Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Electronic Supplementary Information (ESI)

Direct visual detection and quantification of mercury in fresh fish meat using facilely prepared polymeric sensory labels.

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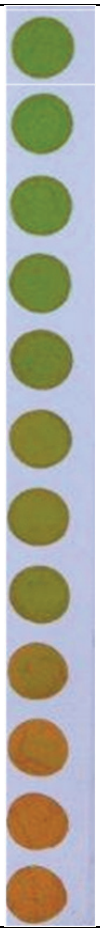
S1.- Titration of Hg(II) with F2 by examining the analysis of the RGB parameters of each disk using a digital picture.

Table S1. RGB data and principal components analysis (**PC1**) of the R and G parameters from photographs taken of the **F2** sensory discs after immersion for 60 min at RT in aqueous solutions (pH = 2.2, KCl–HCl) containing different quantities of Hg(II).

Discs	[Hg(II)], ppb	LOG [Hg(II), ppb]	R	G	B	PC1 (R&G)
	2.00E-01	-0.69897	82	130	12	-0.51541
	2.00E+00	0.30103	91	131	8	-0.90476
	1.00E+01	1	95	135	16	-1.31635
	2.00E+01	1.30103	99	138	14	-1.44587
	1.00E+02	2	97	142	13	-1.17571
	2.00E+02	2.30103	103	142	16	-0.8841
	4.00E+02	2.60205999	100	138	10	-0.63698
	6.00E+02	2.77815125	104	127	20	-0.28418
	8.00E+02	2.90308999	126	125	14	0.01935
	1.00E+03	3	125	128	13	0.14966
	2.00E+03	3.30103	125	124	15	0.82586
	5.00E+03	3.69897	146	116	11	1.57992
	1.00E+04	4	170	110	9	2.10674
	1.50E+04	4.17609126	182	103	16	2.26963
	2.00E+04	4.30103	185	102	10	2.54138

S2.- Mercury analysis in a test sample via the RGB technique using a previously built titration curve.

Table S2. Hg(II) concentrations, RGB parameters and **PC1** of each disk. The test sample with the corresponding RGB and **PC1** data is given at the end of the table.

Discs	[Hg(II)], ppb	LOG [Hg(II), ppb]	R	G	B	PC1 (R&G)
	2.00E+01	1.30	99	138	14	-1.45
	1.00E+02	2.00	97	142	13	-1.18
	8.00E+02	2.90	126	125	14	0.019
	2.00E+03	3.30	125	124	15	0.83
	5.00E+03	3.70	146	116	11	1.58
	1.00E+04	4.00	170	110	9	2.11
	2.00E+04	4.30	185	102	10	2.54
Test	¿?	¿?	103	142	16	-0.88

