Comprehensive extraction method integrated with NMR metabolomics: a new bioactivity screening method for plants, adenosine A1 receptor binding compounds in Orthosiphon stamineus benth

ABSTRACT

A large number of plant metabolites has provided as an incomparable chemical source for drug development. However, the wide range of the polarity of metabolites has been a big obstacle for full use of the chemical diversity. The initial step conventional extraction method by a single solvent does not make use of all the metabolites contained in plants. Also, it takes a long time to confirm the target activity of a single compound because of tedious separation steps. To solve the problem, a new extraction method coupled to NMR-based metabolomics is applied to identify bioactive natural products. A comprehensive extraction method consisting of a continuous flow of solvent mixtures through plant material was developed to provide extracts with a wider chemical variety than those yielded with a single solvent extraction. As the model experiment, 1H NMR spectra of the extracts obtained from the comprehensive extraction of Orthosiphon stamineus were subjected to multivariate data analysis to find its adenosine A1 binding activity. On the basis of the results, two flavonoids from a large number of chemicals were clearly verified to show the adenosine A1 binding activity without any further purification steps. This method could provide a solution to the major drawbacks of natural products in drug development.

Keyword: NMR metabolomics; Orthosiphon stamineus; Comprehensive extraction; Adenosine A1 receptor