Instruction to search natural compounds on CH-NMR-NP

The ‘CH-NMR-NP’ is a charge free service for all users. Please note that required information (name, affiliation, country, email) has to be submitted once to use all functions. The JEOL RESONANCE Inc. is supposed to take responsibility for ‘CH-NMR-NP’ system, however, the copyright of database is held by Dr. Kikuko Hayamizu. Thus JEOL RESONANCE Inc. does not offer any inquiry about ‘CH-NMR-NP’ via phone call or e-mail. Please use dedicated inquiry form on the website.

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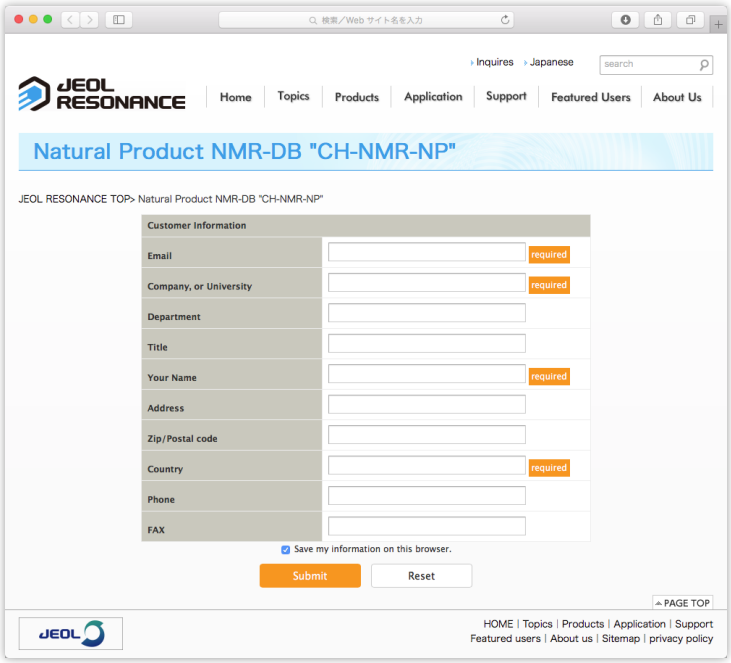
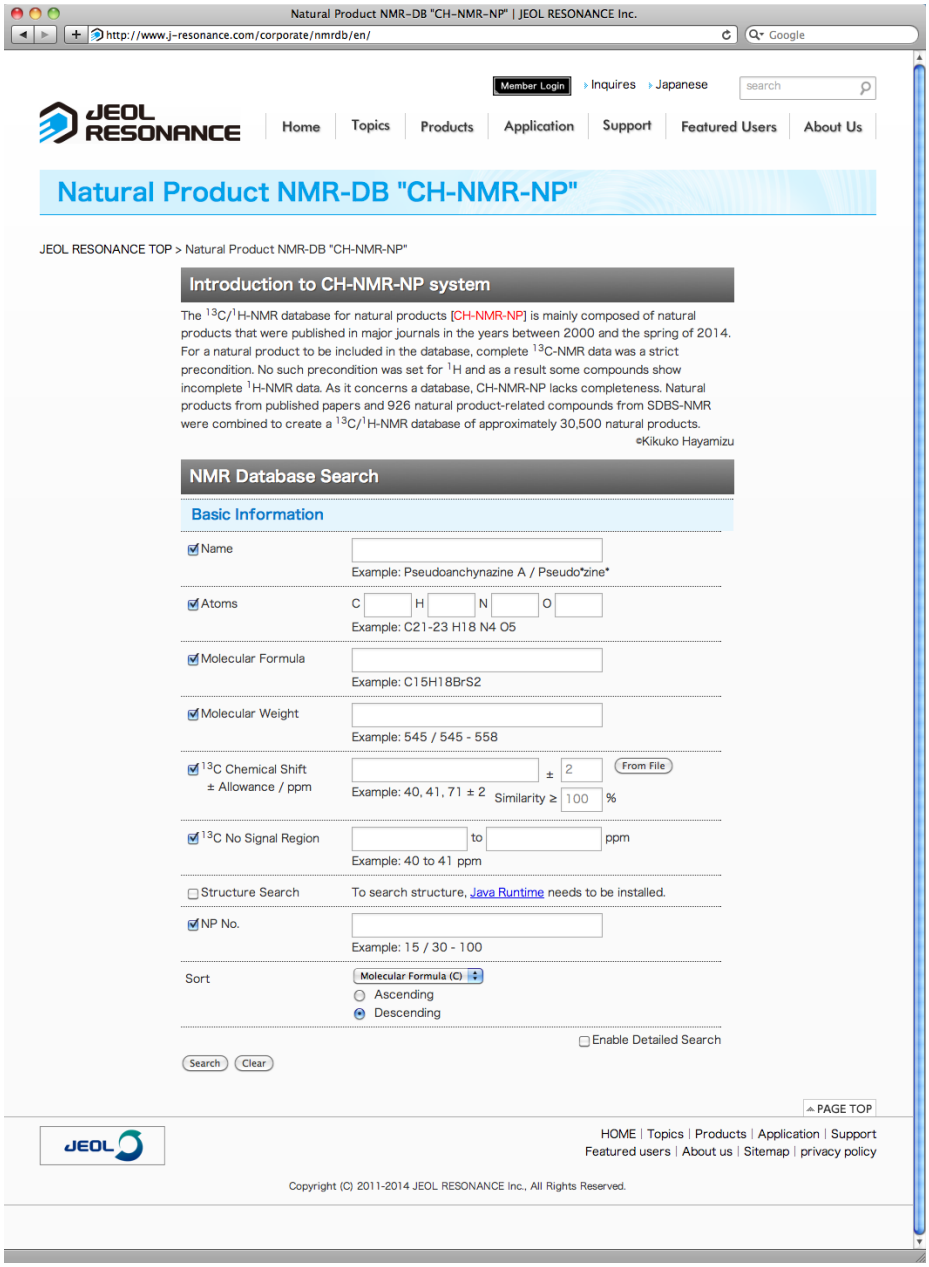
*Mozilla Firefox or Apple Safari are recommended to use for ‘CH-NMR-NP’ as operation checked web bowser.



