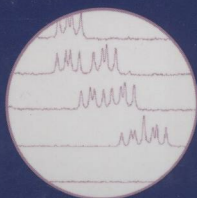


# Discrimination of Chiral Compounds Using NMR Spectroscopy



THOMAS J. WENZEL

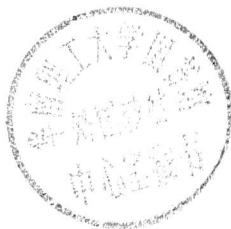
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# DISCRIMINATION OF CHIRAL COMPOUNDS USING NMR SPECTROSCOPY

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SPECTROSCOPY**



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*To Brad and Erica*

# PREFACE

Nuclear magnetic resonance spectroscopy represents one of the most common methods employed for the analysis of chiral compounds. I used over 30 different keywords or combination of keywords as well as numerous CAS numbers in trying to identify articles that describe the development and application of chiral NMR discriminating agents. My search of the literature identified about 3000 publications in which NMR spectroscopy had been employed for the determination of optical purity or assignment of absolute configuration. Many of these reports described new chiral reagents or expanded the applicability of the existing chiral reagents. Many others involved the use of known reagents as tools to analyze a compound of interest to the investigator.

In organizing the manuscript, I had to make a choice between identifying compound classes and then describing particular chiral NMR reagents suitable for analyzing them and identifying chiral NMR reagents and describing the range and types of compounds for which they could be used for analysis. I opted for the latter organization, as too many compounds that were analyzed in the literature were polyfunctional. These polyfunctional substrates often did not have a particular, identifiable functional group that was solely responsible for interaction with the chiral reagent, or bound simultaneously through two sites, thereby resisting easy classification.

In identifying NMR reagents, I opted for a broad coverage so as to show the extensive range of systems that have been used for the analysis of chiral compounds. For those reagents that are the focus of only one or a handful of studies, I generally incorporated a brief discussion of all of the articles I was able to identify. For those chiral discriminating agents that have been extensively applied, which in some cases extend to hundreds of compounds, a discussion of every application was neither

desirable nor feasible. Instead, with these reagents, I focus on aspects that demonstrate the overall utility of the reagent. This required a judgment on my part as to which articles best exemplify the utility of a particular reagent and no doubt reflects some of my own biases as to what is most interesting or important.

This text should be especially useful to the investigator who would like to identify a suitable reagent to analyze the optical purity or assign the absolute configuration of a particular compound. It should also be of use to investigators involved in the development of new chiral NMR discriminating agents who will benefit from the thorough review of prior work in this field.

**THOMAS J. WENZEL**



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