Balancing Chemical Equations and Calculation of Molecular Weight

MatDeck can be used to obtain the molecular formula of a compound by its name, IUPAC name, or SMILES. In this example we show Ethanol fermentation, also called alcoholic fermentation, which converts sugars such as glucose into ethanol and carbon dioxide. Therefore, we need the molecular formula of Glucose, Ethanol, and Carbon dioxide, which are obtained by using the function chem_smiles_to_formula() and its compound name. The formula is obtained as a string, and can be stored as a variable.

```
glucose := chem_smiles_to_formula("glucose")
co2f := chem_smiles_to_formula("carbon dioxide")
ethanolf := chem_smiles_to_formula("ethanol")
```

MatDeck comes implemented with several functions that can help you determine if a chemical equations feasible or not, and help you find the balance the equation if a reaction is feasible. There is an easy way to balance the equation. The procedure is given in two steps:

- Create the equation that you want to be balanced, use the Ctrl. + = key combination to create an equal sign.
- Position the mouse cursor above the equal sign and right click the Equal sign, it will transform to a dart and the equation will be balanced (if the reaction is feasible)

However, chemical equations are expected to be symbolic. Therefore, we have to convert string formulas into symbolic values, which is done using the str2symbol(variable, true/false) function. Here a variable is a string value which is then converted to a symbolic value, and the other argument is used as true if we want to skip spaces in a given string. The formula in the canvas is obtained by converting string variables into symbolic values.

$$C6H12O6 \rightarrow 2\ C2H6O + 2\ CO2$$

Molecular Weight used in the calculation

We can easily calculate the molecular mass of all the compounds used in a chemical reaction. The function chem_smiles_to_mweight("given name") is used to obtain molecular weight. The molecular weight for compounds in given reactions are below.

```
mwEthanol := chem_smiles_to_mweight("ethanol")
mwCO2 := chem_smiles_to_mweight("carbon dioxide")
mwGlucose := chem_smiles_to_mweight("glucose")
```

Next, we can calculate how much of Ethanol we can get from **1g** of Glucose. We can use the balanced equation obtained above, and their molecular weights to perform calculus.

$$mEthanol := \frac{2 \cdot mwEthanol}{mwGlucose} \cdot 1\ g$$

$$mEthanol = 0.511\ g$$