

Instruction to search natural compounds on CH-NMR-NP

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* Mozilla Firefox or Apple Safari are recommended to use for 'CH-NMR-NP' as operation checked web browser.

Compound Search

Here is the initial page for database search.

Natural Product NMR-DB "CH-NMR-NP"

Introduction to CH-NMR-NP system

The $^{13}\text{C}/^1\text{H}$ -NMR database for natural products [CH-NMR-NP] is mainly composed of natural products that were published in major journals in the years between 2000 and the spring of 2014. For a natural product to be included in the database, complete ^{13}C -NMR data was a strict precondition. No such precondition was set for ^1H and as a result some compounds show incomplete ^1H -NMR data. As it concerns a database, CH-NMR-NP lacks completeness. The number of the compounds in natural products compiled from the published papers is about 29,500. Additionally, about 6,000 organic compounds with $^1\text{H}/^{13}\text{C}$ spectral patterns were compiled from SDBS-NMR, and the total number of the compounds is approximately 35,500.

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[Introduction](#) [Instruction \(PDF\)](#) [Inquiry Form](#)

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NMR Database Search

Basic Information

Name
Example: Pseudoenchynazine / Pseudo*zine*

Atoms C H N O
Example: C21-23 H18 N4 O5

Molecular Formula
Example: C15H18BrS2

Molecular Weight
Example: 545 / 545 - 558

^{13}C Chemical Shift \pm Allowance / ppm \pm
Example: 40, 41, 71 \pm 2 Similarity \geq %

^{13}C No Signal Region to ppm
Example: 40 to 41 ppm

Structure Search To search a partial structure, please check the box and draw a partial structure on the molecular editor at the bottom of the page. Please see page 6 in [the instruction manual](#) if the structure search doesn't work well.

NP No.
Example: 15 / 30 - 100

CAS Registry No.
Example: 59392-53-9 / 5932-*

Sort Ascending Descending

Enable Detailed Search

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The Name (compound name), Atoms and Molecular Formula, Molecular Weight, ^{13}C Chemical Shift, ^1H Chemical Shift, No Signal Region, Partial Structure, classification number (NP No.) can be used as query items. Each item is used as a logical AND operator. ^1H chemical shift search can be used when the Enable Detailed Search check box was clicked.

Name

Name

Pseudo

Example: Pseudoanchynazine / Pseudo*zine*

A compound name is used as a query. The compound name is usually a trivial name, which is described in the original paper, but some of them may be a chemical name (IUPAC Name, etc.). A search word is a partial match retrieval, but '*' or '!' can be used as wildcard character. A '*' matches any number of character, and a '!' matches only one character. When using wildcard character, a search word will be an exact word.

Atoms

Atoms

C 21-23 H N O

Example: C21-23 H18 N4 O5

The number of atoms of carbon, hydrogen, nitrogen and oxygen are used as a query. The other element should be set in the 'Molecular Formula' form. An atom number can be specified as a range. For example, '21-23' at 'C' searches compounds that have carbons from 21 to 23. The '-21' at 'C' searches compounds that have not exceeding 21 carbons. The '23-' at 'C' searches compounds that have more than 23 carbons. The '0' searches compounds that contain none of the specified element.

Molecular Formula

Molecular Formula

C15H18BrS2

Example: C15H18BrS2

A molecular formula is used as a query. It is case insensitive, and an order of elements has no limitation. The range specification cannot be used, but '0' searches compounds that contain none of the specified element. For example, 'C15H18BrS2' and 'BrS2c15h18' find the same compounds.

Molecular Weight

Molecular Weight

545-558

Example: 545 / 545 - 558

A molecular weight is used as a query. The value can be range specified. The value in the database is rounded.

