ISSTOX Guidance for use:

Each toxicological endpoint is represented by a separate database. Each database consists of three files, that can be downloaded separately (e.g., ***ISSCAN_vvv_nnn_ddddddd.xls***, ***ISSCAN_vvv_nnn_ddddddd.pdf***, ***ISSCAN_vvv_nnn_ddddddd.sdf)***.

The file names provide information on the version number, the number of chemicals, and the date. For example, ***ISSCAN_v1a_774_10Dec04.xls*** is version v1a, contains 774 chemicals, and was prepared on December 10, 2004.

The file ***ISSCAN_vvv_nnn_ddddddd.xls*** can be read with the program Microsoft Excel. For each chemical, it reports various identifiers together with the toxicological data.

The file ***ISSCAN_vvv_nnn_ddddddd.pdf*** can be read with the program Adobe Acrobat Reader, and reports the 2D chemical structure.

The file ***ISSCAN_vvv_nnn_ddddddd.sdf*** can be read with a series of specialized programs. In addition to the information reported in the file ***ISSCAN_vvv_nnn_ddddddd.xls***, it contains the chemical structures in the format .sdf (structure-data file).

This database can be used for different purposes. As basic application, the .xls file can be searched through names (and synonyms), and CAS number. The chemical structures, in the common graphical format can be found in the file .pdf.

A specific characteristic of these databases is that the chemical structures are coded both in the SMILES and .sdf formats. These codes can be read by a series of specialized programs (e.g., Chemoffice, Sybyl, Maestro, Insight II, Tsar, Daylight Toolkits, etc…). Their capabilities range from e.g., 3D visualization, to the calculation of molecular properties and descriptors that can be used in the study of the relationships between chemical structure and biological activity (Quantitative Structure-Activity Relationships, QSAR).

In addition, particularly important for the role of these databases as decision support system is the possibility of searching by substructures and functional groups, and of reading them as relational databases. This permits the combination of chemical with biological interrogations. For this goal, the file .sdf has to be read with Chemical Relational Database (CRD) programs (e.g., Leadscope, Chemfolder, Hyleos).

More information on the above programs and on the concept of Chemical Relational Databases can be found in the DSSTox site(http://www.epa.gov/nheerl/dsstox/).

Important: The commercial programs cited above should not be considered as endorsed by this project team. They are listed only for information, in no preference order, and as examples of a wider range of programs.

Disclaimer and a cautionary word

The information contained in these databases has been carefully checked, and, when existing, more sources have been considered and compared. However, the project team cannot guarantee accuracy, and will appreciate any suggestion to improve the database.

For particularly significant uses (e.g., regulatory activity), the user is invited to examine the original source of data, and consider that the summary, final outcome of a toxicological assay is usually a simplification of a large and articulated amount of experimental results.

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