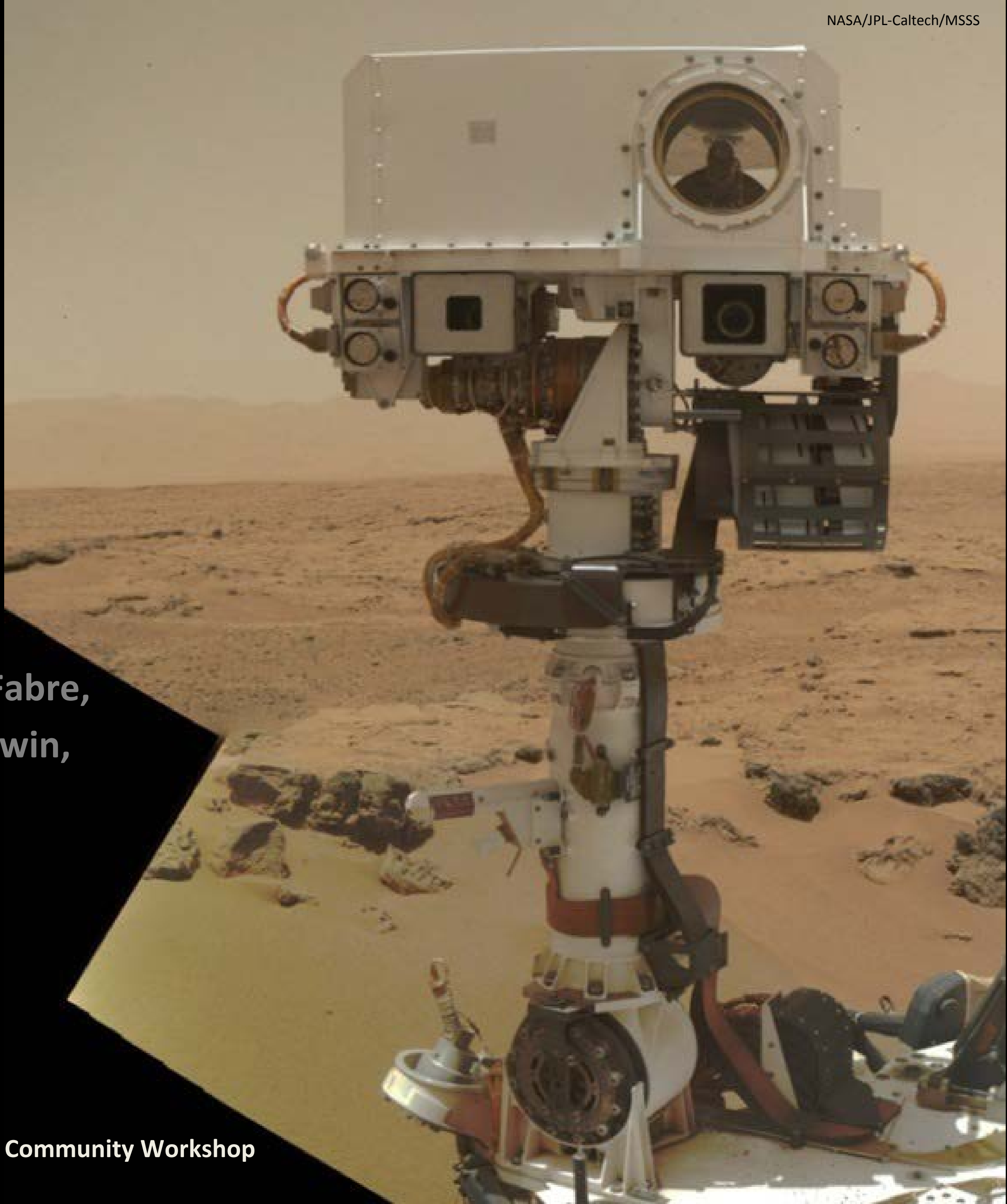
LPSC, ChemCam workshop March 18th, 2015

ChemCam data processing – Advanced processing



R. Anderson, S. Bender, S. Clegg, A. Cousin, D. Dyar, B. Ehlmann, C. Fabre, O. Forni, O. Gasnault, J. Lasue, E. Lewin, S. Maurice, N. Melikechi, R. Wiens, and the ChemCam Team

