# Pentacene Organic Semiconductors with Small HOMO-LUMO Gaps

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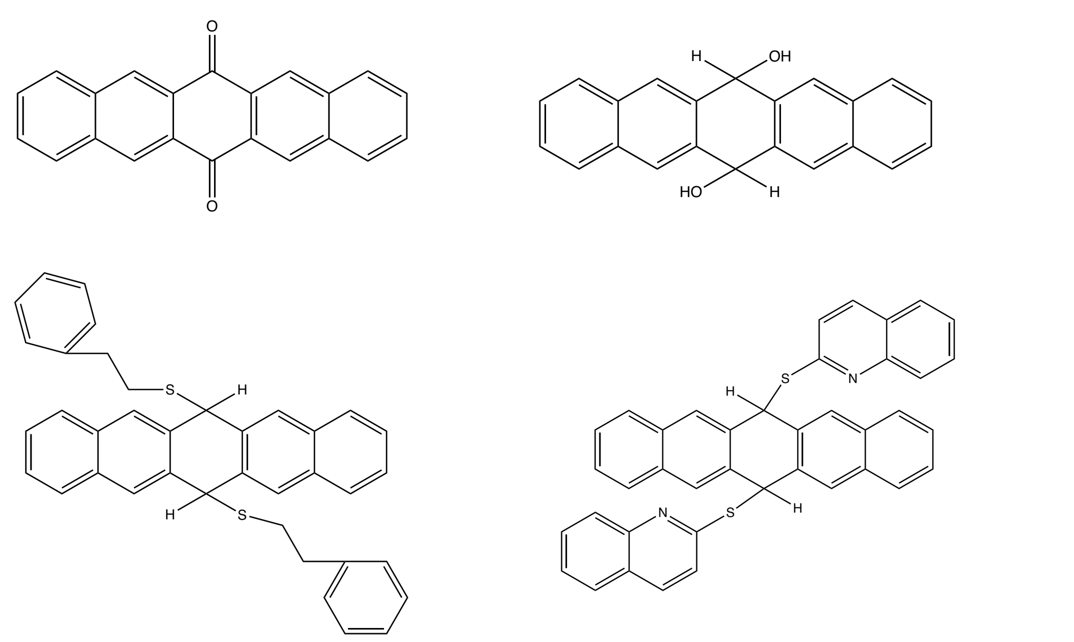
## Introduction

