



HAL
open science

Basics of Fourier Transform Applied to NMR Spectroscopy: An Interactive Open-Source Web Application

Yannick Esvan, Waël Zeinyeh

► **To cite this version:**

Yannick Esvan, Waël Zeinyeh. Basics of Fourier Transform Applied to NMR Spectroscopy: An Interactive Open-Source Web Application. *Journal of Chemical Education*, 2020, 97 (1), pp.263-264. 10.1021/acs.jchemed.9b00502 . hal-04800927

HAL Id: hal-04800927

<https://hal.science/hal-04800927v1>

Submitted on 24 Jan 2025

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.

Basics of Fourier Transform Applied to NMR Spectroscopy: An Interactive Open-Source Web Application

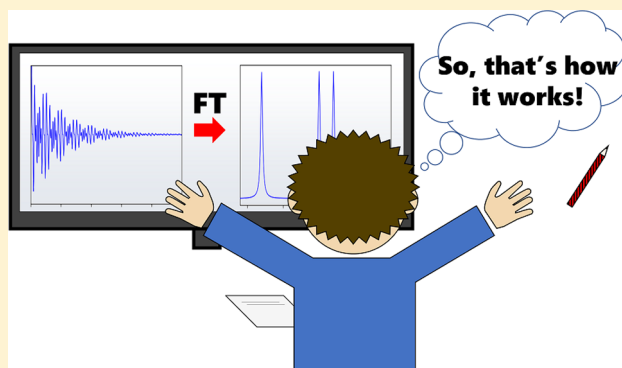
Yannick J. Esvan[†] and Wael Zeinyeh^{*,‡,§}

[†]Charnwood Molecular Ltd., Nottingham NG1 1GF, United Kingdom

[‡]Université de Lyon, Université Claude Bernard Lyon 1, Lyon Neuroscience Research Center, CNRS UMR5292, INSERM U1028, 59 bd Pinel 69677 Bron Cedex, France

Supporting Information

ABSTRACT: The Fourier transformation (FT) is a mathematical process frequently encountered by chemistry students. However, it remains an automated background process perceived by many students as difficult to understand. In this paper we present a simple open-source web application, which can help students to understand the basics of the FT applied to nuclear magnetic resonance (NMR) spectroscopy.



KEYWORDS: Second-Year Undergraduates, Analytical Chemistry, Computer-Based Learning, Distance Learning/Self Instruction, NMR Spectroscopy, Fourier Transform Techniques

Over the past 40 years, several publications in this *Journal* aimed at helping students to understand the theory of Fourier transformation (FT) and its applications in analytical chemistry. One solution frequently proposed by authors was the use of computer simulations, and this started even in the early age of personal computers.^{1,2} Later, interactive simulations based on MathCad (Parametric Technology Corporation) appeared,^{3,4} followed by more recent interactive Excel (Microsoft) spreadsheets.^{5,6}

However, both MathCad and Excel approaches require an additional guided tutorial, and the users have to be familiar with the basics of these two computer programs. Moreover, the two approaches produce static images and lack visual animations. Finally, both programs are not free and might not be accessible for students all over the world (although free alternatives might be available, from which compatibility issues may arise).

Here we report a free web application that explains the FT applied to an NMR signal, in a visual and animated fashion, without the need for a guided tutorial nor for deep computational knowledge (Figure 1).

A step-by-step strategy allows the student to

- Observe the evolution of the free induction decay (FID) when adding new frequencies
- Visualize an animated demonstration of the FT and the construction of the spectrum
- Study the effect on the spectrum of parameters modification (e.g., adding background noise or changing acquisition time)

The transition between steps is based on pop-up messages that explain the principles of the different operations and guide the user intuitively.

The source code of the software was written in Python, a free open-source programming language,⁷ and can be found on GitHub.⁸ Additionally, the software was deployed as a web application hosted on the Pythonanywhere.com server⁹ and can be executed in all recent Internet browsers (including mobile phone and tablet browsers) without any knowledge in programming languages. More experienced teachers and students will be able to adapt and/or improve the software by modifying the source code.

TEACHING VALUE AND RESULTS

The software was initially intended for second year pharmacy students, for whom the time allocated to the NMR course is brief and does not allow an in-depth explanation of the FT process. Nevertheless, our experience has shown that the software can find a widespread application.

