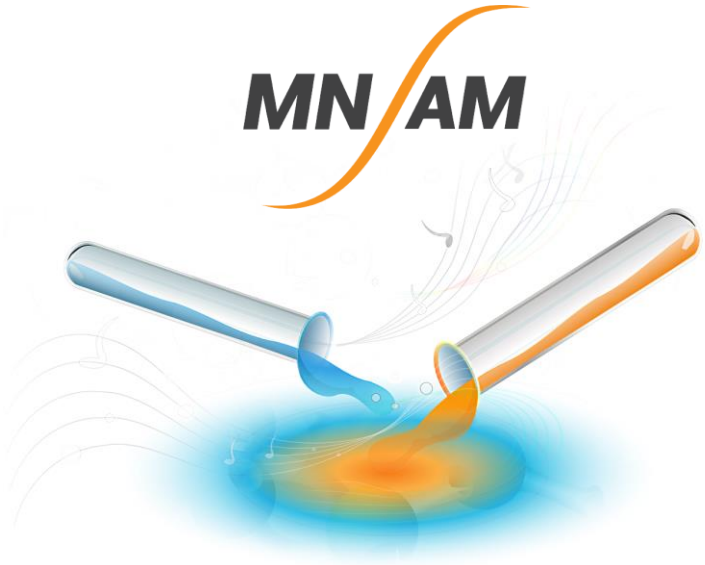


Chemotype Editor

Getting Started

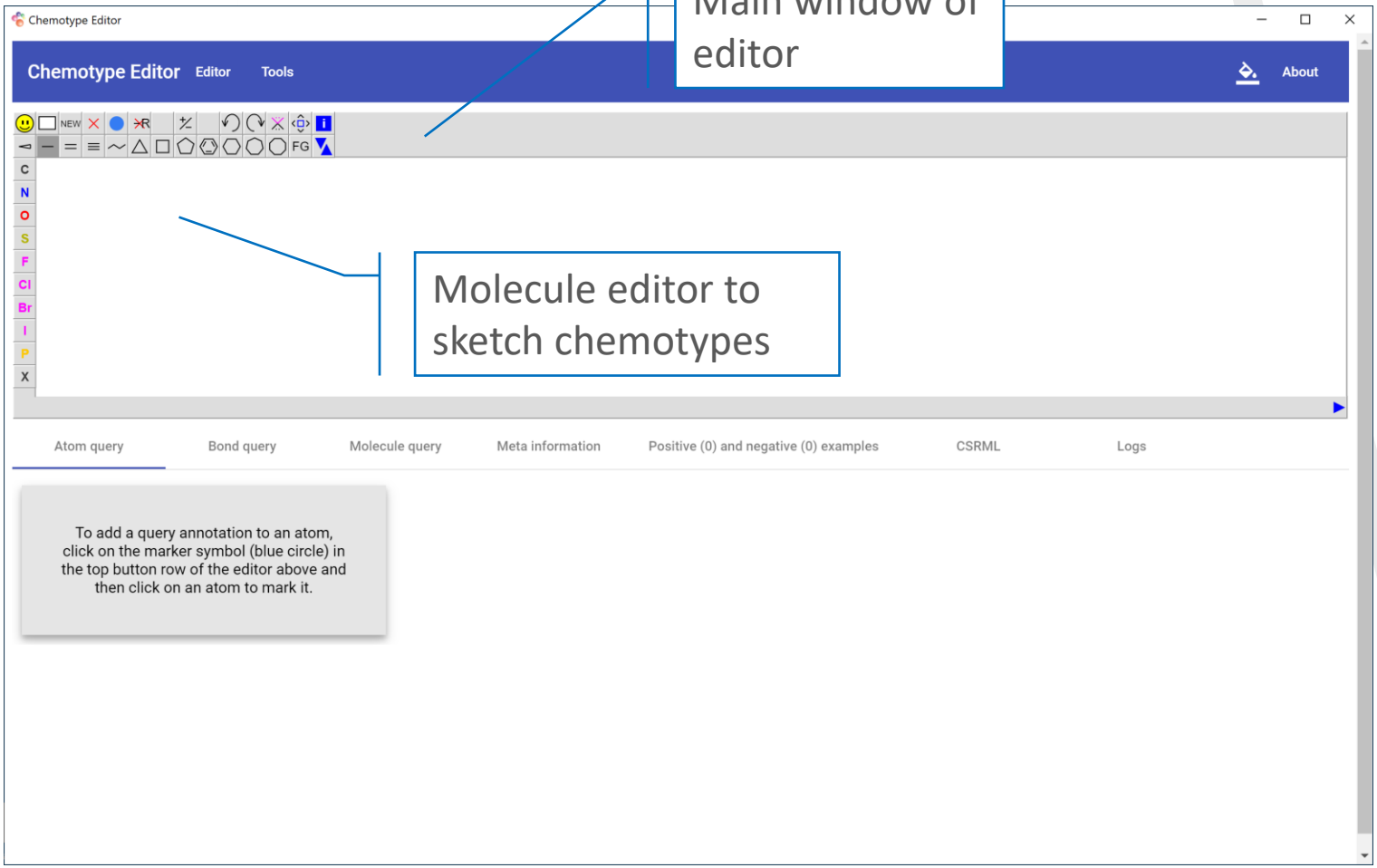
September 2023

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

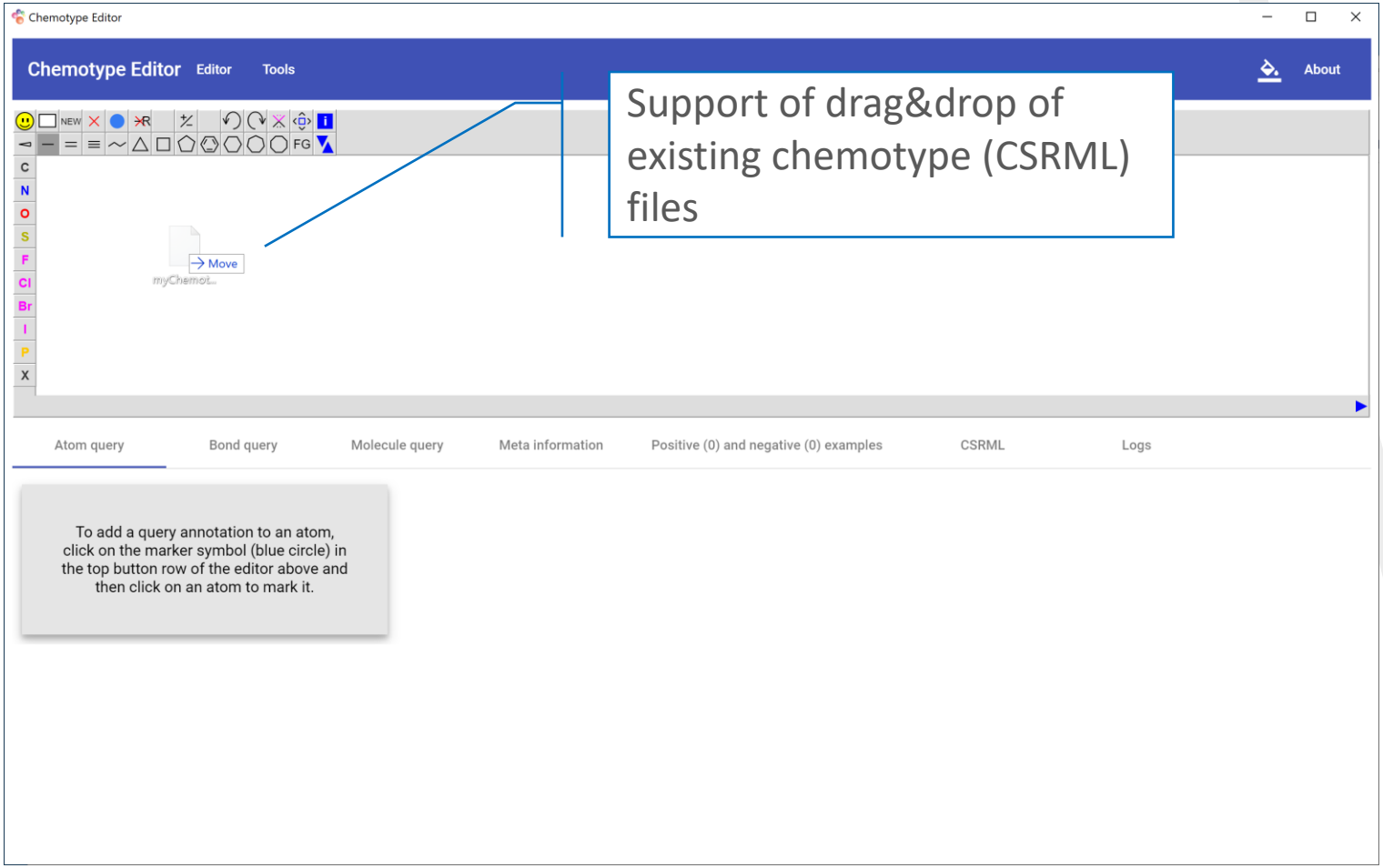
Chemotype Editor

- Start page



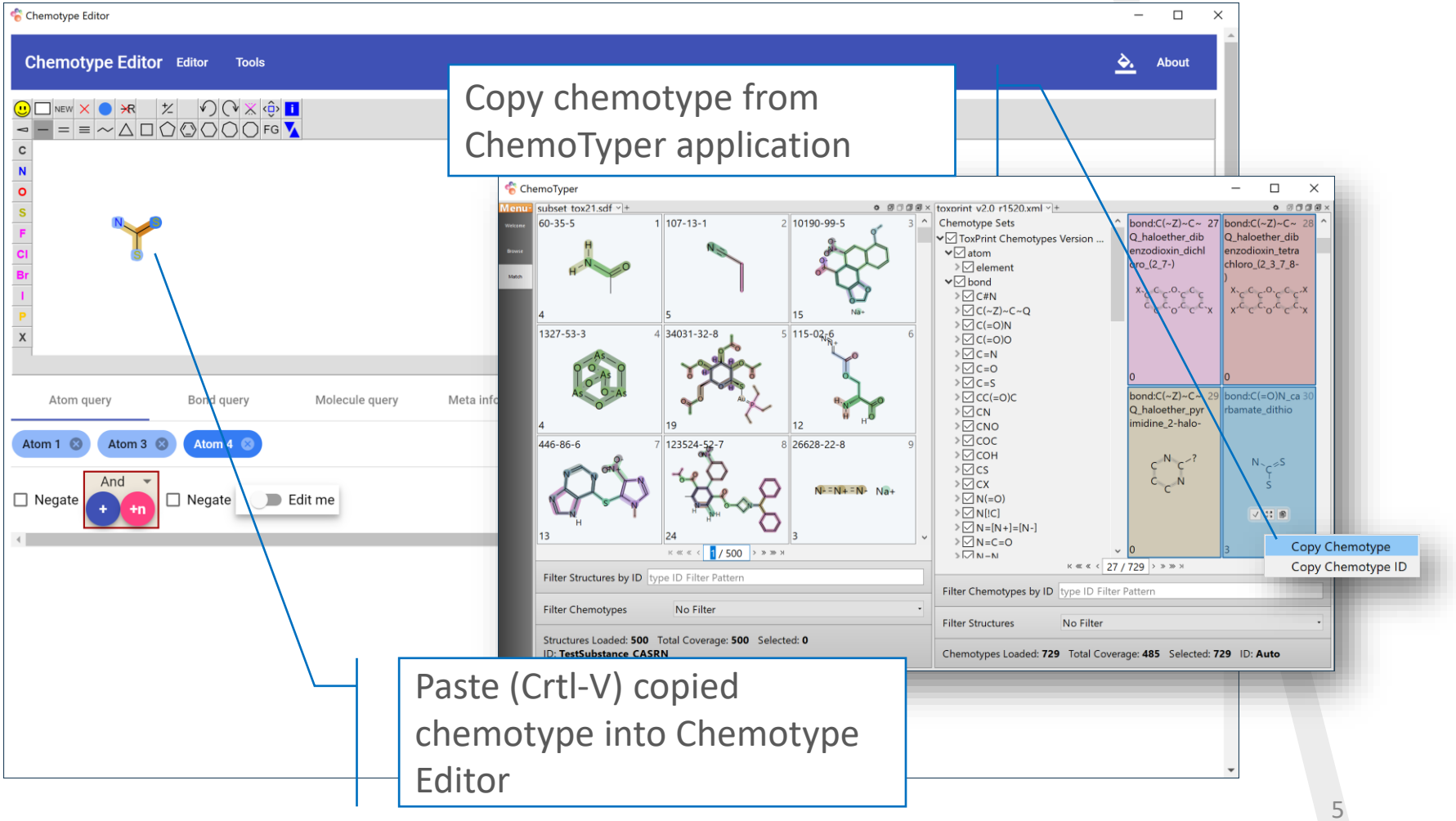
