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In-situ studies into the characterisation and degradation of blue ballpoint inks by diffuse reflectance visible spectroscopy

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Supporting Information

Table S1: Blue ballpoint pens utilised in study

Pen No.	Pen Type	Pen No.	Pen Type
1*	Bic Cristal M	19	Pilot G-2 05
2	Papermate Ink Joy 100	20	Pilot Super Grip
3	Artline Ikonic	21*	Uniball Power Tank
4	Deer Ultrafine	22*	Pilot BPS-GP
5	Artline 7210	23	PaperMate Profile
6	PaperMate Kilometrico	24*	Bic Pro Plus
7	Bic ReAction	25*	PaperMate Flexgrip Elite
8	Celco Retractable	26*	Pentel Rolly
9	Bic Orange Fine	27	PaperMate Kilometrico Elite
10	Keji Ballpoint	28*	Staedtler Triplus 426
11*	Office Basics Ballpoint	29	Staedtler Stick Click Retractable
12	Artline Smoove	30	Pilot BP-145
13*	J.Burrows Ballpoint	31	PaperMate Flexgrip Ultra
14	Bic Round Stic	32*	PaperMate Ink Joy 300
15	Artline Flow 4-Colour Retractable	33*	Office Choice Retractable
16	Artline Clix 4-Colour	34	Cos Capped Ballpoint
17	Bic Cristal M Easy Glide	35	Staedtler 430
18*	Bic Economy		

Pens marked with an asterisk (*) also selected for preparation of validation samples.

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Table S2: Correct vs. incorrect classifications of calibration data using a four-PC LDA model. The overall classification accuracy was 97.7 %.

Pen No.	Correct Classifications	Incorrect Classifications	% Correct
1	5	0	100
2	5	0	100
3	5	0	100
4	5	0	100
5	5	0	100
6	5	0	100
7	5	0	100
8	5	0	100
9	4	1 (Predicted as Pen 18)	80
10	5	0	100
11	5	0	100
12	5	0	100
13	5	0	100
14	5	0	100
15	5	0	100
16	5	0	100
17	5	0	100
18	4	1 (Predicted as Pen 9)	80
19	5	0	100
20	5	0	100
21	5	0	100
22	4	1 (Predicted as Pen 30)	80
23	5	0	100
24	4	1 (Predicted as Pen 7)	80
25	5	0	100
26	5	0	100
27	5	0	100
28	5	0	100
29	5	0	100
30	5	0	100
31	5	0	100
32	5	0	100
33	5	0	100
34	5	0	100
35	5	0	100
Total	171	4	97.7

Figure S1: Photograph of ink sample prepared using parallel lines deposited onto white copy paper.



Figure S2: 3-dimensional PCA projection plot showing the distribution of fresh vs. aged inks following two months stored in the dark, open to air.

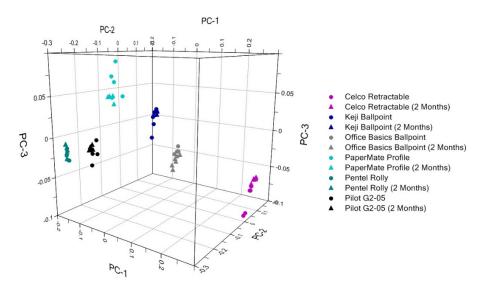


Figure S3: 3-dimensional PCA projection plot showing the distribution of fresh vs. aged inks following two months stored in the dark, sealed in plastic archive sheets.

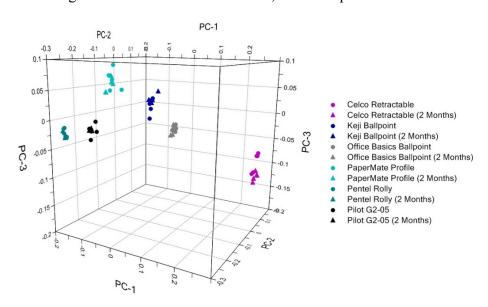


Figure S4: Factor loadings of the first three PCs for PCA conducted on the population of blue ballpoint pens.

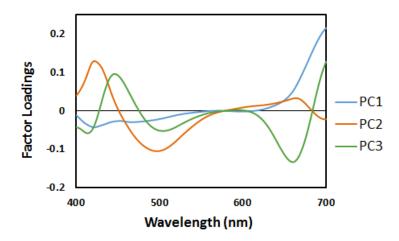


Figure S5: Normalised diffuse reflectance visible spectra obtained from PaperMate Profile ink on copy paper, both freshly deposited and following one week of natural ageing stored under open light.

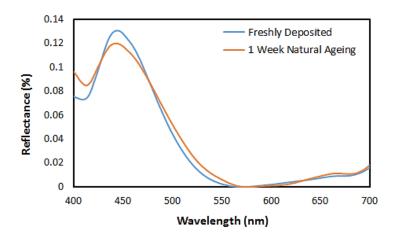


Figure S6: Normalised diffuse reflectance visible spectra obtained from PaperMate Profile ink on copy paper, both freshly deposited and following 24 hours of thermal ageing.

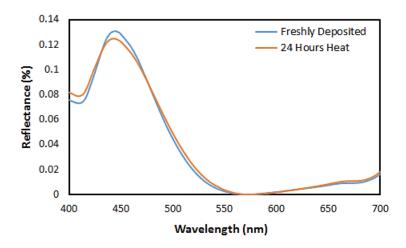


Figure S7: Normalised diffuse reflectance visible spectra obtained from PaperMate Profile ink on copy paper, both freshly deposited and following 24 hours of UV irradiation.

