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         PROFILE = C:\CHEMADDER\PROFILE\SEARCHPROFILE.TXT

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&INC C:\CHEMADDER\URINE\CITRATE.ASL                    POPULATION=  0.72  ***
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&INC C:\CHEMADDER\URINE\ME3-AMINE-OXIDE.ASL            POPULATION=  0.32  ***
&INC C:\CHEMADDER\URINE\TAURINE.ASL                    POPULATION=  0.29  ***
&INC C:\CHEMADDER\URINE\CYSTEINE.ASL                   POPULATION=  0.23  ***
&INC C:\CHEMADDER\URINE\CREATINE.ASL                   POPULATION=  0.16  ***
&INC C:\CHEMADDER\URINE\HISTIDINE.ASL                  POPULATION=  0.15  ***
&INC C:\CHEMADDER\URINE\GLYCOLATE.ASL                  POPULATION=  0.15  ***
&INC C:\CHEMADDER\URINE\ISOCITRATE.ASL                 POPULATION=  0.17
&INC C:\CHEMADDER\URINE\GLUCOSE.ASL                    POPULATION=  0.13  ***
&INC C:\CHEMADDER\URINE\GLUTAMINE.ASL                  POPULATION=  0.13  ***
&INC C:\CHEMADDER\URINE\ETHANOLAMINE.ASL               POPULATION=  0.13  ***
&INC C:\CHEMADDER\URINE\ARABINITOL.ASL                 POPULATION=  0.11  **
&INC C:\CHEMADDER\URINE\MANNITOL.ASL                   POPULATION=  0.11
&INC C:\CHEMADDER\URINE\TRIGONELLINE.ASL               POPULATION=  0.11  ***
...
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&INC C:\CHEMADDER\URINE\13-DINH2-PROPANE.ASL           POPULATION=  0.01
&INC C:\CHEMADDER\URINE\TRANS-FERULATE.ASL             POPULATION=  0.01
&INC C:\CHEMADDER\URINE\MALEATE.ASL                    POPULATION=  0.0

&END of FILE
```

HOLISTIC qQMSA - A NEW DIMENSION OF QMSA:

R. Laatikainen and P. Laatikainen

SPIN DISCOVERIES Ltd, Kuopio, Finland

http://chemadder.com

HOLISTIC qQMSA

A few clicks from a set of data to a presentation!

- qQMSA = quantitative Quantum Mechanical Spectral Analysis
- ASL = Adaptive Spectral Library: NMR Spectra are stored as spectral parameters, so that the spectrum (since it has been analyzed once) can be simulated in any field

HOLISTIC qQMSA: combined analysis of N spectra yields more & better information than N independent analyses for the same spectra !

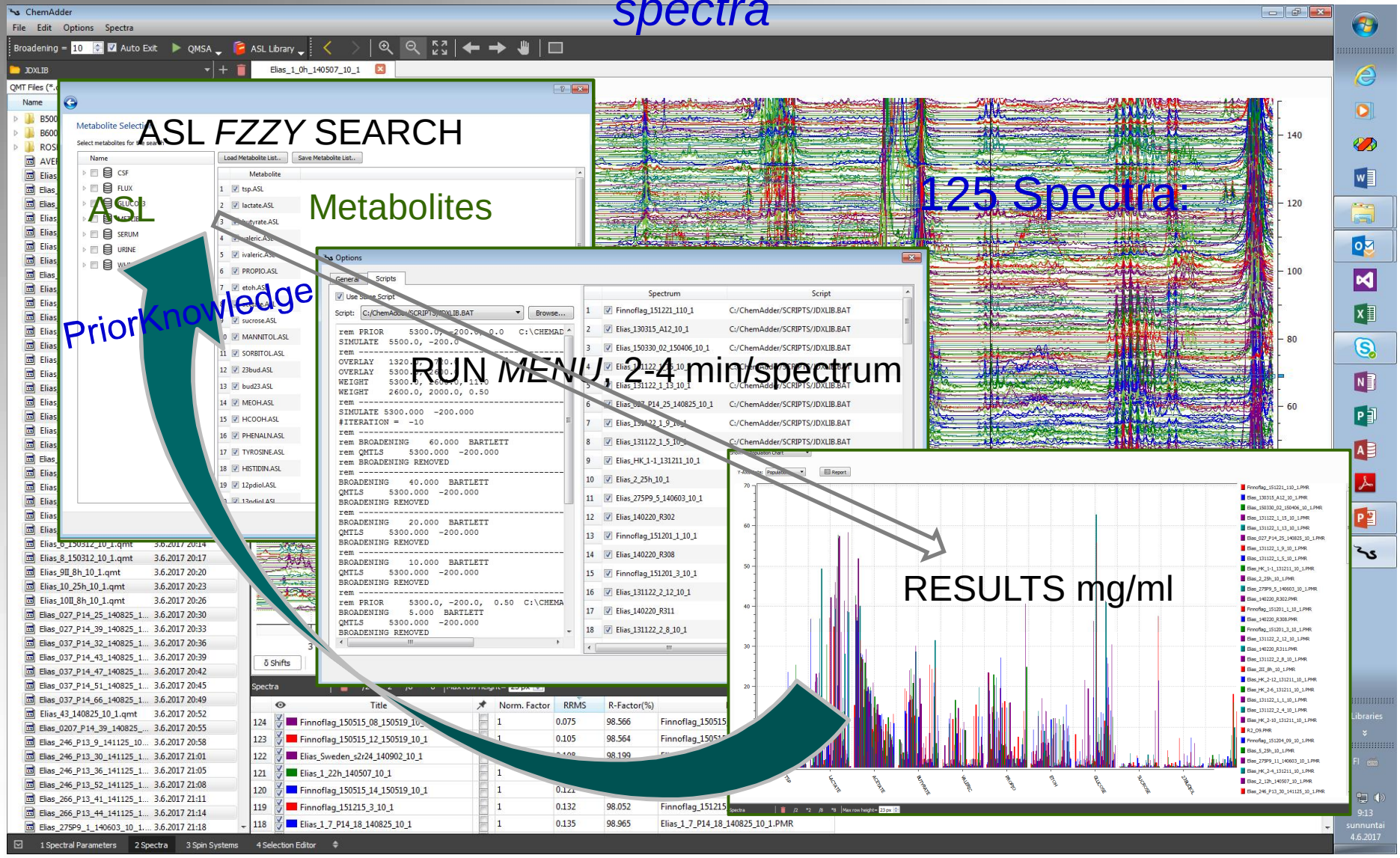
- **The fundamental PROBLEM of qQMSA**: chemical shifts depend on sample !
  - Ranges typically < 0.01 ppm, but even 0.10 ppm for some common metabolites.

- **The SOLUTION**: ***PatternSearch*** and ***PriorKnowledge*** **algorithms** ***(=FZZY Search)***, are based on the fact that the variations are not independent but they correlate.
- The more spectra have been analysed, the better correlations => **HOLISTICS**
  - Batch analysis, < 2-5 min/sample

A few clicks from spectra to diagram !

See video: http://www.chemadder.com/software.html

HOLISTICS: *simultaneous analysis of N spectra yields more & better information than N independent analyses for the same spectra*



The more spectra analysed, the better model!

RECIPE (PMR-file) after *FZZY* SEARCH

AVERAGE.PMR - Notepad

File Edit Format View Help

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&SpinAdder SEARCH file
*ChemAdder2017.05 C:\CHEMADDER\JDXLIB\AVERAGE.PMR
%SEARCH FILE

&CONTROL PARAMETERS & FIT INFO
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           FIELD =   600.402822
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  SCALING FACTOR =     1.000000
  REFERENCE MMOL =       9.0000
   CONCENTRATION =      42.1216
      LINE WIDTH =        3.300
        GAUSSIAN =        0.000
            RMS =         0.143
    R-FACTOR(%) =        98.522

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&CONSTRAINTS (in equations X0 = 1.0)
 IGNORE(PPM): 5.15 to 4.70

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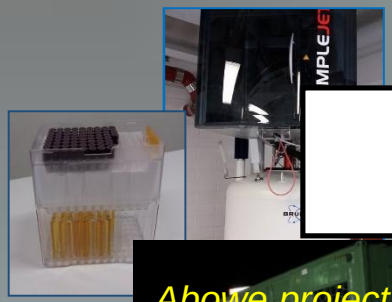
HOLISTIC CYCLE of bioproduct analysis with ChemAdder



SPECTRA (N)
JDX-files

Targeted ASL
Metabolites(M)

FZZY SEARCH ENGINE

SHIFTS, etc.

SELECTED metabolites
ASL files with initial populations

ChemAdder

MENU (script)

