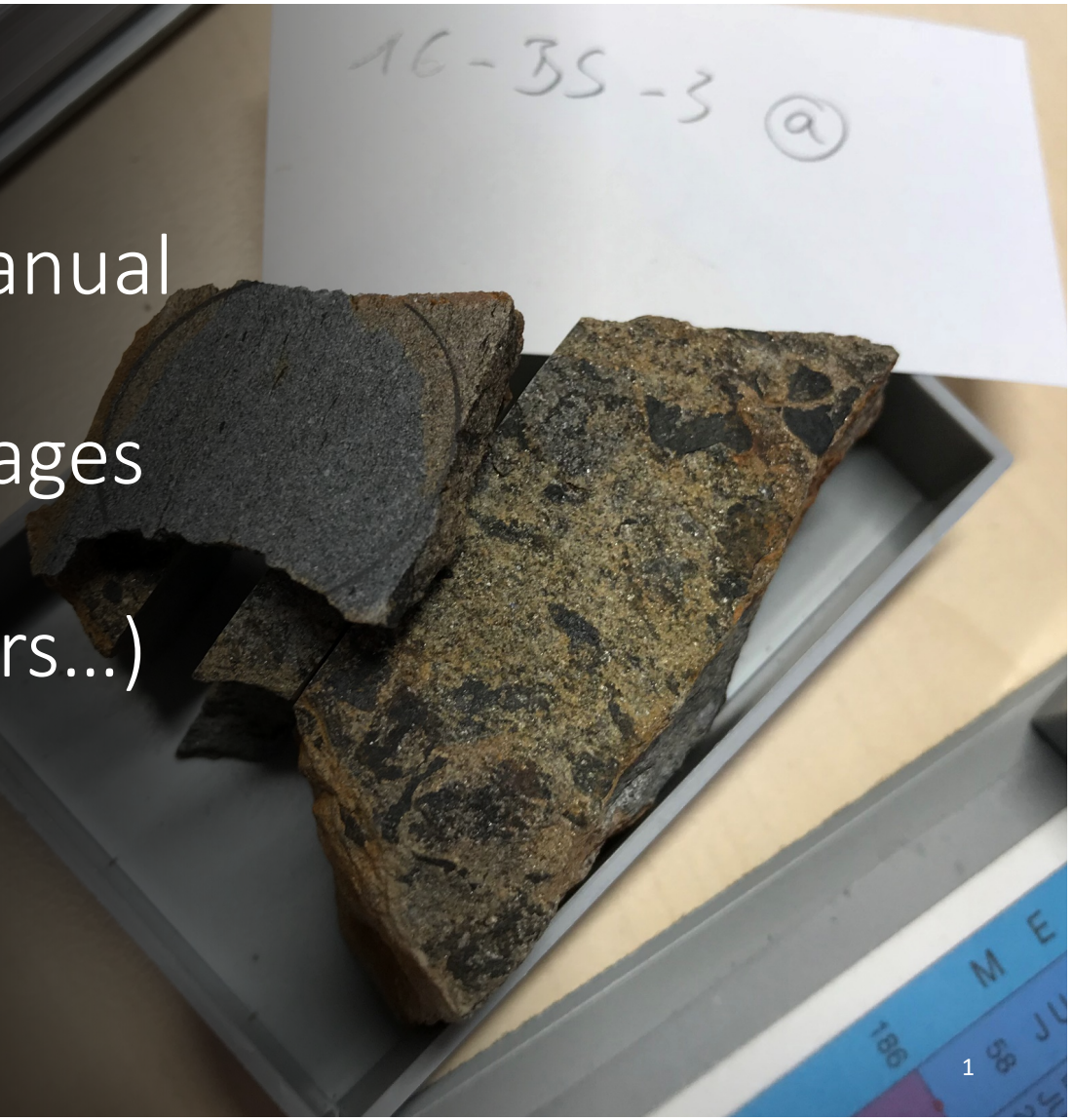
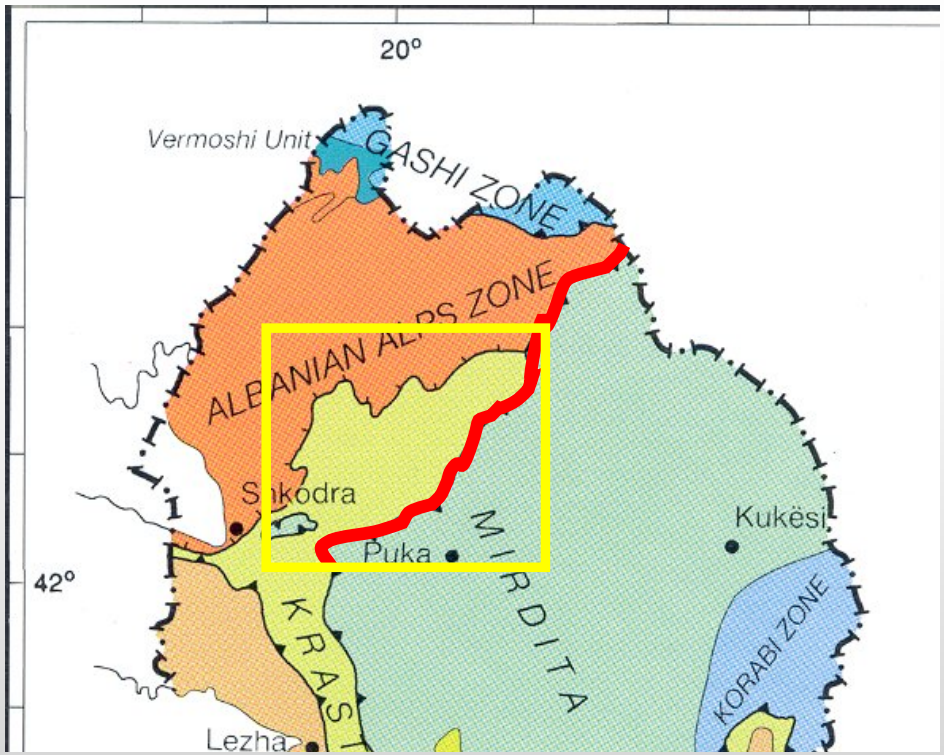
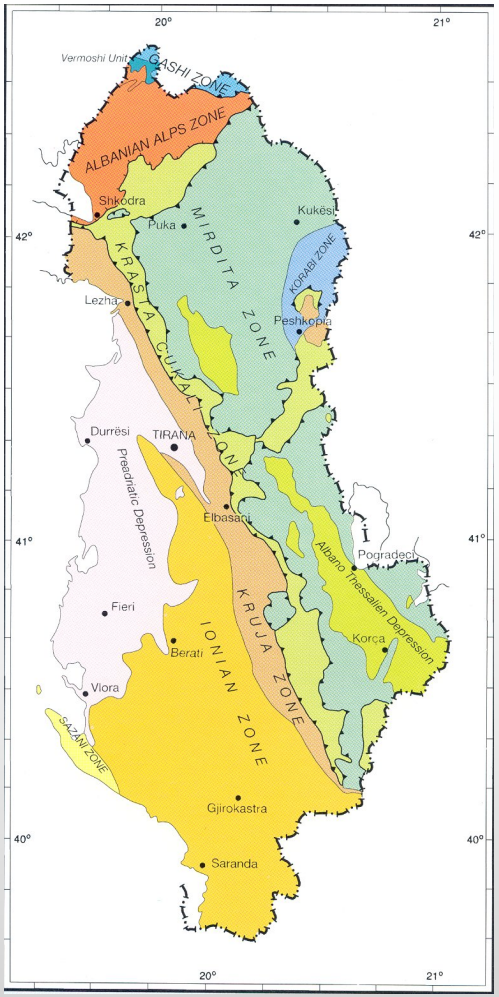
Semi-automated vs. manual evaluation of RSCM – benefits and disadvantages detected by statistical analysis (amongst others…)

A field study from Northern Albania

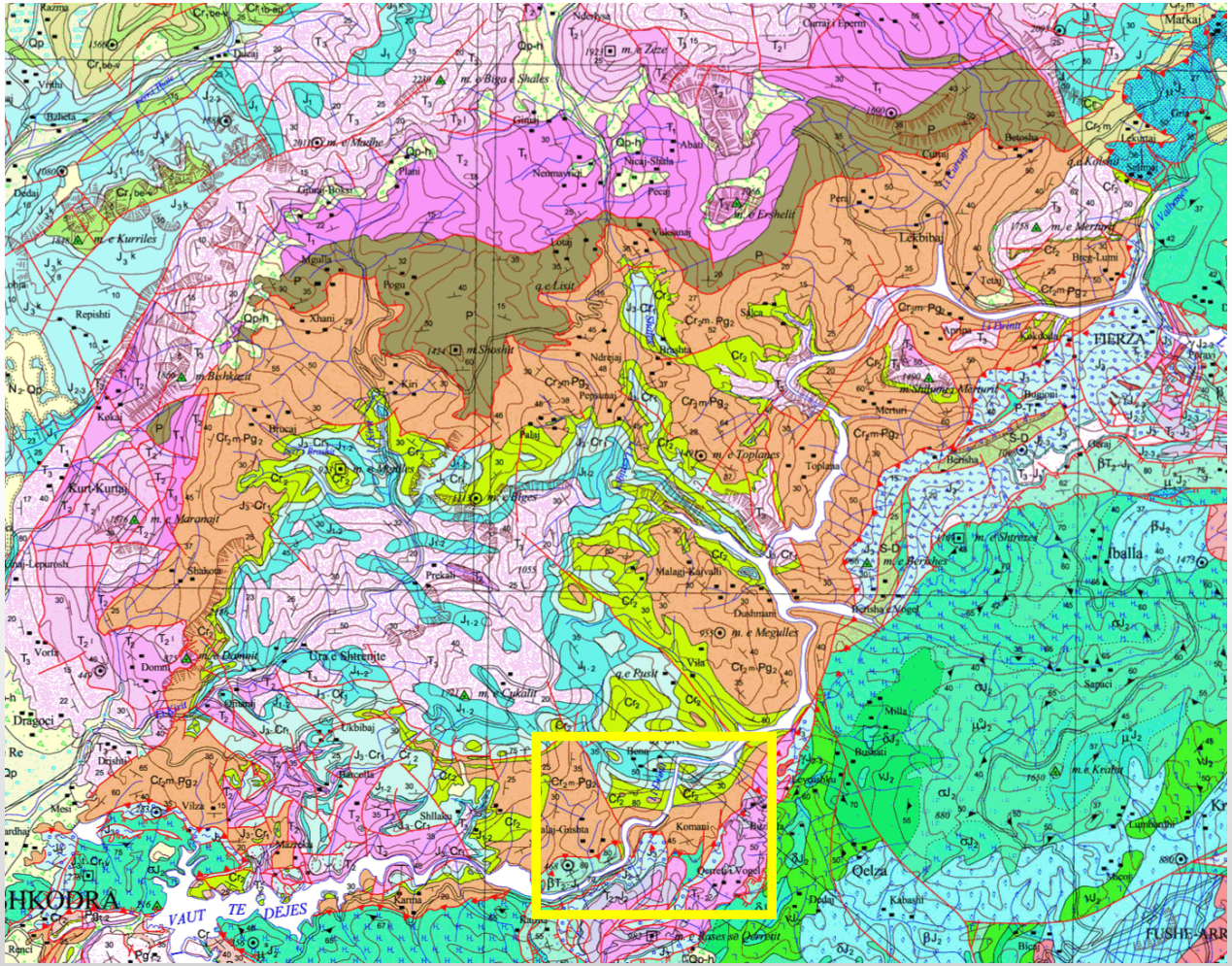


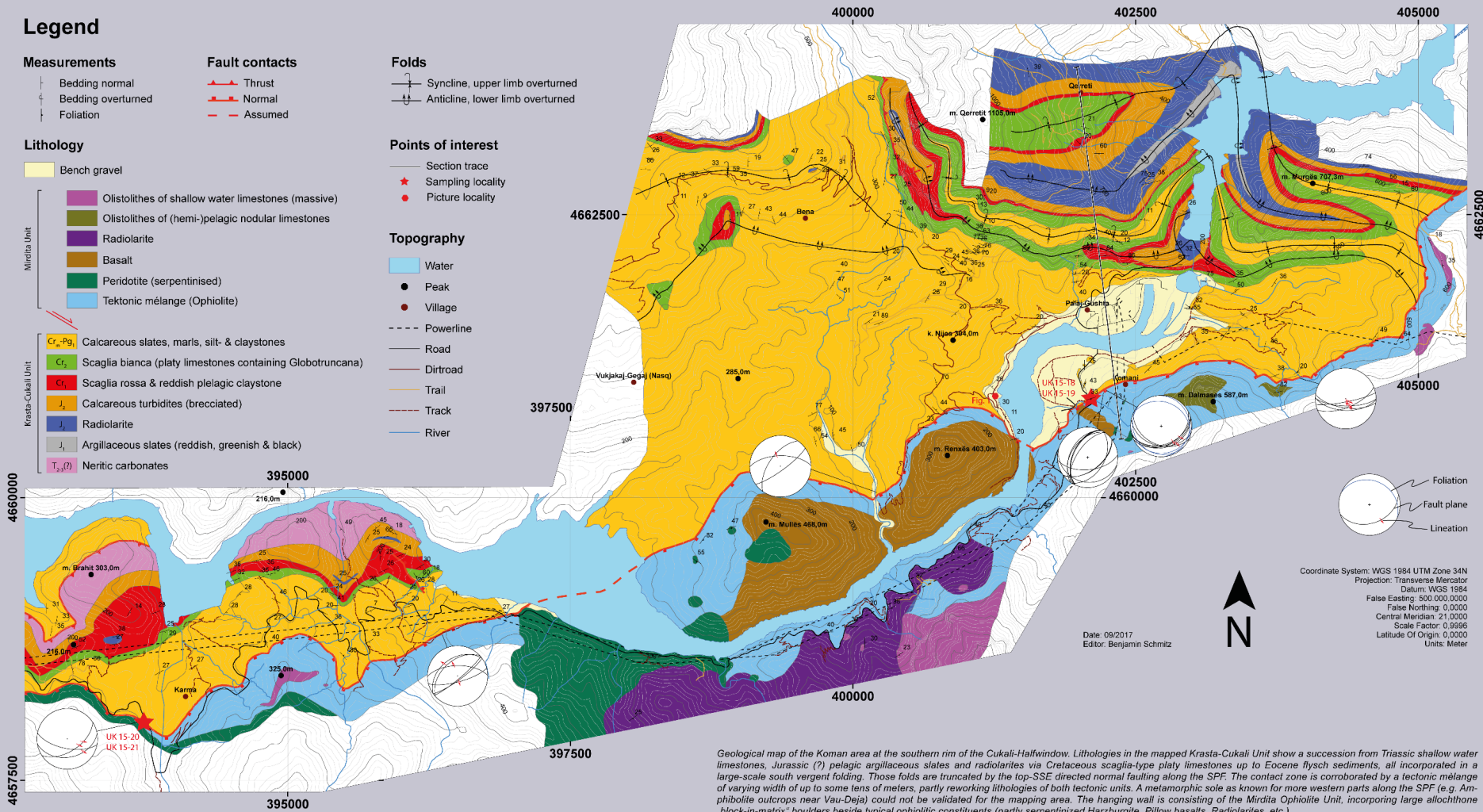
Study area


20°
Vermoshi Unit
GASHI ZONE
ALBANIAN ALPS ZONE
Shkodra
Puka
MIRDITA
Kukësi
42°
KRASTA
KORABI ZONE
Lezha

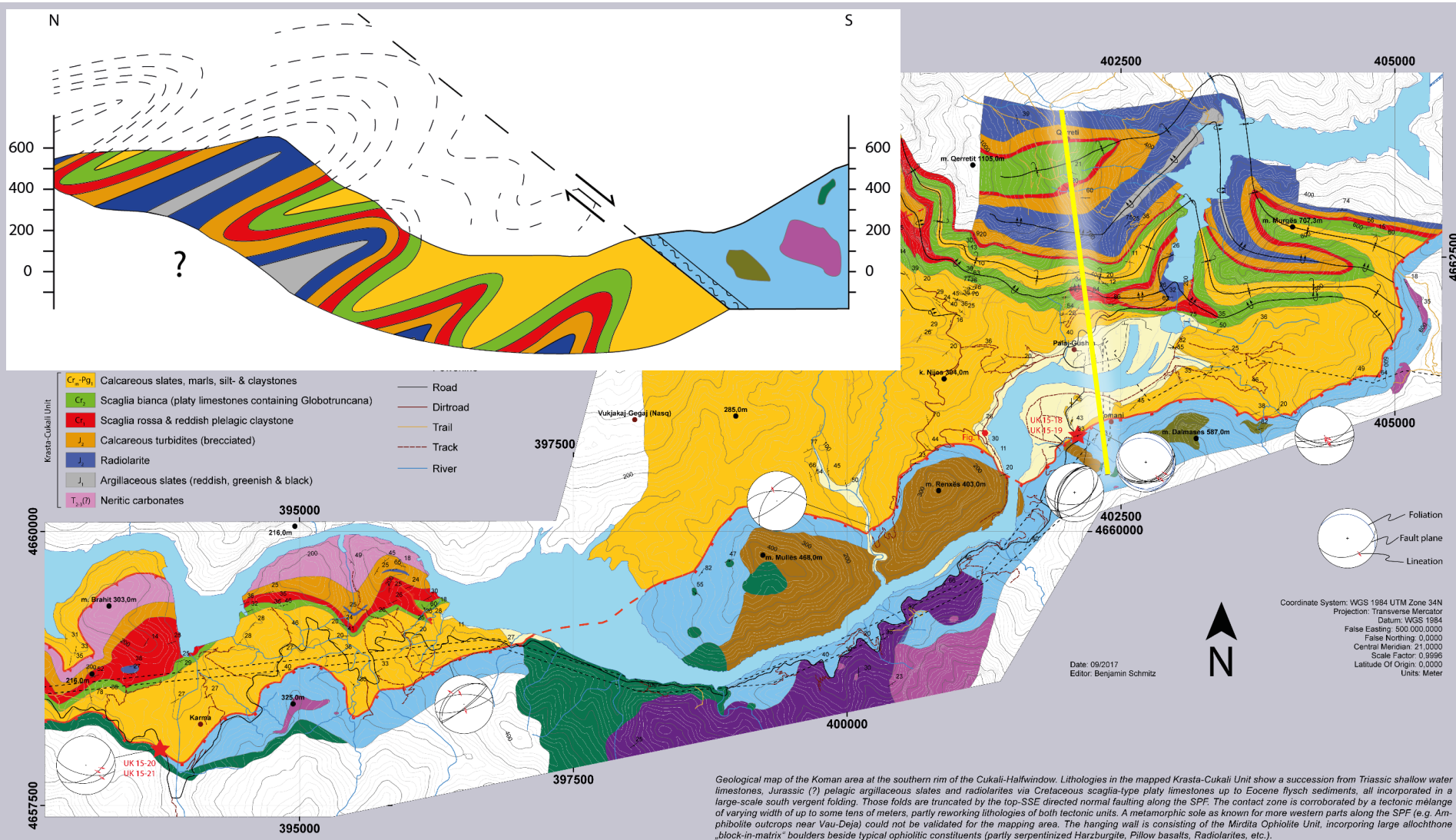

20°
21°
Vermoshi Unit
GASHI ZONE
ALBANIAN ALPS ZONE
Shkodra
Puka
Kukësi
MIRDITA ZONE
KORABI ZONE
42°
Lezha
KRASTA CUKALI ZONE
Peshkopia
Durrësi
TIRANA
Peridriatic Depression
Elbasani
Pogradeci
Albano Thessalian Depression
41°
Fieri
Berati
KRUJA ZONE
IONIAN ZONE
Korça
Vlora
SAZANI ZONE
Gjirokastra
40°
Saranda

Study area





Geological map of the Koman area at the southern rim of the Cukali-Halfwindow. Lithologies in the mapped Krasta-Cukali Unit show a succession from Triassic shallow water limestones, Jurassic (?) pelagic argillaceous slates and radiolarites via Cretaceous scaglia-type platy limestones up to Eocene flysch sediments, all incorporated in a large-scale south vergent folding. Those folds are truncated by the top-SSE directed normal faulting along the SPF. The contact zone is corroborated by a tectonic mélange of varying width of up to some tens of meters, partly reworking lithologies of both tectonic units. A metamorphic sole as known for more western parts along the SPF (e.g. Amphibolite outcrops near Vau-Deja) could not be validated for the mapping area. The hanging wall is consisting of the Mirdita Ophiolite Unit, incorporing large allochthone „block-in-matrix" boulders beside typical ophiolitic constituents (partly serpentinized Harzburgite, Pillow basalts, Radiolarites, etc.).



