



Chemotype Editor

Getting Started

September 2023

MN/AM Introduction & Installation

▶ ChemoType Editor

- ▷ Version 0.0.9
- ▷ October 19, 2020

▶ System requirements

- ▷ Windows 7/8/8.1/10 or later, 64bit
- ▷ Intel Pentium 4 processor or later, SSE2 capable

▶ Installation

- ▷ Copy the Windows ZIP file on your Windows computer, *e.g.*, on your desktop, and extract the ZIP file
- ▷ Open the newly generated directory "chemotype-editor-win32-x64.<versionNumber>" in the Windows Explorer
- ▷ Double-click the file "chemotype-editor.exe" to start the application

MN/AM Chemotype Editor

► Start page

The screenshot shows the MN/AM Chemotype Editor application window. The title bar reads "Chemotype Editor". The menu bar includes "Chemotype Editor", "Editor", and "Tools". On the right of the menu bar are icons for saving and an "About" button. Below the menu bar is a toolbar with various icons for creating and editing chemical structures, including a "NEW" button, a blue circle marker, and a blue square marker. To the left of the main canvas is a vertical sidebar with buttons for chemical elements: C, N, O, S, F, Cl, Br, I, P, and X. The main canvas is a large white area for sketching chemotypes. Below the canvas is a horizontal tab bar with the following tabs: "Atom query", "Bond query", "Molecule query", "Meta information", "Positive (0) and negative (0) examples", "CSRML", and "Logs". The "Atom query" tab is currently selected. A text box in the lower-left corner of the window provides instructions: "To add a query annotation to an atom, click on the marker symbol (blue circle) in the top button row of the editor above and then click on an atom to mark it."

Main window of editor

Molecule editor to sketch chemotypes

To add a query annotation to an atom, click on the marker symbol (blue circle) in the top button row of the editor above and then click on an atom to mark it.

MN/AM Chemotype Editor

► Load existing chemotype files

The screenshot displays the Chemotype Editor application window. The title bar reads "Chemotype Editor". The menu bar includes "Chemotype Editor", "Editor", and "Tools". On the right of the menu bar is an "About" button. Below the menu bar is a toolbar with various icons for editing and querying. A vertical sidebar on the left contains a list of chemical elements: C, N, O, S, F, Cl, Br, I, P, and X. The main workspace shows a file icon labeled "myChemotL..." with a "Move" button next to it. A blue line points from a text box to this icon. The text box contains the text: "Support of drag&drop of existing chemotype (CSRML) files". At the bottom of the window is a tabbed interface with the following tabs: "Atom query", "Bond query", "Molecule query", "Meta information", "Positive (0) and negative (0) examples", "CSRML", and "Logs". The "Atom query" tab is currently selected. A grey text box in the lower-left corner of the workspace contains the following text: "To add a query annotation to an atom, click on the marker symbol (blue circle) in the top button row of the editor above and then click on an atom to mark it."

Support of drag&drop of existing chemotype (CSRML) files

To add a query annotation to an atom, click on the marker symbol (blue circle) in the top button row of the editor above and then click on an atom to mark it.

- ▶ Copy & paste chemotype from ChemoTyper application

The screenshot displays two software interfaces. On the left is the 'Chemotype Editor' with a toolbar and a workspace showing a chemical structure. On the right is the 'ChemoTyper' application, which shows a grid of chemical structures and a list of chemotypes on the right side. A blue line connects the 'Copy Chemotype' button in the ChemoTyper interface to the 'Chemotype Editor' workspace, indicating the workflow for copying and pasting chemotypes.

