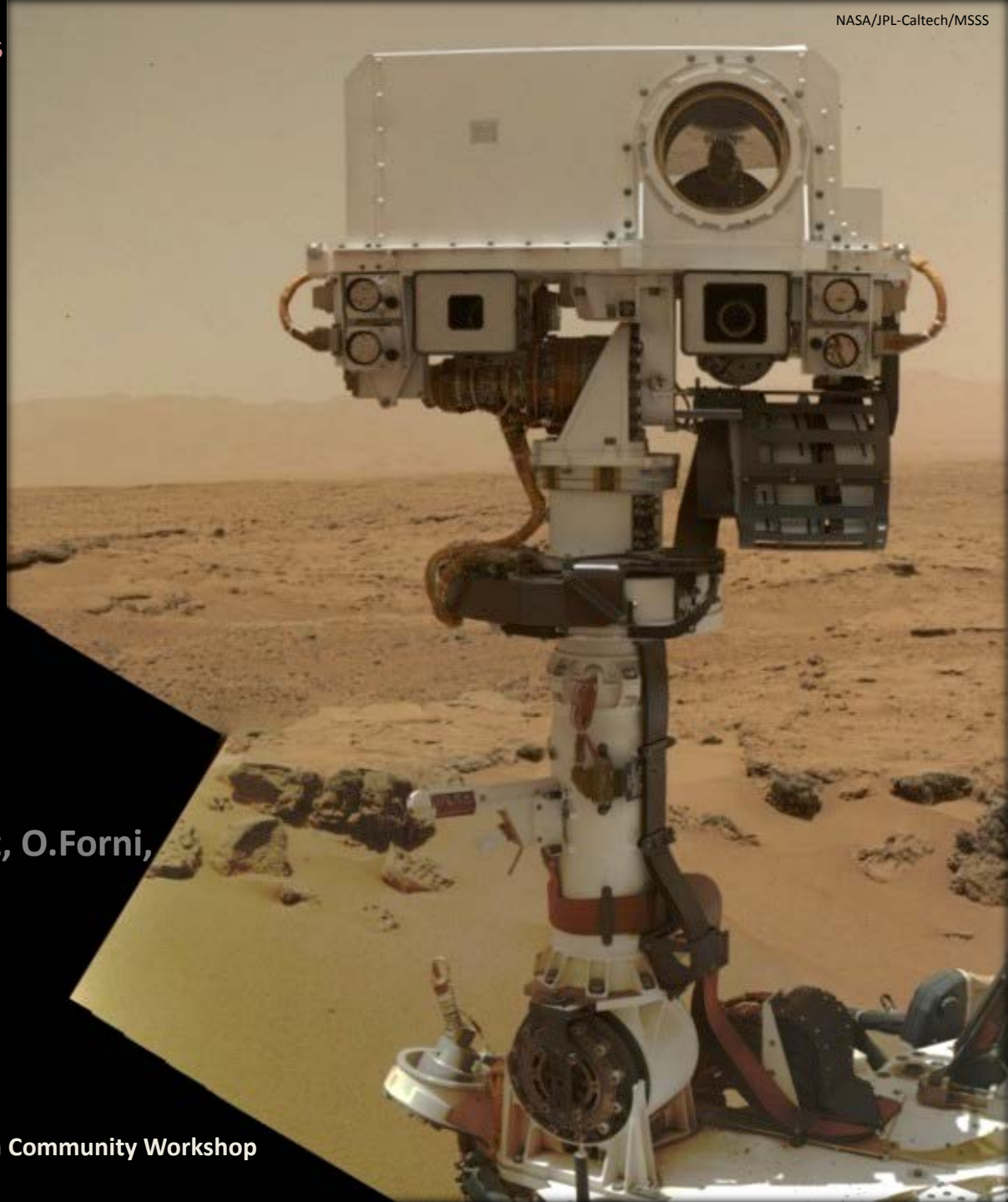
Lunar and Planetary Science Conference, March 18th, 2015

COMMUNITY USER WORKSHOP ON PLANETARY LIBS (CHEMCAM) DATA

C-QuEST

Software



Agnes.cousin@irap.omp.eu

A. Cousin, S. Maurice, O. Gasnault, O.Forni, R. Wiens and ChemCam team

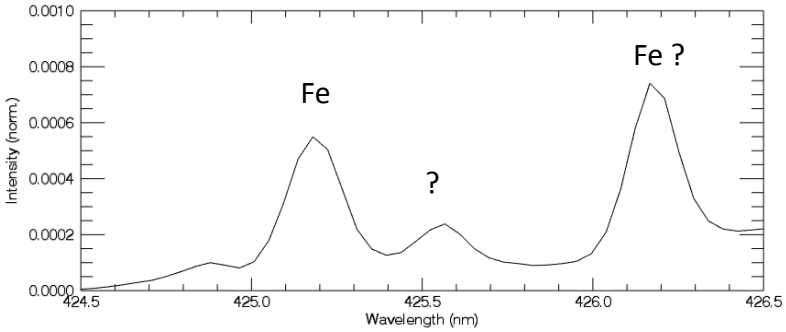
What is C-QuEST ?

Definition

- ChemCam Quick Element Search Tool
- Library of ChemCam emission lines for 32 elements

Why use it ?

- Search for specific element in spectral database
- Search for specific spectral range
- Visualize an elemental synthetic spectrum



LIBS emission lines database

Why doing an emission lines library ?

