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# Live overview of the Relaxometry software REX

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Università La Sapienza, Roma, Italy  
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**Extra Byte**  
>in spin we trust

# What is Rex

A universal **software package** for **NMR Relaxometry** data processing and analysis. It provides support to:

- Scientists who research NMR relaxation phenomena as such
- And those who research molecular dynamics and aggregation
- Developers of specific relaxometry applications for end-users (e.g. in industrial environment)

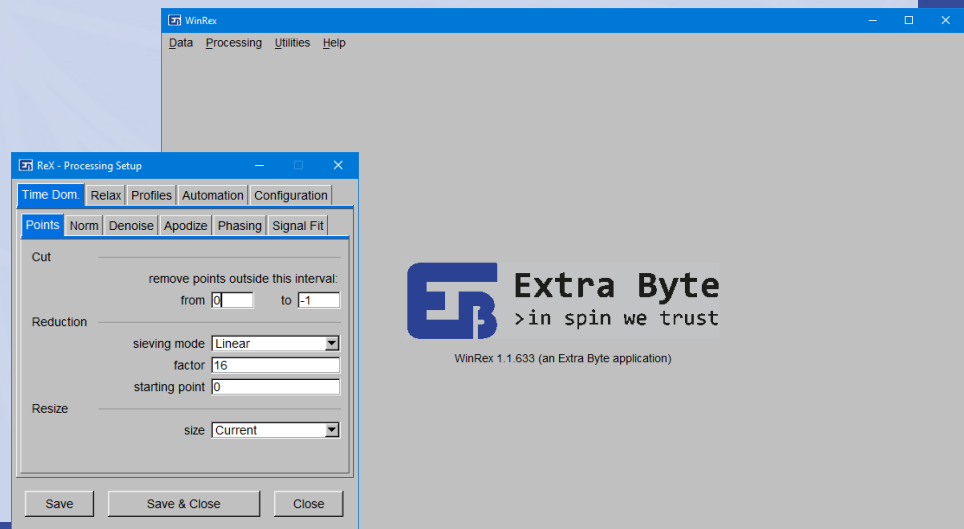
Rex is a **community-oriented** software. This means:

- It's **vendor-independent** and **vendor-agnostic**:  
it can import data from any source, either vendors data format and plain text file (though not all vendors are supported yet)
- Strongly **collaborative purpose** with users:  
Rex grows under NMR community requests (code addition, improvement...)

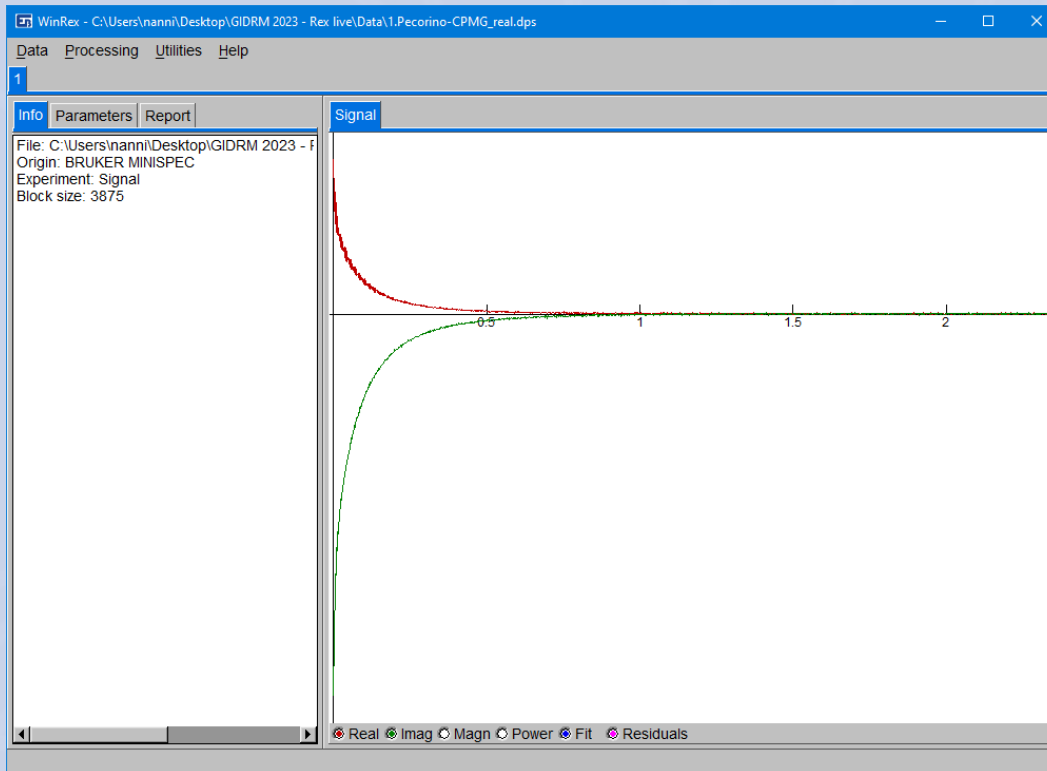
# Current state of the art

**Rex 1.1** offers support for many tasks:

- Suppression of experimental artifacts (group delay, anomalous points ...)
- Denoising (noise reduction filters)
- TD-signal phasing
- FID analysis (components quantification)
- Relaxation curves fitting (Discrete/Continuous ILT)
- Variable Frequency NMRD profiles (FFC)
- Simultaneous fit
- Automation
- Data simulation
- Practical GUI (data visualization, commands setup ...)



