Supplementary Materials

The Yxy colour space parameters as novel signalling tools for digital imaging sensors in the analytical laboratory

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Color models and color spaces:

The color model is an abstract mathematical model describing the way colors can be represented as tuples of numbers; e.g., triples in RGB (Red, Green, Blue). When a color model is associated with a proper mapping function; i.e., a precise description of how the component set of colors are to be interpreted (viewing conditions … etc.), the resulting combination of colors is called a color space. The International commission on illumination (CIE) adopted the RGB (Red, Green and Blue) as a primary colour model. For images with 8-bit depth per channel, R, G, and B take values from 0 to 255, where R=G=B=0 give black color and R=G=B=255 give white color. This color system cannot represent all the colors that the human eye can see, where some colors need to have negative RGB primaries value. Thus, the CIE derived XYZ color space by mathematical conversion of RGB and linear rgb values and assuming a γ-correction of 2.2. In this space, Y defines the luminance (lightness or brightness) and the XZ plane contains all possible chromaticities of that lightness.

$r = (R/255)\text{^}2.2$ (1)

$g = (G/255)\text{^}2.2$ (2)

$b = (B/255)\text{^}2.2$ (3)

$X = 0.3933r + 0.3651g + 0.1903b$ (4)

$Y = 0.212r + 0.71010g + 0.0858b$ (5)

$Z = 0.0182r + 0.1117g + 0.9570b$ (6)

Further, the CIE-Y*xy* is a lightness-chromaticity color space derived from the normalization of the XYZ values, where the Y is the lightness (having the same Y value in XYZ color space) and x, y are chromaticity coordinates.

$x = X/(X + Y + Z)$ (7)

$y = Y/(X + Y + Z)$ (8)

On the other hand, the CMY (Cyan, Magenta, and Yellow) parameters can have values from 0 to 1; when C=M=Y=0 this gives a white color and when C=M=Y=1 this gives a black color. The CMY color space values can be derived as follows:

$C = 1 - R/255$ (9)

$M = 1 - G/255$ (10)

$Y = 1 - B/255$ (11)

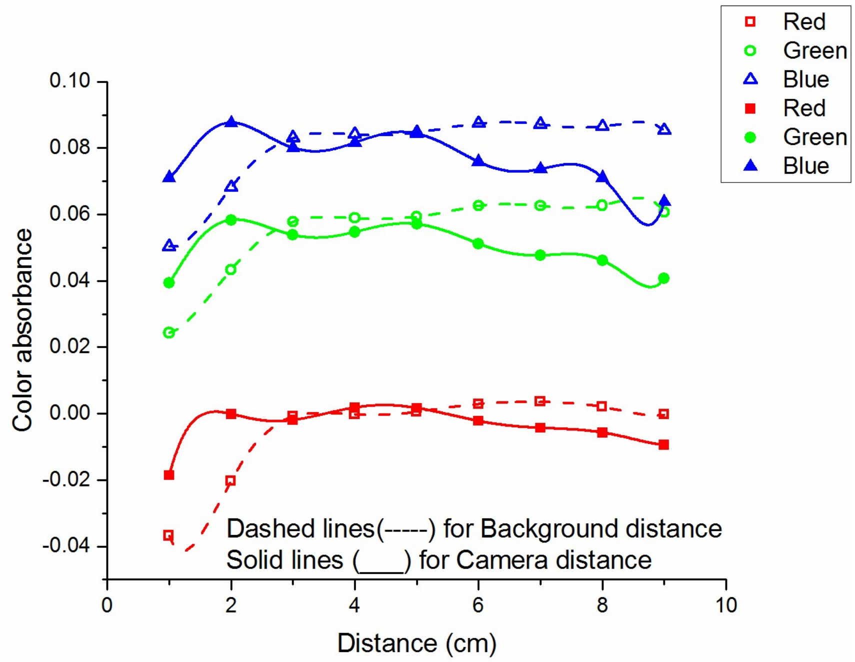

Fig. S1. Effects of the cuvette-background diffuser distance (dotted lines) and camera-cuvette distance (solid lines) on the colour absorbances of the Fe-phenanthroline system.

