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The acquisition and processing of voluminous spectral reflectance measurements of soils and powders for national datasets

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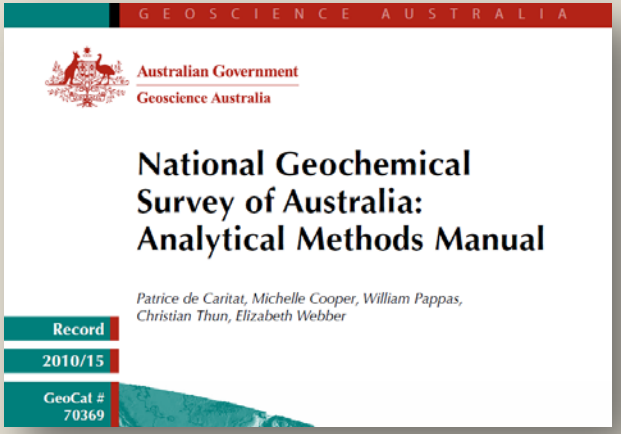
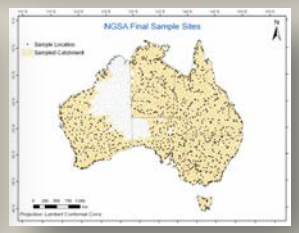
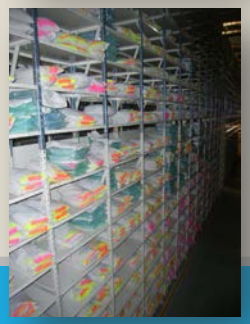
Introduction: Collection of large spectral datasets

- National database of >1300 soil samples from across Australia, which had been chemistry analysed.
- Publicly available spectral data to compliment the geochemistry and soil properties.
- Develop a method to collect, capture and deliver a large spectral dataset with the associated data.
- Standardized method of collection for other projects.

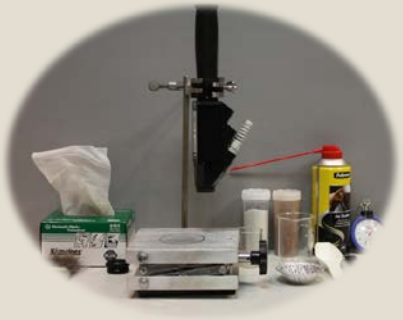






- Patrice de Caritat, Geoscience Australia http://www.ga.gov.au/energy/projects/national-geochemical-survey.html
- Sampling conducted in collaboration with the State and Territory Geological Surveys.
- Initiated due to lack of geochemical coverage available for Australia and because such a data layer is fundamental to successful mineral exploration .
- Transported regolith samples at the outlet of large catchments.
- Sampled at two depths:
  - 0-10 cm below the surface;
  - 60 and 80 cm depth.
- 1390 catchments covering 91 % of Australia.
- Samples were dried, riffle split and sieved >2000 µm.
- 60 elements using mainly XRF and collision cell ICP-MS.
- Archival of split of each bulk sample.

Instrumentation



- Visible-near-shortwave infrared
  - Panalytical ASD FieldSpec4 with high intensity contact probe.
  - Labsphere 99% Spectralon (PTFE) reflectance standard (2 inch round).
  - Lab jack and retort stand.
- Mid-longwave infrared
  - Bruker Vertex 70 and 80v FTIR spectrometer.
    - KBr beam splitter
  - Bruker A562 gold coated integrating sphere.
  - MCT detector with 2mm area.
  - Bruker integrating sphere sample cups (25 mm diameter, 3mm deep).
- Software
  - RS3, ViewSpec Pro, TSG
  - OPUS,
  - SPECCHIO.

Standards

- Lucky Bay (Western Australia) beach sand (quartz)
- Clay Mineral Society KGa-1b Washington County, Georgia, USA well crystalline Kaolinite
- Bruker diffuse gold coated reference

- Wavelength checking
  - REE doped Spectralon
  - HgAr lamp
  - Mylar
  - CO_2 and H_2O gases