Login Dialog

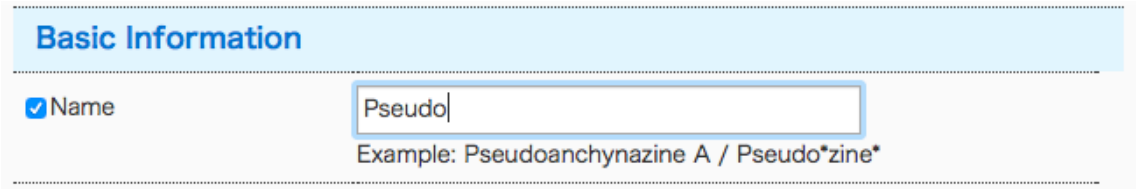
Compound Search

Here is the initial page for database search.



The Name (compound name)、Atoms and Molecular Formula、Molecular Weight、^{13}C Chemical Shift、^{1}H 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

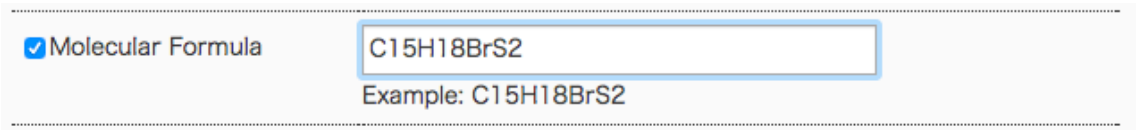


A compound name is used as a query. The compound name is usually a trivial name, which is described in the original paper, but some of them may be a chemical name (IUPAC Name, etc.). A search word is a partial match retrieval, but '*' or '!' can be used as wildcard character. A '*' matches any number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

Atoms

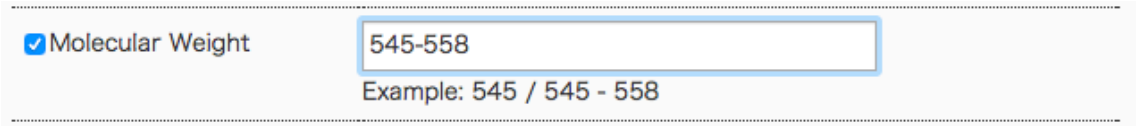
The number of atoms of carbon, hydrogen, nitrogen and oxygen are used as a query. The other element should be set in the 'Molecular Formula' form. A atom number can be specified as a range. For example, '21-23' at 'C' searches compounds that have carbons from 21 to 23. The '-21' at 'C' searches compounds 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 specified element.

