

2025

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

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<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 – CO<sub>2</sub>], and [Carminic acid – CO<sub>2</sub> – 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>