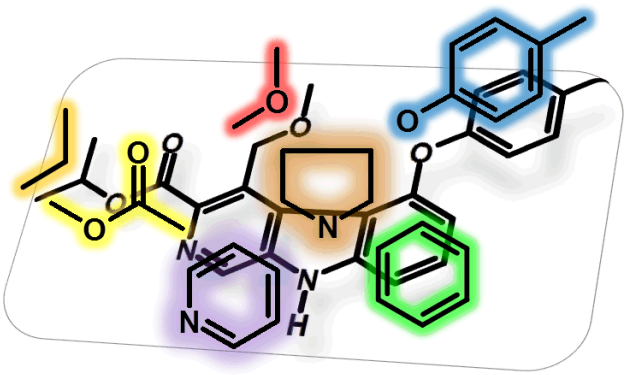
ChemoTyper

Chemotype Your Molecular Datasets

ChemoTyper is an interactive tool that enables the searching and highlighting of chemical chemotypes (substructures or subgraphs) in datasets of molecules for grouping, filtering and categorization purposes. **ChemoTyper** visualizes chemical structures (provided, e.g., in SD or SMILES format) and chemotypes that are stored in XML-based documents and specified in CSRML (Chemical Subgraph and Reaction Markup Language). The chemotype matches can be visually inspected by highlighted positive matches in the molecules color-coded by the corresponding chemotype.

ChemoTyper houses the ToxPrint chemotype library, a public set of chemotypes developed by Chihae Yang and Altamira LLC for the U.S. FDA, Center for Food Safety and Applied Nutrition (CFSAN), Office of Food Additive Safety (OFAS).



Chemical structures that match the same chemotypes can be exported as subsets in SD or text-based file formats and vice versa. Furthermore, **ChemoTyper** can be used for fingerprinting of chemical structures against chemotypes. The fingerprints are exported in a spreadsheet-compatible file format for further analysis.

Key Features

- Applicable to a broad range of chemical compound classes
- Fast and efficient performance and display of multiple chemotype matches
- Houses the ToxPrint chemotypes library containing over 700 predefined chemotypes
- Support by the MOSES chemoinformatics library for application of structural fragments (substructures) with embedded physicochemical properties (chemotypes)
- Several options to influence the filtering and subset generation process
- Fingerprinting against chemotypes

Areas of Application

- Predictive and computational toxicology
- Risk and safety assessment of chemical substances
- Profiling of chemical datasets, databases and inventories and subset generation
- Development of chemical categories and read-across applications
- Threshold of toxicological concern (TTC) applications
- Quantitative structure activity and property relationships (QSAR and QSPR)

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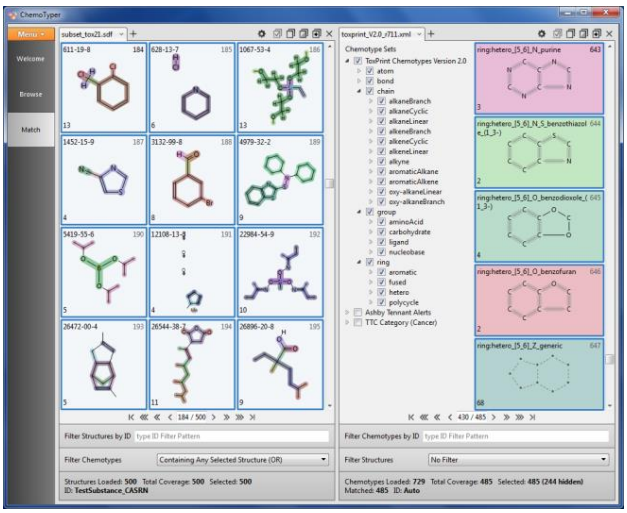
ChemoTyper provides an easy-to use graphical user interface. Structures and chemotypes are displayed in separate panels and the positive matches are highlighted by different colors. Chemotypes can be selected individually or by groups in a tree view organized in a chemically intuitive hierarchy.

A series of options enables the user to change the chemotype matching logic if multiple chemotypes are selected to fine-tune grouping or subset generation experiments.

The integrated ToxPrint chemotypes library covers the following areas of application.

- Generic fragments for atom, bond, ring, functional group types including regulatory structural categories, such as the FDA Redbook categories and EPA pesticide categories
- Structural alerts, such as genotoxic carcinogenicity (*e.g.*, Ashby-Tennant)
- TTC categories, such as cancer TTC categories



The ChemoTyper application was developed under a contract from the U.S. FDA, Center for Food Safety and Applied Nutrition (CFSAN), Office of Food Additive Safety.

Technical Features

- Graphical user interface
- Configurable user interface and chemical structure and chemotype display options
- CSRML reference implementation available for integration of chemotype matching procedure into own software applications

References

- C. Yang *et al. J. Chem. Inf. Model.* **2015**, *55*, 510-528 (DOI: 10.1021/ci500667v)
- A.M. Richard *et al. Chem. Res. Toxicol.* **2016**, *29*, 1225-1251 (DOI: 10.1021/acs.chemrestox.6b00135)

System Requirements

ChemoTyper is available for Microsoft® Windows® (7, 8, 10, 32 bit).

It is recommended to have the latest service pack installed.

Evaluation

ChemoTyper (including the CSRML reference implementation) can be downloaded free of charge at chemotyper.org after registration.

The ToxPrint chemotypes library can be downloaded free of charge at toxprint.org after registration.

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