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Research Article

Useful Irregularity Indices in QSPR Study for Bismuth Tri-Iodide

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Topological indices give us a mathematical language to study molecular structures. They convert a chemical compound into a single number which foresees properties, for example, boiling points, viscosity, and the radius of gyrations. Drugs and other chemical compounds are often modeled as various polygonal shapes, trees, and graphs. In this paper, we will compute some irregularity indices for bismuth tri-iodide chain and sheet that are useful in the quantitative structure-activity relationship.

1. Introduction

In discrete mathematics, graph theory in general not only is the study of different properties of objects but also tells us about objects having same properties as the investigating object. These properties of different objects are of main interest. In particular, graph polynomials related to graph are rich in information. Mathematical tools like polynomials and topological-based numbers [1–5] have significant importance to collect information about properties of chemical compounds. We can find out many hidden information about compounds through these tools. Multifold graph polynomials are presented in the literature. Actually, topological indices are numeric quantities that tell us about the whole structure of graph. There are many topological indices that help us to study physical and chemical reactivities and biological properties [6–12]. Wiener, in 1947, firstly introduced the concept of topological index while working on boiling point. In particular, Hosoya polynomial plays an important in the area of distance-based topological indices, and we can find out the Wiener index, hyper-Wiener index, and Tratch–Stankevich–Zefirov index by Hosoya polynomial. For more about topological indices, refer [5, 13–35].

BiI_3 is an inorganic compound which is the result of the reaction of iodine and bismuth, which inspired the enthusiasm for subjective inorganic investigations [36]. BiI_3 is an excellent inorganic compound and is very useful in "qualitative inorganic analysis" [37]. It was proved that Bi-doped glass optical strands are one of the most promising dynamic laser media. Different kinds of Bi-doped fiber strands have been created and have been used to construct Bi-doped fiber lasers and optical loudspeakers [38].

Layered BiI_3 gemstones are considered to be a three-layered stack structure in which a plane of bismuth atoms is sandwiched between iodide particle planes to form a continuous I-Bi-I plane [39]. The periodic superposition of the diamond-shaped three layers forms BiI_3 crystals with R-3 symmetry [40, 41]. A progressive stack of I-Bi-I layers forms a symmetric hexagonal structure [42], and jewel of BiI_3 was integrated in [43]. In Figures 1 and 2, main cycles are C_4^1 and C_4^2, central cycles are C_4^3 and C_4^6, and base cycles are C_4^4 and C_4^5.

TI is known as the irregularity index, [44] if TI of graph is greater than or equal to zero and TI of graph is equal to zero if and only if graph is regular. The irregularity indices are given below. All these irregularity indices belong to degree-based topological invariants except IRM2 (G) and are used in QSAR.

(1) $\mathrm{VAR}(G) = \sum_{u\epsilon V} (d_u - (2m/n))^2 = (M_1(G)/n) - (2m/n)^2$

(2) $\mathrm{AL}(G) = \sum_{uv\in E(G)} |d_u - d_v|$

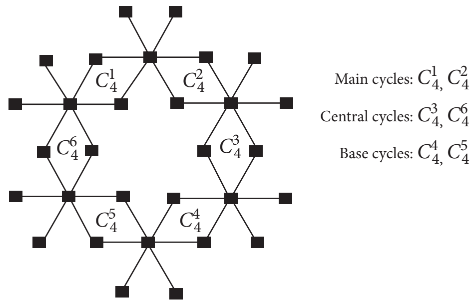

Figure 1: Unit cell (bismuth tri-iodide).

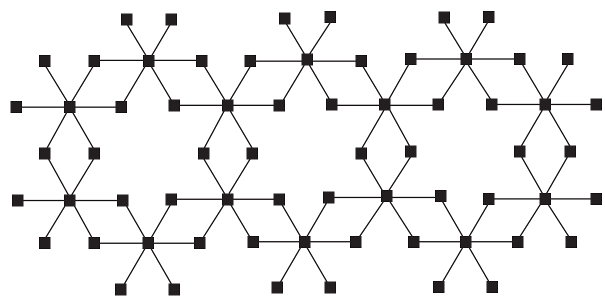

Figure 2: Chain for $m = 3$ (bismuth tri-iodide).

