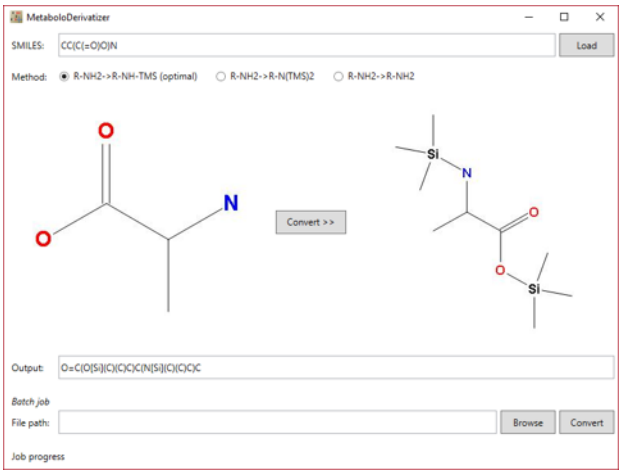
MetaboloDerivatizer tutorial

Objective

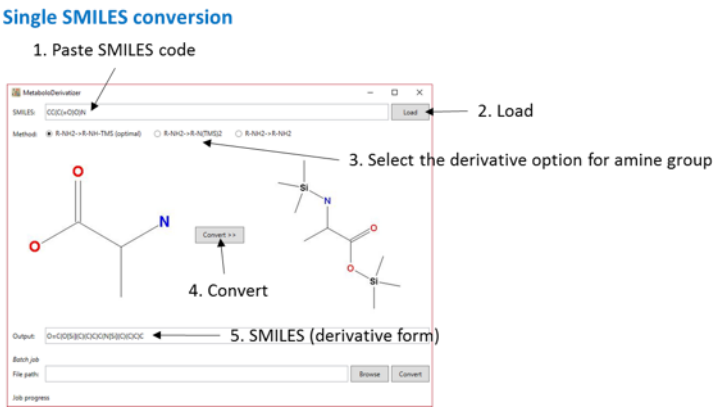
Methoxyamine hydrochloride (MeOX) and *N*-Methyl-*N*-(trimethylsilyl)trifluoroacetamide (MSTFA) are commonly used for the derivatization of small molecules to decrease boiling points and increase stability for GC-MS analysis. Therefore, it is important to theoretically consider the TMS- and MeOX form of small molecules to predict their retention time- and fragmentation behaviours as well as to calculate their chemical properties. Therefore, the converter from the original structure form to the MeOX- and TMS derivative structure was developed. This converter accepts the SMILES code for structure description, and it generates the derivatized form as SMILES.

Main window



Graphical user interface of MetaboloDerivatizer was simply developed for checking the compound structures. It provides two functions; one for single SMILES convert and the other for batch SMILES conversion.

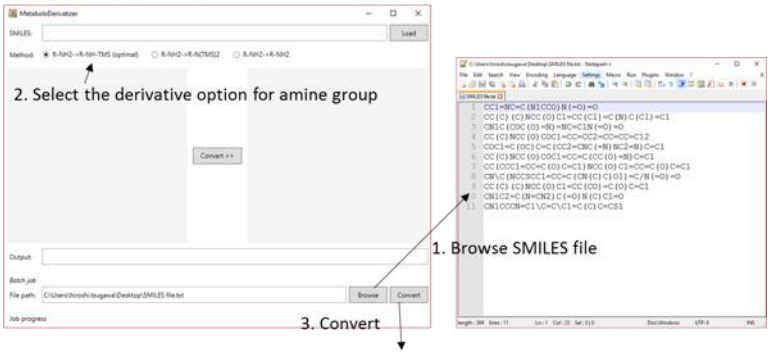
Quick tutorial



1. Paste a SMILES code in TextBox of top-panel, then click 'Load'. -> The structure will be generated on the left-panel.
2. Click 'Convert', and then the derivatized from and the SMILES code will be generated.

* Three options: 1) R-NH2 -> R-N-2TMS, 2) R-NH2 -> R-NH-TMS (the usual form of amine-TMS at the general condition), and 3) R-NH2 -> R-NH2

Batch SMILES conversion



1. Prepare SMILES list. (Do not put any header on the text, and prepare one SMILES in one row. *See the example file.)
2. Click 'Batch convert', and the result will be generated in the same directory.