

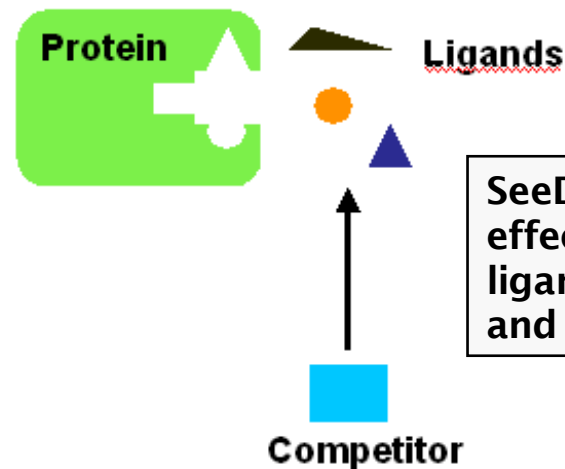
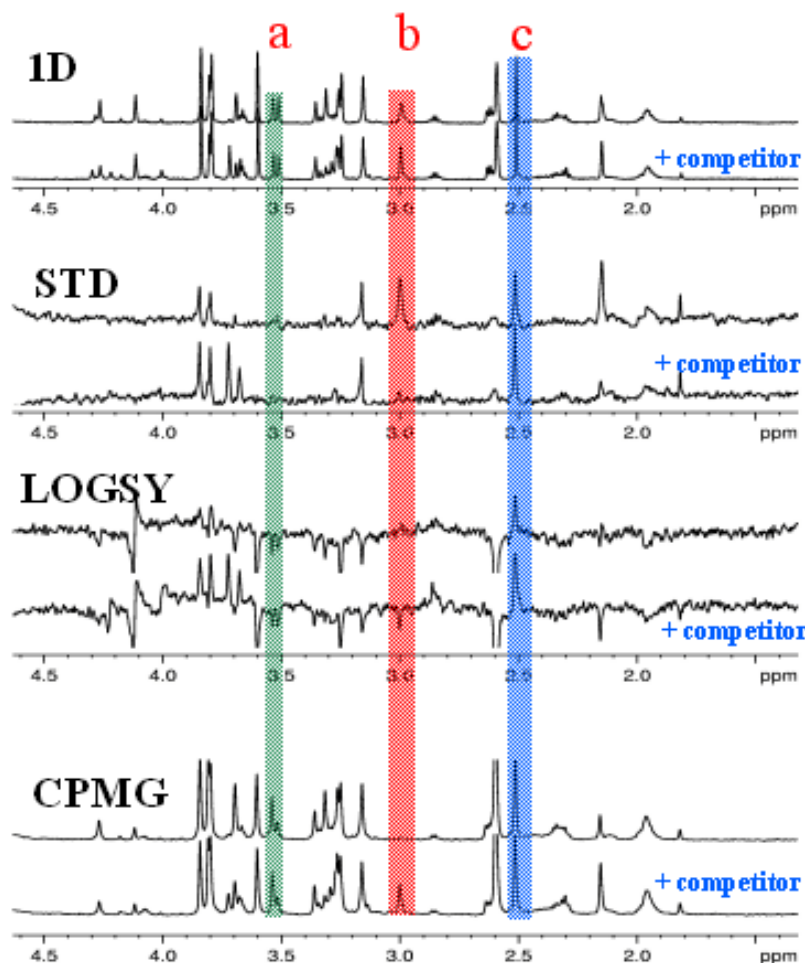
The screenshot shows the Amix-Viewer software interface (version 3.7) with a menu open. The menu items include: Combichem, Quality Control, Buckets, Statistics, Match, Multi Integrate, Algebra, M+T, Analytical Profiler, Spectra bases, Database, Prepare data, and AUREMOL. Red arrows point from the menu items to various windows in the background, which display NMR spectra and analysis results. In the foreground, there is a diagram illustrating a protein-ligand interaction. The diagram shows a green protein structure with a blue ligand and a red competitor. Text next to the diagram states: "Ligands added, it is unknown if they bind" and "Competitor added, it is known that it binds". Below the diagram is a box labeled "Method:" containing the following text: "Analyse series of 1D experiments", "Does the Ligand bind?", and "Ligand replaced, correct binding place?". To the right of the diagram is a yellow cylindrical icon labeled "B-BIOREFCODE" containing a chemical structure and a spectrum.

