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# Computation of Multiplicative Descriptors of Some Agricultural Pesticides

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## Abstract

**Objective:** To examine various degree-based multiplicative descriptors of some agricultural pesticides. **Methods:** To compute the main results, the method of analytical techniques, degree counting method, edge and vertex partition method, and graphical-theoretical tools is used to evaluate the agricultural pesticides. **Findings:** Various degree-based multiplicative indices analytical expressions have been obtained. **Novelty:** Pesticides are combinations of chemicals or mixtures that are primarily used in agriculture and this study creates a simple and exact method of estimating and ranking the potentially hazardous chemicals. The relationship between the chemical compounds and their properties is determined by topological descriptors. The topological indices of agricultural pesticides are plotted and compared with each other.

**Keywords:** Agricultural pesticides; Edge partition; Multiplicative indices

## 1 Introduction

In graph theory, the chemical compounds are described as a graph where atoms are defined as vertices and bonds are indicated as edges. Cheminformatics is a unification of mathematics and chemistry. In chemistry, it is critical to know the properties of the chemical compounds, to track the process and operational efficiency. A topological index describes a physicochemical property of compounds. In the QSAR/QSPRs study, the properties of molecular structure such as toxicity parameters, and photophysical, are evaluated by structural characterization. The structural properties such as boiling point, flash point, molar refraction, osmotic coefficients, polarizability, critical pressure, etc., can be evaluated by topological indices [1,2]. Topological indices can therefore be used to quantitatively analyze and understand different chemical structures and chemical networks [3]. Thus, topological indices enable us to evaluate and compute the chemical structure and its networks in more detail.

Globally, approximately more than 2 billion people are active in agriculture, and most use pesticides to guard their crops and products. Pesticides are defined as "Chemical substance used to prevent, destroy, repel or mitigate any pest ranging from insects (i.e., insecticides), rodents (i.e., rodenticides) and weeds (herbicides) to microorganisms (i.e., algicides, fungicides or bactericides" [4]. Many pesticides have been implicitly equated with their overall risks because of their acute effects on human health. The toxicological testing of an active ingredient is usually limited. To estimate and rank the potentially hazardous chemicals, it is essential to develop an accurate and simple method. Most pesticides are carcinogenic, which is a cancer risk. Thus, it is critical need to analyze and understand the structural properties of agricultural pesticides. In this article, we discuss some agricultural pesticides such as Azadirachtin denoted as $(\rho Za)$, Avermectin b1a as $(\rho Av)$, Salannin as $(\rho Sa)$, Spinosyns as $(\rho Sp)$, Brucine as $(\rho Br)$ and Difethialone as $(\rho Di)$. And the molecular structure of the above chemical compounds is given.

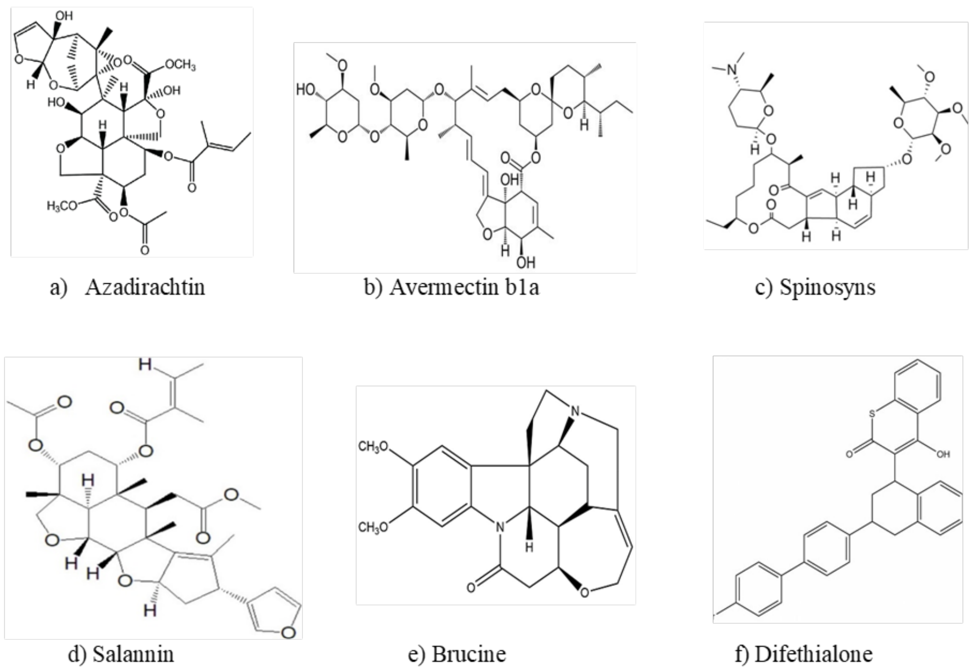


**Fig 1. The molecular structure of some agricultural pesticides**

Azadirahtin, $C_{35}H_{44}O_{16}$ is an insecticide that is extracted from the neem seed. The chemists J. H. Butterworth and E. D. Morgan exposed the molecule azadirahtin and it is finally produced by the research group Stephen V. Ley and his co-workers[5]. The substance is primarily an antifeedant and growth disruptor, being active in affecting over 200 species of insects, initially as a feeding inhibitor for the desert locust (*Schistocerca gregaria*). African cotton leafworms (*Spodoptera littoralis*) are resistant to a commonly used biological pesticide, *Bacillus thuringiensis*, and exhibit considerable toxicity towards azadirachtin.

Avermectin b1a, $C_{48}H_{74}O_{14}$ is insecticides to kill parasitic worms and insects. In 1978, from a soil sample, an actinomycete was extracted at Kitasato Institute and that compound was *Streptomyces avermitilis*[6]. We isolated eight different avermectins from four homologous compounds with an a-component and b-component in different ratios, usually 80:20 to 90:10. Other chemical compounds derived from avermectins namely ivermectin, abamectin, eprinomectin, doramectin, and selamectin.

