Dynamic Center

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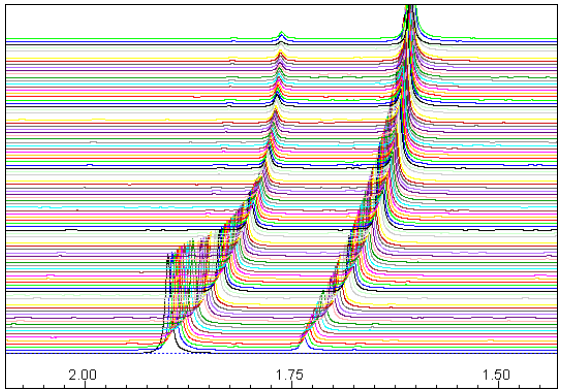
Motivation

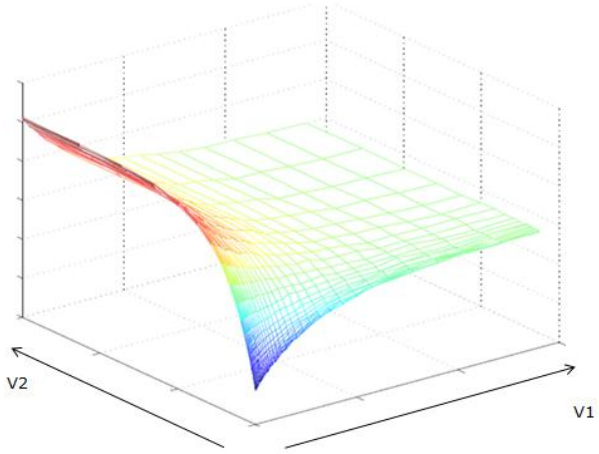
- **Easy-to-use** software to analyze all kinds of dynamics data in an **identical** way.
- **Replacement of older software components** which are either out of date or inconvenient to use.
- **Enhancement** of **functionality** and **quality.**
- Improvements regarding **automation**.

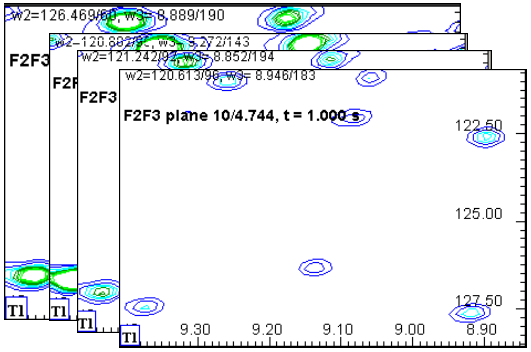
Possible Applications

Dynamics is regarded as a **synonym**: We talk about all kinds of spectra containing signal intensities that depend on one or more variables which are not Fourier transformed.