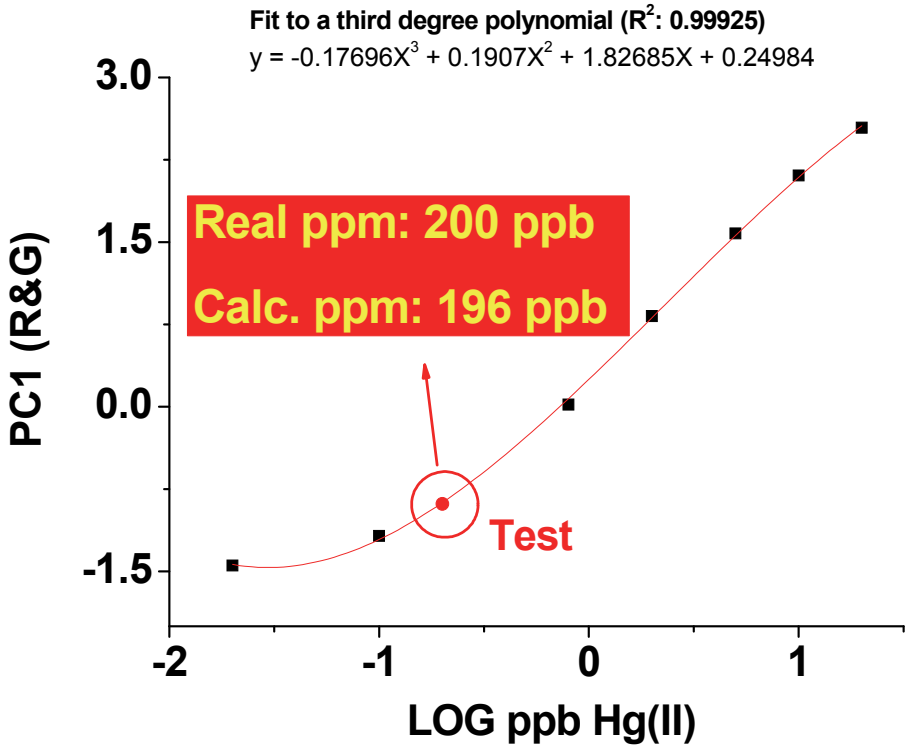


Figure S3. Variation of the **PC1** *vs* the logarithm of the Hg(II) concentration. Upon fitting with a third-degree polynomial, the mercury concentration in the test sample was calculated.

S3.- Selectivity study of F2.

Cs(I) caesium nitrate (Fluka, 99%)	**Mn(II)** manganese (II) nitrate hexahydrate (Alfa Aesar, 98%)	**Ba(II)** barium chloride dihydrate (LabKem, 99%)	**Zn(II)** zinc nitrate hexahydrate (Aldrich, 98%)	**Co(II)** cobalt(II) nitrate hexahydrate (LabKem, 98%)	**NH_4(I)** ammonium nitrate (Aldrich, 98%)	**Cr(III)** chromium(III) nitrate nonahydrate (Alfa Aesar, 98.5%)	**Cu(II)** copper(II) nitrate trihydrate (Aldrich, 98%)
Rb(I) rubidium nitrate (Aldrich, 99.7%)	**Dy(III)** dysprosium(III) nitrate hydrate (Alfa Aesar, 99.9%)	**Li(I)** lithium chloride (Aldrich, 99%)	**Ce(III)** cerium(III) nitrate hexahydrate (Alfa Aesar, 99.5%)	**Zr(II)** zirconium(IV) chloride (Alfa Aesar, 98%)	**Mg(II)** magnesium nitrate hexahydrate (LabKem, 98%)	**La(III)** lanthanum(III) nitrate hexahydrate (Alfa Aesar, 99.9%)	**Hg(II)** mercury(II) nitrate monohydrate (Scharlab, 99%)
K(I) potassium nitrate (Aldrich, 99%)	**Sm(III)** samarium(III) nitrate hexahydrate (Alfa Aesar, 99.9%)	**Al(III)** aluminium nitrate nonahydrate (Aldrich, 98%)]	**Nd(III)** neodymium(III) nitrate hexahydrate (Alfa Aesar, 99.9%)	**Pb(II)** lead(II) nitrate (Fluka, 99%)	**Na(I)** sodium nitrate (LabKem, 99%)	**Sr(II)** strontium nitrate (Alfa Aesar, 98%)	**Ni(II)** nickel(II) nitrate hexahydrate (VWR, 99%)

