

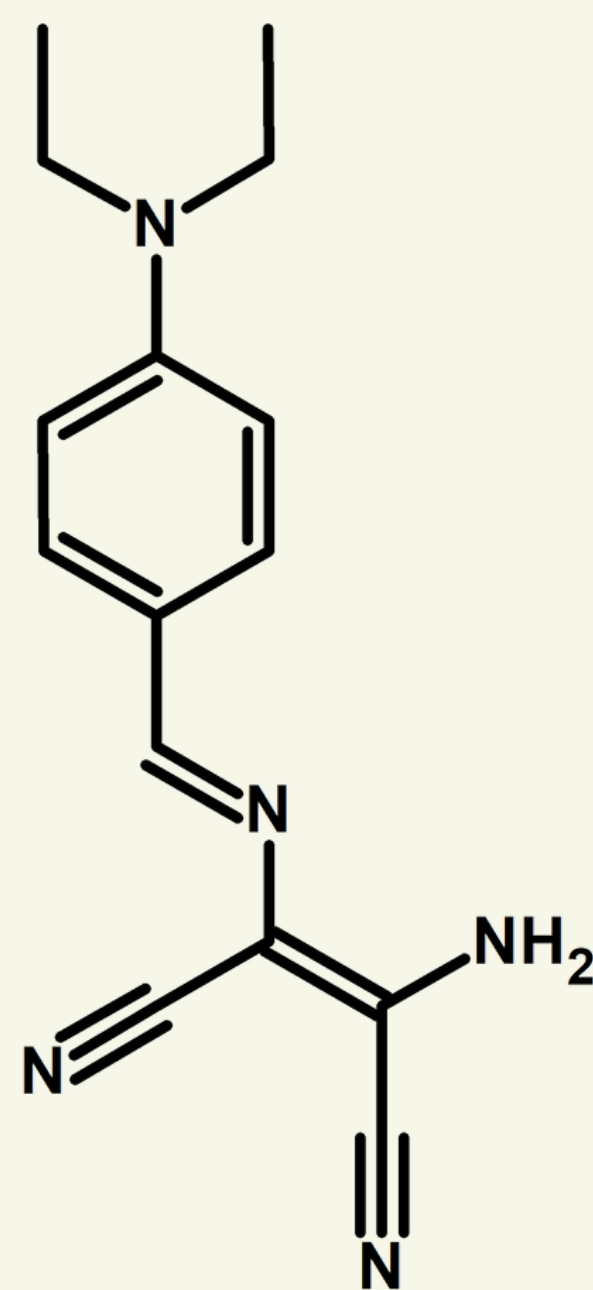
INVESTIGATING A COVALENTLY CONNECTED DIMER OF AN AGGREGATION INDUCED EMISSION (AIE) CHROMOPHORE FOR ENERGY EFFICIENT OPTOELECTRONICS

