



HAL
open science

A robust and prior knowledge independent method to interpret non-negative least squares (NNLS) T2 relaxation results

Guilhem Pages, Amidou Traore, J.-M. Bonny

► **To cite this version:**

Guilhem Pages, Amidou Traore, J.-M. Bonny. A robust and prior knowledge independent method to interpret non-negative least squares (NNLS) T2 relaxation results. 14. International Conference on the Applications of Magnetic Resonance in Food Science, Sep 2018, Rennes, France. hal-02736963

HAL Id: hal-02736963

<https://hal.inrae.fr/hal-02736963>

Submitted on 2 Jun 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

ABSTRACT SUBMISSION

30 April, 2018

Deadline for abstract submission for oral presentations

15 Juin, 2018

Deadline for abstract submission for poster presentations

Abstracts have to be sent by e-mail as attached files (PDF) to the secretariat of
MRFOOD2018
mrfood2018@irstea.fr

Abstracts may include: Tables, Schemes, Figures and References.

To maintain a consistent appearance, all abstracts must be prepared in the following style (**see also the template in the next page**):

- maximum space limit is half page
- maximum usable area is 16.0 cm wide and 12.0 cm high
- times new roman font (symbol font for special characters)
- 14 point boldface font for the title
- 12 point underlined font for presenting Author (12 point normal font for other Authors, if any)
- 12 point *italic font* for affiliations
- affiliations distinguished by superscript numbers if necessary
- one blank line left between address and the beginning of the abstract
- one blank line left between the end of the abstract and references/acknowledgment (if present).

Proposed session (select one):

- NMR/MRI development and signal processing
- Food Physics
- Postharvest Technologies
- Food Technologies
- Foodomics and Food Chemistry

Presentation preference*:

- oral
- poster

* Select the option "Oral presentation" to indicate that you would like your abstract to be considered for an oral presentation

- Paper submission in Magnetic Resonance in Chemistry (**before the 1st of September 2018**)

A robust and prior knowledge independent method to interpret non-negative least squares (NNLS) T_2 relaxation results

Guilhem Pagès, Amidou Traoré, Jean-Marie Bonny

AgroResonance, UR 370 QuaPA, INRA, F-63122 Saint-Genés-Champanelle

The fitting of an NMR signal decay in a weighted sum of exponentials is an ill-posed problem, i.e. different sets of relaxation times and amplitudes will lead to the same least-squares distance between the model and the experimental noisy data. To analyze such data, the classical pipe consists in performing a non-negative least squares (NNLS) algorithm combined with a regularization to smooth the T_2 distribution. However, a critical step of this approach deals with the choice of the operator and then of the corresponding regularization parameter which significantly affects the T_2 distribution. These parameters are usually chosen based on the operator experience as well as prior knowledge on the sample.

In this work, we propose to analyze NNLS results without regularization to circumvent these drawbacks. Our approach is based on the analysis of NNLS outputs by cumulative distribution functions (cdf) and not by probability density functions (pdf) as it is usually done. This concept is validated in different simulations for which the true T_2 distributions are built from discrete to continuous functions. Simulation results showed that the T_2 amplitude measured at a plateau of the cdf is unbiased and (almost) independent of both the decomposition basis and the signal-to-noise ratio. This observation allows to quantitatively interpret the NNLS inversions, especially when the true distribution is continuous. We suggest that NNLS by itself suffices in many situations, provided that cdf plateau can be discernable. The degrees of freedom to adjust in the method are then limited to the decomposition basis. To exemplify, this pragmatic and fruitful approach is applied on real NMR data obtained by spectroscopy and imaging.