AWRI and Vintessential Grape and Wine Analysis

Method Comparison

National Wine and Grape Industry Centre,
Charles Sturt University

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Project: Method Comparison

AWRI and Vintessential Grape and Wine Analysis

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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
9	A2008071/02B		White	2	2	0	2	0	0	8

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	AWRI Analyte	Vintessential Analyte
4-methylguaiacol	4-MG	Cresol rutinoside	m-cresol
Guaiacol	Guaiacol		o-cresol
m-cresol	m-cresol		p-cresol
Methyl syringol	4-MS		Total cresol
o-cresol	o-cresol	Guaiacol rutinoside	Guaiacol
p-cresol	p-cresol	Methylguaiacol rutinoside	4-MG
Syringol	Syringol	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.
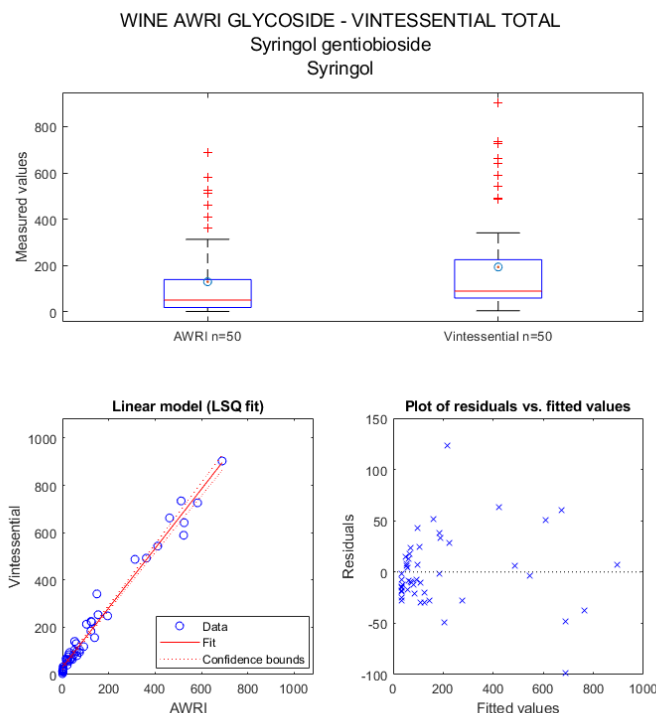
Box plot to show the range of data. Boxes are the 25-75th quartile range, red line is the median value and circle the mean value. Box whiskers show 1.5 x the interquartile range and red crosses are outliers samples i.e. have values beyond this range.

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

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

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 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

Dataset	AWRI	Vintessential	R2	Convert AWRI to Vintessential		Convert Vintessential to AWRI	
				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

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Dataset	AWRI	Vintessential	R2	Convert AWRI to Vintessential		Convert Vintessential to AWRI	
				Intercept	Gradient	Intercept	Gradient
	Guaiacol rutinoside	Guaiacol	0.77	10.44	1.4	-3.39	0.55
	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

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Dataset	AWRI	Vintessential	R2	Convert AWRI to Vintessential		Convert Vintessential to AWRI	
				Intercept	Gradient	Intercept	Gradient
	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
	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=',
```

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```matlab
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)]);
```
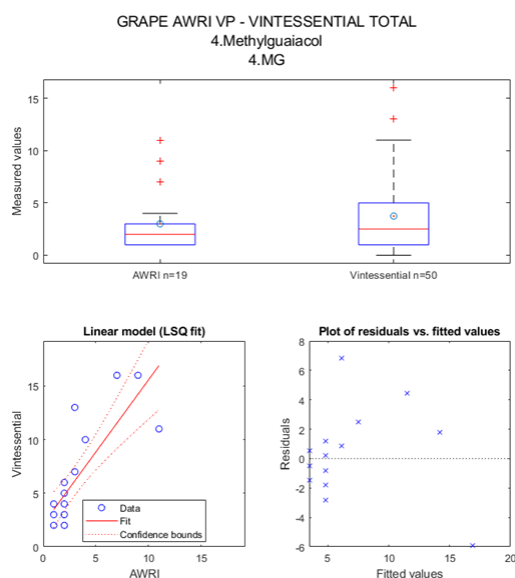
```
        display(['Critical t-value = ', num2str(critT)]);
        display(['Probability of difference in means between groups = ', num2str(p)]);
        if h==0
            display('No significant difference in means at the 5% significance level')
        else
            display('Significant mean differences between samples sets');
        end

    end
    cntr=cntr+1;
end

display('END');
```

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Results

GRAPE AWRI VP - VINTESSENTIAL TOTAL
4.Methylguaiacol
4.MG

{'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
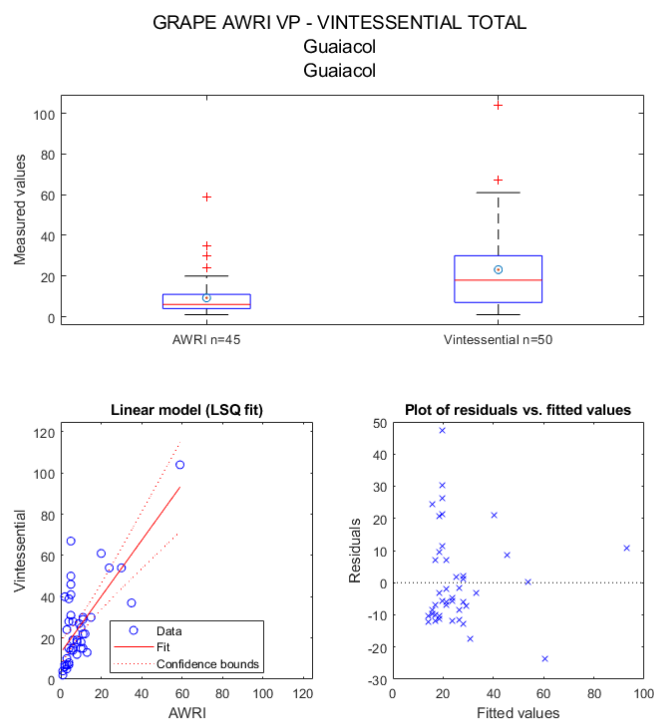t-value = -4.7287
Degrees of Freedom = 18
Critical t-value = 1.7341
Probability of difference in means between groups = 0.00016759
Significant mean differences between samples sets

AWRI and Vintessential
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GRAPE AWRI VP - VINTESSENTIAL TOTAL
Guaiacol
Guaiacol

{'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
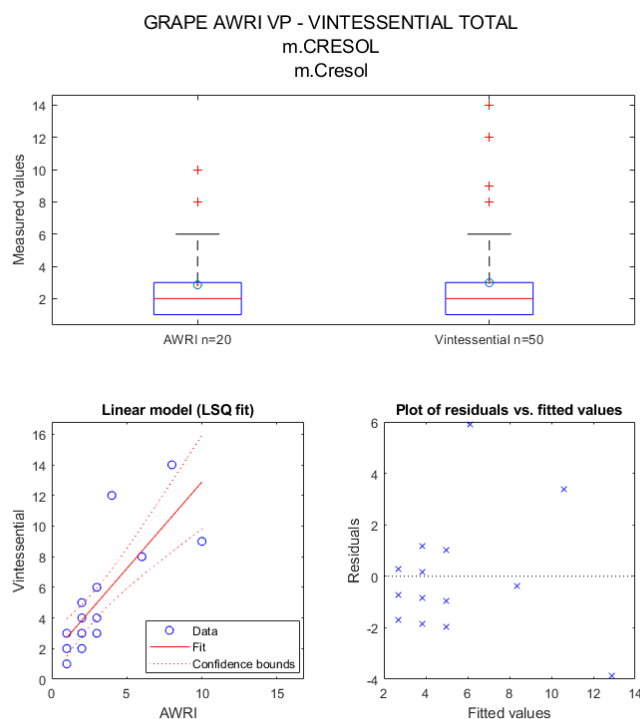Significant variance differences between samples sets
t-value = -7.3127
Degrees of Freedom = 44
Critical t-value = 1.6802
Probability of difference in means between groups = 3.989e-09
Significant mean differences between samples sets

GRAPE AWRI VP - VINTESSENTIAL TOTAL
m.CRESOL
m.Cresol

{'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
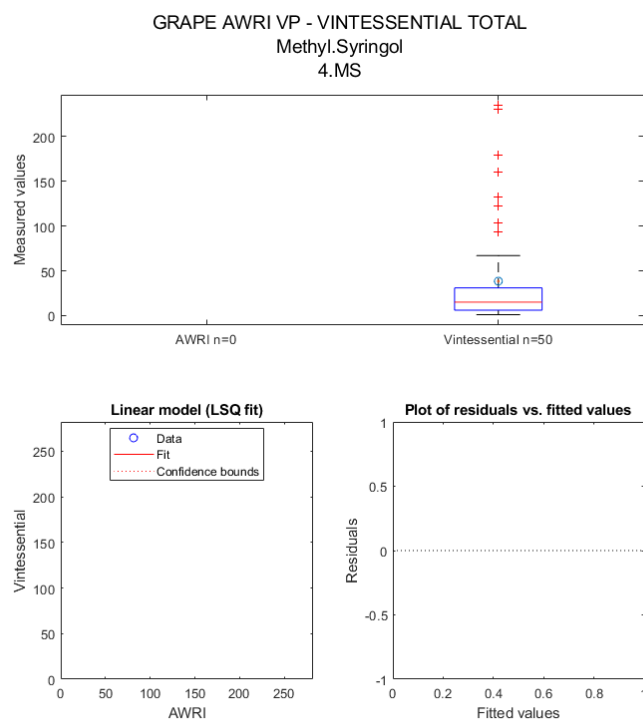t-value = -4.2781
Degrees of Freedom = 19
Critical t-value = 1.7291
Probability of difference in means between groups = 0.00040615
Significant mean differences between samples sets
Warning: Regression design matrix is rank deficient to within machine precision.

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GRAPE AWRI VP - VINTESSENTIAL TOTAL
Methyl.Syringol
4.MS

{'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
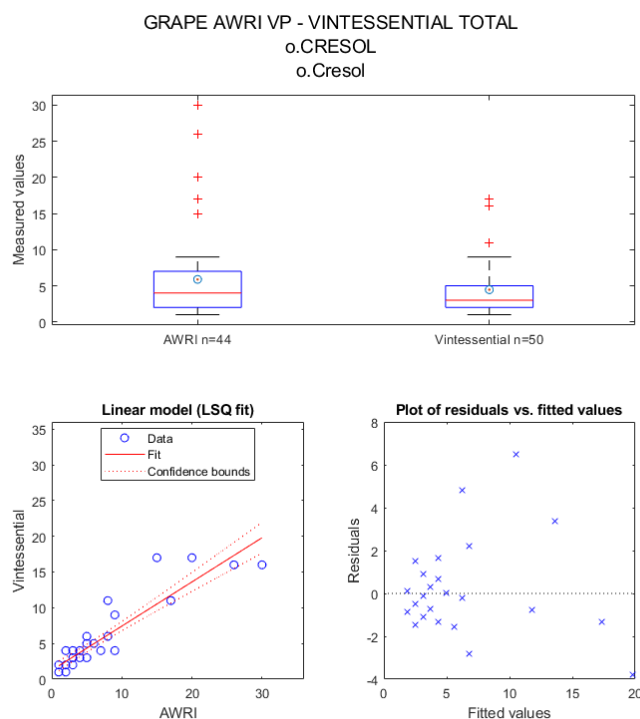Significant variance differences between samples sets
t-value = NaN
Degrees of Freedom = 0
Critical t-value = NaN
Probability of difference in means between groups = NaN
Significant mean differences between samples sets

GRAPE AWRI VP - VINTESSENTIAL TOTAL
o.CRESOL
o.Cresol

Linear model (LSQ fit)

Plot of residuals vs. fitted values

{'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
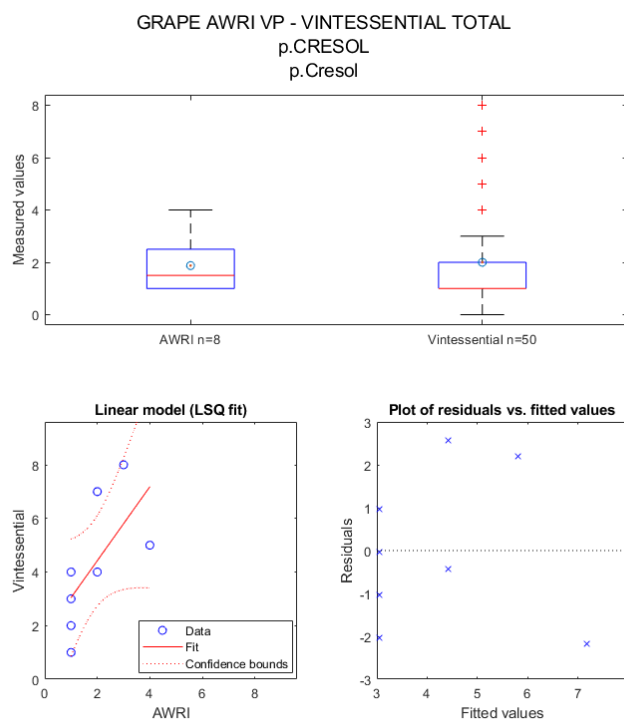Significant variance differences between samples sets
t-value = 2.1914
Degrees of Freedom = 43
Critical t-value = 1.6811
Probability of difference in means between groups = 0.033892
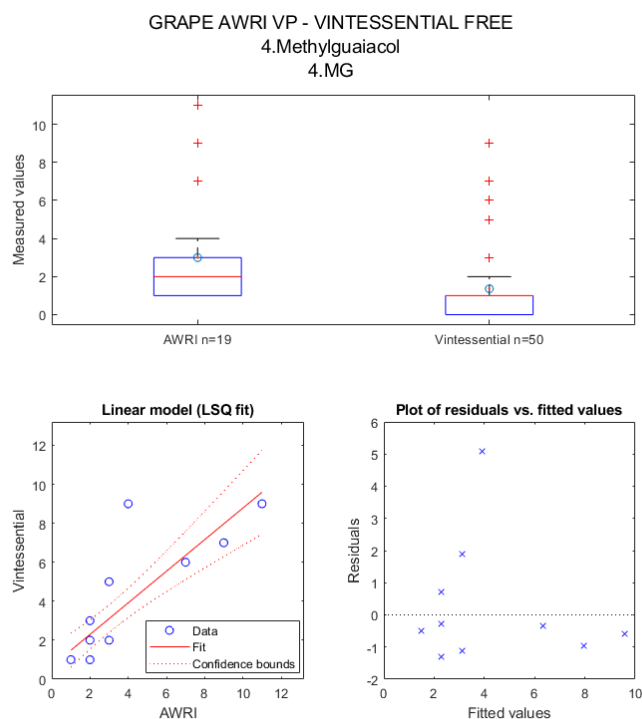Significant mean differences between samples sets

