Supporting Information

Colorimetric sensing of calcium carbide over banana peel using 5,5′-dithiobis-(2-nitrobenzoic acid) (DTNB) as rapid chemoreceptor: A point of care tool for food fraud analysis

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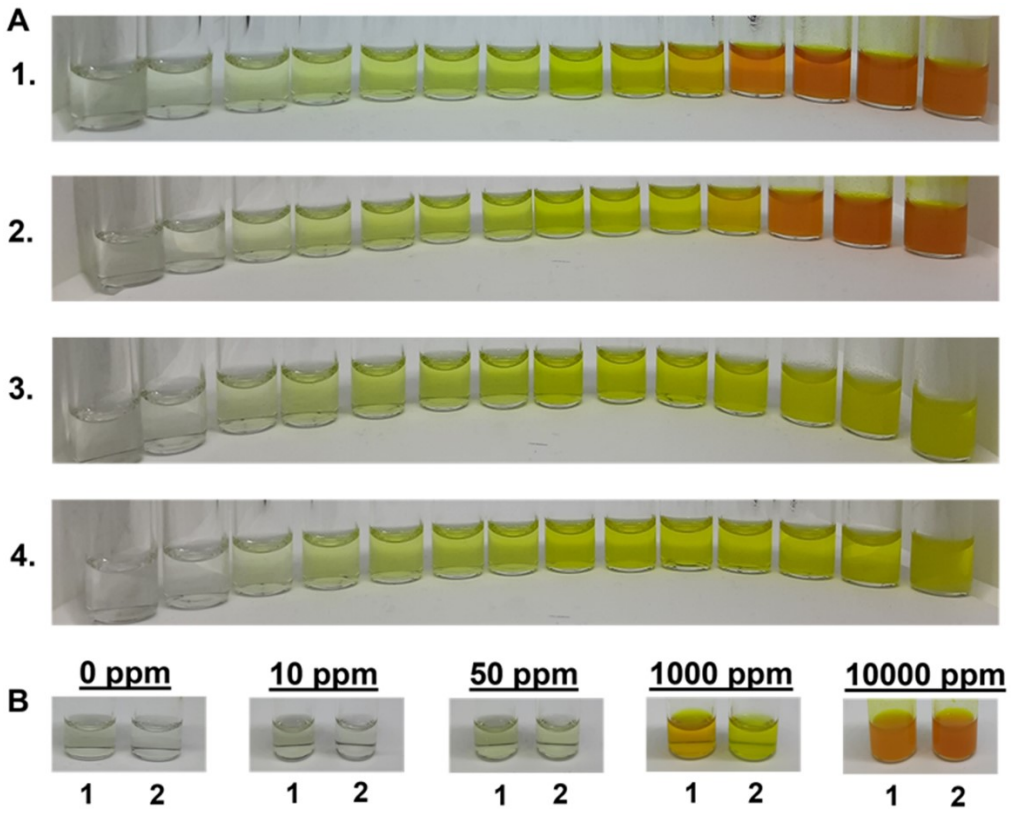

Fig. S1 (A) Optimization of concentration, volume, and pH of DTNB and CaC_2 for different concentrations (0, 10, 50, 100, 150, 200, 250, 500, 750, 1000, 20000, 4000, 6000, and 10000 ppm). 15mM DTNB 9 pH (150 µL), CaC_2 (850 µL) condition showed the highest intensity of colorimetric signals among all four cases i.e., 1. 15mM DTNB 9 pH (150 µL), CaC_2 (850 µL), 2. 15mM DTNB 7 pH (150 µL), CaC2 (850 µL), 3. 0.5mM DTNB 9 pH (150 µL), CaC2 (850 µL), 4. 0.5mM DTNB 7 pH (150 µL), CaC_2 (850 µL, and **(B)** Optimization of pH 9 (1) & 7 (2), pH 9 showed the high intensity of color at lower concentration of CaC_2.

