Palaeontographica, Abt. B: Palaeobotany – Palaeophytology
Vol. 295, Issues 4–6: 91–133
Stuttgart, November 2017

Article

3D chemometric model and frond architecture of *Alethopteris ambigua* (Medullosales): Implications for reconstruction and taxonomy

by

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With 20 text-figures and 10 tables, and 3 appendix tables

Abstract

The postulated relationship between chemistry and frond architecture is further tested based on a 450 mm frond segment *Alethopteris ambigua* Lesquereux pars from the Sydney Coalfield (Canada), this being the largest specimen known for this species. Micromorphology demonstrated amphistomatic rachides with larger anomocytic stomata than on the hypostomatic pinnules, and rachial epidermal cells that are irregularly elongate to polygonal-rectangular, intermingled with more rectangular isodiametric cells, with hardly any change over the segment. Functional groups or chemical structural groups, however, are continuously variable over the frond segment, allowing meaningful comparisons between frond parts. Based on these data, a three-dimensional "model" is derived which explains the relationship between the frond architecture and changes in chemical structural groups. Furthermore, the aromatic-rich compounds correlate with robust and stiffer proximal frond parts, whereas the aliphatic-rich compounds correlate with the slender and flexible distal parts. The former reflects lignin-related compounds in the basal part of the frond, and the latter tannin and resin-like chemicals as secondary metabolites in pinnules and midveins as the defense against herbivory. Strengthening the relationship between the hypothesized fossil chemistry-frond architecture is the testable prediction of chemistry of the "missing parts" in the likely quadripinnate *A. ambigua* frond, i.e. the petiole, frond bifurcation, and their adjacent proximal and most robust parts.

Keywords: *Alethopteris*; frond; cuticles; chemistry; Carboniferous; FTIR; chemometrics; chemical composition

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DOI: 10.1127/palb/2017/0056
2194-900X/17/0295/0056 $ 19.35

DOI:10.1127/palb/295/2017/91