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

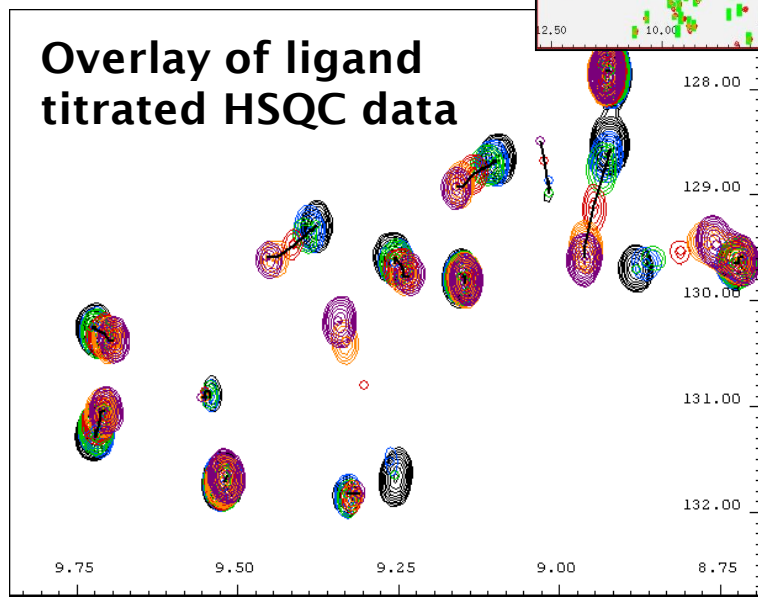
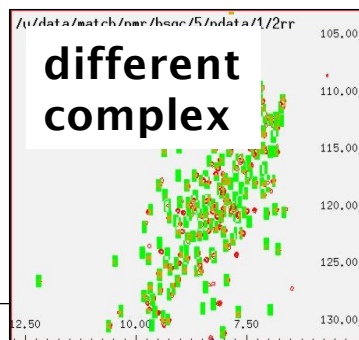
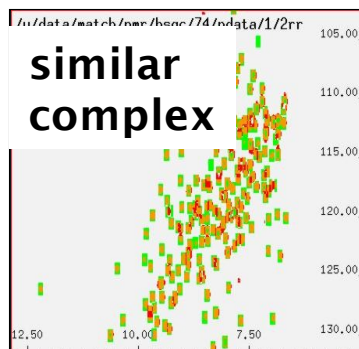
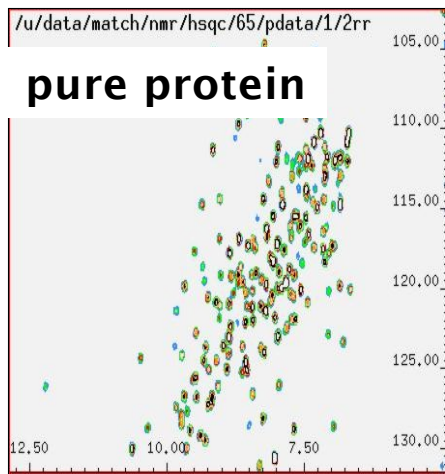
# Amix-Drug-Discovery 1