Molecular Formula



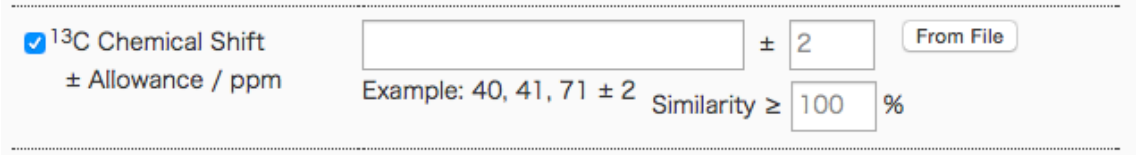
A molecular formula is used as a query. It is case insensitive, and an order of elements has no limitation. The range specification cannot be used, but '0' searches compounds that contain none of specified element. For example, 'C15H18BrS2' and 'BrS2c15h18' find same compounds.

Molecular Weight



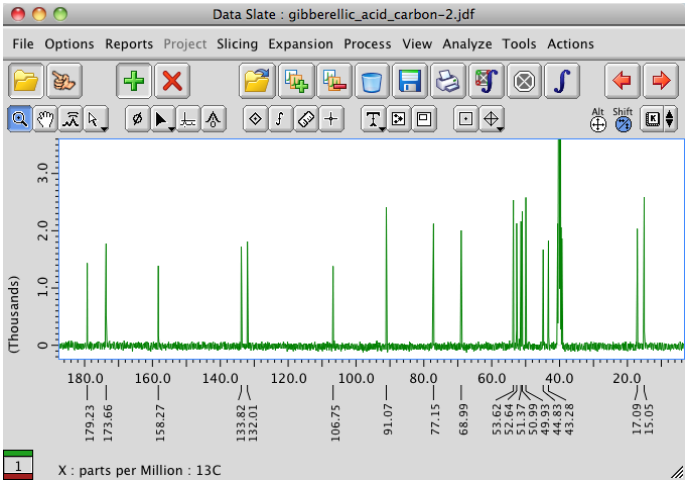
A molecular weight is used as a query. The value can be range specified. The value in the database is rounded.

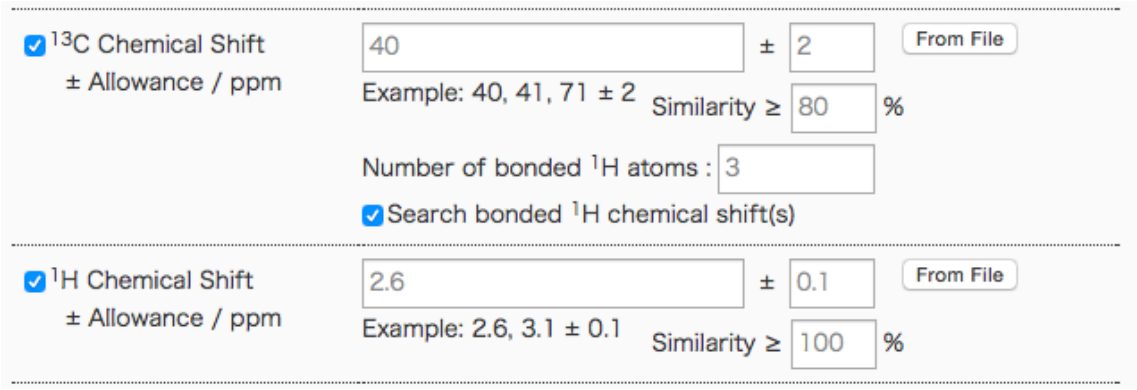
^{13}C Chemical Shift



A 13C 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.

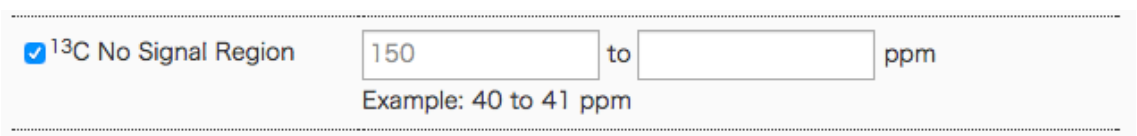




When using the 'Enable Detailed Search', the number of bonded 1H atoms (multiplicity of carbon) can be specified. For example, the '3' should be specified in this field, if the searching 13C chemical shift is CH3. Comma-delimited specification can be used to specify this for multiple carbon signals. 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.

