

Supporting Information For:

Screening of Cosmetic Ingredients from Authentic Formulations and Environmental Samples with Desorption Electrospray Ionization Mass Spectrometry

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<u>Table of Contents</u>	<u>Page</u>
<i>Figure S-1. Structures for Target Cosmetic Analytes</i>	2
<i>Figure S-2. Negative-Ion DESI-MS of Clearasil[®] Acne Treatment Cream</i>	3
<i>Figure S-3. Positive-Ion Thermally-Assisted DESI-MS of Clearasil[®] Acne Treatment Cream Dissolved in Water</i>	4
<i>Table S-1. Ingredients List for Clearasil[®] Acne Treatment Cream</i>	5
<i>Table S-2. Ingredients List for L’Oreal[®] Superior Preference[®] Preference[®] les True Brunettes Color Gel</i>	6
<i>References</i>	7

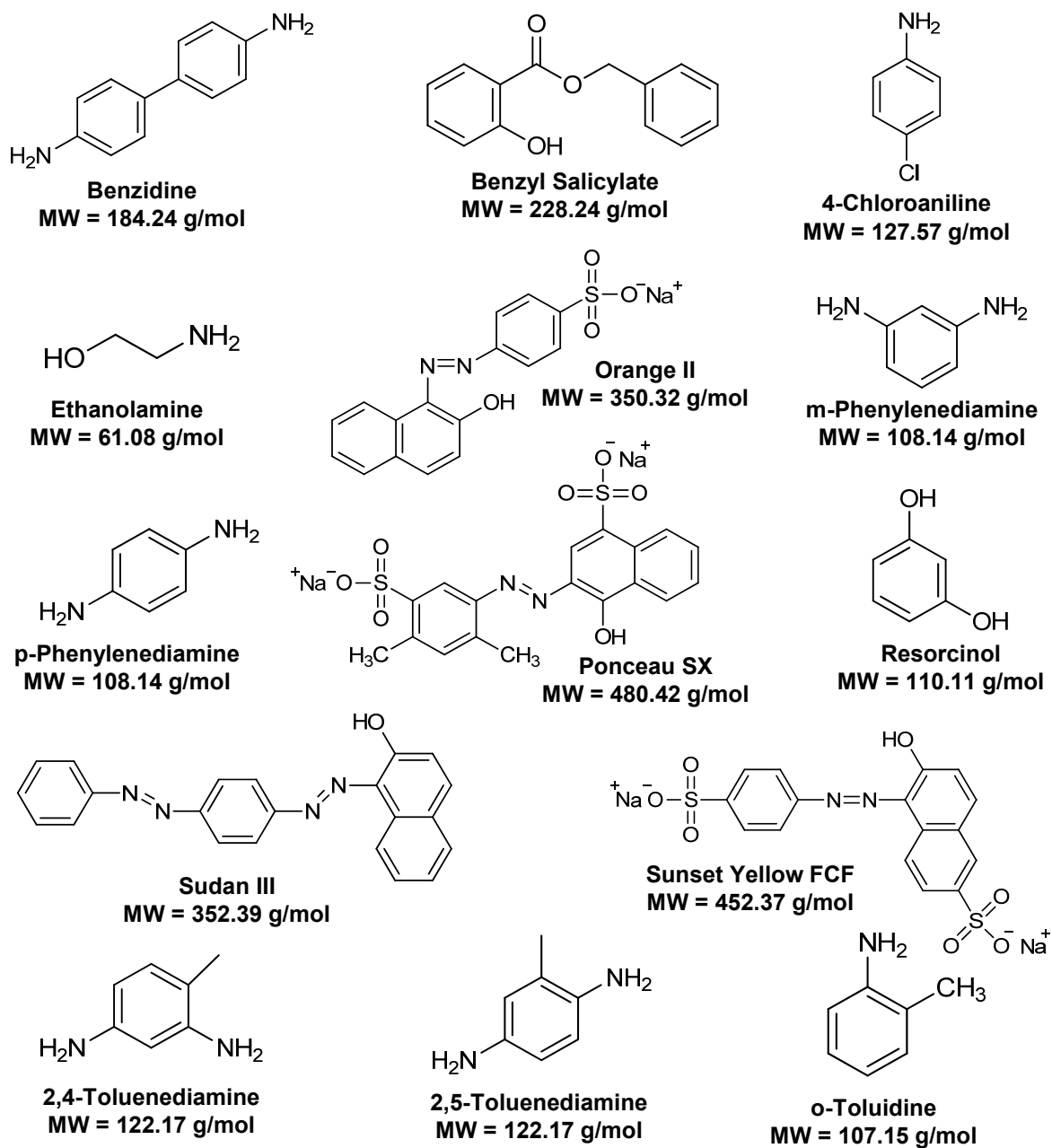


Figure S-1. Structures for target cosmetic analytes

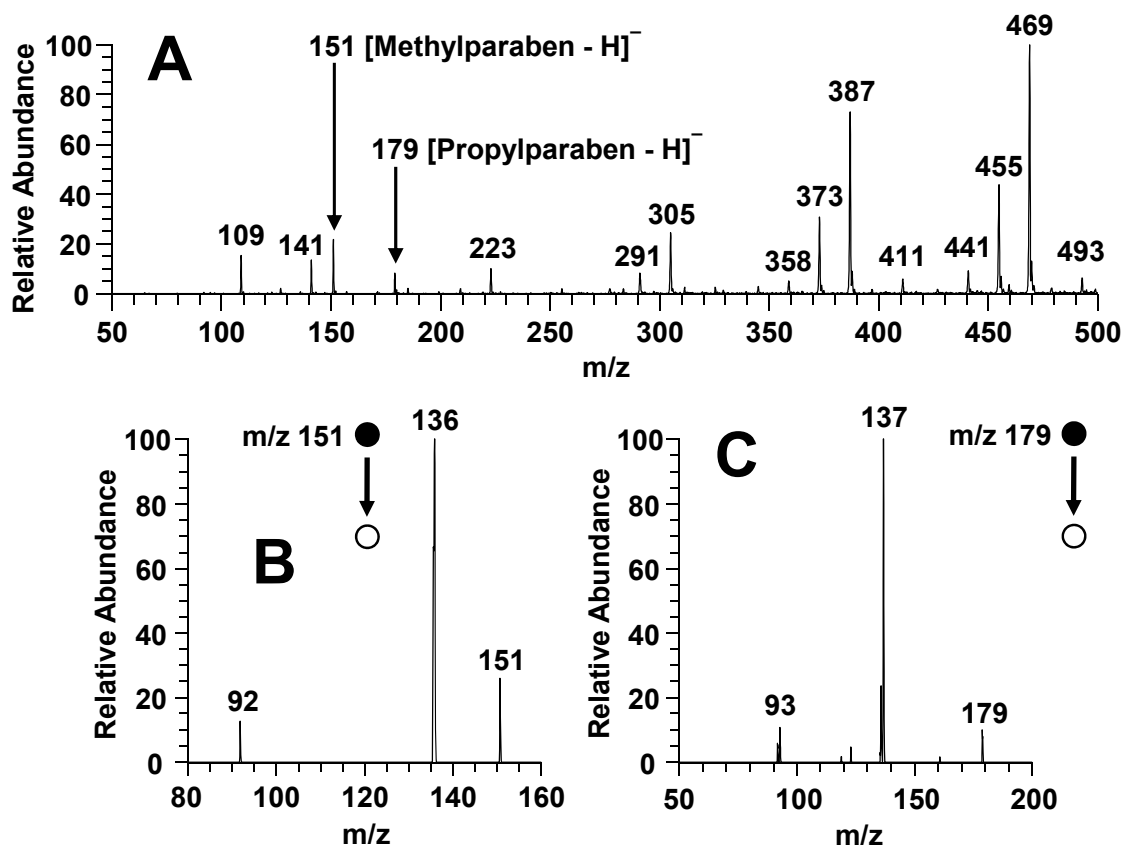


Figure S-2. (a) Negative-ion DESI mass spectrum of Clearasil[®] Adult Tinted Acne Treatment Cream, showing the deprotonated methylparaben at m/z 151 and deprotonated propylparaben m/z at 179. (b) MS² of the m/z 151 precursor gives the major transitions at m/z 136 and 92, corresponding to the loss of a methyl group and a C₂H₃O₂ moiety, respectively. (c) MS² of the m/z 179 precursor gives the major transitions at m/z 137 (loss of propene) and at m/z 93, corresponding to the loss of C₄H₆O₂ to leave the deprotonated phenol ion. Generated spectra were similar to that reported in literature.¹

