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Quantitative Relationship between Autocorrelation Topological Index and Biological Activity of Organic Compounds based on Multi Biomarker Pollution Index Method

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Abstract: As an early warning system for the long-term toxic effects of pollutants, multiple biomarkers have been widely used in environmental monitoring and evaluation. Based on the multi biomarker pollution index(MBPI) method, this paper proposes the autocorrelation topological index(ATI), and analyzes the quantitative relationship(QR) between it and the biological activity of organic substances. Firstly, the MBPI method is briefly introduced, and the quantitative analysis of organic organisms in the MBPI method is carried out, with emphasis on the GC-MS detection and analysis of organic substances; Then, the calculation method of ATI is proposed and analyzed; Finally, through the topological index method, taking penicillin as an example, the QR of its biological activity is discussed, which has important guiding significance for the future study of organic pollution.

1. Introduction

Biomarkers, as an early warning system for long-term toxic effects of pollutants, have been widely used in environmental monitoring and evaluation. However, in the field environment, organisms are often affected by a variety of ways and pollutants, which may add, multiply and antagonize each other. Therefore, when applying biomarkers, it is necessary to consider each influencing factor that may cause their changes. In order to overcome the uncertainty of the change of a single biomarker and evaluate the environmental quality of a region more reasonably, this paper studies and analyzes the QR between ATI and organic biological activity based on the MBPI method.

Based on the QR between ATI and biological activity of organic compounds by MBPI method,

many scholars at home and abroad have studied this. Uluturhan E and others put forward the concept of "total biomarker index" for the first time in the report of the results of the Biomar project funded by the European Union. After improvement, the MPI index was formed and applied to the marine environmental quality evaluation of the Baltic Sea and the Mediterranean coastal waters in Europe, confirming the reliability of this method in evaluating the marine environmental quality and grading [1]. Blanco rayon e et al. Calculated HSI based on the responses of seven biomarkers in Mytilus edulis, and comprehensively evaluated the health status of organisms. The results showed that HSI could distinguish the health status of organisms at different sites, and the results were consistent with the results of other biomarker index evaluation methods [2]. Blazquez Palli n et al. Used Ruditapes rugulosa as an indicator to evaluate the pollution status of riaformosa lagoon in Portugal, measured six biomarkers in Ruditapes, and calculated two biomarker indexes of IBR and HSI. The study found that HSI can effectively distinguish the pollution degree of different stations and seasons, and the evaluation results are consistent with the evaluation conclusion of IBR method [3].

This paper briefly introduces the MBPI method, analyzes the QR between the ATI and the biological activity of organic substances, discusses the ATI, takes the organic anthocyanins as an example, studies the influence of temperature, pH and common metal ions on the stability of anthocyanins in purple onion, and carries out qualitative and quantitative analysis and biological activity research on anthocyanins, The antioxidant activity and inhibition of A. glucosidase activity were analyzed [4-5].

2. QR between ATI and Biological Activity of Organic Compounds based on MBPI Method

2.1. Application of Multi Biomarker Index in Quantitative Analysis of Biological Activity of Organic Substances

As an early warning system for the long-term toxic effects of pollutants, biomarkers have been widely used in environmental monitoring and evaluation. However, due to the comprehensive impact of a variety of pollutants, these pollutants may add, multiply and antagonize each other. Therefore, the application of biomarkers needs to consider each influencing factor that may cause its change. In order to overcome the uncertainty of the change of a single biomarker and evaluate the environmental quality of a region more reasonably, these methods are mainly applied to the QR analysis of the biological activity of organic substances because they are mainly established and developed in some environmental monitoring projects in which organic organisms are the main monitoring organisms [6-7].

2.2. Quantitative Analysis of Organic Organisms based on MBPI Method

Many new and priority pollutants have been detected in ROC, but the final qualitative analysis of pollutants and the quantitative analysis of their concentration have not been given. This paper studies the qualitative and quantitative analysis of new and priority pollutants by lle-gc-ms [8].

This section intends to detect monochloromethane, monochloromethane, tribromomethane and 1,1,2,2-tetrachloroethane. Main reagents and materials are shown in Table 1.

