

Retrieval of Medicinal Chemical Information

W. Jeffrey Howe, EDITOR

The Upjohn Company

Margaret M. Milne, EDITOR

Smith, Kline, and French

Ann F. Pennell, EDITOR

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Retrieval Of Medicinal Chemical Information

William Jeffrey Howe, Margaret M. Milne, Ann F. Pennell, American Chemical Society. Division of Computers in Chemistry, American Chemical Society. Division of Chemical Information

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Library of Medicine Programs and Services National Library of Medicine (U.S.), 1990 **Current Catalog** National Library of Medicine (U.S.), 1979 First multi year cumulation covers six years 1965 70 **Information Retrieval in**

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Brown, 2013-11-06 This first systematic treatment of the concept and practice of scaffold hopping shows the tricks of the trade and provides invaluable guidance for the reader's own projects The first section serves as an introduction to the topic by describing the concept of scaffolds their discovery diversity and representation and their importance for finding new chemical entities The following part describes the most common tools and methods for scaffold hopping whether topological shape based or structure based Methods such as CATS Feature Trees Feature Point Pharmacophores FEPOPS and SkelGen are discussed among many others The final part contains three fully documented real world examples of successful drug development projects by scaffold hopping that illustrate the benefits of the approach for medicinal chemistry While most of the case studies are taken from medicinal chemistry chemical and structural biologists will also benefit greatly from the

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