



BIOTRANSFORMATION OF EPOXYISOPHORONE BY *ASPERGILLUS WELWITSCHIAE*

Lucas B. Filizzola^{1*}, Lucas P. Dutra^{1*}, Aristóteles Goes Neto^{2*}, Diogo M. Vidal^{1*}

lucasbauer926@gmail.com

¹Departamento de química UFMG; ²Instituto de ciências biológicas, UFMG

Biotransformation is a sustainable alternative for obtaining products with economic interest, once affordable reagents, such as isophorone and epoxyisophorone, may be employed to produce complex compounds, which are present in cosmetic, pharmaceutical and food industry. Fungi from *Aspergillus* genus are notorious microorganisms capable of performing such processes in a regio- and stereoselective manner. *A. niger*, for example, is a commonly strain employed in these biotransformation experiments. *A. welwitschiae* is a close related species to *A. niger*, which has never been exploited as biocatalyst. Thus, in this work epoxyisophorone was biotransformed by this fungus. The strain was pre-fermented in six 250 mL Erlenmeyers flasks filled with 100 mL of malt extract (30g/L). It was added 4 mL of a 25 mg/mL of epoxyisophorone DMSO solution in one sterile (positive control) and five inoculated media. To one of the inoculated media it was added 4 mL of DMSO (negative control). These cultures were fermented for more 96 h in the same conditions described above. After the fermentation period 1 mL of each media were extracted with 3x500 µL of ethyl acetate for GC-MS analysis. Using the authentic hydrocarbons C10 until C26 pattern and comparing the mass spectrogram and retention index time on the literature it was possible to identified 3 peaks relating respectively to cyclohexanone 5-methyl-2-1-methylethyl (1a) with R_T 11,10 min, Cyclohex-2-en-1-one, 2-hydroxy-, 3,5,5-trimethyl R_T 11,75 min (1b) and ciclohexanone 3,3,5-trimethyl R_T 14,60 min (1c). Searching on WILEY7, FFNSC and NIST147 to compare the mass spectrum, it was observed 84% similarity for the compound 1a, 99% for 1b and 88% for 1c. The Retention index was also calculated, 1125 (a), 1152 (1b) and 1291 (1c), on NIST webbook it was found 1128, 1149.8 and 1285, respectively. Among this peak it was observed other 5 peaks relating to possible products wich, with the analysis method and database available, was not possible to identify.

Keywords: Biotransformation, epoxyisophorone, sustainable, regio and stereo reactions