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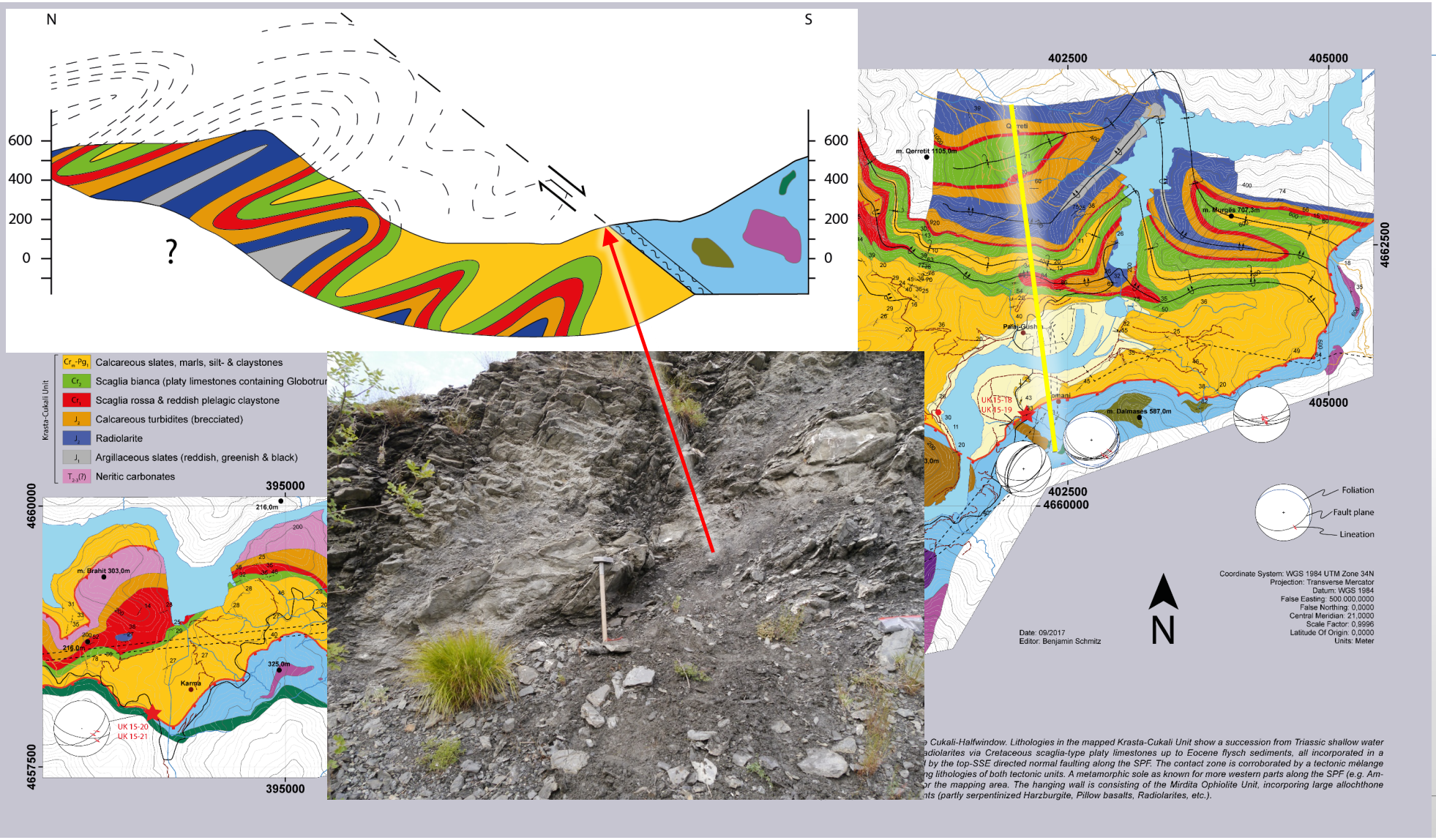

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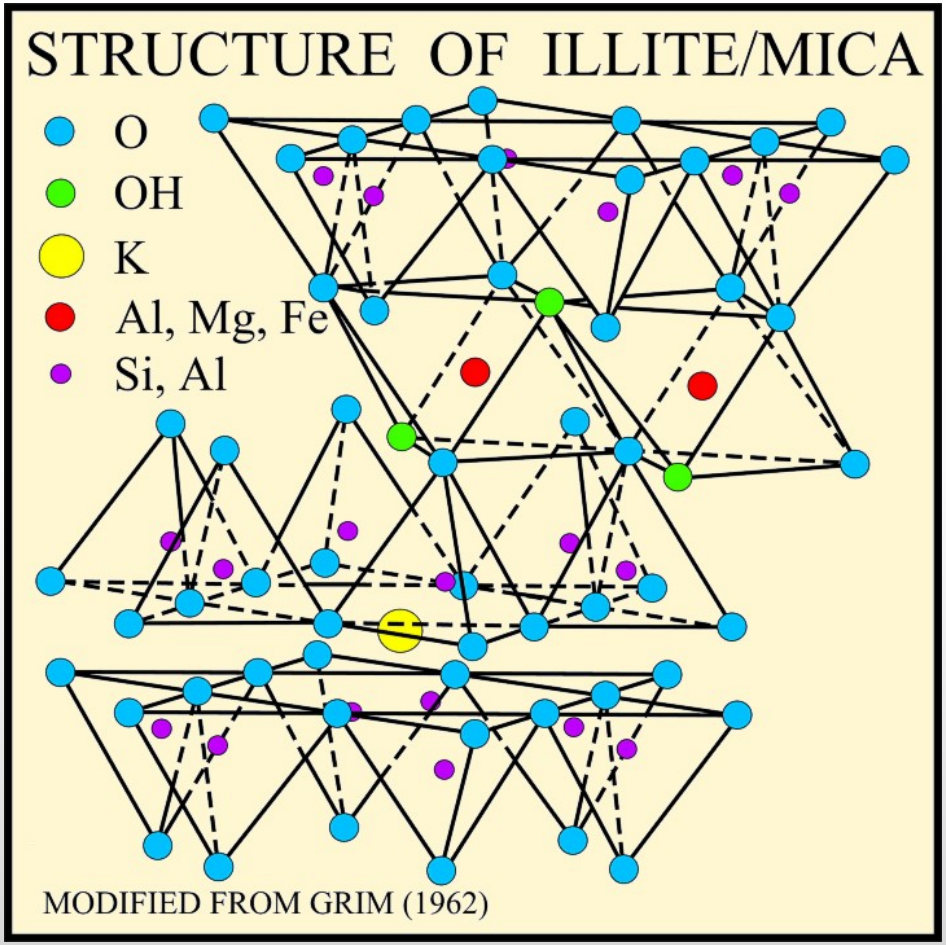
Illite
$K_2Al_4(Si_6Al_2O_{20})(OH_4)$

TOT sheet silicate

Isotope	Occurrence	$T_{1/2}$
^{39}K	93,26 %	stable
^{40}K	0,0117 %	1,248 x 10^9 a
^{41}K	6,73 %	stable



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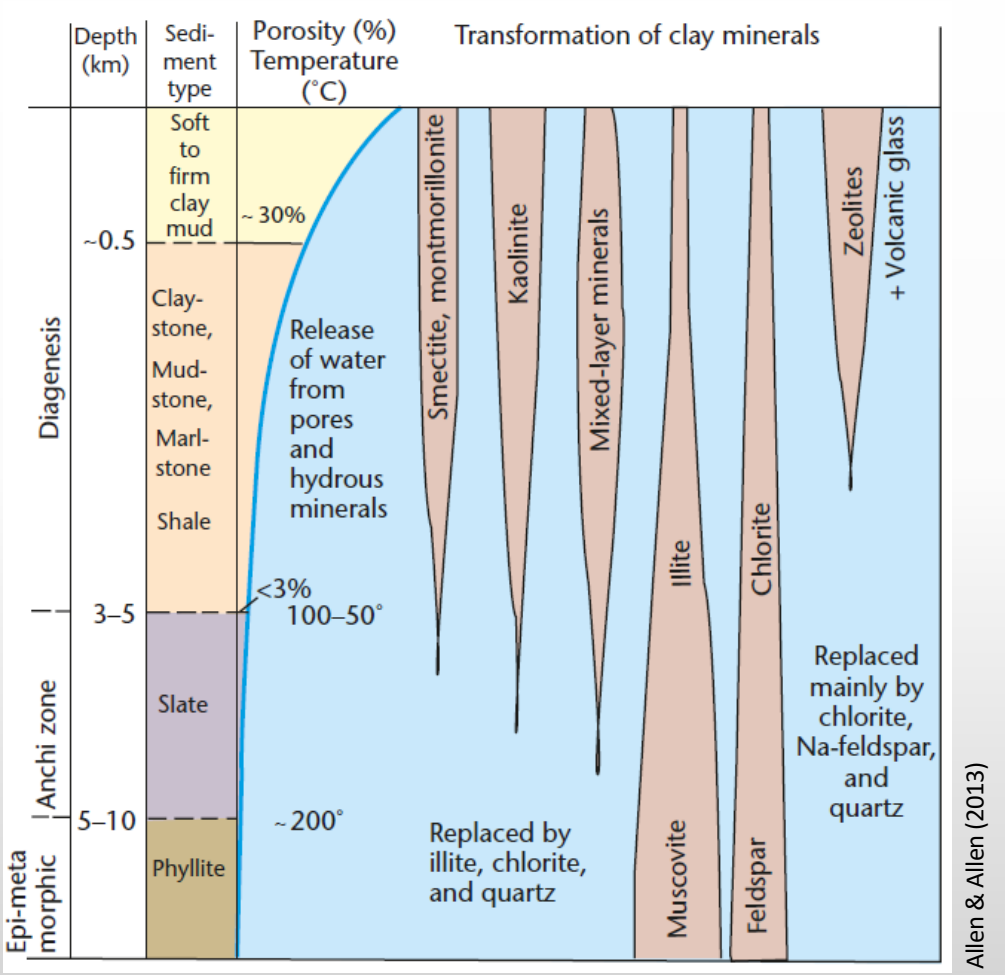
Forming conditions:

- ≥ 60°: Smectite + K-Feldspar → Illite
- ≥ 100-120°: Kaolinite + K-Feldspar → Illite

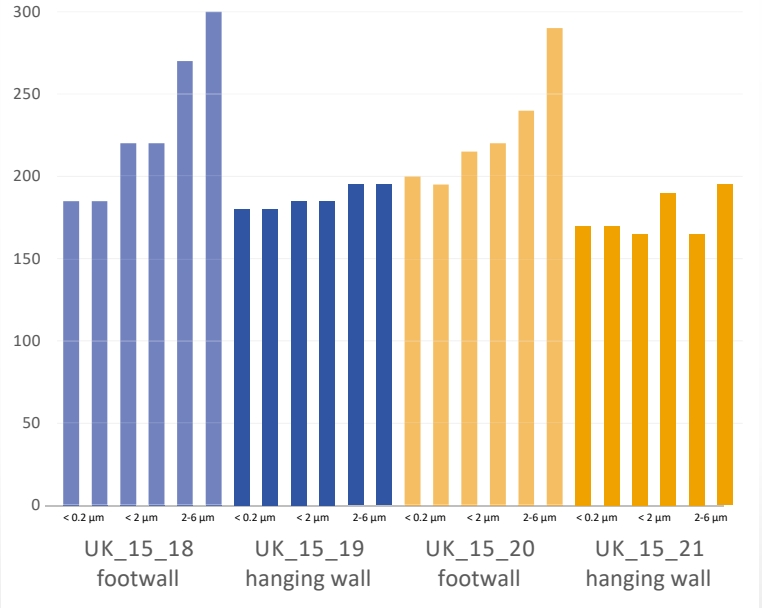


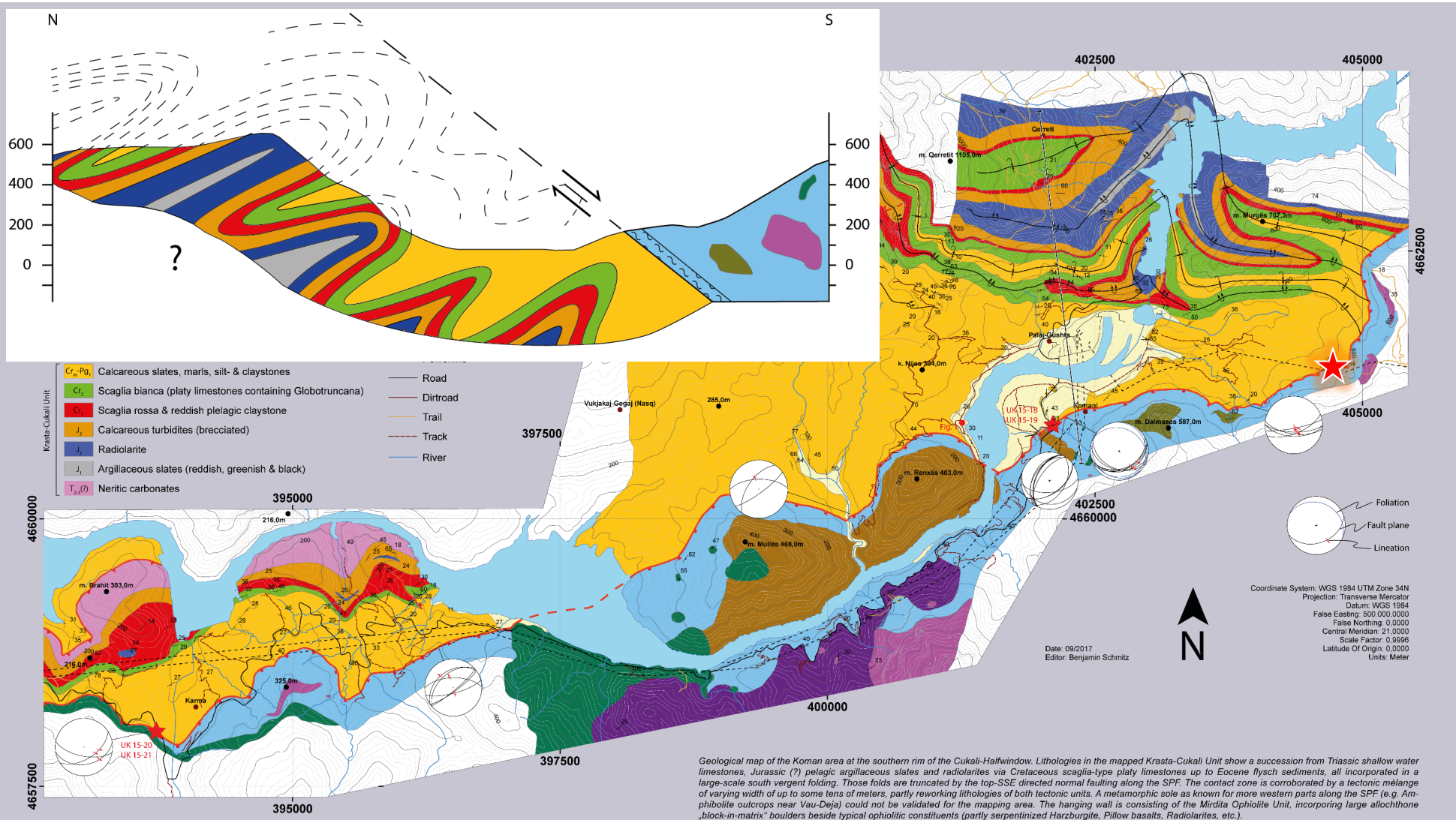
K-Ar dating and Illite

Sample	Location	K2O [Wt. %]	40 Ar * [nl/g] STP	40 Ar * [%]	Age [Ma]	2s-Error [Ma]	2s-Error [%]
UK 15-18 <0.2µm		5.13	8.83	91.46	52.6	0.7	1.2
UK 15-18 <2µm	footwall	5.00	11.83	92.27	72.0	0.9	1.3
UK 15-18 2-6µm		3.88	11.06	95.92	86.4	1.2	1.4
UK 15-19 <0.2µm		3.33	5.43	85.30	50.0	0.7	1.4
UK 15-19 <2µm	hanging wall	3.55	7.47	86.19	64.2	1.0	1.5
UK 15-19 2-6µm		3.50	7.96	88.05	69.2	0.8	1.1
UK 15-20 <0.2µm		3.88	10.74	83.12	83.9	1.1	1.3
UK 15-20 <2µm	footwall	4.10	14.43	91.45	105.9 ?	1.7	1.6
UK 15-20 2-6µm		5.21	15.63	91.14	90.7	1.0	1.1
UK 15-21 <0.2µm		5.42	8.35	90.91	47.1	0.5	1.1
UK 15-21 <2µm	hanging wall	4.93	9.78	93.41	60.5	0.8	1.3
UK 15-21 2-6µm		5.14	10.67	95.71	63.3	1.1	1.7

