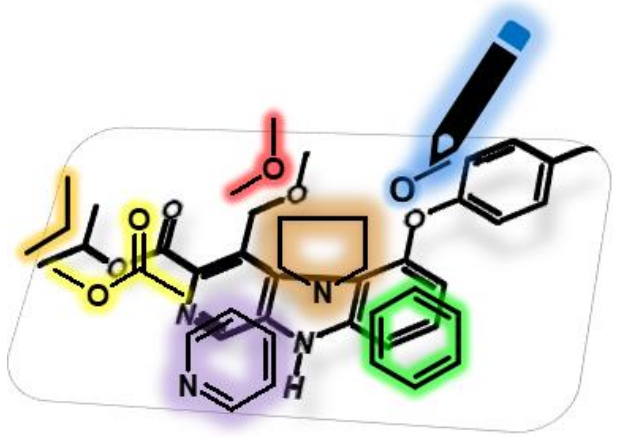


Short Tutorial for Chemotype Editor

October 2023

MN AM

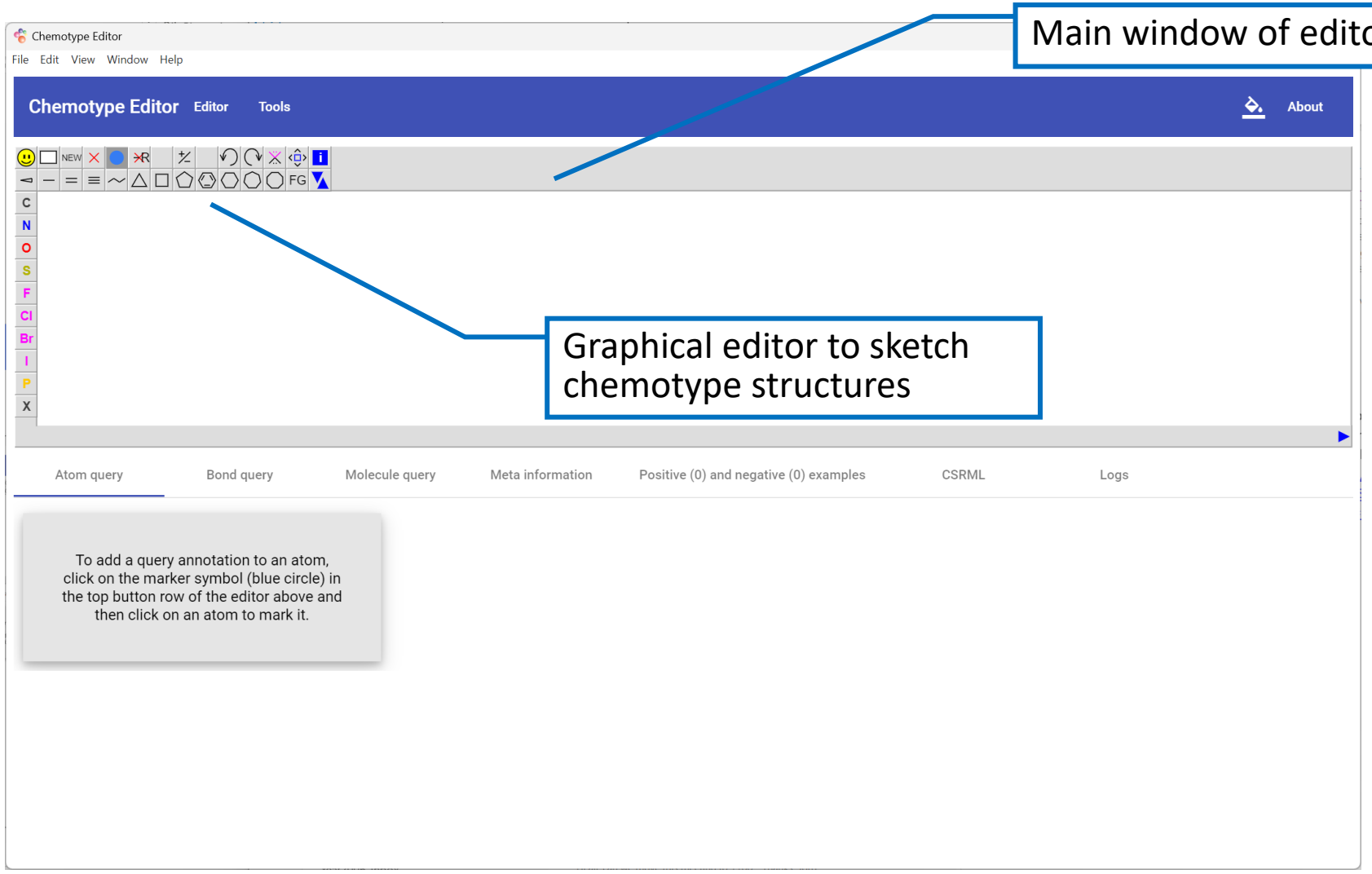
Introduction

- 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

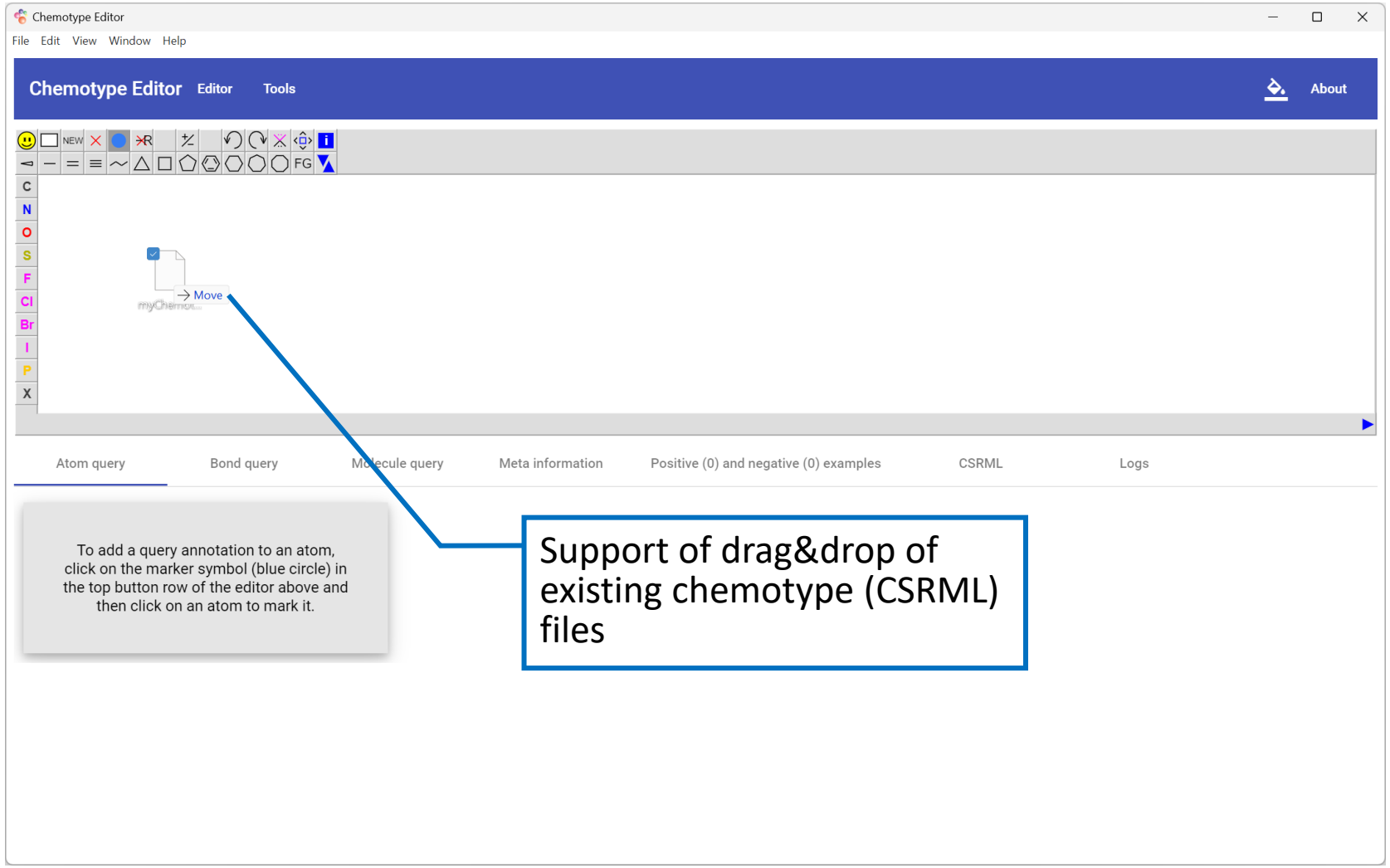
Installation