Chemotype Editor

- Load existing chemotype files



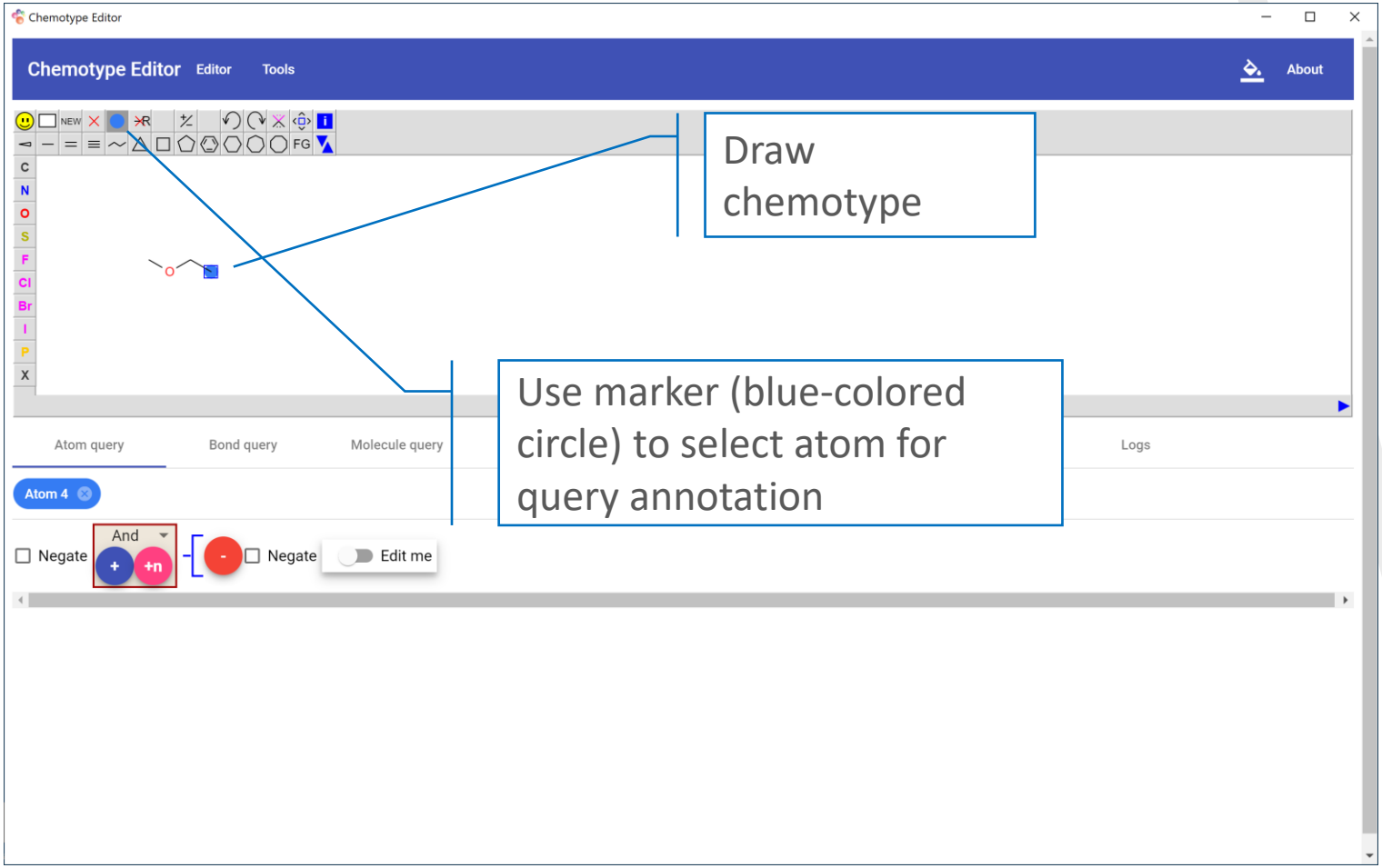
Chemotype Editor

- Copy & paste chemotype from ChemoTyper application



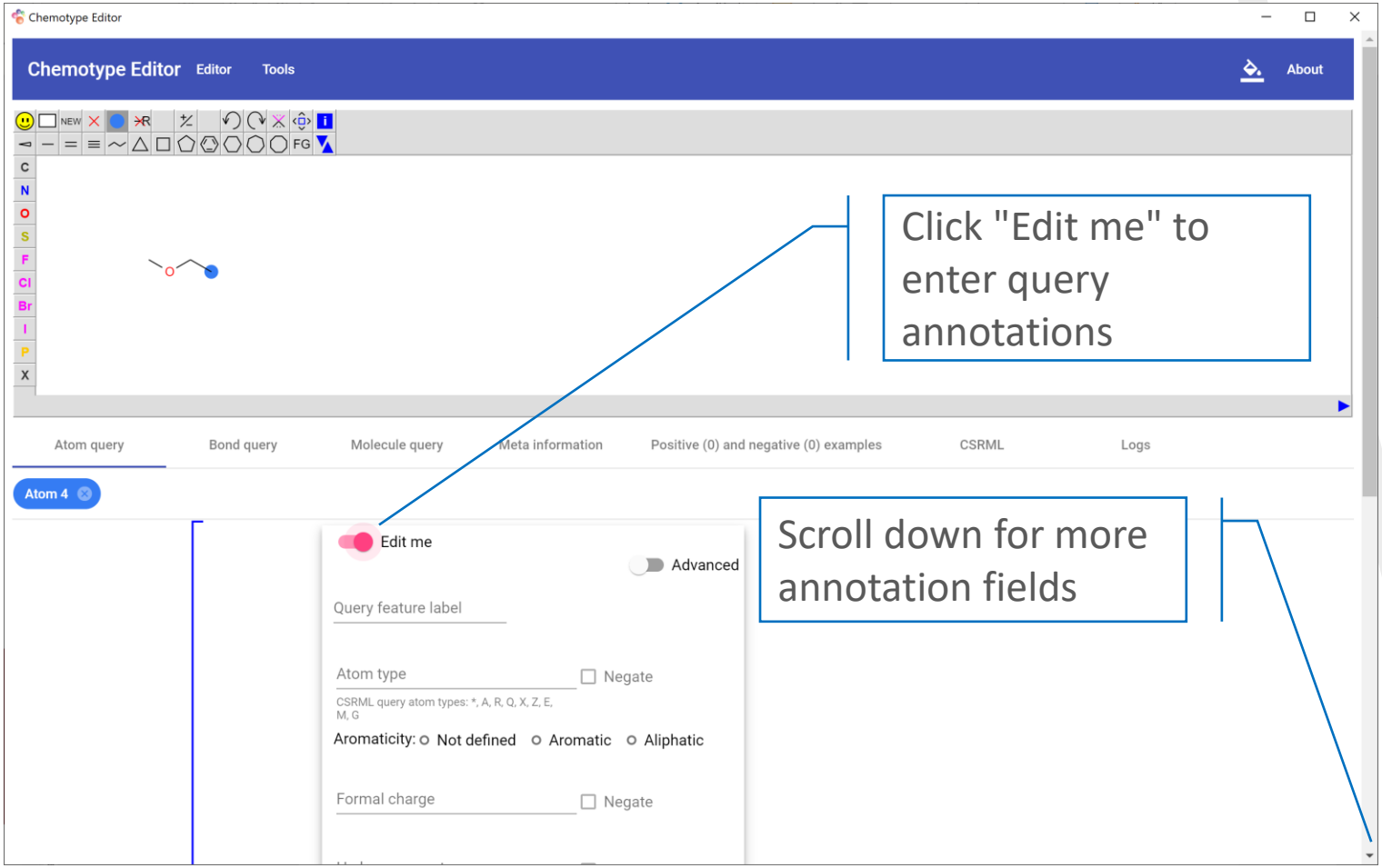
Chemotype Editor

- Draw chemotype and edit atom query annotations



