Supporting Information for:

Berberine isolation from *Coscinium fenestratum*: optical, electrochemical, and computational studies

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1. TD-DFT calculations of absorption spectra – additional detail

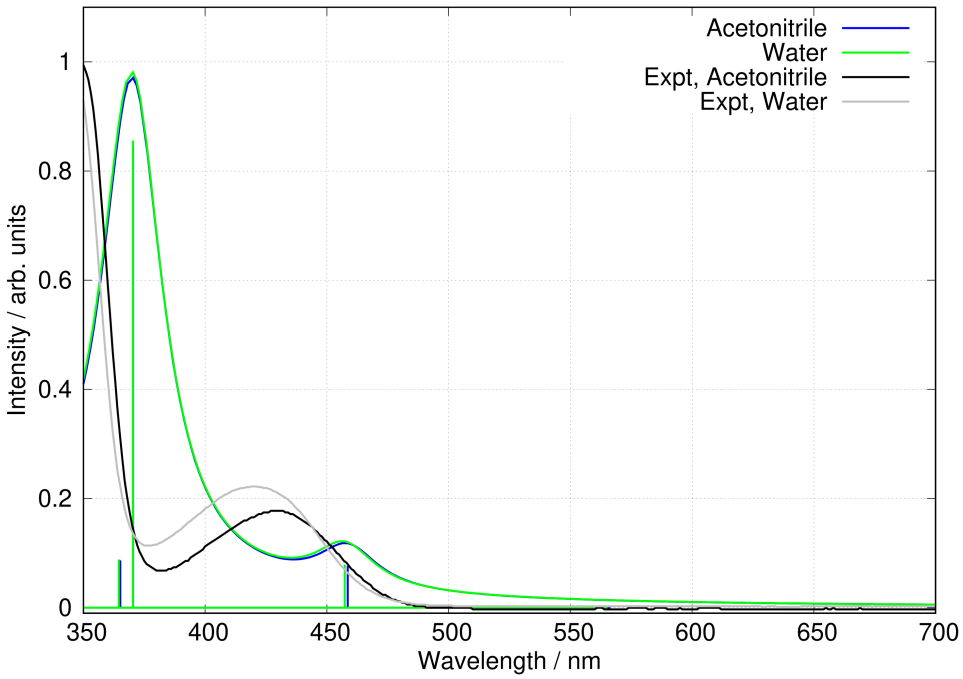

Figure S1: Simulated absorption spectra of the berberine cation in water, acetonitrile, and vacuum. The model chemistry was B3LYP/6-31G(d). The figure presents a zoomed-in region of the spectrum (Fig. 7. main manuscript) showing the $S_0 \rightarrow S_1$ transition more clearly.

