

19009-36

Handbook of Proton-NMR Spectra and Data

Volume 9

Edited by
Asahi Research Center Co., Ltd.
Tokyo, Japan

1A

Supervised by
Shin-ichi Sasaki
Toyohashi University of Technology
Aichi, Japan

1986



Academic Press, Inc.

(Harcourt Brace Jovanovich, Publishers)

Tokyo Orlando San Diego New York
London Toronto Montreal Sydney

0885100

COPYRIGHT© 1986, BY ACADEMIC PRESS JAPAN, INC.
ALL RIGHTS RESERVED.

NO PART OF THIS PUBLICATION MAY BE REPRODUCED OR TRANSMITTED IN ANY FORM OR BY ANY
MEANS ELECTRONIC OR MECHANICAL INCLUDING PHOTOCOPY RECORDING OR ANY INFORMA-
TION STORAGE AND RETRIEVAL SYSTEM WITHOUT PERMISSION IN WRITING FROM THE
PUBLISHER.

ACADEMIC PRESS JAPAN, INC.
Hokoku Bldg. 3-11-13, Iidabashi, Chiyoda-ku, Tokyo 102

United States Edition published by ACADEMIC PRESS, INC.
Orlando, Florida 32887

United Kingdom Edition published by ACADEMIC PRESS, INC. (LONDON) LTD.,
24/28 Oval Road, London NW1 7DX

ISBN: 0-12-064509-2
Library of Congress Catalog Card Number: 85-61909

PRINTED IN JAPAN

86 87 88 89 9 8 7 6 5 4 3 2 1

A User's Guide

This data handbook has been planned as a part of projected open-ended series, with publication of additional data books scheduled upon completion of further data compilation. The handbook consists of proton-NMR spectra and data for 4,000 organic compounds, divided into five volumes with 800 entries each. The handbook is divided into data sections and index sections.

1. Proton-NMR Spectra and Data Sections

All data entries are in the form:

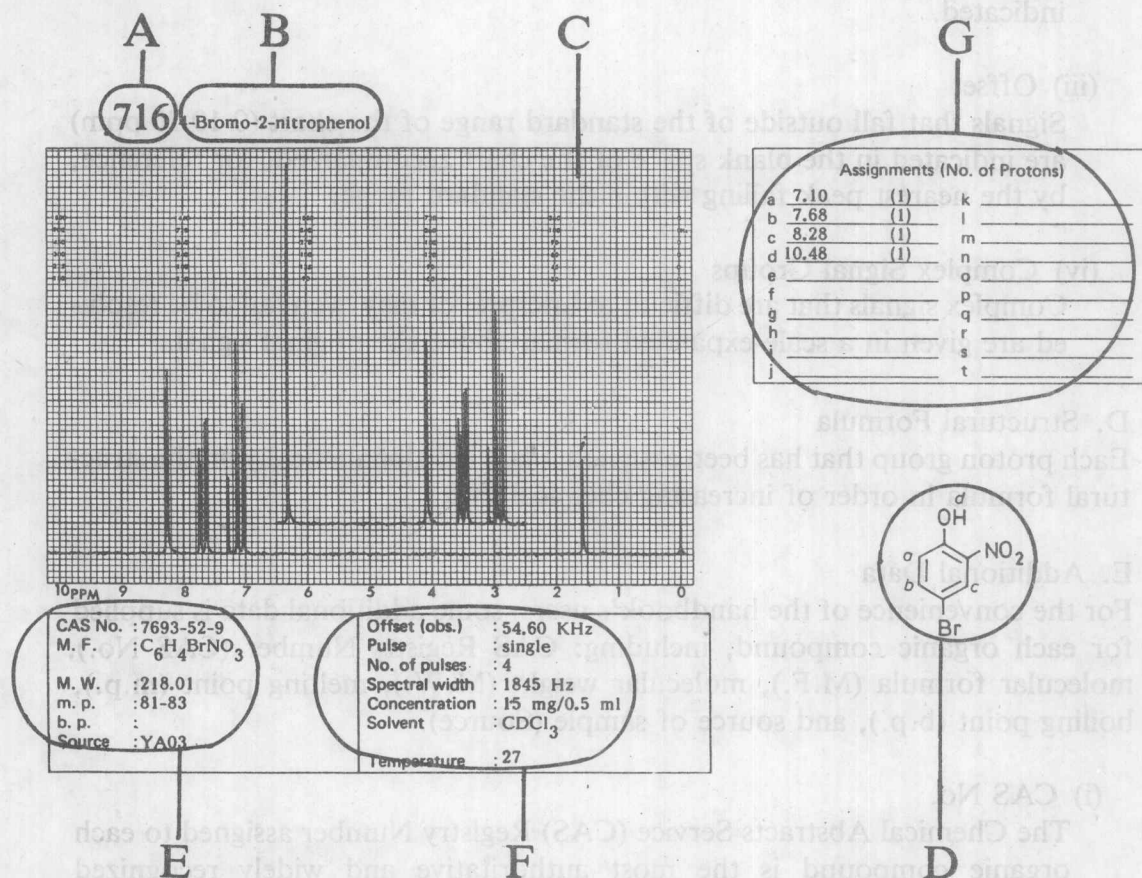


Figure 1. Illustration of Spectral Data

A. Spectrum Number

The organic compounds for which spectral data are provided are arranged in order of molecular complexity, from simpler to more complex. Each entry is assigned a number in sequence which serves as a key for easy indexing and quick reference.

B. Chemical Name

In general, all chemical names are in accord with the IUPAC nomenclature system. There are, however, some compounds that are more frequently referred to by trivial names, such as vanillin. In these cases, the trivial name is used.

C. Spectrum

(i) Units

For easy recognition of peak positions of signals, the smallest unit of the spectrum chart is 0.1 ppm (9 Hz).

(ii) Impurities

Signals resulting from a trace amount of impurities in the sample are indicated by the letter "i" over the signal in question. Signals resulting from impurities in the solvent, however, such as CHCl_3 in CDCl_3 , are not indicated.

(iii) Offset

Signals that fall outside of the standard range of the chart (0-10.20 ppm) are indicated in the blank space of the chart accompanied, for reference, by the nearest peak falling within the standard range.

(iv) Complex Signal Groups

Complex signals that are difficult to interpret or may even fail to be resolved are given in a scale-expanded format above the original signal.

D. Structural Formula

Each proton group that has been assigned is labeled alphabetically on the structural formula in order of increasing chemical shift.

E. Additional Data

For the convenience of the handbook's users, some additional data is supplied for each organic compound, including: CAS Registry Number (CAS No.), molecular formula (M.F.), molecular weight (M.W.), melting point (m.p.), boiling point (b.p.), and source of sample (Source).

(i) CAS No.

The Chemical Abstracts Service (CAS) Registry Number assigned to each organic compound is the most authoritative and widely recognized chemical identification number. As a result, it is extremely helpful as a link

to information available in many other database systems such as CAS-ONLINE and CIS, among others.

(ii) Molecular Formula

Molecular formulas are arranged according to the Hill system, that is, C before H, with all other elements in alphabetical order.

(iii) Molecular Weight

Average molecular weights derived from average atomic weights are given.

(iv) Melting and Boiling Points

Both values are recorded in Celsius, based on the literature or data recorded by sample suppliers. In the case of compounds that decompose, the decomposition point is given, as, for example, 250 dec.

(v) Source of Sample

Sample suppliers are recorded in a four-letter code. Full identification of suppliers is provided in Chart 5.

F. Spectrum Measurement

(i) Spectrometer

The spectrometer used for all measurements is an FX-90Q manufactured by JEOL Ltd. This is a modern Pulse Fourier Transform spectrometer. The 90 MHz spectrometer is the most widely used spectrometer at present.

