An open-source portable device for the determination of fluoride in drinking water.

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Sample holder schemas

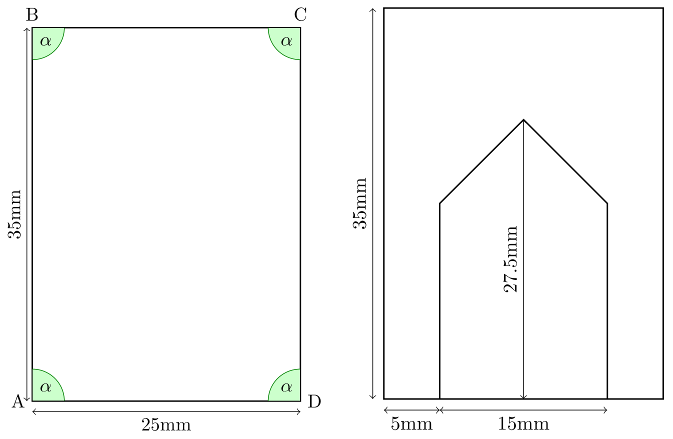
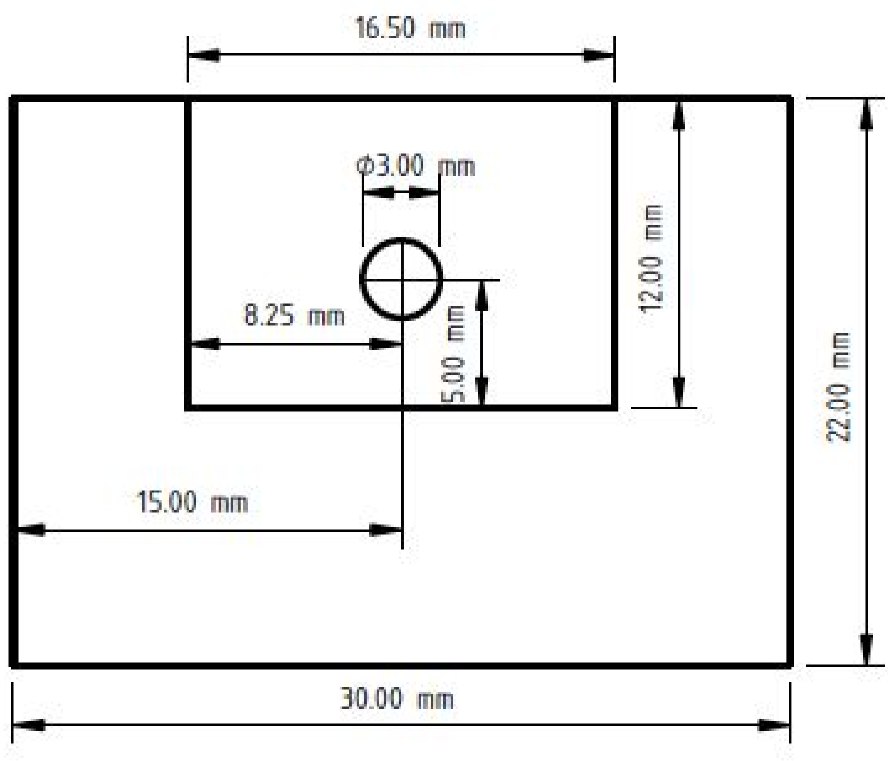
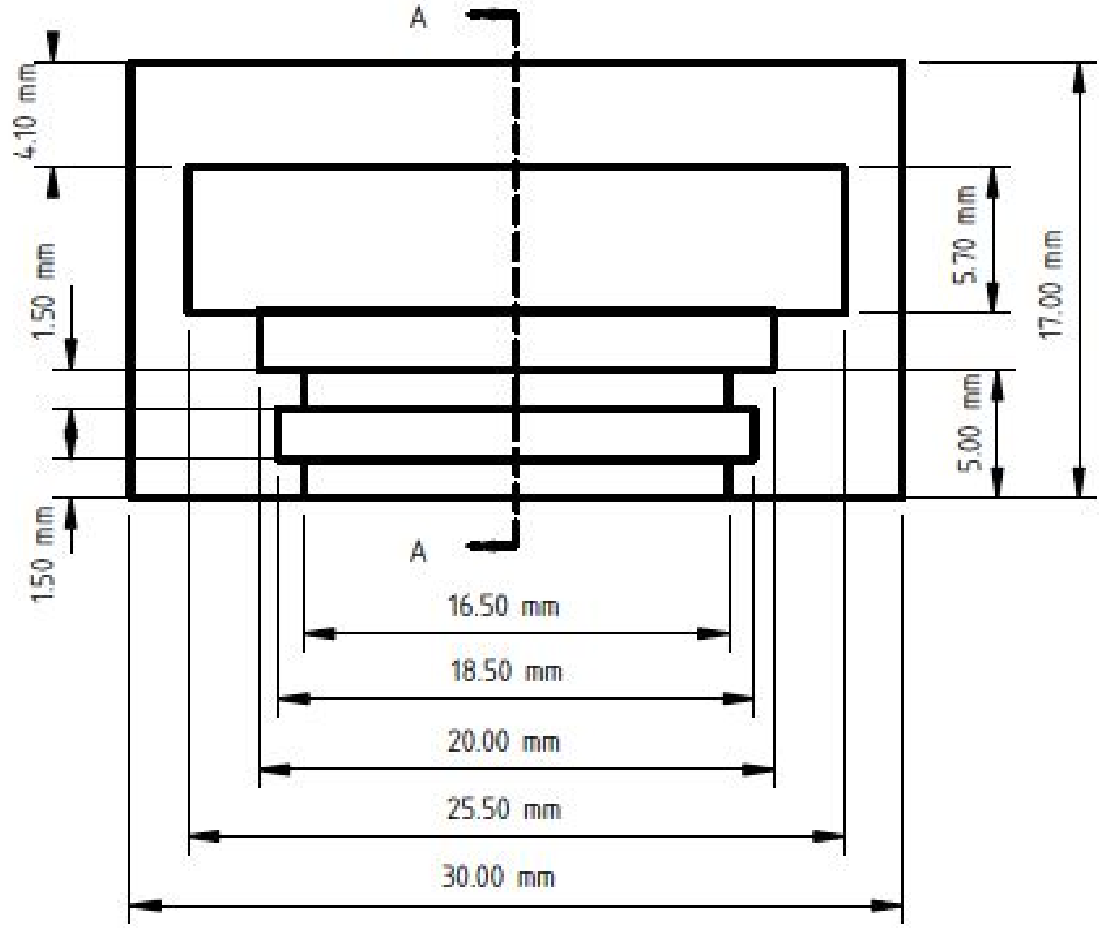
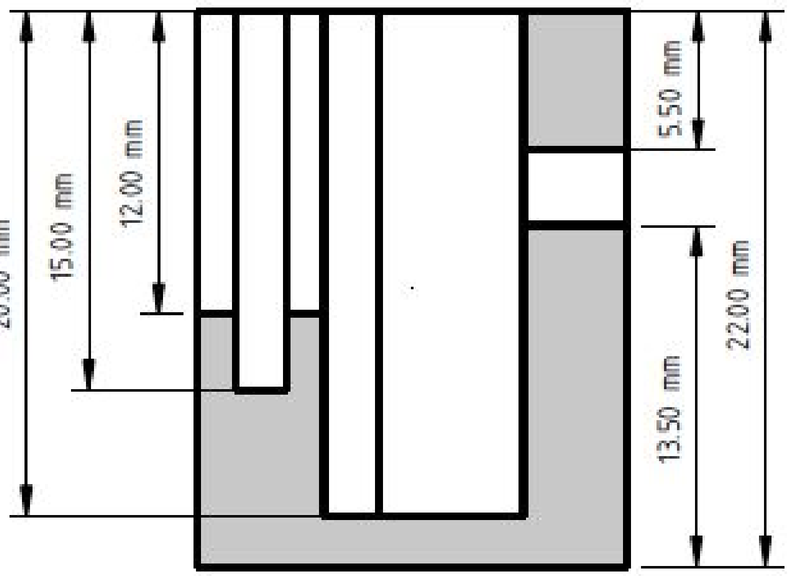


