# Handbook of Proton-NMR Spectra and Data

## Volume 9

Edited by

Asahi Research Center

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## Volume 9

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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:

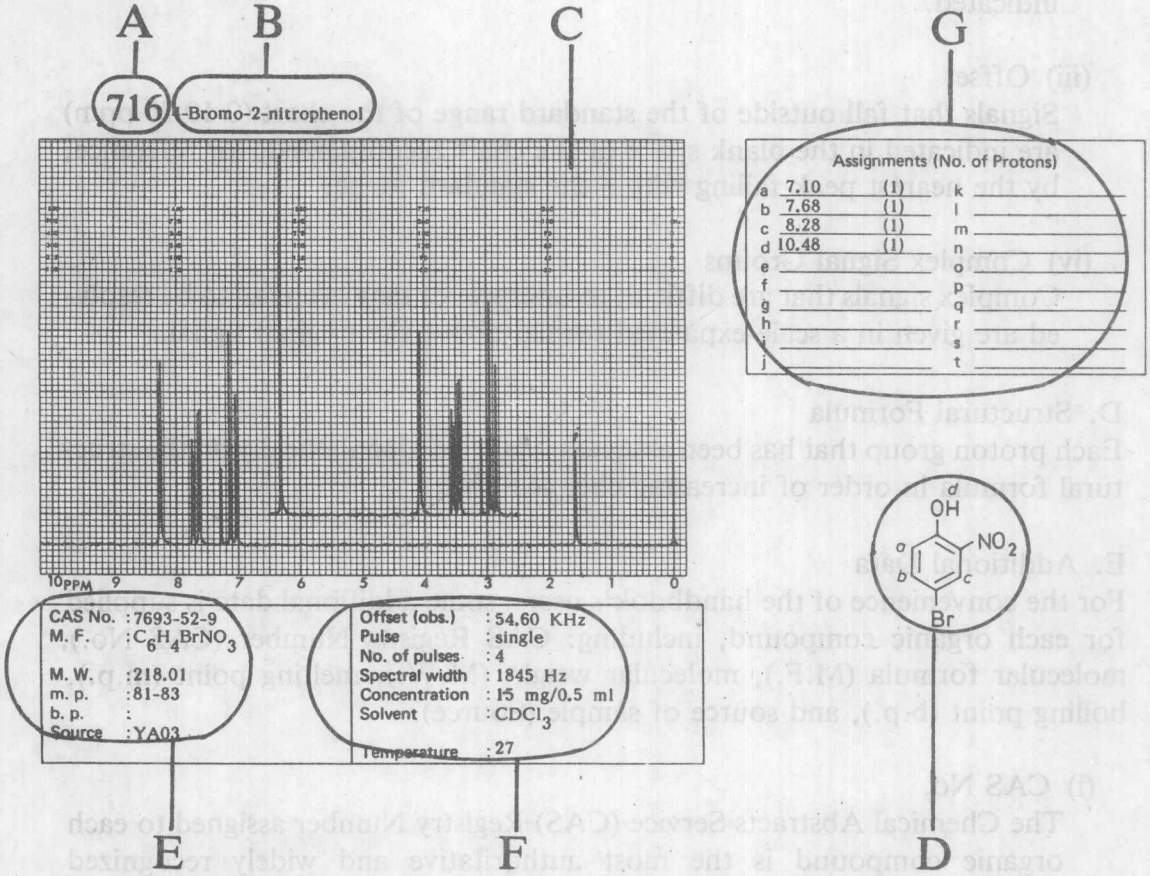


Figure 1. Illustration of Spectral Data

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 — $^1H \leqq 0.2$ 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-$d_4$. 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. $\alpha$ position) and next nearest neighbors (e.g. $\beta$ 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.

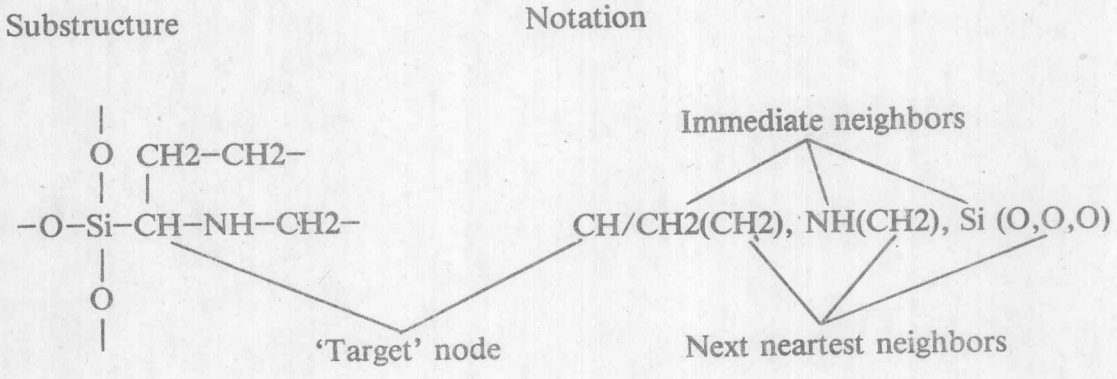


Figure 2. Substructure Notation

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.