Example:
Kinetics using
pseudo 2D data

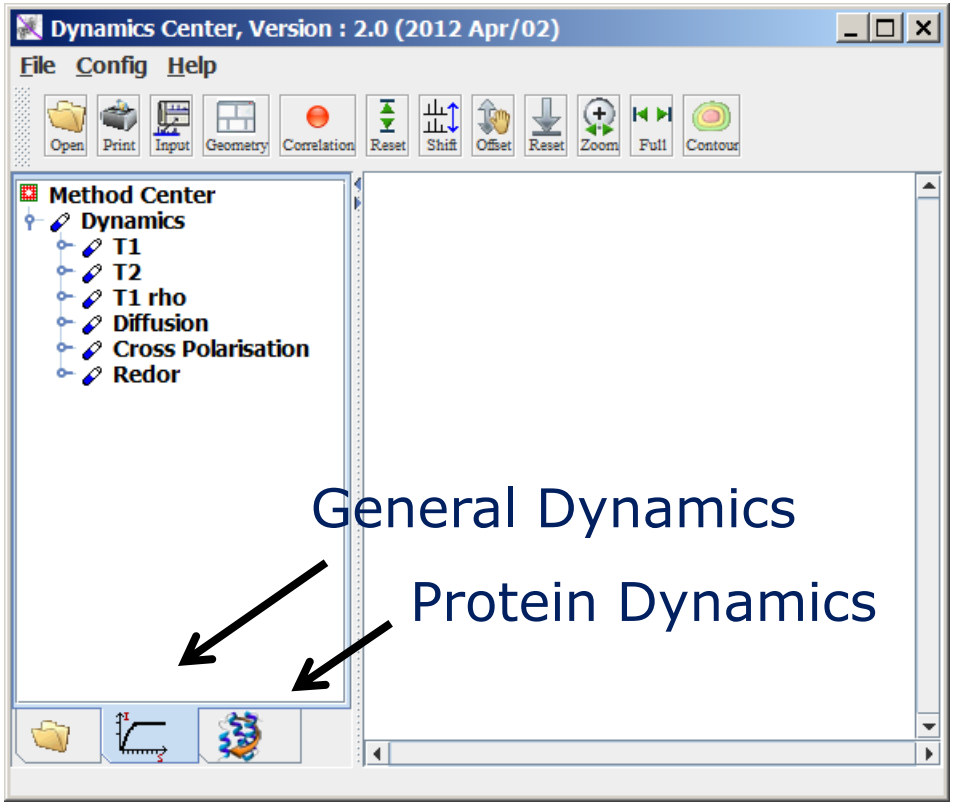




Example:
Relaxation
Using pseudo
3D data

Example:
Data depending
on 2 non-transformed
Variables, e.g. T1/T2,
T1/D, D/D

Dynamics Center 2.0

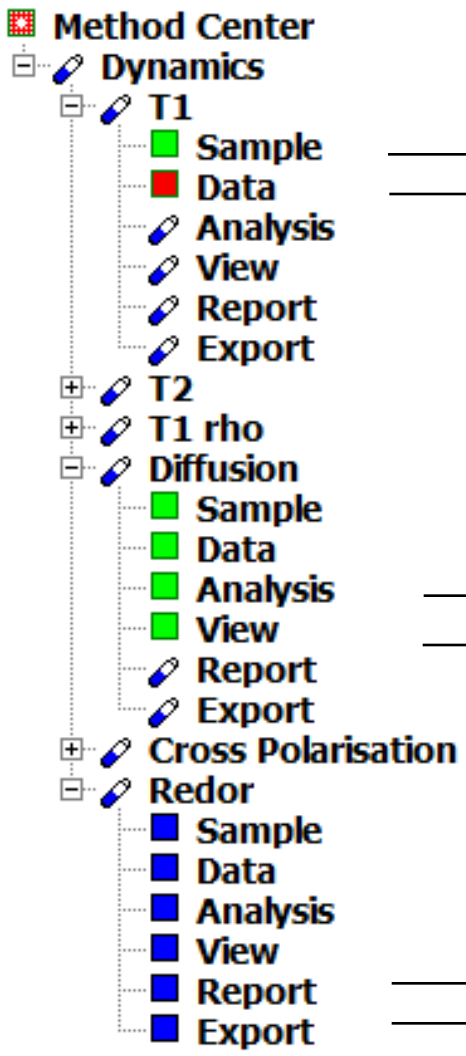


KLZ

BER

- Introduced at ENC 2012
- Runs standalone
- Identical handling of all methods
- General Dynamics
  T_1, T_2, T_{1rho}, Diffusion, CP, REDOR
- Protein Dynamics
  T_1, T_2, T_{1rho}, R_{ex}, hetNOE, modeling backbone dynamics
- Method oriented work flow

Workflow identical for all methods



sample information, protein-**sequence**, -**structure**

spectra, parameters, pulse program **peak/integral** analysis

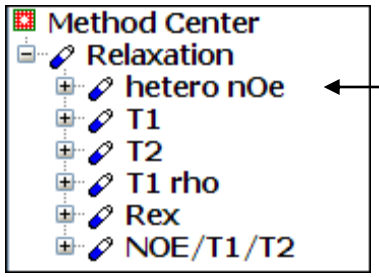
fit of parameters, **error analysis, ILT**

user defined display, spectra, histograms, fit curves, DOSY plots

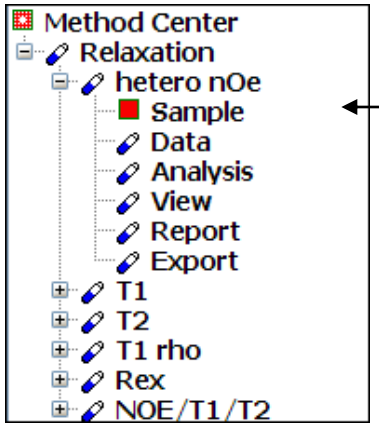
PDF report

Text and **EXCEL** export of results and used data

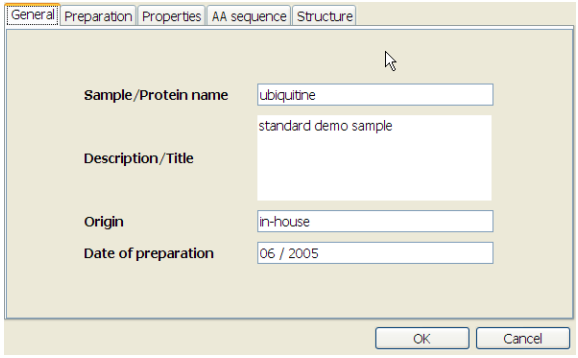
Executing a method

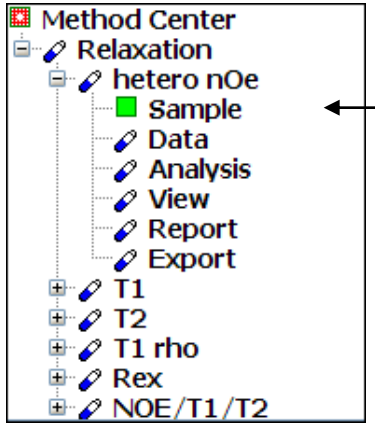


- The method tree works like the File **Explorer** Tree, left click to **node** to open a method



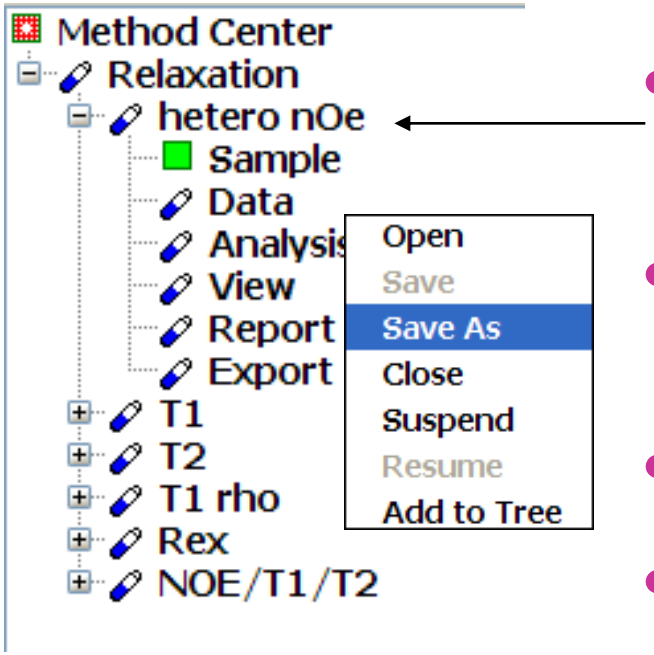
- left click to **leaf** to execute a component, e.g. Sample. It turns **red** until dialogs or calculations are finished.





