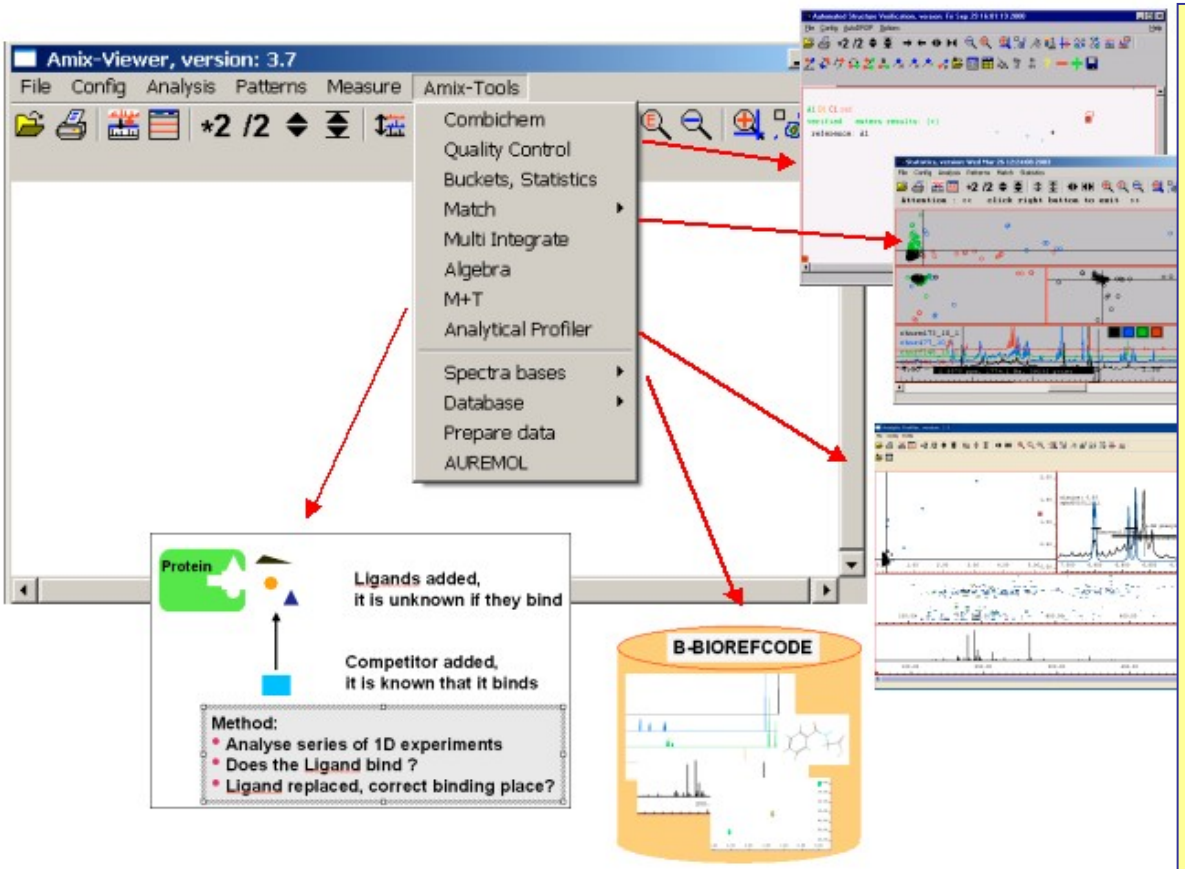
# AMIX

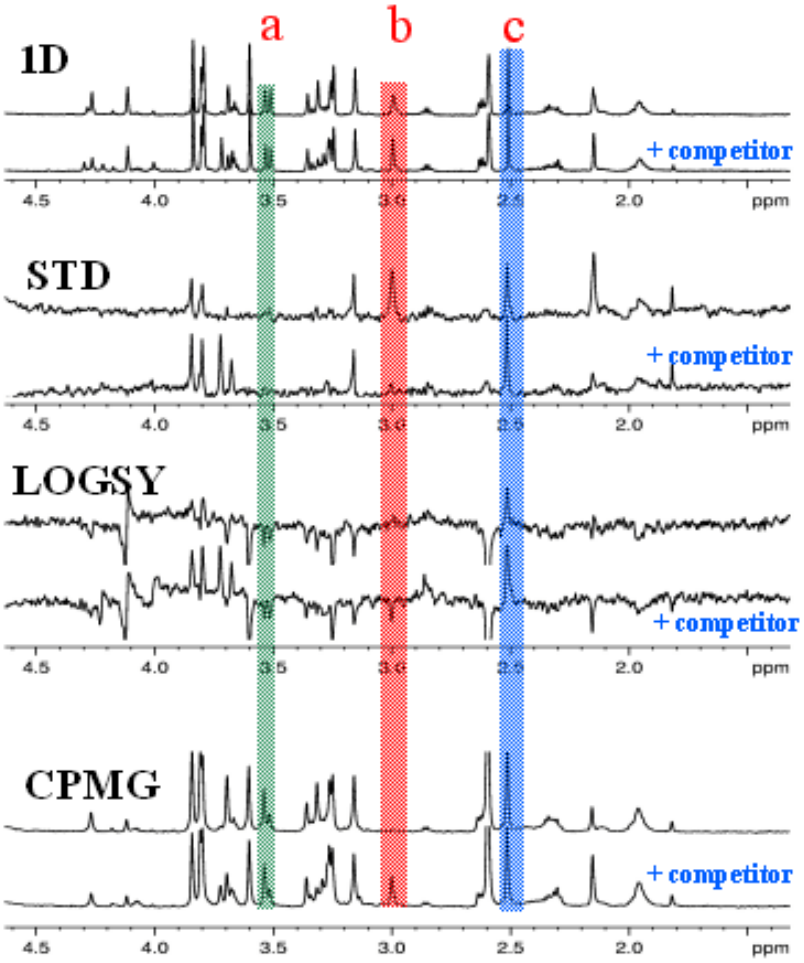


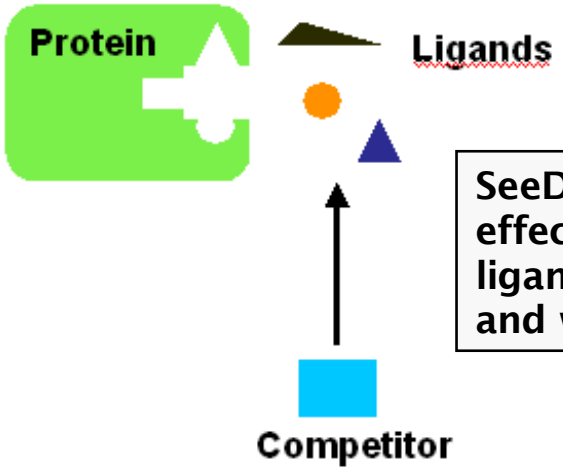

Apart from offering standard techniques for general data analysis, AMIX is designed to provide solutions for special applications.

Examples are:

- Drug Discovery
- Quality Control
- Hyphenation
- Metabolomics
- Spectra bases

# Amix-Drug-Discovery1



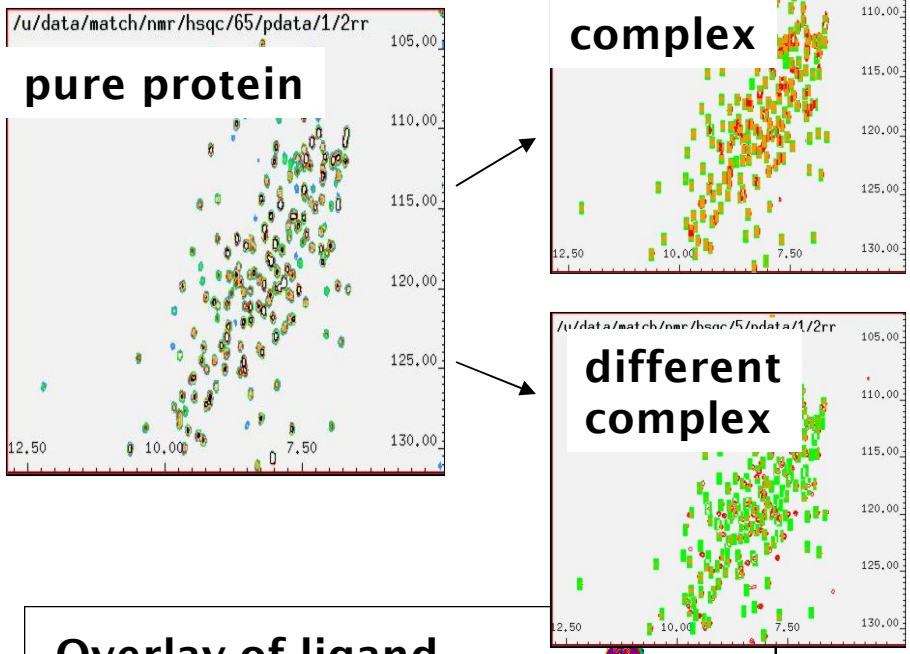



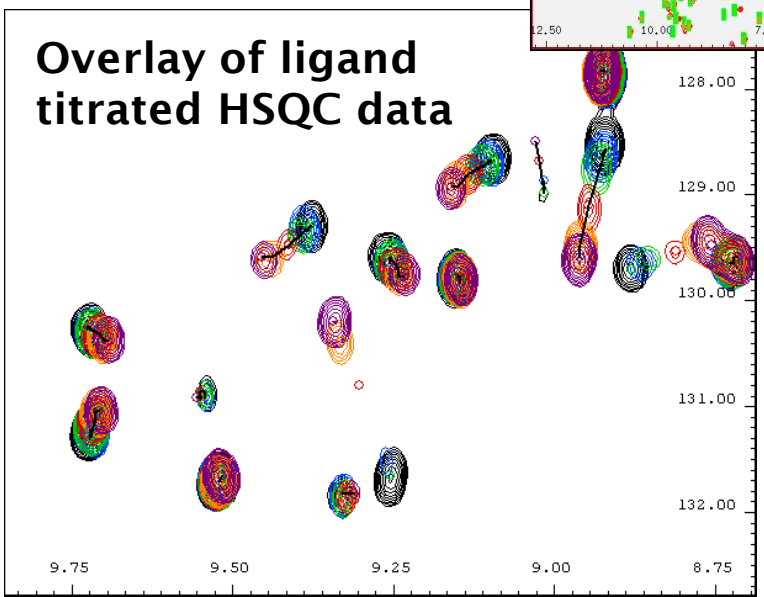

SeeDs exploits the effect of binding to ligand spectra with and without competitor

## Implementation of

- automated SeeDs method
- ligand spectra automatically prepared and stored in sbase
- Set of 1D experiments run with and without competitor to verify correct binding site
- automated analysis of spectra and detection of binders

