Mixtures

OCHEM supports mixtures.

In order that compounds will be recognized as a mixture, it should be uploaded by indicating MIXTURES as the column name. Mixture is specified as several space separated SMILES, e.g.

MIXTURES
CCC C1CCC1C
CCC;0.5 C1CCC1C;0.5
CCC;0.8 C1CCC1C;0.2

The first and second rows are identical for OCHEM: if molar fractions are not provided, we will assume that equilateral molar concentrations were used for all components. The third row has a compound with molar fraction of propane (CCC) is 0.8 and molar fraction of Methylcyclobutane (C1CCC1C) is 0.2.

The sum of molar fractions should be always 1. Upload of data with "MIXTURE" column will automatically create Condition "MIXTURES" with SMILES and molar fraction of individual components of the mixture. Currently this is the only way to upload mixtures: their editing in the browser is not possible. The data with mixture will be automatically recognized by OCHEM and will allow to select different descriptor averaging, (see Ref 1). The current format allows to easily mix both pure and mixtures for model development.

We also simplified processing options for mixtures and left only three options:

1. No processing of descriptors (assumption is that respective descriptor calculation programs or data analysis may do it in the future: currently no such algorithms are supported in OCHEM and using this option will result in an error)
2. Sum of descriptors averaged by molar fractions (if fraction are not provided, equal molar fractions are assumed for all components of the mixture)
3. Sum and difference of descriptors - this option is only available for binary mixtures

For options **1** and **2** the molar fractions are provided as descriptors to the respective modelling algorithms.

This format supersede the one originally described in ref 1. The models from that publication were recalculated based on the new format.

1) Oprisiu I, Novotarskyi S, Tetko IV (2013) Modeling of non-additive mixture properties using the Online CHEmical database and Modeling environment (OCHEM). J Cheminform 5 (1):4. doi:10.1186/1758-2946-5-4