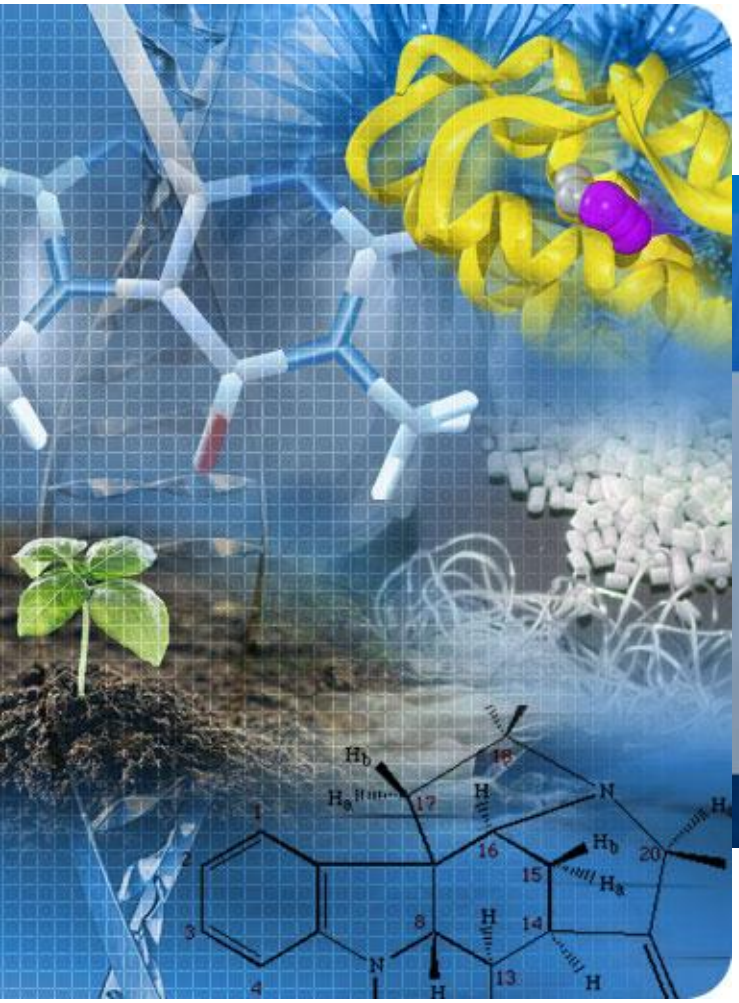


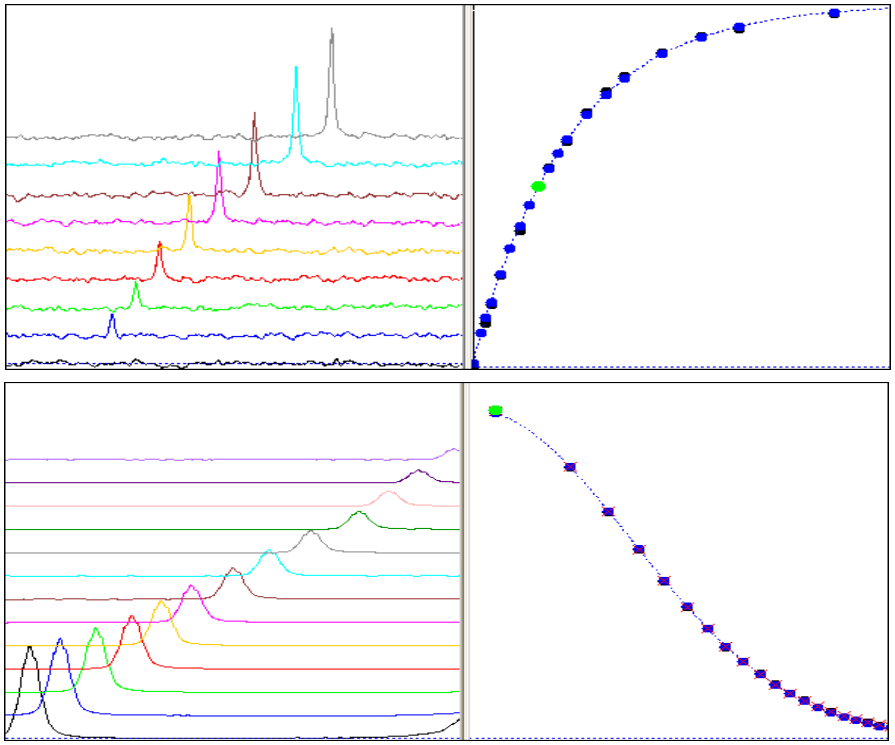
Dynamics Center

Eric Johnson

Symposium on Frontiers in Biomolecular NMR
Vanderbilt University
May 4, 2012

Dynamics

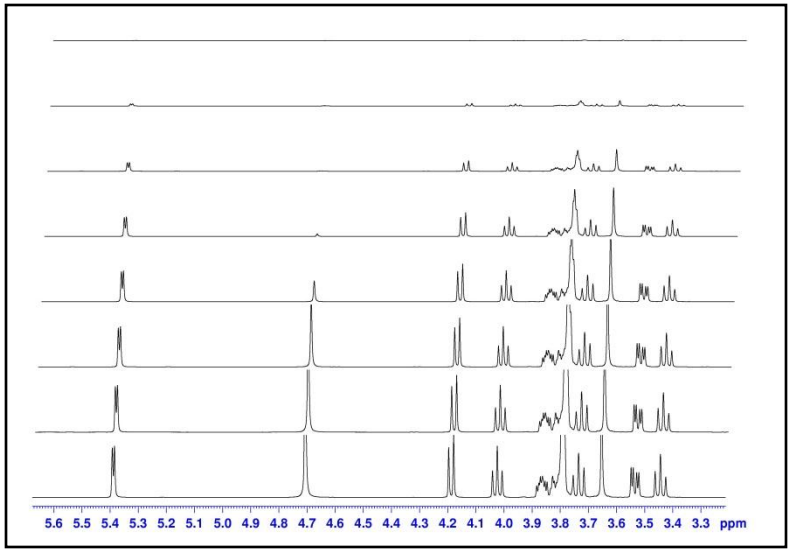
As “dynamics experiments” we regard a wide range of experiments where:
Series of spectra measured with dependence on **at least one variable** that is **not Fourier transformed**, e.g.

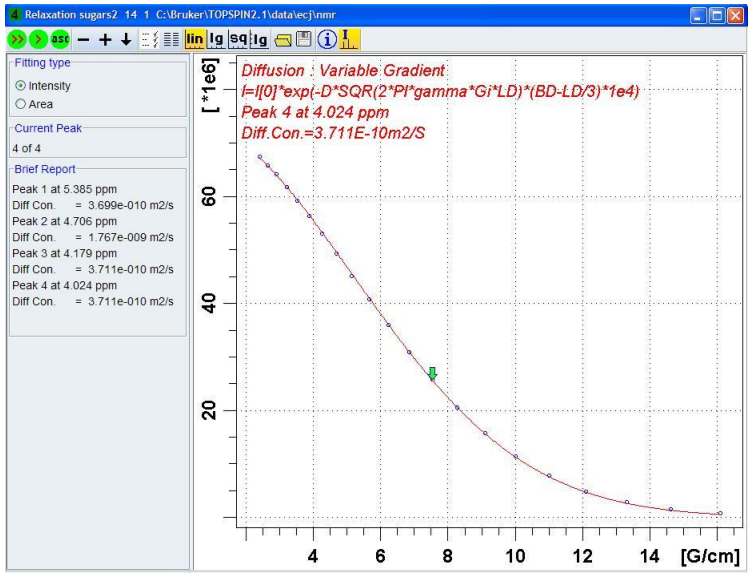


Relaxation:
signal amplitude as a function of mixing time

Diffusion:
signal amplitude as a function of gradient strength

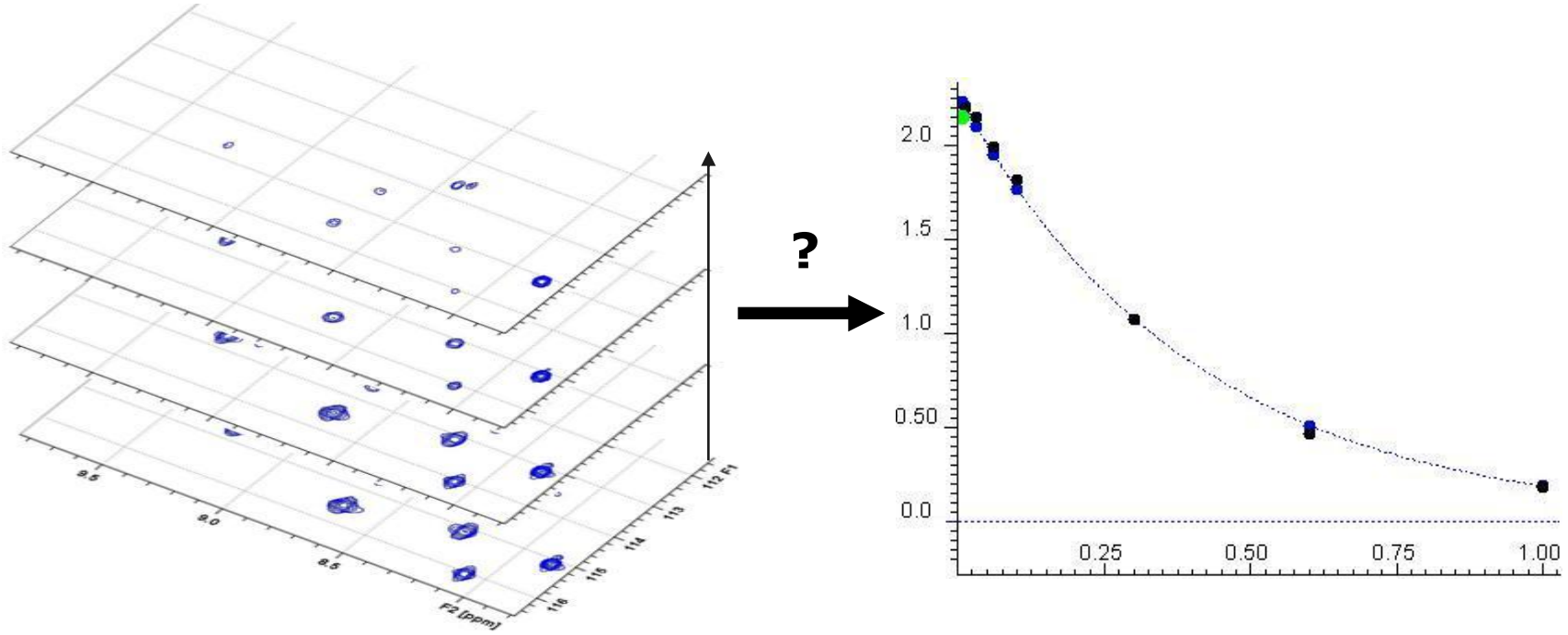
Analysis of small molecule relaxation data





T1/T2 Relaxation Guide has long been part of Topspin

Analysis of protein relaxation data

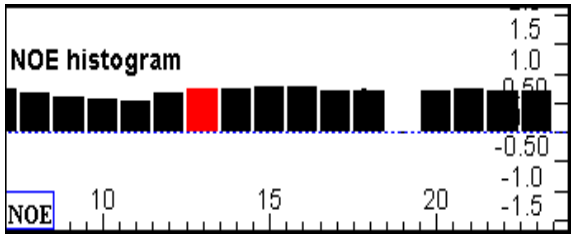


How do we go from 2D spectra (or pseudo-3D) to curve fitting?

Hetero nuclear relaxation experiments

method pulse program

NOE hsqcnoef3gpsi

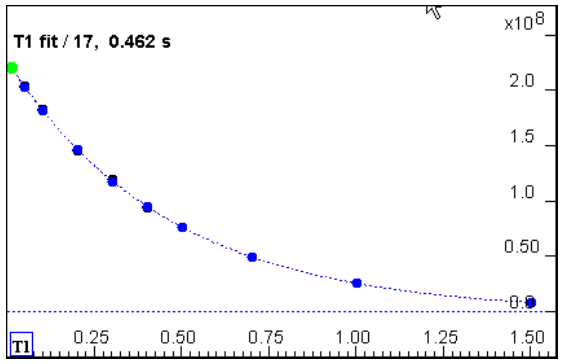


ratio

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

T_1 hsqct1etf3gpsi3d

T_2 hsqct2etf3gpsi3d



fit

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

T_{1rho} hsqctretf3gpsi3d

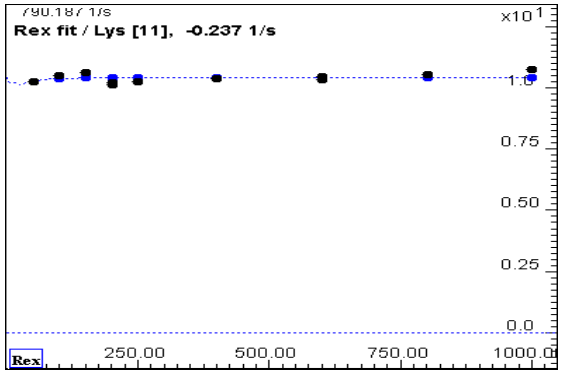
add. calculation

(T_2 from T_1, T_{1rho})

R_{ex} hsqcrexetf3gpsi3d

JACS 123, 11341, 2001

(2 sites, slow exchange)

