Feedbacks from user-oriented tools: CASSIS

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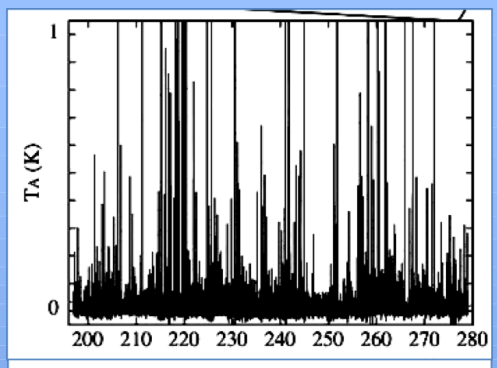
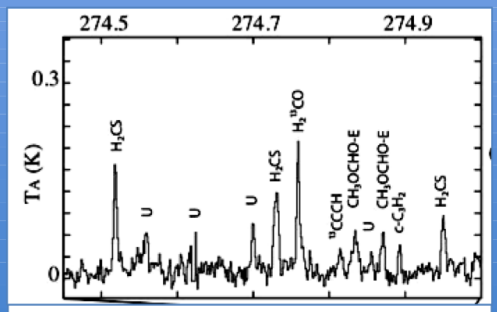
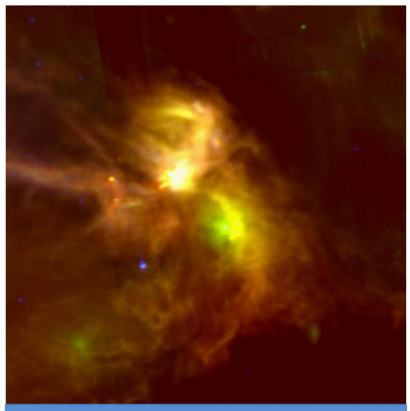
OBSERVATIONS



STEP 1: Observe the spectrum of the source.
Tool: telescope

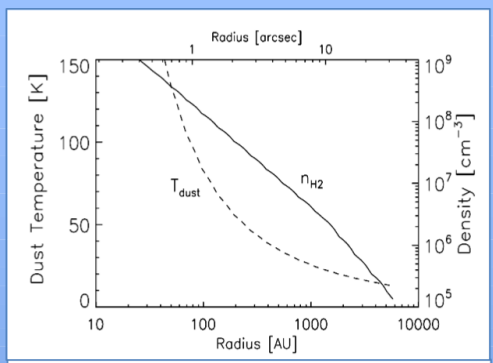


STEP 2: Identify the lines and species.
Tool: spectroscopic data

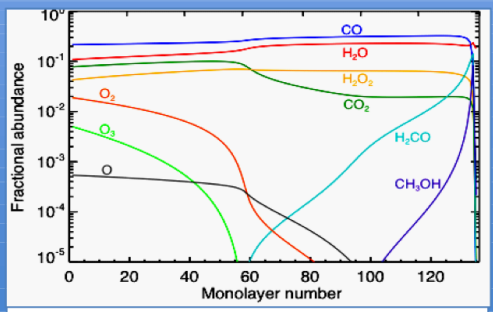


ASTROPHYSICAL OBJECT

TOOLS & MODELS



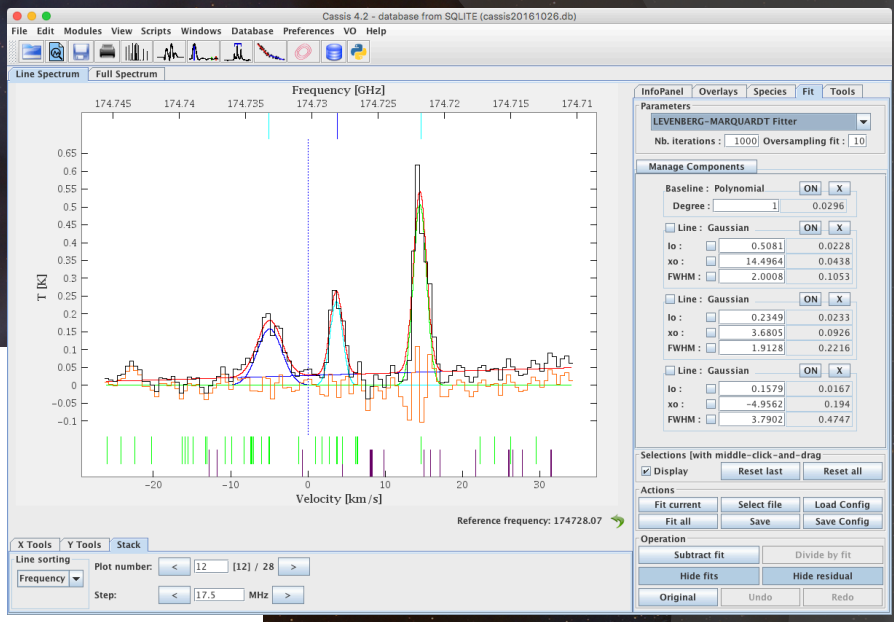
STEP 3: Derive the physical and chemical structure.
Tool: radiative transfer models



STEP 4: Understand the chemical structure.
Tool: astrochemical models

CASSIS (Centre d'Analyse Scientifique de Spectres Instrumentaux et Synthétiques):

http://cassis.irap.omp.eu/



Astrophysical template (fixed parameters N, T_k, T_{ex}, N_{H2}, Δv, choice of the molecule…)

Observed spectra (laboratory or telescope) SSAP protocol (IVOA)

CASSIS

- LTE model and Radex
- Parameters to vary: N, T_k, T_{ex}, n_{H2}, Δv, choice of the molecule and telescope, beam dilution…

Spectroscopic and molecular databases (JPL, CDMS, NIST)

TAP protocol (IVOA)

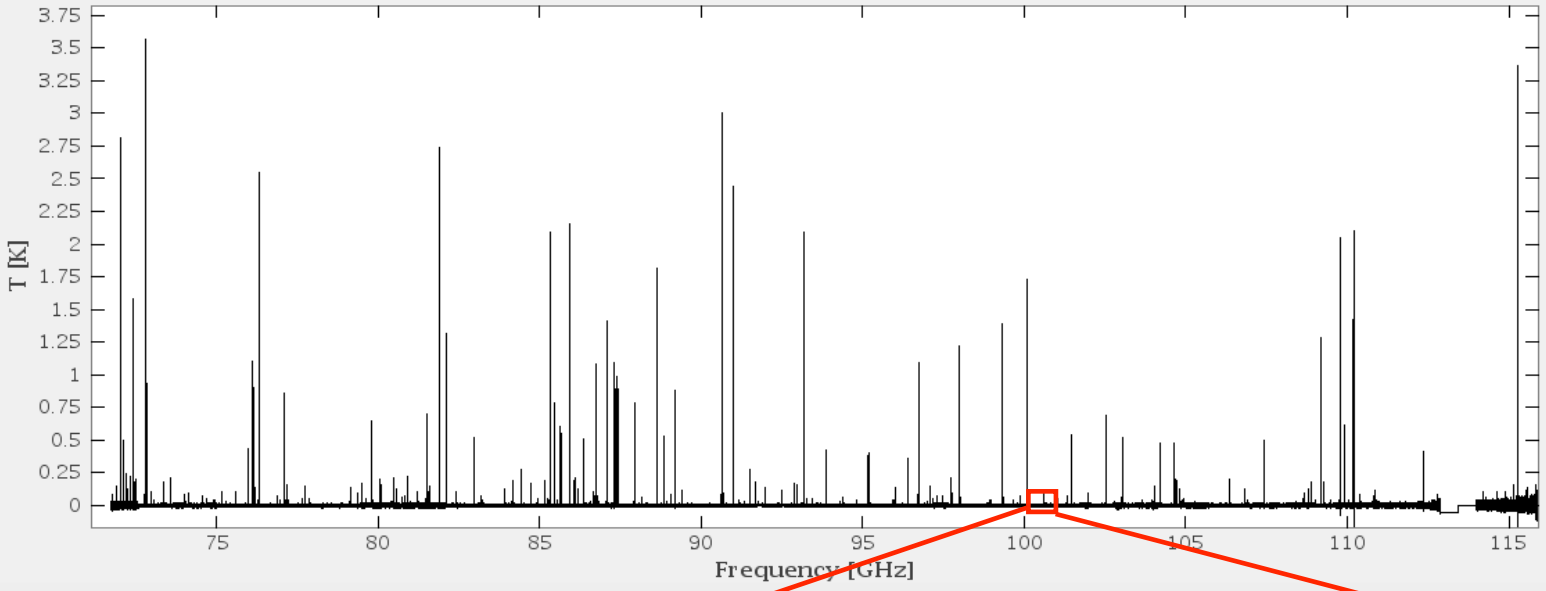
VAMDC Virtual Atomic and Molecular Data Centre