Fig S1 – Sample holder schema used for color intensity quantification in test strips defined in figure 1. Left) back side of the sample holder, right) front side of the sample holder, and cotton substrate dimensions.α=90°.




A
A
4.10 mm
1.50 mm
1.50 mm
5.70 mm
5.00 mm
17.00 mm
16.50 mm
18.50 mm
20.00 mm
25.50 mm
30.00 mm


20.00 mm
15.00 mm
12.00 mm
5.50 mm
13.50 mm
22.00 mm

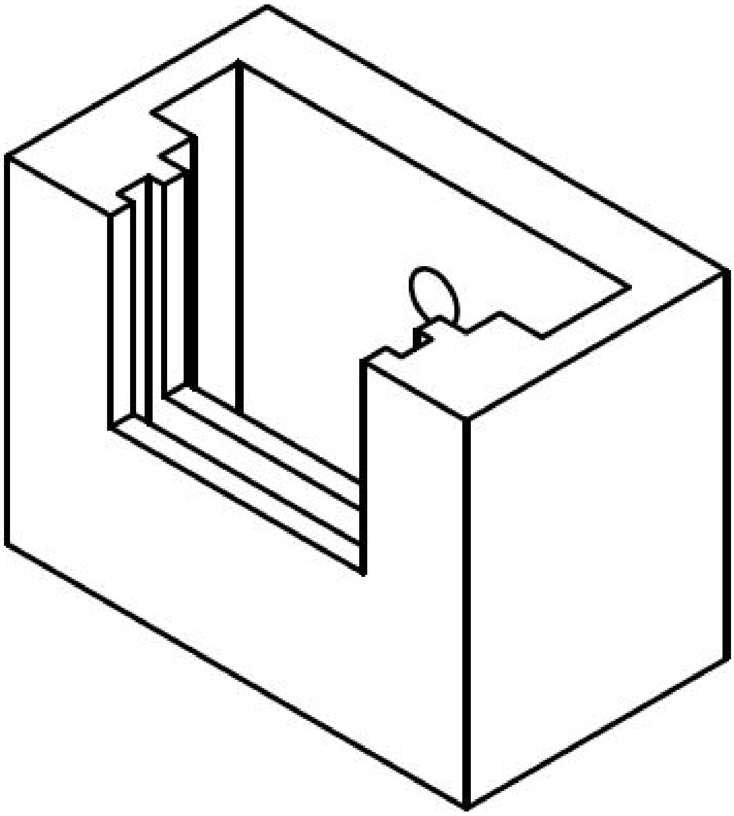


Fig S2 – Technical -drawing, front, top, cut along A-A and perspective view, of the of the LED and ISL29125 holder.

Complexes stability constants

	Fe-SCN [1]	Fe-F [2]
log β1	2.09	5.5
log β2	3.30	9.7
log β3		12.7
log β4		14.9
log β5		15.4

Table S1 –Stability constants of Fe/SCN and Fe/F complex.

Visible spectra

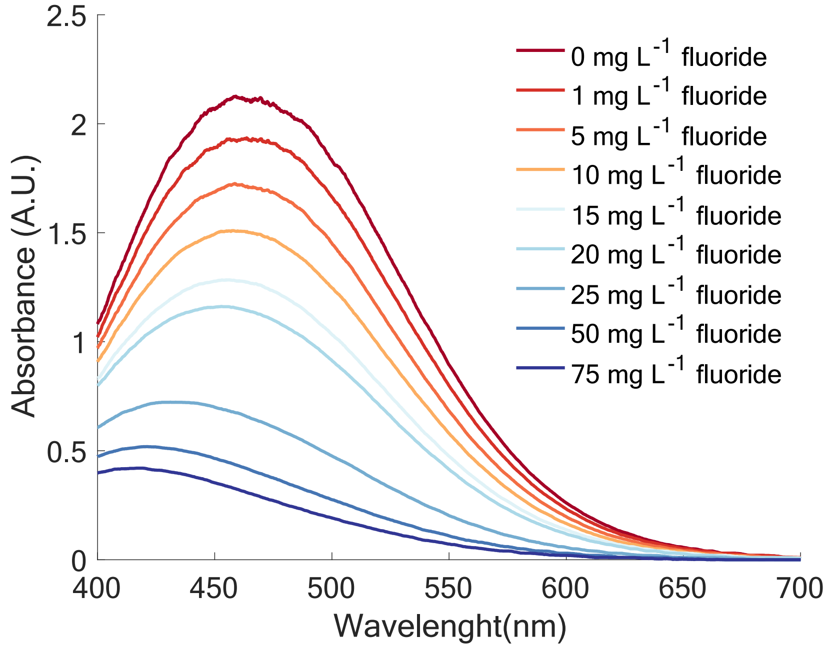


Fig S3 – Visible absorption spectra of Fe-SCN system with different concentrations of fluorides.

