



## ***Splatalogue Quickstart Guide***

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**PURPOSE:** The purpose of this document is to provide a brief overview of the functionality of the Splatalogue homepage available at [www.splatalogue.net](http://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](http://www.splatalogue.net/SLAPNotes.html). 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 send an email to [splatalogue@nrao.edu](mailto:splatalogue@nrao.edu).

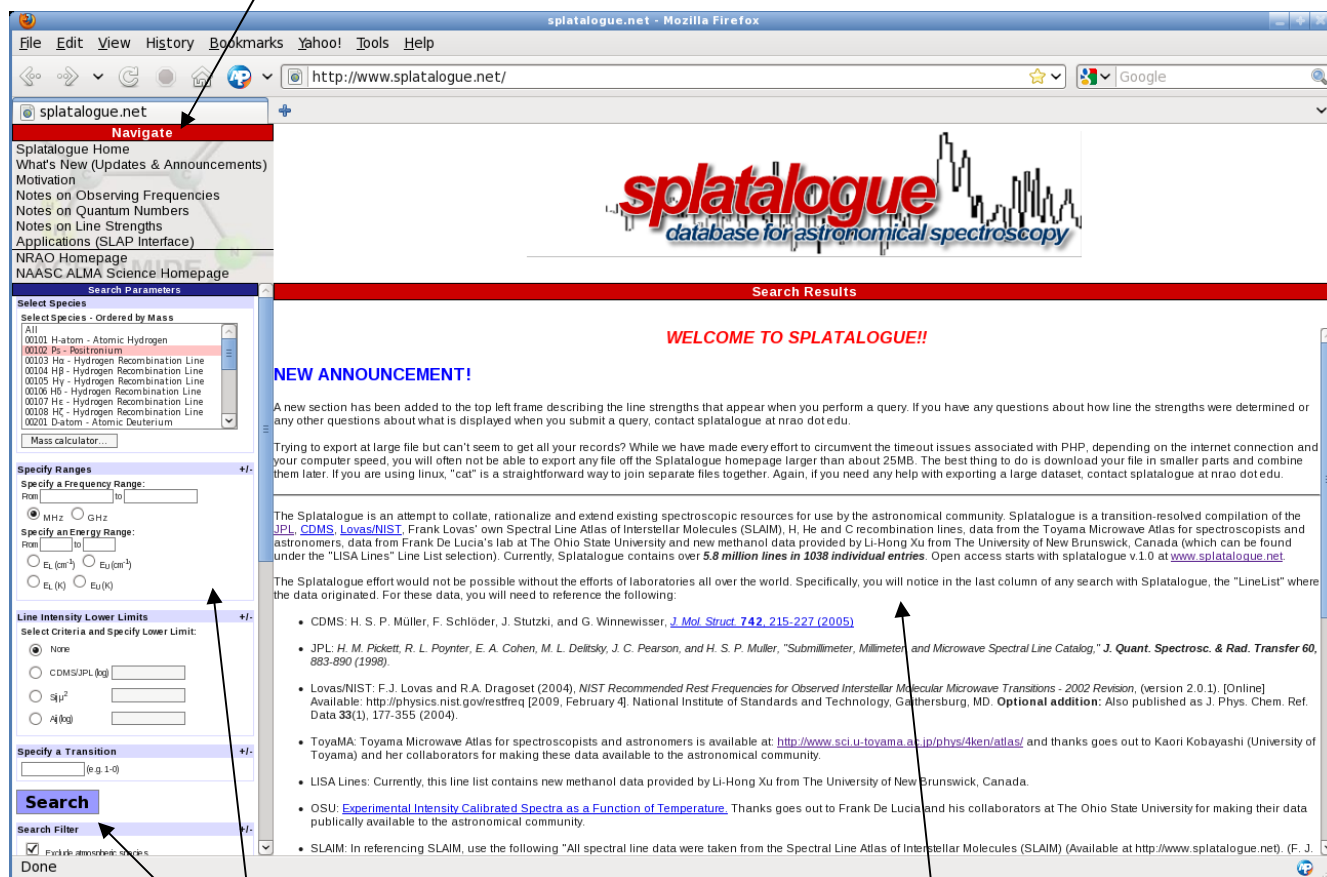
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## BASIC NAVIGATION

When arriving at the Splatalogue homepage at [www.splatalogue.net](http://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) "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.

