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Isoelectric point and electric charge determination of proteins: application to the analysis of biochemical parameters in major burn patients

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There are several methods for the theoretical determination of the isoelectric point (*pI* value) of proteins and other macromolecules. We propose here a new method for the *pI* determination. The program called PICAL (*pI* CALculation), written in the programming language Visual Basic, has the following main characteristics: take into account all the amino acid residues of the protein, has the same accuracy of other methods, uses a much simpler approach to obtain the *pI* value of any macromolecule, makes it possible to work with protein databases and determines the electric charge of proteins with different pH values. By way of example we described the process of determining the charge of all the enzymes classified in the six groups of the EC (Enzyme Commission), in the acidosis - alkalosis range ($\text{pH} = 7.1 - 7.7$), in addition to other plasmatic proteins. Another different option approached also here, is the use of PICAL in the calculation of the *pI* value and protein electric charge for didactical purposes.

The determination of the charge of proteins and other macromolecules has been also focused with a clinical perspective in major burn patients. This type of pathology requires a multidisciplinary approach from different hospital specializations. Amongst factors of great importance and intimately related to the medical view of these patients are, generalized oedema, electrolytic alterations, and an accelerated metabolic state which are all part of the physiopathology of burns. Applying the biochemical knowledge described above to this problem, a retrospective study was carried out on 118 patients admitted between 2006 and 2008 to the Major Burns Unit of the Unfallkrankenhaus Berlin Hospital. A statistical analysis was carried out using 13 biochemical parameters (pH , $[\text{HCO}_3^-]$, $[\text{Na}^+]$, $[\text{K}^+]$ etc), identifying the clinical variables (age, TBSA, depth of burn etc) that modify these parameters. In addition, the probability of death was determined by means of multivariate analyses using clinical and biochemical data. Finally, by means of PICAL software, the electric charge of each patient's plasma was calculated considering the proper biochemical parameter.

All the software described in this study is available free at:

<http://www.andresmaldonado.es/pical.htm>