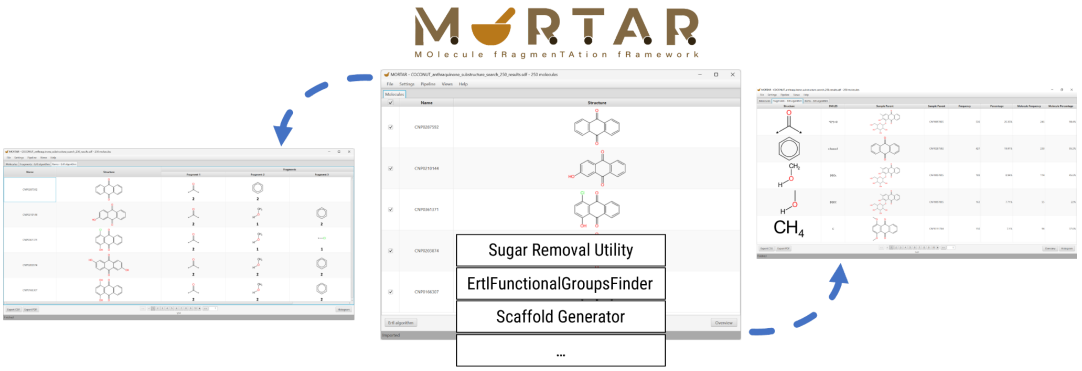
MORTAR – A Rich Client Application for *in silico* Molecule Fragmentation

Felix Bänsch [1,2], Jonas Schaub [1,2], Betül Sevindik [1], Samuel Behr [1], Julian Zander [1], Christoph Steinbeck [2], Achim Zielesny [1]

1 Institute for Bioinformatics and Cheminformatics, Westphalian University of Applied Sciences, Recklinghausen, Germany
2 Institute for Inorganic and Analytical Chemistry, Friedrich Schiller University, Jena, Germany

The process of developing and implementing computational algorithms to extract specific substructures from molecular graphs, known as *in silico* molecular fragmentation, is a repetitive task that involves multiple iterations of applying a set of rules to relevant structural data, followed by checking and adjusting the results. This requires a computational workflow that includes data import, fragmentation algorithm integration, and result visualization. When developing a new algorithm, this workflow is not readily available and must be built from scratch.



To address this problem, this work presents MORTAR (MOlecule fRagmenTAtion fRamework) [1], an open Java-based graphical user interface application that supports the development of new *in silico* molecule fragmentation algorithms as well as their availability after publication. The MORTAR application provides various visualization options for the fragmentation results of a group of molecules and basic analysis functions. Fragmentation algorithms can be integrated and developed within MORTAR using a special wrapper class. In addition, any combination of the available fragmentation methods can be used to run fragmentation pipelines. Currently, three fragmentation methods are integrated in MORTAR: ErtlFunctionalGroupsFinder [2], Sugar Removal Utility [3], and Scaffold Generator [4]. All cheminformatics functionality within MORTAR is implemented using the Chemistry Development Kit (CDK).

[1] F. Bänsch, J. Schaub, B. Sevindik, S. Behr, J. Zander, C. Steinbeck, A. Zielesny, J Cheminform., 2023, 15, 1
[2] S. Fritsch, S. Neumann, J. Schaub, C. Steinbeck, A. Zielesny, J Cheminform., 2019, 11, 37
[3] J. Schaub, A. Zielesny, C. Steinbeck, M. Sorokina, J Cheminform., 2020, 12, 67
[4] J. Schaub, J. Zander, A. Zielesny, C. Steinbeck, J Cheminform., 2022, 14, 79