Synthetic spectra, Line identification, Automatic adjustment (MCMC, χ^2), Rotational diagram

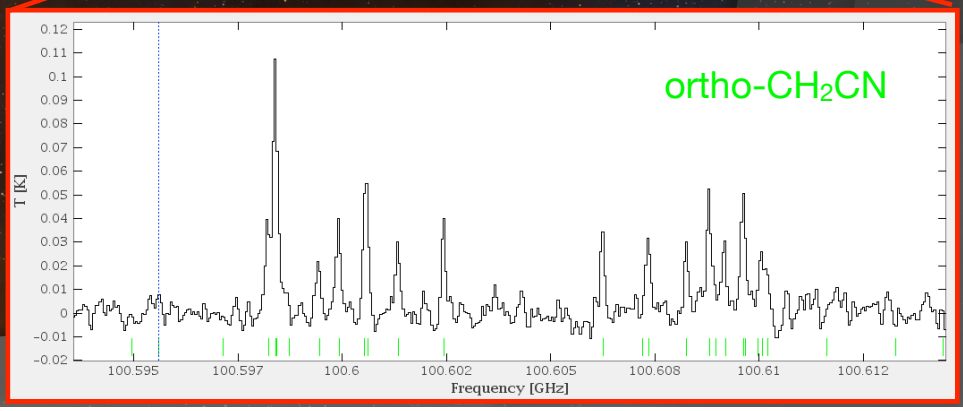
+ CASSIS own databases with:

1) ortho / para / A / E separation
2) HFS
3) ~80 entries for Radex compatible collisional files

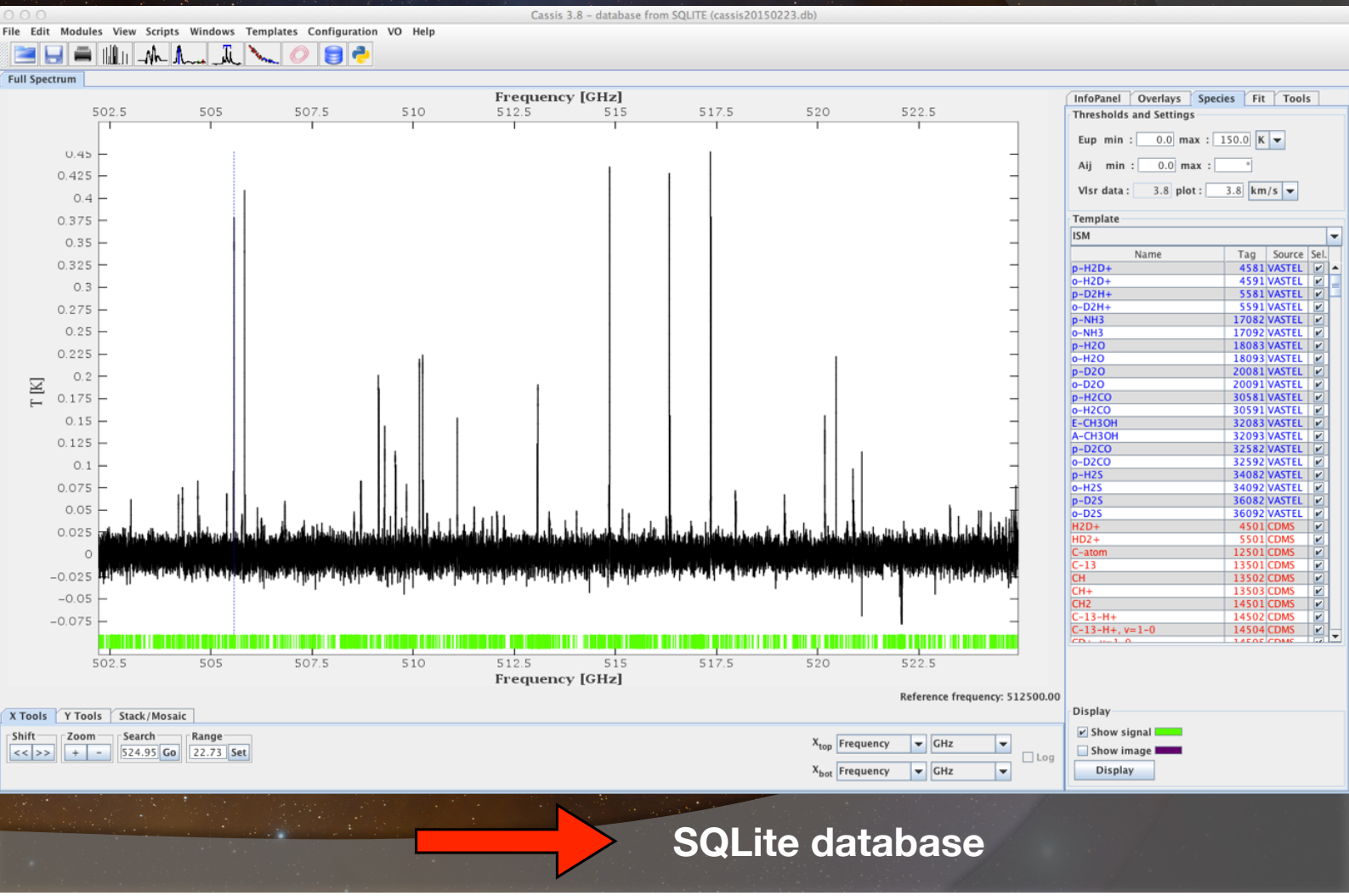
I. Line Identification



- JPL standalone
- CDMS standalone
- Your own database
- VAMDC: NIST, JPL, VALD, CDMS etc…