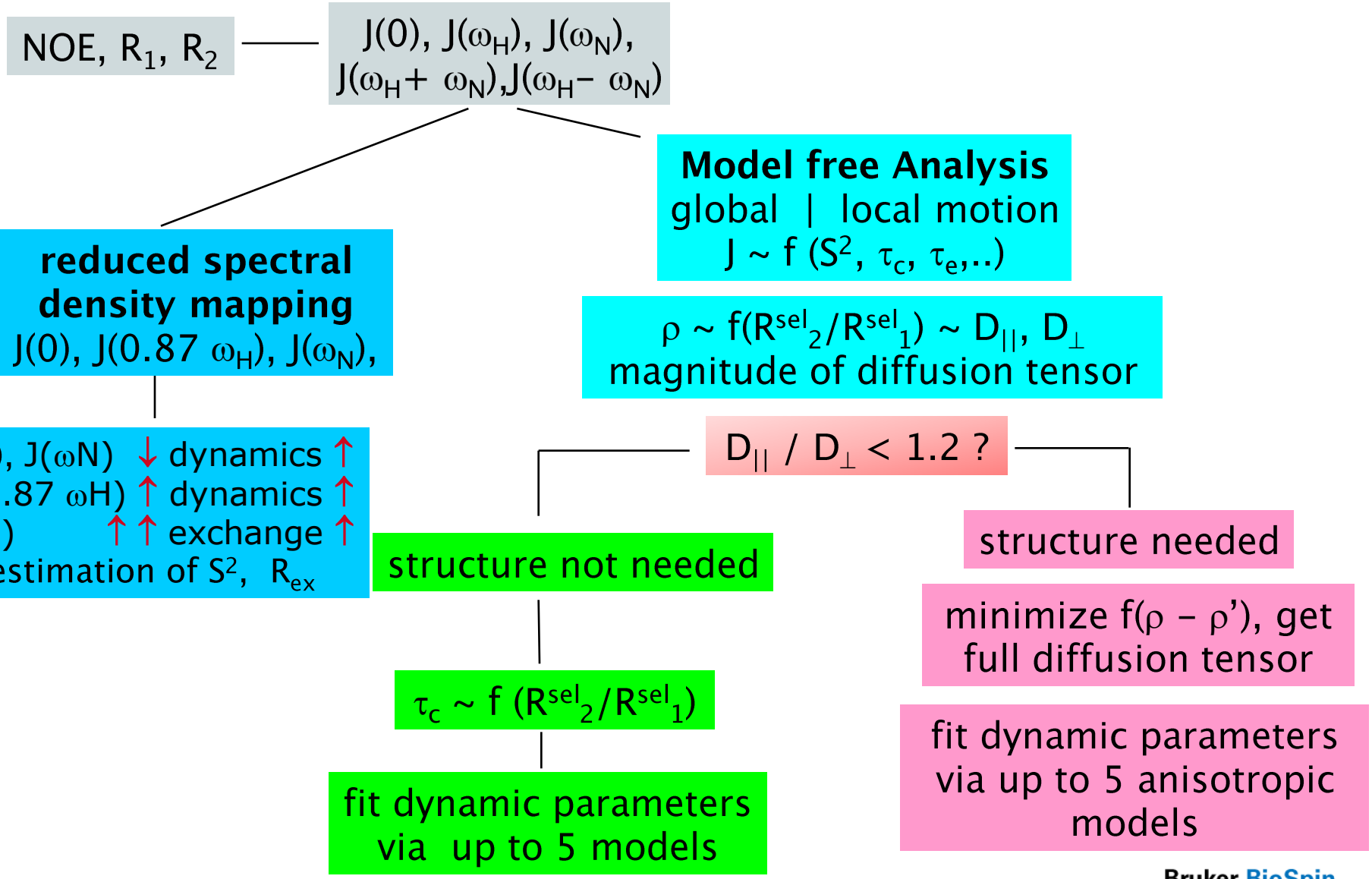


fit

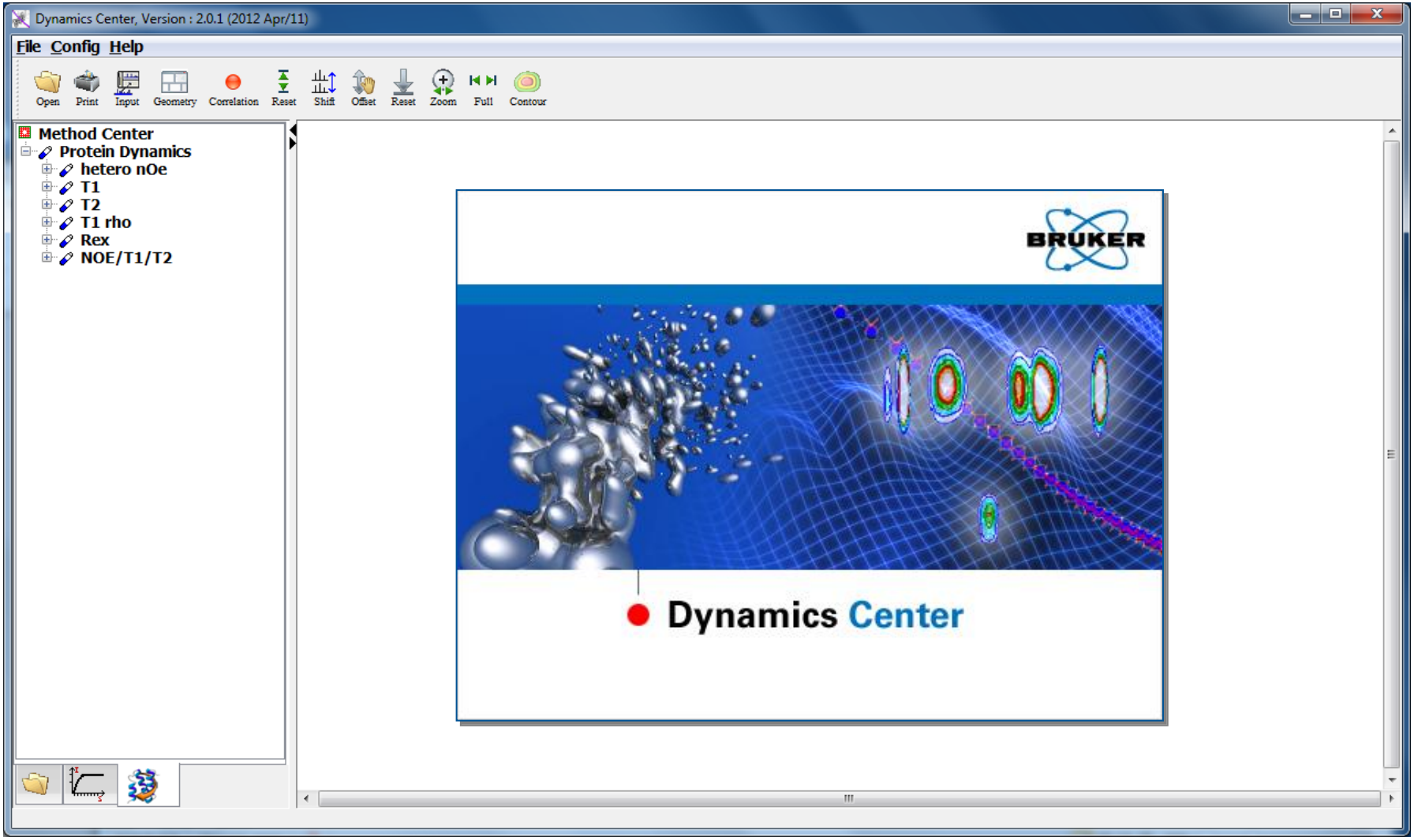
$$R^{eff}(\tau_{cp}) = R_0 + K_{ex} * (1 - \frac{\sin(\delta\omega\,\tau_{cp})}{\delta\omega\,\tau_{cp}})$$

model selection

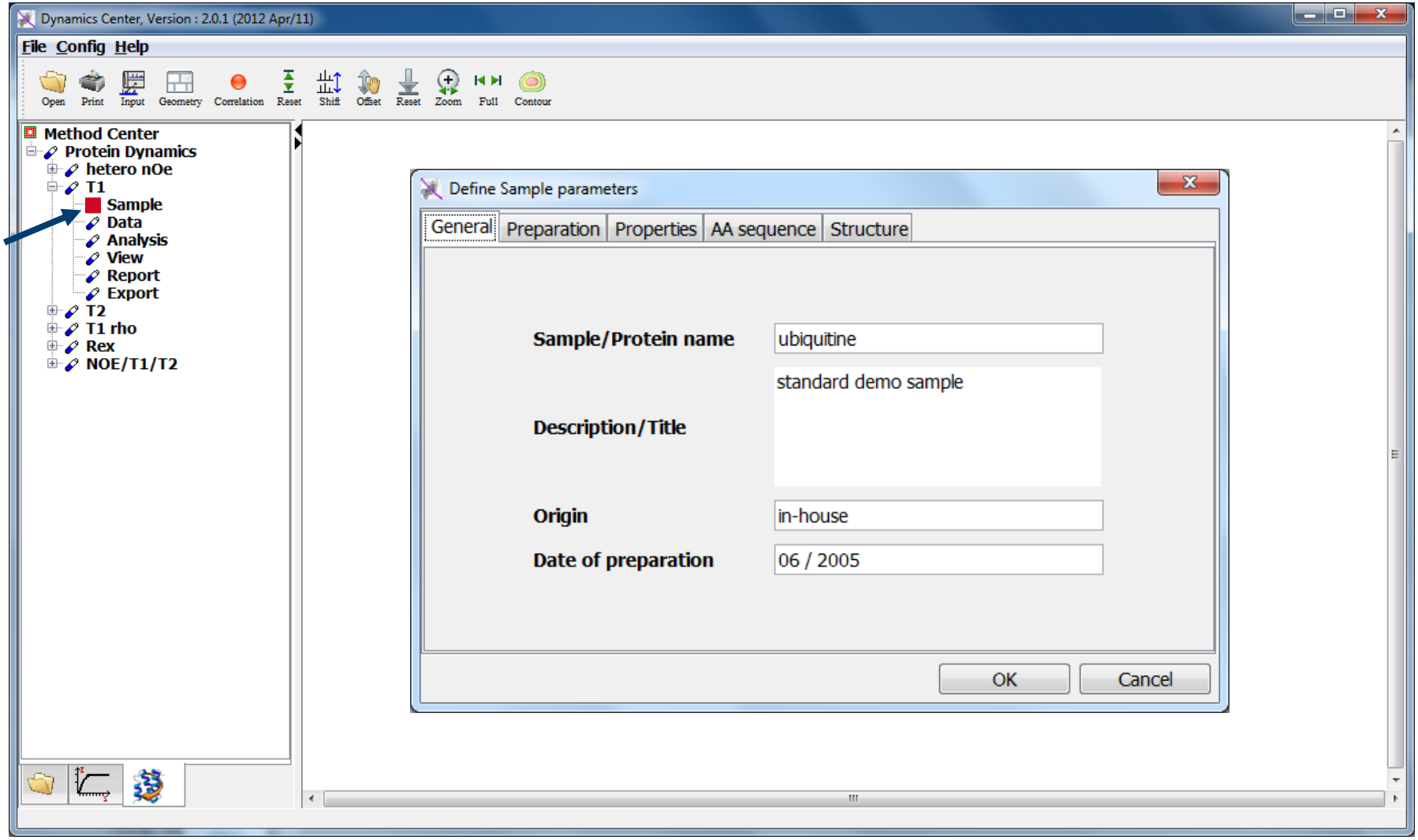
From Relaxation to Dynamics



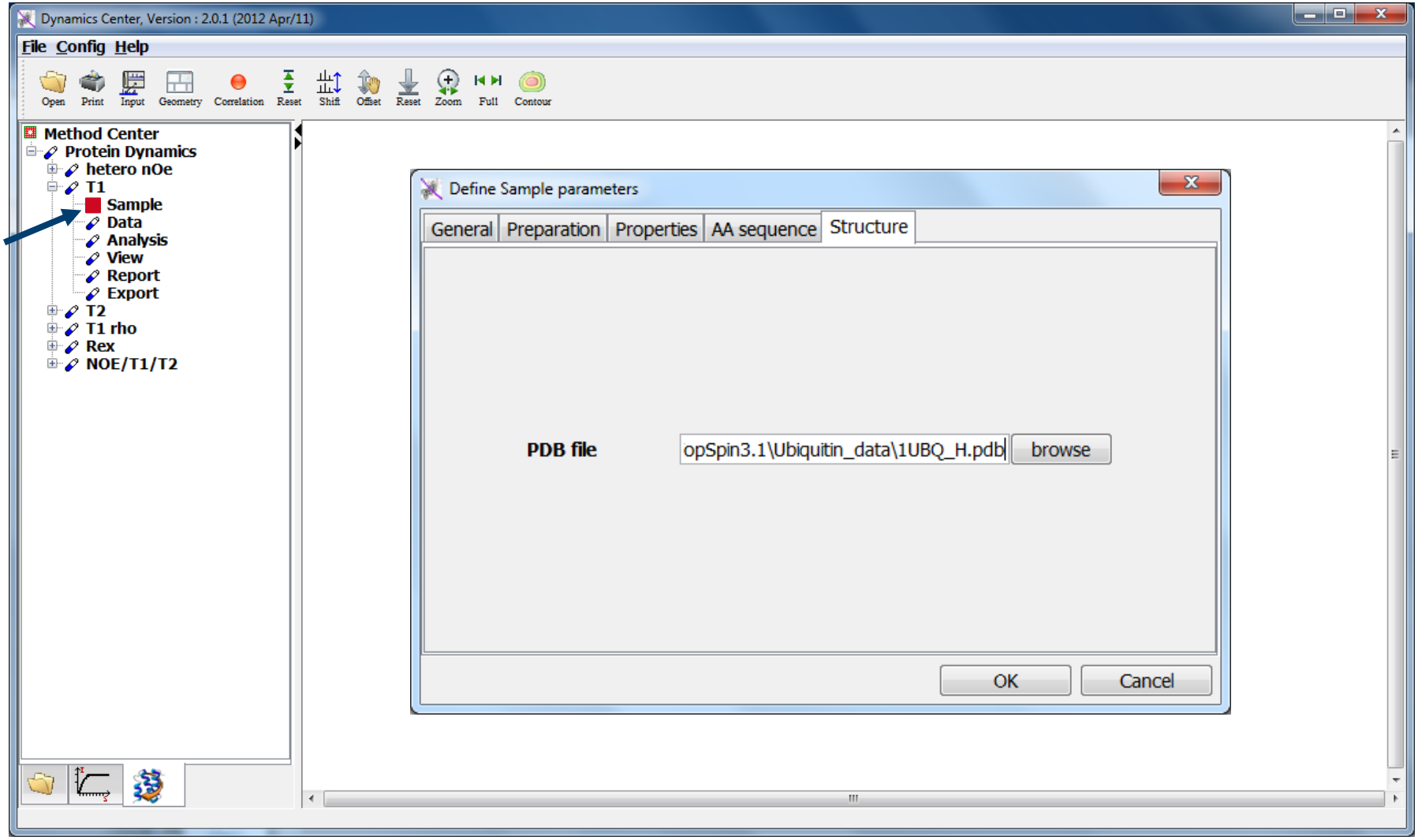
The New Dynamics Center...



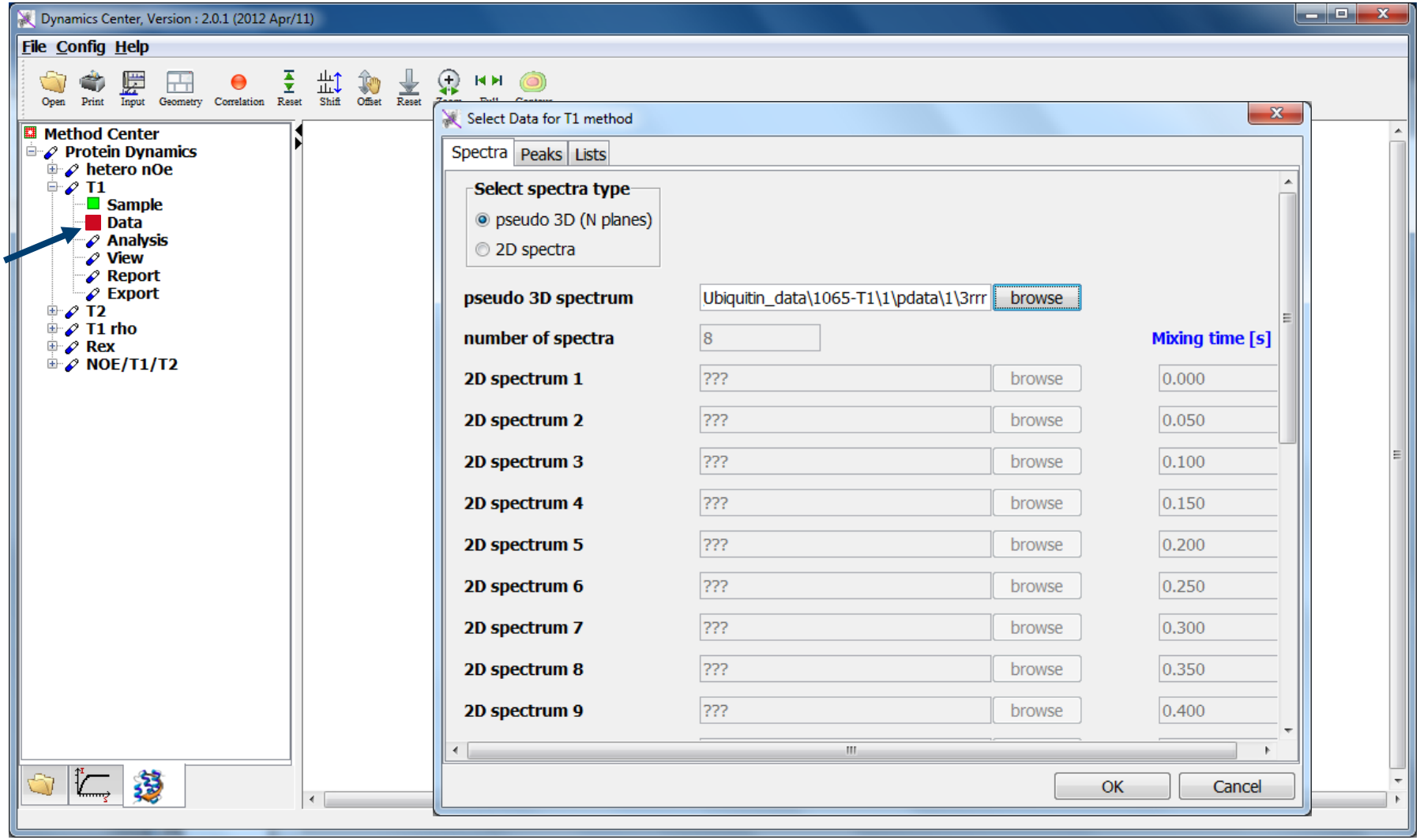
The New Dynamics Center...



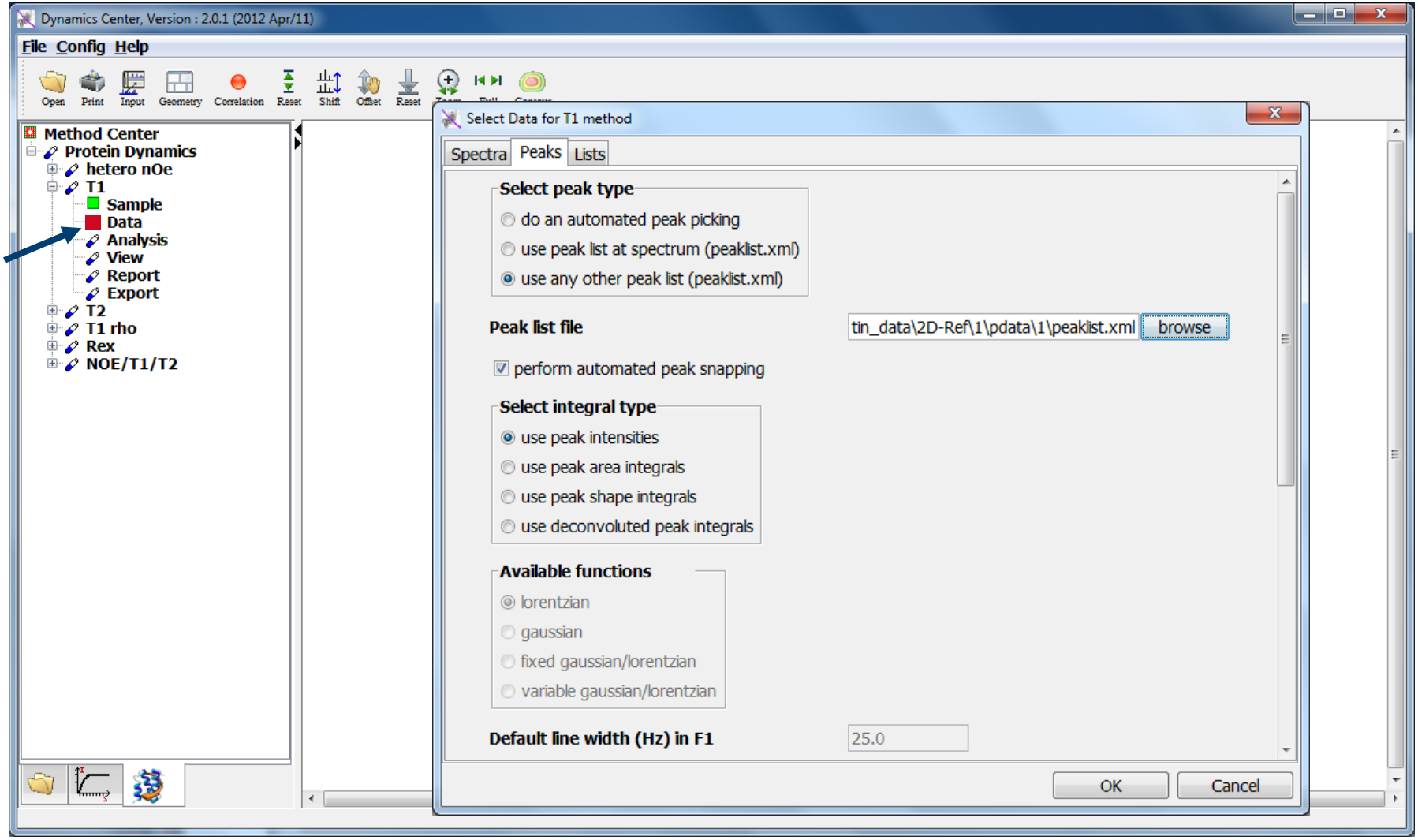
The New Dynamics Center...



