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Indole alkaloid profiles in ergot (*Claviceps purpurea*): Is there a link between chemotype, genetic group and ecology?

Silvio Uhlig[1], **Mariell Negard**[1,2], **Havard Kauserud**[2], **Klaus Hoiland**[2], **Tom Andersen**[2] and **Trude Vralstad**[1,2]
[1]Norwegian Veterinary Institute, Norway
[2]Department of Biosciences, University of Oslo, Norway

Clavicepspurpurea is a phytopathogenicascomycete that parasitizes various grasses within the Poaceae, most notably rye. In late summer, the fungus replaces the grain of an infected host plant with a so-called sclerotium containing toxic indole-alkaloids. Previously, three different genetic groups (G1-G3) with divergent habitat preferences and alkaloid chemistry have been detected, often referred to as *C. purpurea* ecotypes and chemoraces.

The main aims of this study were to analyze the genetic variation in *C. purpurea* in Norway, characterize the indole-alkaloid profiles in relation to genetic groups, and reveal the relationships between genetic groups, chemoraces and ecology.

In total, 596 sclerotia from 14 different grass species were subjected to various analyses, including a sclerotial floating test, genetic analyses from which rDNA ITS and partial beta tubulin sequences were generated. Furthermore, the indole-alkaloid profiles (peptide ergot alkaloids and indole-diterpenoids) were analysed using HPLC-MS.All sclerotia were cut in halves in order to analyze one half genetically and one half chemically.

Phylogenetic analyses and haplotype networks of genetic data supported one new (G4) genetic group of *C. purpurea*in addition to the three known (G1-G3). Furthermore, G1, G2 and G4 were present in Norway while G3 was absent. The new G4 genetic group was supported also from chemical and ecological data. G4 produced sclerotia that were consistently floating, and was predominantly found in very wet habitats on *Moliniacaerulea*, and occasionally also in saline habitats on *Leymusarenarius*. The G4 indole-diterpenoid profile resembled that of G2, but the peptide ergot alkaloid profile of the formerdiffered in high amounts of the ergopeptamergosedmam, the lactam congener of ergosedmine.A consistent presence of indole-diterpenoids in sclerotia from the G2 and G4 genetic groups was demonstrated, while these compounds with few exceptions were absent in the G1 genetic group. This study supports that the alkaloid chemistry in *C. purpurea*is a function of the genetic group.The indole-alkaloid profiles in*C. purpurea*sclerotiacould even be used for assignment to a specific genetic group.

While G1 and G2 were found on numerous host plants and in different habitats, G3 and G4 seem to be more host and habitat specific. Co-occurrence of up to three genetic groups on the same host plant within the same habitat was observed (i.e. G1, G2 and G4). Thus, our results suggest that the four groups G1-G4 in the *C. purpurea* complex represent four biological (cryptic) species rather than only ecotypes.

silvio.uhlig@vetinst.no