Theoretical Analysis of Organic Synthesis Involving Azo-Dyes

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INTRODUCTION

- **The purpose of this project is to detail how chemists make certain chemicals (which in this circumstance is azo-dyes) using retrosynthetic analysis and organic synthesis**
- **Man-made/synthetic products like azo-dyes can be used across various industries and fields**
- **Azo-dyes are preferable because of their viability in mass production and cost-effectiveness**

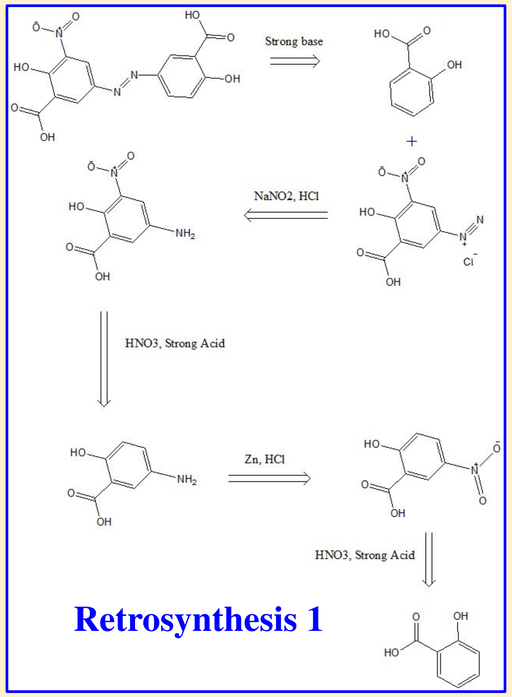
RESEARCH METHODOLOGIES

- This research is mainly qualitative and uses pre established theoretical literature to make retrosynthesis
- The quantitative data is made by finding the yields of reactions in a part of the synthesis that have already been done
- The main **criteria for making the retrosynthesis, is that they use high yielding steps that are cost-effective and rather accessible**
- **With each step in a synthesis the overall yield is decreased**

DATA AND FINDINGS

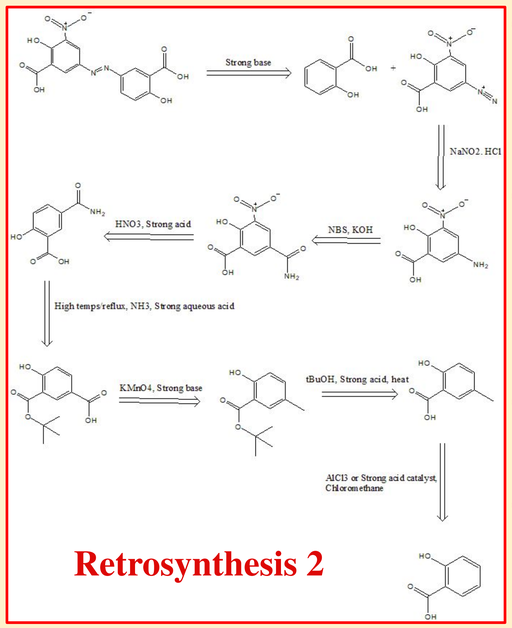
- These two retrosynthetic schemes were made using mostly previous knowledge of Organic chemistry
- **For this specific azo-dye, synthesis presents many challenges** because of molecular asymmetry in one specific spot where the rest of the molecule is identical to the other half
- Many different methods like protecting groups can be used to allow for better selectivity
- Using **retrosynthesis to work backwards from the product is much easier than working from a desired reactant to the product**
- Salicylic acid being the main source of carbon makes both syntheses more cost effective

DISCUSSION, ANALYSIS, AND EVALUSATION



Retrosynthesis 1

- **This synthesis takes less steps**
- **The reactions are slightly less favorable so the yields may be lower in reality**
- **There is no need for protecting groups to enhance selectivity**
- **This still uses salicylic acid as the main fragment and diazotization with coupling**



Retrosynthesis 2

- **This synthesis uses a different approach to making the amine for azo-coupling**
- **A Hofmann rearrangement is used for better selectivity more yields to one specific product**
- **A protecting group is used for better selectivity**
- **A friedel crafts alkylation is used to add the methyl group**

	Cost	Yields	Steps
#1	Low	Lower	5
#2	Higher	Higher	8

CONCLUSIONS, IMPLICATIONS, AND NEXT STEPS

Overall analysis

- Although the first retrosynthesis has less steps, the difficulty with selectivity for the nitration steps makes it potentially have lower overall yields
- The second retrosynthesis has better selectivity and the researched reactions are more common with most likely heightened overall yields despite more steps
- **In terms of yields, cost effectiveness, and accessibility these two syntheses balance out and end up around equal**

What are the next steps?

- Now that multiple syntheses have been proposed for this azo-dye, it is possible to use these retrosyntheses as a baseline for real life synthesis
- **If this azo-dye is synthesized, it can be considered for practical use** in many different industries, like textiles and even food or medications
- Medical applications of this azo-dye are yet to be considered, but the two salicylic acid groups on the molecule would suggest that this molecule might have the potential to be used as a medication
- **This research starts the inquiry into this specific molecule which otherwise does not have any attention drawn to it**

ACKNOWLEDGEMENTS / REFERENCES

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