Dr. Rodionova Oxana Yevgenevna.
N.N. Semenov Institute of Chemical Physics RAS,
Kosygin 4, 119991,
Moscow, Russia

PROFILE

Dr. Rodionova Oxana Yevgenevna is a Leading Researcher at the Semenov Institute of Chemical Physics of Russian Academy of Science, Russian Chemometrics Society (ICP RAS). Basically an engineer in Mathematics from Moscow Institute of Electronic Machines Building, Moscow, she went on to complete her Ph.D in Numerical Mathematics from Calculation Centre of Russian Academy of Sciences and her Doctor of Science in Instruments and Methods of Experimental Physics, from Institute for Analytical Instrumentation, St. Petersburg.

Dr.Oxana's area of expertise is in Chemometrics, Numerical Methods and Mathematical Physics. She is a member of Commission on Chemometrics, South African Chemometric Society(SACS), Science Secretary of Commission on Chemometrics, Russian Chemometric Society and International Chemometric Society and a much invited speaker for various conferences and workshops all over the world. She has given over 50 lectures in various conferences and workshops.

Dr.Oxana is the member of the editorial board of Journal of Chemometrics and a peer reviewer for a variety of journals incuding, Trends in Analytical Chemistry, Journal of Chemometrics, Chemometrics and Intelligent Laboratory Systems and Analytical Chemistry. She possesses over 70 pubications in reputed journals, 15 books and chapters and has received 15 projects and grants.

HOW DO NEAR INFRARED SPECTROSCOPY (NIR) AND CHEMOMETRICS HELP IN PHARMACEUTICAL APPLICATIONS?

Abstract:

The NIR-based approach is a widely-spread technique that is used in modern pharmaceutical applications. It provides possibility for rapid and non-destructive analysis of a remedy as a whole object and helps to reveal various violations in product manufacturing. The efficiency of the approach depends on two critical issues. They are NIR instrument and chemometric method used for data processing.

What issue is more important? Should we pay more attention to the spectrometer and parameters of the spectra acquisition such as very high resolution and very low S/N ratio? Or should we input more effort in the spectra preprocessing, variable selection, and data modeling? Of course this is very problem dependent. These issues are analyzed on the example of classification of the final product, i.e. intact tablets. The results of application of different spectrometers and various chemometric approaches are compared. It is shown that an appropriate chemometric methods help to yield satisfactory results even for the simpler instrument. The new developed classification method called DD_SIMCA provides satisfactory results in separation of various manufacturers of similar drugs for different spectrometers. The possibility to assess the Type I and the Type II errors provide a quantitative assessment of the risk of wrong decisions and can be employed for the science-based risk assessment. The same approach can also be used on various stages of PAT applications, where the process state is continuously monitoring in order to keep it within the control limits. A sound decision should be based on the quantitative risk assessment and accounts for representative data sets, multivariate procedure for development and validation. The decision should be data-driven and employ modern chemometric and statistic tools designed for such purposes.