

Synthesis of Complex Polyaromatic Molecules from asymmetric Substituted Pyrene.

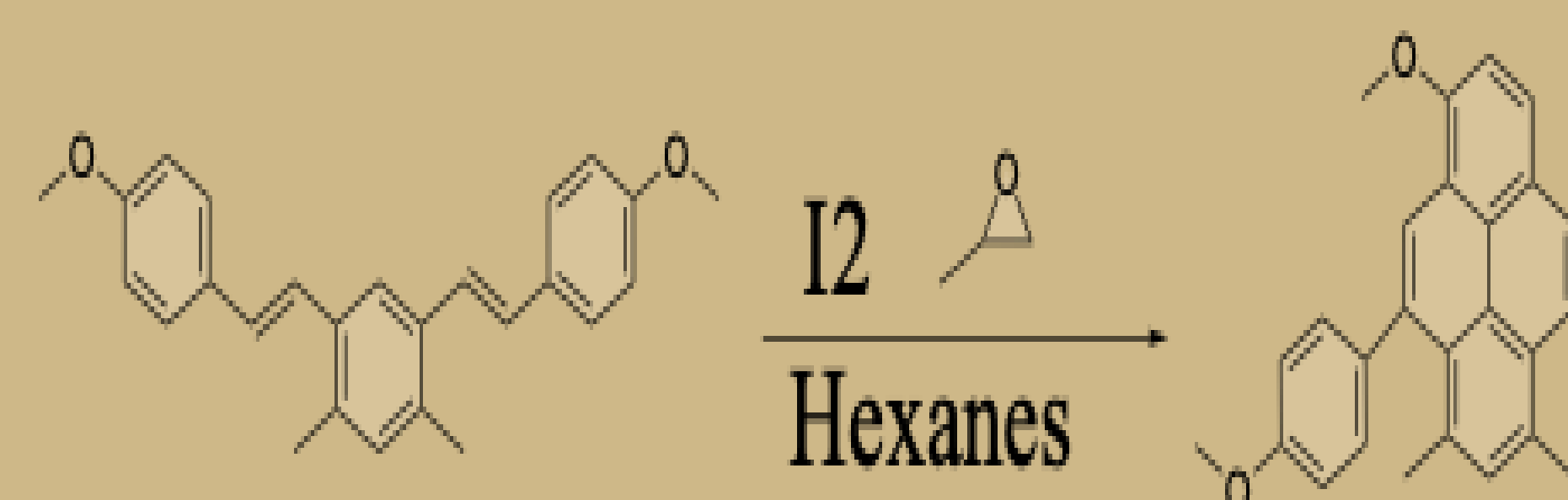
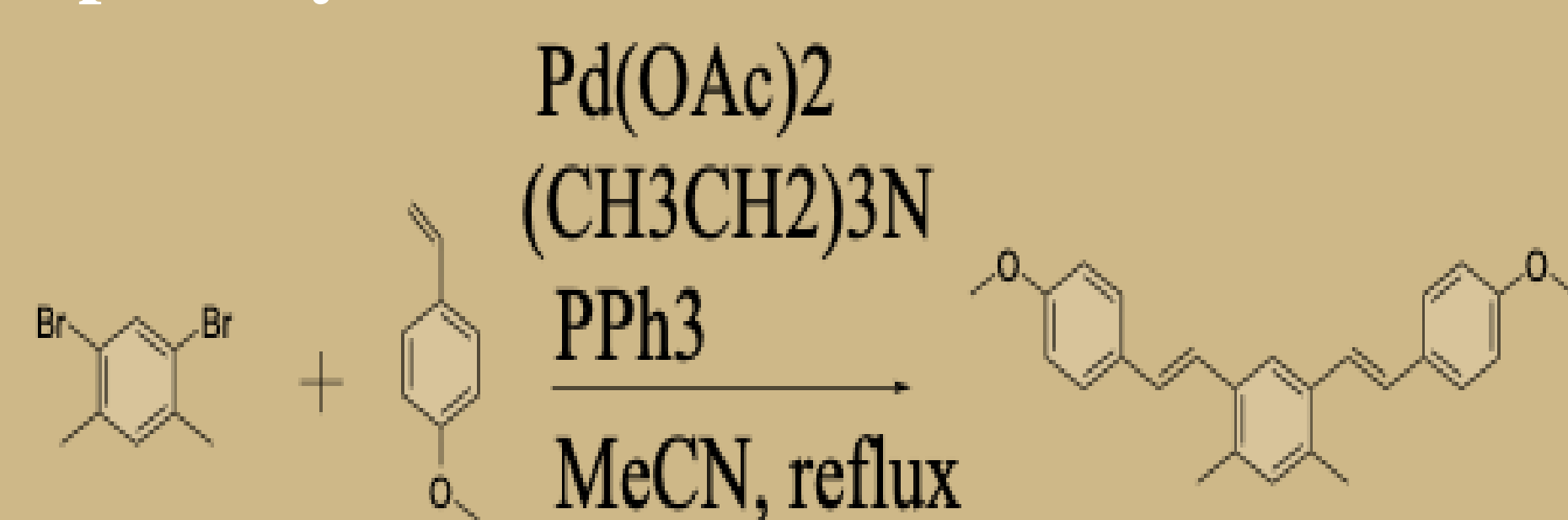
Alejandro Orozco¹, Dr. Nikolas Dos Santos¹

