

A Royal Mystery: a Multianalytical Approach for Dyestuff Identification in Seventeenth Century Waistcoats

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Supplementary Materials

Table S1: HPLC-ESI-Q-Orbitrap-MS sample dye analysis

Sample	Compound	[M-H] ⁻ (m/z)	[M-H] ⁺ (m/z)	MS ² (m/z)
London Museum silk (A27050)	Animal and/or microbial contamination*	202.08	-	-
Drummond Castle silk (DC001)	4-hydroxybenzoic acid	137.03	-	93.05
	Daphnetin	179.01	-	133.05
Drummond Castle silk (DC004)	4-hydroxybenzoic acid	137.03	-	93.05
	Daphnetin	179.01	-	133.05

* m/z signal may be related with animal and/or microbial contamination:

a) m/z 202.07 or 202.08 – D-glucosamine+Na⁺

D-glucosamine (D-GlcN) is an amino sugar and a prominent precursor in the biochemical synthesis of glycosylated proteins and lipids.

Reference: Shaala L.A., Asfour H.Z., Youssef D.T.A., Zóltowska-Aksamitowska S., Wysokowski M., Tsurkan M., Galli R., Meissner, H., Petrenko I., Tabachnick K., Ivanenko V.N., Bechmann N., Muzychka L.V., Smolii O.B., Martinovic' R., Joseph Y., Jesionowski T. and Ehrlich H., New Source of 3D Chitin Scaffolds: The Red Sea Demosponge *Pseudoceratina arabica* (Pseudoceratinidae, Verongiida). *Mar. Drugs* **2019**, 17, 92.

b) m/z 202.07 or 202.08 – (b1,3)- linked GlcNAc residue

c) Acetylglucosamine (GlcNAc) is an amide derivative of the glucose. It is part of a biopolymer in the bacterial cell wall. GlcNAc is the monomeric unit of the polymer chitin, which forms the exoskeletons of arthropods like insects and crustaceans.

Reference: Seymour J.L., Costello C.E. and Zaia J., The Influence of Sialylation on Glycan Negative Ion Dissociation and Energetics. J. Am. Soc. Mass Spectrom. **2006**, 17, 844–854.