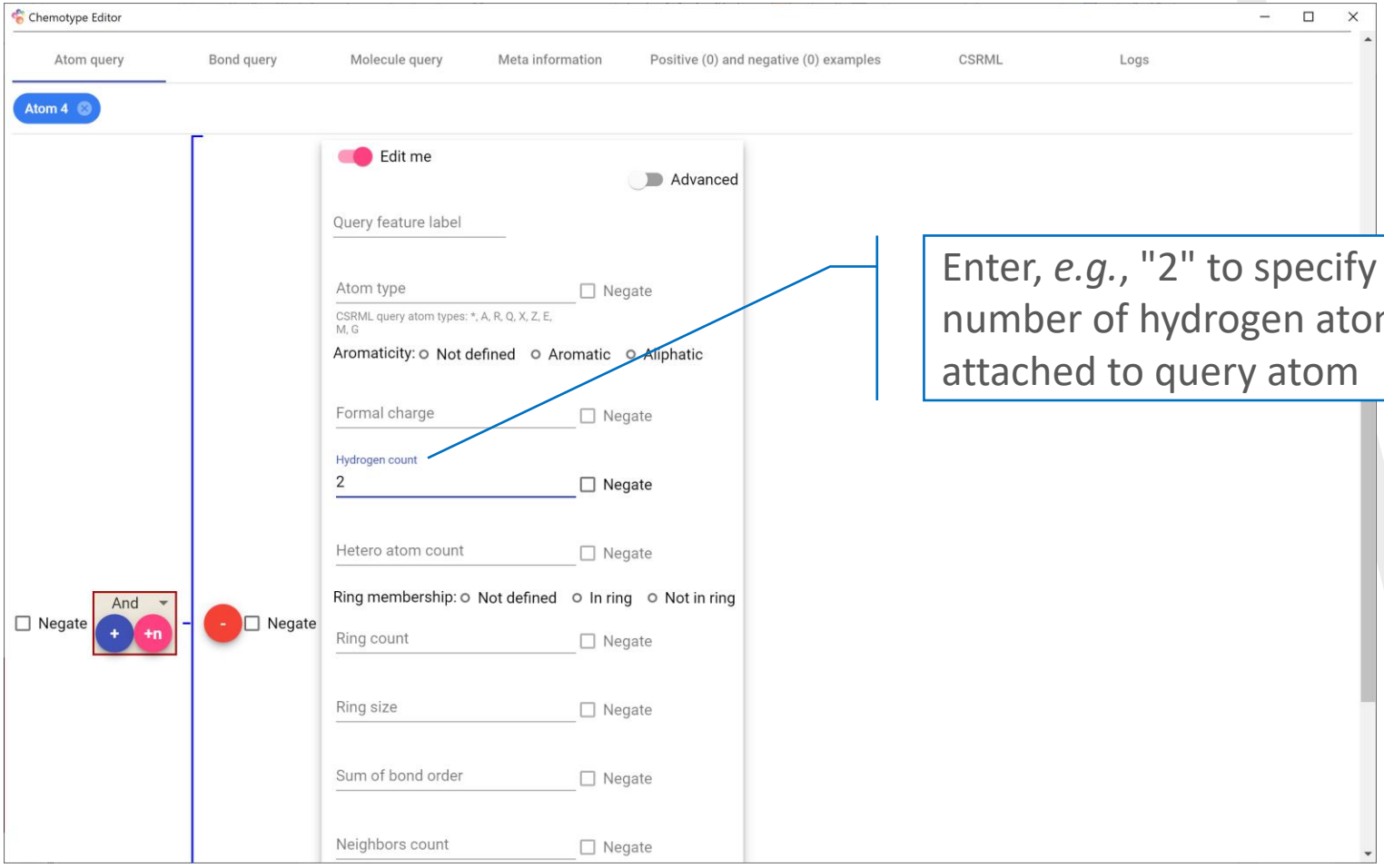
Chemotype Editor

- Atom query annotations



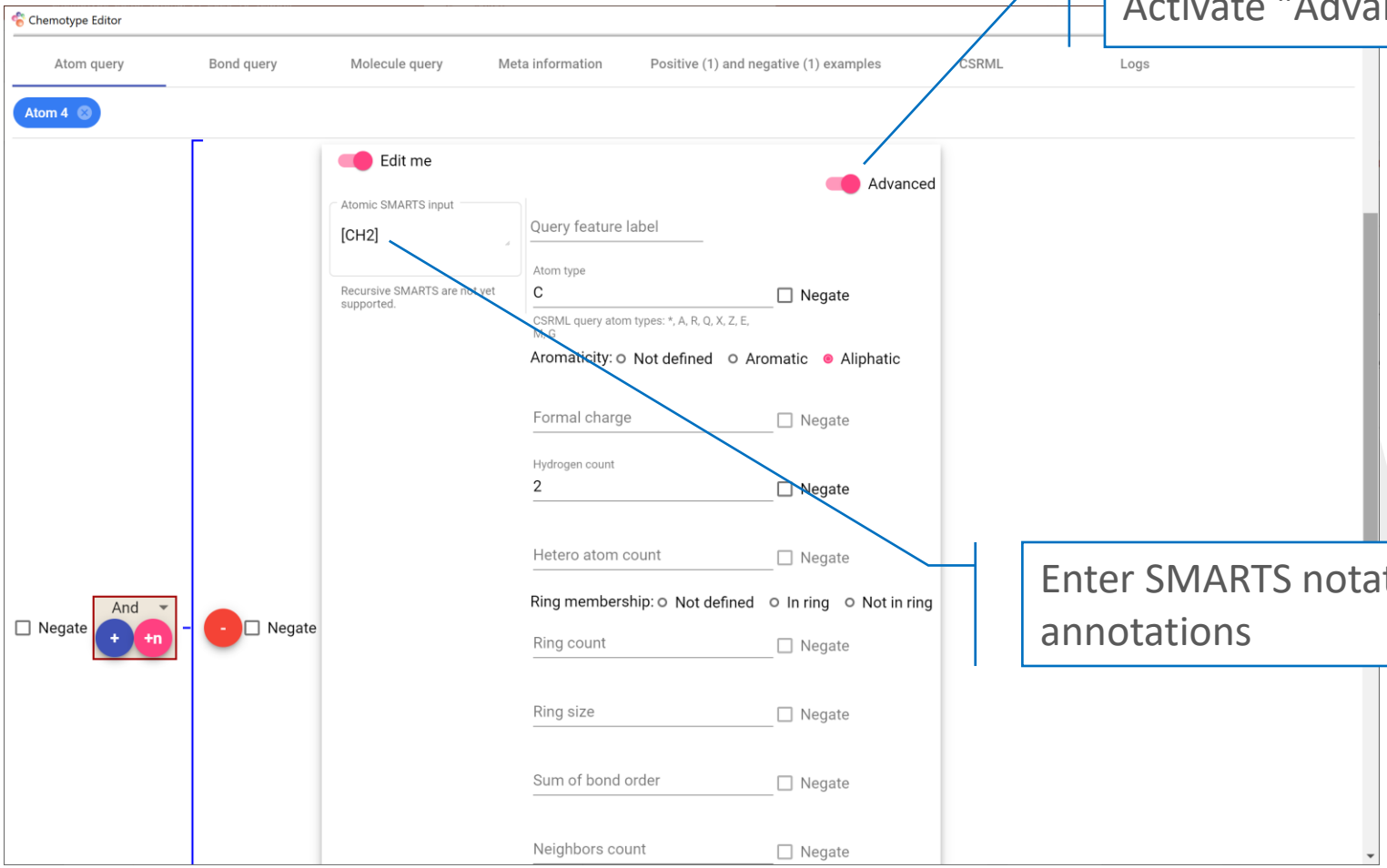
Chemotype Editor

- Atom query annotations



Chemotype Editor

- Atom query annotations from SMARTS

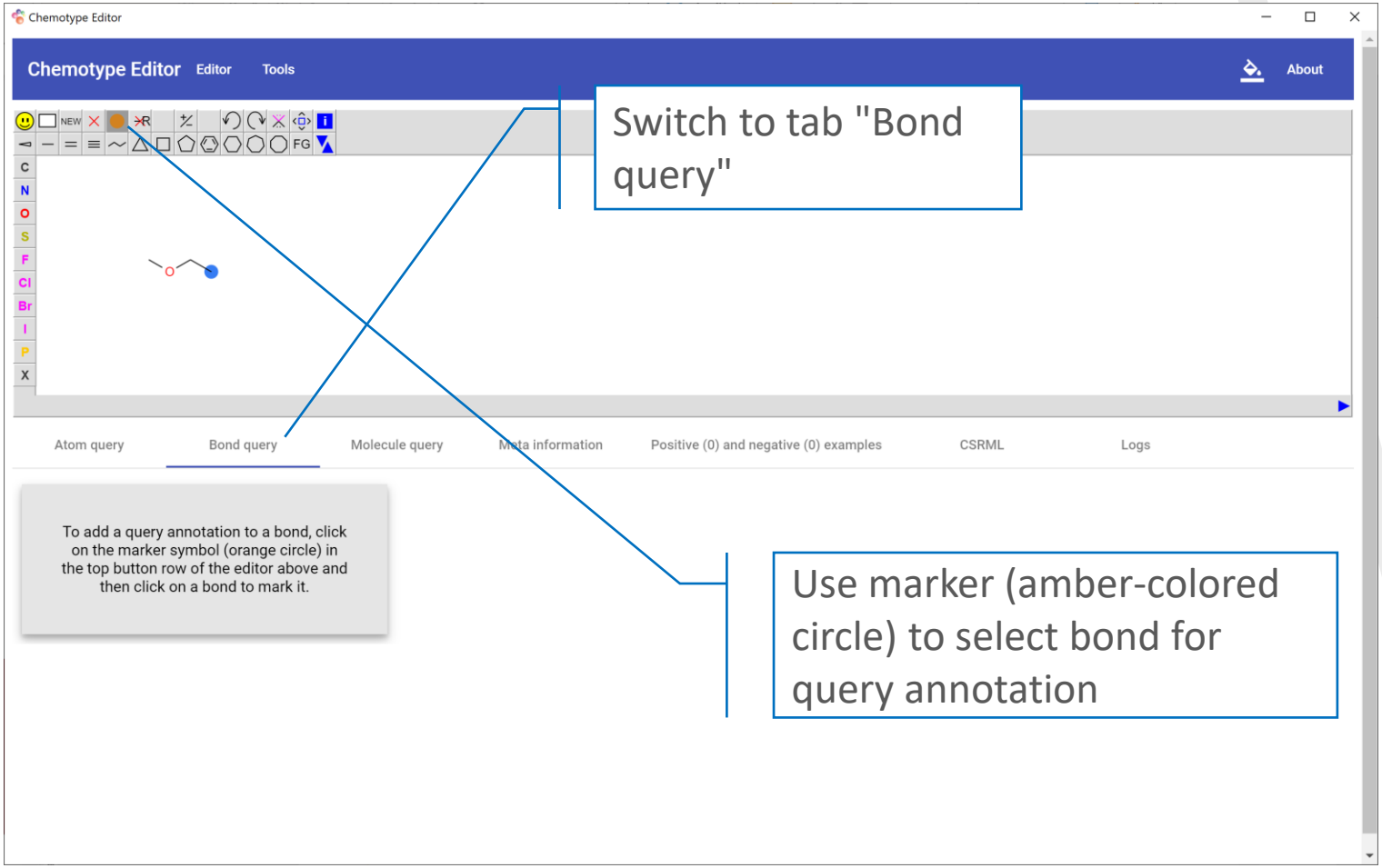


Activate "Advanced"

