

Real-Time Multi-Exponential Component Analysis in TD and FFC NMR Relaxometry

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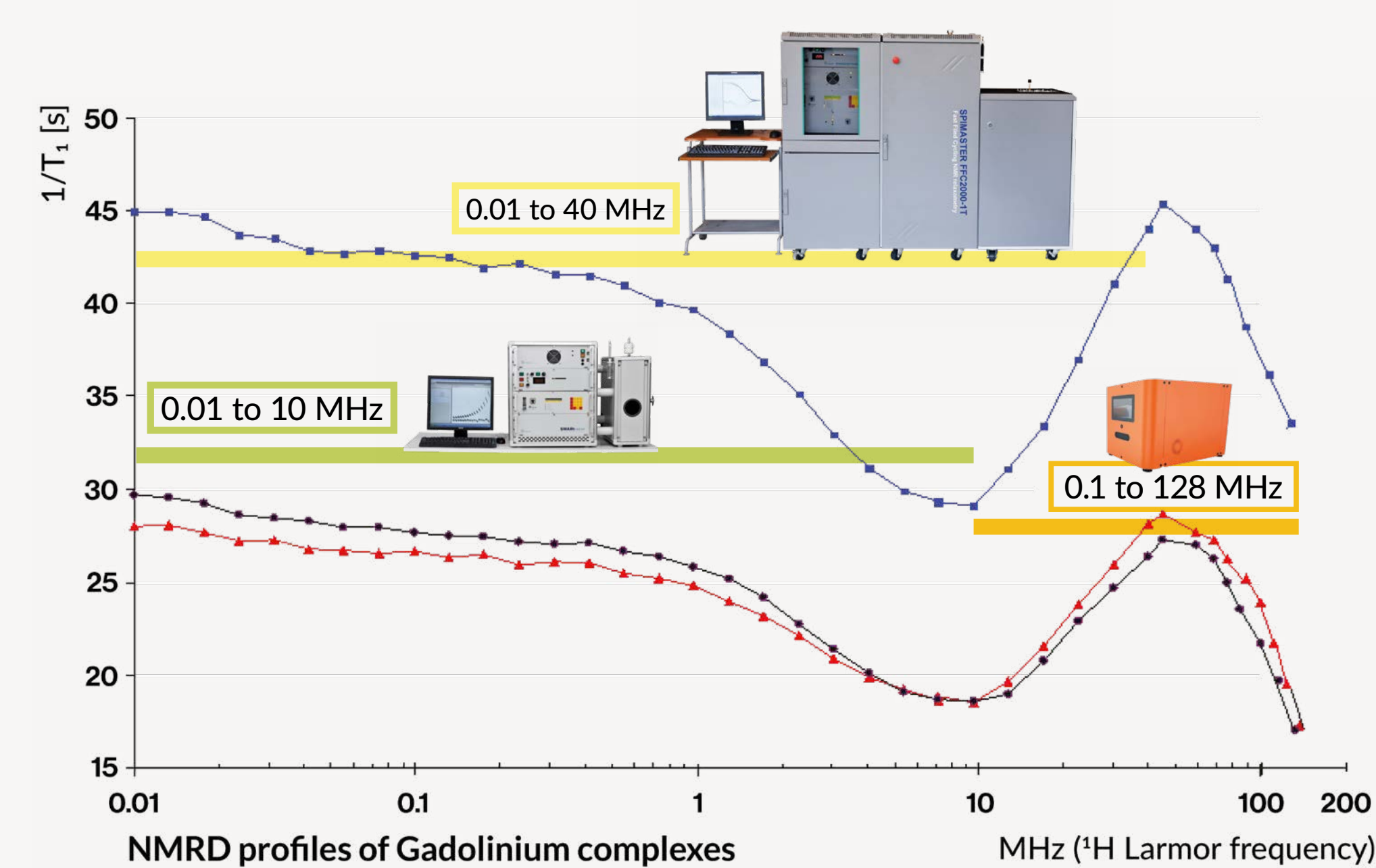
1. Introduction