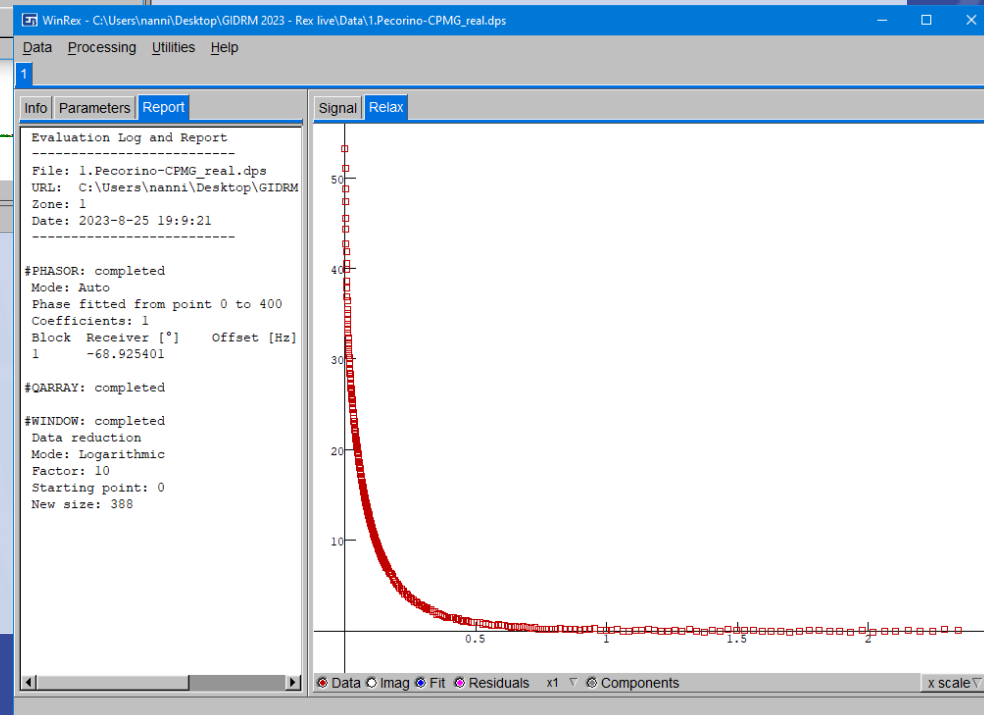
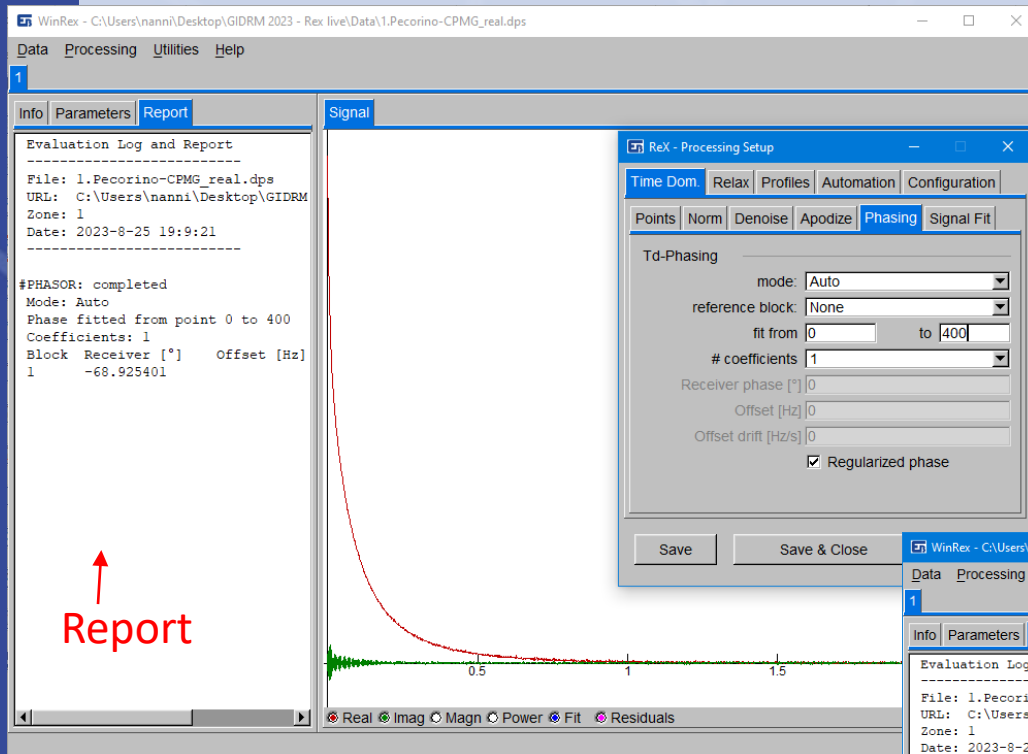
# Example 1. CPMG



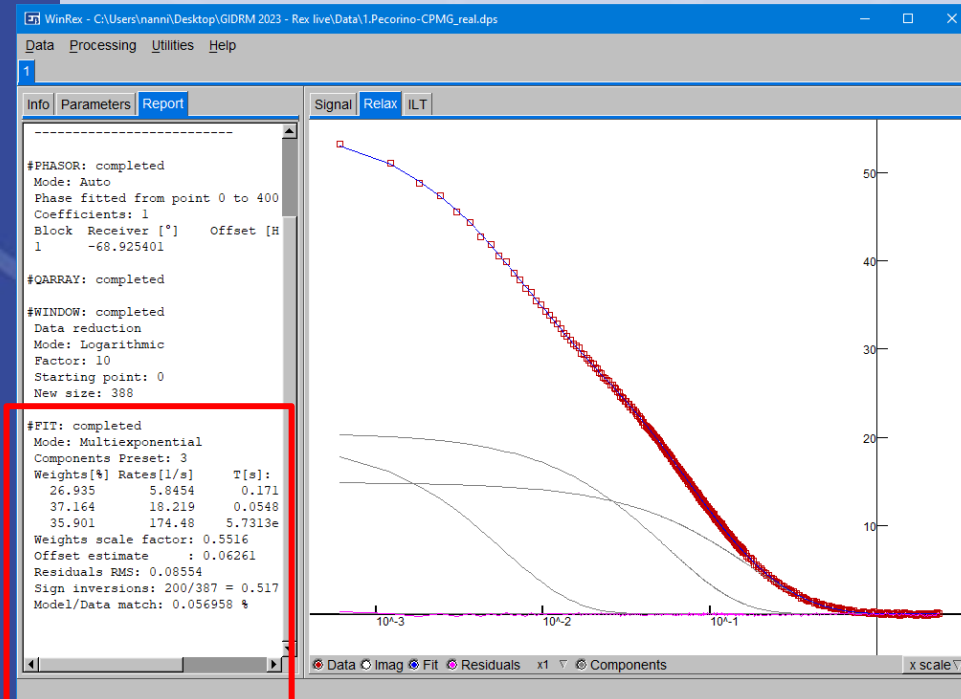
Sample:  
Pecorino Sardo DOP  
cheese

# 1. CPMG

-> Time-domain phasing



-> Points reduction (sieving)



# Inverse Laplace

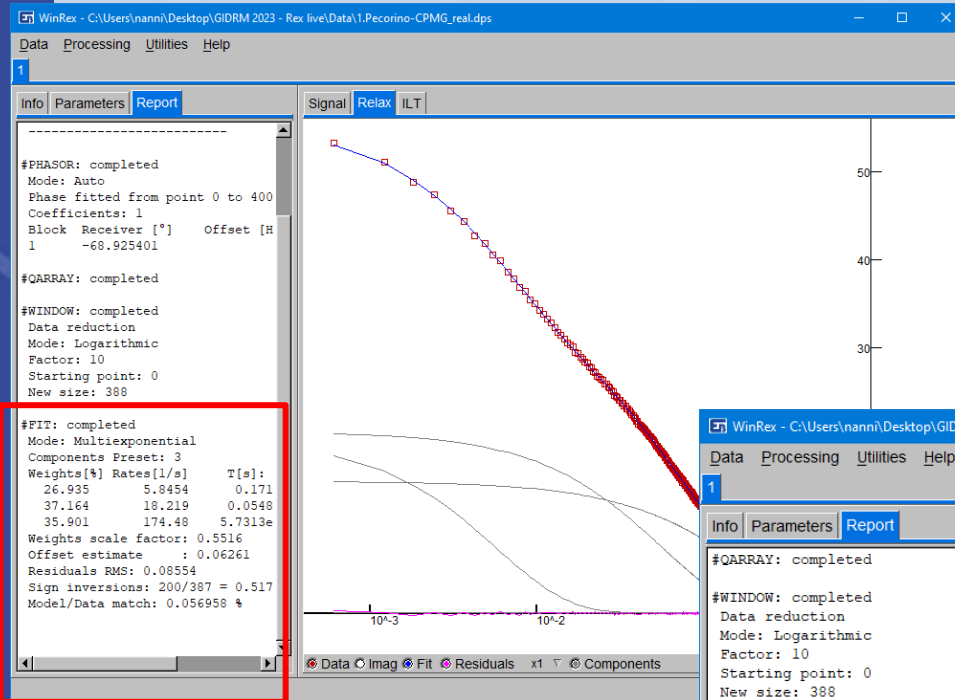
-> Multi-exponential fitting  
(Discrete ILT)

