Charles Sturt University

AWRI and Vintessential
Grape and Wine Analysis

Smoke Method Comparison

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Project: Smoke Method Comparison

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Contents

Statistical Comparison of Methods

Preamble

Extensive and catastrophic bushfires in south east Australia during the 2020 vintage severely impacted the quality of grapes available for wine production. Previous research has demonstrably linked the presence of a suite of volatile phenolic compounds and their glycosylated precursors present in grapes to deleterious wine sensory outcomes. A range of freely volatile, bound or precursor compounds are typically also present in wines made from affected grapes.

Several analytical approaches have been independently developed and deployed by commercial laboratories to enable grape growers to assess the impact of vine smoke exposure upon grape composition. Some differences in sample preparation and analytical approaches are used between laboratories and the basis of this report is to make comparison of sample analysis across two laboratories from identical grape and wine samples. The nature of the sample matrix, sample preparation prior to distribution to the laboratories and individual analytical sample treatments are important factors that may influence the overall variance associated with the results. Liquid samples, such as wines, can be expected to be more homogenous in composition compared to grapes if reasonable mixing and sample storage has occurred. Solids, slurries and composite samples, such as grapes, are typically more heterogenous in composition and this should be a consideration for inferences' from this report.

The basis of this report is a without prejudice comparison of analytical values from two laboratories. No specific inferences or conclusions are made regarding the value of methods for the purposes of assessing smoke exposure of vines and subsequent grape composition.

Report interpretation

To make meaningful comparison of different methods for analytical results two questions need to be considered

1. Do the methods differ substantially i.e. are results from identical samples significantly different?
2. If the results from the methods are different, what is the nature of the difference and how to describe the difference between the methods.

It is reasonable to consider that two methods applied to the same samples would produce exactly the same analytical outcome and the correlation between sample sets would be perfect. In practise this never arises.

From a statistical hypothesis perspective, we can frame the first question to test

- differences of means of the two sample sets (paired t-test, 2 tail)
- differences between variances associated with the two samples sets (F-test)

If the two analytical procedures are the same, we can expect that there will be no significant differences between the means or variance of the results for the two sets of data at a chosen level of certainty (in this case alpha is 5%).

A word of caution. Two procedures may have similar means and sample variances, i.e. appear to provide the same results, but may still be different, conversely two methods may appear to give similar results but may in fact be statistically different. The ability to determine a significant difference between sample sets is dependent on the number of samples, which thereby determines the degrees of freedom associated with probability distributions used to test the hypothesis. Thus the number of samples with matching data will determine the overall level of (un)certainty when assessing the results of comparison tests.

To determine how methods differ a simple linear regression using a least squares fit of the data can be used. In an ideal comparison, the data when plotted as paired samples will produce a perfect straight line with a gradient of one and which passes through the origin of the *xy* axis. Rarely does this occur.

From the linear regression diagnostics several interpretive results can be determined

- R2 values indicate the goodness of fit of the data and overall percent of data variance able to be modelled using the regression equation.
- 'Terms' or the gradient of the least squares line of best fit that indicates the rate of change in values from one method in comparison to the other method over the analytical range. Typically this value is a constant multiplier to analytical value to convert one method result to another. For the purpose of this report there is only one term for each analytical method comparison.
- Intercept values indicate a **constant** difference between the two methods which could be either added to or subtracted from samples when 'converting' values from one method to another, once the output of the multiplier term has been derived. (see caveat below for residuals).
- Residuals should be examined for all samples. The residuals represent the differences for each paired sample between two methods. Expanding residuals across the fitted analytical range indicate proportional errors associated with the methods. Proportional errors are difficult to determine precisely and when present indicate that correction by applying a constant term (intercept) to analytical values may lead to significant inaccuracies, particularly at the higher end of the analytical range.

Data Format

Vintessential data was supplied in spreadsheet format (150 row x 10 columns) with values presented as 'total', 'free' and 'bound' being the difference between total and free. Two tables were presented one each for grape and wine analysis. Samples were in chronological order and columns rearranged to match the AWRI variable order, with an example shown below. Excel data was imported into Matlab and extracted into six separate data tables representing either grape or wine, total, free or bound values. An additional data column was created for these tables representing the total sum of the cresol (ortho, meta & para) isotopes.

	A	B	C	D	E	F	G	H	I	J
1	**Results: Wine**									
2										
3	Sample ID	Date	Sample	4-MG	Guaiacol	m-Cresol	4-MS	o-Cresol	p-Cresol	Syringol
4	A2008071/01T	17-Aug	White	5	14	4	21	3	3	63
5	A2008071/01F	17-Aug	White	1	4	2	1	2	2	3
6	A2008071/01B		White	4	10	2	20	1	1	60
7	A2008071/02T	17-Aug	White	2	4	1	3	1	1	10
8	A2008071/02F	17-Aug	White	0	2	1	1	1	1	2

AWRI data was supplied as four separate sreadsheet pages with samples in chronological order. The four spreadsheets represented the analytical results for volatile phenol analysis for grapes and wine and the glycosydically bound fraction of volatile phenols in grape and wine.

Values reported from AWRI were in the form of <x where x represents either the limit of quantification or limit of detection (not specifcally stated). These values represent a small dilema for method comparison and validation as a reported value of <x is not a true value, and cannot be substituted with the lower boundary of the reported analytical range (i.e. x). To enable the two datasets to be compared, values reported a <x were replaced with NaN (not a number) and this enables the statistical modelling software to ignore these samples. Effectively the confidence of the hypothesis testing is lowered as the number of degrees of freedom are reduced. An example of the AWRI dataset for wine samples is presented below.

	A	B	C	D	E	F	G	H	I
1	Sample ID	Sample Description	4 - Methylguaiacol	Guaiacol	m-CRESOL	Methyl Syringol	o-CRESOL	p-CRESOL	Syringol
2	AE96978	WINE_01	NaN	3	2	NaN	2	1	1
3	AE96979	WINE_02	NaN	NaN	NaN	NaN	NaN	NaN	NaN
4	AE96980	WINE_03	1	5	3	NaN	3	2	NaN
5	AE96981	WINE_04	NaN	2	1	NaN	2	NaN	1
6	AE96982	WINE_05	NaN	1	NaN	NaN	2	NaN	NaN
7	AE96983	WINE_06	NaN	NaN	NaN	NaN	NaN	NaN	NaN
8	AE96984	WINE_07	NaN	1	NaN	NaN	NaN	NaN	1
9	AE96985	WINE_08	NaN	2	1	NaN	2	NaN	NaN
10	AE96986	WINE_09	NaN	2	1	NaN	2	NaN	NaN
11	AE96987	WINE_10	4	11	8	4	9	2	9
12	AE96988	WINE_11	2	5	4	9	5	1	13
13	AE96989	WINE_12	4	13	9	2	10	2	6

Dataset comparison

A table of dataset comparisons is presented below.

AWRI Dataset	Vintessential Dataset
Grape Volatile Phenols	Grape Volatile Phenols – Total
	Grape Volatile Phenols – Free
	Grape Volatile Phenols – Bound
Grape Glyosidic Phenols	Grape Volatile Phenols – Bound
	Grape Volatile Phenols – Total
Wine Volatile Phenols	Wine Volatile Phenols – Total
	Wine Volatile Phenols – Free
	Wine Volatile Phenols – Bound
Wine Glyosidic Phenols	Wine Volatile Phenols – Bound
	Wine Volatile Phenols – Total

A table of matched analytes for each data set is presented below.

AWRI Analyte	Vintessential Analyte
4-methylguaiacol	4-MG
Guaiacol	Guaiacol
m-cresol	*m*-cresol
Methyl syringol	4-MS
o-cresol	*o*-cresol
p-cresol	*p*-cresol
Syringol	Syringol

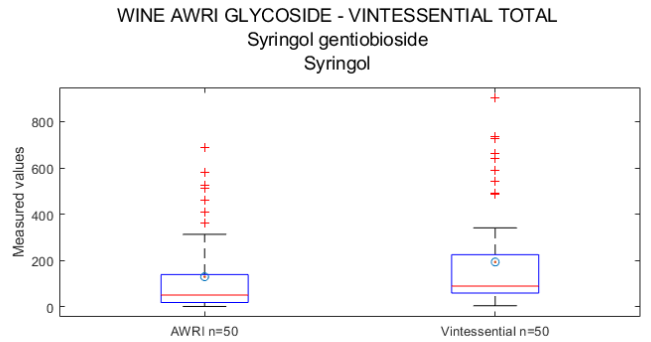
AWRI Analyte	Vintessential Analyte
Cresol rutinoside	*m*-cresol
	o-cresol
	p-cresol
	Total cresol
Guaiacol rutinoside	Guaiacol
Methylguaiacol rutinoside	4-MG
Methylsyringol gentiobioside	4-MS
Phenol rutinoside	No matching analyte
Syringol gentiobioside	Syringol

Software

All statistical modelling was conducted using Matlab (The Mathworks, Natick, MA) version 9.5.0.10033004 (R2018b) Update 2 with the Statistics and Machine Learning Toolbox version 11.4.

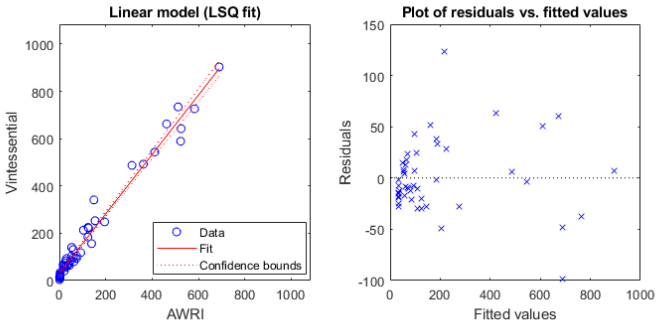
Example Interpretation

The following worked example provides some insight to interpretation of the method comparisons. This working example shows the comparison of wine samples for Syringol gentiobioside as measured by the AWRI to the total Syringol reported by Vintessential.



Box plot to show the range of data. Boxes are the 25-75th quartile range, red line is the median value and circle the mean value. Box whiskers show 1.5 x the interquartile range and red crosses are outliers samples i.e. have values beyond this range.

n = number of samples with reported values for each laboratory dataset



Linear model (LSQ) fit shows the relationship between the two laboratory datasets.

Residual versus fitted values show the difference between the calculated and reported values as a function of analytical range. Larger residuals at the higher analytical range indicate a proportional analytical error. If larger residuals are evenly distributed the proportional error is associated with both data sets, whereas a skewed (more + or -) increasing residual infers the proportional error is confined to one dataset.

{'WINE AWRI GLYCOS…'} {'Syringol gentiob…'} {'Syringol'}

Label check for datasets and matching variables.

Linear regression model:
Vintessential ~ 1 + AWRI

Regression model using only linear terms

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	30.725	6.1334	5.0094	7.8069e-06
AWRI	1.2561	0.027723	45.309	4.7418e-41

Intercept 30.725 = constant difference between Vintessential and AWRI results. This is evident in comparison of the means shown in the box plots.

AWRI 1.2561 = 'gradient' of the linear regression equation to convert the AWRI values to an equivalent Vintessential result. So in this example an AWRI reported value of 100 is equivalent to (1.2561*100) + 30.725 = 156.3 from Vintessential.

Number of observations: 50, Error degrees of freedom: 48
Root Mean Squared Error: 35.2
R-squared: 0.977, Adjusted R-Squared 0.977
F-statistic vs. constant model: 2.05e+03, p-value = 4.74e-41
F value = 0.61931
Degrees of Freedom = 49 & 49
Critical F value = 1.6073
Probability of difference in variance between groups = 0.096785
No significant difference in variances at the 5% significance level
t-value = -7.7809
Degrees of Freedom = 49
Critical t-value = 1.6766
Probability of difference in means between groups = 4.1384e-10
Significant mean differences between samples sets

Outcome of F-Test for differences in variance between the two datasets for each comparison.

Outcome of t-Test for differences in between means for the two datasets for each comparison.

Hypothesis test are assessed at the 5% level.

Compiled Results Tables

Grape analysis method comparisons and conversions

				Convert AWRI to Vintessential		Convert Vintessential to AWRI	
Dataset	AWRI	Vintessential	R2	Intercept	Gradient	Intercept	Gradient
GRAPE AWRI VP - VINTESSENTIAL TOTAL							
	4.Methylguaiacol	4.MG	0.66	2.12	1.34	-0.04	0.49
	Guaiacol	Guaiacol	0.49	12.88	1.36	0.05	0.36
	m.CRESOL	m.Cresol	0.65	1.58	1.13	0.07	0.58
	Methyl.Syringol	4.MS	0	0	0	0	0
	o.CRESOL	o.Cresol	0.83	1.25	0.62	-0.7	1.35
	p.CRESOL	p.Cresol	0.43	1.66	1.38	0.56	0.31
GRAPE AWRI VP - VINTESSENTIAL FREE							
	4.Methylguaiacol	4.MG	0.73	0.67	0.81	0.21	0.9
	Guaiacol	Guaiacol	0.92	2.07	0.98	-1.15	0.93
	m.CRESOL	m.Cresol	0.9	0.31	0.98	-0.01	0.92
	Methyl.Syringol	4.MS	0	0	0	0	0
	o.CRESOL	o.Cresol	0.87	0.76	0.7	-0.2	1.25
	p.CRESOL	p.Cresol	0.9	-0.01	1.14	0.2	0.79
GRAPE AWRI VP - VINTESSENTIAL BOUND							
	4.Methylguaiacol	4.MG	0.27	1.45	0.53	1.44	0.51
	Guaiacol	Guaiacol	0.07	10.8	0.38	6.59	0.19
	m.CRESOL	m.Cresol	0.06	1.27	0.15	2.22	0.37
	Methyl.Syringol	4.MS	0	0	0	0	0
	o.CRESOL	o.Cresol	0.22	0.49	-0.08	5.89	-2.64
	p.CRESOL	p.Cresol	0.02	1.68	0.24	1.66	0.1
GRAPE AWRI GLYCOSIDE - VINTESSENTIAL BOUND							
	Cresol rutinoside	m.Cresol	0.35	0.65	0.08	4.6	4.47
	Cresol rutinoside	o.Cresol	0.04	0.27	-0.02	11.6	-1.92
	Cresol rutinoside	p.Cresol	0.34	0.51	0.07	5.09	4.85
	Cresol rutinoside	Total.cresol	0.18	1.43	0.13	7.51	1.39
	Guaiacol rutinoside	Guaiacol	0.47	5.78	0.79	2.16	0.59
	Methylguaiacol rutinoside	4.MG	0.49	0.88	0.08	5.14	5.94
	Methylsyringol gentiobioside	4.MS	0.92	8.84	1.31	-4.01	0.71
	Syringol gentiobioside	Syringol	0.91	25.27	0.71	-17.09	1.28
GRAPE AWRI GLYCOSIDE - VINTESSENTIAL TOTAL							
	Cresol rutinoside	m.Cresol	0.53	1.03	0.19	2.57	2.81
	Cresol rutinoside	o.Cresol	0.48	1.55	0.28	3.38	1.72
	Cresol rutinoside	p.Cresol	0.56	0.82	0.11	0.97	4.96
	Cresol rutinoside	Total.cresol	0.18	1.43	0.13	7.51	1.39
	Guaiacol rutinoside	Guaiacol	0.77	10.44	1.4	-3.39	0.55

Dataset	AWRI	Vintessential	R2	Convert AWRI to Vintessential		Convert Vintessential to AWRI	
				Intercept	Gradient	Intercept	Gradient
	Methylguaiacol rutinoside	4.MG	0.78	0.9	0.16	-0.08	5.02
	Methylsyringol gentiobioside	4.MS	0.92	9.02	1.31	-4.12	0.7
	Syringol gentiobioside	Syringol	0.91	26	0.72	-18.03	1.28

Wine analysis method comparisons and conversions

Dataset	AWRI	Vintessential	R2	Convert AWRI to Vintessential		Convert Vintessential to AWRI	
				Intercept	Gradient	Intercept	Gradient
WINE AWRI VP - VINTESSENTIAL TOTAL							
	4.Methylguaiacol	4.MG	0.62	7.36	1.7	-0.96	0.37
	Guaiacol	Guaiacol	0.75	21.93	1.77	-4.41	0.42
	m.CRESOL	m.Cresol	0.85	2.19	1.33	-0.51	0.64
	Methyl.Syringol	4.MS	0.13	101.14	6.46	2.58	0.02
	o.CRESOL	o.Cresol	0.95	1.03	1.03	-0.61	0.92
	p.CRESOL	p.Cresol	0.41	4.19	1.02	0.38	0.41
WINE AWRI VP - VINTESSENTIAL FREE							
	4.Methylguaiacol	4.MG	0.99	0.19	1.2	-0.11	0.83
	Guaiacol	Guaiacol	1	0.82	1.26	-0.6	0.79
	m.CRESOL	m.Cresol	0.94	0.09	0.95	0.26	0.99
	Methyl.Syringol	4.MS	0.98	1.06	1.32	-0.71	0.75
	o.CRESOL	o.Cresol	0.99	-0.07	1.14	0.14	0.87
	p.CRESOL	p.Cresol	0.98	0.58	0.89	-0.56	1.1
WINE AWRI VP - VINTESSENTIAL BOUND							
	4.Methylguaiacol	4.MG	0.12	7.17	0.5	2.33	0.24
	Guaiacol	Guaiacol	0.2	21.11	0.51	7.72	0.39
	m.CRESOL	m.Cresol	0.31	2.1	0.37	2.38	0.82
	Methyl.Syringol	4.MS	0.09	100.08	5.15	3.17	0.02
	o.CRESOL	o.Cresol	0.15	1.1	-0.11	7	-1.41
	p.CRESOL	p.Cresol	0.01	3.62	0.13	3.21	0.08
WINE AWRI GLYCOSIDE - VINTESSENTIAL BOUND							
	Cresol rutinoside	m.Cresol	0.78	0.16	0.24	2.77	3.3
	Cresol rutinoside	o.Cresol	0.02	0.21	0.02	14.25	1
	Cresol rutinoside	p.Cresol	0.56	0.47	0.19	5.04	2.95
	Cresol rutinoside	Total.cresol	0.54	0.84	0.44	5.66	1.23
	Guaiacol rutinoside	Guaiacol	0.55	10.23	1.17	2.57	0.47
	Methylguaiacol rutinoside	4.MG	0.75	1.81	0.21	0.01	3.54
	Methylsyringol gentiobioside	4.MS	0.88	13.11	4.31	-0.97	0.2

				Convert AWRI to Vintessential		Convert Vintessential to AWRI	
Dataset	AWRI	Vintessential	R2	Intercept	Gradient	Intercept	Gradient
	Syringol gentiobioside	Syringol	0.97	23.55	1.22	-15.27	0.8
WINE AWRI GLYCOSIDE - VINTESSENTIAL TOTAL							
	Cresol rutinoside	m.Cresol	0.89	0.28	0.55	1.13	1.64
	Cresol rutinoside	o.Cresol	0.76	1.19	0.43	1.46	1.77
	Cresol rutinoside	p.Cresol	0.91	1.19	0.33	-1.88	2.72
	Cresol rutinoside	Total.cresol	0.54	0.84	0.44	5.66	1.23
	Guaiacol rutinoside	Guaiacol	0.84	11.42	2.58	-1.17	0.33
	Methylguaiacol rutinoside	4.MG	0.95	1.45	0.37	-2.45	2.54
	Methylsyringol gentiobioside	4.MS	0.91	14.65	4.53	-1.56	0.2
	Syringol gentiobioside	Syringol	0.98	30.72	1.26	-20.95	0.78

Code

Get data

```
% Vintessential AWRI ring test sample comparison
% data columns sorted for free phenols in excel so variables are in identical columns
% {'4 - Methylguaiacol';'Guaiacol';'m-CRESOL';'Methyl Syringol';'o-CRESOL';'p-CRESOL';'Syringol'}
%  AWRI GLYCOSIDES {'Cresol rutinoside';'Guaiacol rutinoside';'Methylguaiacol rutinoside';'Methylsyringol
gentiobioside';'Phenol rutinoside';'Syringol gentiobioside'}
%
% Vintessential data provided in lines of 3 for each sample with each line
% being:
% SAMPLE ID: TOTAL
% SAMPLE ID: FREE
% SAMPLE ID: BOUND
% extract vintessesntial data into three sample matricees (total; free & bound)

idx_total=1:3:150;
idx_free=2:3:150;
idx_bound=3:3:150;

VINT_GRAPE_VP_TOTAL=VINT_GRAPE_VP(idx_total,:);
VINT_GRAPE_VP_FREE=VINT_GRAPE_VP(idx_free,:);
VINT_GRAPE_VP_BOUND=VINT_GRAPE_VP(idx_bound,:);

VINT_WINE_VP_TOTAL=VINT_WINE_VP(idx_total,:);
VINT_WINE_VP_FREE=VINT_WINE_VP(idx_free,:);
VINT_WINE_VP_BOUND=VINT_WINE_VP(idx_bound,:);
```

