

Handbook of Proton-NMR Spectra and Data Volume 3

Edited by
Asahi Research Center

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Handbook of Proton-NMR Spectra and Data Volume 3

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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:

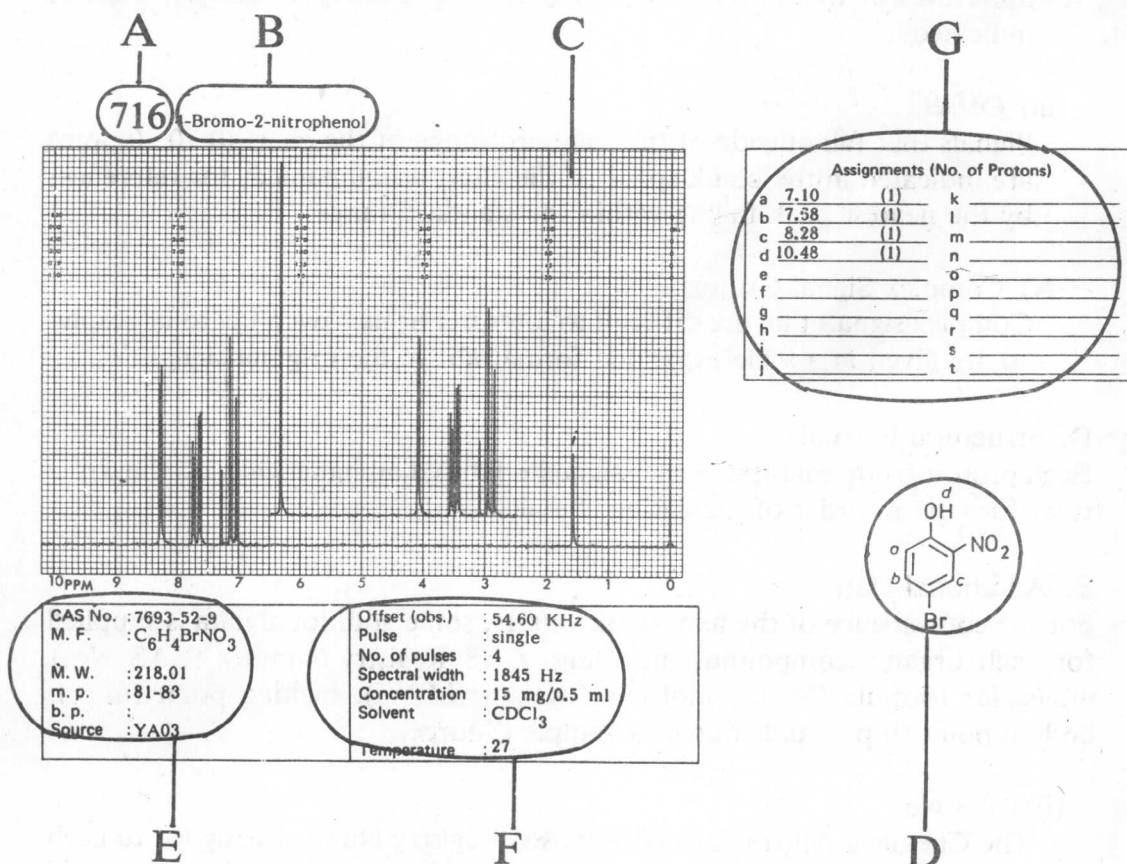


Figure 1. Illustration of Spectral Data

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.

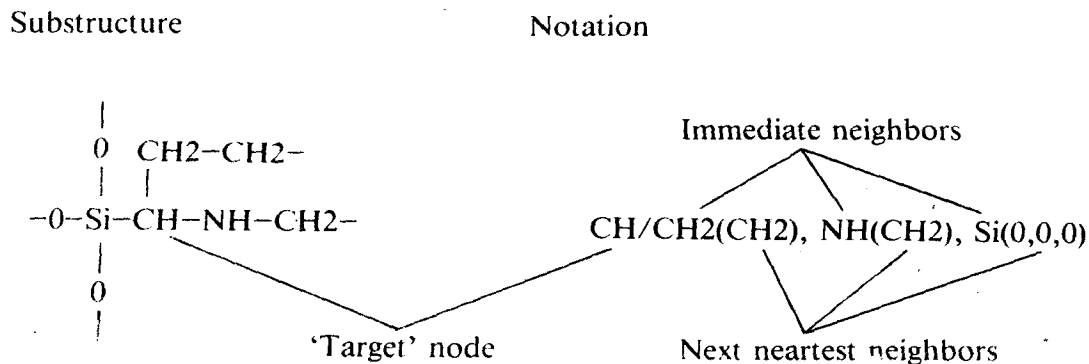


Figure 2. Substructure Notation

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. 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