eastern sampling site

western sampling site





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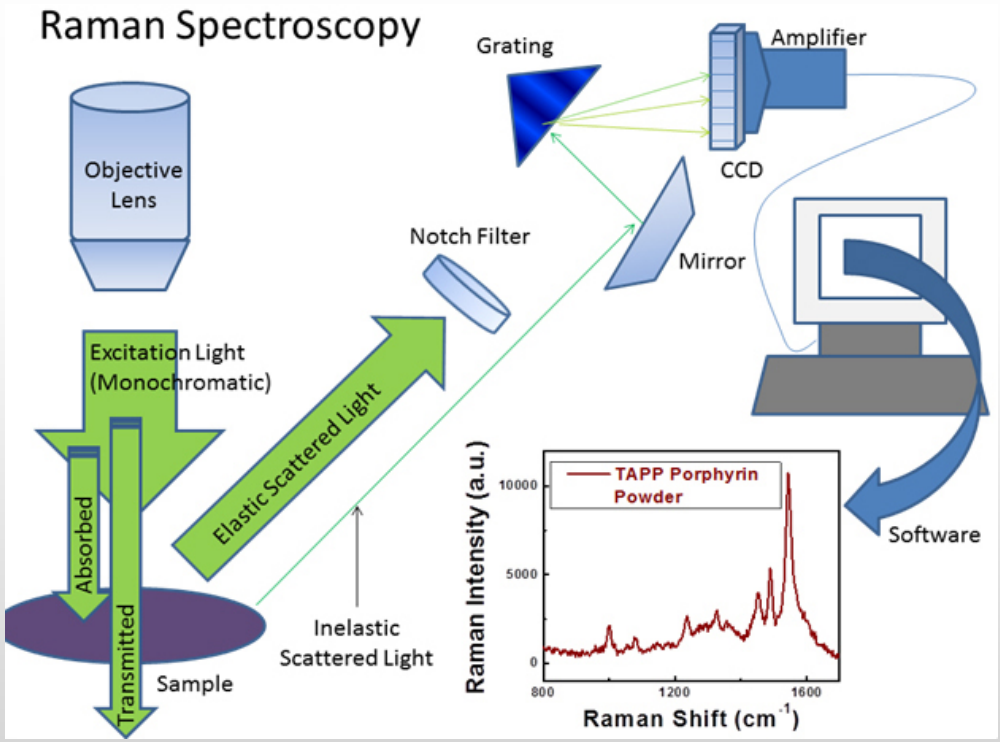
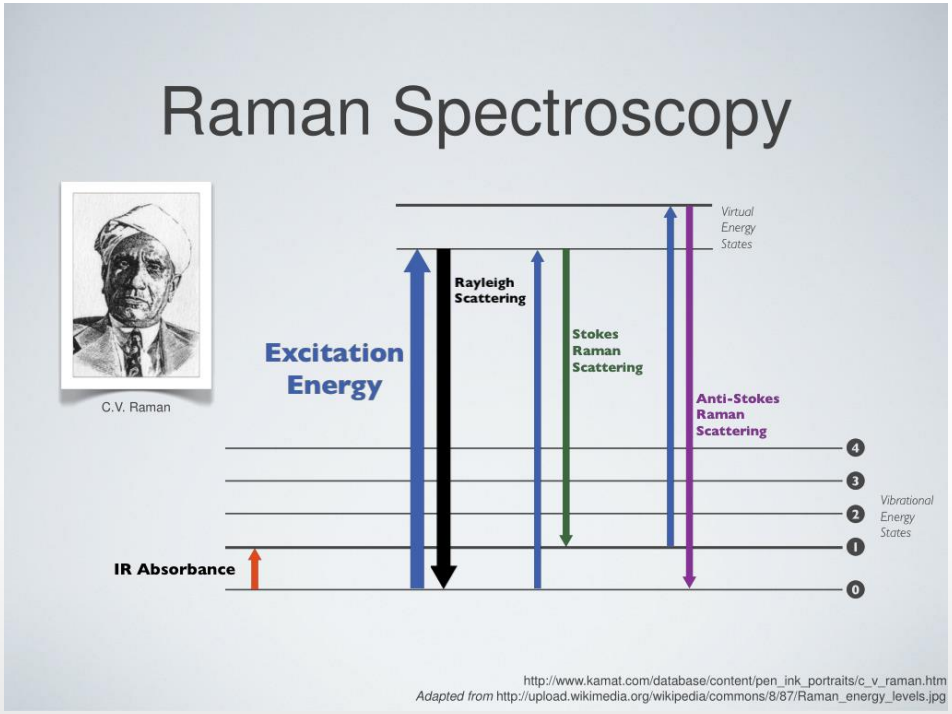
Sampling

Preparation

- standard polished thin section (as for microprobe analysis – DON'T use diamond polish!)
- or polished surfaces

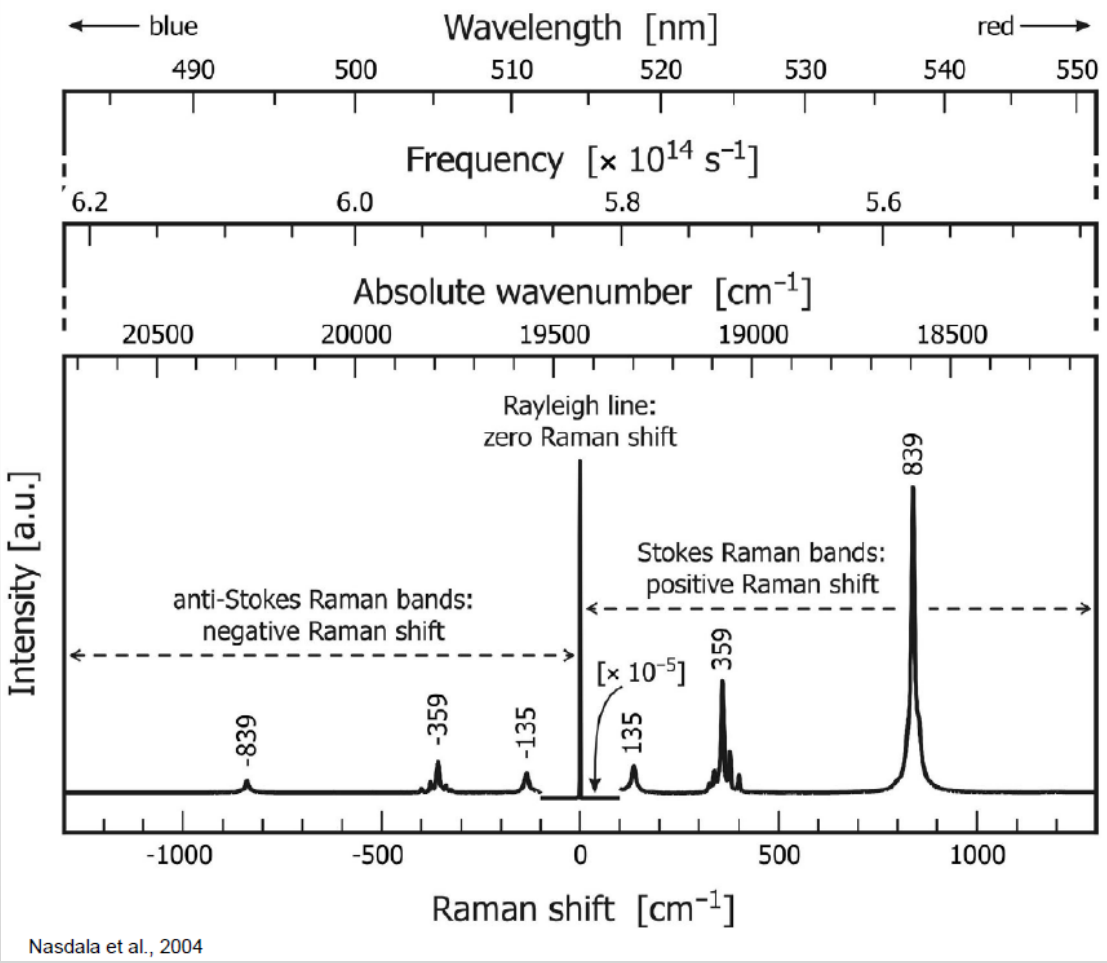
Raman





http://www.kamat.com/database/content/pen_ink_portraits/c_v_raman.htm
Adapted from http://upload.wikimedia.org/wikipedia/commons/8/87/Raman_energy_levels.jpg

Raman



Nasdala et al., 2004

Wavenumber: $1/\lambda$ [cm^{-1}]

Absolute wavenumber:

514.5 nm = 19436.35 cm^{-1}

Raman shift:

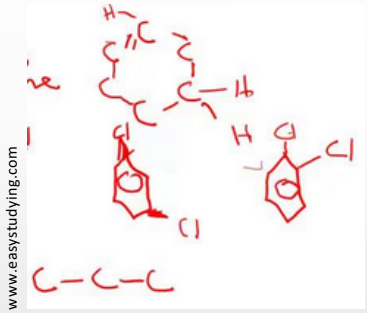
Deviation of the Raman scattered light with respect to the excitation wavelength

RSCM

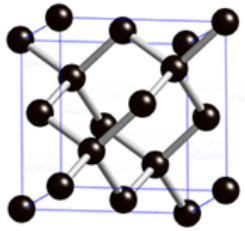

www.thrillist.com

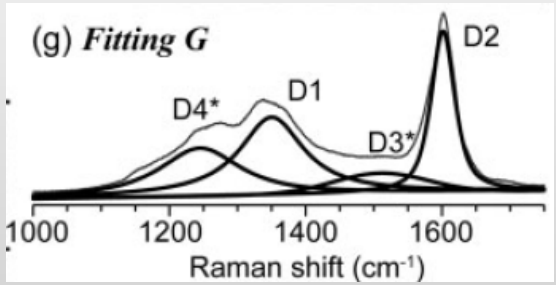
(+ p,) T


www.legacyonlinemarketing.com


www.easystudying.com

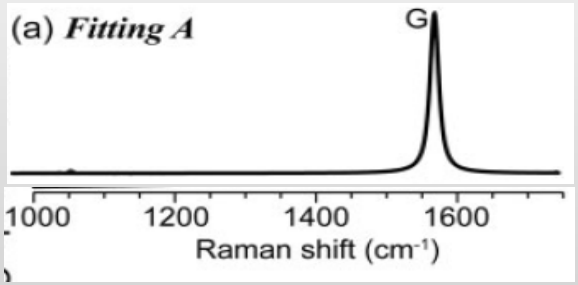
(+ p,) T


www.wikimedia.org



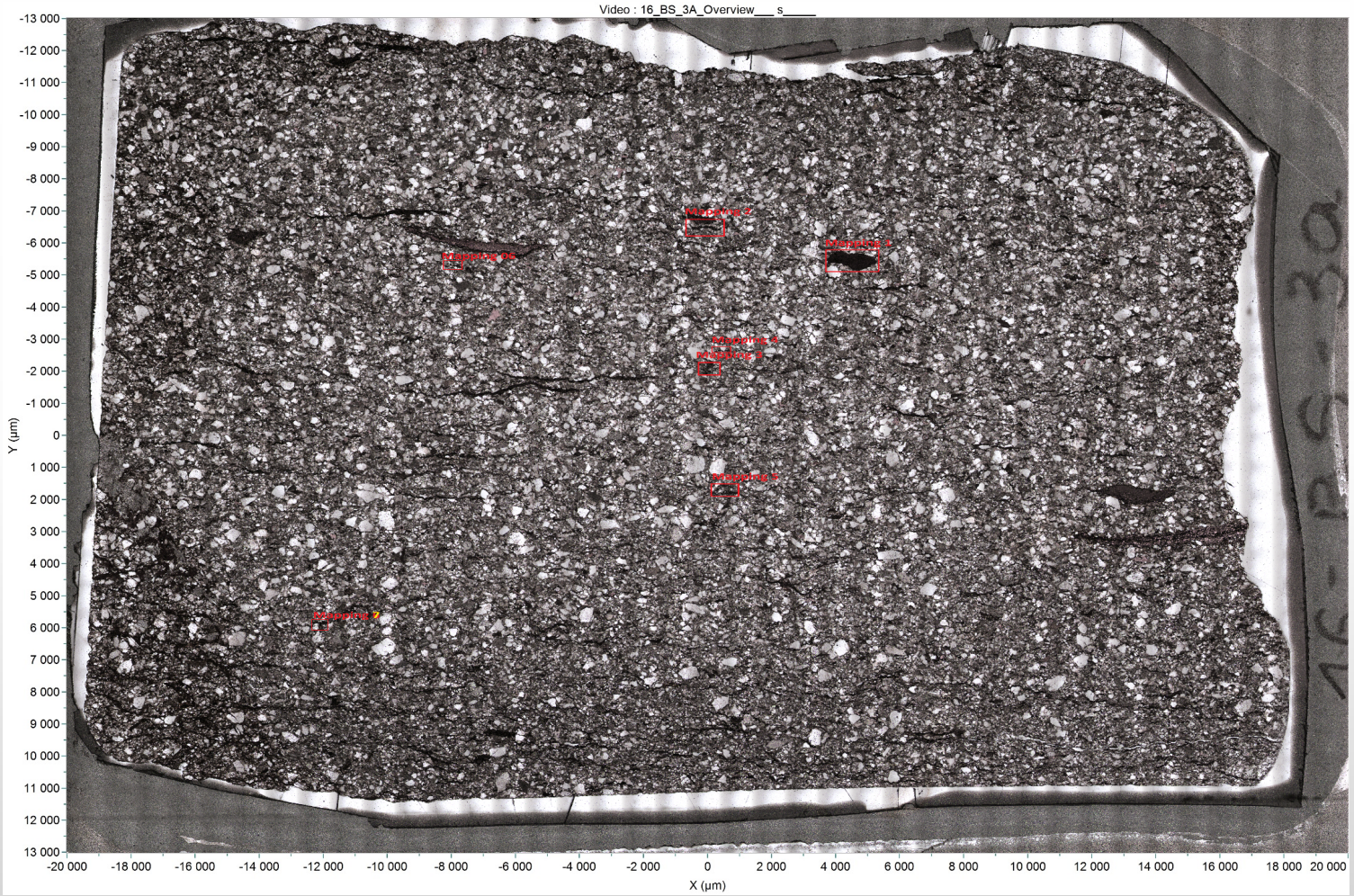
Kouketsu et al. (2014)

(+ p,) T



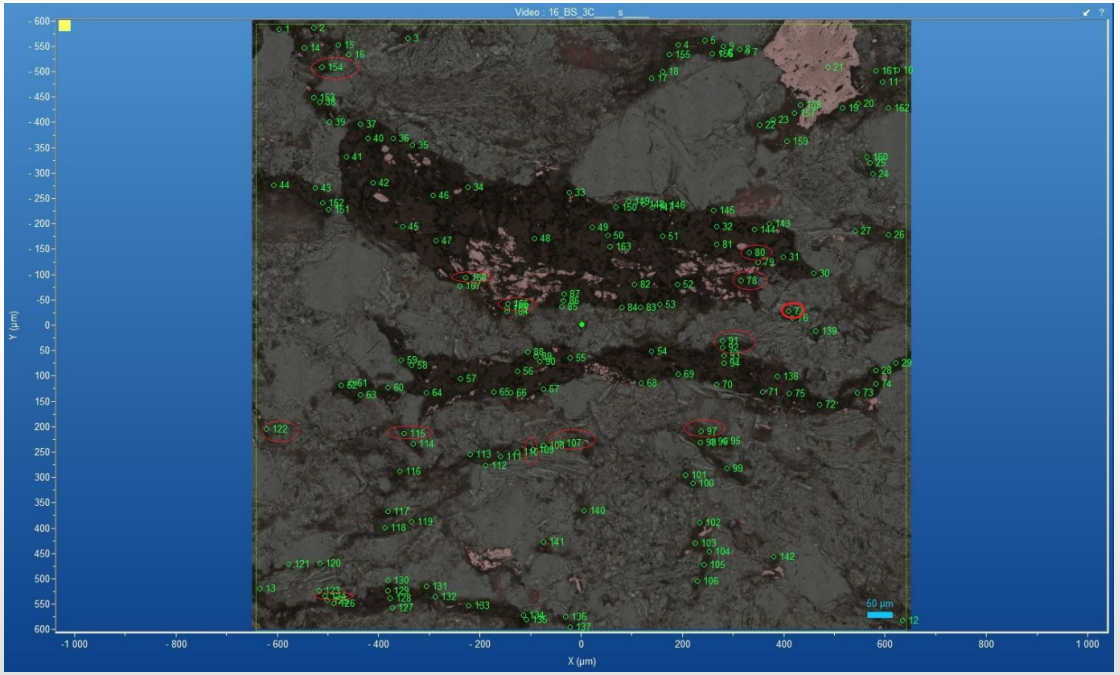
Kouketsu et al. (2014)