3) "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.

The screenshot shows the 'Search Parameters' frame with a blue header. Below the header is the 'Select Species' section, which has a title 'Select Species - Ordered by Mass'. It contains a list box with the following items: 'All', '00101 H-atom - Atomic Hydrogen', '00102 Ps - Positronium' (highlighted in red), '00103 H $\alpha$  - Hydrogen Recombination Line', '00104 H $\beta$  - Hydrogen Recombination Line', '00105 H $\gamma$  - Hydrogen Recombination Line', '00106 H $\delta$  - Hydrogen Recombination Line', '00107 H $\epsilon$  - Hydrogen Recombination Line', '00108 H $\zeta$  - Hydrogen Recombination Line', and '00201 D-atom - Atomic Deuterium'. Below the list box is a text input field labeled 'Enter Molecular Formula (Case sensitive)' and a 'Calculate' button. At the bottom of this section is a button labeled 'Mass calculator...'. Arrows from external text blocks point to the list box and the 'Calculate' button.

There are 1038 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.

The screenshot shows two sections of the 'Search Parameters' frame. The top section is 'Specify Ranges' with a '+/-' icon. It contains two sub-sections: 'Specify a Frequency Range:' with 'From' and 'to' input fields and radio buttons for 'MHz' (selected) and 'GHz'; and 'Specify an Energy Range:' with 'From' and 'to' input fields and radio buttons for 'E<sub>L</sub> (cm<sup>-1</sup>)', 'E<sub>U</sub> (cm<sup>-1</sup>)', 'E<sub>L</sub> (K)', and 'E<sub>U</sub> (K)'. The bottom section is 'Line Intensity Lower Limits' with a '+/-' icon. It contains a sub-section 'Select Criteria and Specify Lower Limit:' with radio buttons for 'None' (selected), 'CDMS/JPL (log)' (with an input field), 'S<sub>ij</sub>  $\mu^2$ ' (with an input field), and 'A<sub>ij</sub> (log)' (with an input field). Below these sections is a 'Specify a Transition' section with a '+/-' icon and an input field with '(e.g. 1-0)' as a hint. At the bottom of the frame is a large blue button labeled 'Search'. Arrows from external text blocks point to the 'Specify Ranges' section, the 'Line Intensity Lower Limits' section, and the 'Search' button.

Limit your searches by entering:  
A frequency range  
An energy range  
A line strength range  
Or a transition

Note, you can only search 1 type of line strength in a given search. This, you cannot limit the line strength in A<sub>ij</sub> AND S<sub>ij</sub> $\mu^2$ .

Finally, the SEARCH button is clearly marked and highlighted.

**Search Filter** +/-

- ☒ Exclude atmospheric species
- ☒ Exclude potential interstellar species
- ☒ Exclude probable interstellar species
- ☐ Include known AST species
- ☐ Show ONLY NRAO Recommended Freq

**Line List Display** +/-

- ☒ Lovas/NIST ☒ SLAIM ☒ JPL ☒ CDMS
- ☒ ToyaMA ☒ OSU ☒ Recombination Lines
- ☒ LISA Lines

**Line Strength Display** +/-

- ☒ CDMS/JPL Intensity ☐  $S_{ij} \mu^2$  ☐  $S_{ij}$  ☐  $A_{ij}$
- ☒ Lovas/AST

**Energy Levels** +/-

- ☒  $E_{lower} (cm^{-1})$  ☐  $E_{lower} (K)$  ☐  $E_{upper} (cm^{-1})$
- ☐  $E_{upper} (K)$