# Chart 1. The Chemical Name Index

# Chart 2. The Molecular Formula Index

# 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. |
|---|---|---|
| CH2/CH(CH3,CH3),NH(C=O) | 3.09 | 5014 |
| CH2/CH(CH3,CH3),NH(C=O) | 3.09 | 5561 |
| CH2/CH(CH3,CH3),NH(C=O) | 3.09 | 5562 |
| CH2/CH(A,OH),NH(CH2) | ca. 3.32 | 5485 |
| CH2/CH(CH,NH2),OH | 3.29 | 5184 |
| CH2/CH(CH2,CH),O(CH3) | 4.22 | 5535 |
| CH2/CH(CH,O),O(C) | 3.40- 4.40 | 4987 |
| CH2/CH(CH3,CH3),S(S) | 2.60 | 5028 |
| CH2/CH(CH2U,CH),S(CH2) | 1.50- 2.01 | 5181 |
| CH2/CH(CH2,O),Br | 3.29- 3.81 | 5509 |
| CH2/CH(CH,O),I | 3.07- 3.40 | 5477 |
| CH2/C(CH3,CH3,CH3),C(CH3,CH3,NH2) | 1.44 | 5031 |
| CH2/C(CH3,CH3,OH),CH=(E)(CH=(E)) | ca. 2.15 | 5554 |
| CH2/C(CH3,CH3,OH),CH=(E)(CH=(E)) | 2.17 | 5552 |
| CH2/C(CH3,CH3,NH2),A(AH,AH) | 2.66 | 5478 |
| CH2/C(CH3,CH3,CH=),C=O(C=) | 2.67 | 5460 |
| CH2/C(CH3,CH2,CH2),C=O(NH) | 2.43 | 4965 |
| CH2/C(CH3,CH2,CH2),C=O(OH) | 2.30 | 4991 |
| CH2/C(CH3,CH2,CH=),C=O(C) | 2.03 | 5465 |
| CH2/C(F,F,F),O(C=O) | 4.73 | 5063 |
| CH2/C(CH3,CH3,A),Cl | 3.65 | 5425 |
| CH2/CH=(CH2=),A(AH,A) | 3.37 | 5400 |
| CH2/CH=(CH=),A(AH,A) | 3.40 | 5071 |
| CH2/CH=(CH2=),NH(A) | 3.79 | 5165 |
| CH2/CH=(CH2=),NH(C=O) | 3.74 | 5495 |
| CH2/CH=(CH2=),NH(SO2) | 3.60 | 5434 |
| CH2/CH=(CH2=),O(A) | 4.53 | 5056 |
| CH2/CH=(CH2=),O(A) | 4.61 | 5332 |
| CH2/CH=(CH2=),O(C=O) | 4.75 | 5366 |
| CH2/CH=(CH2=),O(C=O) | 4.87 | 5103 |
| CH2/CH=(CH2=),S(A) | 3.51 | 5422 |
| CH2/CH=(CH2=),S(A) | 3.55 | 5162 |
| CH2/CH=(E)(CH=(E)),C=(CH3,CH2=) | 2.70 | 5520 |
| CH2/CH=(E)(CH=(E)),OH | 4.15 | 4960 |
| CH2/CH=(E)(C=(E)),OH | 4.16 | 5530 |
| CH2/CH=(E)(CH=(E)),O(A) | 4.46 | 5325 |
| CH2/CH=(E)(CH=(E)),O(C=O) | 4.53 | 5532 |
| CH2/CH=(Z)(CH=(Z)),O(C=O) | 4.68 | 4962 |
| CH2/C=(CH2,N=),A(AH,A) | 3.86 | 5100 |
| CH2/C=(NH2,=S),A(AH,AH) | 4.11 | 4910 |
| CH2/C=(CH2,CH2=),C=O(O) | 3.00 | 5253 |
| CH2/C=(CH2,N=),C=O(N) | 3.59 | 5354 |
| CH2/C=(CH2,N=),C=O(N) | 3.61 | 5328 |
| CH2/C=(CH=,A),C=O(OH) | 3.53 | 5336 |
