

**MICROWAVE DIELECTRIC SPECTRA AND THE  
COMPOSITION OF FOODS:  
PRINCIPAL COMPONENT ANALYSIS VERSUS  
ARTIFICIAL NEURAL NETWORKS.**

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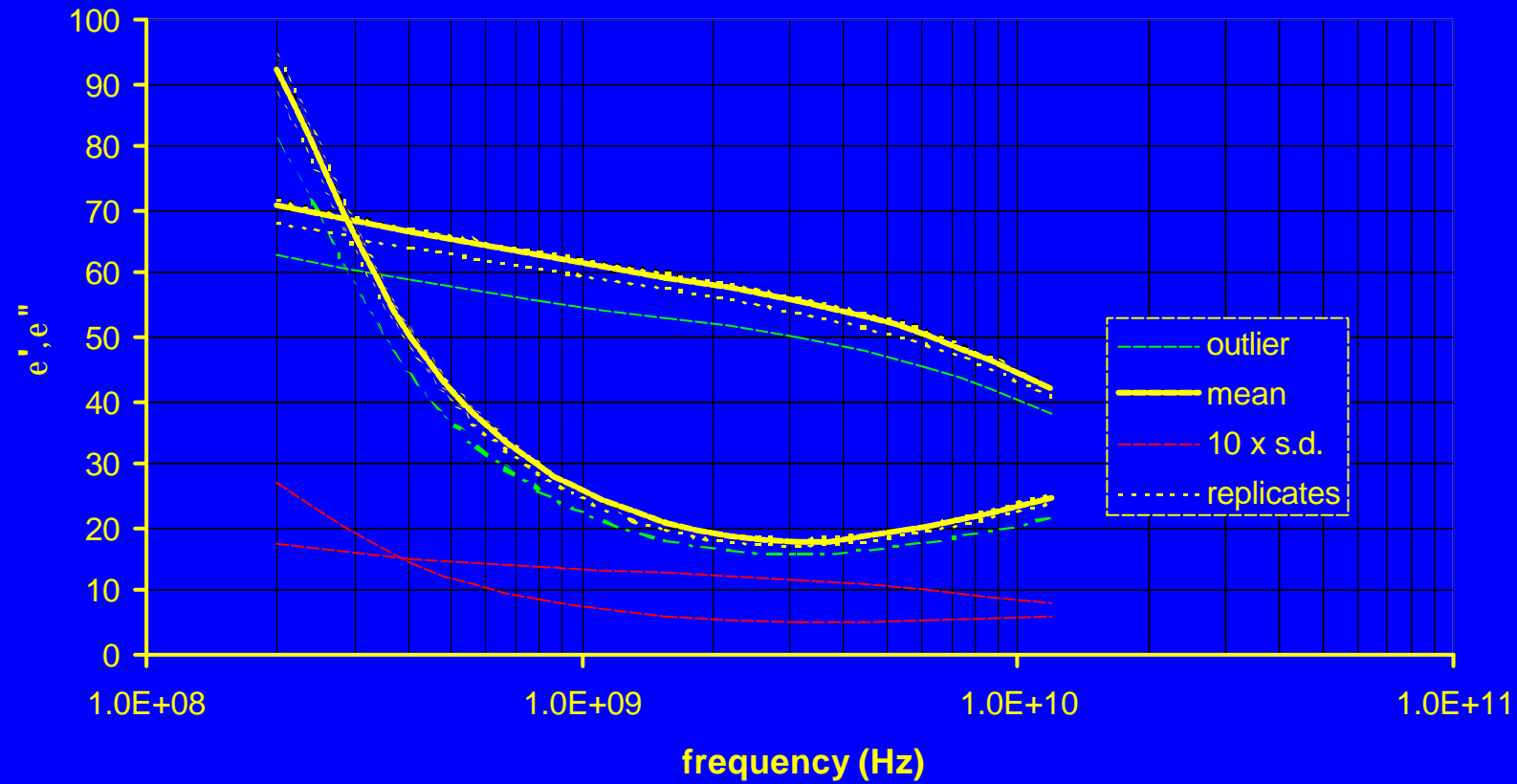
## Complex dielectric permittivity