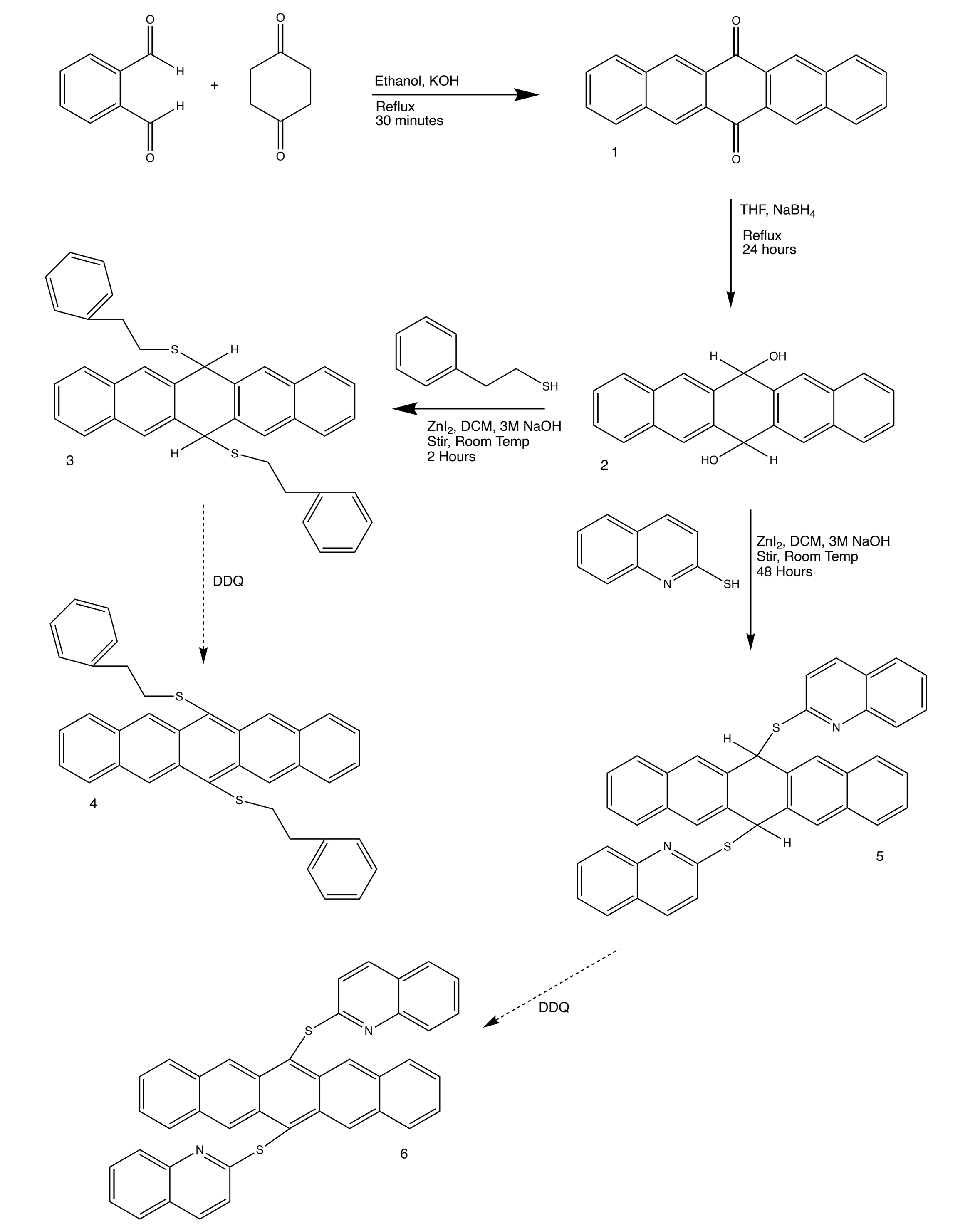
One third of all energy costs worldwide are associated with lighting. Conventional lighting is inefficient and utilizes environmental toxins such as heavy metals. Organic semiconductors offer an alternative path to safe, low-cost, broad spectrum energy efficient lighting via the construction of organic light emitting devices. Pentacene and its derivatives are considered benchmark organic semiconductors because of their small HOMO-LUMO gaps and high charge carrier mobility. I have synthesized and characterized several pentacene derivatives as well as their precursors.



## Objectives

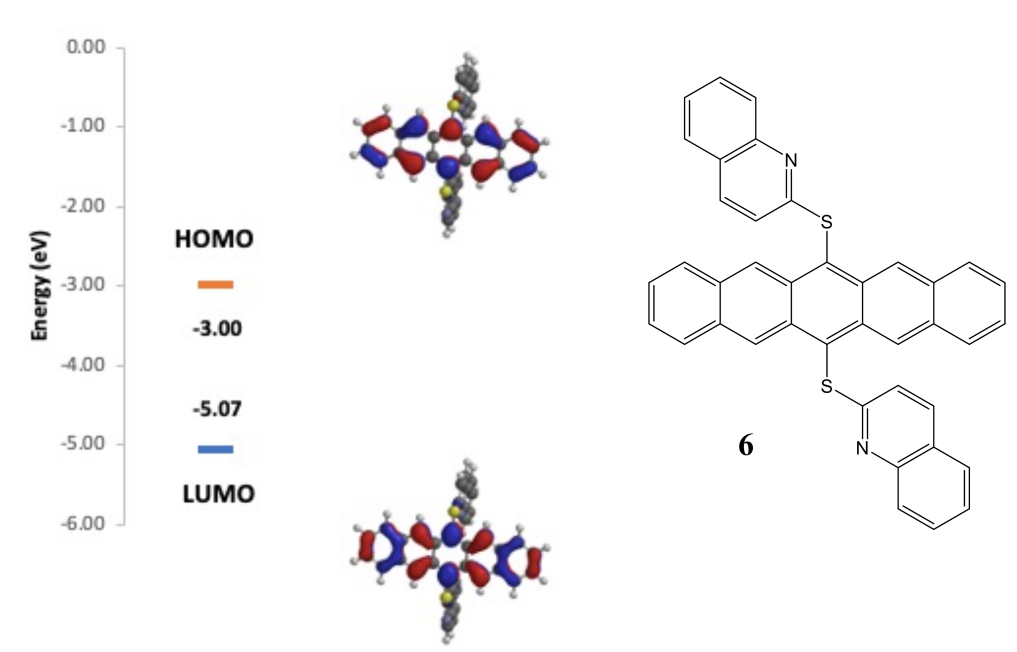
- Perform computational chemistry calculations on a series of pentacene derivatives
- Identify substituent effects on pentacene electronic properties
- Choose target pentacene derivatives with small HOMO-LUMO gaps and plan their syntheses
- Synthesize and purify target compounds
- Characterize newly synthesized compounds by IR and NMR spectroscopies