Sensor spectra response

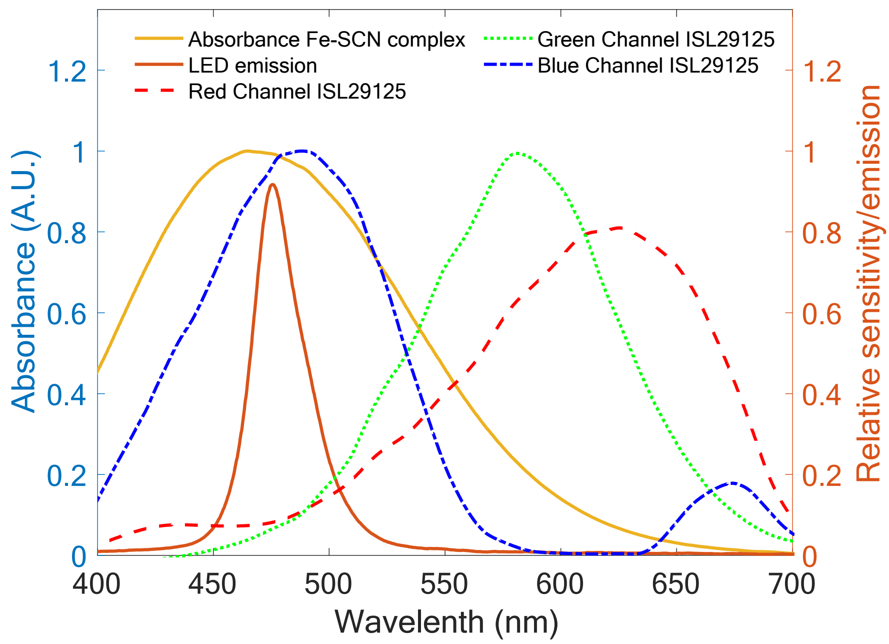


Fig S4 - Normalized spectral response for ambient light sensing for ISL29125 sensor, LED emission and Fe-SCN complex absorbance in the visible region.

Water quality parameters

Sampling location and fluoride content

Sample Number	Type	Latitude	Longitude	Altitude (m)	pH	Fluoride (mg/L) Ionic chromatography	Fluoride (mg/L) Proposed method
1	Groundwater	-3.376808	36.664889	1377	7.31	2.8	2.4 ±0.8
2	Groundwater	-3.407544	36.675525	1312	7.48	5.6	5.8±0.7
3	Groundwater	-3.445592	36.706356	1245	8.01	7.2	8±1
4	Groundwater	-3.370583	36.712331	1435	6.76	0.7	0.8±0.7
5	Groundwater	-3.400758	36.658033	1328	7.71	4.1	3.8±0.7
6	Groundwater	-3.346325	36.684417	1504	7.09	2.1	2.8±0.7
7	Groundwater	-3.390725	36.736778	1355	7.33	1.5	1.3±0.6
8	Groundwater	-3.3655	36.716786	1465	6.88	0.8	0.6±0.6
9	Groundwater	-3.397025	36.724722	1323	7.15	1.6	1.0±0.7

Table S2a – Sampling location, pH and fluoride content of natural water samples.

Sample Number	Anions (mg/L)			Cations (mg/L)			
	Cl^-	NO_3^-	SO_4^-	Na^+	K^+	Mg^{2+}	Ca^{2+}
1	67.0	198.9	46.7	167.6	67.4	14.3	56.9
2	68.3	53.4	24.7	221.0	40.6	11.6	36.6
3	15.7	10.3	6.4	178.6	17.0	2.6	7.4
4	40.1	147.5	25.1	43.8	15.8	23.1	53.1
5	17.9	8.1	17.0	217.3	29.5	6.8	18.4
6	52.2	127.9	48.5	122.9	33.0	12.9	35.9
7	30.8	50.0	16.3	31.8	5.2	22.2	39.8
8	30.0	95.6	8.4	34.9	10.2	13.8	37.5
9	27.5	56.3	3.2	52.4	10.0	27.4	49.7

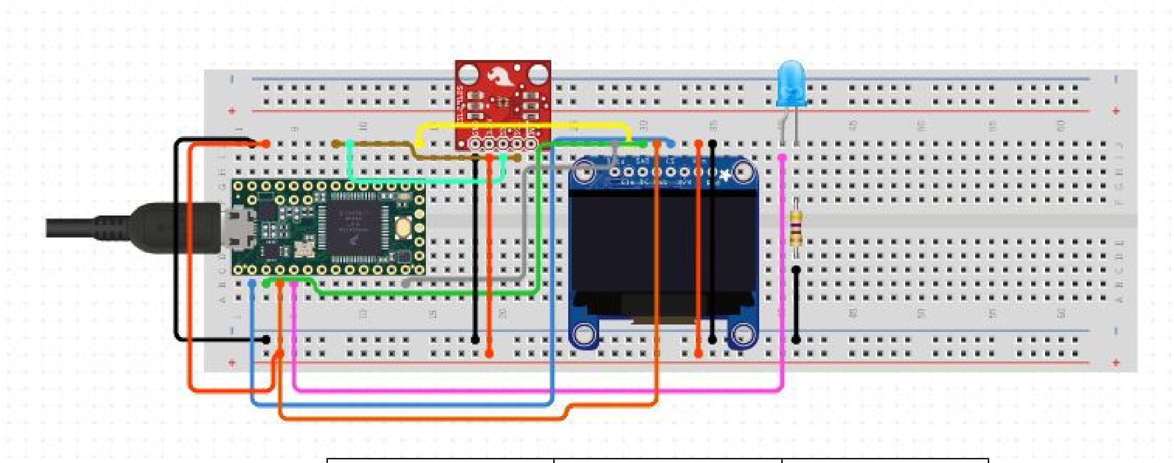
Table S2b – Anion and cation content of natural water samples.