$$\epsilon_f^* = \epsilon_f' - j\epsilon_f''$$

Dispersion, energy storage

Loss factor, energy dissipation

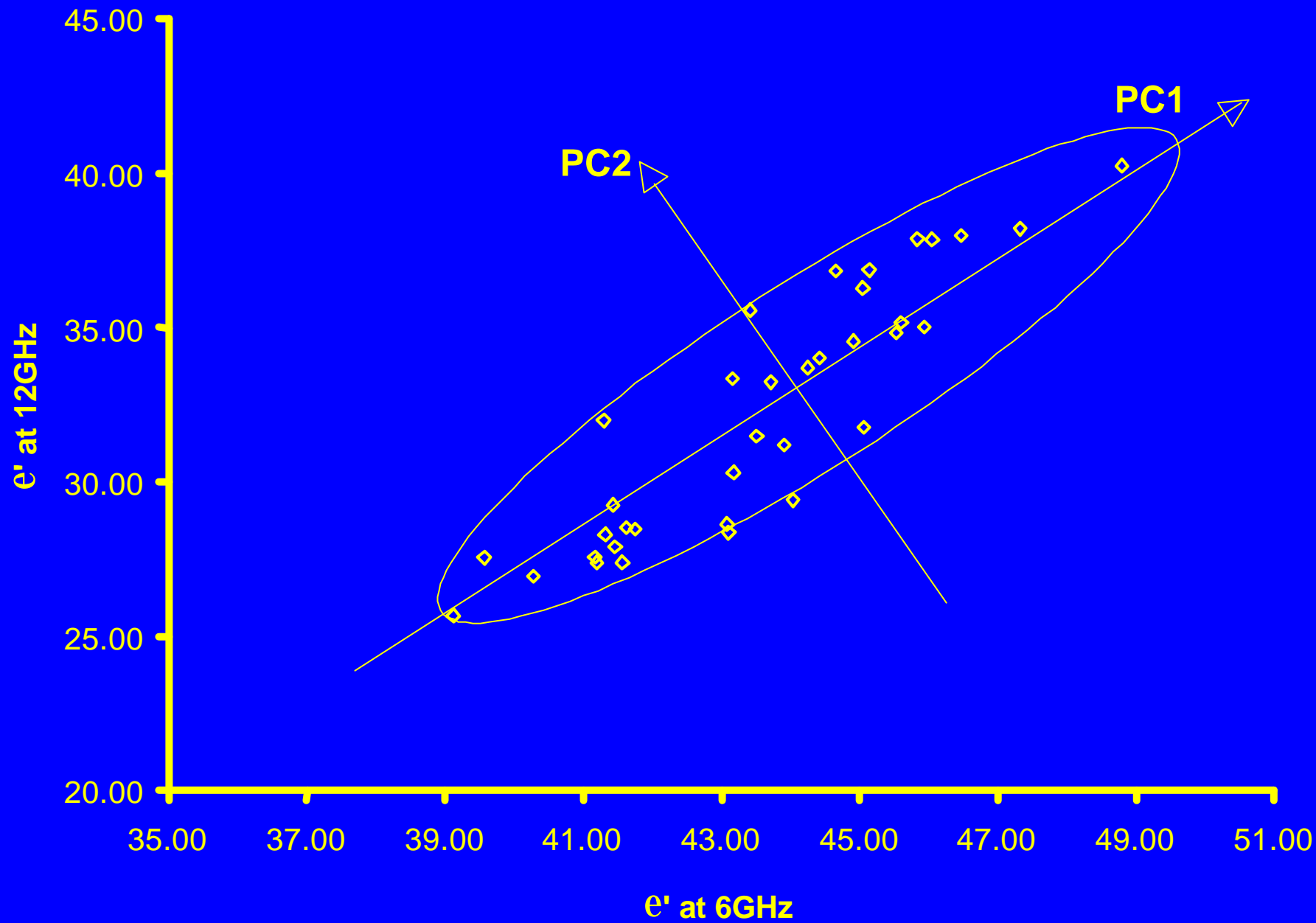
## Dielectric spectra for Chicken at 30°C: 2 hours in 2% polyphosphate



# Multivariate analysis

## Principal Component Analysis (PCA)

$$Y_j = c_{1j}X_1 + c_{2j}X_2 + \dots + c_{pj}X_p \dots$$



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Data reduction:  $n$  values of  $Y$  replace  $p > n$  values of  $X$

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## Principal component Regression (PCR)

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Data reduction:  $n$  values of  $Y$  replace  $p > n$  values of  $X$



## Principal component Regression (PCR)

$k$  responses  $y$ ,  $n$  Principal Components  $Y$

$$y_k = a_k + \sum_{i=1}^n b_{ki} Y_i$$

# Partial Least Squares Regression (PLSR)

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Similar to PCR but  $y$  values included in optimisation process.

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Similar to PCR but  $y$  values included in optimisation process.