Department of Chemistry, Florida State University



Introduction

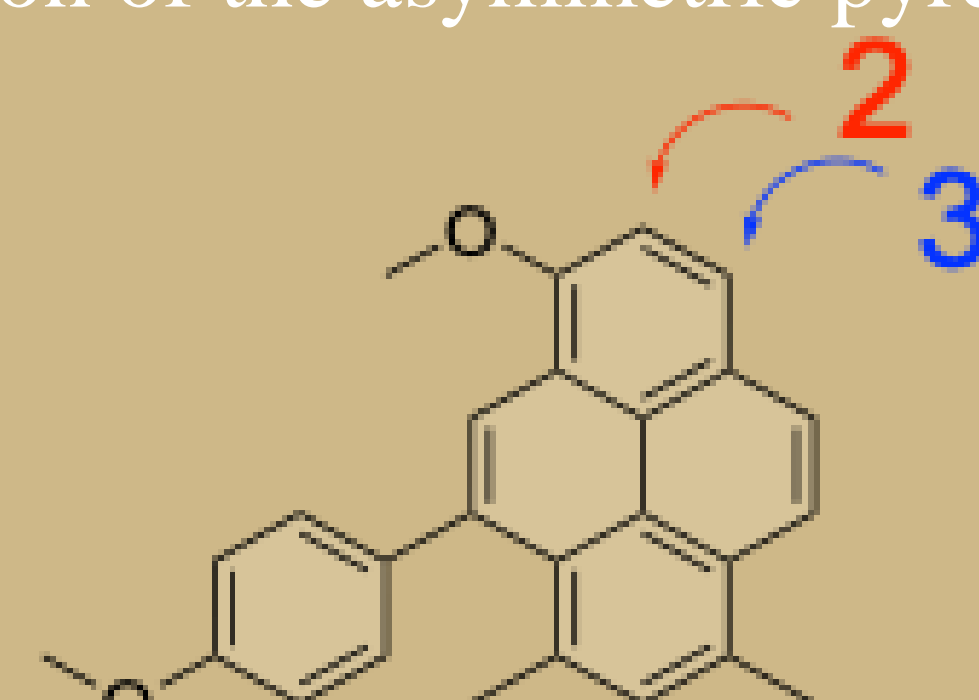
- Investigating the synthesis and functionalization of pyrene derivatives, which are valuable in materials science and organic electronics.
- Worked with **Dr. Nikolas Dos Santos** to synthesize and analyze pyrene-based compounds on various scales through the use of **Heck cross-coupling and Mallory photocyclization**.