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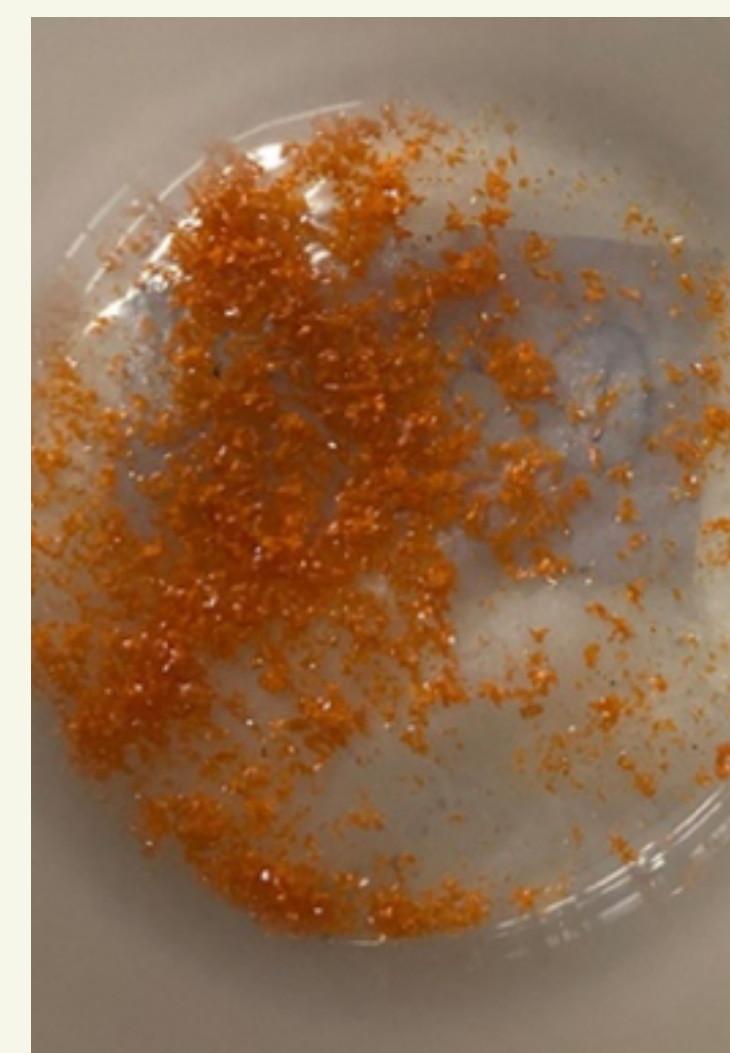
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INTRODUCTION

Our recent reports on the investigation of inversion symmetry-driven aggregation-induced emission (AIE) has opened up never reported applications in optoelectronics, mechanical memory, and quantum information sciences.



- In this work, I focused on A3MN (2-amino-3-((E)-(4-(diethylamino)benzylidene)amino)maleonitrile), a well-studied AIE molecule with distinctive optical properties driven by inversion symmetry.
- Goal:** Form dimers and investigate how such structural modifications could influence its behavior.



RESEARCH OBJECTIVE

- Investigate dimerization of A3MN molecules using a di-carboxylic linker.
- Understand how covalent linking affects absorbance and fluorescence properties.

METHODOLOGY

Dimerization strategy: Oxalic acid as linker between two A3MN molecules through amide bond formation