**Frequency Error Limit** +/-

- ☐ No Frequency Displayed w/ Error > 50 MHz

Limit the number of species displayed by excluding those species that have not yet 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** +/-

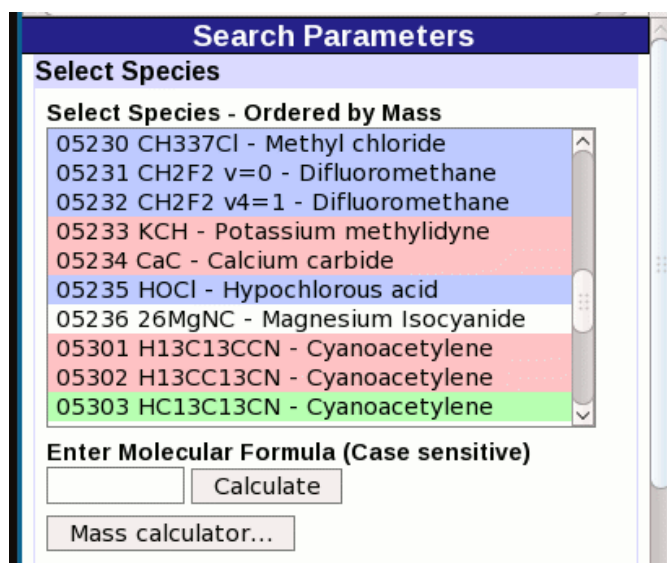
- ☐ No HFS Display ☐ Display HFS Intensity
- ☐ Display Unresolved Quantum Numbers
- ☐ Display Upper State Degeneracy
- ☐ Display Molecule Tag
- ☐ Display Quantum Number Code
- ☐ Display Lovas Lab Ref ☐ Display Lovas Obs Ref
- ☐ Display Ordered Frequency ONLY
- ☐ Display NRAO Recommended Frequencies

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 <sub>L</sub> (cm <sup>-1</sup> )	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...). Please email [splatalogue@nrao.edu](mailto:splatalogue@nrao.edu) on using these different telescope color schemes as they are not fully implemented off the splatalogue.net homepage.

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:

### Select Species - Ordered by Mass

06003	cis-CH <sub>2</sub> OHCHO v=0	- Glycolaldehyde
06004	cis-CH <sub>2</sub> OHCHO v=1	- Glycolaldehyde
06005	cis-CH <sub>2</sub> OHCHO v=2	- Glycolaldehyde
06006	cis-CH <sub>2</sub> OHCHO v=3	- Glycolaldehyde
06007	CH <sub>3</sub> OCHO v=0	- Methyl Formate
06008	CH <sub>3</sub> OCHO v=1	- Methyl Formate
06009	CH <sub>3</sub> COOH v=0	- Acetic Acid
06010	CH <sub>3</sub> COOH v=1	- Acetic Acid
06011	Ga-n-C <sub>3</sub> H <sub>7</sub> OH	- n-Propanol
06012	Na <sup>37</sup> Cl v = 0	- Sodium chloride

### Enter Molecular Formula (Case sensitive)

CH<sub>3</sub>OCHO    Calculate

Species ID like "060"

Mass calculator...

CH<sub>3</sub>OCHO 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 CH<sub>3</sub>OCHO 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<sup>+</sup> 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 <sup>13</sup>C<sup>18</sup>O, 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:

Search Parameters		Search Results							
<div>Select Species</div> <div>Select Species - Ordered by Mass</div> <div>02811 H2C-N - Methylene amidogen</div> <div>02812 H2C-C - Ethynylidene</div> <div>02813 CO v = 1 - Carbon Monoxide</div> <div>02814 CO v = 2 - Carbon Monoxide</div> <div>02815 CO v = 3 - Carbon Monoxide</div> <div>02816 CO+ - Carbon Monoxide Ion</div> <div>02817 H2CN - Cyanogen</div> <div>02818 C2H2 - Acetylene</div> <div>02819 H2O - Oxidane</div> <div>02901 H2CO v = 0 - Hydrogen cyanide</div> <div>Enter Molecular Formula (Case sensitive)</div> <div>CO <input type="text"/> Calculate</div> <div>Species ID like "028"</div> <div>Mass calculator...</div>		<div>Found 242 lines, showing 1 - 242</div> <div>Click on the chemical formula below for more information about that species.</div>							
	Species	Chemical Name	Freq in MHz (Err)	Meas Freq in MHz (Err)	Resolved QNs	CDMS/JPL Intensity	Lovas/AST Intensity	El (cm-1)	Linelist
1	<a href="#">CO v=0</a>	Carbon Monoxide		115271.20180 (0.0005)	1-0	-5.01050		0.00000	CDMS
2	<a href="#">CO v=0</a>	Carbon Monoxide		115271.20180 (0.0005)	1-0	-5.01050		0.00000	JPL
3	<a href="#">CO v=0</a>	Carbon Monoxide	115271.20200 (1)		1-0	0.00000	60.00000	0.00000	Lovas
4	<a href="#">CO v=0</a>	Carbon Monoxide	115271.20200 (0)		1-0	0.00000		0.00000	SLAIM
5	<a href="#">CO v=0</a>	Carbon Monoxide		230538.00000 (0.0005)	2-1	-4.11970		3.84500	CDMS
6	<a href="#">CO v=0</a>	Carbon Monoxide		230538.00000 (0.0005)	2-1	-4.11970		3.84500	JPL
7	<a href="#">CO v=0</a>	Carbon Monoxide	230538.00000 (1)		2-1	0.00000	70.00000	0.00000	Lovas
8	<a href="#">CO v=0</a>	Carbon Monoxide	230538.00000 (0)		2-1	0.00000		3.84500	SLAIM
9	<a href="#">CO v=0</a>	Carbon Monoxide		345795.98990 (0.0005)	3-2	-3.61180		11.53500	CDMS
10	<a href="#">CO v=0</a>	Carbon Monoxide		345795.98990 (0.0005)	3-2	-3.61180		11.53500	JPL
11	<a href="#">CO v=0</a>	Carbon Monoxide	345795.99000 (1)		3-2	0.00000	70.00000	0.00000	Lovas
12	<a href="#">CO v=0</a>	Carbon Monoxide	345795.99000 (0)		3-2	0.00000		11.53500	SLAIM
13	<a href="#">CO v=0</a>	Carbon Monoxide	461040.76800 (1)		4-3	0.00000	60.00000	0.00000	Lovas
14	<a href="#">CO v=0</a>	Carbon Monoxide	461040.76800 (0)		4-3	0.00000		23.06900	SLAIM
15	<a href="#">CO v=0</a>	Carbon Monoxide		461040.76820 (0.0005)	4-3	-3.26570		23.06950	CDMS
16	<a href="#">CO v=0</a>	Carbon Monoxide		461040.76820 (0.0005)	4-3	-3.26570		23.06950	JPL
17	<a href="#">CO v=0</a>	Carbon Monoxide		576267.93050 (0.0005)	5-4	-3.01180		38.44810	CDMS
18	<a href="#">CO v=0</a>	Carbon Monoxide		576267.93050 (0.0005)	5-4	-3.01180		38.44810	JPL
19	<a href="#">CO v=0</a>	Carbon Monoxide	576267.93100 (0)		5-4	0.00000		38.44800	SLAIM
20	<a href="#">CO v=0</a>	Carbon Monoxide	691473.07600 (1)		6-5	0.00000	100.00000	0.00000	Lovas
21	<a href="#">CO v=0</a>	Carbon Monoxide	691473.07600 (0)		6-5	0.00000		57.67000	SLAIM
22	<a href="#">CO v=0</a>	Carbon Monoxide		691473.07630 (0.0005)	6-5	-2.81930		57.67040	CDMS
23	<a href="#">CO v=0</a>	Carbon Monoxide		691473.07630 (0.0005)	6-5	-2.81930		57.67040	JPL
24	<a href="#">CO v=1</a>	Carbon Monoxide	806651.80100 (1)		7-6	0.00000	110.00000	0.00000	Lovas
25	<a href="#">CO v=1</a>	Carbon Monoxide	806651.80100 (0)		7-6	0.00000		80.73500	SLAIM
26	<a href="#">CO v=1</a>	Carbon Monoxide		806651.80600 (0.005)	7-6	-2.67160		80.73540	CDMS
27	<a href="#">CO v=1</a>	Carbon Monoxide		806651.80600 (0.005)	7-6	-2.67160		80.73540	JPL
28	<a href="#">CO v=1</a>	Carbon Monoxide		921799.70000 (0.005)	8-7	-2.55900		107.64240	CDMS
29	<a href="#">CO v=1</a>	Carbon Monoxide		921799.70000 (0.005)	8-7	-2.55900		107.64240	JPL