(A)
(B)
(C)

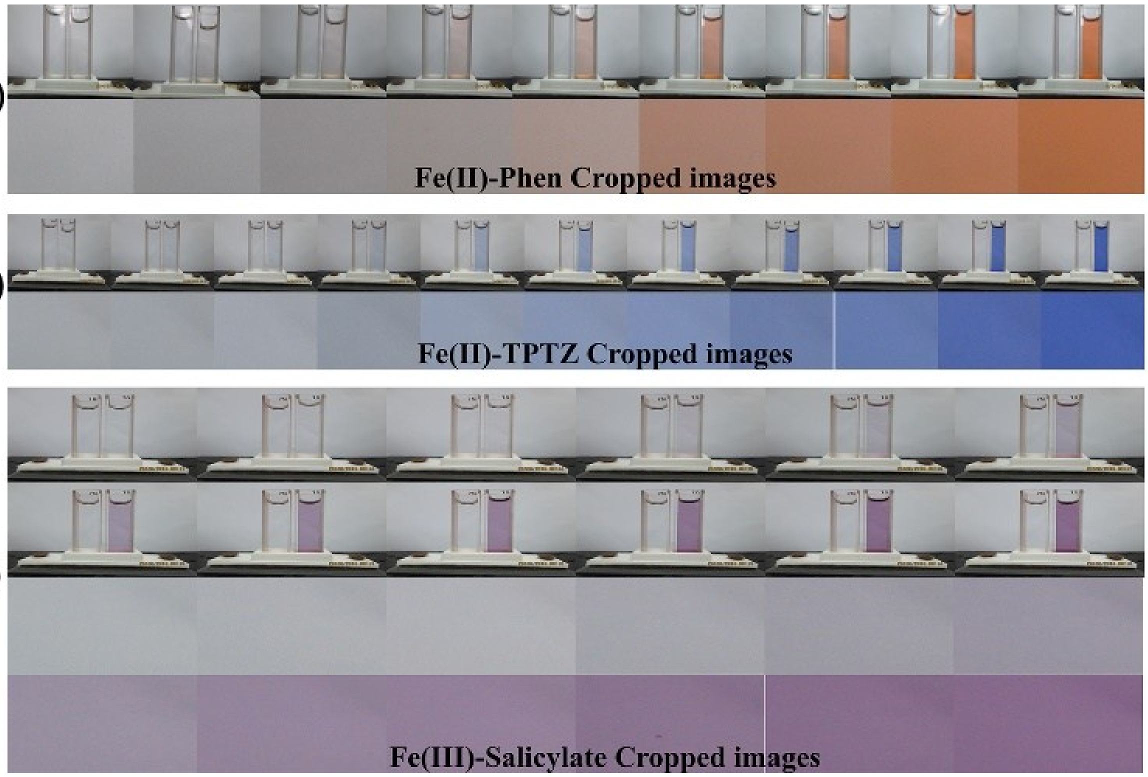

Fig. S2. Digital camera images and cropped areas of Fe(II)-phenanthroline standard solutions of 0.0-3.0 mg L^{-1} Fe (A), Fe(II)-TPTZ standard solutions of 0.0-2.0 mg L^{-1} Fe (B), and Fe(III)-salicylate standard solutions of 0.0-18.0 mg L^{-1} Fe (C) obtained according to the recommended procedures. Captured images were arbitrarily compressed to fit into the page margins; however, for image processing, the original uncompressed images were used.

