Rapid Soil Analysis by Mid-Infrared Spectroscopy Training Course

01. COURSE INTRODUCTION

Anthony Ringrose-Voase

May 2018

Agriculture and Food

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Australian Government

Australian Centre for International Agricultural Research

Training course objectives

To train participants in the use of mid-infrared spectroscopy (MIR) to rapidly characterize soil

- Role of rapid soil analysis in a soil survey context
- Operation of MIR
- Calibration of MIR and prediction of soil properties

Course outline

Seminar on “Rapid Soil Analysis by Mid-Infrared Spectroscopy”

1. What is MIR spectroscopy?
   - Demonstration of MIR operation (video)
2. MIR calibration
   - Demonstration of MIR calibration
   - Demonstration of soil property estimation by MIR
3. Role of rapid soil analysis in digital soil mapping
4. MIR calibration strategies

Course outline

Hands-on training course

1. Course outline	Monday PM
2. What is MIR spectroscopy?	
3. Role of rapid soil analysis in digital soil mapping	
4. Setting up MIR spectrometer and software	Tuesday AM
5. Sample preparation	Tuesday PM
6. Safety	
7. Acquiring MIR spectra from soil specimens	
8. Calibration	Wednesday
9. MIR calibration strategies	
10. Calibration and optimization	Thursday
11. Soil property estimation	Friday

Course outline

The course will consist of:

- Lectures
  - Background to theory and practice of MIR spectroscopy
    - Seminar
- Instructions
  - Demonstrations of practical aspects of MIR spectroscopy
- Practicals
  - Opportunities for participants to learn-by-doing

Training course objectives

At the end of this course you will be able to:

- Understand the principles of MIR spectroscopy as applied to rapid soil analysis
- Be able to:
  - Prepare soil specimens for MIR spectroscopy
  - Acquire MIR spectra from soil specimens
  - Develop MIR calibrations for different soil properties
  - Predict soil properties from MIR spectra
- Understand the role of MIR spectroscopy in soil survey and land evaluation

Rapid Soil Analysis by Mid-Infrared Spectroscopy Training Course

02. WHAT IS MIR SPECTROSCOPY?

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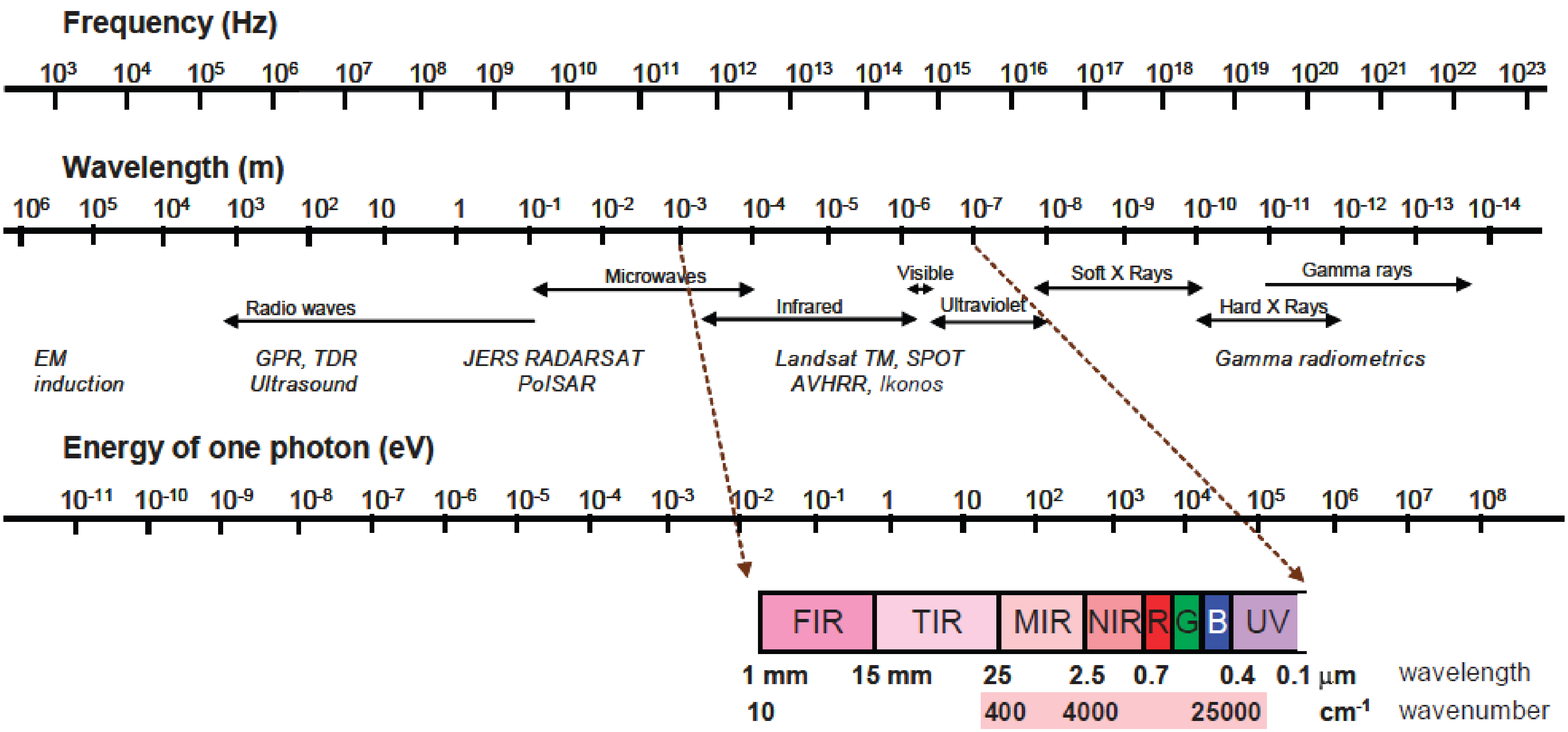
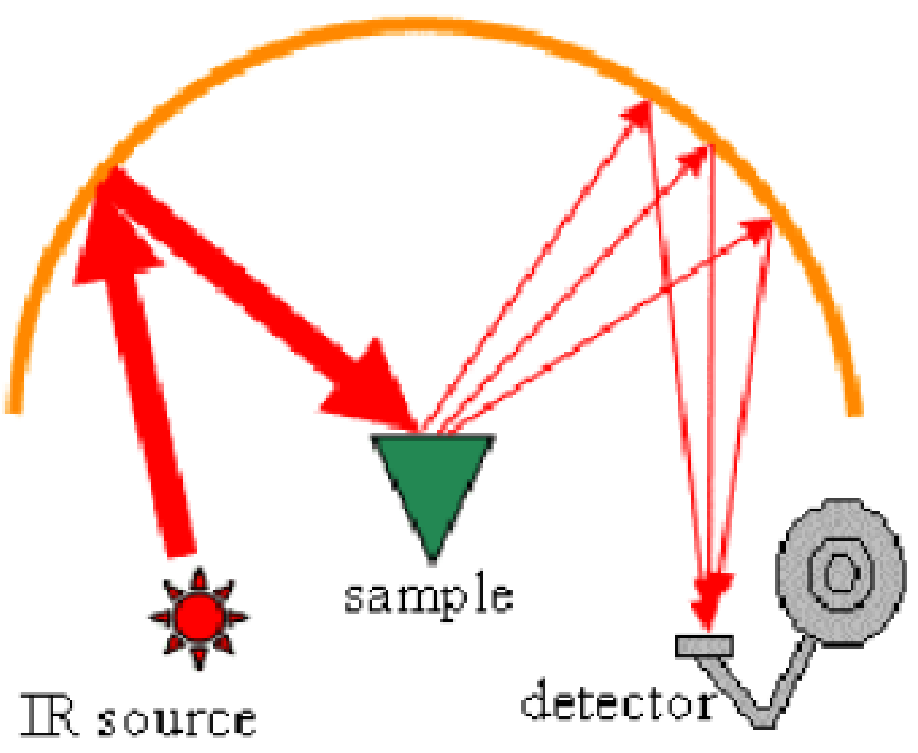
Range of electromagnetic radiation available for rapid soil measurement



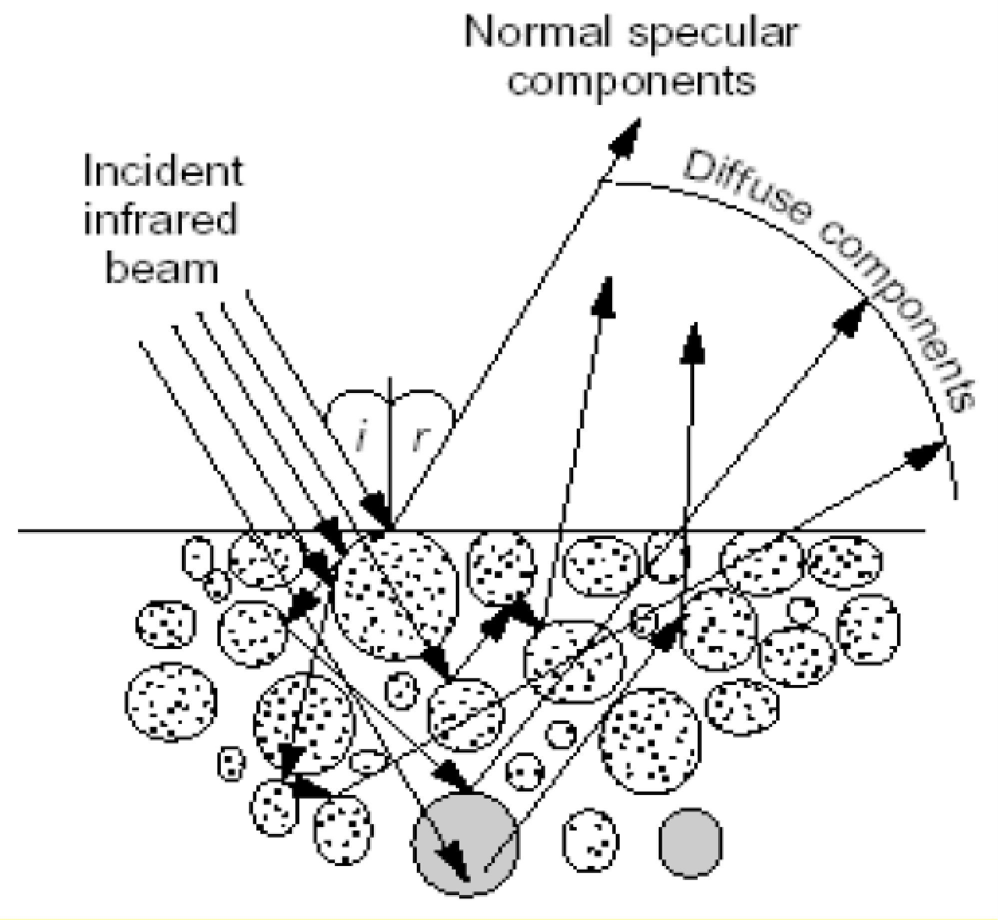
MIR reflectance spectroscopy

- Infrared light is shone at a finely ground soil specimen
- Infrared light is scattered and reflected by soil
- Reflected infrared light is measured by a detector



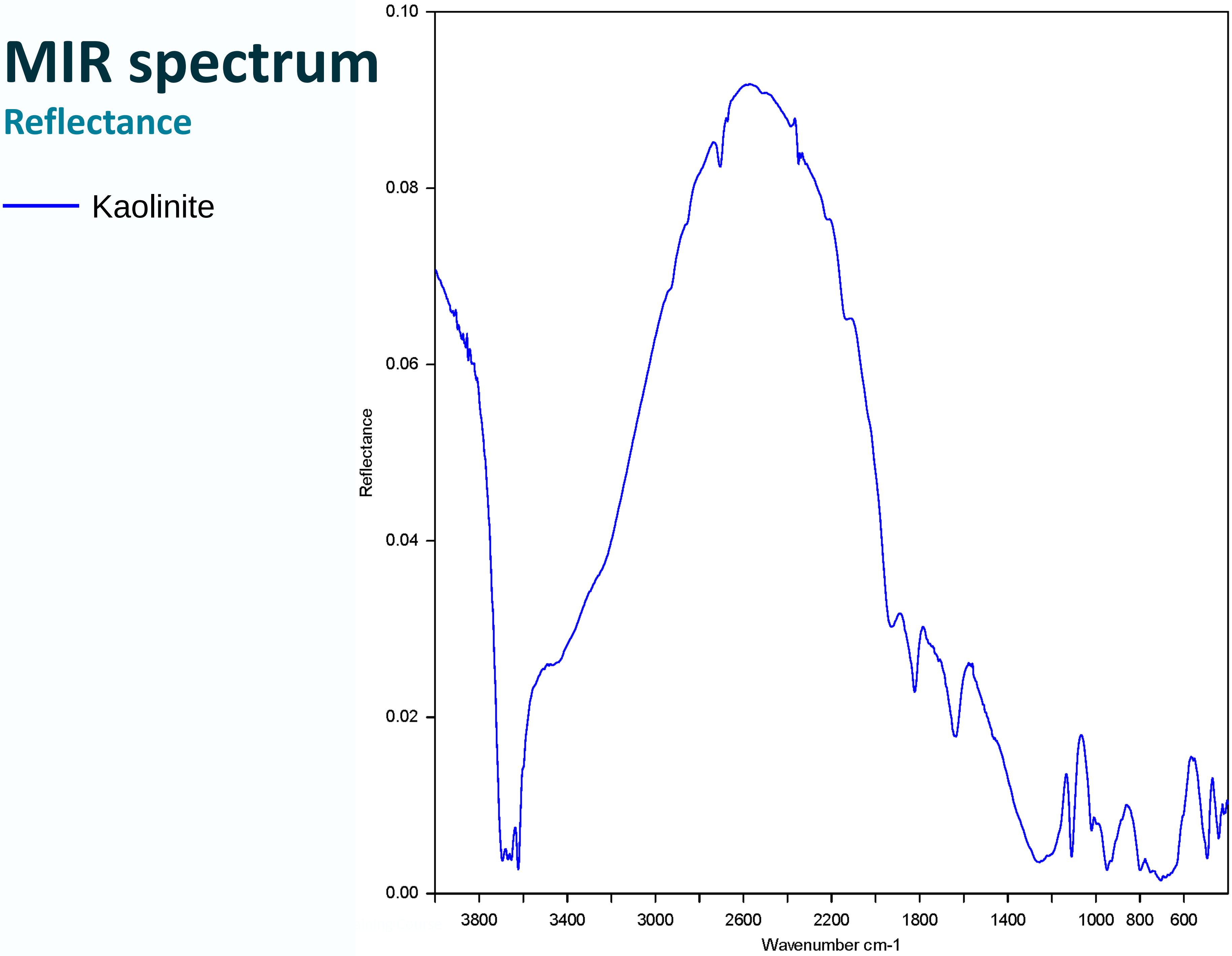
MIR reflectance spectroscopy

Needs dry fine soil particles



MIR spectrum

Reflectance



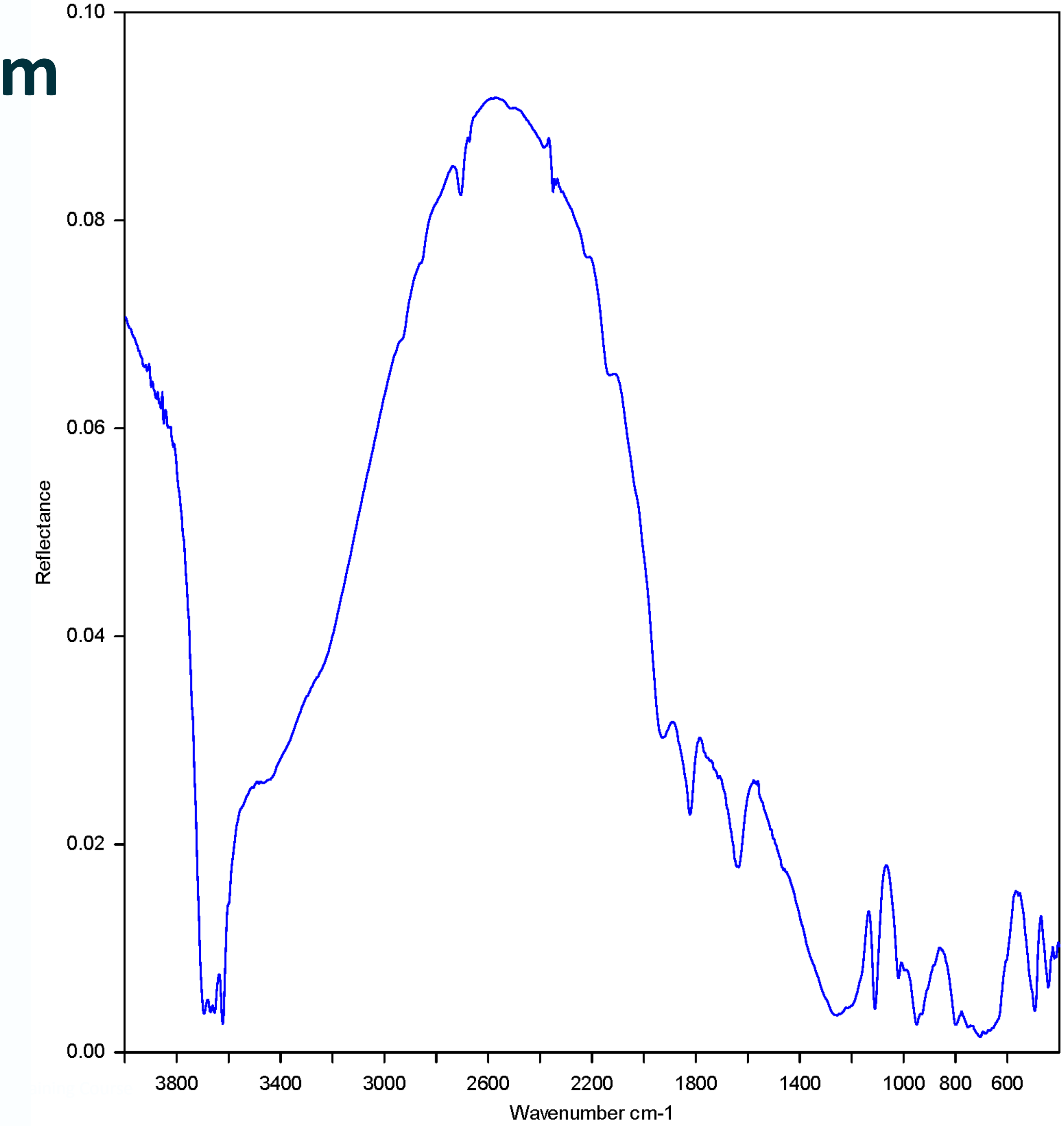
MIR reflectance spectroscopy

- Some of the infrared light is absorbed by substances in the soil specimen
  - Different substances absorb specific infrared wavelengths
  - Which wavelengths are absorbed depends on chemical bonds of the substance
  - In the infrared light reflected by the specimen, the intensity of these wavelengths is reduced
- Reduction in intensity is proportional to the concentration of the substance
- The reflectance spectrum carries information about the concentrations of the substances in the soil specimen
  - Like a fingerprint

MIR spectrum

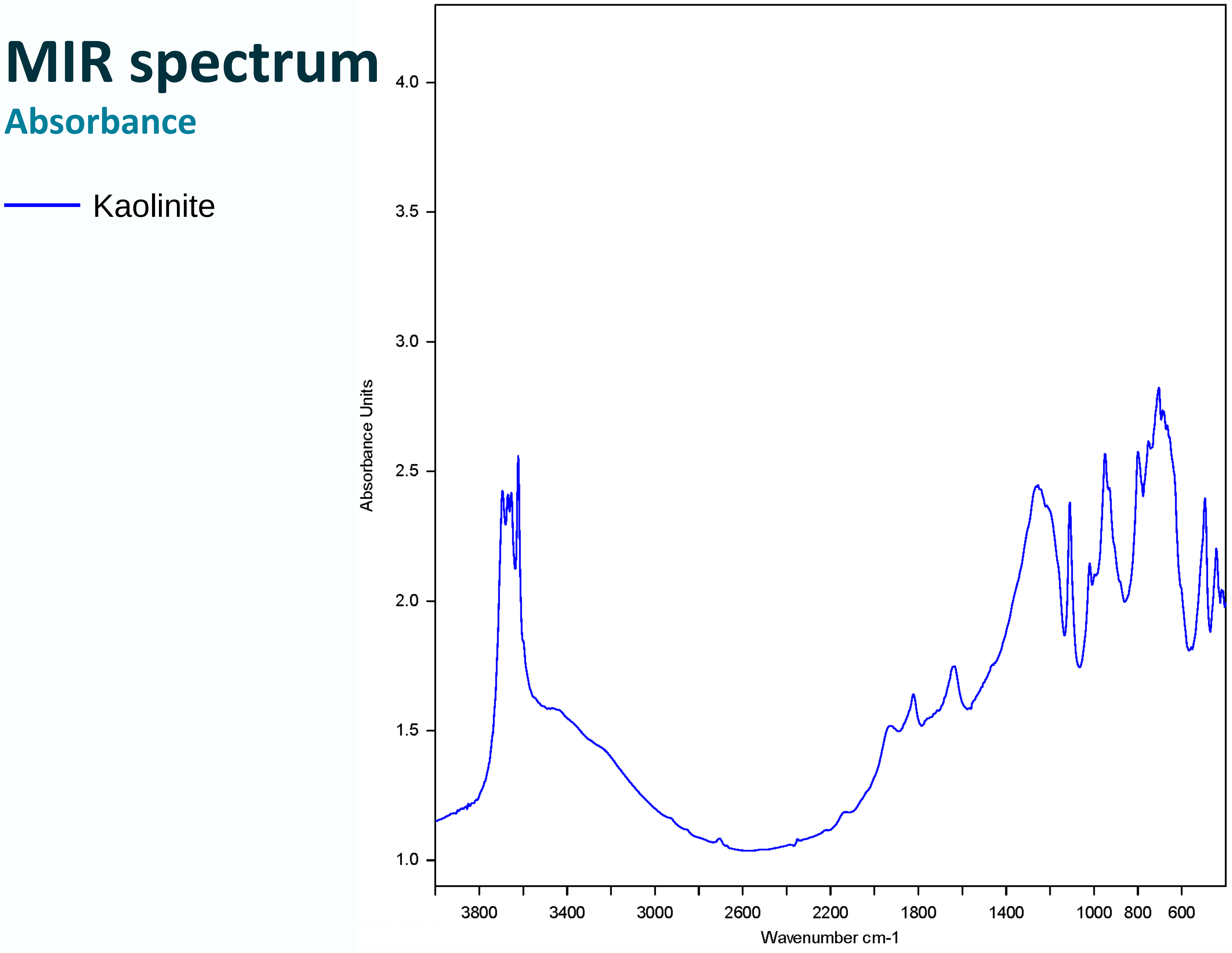
Reflectance

— Kaolinite



MIR spectrum

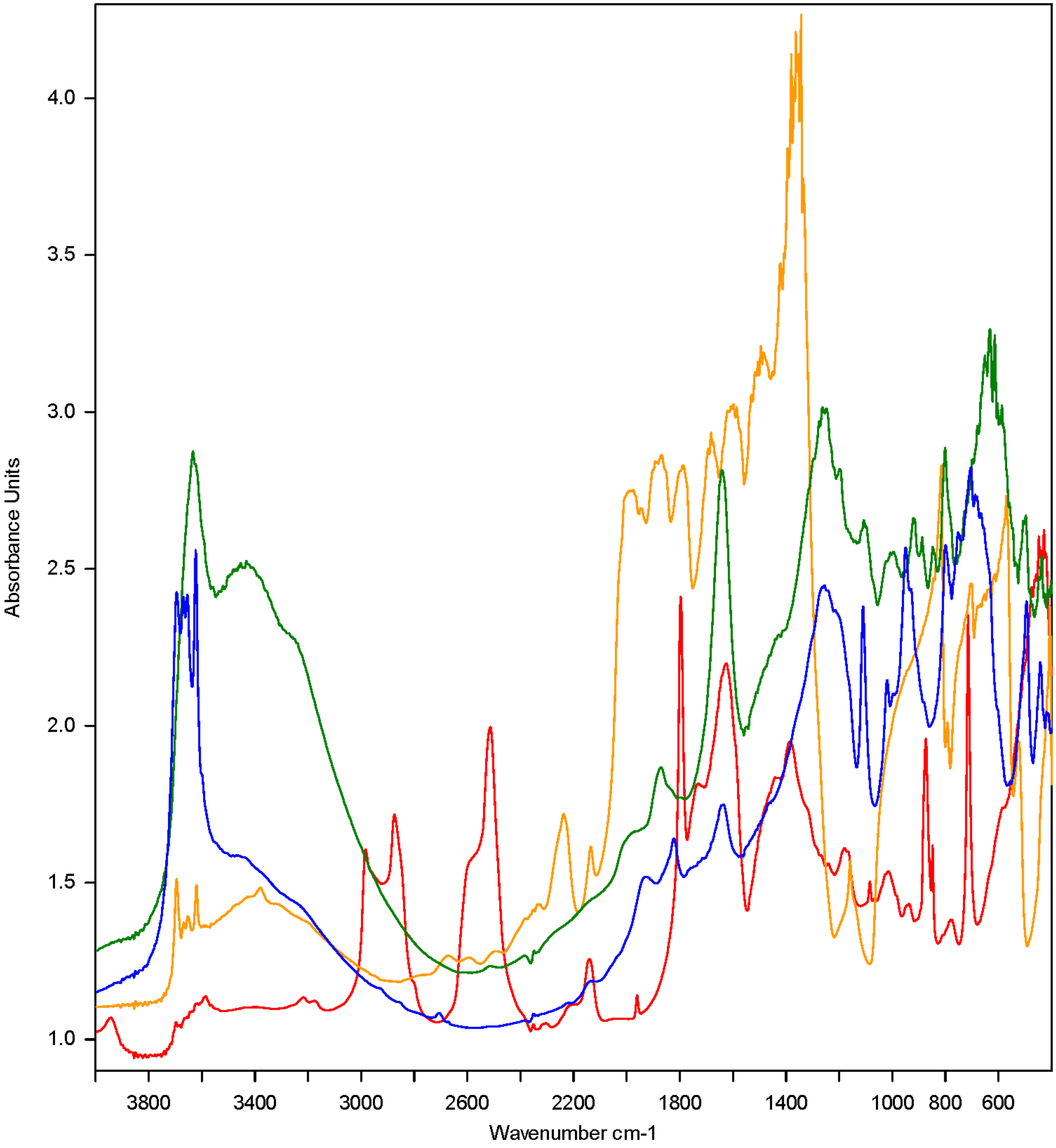
Absorbance



MIR spectra

Absorbance

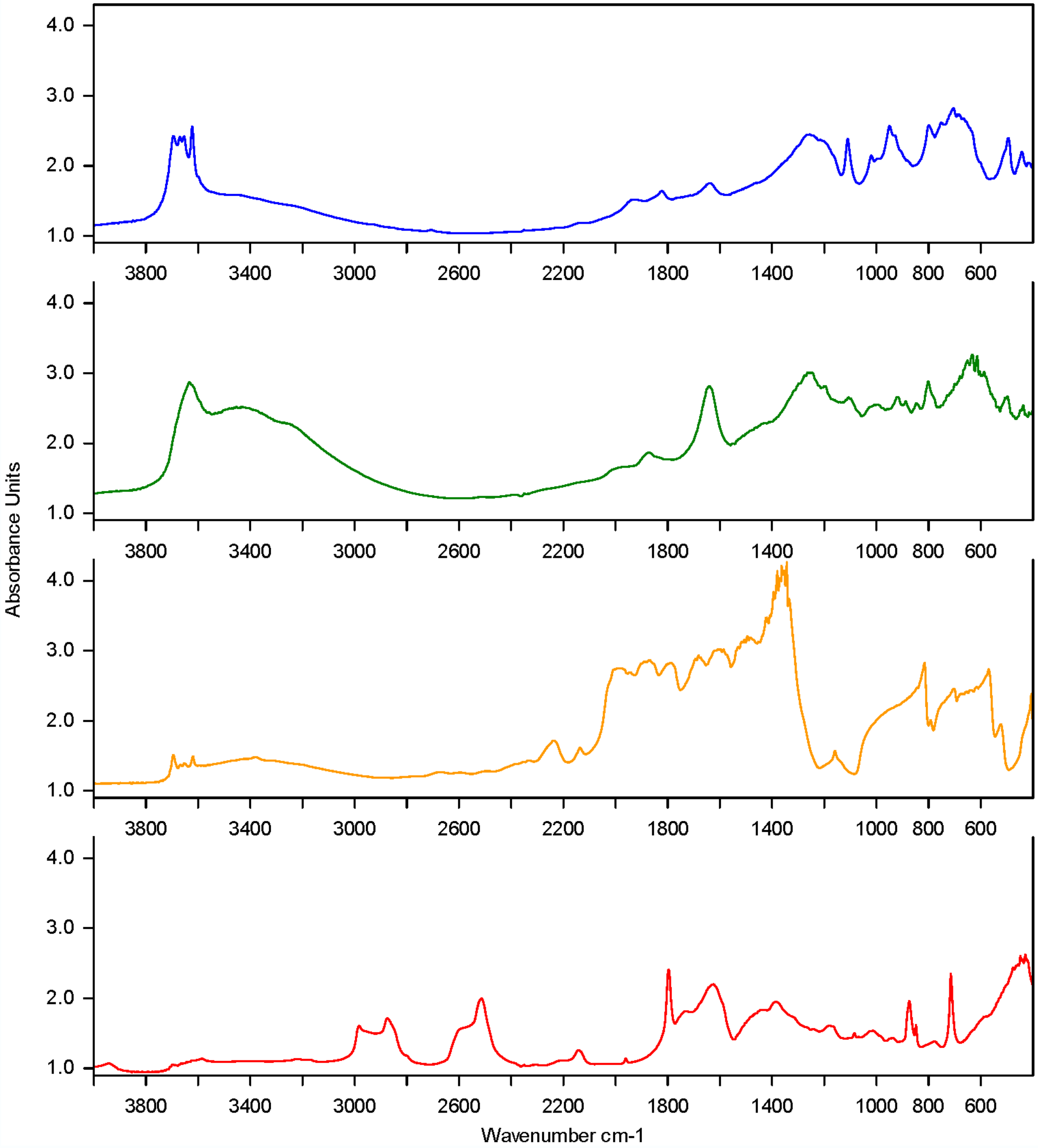
- Kaolinite
- Smectite
- Sand
- Carbonate



MIR spectra

Absorbance

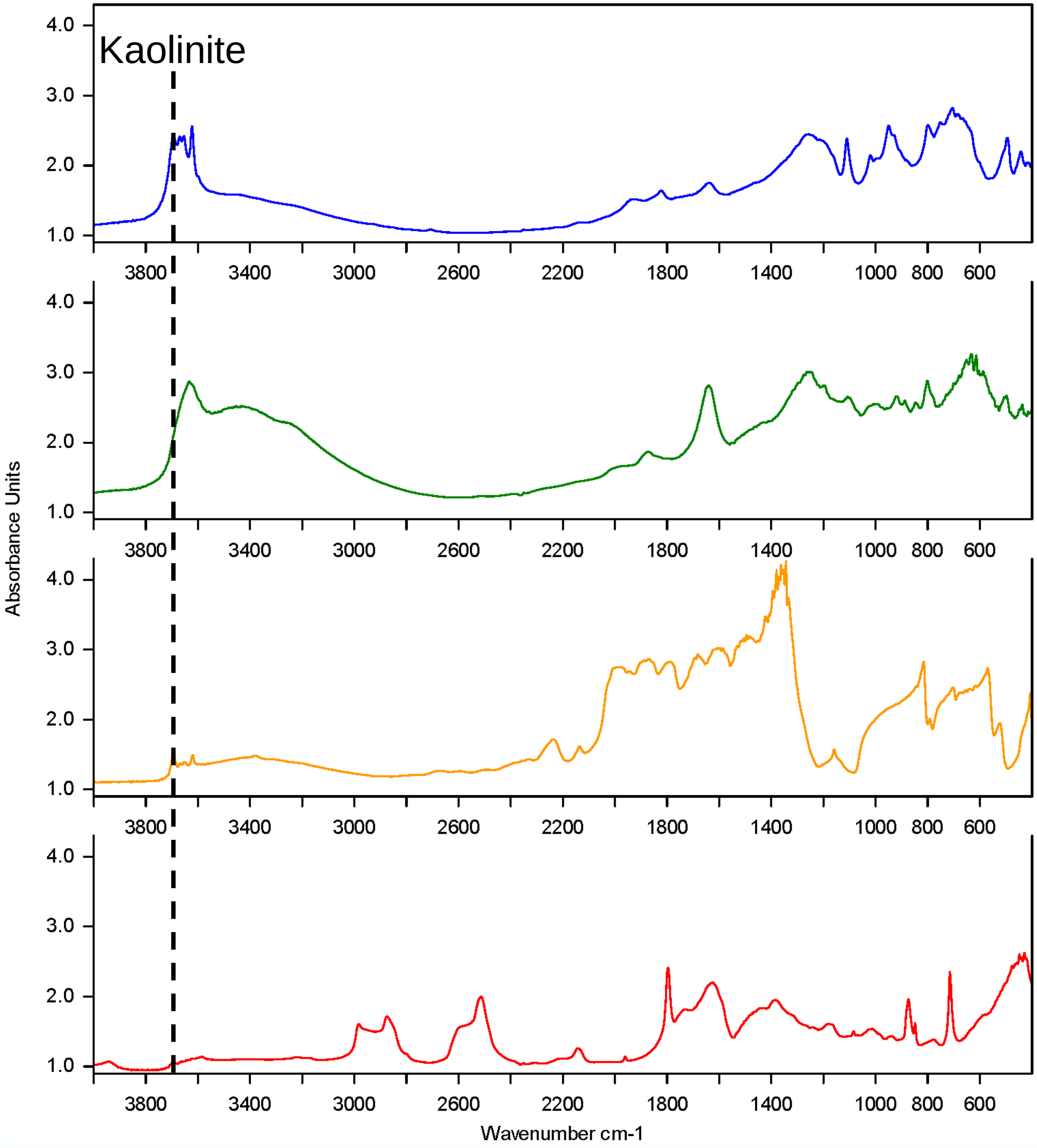
- — Kaolinite
- — Smectite
- — Sand
- — Carbonate



