Antimicrobial Properties of Isomers of Benzofuranylethanol

Nick Cheatwood, Jessica Bronstad, and Michele Harris

STEPHEN F. AUSTIN STATE UNIVERSITY
Department of Chemistry and Biochemistry

ABSTRACT

A biotransformation reaction is a chemical conversion of a substance into a desired product with the aid of whole, living cells containing the necessary enzymes. In additions to living cells, other substances, such as vegetable strips, will also catalyze biotransformation reactions. Advantages of biotransformation reactions include the following: the ability to recycle material, the use of less hazardous chemicals, the ability to compost vegetable strips, the use of inexpensive materials that are locally available, and the ability to produce a single isomer. The biotransformation reaction for the conversion of benzofuranyl methyl ketone (BMK) to (-)-benzofuranylethanol (BMA) using carrot strips as the catalyst has been characterized. The reaction is known to produce a single isomer of the BMA. Some isomers, called enantiomers, are molecules that are mirror images of each other. The two mirror image molecules of this type are known to react in biological systems in different ways. Carrots strips have been used to produce only one of the mirror image molecules, and this molecule of BMA has been shown to have antimicrobial properties. Currently, we are exploring the use of other vegetable strips to determine if the other mirror image molecule of BMA can be synthesized. The goal is to determine if the other isomer has similar or different antimicrobial properties than the isomer produced by carrots. The antimicrobial properties of the two mirror image molecules will be compared

Reaction

benzofuran-2-yl methylketone (BMK)

(-)-benzofuranyl)ethanol (BMA)

Enantiomers

Chiral molecules exhibit "handedness", also called enantiomers. The molecules have identical formulas and properties, but different spatial positioning and function.

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Methods

Preparation of S-BMA by carrot

- 8 g of carrot strips were mixed with 25 mg of ketone (1.6 X 10^{-4} moles) in 25 mL of dH_2O and placed on rotisserie for two hours.
- These samples were then vacuum filtered. The filtrate was extracted into ethyl acetate. TLC (thin layer chromatography was used to verify presence of BMA.

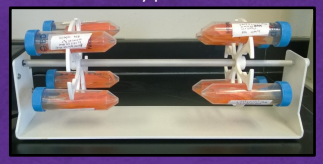

Figure 1. Rotisserie

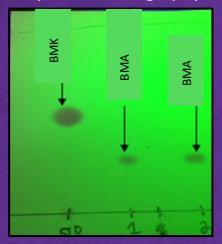

Figure 2. TLC plate

- Ethyl acetate was removed which left the crude BMA product which is a dark orange.
- The crude BMA was purified using silica gel chromatography.
- Purified BMA was eluted with a hexane:ethyl acetate mixtures, and pure BMA fractions pooled.

Figure 3. BMA prep

Preparation of R-BMA by potato and radish

- 8 g of potato (or radish) chunks were mixed with 25 mL of dH_2O and 25 mg of BMK for 48 hours.
- The same procedure for carrots were followed.

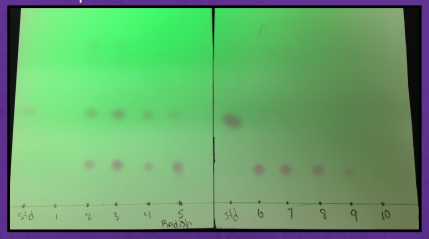

Figure 4. TLC Results from radish prep after silica gel chromatography

Testing Optical Purity of the Sample

- The purified sample was tested for optical rotation using a Jasco P1010 polarimeter.
- 10 mg of each purified sample was dissolved in 10 mL of chloroform and the specific optical rotation (O.R.) was measured

Results

Results of other plants to try to make R-BMA

Plant Type	BMA produced	Specific O.R.
Carrot	Yes	-16.02
Apple	No	--
Sweet Potato	No	--
Potato	Yes	-0.7413
Radish	Yes	-8.953

Discussion

The Specific O.R. for S-BMA has been reported in the literature to be -16.4. The work in our lab is in close agreement with the literature value. We have tested the antimicrobial properties of the pure S-BMA and found it did inhibit the growth both bacteria and Baker's yeast.

The Specific O.R. of pure R-BMA is +16.4. The TLC shown in Figure 4 indicates that radish does produce BMA, but it apparently produces a mixture of R- and S-BMA since the Specific O.R. was -8.953 instead of the expected +16.4. BMA was also produced from potato (results not shown); and its Specific O.R. was –0.7413. We assume potato makes almost equal amounts of both the R-BMA and the S-BMA. We plan to use HPLC with a chiral column to separate the R- and the S-BMA. Once that is accomplished, we will then compare the antimicrobial properties of the R-isomer to the S-isomer.

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