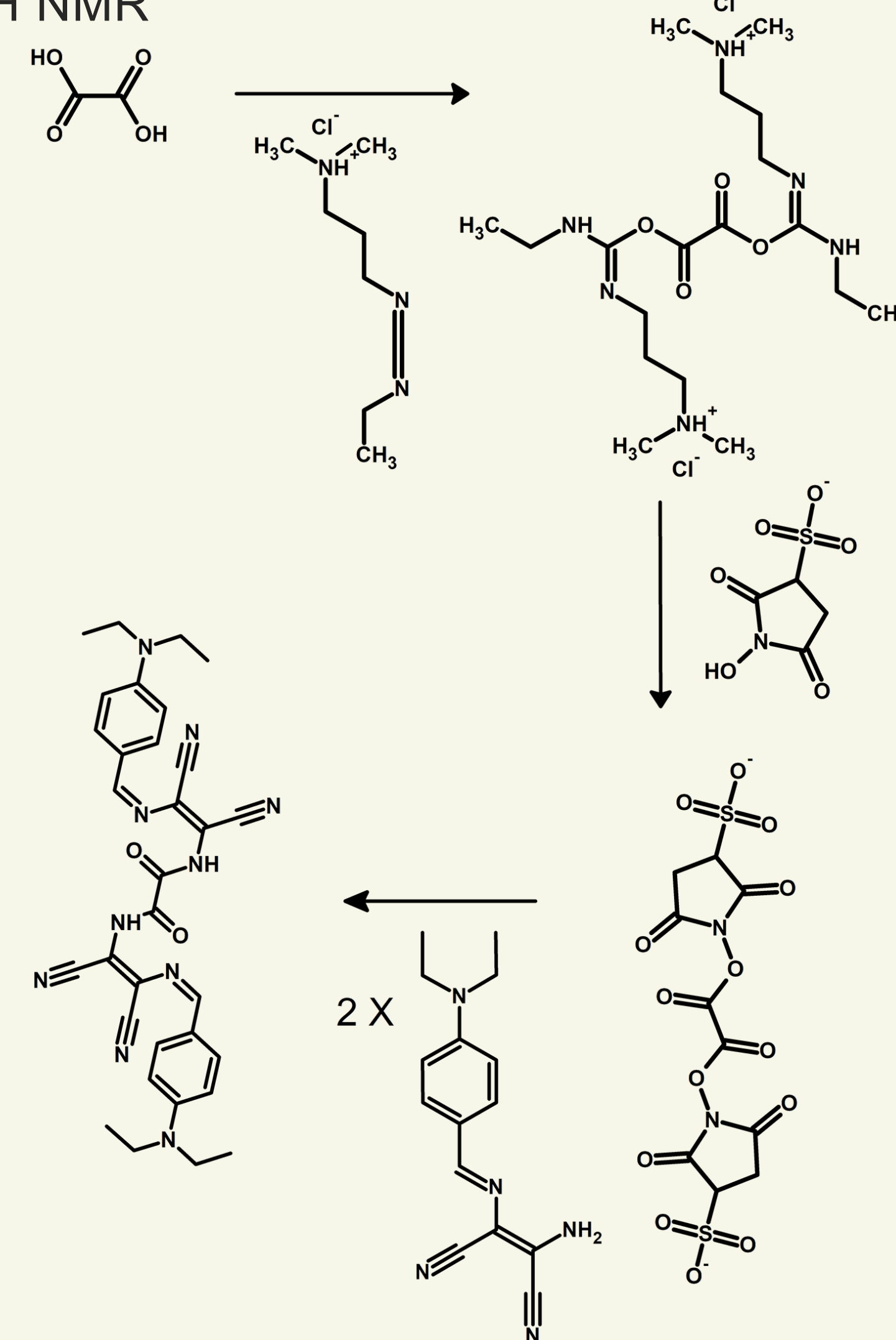
Coupling agents used:

- EDC (1-ethyl-3-(3-dimethylaminopropyl)carbodiimide).
- NHS (N-hydroxysuccinimide)

Reaction design: Two A3MN molecules bound to the two ends of oxalic acid through the primary amine group.

Characterization techniques:

- UV-Visible absorbance spectra.
- Fluorescence spectra.
- ¹H NMR



RESULTS AND DISCUSSION

UV-Vis Spectra (Figure 01):

- A slight drop in absorbance intensity and broadening of the shoulder of the absorbance peak was observed after dimerization.
- This reduction suggests a loss of free A3MN molecules from the reaction mixture, as some have participated in dimer formation.
- Additionally, a new red-shifted peak appeared, further indicating the possible formation of the dimer. (IP protection underway)
- These spectral changes point to structural modifications but require further detailed analysis.

