



## Abstract Nuclear Magnetic Resonance Metabolomics of Three Tomato Cultivars<sup>†</sup>

Cătălin Duduianu<sup>1,2</sup>, Calin Deleanu<sup>1,3</sup>, Liliana Adriana Pairault<sup>4</sup>, Alina Nicolescu<sup>3,\*</sup> and Florin Oancea<sup>5,\*</sup>

- <sup>1</sup> "Costin D. Nenitescu" Institute of Organic and Supramolecular Chemistry, Spl. Independentei 202-B, RO-060023 Bucharest, Romania
- <sup>2</sup> Faculty of Applied Chemistry and Material Science, National University of Science and Technology Politehnica of Bucharest, Str. Polizu 1, RO-011061 Bucharest, Romania
- <sup>3</sup> "Petru Poni" Institute for Macromolecular Chemistry, Aleea Grigore Ghica Voda 41A, RO-700487 Iasi, Romania
- <sup>4</sup> Amia Import-Export, Str. Gorunului 7, RO-075100 Otopeni, Romania
- <sup>5</sup> National Institute for Research & Development in Chemistry and Petrochemistry—ICECHIM, Spl. Independentei 202, RO-060201 Bucharest, Romania
- \* Correspondence: alina@icmpp.ro (A.N.); florin.oancea@icechim.ro (F.O.)
- <sup>+</sup> Presented at the 19th International Symposium "Priorities of Chemistry for a Sustainable Development", Bucharest, Romania, 11–13 October 2023.

Keywords: tomato; NMR spectroscopy; metabolite; concentration

With the continuous increase in the popularity of vegetarianism and veganism, either as a diet or lifestyle, fruits and vegetables are becoming essential components of human nutrition. Among vegetables, tomato (*Solanum lycopersicum* L.), consumed either as fresh fruit or as processed products, is one of the most frequently consumed, mainly due to its availability, accessible price and healthy metabolites, such as folate, vitamin C, potassium, phenolic compounds, carotenoids and lycopene. Tomato consumption has been associated with a reduced onset of cardiovascular disease and certain cancers. These health benefits have been attributed to different metabolites and interactions in tomato. Owing to its short life cycle, tomato has become the model plant for different environmental studies.

This study aims to characterize the composition of metabolites in fresh tomatoes from different cultivars.

Tomato fruits from three cultivars (Signora, Arawak and Cherry) grown by different Romanian producers were analyzed through NMR spectroscopy. Aqueous extracts were obtained by squeezing 2–3 fresh tomato fruits from the same cultivar in a juicer with a snail. The obtained liquid extracts were centrifuged in order to remove any solid particles. For NMR analysis, 0.9 mL of liquid was mixed with 0.1 mL of phosphate buffer in D2O containing TSP as an internal standard. Signal assignments were performed based on reference spectra and literature data, with 16 metabolites being identified and quantified (Figure 1).

Concentrations of 16 metabolites were determined for the three cultivars. No significant differences between cultivar were obtained for valine, leucine, isoleucine, tyrosine or malic acid. For the rest of metabolites, including phenylalanine, threonine, alanine, asparagine, gamma-aminobutyrate, glutamate, glutamine, citric acid, glucose and fructose, the concentrations were cultivar-dependent. The most significant differences were obtained for cherry tomatoes in the case of asparagine, gamma-aminobutyrate and citric acid.

The identification of several metabolites present in freshly squeezed tomato juice without any separation step was described. Some metabolites that presented significant concentration differences among cultivars can be used as variety markers.



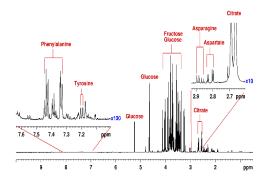
Citation: Duduianu, C.; Deleanu, C.; Pairault, L.A.; Nicolescu, A.; Oancea, F. Nuclear Magnetic Resonance Metabolomics of Three Tomato Cultivars. *Proceedings* **2023**, *90*, 31. https://doi.org/10.3390/ proceedings2023090031

Academic Editors: Mihaela Doni and Radu Claudiu Fierăscu

Published: 13 December 2023



**Copyright:** © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/).



**Figure 1.** 1H NMR spectrum of the tomato aqueous extract with two enlarged regions for better visualization of metabolites' signals.

Author Contributions: Conceptualization, A.N., C.D. (Calin Deleanu), F.O.; methodology, A.N.; formal analysis, A.N., C.D. (Cătălin Duduianu); investigation, A.N., C.D. (Cătălin Duduianu), L.A.P.; writing—original draft preparation, A.N.; writing—review and editing, A.N., C.D. (Calin Deleanu), F.O.; funding acquisition, A.N., F.O. All authors have read and agreed to the published version of the manuscript.

**Funding:** The research leading to these results received funding from the NO Grants 2014-2021, under the project RO-NO-2019-0540 (STIM4+), contract 14/2020.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

**Data Availability Statement:** Further data may be obtained by request for the corresponding authors. Extensive dataset will be published in a forthcoming paper.

Conflicts of Interest: The authors declare no conflict of interest.

**Disclaimer/Publisher's Note:** The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.