name	No.	name	No.
3-carboxylate	3417	2-Hydroxy-4-(octyloxy)benzophenone	3867
1-(5-Ethyl-2-methyl-1-pyridinio)-1-ethoxycarbonyl-		17beta-Hydroxy-3-oxoandrostane	3784
1-[(methylthio)thiocarbonyl]methanide	3328	2-(4-Hydroxyphenyl)-1,3-benzothiazin-4(3H)-one	3243
7-Ethyl-2-methyl-4-undecanol	3368	2-Hydroxy-2-phenylbutyl para-toluenesulfonate	3648
Ethyl myristate	3575	3-Hydroxy-2-phenyl-4H-chromen-4-one	3387
Ethyl oleate	3835	3-(4-Hydroxyphenyl)isochroman	3432
Ethyl palmitate	3731	2-(3-Hydroxyphenyl)-3-methyl-1,3-benzothiazin-4(3H)-one	
1-Ethyl-2-phenylindole	3538	1,1-dioxide	3419
Ethyl stearate	3843	3-(4-Hydroxyphenyl)-2-phenylacrylic acid	3408
3-(1-Ethylthio-1-mercaptomethylene)-1-phenyl-		3-(4-Hydroxyphenyl)-2-phenylpropionic acid	3439
2,3-dihydroindolizin-2-one	3618	3-Hydroxy-3-phenyl-3-ortho-tolylpropionic acid	3549
Ethyl 4-tosyloxybenzoate	3552	11alpha-Hydroxyprogesterone	3871
17alpha-Ethynyl-3-hydroxy-1,3,5(10)-estratrien-17beta-ol	3826	(3-Hydroxypropyl)triphenylphosphonium bromide	3862
17alpha-Ethynyl-3-oxoestr-4-en-17beta-ol	3827	2'-Hydroxy-3,4,5-trimethoxy-3',5'-dimethylchalcone	3824
17alpha-Ethynyl-3-oxo-4-estrenyl acetate	3886	2'-Hydroxy-3',4,5'-trimethylchalcone	3703
Fluoranthene	3494	1-Iodoheptadecane	3581
Fluorescein	3802	1-Iodoctadecane	3737
1-(2-Furyl)-3-(2-hydroxy-3,5-dimethylphenyl)-2-propen-1-one	3436	Isobutyl decanoate	3361
Heptadecanamide	3664	Isobutyl laurate	3578
Heptadecane	3666	Isobutyl myristate	3732
1-Heptadecanol	3667	Isobutyl palmitate	3844
2-Heptadecyl-2-imidazoline	3839	N-Isobutyltridecanamide	3665
Heptanedianilide	3777	4-Isobutyryl-2-methylanisole 2,4-dinitrophenylhydrazine	3710
Heptanoic anhydride	3352	N-Isohexyltridecanamide	3795
Heptyl decanoate	3660	alpha-Isopropoxybenzyl phenyl ketone	3639
Heptyl 4-hydroxybenzoate	3334	3-(4-Isopropyl)benzoyl-2-methylpropionic acid	3320
4-Heptyloxybenzaldehyde	3333	9-Isopropylcarbazole	3443
Heptyltriphenylphosphonium bromide	3931	Isopropyl decanoate	3210
2-Heptylundecanilide	3920	4-Isopropyl-5,8-dimethyl-1,2,3,4-tetrahydro-1-naphthalenone	3460
Hexacosane	3952	4-Isopropyl-5,8-dimethyl-1,2,3,4-tetrahydro-1-naphthol	3464
Hexadecane	3583	4,4'-Isopropylidenebis(2,6-dibromophenol)	3397
Hexadecanethiol	3586	4,4'-Isopropylidenebis(2,6-dichlorophenol)	3400
Hexadecanoic acid	3576	4,4'-Isopropylidenediphenol	3454
1-Hexadecanol	3585	7-Isopropyl-3-methoxy-1-methylnaphthalene	3458
Hexadecylamine	3590	6-Isopropyl-4-methyl-2-naphthol	3312
Hexaethylbenzene	3718	2-Isopropyl-5-methylphenyl 3,5-dinitrobenzoate	3623
2,6,10,15,19,23-Hexamethyltetracosane	3982	2-Isopropyl-5-methylphenyl para-toluenesulfonate	3647
Hexanedianilide	3708	Isopropyl myristate	3661
Hexatriacontane	3996	N-Isopropylundecanamide	3365
2-Hexyldecanoic acid	3577	Laurenisol acetate	3650
3beta-Hydroxyandrost-5-en-17-one	3780	Magnesium phenoxylacetate	3528
4-(2-Hydroxybenzylideneimino)-1,5-dimethyl-2-phenyl-		3-para-Menthyl 3-hydroxy-3,3-diphenylpropionate	3932
