

## LIST OF FIGURES

Figure		Page
1	Fish sauce production .....	6
2	An overview of the electromagnetic spectrum .....	14
3	Principle of NIR measurement .....	15
4	NIR measuring modes .....	16
5	Flow diagram of NIR calibration and validation process .....	18
6	Principal component decomposition. The new axes called principal components ( $PC_i$ ) are linear combinations of the original variables ( $X_i$ ), calculated so that the first PCs point in the direction of greatest dispersion of the samples.....	23
7	Scheme for explanation of Principal Components Analysis (PCA). PCA is based on a decomposition of the data matrix $\mathbf{X}$ into two matrices $\mathbf{V}$ and $\mathbf{U}$ . The matrix $\mathbf{V}$ is usually called the loadings matrix, and the matrix $\mathbf{U}$ is called the scores matrix.....	24
8	Scheme for explanation of Factor Analysis (FA). FA is based on a decomposition of the data matrix $\mathbf{X}$ into two matrices $\mathbf{V}$ and $\mathbf{U}$ . The matrices $\mathbf{U}$ and $\mathbf{V}$ are called scores and loading matrices, respectively.....	26
9	PLS component decomposition. PLS models are based on principal components of both the independent data $\mathbf{X}$ and the dependent data. $\mathbf{Y}$ . The matrices $\mathbf{t}$ and $\mathbf{u}$ are the principal component scores of the $\mathbf{X}$ and the $\mathbf{Y}$ data matrix. A regression set up between both scores called PLSR model.....	28
10	Scheme for explanation of Partial least squares (PLS) regression. The matrix $\mathbf{X}$ is decomposed into a matrix $\mathbf{T}$ (the score matrix) and a matrix $\mathbf{P}'$ (the loadings matrix) plus an error matrix $\mathbf{E}$ . The matrix $\mathbf{Y}$ is decomposed into $\mathbf{U}$ and $\mathbf{Q}$ and the error term $\mathbf{F}$ . These two equations are called <i>outer relations</i> . The goal of the PLS algorithm is to minimize the norm of $\mathbf{F}$ while keeping the correlation between $\mathbf{X}$ and $\mathbf{Y}$ by the <i>inner relation</i> $\mathbf{U} = \mathbf{BT}$ .....	29

### LIST OF FIGURES (continued)

Figure		Page
11	Scheme for explanation of MWPLSR. The sums of squared residuals (SSR) are calculated with the PLS models; $SSR_i = (y_i - X_i \hat{b}_i)^t (y_i - X_i \hat{b}_i)$ . Log(SSR) is plotted as a function of the position of the window.....	31
12	Scheme for explanation of SCMWPLS.....	32
13	The boundaries are obtained by linear discriminant function.....	34
14	SIMCA classification of two classes as shown in the soft modeling representation of the data. SIMCA uses PCA as a starting point. An unknown sample is identified by its position within a class.....	35
15	KNN classification (a) 1-NN classification, (b) 3-NN Classification. An unknown object $u$ is classified in the group which the object's nearest neighbor belong.....	37
16	Architectures of (a) biological neurons and (b) artificial neural networks .....	38
17	Block diagram of quantitative modeling process for chemical and physical properties.....	42
18	Block diagram of classification modeling process.....	44
19	Block diagram for prediction of chemical and physical properties with developed SCMWPLS models using NIR spectra.....	52
20	Block diagram of quantitative modeling process for sensory properties .....	54
21	NIR transfectance spectra of 100 Thai fish sauce samples. (a) the NIR region of 1100-2500 nm and (b) the NIR region of 1100-1900 and 2000-2440 was used for chemometric analysis.....	59
22	Residue lines for total nitrogen content of Thai fish sauces obtained by moving window partial least square regression (MWPLSR). The shade areas are final informative regions.....	60
23	Residue lines for chemical and physical parameters of Thai fish sauces obtained by moving window partial least squares regression (MWPLSR). The shade areas are final informative regions.....	62

