Markush Technology Breakthroughs

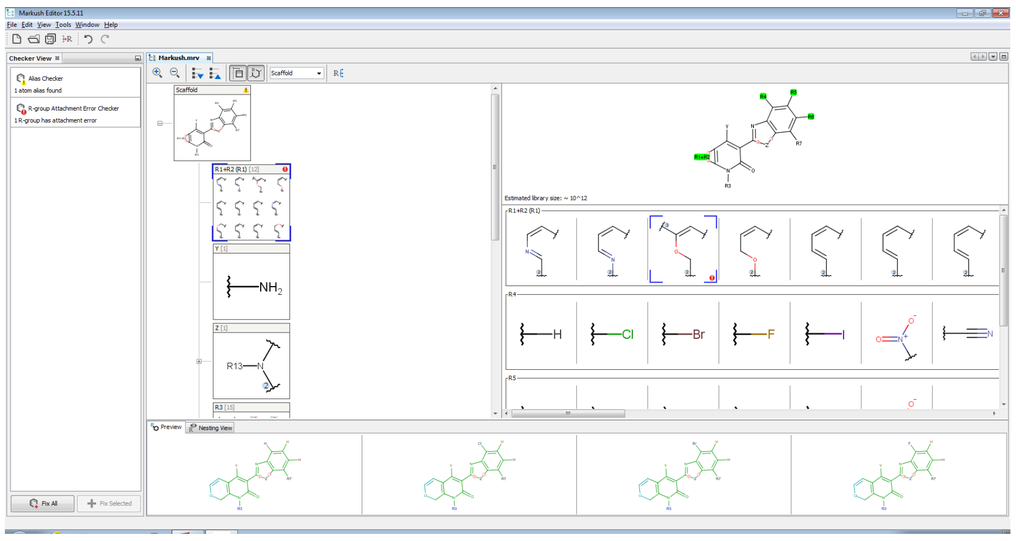
Árpád Figyelmesi, Gábor Botka, János Kendi, Péter Kovács

Overview

Markush structures are widely used in combinatorial chemistry and chemical patents to define large chemical spaces. ChemAxon released the first version of Markush Search & Enumeration in 2008 and is well-known about its market-leader Markush technology since that.

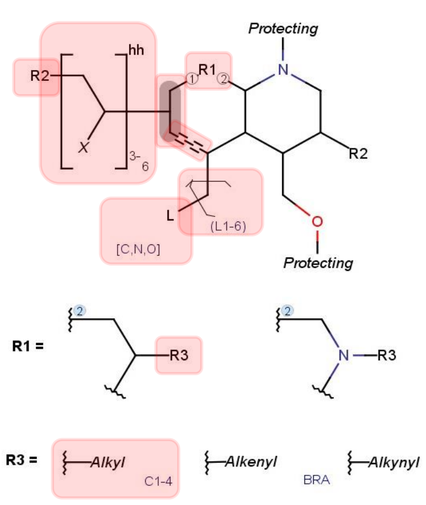
Markush Editor

Marvin and MarvinJS as general drawing tools are perfect for handling smaller Markush structures but not for structures with hundreds of fragments. Markush Editor is designed for creation and visualization of complex combinatorial and patent Markush structures. The hierarchic R-group representation, built-in interactive preview, structure checker and enumeration make it extremely powerful in this field.



Representation

ChemAxon's market-leader Markush representation supports all important structure variations, such as atom list, bond list, position variation
bond, link nodes and repetition units. Complex Markush features, such as multiply-connected R-groups, heavily nested R-groups, R-group bridging and homology groups are also supported.

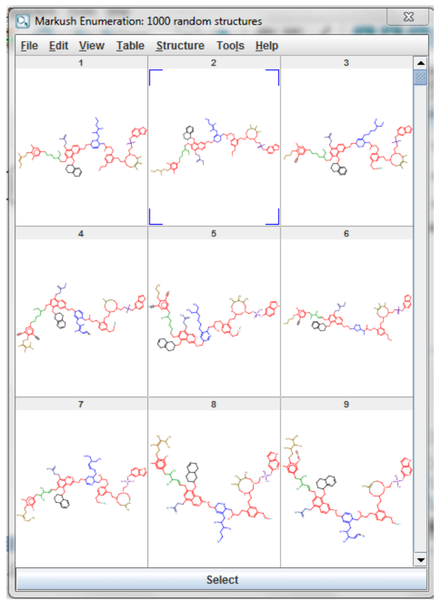


Search and Hit Coloring

Markush Search can be used to search in a large chemical space defined by generic Markush structures, without actually enumerating the explicit compounds. This approach enables the exploration of extremely large Markush spaces, which would be unthinkable by traditional search techniques. Hit coloring and automatic structure alignment make the visualization of the search results easier.

