THE CAUSALITY OF MONOSODIUM GLUTamate
Fourier Transform Infrared (FTIR) ABSORBANCE PATTERN WITH WAVE PEAKS FROM SEVERAL SEASONING PRODUCTS (Savoury Flavors)

Mujianto1, Wignyanto2, Sri Kumalaningsih2, Aulanni’am3
1Agriculture Industry Technology, Wijaya Kusuma University of Surabaya
2Agriculture Industry Technology, Brawijaya University
3Veterinary Medicine, Brawijaya University
mujianto@uwks.ac.id

ABSTRACT

This study is aimed to find out the causality of raw materials, food additives and supportive materials used to produce several products of seasoning products available at commercial market and their direct correlation with monosodium glutamate (MSG) as flavor enhancing ingredient. An observation is taken to randomly collect 9 (nine) brands of seasoning (savory flavors) using Fourier Transform Infrared (FTIR) spectroscopy. The results of observation are processed using main component analysis and hierarchical cluster analysis. The results of study show that 9 (nine) brands of seasoning (savory flavors) are made from food additives and supportive material which score of eigenvalues is equal to 8.854 or 98.374 of variant and there is a direct causality with synthetic flavor enhancing ingredient (2 MSG variants). Such direct causative direct correlation applies to seasoning with grilled chicken flavor (SF7), seasoning with salted cheese flavor (SF5), seasoning with roasted beef flavor (SF3), seasoning with barbeque flavor (SF9), seasoning with tiroamis flavor (SF6), seasoning with spicy corn flavor (SF10) and monosodium glutamate (MSG) with eigenvalues score is 7.416 or 67.416% of variant. Balado flavored seasoning (SF8), cheese flavored seasoning (SF4), sweet spicy flavored seasoning (SF11) and Chinese flavor enhancing ingredient have direct causality with Chinese flavor enhancing ingredient, which eigenvalues score, is 1.517 or 13.792% of variant. Monosodium glutamate (SF1) and Chinese flavor enhancing ingredient have similarity of eigenvalues score is 1.108 or 10.071% of variant.

Keywords: Fourier Transform Infrared (FTIR), principal component analysis (PCA), hierarchical cluster analysis (HCA), savory flavors, MSG, and causality.

INTRODUCTION

Fast food is not new the only difference in pre-historic times was that it ran on two or four legs. The history of Man is reflected in the changes in eating tastes and habits throughout the world, but much of what we think of as innovative and modern, has, in fact, been around for centuries, if not millennia. (Grove, 2010). Seasoning (savory flavor) is commonly used as the seasoning of snacks or crispy snacks. One of the first flavorings used on crisps was in the 1950s when barbecue flavoring was developed for crisps in the U.S.A. This was followed by sour cream and onion flavor because of the popularity in the same country of “dips.” The main flavor enhancer used is monosodium glutamate (E621) in a fine crystal or powder form. Used to a lesser extent are the ribonucleotides (E627, E621, E635) which are nominally added in combination with monosodium glutamate. (Church, 1999). Today more than 2,000 synthetic organic chemicals are used by the flavorists to create high quality flavors. The flavor we appreciate is developed by heating the food to a certain temperature for a certain amount of time (Manley, Choudhury, & Mazeiko, 1999). To-day more than 2,000 synthetic organic chemicals are used by the flavorists to create high quality flavors. The flavor we appreciate is developed by heating the food to a certain temperature for a certain amount of time (Manley, Choudhury, & Mazeiko, 1999). Today more than 2,000 synthetic organic chemicals are used by the flavorists to create high quality flavors. The flavor we appreciate is developed by heating the food to a certain temperature for a certain amount of time (Manley, Choudhury, & Mazeiko, 1999). Today more than 2,000 synthetic organic chemicals are used by the flavorists to create high quality flavors. The flavor we appreciate is developed by heating the food to a certain temperature for a certain amount of time (Manley, Choudhury, & Mazeiko, 1999). 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the 3300-2800 cm\(^{-1}\) spectral range. The 1950-1450 cm\(^{-1}\) region exhibits IR absorption from a wide variety of double-bonded chemical groups. In the food industry NIR spectroscopy is the most common in-line method to monitor moisture, oil, fat and protein to analyze grains, feeds, meat, dairy and other products. Metabolites in leaves of spice plants can be determined by using NIR reflectance measurements. Accuracy and precision achieved are better than ± 0.2 %. On-line measurements are also made for diverse snack food products. (Valdas Sablinskas, 2003). This protein was chosen as an example because it consists of two sub-domains, an amino-terminal domain that is largely α-helical, and a carboxy terminal domain that is largely β-sheet. (Gordon S. Rule, 2006). Proteins are used in the food industries as substitutes for lipids. But the addition of proteins produces different effects in function of the medium and the matrices. Different sorts of proteins are used: milk proteins (\(\beta\)-lactoglobulin, bovine serum albumin, casein), egg albumin, gelatin and soy proteins. (Andree Voilley, 2006). Starches and films based on native and modified starches were characterized by FTIR spectroscopy and the results revealed that employed reactions can add hydrophobic functional groups to improve the water resistance of the biodegradable films based on starches. (Torrenegra, Solano, Herrera, León, & Pajaro, 2018). Maternal MSG intake increased the duration of trial and the number of false trial of offspring in Sprague Dawley rats. (Ün & Büyükuslu, 2018). MSG has an effect on cognitive function. Furthermore, the patients with improved questionnaires about palatability survey showed greater improvement in cognitive function. (Kouzuki, Taniguchi, Matsumoto, & Urankami, 2019). Monosodium Glutamate is a silent toxin in our food, especially our kids’ food. Some of the products in the market contain MSG in a level exceed the European limit. (Abdel Moneim, Yassa, Makboul, & Mohamed, 2018). A very popular snacks are Original, Barbeque (Chicken/Beef), Balado, Cheese, Corn, Sweet (Chocolate/Strawberry), Western tonality eq. Pizza, Teriyaki, Burger Spaghetti, (Sutata, 2012).

