

**SUPPLEMENTARY INFORMATION - USE OF PLASTIC-BASED
ANALYTICAL DEVICE, SMARTPHONE AND CHEMOMETRIC
TOOLS TO DISCRIMINATE AMINES**

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Chemicals, materials and instrumentation

Triethylamine, isobutylamine, isopentylamine, putrescine, tyramine, cadaverine, cellulose acetate, acetone, bromophenol blue, thymol blue, chlorophenol red, alizarin, methyl red and polyoxyethylenesorbitan monolaurate (Tween® 20) were all purchased from Sigma-Aldrich (Poole, UK). The photographs of membranes were taken with the built-in camera of an Apple iPhone 4S. Additionally, a closed chamber was fabricated using black poly(methyl methacrylate) to control the light conditions during image acquisition and to fix the focal distance. The PMMA structure was designed using CorelDraw X6 software (Corel Corporation, Ottawa, Canada) and was cut using a gravograph laser cutter machine (Gravograph, La Chapelle St Luc, France). The light was produced by four white LEDs passed through a series of transparent sandblasted poly(methyl methacrylate) sheets to optimize the distribution of light over the sample. More information about the support schematics with the dimensions and photographs of the support with the smartphone can be found in our previously published article¹.

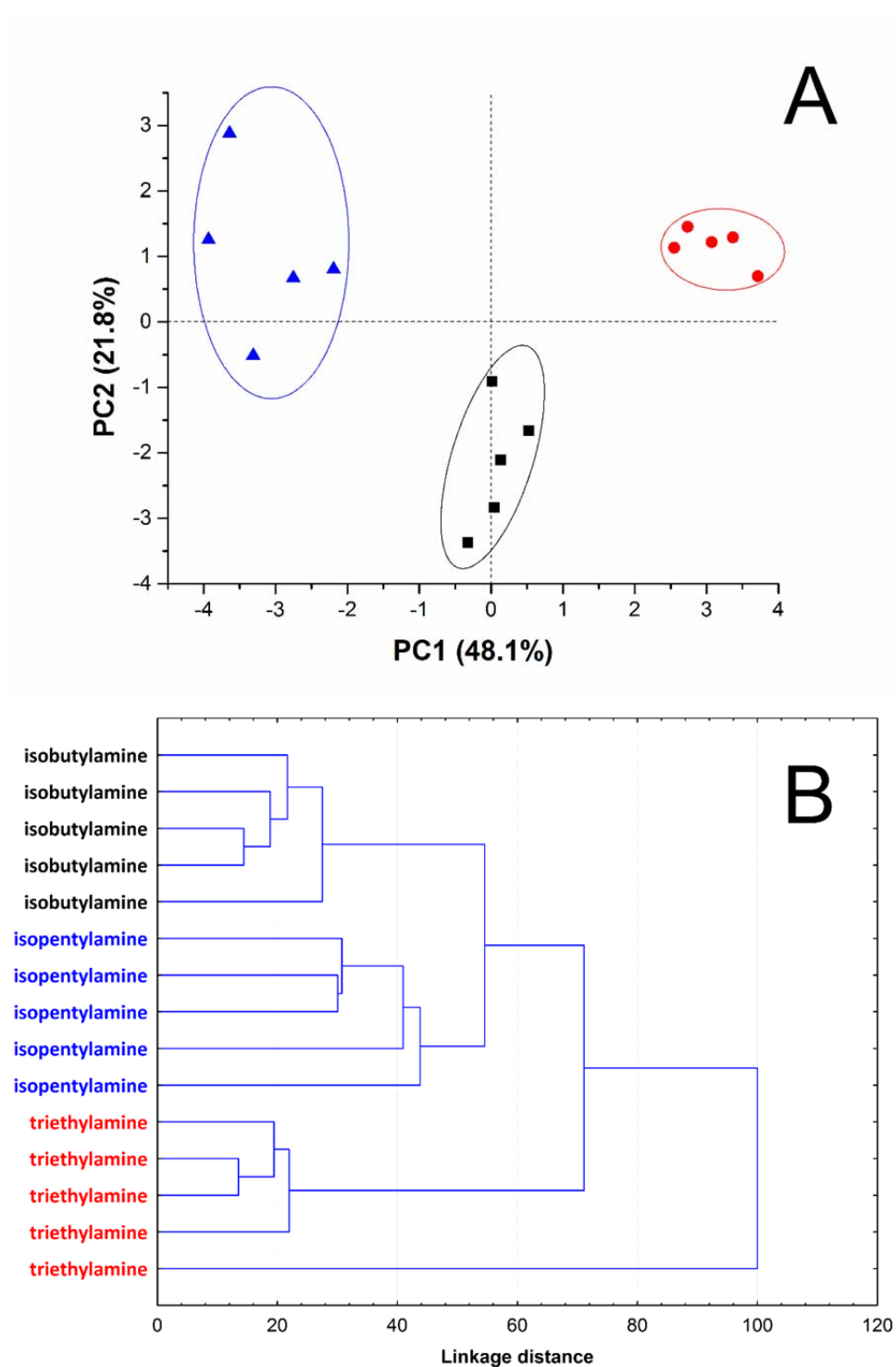


Figure S1 – PCA scores plot obtained from the RGB values extracted from the coloured membranes with 5 pH indicators in contact with three different amines (■ – isobutylamine; ● – triethylamine and ▲ – isopentylamine) at a concentration of 2.5 ppm. (B) HCA plot.