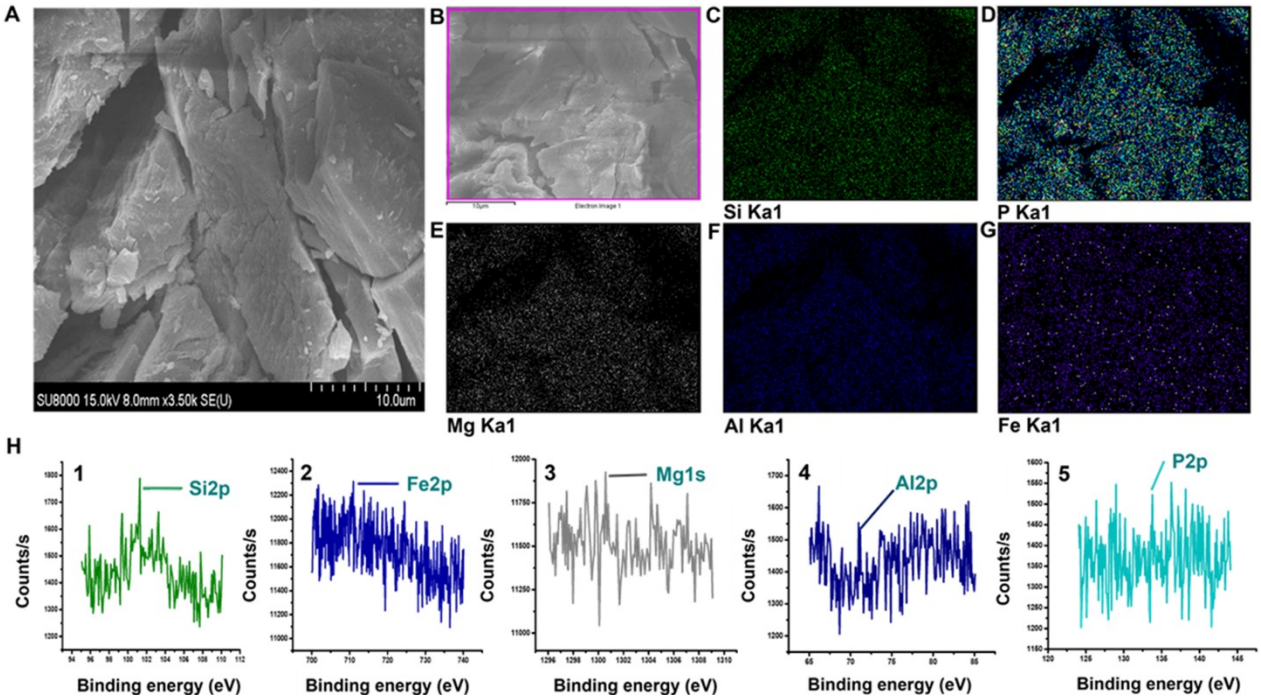

Fig. S2 (A) SEM image of CaC_2 at 10 µm. **(B–G)** Distribution of all elements and their core level studies based on SEM mapping. **(H-1–5)** XPS data of CaC_2.

Table S1 High content of sulfur impurities were detected using X-ray fluorescence (XRF) analysis which is responsible for the colorimetric detection of CaC_2.

Analyte	Results (ppm)
Ca	680,500
S	108,400
Si	56,100
Al	52,900
Fe	52,100
Sr	49,700
P	49,600
Mg	0.00