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GRAPE AWRI VP - VINTESSENTIAL TOTAL
p.CRESOL
p.Cresol

{'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

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GRAPE AWRI VP - VINTESSENTIAL FREE
4.Methylguaiacol
4.MG

{'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
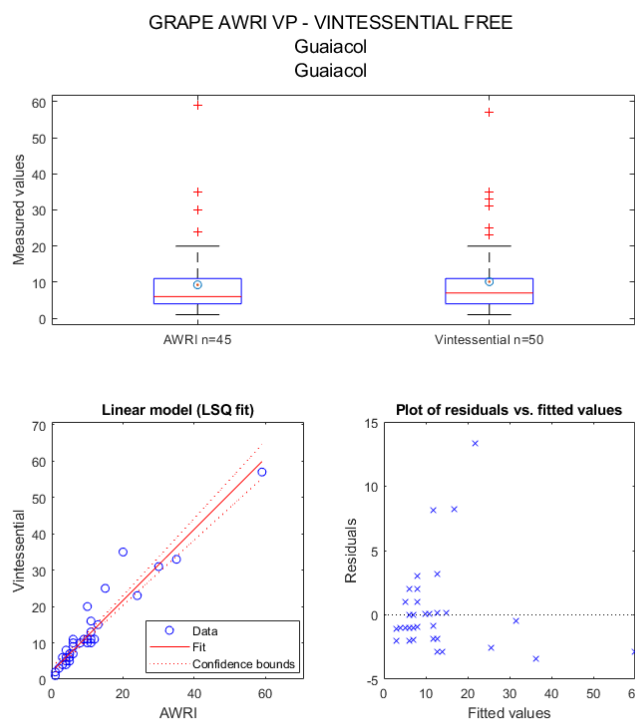No significant difference in variances at the 5% significance level
t-value = -0.30113
Degrees of Freedom = 18
Critical t-value = 1.7341
Probability of difference in means between groups = 0.76677
No significant difference in means at the 5% significance level

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GRAPE AWRI VP - VINTESSENTIAL FREE
Guaiacol
Guaiacol

{'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
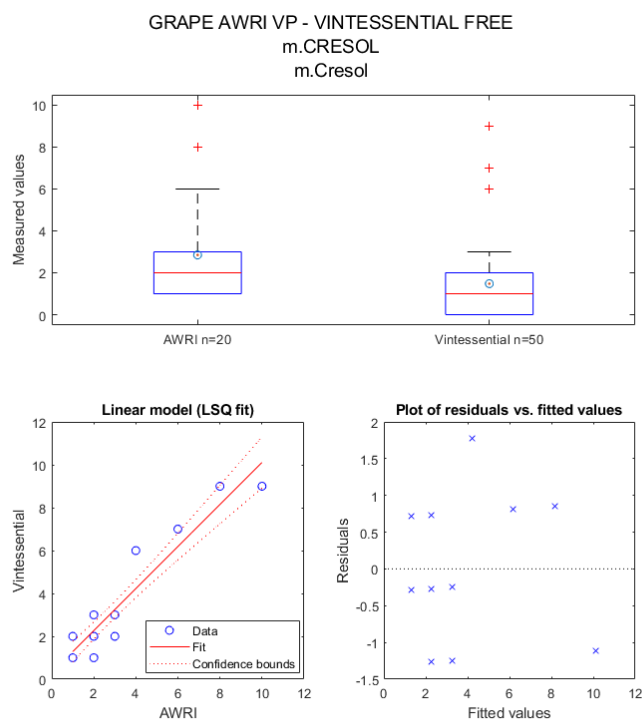No significant difference in variances at the 5% significance level
t-value = -4.0701
Degrees of Freedom = 44
Critical t-value = 1.6802
Probability of difference in means between groups = 0.00019226
Significant mean differences between samples sets

GRAPE AWRI VP - VINTESSENTIAL FREE
m.CRESOL
m.Cresol

{'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
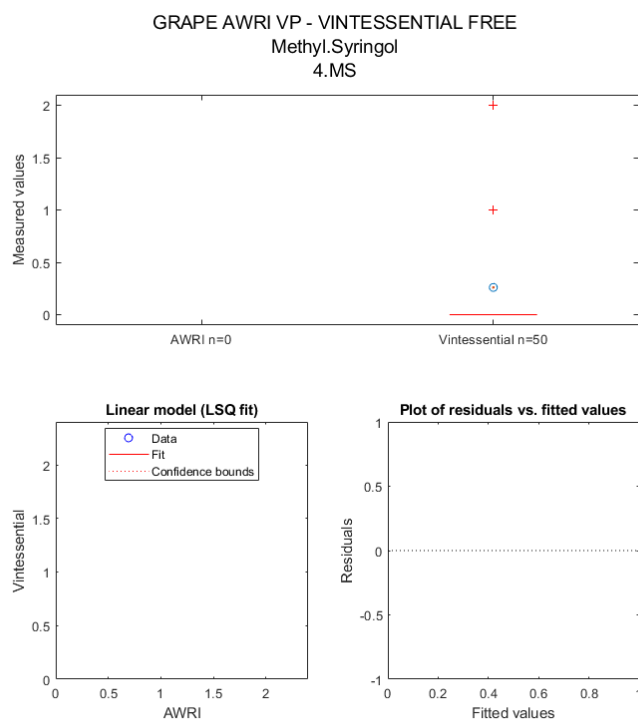t-value = -1.4217
Degrees of Freedom = 19
Critical t-value = 1.7291
Probability of difference in means between groups = 0.17132
No significant difference in means at the 5% significance level
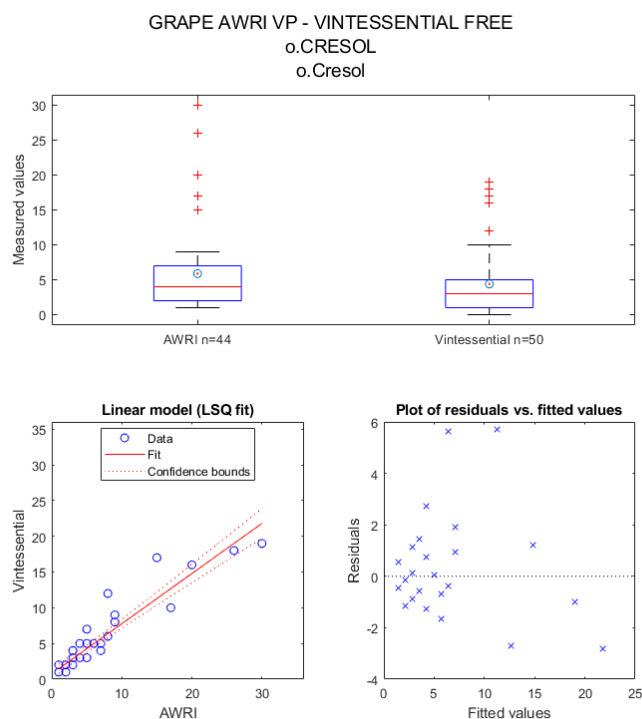Warning: Regression design matrix is rank deficient to within machine precision.

AWRI and Vintessential
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GRAPE AWRI VP - VINTESSENTIAL FREE
Methyl.Syringol
4.MS

{'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
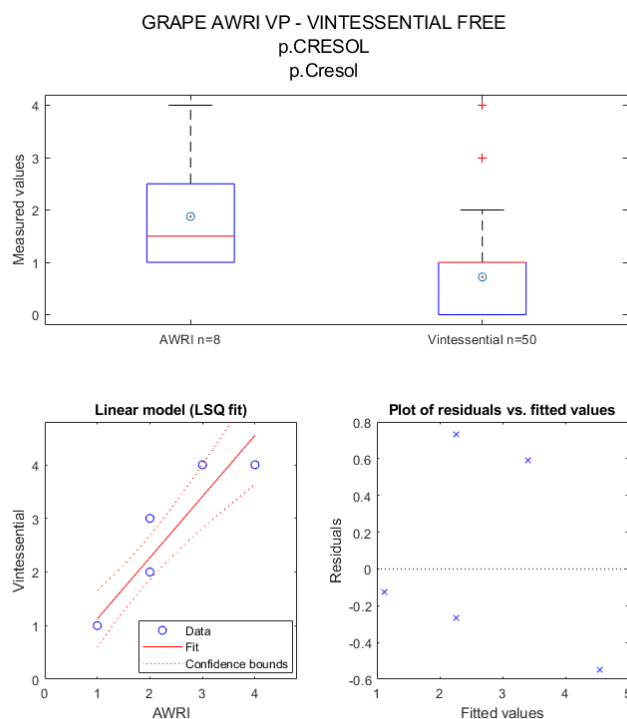Degrees of Freedom = 0
Critical t-value = NaN
Probability of difference in means between groups = NaN
Significant mean differences between samples sets

AWRI and Vintessential
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GRAPE AWRI VP - VINTESSENTIAL FREE
o.CRESOL
o.Cresol

{'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

AWRI and Vintessential
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GRAPE AWRI VP - VINTESSENTIAL FREE
p.CRESOL
p.Cresol


```
    {'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
```
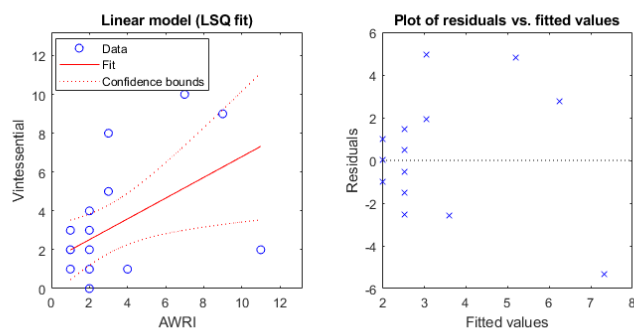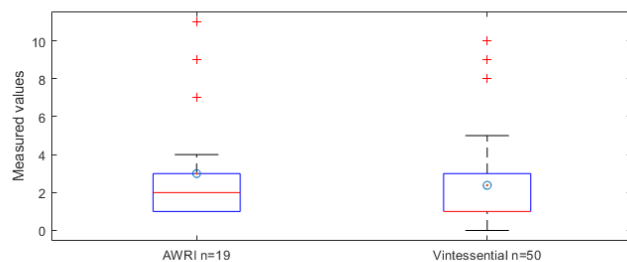
GRAPE AWRI VP - VINTESSENTIAL BOUND
4.Methylguaiacol
4.MG


```
    {'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
```
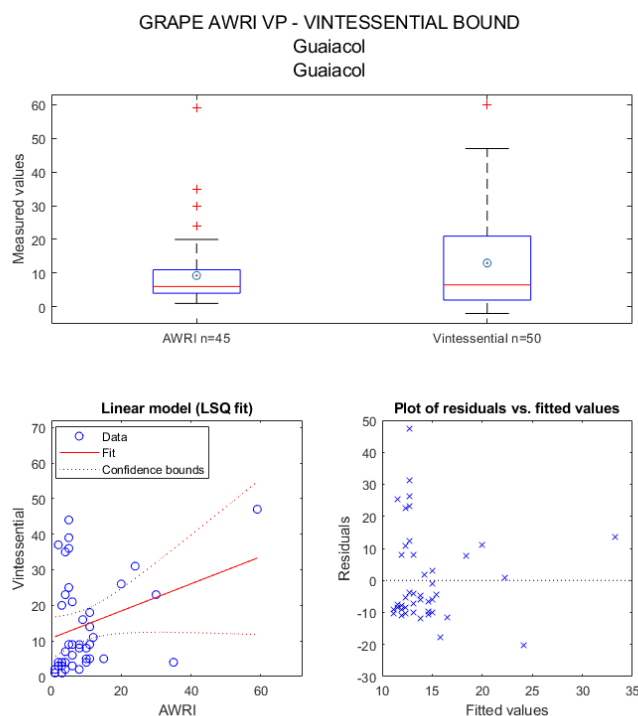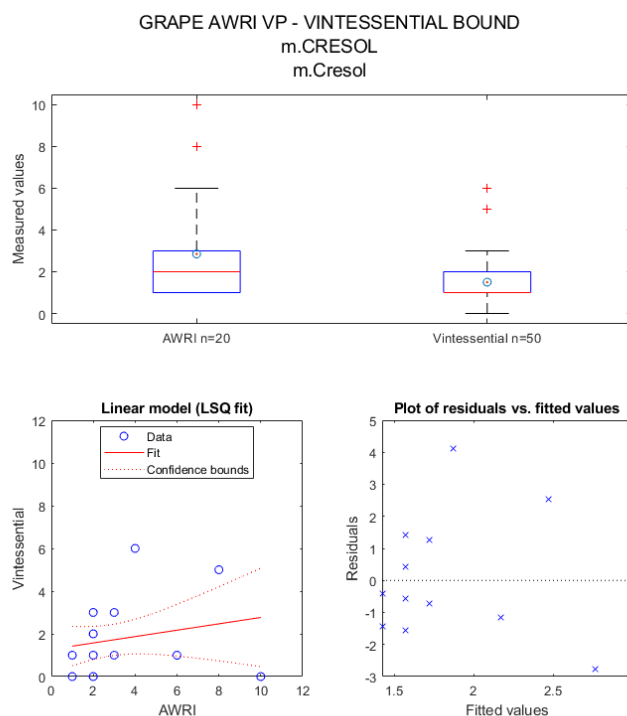
GRAPE AWRI VP - VINTESSENTIAL BOUND
Guaiacol
Guaiacol


```
    {'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 - VINTESSENTIAL BOUND
m.CRESOL
m.Cresol