NIST

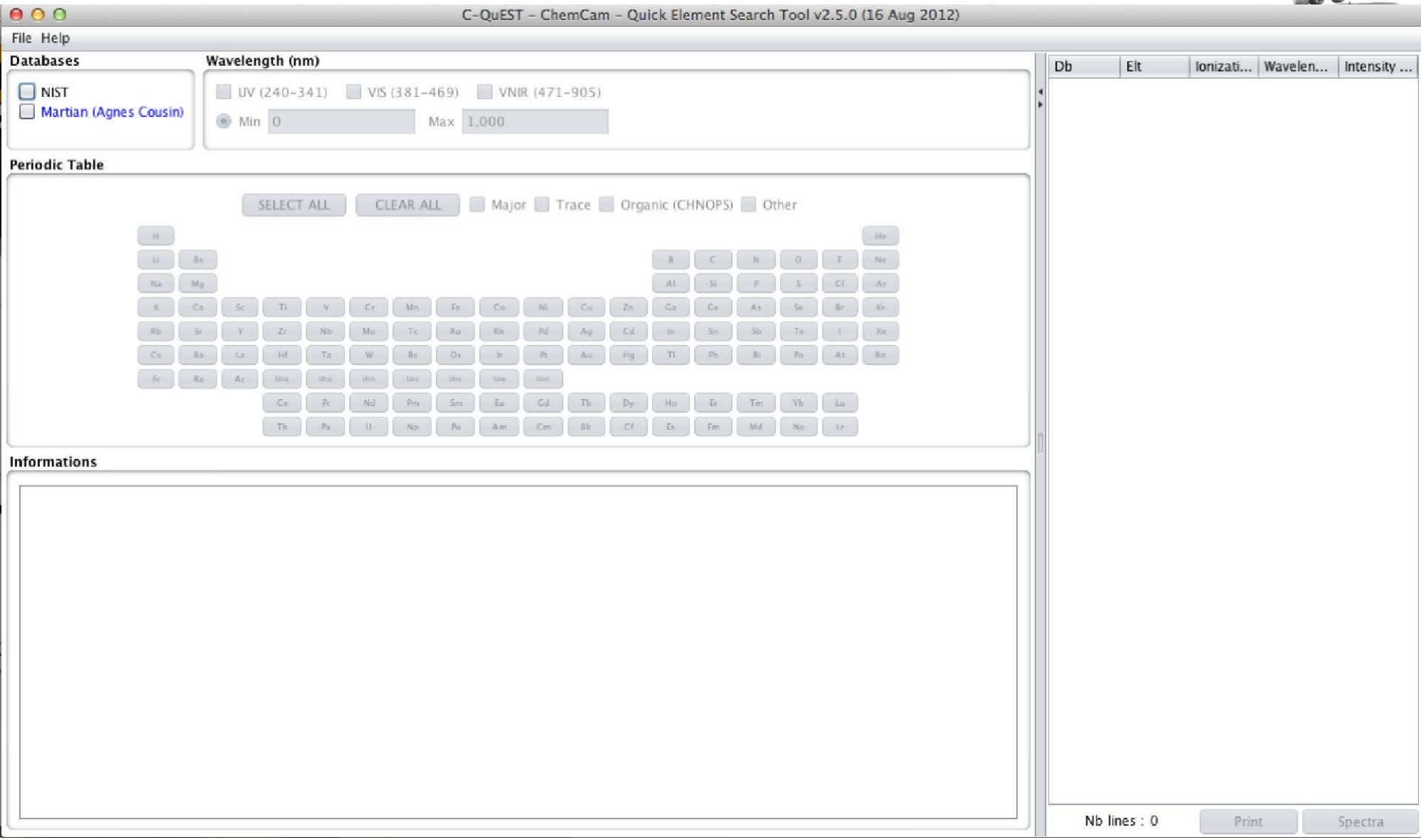
Not LIBS specific
Vacuum and Ambient

CREOSA

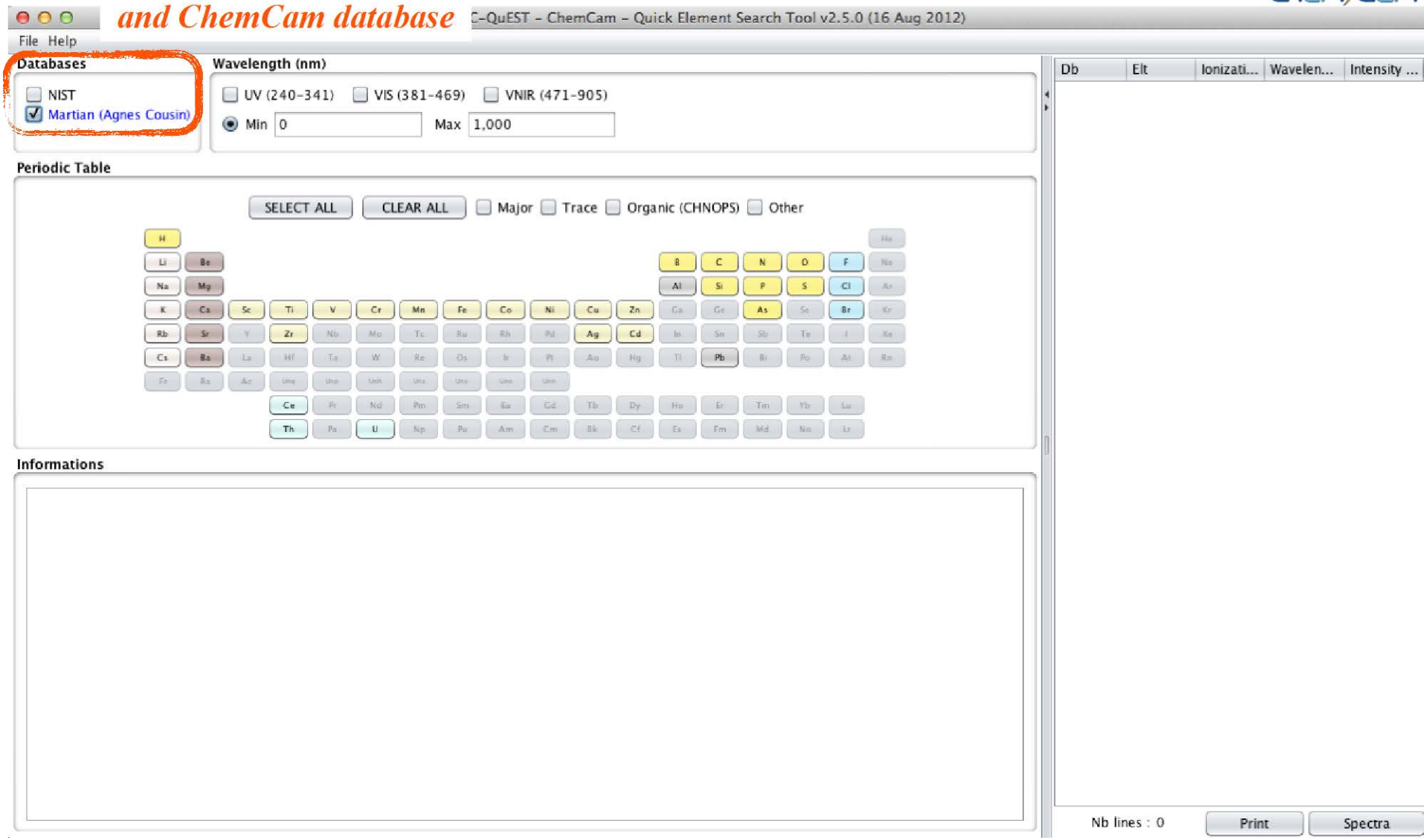
LIBS specific
Helium

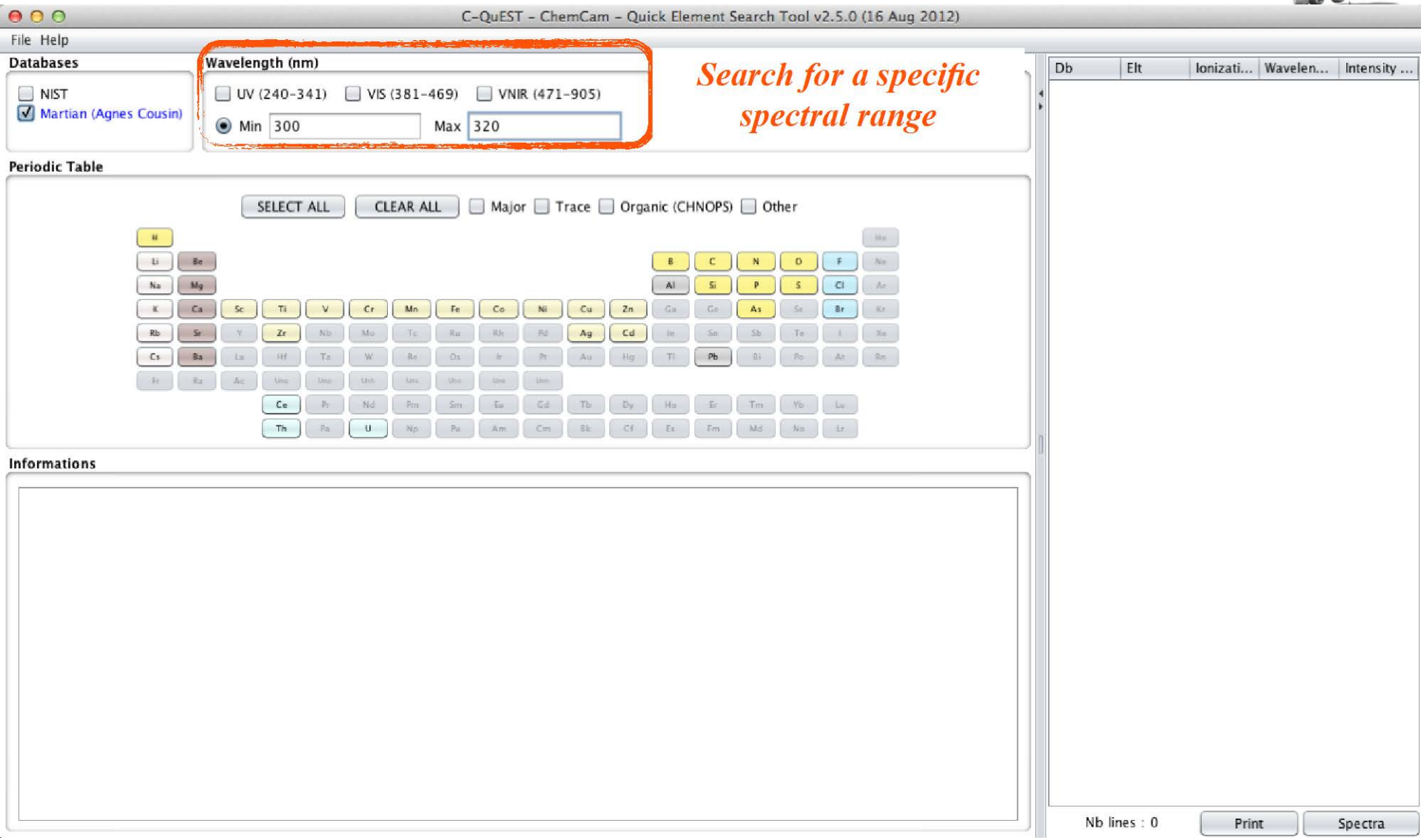
Emission lines are dependent on the experimental conditions
(Pressure, Laser Energy, ..)

Need for a specific Martian database
Subset of the NIST database


C-QuEST – ChemCam – Quick Element Search Tool v2.5.0 (16 Aug 2012)
File Help
Databases
NIST
Martian (Agnes Cousin)
Wavelength (nm)
UV (240-341)
VIS (381-469)
VNIR (471-905)
Min 0
Max 1,000
Periodic Table
SELECT ALL
CLEAR ALL
Major
Trace
Organic (CHNOPS)
Other
Informations
Db
Elt
Ionizati...
Wavelen...
Intensity ...
Nb lines : 0
Print
Spectra

Choice between NIST and ChemCam database

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Databases
NIST
Martian (Agnes Cousin)
Wavelength (nm)
UV (240-341)
VIS (381-469)
VNIR (471-905)
Min 300
Max 320
Search for a specific spectral range
Periodic Table
SELECT ALL
CLEAR ALL
Major
Trace
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Wavelen...
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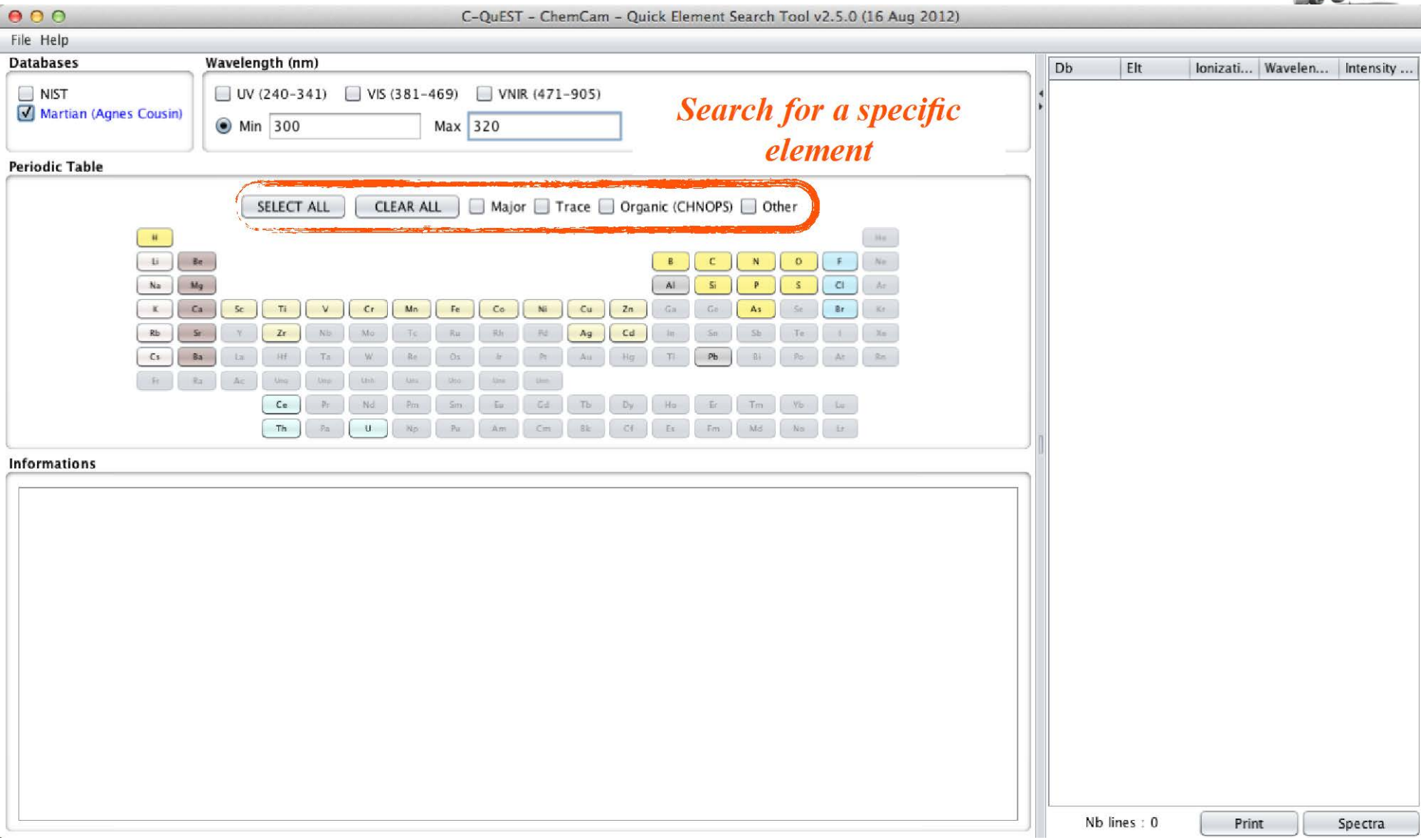
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Min 300
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Search for a specific element
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C-QuEST – ChemCam – Quick Element Search Tool v2.5.0 (16 Aug 2012)

File Help

Databases

- [ ] NIST
- [x] Martian (Agnes Cousin)

Wavelength (nm)

- [ ] UV (240-341)
- [ ] VIS (381-469)
- [ ] VNIR (471-905)
- (•) Min 300 Max 320

Periodic Table

SELECT ALL | CLEAR ALL | [x] Major [x] Trace [x] Organic (CHNOPS) [x] Other

Informations

The most intense one is at 455.53 nm. There are some interferences with Ti lines, but no confusion. This is the line that ensures the presence of Ba in a spectrum.

