

CLASSIFICATION OF BALLPOINT PEN INKS BASED ON SELECTIVE EXTRACTION AND SUBSEQUENT DIGITAL COLOR AND CLUSTER ANALYSES

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Supplementary information

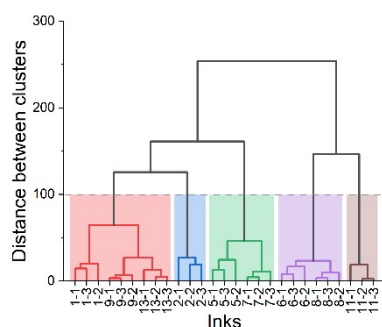


Fig. S1. HCA based on the first two PCs of the data set for evaluation of repeatability. The first digit of an abscissa label is the number of a pen; the second digit is the number of a replicate stroke.

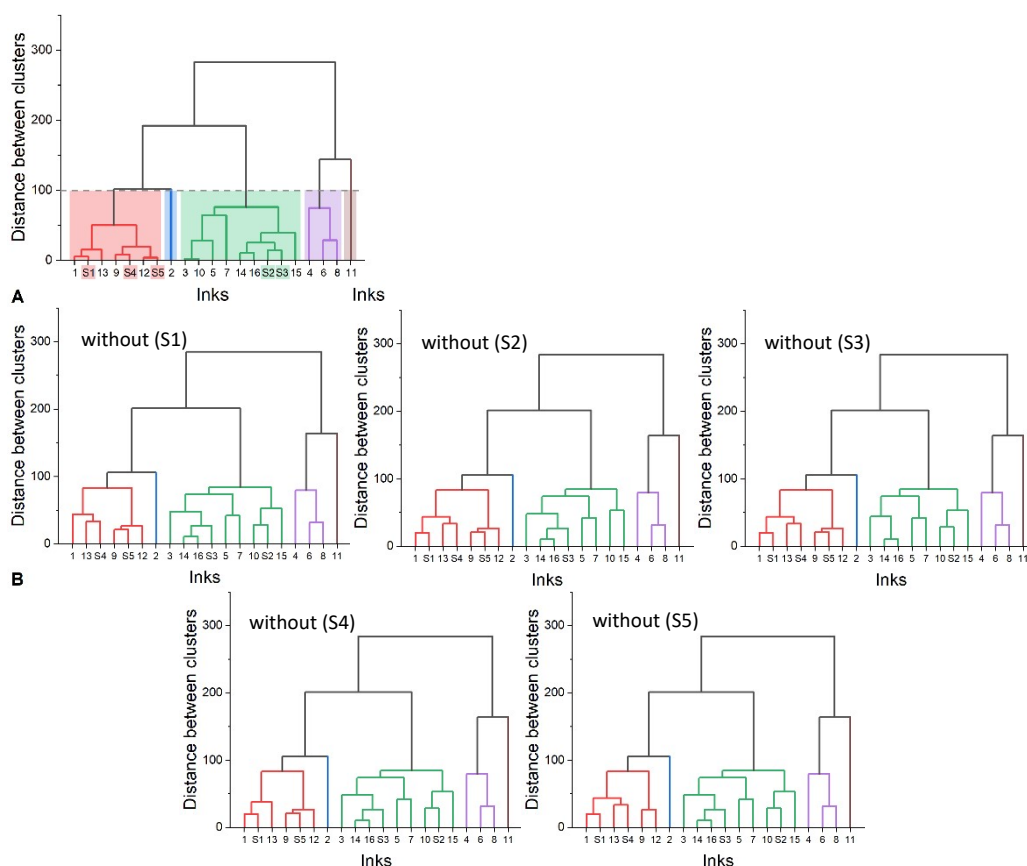


Fig. S2. (A): HCA based on the first two PCs of the original data set augmented with five unknown ink samples (S1)–(S5) (highlighted abscissa labels); (B): the results of “leave-one-out” cross-validation for samples (S1)–(S5).

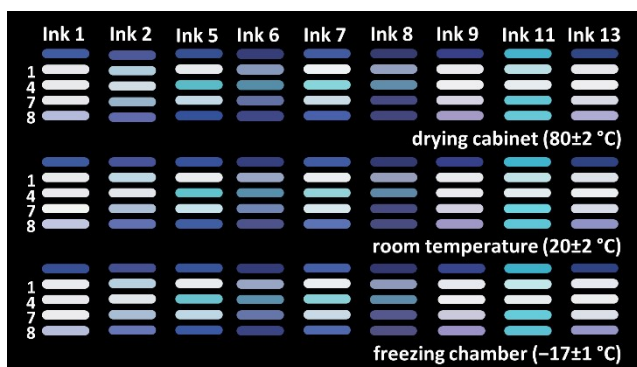


Fig. S3. Average color of ink strokes stored for 7 days at different temperatures prior to (raw) and after selective extraction with (1), (4), (7) extractants.

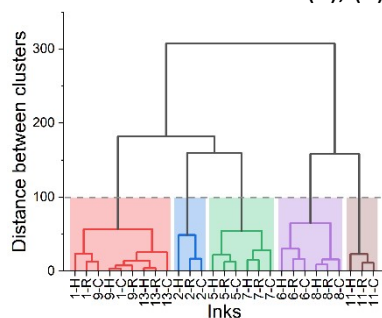


Fig. S4. HCA based on the first two PCs of the ink samples stored for 7 days at the following temperatures: -17 ± 1 °C (C), 20 ± 2 °C (R), and 80 ± 2 °C (H).

