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Anthony Remijan, Robin Pulliam

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ABSTRACT

The purpose of the Splatalogue User Guide is to provide a brief overview of the functionality of the Splatalogue homepage available at www.splatalogue.net. For more detailed information about how to access the Splatalogue database via the VAO SLAP interface, please visit: www.splatalogue.net/SLAPNotes.html. For any other information about accessing the Splatalogue database that goes beyond what is found in this document, or any other questions about conducting searches or exporting the data, please submit a helpdesk ticket to Splatalogue through the ALMA Science Portal found at http://www.almascience.org. Once at the site, select your preferred ALMA regional center (ARC) and on the left side of the subsequent webpage, under "User Services at ARCs," click on Helpdesk.

Splatalogue Quickstart Guide

Anthony J. Remijan
Robin L. Pulliam
NRAO

STATUS: v3.0

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TABLE OF CONTENTS:

Basic Navigation	3
Definition of the Color Schemes	6
Searching for a molecule by molecular mass	8
Performing a query on a selected molecule	9
Performing a query over a frequency range	11
Exporting the data	14
Further Examples and Splatalogue User "Homework"	15

BASIC NAVIGATION

When arriving at the Splatalogue homepage at www.splatalogue.net, you will find it broken up into a series of frames. Figure 1 below shows a screenshot of the frames and gives a description of the content of each frame:

1) "Navigation" Frame – links to various notes, announcements and services available to users in Splatalogue.

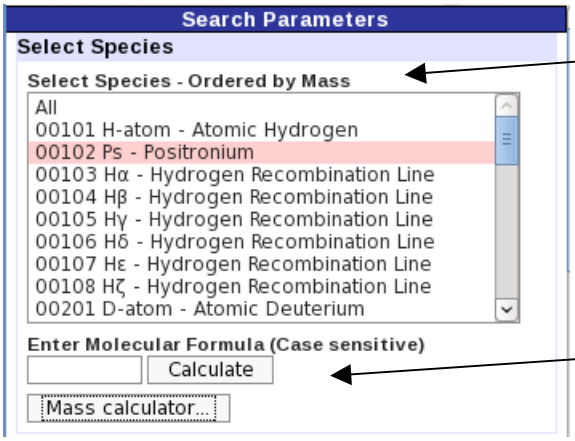
2) "Data Version" Frame – allows the user to navigate between different versions (updates) of molecular species within the database

3) "Search Parameters" Frame – enter the search parameters and various display settings for your search. Once you are satisfied with your search parameters, hit the Search button.

4) "Search Results" Frame – the main display of Splatalogue. This frame will update as new searches and different parameters are set in the "Search Parameters" frame. It is also the front page of Splatalogue so new announcements and updates will appear here first before migrating to the "What's New" page available in the "Navigation" frame.

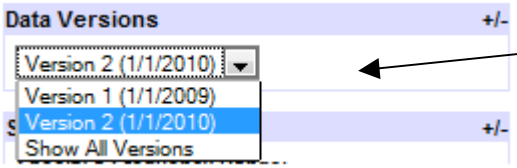
"Search Parameters" Frame:

The "Search Parameters" frame is broken up into 2 categories: Inputs for searches and inputs for display. The top part of the frame is reserved for inputs for searches and the bottom part of the frame is reserved for all the display settings and parameters available to a user. In this frame, you will find the important SEARCH button that will execute your query. Below we illustrate the various search inputs and displays available for users.