58: Cerium

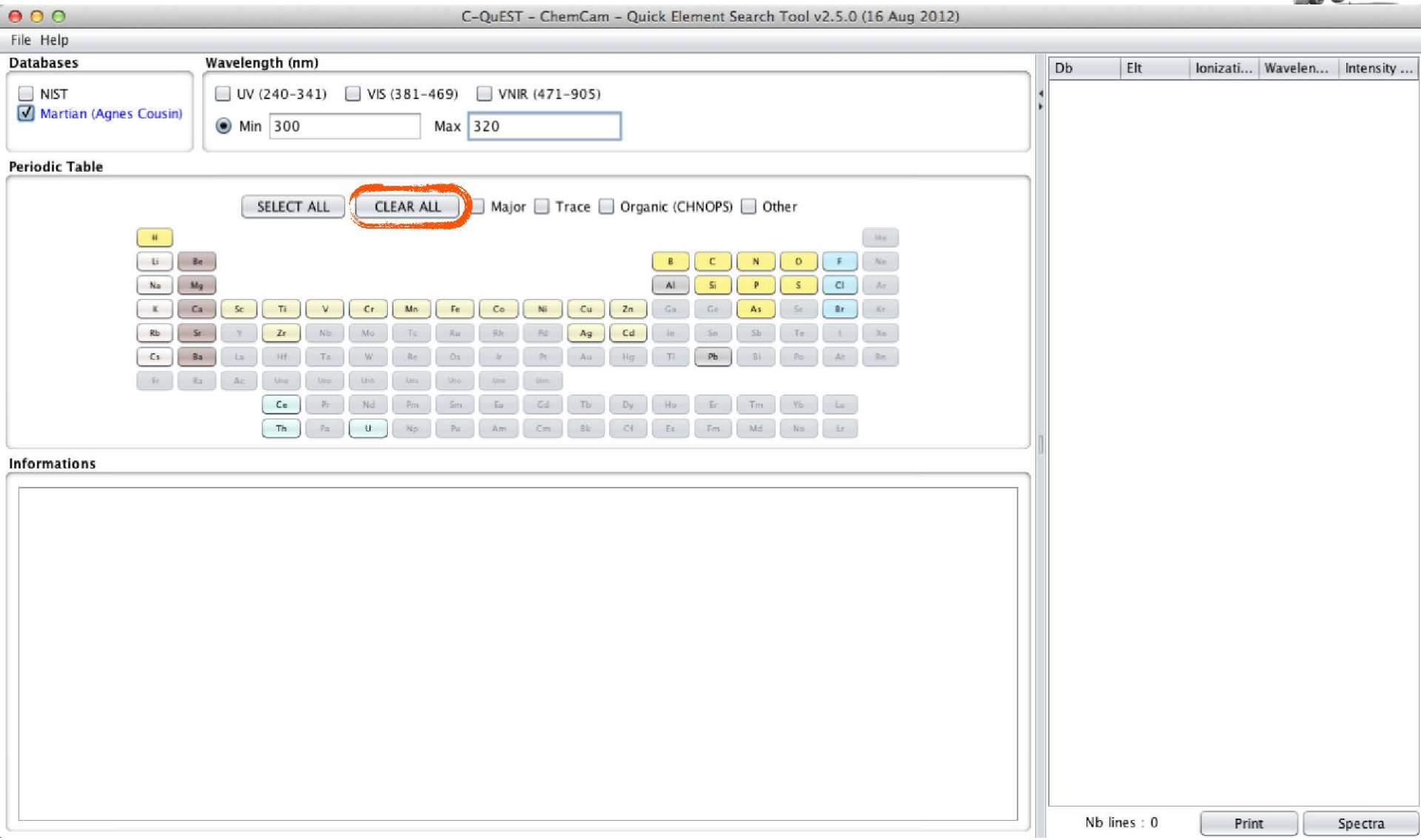
82: Lead

90: Thorium

92: Uranium

Db	Elt	Ioniza...	Wavele... ▲	Intensity ...
Martian	Fe	I	300.039	76.994
Martian	V	II	300.207	522.527
Martian	Ni	I	300.337	11.184
Martian	Fe	II	300.352	258.952
Martian	Ni	I	300.451	236.055
Martian	Mn	I	300.854	28.107
Martian	Fe	I	300.902	86.970
Martian	Cu	I	301.172	8.228
Martian	Mn	I	301.204	41.185
Martian	Mn	I	301.226	41.185
Martian	Ni	I	301.288	288.071
Martian	Fe	III	301.405	10.424
Martian	Mn	I	301.555	43.700
Martian	Ti	II	301.807	2.619
Martian	Ni	I	302.002	39.155
Martian	Mn	II	302.080	476.444
Martian	Fe	I	302.137	204.569
Martian	Fe	I	302.152	132.304
Martian	Fe	I	302.195	132.304
Martian	Mn	I	302.363	182.195
Martian	Fe	I	302.672	60.710
Martian	Ti	II	303.061	2.221
Martian	Mn	II	303.194	594.236
Martian	V	II	303.433	886.474
Martian	V	II	303.470	886.474
Martian	Mn	II	303.623	360.566
Martian	Zn	I	303.666	36.211
Martian	Cu	I	303.698	8.539
Martian	Fe	I	303.827	46.509
Martian	Ni	I	303.882	11.184
Martian	Mn	I	304.148	334.049
Martian	Fe	I	304.252	28.551
Martian	Mn	I	304.546	209.186
Martian	Ti	II	304.757	1.760
Martian	Mn	I	304.793	209.186
Martian	Fe	I	304.849	11.184
Martian	V	II	304.911	1,097.2...
Martian	Mn	II	305.154	349.718
Martian	Ni	I	305.170	189.878
Martian	V	II	305.428	117.904
Martian	Ni	I	305.520	41.308
Martian	Mn	I	305.525	42.558

Nb lines : 126 | Print | Spectra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Ionizati...
Wavelen...
Intensity ...
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Spectra

C-QuEST – ChemCam – Quick Element Search Tool v2.5.0 (16 Aug 2012)

File Help

Databases

- [ ] NIST
- [x] Martian (Agnes Cousin)

Wavelength (nm)

- [ ] UV (240-341) [ ] VIS (381-469) [ ] VNIR (471-905)
- (•) Min 300 Max 320

Periodic Table

SELECT ALL | CLEAR ALL | [x] Major | [ ] Trace | [ ] Organic (CHNOPS) | [ ] Other

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Unq	Unp	Unh	Uns	Uno	Une	Unn								
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

Informations

nm. If these two lines are not observed, the sample does not contain K.

20: Calcium

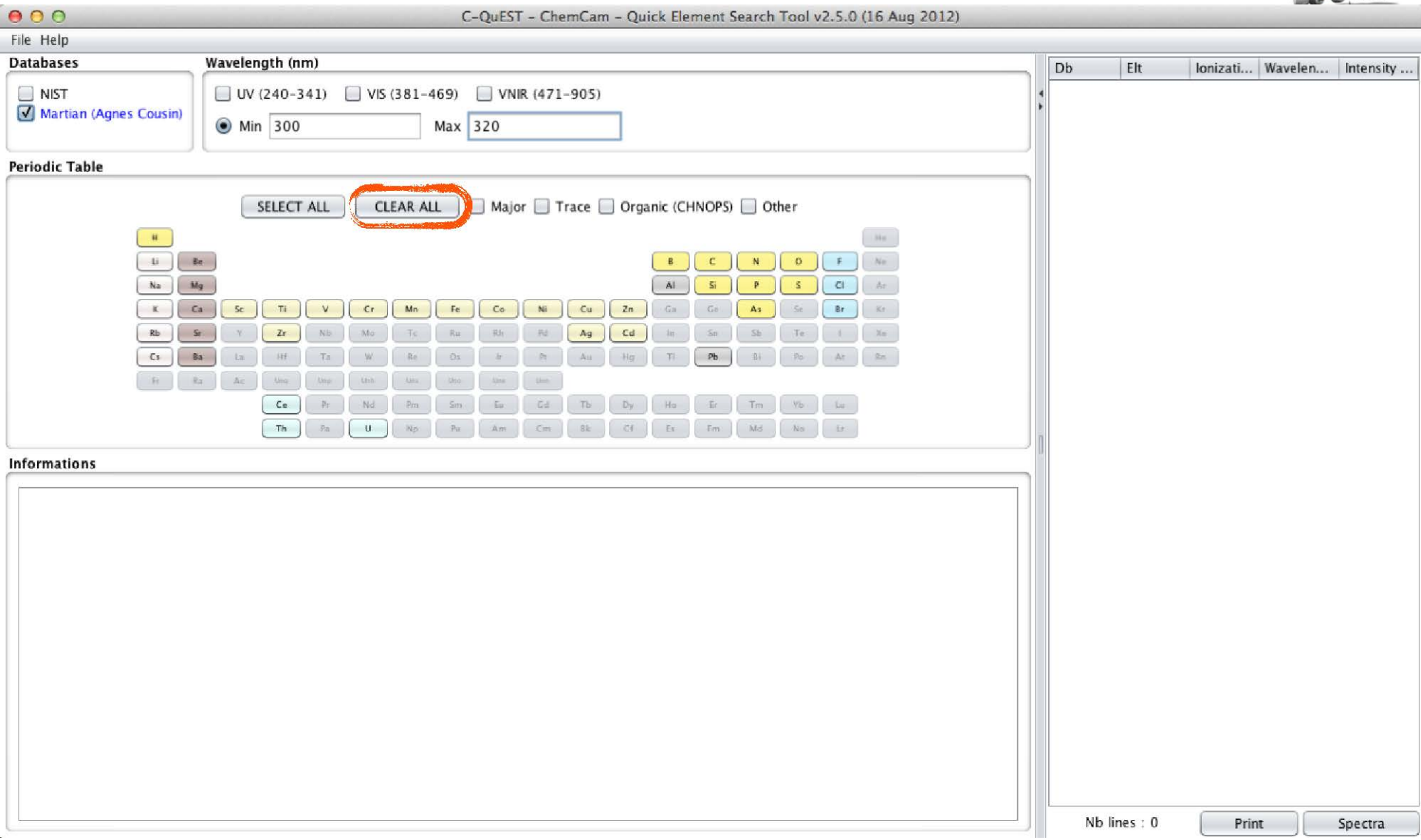
Ca shows several important lines.
Here are the most ones, observed for each spectral range :
- UV : 315.978 nm and 318.025 nm
- VIS : 393.477 nm, 396.959 nm and 422.792 nm are the most important among others
- VNIR : lot of Ca lines. The most easy ones to detect are the triplet at 610.441, 612.39 and 616.3 nm with an increasing intensity, and a second triplet at 644.085, 645.159 and 646.436-646.557 nm with a decreasing intensity.