(ii) Specifications

The specifications for the spectrometer are as follows:

• Magnetic field	21100 gauss
• Observation frequency	89.55-89.65 MHz
• NMR lock	D2 internal lock
• Insert coil	5 mm diameter
• Resolution	$^1\text{H} \leq 0.2 \text{ Hz}$
• Pulse mode	Single
• Accumulation times	Four (average)
• Data points	16 K

(iii) Measurement Conditions

Spectra measurements are carried out under constant conditions as much as possible. Measurement is carried out, as a rule, at 27°C. In most cases, the solvent used is CDCl_3 ; D_2O , DMSO-d_6 , or polysol, a mixture of CDCl_3 and DMSO-d_6 which is used as a solvent for compounds that do not dissolve in CDCl_3 . Tetramethylsilane (TMS) is employed as the internal standard except when the solvent is D_2O , in which case 3-(trimethylsilyl)propionic acid- d_4 sodium salt (TSP- d_4) is employed.

G. Assignment

Assignment is carried out in order of increasing chemical shift relative to TMS or TSP-d₄. Related proton groups are identified with letters of the alphabet for easy correlation.

Integration curves have been omitted from the spectra chart because of the problem of poor legibility. The number of assigned protons is recorded instead in parentheses following the chemical shift value.

Determination of the chemical shift value has been carried out by standard methods. In addition, digital output from the spectrometer has been referred to. For those multiplets for which first-order approximation is sufficient, the center of the multiplets has been regarded as the chemical shift. For those which clearly exhibit a second-order signal pattern, when all the signals constituting the multiplet can be positively identified, the first approximation or the center of the multiplet is regarded as the chemical shift.

Spin-spin coupled multiplets with complex overlapping are represented by the appropriate signal range, as, for example, 7.22-8.54.

When assignment is difficult because of similar chemical environments of proximate molecular structures or overlapping signals, the several alternative assignment values are each marked with an asterisk and a number which indicates that other asterisked values of the same number may be interchangeable.

When no appropriate signal is observable throughout the entire spectrum, the proton group is marked u.o. (unobserved). When the appropriate signal clearly overlaps with another signal and the chemical shift value is difficult to determine, the proton group is marked u.d. (undetermined). When the precise chemical shift value cannot be determined but an extremely close approximation is possible, the value is marked with the prefix ca. (circa).

2. Index Sections

Thorough, carefully prepared indexes are crucial tools for effective use of any data collection. Four types of exhaustive indexes accompany the present handbook, designed for quick and convenient cross checking, in a handy format that provides extremely useful combinations of data at a glance and greatly enhances the use of the entire handbook. The indexes and the data they contain are as follows:

Table 1

Index Name	First Column	Second Column	Third Column
Chemical Name Index	Chemical name	Spectrum No.	
Molecular Formula Index	Molecular formula	Chemical name	Spectrum No.
Substructure Index	Substructure	Chemical shift	Spectrum No.
Chemical Shift Index	Chemical shift	Substructure	Spectrum No.

A. Chemical Name Index

All chemical names are in alphabetical order. Numerals, Greek characters,

and codes indicating substitution positions (such as 1-, beta-, N-, etc.) and geometrical, stereochemical, and optical isomeric prefixes (such as cis-, endo-, levo-, etc.) are disregarded in alphabetization. Each name is followed by a spectrum number, as can be seen in the sample page of the Chemical Name Index (Chart 1).

B. Molecular Formula Index

When the desired organic compound cannot be found in the Chemical Name Index or its nomenclature is unclear, it becomes necessary to look for a compound by means of its molecular formula. This is just the case for which the Molecular Formula Index was designed. Molecular formulas are listed following the Hill system, in order of complexity. When several compounds have the same molecular formula, the different compounds are listed in alphabetical order, as can be seen in the sample page of the Molecular Formula Index (Chart 2). The spectrum number is also provided for easy cross reference to the data handbook.

C. Substructure Index

Determining what sorts of proton correspond to the various signals within a spectrum, investigating their chemical environments, and suggesting models for their structure are all very important parts of spectral analysis.

A unique notation system for representing substructure has been developed in the Substructure Index to allow easy correlation of the chemical environments of protons and chemical shift, and at the same time permit fast consideration of a wide variety of model structures.

In the substructure notation of the index, the proton group which is assigned as the TARGET is grouped with its neighbors (e.g. α position) and next nearest neighbors (e.g. β position). The TARGET occupies the head position of the substructure notation, as can be seen in Fig. 2. It is followed by the neighboring atoms, given outside parentheses; the next-nearest atoms are written inside parentheses.

Substructure

Notation

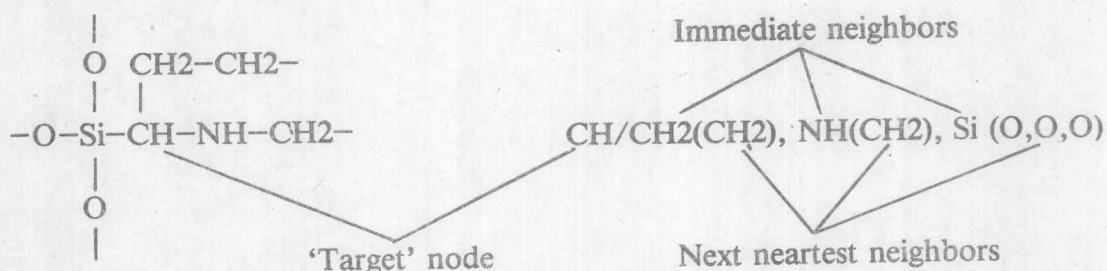


Figure 2. Substructure Notation

All non-identical substructures relating to a particular TARGET are cited in the index. In order to simplify the substructure notation, single bonds have not been represented. Code for other atomic groups is found in Chart 3-1, as is their order of priority. Chart 3-2 shows a sample page of the Substructure Index. ('CH₂U' indicates that two protons of the methylene group are unequivalent.) For the user's convenience, chemical shift value and spectrum number are also provided for each entry.

D. Chemical Shift Index

Entries on the Chemical Shift Index are arranged in order of increasing delta value (ppm). For easy correlation of chemical shift with substructure, substructure notations are listed for each entry as well. Chart 4 shows a sample page of the Chemical Shift Index.

Determining what sorts of proton correspond to the various signals within a spectrum, investigating their chemical environments, and suggesting models for their structure are all very important parts of spectral analysis. A unique notation system for representing substructure has been developed in the Substructure Index to allow easy correlation of the chemical environments of protons and chemical shifts, and at the same time permit fast consideration of a wide variety of model structures. In the substructure notation of the index, the proton group which is assigned as the TARGET is grouped with its neighbors (e.g. a position) and next nearest neighbors (e.g. a position). The TARGET occupies the head position of the substructure notation, as can be seen in Fig. 2. It is followed by the neighboring atoms, given outside parentheses; the next-nearest atoms are written inside parentheses.