^{13}C Chemical Shift

^{13}C Chemical Shift

± Allowance / ppm

Example: 40, 41, 71 ± 2

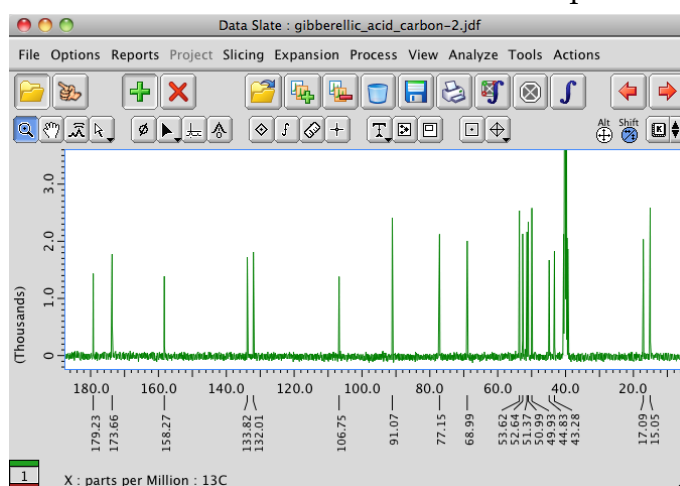
± 2

From File

Similarity ≥ 100 %

A ^{13}C chemical shift (ppm unit) is used as a query. The multiple chemical shifts can be set by comma-delimited format. An allowance is applied to all chemical shifts. All chemical shifts are used as logical AND operators, however, similarity can loosen search condition. For example, 3 chemical shifts with 70% similarity searches compounds have 2 of 3 specified chemical shifts.

The 'From File' button can be used for setting chemical shifts list. The chemical shifts list is automatically set, when a "peak picked carbon spectrum" is specified. A specified file must be a .jdf file (Delta NMR software format). The solvent peak markers are recommended to be eliminated before uploading because database does not include solvent peaks.



<input checked="" type="checkbox"/> ¹³ C Chemical Shift ± Allowance / ppm	<input type="text" value="40"/> ± <input type="text" value="2"/>	<input type="button" value="From File"/>
	Example: 40, 41, 71 ± 2	Similarity ≥ <input type="text" value="80"/> %
	Number of bonded ¹ H atoms : <input type="text" value="3"/>	
	<input checked="" type="checkbox"/> Search bonded ¹ H chemical shift(s)	

<input checked="" type="checkbox"/> ¹ H Chemical Shift ± Allowance / ppm	<input type="text" value="2.6"/> ± <input type="text" value="0.1"/>	<input type="button" value="From File"/>
	Example: 2.6, 3.1 ± 0.1	Similarity ≥ <input type="text" value="100"/> %

When using the 'Enable Detailed Search', the number of bonded ¹H atoms (multiplicity of carbon) can be specified. For example, the '3' should be specified in this field, if the searching ¹³C chemical shift is CH₃. Comma-delimited specification can be used to specify this for multiple carbon signals. When the multiplicities of some carbons are unclear, those carbons should be allocated at the back. For example, if the ¹³C chemical shifts are '40, 41, 71' and these multiplicities are 'CH₃, CH₂, unclear', this field should be '3, 2'. When the 'Search bonded ¹H chemical shift(s)' is on, it searches compounds that have specified ¹³C bonding to specified ¹H. A manner of array in the fields is same as 'number of bonded ¹H atoms', but if ¹H of CH₂ are non-equivalent, two same ¹³C chemical shifts should be specified. For example, to search compounds that have ¹³C at 72 ppm is bonded to ¹H at 3.9 ppm and 4.4 ppm, put '72,72' in ¹³C chemical shift field and '7.9, 4.4' in ¹H chemical shift field. Please note that there are a lot of compounds that have not enough ¹H chemical shift information in the database.

¹³C No Signal Region

<input checked="" type="checkbox"/> ¹³ C No Signal Region	<input type="text" value="150"/> to <input type="text"/>	ppm
	Example: 40 to 41 ppm	