Chemotype Editor

Editor Tools

Chemotype Editor

Copy chemotype from ChemoTyper application

ChemoTyper

Menu: subset tox21.sdf

Chemotype Sets

- ☒ ToxPrint Chemotypes Version ...
- ☒ atom
- ☒ element
- ☒ bond
- ☒ C#N
- ☒ C(-Z)-C-Q
- ☒ C(=O)N
- ☒ C(=O)O
- ☒ C=N
- ☒ C=O
- ☒ C=S
- ☒ CC(=O)C
- ☒ CN
- ☒ CNO
- ☒ COC
- ☒ COH
- ☒ CS
- ☒ CX
- ☒ N(=O)
- ☒ N(C)
- ☒ N=[N+]=[N-]
- ☒ N=C=O
- ☒ N=N

Chemotypes Loaded: 729 Total Coverage: 485 Selected: 729 ID: Auto

Paste (Ctrl-V) copied chemotype into Chemotype Editor

MN/AM Chemotype Editor

- ▶ Draw chemotype and edit atom query annotations

The screenshot displays the MN/AM Chemotype Editor software interface. At the top is a blue header bar with the title "Chemotype Editor" and tabs for "Editor" and "Tools". Below the header is a toolbar containing various icons for drawing and editing chemical structures. On the left side, there is a vertical element menu with buttons for Carbon (C), Nitrogen (N), Oxygen (O), Sulfur (S), Fluorine (F), Chlorine (Cl), Bromine (Br), Iodine (I), Phosphorus (P), and Xenon (X). The main workspace shows a chemical structure of an ether (CH₃-O-CH₂-) with a blue circle highlighting the terminal carbon atom. Two blue lines with text boxes provide instructions: one points to the toolbar and says "Draw chemotype", and the other points to the blue circle and says "Use marker (blue-colored circle) to select atom for query annotation". Below the workspace are three tabs: "Atom query", "Bond query", and "Molecule query". The "Atom query" tab is active, showing a query editor with a dropdown menu set to "And", two buttons labeled "+" and "+n", a checkbox for "Negate", a red circle icon, another "Negate" checkbox, and an "Edit me" button. A "Logs" panel is visible on the right side of the interface.

MN/AM Chemotype Editor

► Atom query annotations

The screenshot displays the MN/AM Chemotype Editor interface. At the top, there is a blue header bar with the title "Chemotype Editor" and tabs for "Editor" and "Tools". Below the header is a toolbar with various icons for creating and editing chemical structures. On the left side, there is a vertical menu with element symbols: C, N, O, S, F, Cl, Br, I, P, and X. The main workspace shows a chemical structure of a methoxy group (CH₃O-). Below the workspace, there are several tabs: "Atom query", "Bond query", "Molecule query", "Meta information", "Positive (0) and negative (0) examples", "CSRML", and "Logs". The "Atom query" tab is selected, and a sub-tab "Atom 4" is active. A pop-up window titled "Edit me" is open, showing fields for "Query feature label", "Atom type" (with a "Negate" checkbox), "CSRML query atom types" (with a list: *, A, R, Q, X, Z, E, M, G), "Aromaticity" (with radio buttons for "Not defined", "Aromatic", and "Aliphatic"), and "Formal charge" (with a "Negate" checkbox). A blue line points from the text "Click 'Edit me' to enter query annotations" to the "Edit me" button. Another blue line points from the text "Scroll down for more annotation fields" to the bottom of the "Edit me" window.

Chemotype Editor Editor Tools

Click "Edit me" to enter query annotations

Atom query Bond query Molecule query Meta information Positive (0) and negative (0) examples CSRML Logs

Atom 4

Edit me

Advanced

Query feature label

Atom type ☐ Negate

CSRML query atom types: *, A, R, Q, X, Z, E, M, G

Aromaticity: ☐ Not defined ☐ Aromatic ☐ Aliphatic

Formal charge ☐ Negate

Scroll down for more annotation fields

► Atom query annotations

Chemotype Editor

Atom query Bond query Molecule query Meta information Positive (0) and negative (0) examples CSRML Logs