Figure 2. Substructure Notation

Chart 1. The Chemical Name Index

name	No.	name	No.
3-Methyl-2-nitrobenzoyl chloride	4822	3-Phenyl-1,3-butanediol	5466
Methyl 4-nitrophenylacetate	5108	1-Phenyl-1,3-butanedione	5360
2-Methyl-2-nonanol	5577	1-Phenyl-2-butanone	5402
(E)-2-Methyl-4-nonen-2-ol	5554	1-Phenyl-1-butyne	5341
2-Methyl-2-(3-oxobutyl)cyclopentane-1,3-dione	5468	cis-2-Phenylcyclopropane-1-carboxylic acid	5361
4-Methyl-3-(3-oxobutyl)-4-pentenal	5503	trans-2-Phenylcyclopropane-1-carboxylic acid	5362
Methyl (2-oxocyclohexane)acetate	5225	2-Phenyl(2- ² H ₁)-1,3-dioxane	5379
Methyl 8-oxo-1,4-dioxaspiro[4.5]decane-7-carboxylate	5472	(1-Phenylethyl)oxamohydrazide	5439
2-Methyl-2-pentenal dimethyl acetal	5009	Phenylglyoxylic acid	4834
4-Methyl-trans-perhydroquinoline	5544	4-Phenyl-3-oxolen-2-one	5319
1-Methyl-3-phenylpropylamine	5482	2-Phenylperhydro-1,2-oxazine-3,5-dione	5337
1-Methyl-5-phenyl-1H-tetrazole	4880	2-Phenylperhydro-1,2-oxazine-3,5-dione 5-oxime	5354
5-Methyl-1-phenyl-1H-tetrazole	4881	N-Phenylpiperazine	5448
Methyl 3-(phenylthio)-3-(² H ₁)propenoate	5329	3-Phenylpropionaldehyde	5134
2-(2-Methyl-2-propenyl)cyclohexanone	5497	2-Phenylpropionamide	5167
N'-Methylpyridine-2,3-dicarboximide	4832	DL-2-Phenylpropionic acid	5142
6-Methyl-2-(2-pyridyl)-1,3-thiazin-4-one	5311	2-Phenylsuccinic acid	5369
2-[2-(Methylthio)phenyl]ethylammonium chloride	5215	3-(Phenylsulfonyl)propionic acid	5159
Methyl para-tolyl sulfone	4924	3-Phenylthiazolidine-2,4-dione	5068
Methyl para-tolyl sulfoxide	4921	(2-Phenyl)thioacetamide	4910
3-Methyl-1-para-tolyltriazeno	4944	3-(Phenylthio)propionic acid	5144
Methyl 3-(trimethylsilylmethyl)-3-butenolate	5253	4-Phenyl-1,2,4-triazolidine-3,5-dione	4863
Naphthalene	5300	1-Phenylvinyl acetate	5363
2,3-Naphthalenediol	5316	Phenyl vinyl sulfone	4888
2,6-Naphthalenediol	5317	Phenyl vinyl sulfoxide	4884
2,7-Naphthalenediol	5318	exo-2-Pinen-4-ol	5498
1-Naphthalenesulfonyl chloride	5293	Potassium 1,4-dioxo-1,4-dihydronaphthalene-2-sulfonate	5280
Naphthionic acid	5338	Potassium hydrogen phthalate	4810
1-Naphthylamine	5331	Potassium 3-indoleacetate	5307
3,3',3''-Nitrilotripropionamide	5247	2-Propionoxybenzoic acid	5370
3'-Nitroacetophenone oxime	4878	Propyl 2-furoate	4925
4-Nitrobenzyl chloroformate	4823	N-Propylheptanamide	5568
4-Nitro-1-naphthoic acid	5591	N-Propylhexanamide	5267
2-(3-Nitrophenoxy)-5-nitropyridine	5593	N-Propylisovaleramide	5017
2-(2'-Nitrophenoxy)pyridine	5598	N-Propyl-4-methylpentanamide	5268
5-Nitro-2-phenoxy-pyridine	5599	4-Propylphenol	5188
2-Nitrophenylacetic acid	4860	2-Propylpyridine	4935
2-(4-Nitrophenyl)-1,3-dithiolane	5104	Propyl 3,4,5-trihydroxybenzoate	5421
4-Nitroquinoline 1-oxide	5051	N-Propylvaleramide	5018
Nitroterephthalic acid	4814	1-Propynylbenzene	5072
4-Nitro-2-vinylaniline	4876	2-Propynyl 3,5-dinitrobenzoate	5284
Nonanenitrile	5241	2-Propynyl 2-oxanyl ether	4961
(Z)-6-Nonenol	5249	N ¹ -Pyridinio-N ² -(ethoxycarbonyl)acetamidin-N ¹ -ide	5440
Nonylamine	5276	4-(1-Pyrrolidinyl)-3-penten-2-one	5227
Nonyl chloroformate	5541	4-(1-Pyrrolidinyl)pyridine	5182
2-Nonyne	5230	Quinazoline	4828
3-Nonyne	5231	2,4-Quinolinediol	5067
4-Nonyne	5232	2-Quinolinel	5064
4-Nonyl-3-one	5221	8-Quinolyl methanesulfonate	5339
2,2,3,3,4,4,5,5-Octafluoro-2'-hydroxy-4'-nitrovaleranolide	5587	Sodium 4-acetamidobenzenesulfinate	4873
Octanal	5008	Sodium (2-carbamoylphenoxy)acetate	5074
Octanedioic acid	4992	Sodium 5,5-diethyl-4,6-dioxo-3,4,5,6-tetrahydropyrimidin-2-olate	4943
1,3-Octanediol	5026	Sodium 4-dimethylaminophenyldiazosulfonate	4920
Octanethiol	5027	Sodium 1-naphthol-5-sulfonate	5298
(E)-2-Octene	4998	Sodium 2-naphthol-6-sulfonate	5299
2-Octyne	4970	Sodium 1-nonanesulfonate	5269
3-Octyne	4971	Sodium octanoate	4995
1-Octyn-3-ol	4981	Spiro[3.3]heptane-2,6-dicarboxylic acid	5202
2-Octyn-1-ol	4982	Spiro[4.4]nona-2,7-diene-1,6-dione	5077
7-Oxabicyclo[2.2.1]heptane-2,3-dicarboxylic acid	4928	Terephthalaldehydic acid	4835
1-Oxaspiro[4.5]dec-3-en-2-one	5195	Terephthalamide	4877
(3-Oxa-5-thiahexyl)benzene	5461	Tetraethylgermane	5037
4-Oxatricyclo[5.2.1.0 ^{2,6}]dec-8-en-3-one	5141	Tetraethyl orthocarbonate	5275
3-(3-Oxobutyl)cyclohexanone	5504	5,6,7,8-Tetrahydro-4H-cyclohepta[c]furan-6-one	5143
7-Oxo-1,3,5-cycloheptatrienyl thiocyanate	4811	1,2,3,4-Tetrahydroisoquinoline	5166
1,1,4,7,7-Pentamethyl-diethylenetriamine	5278	1,2,3,4-Tetrahydro-1-naphthol	5403
2,5,8,11,14-Pentaoxapentadecane	5581	5,6,7,8-Tetrahydro-1-naphthylamine	5427
N-Pentylbutyramide	5265	1,2,4,5-Tetrakis(bromomethyl)benzene	5347
N-Pentylisobutyramide	5266	4,4',5,5'-Tetrakis(methylthio)-2,2'-bi-1,3-dithiolylidene	5423
N-Pentylisovaleramide	5566	2,3,4,5-Tetramethylaniline	5483
N-Pentylpropionamide	5016	Tetramethyl-para-benzoquinone	5410
N-Pentylvaleramide	5567	1,1,3,3-Tetramethylbutylamine	5031
2-(1-Perhydroazocinyl)ethylguanidine sulfate	5572	1,1,3,3-Tetramethyl-1,3-divinyl-disilazane	5035
2-Phenoxyethyl acetate	5416	1,1,3,3-Tetramethyl-1,3-divinyl-disiloxane	5025
Phenylacetamide	4901	Tetramethylene diacetate	4993
D-Phenylalanine	5168		