- 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

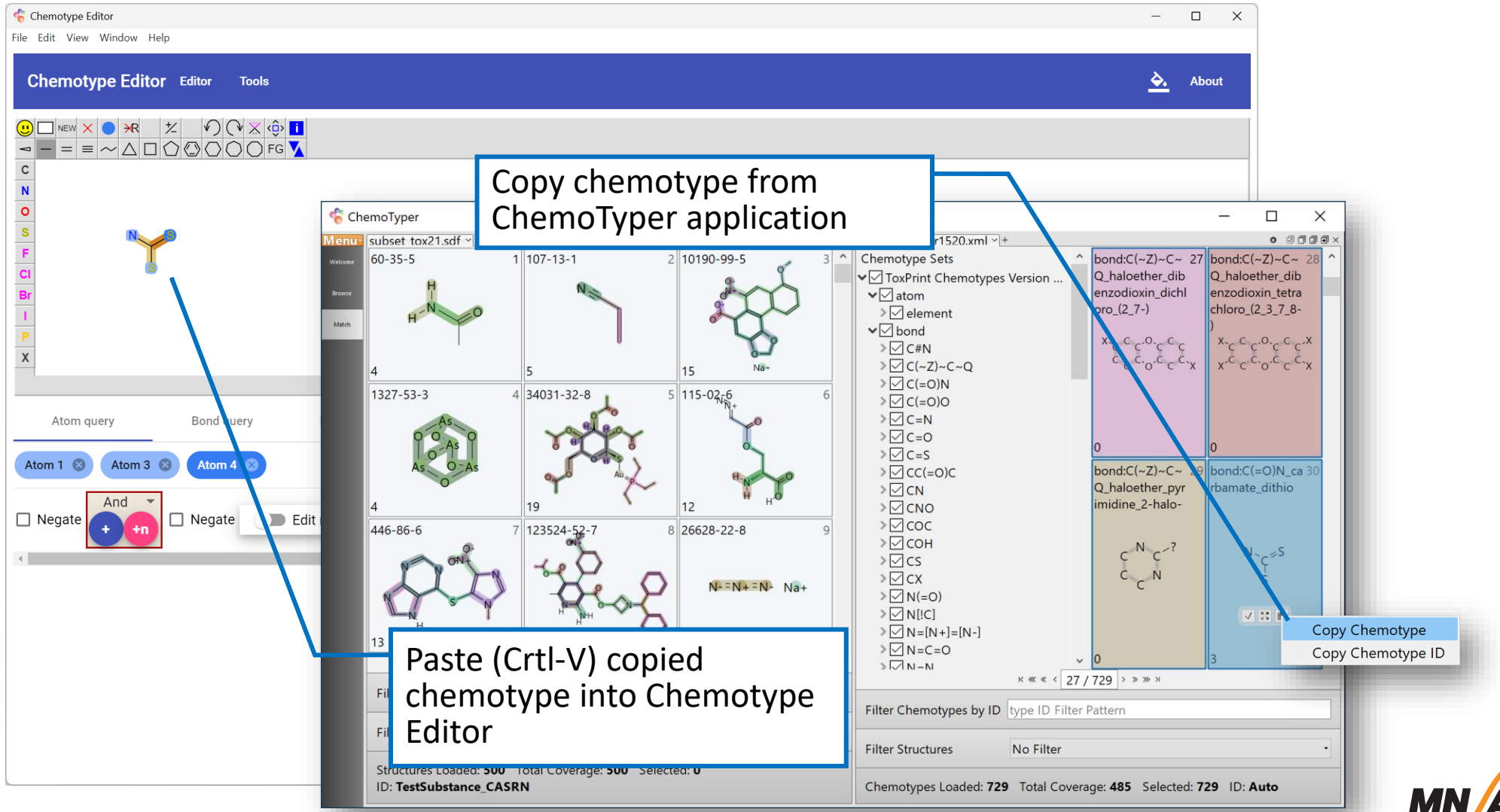
Start Page



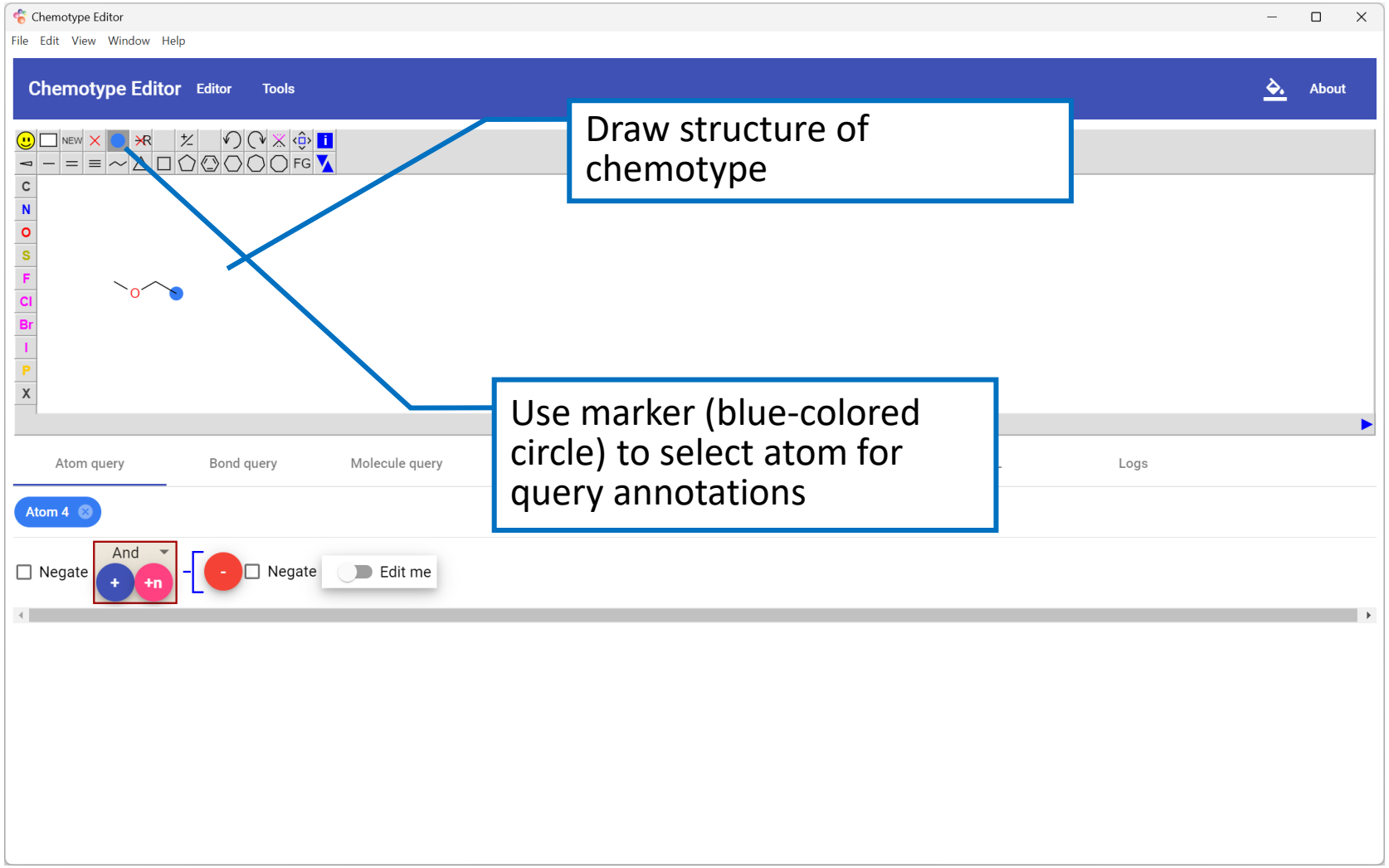
Load Chemotype File



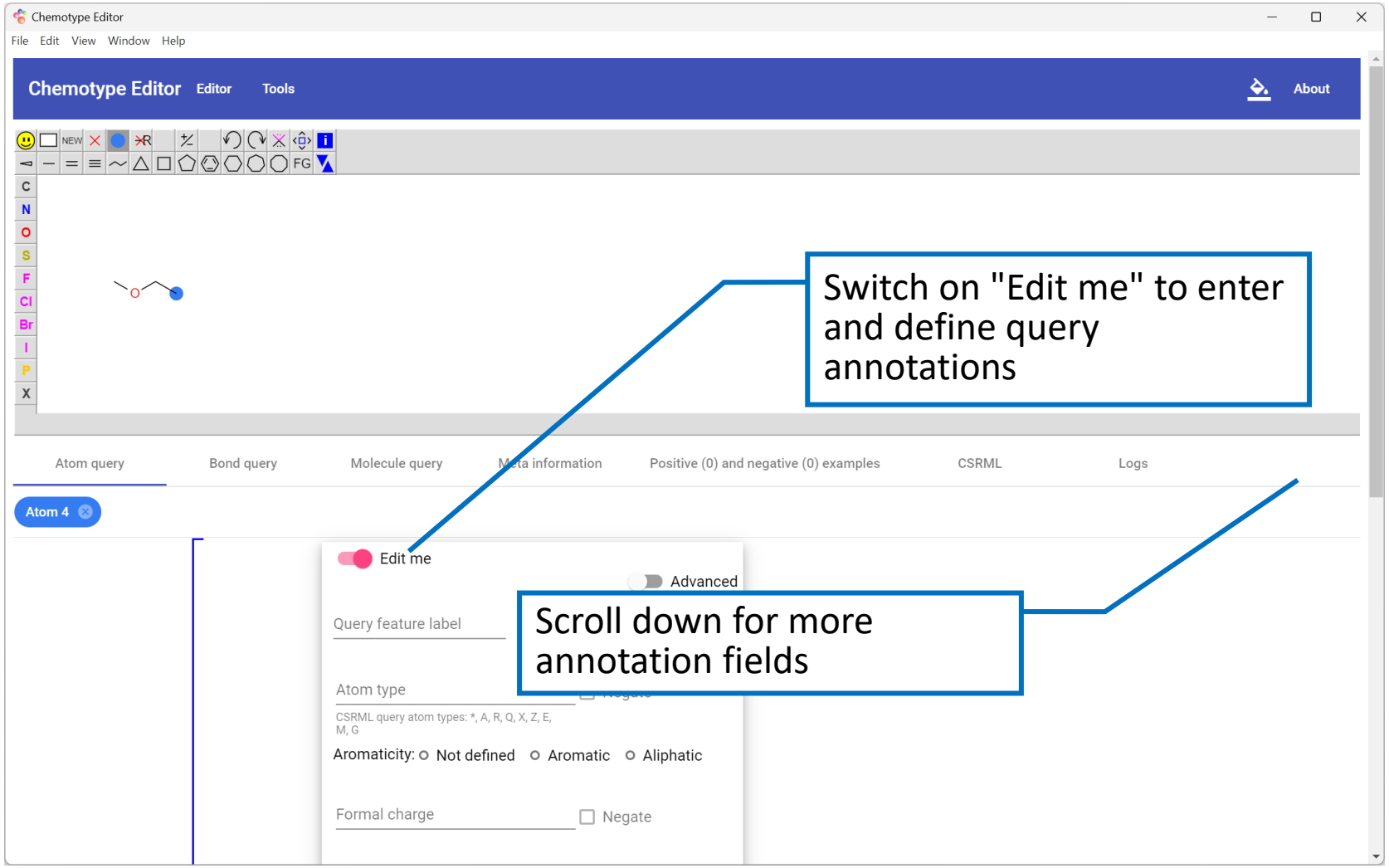
Copy&Paste Chemotype from ChemoTyper Application