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:

### Select Species - Ordered by Mass

02810	HCNH+ - Iminomethylium
02811	H2CN - Methylene amidogen
02812	CO v = 0 - Carbon Monoxide
02813	CO v = 1 - Carbon Monoxide
02814	CO v = 2 - Carbon Monoxide
02815	CO v = 3 - Carbon Monoxide
02816	CO+ - Carbon Monoxide Ion
02817	13C15N - Cyanogen
02818	C2D2 - Acetylene
02819	HBO - Oxyborane

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:

**Search Parameters**

Select Species - Ordered by Mass

0010 H-atom - Atomic Hydrogen  
00102 Ps - Positronium  
00103 H $\alpha$  - Hydrogen Recombination Line  
00104 H $\beta$  - Hydrogen Recombination Line  
00105 H $\gamma$  - Hydrogen Recombination Line  
00106 H $\delta$  - Hydrogen Recombination Line  
00107 H $\epsilon$  - Hydrogen Recombination Line  
00108 H $\zeta$  - Hydrogen Recombination Line  
0020 Dalton - Atomic Deuterium

Enter Molecular Formula (Case sensitive)  
CO   
Species ID like 1026\*

**Specify Ranges**

Specify a Frequency Range:  
From 114.271 to 116.271  
☐ MHz ☒ GHz

Specify an Energy Range:  
From  to   
☐ E<sub>L</sub> (cm<sup>-1</sup>) ☐ E<sub>U</sub> (cm<sup>-1</sup>)  
☐ E<sub>L</sub> (K) ☐ E<sub>U</sub> (K)

**Line Intensity Lower Limits**

Select Criteria and Specify Lower Limit:

☒ None  
☐ CDMS/JPL (kg)  
☐ JPL  
☐ All (kg)

**Specify a Transition**  
 (e.g. 1-0)

**Search Results**

Found 3192 lines from 114.271 - 116.271 GHz, showing 1 - 500 Next >  
Click on the chemical formula below for more information about that species.