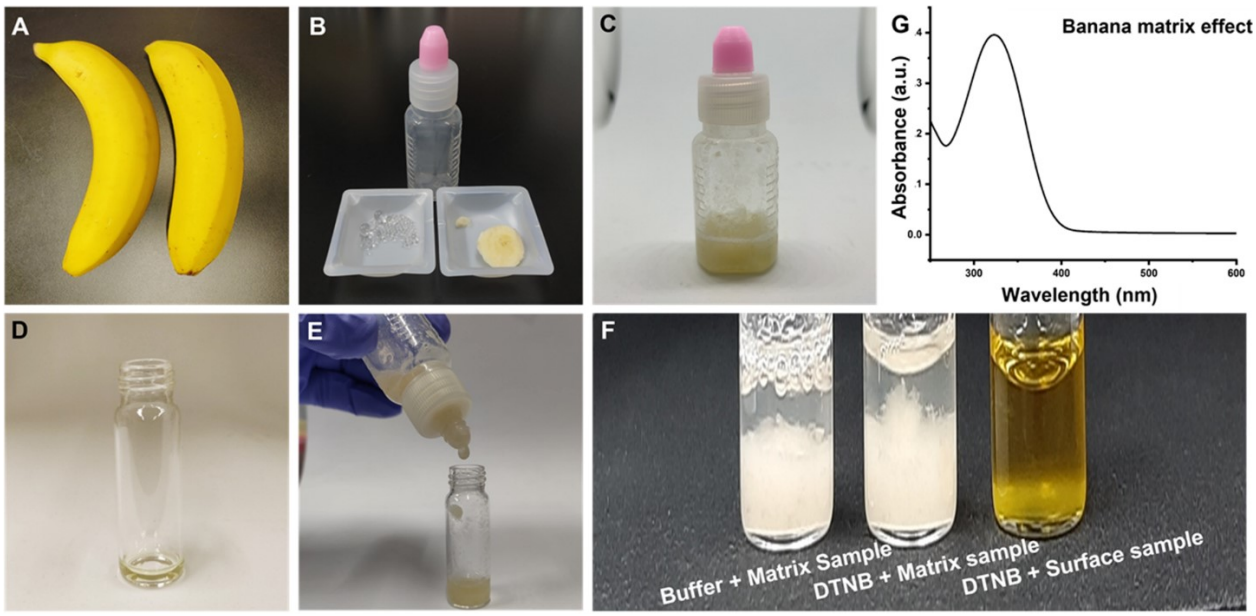

Fig. S3 (A-F) Procedure to cross-check and confirm the selectivity and performance of the developed sensor for matrix effect and **(G)** UV-Spectra of matrix effect, which confirms banana matrix does not play any role in colorimetric signal. Thus, banana matrix has no effect.

Table S2 Quantification of sulfhydryl concentrations in unknown solutions

Standard sample (CaC_2)			Unknown sample (CaC_2)		
Sr. No.	**Sulfhydryl concentration (ppm)**	**CaC_2 Concentration (ppm)**	**Sr. No.**	**Sulfhydryl concentration (ppm)**	**CaC_2 Concentration (ppm)**
	323 nm			323 nm	
1	0	0			
2	0.05	10			
3	0.174	50			
4	0.25	100			
5	0.55	500	3	0.778	654.0877
6	1.38	1000			
7	3.55	2000	4 and 1	4.73 and 5.72	2664.78 and 3222.5
8	6.90	4000	2	7.53	4365.21

To calculate the sulfhydryl concentration in moles/L of unknown sample. The reported molar absorptivity (molar extinction coefficient, which is expressed in units of M^{-1} cm^{-1} of TNB in this buffer system at 412nm is 14,150.2 Molar absorptivity, E, is defined as follows:

$E = A/bc$ (1).

where A = absorbance, b = path length in centimeters, c = concentration in moles/liter (M)

Solving for concentration gives the following formula: $c = A/b\ E$ (2).

For unknown sample (a), applied equation (2); A = 0.294, b = 1cm and E = 14,150 M^{-1} cm^{-1}. Therefore, $c = 0.294/1(14,150) = 2.07\times10^{-5}$ M.

