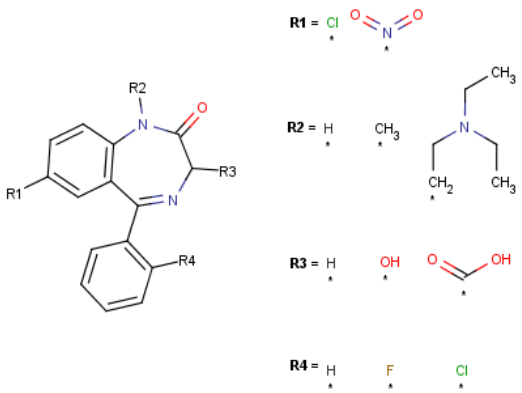
Creating and understanding Markush libraries

The New Markush Editor

Árpád Figyelmesi

Motivation

Markush structures are widely used in combinatorial chemistry and patents to define large chemical spaces.



United States Patent [19]
Bitonti et al.

[11] **Patent Number: 5,681,863**
[45] **Date of Patent: Oct. 28, 1997**

[54] **NON-METABOLIZABLE CLOMIPHENE ANALOGS FOR TREATMENT OF TAMOXIFEN-RESISTANT TUMORS**

[75] Inventors: **Alan J. Bitonti**, Maineville; **Russell J. Baumann**, Cincinnati, both of Ohio

[73] Assignee: **Merrell Pharmaceuticals Inc.**, Cincinnati, Ohio

[21] Appl. No.: **350,192**

[22] Filed: **Dec. 5, 1994**

Related U.S. Application Data

[62] Division of Ser. No. 196,817, Feb. 10, 1994, Pat. No. 5,410,080, which is a continuation of Ser. No. 945,305, Sep. 15, 1992, abandoned.

[51] **Int. Cl.**[6] **A61K 31/135**
[52] **U.S. Cl.** **514/648**; 514/649
[58] **Field of Search** 514/648, 649

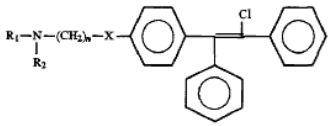
[56] **References Cited**

3,631,109	12/1971	O'Sega et al.	260/570.9
4,696,949	9/1987	Toivola et al.	514/644
4,839,155	6/1989	McCague	514/651
5,114,951	5/1992	King et al.	514/290
5,130,424	7/1992	Weintraub	540/28

Primary Examiner—Jerome D. Goldberg
Attorney, Agent, or Firm—Nelsen L. Lentz

[57] **ABSTRACT**

Compounds of the formula:

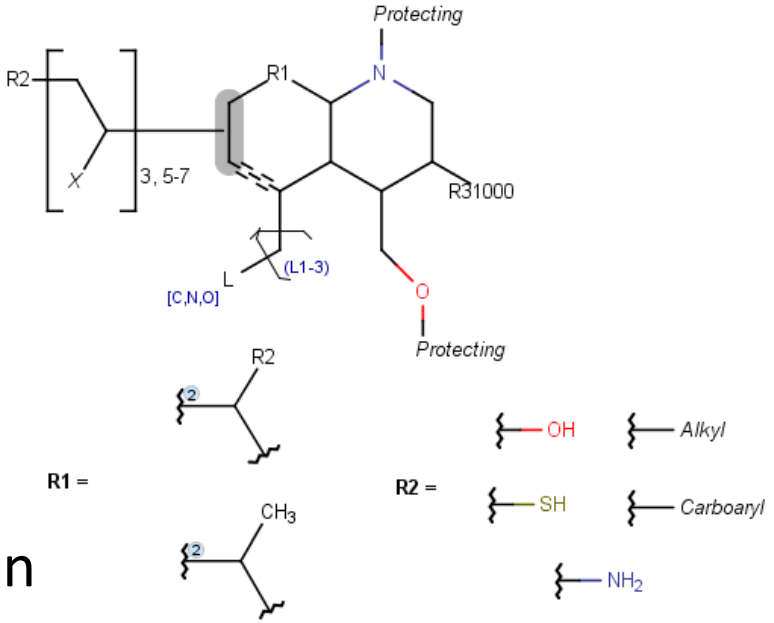


wherein R_1 and R_2 are each selected from the group consisting of C_1–C_2 lower alkyl; X is NH or S; and n is a whole number within the range of 1–4 inclusive; and when n=0, X is $(CH_2)_3$ and the pharmaceutically acceptable salts thereof

