Molecular Shuttles

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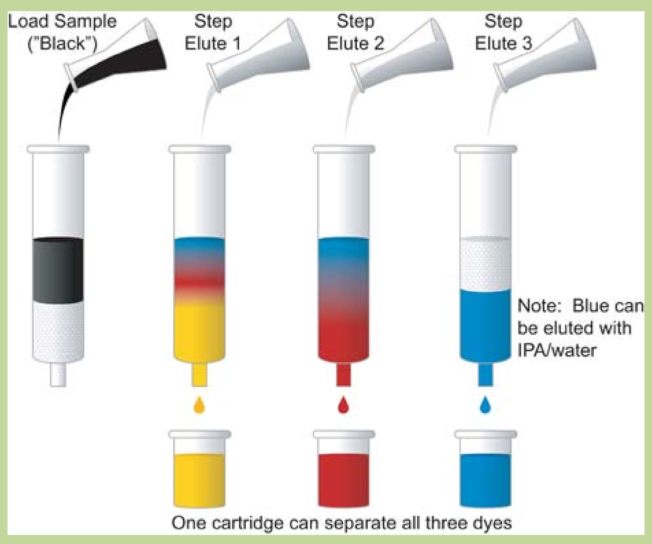
Abstract

Our goal is to create a light sensitive molecule that can function as a retinal prosthetic. When stimulated by light, the molecule will be able to shuttle ions across the cell membrane in a process similar to photosynthesis. In particular, sodium shuttling is important because sodium ions play a significant role in stimulating nerve cells. This ion shuttling also has applications in fuel cell technology because the molecule functions similarly to photosynthesis in that light energy is stored as chemical energy, which can be harvested later. Thus far, I have synthesized several starting materials necessary for the project and have assisted in the synthesis and purification of several steps of the formation of this novel molecule. I have also created a crown anthraquinone for comparison testing. The implications of this molecule are far reaching, in the medical field and in terms of green technology.

The molecule is composed of three parts. The porphyrin reacts to the presence of light, and the electrical charge splits. The positive charge will be directed to the carotenoid, while the negative charge goes to the crown anthraquinone. The splitting of charge is necessary; while the charge is split the molecule can do work. As the negative charge is directed to the crown anthraquinone, positive sodium ions are allowed to cross a cell membrane. Sodium ions stimulate neural cells in the eye, allowing the it to function as a retinal prosthetic.

Experimental Methods

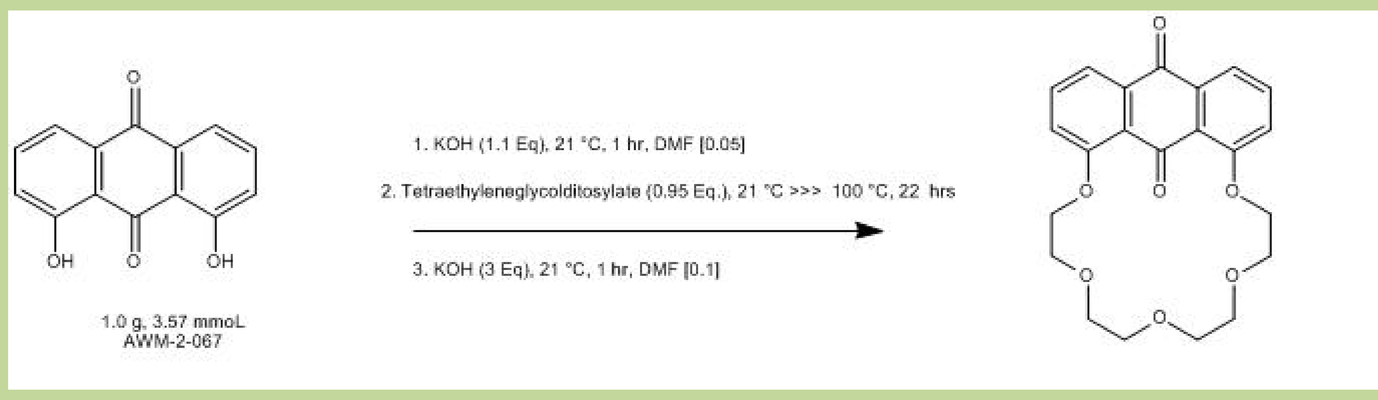
Successful chemical yields are around 80-90%, and the crown anthraquinone in particular has low yields. For a variety of reasons, a hundred percent yield is an unrealistic expectation. The other portion, the other 10-20% of the reaction contains undesirable side products, including unreacted starting material and possibly contaminates. This portion of the reaction needs to be separated out though a process called column chromatography. In column chromatograph, the reaction mixture is loaded onto a column of silica or alumina and the mobile phase, which is a liquid, goes through the column. A gradient of mobile phases and different mobile phases can be used to elute different compounds off of the column at different times. Compounds come out of the column based on their affinity to the mobile phase and are collected as fractions. These fractions are then analyzed to check their composition by Nuclear Magnetic Resonance, or NMR. NMR is a way to find the chemical structure of a compound, and thus find the identity of the substance. Magnetic nuclei, specifically in this case ^{1}H, radiate energy back when hit with electromagnetic pulses in a magnetic field. The frequency of the radiated energy is unique to the atom. By comparing the energy frequency to known standards, the structure of a compound can be determined.