# Amix-Drug-Discovery2

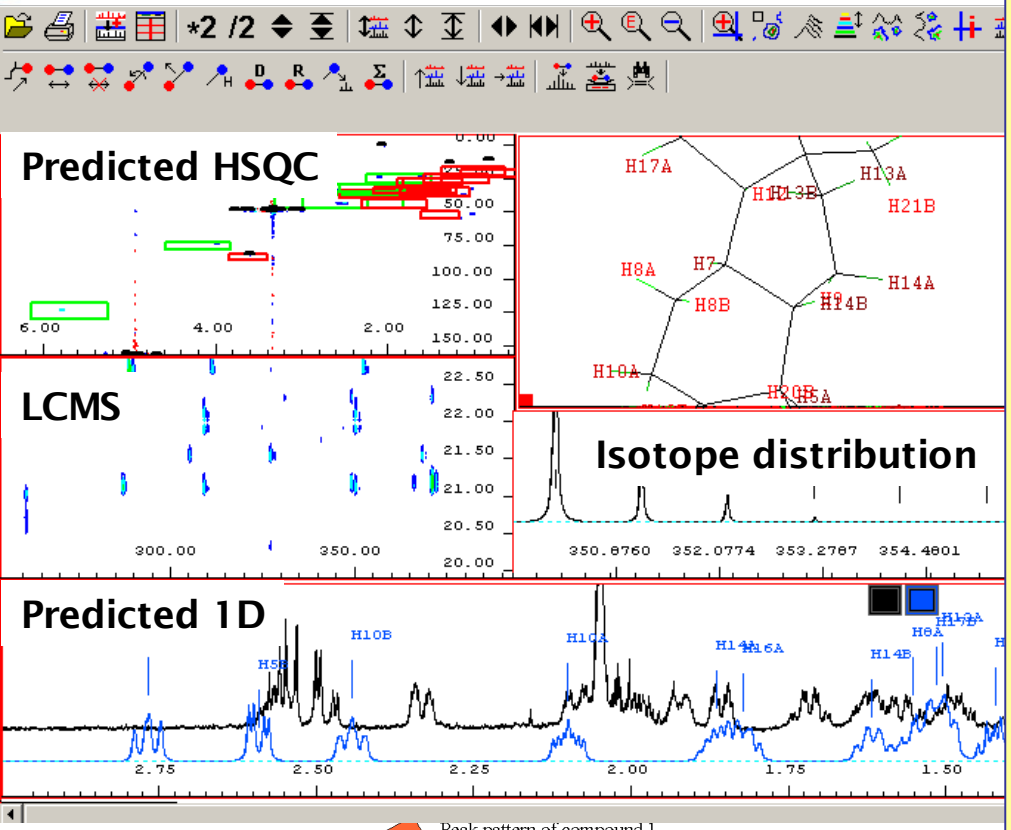


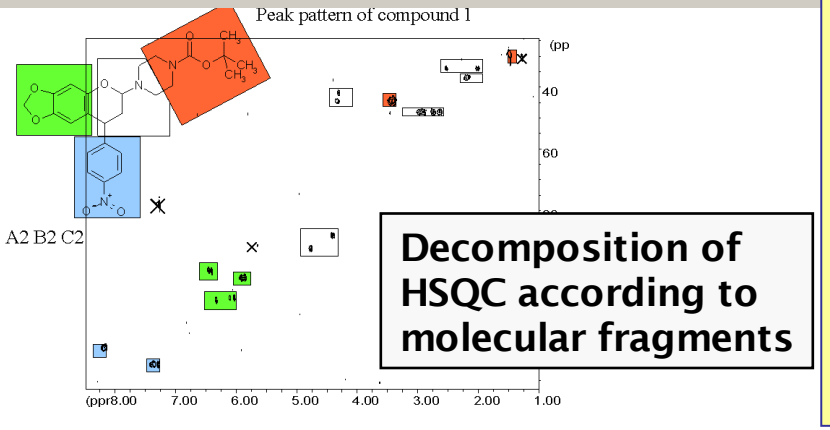




## Implementation of

- automated HSQC comparison to find binders
- optional cross-check with PCA
- semi-automated transfer of peak assignment
- automated 2D peak tracing in titration data
- tabulated output to calculate binding constants

# Amix-NMR-MS-Verification




Decomposition of HSQC according to molecular fragments

## Verification of

- combinatorial data with patented AutoDROP
- parallel synthesis data with scaffold method
- arbitrary data by comparison with PERCH shift predictions