2. FTIR Spectra of isolated and commercial berberine

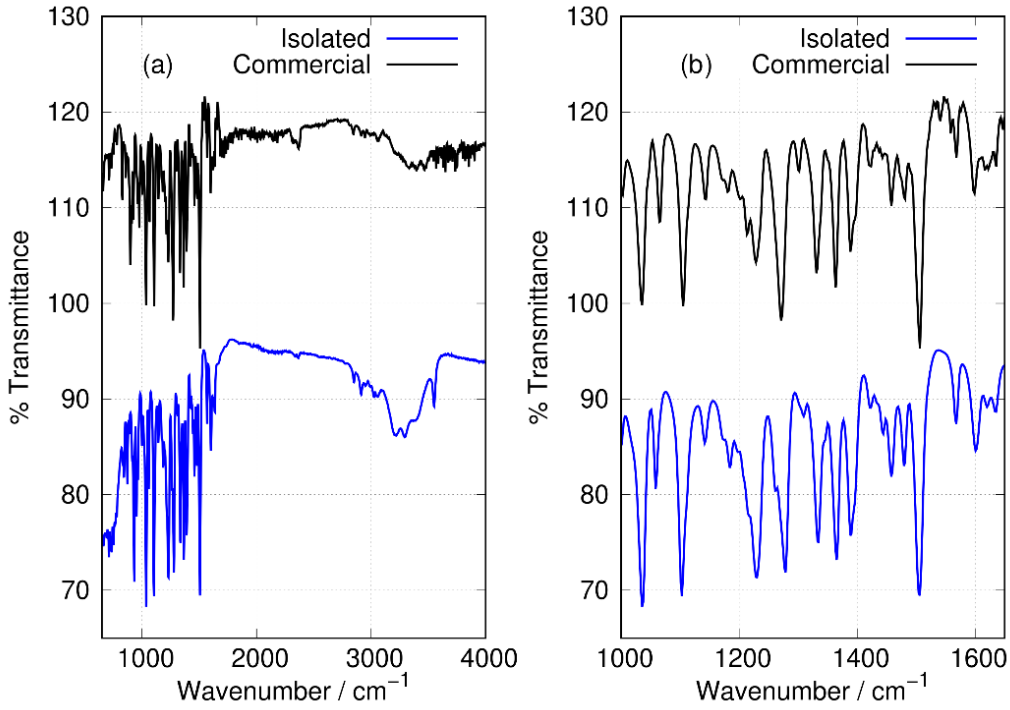

Figure S2: *(a) FTIR spectra of the purified, isolated product and of a commercial sample of berberine chloride. (b) The fingerprint region of the FTIR spectra. The resolution was 4 cm^{-1} in both cases and the spectra are offset on the y-axis for clarity.*

3. SEM Images of crystals of the isolated berberine chloride

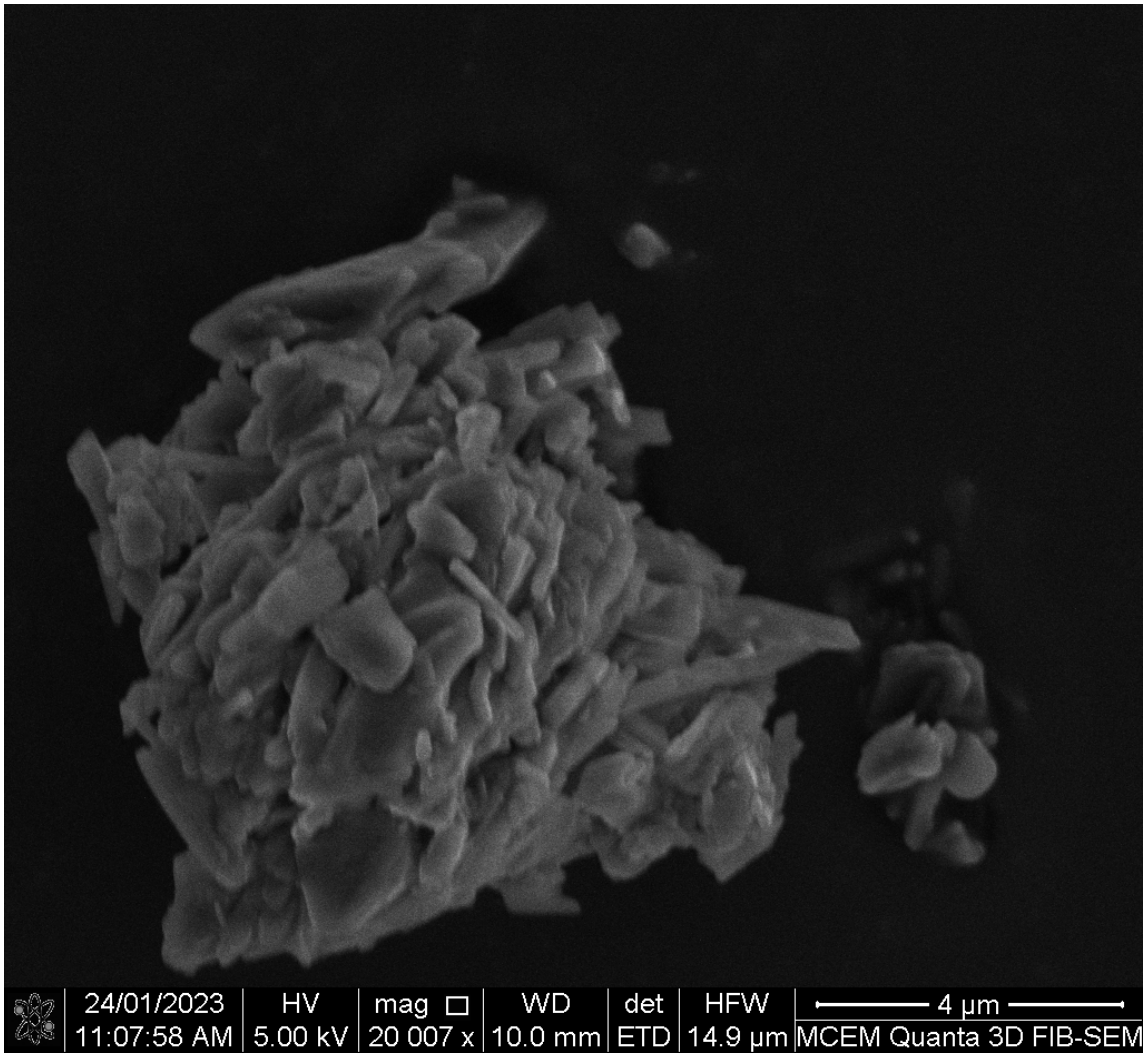

Figure S3: *Electron micrograph of crystals of berberine chloride isolated from Coscinium fenestratum.*