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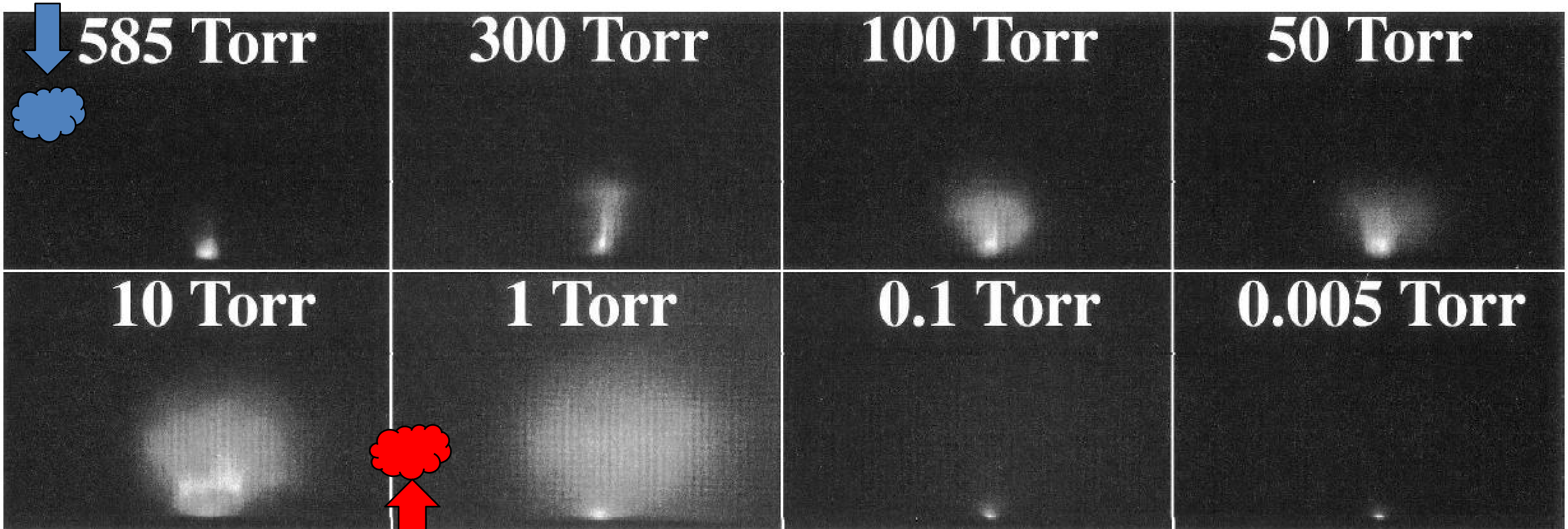
Mars conditions vs. experimental conditions

- Temperature variations can shift λ. Corrected automatically to better than 0.2 pix. MVA models errors increase <10% (Wiens et al. 2013)
- Pressure change (~40 Pa) has negligible effect on the plasma intensity and temperature.
- On-target energy density (related to focus, distance, target properties, etc.) influences plasma conditions
    - Ongoing work to asses and correct for this
- Note: all calibration data on Earth are collected under Mars conditions

Evolution of LIBS plasma with pressure

Earth atmospheric pressure (760 Torr)



Mars atmospheric pressure (5-7 Torr)

Lunar surface pressure (10^{-8}-10^{-12} Torr)

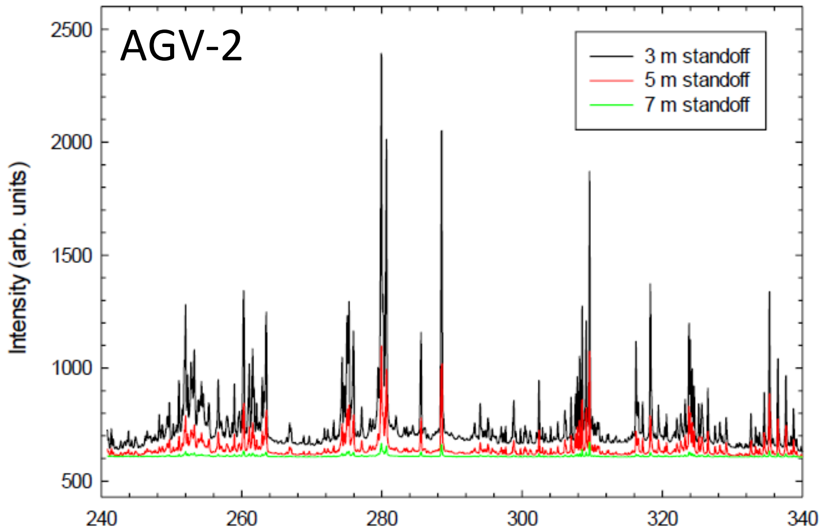
REMS Mars daytime variation 40 Pa ~ 0.3 Torr

Knight et al. 2000: Al I emission at 394.4 nm, Los Alamos soil; gated window between 50ns and 200ns.
See also: Clegg et al., 2007; Mezzacappa et al., LIBS 2010; Lasue et al., LPSC 2011

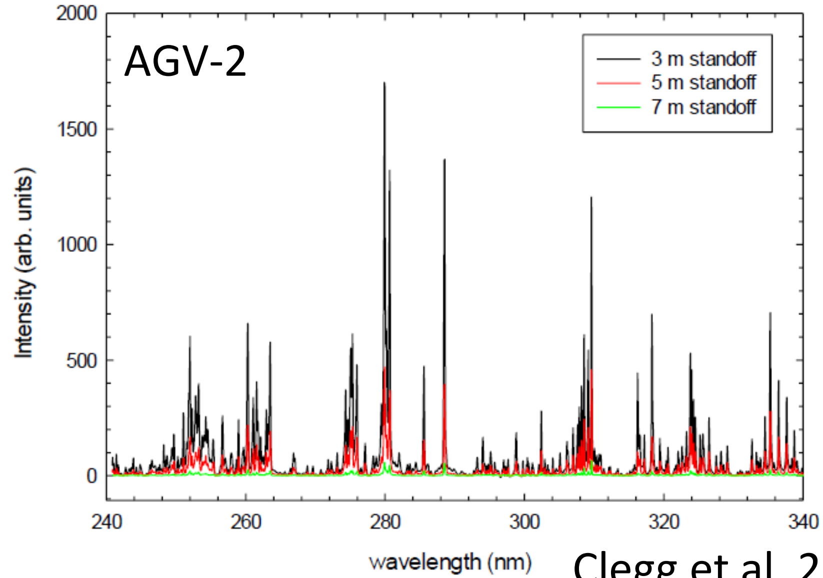
AGV-2 Calibration Spectra at 3, 5, and 7 m Standoff Distance