➢ automated peak annotation

➢ link between atoms and peaks

➢ mass search in LC-MS data

➢ comparison of LC-MS and calc. isotope distribution

# Amix-Hyphenation

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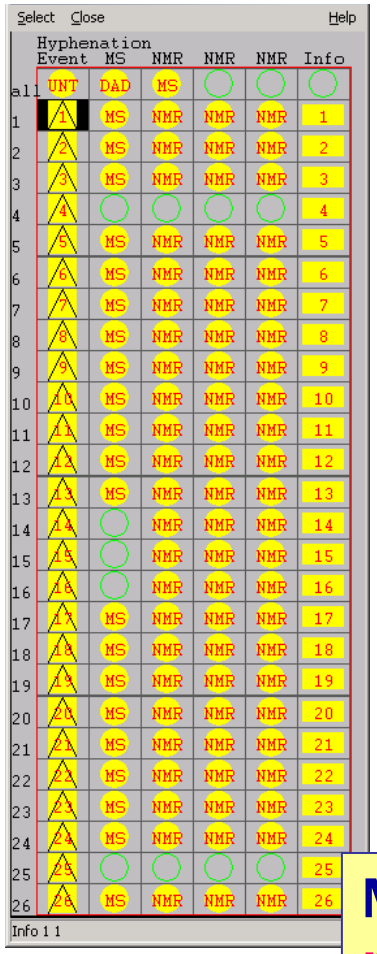
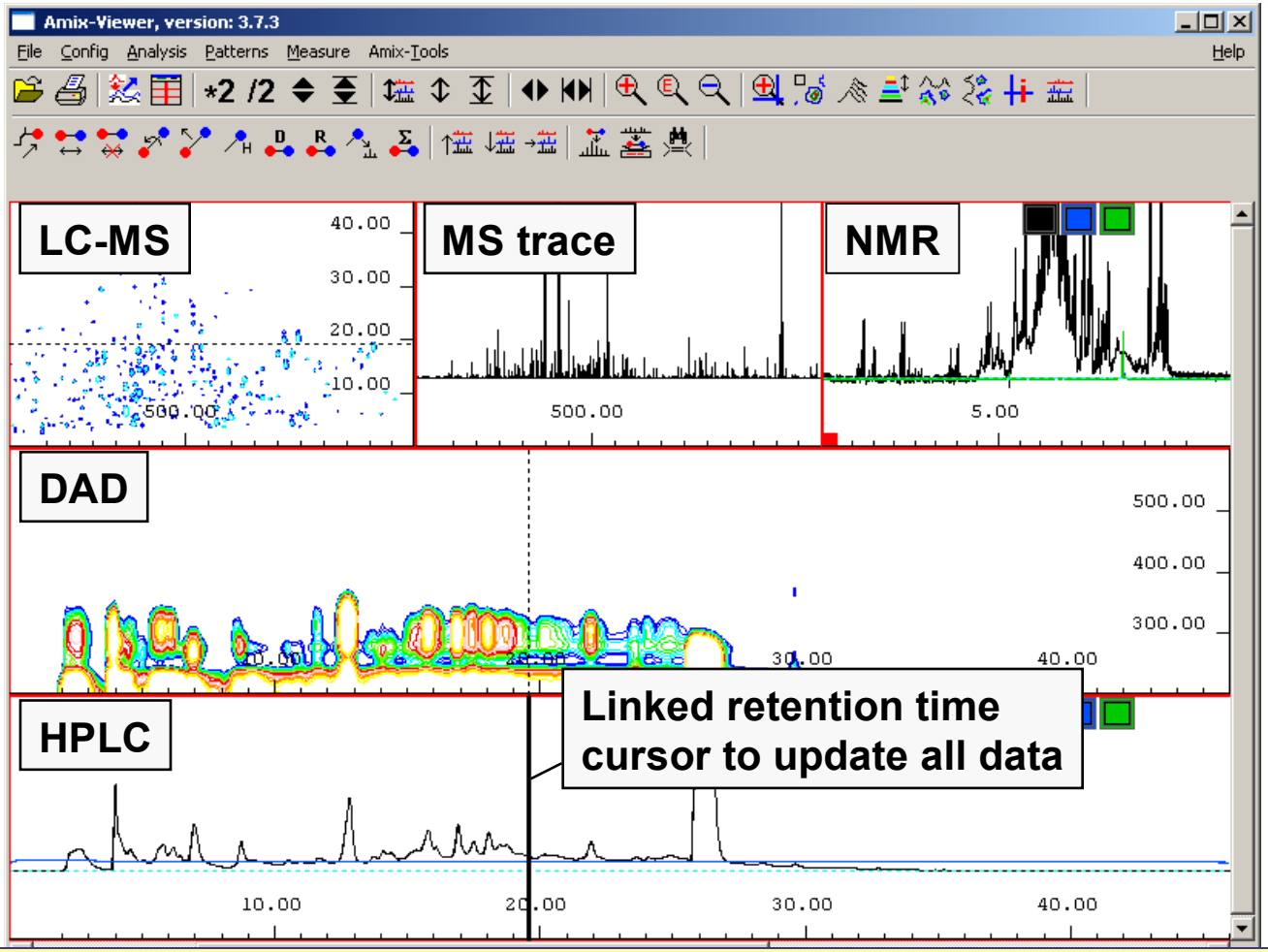
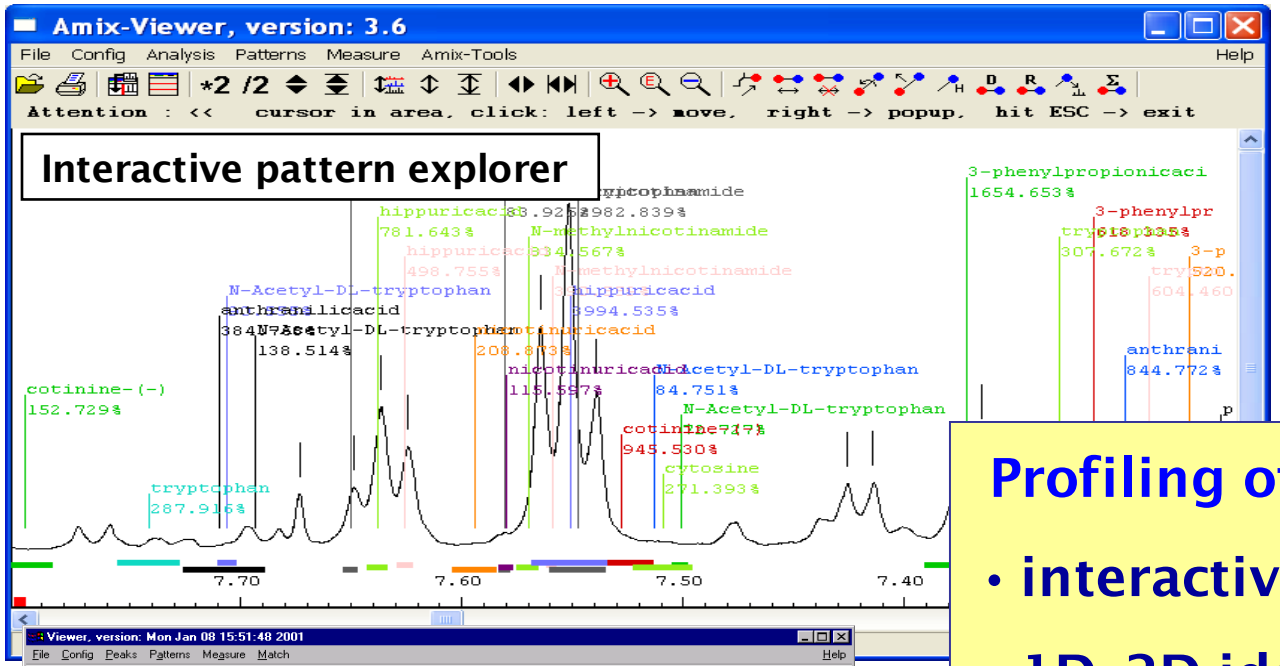
Hyphenation panel