- when getting **green** you can continue with the next leaf

Project: Application of a Method to Data



- get **Popup menu** with right mouse button click, select:
- **Save** or **Save As** to store the details of a project to disk
- **Open** to load a project
- **Suspend/Resume** to simplify display
- **Add to Tree** to get multiple instances of a method, e.g. several T1 methods.

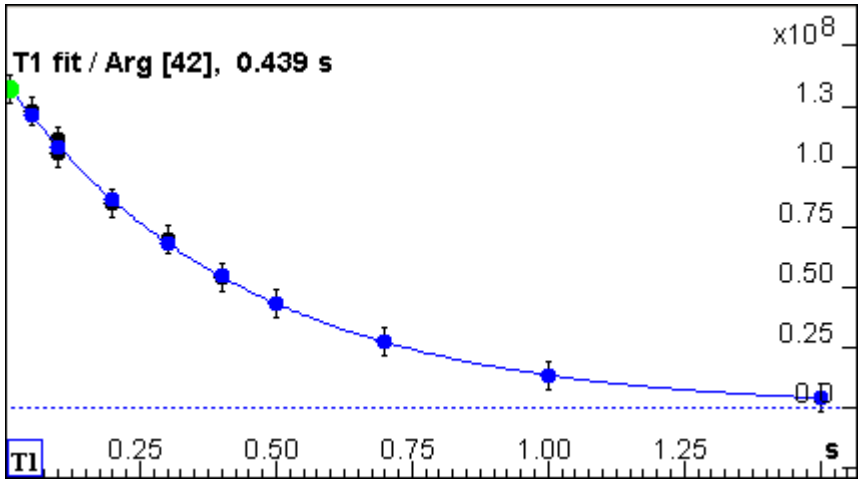
Error Analysis

- error of Y values via S/N, repetition experiments

Available repetition experiments can also be used to estimate systematic errors in the data. Peak intensities/integrals are compared.

Select error calculation method

- (•) systematic error from variance averaging
- ( ) systematic error from worst case estimate per peak



- errors of fitted parameters

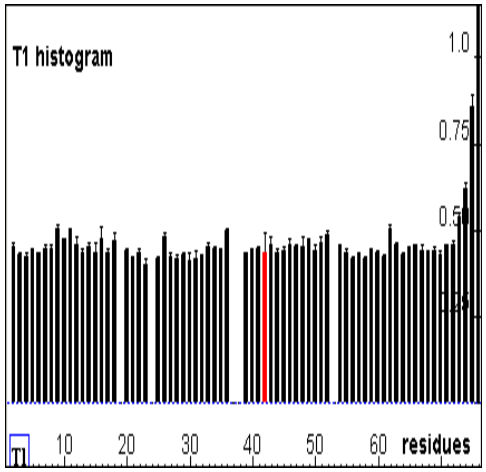
Fit parameter error estimation can be based on different methods

Select error estimation method

- ( ) error estimation by fit
- (•) error estimation by weighted fit
- ( ) error estimation by Monte Carlo simulation

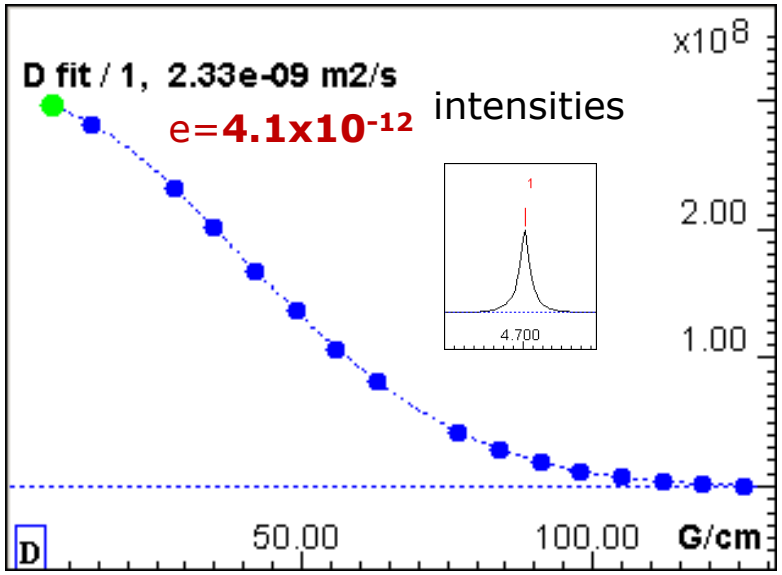
Fitted parameters are calculated and given with a confidence interval