RSCM

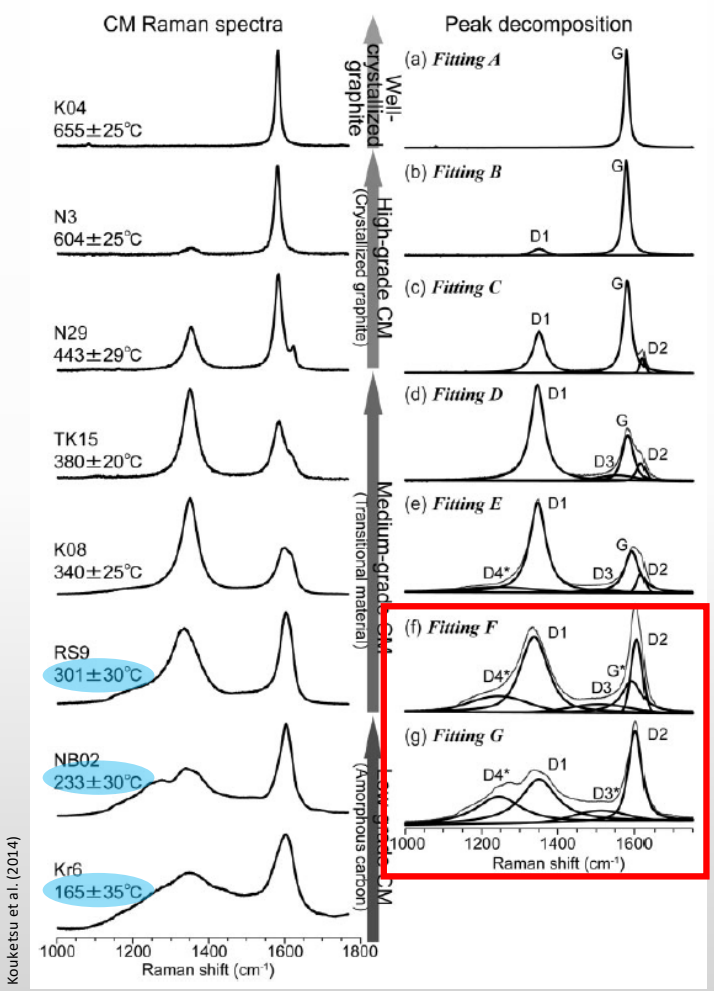

Video : 16_BS_3A_Overview___s_____
Y (µm)
X (µm)
-13 000
-12 000
-11 000
-10 000
-9 000
-8 000
-7 000
-6 000
-5 000
-4 000
-3 000
-2 000
-1 000
0
1 000
2 000
3 000
4 000
5 000
6 000
7 000
8 000
9 000
10 000
11 000
12 000
13 000
-20 000
-18 000
-16 000
-14 000
-12 000
-10 000
-8 000
-6 000
-4 000
-2 000
0
2 000
4 000
6 000
8 000
10 000
12 000
14 000
16 000
18 000
20 000

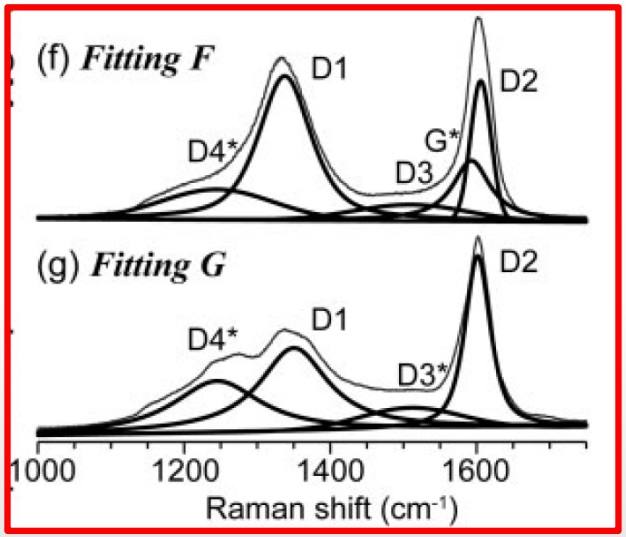
Finding the right spot

- Covered by transparent mineral
  - not too close to the surface
  - not too deep



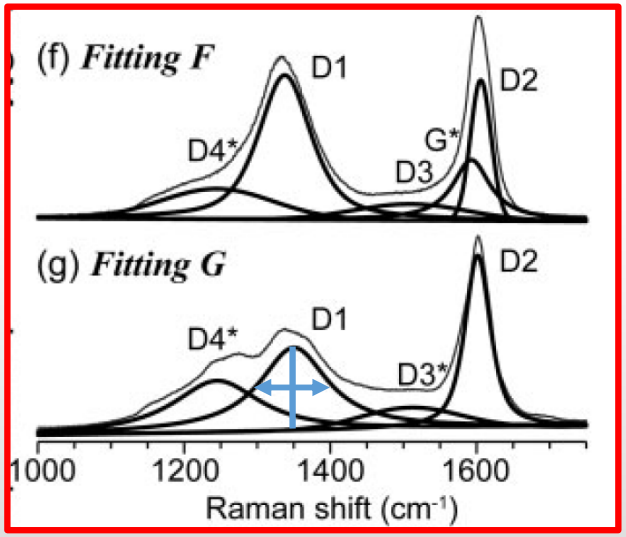
RSCM


CM Raman spectra
Peak decomposition
K04
655±25°C
N3
604±25°C
N29
443±29°C
TK15
380±20°C
K08
340±25°C
RS9
301±30°C
NB02
233±30°C
Kr6
165±35°C
Well-crystallized graphite
High-grade CM (Crystallized graphite)
Medium-grade CM (Transitional material)
Low-grade CM (Amorphous carbon)
(a) Fitting A
(b) Fitting B
(c) Fitting C
(d) Fitting D
(e) Fitting E
(f) Fitting F
(g) Fitting G
G
D1
D2
D3
D4*
G*
D3*
1000
1200
1400
1600
1800
Raman shift (cm-1)
Kouketsu et al. (2014)

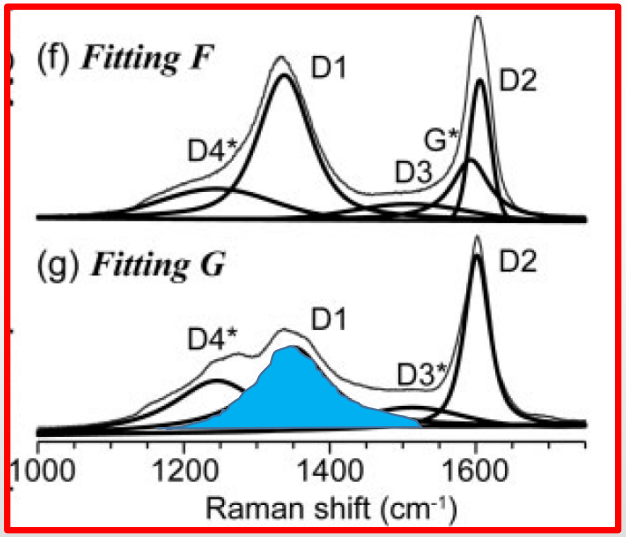

(f) Fitting F
D1
D2
D4*
G*
D3
(g) Fitting G
D2
D1
D4*
D3*
1000
1200
1400
1600
Raman shift (cm-1)

RSCM

FWHM



Area



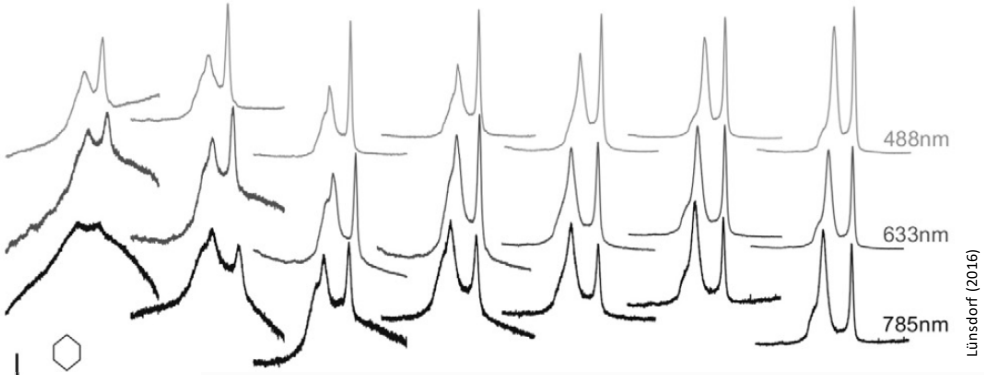
Kouketsu et al. (2014)

Existing thermometers

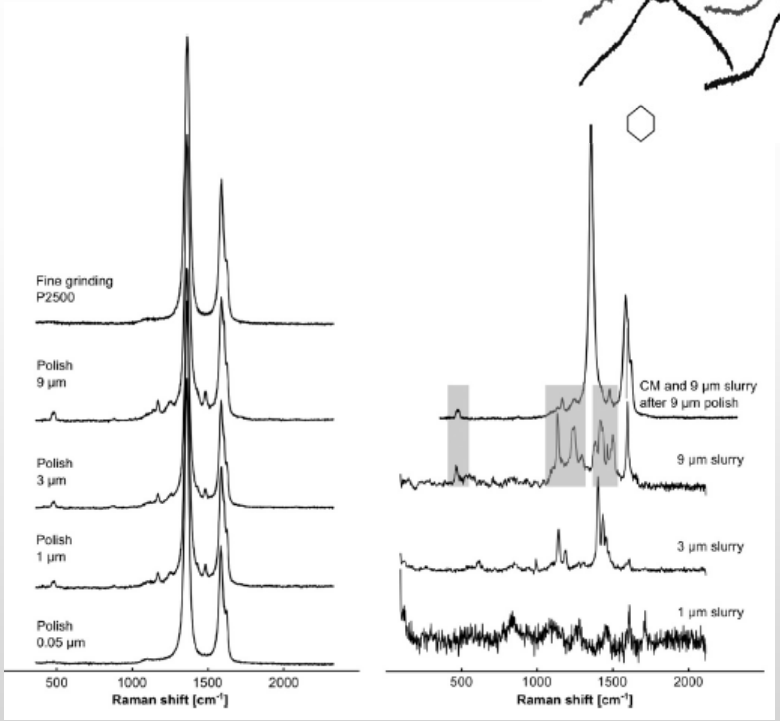
In Jena:
- 457 nm
- 532 nm
- 633 nm
- 785 nm

Thermometer	Laser	T range	Method
Beyssac et al. (2002a)	514.5 nm	330-650°C	height & area
Kouketsu (2014)	532 nm	165-665°C	FWHM
Lahfid (2010)	514.5 nm	200-320°C	area
Lünsdorf (2016)	488 nm (& others)	160-600°C	STA & height
Rahl (2005)	532 nm	100-700°C	area
Scharf (2013)	514.5 nm	100-700°C	height & area

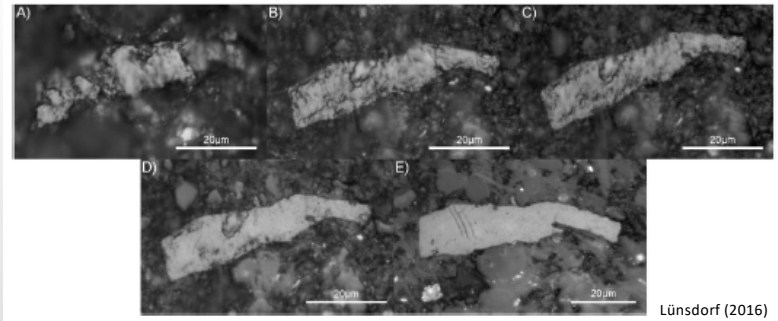
Lünsdorf



Lünsdorf (2016)



Lünsdorf (2016)



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IFORS

Iterative fitting of raman spectroscopy

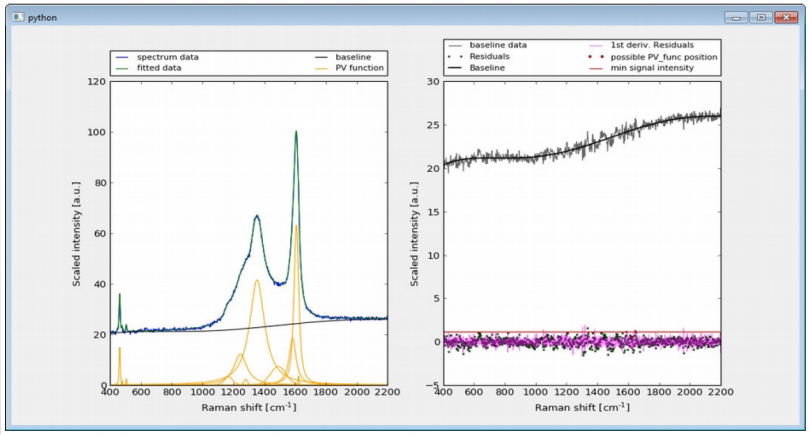


Figure 5: The live-view window showing a curve-fit in progress.

+

- (semi-)automated fitting
- (semi-)automated T estimation
- very fast

-

- partly “black box”
- config-file
- (no GUI) – cmd line based
- requires calibration !

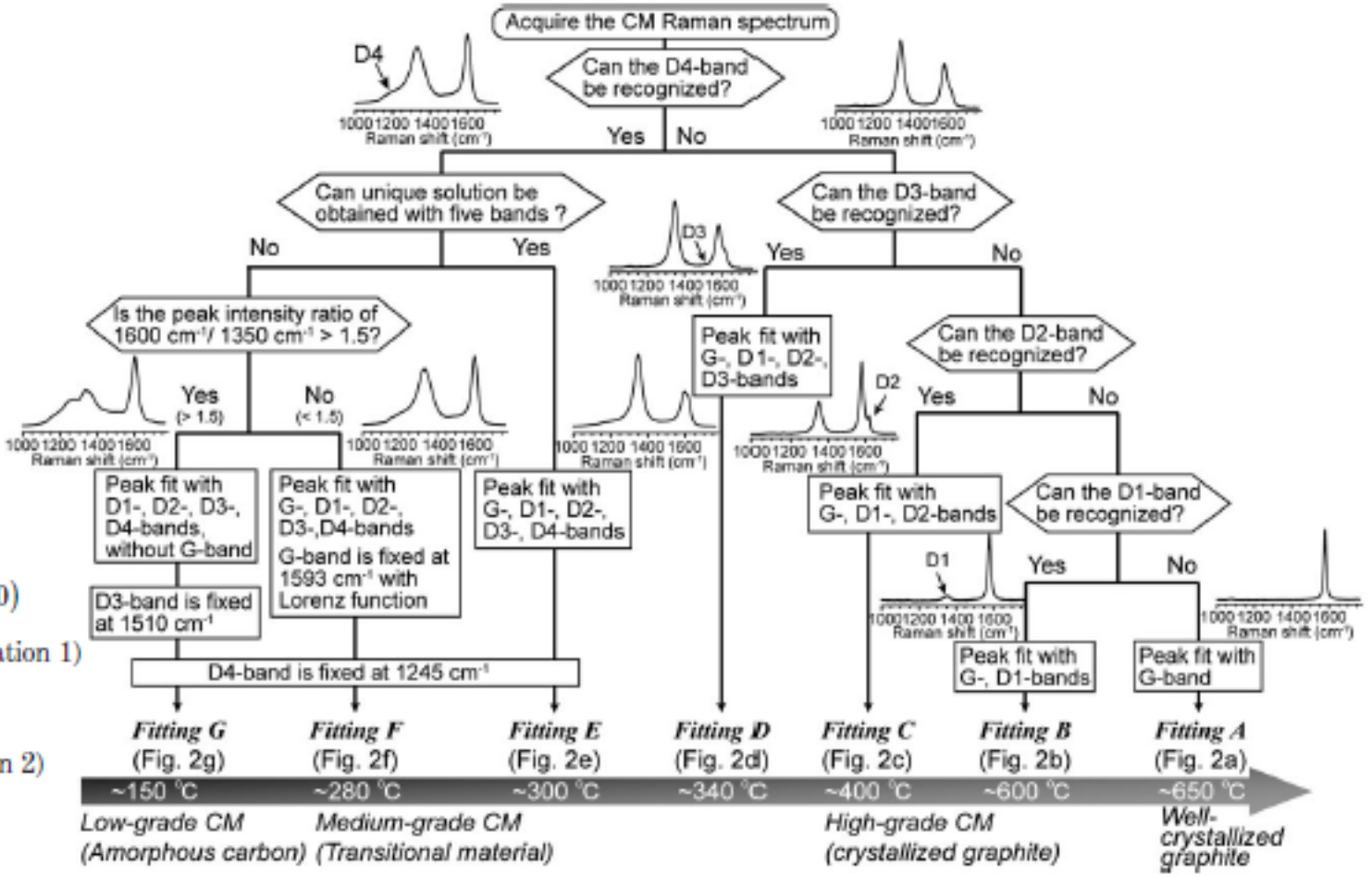
Kouketsu

$$T\,(^{\circ}\mathrm{C}) = -2.15(\mathrm{FWHM\text{-}D1}) + 478$$
$$(\text{coefficient of determination } R^2 = 0.970)$$