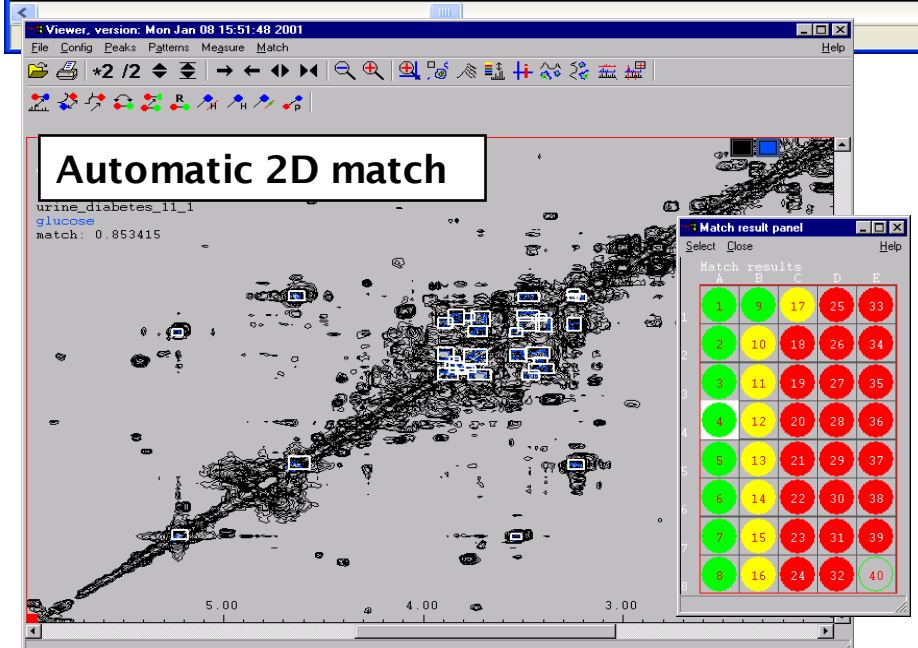



Management and data selection via Hyphenation panel. Parallel analysis of of LC-MS data, MS traces, NMR, UV and HPLC data measured under HyStar control.