```
     {'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.
```
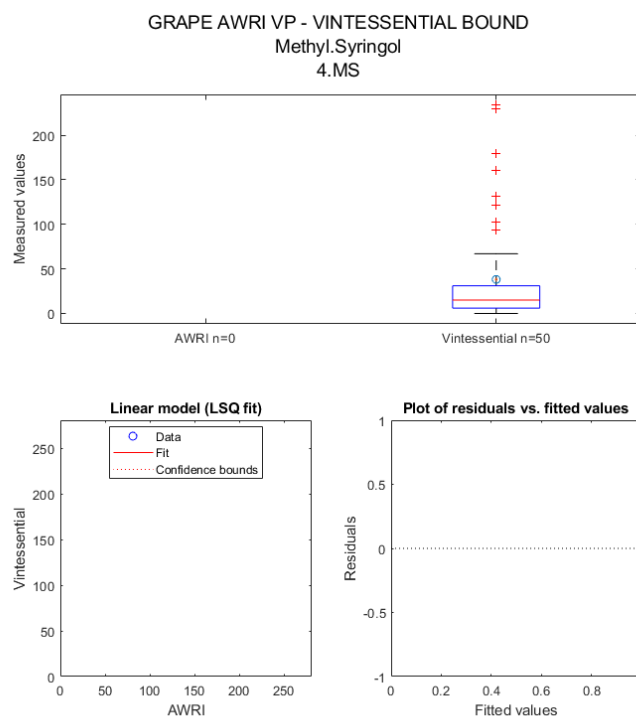
GRAPE AWRI VP - VINTESSENTIAL BOUND
Methyl.Syringol
4.MS

{'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
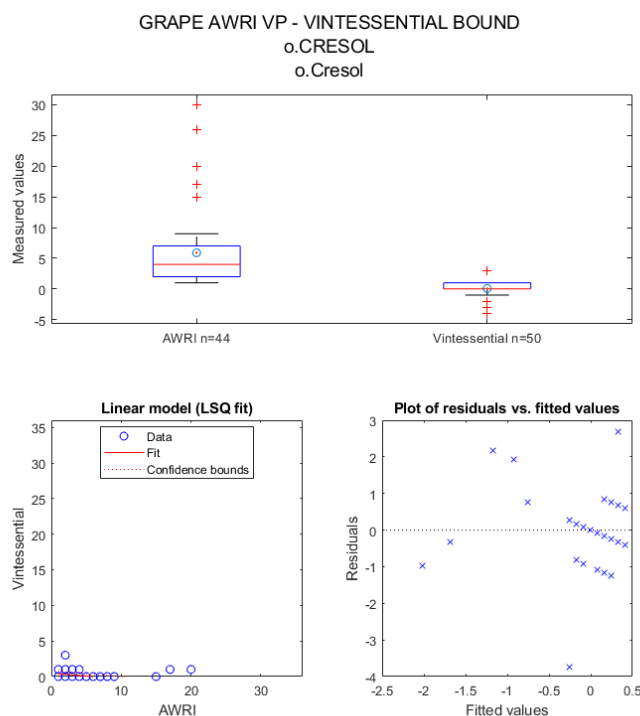Significant variance differences between samples sets
t-value = NaN
Degrees of Freedom = 0
Critical t-value = NaN
Probability of difference in means between groups = NaN
Significant mean differences between samples sets

GRAPE AWRI VP - VINTESSENTIAL BOUND
o.CRESOL
o.Cresol


```
{'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
```
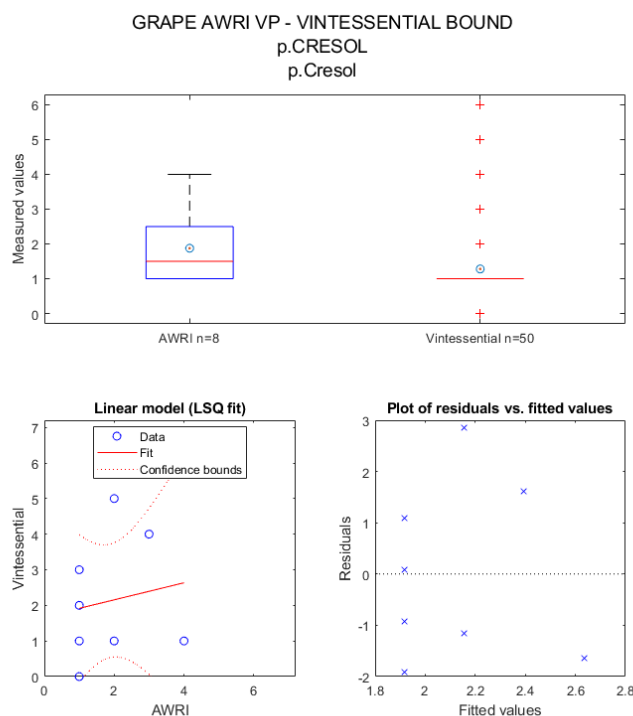
GRAPE AWRI VP - VINTESSENTIAL BOUND
p.CRESOL
p.Cresol


```
    {'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
```
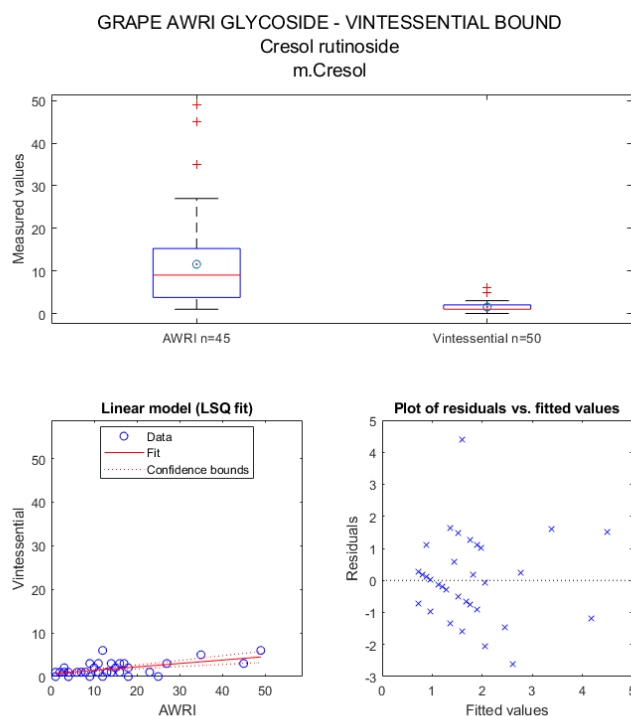
GRAPE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Cresol rutinoside
m.Cresol

{'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
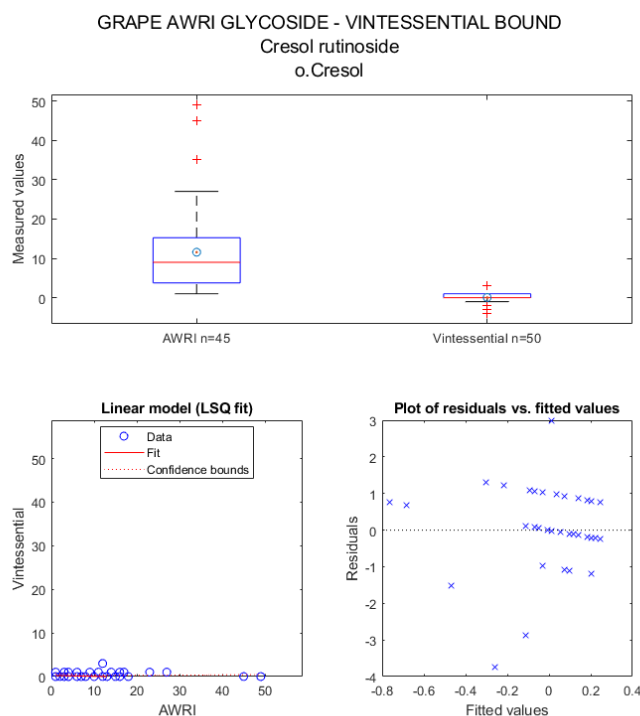Significant variance differences between samples sets
t-value = 6.648
Degrees of Freedom = 44
Critical t-value = 1.6802
Probability of difference in means between groups = 3.7571e-08
Significant mean differences between samples sets

GRAPE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Cresol rutinoside
o.Cresol


```
    {'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
```
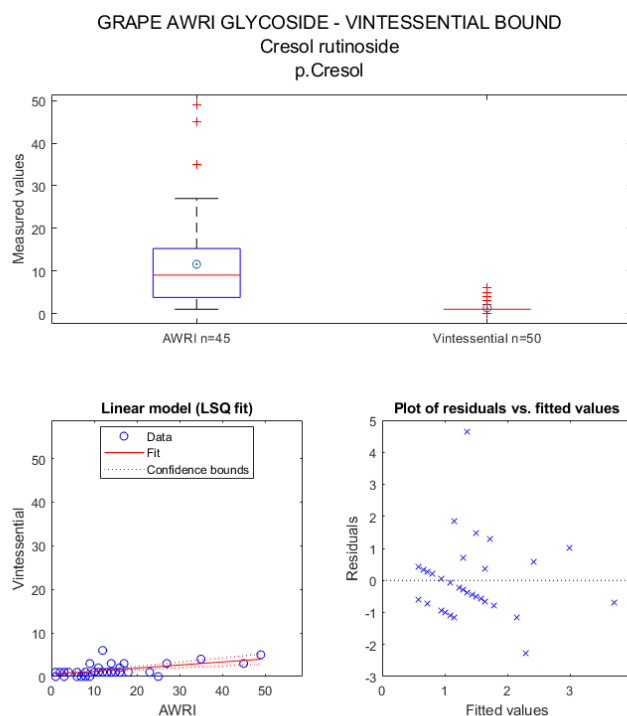
GRAPE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Cresol rutinoside
p.Cresol


```
{'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
```
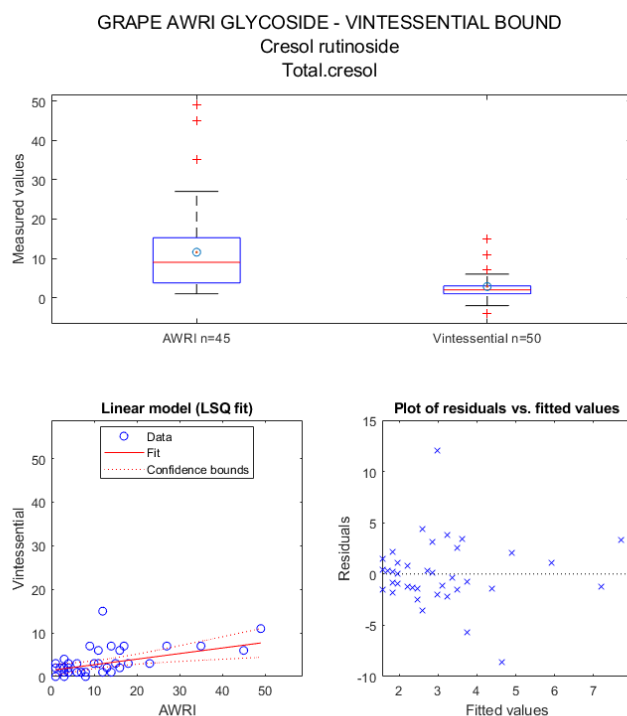
GRAPE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Cresol rutinoside
Total.cresol

        {'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
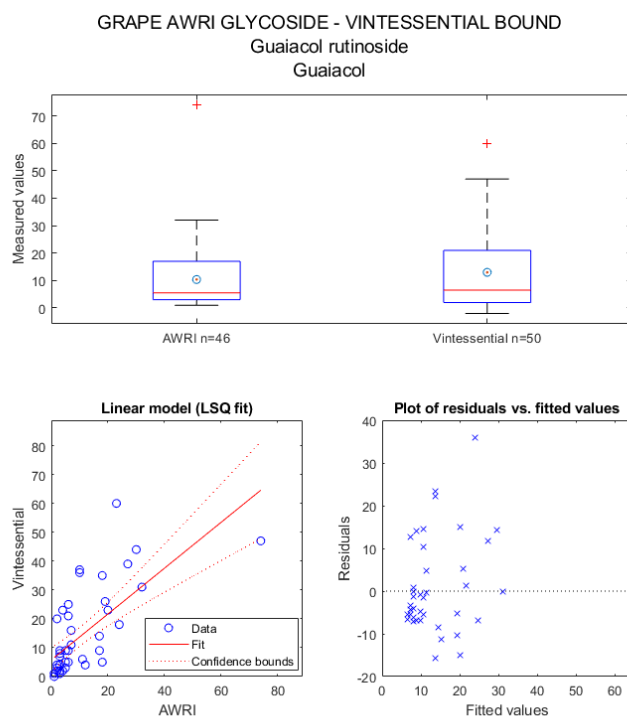Significant variance differences between samples sets
t-value = 5.8319
Degrees of Freedom = 44
Critical t-value = 1.6802
Probability of difference in means between groups = 5.9575e-07
Significant mean differences between samples sets

GRAPE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Guaiacol rutinoside
Guaiacol


```
    {'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
```
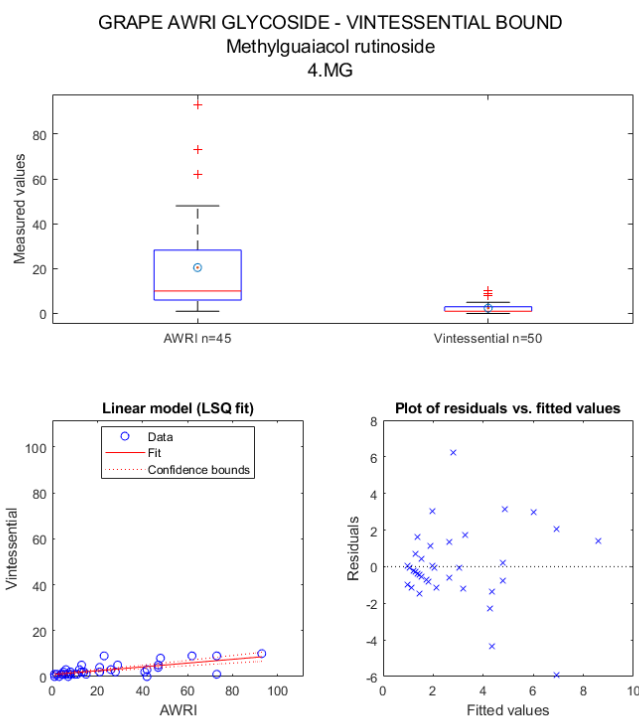
GRAPE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Methylguaiacol rutinoside
4.MG

{'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
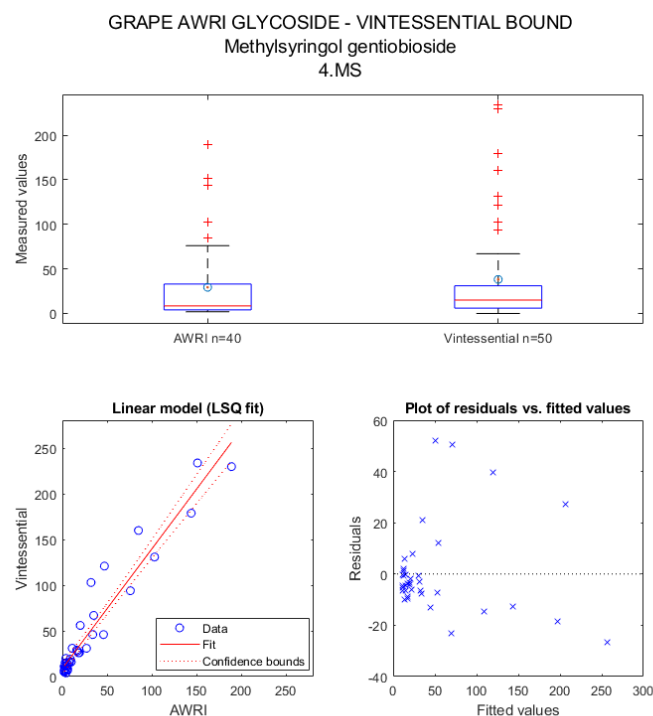Significant variance differences between samples sets
t-value = 5.8411
Degrees of Freedom = 44
Critical t-value = 1.6802
Probability of difference in means between groups = 5.775e-07
Significant mean differences between samples sets

GRAPE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Methylsyringol gentiobioside
4.MS