This value represents the concentration of the solution in the spectrophotometric cuvette. To calculate the concentration of the unknown sample, it is necessary to account for dilution factors as follows:

The total volume of the solution is measured as follows

0.85 mL of unknown sample + 0.15 mL of Ellman's Reagent Solution = 1 mL of solution

If the concentration of the assay solution is 2.07×10^{-5} M, then 1mL of that solution contains

$1mL \times 1\ L/1000\ mL \times (2.07\times10^{-5}\ M) = 2.07\times10^{-8}\ M$

This 2.07×10^{-8} M of sulfhydryl in the assay solution were contributed by the original 0.85 mL sample. Therefore, the concentration of free sulfhydryl in the original unknown sample is

$2.07\times10^{-8}\ M/0.85\ mL\times1000\ mL/L = 2.4\times10^{-5}$ M

Further applied blank correction for the unknown sample to get the final value

2.94×10^{-5} M (blank) - 2.4×10^{-5} M = 5.88×10^{-6} M

Similarly for unknown sample b, c, and d free sulfhydryl concentration is -7.58×10^{-6} M, 2.25×10^{-6} M, and 1.27×10^{-5} M respectively.

Finally, to convert M to g/L

5.88×10^{-6} M×396.34 (molar mass of DTNB) × 1000 = 5.72 g/l

As we know, 1g/l=1ppm. So, 5.72 g/l = 5.72 ppm

Thus, unknown sample b, c, and d free sulfhydryl concentration in ppm is 7.53 ppm, 3.6 ppm, and 4.73 ppm, respectively.

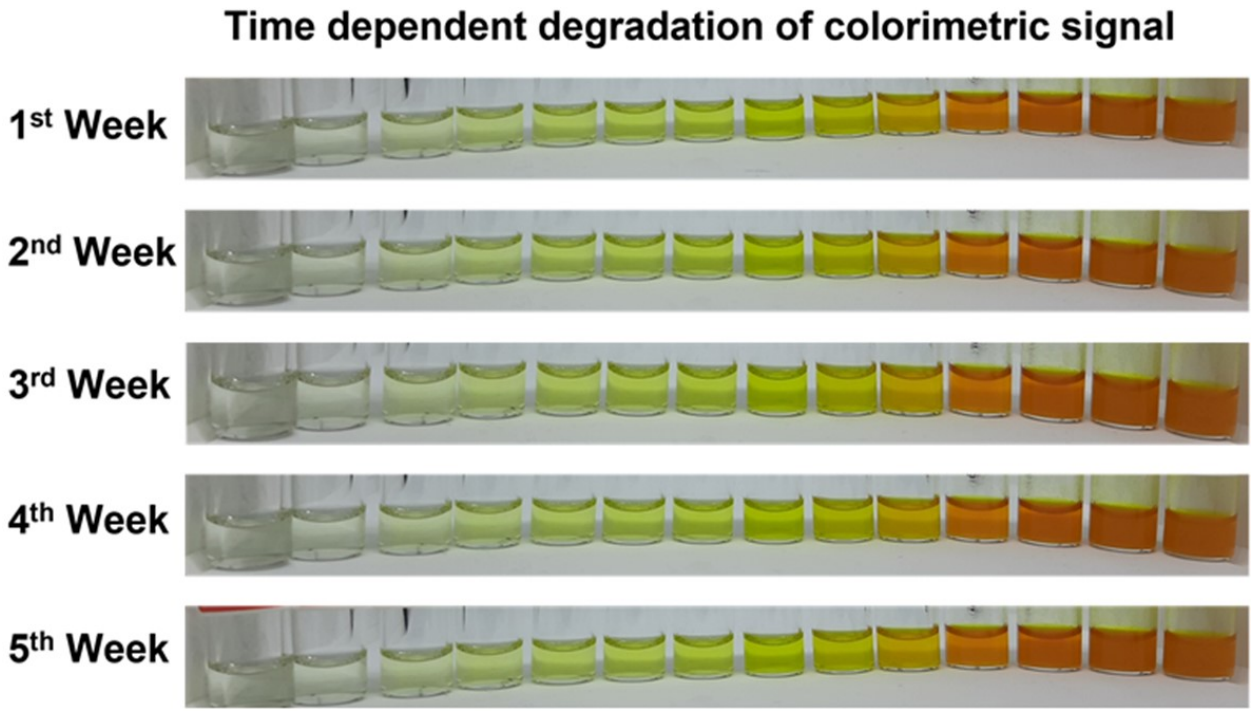

Fig. S4 Time dependent degradation of color till 5 weeks. Until 5th week there no color change noticed, as a result it is concluded that, presented assay is highly stable.