MATERIAL AND METHOD

The materials of study are 9 (nine) types of seasoning and 2 (two) variants of MSG bought at commercial markets in Surabaya. Fourier Transform Infrared (FTIR) spectroscopy absorbance observation results are processed using OriginLab software of version 8.5. Main component analysis and hierarchical cluster analysis shall use SPSS 24 software.

RESULT AND DISCUSSION

The similarity of Raw Materials, Food Additives and Supportive Materials of several Seasonings.

The method applied to see the similarity of raw materials, food additives and supportive materials of several seasonings available at commercial markets is by observing the absorbance pattern of Fourier Transform Infrared (FTIR) spectroscopy and main component analysis and hierarchical cluster analysis. Main component analysis is used to identify data pattern, data similarity, and several data differences. PCA is an efficient method for data reduction in particular in spectroscopy. (Gauglitz, 2003).

Figure 1. Absorbance pattern (spectrogram) of 9 seasonings (SF1, SF2, SF3, SF4, SF5, SF6, SF7, SF8, and SF9)

The results of observation on the absorbance pattern of 9 (nine) seasonings observed using FTIR spectroscopy can be seen in figure 1.

Table 1. Data Description of 9 (nine) Seasonings

| Seasoning | Mean          | Std. Deviation | Analysis | Missing |
|-----------|---------------|----------------|----------|---------|
| SF1       | 6.240484E1    | 27.2239489     | 1868     | 0       |
| SF2       | 6.632622E2    | 27.1328001     | 1868     | 0       |
| SF3       | 6.147111E1    | 28.4859968     | 1868     | 0       |
| SF4       | 6.035580E1    | 27.6772807     | 1868     | 0       |
| SF5       | 6.117411E1    | 27.5141804     | 1868     | 0       |
| SF6       | 6.577228E1    | 26.7806416     | 1868     | 0       |
| SF7       | 6.247482E1    | 27.9477148     | 1868     | 0       |
| SF8       | 5.877258E1    | 27.0461450     | 1868     | 0       |
| SF9       | 6.566655E1    | 27.0850254     | 1868     | 0       |
Fourier Transform Infrared (FTIR) spectroscopy absorbance pattern of 9 (Nine) seasonings (SF1, SF2, SF3, SF4, SF5, SF6, SF7, SF8, and SF9) on wavelength from 400 cm$^{-1}$ to 4,500 cm$^{-1}$ in the above figure 1 shows that there is pattern similarity. The results of main component analysis on 9 (Nine) seasonings (SF1, SF2, SF3, SF4, SF5, SF6, SF7, SF8, and SF9) aimed to find out the similarity of raw materials, food additives and supportive materials used in seasoning formulation process indicate that 9 (Nine) seasonings (SF1, SF2, SF3, SF4, SF5, SF6, SF7, SF8, and SF9) contain raw materials, food additives, and supportive materials those have similarity.