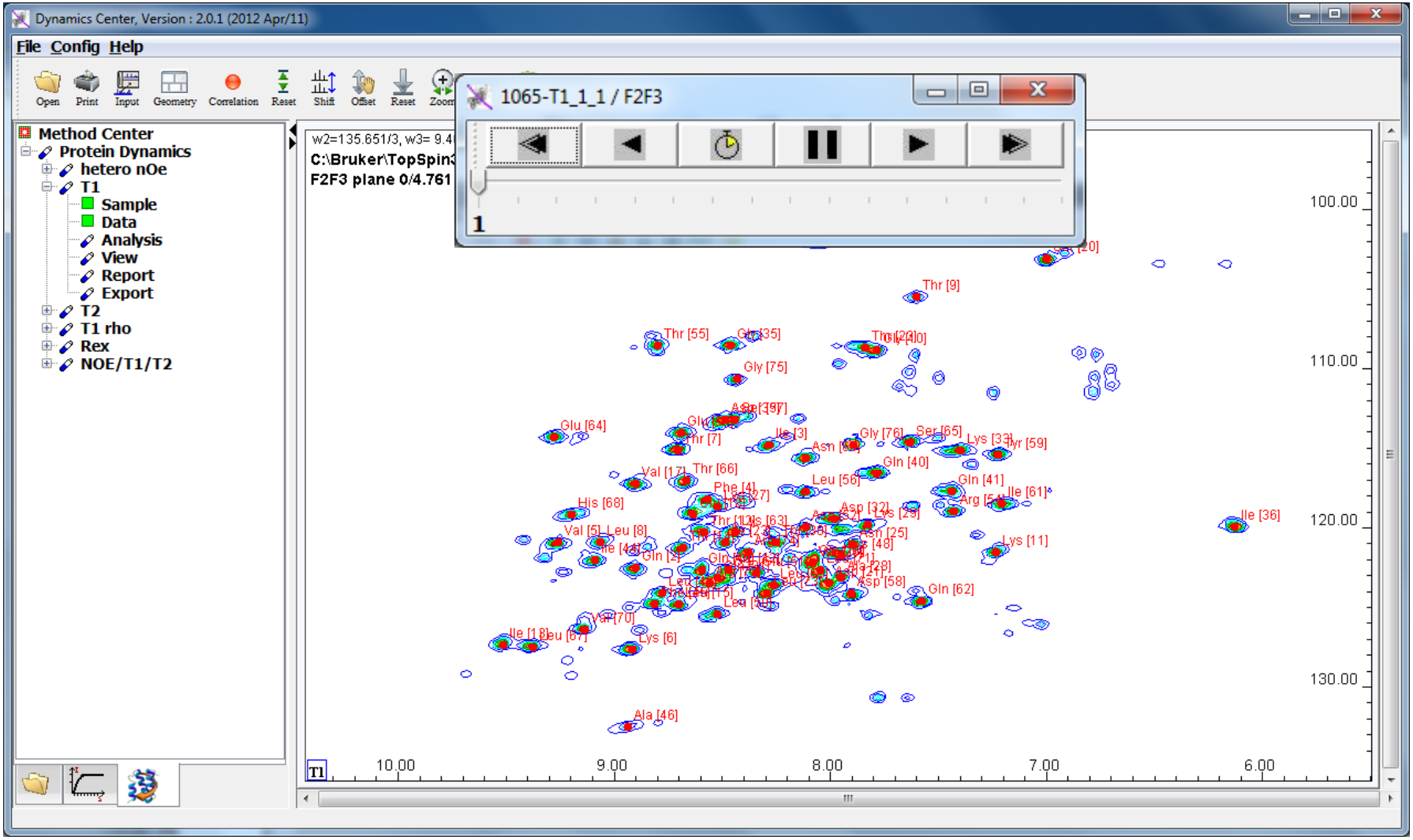
The New Dynamics Center...



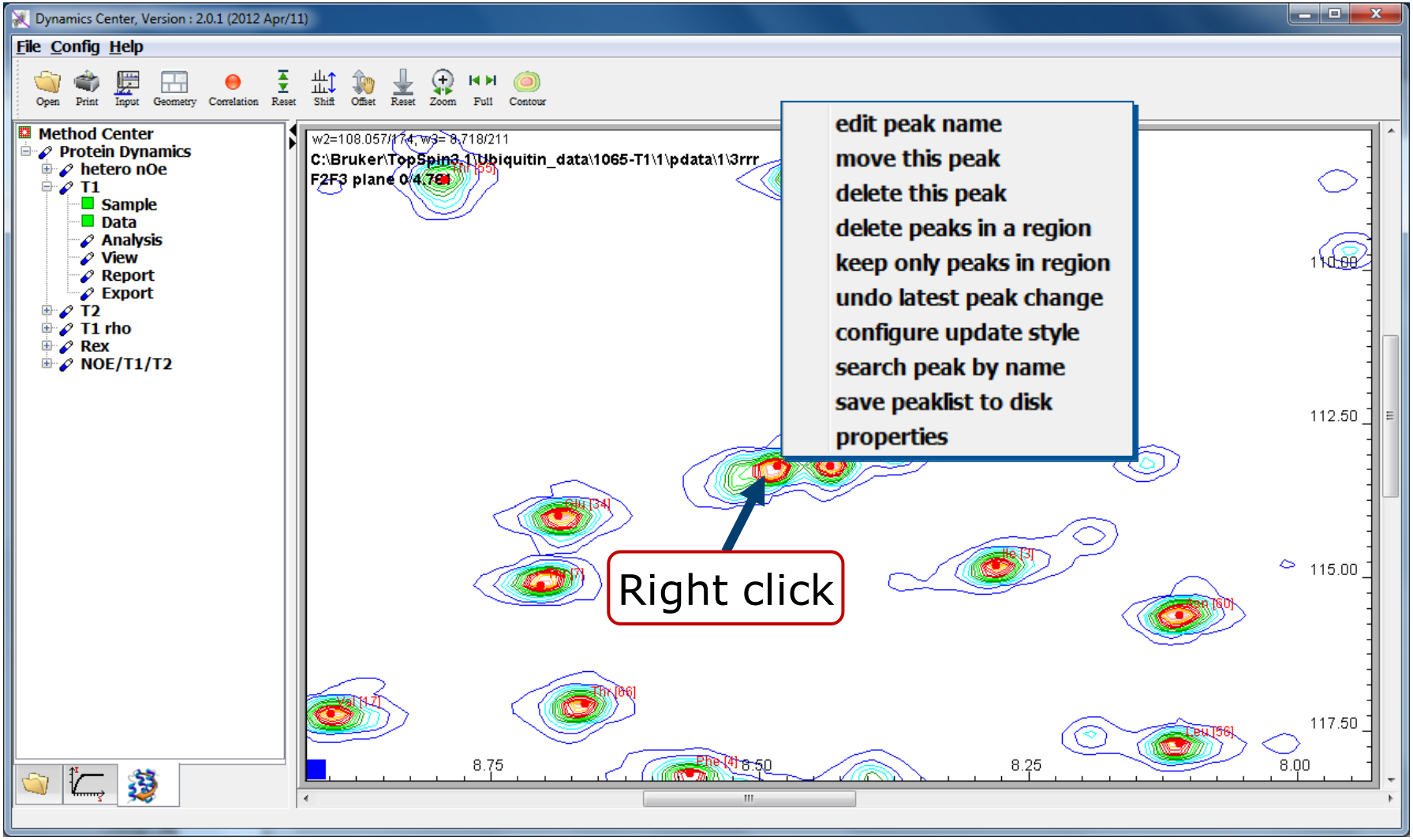
The New Dynamics Center...



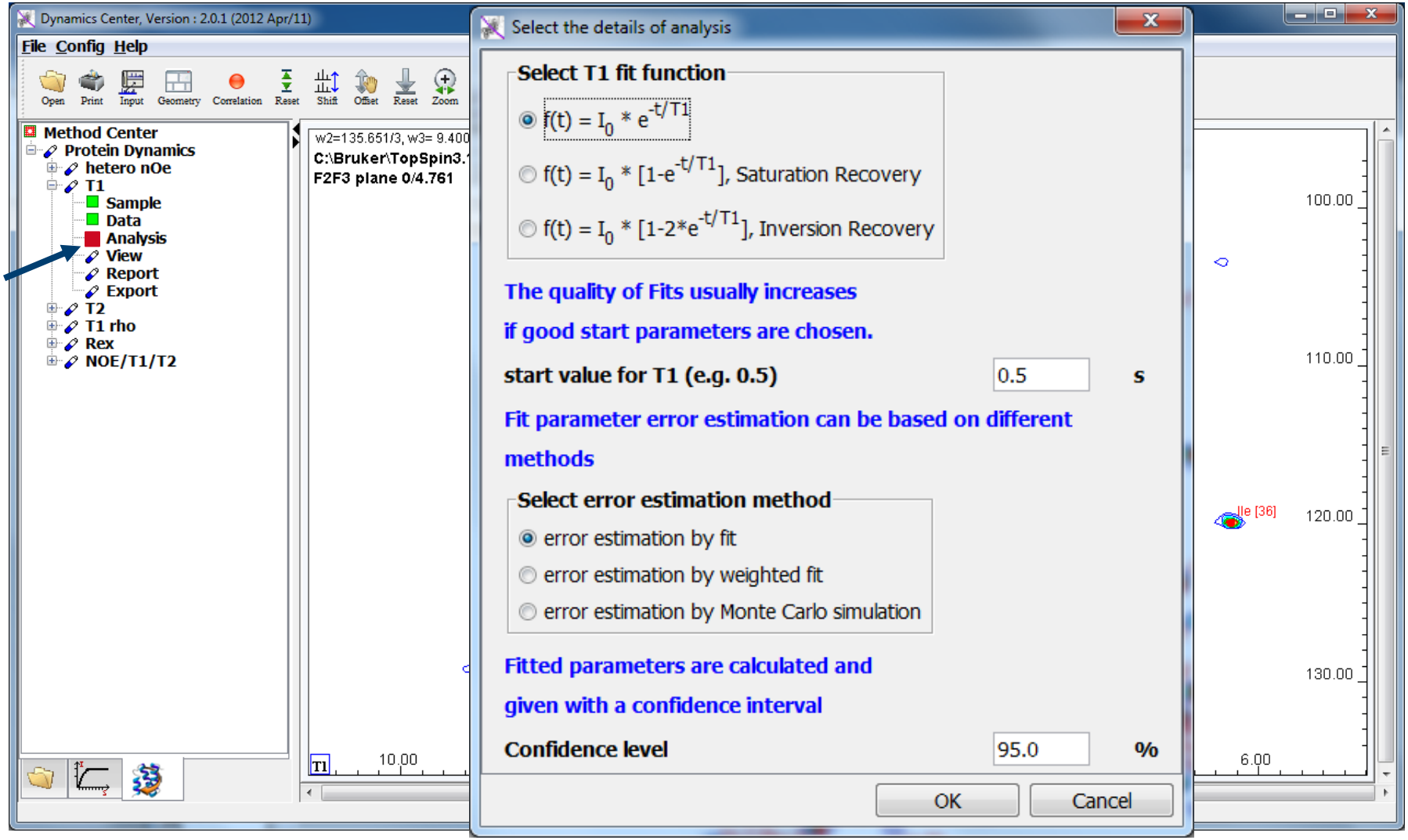
The New Dynamics Center...



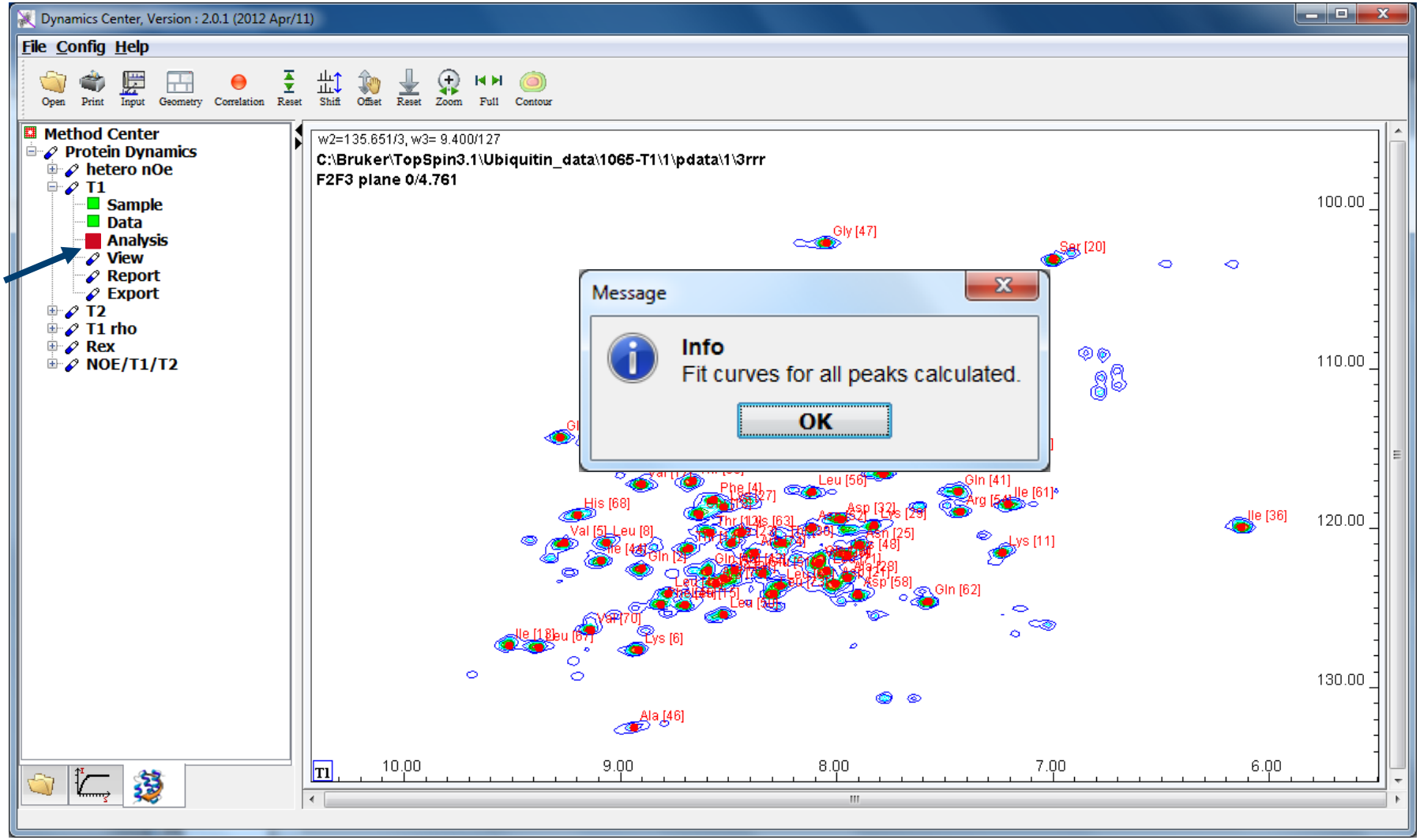
The New Dynamics Center...



