

Short Tutorial for Chemotype Editor

October 2023

Introduction



- ChemoType Editor
 - Version 0.0.9
 - October 19, 2020
- System requirements
 - Windows 10/11 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

1 Quick Start Page

- 2 Load ToxPrint Chemotypes
- 3 Inspect ToxPrint Chemotypes
- 4 Load Structure File
- 5 Matching Results
- 6 Chemotype Sub-Setting
- 7 Structure Sub-Setting
- 8 Further Information

Start Page

Chemotype Editor

File Edit View Window Help

Chemotype Editor Editor Tools

About

Graphical editor to sketch chemotype structures

Main window of editor

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

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.

1 Quick Start Page

2 Load ToxPrint
Chemotypes

3 Inspect ToxPrint
Chemotypes

4 Load Structure File

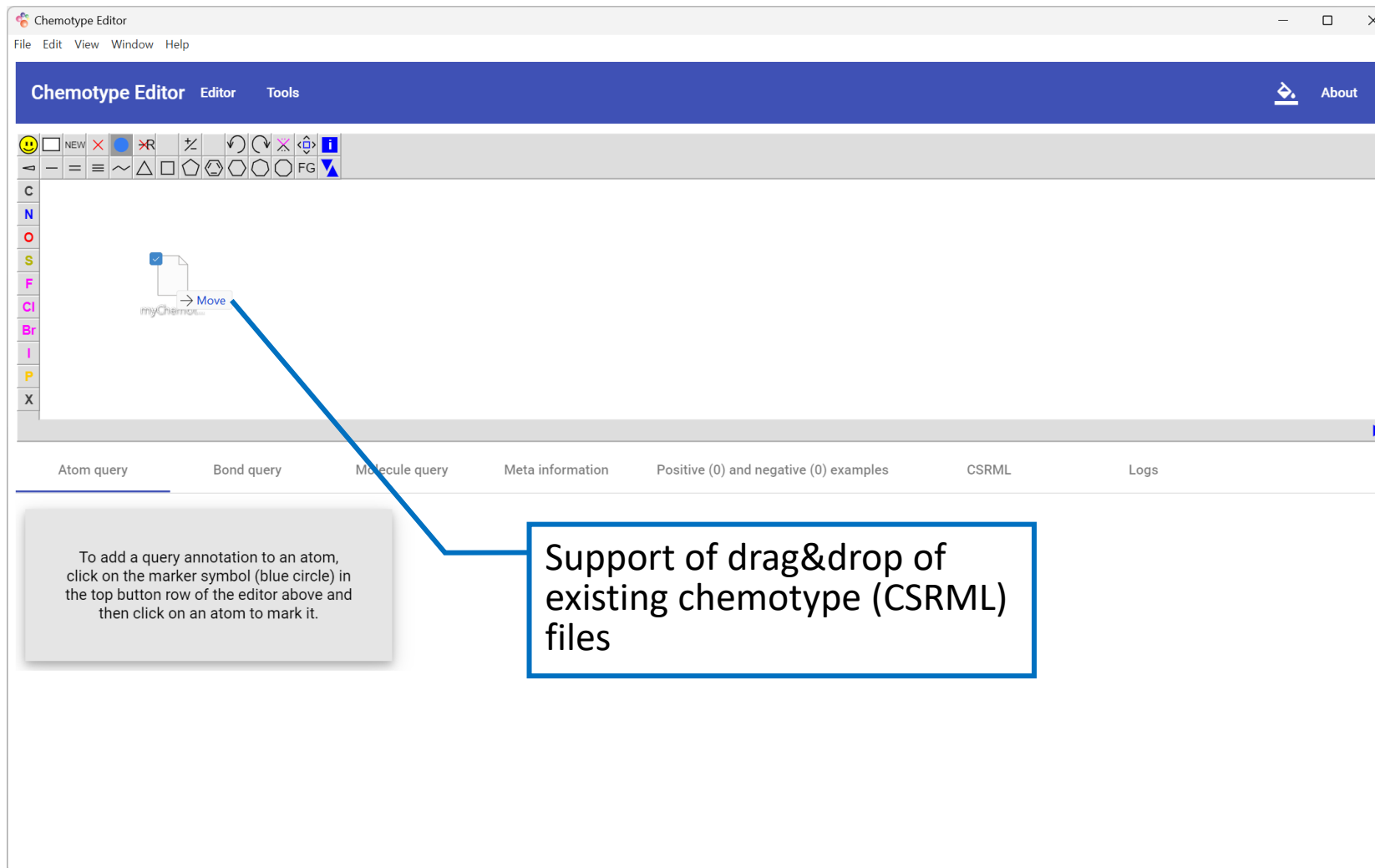
5 Matching Results

6 Chemotype Sub-Setting

7 Structure Sub-Setting

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Load Chemotype File



The screenshot shows the Chemotype Editor application window. The title bar reads "Chemotype Editor". The menu bar includes "File", "Edit", "View", "Window", and "Help". The main toolbar contains icons for "NEW", "COPY", "PASTE", "ERASE", "REDO", "UNDO", "SELECT", "LONE PAIR", "HIGHLIGHT", and "FG". A vertical sidebar on the left lists chemical elements: C, N, O, S, F, Cl, Br, I, P, and X. The central workspace displays a file icon labeled "myChemot..." with a "Move" tooltip. A blue arrow points from this icon to a text box. Below the workspace is a tabbed interface with tabs for "Atom query", "Bond query", "Molecule query", "Meta information", "Positive (0) and negative (0) examples", "CSRML", and "Logs".

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

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Copy&Paste Chemotype from ChemoTyper Application

The image shows two overlapping software windows. The background window is 'ChemoTyper', which displays a grid of chemical structures. A blue box highlights one of the structures, and a callout points to it with the text 'Copy chemotype from ChemoTyper application'. The foreground window is 'ChemoType Editor', which has a toolbar and a main editing area. A blue box highlights the 'And' button in the 'Atom query' section, with a callout pointing to it that says 'Paste (Ctrl-V) copied chemotype into ChemoType Editor'. On the right side of the ChemoTyper window, there is a 'Chemotype Sets' panel. A blue box highlights a specific chemotype entry, and a callout points to it with the text 'Copy Chemotype' and 'Copy Chemotype ID'. The bottom of the ChemoTyper window shows statistics: 'Structures Loaded: 500 Total Coverage: 500 Selected: 0 ID: TestSubstance_CASRN' and 'Chemotypes Loaded: 729 Total Coverage: 485 Selected: 729 ID: Auto'.