Fast Field Cycling (FFC) and Time-Domain (TD) NMR relaxometry are widely used to investigate molecular dynamics in heterogeneous systems such as porous materials, polymers, foods, and biological tissues. In many cases, longitudinal relaxation cannot be accurately described by a single exponential decay because multiple molecular environments contribute distinct relaxation components. Traditional workflows typically perform multi-exponential analysis only after the experiment has finished, requiring export of data to external software. This separation between acquisition and analysis increases processing time and may delay scientific interpretation. To address this limitation, multi-exponential relaxation fitting has been integrated directly into the Storm6 acquisition environment, enabling real-time analysis of relaxation data during TD and FFC experiments.

2. Instrumentation Platform

The Storm6 software platform developed by Stelar s.r.l [2] supports advanced NMR relaxometry experiments using a range of Fast Field Cycling instruments, including SMARtracer, SPINMASTER, and the 3Tracer high-field system, developed in collaboration with HTS-110 [3] extends the accessible Larmor frequency to 128 MHz (3 Tesla).

By combining these systems within a unified platform, users can obtain NMRD profiles covering an exceptionally wide frequency range, from approximately 10 kHz up to 128 MHz, enabling the investigation of molecular dynamics across several orders of magnitude in correlation times (FIGURE 01).



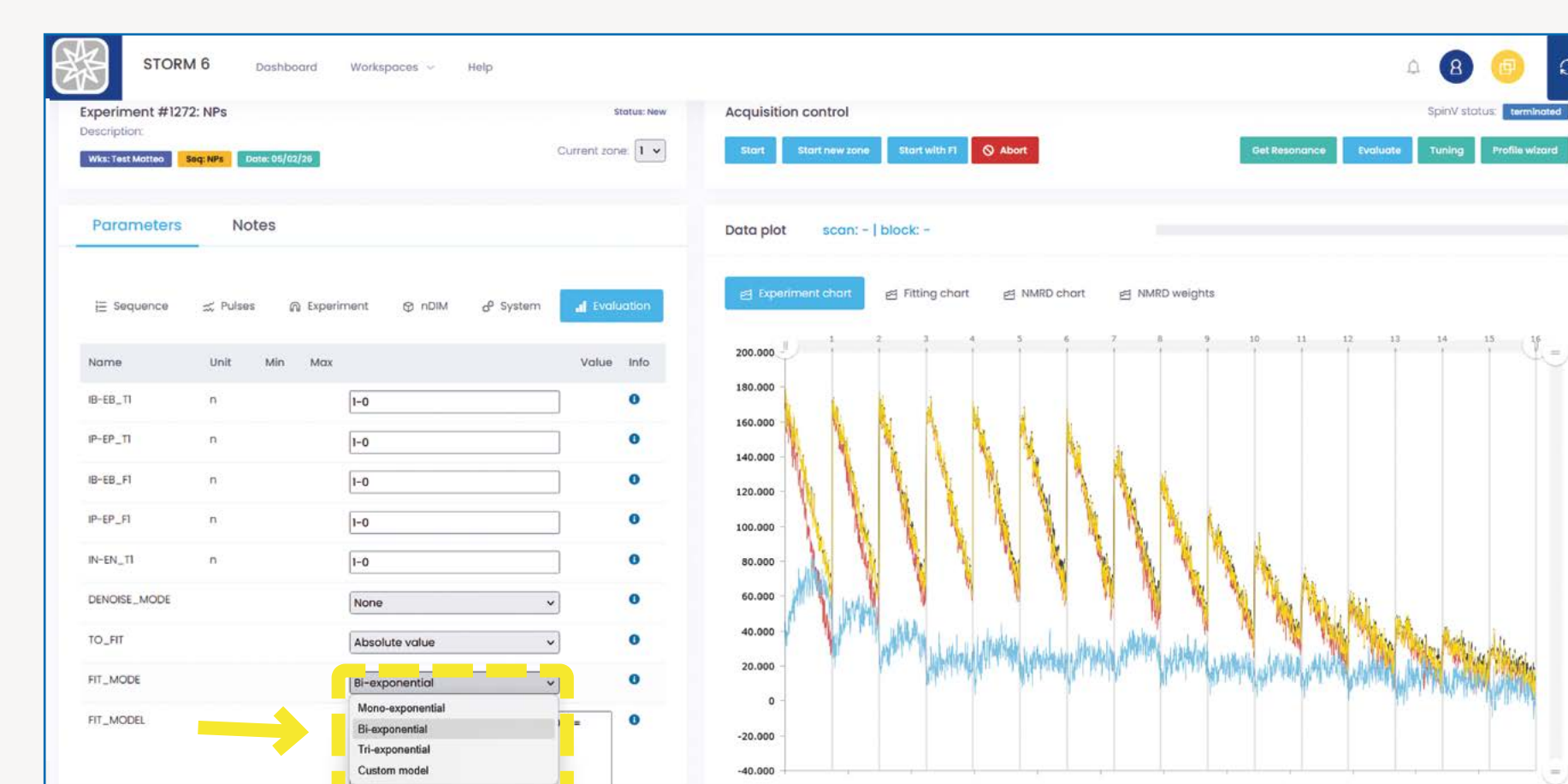
► FIGURE 01. Stelar Instruments cover wide range of molecular dynamics from 10 kHz up to 128 MHz.

