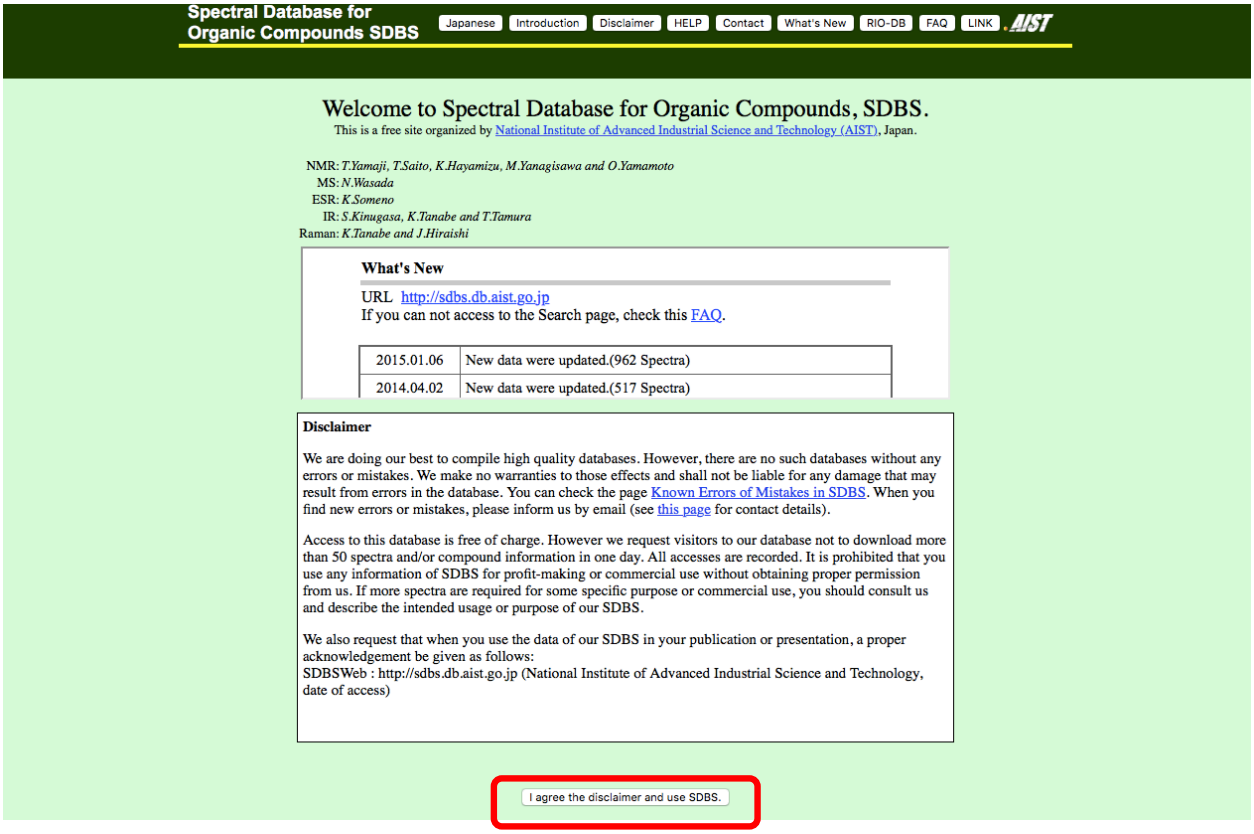
Working with the *Spectral Database of Organic Compounds*

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 ^{1}H 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.

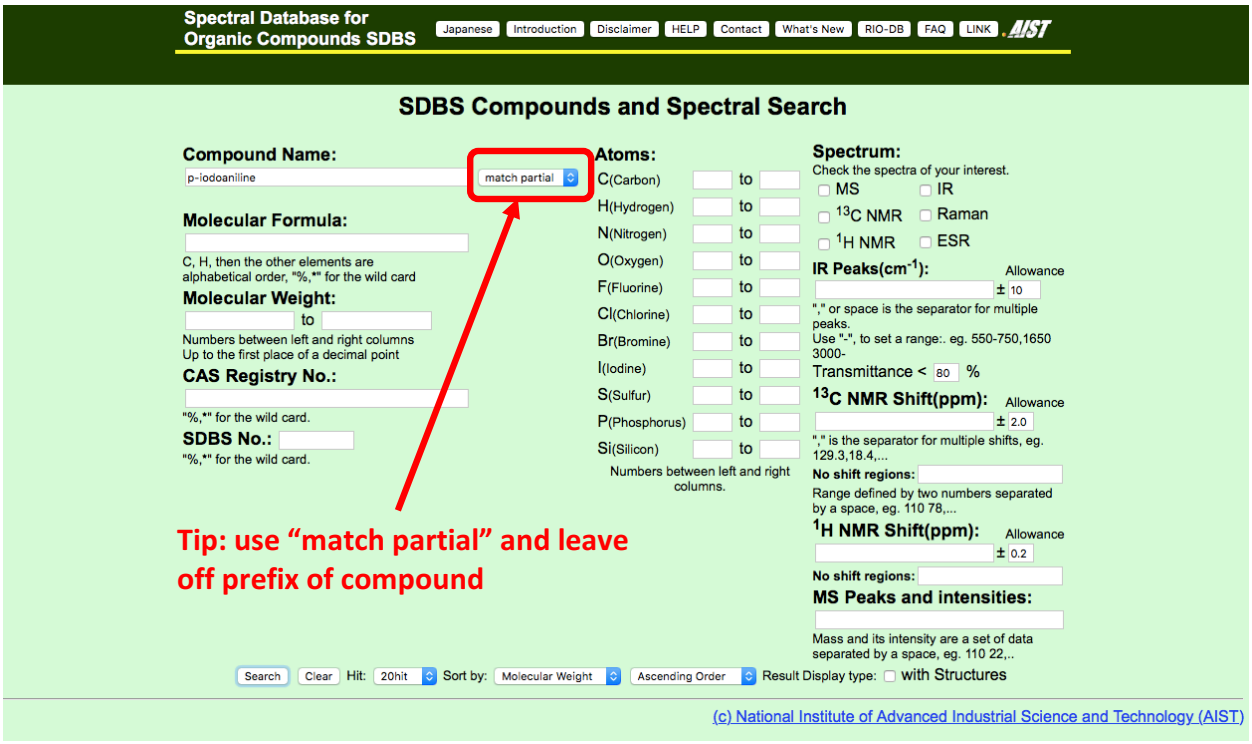
Site Link: http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi

