[C;R](=[O;R0])[C;R]([N;R0][C;R0](=[O;R0])[C;R0][N;R0])[N;R]=[C;R]([c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2)[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:31
256	[O;R0][C;R0]([C;R0][C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[C;R]2[C;R][C;R][C;R]2[C;R0]
257	[N;R0][C;R0]([C;R0][N;R0][C;R]1[C;R][N;R]([C;R0])[c;R]:[c;R][C;R][C;R]1)[C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
258	[N;R0]([C;R0]=[O;R0])[C;R0]([C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[C;R0](=[O;R0])[N;R0][C;R0][c;R]2:[n;R]:[c;R]3:[c;R]:[c;R]:[c;R]:[n;R]:[c;R]:3:[n;R]:2

Category: Purinoceptors

Template_ID	TEMPLATE_SMARTS
259	[O;R0]=[C;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1[C;R0])[N;R0][C;R0][C;R]23[C;R][C;R]4[C;R][C;R]([C;R][C;R]([C;R]4)[C;R]2)[C;R]3
260	[N;R0]([C;R0][C;R0])[S;R0](=[O;R0])(=[O;R0])[c;R]1:[c;R]:[c;R]:[c;R]:[c;R]2:[c;R]:[n;R]:[c;R]:[c;R]:[c;R]:1:2

Category: Sulfonylurea

Template_ID	TEMPLATE_SMARTS
261	[O;R0]=[S;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)(=[O;R0])[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
262	[C;R0][C;R0]([O;R0])([C;R0](=[O;R0])[N;R0][c;R]1:[c;R]:[c;R]:[c;R]:([c;R]:[c;R]:1)[S;R0](=[O;R0])(=[O;R0])[N;R,R0])[C;R0]([F;R0])([F;R0])[F;R0]
263	[O;R0][C;R]1[C;R][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[O;R][C;R]1([C;R0])[C;R0]