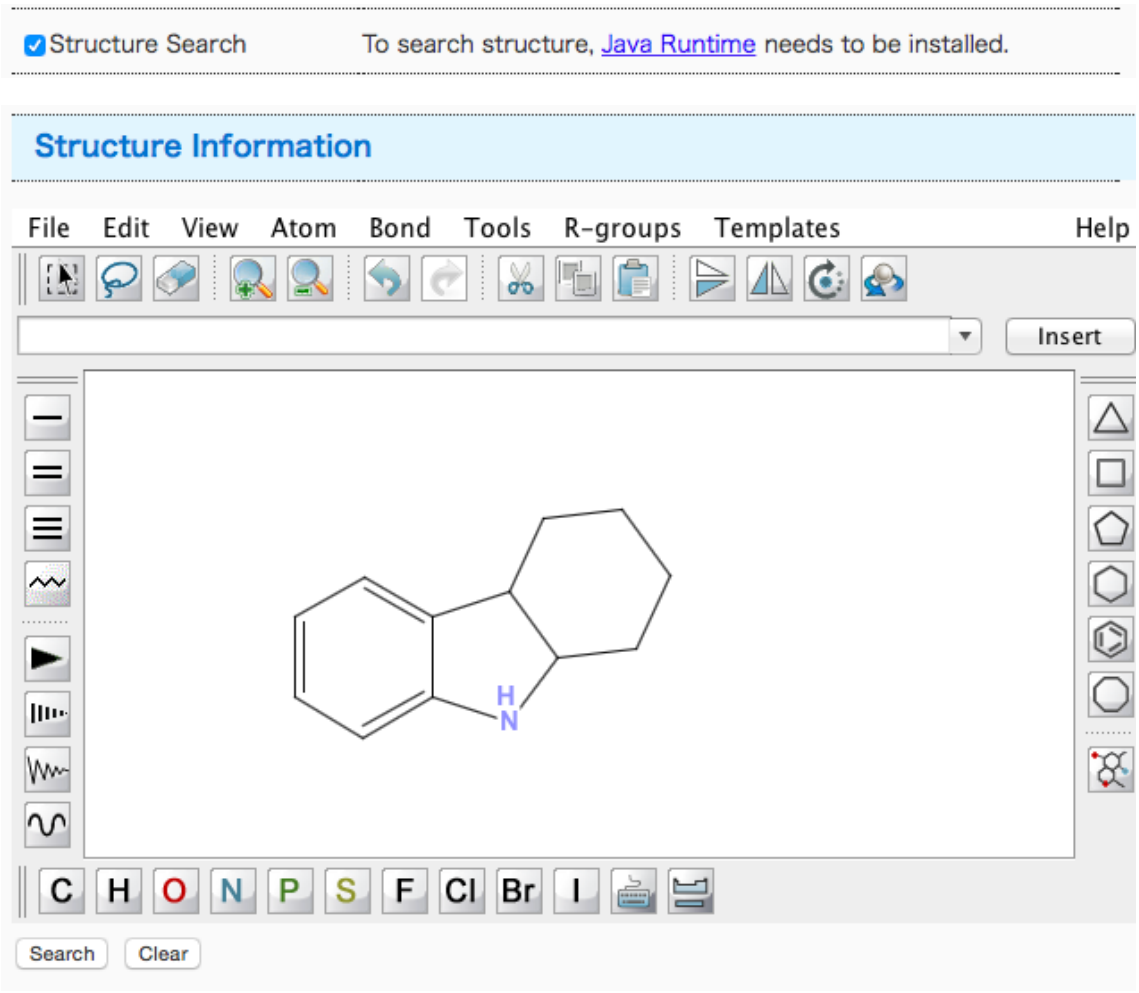
Please note that there are a lot of compounds that have not enough 1H chemical shift information in the database.