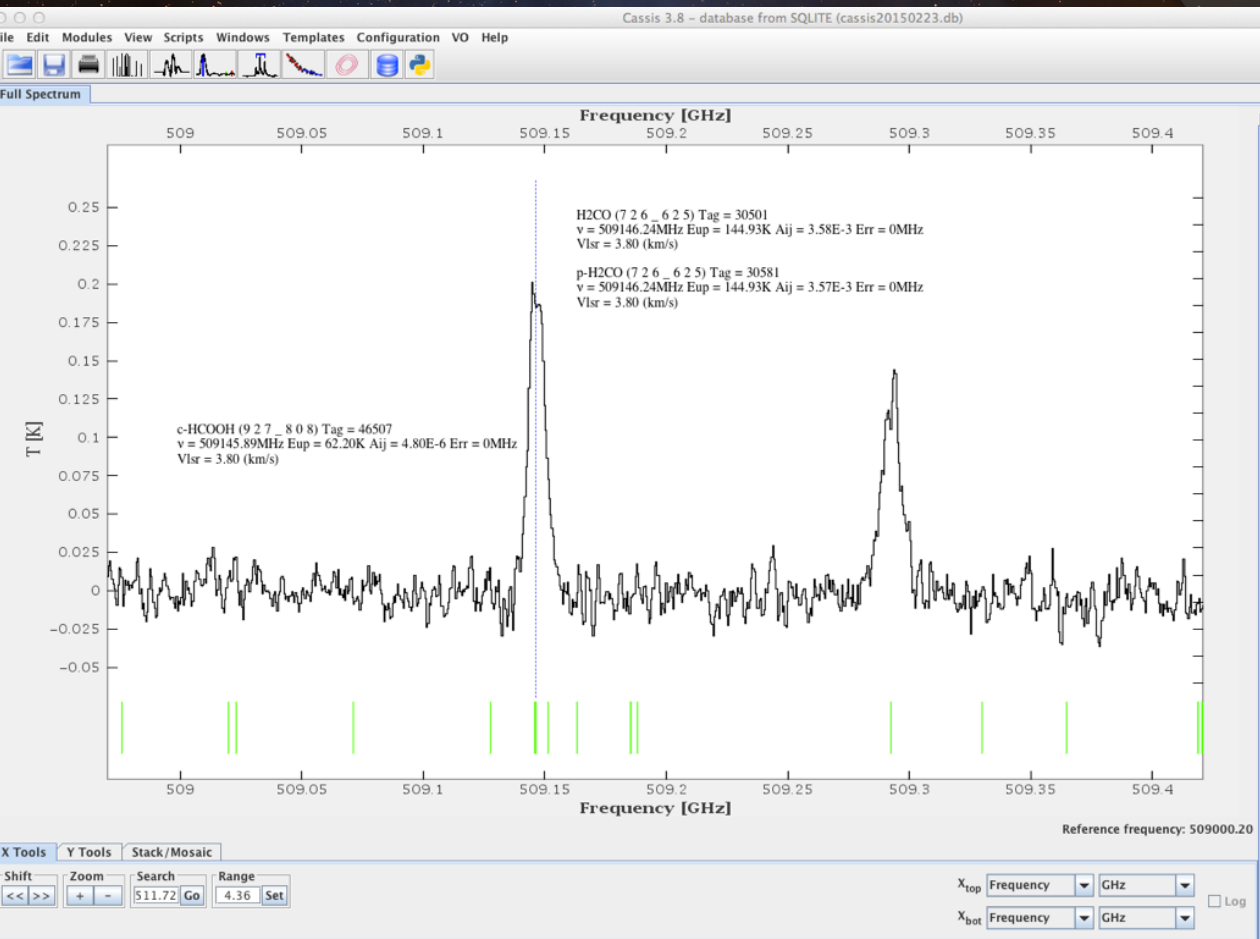


I. Line Identification



SQLite database

I. Line Identification



SQLite database

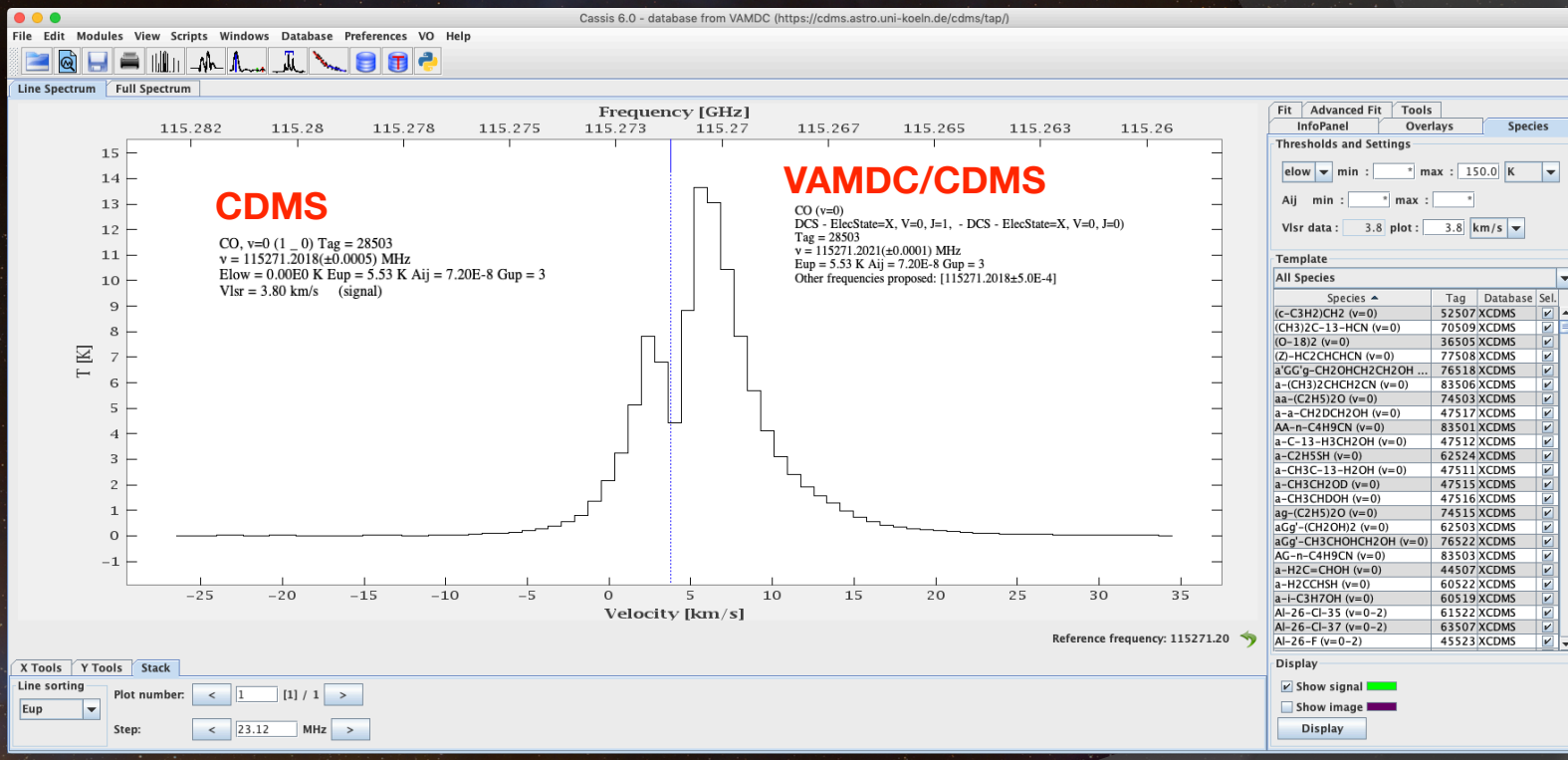
I. Line Identification: Databases and interoperability

The astronomers need: atomic, molecular databases

Local database (SQLite), built on CDMS, JPL, NIST, and private databases (lab or computations), database with nuclear spin state (ortho, para, A and E): *very quick*
CASSIS sometimes finds incoherences in the databases

Access to the CDMS, JPL, NIST and VALD databases linked through VAMDC: *very slow*
Questions:
1) Define the best value for the frequency: EXP, THEO…
2) Within CASSIS, we must retrieve everything, references included: not "useful" for a quick line identification! Too time consuming. Solution: json?
3) Through the portal, is it possible to select a database only? And define criteria?
4) Retrieve a whole SQLite database from VAMDC with regular updates? How big?

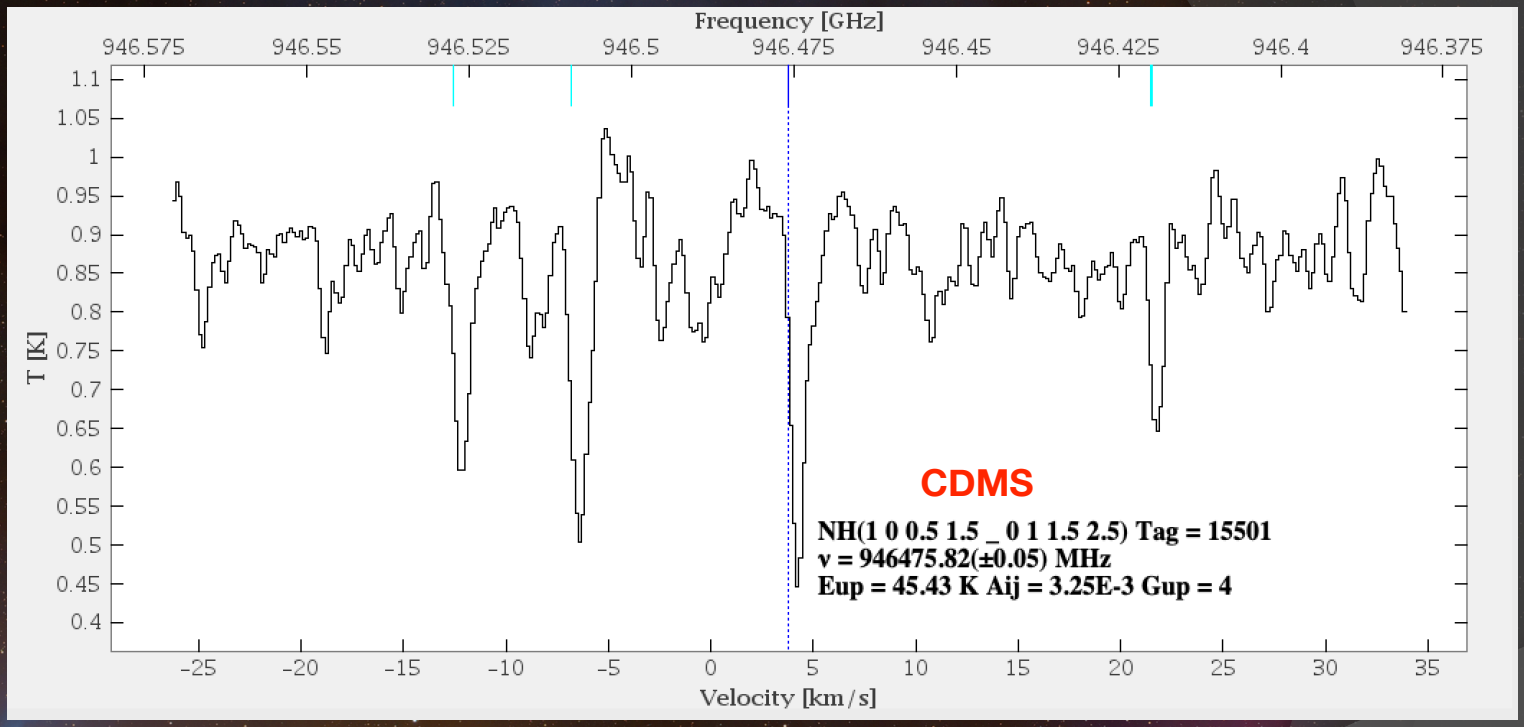
I. Line Identification: VAMDC Access to CDMS



VAMDC: not limited for example for the 3 digit limit on the statistical weigh

When many frequencies available, we choose the one with the lowest uncertainty.