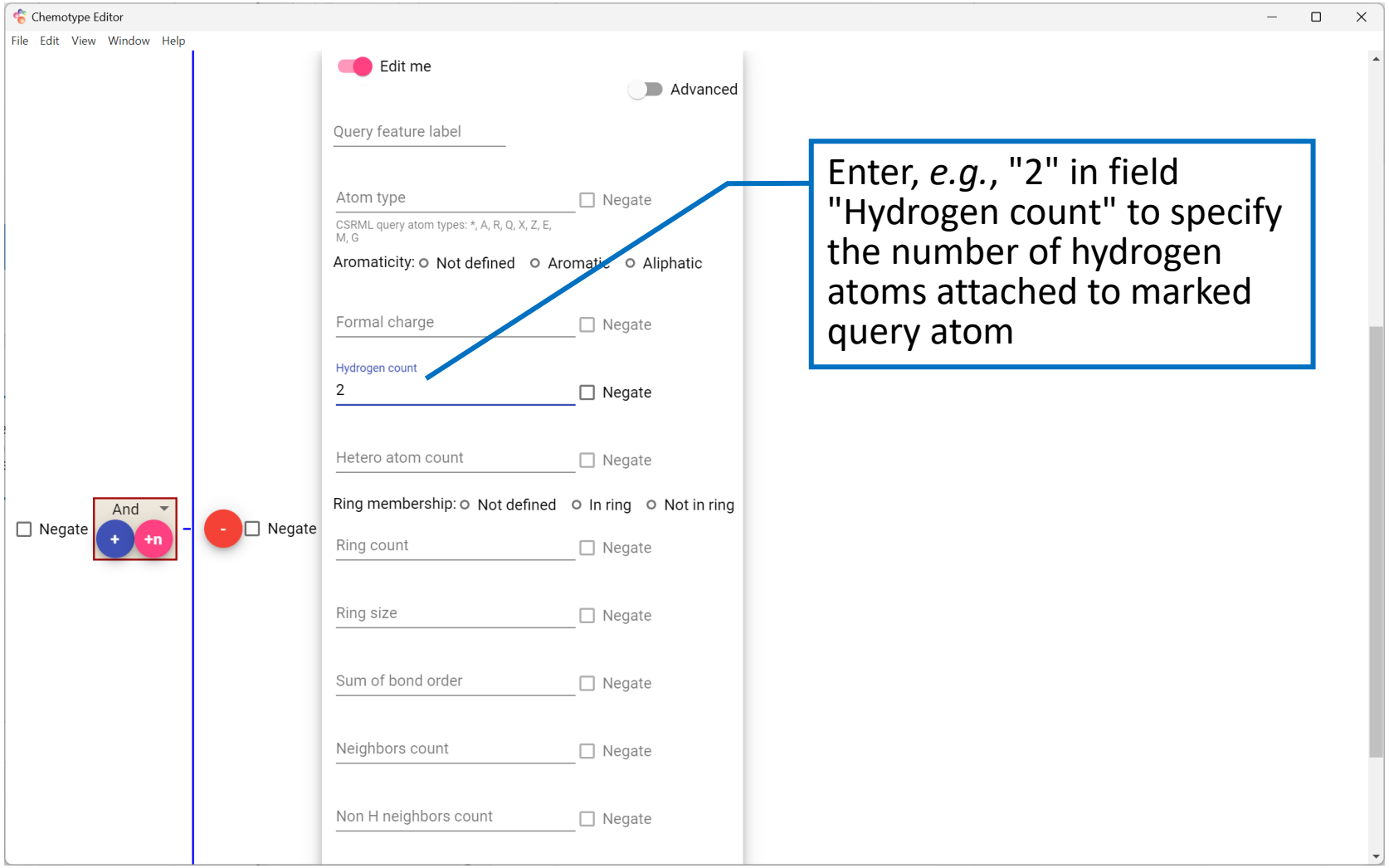
Draw Chemotype Structure



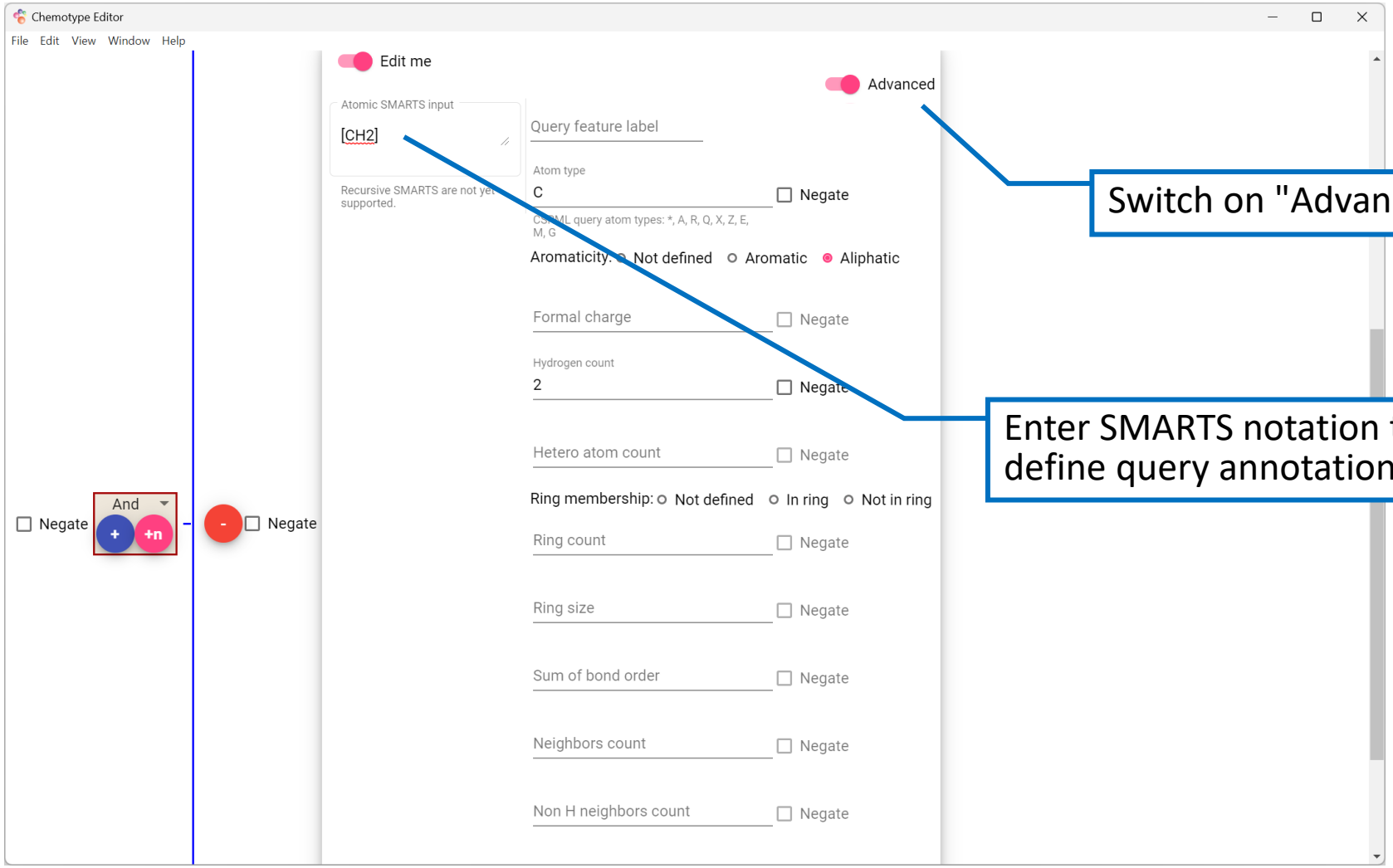
Atom Query Annotations



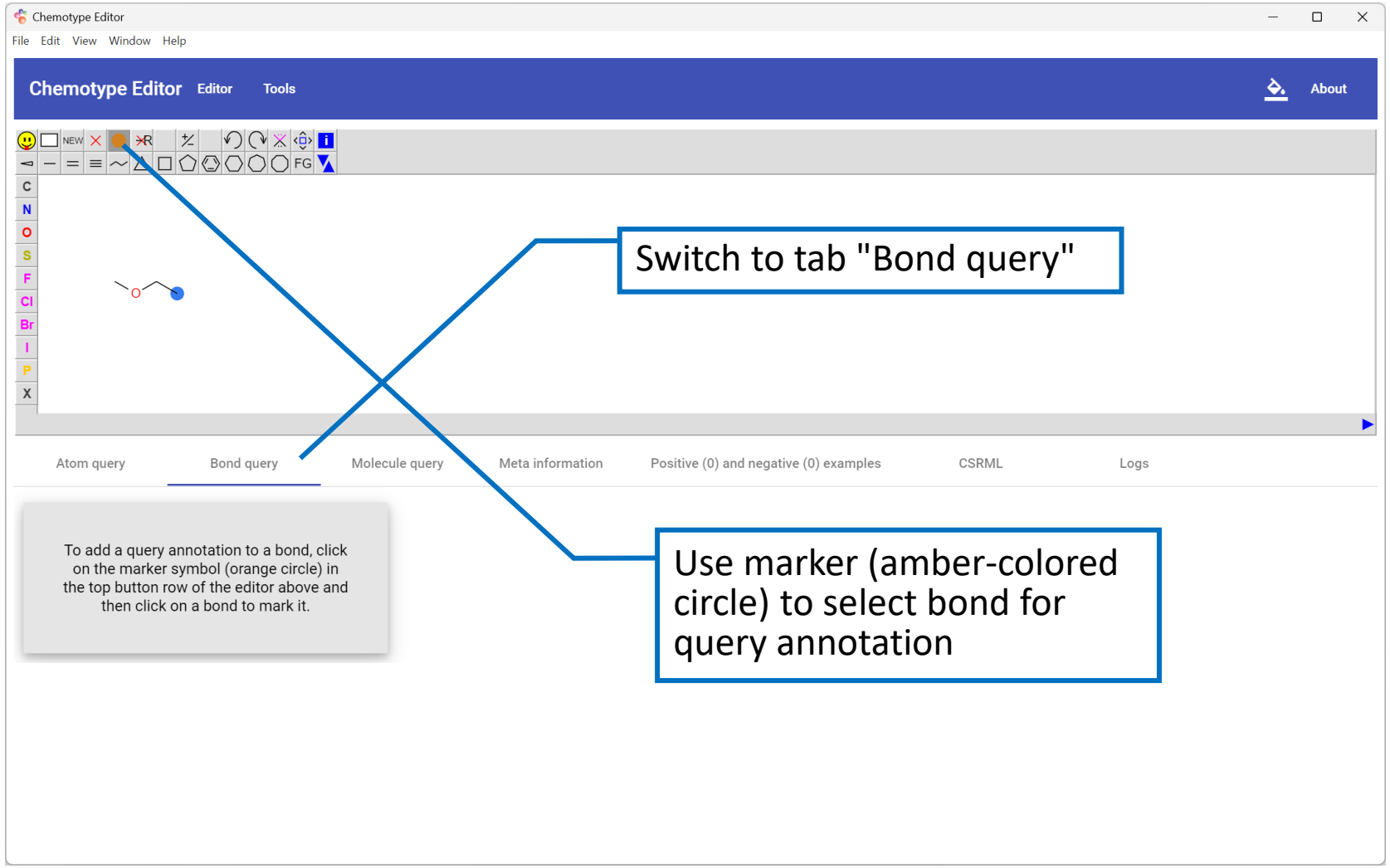