Table 1. Reagents and materials

Reagent	Purity	Specifications
Monochloromethane Bromide In Methanol	National Standard Sample	0.922mg/Ml;2ml
Dichlorodibromomethane In Methanol	National Standard Sample	1.17mg/Ml;2ml
Tribromomethane In Methanol	National Standard Sample	1.03mg/Ml;2ml
1,1,2,2-Tetrachloroethane In Methanol	National Standard Sample	0.931mg/Ml;2ml
P-Fluorobromobenzene In Methanol	Standard	250μg/Ml;1ml

2.2.1. Preparation of Stock Solution

Open the ampoule bottles containing bromodichloromethane, Chlorodibromomethane, tribromomethane and 1,1,2,2-tetrachloroethane in Table 1, transfer 1.5ml of each target into a 10ml volumetric flask through a 2ml pipette, and fix the volume to 10ml through acetone. Then the concentrations of monochloromethane, monochloromethane, tribromomethane and 1,1,2,2-tetrachloroethane stock solutions are 0.138, 0.176, 0.155 and 0.140mg/ml respectively. For the internal standard p-fluorobromobenzene, open the ampoule bottle, transfer 0.5ml to 10ml volumetric flask through a 1ml pipette, and dilute to 10ml through acetone, then the concentration of the stock solution is 12.5 μg / ml [9-10].

2.2.2. Preparation of Working Solution

0.5ml of each stock solution is put into a 10ml volumetric flask, and 1ml of the internal standard p-fluorobromobenzene stock solution is added to the volumetric flask, and then the volume is fixed to 10ml through methyl tert butyl ether. Then the concentrations of monochloromethane, monochloromethane, tribromomethane, 1,1,2,2-tetrachloroethane and p-fluorobromobenzene in the working solution are 6.9, 8.8, 7.75, 7 and 1.25mg/l respectively.

2.2.3. Pretreatment of Water Samples

Take 30mlroc and put it into a 60mlepa sample bottle, add 3.0ml of methyl tertiary butyl ether (MTBE), add 10g of anhydrous sodium sulfate (during the dosing process, the bottle should be tilted properly to avoid anhydrous sodium sulfate from accumulating at the bottom of the bottle and condensing into blocks), shake violently for 4min, and let it stand for 5min [11]. Then take 1.0ml of the upper organic phase, add 2 μl of p-fluorobromobenzene working solution, and store it in the refrigerator at 4 ℃ until GC-MS analysis. The concentration ratio of water sample is 10:1 [12].

2.3. GC-MS Detection and Analysis of Organic Matter

Quantitative analysis is carried out by means of selective ion scanning (SIM). The temperature rise procedure of the column box is: 40 ℃, hold for 3 minutes, 10 ℃ /min rises to 280 ℃, hold for 3 minutes, and the solvent delay time is 7 minutes. The ion parameters scanned by the internal standard (naphthalene-d8) and the recovery indicator (p-terphenyl-d14) added in this section in SIM mode are listed in Table 2 [13].

Table 2. Ion parameters of naphthalene-d8 and p-terphenyl-d14 in SIM mode

Material	English name	CAS No	Quantitative ion (m/z)	Reference ion (m/z)
Naphthalene-d8	Naphthalene-d8	1146-65-2	136	68
P-terphenyl-d14	p-Terphenyl-d14	1718-51-0	244	122,212

GC-MS analysis of disinfection by-products was carried out by GC-MS instrument equipped with Agilent 6890n gas chromatograph and 5975 mass spectrometer detector. The temperature rise procedure of the column box in full scan mode (scan) and selective ion scan (SIM) mode is: 35 ℃, hold for 3min, and rise to 280 ℃ at 20 ℃ /min [14-15]. The solvent delay time is 3min, and the ion parameters scanned in SIM mode are shown in Figure 1.

