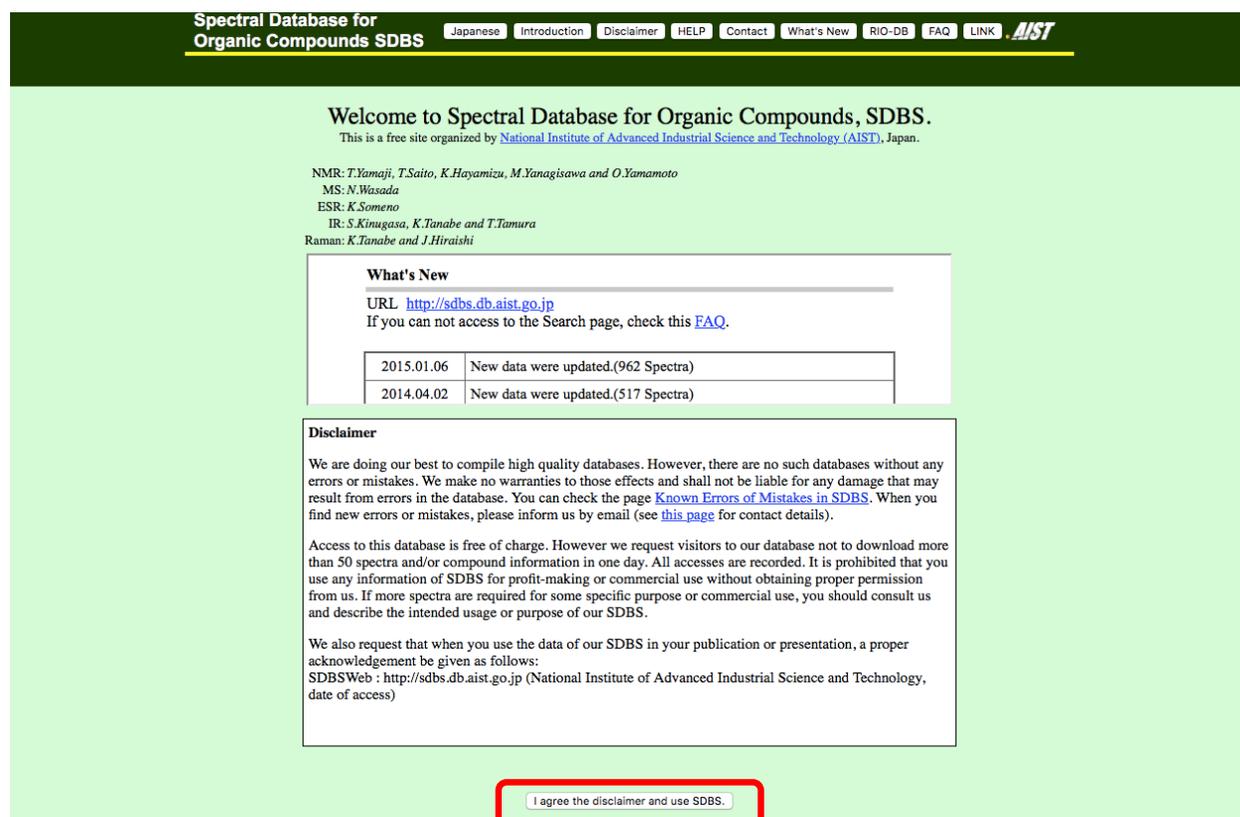


Working with the Spectral Database of Organic Compounds

The Spectral Database of Organic Compounds is a free site organized and maintained by the National Institute of Advanced Industrial Science and Technology in Japan. It is a repository of organic molecules and their spectra including ^1H NMR, ^{13}C NMR, FT-IR, and mass spectrum. It is an incredibly useful site for locating these pieces of data for simple organic molecules.

Site Link: http://sdfs.db.aist.go.jp/sdfs/cgi-bin/cre_index.cgi

Step #1: Read and acknowledge the disclaimer



Spectral Database for Organic Compounds SDBS Japanese Introduction Disclaimer HELP Contact What's New RIO-DB FAQ LINK AIST

Welcome to Spectral Database for Organic Compounds, SDBS.
This is a free site organized by National Institute of Advanced Industrial Science and Technology (AIST), Japan.

NMR: T.Yamaji, T.Saito, K.Hayamizu, M.Yanagisawa and O.Yamamoto
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Raman: K.Tanabe and J.Hiraishi

What's New
URL <http://sdfs.db.aist.go.jp>
If you can not access to the Search page, check this [FAQ](#).

2015.01.06	New data were updated.(962 Spectra)
2014.04.02	New data were updated.(517 Spectra)

Disclaimer
We are doing our best to compile high quality databases. However, there are no such databases without any errors or mistakes. We make no warranties to those effects and shall not be liable for any damage that may result from errors in the database. You can check the page [Known Errors of Mistakes in SDBS](#). When you find new errors or mistakes, please inform us by email (see [this page](#) for contact details).

Access to this database is free of charge. However we request visitors to our database not to download more than 50 spectra and/or compound information in one day. All accesses are recorded. It is prohibited that you use any information of SDBS for profit-making or commercial use without obtaining proper permission from us. If more spectra are required for some specific purpose or commercial use, you should consult us and describe the intended usage or purpose of our SDBS.