Atom Query Annotations



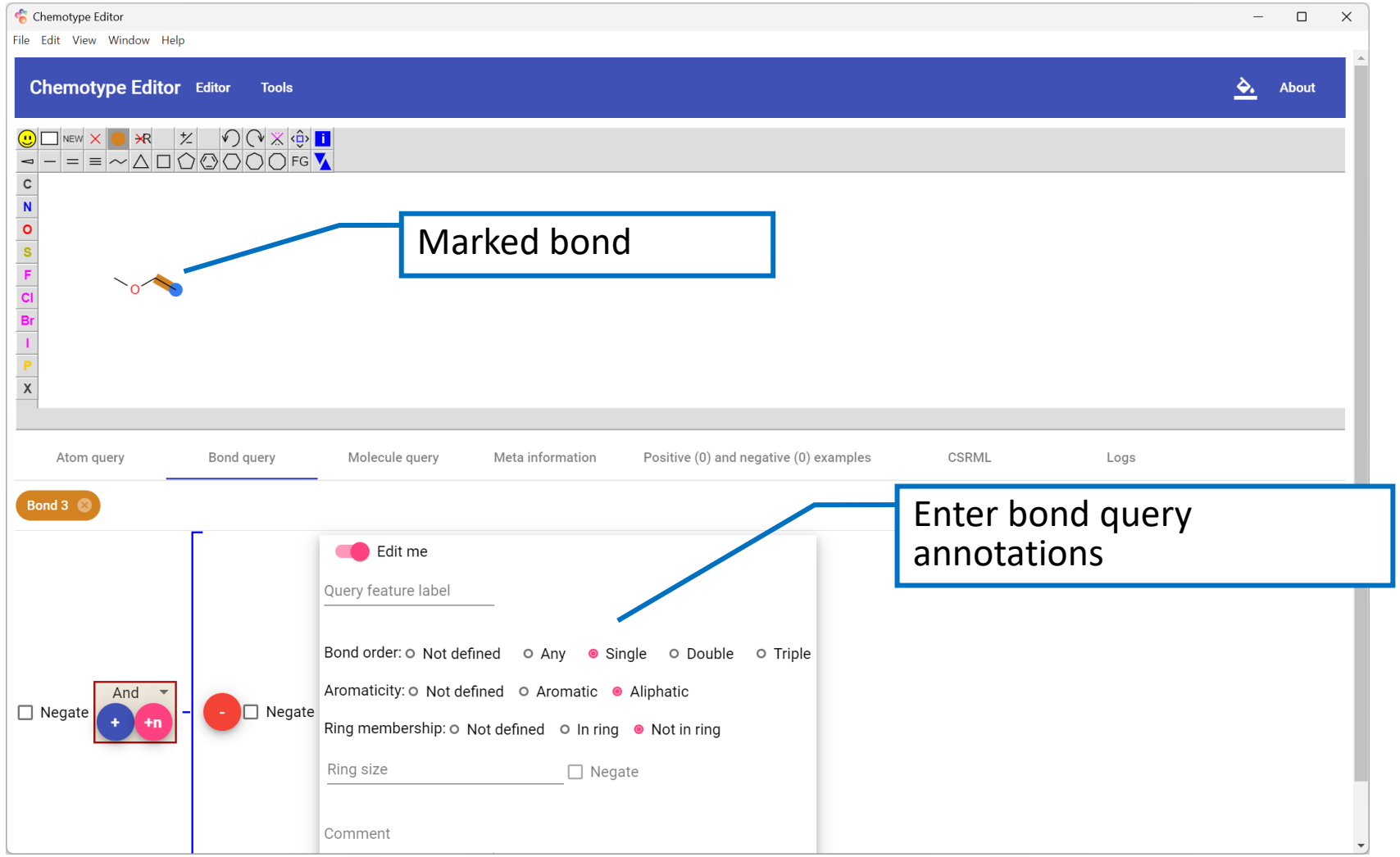
Atom Query Annotations



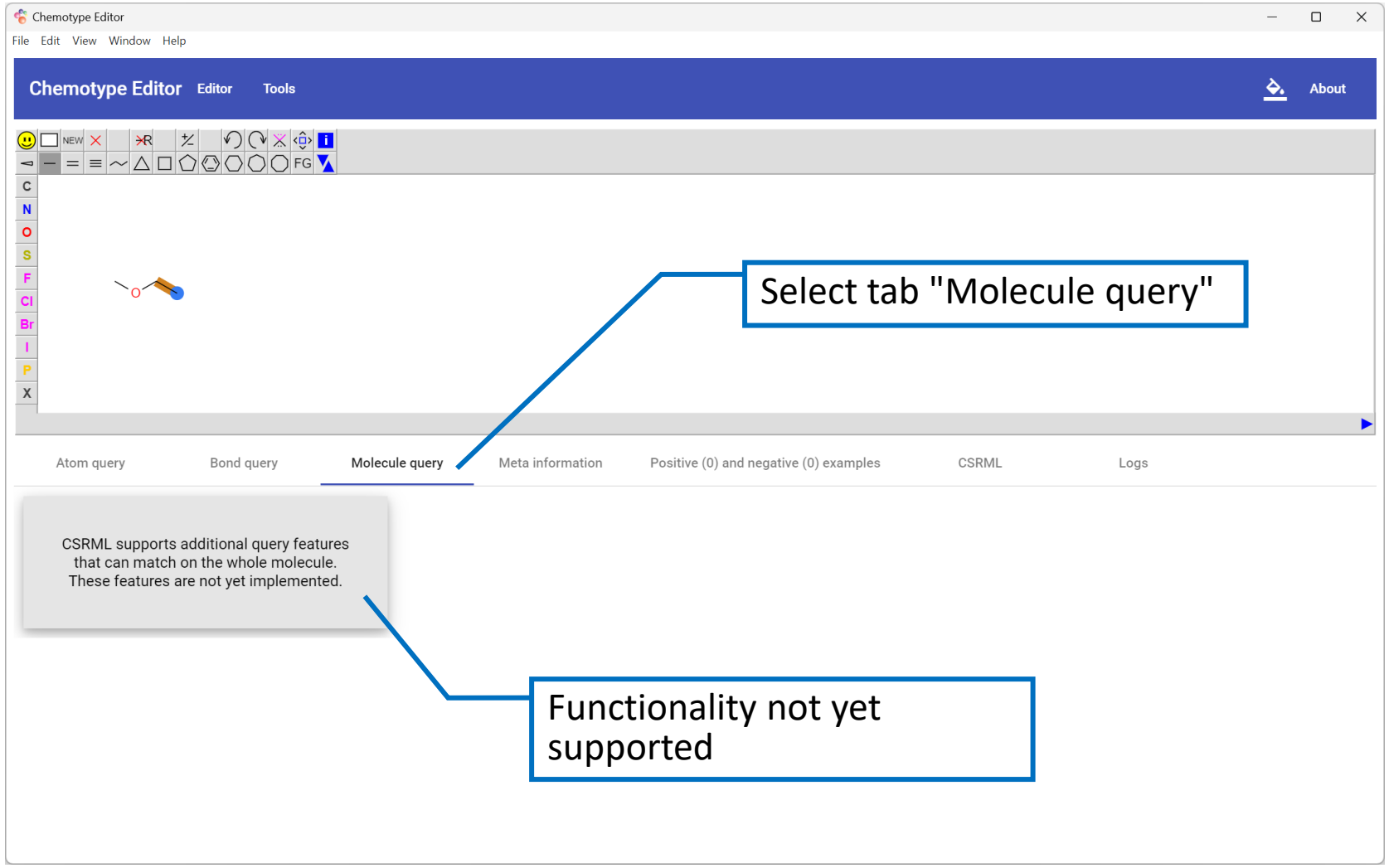
Bond Query Annotations



