SUPPLEMENTARY MATERIAL

Infrared Spectroscopic and Chemometric Approach for Identifying Binding Medium in Sukias mansion’s Wall Paintings

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This paper addresses the application of infrared spectroscopy in combination with chemometrics to identify wall painting’s binding medium while employing pattern recognition techniques to process FTIR dataset of complex samples. In this regard, based on the historical documents and previous researches, firstly 56 standard samples were prepared to represent strata of Persian wall paintings in the safavid period in addition to real historic samples from the case study; Sukias mansion. Then, each sample was analyzed by the means of FTIR and chemometrics. Finally SIMCA was applied to the whole region of studied IR spectra which predicted egg yolk as binding medium of Sukias mansion samples.

Keywords: Binding medium, Chemometrics, FTIR, Persian wall painting, safavid period

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Table S1. FTIR characteristic bands of standard samples materials (Derrick et al. 2000; Stuart 2004; Stuart 2007)

| Binding medium | Vibrational wavenumber (cm\(^{-1}\)) | Description Assignment |
|----------------|---------------------------------------|------------------------|
| Gum Arabic     | 1300-900                              | C–O stretching band    |
|                | 1480-1300                             | C–H bending band       |
|                | 1650                                  | O–H bending band       |
|                | 3000-2800                             | CH\(_2\) asymmetric stretching band |
|                | 3600-3200                             | O–H stretching band of carbohydrates |
| Linseed Oil    | 1378, 1460                            | CH\(_3\) asymmetric bending band |
|                | 1750-1740                             | C=O stretching band    |
|                | 2850, 2930                            | CH\(_2\) asymmetric stretching band |
|                | 3020                                  | =C–H stretching band   |
| Egg Yolk       | 1450                                  | C–N bending band       |
|                | 1550                                  | 60% N–H bending band; 40% C–N stretching band |
|                | 1650                                  | 80% C=O stretching band; 10% C–N stretching band; 10% N–H bending band |
|                | 2850, 2930                            | CH\(_2\) asymmetric stretching band |
|                | 3110, 3300                            | N–H stretching band in resonance with overtone (2 × amide II) |
| Indigo         | 1620-1420                             | Aromatic bands        |
|                | 1700-1550                             | C=O stretching band    |
|                | 3100-2800                             | C–H stretching band    |
| Binding medium | Vibrational wavenumber (cm⁻¹) | Description Assignment |
|----------------|-------------------------------|------------------------|
| Chalk          | 910-850                       | O–C–O bending band     |
|                | 1490-1370                     | CO₃²⁻ stretching band  |
| White Lead     | 693–683                       | Bending bands          |
|                | 1047–1045                     | O–H bending band       |
|                | 1400                          | C=O stretching band    |
|                | 3535–3530                     | O–H band               |

Table S1. (Continued)

| Binding medium   | Vibrational wavenumber (cm⁻¹) | Description Assignment |
|------------------|-------------------------------|------------------------|
| Gypsum           | ~620                          | SO₄²⁻ bending band     |
|                  | 1140-1080                     | asymmetric SO₄²⁻ stretching band |
|                  | 3700-3200                     | asymmetric and symmetric O–H stretching band |
| Ultramarine Blue | 800-400                       | bending bands          |
|                  | 1150-950                      | overlapping stretching bands for Si–O–Si and Si–O–Al |
| Red Ochre        | 800-400                       | bending bands          |
|                  | 1200-1050                     | overlapping stretching bands for Si–O–Si band |

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