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

## Implementation of

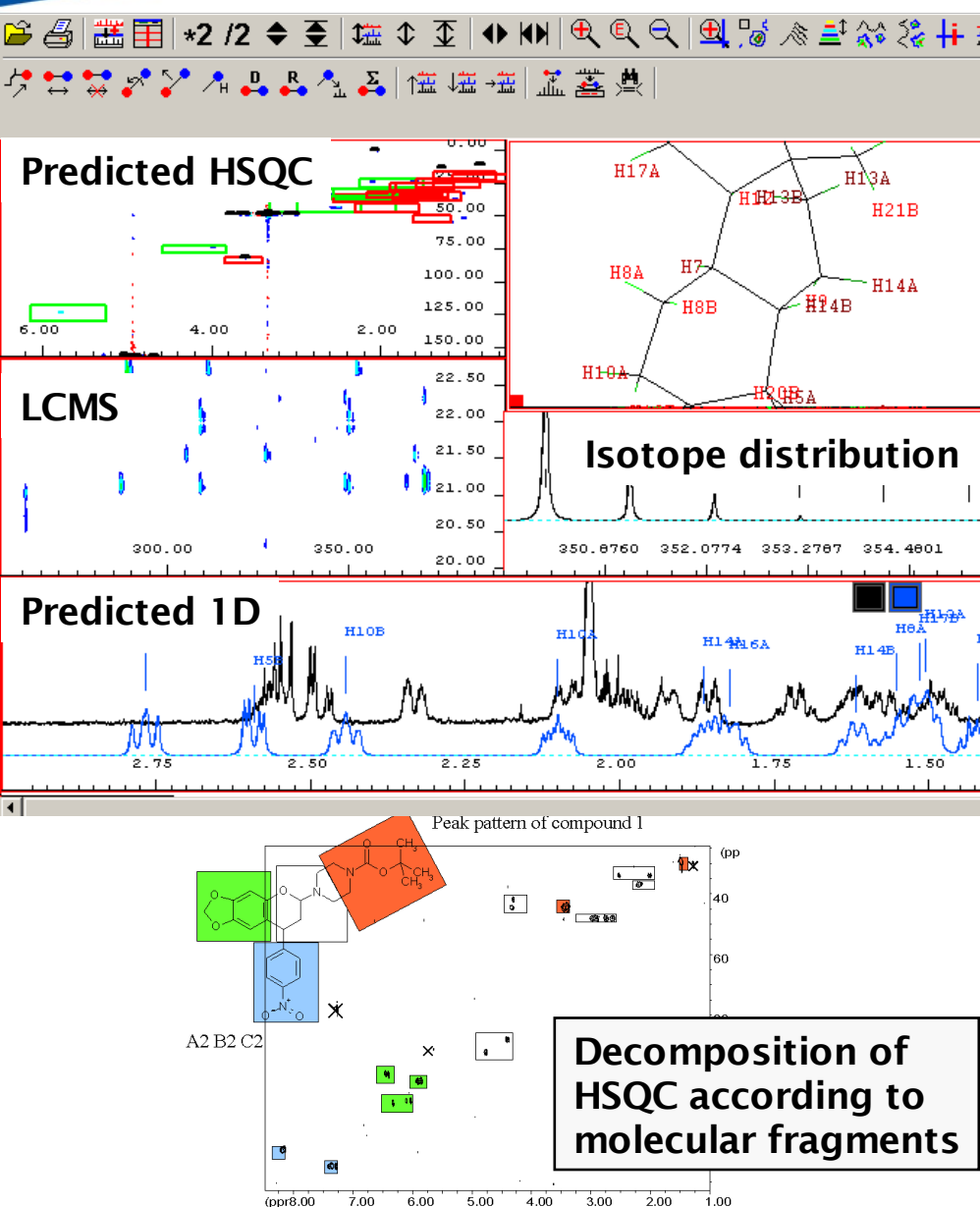
- automated **SeeDs** method
- ligand spectra automatically prepared and stored in sbase
- Set of 1D experiments run with and without competitor to verify correct binding site
- automated analysis of spectra and detection of binders