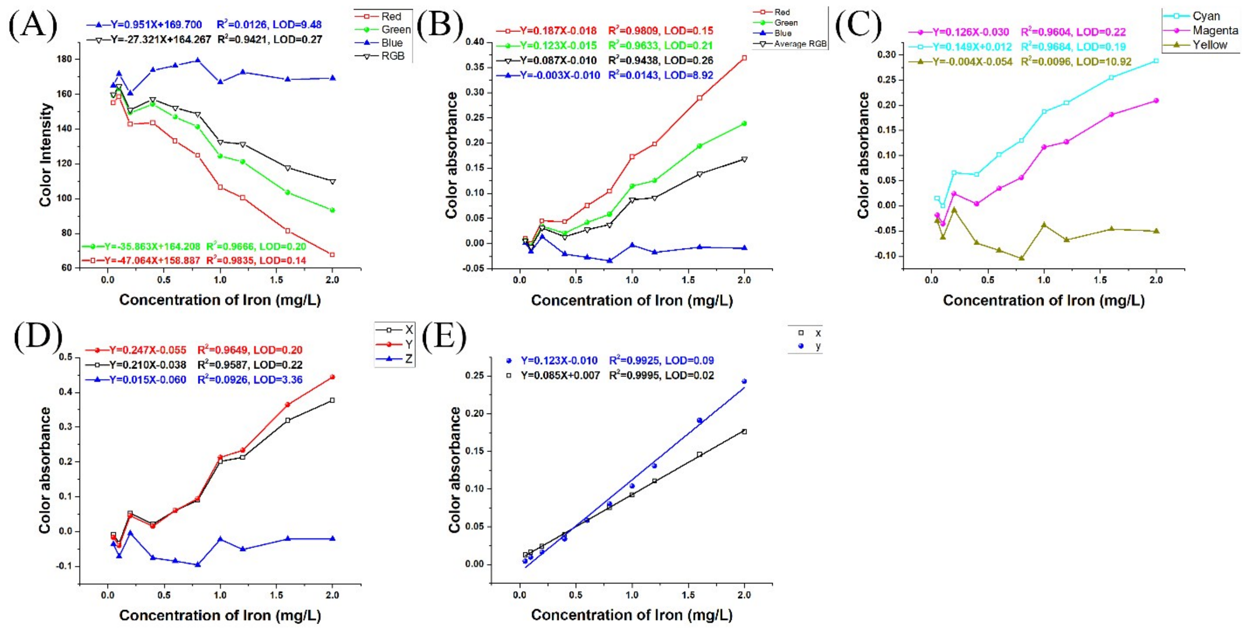

Fig. S3. Calibration curves of the Fe(II)-TPTZ system; responses are (A) RGB intensity, (B) RGB colour absorbance, (C) CMY colour absorbance, (D) tristimulus XYZ colour absorbance, and (E) Yxy colour absorbance. The other conditions tested are those shown in Fig. S2.