```
    {'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
```
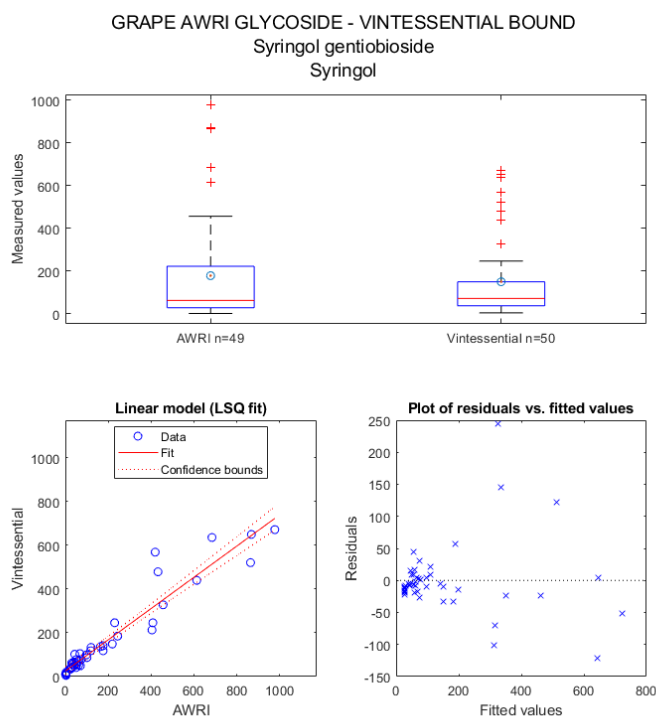
GRAPE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Syringol gentiobioside
Syringol


```
    {'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
```
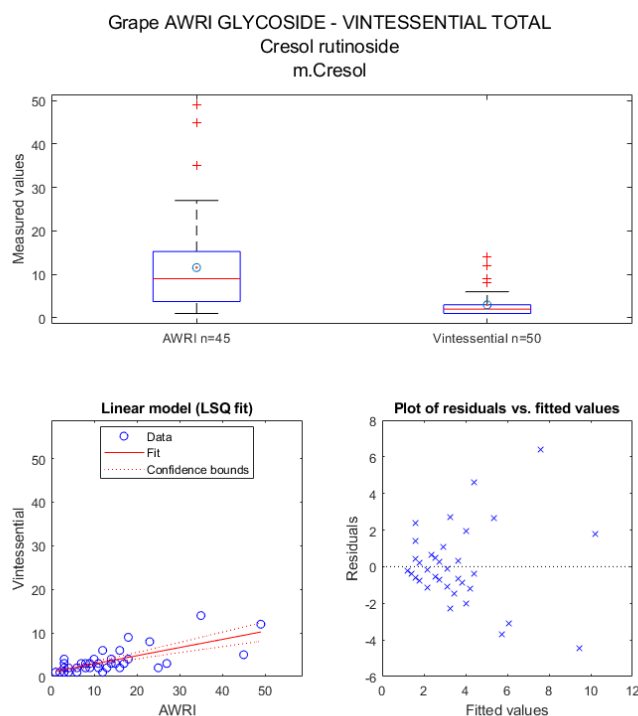
Grape AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Cresol rutinoside
m.Cresol


```
    {'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
```
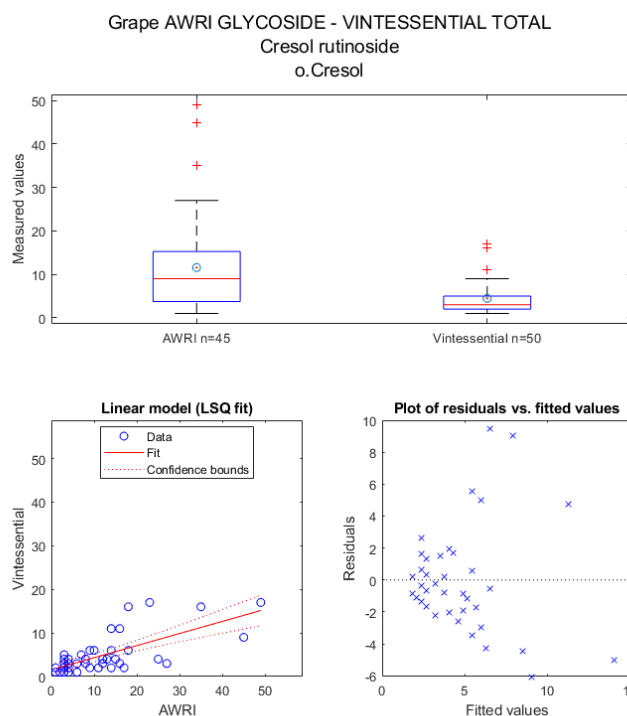
Grape AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Cresol rutinoside
o.Cresol


```
    {'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
```
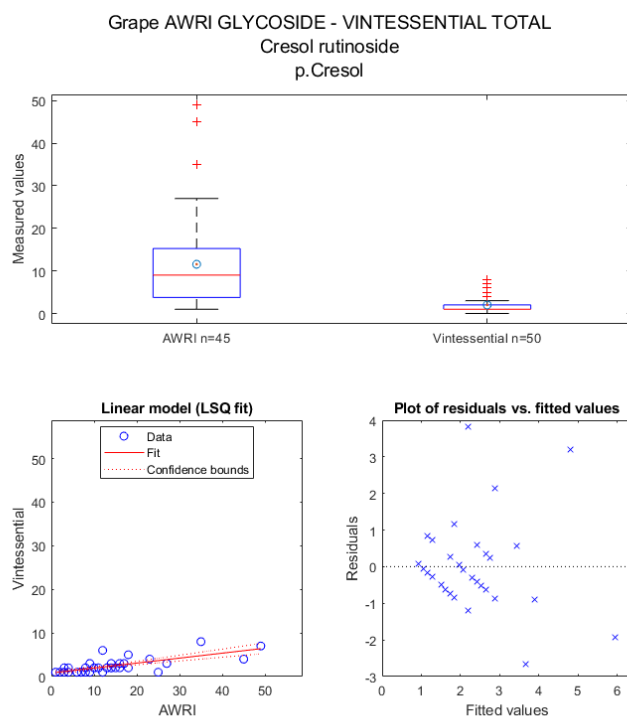
Grape AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Cresol rutinoside
p.Cresol

```
     {'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
```
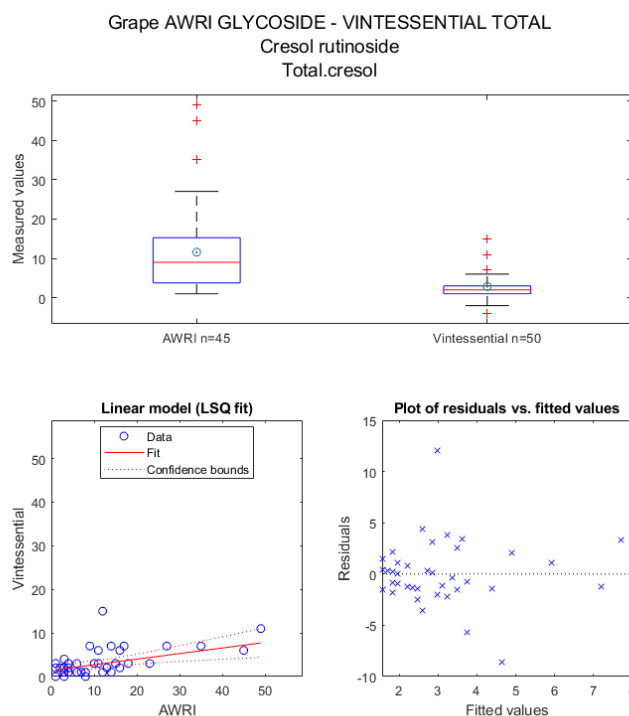
Grape AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Cresol rutinoside
Total.cresol


```
    {'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
```
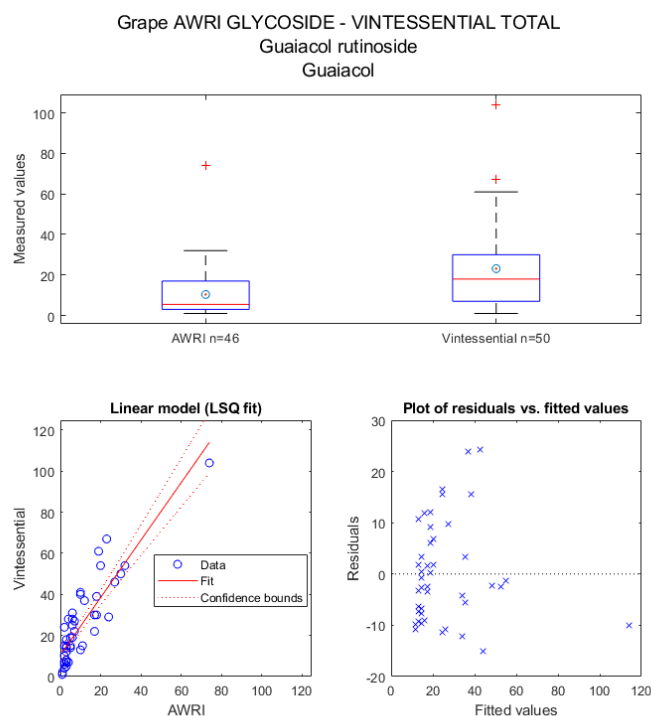
Grape AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Guaiacol rutinoside
Guaiacol


```
    {'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
```
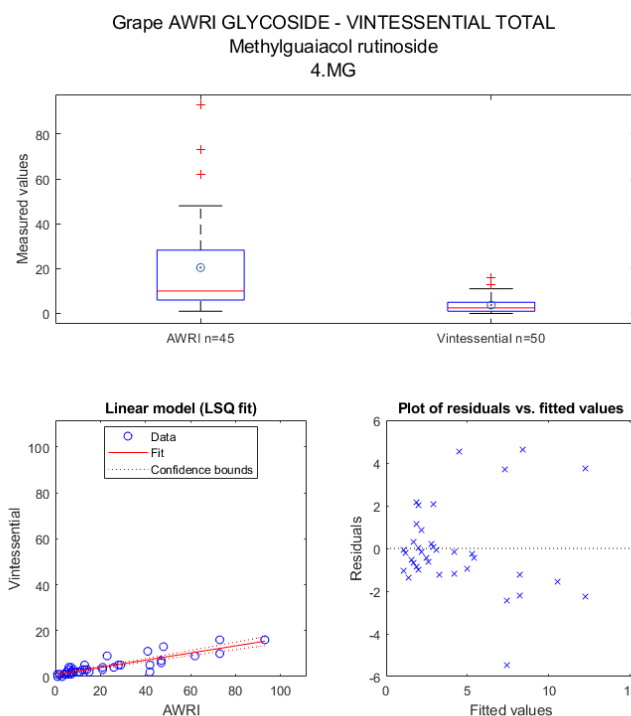
Grape AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Methylguaiacol rutinoside
4.MG


```
     {'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
```
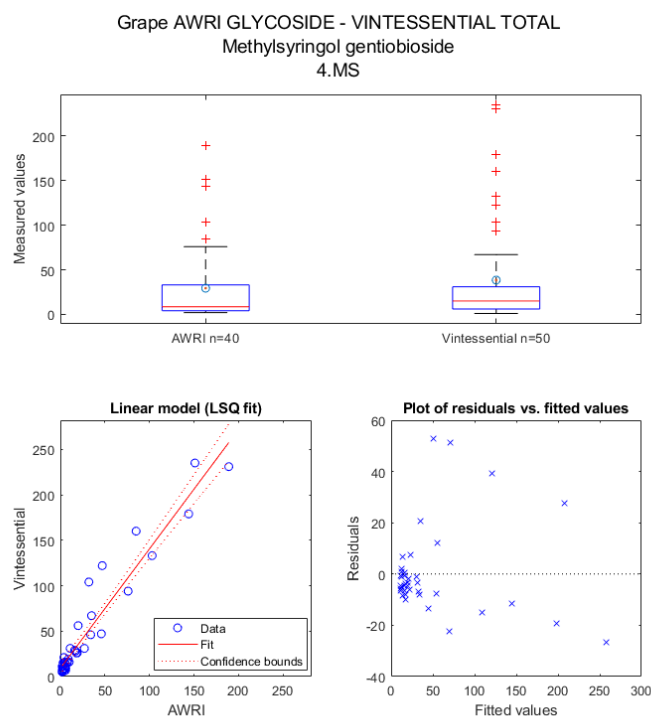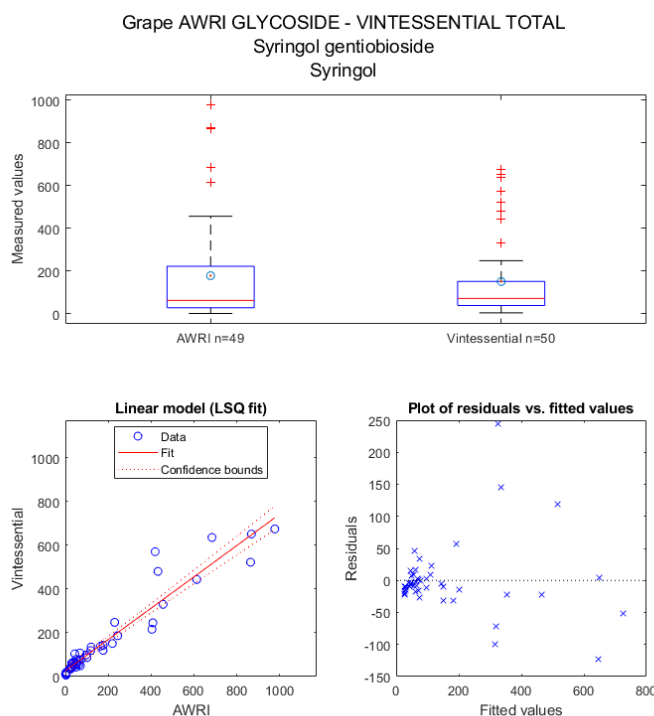
Grape AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Methylsyringol gentiobioside
4.MS