| CH2/C=(CH=,A),C=O(O) | 3.67 | 5307 |
| CH2/C=(CH2,N=),O(N) | 5.00 | 5354 |
| CH2/C=(CH2,N=),O(N) | 5.10 | 5328 |
| CH2/C=(CH=,A),O(C=O) | 5.23 | 5319 |
| CH2/C=(CH=,O),S(S) | 3.71 | 5364 |
| CH2/C=(CH=,C=),Br | 4.46 | 5324 |
| CH2/C=(CH=,C=),Br | 4.53 | 5343 |
| CH2/C=(CH=,C=),Br | 4.55 | 5324 |
| CH2/C=(CH=,C=),Br | 4.60 | 5343 |
| CH2/C=(CH=,C=O),Br | 4.46 | 5324 |
| CH2/C=(CH=,C=O),Br | 4.53 | 5343 |
| CH2/C=(CH=,C=O),Br | 4.55 | 5324 |
| CH2/C=(CH=,C=O),Br | 4.60 | 5343 |
| CH2/C=(CH2,CH2=),Si(CH3,CH3,CH3) | 1.63 | 5253 |
| CH2/C=(E)(CH=(E),C=O),C=O(O) | 3.98 | 5204 |
| CH2/C=(E)(CH3,CH=(E)),OH | 4.00 | 5530 |
| CH2/C#(#N),A(AH,AH) | 3.61 | 4874 |
| CH2/C#(#N),A(AH,AH) | 3.68 | 5102 |
| CH2/C#(#N),A(AH,AH) | 3.71 | 5096 |
| CH2/C#(#N),A(AH,AH) | 3.72 | 4805 |
| CH2/C#(#N),A(AH,AH) | 3.80 | 5308 |
| CH2/C#(#N),A(AH,A) | 3.68 | 5101 |
| CH2/C#(#N),A(AH,A) | 3.81 | 4803 |
| CH2/C#(#N),A(A,A) | 4.02 | 4804 |
| CH2/C#(#N),C=O(N) | 3.39 | 5113 |
| CH2/C#(C#),OH | 4.25 | 4982 |
| CH2/C#(CH#),O(CH) | ca. 4.27 | 4961 |
| CH2/C#(CH#),O(C=O) | 5.09 | 5284 |
| CH2/C#(C#),Br | 3.93 | 4964 |
| CH2/A(AH,AH),C=O(CH2) | 3.69 | 5402 |
| CH2/A(AH,AH),C=O(NH2) | 3.58 | 4901 |
| CH2/A(AH,AH),C=O(OH) | 3.63 | 4851 |
| CH2/A(AH,AH),C=O(OH) | 3.64 | 4852 |
| CH2/A(AH,AH),C=O(O) | 3.74 | 5108 |
| CH2/A(AH,A),C=O(C=O) | 4.58 | 5046 |
| CH2/A(AH,A),C=O(N) | 3.50 | 5099 |
| CH2/A(AH,A),C=O(OH) | 3.80 | 4824 |
| CH2/A(AH,A),C=O(OH) | 4.02 | 4860 |
| CH2/A(AH,AH),NH2 | 3.69 | 4950 |
| CH2/A(AH,AH),NH2 | 3.80 | 4939 |
| CH2/A(AH,AH),NH2 | 3.81 | 4933 |
| CH2/A(AH,AH),NH2 | 3.84 | 4938 |
| CH2/A(AH,AH),NH2 | 3.90 | 4949 |
| CH2/A(AH,A),NH2 | 3.82 | 4937 |
| CH2/A(AH,AH),NH(CH3) | 3.75 | 4934 |
| CH2/A(AH,AH),NH(CH2) | 3.80 | 5208 |
| CH2/A(AH,AH),NH(CH2) | 3.80 | 5219 |
| CH2/A(AH,AH),NH(CH2) | 3.82 | 4952 |
| CH2/A(AH,AH),NH(CH) | 3.79 | 5481 |
| CH2/A(AH,AH),NH(C=O) | 4.43 | 5428 |
| CH2/A(AH,A),NH(CH2) | 4.00 | 5166 |
| CH2/A(AH,AH),N(CH3,CH3,CH3,+) | 5.06 | 5492 |
| CH2/A(AH,AH),OH | 4.48 | 4922 |