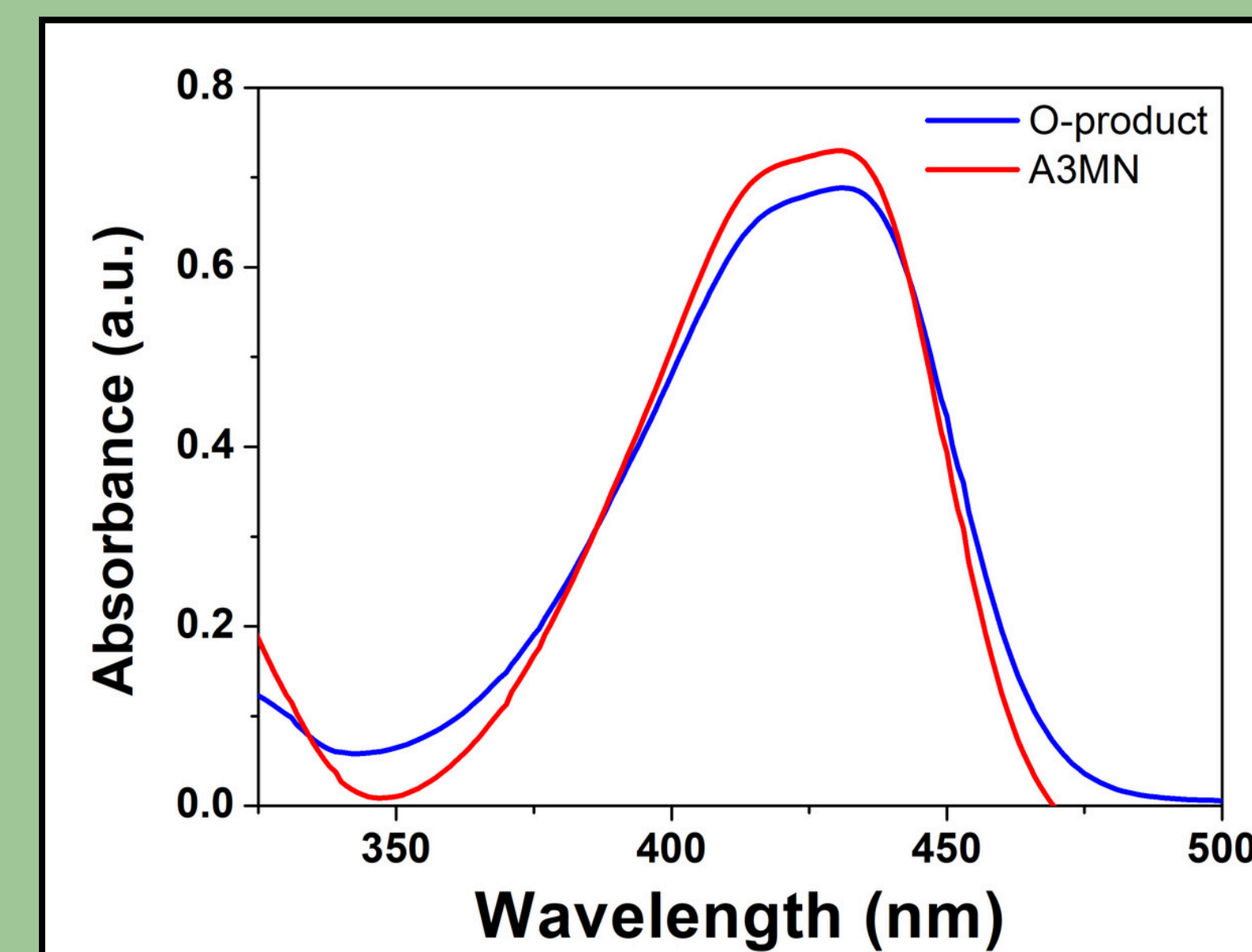


Figure 01

Fluorescence Spectra (Figure 02):

- Free A3MN exhibits high fluorescence intensity with peaks at 352 nm, 496 nm, and 696 nm.
- O-product (dimer) shows a ~6× reduction in fluorescence intensity (496 nm emission)

