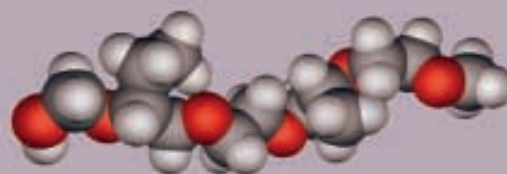


Designing a Better Detergent

Multivariate QSAR techniques were used to characterise non-ionic surfactants and then to design new detergents with improved properties.

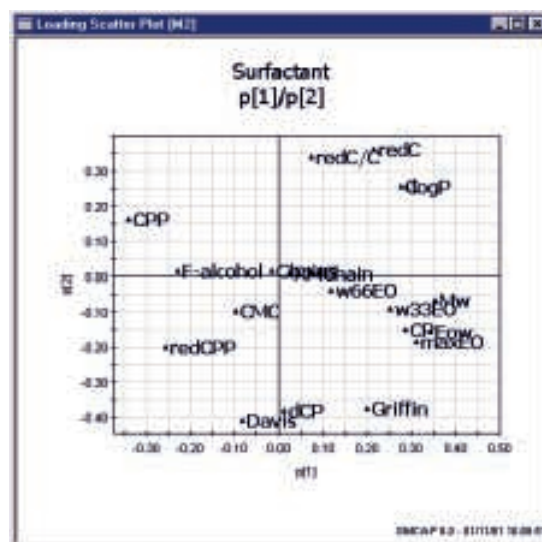
The aim of the study was to find a surfactant with good washing performance but without undesirable toxicity or biodegradability. Non-ionic surfactants typically consist of ethoxylated fatty alcohols. These surfactants are manufactured using a polymerisation process that gives a distribution of chain lengths (technical blends) rather than single compounds.



1. Multivariate Characterisation

To characterise the detergents a number of physico-chemical descriptors were chosen as well as some HPLC chromatographic parameters. The latter described the ethylene oxide content and the molecular weight distribution of the surfactant blend.

Principal Component Analysis (PCA) of 38 surfactant blends with 19 descriptors gave two components. The first principal component was related to surfactant lipophilicity while the second component reflected the hydrophobic/hydrophilic balance (Fig 1).



PCA of detergent physical properties.

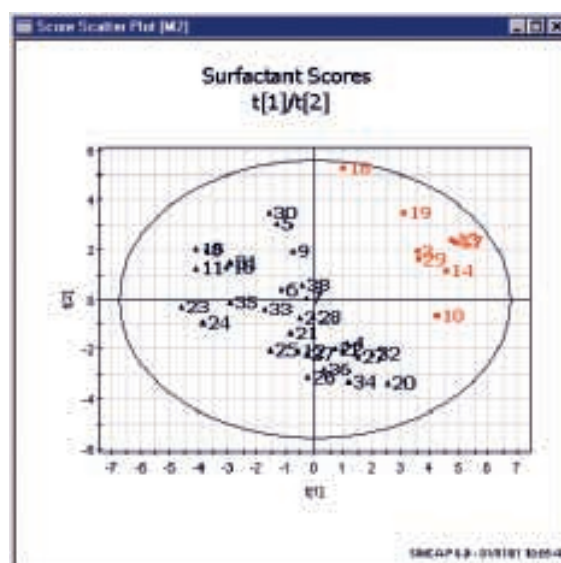
2. Detection of Clusters

A grouping of highly lipophilic surfactants was located in the upper right hand area (Fig 2). These were found to be too lipophilic for the objective and so were removed from the model and a new PCA model computed.

3. Selection of molecules for testing

The scores from the second PCA model were used to select 10 representative surfactants for further testing. The responses measured in the tests were:

- YDet:** % removed soil
- YConc:** optimal washing concentration
- YTemp:** optimal wash temperature
- YTox:** (LC₅₀) acute toxicity towards a fairy shrimp



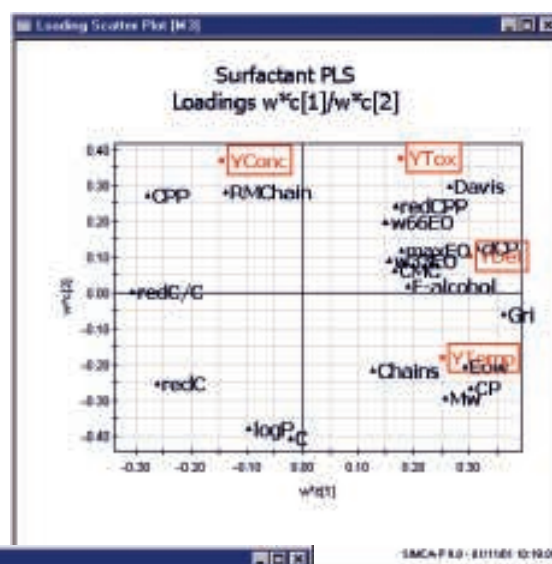
PCA Score plot showing a group of lipophilic compounds

4. Assessing the influence of molecular parameters

A *Partial Least Squares Regression (PLS)* model was built using the test results as the Y matrix. Interpretation of the model showed the relationship between the molecular properties and each of the Y variables.

A reliable model was used to make predictions, which identified the most promising area in multivariate space where surfactants with the best properties could be found.

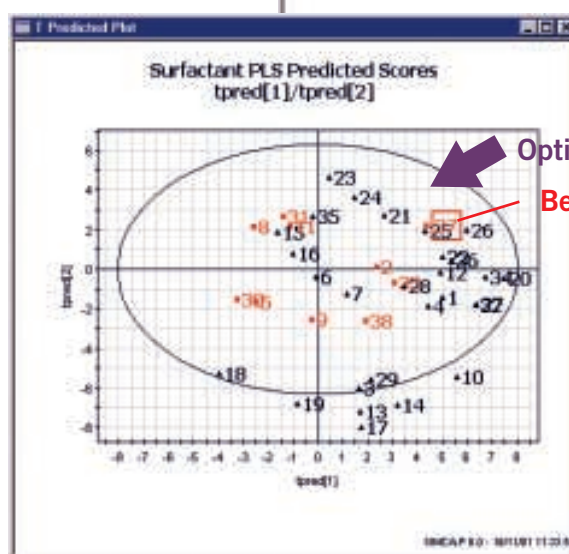
Predictions were made on the **28 non-tested surfactants** and structures with the most potential were identified for further testing.



5. Product Optimisation

The optimisation of surfactants continued until a final product was identified. This approach was so successful that it has recently been repeated on another set of novel compounds.

This research was carried out at AKZO Nobel, Surface Chemistry, Stenungsund, Sweden. Details may be found in the paper by Lindgren, Å., Sjöström, M., and Wold, S (1996) *Quantitative Structure-Effect Relationships for some Technical Non-ionic Surfactants*, JAOCS, 7, 863-875.



Plots superimposing responses and factors.

Optimum region
Best tested

Plot showing training set and prediction set.

Conclusions

- Principal Component Analysis can overview molecular property data and identify clusters and groups.
- The scores from PCA are useful to select representative molecules for testing, ensuring maximum chemical diversity and minimising the number of compounds that need to be tested.
- Partial Least Squares Regression (PLS) can be used to model biological responses/product performance and make predictions for untested molecules. In this way multivariate techniques can help you reduce costs, time and resources.

SIMCA-P is our state-of-the-art “point and click” software for multivariate modelling and analysis. Huge data sets are quickly reduced to a few informative graphs.



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