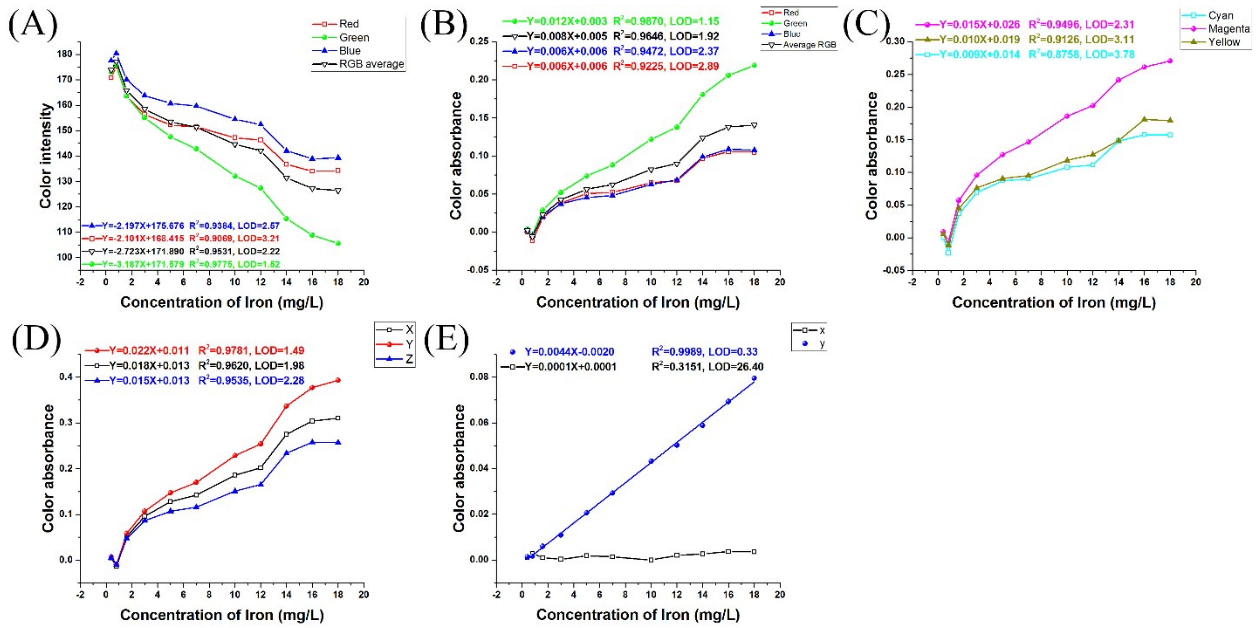

Fig. S4. Calibration curves of the Fe(III)-salicylate System; responses are (A) RGB intensity, (B) RGB colour absorbance, (C) CMY colour absorbance, (D) tristimulus XYZ colour absorbance, and (E) Yxy colour absorbance. The other conditions tested are those shown in Fig. S2.