^{13}C No Signal Region



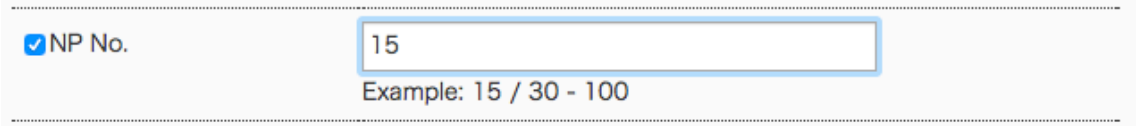
A no signal region of 13C chemical shift (ppm unit) is used as a query.

Structure Search



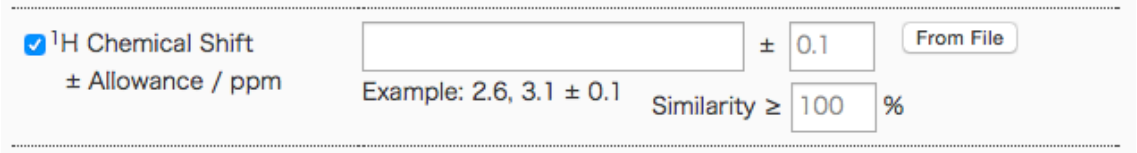
A partial structure is used as a query. The free java applet 'JChempaint' and 'pgchem::tigress' are used for structure drawing and structure search respectively. Thus java runtime needs to be installed to use partial structure search. Additionally, it is necessary to add 'http://www.j-resonance.com/' into the 'exception site list' at security tab of Java control panel.

NP No.



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

^{1}H Chemical Shift (w/ Enable Detailed Search)

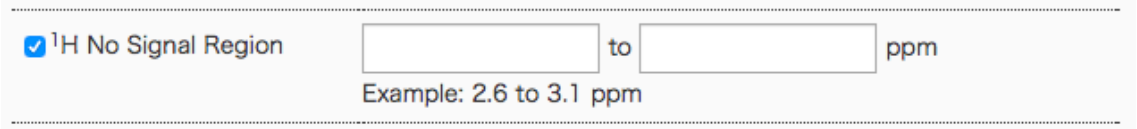


A 1H chemical shift (ppm unit) is used as a query. The multiple chemical shifts can be set by comma-delimited format. An allowance is applied to all chemical shifts. All chemical shifts are used as logical AND operators, however, similarity can loosen search condition. For example, 3 chemical shifts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

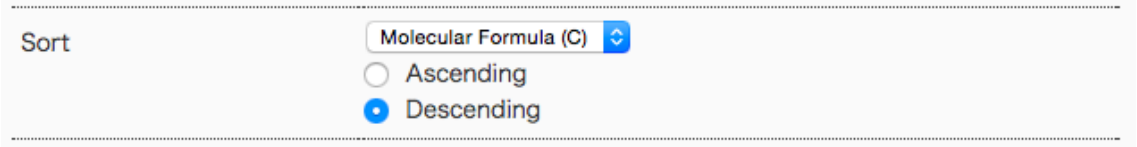
*Please note that proton *J*-splitting are not considered and there are a lot of compound that have not enough 1H chemical shift information.

