Last Wave? – Reference Books Go Digital

The Next Step at Major Reference Works

Global Major Reference Works (CMRW)

225th ACS Meeting, New Orleans 23rd – 27th March 2003
What does „Global“ stand for?

Different data sources combined in one application

What does „Global Major Reference Works“ stand for?

Different major reference works combined in one application

- Retrieval of structures, reactions and text of several data sources at the same time using one application
1. Which Reference Works are included?
2. The Production of single electronic MRW's
3. The Concept of Global-MRW
4. Workflow Example
5. About InfoChem
Which Reference Works are included?

- **Thieme:** Science of Synthesis - Successor of "Houben-Weyl"
  - **planned:** 48 volumes with 250,000 reactions 4-6 volumes / year  → Finished 2008
  - **currently available:** 8 volumes (1,2,4,5,9,10,11,12) with 28,200 reactions
Which Reference Works are included?

John Wiley:

Encyclopedia of Reagents for Organic Synthesis

- 8 volumes
- 52,000 reactions
- 2 updates / year with 2,000 reactions
- Update of the electronic version started in 2002
- Further update March 2003
Which Reference Works are included?

- Springer: Comprehensive Asymmetric Catalysis
  - 3 volumes
  - 6,600 reactions
  - next update winter 02/03 with 600 reactions
The Production of single electronic MRWs
Production of the electronic Version

Database Building

Print Version

Structure / RXN Database

Connection Table

Stored details
- Structures/RXN
- Factual Data
- Catalysts
- Solvents

Search and Retrieval System

InfoChem

InfoChem

InfoChem

Index-Files
The Heart of MRW
The Linking

Electronic Database

Index-Files of the Structure/RXN Database

InfoChem Search Engine (ICSE)

Essential:
- Storing the information where the record is located in the print version

Electronic Version

HTML-Document

InfoChem produces:
- Table of Contents
- Full text index
- Hidden HTML Anchors
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Essential:
Storing the information where the record is located in the print version

Publisher

Electronic Version

Print Version

InfoChem

Electronic Database

Structure/RXN Database

HTML-Document

Location

Link
The Architecture of MRW

Electronic Versions of MRWs

- searchable Database in the Background
- Interface of a single MRW
- Database and HTML are linked together
The Powerful Search Index

What have we achieved?
What distinguishes this approach from a typical text book in chemistry?

- The database created is used as a very powerful new index to the text
- Access to structure and substructure searching
The Concept of Global Major Reference Works (GMRW)
The Architecture of Global-MRW

GMRW Software

- One Application
- Global Search
- Navigation, Browsing, Retrieval in Each Individual MRW

Internet/Intranet http Server

InfoChem‘s Global MRW Software: Search Engine and the electronic MRWs:

- InfoChem Search Engine (ICSE)
- Index-Files

Client
Workflow Example
Synthesis - A Workflow Example

Synthetic Problem

Required information:

- general information about reaction or synthesis strategies
Synthesis - A Workflow Example

Query

- Select global (Search All) or specific MRW
- Select Type of Structure or RXN Query (ISISDraw starts automatically)
- Draw query and Transfer query

Client
Synthesis - A Workflow Example

Query

- Submit query
- Get global hitlist
- Select MRW

Major Reference Works

VRW - Major Reference Works

Results from All Licensed MRW Publications

- CAC 16 Hits
- EROS 41 Hits
- Science of Synthesis 1 Hit

Note: Science of Synthesis works with Internet Explorer only

Return to Query
New Query

Hints & Tips
Synthesis - A Workflow Example

Secondary literature

- Jump directly to the MRW-HTML
- Jump back to hitlist

Chiral aluminol so far been developed for...
Synthesis - A Workflow Example

For additional information select another MRW

Major Reference Works

- CAC
- EROS
- Science of Synthesis

MRW - Major Reference Works

Results from All Licensed MRW Publications

- CAC 16 Hits
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Return to Query

New Query

Hints & Tips
Lanthanide Shift Reagents

\[
\text{Eu(fod)}_3, \quad M = \text{Eu} \\
\text{Yb(fod)}_3, \quad M = \text{Yb} \\
\text{Eu(hfc)}_3, \quad R = \text{CF}_2\text{CF}_2\text{CF}_3 \\
\text{Eu(tfc)}_3, \quad R = \text{CF}_3
\]

(17631-58-4) \cdot \text{C}_2\text{H}_6\text{EuF}_3\text{O}_6 \cdot \text{Eu(fod)}_3 \cdot (\text{MW 1037.50}) (\text{Yb(fod)}_3)

(18323-96-1) \cdot \text{C}_2\text{H}_6\text{EuF}_3\text{O}_6 \cdot \text{Yb(fod)}_3 \cdot (\text{MW 1058.58}) (\text{Eu(hfc)}_3)

(34788-82-4) \cdot \text{C}_2\text{H}_6\text{EuF}_3\text{O}_6 \cdot \text{Eu(hfc)}_3 \cdot (\text{MW 1193.73}) (\text{Eu(tfc)}_3)

(34830-11-1) \cdot \text{C}_2\text{H}_6\text{EuF}_3\text{O}_6 \cdot \text{Eu(tfc)}_3 \cdot (\text{MW 894.72})

(mild Lewis acids capable of catalyzing a variety of synthetic transformations)

Alternate Names: \text{Eu(fod)}_3 = \text{tris}(6,7,8,8,8,8\text{-heptanofuro-2,2-dimethyl-3,5-octanedionato})\text{europium}; \text{Yb(fod)}_3 = \text{tris}(6,7,8,8,8,8\text{-heptanofuro-2,2-dimethyl-3,5-octanedionato})\text{yterbium}; \text{Eu(hfc)}_3 = \text{tris}(3\text{-heptanofropylyldihydroxymethylene})\text{-} (+ + -)\text{-camphorato} \text{europium}; \text{Eu(tfc)}_3 = \text{tris}(3\text{-trifluoromethyl} \text{dihydroxymethylene})\text{-} (+ + -)\text{-camphorato} \text{europium}
The starting question was:
How to synthesis this target molecule?

The resulting suggestions are:

**Science of Synthesis:**
- This cycle is the result of a Hetero-Diels-Alder reaction
- Lanthanide complexes are most suitable
- For enantioselective Hetero-Diels-Alder reaction use specified catalysts

**e-Eros:**
- Assembly of potential Lanthanide Schifft Reagents suitable for Hetero-Diels-Alder reactions

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**Target Molecule**

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About InfoChem

A software company founded in 1989

Production of structural and reaction databases

Development of Internet/Intranet versions of printed major reference works (MRW)

Development of specialized chemistry software tools

Since 1991 a part of Springer-Verlag (Heidelberg)

Since Springer-Verlag has been taken over by Bertelsmann in 1998 InfoChem has become part of the Bertelsmann group
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