Sample Number	EC (mS/m)	ORP (mV)	DO (mg/L)	Alkalinity (meq/L)
1	136.5	197	1.72	6.26
2	169.9	218	1.76	8.95
3	78.4	175	3.92	7.25
4	69.7	268	2.22	2.72
5	105.7	174	2.13	9.57
6	91.0	158	3.62	4.10
7	50.6	184	2.63	3.04
8	48.5	180	1.85	1.95
9	66.7	176	1.56	5.10

Table S2c – Electrical conductivity (EC), Oxidation Reduction Potential (ORP), dissolved oxygen (DO) and alkalinity of natural water samples.

Arduino circuit

Connection on the protoboard



Arduino	OLED	ISL29125
5V	VCC	--
3V3	--	3.3V
GND	GND	GND
A4	SDA	SDA
A5	SCL	SCL

Fig S5 – Connection diagram used in the Arduino circuit

PCB design

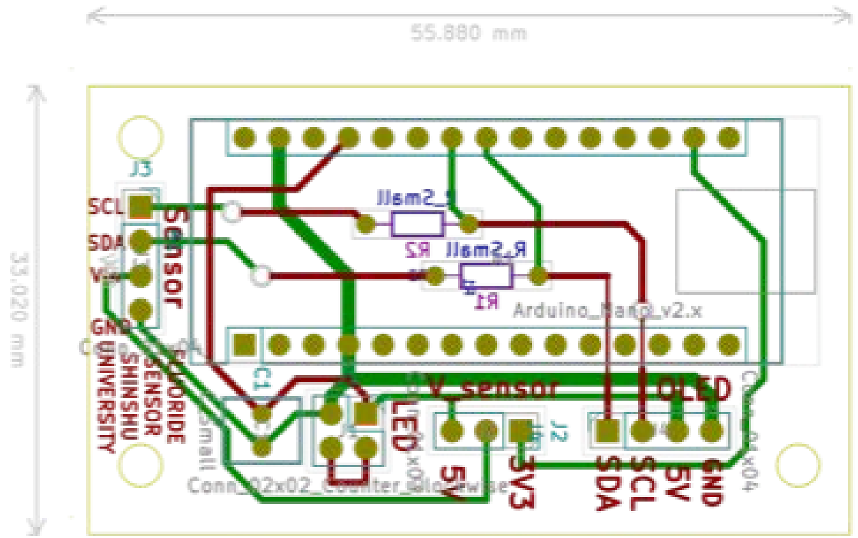


Figure S6 – PCB design for the fluoride sensor. R1 and R2 are 100Ω, C1 is 0.1µF, LED is a socket for the LED and a resistance to control the light emission intensity, and V_sensor is a jumper to regulate voltage for the sensor, ISL29125 sensor is 3.3V.

Calibration curve using ISL29125

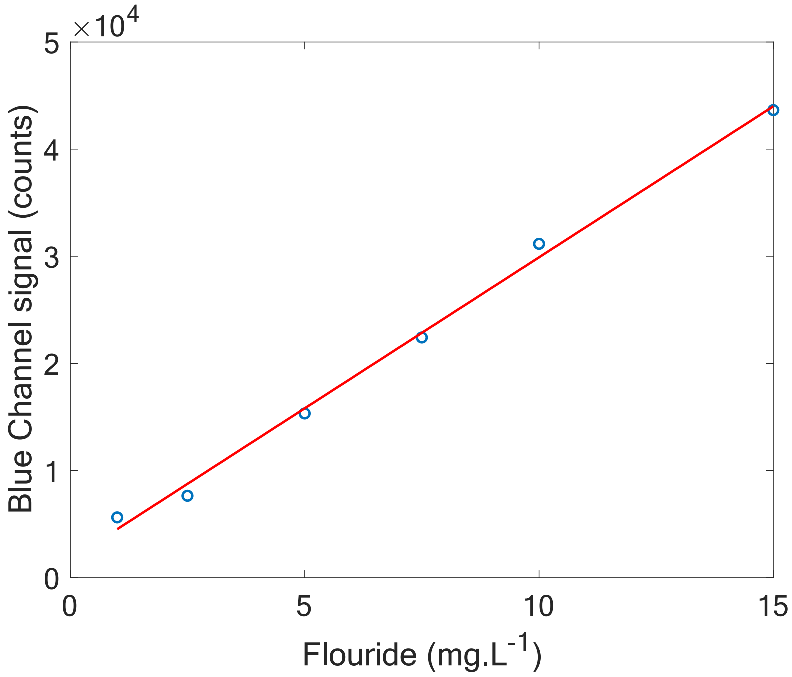


Fig S7 – Calibration curve of Fe-SCN / fluoride system in solution using ISL29125 sensor as detector and OSB5DL3E34B LED as light source.