Method

- Spectrometer preparation
- Sample preparation
- Measurement
- QA
- Processing
- Archiving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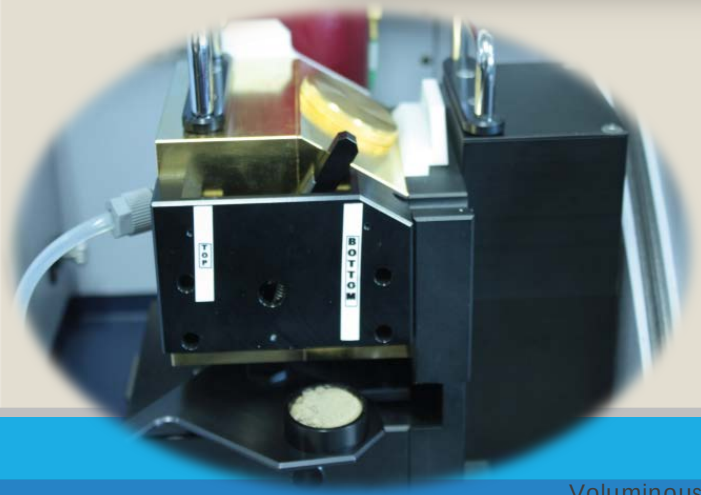
TOP
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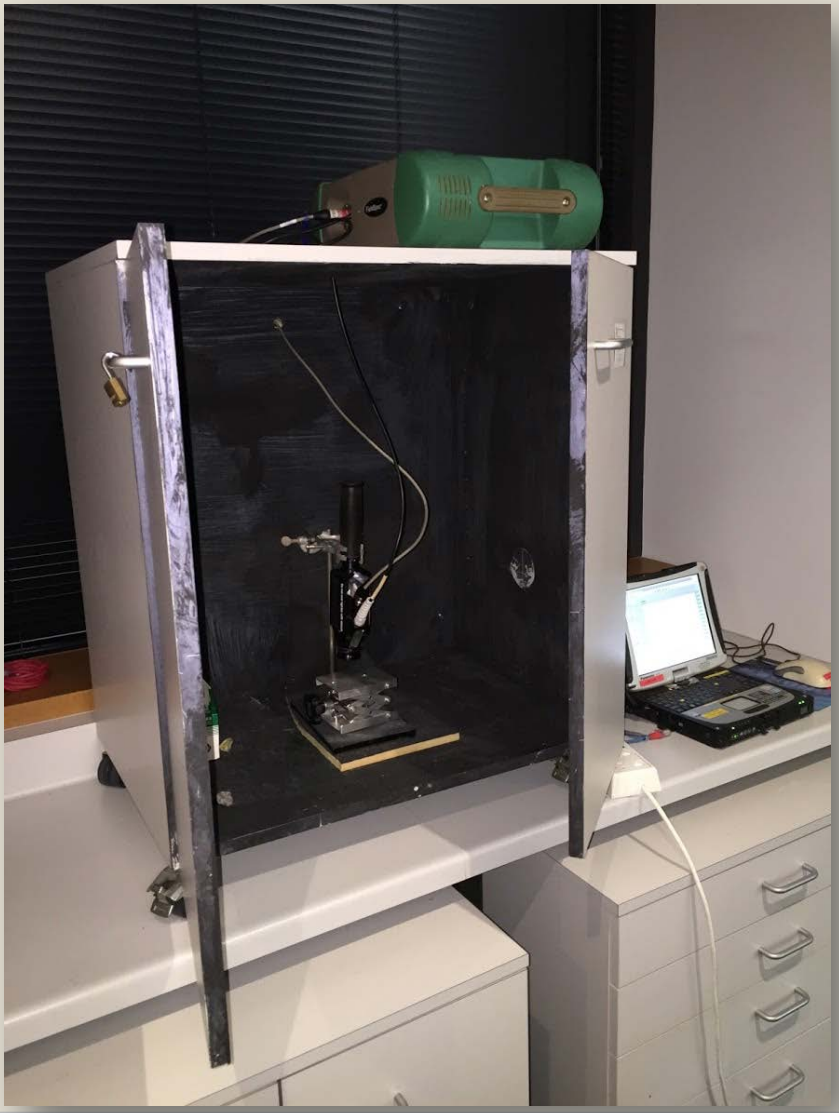
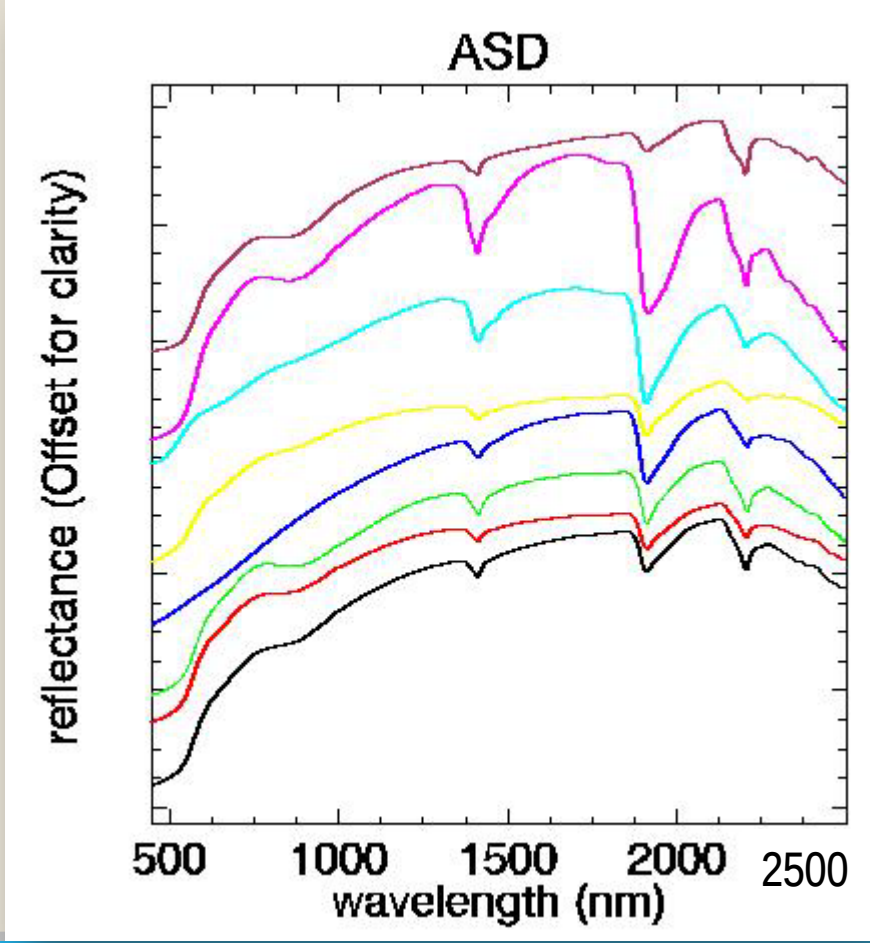