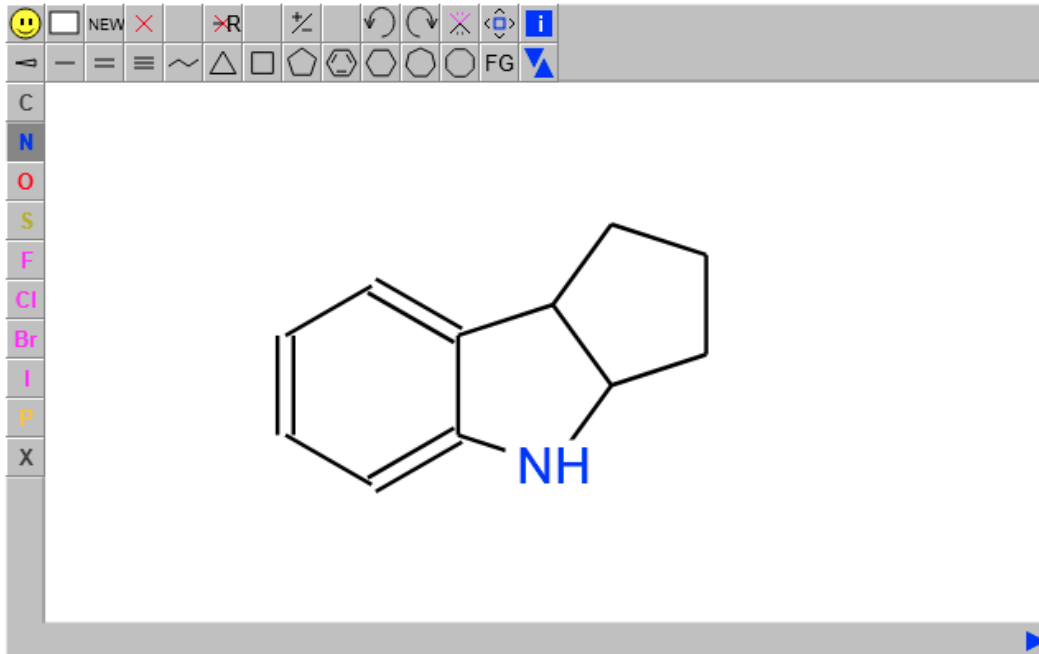
A no signal region of ¹³C chemical shift (ppm unit) is used as a query.

Structure Search

Structure Search

To search a partial structure, please check the box and draw a partial structure on the molecular editor at the bottom of the page. Please see page 6 in [the instruction manual](#) if the structure search doesn't work well.

Structure Information



A partial structure is used as a query. The JavaScript 'JSME Molecular Editor' and 'RDKit cartridge' are used for structure drawing and structure search respectively.

NP No.

NP No.

Example: 15 / 30 - 100

A classification number (NP No.) is used as a query. NP No. can be range specified.

¹H Chemical Shift (w/ Enable Detailed Search)

¹H Chemical Shift ±
± Allowance / ppm Example: 2.6, 3.1 ± 0.1 Similarity ≥ %

A ¹H chemical shift (ppm unit) is used as a query. The multiple chemical shifts can be set by comma-delimited format. An allowance is applied to all chemical shifts. All chemical shifts are used as logical AND operators, however, similarity can loosen search condition. For example, 3 chemical shifts with 70% similarity searches compounds have 2 of 3 specified chemical shifts.

The 'From File' button can be used for setting chemical shifts list. The chemical shifts list is automatically set, when a "peak picked proton spectrum" is specified. A specified file must be a .jdf file (Delta NMR software format).

*Please note that proton *J*-splitting are not considered and there are a lot of compound that have not enough ¹H chemical shift information.

¹H No Signal Region (w/ Enable Detailed Search)

¹H No Signal Region to ppm
Example: 2.6 to 3.1 ppm

A no signal region of ¹H chemical shift (ppm unit) is used as a query.