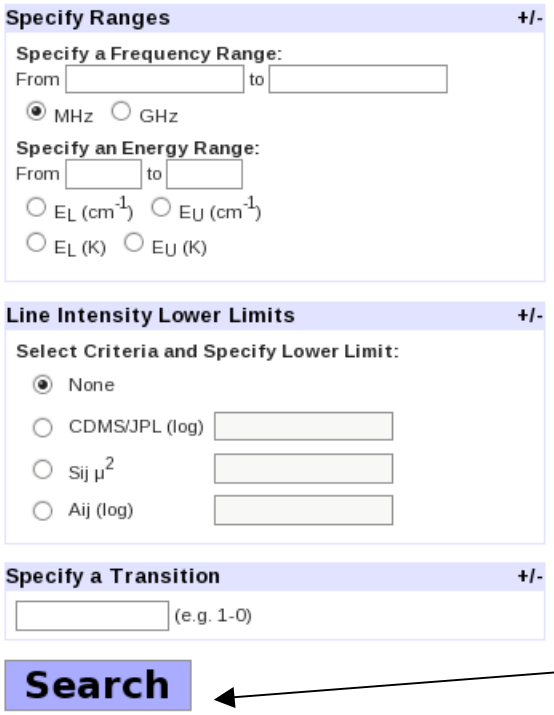


There are over 1040 individual entries a user can search on in Splatalogue. These are contained in a Pulldown Menu and ordered by molecular mass.

The molecular mass calculator will help you find the species of interest. Its use is described in more detail below.



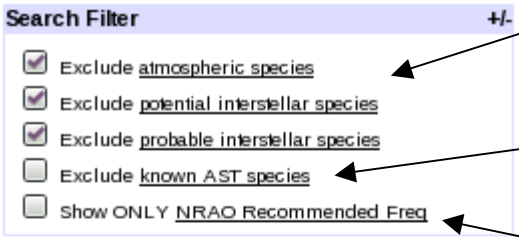
Currently, two data versions are available in Splatalogue. New updated molecular information from other databases are uploaded as Version 2, and older information is then placed in Version 1. You can display Version 1, Version 2, or all Versions of molecular species currently available within Splatalogue by selecting the appropriate pull down menu.



Limit your searches by entering:
- frequency range
- energy range
- line strength range
- transition

Note you can only search 1 type of line strength in a given search (ie. Sijmu2 OR Aij, NOT both).

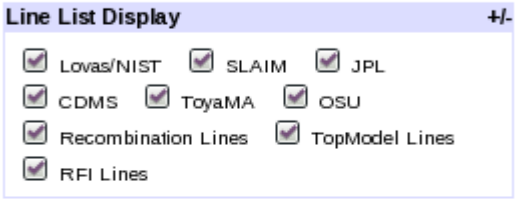
Finally, the SEARCH button is clearly marked and highlighted.



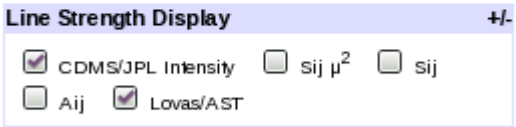
Limit the number of species displayed by excluding those species that have not yet been detected in space.

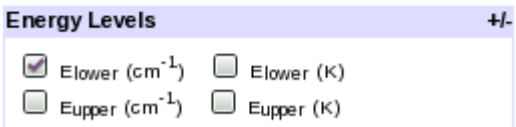
Select to EXCLUDE all currently known molecular species that have been detected in space.

Also, show only the NRAO Recommended frequency for a given transition.



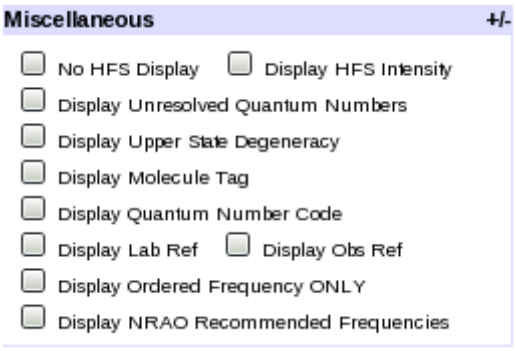
Select the Line List that is searched on and displayed.





Select the type of energy level (lower or upper) and line strength displayed along with the type of units.