(3) $\mathrm{IR1}(G) = \sum_{u\in V}(d_u)^3 - (2m/n)\sum_{u\in V}(d_u)^2 = F(G) - (2m/n)M_1(G)$

(4) $\mathrm{IR2}(G) = \sqrt{(\sum_{uv\in E(G)} d_u d_v/m)} - (2m/n) = \sqrt{(M_2(G)/m)} - (2m/n)$

(5) $\mathrm{IRF}(G) = \sum_{uv\in E(G)}(d_u - d_v)^2 = F(G) - 2M_2(G)$

(6) $\mathrm{IRFW}(G) = (\mathrm{IRF}(G)/M_2(G))$

(7) $\mathrm{IRA}(G) = \sum_{uv\in E(G)}(d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G)$

(8) $\mathrm{IRB}(G) = \sum_{uv\in E(G)}(d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2\mathrm{RR}(G)$

(9) $\mathrm{IRC}(G) = (\sum_{uv\in E(G)}\sqrt{d_u d_v}/m) - (2m/n) = (\mathrm{RR}(G)/m) - (2m/n)$

(10) $\mathrm{IRDIF}(G) = \sum_{uv\in E(G)}|(d_u/d_v) - (d_v/d_u)| = \sum_{i<j} m_{i,j}((j/i) - (i/j))$

(11) $\mathrm{IRL}(G) = \sum_{uv\in E(G)}|\ln d_u - \ln d_v| = \sum_{i<j} m_{i,j} ln(j/i)$

(12) $\mathrm{IRLU}(G) = \sum_{uv\in E(G)}|d_u - d_v|/\min(d_u, d_v) = \sum_{i<j} m_{i,j}\ln((j-i)/i)$

(13) $\mathrm{IRLF}(G) = \sum_{uv\in E(G)}|d_u - d_v|/\sqrt{(d_u d_v)} = \sum_{i<j} m_{i,j}((j-i)/\sqrt{ij})$

(14) $\mathrm{IRLA}(G) = 2\sum_{uv\in E(G)}|d_u - d_v|/(d_u + d_v) = 2\sum_{i<j} m_{i,j}((j-i)/(i+j))$

(15) $\mathrm{IRD1}(G) = \sum_{uv\in E(G)}\ln 1 + |d_u - d_v| = \sum_{i<j} m_{i,j}\ln(i+j-1)$

(16) $\mathrm{IRGA}(G)\sum_{uv\in E(G)}\ln((d_u + d_v)/2\sqrt{d_u d_v}) \sum_{i<j} m_{i,j}((i+j)/2\sqrt{ij})$

M_1, M_2, R, RR, and F are first Zagreb index, second Zagreb index, Randić index, reverse Randić index, and forgotten index, respectively [45–49]. It can be noted that many irregularity indices are constructed with the help of many known TIs.

2. Methodology

To compute our results, first we construct graphs of bismuth tri-iodides and count number of vertices and edges. Secondly, we divide the edge set into different classes with respect to the degrees of end vertices. By applying definitions and using edge division, we computed our results. Finally, we plotted our results to see the dependence on the involved parameters. We used Maple 2015 for plotting our results.

3. Irregularity Indices for Bismuth Tri-Iodide

3.1. Irregularity Indices for Bismuth Tri-Iodide Chain $m - BiI_3$. The unit cell of bismuth tri-iodide is given in Figure 1, and the algebraic graph of bismuth tri-iodide chain $m - \mathrm{BiI}_3$ is shown in Figure 2. For bismuth tri-iodide chain, $|V(m - \mathrm{BiI}_3)| = 6(3m+2)$ and $|E(m - \mathrm{BiI}_3)| = 12(2m+1)$. There are two types of edges in edge set present in the bismuth tri-iodide chain $m - \mathrm{BiI}_3$ given in Table 1.

Theorem 1. *Let $m - BiI_3$ be the bismuth tri-iodide chain. The irregularity indices are*

(1) $\mathrm{VAR}(m - \mathrm{BiI}_3) = 2(45m^2 + 64m + 20)/3(3m+2)^2$

(2) $\mathrm{AL}(m - \mathrm{BiI}_3) = 100m + 56$

Table 1: Partition of $E(m-\mathrm{BiI}_3)$.

(d_u, d_v)	Frequency
(1, 6)	$4m+8$
(2, 6)	$20m+4$

(3) $\mathrm{IR1}(m-\mathrm{BiI}_3) = 8(55m^2+151m+70)/(3m+2)$

(4) $\mathrm{IR2}(m-\mathrm{BiI}_3) = 1/(\sqrt{6m+3})(3m+2)((\sqrt{66m+24})(3m+2)-(8m+4)(\sqrt{6m+3}))$

(5) $\mathrm{IRF}(m-\mathrm{BiI}_3) = 120m+264$

(6) $\mathrm{IRFW}(m-\mathrm{BiI}_3) = (120m+264)/(264m+96)$

(7) $\mathrm{IRA}(m-\mathrm{BiI}_3) = (1/3)((24-20\sqrt{3}-4\sqrt{6})m+(36-4\sqrt{3}-8\sqrt{6}))$

(8) $\mathrm{IRB}(m-\mathrm{BiI}_3) = (188-8\sqrt{3}-8\sqrt{6})m+(88-16\sqrt{3}-16\sqrt{6})$