```
    {'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 GLYCOSIDE - VINTESSENTIAL TOTAL
Syringol gentiobioside
Syringol

{'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
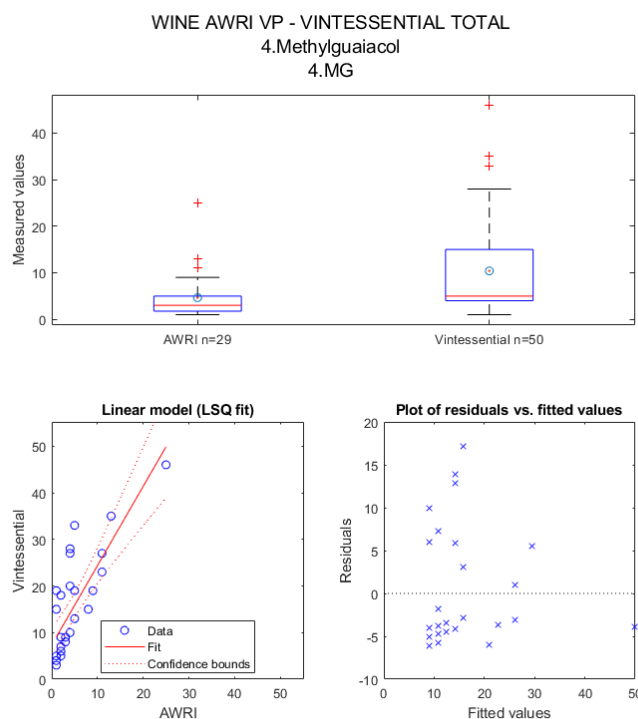Significant variance differences between samples sets
t-value = 1.9084
Degrees of Freedom = 48
Critical t-value = 1.6772
Probability of difference in means between groups = 0.062328
No significant difference in means at the 5% significance level

AWRI and Vintessential
Grape and Wine Analysis | Method Comparison
National Wine and Grape Industry Centre, Charles Sturt University

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WINE AWRI VP - VINTESSENTIAL TOTAL
4.Methylguaiacol
4.MG

{'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
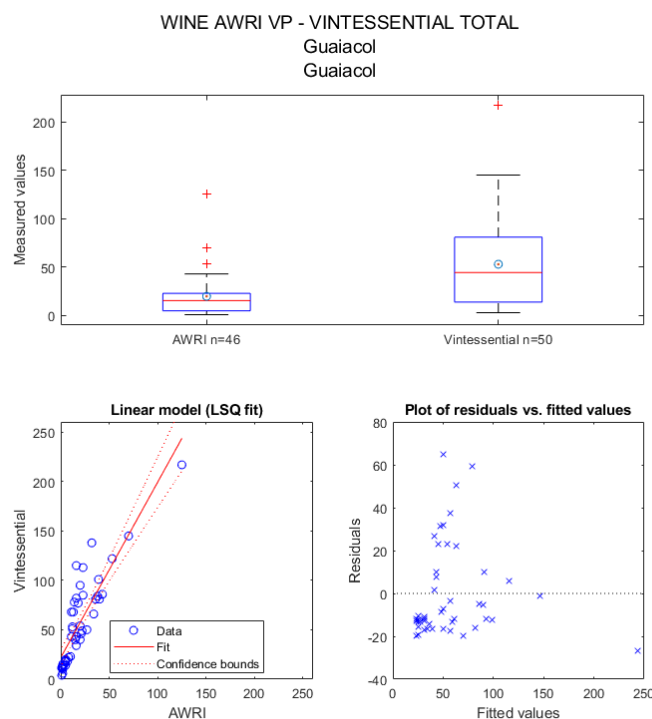Significant variance differences between samples sets
t-value = -7.4307
Degrees of Freedom = 28
Critical t-value = 1.7011
Probability of difference in means between groups = 4.3037e-08
Significant mean differences between samples sets

AWRI and Vintessential
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WINE AWRI VP - VINTESSENTIAL TOTAL
Guaiacol
Guaiacol

{'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
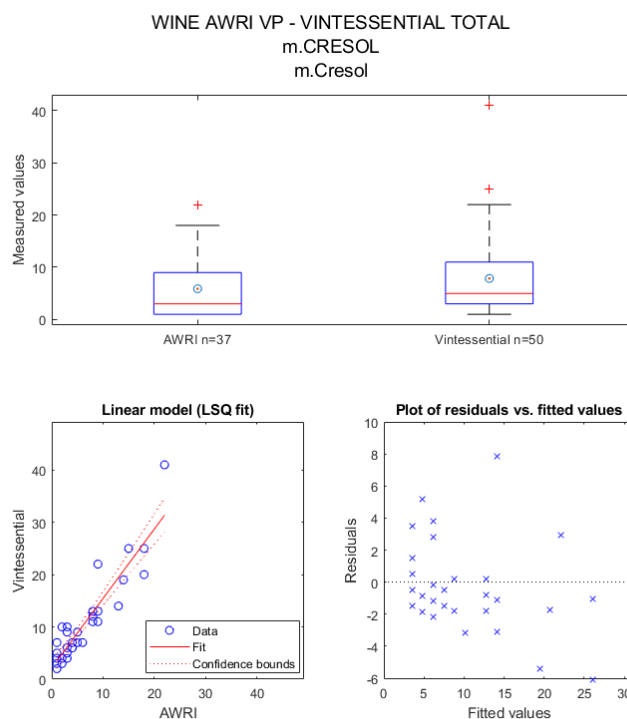
WINE AWRI VP - VINTESSENTIAL TOTAL
m.CRESOL
m.Cresol

{'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
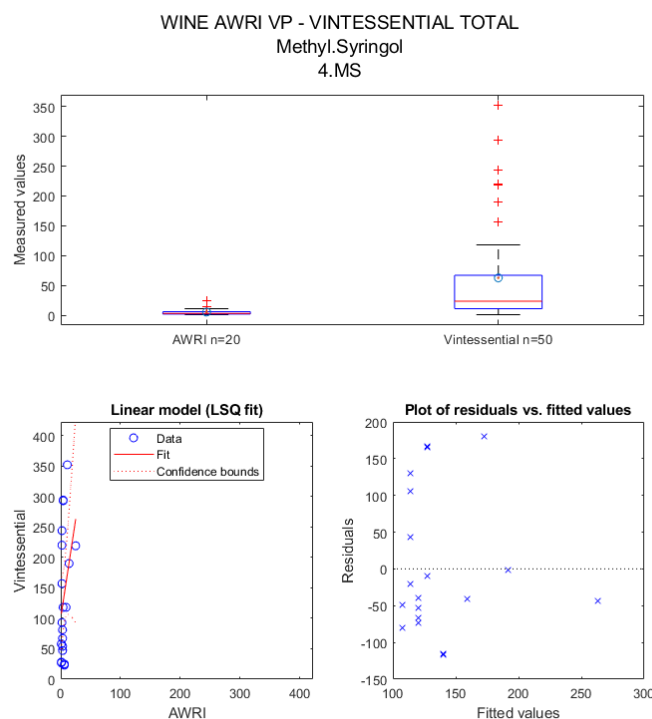Significant variance differences between samples sets
t-value = -6.8465
Degrees of Freedom = 36
Critical t-value = 1.6883
Probability of difference in means between groups = 5.2237e-08
Significant mean differences between samples sets

AWRI and Vintessential
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WINE AWRI VP - VINTESSENTIAL TOTAL
Methyl.Syringol
4.MS

{'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
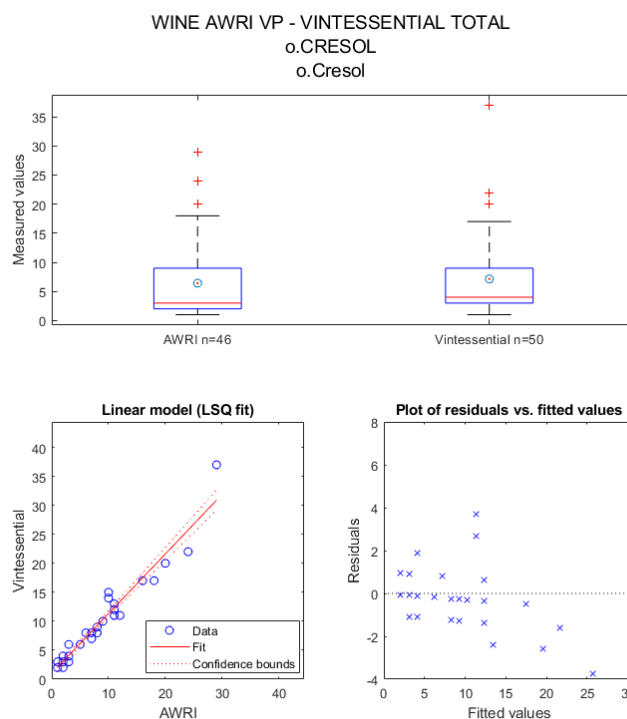Significant variance differences between samples sets
t-value = -5.7098
Degrees of Freedom = 19
Critical t-value = 1.7291
Probability of difference in means between groups = 1.6712e-05
Significant mean differences between samples sets

AWRI and Vintessential
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WINE AWRI VP - VINTESSENTIAL TOTAL
o.CRESOL
o.Cresol

{'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
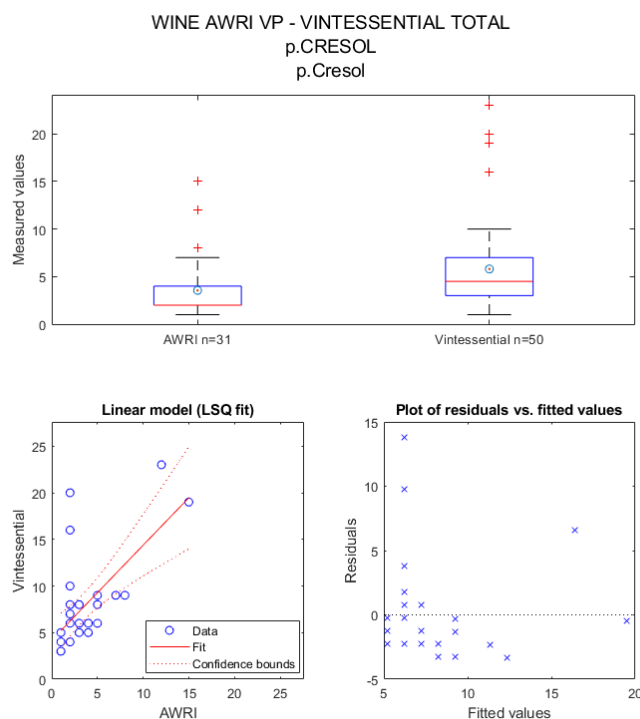
WINE AWRI VP - VINTESSENTIAL TOTAL
p.CRESOL
p.Cresol

{'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
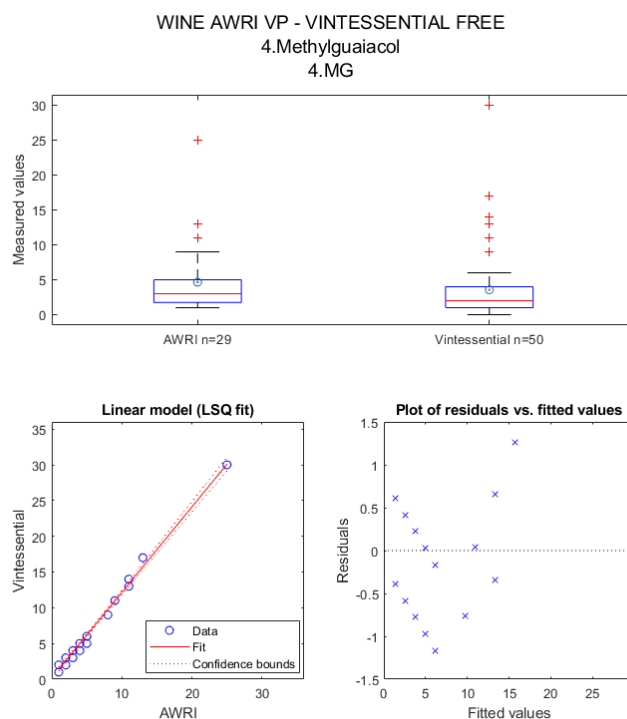Significant variance differences between samples sets
t-value = -6.0814
Degrees of Freedom = 30
Critical t-value = 1.6973
Probability of difference in means between groups = 1.1108e-06
Significant mean differences between samples sets

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WINE AWRI VP - VINTESSENTIAL FREE
4.Methylguaiacol
4.MG