MIR spectra

Absorbance

- 🟦 Kaolinite
- 🟩 Smectite
- 🟧 Sand
- 🟥 Carbonate



MIR spectra

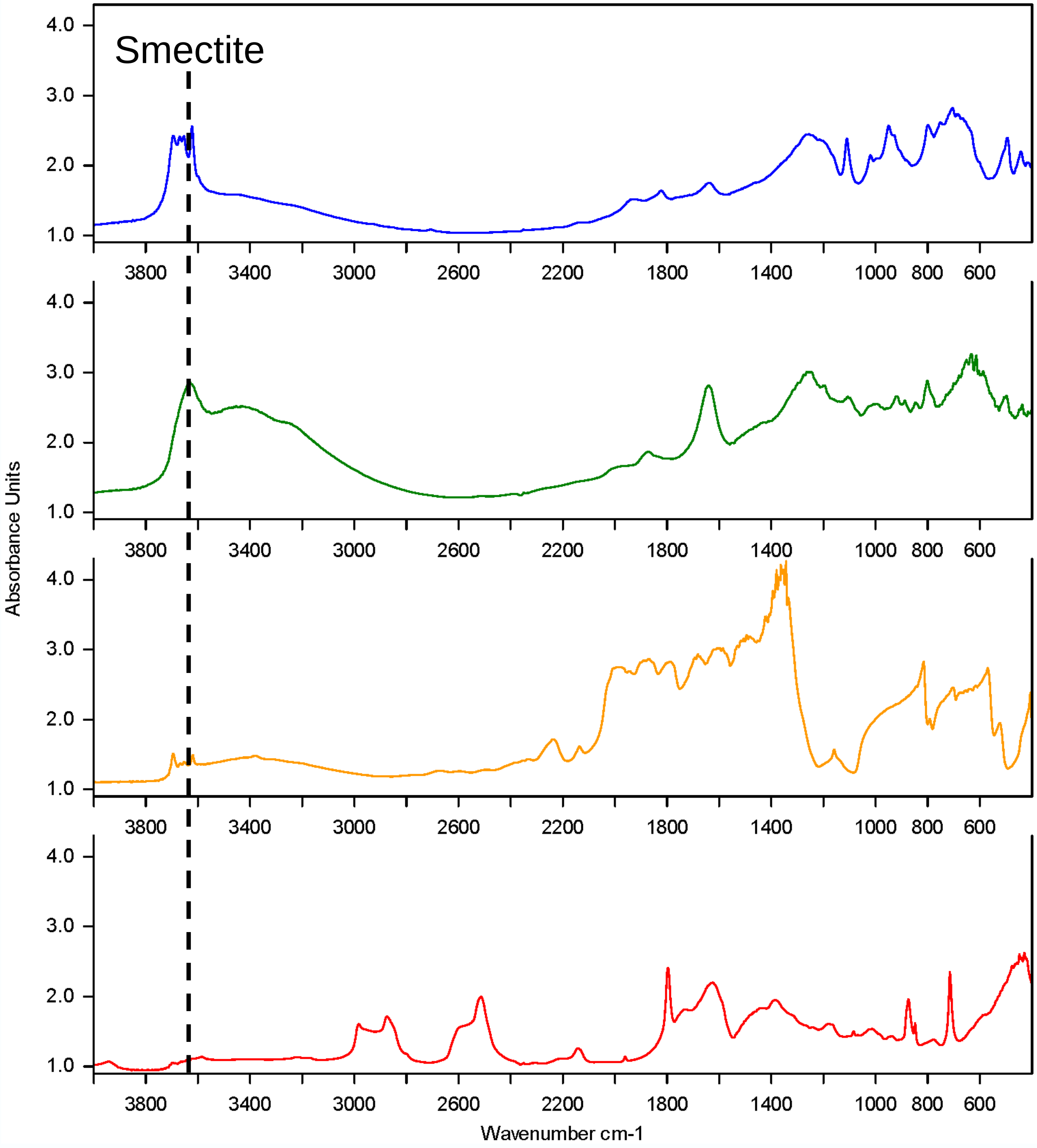
Absorbance

🟦 Kaolinite

🟩 Smectite

🟧 Sand

🟥 Carbonate



MIR spectra

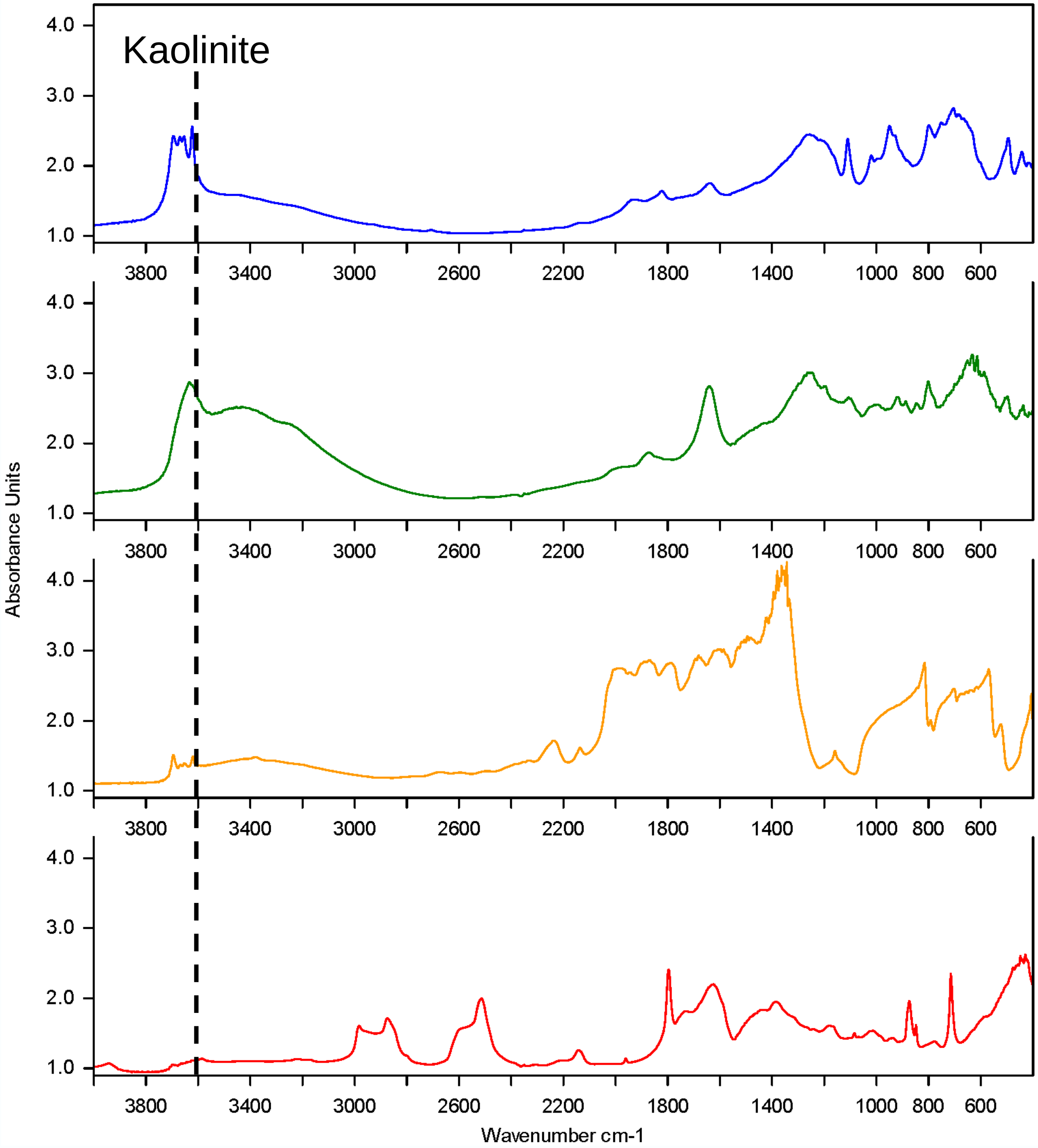
Absorbance

Kaolinite

Smectite

Sand

Carbonate



MIR spectra

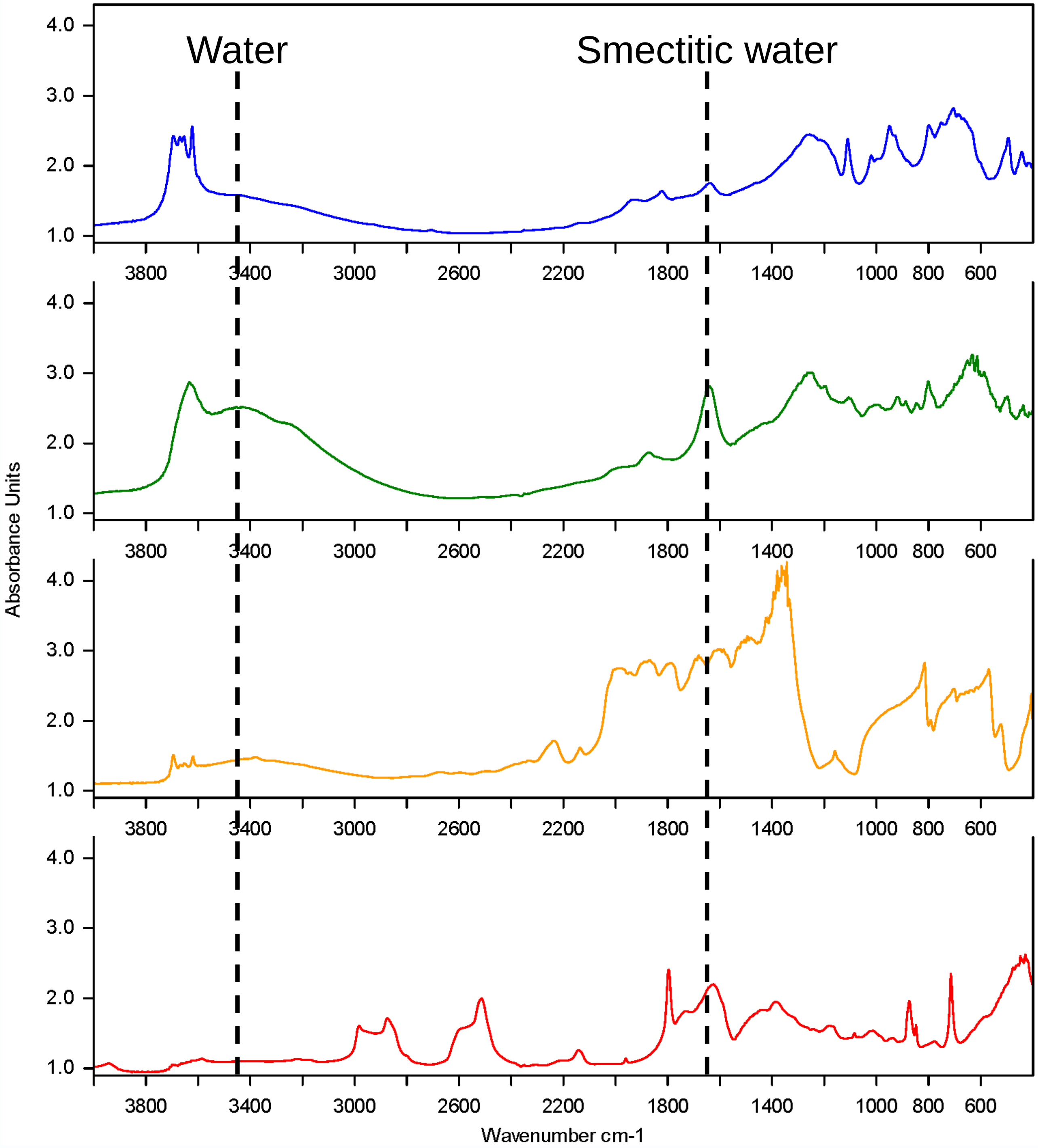
Absorbance

— Kaolinite

— Smectite

— Sand

— Carbonate



MIR spectra

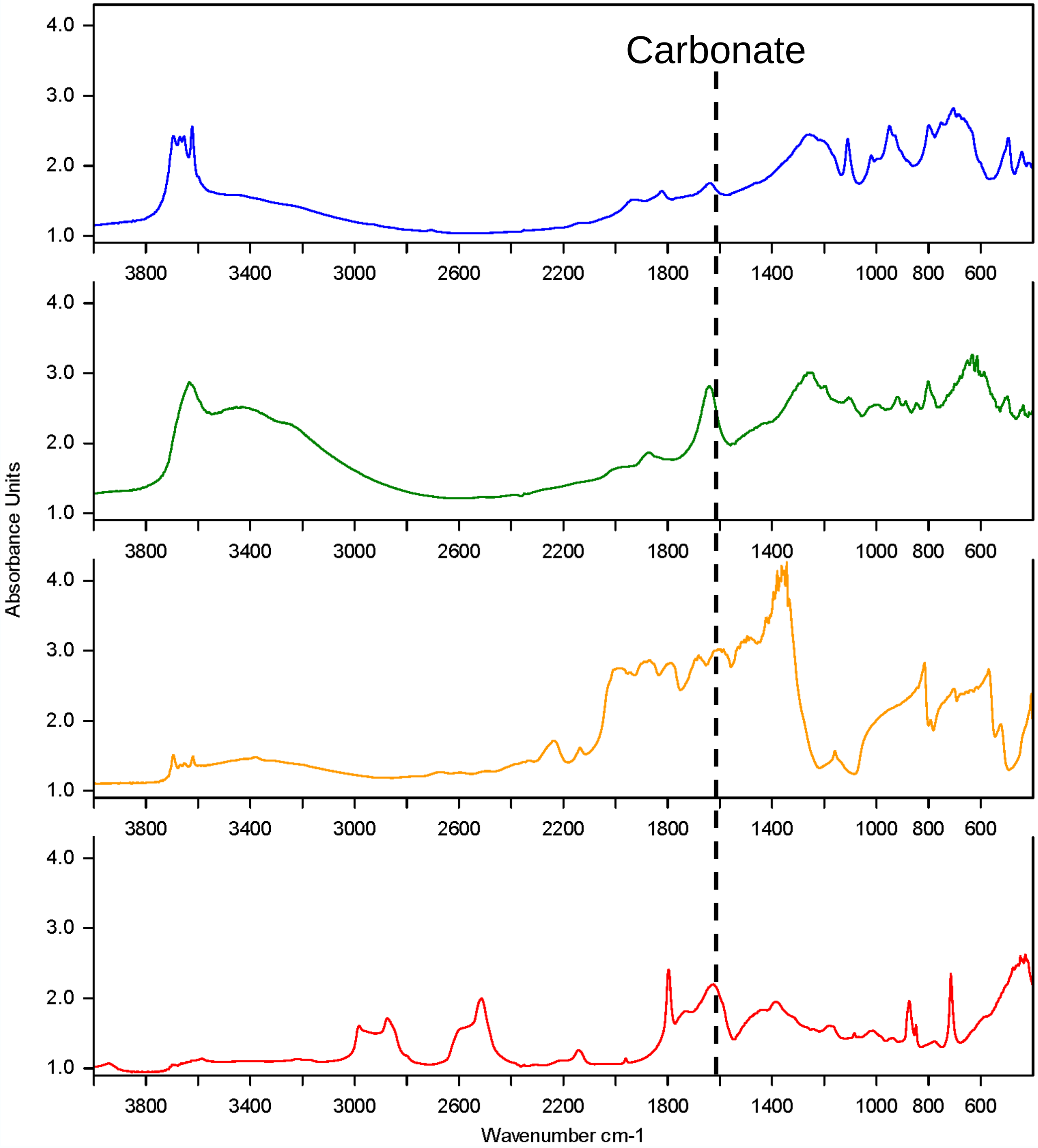
Absorbance

Kaolinite

Smectite

Sand

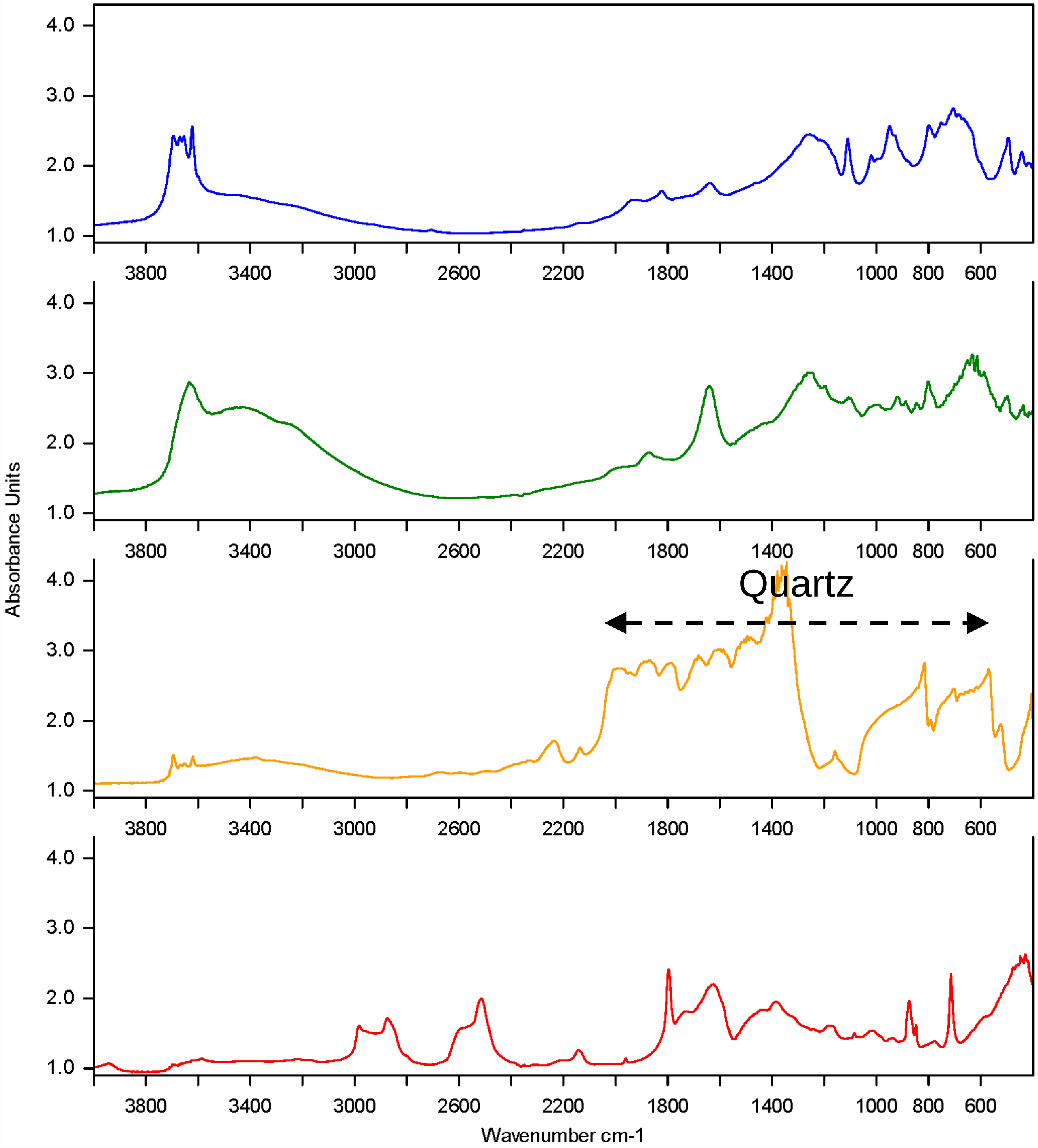
Carbonate



MIR spectra

Absorbance

- Kaolinite
- Smectite
- Sand
- Carbonate



MIR reflectance spectroscopy

- Spectra of real soil is a complicated mixture of peaks
  - Dependent on the concentrations of different substances

MIR spectra

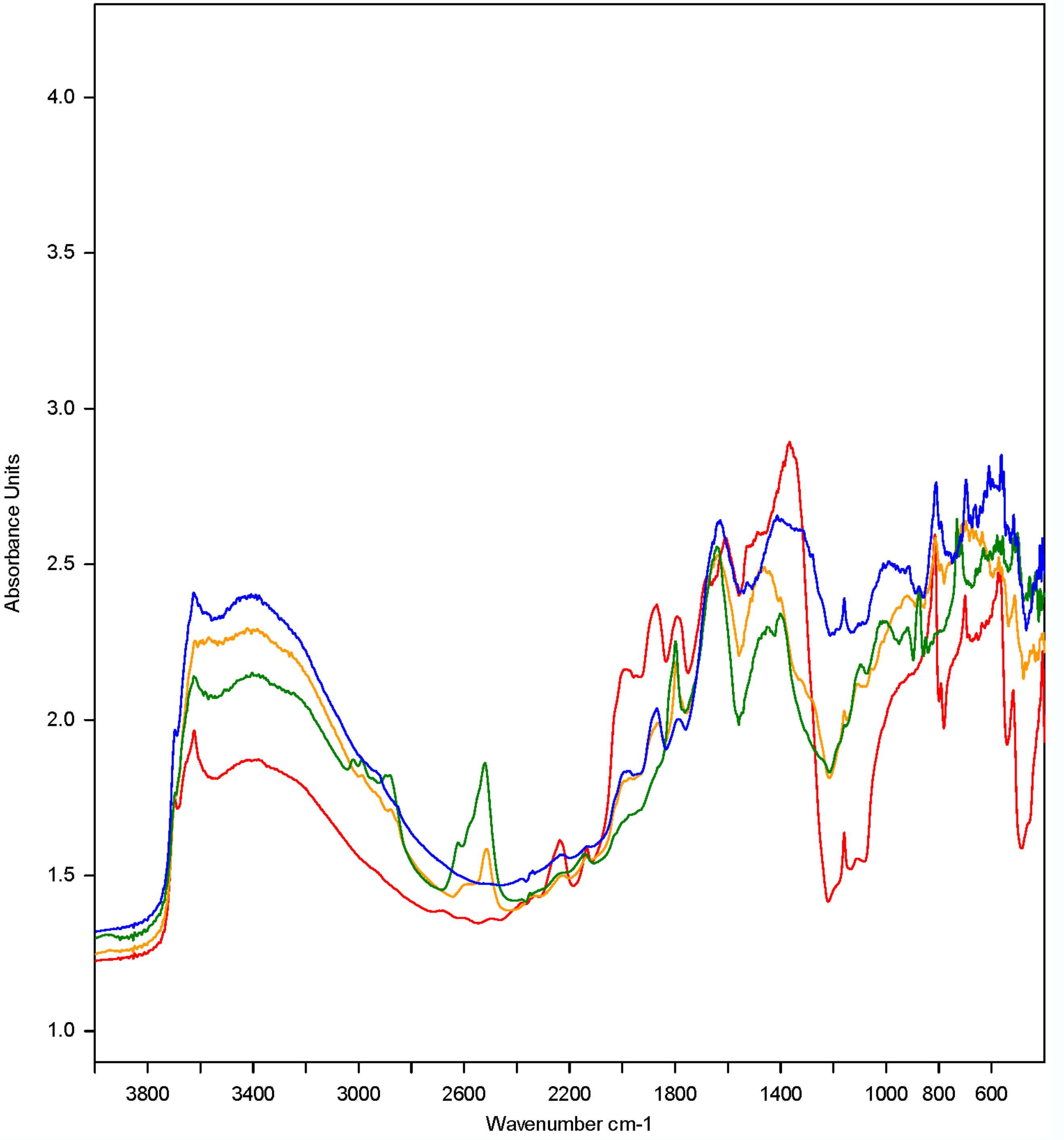
Absorbance

— Clay topsoil

— Clay loam subsoil

— Silty loam topsoil

— Loamy sand topsoil



MIR reflectance spectroscopy

- Spectra of real soil is a complicated mixture of peaks
  - Dependent on the concentrations of different substances
- These concentrations are usually estimated statistically
  - Process is called calibration
  - Uses a training set to ‘teach’ the system
    - Usually a small subset is selected
    - Training set is analysed by conventional laboratory methods
  - A statistical calibration is developed using “partial least squares”
    - Calibrations are developed for each soil property of interest

- This allows a range of soil properties can be estimated from the MIR spectra of the remaining soils

MIR reflectance spectroscopy

- Substances that can be estimated include:
  - Clay
  - Silt
  - Sand
  - Organic carbon
  - Total nitrogen
  - pH
  - Exchangeable cations and CEC
  - Iron
- Other properties related to the above **may** be estimated in a given region
  - Phosphorus buffering index (PBI)
  - Plant available water capacity

MIR reflectance spectroscopy

Benefits

- Minimum soil preparation
  - Only drying and grinding to <0.5 mm
  - No extracts or wet chemistry
- Requires only small sample (teaspoon)

- MIR spectrum acquired for each soil sample is used to estimate many soil properties
  - Each soil property requires a one-off calibration against conventional measurements
  - Once calibrations are developed several soil properties can be predicted simultaneously

- Stored spectra can be used to predict additional soil properties when new calibrations become available

MIR reflectance spectroscopy

Benefits

- Spectrum for one sample acquired in < 5 minutes
  - Allows rapid estimation of many soil properties for large number of samples

- For example: Soil survey of Pyawbwe Township, Myanmar produced 4000 samples
  - Characterisation by conventional analysis would not be possible
    - Time
    - Cost
  - Characterisation by MIR spectroscopy
    + conventional analysis of subset about 100 samples
  - Cost conventional analysis: AUD 170 per sample
    - Total AUD 17,000
  - If used to calibrate MIR and estimate properties for remaining 3900 samples
    - Effective cost: AUD 17,000/4000 = AUD 4.25

- Cost of MIR spectrometer is less than many conventional analytical instruments

Deployment of MIR capability

Recent technological advances mean MIR instruments are relatively inexpensive to buy and run

- Will be commissioned:
  - Koronivia Research Station
- Equipment:
  - Small oven to air-dry samples at 60°C
  - Several agate mortars & pestles
  - Small MIR spectrometer (size of a shoe box)
  - Computer to
    - control spectrometer
    - capture results
    - develop calibrations

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03. ROLE OF RAPID SOIL ANALYIS IN DIGITAL SOIL MAPPING

Anthony Ringrose-Voase
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Types of soil measurement

In conventional soil survey the information collected at each observation site includes:

- Soil profile morphology descriptions: All sites
- Laboratory measurements of soil properties: A few ‘representative’ sites
  - Laboratory analysis is: time-consuming
    expensive

Laboratory analysis in a survey context

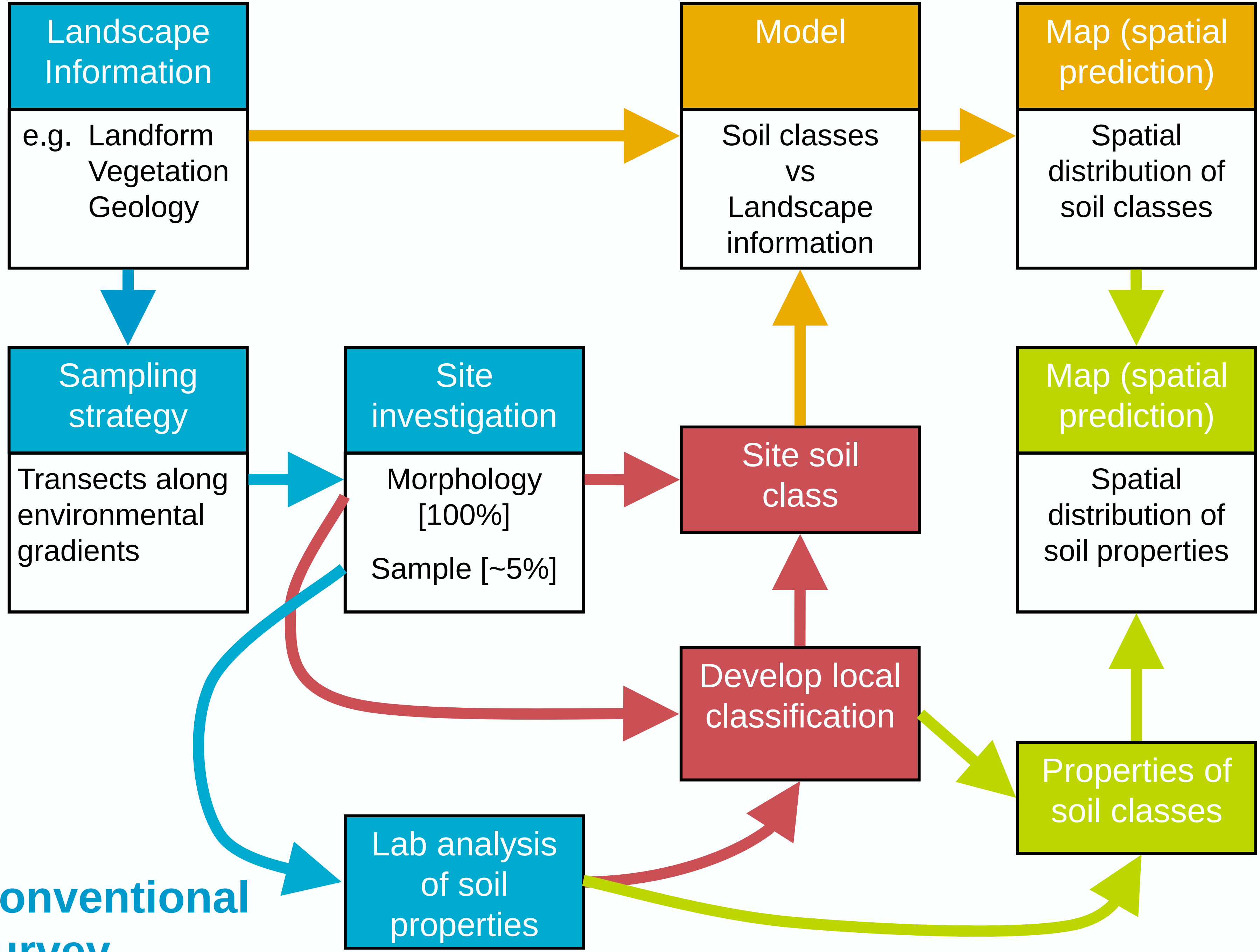
Uses of laboratory analysis

- Assisting with soil classification
  - Required by some taxonomic systems (including Soil Taxonomy)
- Determine properties of each soil class

Why are they necessary?

- Because they directly reflect the function of the soil
  - Usually more important than morphology
- Required for some aspects of land suitability assessment
- Required to guide advice on land management practices

Conventional survey



Landscape Information

e.g. Landform
Vegetation
Geology

Sampling strategy

Transects along environmental gradients

Site investigation

Morphology [100%]

Sample [~5%]

Lab analysis of soil properties

Site soil class

Develop local classification

Model

Soil classes
vs
Landscape information

Map (spatial prediction)

Spatial distribution of soil classes

Map (spatial prediction)

Spatial distribution of soil properties

Properties of soil classes

Types of soil measurement

In conventional soil survey the information collected at each observation site includes:

- Soil profile morphology descriptions: All sites
- Laboratory measurements of soil properties: A few ‘representative’ sites

In digital soil surveys the collected information collected:

- Soil profile morphology descriptions: All sites
- Rapid soil measurements: All sites
- Laboratory measurements of soil properties: A few ‘calibration’ specimens

Role of rapid measurement

Measurement is ‘rapid’

- Like morphology, can be done on all samples from all sites

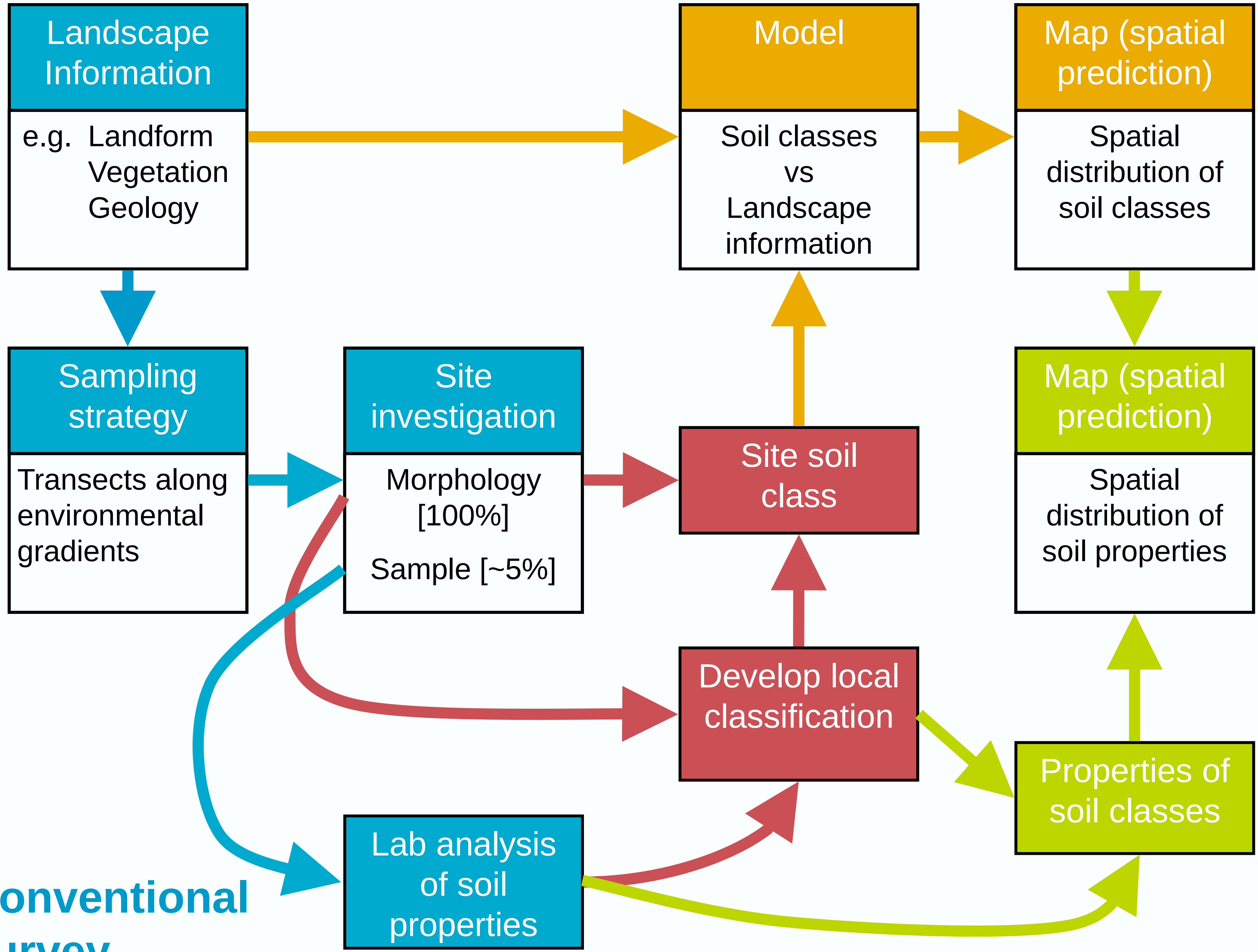
Provides:

- Quantitative data
- Unlike morphology, measures soil properties of interest to farmers, hydrologists, land use planners etc.

