

NeuroDeveloper™

Software designed for the

Classification of Spectroscopic Data

with Artificial Neural Networks

**Amazing where
you can go in :**

spectroscopic imaging

pharmaceutical research

biotechnology

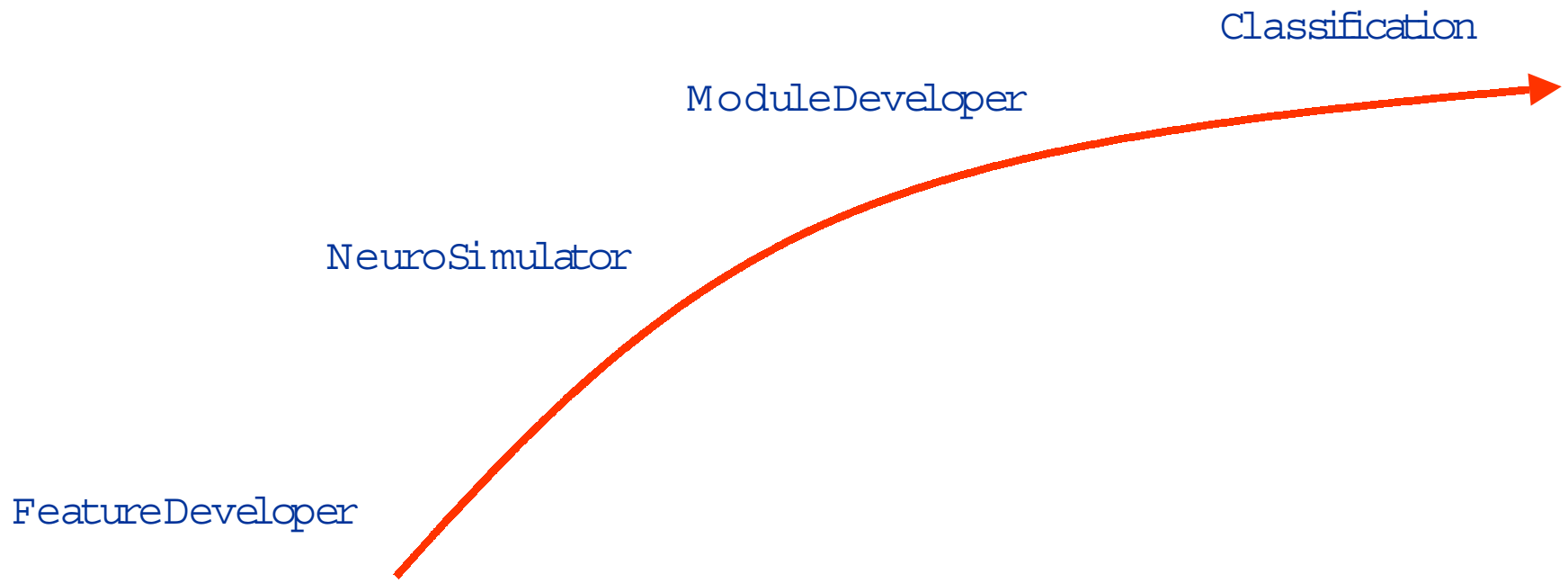
