Dynamics Center 2.3

Advances in Automated Data Analysis

Apart from dragging and dropping project files or xml interface files on the method tree, the Dynamics Center (DC) offers the unique option to set all parameters from external programs at runtime and trigger a complete analysis. This allows a flexible integration of the DC into all kinds of automation environments. Technically, the DC runs as a server which accepts input through a communication channel. The DC can for example be used from TopSpin, via a tool bar containing elements for automatic processing, manual peak picking and automated analysis in Dynamics Center. Standard analysis parameters are supplied internally.
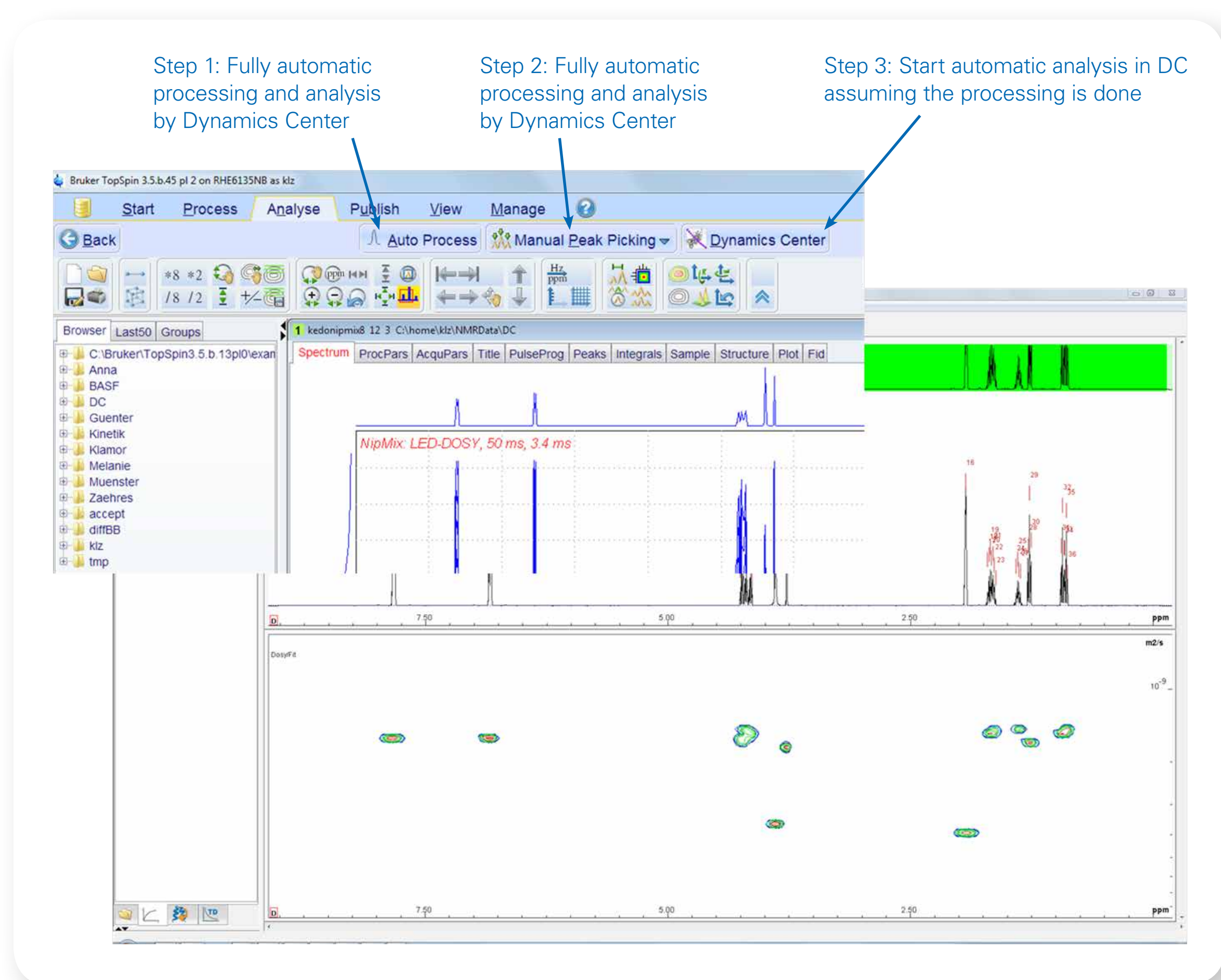