## 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



## 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

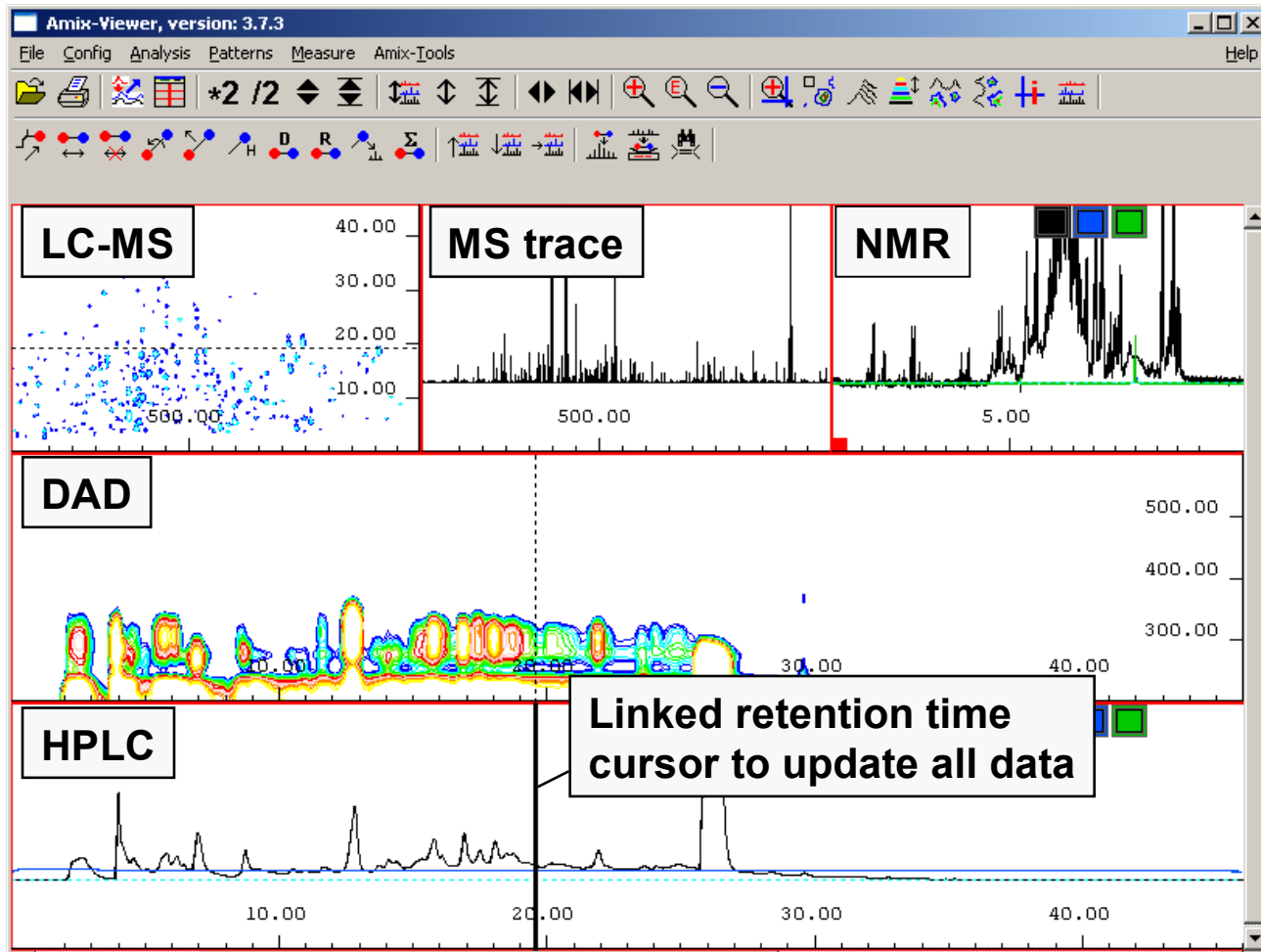


## Hyphenation panel

Select Close Help

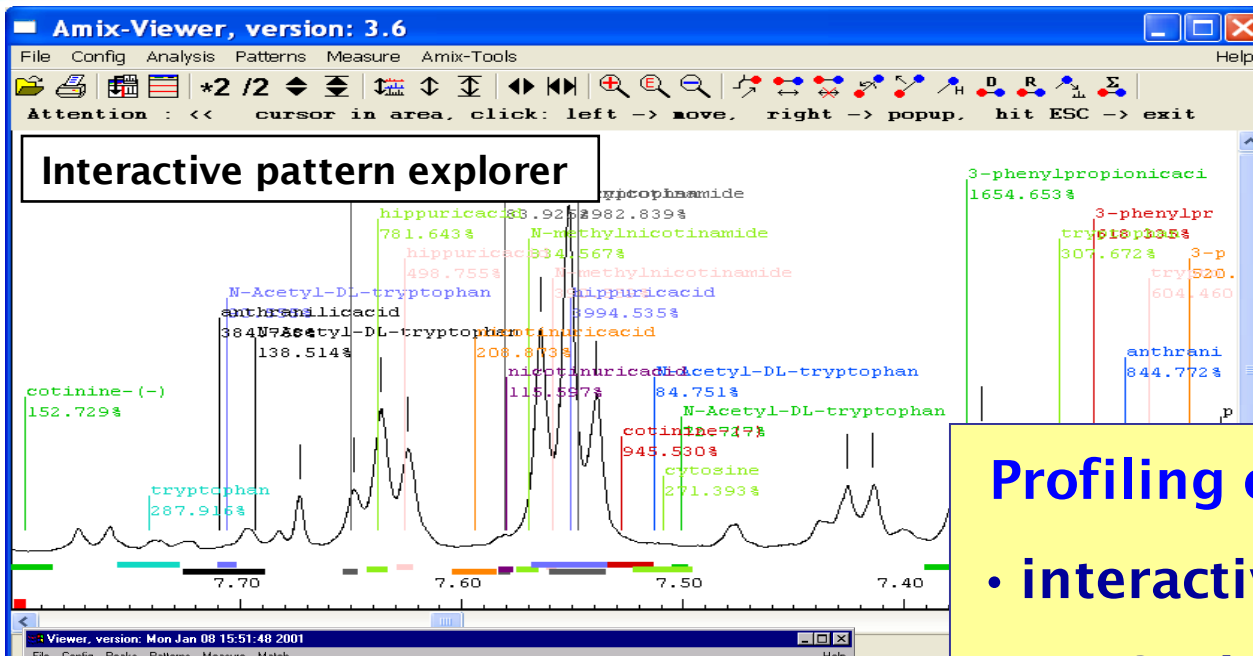
Hyphenation	MS	NMR	NMR	NMR	Info	
UNT	DAD	MS	○	○	○	
1	▲	MS	NMR	NMR	NMR	1
2	▲	MS	NMR	NMR	NMR	2
3	▲	MS	NMR	NMR	NMR	3
4	▲	○	○	○	○	4
5	▲	MS	NMR	NMR	NMR	5
6	▲	MS	NMR	NMR	NMR	6
7	▲	MS	NMR	NMR	NMR	7
8	▲	MS	NMR	NMR	NMR	8
9	▲	MS	NMR	NMR	NMR	9
10	▲	MS	NMR	NMR	NMR	10
11	▲	MS	NMR	NMR	NMR	11
12	▲	MS	NMR	NMR	NMR	12
13	▲	MS	NMR	NMR	NMR	13
14	▲	○	NMR	NMR	NMR	14
15	▲	○	NMR	NMR	NMR	15
16	▲	○	NMR	NMR	NMR	16
17	▲	MS	NMR	NMR	NMR	17
18	▲	MS	NMR	NMR	NMR	18
19	▲	MS	NMR	NMR	NMR	19
20	▲	MS	NMR	NMR	NMR	20
21	▲	MS	NMR	NMR	NMR	21
22	▲	MS	NMR	NMR	NMR	22
23	▲	MS	NMR	NMR	NMR	23
24	▲	MS	NMR	NMR	NMR	24
25	▲	○	○	○	○	25
26	▲	MS	NMR	NMR	NMR	26