combinatorial chemistry

process control

quality control

Use the 4 integrated software modules

for spectroscopic data evaluation

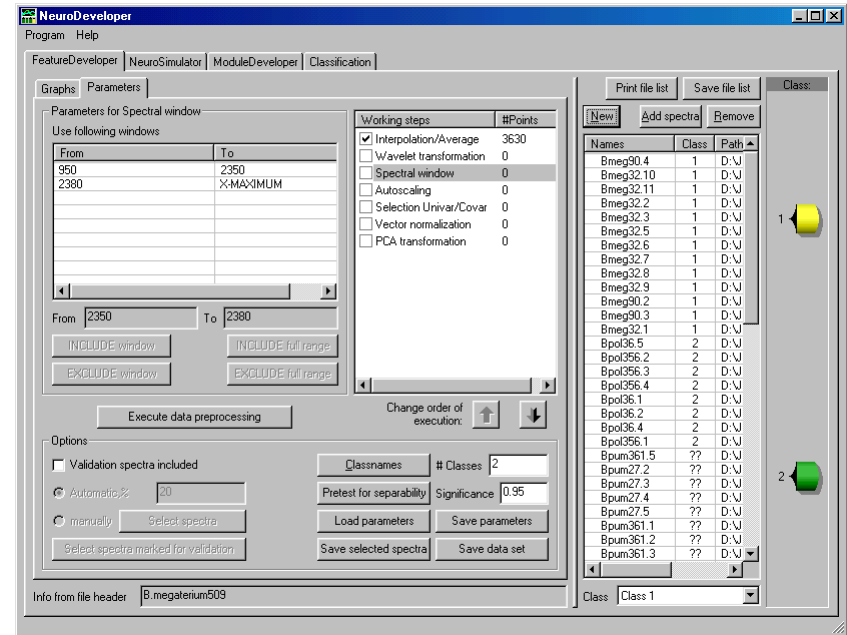
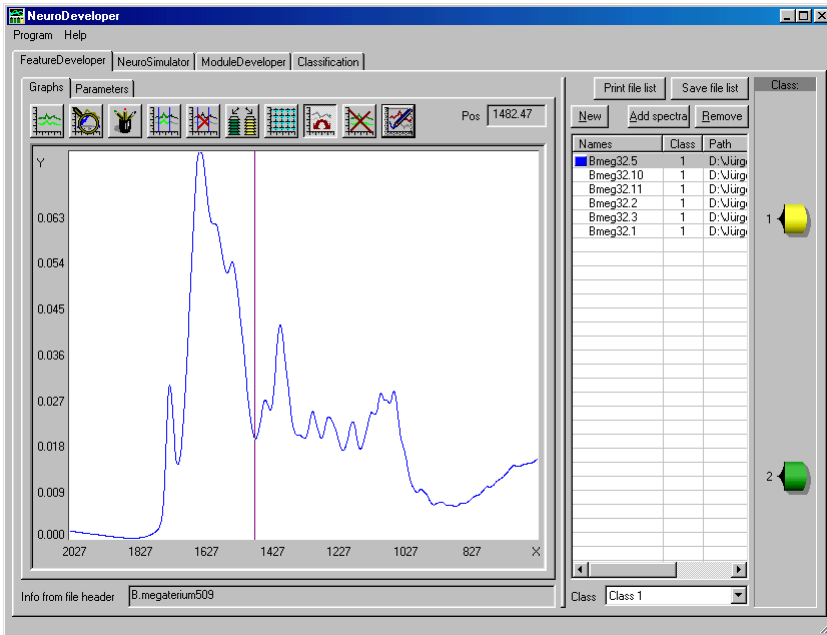