Atom 4

☐ Negate And ☒ + ☒ +n - ☐ Negate

☒ Edit me ☐ Advanced

Query feature label

Atom type ☐ Negate
CSRML query atom types: *, A, R, Q, X, Z, E, M, G

Aromaticity: ☐ Not defined ☐ Aromatic ☐ Aliphatic

Formal charge ☐ Negate

Hydrogen count 2 ☐ Negate

Hetero atom count ☐ Negate

Ring membership: ☐ Not defined ☐ In ring ☐ Not in ring

Ring count ☐ Negate

Ring size ☐ Negate

Sum of bond order ☐ Negate

Neighbors count ☐ Negate

Enter, *e.g.*, "2" to specify the number of hydrogen atoms attached to query atom

► Atom query annotations from SMARTS

Chemotype Editor

Atom query Bond query Molecule query Meta information Positive (1) and negative (1) examples CSXML Logs

Atom 4

☒ Edit me

Atomic SMARTS input
[CH2]

Recursive SMARTS are not yet supported.

Query feature label

Atom type
C ☐ Negate

CSXML query atom types: *, A, R, Q, X, Z, E, M, G

Aromaticity: ☐ Not defined ☐ Aromatic ☒ Aliphatic

Formal charge ☐ Negate

Hydrogen count
2 ☐ Negate

Hetero atom count ☐ Negate

Ring membership: ☐ Not defined ☐ In ring ☐ Not in ring

Ring count ☐ Negate

Ring size ☐ Negate

Sum of bond order ☐ Negate

Neighbors count ☐ Negate

☐ Negate ☒ And ☒ + ☒ +n ☒ - ☐ Negate

☒ Advanced

Activate "Advanced"

Enter SMARTS notation to set annotations

► Bond query annotations

The screenshot displays the Chemotype Editor application window. The interface includes a menu bar with 'Chemotype Editor', 'Editor', and 'Tools'. Below the menu is a toolbar with various icons for editing and querying. A vertical sidebar on the left lists chemical elements: C, N, O, S, F, Cl, Br, I, P, and X. The main workspace shows a chemical structure with an ether bond (C-O-C) and a blue atom. The 'Bond query' tab is selected at the bottom, with other tabs including 'Atom query', 'Molecule query', 'Meta information', 'Positive (0) and negative (0) examples', 'CSRML', and 'Logs'. Annotations are present: a box pointing to the 'Bond query' tab says 'Switch to tab "Bond query"', a box pointing to the marker icon in the toolbar says 'To add a query annotation to a bond, click on the marker symbol (orange circle) in the top button row of the editor above and then click on a bond to mark it.', and a box pointing to the blue atom in the structure says 'Use marker (amber-colored circle) to select bond for query annotation'.

Chemotype Editor

Chemotype Editor Editor Tools

Switch to tab "Bond query"

To add a query annotation to a bond, click on the marker symbol (orange circle) in the top button row of the editor above and then click on a bond to mark it.

Use marker (amber-colored circle) to select bond for query annotation

Atom query Bond query Molecule query Meta information Positive (0) and negative (0) examples CSRML Logs

▶ Bond query annotations

Marked bond

The screenshot displays the Chemotype Editor application. At the top, a blue header bar contains the title "Chemotype Editor" and tabs for "Editor" and "Tools". Below the header is a toolbar with various icons for creating and editing chemical structures. On the left side, a vertical menu lists chemical elements: C, N, O, S, F, Cl, Br, I, P, and X. The main workspace shows a chemical structure with a bond highlighted in blue. A blue line points from the "Marked bond" label to this bond. Below the workspace, a horizontal tab bar includes "Atom query", "Bond query", "Molecule query", "Meta information", "Positive (0) and negative (0) examples", "CSRML", and "Logs". The "Bond query" tab is active, showing a "Bond 3" button. The bond query panel includes a "Query feature label" field, a "Bond order" section with radio buttons for "Not defined", "Any", "Single" (selected), "Double", and "Triple", an "Aromaticity" section with radio buttons for "Not defined", "Aromatic", and "Aliphatic" (selected), a "Ring membership" section with radio buttons for "Not defined", "In ring", and "Not in ring", a "Ring size" field with a "Negate" checkbox, and a "Comment" field. A blue line points from the "Enter bond query annotations" label to the "Aliphatic" radio button. On the left of the panel, there are checkboxes for "Negate" and a box containing "And", "+", and "+n" buttons.

