How to use UltraFine+® Next Gen Analytics QA/QC – The UltraFine+ Standard (QC_UFF_320)

Why is QA/QC important?

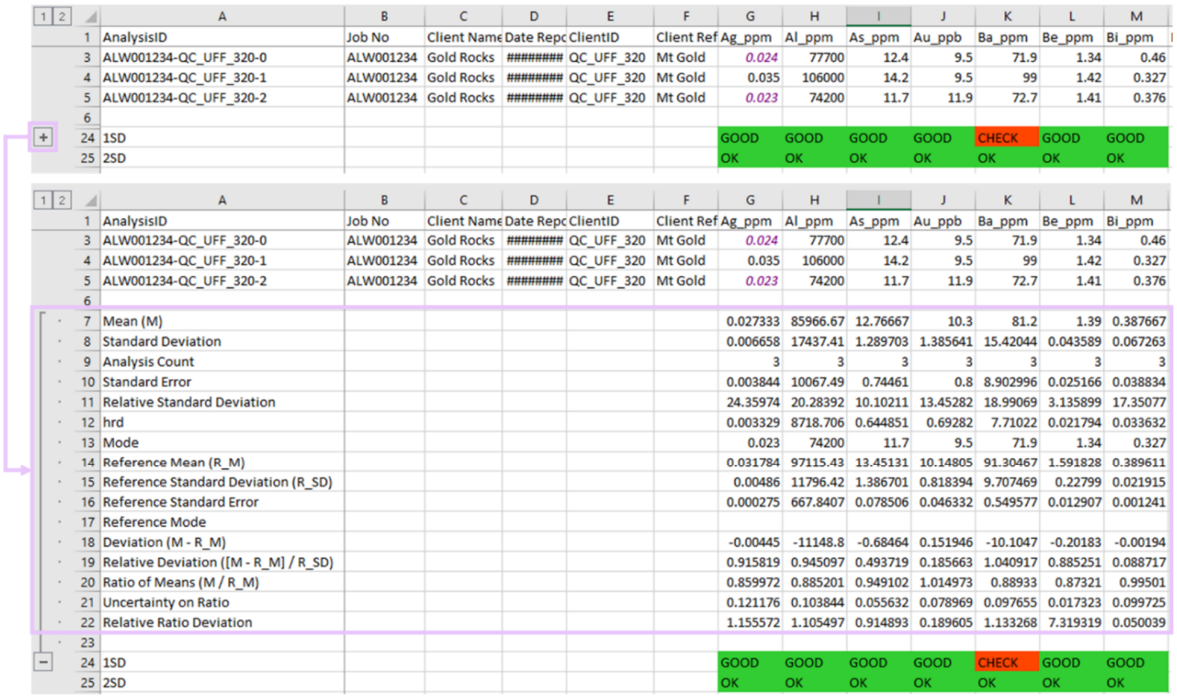
The precision and accuracy of your soil analyses may impact how you interpret your data. Data interpretation can be a tedious manual process, especially when working with many hundreds or thousands of analytical results. This is why we developed a range of statistical QA/QC metrics for CSIRO's UltraFine+® standard, QC_UFF_320. The outputs are designed to provide an overview of analytical quality and repeatability. We use a "traffic light system" to classify measures of the accuracy of the analyses to give you a rapid, first-pass indication of the quality of your analyses.

Where do I find the QA/QC for my samples?

The file *standards_QAQC.xlsx* is in your *Data Package* under *1 Data → QAQC*. The file contains three tabs for geochemistry, VNIR and FTIR analyses (note that the standards are not analysed for size distribution as the UltraFine+® standard is specifically designed to be <2 µm). Automation of the QA/QC workflow requires availability of UltraFine+® standard analyses and consistent formatting of input data. Where this is not provided, your *Data Package* will not include QA/QC.

The Traffic Light System – Geochemistry

Our "traffic light system" is intended to give you a rapid overview of the accuracy of your analyses and whether there is anything you might want to investigate further. For your geochemistry standards analyses, your traffic light is either green or red to indicate whether standards analyses for your data are within one and two standard deviations from the mean of the reference standard, respectively (Figure 1). The mean reference standard values are derived from 312 analyses of the UltraFine+® standard reference material (QC_UFF_320). If everything is green, there is nothing to worry about. If some elements are flagged in red, the first consideration is imprecision close to the detection limit, as this might compromise results. To make this process easy, analyses in ***purple*** font indicate that the value is less than 10 times the detection limit (Figure 1). In addition, analyses in ***green*** font indicate values below the detection limit. These values have been replaced with half the detection limit. Red flags for individual elements can indicate that this element may have been consistently under- or over-reported, and this should be considered when you interpret your geochemical analyses. You can access more detailed information by clicking on the + symbol to open the drop-down calculations (Figure 1) and refer to the table below for an explanation of the calculated parameters. If there are consistent red flags for both one and two standard deviations, the first step would be to check whether this is due to a specific batch effect. If consistent red flags occur across multiple batches for multiple elements, you may want to contact the laboratory for further clarification.