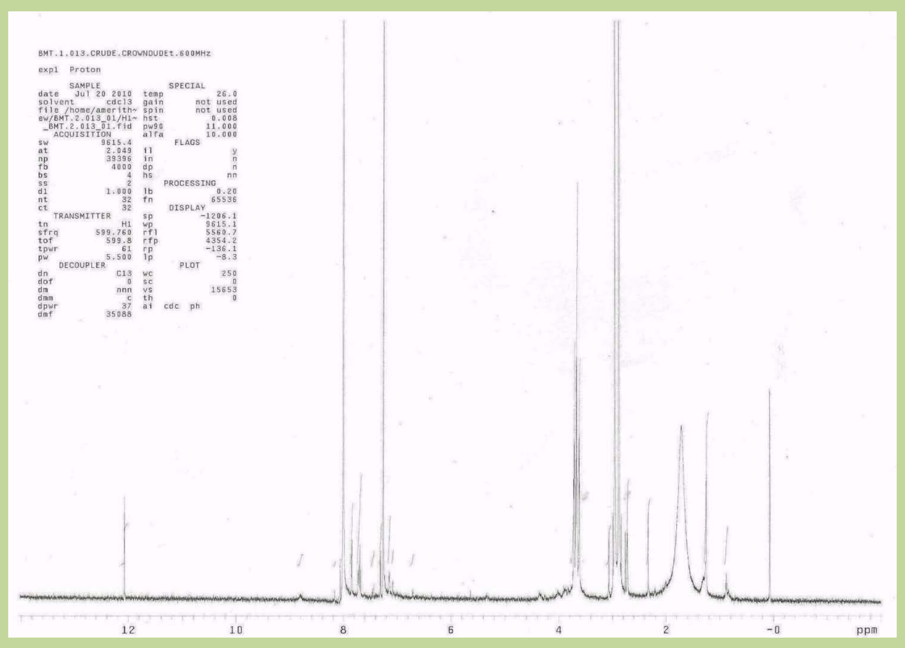
Example of column chromatography on an ink cartridge separating out colored fractions

NMR at Pacific Northwest National Laboratory

Formation of 18 Crown 6 Anthraquinone

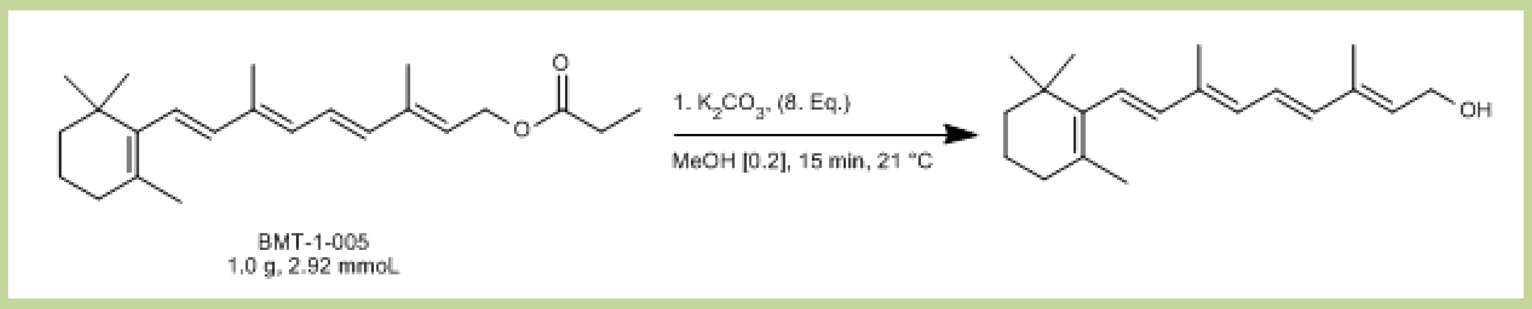


The molecule formed is an 18 crown 6 anthraquinone. 18 refers to the number of atoms in the molecule, while 6 refers to the number of oxygen. This crown is selective in particular to potassium ions. This molecule will be used as a standard for comparison against the sodium specific crowns in physical tests. Below is the NMR of the crude reaction mixture.



NMR of crude reaction mixture. Impurity peaks such as water, and residual solvent (DMF) are also present. This reaction mixture needs to be purified by column chromatography.

Formation of All-trans Retinol



This reaction reduces the ester retinyl propionate to all-trans retinol. This reaction is noteworthy because it uses a mild and environmentally friendly reducing agent, potassium carbonate, instead of harsh, and dangerous chemicals like lithium aluminum hydride which can cause fires and explosions if used improperly. Although all-trans retinol is commercially available, it sells for approximately $300/gram, while retinyl propionate is $40/100 grams providing ample financial incentive.

Conclusions

Thus far, a crown anthraquinone for physical comparison tests has been synthesized. Starting materials including all-trans retinol have been created for creation of the final product. Continuing research will focus on creating other standards of crown anthraquinone, coupling the final molecule together, and biological and physical tests to determine how the molecule works.

Acknoledgements

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