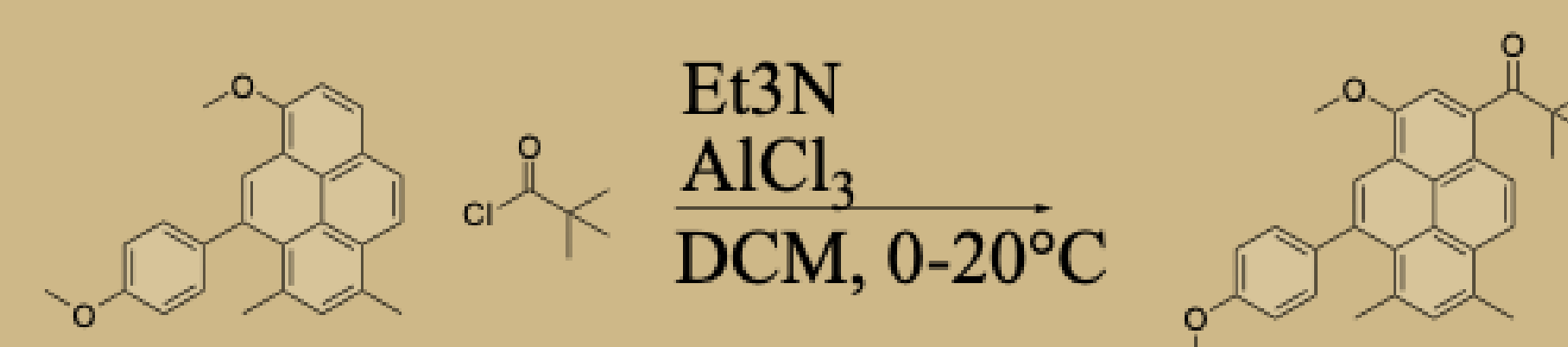
- Applied **advanced synthetic techniques**, including controlled bromination, cross-coupling reactions, and photochemical-cyclizations to investigate regioselectivity enabling precise molecular design.
- Plan to implement **Scholl reaction** and **pyrene aggregation behavior** for possible applications in electronic and optical materials.
- Understanding these **synthetic transformations** will facilitate the design of PAHs with **tunable electronic and optical properties**.
- Potential contributions to **organic semiconductors, fluorescence materials, and supramolecular chemistry**.
- NMR spectroscopy will be the primary method of characterization.

Experimental Plan

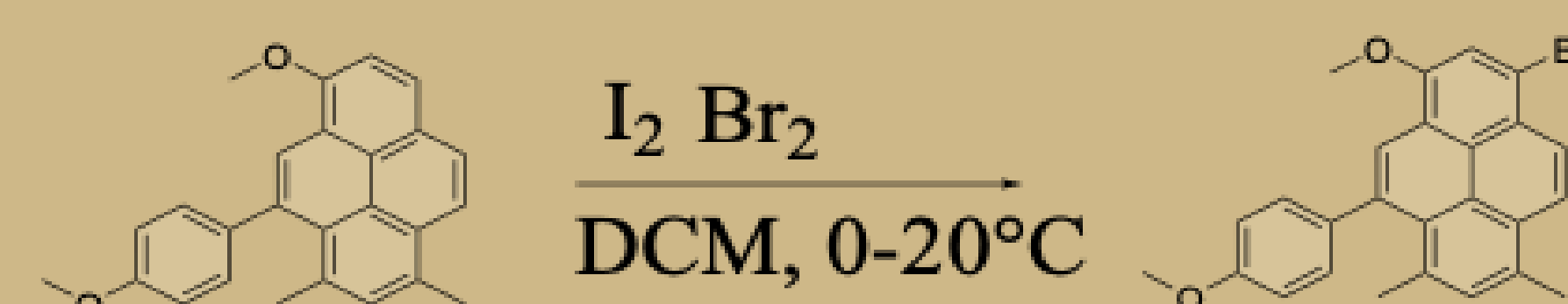
- To further explore the functionalization potential of methoxy-substituted pyrenes, bromination and Friedel–Crafts reactions were conducted to determine whether substitution occurs at the second or third position of the asymmetric pyrene core.



- Friedel–Crafts of the asymmetrically substituted pyrene aimed to explore selective functionalization at the 3rd position of the pyrene core.