FeatureDeveloper

Extensive Data-Preprocessing Tools

Graphical Display
Interactive Spectra Control

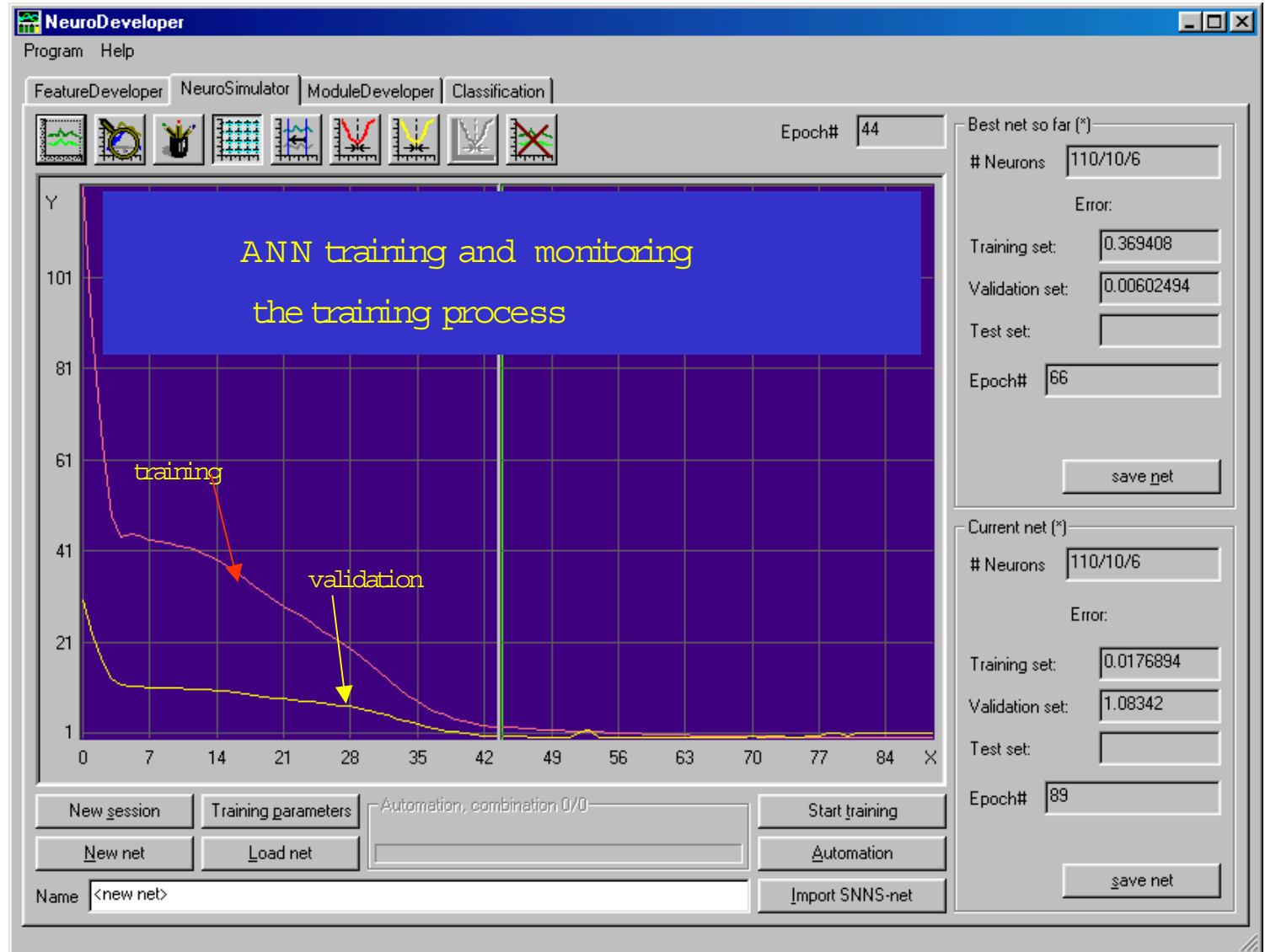
Feature Selection
and data preprocessing



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



NeuroSimulator

- 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

The screenshot displays the NeuroDeveloper software interface. The main window shows a graph with a purple bar chart and a yellow line graph. Overlaid on this is the 'Automation' dialog box, which is used for configuring a neural network. The dialog box contains a table for layer configuration, checkboxes for 'Random weight initialization' and 'Shortcut connections', and a 'Try # initializations' field. A blue callout box on the left contains the text 'Network setup and automated network optimization' with red arrows pointing to the layer configuration table and the 'Try # initializations' field. The background window shows the 'NeuroSimulator' tab selected, with a toolbar and a status bar indicating 'Epoch# 52' and 'Best net so far (*)' with a neuron count of '110/10/6' and an error of '0.219747'.

Automation

Layer:	From	To	stepsize	Activation function
Input layer	50	110	1	Available: 110
Hidden layer 1	5	15	1	Logistic-function
Hidden layer 2				
Hidden layer 3				
Hidden layer 4				
Output layer		6		Logistic-function

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

Buttons: New automation, Load automation, Start training, Cancel

Network setup
and automated
network optimization

ModuleDeveloper

The screenshot shows the NeuroDeveloper software interface. The window title is "NeuroDeveloper". The menu bar includes "Program" and "Help". The main window has tabs for "FeatureDeveloper", "NeuroSimulator", "ModuleDeveloper", and "Classification".

The main area displays a hierarchical tree structure under "Bacteria_Ident". The tree includes the following categories and species:

- Bacillus Species
 - B. megaterium
 - B. polymyxa
 - B. pumilus
 - B. simplex
 - B. spaericus
 - B. subtilis (highlighted)
- Pseudomonads. spezies
 - P. acidovorans
 - P. aeromonas
 - P. auricula
 - P. cepacia
 - cepacia 10856
 - cepacia 17765
 - cepacia 25416
 - cepacia 25608
 - cepacia 27515
 - cepacia 39356
 - P. delafieldii
 - P. diminuta
 - P. fluorescens
 - P. maltophilia
 - P. palleroni
 - P. pseudoalc.
 - P. testosteroni
- Genera Staphylococcus

Four red arrows point from a central blue text box to the "B. subtilis", "Pseudomonads. spezies", "P. cepacia", and "Genera Staphylococcus" nodes in the tree.

