XRF INTER-COMPARISONS

IMPROVE Steering Committee Meeting

2021.11.9 – 2021.11.10

Nicole Hyslop, Chimnoy Sarkar, Nicholas Spada, Colleen Rosales

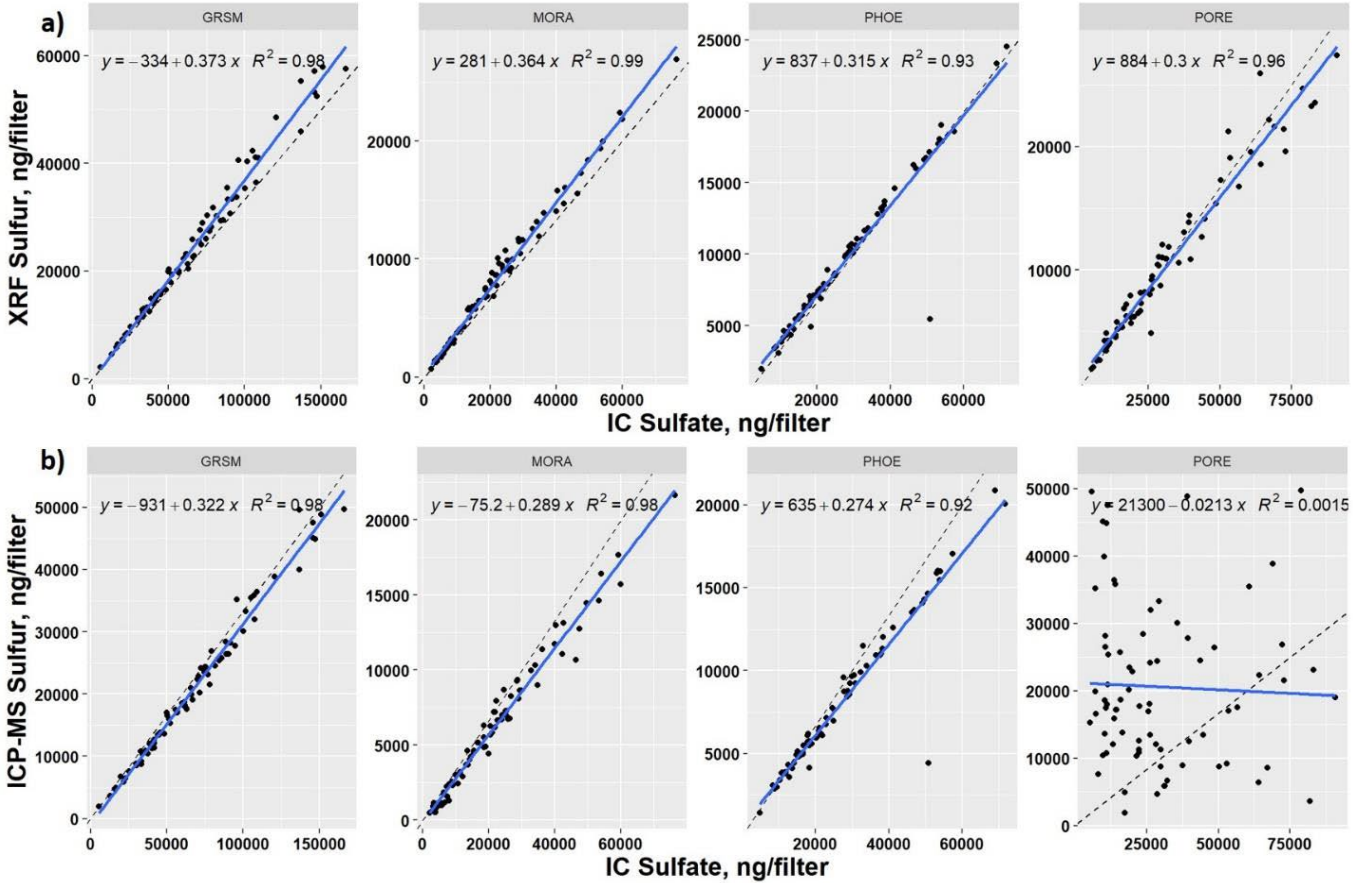
UCDAVIS

AIR QUALITY RESEARCH CENTER

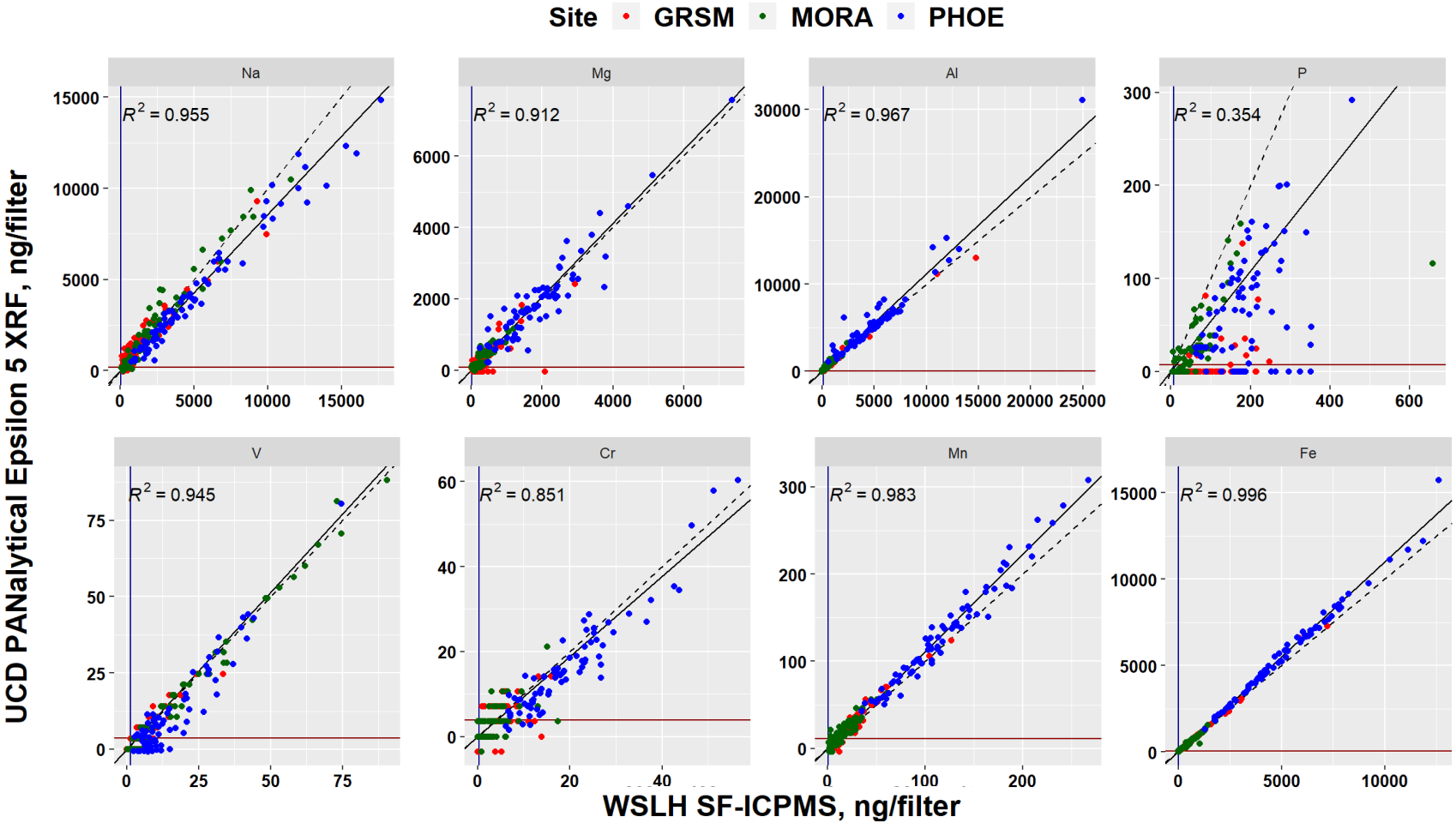
Two X-Ray Fluorescence (XRF) Inter-comparisons