Enter SMARTS notation to set annotations

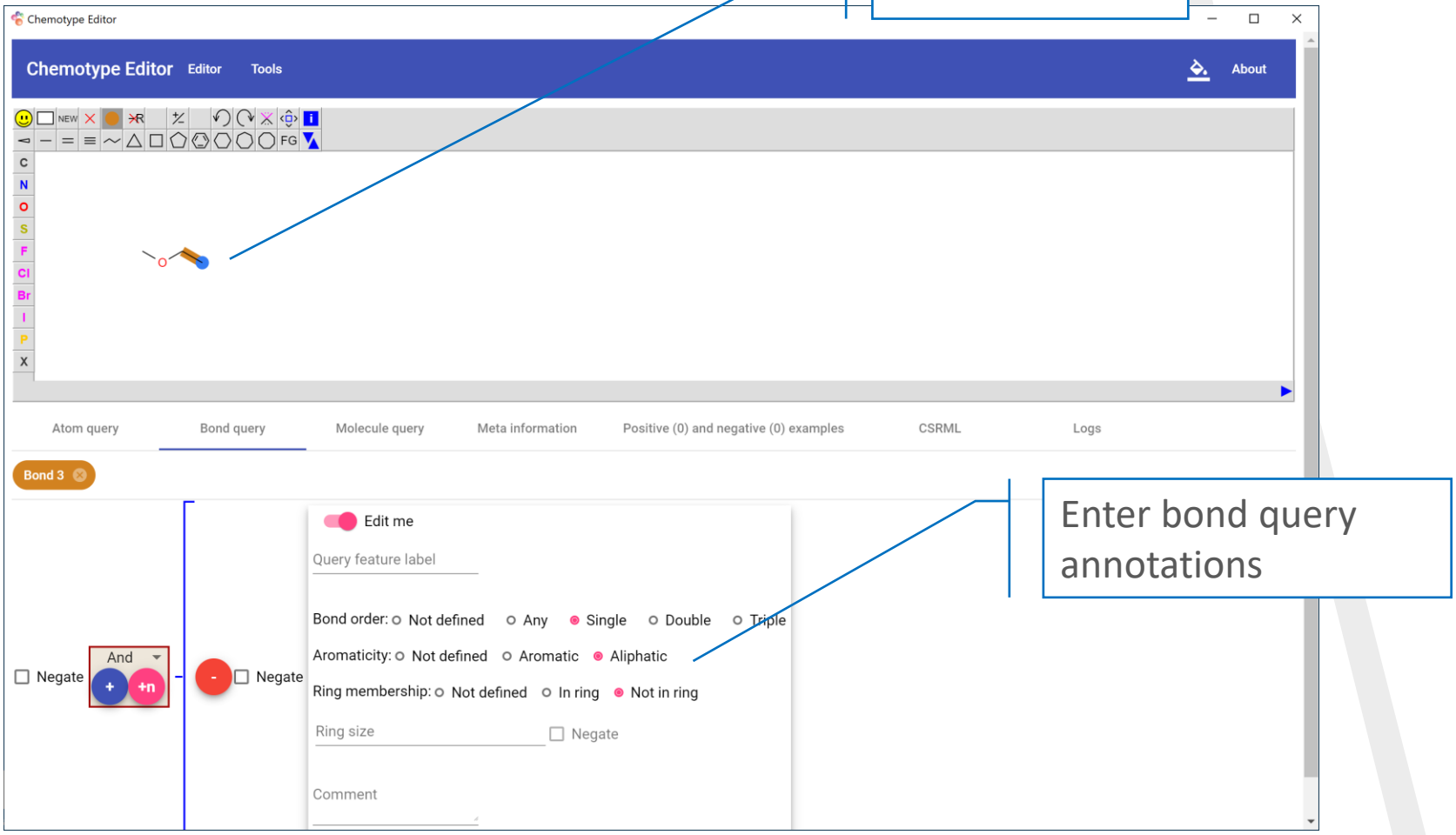
Chemotype Editor

- Bond query annotations



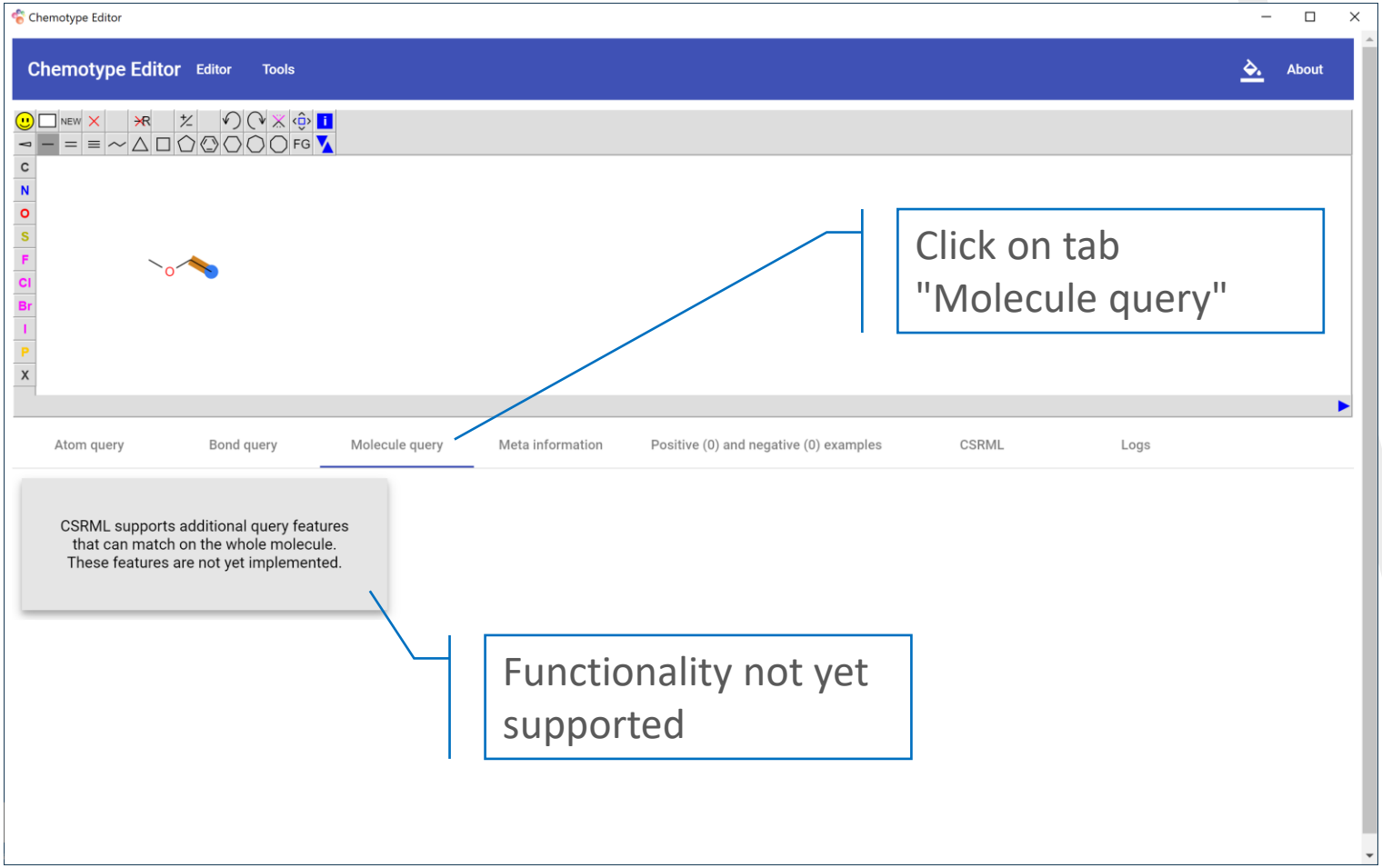
Chemotype Editor

- Bond query annotations