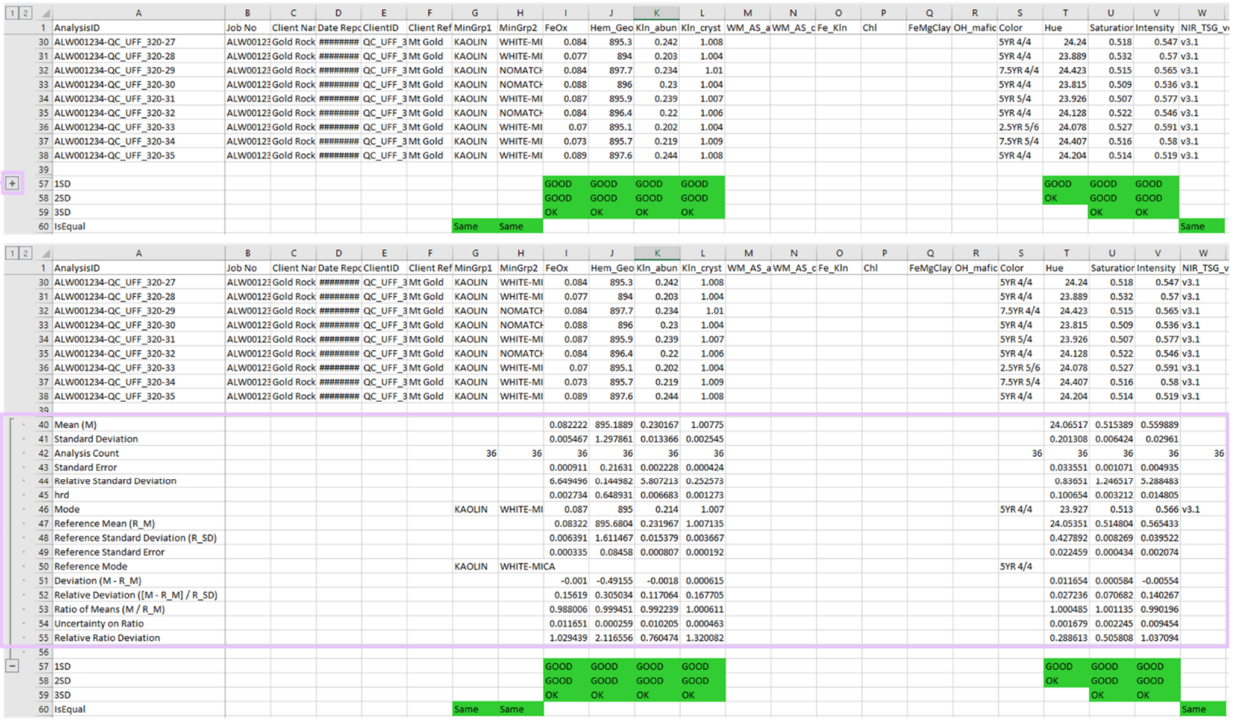
	A	B	C	D	E	F	G	H	I	J	K	L	M
1	AnalysisID	Job No	Client Name	Date Repc	ClientID	Client Ref	Ag_ppm	Al_ppm	As_ppm	Au_ppb	Ba_ppm	Be_ppm	Bi_ppm
3	ALW001234-QC_UFF_320-0	ALW001234	Gold Rocks	########	QC_UFF_320	Mt Gold	0.024	77700	12.4	9.5	71.9	1.34	0.46
4	ALW001234-QC_UFF_320-1	ALW001234	Gold Rocks	########	QC_UFF_320	Mt Gold	0.035	106000	14.2	9.5	99	1.42	0.327
5	ALW001234-QC_UFF_320-2	ALW001234	Gold Rocks	########	QC_UFF_320	Mt Gold	0.023	74200	11.7	11.9	72.7	1.41	0.376
6													
24	1SD						GOOD	GOOD	GOOD	GOOD	CHECK	GOOD	GOOD
25	2SD						OK	OK	OK	OK	OK	OK	OK