Spinosyn is an insecticide extracted from the fermentation of two species of *Saccharopolyspora*. Polyketide-derived tetracyclic macrolides are appended with two saccharides, and they exhibit potent insecticidal activities against a broad range of plant and crop pests. The spinosyn insecticides show greater selectivity toward target insects than many other insecticides and less activity towards mammals, aquatic animals, and birds. Spinosyn A, $C_{41}H_{65}O_{10}$ is a key component in fermentation. The polyketide framework would be formed biosynthetically by exchanging acetate and propionate at appropriate times.

Salannin, $C_{34}H_{44}O_{09}$ is an insecticide synthesized from leaves of Meliaceae, forbids the growth of insects. As larval growth was inhibited, neonate and component star larvae ceased feeding. Aside from inhibiting cell factors, a protein that increases the proliferation of cancer cells and salannin also inhibits fatty acid synthase, which produces prostaglandins.

Brucine, $C_{23}H_{26}N_2O_4$ is an alkaloid most commonly found in the *Strychnos nux-vomica* tree, which is closely related to strychnine. The toxic effects of brucine are rare, since it is usually consumed with strychnine, which is more toxic than brucine. *Brucea antidysenterica*, brought back from Ethiopia by James Bruce, is the genus that bears the name Brucine. Difethialone, $C_{31}H_{23}BrO_2S$ is a rodenticide produced mainly to kill a rat.

One of the main objectives of quantitative structure-activity relationships, QSAR, is to predict organic compounds' biological properties. A well-characterized molecular structure and the selection of appropriate molecular descriptors are key factors determining the success of these methods. The objective of our study is to determine the relationship between molecular topology and the lethal toxicity of pesticides. Recently, by multiplicative indices, the properties of drugs are analyzed[7–9].

## 2 Methodology

Let $\zeta = (V,\ E)$ where $V$ and $E$ be the set of vertices and edges respectively. Let $\mu \in V(\zeta)$, then the degree of m is the number of edges incident to the vertex m, denoted as $\delta(\mu)$. If any two vertices $\mu$ and $\gamma$ of connected graph, $\zeta$ is adjacent then they are connected by edge $\mu\gamma$. A degree-based structural characterization is extended by Consonni and Todeschini, to include multiplicative topological indices form[10]. In recent times, the multiplicative indices grabbing attention[11,12]. Randić degree-based indices are widely used topological descriptors, introduced by Milan Randić[13].

$R(\zeta) = \sum_{\mu\gamma\,\varepsilon\, E(\zeta)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}}$

Among several existing topological indices, the Randić index has numerous applications and is widely applied in medicinal chemistry. The multiplicative Randić index[14] is given by the following formula:

$RCII(\zeta) = \prod_{\mu\gamma\,\varepsilon\, E(\zeta)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}}$

Defining the multiplicative Harmonic index[15] and multiplicative sum connectivity index[16] as follows:

$SCII(\zeta) = \prod_{\mu\gamma\,\varepsilon\, E(\zeta)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}}$

and

$HII(\zeta) = \prod_{\mu\gamma\,\varepsilon\, E(\zeta)} \frac{2}{\delta(\mu)+\delta(\gamma)}$

Atom bond connectivity (ABC) index was introduced by Estrada et al.[17] and multiplicative atomic bond connectivity index[18] is defined as

$ABCII(\zeta) = \prod_{\mu\gamma\,\varepsilon\, E(\zeta)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}}$

Geometric arithmetic (GA) index was presented by Vukicevic and Furtula in[19], whose multiplicative geometric arithmetic index[18] as:

$GAII(\zeta) = \prod_{\mu\gamma\,\varepsilon\, E(\zeta)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)}$

In addition, kulli[20] introduced the concept of multiplicative sum connectivity F-index and multiplicative product connectivity F-index are presented as

$SFII(\zeta) = \prod_{\mu\gamma\,\varepsilon\, E(\zeta)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}}$

and

$PFII(\zeta) = \prod_{\mu\gamma\,\varepsilon\, E(\zeta)} \frac{1}{\sqrt{\delta(\mu)^2\times\delta(\gamma)^2}}$

A hyper Zagreb (HM) index was presented by Shirdel et al. in[21] and its multiplicative is defined as

$HMII(\zeta) = \prod_{\mu\gamma\,\varepsilon\, E(\zeta)} (\delta(\mu)+\delta(\gamma))^2$

Gutman et al.[22] introduced the first and second Zagreb indices in 1975**.** This pair of indices is among the oldest degree-depending descriptors, and their properties have been extensively examined. Eliasi et al.[12] defined a new multiplicative version of the first Zagreb index as follows:

$\Pi_1^*(\zeta) = \prod_{\mu\gamma\,\varepsilon\, E(\zeta)} (\delta(\mu)+\delta(\gamma))$

The multiplicative second Zagreb index is explained in[23] is defined as follows:

$\Pi_2(\zeta) = \prod_{\mu\gamma\,\varepsilon\, E(\zeta)} (\delta(\mu)\times\delta(\gamma))$

## 3 Degree-based Multiplicative Indices

In this section, the multiplicative degree-based indices for six pesticides namely Azadirachtin, brucine, difethialone, Avermectin b1a, Spinosyns, Salannin have been evaluated.

**Theorem 1**. Let $G = \rho Za$, then $RCII(\rho Za) = 5.5449\times10^{-16}$, $SCII(\rho Za) = 1.0288\times10^{-21}$, $HII(\rho Za) = 7.6263\times10^{-26}$, $ABCII(\rho Za) = 0.0257$, $GAII(\rho Za) = 0.0421$, $HMII(\rho Za) = 2.2855\times10^{86}$, $SFII(\rho Za) = 2.8322\times10^{-30}$, $PFII(\rho Za) =$

$3.2811\times10^{-48}$ ,$\Pi_1^*(\rho Za)$ =$1.5118\times10^{43}$ ,$\Pi_2(\rho Za) = 3.0477\times10^{47}$.

