Experimental and theoretical study of nitro compounds to aromatic alcohol: a sustainable biocatalytic transformation from Amazonian fungi

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INTRODUCTION

The ability of natural products to provide new compounds with applications in various fields, including biology, pharmacology, and materials science, has attracted much attention in recent years. In this study, we explored the extraction of the 1-nitro-2-phenylethane (NPE) compound from Aniba canelilla and its biotransformation to 2-phenylethanol (PE) by fungi species from the Brazilian Amazon. In addition, we performed computational analyzes to track changes in molecular properties.[1]

METHODS

The nitrogenous compound was obtained from the essential oil of *Aniba canelilla*. The biotransformation reactions were carried out using four species of fungi: *Aspergillus flavus*, *Colletotrichum sp.*, *Lasiodiplodia caatinguensis,* and *Rigidoporus lineatus*. After an incubation period of 7 days at 32 °C on an orbital shaker (130 rpm), 50 mg of 1-nitro-2-phenylethane diluted in 100 mL of dimethylsulfoxide (DMSO) was added to the reaction vessels. Aliquots (2 mL) were taken and analyzed by GC-MS (pulverized silicon capillary column, RTX-5MS 30 m 0.25 mm 0.25 m). FTIR spectra of 1-nitro-2-phenylethane and 2-phenylethanol were obtained using total attenuated reflection (ATR). The NPE and PE FTIR spectra were obtained using an Agilent CARY 630 spectrometer in the spectral region between 400 and 650 cm^{-1}.

Calculations were performed in the Gaussian 09[2] program while the DICE[3] code was used to perform the s-MC-QM sequence and generate the liquid environment using default parameters. The interactions were described by coupling the Lennard-Jones and Coulomb potentials using the All-Atom Optimized for Liquid-State Simulations (AA-OPLS) force field. All reactive parameters and electrical excitations were calculated using Density Functional Theory, M06-2X/6-311++G(d,p). [4,5]

RESULTS

The finds show that the biotransformation of NPE into PE using the four tested fungal species was successful, as evidenced by an improvement in the nonlinear optical response of PE in comparison to N2PE. We also note that interactions with solvents affect the vibrational spectra of the donor and acceptor groups of compounds and that bioconversion affects the molecular reactivity of the compound.

CONCLUSIONS

This study showed that using fungal species to biotransform NPE into PE is a promising technique. In addition, Monte Carlo simulations and vibrational analyses help us understand changes to the molecular properties that occur throughout the biotransformation.

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