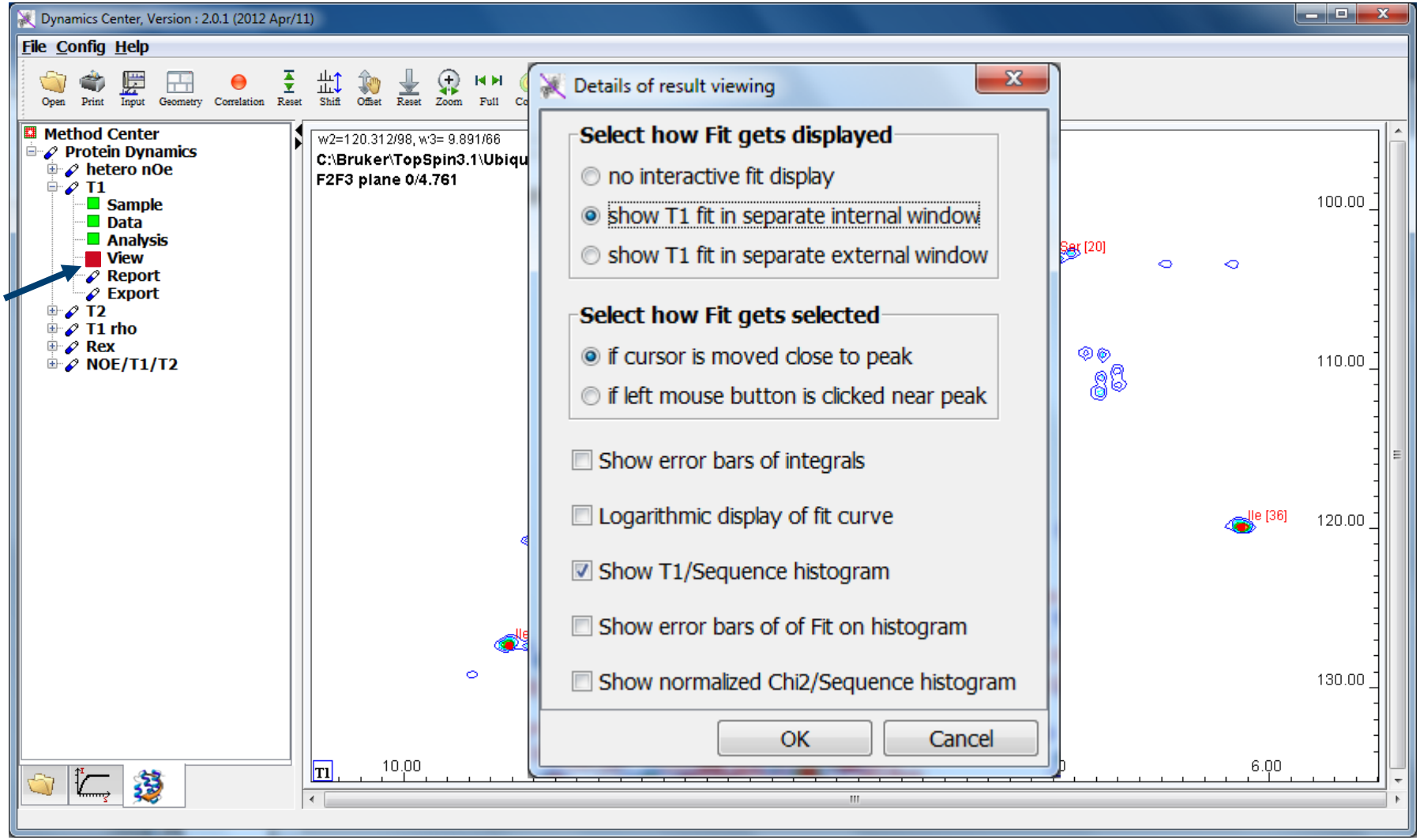
The New Dynamics Center...



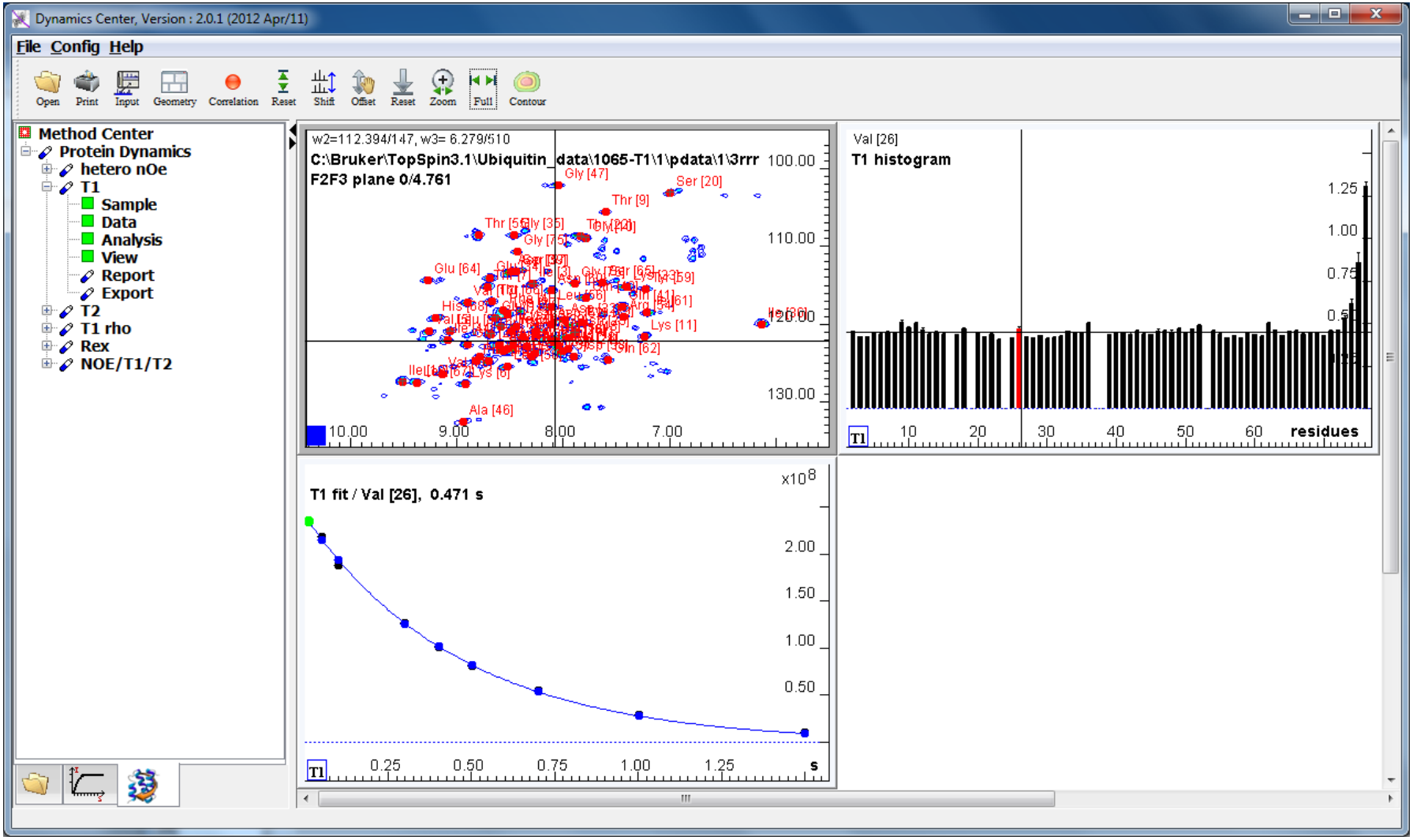
The New Dynamics Center...



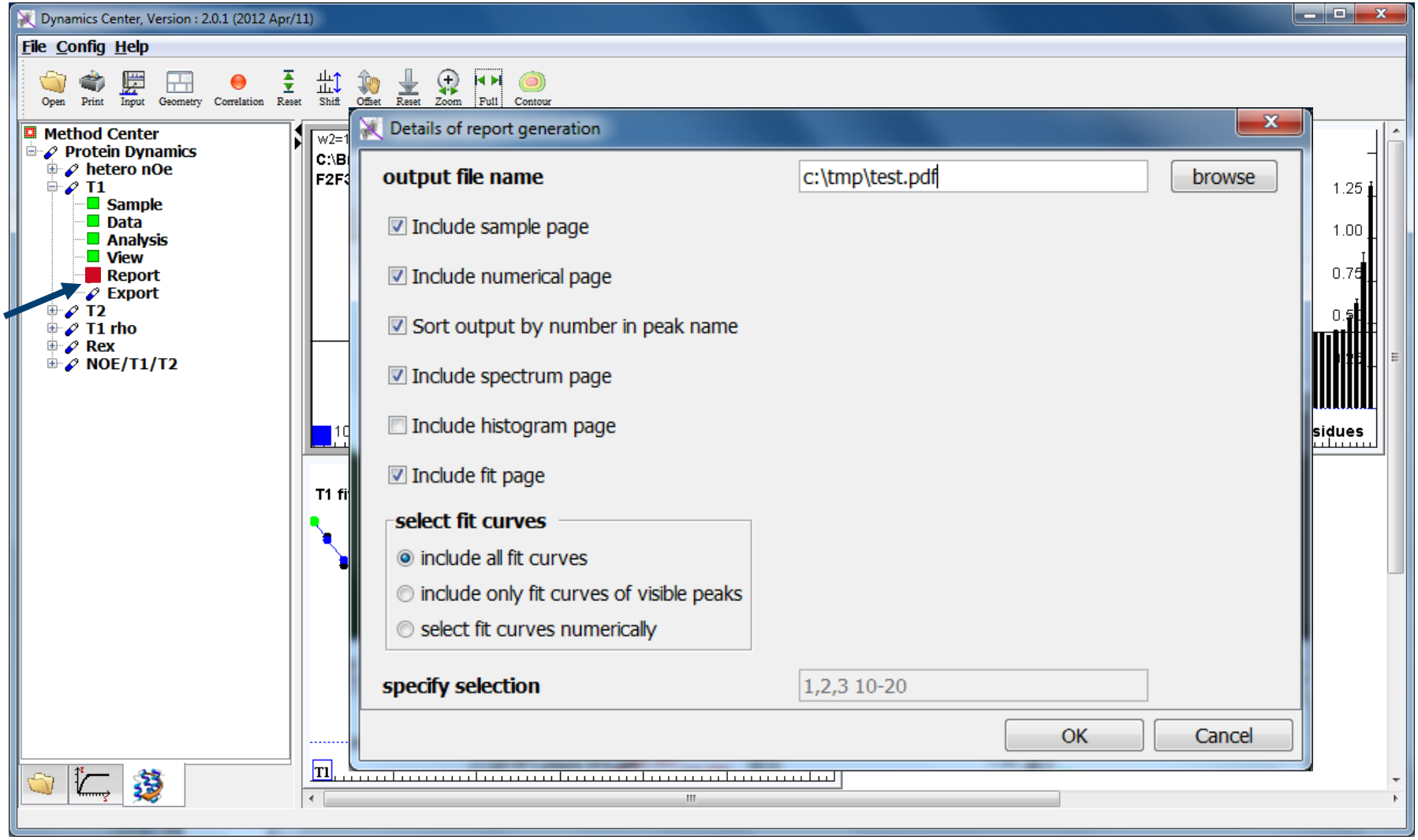
The New Dynamics Center...



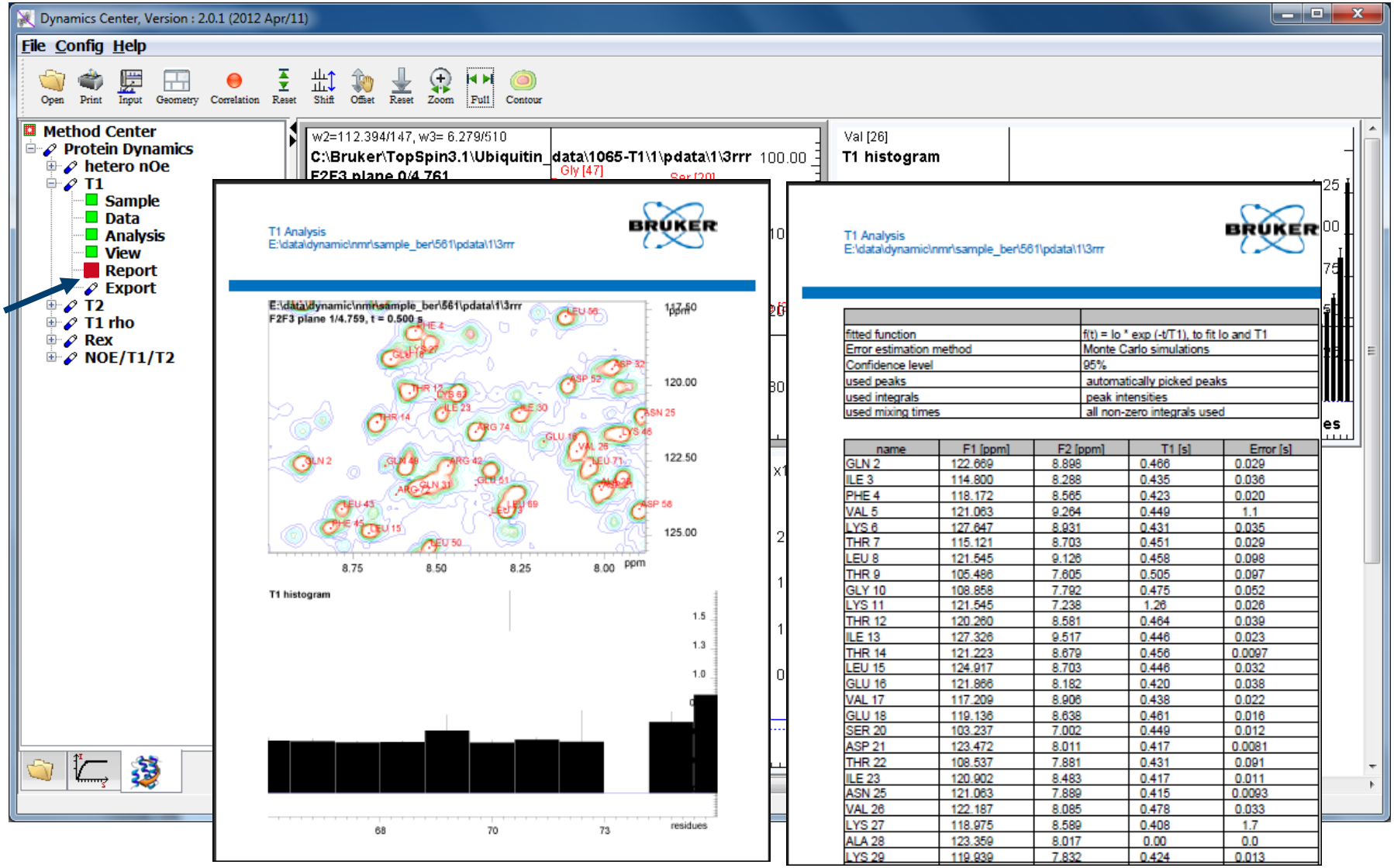
The New Dynamics Center...



The New Dynamics Center...

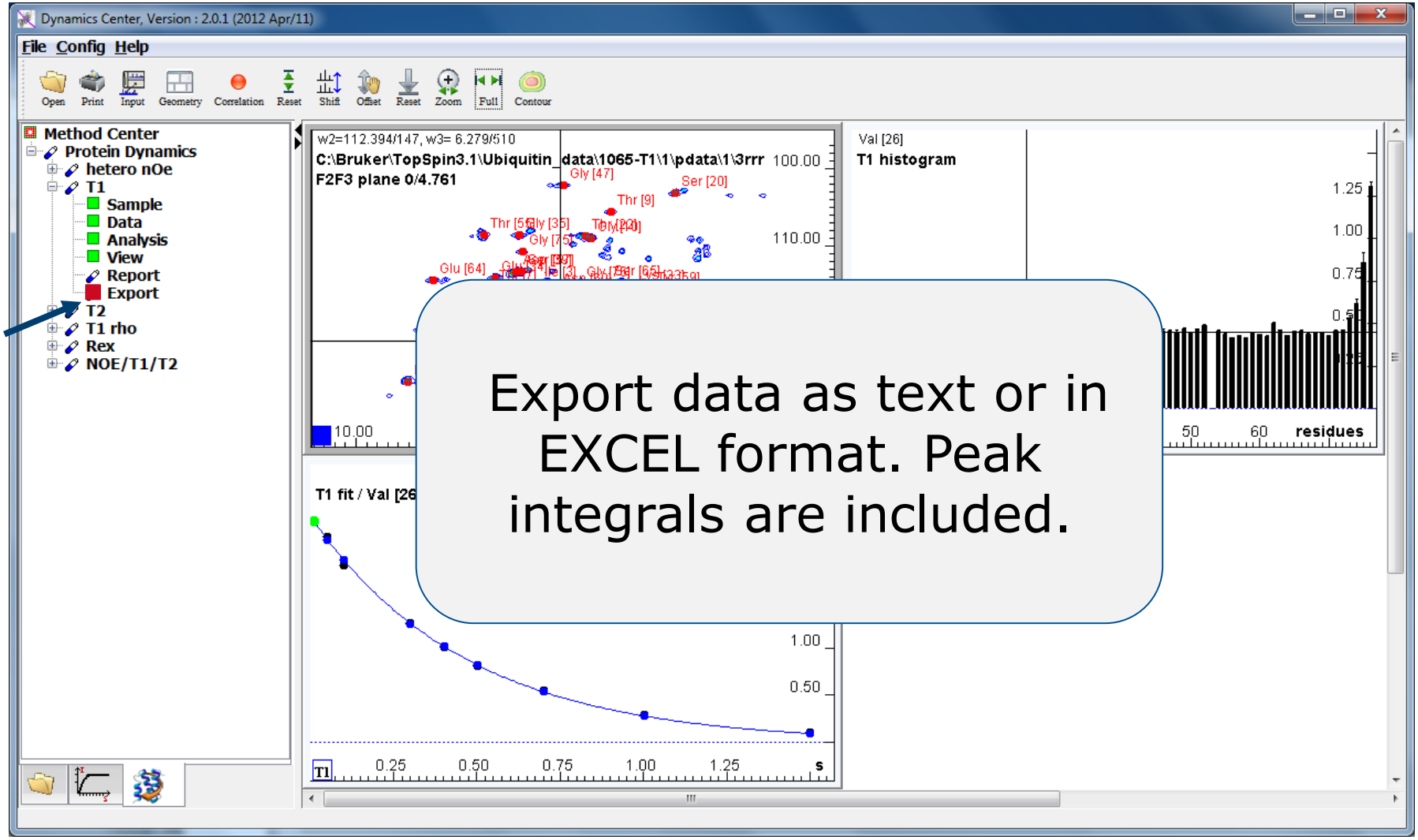


The New Dynamics Center...