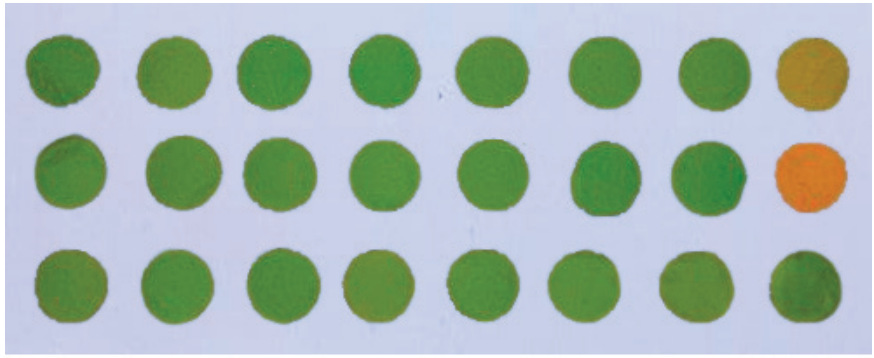


Figure S4. 8 mm discs of **F2** photographed after immersing for 24 hours at room temperature in a 10^{-3} M solution of each cation buffered at pH 2.2. The table shows the name of each salt with the supplier and purity.

CN^- (Sodium cyanide (Aldrich, >97%)	**$CH3COO^-$** Sodium acetate (Aldrich, >99%)	**OH^-** Lithium hydroxide (Aldrich, >98%)	**F^-** Sodium fluoride (Aldrich,)	**ClO_4^-** Potassium perchlorate (Aldrich, >99%)	**$C_{12}H_{25}SO_4^-$** Sodium dodecyl sulfate (Aldrich, >98.5%)	**$CH_3CH_2O^-$** Sodium Ethoxide (Aldrich, 95%)	**$HOOCC6H4COO^-$** Potassium hydrogen phthalate (Aldrich, 99.95%)
$P_2O_7^{4-}$ Sodium pyrophosphate tetrabasic (Aldrich, >95%)	**$S_2O_8^{2-}$** Potassium persulfate (Aldrich, >99%)	**$CH3SO3^-$** Sodium methanesulfonate (Aldrich, 98%)	**$H_2P_2O_7^{2-}$** Sodium pyrophosphate dibasic (Aldrich, >99%)	**$CF_3SO_3^-$** Lithium trifluoromethanesulfonate (Aldrich, 96%)	**$CH_3C_6H_4SO_3^-$** Sodium p-toluenesulfonate (Aldrich, 95%)	**Br^-** Potassium bromide (Aldrich, >99%)	**SCN^-** Potassium thiocyanate (Aldrich, >99%)
$C_2O_4^{2-}$ Potassium oxalate monohydrate (Aldrich, >98.5%)	**CO_3^{2-}** Sodium carbonate (Aldrich, >99%)	**$C_6H_5COO^-$** Sodium benzoate (Aldrich, >99.5%)	**$H_2PO_4^-$** Lithium phosphate monobasic (Aldrich, 99%)	**SO_4^{2-}** Sodium sulfate (Aldrich, 99%)	**$C_2H_2ClO_2^-$** Sodium chloroacetate (Aldrich, 98%)	**CF_3COO^-** Sodium trifluoroacetate (Aldrich, >99%)	

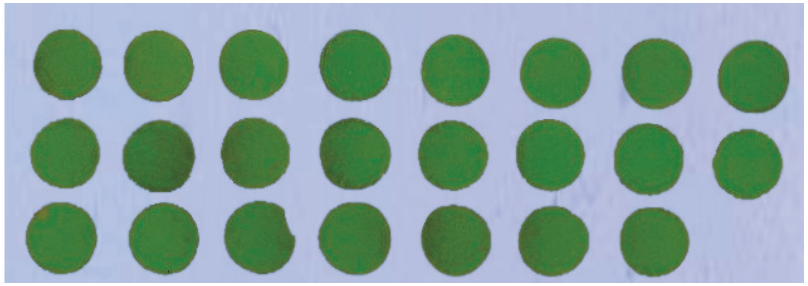


Figure S5. 8 mm discs of **F2** photographed after immersing for 24 hours at room temperature in a 10^{-3} M solution of each anion buffered at pH 2.2. The table shows the name of each salt with the supplier and purity.