Info 1 1

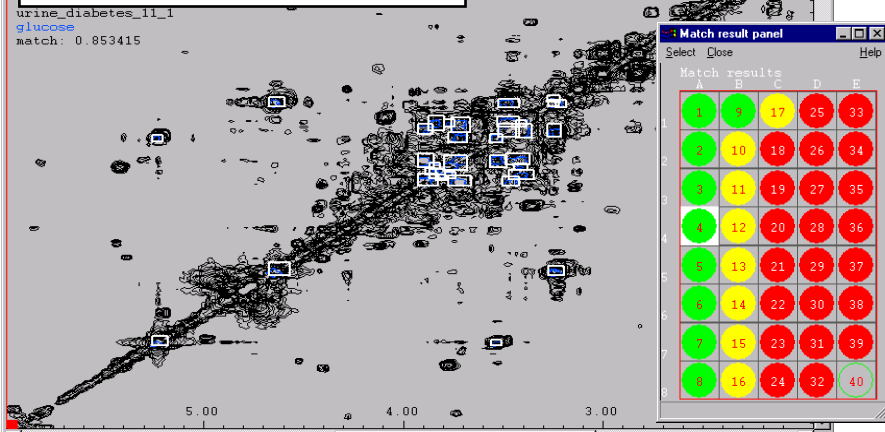


Management and data selection via **Hyphenation panel**. Parallel analysis of of LC-MS data, MS traces, NMR, UV and HPLC data measured under **HyStar** control.

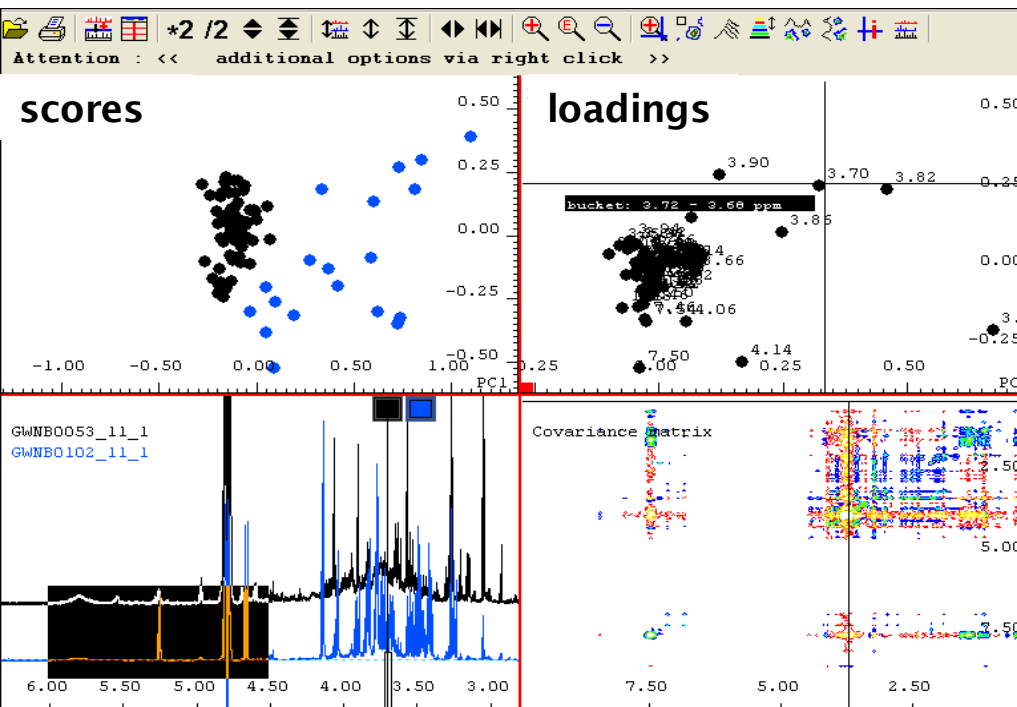
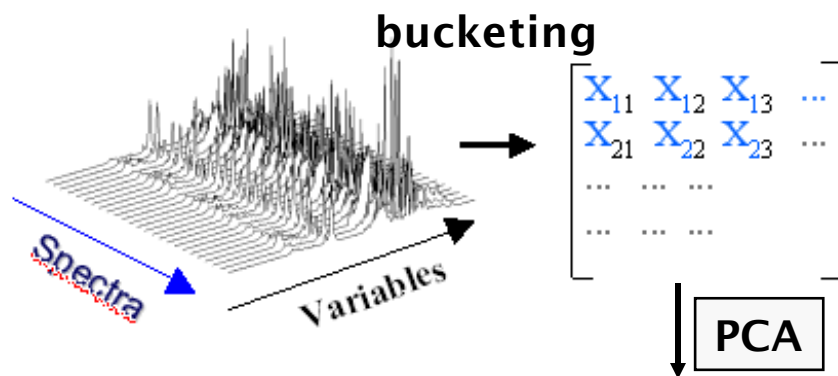
# Amix-Profiling