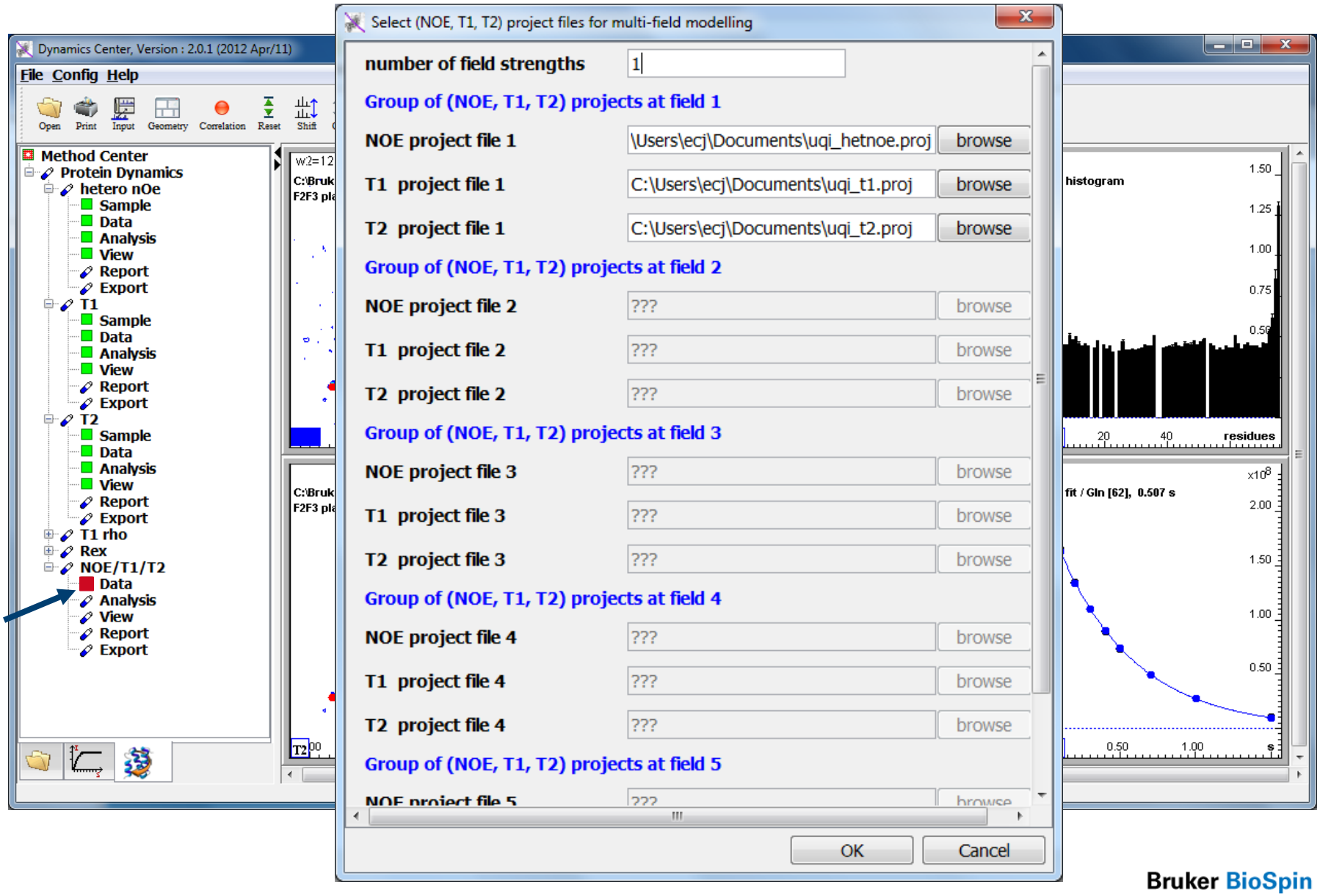


name	F1 [ppm]	F2 [ppm]	T1 [s]	Error [s]
GLN 2	122.669	8.898	0.466	0.029
ILE 3	114.800	8.288	0.435	0.036
PHE 4	118.172	8.565	0.423	0.020
VAL 5	121.063	9.264	0.449	1.1
LYS 6	127.647	8.931	0.431	0.035
THR 7	115.121	8.703	0.451	0.029
LEU 8	121.545	9.126	0.458	0.098
THR 9	105.486	7.605	0.505	0.097
GLY 10	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

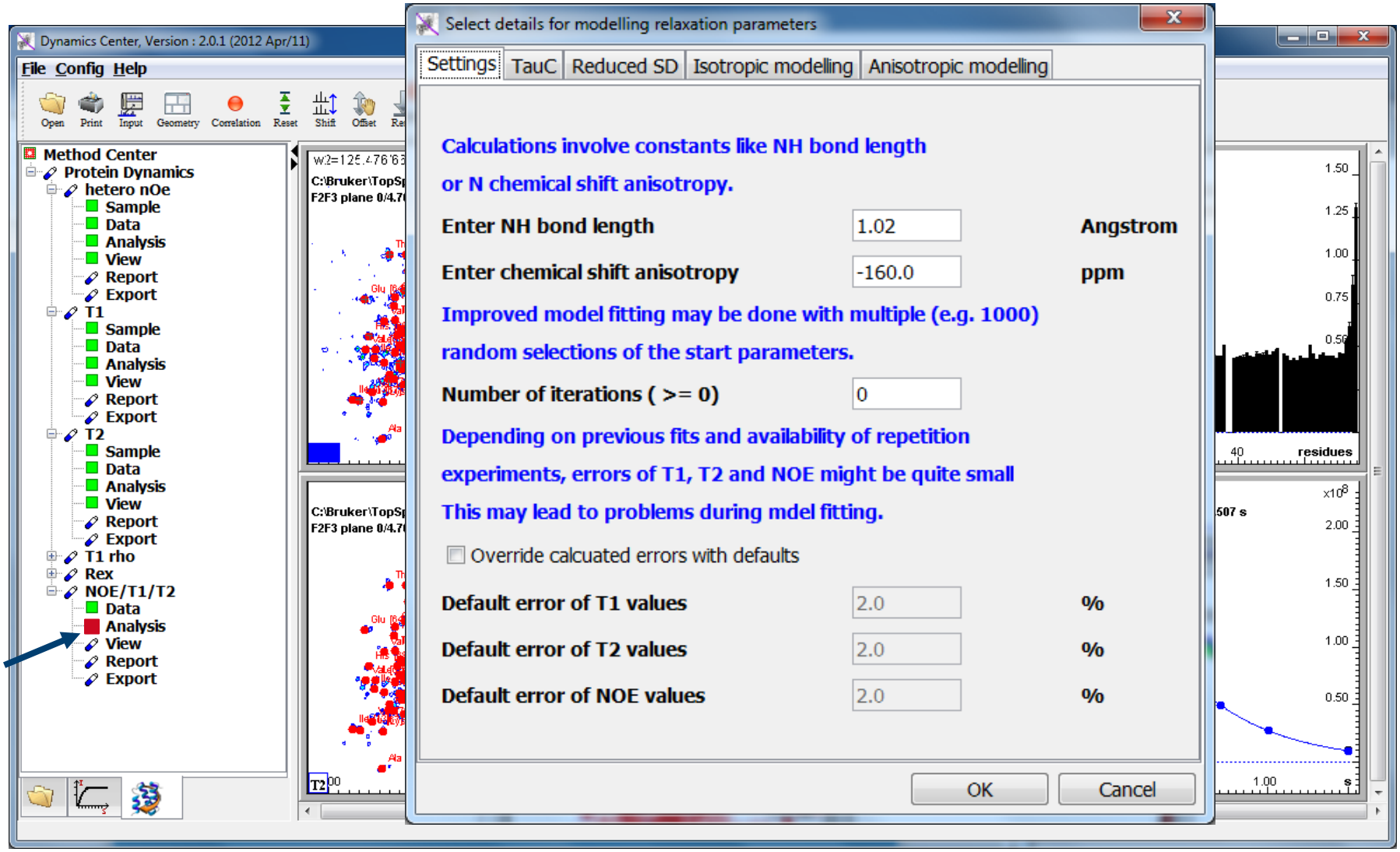
The New Dynamics Center...



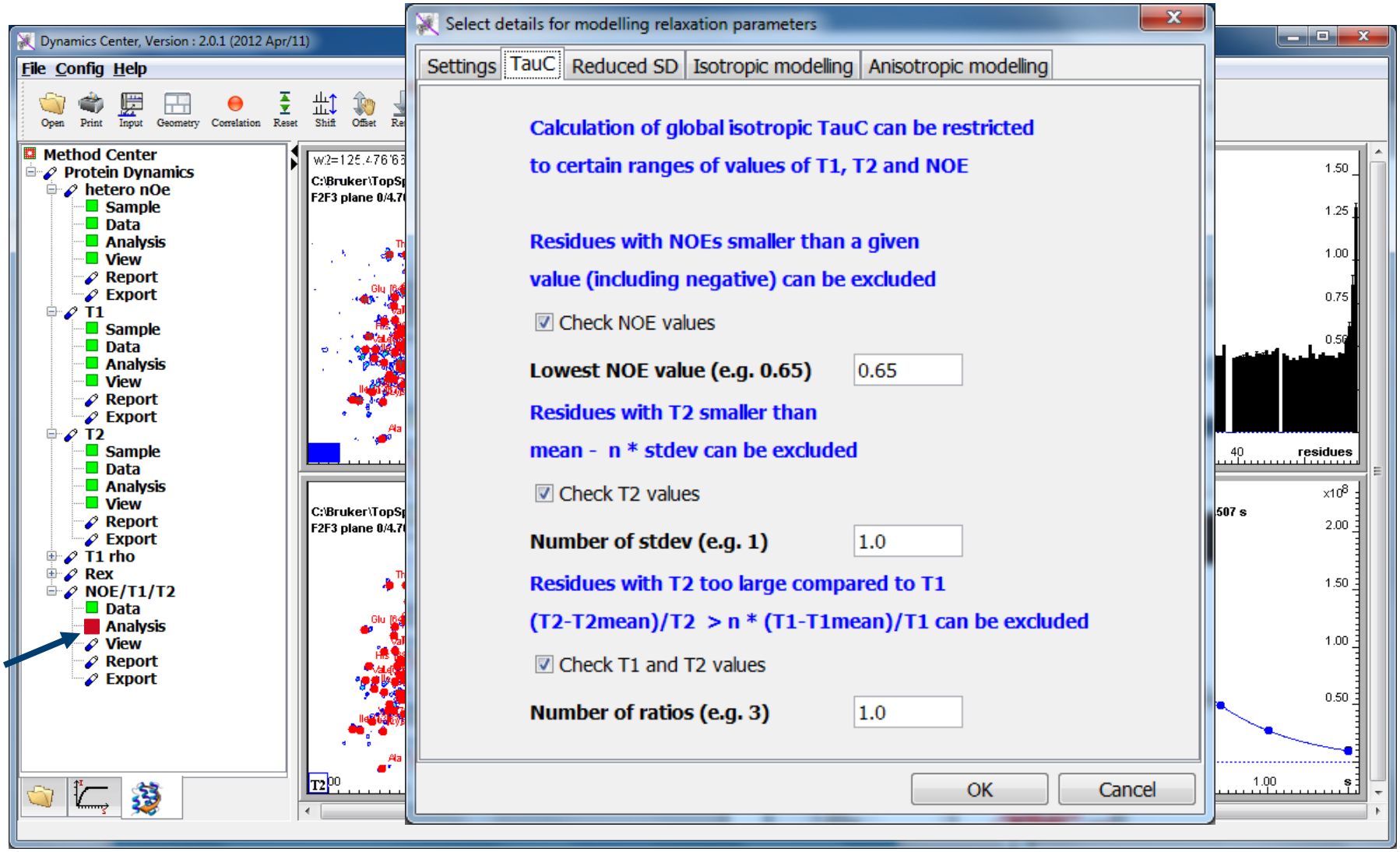
The New Dynamics Center...



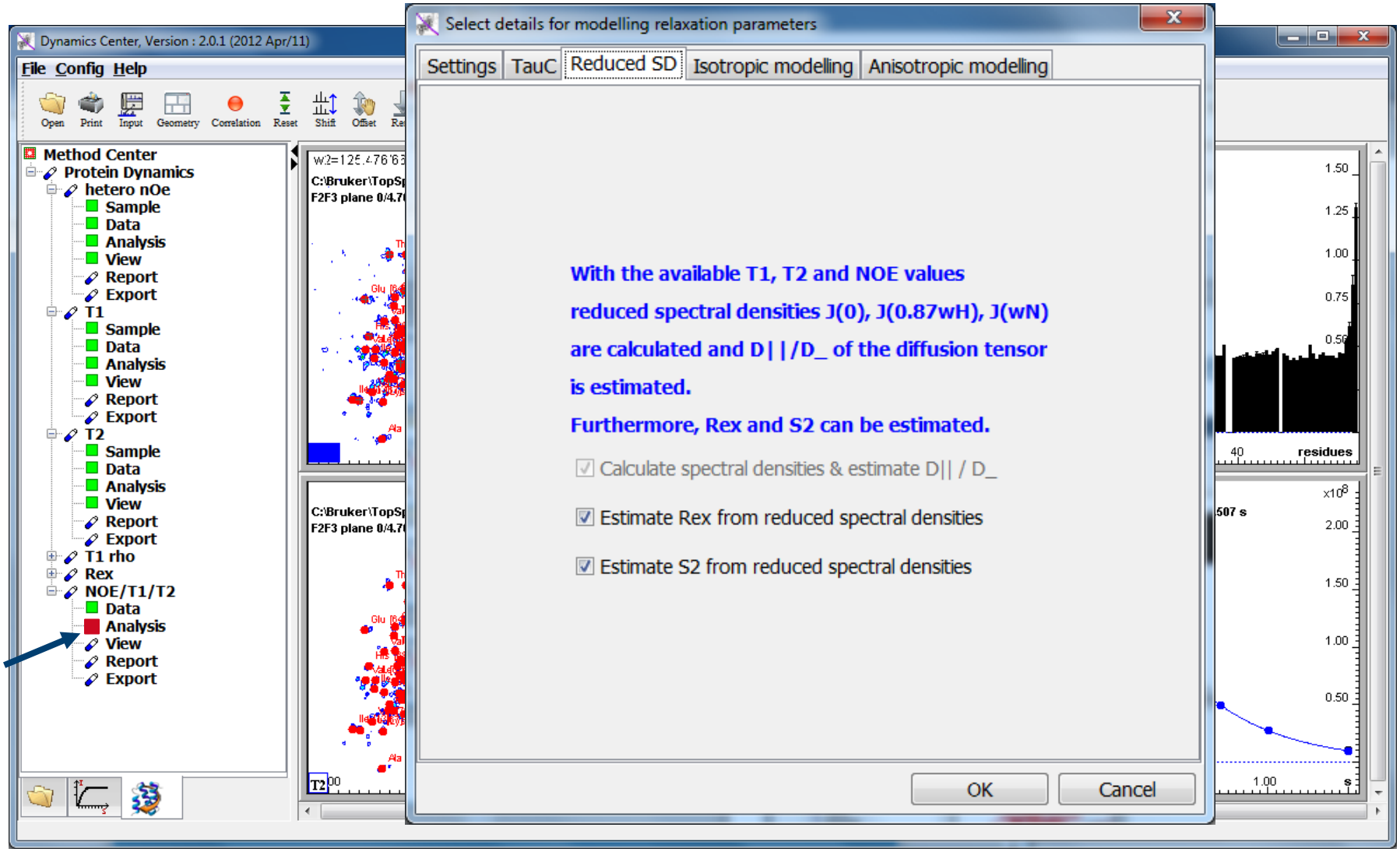
The New Dynamics Center...



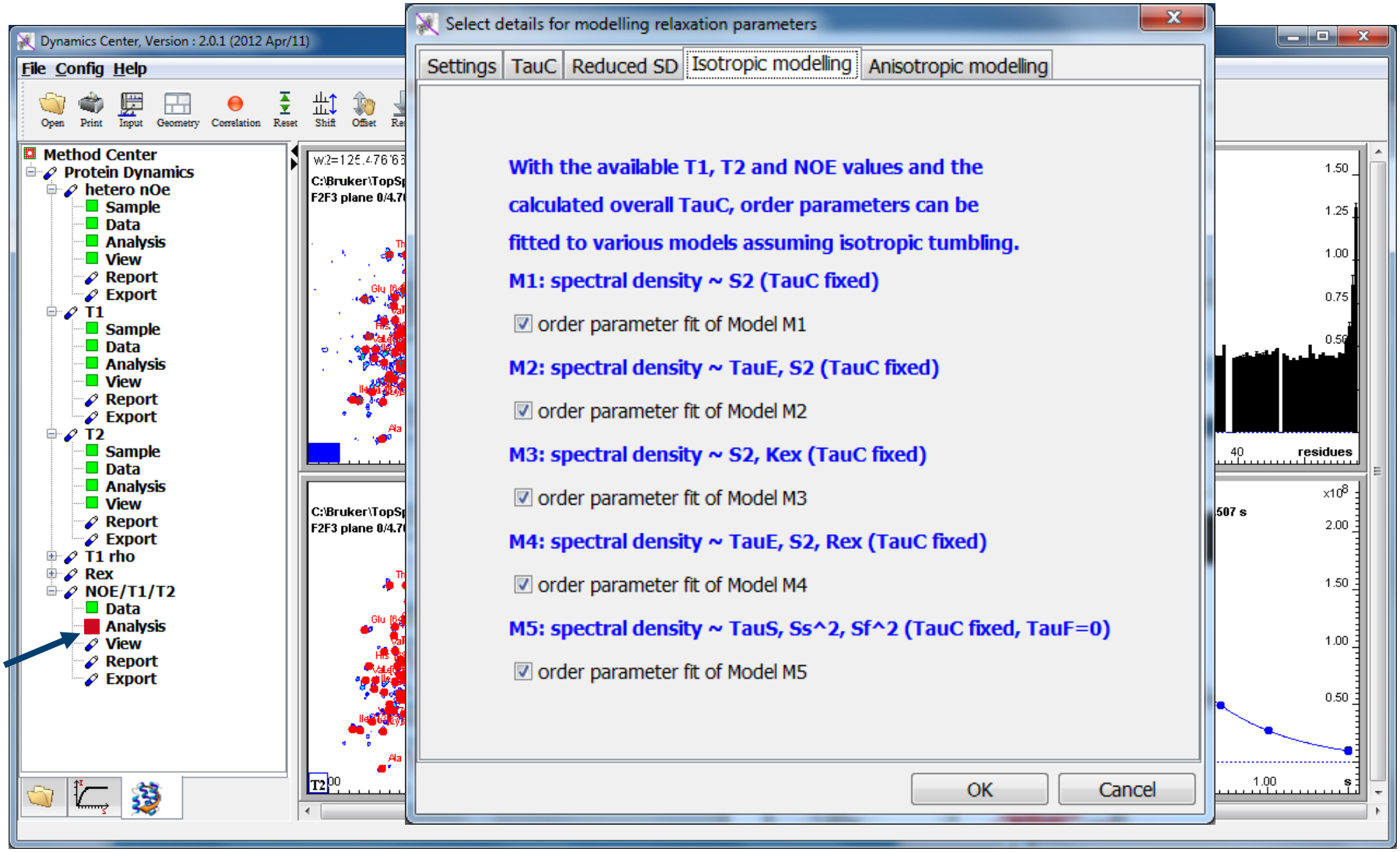
The New Dynamics Center...



