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The Analysis and Characterization of Phenolic Compounds via Cytochrome P450 Enzymatic Processes

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Introduction

This research is about how compounds that are found in pesticides and other industrial products can affect our health. In this research we specifically focused on phenolic compounds that are shown in Figure 1, to learn how our body breaks down these compounds, when it enters our body, through Cytochrome P450 that are found inside our liver.

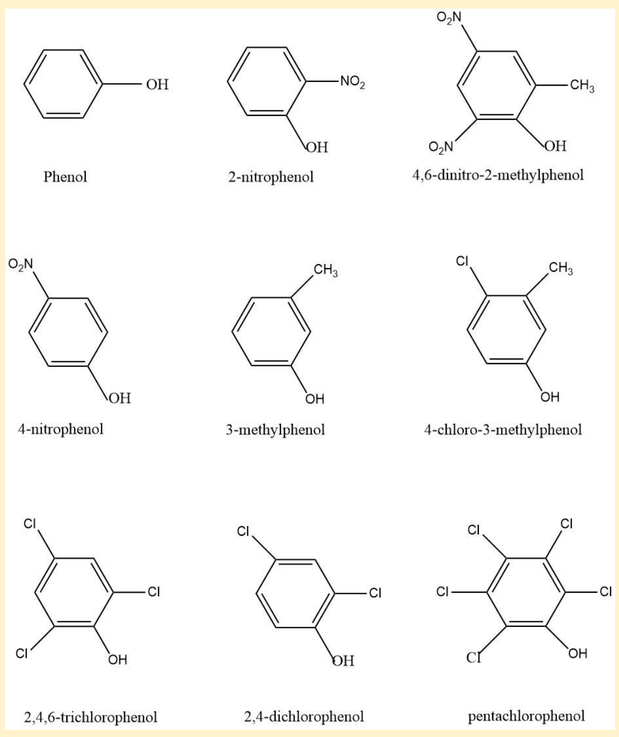

Figure 1: Phenolic Compounds

Research Question

How will the products of catalyzed cytochrome P450 with phenolic compounds in the environment affect the human body?

Methods

A method to resolve the research question consist of two different sections. The first section, theoretical part, begins with the prediction of the breakdown of the phenolic compound by the cytochrome P450. An example of a phenolic compound, phenol, is shown in Figure 2.The second section, we will be using Gas Chromatography-Mass Spectrometry (GC-MS) to verify our prediction.

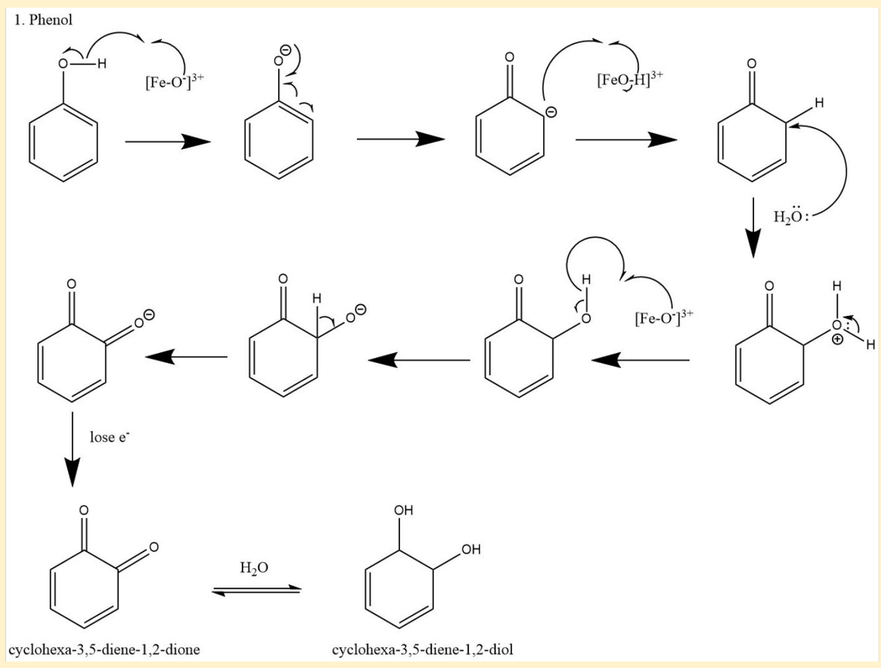

Figure 2: Mechanism of Phenol via Cytochrome P450

Results and Discussion

After the theoretical prediction of the phenolic compounds catalyzed reaction by cytochrome P450, we came up with list of products from alcohol and ketone functional group which are shown below in Figure 3 and Figure 4.

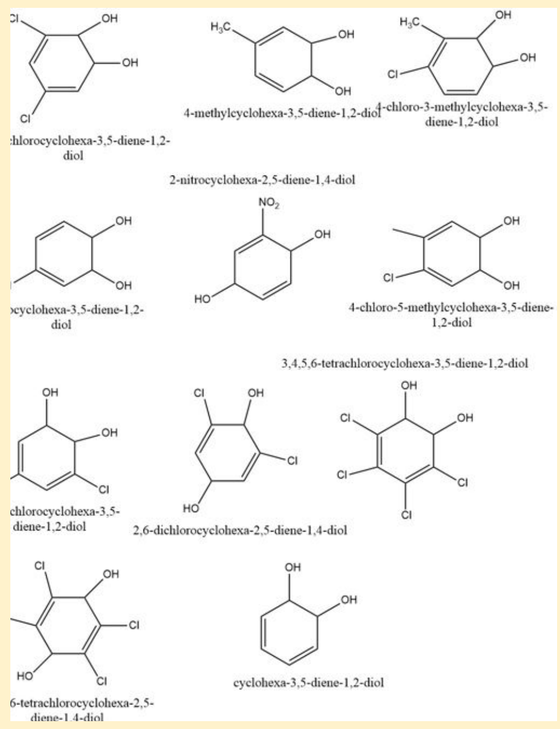

Figure 3: Alcohol Products

Ketone products

1. Cyclohexa-3,5-diene-1,2-dione
2. 3-methylcyclohexa-3,5-diene-1,2-dione
3. 4-methylcyclohexa-3,5-diene-1,2-dione
4. 2-methylcyclohexa-2,5-diene-1,4-dione
5. 3-nitrocyclohexa-3,5-diene-1,2-dione
6. 2-nitrocyclohexa-2,5-diene-1,4-dione
7. 3,5-dichlorocyclohexa-3,5-diene-1,2-dione
8. 2-chlorocyclohexa-2,5-diene-1,2-dione
9. 4-chlorocyclohexa-3,5-diene-1,2-dione
10. 4-chloro-5-methylcyclohexa-3,5-diene-1,2-dione
11. 4-chloro-3-methylcyclohexa-3,5-diene-1,2-dione
12. 2,6-dichlorocyclohexa-2,5-diene-1,2-dione
13. 4-nitrocyclohexa-3,5-diene-1,2-dione
14. Benzoquinone (cyclohexa-2,5-diene-1,4-dione)
15. 2-methyl-6-nitrocyclohexa-2,5-diene-1,4-dione
16. 3-methyl-5-nitrocyclohexa-3,5-diene-1,2-dione
17. 3,4,5,6-tetrachlorocyclohexa-3,5-diene-1,2-dione
18. 2,3,5,6-tetrachlorocyclohexa-2,5-diene-1,4-dione

Figure 4: Ketone Products

Future Work

- Experimental approach using GC-MS for the analysis of the parent compounds and their reactive catalyzed species.
- Data analysis between theoretical and experimental
- Calibration curves
- Analysis of human urine and blood

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