Working with datasets

Baskets definition

OCHEM allows to combine experimental records into reusable sets. Such sets of records are referred to as *baskets.*
Baskets have names and user can virtually have as many baskets as required. Baskets are typically used as
training or validation sets for the development of QSAR models.

Baskets as sets of molecules

Usually, baskets contain the experimental data records. However, baskets can contain molecules without any
experimental data attached.
In this case, baskets serve as sets of molecules.