Sort

Sort ▾
 Ascending
 Descending

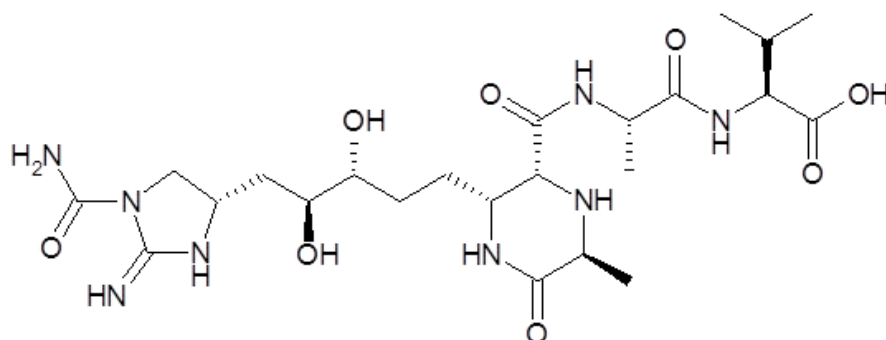
Search result is sorted in descending order of carbon number as a default. The compounds of same carbon number are sorted in descending of number of hydrogen, nitrogen, oxygen, in that order. The NP No., compound name (alphabetical), number of atoms (CHNO), molecular weight, similarity can be used for sorting in ascending or descending order.

Search Result

Search Results

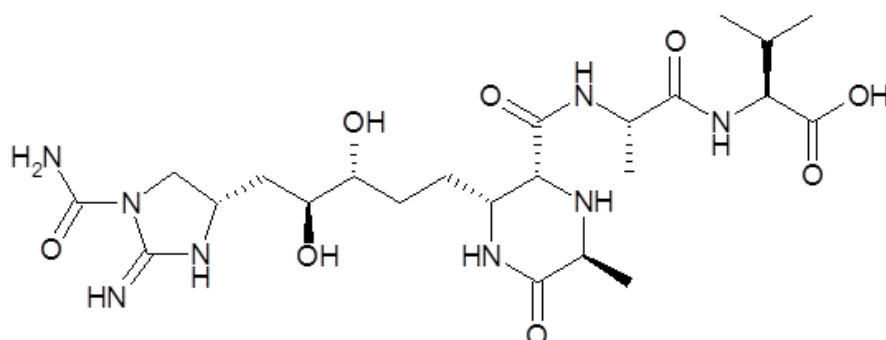
18 Found. [Back to Search](#)

1/18 **guadinomine C1**



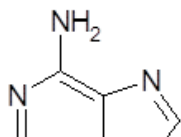
NP No. : 21142, Molecular Formula : $C_{23}H_{40}N_8O_8$, Solvent : D_2O

2/18 **guadinomine C2**



NP No. : 21142, Molecular Formula : $C_{23}H_{40}N_8O_8$, Solvent : D_2O

3/18 **sinefungin VA**

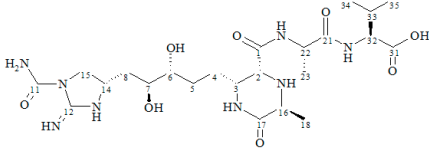


In the search result list, the compound name, structure, NP No., molecular formula, and solvent are displayed for each compounds. When clicking the compound name or structure, detailed data will be displayed on a new window.

Detailed data display

Natural Product NMR-DB "CH-NMR-NP"

Structure



Assignment List

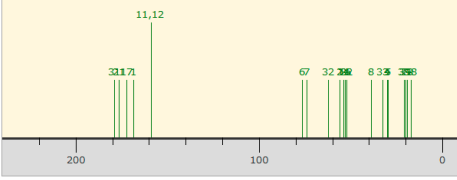
No.	¹³ C Shift /ppm	Carbon Type	¹ H Shift /ppm	¹ H Pattern /Hz
1	168.4	C		
2	56.0	CH	4.43	d 3.4
3	53.8	CH	3.97	m
4	30.3	CH ₂	1.71	m
5	29.6	CH ₂	1.57	m
6	76.7	CH	3.48	m
7	74.1	CH	3.61	m
8	38.8	CH ₂	1.93	ddd 14 5.6 2.1
			1.77	m
11	158.9	C		
12	158.9	C		
14	54.0	CH	4.23	m
15	53.1	CH ₂	4.23	dd 8.4 8.4
			3.79	dd 8.5 5.6
16	53.3	CH	4.17	q 7.0
17	172.1	C		
18	17.0	CH ₃	1.55	d 6.9
21	176.6	C		
22	52.2	CH	4.44	q 7.0
23	19.2	CH ₃	1.39	d 7.0
31	179.0	C		
32	62.4	CH	4.07	d 7.0
33	32.6	CH	2.11	dsep 6.9 6.5
34	20.1	CH ₃	0.92	d 6.9
35	21.1	CH ₃	0.92	d 6.9