The central blue text box contains the following text:

add individual ANNs
graphically to a complex
hierarchy and modular library

On the right side of the interface, there is an "Options" panel with the following buttons:

- New top level net
- Load subnet
- Delete subnet
- Save net

At the bottom of the window, there are two input fields:

- Class name: B. subtilis
- Net name: Pseudomonads. spezies

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

The screenshot displays the NeuroDeveloper software interface, specifically the Classification module. The interface is divided into several sections:

- Graph (Left):** A bar chart showing the distribution of spectra across different classes. The x-axis represents the percentage of spectra (0 to 100%), and the y-axis represents the number of spectra (No.). A yellow bar highlights a specific class, and a red arrow points to it from the callout box.
- Table (Right):** A table listing the classified spectra, including their names, classes, classifications, and paths.
- Control Panel (Bottom):** A panel for configuring the classification process, including fields for the selected class, evaluation method, and subnetwork.

Table Data:

Names	Class	Classification	Path
Bmeg32.10	1.1	B. megaterium	D:\Würgen\usa...
Bmeg32.11	1.1	B. megaterium	D:\Würgen\usa...
Bmeg90.10	1.1	B. megaterium	D:\Würgen\usa...
Bmeg90.11	1.1	B. megaterium	D:\Würgen\usa...
Bpol356.10	1.2	B. polymyxa	D:\Würgen\usa...
Bpol356.11	1.2	B. polymyxa	D:\Würgen\usa...
Bpol36.10	1.2	B. polymyxa	D:\Würgen\usa...
Bpol36.111	1.2	B. polymyxa	D:\Würgen\usa...
Bpum27.10	1.3	B. pumilus	D:\Würgen\usa...
Bpum361.10	1.3	B. pumilus	D:\Würgen\usa...
Bpum361.11	1.3	B. pumilus	D:\Würgen\usa...
Bsim1321.10	1.4	B. simplex	D:\Würgen\usa...
Bsim1322.10	1.4	B. simplex	D:\Würgen\usa...
Bsim1322.11	1.4	B. simplex	D:\Würgen\usa...
Bsim1323.10	1.4	B. simplex	D:\Würgen\usa...
Bsim1323.11	1.?	<failed>	D:\Würgen\usa...
Bsim1323.12	1.4	B. simplex	D:\Würgen\usa...
Bsph28.10	1.5	B. spaericus	D:\Würgen\usa...
Bsph28.11	1.5	B. spaericus	D:\Würgen\usa...
Bsph396.10	1.5	B. spaericus	D:\Würgen\usa...
Bsph396.11	1.5	B. spaericus	D:\Würgen\usa...
Bsub10.10	1.6	B. subtilis	D:\Würgen\usa...
Bsub1089.10	1.6	B. subtilis	D:\Würgen\usa...
Bsub1090.11	1.6	B. subtilis	D:\Würgen\usa...
Bsub675.10	1.6	B. subtilis	D:\Würgen\usa...

Control Panel:

- Info: B.polymyxa36
- Extrapolation (%): 100
- Evaluation: B. polymyxa
- WTA:
- 402040:
- Subnet: Bacillus Species
- Net topology:
- Class names:

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



NEW

- interfacing the Bruker OPUS TM software for data evaluation and Imaging based on NeuroDeveloper TM ANNs.
- access full compatibility for macros, image display and reports in OPUS TM in data evaluation with NeuroDeveloper TM ANNs

Innovative Solutions for Today`s Challenges in Chemometrics

Fore more information contact

in Europe

Synthon KG

Analytics and pattern recognition

Karl-Christ-Str. 39

69118 Heidelberg

Germany

email: info@synthon-analytics.com

www.synthon-analytics.com

Phone: +49 -(0)- 6221-893372

in USA

Bruker Optics Inc.

19 Fortune Drive

Manning Park

Billerica, MA 01821

USA

sales@bruker.com

www.bruker.com/optics

(978) 667-9580