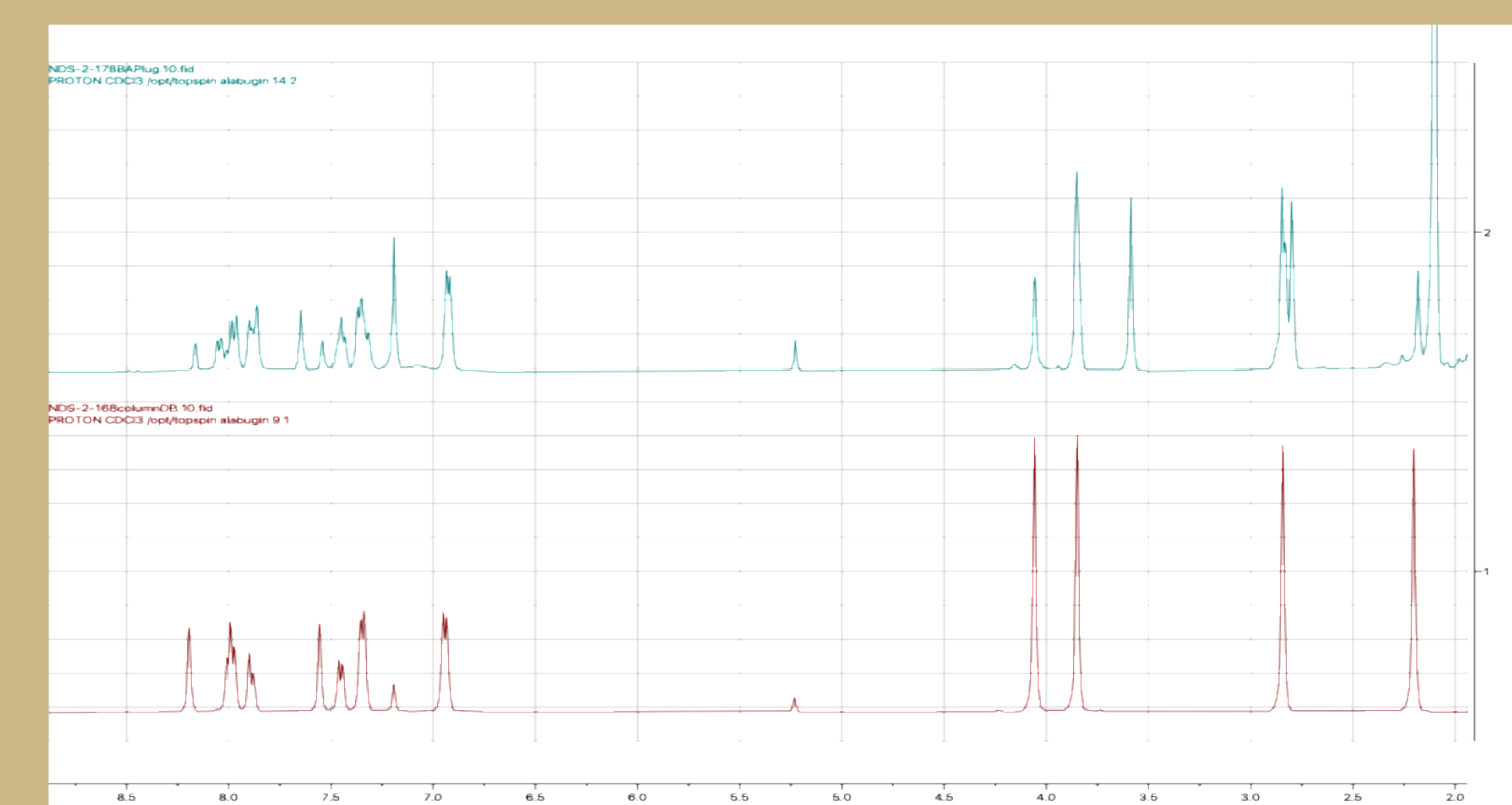
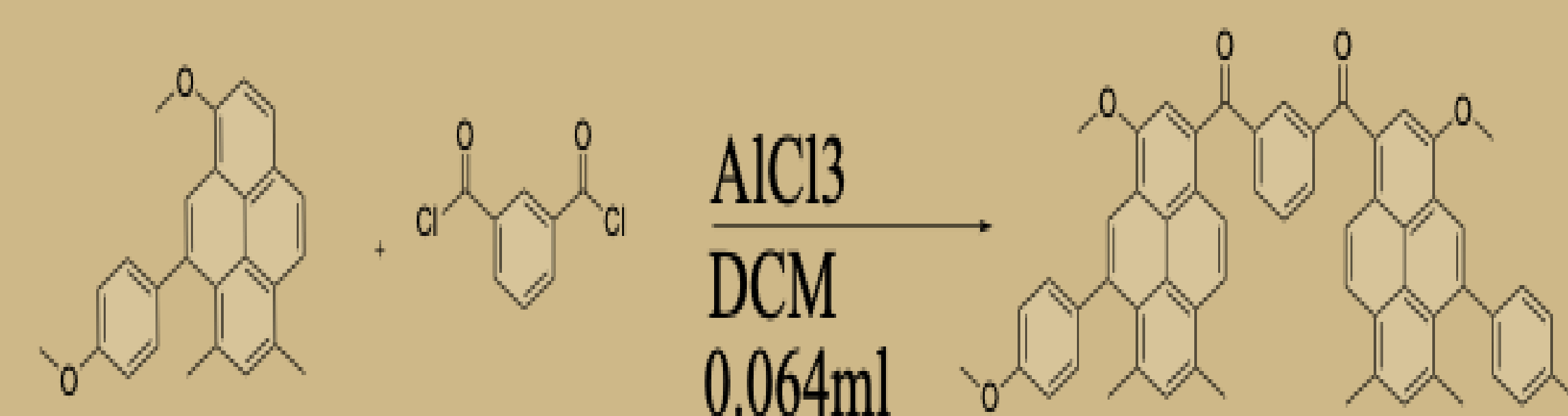
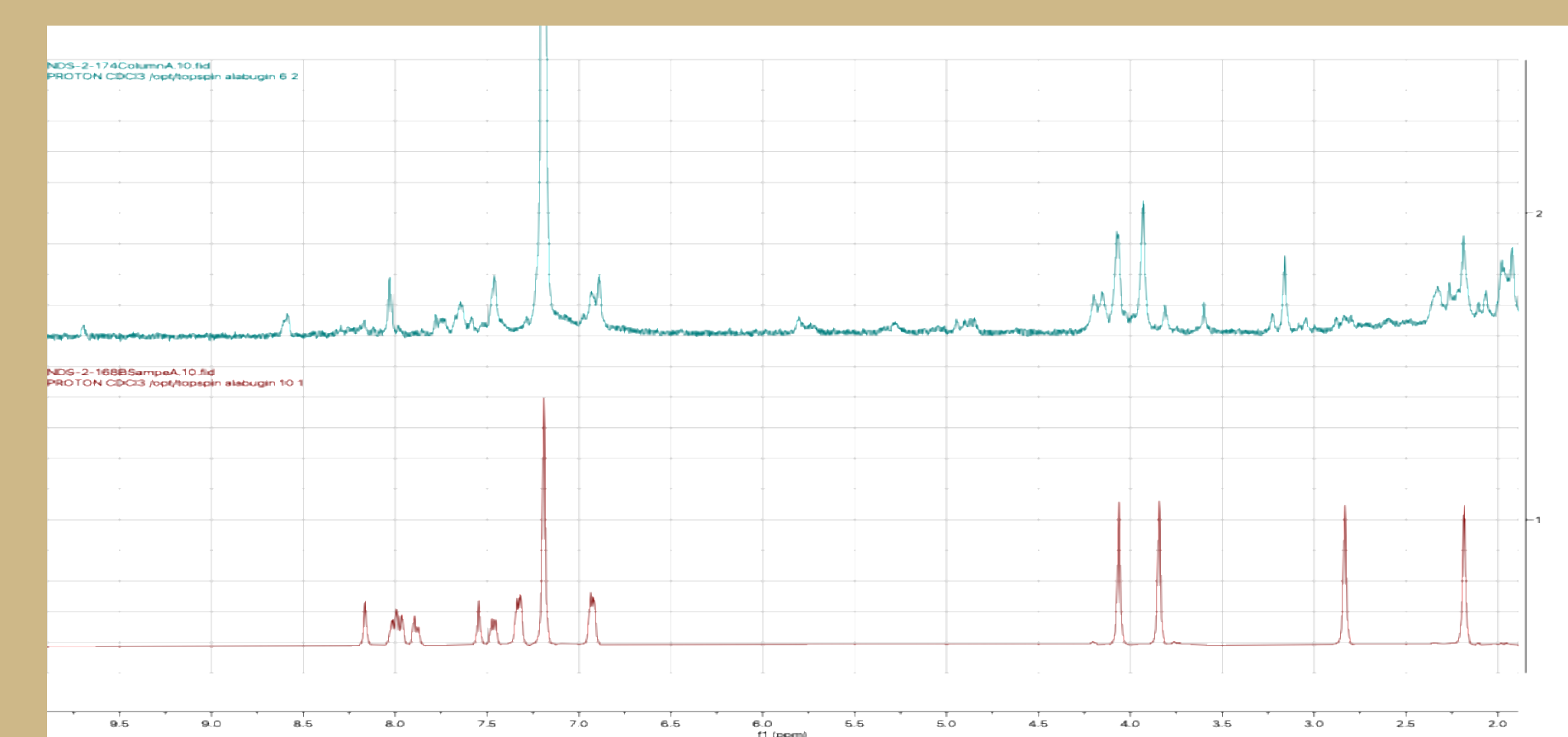
