

NEUROTOXKB

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NeurotoxKB is an important class of hazardous chemicals. They are a significant concern due to the kind of damage they can cause in the body. Neurological damage is often irreversible, hence any exposure to potential neurotoxins is a severe concern. We built NeurotoxKB as a resource to assist in the identification of potential neurotoxins, compile the data necessary for research and informed policy decisions, and aid in the environmental monitoring of neurotoxins. We have compiled and curated potential neurotoxins among environmental chemicals from four well-established lists, namely, US EPA report (1976), Mundy et al (2015), Auer et al (2016), and Grandjean and Landrigan (2014) on neurotoxins. The chemicals from these four lists have been filtered based on their experimental evidence for neurotoxicity, the target organ, and the origin of the chemical (biological or xenobiotic).

Simple search

Physicochemical filter

Chemical similarity filter

Chemical name

For example: 'Malathion'

Chemical identifier (PubChem or CAS)

For example: '58-89-9' or '991'

Search

Simple search

Physicochemical filter

Chemical similarity filter

Molecular weight

Choose here

LogP

Choose here

TPSA

Choose here

Hydrogen bond acceptors (HBA)

Choose here

Hydrogen bond donors (HBD)

Choose here

Heavy atoms

Choose here

Heteroatoms

Choose here

Rotatable bonds

Choose here

Search

Simple search

Physicochemical filter

Chemical similarity filter

Enter SMILES

Search

Choose fingerprint

Choose here

Environmental source

Chemical classification

Presence in chemical regulation or guideline

Presence in human biospecimen

6 BROAD CATEGORIES

Agriculture and farming

Consumer products

Industry

Intermediates

Medicine and healthcare

Pollutant

41 SUB-CATEGORIES