Create Datasets

for each dataset do box plots for each variable do F-test for variance do t-test for means plot xy with linear regression find intercept and gradient inspect residuals

```
% For glycosides the comparison are not as easy to determine so the following comparisons are made for both total and bound fractions:
% Cresol rutinoside: m_cresol
% Cresol rutinoside: o_cresol
% Cresol rutinoside: p_cresol
% Cresol rutinoside: Sum of cresol
% Guaiacol rutinoside: guaiacol
% Methylguaiacol rutinoside: 4-MG
% Methylsyringol gentiobioside: 4-MS
% Phenol rutinoside: NO IDENTIFIED ANALOGUE
% Syringol gentiobioside: Syringol
%For glycolyated compund comparison
gly_var_sel=[1 3; 1 5; 1 6; 1 8; 2 2; 3 1; 4 4; 6 7]; % AWRI glycosylated column 1 Vintessential total column 2

% create sum of cresols
idx_sum=[3 5 6];

VINT_GRAPE_VP_BOUND(:,8)=sum(VINT_GRAPE_VP_BOUND(:,idx_sum),2);
VINT_GRAPE_VP_TOTAL(:,8)=sum(VINT_GRAPE_VP_BOUND(:,idx_sum),2);
VINT_WINE_VP_BOUND(:,8)=sum(VINT_WINE_VP_BOUND(:,idx_sum),2);
VINT_WINE_VP_TOTAL(:,8)=sum(VINT_WINE_VP_BOUND(:,idx_sum),2);

%For volatiles phenols column comparisons
vol_phenol_var_sel=[1 1; 2 2; 3 3; 4 4; 5 5; 6 6]; %AWRI_xxx_VP column 1 VINTESSENTIAL_FREE_VP column 2

% do GRAPE DATA SETS AWRI GRAPE VP & VINT_GRAPE_VP_FREE
% create global dataset for easy DS selection
smp_global.data{1,1}=AWRI_GRAPE_VP;
smp_global.data{1,2}=AWRI_GRAPE_GLY;
smp_global.data{1,3}=AWRI_WINE_VP;
smp_global.data{1,4}=AWRI_WINE_GLY;
smp_global.data{1,5}=VINT_GRAPE_VP_TOTAL;
smp_global.data{1,6}=VINT_GRAPE_VP_FREE;
smp_global.data{1,7}=VINT_GRAPE_VP_BOUND;
smp_global.data{1,8}=VINT_WINE_VP_TOTAL;
smp_global.data{1,9}=VINT_WINE_VP_FREE;
smp_global.data{1,10}=VINT_WINE_VP_BOUND;


ds_compare=[1 5; 1 6; 1 7; 2 7; 2 5; 3 8; 3 9; 3 10; 4 10; 4 8];
smp_global.var_sel{1,1}=vol_phenol_var_sel;
smp_global.var_sel{1,2}=vol_phenol_var_sel;
smp_global.var_sel{1,3}=vol_phenol_var_sel;
smp_global.var_sel{1,4}=gly_var_sel;
smp_global.var_sel{1,5}=gly_var_sel;
smp_global.var_sel{1,6}=vol_phenol_var_sel;
```

```
smp_global.var_sel{1,7}=vol_phenol_var_sel;
smp_global.var_sel{1,8}=vol_phenol_var_sel;
smp_global.var_sel{1,9}=gly_var_sel;
smp_global.var_sel{1,10}=gly_var_sel;

smp_global.lbl{1,1}=lbl_awri_grape_vp; smp_global.lbl{2,1}=lbl_vint_grape;
smp_global.lbl{1,2}=lbl_awri_grape_vp; smp_global.lbl{2,2}=lbl_vint_grape;
smp_global.lbl{1,3}=lbl_awri_grape_vp; smp_global.lbl{2,3}=lbl_vint_grape;
smp_global.lbl{1,4}=lbl_awri_grape_gly; smp_global.lbl{2,4}=lbl_vint_grape;
smp_global.lbl{1,5}=lbl_awri_grape_gly; smp_global.lbl{2,5}=lbl_vint_grape;
smp_global.lbl{1,6}=lbl_awri_grape_vp; smp_global.lbl{2,6}=lbl_vint_grape;
smp_global.lbl{1,7}=lbl_awri_grape_vp; smp_global.lbl{2,7}=lbl_vint_grape;
smp_global.lbl{1,8}=lbl_awri_grape_vp; smp_global.lbl{2,8}=lbl_vint_grape;
smp_global.lbl{1,9}=lbl_awri_grape_gly; smp_global.lbl{2,9}=lbl_vint_grape;
smp_global.lbl{1,10}=lbl_awri_grape_gly; smp_global.lbl{2,10}=lbl_vint_grape;
```

Do comparisons and plot results

```
% create data collection ds
ds_results.compare={};
ds_results.R2=[];
ds_results.intercept=[];
ds_results.slope_awri=[];

cntr=1;


for vito=1:(numel(ds_compare)/2)
    ds1=smp_global.data{1,ds_compare(vito,1)};
    ds2=smp_global.data{1,ds_compare(vito,2)};
    lbl_1=smp_global.lbl{1,vito};
    lbl_2=smp_global.lbl{2,vito};

    var_com=smp_global.var_sel{1,vito};

    ncompare=numel(var_com);

    % loop over columns
    for toto=1:ncompare/2

        % get columns of data
        clear temp;
        temp(:,1)=ds1(:,var_com(toto,1)); temp(:,2)=ds2(:,var_com(toto,2));
        xn=sum(~isnan(temp));

        % get labels
        lbl_compar{toto,1}=lbl_1(var_com(toto,1)); lbl_compar{toto,2}=lbl_2(var_com(toto,2));

        % do box plots;
```

```
figure;
set(gcf, 'PaperPositionMode', 'manual');
%pu = get(gcf,'PaperUnits');
%pp = get(gcf,'PaperPosition');
set(gcf, 'Units', 'centimeters'); %sets dimensions to centimetres
set(gcf, 'Position', [2 1 20 20]); %creates image of dimensions last 2 values in cm in x y dimension
subplot(2,2,[1 2]);
boxplot(temp, 'Labels', {['AWRI n=', num2str(xn(1))], ['Vintessential n=', num2str(xn(2))]}); hold on;

%suptitle
suptitle([lbl_suptitle{vito} lbl_compar{toto,1} lbl_compar{toto,2}]);
ylabel('Measured values');

% get means
xm=mean(temp, 'omitnan');

% plot xm
scatter(1:2,xm, 'o'); scatter(1:2, xm, '.'); % plot means

%get limits for plots
xmax=max(temp);

% get linear model
md=fitlm(temp(:,1), temp(:,2),'linear', 'VarNames', {'AWRI', 'Vintessential'});
subplot(2,2,3)
h=plot(md, 'Marker', 'o'); hold on;
xlim([0, max(xmax)*1.2]);
ylim([0, max(xmax)*1.2]);
title('Linear model (LSQ fit)');
%title(horzcat(['Grape: Free', lbl_compar{1,1} lbl_compar{1,2}]));

% do plot for residuals
subplot(2,2,4);
plotResiduals(md, 'fitted')

% display model diagnostics

display([lbl_suptitle{vito} lbl_compar{toto,1} lbl_compar{toto,2}]); % get model headers to match figures
display(md);

ds_results.compare(cntr,:)=horzcat(lbl_suptitle{vito}, lbl_compar{toto,1}, lbl_compar{toto,2}); % get lables for results tables
ds_results.R2(cntr)=md.Rsquared.Ordinary;
ds_results.slope_awri(cntr)=md.Coefficients.Estimate(2,1);
ds_results.intercept(cntr)=md.Coefficients.Estimate(1,1);

% do F-test
[h,p,ci,stats] = vartest2(temp(:,1),temp(:,2));
critF=finv(0.95, stats.df1, stats.df2);
display(['F value = ', num2str(stats.fstat)]);
display(['Degrees of Freedom = ', num2str(stats.df1), ' & ', num2str(stats.df2)]);
```

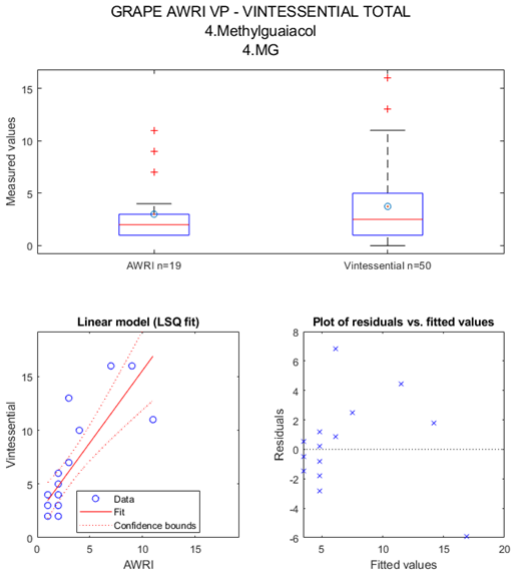
```
        display(['Critical F value = ', num2str(critF)]);
        display(['Probability of difference in variance between groups = ', num2str(p)]);
        if h==0
            display('No significant difference in variances at the 5% significance level')
        else
            display('Significant variance differences between samples sets');
        end

        % do t-test
        [h,p,ci,stats] = ttest(temp(:,1),temp(:,2),'Alpha',0.05);
        critT=tinv(0.95,stats.df);
        display(['t-value = ', num2str(stats.tstat)]);
        display(['Degrees of Freedom = ', num2str(stats.df)]);
        display(['Critical t-value = ', num2str(critT)]);
        display(['Probability of difference in means between groups = ', num2str(p)]);
        if h==0
            display('No significant difference in means at the 5% significance level')
        else
            display('Significant mean differences between samples sets');
        end

    end
    cntr=cntr+1;
end

display('END');
```

Results



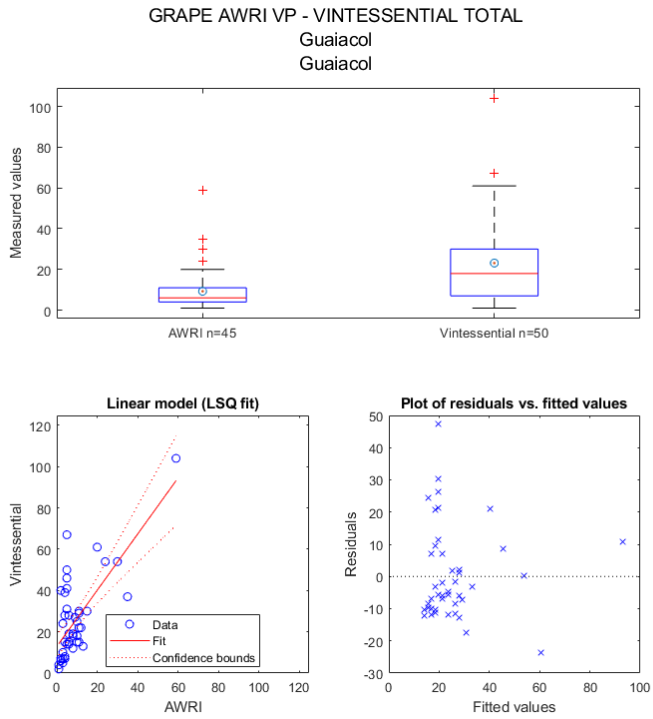
{'GRAPE AWRI VP - …'} {'4.Methylguaiacol'} {'4.MG'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	2.1241	0.94897	2.2383	0.038871
AWRI	1.3446	0.2316	5.8057	2.108e-05

Number of observations: 19, Error degrees of freedom: 17
Root Mean Squared Error: 2.82
R-squared: 0.665, Adjusted R-Squared 0.645
F-statistic vs. constant model: 33.7, p-value = 2.11e-05
F value = 0.54918
Degrees of Freedom = 18 & 49
Critical F value = 1.8185
Probability of difference in variance between groups = 0.16454
No significant difference in variances at the 5% significance level
t-value = -4.7287
Degrees of Freedom = 18
Critical t-value = 1.7341
Probability of difference in means between groups = 0.00016759
Significant mean differences between samples sets



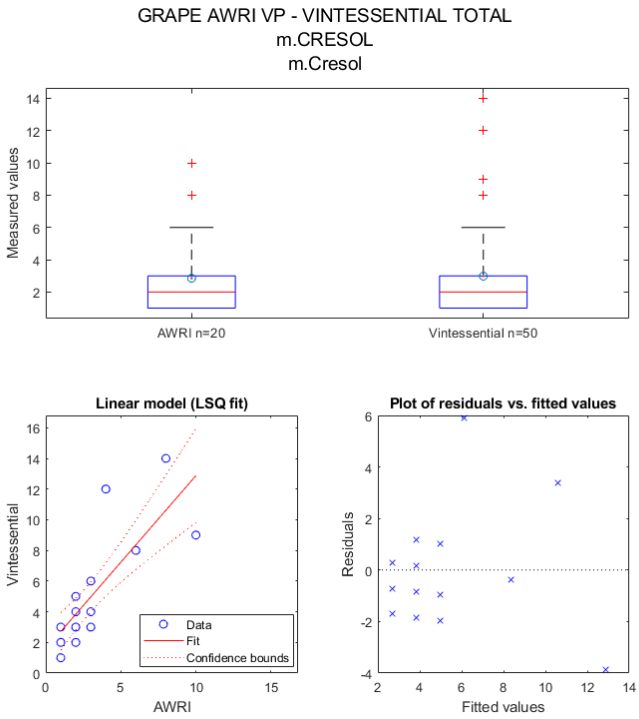
{'GRAPE AWRI VP - …'} {'Guaiacol'} {'Guaiacol'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	12.875	2.9213	4.4074	6.8574e-05
AWRI	1.3612	0.21091	6.4537	7.9932e-08

Number of observations: 45, Error degrees of freedom: 43
Root Mean Squared Error: 14.6
R-squared: 0.492, Adjusted R-Squared 0.48
F-statistic vs. constant model: 41.7, p-value = 7.99e-08
F value = 0.25925
Degrees of Freedom = 44 & 49
Critical F value = 1.6232
Probability of difference in variance between groups = 1.2897e-05
Significant variance differences between samples sets
t-value = -7.3127
Degrees of Freedom = 44
Critical t-value = 1.6802
Probability of difference in means between groups = 3.989e-09
Significant mean differences between samples sets



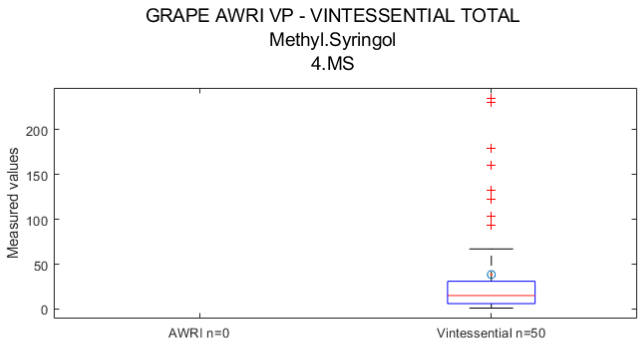
{'GRAPE AWRI VP - …'} {'m.CRESOL'} {'m.Cresol'}

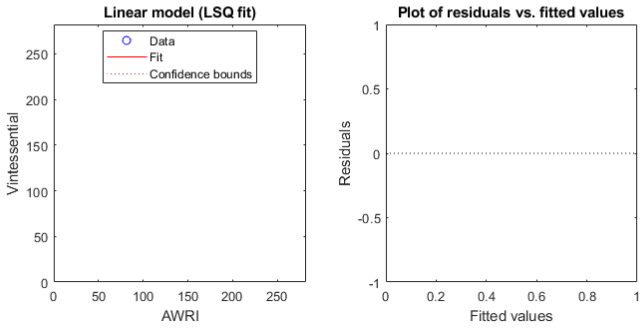
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.5805	0.71929	2.1973	0.041327
AWRI	1.1296	0.19328	5.8446	1.5516e-05

Number of observations: 20, Error degrees of freedom: 18
Root Mean Squared Error: 2.07
R-squared: 0.655, Adjusted R-Squared 0.636
F-statistic vs. constant model: 34.2, p-value = 1.55e-05
F value = 0.80064
Degrees of Freedom = 19 & 49
Critical F value = 1.8029
Probability of difference in variance between groups = 0.60944
No significant difference in variances at the 5% significance level
t-value = -4.2781
Degrees of Freedom = 19
Critical t-value = 1.7291
Probability of difference in means between groups = 0.00040615
Significant mean differences between samples sets
Warning: Regression design matrix is rank deficient to within machine precision.





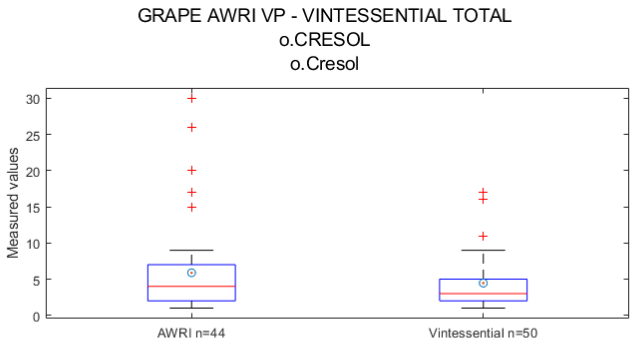
{'GRAPE AWRI VP - …'} {'Methyl.Syringol'} {'4.MS'}

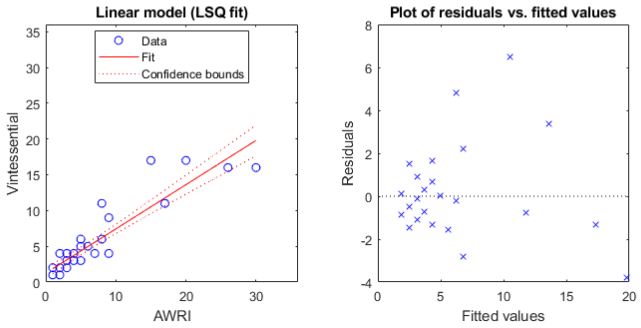
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0	0	NaN	NaN
AWRI	0	0	NaN	NaN

Number of observations: 0, Error degrees of freedom: 0
R-squared: NaN, Adjusted R-Squared NaN
F-statistic vs. constant model: NaN, p-value = NaN
F value = NaN
Degrees of Freedom = 0 & 49
Critical F value = NaN
Probability of difference in variance between groups = NaN
Significant variance differences between samples sets
t-value = NaN
Degrees of Freedom = 0
Critical t-value = NaN
Probability of difference in means between groups = NaN
Significant mean differences between samples sets





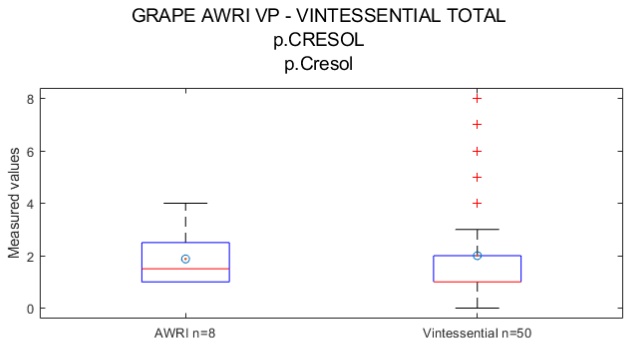
{'GRAPE AWRI VP - …'} {'o.CRESOL'} {'o.Cresol'}

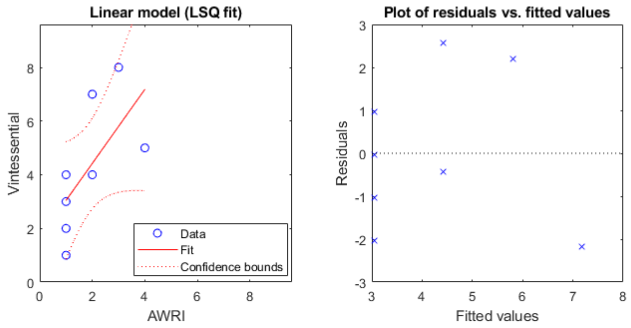
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.2484	0.36919	3.3813	0.0015697
AWRI	0.61804	0.04265	14.491	6.0907e-18

Number of observations: 44, Error degrees of freedom: 42
Root Mean Squared Error: 1.8
R-squared: 0.833, Adjusted R-Squared 0.829
F-statistic vs. constant model: 210, p-value = 6.09e-18
F value = 2.2941
Degrees of Freedom = 43 & 49
Critical F value = 1.6268
Probability of difference in variance between groups = 0.0053235
Significant variance differences between samples sets
t-value = 2.1914
Degrees of Freedom = 43
Critical t-value = 1.6811
Probability of difference in means between groups = 0.033892
Significant mean differences between samples sets





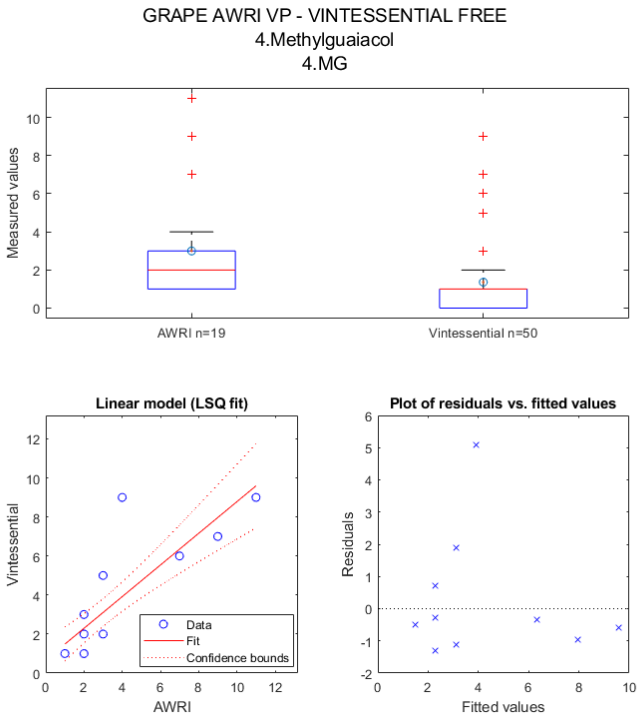
{'GRAPE AWRI VP - …'} {'p.CRESOL'} {'p.Cresol'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.662	1.4008	1.1865	0.28028
AWRI	1.3803	0.65135	2.1191	0.078379

Number of observations: 8, Error degrees of freedom: 6
Root Mean Squared Error: 1.94
R-squared: 0.428, Adjusted R-Squared 0.333
F-statistic vs. constant model: 4.49, p-value = 0.0784
F value = 0.48535
Degrees of Freedom = 7 & 49
Critical F value = 2.2032
Probability of difference in variance between groups = 0.31882
No significant difference in variances at the 5% significance level
t-value = -3.6374
Degrees of Freedom = 7
Critical t-value = 1.8946
Probability of difference in means between groups = 0.0083162
Significant mean differences between samples sets



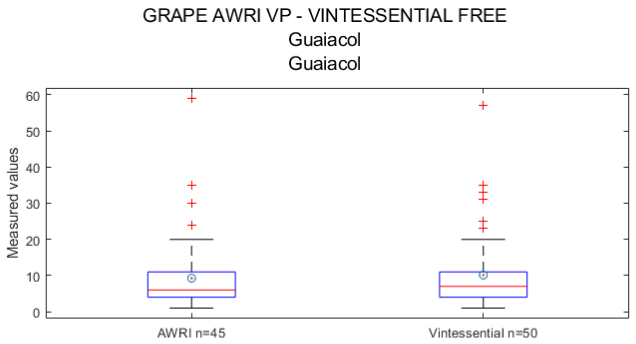
{'GRAPE AWRI VP - …'} {'4.Methylguaiacol'} {'4.MG'}