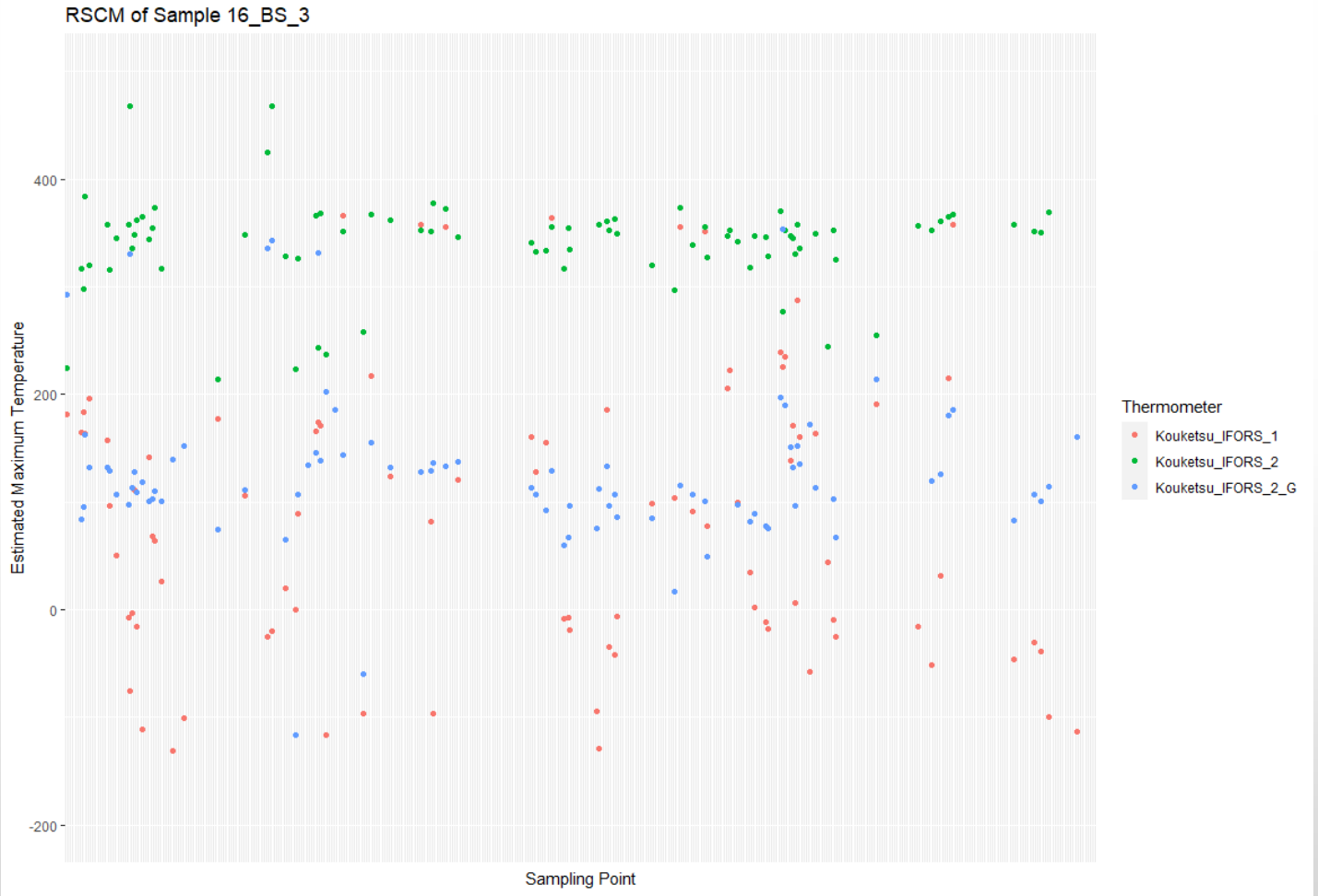
(Equation 1)

$$T\,(^{\circ}\mathrm{C}) = -6.78(\mathrm{FWHM\text{-}D2}) + 535$$
$$(R^2 = 0.968)$$

(Equation 2)



Results Kouketsu IFORS

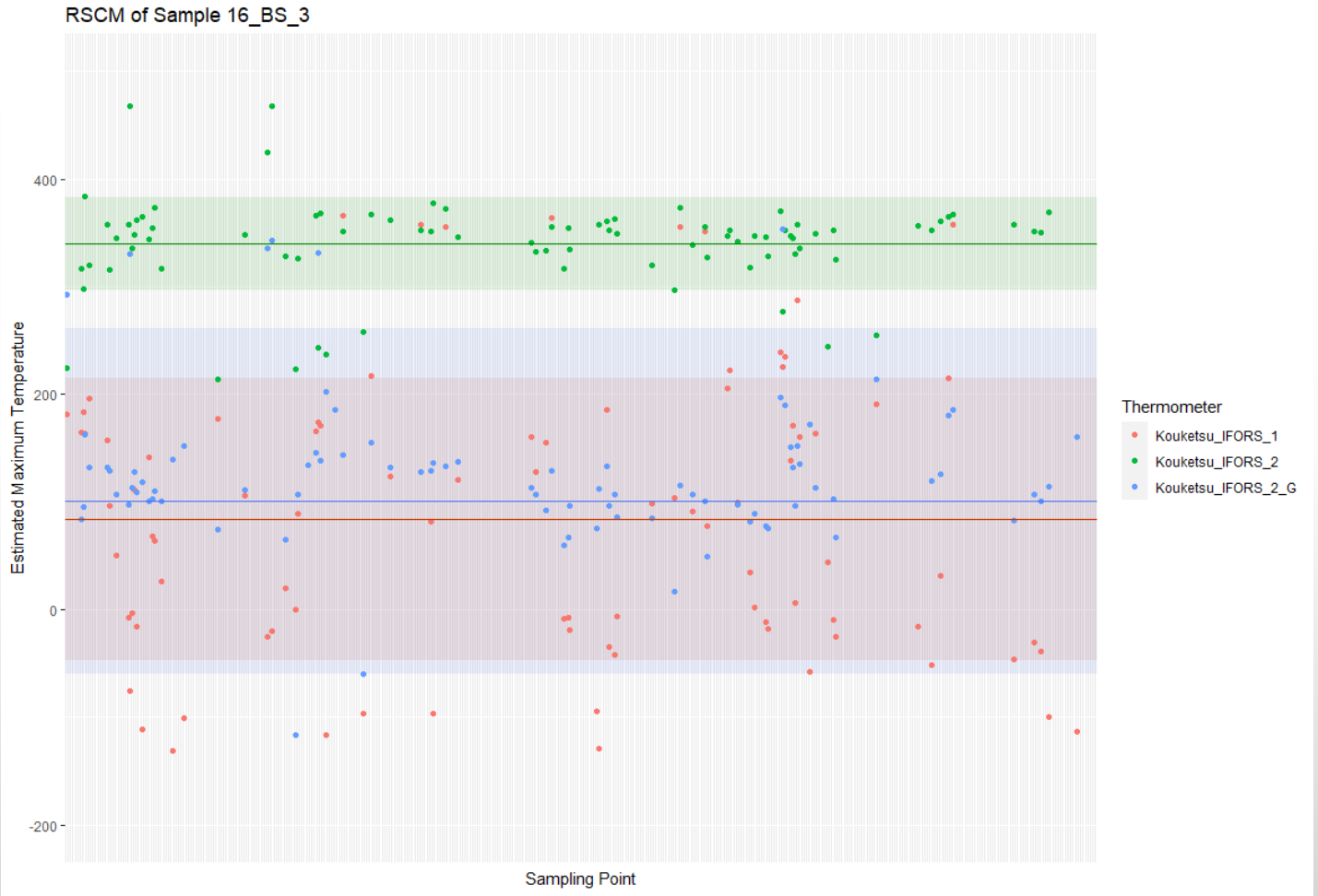


Results Kouketsu IFORS

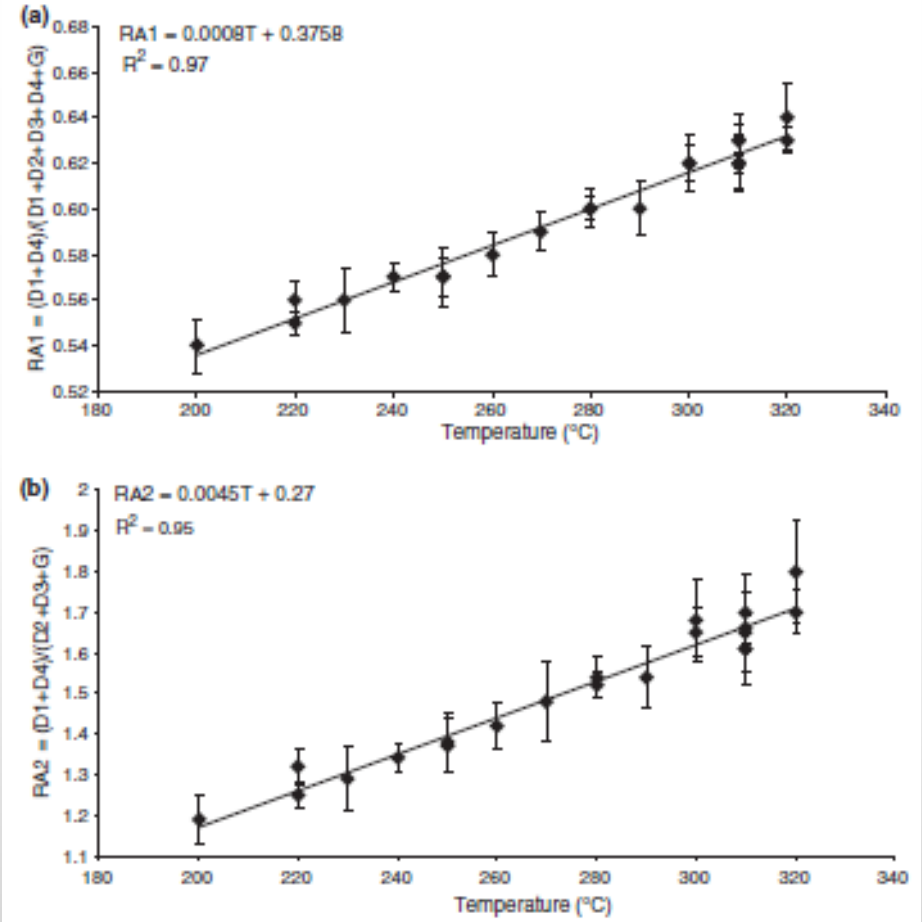
$\bar{x}$ = 340°C
σ = 43°C

$\bar{x}$ = 101°C
σ = 160°C

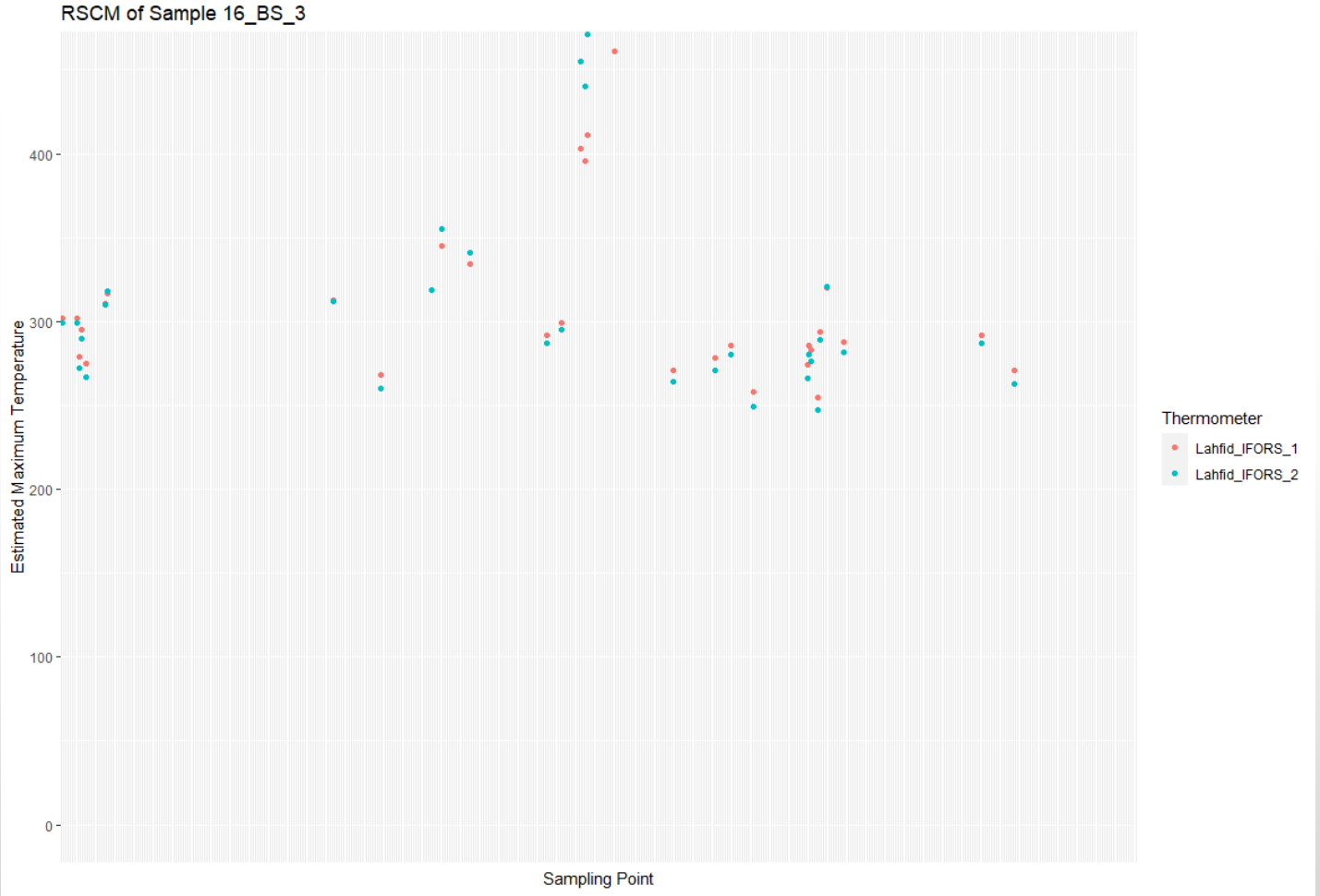
$\bar{x}$ = 84°C
σ = 131°C



Lahfid

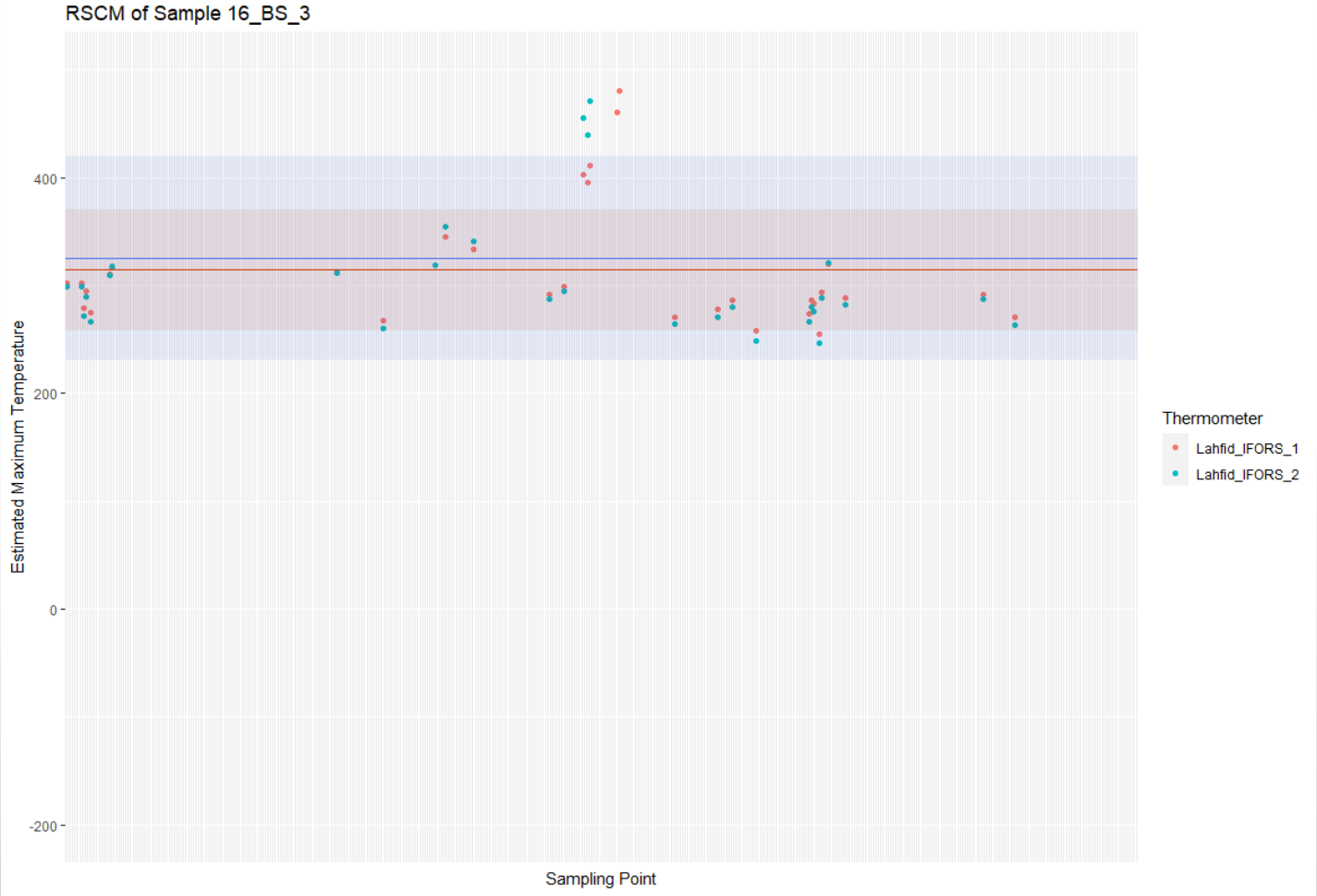

(a)
RA1 = 0.0008T + 0.3758
R² = 0.97
RA1 = (D1+D4)/(D1+D2+D3+D4+G)
Temperature (°C)
(b)
RA2 = 0.0045T + 0.27
R² = 0.95
RA2 = (D1+D4)/(D2+D3+G)
Temperature (°C)

