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報告書

# 平成30年度「日本薬局方の試験法等に関する研究」研究報告
# ケモメトリックスの日本薬局方への導入に関する研究*2

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# Study on the Introduction of Chemometrics into the Japanese Pharmacopoeia*2

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**Summary**

The purpose of this study was to facilitate the introduction of chemometrics into the Japanese pharmacopoeia. US and European pharmacopoeias already include a chapter on chemometrics. They say that specificity, linearity, range, accuracy, precision, and robustness are required for the evaluation of chemometrics models in the method validation. Based on these requirements, a comparative study of the content uniformity test between the conventional test and PAT with chemometrics was performed. The UV method was used for the conventional test and transmission Raman spectroscopy was used for PAT with chemometrics. Partial least-squares regression (PLSR) with standard normal variate (SNV) spectral pretreatment was used for chemometrics. 100 tablets containing 20% acetaminophen and 80% lactose monohydrate were measured using both methods. The quantitative results obtained by transmission Raman with chemometrics were highly correlated to those obtained by the conventional UV method and showed sufficient accuracy and precision for pharmaceutical quantification.

**Key words**

Chemometrics, Transmission Raman spectroscopy, Process analytical technology, Acetaminophen