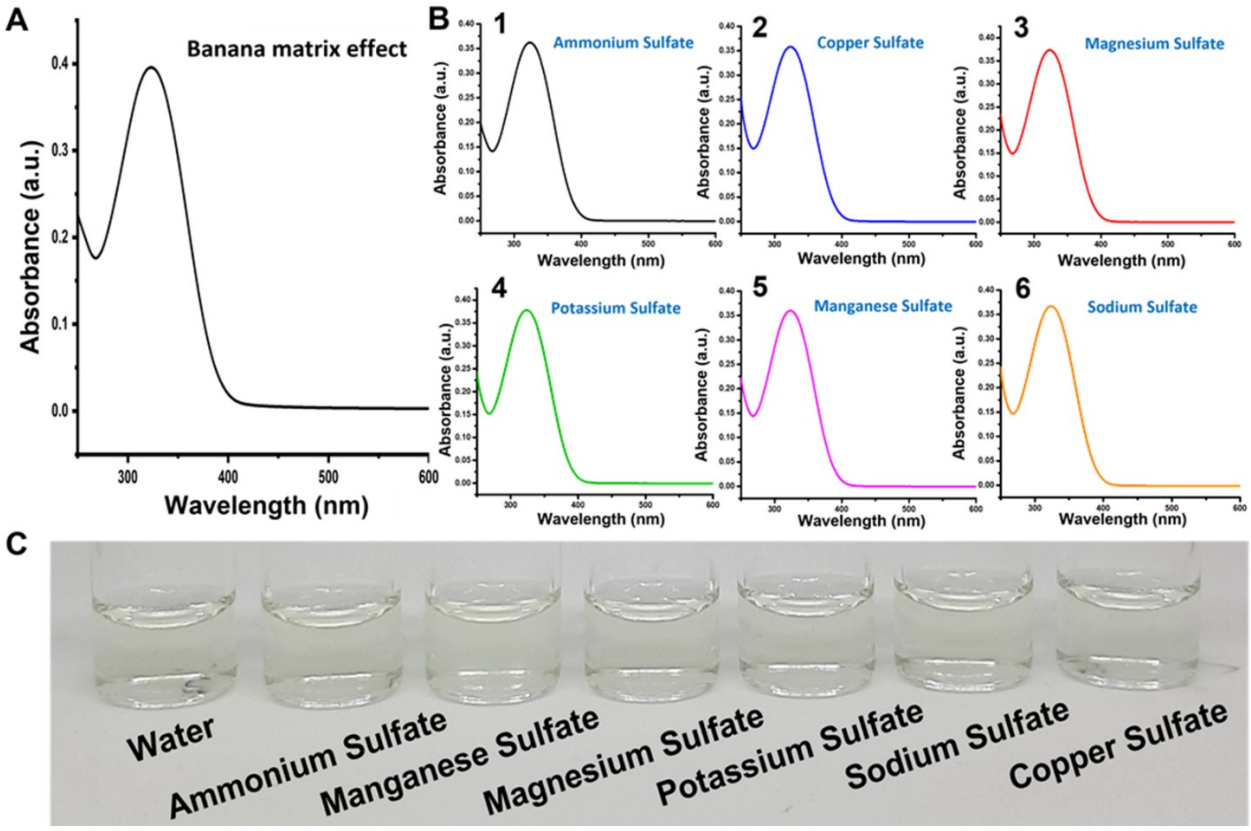

Fig. S5 (A) No interference effect of banana matrix in the presented assay, **(B)** UV-Spectra of other sulfates salts for cross check and **(C)** Colorimetric assay of other sulfate salts (no interference).