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Draw Chemotype Structure

The screenshot displays the Chemotype Editor application window. The interface includes a menu bar (File, Edit, View, Window, Help), a toolbar with various drawing tools, and a vertical element list on the left (C, N, O, S, F, Cl, Br, I, P, X). A chemical structure is shown in the main workspace, with a blue circle highlighting a specific atom. Below the workspace, there are tabs for Atom query, Bond query, and Molecule query. The Atom query tab is active, showing a query editor with a dropdown menu set to 'And', a 'Negate' checkbox, and a 'Edit me' button. A red box highlights the '+' and '+n' buttons in the query editor. Two callout boxes provide instructions: one points to the drawing toolbar with the text 'Draw structure of chemotype', and another points to the blue circle on the atom with the text 'Use marker (blue-colored circle) to select atom for query annotations'.

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Atom Query Annotations

The screenshot shows the Chemotype Editor application window. The main toolbar includes icons for smiley, new, delete, copy, paste, undo, redo, and atom query. The left sidebar lists chemical elements: C, N, O, S, F, Cl, Br, I, P, X. The main workspace displays a chemical structure fragment. Below the workspace is a tabbed interface with 'Atom query' selected. A 'Atom 4' button is visible. The 'Edit me' dialog box is open, showing fields for 'Query feature label', 'Atom type', 'CSRML query atom types', 'Aromaticity', and 'Formal charge'. The 'Edit me' toggle is turned on, and the 'Advanced' toggle is also visible.

Switch on "Edit me" to enter and define query annotations

Scroll down for more annotation fields

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Atom Query Annotations

Chemotype Editor

File Edit View Window Help

☒ 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

Non H neighbors count _____ ☐ Negate

☐ Negate And + +n - ☐ Negate

Enter, e.g., "2" in field "Hydrogen count" to specify the number of hydrogen atoms attached to marked query atom

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Atom Query Annotations

Chemotype Editor

File Edit View Window Help

☒ Edit me

Atomic SMARTS input

[CH2]

Recursive SMARTS are not yet supported.