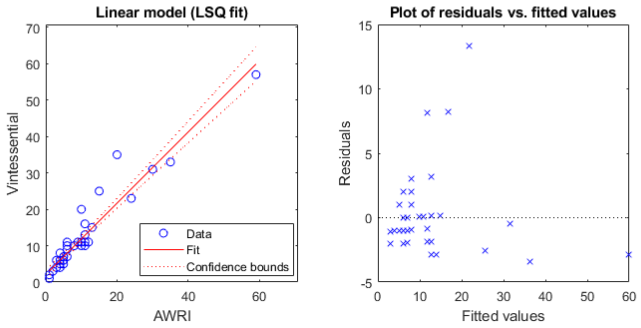
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.67283	0.49347	1.3635	0.19052
AWRI	0.81081	0.12043	6.7325	3.5106e-06

Number of observations: 19, Error degrees of freedom: 17
Root Mean Squared Error: 1.47
R-squared: 0.727, Adjusted R-Squared 0.711
F-statistic vs. constant model: 45.3, p-value = 3.51e-06
F value = 1.7253
Degrees of Freedom = 18 & 49
Critical F value = 1.8185
Probability of difference in variance between groups = 0.13337
No significant difference in variances at the 5% significance level
t-value = -0.30113
Degrees of Freedom = 18
Critical t-value = 1.7341
Probability of difference in means between groups = 0.76677
No significant difference in means at the 5% significance level





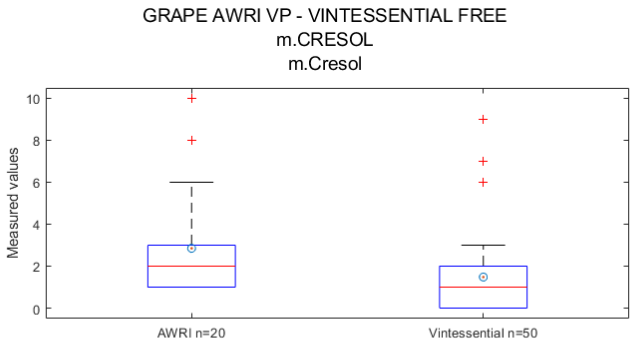
{'GRAPE AWRI VP - …'} {'Guaiacol'} {'Guaiacol'}

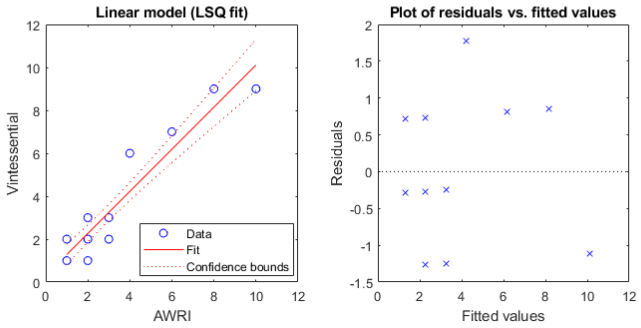
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	2.0728	0.63024	3.289	0.002011
AWRI	0.98015	0.045502	21.541	1.156e-24

Number of observations: 45, Error degrees of freedom: 43
Root Mean Squared Error: 3.14
R-squared: 0.915, Adjusted R-Squared 0.913
F-statistic vs. constant model: 464, p-value = 1.16e-24
F value = 0.97088
Degrees of Freedom = 44 & 49
Critical F value = 1.6232
Probability of difference in variance between groups = 0.92449
No significant difference in variances at the 5% significance level
t-value = -4.0701
Degrees of Freedom = 44
Critical t-value = 1.6802
Probability of difference in means between groups = 0.00019226
Significant mean differences between samples sets





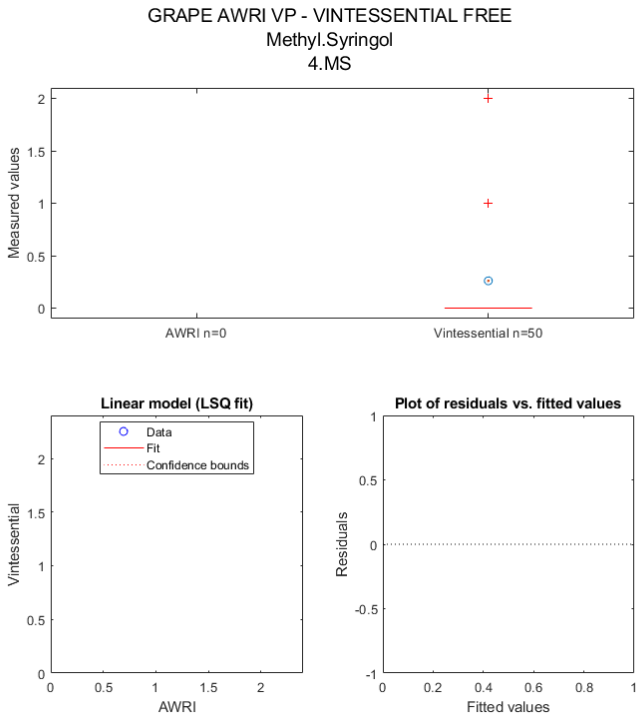
{'GRAPE AWRI VP - …'} {'m.CRESOL'} {'m.Cresol'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.30598	0.28041	1.0912	0.28958
AWRI	0.98036	0.075347	13.011	1.3574e-10

Number of observations: 20, Error degrees of freedom: 18
Root Mean Squared Error: 0.806
R-squared: 0.904, Adjusted R-Squared 0.899
F-statistic vs. constant model: 169, p-value = 1.36e-10
F value = 1.3522
Degrees of Freedom = 19 & 49
Critical F value = 1.8029
Probability of difference in variance between groups = 0.39207
No significant difference in variances at the 5% significance level
t-value = -1.4217
Degrees of Freedom = 19
Critical t-value = 1.7291
Probability of difference in means between groups = 0.17132
No significant difference in means at the 5% significance level
Warning: Regression design matrix is rank deficient to within machine precision.



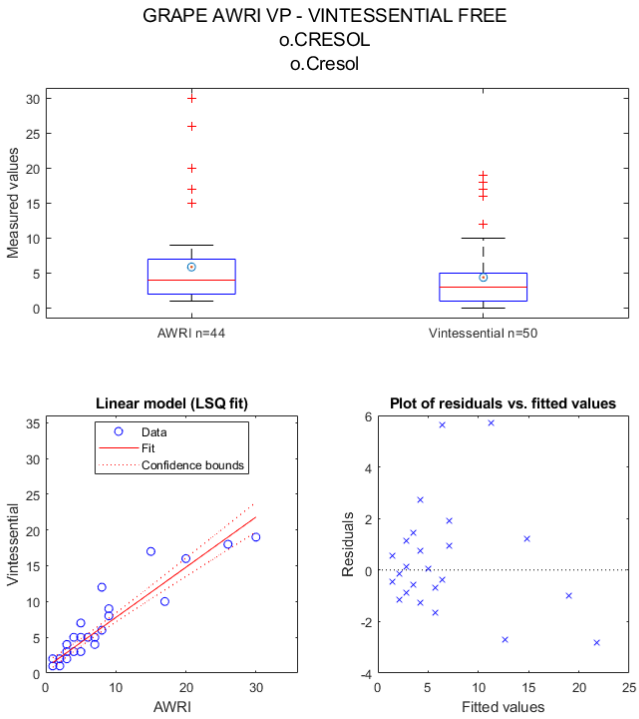
{'GRAPE AWRI VP - …'} {'Methyl.Syringol'} {'4.MS'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0	0	NaN	NaN
AWRI	0	0	NaN	NaN

Number of observations: 0, Error degrees of freedom: 0
R-squared: NaN, Adjusted R-Squared NaN
F-statistic vs. constant model: NaN, p-value = NaN
F value = NaN
Degrees of Freedom = 0 & 49
Critical F value = NaN
Probability of difference in variance between groups = NaN
Significant variance differences between samples sets
t-value = NaN
Degrees of Freedom = 0
Critical t-value = NaN
Probability of difference in means between groups = NaN
Significant mean differences between samples sets



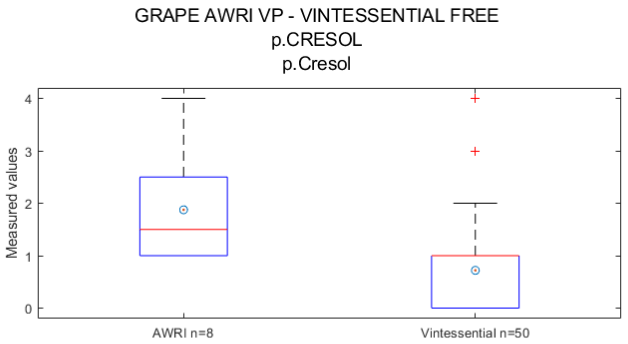
{'GRAPE AWRI VP - …'} {'o.CRESOL'} {'o.Cresol'}

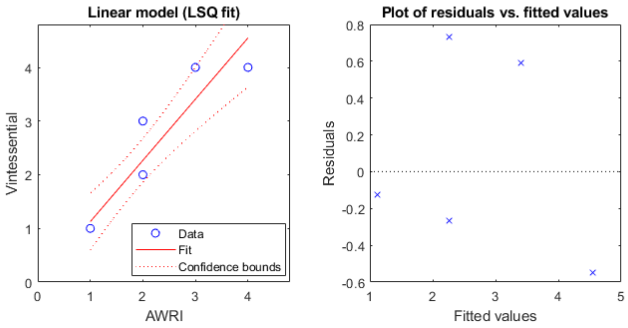
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.75684	0.35629	2.1242	0.039582
AWRI	0.70154	0.04116	17.044	1.7621e-20

Number of observations: 44, Error degrees of freedom: 42
Root Mean Squared Error: 1.73
R-squared: 0.874, Adjusted R-Squared 0.871
F-statistic vs. constant model: 291, p-value = 1.76e-20
F value = 1.8598
Degrees of Freedom = 43 & 49
Critical F value = 1.6268
Probability of difference in variance between groups = 0.036423
Significant variance differences between samples sets
t-value = 2.5811
Degrees of Freedom = 43
Critical t-value = 1.6811
Probability of difference in means between groups = 0.013344
Significant mean differences between samples sets





{'GRAPE AWRI VP - …'} {'p.CRESOL'} {'p.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	-0.014085	0.3391	-0.041535	0.96822
AWRI	1.1408	0.15768	7.2352	0.00035377

Number of observations: 8, Error degrees of freedom: 6

Root Mean Squared Error: 0.47

R-squared: 0.897, Adjusted R-Squared 0.88

F-statistic vs. constant model: 52.3, p-value = 0.000354

F value = 1.4764

Degrees of Freedom = 7 & 49

Critical F value = 2.2032

Probability of difference in variance between groups = 0.39553

No significant difference in variances at the 5% significance level

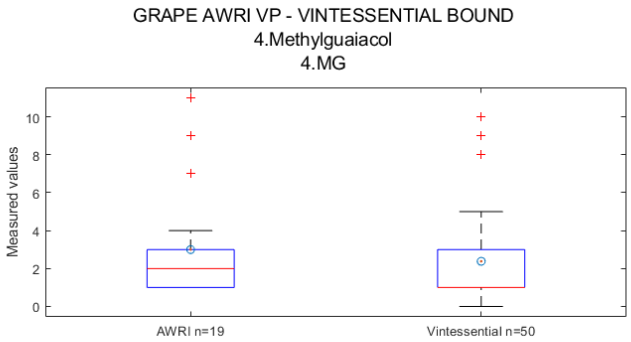
t-value = -1.5275

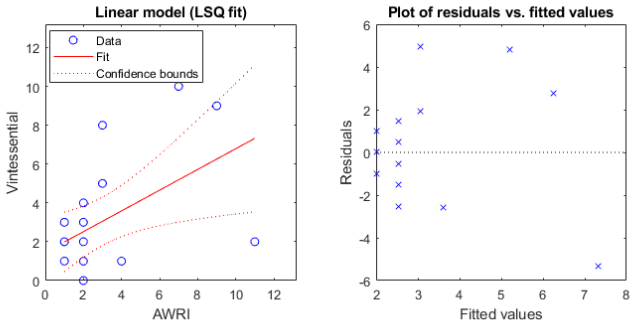
Degrees of Freedom = 7

Critical t-value = 1.8946

Probability of difference in means between groups = 0.17047

No significant difference in means at the 5% significance level





{'GRAPE AWRI VP - …'} {'4.Methylguaiacol'} {'4.MG'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.4513	0.86751	1.6729	0.11264
AWRI	0.53378	0.21172	2.5212	0.021972

Number of observations: 19, Error degrees of freedom: 17

Root Mean Squared Error: 2.58

R-squared: 0.272, Adjusted R-Squared 0.229

F-statistic vs. constant model: 6.36, p-value = 0.022

F value = 1.2443

Degrees of Freedom = 18 & 49

Critical F value = 1.8185

Probability of difference in variance between groups = 0.53156

No significant difference in variances at the 5% significance level

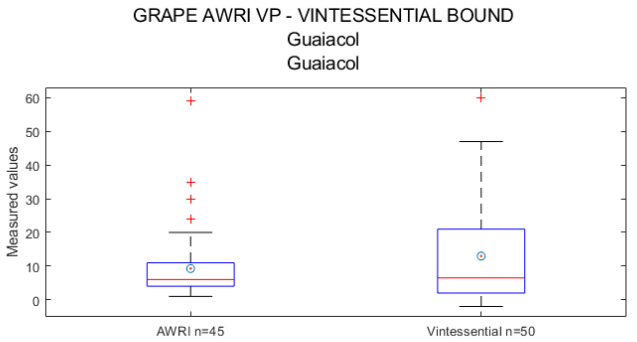
t-value = -0.080845

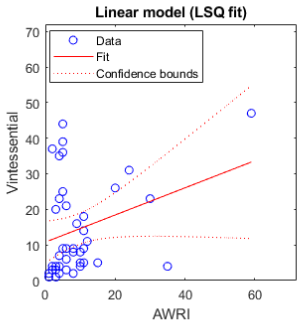
Degrees of Freedom = 18

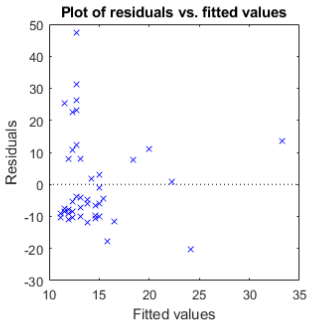
Critical t-value = 1.7341

Probability of difference in means between groups = 0.93646

No significant difference in means at the 5% significance level







{'GRAPE AWRI VP - …'} {'Guaiacol'} {'Guaiacol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	10.803	2.9052	3.7183	0.00057577
AWRI	0.38102	0.20975	1.8165	0.076265

Number of observations: 45, Error degrees of freedom: 43

Root Mean Squared Error: 14.5

R-squared: 0.0713, Adjusted R-Squared 0.0497

F-statistic vs. constant model: 3.3, p-value = 0.0763

F value = 0.50382

Degrees of Freedom = 44 & 49

Critical F value = 1.6232

Probability of difference in variance between groups = 0.022572

Significant variance differences between samples sets

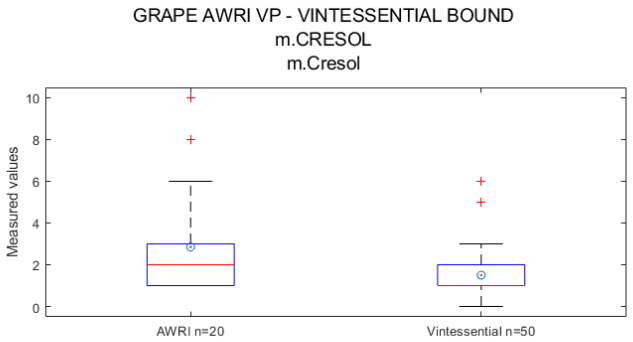
t-value = -2.1645

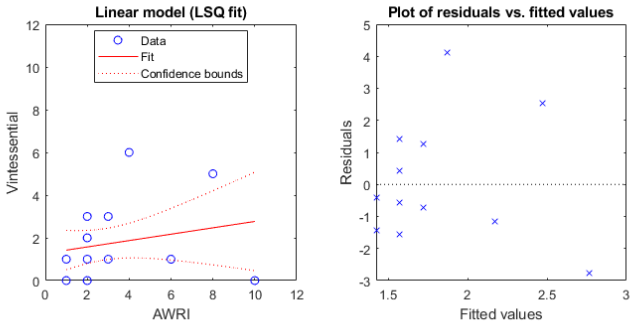
Degrees of Freedom = 44

Critical t-value = 1.6802

Probability of difference in means between groups = 0.035891

Significant mean differences between samples sets





{'GRAPE AWRI VP - …'} {'m.CRESOL'} {'m.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.2746	0.54146	2.3539	0.03014
AWRI	0.14928	0.14549	1.026	0.31847

Number of observations: 20, Error degrees of freedom: 18

Root Mean Squared Error: 1.56

R-squared: 0.0553, Adjusted R-Squared 0.00277

F-statistic vs. constant model: 1.05, p-value = 0.318

F value = 3.1937

Degrees of Freedom = 19 & 49

Critical F value = 1.8029

Probability of difference in variance between groups = 0.0011056

Significant variance differences between samples sets

t-value = 1.9928

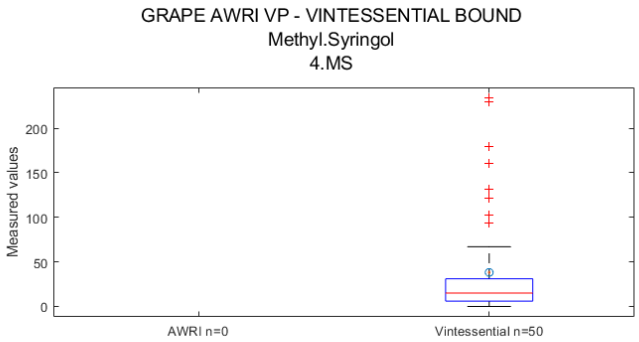
Degrees of Freedom = 19

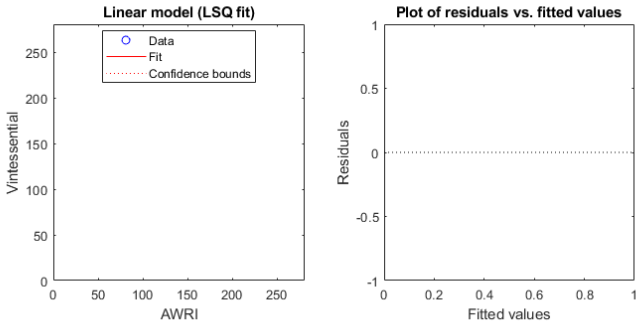
Critical t-value = 1.7291

Probability of difference in means between groups = 0.060849

No significant difference in means at the 5% significance level

Warning: Regression design matrix is rank deficient to within machine precision.





{'GRAPE AWRI VP - …'} {'Methyl.Syringol'} {'4.MS'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0	0	NaN	NaN
AWRI	0	0	NaN	NaN

Number of observations: 0, Error degrees of freedom: 0

R-squared: NaN, Adjusted R-Squared NaN

F-statistic vs. constant model: NaN, p-value = NaN

F value = NaN

Degrees of Freedom = 0 & 49

Critical F value = NaN

Probability of difference in variance between groups = NaN

Significant variance differences between samples sets

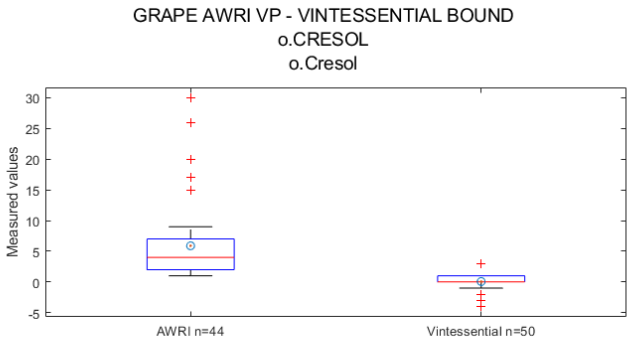
t-value = NaN

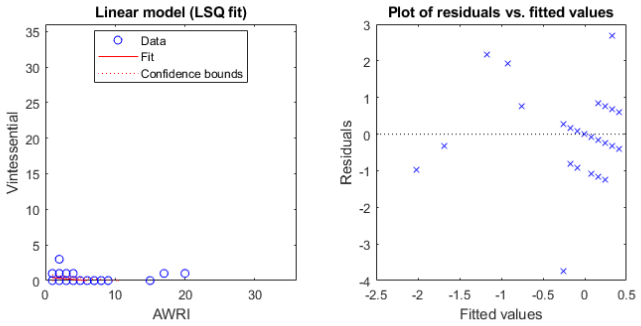
Degrees of Freedom = 0

Critical t-value = NaN

Probability of difference in means between groups = NaN

Significant mean differences between samples sets





{'GRAPE AWRI VP - …'} {'o.CRESOL'} {'o.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.49152	0.20959	2.3451	0.023821
AWRI	-0.083501	0.024213	-3.4487	0.0012942

Number of observations: 44, Error degrees of freedom: 42

Root Mean Squared Error: 1.02

R-squared: 0.221, Adjusted R-Squared 0.202

F-statistic vs. constant model: 11.9, p-value = 0.00129

F value = 34.3378

Degrees of Freedom = 43 & 49

Critical F value = 1.6268

Probability of difference in variance between groups = 9.5891e-25

Significant variance differences between samples sets

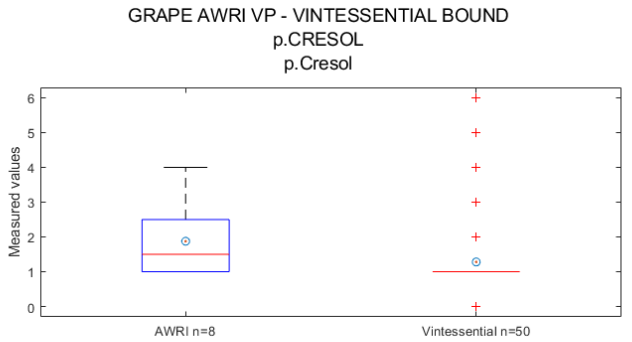
t-value = 5.555

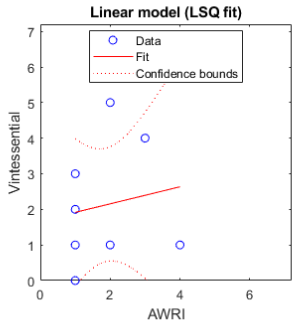
Degrees of Freedom = 43

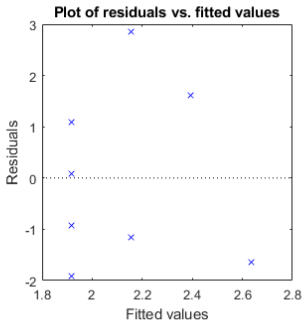
Critical t-value = 1.6811

Probability of difference in means between groups = 1.6166e-06

Significant mean differences between samples sets







{'GRAPE AWRI VP - …'} {'p.CRESOL'} {'p.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.6761	1.33	1.2602	0.25439
AWRI	0.23944	0.61844	0.38716	0.71199