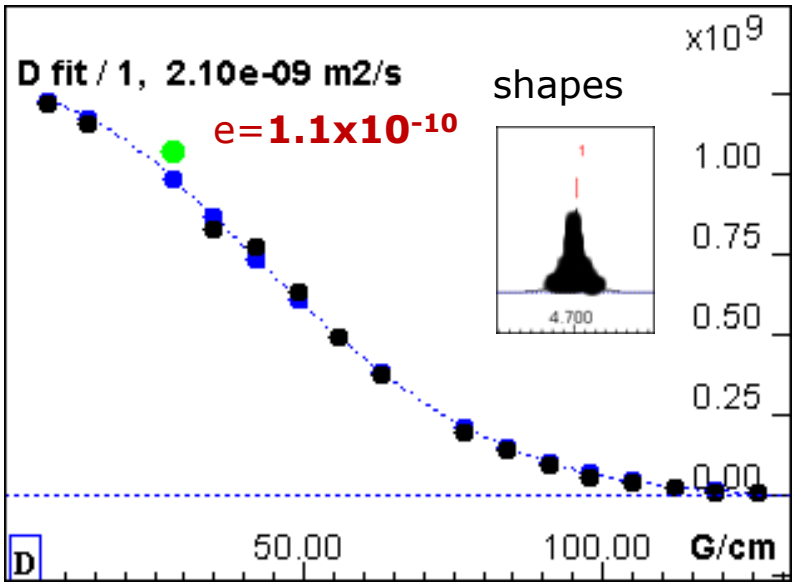
Confidence level 95.0 %

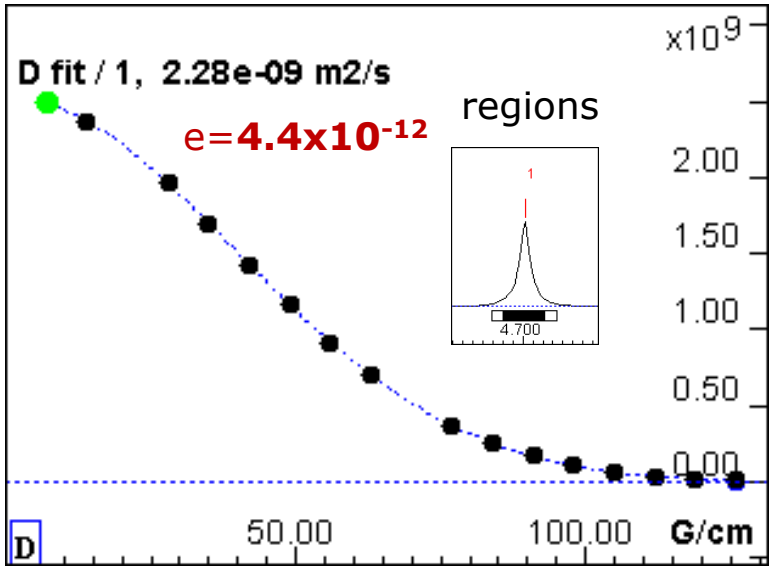


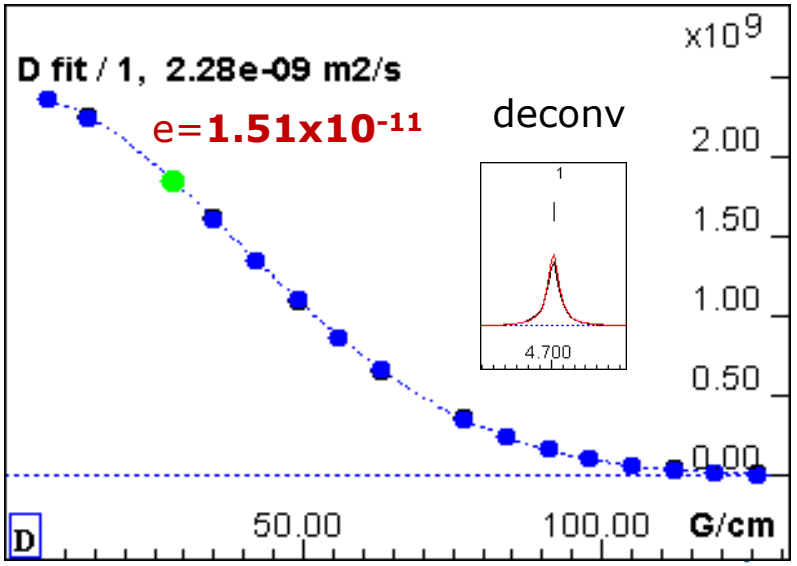
D [m2/s]	error
3.82e-10	2.979e-12
2.31e-10	1.503e-12
3.57e-10	1.306e-11
3.80e-10	4.461e-12
3.83e-10	3.645e-12
2.34e-10	1.568e-12
2.34e-10	9.702e-12
3.56e-10	6.383e-12
3.44e-10	6.766e-12
3.23e-10	1.181e-11
3.48e-10	1.183e-11
3.51e-10	8.515e-12
3.79e-10	5.276e-12
3.85e-10	2.974e-12
3.80e-10	4.052e-12