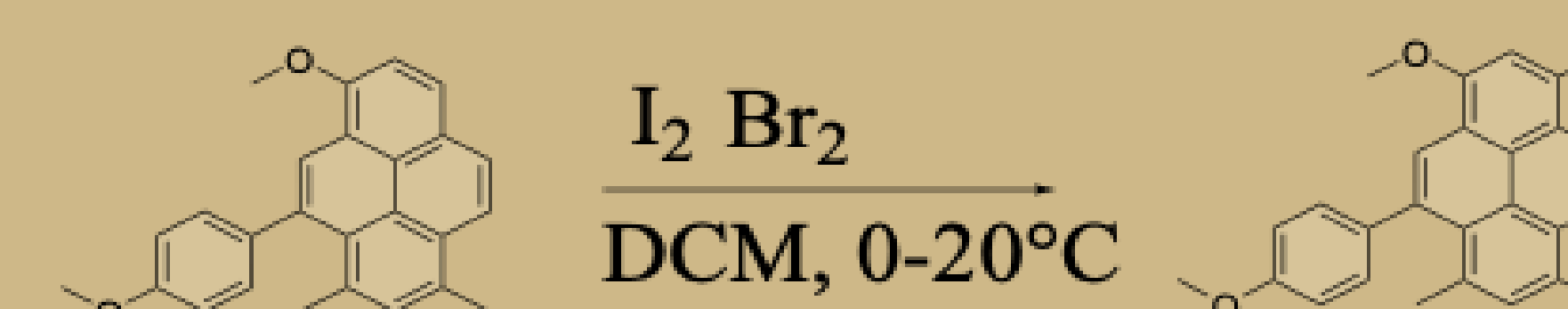
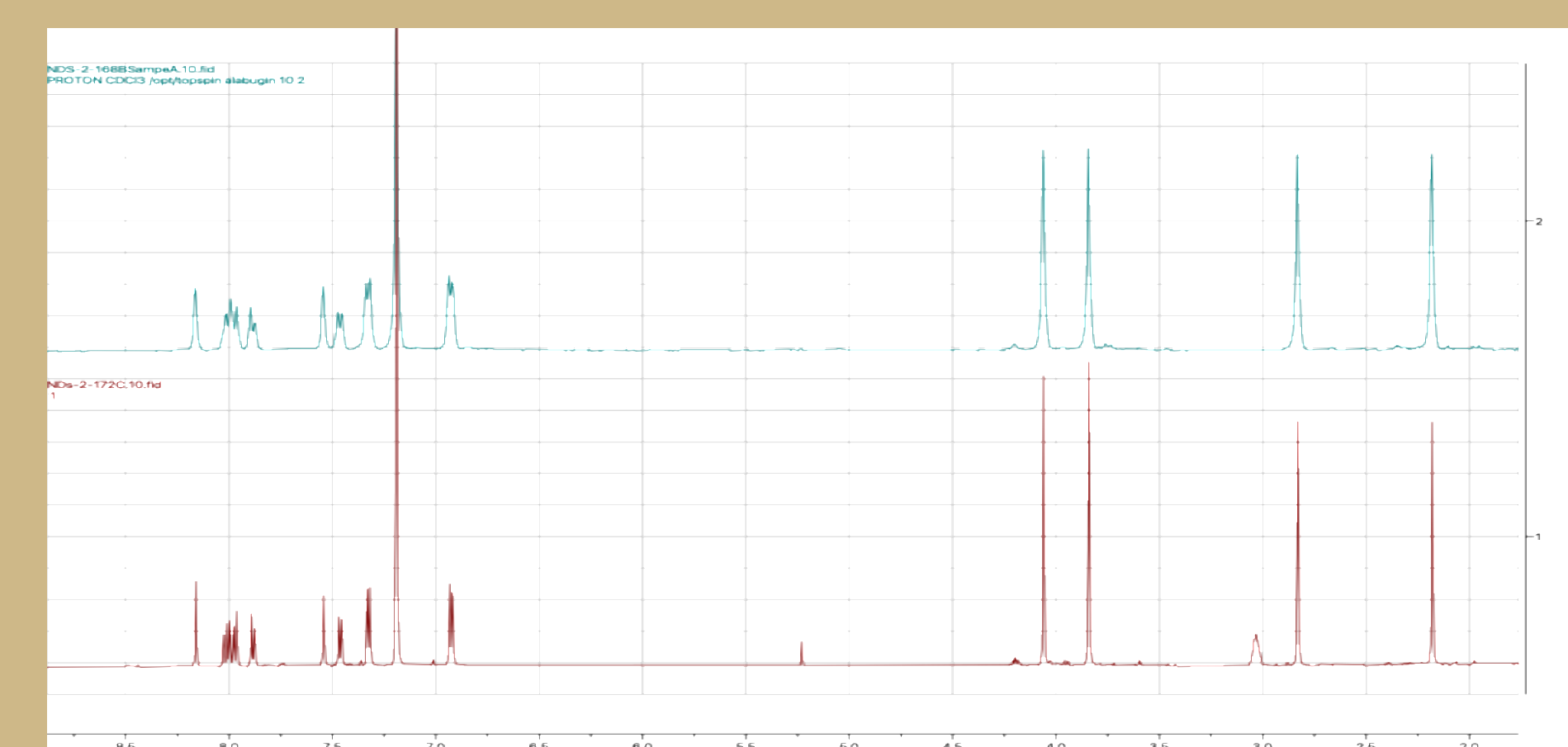
- Bromination was conducted to investigate selective functionalization at specific positions on the pyrene core.



