Supplemental

Liquid Chromatography-Mass Spectrometry (LC-MS) analysis of dyes formed by in situ oxidative methods then purified by absorption and extraction from hair wefts

M. John Plater* and Andrea Raab, Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen, AB24 3UE, UK

*Correspondence to m.j.plater@abdn.ac.uk

G1 = Gradient 1
G2 = Gradient 2

File 1
Figure S 17 Chart 2 G1 Bandrowski’s base 2
Figure S 18 Chart 3 G1 Bandrowski’s base 2
Figure S 19 Chart 4 G1 Bandrowski’s base 2

File 2
Figure S 20 Chart 1 G2 Bandrowski’s base 2
Figure S 21 Chart 2 G2 Bandrowski’s base 2
Figure S 22 Chart 3 G2 Bandrowski’s base 2
Figure S 23 Chart 4 G2 Bandrowski’s base 2

File 3
Figure S 24 Chart 1 G2 Honey Blonde
Figure S 25 Chart 2 G2 Honey Blonde
Figure S 26 Chart 3 G2 Honey Blonde
Figure S 27 Chart 4 G2 Honey Blonde

File 4
Figure S 28 Chart 1 G2 Light Brown Warm
Figure S 29 Chart 2 G2 Light Brown Warm
Figure S 30 Chart 3 G2 Light Brown Warm
Figure S 31 Chart 4 G2 Light Brown Warm

File 5
Figure S 32 Chart 1 G2 Dark Brown
Figure S 33 Chart 2 G2 Dark Brown
Figure S 34 Chart 3 G2 Dark Brown
Figure S 35 Chart 4 G2 Dark Brown
Figure S 17 Chart 2 G1 Bandrowski’s base (WIRZEC) 2

Figure S 18 Chart 3 G1 Bandrowski’s base (WIRZEC) 2
Figure S 19 Chart 4 G1 Bandrowski’s base (WIRZEC) 2

Figure S 20 Chart 1 G2 Bandrowski’s base (WIRZEC) 2
**Figure S 21** Chart 2 G2 Bandrowski’s base (WIRZEC) 2

**Figure S 22** Chart 3 G2 Bandrowski’s base (WIRZEC) 2
Figure S 23 Chart 4 G2 Bandrowski’s base (WIRZEC) 2
Figure S 24 Chart 1 G2 Honey Blonde

Figure S 25 Chart 2 G2 Honey Blonde
Figure S 26 Chart 3 G2 Honey Blonde

Figure 4

Figure S 27 Chart 4 G2 Honey Blonde
Figure S 28 Chart 1 G2 Light Brown Warm

Figure S 29 Chart 2 G2 Light Brown Warm
Figure S 30 Chart 3 G2 Light Brown Warm

Figure S 31 Chart 4 G2 Light Brown Warm
Figure S 32 Chart 1 G2 Dark Brown

Figure S 33 Chart 2 G2 Dark Brown
**Figure S 34 Chart 3 G2 Dark Brown**

**Figure S 35 Chart 4 G2 Dark Brown**
Cetylpyridinium chloride 1S (Figure S25, S29 and S33) (red trace) (M + H, 304.2998, Calc 304.2998); Linolenyltrimethylammonium chloride 2S (Figure S33) (grey trace) (M + H, 306.3155, Calc 306.3155); Linoleyltrimethylammonium chloride 3S (Figure S33) (green trace) (M + H, 308.3313, Calc 308.3312); Oleyltrimethylammonium chloride 4S (Figure S33) (grey trace) (M + H, 310.3468, Calc 310.3468); Docosyltrimethylammonium chloride 5S (Figure S35) (light blue trace) (M + H, 368.4252, Calc 368.4251); Didodecyltrimethylammonium chloride 6S (Figure S27, S31 and S35) (brown trace) (M + H, 382.4408, Calc 382.4407).

| Compound | Quaternary ammonium salts identified from the LC-MS analyses | Accurate mass | Calculated mass |
|----------|-------------------------------------------------------------|---------------|-----------------|
| 1S       | ![Cetylpyridinium chloride](chemical_formula_1S.png)        | 304.2998 (M+) | 304.2998 (M+)   |
| 2S       | ![Linolenyltrimethylammonium chloride](chemical_formula_2S.png) | 306.3155 (M+) | 306.3155 (M+)   |
| 3S       | ![Linoleyltrimethylammonium chloride](chemical_formula_3S.png) | 308.3313 (M+) | 308.3312 (M+)   |
| 4S       | ![Oleyltrimethylammonium chloride](chemical_formula_4S.png) | 310.3468 (M+) | 310.3468 (M+)   |
| 5S       | ![Docosyltrimethylammonium chloride](chemical_formula_5S.png) | 368.4252 (M+) | 368.4251 (M+)   |
| 6S       | ![Didodecyltrimethylammonium chloride](chemical_formula_6S.png) | 382.4408 (M+) | 382.4407 (M+)   |
| Chemical Formula: $C_{26}H_{56}NCl$ |
|-----------------------------------|
| Didodecyldimethylammonium chloride |

**Table 1S** Quaternary ammonium salts identified by LC-MS analysis of coloured hair wefts extracted with dichloromethane:trifluoroacetic acid (75:25).