**Proof:** Let Azadirachtin be the chemical graph $G = \rho Za$ consists of 52 vertices and 58 edges. In $\rho Za$, degree 2 for 15 vertices, degree 3 for 14 vertices, degree 4 for 7 vertices and degree 1 for 16 vertices. From the Figure 2, nine classes of edge partition are obtained by considering the degree of the end vertices. In the first edge partition, $E_1$ has 4 edges, $\mu\gamma\, \varepsilon\, E(\rho Za)$ where $\delta(\mu) = 2$ and $\delta(\gamma) = 2$. In the second edge partition, $E_2$ has 15 edges $\mu\gamma$, where $\delta(\mu) = 2$ and $\delta(\gamma) = 3$. In the third edge partition, $E_3$ has 3 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 3$. In the fourth edge partition, $E_4$ has 14 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\delta(\gamma) = 3$. In the fifth edge partition, $E_5$ has 6 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\delta(\gamma) = 2$. In the sixth edge partition, $E_6$ has 9 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 1$. In the seventh edge partition, $E_7$ has 3 edges $\mu\gamma$, where $\delta(\mu) = 2$ and $\delta(\gamma) = 1$. In the eighth edge partition, $E_8$ has 4 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\delta(\gamma) = 1$. In the ninth edge partition, $E_9$ has 2 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\gamma = 4$.

$$\mathrm{RC}II(\rho Za) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Za)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}}$$

$$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Za)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Za)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Za)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Za)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_5(\rho Za)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Za)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Za)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_8(\rho Za)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_9(\rho Za)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}}$$

$$= \left(\tfrac{1}{2}\right)^4 \times \left(\tfrac{1}{\sqrt{6}}\right)^{15} \times \left(\tfrac{1}{3}\right)^3 \times \left(\tfrac{1}{2\sqrt{3}}\right)^{14} \times \left(\tfrac{1}{2\sqrt{2}}\right)^6 \times \left(\tfrac{1}{\sqrt{3}}\right)^9 \times \left(\tfrac{1}{\sqrt{2}}\right)^3 \times \left(\tfrac{1}{2}\right)^4 \times \left(\tfrac{1}{4}\right)^2 = 5.5449\times10^{-16}$$

$$\mathrm{SC}II(\rho Za) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Za)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}}$$

$$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Za)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Za)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Za)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Za)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_5(\rho Za)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Za)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Za)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_8(\rho Za)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_9(\rho Za)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}}$$

$$= \left(\tfrac{1}{2}\right)^4 \times \left(\tfrac{1}{\sqrt{5}}\right)^{15} \times \left(\tfrac{1}{\sqrt{6}}\right)^3 \times \left(\tfrac{1}{\sqrt{7}}\right)^{14} \times \left(\tfrac{1}{\sqrt{6}}\right)^6 \times \left(\tfrac{1}{2}\right)^9 \times \left(\tfrac{1}{\sqrt{3}}\right)^3 \times \left(\tfrac{1}{\sqrt{5}}\right)^4 \times \left(\tfrac{1}{2\sqrt{2}}\right)^2 = 1.0288\times10^{-21}$$

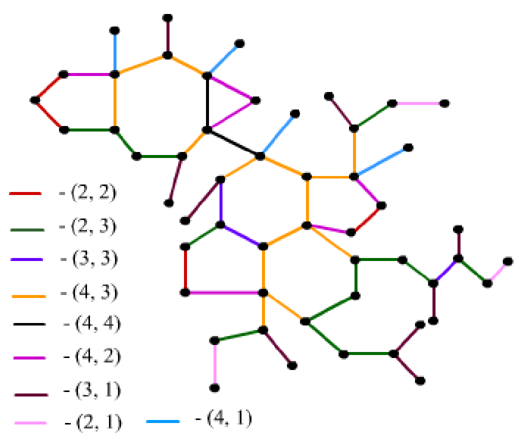


**Fig 2. The edge partition of Azadirachtin, $\rho Za$ based on degree of end vertices**

$$\mathrm{H}II(\rho Za) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Za)} \frac{2}{\delta(\mu)+\delta(\gamma)}$$

$$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Za)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Za)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Za)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Za)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_5(\rho Za)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Za)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Za)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_8(\rho Za)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_9(\rho Za)} \frac{2}{\delta(\mu)+\delta(\gamma)}$$

$$= \left(\tfrac{1}{2}\right)^4 \times \left(\tfrac{2}{5}\right)^{15} \times \left(\tfrac{1}{3}\right)^3 \times \left(\tfrac{2}{7}\right)^{14} \times \left(\tfrac{1}{3}\right)^6 \times \left(\tfrac{1}{2}\right)^9 \times \left(\tfrac{2}{3}\right)^3 \times \left(\tfrac{2}{5}\right)^4 \times \left(\tfrac{1}{4}\right)^2 = 7.6263\times10^{-26}$$

$$\mathrm{ABC}II(\rho Za) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Za)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}}$$

$$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Za)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Za)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Za)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Za)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Za)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Za)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_5(\rho Za)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_8(\rho Za)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon\, E_9(\rho Za)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}}$$

$= \left(\frac{1}{\sqrt{2}}\right)^4 \times \left(\frac{1}{\sqrt{2}}\right)^{15} \times \left(\frac{2}{3}\right)^3 \times \left(\frac{\sqrt{5}}{2\sqrt{3}}\right)^{14} \times \left(\frac{1}{\sqrt{2}}\right)^6 \times \left(\frac{\sqrt{2}}{\sqrt{3}}\right)^9 \times \left(\frac{1}{\sqrt{2}}\right)^3 \times \left(\frac{\sqrt{3}}{2}\right)^4 \times \left(\frac{\sqrt{3}}{2\sqrt{2}}\right)^2 = 0.0257$

$GAII(\rho Za) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Za)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)}$

