

# Accelerating Biomolecular Nuclear Magnetic Resonance Assignment with A\*

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# Overview

- 1 Introduction
  - Nuclear Magnetic Resonance Spectroscopy
- 2 Assignment Process
  - Data Collection
  - Manual Assignment
- 3 Automation
  - Algorithm Design
- 4 Conclusion
  - Results
  - Outlook



# Title



# Title





# Title



# Title

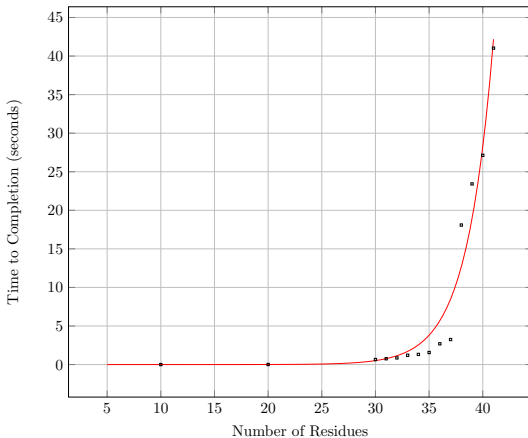




# Title



# Time of Assignment





# Assignment Issues

- Missing data decreases accuracy
  - increases assignment time

# Future Goals

- Parallelization
  - Decrease assignment time
  - Allow for larger data sets
- Machine learning
  - Increase accuracy of assignment
  - Optimize cost calculation



# Bibliography