

Library Handbook for Organic Chemists

Library Handbook for Organic Chemists

Andrew J. Poss

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Andrew J. Poss

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*“Two weeks in the laboratory will
save you three hours in the library.”*

*From Professor Samuel Danishefsky’s lecture
on Quadrone at the University of Rochester.*

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PREFACE

Library Handbook for Organic Chemists is an effort to bridge the gap between the needs of the research scientist and the predicaments of today's libraries. Science libraries vary in collection size, completeness, and budget. Many libraries have incomplete sets of the large expensive series such as Beilstein's, Houben-Weyl, or Rodd's. These collections are often missing important indexes and are thus rendered useless to the chemical searcher. Furthermore, it is either too late or still too expensive to complete these series. An incomplete reference collection may hold the answers to a scientist's questions, but they have no means to access the information. This book introduces the Index to the Table of Contents and provides it to as many sources as possible. The Index to the Table of Contents is expected to make incomplete collections useful to researchers. For example, if your library has a partial collection of Houben-Weyl, say Volumes 1–12, you would have to search the index in each volume to determine if the information you seek is available in this collection. The cumulative index was not published until Volume 16. By checking the Index to the Table of Contents in the Houben-Weyl section of this book, you can determine which volume to look up your desired information or borrow that volume by interlibrary loan if it is not readily available.

Throughout the book, Library of Congress call numbers are provided to aid the researcher in finding references. The journal section lists the call numbers for journals because some libraries continue to file scientific journals by call number, not alphabetically by title. (*An excellent way to turn three hours into six hours.*) Information searching is becoming only a mouse click away from the laboratory. Researchers can start their library searches without ever leaving their desk by making use of the Internet web sites and searchable CD-ROMs mentioned throughout the text.

Section A is a link between commonly asked questions or needed information and the chemical library sources available. Section B is an expansion of each secondary library source with suggestions for easy

access, indexes available, organization, and indexes to their table of contents to make the user more familiar with the resource. Section C is an index of all review articles published in *Tetrahedron* and *Synthesis* journals. Although these reviews can be accessed through other reference materials, they constitute many of the concepts of organic chemistry and quick access to them could lead the searcher to his quest faster than other reference sources.

This book is expected to streamline and organize the process of searching the chemical literature. It represents an effort to ensure that the correct reference works and all possible sources are consulted during a search. For those using computer searching, it is expected to help in selecting databases and to aid in searching. This book should be the first reference source a researcher uses when beginning a literature search and the last book he or she consults near its completion. It is written and organized so that a searcher does not have to read the entire book or even an entire section to understand and search the chemical literature. Each section of the book is designed for quick assimilation of the information necessary to find a reference.

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Buffalo, N.Y., 2000

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I express my deepest appreciation to “Beany Mae” for her support and encouragement during the preparation of this text.

I also acknowledge the publishers and database companies for their permission to reproduce information found in this book.

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Beilstein-Institut	Beilstein’s Handbuch der Organischen Chemie
CRC Press	CRC Handbook of Chemistry and Physics; CRC Handbook of Data on Organic Compounds
The Dialog Corporation	Dictionary of Organometallic Compounds; Dictionary of Organic Compounds

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John Wiley & Sons Limited	Encyclopedia of Reagents for Organic Synthesis
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B.1.

Aldrich Catalog/Handbook of Fine Chemicals:

TP202.A38

- compound name and structure
- physical properties
- chemical and spectroscopic references

The Catalog/Handbook contains information on only those chemicals sold by Aldrich Chemical Company.

EASY ACCESS

— For a chemical, look in the Molecular Formula Index for the systematic name and page number.

INDEXING

In the **Chemicals Section**, all chemicals contained in the catalog are listed by a systematic name in alphabetical order. Prefixes, i.e., *bis*, *tris*, *tetra*, etc., are part of the chemical name. Descriptors, i.e., *R*, *S*, *cis*, *trans*, *tert*, etc., are not used in alphabetizing the chemical name. Commonly used names and acronyms are cross-referenced to the systematic name and catalog page where they can be found.

The **Molecular Formula Index** lists all chemicals contained in the Aldrich Catalog by Hill molecular formula. For each formula, the products are arranged in alphabetical order along with the catalog page number where the entry can be found. Formulas are arranged by citing carbons in ascending order, then hydrogens, and finally the remaining elements in alphabetical order. If carbon is not present, the elements are arranged in alphabetical order. Metal salts of acids, alcohols, and amines, and hydrochlorides, acetates, etc., or bases, are indexed at the formulas of the substances from which they are derived.

The **CAS Number Cross-Reference Index** lists Chemical Abstracts Service Registry Numbers in ascending order together with the corresponding Aldrich Catalog page number.

CD-ROM

The *Sigma-Aldrich Chemical Directory on CD-ROM* contains all the chemicals available from the Sigma-Aldrich Corporation, including the Library of Rare Chemicals. It can be searched by text, physical properties, or structure. The text search uses chemical name or synonym, molecular formula, molecular weight, or Sigma-Aldrich product number. Density, refractive index, boiling point, and melting point searches are available under physical properties. Structure searches can be either imported or drawn on the screen.