| CH2/A(AH,AH),OH | 4.52 | 4889 |
| CH2/A(AH,AH),OH | 4.61 | 5469 |
| CH2/A(AH,AH),OH | 4.76 | 5151 |
| CH2/A(AH,A),OH | 4.52 | 5194 |
| CH2/A(AH,A),OH | 4.53 | 5198 |
| CH2/A(AH,A),OH | 4.69 | 5199 |
| CH2/A(AH,A),OH | 4.80 | 5197 |
| CH2/A(AH,TPL),OH | 4.60 | 5092 |
| CH2/A(A,A),OH | 4.61 | 4941 |
| CH2/A(AH,AH),O(CH2) | 4.57 | 5192 |
| CH2/A(AH,AH),O(CH2) | 4.59 | 5164 |
| CH2/A(AH,AH),O(C=O) | 5.10 | 4904 |
| CH2/A(AH,AH),O(C=O) | 5.40 | 4823 |
| CH2/A(AH,A),O(C=O) | 5.20 | 5368 |
| CH2/A(AH,AH),SH | 3.72 | 4930 |
| CH2/A(AH,A),SH | 3.81 | 5473 |
| CH2/A(AH,AH),S(C=) | 4.59 | 4919 |
| CH2/A(AH,AH),SO2(CH3) | 4.14 | 5486 |
| CH2/A(AH,AH),SO2(Cl) | 4.84 | 4898 |
| CH2/A(AH,A),SO2(Cl) | 4.96 | 5163 |
| CH2/A(AH,AH),P=(O,O,=O) | 3.18 | 5216 |
| CH2/A(AH,AH),Br | 4.50 | 4895 |
| CH2/A(AH,A),Br | 4.60 | 5347 |
| CH2/A(AH,AH),D | 2.29 | 5117 |
| CH2/C=O(CH2),C=O(CH) | 3.40 | 5501 |
| CH2/C=O(CH2),C=O(N) | 3.80 | 5305 |
| CH2/C=O(CH2),C=O(N) | 3.80 | 5337 |
| CH2/C=O(CH2),C=O(N) | 3.81 | 5304 |
| CH2/C=O(CH2),C=O(O) | 3.62 | 5226 |
| CH2/C=O(CH),C=O(O) | 3.50 | 5506 |
| CH2/C=O(C),C=O(C=) | 6.47 | 4808 |
| CH2/C=O(O),C=O(O) | 3.31 | 5239 |
| CH2/C=O(NH),NH(C=O) | 3.87 | 5394 |
| CH2/C=O(OH),NH(C=O) | 3.88 | 5125 |
| CH2/C=O(OH),NH(C=O) | 3.92 | 5387 |
| CH2/C=O(O),NH(C=O) | 4.53 | 4955 |
| CH2/C=O(OH),N(CH2,CH2) | 3.63 | 5426 |
| CH2/C=O(O),N(CH2,CH2) | 3.16 | 5488 |
| CH2/C=O(O),N(CH2,CH2) | 3.38 | 5393 |
| CH2/C=O(O),N(CH2,CH2) | 3.63 | 5426 |
| CH2/C=O(CH3),N(*(AH,AH,+) | 5.94 | 4913 |
| CH2/C=O(O),OH | 4.40 | 5323 |
| CH2/C=O(CH2),O(N) | 4.56 | 5337 |
| CH2/C=O(CH2),O(N) | 4.57 | 5305 |
| CH2/C=O(CH2),O(N) | 4.69 | 5304 |
| CH2/C=O(A),O(C=O) | 5.43 | 5323 |
| CH2/C=O(OH),O(A) | 4.61 | 5152 |
| CH2/C=O(OH),O(A) | 4.66 | 5417 |
| CH2/C=O(OH),O(A) | 4.71 | 5158 |
| CH2/C=O(OH),O(A) | 4.75 | 4826 |
| CH2/C=O(O),O(A) | 4.62 | 5074 |
| CH2/C=O(O),O(A) | 4.62 | 5378 |
| CH2/C=O(N),S(C=) | 3.19 | 5333 |
| CH2/C=O(N),S(C=) | 4.22 | 5334 |
| CH2/C=O(N),S(C=O) | 4.13 | 5068 |