Arduino program

Full code to use an OLED screen and serial port data export.

```
#include <Wire.h>
#include "SFE_ISL29125.h"
#include <Adafruit_SSD1306.h>
#include <Adafruit_GFX.h>

// Wiring: SDA pin is connected to A4 and SCL pin to A5.
// Declare sensor object
SFE_ISL29125 RGB_sensor;

// Comment to eliminate the OLED from the device
// Wiring: SDA pin is connected to A4 and SCL pin to A5.
#define SCREEN_WIDTH 128 // OLED display width, in pixels
#define SCREEN_HEIGHT 64 // OLED display height, in pixels
Adafruit_SSD1306 display(SCREEN_WIDTH, SCREEN_HEIGHT, &Wire, -1);
//
void setup()
{
  // Initialize serial communication
  Serial.begin(115200);

  // Initialize the ISL29125 with simple configuration so it starts
sampling
```

```
  if (RGB_sensor.init())

if(!display.begin(SSD1306_SWITCHCAPVCC, 0x3C)) { // Address 0x3D for 128x64
  Serial.println(F("SSD1306 allocation failed"));
  for(;;);
}

// Comment to eliminate the OLED from the device
delay(2000);
display.clearDisplay();
display.setTextColor(WHITE);

// Initial text
  display.setTextSize(1.5);
  display.setTextColor(SSD1306_WHITE);
  display.setCursor(0,0);
  display.print("Fluoride sensor");
  display.setCursor(0,16);
  display.print("Shinshu University");
  display.setCursor(0,32);
  display.println("v 1.03");
  display.setCursor(0,0);
  display.display(); // actually display all of the above
  Serial.println("Fluoride sensor");
  Serial.println("Shinshu University");
  Serial.println();

delay(2000);
display.clearDisplay();
//
  {
    Serial.println("Sensor Initialization:");
    Serial.println("Successful\n\r");
  }
}

// Read sensor values for each color and print them to serial monitor
void loop()
{
  // Read sensor values (16 bit integers)
 unsigned int blue = RGB_sensor.readBlue();

delay(100);

if (blue <= 27589) { // replace this values with your calibration curve
// Measurement results
// Comment to eliminate the OLED from the device
  display.setTextSize(3);
  display.setTextColor(SSD1306_WHITE);
  display.setCursor(0,0);
  display.print("Water");
  display.setTextSize(3);
  display.setCursor(0,32);
  display.print("OK");
  display.display();
  delay(4000);
  display.clearDisplay();
//
  Serial.print((blue-float(23165))/float(2949),1); // Idem
  Serial.println("ppm");
  Serial.println("WATER OK - Fluoride < 1.5ppm");
```

```
  Serial.println();
  }
else if (blue > 27589) { // replace this values with your calibration curve
// Measurement results
// Comment to eliminate the OLED from the device
  display.setTextSize(3);
  display.setTextColor(SSD1306_WHITE);
  display.setCursor(0,0);
  display.print("Don't");
  display.setTextSize(3);
  display.setCursor(0,32);
  display.print("Drink");
  display.display();
  delay(4000);
  display.clearDisplay();
//
  Serial.print((blue-float(23165))/float(2949),1); // Idem
  Serial.println("ppm");
  Serial.println("DON'T DRINK - Fluoride > 1.5ppm");
  Serial.println();
  }

}
\
```

Chemical interferences

Anions

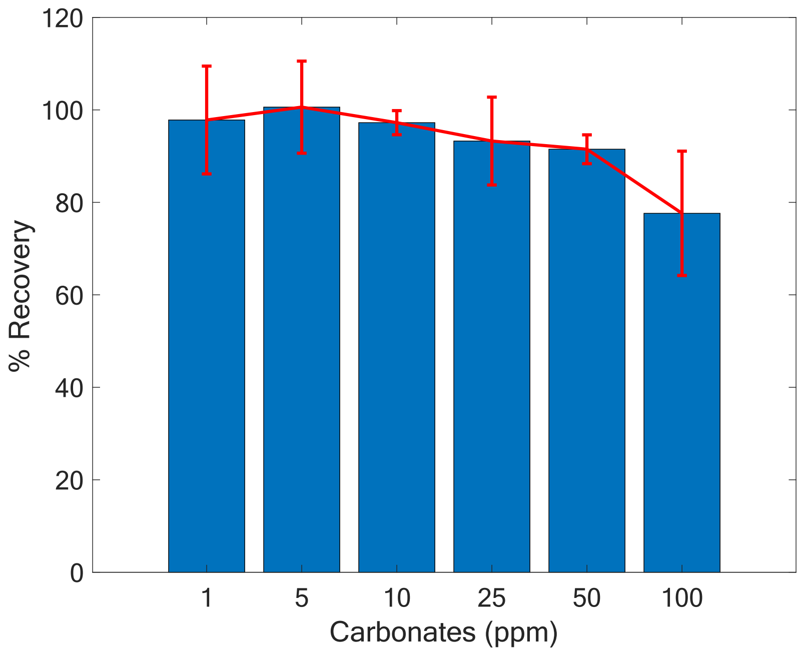


Fig S8 – Influence of carbonate interference in fluoride quantification, $[F^-]$ = 5ppm.

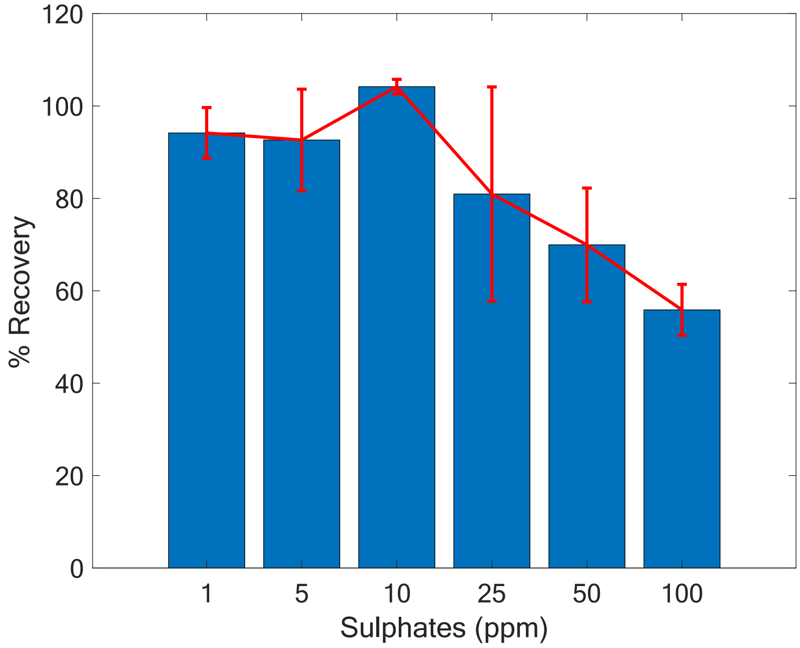


Fig S9 – Influence of sulphate interference in fluoride quantification, $[F^-]$ = 5ppm.