Automatic research of the  
components

Results

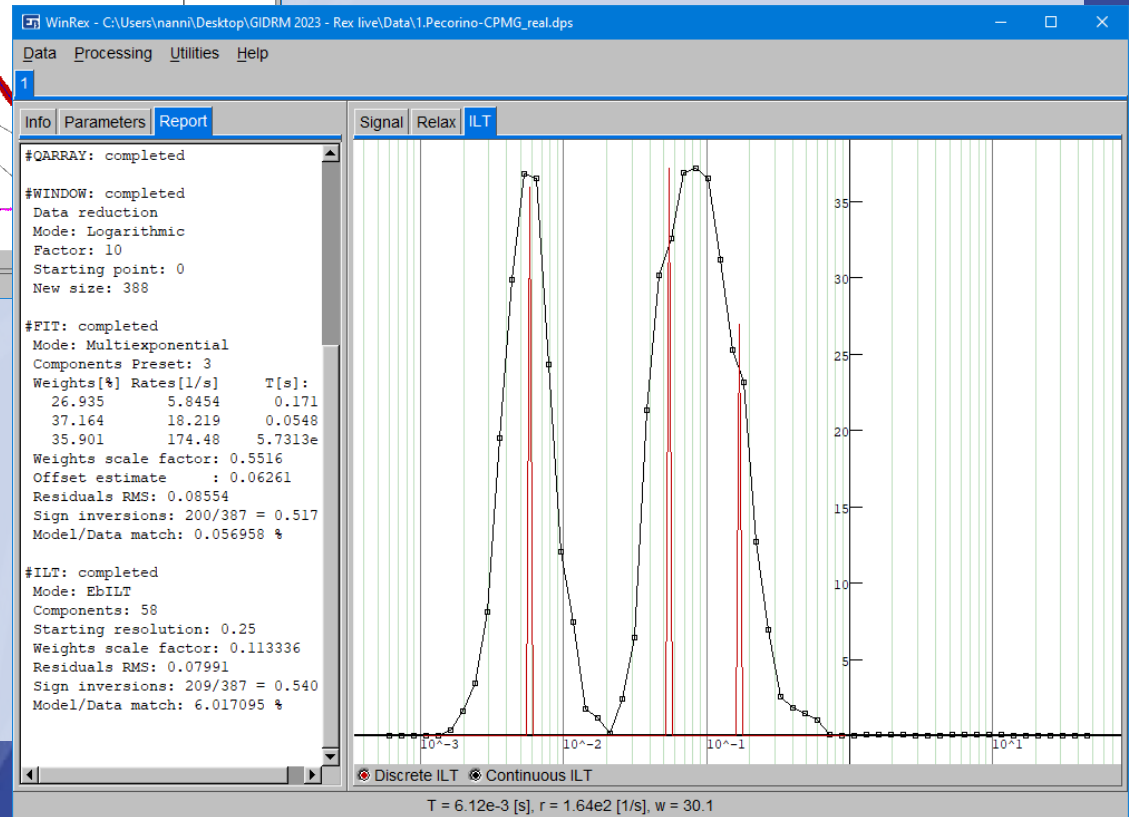
# Inverse Laplace

-> Multi-exponential fitting  
(Discrete ILT)



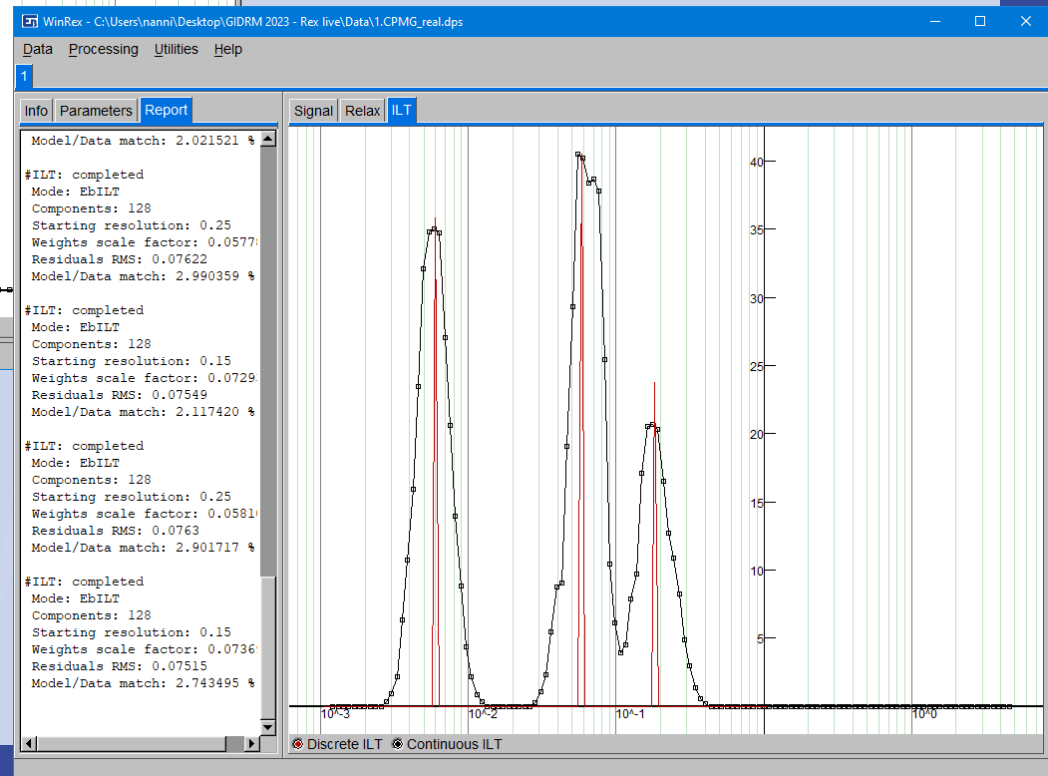
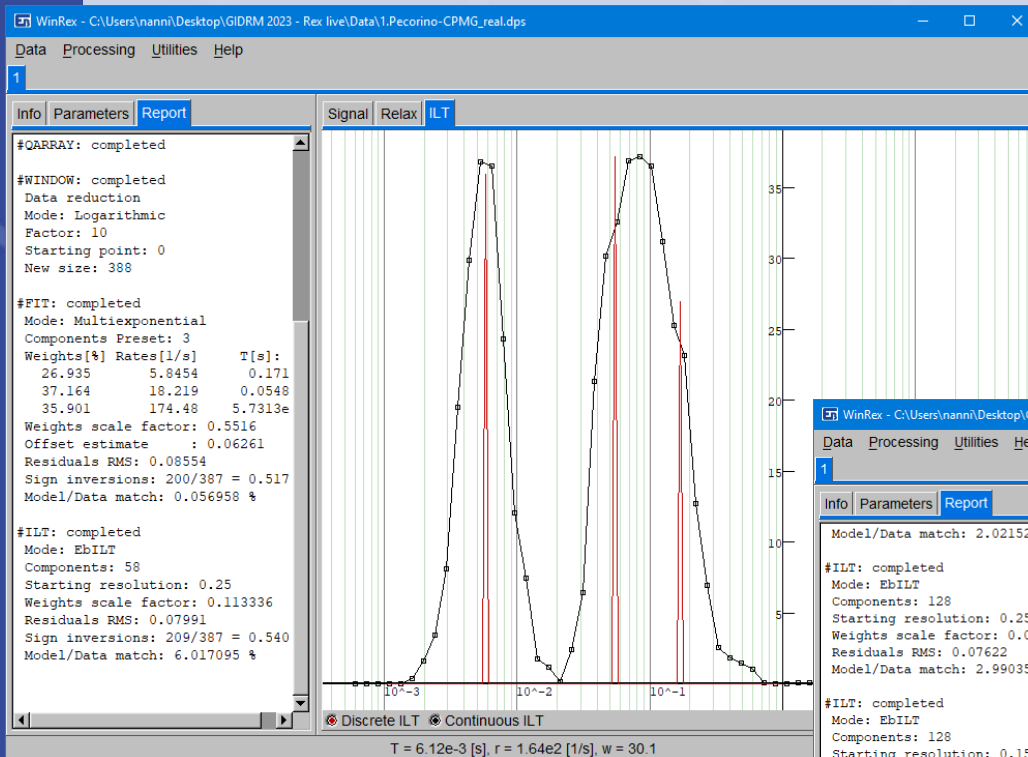
Results