{'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
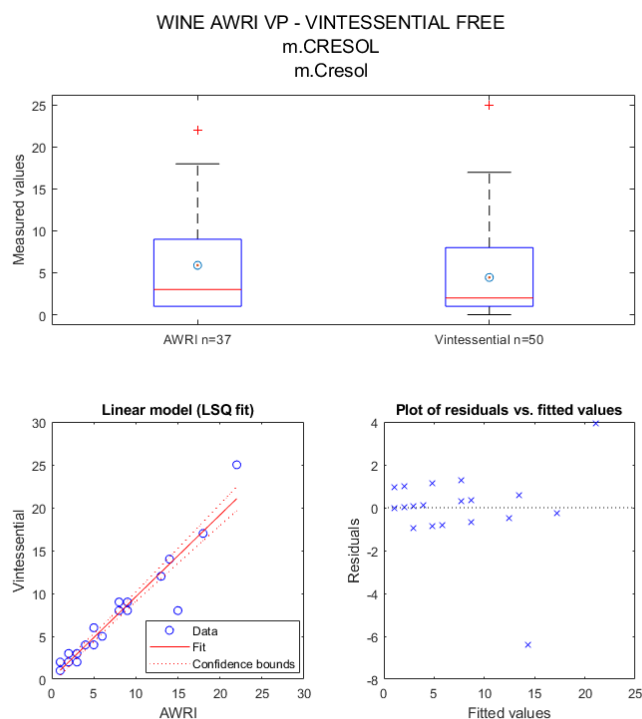Significant mean differences between samples sets
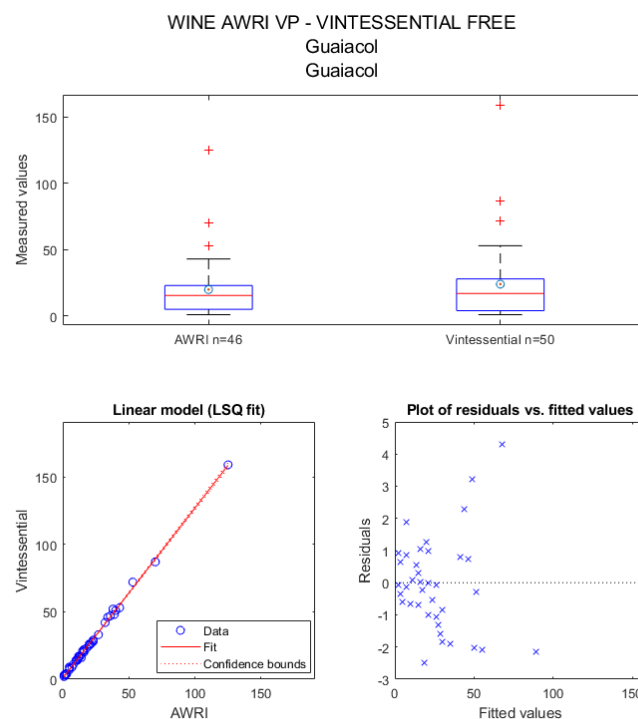
WINE AWRI VP - VINTESSENTIAL FREE
Guaiacol
Guaiacol

{'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
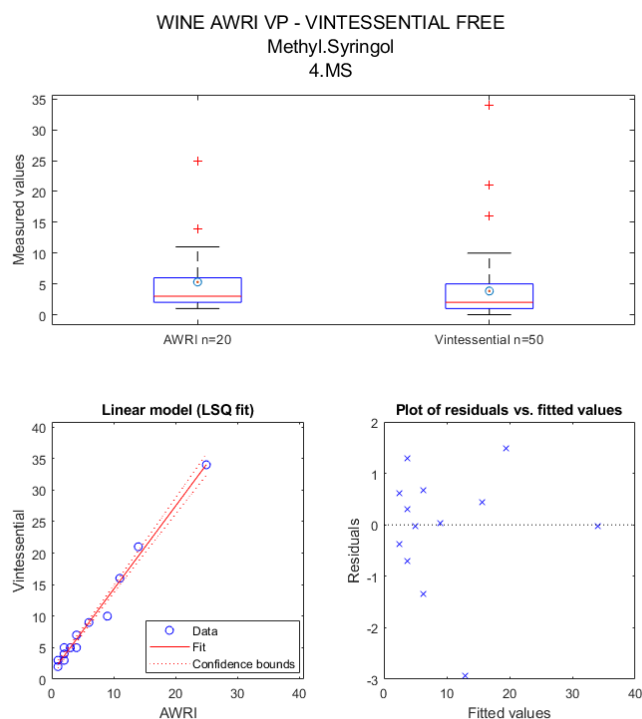Significant mean differences between samples sets

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WINE AWRI VP - VINTESSENTIAL FREE
m.CRESOL
m.Cresol

Linear model (LSQ fit)

Plot of residuals vs. fitted values

{'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
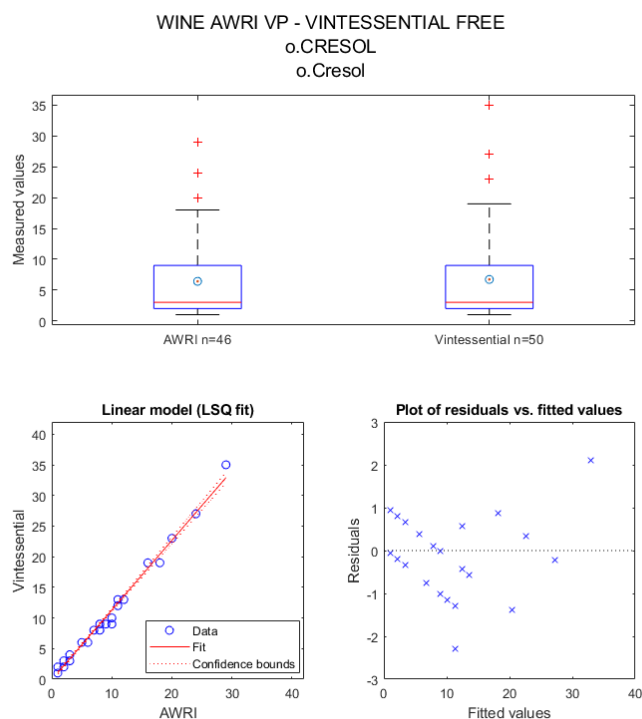No significant difference in means at the 5% significance level

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WINE AWRI VP - VINTESSENTIAL FREE
Methyl.Syringol
4.MS

{'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

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WINE AWRI VP - VINTESSENTIAL FREE
o.CRESOL
o.Cresol

{'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
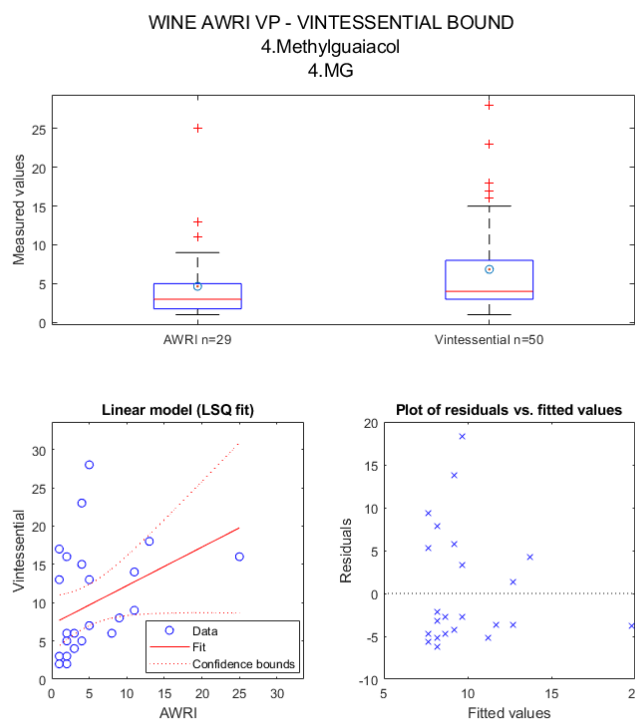Significant mean differences between samples sets
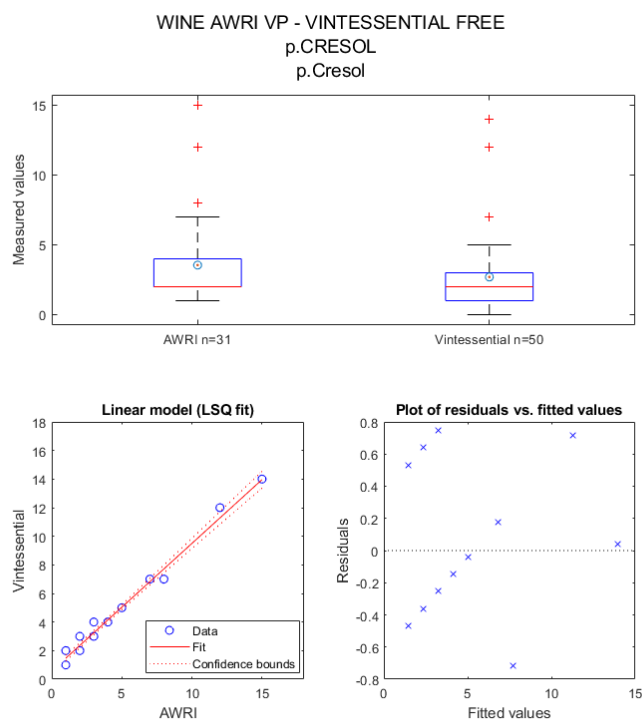
WINE AWRI VP - VINTESSENTIAL FREE
p.CRESOL
p.Cresol

Linear model (LSQ fit)

Plot of residuals vs. fitted values

{'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

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WINE AWRI VP - VINTESSENTIAL BOUND
4.Methylguaiacol
4.MG


```
   {'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
```
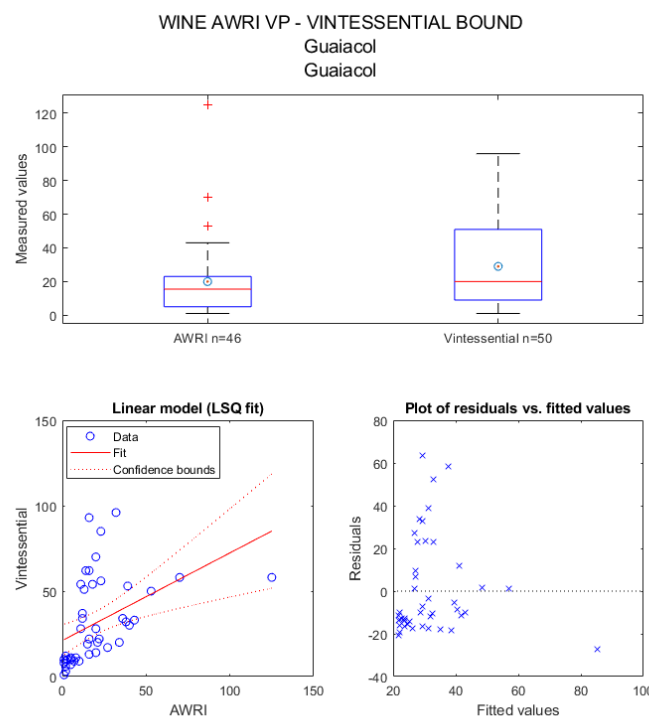
WINE AWRI VP - VINTESSENTIAL BOUND
Guaiacol
Guaiacol

{'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
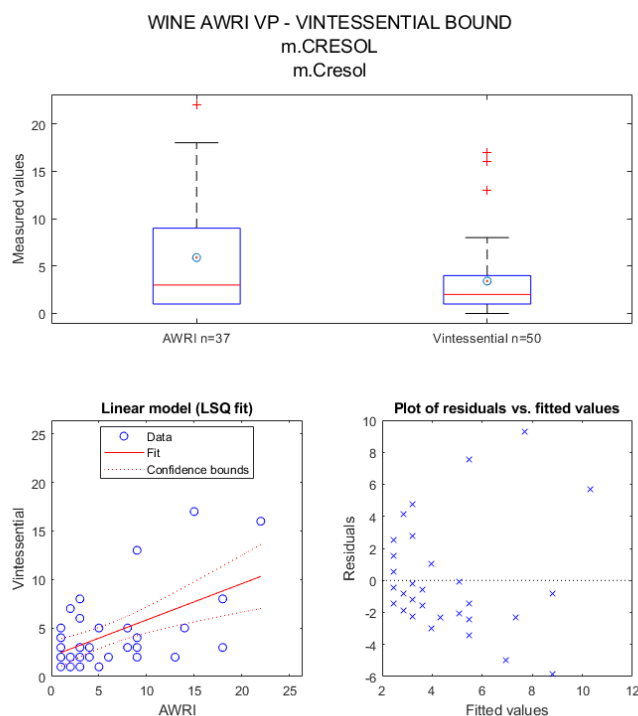No significant difference in variances at the 5% significance level
t-value = -3.1005
Degrees of Freedom = 45
Critical t-value = 1.6794
Probability of difference in means between groups = 0.0033285
Significant mean differences between samples sets