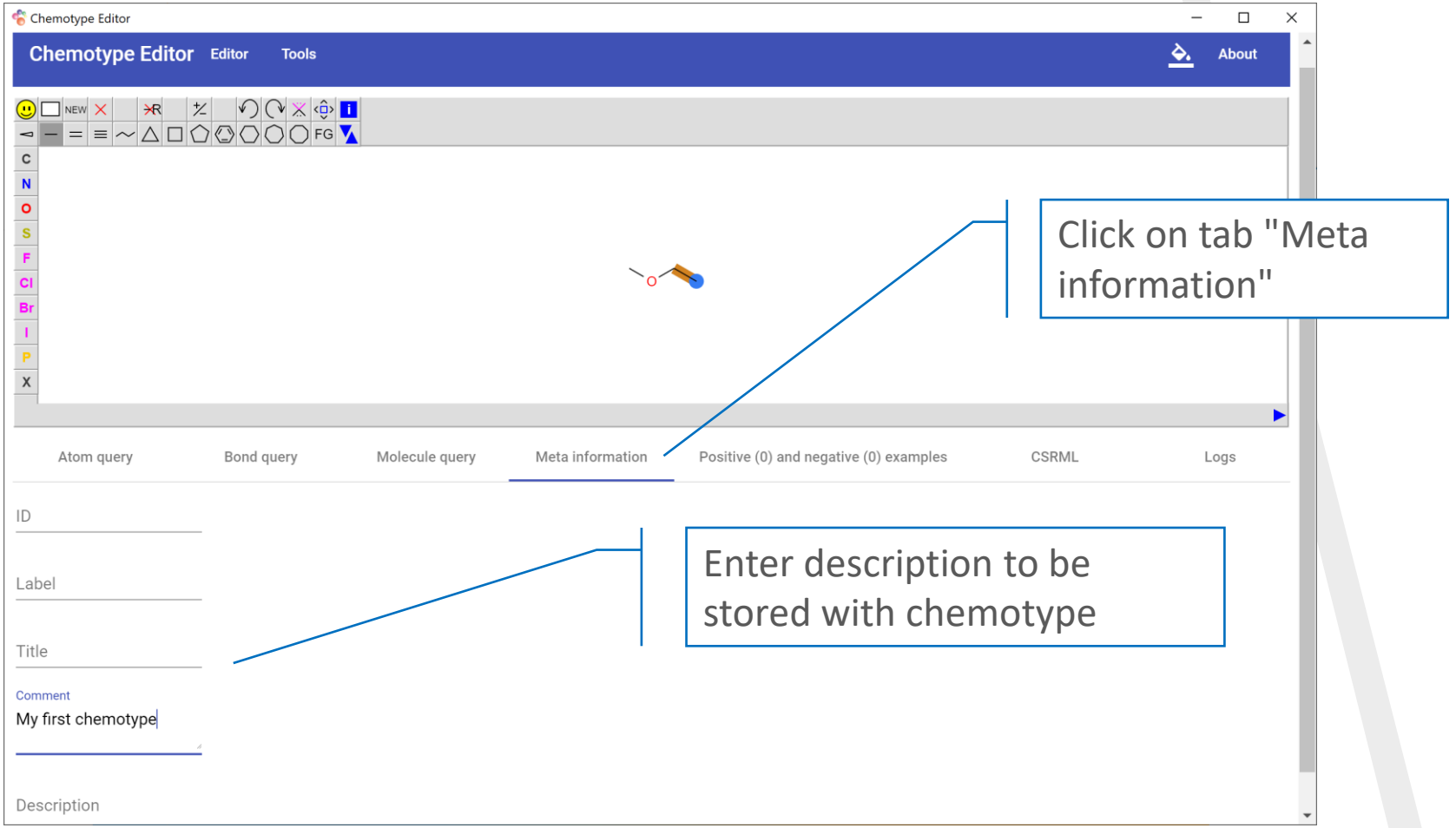
Chemotype Editor

- Molecule query annotations



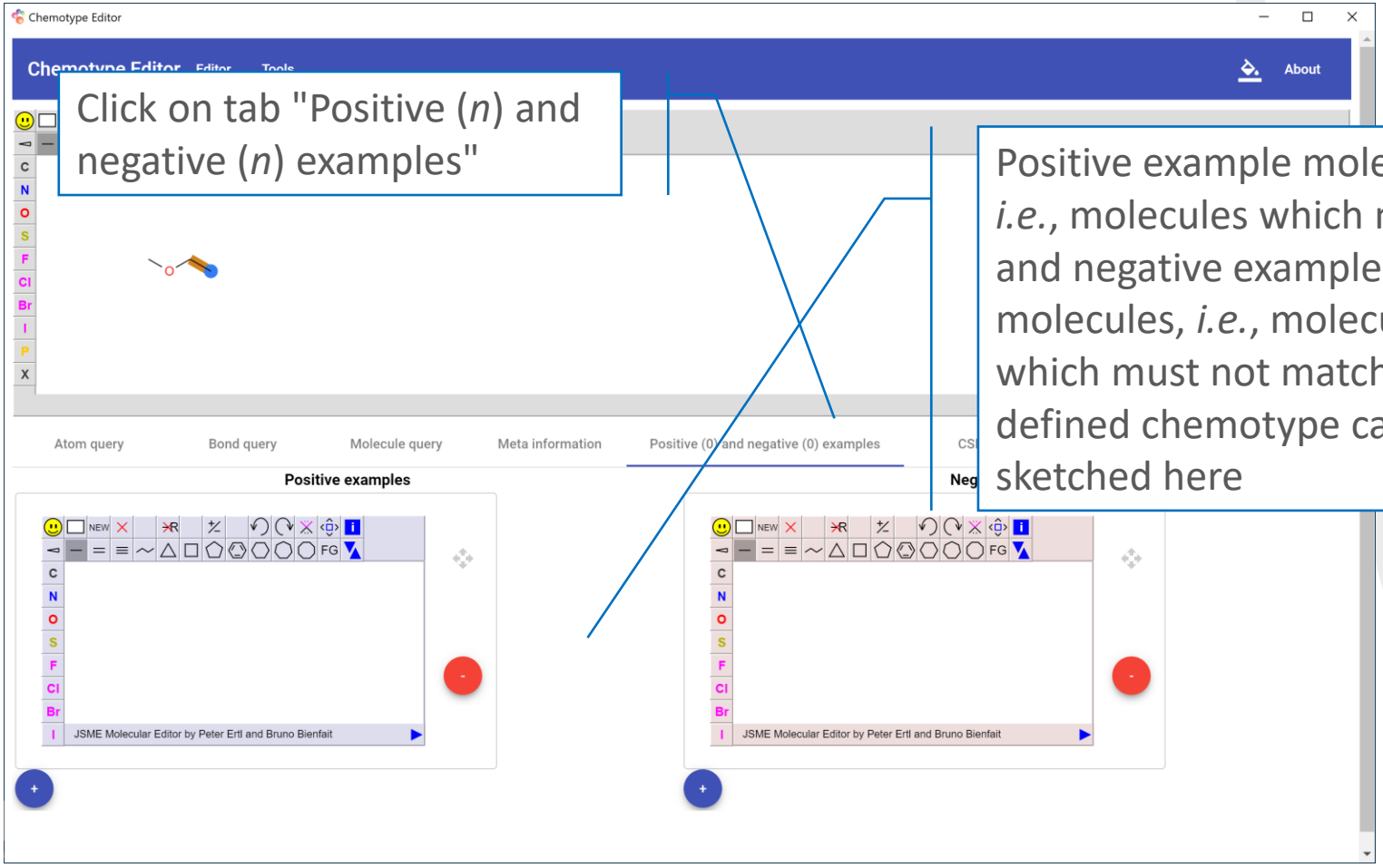
Chemotype Editor

- Meta information



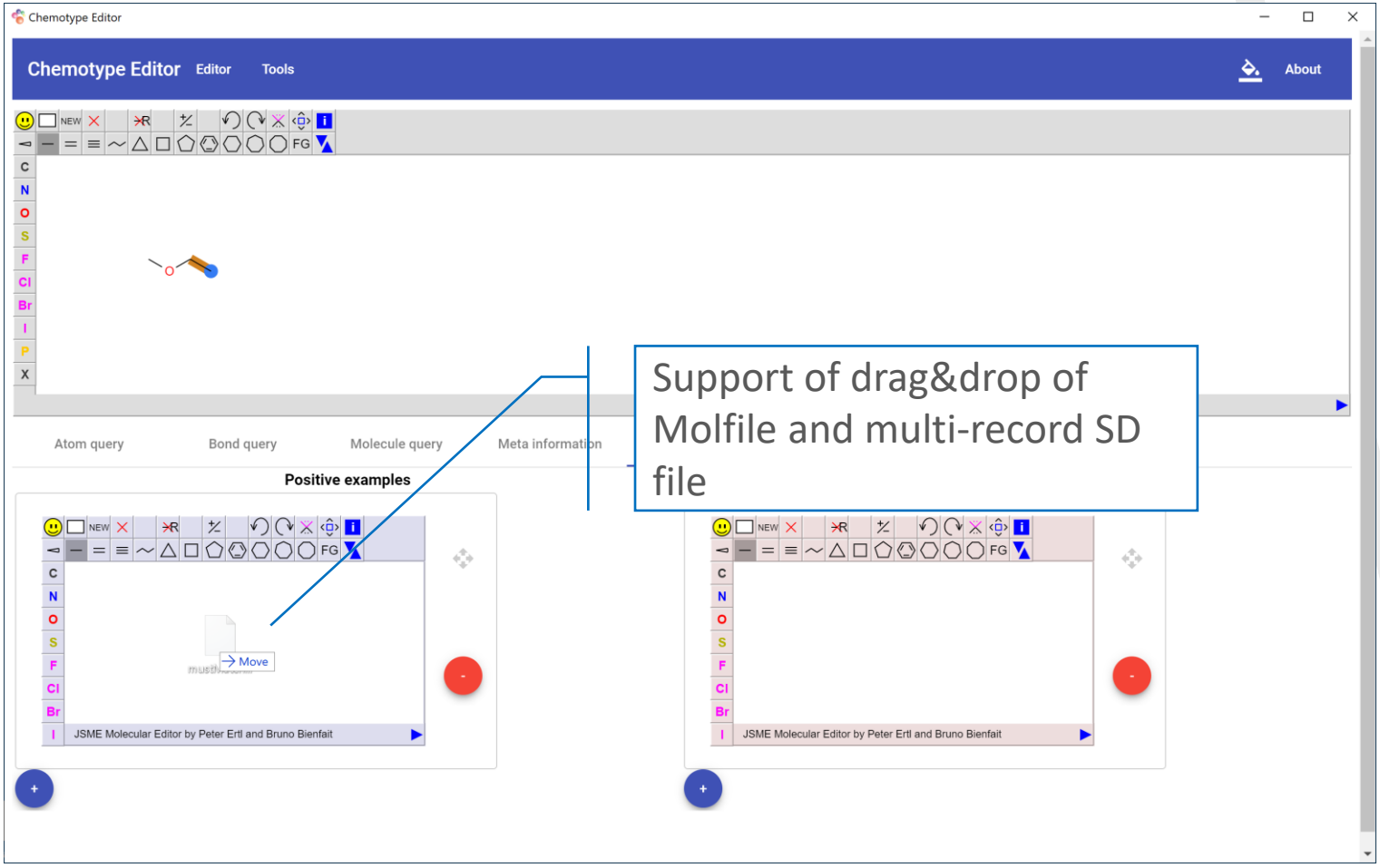
Chemotype Editor