### Automatic 2D match



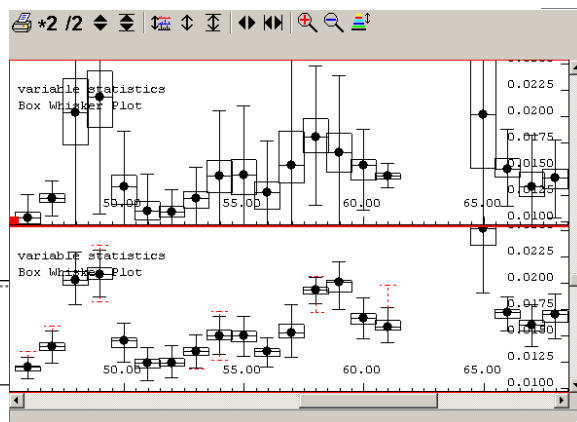
- Profiling of mixtures includes
- interactive pattern explorer
- 1D, 2D identification via spectra bases
- automated data matching techniques
- 1D, 2D quantification
- user defined protocols
- Confirmation via MS data



## 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

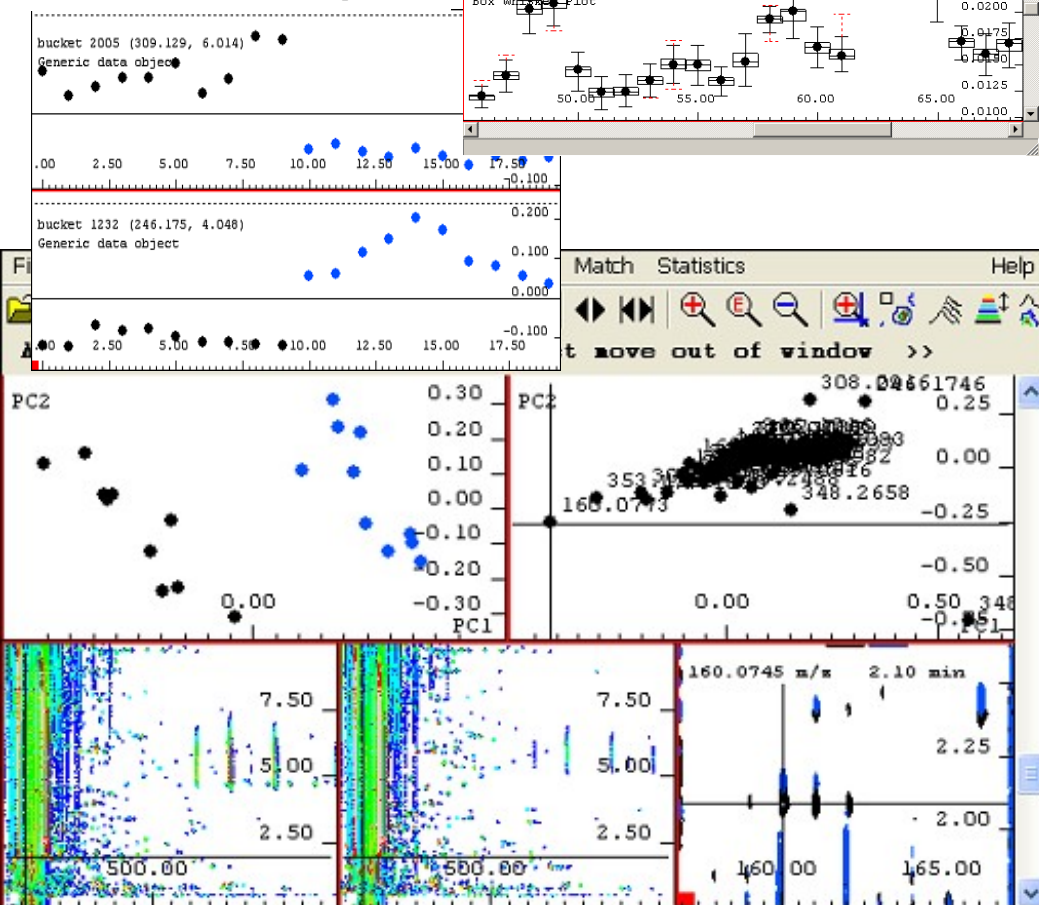