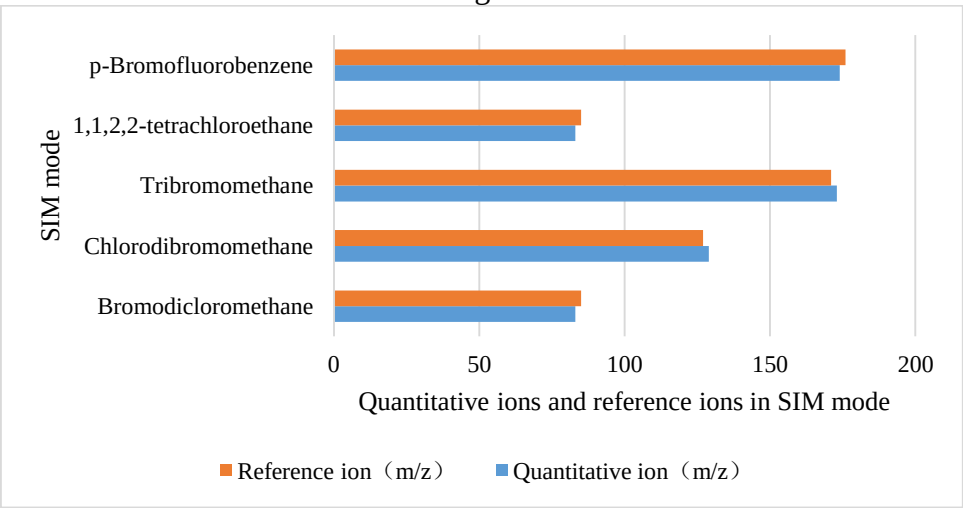

Figure 1. Quantitative ions and reference ions in SIM mode

The concentration of the substance to be measured is roughly estimated by the peak abundance ratio. Due to the low concentration multiple, the abundance of the chromatogram is very low. Moreover, in the column box heating rate of 20 ℃ /min, the chromatographic peaks of bromodichloromethane and Chlorodibromomethane are bifurcated [16]. Therefore, in order to reduce or even eliminate this phenomenon, it is necessary to increase the heating rate. Considering the above test results and in the analysis and detection, ECD has higher sensitivity and more development potential than MSD. Combined with the existing research conditions, the detection of disinfection by-products will not be further studied [17-18].

3. ATI

ATI is derived from the concept of autocorrelation function in mathematics. In mathematics, the autocorrelation function g (s) of function f (x) on interval AB is defined as:

$$G(s)=\int_{AB} G(x)G(x+t)dx \tag{1}$$

If f (x) moves a to the left, then:

$$G(s)=\int_{AB} g(x+a)g(x+a+s)dx\underline{\underline{y=x+a}}\int_{AB} g(y)g(y+1)dx$$

$$\underline{\underline{dy = dx}}\int_{AB} g(y)g(y+s)dy = \int_{AB} g(x)g(x|+s)dx \quad (2)$$

Formula (2) reflects the topological invariance of F (T), which can be used to define the topological invariants for generating molecular graphs. For the topological spatial structure of molecular graph, the autocorrelation function is defined as:

$$G(s) = \sum g(i)g(j) = \sum g(i)g(i+s) \quad (3)$$

In formula (3), t is the path length, representing the order of the index; I and j are two nodes separated by the length of T path; F (I) and f (J) are some physical and chemical properties of nodes I and J; F (T) refers to the distribution of this physical and chemical property.

4. QR between ATI and Biological Activity of Organic Compounds

4.1. Analysis of Antioxidant Activity

In this paper, the antioxidant capacity of Anthocyanins Extracted from purple onion, black bean peel and cyanidin 3-o-glucoside were determined by scavenging abts+ and dpph+ in vitro, and the antioxidant capacity of anthocyanins was comprehensively evaluated.

Table *3. The biological IC50 values of organic matter are listed in the table*

	Abts+ clearance	Dpph+ clearance	A-glucosidase inhibition rate
Purple onion	12.12+0.61	48.63+2.43	47.16+2.36
Black bean peel	16.67+0.83	38.81+1.94	39.45+1.97
Cyanidin 3-O-Glucoside	50.15+2.51	52.82+2.64	444.13+22.21
VC	98.68+4.93	139.8846.99	-
Acarbose	-	-	24.18+1.21

Table 3 shows that compared with the abts+ and dpph+ scavenging activities of VC, the ICSO value of organic biological extract is significantly lower than that of VC. The abts+ scavenging ability is about 8.14 times that of VC, and the dpph+ scavenging ability is about 2.88 times that of VC. Compared with VC, the ICSO value of black bean peel anthocyanin extract was lower than VC. The ability to remove abts+ is about 5.92 times that of VC, and the ability to remove dpph+ is about 3.6 times that of VC. It shows that the antioxidant capacity of anthocyanin extract from purple onion and black bean peel is stronger than that of VC. In addition, the ability of anthocyanins to scavenge free radicals increased with the decrease of glycosyl units and the increase of aglycone hydroxyl groups.

Anthocyanins have strong antioxidant properties due to their highly conjugated system in structure, which is the most prominent among many pharmacological activities of anthocyanins. In addition to preventing the damage of free radicals to human cells, anthocyanins are also the basis for the treatment of a series of major diseases such as cancer, cardiovascular disease and so on. Therefore, it is of great significance to study the antioxidant capacity of anthocyanins, including the mechanism of antioxidant effect and the relationship with other major diseases. The antioxidant

mechanism of anthocyanins has been found, such as by scavenging free radicals or forming complexes with metal ions. Anthocyanins are the most effective natural free radical scavengers at present. Their ability to scavenge free radicals is stronger than the positively charged oxygen atoms in the widely circulated antioxidants VC and ve anthocyanins, making them an effective and unique hydrogen donor antioxidant, which can effectively quench free radicals and terminate the chain reaction that causes oxidative damage.