-> Continuous ILT



# Continuous ILT

One parameter sets the initial resolution



ILT distribution results with different resolution parameter

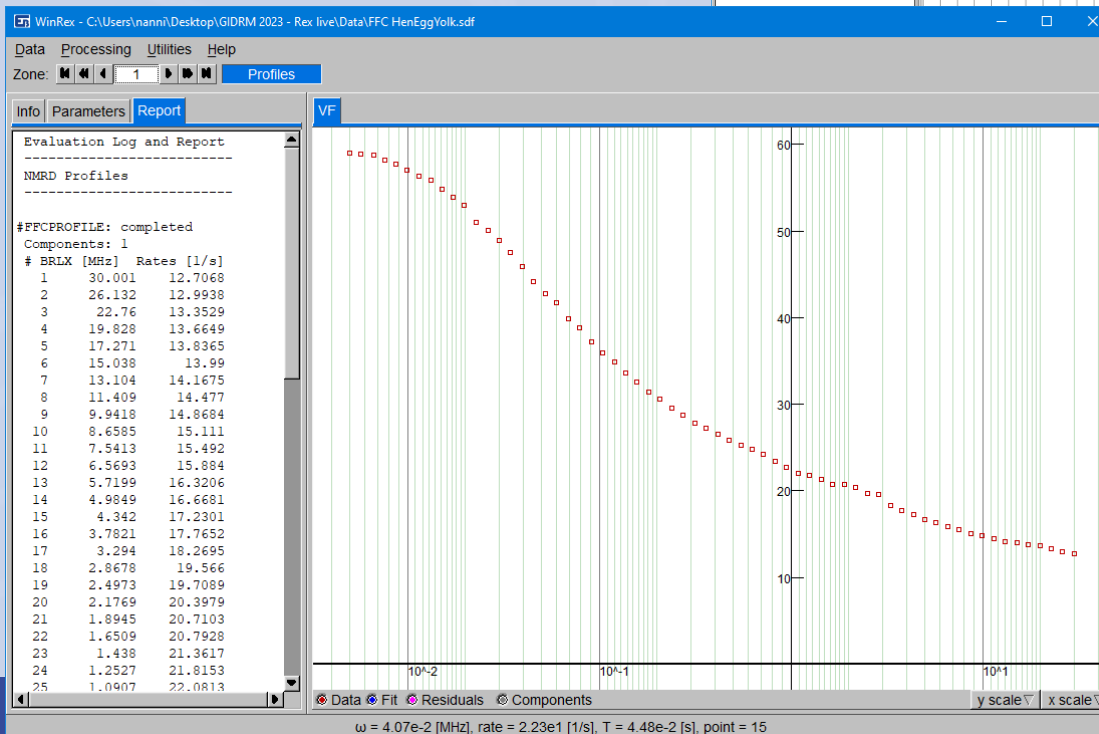
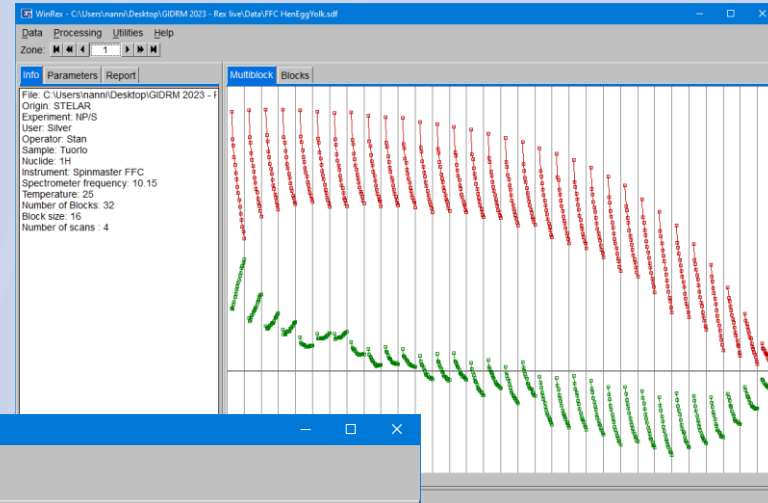


# Ex 2. NMRD Profile

Sample: Hen egg yolk

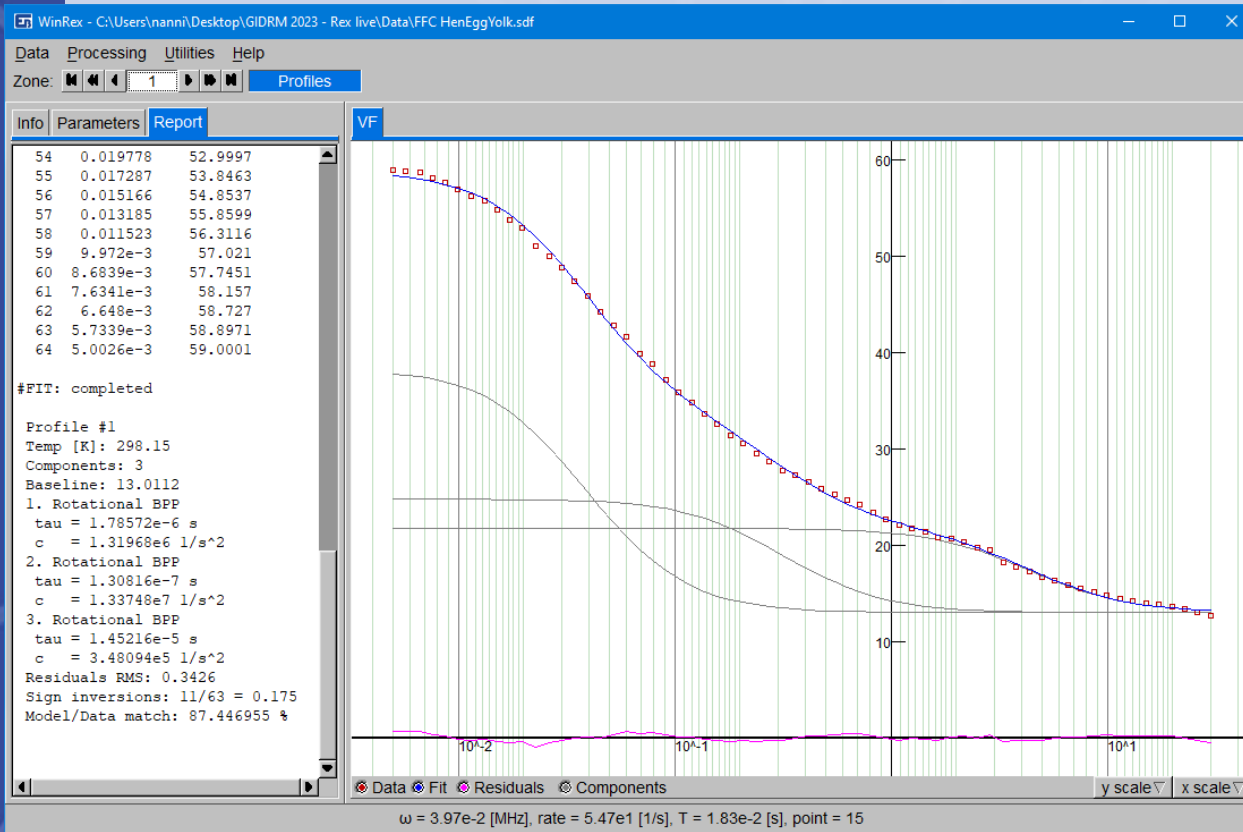
Profile built from  
Fast Field Cycling (FFC) data