# Amix-Profiling

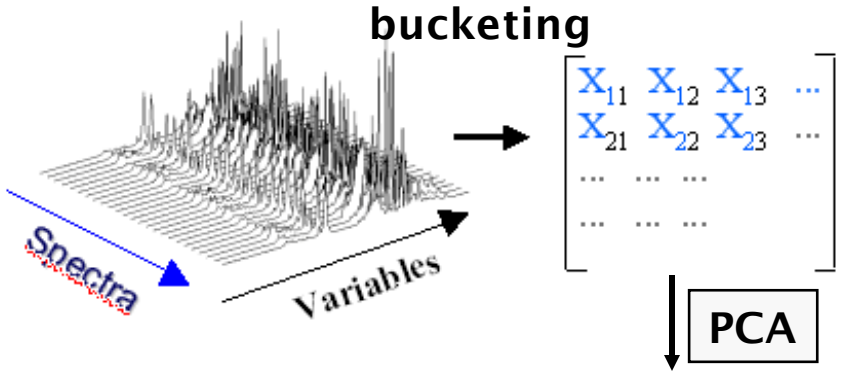


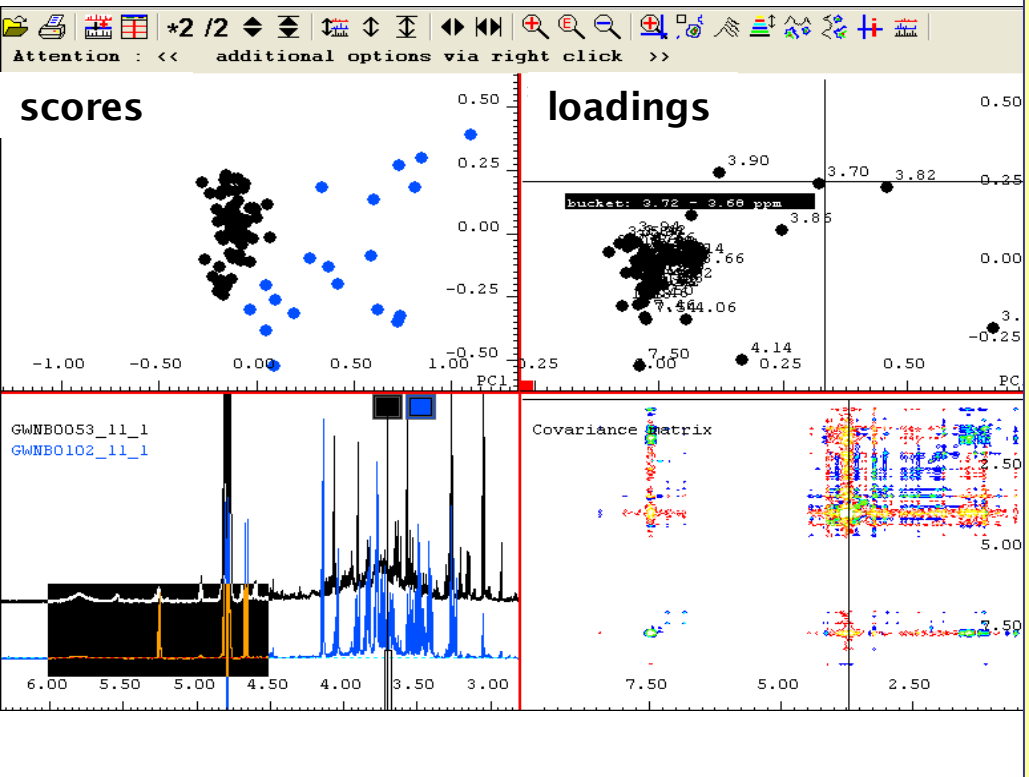




## Profiling of mixtures includes

- interactive pattern explorer
- 1D, 2D identification via spectra bases
- automated data matching techniques
- 1D, 2D quantification
- user defined protocols
- Confirmation via MS data

# Amix-Metabolomics




## Features

- applies to NMR, MS and HPLC data
- different bucketing methods
- unit-variate analysis