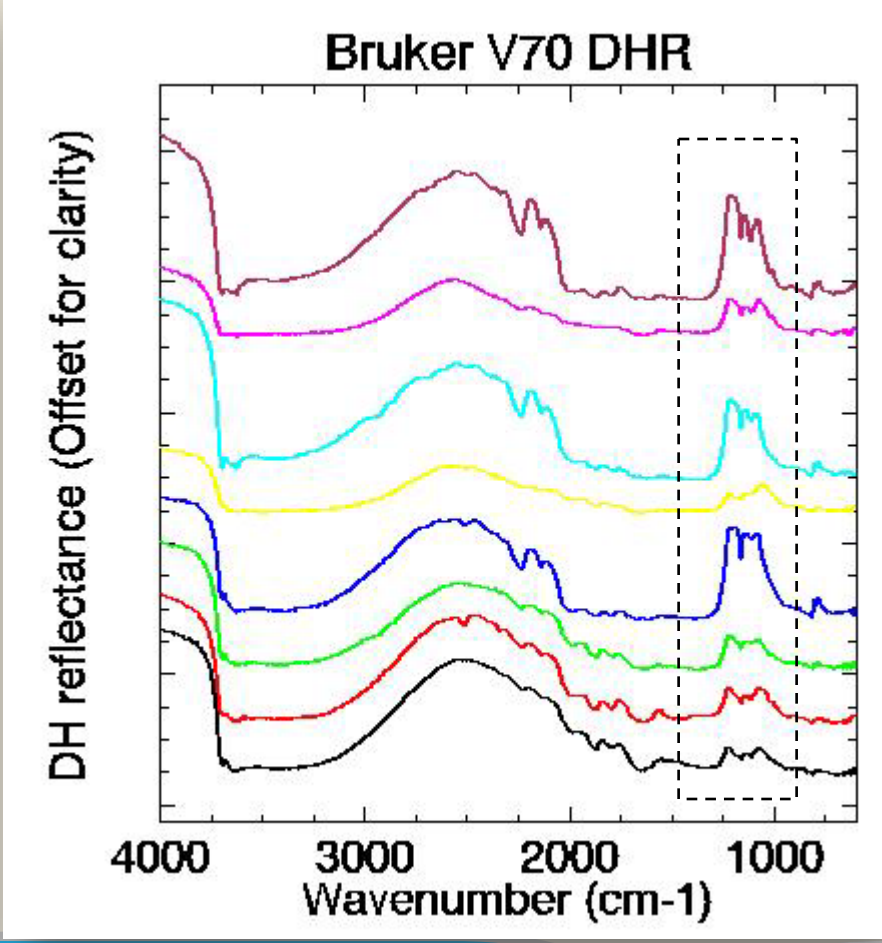

Unit 16446


3.5.1 HI CONTACT
PROBE

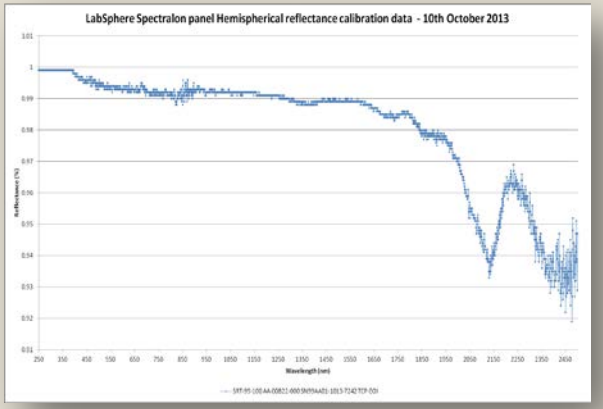

Unit 1

Examples of NGSA soil spectra





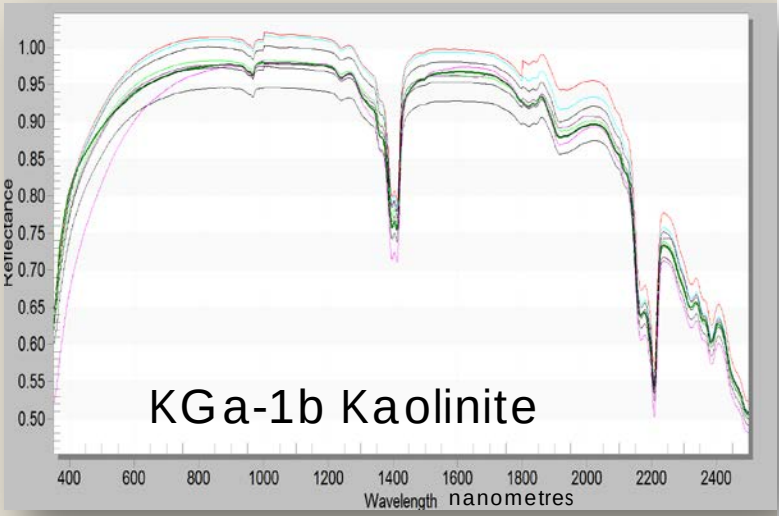
Processing

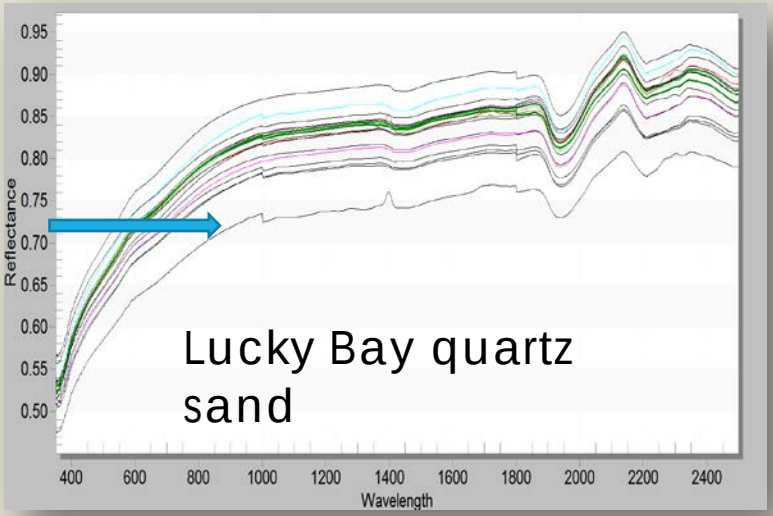


- VNIR-SWIR
  - Step-correction
  - Relative to Absolute reflectance (using Spectralon calibration file)
- FTIR
  - Subsetting to remove long wavelength noisy data (>500cm^{-1})