## Relaxation rate vs Frequency



Automation:  
execute a list of  
commands for  
each frequency

## 2. NMRD Profile

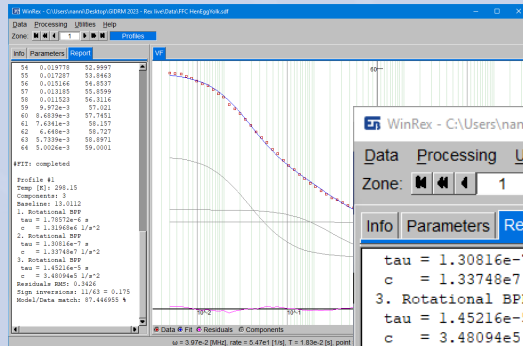


a) Fit with 3 BPP

$$\text{BPP} = c \left[ \frac{4\tau}{1+4(\omega\tau)^2} + \frac{\tau}{1+(\omega\tau)^2} \right]$$

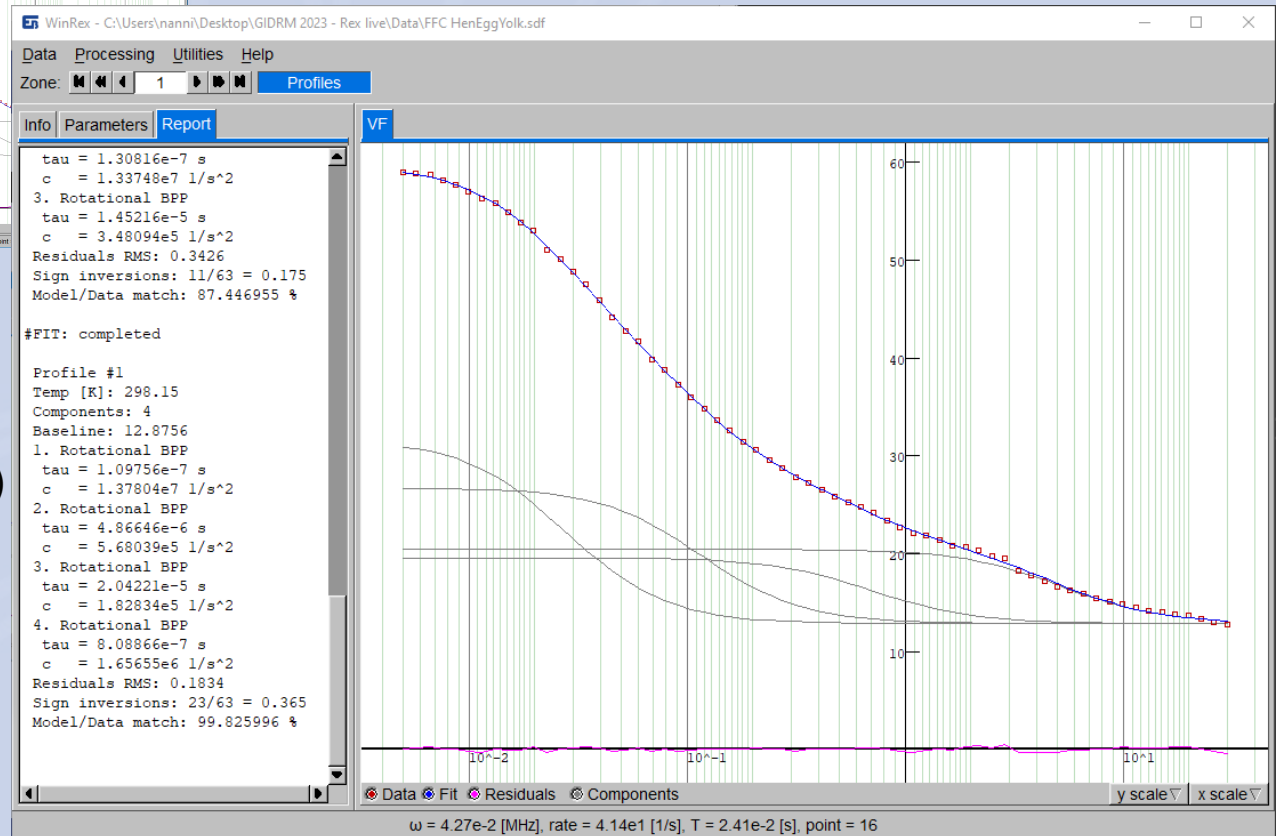
# 2. NMRD Profile

a)

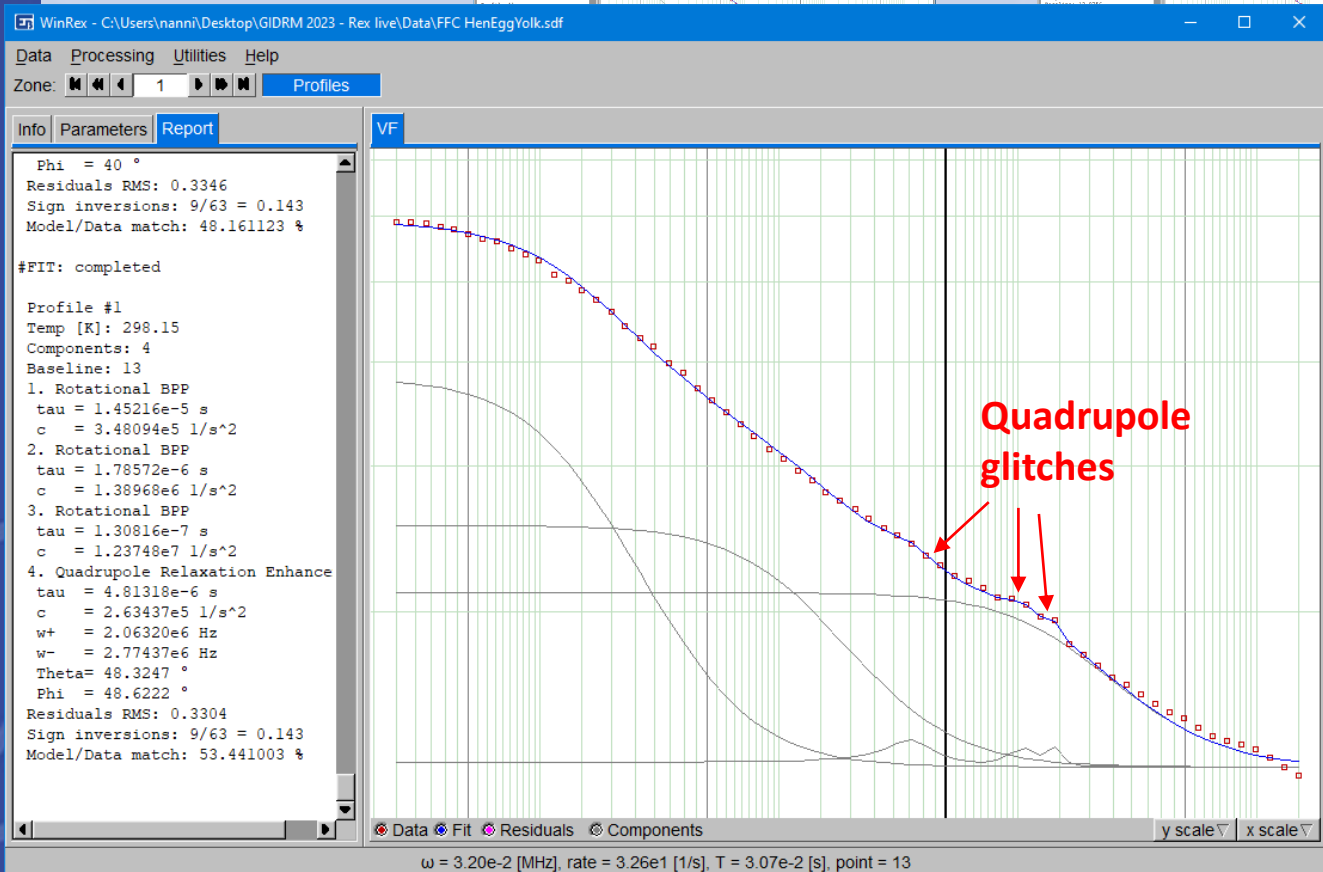
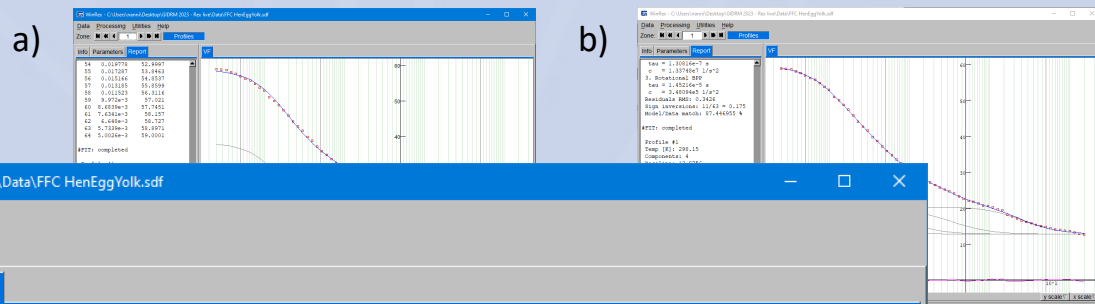