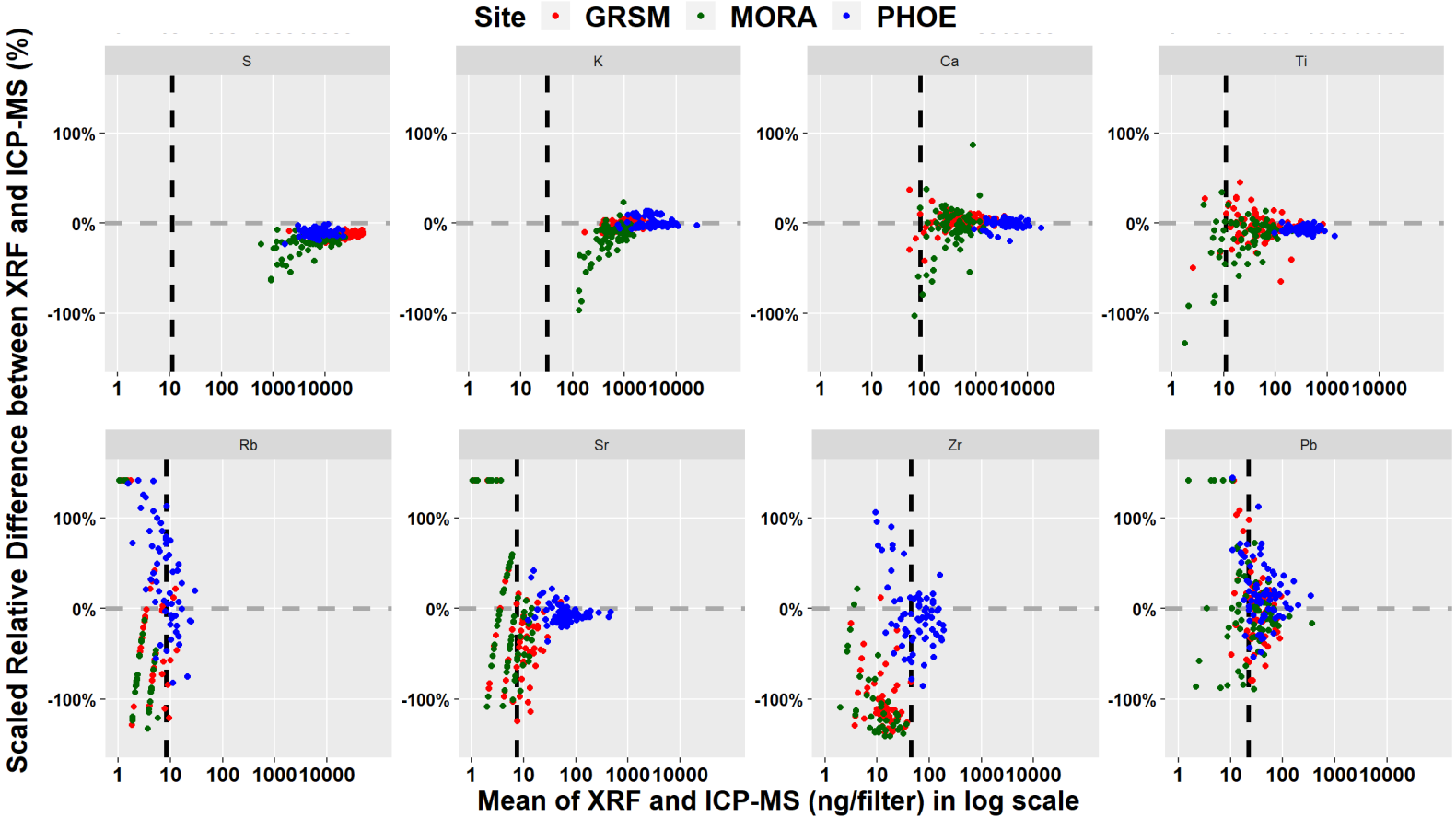
- UCD XRF versus Wisconsin State Laboratory of Hygiene (WSLH) Sector-Field Inductively Coupled Plasma Mass Spectrometry (ICP-MS)
  - 300 samples from 4 IMPROVE sites
  - 20 overlapping elements
  - Lab analyses completed in 2019, manuscript submitted in 2021
- UCD XRF versus RTI XRF and ICP-MS: 3-way comparison
  - 400 samples from Chemical Speciation Network (CSN) samples
    - From all sites in network to cover the range of source profiles
    - Represent range of loadings
    - Collocated samples to assess intra- and inter-instrument uncertainties
  - ICP-MS analysis is on-going

