

New on DiscoveryGate®

View full reaction schemes in select synthetic reaction databases

Chemists using the DiscoveryGate® platform now have a unique new tool that provides a dramatic visual aid in synthesis planning. The ChemInform Reaction Library and MDL® Solid-Phase Organic Reactions databases (both produced by FIZ CHEMIE Berlin) offer full reaction scheme views, allowing researchers to quickly evaluate the utility of a given reaction in the synthesis of new target molecules.

“When viewing a reaction result from a search, synthetic chemists must judge the suitability of the reaction for their particular synthetic problem,” says Dr. Terry Wright, Chemistry Database Product Manager for Elsevier MDL. “If their molecules are

structurally different from the search result, this can be difficult to evaluate.”

The full scheme display shows the reaction in context of the overall strategy described in the reference. “This can demonstrate the effects of substituents, such as electronic or steric, on the course of the reaction,” says Wright. “This information often provides indications of the suitability of the reaction for a new purpose.”

“Another advantage of viewing a reaction in the context of an overall synthetic scheme is that chemists may find that all or portions of this scheme may also be useful to their synthetic needs, thereby reducing time spent searching for individual reactions to build a synthetic route,” says Wright.

www.discoverygate.com

Finding similar reactions

With a single search on the DiscoveryGate platform, chemists can review reactions in one data source and then link directly to similar types of reactions in other sources. This interlinking between chemistry and synthetic methodology databases and Integrated Major Reference Works creates the industry's most

advanced system for selecting and evaluating synthetic methods.

For chemists, this unique functionality can significantly simplify and accelerate synthesis planning. To get more information and sign up for a free evaluation, click Reaction Linking Evaluation on www.mdl.com.

Case study

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

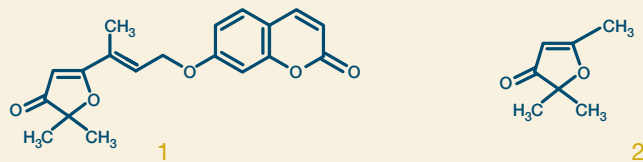


Figure 1: Geiparvarin (1) and core target structure (2)

A search for the basic ring structure in ChemInform Reaction Library 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 from the article can help in evaluating the reaction further (Figure 3).

The full reaction scheme shows the reaction in the context of the overall synthetic strategy from the article (highlight A, Figure 3). Now we can see the effect of various substituents on the course of the reaction (highlight B). We also see methods for preparation of the precursors to our target and various reaction conditions used (highlight C). Viewing the full reaction scheme, makes it much easier to evaluate the scope of a reaction.

ChemInform Reaction Library

Reaction Details (hide)

RXC06014246 Reaction Variation 1 of 1

Product no.	% Yield	Grade	%Cs	%ds	%de	%ee	Reaction no.	Reactant Grade
1	93		100					

Step no.	Catalysts and Solvents	Catalyst ID	Solvent ID
1	02 PdCl ₂ /CuCl/NaH ₂ PO ₄ (1:1:1) (cat.) DME	5896 6100 8042 20931	5855

Detailed Data

External Registry No. 1060913907 Path A Step 2 Of 2

Export

REITER, M., TURNER, H., MILLS-WEBB, R., GOUVARNEUR, V., *J. Org. Chem.* (JOCFAH) 2005, 70 (21), 8478-8485.

Figure 2: Reaction details for preparation of a furan-3(2H)-one

The full scheme also describes a similar synthetic scheme to closely related dihydropyranones (highlight D). These compounds would not have been retrieved by the original reaction search.

This enhancement to the ChemInform Reaction Library and Solid-Phase Organic Reactions databases on DiscoveryGate provides a powerful tool for synthetic chemists. "By looking at the full reaction scheme you can quickly evaluate the potential value of a reaction in designing syntheses," says Wright. "And with DiscoveryGate you can add these images to reports, and use the rich interlinking between databases to instantly check for relevant chemical sourcing information, material safety data, bioactivity information, similar reactions and more." ■

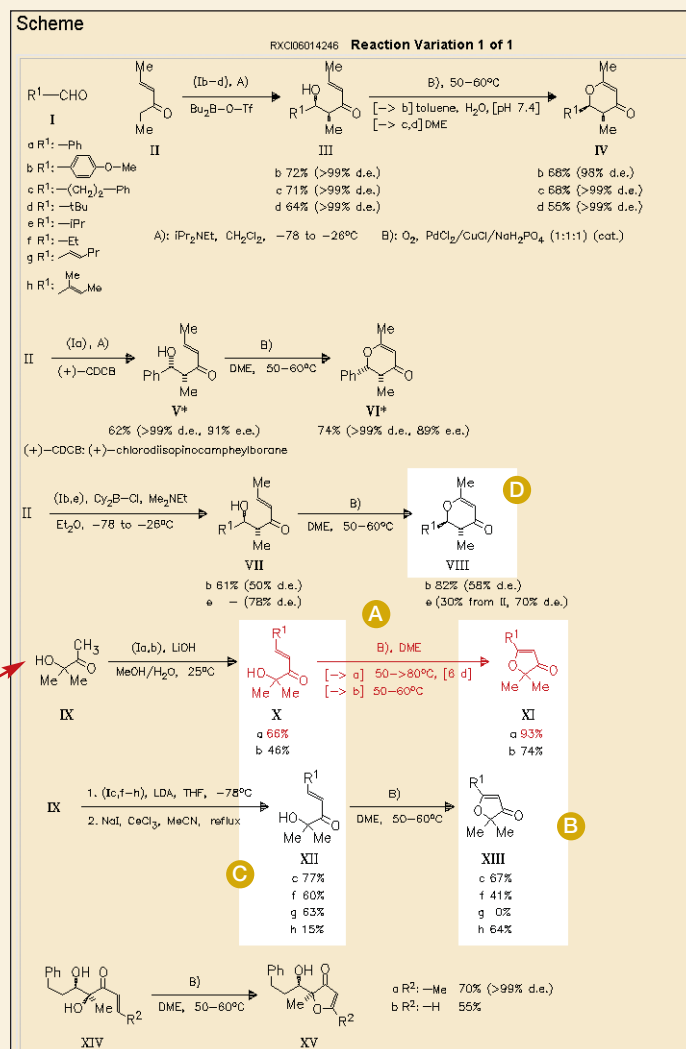


Figure 3: Full reaction scheme showing overall route to furan-3(2H)-ones, reaction conditions and substituent effects on outcome of the synthesis. Also shown is a route to closely related dihydropyranones.



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