# Utilizing volatile organic compounds for early detection of Fusarium circinatum

SND-ID: 2022-134-1. Version: 1. DOI: https://doi.org/10.5878/hc9w-7694

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## Associated documentation

Data\_description.txt (2.13 KB)

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2022-134-1-1.zip (~977.79 MB)

#### Citation

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## Creator/Principal investigator(s)

Ida Nordström - Swedish University of Agricultural Sciences, Southern Swedish Forest Research Center

## **Research principal**

Swedish University of Agricultural Sciences - Southern Swedish Forest Research Center

## Principal's reference number

SLU.ess.2022.IÄ-2

# Description

Fusarium circinatum, a fungal pathogen deadly to many Pinus species, can cause significant economic and ecological losses, especially if it were to become more widely established in Europe. Early detection tools with high-throughput capacity can increase our readiness to implement mitigation actions against new incursions. This study sought to develop a disease detection method based on volatile organic compound (VOC) emissions to detect F. circinatum on different Pinus species. VOCs emitted from four different Fusarium species (Fusarium circinatum, Fusarium graminearum, Fusarium bulbicola and Fusarium oxysporum f.sp. pini) grown on Elliott's media agar (in vitro), and three Pinus species (Pinus radiata, Pinus sylvestris, Pinus pinea) inoculated with either i) Fusarium circinatum or ii) mock treatment (in vivo). The four Fusarium species were grown on media and analysed in order to compare their respective VOCs profiles, while the pinus seedlings were analysed in order to determine whether Fusarium circinatum-inoculated seedlings' VOCs profiles could be distinguished from mock inoculated seedlings. The VOCs were sampled using static headspace sampling, enclosing the samples individually in (relatively inert) high-density poly-ethylene bags along with SPME fibers. Divinylbenzene/carboxen/polydimethylsiloxane SPME fibers needle size was 24 ga, 2 cm long and coated with 30 µm (CAR/PDMS layer), 50 µm (DVB layer) (Merck KGaA, Darmstadt, Germany). Immediately after sampling, the SPME fibers were manually injected through an ultra-inert, splitless, straight, 2 mm liner (Agilent, Santa Clara, USA) on a 6890N GC (Agilent Technologies, Santa Clara, USA) coupled with a 5973 MS (Agilent Technologies, Santa Clara, USA). The column was a HP-5ms ultra inert 60m GC column, 0.25 mm, 0.25 µm, 7 inch cage (Agilent, Santa Clara, USA). A C8-C20 hexane mix (Merck KGaA, Darmstadt, Germany). GC-MS was performed through MSD ChemStation version E.02.02.1431 (Agilent Technologies, Santa Clara, USA) with an initial oven temperature of 50°C, followed by an 8°C/min increase to 100°C, subsequently increasing by 4°C/min to 160°C, a final ramp of 16°C/min to 280°C and hold for 2.5 min. GC-MS data were transformed to .cdf files and processed (ADAP chromatogram builder, chromatogram deconvolution, multivariate curve resolution) and aligned (ADAP aligner) with MZMine 2 (v 2.53). Randomforest was applied to see what (if any) compounds could be useful for distinguishing between mock- or F. circinatum-inoculated seedlings (in vivo), or Fusarium species (in vitro). These compounds were tentatively identified by matching mass spectrometry data and back-calculated retention indices with literature values from authentic standards found in Nist20 and Wiley12 MS databases.

The above described pipeline applied here, entailing gas chromatography – mass spectrometry of VOCs, automated data analysis and machine learning, distinguished diseased from healthy seedlings of Pinus sylvestris and Pinus radiata. In P. radiata, this distinction was possible even before the seedlings became visibly symptomatic, suggesting the possibility for this method to identify latently infected, yet healthy looking plants. Pinus pinea, which is known to be relatively resistant to F.

circinatum, remained asymptomatic and showed no changes in VOCs over 28 days. In a separate analysis of in vitro VOCs collected from different species of Fusarium, we showed that even closely related Fusarium spp. can be readily distinguished based on their VOC profiles. The results further substantiate the potential for volatilomics to be used for early disease detection and diagnostic recognition.