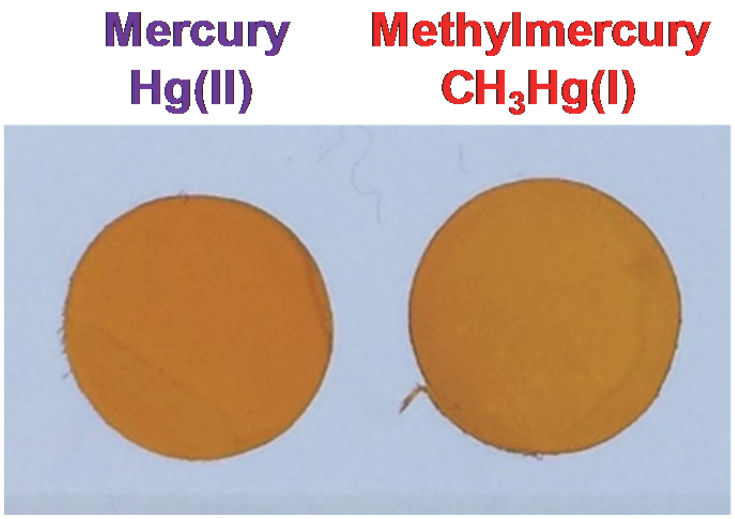


Figure S6. 8 mm discs of **F2** photographed after immersion for 24 hours at room temperature in a 10^{-3} M solution of mercury nitrate monohydrate (left) and methylmercury(II) chloride (right). Due to the insolubility of methylmercury(II) chloride in pure water, the media in this case was MeOH:water-buffer-pH 2.2 (10/90 v/v).

S4.- Response time of F2.

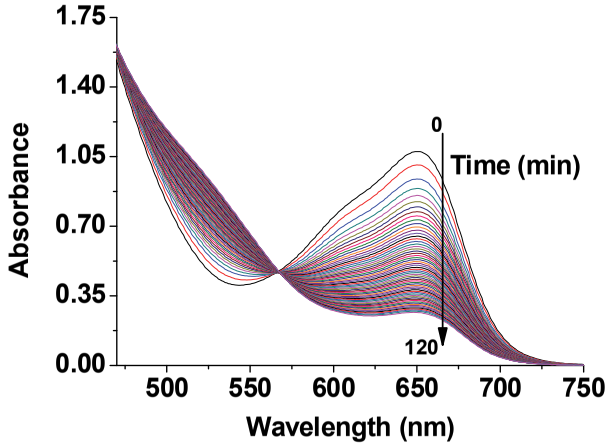


Figure S7. Detection kinetics of Hg(II) by the UV/Vis technique using **F2** as a sensory material (Hg(II) = 20 ppm, water, pH = 2.2). The graphic shows the isosbestic point of the equilibrium between **DZ** and the **DZ_2Hg** complex.

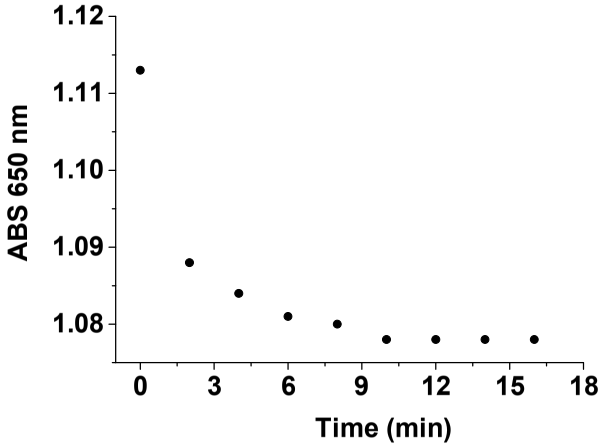


Figure S8. Detection kinetics of Hg(II) by the UV/Vis technique using **F2** as a sensory material (Hg(II) = 20 ppb, water, pH = 2.2).

S5.- Procedure followed for detection of mercury in real fish samples using sensory discs of F2 and the RGB technique.