Chart 2. The Molecular Formula Index

name	No.	name	No.
C ₁₀ H ₁₃ K ₃ N ₂ O ₈ Tripotassium hydrogen ethylenediaminetetraacetate	5426	C ₁₀ H ₁₄ O ₄ 3,4,5-Trimethoxybenzyl alcohol	5469
C ₁₀ H ₁₃ N 5,6,7,8-Tetrahydro-1-naphthylamine	5427	4,7,7-Trimethyl-3-oxo-2-oxabicyclo[2.2.1]heptane-1-carboxylic acid	5470
C ₁₀ H ₁₃ NO N-Benzylpropionamide	5428	C ₁₀ H ₁₄ O ₄ Pd Bis(2,4-pentanedionato-O,O')palladium(II)	5471
3-(Dimethylamino)acetophenone	5429	C ₁₀ H ₁₄ O ₅ Methyl 8-oxo-1,4-dioxaspiro[4.5]decane-7-carboxylate	5472
4-(Dimethylamino)acetophenone	5430	C ₁₀ H ₁₄ S ₂ 4,5-Bis(mercaptomethyl)-ortho-xylene	5473
C ₁₀ H ₁₃ NO ₂ 3-Hydroxy-3-phenylbutyramide	5431	C ₁₀ H ₁₅ Br 2-Bromotricyclo[3.3.1.1 ^{3,7}]decane	5474
Methyl 2-dimethylaminobenzoate	5432	C ₁₀ H ₁₅ Cl 1-Chlorotricyclo[3.3.1.1 ^{3,7}]decane	5475
2,3,4,5-Tetramethyl-1-nitrobenzene	5433	C ₁₀ H ₁₅ D (1- ² H ₁)Tricyclo[3.3.1.1 ^{3,7}]decane	5476
C ₁₀ H ₁₃ NO ₂ S N-Allyl-para-toluenesulfonamide	5434	C ₁₀ H ₁₅ IO ₅ 3-O-Acetyl-5-deoxy-5-iodo-1,2-O-isopropylidene-alpha-D-xylofuranose	5477
C ₁₀ H ₁₃ NO ₃ 3,4-Dimethoxyacetanilide	5435	C ₁₀ H ₁₅ N 1,1-Dimethyl-2-phenylethylamine	5478
L-Tyrosine methyl ester hydrochloride	5436	2-(1-Ethylpropyl)pyridine	5479
C ₁₀ H ₁₃ NO ₃ S 4-(Benzenesulfonyl)morpholine	5437	4-(1-Ethylpropyl)pyridine	5480
C ₁₀ H ₁₃ NO ₄ Methyl 4-amino-2,5-dimethoxybenzoate	5438	N-Isopropylbenzylamine	5481
C ₁₀ H ₁₃ N ₃ O ₂ (1-Phenylethyl)oxamohydrazide	5439	1-Methyl-3-phenylpropylamine	5482
N ¹ -Pyridinio-N ² -(ethoxycarbonyl)acetamidin-N ¹ -ide	5440	2,3,4,5-Tetramethylaniline	5483
C ₁₀ H ₁₃ N ₅ O ₅ Guanosine	5441	C ₁₀ H ₁₅ NO 1-(3-Dimethylaminophenyl)ethanol	5484
C ₁₀ H ₁₄ meta-Cymene	5442	C ₁₀ H ₁₅ NO ₂ 3-(1-Hydroxy-3-azapentyl)phenol hydrochloride	5485
meta-Diethylbenzene	5443	C ₁₀ H ₁₅ NO ₂ S 4-Dimethylaminobenzyl methyl sulfone	5486
ortho-Diethylbenzene	5444	C ₁₀ H ₁₅ NO ₃ Ethyl 3-oxo-2-(2-pyrrolidinylidene)butyrate	5487
para-Diethylbenzene	5445	C ₁₀ H ₁₅ N ₂ Na ₃ O ₇ Trisodium N'-(2-hydroxyethyl)ethylenediamine-N,N,N'-triacetate dihydrate	5488
1-Ethyl-2,4-dimethylbenzene	5446	C ₁₀ H ₁₅ N ₃ O 6-Methyl-4-(1-methylpropylidenehydrazino)-2(1H)-pyridone	5489
C ₁₀ H ₁₄ CaO ₆ Calcium bis(3-methyl-2-oxobutyrate)	5447	C ₁₀ H ₁₅ P Diethylphenylphosphine	5490
C ₁₀ H ₁₄ N ₂ N-Phenylpiperazine	5448	C ₁₀ H ₁₆ (+)-3-Carene	5491
C ₁₀ H ₁₄ N ₂ O N,N-Diethyl-4-nitrosoaniline	5449	C ₁₀ H ₁₆ CIN Benzyltrimethylammonium chloride	5492
4,6,7,8,9,10-Hexahydro-2-methylpyrimidino[1,2-a]azepin-4-one	5450	C ₁₀ H ₁₆ N ₂ N,N-Diethyl-para-phenylenediamine sulfate	5493
C ₁₀ H ₁₄ N ₂ O ₂ N,N-Diethyl-2-nitroaniline	5451	N,N,N',N'-Tetramethyl-para-phenylenediammonium dichloride	5494
C ₁₀ H ₁₄ N ₅ O ₇ P Adenosine 5'-monophosphate	5452	C ₁₀ H ₁₆ N ₂ O ₄ N,N'-Diallyl-L-tartaramide	5495
C ₁₀ H ₁₄ O 2-tert-Butylphenol	5453	C ₁₀ H ₁₆ O Bicyclo[4.4.0]decan-3-one	5496
4-sec-Butylphenol	5454	2-(2-Methyl-2-propenyl)cyclohexanone	5497
2-(1-Hydroxyethyl)-1,4-dimethylbenzene	5455	exo-2-Pinen-4-ol	5498
1,4(8)-para-Menthadien-3-one	5456	Tricyclo[3.3.1.1 ^{3,7}]decan-1-ol	5499
1,8-para-Menthadien-3-one	5457	Tricyclo[3.3.1.1 ^{3,7}]decan-2-ol	5500
7-Methylenebicyclo[3.3.1]nonan-3-one	5458	C ₁₀ H ₁₆ O ₂ 4-tert-Butylcyclohexane-1,3-dione	5501
3,4,5-Trimethylanisole	5459	(Z)-3-Hexenyl crotonate	5502
2,6,6-Trimethyl-2,4-cycloheptadienone	5460	4-Methyl-3-(3-oxobutyl)-4-pentalen	5503
C ₁₀ H ₁₄ OS (3-Oxa-5-thiahexyl)benzene	5461	3-(3-Oxobutyl)cyclohexanone	5504
C ₁₀ H ₁₄ O ₂ 3-Butoxyphenol	5462		
4-Butoxyphenol	5463		
tert-Butylhydroquinone	5464		
1-Methoxy-4-methylbicyclo[2.2.2]oct-5-en-2-one	5465		
3-Phenyl-1,3-butanediol	5466		
C ₁₀ H ₁₄ O ₂ S Isopropyl para-tolyl sulfone	5467		
C ₁₀ H ₁₄ O ₃ 2-Methyl-2-(3-oxobutyl)cyclopentane-1,3-dione	5468		

Chart 3-1. The Code Table of Substructure Notation

Priority	Code	Substructure	Priority	Code	Substructure
1	CH3	-CH ₃	26	=N=	=N=
2	CH2	-CH ₂ -	27	N[*	aromatic nitrogen
3	CH2U	-CH ₂ - a]	28	NO2	-NO ₂
4	CH	-CH<	29	#N	≡N
5	C	>C<	30	OH	-OH
6	CH2=	=CH ₂	31	O	-O-
7	CH=	=CH-	32	=O	=O
8	CH=[E]	=CH- b]	33	SH	-SH
9	CH=[Z]	=CH- c]	34	S	-S-
10	C=	=C<	35	=S	=S or =S<
11	=C=	=C=	36	SO2	-SO ₂
12	#CH	≡CH	37	P	-P<
13	C#	≡C-	38	PH=	=PH
14	AH	d]	39	P=	-P= or >P=
15	A	e]	40	F	-F
16	TRL	f]	41	Cl	-Cl
17	CHO	-CHO	42	Br	-Br
18	C=O	>C=O	43	I	-I
19	=C=O	=C=O	44	As	>As-
20	NH3 ⁺	ammonium cation	45	As=	=As-
21	NH2	-NH ₂	46	Si	>Si<
22	NH	>NH	47	+	cation
23	N	>N-	48	-	anion
24	=NH	=NH	49	.	radical
25	N=	-N=	50	/	chelation
			51	g]	X other atoms

- a) Unequivalent methylene b) Entgegen c) Zusammen
d) Aromatic carbon with proton e) Aromatic carbon without proton
f) -C(OH)-C(O)- in troponoid g) Other element symbols are listed in alphabetical order.