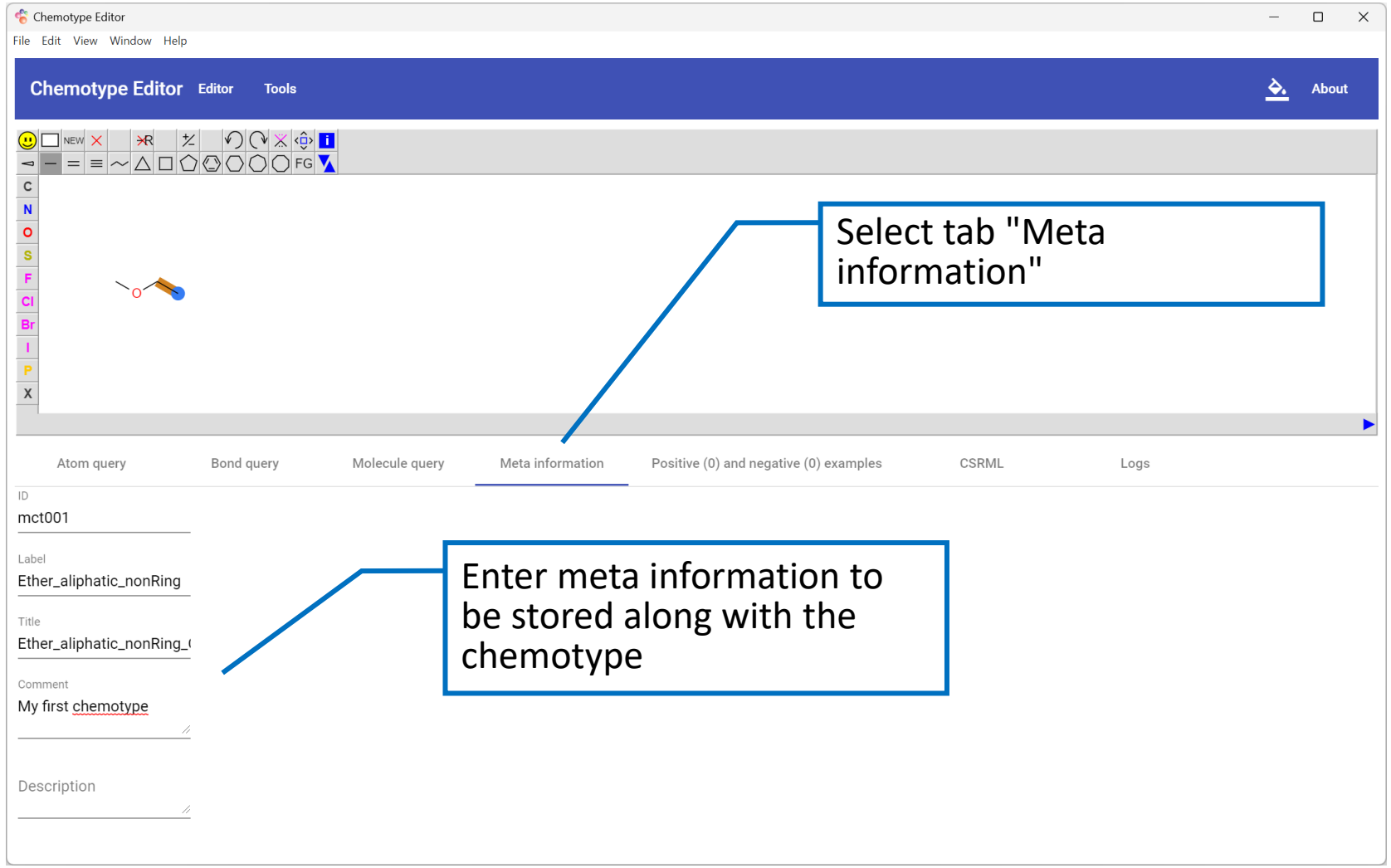
Bond Query Annotations



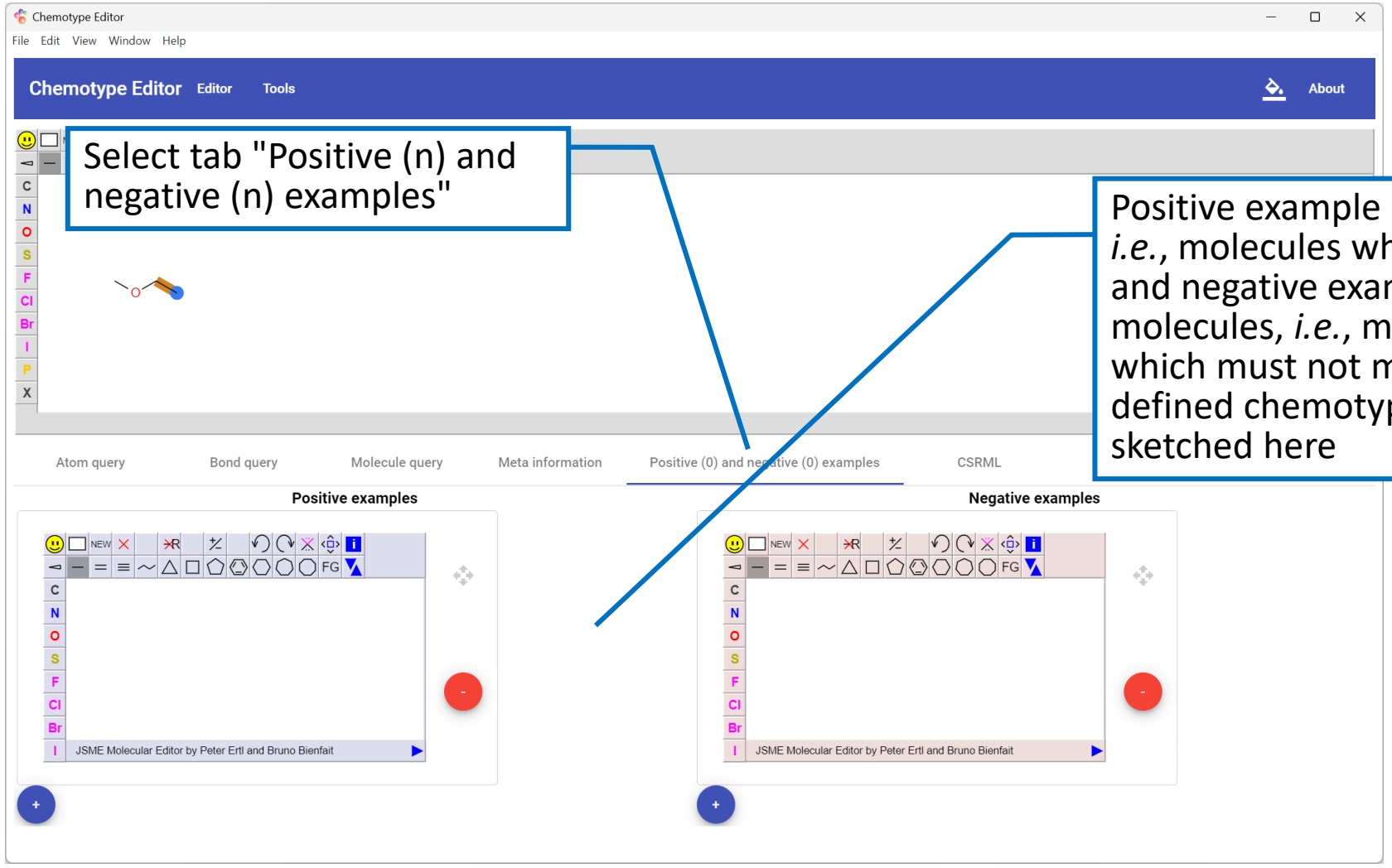
Molecule Query Annotations



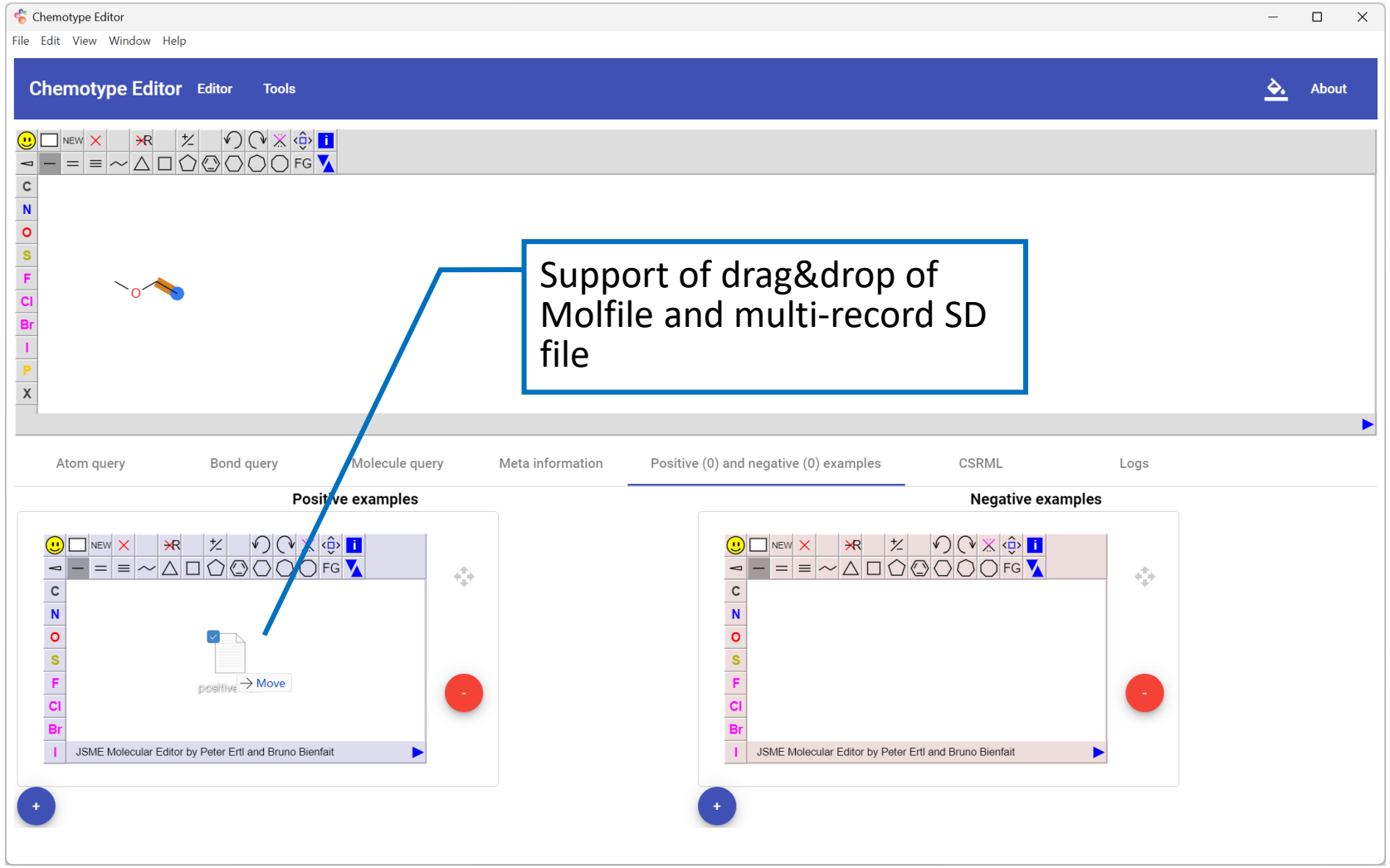
Meta Information



Positive and Negative Match Examples (required)



Positive and Negative Match Examples (required)



Positive and Negative Match Examples (required)