Distance correction

Raw Spectra

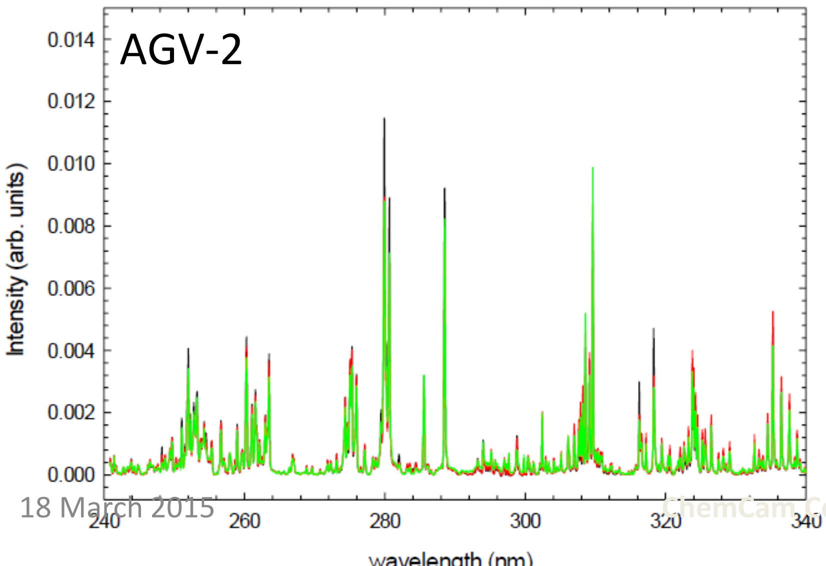


Continuum Removed



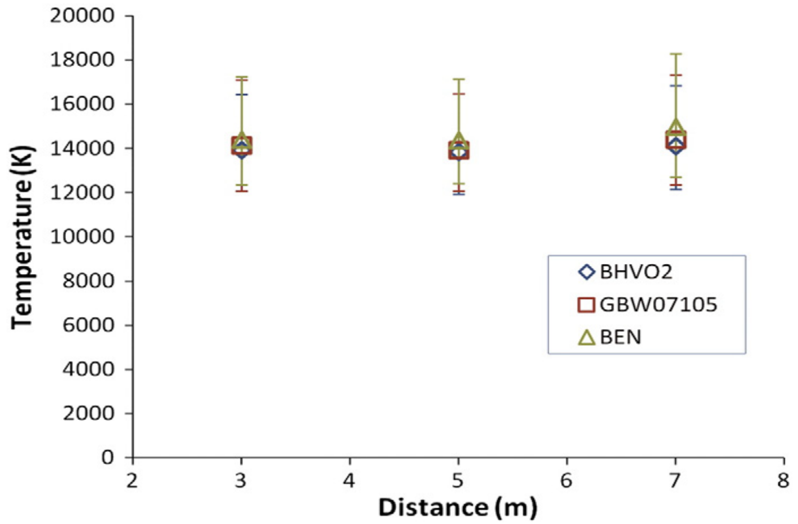
Clegg et al. 2013

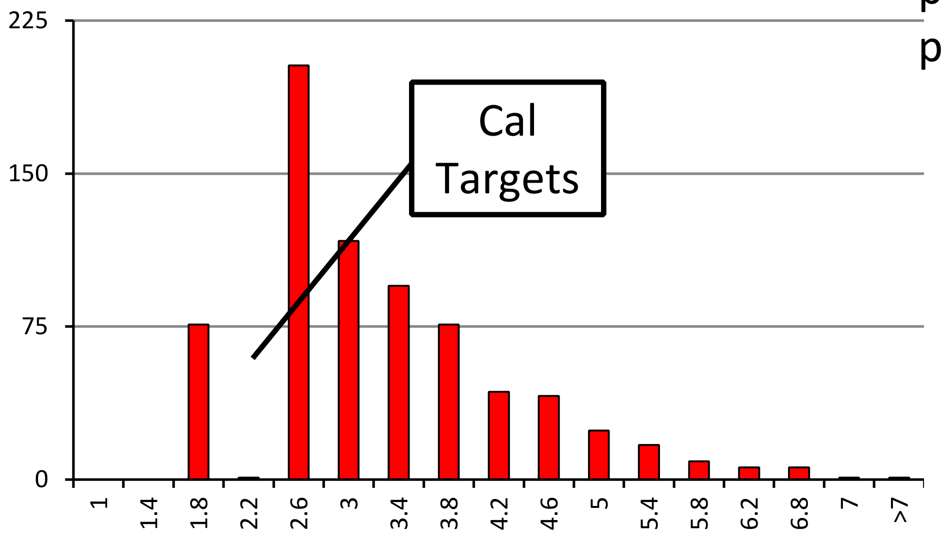
Continuum Removed + Normalized



- Background subtraction, instrument response ($1/r^2$) and normalization correct to 1st order
- Improved distance correction in progress (Melikechi et al., 2014, Mezzacappa et al., 2014)