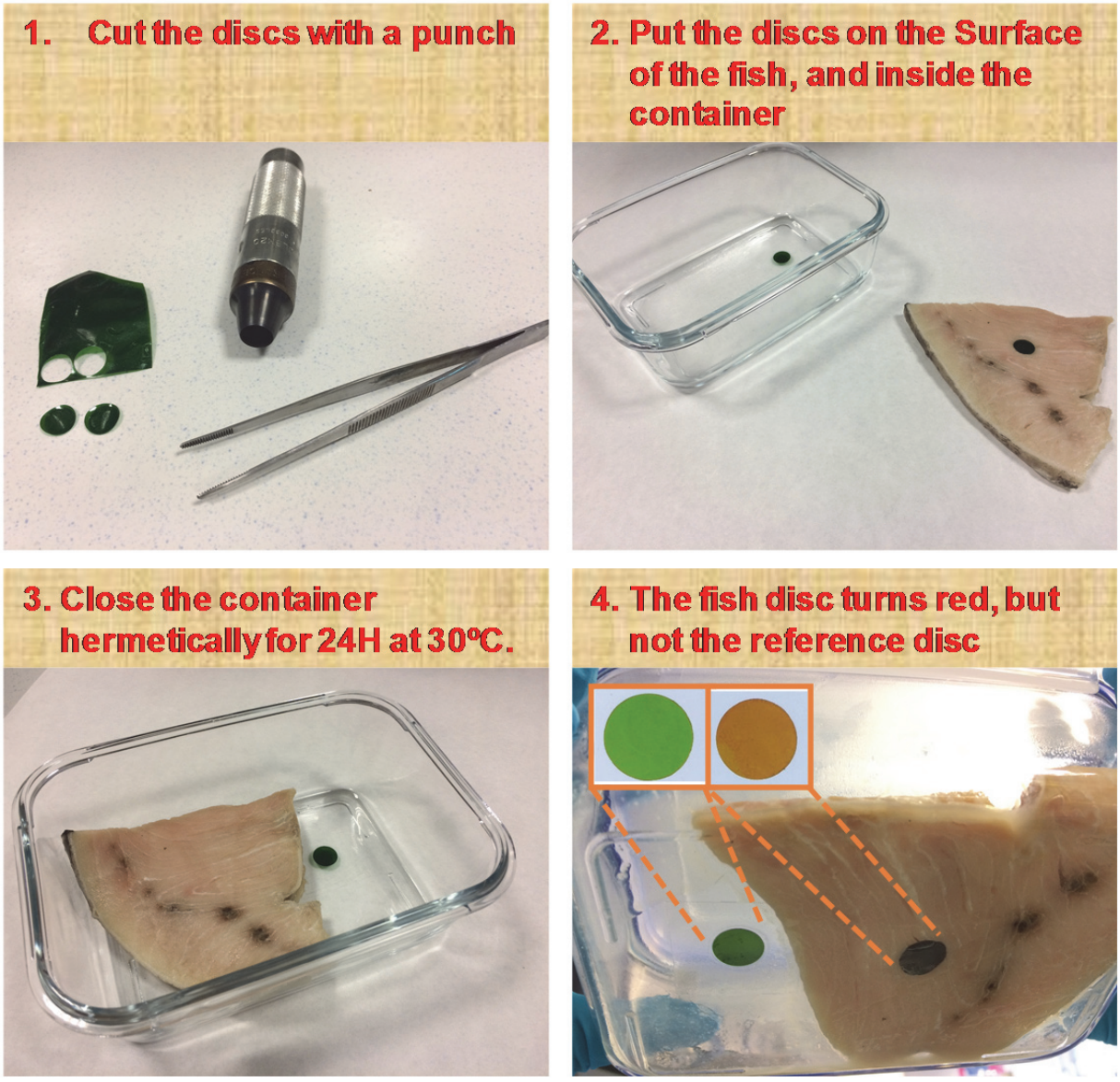
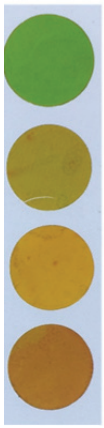


Figure S9. Procedure for measuring the concentration of mercury in real fish samples (for example, swordfish) using 12 mm discs of **F2**. In the fourth step, the two discs were photographed with the retro-illumination device. One of them is a reference (left, no contact with the fish meal), while the other (right) was in contact with the fish meal at 30°C for 24 hours.