- Construct linear combinations of inputs *incorporating*  $y$
- Finds directions with maximum variance and correlation with the output
- Partial least squares regression operates like principal component regression

- **Principal Components Regression**

- Regress on  $n < p$  principal components of  $X$

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  - Regress on  $n < p$  principal components of  $X$
- **Partial Least Squares Regression**
  - Regress on  $n < p$  directions of  $X$  weighted by  $y$

# **Artificial Neural Networks (ANN)**

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$$y = f(X, W)$$

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$X$  variables measured

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$W$  weighting vector or activation function

# **Artificial Neural Networks (ANN)**

Activation function of neurons



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Activation function of neurons:

linear-emulates PCR

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non-linear- more general

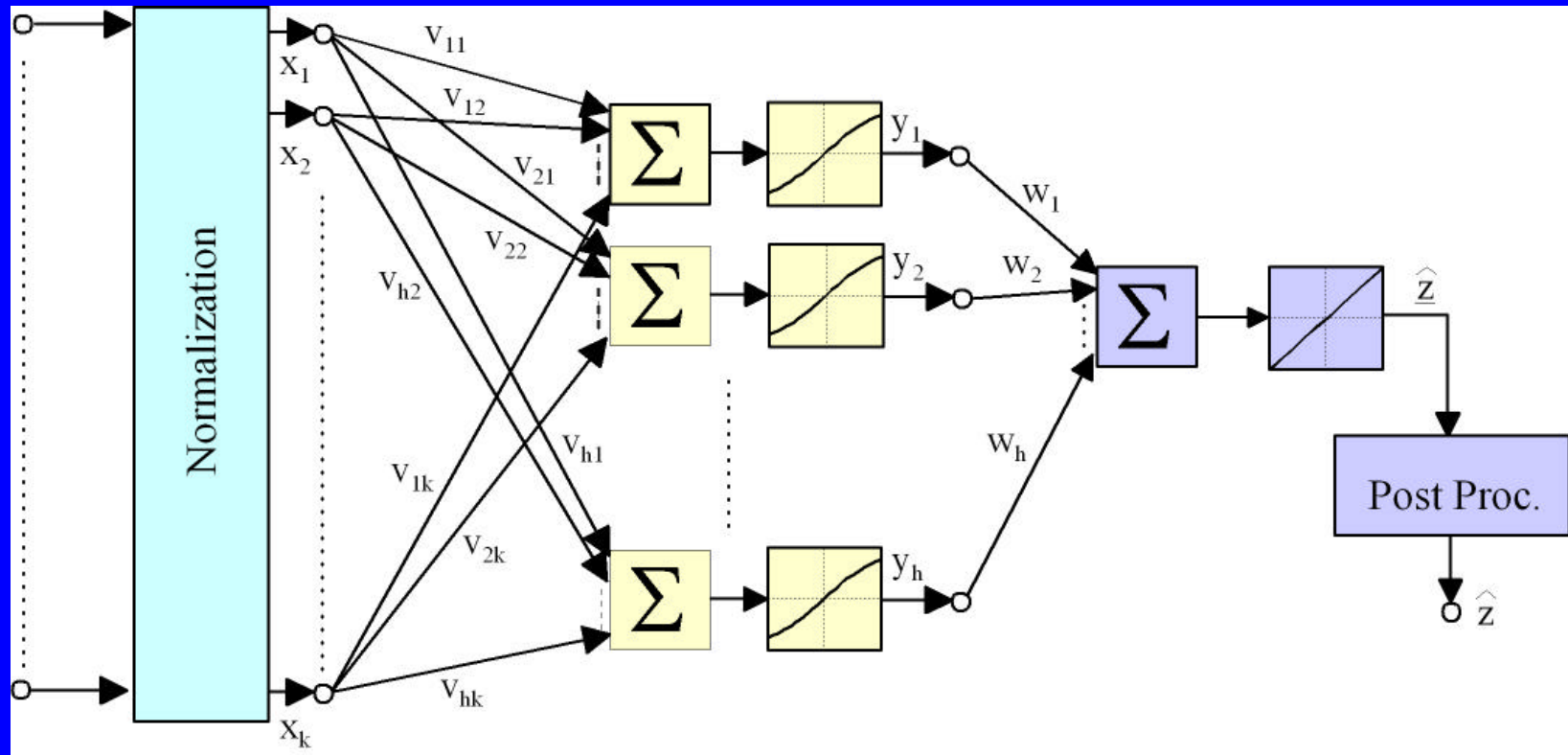
## Artificial Neural Networks (ANN)