- Positive and negative example (required)



Chemotype Editor

- Positive and negative example (required)

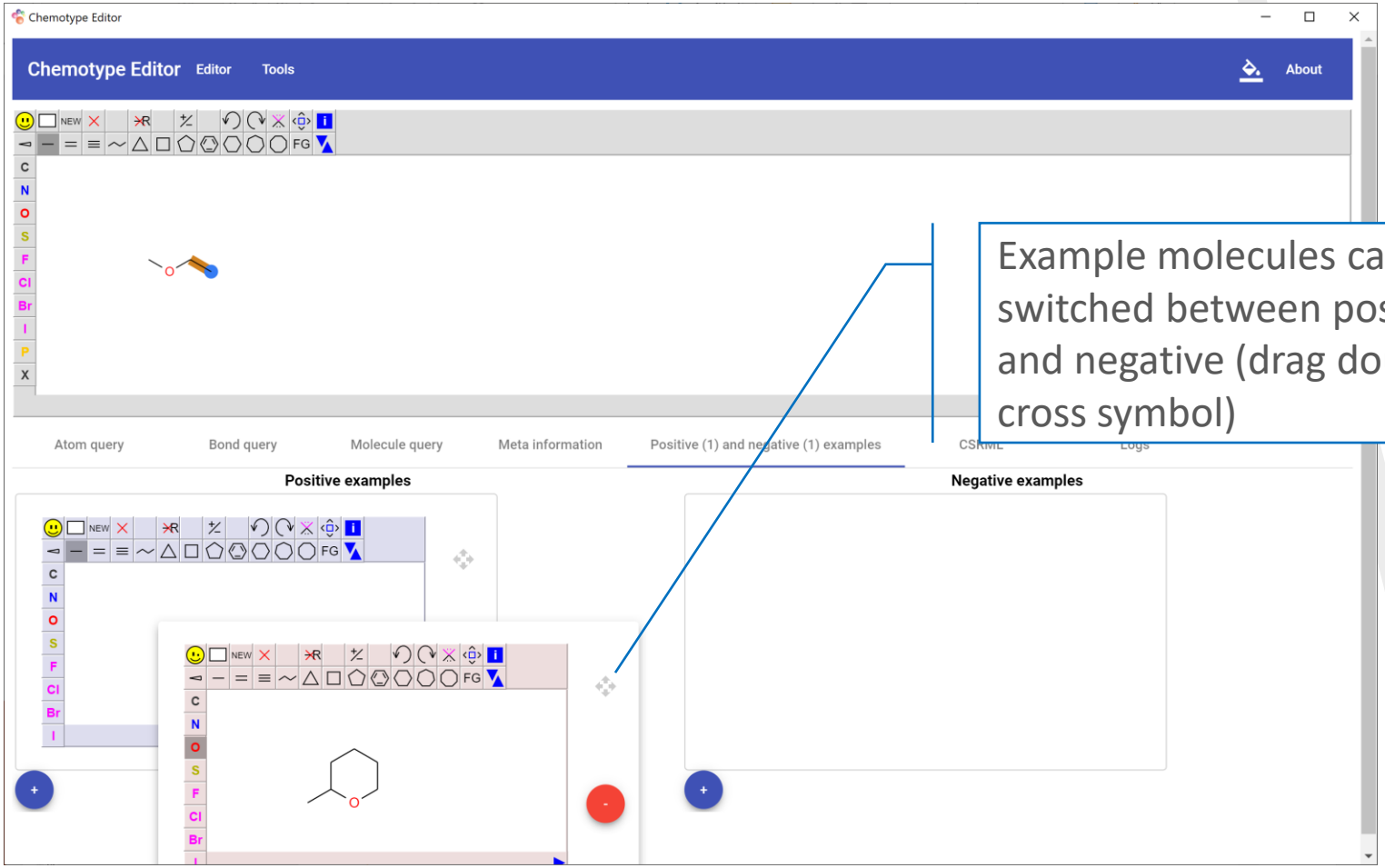


Chemotype Editor

- Positive and negative example (required)