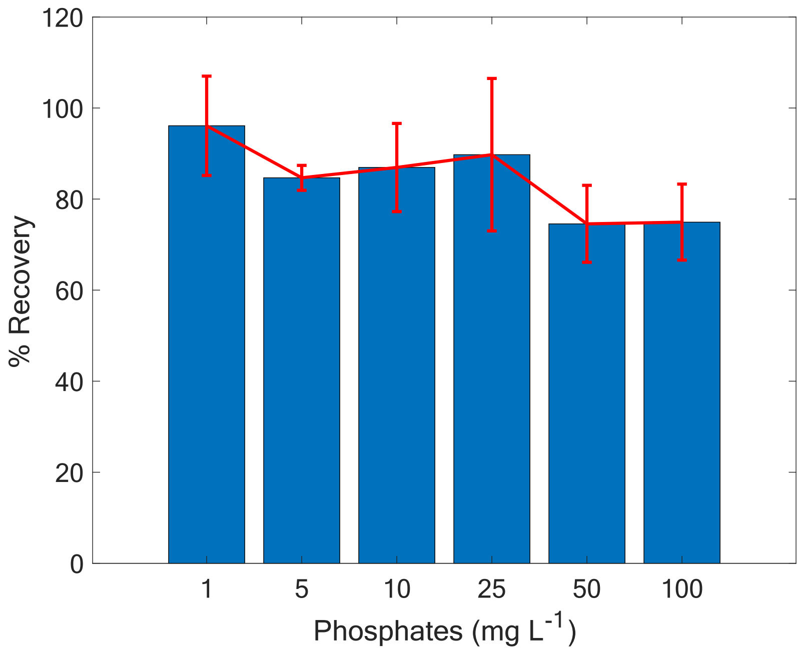


Fig S10 – Influence of phosphate interference in fluoride quantification, $[F^-]$ = 5ppm.

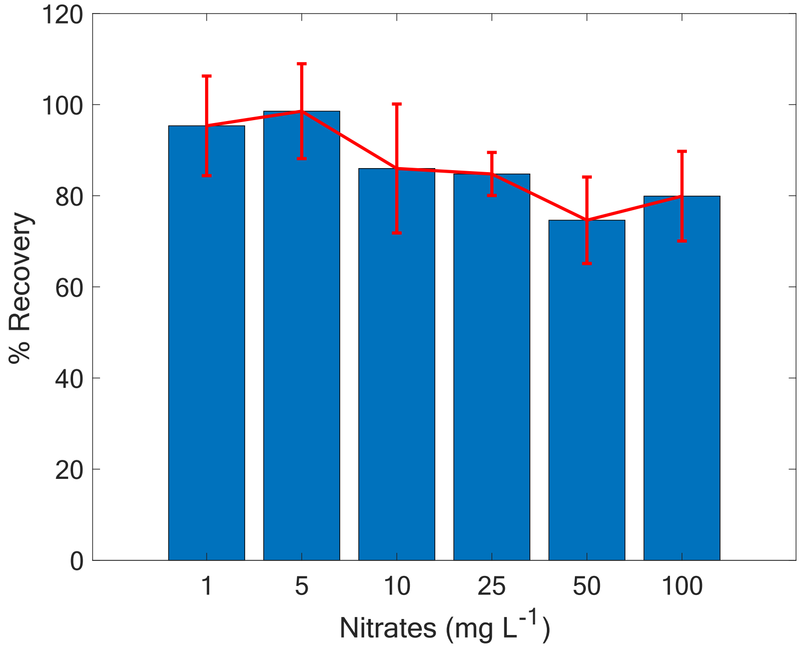


Fig S11 – Influence of nitrate interference in fluoride quantification, [F$^-$] = 5ppm.

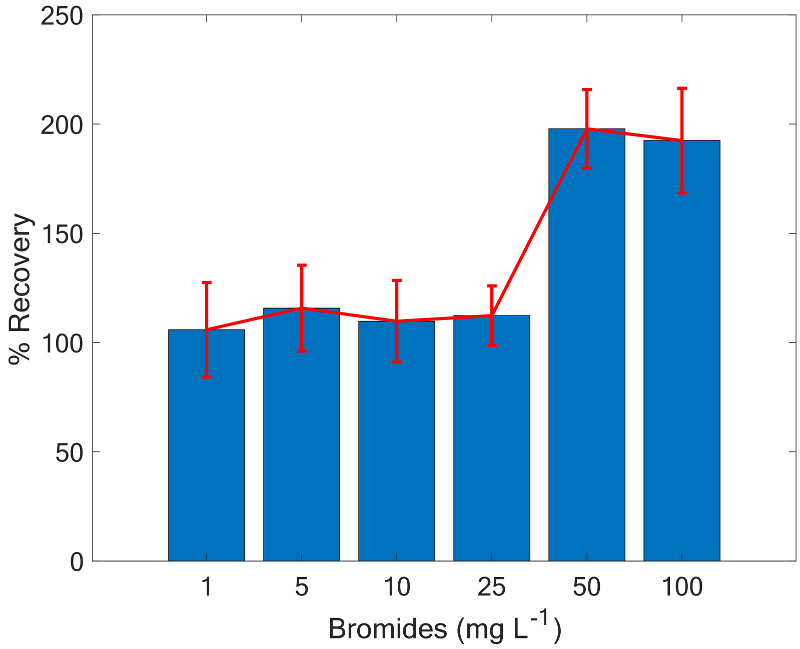


Fig S12 – Influence of bromide interference in fluoride quantification, [F$^-$] = 5ppm.

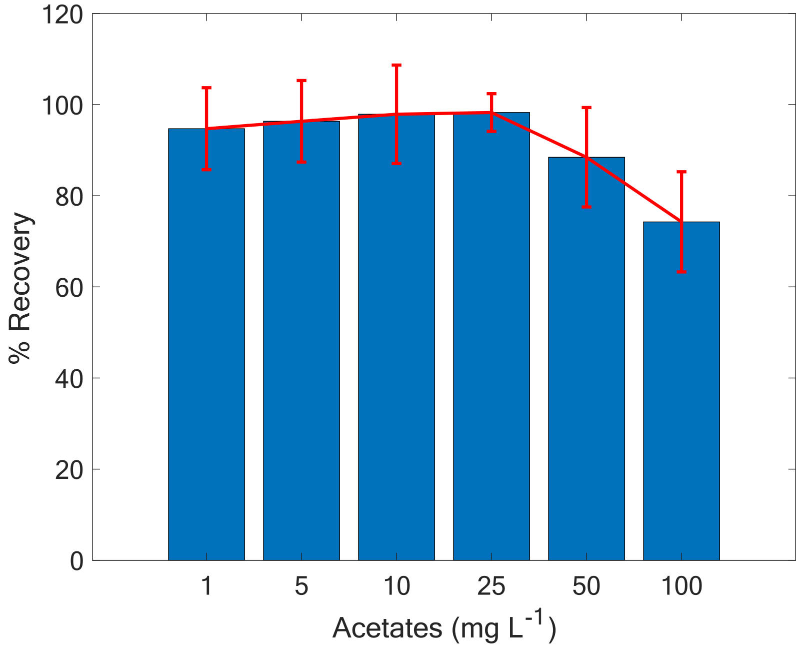


Fig S13 – Influence of acetate in fluoride quantification, [F$^-$] = 5ppm.