$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Za)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Za)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Za)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Za)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times$
$\prod_{\mu\gamma\varepsilon\, E_5(\rho Za)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Za)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times$
$\prod_{\mu\gamma\varepsilon\, E_7(\rho Za)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_8(\rho Za)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon\, E_9(\rho Za)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)}$

$= (1)^4 \times \left(\frac{2\sqrt{6}}{5}\right)^{15} \times (1)^3 \times \left(\frac{4\sqrt{3}}{7}\right)^{14} \times \left(\frac{2\sqrt{2}}{3}\right)^6 \times \left(\frac{\sqrt{3}}{2}\right)^9 \times \left(\frac{2\sqrt{2}}{3}\right)^3 \times \left(\frac{4}{5}\right)^4 \times (1)^2 = 0.0421$

$HMII(\rho Za) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Za)} (\delta(\mu)+\delta(\gamma))^2$

$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Za)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Za)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Za)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Za)} (\delta(\mu)+\delta(\gamma))^2 \times$
$\prod_{\mu\gamma\varepsilon\, E_5(\rho Za)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Za)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Za)} (\delta(\mu)+\delta(\gamma))^2 \times$
$\prod_{\mu\gamma\varepsilon\, E_8(\rho Za)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon\, E_9(\rho Za)} (\delta(\mu)+\delta(\gamma))^2$

$= (16)^4 \times (25)^{15} \times (36)^3 \times (49)^{14} \times (36)^6 \times (16)^9 \times (9)^3 \times (25)^4 \times (64)^2 = 2.2855\times 10^{86}$

$SFII(\rho Za) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}}$

$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times$
$\prod_{\mu\gamma\varepsilon\, E_5(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times$
$\prod_{\mu\gamma\varepsilon\, E_8(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_9(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}}$

$= \left(\frac{1}{\sqrt{8}}\right)^4 \times \left(\frac{1}{\sqrt{13}}\right)^{15} \times \left(\frac{1}{3\sqrt{2}}\right)^3 \times \left(\frac{1}{5}\right)^{14} \times \left(\frac{1}{2\sqrt{5}}\right)^6 \times \left(\frac{1}{\sqrt{10}}\right)^9 \times \left(\frac{1}{\sqrt{5}}\right)^3 \times \left(\frac{1}{\sqrt{17}}\right)^4 \times \left(\frac{1}{4\sqrt{2}}\right)^2 = 2.8322\times 10^{-30}$

$PFII(\rho Za) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2\times\delta(\gamma)^2}}$

$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times$
$\prod_{\mu\gamma\varepsilon\, E_5(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times$
$\prod_{\mu\gamma\varepsilon\, E_8(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_9(\rho Za)} \frac{1}{\sqrt{\delta(\mu)^2\times\delta(\gamma)^2}}$

$= \left(\frac{1}{4}\right)^4 \times \left(\frac{1}{6}\right)^{15} \times \left(\frac{1}{9}\right)^3 \times \left(\frac{1}{12}\right)^{14} \times \left(\frac{1}{8}\right)^6 \times \left(\frac{1}{3}\right)^9 \times \left(\frac{1}{2}\right)^3 \times \left(\frac{1}{4}\right)^4 \times \left(\frac{1}{16}\right)^2 = 3.2811\times 10^{-48}$

$\Pi_1^*(\rho Za) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Za)} (\delta(\mu)+\delta(\gamma))$

$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times$
$\prod_{\mu\gamma\varepsilon\, E_5(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times$
$\prod_{\mu\gamma\varepsilon\, E_8(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_9(\rho Za)} (\delta(\mu)+\delta(\gamma))$

$= (4)^4 \times (5)^{15} \times (6)^3 \times (7)^{14} \times (6)^6 \times (4)^9 \times (3)^3 \times (5)^4 \times (8)^2 = 1.5118\times 10^{43}$

$\Pi_2(\rho Za) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Za)} (\delta(\mu)\times\delta(\gamma))$

$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times$
$\prod_{\mu\gamma\varepsilon\, E_5(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times$
$\prod_{\mu\gamma\varepsilon\, E_8(\rho Za)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_9(\rho Za)} (\delta(\mu)\times\delta(\gamma))$

$= (4)^4 \times (6)^{15} \times (9)^3 \times (12)^{14} \times (8)^6 \times (3)^9 \times (2)^3 \times (4)^4 \times (16)^2 = 3.0477\times 10^{47}$

**Theorem 2.** Let $G = \rho Av$, then $RCII(\rho Av) = 2.21599\times 10^{-23}$, $SCII(\rho Av) = 4.0095\times 10^{-24}$, $HII(\rho Av) = 4.7447\times 10^{-27}$, $ABCII(\rho Av) = 1.2503\times 10^{-9}$, $GAII(\rho Av) = 0.06166$, $HMII(\rho Av) = 3.8695\times 10^{93}$, $SFII(\rho Av) = 8.6936\times 10^{-32}$, $PFII(\rho Av) = 5.9204\times 10^{-51}$, $\Pi_1^*(\rho Av) = 6.2205\times 10^{46}$, $\Pi_2(\rho Av) = 1.6891\times 10^{50}$.

**Proof:** Let Avermectin b1a be the chemical graph $G = \rho Av$ consists of 62 vertices and 68 edges. In $\rho Av$, degree 2 for 23 vertices, degree 3 for 21 vertices, degree 4 for 2 vertices and degree 1 for 16 vertices. From the Figure 3, eight classes of edge partition are obtained by considering the degree of the end vertices. In the first edge partition, $E_1$ has 6 edges, $\mu\gamma\,\varepsilon\,E(\rho Av)$ where $\delta(\mu) = 2$ and $\delta(\gamma) = 2$. In the second edge partition, $E_2$ has 31 edges $\mu\gamma$, where $\delta(\mu) = 2$ and $\delta(\gamma) = 3$. In the third edge partition, $E_3$ has 10 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 3$. In the fourth edge partition, $E_4$ has 2 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\delta(\gamma) = 3$. In the fifth edge partition, $E_5$ has 5 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\delta(\gamma) = 2$. In the sixth edge partition, $E_6$ has 10 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 1$. In the seventh edge partition, $E_7$ has 3 edges $\mu\gamma$, where $\delta(\mu) = 2$ and $\delta(\gamma) = 1$. In the eighth edge partition, $E_8$ has 1 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\delta(\gamma) = 1$.