Activation function of neurons:

linear-emulates PCR

non-linear- more general- sigmoid, tansig or logsig

$$\text{tansig}(n) = \frac{2}{1 + \exp(-2n)} - 1$$



## **Samples and data used**

chicken 1

calibration

144 samples measured in 1994; 72 controls, 72 treated.

validation

72 samples measured in 2000.

chicken 2

calibration

pooled data -106 validation samples.

validation

110 randomly selected samples.

prawns

calibration

152 samples

validation

16 samples prepared at a later date

pork

calibration

167 various types of treated pork, canned, bacon, ham and fresh

validation

18 unknown samples prepared at a later date; 4 leg meat, 4 streaky bacon, 4 ham and 6

**Some results**

	<b>R<sup>2</sup></b>	<b>PCR RMSE</b>	<b>RMSE</b>
		<b>c</b>	<b>v</b>
Chicken 1			
<b>Water</b>	57.0	1.15	0.57
<b>Protein</b>	64.1	1.23	0.79
<b>Added Water</b>	89.5	3.91	2.30
Chicken 2			
<b>Water</b>	69.3	0.75	0.70
<b>Protein</b>	69.0	0.96	0.99
<b>Added Water</b>	90.8	2.69	3.28
Prawns			
<b>Water</b>	82.6	0.65	0.82
<b>Fat</b>	36.8	0.09	0.08
<b>Protein</b>	89.1	0.58	0.92
<b>NaCl</b>	70.5	0.42	0.083
<b>Phosphate</b>	58.3	98.4	63.8
<b>Added Water</b>	74.6	3.06	3.81
Pork			
<b>Water</b>	94.2	1.53	1.43
<b>Fat</b>	95.3	1.59	1.63
<b>Ash</b>	88.6	0.24	0.20
<b>Protein</b>	66.3	1.78	1.38
<b>NaCl</b>	91.8	0.19	0.15
<b>Added Water</b>	54.4	7.60	5.90



