NeuroDeveloper™
Software designed for the
Classification of Spectroscopic Data
with Artificial Neural Networks

Amazing where you can go in:
spectroscopic imaging
pharmaceutical research
biotechnology
combinatorial chemistry
process control
quality control
Use the 4 integrated software modules for spectroscopic data evaluation.
FeatureDeveloper

Extensive Data-Preprocessing Tools

Graphical Display
Interactive Spectra Control

Feature Selection and data preprocessing
FeatureDeveloper

- treat your spectra with various preprocessing techniques

- perform a wavelength selection using univariate and multivariate criteria

- compress spectra with the Wavelet transform or Principal Component Analysis

- combine different techniques of data pretreatment, wavelength selection and compression

- display spectra and various results from data preprocessing and wavelength selection

- optimize the feature selection procedure using a rapid pretest for class separability

- get a full report of data preprocessing steps and selected wavelengths

- direct access to Bruker OPUS files, JCAMP or ASCII format
NeuroSimulator

ANN training and monitoring the training process
- monitor the training a validation process graphically

- classify your spectra with one of the most powerful training algorithms for neural networks (Rprop)

- compare the efficiency of different ANN architectures

- automate the extensive search of the most appropriate ANN architecture

- use the automation procedure to statistically evaluate your ANN setup

- use the backtracking option to reset a ANN to any user defined training cycle
**NeuroSimulator**

Network setup and automated network optimization

<table>
<thead>
<tr>
<th>Layer</th>
<th>From</th>
<th>To</th>
<th>stepsize</th>
<th>Activation function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Input layer</td>
<td>50</td>
<td>110</td>
<td>1</td>
<td>Available: 110</td>
</tr>
<tr>
<td>Hidden layer 1</td>
<td>5</td>
<td>15</td>
<td>1</td>
<td>Logistic-function</td>
</tr>
<tr>
<td>Hidden layer 2</td>
<td></td>
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<tr>
<td>Hidden layer 3</td>
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<tr>
<td>Hidden layer 4</td>
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<tr>
<td>Output layer</td>
<td></td>
<td></td>
<td></td>
<td>Logistic-function</td>
</tr>
</tbody>
</table>

- # Hidden layers: 1
- Random weight initialization from -1 and 1
- Try # initializations: 100
- File: Test_automation1
- Combinators: 1/67100

![NeuroSimulator GUI](image)
ModuleDeveloper

add individual ANNs graphically to a complex hierarchy and modular library
ModuleDeveloper

- decompose complex and large scale classification tasks gradually
  by building hierarchical organized, multiple neural networks with individual
  and optimized data preprocessing

- combine and connect multiple neural networks of any degree of complexity to
  one library for evaluation with the graphical interface. No programming is needed.
Classification

Classify unknown spectra
Classification

- evaluate single ANNs or hierarchical libraries using an arbitrary amount of unknown spectra
- get access to every classification level in hierarchical neural networks
- create a detailed report and documentation of the classification results
- interfacing the Bruker OPUS™ software for data evaluation and Imaging based on NeuroDeveloper™ ANNs.
- access full compatibility for macros, image display and reports in OPUS™ in data evaluation with NeuroDeveloper™ ANNs
Innovative Solutions for Today`s Challenges in Chemometrics

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