	Species	Chemical Name	Freq in GHz (Err)	Meas Freq in GHz (Err)	Resolved QNs	CDMS/JPL Intensity	Lovas/AST Intensity	E <sub>L</sub> (cm <sup>-1</sup> )	Linelist
1	<a href="#">CH<sub>3</sub>CH<sub>2</sub>CHO</a>	Propanal	114.27176 (0.011)		12(1,12)-11(1,11)	0.00000		21.65100	SLAIM
2	<a href="#"><sup>13</sup>CH<sub>3</sub>CH<sub>2</sub>CN</a>	Ethyl Cyanide	114.28312 (0.0147)		20(7,14)-21(6,15)	-5.27200		94.92200	CDMS
3	<a href="#"><sup>13</sup>CH<sub>3</sub>CH<sub>2</sub>CN</a>	Ethyl Cyanide	114.28316 (0.021)		20(7,14)-21(6,15)	0.00000		94.92200	SLAIM
4	<a href="#">(CH<sub>3</sub>)<sub>2</sub>CO v=0</a>	Acetone	114.28350 (0.3842)		40(14,26)-39(17,23) EE	-8.25380		403.52229	JPL
5	<a href="#">(CH<sub>3</sub>)<sub>2</sub>CO v=0</a>	Acetone	114.28350 (0.3842)		40(15,26)-39(16,23) EE	-8.25380		403.52229	JPL
6	<a href="#"><sup>13</sup>CH<sub>3</sub>CH<sub>2</sub>CN</a>	Ethyl Cyanide	114.28354 (0.0147)		20(7,13)-21(6,16)	-5.27200		94.92200	CDMS
7	<a href="#"><sup>13</sup>CH<sub>3</sub>CH<sub>2</sub>CN</a>	Ethyl Cyanide	114.28358 (0.021)		20(7,13)-21(6,16)	0.00000		94.92200	SLAIM
8	<a href="#">(CH<sub>3</sub>)<sub>2</sub>CO v=0</a>	Acetone	114.29045 (0.528)		36(22,15)-36(21,16) EE	0.00000		370.90400	SLAIM
9	<a href="#">(CH<sub>3</sub>)<sub>2</sub>CO v=0</a>	Acetone	114.29045 (0.2663)		36(22,15)-36(21,16) EE	-5.54950		370.90299	JPL
10	<a href="#">H<sub>2</sub>CCOCHCN</a>	Cyanoallene	114.29071 (10.6284)		72(5,68)-71(6,65)	-5.55630		469.30070	CDMS
11	<a href="#">Unidentified Transition</a>	UNIDENTIFIED	114.29100 (19)		U-114291	0.00000	0.09000	0.00000	Lovas
12	<a href="#">H<sub>2</sub>CCOCHCN</a>	Cyanoallene	114.29101 (0.066)		22(14,9)-21(14,8), F=22-21	0.00000		190.44000	SLAIM
13	<a href="#">H<sub>2</sub>CCOCHCN</a>	Cyanoallene	114.29101 (0.066)		22(14,8)-21(14,7), F=22-21	0.00000		190.44000	SLAIM
14	<a href="#">CH<sub>3</sub>CH<sub>2</sub><sup>13</sup>CN</a>	Ethyl Cyanide	114.29108 (2.698)		9(3,6)-9(2,7), F=8-8	-5.26210		16.52730	JPL
15	<a href="#">H<sub>2</sub>CCOCHCN</a>	Cyanoallene	114.29109 (0.065)		22(14,9)-21(14,8)	0.00000		190.44000	SLAIM

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 3192 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”:

Search Results

Found 1472 lines from 114.271 - 116.271 GHz, showing 1 - 500 Next >  
Click on the chemical formula below for more information about that species.