Query feature label

Atom type

C ☐ Negate

CSML 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

Non H neighbors count ☐ Negate

☐ Negate ☐ Negate

☒ Advanced

Switch on "Advanced"

Enter SMARTS notation to define query annotation

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Bond Query Annotations

Chemotype Editor

File Edit View Window Help

Chemotype Editor Editor Tools

Switch to tab "Bond query"

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

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.

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Bond Query Annotations

The screenshot displays the Chemotype Editor application. At the top, a blue header bar contains the title "Chemotype Editor" and menu options "File", "Edit", "View", "Window", and "Help". Below the header is a toolbar with various icons for creating and editing chemical structures. On the left side, a vertical toolbar 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 and labeled "Marked bond". Below the workspace, a tabbed interface is visible, with the "Bond query" tab selected. This tab displays a query builder for "Bond 3". The query builder includes a "Negate" checkbox, a logical operator dropdown set to "And", and a "Negate" checkbox. A red circle is placed next to the query. A callout box labeled "Enter bond query annotations" points to the query builder. The callout box contains the following options:

- ☒ Edit me
- Query feature label
- Bond order: ☐ Not defined ☐ Any ☒ Single ☐ Double ☐ Triple
- Aromaticity: ☐ Not defined ☐ Aromatic ☒ Aliphatic
- Ring membership: ☐ Not defined ☐ In ring ☒ Not in ring
- Ring size ☐ Negate
- Comment

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Molecule Query Annotations

The screenshot displays the Chemotype Editor application window. The title bar reads 'Chemotype Editor'. Below it is a menu bar with 'File', 'Edit', 'View', 'Window', and 'Help'. A dark blue header bar contains 'Chemotype Editor' on the left and 'About' on the right. Below the header is a toolbar with various icons for creating and editing chemical structures. On the left side of the main workspace is a vertical element palette with buttons for C, N, O, S, F, Cl, Br, I, P, and X. The main workspace shows a chemical structure of an ether. At the bottom is a tabbed interface with the following tabs: 'Atom query', 'Bond query', 'Molecule query' (which is selected and highlighted with a blue underline), 'Meta information', 'Positive (0) and negative (0) examples', 'CSRML', and 'Logs'. A blue line points from a text box 'Select tab "Molecule query"' to the 'Molecule query' tab. Another blue line points from a text box 'Functionality not yet supported' to a grey callout box. The callout box contains the text: 'CSRML supports additional query features that can match on the whole molecule. These features are not yet implemented.'

Select 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

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Meta Information

The screenshot shows the Chemotype Editor application window. The title bar reads 'Chemotype Editor'. The menu bar includes 'File', 'Edit', 'View', 'Window', and 'Help'. The main toolbar contains icons for 'NEW', 'X', 'R', 'Z', 'undo', 'redo', 'copy', 'paste', 'info', and 'FG'. On the left, a vertical element list shows 'C', 'N', 'O', 'S', 'F', 'Cl', 'Br', 'I', 'P', and 'X'. The central workspace displays a chemical structure of an ether. Below the workspace is a tabbed interface with the following tabs: 'Atom query', 'Bond query', 'Molecule query', 'Meta information' (which is selected), 'Positive (0) and negative (0) examples', 'CSRML', and 'Logs'. The 'Meta information' tab contains the following fields:

- ID: mct001
- Label: Ether_aliphatic_nonRing
- Title: Ether_aliphatic_nonRing_t
- Comment: My first chemotype
- Description: (empty)

Two blue callout boxes provide instructions: one points to the 'Meta information' tab with the text 'Select tab "Meta information"', and the other points to the input fields with the text 'Enter meta information to be stored along with the chemotype'.

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Positive and Negative Match Examples (required)

Chemotype Editor

File Edit View Window Help

Chemotype Editor Editor Tools

About

Select 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

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

Positive examples

Negative examples

JSME Molecular Editor by Peter Ertl and Bruno Bienfait

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Positive and Negative Match Examples (required)

Chemotype Editor

File Edit View Window Help

Chemotype Editor Editor Tools

NEW X R Z Q P I

C N O S F Cl Br I P X

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

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

Positive examples

Negative examples

positive -> Move

JSME Molecular Editor by Peter Ertl and Bruno Bienfait

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Positive and Negative Match Examples (required)

The screenshot displays the Chemotype Editor application. The main window has a menu bar (File, Edit, View, Window, Help) and a toolbar with various chemical editing tools. Below the toolbar is a vertical list of element symbols (C, N, O, S, F, Cl, Br, I, P, X). The main canvas shows a chemical structure of an ether. A blue box with a pointer indicates: "At least one positive and one negative example must be provided".