WINE AWRI VP - VINTESSENTIAL BOUND
m.CRESOL
m.Cresol

```
    {'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
```
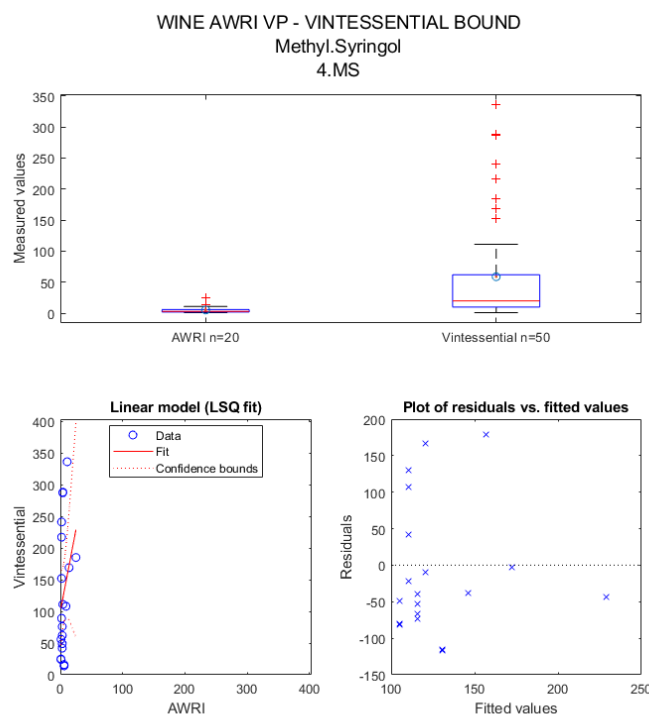
WINE AWRI VP - VINTESSENTIAL BOUND
Methyl.Syringol
4.MS


```
   {'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
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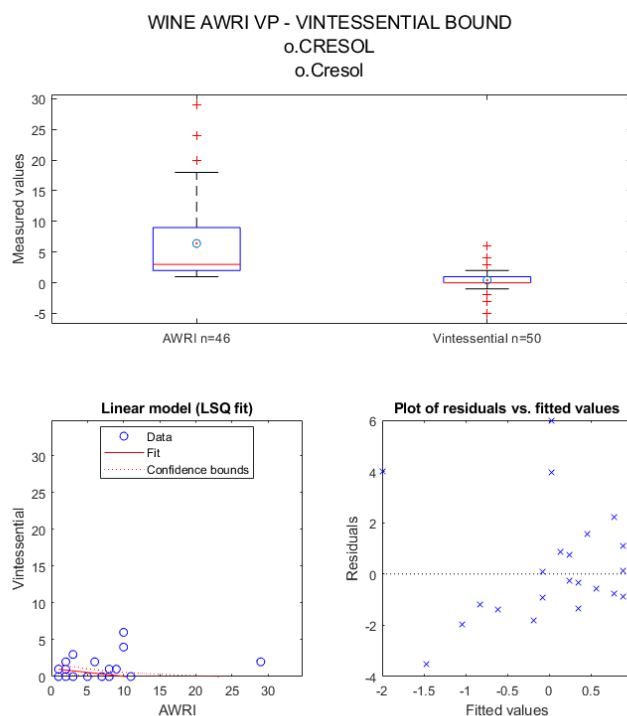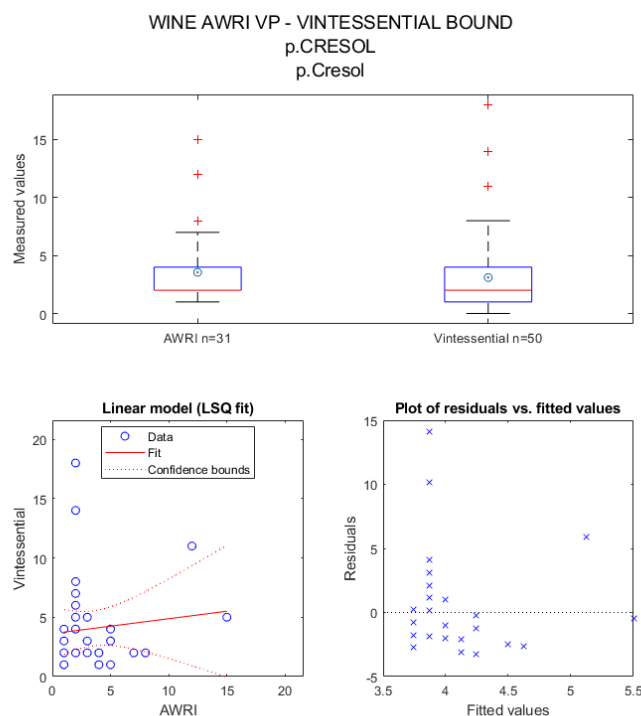
WINE AWRI VP - VINTESSENTIAL BOUND
o.CRESOL
o.Cresol


```
    {'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 - VINTESSENTIAL BOUND
p.CRESOL
p.Cresol


```
    {'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
```
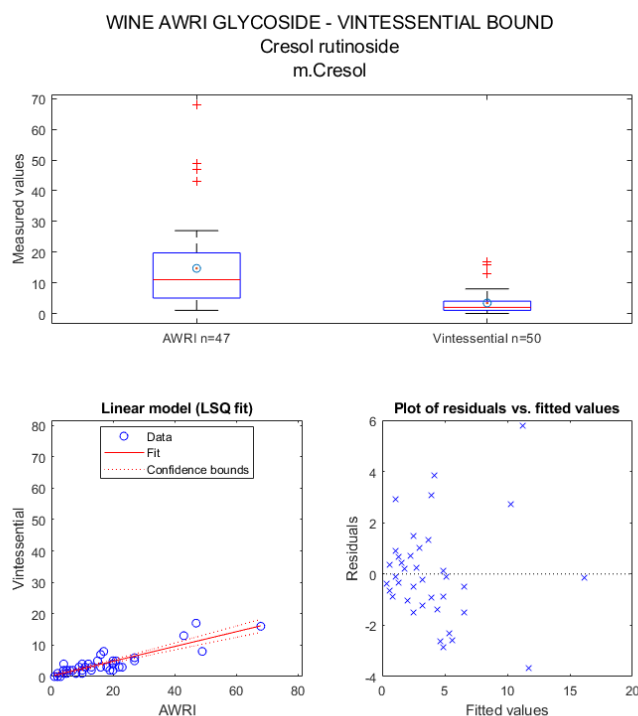
WINE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Cresol rutinoside
m.Cresol


```
    {'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
```
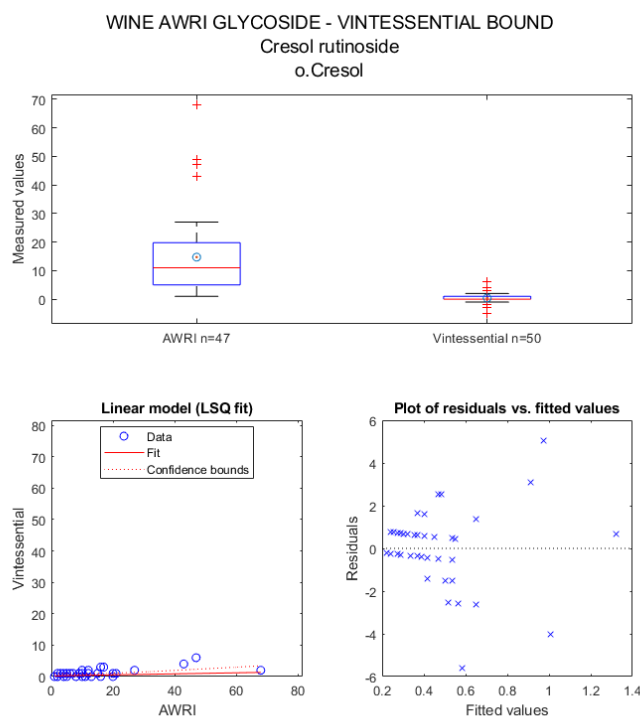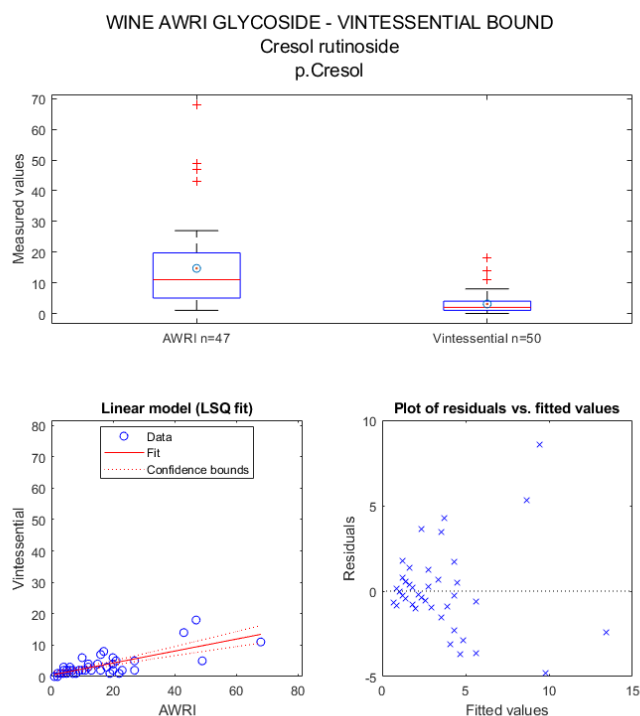
WINE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Cresol rutinoside
o.Cresol


```
    {'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 GLYCOSIDE - VINTESSENTIAL BOUND
Cresol rutinoside
p.Cresol


```
    {'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
```
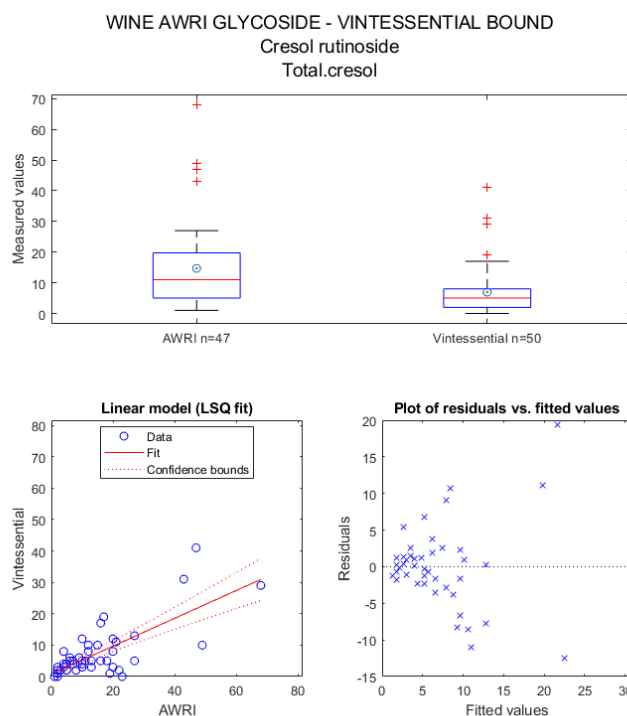
WINE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Cresol rutinoside
Total.cresol

    {'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
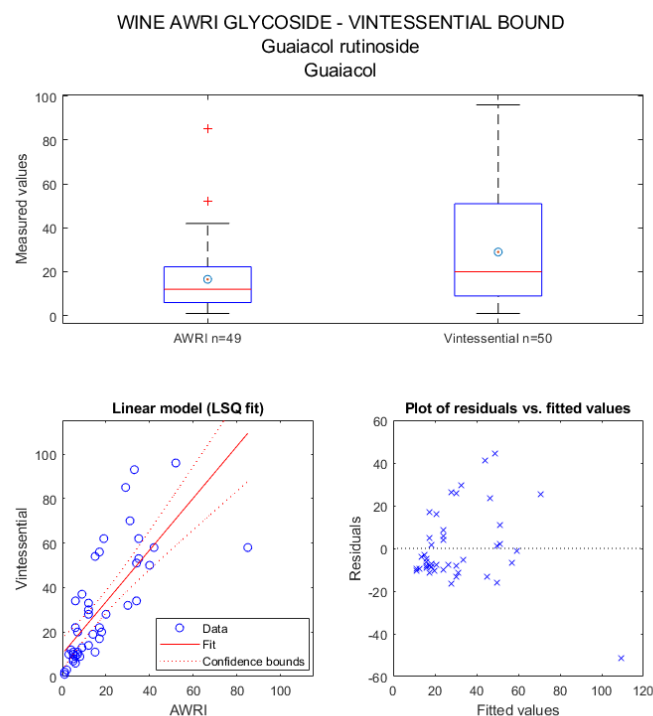Significant variance differences between samples sets
t-value = 5.331
Degrees of Freedom = 46
Critical t-value = 1.6787
Probability of difference in means between groups = 2.8726e-06
Significant mean differences between samples sets

WINE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Guaiacol rutinoside
Guaiacol

{'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
```
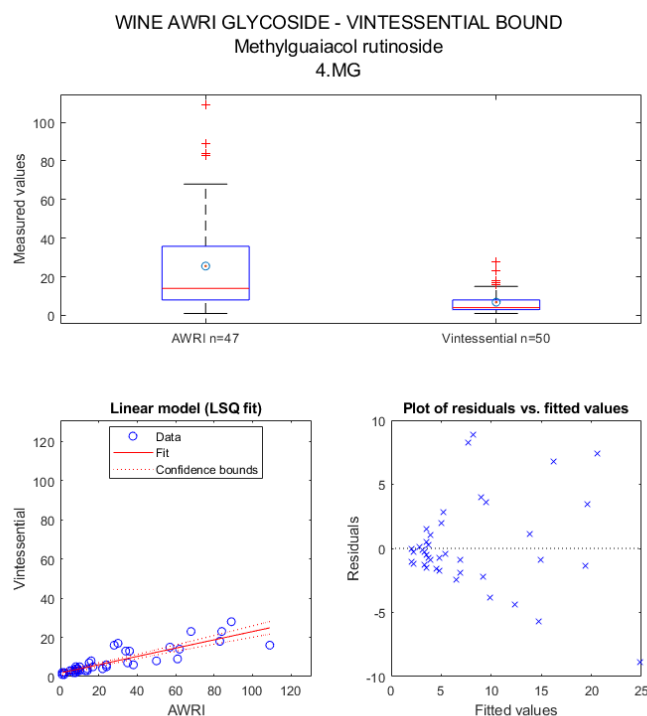
WINE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Methylguaiacol rutinoside
4.MG


```
    {'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
```
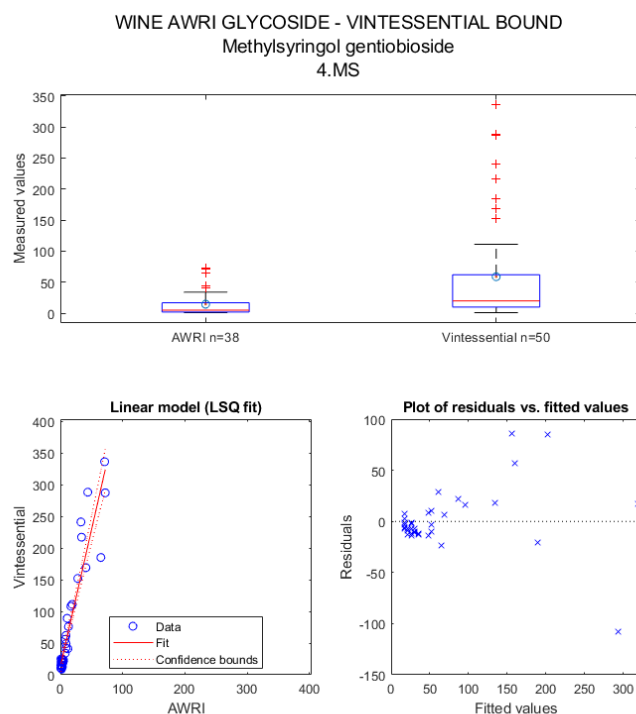
WINE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Methylsyringol gentiobioside
4.MS

Linear model (LSQ fit)