Distance correction

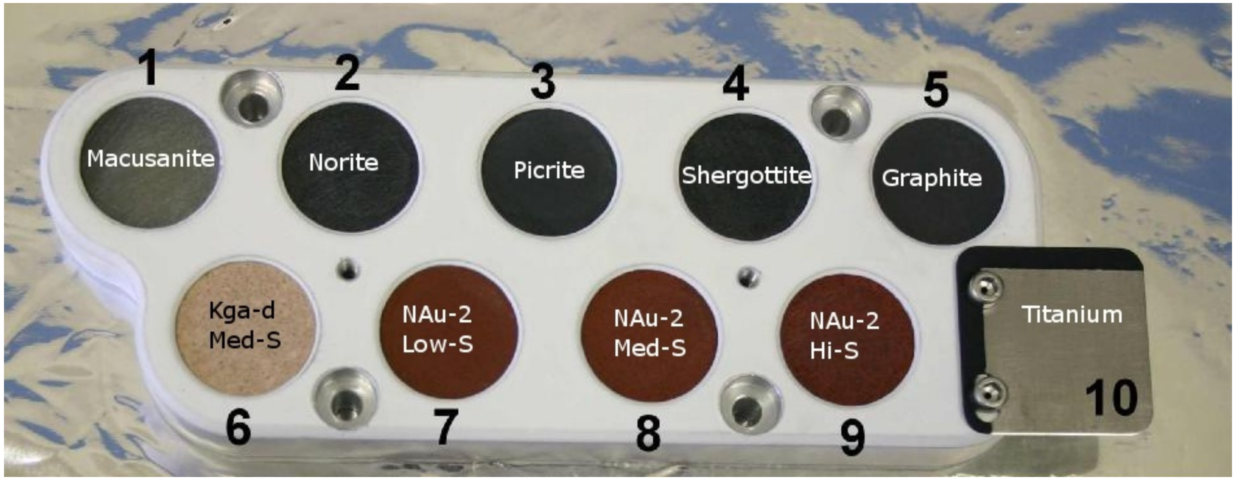




- Plasma temperature is independent of distance
  Wiens et al., 2013
- Most observations between 2m and 4m, but some out to 7m.
- Observations using the arm require strategic planning, but ChemCam observations can be planned tactically
  - Allows rapid response to interesting targets
  - >200,000 laser shots to date

Univariate calibration

- Use strength of a single emission line to predict the composition for a given element
- Useful alternative to multivariate method, especially for minor/trace elements
- Use calibration targets on the rover to build the regression
    - different laser energies require different models

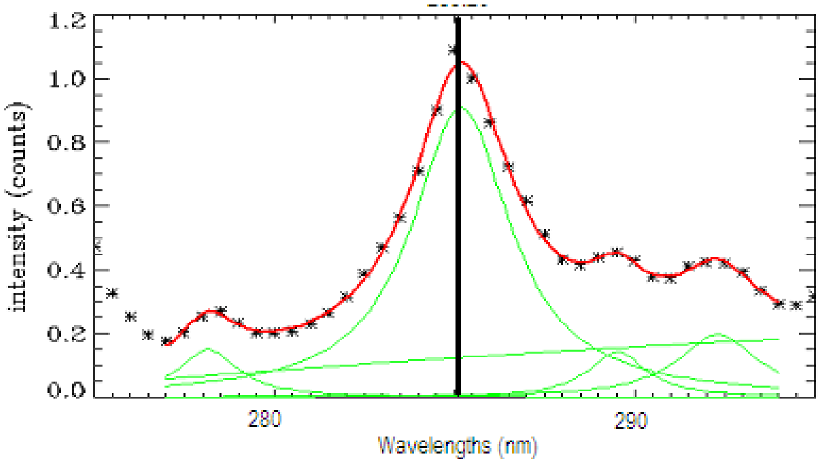


1. Macusanite volcanic glass
2. Norite synthetic glass
3. Picrite synthetic glass
4. Shergottite synthetic glass
5. Graphite
6. Kaolinite ceramic
7. Nontronite ceramic
8. Titanium plate (diagnostics)

