Electronic Supplementary Information

Applying multivariate analysis to x-ray diffraction computed tomography: the study of medieval applied brocades.

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Figure S1: Pietà (MON), castle of Montrottier in Lovagny (Haute-Savoie, France), circa 1500, H. 57; l.64; d.20 cm. The locations and denominations of the microsamples are noted in red.



Figure S2: XRF spectrum obtained by summing all measured spectra. The intensity is on a logarithmic scale. The main fluorescence lines are indicated.



Figure S3: Results of the Search-Match phase identification for sample S157-layer02 using the EVA software. Top: full pattern, bottom: zoom on the low angle part.



Figure S4: comparison of the experimental sum data with the reconstructed sum pattern after MCR-ALS decomposition using 9 (top) or 6 (center) components and after NMF decomposition with 6 components (bottom). Blue circles: experimental pattern, orange line: calculated, green line: difference (shifted by -10% of the maximum).



Figure S5: The components found by MCR-ALS for the 9 components case. Components 0 to 8 from left to right and top to bottom. For each component are shown from left to right the component pattern, the sinogram and tomographic reconstruction of the component concentration.



Figure S6: The components found by MCR-ALS for the 6 components case. Components 0 to 5 from

left to right and top to bottom. For each component are shown from left to right the component pattern, the sinogram and tomographic reconstruction of the component concentration.



Figure S7: Part of the patterns for component 1 and 4 found by MCR-ALS with 9 components. All peaks can be indexed as gypsum. A 2 θ -dependent shift is clearly visible, which can be attributed to a displacement of the diffraction center.



Figure S8: The components found by NMF for the 6 components case. Components 0 to 5 from left to right and top to bottom. For each component are shown from left to right the component pattern, the sinogram and tomographic reconstruction of the component concentration.



Figure S9: Results of the Search-Match phase identification for sample S157-layer02 using the EVA software, for the 6 components found by NMF.



Figure S10: Tomographic reconstruction of the concentrations of the 11 phases obtained by supervised MCR-ALS analysis. From left to right and top to bottom: gypsum, cinnabar, beeswax, romarchite, cassiterite, cerussite, hydrocerussite, gold, chlorargyrite, goethite, minium. The approximate sample shape is shown as a grey line.