Below the main canvas are several tabs: 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 sub-panels:

- Positive examples:** Contains a chemical structure of an ether (isopropyl ethyl ether) and a red minus button.
- Negative examples:** Contains a chemical structure of a cyclic ether (tetrahydrofuran) and a red minus button.

Each sub-panel also has its own toolbar and element list, and a blue plus button is located at the bottom left of each panel.

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Positive and Negative Match Examples (required)

The screenshot displays the Chemotype Editor application. The main window has a menu bar (File, Edit, View, Window, Help) and a toolbar with various chemical editing tools. Below the toolbar is a vertical element palette with atoms C, N, O, S, F, Cl, Br, I, P, and X. The main canvas shows a chemical structure of an ether. 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'. The 'Positive examples' panel contains two smaller chemical structure editors, each with its own toolbar and element palette. The first editor shows a branched ether, and the second shows a cyclic ether. The 'Negative examples' panel is currently empty. A blue callout box with a pointer indicates that example molecules can be switched between positive and negative by dragging a double cross symbol.

Chemotype Editor

File Edit View Window Help

Chemotype Editor Editor Tools

NEW X R Z Q P I

C N O S F Cl Br I P X

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

Positive examples

Negative examples

Example molecules can be switched between positive and negative (drag double cross symbol)

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Positive and Negative Match Examples (required)

The screenshot displays the Chemotype Editor application. The main window has a menu bar (File, Edit, View, Window, Help) and a toolbar with various chemical editing tools. Below the toolbar is a vertical element palette with atoms (C, N, O, S, F, Cl, Br, I, P, X). The main canvas shows a chemical structure of an ether. Below the canvas 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 sub-panels: 'Positive examples' and 'Negative examples'. Each sub-panel contains a smaller version of the Chemotype Editor interface. In the 'Positive examples' panel, a chemical structure of an ether is shown, and a red minus button is visible. In the 'Negative examples' panel, a chemical structure of a cyclic ether is shown, and a red minus button is visible. A blue line connects the red minus button in the 'Negative examples' panel to a text box that says '...or existing can be deleted'. Another blue line connects the text box 'Further example molecules can be added...' to the 'Negative examples' panel.

Further example molecules can be added...

...or existing can be deleted

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Positive and Negative Match Examples

The image displays two software windows: **Chemotype Editor** and **ChemoTyper**.

Chemotype Editor (top left) shows a chemical structure editor with a toolbar and a list of elements (C, N, O, S, F, Cl, Br, I, P, X). A callout box points to the toolbar with the text: "Copy structure from ChemoTyper application".

ChemoTyper (bottom right) shows a window with a list of chemotypes and their matches. A callout box points to the "Copy Structure" button with the text: "Copy Structure".

Below the Chemotype Editor, there is a section titled "Positive examples" showing a chemical structure of an ether. A callout box points to this structure with the text: "Paste (Ctrl-V) copied structure into positive example panel".

The ChemoTyper window also displays a list of chemotypes and their matches, including:

- chain:alkaneBr 422
- anch_isopropyl_C3
- chain:alkaneC 432
- clac_ethyl_C2(c onnect_noZ)
- chain:alkaneLin 437
- group:carbohy 544
- ear_ethyl_C2(H gt_1)
- drate_hexopyra nose_generic
- ring:hetero_[6]_668
- ring:hetero_[6]_669
- O_pyran_gener ic
- Z_1+

The bottom of the ChemoTyper window shows a summary: "Chemotypes Loaded: 729 Total Coverage: 8 Selected: 8 (721 hidden) Matched: 8 ID: Auto".

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CSRML = Chemical
Substructure and
Reaction Markup
Language

Chemotype in CSRML

The screenshot shows the Chemotype Editor window. The top menu bar includes File, Edit, View, Window, and Help. Below the menu is a toolbar with various icons for creating and editing chemical structures. On the left side, there is a vertical toolbar with element symbols: C, N, O, S, F, Cl, Br, I, P, and X. The main workspace displays a chemical structure of an ether. Below the workspace is a tabbed interface with the following tabs: Atom query, Bond query, Molecule query, Meta information, Positive (1) and negative (1) examples, **CSRML**, and Logs. The CSRML tab is active, showing the generated CSRML code. A callout box points to the CSRML tab with the text "Select tab 'CSRML'". Another callout box points to the CSRML code with the text "Inspect generated CSRML code".