1D Peak Integration Techniques

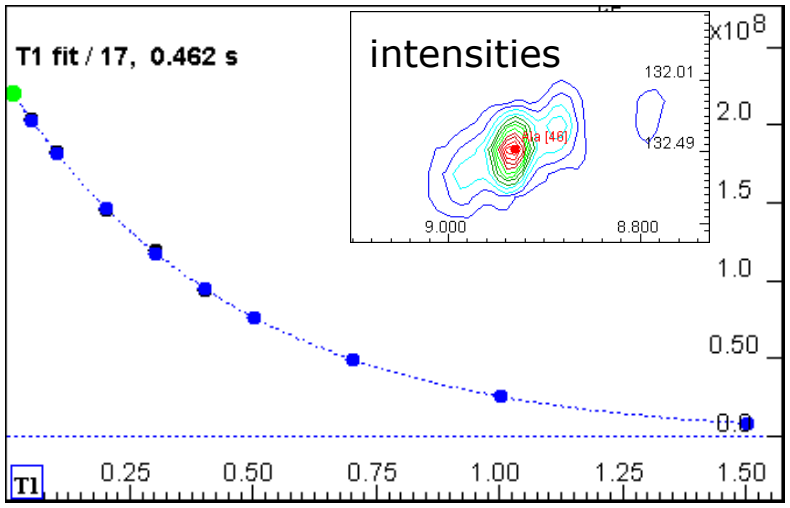


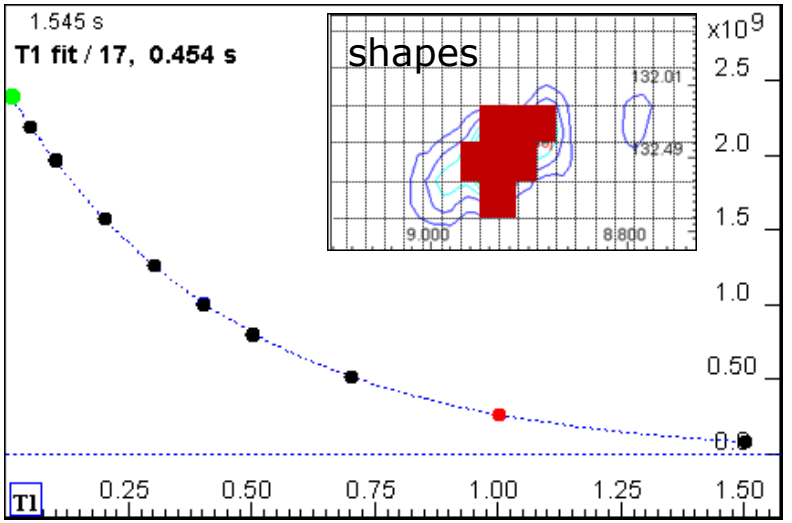


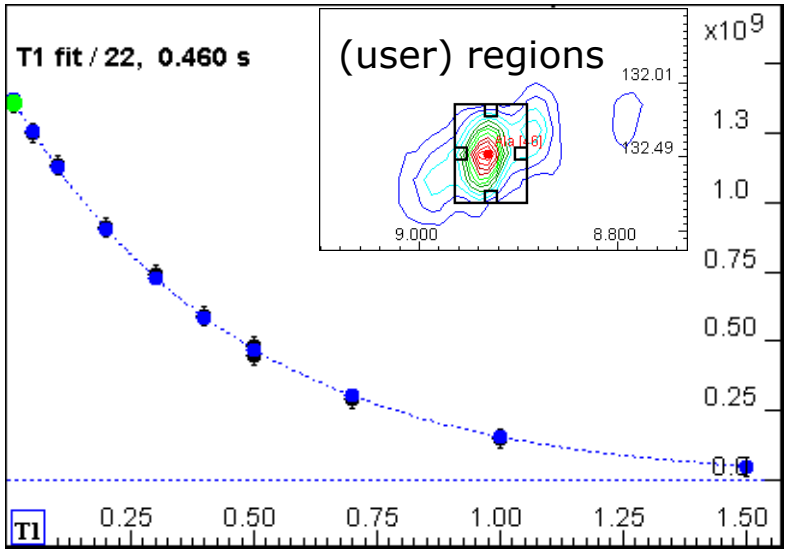


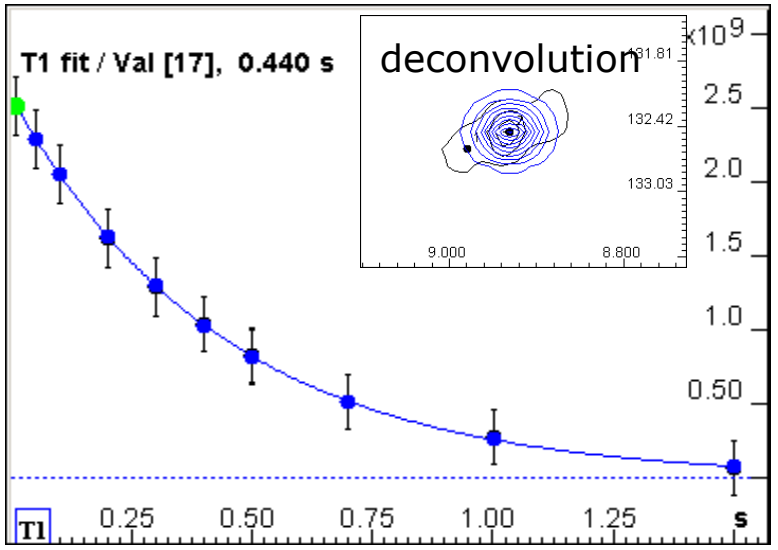


2D Peak Integration Techniques

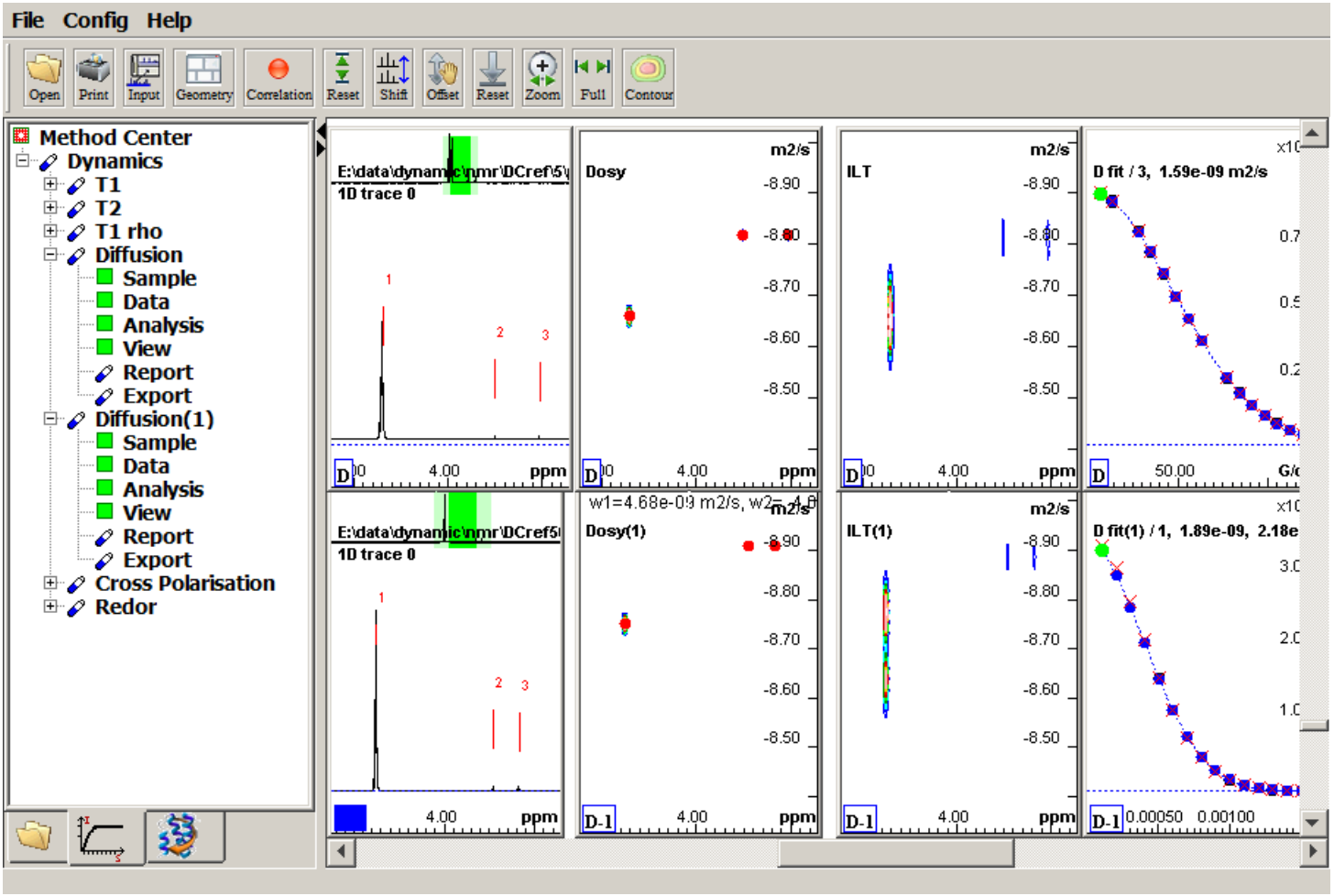








