Title: Rapid and non-invasive diagnosis of the presence of coronary artery disease based on 1H-NMR spectra of human blood plasma using supervised self-organizing map

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Abstract: Coronary artery disease (CAD) is a major cause of mortality and morbidity in developed countries, affecting as many as one in three individuals before the age of 70 years [1]. Despite a slight decrease in prevalence that has occurred over the past decade, it still contributes to nearly 15% of deaths [2]. Although a wide range of risk factors for coronary disease have been identified from population studies, these measures, singly or in combination, are insufficiently powerful to provide a reliable, noninvasive diagnosis of the presence of coronary disease [3]. Techniques such as genomics, proteomics and metabonomics (a systems approach to examining the changes in hundreds or thousands of low-molecular-weight metabolites in an intact tissue or bio fluid) offer the prospect of efficiently discriminating individuals who have special disease or toxic states. The NMR based technique offers several clear advantages in the clinical goals. It can be carried out on standard preparations of serum, plasma or urine samples [4-6]. In this work, supervised Kohonen artificial neural networks (SKANN) as a supervised self-organizing map (SOM) [7-12] is used as a non-linear modeling and visualizing method to analyze proton nuclear magnetic resonance (1H-NMR) spectroscopy data which obtained from human blood plasma samples. The goal of this study is human disease diagnosis and classifying CAD samples on basis of visualizing the relationship between different spectral patterns. Samples were collected after angiography and included patients with CAD and non-findings individuals (healthy cases) (64 samples with 2 classes). In this study, the oblique rotation (OR) [15] was implemented on the selected factors to transform them linearly to obtain the optimal discriminative factors. The optimal factors were introduced as input to SKANN [9-12] and also, partial least squares-discriminant analysis (PLS-DA) [11, 16] as non-linear and linear classification methods, respectively. Classification results were calculated and evaluated by cross validation and external test set and compared together. The best result obtained using SKANN. All the training and cross validated samples were successfully classified using proposed method. Percent of correct classified samples for test samples were 0.92 and 0.86 using SKANN and PLS-DA, respectively. It can be concluded that the combination of chemometrics approaches and SKANN [9-12] and PLS-DA [11, 16] as non-linear and linear classification methods, respectively. Classification results were calculated and evaluated by cross validation and external test set and compared together. The best result obtained using SKANN. All the training and cross validated samples were successfully classified using proposed method. Percent of correct classified samples for test samples were 0.92 and 0.86 using SKANN and PLS-DA, respectively. Classification (Chemometrics), Supervised self-organizing map, Nuclear magnetic resonance spectroscopy, Genetic Algorithm, PLS-DA.

Presentation: Poster