# Chart 4. The Chemical Shift Index

| chemical shift | substructure | No. |
|---|---|---|
| 1.50- 2.50 | CH2/CH(CH2,C=O),CH=(C=) | 4976 |
| 1.50- 2.50 | CH/CH2(CH2),CH2(CH=),C=O(NH) | 4976 |
| 1.50- 2.90 | CH2/CH2(C=O),CH(C,C=O) | 5501 |
| 1.50- 2.90 | CH2/CH2(CH),C=O(CH2) | 5501 |
| 1.50- 2.90 | CH/CH2(CH2),C(CH3,CH3,CH3),C=O(CH2) | 5501 |
| 1.51 | CH3/CH(A,C=O) | 5142 |
| 1.51 | CH3/CH(A,C=O) | 5167 |
| 1.51 | NH2/CH2(A) | 4949 |
| ca. 1.52 | CH2/CH2(CH3),CH2(C=O) | 5260 |
| 1.52 | CH/CH3,CH3,CH2(CH=(E)) | 5520 |
| 1.52- 2.00 | CH2/CH2(CH2),CH(CH2,NH) | 5257 |
| 1.53 | CH3/C(CH3,CH3,O) | 5539 |
| 1.53 | CH3/C(CH3,O,O) | 5477 |
| 1.53 | CH2/CH3,CH2(NH) | 5017 |
| 1.53 | CH2/CH3,CH2(NH) | 5568 |
| 1.53 | CH2/CH2(CH2),CH2(CH) | 4984 |
| 1.53 | CH2/CH2(CH2),CH(CH2U,O) | 4984 |
| 1.53 | CH2/CH(CH,CH=),CH(CH,CH=) | 5105 |
| ca. 1.53 | CH/CH3,CH3,CH(CH3,CH2) | 5270 |
| ca. 1.53 | CH/CH3,CH2(CH2),CH(CH3,CH3) | 5270 |
| 1.53 | NH2/CH2(A) | 4938 |
| 1.53- 2.00 | CH2/CH2(CH2),CH2(CH2) | 5450 |
| 1.53- 2.00 | CH2/CH2(CH2),CH2(C=) | 5450 |
| 1.53- 2.00 | CH2/CH2(CH2),CH2(N) | 5450 |
| 1.54 | CH3/CH(C=O,NH) | 5384 |
| 1.54 | CH3/C(C=O,O,O) | 5255 |
| 1.54 | CH2/CH2(CH2),CH2(C=O) | 4995 |
| ca. 1.54 | CH/CH3,CH3,CH2(CH=(E)) | 5519 |
| 1.55 | CH3/CH(A,NH) | 5439 |
| 1.55 | CH3/CH(C=O,NH2) | 5001 |
| 1.55 | CH3/CH(C=O,NH2) | 5003 |
| 1.55 | CH3/CH(C=O,NH2) | 5245 |
| 1.55 | CH2/CH3,CH(CH3,A) | 5454 |
| 1.55 | CH2/CH2(CH2),CH2(SH) | 5027 |
| ca. 1.55 | CH/CH3,CH3,C=O(NH) | 5262 |
| 1.56 | CH3/CH(C=O,NH2) | 5002 |
| ca. 1.56 | CH2/CH2(CH=),C(CH3,CH=,OH) | 5526 |
| 1.57 | CH3/CH(CH3,N) | 5395 |
| 1.58 | CH3/C(CH2U,A,OH) | 5431 |
| ca. 1.58 | CH2/CH2(CH2),CH2(C#) | 5241 |
| 1.58 | CH2/CH2(C=O),CH(CH2,C) | 5220 |
| 1.58- 1.92 | CH2/CH2(CH2),CH(C=O,NH) | 5246 |
| 1.59 | CH3/CH2(N) | 5127 |
| 1.59 | CH3/C(CH2,A,OH) | 5466 |
| 1.60 | CH3/C=(CH3,CH=) | 5526 |
| 1.60 | CH3/C=(CH2,CH=) | 5491 |
| 1.60 | CH3/C=(CH,CH=) | 5009 |
| 1.60 | CH2/CH3,CH2(A) | 5188 |
| ca. 1.60 | CH2/CH3,CH2(C=O) | 5551 |
| ca. 1.60 | CH2/CH3,CH2(NH) | 5267 |
| ca. 1.60 | CH2/CH2(CH2),CH2(C=O) | 5551 |
| ca. 1.60 | CH/CH3,CH3,CH2(CH2) | 4969 |
| 1.60 | CH/CH3,CH2(CH3),CH2(CH) | 5021 |
| 1.60 | NH/CH2(CH2),CH2(CH2) | 5448 |
| 1.60 | OH/CH(CH2,CH) | 5524 |
| 1.60- 1.90 | CH2/CH2(CH3),CH(C=O,NH) | 5001 |
| 1.60- 2.00 | CH2/CH2(CH2),CH(C=O,OH) | 5010 |
| 1.60- 2.66 | CH2/CH2(C),C(CH3,C,C=O) | 5470 |
| 1.60- 2.66 | CH2/CH2(C),C(C,C=O,O) | 5470 |
| 1.61 | CH3/C=(CH3,CH=) | 5527 |
| 1.61 | CH2/CH2(CH3),CH2(NH) | 5012 |
| 1.62 | CH3/C=(CH3,CH=) | 5007 |
| 1.62 | CH3/C=(CH3,CH=) | 5236 |
| ca. 1.62 | CH2/CH3,CH(CH2,A) | 5480 |
| 1.62 | CH2/CH2(CH2),CH2(CHO) | 5008 |
| ca. 1.62 | CH2/CH2(CH2),CH2(C=O) | 5561 |
| 1.62 | CH2/CH2(CH2),CH2(NH) | 5559 |
| 1.63 | CH3/C(CH3,CH3,O) | 4953 |
| ca. 1.63 | CH2/CH2(CH2),NH(CH2) | 5032 |
| 1.63 | CH2/C=(CH2,CH2=),Si(CH3,CH3,CH3) | 5253 |
| 1.63 | NH2/CH2(A) | 4937 |
| 1.64 | CH2/CH2(A),CH(CH3,NH2) | 5482 |
| ca. 1.64 | CH2/CH2(C=O),CH(CH2,C=) | 5503 |
| 1.65 | CH3/CH=(E)(CH=(E)) | 4998 |
| 1.65 | CH3/C=(CH,CH2=) | 5503 |
| 1.65 | CH2/CH3,CH2(C=O) | 5273 |