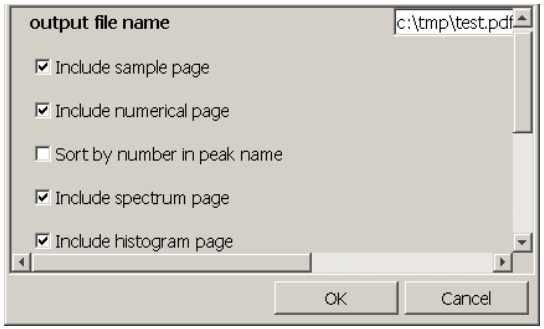
Working with Multiple Methods

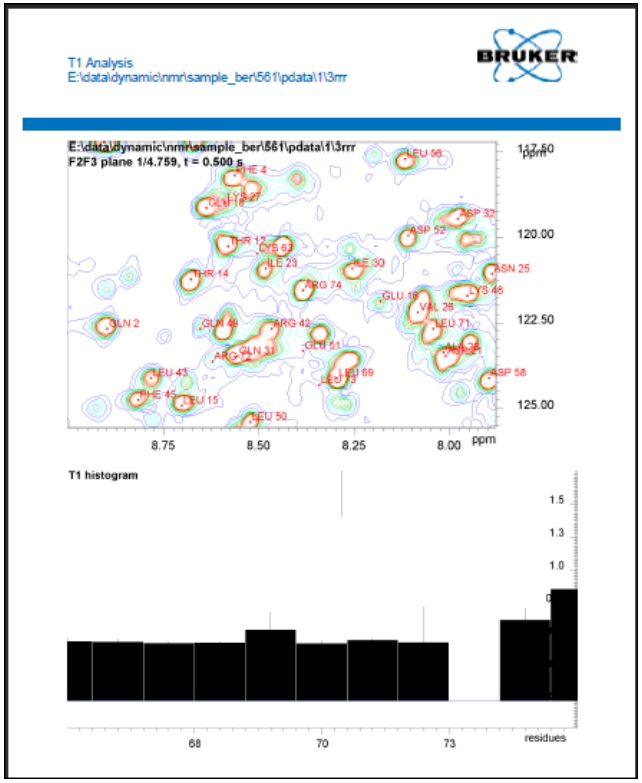


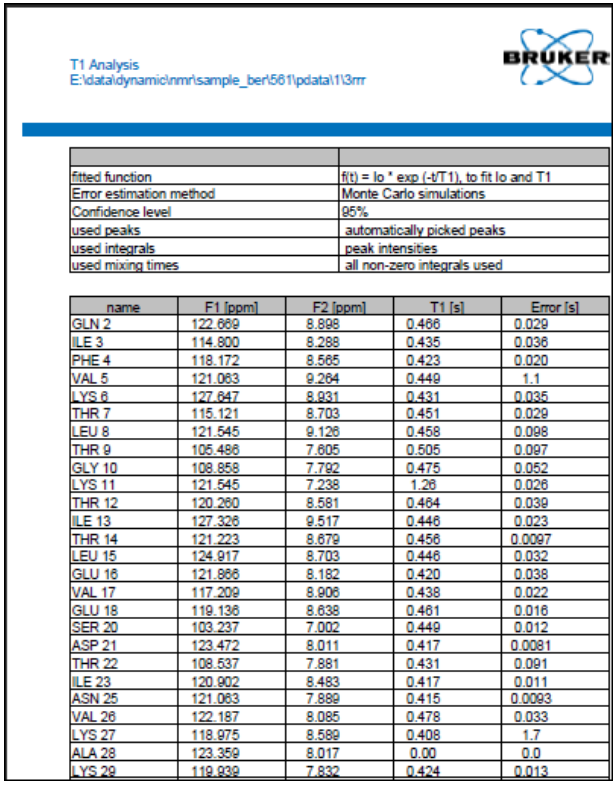
- Different methods
- Multiple instances of the same method
- Compare analyses
- Compare data acquired differently ~optimization