All these lines are well defined with no interferences.
The most important Ca lines in all the spectrum are those at 393.477 nm and 396.959 nm, but they can suffer some auto-absorption effects.

26: Iron

Db	Elt	Ionizati...	Wavele... ▲	Intensity ...
Martian	Fe	I	300.039	76.994
Martian	Fe	II	300.352	258.952
Martian	Fe	I	300.902	86.970
Martian	Fe	III	301.405	10.424
Martian	Fe	I	302.137	204.569
Martian	Fe	I	302.152	132.304
Martian	Fe	I	302.195	132.304
Martian	Fe	I	302.672	60.710
Martian	Fe	I	303.827	46.509
Martian	Fe	I	304.252	28.551
Martian	Fe	I	304.849	11.184
Martian	Fe	I	305.833	132.755
Martian	Fe	I	305.998	11.184
Martian	Fe	I	306.814	53.376
Martian	Fe	I	307.661	84.976
Martian	Al	I	308.305	797.742
Martian	Al	II	308.941	44.827
Martian	Fe	I	309.247	10.839
Martian	Al	I	309.361	718.594
Martian	Al	I	309.374	1,369.8...
Martian	Mg	I	309.388	46.616
Martian	Na	II	309.645	69.978
Martian	Mg	I	309.779	94.835
Martian	Fe	I	310.120	88.149
Martian	Na	II	312.612	80.808
Martian	Fe	II	315.512	77.237
Martian	Ca	II	315.978	449.694
Martian	Fe	III	317.501	4.460
Martian	Fe	III	317.893	37.426
Martian	Ca	II	318.025	700.170
Martian	Fe	I	318.582	11.853
Martian	Fe	I	319.422	56.373
Martian	Si	II	319.561	254.413
Martian	Fe	I	319.785	46.588

Nb lines : 34 | Print | Spectra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Martian (Agnes Cousin)
Wavelength (nm)
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VIS (381-469)
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Min 300
Max 320
Periodic Table
SELECT ALL
CLEAR ALL
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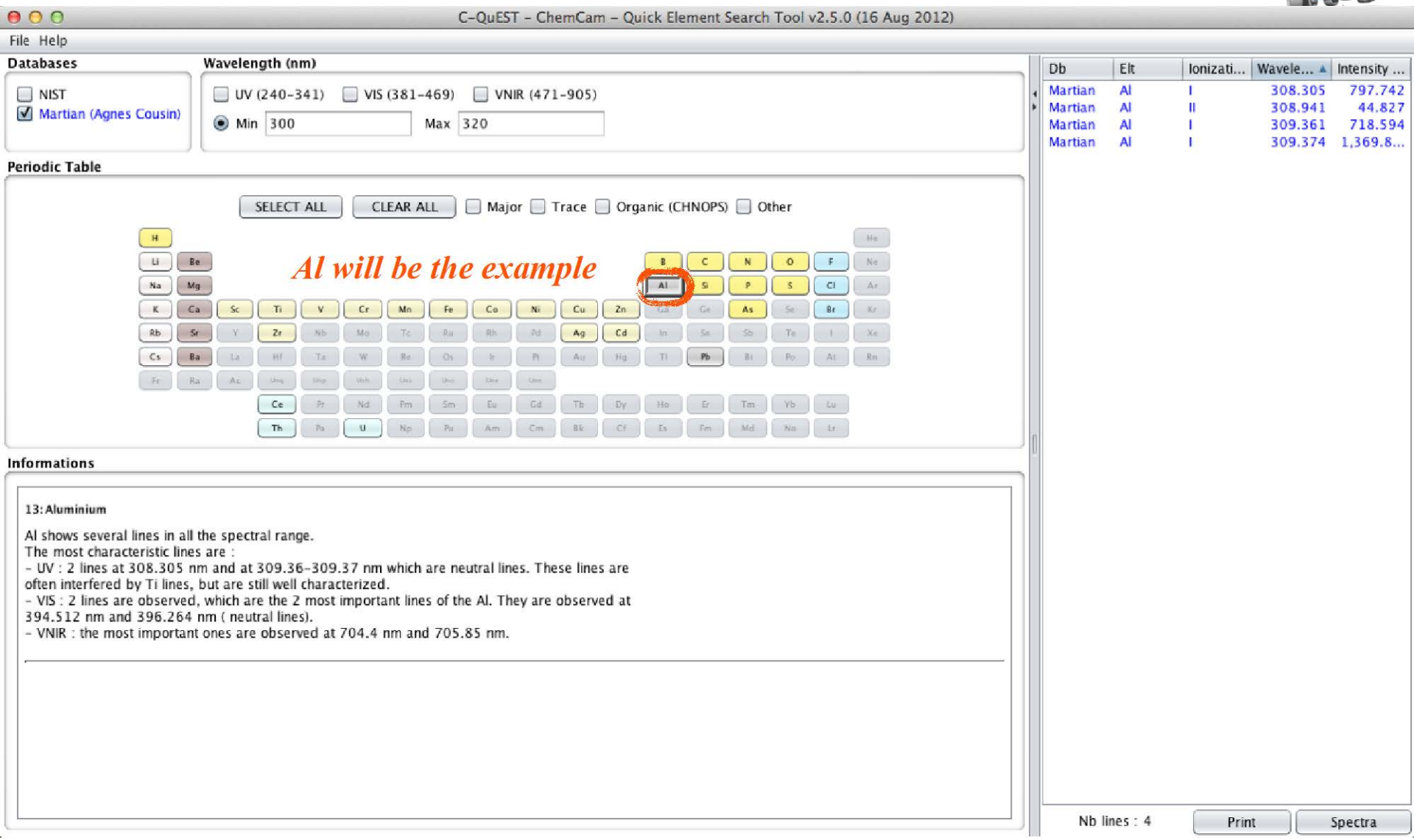
Trace
Organic (CHNOPS)
Other
Informations
Db
Elt
Ionizati...
Wavelen...
Intensity ...
Nb lines : 0
Print
Spectra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Min 300
Max 320
Periodic Table
SELECT ALL
CLEAR ALL
Major
Trace
Organic (CHNOPS)
Other
Al will be the example
Informations
13: Aluminium
Al shows several lines in all the spectral range.
The most characteristic lines are :
- UV : 2 lines at 308.305 nm and at 309.36-309.37 nm which are neutral lines. These lines are often interfered by Ti lines, but are still well characterized.
- VIS : 2 lines are observed, which are the 2 most important lines of the Al. They are observed at 394.512 nm and 396.264 nm (neutral lines).
- VNIR : the most important ones are observed at 704.4 nm and 705.85 nm.
Db
Elt
Ionizati...
Wavele...
Intensity ...
Martian Al I 308.305 797.742
Martian Al II 308.941 44.827
Martian Al I 309.361 718.594
Martian Al I 309.374 1,369.8...
Nb lines : 4
Print
Spectra

C-QuEST – ChemCam – Quick Element Search Tool v2.5.0 (16 Aug 2012)

File Help

Databases

- [ ] NIST
- [x] Martian (Agnes Cousin)

Wavelength (nm)

- [ ] UV (240-341) [ ] VIS (381-469) [ ] VNIR (471-905)
- (•) Min 300 Max 320

Periodic Table

SELECT ALL | CLEAR ALL | [ ] Major [ ] Trace [ ] Organic (CHNOPS) [ ] Other

Informations

13: Aluminium

Al shows several lines in all the spectral range.
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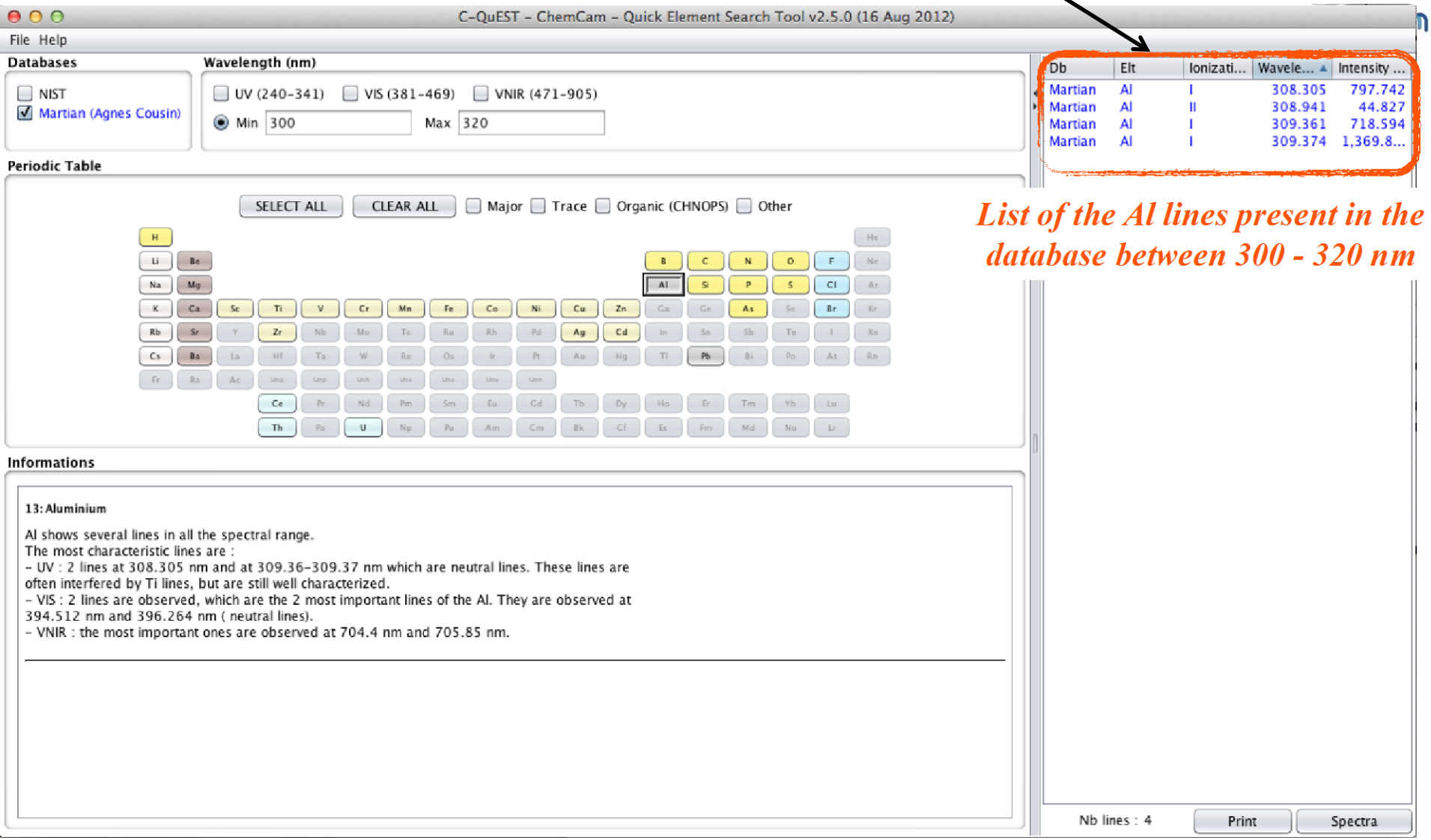
Db	Elt	Ionizati...	Wavele...	Intensity ...
Martian	Al	I	308.305	797.742
Martian	Al	II	308.941	44.827
Martian	Al	I	309.361	718.594
Martian	Al	I	309.374	1,369.8...

