Supporting Information

Molecular taphonomy of heme: Chemical degradation of hemin under presumed fossilization conditions

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I. ^{1}H-NMR and ^{13}C-NMR spectra of isolated hematinic acid

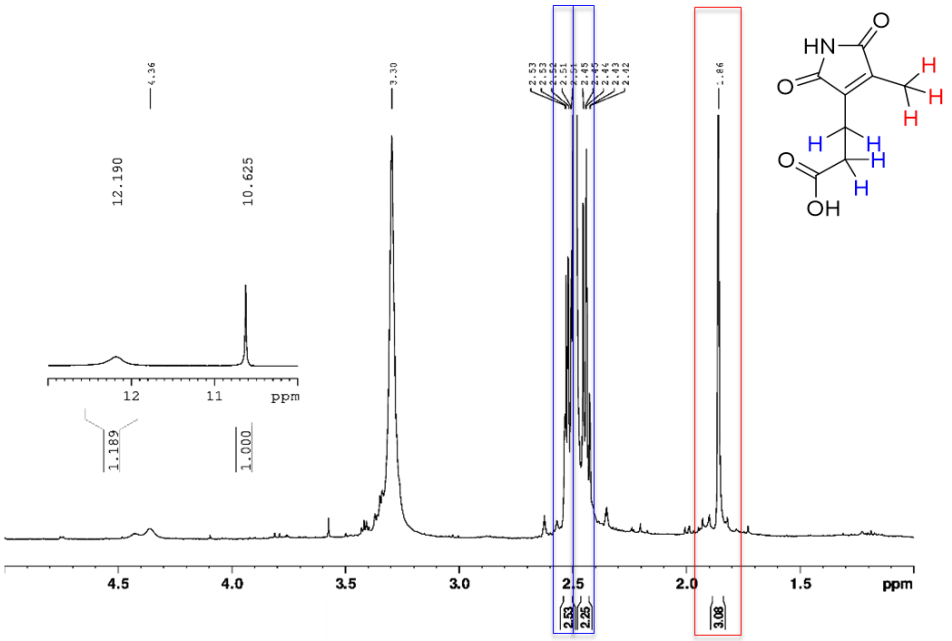

Figure S1. ^{1}H NMR spectrum of isolated hematinic acid determined in DMSO-d_6.

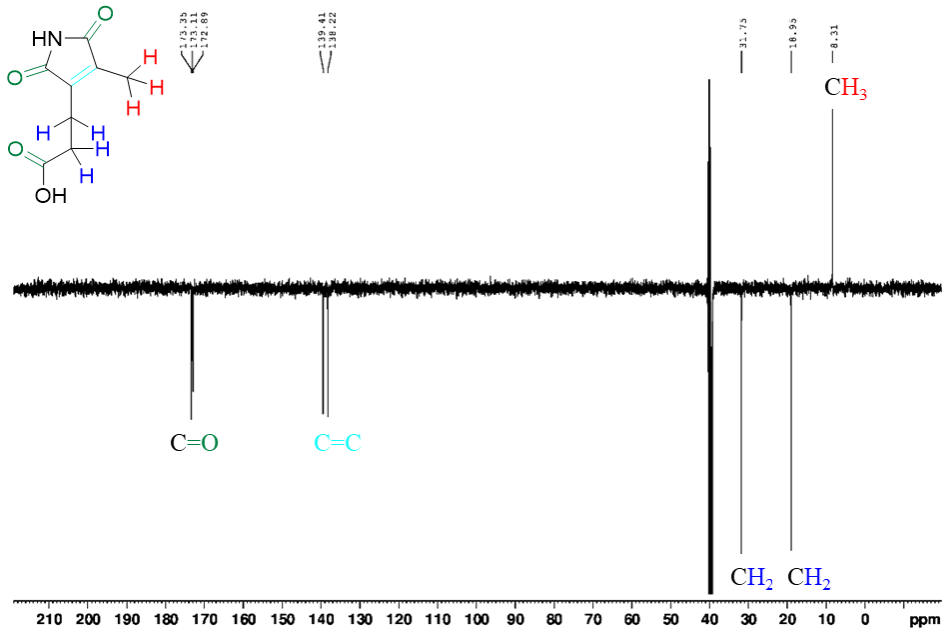

Figure S2. ^{13}C NMR spectrum (attached proton test, APT) of isolated hematinic acid determined in DMSO-d_6.

