Data Article

Data on spot–kits versus titration method for iodine determination in salt: Performance and validity

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Abstract

The aim of this data is comparison of achieved data from salt iodine measurement by titration method with using sodium thiosulfate in presence of lugol's reagent and commercial spot- kit. Titration measurement was carried out in two different laboratories using standard samples. 437 samples including 20 commercial brands were collected throughout Iran. The iodine contents of the samples were measured by both the titration method and two most frequently used spot-kit brands in Iran. There is no significant difference between the results obtained from the two brands of spot-kits (ICC = 0.797). The kits sensitivity for determination of negative samples was high (more than 0.9) but by increasing the iodine concentration up to 15 ppm, the kits’ sensitivity was decreased. These findings indicate that the titration method is necessary for quantitative purposes, especially for concentrations higher than 30 ppm. However, spot-kits are suitable for qualitative and semi-quantitative measurements.

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Specifications table

| Subject area          | Food Chemistry          |
|-----------------------|-------------------------|
| More specific subject area | Iodine determination |
| Type of data         | Tables, Figure          |
| How data was acquired | 20 random commercial brands including 437 samples were gathered around the Iran and their iodine contents were measured by titration method in two different labs for validation of measured values. |
| Data format          | Raw, Analyzed           |
| Experimental factors | The mentioned parameters above, in abstract section, were analyzed according to the standards. |
| Experimental features | Iodine determination in salt |
| Data source location | Tehran University of Medical Sciences, Tehran, Iran |
| Data accessibility   | The data are available with this article |
| Related research article | Pandav CS, Arora NK, Krishnan A, Sankar R, Pandav S, Karmarkar MG. Validation of spot-testing kits to determine iodine content in salt. Bulletin of the World Health Organization. 2000;78(8):975-80. |

Value of the data

- This data can be used for insure health managers that spot kits have appropriate validity for salt iodine concentration monitoring programs.
- As this data is shown, spot-kits are cost effective method for rapid monitoring of salt iodine concentration in low income countries.
- This data is useful for comparison of available commercial spot-kits, produced around the world for determination of invalid commercial brands.

1. Data

The values of iodine content of real samples measured by both the reference method and the spot-kits A and B are shown in Tables 1 and 2, in four different ranges: 0 to ≤ 8, 8 to ≤ 15, 15 to ≤ 30 and ≥ 30 ppm. Linear regression fit of the iodine values measured by the titration method, as reference method, in two different labs gave an R² value of 0.9537. Therefore results achieved from the titration method are valid. Tables 3 and 4 contain sensitivity, specificity, positive predictive values (PPV) and negative predictive values (NPV) of the spot-kit A and spot-kit B. Tables 3 and 4 have two categories including presence or absence of iodine (0 ppm or not) and presence or absence of significant amount of iodine (≤ 15 ppm or > 15 ppm). In order to compare the two brands of spot-kits, the interclass correlation (ICC) analysis was performed using the results shown in Tables 1 and 2. The outcome of ICC is summarized in Table 5.

Table 1
Comparison of the titration method and spot-kit A in determination of iodine content in salt.

| Spot-testing kit A (ppm of iodine) | Iodine concentration by iodometric titration (ppm) | Total |
|-----------------------------------|--------------------------------------------------|-------|
|                                   | 0 to ≤ 8 | 8 to ≤ 15 | 15 to ≤ 30 | ≥ 30 |       |
| 0 to ≤ 8                          | 19       | 10        | 55         | 41   | 125(28) |
| 8 to ≤ 15                         | 2        | 6         | 88         | 101  | 197(45) |
| 15 to ≤ 30                        | 0        | 0         | 37         | 78   | 115(26) |
| ≥ 30                              | 0        | 0         | 0          | 0    | 0(0)   |
| Total                             | 21(4.8)  | 16(3.66)  | 180(41.1)  | 220(50.34) | 437    |
Table 2
Comparison of the titration method and spot-kit B in determination of iodine content in salt.