We also request that when you use the data of our SDBS in your publication or presentation, a proper acknowledgement be given as follows:
SDBSWeb : <http://sdfs.db.aist.go.jp> (National Institute of Advanced Industrial Science and Technology, date of access)

Step #2: Using the tool bar on the left side the of screen insert the name, molecular formula, molecular weight or CAS number. If you are using the name, it may be advantageous to leave off any prefix and widen the search using the “match partial” search (this option may be selected in the drop down menu to the left of the name field).

For example – If you are searching for 4-iodoaniline, placing the full name in the name field yields no results. This is because 4-iodoaniline is filed under p-iodoaniline. Therefore, its much easier to search “iodoanilen” and then scan through the result to find the desired substitution pattern.

Spectral Database for Organic Compounds SDBS [Japanese](#) [Introduction](#) [Disclaimer](#) [HELP](#) [Contact](#) [What's New](#) [RIO-DB](#) [FAQ](#) [LINK](#) 

SDBS Compounds and Spectral Search

Compound Name:
p-iodoaniline match partial

Molecular Formula:

Molecular Weight:
_____ to _____
Numbers between left and right columns
Up to the first place of a decimal point

CAS Registry No.:

SDBS No.:

Atoms:

C(Carbon) to

H(Hydrogen) to

N(Nitrogen) to

O(Oxygen) to

F(Fluorine) to

Cl(Chlorine) to

Br(Bromine) to

I(Iodine) to

S(Sulfur) to

P(Phosphorus) to

Si(Silicon) to

Numbers between left and right columns.

Spectrum:
Check the spectra of your interest.

MS IR

¹³C NMR Raman

¹H NMR ESR

IR Peaks(cm⁻¹): Allowance
_____ ± 10
" " or space is the separator for multiple peaks.
Use "-", to set a range.: eg. 550-750,1650-3000-

Transmittance < 80 %

¹³C NMR Shift(ppm): Allowance
_____ ± 2.0
" " is the separator for multiple shifts, eg. 129.3,18.4,...

No shift regions: _____

Range defined by two numbers separated by a space, eg. 110 78,...

¹H NMR Shift(ppm): Allowance
_____ ± 0.2

No shift regions: _____

MS Peaks and intensities: _____

Mass and its intensity are a set of data separated by a space, eg. 110 22,...

Tip: use "match partial" and leave off prefix of compound

Hit: 20hit

(c) National Institute of Advanced Industrial Science and Technology (AIST)

Step #3: scan through the results to find the desired compound. In the search results, you will see a hyperlinked Y under each analysis type if it is SDBS has it on file. There will be a N for those items not yet archived.

SDBS Search Results: 1 - 1 out of 1 hits Sort by:

SDBS No	Molecular Formula	Molecular Weight	MS	CNMR	HNMR	IR	Raman	ESR	Compound Name
2869	C6H6IN	219.0	Y	Y	Y	Y	N	Y	p-iodoaniline

Clicking on the desired analysis will bring up a spectrum and picture of the compound with each atom type numbered. The chemical shifts/mass values will be giving in a table below the structure. The tool bar on the left will allow you to jump from one type of analysis to another.

SDBS Information

SDBS No.: 2869

 Compound Name:
p-iodoaniline

 Molecular Formula: C₆H₆IN

Molecular Weight: 219.0

 CAS Registry No.:
540-37-4

Derivatives:

display in a separate page

[SDBS Structures Web \(on trial since 2013-05-14\)](#)
Spectral Code:
[Mass :](#)
[¹³C NMR : in CDCl₃](#)
[¹H NMR : 90 MHz in CDCl₃](#)
[¹H NMR : parameter in acetone](#)
[IR : KBr disc](#)
[IR : liquid film](#)
[IR : CCl₄ solution](#)
[IR : nujol mull](#)
[ESR : OXIDATION WITH PERBENZOIC ACID](#)
[Chemical Information:](#)
[Return to Search:](#)
[Return to Result:](#)

¹H NMR
Solvent info may be found
on tin the toolbar on the

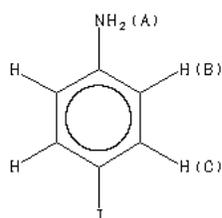
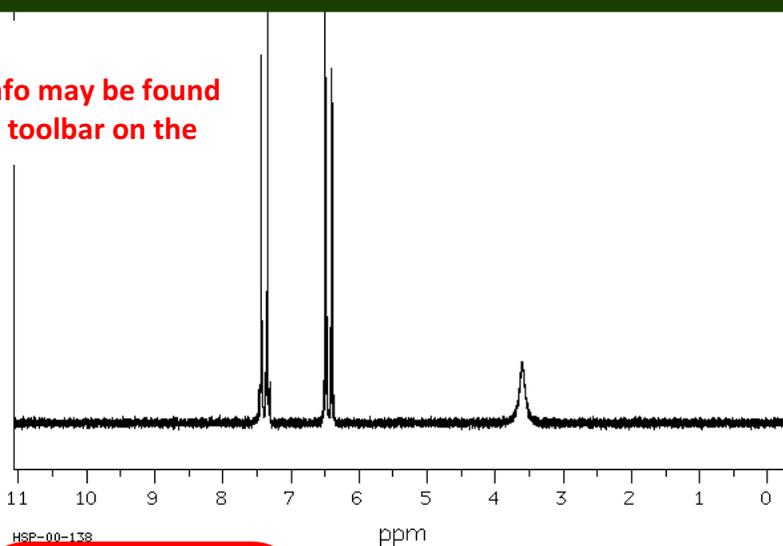


Table of chemical shifts

Assign.	Shift (ppm)
A	3.61
B	6.449
C	7.389