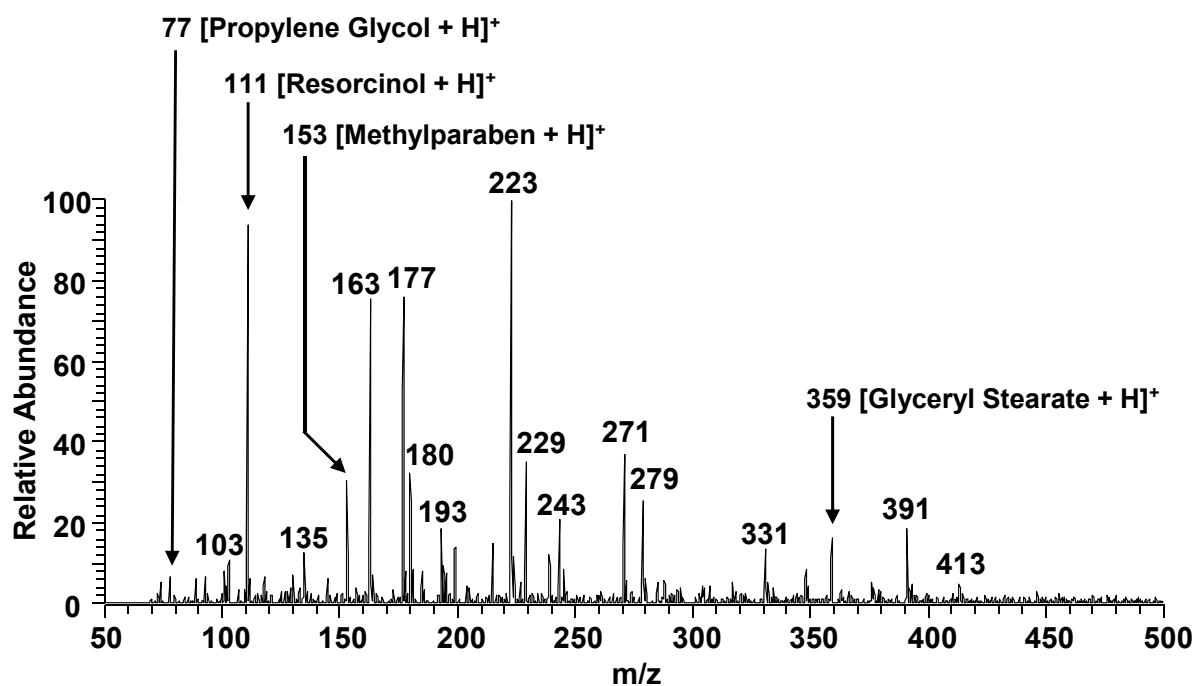


Figure S-3. Positive-ion thermally-assisted DESI mass spectrum of Clearasil[®] Adult Tinted Acne Treatment Cream dissolved in tap water. For this experiment, 5.5 mg of the composition was dissolved in tap water and directly analyzed (final concentration of active ingredient resorcinol was approx. 1.1 ppm). The ingredients propylene glycol, resorcinol, methylparaben, and glyceryl stearate can be seen as protonated molecules at m/z 77, 111, 153, and 359, respectively. Interestingly, data obtained on the dissolved face cream with thermal assistance yielded similar results to that obtained from surface residues with traditional DESI-MS. Spectral peaks for resorcinol and other ions at low m/z values are seen with increased intensity under thermal assistance.

Table S-1. Cosmetic Ingredients List for Clearasil[®] Adult Tinted Acne Treatment Cream

Ingredients
<i>Actives</i>
Resorcinol 2%
Sulfur 8%
<i>Inactives</i>
Water
Alcohol Denat.
Bentonite
Glyceryl Stearate SE
Propylene Glycol
Isopropyl Myristate
Fragrance
Simethicone
Methylparaben
Propylparaben
Titanium Dioxide
Iron Oxides

Table S-2. Cosmetic Ingredients List for L'Oreal® Superior Preference® True Brunettes Color Gel

Ingredients: Color Gel
Oleic Acid
Water
Cocamide Mipa
Octyldodecanol
Benzyl Alcohol
Alcohol Denat.
Ethanolamine
Ammonium Hydroxide
Oleth-30
Hexadimethrine Chloride
Mea-Laureth Sulfate
Parfum/fragrance
Sodium Metabisulfite
Isopropanolamine
EDTA
Resorcinol
Erythorbic Acid
p-Phenylenediamine
2,4-Diaminophenoxyethanol HCl
Alpha-Isomethyl Ionone
Eugenol
m-Aminophenol
Linalool
Citronellol
Hydroxypropyl Bis(N-Hydroxy- Ethyl-P-Phenylenediamine) HCl

References

1. A. Peck, Analytical methods for the determination of persistent ingredients of personal care products in environmental matrices, *Anal Bioanal Chem*, 2006, **386**, 907-939.