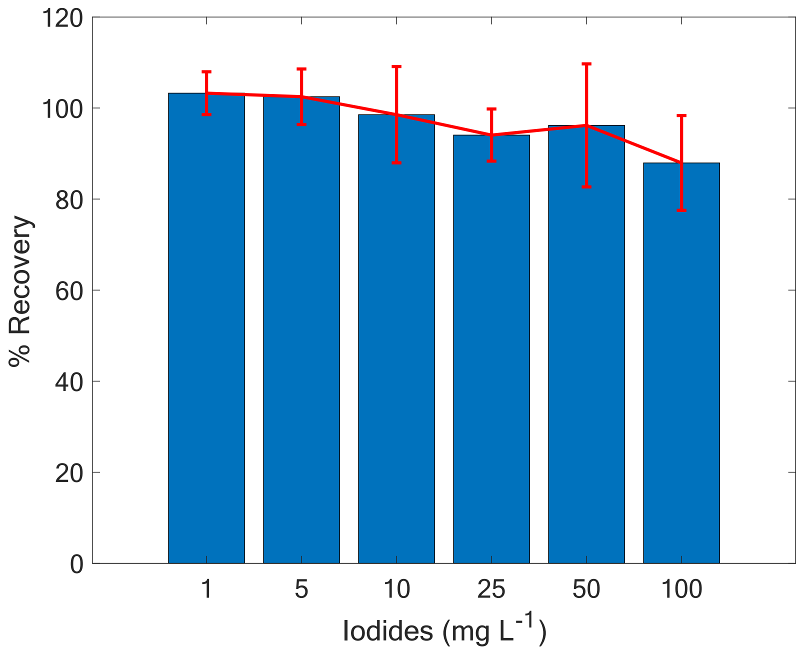


Fig S14 – Influence of iodide in fluoride quantification, [F$^-$] = 5ppm.

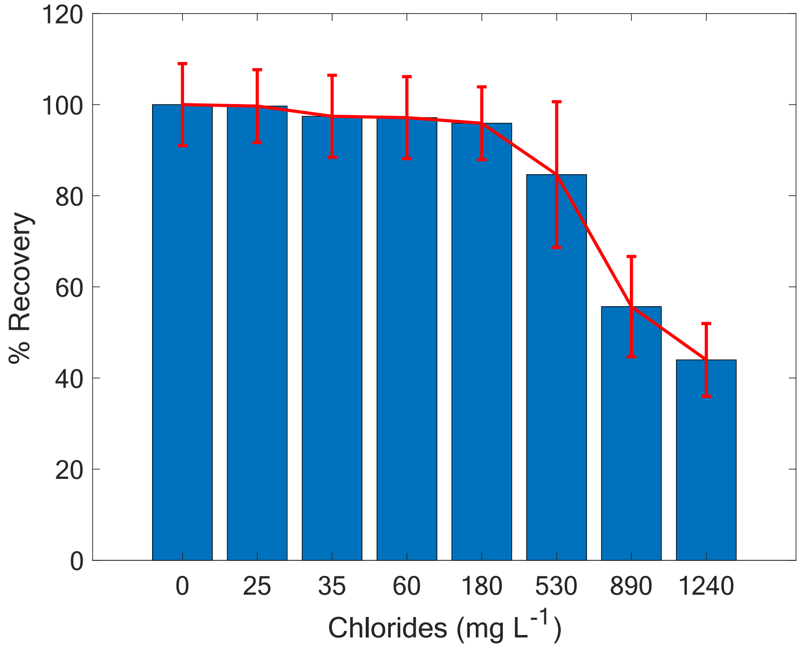


Fig. S15- Influence of Chlorides in fluoride quantification, [F^-] = 5ppm

Cations

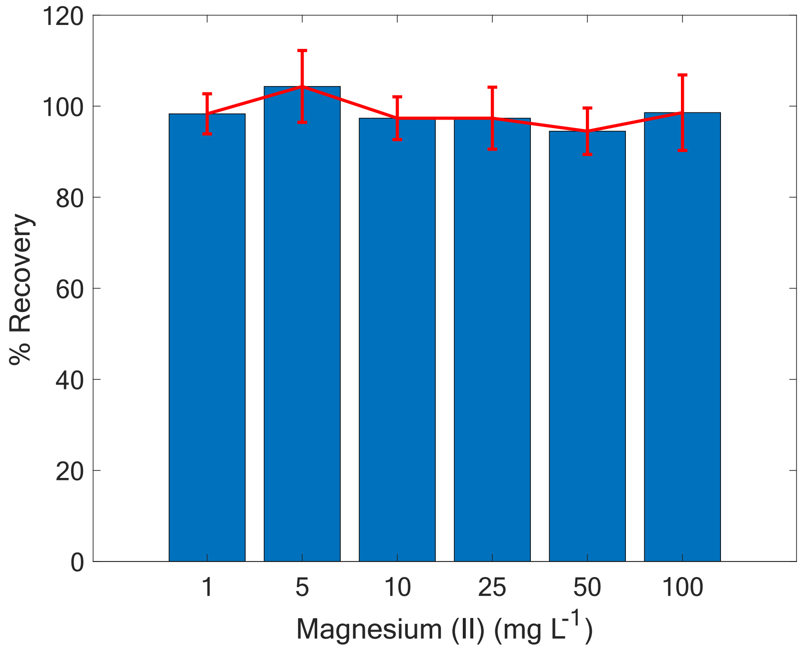


Fig S16 – Influence of magnesium (II) interference in fluoride quantification, [F^-] = 5ppm.