Report & Export

- Configurable



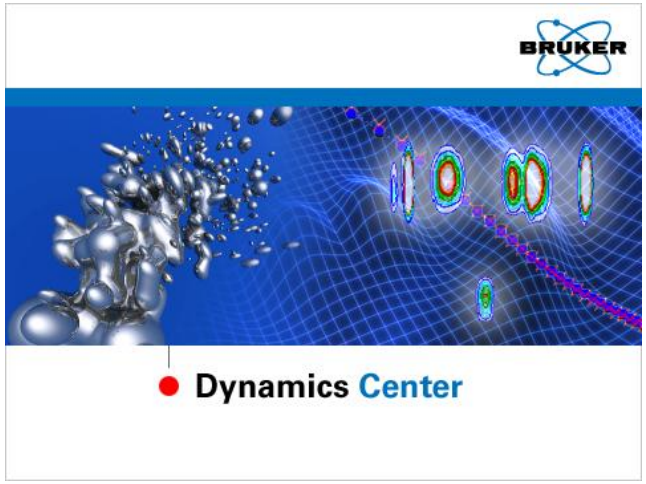




fitted function	f(t) = Io * exp (-t/T1), to fit Io and T1
Error estimation method	Monte Carlo simulations
Confidence level	95%
used peaks	automatically picked peaks
used integrals	peak intensities
used mixing times	all non-zero integrals used

name	F1 [ppm]	F2 [ppm]	T1 [s]	Error [s]
GLN 2	122.669	8.898	0.466	0.029
ILE 3	114.800	8.288	0.435	0.036
PHE 4	118.172	8.565	0.423	0.020
VAL 5	121.063	9.264	0.449	1.1
LYS 6	127.647	8.931	0.431	0.035
THR 7	115.121	8.703	0.451	0.029
LEU 8	121.545	9.126	0.458	0.098
THR 9	105.486	7.605	0.505	0.097
GLY 10	108.858	7.792	0.475	0.052
LYS 11	121.545	7.238	1.26	0.026
THR 12	120.260	8.581	0.464	0.039
ILE 13	127.326	9.517	0.446	0.023
THR 14	121.223	8.679	0.456	0.0097
LEU 15	124.917	8.703	0.446	0.032
GLU 16	121.866	8.182	0.420	0.038
VAL 17	117.209	8.906	0.438	0.022
GLU 18	119.136	8.638	0.461	0.016
SER 20	103.237	7.002	0.449	0.012
ASP 21	123.472	8.011	0.417	0.0081
THR 22	108.537	7.881	0.431	0.091
ILE 23	120.902	8.483	0.417	0.011
ASN 25	121.063	7.889	0.415	0.0093
VAL 26	122.187	8.085	0.478	0.033
LYS 27	118.975	8.589	0.408	1.7
ALA 28	123.359	8.017	0.00	0.0
LYS 29	119.939	7.832	0.424	0.013

- PDF Report
- Export
  - **Text** or **XLS**
  - integrals & errors included
  - all information to redo calculation
  - interface to relax and SIMPSON



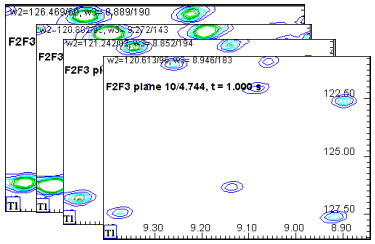
Protein Dynamics

(Wolfgang Bermel, Clemens Anklin, Daniel Matthieu)

Standard workflow

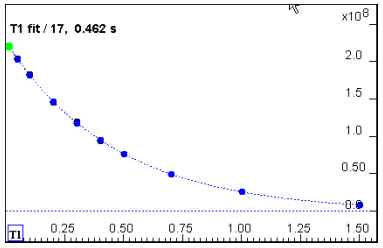
acquisition and processing of [pseudo 3D] data

conventional, NUS



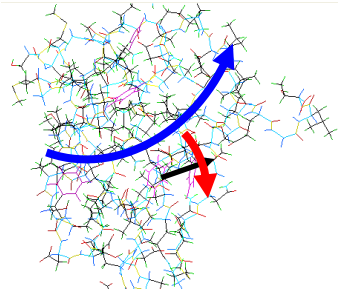
peak integrals as function of mixing times, RF strengths

peak analysis, esp. integration



extraction of relaxation parameters

simple calculation or fit



translation into motional parameters

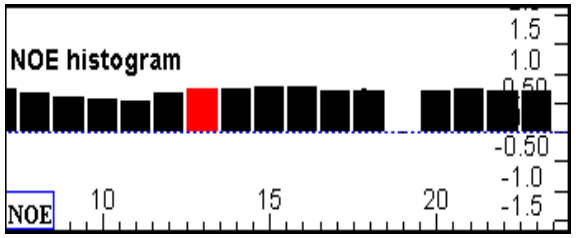
relaxation parameters

spectral densities of motions modeled with (S2, τ_c, τ_i, ..)