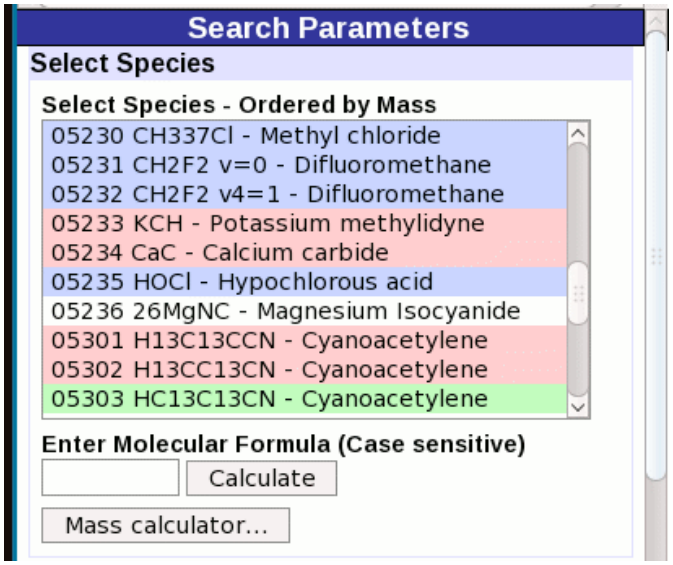
Option to not search on any transition where the error in the frequency is over 50 MHz.



Miscellaneous search filters and displays. You have the option to display only 1 frequency instead of both the predicted and measured values as well as displaying the NRAO recommended frequency. The recommended frequency will be highlighted in the main frame with a "SPLAT": 

DEFINITIONS OF COLOR SCHEMES

In both the species pulldown menu and in the main display frame off the Splatalogue homepage, we use different color schemes to guide a user. In the molecule pulldown menu, you will see species highlighted by difference background colors:



BLUE
(atmospheric)

RED
(possible)

WHITE
(known)

GREEN
(probable)

The definitions of each of these different categories are given below:

Atmospheric Molecule – Self explanatory

- Omitted from search by default

"Potential" Astronomical Molecule

- These species have the potential to be found in astronomical environments but only through a dedicated search and are unlikely to appear in cursory spectral line surveys. Such molecules include amino-ethanol, GLYCINE conformers!
- Omitted from search by default

"Probable" Astronomical Molecules

- These species are mostly isotopomers or higher vibrational states of known astronomical molecules that given the high sensitivity of existing and future receivers, may show up in spectral line passbands. Such molecules include, high v states of CO, SiO, SiS, CS, etc… 13 isotopes of ethyl cyanide and methyl formate.
- Omitted from search by default

"Known" Astronomical Molecules – Self explanatory

- Included in search by default

To "turn on" searching for molecules in the atmospheric, potential or probable categories, you can uncheck the appropriate box available in the search filters. When a search is performed and the data are displayed in the main "Search Results" frame, many transitions will have a different color background as shown below:

Species	Chemical Name	Freq in MHz (Err)	Meas Freq in MHz (Err)	Resolved QNs	CDMS/JPL Intensity	Lovas/AST Intensity	E_L (cm^{-1})	Linelist
CO v = 0	Carbon Monoxide		115271.20180 (0.0005)	1-0	-5.01050		0.00000	CDMS
CO v = 0	Carbon Monoxide		115271.20180 (0.0005)	1-0	-5.01050		0.00000	JPL
CO v = 0	Carbon Monoxide	115271.20200 (1)		1-0	0.00000	60.00000	0.00000	Lovas
CO v = 0	Carbon Monoxide	115271.20200 (0)	115271.20200 (0.001)	1- 0	0.00000		0.00000	SLAIM
CO v = 0	Carbon Monoxide		230538.00000 (0.0005)	2-1	-4.11970		3.84500	CDMS
CO v = 0	Carbon Monoxide		230538.00000 (0.0005)	2-1	-4.11970		3.84500	JPL
CO v = 0	Carbon Monoxide	230538.00000 (1)		2-1	0.00000	70.00000	0.00000	Lovas
CO v = 0	Carbon Monoxide	230538.00000 (0)	230538.00000 (0.001)	2- 1	0.00000		3.84500	SLAIM
CO v = 0	Carbon Monoxide		345795.98990 (0.0005)	3-2	-3.61180		11.53500	CDMS
CO v = 0	Carbon Monoxide		345795.98990 (0.0005)	3-2	-3.61180		11.53500	JPL
CO v = 0	Carbon Monoxide	345795.99000 (1)		3-2	0.00000	70.00000	0.00000	Lovas
CO v = 0	Carbon Monoxide	345795.99000 (0)	345795.99000 (0.001)	3- 2	0.00000		11.53500	SLAIM
CO v = 0	Carbon Monoxide	461040.76800 (1)		4-3	0.00000	60.00000	0.00000	Lovas
CO v = 0	Carbon Monoxide	461040.76800 (0)	461040.76800 (0.001)	4- 3	0.00000		23.06900	SLAIM
CO v = 0	Carbon Monoxide		461040.76820 (0.0005)	4-3	-3.26570		23.06950	CDMS
CO v = 0	Carbon Monoxide		461040.76820 (0.0005)	4-3	-3.26570		23.06950	JPL
CO v = 0	Carbon Monoxide		576267.93050 (0.0005)	5-4	-3.01180		38.44810	CDMS
CO v = 0	Carbon Monoxide		576267.93050 (0.0005)	5-4	-3.01180		38.44810	JPL
CO v = 0	Carbon Monoxide	576267.93100 (0)	576267.93100 (0.001)	5- 4	0.00000		38.44800	SLAIM
CO v = 0	Carbon Monoxide	691473.07600 (1)		6-5	0.00000	100.00000	0.00000	Lovas
CO v = 0	Carbon Monoxide	691473.07600 (0)	691473.07600 (0.001)	6- 5	0.00000		57.67000	SLAIM
CO v = 0	Carbon Monoxide		691473.07630 (0.0005)	6-5	-2.81930		57.67040	CDMS
CO v = 0	Carbon Monoxide		691473.07630 (0.0005)	6-5	-2.81930		57.67040	JPL
CO v = 0	Carbon Monoxide	806651.80100 (1)		7-6	0.00000	110.00000	0.00000	Lovas
CO v = 0	Carbon Monoxide	806651.80100 (0)	806651.80600 (0.005)	7- 6	0.00000		80.73500	SLAIM
CO v = 0	Carbon Monoxide		806651.80600 (0.005)	7-6	-2.67160		80.73540	CDMS
CO v = 0	Carbon Monoxide		806651.80600 (0.005)	7-6	-2.67160		80.73540	JPL
CO v = 0	Carbon Monoxide		921799.70000 (0.005)	8-7	-2.55900		107.64240	CDMS
CO v = 0	Carbon Monoxide		921799.70000 (0.005)	8-7	-2.55900		107.64240	JPL
CO v = 0	Carbon Monoxide	921799.70400 (0.001)	921799.70000 (0.005)	8- 7	0.00000		107.64200	SLAIM
CO v = 0	Carbon Monoxide	1036912.38500 (1)		9-8	0.00000	17.50000	0.00000	Lovas

The color scheme used in this frame highlights the specific ALMA bands those frequencies fall in. For example, the top four lines have a "bright blue background". In this case, this color background is used for ALMA Band 3 (86-115 GHz). The "green background" that highlights the CO 3-2 line is representative of ALMA Band 7 (275-373 GHz).

By default, we highlight the ALMA bands. However, Splatalogue has the ability to highlight different bands depending on the telescope used (e.g. the GBT, eVLA, IRAM 30m, etc...). Note: These different telescope color schemes are not fully implemented off the splatalogue.net homepage yet.

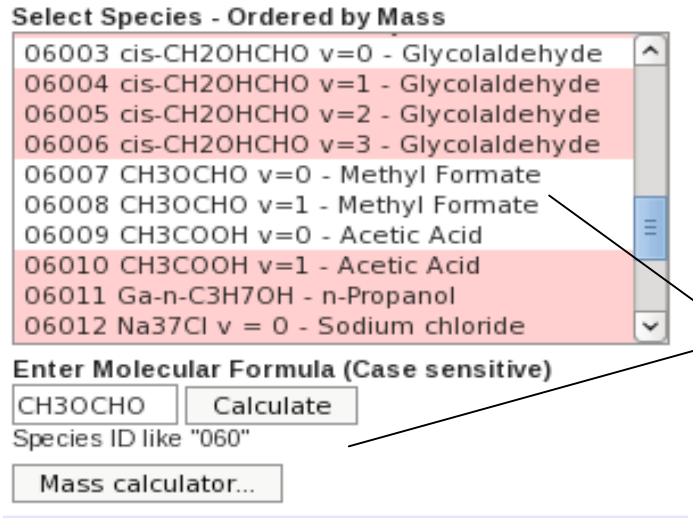
Also note that the color schemes used for the molecule pulldown menu is completely separate from the color scheme used to highlight frequencies in the “Search Results” frame. Meaning, a “BLUE” background in the “Search Results” frame does not designate those molecules and transitions are due to atmospheric molecules.