3-pyrazolone	3697	3-para-Menthyl 3-hydroxy-3-phenylbutyrate	3831
5-(4-Hydroxybenzyl)-3-phenyl-2-thioxo-4-imidazolidone	3530	3-para-Menthyl 4-oxo-4-phenylbutyrate	3829
3beta-Hydroxy-5-cholesten-7-one	3956	2-Methoxybenzaldehyde 4-nitrophenylhydrazine	3274
7beta-Hydroxycholesten-3beta-yl benzoate	3992	3-Methoxybenzaldehyde 4-nitrophenylhydrazine	3275
7alpha-Hydroxycholesterol	3959	2-(4-Methoxybenzylidene)-3(2H)-benzofuranone	3507
7beta-Hydroxycholesterol	3960	5-Methoxycanthin-6-one	3382
3-(4-Hydroxy-3,5-diiodophenyl)-2-phenylpropionic acid	3401	6-Methoxy-2-(2,4-dimethoxybenzylidene)-	
2'-Hydroxy-2,3-dimethoxy-3',5'-dimethylchalcone	3772	3(2H)-benzofuranone	3694
2'-Hydroxy-2,5-dimethoxy-3',5'-dimethylchalcone	3773	4'-Methoxy-1',6'-dimethyl-2'-acetophenone	3455
2'-Hydroxy-3,4-dimethoxy-3',5'-dimethylchalcone	3774	7-Methoxy-3,9-dimethylnaphtho[1,2-b]thiophene	3429
i-(2-Hydroxy-3,5-dimethylphenyl)-1-(4-phenoxyphenyl)-		5-Methoxy-4,7-dimethyl-1,2,3,4-tetrahydro-1-naphthalenone	
2,5-pentadien-1-one	3929	2,4-dinitrophenylhydrazine	3768
i-(2-Hydroxy-3,5-dimethylphenyl)-1-phenyl-2,4-pentadien-		6-Methoxy-2-(4-methoxybenzylidene)-3(2H)-benzofuranone	3611
1-one	3758	2-(2-Methoxy-4-methylphenoxy)-1-(3,4-dimethoxyphenyl)-	
1-Hydroxy-3,3-diphenylpropionic acid	3437	propan-1-ol	3779
2-(1-Hydroxyethyl)-6-methyl-4-phenyl-3-quinolinecarboxylic		1-(2-Methoxy-5-methylphenyl)-3-phenylthiourea	3445
acid lactone	3750	2'-Methoxy-5'-methylpropionophenone	
5-Hydroxy-2-(4-hydroxyphenyl)-7-methoxy-4-chromanone	3536	2,4-dinitrophenylhydrazine	3638
2-Hydroxy-4-methoxybenzophenone	3262	4-Methoxy-2'-nitrochalcone	3524
2'-Hydroxy-4-methoxy-3',5'-dimethylchalcone	3704	4-(4-Methoxyphenoxy)phenyl isothiocyanate	3244
2-(3-Hydroxy-4-methoxyphenyl)-1,3-benzothiazin-4(3H)-one	3414	2-(4-Methoxyphenyl)-1,3-benzothiazin-4(3H)-one 1,1-dioxide	3420
2-(4-Hydroxy-3-methoxyphenyl)-1,3-benzothiazin-4(3H)-one	3415	alpha-(4-Methoxyphenyl)benzyl alcohol	3291
2-(3-Hydroxy-4-methoxyphenyl)-1,3-benzothiazole	3242	2-(4-Methoxyphenyl)-4H-chromen-4-one	3508
3-(3-Hydroxy-4-methoxyphenyl)-3,4-dihydroisocoumarin	3535	7-Methoxy-2-phenyl-4H-chromen-4-one	3509
3-(3-Hydroxy-4-methoxyphenyl)-1-(2-hydroxyphenyl)-		7-Methoxy-3-phenyl-4H-chromen-4-one	3510
1-propanone	3551	3-(4-Methoxyphenyl)-3,4-dihydroisocoumarin	3533
2-(3-Hydroxy-4-methoxyphenyl)-3-methyl-1,3-benzothiazin-		2-Methoxyphenyl 3,5-dinitrobenzoate	3233
4(3H)-one	3541	2-(4-Methoxyphenyl)-3-methyl-1,3-benzothiazin-4(3H)-one	3540
1-(3-Hydroxy-4-methoxyphenyl)-2-phenylethanone	3438	2-(4-Methoxyphenyl)-3-methyl-1,3-benzothiazin-4(3H)-one	
2-(1-Hydroxy-1-methylethyl)-6-methoxy-8-methyl-		1,1-dioxide	3543
1,2,3,4-tetrahydronaphthalene	3466	3-(4-Methoxyphenyl)-2-methyl-1-isoquinolone	3619
1-(2-Hydroxymethyl)phenyl-1-phenylethanol	3453	1-(4-Methoxyphenyl)-3-phenylthiourea	3280
3-(4-Hydroxy-3-nitrophenyl)-3,4-dihydroisocoumarin	3393	6-Methoxy-2-(2,3,4-trimethoxybenzylidene)-3(2H)-	
12-Hydroxyoctadecanoic acid	3734	benzofuranone	3759

