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# Recognition of the 'high quality forgeries' among the medicines: application of NIR spectroscopy and chemometrics

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## ABSTRACT

Counterfeiting causes a huge economic and reputational damage to pharmaceutical companies, as well as poses a significant danger to public health. Fake medicines could be of different type: placebo, the medicines with lower concentration of active substances, the drugs that do not contain the proper concentrations or contain a wrong type of excipients, etc. From the recognition point of view there are also various types of fakes. They are (1) pills/tablets that can be recognized without any instruments, simply by glance, or, at least, by experienced glance; (2) medications with special drug packages, holograms, unique printing on tablet surface, special shapes of pills and capsules; (3) fakes that only can be detected using chemical/physical testing of drugs themselves. The most difficult for revealing are 'the high quality fakes', which have a proper composition but produced by the underground manufactures with violation of technological regulations. For rapid testing we propose application of Near Infrared (NIR) measurements accompanied with chemometric data processing. NIR spectra carry information regarding not only chemical but also physical phenomena. A general approach is to consider a remedy as a whole object, taking into account a complex composition of active ingredients, excipients, as well as manufacturing conditions, such as degree of drying, etc. A newly developed classification method, DD-SIMCA, shows satisfactory results both in revealing counterfeits and in separation of various manufacturers of similar drugs. A real world example presents an analysis of the widely used medication for treating allergies, produced by five various manufacturers, and comparison the results with counterfeited samples (Figure 1). The case study demonstrates that theoretically predicted classifier characteristics, such as the Type I error, α, and the Type II error, β, are confirmed by the real-life calculations. The values of α and β errors provide a quantitative assessment of the risk of wrong decisions and can be employed for the science-based risk assessment.

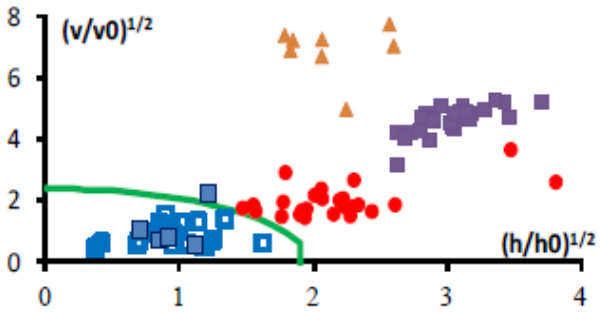


**Figure 1.** The DD-SIMCA plot. The green curve delineates the acceptance area. Outside objects are aliens.

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