Chemistry Plug in - Use cases

MatDecks chemistry functions help users to get various data on chemical compounds including names, IUPAC names, molecular formulas, SMILES representations and molecular images. Obtained chemical molecular formulas can be used to write chemical reactions. MatDeck can also help to balance chemical reactions. The Chemistry functions are based on MatDecks plug in technology.

Obtained names of chemical compounds based on SMILES or common a name

The function chem_smiles_to_names() is used to obtain a list of common names of chemical compounds based on the SMILES string identifier, IUPAC name, or any other common name. The list of common names is obtained in the form of vector.

```
1 names := chem_smiles_to_names("ethyl alcohol")
2 names1 := chem_smiles_to_names("CC(=O)Oc1ccccc1C(O)=O")
```

names = 226 elements vector
names[0] = "ethanol"
names1 = 224 elements vector
names1[0] = "2-acetyloxybenzoic acid"

Obtaining the IUPAC name of chemical compounds based on SMILES or a common name

The function chem_smiles_to_name() can be used to obtain the IUPAC name of chemical compounds based on the SMILES string identifier, IUPAC name, or any other common name. The result is given in the form of string.

```
3 iupac := chem_smiles_to_name("ethyl alcohol")
4 iupac1 := chem_smiles_to_name("CC(=O)Oc1ccccc1C(O)=O")
```

iupac = "ethanol"
iupac1 = "2-acetyloxybenzoic acid"

Obtaining SMILES from a name or a IUPAC name

The function chem_name_to_smiles() is used to obtain the SMILES representation of chemical compounds based on the IUPAC name, or any other common name. The SMILES is presented in the form of string.

```
5 smiles := chem_name_to_smiles("aspirin")
```

smiles = "CC(=O)Oc1ccccc1C(O)=O"

Obtaining the molecular formula from a name or SMILES

The function chem_smiles_to_formula() is used to obtain the molecular formula of a chemical compound based on a SMILES string identifier, IUPAC name, or any other common name. The molecular formula is expressed in the form of string.

```
6 f1 := chem_smiles_to_formula("ethyl alcohol")
7 f2 := chem_smiles_to_formula("CC(=O)Oc1ccccc1C(O)=O")
```

f1 = "C2H6O"
f2 = "C9H8O4"

Obtaining a molecular image from a name or smiles

The first way to obtain a molecular image is to use the chem_smiles_to_image() function; with the option that the function directly returns a widget, which can be embedded within a canvas.

```
8 image1 := chem_smiles_to_image("CC(=O)Oc1ccccc1C(O)=O", "Aspirin", true)
```

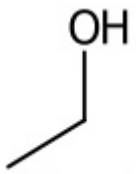
The second way to obtain a molecular image is to use the chem_smiles_to_image() function to get image data, when the image data is manipulated further in the code, it generates an image widget which is embedded within a canvas.

```
9  image2 := chem_smiles_to_image(chem_name_to_smiles("ethyl alcohol"),
   "Ethanol", false)
10 imwid := image_widget(0, image2)
11 set_size(imwid, width(imwid) * 6, height(imwid) * 6)
```

The molecular image can opened outside of the document, if we use the option *show()* for the widget instead of the *embed_widget()* used within a canvas.

```
12 show(image1)
```

Aspirin



Ethanol