DATABASE FOR NITROSAMINES DETECTION IN MARS

File name: db_nitrosamines_20240531
Number of compounds: 28,024
Classification: two classes (linear nitrosamines, cyclic nitrosamines)
Number of MS/MS spectra: 28,024
Type of MS/MS spectra: rule-based fragmentation (virtual)

Details: The database contains the structure, formula, exact mass, MS1, and MS2 information for 28,024 nitrosamines. Both linear and cyclic nitrosamines are included in the database. In particular, the linear nitrosamines included in the database are 27,856, while the cyclic nitrosamines are 168.

Nitrosamines compounds derives from different data sources:

1. nitrosamines reported by Regulatory Agencies (e.g., EMA and FDA);
2. nitrosamines distributed by commercial suppliers;
3. nitrosamines generated in-silico.

Table 1. Number of entries included in the database from the different sources

Source	Entries
Regulatory Agencies	141
Commercial suppliers	209
In silico generation	27,674
	Total number: 28,024

Nomenclature assignation: an identification code (ID) consisting of an alphanumeric string of two letters and 7 number (i.e., NA0000001, NA0000002, NA0000003, etc.) is assigned to each nitrosamine in the database. In addition, a common name is associated to each compound. The schematic common name for linear nitrosamines is NO(N-X/N-Y) where X and Y can represent:

1. aliphatic chains bonded to the *N*-nitroso group. Aliphatic chains are represented in the common name as "C:DB" where C is the number of carbon and DB is the number of double bonds in the chains. Example for *N*-nethylethylamine (NMEA), common name: NO(N-1:0/N-2:0).

2. substituent different from aliphatic chains bonded to the *N*-nitroso group. This kind of substituents are represented in the common name with an alphanumeric string. Example for *N*-nitrosodiphenylamine (NDPhA), common name: NO(N-Ph/N-Ph).

In contrast, the schematic common name for cyclic nitrosamines is NO(C-Z), where Z is an alpha-numeric string. Example for *N*-nitrosomorpholine (NMOR), common name: NO(C-MOR); *N*-nitrosopiperidine (NPIP), common name: NO(C-PIP); and *N*-nitrosopyrrolidine (NPYR), common name: NO(C-PYR).

Fragmentation rules: fragmentation rules was coded from experimental fragmentation of nitrosamines collected from literature[1-3] and from *in-house* acquired data.

References

1. Lijinsky, W., Chemistry and biology of N-nitroso compounds. Cambridge University Press: 1992.
2. Zhao, Y. Y.; Boyd, J.; Hrudey, S. E.; Li, X. F., Characterization of new nitrosamines in drinking water using liquid chromatography tandem mass spectrometry. Environ Sci Technol 2006, 40 (24), 7636-41.
3. Asare, S. O.; Hoskins, J. N.; Blessing, R. A.; Hertzler, R. L., Mass spectrometry based fragmentation patterns of nitrosamine compounds. Rapid Commun Mass Spectrom 2022, 36 (8), e9261