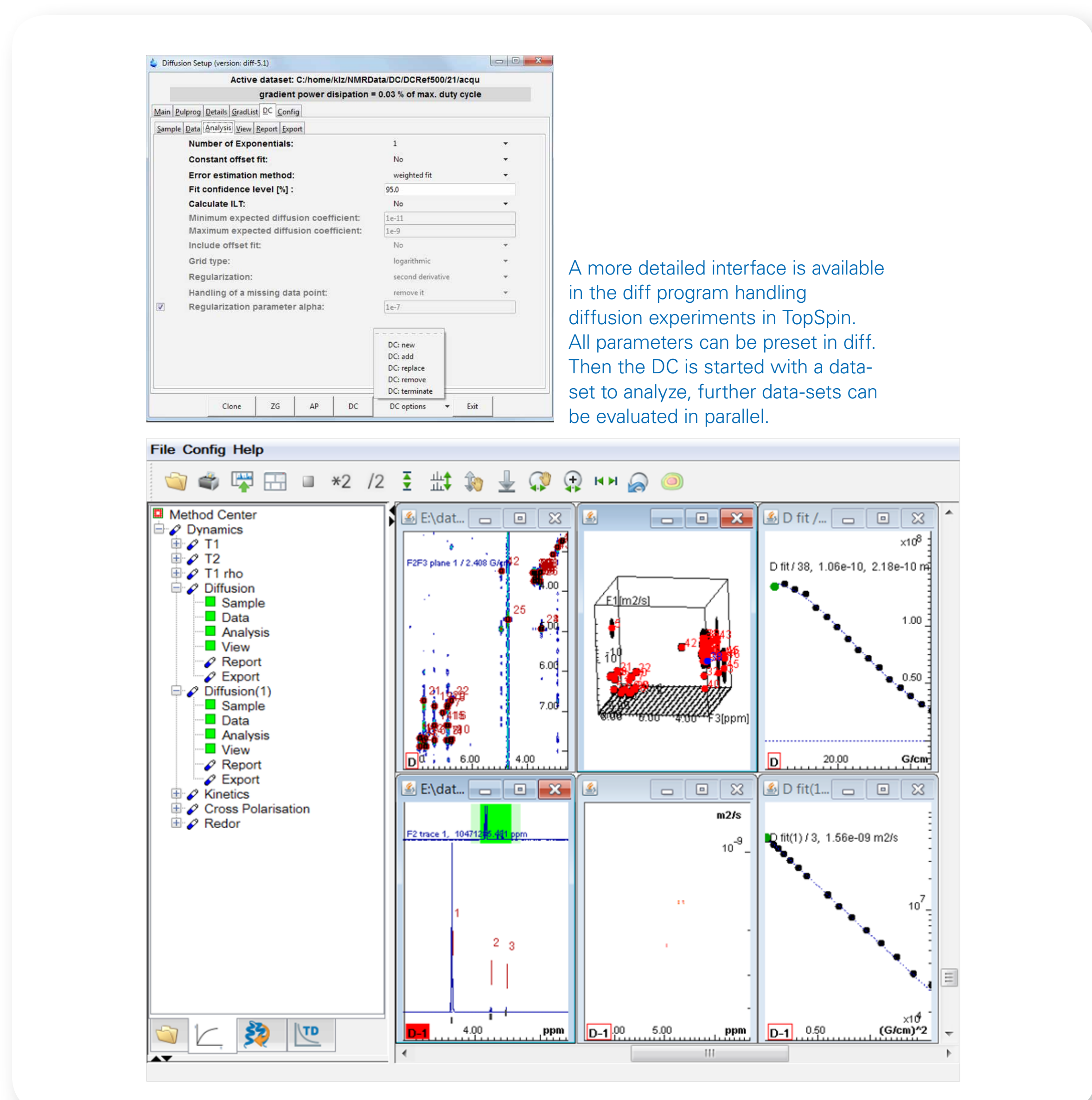Fig. 1 The DC controlled from TopSpin via a tool bar.

Fig. 2 The DC controlled from the diff software.

Time Domain Dynamics

Time Domain Dynamics is a new and exciting tool for the extraction of relaxation information from NMR time domain data recorded with Bruker's benchtop minispec. As part of Dynamics Center, it offers the standard method oriented workflow for easy analysis and reporting.

