MORTAR

MOlecule fRagmenTAtion fRamework

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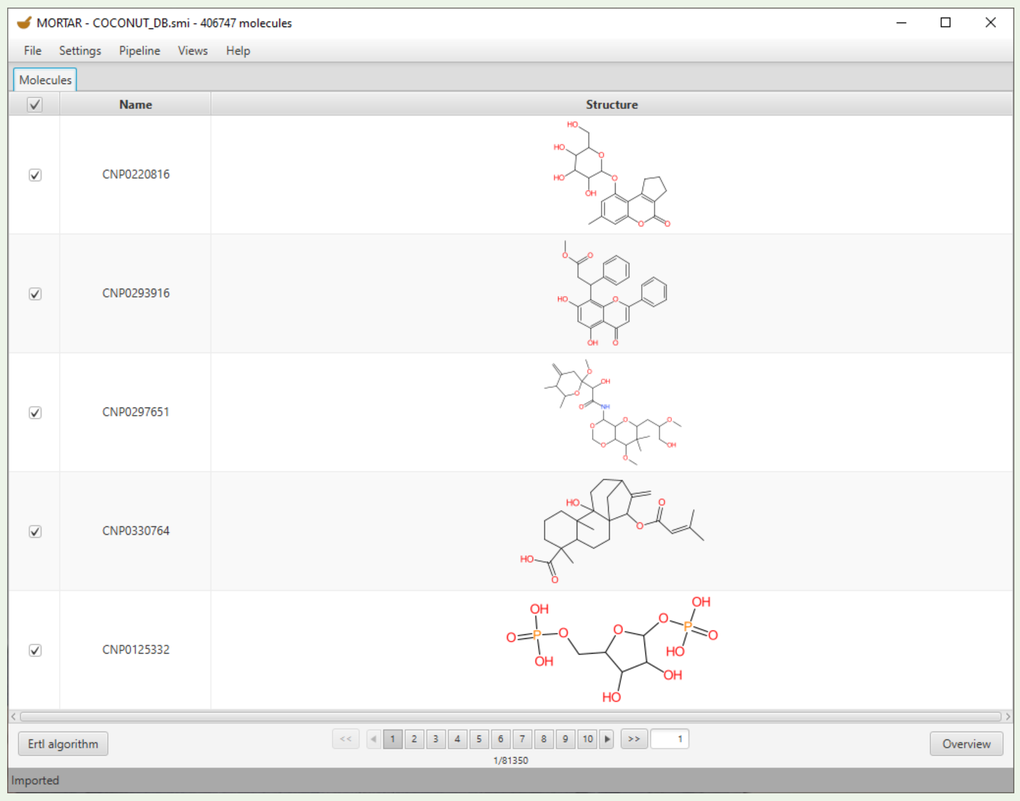
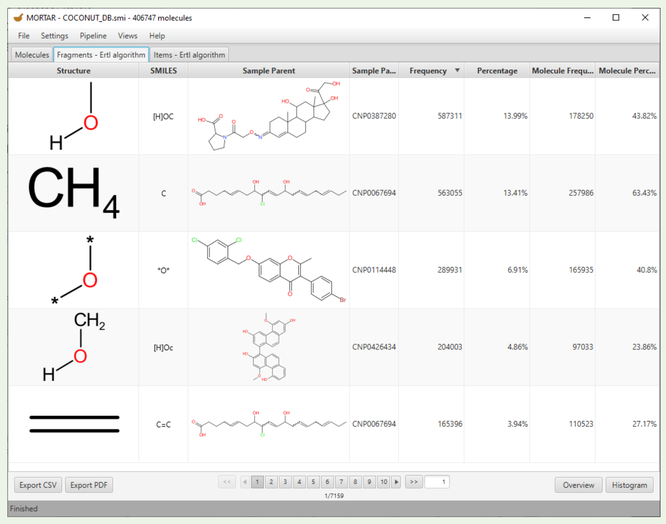
MORTAR (MOlecule fRagmenTation fRamework) [1] is an open-source client application designed to facilitate molecular fragmentation and substructure analysis workflows. No programming skills are required to perform in silico fragmentation studies with MORTAR, as its graphical features allow the visualisation of fragmentation results for individual compounds or entire compound sets. By providing multiple views and analytical functions, MORTAR facilitates the interpretation of fragmentation results. Three integrated methods for substructure analysis and fragmentation are currently available in MORTAR: The ErtlFunctionalGroupsFinder [2] for functional groups detection in organic molecules, the Sugar Removal Utility [3] to unmask a potential drug core by removing sugar moieties and Scaffold Generator [4], a software library for the hierarchical decomposition of the basic molecular structure into chemically valid subunits. MORTAR allows not only the easy integration of custom fragmentation algorithms, but also the development and implementation of new algorithms through the implementation of a MORTAR-specific interface. All cheminformatics functionalities of MORTAR are implemented using the Chemistry Development Kit (CDK). As an open-source software project MORTAR is available on GitHub [5].