ChemAxon

Overview

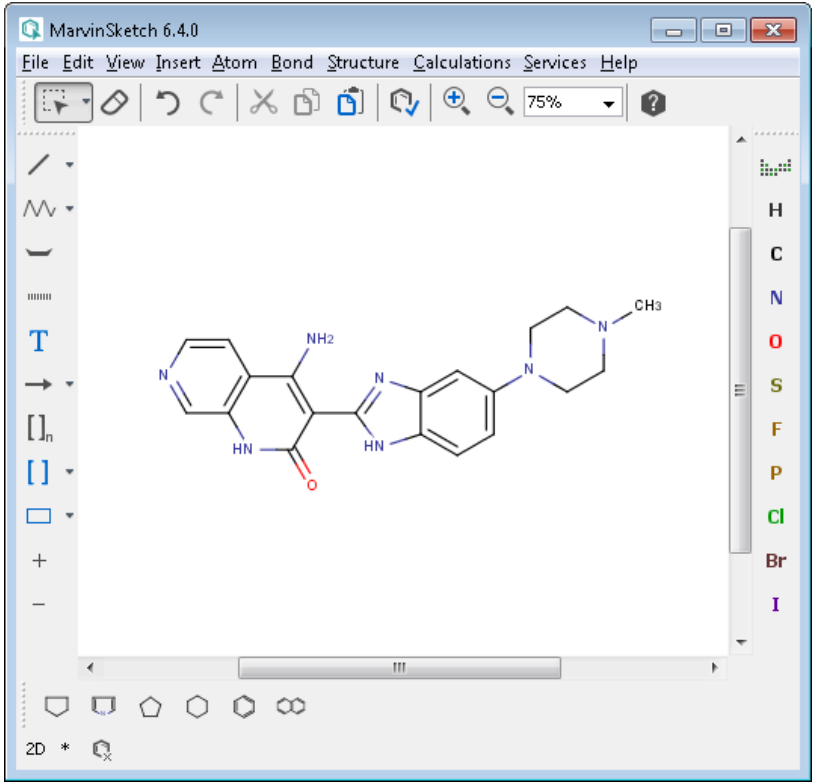
- Market leader Markush technology
  - R-groups
  - Atom lists, bond lists
  - Position variation bond
  - Link nodes
  - Repeating units
  - Homology groups
- Markush enumeration
- Markush search & hit visualization
- R-group decomposition

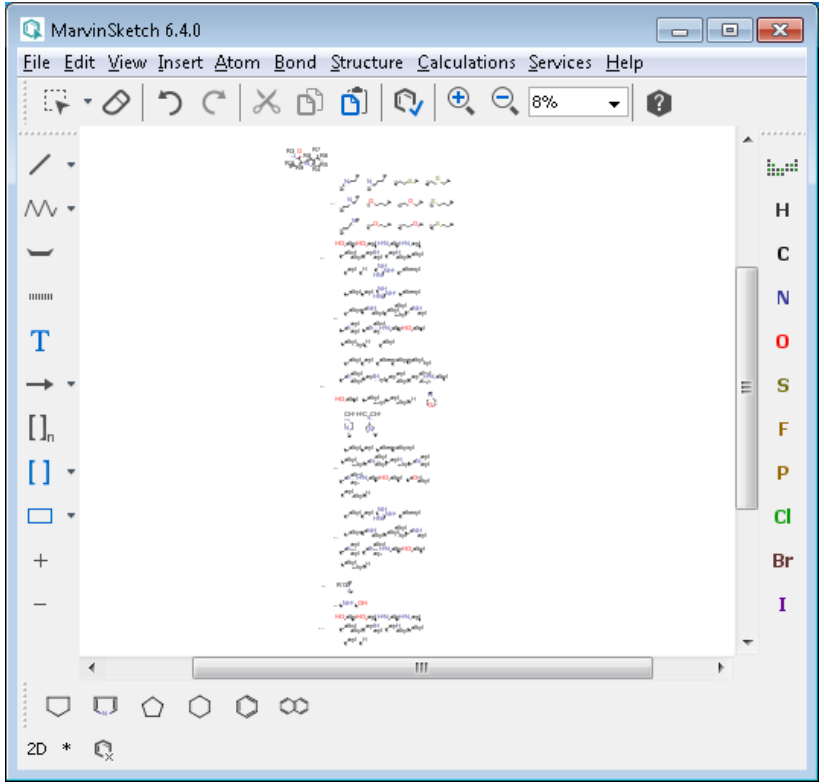


Challenges

- No proper tools for editing complex Markush structures
- Manual processing and analyzing is time consuming and needs special expertise