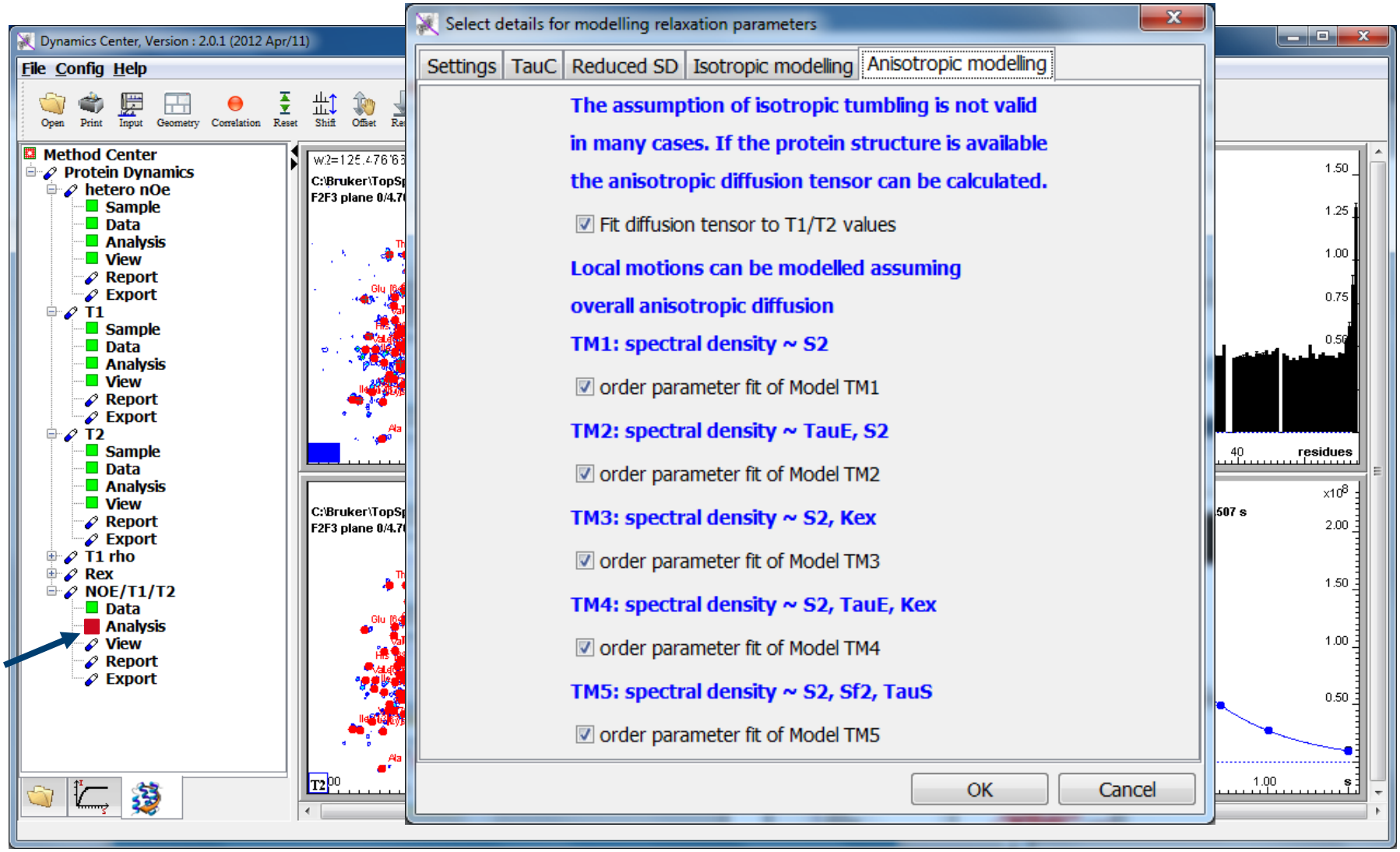
The New Dynamics Center...



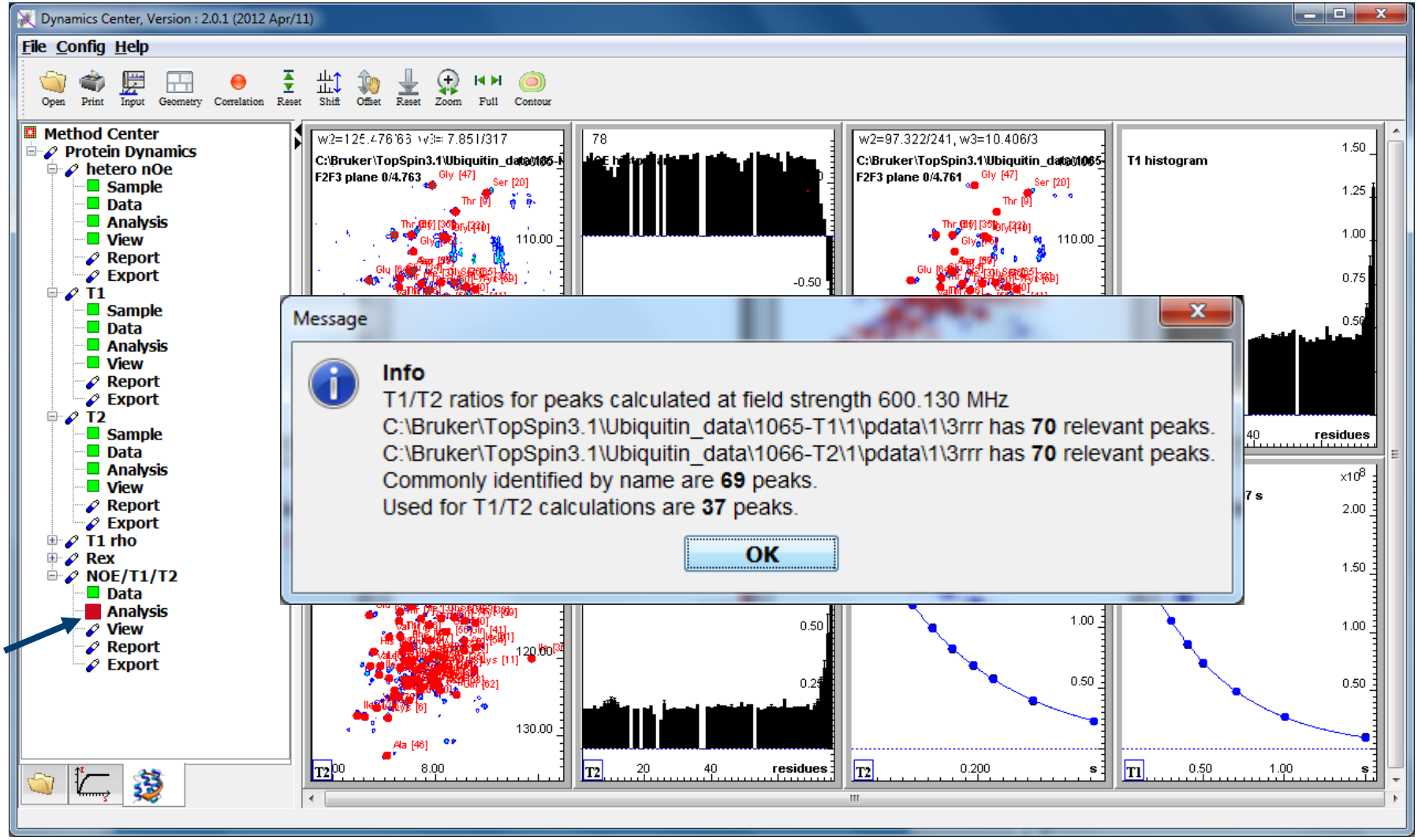
The New Dynamics Center...



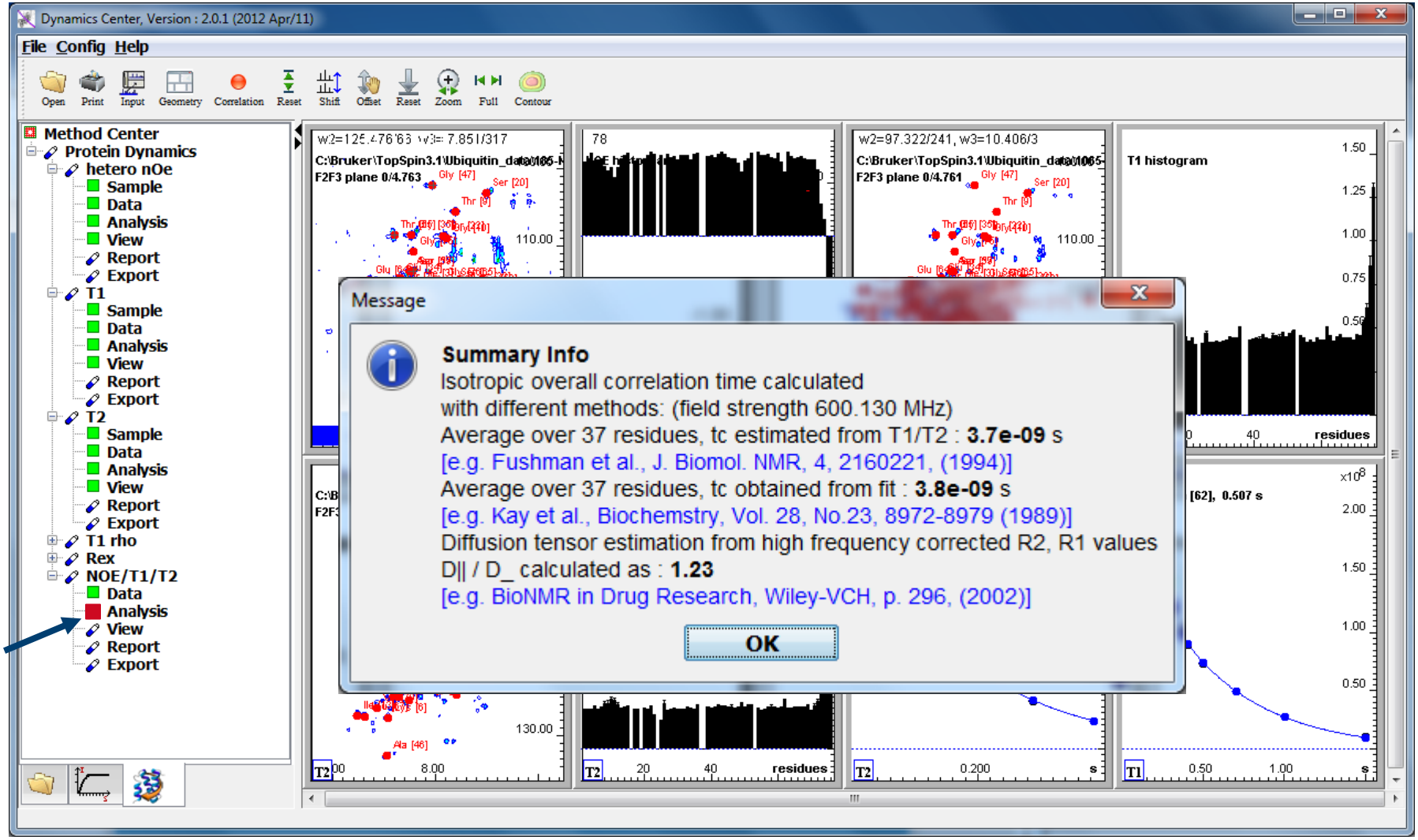
The New Dynamics Center...



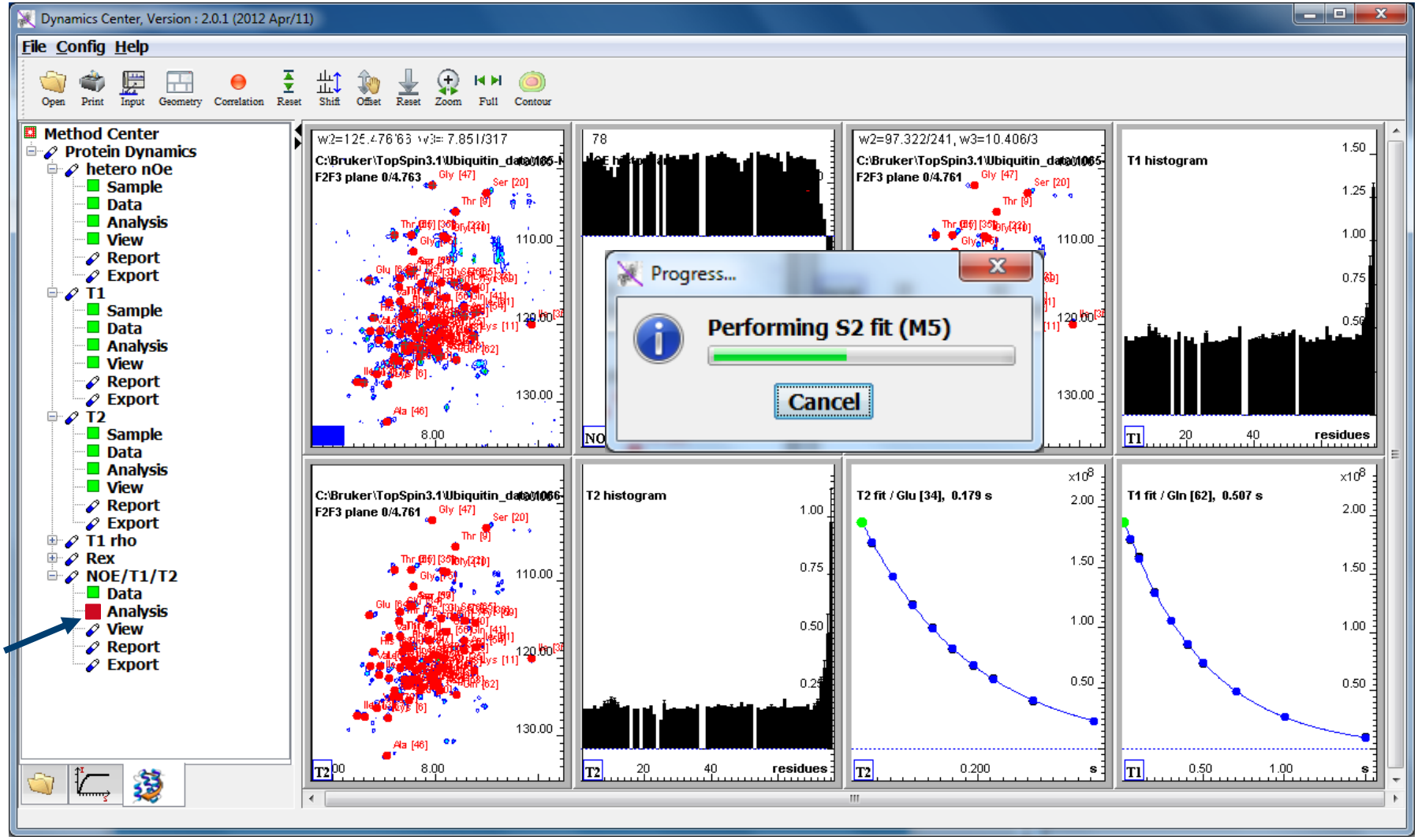
The New Dynamics Center...