Compound Information

Name: guadinomine C1
Molecular Formula: C₂₃H₄₀N₆O₈ Molecular Weight: 556.6
NP No.: 21142 Spectral Key: 21-142
Source: Streptomyces sp. K01-0509
Remarks: fermentation
CAS Registry No.: 1033827-71-2
Solvent: D₂O
¹H Frequency: 600 MHz
Reference: Iwatsuki, M., et al., J. Antibiotics, 61, 230 (2008)
Comments: stereoisomer at C16

Show ¹³C NMR Spectrum

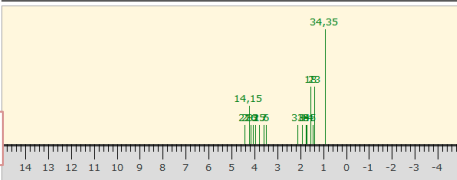
¹³C NMR Spectrum



View Range: 240 to -10 ppm

C CH CH₂ CH₃ APT Show ¹H NMR Shifts

¹H NMR Shifts



View Range: 15 to -5 ppm

1 2 3 ... 10 ... 18

Print Layout

Print Layout display

In a detailed data page, a chemical structure (w/ assignment number), compound information, an assignment List and a ¹³C NMR spectrum are shown as a default. The paging buttons (it follows sorting in search results) located at the page bottom.

- **Chemical Structure**

a chemical structure is corresponding to the original paper. All carbons are numbered for spectrum assignment. Abbreviated partial structure e.g. Acetyl, Benzyl, Glu are transcribed into full structure. The carbon number is corresponding to the original paper, but non-number e.g. alpha, beta, 1', 1'', etc. were replaced into numeric character. A duplicative number is not used for one-to-one assignment to chemical shifts. The equivalent carbons are not numbered.

- **Compound Information**

- **Name** (trivial name or chemical name in the original paper)
Special character including Greek alphabet are replaced into alphameric character. Superscript, subscript, arrows are also replaced. A long authoritative chemical name might be described if it is only written in the paper.
- **Molecular Formula**
Molecular formula formed based on the chemical structure.
- **Molecular Weight**
Molecular formula weight based on the chemical structure. The value after the decimal point might be different from original paper. This is explained as resulting from diverseness of natural abundance at production area.
- **NP No.**
A classification number for each compound.
- **Spectral Key**
Corresponding to spectrum (¹³C NMR and ¹H NMR)
- **Source**
The feed material for the extraction of natural product. Described as an academic name in usual case.
- **Remarks**
A brief comment (plant, fish, shellfish, fungus, etc.) about extraction feed.

- **Characteristic**
The characterization described by author of original paper.
 - **Chemical Name**
An authoritative chemical name as represented by IUPAC name if it is described in the original paper.
 - **CAS Registry No.**
 - **Solvent**
The solvent for NMR experiment, and measurement condition (temperature, pH, etc.) are described. The most of them are 25-35 °C is assumed if temperature is not specified.
 - **¹H Frequency**
An observing frequency of the ¹H NMR (magnetic field of NMR machine). The maximum frequency in the experimental section is used if it is not described for individual data.
 - **Shift Ref.**
A chemical shift reference of NMR spectra. For example, in case of CDCl₃, the description '7.25 / 77.0' means that ¹H signal of residual CHCl₃ was set to 7.25 ppm and ¹³C signal of CDCl₃ was set to 77.0 ppm as according to the paper.
 - **Reference**
An original paper of corresponding data. It is described with first author only. The URL link target is a result of google scholar search.
In case of the 6,000 compounds from SDBS-NMR, reference shows SDBS registry number.
 - **Comments**
A comment by database editor.
- **Assignment List**
Numbering of each ¹³C, chemical shift of ¹³C, carbon type (CH₃, CH₂, CH, C), chemical shift of bonded ¹H, comment including *J* coupling pattern of ¹H and *J* value etc. are described. When using ¹³C Chemical shift query at the compound search, matched ¹³C were highlighted. ¹H chemical shift

on the row without ^{13}C number shows 2nd chemical shift of non-equivalent ^1H or OH/NH. In case of OH/NH, it is specified in comment field.