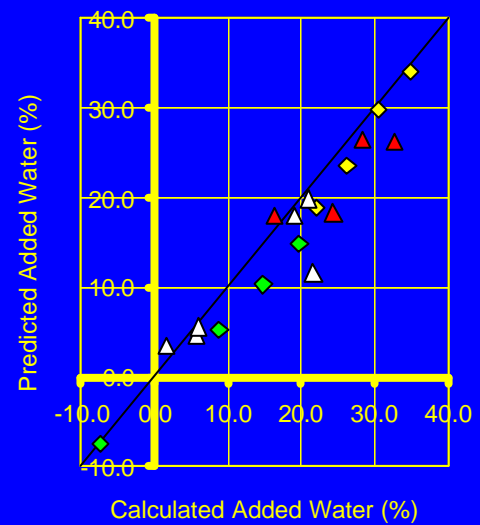
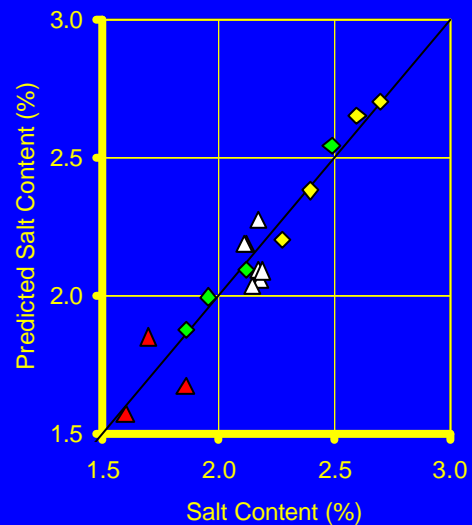
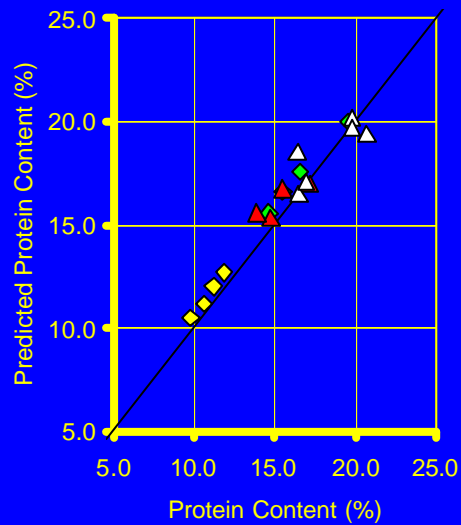
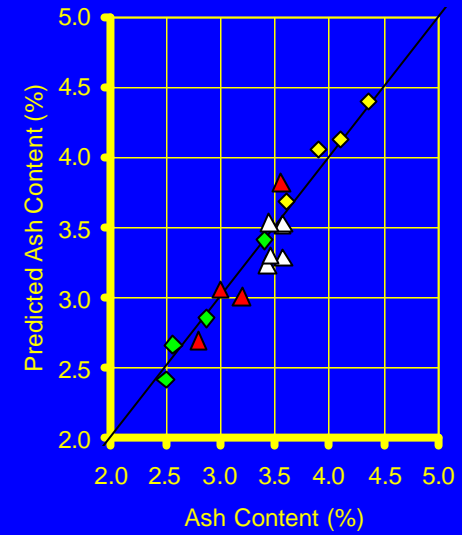
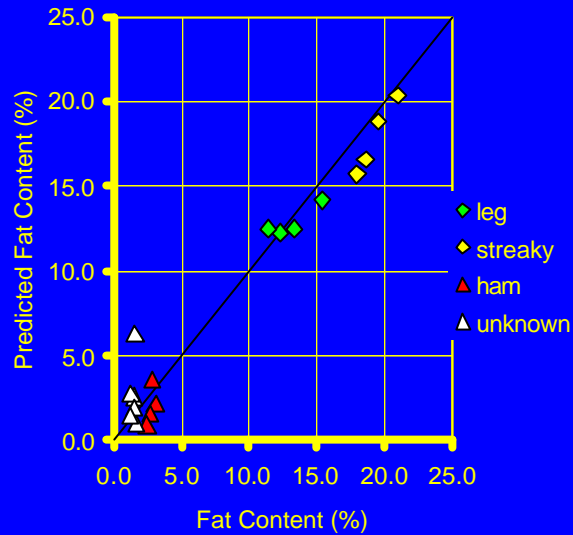
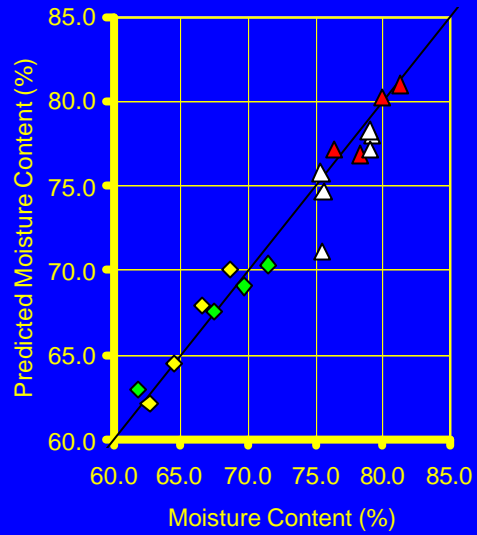
	R <sup>2</sup>	PCR		R <sup>2</sup>	PLSR	
		RMSE	RMSE		RMSE	RMSE
		c	v		c	v
Chicken 1						
<b>Water</b>	57.0	1.15	0.57	69.5	0.97	0.70
<b>Protein</b>	64.1	1.23	0.79	72.7	1.09	1.04
<b>Added Water</b>	89.5	3.91	2.30	90.8	3.66	2.86
Chicken 2						
<b>Water</b>	69.3	0.75	0.70	69.8	0.75	0.74
<b>Protein</b>	69.0	0.96	0.99	67.9	0.97	0.99
<b>Added Water</b>	90.8	2.69	3.28	91.9	2.53	3.30
Prawns						
<b>Water</b>	82.6	0.65	0.82	88.1	0.54	0.81
<b>Fat</b>	36.8	0.09	0.08	44.2	0.08	0.09
<b>Protein</b>	89.1	0.58	0.92	90.0	0.55	0.96
<b>NaCl</b>	70.5	0.42	0.083	83.4	0.031	0.092
<b>Phosphate</b>	58.3	98.4	63.8	58.9	97.6	63.8
<b>Added Water</b>	74.6	3.06	3.81	81.3	2.62	3.80
Pork						
<b>Water</b>	94.2	1.53	1.43	96.0	1.27	1.29
<b>Fat</b>	95.3	1.59	1.63	96.5	1.38	1.56
<b>Ash</b>	88.6	0.24	0.20	93.8	0.18	0.12
<b>Protein</b>	66.3	1.78	1.38	83.6	1.24	1.02
<b>NaCl</b>	91.8	0.19	0.15	94.0	0.17	0.087
<b>Added Water</b>	54.4	7.60	5.90	81.2	4.87	4.11