Nb lines : 4 | Print | Spectra

Information about main emission lines

List of emission lines by database, element, ionization stage, wavelength or intensity



List of the Al lines present in the database between 300 - 320 nm

C-QuEST – ChemCam – Quick Element Search Tool v2.5.0 (16 Aug 2012)

File Help

Databases

- [ ] NIST
- [x] Martian (Agnes Cousin)

Wavelength (nm)

- [ ] UV (240-341)
- [ ] VIS (381-469)
- [ ] VNIR (471-905)
- (•) Min 300 Max 320

Periodic Table

SELECT ALL | CLEAR ALL | [ ] Major [ ] Trace [ ] Organic (CHNOPS) [ ] Other

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Unq	Unp	Unh	Uns	Uno	Une	Unn								
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

Informations

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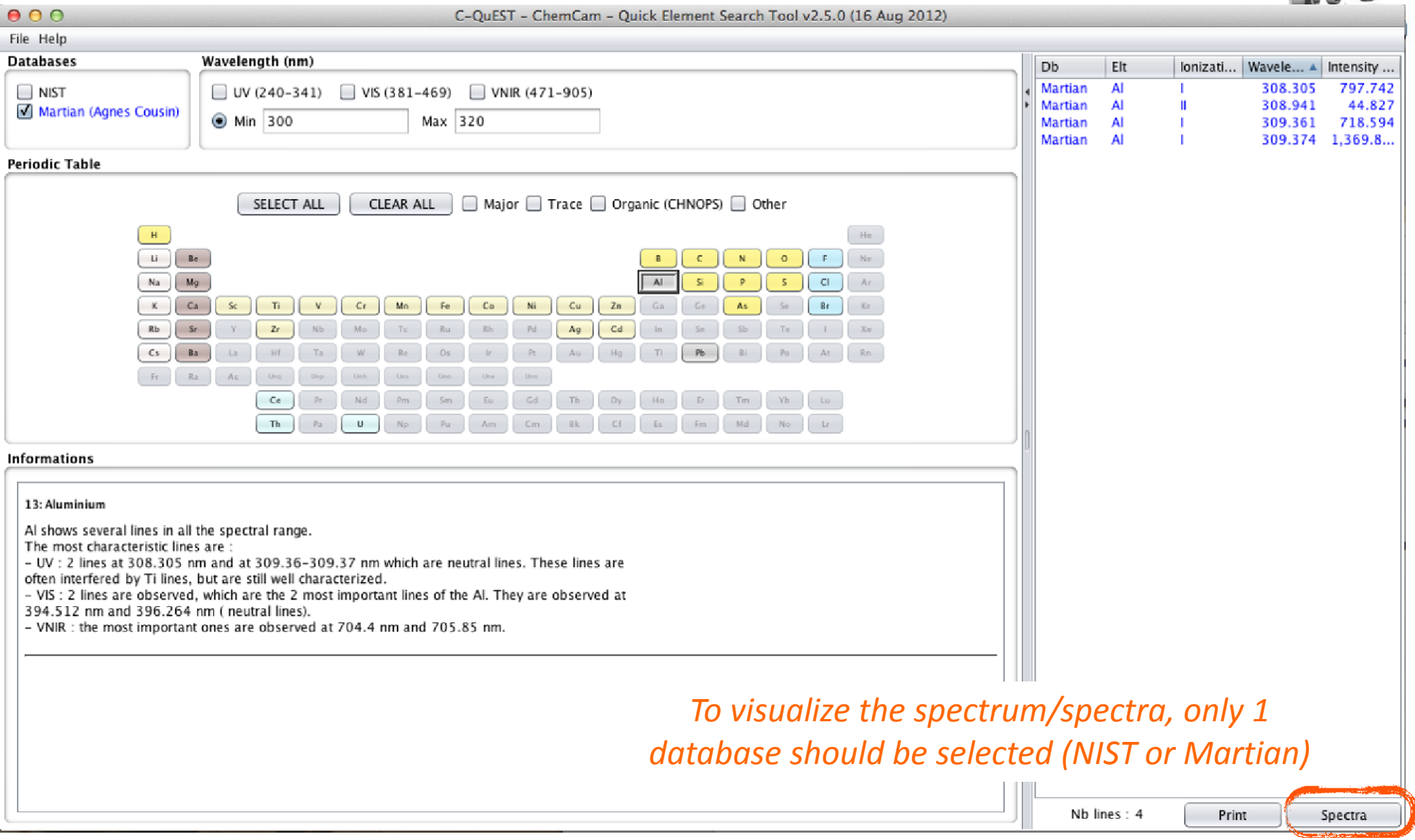
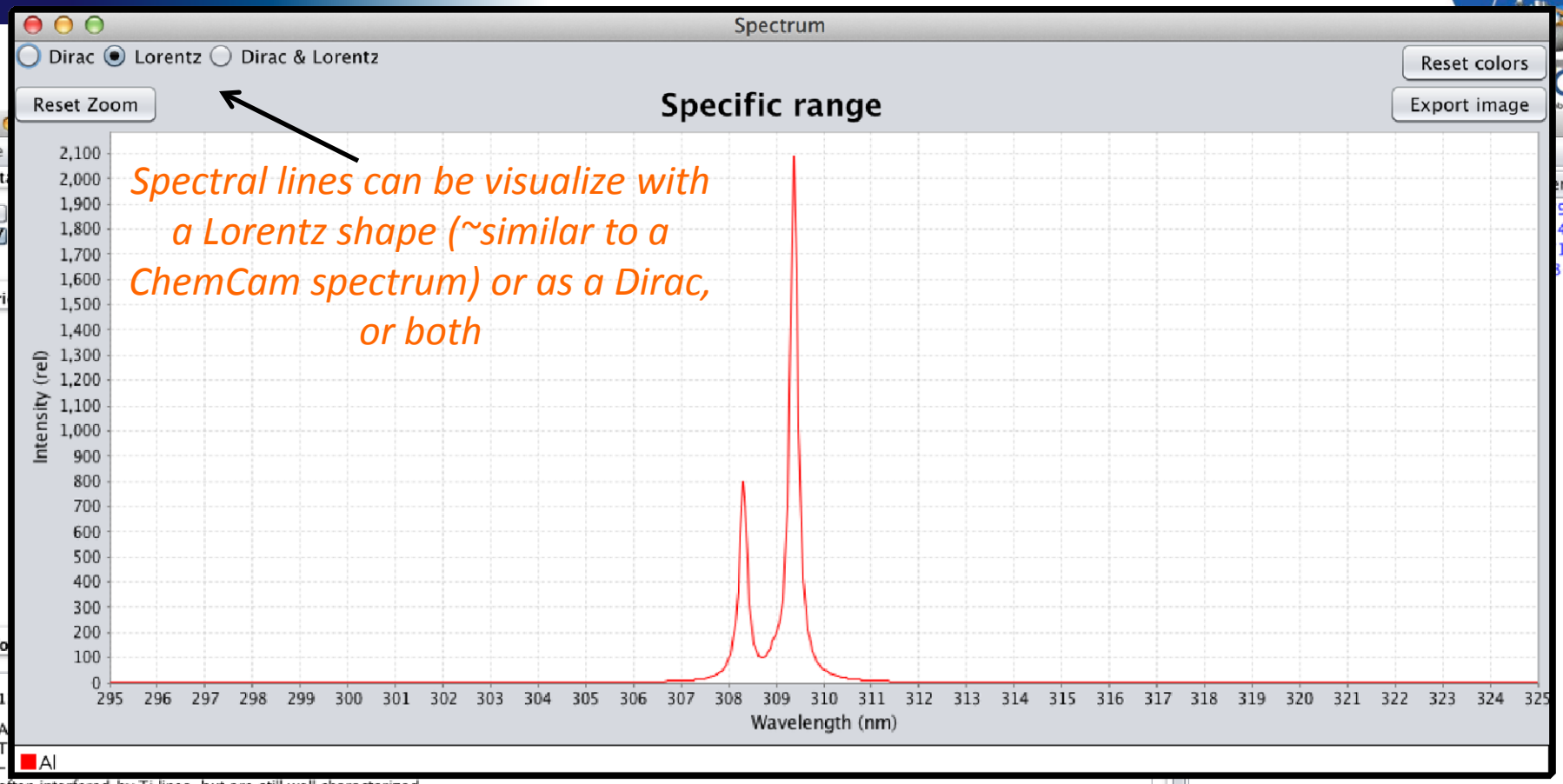
Martian	Al	I	309.361	718.594
Martian	Al	I	309.374	1,369.8...