Plot of residuals vs. fitted values

```
    {'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
```
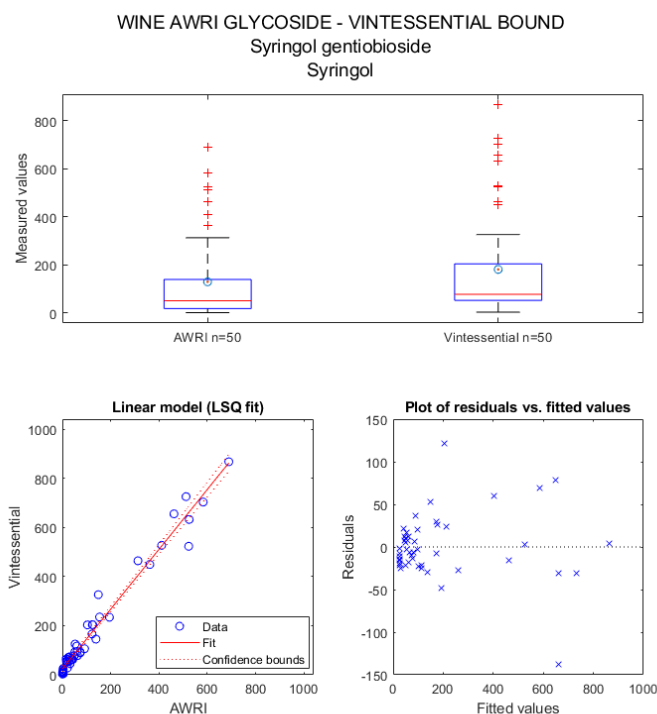
WINE AWRI GLYCOSIDE - VINTESSENTIAL BOUND
Syringol gentiobioside
Syringol

{'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
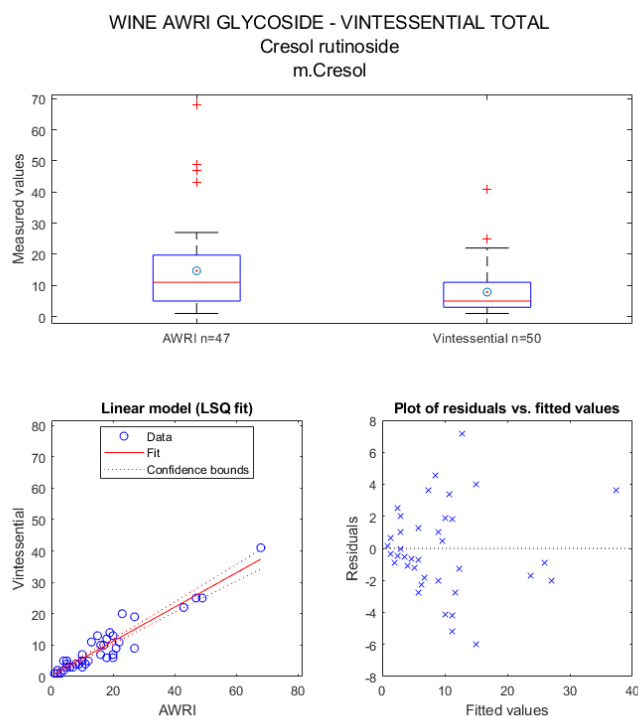No significant difference in variances at the 5% significance level
t-value = -6.7572
Degrees of Freedom = 49
Critical t-value = 1.6766
Probability of difference in means between groups = 1.5776e-08
Significant mean differences between samples sets

WINE AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Cresol rutinoside
m.Cresol


```
    {'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
```
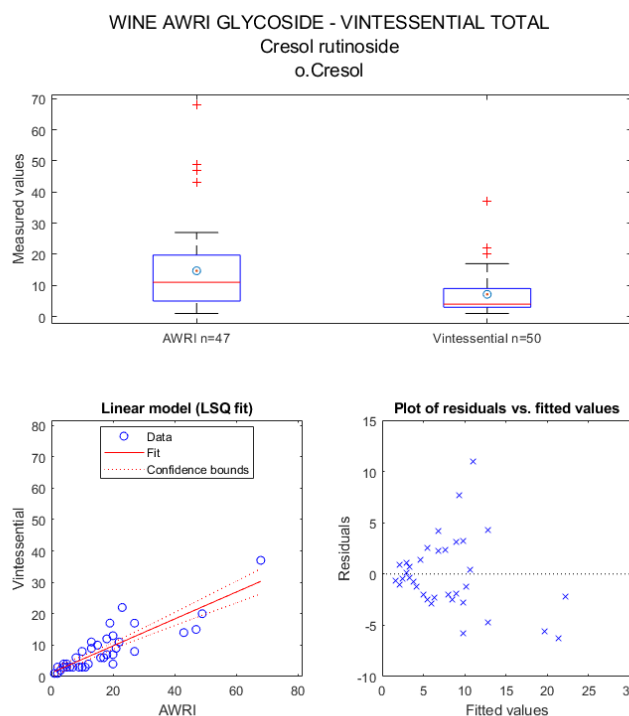
WINE AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Cresol rutinoside
o.Cresol


```
    {'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
```
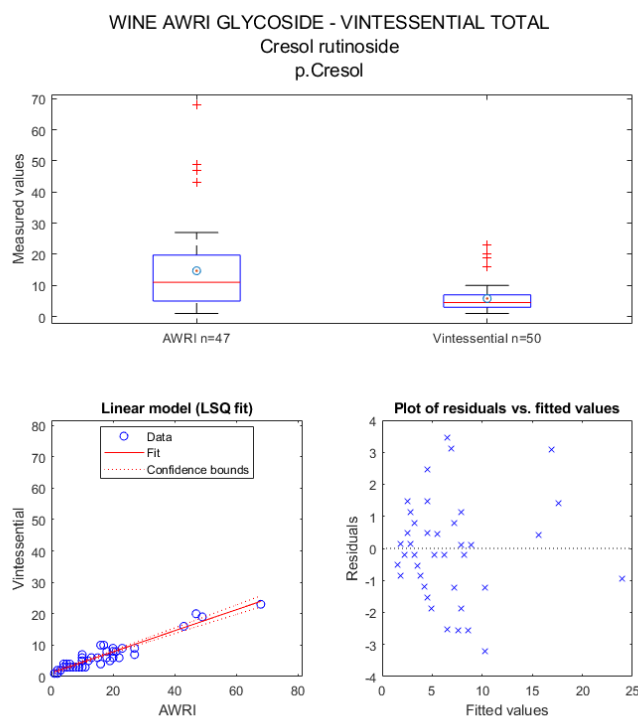
WINE AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Cresol rutinoside
p.Cresol


```
    {'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
```
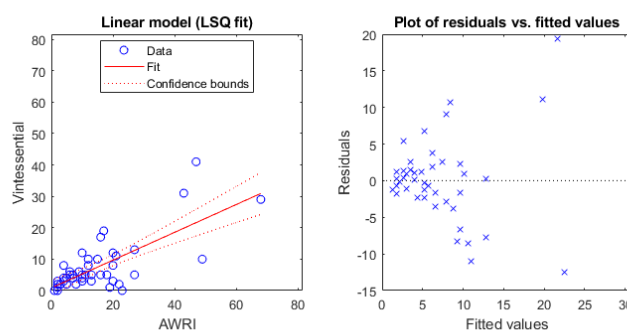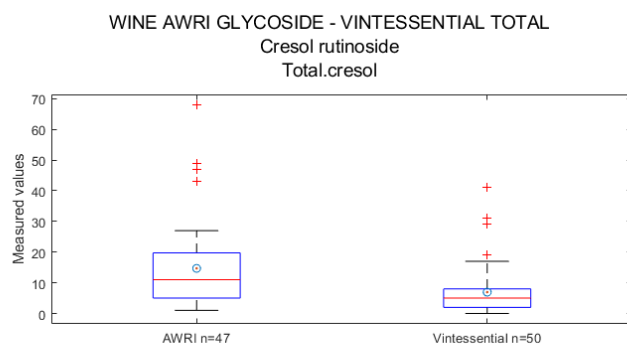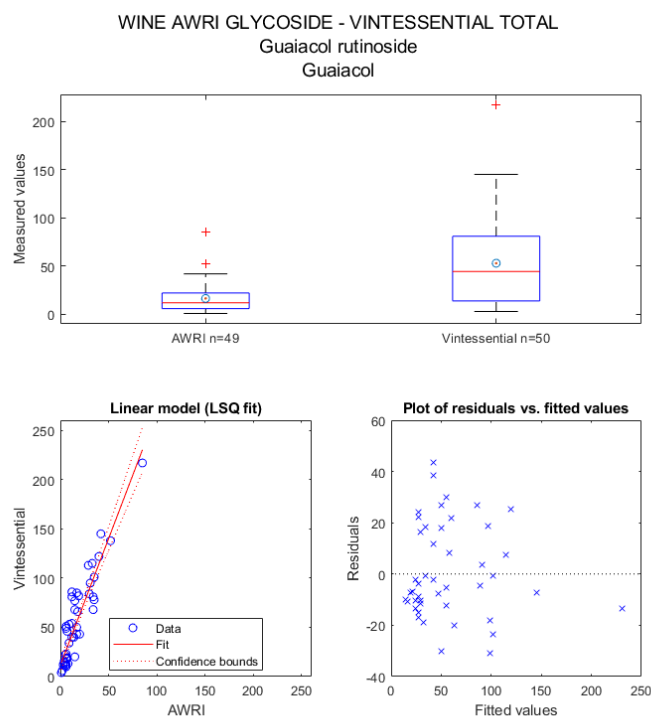
WINE AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Cresol rutinoside
Total.cresol

    {'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 GLYCOSIDE - VINTESSENTIAL TOTAL
Guaiacol rutinoside
Guaiacol


```
    {'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
```
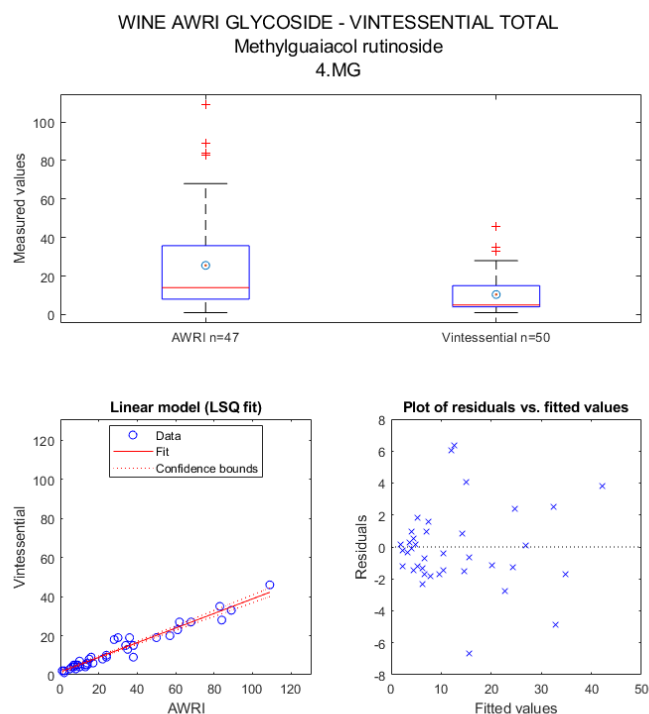
WINE AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Methylguaiacol rutinoside
4.MG

```
    {'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
```
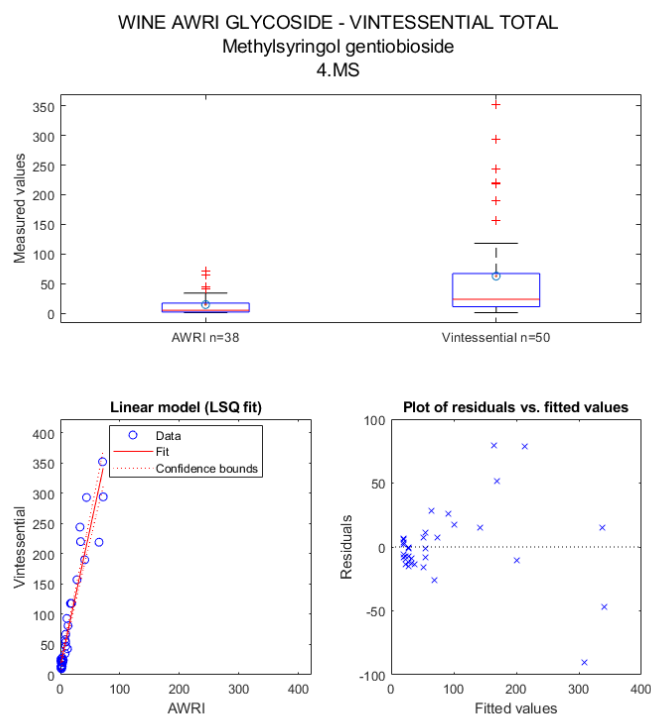
WINE AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Methylsyringol gentiobioside
4.MS


```
    {'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
```
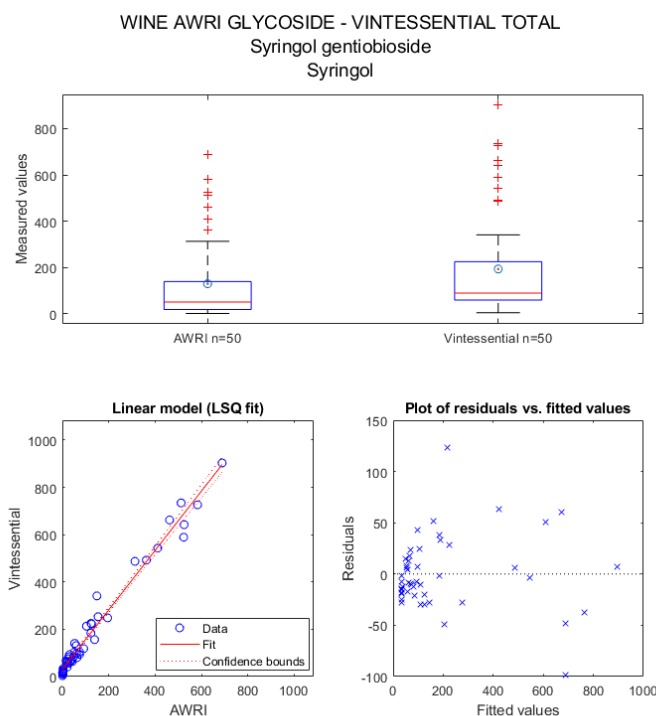
WINE AWRI GLYCOSIDE - VINTESSENTIAL TOTAL
Syringol gentiobioside
Syringol


```
    {'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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