  - Export Bruker binary files as ASCII
  - Wavenumber to nanometre conversion
  - Resampling (if required)
- Import into The Spectral Geologist version 8.
- Mineral scalars processing

Quality control

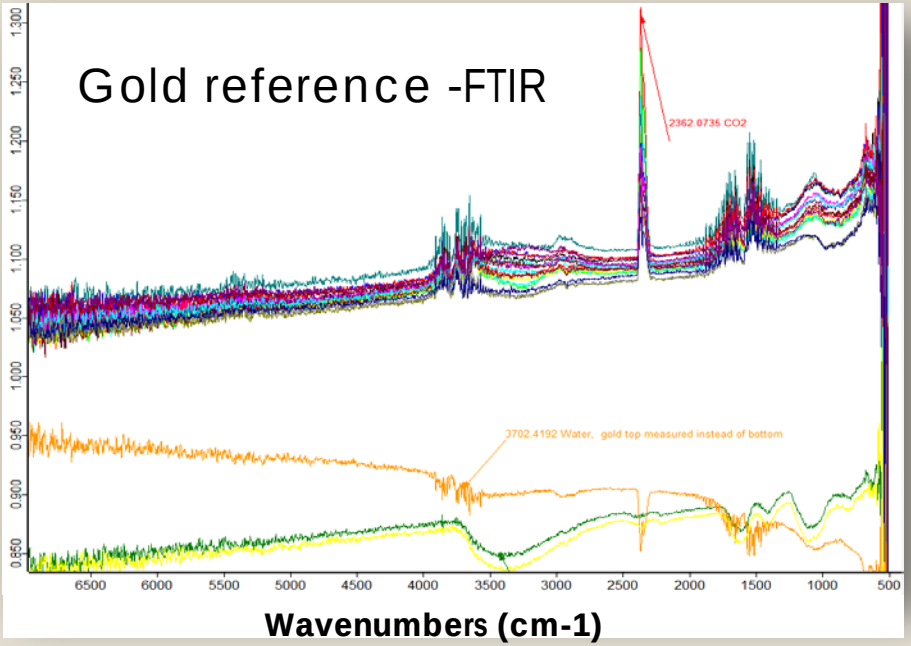
- Visual
- SNR
- File naming (and time of acquisition)
- FTIR signal on the gold reference check
- Reference sample measurement – comparison with past measurements
- Gas absorptions in FTIR