II. High-resolution mass spectra of isolated hematinic acid

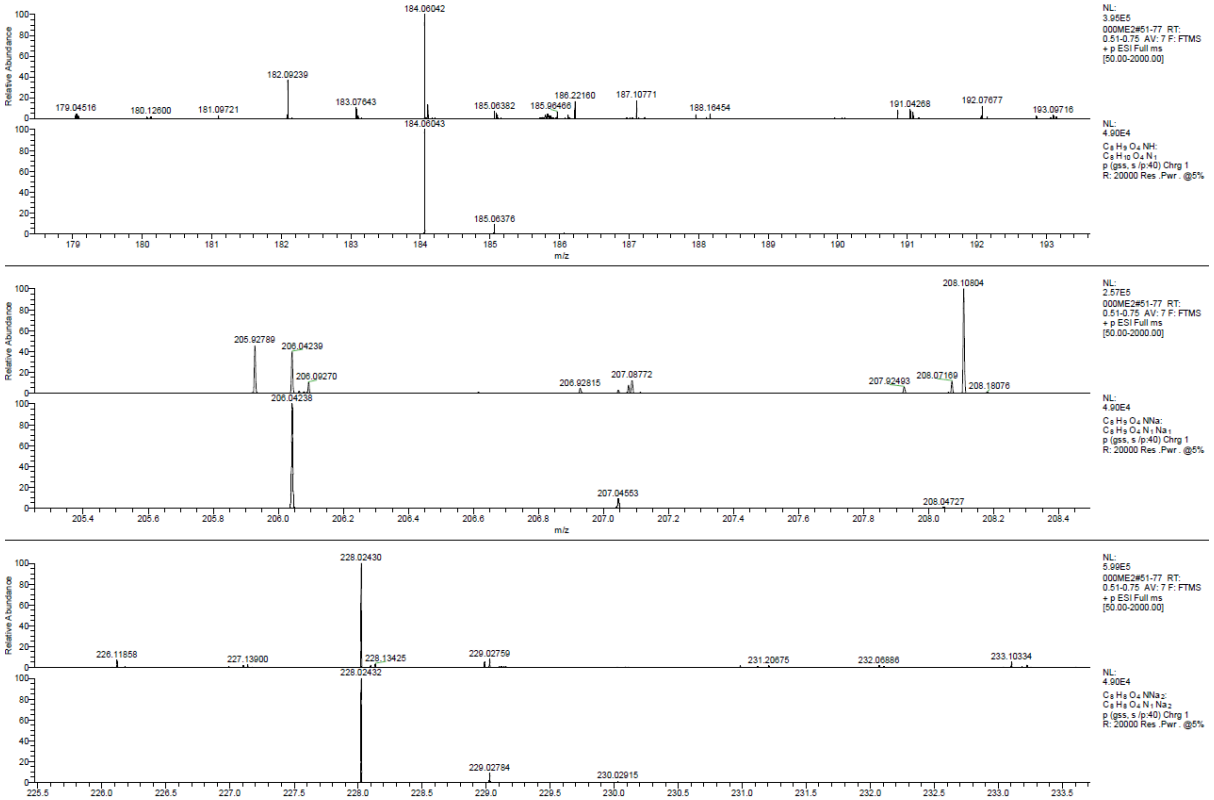

Figure S3. High resolution direct infusion electrospray mass spectra (Orbitrap XL) of isolated hematinic acid showing its molecular ions $[M+H]^+$ at *m/z* 184.06043 (top), $[M+Na]^+$ at *m/z* 206.04239 (top), and $[M+2Na-H]^+$ at *m/z* 228.02430 (bottom). In each case, the measured spectrum is shown above, the calculated one below for comparison.