Chart 2. The Molecular Formula Index

name	No.	name	No.
C_5H_9NO		$C_5H_{11}N$	
Butyl isocyanate	555	Piperidine	601
tert-Butyl isocyanate	556	$C_5H_{11}NO$	
N,N-Dimethylacrylamide	557	N,N-Diethylformamide	602
3-Ethoxypropionitrile	558	2,2-Dimethylpropionamide	603
2-Ethyl-4,5-dihydrooxazole	559	N,N-Dimethylpropionamide	604
1-Methyl-2-pyrrolidinone	560	N-Ethylpropionamide	605
$C_5H_9NO_2$		N-Methylmorpholine	606
L-Proline	561	Valeramide	607
$C_5H_9NO_3$		$C_5H_{11}NO_2$	
5-Amino-4-oxopentanoic acid hydrochloride	562	Betaine	608
$C_5H_9NO_3S$		Butyl carbamate	609
N-Acetyl-L-cysteine	563	N,N-Dimethylglycine methyl ester	610
C_5H_9NS		3-Hydroxy-3-methyl-2-butanone oxime	611
Butyl isothiocyanate	564	Methyl 2-aminobutyrate hydrochloride	612
$C_5H_9N_3O_2S_2$		$C_5H_{11}NO_3$	
1-Methoxycarbonyl-3-[(methylthio)thiocarbonyl]guanidine	565	Amyl nitrate	613
C_5H_{10}		$C_5H_{11}NO_4S$	
Cyclopentane	566	2-Amino-4-(Methylsulfonyl)butyric acid	614
2-Methyl-1-butene	567	$C_5H_{11}O_5P$	
2-Methyl-2-butene	568	Methyl (Dimethoxyphosphoryl)acetate	615
$C_5H_{10}Br_2$		C_5H_{12}	
1,4-Dibromopentane	569	2-Methylbutane	616
1,5-Dibromopentane	570	$C_5H_{12}ClN$	
$C_5H_{10}Cl_2$		3-(Dimethylamino)propylchloride hydrochloride	617
1,5-Dichloropentane	571	$C_5H_{12}N_2$	
$C_5H_{10}N_2$		2-Methylpiperazine	618
3-(Dimethylamino)propionitrile	572	$C_5H_{12}N_2O$	
$C_5H_{10}N_2O$		tert-Butylurea	619
1,3-Dimethyl-2-imidazolidone	573	Tetramethylurea	620
1-Piperazinecarbaldehyde	574	$C_5H_{12}N_2O_2$	
$C_5H_{10}O$		tert-Butyl carbazate	621
Cyclopentanol	575	L-Ornithine dihydrochloride	622
3-Methyl-2-butanone	576	$C_5H_{12}N_2S$	
2-Methyl-3-buten-2-ol	577	1,3-Diethylthiourea	623
2-Methyltetrahydrofuran	578	Tetramethylthiourea	624
3-Pentanone	579	$C_5H_{12}O$	
Tetrahydropyran	580	Butyl methyl ether	625
$C_5H_{10}O_2$		Ethyl propyl ether	626
2,2-Dimethyl-1,3-dioxolane	581	2-Methyl-2-butanol	627
3-Hydroxy-3-methyl-2-butanone	582	3-Methyl-2-butanol	628
Isobutyl formate	583	1-Pentanol	629
Isopropyl acetate	584	2-Pentanol	630
DL-2-Methylbutyric acid	585	3-Pentanol	631
Pivalic acid	586	$C_5H_{12}O_2$	
Propyl acetate	587	Diethoxymethane	632
Tetrahydrofurfuryl alcohol	588	2,2-Dimethoxypropane	633
Valeric acid	589	2,2-Dimethyl-1,3-propanediol	634
$C_5H_{10}O_3$		2-Isopropoxyethanol	635
3-Ethoxypropionic acid	590	1-Methoxy-2-butanol	636
Ethyl L-lactate	591	3-Methoxy-1-butanol	637
2-Methoxyethyl acetate	592	1,5-Pentanediol	638
$C_5H_{10}O_4$		$C_5H_{12}O_3$	
2,2-Bis(hydroxymethyl)propionic acid	593	2,2-Bis(hydroxymethyl)propan-1-ol	639
Methyl dimethoxyacetate	594	3,6-Dioxahexan-1-ol	640
$C_5H_{10}S$		Trimethyl orthoacetate	641
2-Methyltetrahydrothiophene	595	$C_5H_{12}O_4$	
$C_5H_{11}Br$		Pentaerythritol	642
1-Bromopentane	596	$C_5H_{12}O_5$	
$C_5H_{11}Cl$		Xylitol	643
1-Chloro-2,2-dimethylpropane	597	$C_5H_{12}S$	
1-Chloropentane	598	Ethyl propyl sulfide	644
$C_5H_{11}ClO_2$		1-Pentanethiol	645
3-Chloro-1,1-dimethoxypropane	599	$C_5H_{13}ClNa_2O_4P$	
$C_5H_{11}I$		Choline chloride O-(disodium phosphate)	646
1-Iodopentane	600	$C_5H_{13}N$	