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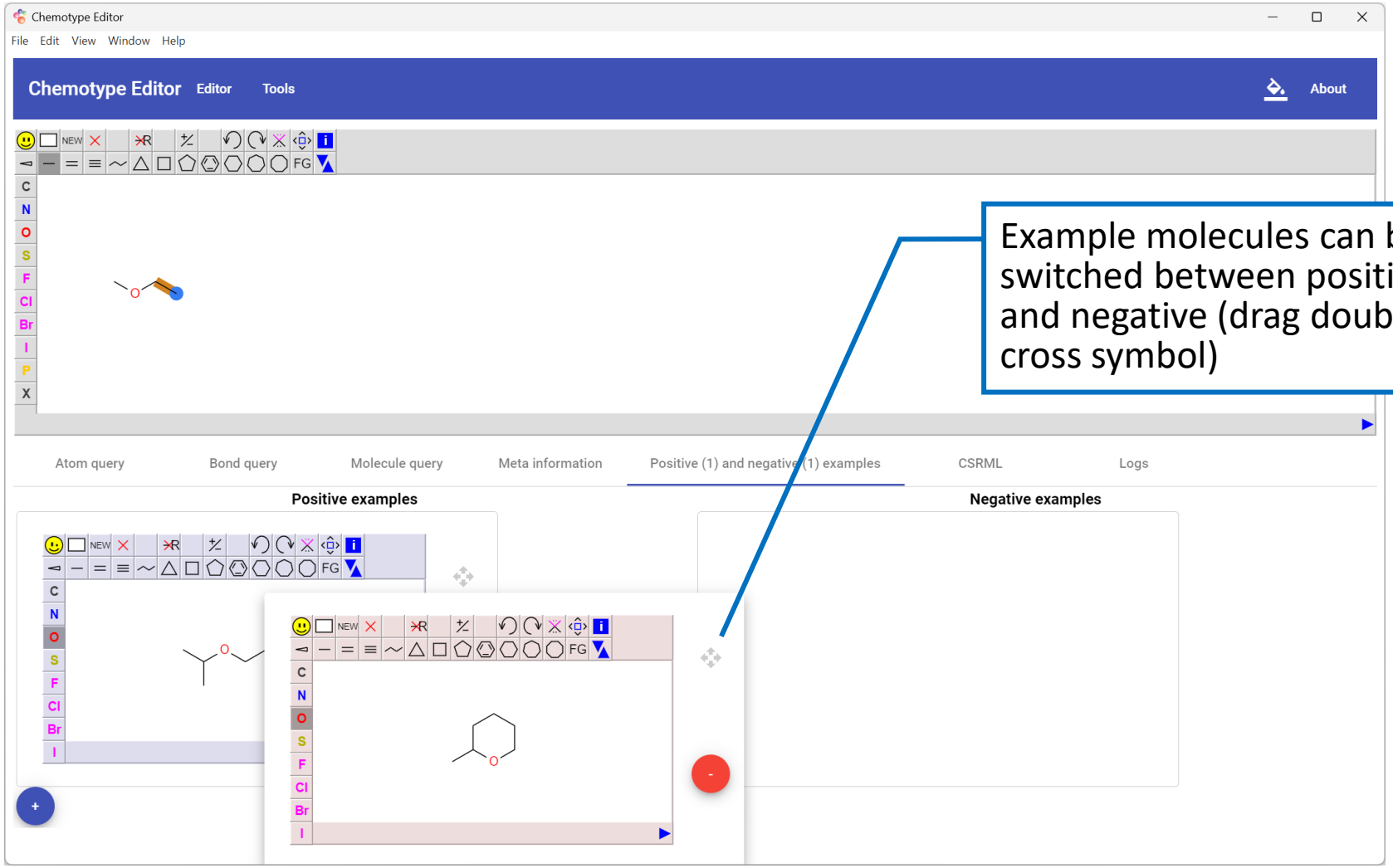

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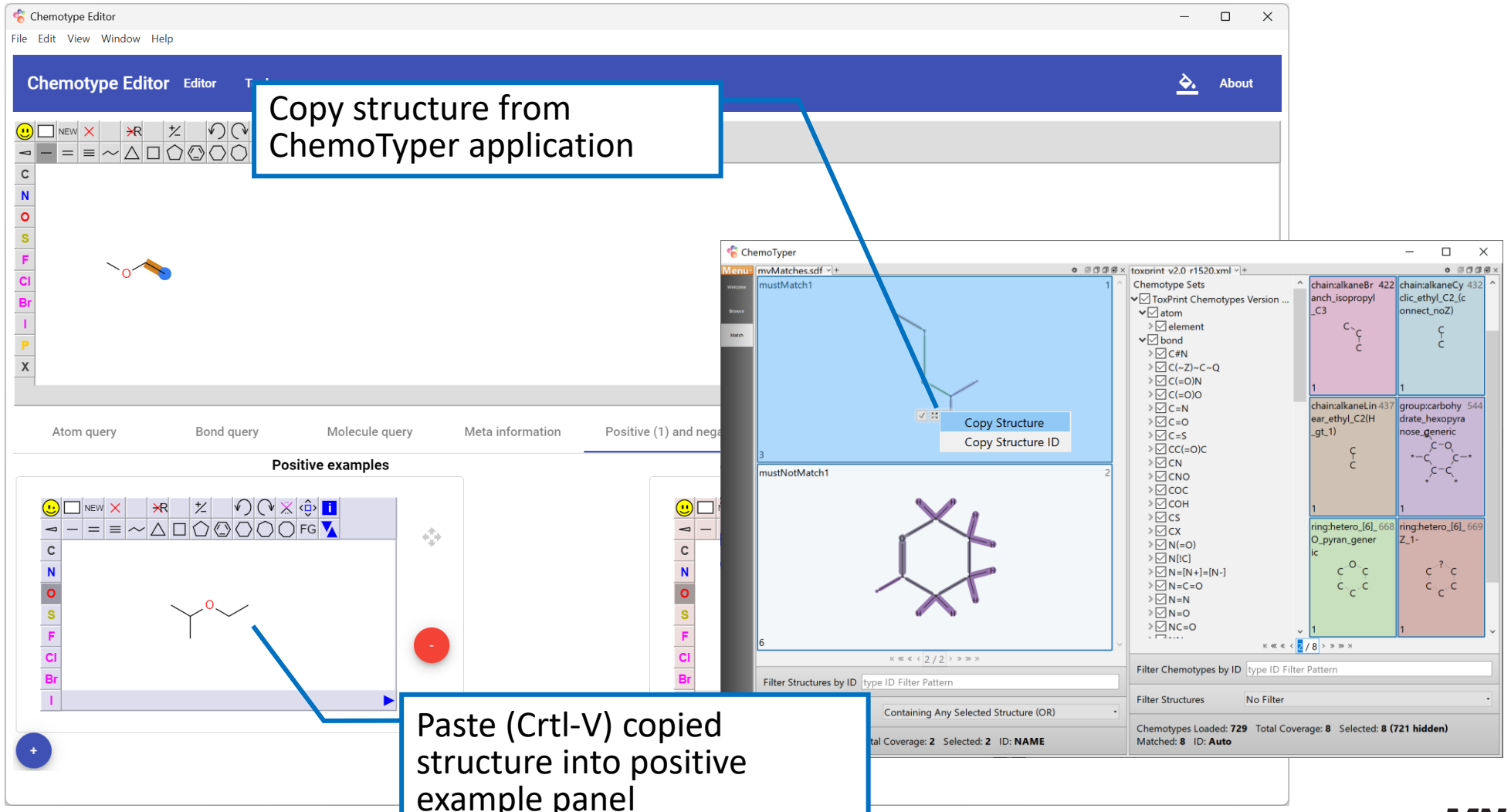
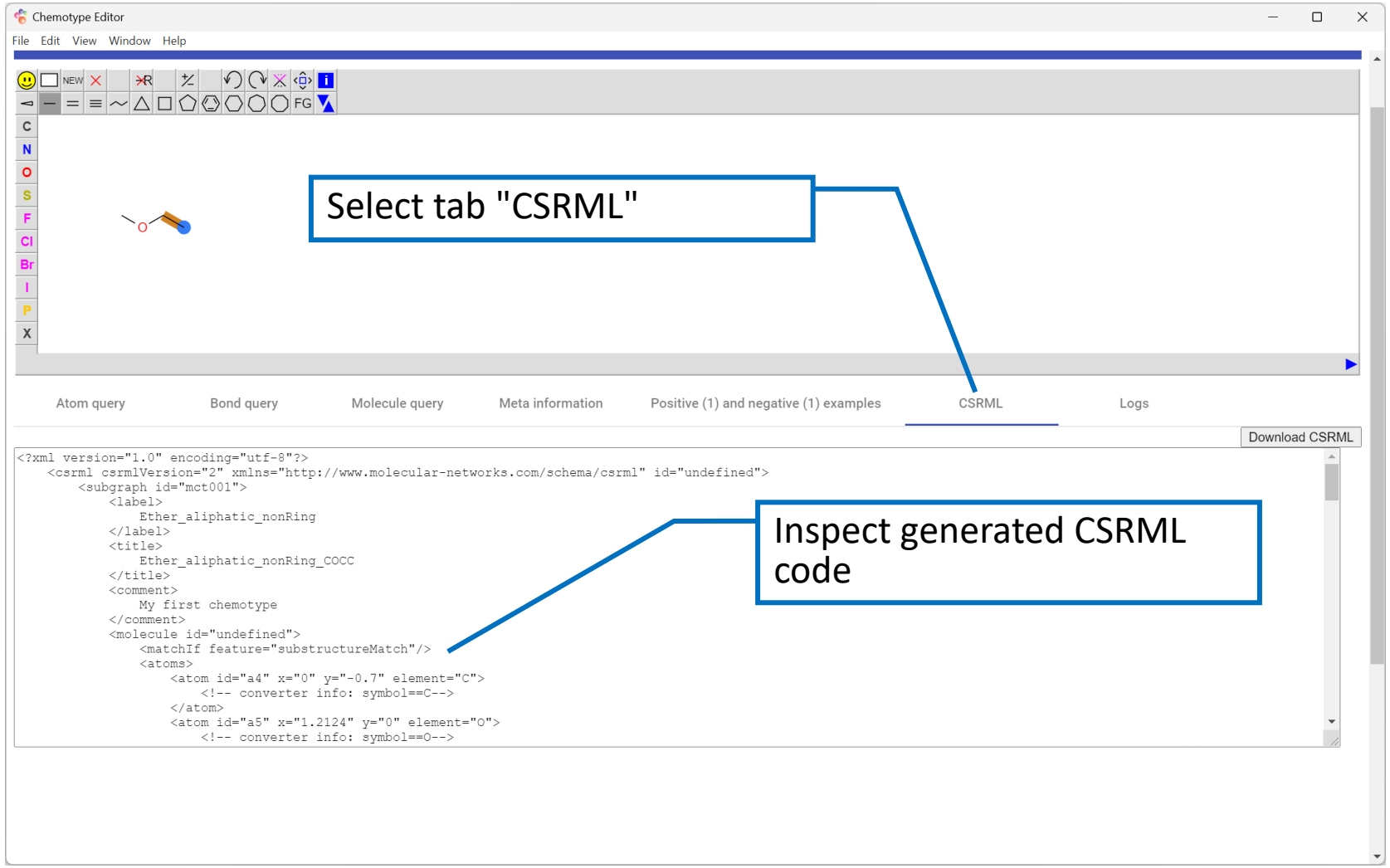
Positive and Negative Match Examples