Enter bond query annotations

► Molecule query annotations

The screenshot displays the Chemotype Editor application window. The title bar reads 'Chemotype Editor'. The menu bar includes 'Chemotype Editor', 'Editor', and 'Tools'. On the right of the menu bar is an 'About' button. Below the menu bar is a toolbar with various icons for creating and editing chemical structures. On the left side, there is a vertical element list with buttons for C, N, O, S, F, Cl, Br, I, P, and X. The main workspace shows a chemical structure of a small molecule. At the bottom, there is a tabbed interface with the following tabs: 'Atom query', 'Bond query', 'Molecule query' (which is the active tab), 'Meta information', 'Positive (0) and negative (0) examples', 'CSRML', and 'Logs'. A blue line points from a text box to the 'Molecule query' tab. Another blue line points from a text box to a grey informational box that appears when the 'Molecule query' tab is active. This box contains the text: 'CSRML supports additional query features that can match on the whole molecule. These features are not yet implemented.'

Click on tab "Molecule query"

CSRML supports additional query features that can match on the whole molecule. These features are not yet implemented.

Functionality not yet supported

MNAM Chemotype Editor

► Meta information

The screenshot displays the MNAM Chemotype Editor application. The main window has a blue header bar with the title "Chemotype Editor" and tabs for "Editor" and "Tools". Below the header is a toolbar with various icons for creating and editing chemical structures. On the left side, there is a vertical menu with element symbols: C, N, O, S, F, Cl, Br, I, P, and X. The central workspace shows a chemical structure of a methyl ether (CH₃-O-CH₃). At the bottom, there is a tabbed interface with the following tabs: "Atom query", "Bond query", "Molecule query", "Meta information" (which is the active tab), "Positive (0) and negative (0) examples", "CSRML", and "Logs". The "Meta information" tab contains several input fields: "ID", "Label", "Title", "Comment" (with a link icon), and "Description". The "Comment" field is currently filled with the text "My first chemotype".

Click on tab "Meta information"

Enter description to be stored with chemotype

MNAM Chemotype Editor

► Positive and negative example (required)

The screenshot displays the MNAM Chemotype Editor software interface. At the top, a blue header bar contains the title 'Chemotype Editor' and a menu with 'Editor' and 'Tools'. Below the header, a vertical toolbar on the left lists chemical elements: C, N, O, S, F, Cl, Br, I, P, and X. The main workspace shows a chemical structure of an ether. Below the workspace, a horizontal tab bar includes 'Atom query', 'Bond query', 'Molecule query', 'Meta information', and 'Positive (0) and negative (0) examples'. The 'Positive (0) and negative (0) examples' tab is selected, revealing two panels: 'Positive examples' on the left and 'Negative examples' on the right. Each panel contains a JSME Molecular Editor by Peter Ertl and Bruno Bienfait, with a red circular button at the bottom right. A callout box points to the tab bar with the text: 'Click on tab "Positive (n) and negative (n) examples"'. Another callout box points to the 'Positive examples' panel with the text: 'Positive example molecules, i.e., molecules which must, and negative example molecules, i.e., molecules which must not match the defined chemotype can be sketched here'.

Click on tab "Positive (n) and negative (n) examples"

Positive example molecules, i.e., molecules which must, and negative example molecules, i.e., molecules which must not match the defined chemotype can be sketched here

► Positive and negative example (required)

The screenshot displays the Chemotype Editor application window. The main editing area shows a chemical structure fragment. Below the main area, there are tabs for 'Atom query', 'Bond query', 'Molecule query', and 'Meta information'. A callout box with a blue border points to a 'Move' button in the 'Positive examples' section, indicating the drag-and-drop functionality for Molfile and multi-record SD files. The interface includes a toolbar with various chemical editing tools and a sidebar with element selection buttons (C, N, O, S, F, Cl, Br, I, P, X). The footer of the editor window reads 'JSME Molecular Editor by Peter Ertl and Bruno Bienfait'.