## Univariate bucket statistics



## 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

## Distribution analysis

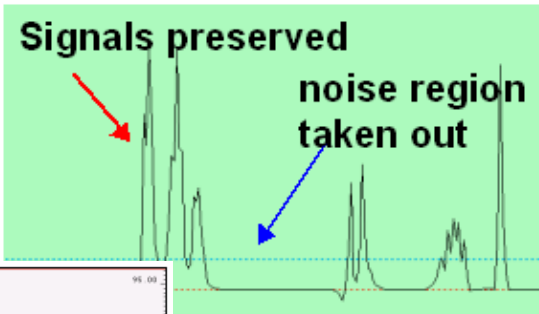




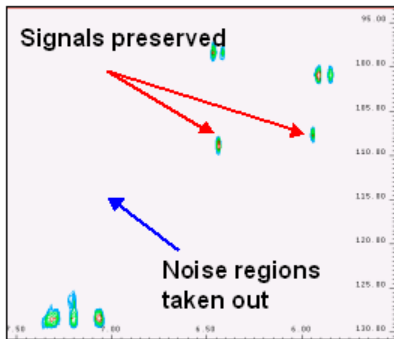
# Amix-Spectra bases



Signals preserved

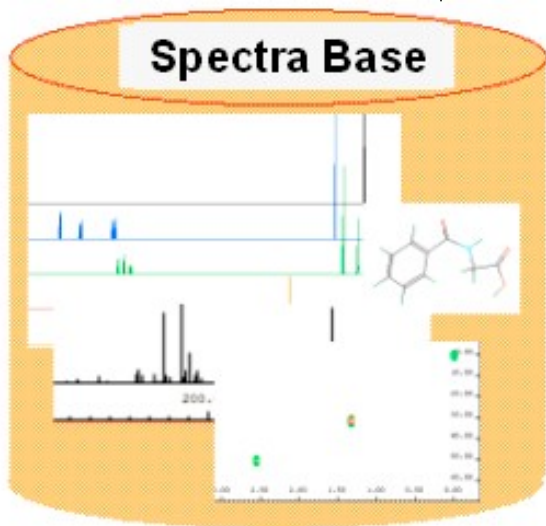


Signals preserved



manual or automated

Spectra Base



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