IC Sulfate Results Used to Validate XRF and ICP-MS Results



Something went wrong with PORE analysis by ICP-MS

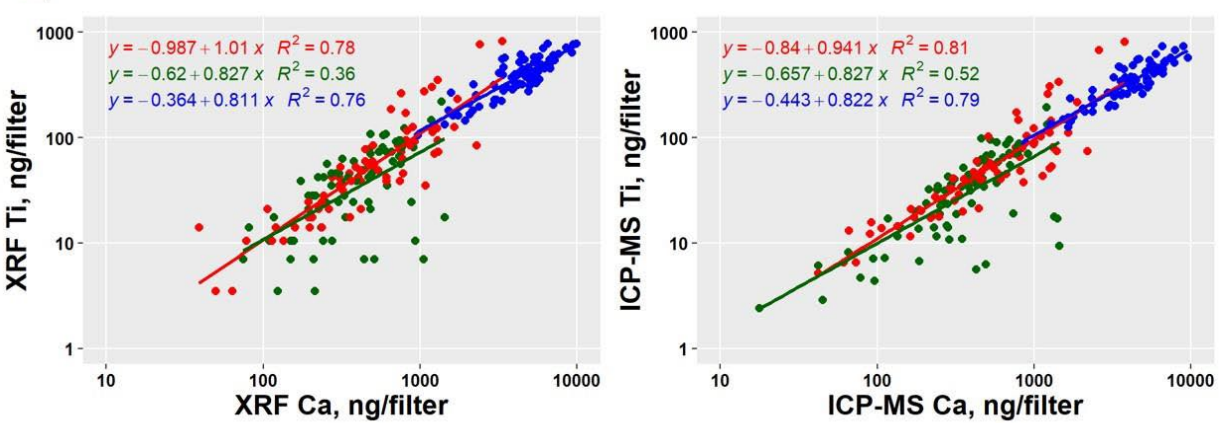

Site GRSM MORA PHOE
Na
R^2 = 0.955
Mg
R^2 = 0.912
Al
R^2 = 0.967
P
R^2 = 0.354
V
R^2 = 0.945
Cr
R^2 = 0.851
Mn
R^2 = 0.983
Fe
R^2 = 0.996
UCD PANalytical Epsilon 5 XRF, ng/filter
WSLH SF-ICPMS, ng/filter



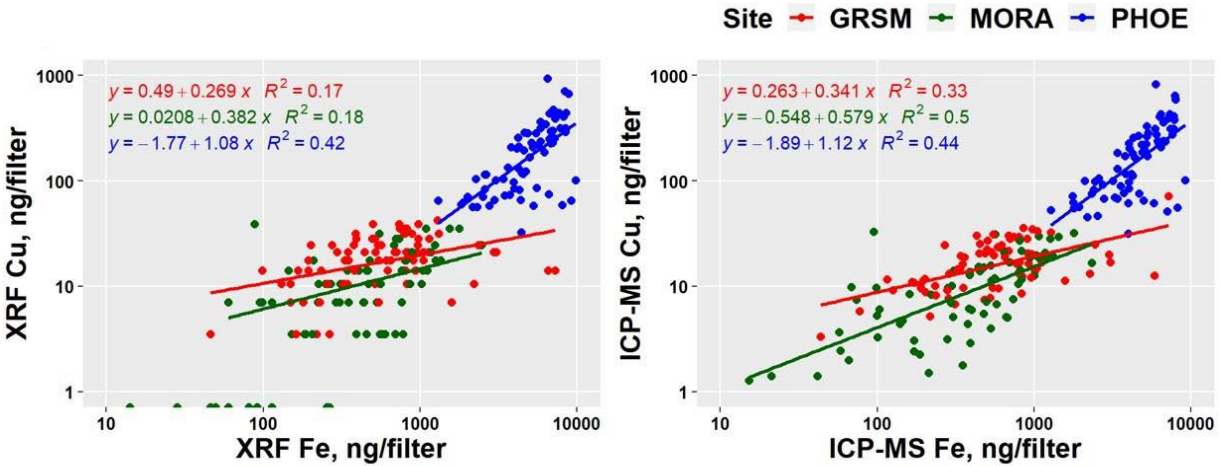
$$Scaled\ Relative\ Difference\ (SRD) = \frac{(XRF_i - ICPMS_i)/\sqrt{2}}{(XRF_i + ICPMS_i)/2}$$