$RCII(\rho Av) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Av)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}}$

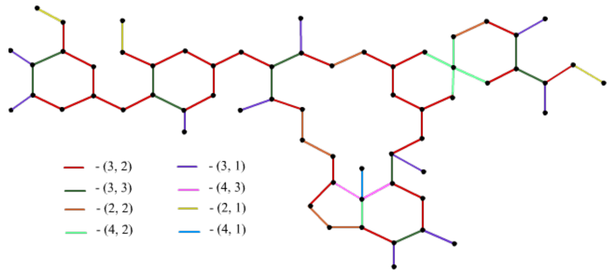


**Fig 3. The edge partition of Avermectin b1a , $\rho Av$ based on degree of end vertices**

$$= \prod_{\mu\gamma\varepsilon E_1(\rho Av)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_2(\rho Av)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_3(\rho Av)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_4(\rho Av)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_5(\rho Av)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_6(\rho Av)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_7(\rho Av)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_8(\rho Av)} \frac{1}{\sqrt{\delta(\mu)\times\delta(\gamma)}}$$

$$= (\tfrac{1}{2})^6 \times (\tfrac{1}{\sqrt{6}})^{31} \times (\tfrac{1}{3})^{10} \times (\tfrac{1}{2\sqrt{3}})^2 \times (\tfrac{1}{2\sqrt{2}})^5 \times (\tfrac{1}{\sqrt{3}})^{10} \times (\tfrac{1}{\sqrt{2}})^3 \times (\tfrac{1}{2})^1 = 2.21599\times 10^{-23}$$

$$\mathrm{SC}II(\rho Av) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Av)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}}$$

$$= \prod_{\mu\gamma\varepsilon E_1(\rho Av)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_2(\rho Av)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_3(\rho Av)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_4(\rho Av)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_5(\rho Av)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_6(\rho Av)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_7(\rho Av)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_8(\rho Av)} \frac{1}{\sqrt{\delta(\mu)+\delta(\gamma)}}$$

$$= (\tfrac{1}{2})^6 \times (\tfrac{1}{\sqrt{5}})^{31} \times (\tfrac{1}{\sqrt{6}})^{10} \times (\tfrac{1}{\sqrt{7}})^2 \times (\tfrac{1}{\sqrt{6}})^5 \times (\tfrac{1}{2})^{10} \times (\tfrac{1}{\sqrt{3}})^3 \times (\tfrac{1}{\sqrt{5}})^1 = 4.0095\times 10^{-24}$$

$$\mathrm{H}II(\rho Av) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Av)} \frac{2}{\delta(\mu)+\delta(\gamma)}$$

$$= \prod_{\mu\gamma\varepsilon E_1(\rho Av)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_2(\rho Av)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_3(\rho Av)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_4(\rho Av)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_5(\rho Av)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_6(\rho Av)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_7(\rho Av)} \frac{2}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_8(\rho Av)} \frac{2}{\delta(\mu)+\delta(\gamma)}$$

$$= (\tfrac{1}{2})^6 \times (\tfrac{2}{5})^{31} \times (\tfrac{1}{3})^{10} \times (\tfrac{2}{7})^2 \times (\tfrac{1}{3})^5 \times (\tfrac{1}{2})^{10} \times (\tfrac{2}{3})^3 \times (\tfrac{2}{5})^1 = 4.7447\times 10^{-27}$$

$$\mathrm{ABC}II(\rho Av) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Av)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}}$$

$$= \prod_{\mu\gamma\varepsilon E_1(\rho Av)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_2(\rho Av)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_3(\rho Av)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_4(\rho Av)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_5(\rho Av)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_6(\rho Av)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_7(\rho Av)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}} \times \prod_{\mu\gamma\varepsilon E_8(\rho Av)} \sqrt{\frac{\delta(\mu)+\delta(\gamma)-2}{\delta(\mu)\times\delta(\gamma)}}$$

$$= (\tfrac{1}{\sqrt{2}})^6 \times (\tfrac{1}{\sqrt{2}})^{31} \times (\tfrac{2}{3})^{10} \times (\tfrac{\sqrt{5}}{2\sqrt{3}})^2 \times (\tfrac{1}{\sqrt{2}})^5 \times (\tfrac{\sqrt{2}}{\sqrt{3}})^{10} \times (\tfrac{1}{\sqrt{2}})^3 \times (\tfrac{\sqrt{3}}{2})^1 = 1.2503\times 10^{-9}$$

$$\mathrm{GA}II(\rho Av) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Av)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)}$$

$$= \prod_{\mu\gamma\varepsilon E_1(\rho Av)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_2(\rho Av)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_3(\rho Av)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_4(\rho Av)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_5(\rho Av)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_6(\rho Av)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_7(\rho Av)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)} \times \prod_{\mu\gamma\varepsilon E_8(\rho Av)} \frac{2\sqrt{\delta(\mu)\times\delta(\gamma)}}{\delta(\mu)+\delta(\gamma)}$$

$$= (1)^6 \times (\tfrac{2\sqrt{6}}{5})^{31} \times (1)^{10} \times (\tfrac{4\sqrt{3}}{7})^2 \times (\tfrac{2\sqrt{2}}{3})^5 \times (\tfrac{\sqrt{3}}{2})^{10} \times (\tfrac{2\sqrt{2}}{3})^3 \times (\tfrac{4}{5})^1 = 0.06166$$

$$\mathrm{HM}II(\rho Av) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Av)} (\delta(\mu)+\delta(\gamma))^2$$

