Partial least squares regression: A valuable method for modeling molecular behavior in hemodialysis

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RESUMEN

The aim of this work was to use the Partial Least Squares Regression (PLS) technique to fit simple models for the interpretation of an underlying complex process. In this study, the technique was used to build a statistical model for molecular kinetic data obtained from hemodialyzed patients. By using PLS we derived statistical linear models for the prediction of the equilibrated urea concentration which would be reached 30-60 min after the end of the dialysis session. Models with an average relative prediction error (RPE) of less than 0.05% were achieved. The model predictive accuracy was evaluated in a cross-center study yielding an RPE < 3%. The chosen model was robust to variations such as sampling extraction time demonstrating a high capacity for modeling kinetics. It also was found to be useful for bedside monitoring. Finally, the PLS technique allowed identification of the most important co-variables in the model and of those patients with outlier patterns in their molecular dynamics.

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