Select tab "CSRML"

Inspect generated CSRML code

```
<?xml version="1.0" encoding="utf-8"?>
<csrml csrmlVersion="2" xmlns="http://www.molecular-networks.com/schema/csrml" id="undefined">
  <subgraph id="mct001">
    <label>
      Ether_aliphatic_nonRing
    </label>
    <title>
      Ether_aliphatic_nonRing_COCC
    </title>
    <comment>
      My first chemotype
    </comment>
    <molecule id="undefined">
      <matchIf feature="substructureMatch"/>
      <atoms>
        <atom id="a4" x="0" y="-0.7" element="C">
          <!-- converter info: symbol==C-->
        </atom>
        <atom id="a5" x="1.2124" y="0" element="O">
          <!-- converter info: symbol==O-->
        </atom>
      </atoms>
    </molecule>
  </subgraph>
</csrml>
```

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CSRML = Chemical
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Reaction Markup
Language

Chemotype in CSRML

The screenshot displays the Chemotype Editor application. The main window shows a chemical structure of an ether. A file save dialog is open, titled "blob:file:///38ae6254-ff43-4e26-8282-6db153f516a2", with the file name "my_first_chemotype.xml" and "All Files (*.*)" selected. The dialog shows the Desktop as the save location. Below the dialog, the CSRML XML output is visible, showing the structure's details and atom coordinates.

Chemotype Editor

File Edit View Window Help

NEW X R Z C F G

Atom query Bond query Molecule query

File name: my_first_chemotype.xml

Save as type: All Files (*.*)

Save Cancel

```
<?xml version="1.0" encoding="utf-8"?>
<csrml csrmlVersion="2" xmlns="http://www.molecul...
  <subgraph id="mct001">
    <label>
      Ether_aliphatic_nonRing
    </label>
    <title>
      Ether_aliphatic_nonRing_COCC
    </title>
    <comment>
      My first chemotype
    </comment>
    <molecule id="undefined">
      <matchIf feature="substructureMatch"/>
      <atoms>
        <atom id="a4" x="0" y="-0.7" element="C">
          <!-- converter info: symbol==C-->
        </atom>
        <atom id="a5" x="1.2124" y="0" element="O">
          <!-- converter info: symbol==O-->
        </atom>
      </atoms>
    </molecule>
  </subgraph>
</csrml>
```

Save chemotype as CSRML
file

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Tools

Select "Tools" to open stack

The screenshot displays the Chemotype Editor web application. The top navigation bar includes 'Chemotype Editor', 'Editor', and 'Tools'. The 'Tools' menu is highlighted, and a callout box points to it with the text 'Select "Tools" to open stack'. Below the navigation bar, there are four tabs: 'Interactive MOL to CSRML converter', 'SDF to CSRML converter', 'SMARTS to CSRML', and 'CSRML to CSRML'. The 'Interactive MOL to CSRML converter' tab is active. A callout box points to this tab with the text 'Various tools (converters) to support editing of chemotypes'. The main workspace shows a chemical structure of a carbonyl group (C=O) with a nitrogen atom (N) attached to the carbon. On the left side of the workspace is a vertical toolbar with icons for various chemical elements (C, N, O, S, F, Cl, Br, I, P, X) and functional groups. At the bottom of the workspace are buttons for 'Clear editor' and 'Download CSRML'. Below the workspace is a text area displaying the CSRML XML output for the structure.

```
<?xml version="1.0" encoding="utf-8"?>
<csrml csrmlVersion="2" xmlns="http://www.molecular-networks.com/schema/csrml" id="csrml0">
  <subgraph id="r00002">
    <molecule id="m1">
      <matchIf feature="substructureMatch"/>
      <atoms>
        <atom id="a1" element="C" x="0" y="-2.1">
          <matchIf feature="aliphaticAtom"/>
        </atom>
        <atom id="a2" element="C" x="1.2124" y="-1.4">
          <matchIf feature="aliphaticAtom"/>
        </atom>
        <atom id="a3" element="N" x="1.2124" y="0">
          <matchIf feature="aliphaticAtom"/>
        </atom>
        <atom id="a4" element="O" x="2.4248" y="-2.1">
          <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

Known Limitations

- 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



Q&A

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THANK
YOU!