Enumeration

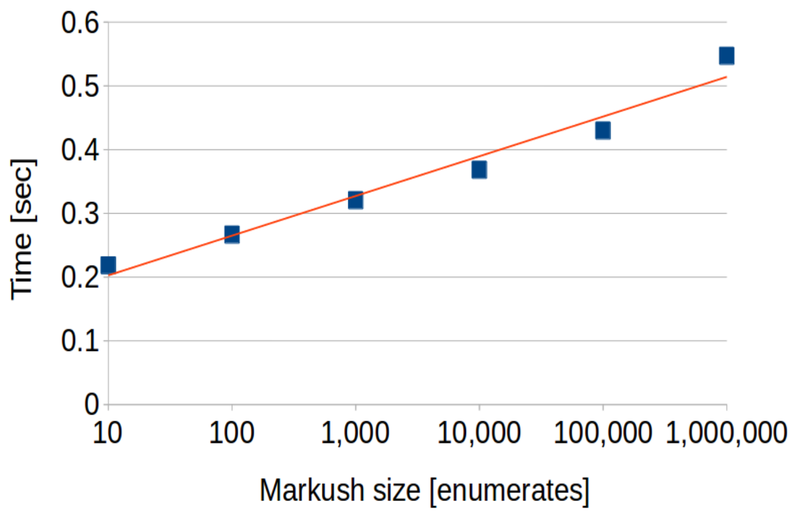
Markush Enumeration is a powerful tool for Markush structure analysis. By interactively guiding the enumeration of the Markush structure, users can quickly understand the covered chemical space. Current enumeration types include full, partial, and random enumeration as well as library size calculation.



Overlap Analysis

NEW

Markush Overlap analysis is capable to calculate the overlapping chemical space between two Markush structures regardless of the complexity of the structures. The percentage of overlap and the Markush representation of the overlapping chemical space can be calculated.



Overlapping chemical space calculation

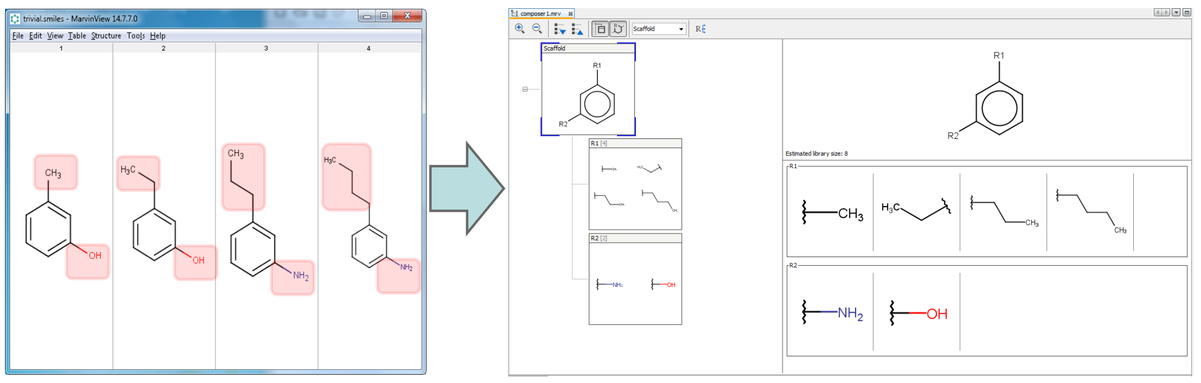
Results:
- Percentage of overlap
- Overlapping Markush

Benefits:
- No enumeration
- No size limitation

Composer

NEW

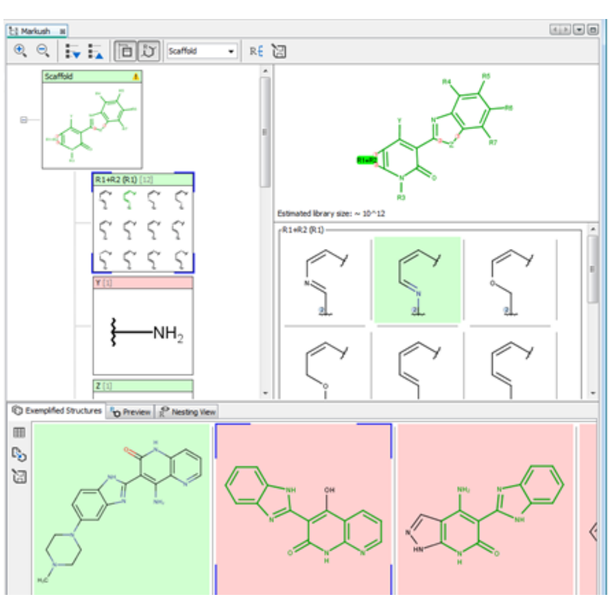
Besides drawing it manually, a Markush structure can be generated automatically from a molecule library using R-group decomposition or the new Composer. Compared with R-group decomposition, Composer can calculate the optimal scaffold automatically and can generate not only combinatorial but also complex patent like Markush structures according the user needs.



Non-hit Visualization

NEW

Markush non-hit visualization technology is capable of highlighting both the matching and non-matching parts in a query structure and in the R-groups of a target Markush structure in the cases when the query does not fully match to the Markush.



Differentiating structure parts visualization in target Markush and Query structure.

Based on Markush Overlap and MCS technologies.

Benefits:
- Easily understandable difference visualization
- Extremely fast comparison

ChemAxon Ltd, 1031 Budapest, Zahony u. 7, Hungary
www.chemaxon.com

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