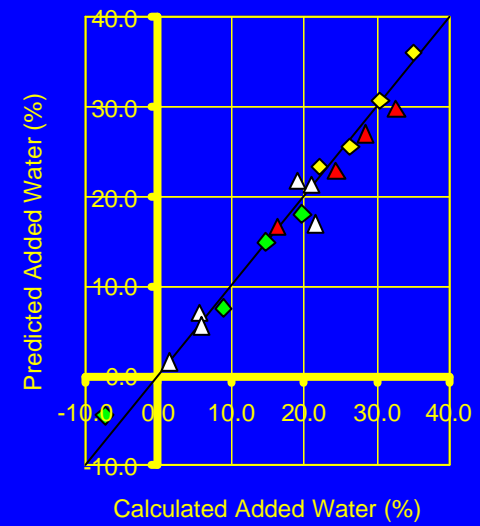
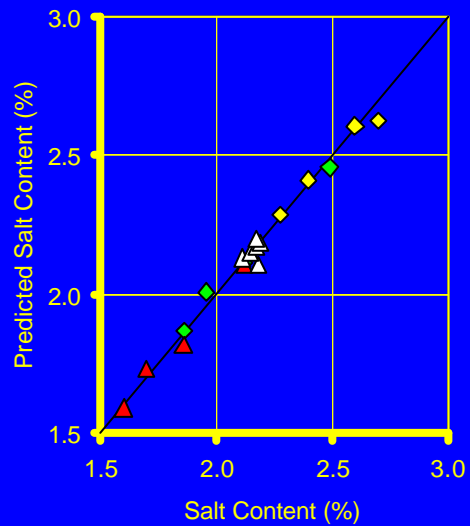
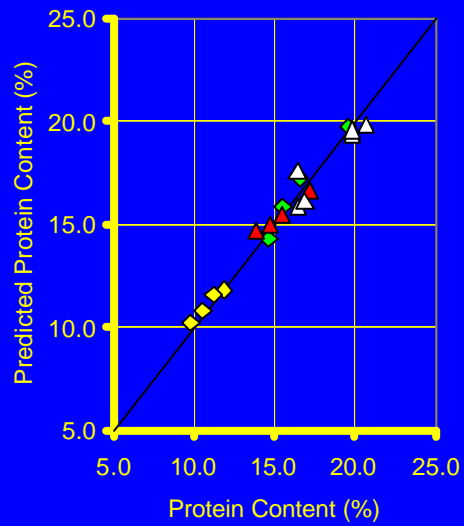
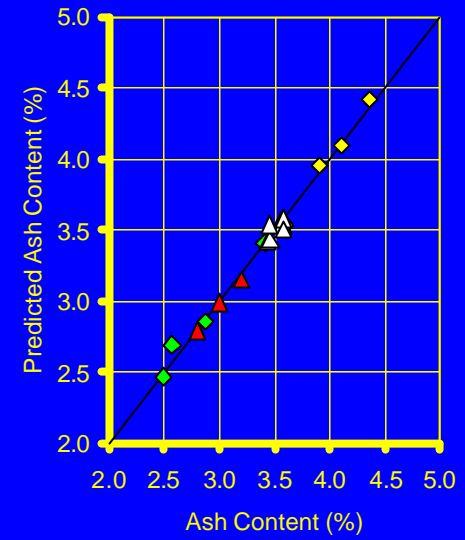
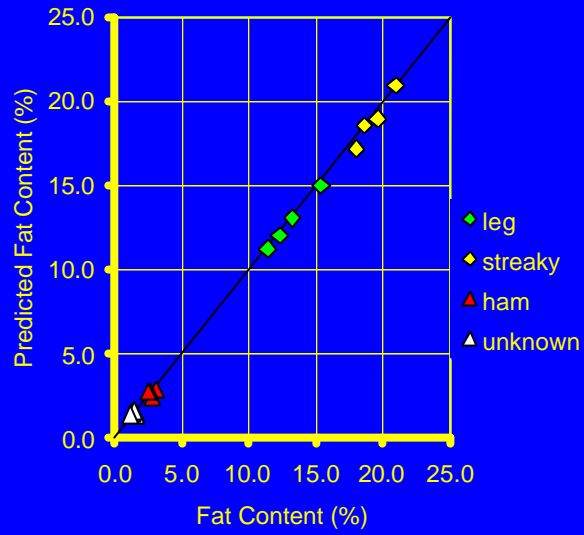
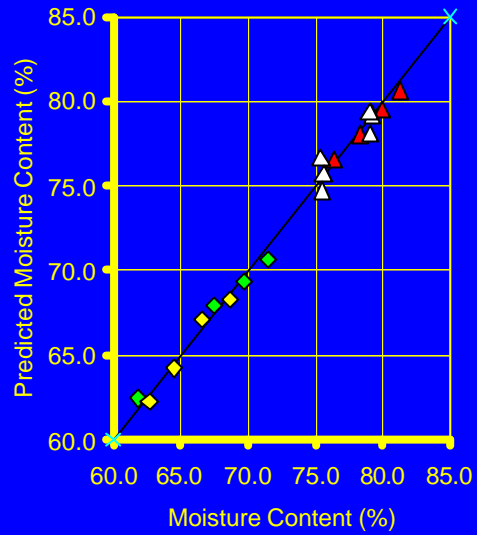
	R <sup>2</sup>	PCR		R <sup>2</sup>	PLSR		ANN (linear)		
		RMSE c	RMSE v		RMSE c	RMSE v	R <sup>2</sup>	RMS E <sub>c</sub>	RMS E <sub>v</sub>
Chicken 1									
<b>Water</b>	57.0	1.15	0.57	69.5	0.97	0.70	80.9	0.77	0.86
<b>Protein</b>	64.1	1.23	0.79	72.7	1.09	1.04	74.5	1.05	1.15
<b>Added Water</b>	89.5	3.91	2.30	90.8	3.66	2.86	92.6	3.29	5.35
Chicken 2									
<b>Water</b>	69.3	0.75	0.70	69.8	0.75	0.74	72.1	0.72	0.73
<b>Protein</b>	69.0	0.96	0.99	67.9	0.97	0.99	71.3	0.92	1.03
<b>Added Water</b>	90.8	2.69	3.28	91.9	2.53	3.30	91.2	2.64	3.25
Prawns									
<b>Water</b>	82.6	0.65	0.82	88.1	0.54	0.81	88.0	0.54	0.81
<b>Fat</b>	36.8	0.09	0.08	44.2	0.08	0.09	44.8	0.081	0.083
<b>Protein</b>	89.1	0.58	0.92	90.0	0.55	0.96	90.8	0.53	0.97
<b>NaCl</b>	70.5	0.42	0.083	83.4	0.031	0.092	75.5	0.038	0.088
<b>Phosphate</b>	58.3	98.4	63.8	58.9	97.6	63.8	60.9	95.2	67.3
<b>Added Water</b>	74.6	3.06	3.81	81.3	2.62	3.80	81.4	2.62	3.70
Pork									
<b>Water</b>	94.2	1.53	1.43	96.0	1.27	1.29	95.2	1.39	1.39
<b>Fat</b>	95.3	1.59	1.63	96.5	1.38	1.56	95.5	1.57	1.61
<b>Ash</b>	88.6	0.24	0.20	93.8	0.18	0.12	90.0	0.23	0.17
<b>Protein</b>	66.3	1.78	1.38	83.6	1.24	1.02	75.6	1.51	1.17
<b>NaCl</b>	91.8	0.19	0.15	94.0	0.17	0.087	92.5	0.19	0.12
<b>Added Water</b>	54.4	7.60	5.90	81.2	4.87	4.11	69.7	6.20	4.85