b) Fit with 4 BPP

(RMSE decreased by 50%)



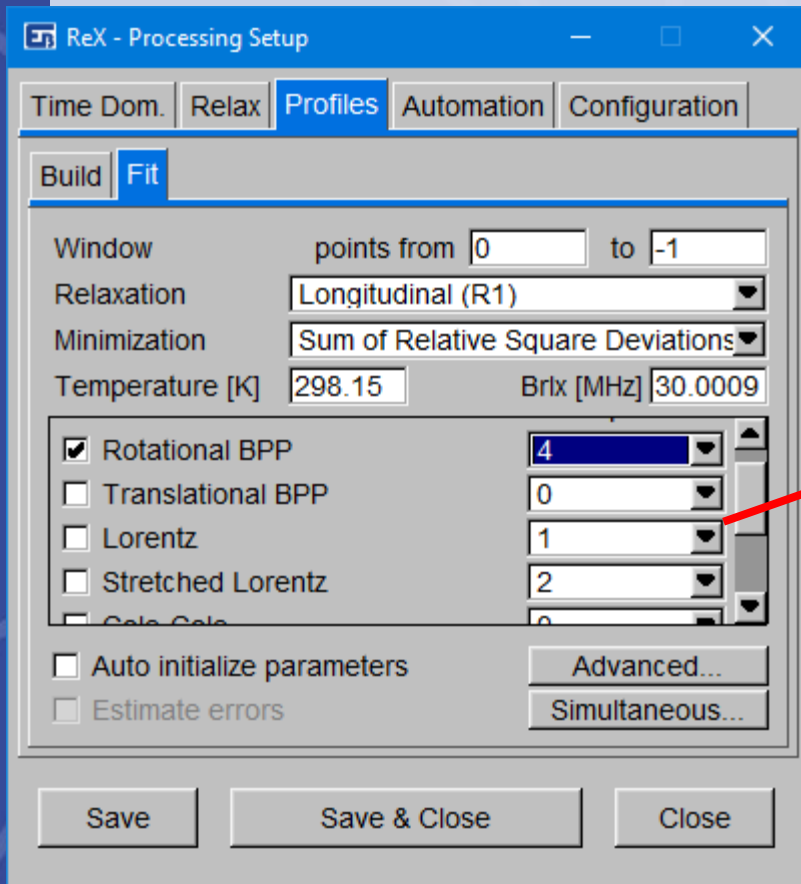
# 2. NMRD Profile



c) Fit with  
3 BPP + QRE  
  
(Quadrupole  
Relaxation  
Enhancement)

## 2. NMRD Profile

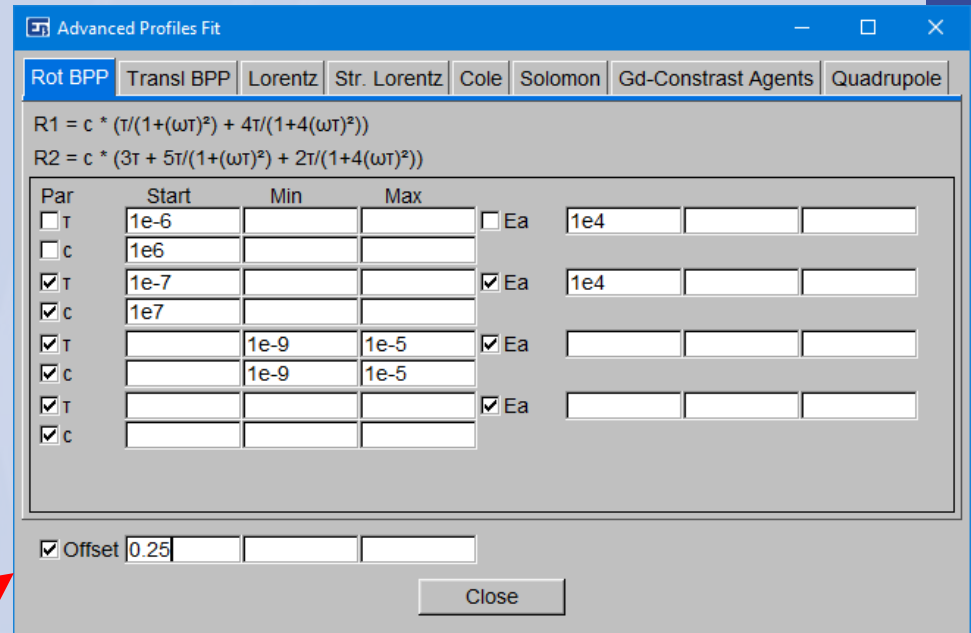
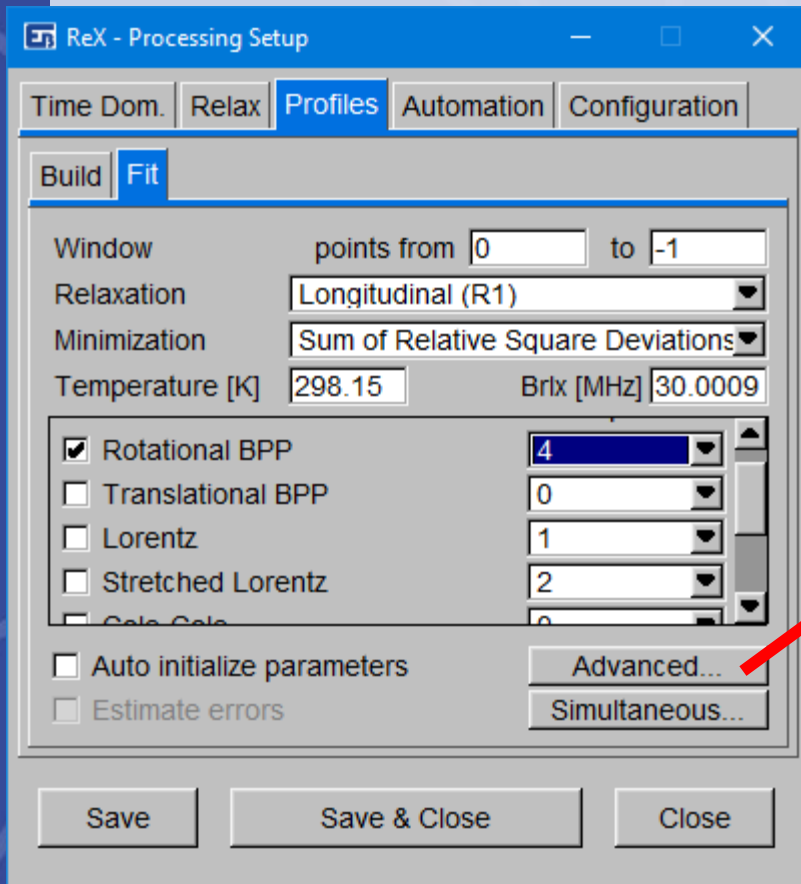
Profiles fitting interface



