CIRX and SPORE synthetic methodology databases
Using Isis or Isentris software

Better, faster synthesis of novel compounds

Search by structure to identify promising starting materials and intermediates, design solution-phase and solid-phase combinatorial libraries and develop plans for entirely novel syntheses. Search over both databases with a single query and integrate in-house data.

The ChemInform Reaction Library (CIRX) helps to deal with the enormous number of published reactions as it does not cover all information available but rather a quintessence based on a careful selection. CIRX provides detailed reaction data selected from about 100 journals. The selection focuses on novel or improved synthetic methods, syntheses of new compounds or classes of substances, and reactions employing new catalysts or reagents. Standard applications of well-known reactions are not covered. To ensure reliable data, the highly qualified ChemInform staff extract the reaction data from both the publication and the supporting material, and occasionally even contact the authors to clarify inconsistencies in the original publications.

ChemInform® RX

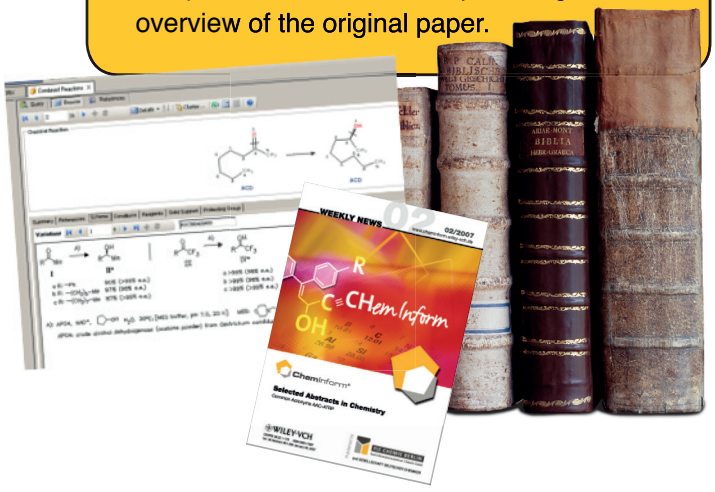
The **ChemInform Reaction Library (CIRX)** provides reactions of interest to synthetic chemists from 1990 to the present and, in combination with RefLib, over one hundred years of chemical literature citations supporting synthetic methodologies. CIRX is the best source for the synthesis of novel organic compounds, providing scope and limitations of reactions and targeted, highly relevant hit sets. CIRX also contains detailed information on chemo-, regio-, and stereo-selective reactions. The RefLib database is included with CIRX and provides reactions abstracted from Theilheimer's Synthetic Methods of Organic Chemistry (1900-1991).

The **Current Synthetic Methodology (CSM)** database is a subset of CIRX containing the most innovative and significant reactions since 1992

SPORE

Solid Phase Organic Reactions (SPORE) describes various aspects of organic reactions performed on solid supports and provides access to the syntheses of small molecules, peptides, and solid-supported reagents. The application, scope and limitations of the solid-phase reactions are delineated by detailed comments and a series of special datafields relating to the polymeric scaffold, linkers, linkage type, protecting groups, and reaction conditions.

There is a long and fascinating history behind the ChemInform product family. It is going back to the legendary German Chemisches Zentralblatt established in 1830, which was the most important reference work for chemists around the world. For decades, scientific editors have prepared abstracts of the research progress in chemistry for this information service. Now the needs of the modern chemists are met in a modern product family combining the traditional printed weekly ChemInform journal with online offers and the inhouse databases ChemInform Reaction Library and SPORE. Due to the print media background, the reaction databases deliver compact reaction schemes providing an overview of the original paper.



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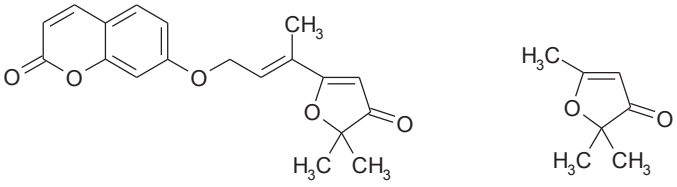
View full reaction schemes

CIRX and SPORE offer full reaction scheme views, enabling researchers to quickly evaluate the utility of a given reaction in the synthesis of new target molecules.

Case Study

Geiparvarin (Figure 1), a potent anti-tumor agent, is one of many natural products containing a furan-3(2H)-one ring. You want to develop a simple route to a number of these heterocycles.