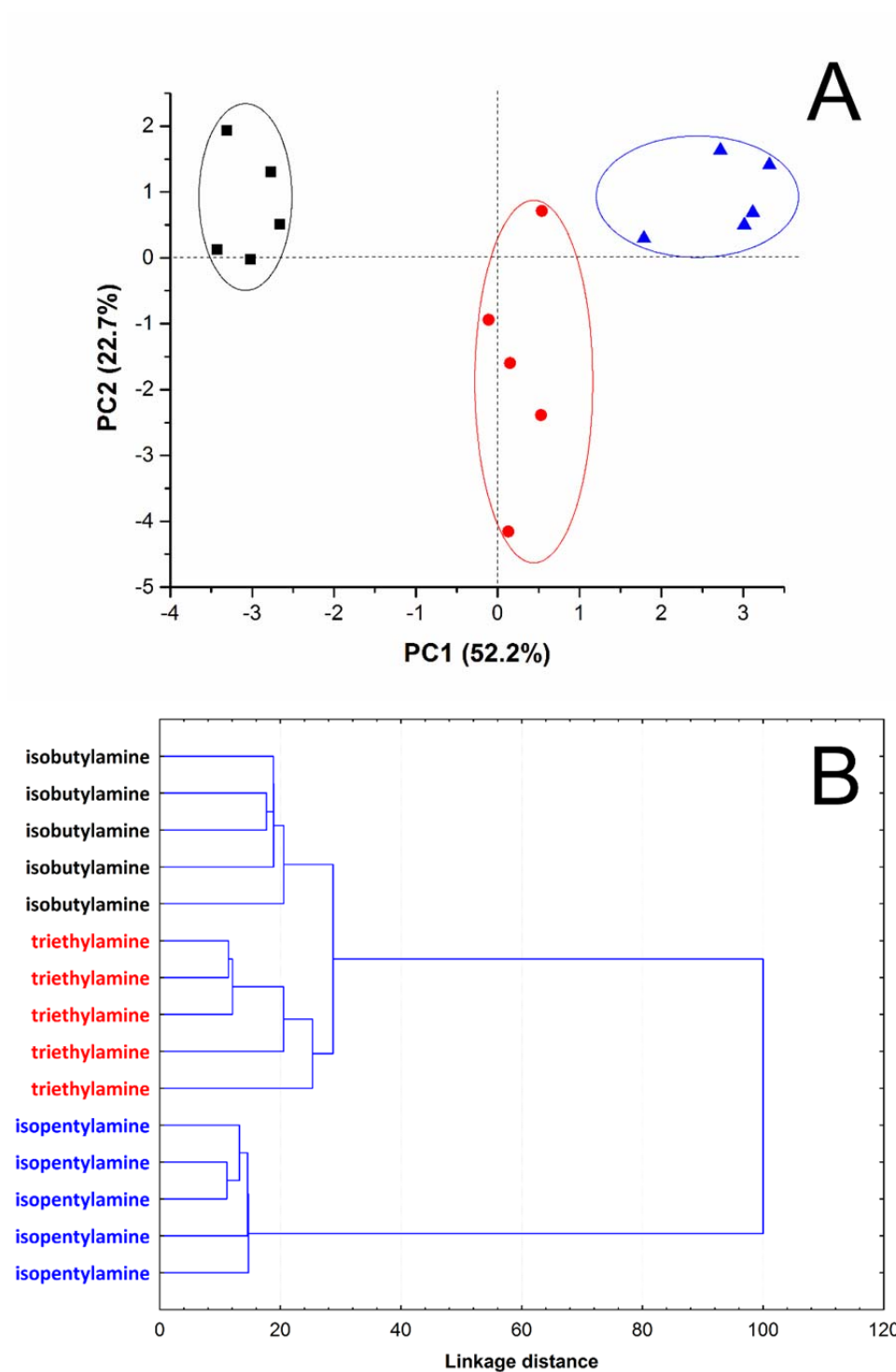


Figure S2 – PCA scores plot obtained from the RGB values extracted from the coloured membranes with 5 pH indicators in contact with three different amines (■ – isobutylamine; ● – triethylamine and ▲ – isopentylamine) at a concentration of 1.0 ppm. (B) HCA plot.