Use element ratios to assess results (continued)

Ti and Ca: soil dust

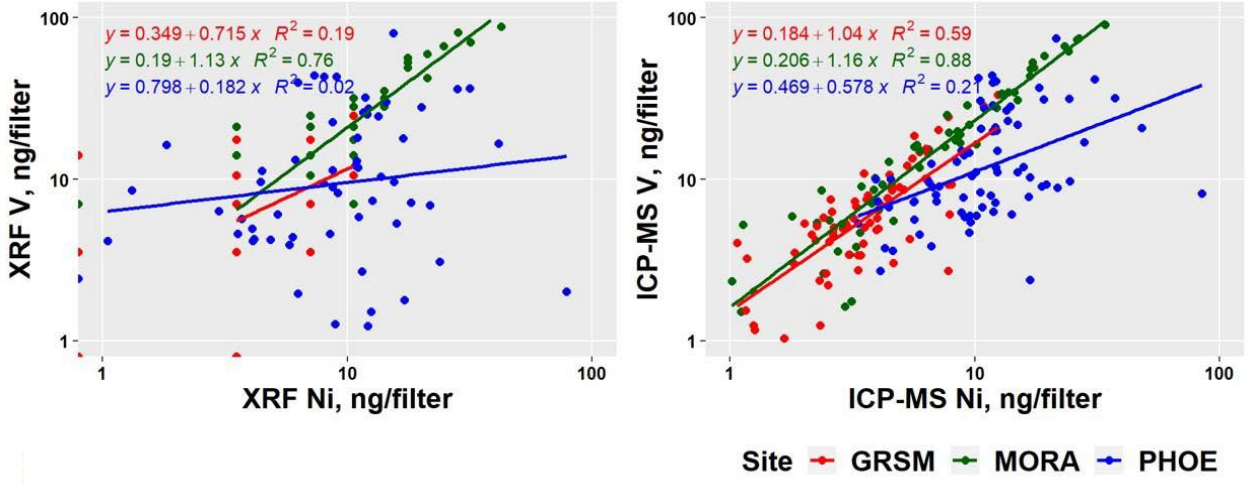


Cu and Fe: vehicular sources

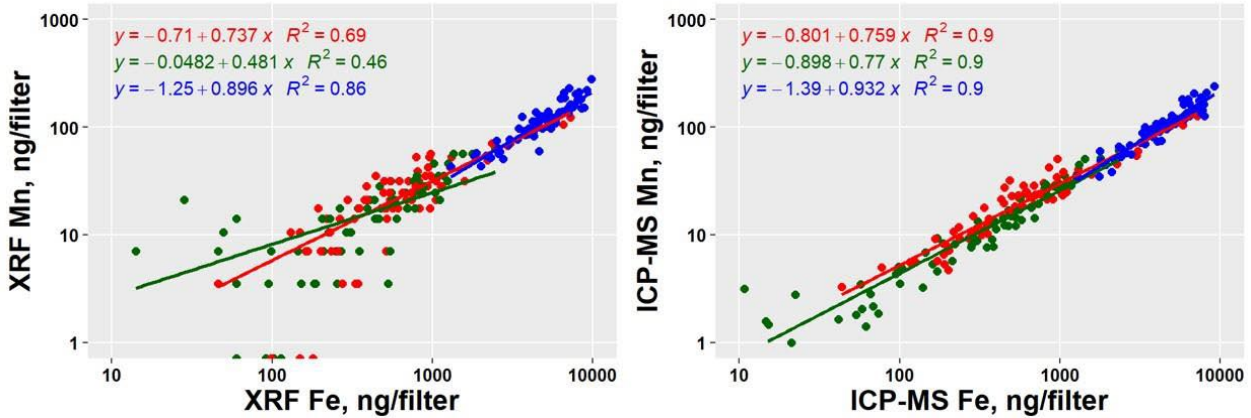


Use element ratios to assess results (continued)