Number of observations: 8, Error degrees of freedom: 6

Root Mean Squared Error: 1.84

R-squared: 0.0244, Adjusted R-Squared -0.138

F-statistic vs. constant model: 0.15, p-value = 0.712

F value = 0.79566

Degrees of Freedom = 7 & 49

Critical F value = 2.2032

Probability of difference in variance between groups = 0.81079

No significant difference in variances at the 5% significance level

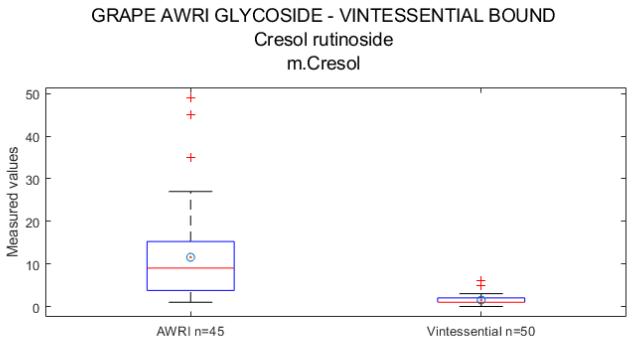
t-value = -0.37048

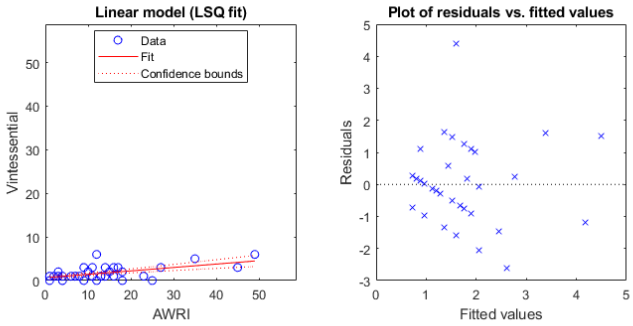
Degrees of Freedom = 7

Critical t-value = 1.8946

Probability of difference in means between groups = 0.72198

No significant difference in means at the 5% significance level





{'GRAPE AWRI GLYCO…'} {'Cresol rutinoside'} {'m.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.65141	0.25689	2.5358	0.014936
AWRI	0.078244	0.016274	4.8078	1.8949e-05

Number of observations: 45, Error degrees of freedom: 43

Root Mean Squared Error: 1.17

R-squared: 0.35, Adjusted R-Squared 0.334

F-statistic vs. constant model: 23.1, p-value = 1.89e-05

F value = 62.6419

Degrees of Freedom = 44 & 49

Critical F value = 1.6232

Probability of difference in variance between groups = 6.1859e-31

Significant variance differences between samples sets

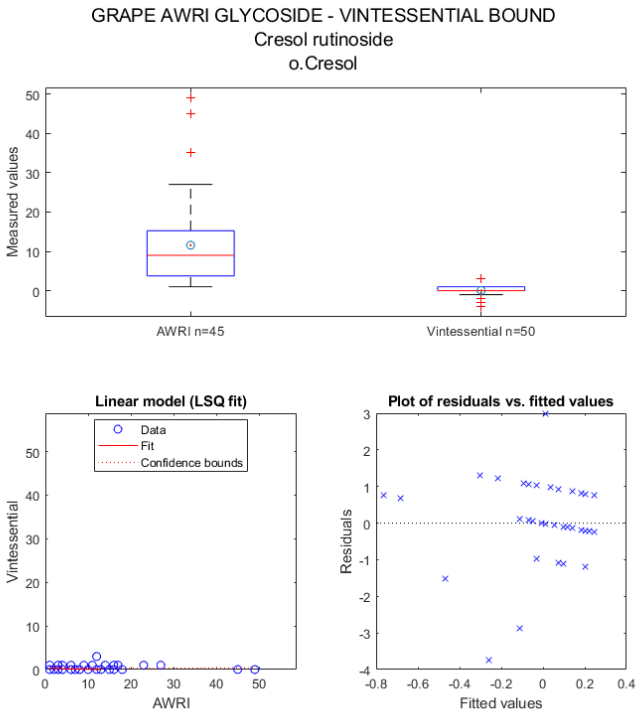
t-value = 6.648

Degrees of Freedom = 44

Critical t-value = 1.6802

Probability of difference in means between groups = 3.7571e-08

Significant mean differences between samples sets



{'GRAPE AWRI GLYCO…'} {'Cresol rutinoside'} {'o.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.26553	0.24674	1.0761	0.28786
AWRI	-0.021056	0.015632	-1.347	0.18505

Number of observations: 45, Error degrees of freedom: 43

Root Mean Squared Error: 1.13

R-squared: 0.0405, Adjusted R-Squared 0.0182

F-statistic vs. constant model: 1.81, p-value = 0.185

F value = 98.5103

Degrees of Freedom = 44 & 49

Critical F value = 1.6232

Probability of difference in variance between groups = 1.2532e-35

Significant variance differences between samples sets

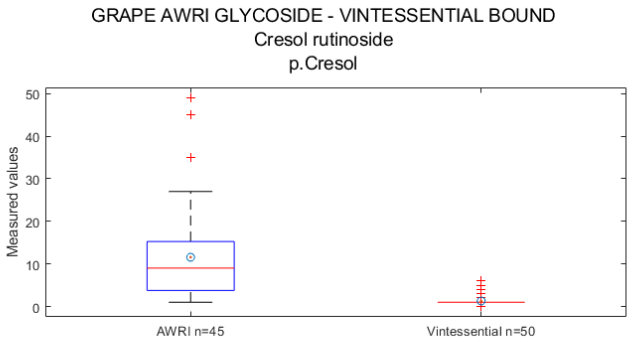
t-value = 6.9331

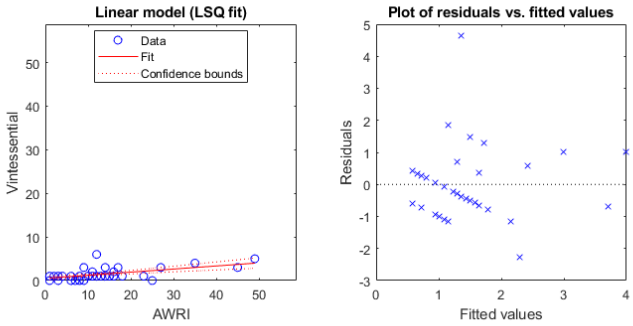
Degrees of Freedom = 44

Critical t-value = 1.6802

Probability of difference in means between groups = 1.4327e-08

Significant mean differences between samples sets





{'GRAPE AWRI GLYCO…'} {'Cresol rutinoside'} {'p.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.51456	0.23568	2.1833	0.034518
AWRI	0.070855	0.014931	4.7455	2.319e-05

Number of observations: 45, Error degrees of freedom: 43

Root Mean Squared Error: 1.08

R-squared: 0.344, Adjusted R-Squared 0.328

F-statistic vs. constant model: 22.5, p-value = 2.32e-05

F value = 74.2107

Degrees of Freedom = 44 & 49

Critical F value = 1.6232

Probability of difference in variance between groups = 1.0991e-32

Significant variance differences between samples sets

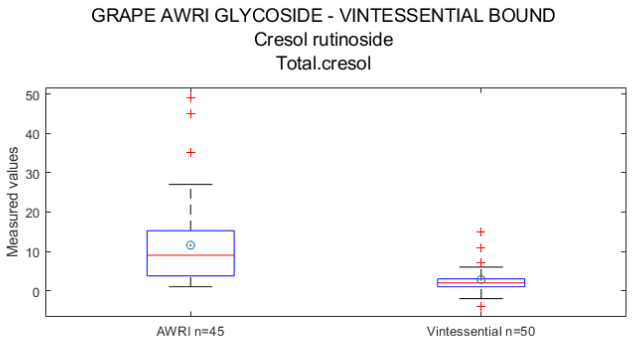
t-value = 6.7494

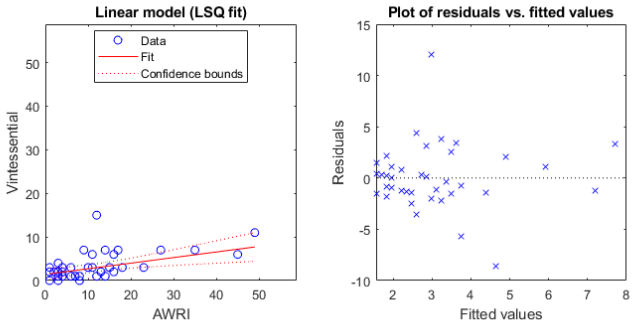
Degrees of Freedom = 44

Critical t-value = 1.6802

Probability of difference in means between groups = 2.6661e-08

Significant mean differences between samples sets





{'GRAPE AWRI GLYCO…'} {'Cresol rutinoside'} {'Total.cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.4315	0.66268	2.1602	0.036378
AWRI	0.12804	0.041983	3.0499	0.0039101

Number of observations: 45, Error degrees of freedom: 43

Root Mean Squared Error: 3.03

R-squared: 0.178, Adjusted R-Squared 0.159

F-statistic vs. constant model: 9.3, p-value = 0.00391

F value = 11.9541

Degrees of Freedom = 44 & 49

Critical F value = 1.6232

Probability of difference in variance between groups = 1.0755e-14

Significant variance differences between samples sets

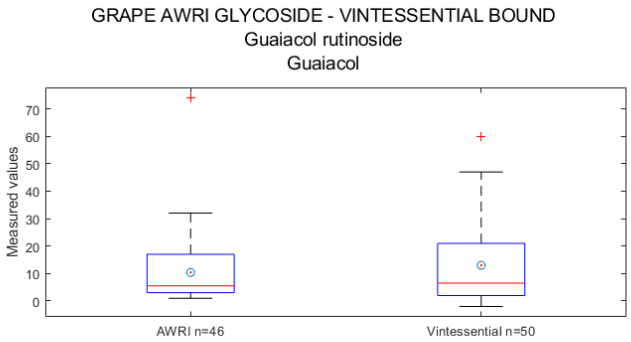
t-value = 5.8319

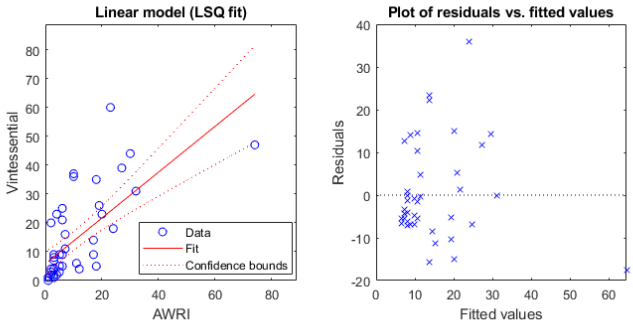
Degrees of Freedom = 44

Critical t-value = 1.6802

Probability of difference in means between groups = 5.9575e-07

Significant mean differences between samples sets





{'GRAPE AWRI GLYCO…'} {'Guaiacol rutinos…'} {'Guaiacol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	5.7831	2.0964	2.7585	0.0084265
AWRI	0.7945	0.12846	6.1848	1.8052e-07

Number of observations: 46, Error degrees of freedom: 44

Root Mean Squared Error: 11

R-squared: 0.465, Adjusted R-Squared 0.453

F-statistic vs. constant model: 38.3, p-value = 1.81e-07

F value = 0.75458

Degrees of Freedom = 45 & 49

Critical F value = 1.6198

Probability of difference in variance between groups = 0.34128

No significant difference in variances at the 5% significance level

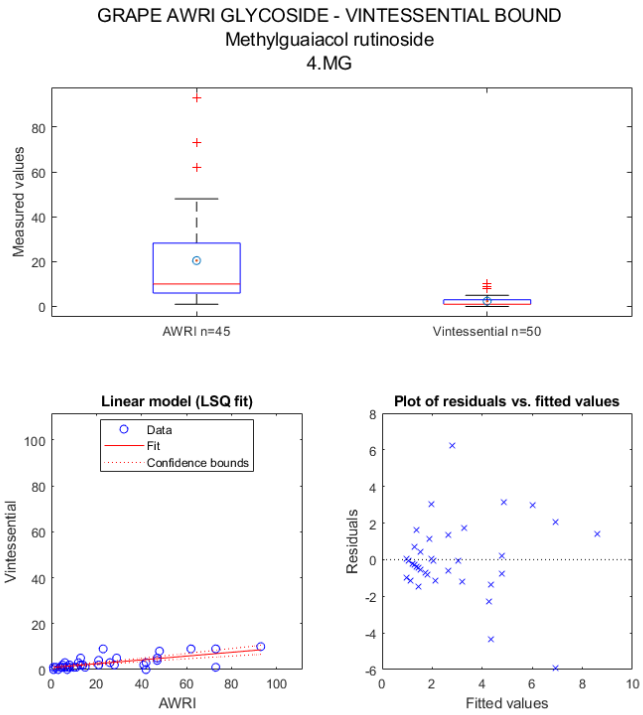
t-value = -2.218

Degrees of Freedom = 45

Critical t-value = 1.6794

Probability of difference in means between groups = 0.031646

Significant mean differences between samples sets



{'GRAPE AWRI GLYCO…'} {'Methylguaiacol r…'} {'4.MG'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.88311	0.386	2.2878	0.027126
AWRI	0.082892	0.012843	6.4543	7.9794e-08

Number of observations: 45, Error degrees of freedom: 43

Root Mean Squared Error: 1.9

R-squared: 0.492, Adjusted R-Squared 0.48

F-statistic vs. constant model: 41.7, p-value = 7.98e-08

F value = 75.1222

Degrees of Freedom = 44 & 49

Critical F value = 1.6232

Probability of difference in variance between groups = 8.2154e-33

Significant variance differences between samples sets

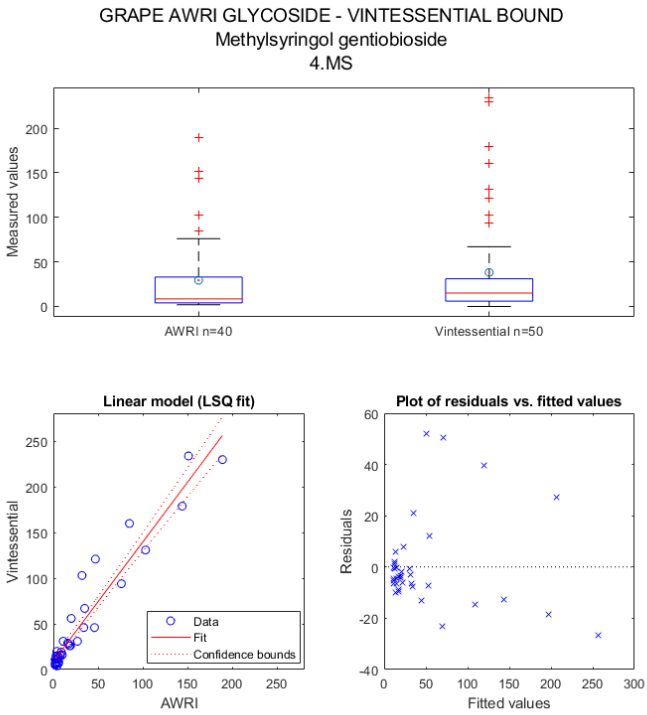
t-value = 5.8411

Degrees of Freedom = 44

Critical t-value = 1.6802

Probability of difference in means between groups = 5.775e-07

Significant mean differences between samples sets



{'GRAPE AWRI GLYCO…'} {'Methylsyringol g…'} {'4.MS'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	8.8426	3.2442	2.7257	0.0096499
AWRI	1.3103	0.060852	21.533	6.8178e-23

Number of observations: 40, Error degrees of freedom: 38

Root Mean Squared Error: 17.1

R-squared: 0.924, Adjusted R-Squared 0.922

F-statistic vs. constant model: 464, p-value = 6.82e-23

F value = 0.60737

Degrees of Freedom = 39 & 49

Critical F value = 1.6428

Probability of difference in variance between groups = 0.10983

No significant difference in variances at the 5% significance level

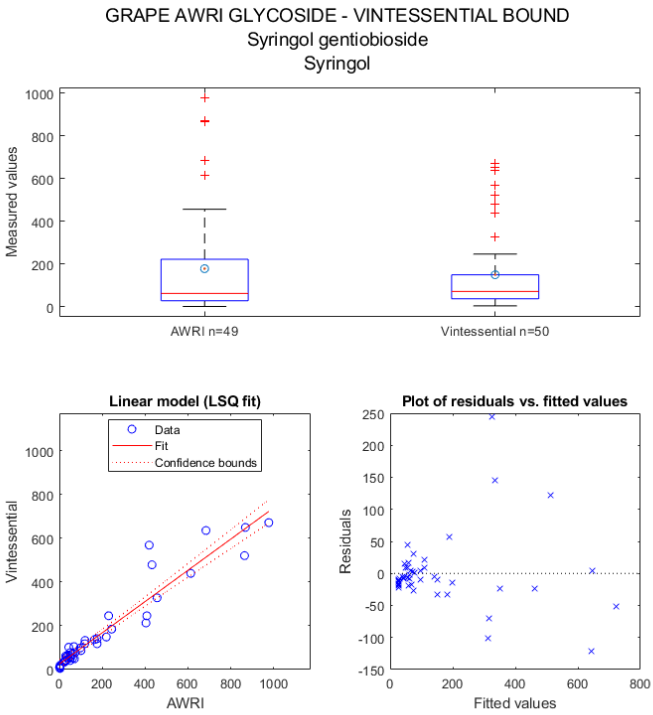
t-value = -5.1737

Degrees of Freedom = 39

Critical t-value = 1.6849

Probability of difference in means between groups = 7.2288e-06

Significant mean differences between samples sets



{'GRAPE AWRI GLYCO…'} {'Syringol gentiob…'} {'Syringol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	25.266	9.7169	2.6002	0.012413
AWRI	0.71456	0.031914	22.39	1.0221e-26

Number of observations: 49, Error degrees of freedom: 47

Root Mean Squared Error: 55.2

R-squared: 0.914, Adjusted R-Squared 0.912

F-statistic vs. constant model: 501, p-value = 1.02e-26

F value = 1.8046

Degrees of Freedom = 48 & 49

Critical F value = 1.6102

Probability of difference in variance between groups = 0.041998

Significant variance differences between samples sets

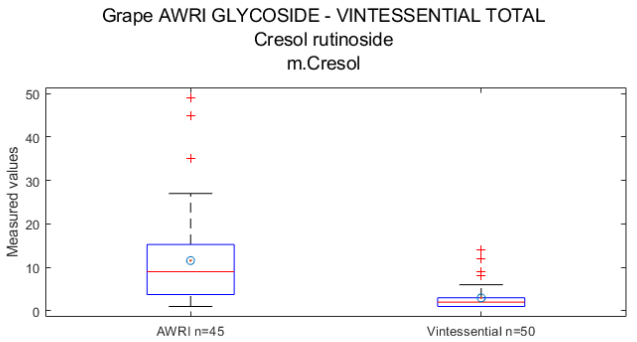
t-value = 1.9868

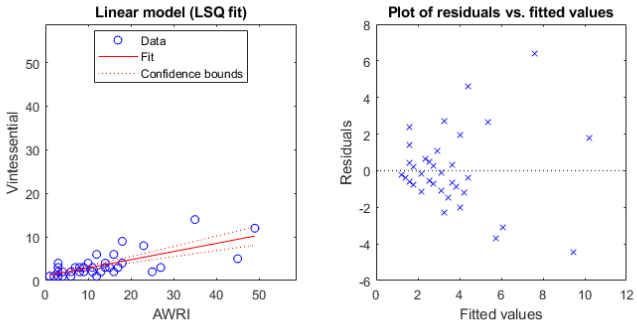
Degrees of Freedom = 48

Critical t-value = 1.6772

Probability of difference in means between groups = 0.052669

No significant difference in means at the 5% significance level





{'Grape AWRI GLYCO…'} {'Cresol rutinoside'} {'m.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.0346	0.428	2.4173	0.019948
AWRI	0.18739	0.027115	6.9108	1.7326e-08

Number of observations: 45, Error degrees of freedom: 43

Root Mean Squared Error: 1.96

R-squared: 0.526, Adjusted R-Squared 0.515

F-statistic vs. constant model: 47.8, p-value = 1.73e-08

F value = 15.7038

Degrees of Freedom = 44 & 49

Critical F value = 1.6232

Probability of difference in variance between groups = 3.3609e-17

Significant variance differences between samples sets

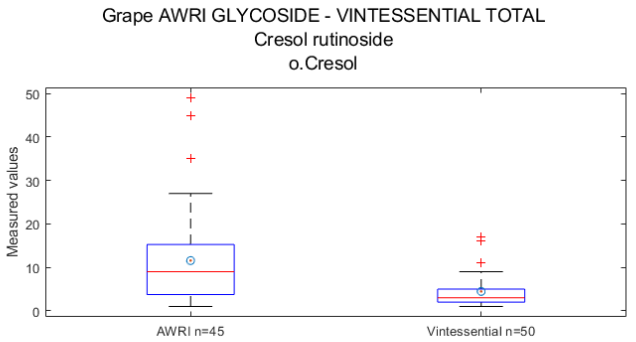
t-value = 6.1964

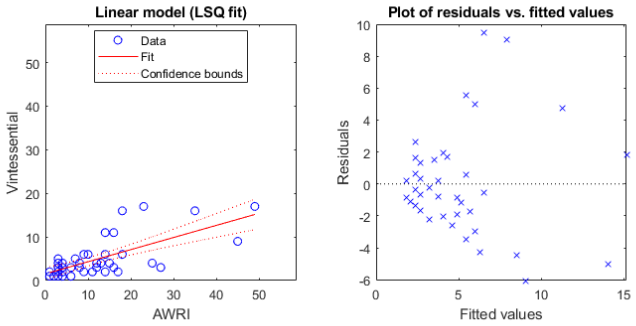
Degrees of Freedom = 44

Critical t-value = 1.6802

Probability of difference in means between groups = 1.7356e-07

Significant mean differences between samples sets





{'Grape AWRI GLYCO…'} {'Cresol rutinoside'} {'o.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.5461	0.69916	2.2114	0.032374
AWRI	0.27774	0.044293	6.2704	1.4774e-07

