

Retrieving Toxicity Data

This module introduces new users to the Toxicity database and the Toxicity Finder application. Participants conduct structure and data searches to retrieve the toxicity data of interest. Using the links to the Metabolite Browser and the LitLink service, participants also learn how to retrieve related metabolic data and reference publications.

Course Objectives

The participant will be able to:

- ◆ Conduct structure and data searches using the Toxicity Finder
- ◆ View chemical, toxicity, and review article data
- ◆ Save, combine, and print search results
- ◆ Connect to the Metabolite Browser and view related metabolic data
- ◆ Connect to the LitLink online service and retrieve related literature references

Prerequisites

None

Course Length

1 day

Examples from the Class

Toxicity Data browse form

The screenshot shows a web-based interface for viewing toxicity data. At the top, there are navigation buttons: 'Forms', 'Query', 'Browse', and 'Update'. Below this, a search bar contains the text '<CHEMICAL>' and '1 of 32'. The main content area is divided into several sections: 'Chemical', 'Toxicity Data', and 'Review'. The 'Toxicity Data' section is currently active, showing a list of search results. The first result is for a chemical with the name 'Trichlohe... 8-ene-3-alpha,4-beta,8-alpha,15-tetra... 12,13-digono... 4,15-Diacetoxy-8-(3-methylbutyryloxy)-12,13-epoxy-4-... 4-beta,15-Diacetoxy-8-alpha-(3-methylbutyryloxy)-3-alpha-hydro...'. Below the name, there are fields for 'RTECS', 'Acute Toxicity', 'Species or Organism Tested' (rat), 'Route of Exposure' (intratracheal), 'Exposure Concentration or Dose' (4 mg/kg), and 'Endpoint' (LD50). A 'Toxic Effects' section lists 'Acute pulmonary edema', 'Other changes (endocrine)', and 'Hemorrhage (blood)'. A 'Select Data Type' dialog box is open over the main content, with the title 'Select Toxicity Data Type'. It contains a list of options: 'Acute Toxicity', 'Mutagenicity', 'Skin/Eye Irritation', 'Tumorigenicity', 'Reproductive Effects', and 'Other Multiple Doses'. The 'OK' and 'Cancel' buttons are at the bottom of the dialog.

Toxicity to Metabolite link

The screenshot shows a web-based interface for linking toxicity data to metabolite data. At the top, there are navigation buttons: 'Chemical', 'Toxicity Data', and 'Review'. The main content area is divided into several sections: 'Chemical', 'Toxicity Data', and 'Review'. The 'Toxicity Data' section is currently active, showing a list of search results. The first result is for a chemical with the name 'C₁₃H₁₁N₃'. Below the name, there are fields for 'Molecular Weight' (209.2510), 'CAS Registry Number' (92-62-6), and 'Beilstein Number' (0166950). A 'Metabolite data' section is visible, showing a transformation from the parent compound to a metabolite. The 'Parent' section shows the chemical structure and name 'Proflavine'. The 'Metabolite' section shows the chemical structure and name 'N-Glucuronidation'. A 'Toxicity/Metabolite Link button' is highlighted in red. Below the 'Metabolite data' section, there is a 'Full Citation' section with a list of references. The first reference is '1 of 3 Plakas, S. M., Said, K. R. E., Benicath, F. A., Mussier, S. M., Hayton, W. L.; Xenobiotica [ENGLAND] 1998, 28 (6), 605'. The second reference is '1 of 3 Pharmacokinetics, tissue distribution and metabolism of acriflavine and proflavine in the channel catfish (Ictalurus punctatus)'. The 'LitLink' button is also visible on the left side of the interface.