TITLE: Identification in silico of anticancer drugs in Actinobacteria

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About of 45% of the drugs obtained of microorganism belong of Actinobacterias, principally of the genus Streptomyces. These drug-producing Microorganisms were isolated of different environments, but those obtained of marine environment have been a new target for the production of secondary metabolites, since these compound requires being more efficient to act on aqueous environment, especially in marine water. The aim was compare the compounds with anticancer and antitumor activity identified by MS-MS in four Actinobacteria against the databank of compounds isolated of Streptomyces. Four bacteria identified as Streptomyces sp (n=2), Gordonia sp (n=1) and Nocardiopsis sp (n=1) selected for the antiproliferative activity, was fermented and obtained the crude extract whit ethyl acetate. The extract was fractioned with methanol, methanol: water, water and ethyl acetate. The fractions was analyzed with UPLC-MS Acquity coupled to mass spectrometry TDQ Acquity (Micromass-Waters Manchester, England) with ionization source ESI with a column Acquity UPLC BEH C18 (2,1 mm x 50mm and 1,7µm particle size). The condition was solvent A (Mili-Q water with formic acid) with the solvent B (Methanol HPLC class). The initial specters obtained was analyzed for search the descript compounds in the databank DoBiscuit. Then the selected mass was analyzed by ESI-MS-MS. Were recognized 48 compounds belonging to the polyketide group, of which 23 were identified in the four microorganisms analyzed. Danurobicin was identified in the fractions of one of the Streptomyces sp. While its analogue Doxorubicin was found exclusively in the genus Streptomyces. Benastatin B and E was identified in Streptomyces sp and Nocardiopsis sp. The genus Gordonia sp synthetize different analogous of Benastatin. Identifying new niches of secondary metabolite synthesis allows to recognize potentially new modifiable organisms and producers of drug analogues. Identifying new niches of secondary metabolite synthesis allows recognizing potentially new modifiable organisms and producers of drug analogues.

Keywords: Streptomyces sp, Gordonia sp, Nocardiopsis sp, Anticancer drugs.

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