

PERCH NMR Software

Turku 16.17.5.2006

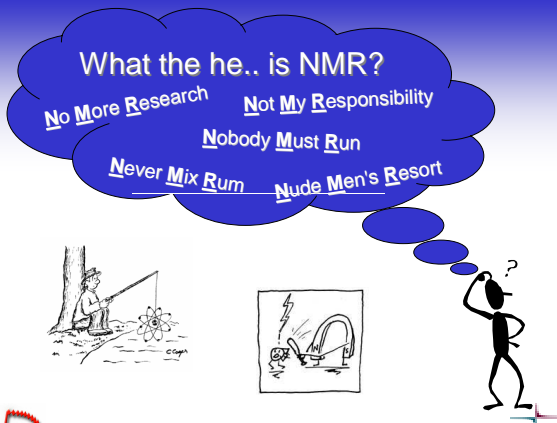


Matthias Niemitz
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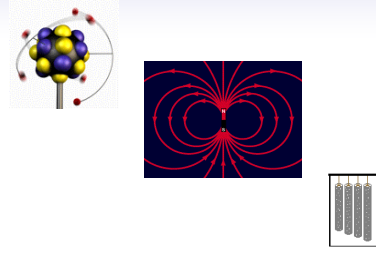


What the he.. is NMR?

No More Research Not My Responsibility
 Nobody Must Run
 Never Mix Rum Nude Men's Resort

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Nuclear Magnetic Resonance








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WHY NMR?

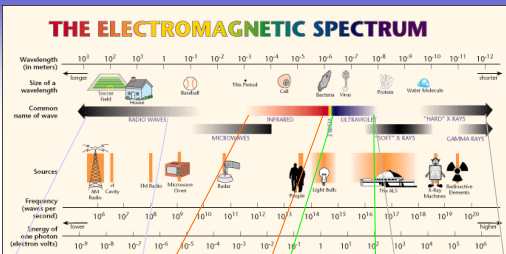
Because there is hardly another technique that is so informative for so many different types of applications, and because there is no other technique that provides so much fun.

Richard R. Ernst
(Nobel Prize in Chemistry 1991)

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THE ELECTROMAGNETIC SPECTRUM





Radio waves: Nuclear spin states (in a magnetic field)

IR: molecular vibrations

UV: valence electronic excitation



X-ray: core electron excitation

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NMR Observables & Information

Observable	Information
• Chemical shifts 1H, 13C, 15N, 31P	Assignments, Secondary Structure
• J-couplings (through bond) 3J(HN, H α), 3J(H α , H β), ...	Dihedral angles: Φ , χ , Karplus curves
• NOE (through space)	Interatomic distances (<5Å)
• Solvent exchange (HN)	Hydrogen bonds
• Relaxation / linewidths 1H, 13C, 15N	Mobility, dynamics conform./chem.exchange
• Residual dipolar couplings	Projection angles

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NMR - Pros & Cons

- + Most utilizable molecular probe
- + Broad range of applications
- + Quantitative
- + Kinetics (dynamics)
- + Non-invasive (in-vivo)
- Cost intensive
- Low sensitivity
- "Demanding interpretation"



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WHY PERCH?

Because there is hardly any other software providing so many unique features for analyzing NMR data that allow you to do things you simply cannot do with any other software.

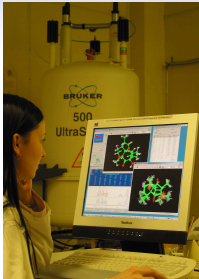
Is it fun?
SURE!



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"Off-Spectrometer" Processing & Analysis



Network
FTP



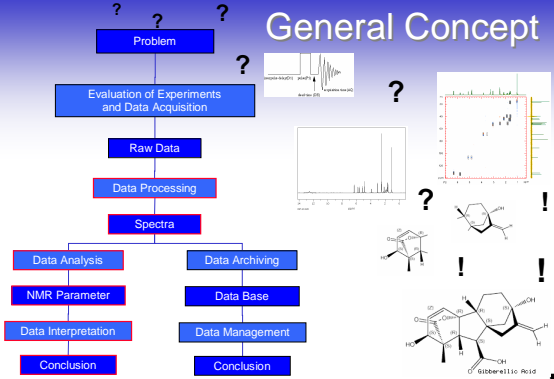
- More flexibility
- Cost saving



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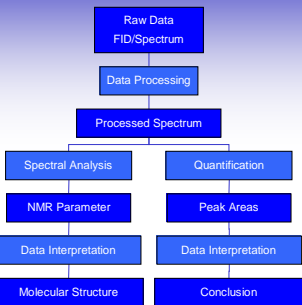
General Concept