(9) $\mathrm{IRC}(m-\mathrm{BiI}_3) = (1/3)(2m+1)(3m+2)((3\sqrt{6}+30\sqrt{3}-48)m^2+(8\sqrt{6}+26\sqrt{3}-48)m+(4\sqrt{6}+4\sqrt{3}-12))$

(10) $\mathrm{IRDIF}(m-\mathrm{BiI}_3) = (1/3)(230m+172)$

(11) $\mathrm{IRL}(m-\mathrm{BiI}_3) = 28.96m+18.68$

(12) $\mathrm{IRLU}(m-\mathrm{BiI}_3) = 60m+48$

(13) $\mathrm{IRLF}(m-\mathrm{BiI}_3) = (1/6)[(20\sqrt{6}+80\sqrt{3})m+(40\sqrt{6}+16\sqrt{3})]$

(14) $\mathrm{IRLA}(m-\mathrm{BiI}_3) = (1/7)(180m+108)$

(15) $\mathrm{IRD1}(m-\mathrm{BiI}_3) = 39.16m+20.72$

(16) $\mathrm{IRGA}(m-\mathrm{BiI}_3) = 4m+3.32$

Proof

$$\begin{aligned}\mathrm{VAR}(m-\mathrm{BiI}_3) &= \sum_{u\epsilon V}\left(d_u-\frac{2m}{n}\right)^2 = \frac{M_1(m-BiI_3)}{n}-\left(\frac{2m}{n}\right)^2\\ &= \left(\frac{188m+88}{18m+12}\right)-\left(\frac{2(24m+12)}{(18m+12)}\right)^2\\ &= \frac{2(45m^2+64m+20)}{3(3m+2)^2},\end{aligned} \tag{1}$$

$$\begin{aligned}\mathrm{AL}(m-\mathrm{BiI}_3) &= \sum_{uv\epsilon E(m-\mathrm{BiI}_3)}|d_u-d_v|\\ &= |1-6|(4m+8)+|2-6|(20m+4)\\ &= 100m+56,\end{aligned} \tag{2}$$

$$\begin{aligned}\mathrm{IR1}(m-\mathrm{BiI}_3) &= \sum_{u\epsilon V} d_u^3-\frac{2m}{n}\sum_{u\epsilon V} d_u^2\\ &= F(G)-\left(\frac{2m}{n}\right)M_1(m-\mathrm{BiI}_3)\\ &= (948m+456)-\frac{2(24m+12)}{18m+12}(188m+88)\\ &= \frac{8(55m^2+151m+70)}{3m+2},\end{aligned} \tag{3}$$

$$\begin{aligned}\mathrm{IR2}(m-\mathrm{BiI}_3) &= \sqrt{\frac{\sum_{uv\epsilon E(m-\mathrm{BiI}_3)} d_u d_v}{m}}-\frac{2m}{n}\\ &= \sqrt{\frac{M_2(m-\mathrm{BiI}_3)}{m}}-\frac{2m}{n}\\ &= \sqrt{\frac{264m+96}{24m+12}}-\left(\frac{2(24m+12)}{18m+12}\right)\\ &= \frac{1}{(\sqrt{6m+3})(3m+2)}((\sqrt{66m+24})\\ &\quad\cdot(3m+2)-(8m+4)(\sqrt{6m+3})),\end{aligned} \tag{4}$$

$$\begin{aligned}\mathrm{IRF}(m-\mathrm{BiI}_3) &= \sum_{uv\epsilon E(m-\mathrm{BiI}_3)}(d_u-d_v)^2\\ &= (1-6)^2(4m+8)+(2-6)^2(20m+4)\\ &= 120m+264,\end{aligned} \tag{5}$$

$$\begin{aligned}\mathrm{IRFW}(m-\mathrm{BiI}_3) &= \frac{\mathrm{IRF}(m-\mathrm{BiI}_3)}{M_2(m-\mathrm{BiI}_3)}\\ &= \frac{120m+264}{264m+96},\end{aligned} \tag{6}$$

$$\begin{aligned}\mathrm{IRA}(m-\mathrm{BiI}_3) &= \sum_{uv\epsilon E(m-\mathrm{BiI}_3)}\left(d_u^{-1/2}-d_v^{-1/2}\right)^2\\ &= n-2R(m-\mathrm{BiI}_3)\\ &= (18m+12)-\left(\frac{1}{6}\sqrt{6}(4m+8)\right.\\ &\quad\left.+\frac{1}{6}\sqrt{3}(20m+4)\right)\\ &= \frac{1}{3}((24-20\sqrt{3}-4\sqrt{6})m\\ &\quad+(36-4\sqrt{3}-8\sqrt{6})),\end{aligned} \tag{7}$$