Chart 3-1. The Code Table of Substructure Notation

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

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

Chart 3-2. The Substructure Index

substructure	chemical shift	No.	substructure	chemical shift	No.
CH=CH=C(O), N=C=	7.43	254	AH/AH(AH), AH(AH)	7.31	778
CH=CH=NH, N=CH=	7.15	120	AH/AH(AH), AH(AH)	7.32	490
CH=CH=NH, N=C=	6.98	283	AH/AH(AH), AH(AH)	7.63	797
CH=CH=NH, N=C=	7.01	525	AH/AH(AH), AH(AH)	7.69	487
CH=CH=N, N=CH=	6.88	282	AH/AH(AH), AH(AH)	ca. 7.77	786
CH=CH=N, N=CH=	6.93	524	AH/AH(AH), AH(AH)	7.85	795
CH=CH=N, N=CH=	7.05	524	AH/AH(AH), AH(A)	6.49	758
CH=CH=N, N=CH=	7.12	502	AH/AH(AH), AH(A)	6.77	774
CH=CH=N, N=CH=	7.12	501	AH/AH(AH), AH(A)	6.80- 7.22	723
CH=CH=N, N=CH=	7.20	501	AH/AH(AH), AH(A)	6.87- 7.37	712
CH=CH=N, N=C=	6.84	522	AH/AH(AH), AH(A)	6.92	726
CH=CH=S, N=C=	6.52	123	AH/AH(AH), AH(A)	7.00	781
CH=CH=CH=O, O(CH=)	7.48	258	AH/AH(AH), AH(A)	7.00- 7.30	773
CH=CH=CH=O, O(C=)	7.27	506	AH/AH(AH), AH(A)	7.14	707
CH=CH=CH=O, O(C=)	7.71	479	AH/AH(AH), AH(A)	7.15	711
CH=CH=CH=O, O(C=)	7.94	482	AH/AH(AH), AH(A)	7.20	737
CH=CH=CH=O, O(N=)	8.51	102	AH/AH(AH), AH(A)	7.22	774
CH=CH=CH=O, S(C=)	7.08	512	AH/AH(AH), AH(A)	7.28	726
CH=CH=CH=O, S(C=)	7.10	242	AH/AH(AH), AH(A)	7.29	707
CH=CH=CH=O, S(C=)	7.67	480	AH/AH(AH), AH(A)	7.29	753
CH=CH=CH=O, S(C=)	7.91	241	AH/AH(AH), AH(A)	7.30- 7.63	729
CH=CH=C=O, S(CH=)	ca. 7.26	240	AH/AH(AH), AH(A)	7.31	778
CH=CH=C=O, S(C=)	7.28	232	AH/AH(AH), AH(A)	7.33	781
CH=CH=N=O, S(C=)	7.09	123	AH/AH(AH), AH(A)	7.35	758
CH=C=CH3, NH, C=CH3, N=	5.82	523	AH/AH(AH), AH(A)	7.38- 7.70	473
CH=C=CH3, O, C=NH2, N=	5.56	287	AH/AH(AH), AH(A)	7.40	495
CH=C=CH=O, N=, C=C=O, BR	7.79	669	AH/AH(AH), AH(A)	7.52	753
CH=C=CH=O, N=, C=C=O, BR	8.28	669	AH/AH(AH), AH(A)	7.63	797
CH=C=C=O, BR, C=S, BR	6.92	230	AH/AH(AH), AH(A)	ca. 7.66	786
CH=C=C=CH3, C=O, C=O(OH)	6.00	509	AH/AH(AH), AH(A)	7.68	476
CH=C=C=CH3, NH, C=O(NH)	5.69	504	AH/AH(AH), AH(A)	7.70- 8.00	733
CH=C=C=CH2, NH, C=O(NH)	5.67	485	AH/AH(AH), AH(A)	7.72	795
CH=C=C=C(OH), C=O(CH3)	5.95	486	AH/AH(AH), AH(A)	7.88	761
CH=C=C=C(OH), C=O(C=)	5.85	771	AH/AH(AH), AH(A)	7.88	756
CH=C=C=C(O, CL), C=O(CH=)	7.04	673	AH/AH(AH), AH(N*)	6.60	495
CH=C=C=C(O, CL), C=O(C=)	7.17	672	AH/AH(AH), AH(N*)	7.21	476
CH=C=C=C(O, BR), C=O(O)	7.20	229	AH/AH(AH), AH(N*)	7.28	473
CH=C=C=CH3, N=, NH(CH=)	6.78	284	AH/AH(AH), AH(N*)	7.29	487
CH=C=C=C(O, F), NH(C=O)	7.76	243	AH/AH(AH), AH(N*)	7.32	490
CH=C=C=N, NO2, N=C=	7.92	517	AH/AH(AH), AH(N*)	7.54	250
CH=C=C=NO2, S, N=C=	8.26	107	AH/AH(AH), AH(N*)	7.58	761
CH=C=C=CH=O, C=O, C=O	8.38	772	AH/AH(A), AH(A)	6.60	791
CH=C=C=CH=O, BR, S(CH=)	ca. 7.26	240	AH/AH(A), AH(A)	6.70	721
CH=C=C=O(NH), N=NH	7.46	106	AH/AH(A), AH(A)	6.78- 7.44	724
CH=NH(CH=), N=CH=	7.73	120	AH/AH(A), AH(A)	6.81	744
CH=NH(CH=), N=C=	7.57	284	AH/AH(A), AH(A)	6.88- 7.17	741
CH=NH(A), N=A	8.72	469	AH/AH(A), AH(A)	6.90	690
CH=NH(A), N=A	8.78	469	AH/AH(A), AH(A)	6.94	788
CH=NH(N=), N=C=	7.48	51	AH/AH(A), AH(A)	7.00- 7.50	683
CH=N(CH3, CH=), N=CH=	7.42	282	AH/AH(A), AH(A)	7.02	727
CH=N(CH2, CH=), N=CH=	7.49	524	AH/AH(A), AH(A)	7.07	682
CH=N(CH=, CH=), N=CH=	7.68	501	AH/AH(A), AH(A)	7.08	775
CH=N(CH=, C=O), N=CH=	8.17	502	AH/AH(A), AH(A)	7.10	719
CH(E)/CH3, CH=E(CH2)	5.68	361	AH/AH(A), AH(A)	7.13	708
CH(E)/CH3, CH=E(C=O)	7.10	296	AH/AH(A), AH(A)	7.13	799
CH(E)/CH2(OH), CH=E(CH3)	5.68	361	AH/AH(A), AH(A)	7.13	697
CH(E)/CH2(OH), CH=E(C=O)	7.07	539	AH/AH(A), AH(A)	7.18	768
CH(E)/CH2(CL), CH=E(CH2)	5.95	278	AH/AH(A), AH(A)	7.20	782
CH(E)/CH2(BR), CH=E(CH2)	5.99	274	AH/AH(A), AH(A)	7.25	738
CH(E)/CH=E(C#), C#(N)	6.31	235	AH/AH(A), AH(A)	7.30	754
CH(E)/CH=E(CH3), C=O(OH)	5.85	296	AH/AH(A), AH(A)	7.40	691
CH(E)/CH=E(CH2), C=O(O)	6.12	539	AH/AH(A), AH(A)	7.45	467
CH(E)/CH=E(C=O), C=O(O)	6.55	236	AH/AH(A), AH(A)	7.52	730
CH(E)/CH=E(CL), CL	6.37	25	AH/AH(A), AH(A)	7.58	751
CH(Z)/CH=Z(C=O), C=O(O)	6.02	237	AH/AH(A), AH(A)	7.85	764
CH(Z)/CH=Z(CL), CL	6.45	26	AH/AH(A), AH(A)	7.91	734
#CH/C#(CH2)	2.06	290	AH/AH(A), AH(N*)	6.08	492
#CH/C#(CH2)	2.33	529	AH/AH(A), AH(N*)	7.08	496
#CH/C#(CH2)	2.50	124	AH/AH(A), AH(N*)	7.19	488
#CH/C#(CH2)	2.52	98	AH/AH(A), AH(N*)	7.20	474
#CH/C#(CH2)	2.53	99	AH/AH(A), AH(N*)	7.22	494
#CH/C#(CH)	2.47	528	AH/AH(A), AH(N*)	7.27	477
#CH/C#(C)	2.42	527	AH/AH(A), AH(N*)	7.48	763
#CH/C#(C=O)	2.88	507	AH/AH(A), AH(S)	6.97	239
#CH/C#(C=O)	3.05	97	AH/AH(N*), AH(N*)	6.60	271
AH/AH(AH), AH(AH)	7.00- 7.30	773	AH/AH(N*), AH(N*)	6.83	253