| chemical shift | substructure | No. |
|---|---|---|
| 1.65 | CH2/CH3,CH2(C=O) | 5532 |
| 1.65 | CH2/CH3,CH2(C=O) | 5533 |
| ca. 1.65 | CH2/CH2(CH3),CH2(A) | 5206 |
| ca. 1.65 | CH2/CH2(CH2),CH(CH2,OH) | 5579 |
| ca. 1.65 | CH2/CH2(CH2),CH(C#,OH) | 4981 |
| ca. 1.65 | CH2/CH2(CH2),CH(C=O,NH) | 4974 |
| 1.65 | CH2U/CH(CH,CH=),CH(CH,CH=) | 5141 |
| 1.65 | CH2U/CH(CH,A),CH(CH,C=O) | 5361 |
| 1.65 | OH/C(CH3,CH3,CH2) | 5554 |
| 1.65- 2.30 | CH2/CH2(C=O),C(CH3,C=,C=O) | 5409 |
| 1.66 | CH3/CH(C=O,O) | 5091 |
| 1.66 | CH3/C=(CH2,CH=) | 4976 |
| 1.66 | CH2/CH3,CH2(CH=) | 5399 |
| ca. 1.66 | CH2/CH2(CH2),CH2(NH) | 5265 |
| 1.67 | CH2/CH3,CH2(O) | 5421 |
| 1.67 | OH/CH(CH,CH) | 5500 |
| 1.67- 1.97 | CH2/CH2(C=O),CH(CH3,C=O) | 4990 |
| 1.68 | CH3/C=(CH3,CH=) | 5526 |
| 1.68 | CH2/CH(CH2,CH2),CH(CH2,CH2) | 5475 |
| 1.68 | OH/CH(CH,CH=) | 5498 |
| 1.68- 2.18 | CH/CH3,CH3,CH(CH2,CH) | 5553 |
| 1.68- 2.18 | CH/CH3,CH2(CH2),CH2(CH) | 5553 |
| 1.68- 2.18 | CH/CH2(CH2),CH(CH3,CH3),CH(CH2,OH) | 5553 |
| 1.69 | CH3/C=(CH3,CH=) | 4999 |
| 1.69 | CH3/C=(CH3,CH=) | 5236 |
| 1.69 | CH3/C=(E)(CH2,CH=(E)) | 5530 |
| 1.69 | CH2/CH3,P=(O,O,=O) | 5036 |
| 1.69 | CH2/CH2(CH2),CH2(S) | 5582 |
| ca. 1.69 | CH2/CH2(OH),CH(CH2,OH) | 5578 |
| 1.70 | CH3/C=(CH3,CH=) | 5007 |
| 1.70 | CH3/C=(CH3,CH=) | 5527 |
| 1.70 | CH3/C=(CH2,CH2=) | 5497 |
| 1.70 | CH2/CH3,CH2(C=O) | 5272 |
| 1.70 | CH2/CH3,CH(C,C=O) | 5254 |
| 1.70 | CH2/CH3,C(C,CH=,OH) | 5505 |
| ca. 1.70 | CH2/CH2(CH2),CH2(CH2) | 5195 |
| ca. 1.70 | CH2/CH2(CH2),CH2(C) | 5195 |
| 1.70 | CH2/CH2(CH2),CH2(O) | 4993 |
| 1.70 | CH2/CH2(OH),CH(CH2,OH) | 5026 |
| ca. 1.70 | CH2/CH2(CH2),C(CH2,CH=,O) | 5195 |
| 1.70 | CH2/CH(CH2,CH2),CH(CH2,CH2) | 5511 |
| 1.70 | CH2U/CH(CH2,S),CH(CH2U,O) | 4983 |
| ca. 1.70 | CH2U/CH(CH,A),CH(CH,C=O) | 5362 |
| ca. 1.70 | CH/CH2U(CH),CH(CH2U,A),C=O(OH) | 5362 |
| 1.70 | OH/CH(CH2U,A) | 5133 |
| 1.70- 2.07 | CH2/CH2(CH),CH2(C=O) | 5529 |
| 1.70- 2.07 | CH2/CH2(CH2),CH(CH2,O) | 5529 |
| 1.71 | CH2/CH3,CH(CH2,A) | 5479 |
| 1.72 | CH3/CH(C=O,O) | 5090 |
| 1.72 | CH3/C=(CH2,CH2=) | 5520 |
| 1.72 | CH3/C=O(CH2U) | 5386 |
| ca. 1.72 | CH2/CH2(CH3),CH2(O) | 5462 |
| 1.72 | CH2/CH2(CH=),CH(CH2,C=O) | 4958 |
| 1.72 | OH/CH(CH,C#) | 4980 |
| 1.72 | SH/CH2(A) | 4930 |
| 1.72- 2.10 | CH/CH3,CH2(CH3),CH(C=O,NH) | 5245 |
| 1.73 | CH3/C(CH3,C#,N=) | 4956 |
| 1.73 | CH3/C=(CH,CH=) | 5498 |
| 1.73 | CH2/CH2(CH3),CH2(O) | 5463 |
| 1.73 | CH2/CH2(CH2),CH2(O) | 5541 |
| 1.73 | CH2/CH2(CH2),CH2(SO2) | 5269 |
| 1.74 | OH/CH2(CH=(E)) | 5530 |
| 1.74 | OH/CH2(C=(E)) | 5530 |
| 1.75 | CH3/C=(CH3,CH=) | 5519 |
| 1.75 | CH3/C=(CH3,C=) | 4940 |
| 1.75 | CH3/C=(CH,CH2=) | 5457 |
| ca. 1.75 | CH/CH3,CH3,CH2(NH) | 5260 |
| 1.76 | CH2/CH3,CH2(A) | 4935 |
| 1.76 | CH2/CH3,CH2(O) | 4925 |
| 1.76 | CH2/CH3,C(O,O,O) | 5274 |
| 1.76 | CH/CH3,CH3,CH2(NH) | 5562 |
| 1.77 | CH3/CH=(E)(CH=(E)) | 5325 |
| 1.77 | CH2/CH2(CH2),CH2(Cl) | 5256 |
| 1.77 | OH/CH(CH3,A) | 5455 |
| 1.78 | CH3/C#(C#) | 4969 |
| 1.78 | CH2/CH2(CH2),CH2(C[illegible] | 5547 |