Choose and combine different models

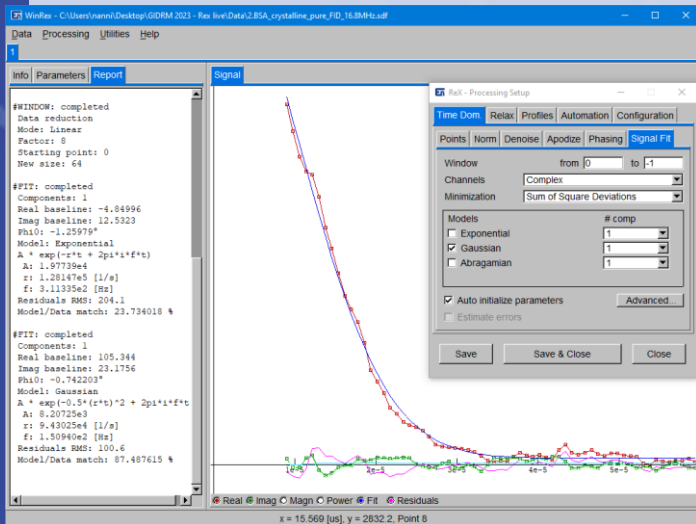
## 2. NMRD Profile

Profiles fitting interface



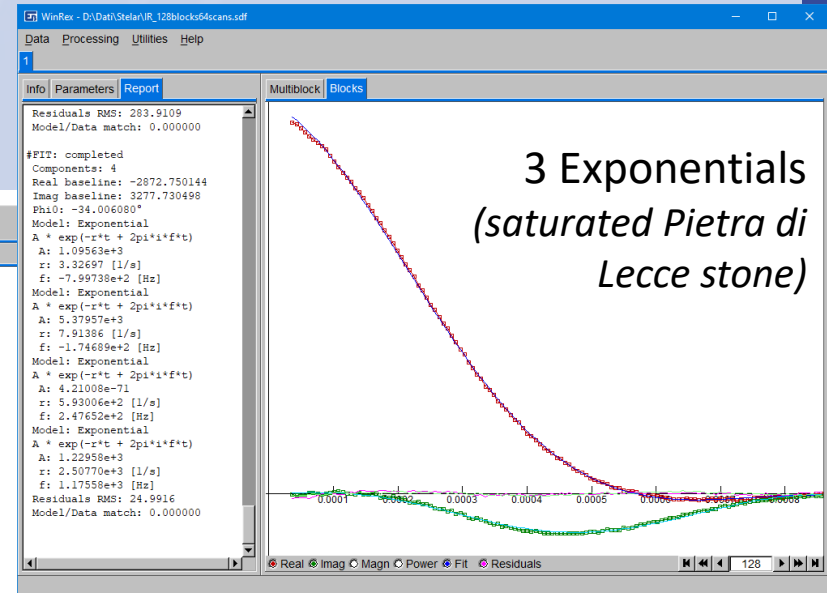
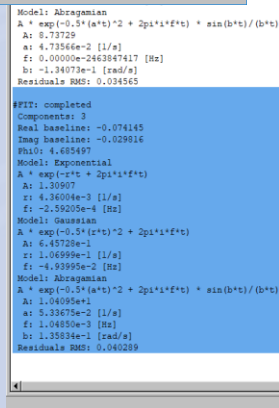
Advanced parameters setting:  
(manual initialization, setting limit values,  
fix any parameter)

# FIDs – fitting examples



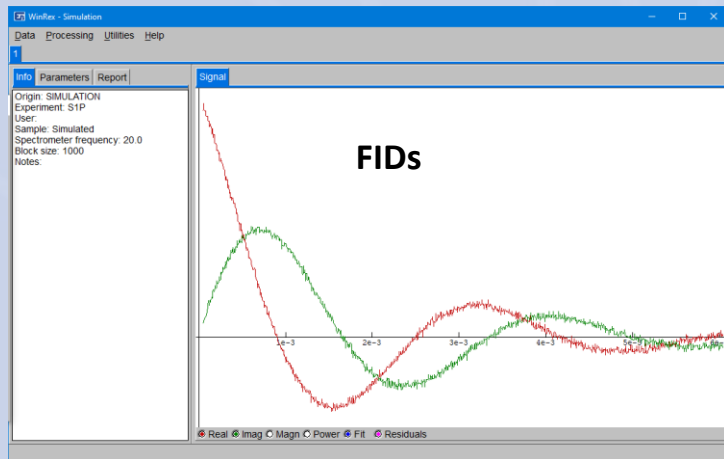
Gaussian (BSA)

Abragamian +  
Gaussian +  
Exponential  
(cellulose)



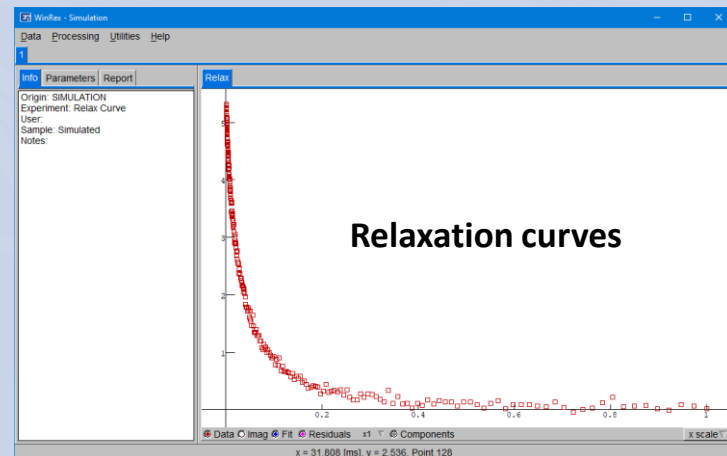
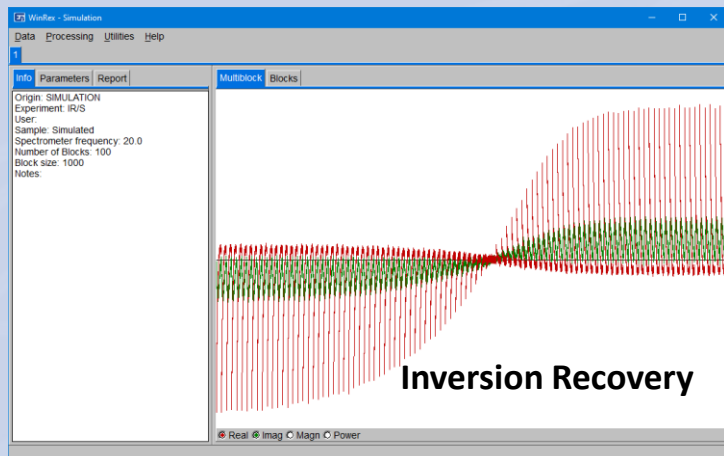
3 Exponentials  
(saturated Pietra di  
Lecce stone)

# Data Simulation



User can set:

- Instrumental parameters (B0, noise ...)
- Experimental parameters (points digitization, receiver phase, pulse width ...)
- Decay properties (weights, frequencies, T1, T2 ...)



