Gas Chromatography-Mass Spectrometry data used to identify aceramic birch bark tar production methods

Introduction:

The dataset contains data collected between September 2019 and September 2023 as part of the Ancient Adhesives project under the European Union's Horizon 2020 research and innovation programme Grant Agreement No. 678 804151 (Grant holder G.H.J.L.). It is being made public to act as supplementary data for a publication and for other researchers to use this data in their own work. Due to the nature of the GC-MS data, all raw files have been supplied which will allow further processing in the original software.

The dataset includes 29 .zip with the raw GC-MS data and four .Xlsx files containing the processed information used in the manuscript. Each .zip file contains the files necessary to open and manipulate the data using the original software Agilent OpenLab 2.5.

List of .zip files containing raw GC-MS data. Within each file, there is a .DX file (for opening with Agilent OpenLab 2.5) and accompanying .ACAML, .DX, .MFX, .BIN, .RX, .PMX, and .AMX files:
210929 HOR_AM3.zip
210927 Vla_PR11.1.zip
210927 Vla_PR11.2.zip
210927 Vla_RSO2.1.zip
210927 Vla_RSO2.2.zip
20230314 Vla CO_2.1.zip
20230314 Vla CO_3.1.zip
20230314 Vla CO_4.1.zip
20230314 Vla CO_5.1.zip
20230314 Vla CO_6.1.zip
20230314 Vla CO_7.1.zip
20230314 Vla PRO_1.1.zip
20230314 Vla PRO_2.1
20230314 Vla PRO_3.1.zip
20230314 Vla PRO_4.1.zip
20230314 Vla PRO_7.1.zip
20230314 Vla PRO_8.1.zip
20230314 Vla PRO_9.1.zip
20230314 Vla RSO_1.1.1.zip
20230314 Vla RSO_1.1.2.zip
20230314 Vla RSO_2.1.1.zip
20230314 Vla RSO_2.1.2.zip
20230314 Vla RSO_2.1.3.zip
20230316 VLA CO_8.1.zip
20230316 VLA CO_16.1.zip
20230316 VLA CO_17.1.zip
20230526 HOR_AM1.zip
20230526 HOR_AM2.zip
20230526 HOR_AM4.zip

List of .Xlsx file containing processed information used in the accompanying publication separated according to the tar production method – ash mound, condensation, pit roll, and raised structure:
HOR ash mound results.xlsx
VLA condensation results.xlsx
VLA pit roll results.xlsx
VLA raised structure results.xlsx

Each sheet contains the complete GC-MS data exported for samples analyzed as well as the MS data and automated molecular data against the National Institute of Standards and Technology (NIST) library.
RT= Retention time (min)
Type = Type of integration. BB = baseline to baseline, BV = baseline to valley, VB = valley to baseline, VV = valley to valley, MV = manual to valley, VM = valley to manual, MB = manual to baseline, MM = manually integrated
Width (min) = Peak width
Area = Peak area
Height = Peak height
Area % = Peak area %
Compound name = compound automatically identified from NIST library using Agilent Openlab corresponding to the RT.
Score = Match factor, or a comparison of the unknown's mass spectrum's peak to those of the peaks in the library's spectra.
Rev. Score = The match factor when the peaks in the unknown's spectrum that are not in the library's known reference spectrum are ignored.
Prob.% = Probability percent that the compound is identified correctly within the NIST library.
CAS # = Chemical Abstracts Service Number – A unique accession number assigned to a given compound
Library Id = Identification number from the NIST mass spectral library