Chart 3-2. The Substructure Index

substructure	chemical shift	No.	substructure	chemical shift	No.
CH ₂ /CH(CH ₃ ,CH ₃),NH(C=O)	3.09	5014	CH ₂ /A(AH,AH),C=O(OH)	3.64	4852
CH ₂ /CH(CH ₃ ,CH ₃),NH(C=O)	3.09	5561	CH ₂ /A(AH,AH),C=O(O)	3.74	5108
CH ₂ /CH(CH ₃ ,CH ₃),NH(C=O)	3.09	5562	CH ₂ /A(AH,A),C=O(C=O)	4.58	5046
CH ₂ /CH(A,OH),NH(CH ₂)	ca. 3.32	5485	CH ₂ /A(AH,A),C=O(N)	3.50	5099
CH ₂ /CH(CH,NH ₂),OH	3.29	5184	CH ₂ /A(AH,A),C=O(OH)	3.80	4824
CH ₂ /CH(CH ₂ ,CH),O(CH ₃)	4.22	5535	CH ₂ /A(AH,A),C=O(OH)	4.02	4860
CH ₂ /CH(CH ₂ ,O),O(C)	3.40- 4.40	4987	CH ₂ /A(AH,AH),NH ₂	3.69	4950
CH ₂ /CH(CH ₃ ,CH ₃),S(S)	2.60	5028	CH ₂ /A(AH,AH),NH ₂	3.80	4939
CH ₂ /CH(CH ₂ U,CH),S(CH ₂)	1.50- 2.01	5181	CH ₂ /A(AH,AH),NH ₂	3.81	4933
CH ₂ /CH(CH ₂ ,O),Br	3.29- 3.81	5509	CH ₂ /A(AH,AH),NH ₂	3.84	4938
CH ₂ /CH(CH ₂ ,O),I	3.07- 3.40	5477	CH ₂ /A(AH,AH),NH ₂	3.90	4949
CH ₂ /C(CH ₃ ,CH ₃ ,CH ₃),C(CH ₃ ,CH ₃ ,NH ₂)	1.44	5031	CH ₂ /A(AH,A),NH ₂	3.82	4937
CH ₂ /C(CH ₃ ,CH ₃ ,OH),CH=(E)(CH=(E))	ca. 2.15	5554	CH ₂ /A(AH,AH),NH(CH ₃)	3.75	4934
CH ₂ /C(CH ₃ ,CH ₃ ,OH),CH=(E)(CH=(E))	2.17	5552	CH ₂ /A(AH,AH),NH(CH ₂)	3.80	5208
CH ₂ /C(CH ₃ ,CH ₃ ,NH ₂),A(AH,AH)	2.66	5478	CH ₂ /A(AH,AH),NH(CH ₂)	3.80	5219
CH ₂ /C(CH ₃ ,CH ₃ ,CH=),C=O(C=)	2.67	5460	CH ₂ /A(AH,AH),NH(CH ₂)	3.82	4952
CH ₂ /C(CH ₃ ,CH ₂ ,CH ₂),C=O(NH)	2.43	4965	CH ₂ /A(AH,AH),NH(CH)	3.79	5481
CH ₂ /C(CH ₃ ,CH ₂ ,CH ₂),C=O(OH)	2.30	4991	CH ₂ /A(AH,AH),NH(C=O)	4.43	5428
CH ₂ /C(CH ₃ ,CH ₂ ,CH=),C=O(C)	2.03	5465	CH ₂ /A(AH,A),NH(CH ₂)	4.00	5166
CH ₂ /C(F,F,F),O(C=O)	4.73	5063	CH ₂ /A(AH,AH),N(CH ₃ ,CH ₃ ,CH ₃ ,+)	5.06	5492
CH ₂ /C(CH ₃ ,CH ₃ ,A),Cl	3.65	5425	CH ₂ /A(AH,AH),OH	4.48	4922
CH ₂ /CH=(CH ₂ =),A(AH,A)	3.37	5400	CH ₂ /A(AH,AH),OH	4.52	4889
CH ₂ /CH=(CH=),A(AH,A)	3.40	5071	CH ₂ /A(AH,AH),OH	4.61	5469
CH ₂ /CH=(CH ₂ =),NH(A)	3.79	5165	CH ₂ /A(AH,A),OH	4.76	5151
CH ₂ /CH=(CH ₂ =),NH(C=O)	3.74	5495	CH ₂ /A(AH,A),OH	4.52	5194
CH ₂ /CH=(CH ₂ =),NH(SO ₂)	3.60	5434	CH ₂ /A(AH,A),OH	4.53	5198
CH ₂ /CH=(CH ₂ =),O(A)	4.53	5056	CH ₂ /A(AH,A),OH	4.69	5199
CH ₂ /CH=(CH ₂ =),O(A)	4.61	5332	CH ₂ /A(AH,A),OH	4.80	5197
CH ₂ /CH=(CH ₂ =),O(C=O)	4.75	5366	CH ₂ /A(AH,TPL),OH	4.60	5092
CH ₂ /CH=(CH ₂ =),O(C=O)	4.87	5103	CH ₂ /A(A,A),OH	4.61	4941
CH ₂ /CH=(CH ₂ =),S(A)	3.51	5422	CH ₂ /A(AH,AH),O(CH ₂)	4.57	5192
CH ₂ /CH=(CH ₂ =),S(A)	3.55	5162	CH ₂ /A(AH,AH),O(CH ₂)	4.59	5164
CH ₂ /CH=(E)(CH=(E)),C=(CH ₃ ,CH ₂ =)	2.70	5520	CH ₂ /A(AH,AH),O(C=O)	5.10	4904
CH ₂ /CH=(E)(CH=(E)),OH	4.15	4960	CH ₂ /A(AH,AH),O(C=O)	5.40	4823
CH ₂ /CH=(E)(C(E)),OH	4.16	5530	CH ₂ /A(AH,A),O(C=O)	5.20	5368
CH ₂ /CH=(E)(CH=(E)),O(A)	4.46	5325	CH ₂ /A(AH,AH),SH	3.72	4930
CH ₂ /CH=(E)(CH=(E)),O(C=O)	4.53	5532	CH ₂ /A(AH,A),SH	3.81	5473
CH ₂ /CH=(Z)(CH=(Z)),O(C=O)	4.68	4962	CH ₂ /A(AH,AH),S(C=)	4.59	4919
CH ₂ /C=(CH ₂ ,N=),A(AH,A)	3.86	5100	CH ₂ /A(AH,AH),SO ₂ (CH ₃)	4.14	5486
CH ₂ /C=(NH ₂ =S),A(AH,AH)	4.11	4910	CH ₂ /A(AH,AH),SO ₂ (Cl)	4.84	4898
CH ₂ /C=(CH ₂ ,CH ₂ =),C=O(O)	3.00	5253	CH ₂ /A(AH,A),SO ₂ (Cl)	4.96	5163
CH ₂ /C=(CH ₂ ,N=),C=O(N)	3.59	5354	CH ₂ /A(AH,AH),P(O,O,O=)	3.18	5216
CH ₂ /C=(CH ₂ ,N=),C=O(N)	3.61	5328	CH ₂ /A(AH,AH),Br	4.50	4895
CH ₂ /C=(CH=,A),C=O(OH)	3.53	5336	CH ₂ /A(AH,A),Br	4.60	5347
CH ₂ /C=(CH=,A),C=O(O)	3.67	5307	CH ₂ /A(AH,AH),D	2.29	5117
CH ₂ /C=(CH ₂ ,N=),O(N)	5.00	5354	CH ₂ /C=O(CH ₂),C=O(CH)	3.40	5501
CH ₂ /C=(CH ₂ ,N=),O(N)	5.10	5328	CH ₂ /C=O(CH ₂),C=O(N)	3.80	5305
CH ₂ /C=(CH=,A),O(C=O)	5.23	5319	CH ₂ /C=O(CH ₂),C=O(N)	3.80	5337
CH ₂ /C=(CH=,O),S(S)	3.71	5364	CH ₂ /C=O(CH ₂),C=O(N)	3.81	5304
CH ₂ /C=(CH=,C=),Br	4.46	5324	CH ₂ /C=O(CH ₂),C=O(O)	3.62	5226
CH ₂ /C=(CH=,C=),Br	4.53	5343	CH ₂ /C=O(CH),C=O(O)	3.50	5506
CH ₂ /C=(CH=,C=),Br	4.55	5324	CH ₂ /C=O(C),C=O(C=)	6.47	4808
CH ₂ /C=(CH=,C=),Br	4.60	5343	CH ₂ /C=O(O),C=O(O)	3.31	5239
CH ₂ /C=(CH=,C=O),Br	4.46	5324	CH ₂ /C=O(NH),NH(C=O)	3.87	5394
CH ₂ /C=(CH=,C=O),Br	4.53	5343	CH ₂ /C=O(OH),NH(C=O)	3.88	5125
CH ₂ /C=(CH=,C=O),Br	4.55	5324	CH ₂ /C=O(OH),NH(C=O)	3.92	5387
CH ₂ /C=(CH=,C=O),Br	4.60	5343	CH ₂ /C=O(O),NH(C=O)	4.53	4955
CH ₂ /C=(CH ₂ ,CH ₂ =),Si(CH ₃ ,CH ₃ ,CH ₃)	1.63	5253	CH ₂ /C=O(OH),N(CH ₂ ,CH ₂)	3.63	5426
CH ₂ /C=(E)(CH=(E),C=O),C=O(O)	3.98	5204	CH ₂ /C=O(O),N(CH ₂ ,CH ₂)	3.16	5488
CH ₂ /C=(E)(CH ₃ ,CH=(E)),OH	4.00	5530	CH ₂ /C=O(O),N(CH ₂ ,CH ₂)	3.38	5393
CH ₂ /C#(N),A(AH,AH)	3.61	4874	CH ₂ /C=O(O),N(CH ₂ ,CH ₂)	3.63	5426
CH ₂ /C#(N),A(AH,AH)	3.68	5102	CH ₂ /C=O(O),N*(AH,AH,+)	5.94	4913
CH ₂ /C#(N),A(AH,AH)	3.71	5096	CH ₂ /C=O(O),OH	4.40	5323
CH ₂ /C#(N),A(AH,AH)	3.72	4805	CH ₂ /C=O(CH ₂),O(N)	4.56	5337
CH ₂ /C#(N),A(AH,AH)	3.80	5308	CH ₂ /C=O(CH ₂),O(N)	4.57	5305
CH ₂ /C#(N),A(AH,A)	3.68	5101	CH ₂ /C=O(CH ₂),O(N)	4.69	5304
CH ₂ /C#(N),A(AH,A)	3.81	4803	CH ₂ /C=O(A),O(C=O)	5.43	5323
CH ₂ /C#(N),A(A,A)	4.02	4804	CH ₂ /C=O(OH),O(A)	4.61	5152
CH ₂ /C#(N),C=O(N)	3.39	5113	CH ₂ /C=O(OH),O(A)	4.66	5417
CH ₂ /C#(N),OH	4.25	4982	CH ₂ /C=O(OH),O(A)	4.71	5158
CH ₂ /C#(CH#),O(CH)	ca. 4.27	4961	CH ₂ /C=O(OH),O(A)	4.75	4826
CH ₂ /C#(CH#),O(C=O)	5.09	5284	CH ₂ /C=O(O),O(A)	4.62	5074
CH ₂ /C#(C#),Br	3.93	4964	CH ₂ /C=O(O),O(A)	4.62	5378
CH ₂ /A(AH,AH),C=O(CH ₂)	3.69	5402	CH ₂ /C=O(N),S(C=)	3.19	5333
CH ₂ /A(AH,AH),C=O(NH ₂)	3.58	4901	CH ₂ /C=O(N),S(C=)	4.22	5334
CH ₂ /A(AH,AH),C=O(OH)	3.63	4851	CH ₂ /C=O(N),S(C=O)	4.13	5068