Results Lahfid IFORS

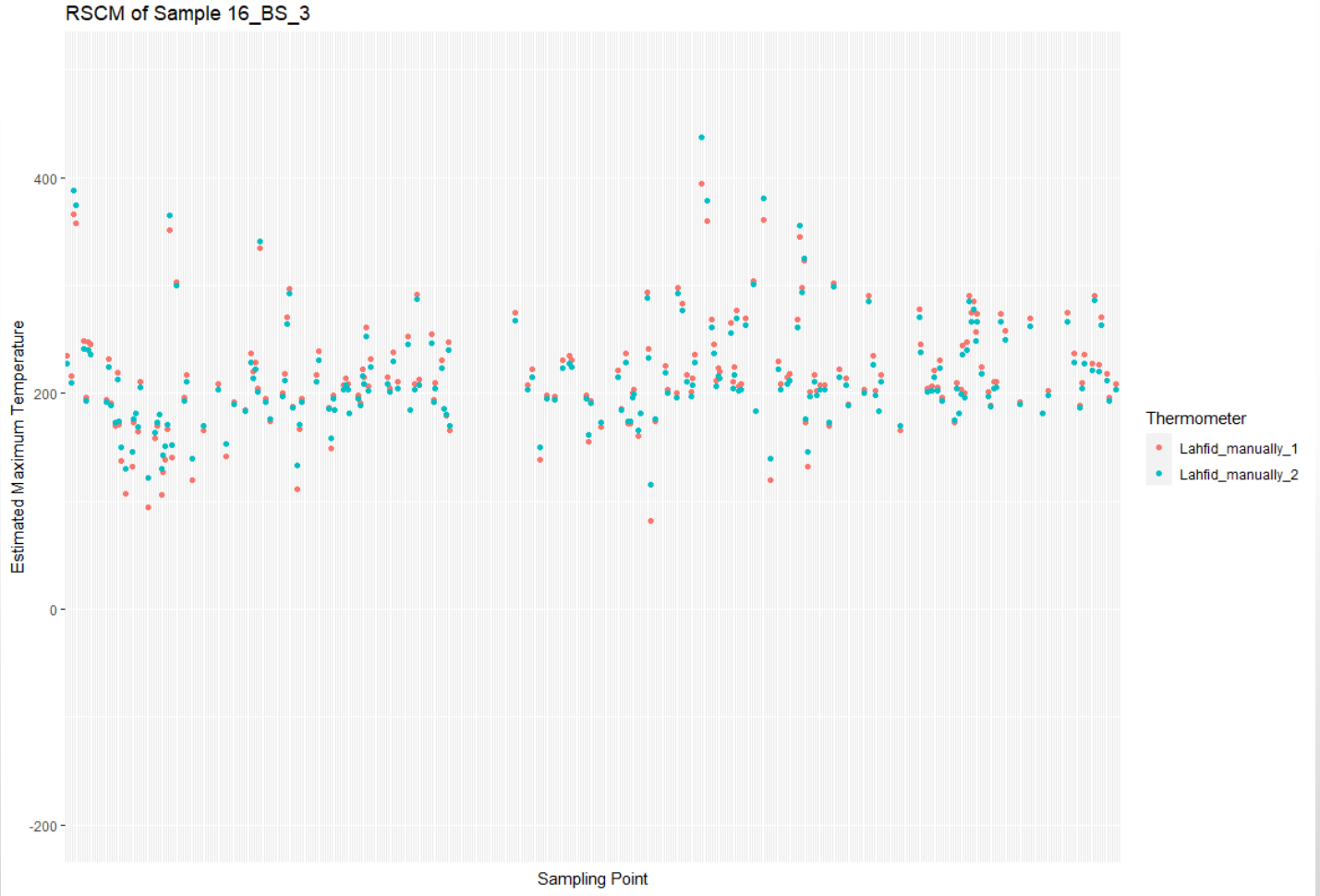


Results Lahfid IFORS

$\bar{x}$ = 325°C
σ = 95°C
$\bar{x}$ = 314°C
σ = 56°C

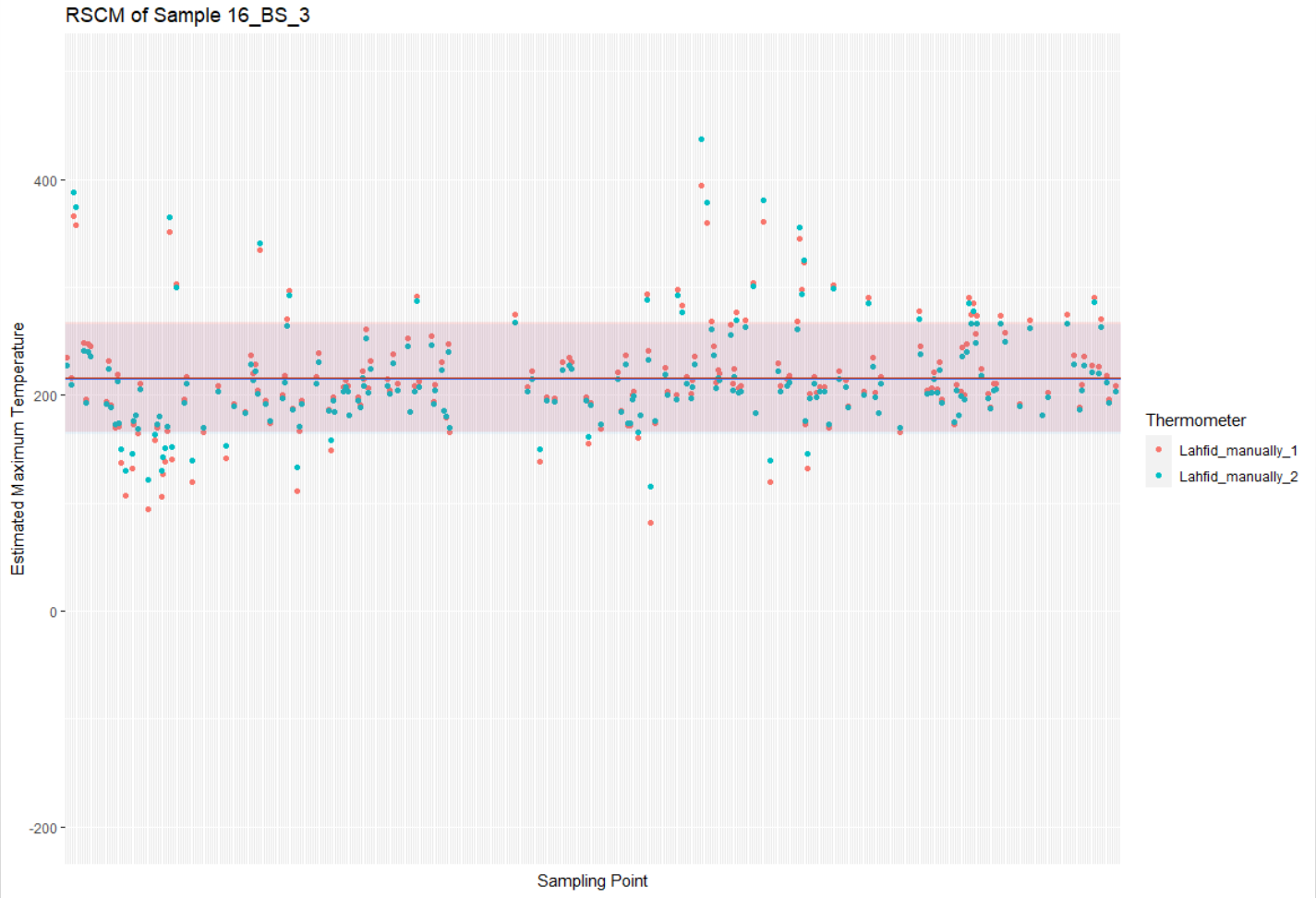


Results Lahfid manually

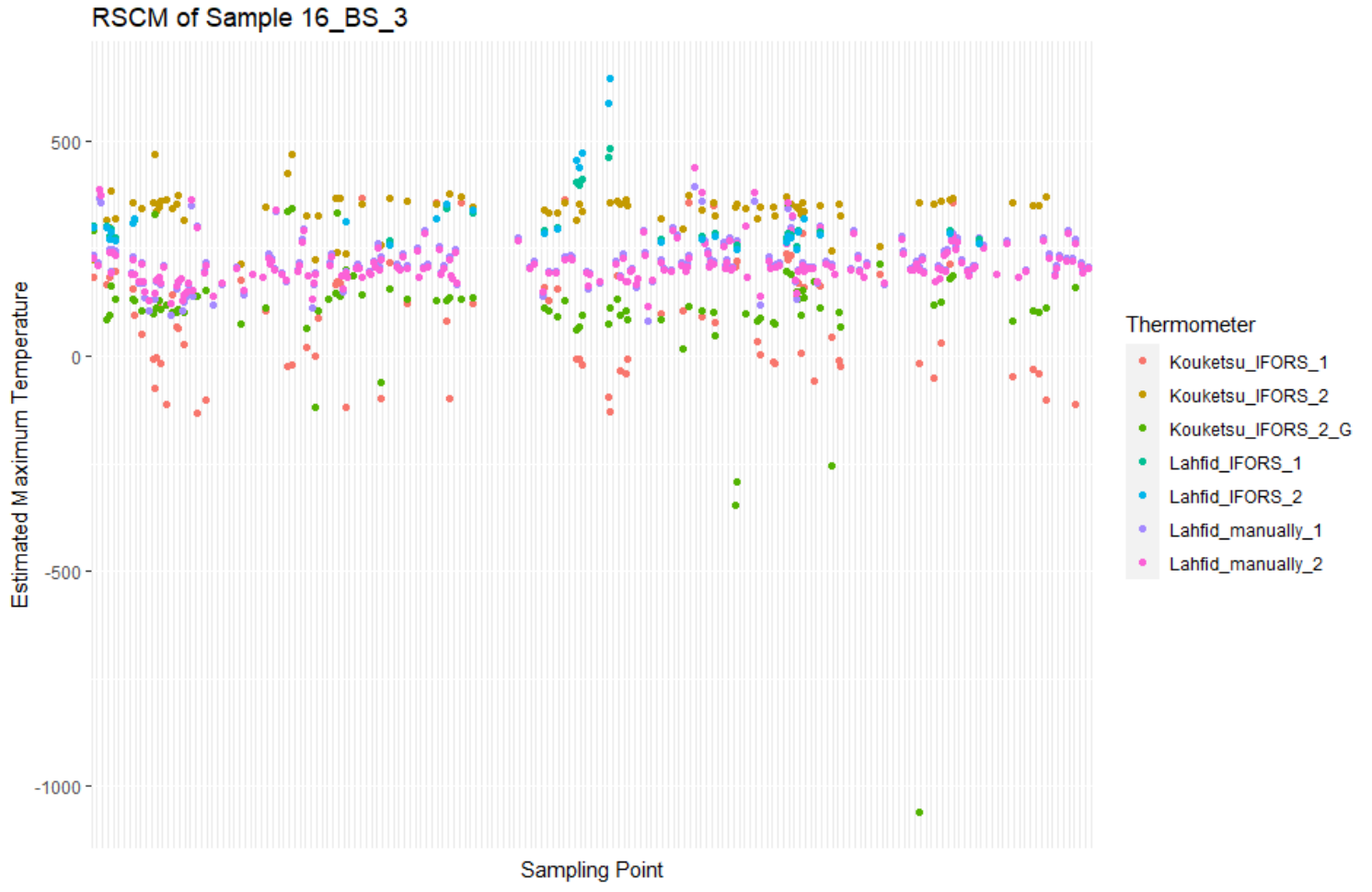


Results Lahfid manually

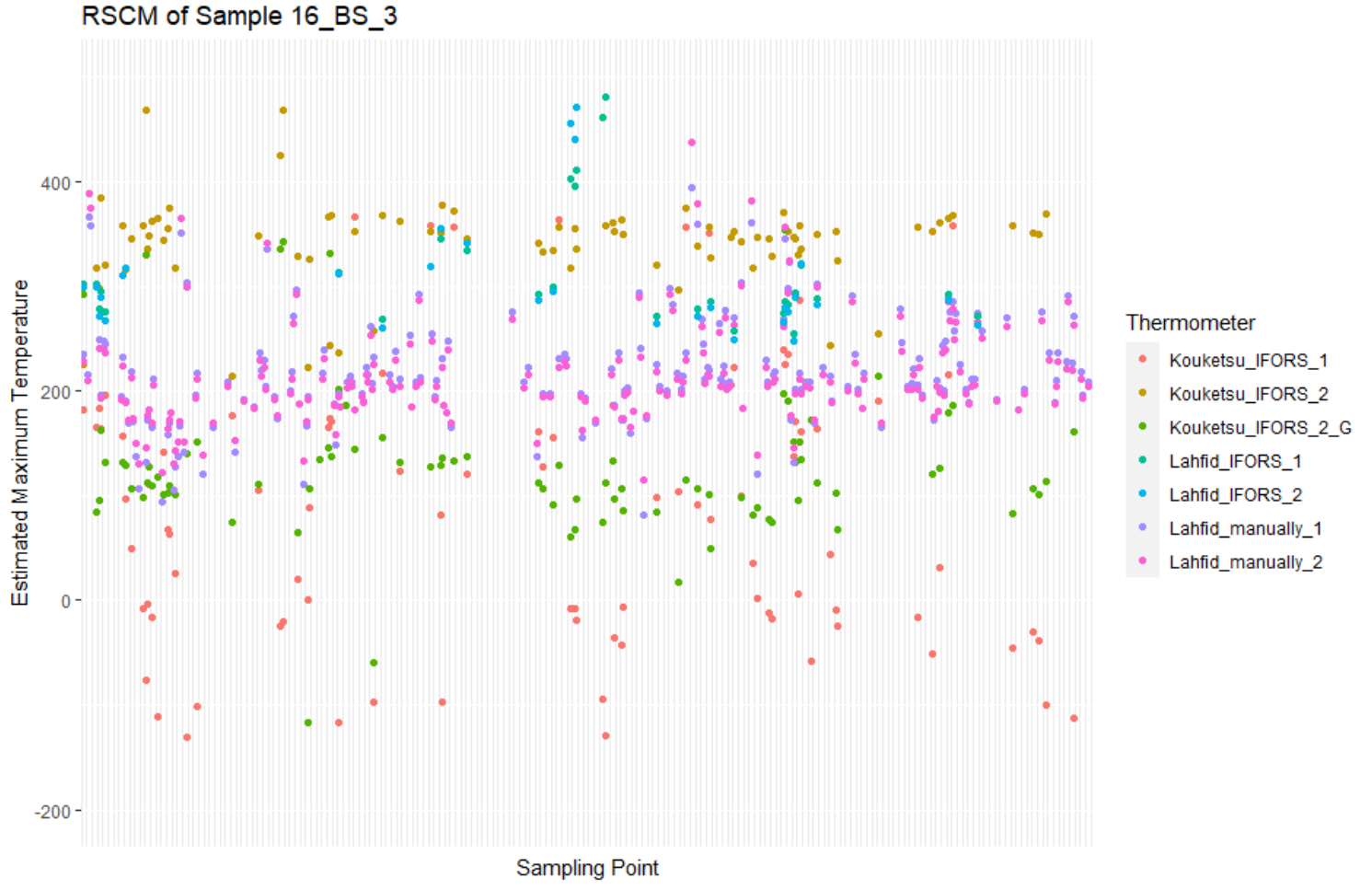
$\bar{x}$ = 216°C
σ = 51°C
$\bar{x}$ = 215°C
σ = 51°C