Number of observations: 45, Error degrees of freedom: 43

Root Mean Squared Error: 3.2

R-squared: 0.478, Adjusted R-Squared 0.465

F-statistic vs. constant model: 39.3, p-value = 1.48e-07

F value = 6.5814

Degrees of Freedom = 44 & 49

Critical F value = 1.6232

Probability of difference in variance between groups = 1.21e-09

Significant variance differences between samples sets

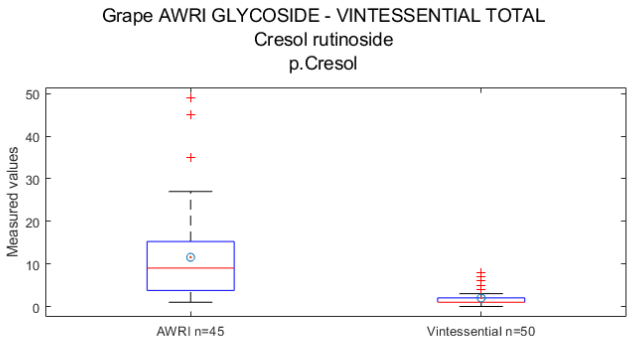
t-value = 5.3885

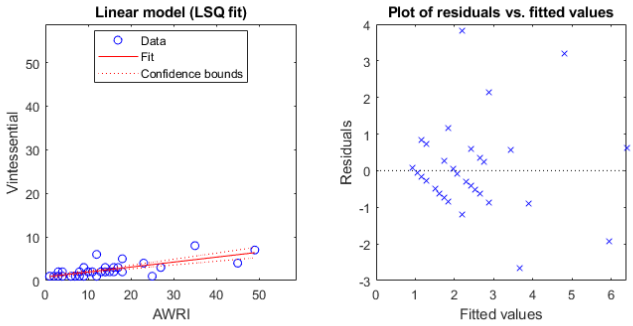
Degrees of Freedom = 44

Critical t-value = 1.6802

Probability of difference in means between groups = 2.648e-06

Significant mean differences between samples sets





{'Grape AWRI GLYCO…'} {'Cresol rutinoside'} {'p.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.8193	0.24045	3.4073	0.0014343
AWRI	0.11371	0.015233	7.4648	2.7499e-09

Number of observations: 45, Error degrees of freedom: 43

Root Mean Squared Error: 1.1

R-squared: 0.564, Adjusted R-Squared 0.554

F-statistic vs. constant model: 55.7, p-value = 2.75e-09

F value = 45.2685

Degrees of Freedom = 44 & 49

Critical F value = 1.6232

Probability of difference in variance between groups = 1.3123e-27

Significant variance differences between samples sets

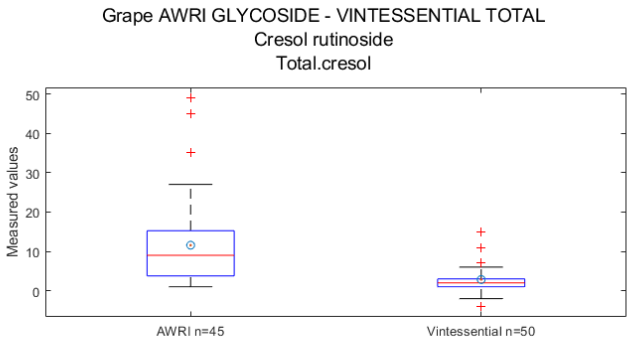
t-value = 6.5169

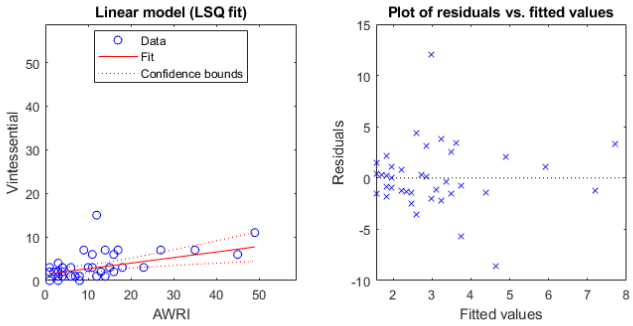
Degrees of Freedom = 44

Critical t-value = 1.6802

Probability of difference in means between groups = 5.8586e-08

Significant mean differences between samples sets





{'Grape AWRI GLYCO…'} {'Cresol rutinoside'} {'Total.cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.4315	0.66268	2.1602	0.036378
AWRI	0.12804	0.041983	3.0499	0.0039101

Number of observations: 45, Error degrees of freedom: 43

Root Mean Squared Error: 3.03

R-squared: 0.178, Adjusted R-Squared 0.159

F-statistic vs. constant model: 9.3, p-value = 0.00391

F value = 11.9541

Degrees of Freedom = 44 & 49

Critical F value = 1.6232

Probability of difference in variance between groups = 1.0755e-14

Significant variance differences between samples sets

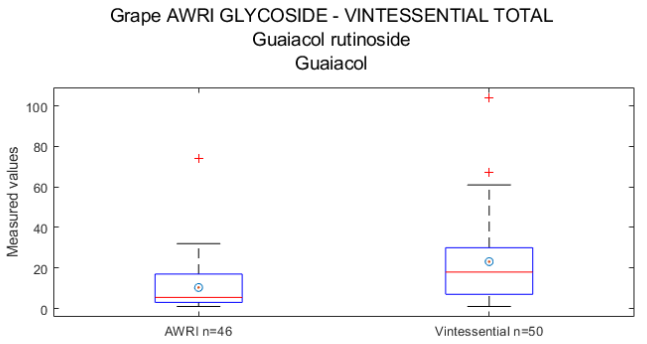
t-value = 5.8319

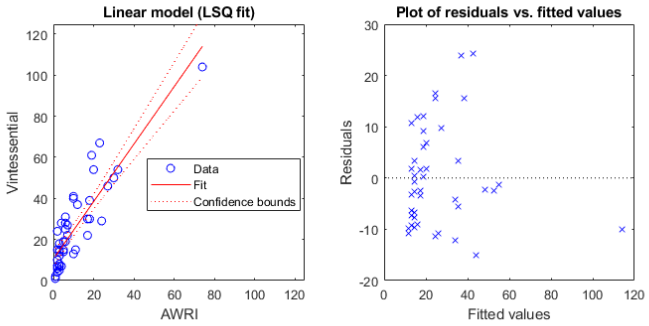
Degrees of Freedom = 44

Critical t-value = 1.6802

Probability of difference in means between groups = 5.9575e-07

Significant mean differences between samples sets





{'Grape AWRI GLYCO…'} {'Guaiacol rutinos…'} {'Guaiacol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	10.442	1.8726	5.5761	1.411e-06
AWRI	1.3997	0.11475	12.199	1.0341e-15

Number of observations: 46, Error degrees of freedom: 44

Root Mean Squared Error: 9.81

R-squared: 0.772, Adjusted R-Squared 0.767

F-statistic vs. constant model: 149, p-value = 1.03e-15

F value = 0.38828

Degrees of Freedom = 45 & 49

Critical F value = 1.6198

Probability of difference in variance between groups = 0.00168

Significant variance differences between samples sets

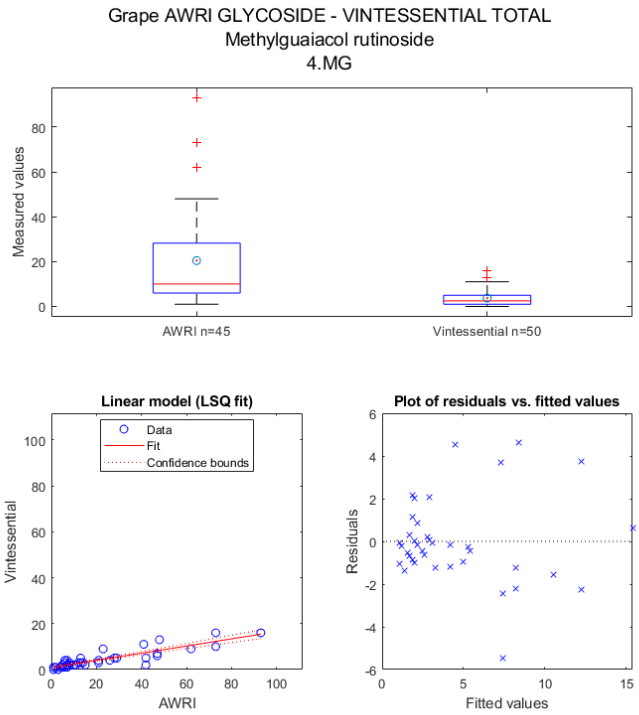
t-value = -9.0321

Degrees of Freedom = 45

Critical t-value = 1.6794

Probability of difference in means between groups = 1.1417e-11

Significant mean differences between samples sets



{'Grape AWRI GLYCO…'} {'Methylguaiacol r…'} {'4.MG'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.90423	0.37688	2.3992	0.020836
AWRI	0.15577	0.01254	12.422	8.072e-16

Number of observations: 45, Error degrees of freedom: 43

Root Mean Squared Error: 1.85

R-squared: 0.782, Adjusted R-Squared 0.777

F-statistic vs. constant model: 154, p-value = 8.07e-16

F value = 33.1548

Degrees of Freedom = 44 & 49

Critical F value = 1.6232

Probability of difference in variance between groups = 1.8295e-24

Significant variance differences between samples sets

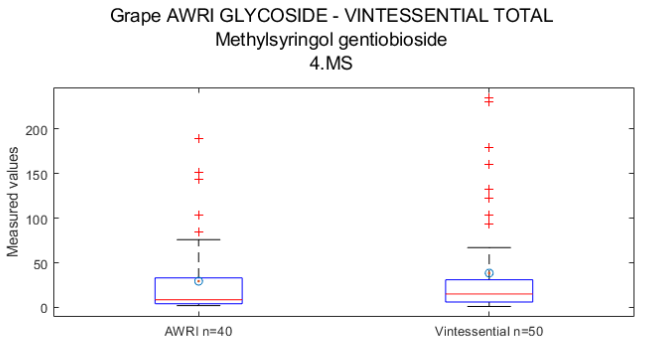
t-value = 5.8056

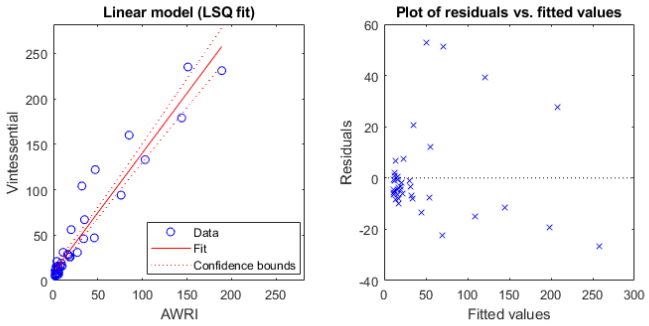
Degrees of Freedom = 44

Critical t-value = 1.6802

Probability of difference in means between groups = 6.5097e-07

Significant mean differences between samples sets





{'Grape AWRI GLYCO…'} {'Methylsyringol g…'} {'4.MS'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	9.016	3.2549	2.77	0.0086254
AWRI	1.3146	0.061054	21.532	6.8228e-23

Number of observations: 40, Error degrees of freedom: 38

Root Mean Squared Error: 17.2

R-squared: 0.924, Adjusted R-Squared 0.922

F-statistic vs. constant model: 464, p-value = 6.82e-23

F value = 0.60327

Degrees of Freedom = 39 & 49

Critical F value = 1.6428

Probability of difference in variance between groups = 0.10514

No significant difference in variances at the 5% significance level

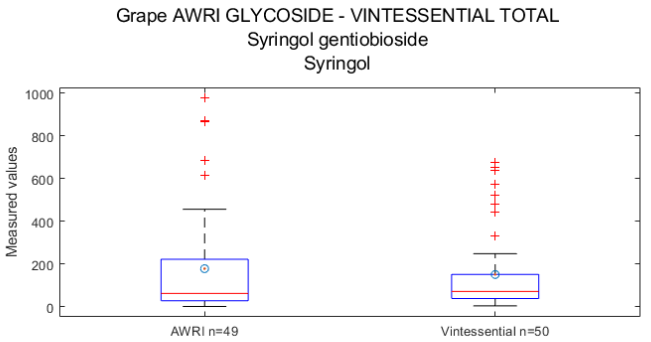
t-value = -5.2204

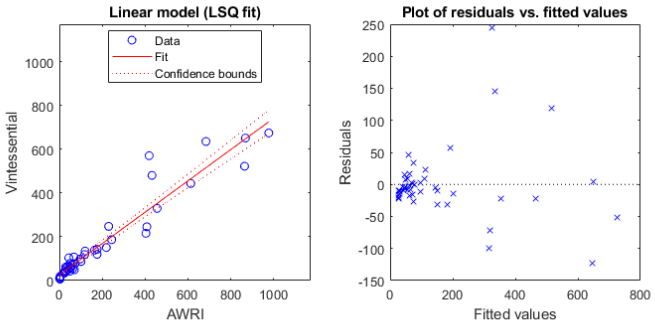
Degrees of Freedom = 39

Critical t-value = 1.6849

Probability of difference in means between groups = 6.2345e-06

Significant mean differences between samples sets





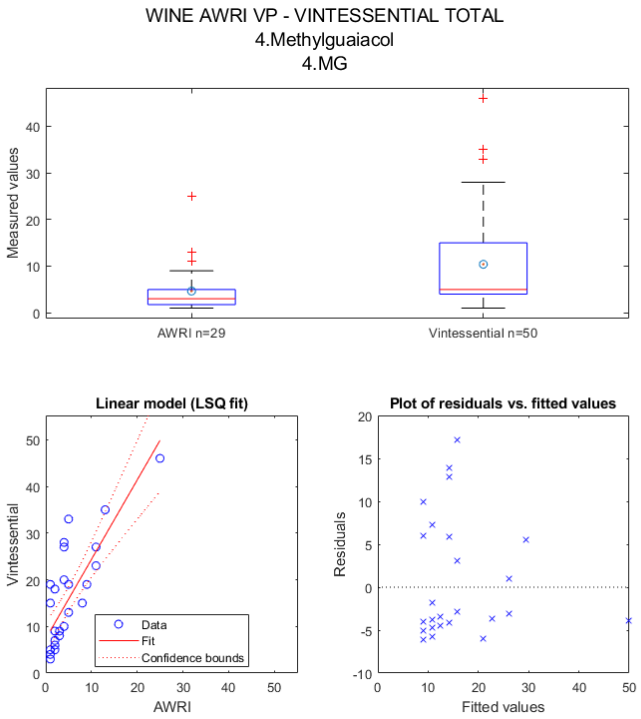
{'Grape AWRI GLYCO…'} {'Syringol gentiob…'} {'Syringol'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	26.005	9.7166	2.6763	0.010216
AWRI	0.71672	0.031914	22.458	8.9644e-27

Number of observations: 49, Error degrees of freedom: 47
Root Mean Squared Error: 55.2
R-squared: 0.915, Adjusted R-Squared 0.913
F-statistic vs. constant model: 504, p-value = 8.96e-27
F value = 1.7945
Degrees of Freedom = 48 & 49
Critical F value = 1.6102
Probability of difference in variance between groups = 0.04397
Significant variance differences between samples sets
t-value = 1.9084
Degrees of Freedom = 48
Critical t-value = 1.6772
Probability of difference in means between groups = 0.062328
No significant difference in means at the 5% significance level



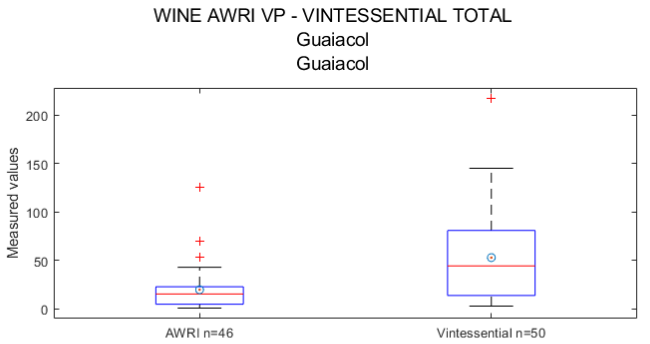
{'WINE AWRI VP - V…'} {'4.Methylguaiacol'} {'4.MG'}

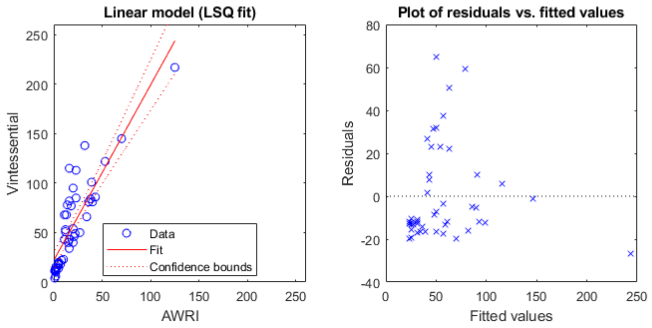
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	7.3619	1.7457	4.2172	0.00024858
AWRI	1.7	0.25371	6.7008	3.4153e-07

Number of observations: 29, Error degrees of freedom: 27
Root Mean Squared Error: 6.92
R-squared: 0.624, Adjusted R-Squared 0.611
F-statistic vs. constant model: 44.9, p-value = 3.42e-07
F value = 0.25096
Degrees of Freedom = 28 & 49
Critical F value = 1.7064
Probability of difference in variance between groups = 0.00020136
Significant variance differences between samples sets
t-value = -7.4307
Degrees of Freedom = 28
Critical t-value = 1.7011
Probability of difference in means between groups = 4.3037e-08
Significant mean differences between samples sets





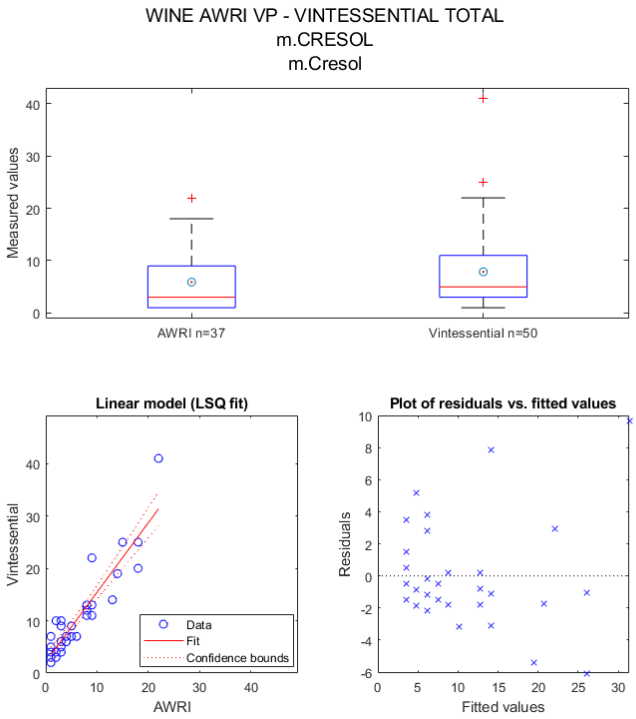
{'WINE AWRI VP - V…'} {'Guaiacol'} {'Guaiacol'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	21.932	4.506	4.8674	1.4923e-05
AWRI	1.7744	0.1529	11.605	5.5842e-15

Number of observations: 46, Error degrees of freedom: 44
Root Mean Squared Error: 22.5
R-squared: 0.754, Adjusted R-Squared 0.748
F-statistic vs. constant model: 135, p-value = 5.58e-15
F value = 0.23345
Degrees of Freedom = 45 & 49
Critical F value = 1.6198
Probability of difference in variance between groups = 2.433e-06
Significant variance differences between samples sets
t-value = -9.0513
Degrees of Freedom = 45
Critical t-value = 1.6794
Probability of difference in means between groups = 1.0727e-11
Significant mean differences between samples sets



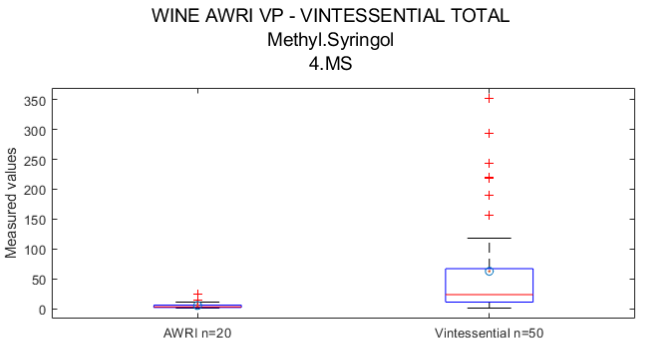
{'WINE AWRI VP - V…'} {'m.CRESOL'} {'m.Cresol'}

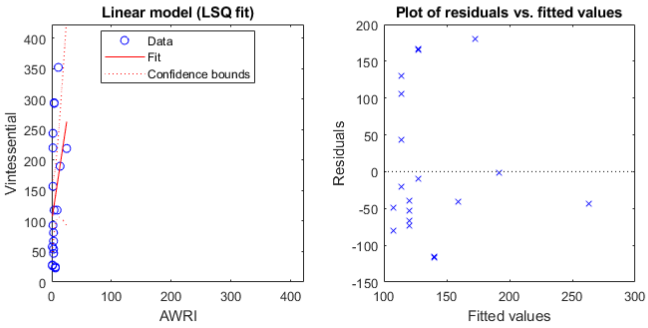
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	2.1857	0.76477	2.8579	0.0071341
AWRI	1.3263	0.09433	14.06	5.7938e-16

Number of observations: 37, Error degrees of freedom: 35
Root Mean Squared Error: 3.2
R-squared: 0.85, Adjusted R-Squared 0.845
F-statistic vs. constant model: 198, p-value = 5.79e-16
F value = 0.51279
Degrees of Freedom = 36 & 49
Critical F value = 1.6567
Probability of difference in variance between groups = 0.038506
Significant variance differences between samples sets
t-value = -6.8465
Degrees of Freedom = 36
Critical t-value = 1.6883
Probability of difference in means between groups = 5.2237e-08
Significant mean differences between samples sets