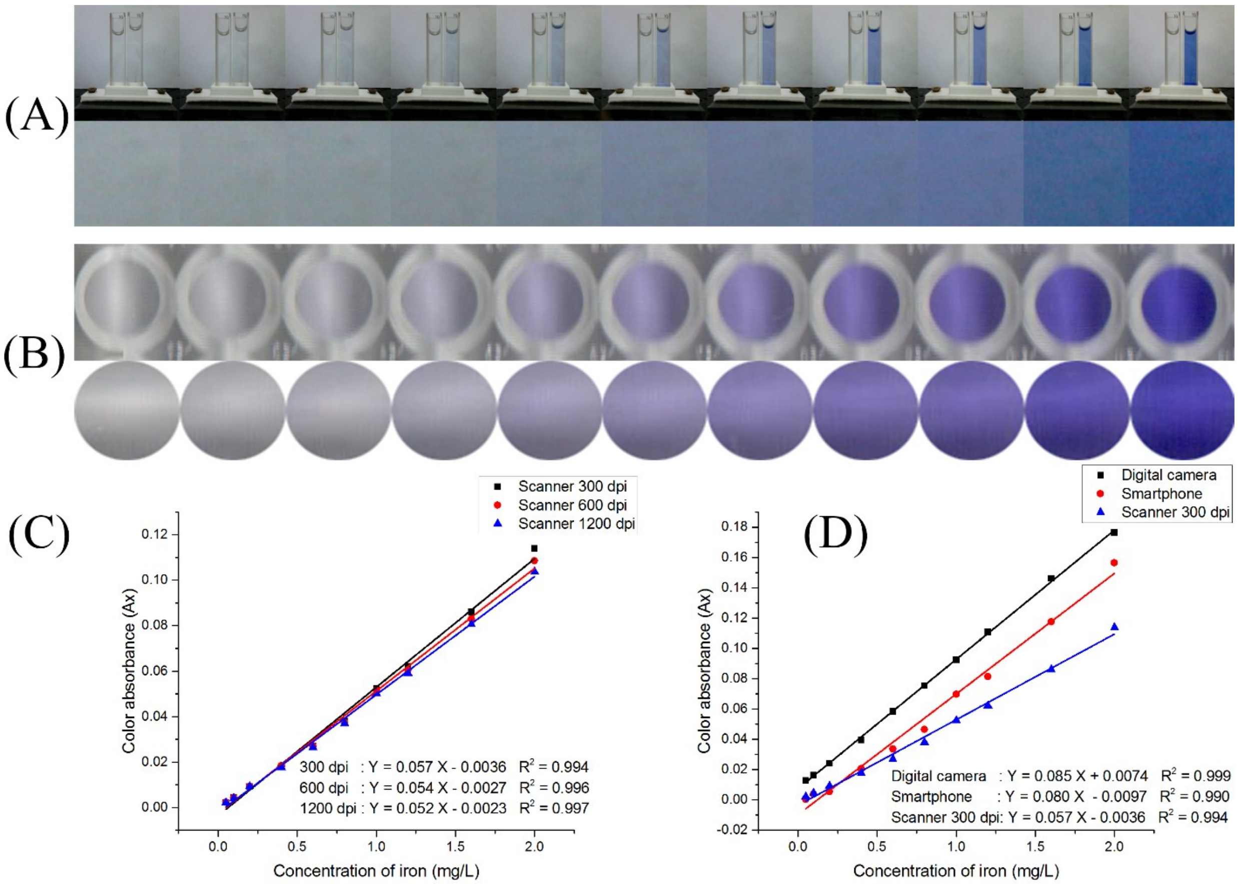

Fig. S5.Digital images and cropped images of Fe(II)-TPTZ standard solutions (0.0-2.0 mg L^{-1} Fe). Images were captured using (A) a Sony Xperia E smartphone with a 3.15 MP camera and (B) the scanner of HP LaserJet Pro M1536dnf MF printer at 1200 dpi. Calibration graphs based on images from the desktop scanner at 300, 600 and 1200 dpi (C) and from different image-capturing devices (D). The other conditions tested are those shown in **Fig. S2**.