I. Line Identification: VAMDC Access to CDMS

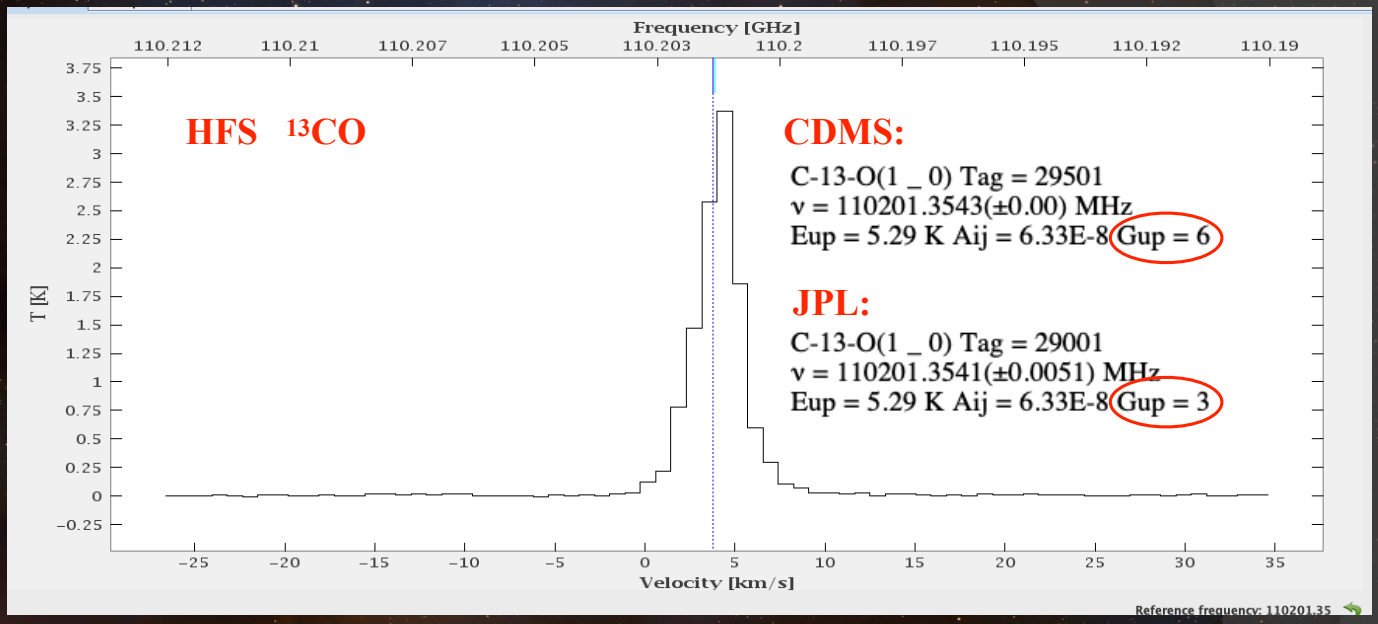


NH from VAMDC decoded in CASSIS:

NH (v=0)(
HUNDB - ElecState=X, S=1.0, F1NuclearSpinRef=N, V=0, FValue=1.5, J=0.0, F1Value=0.5, FNuclearSpinRef=H, N=1, -
HUNDB - ElecState=X, S=1.0, F1NuclearSpinRef=N, V=0, FValue=2.5, J=1.0, F1Value=1.5, FNuclearSpinRef=H, N=0,)
Tag = 15501
ν = 946475.8538(±0.033) MHz
Eup = 45.43 K Aij = 3.25E-3 Gup = 4
Other frequencies proposed: [946475.82±0.05]

9 versus 4 quantum numbers

I. Line Identification: VAMDC Access to CDMS



VAMDC/CDMS

- **DCS - ElecState=X, V=0, FValue=1.5, J=1, FNuclearSpinRef=C-13, - DCS - ElecState=X, V=0, FValue=0.5, J=0, FNuclearSpinRef=C-13**

ν = 110201.3707(±0.0001) MHz, Eup = 5.29 K Aij = 6.33E-8 Gup = 4

Other frequencies proposed: [110201.37039±6.6E-4]

- **DCS - ElecState=X, V=0, J=1, - DCS - ElecState=X, V=0, J=0,**

ν = 110201.3543(±0.00) MHz, Eup = 5.29 K Aij = 6.33E-8 Gup = 6

- **DCS - ElecState=X, V=0, FValue=0.5, J=1, FNuclearSpinRef=C-13, - DCS - ElecState=X, V=0, FValue=0.5, J=0, FNuclearSpinRef=C-13**

ν = 110201.3216(±0.0002) MHz, Eup = 5.29 K Aij = 6.33E-8 Gup = 2

Other frequencies proposed: [110201.3218±7.0E-4]

VAMDC/JPL:

- **DCS - ElecState=X, V=0, J=1, - DCS - ElecState=X, V=0, J=0,)**

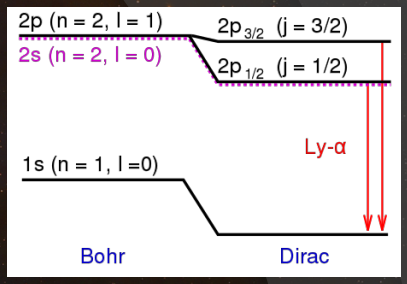
ν = 110201.3541(±0.0051) MHz

Eup = 5.29 K Aij = 6.33E-8 Gup = 3

Factor 2 for the partition function

II. Line Identification: atomic databases

1 simple species, (Lyman-alpha), many different frequencies and A_{ij}, f_{ji}, S_{ik}



CHIANTI: 1 4 1215.670 5.550e-01 6.260e+08 1s 2S1/2 - 2p 2P3/2 Lyman alpha

Chianti/VAMDC:

<SpeciesRef>Xchianti-1</SpeciesRef><Probability><TransitionProbabilityA><Value units="1/s">626000000.0</Value></TransitionProbabilityA><WeightedOscillatorStrength><Value units="unitless">0.555</Value></WeightedOscillatorStrength></Probability>

<ProcessClass></ProcessClass></RadiativeTransition><RadiativeTransition id="Pchianti-R10"><EnergyWavelength><Wavelength methodRef="Mchianti-EXP"><Value units="A">1215.67</Value></Wavelength><Wavelength methodRef="Mchianti-THEO"><Value units="A">1215.02</Value></Wavelength></EnergyWavelength><UpperStateRef>Schianti-3000001</UpperStateRef><LowerStateRef>Schianti-1000001</LowerStateRef>

Kentucky database (Not in VAMDC):

-LAMBDA-VAC-ANG-	-SPECTRUM--	TT	--------TERM---------	---J-J---	----LEVEL ENERGY--CM-1----
1215.6700	H I	E1	1-2	1/2-*	0.00 - 82259.11

VALD/VAMDC:

<SpeciesRef>Xvald-1</SpeciesRef><Probability><Log10WeightedOscillatorStrength><SourceRef>Bvald-CDROM18</SourceRef><Value units="unitless">-0.801</Value></Log10WeightedOscillatorStrength></Probability><ProcessClass></ProcessClass><Broadening name="natural" envRef="Evald-natural"><Comments>Natural Broadening</Comments><SourceRef>Bvald-CDROM18</SourceRef><Lineshape name="lorentzian"><LineshapeParameter name="log(gamma)"><Value units="1/s">8.77</Value></LineshapeParameter></Lineshape></Broadening></RadiativeTransition><RadiativeTransition id="Pvald-R154476610" process="excitation"><EnergyWavelength><Wavelength><Comments>Vacuum wavelength from state energies (RITZ)</Comments><SourceRef>Bvald-CDROM18</SourceRef><Value units="A">1215.67100000</Value><Wavelength><Wavelength><Comments>Vacuum wavelength from measurements (non-RITZ)</Comments><SourceRef>Bvald-CDROM18</SourceRef><Value units="A">1215.67089746</Value></Wavelength></EnergyWavelength><UpperStateRef>Svald-1105790</UpperStateRef><LowerStateRef>Svald-1021407</LowerStateRef>

Some quantum numbers in VALD but not for everything. Also need some de-coding to get the QN listed in the above figure. Not very useful…

II. Line Identification: atomic databases

NIST VAMDC:

<RadiativeTransition id="PASD-R275805"><Comments>Wavelength is for vacuum.</Comments><EnergyWavelength><Wavelength><Value units="A">1215.6699</Value></Wavelength></EnergyWavelength><UpperStateRef>SASD-001001.001.000002</UpperStateRef><LowerStateRef>SASD-001001.001.000001</LowerStateRef><Probability><TransitionProbabilityA><Value units="1/s">6.2648e+08</Value></TransitionProbabilityA><Log10WeightedOscillatorStrength><Value units="unitless">-0.55657</Value></Log10WeightedOscillatorStrength></Probability><ProcessClass></ProcessClass></RadiativeTransition>

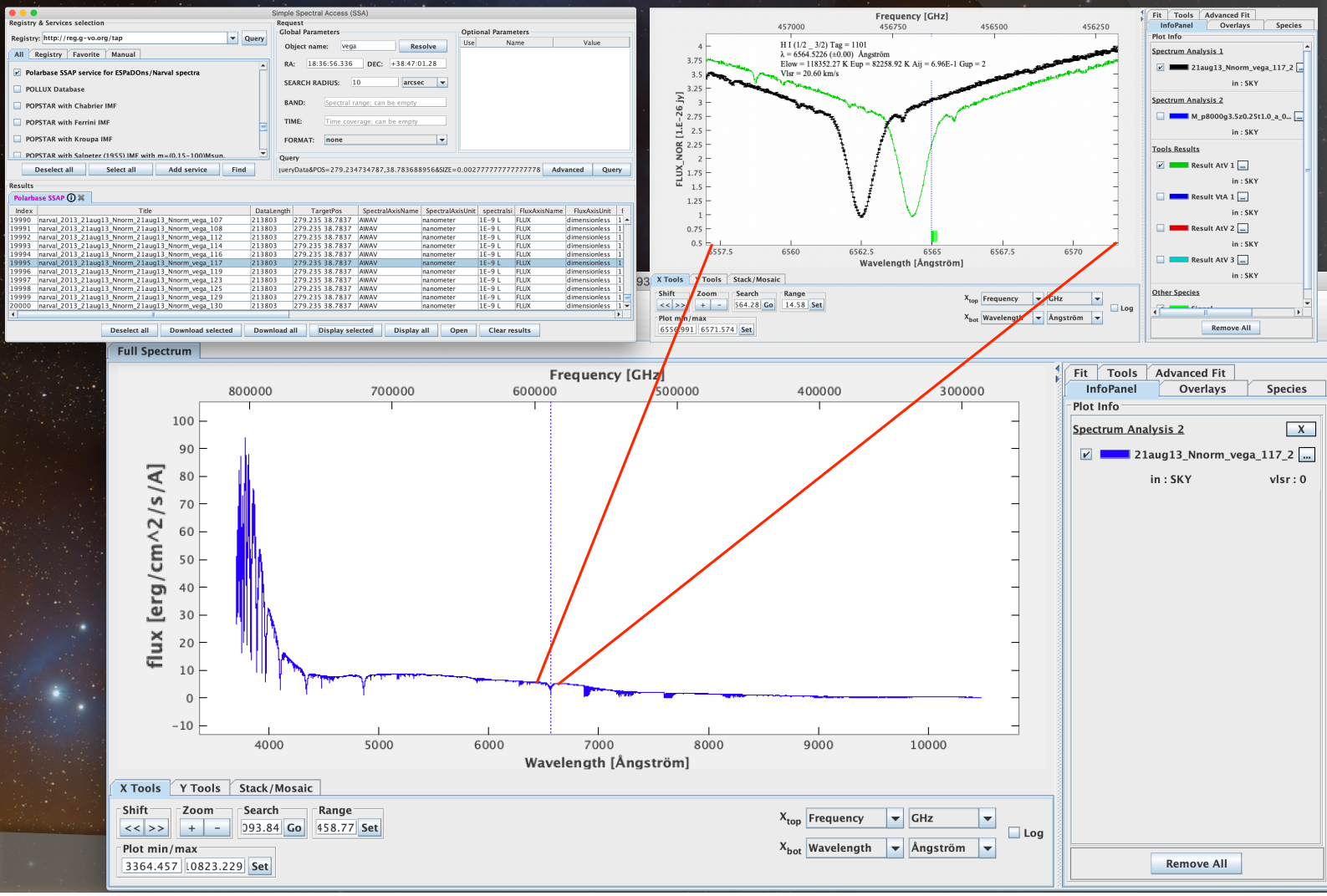
<RadiativeTransition id="PASD-R275807"><Comments>Wavelength is for vacuum.</Comments><EnergyWavelength><Wavelength><Value units="A">1215.6699</Value></Wavelength></EnergyWavelength><UpperStateRef>SASD-001001.001.000004</UpperStateRef><LowerStateRef>SASD-001001.001.000001</LowerStateRef><Probability><TransitionProbabilityA><Value units="1/s">6.2647e+08</Value></TransitionProbabilityA><Log10WeightedOscillatorStrength><Value units="unitless">-0.25555</Value></Log10WeightedOscillatorStrength></Probability><ProcessClass></ProcessClass></RadiativeTransition>

No quantum numbers in NIST/VAMDC!! Not very useful…

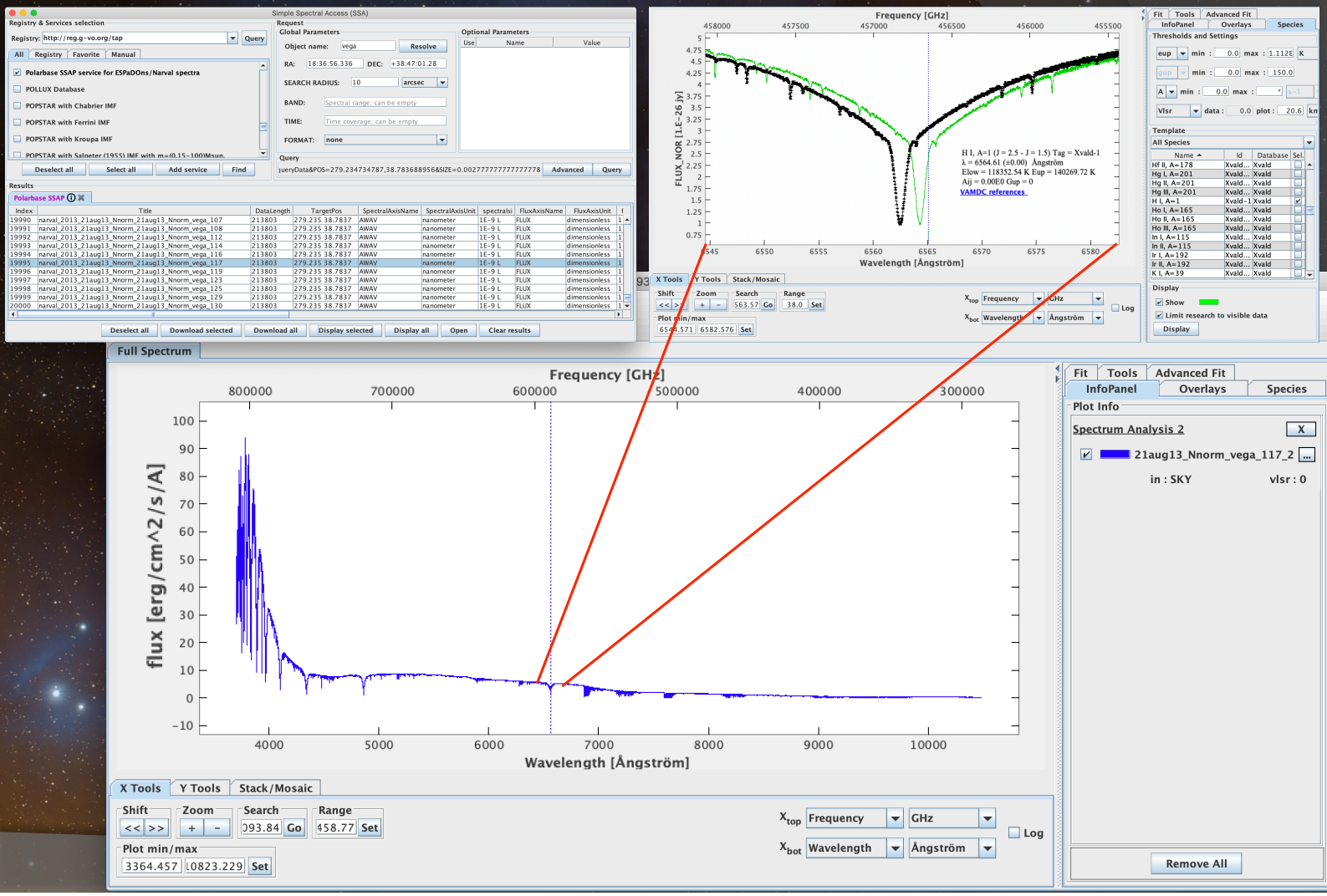
NIST:

Observed	Ritz Wavelength	Aij						
1215.6699	1215.668237310	6.2647e+08	1s	2S	1/2	2p	2P°	3/2
1215.6699	1215.673644608	6.2648e+08	1s	2S	1/2	2p	2P°	1/2

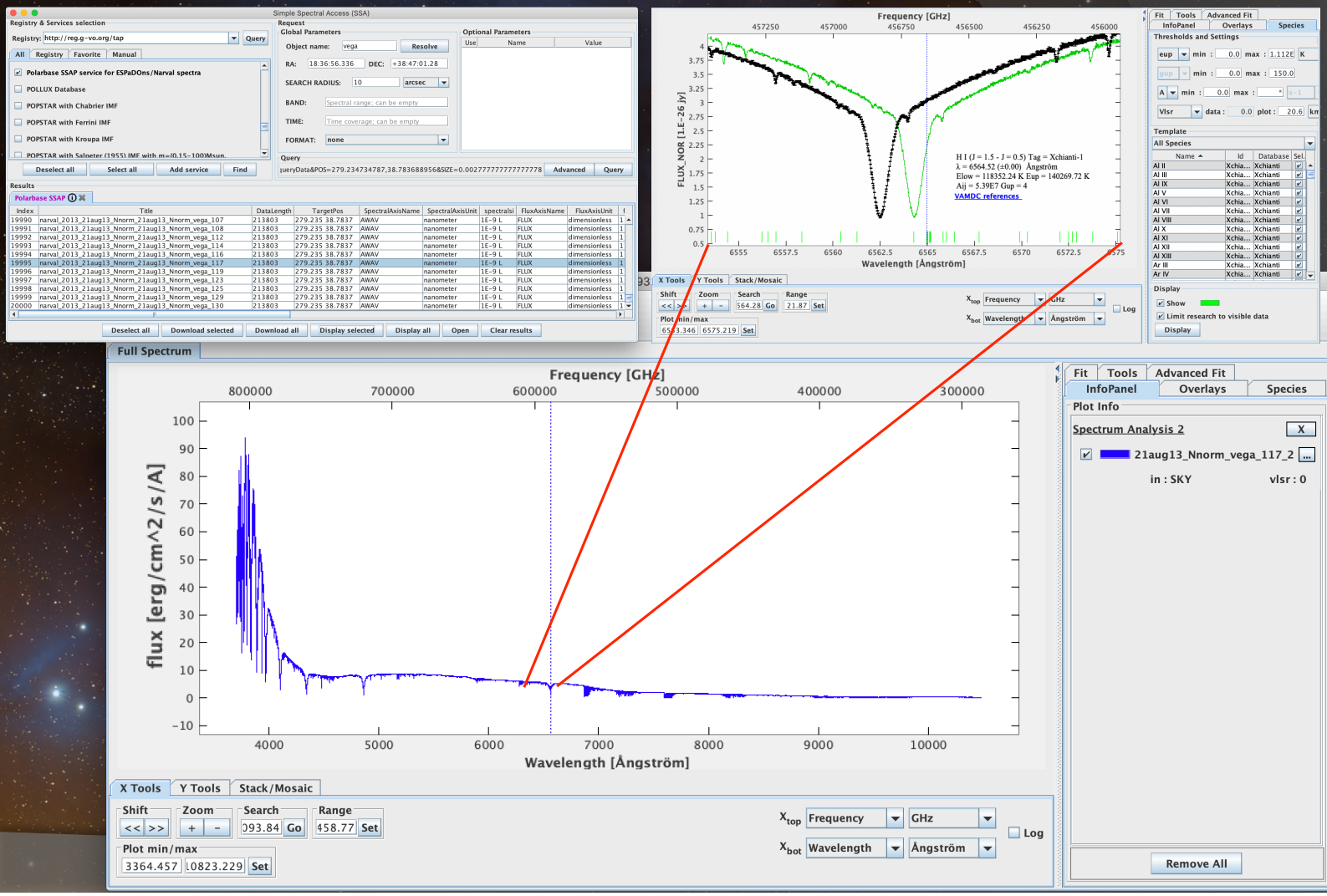
II. Stellar spectra (with CASSIS NIST database)



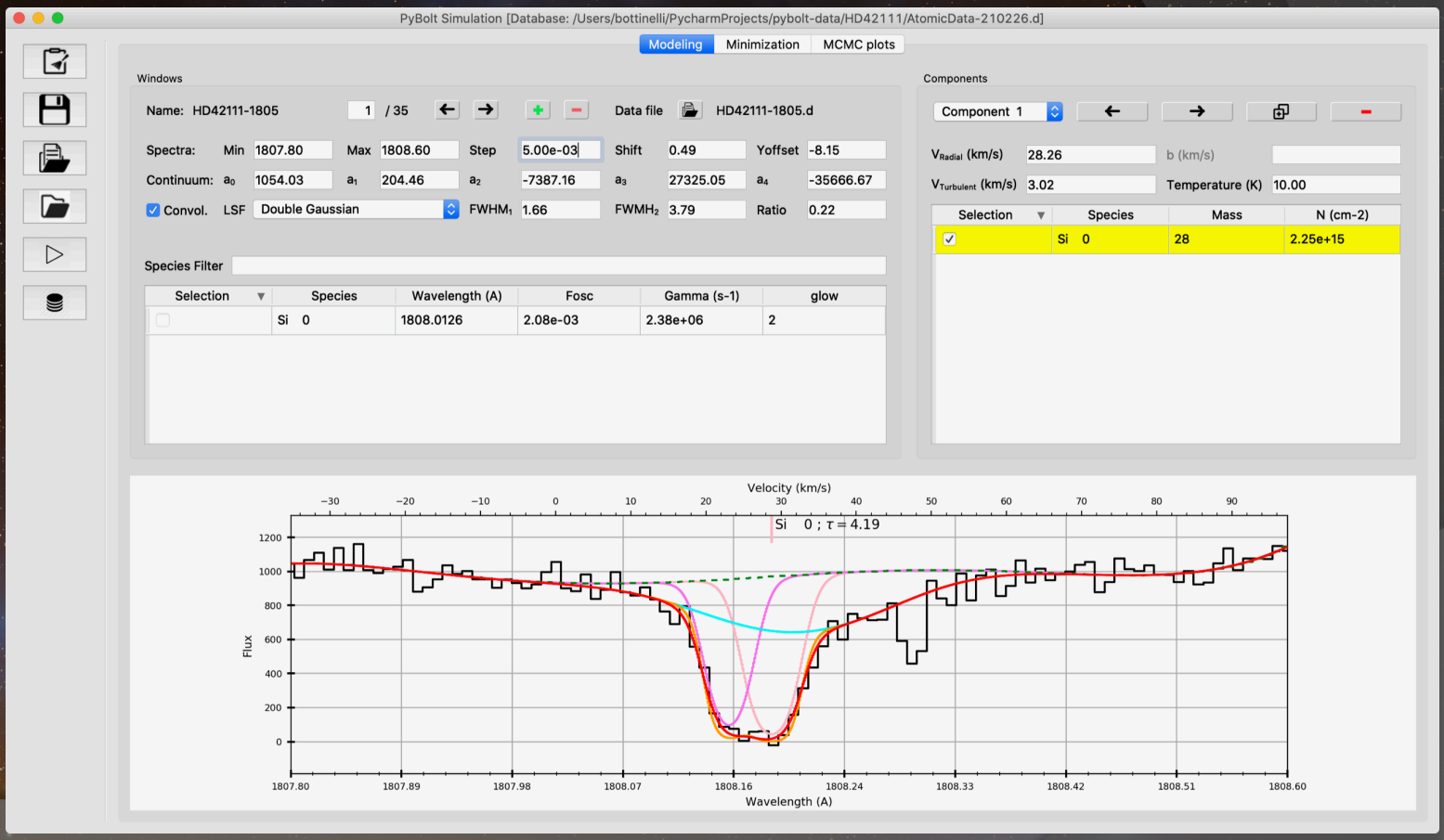
II. Stellar spectra (with VAMDC VALD database)