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	AnalysisID	Job No	Client Name	Date Repc	ClientID	Client Ref	Ag_ppm	Al_ppm	As_ppm	Au_ppb	Ba_ppm	Be_ppm	Bi_ppm
3	ALW001234-QC_UFF_320-0	ALW001234	Gold Rocks	########	QC_UFF_320	Mt Gold	0.024	77700	12.4	9.5	71.9	1.34	0.46
4	ALW001234-QC_UFF_320-1	ALW001234	Gold Rocks	########	QC_UFF_320	Mt Gold	0.035	106000	14.2	9.5	99	1.42	0.327
5	ALW001234-QC_UFF_320-2	ALW001234	Gold Rocks	########	QC_UFF_320	Mt Gold	0.023	74200	11.7	11.9	72.7	1.41	0.376
6													
7	Mean (M)						0.027333	85966.67	12.76667	10.3	81.2	1.39	0.387667
8	Standard Deviation						0.006658	17437.41	1.289703	1.385641	15.42044	0.043589	0.067263
9	Analysis Count						3	3	3	3	3	3	3
10	Standard Error						0.003844	10067.49	0.74461	0.8	8.902996	0.025166	0.038834
11	Relative Standard Deviation						24.35974	20.28392	10.10211	13.45282	18.99069	3.135899	17.35077
12	hrd						0.003329	8718.706	0.644851	0.69282	7.71022	0.021794	0.033632
13	Mode						0.023	74200	11.7	9.5	71.9	1.34	0.327
14	Reference Mean (R_M)						0.031784	97115.43	13.45131	10.14805	91.30467	1.591828	0.389611
15	Reference Standard Deviation (R_SD)						0.00486	11796.42	1.386701	0.818394	9.707469	0.22799	0.021915
16	Reference Standard Error						0.000275	667.8407	0.078506	0.046332	0.549577	0.012907	0.001241
17	Reference Mode												
18	Deviation (M - R_M)						-0.00445	-11148.8	-0.68464	0.151946	-10.1047	-0.20183	-0.00194
19	Relative Deviation ([M - R_M] / R_SD)						0.915819	0.945097	0.493719	0.185663	1.040917	0.885251	0.088717
20	Ratio of Means (M / R_M)						0.859972	0.885201	0.949102	1.014973	0.88933	0.87321	0.99501
21	Uncertainty on Ratio						0.121176	0.103844	0.055632	0.078969	0.097655	0.017323	0.099725
22	Relative Ratio Deviation						1.155572	1.105497	0.914893	0.189605	1.133268	7.319319	0.050039
23													
24	1SD						GOOD	GOOD	GOOD	GOOD	CHECK	GOOD	GOOD
25	2SD						OK	OK	OK	OK	OK	OK	OK

Figure 1: Example QA/QC output and expanded drop-down menu with more detailed information for geochemical analyses of the UltraFine+® standard (QC_UFF_320).

The Traffic Light System – VNIR

Compared to the well-established QA/QC procedures for geochemical analyses, routine protocols for QA/QC of features/scalars derived from VNIR data at the post-processing stage have not been universally established or adopted. Rather, the spectra are visually examined by an expert user and undergo QA/QC during data acquisition and processing in TSG™. However, we have independently reviewed over four hundred VNIR spectra of the QC_UFF_320 standard to enable end-user QA/QC on this data, similar to the geochemical data. Our automated QA/QC compares the standard analyses in your analyses batches to being within one, two or three standard deviations from the mean of the reference standard analyses for most scalars (Figure 2). This is derived from an assessment of the original VNIR spectra and how these spectra relate to the numerical values that are reported. In addition, the *IsEqual* row is used to compare the modal values of categorical properties (non-numerical values). Like the geochemical analyses, if everything is green, there is nothing to worry about. If some scalars are flagged as red you can access more detailed information by clicking on the + symbol to open the drop-down calculations and refer to the table below for an explanation of the calculated parameters. Red flags for individual scalars can indicate that this scalar may not be reliable, this should be considered when you interpret your analyses. These values or anomalous results should be used with caution and checked against other parameters if you are looking to use these numbers to derive a new target for example. If there are consistent red flags for multiple scalars for one, two and three standard deviations, the first step would be to check whether this is due to a specific batch analysis. If consistent red flags across multiple batches occur for multiple scalars, you may want to contact the laboratory for further clarification.