## Reactions




## Spartan Calculations

| Compounds: Pentacenes (Disubstituted on middle ring) Level of theory: Energy B3LYP/6-311+G(d,p)//Opt B3LYP/6-31G(d) | | | | | |
|---|---|---|---|---|---|
| Substituent | Energy/au | LUMO/eV | HOMO/eV | HOMO-LUMO gap/eV | UV wavelength max/ nm |
| Phenylethanethiol | -2262.921 | -2.89 | -4.95 | 2.06 | 697.94 |
| 2-Quinolinethiol | -2445.069 | -3.00 | -5.07 | 2.07 | 685.65 |
| 6,13-Pentacenequinone | -996.310 | -2.88 | -6.58 | 3.7 | 397.41 |
| 6,13-Pentacenediol | -998.699 | -1.82 | -6.25 | 4.43 | 308.57 |

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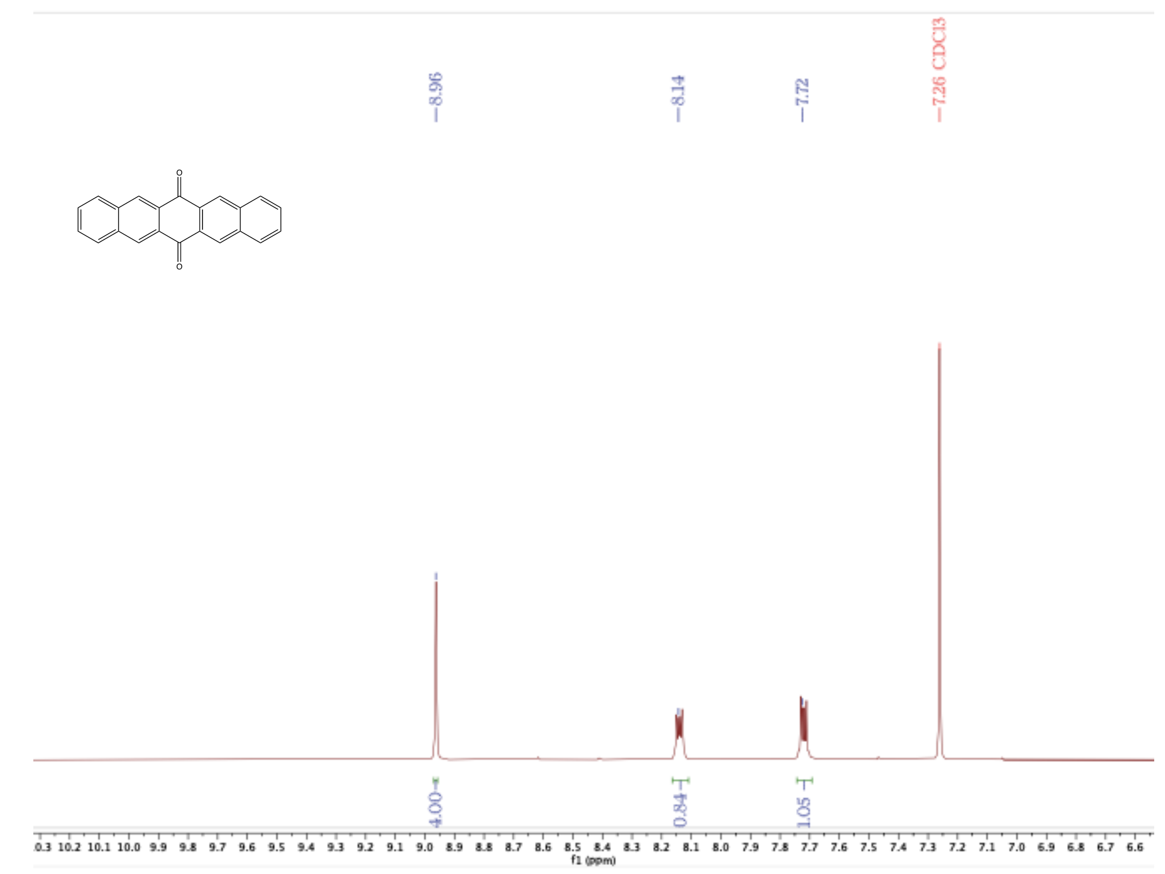
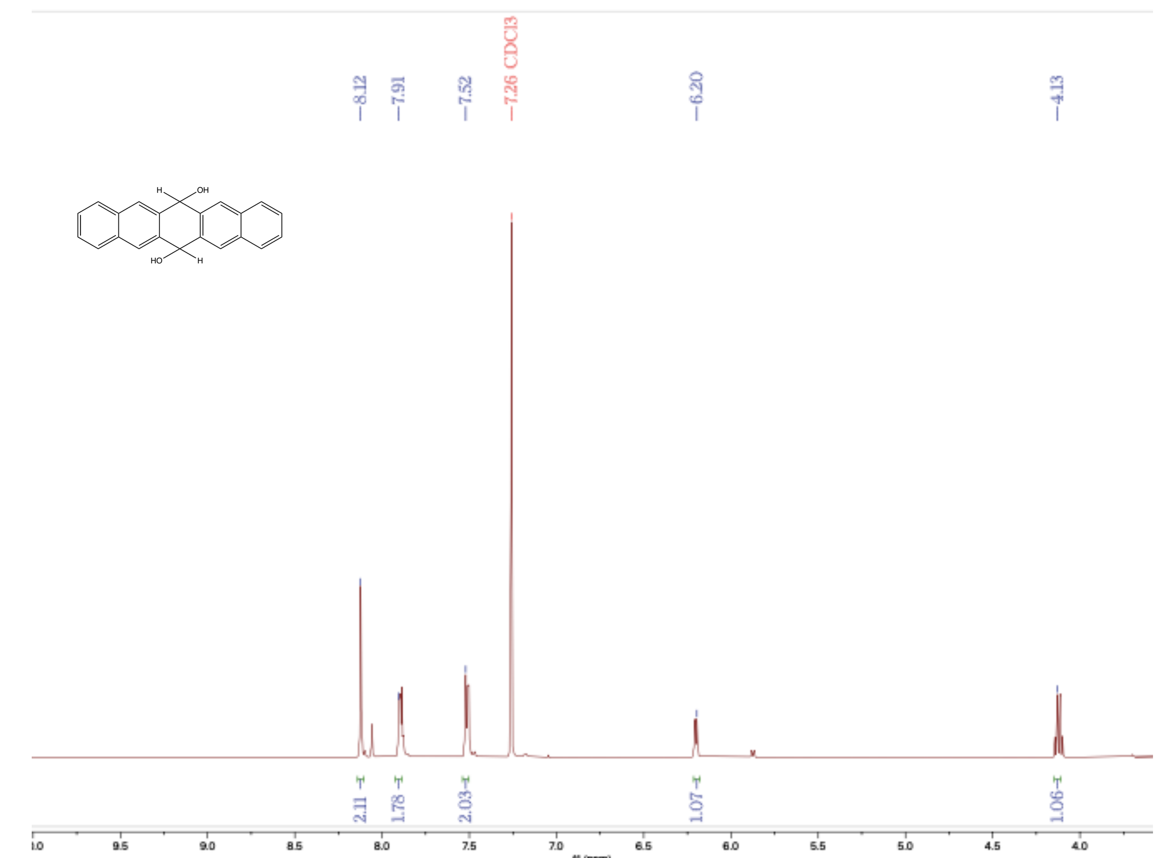
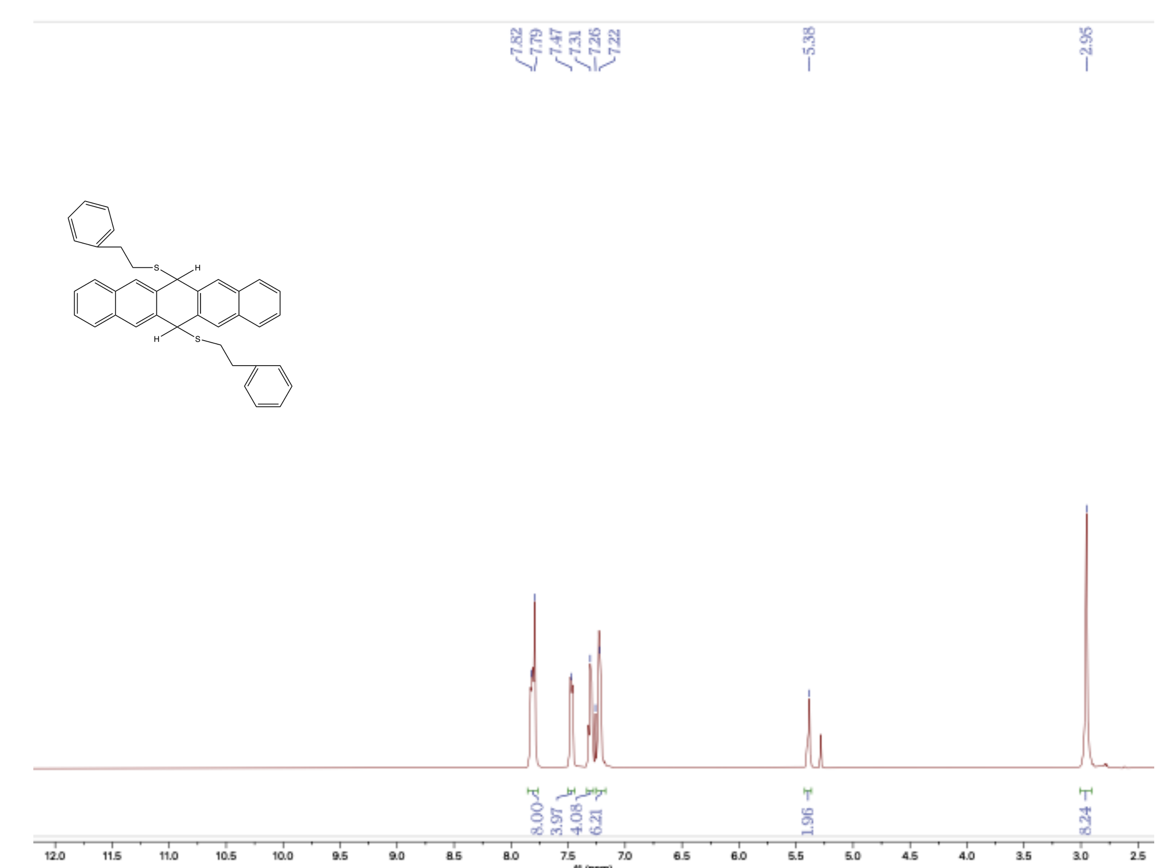
## ¹H NMR Spectra







## Conclusions

- Computational chemistry calculations performed using Spartan'24 software
- Syntheses of target compounds designed
- Precursors to target pentacene derivatives synthesized and purified
- Compounds characterized by IR and NMR spectroscopies

## Next Steps

- Finish syntheses of fully aromatic target compounds by dehydrogenating their precursors
- Purify target compounds
- Investigate target compounds by UV-vis spectroscopy and cyclic voltammetry to experimentally determine their HOMO-LUMO gaps

## References

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2. *Okamoto, T.; Kumagai, S.; Fukuzaki, E.; Ishii, H.; Watanabe, G.; Niitsu, N.; Annaka, T.; Yamagishi, M.; Tani, Y.; Sugiura, H.; Watanabe, T.; Watanabe, S.; Takeya, J. Robust, High-Performance N-Type Organic Semiconductors. Science Advances* ***2020****, 6 (18).* *https://doi.org/10.1126/sciadv.aaz0632*.
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