

Title: Discrimination of *Candida spp* by fluorogenic assay with 6-nitroquinoline associated with FT-IR and chemometrics

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Abstract:

Technics using fluorogenic substrates (FS) are fast, specific and efficient methodologies used in detection of several pathogenic microorganisms in clinical samples in relation to culture methods. In this context, the prospection by novel FS has been constant. Here, we presented the results of discrimination of *Candida spp.* using the bioreduction products of 6-nitroquinoline (6NQ) in association with metabolomics technics: Fourier transform infrared spectroscopy (FT-IR) and chemometrics. 6NQ was synthesized by Skraup condensation of *p*-nitroaniline with glycerol and characterized by spectroscopic methods. Fluorogenic assay was carried out by incubation of culture loop of *Candida spp.* (17 strains, Sabouraud agar, 48h, 37°C) in broth containing 6NQ 1 mM and glucose 1% by 48h at 37 °C. The metabolome of biotransformation products was revealed by 365 nm uv light after treatment of cultures with equal volume of NaCl saturated solution and ethyl acetate 0,4 mL. The set organic fractions was too evaluated by FT-IR and processed by exploratory and classification methods. Ten strains tested positive (*C. albicans*, *C. krusei*, *C. stellacoidea*, *C. tropicalis*, *C. lusitaniae*) emitting blue or yellow fluorescence (associated to metabolome of bioreduction 6NQ derivatives). Principal Component Analysis of FT-IR spectra revealed two groups of positive samples and two groups of negative samples. PC3 separated the positive samples from negatives and PC1 separated the two groups of positive samples. Some species, as *C. krusei* and *C. glabrata*, presented two spectral patterns. The use of Soft Independent Modeling of Class Analogy (SIMCA) allowing the discrimination of the species investigated. The association of fluorogenic assay of 6NQ with FT-IR and chemometrics allowed a better understanding of the potential bioreduction of nitrocompounds of *Candida* and its endogenous metabolism.

Keywords: *Candida spp*, fluorogenic substrates, 6-nitroquinoline

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