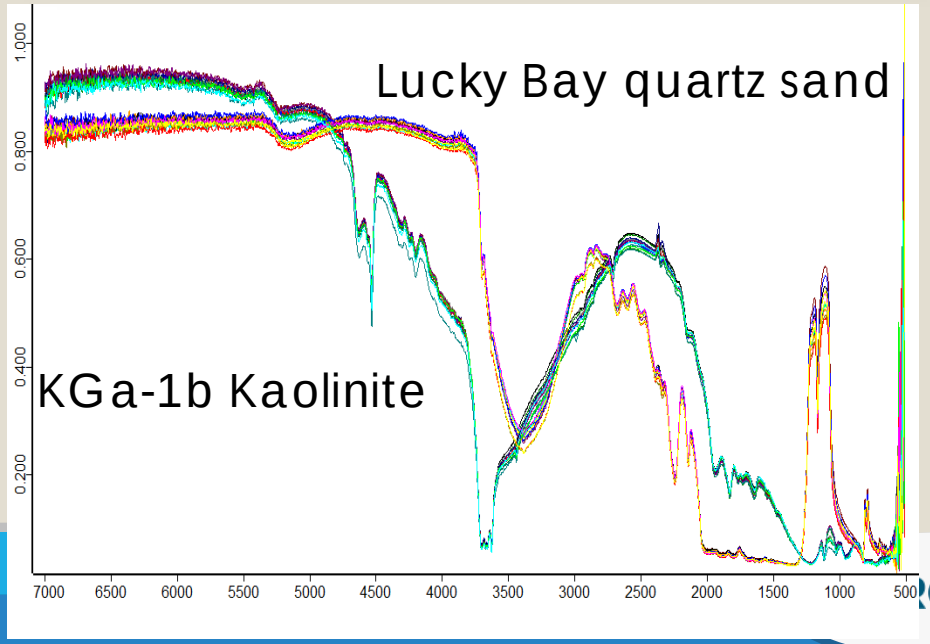




QC Standards

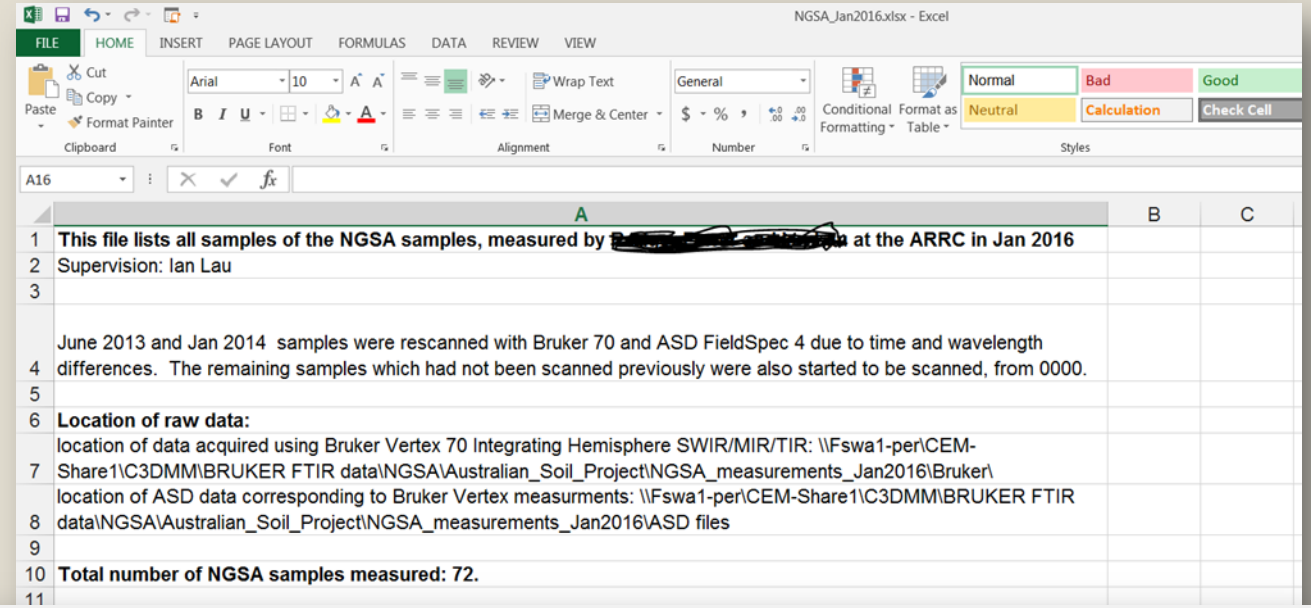
- Checking of standards.
- Both instruments.
- Multiple measurement of standards each day.