References:
1-4: Fabre et al., 2011
6-9: Vaniman et al., 2012

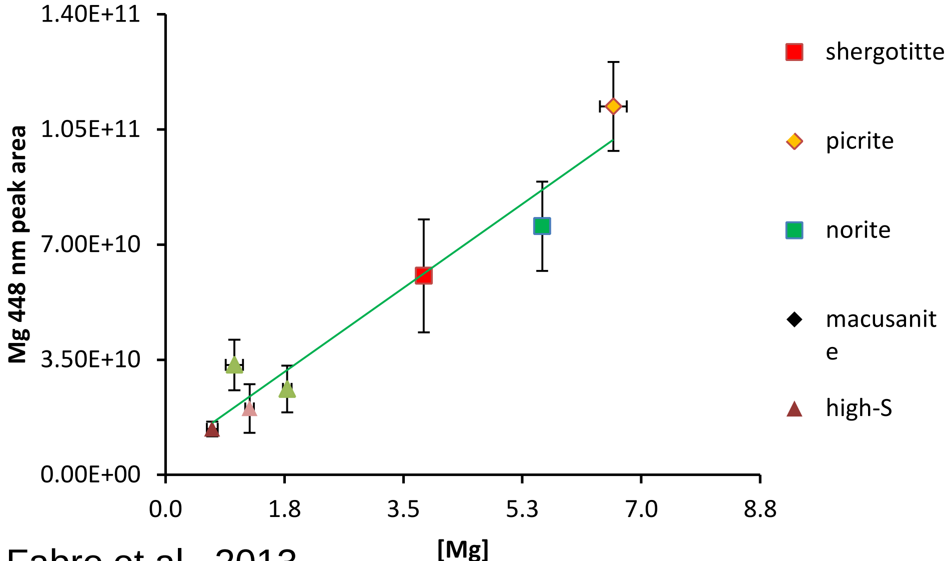
Univariate calibration

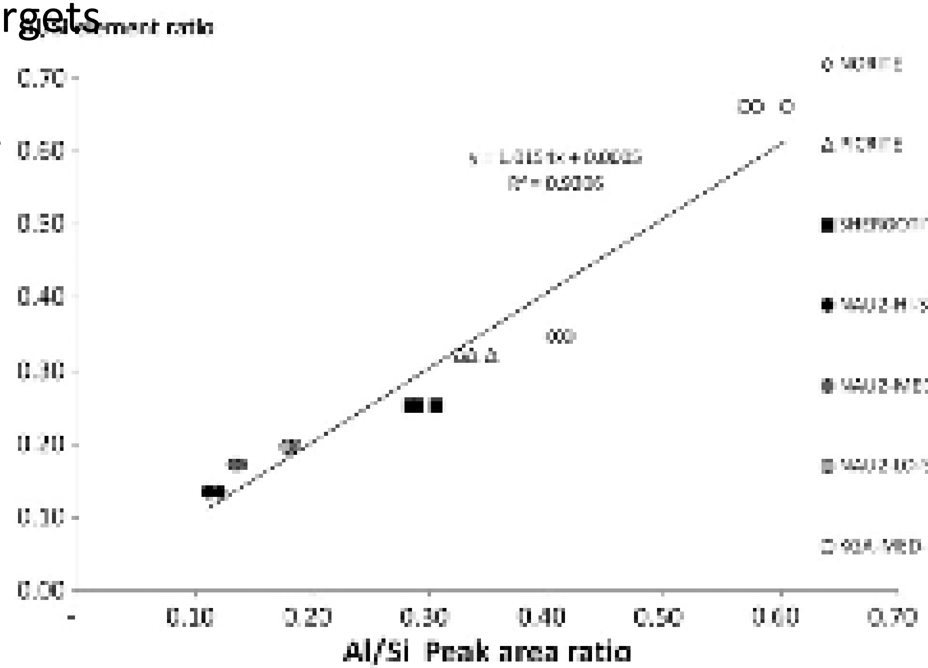
Peak fitting is necessary



- Use Cleaned Calibrated Spectra (CSS)
- Peak fitting is necessary to isolate the emission line of interest, so that calculated peak area is accurate
- Calibration curves plot peak area vs known composition
- Taking ratios of lines can help correct for differences in intensity from different targets

Calibration curves





Fabre et al., 2013

Univariate calibration

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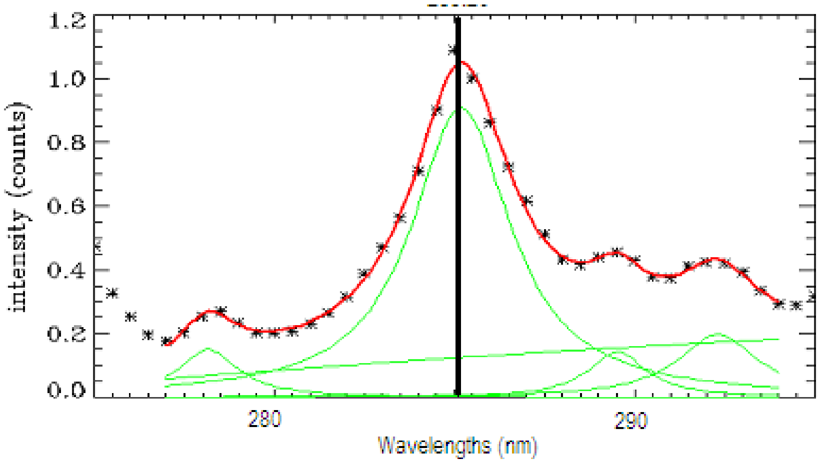