Support of drag&drop of Molfile and multi-record SD file

► Positive and negative example (required)

Chemotype Editor

Chemotype Editor Editor Tools

At least one positive and one negative example must be provided

Atom query Bond query Molecule query Meta information Positive (1) and negative (1) examples CSRML Logs

Positive examples

Negative examples

MNAM Chemotype Editor

► Positive and negative example (required)

The screenshot displays the MNAM Chemotype Editor software. The main window has a title bar 'Chemotype Editor' and a menu bar with 'Editor' and 'Tools'. Below the menu bar is a toolbar with various chemical editing tools. A vertical element menu on the left lists atoms: C, N, O, S, F, Cl, Br, I, P, X. The main editing area shows a small molecule fragment. Below the main area are several tabs: 'Atom query', 'Bond query', 'Molecule query', 'Meta information', 'Positive (1) and negative (1) examples' (which is selected), 'CSML', and 'Logs'. The 'Positive (1) and negative (1) examples' tab contains two sub-panels: 'Positive examples' and 'Negative examples'. The 'Positive examples' panel has its own toolbar and element menu. A callout box with a blue border points to a double cross symbol (a square with an 'X' inside) located in the 'Positive examples' panel, with the text: 'Example molecules can be switched between positive and negative (drag double cross symbol)'. At the bottom of the 'Positive examples' panel, there is a blue '+' button. In the 'Negative examples' panel, there is a red '-' button and a blue '+' button.

MNAM Chemotype Editor

► Positive and negative example (required)

The screenshot displays the MNAM Chemotype Editor software. The main window has a menu bar with 'Chemotype Editor', 'Editor', and 'Tools'. Below the menu is a toolbar with various chemical drawing tools. A vertical element list on the left contains C, N, O, S, F, Cl, Br, I, P, and X. The main canvas shows a small molecule fragment. At the bottom, there are tabs for 'Atom query', 'Bond query', 'Molecule query', 'Meta information', 'Positive (1) and negative (1) examples', 'CSRML', and 'Logs'. The 'Positive (1) and negative (1) examples' tab is active, showing two panels: 'Positive examples' and 'Negative examples'. Each panel contains a smaller version of the Chemotype Editor interface with its own toolbar and element list. The 'Positive examples' panel shows a molecule with SMILES CCOC and has a red minus button and a blue plus button. The 'Negative examples' panel shows a molecule with SMILES CC1OCC1 and also has a red minus button and a blue plus button. A blue line connects the text 'Further example molecules can be added...' to the blue plus button in the 'Negative examples' panel. Another blue line connects the text '...or existing can be deleted' to the red minus button in the 'Positive examples' panel.

Chemotype Editor

Chemotype Editor Editor Tools

Further example molecules can be added...

Positive examples

Negative examples

...or existing can be deleted

MNAM Chemotype Editor

- Copy positive/negative example from ChemoTyper app

The screenshot displays the MNAM Chemotype Editor interface. A callout box points to the 'Copy Structure' button in the ChemoTyper application, which is used to copy a chemical structure. Another callout box points to the 'Paste (Ctrl-V) copied structure into positive example panel' button in the editor. The interface includes a menu bar, a toolbar, and a main workspace. The 'Positive examples' panel is visible at the bottom left, showing a chemical structure and a status bar indicating 'Structure pasted.'.

Copy structure from ChemoTyper application

Copy Structure

Copy Structure ID

Positive examples

Structure pasted.

Paste (Ctrl-V) copied structure into positive example panel

Chemotype Editor

Menu

mustMatch1

mustNotMatch1

Filter Structures by ID type ID Filter Pattern

Filter Chemotypes Containing Any Selected Structure (OR)

Structures Loaded: 2 Total Coverage: 2 Selected: 2 ID: NAME

toxprint v2.0 r1520.xml

Chemotype Sets

☒ ToxPrint Chemotypes Version ...