$$\begin{aligned}\mathrm{IRB}(m-\mathrm{BiI}_3) &= \sum_{uv\epsilon E(m-\mathrm{BiI}_3)} \left(d_u^{1/2}-d_v^{1/2}\right)^2 \\ &= M_1(D_nP_n) - 2\mathrm{RR}(m-\mathrm{BiI}_3) \\ &= (188m+88) - 2(\sqrt{6}(4m+8) \\ &\quad + 2\sqrt{3}(20m+4)) = (188-8\sqrt{3}-8\sqrt{6})m \\ &\quad + (88-16\sqrt{3}-16\sqrt{6}),\end{aligned} \tag{8}$$

$$\begin{aligned}\mathrm{IRC}(m-\mathrm{BiI}_3) &= \frac{\sum_{uv\epsilon E(m-\mathrm{BiI}_3)}\sqrt{d_ud_v}}{m} - \frac{2m}{n} \\ &= \frac{\mathrm{RR}(m-\mathrm{BiI}_3)}{m} - \frac{2m}{n} \\ &= \frac{\sqrt{6}(4m+8)+2\sqrt{3}(20m+4)}{24m+12} \\ &\quad - \frac{2(24m+12)}{18m+12} = \frac{1}{3(2m+1)(3m+2)} \\ &\quad \cdot \left((3\sqrt{6}+30\sqrt{3}-48)m^2\right. \\ &\quad + (8\sqrt{6}+26\sqrt{3}-48)m \\ &\quad \left.+ (4\sqrt{6}+4\sqrt{3}-12)\right),\end{aligned} \tag{9}$$

$$\begin{aligned}\mathrm{IRDIF}(m-\mathrm{BiI}_3) &= \sum_{uv\epsilon E(m-\mathrm{BiI}_3)} \left|\frac{d_u}{d_v}-\frac{d_v}{d_u}\right| \\ &= \left(\left|\frac{1}{6}-\frac{6}{1}\right|\right)(4m+8) + \left(\left|\frac{2}{6}-\frac{6}{2}\right|\right)(20m+4) \\ &= \frac{1}{3}(230m+172),\end{aligned} \tag{10}$$

$$\begin{aligned}\mathrm{IRL}(m-\mathrm{BiI}_3) &= \sum_{uv\epsilon E(m-\mathrm{BiI}_3)} \left|\ln d_u - \ln d_v\right| \\ &= |\ln 1 - \ln 6|(4m+8) + |\ln 2 - \ln 6|(20m+4) \\ &= 28.96m + 18.68,\end{aligned} \tag{11}$$

$$\begin{aligned}\mathrm{IRLU}(m-\mathrm{BiI}_3) &= \sum_{uv\epsilon E(m-\mathrm{BiI}_3)} \frac{|d_u-d_v|}{\min(d_u,d_v)} \\ &= \left(\frac{|1-6|}{1}\right)(4m+8) + \left(\frac{|2-6|}{2}\right)(20m+8) \\ &= 60m+48,\end{aligned} \tag{12}$$

$$\begin{aligned}\mathrm{IRLF}(m-\mathrm{BiI}_3) &= \sum_{uv\epsilon E(m-\mathrm{BiI}_3)} \frac{|d_u-d_v|}{\sqrt{d_u\cdot d_v}} \\ &= \left(\frac{|1-6|}{\sqrt{6}}\right)(4m+8) + \left(\frac{|2-6|}{\sqrt{12}}\right)(20m+8) \\ &= \frac{1}{6}((20\sqrt{6}+80\sqrt{3})m + (40\sqrt{6}+16\sqrt{3})),\end{aligned} \tag{13}$$

$$\begin{aligned}\mathrm{IRLA}(m-\mathrm{BiI}_3) &= \sum_{uv\epsilon E(m-\mathrm{BiI}_3)} 2\frac{|d_u-d_v|}{(d_u+d_v)} \\ &= 2\left(\frac{|1-6|}{1+6}\right)(4m+8) + 2\left(\frac{|2-6|}{2+6}\right) \\ &\quad \cdot (20m+4) \\ &= \frac{1}{7}(180m+108),\end{aligned} \tag{14}$$

$$\begin{aligned}\mathrm{IRD1}(m-\mathrm{BiI}_3) &= \sum_{uv\epsilon E(m-\mathrm{BiI}_3)} \ln\{1+|d_u-d_v|\} \\ &= \ln\{1+|1-6|\}(4m+8) + \ln\{1+|2-6|\} \\ &\quad \cdot (20m+4) \\ &= 39.16m + 20.72,\end{aligned} \tag{15}$$

$$\begin{aligned}\mathrm{IRGA}(m-\mathrm{BiI}_3) &= \sum_{uv\epsilon E(m-\mathrm{BiI}_3)} \ln\left(\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right) \\ &= \ln\left(\frac{1+6}{2\sqrt{1\times 6}}\right)(4m+8) + \ln\left(\frac{2+6}{2\sqrt{2\times 6}}\right) \\ &\quad \cdot (20m+4) \\ &= 4m+3.32.\end{aligned} \tag{16}$$

□

3.2. Graphical Representation of Bismuth Tri-Iodide Chain $m-BiI_3$. Here, we will graphically present results of irregularity indices for bismuth tri-iodide chain $m-\mathrm{BiI}_3$. From these plots, one can observe the behavior of computed results on the involved parameters (Figure 3).