$$= \prod_{\mu\gamma\varepsilon E_1(\rho Av)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon E_2(\rho Av)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon E_3(\rho Av)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon E_4(\rho Av)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon E_5(\rho Av)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon E_6(\rho Av)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon E_7(\rho Av)} (\delta(\mu)+\delta(\gamma))^2 \times \prod_{\mu\gamma\varepsilon E_8(\rho Av)} (\delta(\mu)+\delta(\gamma))^2$$

$$= (16)^6 \times (25)^{31} \times (36)^{10} \times (49)^2 \times (36)^5 \times (16)^{10} \times (9)^3 \times (25)^1 = 3.8695\times 10^{93}$$

$$\mathrm{SF}II(\rho Av) = \prod_{\mu\gamma\,\varepsilon\, E(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}}$$

$$= \prod_{\mu\gamma\varepsilon E_1(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon E_2(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon E_3(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon E_4(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon E_5(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon E_6(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon E_7(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon E_8(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon E_9(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2+\delta(\gamma)^2}}$$

$$= (\tfrac{1}{\sqrt{8}})^6 \times (\tfrac{1}{\sqrt{13}})^{31} \times (\tfrac{1}{3\sqrt{2}})^{10} \times (\tfrac{1}{5})^2 \times (\tfrac{1}{2\sqrt{5}})^5 \times (\tfrac{1}{\sqrt{10}})^{10} \times (\tfrac{1}{\sqrt{5}})^3 \times (\tfrac{1}{\sqrt{17}})^1 = 8.6936\times 10^{-32}$$

$\mathrm{PF}II(\rho Av) = \prod_{\mu\gamma\, \varepsilon\, E(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2 \times \delta(\gamma)^2}}$

$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2\times\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2\times\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2\times\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2\times\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_5(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2\times\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2\times\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2\times\delta(\gamma)^2}} \times \prod_{\mu\gamma\varepsilon\, E_8(\rho Av)} \frac{1}{\sqrt{\delta(\mu)^2\times\delta(\gamma)^2}}$

$= \left(\frac{1}{4}\right)^6 \times \left(\frac{1}{6}\right)^{31} \times \left(\frac{1}{9}\right)^{10} \times \left(\frac{1}{12}\right)^2 \times \left(\frac{1}{8}\right)^5 \times \left(\frac{1}{3}\right)^{10} \times \left(\frac{1}{2}\right)^3 \times \left(\frac{1}{4}\right)^1 = 5.9204\times 10^{-51}$

$\Pi_1^*(\rho Av) = \prod_{\mu\gamma\, \varepsilon\, E(\rho Av)} (\delta(\mu)+\delta(\gamma))$

$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Av)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Av)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Av)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Av)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_5(\rho Av)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Av)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Av)} (\delta(\mu)+\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_8(\rho Av)} (\delta(\mu)+\delta(\gamma))$

$= (4)^6 \times (5)^{31} \times (6)^{10} \times (7)^2 \times (6)^5 \times (4)^{10} \times (3)^3 \times (5)^1 = 6.2205\times 10^{46}$

$\Pi_2(\rho Av) = \prod_{\mu\gamma\, \varepsilon\, E(\rho Av)} (\delta(\mu)\times\delta(\gamma))$

$= \prod_{\mu\gamma\varepsilon\, E_1(\rho Av)} (\delta(\mu)\times\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_2(\rho Av)} (\delta(\mu)\times\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_3(\rho Av)} (\delta(\mu)\times\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_4(\rho Av)} (\delta(\mu)\times\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_5(\rho Av)} (\delta(\mu)\times\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_6(\rho Av)} (\delta(\mu)\times\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_7(\rho Av)} (\delta(\mu)\times\delta(\gamma)) \times \prod_{\mu\gamma\varepsilon\, E_8(\rho Av)} (\delta(\mu)\times\delta(\gamma))$

$= (4)^6 \times (6)^{31} \times (9)^{10} \times (12)^2 \times (8)^5 \times (3)^{10} \times (2)^3 \times (4)^1 = 1.6891\times 10^{50}$

**Theorem 3**. Let $G = \rho Sa$, then $\mathrm{RC}II(\rho Sa) = 3.5974\times 10^{-15}$, $\mathrm{SC}II(\rho Sa) = 1.0712\times 10^{-17}$, $\mathrm{H}II(\rho Sa) = 3.23\times 10^{-20}$, $\mathrm{ABC}II(\rho Sa) = 5.4381\times 10^{-4}$, $\mathrm{GA}II(\rho Sa) = 0.1178$, $\mathrm{HM}II(\rho Sa) = 7.5941\times 10^{67}$, $\mathrm{SF}II(\rho Sa) = 2.2444\times 10^{-25}$, $\mathrm{PF}II(\rho Sa) = 7.5159\times 10^{-38}$, $\Pi_1^*(\rho Sa) = 8.7144\times 10^{33}$, $\Pi_2(\rho Sa) = 1.3305\times 10^{37}$.

**Proof:** Let Salannin be the chemical graph $G = \rho Sa$ consists of 43 vertices and 48 edges. In $\rho Sa$, degree 2 for 14 vertices, degree 3 for 15 vertices, degree 4 for 3 vertices and degree 1 for 11 vertices. From the Figure 4, eight classes of edge partition are obtained by considering the degree of the end vertices. In the first edge partition, $E_1$ has 4 edges, $\mu\gamma\, \varepsilon\, \mathrm{E}(\rho Sa)$ where $\delta(\mu) = 2$ and $\delta(\gamma) = 2$. In the second edge partition, $E_2$ has 17 edges $\mu\gamma$, where $\delta(\mu) = 2$ and $\delta(\gamma) = 3$. In the third edge partition, $E_3$ has 7 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 3$. In the fourth edge partition, $E_4$ has 8 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\delta(\gamma) = 3$. In the fifth edge partition, $E_5$ has 1 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\delta(\gamma) = 2$. In the sixth edge partition, $E_6$ has 6 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 1$. In the seventh edge partition, $E_7$ has 2 edges $\mu\gamma$, where $\delta(\mu) = 2$ and $\delta(\gamma) = 1$. In the eighth edge partition, $E_8$ has 3 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\delta(\gamma) = 1$. A similar computational method of Theorem 1 and 2, is then applied to complete the proof.

