

Markush Search is an add-on for JChem which enables patent and combinatorial chemistry researchers to store and search Markush structures in the same way as other chemical structures. Through supporting Markush features in the chemical editor and query features in the JChem search engine, Markush Search can easily and rationally expand the capture and use of Markush content across your organization.

## Features

### Markush structure

- R-groups (nested to any depth)
- Atom and bond lists
- Link nodes and repeating units
- Position variation bonds
- Homology variation for generic (alkyl, aryl, etc) and user-defined (protecting group, etc) groups

### Searching Markush records

- Markush query features included within MarvinSketch chemical editor
- Sub structure and full structure search

### Working with search results

- Queries are highlighted in the result (relevant parts of scaffold and R-group(s))
- Markush structure hit reduction, expands the generic features overlapping each hit
- Toggle display of R-group definitions

### Complexity - patent and combi-chem

ChemAxon's Markush technology is designed to handle the large chemical spaces often described by a single Markush structure, without enumeration:

- Combinatorial chemical space of at least 10<sup>30</sup>
- Patent chemical space of potentially infinite size (homology groups)

## Integration ready

### Platform

- Runs under all major operating systems
- All major database engines supported
- Choice of interfaces; API (Java and .NET), command line, web service,
- Integrated within JChem toolkit (JChem Base, JChem Web Services)
- Pipeline Pilot and KNIME connectivity

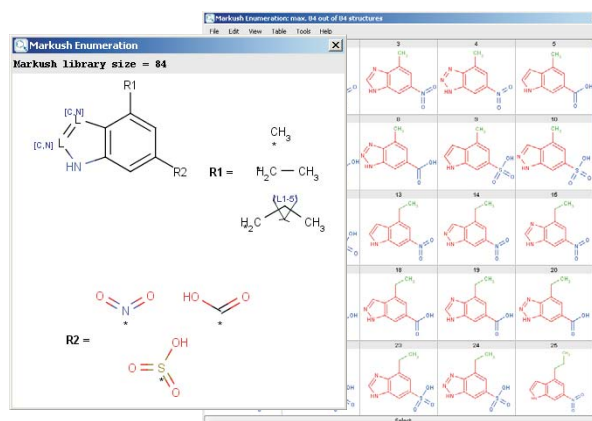
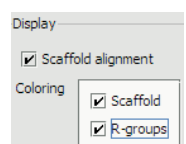
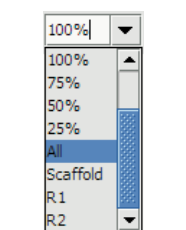
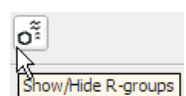
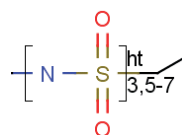
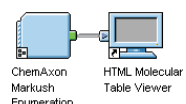
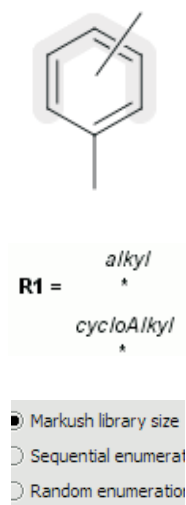
### Applications & web delivery

- Supports integration in applications and web pages (Java Applets, Java Beans, .NET)
- Integrated within ChemAxon's desktop products (Marvin, Instant JChem, JChem for Excel)

## Markush enumeration

As a part of Markush Search, we include the Markush enumeration Calculator Plugin, which allows full, partial and random enumeration of Markush structures as well as calculation of the library size.

- Coloring of scaffold and R-groups
- Alignment of output structures
- Simple selection of structure parts during partial enumeration
- Uniform distribution of random set representatives in chemical space
- Calculate exact or scale of magnitude for the represented chemical library of Markush structures
- Markush code - identifier of enumerated structures

## Feature focus

### Homology Groups

Within patent chemistry, homology groups represent generic description of chemical groups, but often without explicit definitions.

Homology groups are handled by the software:

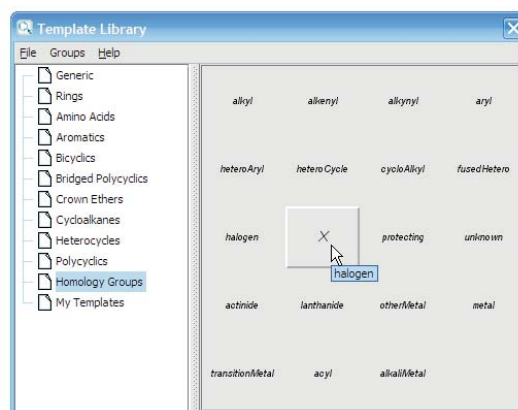
The most common homology groups are available via the MarvinSketch structure editor and custom homology groups can be defined by the user.

#### In Markush search

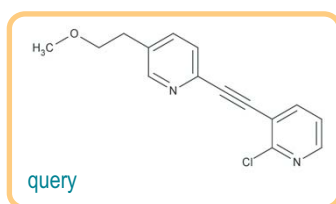
Specific chemical groups used as part of the query will find the corresponding homology group in the database.

#### In Markush enumeration

Homology groups can be enumerated, either as a homology group pseudo atom or using structure definitions. Users can customize structure definition lists for each homology group.

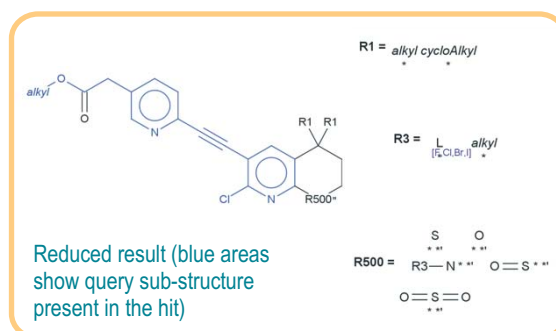
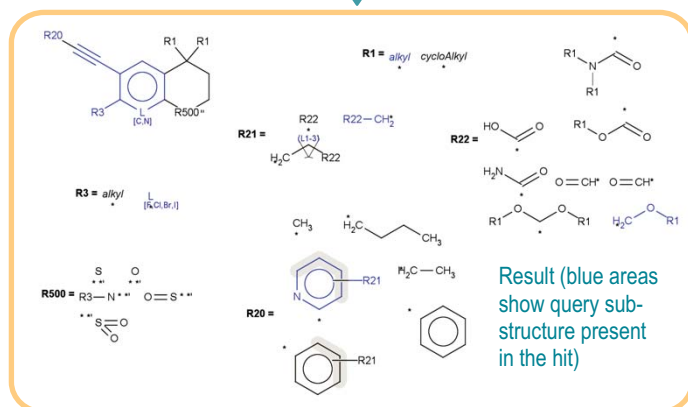


### Markush structure hit reduction



Markush reduction is used to display Markush substructure hits. The visualization expands and highlights the variable parts included in the substructure.

In this example the query and standard and reduced hit results are shown.



## I want to try this



Free evaluation



Free for teaching & academic research



Free for free websites

Markush Search is an add-on for JChem Base, Instant JChem, Marvin and JChem for Excel desktop applications and is already included in the download packages.

We can provide evaluation licensing for you to try out Markush Search and Markush enumeration. Please contact [sales@chemaxon.com](mailto:sales@chemaxon.com) or your local representative.