Not as precise as laboratory measurements

Measurement strategy for soil survey:

- Many, less precise measurements
  are better than
  few precise measurements
- **Because spatial variability of soil properties is large**
  - **Even over short distances**



Landscape Information

e.g. Landform
Vegetation
Geology

Model

Soil classes
vs
Landscape
information

Map (spatial prediction)

Spatial
distribution of
soil classes

Sampling strategy

Transects along
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Site investigation

Morphology
[100%]

Sample [~5%]

Site soil class

Map (spatial prediction)

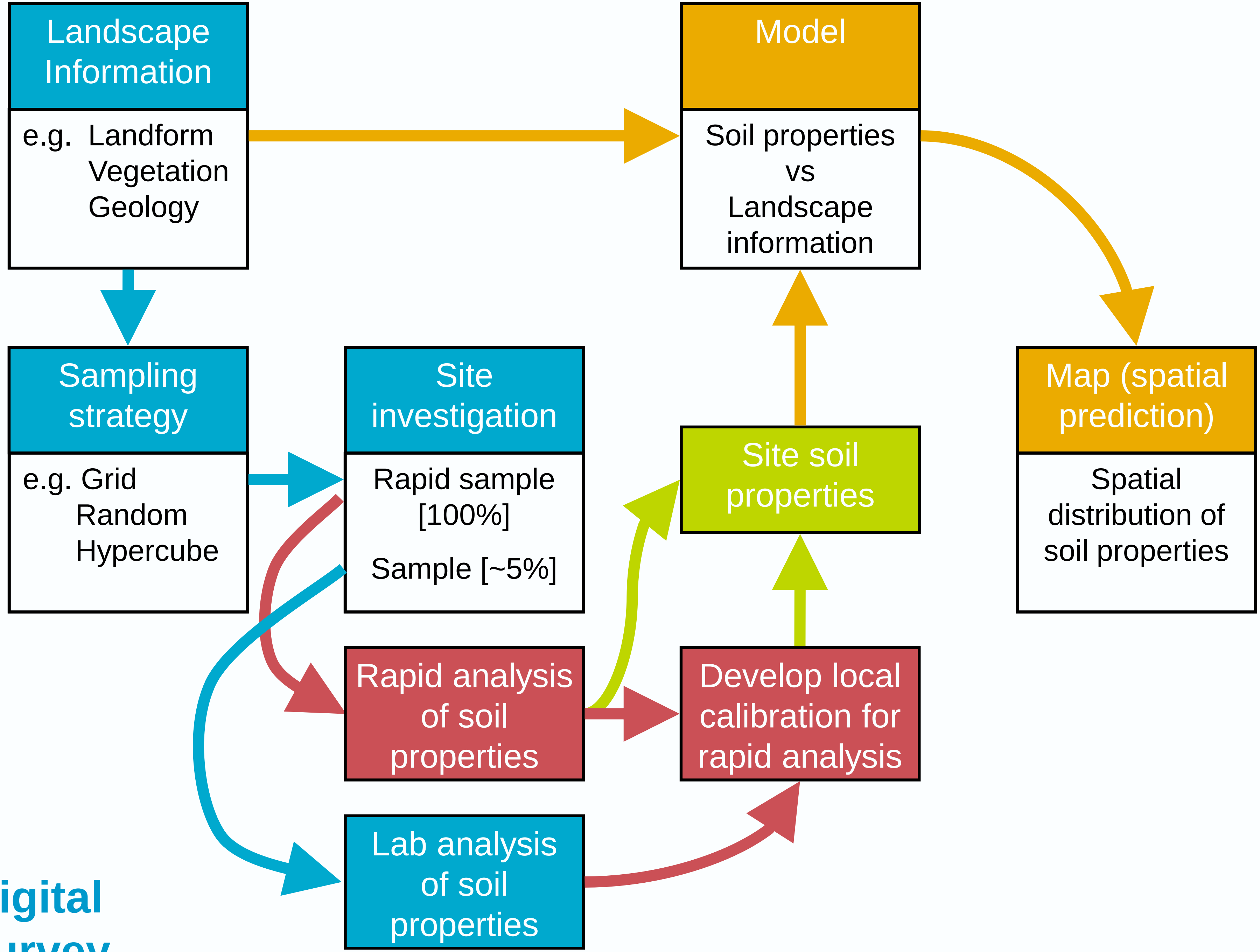
Spatial
distribution of
soil properties

Develop local classification

Properties of soil classes

Lab analysis of soil properties

Conventional survey



Landscape Information

e.g. Landform
Vegetation
Geology

Model

Soil properties
vs
Landscape
information

Sampling strategy

e.g. Grid
Random
Hypercube

Site investigation

Rapid sample
[100%]

Sample [~5%]

Site soil properties

Map (spatial prediction)

Spatial
distribution of
soil properties

Rapid analysis of soil properties

Develop local calibration for rapid analysis

Lab analysis of soil properties

Digital survey

Digital Land Resource Mapping (DLRM)

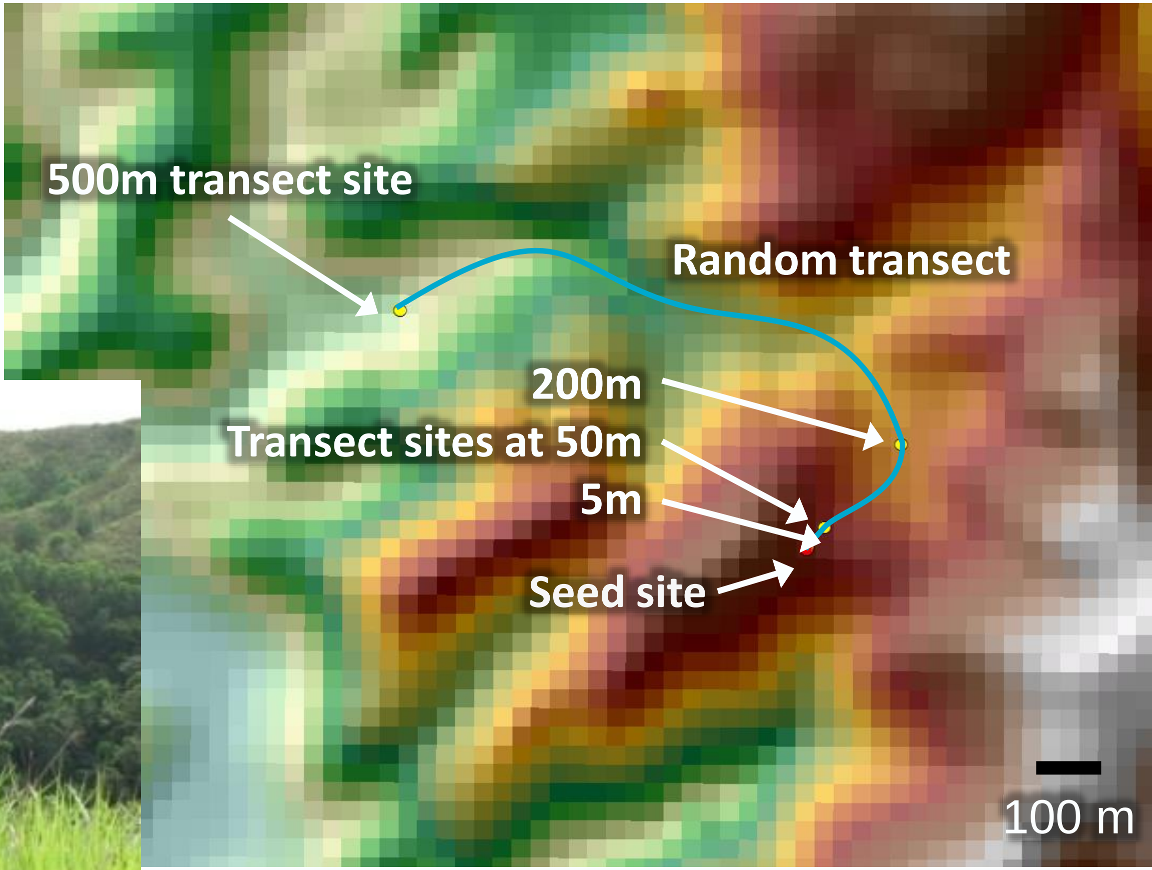
including Digital Soil Mapping (DSM)

Based on 4 pillars:

1. Statistically-based sampling strategy
2. Simplified site and soil profile methods
3. Rapid soil analysis
4. Mapping of soil and land properties using statistical models

1. Statistically-based sampling strategy

Using random transect samples generated on a 30 m digital elevation model (DEM)



2. Simplified site and soil profile methods

Simplified field procedures that can be carried out by non-experts with an emphasis on soil sampling all sites

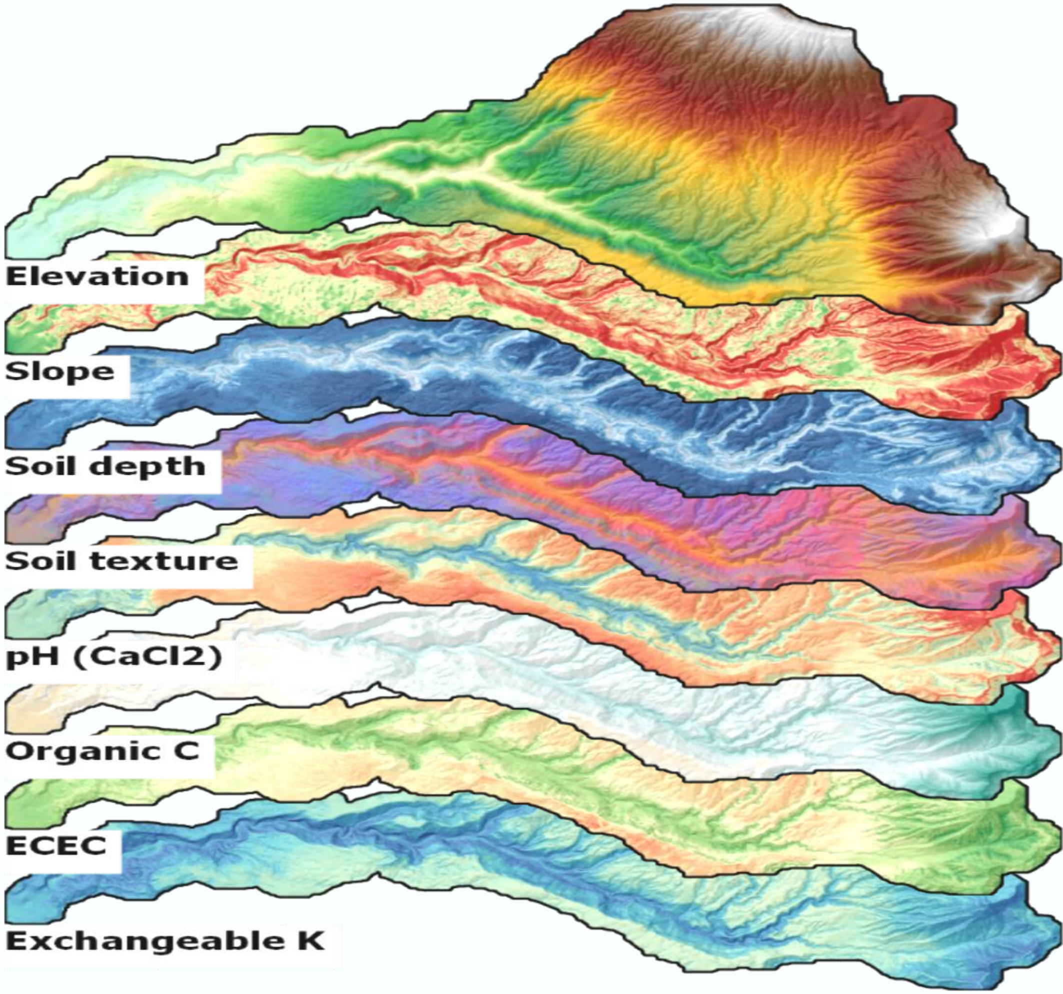
3. Rapid soil analysis

- Uses mid-infrared spectroscopy (MIR)
- Possible to estimate a range of soil properties at all sample sites
  - rather than at a small subset when only conventional laboratory methods are used.

4. Mapping of soil and land properties using statistical models

Numerical methods are used

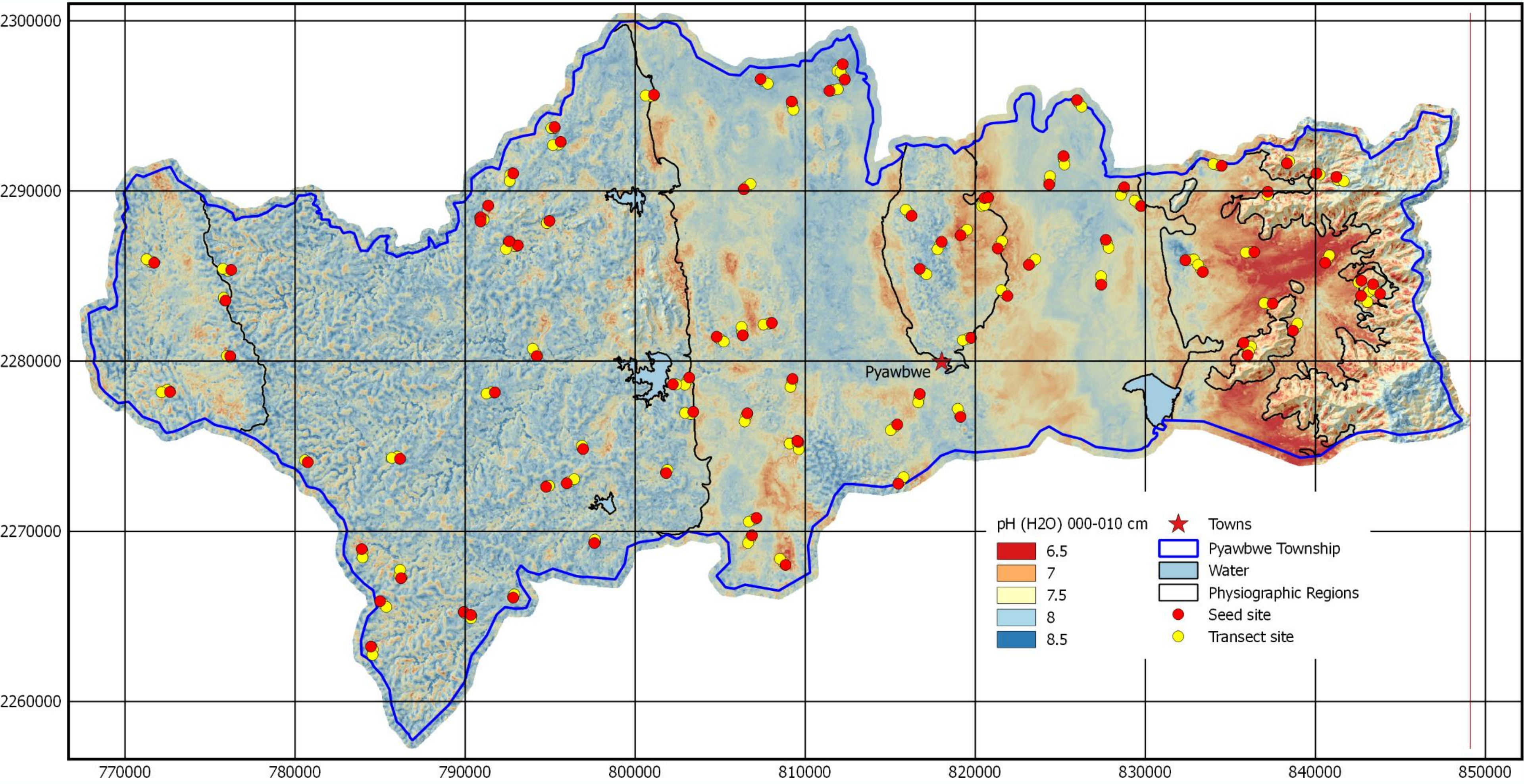
- To predict land and soil properties over the survey area using
  - Measurements at sample sites
  - Terrain attributes (e.g. slope) derived from a 20 m digital elevation model (DEM)
- Produces, not one, but many digital maps such as these



Cabulig watershed, southern Philippines

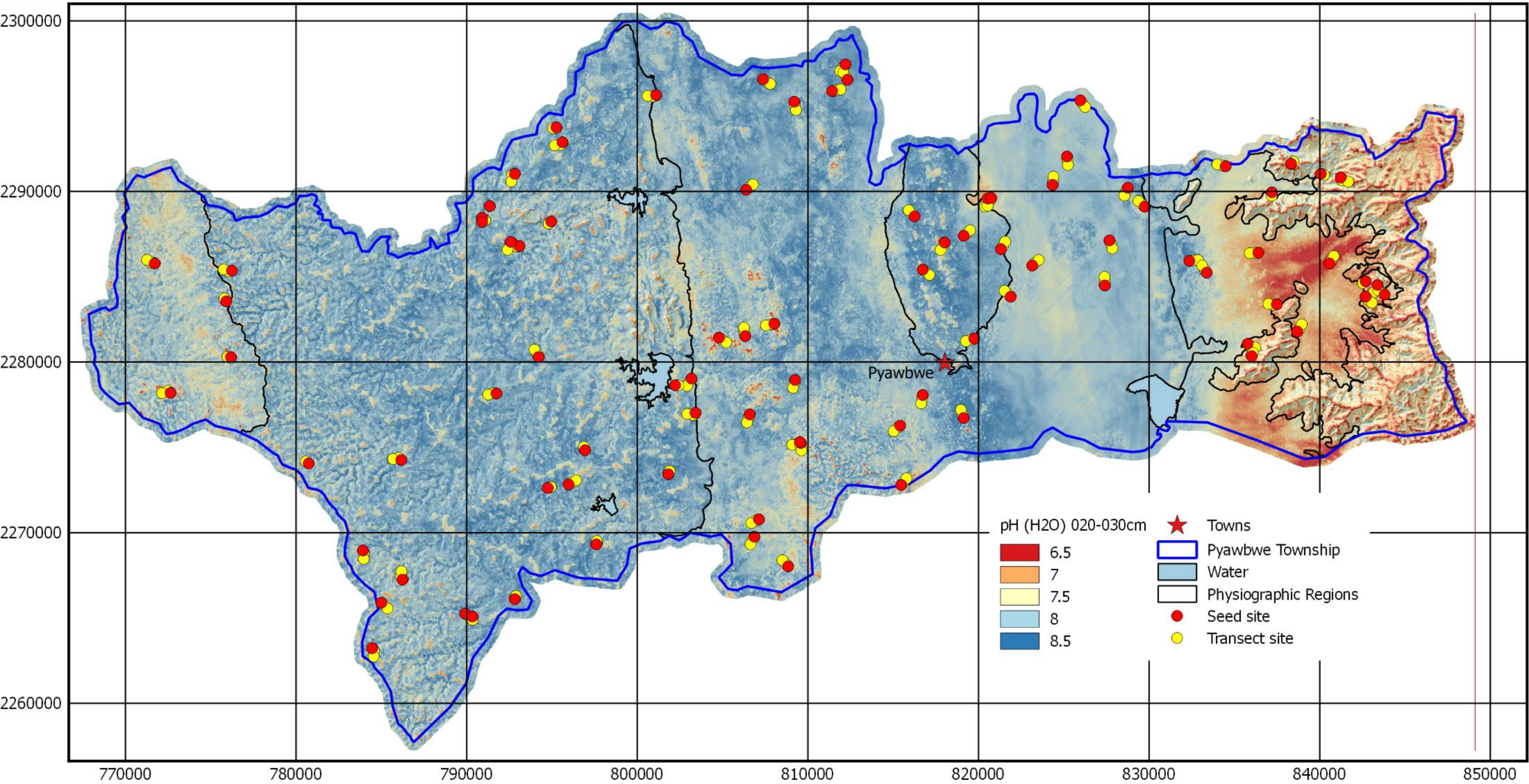
Digital soil map of Pyawbwe Township

pH (1:5 H_2O) at 0 - 10 cm depth



Digital soil map of Pyawbwe Township

pH (1:5 H_2O) at 20 - 30 cm depth



Conclusion

Rapid soil analysis by MIR spectroscopy

- Allows direct mapping of soil properties of interest to land managers

- Instead of mapping soil type based on observations of soil morphology and then inferring soil properties from a measurements on a few examples of each soil type

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04. SAFETY

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Health and safety

Highest priority objective for any project:

- That all staff return home
- Uninjured
- In good health

Outline of presentation

- CSIRO framework for assessing health and safety risks
- Controlling risk
- Risk assessment for field laboratory

Framework for assessing safety

1. Identify a hazard
    - For example, repetitive strain injury due to soil grinding

Framework for assessing safety

2. Assess the consequence of the hazard

- Catastrophic
  - Fatality
  - Serious, permanent disability
- Major
  - Extended absence from work (>1 week)
  - Moderate to severe health effects
- Moderate
  - Temporary absence from work (<1 week)
  - Requires one or more visits to doctor
- Minor
  - Requires first aid
- Insignificant
  - No injury

Framework for assessing safety

3. Assess **likelihood** of hazard
    - Almost certain
        - Daily to several times per week
    - Likely
        - Once per month to several times per year
    - Possible
        - Once per year to several times over 2 years
    - Unlikely
        - Once every 2 to 5 years
    - Rare
        - Once every 5 years or less

Framework for assessing safety

4. Assess **inherent risk**

- Risk that exists in the absence of control measures
- Assessed using consequence and likelihood

Likelihood	Consequence				
	Insignificant	Minor	Moderate	Major	Catastrophic
Almost certain	Mod	Mod	High	High	High
Likely	Mod	Mod	Mod	High	High
Possible	Low	Mod	Mod	High	High
Unlikely	Low	Low	Mod	Mod	High
Rare	Low	Low	Mod	Mod	Mod

Framework for assessing safety

Inherent risk levels

High risk

- Immediate action required

Moderate risk

- Management responsibility must be specified

Low risk

- Manage by routine procedures

Framework for assessing safety

5. Decide on management controls

- Very good
  - Controls are best practice
  - Involve explicit standards
  - Followed all of the time
  - High emphasis on elimination, substitution or engineering controls.
- Reasonable
  - Controls are in place
  - Not followed all of the time
  - May not include best practice
  - High emphasis on administration and protective equipment.
- Poor
  - Few or no controls in place.
  - No standards have been identified.
  - Controls do not address Hierarchy of Control principles.

Framework for assessing safety

6. Assess impact of **management controls**
    - Determines residual risk
    - Risk that exists after application of control measures

Likelihood	**Consequence**				
	Insignificant	Minor	Moderate	Major	Catastrophic
Almost certain	Mod	Mod	High	High	High
Likely	Mod	Mod	Mod	High	High
Possible	Low	Mod	Mod	High	High
Unlikely	Low	Low	Mod	Mod	High
Rare	Low	Low	Mod	Mod	Mod

Framework for assessing safety

Residual risk levels

High	Attend to immediately
Moderate	Attend to in short-term
Low	Attend to in longer term

Hierarchy of control principles

Elimination

- Eliminate the hazard from the workplace altogether

Substitution/modification

- Substitute the hazard with something with lesser risk which will still perform the same task in a satisfactory manner

Isolation

- Isolate the problem from staff
- often by use of separate purpose built rooms, barricades, sound barriers, etc.

Engineering controls

- Re-design equipment, work processes or tools to reduce or eliminate the risk

Hierarchy of control principles

Administrative controls

- Training
- Written work procedures
- Adequate supervision
- Signage
- Maintenance of plant and equipment
- Limitation of exposure time

Personal protective equipment (PPE)

- Provide adequate personal protective equipment.
- Masks, gloves, boots, overalls etc.

Note:

- This is the least preferable method of dealing with a hazard
- It should only be adopted when all other methods are unsuitable.


Least preferred controls

Exercise: Risk assessment for MIR laboratory

Exercise:

1. Identify a hazard you think we might encounter in the field laboratory

Then work through the risk assessment framework for that hazard

2. Consequences
3. Likelihood
4. Inherent risk
5. Management controls
6. Residual risk

Hazards in MIR laboratory

Repetitive strain injury

- Long term pain due to repetitive actions during grinding
- Consequence: Major
- Likelihood: Likely
- Inherent risk: High
- Controls:
  - Staff should be aware of risk and of need to act early
  - Provide ergonomic workstations
  - Regular rest-breaks – rotate activity with other staff
- Consequence: Moderate
- Likelihood: Unlikely
- Residual risk: Moderate

Hazards in MIR laboratory

Electrocution

- Use of electric equipment – oven, MIR spectrometer
- Serious injury, death
- Consequence: Catastrophic
- Likelihood: Unlikely
- Inherent risk: High
- Controls:
  - Use earth
  - Check electric leads for wear and tear
  - Maintain equipment
  - Use approved plugs and sockets
  - Use licensed electrician to change plugs etc.
- Consequence: Catastrophic
- Likelihood: Rare
- Residual risk: Moderate

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05. MIR CALIBRATION STRATEGY

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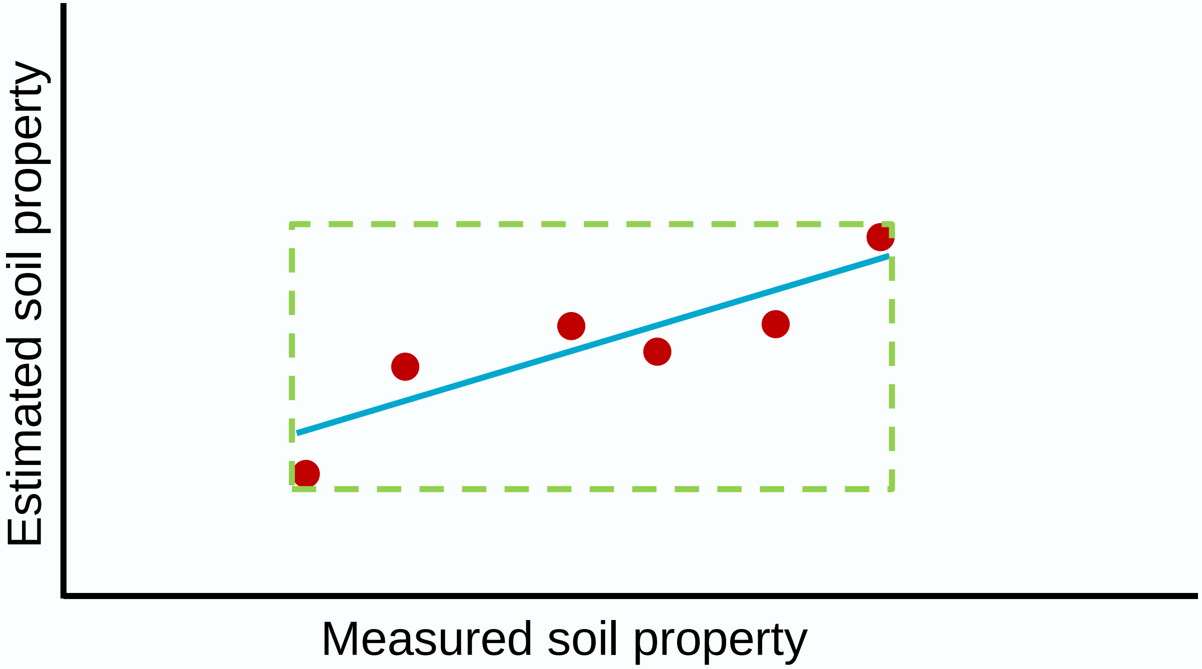
Choice of samples for calibration

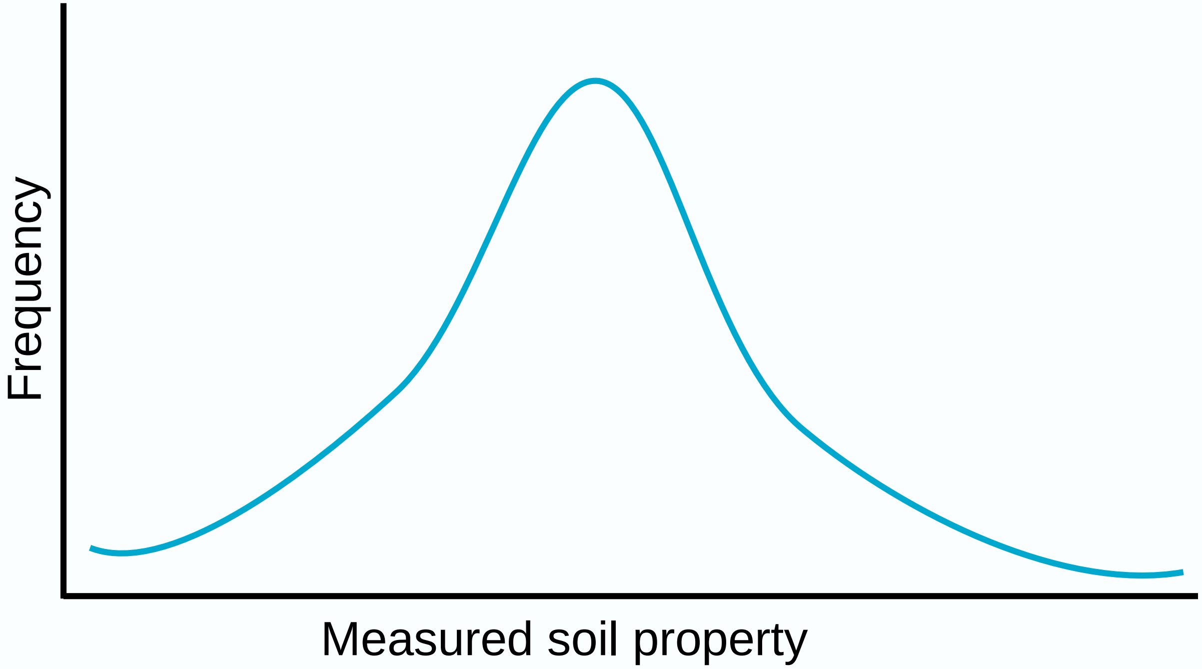
Prediction of a soil property using a calibration is only valid for soil property values within the range of the calibration sample set

- Properties of calibration samples should cover full range encountered in survey area



Choice of samples for calibration

Calibrations are most reliable when statistical distribution of soil properties in the calibration sample set reflects the distribution in the survey area



Calibration strategy for a survey area

- At the outset we have no knowledge of the range or distribution of soil properties in survey area
- Aim to represent the range of soil materials in survey area
- Two stage process
  - Select sampling locations likely to include a wide range of soil materials
  - After acquiring MIR spectra, select samples that cover the range of MIR spectral characteristics

Calibration strategy for a survey area

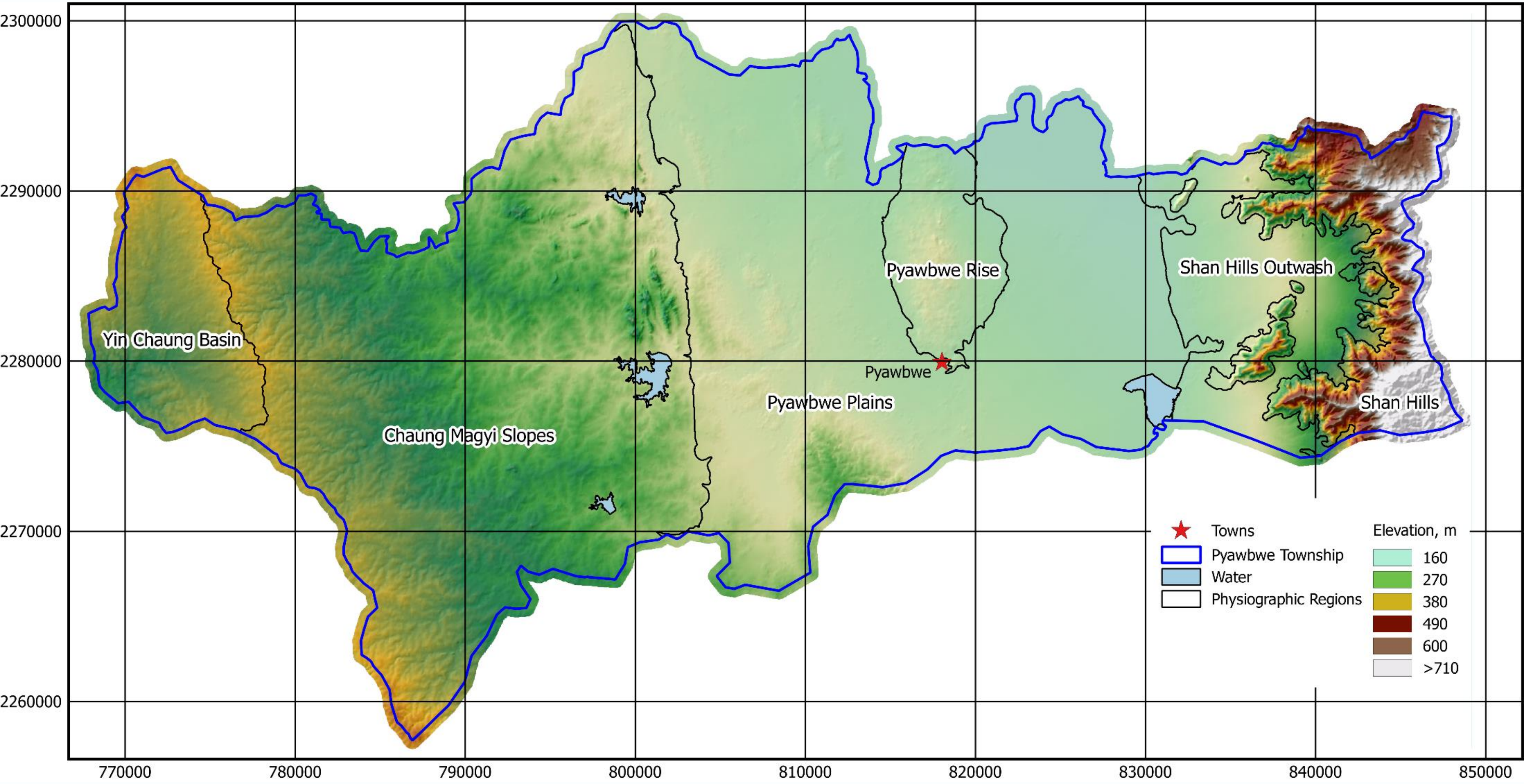
Stage 1

Select sampling locations likely to include a wide range of soil materials

- Stratify landscape at two levels
  - Physiographic regions
  - Landform units

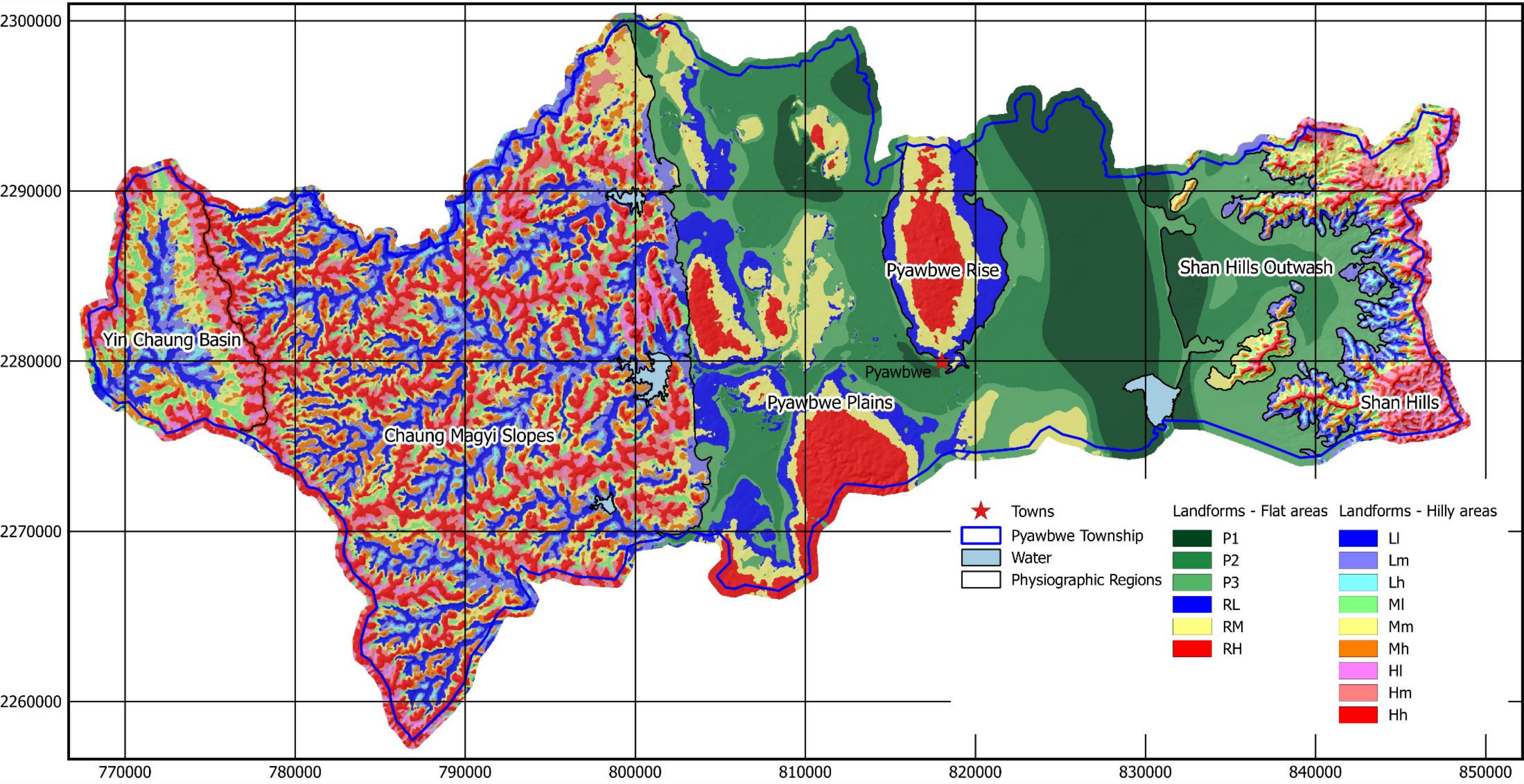
Calibration strategy for a survey area

Stage 1 – Stratification into physiographic regions



Calibration strategy for a survey area

Stage 1 – Stratification of each physiographic region into landform units



Calibration strategy for a survey area

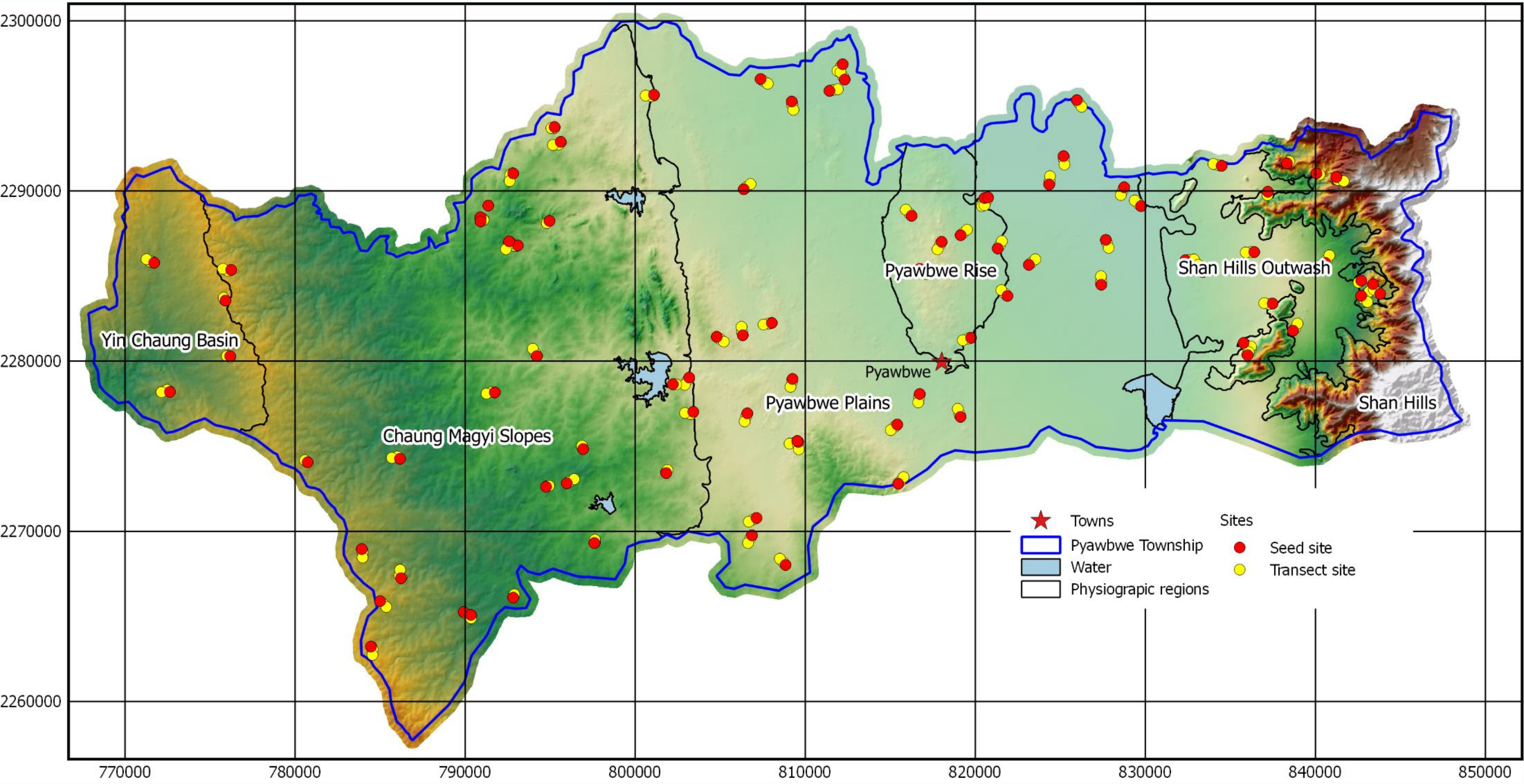
Stage 1

Select sampling locations likely to include a wide range of soil materials

- Stratify landscape at two levels
  - Physiographic regions
  - Landform units
- Randomly locate ‘seed sites’ in each physiographic-landform unit
  - Number of sites proportional to unit area
- Also locate 4 ‘transect sites’ along random transects away from seed site