Hetero nuclear relaxation experiments

method pulse program

NOE hsqcnoef3gpsi

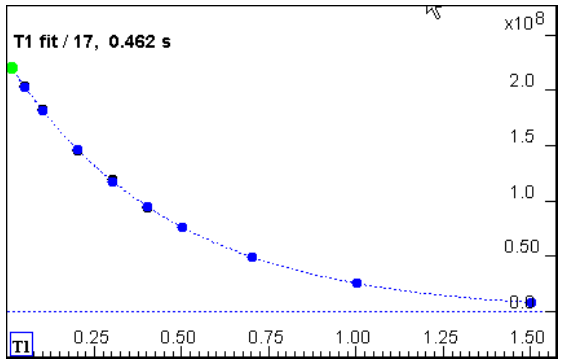


ratio

$$NOE^i = \frac{I^i{}_s}{I^i{}_u}$$

T_1 hsqct1etf3gpsi3d

T_2 hsqct2etf3gpsi3d



fit

$$I(t) = A * e^{-t/B}$$

T_{1rho} hsqctretf3gpsi3d

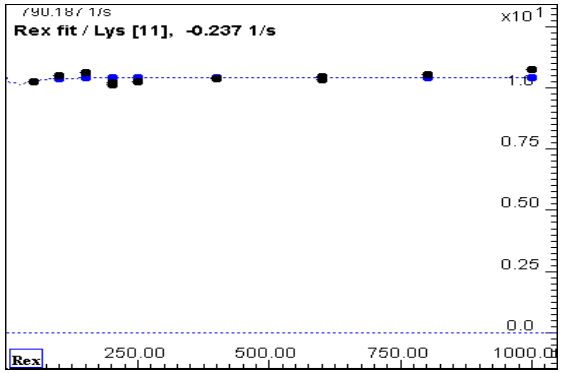
add. calculation

(T_2 from T_1, T_{1rho})

R_{ex} hsqcrexetf3gpsi3d

JACS 123, 11341, 2001

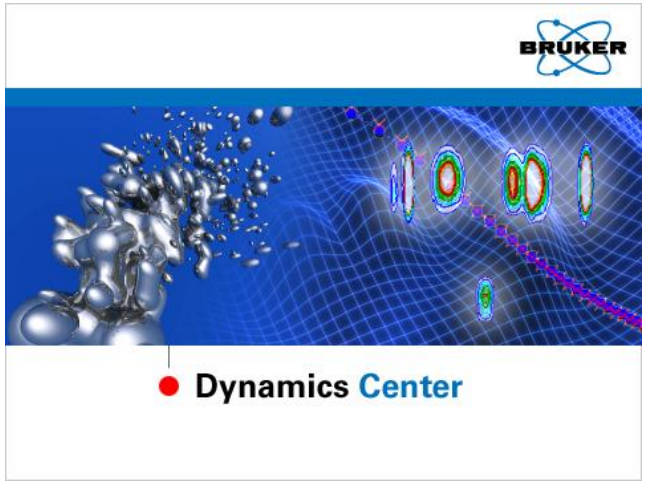
(2 sites, slow exchange)



fit

$$R^{eff}(\tau_{cp}) = R_0 + K_{ex} * (1 - \frac{\sin(\delta\omega\,\tau_{cp})}{\delta\omega\,\tau_{cp}})$$

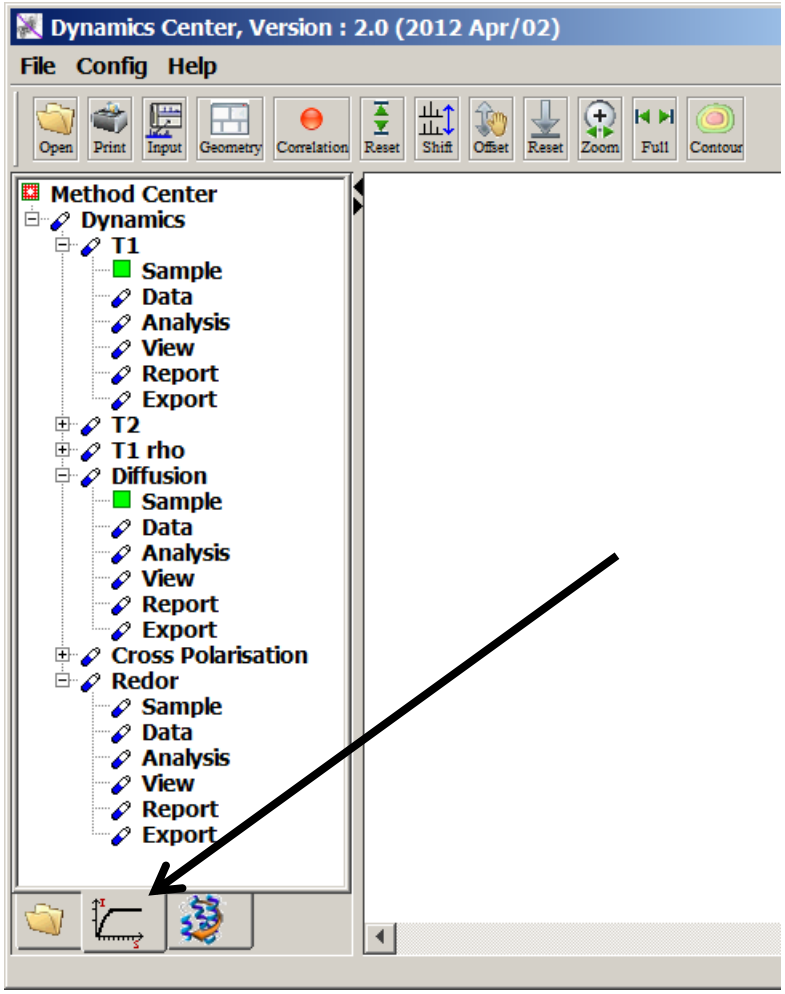
model selection



General Dynamics

(Klaus Zick, Aitor Moreno, Sebastian Wegner,
Robin Stein, Anna Codina)

Overview



- Independent of molecule, includes mixtures
- T_1 T_2, T_{1rho} (1D, $2D^{ps}$, 2D, $3D^{ps}$)
- Diffusion, CP (1D, $2D^{ps}$)
- REDOR ($2D^{ps}$)
- Detailed customization
- Automation, first steps