Metadata

- Records for each set of measurements



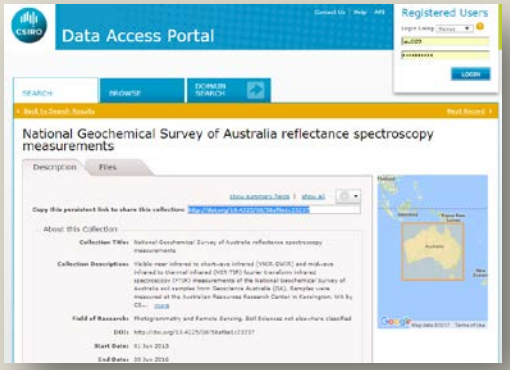
NGSA_Jan2016.xlsx - Excel

	A
1	**This file lists all samples of the NGSA samples, measured by [redacted] at the ARRC in Jan 2016**
2	Supervision: Ian Lau
3	
4	June 2013 and Jan 2014 samples were rescanned with Bruker 70 and ASD FieldSpec 4 due to time and wavelength differences. The remaining samples which had not been scanned previously were also started to be scanned, from 0000.
5	
6	**Location of raw data:**
7	location of data acquired using Bruker Vertex 70 Integrating Hemisphere SWIR/MIR/TIR: \\Fswa1-per\CEM-Share1\C3DMM\BRUKER FTIR data\NGSA\Australian_Soil_Project\NGSA_measurements_Jan2016\Bruker\
8	location of ASD data corresponding to Bruker Vertex measurments: \\Fswa1-per\CEM-Share1\C3DMM\BRUKER FTIR data\NGSA\Australian_Soil_Project\NGSA_measurements_Jan2016\ASD files
9	
10	**Total number of NGSA samples measured: 72.**

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1			Sample Description														Bruker Vertex 80v Integrating Hemisphere SWIR/MIR/TIR		
2	Number	Sample	ASD	project	client	location	rock type	mineral (inferred)		filename	Date	type	comment	crushed soil samples/rock	Aperture:	Beamsplitter:	Optical Filter setting:	Detector setting:	Preamp gain
3																			
4																			
5		Yellow lines indicates when white reference was taken in between respective ASD measurements (WR)																	
6		red indicated 128 resolution, 3 repeated at higher res																	
16		GOLD2	Y	NGSA	Matilda Thomas					GOLD2.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
17	1	TB0151	Y	NGSA	Matilda Thomas					TB0151.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
18	2	TB0158	Y	NGSA	Matilda Thomas					TB0158.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
19	3	TB0163	Y	NGSA	Matilda Thomas					TB0163.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
20	4	TB0165	Y	NGSA	Matilda Thomas					TB0165.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
21	5	TB0176	Y	NGSA	Matilda Thomas					TB0176.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
22	6	TB0178	Y	NGSA	Matilda Thomas					TB0178.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
23	7	TB0181	Y	NGSA	Matilda Thomas					TB0181.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
24	8	TB0182	Y	NGSA	Matilda Thomas					TB0182.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
25	9	TB0183	Y	NGSA	Matilda Thomas					TB0183.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
26	10	TB0185	Y	NGSA	Matilda Thomas					TB0185.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
27	11	TB0189	Y	NGSA	Matilda Thomas					TB0189.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
28	12	TB0192	Y	NGSA	Matilda Thomas					TB0192.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
29	13	TB0193	Y	NGSA	Matilda Thomas					TB0193.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
30	14	TB0194	Y	NGSA	Matilda Thomas					TB0194.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
31	15	TB0196	Y	NGSA	Matilda Thomas					TB0196.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A
32	16	TB0197	Y	NGSA	Matilda Thomas					TB0197.0	20/01/2016	Intergrating Hemisphere	Scanning by Richard with Bruker Vertex 70	crushed soil samples	6mm	KBr	Open	LN-MTCMid	A

Archiving of spectral data

- Current:
  - CSIRO Data Access Portal
    http://doi.org/10.4225/08/58af8e1c23237
    - ASCII (CSV) files for ASD and FTIR data
  - SPECCHIO Spectral Information System
    - Individual spectra with metadata and associated NGSA data
- Future:
  - Auscope Discovery Portal
  - Australian Geoscience Datacube