- **Show ^{13}C NMR Spectrum** (checkbox)

The ON shows ^{13}C NMR spectrum, and OFF hides it. Show/Hide state is reflected on the print layout page.

- **^{13}C NMR Spectrum**

The virtual ^{13}C NMR spectrum with assignment carbon number is shown. When using ^{13}C Chemical shift query at the compound search, matched ^{13}C were highlighted. The intensity of individual peak correspond to the number of carbon. The display range of spectrum can be expanded by drag & drop operation or numerical entry. Click reset button to reset view.

The checkboxes at the bottom (C, CH, CH₂, CH₃) switches Show/Hide corresponding peaks. The APT checkbox switches spectrum to up (CH₃, CH) and down (CH₂, C) view. The 'Show ^1H NMR Shifts' checkbox shows ^1H chemical shift graph.

- 「Download ^{13}C NMR data in Delta format」

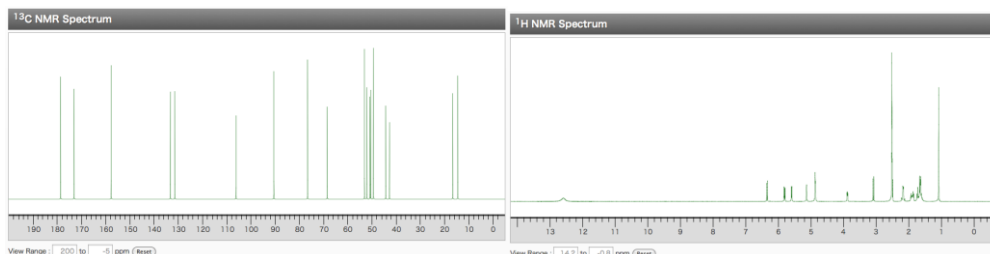
Delta format ^{13}C NMR spectrum data can be downloaded by clicking this link. The downloaded data can be opened by Delta software, and it is easy to compare with measured NMR spectra.

- **^1H NMR Shifts**

The ^1H chemical shifts graph is shown. It is only a isotropic chemical shift, and J splitting pattern is not shown.

- **View ^1H and ^{13}C Spectra**

In case of the 6,000 compounds from SDBS-NMR, measured spectra can be shown.



- **Print Layout**

The print layout without unnecessary information e.g. header/footer, URL links, buttons is shown in a new window. The ON/OFF states of spectra are reflected on a print layout.

gibberellic acid

No.	^{13}C Shift /ppm	Carbon Type	^1H Shift /ppm	^1H Pattern /Hz
1	131.37	CH	6.334	
2	133.18	CH	5.800	
3	68.35	CH	3.874	
			5.58	OH
4	52.97	C		
5	50.37	CH	2.30	
6	50.72	CH	3.075	
7	178.55	C	12.6	OH
8	49.29	C		
9	52.00	CH	1.6	
10	90.43	C		
11	16.47	CH ₂	1.6	
			1.91	
12		CH ₂	1.6	
			1.86	
13	76.50	C	4.87	OH
14	44.18	CH ₂	1.72	
			1.63	
15	42.66	CH ₂	2.15	
			2.18	
16	157.65	C		
17	106.08	CH ₂	5.127	
			4.85	
18	14.42	CH ₃	1.071	
19	173.00	C		

Name: gibberellic acid
Molecular Formula: C₁₉H₂₂O₆ Molecular Weight: 346.4
NP No.: 9089 Spectral Key: 09-089
CAS Registry No.: 77-06-5
Solvent: DMSO-d₆
 ^1H Frequency: 400 MHz(H) / 50.32 MHz(C) Shift Ref.: TMS
SDBS No.: 10779
Comments: CNMR of C12; overlapped with solvent signals.

CH-NMR-NP (^{13}C and ^1H NMR Database of Natural Products)
The CH-NMR-NP System is powered by JEOL Ltd.

- **Paging**

The paging of search result can be done by clicking paging buttons at the page bottom. The page is corresponding to the sorting number of search result.

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