The correlation between the score of eigenvalues and the main component in the above figure indicates that the score of eigenvalues has almost achieve 0 (zero) up to the second main component (F2) and the cumulative % (percentage) of described variant is 99.067%.

Table 3. Component Matrix After Rotation of 9 (nine) Seasonings

| Component | 1       | 2       |
|-----------|---------|---------|
| SF7       | .800    | .596    |
| SF6       | .798    | .596    |
| SF5       | .793    | .603    |
| SF1       | .786    | .611    |
| SF2       | .777    | .624    |
| SF8       | .774    | .613    |
| SF9       | .769    | .631    |
| SF3       | .745    | .659    |
| SF4       | .602    | .798    |

Figure 3 shows that seasonings SF4, SF3, SF9, SF2, SF8, SF1, SF5, SF6 and SF7 have similarity as they are located in 1 (one) quadrant.
Based on table 3 above, the equation for the first (F1) main component that constitutes the similarity function of raw materials, supportive materials and additives of seasoning is as follows:

\[ F1 = 0.793 \, SF5 + 0.798 \, SF6 + 0.800 \, SF7 + 0.774 \, SF8 + 0.769 \, SF9 + 0.786 \, SF1 + 0.777 \, SF2 \, - \, 0.745 \, SF3 \, - \, 0.602 \, SF4 \]  

Remarks:
- F1 = Raw materials, supportive materials and additives similarity of seasoning
- SF1 = Seasoning with grilled chicken flavor
- SF2 = Seasoning with balado flavor
- SF3 = Seasoning with barbeque flavor
- SF4 = Seasoning with spicy corn flavor
- SF5 = Seasoning with cheese flavor
- SF6 = Seasoning with salted cheese flavor
- SF7 = Seasoning with sweet spicy flavor
- SF8 = Seasoning with roasted beef flavor
- SF9 = Seasoning with tiramisu flavor

The seasoning with sweet spicy flavor has the biggest variable coefficient score from the above equation (1) calculation. It indicates that the first (F1) main component as the similarity function of raw materials, supportive materials and additives of seasoning has the most significant direct effect before the next variable coefficients those are SF6, SF5, SF1, SF2, SF8, SF9, SF3, and SF4. The similarity of raw materials, supportive materials and additives of seasoning obtained from absorbance observation on wavelength from 400 cm\(^{-1}\) to 4,500 cm\(^{-1}\) with 16,812 points of observation.

Monosodium Glutamate Fourier Transform Infrared Absorbance Pattern Causality with Several Seasonings (Savory Flavor)

The method used to see the causality between monosodium glutamate absorbance pattern and the absorbance pattern of several types of seasonings (savory flavor) is to observe Fourier Transform Infrared (FTIR) spectroscopy absorbance pattern and to use main component analysis and hierarchical cluster analysis. Some problems alter the accuracy of the mass determination at the centroid. Actually, the experimental peak may contain several of these alterations. Furthermore, peaks with low noise on the signal are used here. (Edmond de Hoffmann, 2007). Three-dimensional Principal Component Analysis (PCA) scores plots and PCA loadings plots were created with the Pirouette Exploratory algorithm and examined to see how well class groupings were accomplished and which independent variables (GC peak area ratios) contributed most to class differentiation. Inspection of dendograms created with the Hierarchical Cluster Analysis (HCA) algorithm helped to visualize sample class grouping and was useful in deciding which independent variables to eliminate in order to improve clustering of similarly abused samples. (N. Millar, 1998).

