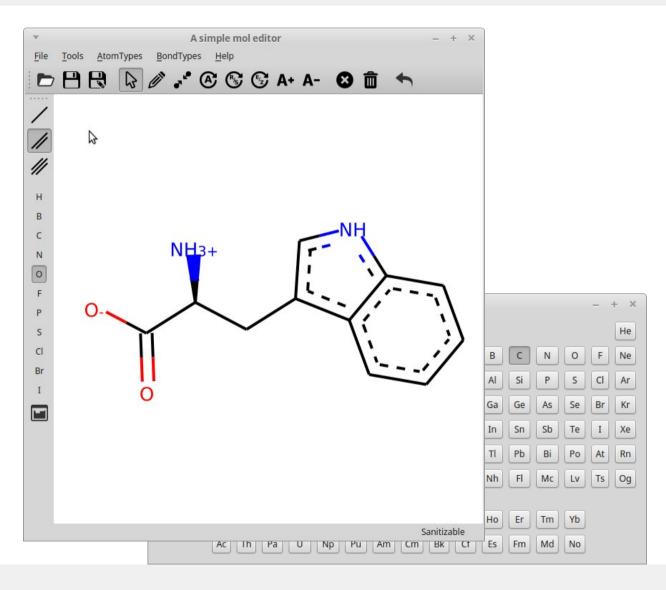


rdEditor: Graphical RDKit molecule editor



Classes

- QtSvg.QSvgWidget (PySide)
 - -Can draw SVG
- MolViewWidget (170 lines)
 - -Draw the molecule + Selection accounting
- MolEditWidget (421 lines)
 - -Mousepress events and methods to edit the molecule
- MainWindow (428 lines)
 - -GUI elements and actions to call methods/set properties on MolEditWidget



QT Signals and Slots

- Use of signals and slots to link events to code execution (QTCore, not GUI)
 - Molviewwidget.mol = Chem.MolFromSmiles('CCCC')
 - @mol.setter => Molviewwidget.molchanged.emit()
 - Molchanged signal bound to slot molviewwidget.sanitize draw()
 - Method updates SVG => show new molecule



Issues

- R/S (after saving/reopening)
- E/Z not implemented

- Molecule jumps around, especially for small molecules (Editor, not drawing program)
- Probably other bugs as well

- Available at https://github.com/EBjerrum/rdeditor
- LGPL v.3 license (as PySide)