We evaluated our web application with pharmacy and organic chemistry undergraduate and graduate students, and also with Ph.D. students and organic chemistry teachers who are not specialized in NMR techniques but are familiar with NMR spectrum interpretation. All of them ignored the details of the

Received: May 28, 2019

Revised: October 17, 2019

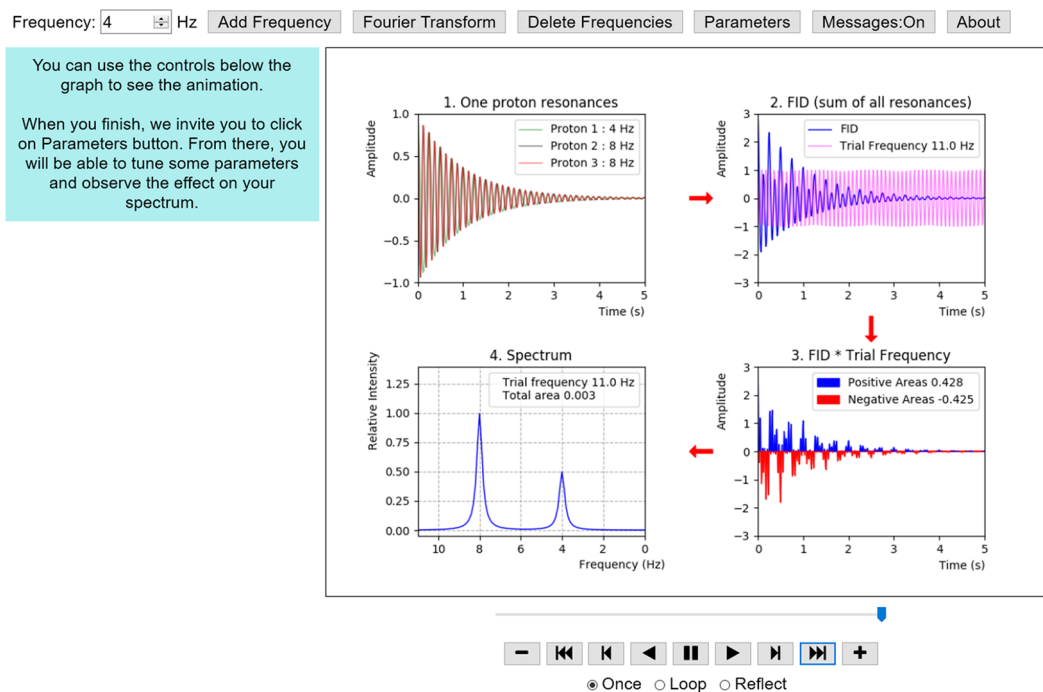


Figure 1. Screen capture of the web application.

FT process before using the application, and the majority recognized understanding its basics after running it.

Even if the application was designed as a self-instruction tool, the students who tested the application subsequently raised discussion with their teachers: A sample of frequent interrogations as well as a guided teaching experience are proposed in the [Supporting Information](#).

CONCLUSION

In conclusion, the proposed application can be considered as a good assistive tool for teachers during their NMR course, in order to introduce the concept of the FT. It allows students to have a full grasp of this mathematical process applied to NMR spectroscopy in a guided and visual fashion, helping them to understand several factors that will ultimately impact the quality of the NMR spectrum they utilize.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the [ACS Publications website](#) at DOI: [10.1021/acs.jchemed.9b00502](https://doi.org/10.1021/acs.jchemed.9b00502).

Teacher's guide to the application, including our teaching experience ([PDF](#), [DOCX](#))

AUTHOR INFORMATION

Corresponding Author

*E-mail: wael.zeinyeh@univ-lyon1.fr.

ORCID

Wael Zeinyeh: 0000-0001-7483-4751

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

We would like to thank all colleagues and students who contributed to the evaluation of the application, in particular, Dr. Anne Denuzière, Dr. Sylvie Radix, Alexandre Bancet, Bruna Gioia, Kevin Grollier, Mathis Larrieu, and Oliver Leadbeater.

REFERENCES

- Estler, R. C. Software simulations of Fourier Transform Experiments. *J. Chem. Educ.* **1991**, *68* (9), A220–A224.
- Blunt, J. W. Principles of Fourier-transform nuclear magnetic resonance. *J. Chem. Educ.* **1983**, *60* (2), 97–98.
- Van Bramer, S. E. An Introduction to the Fourier Transform: IntroFourierTransform.mcd and LectureIntroFT.mcd. *J. Chem. Educ.* **1999**, *76* (2), 286.
- Iannone, M. Exploring Fourier Transform Techniques with Mathcad: FTIntro.mcd, FT2IR.mcd, FT3Pulse.mcd, and FT4FreeInd-Decay.mcd. *J. Chem. Educ.* **1999**, *76* (2), 286.
- Hoffmann, M. M. An Interactive Spreadsheet for Demonstration of Basic NMR and Fourier Transform Concepts. *J. Chem. Educ.* **2009**, *86* (3), 399.
- Shepherd, B.; Bellamy, M. K. A Spreadsheet Exercise To Teach the Fourier Transform in FTIR Spectrometry. *J. Chem. Educ.* **2012**, *89* (5), 681–682.
- Python Software Foundation. <https://www.python.org/> (accessed August 2019).
- https://github.com/waelzeinyeh/FT_EXPLAINED (accessed August 2019).
- URL to run the application: <https://ftnmr.eu.pythonanywhere.com> (accessed August 2019) or https://clarolineconnect.univ-lyon1.fr/icap_website/view/2018 (accessed August 2019).