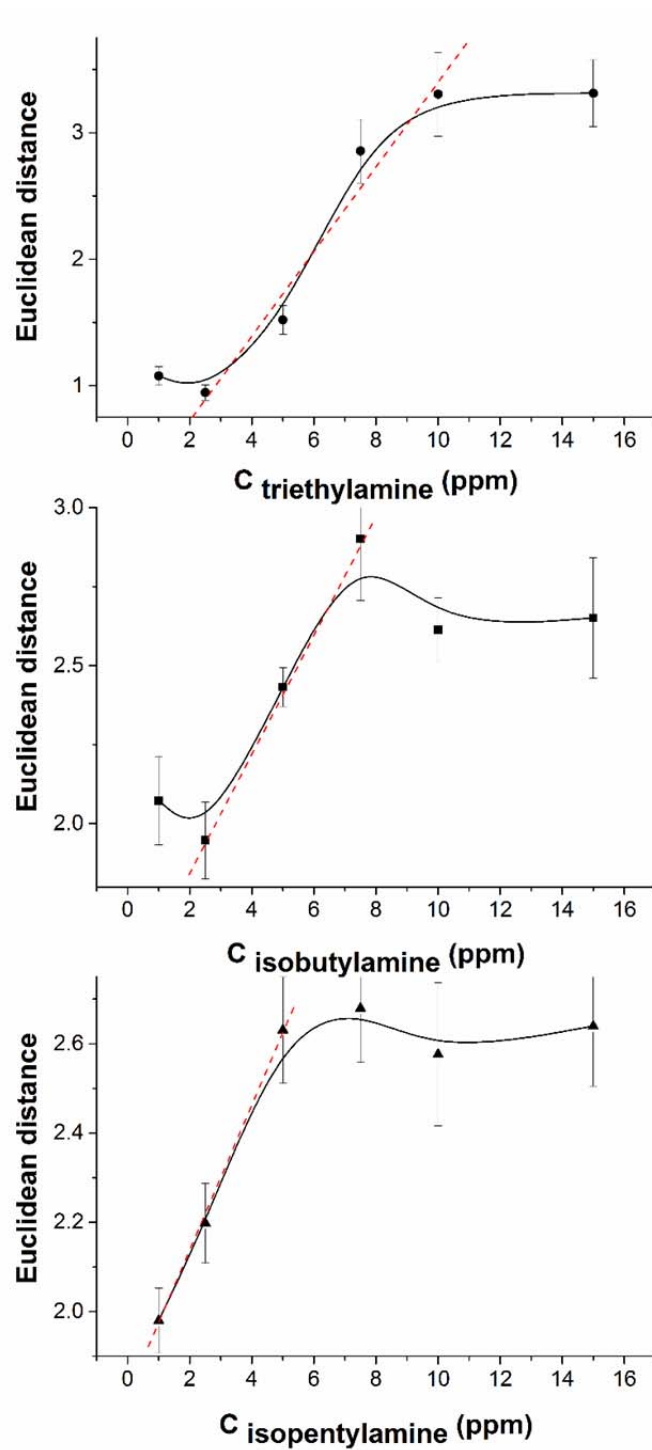


Figure S3 - Calibration curves obtained for the amines using the Euclidean distance (ED) of the RGB values versus concentration. Legend: (■ – isobutylamine; ● – triethylamine and ▲ – isopentylamine). Linear Regression: $ED = 1.47 + 0.19 C_{\text{isobutylamine}}$, $R^2 = 0.99995$; $ED = 0.051 + 0.34 C_{\text{triethylamine}}$, $R^2 = 0.98092$ and $ED = 1.47 + 0.19 C_{\text{isopentylamine}}$, $R^2 = 0.99995$. Number of replicates = 3.

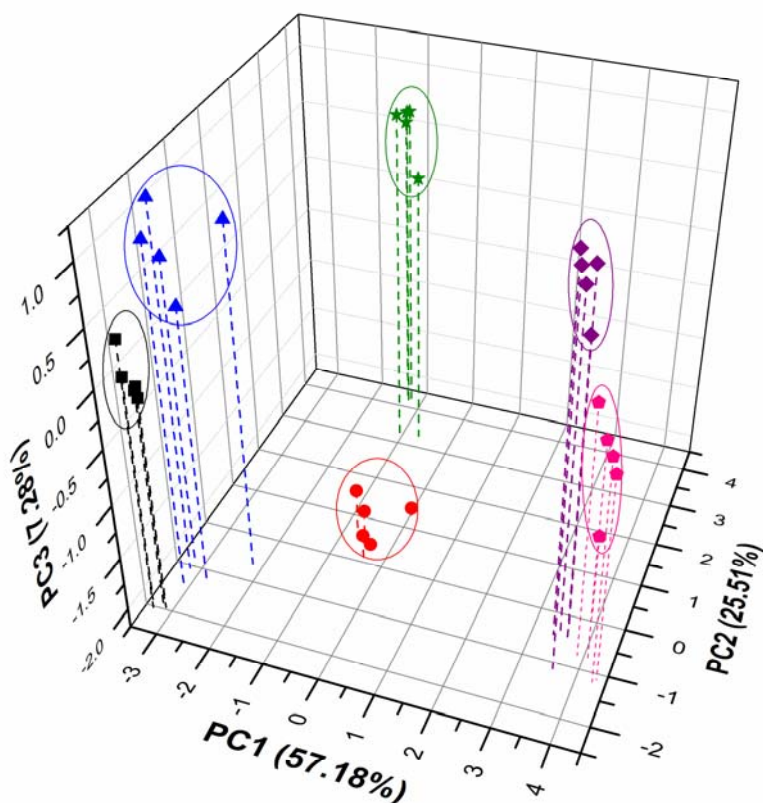


Figure S4 – PCA scores plot obtained from the RGB values extracted from the coloured membranes with 5 pH indicators in contact with all amines studied (◆ – tyramine; ★ – putrescine, ◆ – cadaverine, ■ – isobutylamine; ● – triethylamine and ▲ – isopentylamine) at a concentration of 5 ppm for the isobutylamine, triethylamine and isopentylamine and 65 µg tyramine, 3.6 mg of putrescine and 87 µg cadaverine.

References

1. M. O. Salles, G. N. Meloni, W. R. de Araujo and T. R. L. C. Paixão, *Anal. Methods*, 2014, **6**, 2047-2052.