Chart 4. The Chemical Shift Index

chemical shift	substructure	No.	chemical shift	substructure	No.
1.50- 2.50	CH ₂ /CH(CH ₂ ,C=O),CH=(C=)	4976	1.65	CH ₂ /CH ₃ ,CH ₂ (C=O)	5532
1.50- 2.50	CH/CH ₂ (CH ₂),CH ₂ (CH=),C=O(NH)	4976	1.65	CH ₂ /CH ₃ ,CH ₂ (C=O)	5533
1.50- 2.90	CH ₂ /CH ₂ (C=O),CH(C,C=O)	5501	ca. 1.65	CH ₂ /CH ₂ (CH ₃),CH ₂ (A)	5206
1.50- 2.90	CH ₂ /CH ₂ (CH),C=O(CH ₂)	5501	ca. 1.65	CH ₂ /CH ₂ (CH ₂),CH(CH ₂ ,OH)	5579
1.50- 2.90	CH/CH ₂ (CH ₂),C(CH ₃ ,CH ₃ ,CH ₃),C=O(CH ₂)	5501	ca. 1.65	CH ₂ /CH ₂ (CH ₂),CH(C#OH)	4981
1.51	CH ₃ /CH(A,C=O)	5142	ca. 1.65	CH ₂ /CH ₂ (CH ₂),CH(C=O,NH)	4974
1.51	CH ₃ /CH(A,C=O)	5167	1.65	CH ₂ U/CH(CH,CH=),CH(CH,CH=)	5141
1.51	NH ₂ /CH ₂ (A)	4949	1.65	CH ₂ U/CH(CH,A),CH(CH,CH=)	5361
ca. 1.52	CH ₂ /CH ₂ (CH ₃),CH ₂ (C=O)	5260	1.65	OH/C(CH ₃ ,CH ₃ ,CH ₂)	5554
1.52	CH/CH ₃ ,CH ₃ ,CH ₂ (CH=(E))	5520	1.65- 2.30	CH ₂ /CH ₂ (C=O),C(CH ₃ ,C=,C=O)	5409
1.52- 2.00	CH ₂ /CH ₂ (CH ₂),CH(CH ₂ ,NH)	5257	1.66	CH ₃ /CH(C=O,O)	5091
1.53	CH ₃ /C(CH ₃ ,CH ₃ ,O)	5539	1.66	CH ₃ /C=(CH ₂ ,CH=)	4976
1.53	CH ₃ /C(CH ₃ ,O,O)	5477	1.66	CH ₂ /CH ₃ ,CH ₂ (CH=)	5399
1.53	CH ₂ /CH ₃ ,CH ₂ (NH)	5017	ca. 1.66	CH ₂ /CH ₂ (CH ₂),CH ₂ (NH)	5265
1.53	CH ₂ /CH ₃ ,CH ₂ (NH)	5568	1.67	CH ₂ /CH ₃ ,CH ₂ (O)	5421
1.53	CH ₂ /CH ₂ (CH ₂),CH ₂ (CH)	4984	1.67	OH/CH(CH,CH)	5500
1.53	CH ₂ /CH ₂ (CH ₂),CH(CH ₂ U,O)	4984	1.67- 1.97	CH ₂ /CH ₂ (C=O),CH(CH ₃ ,C=O)	4990
1.53	CH ₂ /CH(CH,CH=),CH(CH,CH=)	5105	1.68	CH ₃ /C=(CH ₃ ,CH=)	5526
1.53	CH/CH ₃ ,CH ₃ ,CH(CH ₃ ,CH ₂)	5270	1.68	CH ₂ /CH(CH ₂ ,CH ₂),CH(CH ₂ ,CH ₂)	5475
ca. 1.53	CH/CH ₃ ,CH ₂ (CH ₂),CH(CH ₃ ,CH ₃)	5270	1.68	OH/CH(CH,CH=)	5498
ca. 1.53	NH ₂ /CH ₂ (A)	4938	1.68- 2.18	CH/CH ₃ ,CH ₃ ,CH(CH ₂ ,CH)	5553
1.53- 2.00	CH ₂ /CH ₂ (CH ₂),CH ₂ (CH ₂)	5450	1.68- 2.18	CH/CH ₃ ,CH ₂ (CH ₂),CH ₂ (CH)	5553
1.53- 2.00	CH ₂ /CH ₂ (CH ₂),CH ₂ (C=)	5450	1.68- 2.18	CH/CH ₂ (CH ₂),CH(CH ₃ ,CH ₃),CH(CH ₂ ,OH)	5553
1.53- 2.00	CH ₂ /CH ₂ (CH ₂),CH ₂ (N)	5450	1.69	CH ₃ /C=(CH ₃ ,CH=)	4999
1.54	CH ₃ /CH(C=O,NH)	5384	1.69	CH ₃ /C=(CH ₃ ,CH=)	5236
1.54	CH ₃ /C(C=O,O,O)	5255	1.69	CH ₃ /C=(E)(CH ₂ ,CH=(E))	5530
1.54	CH ₂ /CH ₂ (CH ₂),CH ₂ (C=O)	4995	1.69	CH ₂ /CH ₃ ,P=(O,O,O=O)	5036
ca. 1.54	CH/CH ₃ ,CH ₃ ,CH ₂ (CH=(E))	5519	1.69	CH ₂ /CH ₂ (CH ₂),CH ₂ (S)	5582
1.55	CH ₃ /CH(A,NH)	5439	ca. 1.69	CH ₂ /CH ₂ (OH),CH(CH ₂ ,OH)	5578
1.55	CH ₃ /CH(C=O,NH ₂)	5001	1.70	CH ₃ /C=(CH ₃ ,CH=)	5007
1.55	CH ₃ /CH(C=O,NH ₂)	5003	1.70	CH ₃ /C=(CH ₃ ,CH=)	5527
1.55	CH ₃ /CH(C=O,NH ₂)	5245	1.70	CH ₃ /C=(CH ₂ ,CH ₂ =)	5497
1.55	CH ₂ /CH ₃ ,CH(CH ₃ ,A)	5454	1.70	CH ₂ /CH ₃ ,CH ₂ (C=O)	5272
1.55	CH ₂ /CH ₂ (CH ₂),CH ₂ (SH)	5027	1.70	CH ₂ /CH ₃ ,CH(C,C=O)	5254
ca. 1.55	CH/CH ₃ ,CH ₃ ,C=O(NH)	5262	1.70	CH ₂ /CH ₃ ,C(C,CH=,OH)	5505
1.56	CH ₃ /CH(C=O,NH ₂)	5002	ca. 1.70	CH ₂ /CH ₂ (CH ₂),CH ₂ (CH ₂)	5195
ca. 1.56	CH ₂ /CH ₂ (CH=),C(CH ₃ ,CH=,OH)	5526	ca. 1.70	CH ₂ /CH ₂ (CH ₂),CH ₂ (C)	5195