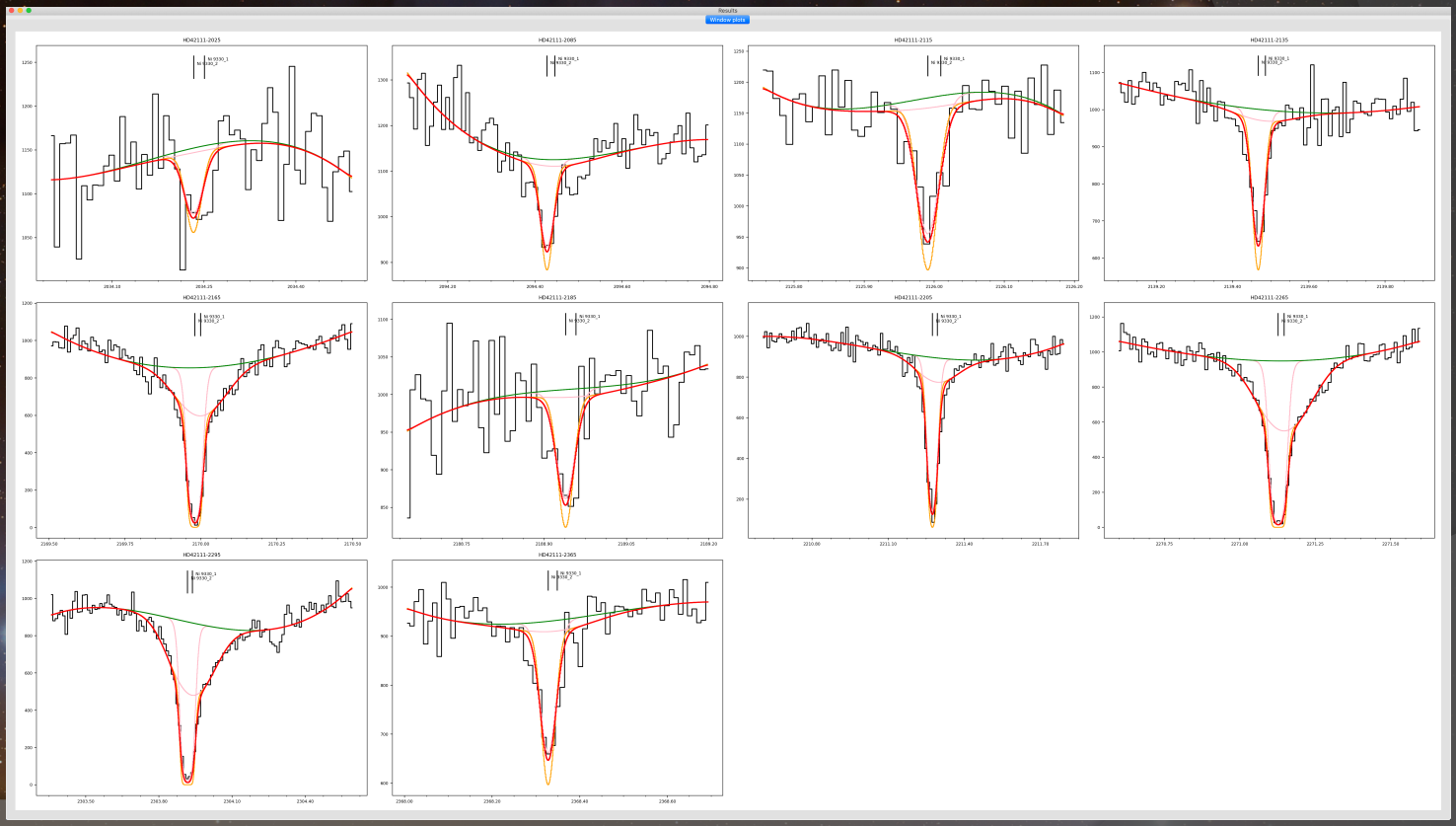
II. Stellar spectra (with VAMDC CHIANTI database)



Absorption spectra (with Ad'Hoc database)
PyBolt module (in progress)



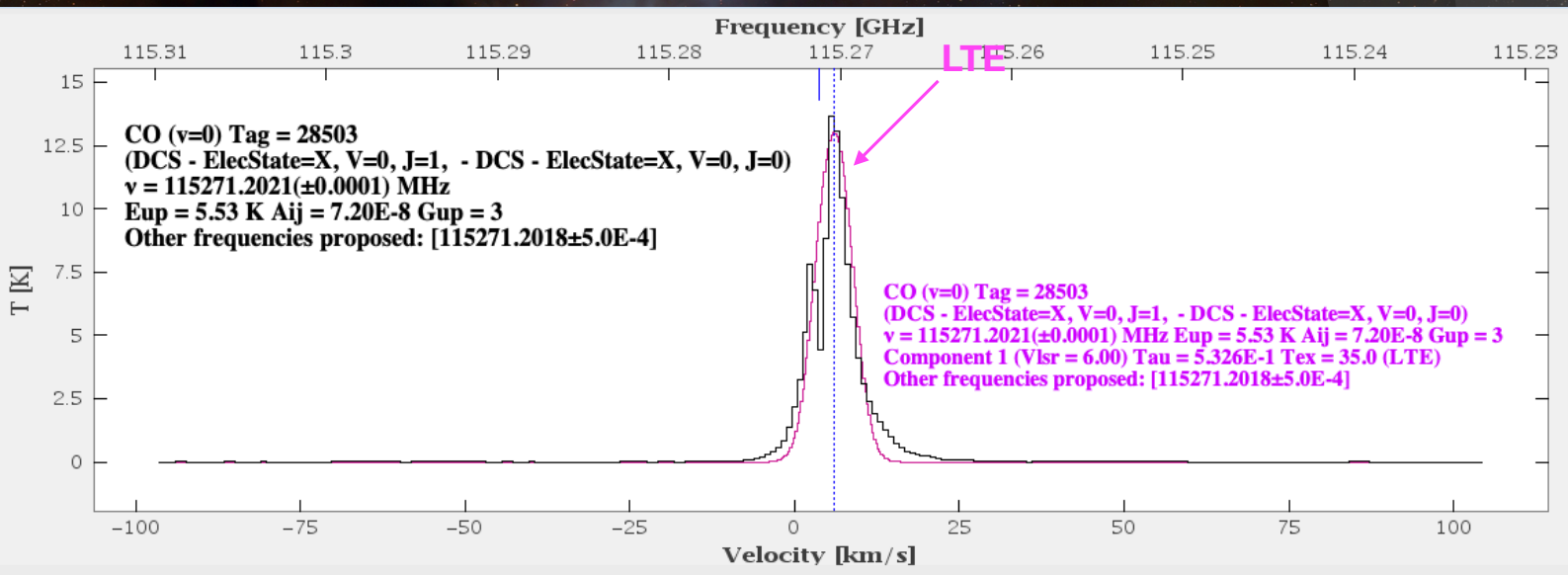
Absorption spectra (with Ad'Hoc database)
PyBolt module (in progress)



III. Radiative transfer: LTE

1) Line identification through VAMDC
2) LTE modelling using the partition function, Aij, gu, frequencies given by VAMDC

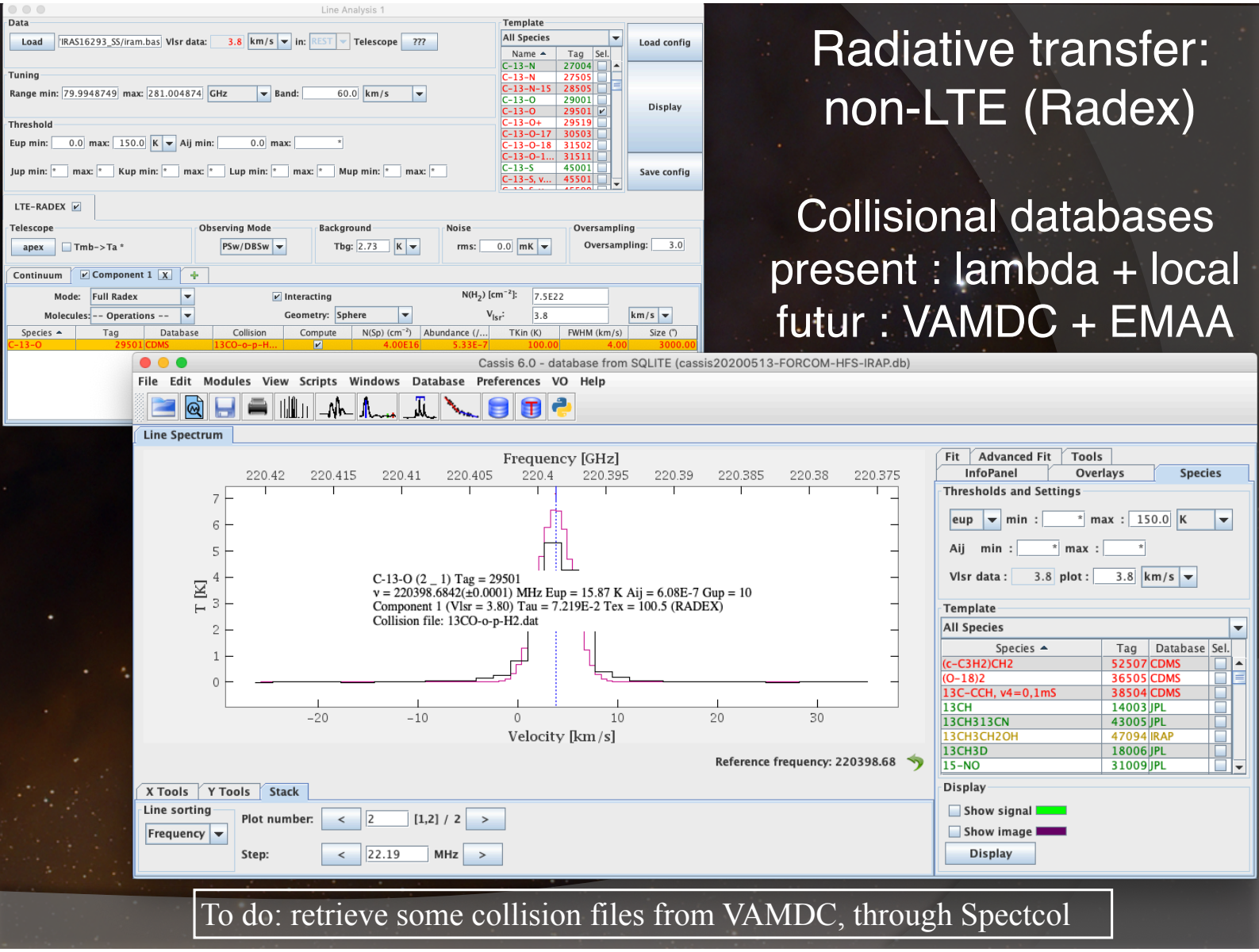
Radiative transfert should be easy through VAMDC, but however much slower