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PERCH's Concept



- Small molecules
- 1D - spectra
- High resolution
- Iterative Spectral Analysis
- Quantification
- Automation

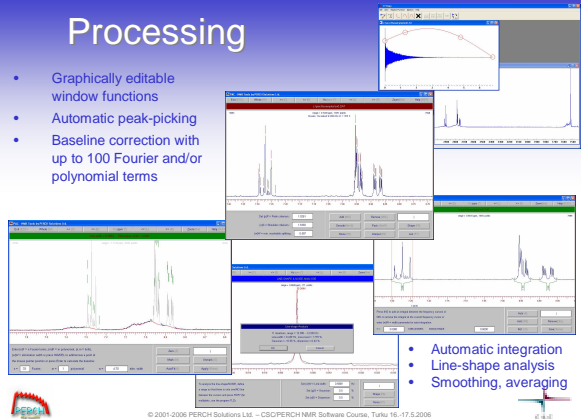


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Processing

- Graphically editable window functions
- Automatic peak-picking
- Baseline correction with up to 100 Fourier and/or polynomial terms



- Automatic integration
- Line-shape analysis
- Smoothing, averaging

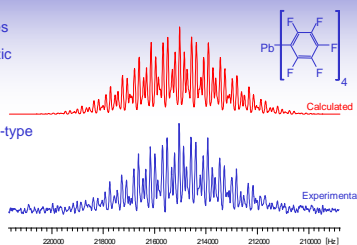


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Spectral Simulation & Analysis

- Up to 100 spin-particles
- Chemical and magnetic equivalence
- X -approximation
- Traditional LAOCOON-type
- Peak-top-fitting
- Integral transforms
- Total-line-shape fitting
- Auto-verification



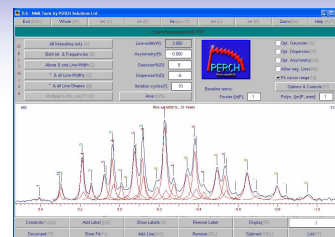
¹⁹F Spectrum of Tetra(pentafluorophenyl)lead(IV)

Klapötke et. al. J. Fluorine Chem.

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Quantitative NMR - qNMR

- Total-line-shape fitting
- Deconvolution
- Graphical peak editing
- Individual line-shapes
- Constraint features
- Multiplet structures
- Complex and structure constraints
- Auto-constraints



Analysis of Overlapping ¹³C-¹H Isotopomers of deuterated L-[3-¹³C] Lactate

Laatikainen et. al. Magn. Reson. in Med.

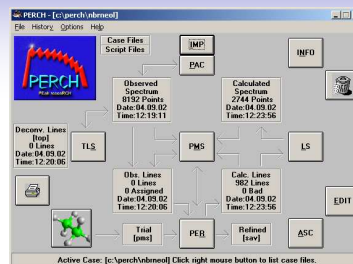
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PERCH NMR Tools

- IMP Imports the original FID or spectrum into the PERCH format.
- FFT Fast Fourier Transformation (Windows program).
- PAC Provides the preparation routines (peak picking, baseline correction, smoothing)
- TLS Total-Line-Shape analysis (deconvolution, STAC for STACKED spectra)
- MMS The 3D-structure editor and proton spectral parameter predictor.
- PMS The graphical spectral parameter editor.
- PER Starts the spectral calculation with the PERCHit iterator.
- LS Simulates the Line Shape.
- APP APPends spectra.
- ASC Converts PERCH-format into ASCII format.

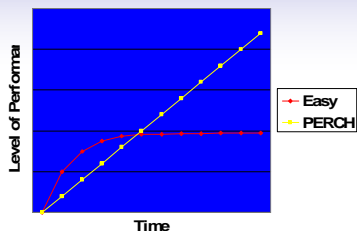
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PERCH Shell



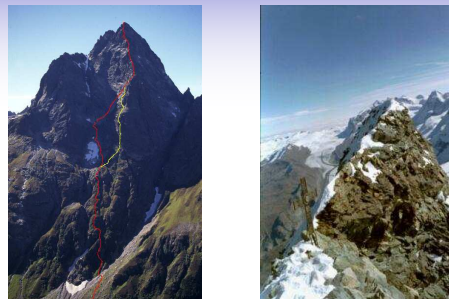
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"Steep Learning Curve"



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Goal



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