

Abstract

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Varmuza K., He Ping, Fang Kai-Tai:

Boosting applied to classification of mass spectral data.

Boosting is a machine learning algorithm that is not well known in chemometrics.

We apply boosting tree to the classification of mass spectral data. In the experiment, recognition of 15 chemical substructures from mass spectral data have been taken into account.

The performance of boosting is very encouraging. Compared with previous result, boosting significantly improves the accuracy of classifiers based on mass spectra.