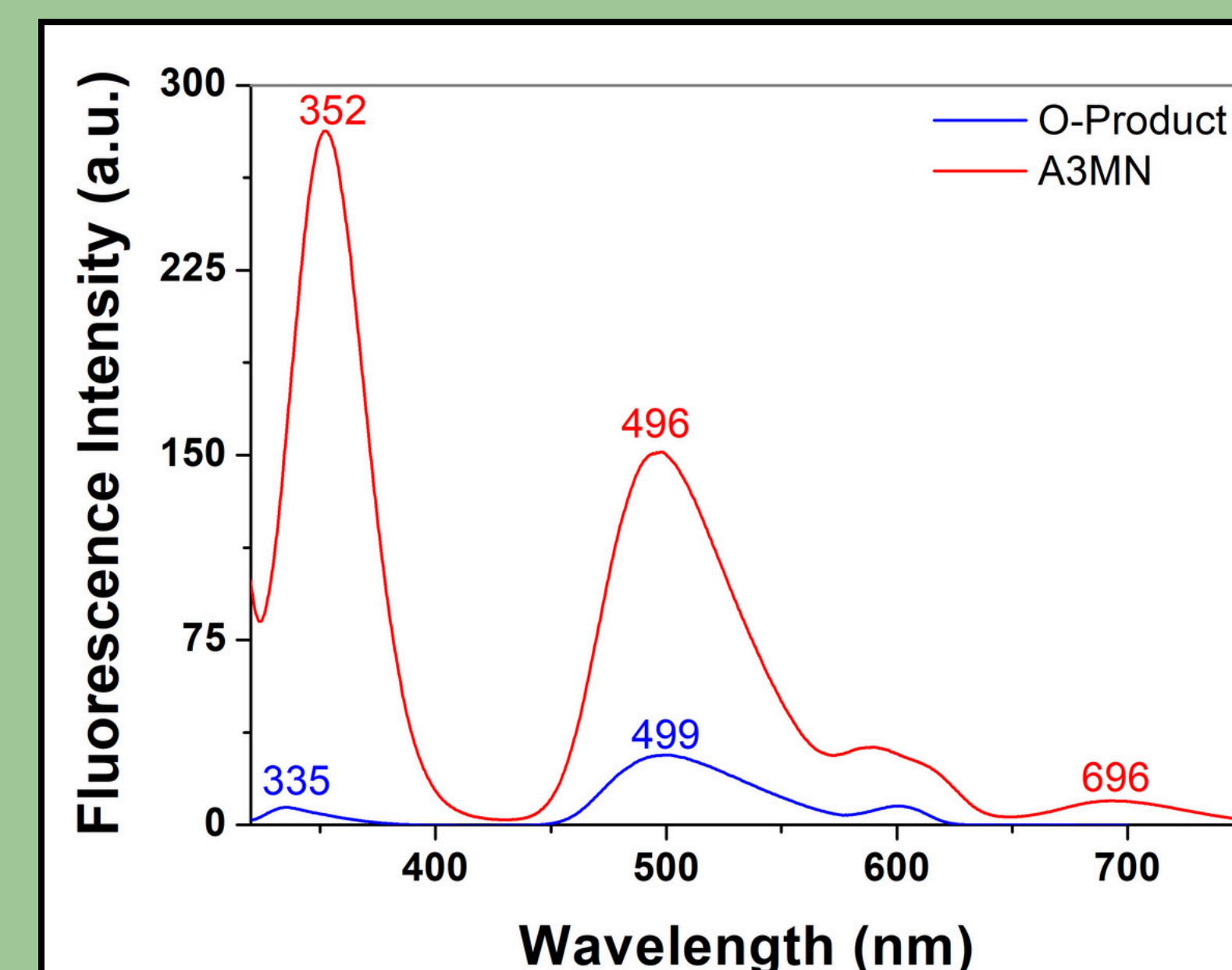


Figure 02

Observations:

- A new red-shifted peak was observed in the UV-Vis spectrum.
- This indicates the possible formation of a new species (dimer/ different form of aggregate) in the reaction mixture.
- The spectral evidence are consistent with the hypothesis that dimerization has occurred.
- ¹H NMR showed no new peaks, suggesting that the core molecular structure remained intact after reaction with oxalic acid, or that the yield of the O-product was too low to be detected.

FUTURE WORK

- Confirming dimer formation using additional characterization methods (e.g., mass spectrometry, X-ray crystallography).
- Exploring different linkers (not just oxalic acid) to see how they influence optical properties.
- Purification of the O-Product formed.
- Tuning fluorescence intensity by modifying the conjugation length or substituents.
- Investigating mechanical memory and data storage potential of AIE-based dimers.

CONCLUSION

- Preliminary findings suggest that A3MN dimerization via oxalic acid is feasible, with spectral evidence pointing toward the formation of a new species.
- Further conformational evidence is required

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