GC-MS data were collected both in vitro (fungal species grown on identical media) and in vivo (pine seedlings inoculated with Fusarium circinatum or mock). This GC-MS data could then be used to compare what volatile compounds were emitted from each sample and, that way, determine whether these "chemical fingerprints" of volatile compound blends differed between fungal species, or sick and healthy pine seedlings, respectively. Each data file therefore contain all the chemical compounds that can be detected by using our instruments (see general description), their mass spectas, relative abundance and retention times. No sorting of these chemical compounds have been performed, nor any other processing of this raw data for publication.

The dataset includes GC-MS data according to the Mass Spectrometry Development Kit (MSDK) data model in NetCDF format. Files can be read in software that uses MSDK, such as AMDIS or MZMine. See <a href="https://msdk.github.io/">https://msdk.github.io/</a> for more possibilities.

There are 5 or 6 replicates for each time point and pine species included in the in vivo-analyses. For the in vitro analyses, there are 3 replicates per fusarium species/media blank and time point.

All in vivo files are named in the format "#DAABB\*" where:

# = days post inoculation (7, 14 or 28)

D = Days

AA = Pine species (Sy=Pinus sylvestris, Ra=Pinus radiata, Pi=Pinus pinea)

BB = Inoculation type (Fc=Fusarium circinatum, Mo=Mock inoculation)

\* = Replicate number (1-6)

Example: 14DPiFc4.CDF = Analysed 14 days post inoculation, Pinus pinea inoculated with F. circinatum, replicate number 4.

All in vitro files are named in the format "AAAA#\*" except the media blank that is named "emabl#\*" where:

AAAA = Fusarium species (fcir=Fusarium circinatum, fgra=Fusarium graminearum, foxy=Fusarium oxysporum f.sp. pini, fbul=Fusarium bulbicola)

# = days post inoculation (7, 14 eller 21)

\* = replicate number (1-3)

Example: fcir72.CDF = Fusarium circinatum, Analysed 7 days post inoculation, replicate number 2

## Data contains personal data

No

## Language

**English** 

Data format / data structure

<u>Numeric</u>

## Species and taxons

<u>Fusarium graminearum schwabe</u> <u>Fusarium bulbicola nirenberg & o'donnell</u> Pinus radiata d. don Pinus sylvestris l. Fusarium circinatum nirenberg & o'donnell Fusarium oxysporum schltdl. Pinus pinea l. Fusarium Pinus

#### **Geographic spread**

Geographic description: Not relevant as the study never involved trees planted other than in pots, and no field samples were collected.

#### **Responsible department/unit**

Southern Swedish Forest Research Center

#### Funding 1

- Funding agency: Carl Tryggers Stiftelse för Vetenskaplig Forskning
- Funding agency's reference number: 18:67

#### Funding 2

- Funding agency: Craafordska stiftelsen
- Funding agency's reference number: 20200631

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• Funding agency: Erasmus+ Staff mobility grant

#### **Funding 4**

• Funding agency: Anna-Britta & Vadim Söderströms resestipendium

#### **Funding 5**

• Funding agency: NordGen Forest SNS scholarships

#### **Funding 6**

- Funding agency: The Swedish Research Council Formas
- Funding agency's reference number: 2018-00966

#### **Funding 7**

• Funding agency: The Royal Swedish Academy of Agriculture and Forestry

#### **Funding 8**

• Funding agency: Stiftelsen fonden för skogsvetenskaplig forskning

#### **Research area**

Engineering and technology (Standard för svensk indelning av forskningsämnen 2011) Chemical sciences (Standard för svensk indelning av forskningsämnen 2011) Microbiology (Standard för svensk indelning av forskningsämnen 2011) Forest science (Standard för svensk indelning av forskningsämnen 2011)

## Keywords

Gas chromatography, Plant health care, Forest health, Plant diseases, Biosecurity, Plant health control, Mass spectrometry, Solid phases, Vocs, Spme, Plant health, Volatile organic compounds, Pathogens, Pine pitch canker, Bio security, Disease detection

#### Accessibility level

Access to data through SND Data are freely accessible

## Use of data

Things to consider when using data shared through SND

Versions Version 1. 2022-12-15

#### Contact for questions about the data

Ida Nordström ida.nordstrom@slu.se

#### **Download metadata**

DataCite DDI 2.5 DDI 3.3 DCAT-AP-SE 2.0 JSON-LD PDF Citation (CSL) File overview (CSV)

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