- multi-variate statistics (PCA, PLS, PLS-DA)
- SIMCA classification
- PLS prediction
- special tools, e.g. covariance analysis
- unique combination with spectroscopy, automated correlation of loadings with spectra base

# Amix-Metabolomics-Specials

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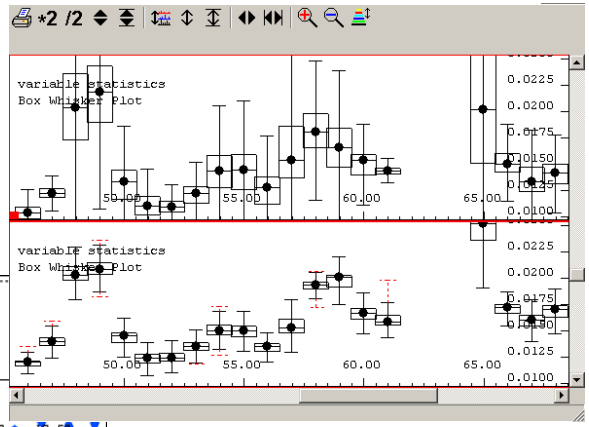
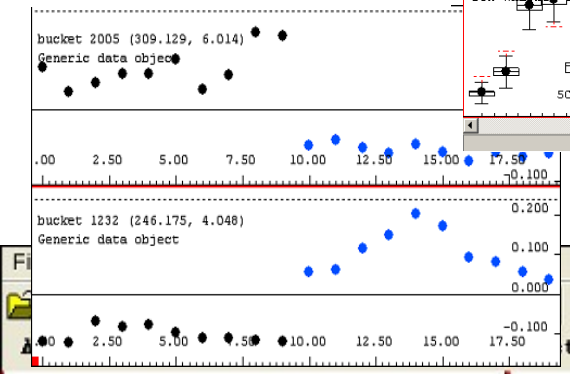
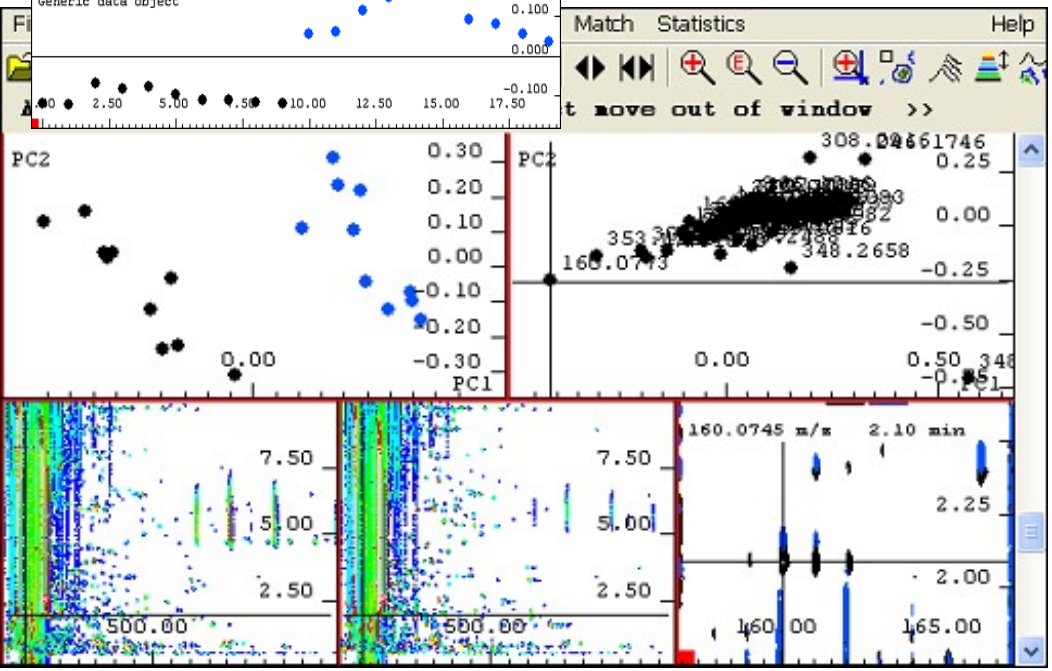
Univariate bucket staistics