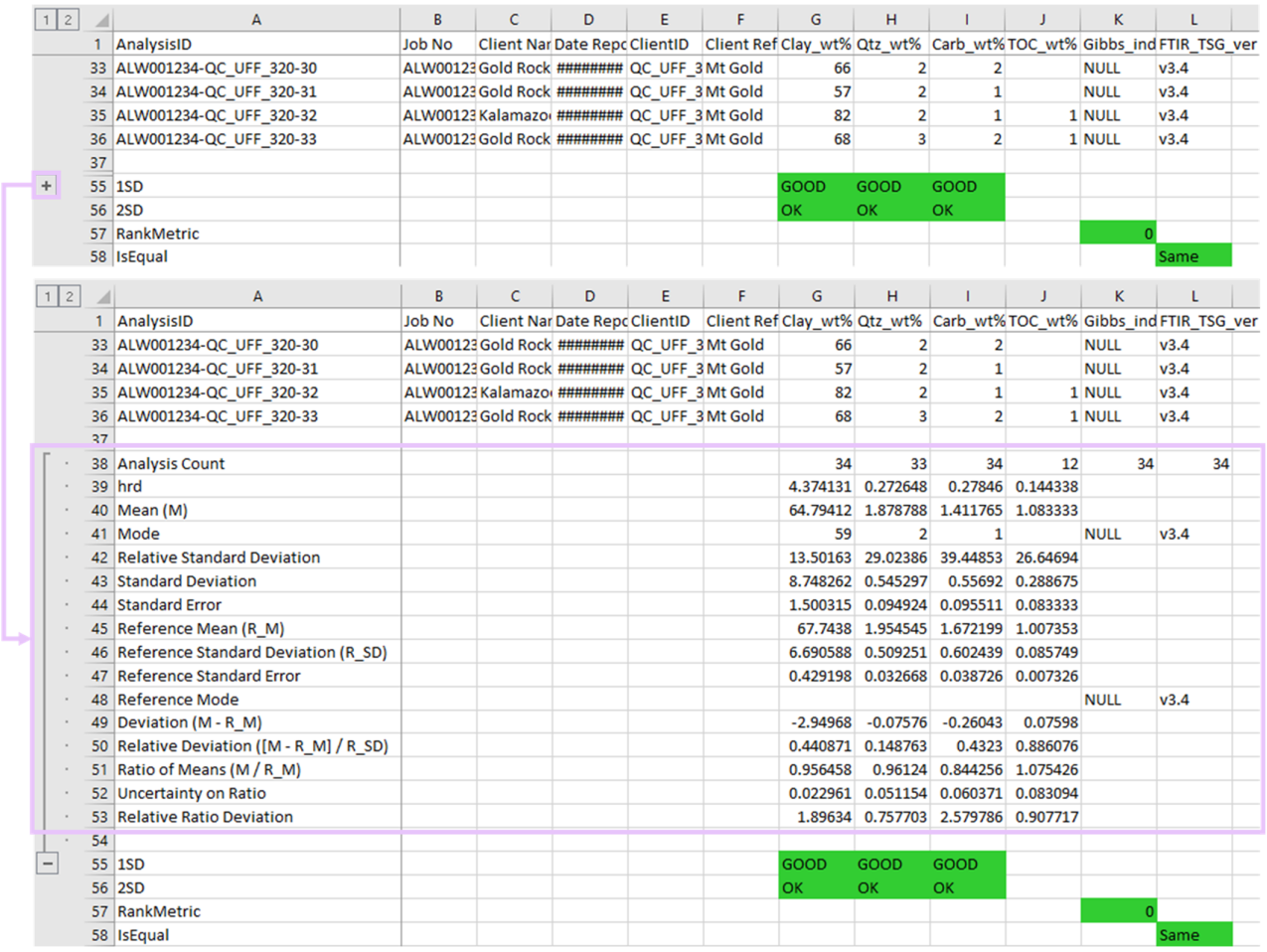
	AnalysisID	Job No	Client Nar	Date Repc	ClientID	Client Ref	MinGrp1	MinGrp2	FeOx	Hem_Geo	Kln_abun	Kln_cryst	WM_AS_a	WM_AS_c	Fe_Kln	Chl	FeMgClay	OH_mafic	Color	Hue	Saturatior	Intensity	NIR_TSG_v
30	ALW001234-QC_UFF_320-27	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.084	895.3	0.242	1.008							5YR 4/4	24.24	0.518	0.547	v3.1
31	ALW001234-QC_UFF_320-28	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.077	894	0.203	1.004							5YR 4/4	23.889	0.532	0.57	v3.1
32	ALW001234-QC_UFF_320-29	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	NOMATCH	0.084	897.7	0.234	1.01							7.5YR 4/4	24.423	0.515	0.565	v3.1
33	ALW001234-QC_UFF_320-30	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	NOMATCH	0.088	896	0.23	1.004							5YR 4/4	23.815	0.509	0.536	v3.1
34	ALW001234-QC_UFF_320-31	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.087	895.9	0.239	1.007							5YR 5/4	23.926	0.507	0.577	v3.1
35	ALW001234-QC_UFF_320-32	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	NOMATCH	0.084	896.4	0.22	1.006							5YR 4/4	24.128	0.522	0.546	v3.1
36	ALW001234-QC_UFF_320-33	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.07	895.1	0.202	1.004							2.5YR 5/6	24.078	0.527	0.591	v3.1
37	ALW001234-QC_UFF_320-34	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.073	895.7	0.219	1.009							7.5YR 5/4	24.407	0.516	0.58	v3.1
38	ALW001234-QC_UFF_320-35	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.089	897.6	0.244	1.008							5YR 4/4	24.204	0.514	0.519	v3.1
39																							
57	1SD								GOOD	GOOD	GOOD	GOOD								GOOD	GOOD	GOOD	
58	2SD								GOOD	GOOD	GOOD	GOOD								OK	GOOD	GOOD	
59	3SD								OK	OK	OK	OK									OK	OK	
60	IsEqual						Same	Same															Same

