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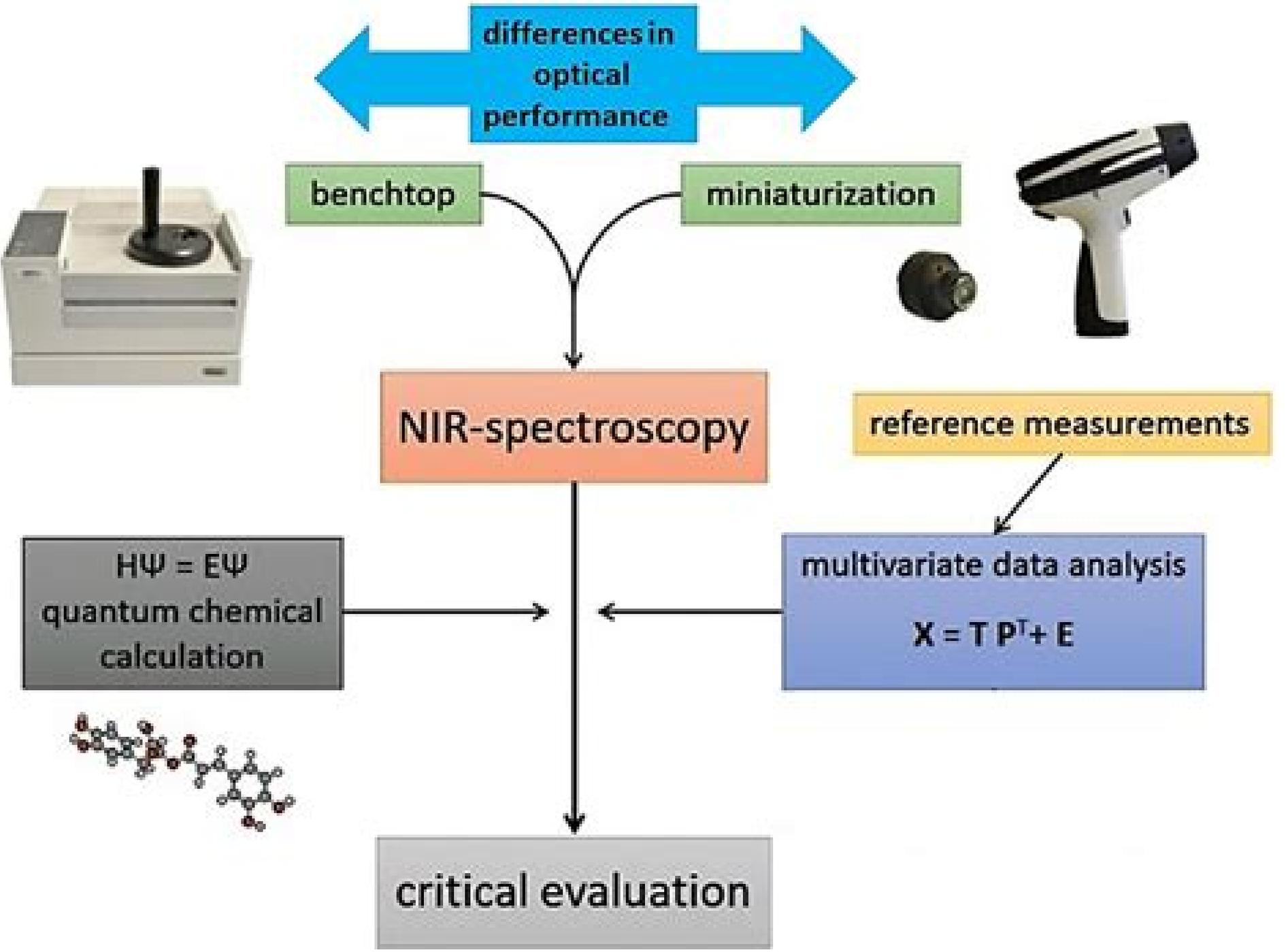
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$H\Psi = E\Psi$
quantum chemical calculation

multivariate data analysis
 $X = T P^T + E$



critical evaluation



Application Of Multivariate Calibration And Nir

Engin Deniz Yalvac



Application Of Multivariate Calibration And Nir:

Multi- and Megavariate Data Analysis Basic Principles and Applications L. Eriksson, T. Byrne, E. Johansson, J. Trygg, C. Vikström, 2013-07-01 To understand the world around us as well as ourselves we need to measure many things many variables many properties of the systems and processes we investigate Hence data collected in science technology and almost everywhere else are multivariate a data table with multiple variables measured on multiple observations cases samples items process time points experiments This book describes a remarkably simple minimalistic and practical approach to the analysis of data tables multivariate data The approach is based on projection methods which are PCA principal components analysis and PLS projection to latent structures and the book shows how this works in science and technology for a wide variety of applications In particular it is shown how the great information content in well collected multivariate data can be expressed in terms of simple but illuminating plots facilitating the understanding and interpretation of the data The projection approach applies to a variety of data analytical objectives i e i summarizing and visualizing a data set ii multivariate classification and discriminant analysis and iii finding quantitative relationships among the variables This works with any shape of data table with many or few variables columns many or few observations rows and complete or incomplete data tables missing data In particular projections handle data matrices with more variables than observations very well and the data can be noisy and highly collinear Authors The five authors are all connected to the Umetrics company www.umetrics.com which has developed and sold software for multivariate analysis since 1987 as well as supports customers with training and consultations Umetrics customers include most large and medium sized companies in the pharmaceutical biopharm chemical and semiconductor sectors

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introducing the material in a readily comprehensible manner A considerable part of the text is dedicated to practical applications including sample preparation and investigations of polymers textiles drugs food and animal feed However special topics such as two dimensional correlation analysis are also covered in separate chapters Written by eight experts in different fields this book presents an introduction to the current state of developments and is valuable to spectroscopists and to practitioners applying NIR spectroscopy as a daily analytical tool

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