Figure 4. FTIR absorbance pattern of 9 (nine) seasoning and 2 (two) variants of MSG

NMR methodology may be used as a rapid method for determining oxidative state of lipids and to estimate the overall changes in the primary and secondary oxidation products. (E.T, 1998). Most consumers of seasoning prefer savory taste as basic taste instead of other taste variants, such as grilled chicken, balado, barbeque, spicy corn, cheese, and salty cheese, sweet spicy and other flavors. Savory taste is organoleptically formed by amino acid (glutamate acid) substance or protein then absorbance observation over wavelength from 2,250 cm\(^{-1}\) to 4,500 cm\(^{-1}\) with absorbance value from 0% to 55% is made as the variable of main component analysis and hierarchical cluster analysis. The purpose is to find out the causality between FTIR absorbance pattern of monosodium glutamate and absorbance pattern of several types of seasoning. Protein is amino acid poly that has R-NH (amine) functional cluster with Fourier transform infrared (FTIR) spectroscopy of amine functional cluster can be identified at wavelength from 2,250 cm\(^{-1}\) to 4,500 cm\(^{-1}\). The distribution of absorbance observation can be seen in table 8. It is started from wavelength of 400 cm\(^{-1}\) to 2,250 cm\(^{-1}\).
with absorbance value from 55% to 100% or \( n (A) \) and from wavelength of 400 cm\(^{-1}\) to 2,250 cm\(^{-1}\) with absorbance value from 0% to 55% or \( n (D) \). It is also from wavelength of 2,250 cm\(^{-1}\) to 4,500 cm\(^{-1}\) with absorbance value from 55% to 100% or \( n (B) \), and from wavelength of 2,250 cm\(^{-1}\) to 4,500 cm\(^{-1}\) with absorbance value from 0% to 55% or \( n (C) \). NMR spectroscopy has become the most powerful and noninvasive physicochemical technique for determining polysaccharide structures, (Steve W. Cui, 2005).

Table 4. 9 (nine) types of Seasoning and 2 (two) Variants of MSG Data Description at Quadrant \( n (C) \)

|        | Mean   | Std Deviation | Analysis N | Missing N |
|--------|--------|---------------|------------|-----------|
| SF1    | 42.2975| 6.30002       | 363        | 65        |
| SF2    | 26.2335| 1.41144       | 257        | 171       |
| SF3    | 29.3081| 15.03878      | 370        | 58        |
| SF4    | 26.9497| 14.84103      | 318        | 110       |
| SF5    | 28.1623| 14.57967      | 382        | 46        |
| SF6    | 27.3903| 15.14527      | 392        | 38        |
| SF7    | 29.9949| 14.88655      | 390        | 38        |
| SF8    | 27.0779| 14.91415      | 321        | 107       |
| SF9    | 28.7189| 14.99221      | 370        | 58        |
| SF10   | 27.4206| 14.00120      | 428        | 0         |
| SF11   | 26.7645| 14.98986      | 327        | 101       |

The test result of KMO value > 0.5 that is of 0.808 > 0.500 means that the variable can be further predicted and analyzed. Bartlett’s test < 0.05 that is of 0.000 < 0.050 indicates that inter variables are highly correlated.

Table 5. KMO Value and Bartlett’s Test

|                           | Kaiser-Meyer-Olkin Measure of Sampling Adequacy | Bartlett’s Test of Sphericity |
|---------------------------|------------------------------------------------|------------------------------|
|                           | .808                                           | 6.627E3                      |
|                           | df                                             | Sig. .000                    |

Variables extraction process with qualified MSA (measure of sampling adequacy) score > 0.5 produces 3 (three) main components. Total score of eigenvalues of those 3 (three) main components is 91.280%.
Table 6. Matrix Component prior to Varimax Rotation

| Component Matrix³ |
|-------------------|
| 1  | 2  | 3   |
| SF6 | .964 | -.176  | .038 |
| SF9 | .959 | -.187  | .012 |
| SF3 | .956 | -.224  | .004 |
| SF5 | .939 | -.288  | -.023 |
| SF7 | .893 | -.417  | -.062 |
| SF11 | .846 | .501   | .057 |
| SF4 | .817 | .553   | .065 |
| SF6 | .809 | .570   | .051 |
| SF10 | .763 | -.391  | -.089 |
| SF2 | .498 | .328   | -.575 |

Factorization or matrix component extraction prior to varimax rotation produces factor 1 (one) that has 10 variables, namely SF6, SF9, SF3, SF5, SF7, SF11, SF4, SF8, and SF10. Factor 2 (two) has 3 variables, namely SF11, SF4, and SF8. Factor 3 (three) has 2 variables, namely SF2 and SF1.