Results compared

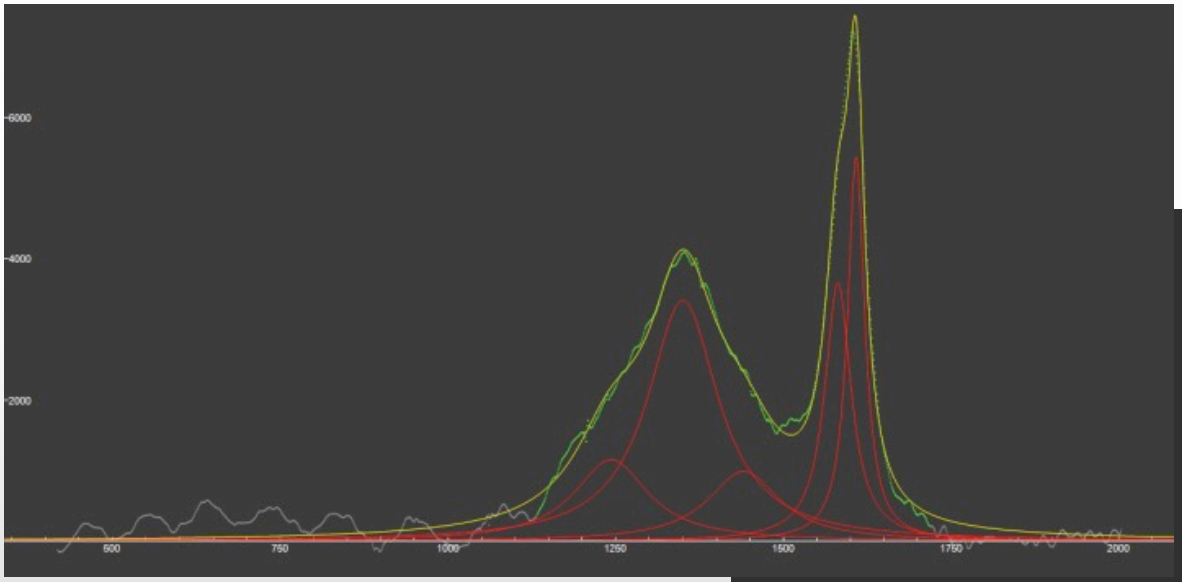


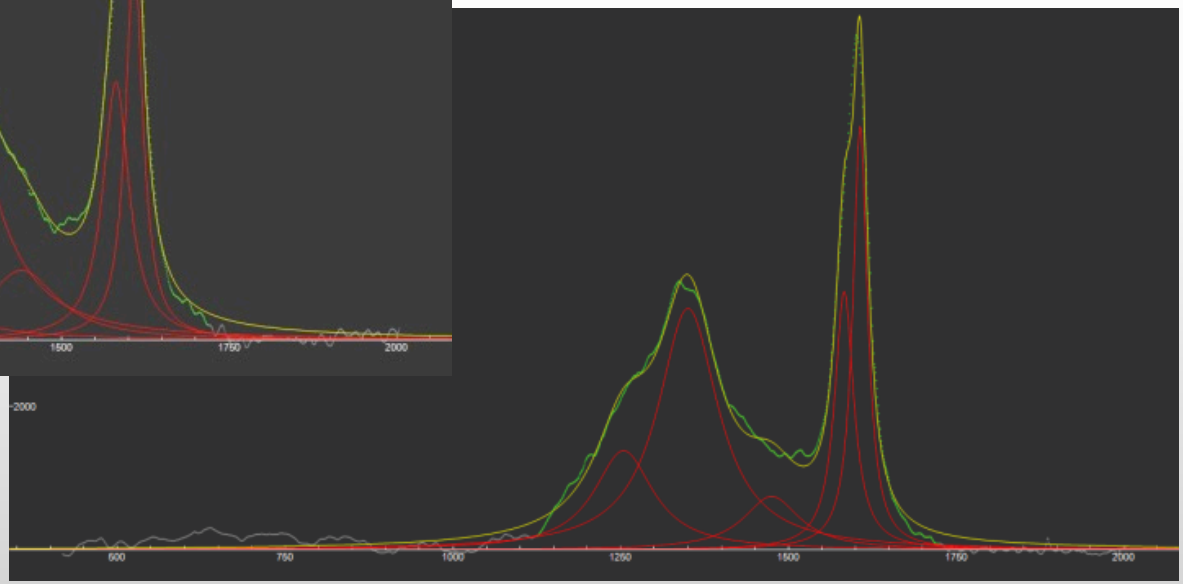
Results compared



Quality management

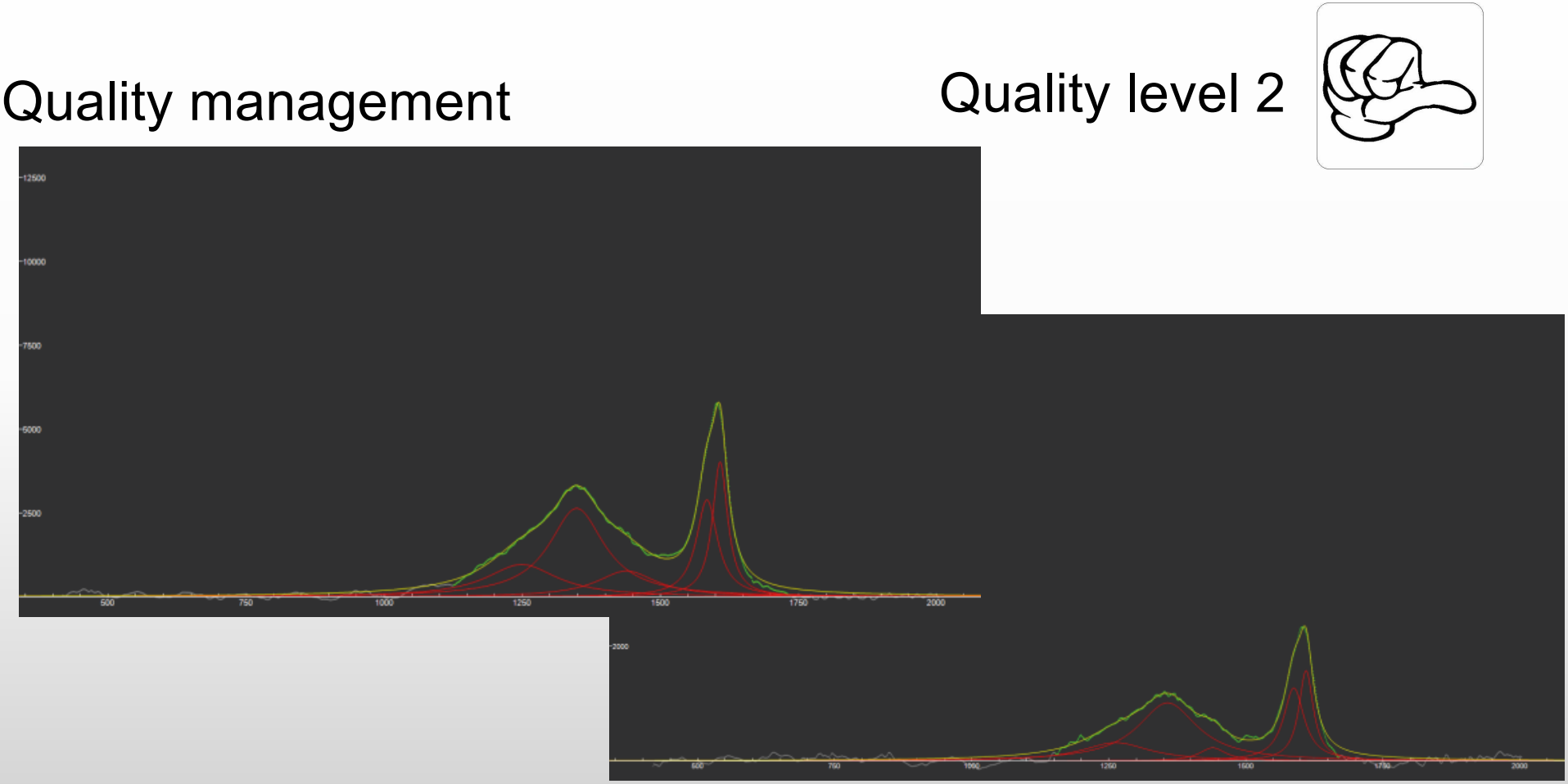
Quality level 1





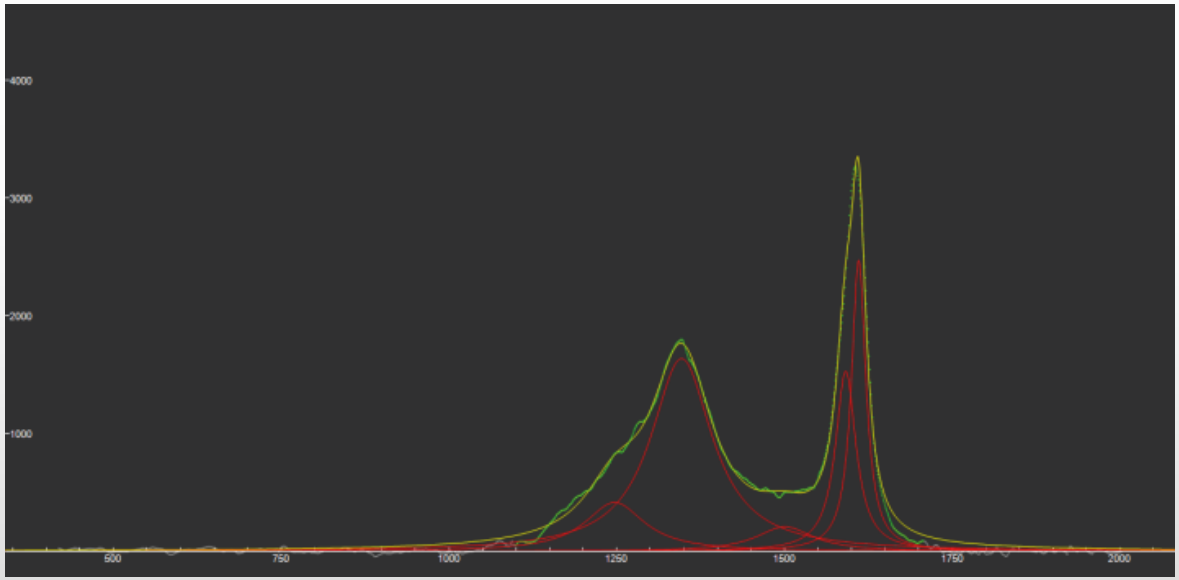
Quality management

Quality level 2

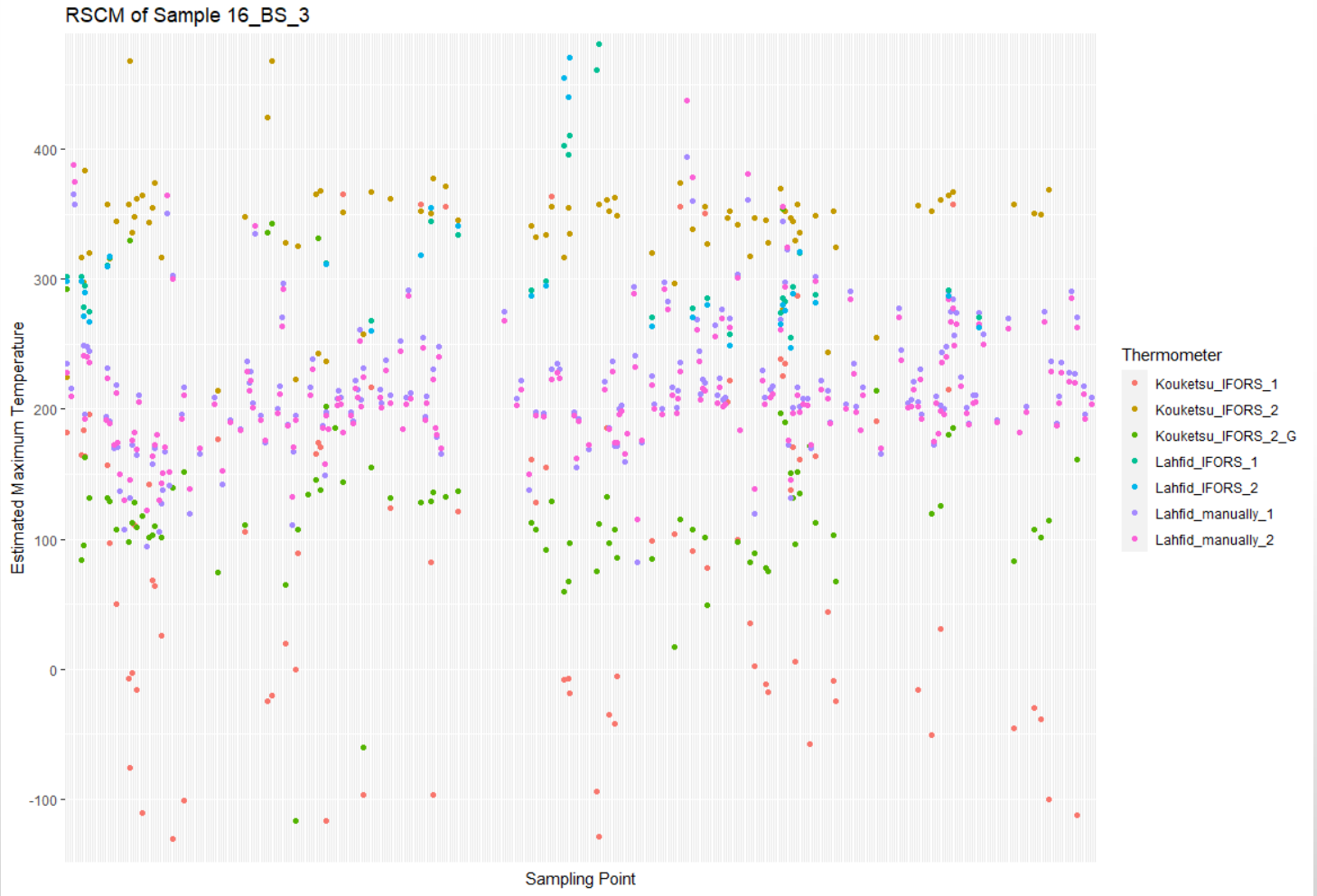


Quality management

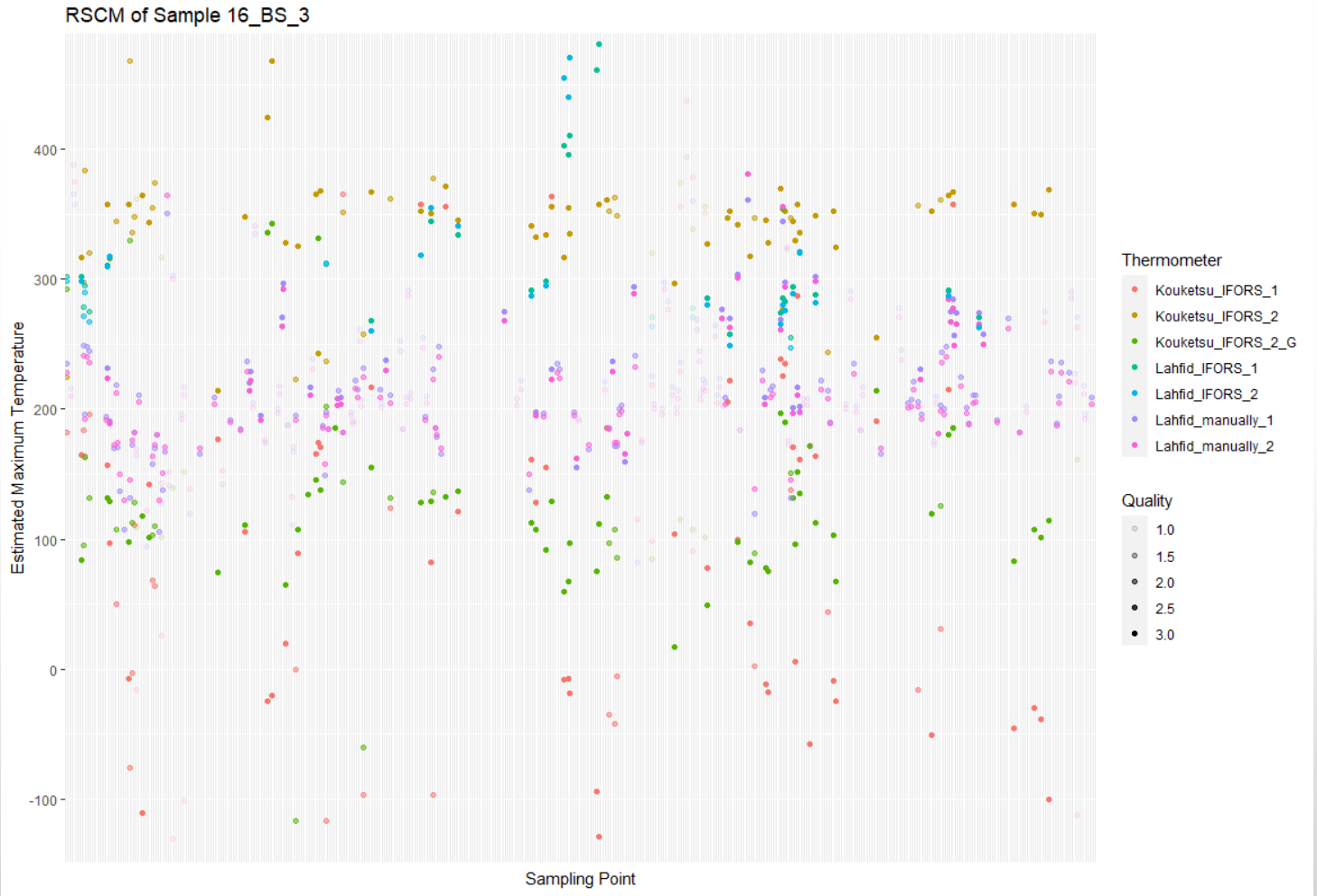
Quality level 3



Results compared

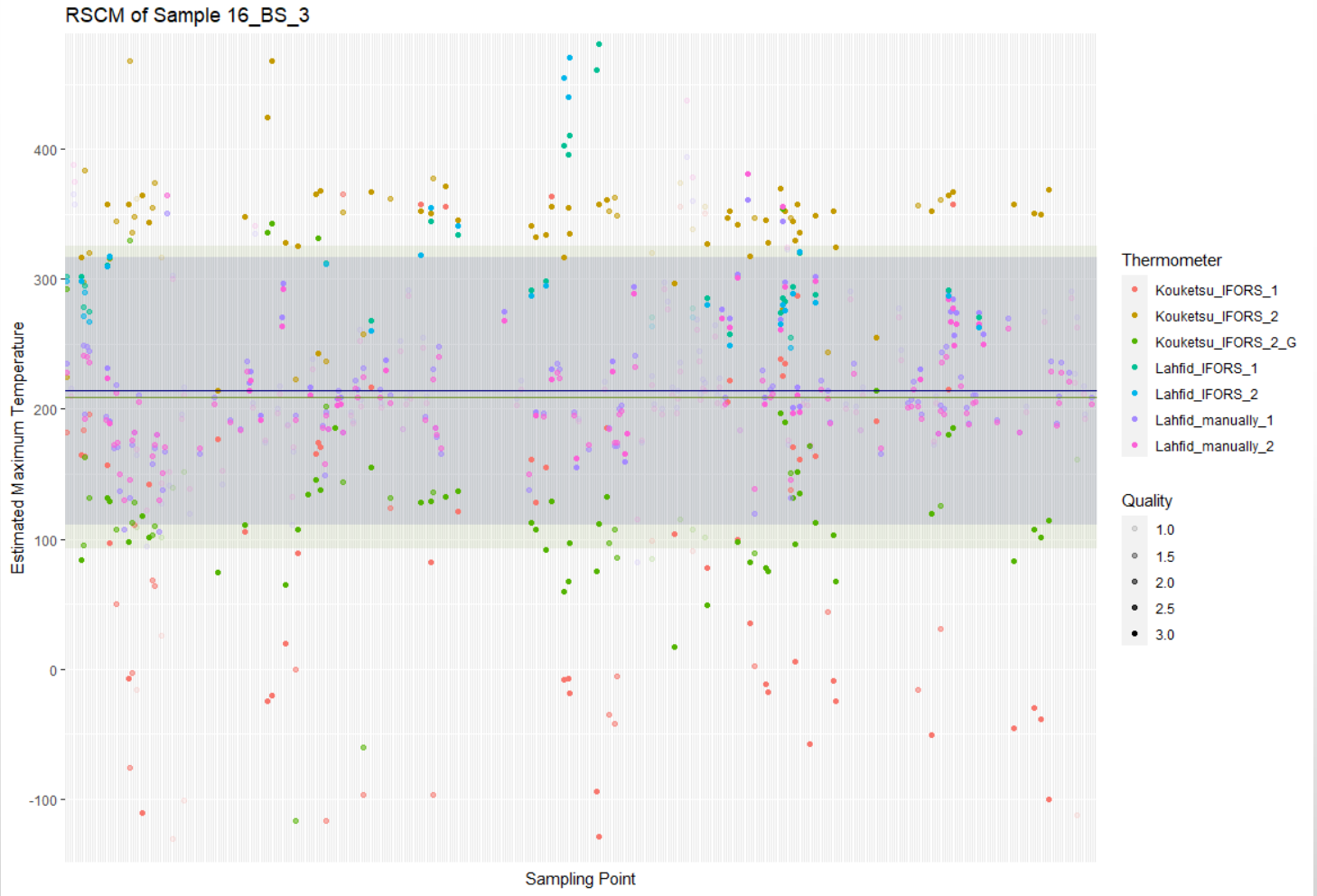


Results compared

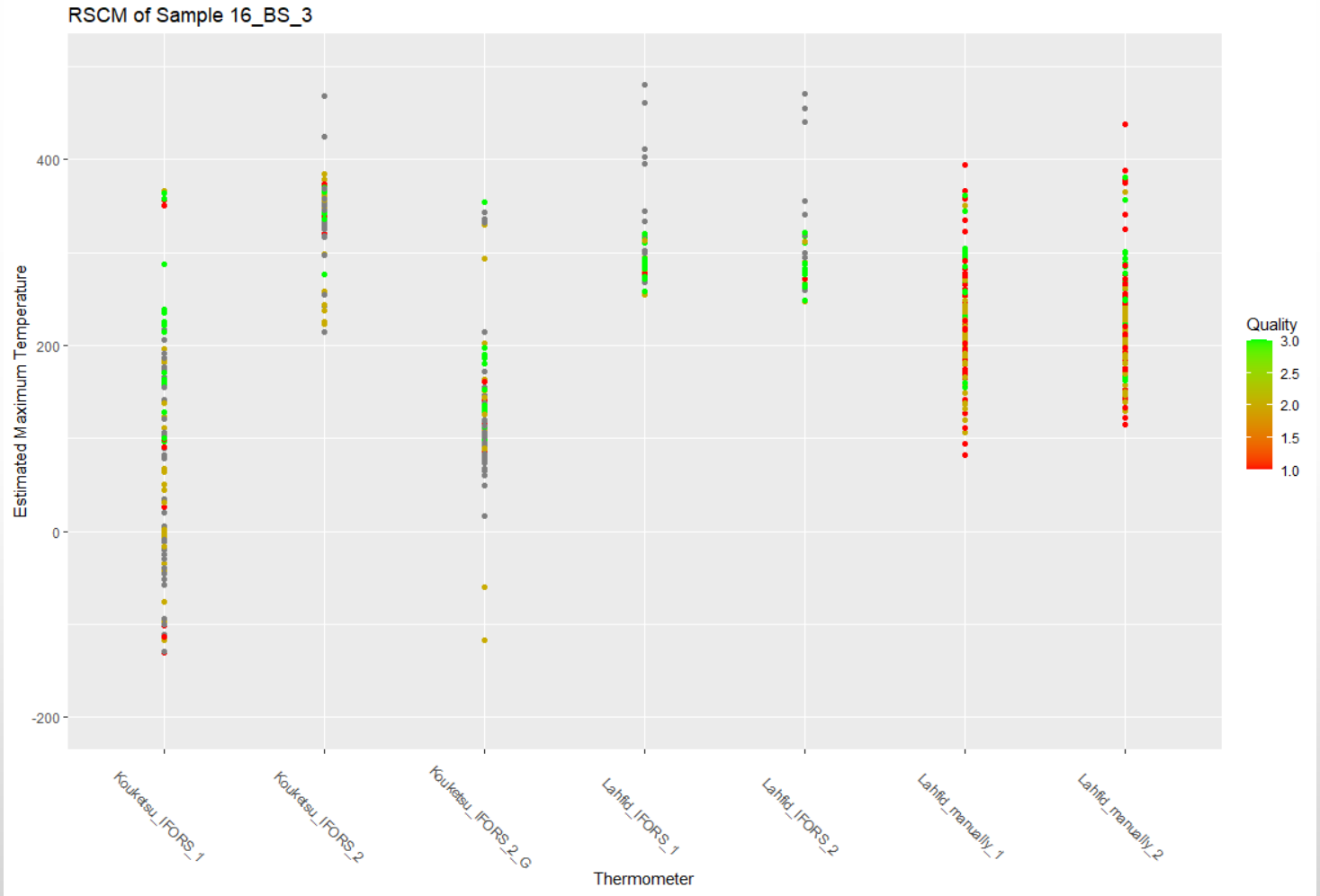


Results compared

$\bar{x}$ = 214°C
σ = 103°C
$\bar{x}$ = 209°C
σ = 116°C

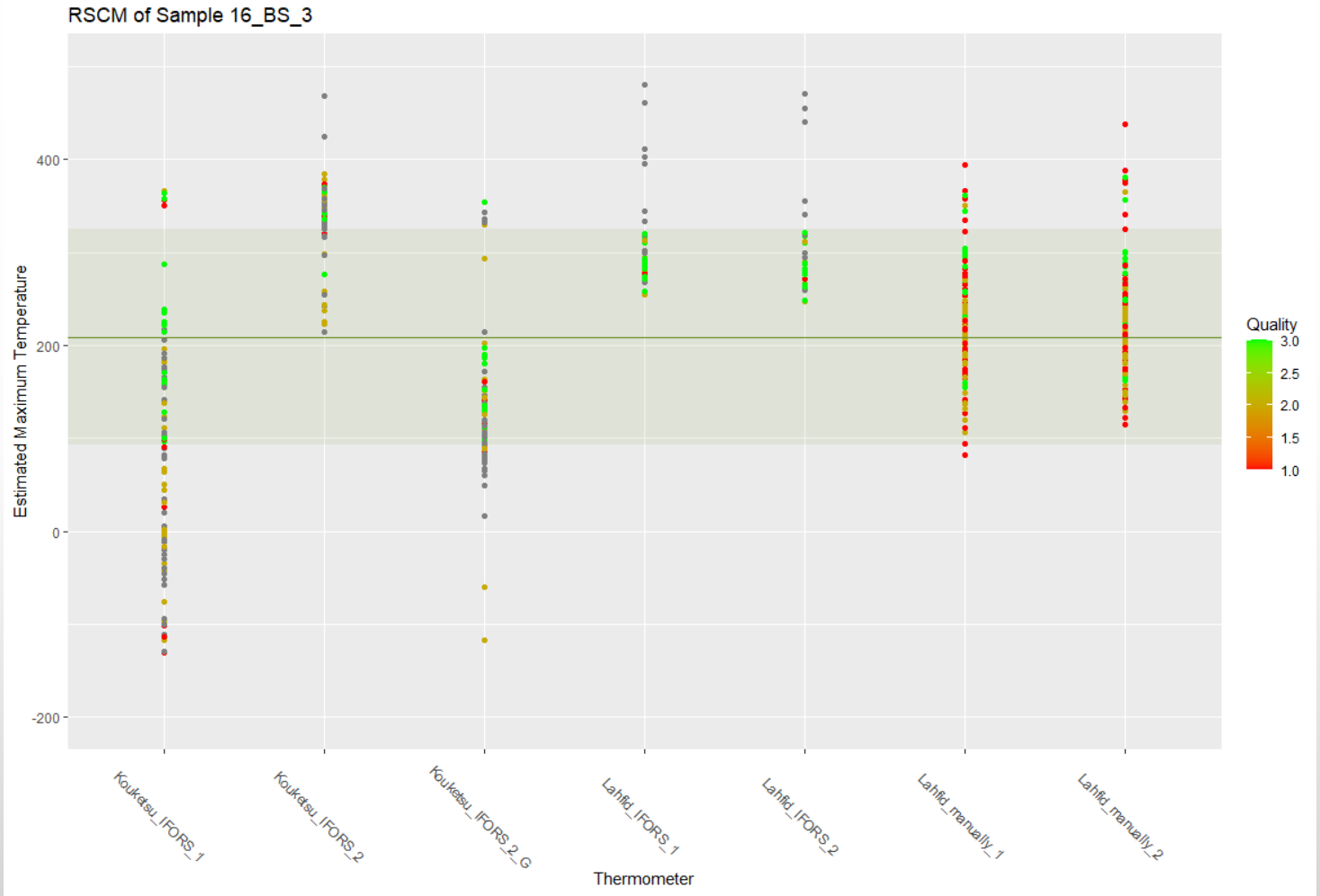


Results compared



Results compared

$\bar{x}$ = 209°C
σ = 116°C



Results compared

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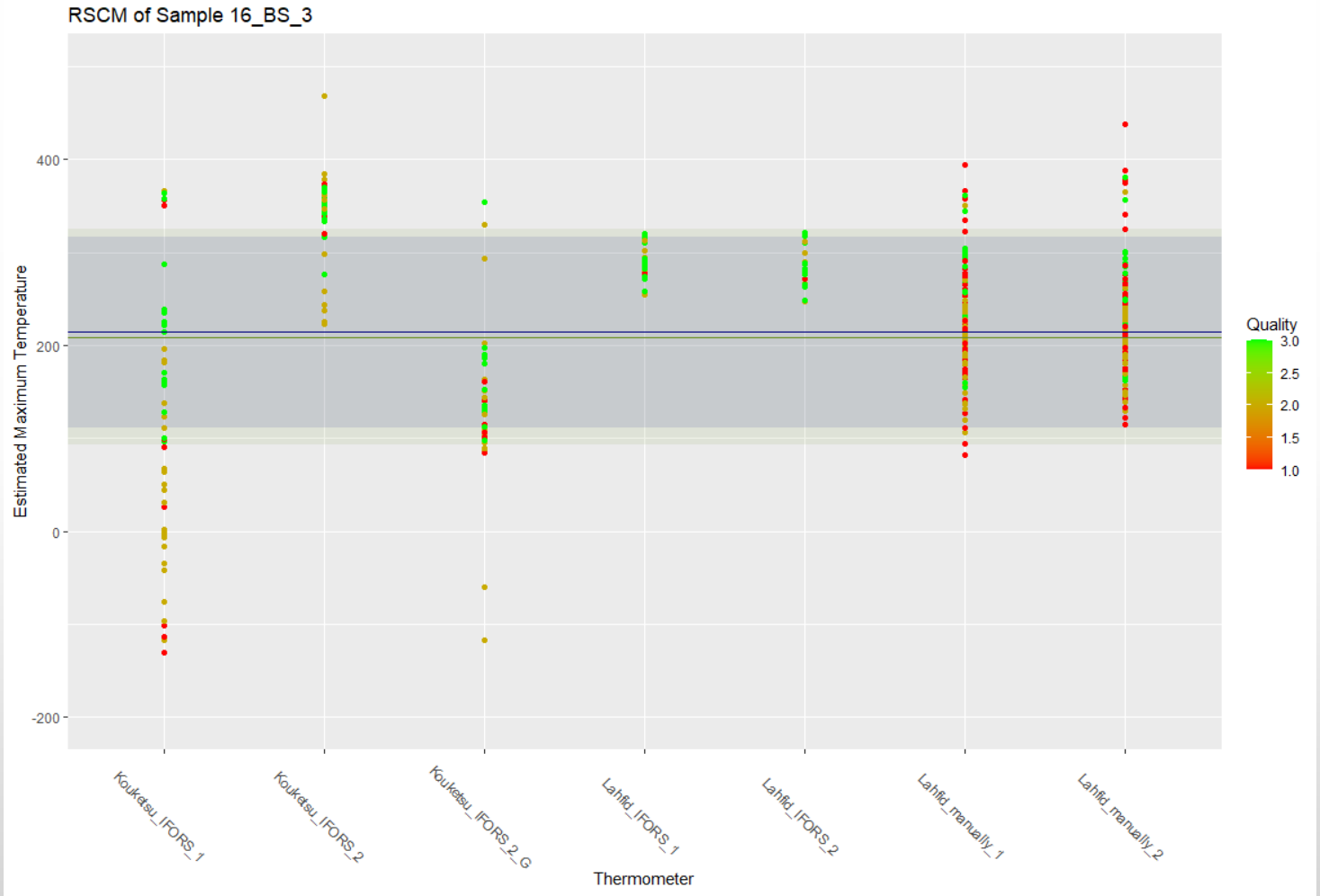
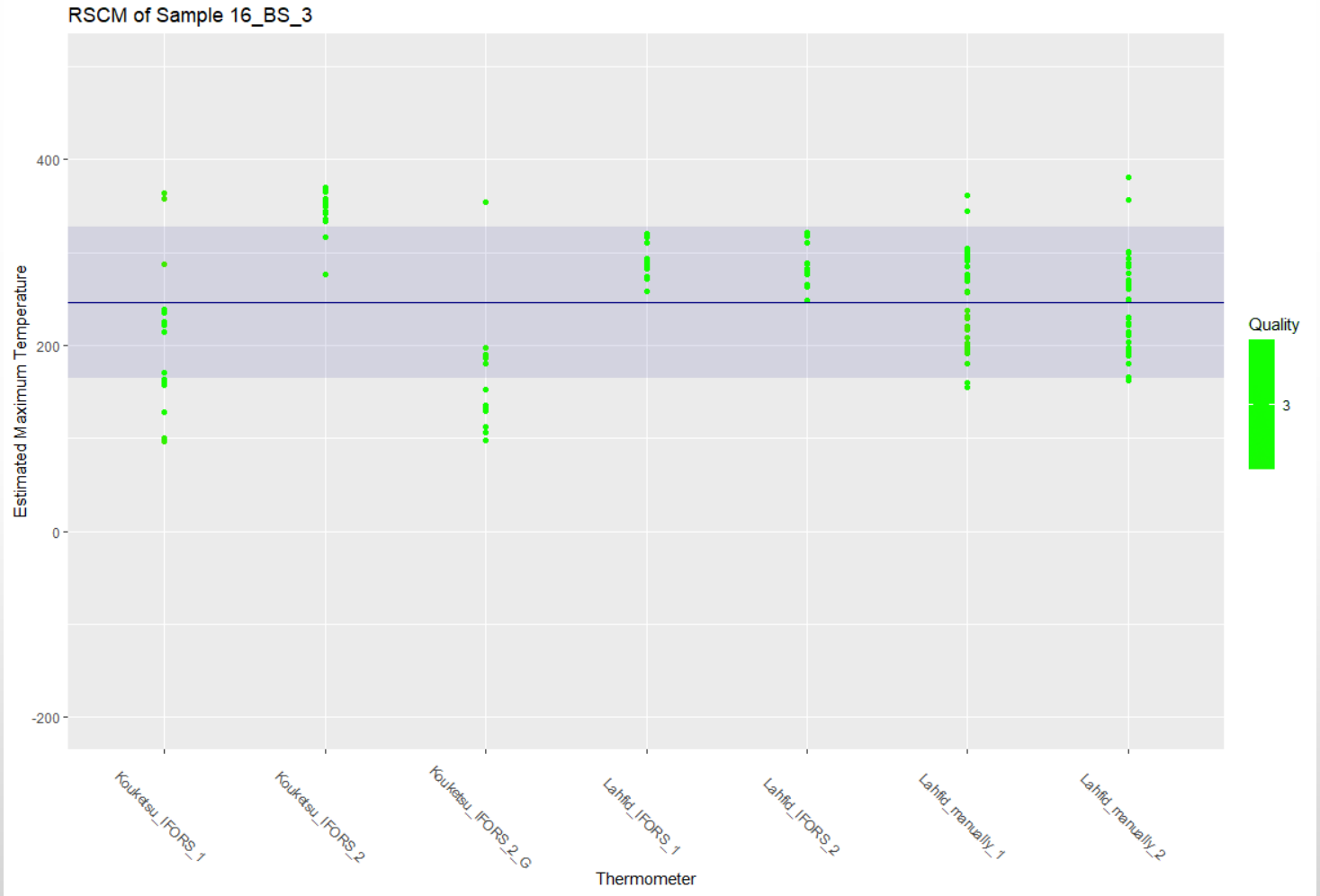
σ = 116°C



Results compared

$\bar{x}$ = 246°C
σ = 81°C



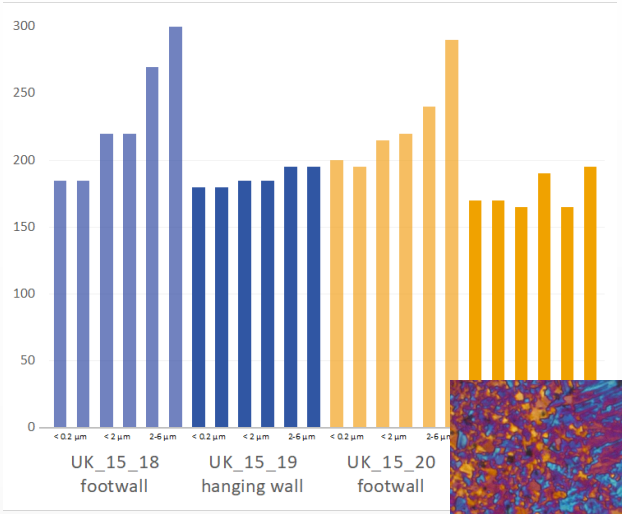
Conclusions

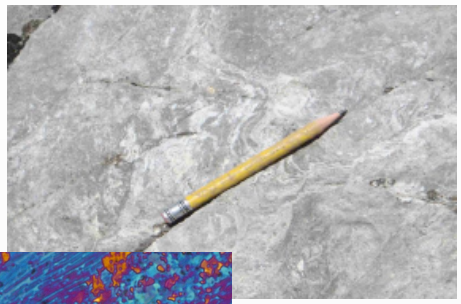