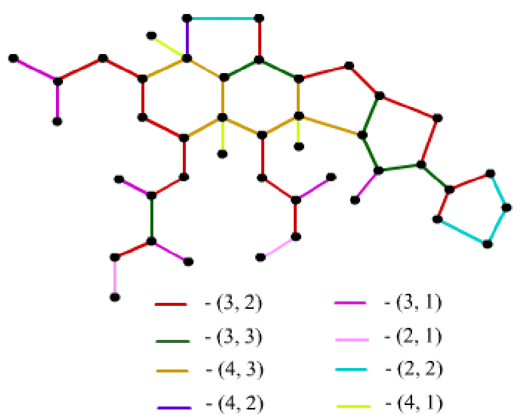


**Fig 4. The edge partition of Salannin, $\rho Sa$ based on degree of end vertices**

**Theorem 4**. Let $G = \rho Sp$, then $\mathrm{RC}II(\rho Sp) = 8.9141\times 10^{-22}$, $\mathrm{SC}II(\rho Sp) = 3.1753\times 10^{-20}$, $\mathrm{H}II(\rho Sp) = 1.4531\times 10^{-22}$, $\mathrm{ABC}II(\rho Sp) = 3.1613\times 10^{-9}$, $\mathrm{GA}II(\rho Sp) = 0.16301$, $\mathrm{HM}II(\rho Sp) = 9.8366\times 10^{77}$, $\mathrm{SF}II(\rho Sp) = 1.3433\times 10^{-27}$, $\mathrm{PF}II(\rho Sp) = 7.9462\times 10^{-43}$, $\Pi_1^*(\rho Sp) = 9.91796\times 10^{38}$, $\Pi_2(\rho Sp) = 1.2585\times 10^{42}$.

**Proof:** Let Spinosyns be the chemical graph $G = \rho Sp$ consists of 57 vertices and 52 edges. In $\rho Sp$, degree 2 for 20 vertices, degree 3 for 21 vertices and degree 1 for 11 vertices. From the Figure 5, five classes of edge partition are obtained by considering the degree of the end vertices. In the first edge partition, $E_1$ has 4 edges, $\mu\gamma\, \varepsilon\, \mathrm{E}(\rho Sp)$ where $\delta(\mu) = 2$ and $\delta(\gamma) = 2$. In the second edge partition, $E_2$ has 28 edges $\mu\gamma$, where $\delta(\mu) = 2$ and $\delta(\gamma) = 3$. In the third edge partition, $E_3$ has 14 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 3$. In the fourth edge partition, $E_4$ has 7 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 1$. In the fifth edge partition, $E_5$ has 4 edges $\mu\gamma$, where $\delta(\mu) = 2$ and $\delta(\gamma) = 1$. A similar computational method of Theorem 1 and 2, is then applied to complete the proof.

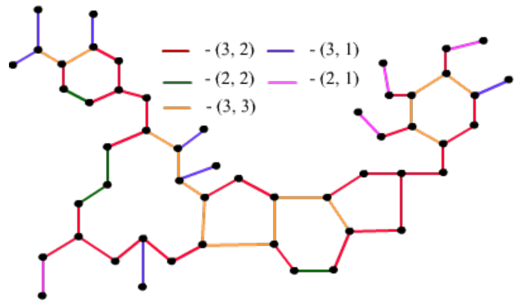


**Fig 5. The edge partition of Spinosyns , $\rho Sp$ based on degree of end nodes**

**Theorem 5**. Let $G = \rho Br$, then RC$II(\rho Br) = 2.0465\times10^{-13}$, SC$II(\rho Br) = 1.6903\times10^{-13}$, H$II(\rho Br) = 5.0206\times10^{-5}$, ABC$II(\rho Br) = 1.9635\times10^{-15}$, GA$II(\rho Br) = 0.51809$, HM$II(\rho Br) = 1.2249\times10^{51}$, SF$II(\rho Br) = 7.2385\times10^{-18}$, PF$II(\rho Br) = 1.4363\times10^{-29}$,$\Pi_1^*(\rho Br) = 3.4999\times10^{25}$,$\Pi_2(\rho Br) = 6.9622\times10^{28}$.

**Proof:** Let Brucine be the chemical graph $G = \rho Br$ consists of 30 vertices and 36 edges. In $\rho Br$, degree 2 for 13 vertices, degree 3 for 13 vertices, degree 4 for 1 vertices and degree 1 for 3 vertices. From the Figure 6, seven classes of edge partition are obtained by considering the degree of the end vertices. In the first edge partition, $E_1$ has 4 edges, $\mu\gamma\,\varepsilon$ E$(\rho Br)$ where $\delta(\mu) = 2$ and $\delta(\gamma) = 2$. In the second edge partition, $E_2$ has 15 edges $\mu\gamma$, where $\delta(\mu) = 2$ and $\delta(\gamma) = 3$. In the third edge partition, $E_3$ has 10 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 3$. In the fourth edge partition, $E_4$ has 3 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\delta(\gamma) = 3$. In the fifth edge partition, $E_5$ has 1 edges $\mu\gamma$, where $\delta(\mu) = 4$ and $\delta(\gamma) = 2$. In the sixth edge partition, $E_6$ has 1 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 1$. In the seventh edge partition, $E_7$ has 2 edges $\mu\gamma$, where $\delta(\mu) = 2$ and $\delta(\gamma) = 1$. A similar computational method of Theorem 1 and 2, is then applied to complete the proof.