Ni and V: oil burning



Mn and Fe: soil dust

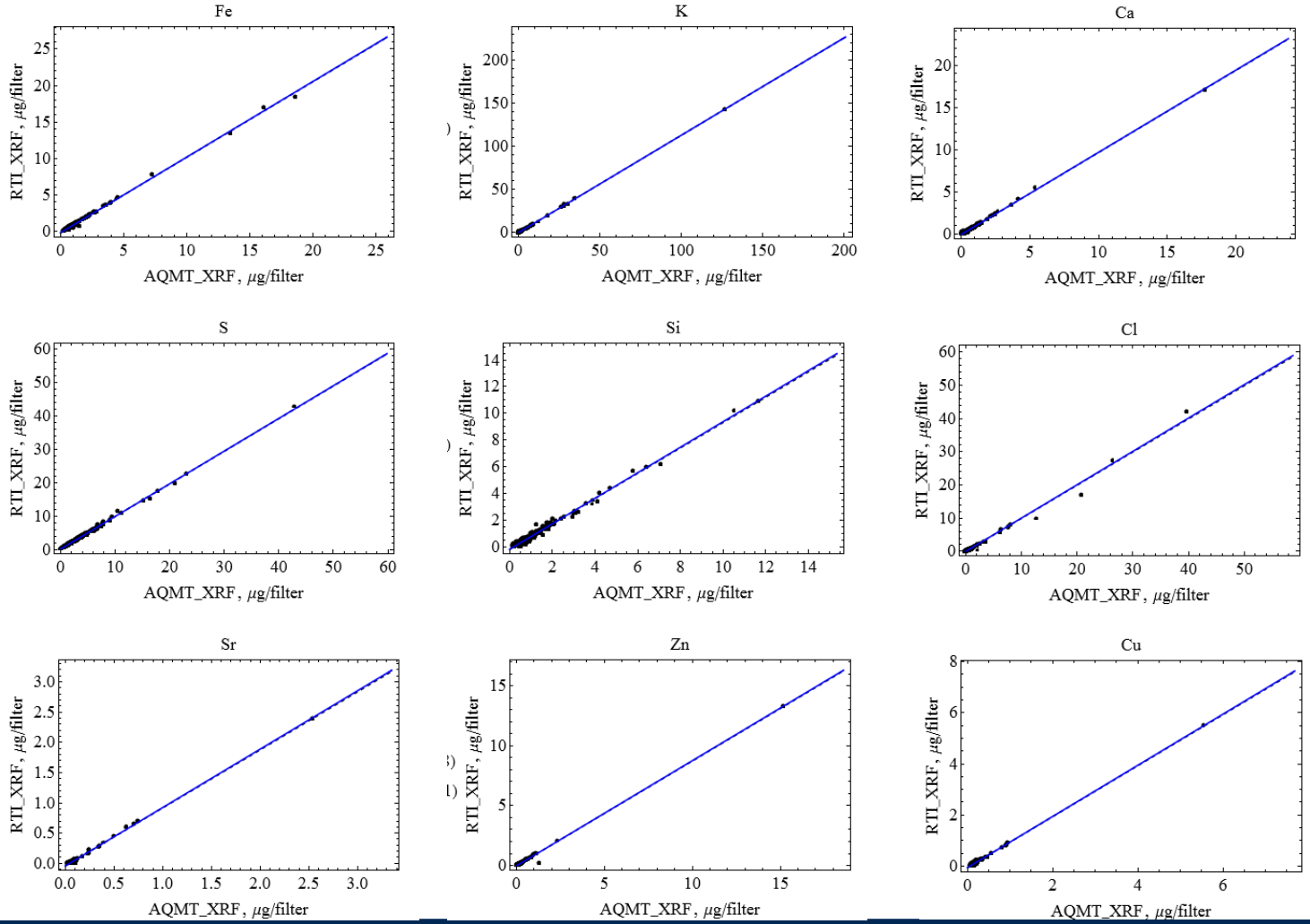


Conclusions from Comparison with WSLH

- Major axis regression between 314 EDXRF and ICP-MS results showed
  - very strong correlations ($r2 > 0.9$) for 13 out of 20 elements (Na, Mg, Al, S, K, Ca, Ti, V, Mn, Fe, Cu, Zn and Sr),
  - strong correlations ($0.8 < r2 < 0.9$) for 3 elements (Cr, Ni and Pb),
  - a weak correlation ($r2 = 0.69$) for one element (Zr), and
  - very weak correlations ($r2 < 0.4$) for three elements (P, As and Rb).
  - Except for Zn, all the elements with strong or very strong correlations had regression slopes within 20% of unity.
- Source-specific element ratios validate that ICP-MS has better MDLs than XRF for several elements