- The double Friedel–Crafts with a benzene bridge was designed to construct a more complex, fused polycyclic aromatic system by linking two pyrene units.



Results



Conclusion

NMR analysis of the bromination and Friedel–Crafts reactions revealed the formation of a product distinct from the starting material. However, due to overlapping signals and the complexity of the resulting spectra, precise characterization using only NMR proved challenging. Additional analytical techniques, such as mass spectrometry (MS) or X-ray crystallography, may be necessary to definitively confirm the structure of the functionalized pyrene derivatives. Further investigation is required to determine whether the regioselectivity of the reaction follows the anticipated substitution pattern at the second or third position of the asymmetric pyrene core. In contrast, the NMR spectra of the product obtained from the double Friedel–Crafts displayed highly promising results. The expected shifts in the aromatic region, along with the disappearance of starting material peaks, suggest successful formation of the desired polycyclic system. The well-resolved spectral data indicate that the reaction proceeded with high selectivity, supporting the feasibility of using this approach for controlled polycyclic aromatic hydrocarbon (PAH) synthesis. Further purification and characterization using 2D NMR techniques and mass spectrometry will help confirm the precise structure and electronic properties of the product.

Acknowledgements

This research study would not have been possible without the opportunity of being a part of the Honors in the Major Program at Florida State University, my graduate mentor Dr. Nikolas Dos Santos, committee members, and my principal investigator, Dr. Alabugin.