Nb lines : 4 | Print | Spectra

To print the list of emission lines



To visualize the spectrum/spectra, only 1 database should be selected (NIST or Martian)



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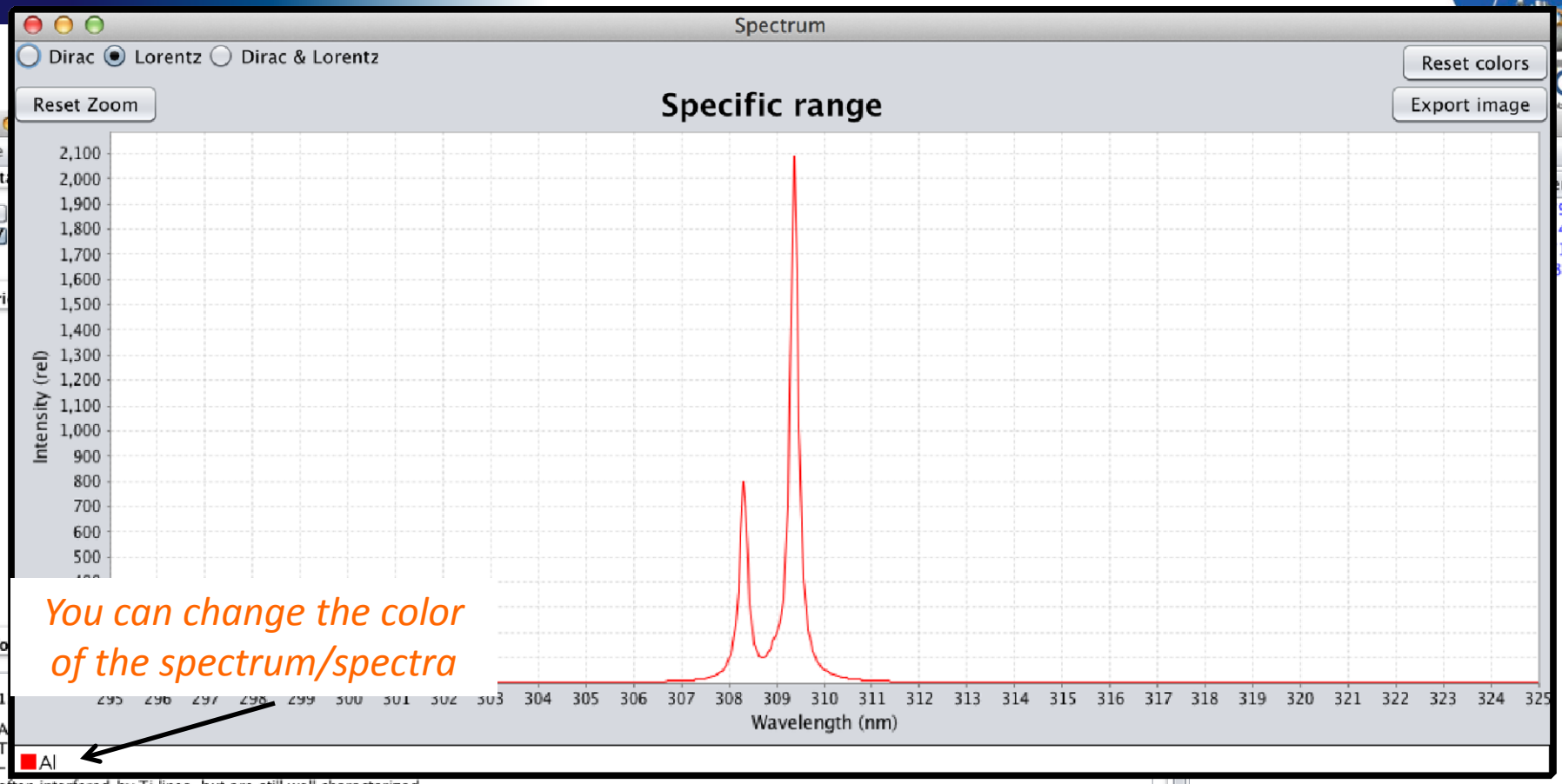
- VNIR : the most important ones are observed at 704.4 nm and 705.85 nm.

Nb lines : 4 Print Spectra



You can change the color of the spectrum/spectra

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- VIS : 2 lines are observed, which are the 2 most important lines of the Al. They are observed at 394.512 nm and 396.264 nm (neutral lines).
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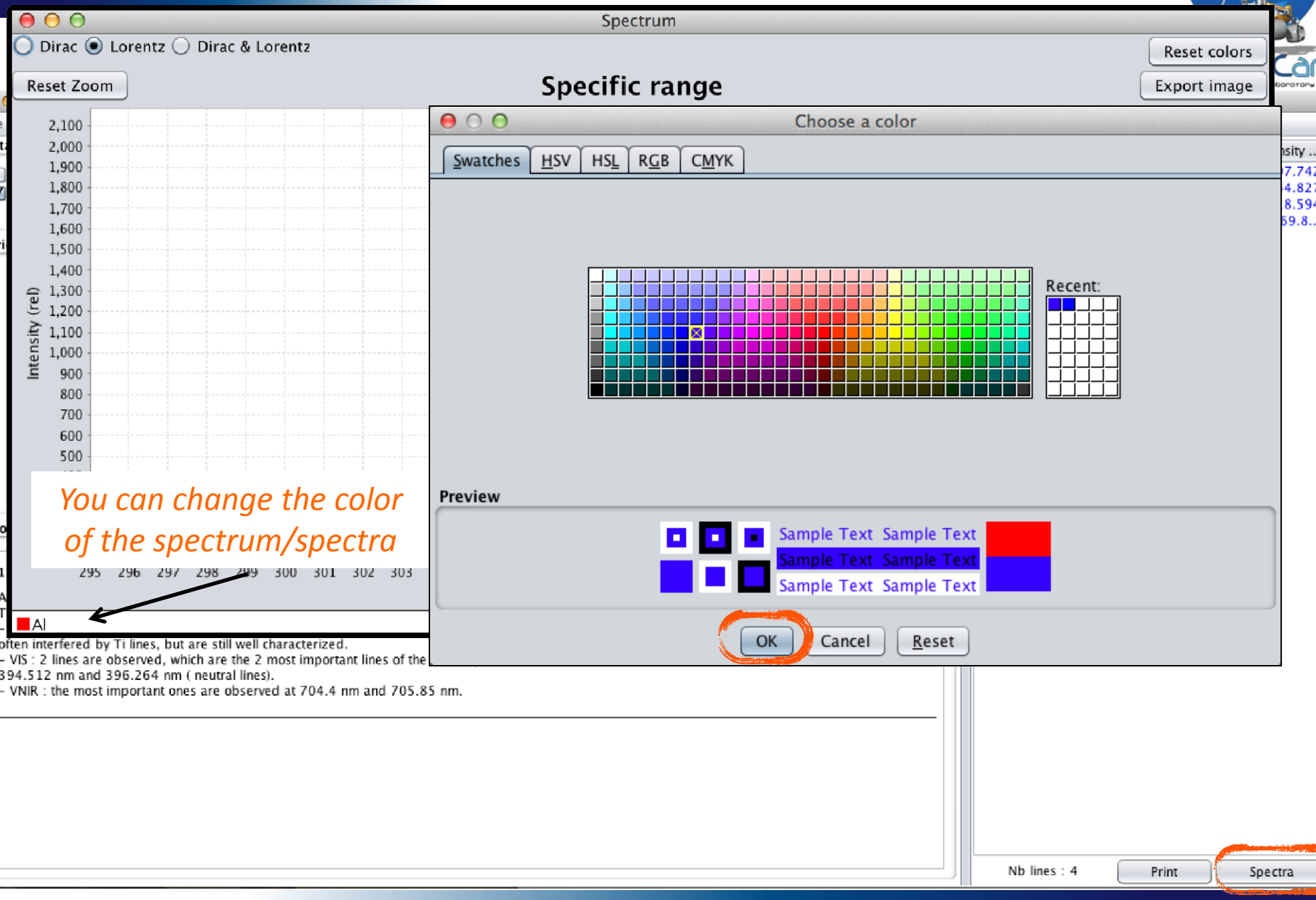
Nb lines : 4 | Print | Spectra