	AnalysisID	Job No	Client Nar	Date Repc	ClientID	Client Ref	MinGrp1	MinGrp2	FeOx	Hem_Geo	Kln_abun	Kln_cryst	WM_AS_a	WM_AS_c	Fe_Kln	Chl	FeMgClay	OH_mafic	Color	Hue	Saturatior	Intensity	NIR_TSG_v
30	ALW001234-QC_UFF_320-27	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.084	895.3	0.242	1.008							5YR 4/4	24.24	0.518	0.547	v3.1
31	ALW001234-QC_UFF_320-28	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.077	894	0.203	1.004							5YR 4/4	23.889	0.532	0.57	v3.1
32	ALW001234-QC_UFF_320-29	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	NOMATCH	0.084	897.7	0.234	1.01							7.5YR 4/4	24.423	0.515	0.565	v3.1
33	ALW001234-QC_UFF_320-30	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	NOMATCH	0.088	896	0.23	1.004							5YR 4/4	23.815	0.509	0.536	v3.1
34	ALW001234-QC_UFF_320-31	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.087	895.9	0.239	1.007							5YR 5/4	23.926	0.507	0.577	v3.1
35	ALW001234-QC_UFF_320-32	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	NOMATCH	0.084	896.4	0.22	1.006							5YR 4/4	24.128	0.522	0.546	v3.1
36	ALW001234-QC_UFF_320-33	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.07	895.1	0.202	1.004							2.5YR 5/6	24.078	0.527	0.591	v3.1
37	ALW001234-QC_UFF_320-34	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.073	895.7	0.219	1.009							7.5YR 5/4	24.407	0.516	0.58	v3.1
38	ALW001234-QC_UFF_320-35	ALW0012	Gold Rock	########	QC_UFF_3	Mt Gold	KAOLIN	WHITE-MI	0.089	897.6	0.244	1.008							5YR 4/4	24.204	0.514	0.519	v3.1
39																							
40	Mean (M)								0.082222	895.1889	0.230167	1.00775								24.06517	0.515389	0.559889	
41	Standard Deviation								0.005467	1.297861	0.013366	0.002545								0.201308	0.006424	0.02961	
42	Analysis Count						36	36	36	36	36	36							36	36	36	36	36
43	Standard Error								0.000911	0.21631	0.002228	0.000424								0.033551	0.001071	0.004935	
44	Relative Standard Deviation								6.649496	0.144982	5.807213	0.252573								0.83651	1.246517	5.288483	
45	hrd								0.002734	0.648931	0.006683	0.001273								0.100654	0.003212	0.014805	
46	Mode						KAOLIN	WHITE-MI	0.087	895	0.214	1.007							5YR 4/4	23.927	0.513	0.566	v3.1
47	Reference Mean (R_M)								0.08322	895.6804	0.231967	1.007135								24.05351	0.514804	0.565433	
48	Reference Standard Deviation (R_SD)								0.006391	1.611467	0.015379	0.003667								0.427892	0.008269	0.039522	
49	Reference Standard Error								0.000335	0.08458	0.000807	0.000192								0.022459	0.000434	0.002074	
50	Reference Mode						KAOLIN	WHITE-MICA											5YR 4/4				
51	Deviation (M - R_M)								-0.001	-0.49155	-0.0018	0.000615								0.011654	0.000584	-0.00554	
52	Relative Deviation ([M - R_M] / R_SD)								0.15619	0.305034	0.117064	0.167705								0.027236	0.070682	0.140267	
53	Ratio of Means (M / R_M)								0.988006	0.999451	0.992239	1.000611								1.000485	1.001135	0.990196	
54	Uncertainty on Ratio								0.011651	0.000259	0.010205	0.000463								0.001679	0.002245	0.009454	
55	Relative Ratio Deviation								1.029439	2.116556	0.760474	1.320082								0.288613	0.505808	1.037094	
56																							
57	1SD								GOOD	GOOD	GOOD	GOOD								GOOD	GOOD	GOOD	
58	2SD								GOOD	GOOD	GOOD	GOOD								OK	GOOD	GOOD	
59	3SD								OK	OK	OK	OK									OK	OK	
60	IsEqual						Same	Same															Same