INTERNET

The **Aldrich Catalog Handbook of Fine Chemicals** is searchable online at the Aldrich internet web site:

<http://www.sigald.sial.com/aldrich/catalog/>

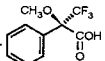
The Aldrich online catalog can be searched by text or physical properties. The text search uses chemical name or synonym, CAS registry number, EINECS number, or Sigma-Aldrich product number. Density, refractive index, boiling point, and melting point searches are available in physical properties searches. The matched response leads to a web page containing the chemical name and synonyms, product number, CAS and EINECS numbers, physical properties, references to Aldrich Spectroscopy Libraries and the Beilstein Handbook, and safety data with precautions.

ORGANIZATION

Compounds are arranged alphabetically by systematic name throughout the book. The **Aldrich Catalog/Handbook of Fine Chemicals** is published every two years by the Aldrich Chemical Company, Inc. Individual catalogs highlighting the following specialty areas are also available: Chiral Products, Combinational Chemistry Products, Dyes, Flavors and Fragrances, Fluorinated Products, High Purity Solvents, Indicators and Intermediates, Inorganics and Organometallics, Polymers, Stable Isotopes, Spectroscopy Products, and Rare Chemicals.

EXAMPLE ENTRY

Key to chemical listings

1	2	3	4	5	6	7	8
27,072-5	Acetone , 99.9+%, HPLC grade [67-64-7]	CH ₃ COCH ₃	FW 58.08	mp -94°	100mL	14.20	
9	bp 56° n _D ²⁰ 1.3590 d 0.791 Fp 1°F(-17°C)	Beil. 1,635	Fieser 2,13 3,4 6,9		1L	18.70	
10	Merck Index 11,58 FT-NMR 1(1),6,31A	FT-IR 1(3),487A	Safety 2,20A	R&S 1(1),447A	6x1L	86.10	
11	RTECS# AL3150000	FLAMMABLE LIQUID	IRRITANT		2L †	28.10	
12	Glass distilled				4x2L †	84.20	
13					4x4L †	135.20	
14					18L †	120.00	20
15							
21	Max. U.V. Abs. (1 cm. cell - vs. H ₂ O)						
	λ (nm)	400	350	340	330		
	A	0.01	0.02	0.10	1.0		
	Water<0.5%						
	Evapn. residue <0.0002%						
		22	23	24	25	26	
15,526-8	(R)-(+)-α-Methoxy-α-(trifluoromethyl)phenylacetic acid, 99%, [99% ee/(GLC)]				100mg	11.25	
	[20445-31-2] [(+)-MTPA] FW 234.17 bp 116-118°/1.5mm n _D ²⁰ 1.4730 d 1.344				250mg	22.50	
27	Fp >230°F(110°C) [α] _D ²⁰ +72° (c=1.6, CH ₃ OH)	FT-IR 1(2)144A	SI 278, E, 8		1g	74.90	
28	Derivatives of this acid are best known for separations, ¹ but have analytical uses on a preparative scale as well. ² (1) Yamaguchi, S. <i>Asymmetric Synthesis</i> ; Morrison, J.D. Ed.; Academic Press: New York, 1983; Vol 1, p128(212,297-5). (2) <i>Tetrahedron</i> 1992, 48, 10531.				5g	262.10	
23,409-5	Methylene Blue, zinc chloride double salt monohydrate [26283-09-0] (Basic				100g	18.25	
29	Blue 9; C.I. 52015) FW 406.01 d 0.980 Fp none λ _{max} 664nm	Merck Index 11,5979	500g	63.00			
30	UV-Vis 450	IRRITANT					
31							
32							
33							
34	Mosher's acid, see α-Methoxy-α-(trifluoromethyl)phenylacetic acid						
35							
	15,526-8						

- | | | |
|--|---|---|
| 1. Aldrich catalog number | 16. Beilstein reference | 27. Catalog entry has structure appearing at the bottom of page |
| 2. Product name | 17. Fieser reference | 28. Use statement including pertinent literature reference |
| 3. Chemical purity | 18. Reference to <i>Sigma-Aldrich Library of Chemical Safety Data</i> | 29. Colour Index number |
| 4. Chemical Abstracts Service Registry Number | 19. Reference to <i>Sigma-Aldrich Library of Regulatory & Safety Data</i> | 30. Reference to <i>Sigma-Aldrich Library of Stains, Dyes & Indicators</i> |
| 5. Linear representation of chemical structure | 20. This quantity of chemical must be shipped via truck | 31. Hazardous properties |
| 6. Formula weight | 21. Product specifications | 32. Wavelength in nanometers at which the maximum absorption of a stain or dye was observed |
| 7. Melting point | 22. Alternate product name | 33. Merck Index reference |
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| 9. Denotes that the chemical is in the EPA inventory under TSCA | 24. Reference to <i>Aldrich Library of FT-IR Spectra</i> | 35. Structure and catalog number |
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| 11. Reference to Registry of Toxic Effects of Chemical Substances | 26. Percent enantiomeric excess/method of determination | |
| 12. Index of refraction | | |
| 13. Reference to <i>Aldrich Library of ¹³C and ¹H FT NMR Spectra</i> | | |
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| 15. Flash point | | |

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