UCD versus RTI XRF

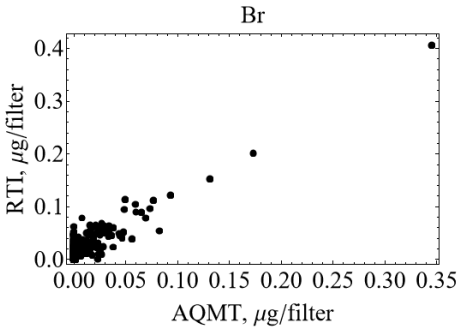
Very good agreement for some elements

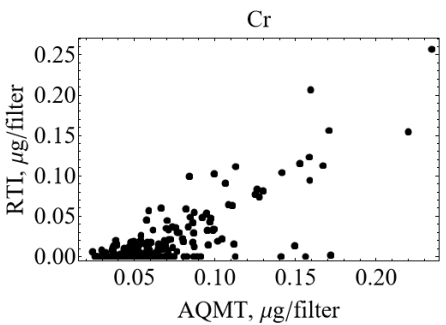


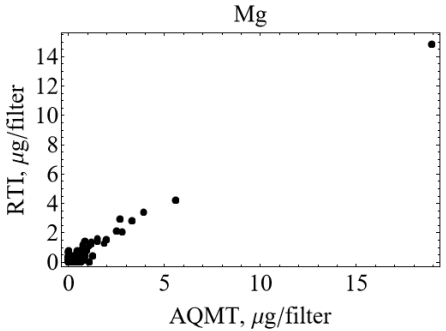
UCD versus RTI XRF

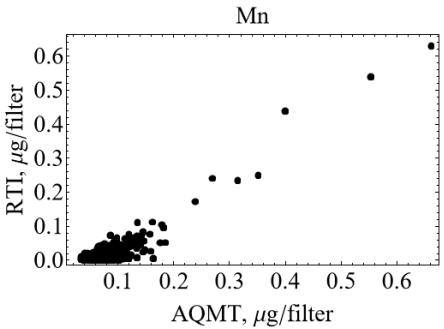
Okay agreement for some elements

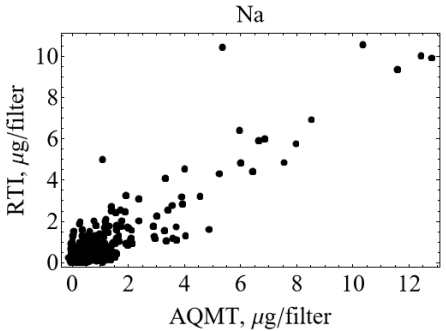
Not so great for some trace elements (not shown)

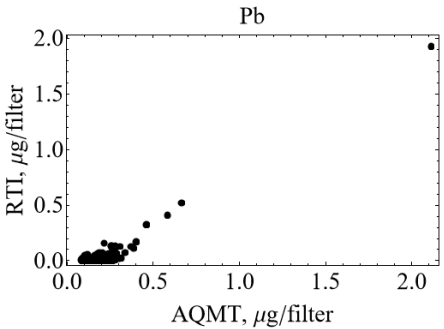


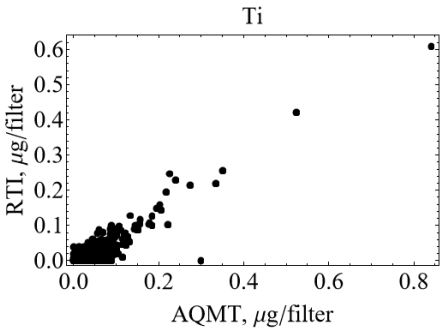












Early Results of RTI XRF versus ICP-MS Comparison