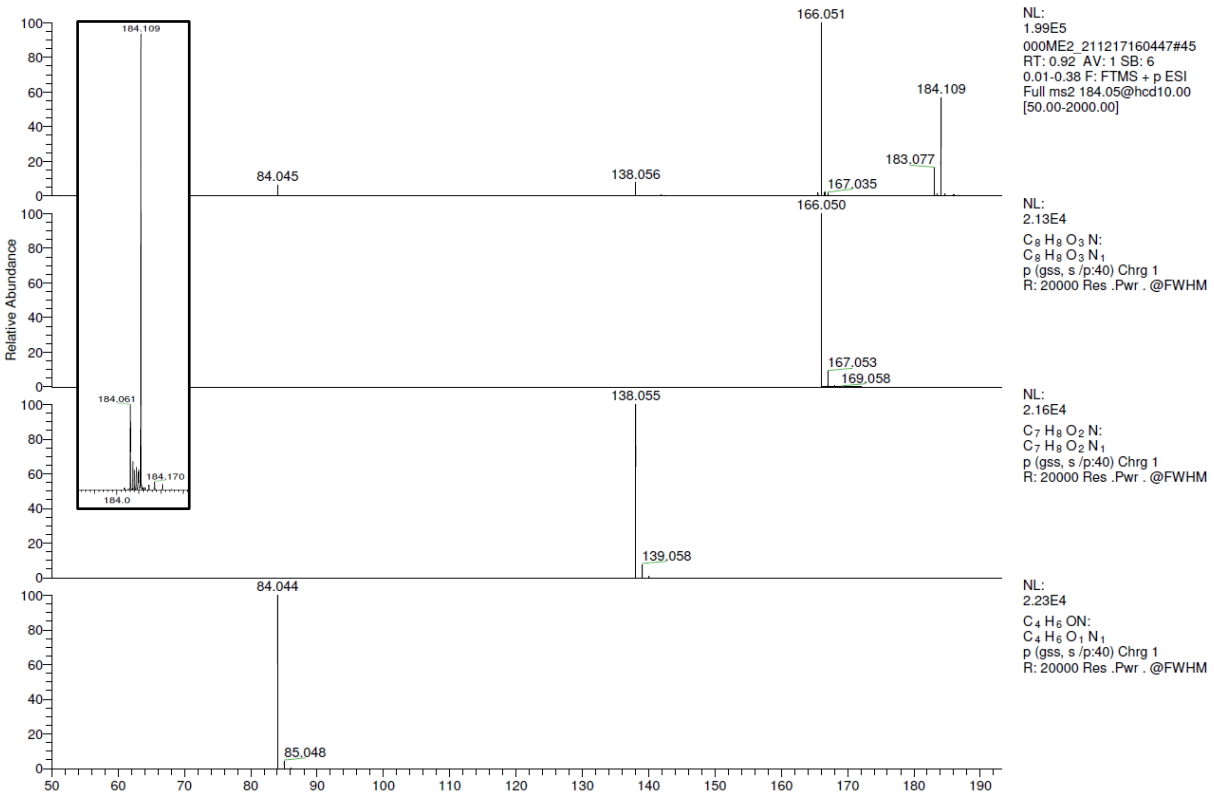

Figure S4. Collision-induced dissociation (CID) high resolution mass spectrum of mass-selected protonated hematinic acid showing its fragmentation pattern starting with consecutive losses of H_2O and CO, calculated spectra for the fragments below for comparison. The inset on the top left shows a zoom into the mass-selected region in the measured CID spectrum. Two signals with *m/z* 184 were present in the original spectrum (see Figure S3 top row), most of the molecular ion of hematinic acid (*m/z* 184.061) was fragmented by CID.