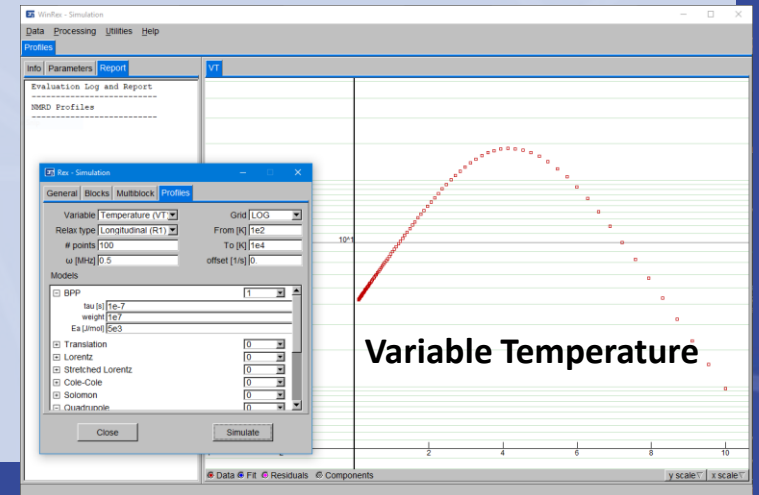
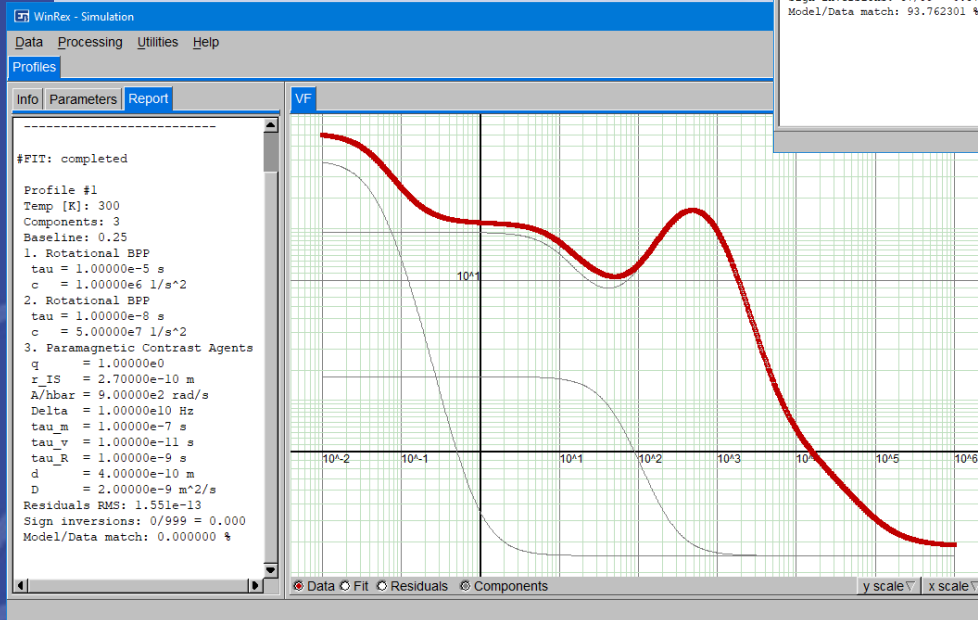
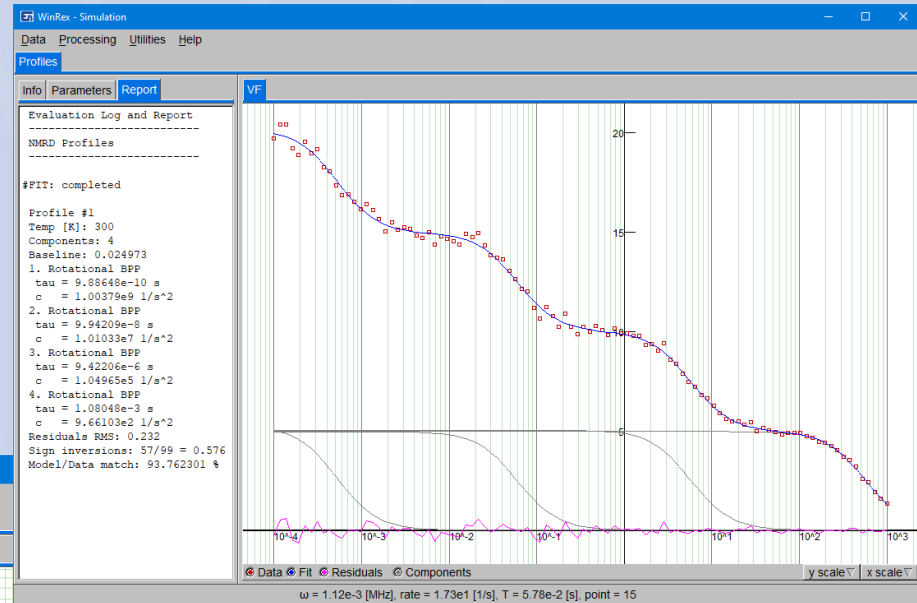


# Data Simulation - NMRD profiles

## Combination of different models:

- BPP
- Empirical formulae (Cole...)
- Quadrupolar Resonance
- Gd-based Contrast Agents
- ...

## Variable Frequency



## Next advancements

- More versatility in fitting tasks
- Improvements in automation procedures
- More support for specific applications

## Webpage

[www.extrabyte.eu/products/rex](http://www.extrabyte.eu/products/rex)

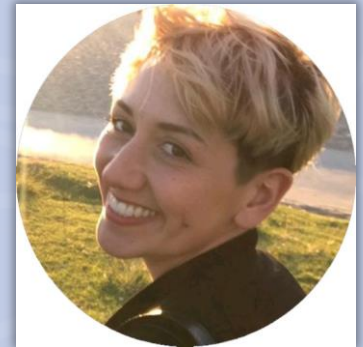
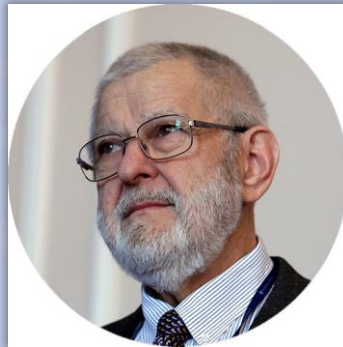
- Installer (Win64)
- Reference manual
- Tutorial, training
- Example data

60 days free trial!



# Thank You for Your Attention!

our team:



**Extra Byte**  
>in spin we trust

visit: [www.extrabyte.eu](http://www.extrabyte.eu)

email: [info@extrabyte.eu](mailto:info@extrabyte.eu)