- Smallest stdv: Lahfid (IFORS)
- Closest to overall mean: Lahfid (manually)

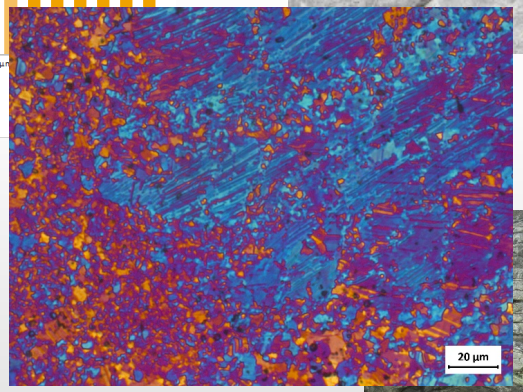
Thermometer	Min.Temp	Max.Temp	Mean.Temp	Stdv	Measurments
Kouketsu_IFORS_1	-131	336	122	132	48
Kouketsu_IFORS_2	223	468	339	43	45
Kouketsu_IFORS_2_G	-293	354	117	117	47
Lahfid_IFORS_1	255	320	289	19	47
Lahfid_IFORS_2	247	321	284	22	47
Lahfid_manually_1	82	394	219	50	382
Lahfid_manually_2	115	438	217	48	382
Kouketsu_IFORS_total	-293	354	192	147	140
Lahfid_IFORS_total	247	321	286	20	94
Lahfid_manually_total	82	438	218	49	764

Supporting indicators

- Illite crystallinity
  - 200°C
- Calcite twins in calcareous mylonite
  - 230°C
- Beginning of shear-folding
  - Brittle-ductile transition zone







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Illite
$K_2Al_4(Si_6Al_2O_{20})(OH_4)$

TOT sheet silicate

Isotope	Occurrence	$T_{1/2}$
^{39}K	93,26 %	stable
^{40}K	0,0117 %	1,248 x 10^9 a
^{41}K	6,73 %	stable

Forming conditions:

- ≥ 60°: Smectite + K-Feldspar → Illite
- ≥ 100-120°: Kaolinite + K-Feldspar → Illite