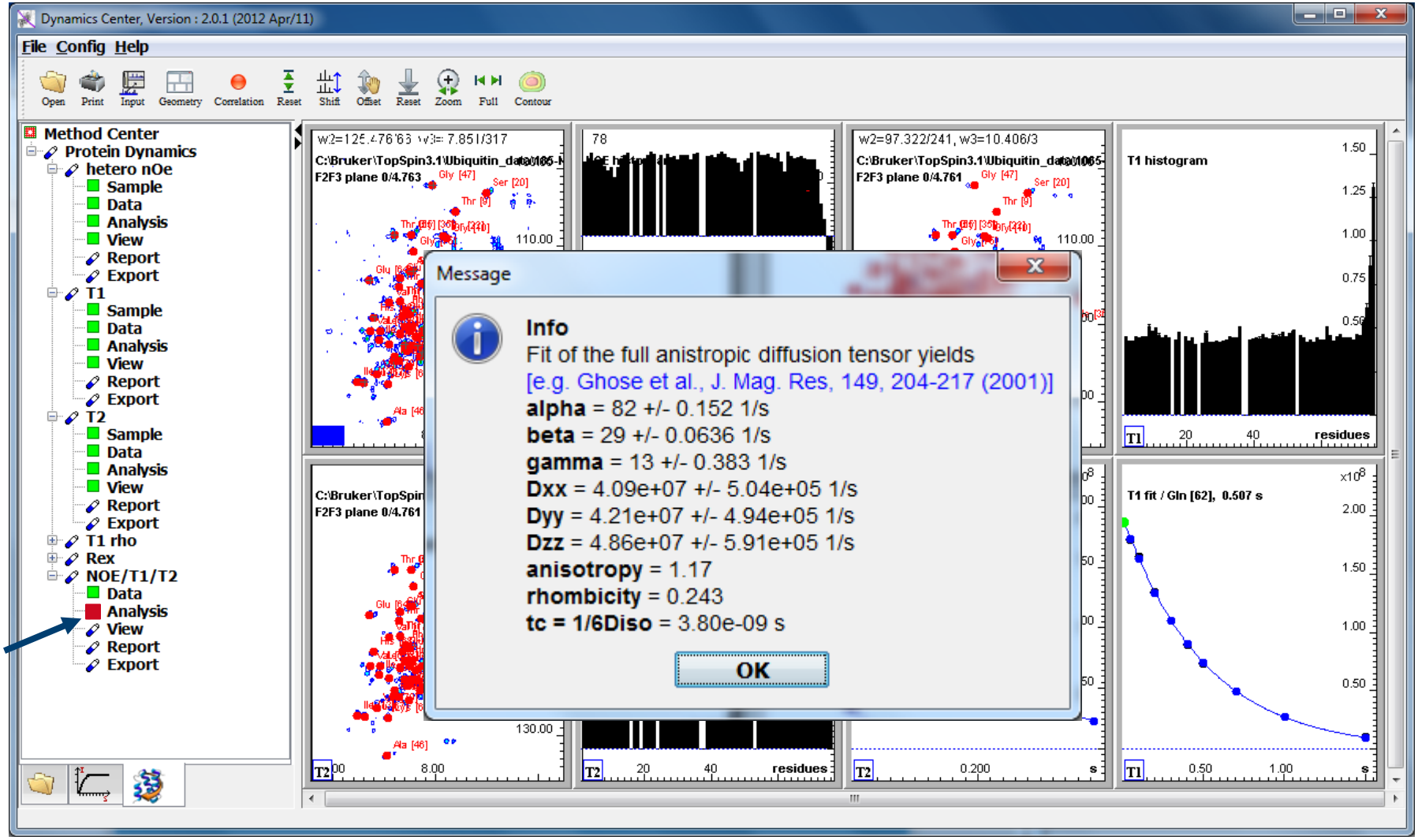
The New Dynamics Center...



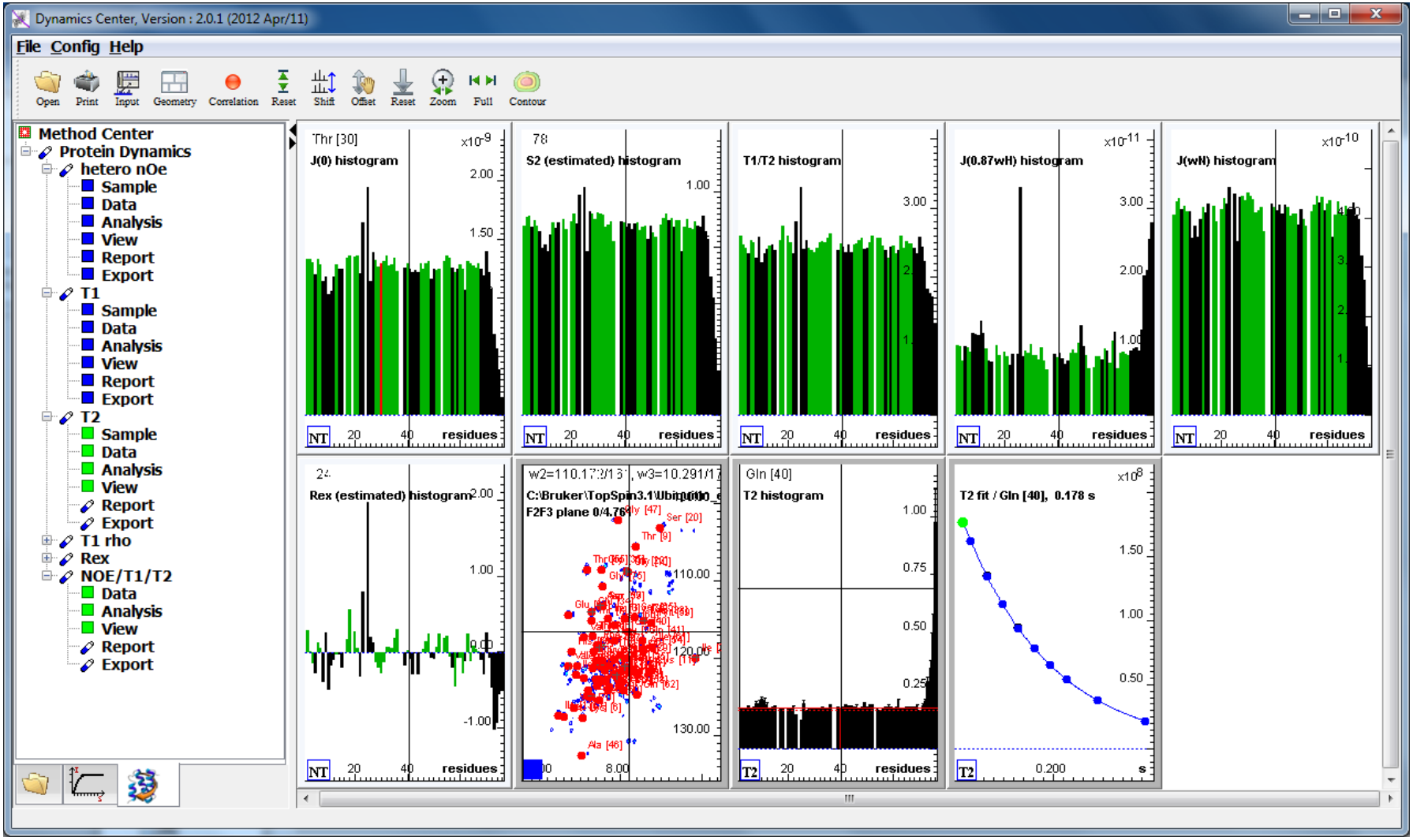
The New Dynamics Center...



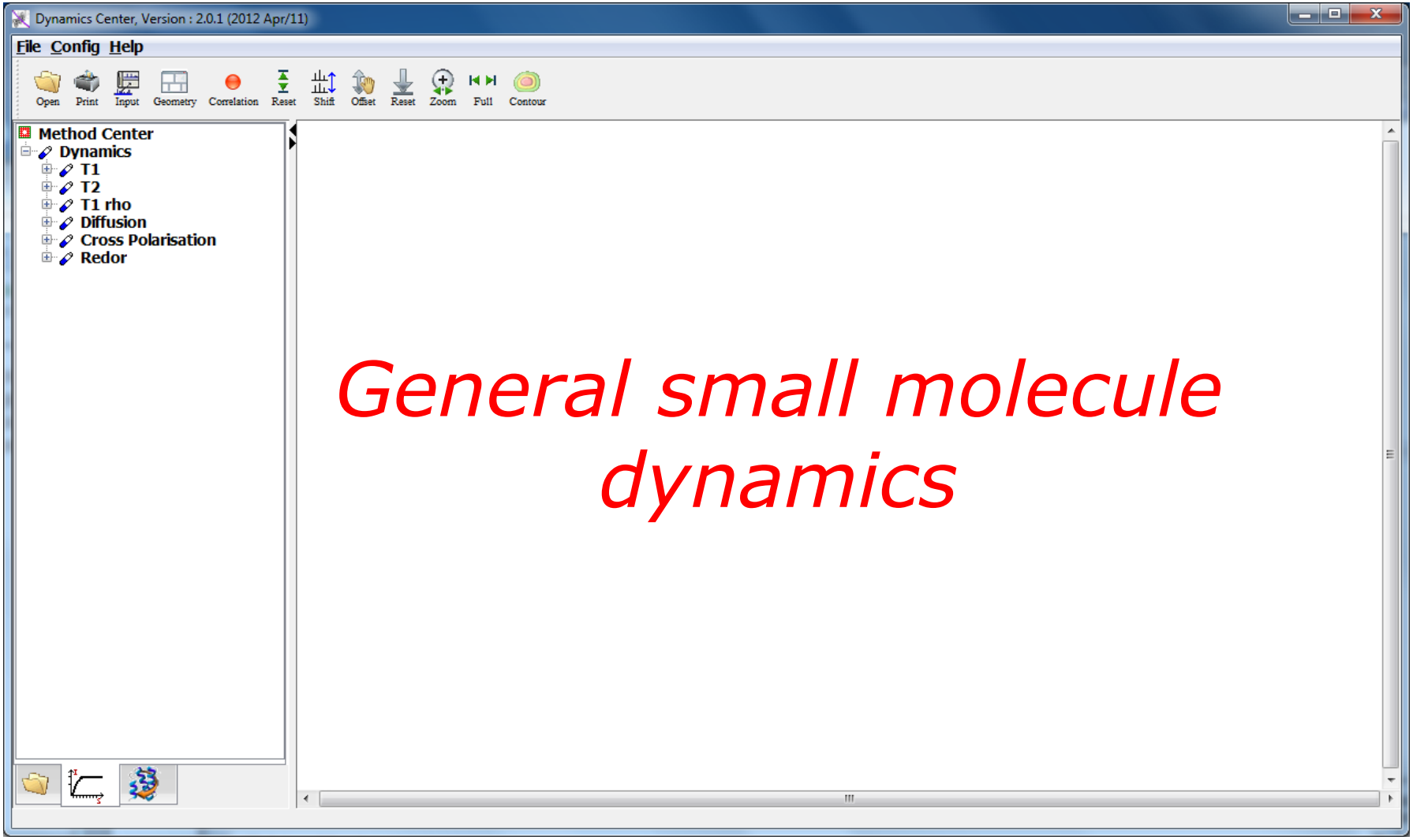
The New Dynamics Center...



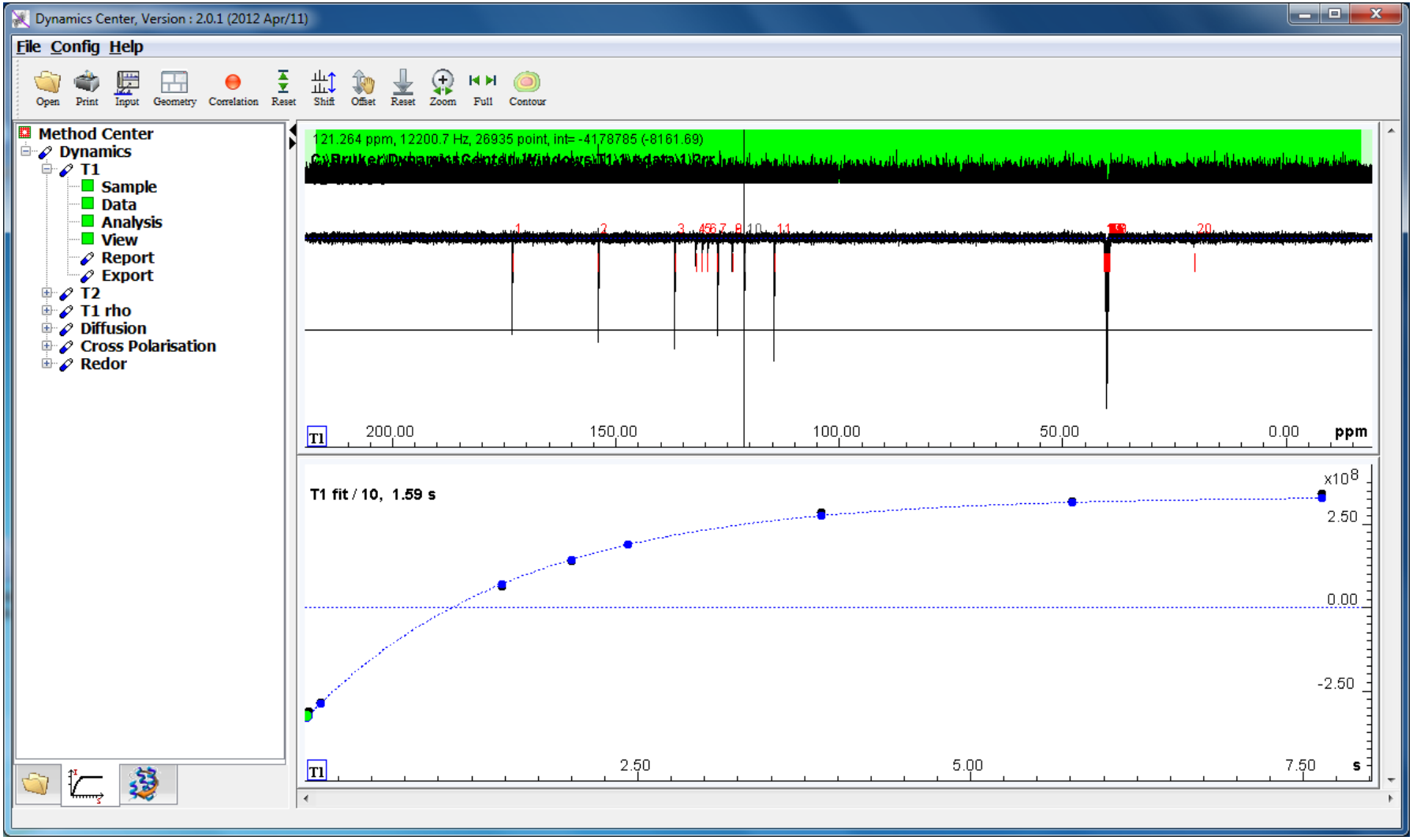
The New Dynamics Center...