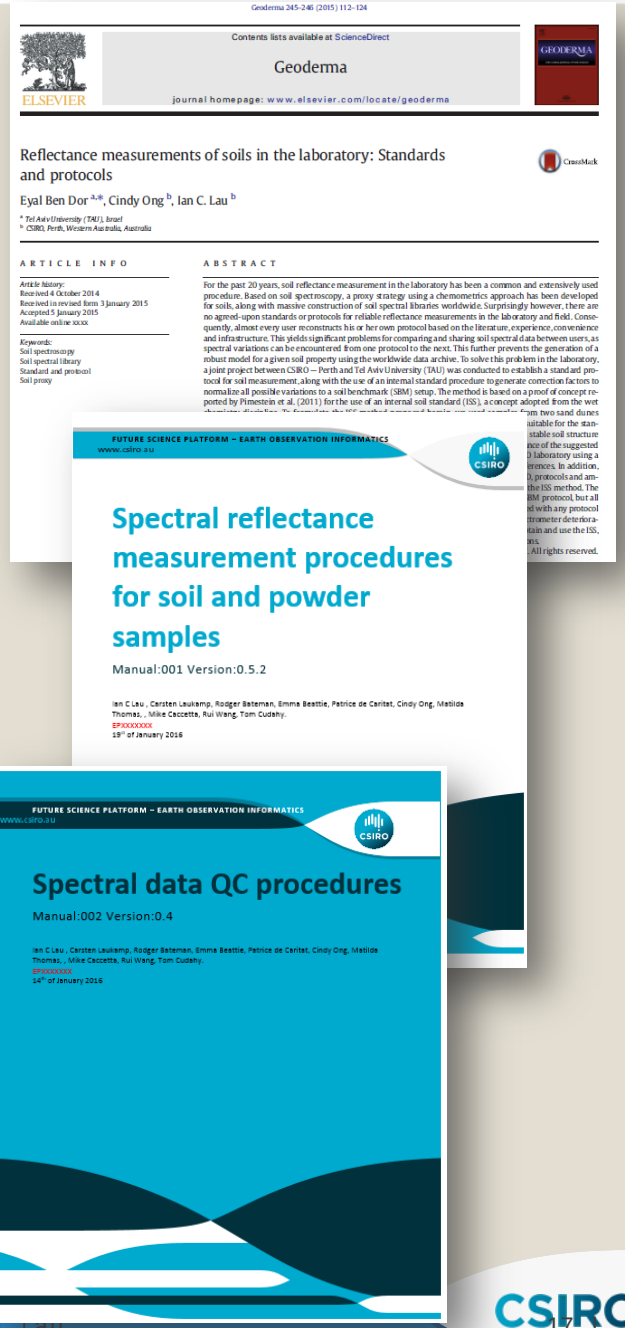


Problems encountered

- Use of different spectrometers (both VNIR-SWIR and FTIR) and detectors.
- Missed samples.
- Stray light in laboratory.
- Dirty Spectralon/poor panel placement.
- Non-vacuum sphere (atmospheric gas).
- Condensation on MCT detector after filling dewar.
- Consistency with packing samples in to sample holder.
- Grain size (sample texture) variations.
- A562 integrating sphere design characteristics.