Distribution analysis




## Special Features

- loadings provide the key for identification of relevant metabolites
- distribution analysis shows separating compounds
- direct search in Spectra Bases
- search in external data bases
- sum formula calculation from mass loadings
- descriptive statistics of bucket variables

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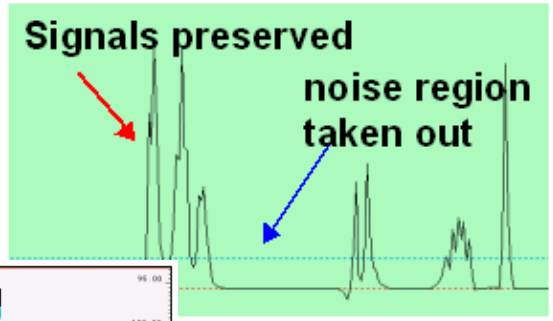
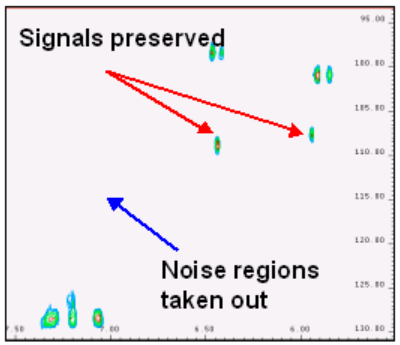
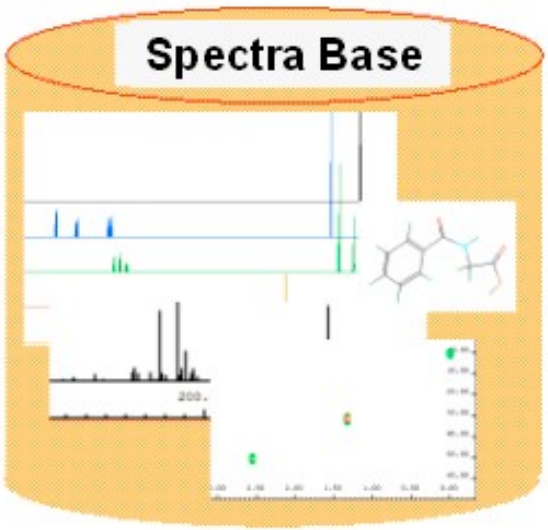
# Amix-Spectra bases

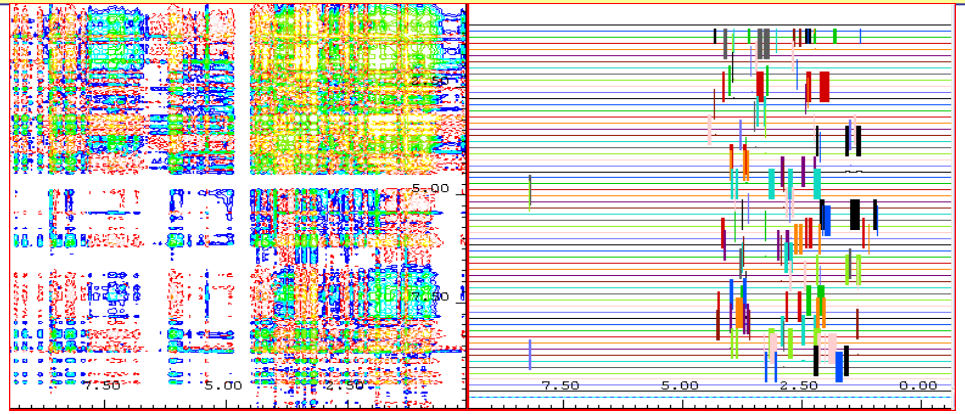



manual or automated




Example usage: automated covariance analysis



## Features

- contains clean and compressed data including molecular structures and multiple name handling
- extremely fast access
- tools to build your own sbases
- complete set of management tools
- SQL interface to ORACLE
- directly linked into Amix-Tool Kits