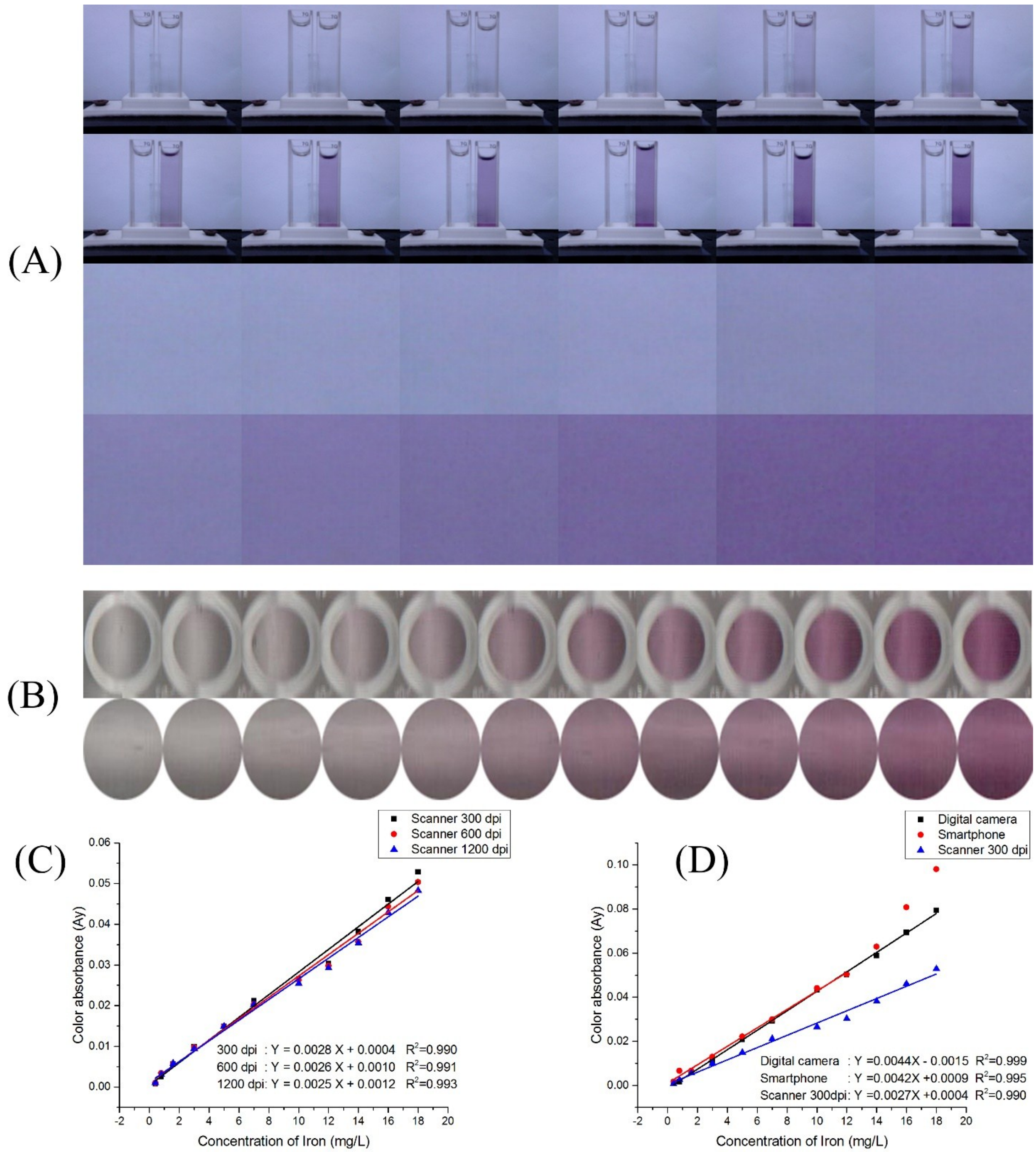

Fig. S6. Digital images and cropped images of Fe(III)-salicylate standard solutions (0.0-18.0 mg L^{-1} Fe). Images captured using (A) a Sony Xperia E smartphone with a 3.15 MP camera and (B) the scanner of HP LaserJet Pro M1536dnf MF printer at 1200 dpi. Calibration graphs based on images from desktop scanner at 300, 600 and 1200 dpi (C), and from different image-capturing devices (D). The other conditions tested are those shown in **Fig. S2**.

Table S 1. Regression parameters for calibration graphs obtained with various non-uniform colour spaces for iron(II) or iron(III) determination using phenanthroline, TPTZ, and salicylate.

		parameter	Intercept ± SD	Slope ± SD	R^2	LOD	LOQ
Fe(II)-Phenanthroline	**Spectrophotometer**		-0.003 ± 0.002	0.219 ± 0.001	0.9998	0.03	0.10
	RGB intensity	I_R	146.900 ± 2.671	9.777 ± 1.587	0.8635	0.82	2.73
		I_G	148.089 ± 2.370	-13.962 ± 1.408	0.9425	0.51	1.70
		I_B	152.160 ± 2.603	-27.443 ± 1.547	0.9813	0.26	0.86
		I_{RGB}	149.050 ± 2.471	-10.543 ± 1.468	0.8968	0.70	2.33
	Y_{xy} Colour Absorbance	A_Y	Same Y in XYZ				
		A_x	-0.006 ± 0.001	0.059 ± 0.001	0.9990	0.07	0.22
		A_y	-0.002 ± 0.001	0.025 ± 0.0004	0.9983	0.09	0.28
Fe(II)-Tripyridyl triazine	**Spectrophotometer**		0.0001 ± 0.001	0.420 ± 0.001	0.9999	0.01	0.03
	RGB intensity	I_R	158.887 ± 2.181	-47.064 ± 2.158	0.9835	0.14	0.46
		I_G	164.208 ± 2.381	-35.863 ± 2.356	0.9666	0.20	0.66
		I_B	169.700 ± 3.003	0.951 ± 2.972	0.0126	9.48	31.59
		I_{RGB}	164.267 ± 2.419	-27.321 ± 2.394	0.9421	0.27	0.89
	Y_{xy} Colour Absorbance	A_Y	Same Y in XYZ				
		A_x	0.007 ± 0.001	0.085 ± 0.001	0.9995	0.02	0.08
		A_y	-0.010 ± 0.004	0.123 ± 0.004	0.9925	0.09	0.31
Fe(III)-Salicylate	**Spectrophotometer**		0.008 ± 0.0035	0.030 ± 0.0003	0.9987	0.35	1.17
	RGB intensity	I_R	168.415 ± 2.250	-2.101 ± 0.224	0.9069	3.21	10.71
		I_G	171.579 ± 1.962	-3.187 ± 0.196	0.9775	1.52	5.07
		I_B	175.676 ± 1.882	-2.197 ± 0.188	0.9384	2.57	8.57
		I_{RGB}	171.890 ± 2.019	-2.723 ± 0.201	0.9531	2.22	7.42
	Y_{xy} Colour Absorbance	A_Y	Same Y in XYZ				
		A_x	0.00010 ± 0.0005	0.00010 ± 0.00001	0.3151	26.40	88.00
		A_y	-0.0020 ± 0.0004	0.00440 ± 0.00005	0.9989	0.33	1.09