Searching for a molecule by molecular mass

Nearly all the publically available catalogs organize molecules in order of increasing molecular mass in amu (e.g. CO has a molecular mass of 28 amu). If a user is searching for transitions of a particular molecule, it will be beneficial to use the “Molecular Mass Calculator” built into Splatalogue to aid in the search.

Each molecule is organized by a unique Splatalogue ID number. An example of a Splatalogue ID is: “02801”. The first 3 numbers designate the molecular mass. In this case “028” refers to a molecule with a molecular mass of 28 amu. The last 2 numbers designate the Splatalogue index number. In this case “01” refers to the first entry for that molecular mass.

To open the mass calculator, click on the “Mass Calculator...” button on the Splatalogue homepage. To find the molecular mass of a molecule using the mass calculator, simply type in the molecular formula and hit the “Calculate” button. You will get the following returned:



CH3OCHO has a molecular mass of 60 amu so you should then scroll down the molecule pulldown menu until you find molecules with Species ID like “060”. Doing so, you will find CH3OCHO has a SplatID of “06007” in the ground vibrational state.

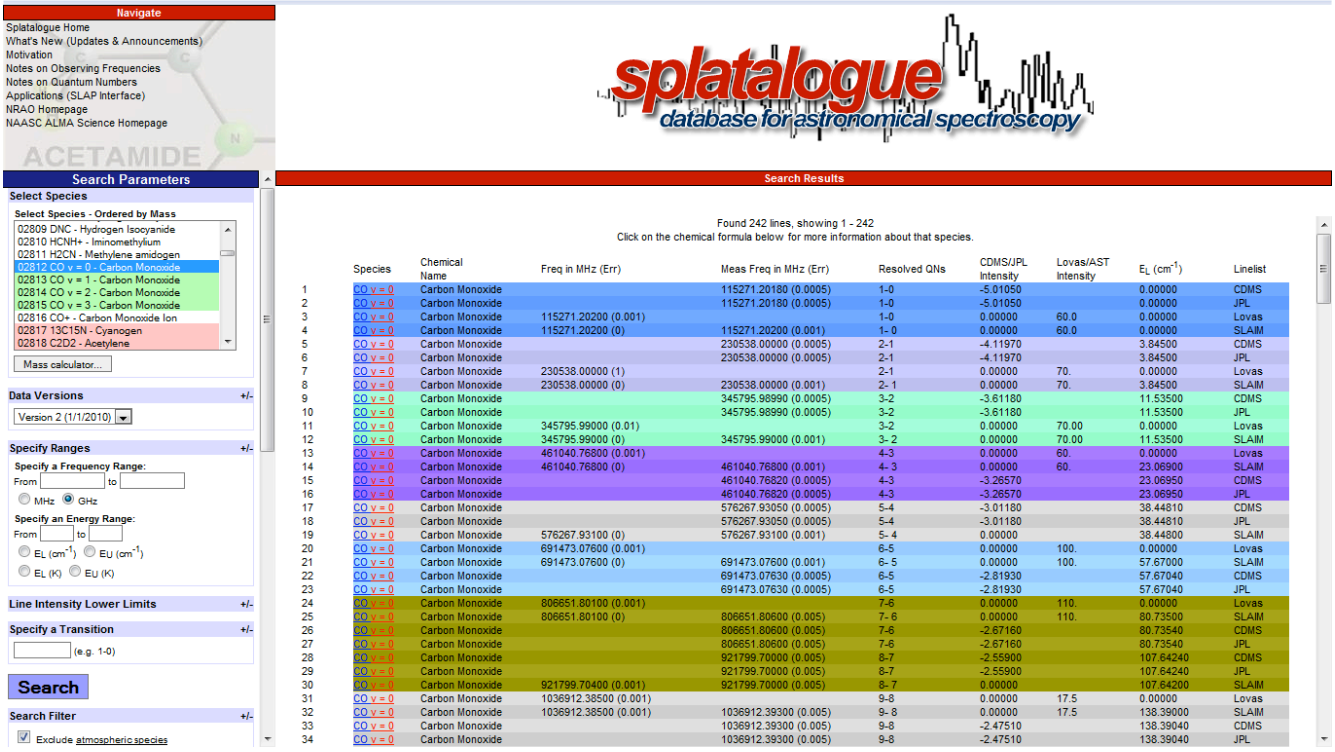
USAGE NOTES:

1. The mass calculator is CASE SENSITIVE. This is because the entire periodic table is contained in the database. SiC (Silicon and Carbon) will have a different mass than SIC (Sulfur, Iodine and Carbon).
2. The mass calculator does not support “+” or “-”. That is, the mass of HCO+ is the same as HCO.

3. The calculator interprets numbers as the total number of atoms in that molecule. It does NOT interpret numbers as an isotopologue number. As an example, if a user types “C15N” in the Mass calculator, they may be trying to find the mass of Carbon plus 15-Nitrogen. However, the calculator will interpret “C15N” as 15 Carbons plus Nitrogen NOT Carbon plus 15-Nitrogen. To find the mass of isotopologues, add the mass of the unknown atom in that molecule. So, search for “C” and it will return 12 add that to 15 for a mass of 27 amu. To find the mass of 13C18O, add 13+18 = 31.

Performing a query on a selected molecule

It is often beneficial to search for all the transitions of a molecule when preparing for an observation. In this case, if a researcher is interested in CO, they would select “CO” from molecule pulldown window and click “SEARCH”. This search is illustrated below as well as the results from the search:

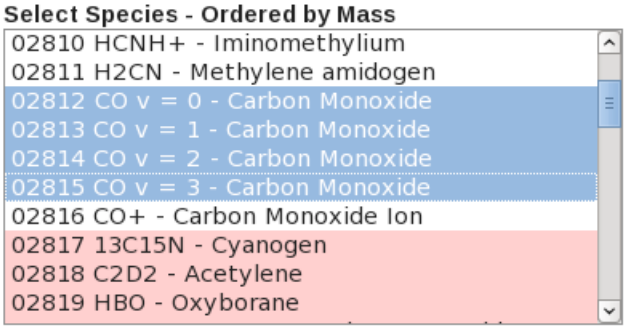


In this case the procedure is:

1. Use the “Mass Calculator...” to find the mass of CO. The mass is 28 amu so search for molecules in the pulldown menu with Splatalogue ID like “028”.
2. “CO v=0” (i.e. CO in the ground vibrational state) has a Splatalogue ID = 02812. Select that molecule (it will highlight).

3. Click the “Search” button and you get the display shown above in the main “Search Results” frame.

A user can also search over many molecular species at the same time. In this case, you hold the “Ctrl” button while selecting molecules from the pulldown menu. As you click on species in the pulldown menu, they will highlight. To select a whole group of species in a row, hold down the “Shift” key, click on the “top” molecule in the row and then the “bottom” molecule in the row. In that case, all molecules between the selected species will be highlighted. In the case below, all the CO species are selected from the v=0 to the v=3 state using the “Shift” key selection. You can see they are all highlighted and will be included in the search:



To perform the search, simply click the “Search” button.