	R <sup>2</sup>	PCR		R <sup>2</sup>	PLSR		ANN (linear)			ANN(non-linear)		
		RMSE	RMSE		RMSE	RMSE	R <sup>2</sup>	RMS	RMS	R <sup>2</sup>	RMSE	RMSE
		c	v		c	v	E <sub>c</sub>	E <sub>v</sub>	c	v		
Chicken 1												
<b>Water</b>	57.0	1.15	0.57	69.5	0.97	0.70	80.9	0.77	0.86	87.2	0.63	0.64
<b>Protein</b>	64.1	1.23	0.79	72.7	1.09	1.04	74.5	1.05	1.15	74.9	1.04	0.77
<b>Added Water</b>	89.5	3.91	2.30	90.8	3.66	2.86	92.6	3.29	5.35	92.1	3.39	1.61
Chicken 2												
<b>Water</b>	69.3	0.75	0.70	69.8	0.75	0.74	72.1	0.72	0.73	83.5	0.55	0.60
<b>Protein</b>	69.0	0.96	0.99	67.9	0.97	0.99	71.3	0.92	1.03	77.2	0.82	0.99
<b>Added Water</b>	90.8	2.69	3.28	91.9	2.53	3.30	91.2	2.64	3.25	96.6	1.63	2.42
Prawns												
<b>Water</b>	82.6	0.65	0.82	88.1	0.54	0.81	88.0	0.54	0.81	78.4	0.73	0.62
<b>Fat</b>	36.8	0.09	0.08	44.2	0.08	0.09	44.8	0.081	0.083	7.6	0.11	0.06
<b>Protein</b>	89.1	0.58	0.92	90.0	0.55	0.96	90.8	0.53	0.97	94.4	0.42	0.74
<b>NaCl</b>	70.5	0.42	0.083	83.4	0.031	0.092	75.5	0.038	0.088	55.7	0.51	0.64
<b>Phosphate</b>	58.3	98.4	63.8	58.9	97.6	63.8	60.9	95.2	67.3	83.9	61.1	58.9
<b>Added Water</b>	74.6	3.06	3.81	81.3	2.62	3.80	81.4	2.62	3.70	80.2	2.70	2.45
Pork												
<b>Water</b>	94.2	1.53	1.43	96.0	1.27	1.29	95.2	1.39	1.39	98.6	0.74	0.59
<b>Fat</b>	95.3	1.59	1.63	96.5	1.38	1.56	95.5	1.57	1.61	98.6	0.88	0.67
<b>Ash</b>	88.6	0.24	0.20	93.8	0.18	0.12	90.0	0.23	0.17	97.5	0.12	0.05
<b>Protein</b>	66.3	1.78	1.38	83.6	1.24	1.02	75.6	1.51	1.17	82.5	0.82	0.60
<b>NaCl</b>	91.8	0.19	0.15	94.0	0.17	0.087	92.5	0.19	0.12	95.1	0.15	0.042
<b>Added Water</b>	54.4	7.60	5.90	81.2	4.87	4.11	69.7	6.20	4.85	90.3	3.50	2.73