3. Real-Time Multi-Exponential Analysis in Storm6

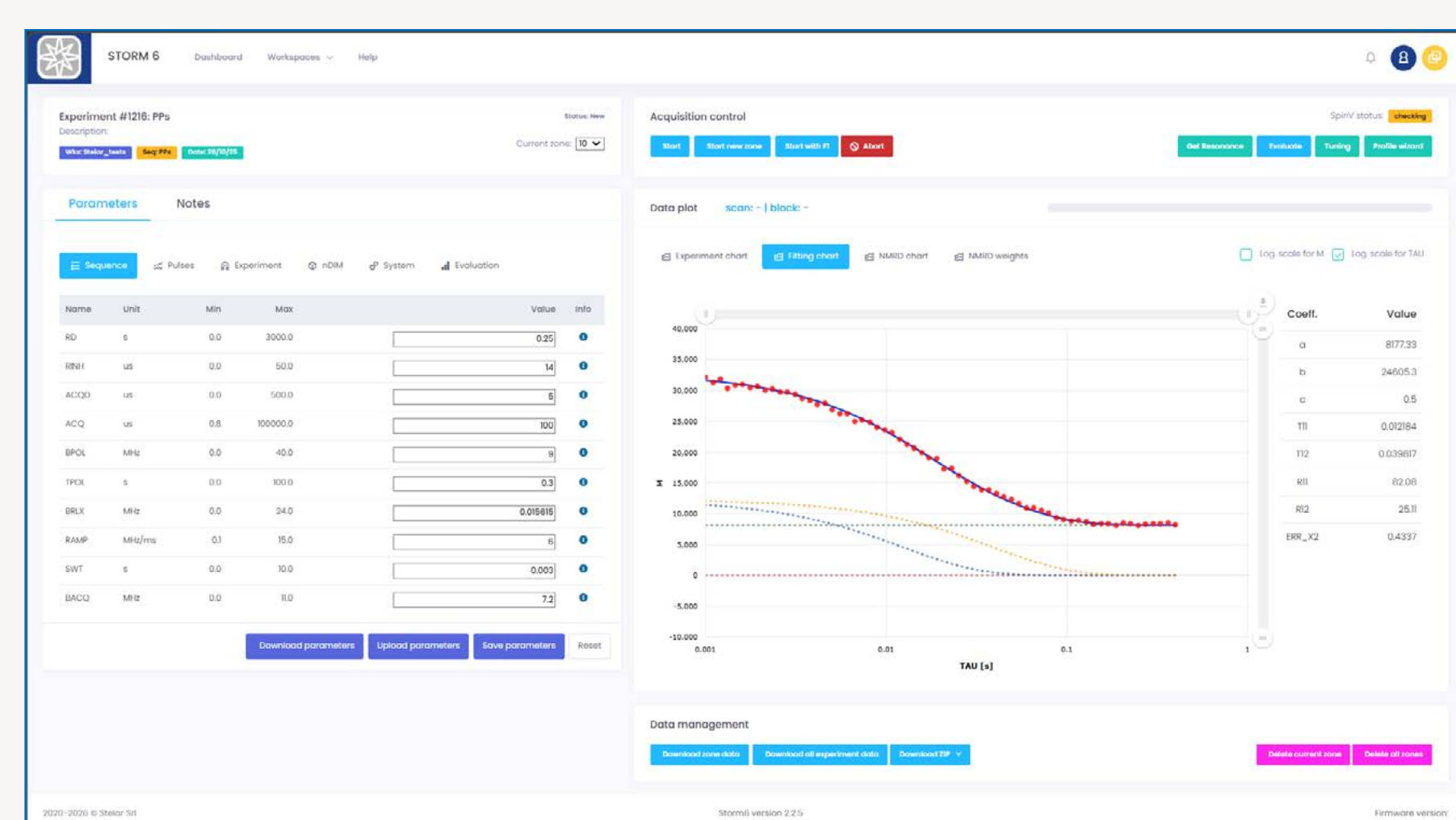
Multi-exponential fitting is implemented in Storm6 through integration of the mathematical fitting framework of OneFitEngine [1] providing fitting models (FIGURE 02) for:

- Mono-exponential
- Bi-exponential
- Tri-exponential
- User-defined functions

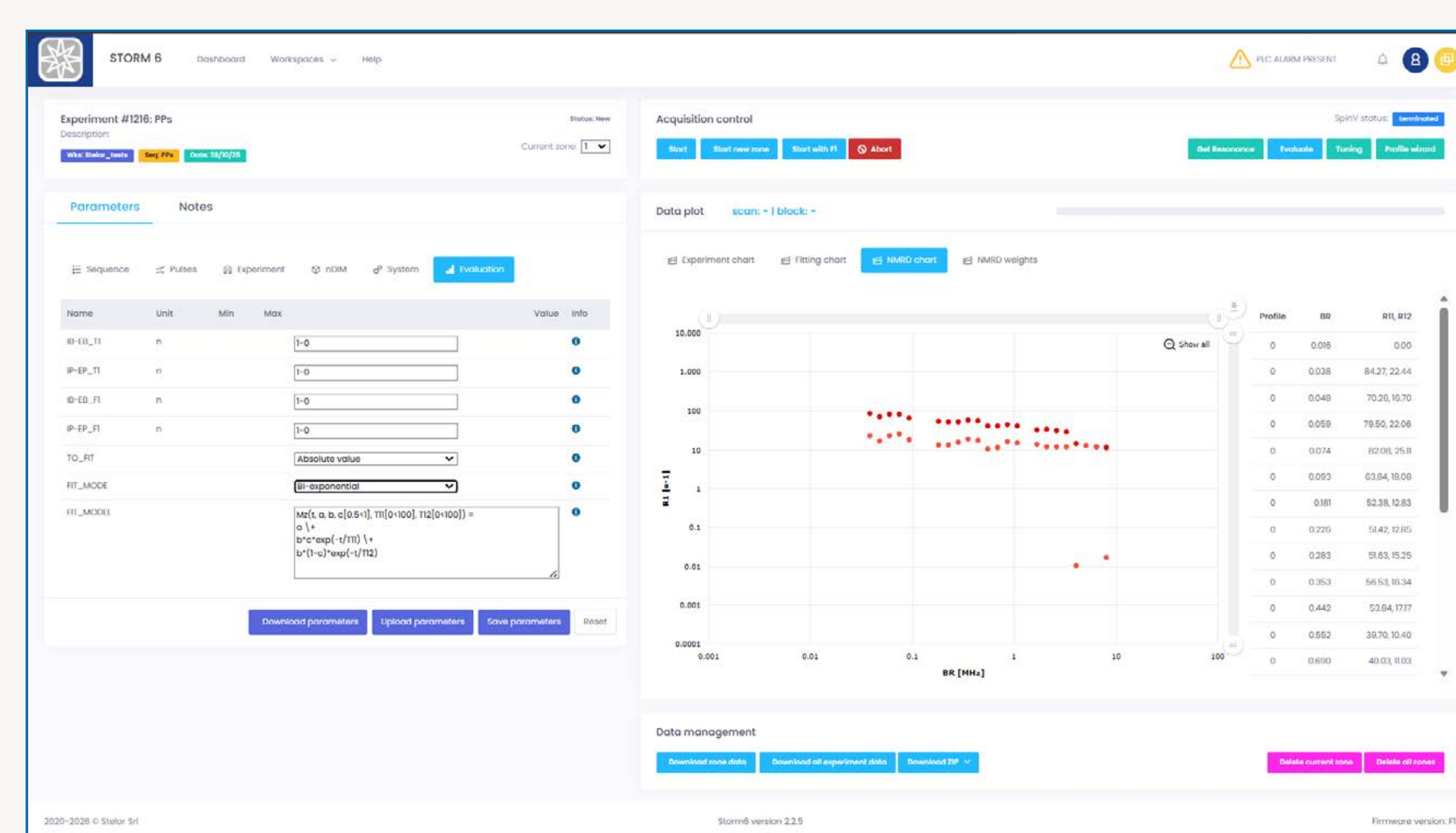
During experiments, the relaxation curve acquired at each magnetic field value is fitted immediately after acquisition. The resulting relaxation rates and component weights are used to update the evolving NMRD profile in real time, enabling rapid identification of multi-component relaxation behaviour (see FIGURES 03 A-C).