Table S10. ICP-MS data corresponding to the total Hg mercury concentrations measured for each type of fish, the RGB parameters obtained from the digital picture, and the **PC1** value that groups the two parameters R and G obtained from the digital colour.



	R	G	B	PC1 (R & G)	LOG ppb Hg(II)
Blank	91	154	10	-1.67	0.11
Salmon	155	138	13	-0.017	1.79
Hake	189	141	9	0.45	2.26
Swordfish	164	107	25	1.24	3.62

S6.- Extraction of mercury from tap water using F2.

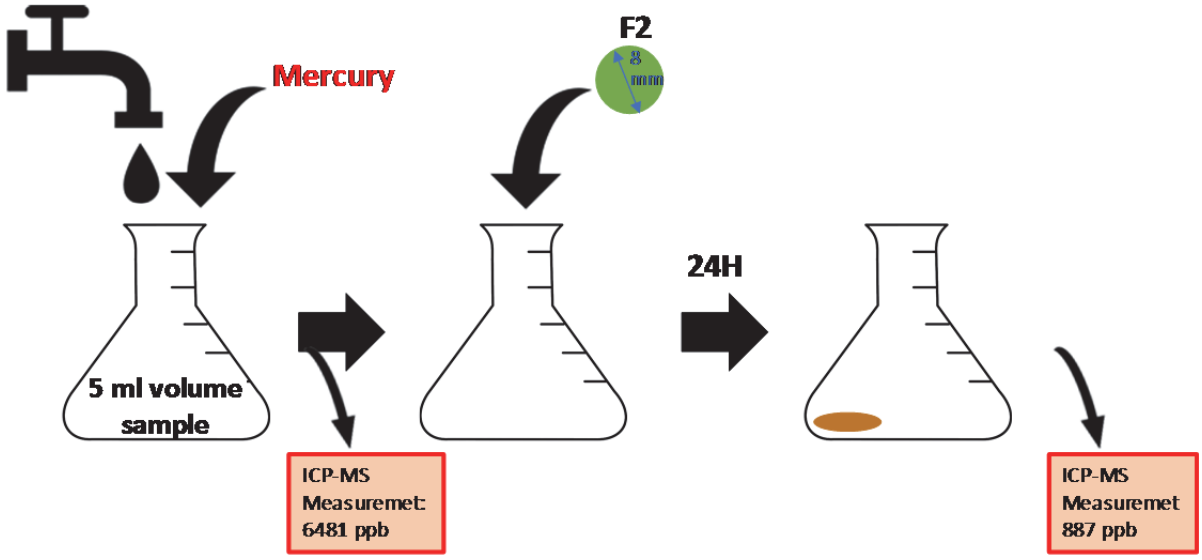


Figure S11. Up) The figure shows the preparation of the samples. First, a 5 ml volume of tap water was buffered at pH 2.2. Then, a small amount of mercury (6 ppm) was added to the solution. The concentration of mercury in this solution was measured with an Agilent 7500 ICP-MS spectrometer. The obtained data (6.5 ppm) correspond to the sum of the added and innate mercury ion concentration in tap water. After that, a 8 mm disk of **F2** was immersed in the solution for 24 hour at room temperature. Finally, the ICP-MS measurement shows an 86% reduction in the mercury concentration (0.9 ppb).

S7.- Images of the homemade retro-illumination device.