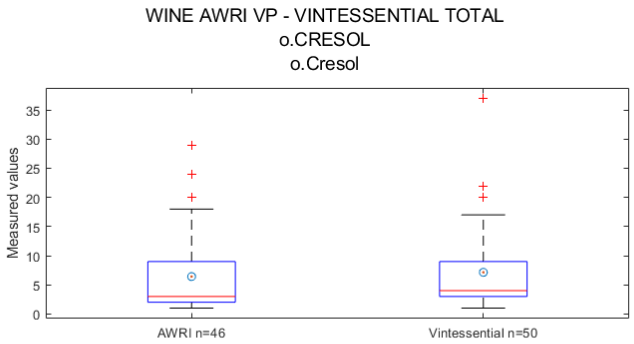
{'WINE AWRI VP - V…'} {'Methyl.Syringol'} {'4.MS'}

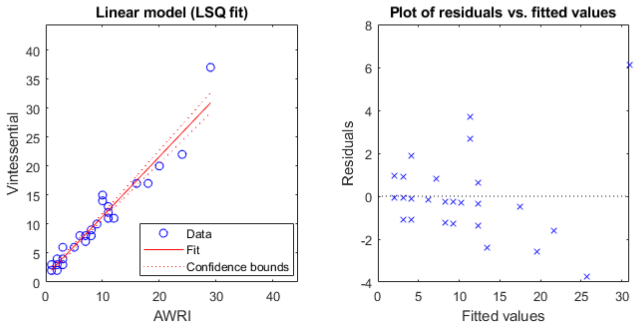
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	101.14	30.538	3.3119	0.0038782
AWRI	6.4643	3.9458	1.6383	0.11872

Number of observations: 20, Error degrees of freedom: 18
Root Mean Squared Error: 99.5
R-squared: 0.13, Adjusted R-Squared 0.0814
F-statistic vs. constant model: 2.68, p-value = 0.119
F value = 0.0042689
Degrees of Freedom = 19 & 49
Critical F value = 1.8029
Probability of difference in variance between groups = 4.3877e-19
Significant variance differences between samples sets
t-value = -5.7098
Degrees of Freedom = 19
Critical t-value = 1.7291
Probability of difference in means between groups = 1.6712e-05
Significant mean differences between samples sets





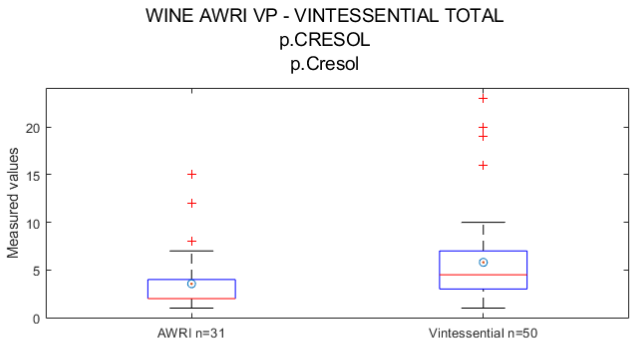
{'WINE AWRI VP - V…'} {'o.CRESOL'} {'o.Cresol'}

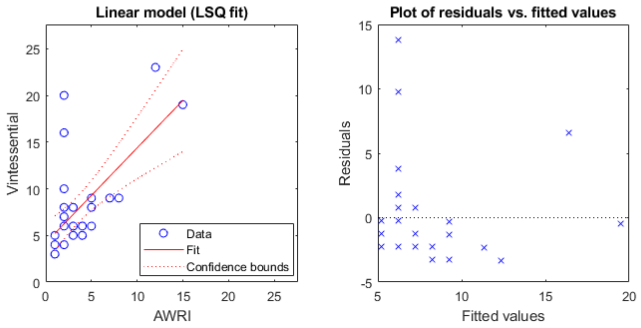
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.0261	0.3293	3.1159	0.003225
AWRI	1.0298	0.036564	28.165	8.7469e-30

Number of observations: 46, Error degrees of freedom: 44
Root Mean Squared Error: 1.57
R-squared: 0.947, Adjusted R-Squared 0.946
F-statistic vs. constant model: 793, p-value = 8.75e-30
F value = 0.91028
Degrees of Freedom = 45 & 49
Critical F value = 1.6198
Probability of difference in variance between groups = 0.75215
No significant difference in variances at the 5% significance level
t-value = -5.2852
Degrees of Freedom = 45
Critical t-value = 1.6794
Probability of difference in means between groups = 3.5393e-06
Significant mean differences between samples sets





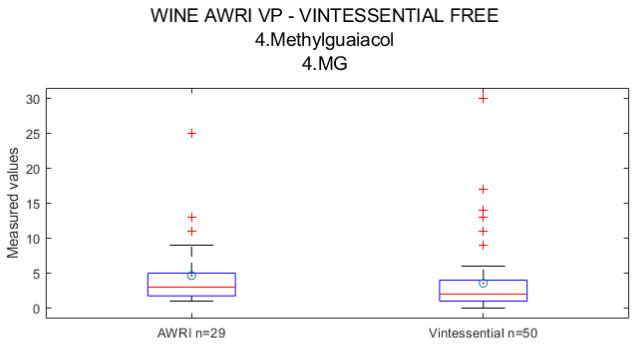
{'WINE AWRI VP - V…'} {'p.CRESOL'} {'p.Cresol'}

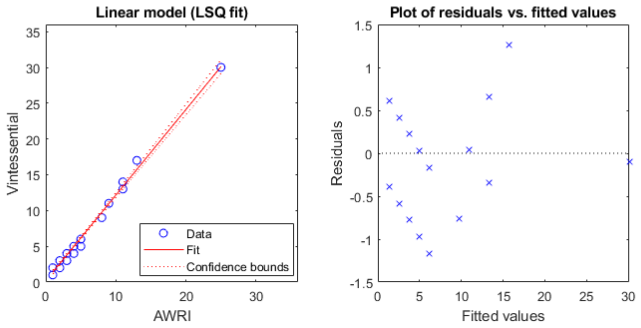
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	4.1937	1.0706	3.9173	0.00050058
AWRI	1.0181	0.22529	4.5191	9.6314e-05

Number of observations: 31, Error degrees of freedom: 29
Root Mean Squared Error: 3.96
R-squared: 0.413, Adjusted R-Squared 0.393
F-statistic vs. constant model: 20.4, p-value = 9.63e-05
F value = 0.44214
Degrees of Freedom = 30 & 49
Critical F value = 1.6918
Probability of difference in variance between groups = 0.019219
Significant variance differences between samples sets
t-value = -6.0814
Degrees of Freedom = 30
Critical t-value = 1.6973
Probability of difference in means between groups = 1.1108e-06
Significant mean differences between samples sets





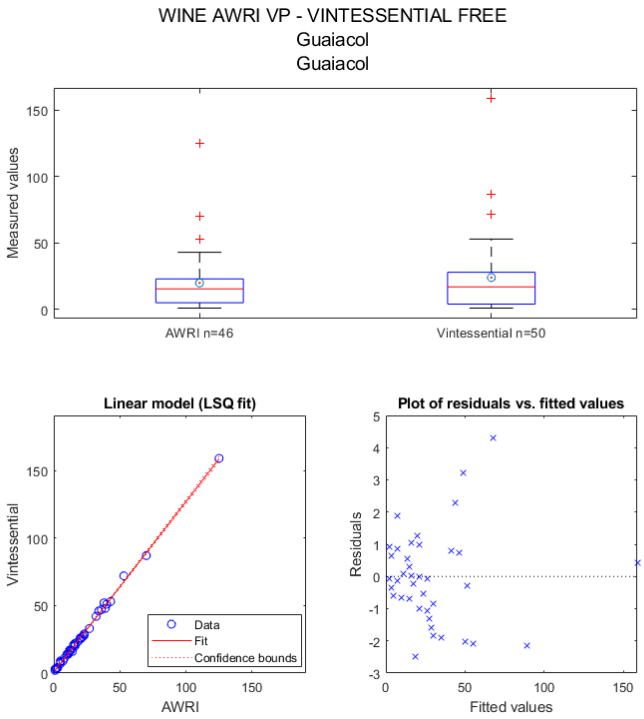
{'WINE AWRI VP - V…'} {'4.Methylguaiacol'} {'4.MG'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.19039	0.15382	1.2378	0.22646
AWRI	1.1961	0.022356	53.505	6.1068e-29

Number of observations: 29, Error degrees of freedom: 27
Root Mean Squared Error: 0.61
R-squared: 0.991, Adjusted R-Squared 0.99
F-statistic vs. constant model: 2.86e+03, p-value = 6.11e-29
F value = 0.92127
Degrees of Freedom = 28 & 49
Critical F value = 1.7064
Probability of difference in variance between groups = 0.8324
No significant difference in variances at the 5% significance level
t-value = -5.0551
Degrees of Freedom = 28
Critical t-value = 1.7011
Probability of difference in means between groups = 2.3853e-05
Significant mean differences between samples sets



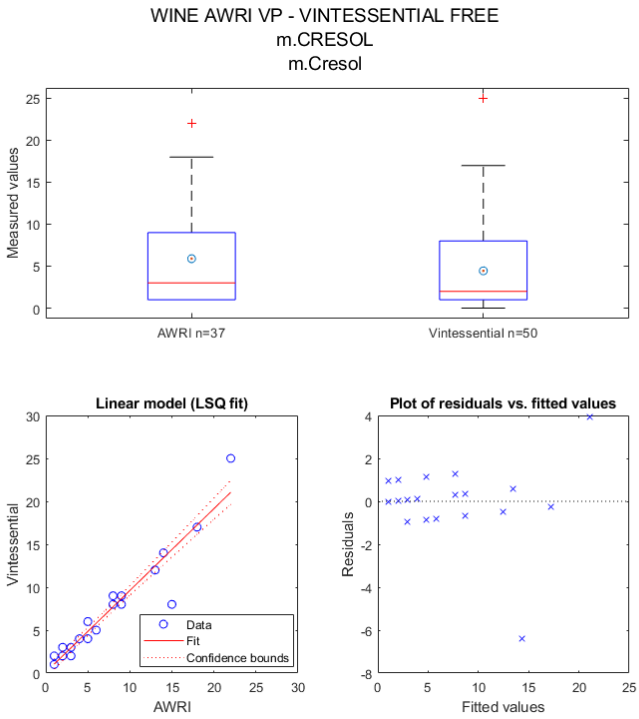
{'WINE AWRI VP - V…'} {'Guaiacol'} {'Guaiacol'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.82065	0.27418	2.9931	0.0045165
AWRI	1.262	0.0093038	135.64	2.4321e-59

Number of observations: 46, Error degrees of freedom: 44
Root Mean Squared Error: 1.37
R-squared: 0.998, Adjusted R-Squared 0.998
F-statistic vs. constant model: 1.84e+04, p-value = 2.43e-59
F value = 0.64197
Degrees of Freedom = 45 & 49
Critical F value = 1.6198
Probability of difference in variance between groups = 0.13493
No significant difference in variances at the 5% significance level
t-value = -6.9396
Degrees of Freedom = 45
Critical t-value = 1.6794
Probability of difference in means between groups = 1.2525e-08
Significant mean differences between samples sets



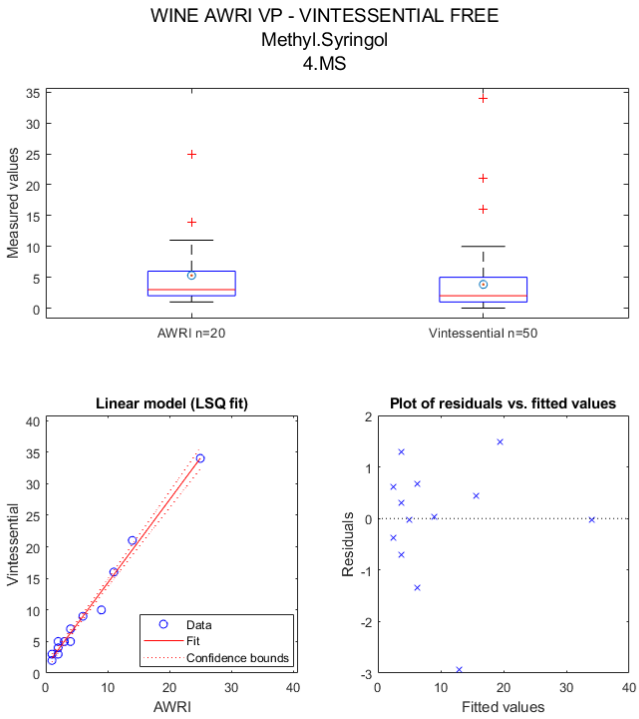
{'WINE AWRI VP - V…'} {'m.CRESOL'} {'m.Cresol'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.086811	0.32654	0.26585	0.79192
AWRI	0.95316	0.040277	23.665	4.0367e-23

Number of observations: 37, Error degrees of freedom: 35
Root Mean Squared Error: 1.36
R-squared: 0.941, Adjusted R-Squared 0.939
F-statistic vs. constant model: 560, p-value = 4.04e-23
F value = 1.1689
Degrees of Freedom = 36 & 49
Critical F value = 1.6567
Probability of difference in variance between groups = 0.60499
No significant difference in variances at the 5% significance level
t-value = 0.83933
Degrees of Freedom = 36
Critical t-value = 1.6883
Probability of difference in means between groups = 0.40682
No significant difference in means at the 5% significance level



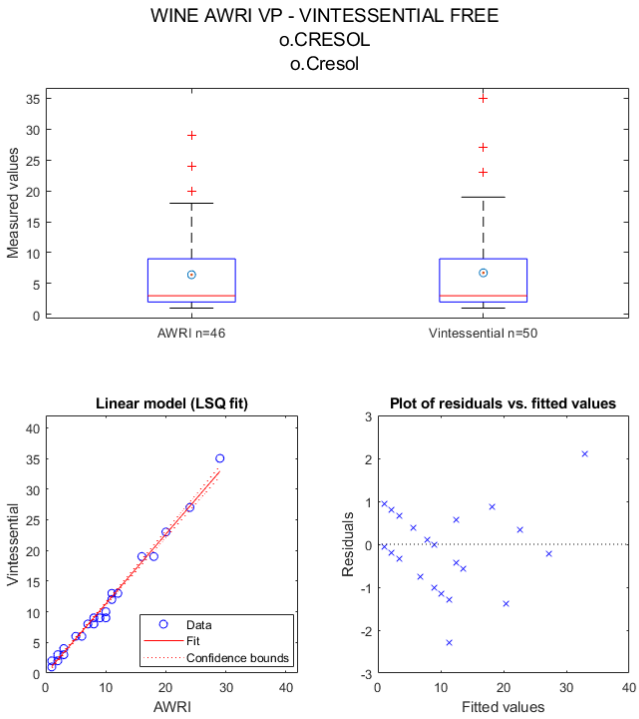
{'WINE AWRI VP - V…'} {'Methyl.Syringol'} {'4.MS'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.063	0.30077	3.5343	0.0023691
AWRI	1.3183	0.038862	33.922	9.1066e-18

Number of observations: 20, Error degrees of freedom: 18
Root Mean Squared Error: 0.98
R-squared: 0.985, Adjusted R-Squared 0.984
F-statistic vs. constant model: 1.15e+03, p-value = 9.11e-18
F value = 0.9513
Degrees of Freedom = 19 & 49
Critical F value = 1.8029
Probability of difference in variance between groups = 0.94211
No significant difference in variances at the 5% significance level
t-value = -5.929
Degrees of Freedom = 19
Critical t-value = 1.7291
Probability of difference in means between groups = 1.0443e-05
Significant mean differences between samples sets



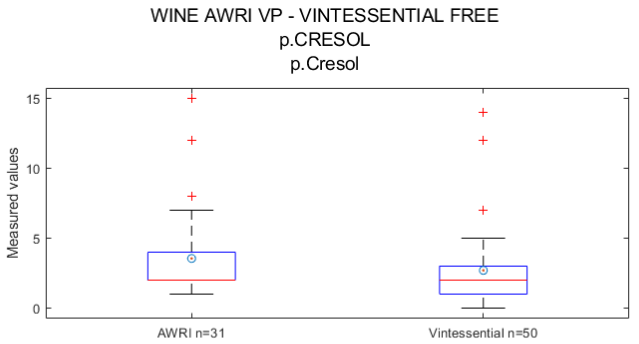
{'WINE AWRI VP - V…'} {'o.CRESOL'} {'o.Cresol'}

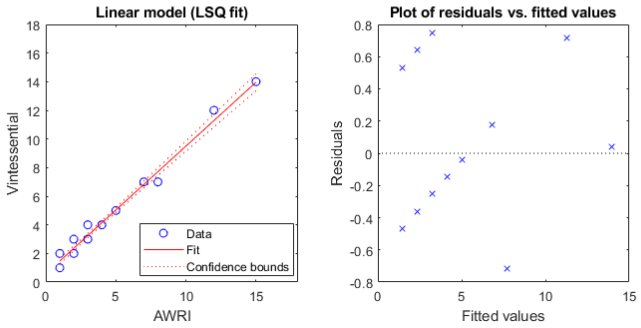
Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	-0.07338	0.16386	-0.44783	0.65647
AWRI	1.1369	0.018194	62.485	1.3024e-44

Number of observations: 46, Error degrees of freedom: 44
Root Mean Squared Error: 0.78
R-squared: 0.989, Adjusted R-Squared 0.989
F-statistic vs. constant model: 3.9e+03, p-value = 1.3e-44
F value = 0.78656
Degrees of Freedom = 45 & 49
Critical F value = 1.6198
Probability of difference in variance between groups = 0.41715
No significant difference in variances at the 5% significance level
t-value = -4.6764
Degrees of Freedom = 45
Critical t-value = 1.6794
Probability of difference in means between groups = 2.6791e-05
Significant mean differences between samples sets





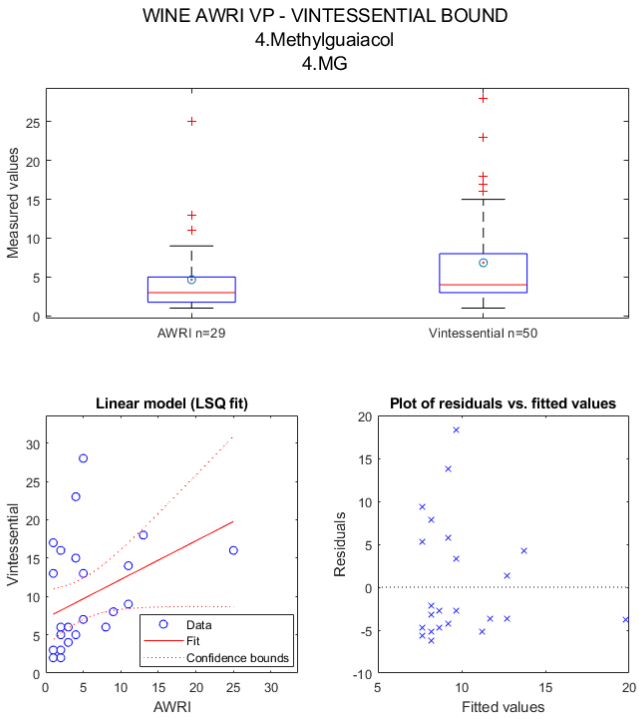
{'WINE AWRI VP - V…'} {'p.CRESOL'} {'p.Cresol'}

Linear regression model:
Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.575	0.115	4.9999	2.5374e-05
AWRI	0.8925	0.024201	36.878	6.4103e-26

Number of observations: 31, Error degrees of freedom: 29
Root Mean Squared Error: 0.426
R-squared: 0.979, Adjusted R-Squared 0.978
F-statistic vs. constant model: 1.36e+03, p-value = 6.41e-26
F value = 1.4768
Degrees of Freedom = 30 & 49
Critical F value = 1.6918
Probability of difference in variance between groups = 0.22136
No significant difference in variances at the 5% significance level
t-value = -1.9853
Degrees of Freedom = 30
Critical t-value = 1.6973
Probability of difference in means between groups = 0.056313
No significant difference in means at the 5% significance level



{'WINE AWRI VP - V…'} {'4.Methylguaiacol'} {'4.MG'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	7.1715	1.7793	4.0306	0.00040809
AWRI	0.50389	0.25858	1.9487	0.061799

Number of observations: 29, Error degrees of freedom: 27

Root Mean Squared Error: 7.06

R-squared: 0.123, Adjusted R-Squared 0.0908

F-statistic vs. constant model: 3.8, p-value = 0.0618

F value = 0.61907

Degrees of Freedom = 28 & 49

Critical F value = 1.7064

Probability of difference in variance between groups = 0.17534

No significant difference in variances at the 5% significance level

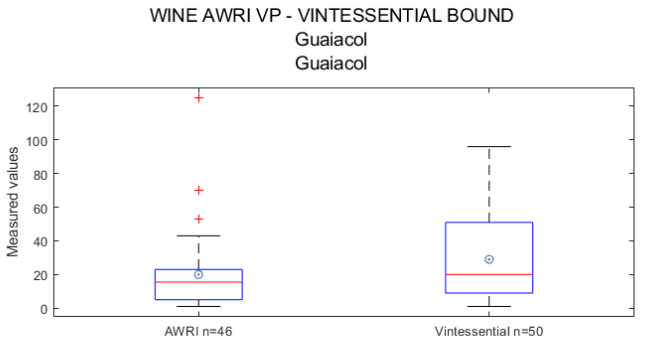
t-value = -3.545

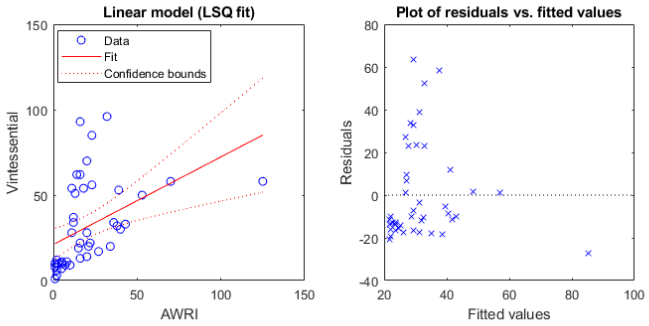
Degrees of Freedom = 28

Critical t-value = 1.7011

Probability of difference in means between groups = 0.0014021

Significant mean differences between samples sets





{'WINE AWRI VP - V…'} {'Guaiacol'} {'Guaiacol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	21.112	4.5561	4.6337	3.1994e-05
AWRI	0.51239	0.1546	3.3143	0.0018457