1

2

Figure 1: Geiparvarin (1) and core target structure (2)

A search for the basic ring structure in CIRX retrieves several reaction records, one of which is shown in Figure 2. Although the method described in Figure 2 looks useful, it is difficult to judge its suitability to targets with different structural features. This is where viewing the full reaction scheme can help in evaluating the reaction further (Figure 3).

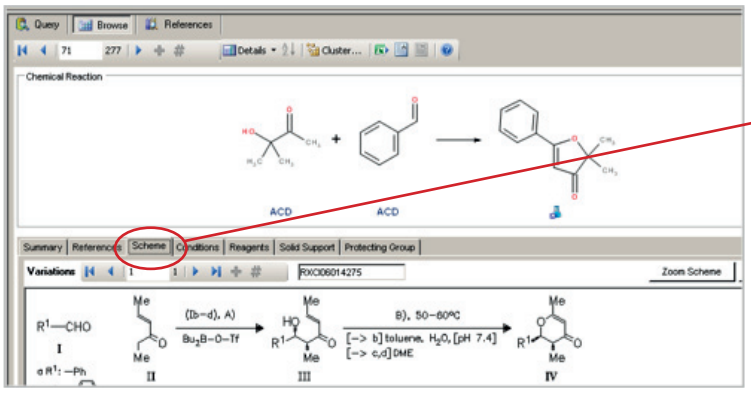


Figure 2: Reaction record for the synthesis of a furan-3(2H)-one

By looking at full reaction schemes, you can easily evaluate the potential value of given reactions in designing syntheses.

The full reaction scheme shows the reaction in the context of the overall synthetic strategy from the article (**A** Figure 3). Now you can see the effect of various substituents on the course of the reaction (**B**). You also see methods for preparation of the precursors to your target and various reaction conditions used. Viewing the full reaction scheme, instead of simply viewing the reaction in isolation, makes it much easier to evaluate the scope of a reaction. The full scheme also describes a similar synthetic scheme to closely related dihydropyranones (**C**). These compounds would not have been retrieved by the original reaction search.

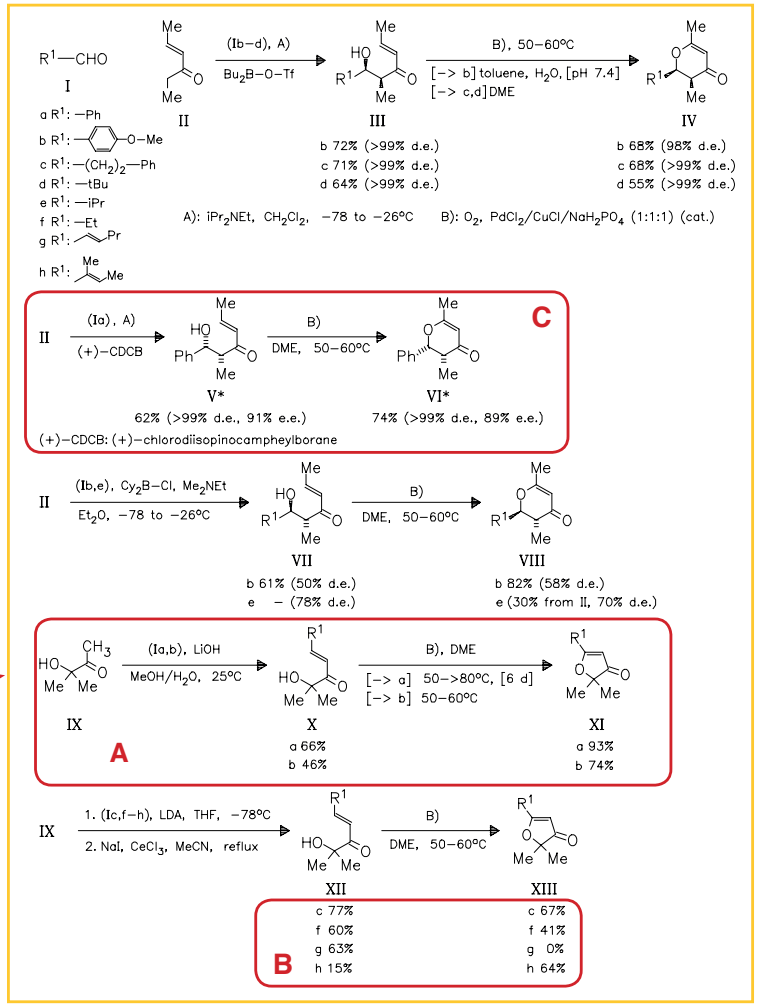


Figure 3: Full reaction scheme showing overall route to furan-3(2H)-ones

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