1.57	CH ₃ /CH(CH ₃ ,N)	5395	1.70	CH ₂ /CH ₂ (CH ₂),CH ₂ (O)	4993
1.58	CH ₃ /C(CH ₂ U,A,OH)	5431	1.70	CH ₂ /CH ₂ (OH),CH(CH ₂ ,OH)	5026
ca. 1.58	CH ₂ /CH ₂ (CH ₂),CH ₂ (C#)	5241	ca. 1.70	CH ₂ /CH ₂ (CH ₂),C(CH ₂ ,CH=O)	5195
1.58	CH ₂ /CH ₂ (C=O),CH(CH ₂ ,C)	5220	1.70	CH ₂ /CH(CH ₂ ,CH ₂),CH(CH ₂ ,CH ₂)	5511
1.58- 1.92	CH ₂ /CH ₂ (CH ₂),CH(C=O,NH)	5246	1.70	CH ₂ U/CH(CH ₂ ,S),CH(CH ₂ U,O)	4983
1.59	CH ₃ /CH ₂ (N)	5127	ca. 1.70	CH ₂ U/CH(CH,A),CH(CH,CH=O)	5362
1.59	CH ₃ /C(CH ₂ ,A,OH)	5466	ca. 1.70	CH/CH ₂ U(CH),CH(CH ₂ U,A),C=O(OH)	5362
1.60	CH ₃ /C=(CH ₃ ,CH=)	5526	1.70	OH/CH(CH ₂ U,A)	5133
1.60	CH ₃ /C=(CH ₂ ,CH=)	5491	1.70- 2.07	CH ₂ /CH ₂ (CH),CH ₂ (C=O)	5529
1.60	CH ₃ /C=(CH,CH=)	5009	1.70- 2.07	CH ₂ /CH ₂ (CH ₂),CH(CH ₂ ,O)	5529
1.60	CH ₂ /CH ₃ ,CH ₂ (A)	5188	1.71	CH ₂ /CH ₃ ,CH(CH ₂ ,A)	5479
ca. 1.60	CH ₂ /CH ₃ ,CH ₂ (C=O)	5551	1.72	CH ₃ /CH(C=O,O)	5090
ca. 1.60	CH ₂ /CH ₃ ,CH ₂ (NH)	5267	1.72	CH ₃ /C=(CH ₂ ,CH ₂ =)	5520
ca. 1.60	CH ₂ /CH ₂ (CH ₂),CH ₂ (C=O)	5551	1.72	CH ₃ /C=O(CH ₂ U)	5386
ca. 1.60	CH/CH ₃ ,CH ₃ ,CH ₂ (CH ₂)	4969	ca. 1.72	CH ₂ /CH ₂ (CH ₃),CH ₂ (O)	5462
1.60	CH/CH ₃ ,CH ₂ (CH ₃),CH ₂ (CH)	5021	1.72	CH ₂ /CH ₂ (CH=),CH(CH ₂ ,C=O)	4958
1.60	NH/CH ₂ (CH ₂),CH ₂ (CH ₂)	5448	1.72	OH/CH(CH,CH#)	4980
1.60	OH/CH(CH ₂ ,CH)	5524	1.72	SH/CH ₂ (A)	4930
1.60- 1.90	CH ₂ /CH ₂ (CH ₃),CH(C=O,NH)	5001	1.72- 2.10	CH/CH ₃ ,CH ₂ (CH ₃),CH(C=O,NH)	5245
1.60- 2.00	CH ₂ /CH ₂ (CH ₂),CH(C=O,OH)	5010	1.73	CH ₃ /C(CH ₃ ,C#N=)	4956
1.60- 2.66	CH ₂ /CH ₂ (C),C(CH ₃ ,C,C=O)	5470	1.73	CH ₃ /C=(CH,CH=)	5498
1.60- 2.66	CH ₂ /CH ₂ (C),C(C,C=O,O)	5470	1.73	CH ₂ /CH ₂ (CH ₃),CH ₂ (O)	5463
1.61	CH ₃ /C=(CH ₃ ,CH=)	5527	1.73	CH ₂ /CH ₂ (CH ₂),CH ₂ (O)	5541
1.61	CH ₂ /CH ₂ (CH ₃),CH ₂ (NH)	5012	1.73	CH ₂ /CH ₂ (CH ₂),CH ₂ (SO ₂)	5269
1.62	CH ₃ /C=(CH ₃ ,CH=)	5007	1.74	OH/CH ₂ (CH=(E))	5530
1.62	CH ₃ /C=(CH ₃ ,CH=)	5236	1.74	OH/CH ₂ (C=(E))	5530
ca. 1.62	CH ₂ /CH ₃ ,CH(CH ₂ ,A)	5480	1.75	CH ₃ /C=(CH ₃ ,CH=)	5519
ca. 1.62	CH ₂ /CH ₂ (CH ₂),CH ₂ (CHO)	5008	1.75	CH ₃ /C=(CH ₃ ,C=)	4940
ca. 1.62	CH ₂ /CH ₂ (CH ₂),CH ₂ (C=O)	5561	1.75	CH ₃ /C=(CH,CH ₂ =)	5457
1.62	CH ₂ /CH ₂ (CH ₂),CH ₂ (NH)	5559	ca. 1.75	CH/CH ₃ ,CH ₃ ,CH ₂ (NH)	5260
1.63	CH ₃ /C(CH ₃ ,CH ₃ ,O)	4953	1.76	CH ₂ /CH ₃ ,CH ₂ (A)	4935
ca. 1.63	CH ₂ /CH ₂ (CH ₂),NH(CH ₂)	5032	1.76	CH ₂ /CH ₃ ,CH ₂ (O)	4925
1.63	CH ₂ /C=(CH ₂ ,CH ₂ =),Si(CH ₃ ,CH ₃ ,CH ₃)	5253	1.76	CH ₂ /CH ₃ ,C(O,O,O)	5274
1.63	NH ₂ /CH ₂ (A)	4937	1.76	CH/CH ₃ ,CH ₃ ,CH ₂ (NH)	5562
1.64	CH ₂ /CH ₂ (A),CH(CH ₃ ,NH ₂)	5482	1.77	CH ₃ /CH=(E)(CH=(E))	5325
ca. 1.64	CH ₂ /CH ₂ (C=O),CH(CH ₂ ,C=)	5503	1.77	CH ₂ /CH ₂ (CH ₂),CH ₂ (Cl)	5256
1.65	CH ₃ /CH=(E)(CH=(E))	4998	1.77	OH/CH(CH ₃ ,A)	5455
1.65	CH ₃ /C=(CH,CH ₂ =)	5503	1.78	CH ₃ /C#(C#)	4969
1.65	CH ₂ /CH ₃ ,CH ₂ (C=O)	5273	1.78	CH ₂ /CH ₂ (CH ₂),CH ₂ (C)	5547