# Chart 5. Code Table of Sample Suppliers

| Code | Name | Appliation |
|---|---|---|
| AB01 | Abe, Nobuo | Akita University |
| AB02 | Abe, Yoshio | Keio University |
| AD01 | Adachi, Kazuo | Osaka Institute of Technology |
| AL | | Aldrich Chemical Co. |
| AN01 | Ando, Masayoshi | Tohoku University |
| AR01 | Arai, Mannosuke | Tohoku University |
| AS01 | Asao, Toyonobu | Tohoku University |
| AS02 | Asami, Masatoshi | Yokohama National University |
| FU01 | | Kao Corporation |
| FU02 | Fujise, Yutaka | Tohoku University |
| FU03 | | Asahi Chemical Industry Co., Ltd. |
| GO01 | Goromaru, Tsuyoshi | The University of Tokushima |
| HA01 | Hamada, Yoshiki | Meijo University |
| HA02 | Hamada, Keinosuke | Nagasaki University |
| HA03 | Harada, Nobuyuki | Tokoku University |
| HA04 | Hagiwara, Hisahiro | Tohoku University |
| HA05 | | Toyo Jozo Co., Ltd. |
| HI01 | Hirose, Yoshiyuki | Science University of Tokyo |
| HI02 | Hirota, Hiroshi | The University of Tokyo |
| HO01 | Horiike, Michio | Kochi University |
| HO02 | | Nippon Kayaku Co., Ltd. |
| HO03 | Iino, Masashi | Tohoku University |
| HO04 | | Hokko Chemical Industry Co., Ltd. |
| IK01 | Ikeda, Masazumi | Osaka University |
| IK02 | Ikariya, Takao | The University of Tokyo |
| IS01 | Ishida, Shin-ichiro | Kanazawa University |
| IS02 | Ishikawa, Yukihiro | Tottori University |
| IS03 | | National Food Research Institute |
| IS04 | Ishiyama, Junichi | Tohoku University |
| IT01 | Ito, Kenji | Toyohashi University of Technology |
| IT02 | Ito, Takashi | Yokohama National University |
| KA | | Kanto Chemical Co., Inc. |
| KA01 | Kan, Takayuki | Hiroshima University |
| KA02 | Kasahara, Akira | Yamagata University |
| KA03 | Kakei, Shoichi | Shinshu University |
| KA04 | Kanno, Shunroku | Yamagata University |
| KA05 | Karube, Akio | Akita National College of Technology |
| KA06 | | Konishiroku Photo Ind. Co., Ltd. |
| KA07 | Kato, Norimoto | Tohoku University |
| KA08 | Kawashima, Takayuki | The University of Tokyo |
| KA09 | Katayama, Hajime | Nigata College of Pharmacy |
| KI01 | Kimura, Yoshiharu | Kyoto University of Industrial Art and Textile |
| KI02 | Kido, Hideo | Tohoku University |
| KI03 | Kitahara, Haruo | Hirosaki University |
| KO01 | Kosugi, Hiroshi | Tohoku University |
| KO02 | Komiya, Sanshiro | Tokyo University of Agriculture and Technology |
| KO03 | Koga, Gen | Ibaraki University |
| KU01 | Kusuyama, Yoshiaki | Wakayama University |
| KU02 | Kurosawa, Kazu | Kumamoto University |
| MA01 | Matoba, Katsuhide | Toyama Medical and Pharmaceutical University |
| MA02 | Machida, Katsunosuke | Kyoto University |