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



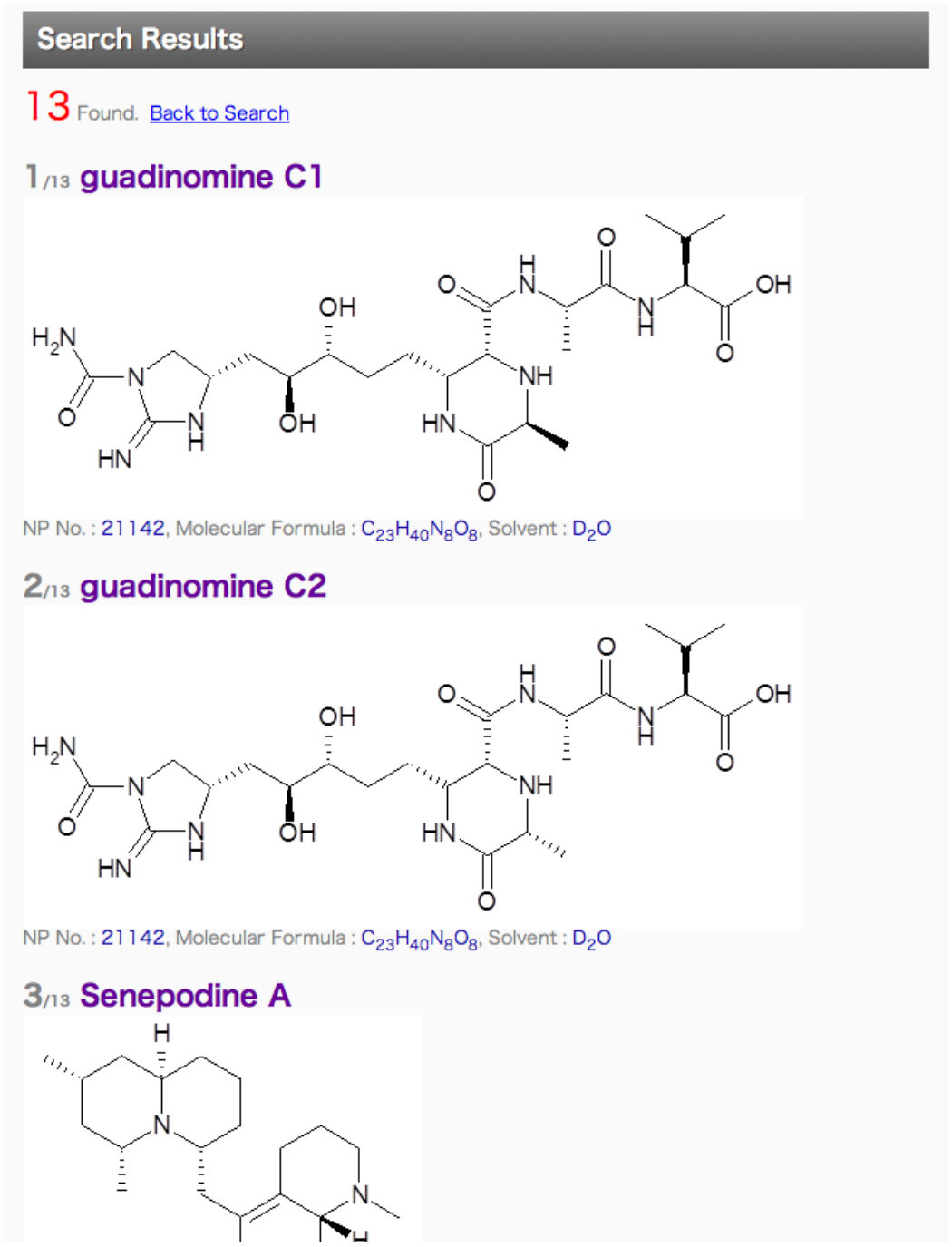
A no signal region of 1H chemical shift (ppm unit) is used as a query.