Table 7. Matrix Component Rotation Results

| Rotated Component Matrix⁴ |
|-----------------------------|
| 1  | 2  | 3  |
| SF7 | .968 | .195  | -.006 |
| SF5 | .926 | .327  | .029 |
| SF3 | .900 | .389  | .054 |
| SF9 | .880 | .420  | .061 |
| SF6 | .875 | .432  | .087 |
| SF10 | .866 | .151  | -.039 |
| SF8 | .308 | .940   | .062 |
| SF4 | .324 | .931   | .077 |
| SF11 | .375 | .907   | .073 |
| SF1 | .144 | .205   | .877 |
| SF2 | .239 | .555   | -.566 |

Main components rotation produces factor 1 (one) that has 6 variables, factor 2 (two) that has 4 variables, and factor 3 that has 2 variables.

F1 = 0.968 SF7 + 0.926 SF5 + 0.900 SF3 +
  0.880 SF9 + 0.875 SF6 + 0.866 SF10

F2 = 0.940 SF8 + 0.931 SF4 + 0.907 SF11 +
  0.555 SF2

F3 = 0.877 SF1 – 0.566 SF2

Remarks:
F1 = Raw materials, supportive materials and additives similarity of seasoning
F2 = Seasoning and Chinese flavor enhancer similarities
F3 = MSG and Chinese flavor enhancer similarities

Principles of the widely used chemometric methods, such as PCA, PCR, and PLS are explained together with their applications in IR spectroscopy, (Gauglitz, 2003)

Figure 7. Component Plot in Rotated Space of 9 (nine) types of seasoning and 2 (two) variants of MSG

Infrared (IR) spectroscopy is a well-established technique in chemical analysis. Infrared radiation is absorbed by molecules, including taste components such as sugars and acids, causing molecular vibrations and rotations at specific wave lengths which depend on the chemical bounds within the molecule, (B.M. Nicolai, A.Berna, K.Beullens, 2008)
### Table 8. Absorbance (Abs) Point Observation Results of Fourier Transform Infrared (FTIR) of Seasoning

| NO | MATERIAL                                           | CODE | \( n(A) \) 400 - 2250 | \( n(B) \) 2250 - 4000 | \( n(C) \) 2250 - 4000 | \( n(D) \) 400 - 2250 | TOTAL ABS POINT |
|----|---------------------------------------------------|------|------------------------|-----------------------|------------------------|------------------------|-----------------|
| 1  | Seasoning with Grilled Chicken Flavor             | SF7  | 496                    | 518                   | 390                    | 465                    | 1869            |
| 2  | Seasoning with Balado Flavor                      | SF8  | 647                    | 587                   | 321                    | 313                    | 1868            |
| 3  | Seasoning with Barbeque Flavor                    | SF9  | 535                    | 538                   | 370                    | 432                    | 1875            |
| 4  | Seasoning with Spicy Corn Flavor                  | SF10 | 548                    | 480                   | 428                    | 412                    | 1868            |
| 5  | Seasoning with Cheese Flavor                      | SF4  | 649                    | 590                   | 318                    | 311                    | 1868            |
| 6  | Seasoning with Salty Cheese Flavor                | SF5  | 512                    | 526                   | 382                    | 448                    | 1868            |
| 7  | Seasoning with Sweet Spicy Flavor                 | SF11 | 637                    | 580                   | 328                    | 323                    | 1868            |
| 8  | Seasoning with Grilled Beef Flavor                | SF3  | 573                    | 537                   | 371                    | 387                    | 1868            |
| 9  | Seasoning with Tiramisu Flavor                    | SF6  | 573                    | 516                   | 392                    | 387                    | 1868            |
| 10 | Monosodium Glutamate (MSG)                        | SF1  | 695                    | 545                   | 363                    | 265                    | 1868            |
| 11 | Chinese Flavor Enhancing Spices                  | SF2  | 763                    | 651                   | 257                    | 210                    | 1881            |

### Figure 8. Combined Absorbance Pattern (spectrogram) of 9 (nine) seasonings (SF1, SF2, SF3, SF4, SF5, SF6, SF7, SF8, and SF9)

