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Journal of the Science of Food and Agriculture
Volume 98, Issue 1, January 2018, Pages 240-252

Comparison of partial least squares and random forests for evaluating relationship between phenolics and bioactivities of Neptunia oleracea (Article)

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Abstract

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BACKGROUND: Neptunia oleracea is a plant consumed as a vegetable and which has been used as a folk remedy for several diseases. Herein, two regression models (partial least squares, PLS; and random forest, RF) in a metabolomics approach were compared and applied to the evaluation of the relationship between phenolics and bioactivities of N. oleracea. In addition, the effects of different extraction conditions on the phenolic constituents were assessed by pattern recognition analysis. RESULTS: Comparison of the PLS and RF showed that RF exhibited poorer generalization and hence poorer predictive performance. Both the regression coefficient of PLS and the variable importance of RF revealed that quercetin and kaempferol derivatives, caffeic acid and vitexin-2-O-rhamnoside were significant towards the tested bioactivities. Furthermore, principal component analysis (PCA) and partial least squares–discriminant analysis (PLS-DA) results showed that sonication and absolute ethanol are the preferable extraction method and ethanol ratio, respectively, to produce N. oleracea extracts with high phenolic levels and therefore high DPPH scavenging and α-glucosidase inhibitory activities. CONCLUSION: Both PLS and RF are useful regression models in metabolomics studies. This work provides insight into the performance of different multivariate data analysis tools and the effects of different extraction conditions on the extraction of desired phenolics from plants. © 2017 Society of Chemical Industry. © 2017 Society of Chemical Industry

Reaxys Database Information

View Compounds

Author keywords

extraction conditions metabolomics Neptunia oleracea partial least squares phenolics random forest

Indexed keywords

EMTREE drug terms: caffeic acid caffeic acid derivative flavonoid glycoside neptunium phenol derivative plant extract vitexin-2-O-rhamnoside

EMTREE medical terms: chemistry comparative study least square analysis metabolomics

MeSH: Caffeic Acids Flavonoids Glycosides Least-Squares Analysis Metabolomics Neptunium Phenols Plant Extracts

Chemicals and CAS Registry Numbers:

caffeic acid, 27323-69-9, 331-39-5; neptunium, 7439-99-8;

caffeic acid; Caffeic Acids; Flavonoids; Glycosides; Neptunium; Phenols; Plant Extracts; vitexin-2-O-rhamnoside

ISSN: 00225142
CODEN: JSFAA
Source Type: Journal
Original language: English
DOI: 10.1002/jsfa.8462
PubMed ID: 28580581
Document Type: Article
Publisher: John Wiley and Sons Ltd

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