Number of observations: 46, Error degrees of freedom: 44

Root Mean Squared Error: 22.8

R-squared: 0.2, Adjusted R-Squared 0.182

F-statistic vs. constant model: 11, p-value = 0.00185

F value = 0.74566

Degrees of Freedom = 45 & 49

Critical F value = 1.6198

Probability of difference in variance between groups = 0.3213

No significant difference in variances at the 5% significance level

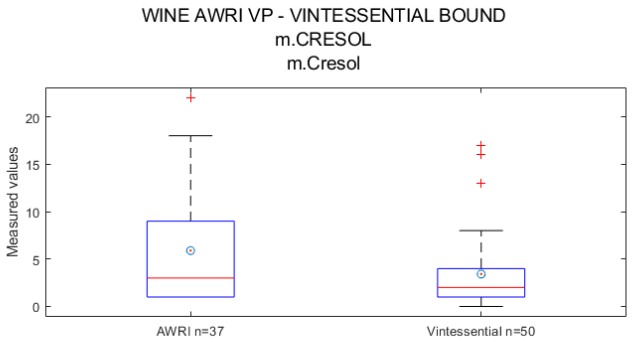
t-value = -3.1005

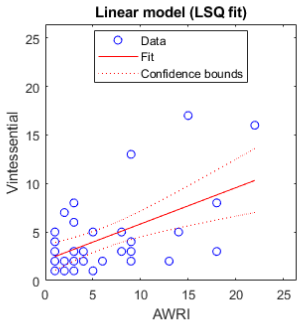
Degrees of Freedom = 45

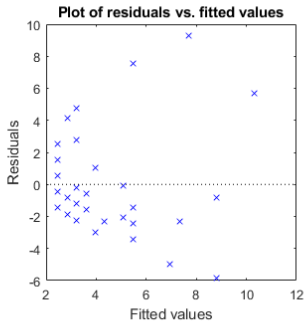
Critical t-value = 1.6794

Probability of difference in means between groups = 0.0033285

Significant mean differences between samples sets







{'WINE AWRI VP - V…'} {'m.CRESOL'} {'m.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	2.0989	0.77176	2.7196	0.010106
AWRI	0.37313	0.095193	3.9197	0.00039358

Number of observations: 37, Error degrees of freedom: 35

Root Mean Squared Error: 3.22

R-squared: 0.305, Adjusted R-Squared 0.285

F-statistic vs. constant model: 15.4, p-value = 0.000394

F value = 2.4024

Degrees of Freedom = 36 & 49

Critical F value = 1.6567

Probability of difference in variance between groups = 0.0044986

Significant variance differences between samples sets

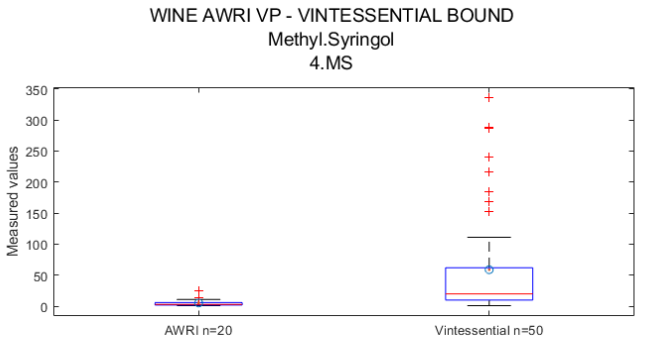
t-value = 2.0387

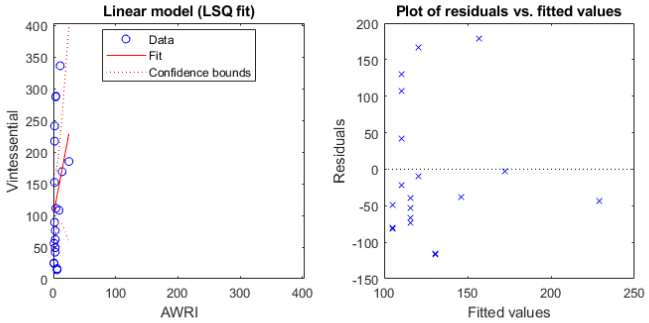
Degrees of Freedom = 36

Critical t-value = 1.6883

Probability of difference in means between groups = 0.04888

Significant mean differences between samples sets





{'WINE AWRI VP - V…'} {'Methyl.Syringol'} {'4.MS'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	100.08	30.56	3.2748	0.0042092
AWRI	5.146	3.9485	1.3033	0.20891

Number of observations: 20, Error degrees of freedom: 18

Root Mean Squared Error: 99.6

R-squared: 0.0862, Adjusted R-Squared 0.0355

F-statistic vs. constant model: 1.7, p-value = 0.209

F value = 0.0046235

Degrees of Freedom = 19 & 49

Critical F value = 1.8029

Probability of difference in variance between groups = 9.3252e-19

Significant variance differences between samples sets

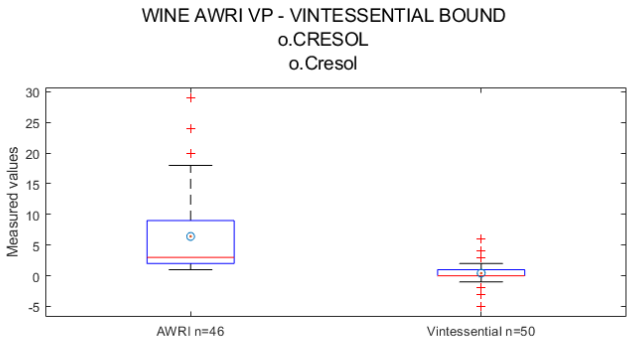
t-value = -5.4658

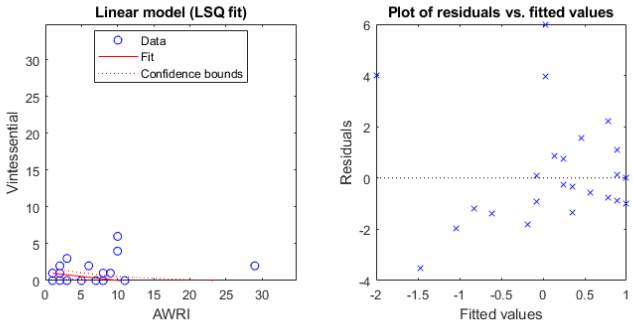
Degrees of Freedom = 19

Critical t-value = 1.7291

Probability of difference in means between groups = 2.8396e-05

Significant mean differences between samples sets





{'WINE AWRI VP - V…'} {'o.CRESOL'} {'o.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.0994	0.34403	3.1958	0.0025809
AWRI	-0.10703	0.0382	-2.8019	0.0075242

Number of observations: 46, Error degrees of freedom: 44

Root Mean Squared Error: 1.64

R-squared: 0.151, Adjusted R-Squared 0.132

F-statistic vs. constant model: 7.85, p-value = 0.00752

F value = 14.0852

Degrees of Freedom = 45 & 49

Critical F value = 1.6198

Probability of difference in variance between groups = 3.0054e-16

Significant variance differences between samples sets

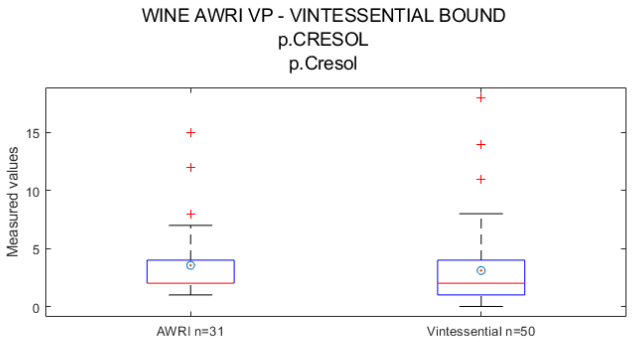
t-value = 5.605

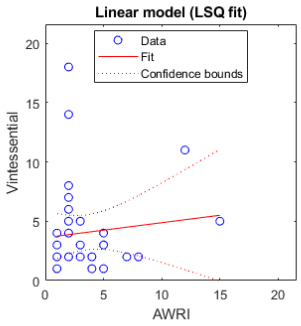
Degrees of Freedom = 45

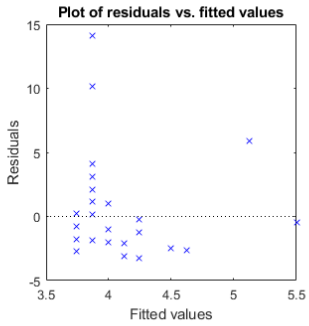
Critical t-value = 1.6794

Probability of difference in means between groups = 1.1998e-06

Significant mean differences between samples sets







{'WINE AWRI VP - V…'} {'p.CRESOL'} {'p.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	3.6187	1.0859	3.3325	0.0023603
AWRI	0.12563	0.22852	0.54973	0.58671

Number of observations: 31, Error degrees of freedom: 29

Root Mean Squared Error: 4.02

R-squared: 0.0103, Adjusted R-Squared -0.0238

F-statistic vs. constant model: 0.302, p-value = 0.587

F value = 0.86242

Degrees of Freedom = 30 & 49

Critical F value = 1.6918

Probability of difference in variance between groups = 0.67496

No significant difference in variances at the 5% significance level

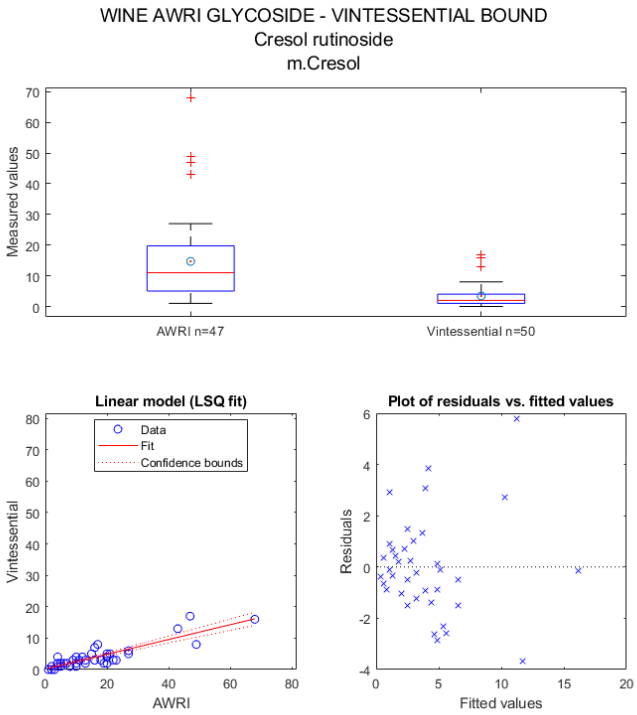
t-value = -0.59248

Degrees of Freedom = 30

Critical t-value = 1.6973

Probability of difference in means between groups = 0.55797

No significant difference in means at the 5% significance level



{'WINE AWRI GLYCOS…'} {'Cresol rutinoside'} {'m.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.15954	0.37726	0.42288	0.6744
AWRI	0.23517	0.01884	12.482	3.238e-16

Number of observations: 47, Error degrees of freedom: 45

Root Mean Squared Error: 1.76

R-squared: 0.776, Adjusted R-Squared 0.771

F-statistic vs. constant model: 156, p-value = 3.24e-16

F value = 14.2304

Degrees of Freedom = 46 & 49

Critical F value = 1.6165

Probability of difference in variance between groups = 2.117e-16

Significant variance differences between samples sets

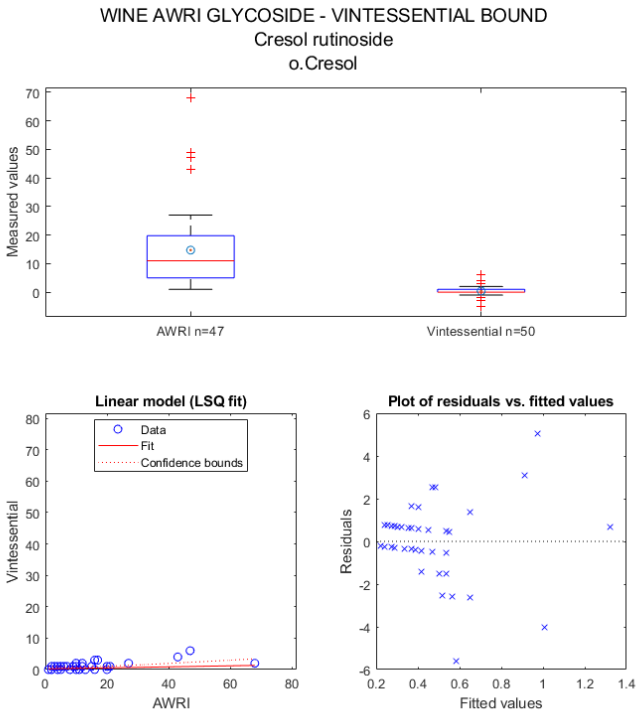
t-value = 7.1342

Degrees of Freedom = 46

Critical t-value = 1.6787

Probability of difference in means between groups = 5.7339e-09

Significant mean differences between samples sets



{'WINE AWRI GLYCOS…'} {'Cresol rutinoside'} {'o.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.20602	0.378	0.54502	0.58843
AWRI	0.016378	0.018877	0.86759	0.39022

Number of observations: 47, Error degrees of freedom: 45

Root Mean Squared Error: 1.76

R-squared: 0.0165, Adjusted R-Squared -0.0054

F-statistic vs. constant model: 0.753, p-value = 0.39

F value = 65.0745

Degrees of Freedom = 46 & 49

Critical F value = 1.6165

Probability of difference in variance between groups = 1.812e-31

Significant variance differences between samples sets

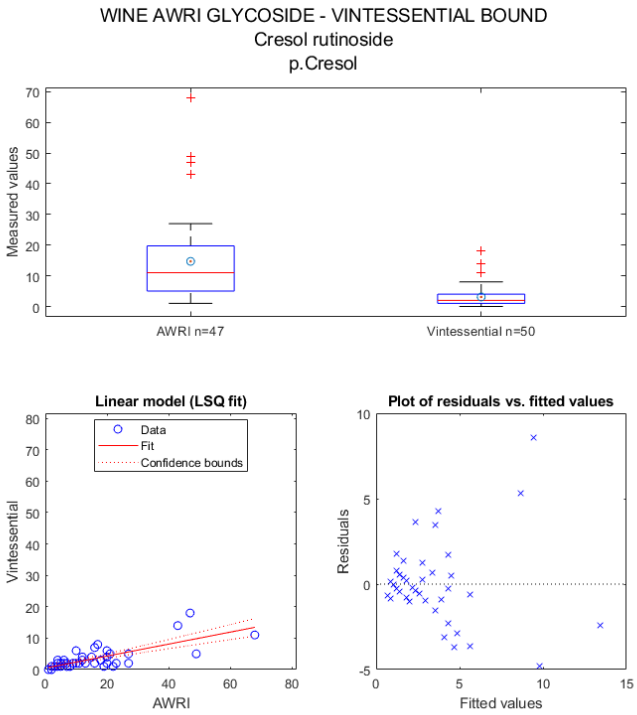
t-value = 7.1714

Degrees of Freedom = 46

Critical t-value = 1.6787

Probability of difference in means between groups = 5.0449e-09

Significant mean differences between samples sets



{'WINE AWRI GLYCOS…'} {'Cresol rutinoside'} {'p.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.47377	0.50207	0.94364	0.35039
AWRI	0.19064	0.025074	7.6033	1.3108e-09

Number of observations: 47, Error degrees of freedom: 45

Root Mean Squared Error: 2.34

R-squared: 0.562, Adjusted R-Squared 0.553

F-statistic vs. constant model: 57.8, p-value = 1.31e-09

F value = 15.7754

Degrees of Freedom = 46 & 49

Critical F value = 1.6165

Probability of difference in variance between groups = 2.3136e-17

Significant variance differences between samples sets

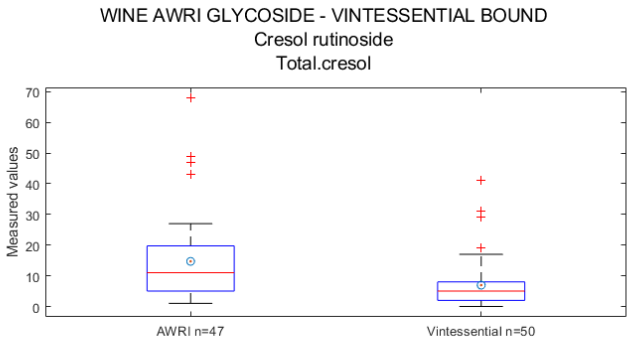
t-value = 6.8957

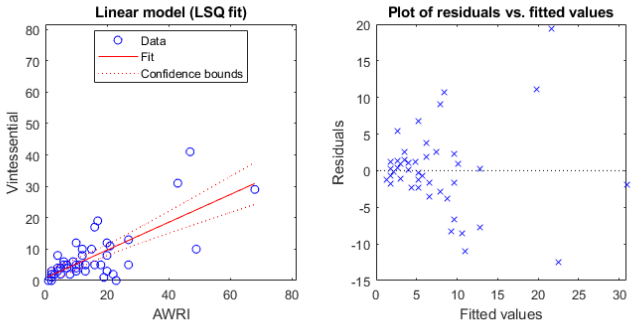
Degrees of Freedom = 46

Critical t-value = 1.6787

Probability of difference in means between groups = 1.3067e-08

Significant mean differences between samples sets





{'WINE AWRI GLYCOS…'} {'Cresol rutinoside'} {'Total.cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.83933	1.207	0.69537	0.4904
AWRI	0.44219	0.060279	7.3357	3.247e-09

Number of observations: 47, Error degrees of freedom: 45

Root Mean Squared Error: 5.62

R-squared: 0.545, Adjusted R-Squared 0.534

F-statistic vs. constant model: 53.8, p-value = 3.25e-09

F value = 2.8496

Degrees of Freedom = 46 & 49

Critical F value = 1.6165

Probability of difference in variance between groups = 0.00041172

Significant variance differences between samples sets

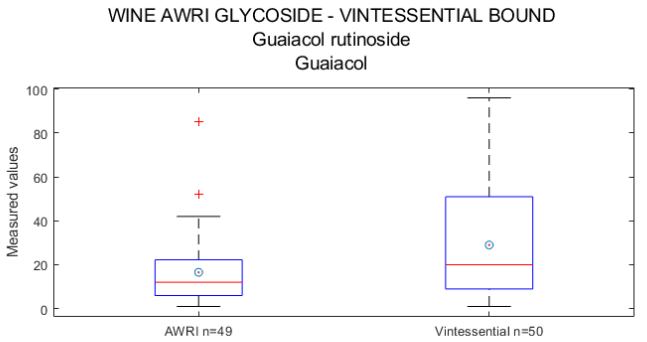
t-value = 5.331

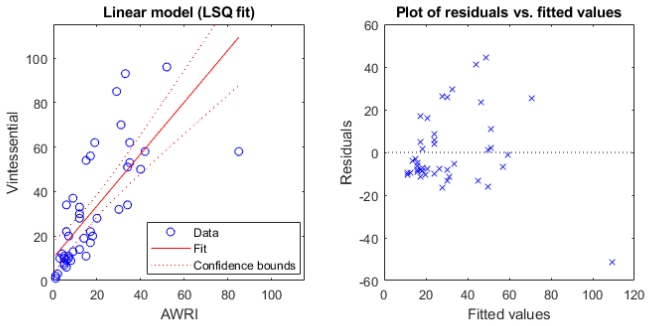
Degrees of Freedom = 46

Critical t-value = 1.6787

Probability of difference in means between groups = 2.8726e-06

Significant mean differences between samples sets





{'WINE AWRI GLYCOS…'} {'Guaiacol rutinos…'} {'Guaiacol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	10.233	3.528	2.9005	0.00565
AWRI	1.1659	0.15326	7.6078	9.861e-10

Number of observations: 49, Error degrees of freedom: 47

Root Mean Squared Error: 17.2

R-squared: 0.552, Adjusted R-Squared 0.542

F-statistic vs. constant model: 57.9, p-value = 9.86e-10

F value = 0.40469

Degrees of Freedom = 48 & 49

Critical F value = 1.6102

Probability of difference in variance between groups = 0.0020887

Significant variance differences between samples sets

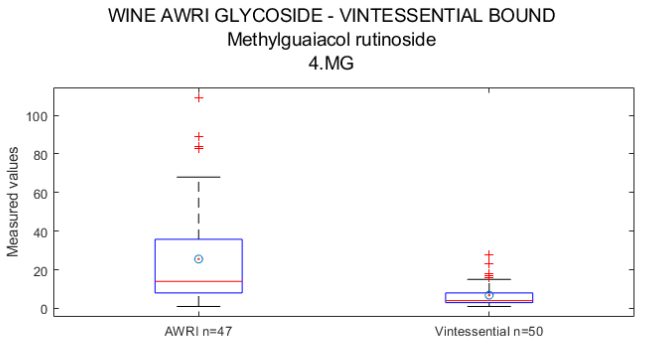
t-value = -5.2838

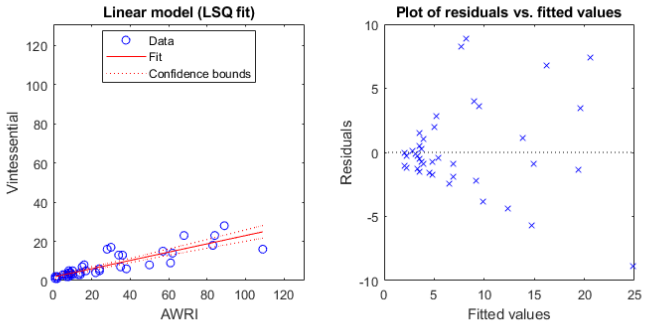
Degrees of Freedom = 48

Critical t-value = 1.6772

Probability of difference in means between groups = 3.0474e-06

Significant mean differences between samples sets





{'WINE AWRI GLYCOS…'} {'Methylguaiacol r…'} {'4.MG'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.8135	0.67482	2.6874	0.010057
AWRI	0.21147	0.018282	11.567	4.4849e-15