### LIST OF FIGURES (continued)

Figure		Page
24	The average NIR transfectance in the spectra region of 2264-2428 nm corresponding to the total nitrogen content for three groups of Thai fish sauces.....	77
25	Three groups scatter plots obtained by the Linear Discriminant Analysis (LDA) classified model (□: standard pure fish sauces (SPF), ●: standard mixed fish sauces (SMF), Δ: out of standard fish sauces (OF)).....	79
26	Factor loadings for the first two factors extracted from the NIR region of 2264-2428 nm using factor analysis; (a) Factor 1 and (b) Factor 2. The extraction and rotation methods used in factor analysis were principal component analysis and Varimax with Kaiser Normalization methods, respectively.....	81
27	Factor score coefficients based on the first two factors extracted from the NIR region of 2264-2428 nm using factor analysis; (a) Factor 1 and (b) Factor 2. The extraction and rotation methods used in factor analysis were principal component analysis and Varimax with Kaiser Normalization methods, respectively.....	82
28	Distribution of 100 fish sauce sample based on factor scores of the first two factors calculated from the spectra region of 2264-2428 nm ( □: standard pure fish sauces, ●: standard mixed fish sauces, Δ: out of standard fish sauces).....	83
29	Three groups scatter plots obtained by the Factor Analysis- Linear Discriminant Analysis (FALDA) classified model ( □: standard pure fish sauces (SPF), ●: standard mixed fish sauces (SMF), Δ: out of standard fish sauces (OF)).....	85
30	Cooman's plot of the classification models performed on the region of 2264- 2428 nm using the test set (n=20); □: standard pure fish sauces, ○: standard mixed fish sauces, Δ : out of standard fish sauces.....	88

### LIST OF FIGURES (continued)

Figure		Page
31	Corrective classification rate versus K(from K=1 to K=15).....	89
32	Diagram showing the network structure with 83 wavelength input variables. This is a network comprising four hidden neurons and a single output neuron. Transfer functions ( $f_i$ ) for hidden and output layers are LOGSIG ( $f_1$ ) and PURELIN ( $f_2$ ), respectively. The weights to layer from input ( $W_i$ ) are given in an Appendix C.....	92
33	The sensory profiles of Thai pure fish sauce and mixed fish sauce based on generic descriptive analysis test. The distance from the center is the mean value for the attributes.....	101
34	Clustering of 20 fish sauces based on their sensory properties (P, pure fish sauce; M, mixed fish sauce) using cluster analysis.....	103
35	Scores for the twenty fish sauce samples and correlation coefficients of the fifteen sensory attributes with principal component 1 and 2. (P, pure fish sauce; M, mixed fish sauce).....	105
36	Scores for the twenty fish sauce samples and correlation coefficients of the fifteen sensory attributes with principal component 1 and 3. (P, pure fish sauce; M, mixed fish sauce.....	106
37	NIR tranflectance spectra of 20 Thai commercial fish sauce samples.....	108
38	NIR spectra loadings for the first two principal components performed by principal component analysis (PCA).....	109
39	Scores for the twenty fish sauce samples and correlation coefficients of the sensory attributes and NIR spectra with principal component 1 and 2. (P, pure fish sauce; M, mixed fish sauce).....	112
40	Scores for the twenty fish sauce samples and correlation coefficients of the sensory and chemical attributes with principal component 1 and 2. (P, pure fish sauce; M, mixed fish sauce).....	118

## LIST OF FIGURES (continued)

Figure	Page
41 Scores for the twenty fish sauce samples and correlation coefficients of the sensory and physical attributes with principal component 1 and 2. (P, pure fish sauce; M, mixed fish sauce).....	123
42 Residue lines for brown color of Thai fish sauces obtained by moving window partial least squares regression (MWPLSR). The shade areas are final informative regions.....	128
43 Residue lines for five aromatic descriptors of Thai fish sauces obtained by moving window partial least squares regression (MWPLSR). The shade areas are final informative regions. (a) sweet aromatic, (b) caramelized aromatic, (c) fermented aromatic, (d) fishy aromatic, and (e) musty aromatic.....	129
44 Residue lines for four taste descriptors of Thai fish sauces obtained by moving window partial least squares regression (MWPLSR). The shade areas are final informative regions. (a) sweet taste, (b) salty taste, (c) bitter taste, and (d) umami taste.....	132
45 Residue lines for three aftertaste descriptors of Thai fish sauces obtained by moving window partial least squares regression (MWPLSR). The shade areas are final informative regions. (a) sweet aftertaste, (b) salty aftertaste, and (c) bitter aftertaste.....	135
46 Residue lines for two flavor descriptors of Thai fish sauces obtained by moving window partial least squares regression (MWPLSR). The shade areas are final informative regions. (a) caramelized flavor and (b) fishy flavor.....	137
 <b>Appendix Figure</b>	
B1 NIR instrument was used in this study (a) an InfraAlyzer 500 spectrometer and (b) a 0.3 mm British cup.....	172