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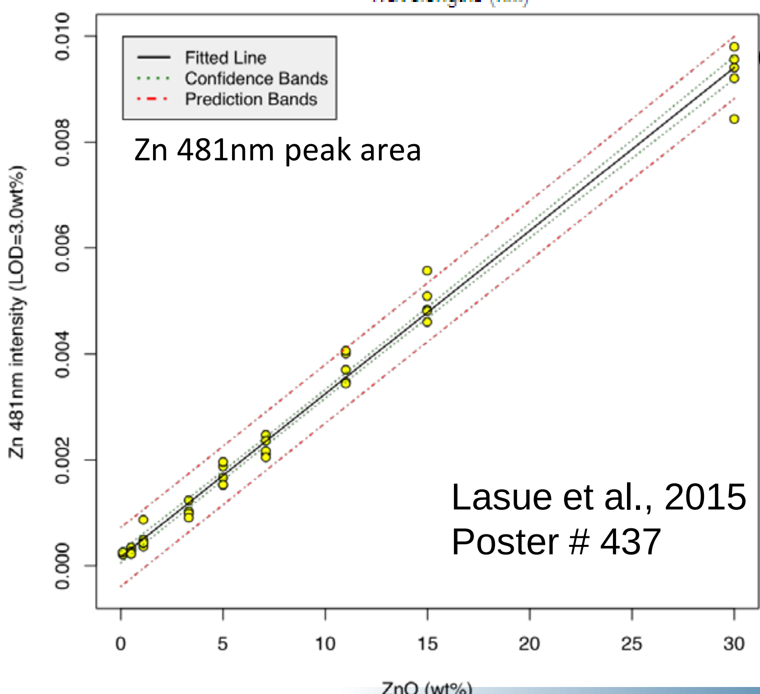
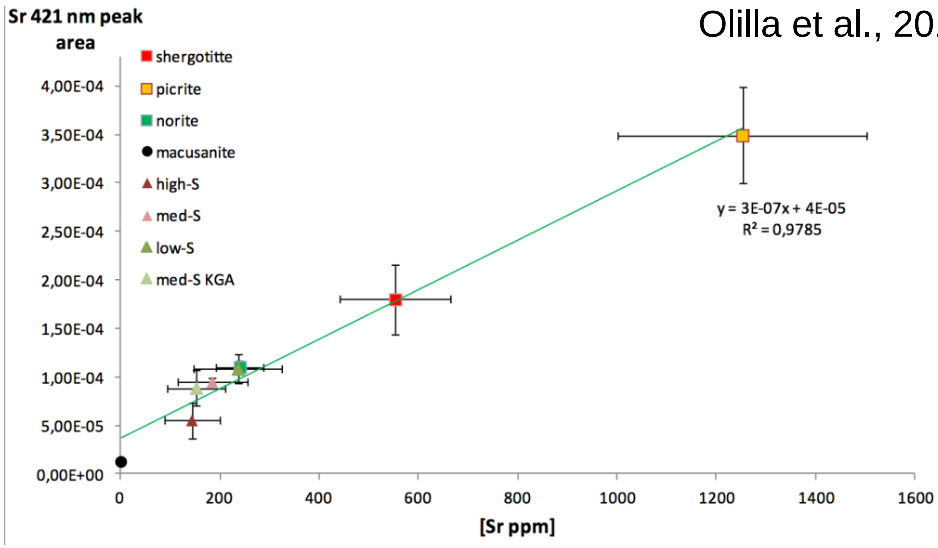