Spectrum
Dirac
Lorentz
Dirac & Lorentz
Reset colors
Reset Zoom
Specific range
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Swatches
HSV
HSL
RGB
CMYK
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Preview
Sample Text Sample Text
Sample Text Sample Text
Sample Text Sample Text
OK
Cancel
Reset
Intensity (rel)
2,100
2,000
1,900
1,800
1,700
1,600
1,500
1,400
1,300
1,200
1,100
1,000
900
800
700
600
500
295 296 297 298 299 300 301 302 303
Al
You can change the color of the spectrum/spectra
often interfered by Ti lines, but are still well characterized.
- VIS : 2 lines are observed, which are the 2 most important lines of the
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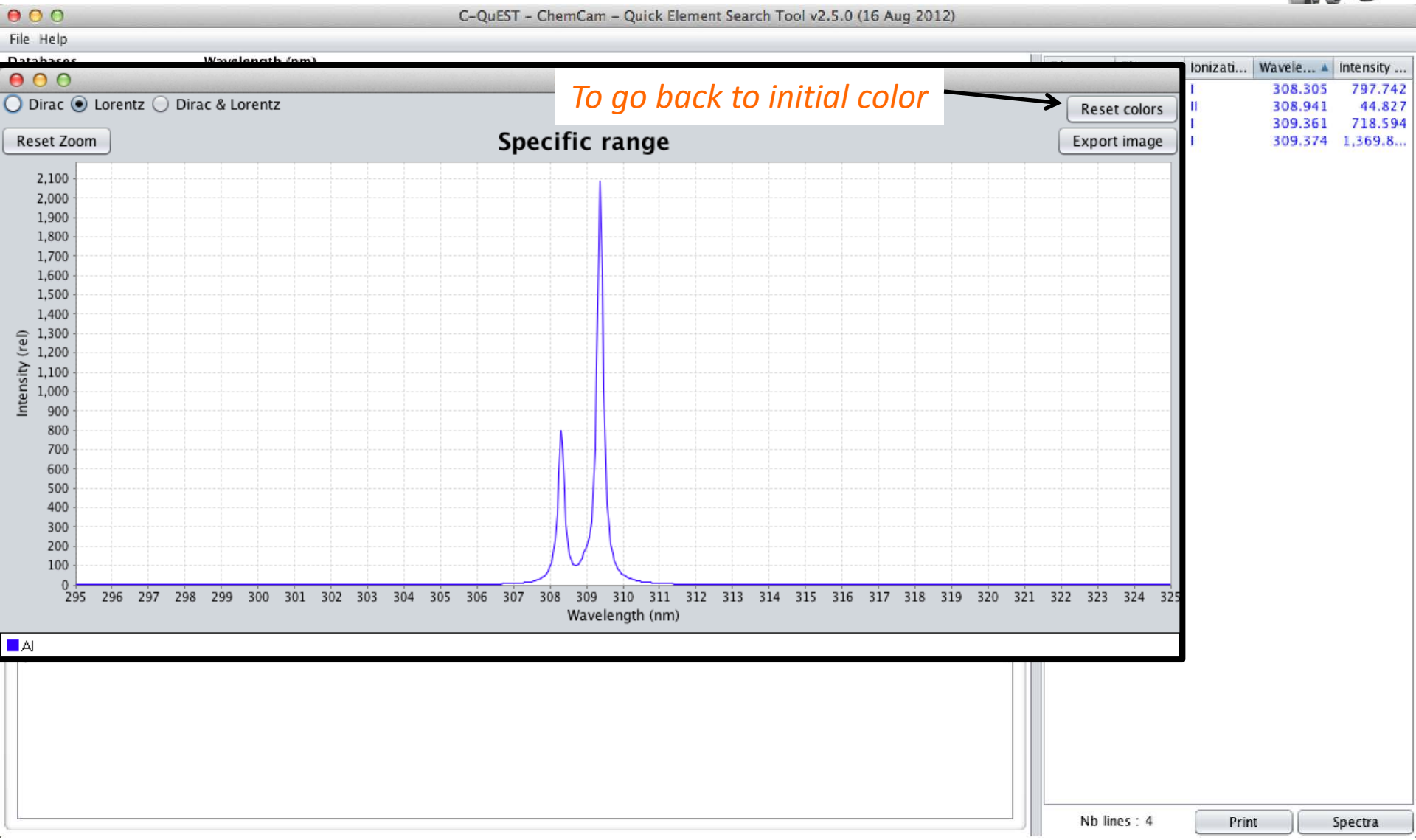
- VNIR : the most important ones are observed at 704.4 nm and 705.85 nm.
Nb lines : 4
Print
Spectra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File Help
To go back to initial color
Dirac
Lorentz
Dirac & Lorentz
Reset colors
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Wavelength (nm)
Al
Ionizati...
Wavele...
Intensity ...
I 308.305 797.742
II 308.941 44.827
I 309.361 718.594
I 309.374 1,369.8...
Nb lines : 4
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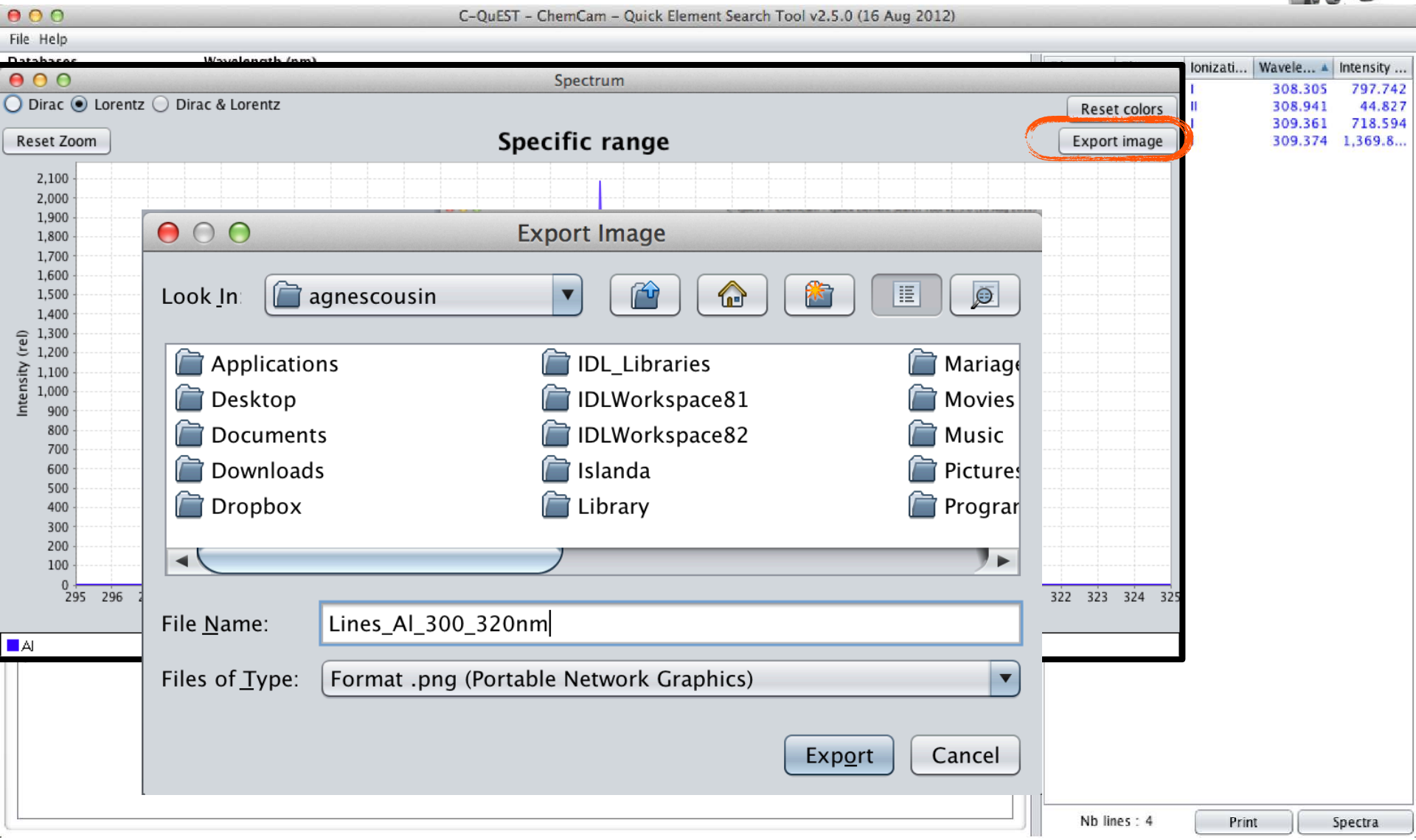
Spectra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Spectrum
Dirac Lorentz Dirac & Lorentz
Reset Zoom
Specific range
Reset colors
Export image
Intensity (rel)
Export Image
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Applications
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Documents
Downloads
Dropbox
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IDLWorkspace81
IDLWorkspace82
Islanda
Library
Movies
Music
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Ionizati...
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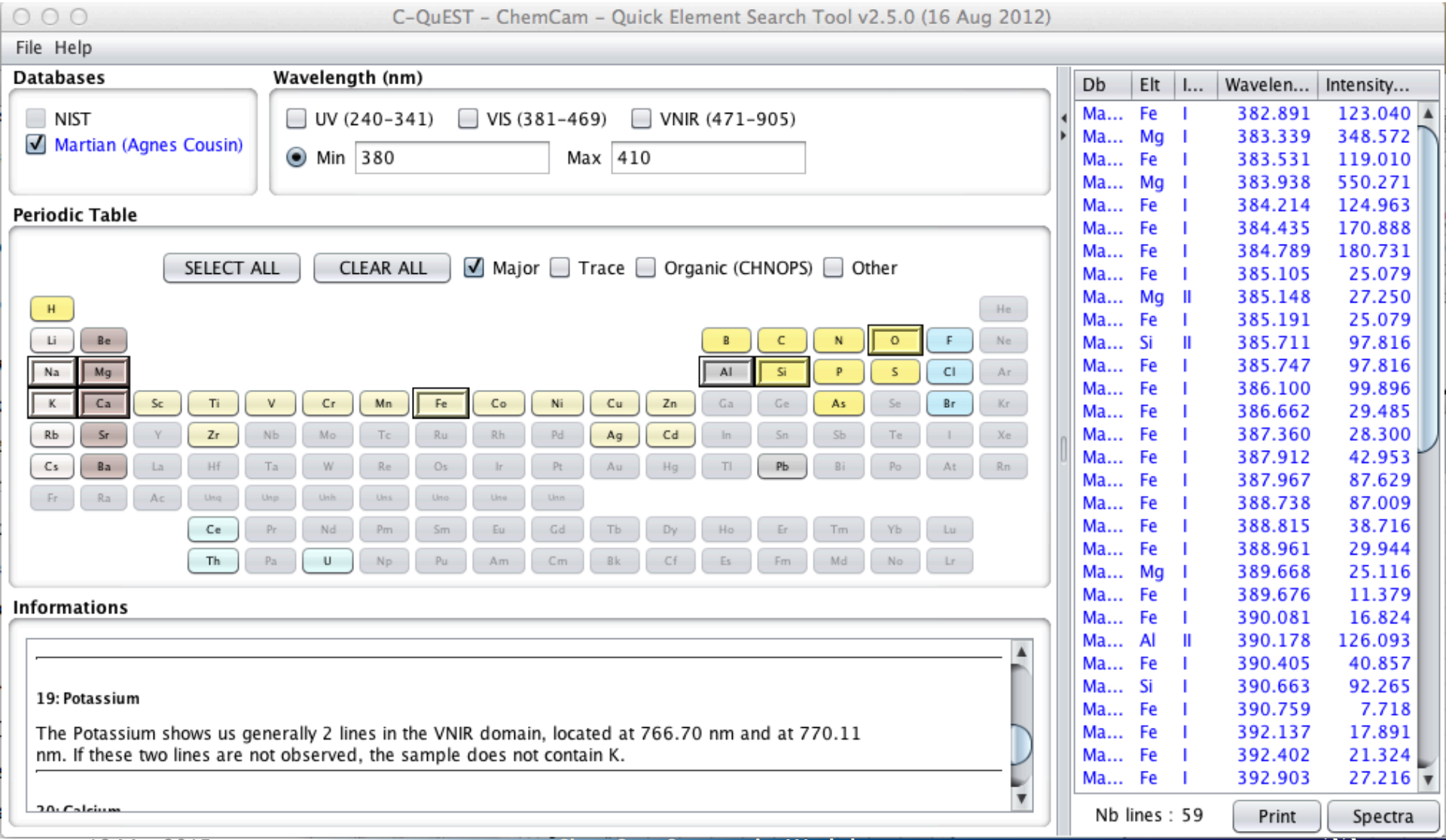
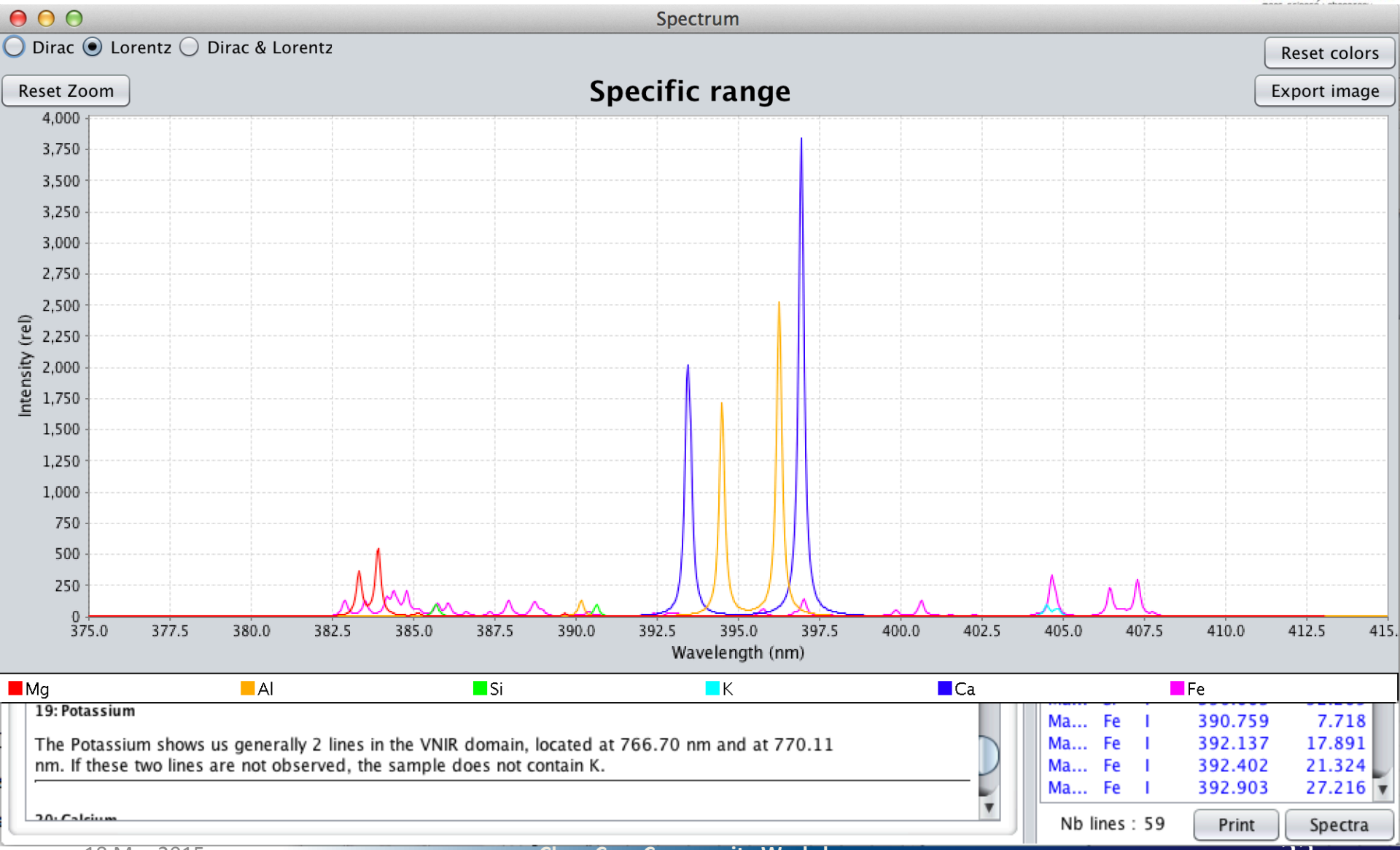
Intensity ...
308.305 797.742
308.941 44.827
309.361 718.594
309.374 1,369.8...
Al
Nb lines : 4
Print
Spectra