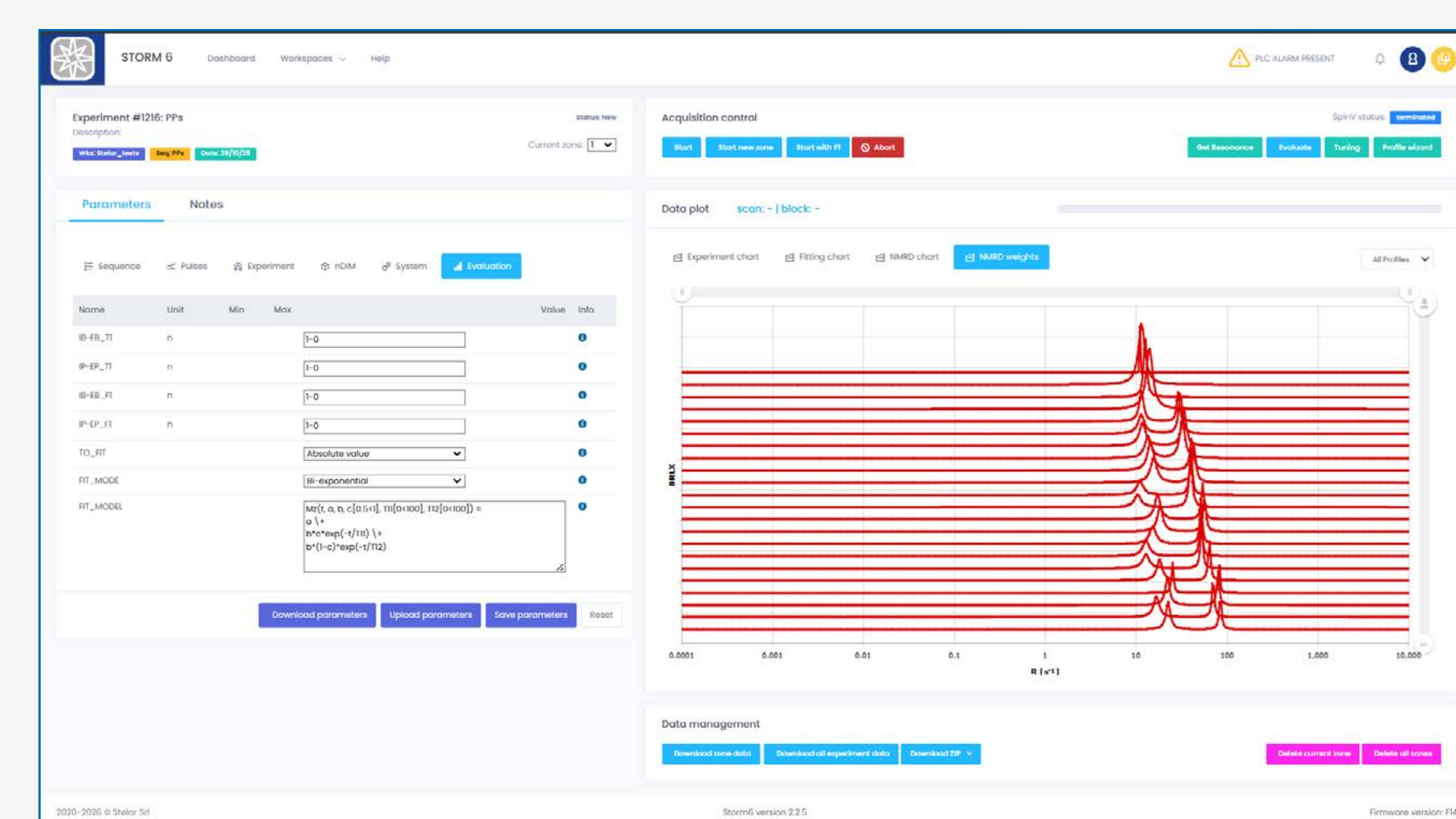
▲ FIGURE 02. Users can set the experiment parameters in the parameters list for acquisition and can select the model to fit the acquired data. Data can be fitted using mono-exponential, bi-exponential, tri-exponential, or any custom model, based on the guidelines of OneFitEngine.