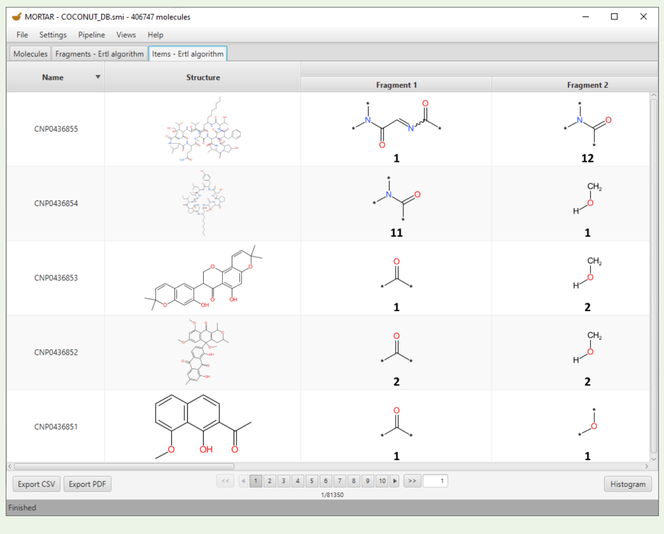
MORTAR main view (screenshot) with a paginated overview of the open COCONUT database of natural products.

Fragmentation Results



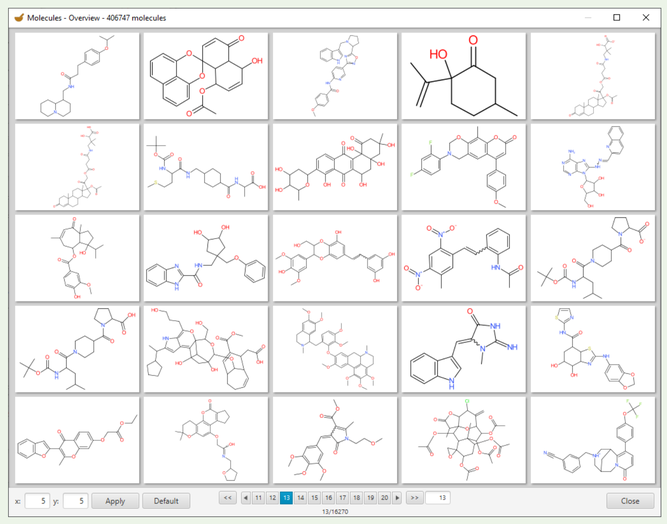
Fragments tab:
Functional groups of the natural products from the COCONUT database are generated with ErtlFunctionalGroupsFinder as shown in this screenshot: In addition to 2D structure and SMILES, a randomly selected parent molecule is shown. Frequencies of the functional group fragments are evaluated and can be used for sorting purposes.

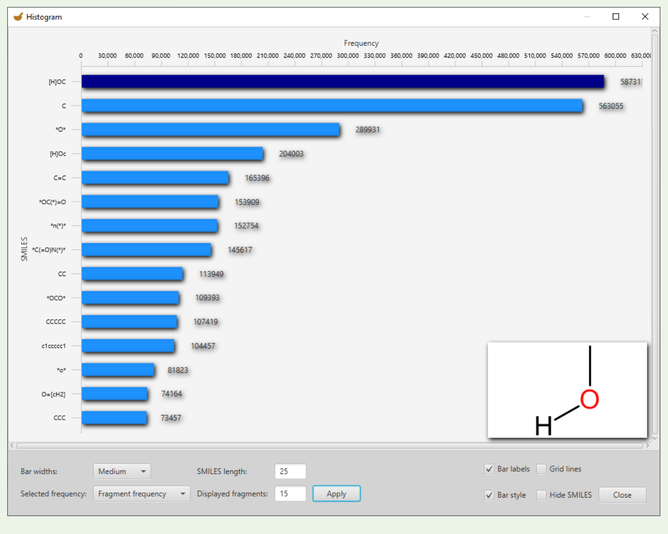
Items tab:
Functional group fragments for each molecule together with their frequencies (screenshot). The Fragments and Items tabs can be exported as either a csv file or a PDF document. The csv file contains only SMILES and corresponding frequencies, while the pdf file contains the 2D structures displayed in the view in addition to the SMILES and frequencies.



Alternative and Analytic Views

Overview:
A screenshot of the grid-based visualisation of the molecular structures of the COCONUT, as an alternative view that allows faster inspection than in the list-based MORTAR main window. The imported molecule set, generated fragment sets, fragments of a single molecule and all parent molecules of a single fragment can be visualised in this way.





Histogram:
A histogram showing the fragment frequencies of the functional groups of COCONUT in descending order, as shown in this screenshot, generated with the ErtlFunctional-GroupsFinder. When the mouse is moved over a bar, the corresponding fragment structure is displayed as a 2D structure in the lower right corner. In addition to the absolute frequency of a fragment, the frequency in how many molecules it occurs can be displayed.

[1] Bänsch, F., Schaub, J., Sevindik, B., Behr, S., Zander, J., Steinbeck, C., Zielesny, A. MORTAR: a rich client application for in silico molecule fragmentation. J Cheminform 15, 1 (2023).
[2] Fritsch, S., Neumann, S., Schaub, J. et al. ErtlFunctionalGroupsFinder: automated rule-based functional group detection with the Chemistry Development Kit (CDK). J Cheminform 11, 37 (2019).
[3] Schaub, J., Zielesny, A., Steinbeck, C. et al. Too sweet: cheminformatics for deglycosylation in natural products. J Cheminform 12, 67 (2020).
[4] Schaub J, Zander J, Zielesny A, Steinbeck C. Scaffold Generator: a Java library implementing molecular scaffold functionalities in the Chemistry Development Kit (CDK). J Cheminform 14, 79 (2022).
[5] MORTAR, https://github.com/FelixBaensch/MORTAR, Accessed 28 February 2023

MORTAR v1.1