Boston University

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BU Research Data BU Research Data

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Dataset for article: the chemical identification of cochineal production tools in archaeological environments: preservation, degradation, and contamination

https://hdl.handle.net/2144/50791

"Downloaded from OpenBU. Boston University's institutional repository."

Guide to Data

Spreadsheet 1: Experimental Archaeology Data.

1) Sample Information
    a. Samples are vertically clustered into 3 groups: standards/comparative samples, fresh artifacts, and buried artifacts.
2) Raw Computer Data
    a. BPC = Base Peak Chromatogram.
    b. EIC = Extracted Ion Chromatogram.
    c. All numerical data and spectra were collected using Agilent MassHunter software. The images of EIC's of m/z 475, 447, and 457 for samples M1, M4, and M7 were generated using Peaksel due to computer error for those three files.
    d. RT: Retention Time.
3) Anthraquinones only
    a. Data from "Raw Computer Data" that pertains to the molecules carminic acid, dcII, dcIV, dcVII, dcIV – O, dcVII – O, [Carminic acid – CO2], and [Carminic acid – CO2 – 90 Da]. CA = carminic acid.
    b. * = peaks were visible to the human eye but not identified by computer software.
        i. * = peaks were manually identified/measured.
        ii. *--- = peaks were not measured manually.
    c. N.D. = None detected.
    d. I.A. = Integrated Area.
4) Noise Calculations
    a. Due to variation between software programs in S/N calculations, noise was measured manually. A standard method of manually approximating noise, or the standard deviation of the baseline, is to measure the peak-to-peak value of baseline noise over one minute (Wells et al. 2023). To lower error associated with this method, peak-to-peak values were measured at three separate points, then averaged.
        i. N1, N2, N3: First, second, and third peak-to-peak measurement.
        ii. Time N1, Time N2, Time N3: One minute range over which N1, N2, and N3 were measured.
        iii. Noise: Average of N1, N2, and N3.
    b. S/N: Signal (Peak Height)/Noise.
        i. If S/N > 3.3, then it is above the LOD (limit of detection.)
        ii. If S/N > 10, then it is above the LOQ (limit of quantification).
    c. N/A: Not Applicable. Noise was not measured for samples for which no analyte was detected.
5) Data for Use in Article
    a. N.D. = No analyte was detected. This includes those samples for which a peak was identified, but it fell below the limit of detection (<LOD) – i.e., it could not be reliably differentiated from baseline noise.
    b. LOD<x<LOQ = the analyte was detected, but it fell below the limit of quantification; therefore, numerical values for the peak's height and area are not reported.

Spreadsheet 2: Archaeological Artifact Data

1) Artifact Information
2) Lab Data
3) Raw Computer Data
    c. For all samples, EIC's of m/z = 491 amu and 475 amu are reported. Only for samples CT6I and 6A are integration peak lists and EIC's of m/z = 447 amu and 357 amu reported as well.
    d. All numerical data and spectra were collected using Agilent MassHunter software. The image of EIC's of m/z 475 for sample CT3I was generated using Peaksel due to computer error for that file.
4) Data for Use in Article
    a. Noise, S/N, and cutoff values for LOD and LOQ are the same as in Spreadsheet #1.

Wells, G., Harry Prest, and Charles William Rust IV.
2023 Signal, Noise, and Detection Limits in Mass Spectrometry. *Technical Overviews: Chemical Analysis*. Publication Part Number: 5990-7651 EN. Agilent Technologies, Inc.
https://www.agilent.com/cs/library/technicaloverviews/public/5990-7651EN.pdf