▲ FIGURE 03A. Fitting-chart of multi-exponential fit.
 ••••• Red dots: experimental data
 — Blue line: fitting curve
 - - - - - Dashed colored lines: fitting components



▲ FIGURE 03B. The real-time NMRD profile shows the relaxation behavior of individual components across selected magnetic field strengths.



▲ FIGURE 03C. Complementary to the NMRD profile, the real-time field-dependent weights of multi-exponential components are also plotted.

4. Conclusions

The integration of real-time multi-exponential fitting into the Storm6 platform represents a major advancement in Time Domain (TD), High Field (HF) and Fast Field Cycling (FFC) NMR relaxometry workflows. By embedding flexible analysis directly within the acquisition environment, the traditional separation between data collection and post-processing is removed, enabling immediate identification of multi-component relaxation behavior during experiments. Combined with Stelar Fast Field Cycling instrumentation and HTS-110 high-field magnetic systems, the pre-

sented platform enables NMRD measurements over an exceptionally wide frequency range (~10 kHz to 128 MHz, 3T). From a technological, academic and Industrial perspective, Storm6 introduces a fully integrated relaxometry environment, where acquisition, analysis, and visualization operate in real time. By closing the gap between acquisition and analysis, the platform modernizes the experimental workflow, improving efficiency, reproducibility, and enabling faster, more informed scientific discovery.

References

- [1] Pedro J Sebastião, 2014, *Eur. J. Phys.*, 35, 015017
- [2] <https://www.stelar.it/products-page/>
- [3] <https://www.hts-110.com/product/3t-metrology-magnet/>

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