Classification of Antitumor Polyphenolic Compounds by FTIR Spectroscopy

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Polyphenolic compounds constitute one of the largest groups of plant metabolites. They display a vast array of molecular structures and cellular effects. In the past few decades, significant advances enabled researchers to investigate the potential use of these phytochemicals to treat or manage a plethora of chronic diseases including inflammatory diseases, cardiovascular abnormalities and various types of cancer (1). Antitumor properties of some of them such as curcumin have already been demonstrated. Traditionally, new drugs are evaluated for their potential to inhibit the proliferation of cancer cell lines. This approach is obviously not sufficient, and molecules with new modes of action are especially needed. Before setting up any advanced test on animals or clinical trials, and considering the large number of natural polyphenolic compounds already discovered, a preliminary classification of these molecules, preferentially based on induced cell metabolic modifications, is required. With such a classification, it should be possible to combine molecules acting on diverse signal transduction or biochemical pathways to create more efficient treatments. The aim of this work is to establish a classification method of polyphenolic compounds based on their mechanisms of action on cancer cell lines by FTIR spectroscopy using a high-throughput FT-IR spectrometer. This FTIR information is particularly rich as it originates at the same time from the genome, proteome, lipidome and metabolome. In this project, we will examine the effects of various polyphenols on 4 breast cancer cell lines presenting a growing invasive character. These cell lines are HBL-100, MCF-7, SK-BR-3 and MDA-MB-231.

Infrared spectra of cultivated cells exposed to polyphenols at their IC_{50} concentrations provide a precise signature of the global cell composition after treatment. It has been recently demonstrated in our laboratory that the infrared spectrum of cells exposed to well-characterized anticancer drugs provides a fingerprint representative of the metabolic changes induced by the drugs (2,3). As a first step in this procedure, we are working on the improvement of the quality of the IR spectra recorded by the high-throughput FTIR spectrometer (HTS). In particular we compare HTS absorbance spectra with imaging absorbance spectra of individual cells from the same cell smear in an attempt to understand the variable quality of HTS spectra. To do so, the program “Kinetics” running under Matlab carried out the processing of all the spectra acquired and unsupervised multivariate statistical analysis (hierarchical classification) used to classify them.

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