Step #1: Read and acknowledge the disclaimer

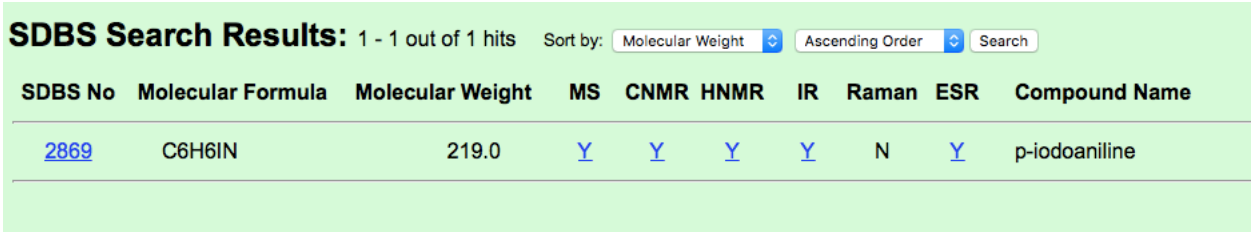


Step #2: Using the tool bar on the left side the of screen insert the name, molecular formula, molecular weight or CAS number. If you are using the name, it may be advantageous to leave off any prefix and widen the search using the "match partial" search (this option may be selected in the drop down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



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 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: C_6H_6IN

Molecular Weight: 219.0

CAS Registry No.:
540-37-4

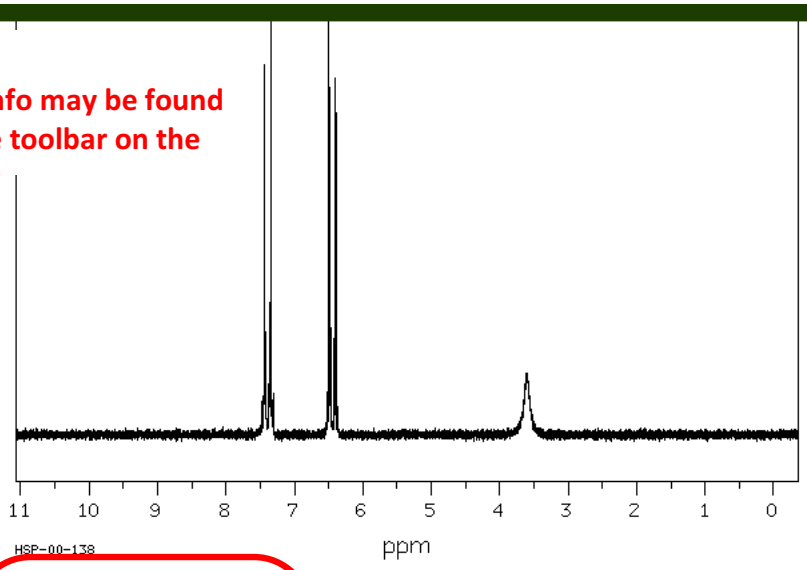
Derivatives:
display in a separate page
SDBS Structures Web (on trial since 2013-05-14)

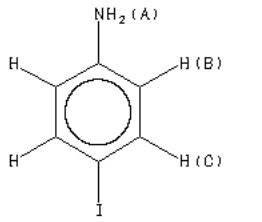
Spectral Code:
Mass :
^{13}C NMR : in $CDCl_3$
^{1}H NMR : 90 MHz in $CDCl_3$
^{1}H NMR : parameter in acetone
IR : KBr disc
IR : liquid film
IR : CCl_4 solution
IR : nujol mull
ESR : OXIDATION WITH PERBENZOIC ACID

Chemical Information:

Return to Search:
Return to Result:

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





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

Table of chemical shifts