Chart 4. The Chemical Shift Index

chemical shift	substructure	No.	chemical shift	substructure	No.
ca. 5.87	NH/CH ₃ , C=O(CH ₂)	401	6.44	AH/AH(N*), A(AH, NH ₂)	484
5.87	OH/A(A, A)	687	6.45	CH ₂ =/CH=C=O	533
5.90	CH/CH ₃ , CL, CL	47	6.45	CH=(Z)/CH=(Z)(CL), CL	26
5.90	CH ₂ =/C=CH ₂ , C=O	510	6.47	AH/AH(AH), A(NH ₂ , N*)	495
5.90	CH=/CH ₂ (O), CH=(CH ₂)	291	6.49	CH=/CH ₂ =, O(CH ₂)	322
5.90	OH/A(A, A)	721	6.49	AH/AH(AH), AH(A)	758
5.92	CH=/CH ₂ (O), CH ₂ =	292	6.50	AH/AH(A), A(AH, NH ₂)	792
5.93	CH ₂ =/CH=C=O	508	6.50	NH ₂ /C=O(C=O)	341
5.93	CH=/CH(CH ₃ , OH), CH ₂ =	362	6.50-9.00	OH/A(AH, A)	767
5.93	CH=/CH(CH ₃ , CL), CH ₂ =	318	6.51	CH/C(C, CL, CL), CL, CL	91
5.94	CH=/CH ₂ (O), CH ₂ =	531	6.52	CH=/CH=(S), N=C=	123
5.94	NH/C=O(O), NH ₂	621	6.52	AH/AH(A), A(NH ₂ , N*)	494
5.95	CH=/CH=(CH=), C=(CH ₃ , O)	506	6.53	AH/AH(N*), A(AH, NH ₂)	497
5.95	CH=/C=C(OH), C=O(CH ₃)	486	6.53	OH/A(A, A)	696
5.95	CH=(E)/CH ₂ (CL), CH=(E)(CH ₂)	278	6.55	CH ₂ =/CH=C=O	508
5.96	CH=/CH ₂ (NH ₂), CH ₂ =	190	6.55	CH=(E)/CH=(E)(C=O), C=O(O)	236
5.96	CH=/CH ₂ (CL), CH ₂ =	134	6.55	AH/A(AH, NH ₂), A(N*, CL)	484
5.97	AH/AH(A), A(AH, O)	759	6.56	AH/A(AH, NH ₂), A(AH, CL)	793
5.98	CH/CH(CL, CL), CL, CL	31	6.58	AH/AH(AH), A(AH, OH)	799
5.98	CH/C=O(O), CL, CL	116	6.58	AH/AH(AH), A(AH, F)	799
5.98	CH=/CH=(N=), C=(CH ₃ , O)	266	6.60	AH/AH(AH), AH(N*)	495
5.99	CH=(E)/CH ₂ (BR), CH=(E)(CH ₂)	274	6.60	AH/AH(A), AH(A)	791
ca. 5.99	NH/CH ₃ , C=O(CH ₃)	193	6.60	AH/AH(N*), AH(N*)	271
6.00	CH=/CH ₂ (OH), CH ₂ =	169	6.60	AH/A(AH, NH ₂), A(A, CL)	794
6.00	CH=/C=CH ₃ , C=O, C=O(OH)	509	6.62	CH=/CH ₂ =, C=O(N)	557
6.00-9.90	OH/C=O(CH ₂)	309	6.62	CH=/CH ₂ =, N(CH ₃ , CH ₃)	395
6.00-9.90	OH/C=O(CH)	309	6.63	CH=/CH=C=, CH=O	479
6.01	CH=/C(CH ₃ , CH ₃ , OH), CH ₂ =	577	6.63	AH/AH(AH), A(A, NH ₂)	788
6.02	CH/C=O(OH), CL, CL	28	6.64	AH/AH(A), A(A, NH ₂)	748
6.02	CH=/CH ₂ (BR), CH ₂ =	128	6.65	CH ₂ =/CH=C=O	100
6.02	CH=(Z)/CH=(Z)(C=O), C=O(O)	237	6.65	AH/AH(A), A(A, NH ₂)	777
6.06	CH/C(O, F, F), F, CL	110	6.65	AH/A(AH, OH), A(AH, F)	799
6.07	CH/C=O(O), CL, CL	19	6.68	CH=/CH=C=, CH=O	482
6.07	CH=/CH=(NH), C=(CH ₃ , N=)	285	6.68	AH/AH(AH), A(AH, OH)	799
6.08	CH/CH(BR, BR), BR, BR	23	6.68	AH/AH(AH), A(AH, F)	799
6.08	CH/C=O(NH ₂), BR, BR	34	6.68	AH/AH(A), A(AH, CL)	790
6.08	AH/AH(A), AH(N*)	492	6.70	AH/AH(A), AH(A)	721