4. Irregularity Indices for Bismuth Tri-Iodide Sheet $\mathrm{BiI}_3\,(m\times n)$

The algebraic graph of bismuth tri-iodide sheet $\mathrm{BiI}_3\,(m\times n)$ is shown in Figure 4. For bismuth tri-iodide sheet, $|V\,(\mathrm{BiI}_3\,(m\times$

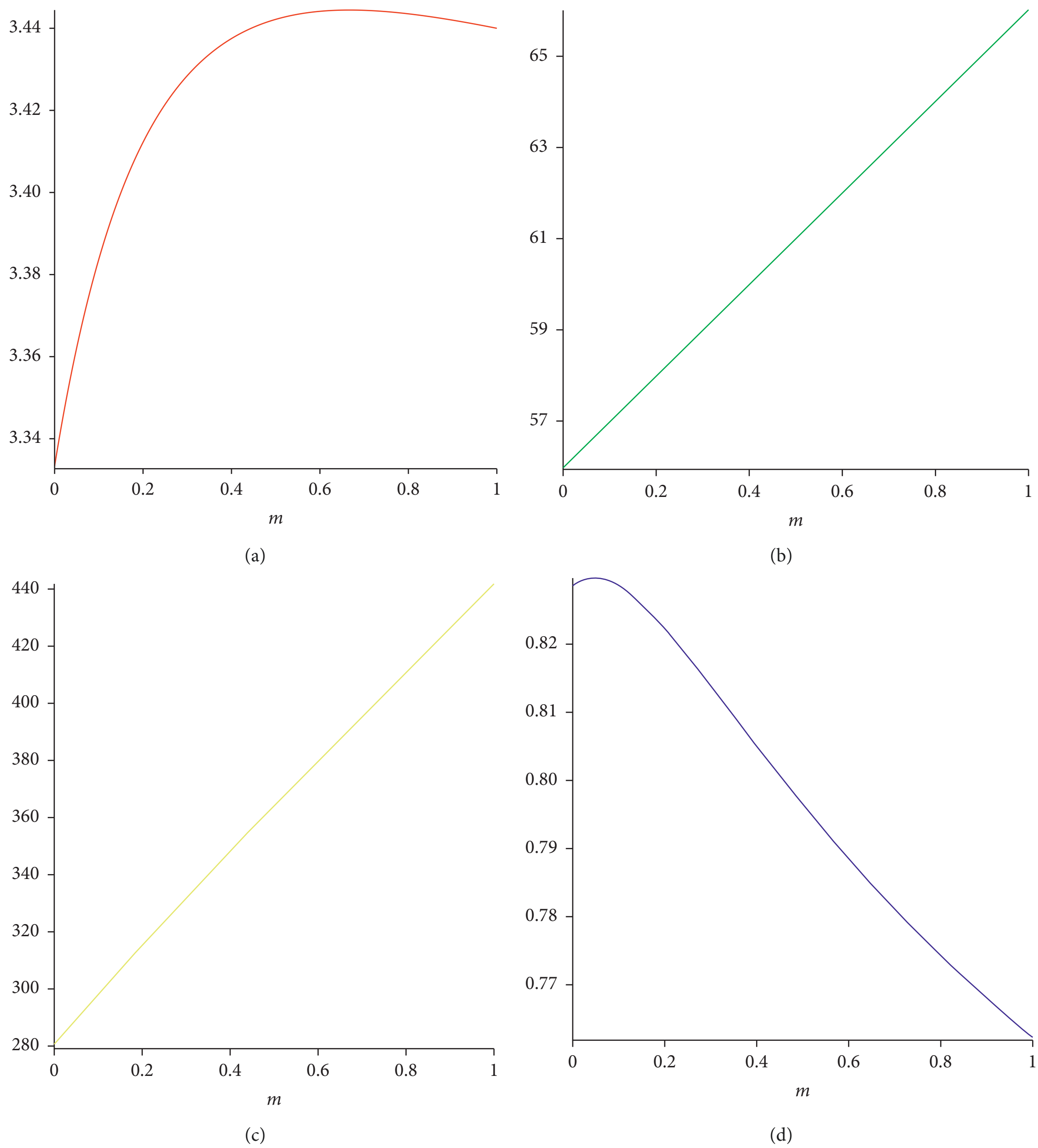

FIGURE 3: Continued.