```
SIMULATE 500
BROADENING 50
REGRESSION 5000 1000
QMTLS 5000 1000
REM BROADENING
QMTLS 5000 1000
#LINEWIDTH OPTIMIZED = F
QMTLS 5000 1000
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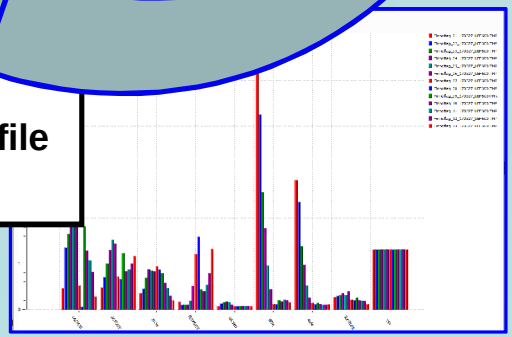
SpinAdder (qQMSA)

CONCENTRATIONS:
diagram, txt-, csv- or xlsx-file
(in mg/ml)



TARGETED RECIPE (PMR file in include format) FOR URINE

The metabolites are given in order of typical abundances and finding probabilities (here from **Bouatra, S. et al**. *The human urine metabolome*. **PLoS ONE** 8, e73076, 2013):

```
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       BATCHFILE = C:\CHEMADDER\SCRIPTS\URINE.BAT                  = The MENU (SCRIPT file) for analysis
         PROFILE = C:\CHEMADDER\PROFILE\SEARCHPROFILE.TXT          = Defaults for iteration
  REFERENCE MMOL = 9.292

&INC C:\CHEMADDER\URINE\HIPPURATE.ASL                 POPULATION=  0.82  ***  = 100% probability
&INC C:\CHEMADDER\URINE\CITRATE.ASL                   POPULATION=  0.72  ***
&INC C:\CHEMADDER\URINE\GLYCINE.ASL                   POPULATION=  0.38  ***
&INC C:\CHEMADDER\URINE\ME3-AMINE-OXIDE.ASL           POPULATION=  0.32  ***
&INC C:\CHEMADDER\URINE\TAURINE.ASL                   POPULATION=  0.29  ***
&INC C:\CHEMADDER\URINE\CYSTEINE.ASL                  POPULATION=  0.23  ***
&INC C:\CHEMADDER\URINE\CREATINE.ASL                  POPULATION=  0.16  ***
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&INC C:\CHEMADDER\URINE\GLYCOLATE.ASL                 POPULATION=  0.15  ***
&INC C:\CHEMADDER\URINE\ISOCITRATE.ASL                POPULATION=  0.17       < 50% probability
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&END of FILE                                                          Totally >200 metabolites
```

Under testing …


http://chemadder.com