| Spot-testing kit B (ppm of iodine) | Iodine concentration by iodometric titration (ppm) | Total |
|-----------------------------------|--------------------------------------------------|-------|
|                                   | 0 to \( \leq 8 \) | 8 to \( \leq 15 \) | 15 to \( \leq 30 \) | \( \geq 30 \) |
| 0 to \( \leq 8 \)                | 19 | 9 | 56 | 38 | 122(27) |
| 8 to \( \leq 15 \)               | 2 | 7 | 85 | 100 | 194(44) |
| 15 to \( \leq 30 \)              | 0 | 0 | 39 | 82 | 121(27) |
| \( \geq 30 \)                    | 0 | 0 | 0 | 0 | 0(0) |
| Total                             | 21(4.8) | 16(3.66) | 180(41.1) | 220(50.34) | 437 |

Table 3
Spot-kit A validation using as a qualitative method.

| Interpretation of test | Indicators |
|------------------------|------------|
|                        | Sensitivity | Specificity | PPV\(^a\) | NPV\(^b\) |
| Iodine absence (0 ppm) | 0.96 (0.93–0.97) | 0.78 (0.4–0.97) | 0.99 (0.98–1) | 0.06 (0.03–0.1) |
| Iodine presence (> 0 ppm) | 0.76 (0.72–0.8) | 0.85 (0.68–0.95) | 0.98 (0.96–0.99) | 0.23 (0.15–0.31) |

\(^a\) Positive predictive value.  
\(^b\) Negative predictive value.

Table 4
Spot-kit B validation using a qualitative method.

| Interpretation of test | Indicators |
|------------------------|------------|
|                        | Sensitivity | Specificity | PPV | NPV |
| Iodine absence (0 ppm) | 0.91 (0.88–0.94) | 0.89 (0.52–1) | 1 (0.99–1) | 0.19 (0.08–0.31) |
| Iodine presence (> 0 ppm) | 0.76 (0.72–0.81) | 0.82 (0.65–0.93) | 0.98 (0.96–0.99) | 0.23 (0.15–0.31) |

Table 5
Summary of the ICC analysis of the results obtained from the two spot-kits.

| Kinds of test | Agreement |
|---------------|-----------|
| Test model    | One way   |
| Number of samples | 437    |
| ICC           | 0.797     |
| Rater         | 2         |
| Confidence interval | 0.95 |
| ICC range     | 0.761–0.829 |
| \( \alpha \)  | 0.887     |
2. Experimental design, material and methods

2.1. Setting up a calibration plot using the reference method

In order to set up a calibration plot using the titration method, as reference method, 200 g NaCl (analytical grade, MERK, GERMANY) was dissolved in 1000 mL distilled water and divided into four 250 mL aliquots. 10, 20, 40 and 80 μg potassium iodate (KIO₃) were added to each of the aliquots. Then, 1 mL H₂SO₄ (2 N) and 5 mL KI (10% w/v) were added to each aliquot and the mellow yellow color appeared. After 10 minutes in the dark, the solutions were titrated by 0.005 N Na₂S₂O₃ until light yellow color appeared. Then some drops of lugol’s iodine indicator were added and titration was continued until the solution turned colorless. The consumed volume of Na₂S₂O₃ was used to calculate iodine concentration according to Eq. (1) [1–10]:

\[ I = \left( \frac{V \times F \times 0.1058}{W} \right) \times 1000 \]  (1)

\( I \) = iodine concentration (μg/kg), \( V \) = consumed volume of Na₂S₂O₃ (mL), \( F \) = modifying coefficient for Na₂S₂O₃ solution, \( W \) = weight of dry salt sample (g)

The measured values were fitted against the real values of standard solutions in a linear regression model and the \( R^2 \) was achieved.

2.2. Measurement of the iodine contents of real samples

After setting up a calibration plot using the titration method, iodine contents of real samples were measured by titration method. In this step, 20 random commercial brands including 437 samples were gathered around the Iran and their iodine contents were measured by this method in two different labs for validation of measured values. The results obtained in both labs were fitted in a linear regression model. Achieved \( R^2 \) was 0.993 that shows there is not any significant differences between achieved data in two labs.

In the next step, the iodine content of all the samples were measured by two available brands of spot-kits. To this purpose, one drop of each kit’s indicator was added to the samples to produce color. Produced color was compared to a color standard series. In order to determine the degree of agreement between two kits, the interclass correlation (ICC) statistical analysis was done. Also, sensitivity, specificity, positive predictive value (PPV) and negative predictive value (NPV) were calculated for determination of validity of results obtained from the kits. All the statistical analyses were done in R software environment (version 3.4.3).

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Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.10.001.
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