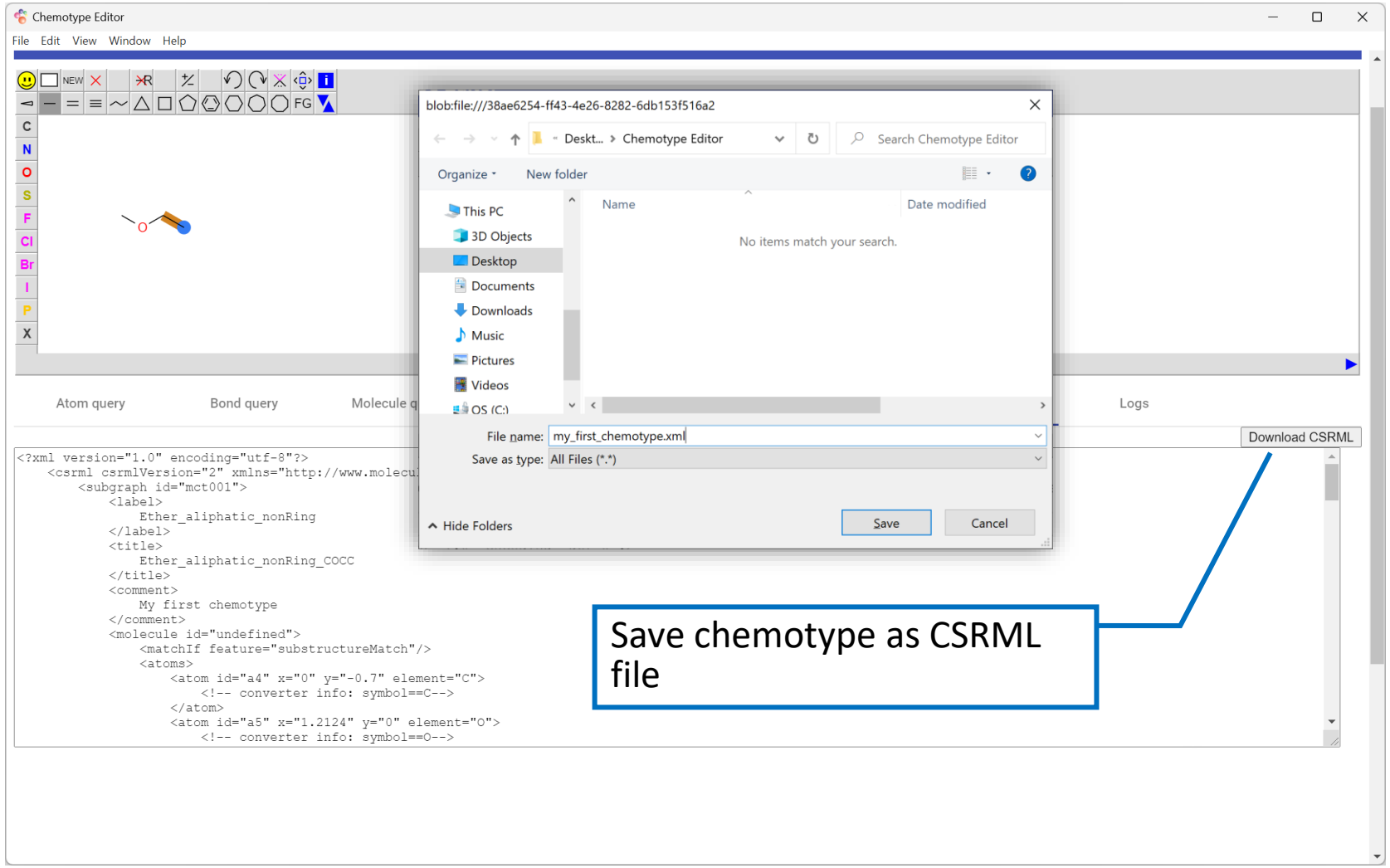


Chemotype in CSRML



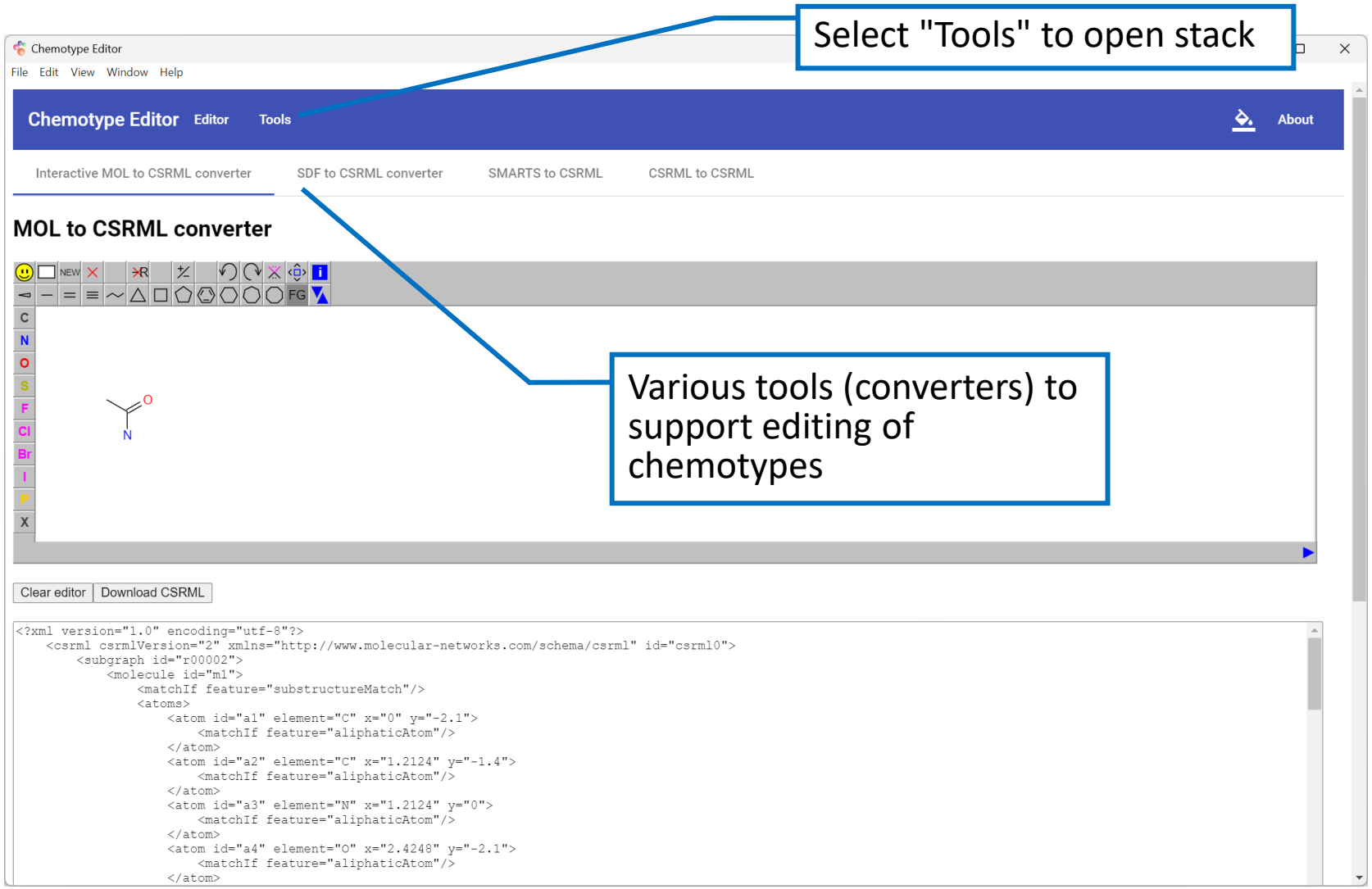
CSRML = Chemical Substructure and Reaction Markup Language

Chemotype in CSRML



CSRML = Chemical Substructure and Reaction Markup Language

Tools



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

THANK YOU!

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