Lessons learnt

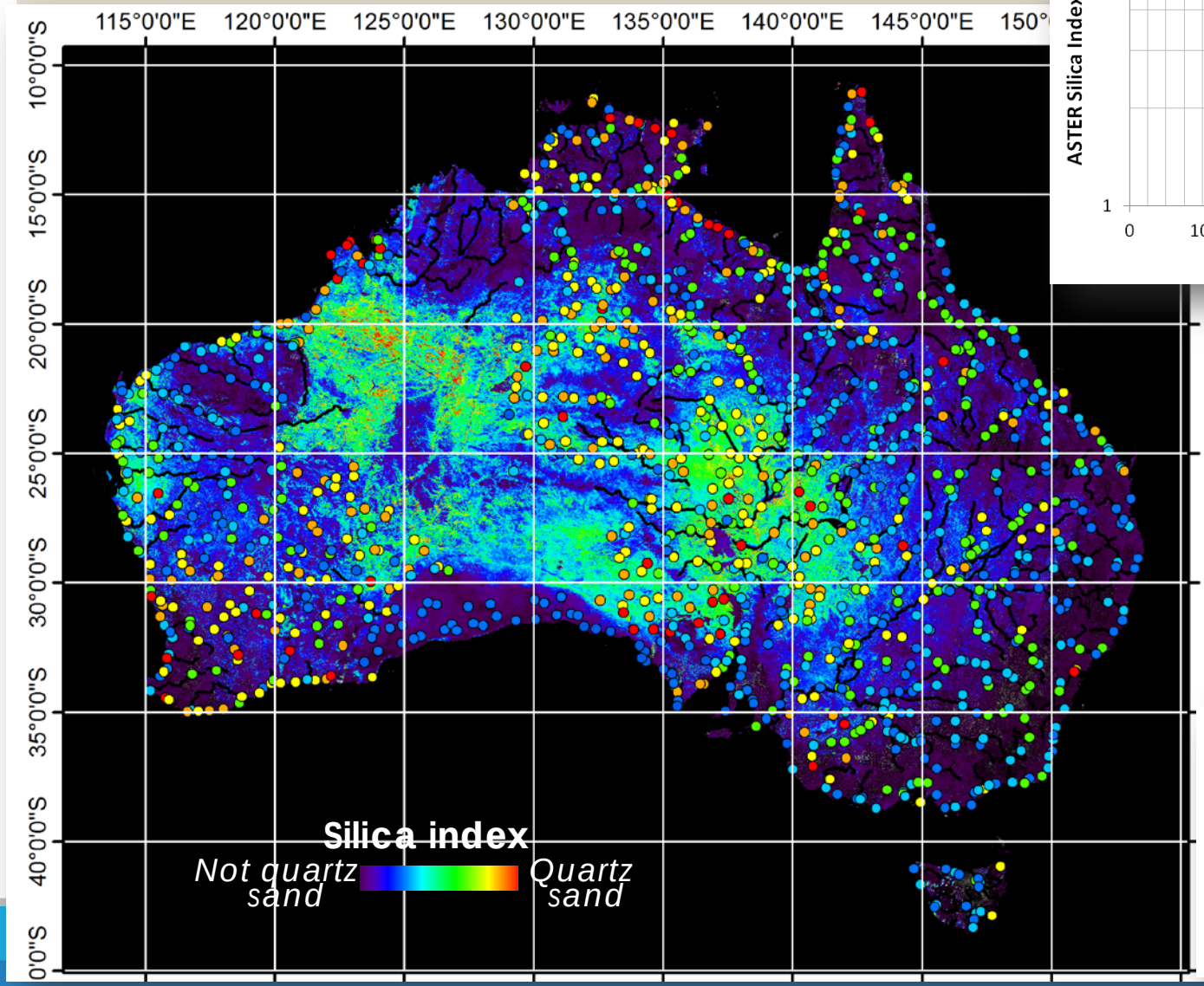
- Dedicated spectrometers and accessories to a campaign.
- Consistent use of same white reference and maintaining it to a high standard.
- Record detailed metadata (white reference, instruments, operator, lab conditions).
- Regular QA of data (daily at a minimum)
- Regular reference sample measurement for QC (multiple daily).
- Archive spectra and meta data regularly.

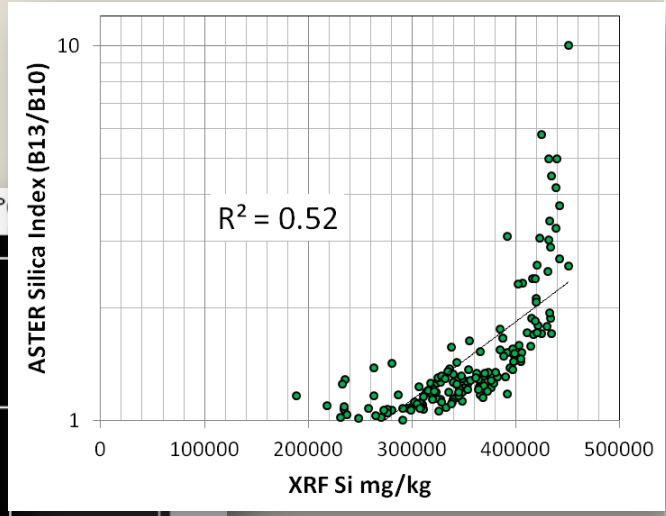


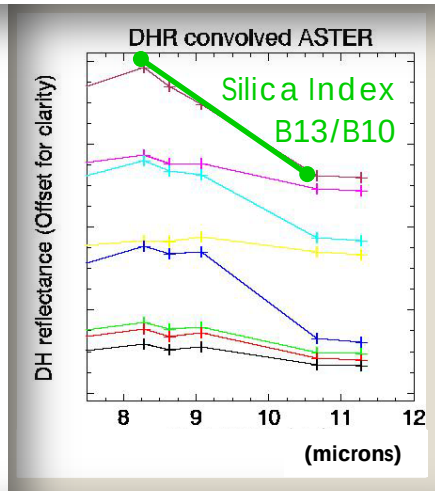
Example

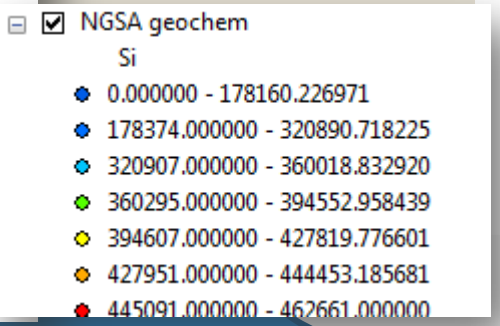
ASTER geoscience map validation using NGSA spectral data

NGSA Si_{XRF} and ASTER Silica









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