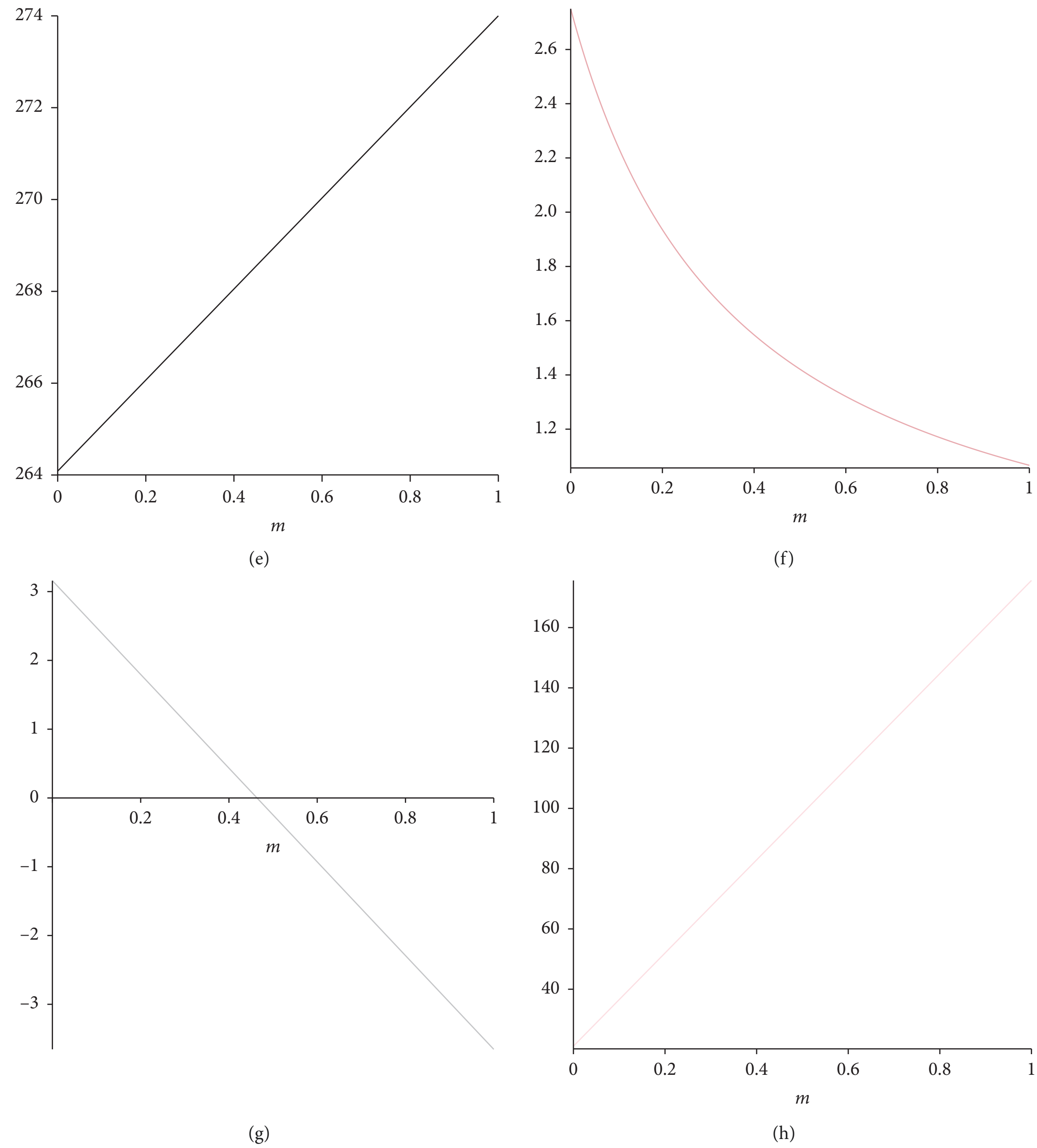

Figure 3: Continued.