Chart 5. Code Table of Sample Suppliers

Code	Name	Appliation	Code	Name	Appliation
AB01	Abe, Nobuo	Akita University	NA01	Nakasuga, Noriyuki	Nagoya University
AB02	Abe, Yoshio	Keio University	NA02	Nakagawa, Shigeki	Nippon University
AD01	Adachi, Kazuo	Osaka Institute of Technology	NA03	Hoshino, Masamatsu	Saitama University
AL		Aldrich Chemical Co.	NA04	Nagata, Masanori	Toyama Medical and Pharmaceutical University
AN01	Ando, Masayoshi	Tohoku University	NI01	Nishimura, Jun	Kyoto University of Industrial Art and Textile
AR01	Arai, Mannosuke	Tohoku University	NI02	Nishiyama, Shigeru	Keio University
AS01	Asao, Toyonobu	Tohoku University	NO01	Nonaka, Tsutomu	Tokyo Institute of Technology
AS02	Asami, Masatoshi	Yokohama National University	NO02	Nomura, Keiichi	Toyama Medical and Pharmaceutical University
FU01		Kao Corporation			
FU02	Fujise, Yutaka	Tohoku University			
FU03		Asahi Chemical Industry Co., Ltd.			
GO01	Goromaru, Tsuyoshi	The University of Tokushima	NU01		Numazu College of Technology
HA01	Hamada, Yoshiki	Meijo University	OG01	Ogino, Hiroshi	Tohoku University
HA02	Hamada, Keinosuke	Nagasaki University	OJ01	Ojima, Juro	Toyama University
HA03	Harada, Nobuyuki	Tokoku University	OO01	Osawa, Keisuke	Tohoku Pharmaceutical College
HA04	Hagiwara, Hisahiro	Tohoku University	OO02	Onuma, Hiroshi	Akita University
HA05		Toyo Jozo Co., Ltd.	OO03	Omura, Satoshi	Kitasato University
HI01	Hirose, Yoshiyuki	Science University of Tokyo	OO04		BASF Japan Co., Ltd.
HI02	Hirota, Hiroshi	The University of Tokyo	OZ01	Ozawa, Fumiyuki	Tokyo Institute of Technology
H001	Horiike, Michio	Kochi University	SA01	Sato, Gen	Sophia University
H002		Nippon Kayaku Co., Ltd.	SA02		Fuji Photo Film Co., Ltd.
H003	Iino, Masashi	Tohoku University	SA03	Sato, Masaru	Saitama University
H004		Hokko Chemical Industry Co., Ltd.	SA04		Konishiroku Photo Ind. Co., Ltd.
IK01	Ikeda, Masazumi	Osaka University	SA05	Minabe, Masahiro	Utsunomiya University
IK02	Ikariya, Takao	The University of Tokyo	SE01	Senda, Yasuhisa	Yamagata University
IS01	Ishida, Shin-ichiro	Kanazawa University	SI01	Shibata, Hisao	Shinshu University
IS02	Ishikawa, Yukihiro	Tottori University	SI02		Asahi Chemical industry Co., Ltd.
IS03		National Food Research Institute	SU01	Suzuki, Minoru	Hokkaido University
IS04	Ishiyama, Junichi	Tohoku University	SU02	Suzuki, Toshio	Akita University
IT01	Ito, Kenji	Toyohashi University of Technology	SU03	Suzuki, Kanji	Tokyo Institute of Technology
IT02	Ito, Takashi	Yokohama National University	SU04		Sumitomo Chemical Co., Ltd.
KA		Kanto Chemical Co., Inc.	SU05		Nippon Soda Co., Ltd.
KA01	Kan, Takayuki	Hiroshima University	TA01	Takatori, Masayuki	Fukushima University
KA02	Kasahara, Akira	Yamagata University	TA02	Tabei, Katsumi	Tokyo College of Pharmacy
KA03	Takei, Shoichi	Shinshu University	TA03		Zeria Pharmaceutical Co., Ltd.
KA04	Kanno, Shunroku	Yamagata University	TA04	Tanaka, Kuniyoshi	Kinki University
KA05	Karube, Akio	Akita National College of Technology	TA05	Takeda, Kei	Toyama Medical and Pharmaceutical University
KA06		Konishiroku Photo Ind. Co., Ltd.	TA06		Asahi Chemical Industry Co., Ltd.
KA07	Kato, Norimoto	Tohoku University	TO		Tokyo Kasei Kogyo Co., Ltd.
KA08	Kawashima, Takayuki	The University of Tokyo	TS01		Sumitomo Bakelite Co., Ltd.
KA09	Katayama, Hajime	Nigata College of Pharmacy	TS02	Tsunetsugu, Josuke	Saitama University
KI01	Kimura, Yoshiharu	Kyoto University of Industrial Art and Textile	TS03		Asahi Chemical Industry Co., Ltd.
KI02	Kido, Hideo	Tohoku University	UE01	Uehara, Tadao	Tohoku University
KI03	Kitahara, Haruo	Hirosaki University	YA01	Yasuda, Seiichi	Nagoya University
KO01	Kosugi, Hiroshi	Tohoku University	YA02		Central Glass Co., Ltd.
KO02	Komiya, Sanshiro	Tokyo University of Agriculture and Technology	YA03	Yamato, Masatoshi	Okayama University
KO03	Koga, Gen	Ibaraki University	YA04	Yamamoto, Yutaka	Tohoku Pharmaceutical College
KU01	Kusuyama, Yoshiaki	Wakayama University	YA05	Yasunami, Masafumi	Tohoku University
KU02	Kurosawa, Kazu	Kumamoto University	YA06	Yamada, Yoichi	Utsunomiya University
MA01	Matoba, Katsuhide	Toyama Medical and Pharmaceutical University	YA07	Yashima, Shigetaka	Hokkaido University
MA02			YO01		Maruzen Petrochemical Co., Ltd.
MA03	Machida, Katsunosuke	Kyoto University	YO02		The Green Cross Corporation
MA04	Maruyama, Masao	Miyagi University of Education			
MA05	Matsuda, Sumu	Hirosaki University			
MA06	Maruyama, Kazuhiro	Kyoto University			
ME01	Meguro, Hiroshi	Tohoku University			
MO01	Mochida, Kunio	Gakushuin University			
MO02		Fujisawa Pharmaceutical Co., Ltd.			
MO03	Morita, Yasuo	Tohoku Pharmaceutical College			

Contents

A User's Guide	vii
Proton-NMR Spectra and Data	1
Chemical Name Index	403
Molecular Formula Index	411
Substructure Index	425
Chemical Shift Index	469

Proton-NMR Spectra and Data