	Species	Chemical Name	Freq in GHz (Err)	Meas Freq in GHz (Err)	Resolved QNs	CDMS/JPL Intensity	Lovas/AST Intensity	E <sub>L</sub> (cm <sup>-1</sup> )	Linelist
1	CH <sub>3</sub> CH <sub>2</sub> CHO	Propanal	114.27176 (0.011)		12(1,12)-11(1,11)	0.00000		21.65100	SLAIM
2	<sup>13</sup> CH <sub>3</sub> CH <sub>2</sub> CN	Ethyl Cyanide	114.28316 (0.021)		20(7,14)-21(6,15)	0.00000		94.92200	SLAIM
3	(CH <sub>3</sub> ) <sub>2</sub> CO v=0	Acetone	114.28350 (0.3842)		40(14,26)-39(17,23) EE	-8.25380		403.52229	JPL
4	(CH <sub>3</sub> ) <sub>2</sub> CO v=0	Acetone	114.28350 (0.3842)		40(15,26)-39(16,23) EE	-8.25380		403.52229	JPL
5	<sup>13</sup> CH <sub>3</sub> CH <sub>2</sub> CN	Ethyl Cyanide	114.28358 (0.021)		20(7,13)-21(6,16)	0.00000		94.92200	SLAIM
6	(CH <sub>3</sub> ) <sub>2</sub> CO v=0	Acetone	114.29045 (0.2663)		36(22,15)-36(21,16) EE	-5.54950		370.90299	JPL
7	H <sub>2</sub> CCCHCN	Cyanoallene	114.29071 (0.6284)		72(5,68)-71(6,65)	-5.55630		469.30070	CDMS
8	H <sub>2</sub> CCCHCN	Cyanoallene	114.29133 (0.011)		22(14,8)-21(14,7)	-3.95390		190.55560	CDMS
9	H <sub>2</sub> CCCHCN	Cyanoallene	114.29133 (0.011)		22(14,9)-21(14,8)	-3.95390		190.55560	CDMS
10	CH <sub>3</sub> <sup>13</sup> CH <sub>2</sub> CN	Ethyl Cyanide	114.29767 (0.013)		14(6,9)-15(5,10)	0.00000		54.50900	SLAIM
11	gGa-(CH <sub>2</sub> OH) <sub>2</sub>	Ethylene Glycol	114.29813 (0.0013)		12(1,12) v=1 - 11(0,11) v=1	-5.11830		21.67260	CDMS
12	os-CH <sub>2</sub> OHCHO v=0	Glycolaldehyde	114.29861 (0.6682)		77(13,65)-78(10,68)	-7.75470		1236.89330	JPL
13	CH <sub>3</sub> <sup>13</sup> CH <sub>2</sub> CN	Ethyl Cyanide	114.29863 (0.013)		14(6,8)-15(5,11)	0.00000		54.50900	SLAIM
14	gGa-(CH <sub>2</sub> OH) <sub>2</sub>	Ethylene Glycol	114.29946 (0.0013)		12(1,12) v=0 - 11(0,11) v=0	-5.07730		21.44000	CDMS
15	g-CH <sub>2</sub> CH <sub>2</sub> OH	gauche-Ethanol	114.30163 (0.0066)		11(2,10)-11(1,11), v=0-0	-7.09670		77.07720	JPL
16	(CH <sub>3</sub> ) <sub>2</sub> CO v=0	Acetone	114.30220 (0.4412)		40(14,26)-39(17,23) AA	-8.67880		403.55084	JPL
17	(CH <sub>3</sub> ) <sub>2</sub> CO v=0	Acetone	114.30220 (0.4412)		40(15,26)-39(16,23) AA	-8.45700		403.55088	JPL
18	NH <sub>2</sub> CHO	Formamide	114.30425 (0.004)		10(1,9)-10(0,10)	0.00000		38.45400	SLAIM
19	CH <sub>3</sub> CHO v=1	Acetaldehyde	114.30621 (0.01)		6(1,6)-5(1,5) E	0.00000		152.67700	SLAIM
20	CH <sub>3</sub> NH <sub>2</sub>	Methylamine	114.30946 (0.018)	114.30947 (0.02)	24(8)E1-1-25(7)E1-1	0.00000		612.46400	SLAIM
21	S <sub>2</sub> O <sub>2</sub> v=0	Sulfur Dioxide	114.31198 (2.2457)		82(8,74)-83(7,77)	-9.88620		2306.85000	CDMS
22	c-HCC <sup>13</sup> CH	Cyclopropenylidene	114.31264 (0.0234)		7(4,3)-7(3,4)	-3.42810		52.40080	JPL
23	CH <sub>3</sub> <sup>13</sup> CHCN	Vinyl Cyanide	114.31366 (1.6449)		54(3,51)-55(2,54)	-6.63840		483.44893	CDMS

By “Showing” only the recommended frequencies, the number of lines was reduced to 1492. 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 Splatologue, select “Notes on Observing Frequencies” from the “Navigation” Frame.

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

Search Results

Found 3192 lines from 114.271 - 116.271 GHz, showing 1 - 500 Next >  
Click on the chemical formula below for more information about that species.