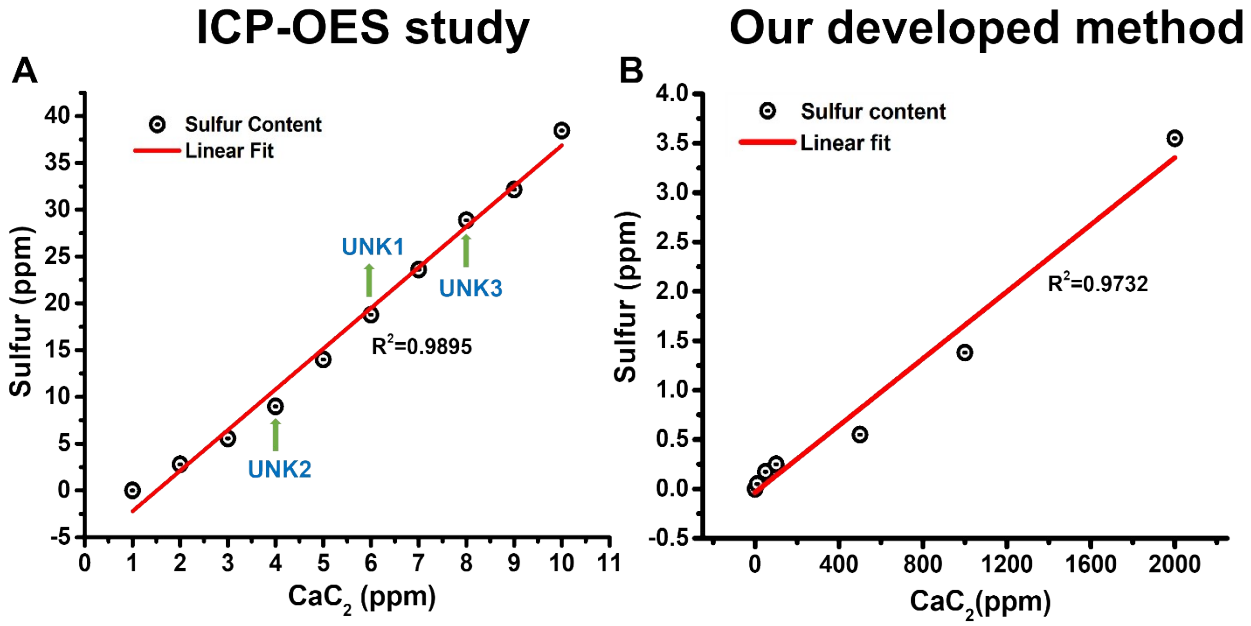

Fig. S6 Comparative study and validation of our developed method. **(A)** Inductively coupled plasma optical emission spectroscopy (ICP-OES) analysis of sulfur content in standard and unknown (UNK) concentration of CaC_2 and **(B)** our developed DTNB sensor analysis of sulfur content in standard concentration of CaC_2. Both methods follows a linear pattern for detecting sulfur content in CaC_2 samples. Thus, our method is precise and validate for detecting CaC_2 in artificially ripened fruit.

Table S3 Validation data of developed method compared with ICP-OES

CaC_2 concentration (ppm)	Developed method			ICP-OES conventional analysis of trace sulfur (ppm)
	Absorbance		Color development	
	323 nm	412 nm		
	DTNB	TNB		
0 ppm	0.354	0	No	0 ppm
10 ppm	0.352	0	No	2.802 ppm
50 ppm	0.348	0	Yes	5.56 ppm
100 ppm	0.34	0	Yes	13.994 ppm
500 ppm	0.343	0	Yes	23.61 ppm
1000 ppm	0.319	0.058	Yes	32.16 ppm
2000 ppm	0.244	0.189	Yes	38.46 ppm