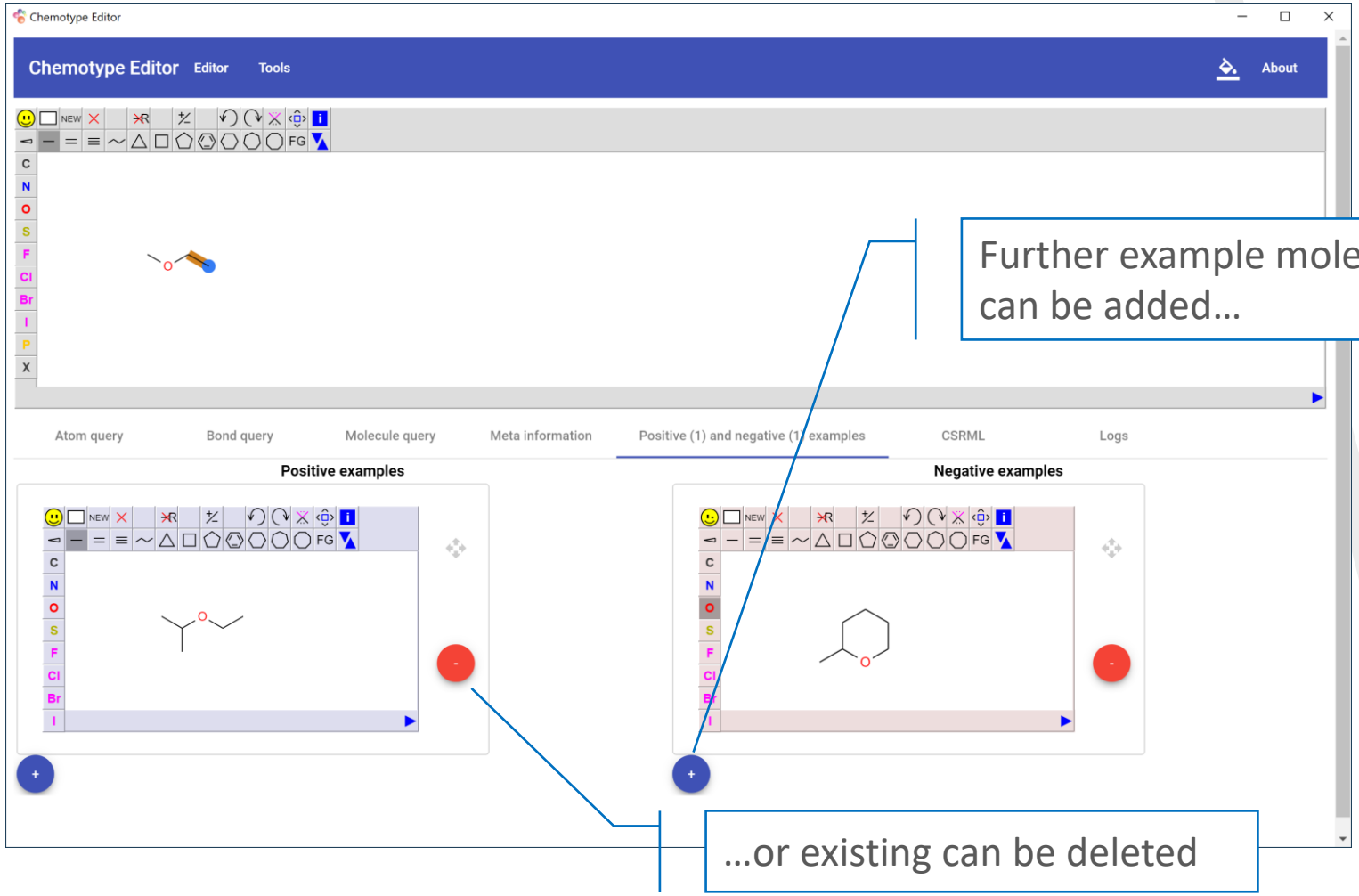
Chemotype Editor

- Positive and negative example (required)



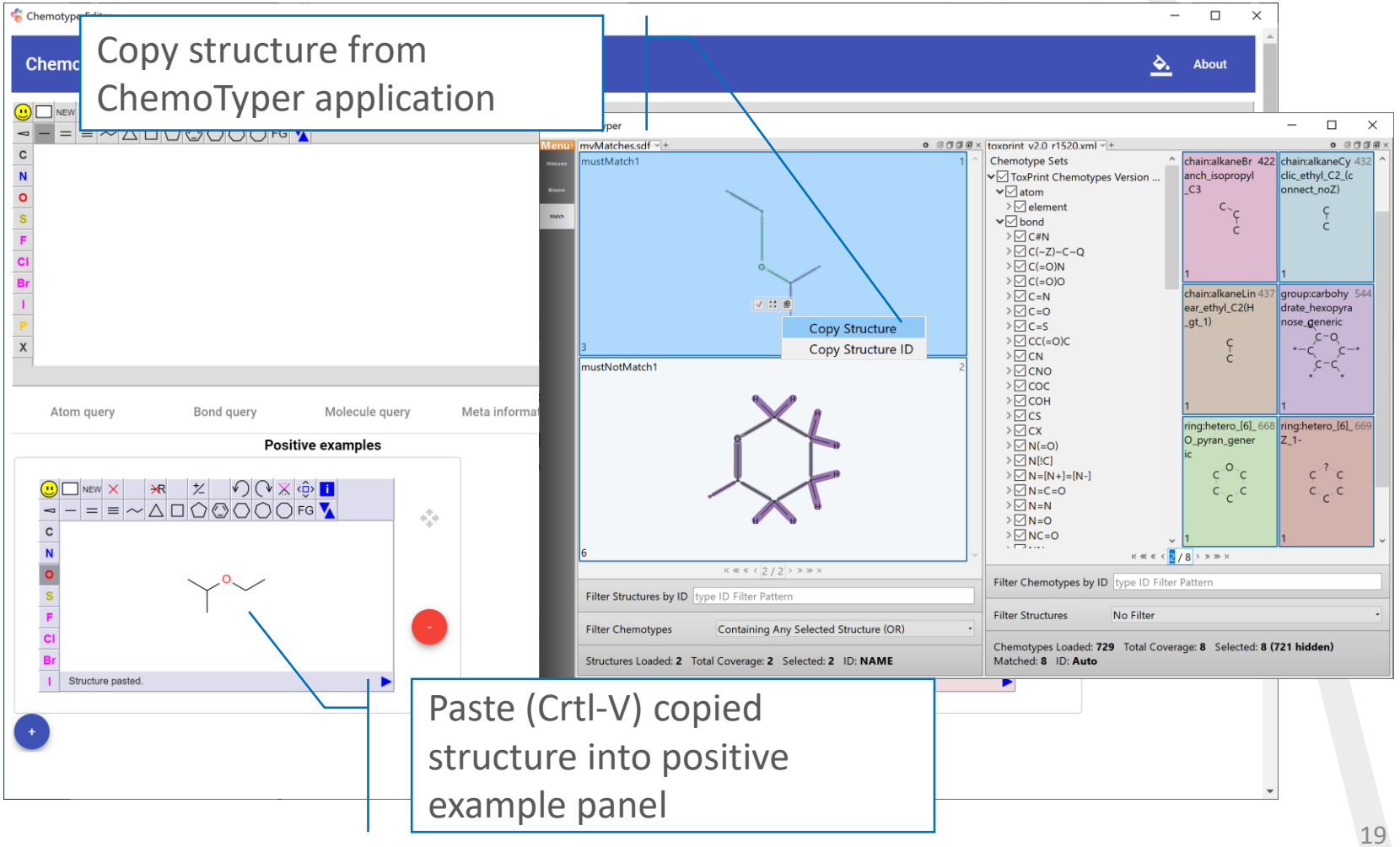
Chemotype Editor

- Positive and negative example (required)



