Analysis of Synthetic Approaches toward Glyoxylic Acids

Biography

Dr. Charlotte Gers (right) studied Chemistry at Heinrich-Heine-Universität Düsseldorf, Germany. She obtained her Ph.D. with Prof. Thomas J. J. Müller in May 2014. Her studies focus on one-pot synthesis and photophysical investigations of fluorescent quinoxaline derivatives.

Franziska Merkt, B.Sc., (left) is currently engaged in her Master thesis on quinoxaline dyes in the group of Prof. Thomas J. J. Müller at Heinrich-Heine-Universität Düsseldorf, Germany.

Institution

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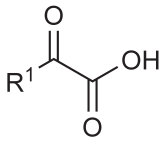
Abstract

In this case study, we investigated possible synthetic approaches toward glyoxylic acids (Scheme 1) with *Science of Synthesis* Online. The search was based on Section 20.2.5 (2-Oxo- and 2-Imino-Substituted Alkanoic Acids) and the structure-based query tool. The results of both approaches will be discussed and compared.



Scheme 1 General Structure of Glyoxylic Acids

Discussion

Glyoxylic acids are valuable starting materials for our one-pot syntheses toward various quinoxalines. However, only a small variety of derivatives is commercially available. In order to increase the substrate scope of our one-pot reactions, we became interested in synthetic methods for such compounds, especially aryl-substituted derivatives.

The aim of this case study was to identify possible synthetic approaches toward glyoxylic acids, which allow the introduction of a large variety of aromatic substituents, preferably starting from commercially available or easily accessible substances.

Science of Synthesis Online offers a comprehensive chapter (Section 20.2.5, 2-Oxo- and 2-Imino-Substituted Alkanoic Acids) on the synthesis of glyoxylic acids. This chapter is divided into four categories: hydrolysis (Section 20.2.5.1.1), oxidation (Section 20.2.5.1.2), Friedel–Crafts acylation (Section 20.2.5.1.3), and aldol condensations of pyruvic acid with benzaldehydes (Section 20.2.5.1.4) and provides 13 basic methods and 49 citations in total (Scheme 2). Each chapter and subchapter can be reached by navigation through the tree structure. The well-organized data in combination with intuitive chapter titles facilitates the localization of required details in a quick and comfortable manner. The chapter-based search is a useful tool to acquire a general overview of a topic.

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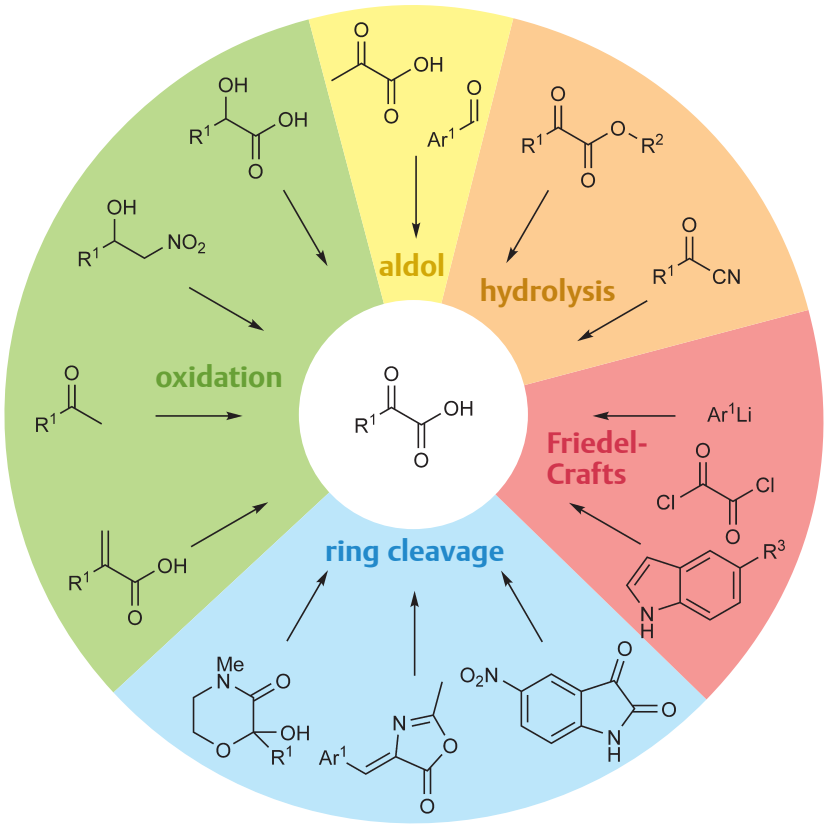

Scheme 2 Synthetic Approaches toward Glyoxylic Acids Divided into Reactivity-Based Subclasses

Additionally, the structure-based query tool was used to search for synthetic approaches toward glyoxylic acids. This tools enables general structure searches by using R or A as substituents, but also searches for specific structures such as R^1 = Ph. The results can be refined by setting filters. This tool enables a more straightforward search compared to the chapter-based method. Glyoxylic acid syntheses were located in ten other subchapters. Searching for those by browsing through the chapters, would have been a tedious task.

Each of the subchapters contains general information on a specific synthetic method, e.g. reaction conditions, yields, tolerated functional groups, and the corresponding literature. Additionally, experimental details are given, which offers an ideal starting point for the synthesis of novel and known derivatives.

Conclusion

Science of Synthesis Online provided a good overview of glyoxylic acid syntheses quickly and comfortably. A comprehensive data set was obtained by combining the chapter-based search with the structure-based query tool. The well-organized structure of the available data is very user-friendly. The review-like character of the product in combination with a vast amount of experimental detail is highly suited to locating the most efficient and diversity-oriented methods for the synthesis of starting materials.