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Molecular fragments chemoinformatics

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The description of chemical structures as a collection of connected molecular fragments is a basic requirement of coarse grained simulation methods like molecular fragment dynamics. These methods use molecular fragments as their basic interacting entities ("atoms") and allow the modelling and investigation of very large chemical systems. Therefore a molecular fragments chemoinformatics is in need that supports the fragment-based representation of chemical structures as well as the elementary operations upon them. The poster outlines definitions and approaches to tackle these issues from an adequate molecular line notation up to the graphical representation of simulation boxes.

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