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# Artificial neural networks applied to quantitative elemental analysis of organic material using PIXE

R. Correa [a], M.A. Chesta [b,*], J.R. Morales [c], M.I. Dinator [c], I. Requena [d], I. Vila [e]

[a] Universidad Tecnológica Metropolitana, Departamento de Física, Av. José Pedro Alessandri 1242, Ñuñoa, Santiago, Chile
[b] Universidad Nacional de Córdoba, Facultad de Matemática, Astronomía y Física, Medina Allende s/n Ciudad Universitaria, 5000 Córdoba, Argentina
[c] Universidad de Chile, Facultad de Ciencias, Departamento de Física, Las Palmeras 3425, Ñuñoa, Santiago, Chile
[d] Universidad de Granada, Departamento de Ciencias de la Computación e Inteligencia Artificial, Daniel Saucedo Aranda s/n, 18071 Granada, Spain
[e] Universidad de Chile, Facultad de Ciencias, Departamento de Ecología, Las Palmeras 3425, Ñuñoa, Santiago, Chile

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**Abstract**

An artificial neural network (ANN) has been trained with real-sample PIXE (particle X-ray induced emission) spectra of organic substances. Following the training stage ANN was applied to a subset of similar samples thus obtaining the elemental concentrations in muscle, liver and gills of *Cyprinus carpio*. Concentrations obtained with the ANN method are in full agreement with results from one standard analytical procedure, showing the high potentiality of ANN in PIXE quantitative analyses.


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*Keywords:* Artificial neural networks; PIXE

## 1. Introduction

Developments from artificial intelligence like artificial neural networks, ANN, can be regarded as an engineering procedure emulating the human brain activity. It can be defined as a set of non-linear and non-stationary interconnection of elemental processes able to carry out at least one of the following functions: training, remembrance and generalization, or, abstraction of substantial properties. The fundamentals of the ANN technique have been described elsewhere [1,2] and several commercial and free codes are accessible nowadays.

Applications of ANN to atomic and nuclear physics has increased during the last two decades [3–13], mainly in problems related to nuclear reactors. The most used paradigms in artificial intelligence applications to nuclear science and particle physics are the expert system, genetic algorithms, fuzzy system, neural networks and hybrid system. Some applications to α, γ and X-ray spectra have been reported in the last decade [14–17]. Further application of ANN in other cases where strong non-lineal effects are present like in the spectral analyses generated in analytical techniques like PIXE [18,19] and XRF (X-ray fluorescence) [20,21] are scarce and in BIXE spectra (beta induced X-ray emissions) remain unexplored [22,23]. In [24,25] a review of applications of ANN and its potentialities in atomic and nuclear physics is shown.

A case where the potentialities of ANN seem to be most convenient is in the repetitive analysis of many spectra presenting similar patterns with specific differences. A typical

* Corresponding author. Tel.: +54 351 4334052; fax: +54 351 4334054.
*E-mail addresses:* rcorrea@utem.cl (R. Correa), chesta@famaf.unc.edu.ar (M.A. Chesta), rmorales@uchile.cl (J.R. Morales), mdinator@uchile.cl (M.I. Dinator), requena@decsai.ugr.es (I. Requena), limnolog@uchile.cl (I. Vila).

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case is presented in the elemental analysis of samples of unknown composition using energy dispersive XRF spectroscopy. Their respective spectra present peaks of known energy but different intensities containing information required to the evaluation of the elemental concentrations in each sample.

PIXE is a well established analytical method that allows the determination of concentrations in the range of mg/kg [26,27]. One of the factors that define the quality of the analysis is the ability to determine the correct amount of counts in each peak. Usually this is accomplished by the use of some reliable computer code, like AXIL [28].

Additional inputs of the proper physical parameters involved in the irradiation like beam intensity, detector efficiency, geometrical parameters, etc., permit the determination of the elemental concentrations.

The purpose of this work has been to take advantage of the non-linear properties and the neural network ability to learn and generalize together with its fast response. Samples of fish tissues were irradiated with protons to determine their elemental concentrations as part of a study of metal bioaccumulation by fishes. Several PIXE spectra were obtained from muscle, liver and gills samples of *Cyprinus Carpio*. A part of the samples set was analyzed by the standard method and later used to train the ANN for further calculations. Without assumptions about the distribution of data it was possible to detect elements (P, S, K, Ca, Fe, Zn) and determine their concentration in these organic samples obtained from fishes captured in Rapel Lake in Chile.