Calibration strategy for a survey area

Stage 1 – Stratified-random sampling strategy



Calibration strategy for a survey area

Stage 1

Select sampling locations likely to include a wide range of soil materials

- Stratify landscape at two levels
  - Physiographic regions
  - Landform units
- Randomly locate ‘seed sites’ in each physiographic-landform unit
  - Number of sites proportional to unit area
- Also locate 4 ‘transect sites’ along random transects away from seed site

- Specimen collection
  - Seed sites: MIR specimen + bag specimen (Pyawbwe – 498 specimens)
  - Transect sites: MIR specimen only (Pyawbwe – 3561 specimens)

(Pyawbwe – 4059 total)

Calibration strategy for a survey area

Stage 2

From seed site specimens select specimens that cover the range of MIR spectral characteristics

- Scan all MIR specimens from seed sites
  - (Pyawbwe – 498 specimens)
- Analyse MIR spectra
  - Using principal component analysis
- Select a sub set of ~100 specimens that cover range of principal components
  - Using Kennard Stone sampling method

Calibration strategy for a survey area

- Conventional analysis of bag specimens for selected MIR spectra
  - 104 specimens (out of all seed site specimens – 498 in Pyawbwe)
- Develop calibrations for each soil property of interest
- Scan MIR specimens from transect sites
  - (3561 specimens in Pyawbwe)
- Estimate soil properties for unanalysed specimens using calibrations
  - Pyawbwe: 3561 transect specimens + 394 seed specimens = 3955 specimens
- Outliers with unreliable estimates are automatically identified
  - Can be removed if desired
  - Or sent for conventional analysis to update calibration

Types of calibration strategies

- Survey area calibrations
  - As above (e.g. for township, catchments)
- Regional calibrations
  - E.g. Central Dry Zone
  - Start with calibration for a survey area
  - Gradually add sites for other areas in the region
  - Incrementally update calibrations
- National calibration
  - Use: Existing database of soil test values within a country
    Archive of soil specimens (from surveys, agronomy trials etc.)
- Global calibration

Types of calibration strategies

General rule:

- Local calibrations will generally give more accurate estimates than regional, national or global calibrations
  - But are limited to the calibration area
- Spectra should be archived together with soil specimens
  - Allows calibrations to be developed for new soil properties in the future
- Most effective if different institutions share spectra and results to build up databases of soil properties and MIR spectra

Rapid Soil Analysis by Mid-Infrared Spectroscopy Training Course

06. MIR CALIBRATION

Anthony Ringrose-Voase

May 2018

Agriculture and Food

www.csiro.au

CSIRO

Australian Government

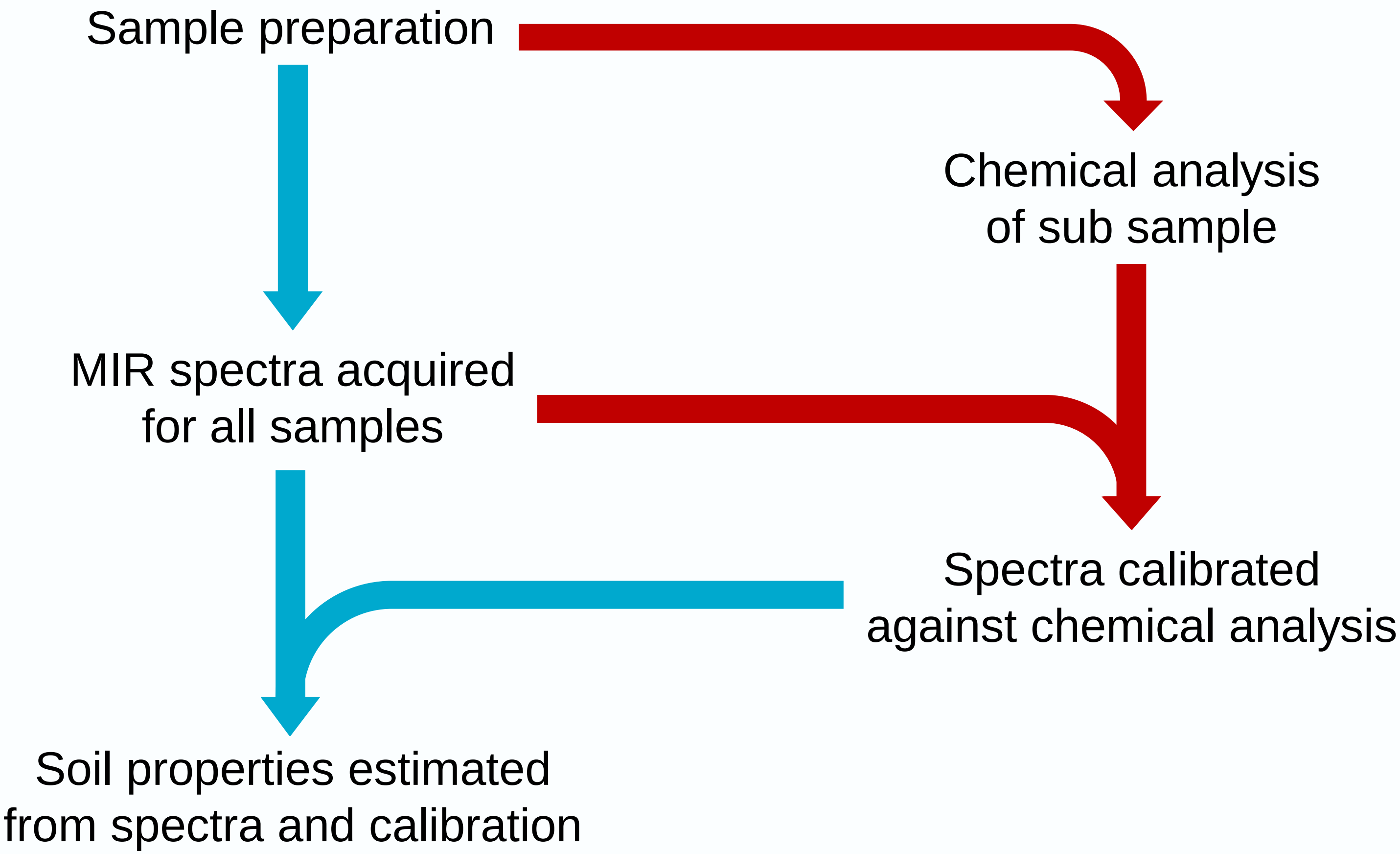
Australian Centre for International Agricultural Research

Purpose of MIR calibration

- To correlate measured MIR spectra with soil properties measured by conventional analysis
- To use this correlation to estimate these properties for soil samples for which there is no conventional analysis

- The whole spectrum is used in correlation
- The correlation is done by partial least square regression

MIR Process to measure soil properties



Sample preparation

Chemical analysis of sub sample

MIR spectra acquired for all samples

Spectra calibrated against chemical analysis

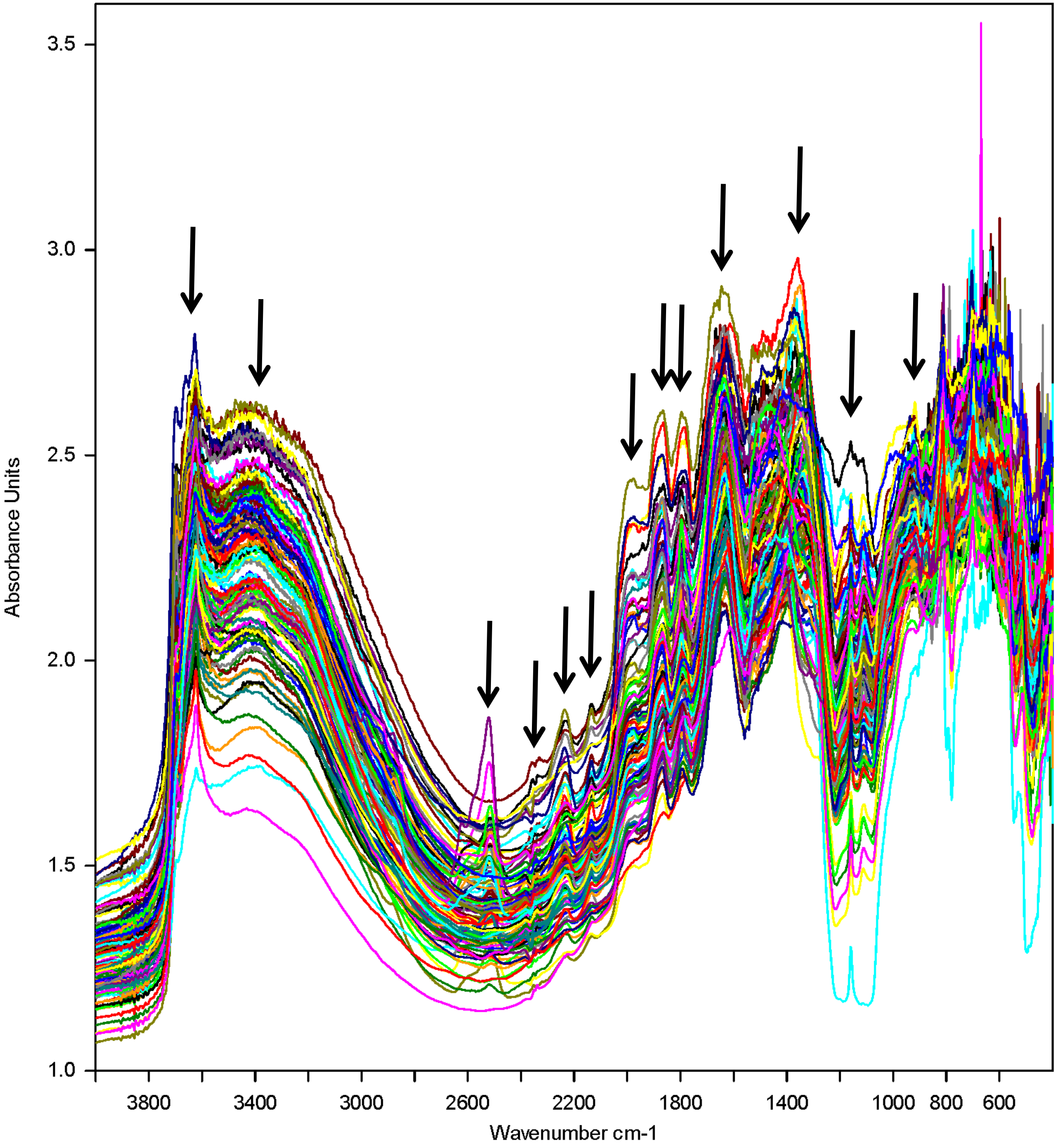
Soil properties estimated from spectra and calibration

MIR spectra of 104 samples

Pyawbwe Township, Myanmar

Many parts of the spectra follow a similar pattern

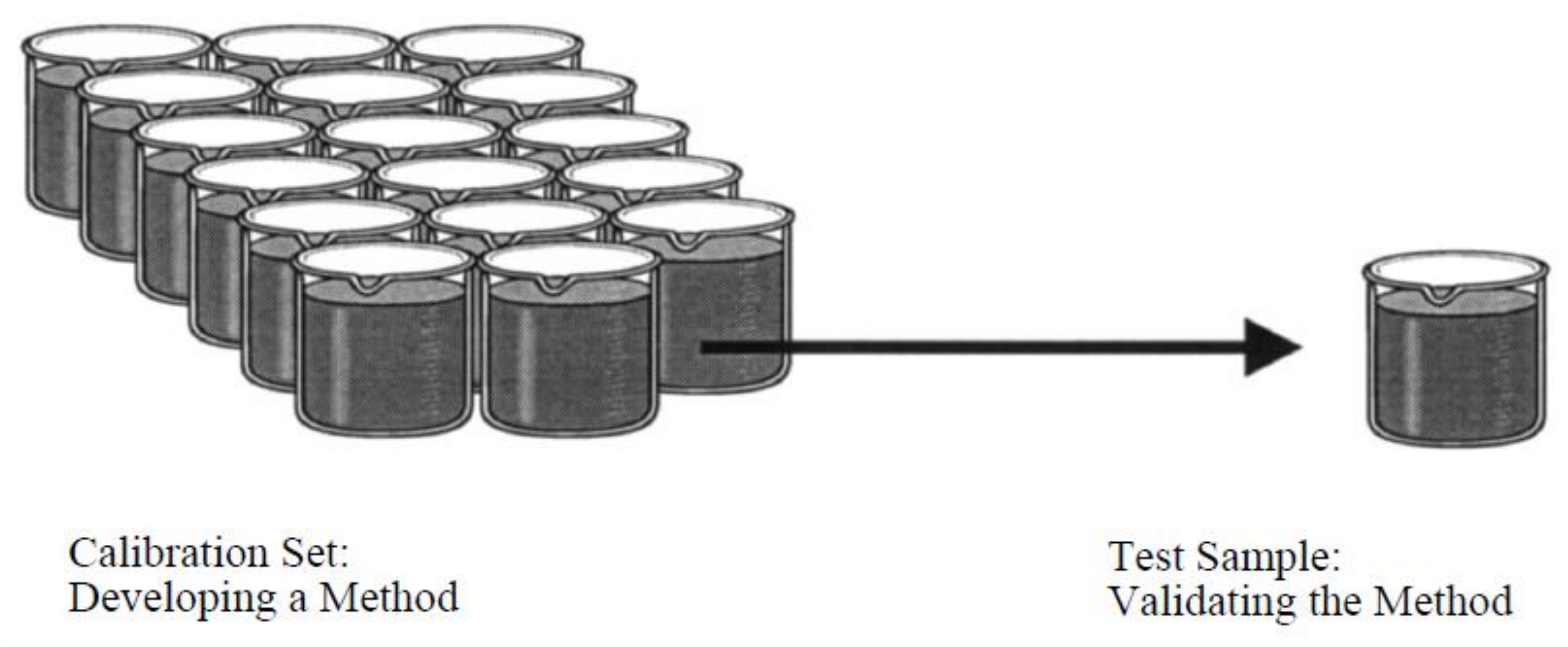
- Therefore much is redundant information
- The whole spectra can be described by a few principal components



Cross-validation

Checking the quality of a calibration

- Calibration is run many times
  - Each time one sample is removed and used for validation
- Good method when short of samples: minimum of ~60 required for a calibration



Residual prediction deviation (RPD)

Assessment of calibration

- RPD = Standard deviation/Root mean square error of prediction
- Related to R^2
- Indicates quality of prediction:

< 1.5	Poor
1.5-2.0	Indicator
2.0-3.0	Good
> 3.0	Analytical quality

MIR prediction for soil samples

Cabulig watershed, southern Philippines

Soil attribute	RPD	Prediction quality
Organic carbon	3.1	Analytical quality
pH (1:5 H_2O)	2.8	Good quality
Exchangeable Mg	2.7	Good quality
Exchangeable acid	2.3	Good quality
Sum exchangeable cation	2.3	Good quality
Clay content	2.2	Good quality
Exchangeable Ca	2.2	Good quality
ECEC	2.0	Good quality
Sand content	1.8	Indicator
Exchangeable K	1.5	Indicator
Silt	1.4	Poor
Olsen P	1.3	Poor

MIR prediction for soil samples

Inabanga watershed, southern Philippines

Soil attribute	RPD	Prediction quality	*(Cabulig)*
Organic carbon	2.1	Good quality	*(Analytical quality)*
pH (1:5 H_2O)	2.0	Good quality	*(Good quality)*
Exchangeable Mg	2.1	Good quality	*(Good quality)*
Exchangeable acid	1.7	Indicator	*(Good quality)*
Sum exchangeable cation	3.8	Analytical quality	*(Good quality)*
Clay content	1.8	Indictor	*(Good quality)*
Exchangeable Ca	3.4	Analytical quality	*(Good quality)*
ECEC	3.4	Analytical quality	*(Good quality)*
Sand content	1.7	Indicator	*(Indicator)*
Exchangeable K	1.6	Indicator	*(Indicator)*
Silt	1.4	Poor	*(Poor)*
Olsen P	1.1	Poor	*(Poor)*

Calibration process

- Make a table of spectra of calibration samples
- Make a table of laboratory results
- Check match of calibration and lab analysis
- Calculate calibration
- Validate
- Optimize

Rapid Soil Analysis by Mid-Infrared Spectroscopy Training Course

07. MIR CALIBRATION INSTRUCTIONS

Anthony Ringrose-Voase

May 2018

Agriculture and Food

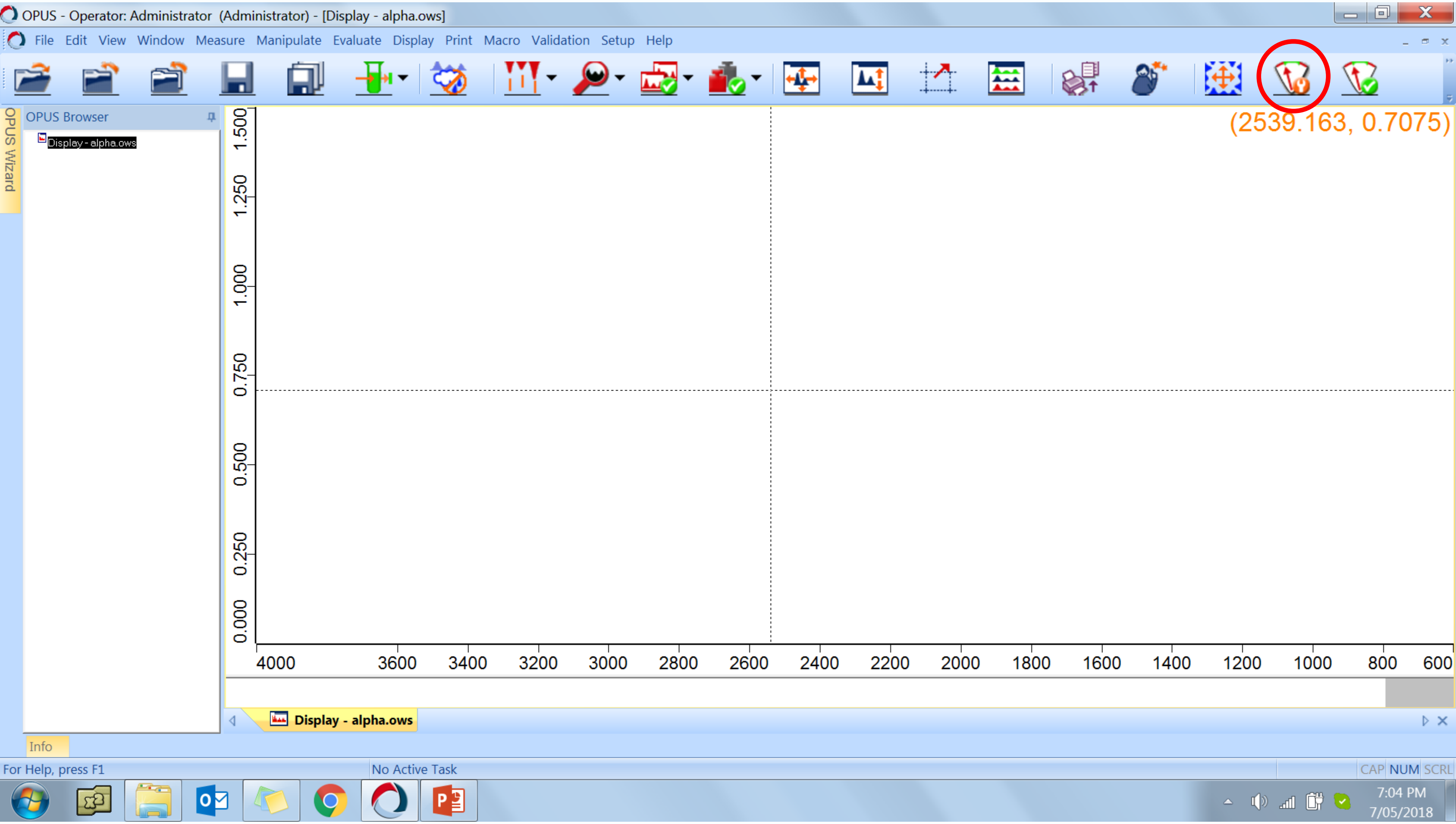
www.csiro.au

Australian Government

Australian Centre for International Agricultural Research

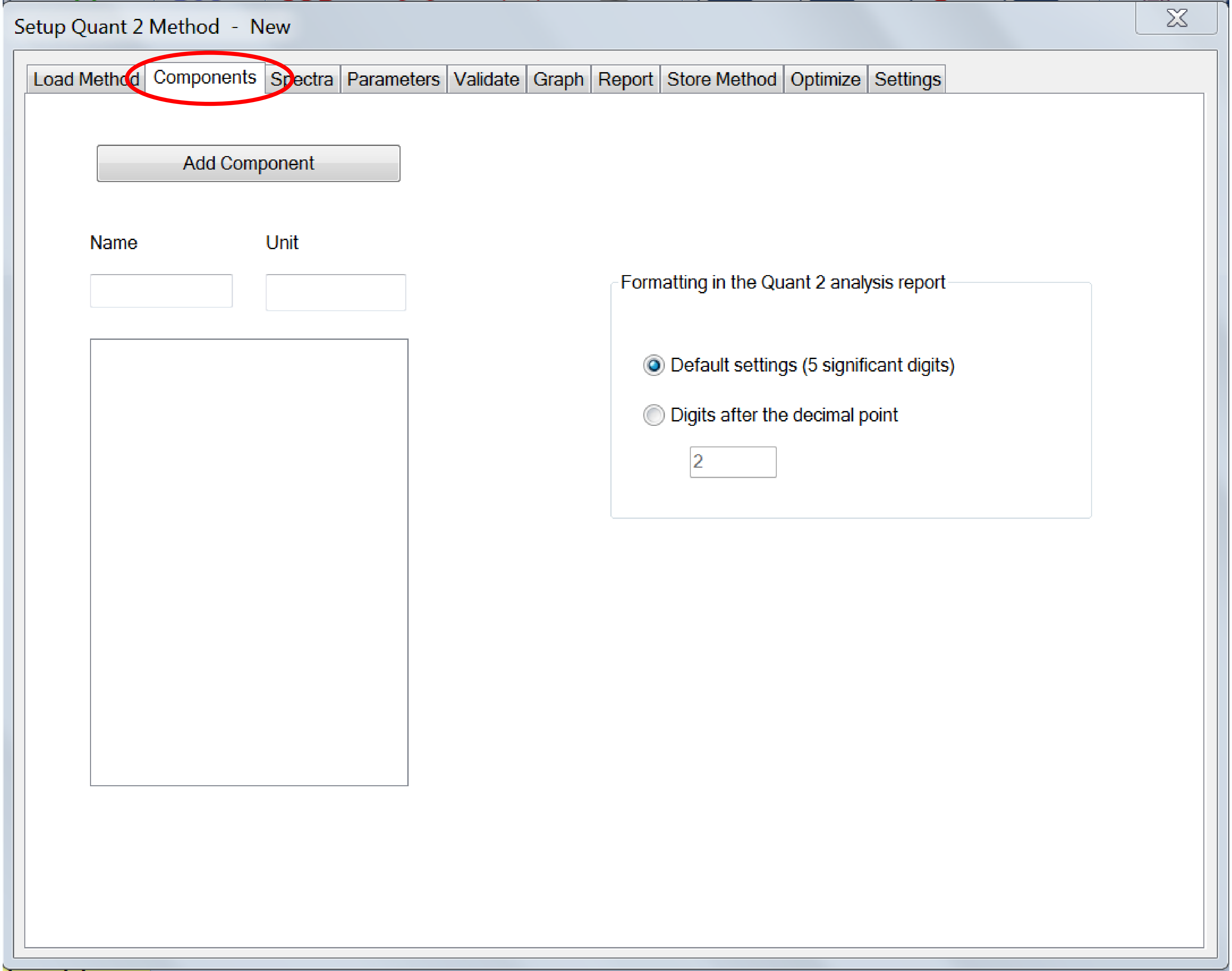
MIR Calibration with OPUS Quant 2 module

Start Quant 2



First create a calibration template

- Template will contain:
  - List of soil properties for which there are calibration data
  - List of calibration spectra
    - How many replicate spectra there are for each sample
  - Calibration data
  - Other calibration settings
- Setting up a template correctly makes it easier to perform the calibrations in a standard way



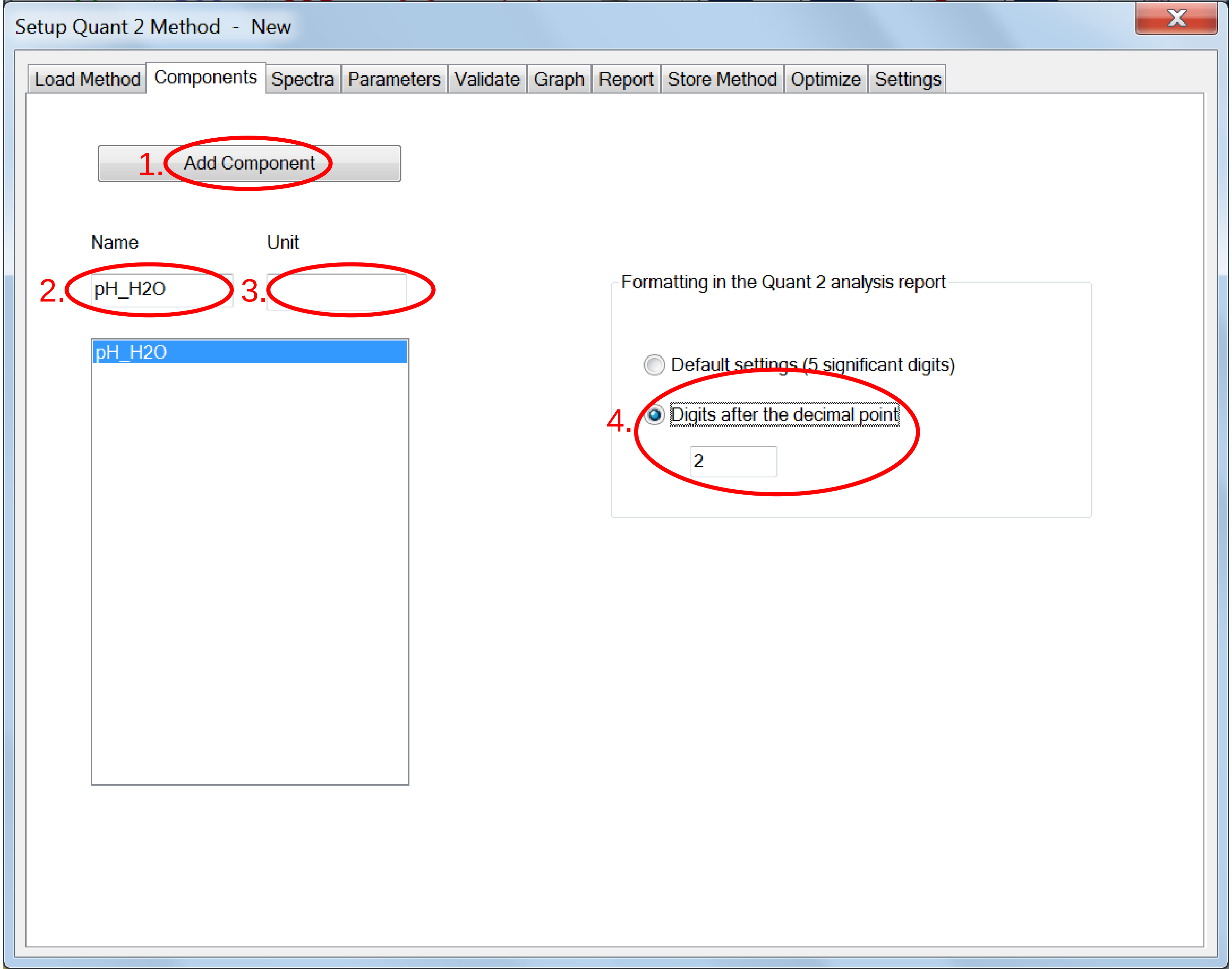
Setup Quant 2 Method - New

Formatting in the Quant 2 analysis report

● Default settings (5 significant digits)

○ Digits after the decimal point

2



2. Name: pH_H2O

3. Unit:

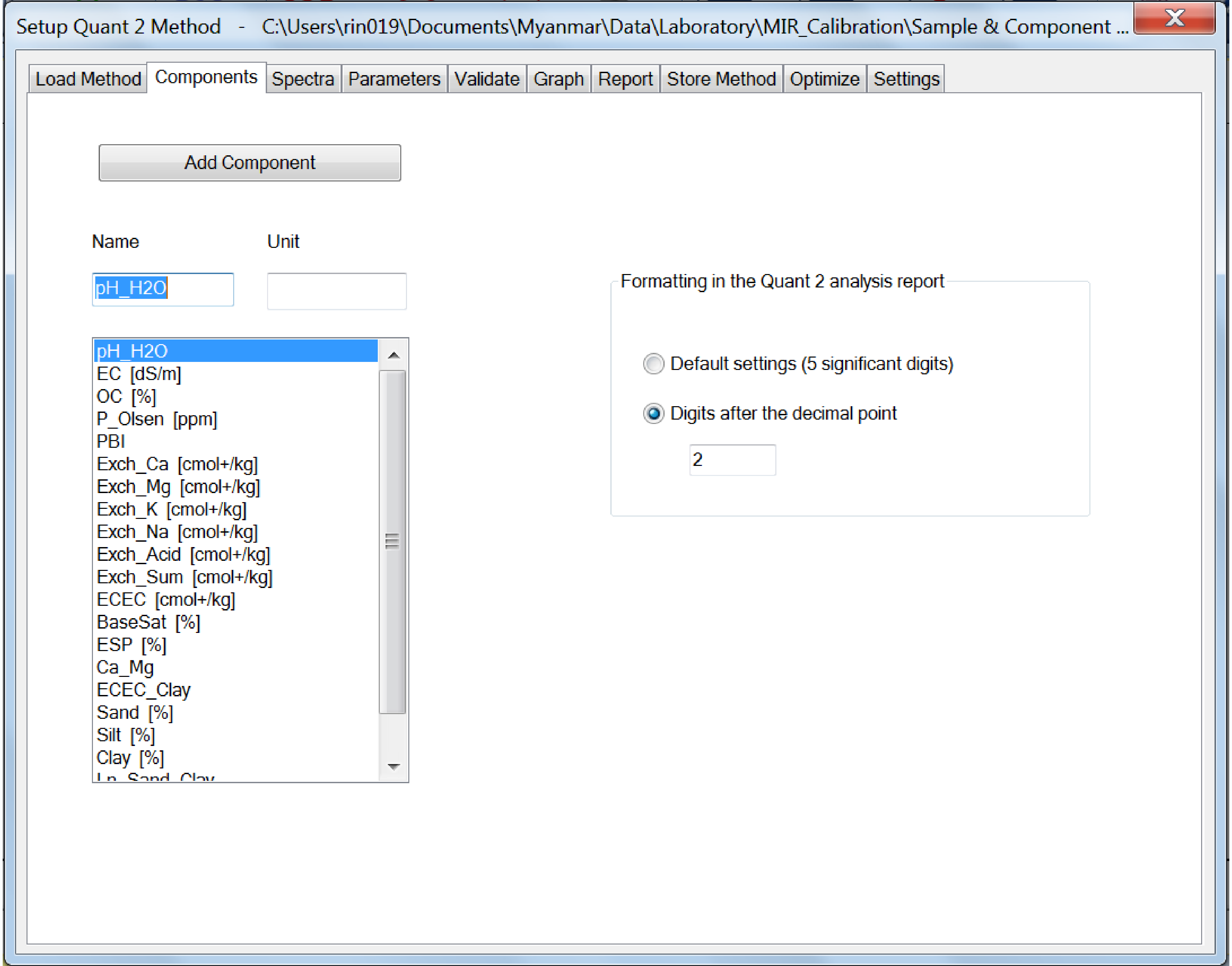
pH_H2O

Formatting in the Quant 2 analysis report

○ Default settings (5 significant digits)

4. ● Digits after the decimal point

2



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

Name: pH_H2O

Unit:

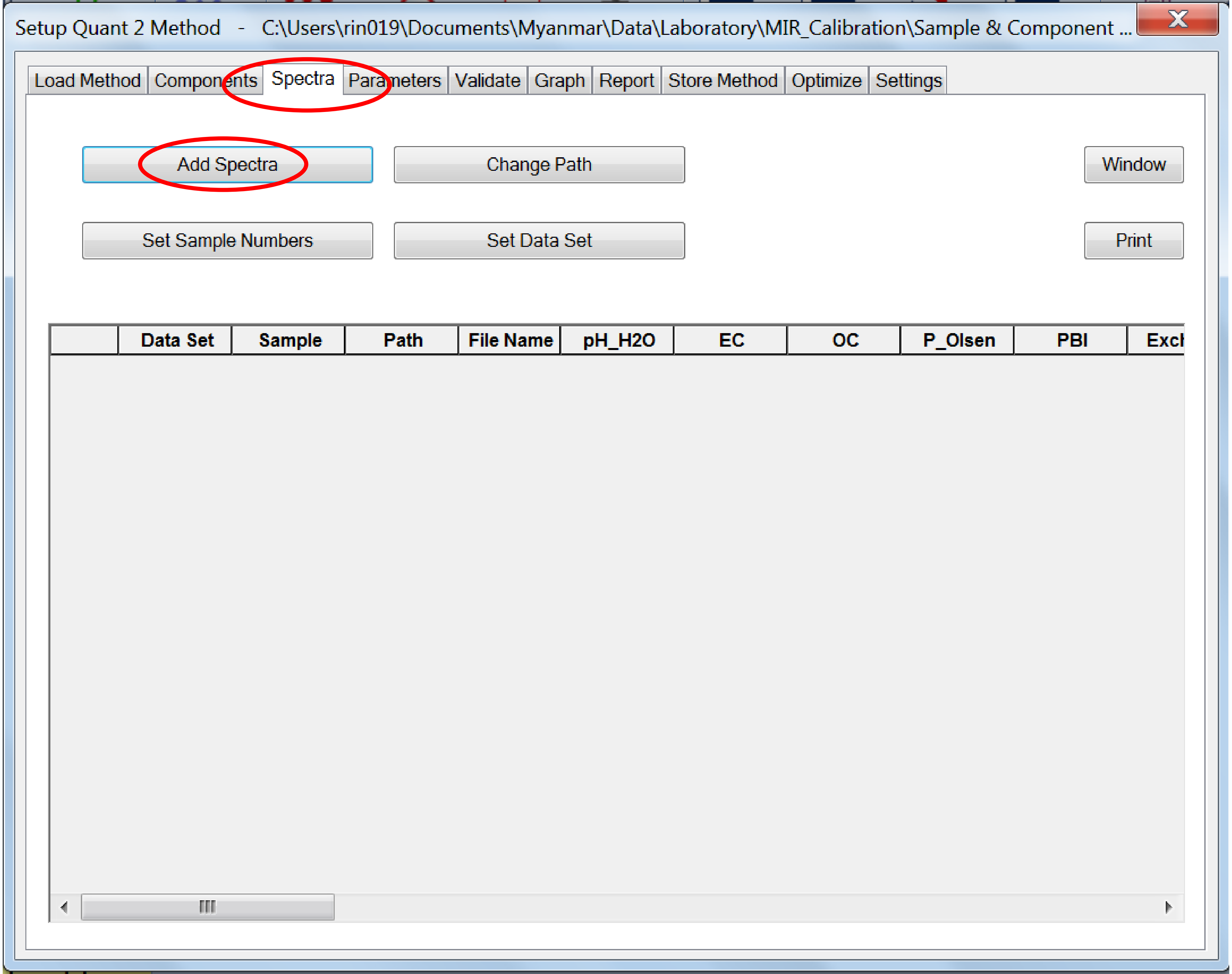
- pH_H2O
- EC [dS/m]
- OC [%]
- P_Olsen [ppm]
- PBI
- Exch_Ca [cmol+/kg]
- Exch_Mg [cmol+/kg]
- Exch_K [cmol+/kg]
- Exch_Na [cmol+/kg]
- Exch_Acid [cmol+/kg]
- Exch_Sum [cmol+/kg]
- ECEC [cmol+/kg]
- BaseSat [%]
- ESP [%]
- Ca_Mg
- ECEC_Clay
- Sand [%]
- Silt [%]
- Clay [%]

Formatting in the Quant 2 analysis report

○ Default settings (5 significant digits)

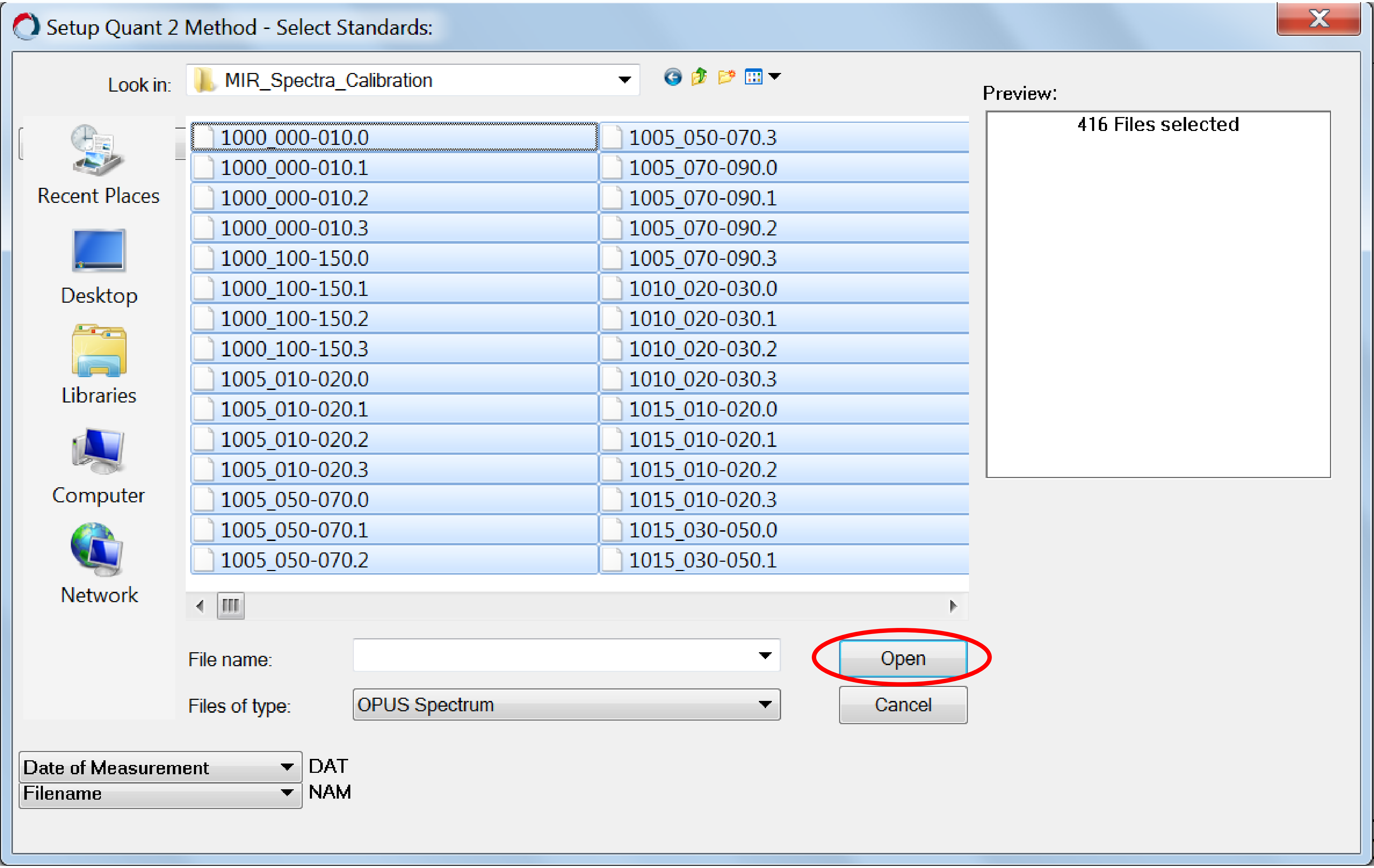
● Digits after the decimal point

2



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

	Data Set	Sample	Path	File Name	pH_H2O	EC	OC	P_Olsen	PBI	Excl



Look in: MIR_Spectra_Calibration

1000_000-010.0
1000_000-010.1
1000_000-010.2
1000_000-010.3
1000_100-150.0
1000_100-150.1
1000_100-150.2
1000_100-150.3
1005_010-020.0
1005_010-020.1
1005_010-020.2
1005_010-020.3
1005_050-070.0
1005_050-070.1
1005_050-070.2
1005_050-070.3
1005_070-090.0
1005_070-090.1
1005_070-090.2
1005_070-090.3
1010_020-030.0
1010_020-030.1
1010_020-030.2
1010_020-030.3
1015_010-020.0
1015_010-020.1
1015_010-020.2
1015_010-020.3
1015_030-050.0
1015_030-050.1

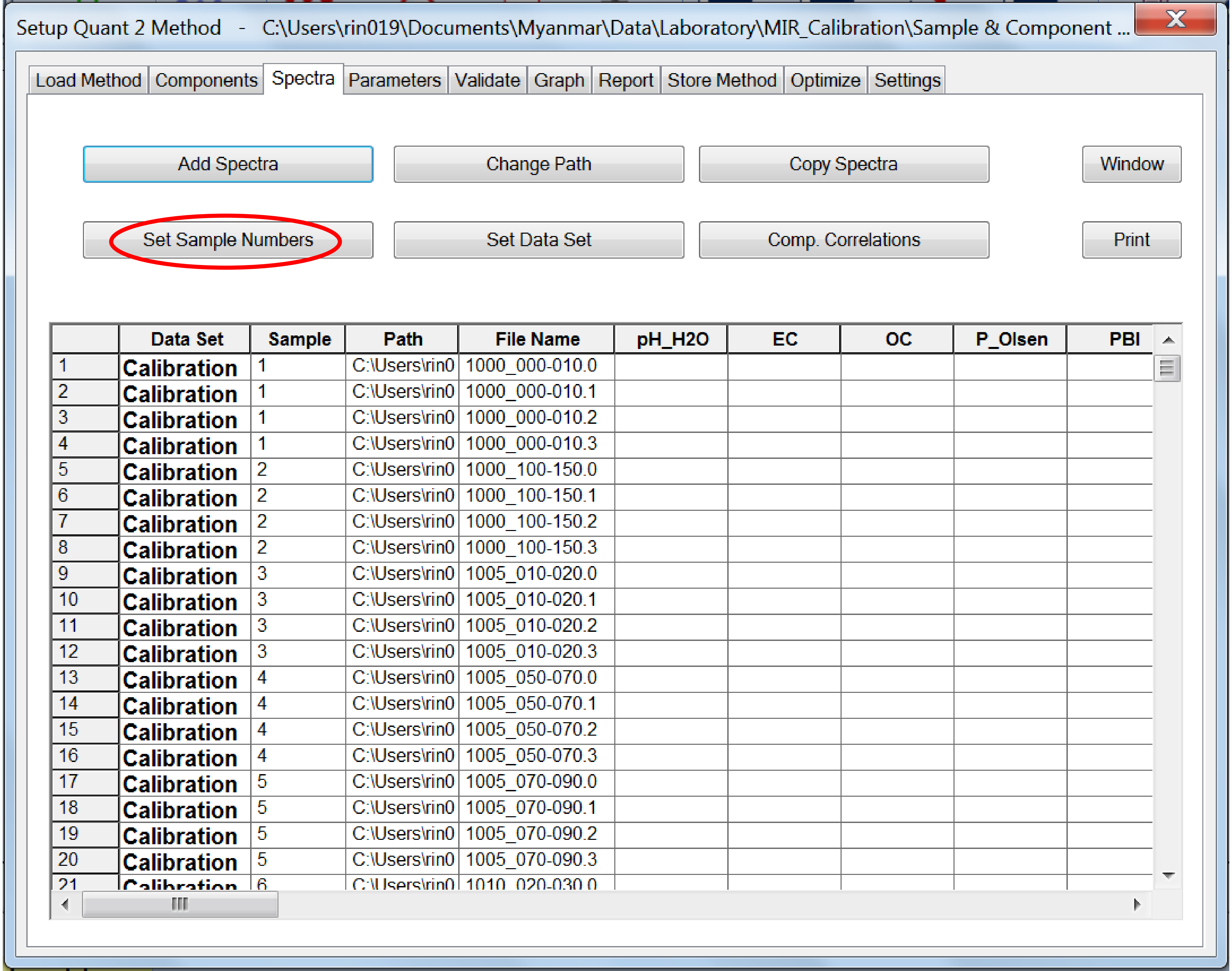
Preview: 416 Files selected

File name:

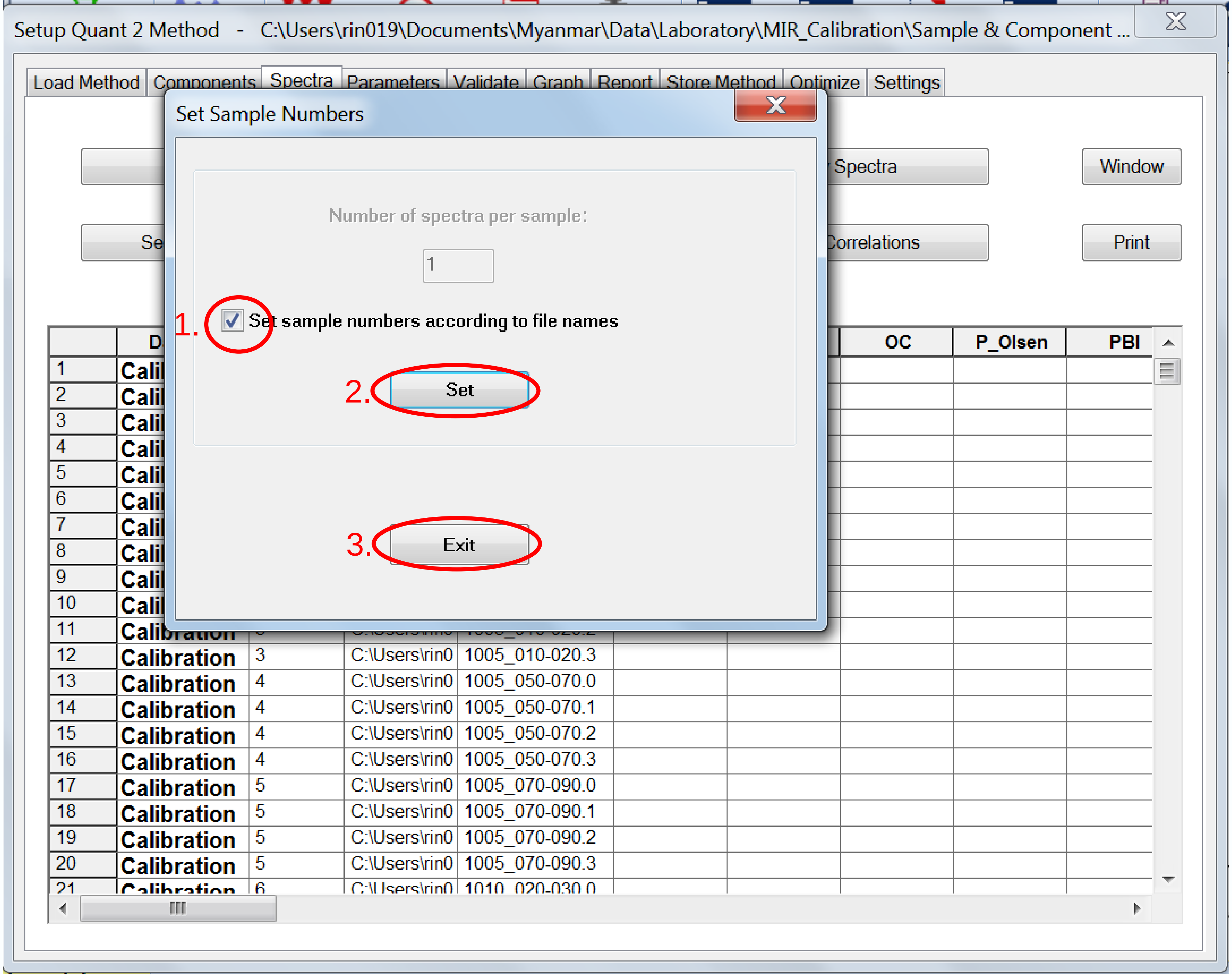
Files of type: OPUS Spectrum

Date of Measurement DAT
Filename NAM

- Hint: Click first spectra then <Ctrl A> to select all spectra in folder



	Data Set	Sample	Path	File Name	pH_H2O	EC	OC	P_Olsen	PBI
1	Calibration	1	C:\Users\rin0	1000_000-010.0					
2	Calibration	1	C:\Users\rin0	1000_000-010.1					
3	Calibration	1	C:\Users\rin0	1000_000-010.2					
4	Calibration	1	C:\Users\rin0	1000_000-010.3					
5	Calibration	2	C:\Users\rin0	1000_100-150.0					
6	Calibration	2	C:\Users\rin0	1000_100-150.1					
7	Calibration	2	C:\Users\rin0	1000_100-150.2					
8	Calibration	2	C:\Users\rin0	1000_100-150.3					
9	Calibration	3	C:\Users\rin0	1005_010-020.0					
10	Calibration	3	C:\Users\rin0	1005_010-020.1					
11	Calibration	3	C:\Users\rin0	1005_010-020.2					
12	Calibration	3	C:\Users\rin0	1005_010-020.3					
13	Calibration	4	C:\Users\rin0	1005_050-070.0					
14	Calibration	4	C:\Users\rin0	1005_050-070.1					
15	Calibration	4	C:\Users\rin0	1005_050-070.2					
16	Calibration	4	C:\Users\rin0	1005_050-070.3					
17	Calibration	5	C:\Users\rin0	1005_070-090.0					
18	Calibration	5	C:\Users\rin0	1005_070-090.1					
19	Calibration	5	C:\Users\rin0	1005_070-090.2					
20	Calibration	5	C:\Users\rin0	1005_070-090.3					
21	Calibration	6	C:\Users\rin0	1010_020-030.0					



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

Set Sample Numbers

Number of spectra per sample:

1

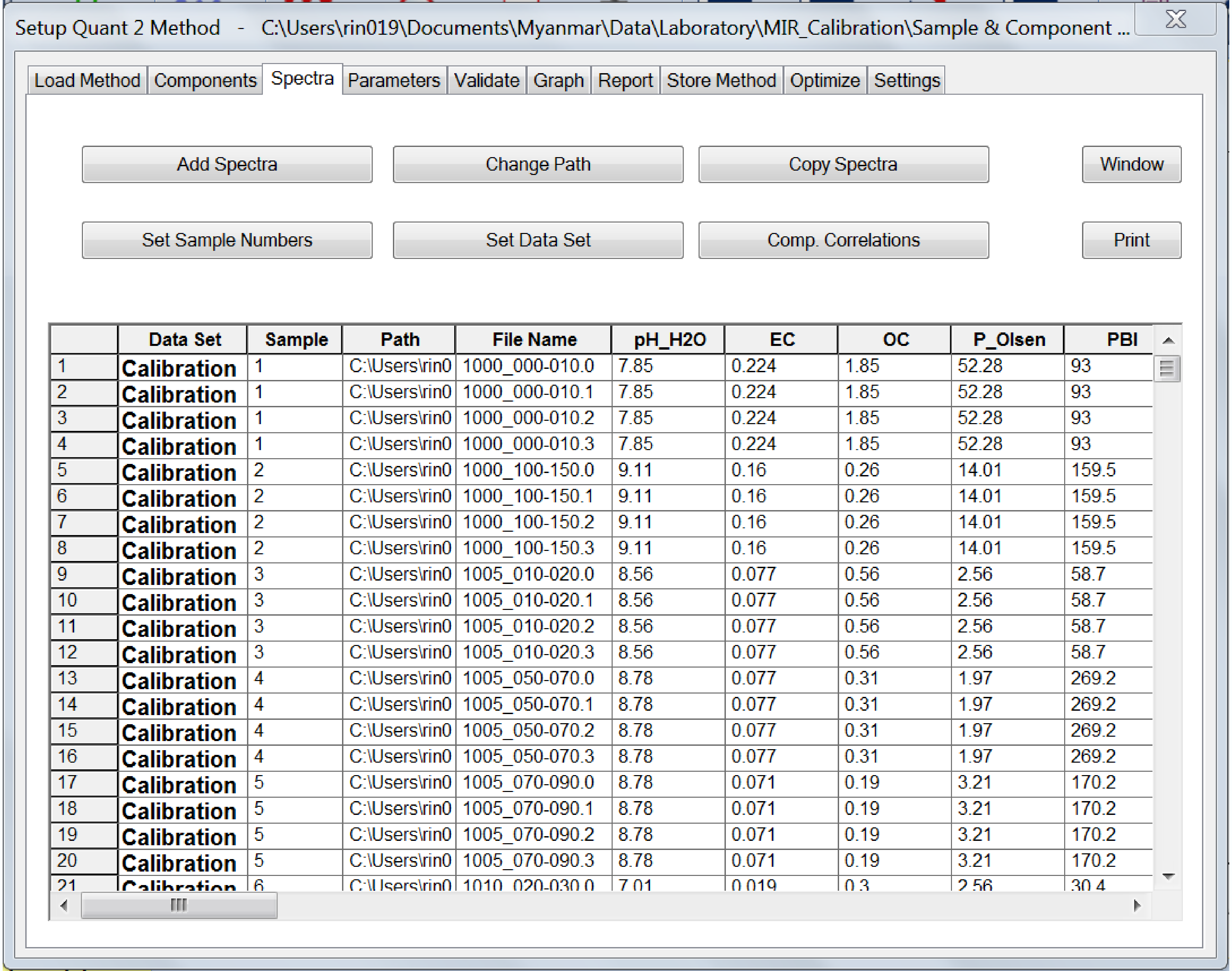
1. ☑ Set sample numbers according to file names

2. Set

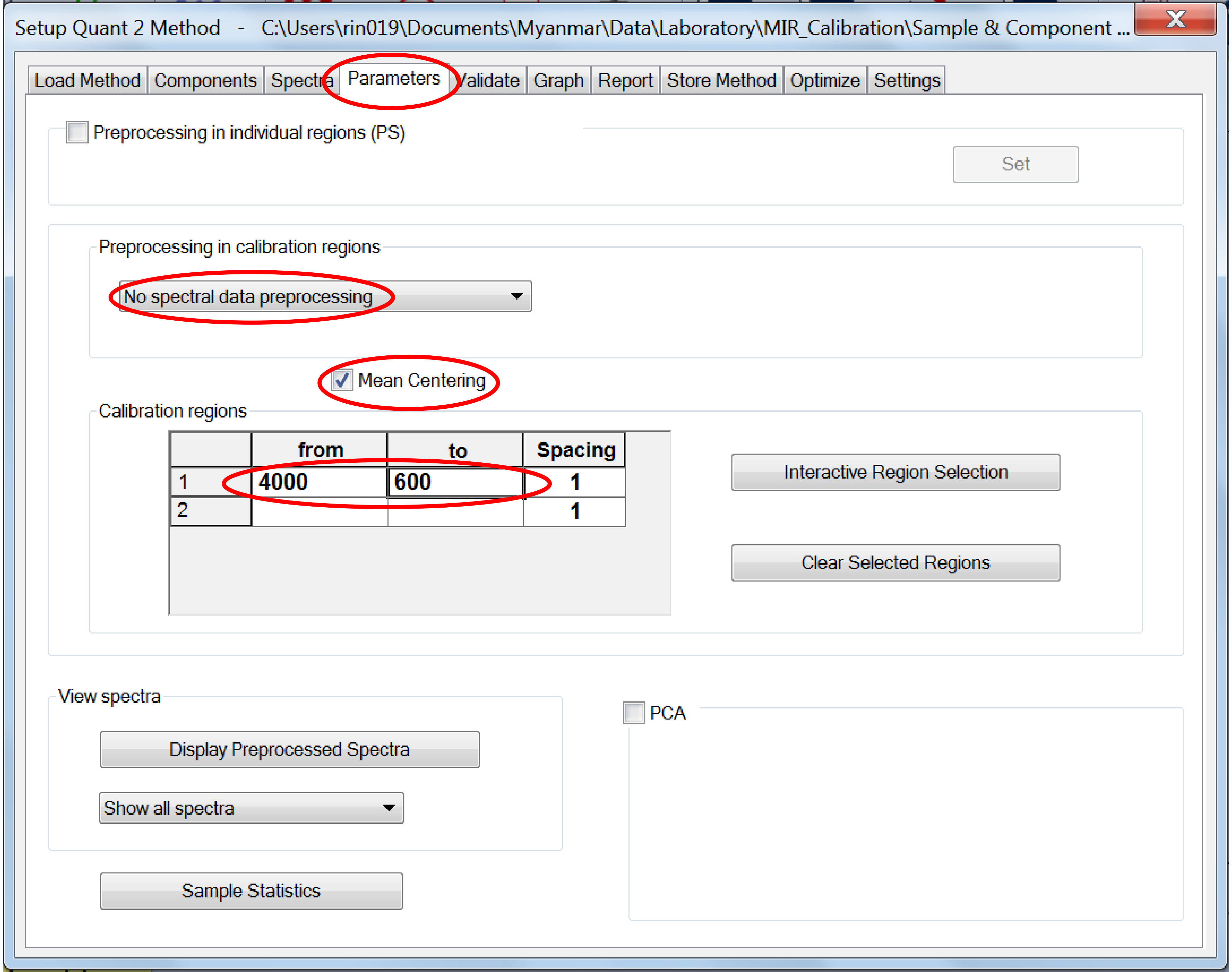
3. Exit

	D						OC	P_Olsen	PBI
1	Cali								
2	Cali								
3	Cali								
4	Cali								
5	Cali								
6	Cali								
7	Cali								
8	Cali								
9	Cali								
10	Cali								
11	Calibration								
12	Calibration	3	C:\Users\rin0	1005_010-020.3					
13	Calibration	4	C:\Users\rin0	1005_050-070.0					
14	Calibration	4	C:\Users\rin0	1005_050-070.1					
15	Calibration	4	C:\Users\rin0	1005_050-070.2					
16	Calibration	4	C:\Users\rin0	1005_050-070.3					
17	Calibration	5	C:\Users\rin0	1005_070-090.0					
18	Calibration	5	C:\Users\rin0	1005_070-090.1					
19	Calibration	5	C:\Users\rin0	1005_070-090.2					
20	Calibration	5	C:\Users\rin0	1005_070-090.3					
21	Calibration	6	C:\Users\rin0	1010_020-030.0					

- In Excel ensure that any missing values are BLANK
- Copy calibration data in Excel
- Paste into OPUS
- CHECK that the data is lined up against the correct sample names
- Check again
- And again
  - It is really important that OPUS matches the correct data with each spectrum



	Data Set	Sample	Path	File Name	pH_H2O	EC	OC	P_Olsen	PBI
1	**Calibration**	1	C:\Users\rin0	1000_000-010.0	7.85	0.224	1.85	52.28	93
2	**Calibration**	1	C:\Users\rin0	1000_000-010.1	7.85	0.224	1.85	52.28	93
3	**Calibration**	1	C:\Users\rin0	1000_000-010.2	7.85	0.224	1.85	52.28	93
4	**Calibration**	1	C:\Users\rin0	1000_000-010.3	7.85	0.224	1.85	52.28	93
5	**Calibration**	2	C:\Users\rin0	1000_100-150.0	9.11	0.16	0.26	14.01	159.5
6	**Calibration**	2	C:\Users\rin0	1000_100-150.1	9.11	0.16	0.26	14.01	159.5
7	**Calibration**	2	C:\Users\rin0	1000_100-150.2	9.11	0.16	0.26	14.01	159.5
8	**Calibration**	2	C:\Users\rin0	1000_100-150.3	9.11	0.16	0.26	14.01	159.5
9	**Calibration**	3	C:\Users\rin0	1005_010-020.0	8.56	0.077	0.56	2.56	58.7
10	**Calibration**	3	C:\Users\rin0	1005_010-020.1	8.56	0.077	0.56	2.56	58.7
11	**Calibration**	3	C:\Users\rin0	1005_010-020.2	8.56	0.077	0.56	2.56	58.7
12	**Calibration**	3	C:\Users\rin0	1005_010-020.3	8.56	0.077	0.56	2.56	58.7
13	**Calibration**	4	C:\Users\rin0	1005_050-070.0	8.78	0.077	0.31	1.97	269.2
14	**Calibration**	4	C:\Users\rin0	1005_050-070.1	8.78	0.077	0.31	1.97	269.2
15	**Calibration**	4	C:\Users\rin0	1005_050-070.2	8.78	0.077	0.31	1.97	269.2
16	**Calibration**	4	C:\Users\rin0	1005_050-070.3	8.78	0.077	0.31	1.97	269.2
17	**Calibration**	5	C:\Users\rin0	1005_070-090.0	8.78	0.071	0.19	3.21	170.2
18	**Calibration**	5	C:\Users\rin0	1005_070-090.1	8.78	0.071	0.19	3.21	170.2
19	**Calibration**	5	C:\Users\rin0	1005_070-090.2	8.78	0.071	0.19	3.21	170.2
20	**Calibration**	5	C:\Users\rin0	1005_070-090.3	8.78	0.071	0.19	3.21	170.2
21	**Calibration**	6	C:\Users\rin0	1010_020-030.0	7.01	0.019	0.3	2.56	30.4



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

☐ Preprocessing in individual regions (PS)

Preprocessing in calibration regions

No spectral data preprocessing

☑ Mean Centering

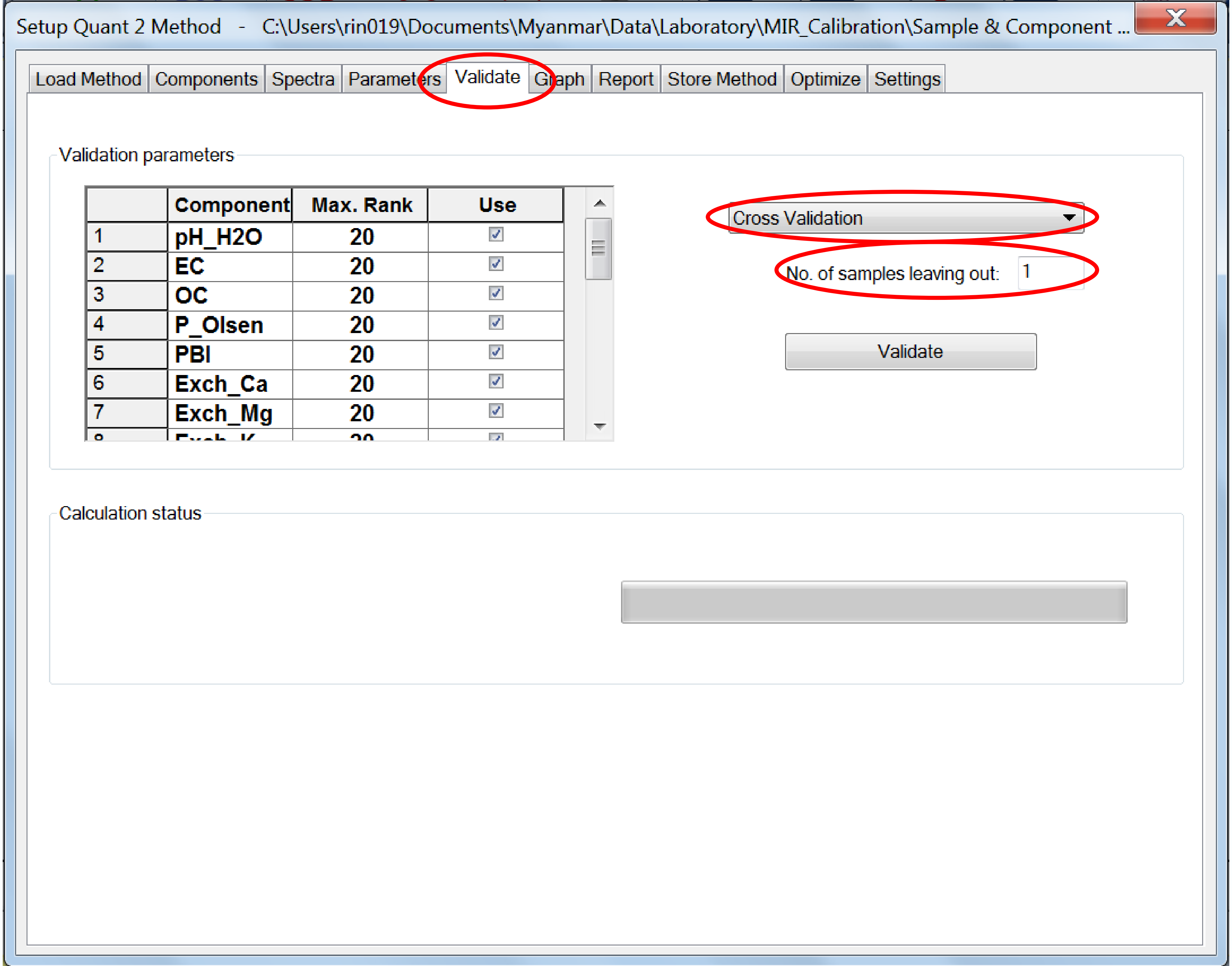
Calibration regions

	from	to	Spacing
1	4000	600	1
2			1

View spectra

Show all spectra

☐ PCA



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

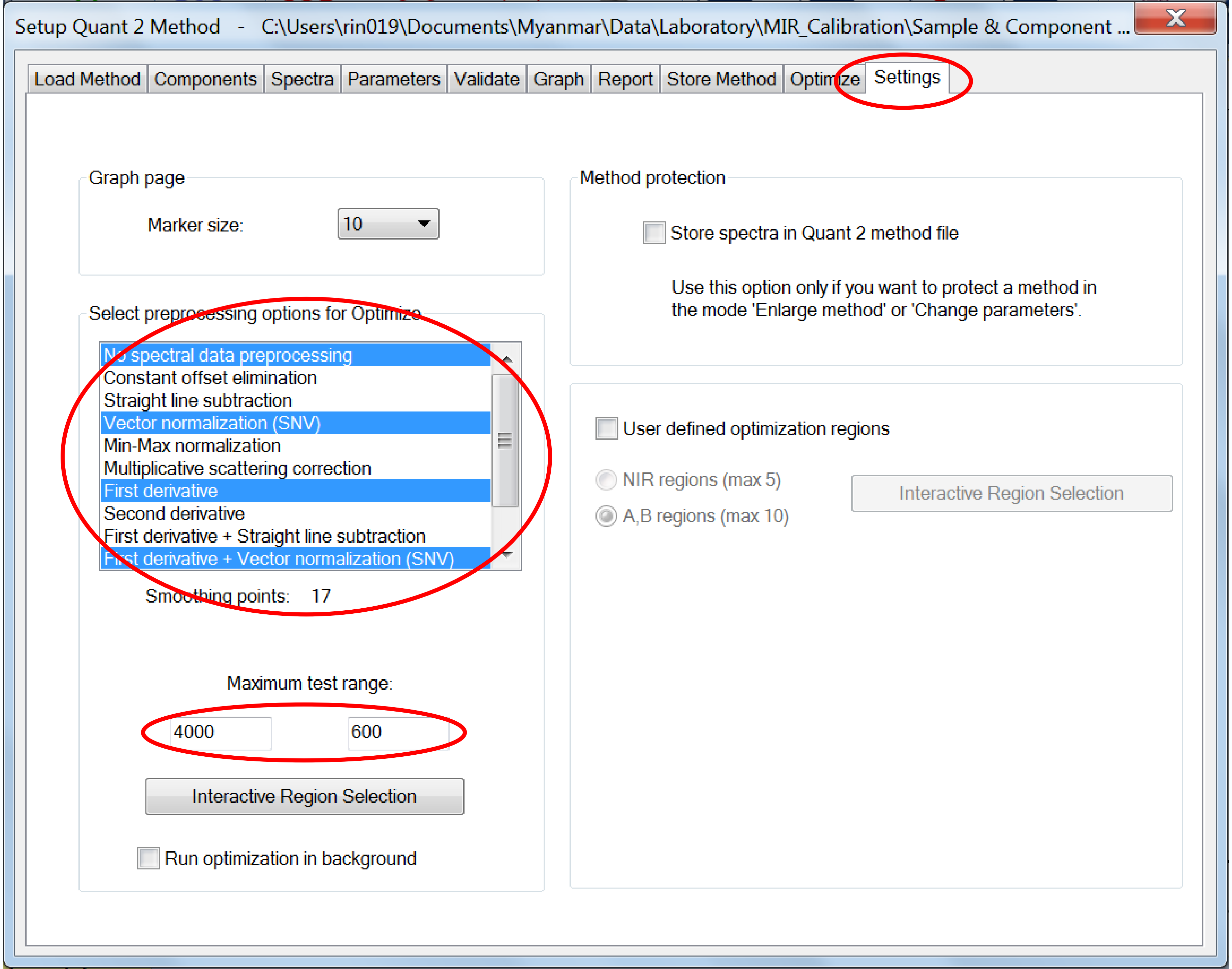
Validation parameters

	Component	Max. Rank	Use
1	pH_H2O	20	☑
2	EC	20	☑
3	OC	20	☑
4	P_Olsen	20	☑
5	PBI	20	☑
6	Exch_Ca	20	☑
7	Exch_Mg	20	☑
8	Exch_K	20	☑