Sort



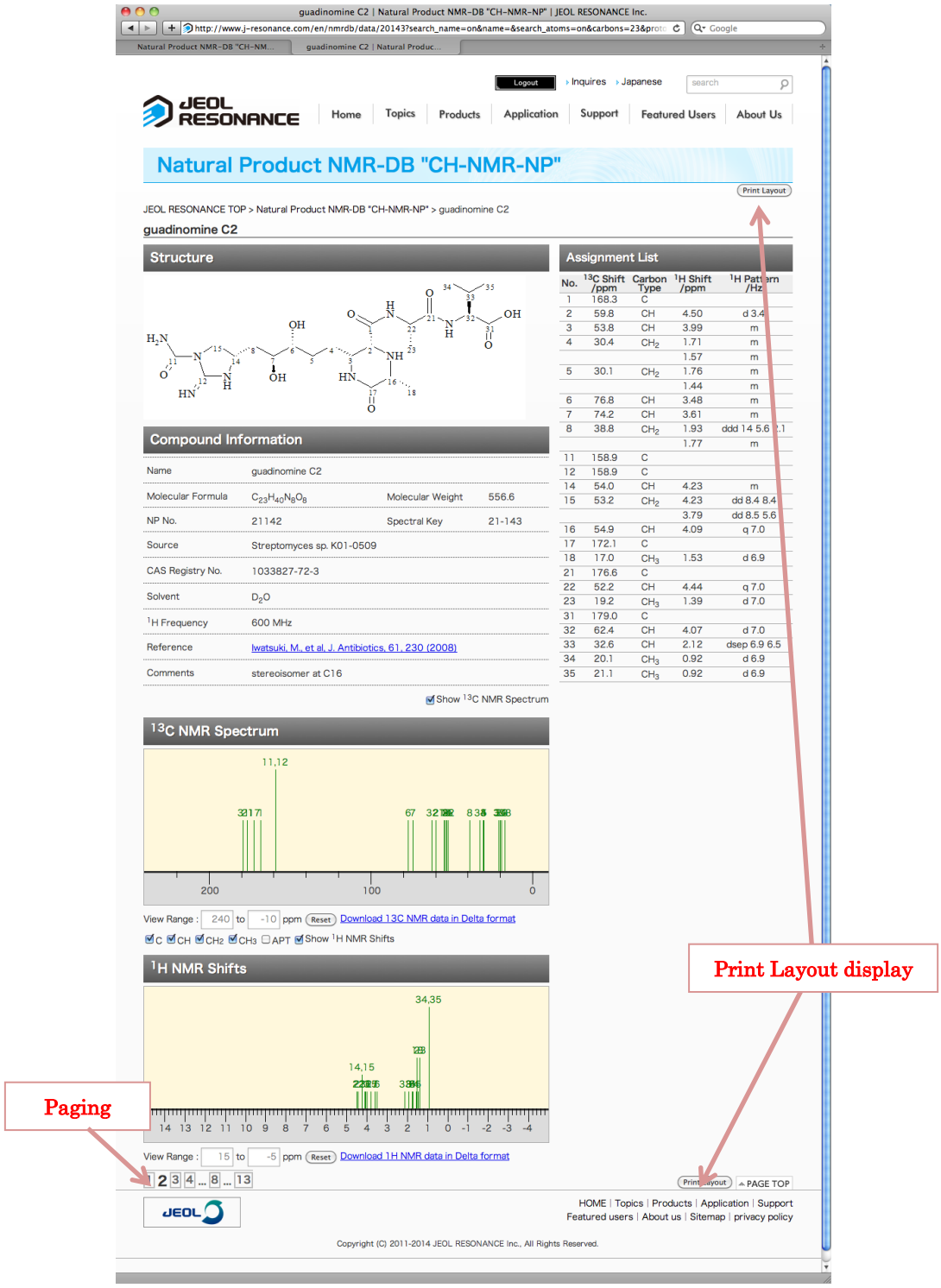
Search result is sorted in descending order of carbon number as a default. The compounds of same carbon number are sorted in descending of number of hydrogen, nitrogen, oxygen, in that order. The NP No., compound name (alphabetical), number of atoms (CHNO), molecular weight, similarity can be used for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

Search Result



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. (site login required)

Detailed data 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 (^{13}C NMR and ^{1}H 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.
- **^{1}H Frequency**

  An observing frequency of the ^{1}H 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 $CDCl_3$, the description '7.25 / 77.0' means that ^{1}H signal of residual $CHCl_3$ was set to 7.25 ppm and ^{13}C signal of $CDCl_3$ 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 ^{13}C, chemical shift of ^{13}C, carbon type (CH_3, CH_2, CH, C), chemical shift of bonded 1H, comment including *J* coupling pattern of ^{1}H and J value etc. are described. When using 13C Chemical shift query at the compound search, matched 13C were highlighted. ^{1}H chemical shift on the row without ^{13}C number shows 2nd chemical shift of

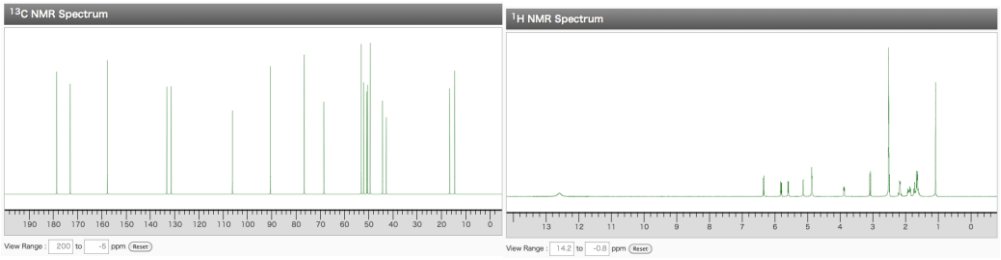
non-equivalent ^{1}H or OH/NH. In case of OH/NH, it is specified in comment field.