## 2. Analysis

The analysis was performed in two phases. First, one in which PIXE spectra were used to train the ANN and a second one in which the application of ANN independently produced results that were compared with those obtained by standard methodology.

PIXE spectra from muscle, liver and gills samples were used together with proper experimental data like average beam intensity, irradiation times, target masses, plus cross-sections values and detection system sensitivity, to determine elemental concentrations. As mentioned above, the amount of counts in each peak is currently used to determine the elemental concentration. Here, a slightly different approach has been used based on the fact that ANN application disregards additive constants. Then considering the observation that the background contribution at the peak is rather constant for equal irradiation times, the use of the maximum value at the peak channel as an input in ANN calculations, simplifies data handling and provides equivalent results as those obtained when the full area is used. These values and the already known concentrations were given as an input and output data respectively in the ANN training phase. Fig. 1 shows the flux diagram followed in each phase.

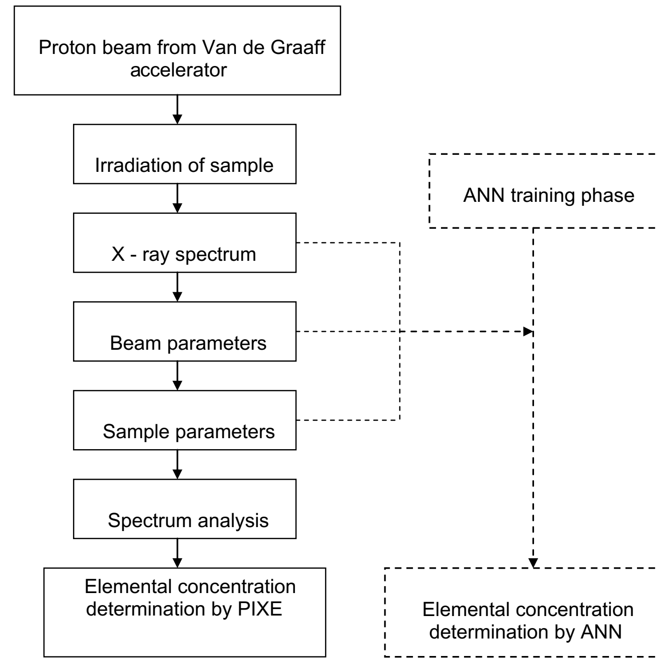


Fig. 1. Flux diagram showing the relationship between ANN inputs and the classical PIXE experimental steps.

### 2.1. PIXE analysis

The PIXE applications were performed at the Center for Experimental Physics, Faculty of Sciences, University of Chile, using the KN 3750 Van de Graaff electrostatic accelerator. Twenty one biological samples from a (*C. Carpio*) fish were prepared by digestion with $HNO_3$ and deposited on 8.4 μm thickness Kapton films for later irradiation with a 2.0 MeV proton beam. The X-ray photons emitted from the samples were detected by a Si(Li) detector (FWHM = 180 eV at 5.9 keV) coupled to conventional electronic units and MCA. The detector was placed at 90° angle with respect to the incident beam. A typical spectrum from a liver sample is shown in Fig. 2, where the characteristic Kα and Kβ peaks appear over the continuous

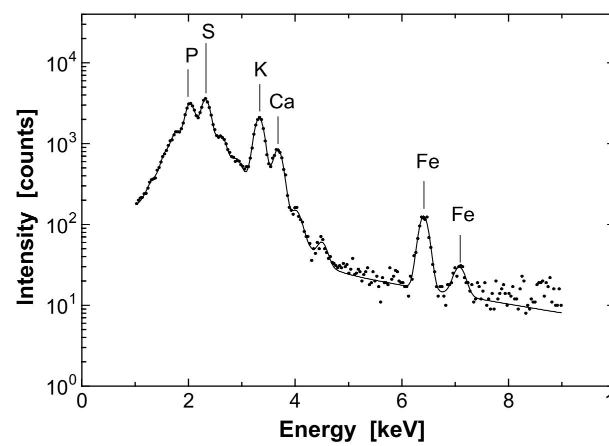


Fig. 2. Typical PIXE spectrum of a liver sample from fish *C. carpio*, using 2.0 MeV protons. The solid line is a fit given by AXIL.