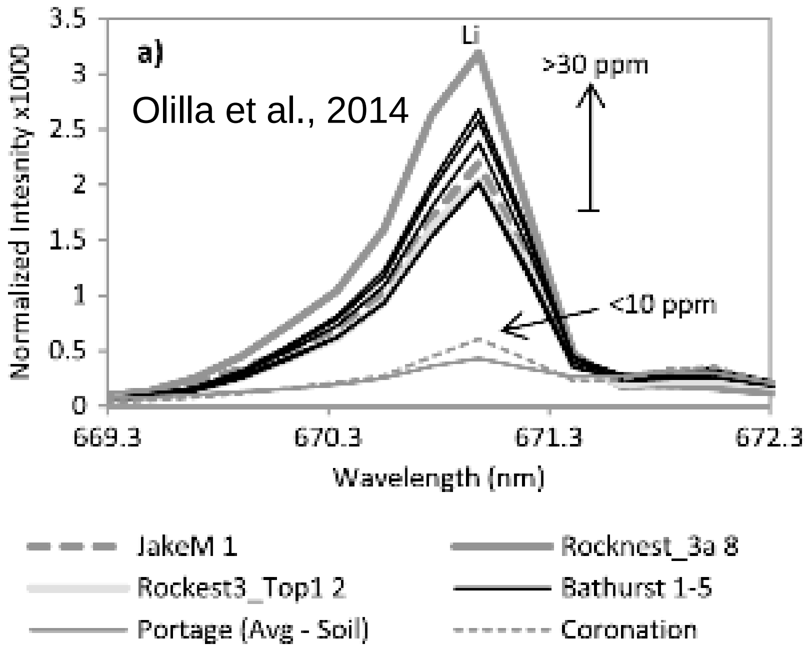
Lasue et al., 2015
Poster # 437

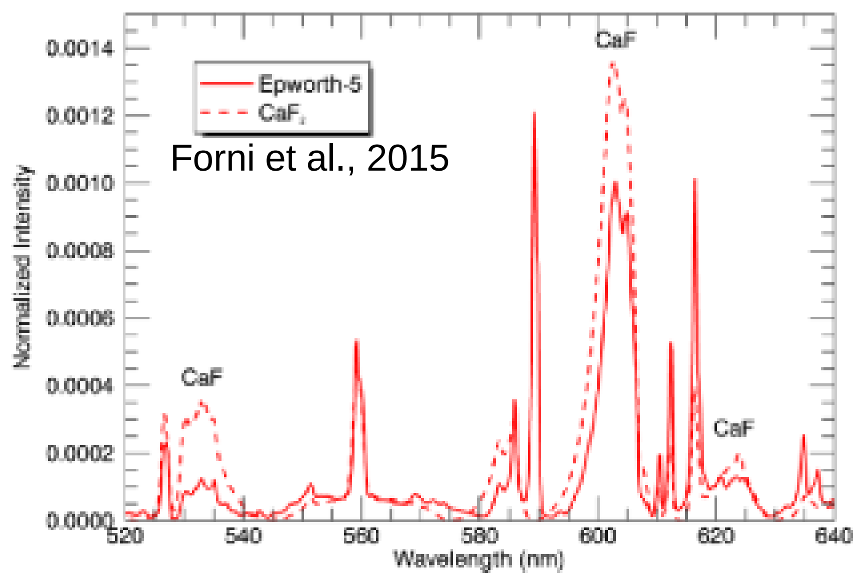
Olilla et al., 2014



Trace elements

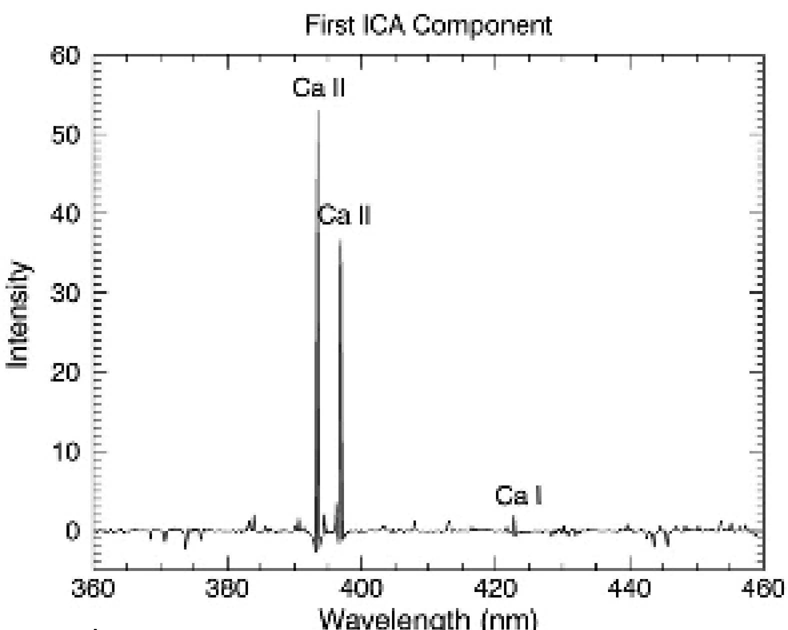
- ChemCam can detect minor and trace elements, including: Li, Ba, Sr, Rb, Mn, F, Zn, S
- Univariate models and/or restricted-range PLS can be used to get approximate quantitative measurements
- Using the full wavelength range in PLS doesn't perform as well: strong lines dominate



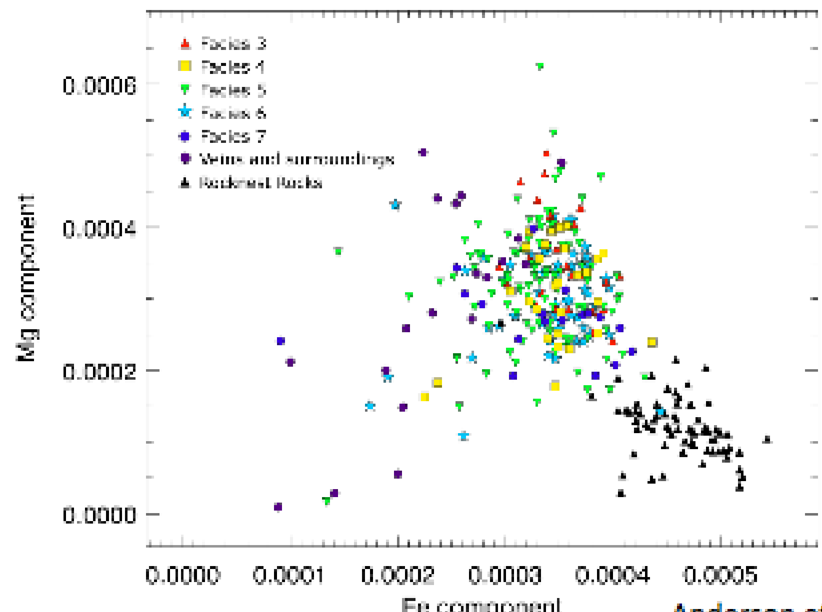


Independent Component Analysis

- Similar to PCA, but seeks to minimize statistical dependence between components
  - Does not assume a Gaussian distribution as PCA does
  - Results in loadings that isolate individual elements→ easier to read scores plots than PCA
    - Axes are a qualitative measure of signal from one element