- **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 13C Chemical shift query at the compound search, matched 13C 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, CH_2, CH_3) switches Show/Hide corresponding peaks. The APT checkbox switches spectrum to up (CH_3, CH) and down (CH_2, C) view. The 'Show ^{1}H NMR Shifts' checkbox shows 1H chemical shift graph.
  - 「Download 13C 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.

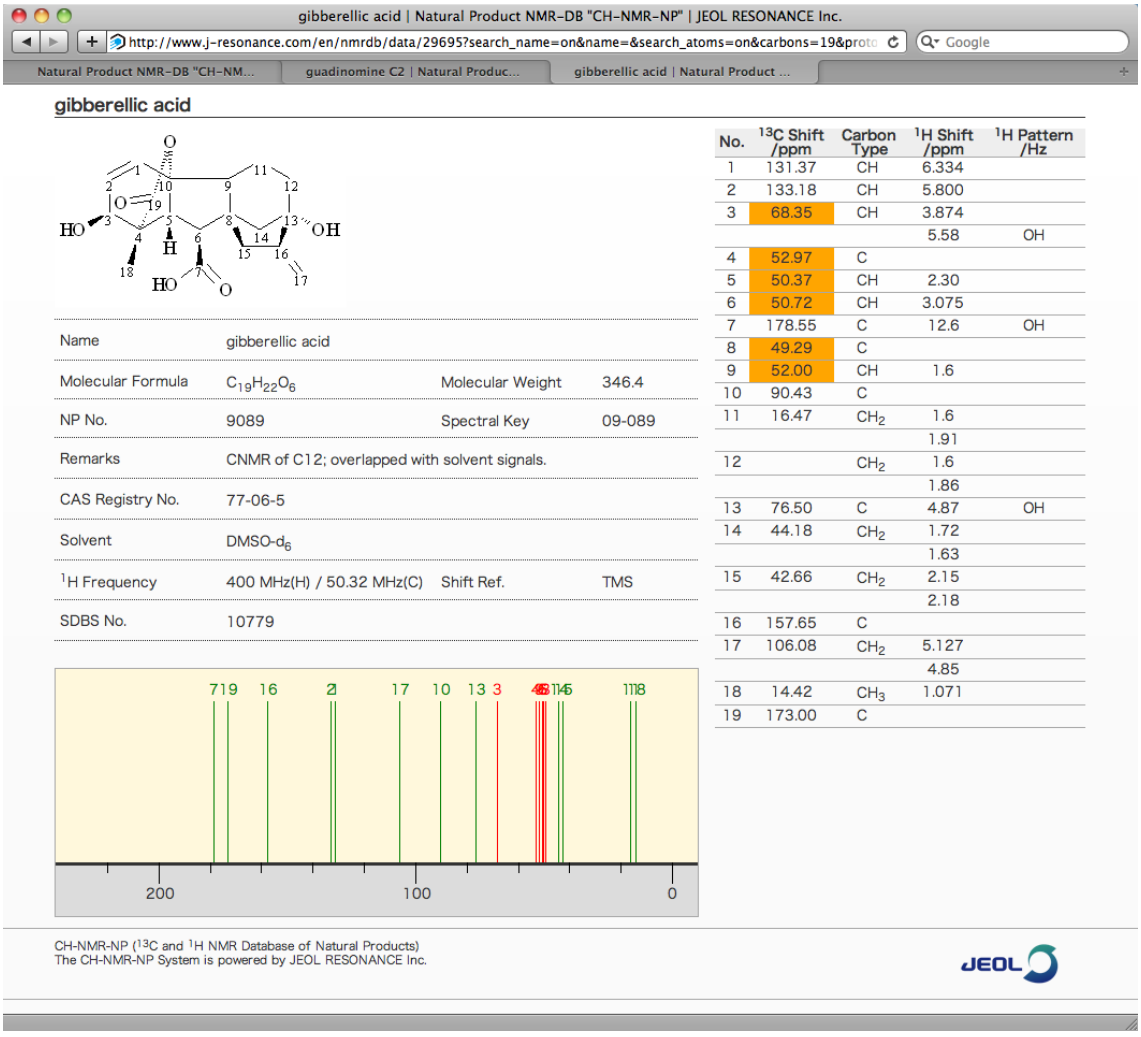
- **^{1}H NMR Shifts**
  The ^{1}H chemical shifts graph is shown. It is only a isotropic chemical shift, and *J* splitting pattern is not shown.

- **View 1H and 13C 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.



- **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.