☒ atom

☒ element

☒ bond

☒ C#N

☒ C(-Z)-C-Q

☒ C(=O)N

☒ C(=O)O

☒ C=N

☒ C=O

☒ C=S

☒ CC(=O)C

☒ CN

☒ CNO

☒ COC

☒ COH

☒ CS

☒ CX

☒ N(=O)

☒ N[IC]

☒ N=[N+]=[N-]

☒ N=C=O

☒ N=N

☒ N=O

☒ NC=O

chain:alkaneBr 422

anch_isopropyl_C3

chain:alkaneLin 437

ear_ethyl_C2(H_gt_1)

ring:hetero_161_668

O_pyrans_gener

chain:alkaneCy 432

clac_ethyl_C2(c_omnect_noZ)

group:carbohy

drate_hexopyra

nose_generic

ring:hetero_161_669

Z_1-

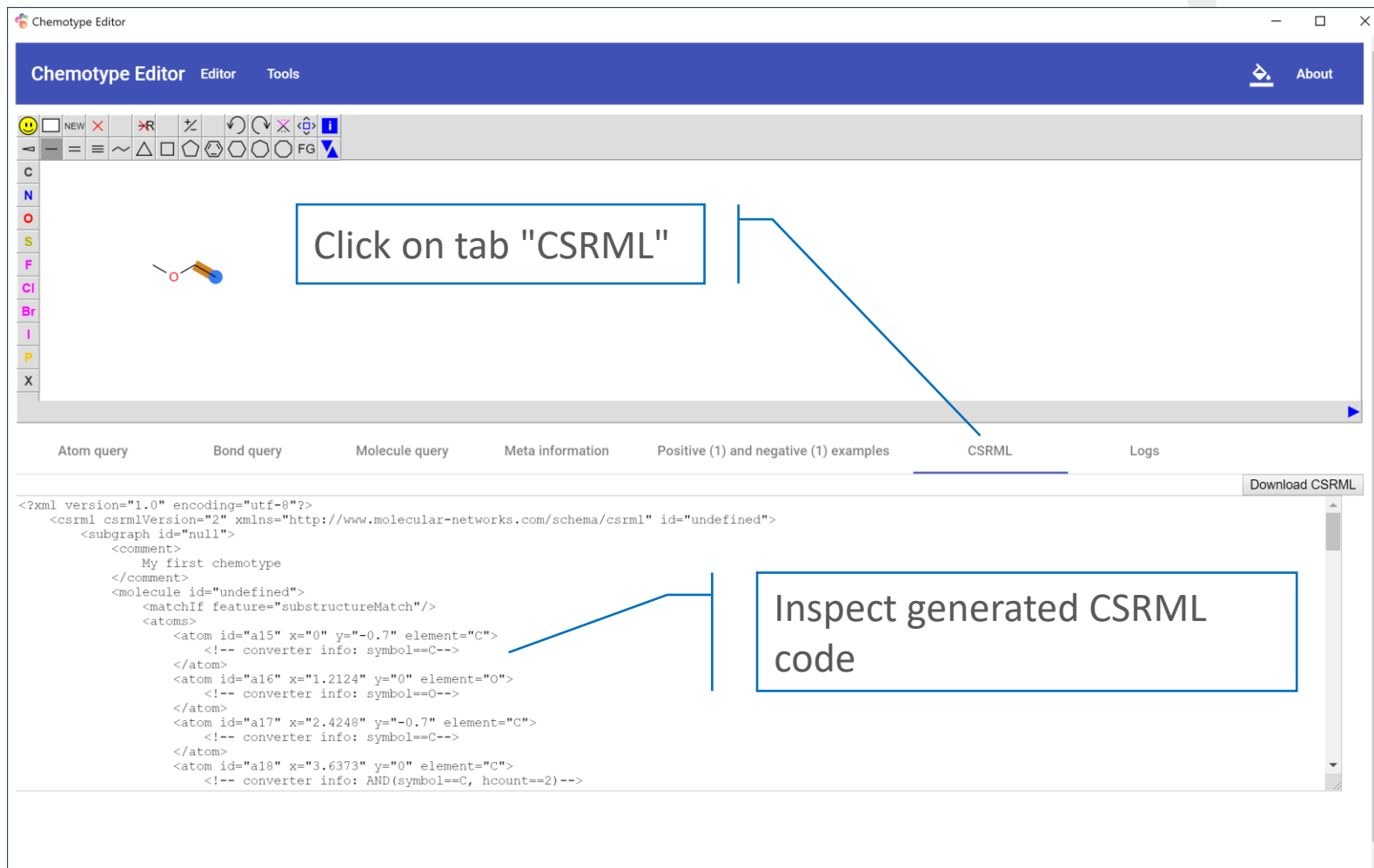
Filter Chemotypes by ID type ID Filter Pattern