Category: Transient receptor potential

Template_ID	TEMPLATE_SMARTS

Template_ID	TEMPLATE_SMARTS
264	[O;R0]=[C;R0][N;R0][C;R0][C;R0][c;R]1:[c;R]:[n;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1:2
265	[O;R0]=[C;R0][N;R0][c;R]1:[n;R]:[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2:[s;R]:1
266	[O;R0]=[C;R0][N;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]2:[c;R]:[n;R]:[c;R]:[c;R]:[c;R]:1:2
267	[O;R0]=[C;R0]([N;R0][C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:1)[N;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
268	[O;R0][c;R]1:[c;R]:[c;R](-[c;R]2:[c;R]:[c;R]:[c;R]([C;R0]):[c;R]:[c;R]:2):[n;R]:[c;R]:[n;R]:1
269	[O;R0]=[C;R0]([N;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:1)[N;R]2[C;R][C;R][N;R][C;R][C;R]2
270	[N;R0][C;R0](=[O;R0])[N;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]2:[n;R]:[n;R]:[c;R]:[c;R]:1:2
271	[N;R0][C;R0](=[O;R0])[N;R]1[C;R][C;R][N;R]([C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[n;R]:2
272	[N;R0][C;R0](=[O;R0])[C;R]1[C;R][C;R][N;R]([C;R][C;R]1)[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2
273	[O;R0]=[C;R0]([N;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:1)[C;R]2[C;R][C;R][N;R][C;R][C;R]2
274	[O;R0]=[C;R0]([N;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:1)[C;R]2=[C;R][C;R][N;R][C;R][C;R]2
275	[O;R0][c;R]1:[c;R]:[c;R]:[c;R](-[c;R]:[c;R]:1)[C;R0][N;R0][C;R0][C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
276	[O;R0]=[C;R0]([c;R]1:[n;R]:[c;R]:[s;R]:[c;R]:1)[N;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
277	[N;R0]([c;R]1:[c;R]:[c;R](-[c;R]2:[c;R]:[c;R]:[c;R]([C;R0]):[c;R]:[c;R]:2):[n;R]:[c;R]:[n;R]:1)[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:3
278	[O;R0]=[C;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:1)[N;R0][c;R]2:[c;R]:[c;R]:[c;R]:[n;R]:[c;R]:2
279	[N;R0][c;R]1:[c;R]:[c;R]:[c;R]2[O;R][C;R][C;R][O;R][c;R]:2:[c;R]:1
280	[N;R0][C;R0]([c;R]1:[n;R]:[c;R]([C;R0][c;R]2:[c;R](-[c;R]:[c;R]:[c;R]:[c;R]:2[Cl;R0])[Cl;R0]):[s;R]:[c;R]:1)=[O;R0]
281	[O;R0]=[C;R0]([N;R0][C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:1)[C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
282	[O;R0]=[C;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[n;R]:1)[N;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
283	[O;R0]([c;R]1:[c;R]:[c;R]2:[n;R]:[c;R]:[n;R]:[c;R]:2:[c;R]:[c;R]:1)[C;R0]
284	[c;R]1:[c;R]:[c;R]:[c;R]([N;R0][C;R0](=[O;R0])[c;R]2:[c;R]:[n;R]:[c;R]([C;R0][c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:3):[n;R]:2):[c;R]:[c;R]:1
285	[O;R0]=[C;R0]([N;R]1[C;R][C;R][C;R][C;R]1)[N;R0][c;R]2:[c;R]:[c;R]:[c;R](-[c;R]:[c;R]:2)[C;R0]([F;R0])([F;R0])[F;R0]
286	[O;R0]=[C;R0]([c;R]1:[c;R]:[c;R]:[c;R]:[n;R]:1)[N;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
287	[N;R0]#[C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[n;R]:[c;R]:1[N;R]2[C;R][C;R][N;R][C;R][C;R]2
288	[O;R0]=[C;R0]([N;R0][C;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:1)[N;R0][C;R0][c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:2
289	[c;R]1:[c;R]:[c;R]:[c;R](-[c;R]:[c;R]:1)-[c;R]2:[n;R]:[c;R]3:[c;R]:[c;R](-[c;R]:[c;R]:[c;R]:3:[n;R]:2)-[c;R]4:[n;R]:[c;R]:[c;R]:[c;R]:4
290	[O;R0]=[C;R0]([c;R]1:[c;R]:[c;R]:[c;R]([O;R0][C;R0]([F;R0])([F;R0])[F;R0]):[c;R]:[c;R]:1)[N;R0][C;R0][C;R0][N;R]2[C;R][C;R][C;R]3:[c;R]:[c;R]:[c;R]:[c;R]:2:3

Template_ID	TEMPLATE_SMARTS
291	[O;R0][c;R]1:[c;R]:[c;R]:[n;R]:[n;R]:1-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[C;R0]([F;R0])([F;R0])[F;R0]
292	[N;R0][C;R0]([N;R]1[C;R][C;R][N;R]([c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[C;R0]([F;R0])([F;R0])[F;R0])[C;R][C;R]1)=[O;R0]
293	[O;R0][c;R]1:[c;R]:[c;R]:[c;R]:[c;R]:[c;R](-[c;R]2:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:2[C;R0]([C;R0])[C;R0]):[c;R]:1
294	[O;R0][c;R]1:[n;R]:[c;R]:[n;R]:[c;R]2:[c;R]:[c;R]([C;R0]([C;R0])[C;R0]):[c;R]:[c;R]:[c;R]:1:2-[c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3
295	[c;R]1:[c;R]:[c;R]:[c;R]2:[n;R]:[c;R](:[n;R]:[c;R]:2:[c;R]:1)[N;R]3[C;R][C;R][N;R][C;R][C;R]3[a,A]
296	[N;R0][c;R]1:[c;R]2:[n;R]:[c;R]([N;R0][c;R]3:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:[c;R]:3):[s;R]:[c;R]:2:[n;R]:[c;R]:[n;R]:1
297	[N;R0][c;R]1:[n;R]:[c;R]2:[c;R]([O;R0][c;R]3:[c;R]:[c;R]:[n;R]:[c;R]:[n;R]:3):[c;R]:[c;R]:[c;R]:[c;R]:2:[s;R]:1