Cross Validation

No. of samples leaving out: 1

Calculation status



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

Graph page

Marker size: 10

Select preprocessing options for Optimize

- No spectral data preprocessing
- Constant offset elimination
- Straight line subtraction
- Vector normalization (SNV)
- Min-Max normalization
- Multiplicative scattering correction
- First derivative
- Second derivative
- First derivative + Straight line subtraction
- First derivative + Vector normalization (SNV)

Smoothing points: 17

Maximum test range: 4000 600

☐ Run optimization in background

Method protection

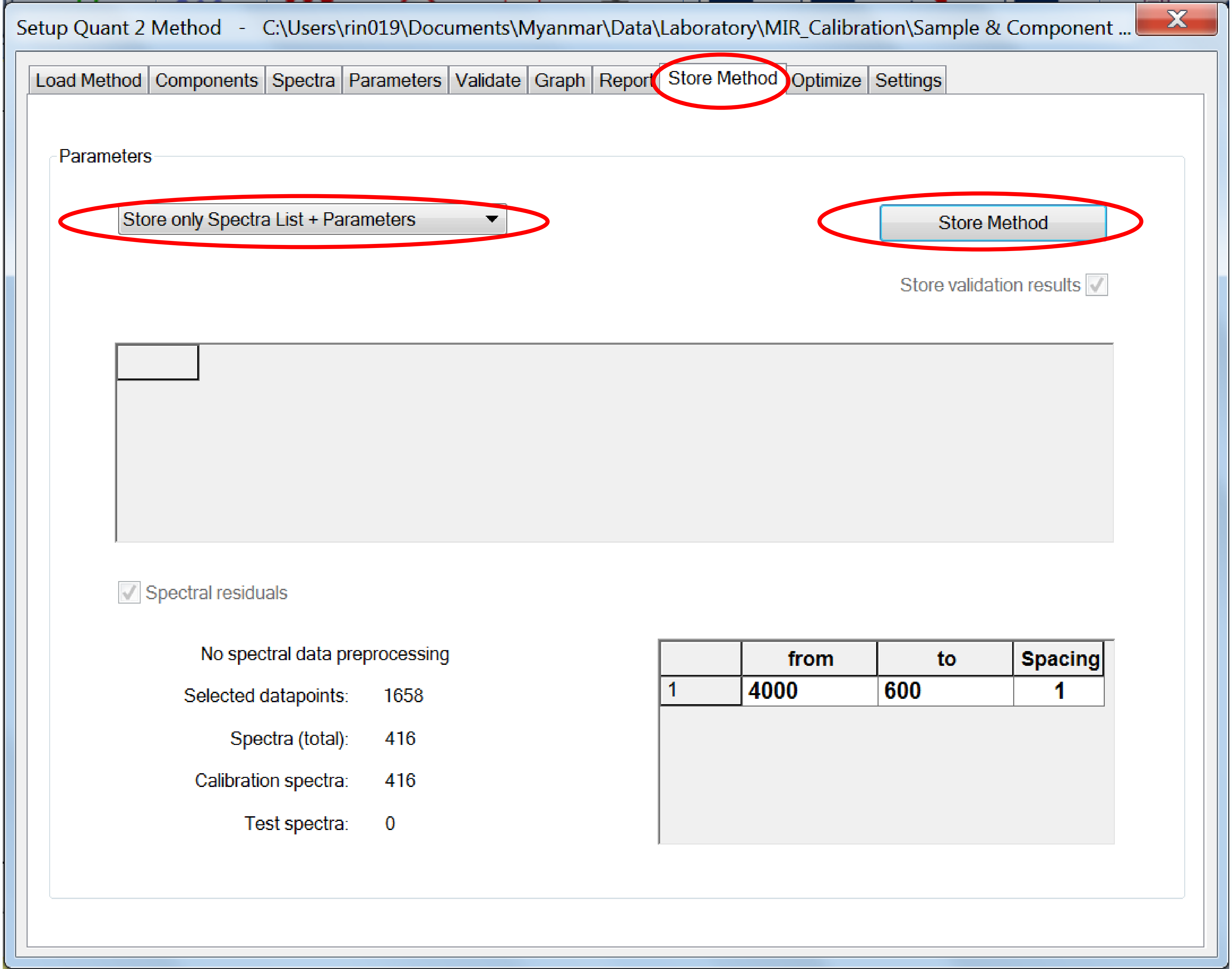
☐ Store spectra in Quant 2 method file

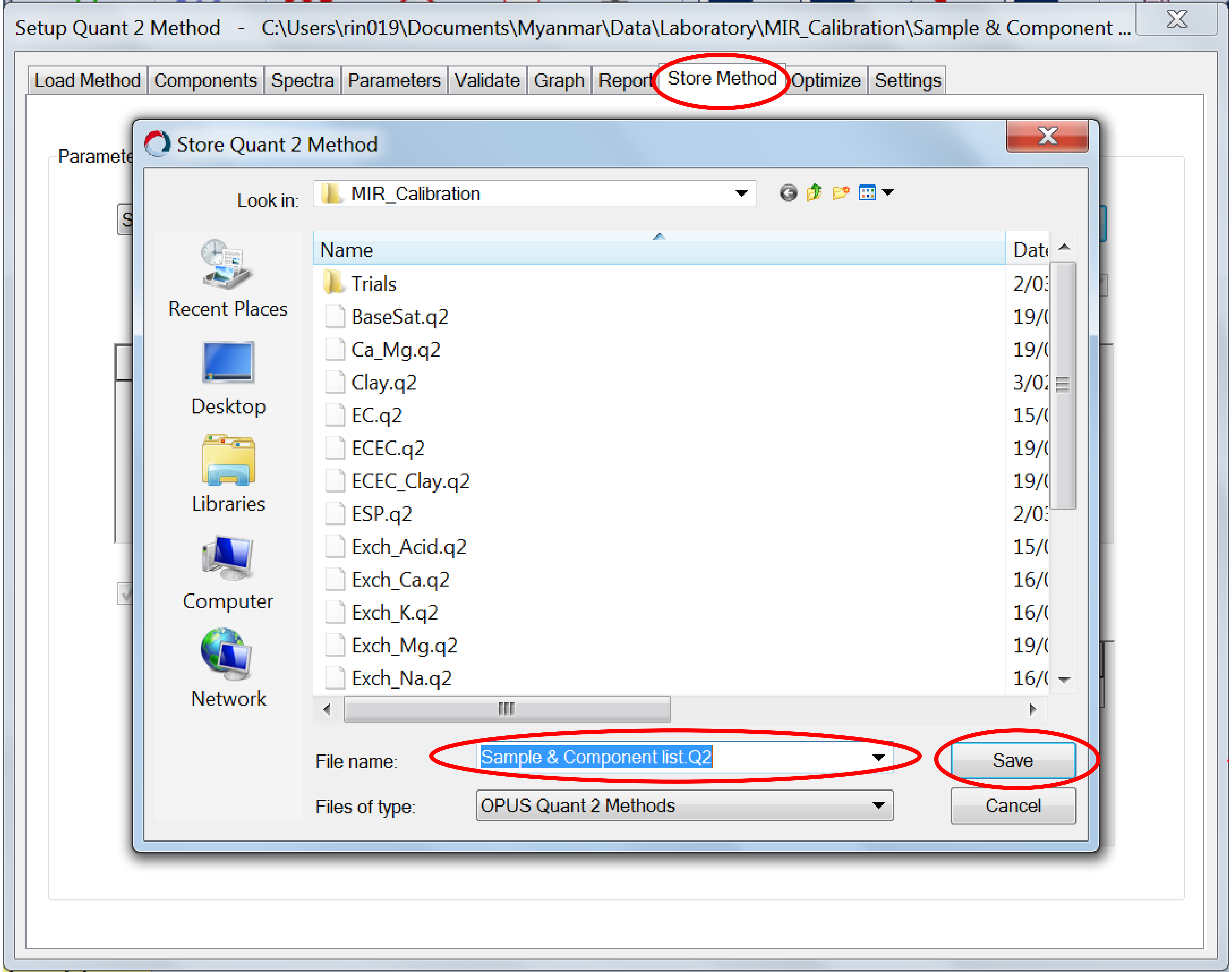
Use this option only if you want to protect a method in the mode 'Enlarge method' or 'Change parameters'.

☐ User defined optimization regions

○ NIR regions (max 5)

● A,B regions (max 10)



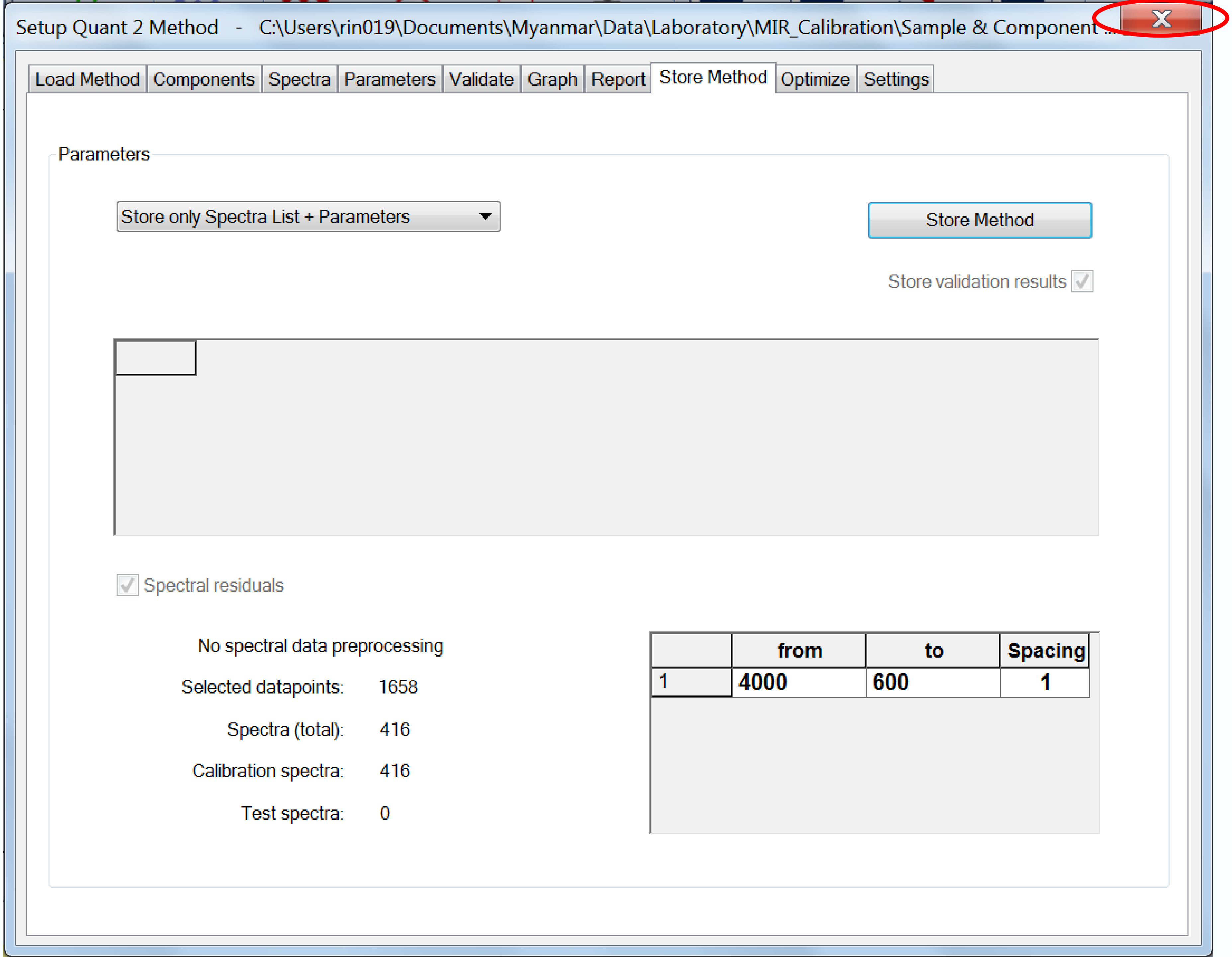


Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

Look in: MIR_Calibration

File name: Sample & Component list.Q2

Files of type: OPUS Quant 2 Methods



Store only Spectra List + Parameters

Store validation results ☑

☑ Spectral residuals

No spectral data preprocessing

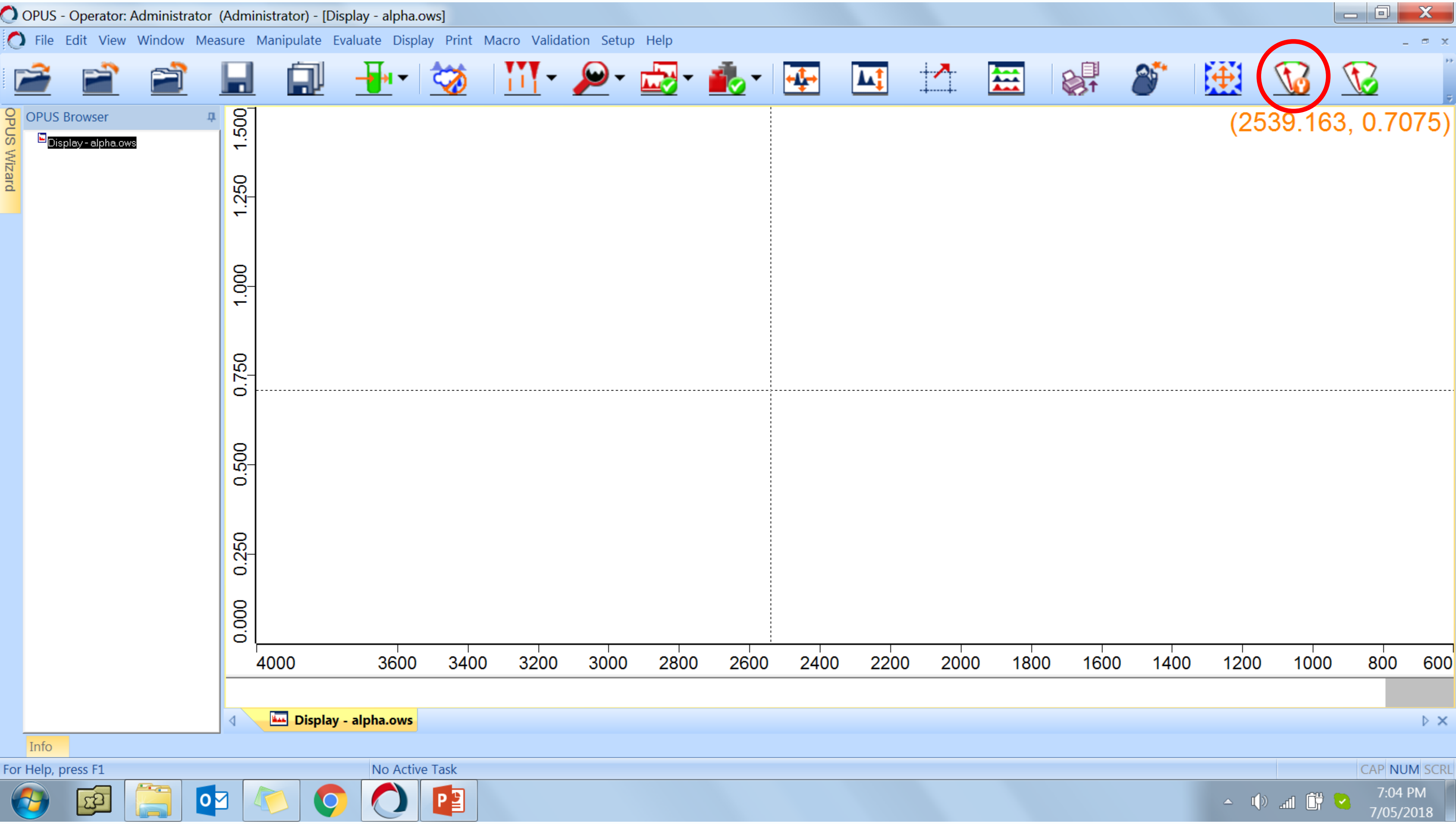
Selected datapoints:	1658
Spectra (total):	416
Calibration spectra:	416
Test spectra:	0

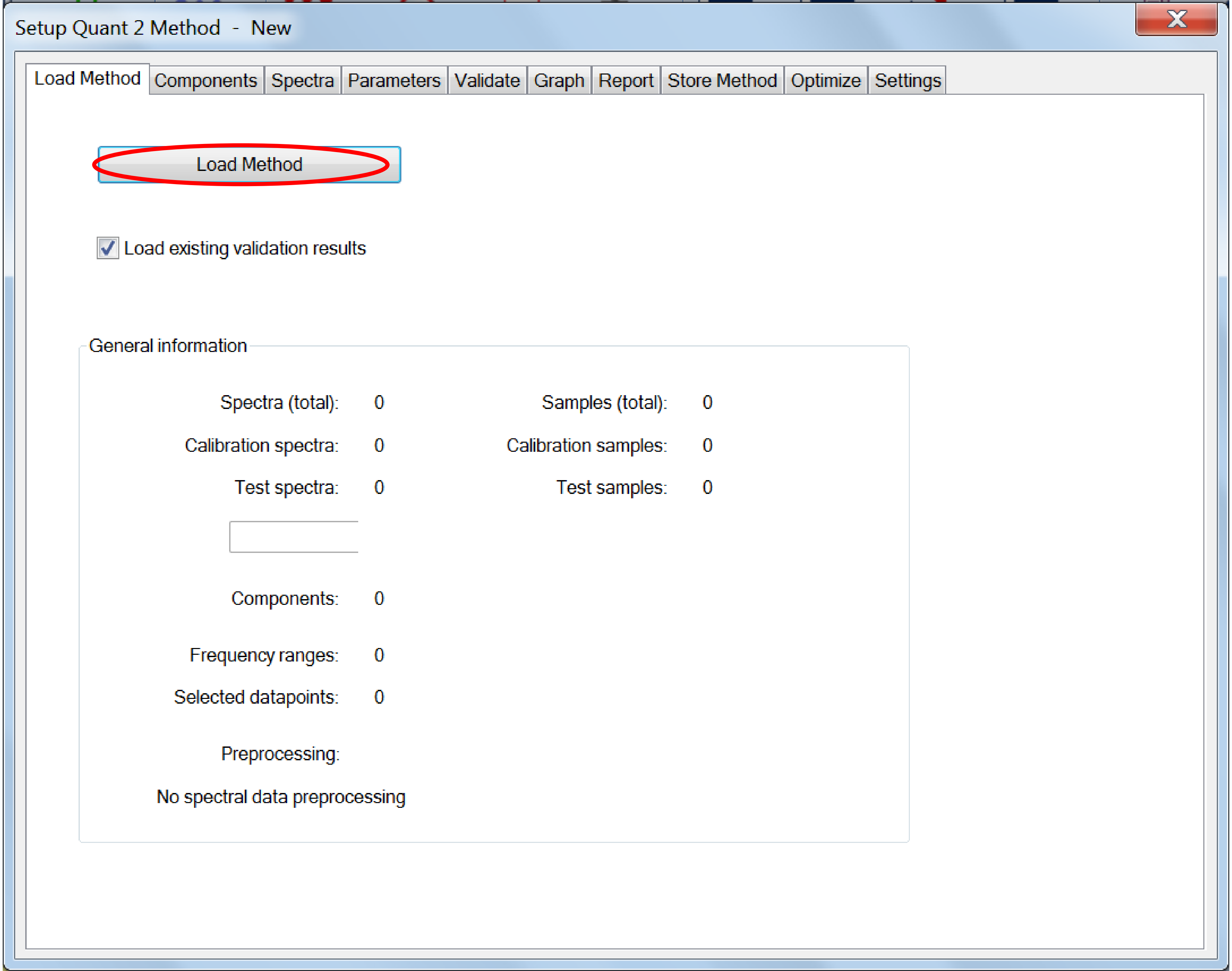
	from	to	Spacing
1	4000	600	1

- This completes setting up the calibration template

Calibrate each soil property in turn

In this example calibrate pH_H2O





☑ Load existing validation results

General information

Spectra (total): 0

Samples (total): 0

Calibration spectra: 0

Calibration samples: 0

Test spectra: 0

Test samples: 0

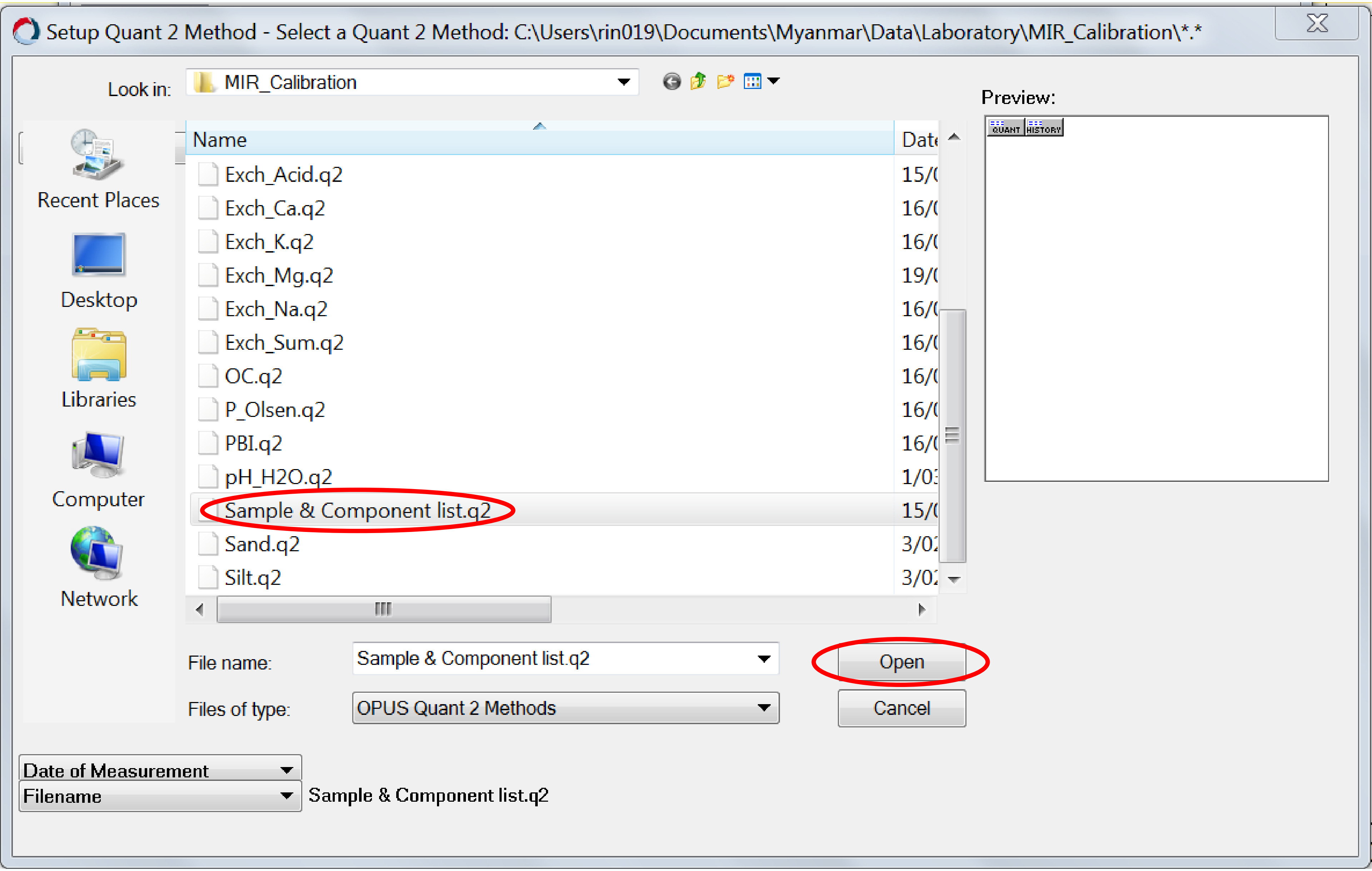
Components: 0

Frequency ranges: 0

Selected datapoints: 0

Preprocessing:

No spectral data preprocessing



Setup Quant 2 Method - Select a Quant 2 Method: C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration*.*

Look in: MIR_Calibration

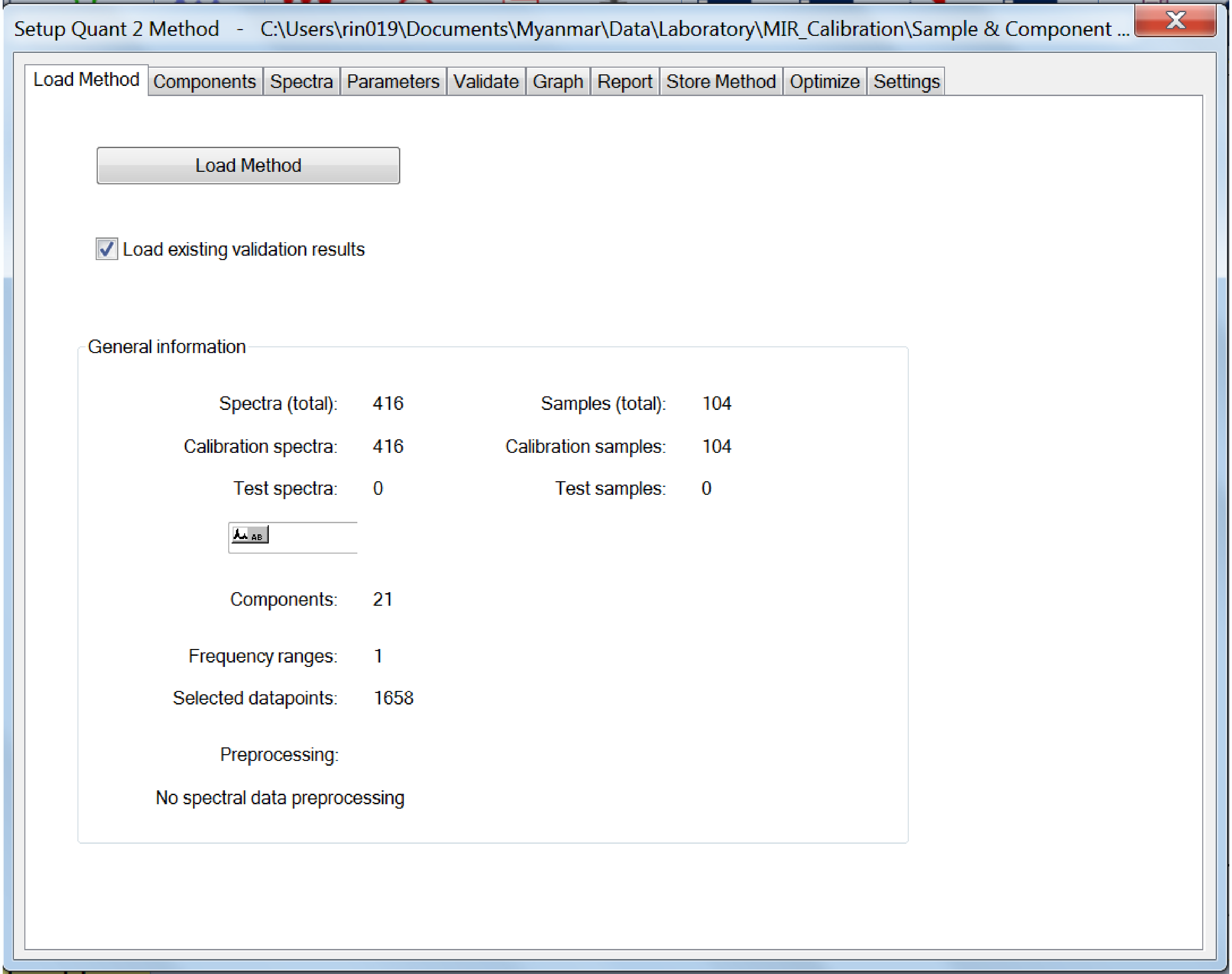
Name	Dat
Exch_Acid.q2	15/
Exch_Ca.q2	16/
Exch_K.q2	16/
Exch_Mg.q2	19/
Exch_Na.q2	16/
Exch_Sum.q2	16/
OC.q2	16/
P_Olsen.q2	16/
PBI.q2	16/
pH_H2O.q2	1/0
Sample & Component list.q2	15/
Sand.q2	3/0
Silt.q2	3/0

File name: Sample & Component list.q2

Files of type: OPUS Quant 2 Methods

Date of Measurement

Filename: Sample & Component list.q2



☑ Load existing validation results

General information

Spectra (total): 416
Calibration spectra: 416
Test spectra: 0

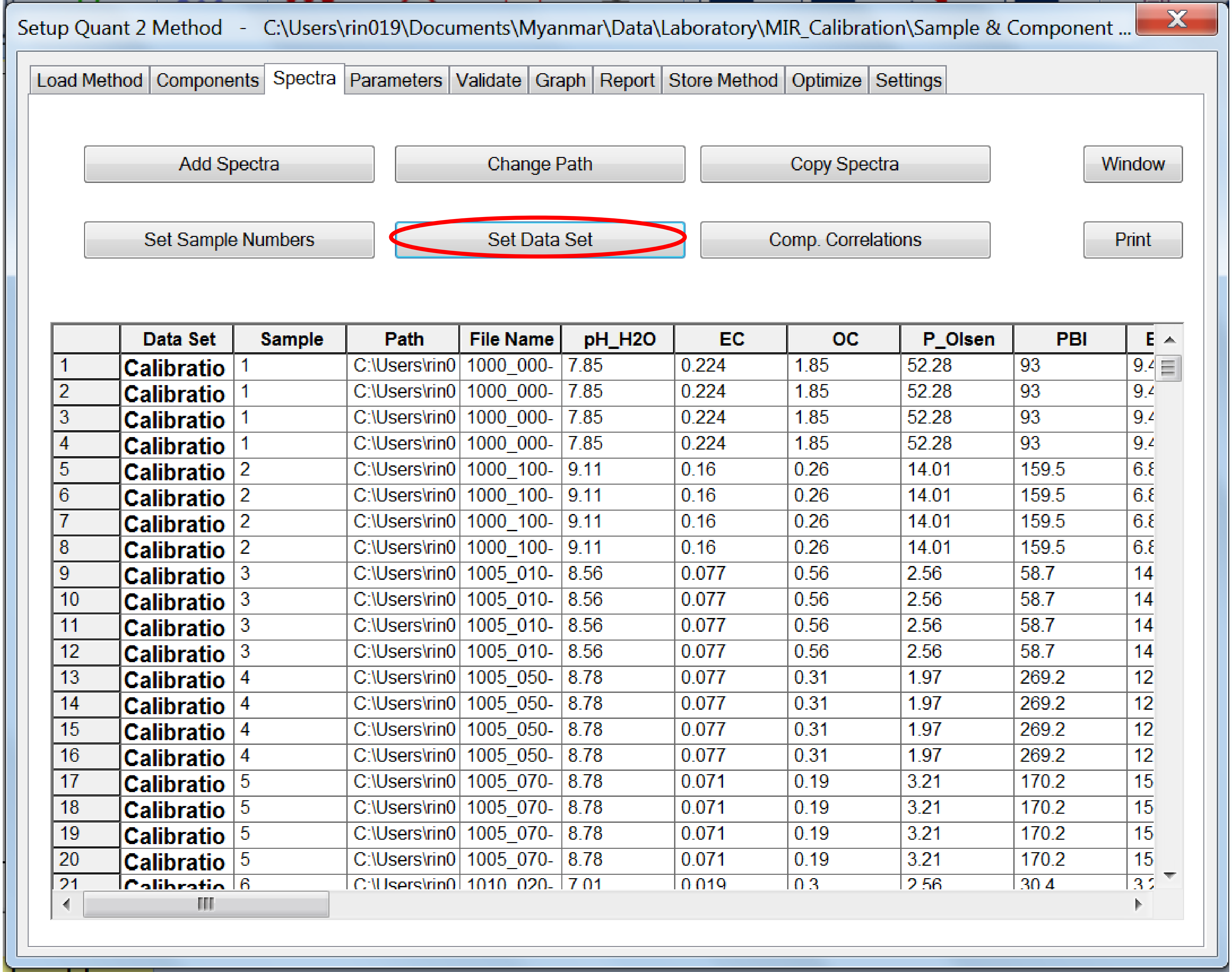
Samples (total): 104
Calibration samples: 104
Test samples: 0

Components: 21

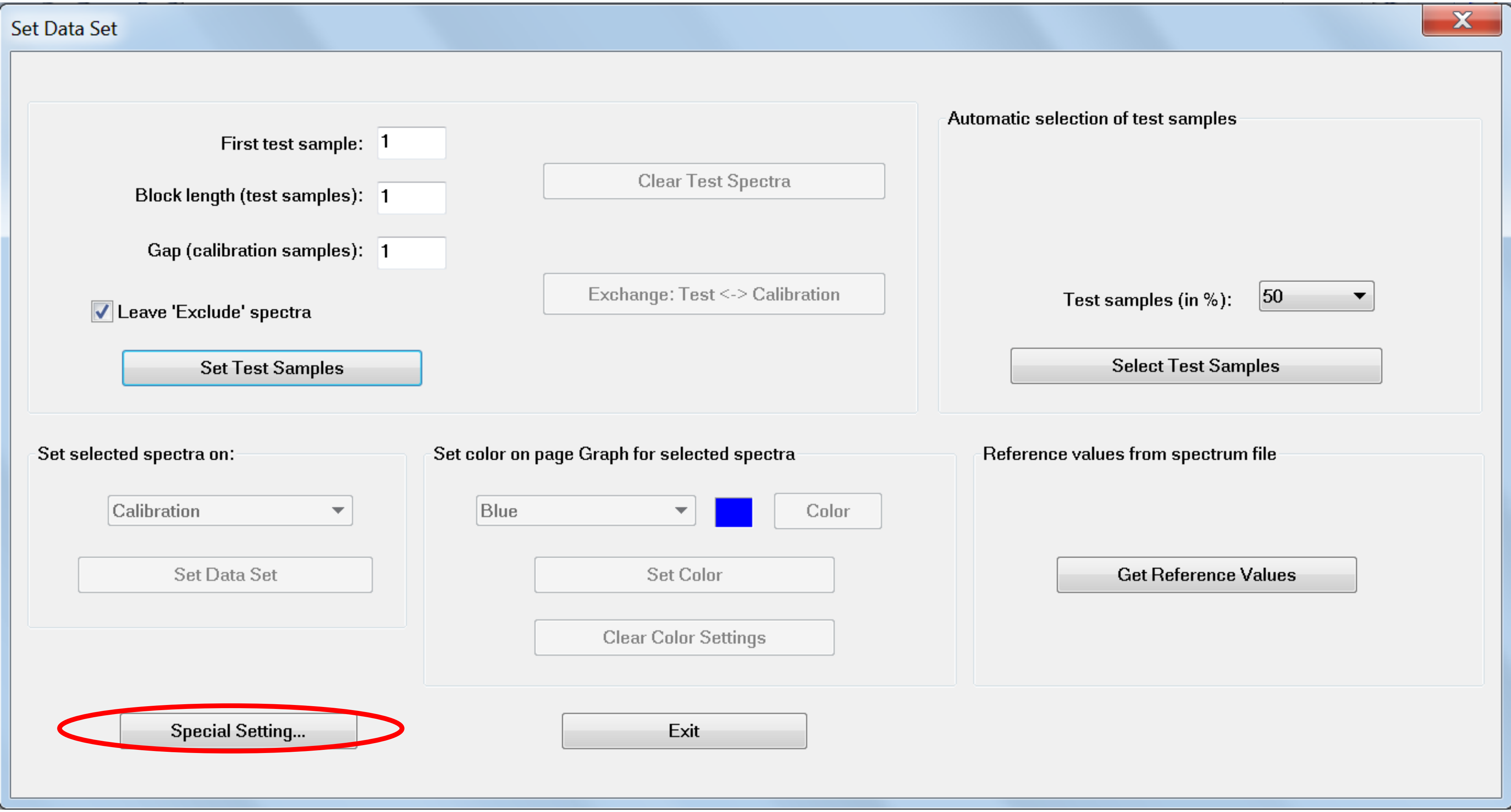
Frequency ranges: 1
Selected datapoints: 1658