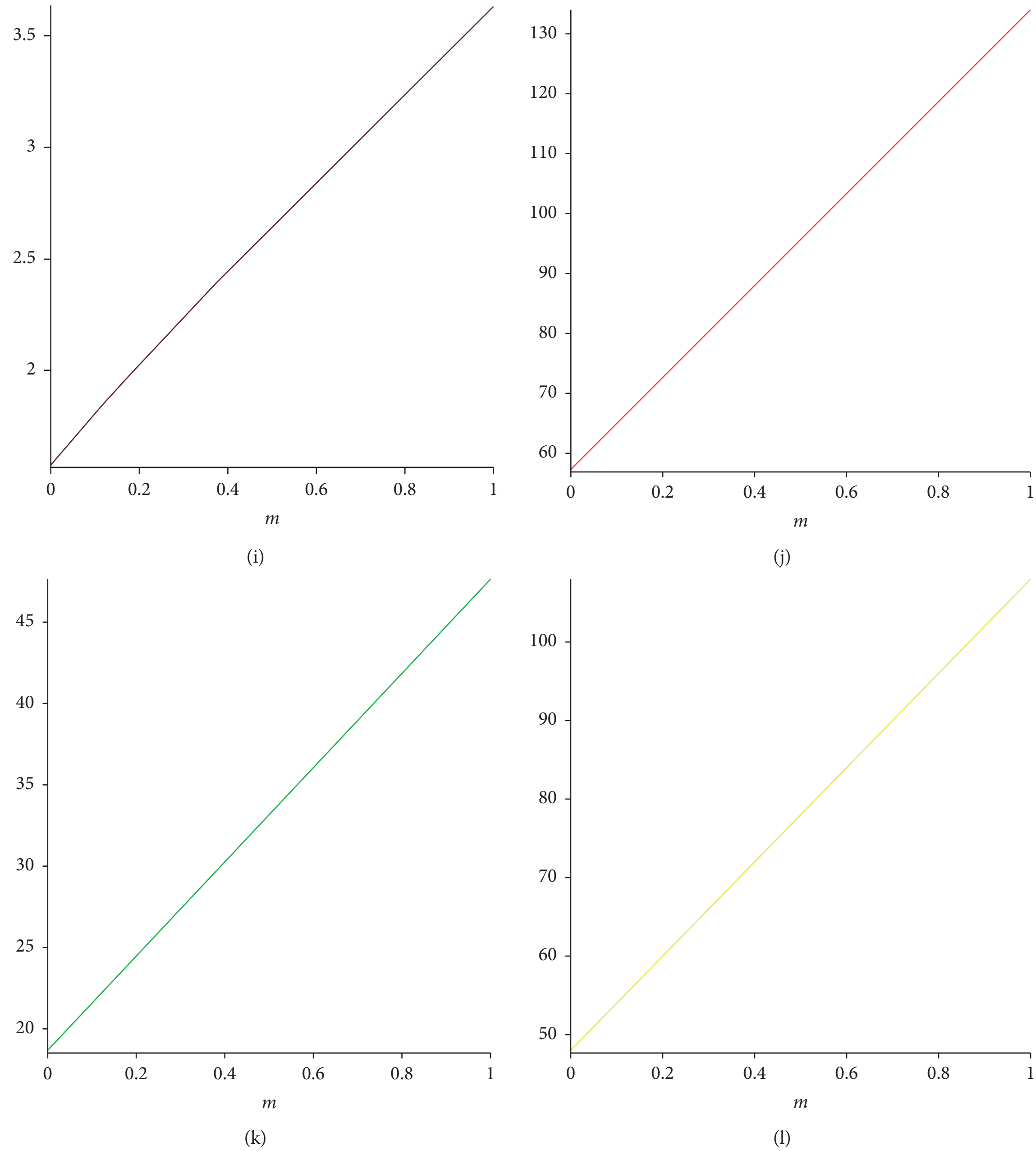

FIGURE 3: Continued.