Filter Structures No Filter

Chemotypes Loaded: 729 Total Coverage: 8 Selected: 8 (721 hidden)

Matched: 8 ID: Auto

► Resulting CSRML code



The screenshot displays the Chemotype Editor application. The top menu bar includes "Chemotype Editor", "Editor", and "Tools". A toolbar with various icons is located below the menu. On the left, a vertical toolbar lists chemical elements: C, N, O, S, F, Cl, Br, I, P, and X. The main workspace shows a chemical structure of a small molecule. A blue box with the text "Click on tab 'CSRML'" has an arrow pointing to the "CSRML" tab in the bottom panel. The bottom panel contains several tabs: "Atom query", "Bond query", "Molecule query", "Meta information", "Positive (1) and negative (1) examples", "CSRML", and "Logs". The "CSRML" tab is active, displaying XML code. A blue box with the text "Inspect generated CSRML code" has an arrow pointing to the XML code. A "Download CSRML" button is visible in the top right of the CSRML tab area.

Chemotype Editor

Chemotype Editor Editor Tools

NEW

C N O S F Cl Br I P X

Click on tab "CSRML"

Atom query Bond query Molecule query Meta information Positive (1) and negative (1) examples CSRML Logs

Download CSRML

```
<?xml version="1.0" encoding="utf-8"?>
<csrml csrmlVersion="2" xmlns="http://www.molecular-networks.com/schema/csrml" id="undefined">
  <subgraph id="null">
    <comment>
      My first chemotype
    </comment>
    <molecule id="undefined">
      <matchIf feature="substructureMatch"/>
      <atoms>
        <atom id="a15" x="0" y="-0.7" element="C">
          <!-- converter info: symbol==C-->
        </atom>
        <atom id="a16" x="1.2124" y="0" element="O">
          <!-- converter info: symbol==O-->
        </atom>
        <atom id="a17" x="2.4248" y="-0.7" element="C">
          <!-- converter info: symbol==C-->
        </atom>
        <atom id="a18" x="3.6373" y="0" element="C">
          <!-- converter info: AND(symbol==C, hcount==2)-->
        </atom>
      </atoms>
    </molecule>
  </subgraph>
</csrml>
```

Inspect generated CSRML code

MN/AM Chemotype Editor

► Download CSRML file

The screenshot displays the Chemotype Editor application. The main window shows a chemical structure (a benzene ring with a substituent) and a toolbar with various editing tools. A file save dialog is open, showing the file name "my_first_chemotype.xml" and the save location "Desktop". The dialog also shows a search bar and a "Save" button. Below the main window, the CSRML XML output is displayed, showing the structure's metadata and atom coordinates.