	Species	NRAO Recommended	Chemical Name	Freq in GHz (Err)	Meas Freq in GHz (Err)	Resolved QNs	CDMS/JPL Intensity	Lovas/AST Intensity	E <sub>L</sub> (cm <sup>-1</sup> )	Linelist
1	CH <sub>3</sub> CH <sub>2</sub> CHO	*	Propanal	114.27176 (0.011)		12(1,12)-11(1,11)	0.00000		21.65100	SLAIM
2	<sup>13</sup> CH <sub>3</sub> CH <sub>2</sub> CN	*	Ethyl Cyanide	114.28312 (0.0147)		20(7,14)-21(6,15)	-5.27200		94.92200	CDMS
3	<sup>13</sup> CH <sub>3</sub> CH <sub>2</sub> CN	*	Ethyl Cyanide	114.28316 (0.021)		20(7,14)-21(6,15)	0.00000		94.92200	SLAIM
4	(CH <sub>3</sub> ) <sub>2</sub> CO v=0	*	Acetone	114.28350 (0.3842)		40(14,26)-39(17,23) EE	-8.25380		403.52229	JPL
5	(CH <sub>3</sub> ) <sub>2</sub> CO v=0	*	Acetone	114.28350 (0.3842)		40(15,26)-39(16,23) EE	-8.25380		403.52229	JPL
6	<sup>13</sup> CH <sub>3</sub> CH <sub>2</sub> CN	*	Ethyl Cyanide	114.28354 (0.0147)		20(7,13)-21(6,16)	-5.27200		94.92200	CDMS
7	<sup>13</sup> CH <sub>3</sub> CH <sub>2</sub> CN	*	Ethyl Cyanide	114.28358 (0.021)		20(7,13)-21(6,16)	0.00000		94.92200	SLAIM
8	(CH <sub>3</sub> ) <sub>2</sub> CO v=0	*	Acetone	114.29045 (0.528)		36(22,15)-36(21,16) EE	0.00000		370.90400	SLAIM
9	(CH <sub>3</sub> ) <sub>2</sub> CO v=0	*	Acetone	114.29045 (0.2663)		36(22,15)-36(21,16) EE	-5.54950		370.90299	JPL
10	H <sub>2</sub> CCCHCN	*	Cyanoallene	114.29071 (0.6284)		72(5,68)-71(6,65)	-5.55630		469.30070	CDMS
11	Unidentified Transition		UNIDENTIFIED	114.29100 (19)		U-114291	0.00000	0.09000	0.00000	Lovas
12	H <sub>2</sub> CCCHCN		Cyanoallene	114.29101 (0.066)		22(14,9)-21(14,8), F=22-21	0.00000		190.44000	SLAIM
13	H <sub>2</sub> CCCHCN		Cyanoallene	114.29101 (0.066)		22(14,8)-21(14,7), F=22-21	0.00000		190.44000	SLAIM
14	CH <sub>3</sub> CH <sub>2</sub> <sup>13</sup> CH		Ethyl Cyanide	114.29108 (2.698)		9(3,6)-9(2,7), F=8-8	-5.26210		16.52730	JPL
15	H <sub>2</sub> CCCHCN		Cyanoallene	114.29109		22(14,9)-21(14,8)	0.00000		190.44000	SLAIM

Notice now we return to the 3192 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:

700  
500

[H<sub>2</sub>CCCHCN](#)

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

Field Separator	Range
<input checked="" type="radio"/> Tab	<input checked="" type="radio"/> All Records
<input type="radio"/> Comma	<input type="radio"/> Current Page
<input type="radio"/> Colon	
<input type="radio"/> Ampersand (TeX)	
<input type="button" value="Export"/>	

### Exporting notes:

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 available 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](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<sub>3</sub>, CH<sub>3</sub>OH, CH<sub>3</sub>OCHO and CH<sub>3</sub>CH<sub>2</sub>CN.
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<sup>2</sup>. (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<sup>-1</sup> AND line strengths greater than 0.001 D<sup>2</sup>.
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<sub>ij</sub>μ<sup>2</sup> 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](http://www.splatalogue.net).