Preprocessing:

No spectral data preprocessing



	Data Set	Sample	Path	File Name	pH_H2O	EC	OC	P_Olsen	PBI	E
1	**Calibratio**	1	C:\Users\rin0	1000_000-	7.85	0.224	1.85	52.28	93	9.4
2	**Calibratio**	1	C:\Users\rin0	1000_000-	7.85	0.224	1.85	52.28	93	9.4
3	**Calibratio**	1	C:\Users\rin0	1000_000-	7.85	0.224	1.85	52.28	93	9.4
4	**Calibratio**	1	C:\Users\rin0	1000_000-	7.85	0.224	1.85	52.28	93	9.4
5	**Calibratio**	2	C:\Users\rin0	1000_100-	9.11	0.16	0.26	14.01	159.5	6.8
6	**Calibratio**	2	C:\Users\rin0	1000_100-	9.11	0.16	0.26	14.01	159.5	6.8
7	**Calibratio**	2	C:\Users\rin0	1000_100-	9.11	0.16	0.26	14.01	159.5	6.8
8	**Calibratio**	2	C:\Users\rin0	1000_100-	9.11	0.16	0.26	14.01	159.5	6.8
9	**Calibratio**	3	C:\Users\rin0	1005_010-	8.56	0.077	0.56	2.56	58.7	14
10	**Calibratio**	3	C:\Users\rin0	1005_010-	8.56	0.077	0.56	2.56	58.7	14
11	**Calibratio**	3	C:\Users\rin0	1005_010-	8.56	0.077	0.56	2.56	58.7	14
12	**Calibratio**	3	C:\Users\rin0	1005_010-	8.56	0.077	0.56	2.56	58.7	14
13	**Calibratio**	4	C:\Users\rin0	1005_050-	8.78	0.077	0.31	1.97	269.2	12
14	**Calibratio**	4	C:\Users\rin0	1005_050-	8.78	0.077	0.31	1.97	269.2	12
15	**Calibratio**	4	C:\Users\rin0	1005_050-	8.78	0.077	0.31	1.97	269.2	12
16	**Calibratio**	4	C:\Users\rin0	1005_050-	8.78	0.077	0.31	1.97	269.2	12
17	**Calibratio**	5	C:\Users\rin0	1005_070-	8.78	0.071	0.19	3.21	170.2	15
18	**Calibratio**	5	C:\Users\rin0	1005_070-	8.78	0.071	0.19	3.21	170.2	15
19	**Calibratio**	5	C:\Users\rin0	1005_070-	8.78	0.071	0.19	3.21	170.2	15
20	**Calibratio**	5	C:\Users\rin0	1005_070-	8.78	0.071	0.19	3.21	170.2	15
21	**Calibratio**	6	C:\Users\rin0	1010_020-	7.01	0.019	0.3	2.56	30.4	3.2



First test sample: 1

Block length (test samples): 1

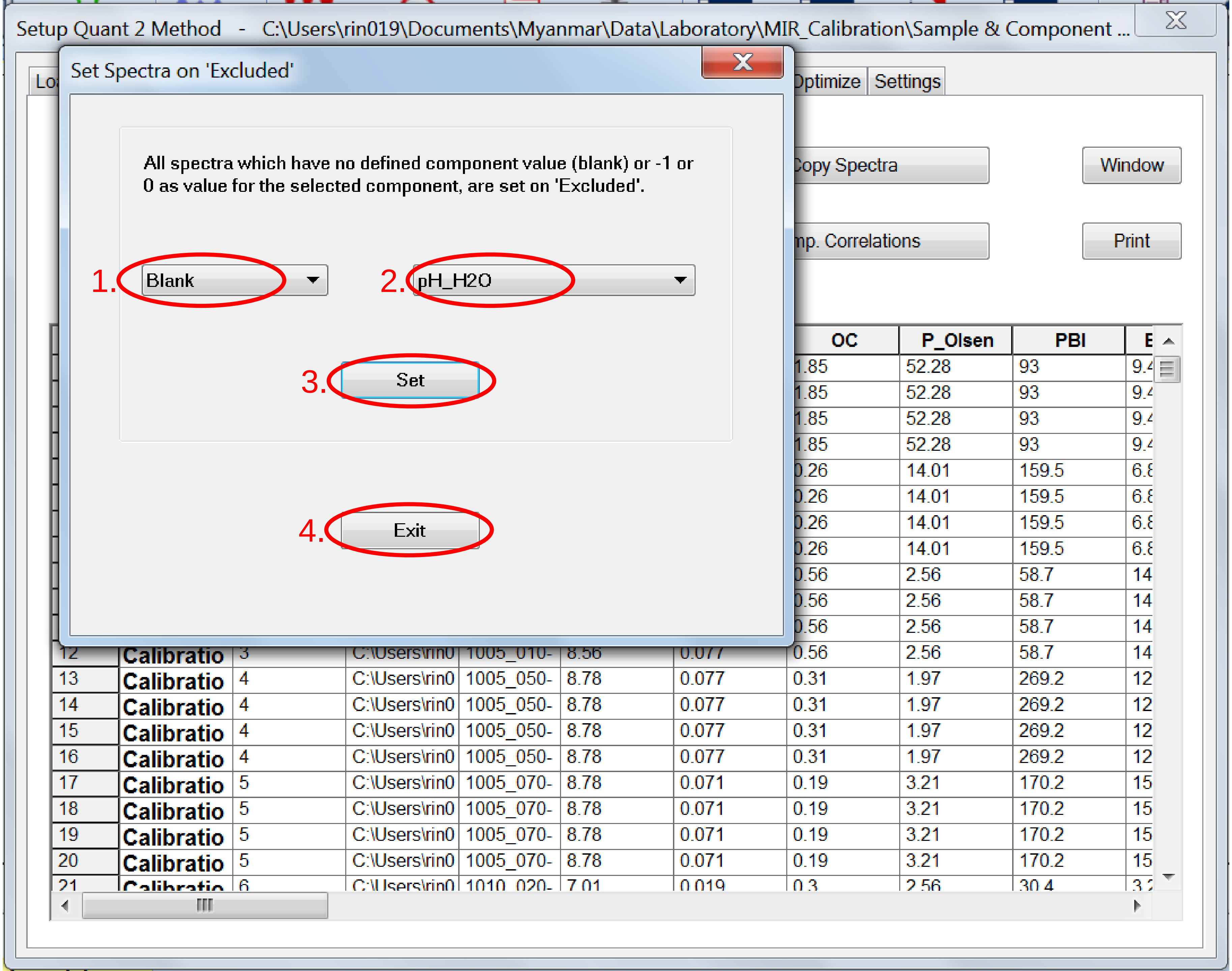
Gap (calibration samples): 1

☑ Leave 'Exclude' spectra

Test samples (in %): 50

Calibration

Blue


Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

Set Spectra on 'Excluded'

All spectra which have no defined component value (blank) or -1 or 0 as value for the selected component, are set on 'Excluded'.

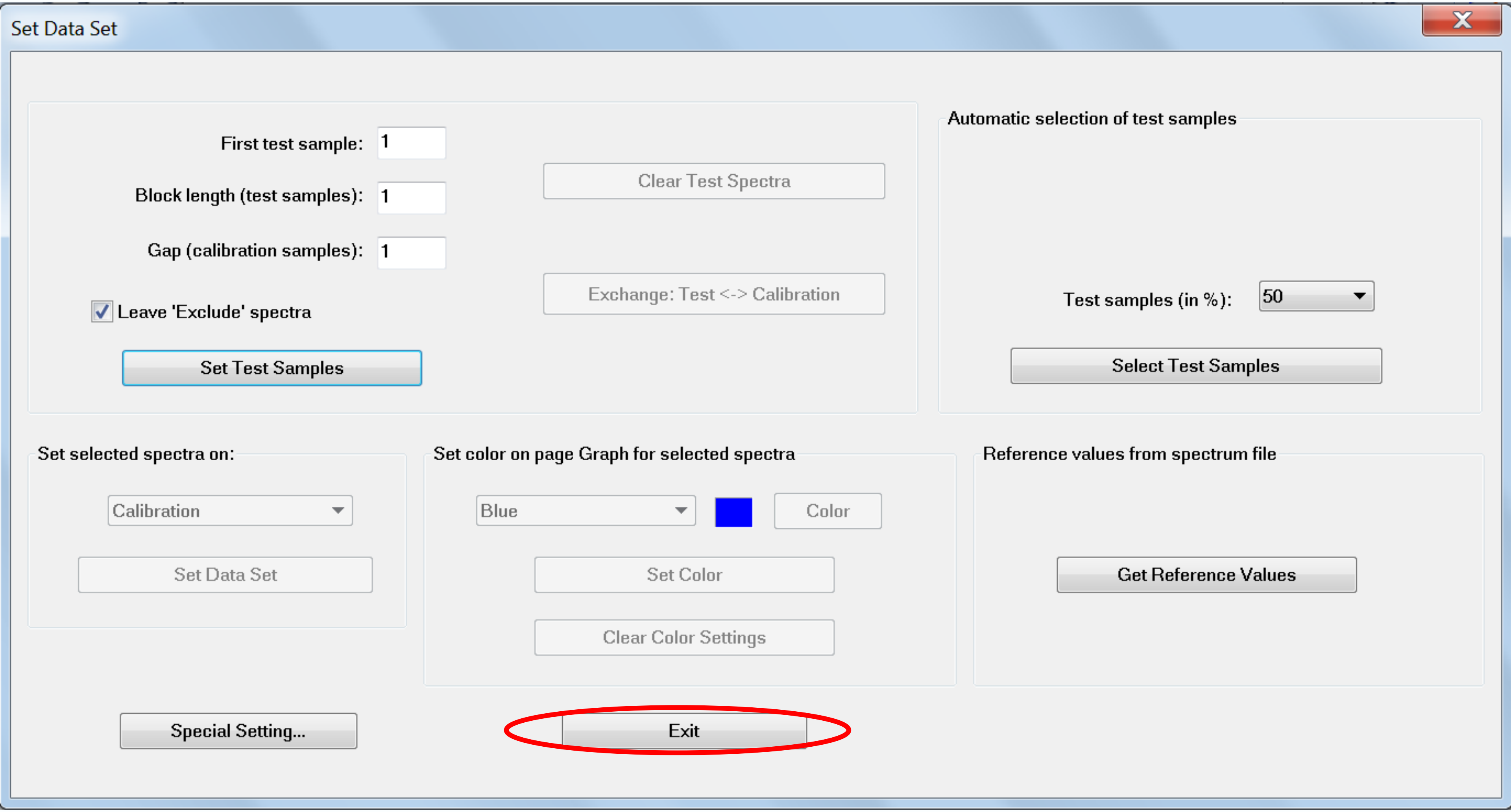
1. Blank

2. pH_H2O

3. Set

4. Exit

							OC	P_Olsen	PBI	E
							1.85	52.28	93	9.4
							1.85	52.28	93	9.4
							1.85	52.28	93	9.4
							1.85	52.28	93	9.4
							0.26	14.01	159.5	6.8
							0.26	14.01	159.5	6.8
							0.26	14.01	159.5	6.8
							0.26	14.01	159.5	6.8
							0.56	2.56	58.7	14
							0.56	2.56	58.7	14
							0.56	2.56	58.7	14
12	Calibratio	3	C:\Users\rin0	1005_010-	8.56	0.077	0.56	2.56	58.7	14
13	Calibratio	4	C:\Users\rin0	1005_050-	8.78	0.077	0.31	1.97	269.2	12
14	Calibratio	4	C:\Users\rin0	1005_050-	8.78	0.077	0.31	1.97	269.2	12
15	Calibratio	4	C:\Users\rin0	1005_050-	8.78	0.077	0.31	1.97	269.2	12
16	Calibratio	4	C:\Users\rin0	1005_050-	8.78	0.077	0.31	1.97	269.2	12
17	Calibratio	5	C:\Users\rin0	1005_070-	8.78	0.071	0.19	3.21	170.2	15
18	Calibratio	5	C:\Users\rin0	1005_070-	8.78	0.071	0.19	3.21	170.2	15
19	Calibratio	5	C:\Users\rin0	1005_070-	8.78	0.071	0.19	3.21	170.2	15
20	Calibratio	5	C:\Users\rin0	1005_070-	8.78	0.071	0.19	3.21	170.2	15
21	Calibratio	6	C:\Users\rin0	1010_020-	7.01	0.019	0.3	2.56	30.4	3.2



Set Data Set

First test sample: 1

Block length (test samples): 1

Gap (calibration samples): 1

☑ Leave 'Exclude' spectra

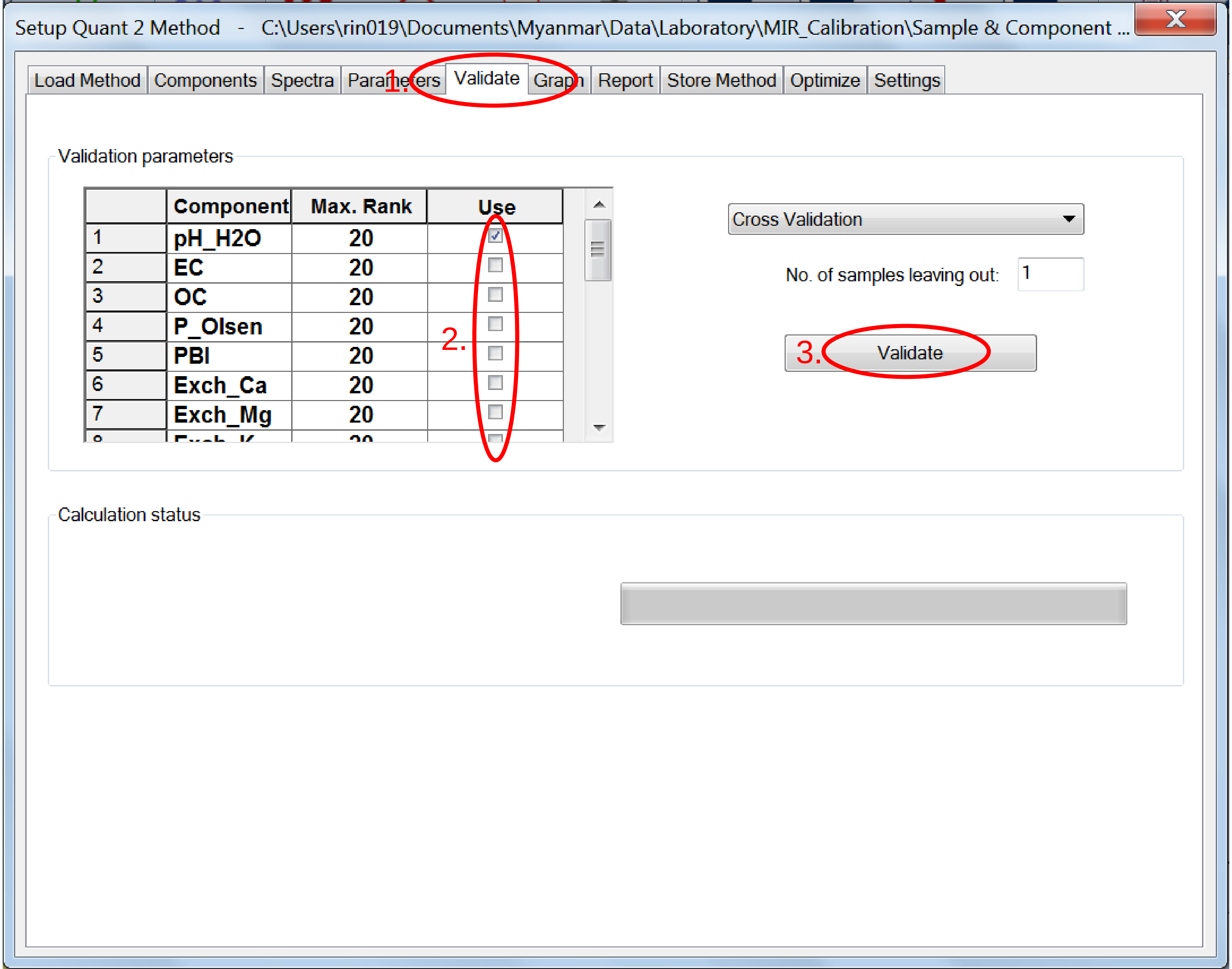
Automatic selection of test samples

Test samples (in %): 50

Set selected spectra on: Calibration

Set color on page Graph for selected spectra: Blue

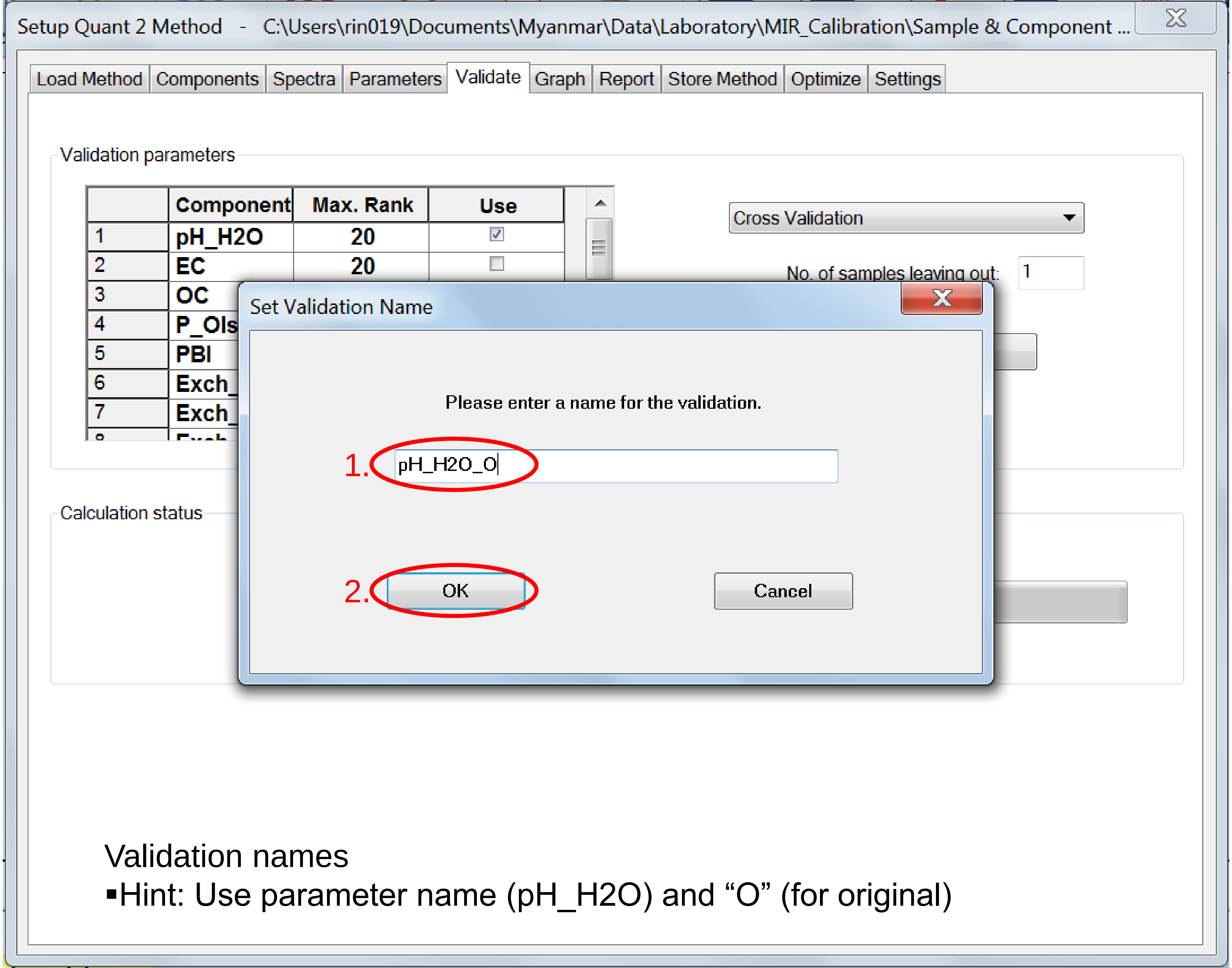
Reference values from spectrum file



	Component	Max. Rank	Use
1	pH_H2O	20	☑
2	EC	20	☐
3	OC	20	☐
4	P_Olsen	20	☐
5	PBI	20	☐
6	Exch_Ca	20	☐
7	Exch_Mg	20	☐
8	Exch_K	20	☐

Cross Validation

No. of samples leaving out: 1



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

Validation parameters

	Component	Max. Rank	Use
1	pH_H2O	20	☑
2	EC	20	☐
3	OC		
4	P_Ols		
5	PBI		
6	Exch_		
7	Exch_		

Cross Validation

No. of samples leaving out: 1

Calculation status

Set Validation Name

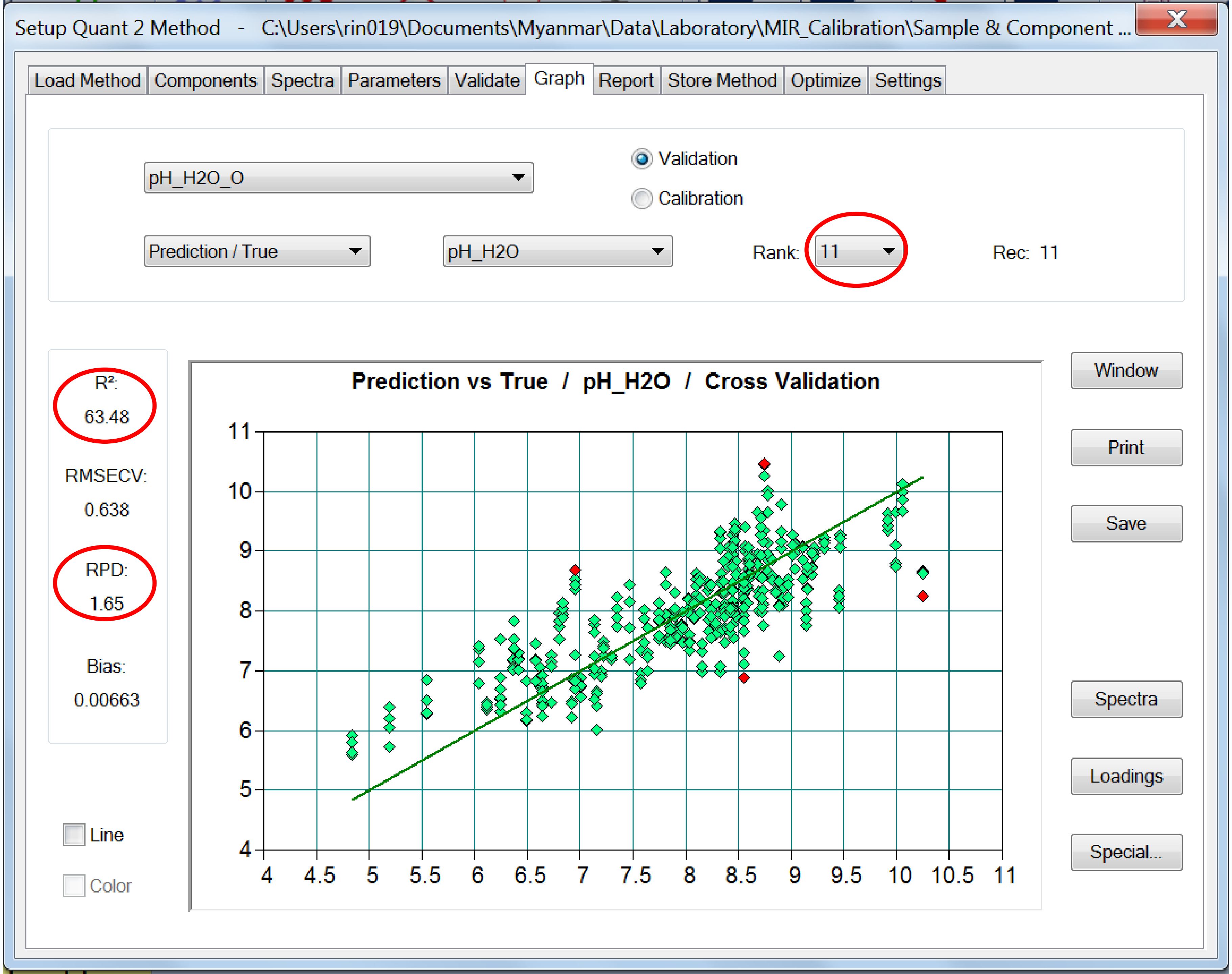
Please enter a name for the validation.

1. pH_H2O_O

2. OK

Validation names

- Hint: Use parameter name (pH_H2O) and “O” (for original)



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

pH_H2O_O

● Validation

○ Calibration

Prediction / True

pH_H2O

Rank: 11

Rec: 11

R²: 63.48

RMSECV: 0.638

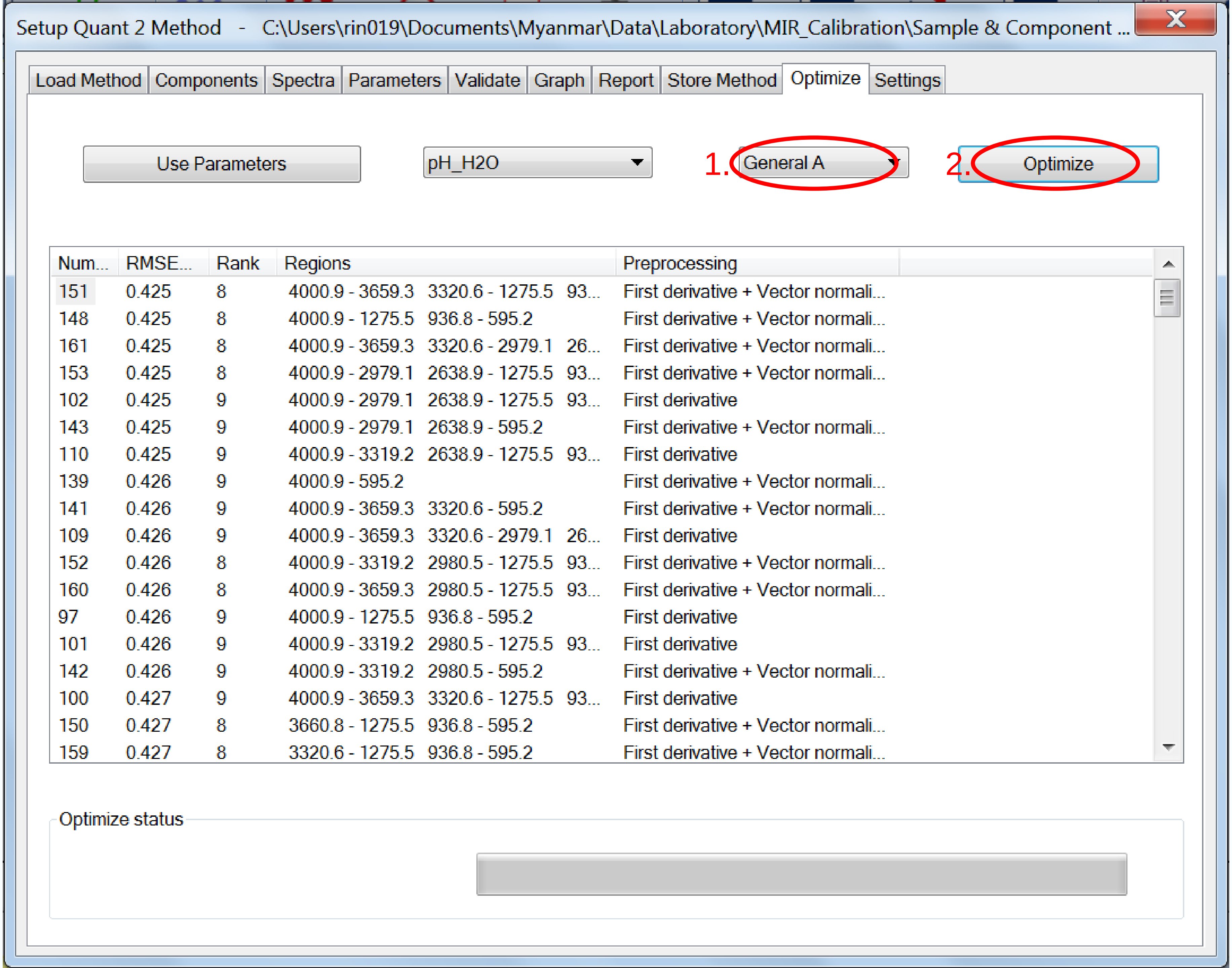
RPD: 1.65

Bias: 0.00663

☐ Line

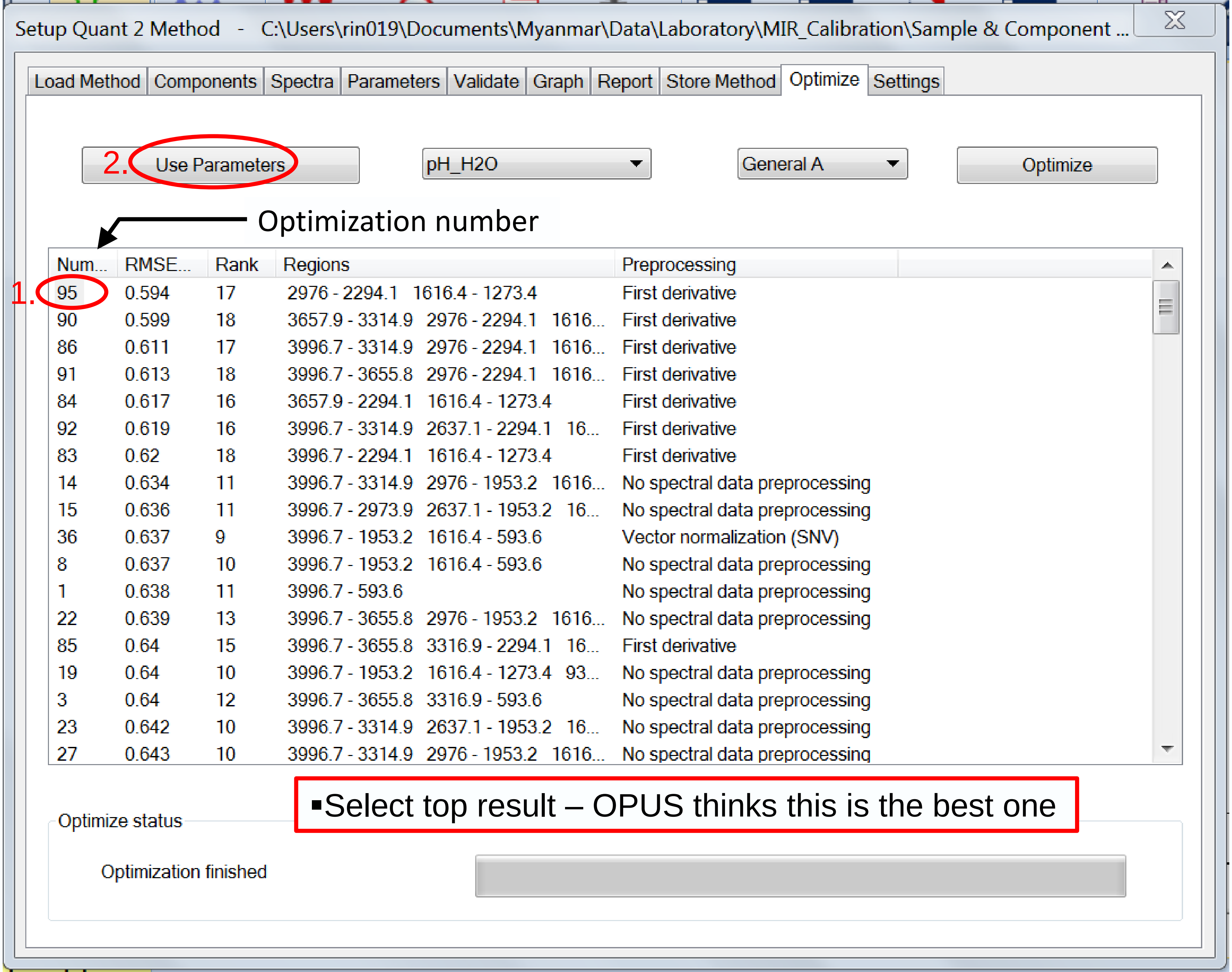
☐ Color

- Next optimize the calibration



Num...	RMSE...	Rank	Regions	Preprocessing
151	0.425	8	4000.9 - 3659.3 3320.6 - 1275.5 93...	First derivative + Vector normali...
148	0.425	8	4000.9 - 1275.5 936.8 - 595.2	First derivative + Vector normali...
161	0.425	8	4000.9 - 3659.3 3320.6 - 2979.1 26...	First derivative + Vector normali...
153	0.425	8	4000.9 - 2979.1 2638.9 - 1275.5 93...	First derivative + Vector normali...
102	0.425	9	4000.9 - 2979.1 2638.9 - 1275.5 93...	First derivative
143	0.425	9	4000.9 - 2979.1 2638.9 - 595.2	First derivative + Vector normali...
110	0.425	9	4000.9 - 3319.2 2638.9 - 1275.5 93...	First derivative
139	0.426	9	4000.9 - 595.2	First derivative + Vector normali...
141	0.426	9	4000.9 - 3659.3 3320.6 - 595.2	First derivative + Vector normali...
109	0.426	9	4000.9 - 3659.3 3320.6 - 2979.1 26...	First derivative
152	0.426	8	4000.9 - 3319.2 2980.5 - 1275.5 93...	First derivative + Vector normali...
160	0.426	8	4000.9 - 3659.3 2980.5 - 1275.5 93...	First derivative + Vector normali...
97	0.426	9	4000.9 - 1275.5 936.8 - 595.2	First derivative
101	0.426	9	4000.9 - 3319.2 2980.5 - 1275.5 93...	First derivative
142	0.426	9	4000.9 - 3319.2 2980.5 - 595.2	First derivative + Vector normali...
100	0.427	9	4000.9 - 3659.3 3320.6 - 1275.5 93...	First derivative
150	0.427	8	3660.8 - 1275.5 936.8 - 595.2	First derivative + Vector normali...
159	0.427	8	3320.6 - 1275.5 936.8 - 595.2	First derivative + Vector normali...

