# Article information:

ML-J-DP4: An Integrated Quantum Mechanics-Machine Learning Approach for Ultrafast NMR Structural Elucidation | Organic Letters
<https://pubs.acs.org/doi/10.1021/acs.orglett.2c01251>

# Article summary:

1. The determination of molecular structure is essential in many areas of chemistry, and NMR calculations using DFT approaches have emerged as powerful tools to facilitate the structural assignment of complex molecules.

2. A new machine-learning based approach has been developed that accelerates J-DP4 (one of the state-of-the-art methods in structural elucidation) by 2 orders of magnitude.

3. The results obtained with this approach provide strong evidence for the inclusion of Karplus-type 3JHH values in the J-DP4 architecture, resulting in significant time savings.

# Article rating:

Appears well balanced: The article presents the information in a reliable and balanced way, without biases and prejudices. The claims made in the article are well supported and, where applicable, all sides of the argument are given opportunity to present their point of view. The article appears trustworthy and reliable.

# Article analysis:

The article provides a detailed overview of an integrated quantum mechanics-machine learning approach for ultrafast NMR structural elucidation, and presents a proof-of-principle study demonstrating its potential to accelerate J-DP4 by two orders of magnitude. The article is well written and provides a comprehensive description of the methodology used, as well as a thorough analysis and discussion of the results obtained.

The authors present their findings objectively and without bias, providing evidence to support their claims and exploring possible counterarguments where appropriate. They also acknowledge potential limitations such as computational cost and accuracy issues associated with lower levels of theory used for NMR calculations. Furthermore, they provide sufficient detail on their methodology so that readers can assess its reliability and trustworthiness for themselves.

In conclusion, this article is reliable and trustworthy due to its objective presentation of findings, thorough analysis and discussion, acknowledgement of potential limitations, and provision of sufficient detail on methodology used.

# Topics for further research:

* Quantum Mechanics-Machine Learning
* Ultrafast NMR Structural Elucidation
* J-DP4 Acceleration
* Computational Cost of NMR Calculations
* Accuracy Issues in NMR Calculations
* Machine Learning Applications in Chemistry

# Report location:

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