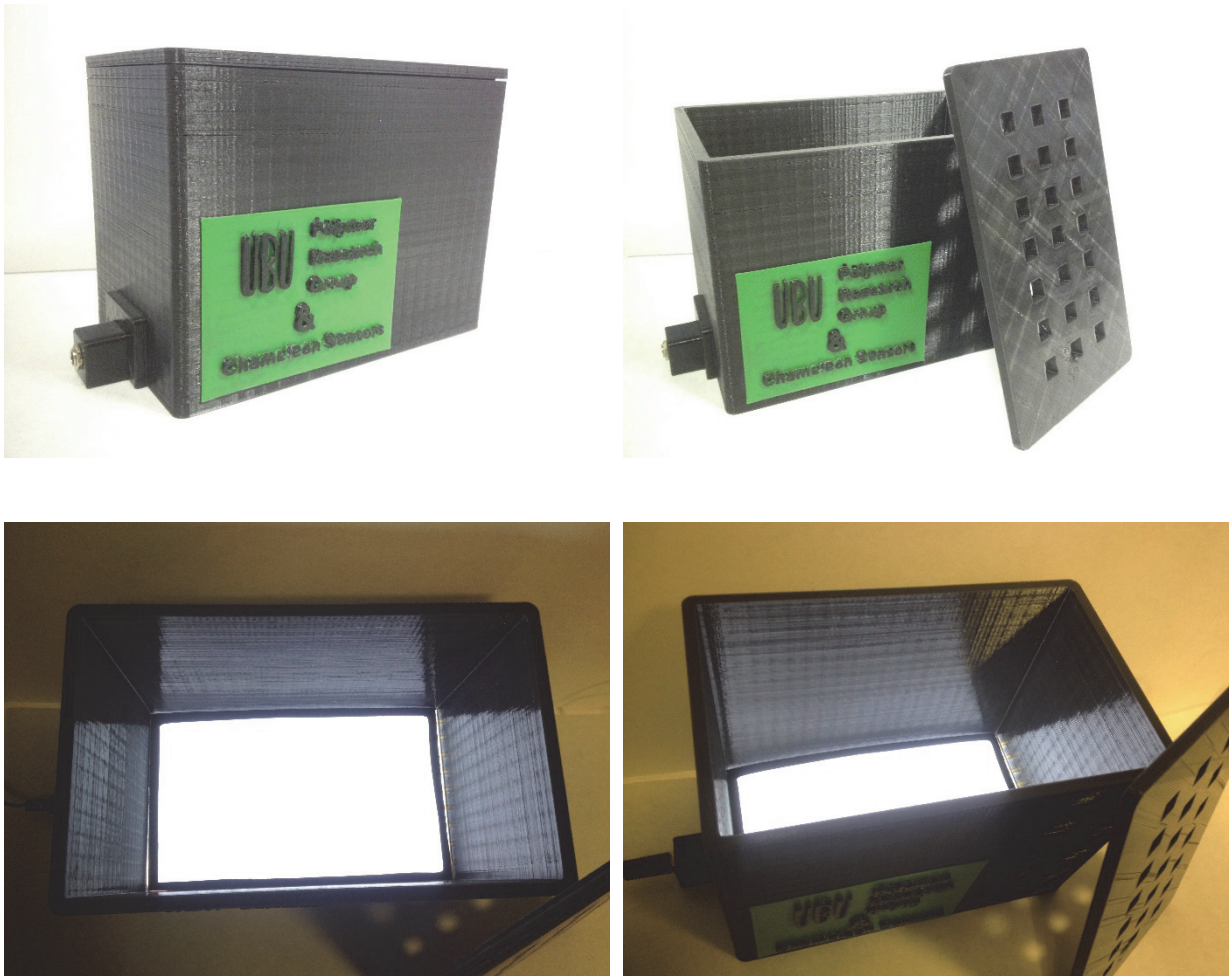


Figure S12. Images of the retro-illumination device. The closed box was prepared with a Prusa i3 steel 3D printer. The holes in the cap allowed us to take clear pictures, without shaking the camera. The light at the bottom is the illumination system of an old tablet.

S8.- Overall migration results as described in Commission Regulation (EU) No 10/2011 (and amendments) relating to plastic materials and articles intended to come into contact with food.