- Now wait a long time (sometimes hours)



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

2. Use Parameters

Optimization number

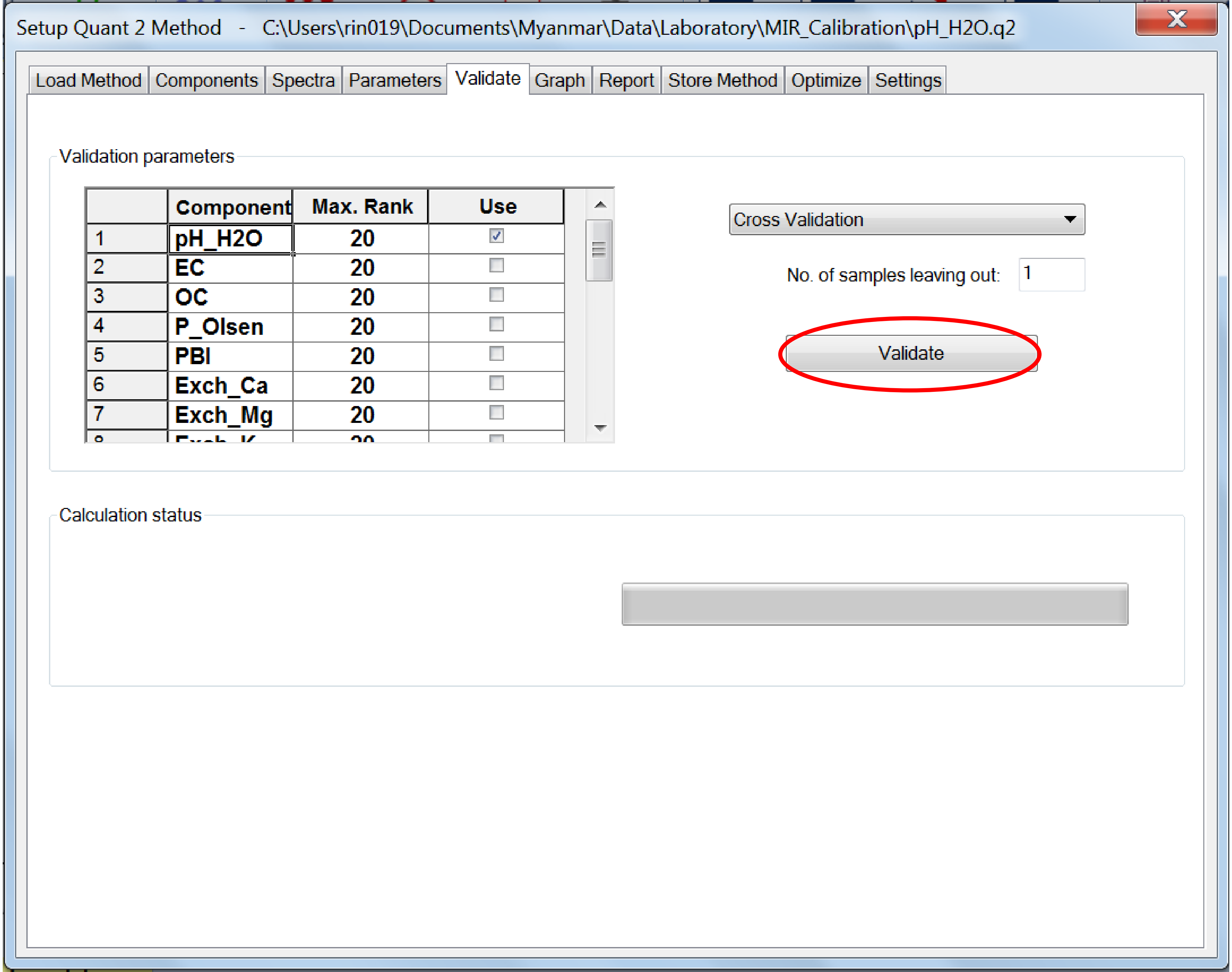
1.

Num...	RMSE...	Rank	Regions	Preprocessing
95	0.594	17	2976 - 2294.1 1616.4 - 1273.4	First derivative
90	0.599	18	3657.9 - 3314.9 2976 - 2294.1 1616...	First derivative
86	0.611	17	3996.7 - 3314.9 2976 - 2294.1 1616...	First derivative
91	0.613	18	3996.7 - 3655.8 2976 - 2294.1 1616...	First derivative
84	0.617	16	3657.9 - 2294.1 1616.4 - 1273.4	First derivative
92	0.619	16	3996.7 - 3314.9 2637.1 - 2294.1 16...	First derivative
83	0.62	18	3996.7 - 2294.1 1616.4 - 1273.4	First derivative
14	0.634	11	3996.7 - 3314.9 2976 - 1953.2 1616...	No spectral data preprocessing
15	0.636	11	3996.7 - 2973.9 2637.1 - 1953.2 16...	No spectral data preprocessing
36	0.637	9	3996.7 - 1953.2 1616.4 - 593.6	Vector normalization (SNV)
8	0.637	10	3996.7 - 1953.2 1616.4 - 593.6	No spectral data preprocessing
1	0.638	11	3996.7 - 593.6	No spectral data preprocessing
22	0.639	13	3996.7 - 3655.8 2976 - 1953.2 1616...	No spectral data preprocessing
85	0.64	15	3996.7 - 3655.8 3316.9 - 2294.1 16...	First derivative
19	0.64	10	3996.7 - 1953.2 1616.4 - 1273.4 93...	No spectral data preprocessing
3	0.64	12	3996.7 - 3655.8 3316.9 - 593.6	No spectral data preprocessing
23	0.642	10	3996.7 - 3314.9 2637.1 - 1953.2 16...	No spectral data preprocessing
27	0.643	10	3996.7 - 3314.9 2976 - 1953.2 1616...	No spectral data preprocessing

- Select top result – OPUS thinks this is the best one

Optimize status

Optimization finished



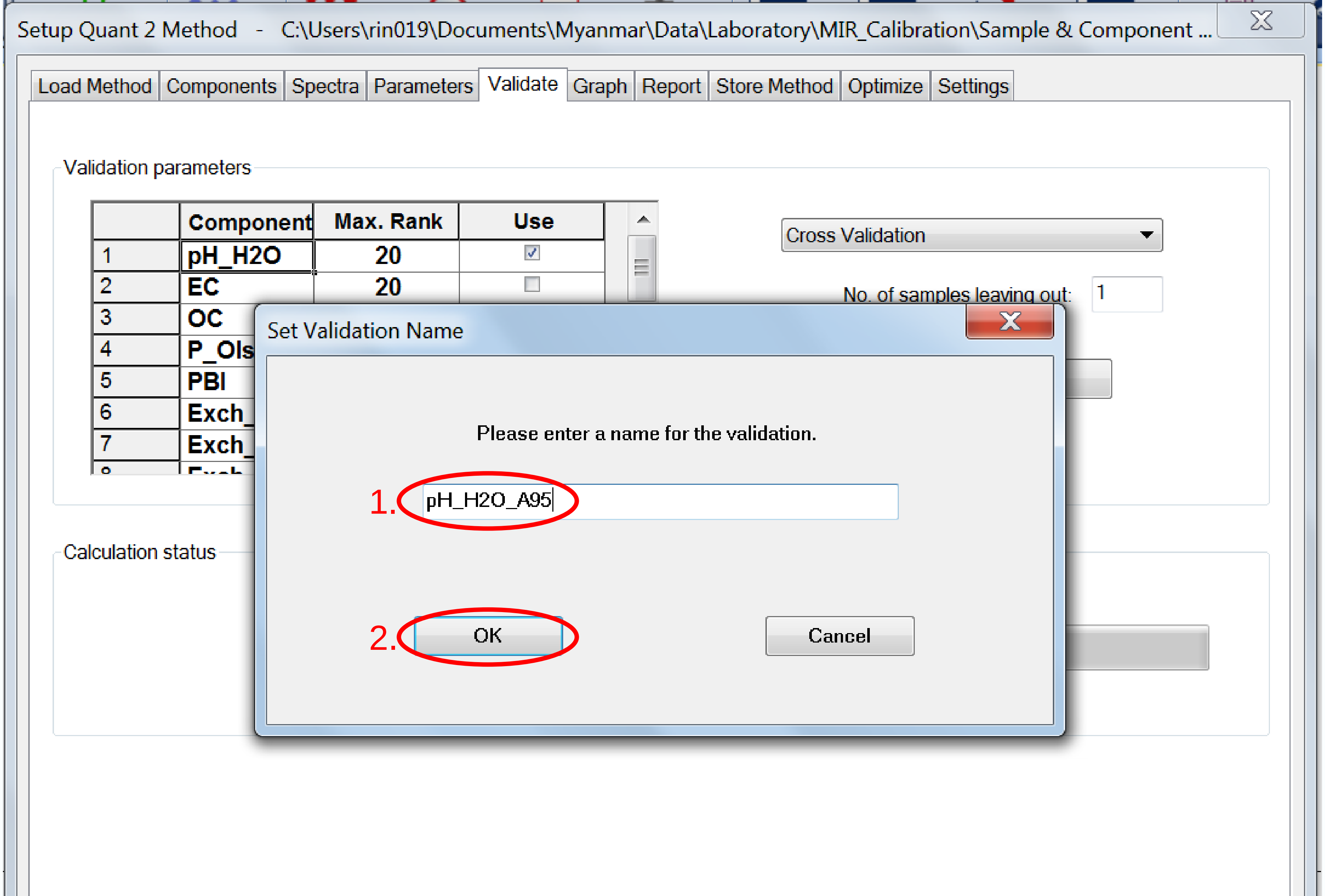
Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\pH_H2O.q2

Validation parameters

	Component	Max. Rank	Use
1	pH_H2O	20	☑
2	EC	20	☐
3	OC	20	☐
4	P_Olsen	20	☐
5	PBI	20	☐
6	Exch_Ca	20	☐
7	Exch_Mg	20	☐
8	Exch_K	20	☐

Cross Validation

No. of samples leaving out: 1



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

Validation parameters

	Component	Max. Rank	Use
1	pH_H2O	20	☑
2	EC	20	☐
3	OC		
4	P_Ols		
5	PBI		
6	Exch_		
7	Exch_		

Cross Validation

No. of samples leaving out: 1

Calculation status

Set Validation Name

Please enter a name for the validation.

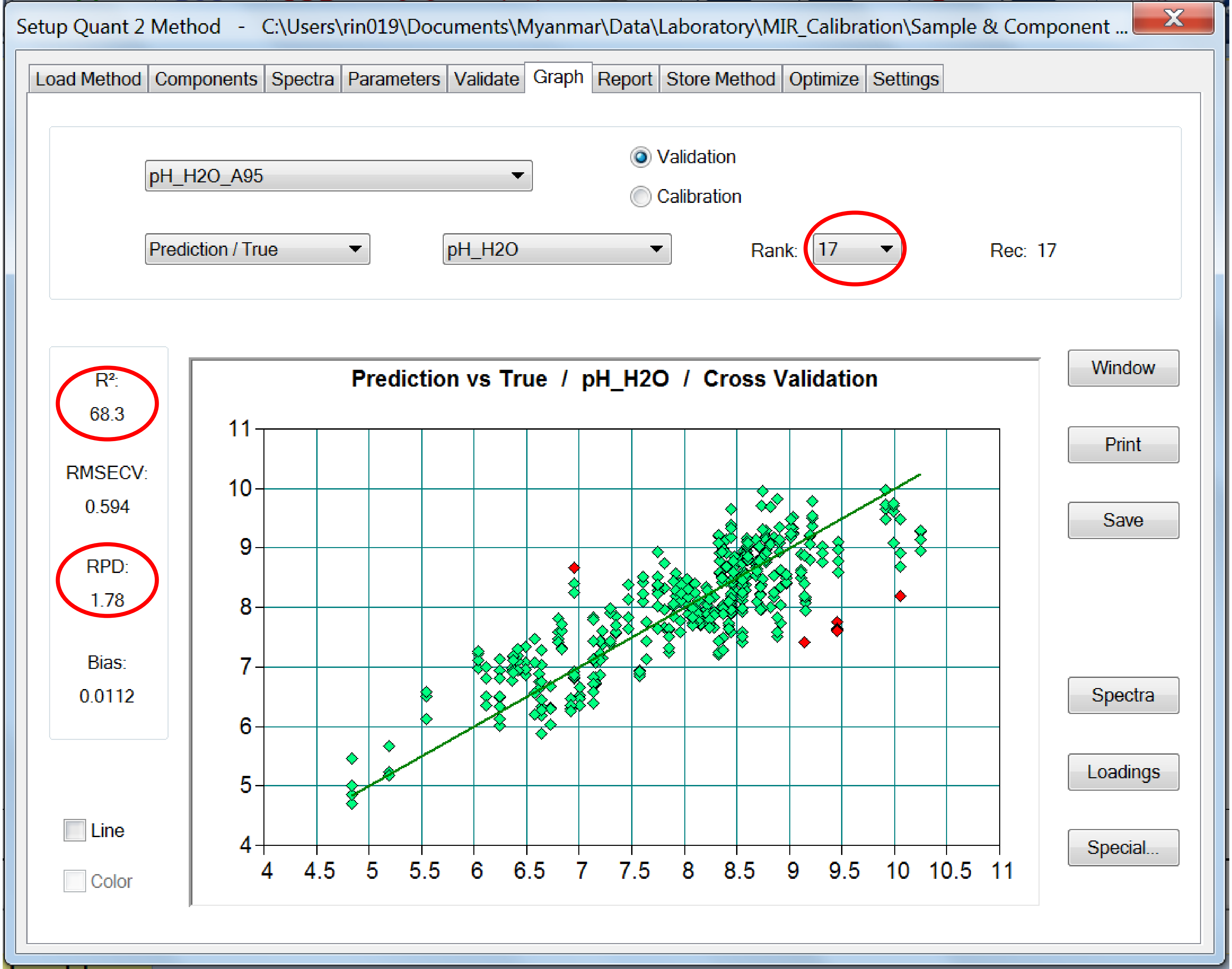
1. pH_H2O_A95

2. OK

Cancel

Validation names

- Hint: Use parameter name and “A95” (95 was optimization number)



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

pH_H2O_A95

● Validation
○ Calibration

Prediction / True

pH_H2O

Rank: 17

Rec: 17

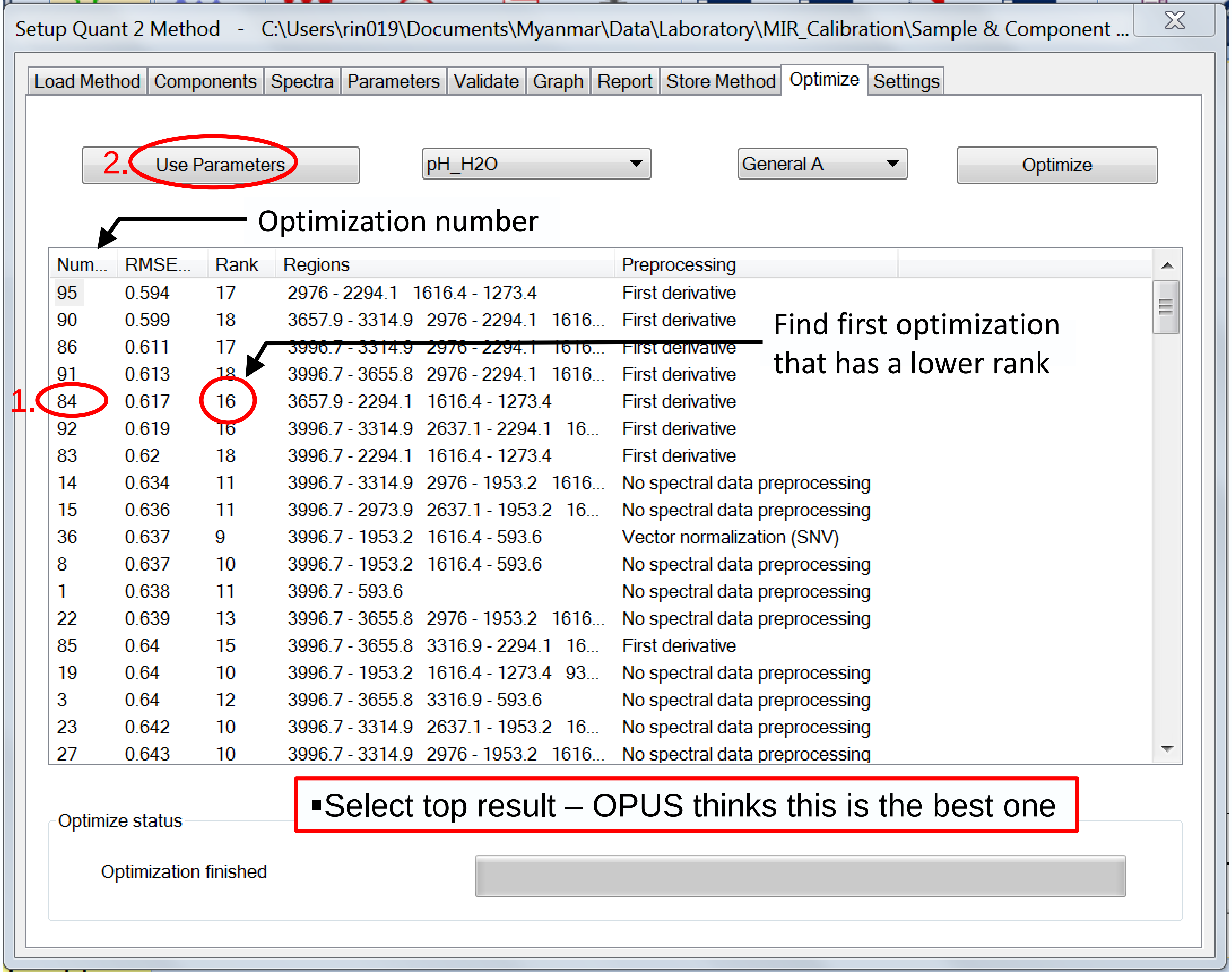
R²: 68.3

RMSECV: 0.594

RPD: 1.78

Bias: 0.0112

☐ Line
☐ Color



Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

2.

Optimization number

Find first optimization that has a lower rank

1.

Num...	RMSE...	Rank	Regions	Preprocessing
95	0.594	17	2976 - 2294.1 1616.4 - 1273.4	First derivative
90	0.599	18	3657.9 - 3314.9 2976 - 2294.1 1616...	First derivative
86	0.611	17	3996.7 - 3314.9 2976 - 2294.1 1616...	First derivative
91	0.613	18	3996.7 - 3655.8 2976 - 2294.1 1616...	First derivative
84	0.617	16	3657.9 - 2294.1 1616.4 - 1273.4	First derivative
92	0.619	16	3996.7 - 3314.9 2637.1 - 2294.1 16...	First derivative
83	0.62	18	3996.7 - 2294.1 1616.4 - 1273.4	First derivative
14	0.634	11	3996.7 - 3314.9 2976 - 1953.2 1616...	No spectral data preprocessing
15	0.636	11	3996.7 - 2973.9 2637.1 - 1953.2 16...	No spectral data preprocessing
36	0.637	9	3996.7 - 1953.2 1616.4 - 593.6	Vector normalization (SNV)
8	0.637	10	3996.7 - 1953.2 1616.4 - 593.6	No spectral data preprocessing
1	0.638	11	3996.7 - 593.6	No spectral data preprocessing
22	0.639	13	3996.7 - 3655.8 2976 - 1953.2 1616...	No spectral data preprocessing
85	0.64	15	3996.7 - 3655.8 3316.9 - 2294.1 16...	First derivative
19	0.64	10	3996.7 - 1953.2 1616.4 - 1273.4 93...	No spectral data preprocessing
3	0.64	12	3996.7 - 3655.8 3316.9 - 593.6	No spectral data preprocessing
23	0.642	10	3996.7 - 3314.9 2637.1 - 1953.2 16...	No spectral data preprocessing
27	0.643	10	3996.7 - 3314.9 2976 - 1953.2 1616...	No spectral data preprocessing

- Select top result – OPUS thinks this is the best one

Optimize status

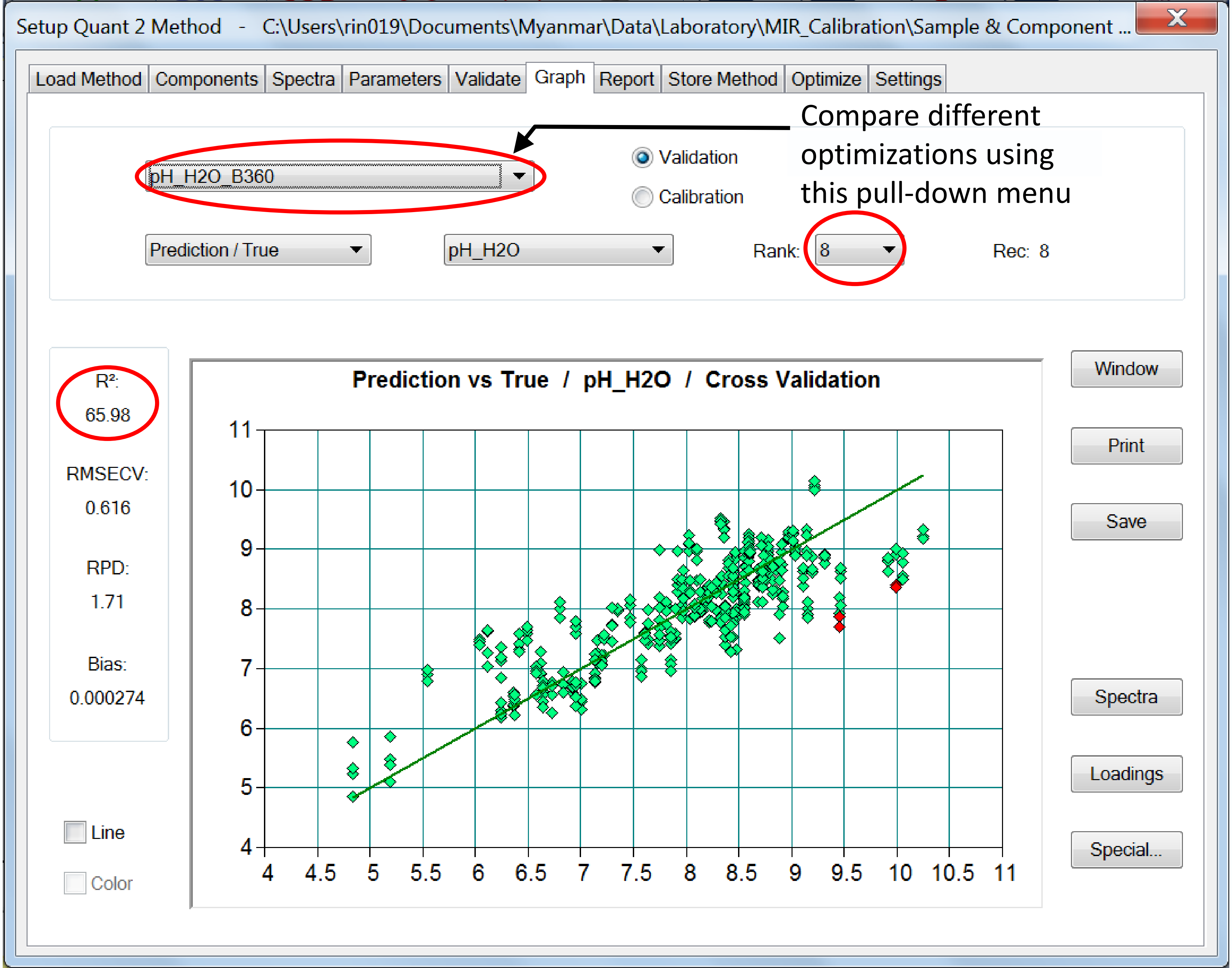
Optimization finished

- Validate first optimization that has a lower rank
- Examine R^2. If it is less that 1% lower that the top optimization:
  - Consider using it instead the top optimization

- Next Select <General B> on the Optimize sheet
- Wait while the optimization runs

- When finished, select top optimization and validate
- Then select first optimization that has a lower rank and validate

- On the Graph sheet, compare R^2 and rank of all the selected optimizations and choose which to use as a calibration



Compare different optimizations using this pull-down menu

Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

pH_H2O_B360

● Validation

○ Calibration

Prediction / True

pH_H2O

Rank: 8

Rec: 8

R²: 65.98

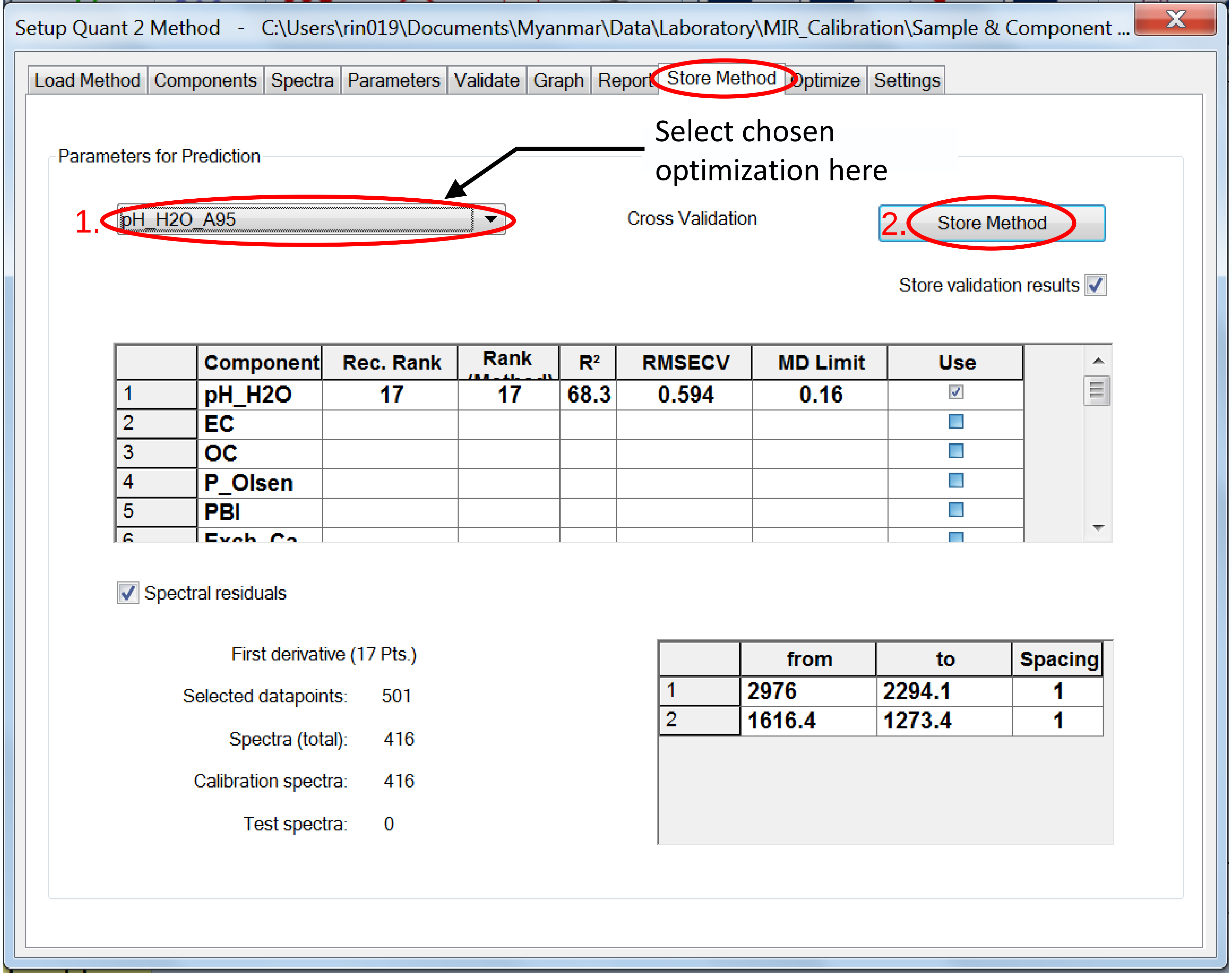
RMSECV: 0.616

RPD: 1.71

Bias: 0.000274

☐ Line

☐ Color



Select chosen optimization here

Parameters for Prediction

1. pH_H2O_A95

Cross Validation

2. Store Method

Store validation results ☑

	Component	Rec. Rank	Rank (Method)	R²	RMSECV	MD Limit	Use
1	pH_H2O	17	17	68.3	0.594	0.16	☑
2	EC						☐
3	OC						☐
4	P_Olsen						☐
5	PBI						☐
6	Exch_Ca						☐

☑ Spectral residuals

First derivative (17 Pts.)

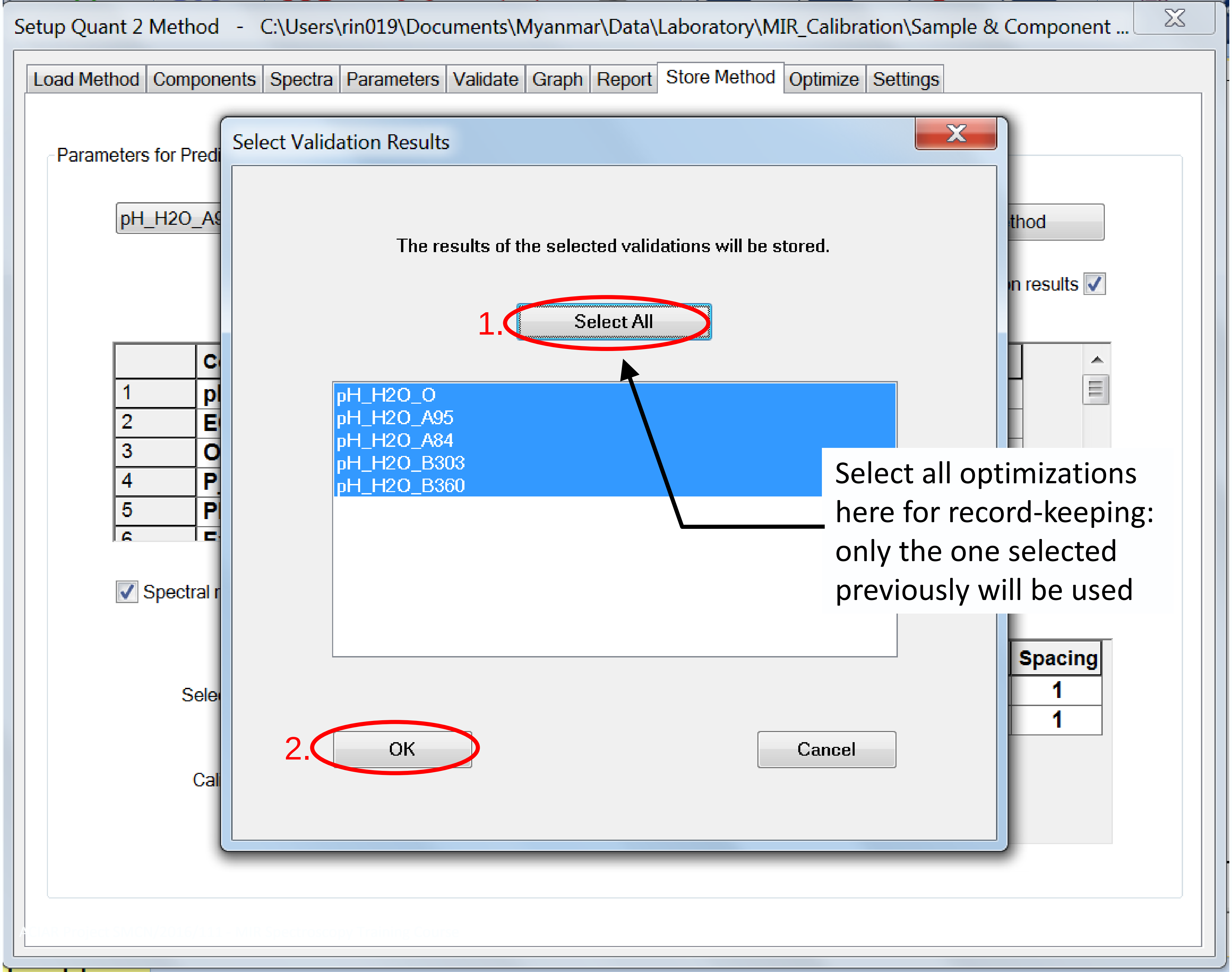
Selected datapoints: 501

Spectra (total): 416

Calibration spectra: 416

Test spectra: 0

	from	to	Spacing
1	2976	2294.1	1
2	1616.4	1273.4	1



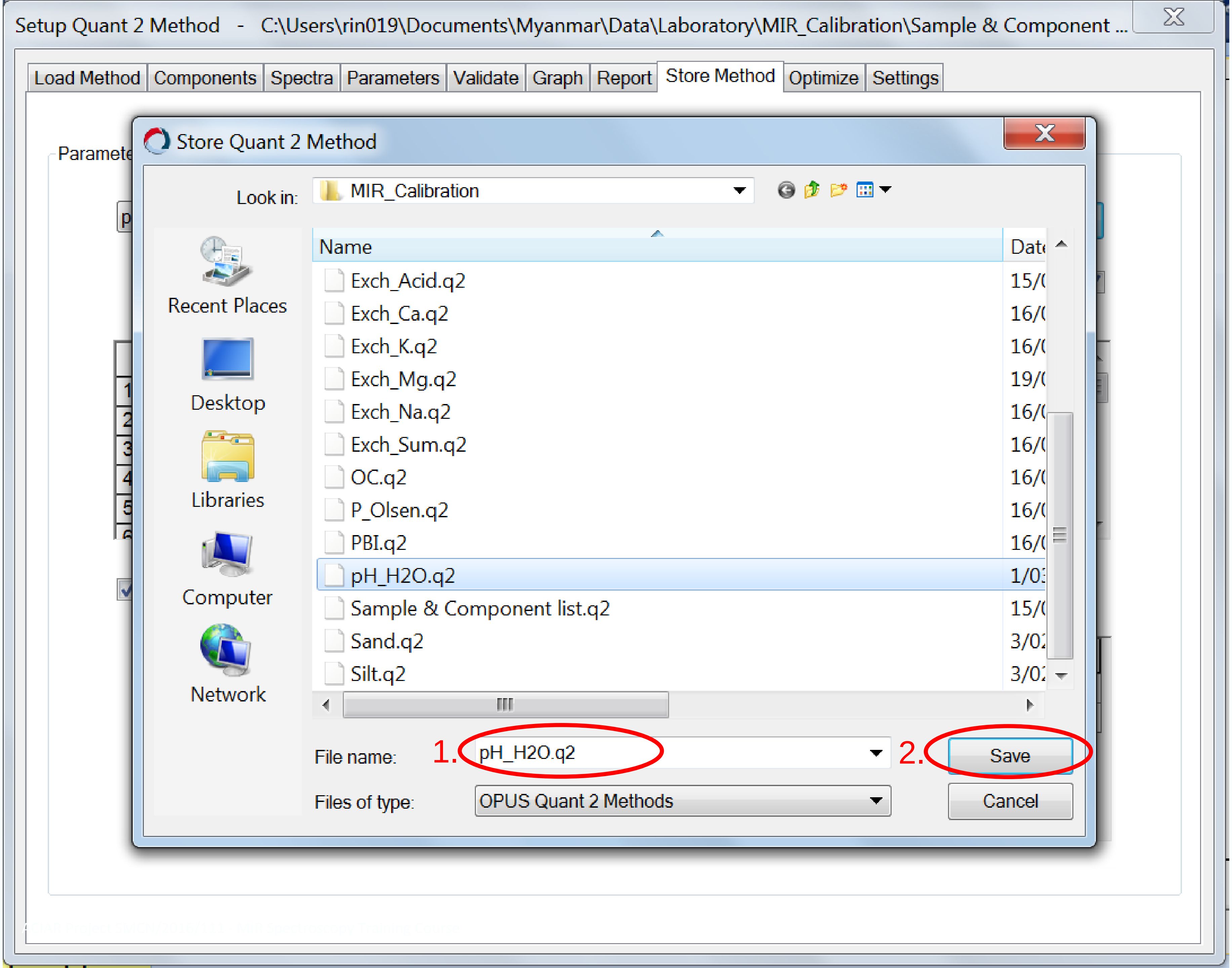
Setup Quant 2 Method - C:\Users\rin019\Documents\Myanmar\Data\Laboratory\MIR_Calibration\Sample & Component ...

Select Validation Results

The results of the selected validations will be stored.

pH_H2O_O
pH_H2O_A95
pH_H2O_A84
pH_H2O_B303
pH_H2O_B360

Select all optimizations here for record-keeping: only the one selected previously will be used



Name	Date
Exch_Acid.q2	15/
Exch_Ca.q2	16/
Exch_K.q2	16/
Exch_Mg.q2	19/
Exch_Na.q2	16/
Exch_Sum.q2	16/
OC.q2	16/
P_Olsen.q2	16/
PBI.q2	16/
pH_H2O.q2	1/0
Sample & Component list.q2	15/
Sand.q2	3/0
Silt.q2	3/0

File name: pH_H2O.q2

Files of type: OPUS Quant 2 Methods

- The chosen calibration is now saved as a “Method”, and can be used to predict the pH of other samples based on their MIR spectra

Thank you

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Principal Research Consultant

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