Molecular representations and molecular descriptors

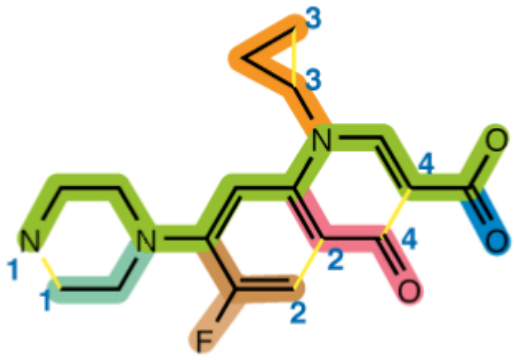
SMILES strings

The simplified molecular input line-entry system (SMILES) is a specification in the form of a line notation for describing the structure of one or more molecules, using short ASCII strings. SMILES strings can be imported by most molecule editors for conversion back into two-dimensional drawings or three-dimensional models of the molecules.

In brief (Figure 1)

- Atoms are represented by their atomic symbols, with the possibility to omit H;
- Single, double, triple and aromatic bonds can be represented with the following symbols: “−”, “=”, “#”, and “:”, respectively. Single bonds can be omitted.
- Branches are specified by enclosures in parentheses;
- Cyclic structures are represented by breaking one single or aromatic bond in each ring and starting from one of the ring atoms. Ring “opening”/”closure” bonds are then indicated by a digit immediately following the atomic symbol at each ring closure. Aromaticity on carbon atoms can be written with lower-case letters or by alternating single and double bonds (Kekulé notation). For instance, benzene can be both written as “c1ccccc1” and “C1=CC=CC=C1”;
- Local chirality can be specified using the symbols “/” and “\”. For instance, E- and Z-1,2-difluoroethene can be written as F/C=C/F and F/C=C\F, respectively. Additionally, tetrahedral centers are often indicated using “@” (or “@@”), following the atomic symbol of the chiral atom. “@” indicates that the listed neighbors are arranged anticlockwise, while “@@” that they appear in a clockwise order.
- The chosen atom order for generating the SMILES does not affect the encoded 2D structure. However, several types of standardized (also known as canonicalized) SMILES generation procedures exist.

C



D

N1CCN(CC1)C(C(F)=C2)=CC(=C2C4=O)N(C3CC3)C=C4C(=O)O

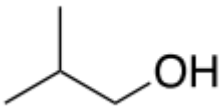
Figure 1. Example of the calculation of a SMILES string. Image from https://chejunkie.com/knowledge-base/convert-cas-registry-number-other/.

You can find a summary of the SMILES theory here: https://www.daylight.com/dayhtml/doc/theory/theory.smiles.html

SMILES strings: exercise 1

Which of the following molecular depictions corresponds to the reported SMILES string?

SMILES:

A. 

SMILES: C1=CC(=CC(=C1)Br)OC(F)(F)F

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""
```

```
ans =
""
```

SMILES strings: exercise 2

Calculate molecular descriptors for the following molecule, expressed as SMILES string:

SMILES string: "ClC(C)CC1=CC=C(C=C1)C(C)C(=O)O"

Complete the code below, to compute the following descriptors:

- "nCl": number of Chlorine atoms

- "nC": number of Carbon atoms
- "nDB": number of double bonds
- "nO": number of oxygens

```
smiles = 'ClC(C)CC1=CC=C(C=C1)C(C)C(=O)O';
```

```
smiles =
'ClC(C)CC1=CC=C(C=C1)C(C)C(=O)O'
```