### Table 9. Interpretation Results of FTIR Absorbance Pattern Variable of Seasoning from 16,812 Observation Points

| NO | VARIABLE | FACTOR                                                                 | EIGEN VALUES | LOADING FACTOR | % VARIANCE | CUMULATIVE % |
|----|----------|------------------------------------------------------------------------|--------------|----------------|------------|--------------|
| 1  | SF1      | The similarity of raw materials, supportive materials and additives those compile product composition \( (F_1) \) | 8,854        | 0.78600        | 98.374     | 98.374       |
| 2  | SF2      |                                                                        |              | 0.77700        |            |              |
| 3  | SF3      |                                                                        |              | 0.74500        |            |              |
| 4  | SF4      |                                                                        |              | 0.60200        |            |              |
| 5  | SF5      |                                                                        |              | 0.73900        |            |              |
| 6  | SF6      |                                                                        |              | 0.79800        |            |              |
| 7  | SF7      |                                                                        |              | 0.80000        |            |              |
| 8  | SF8      |                                                                        |              | 0.77400        |            |              |
| 9  | SF9      |                                                                        |              | 0.76900        |            |              |
Table 10. Interpretation Results of FTIR Absorbance Pattern Variable from 20,569 Observation Points

| NO | VARIABLE | FACTOR | EIGEN VALUES | LOADING FACTOR | % VARIANCE | CUMULATIVE % |
|----|----------|--------|--------------|----------------|-------------|--------------|
| 1  | MSG      |        |              | 9,81625        | 0.21263     | 89.24        | 89.24        |
| 2  | VC       |        |              |                | 0.25170     |              |              |
| 3  | SF1      |        |              |                | 0.31753     |              |              |
| 4  | SF2      |        |              |                | 0.31444     |              |              |
| 5  | SF3      |        |              |                | 0.31419     |              |              |
| 6  | SF4      |        |              |                | 0.30737     |              |              |
| 7  | SF5      |        |              |                | 0.31742     |              |              |
| 8  | SF6      |        |              |                | 0.31589     |              |              |
| 9  | SF7      |        |              |                | 0.31644     |              |              |
| 10 | SF8      |        |              |                | 0.31522     |              |              |
| 11 | SF9      |        |              |                | 0.31366     |              |              |
| 12 | MSG      |        | 0.99828      | 0.73026        | 9.08        | 98.31        |
| 13 | VC       |        | 0.58588      |                |             |              |

Table 11. Interpretation Results of FTIR Absorbance Pattern Variable from 3,920 Observation Points at Wavelength from 2,250 cm\(^{-1}\) to 4,500 cm\(^{-1}\)

| NO | VARIABLE | FACTOR | EIGEN VALUES | LOADING FACTOR | % VARIANCE | CUMULATIVE % |
|----|----------|--------|--------------|----------------|-------------|--------------|
| 1  | SF7      |        | 7,416        | 0.968          | 67.416      | 67.416       |
| 2  | SF5      |        |              | 0.926          |             |              |
| 3  | SF3      |        |              | 0.900          |             |              |
| 4  | SF9      |        |              | 0.880          |             |              |
| 5  | SF6      |        |              | 0.875          |             |              |
| 6  | SF10     |        |              | 0.866          |             |              |
| 7  | SF8      |        |              | 0.940          | 13.792      | 81.208       |
| 8  | SF4      |        |              | 0.931          |             |              |
| 9  | SF11     |        |              | 0.907          |             |              |
| 10 | SF2      |        | 1,517        | 0.555          |             |              |
| 11 | SF1 (MSG)|        |              | 0.877          | 10.071      | 91.28        |
| 12 | SF2 (VC)|        |              | 0.566          |             |              |
Figure 9. (A) Cluster analysis (hierarchical cluster analysis), (B) Main Component Analysis and (C) 9 (nine) Seasonings and 2 (two) MSG variants Combined Spectrogram.
Figure 10. (A) Functional cluster distribution at various wavelengths, (B) functional cluster radar at various wavelengths, and (C) the absorbance pattern of 9 seasonings and 2 monosodium glutamate variants.
CONCLUSION

1. FTIR absorbance pattern and main component analysis observation results and hierarchy component analysis of 9 (nine) seasonings indicate that they are made from the same raw materials, supportive materials, and additives.

2. Those 9 (nine) seasonings studied all contain monosodium glutamate (MSG) flavor enhancing ingredient.

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