The overall migration was measured as described in Commission Regulation (EU) No 10/2011 (and amendments) relating to plastic materials and articles intended to come into contact with food.
The test methods followed:

- EN 1186-1; *Guide to the selection of conditions and test methods for overall migration.*
- EN 1186-2; *Test methods for overall migration into olive oil by total immersion.*
- EN 1186-3; *Test methods for overall migration into aqueous food simulants by total immersion.*

Aggressive contact conditions were used. Therefore, testing was performed at OM6 for 4 hours at 100°C or reflux temperature. This condition represents the worst case scenario for testing with simulants.

Simulant	**Test condition**
10% ethanol (simulant A)	4 hours at reflux
3% acetic acid (simulant B)	4 hours at reflux
Olive oil (simulant D2)	4 hours at 100°C

F2			
Contact area: 0.6 dm² Volume simulant: 100 ml			
Method	**EN 1186-3**	**EN 1186-3**	**EN 1186-2**
Migration media	**3% acetic acid**	**10% ethanol**	**olive oil**
Migration, mg/dm^2	0.7	5.9	4.8

The overall migration results obtained for **F1** were found to be in compliance with the restriction for the overall migration limit (< 10 mg/dm^2) as defined in Commission Regulation (EU) No 10/2011 for food contact materials for tests performed under the abovementioned test conditions.

S9.- Thermogravimetric analysis of F2.

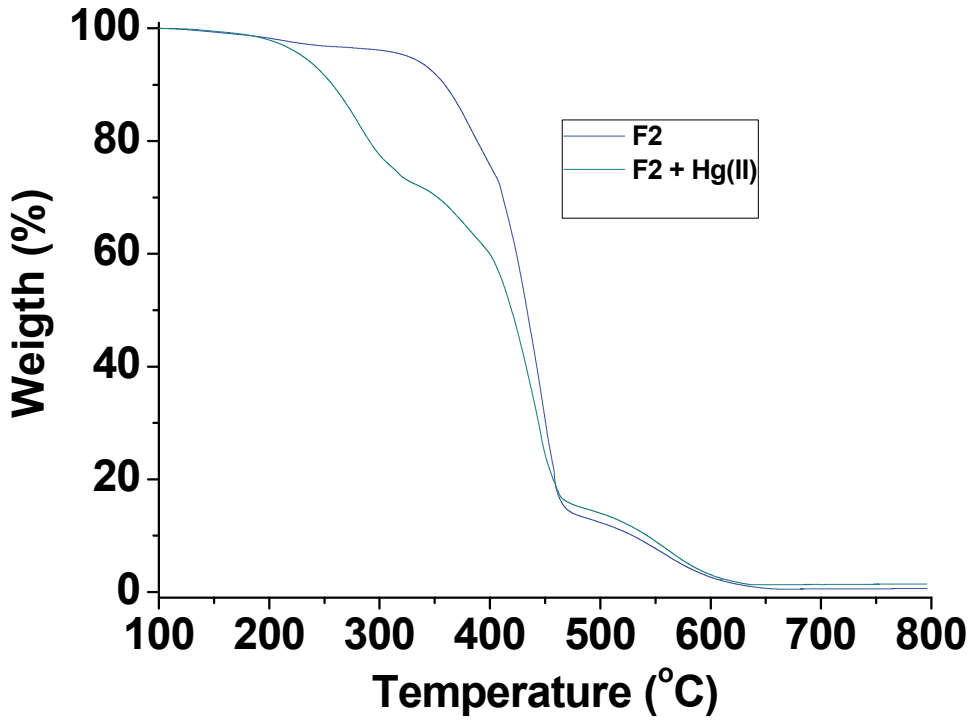


Figure S13. Thermogravimetric curves at 10°C/min for **F2** before and after immersion in a 10^{-3} M solution of $Hg(NO_3)_2 \cdot H_2O$. Atmosphere = synthetic air.