Performing a query over a frequency range

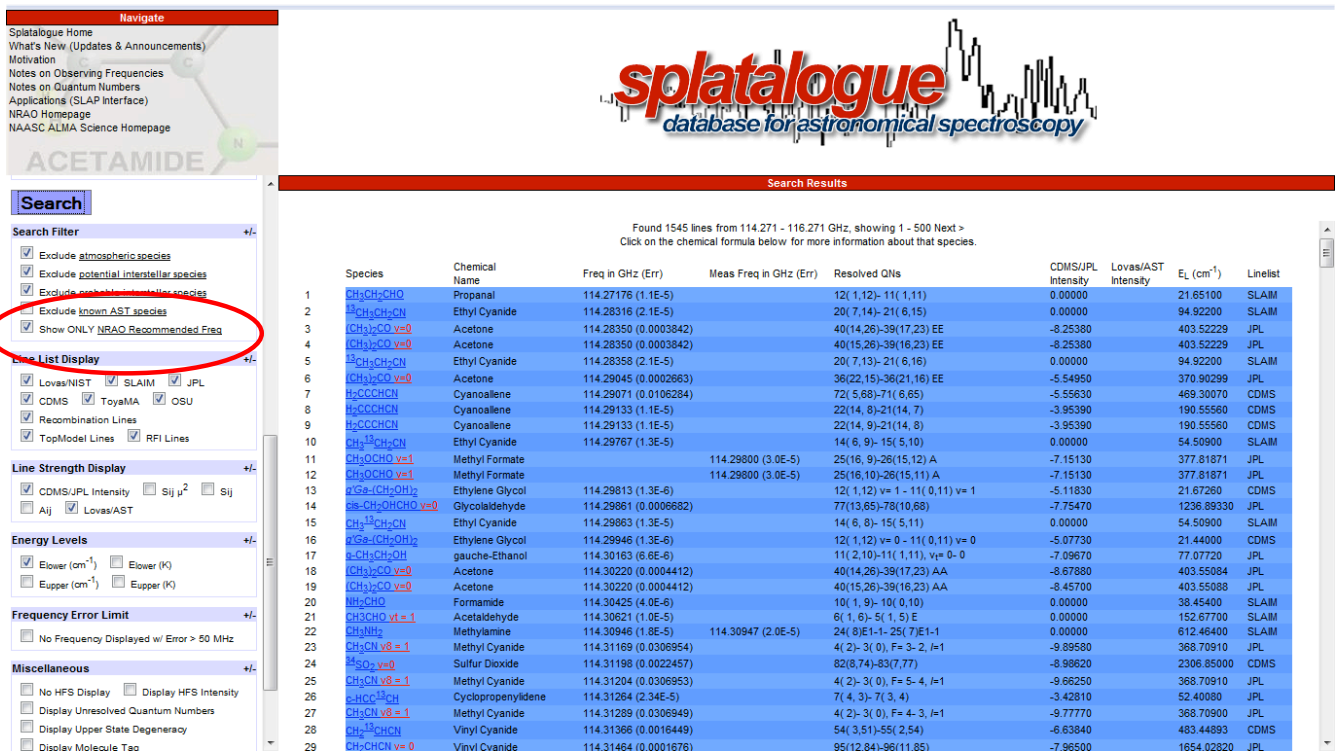
It is also useful when preparing an observation to know what other transitions of molecules are in the passband of your primary search target. In the example below, a search is conducted between 114.271 GHz and 116.271 GHz. That is, we are investigating the other transitions within +/- 1 GHz of the CO v=0, J=1-0 transition. This search is illustrated below as well as the results from the search:

In this case, the procedure is:

1. Select “All” molecules from the pulldown menu
2. Enter a frequency range of 114.271 to 116.271 and highlight the “GHz” radio button
3. Click the “Search” button and you get the following display in the main “Search Results” frame.
4. NOTE: Remember that by default, Splatalogue will display ONLY the known astronomical molecules. If a user wants to utilize the entire dataset including the atmospheric, potential and probable molecules in their search, they need to “uncheck” these options under the “Search Filter” options.

In this case, Splatalogue found 3375 transitions in the selected frequency range. What you can notice though is that Splatalogue reports transitions and frequencies of molecules from ALL catalogs contained in the database. To limit the search or to flag the NRAO recommended frequency of a given transition, a user can select either “Show ONLY NRAO Recommended Frequency” from the “Search Filter” section or “Display NRAO Recommended Frequency” from the “Miscellaneous” section.