Example with several elements



Example with several elements



TIPS

- To visualize a synthetic spectrum, it is better to select only 1 spectral range (UV, VIS or VNIR) :
  - Data acquired with commercial spectrometers without a demultiplexer (each spectral range acquired separately)
  - Total intensity from one domain to another can be different

Backup slides

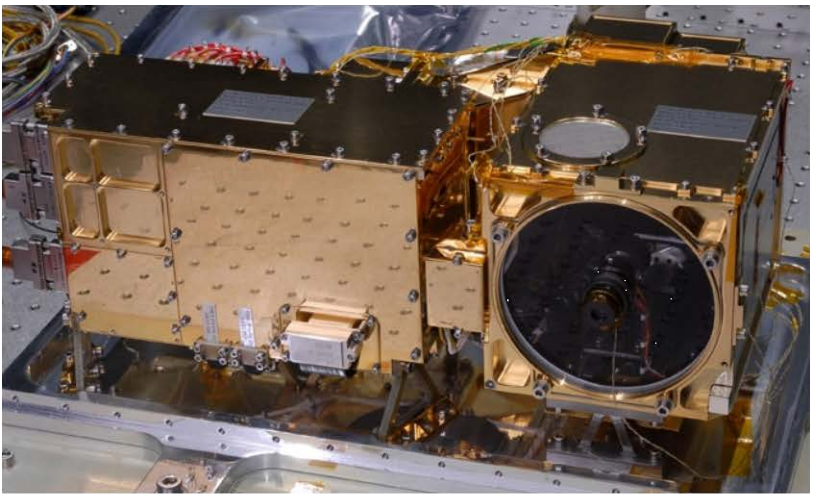
Ground Station

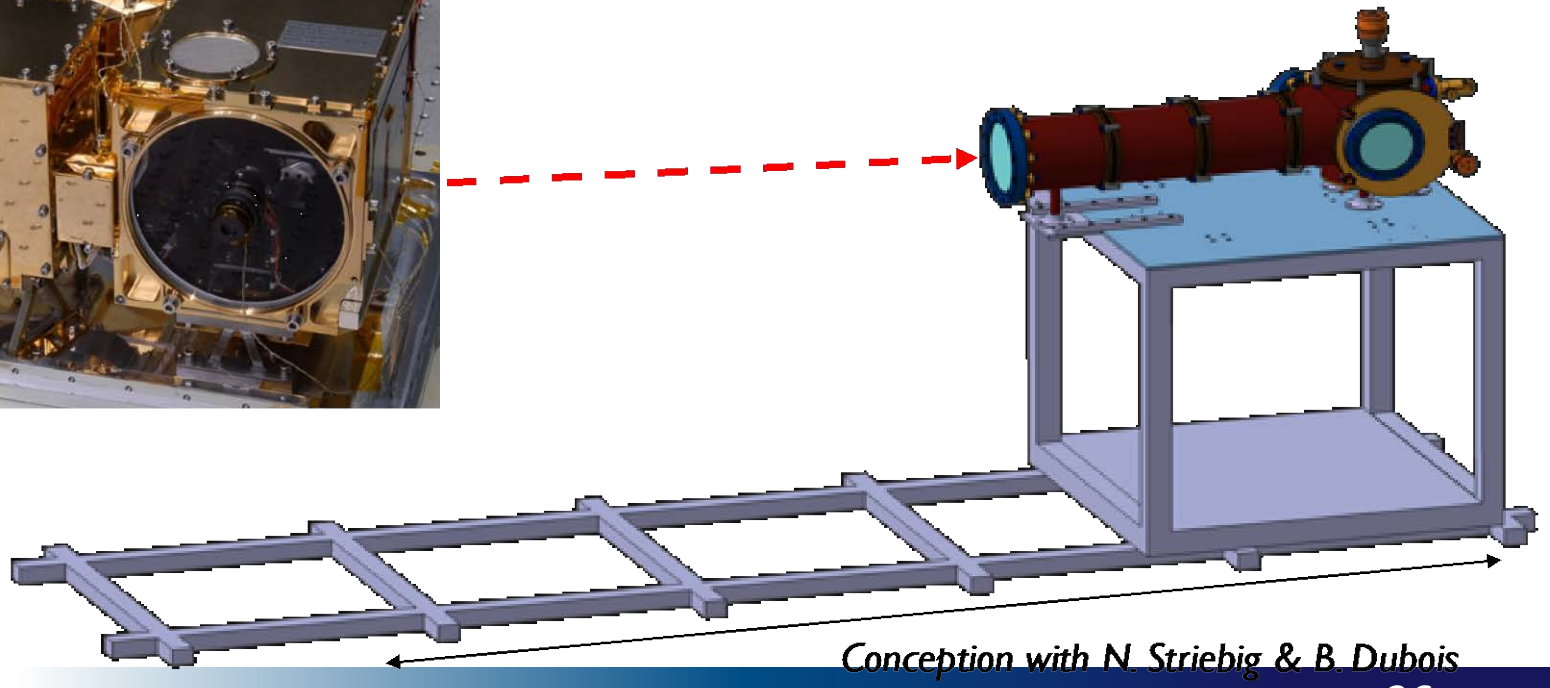
ChemCam

- Mast Unit : Engineering & Qualification Model (EQM)
- Body Unit: Commercial spectrometers (same resolution as flight Model)

Mars

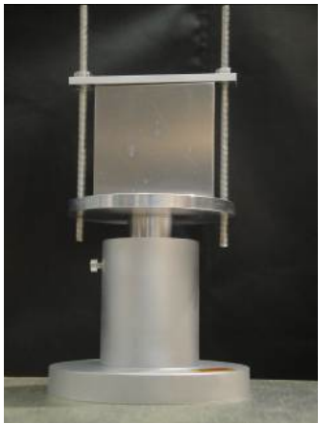
- 6 mbars
- Mars atmosphere (95.7 % CO_2, 2.7 % N_2, 1.6 % Ar)





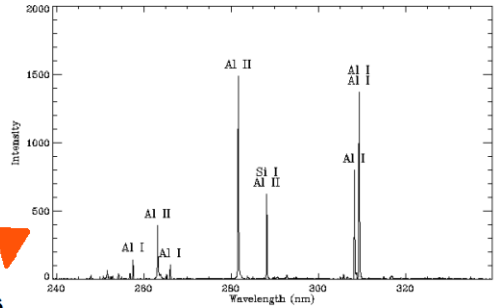
Emission Lines Database Creation

Characterized sampled

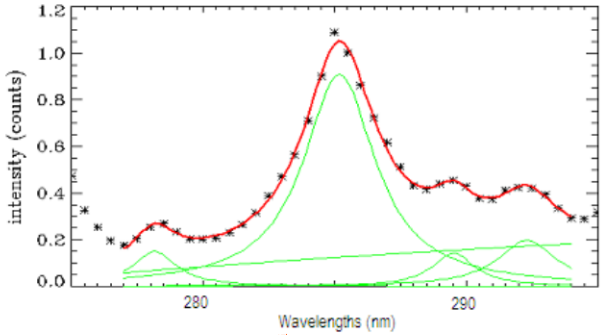


Processing

Line identification with NIST



Line fitting



Database creation

Element	Ext	OBS. Wave	OBS. Int.	Env.	Target
Al	I	257.570	143.582	MARS	Al/Si
Sr	II	421.682	327.219	MARS	Calib.
F	II	402.578	66.9510	MARS	Fluorine

Type of target	**Pure targets**	**Geological targets**	**Specific Atmospheres**
Elements *(Increasing Z)*	C, Al, Si, Ti, Mn, Fe, Ni, Cu, Pb	H, Li, Be, B, F, Na, Mg, P, S, Cl, K, Ca, V, Cr, Zn, As, Rb, Sr, Cs, Ba	N, Ar O

32 elements, 1336 emission lines