# what do you want? <br> oder: wie sich die ergebnisse interpretieren ?! 

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## If all you have got is a hammer ...

...everything looks like a nail
(1) We'd like to find out about Metabolomics
(2) We know Petri Nets
(3) We know Bayesian Nets

Can we do (1) using (2)+ ? ??

If the only tool you have is a hammer...

then everything looks like a nail!
(1) GC / LC Separation
(2) Ionisation \& Acceleration
(3) Mass Detection
4. Peaks with retention time and $m / z$ Value

Fingerprinting Phenotypic Features
Target Analysis Individual Metabolites
Metabolite Profiling Quantification of Metabolite subset
Metabolomics "Comprehensive" Quantification

## Mass Spectrometry

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## Bioconductor [G|L]CMS = XCMS

- Siuzdak\&Abagyan @ Scripps
- Bioconductor (optimised C)
- Peak alignment
- Peak integration
- "Differential" metabolites
- RServe Web Frontend underway



## Bioconductor [G|L]CMS = XCMS

Retention Time Deviation vs. Retention Time

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Filtered with Second Derivative Gaussian

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- Metabolites
- Proteins/Enzymes/Genes
- Reactions:
- Stoichiometry
- Kinetics
- Mass Action
- Michaelis Menten
- Hill-type kinetics
- Kinetic Constants

What we measure:

- Metabolite Profiles
- Fluxes
- Proteomics
- Enzyme Activity
- Transcripts
tinyhttp://eot.bu.edu/ccb/Kinetics/index.htm
Mass action kinetics state:

$$
\begin{equation*}
r=k_{S} \times S \tag{1}
\end{equation*}
$$

Hill type
Michaelis-Menten:

- reversible or irreversible reactions

$$
\begin{equation*}
v=\frac{V_{\max } S}{K_{m}+S} \tag{2}
\end{equation*}
$$

- more than one substrate
- competitive inhibitors

$$
\begin{equation*}
r=\frac{k_{c a t} E S}{K_{m}+S} \tag{3}
\end{equation*}
$$

- non competitive inhibitors

A riboswitch is a part of an mRNA molecule that can directly bind a small target molecule, and affects the gene's activity. An mRNA that contains a riboswitch is directly involved in regulating its own activity.
http://en.wikipedia. org/wiki/Riboswitch

- activation / repression
- transcription termination
- translation initiation
- self-cleavage (ribozyme that cleaves itself)
- mostly eubacteria
- some in eukaryotes
- similar in archaea


The only thing we measure are Metabolite-"concentrations" under various conditions:

- Is there a way to infer Pathways ?
- Is there a way to infer Activation / Inhibition of Reactions ?
- What experiments are needed to infer these ?
- Time Series ?
- Knock-Outs ?
- Can we find Gene Regulation by Metabolites ?

