

The dataset contains data collected 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.

The dataset includes eight .zip with the raw GC-MS data and one .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 files containing GC-MS data. Within each .zip file, there is a .DX file (for opening with Agilent OpenLab 2.5) and accompanying .ACAML, .DX, .MFX, .BIN, .RX, .PMX, and .AMX files.

20220718 SBF17_1.zip
20220718 SBF23_2.zip
20230316 SBF_15.zip
20230316 SBF_27.2.zip
230404 SBF 14.1.zip
230404 SBF 2.1.zip
230404 SBF 5.1.zip
230421 SBF 20.1.zip
SBF GC-MS samples.xlsx

In the .Xlsx file, 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