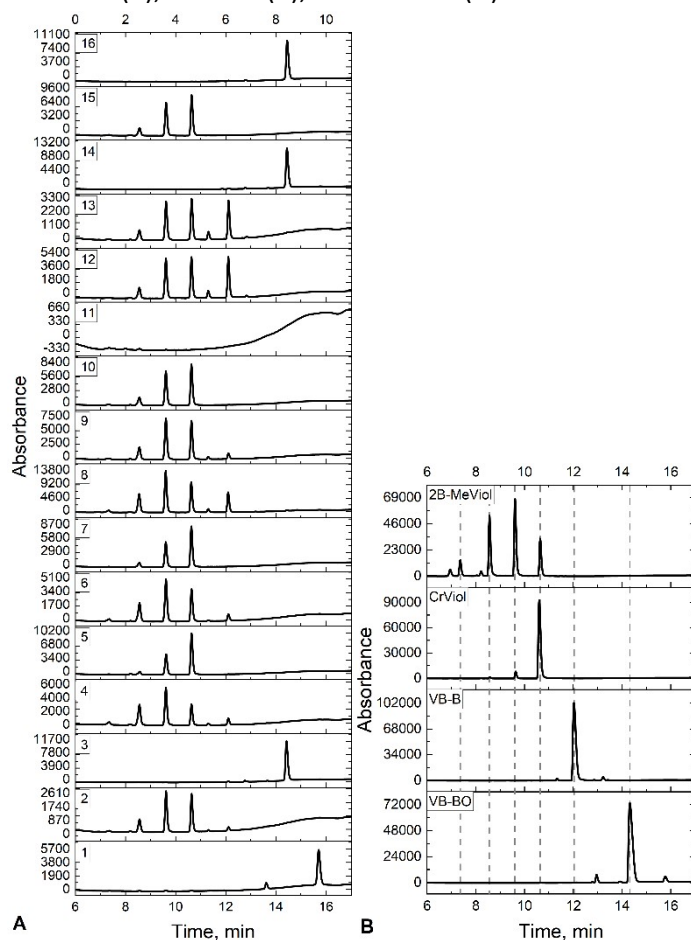


Fig. S5. Raw HPLC data of inks (1)–(16) (A) and of individual standards (B) from 6 to 17 min; wavelength 575 nm. Denotation: 2B-MeViol — Methyl violet 2B ($C_{24}H_{28}ClN_3$), CrViol — Crystal violet ($C_{25}N_3H_{30}Cl$), VB-B — Victoria blue B ($C_{33}H_{32}N_3Cl$), VB-BO — Victoria blue BO ($C_{33}H_{40}N_3Cl$).

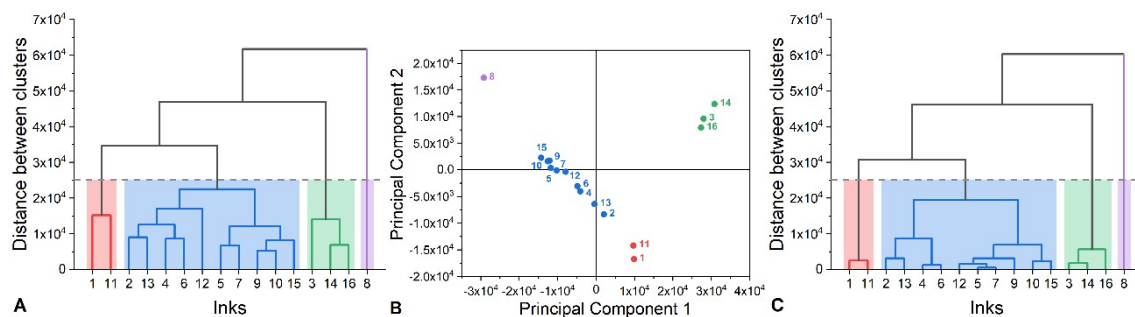


Fig. S6. HCA (A), score plot (B) and HCA based on the first two PCs (C) of the ink samples obtained from the raw chromatography data (1595-dimensional array).

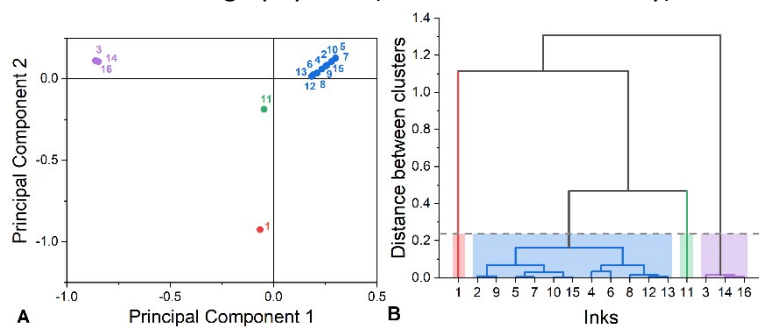


Fig. S7. Score plot (A) and HCA based on the first two PCs (B) obtained from six most illustrative peaks in normalized chromatograms.