Figure 2: Example QA/QC output and expanded drop-down menu with more detailed information for VNIR analyses of QC_UFF_320 standard analyses. Note that Colour is derived from Hue, Saturation and Intensity and, therefore, rules are applied to those columns but not to the Colour column.

The Traffic Light System – FTIR

As is the case with VNIR data, routine protocols for QA/QC of features derived from FTIR data at the post-processing stage are not universally established, and the spectra are visually examined by an expert user and undergo QA/QC during data acquisition and processing in TSG™. We have independently reviewed over two hundred FTIR spectra of the QC_UFF_320 standard to enable the end-user to carry out QA/QC on this data. Our automated QA/QC workflow indicates whether the mean of standard analyses in your analysis batches is within one and two standard deviations, respectively, from the mean of the reference standard analyses for most scalars (Figure 3). This is derived from an assessment of the original FTIR spectra and how these spectra relate to the numerical values that are reported. In addition, the *RankMetric* row is used for the ordinal/ranking analysis output for Gibbsite (with possible values NULL, 1, 2, 3 indicating increasing unquantified abundances), as Gibbsite should not be present in the QC_UFF_320 material. Like the geochemical analyses, if everything is green, there is nothing to worry about. If some scalars are flagged red you can access more detailed information by clicking on the + symbol to open the drop-down calculations and refer to the table below for an explanation of the calculated parameters. Red flags for individual scalars can indicate that this scalar may not be reliable, this should be considered when you interpret your analyses. These values or anomalous results should be used with caution and checked against other parameters if looking to use these numbers to derive a new target for example. If there are consistent red flags for multiple scalars for one and two standard deviations, the first step would be to check whether this is due to a specific batch. If consistent red flags occur across multiple batches for multiple scalars, you may want to contact the lab for further clarification.



	A	B	C	D	E	F	G	H	I	J	K	L
1	AnalysisID	Job No	Client Nar	Date Repc	ClientID	Client Ref	Clay_wt%	Qtz_wt%	Carb_wt%	TOC_wt%	Gibbs_ind	FTIR_TSG_ver
33	ALW001234-QC_UFF_320-30	ALW00123	Gold Rock	########	QC_UFF_3	Mt Gold	66	2	2		NULL	v3.4
34	ALW001234-QC_UFF_320-31	ALW00123	Gold Rock	########	QC_UFF_3	Mt Gold	57	2	1		NULL	v3.4
35	ALW001234-QC_UFF_320-32	ALW00123	Kalamazo	########	QC_UFF_3	Mt Gold	82	2	1	1	NULL	v3.4
36	ALW001234-QC_UFF_320-33	ALW00123	Gold Rock	########	QC_UFF_3	Mt Gold	68	3	2	1	NULL	v3.4
37												
55	1SD						GOOD	GOOD	GOOD			
56	2SD						OK	OK	OK			
57	RankMetric										0	
58	IsEqual											Same