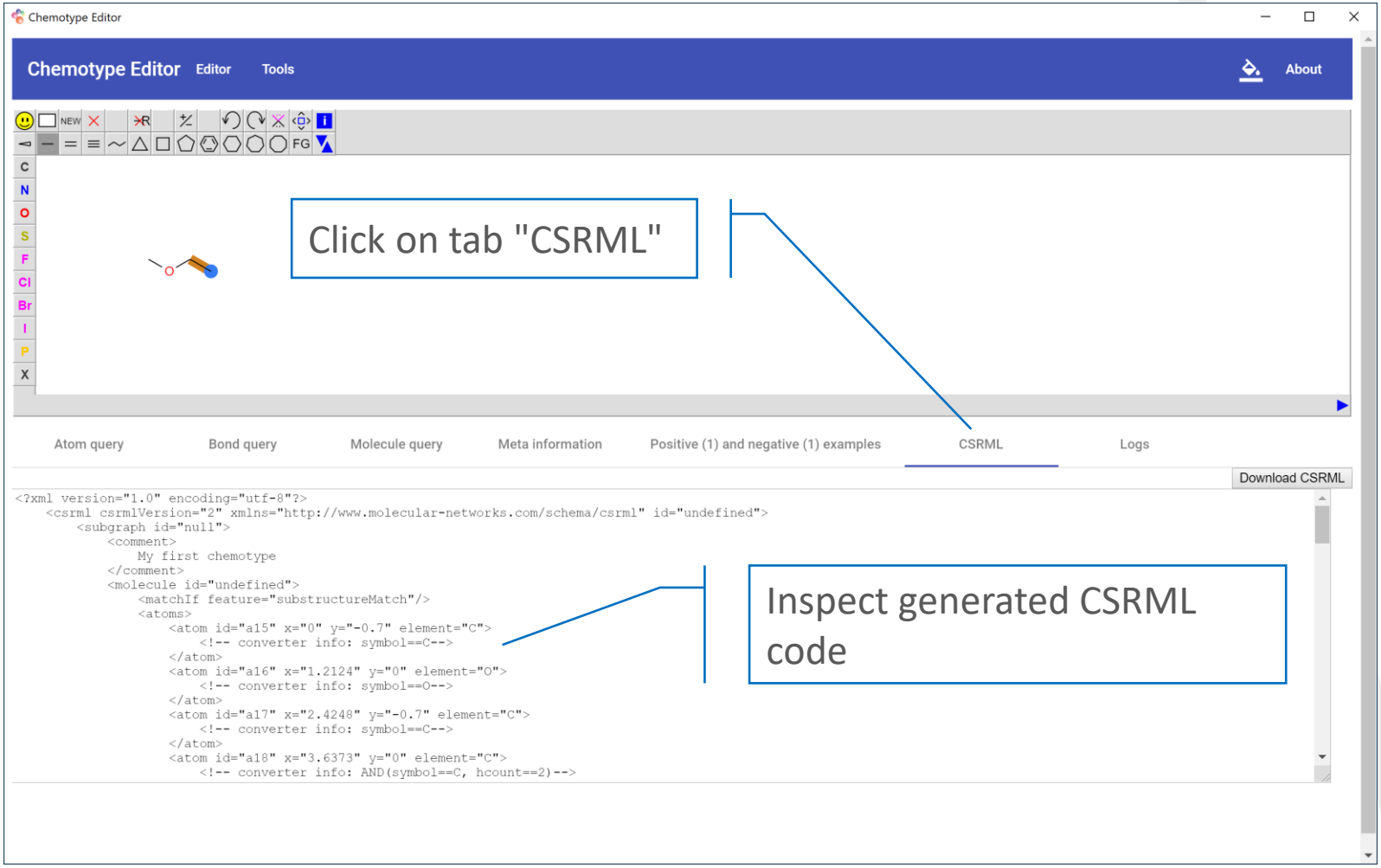
Chemotype Editor

- Copy positive/negative example from ChemoTyper app



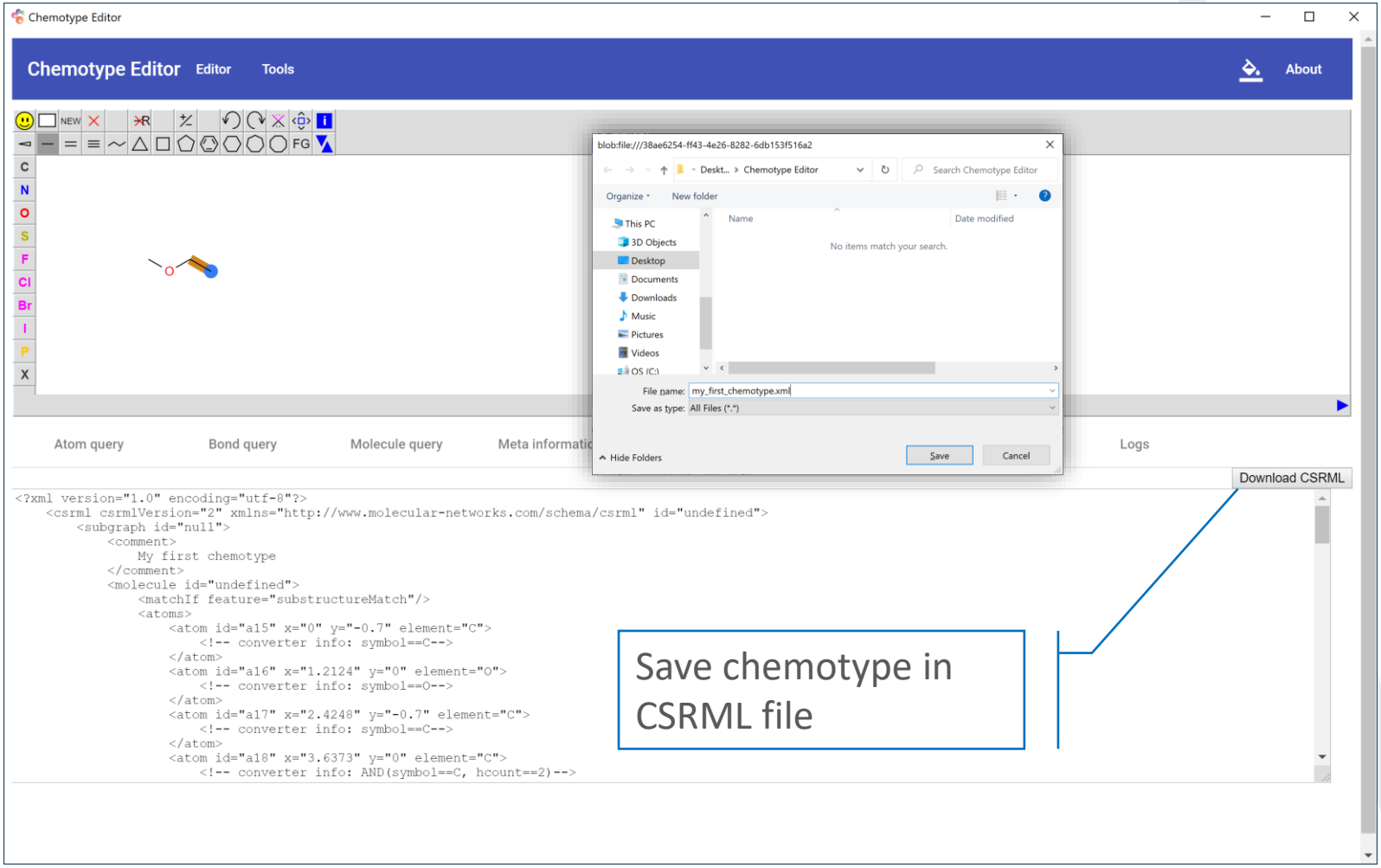
Chemotype Editor

- Resulting CSRML code



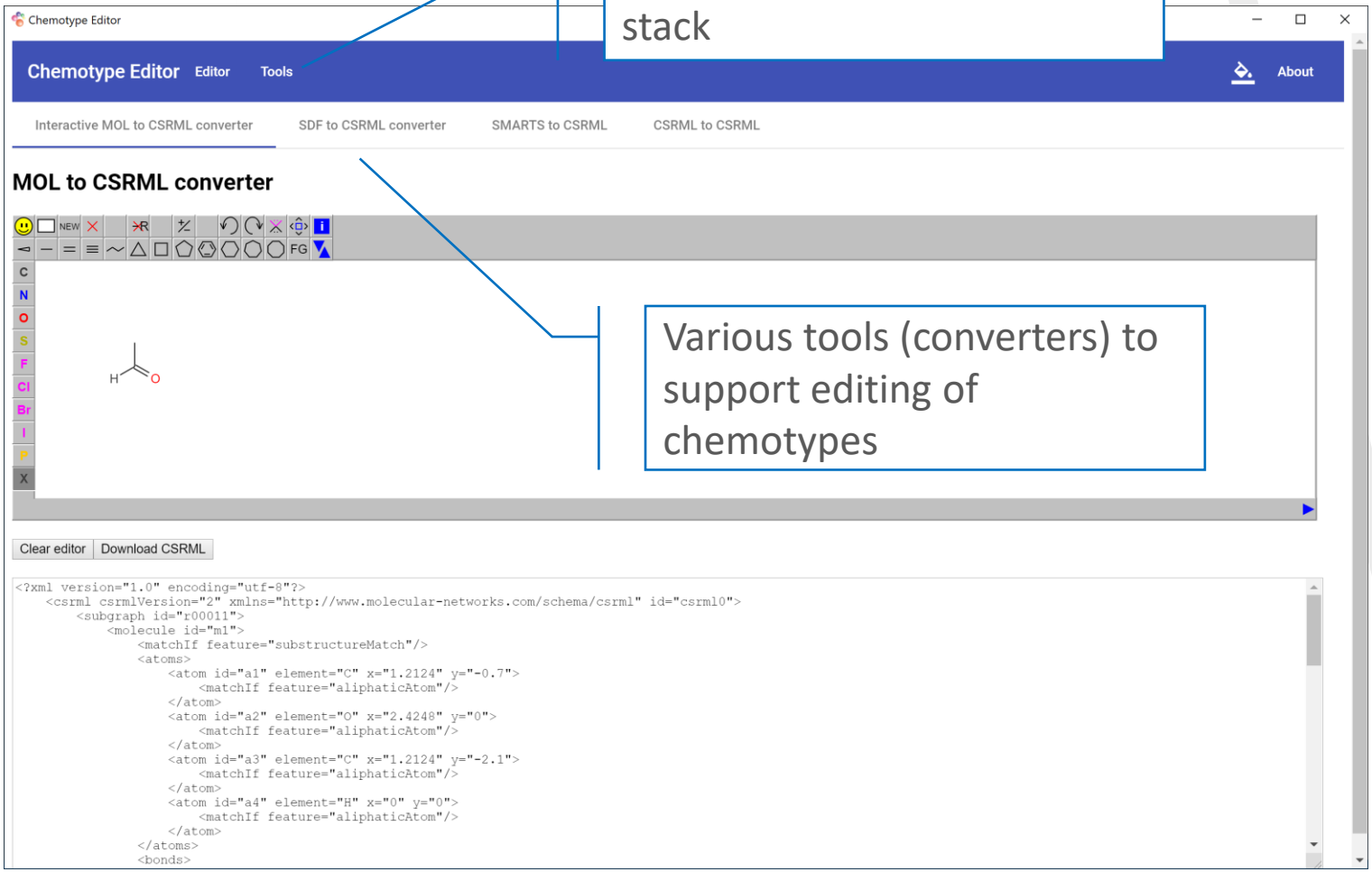
Chemotype Editor

- Download CSRML file



Chemotype Editor

- Tools



Click on "Tools" to open tool stack

Various tools (converters) to support editing of chemotypes

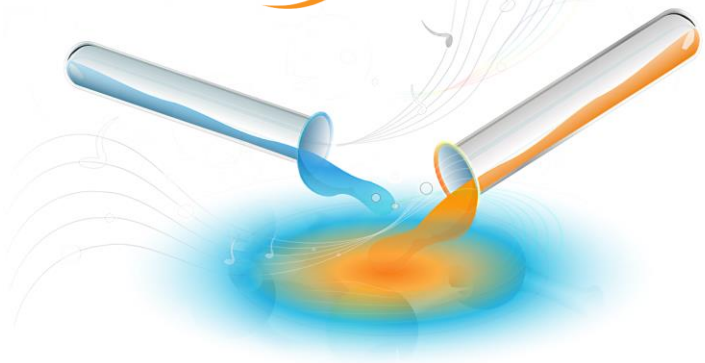
Chemotype Editor

- 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

Chemotype Editor

- 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

MN AM



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