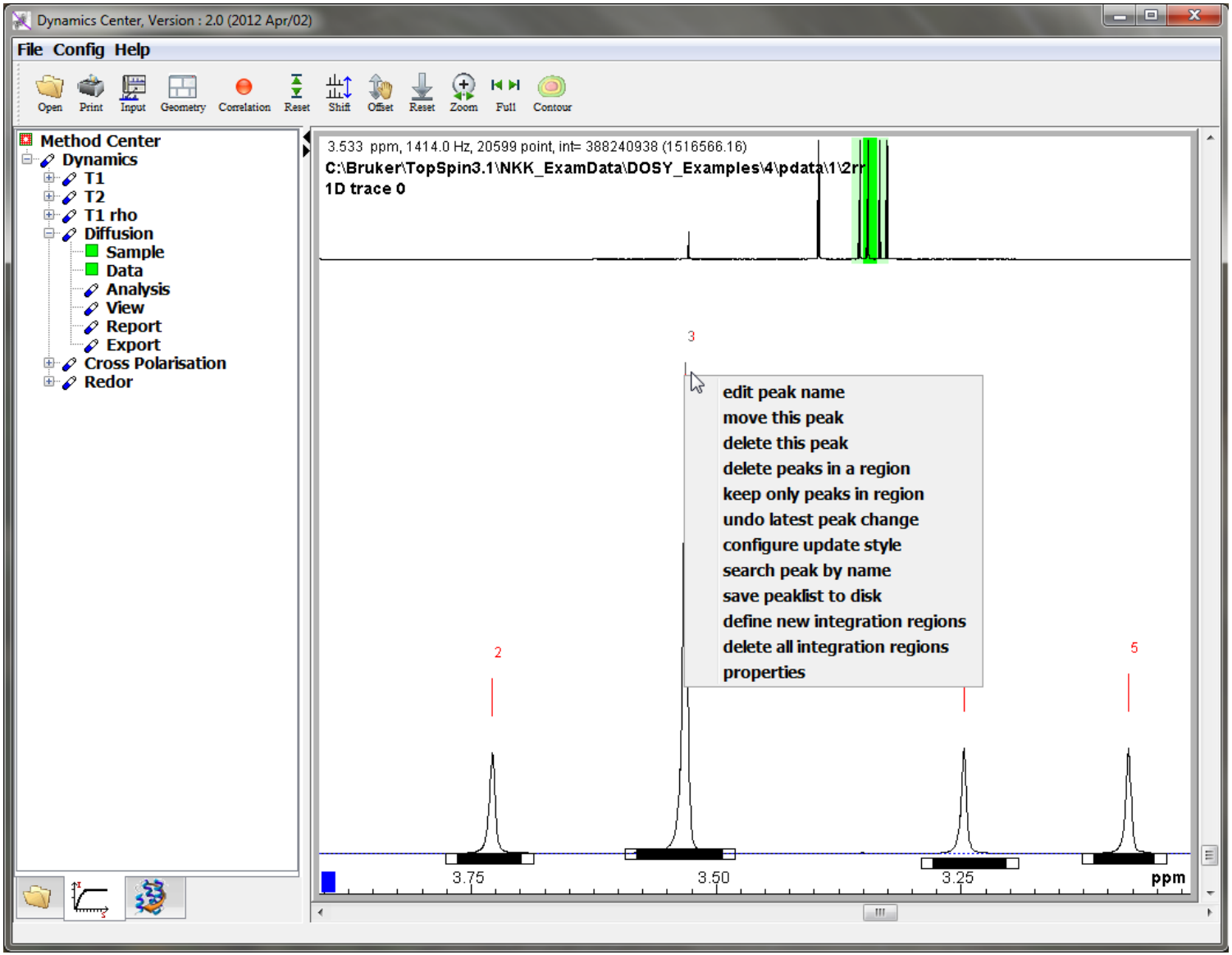
New in Dynamics Center v2.0



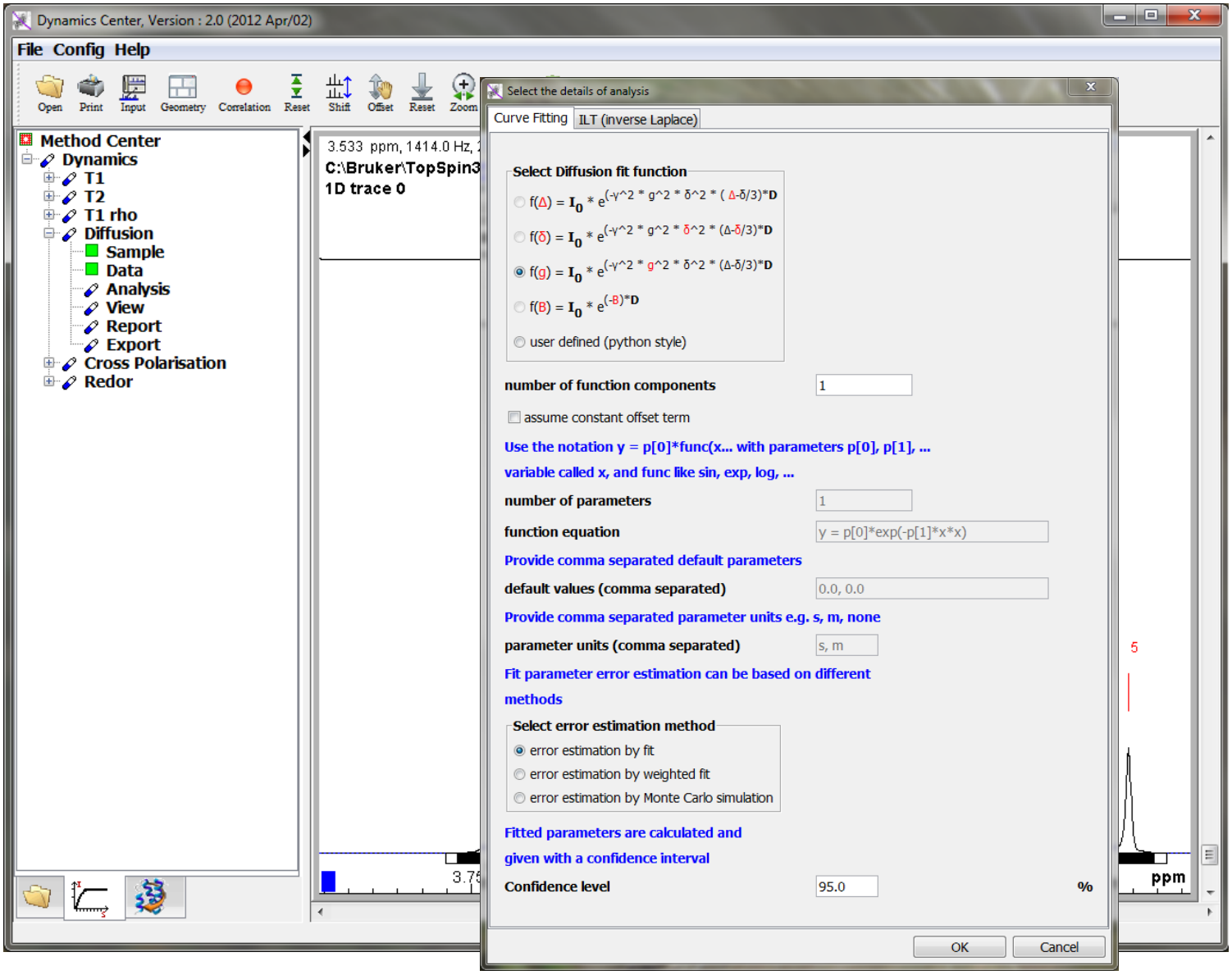
New in Dynamics Center v2.0



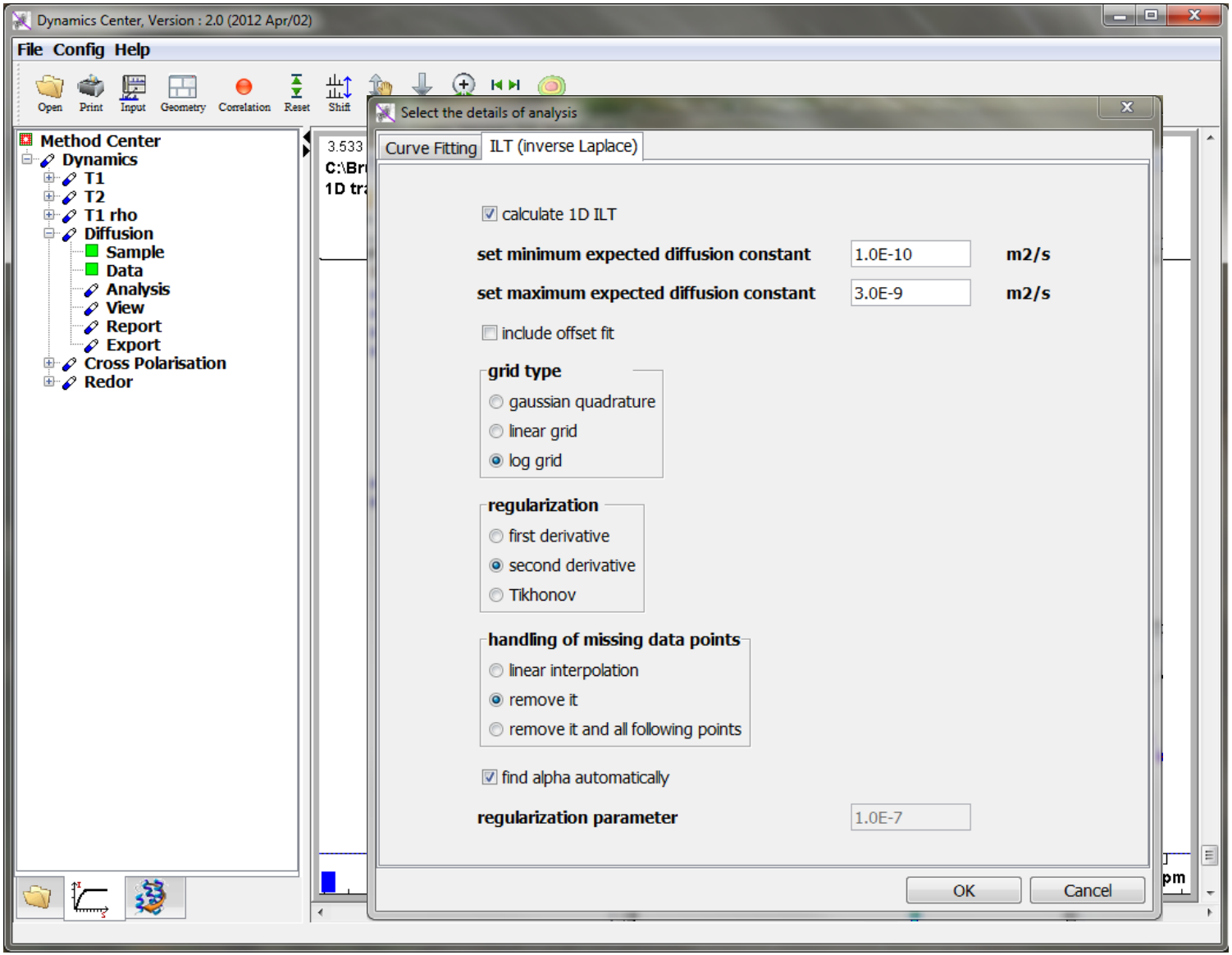
Inclusion of Diffusion analysis



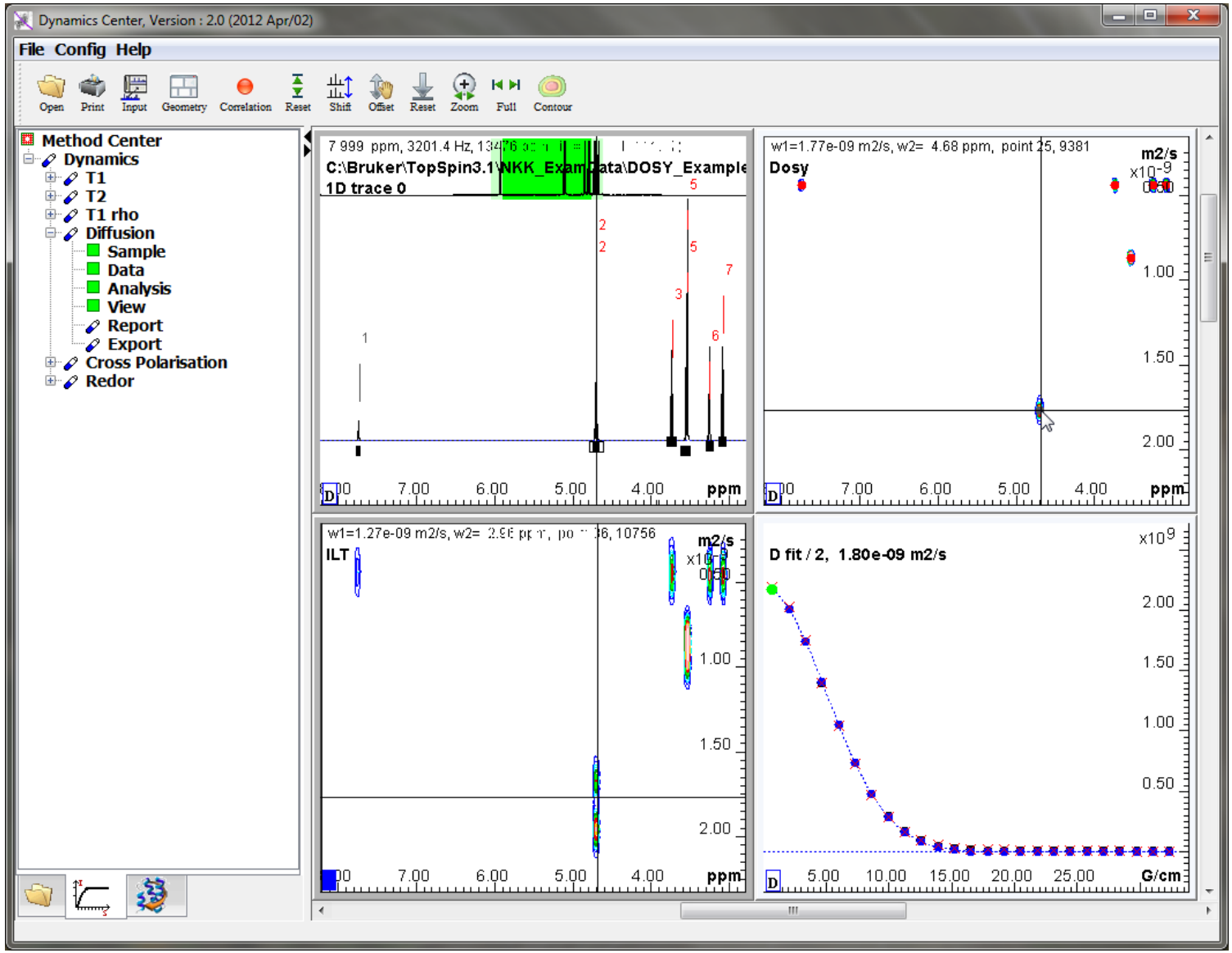
Inclusion of Diffusion analysis



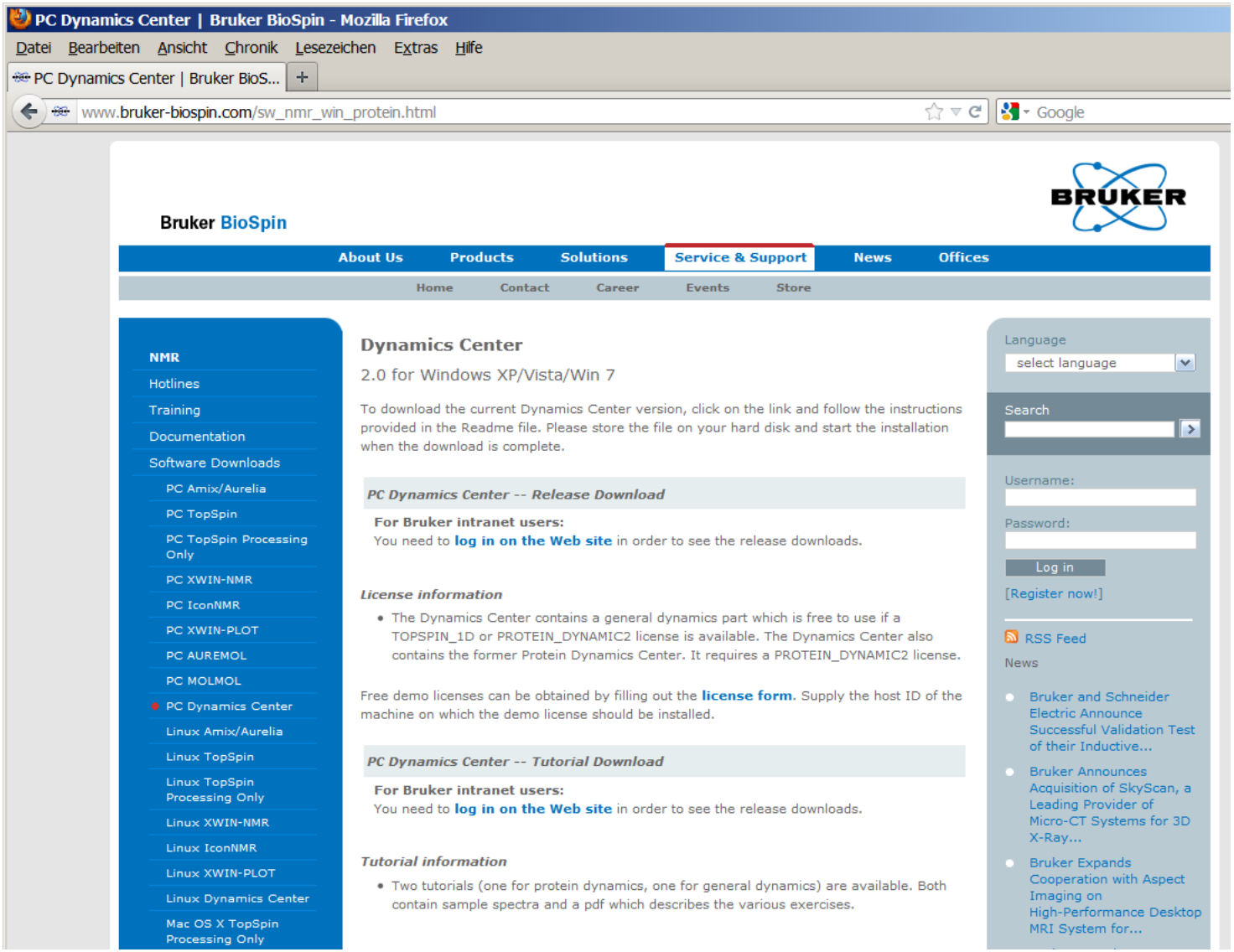
Inclusion of diffusion analysis



Inclusion of diffusion analysis



Availability



Summary

Dynamics Center 2.0 now available

- On http://www.bruker-biospin.com/sw_nmr_win_protein.html
- On Bruker software DVD TS 3.1 PL6
- Directly in TS (starting TS 3.2)

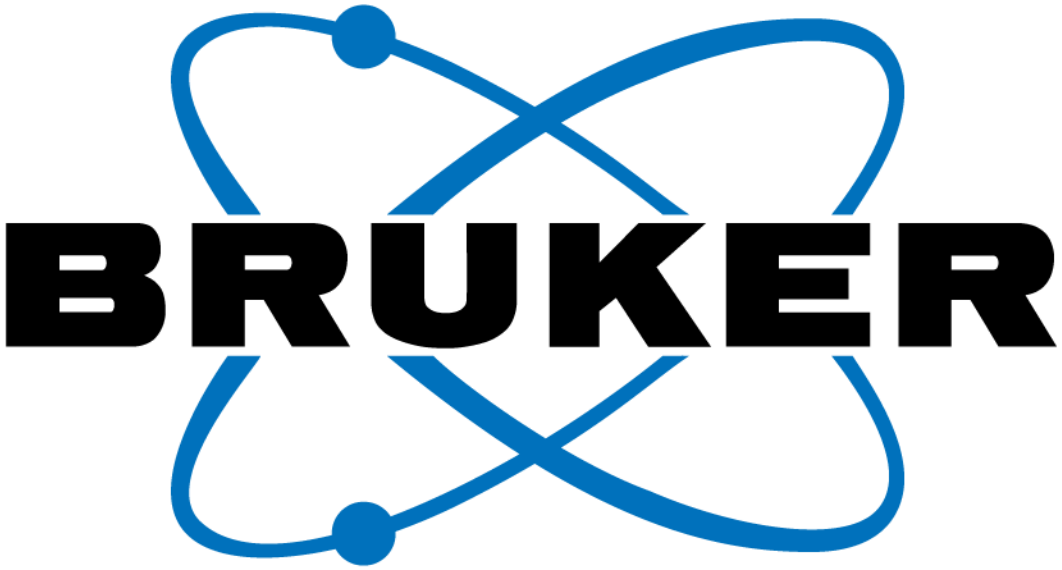
Licenses

- General dynamics is free.
- Protein dynamics needs license PROTEIN_DYNAMIC2

Platforms

- Windows XP/Vista/7
- Linux CentOS 5

Thank You



www.bruker-biospin.com