In the illustration below, we will "***Show*** ONLY NRAO Recommended Frequency":



By "Showing" only the recommended frequencies, the number of lines was reduced to 1545. This is because NRAO has recommended only one frequency for each transition of every known astronomical molecule. For more information on this procedure and notes on the frequencies displayed in Splatalogue, select "Notes on Observing Frequencies" from the
"Navigation" Frame.

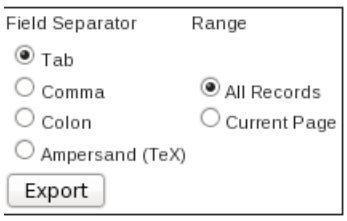
In the following illustration, we “***Display*** the NRAO recommended Frequency”:

Notice now we return to the 3375 transitions but the recommended frequency is now highlighted with a “SPLAT”.

Exporting the data

Once you are satisfied with the search and you have turned on (or off) the display parameters of your choice, you can download the data in various formats. Scrolling down the main "Search Results" frame, you find:

Exporting notes:



The user has the option to select the field delimiters and the range of data to export.

1. While we have made every effort to circumvent the timeout issues associated with PHP, depending on the internet connection and your computer speed, you will often not be able to export any file off the Splatalogue homepage larger than about 25MB. The best thing to do is download your file in smaller parts and combine them later. If you are using linux, "cat" is a straightforward way to join separate files together.
2. If you want to import your dataset from Splatalogue into CASA, then you will need to download the files in a Tab delimited format with the following fields:
    1. Species (chemical formula)
    2. Flag indicating it is an NRAO recommended rest frequency
    3. Name (chemical name)
    4. Rest Frequency (GHz) (This is the NRAO recommended frequency, in many cases alternative frequencies are availabe in other spectral line catalogs and the full list in Splatalogue, see http://www.cv.nrao.edu/php/splat/SPLATFrequency.html for more information).
    5. Resolved Quantum Number (for more details see http://www.cv.nrao.edu/php/splat/QuantumCode.html)
    6. CDMS/JPL Intensity (not available for all species, evaluated at 300 K))
    7. Sijmu^2 (Debye, available for all molecular species)
    8. Log10(Aij) (Einstein A coefficient, available for all molecular species)
    9. E_lower (K)
    10. E_upper (K)
    11. Original spectral line catalog (see http://www.splatalogue.net/ for references)

NOTE: These instructions are relevant for the October 2010 release of CASA. For more information on importing data into casa and the offline version of Splatalogue contained in CASA visit:
https://safe.nrao.edu/wiki/bin/view/ALMA/CASA_Offline_Splat_list

Further Examples and Splatalogue User "Homework"

1. Using the mass calculator, find the molecular mass of the well known interstellar molecules like CO, NH_3, CH_3OH, CH_3OCHO and CH_3CH_2CN.
2. Having the mass of CO, select that molecule from the list and find all the available transitions, (ie. All frequencies) of CO in the known catalogs.
3. Find the NRAO recommended frequencies for CO.
4. Find and display the transitions of CO with an upper state energy greater than 50 K.
5. Find and display the transitions of CO with line strengths greater than 0.2 D^2. (NOTE: make sure you turn off 4) first!)
6. Find and display the transitions of CO with an upper state energy less than 30 cm^{-1} AND line strengths greater than 0.001 D^2.
7. Export the results in 6) in a tab delimited .csv file.
8. Go back to the search defaults. You can just reload the Splatalogue homepage.
9. Select "all" molecules and under the search options, "uncheck" the atmospheric, potential and probable molecule boxes. Search for all transitions between 201 and 202 GHz. How many transitions are there between those frequencies?
    1. "check" the atmospheric box – redo the search. How many transitions are there now?
    2. "check" the atmospheric and potential boxes – redo the search. How many transitions are there now?
    3. "check the atmospheric, potential and probable boxes – redo the search. How many transitions are there now?
10. Find the NRAO recommended frequencies in that frequency range.
11. Find and display the transitions that may be populated in a hot molecular cloud core of 200 K.
12. Display the line strength of all the transitions in $S_{ij}\,\mu^2$ instead of the default values.
13. Export the results in 12) in an ampersand delimited .csv file.

Answers to the "homework" will be made available off the Splatalogue homepage at www.splatalogue.net.