Rule-based *in-silico* Fragmentation for the Analysis of Natural Product Chemical Space

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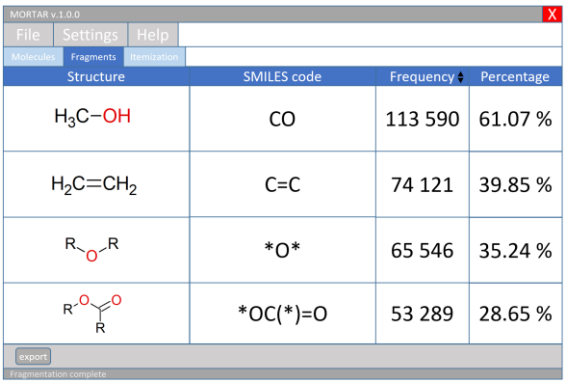
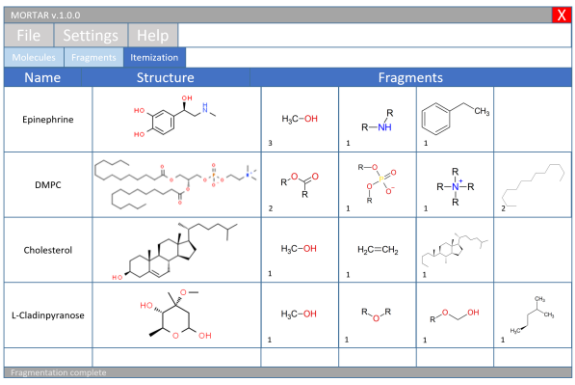
The *in-silico* analysis of chemical compound collections based on substructures extracted according to a defined set of rules (fragmentation) is a method used in various areas of cheminformatics. Examples of application are drug design [1], structural classification of compounds [2], and the structural investigation of functional groups [3].
This project aims at the development of an algorithm for extracting characteristic fragments from natural product structures to study their chemical space. The initial idea is to adapt the Ertl algorithm for automatic functional group identification in organic compounds [4,5], thus using functional groups as a basis for the extracted fragments.
To support the refinement of the fragmentation algorithm, a Java rich client application will be developed. The application named *MORTAR* ('MOlecule fRagmenTAtion fRamework') will provide extensive graphical functions for visualizing fragmentation results based on single compounds and entire compound collections:





The ultimate aim of this project is to improve our understanding of chemical motives in natural products in order to create better computer-assisted structure elucidation systems.

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[3] P. Ertl, T. Schuhmann, *J. Nat. Prod.*, **2019**, *82*, 1258–1263.
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