Forni et al., 2013



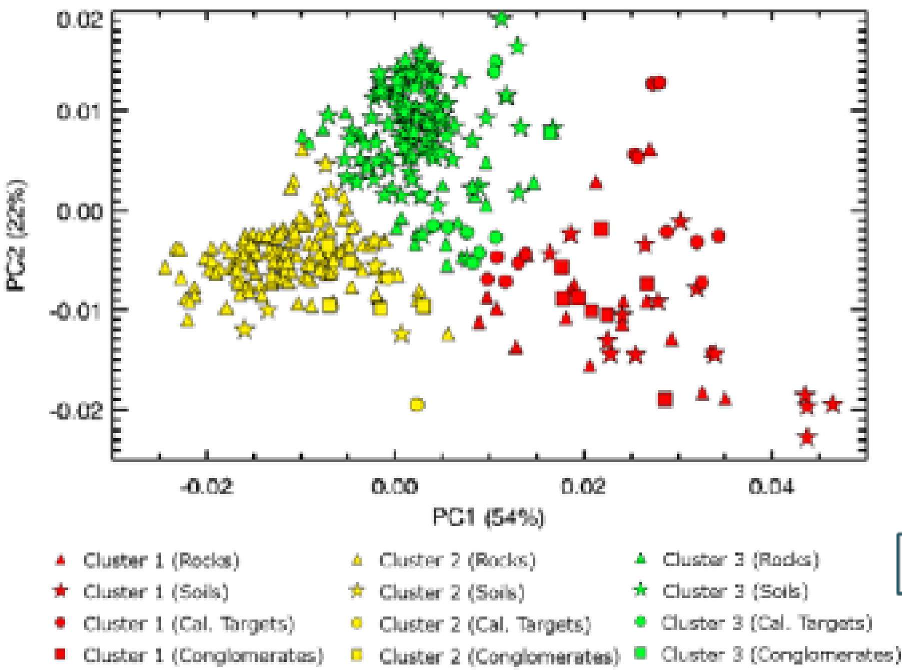
Anderson et al., 2014

Clustering / Classification

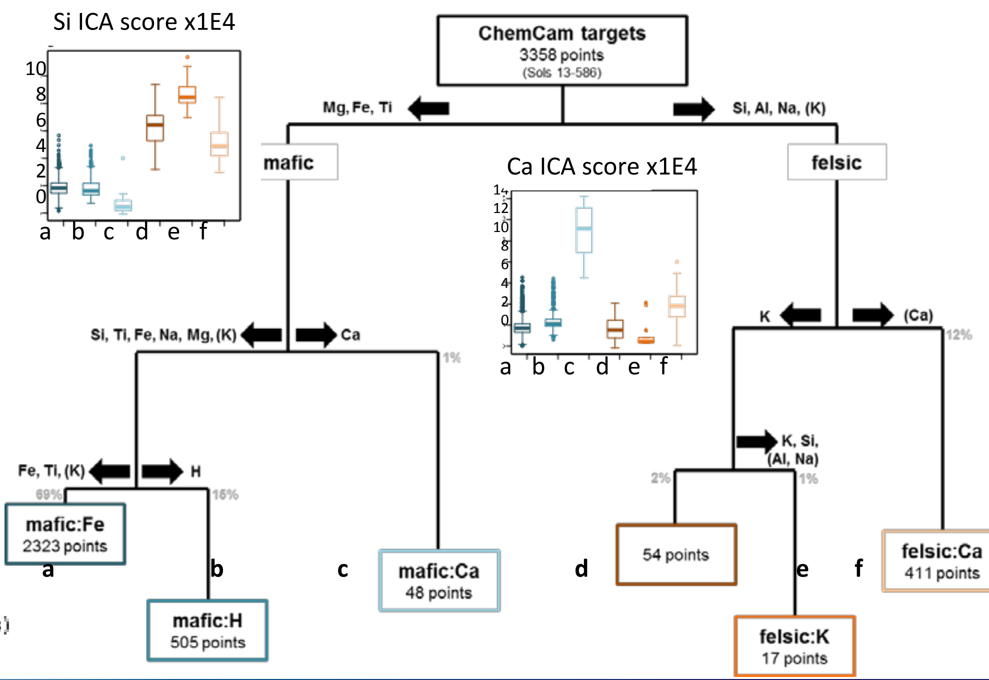
- Many different methods!
- Many use ICA or PCA scores as input
- Non linear projection can be used (Lasue et al. 2011)

- Unsupervised:
  - Hierarchical clustering
  - K-means clustering
- Supervised:
  - SIMCA
  - PLS-DA

Gasnault et al., 2015
Poster # 2789



Anderson et al., 2013 LPSC



Software options

- Unscrambler
  - Pro: capable of most multivariate analysis methods, relatively user-friendly
  - Con: proprietary, expensive, not scriptable
- Programming languages:
  - **IDL**
    - **Primary language currently used by the CCAM team**
    - Pro: scriptable, has functions for some methods described
    - Con: expensive, learning curve, doesn't have functions for all methods
  - **Python/Numpy/SciPy => next step**
    - Pro: free, scriptable, many libraries for multivariate analysis, widely used
    - Con: learning curve
  - R
    - Pro: very large library of statistical functions, free, widely used
    - Con: learning curve
- Many others!
- Questions? Ask a CCAM team member!
  My Email: jlasue@irap.omp.eu (full list available)

To be continued with
Multivariate Quantitative Predictions

Thank you