

# 2D visualizing and navigation in fragment-based chemistry spaces

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Fragment-based chemistry spaces consist of a set of fragments and a set of rules which specify how the fragments can be connected. These spaces can be the underlying search space for typical tasks in pharmaceutical research like library design, de novo design or lead optimization. Since the fragment spaces may become very large it would be useful to have a tool to visualize and navigate in fragment-based chemistry spaces.

We present the tool FragView developed for these tasks. FragView allows the user to visualize fragments as 2D structure diagrams. To overcome the problem of visualizing large fragment spaces the tool allows to reduce the set of shown fragments to those with desirable features. For example, the user can specify allowed ranges for physicochemical properties like number of atoms or link types. To have a better overview of fragments with compatible link types, it is possible to orientate the fragments according to their links employing an algorithm for constrained structure diagram generation[1]. Further on, the fragments can be inspected in a spreadsheet which allows the user to see all fragment attributes like number of atoms or number of links.

Beside visualization and orientation of fragments, FragView can also be used to build up new fragments according to the rules of the chemistry space[2]. This can be done by explicitly selecting two or more fragments which will then be connected in all possible combinations. For a more automated build up, two subsets of fragments with desirable properties can be selected by means of a query. Each fragment of the first set would then be connected with every compatible fragment of the second set. Since the new generated fragments are also part of the fragment space, all operations of the program can be used in an iterative fashion, e.g. the new fragments can be used to build up further fragments.

The functionality of FragView will be shown on sample chemistry spaces resulting from combinatorial chemistry programs and compound shredding (RECAP-Procedure).

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## References

- [1] Fricker PC, Gastreich M, Rarey M, *J. Chem. Inf. Comput. Sci.*, 2004, **44**, 1065.
- [2] Rarey M, Stahl M, *J. Comput.-Aided Mol. Design*, 2001, **15**, 497.