4.2. Inhibition A. Analysis of Glucosidase Activity

Using 4.mug as the substrate, the anthocyanin extract of purple onion and black bean peel and cyanidin monomer cyanidin 3.o. glucoside were studied. The ICSO value was calculated according to the plot of concentration inhibition rate curve. The ICSO value was used to compare the inhibition ability of the enzyme.

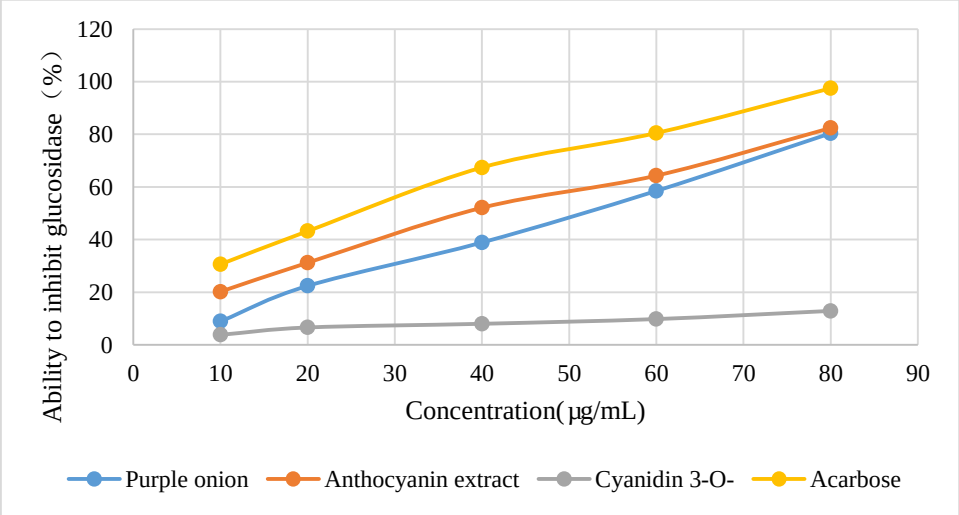

Figure 2. Ability to inhibit glucosidase

It can be seen from the above figure that the smaller the IC50 value is, the better the q The greater the inhibition of glucosidase. The anthocyanin extract of purple onion and black bean peel has a certain inhibitory effect on Q. glucosidase, and the inhibitory ability has a significant dose-response relationship with anthocyanin concentration. With the increasing concentration of anthocyanin, the inhibitory ability of anthocyanin on the enzyme is becoming stronger and stronger. The ICSO value of purple onion and black bean peel extracts on the inhibition of Ru glucosidase was higher than acarbose. In addition to anthocyanins, there are other compounds, which interfere, resulting in purple ocean and black bean skin anthocyanin extracts showing weaker Q than acarbose Glucosidase inhibition. However, anthocyanin extracts from purple onion and black bean peel still showed the potential to inhibit Q. glucosidase. The IC50 value of cornflower 3.o. glucoside on the inhibition of Q. glucosidase is also higher than acarbose, indicating that the inhibition ability of cornflower 3.o. glucoside is not as good as acarbose. But cyanidin 3.o. glucoside has no effect on a Glucosidase shows inhibition. The inhibition ability has an obvious dose-response relationship with anthocyanin concentration. With the increasing concentration of anthocyanin, the inhibition ability of glucosidase becomes stronger and stronger. Cyanidin 3.o. glucoside shows the potential to inhibit Q. glucosidase, which can provide theoretical support for anthocyanins in the treatment of diabetes.

5. Conclusion

This paper studies and analyzes the QR between ATI and biological activity of organic compounds based on MBPI method. Although some conclusions are reached through experiments, there are many deficiencies in the separation and purification of organic organisms and the preparation of monomers due to the limitation of time and equipment: due to the time relationship and the total amount of monomer compounds produced are less, Therefore, the screening of antioxidant and hypoglycemic activities of monomer compounds in vitro is still in progress; The lack of reasonable pharmacological activity tracking means and the failure of the research process to cooperate closely in time with the guidance of reasonable pharmacological activity tracking means make the research process more blind. At present, there are few studies on the use of biomarker index for marine environmental quality assessment in China. In the future, we should combine the pollution characteristics of our country, select appropriate indicator organisms and sensitive biomarker index system, apply and develop comprehensive biomarker index, and develop comprehensive evaluation technology and methods of environmental quality based on a series of biomarkers, so as to provide scientific basis for environmental pollution control and environmental management in our country.

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Data Availability

The datasets used during the current study are available from the corresponding author on reasonable request.

Conflict of Interest

The author states that this article has no conflict of interest.

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