6.09	CH=/CH ₂ (SO ₂), CH=(CH ₂)	302	6.70	AH/AH(A), A(A, NH ₂)	789
6.09	NH ₂ /A(AH, A)	779	6.71	AH/A(A, OH), A(A, OH)	747
ca. 6.10	NH ₂ /C=O(C=)	335	6.73	CH=/CH=C=O, C=O(NH)	245
6.11	CH ₂ =/CH=C#	101	6.73	AH/AH(AH), A(A, OH)	492
6.12	CH=(E)/CH=(E)(CH ₂), C=O(O)	539	6.73	AH/AH(A), A(AH, OH)	776
6.13	CH/C(CL, CL, CL), CL, CL	21	6.73	AH/AH(AH, CL), A(AH, CL)	793
6.13	CH/C=O(CL), CL, CL	20	6.74	AH/AH(A), A(AH, OH)	784
6.13	CH=/CH ₂ =, C=O(O)	533	6.75-7.11	AH/AH(A), A(AH, NH ₂)	798
6.15	CH ₂ =/C=C#(CL)	93	6.75-7.11	AH/AH(A), A(A, F)	798
6.15	CH=/CH ₂ =, C=O(O)	299	6.77	AH/AH(AH), AH(A)	774
6.15	NH/CH ₂ (CH ₃), C=(NH, =S)	623	6.77	AH/AH(AH), A(AH, OH)	782
6.17	CH/CH(CH ₂ , CL), CL, CL	118	6.77	AH/AH(A), A(AH, F)	800
6.17	NH ₂ /C=O(NH)	413	6.77	AH/A(AH, OH), A(AH, CL)	745
6.20	CH ₂ =/CH=C=O	100	6.77	AH/A(AH, CL), A(A, NH ₂)	790
6.22	AH/AH(N*), A(AH, OH)	489	6.78	CH=/CH=(CH=), C=(CH ₃ , S)	512
6.24	CH ₂ =/C=C#(CL)	93	6.78	CH=/C=CH ₃ , N=, NH(CH=)	284
6.24	OH/A(AH, A)	731	6.78	AH/AH(AH), A(AH, BR)	775
ca. 6.25	CH=/CH ₂ =, C=O(O)	508	6.78	AH/AH(A), A(AH, OH)	783
6.25	CH=/CH=C=, CH=O	506	6.78	AH/A(AH, NH ₂), A(A, CL)	792
6.26	CH/C(CH, CL, CL), CL, CL	94	6.78	NH ₂ /SO ₂ (CH ₃)	16
6.27	CH ₂ =/CH=C#(CL)	101	6.78-7.44	AH/AH(A), AH(A)	724
6.27	CH ₂ =/C=CH ₃ , C=O	298	6.78-7.44	AH/AH(AH), A(AH, F)	724
6.29	CH ₂ =/CH=N	395	6.78-7.44	AH/AH(AH), A(AH, CL)	724
6.29	NH ₂ /C=(N=, S)	166	6.78-7.44	AH/A(AH, F), A(AH, CL)	724
6.30	CH ₂ =/CH=C=O	557	6.79	AH/AH(A), A(A, NH ₂)	779
6.31	CH=(E)/CH=(E)(C#), C#(N)	235	6.80	AH/AH(AH), A(A, O)	758
6.32	AH/AH(AH), A(A, CL)	781	6.80	AH/AH(A), A(A, OH)	785
6.35	CH=/CH=(NH), CH=(N=)	121	6.80	AH/A(AH, CL), A(A, OH)	785
6.35	CH=/CH=C=, C=O(O)	772	6.80	AH/A(A, NH ₂), A(A, CL)	739
6.35	NH/CH ₃ , C=(NH, =S)	206	6.80-7.22	AH/AH(AH), AH(A)	723
6.37	CH=/CH ₂ =, C=O(CL)	100	6.81	AH/AH(A), AH(A)	744
6.37	CH=(E)/CH=(E)(CL), CL	25	6.82	AH/AH(AH), A(A, CL)	788
6.39	CH ₂ =/CH=C=O	299	6.82	AH/A(A, NH ₂), A(A, CL)	796
6.39	CH ₂ =/C=CH ₂ , C=O	510	6.82	AH/A(A, O), A(A, CL)	677
6.40	CH=/CH=(N=), CH=O	102	6.83	AH/AH(N*), AH(N*)	253
6.40	NH/C=O(O), NH ₂	205	6.83	AH/AH(AH), A(AH, OH)	491
6.41	CH=/CH=(CH=), CH=O	258	6.84	CH=/CH=(N=), N(CH ₃ , C=)	522
6.42	CH/C=O(NH ₂), CL, CL	36	6.84	CH=/CH=(N), N=C=	522
6.44	AH/AH(A), A(NH ₂ , N*)	483	6.85	AH/AH(AH), N*(A)	492

