CPCA Scoring

CPCA Classification ver.
Name of the product: XXXXXXX
Writer: YYYYYY

Paste the structure of the compound *

* For chemical information and draw structure (https://pubchem.ncbi.nlm.nih.go

Credit: Yosuke Mino & Lucas Mauriz

Please input the information of the product in the boxes.

1.Does N-Nitrosamine have any hydrogens on its α-carbons?

2.Does N-Nitrosamine have more than one α-hydrogen on one or both sides of N-nitroso group?

3.Does N-Nitrosamine have a tertiary α-carbon?

Category:
AI = ng/day

4. Please check the following features included in the compounds.

4-1. alfa-Hydrogen Score

What count of Hydrogen Atoms on Each alfa-carbon, Lowest First?

Score:

4-2. Deactivating Feature Score

Carboxylic acid group anywhere on molecule?

Score:

What ring system is included?

Score:

Chains of ≥5 consecutive non-hydrogen atoms (cyclic or acyclic) on both side of acyclic N-nitroso group?
Not more than 4 atoms in each chain may be in the same ring?

Score:

Electron-withdrawing group** bonded to α-carbon of N-nitroso group (cyclic or acyclic)?

Score:

Hydroxyl group bonded to β-carbon*** of N-nitroso group (cyclic or acyclic)?

Score:

4-3. Activating Feature Score

Aryl group bonded to α-carbon (i.e., benzylic or pseudo-benzylic substituent on N-nitroso group

Score:

Methyl group bonded to β-carbon (cyclic or acyclic)?

Score:

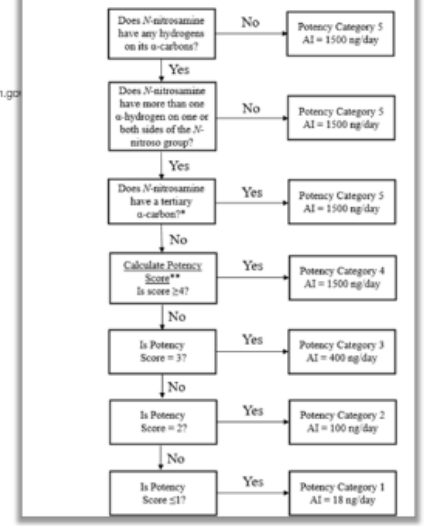
Potency Score:

Category:
AI = ng/day

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CPCA Workflow

Figure 2. Flowchart to Predict the Potency Category of an *N*-nitrosamine



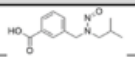
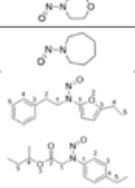
alfa-Hydrogen Score

Table 2. Count of hydrogen atoms on each α-carbon (lowest count first) and corresponding α-Hydrogen Score. Examples are intended to be illustrative only and are not intended to be exhaustive.

Count of Hydrogen Atoms on Each α-Carbon, Lowest First	Example	α-Hydrogen Score
0,2		3*
0,3		2
1,2		3
1,3		3
2,2		1
2,3		1

*A score of 3 applies when the methylene α-carbon is not part of an ethyl group. If the methylene α-carbon is part of an ethyl group, a score of 2 should be applied.

Deactivating Feature Score

Deactivating Feature	Example	Individual Deactivating Feature Score
Carboxylic acid group anywhere on molecule		+3
N-nitroso group in a pyrrolidine ring		+3
N-nitroso group in a 6-membered ring containing at least one sulfur atom		+3
N-nitroso group in a 5- or 6-membered ring*		+2
N-nitroso group in a morpholine ring		+1
N-nitroso group in a 7-membered ring		+1
Chains of ≥5 consecutive non-hydrogen atoms (cyclic or acyclic) on both side of acyclic *N*-nitroso group. Not more than 4 atoms in each chain may be in the same ring.		+1
Electron-withdrawing group** bonded to α-carbon on only one side of *N*-nitroso group (cyclic or acyclic)		+1
Electron-withdrawing groups** bonded to α-carbons on both sides of *N*-nitroso group (cyclic or acyclic)		+2
Hydroxyl group bonded to β-carbon*** on only one side of *N*-nitroso group (cyclic or acyclic)		+1
Hydroxyl group bonded to β-carbons*** on both sides of *N*-nitroso group (cyclic or acyclic)		+2

Activating Feature Score

Activating Feature	Example	Individual Activating Feature Score
Aryl group bonded to α-carbon (i.e., benzylic or pseudo-benzylic substituent on *N*-nitroso group)		-1
Methyl group bonded to β-carbon (cyclic or acyclic)		-1