



Computational study correlating trace elements concentration and electron density in tumoral canine mammary tissues

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Background, Motivation and Objective. Canine life expectancy had a significant growth in recent years, mainly due to a higher demand for veterinary monitoring, vaccination, and appropriate dieting. As a result, several age-related diseases have arisen, such as neoplasms, a pathology that causes great interference in animal health and welfare ^[1]. Thus, the importance of investigating canine breast tumors lies in the rising awareness of caregivers regarding their pet's health, as well as the possible similarities with human tissues ^[1,2]. It is known that tumors are caused by chemical and biochemical changes in cells with consequences on the tissues and structures that constitutes it ^[2]. X-ray fluorescence (XRF) is one of the most used techniques for obtaining information about chemical elements in a tumor tissue sample, mainly because it allows the analysis of several elements simultaneously ^[2]. However, X-ray fluorescence experiments are not sensitive to elements of low atomic number, such as carbon and oxygen, major constituents of breast tissues. Consequently, no information about the morphology and composition of the tissue matrix are obtained, whose changes can be associated to the presence of neoplasias ^[3]. Nevertheless, this limitation of XRF techniques can be overcome by other techniques, such as Compton scattering, widely reported as an important tool for characterization of materials, since it allows assessing their electron densities ^[3]. This work aims to study by Monte Carlo computational simulation the determination of trace elements concentration and electron density by using XRF and Compton scattering spectroscopic techniques respectively. It is expected that this study can serve as a basis for performing experimental measurements on canine mammary tissues, correlating the information about the metabolic and biological processes associated to cancer dissemination.

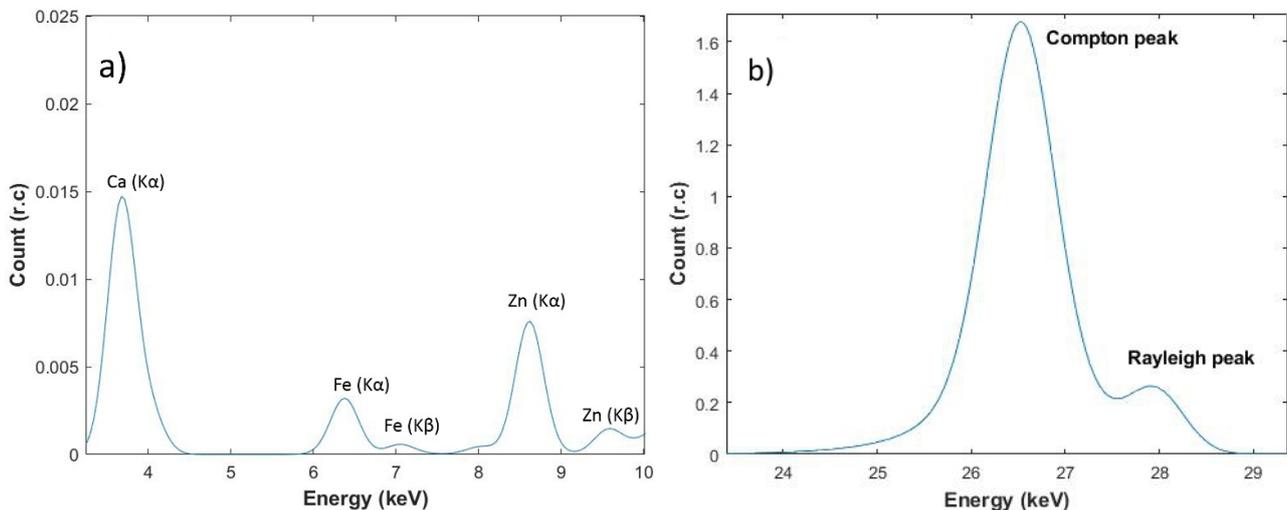
Methods. The XRF and Compton scattering simulations are performed by the XPMC (X-ray Monte Carlo program) ^[4]. The sample consists of an external cylinder of 2.0 cm in diameter and 1.0 cm in height, with a carcinoma composition. The typical concentration interval for each element: calcium, copper, iron and zinc typical of a carcinoma, are obtained from the literature ^[2] and included in the sample to simulate the presence of these chemical elements, which are characteristic upon carcinogenic activity in this type of tumor. Also, these concentration values are used in this study for comparison purposes. The simulations are performed using several energies, ranging from 10 to 30 keV. The XRF and scattering spectra are recorded by a 5.0 x 5.0 mm² square detector, positioned at $\theta = 45^\circ$. An in-house computational program is implemented to automate the curve fitting process for obtaining the areas (count) of the XRF and Compton peaks from which the element trace concentrations and electron densities are determined, respectively.

Results. Examples of fluorescence (a) and Compton (b) spectra obtained by the simulations are shown by figure 1. The area (count) under each fluorescence peaks is related to the concentration of the trace element while the area of Compton peak is related to the electron density of the tissue. The computational simulations show that the XRF technique is able to determine the trace

elements concentration with good accuracy (errors <3.0%). On the other hand, the electron densities are determined with an error around $\pm 2\%$ (including statistical and calibration errors).

Discussion and Conclusions. The computational results obtained by fluorescence simulations proves to be sensitive to the typical concentration of the investigated trace elements. The variations of these concentration in the tissues is associated with carcinogenic process and its determination brings important diagnostic information. In addition, from the scattering simulation it is possible to determine the electron density of the sample, which confirms the technique as a tool for studies involving morphology and composition of the tissue matrix. Thus, this study shows the possibility of combining fluorescence and scattering techniques for characterization of biological samples.

Figure 1: Example of spectra obtained by the simulations: (a) Fluorescence and (b) scattering. (r.c: relative count).



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Keywords. Fluorescence; X-ray scattering; canine breast cancer; simulation.

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