| MA03 | Maruyama, Masao | Miyagi University of Education |
| MA04 | Matsuda, Sumu | Hirosaki University |
| MA05 | 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 |
| NA01 | Nakasuga, Noriyuki | Nagoya University |
| NA02 | Nakagawa, Shigeki | Nippon University |
| NA03 | Hoshino, Masamatsu | Saitama University |
| NA04 | Nagata, Masanori | Toyama Medical and Pharmaceutical University |
| NI01 | Nishimura, Jun | Kyoto University of Industrial Art and Textile |
| NI02 | Nishiyama, Shigeru | Keio University |
| NO01 | Nonaka, Tsutomu | Tokyo Institure of Technology |
| NO02 | Nomura, Keiichi | Toyama Medical and Pharmaceutical University |
| NU01 | | Numazu College of Technology |
| OG01 | Ogino, Hiroshi | Tohoku University |
| OJ01 | Ojima, Juro | Toyama University |
| OO01 | Osawa, Keisuke | Tohoku Pharmaceutical College |
| OO02 | Onuma, Hiroshi | Akita University |
| OO03 | Omura, Satoshi | Kitasato University |
| OO04 | | BASF Japan Co., Ltd. |
| OZ01 | Ozawa, Fumiyuki | Tokyo Institute of Technology |
| SA01 | Sato, Gen | Sophia University |
| SA02 | | Fuji Photo Film Co., Ltd. |
| SA03 | Sato, Masaru | Saitama University |
| SA04 | | Konishiroku Photo Ind. Co., Ltd. |
| SA05 | Minabe, Masahiro | Utsunomiya University |
| SE01 | Senda, Yasuhisa | Yamagata University |
| SI01 | Shibata, Hisao | Shinshu University |
| SI02 | | Asahi Chemical industry Co., Ltd. |
| SU01 | Suzuki, Minoru | Hokkaido University |
| SU02 | Suzuki, Toshio | Akita University |
| SU03 | Suzuki, Kanji | Tokyo Institute of Technology |
| SU04 | | Sumitomo Chemical Co., Ltd. |
| SU05 | | Nippon Soda Co., Ltd. |
| TA01 | Takatori, Masayuki | Fukushima University |
| TA02 | Tabei, Katsumi | Tokyo College of Pharmacy |
| TA03 | | Zeria Pharmaceutical Co., Ltd. |
| TA04 | Tanaka, Kuniyoshi | Kinki University |
| TA05 | Takeda, Kei | Toyama Medical and Pharmaceutical University |
| TA06 | | Asahi Chemical Industry Co., Ltd. |
| TO | | Tokyo Kasei Kogyo Co., Ltd. |
| TS01 | | Sumitomo Bakelite Co., Ltd. |
| TS02 | Tsunetsugu, Josuke | Saitama University |
| TS03 | | Asahi Chemical Industry Co., Ltd. |
| UE01 | Uehara, Tadao | Tohoku University |
| YA01 | Yasuda, Seiichi | Nagoya University |
| YA02 | | Central Glass Co., Ltd. |
| YA03 | Yamato, Masatoshi | Okayama University |
| YA04 | Yamamoto, Yutaka | Tohoku Pharmaceutical College |
| YA05 | Yasunami, Masafumi | Tohoku University |
| YA06 | Yamada, Yoichi | Utsunomiya University |
| YA07 | Yashima, Shigetaka | Hokkaido University |
| YO01 | | Maruzen Petrochemical Co., Ltd. |
| YO02 | | The Green Cross Corporation |

# Contents

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