4. Energy dispersive X-ray Analysis of the isolated berberine chloride

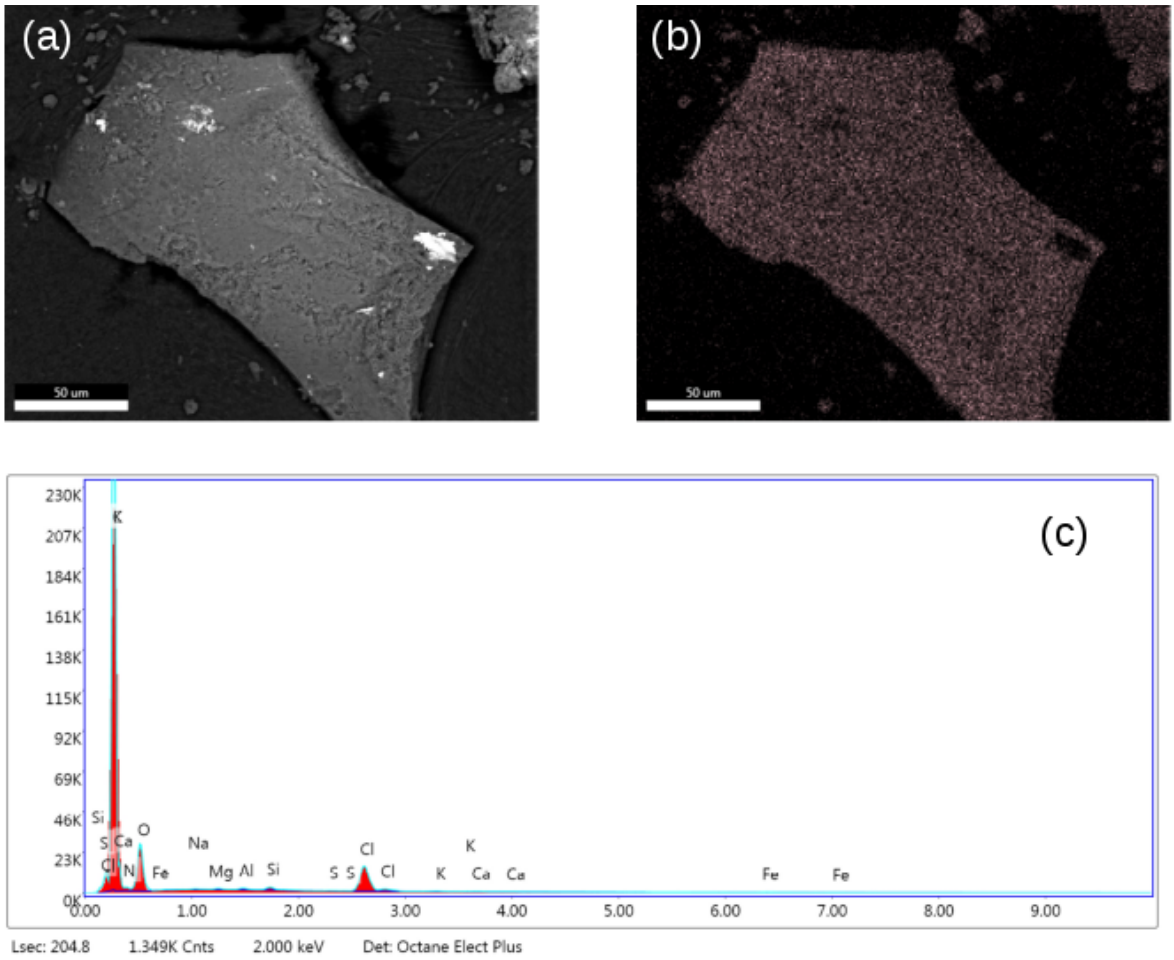

Figure S4: *Electron microscopy and energy-dispersive X-ray spectra of crystals of berberine chloride isolated from Coscinium fenestratum. (a) Electron micrograph of a crystallite. (b) False colour EDX map of Cl Ka and (c) EDX spectrum, Intensity / kcounts against energy. In (a) and (b) the scale bar represents 50 µm.*

These maps and spectra confirm the presence of chloride as the counteranion in the isolated berberine samples.