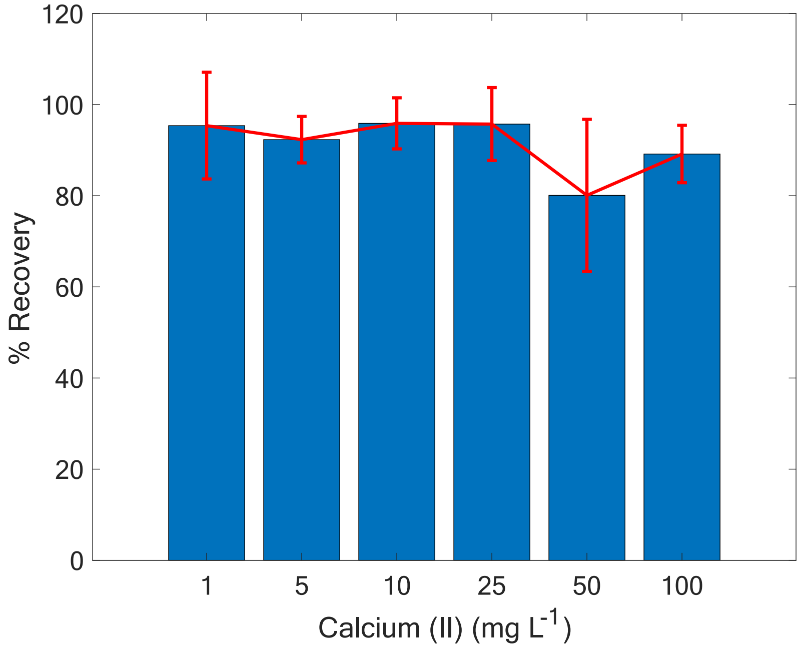


Fig S17 – Influence of calcium (II) interference in fluoride quantification, [F^-] = 5ppm.

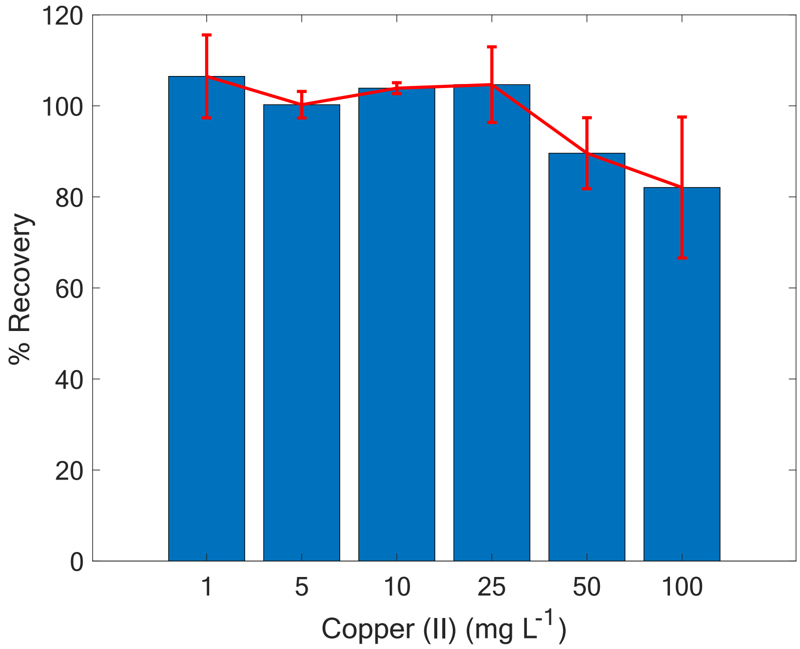


Fig S18 – Influence of copper (II) interference in fluoride quantification, [F^-] = 5ppm.

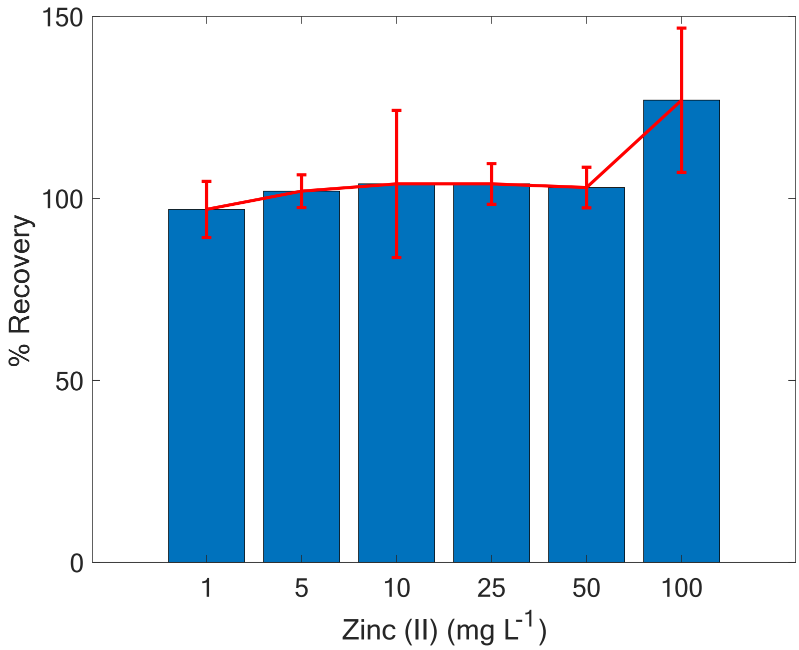


Fig S19 – Influence of zinc (II) interference in fluoride quantification, [F^-] = 5ppm.

References

(1) Complexation of Iron(III) with Thiocyanate Ions in Aqueous Solution https://www.jstage.jst.go.jp/article/analsci1985/8/4/8_4_521/_article (accessed Jun 8, 2020).

(2) Arribas Jimeno, S.; Hernandez Mendez, J.; Lucena Conde, F.; Burriel Marti, F. *Química analítica cualitativa*, Paraninfo.; 2002.