Chemotype Editor

Chemotype Editor Editor Tools

Atom query Bond query Molecule query Meta information

Download CSRML

Save chemotype in CSRML file

```
<?xml version="1.0" encoding="utf-8"?>
<csrml csrmlVersion="2" xmlns="http://www.molecular-networks.com/schema/csrml" id="undefined">
  <subgraph id="null">
    <comment>
      My first chemotype
    </comment>
    <molecule id="undefined">
      <matchIf feature="substructureMatch"/>
      <atoms>
        <atom id="a15" x="0" y="-0.7" element="C">
          <!-- converter info: symbol==C-->
        </atom>
        <atom id="a16" x="1.2124" y="0" element="O">
          <!-- converter info: symbol==O-->
        </atom>
        <atom id="a17" x="2.4248" y="-0.7" element="C">
          <!-- converter info: symbol==C-->
        </atom>
        <atom id="a18" x="3.6373" y="0" element="C">
          <!-- converter info: AND(symbol==C, hcount==2)-->
        </atom>
      </atoms>
    </molecule>
  </subgraph>
</csrml>
```

MNAM Chemotype Editor

Tools

Click on "Tools" to open tool stack

The screenshot displays the Chemotype Editor application window. The top menu bar includes 'Chemotype Editor', 'Editor', 'Tools', and 'About'. Below the menu bar, a sub-menu for 'Tools' is open, showing options: 'Interactive MOL to CSRML converter', 'SDF to CSRML converter', 'SMARTS to CSRML', and 'CSRML to CSRML'. The 'Interactive MOL to CSRML converter' tool is selected and active. The main workspace shows a chemical structure of a methyl ketone (CH₃-C(=O)-H). A vertical toolbar on the left contains buttons for various chemical elements (C, N, O, S, F, Cl, Br, I, P, X). A text box with a blue border points to the 'Tools' menu, stating 'Click on "Tools" to open tool stack'. Another text box with a blue border points to the 'MOL to CSRML converter' tool, stating 'Various tools (converters) to support editing of chemotypes'. At the bottom, there are buttons for 'Clear editor' and 'Download CSRML', and a text area displaying the CSRML XML output for the structure.

MOL to CSRML converter

Clear editor | Download CSRML

```
<?xml version="1.0" encoding="utf-8"?>
<csrml csrmlVersion="2" xmlns="http://www.molecular-networks.com/schema/csrml" id="csrml0">
  <subgraph id="r00011">
    <molecule id="m1">
      <matchIf feature="substructureMatch"/>
      <atoms>
        <atom id="a1" element="C" x="1.2124" y="-0.7">
          <matchIf feature="aliphaticAtom"/>
        </atom>
        <atom id="a2" element="O" x="2.4248" y="0">
          <matchIf feature="aliphaticAtom"/>
        </atom>
        <atom id="a3" element="C" x="1.2124" y="-2.1">
          <matchIf feature="aliphaticAtom"/>
        </atom>
        <atom id="a4" element="H" x="0" y="0">
          <matchIf feature="aliphaticAtom"/>
        </atom>
      </atoms>
    </molecule>
  </subgraph>
</csrml>
```

► Tools

- ▶ Interactive MOL to CSRML converter
 - Generates CSRML code from uploaded Mol/SD file or sketched structure
- ▶ SDF to CSRML converter
 - Batch conversion of SD to CSRML files
 - Supports multi-record files
- ▶ SMARTS to CSRML converter
 - Generates CSRML code from entered SMARTS strings
- ▶ CSRML to CSRML (converter)
 - "Round trip" to check if interpretation and generation of CSRML works correctly

▶ Known limitations

- ▷ One chemotype at a time
 - Editing of multiple chemotype (files) not supported
- ▷ Molecule query annotations not yet supported
- ▷ Query feature label and comment fields in atom and bond query annotations not yet stored/exported
- ▷ No check for valid positive or negative examples
 - No actual match performed
- ▷ Editing CSRML code in tab "CSRML" has no impact
 - Does not change any annotations, examples, etc in other tabs and is not exported
- ▷ Recursive SMARTS not yet supported
- ▷ Annotations with physicochemical properties not yet supported



Molecular Networks GmbH (Germany) and
Altamira LLC (USA)
Neumeyerstr. 22-34, 90411 Nürnberg, Germany
470 W Broad St, Unit #5007, Columbus,
Ohio 43215, USA
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