	A	B	C	D	E	F	G	H	I	J	K	L
1	AnalysisID	Job No	Client Nar	Date Repc	ClientID	Client Ref	Clay_wt%	Qtz_wt%	Carb_wt%	TOC_wt%	Gibbs_ind	FTIR_TSG_ver
33	ALW001234-QC_UFF_320-30	ALW00123	Gold Rock	########	QC_UFF_3	Mt Gold	66	2	2		NULL	v3.4
34	ALW001234-QC_UFF_320-31	ALW00123	Gold Rock	########	QC_UFF_3	Mt Gold	57	2	1		NULL	v3.4
35	ALW001234-QC_UFF_320-32	ALW00123	Kalamazo	########	QC_UFF_3	Mt Gold	82	2	1	1	NULL	v3.4
36	ALW001234-QC_UFF_320-33	ALW00123	Gold Rock	########	QC_UFF_3	Mt Gold	68	3	2	1	NULL	v3.4
37												
38	Analysis Count						34	33	34	12	34	34
39	hrd						4.374131	0.272648	0.27846	0.144338		
40	Mean (M)						64.79412	1.878788	1.411765	1.083333		
41	Mode						59	2	1		NULL	v3.4
42	Relative Standard Deviation						13.50163	29.02386	39.44853	26.64694		
43	Standard Deviation						8.748262	0.545297	0.55692	0.288675		
44	Standard Error						1.500315	0.094924	0.095511	0.083333		
45	Reference Mean (R_M)						67.7438	1.954545	1.672199	1.007353		
46	Reference Standard Deviation (R_SD)						6.690588	0.509251	0.602439	0.085749		
47	Reference Standard Error						0.429198	0.032668	0.038726	0.007326		
48	Reference Mode										NULL	v3.4
49	Deviation (M - R_M)						-2.94968	-0.07576	-0.26043	0.07598		
50	Relative Deviation ([M - R_M] / R_SD)						0.440871	0.148763	0.4323	0.886076		
51	Ratio of Means (M / R_M)						0.956458	0.96124	0.844256	1.075426		
52	Uncertainty on Ratio						0.022961	0.051154	0.060371	0.083094		
53	Relative Ratio Deviation						1.89634	0.757703	2.579786	0.907717		
54												
55	1SD						GOOD	GOOD	GOOD			
56	2SD						OK	OK	OK			
57	RankMetric										0	
58	IsEqual											Same

Figure 3: Example QA/QC output for FTIR analyses of QC_UFF_320 standard analyses with drop-down menu for more information.

What do the parameters in the QA/QC drop down menu mean and how were they calculated?

Parameter	Formulae	Definition
Analysis Count	n	The total count of all available QC_UFF_320 analyses for the specific analyte
Mean (M)	$\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$	The mean (or average) of all available QC_UFF_320 analyses
Standard Deviation	$s = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - \overline{x})}$	Measures how dispersed the data is in relation to the mean; low values indicate the analyses are clustered around the mean (are more precise); high values indicate the analyses exhibit greater variation
Standard Error	$s_{\overline{x}} = \frac{s}{\sqrt{n}}$	The standard deviation of the sample population which measures the accuracy with which a sample represents a population
Relative Standard Deviation	$100\frac{s}{\overline{x}}$	Percentage value describing the spread of analyses as a proportion of the Mean
hrd	$100\frac{\lvert x_a - x_b \rvert}{x_a + x_b}$	Half absolute relative difference between two estimates of a value
Mode		The most common value for a specific analyte; typically only used for categorical/ordinal data

