



Detection and partial structure elucidation of basic taxoids from *Taxus wallichiana* by electrospray ionization tandem mass spectrometry.

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A sensitive method for the detection and characterization of basic taxoids from the ethyl acetate extract of *Taxus wallichiana* has been described. A combined analysis of the fragmentation spectra of 3 purified standard basic taxoids and the substructure analysis of 139 previously reported taxoids provided information on typical primary and secondary product ions that are generated by CID mass spectrometry of basic taxoids. Precursor-scan analysis of selected product ions allowed for the detection of 57 basic taxoids from the ethyl acetate extract of *T. wallichiana*, 45 of which have not been reported. The method described in this paper provides a fast method for the "dereplication" of natural products. The mass spectrometric data derived by this method was sufficient for the partial structure elucidation of novel basic taxoids. The method presented in this paper can be easily adapted into a high-throughput screening protocol for the identification and characterization of bioactive natural products.

Słowa kluczowe

Fragmentation, Ions, Mass spectrometry, Organic compounds, Scaffolds

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