Radiative transfer: non-LTE (Radex)

Collisional databases present : lambda + local

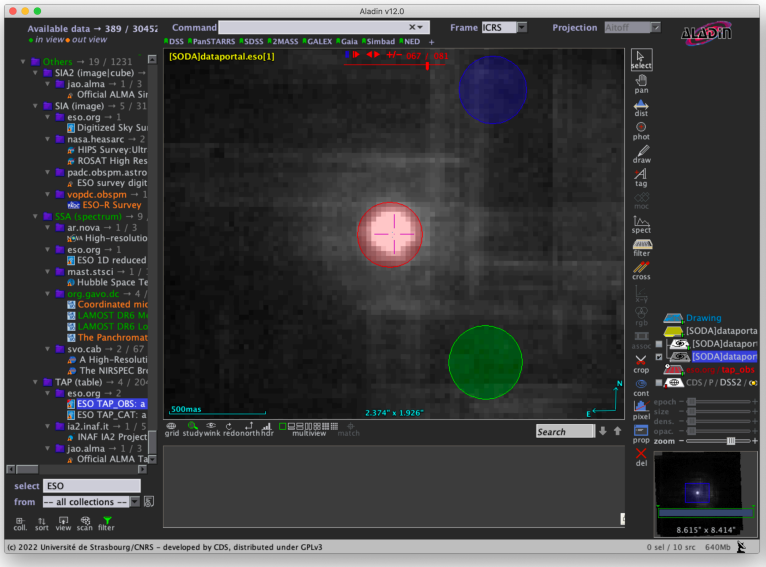
futur : VAMDC + EMAA

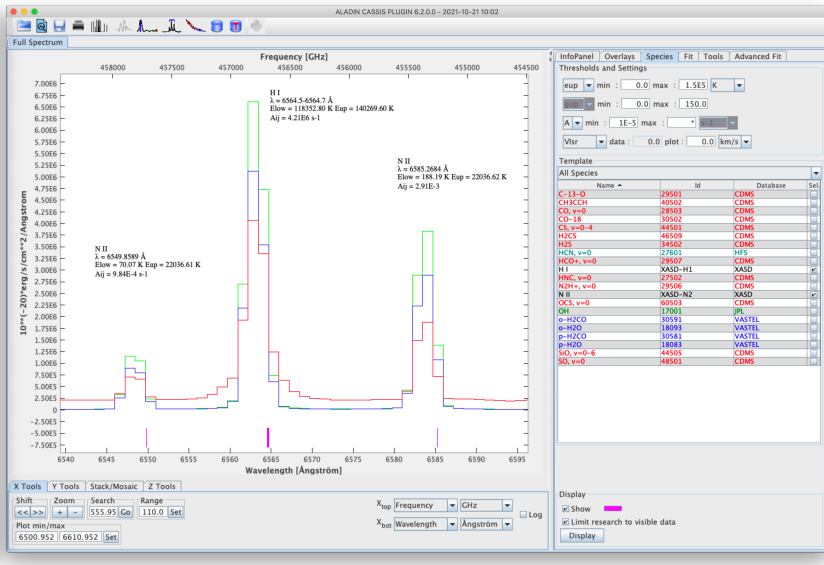


To do: retrieve some collision files from VAMDC, through Spectcol

IV. The Aladin connection: VO

https://aladin.u-strasbg.fr/ developed by CDS Aladin team (Centre de Données Astronomiques de Strasbourg)
Select database for the cube (E.g. MUSE with ESO ObsTAP) and extract a data sub-cube (ESO SODA: datalink): define a polygon, extract the spectrum from the polygon and send to CASSIS (cursors and spectral profiles are synchronised between the two applications)





http://cassis.irap.omp.eu/?page=publicationsandtalks
https://wiki.ivoa.net/internal/IVOA/InterOpNov2021Apps/2021-IVOA-Northern-Fall-interop-CASSIS-Aladin-Plugin-final.mp4
http://cassis.irap.omp.eu/download/presentations/Cassis_Adass_2021_D3-001.pdf

III. The Aladin connection: VO

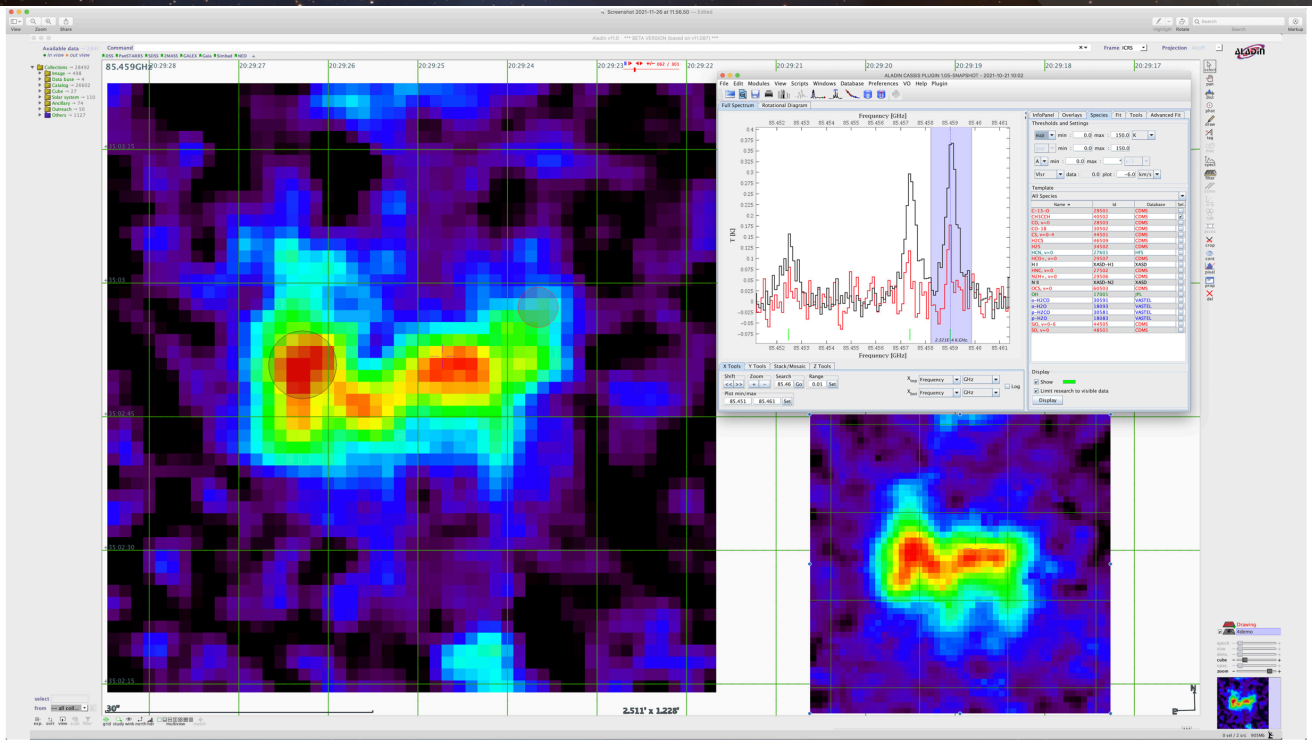


Figure 2. Selected areas on the cube field in Aladin (left) with the corresponding spectra in CASSIS (top right) and integrated spectral plane in Aladin driven by the blue limits set on the spectrum into the CASSIS window (bottom right).