Parameter	Formulae	Definition
Reference Mean (R_M)	$\mu_{ref} = \frac{1}{N}\sum_{i=1}^{N} x_i$	The mean of the QC_UFF_320 standard calculated from a static set of 312 analyses for 49 elements.
Reference Standard Deviation (R_SD)	$\sigma_{ref} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \overline{x})}$	The standard deviation of the QC_UFF_320 standard calculated from a static set of 312 analyses for 49 elements.
Reference Standard Error	$\sigma_{\mu_{ref}} = \frac{s\sigma_{ref}}{\sqrt{n_{ref}}}$	The standard deviation of the reference analysis population (the 312 QC_UFF_320 analyses)
Reference Mode		The most common value or a specific analyte in the reference data set (the 312 QC_UFF_320 analyses); typically only used for categorical/ordinal data.
Deviation (M - R_M)	$D = \mu - \mu_{ref}$	The difference between the mean of the reference material analyses for this site (M) relative to the mean of a static set of 312 analyses for 49 elements (R_M)
Relative Deviation ([M - R_M] / R_SD)	$\frac{D}{\sigma_{ref}}$	The relative difference between the means (M, R_M), expressed as the Deviation (above, M-R_M) scaled by the standard deviation of the reference set (R_SD) to give an estimate of 'standard deviations from unity'
Ratio of Means (M / R_M)	$R = \frac{\mu}{\mu_{ref}}$	The ratio between the mean of the reference material analyses for this site (M) relative to the mean of a static set of 312 analyses for 49 elements (R_M)
Uncertainty on Ratio	$\sigma_R = R\sqrt{\frac{{\sigma_{\mu_{ref}}}^2}{\mu_{ref}} + \frac{s_{\overline{x}}^2}{\overline{x}}}$	The uncertainty on the ratio of means (M/R_M) estimated by propagated uncertainties (1σ)
Relative Ratio Deviation	$\frac{R-1}{\sigma_R}$	An estimate of how far the means are from equality (a ratio of one, or unity) expressed in terms of the uncertainty on the ratio (σ); values greater than two likely indicate significant differences between the means
IsEqual		Whether two categorical data values are the same (e.g., mineral groups, software versions)
RankMetric		Rank differences between two ordinal values, used here to compare the modal Gibbsite index (with ordinal values [NULL, 1, 2, 3])
1SD	$\left\lvert\frac{D}{s_{ref}}\right\rvert < 1$	Indicates whether the Mean of the QC_UFF_320 analyses in this batch is within one (1) standard deviation of the Mean of the reference standard values (calculated from 312 QC_UFF_320 analyses)
2SD	$\left\lvert\frac{D}{s_{ref}}\right\rvert < 2$	Indicates whether the Mean of the QC_UFF_320 analyses in this batch is within two (2) standard deviations of the Mean of the reference standard values (calculated from 312 QC_UFF_320 analyses)
3SD	$\left\lvert\frac{D}{s_{ref}}\right\rvert < 3$	Indicates whether the Mean of the QC_UFF_320 analyses in this batch is within three (3) standard deviations of the Mean of the reference standard values (calculated from 312 QC_UFF_320 analyses)

Why is QA/QC missing for some data?

The QC_UFF_320 standard is not analysed for pH and EC (or sizing) as these analyses are carried out on bulk samples. Therefore, pH and EC are not part of the standards QA/QC. However, they are part of the duplicate QA/QC.

As the elements Br, I and Pd were not part of the original UltraFine+® analysis method, we do not currently have sufficient analyses on the QC_320_UFF standard material to create a statistically relevant mean.

Columns for some VNIR scalars are empty as the QC_UFF_320 standard was initially developed for geochemical analyses. As the UltraFine+® Next Gen Analytics project has progressed and the VNIR method for soil samples has improved, additional

scalars are added which do not report numbers (i.e., the UltraFine+® standard does not contain chlorite, hence this column should be empty). Occasionally, very low numbers of some scalars may occur in individual standard analyses.

Why is there no automated QA/QC on CRMs?

Since the UltraFine+® method uses only the <2 µm soil fraction, we cannot currently use CRMs for the whole process (sieving these to <2 µm would change the results rendering them incomparable to the certified reference values). Hence, we have developed the UltraFine+® Standard (currently QC_320_UFF, to be replaced with QC_422 in the future). This standard has been generated by blending representative soil types from across Australia and we have tested this standard with over 300 analyses for ICP-OES/MS and spectral analyses. While CRMs can be incorporated into the geochemistry analytical steps, expect that the UltraFine+® method will usually report slightly higher concentrations of many metals (due to the more aggressive closed vessel aqua regia approach compared to open block). Our industry partner LabWest have tested this on several commonly submitted CRMs and a table can be found here.

I want to do my own QA/QC – can I have the mean values of the UltraFine+® standard?

You can download excel spreadsheets of the mean standard values on our webpage under Other Resources. For geochemical analyses of the UltraFine+® standard we have also calculated tolerance and confidence intervals. These are also available for VNIR data. However, at the time of writing this guide, the FTIR data is only semi-quantitative in nature, and we therefore do not supply confidence or tolerance intervals for this data.

The methods for VNIR and FTIR data acquisition have been developed as part of the UltraFine+® Next Gen Analytics project and are still subject to ongoing research. Hence, scalars are regularly being improved when updated TSG™ versions are rolled out and this has flow-on effects on the end-user QA/QC of this data. This is similar to the improvement of detection limits for geochemical analyses and we, therefore, re-process the UltraFine+® standard analyses with each TSG™ update to derive the correct reference means for QA/QC. Please download the mean values for the correct TSG™ version your data has been processed with. This data is available for NIR TSG™ v. 3.1 and onwards, and for FTIR TSG™ v. 3.3 and onwards.