Number of observations: 47, Error degrees of freedom: 45

Root Mean Squared Error: 3.34

R-squared: 0.748, Adjusted R-Squared 0.743

F-statistic vs. constant model: 134, p-value = 4.48e-15

F value = 16.9029

Degrees of Freedom = 46 & 49

Critical F value = 1.6165

Probability of difference in variance between groups = 5.1691e-18

Significant variance differences between samples sets

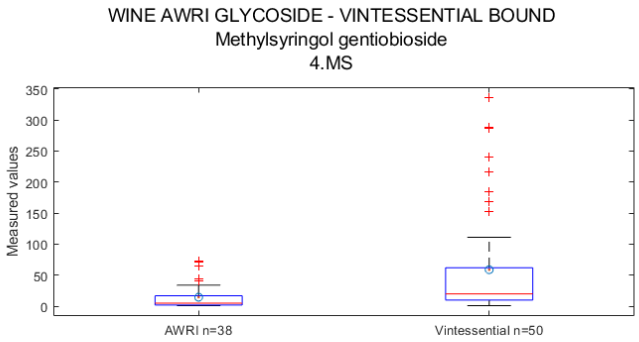
t-value = 5.8407

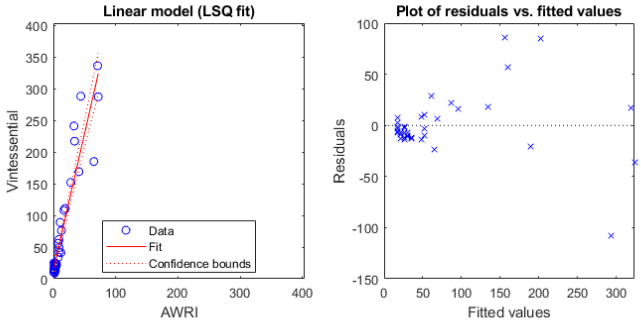
Degrees of Freedom = 46

Critical t-value = 1.6787

Probability of difference in means between groups = 5.0145e-07

Significant mean differences between samples sets





{'WINE AWRI GLYCOS…'} {'Methylsyringol g…'} {'4.MS'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	13.105	6.4086	2.0449	0.048225
AWRI	4.3105	0.26211	16.445	2.5447e-18

Number of observations: 38, Error degrees of freedom: 36

Root Mean Squared Error: 31.7

R-squared: 0.883, Adjusted R-Squared 0.879

F-statistic vs. constant model: 270, p-value = 2.54e-18

F value = 0.054632

Degrees of Freedom = 37 & 49

Critical F value = 1.6518

Probability of difference in variance between groups = 3.7682e-15

Significant variance differences between samples sets

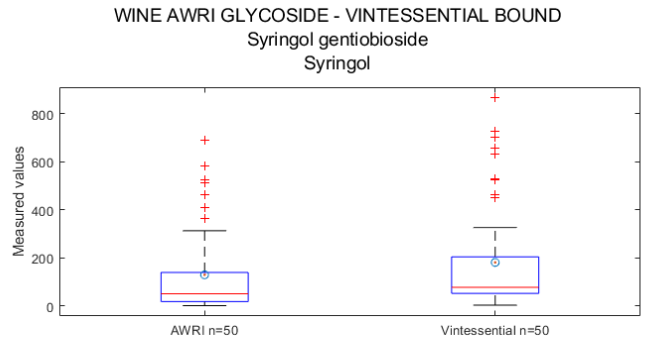
t-value = -5.1892

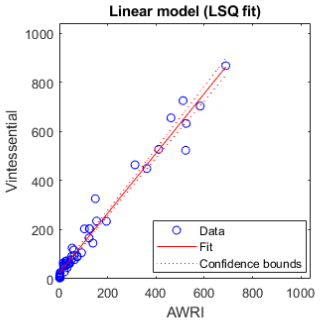
Degrees of Freedom = 37

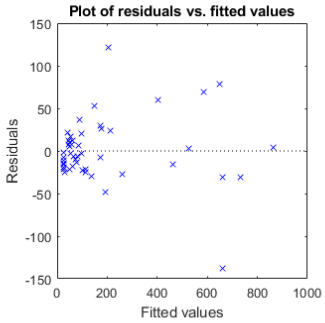
Critical t-value = 1.6871

Probability of difference in means between groups = 7.8516e-06

Significant mean differences between samples sets







{'WINE AWRI GLYCOS…'} {'Syringol gentiob…'} {'Syringol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	23.55	6.5226	3.6105	0.00072835
AWRI	1.2174	0.029482	41.293	3.6571e-39

Number of observations: 50, Error degrees of freedom: 48

Root Mean Squared Error: 37.4

R-squared: 0.973, Adjusted R-Squared 0.972

F-statistic vs. constant model: 1.71e+03, p-value = 3.66e-39

F value = 0.65624

Degrees of Freedom = 49 & 49

Critical F value = 1.6073

Probability of difference in variance between groups = 0.14389

No significant difference in variances at the 5% significance level

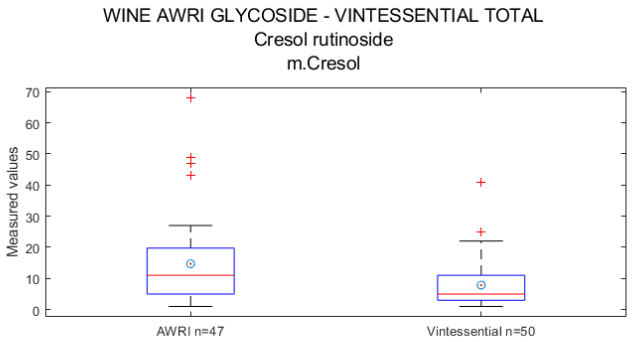
t-value = -6.7572

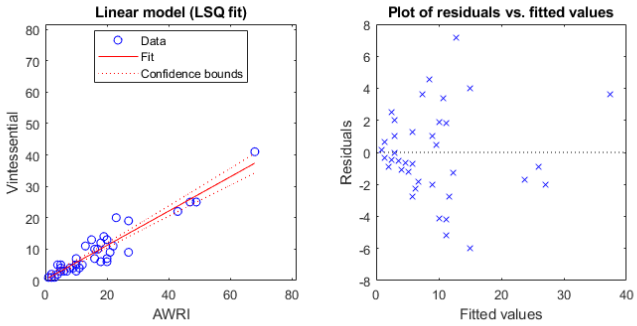
Degrees of Freedom = 49

Critical t-value = 1.6766

Probability of difference in means between groups = 1.5776e-08

Significant mean differences between samples sets





{'WINE AWRI GLYCOS…'} {'Cresol rutinoside'} {'m.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.28116	0.56693	0.49594	0.62235
AWRI	0.54528	0.028312	19.259	2.3242e-23

Number of observations: 47, Error degrees of freedom: 45

Root Mean Squared Error: 2.64

R-squared: 0.892, Adjusted R-Squared 0.889

F-statistic vs. constant model: 371, p-value = 2.32e-23

F value = 3.0375

Degrees of Freedom = 46 & 49

Critical F value = 1.6165

Probability of difference in variance between groups = 0.00018474

Significant variance differences between samples sets

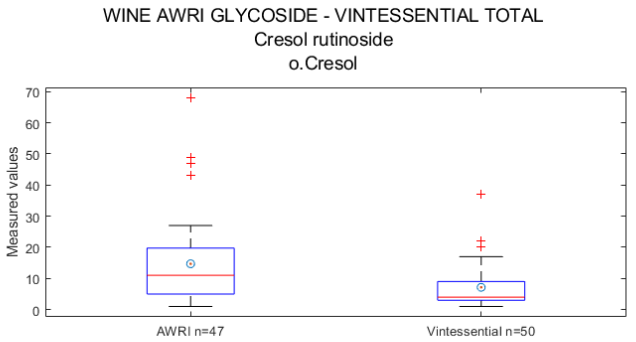
t-value = 6.4837

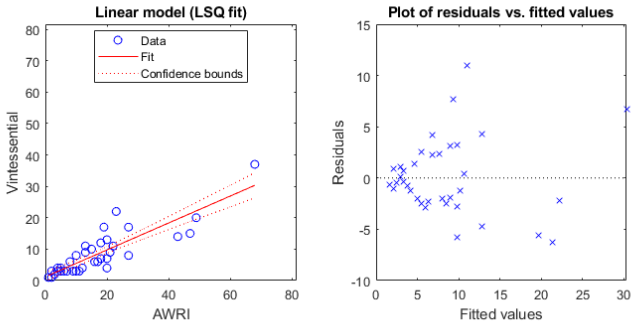
Degrees of Freedom = 46

Critical t-value = 1.6787

Probability of difference in means between groups = 5.4353e-08

Significant mean differences between samples sets





{'WINE AWRI GLYCOS…'} {'Cresol rutinoside'} {'o.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.1946	0.72438	1.6492	0.10608
AWRI	0.42815	0.036176	11.835	2.0532e-15

Number of observations: 47, Error degrees of freedom: 45

Root Mean Squared Error: 3.37

R-squared: 0.757, Adjusted R-Squared 0.751

F-statistic vs. constant model: 140, p-value = 2.05e-15

F value = 4.2056

Degrees of Freedom = 46 & 49

Critical F value = 1.6165

Probability of difference in variance between groups = 1.8618e-06

Significant variance differences between samples sets

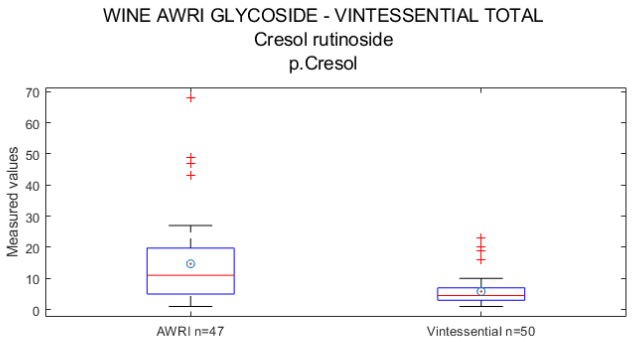
t-value = 5.7928

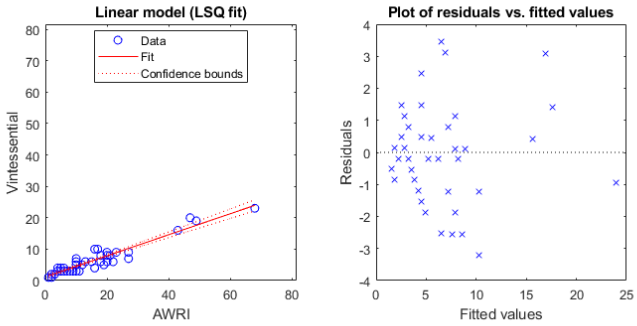
Degrees of Freedom = 46

Critical t-value = 1.6787

Probability of difference in means between groups = 5.9147e-07

Significant mean differences between samples sets





{'WINE AWRI GLYCOS…'} {'Cresol rutinoside'} {'p.Cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.1867	0.31688	3.7449	0.00051072
AWRI	0.33462	0.015825	21.145	5.2318e-25

Number of observations: 47, Error degrees of freedom: 45

Root Mean Squared Error: 1.47

R-squared: 0.909, Adjusted R-Squared 0.907

F-statistic vs. constant model: 447, p-value = 5.23e-25

F value = 8.0877

Degrees of Freedom = 46 & 49

Critical F value = 1.6165

Probability of difference in variance between groups = 2.089e-11

Significant variance differences between samples sets

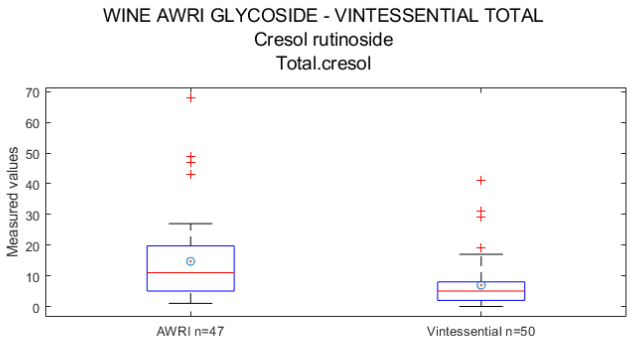
t-value = 6.3647

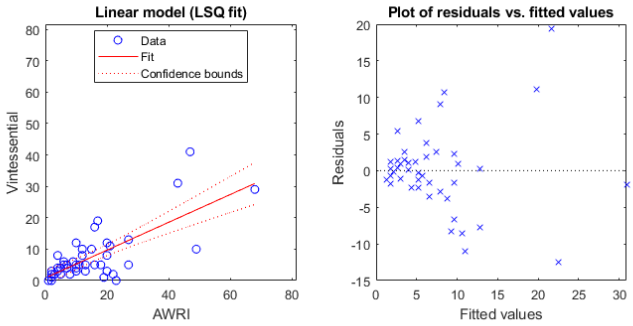
Degrees of Freedom = 46

Critical t-value = 1.6787

Probability of difference in means between groups = 8.2059e-08

Significant mean differences between samples sets





{'WINE AWRI GLYCOS…'} {'Cresol rutinoside'} {'Total.cresol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	0.83933	1.207	0.69537	0.4904
AWRI	0.44219	0.060279	7.3357	3.247e-09

Number of observations: 47, Error degrees of freedom: 45

Root Mean Squared Error: 5.62

R-squared: 0.545, Adjusted R-Squared 0.534

F-statistic vs. constant model: 53.8, p-value = 3.25e-09

F value = 2.8496

Degrees of Freedom = 46 & 49

Critical F value = 1.6165

Probability of difference in variance between groups = 0.00041172

Significant variance differences between samples sets

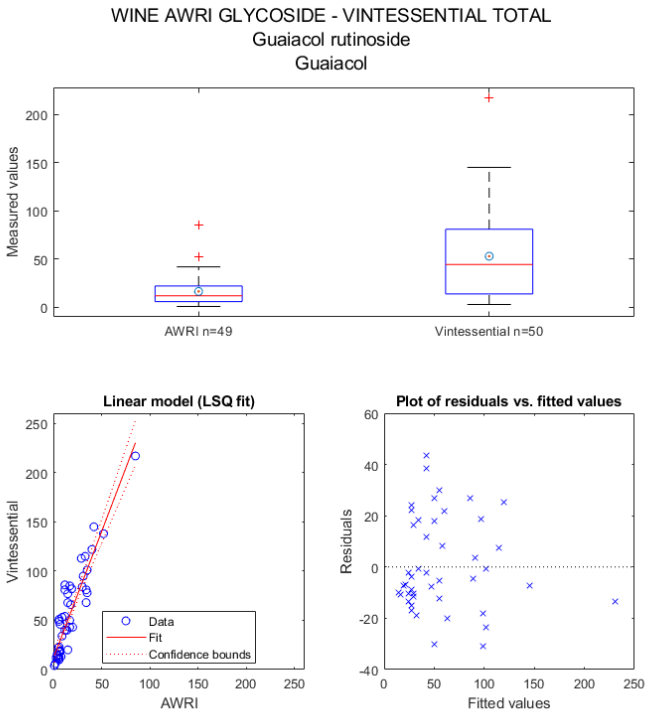
t-value = 5.331

Degrees of Freedom = 46

Critical t-value = 1.6787

Probability of difference in means between groups = 2.8726e-06

Significant mean differences between samples sets



{'WINE AWRI GLYCOS…'} {'Guaiacol rutinos…'} {'Guaiacol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	11.416	3.7104	3.0767	0.0034852
AWRI	2.5754	0.16118	15.979	1.2651e-20

Number of observations: 49, Error degrees of freedom: 47

Root Mean Squared Error: 18.1

R-squared: 0.845, Adjusted R-Squared 0.841

F-statistic vs. constant model: 255, p-value = 1.27e-20

F value = 0.1267

Degrees of Freedom = 48 & 49

Critical F value = 1.6102

Probability of difference in variance between groups = 3.5618e-11

Significant variance differences between samples sets

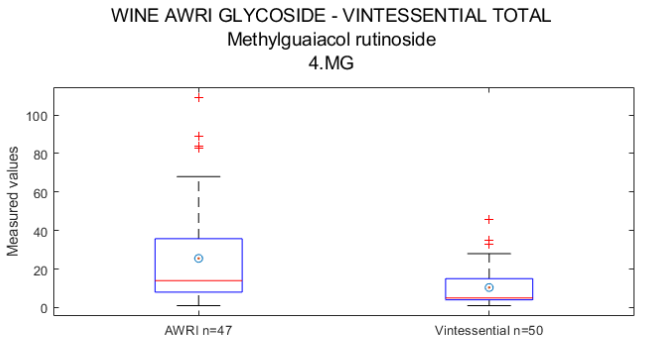
t-value = -8.4362

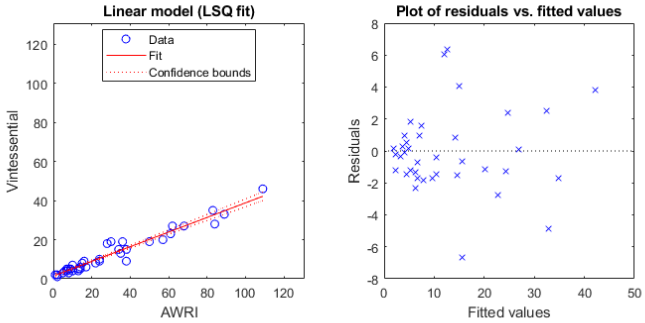
Degrees of Freedom = 48

Critical t-value = 1.6772

Probability of difference in means between groups = 4.8656e-11

Significant mean differences between samples sets





{'WINE AWRI GLYCOS…'} {'Methylguaiacol r…'} {'4.MG'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.4516	0.46549	3.1185	0.0031667
AWRI	0.37398	0.012611	29.655	3.5367e-31

Number of observations: 47, Error degrees of freedom: 45

Root Mean Squared Error: 2.3

R-squared: 0.951, Adjusted R-Squared 0.95

F-statistic vs. constant model: 879, p-value = 3.54e-31

F value = 6.852

Degrees of Freedom = 46 & 49

Critical F value = 1.6165

Probability of difference in variance between groups = 4.726e-10

Significant variance differences between samples sets

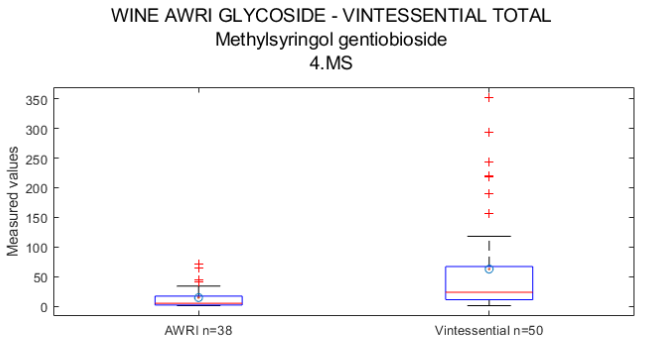
t-value = 5.8529

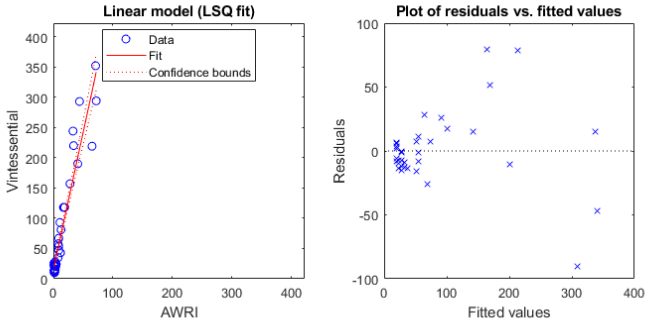
Degrees of Freedom = 46

Critical t-value = 1.6787

Probability of difference in means between groups = 4.8083e-07

Significant mean differences between samples sets





{'WINE AWRI GLYCOS…'} {'Methylsyringol g…'} {'4.MS'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	14.648	5.9429	2.4649	0.01861
AWRI	4.5349	0.24306	18.657	4.3101e-20

Number of observations: 38, Error degrees of freedom: 36

Root Mean Squared Error: 29.4

R-squared: 0.906, Adjusted R-Squared 0.904

F-statistic vs. constant model: 348, p-value = 4.31e-20

F value = 0.050442

Degrees of Freedom = 37 & 49

Critical F value = 1.6518

Probability of difference in variance between groups = 9.7441e-16

Significant variance differences between samples sets

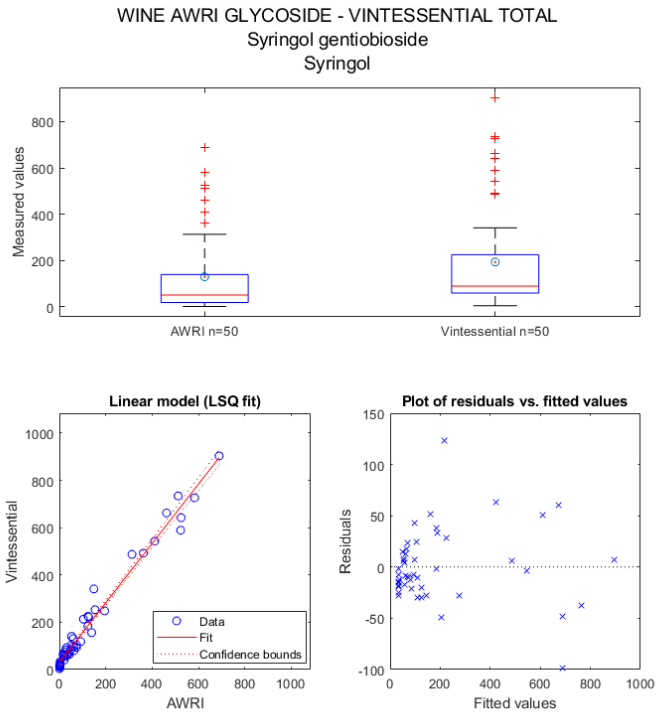
t-value = -5.3638

Degrees of Freedom = 37

Critical t-value = 1.6871

Probability of difference in means between groups = 4.5631e-06

Significant mean differences between samples sets



{'WINE AWRI GLYCOS…'} {'Syringol gentiob…'} {'Syringol'}

Linear regression model:

Vintessential ~ 1 + AWRI

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	30.725	6.1334	5.0094	7.8069e-06
AWRI	1.2561	0.027723	45.309	4.7418e-41

Number of observations: 50, Error degrees of freedom: 48

Root Mean Squared Error: 35.2

R-squared: 0.977, Adjusted R-Squared 0.977

F-statistic vs. constant model: 2.05e+03, p-value = 4.74e-41

F value = 0.61931

Degrees of Freedom = 49 & 49

Critical F value = 1.6073

Probability of difference in variance between groups = 0.096785

No significant difference in variances at the 5% significance level

t-value = -7.7809

Degrees of Freedom = 49

Critical t-value = 1.6766

Probability of difference in means between groups = 4.1384e-10

Significant mean differences between samples sets

END

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