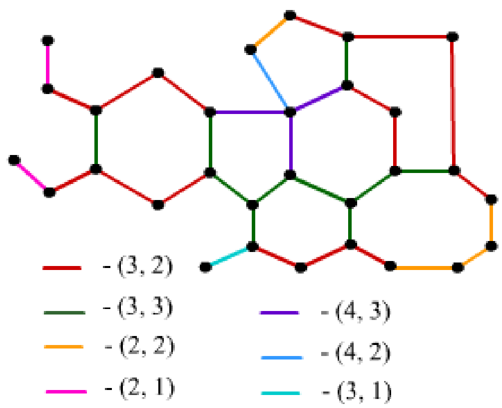


**Fig 6. The edge partition of Brucine , $\rho Br$ based on degree of end nodes**

**Theorem 6**. Let $G = \rho Di$, then RC$II(\rho Di) = 9.4747\times10^{-16}$, SC$II(\rho Di) = 1.9688\times10^{-14}$, H$II(\rho Di) = 4.2619\times10^{-16}$, ABC$II(\rho Di) = 8.6422\times10^{-7}$, GA$II(\rho Di)$ =0.4498 , HM$II(\rho Di) = 6.6558\times10^{54}$, SF$II(\rho Di) = 1.0462\times10^{-19}$, PF$II(\rho Di) = 8.977\times10^{-31}$,$\Pi_1^*(\rho Di) = 2.5799\times10^{27}$,$\Pi_2(\rho Di) = 1.11395\times10^{30}$.

**Proof:** Let Difethialone be the chemical graph $G = \rho Di$ consists of 35 vertices and 40 edges. In $\rho Di$, degree 2 for 19 vertices, degree 3 for 13 vertices and degree 1 for 3 vertices. From the Figure 7, four classes of edge partition are obtained by considering the degree of the end vertices. In the first edge partition, $E_1$ has 10 edges, $\mu\gamma\,\varepsilon$ E$(\rho Sp)$ where $\delta(\mu) = 2$ and $\delta(\gamma) = 2$. In the second edge partition, $E_2$ has 18 edges $\mu\gamma$, where $\delta(\mu) = 2$ and $\delta(\gamma) = 3$. In the third edge partition, $E_3$ has 9 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 3$. In the fourth edge partition, $E_4$ has 3 edges $\mu\gamma$, where $\delta(\mu) = 3$ and $\delta(\gamma) = 1$. A similar computational method of Theorem 1 and 2, is then applied to complete the proof.

## 4 Discussion

Our main outcome is estimation of multiplicative topological indices of some agricultural pesticides. To compute the main results, the method of analytical techniques, degree counting method, edge and vertex partition method and graphical-

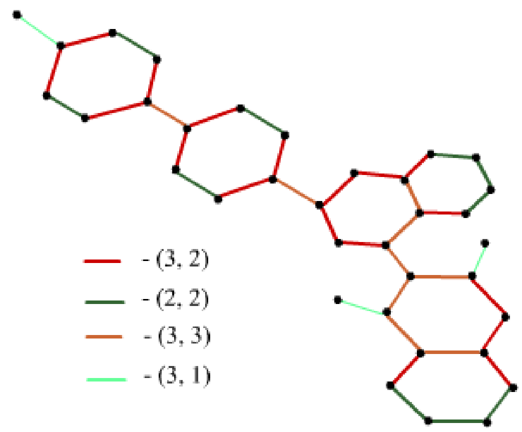


**Fig 7. The edge partition of Difethialone , $\rho Di$ based on degree of end nodes**

theoretical tools is used. Initially, first count the vertices and edges of the given chemical agricultural pesticides. As a result of the symmetry of chemical structures, vertex partitions and edge partitions based on the degree of end nodes are determined. Topological indices of Azadirachtin ($\rho Za$), Avermectin b1a ($\rho Av$) , Salannin ($\rho Sa$), Spinosyns ($\rho Sp$) , Brucine ($\rho Br$) and Difethialone ($\rho Di$) were computed using these edge partitions. The graphical comparison among the indices also plotted using MATLAB. Refer Figure 8 for the same.

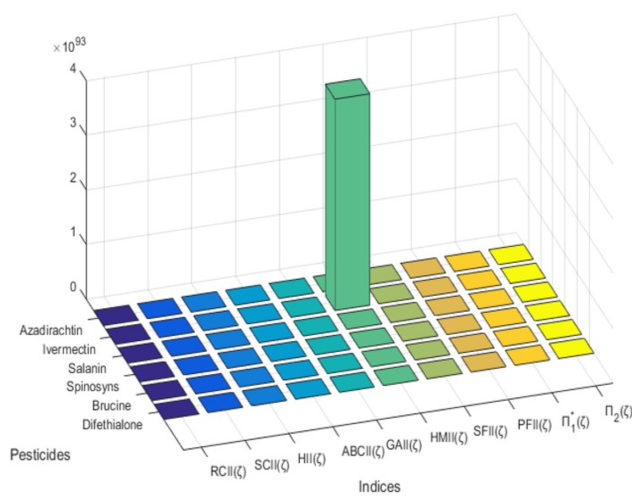


**Fig 8. The graphical comparison of pesticides and indices**

## 5 Conclusion

In this article, multiplicative degree based namely multiplicative Randic index, multiplicative Harmonic index, multiplicative sum connectivity index, multiplicative atomic bond connectivity index, multiplicative geometric arithmetic index, multiplicative sum connectivity F-index, multiplicative product connectivity F-index, multiplicative hyper Zagreb index, multiplicative first and second Zagreb index of Azadirachtin($\rho Za$), Avermectin b1a,($\rho Av$) , Salannin ($\rho Sa$), Spinosyns ($\rho Sp$) , Brucine ($\rho Br$) and Difethialone ($\rho Di$) has been computed. It is possible that the computed numerical values help gain a deeper understanding of nature and behaviour of pesticides. This alternative approach for toxicity prediction of compounds which ease the chemist to examine the function of pesticides.

## 6 Declaration

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