Multiple samples or different fitting functions can be analyzed in parallel.
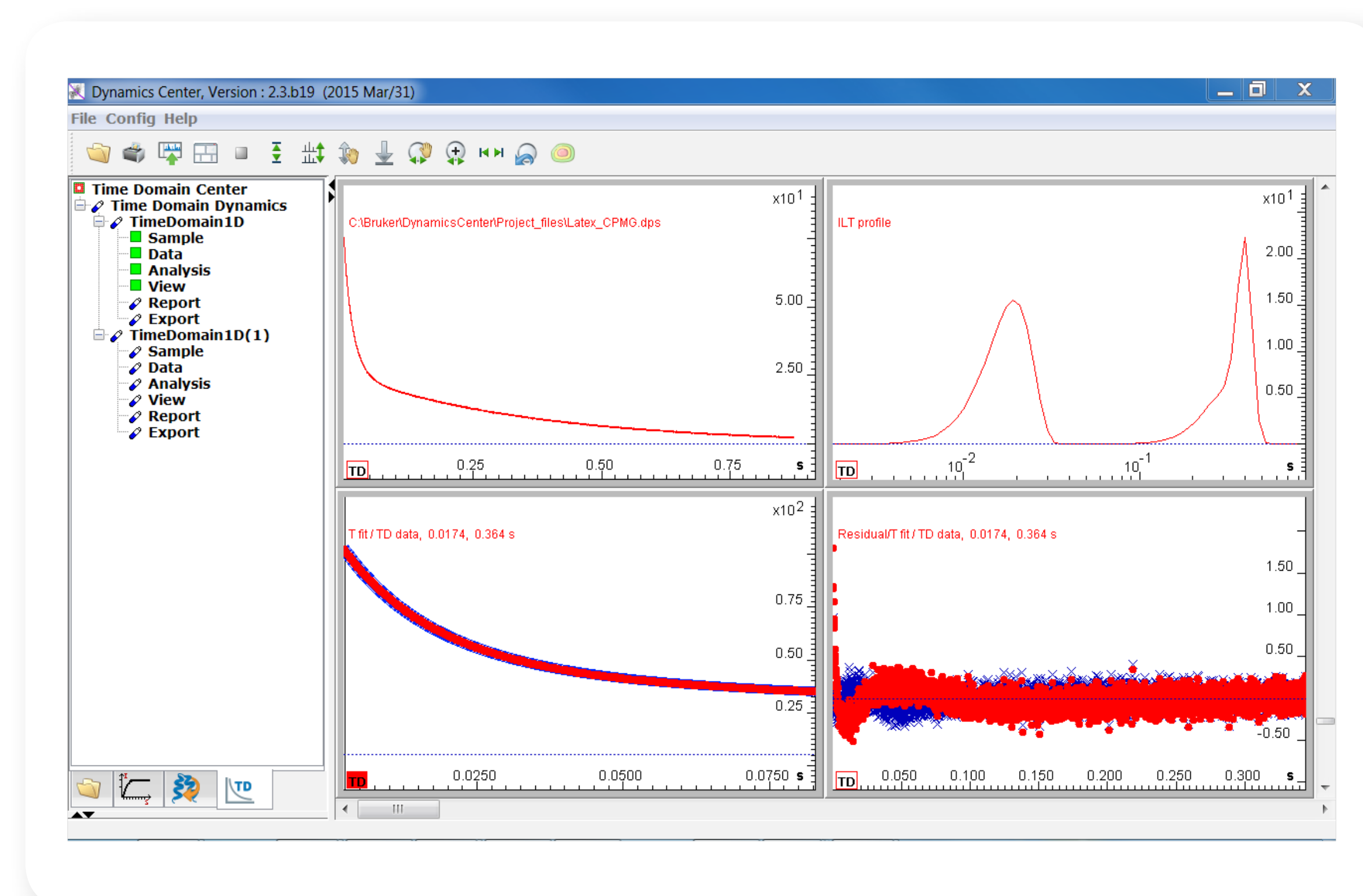

Fig. 3 Top left: Experimental T_2 relaxation decay.
Top right: Distribution of T_2 relaxation times resulting from Inverse Laplace Transformation (ILT).
Bottom left: Fitted decay curve.
Bottom right: Residuals from curve fitting and ILT.

The predefined library in Time Domain Dynamics contains functions commonly used in NMR relaxometry and polymer analysis, e.g. for the analysis of the cross-link density in rubbers or the morphology of polyolefins.

The software is ideally suited for method development and additionally provides the infrastructure for automated analysis of large sample batches.

Summary

- Unified, easy-to-use workflow for all kinds of relaxation, diffusion and kinetics analyses
- Client/Server architecture for usage in anyprogramming environment
- Highly efficient multiple, parallel analysis of any types of spectra: series of 1Ds / 2Ds, pseudo 2Ds, pseudo 3Ds and time domain data
- Automatic data fitting and best model selection
- Library of predefined fitting functions
- Option for user defined fitting functions
- Powerful algorithm for Inverse Laplace Transformation
- Unique interactive multi spectra display features
- Easy data opening by drag and drop
- New release version Dynamics Center 2.3
- Available on Windows, Linux and Mac