	R <sup>2</sup>	PCR		R <sup>2</sup>	PLSR		ANN (linear)			ANN(non-linear)		
		RMSE	RMSE		RMSE	RMSE	R <sup>2</sup>	RMS	RMS	R <sup>2</sup>	RMSE	RMSE
		c	v		c	v	E <sub>c</sub>	E <sub>v</sub>	c	v		
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<b>Water</b>	57.0	1.15	0.57	69.5	0.97	0.70	80.9	0.77	0.86	87.2	0.63	0.64
<b>Protein</b>	64.1	1.23	0.79	72.7	1.09	1.04	74.5	1.05	1.15	74.9	1.04	0.77
<b>Added Water</b>	89.5	3.91	2.30	90.8	3.66	2.86	92.6	3.29	5.35	92.1	3.39	1.61
Chicken 2												
<b>Water</b>	69.3	0.75	0.70	69.8	0.75	0.74	72.1	0.72	0.73	83.5	0.55	0.60
<b>Protein</b>	69.0	0.96	0.99	67.9	0.97	0.99	71.3	0.92	1.03	77.2	0.82	0.99
<b>Added Water</b>	90.8	2.69	3.28	91.9	2.53	3.30	91.2	2.64	3.25	96.6	1.63	2.42
Prawns												
<b>Water</b>	82.6	0.65	0.82	88.1	0.54	0.81	88.0	0.54	0.81	78.4	0.73	0.62
<b>Fat</b>	36.8	0.09	0.08	44.2	0.08	0.09	44.8	0.081	0.083	7.6	0.11	0.06
<b>Protein</b>	89.1	0.58	0.92	90.0	0.55	0.96	90.8	0.53	0.97	94.4	0.42	0.74
<b>NaCl</b>	70.5	0.42	0.083	83.4	0.031	0.092	75.5	0.038	0.088	55.7	0.51	0.64
<b>Phosphate</b>	58.3	98.4	63.8	58.9	97.6	63.8	60.9	95.2	67.3	83.9	61.1	58.9
<b>Added Water</b>	74.6	3.06	3.81	81.3	2.62	3.80	81.4	2.62	3.70	80.2	2.70	2.45
Pork												
<b>Water</b>	94.2	1.53	1.43	96.0	1.27	1.29	95.2	1.39	1.39	98.6	0.74	0.59
<b>Fat</b>	95.3	1.59	1.63	96.5	1.38	1.56	95.5	1.57	1.61	98.6	0.88	0.67
<b>Ash</b>	88.6	0.24	0.20	93.8	0.18	0.12	90.0	0.23	0.17	97.5	0.12	0.05
<b>Protein</b>	66.3	1.78	1.38	83.6	1.24	1.02	75.6	1.51	1.17	82.5	0.82	0.60
<b>NaCl</b>	91.8	0.19	0.15	94.0	0.17	0.087	92.5	0.19	0.12	95.1	0.15	0.042
<b>Added Water</b>	54.4	7.60	5.90	81.2	4.87	4.11	69.7	6.20	4.85	90.3	3.50	2.73

# **Comparison of PCR and ANN**





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