General structure editors

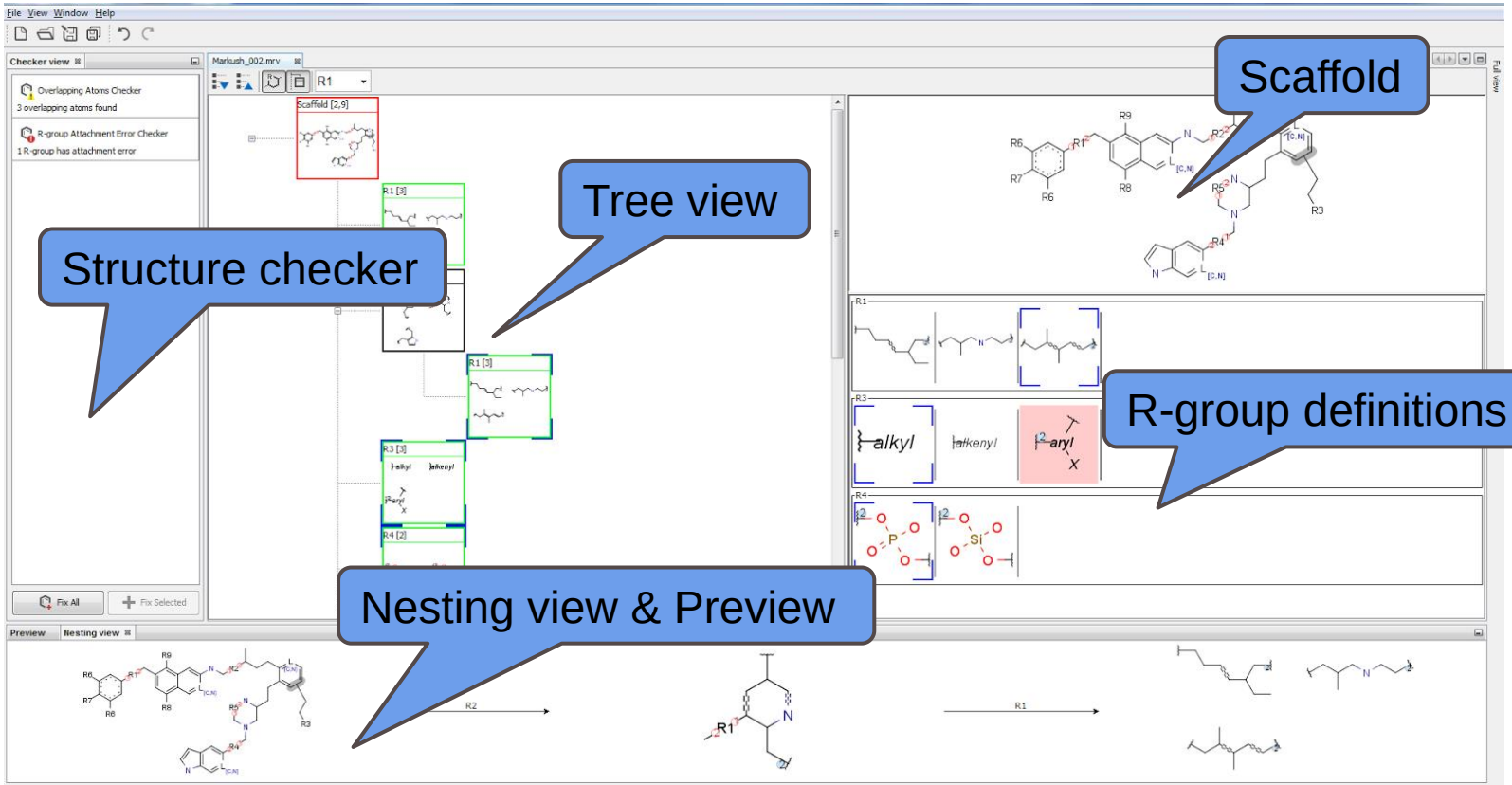




Markush Editor

- Editing complex patent Markush structures
- Hierarchical representation of fragments' relationships
- Visualization of nesting view, preview
- Editing individual fragments separately
- Integrated structure checker
- Available as a desktop application and as an integratable component

Markush Editor



Coming soon in Markush Editor

- Markush composer function
- New Markush structure checker functions
- Markush standardization
- Alias handling

Coming soon in Markush technology

- Markush overlap analysis

  Percentage of overlap and representation of overlapping chemical space
- Markush non-hit visualization

  Visualization of distinguishing structure parts
- ChemCurator

  http://www.chemaxon.com/wp-content/uploads/2014/05/ChemAxon-Patent-Curation.pdf

US UGM 2014

Markush Session at ChemAxon US UGM, September 25-26, Cambridge, MA

We launch ChemCurator and overview existing Markush Editor, search and enumeration technologies

User presentations from Merck and Novartis, including (provisional)

- "Construction of a vast virtual library powered by ChemAxon's Markush Search Platform and its utility in molecular design - Zhengwei Peng, Merck & Co.
- The needs and challenges related to in-depth analysis of patent molecular spaces to support drug discovery projects. -Zhengwei Peng, Merck & Co.
- Placeholder topic: Markush search - Gregory Landrum, Novartis

Thank you for your attention

Tutorial

http://www.chemaxon.com/library/markush-editor-6-3-version/

User guide

https://docs.chemaxon.com/display/markusheditor063/User%27s+Guide

Download page

http://www.chemaxon.com/download/markush-editor/

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