Chart 5. Code Table of Sample Suppliers

Code	Name	Appliation	Code	Name	Appliation
AB01	Abe, Nobuo	Akita University	MO02		Fujisawa Pharmaceutical Co., Ltd.
AB02	Abe, Yoshio	Keio University	MO03	Morita Yasuo	Tohoku Pharmaceutical College
AD01	Adachi, Kazuo	Osaka Institute of Technology	NA01	Nakasuga, Noriyuki	Nagoya University
AL		Aldrich Chemical Co.	NA02	Nakagawa, Shigeki	Nippon University
AN01	Ando, Masayoshi	Tohoku University	NA03	Hoshino, Masamatsu	Saitama University
AR01	Arai, Mannosuke	Tohoku University	NI01	Nishimura, Jun	Kyoto University of Industrial Art and Textile
AS01	Asao, Toyonobu	Tohoku University	NI02	Nishiyama, Shigeru	Keio University
FU01		Kao Corporation	NO01	Nonaka, Tsutomu	Tokyo Institute of Technology
FU02	Fujise, Yutaka	Tohoku University	NU01		Numazu College of Technology
GO01	Goromaru, Tsuyoshi	The University of Tokushima	OG01	Ogino, Hiroshi	Tohoku University
HA01	Hamada, Yoshiki	Meijo University	OJ01	Ojima, Juro	Toyama University
HA02	Hamada, Keinosuke	Nagasaki University	OO01	Osawa, Keisuke	Tohoku Pharmaceutical College
HA03	Harada, Nobuyuki	Tohoku University	OO02	Onuma, Hiroshi	Akita University
HA04	Hagiwara, Hisahiro	Tohoku University	OO03	Omura, Satoshi	Kitasato University
HI01	Hirose, Yoshiyuki	Science University of Tokyo	OZ01	Ozawa, Fumiyuki	Tokyo Institute of Technology
HI02	Hirota, Hiroshi	The University of Tokyo	SA01	Sato, Gen	Sophia University
HO01	Horiike, Michio	Kochi University	SA02		Fuji Photo Film Co., Ltd.
II01	Iino, Masashi	Tohoku University	SA03	Sato, Masaru	Saitama University
IK01	Ikeda, Masazumi	Osaka University	SA04		Konishiroku Photo Ind. Co., Ltd.
IK02	Ikariya, Takao	The University of Tokyo	SA05	Minabe, Masahiro	Utsunomiya University
IS01	Ishida, Shin-ichiro	Kanazawa University	SE01	Senda, Yasuhisa	Tohoku University
IS02	Ishikawa, Yukihiro	Tottori University	SI01	Shibata, Hisao	Shinshu University
IT01	Ito, Keiji	Toyohashi University of Technology	SU01	Suzuki, Minoru	Hokkaido University
IT02	Ito, Takashi	Yokohama National University	SU02	Suzuki, Toshio	Akita University
KA		Kanto Chemical Co., Inc.	SU03	Suzuki, Kanji	Tokyo Institute of Technology
KA01	Kan, Takayuki	Hiroshima University	TA01	Takatori, Masayuki	Fukushima University
KA02	Kasahara, Akira	Yamagata University	TA02	Tabei, Katsumi	Tokyo College of Pharmacy
KA03	Kakei, 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	TO		Tokyo Kasei Kogyo Co., Ltd.
KA06		Konishiroku Photo Ind. Co., Ltd.	TS01		Sumitomo Bakelite Co., Ltd.
KA07	Kato, Norimoto	Tohoku University	TS02	Tsunetsugu, Josuke	Saitama University
KI01	Kimura, Yoshiharu	Kyoto University of Industrial Art and Textile	UE01	Uehara, Tadao	Tohoku University
KI02	Kido, Hideo	Tohoku 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	YO01		Maruzen Petrochemical Co., Ltd.
MA02	Machida, Katsunosuke	Kyoto University	YO02		The Green Cross Corporation
MA03	Maruyama, Masao	Miyagi University of Education			
MA04	Matsueda, Sumu	Hirosaki University			
MA05	Maruyama, Kazuhiro	Kyoto University			
MO01	Mochida, Kunio	Gakushuin University			

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