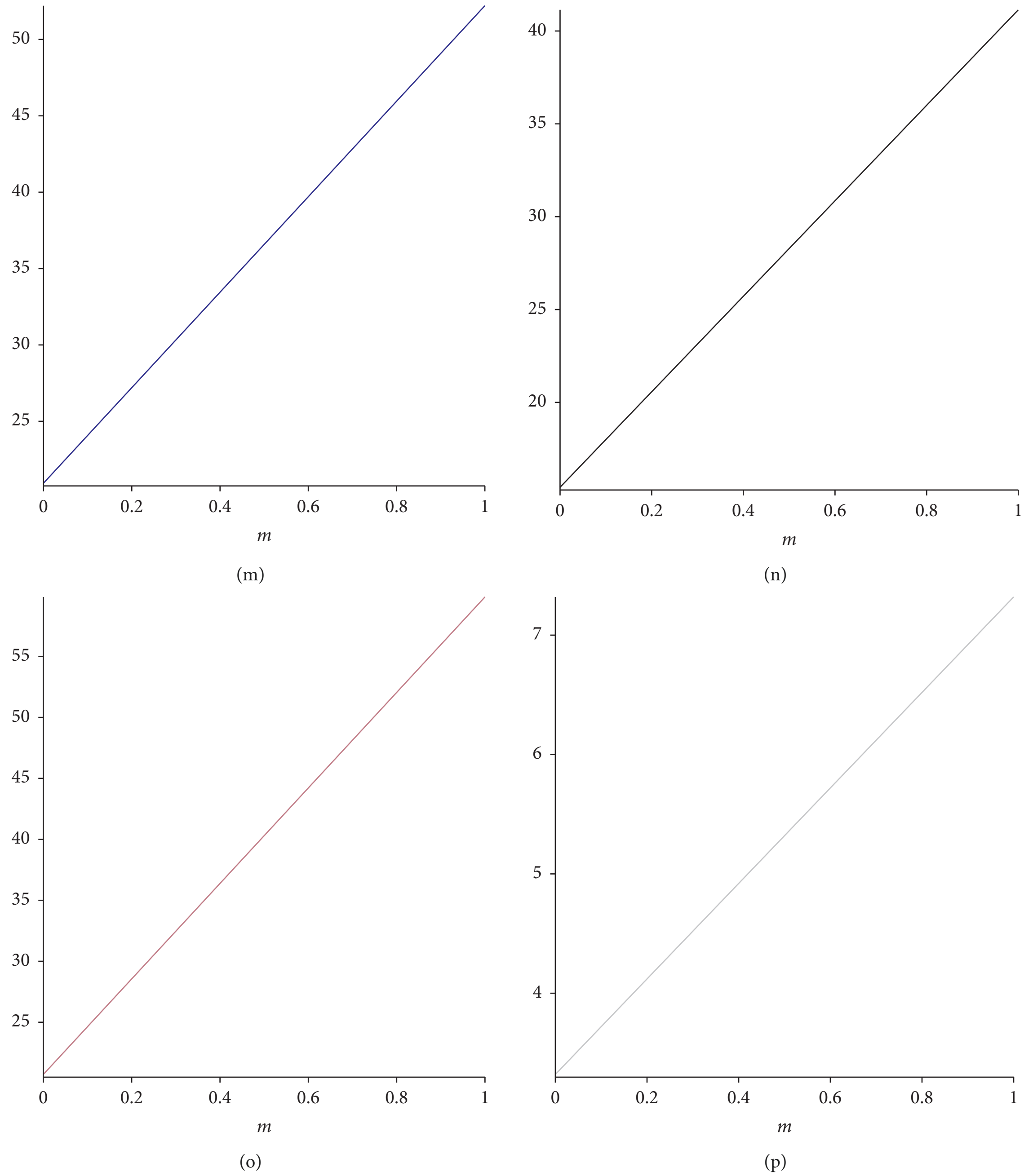

Figure 3: (a) VAR $(m - BiI_3)$; (b) AL $(m - BiI_3)$; (c) IR1 $(m - BiI_3)$; (d) IR2 $(m - BiI_3)$; (e) IRF $(m - BiI_3)$; (f) IRFW $(m - BiI_3)$; (g) IRA $(m - BiI_3)$; (h) IRB $(m - BiI_3)$; (i) IRC $(m - BiI_3)$; (j) IRDIF $(m - BiI_3)$; (k) IRL $(m - BiI_3)$; (l) IRLU $(m - BiI_3)$; (m) IRLF $(m - BiI_3)$; (n) IRLA $(m - BiI_3)$; (o) IRD1 $(m - BiI_3)$; (p) IRGA $(m - BiI_3)$.

$n))| = 11mn + 10m + 7n + 2$ and $|E(BiI_3(m \times n))| = 18mn + 12m + 6n$. There are two types of edges in edge set present in bismuth tri-iodide sheet $BiI_3(m \times n)$, as given in Table 2.

Theorem 2. *Let $BiI_3(m \times n)$ be the bismuth tri-iodide sheet. The irregularity indices are*

(1) $\mathrm{VAR}(BiI_3(m \times n)) = 2(177m^2n^2 + 392m^2n - 402mn^2 + 172m^2 - 288mn - 387n^2 + 72m - 104n - 4)/(11mn + 10m + 7n + 2)^2$

(2) $\mathrm{AL}(BiI_3(m \times n)) = 66mn + 52m - 30n + 4$

(3) $\mathrm{IR1}(BiI_3(m \times n)) = 2(1425m^2n^2 + 2868m^2n + 914mn^2 + 1236m^2 + 712mn - 1007n^2 + 456m - 460n - 12)/(11mn + 10m + 7n + 2)$

(4) $\mathrm{IR2}(BiI_3(m \times n)) = (1/(\sqrt{18mn + 12m + 6n})(11mn + 10m + 7n + 2))[(\sqrt{252mn + 468m - 442n - 12})(11mn + 10m + 7n + 2) - 2(18mn + 12m + 6n)(\sqrt{18mn + 12m + 6n})]$

(5) $\mathrm{IRF}(BiI_3(m \times n)) = 246mn + 228m - 82n + 36$

(6) $\mathrm{IRFW}(BiI_3(m \times n)) = (246mn + 228m - 82n + 36)/(252mn + 120m - 180n - 24)$

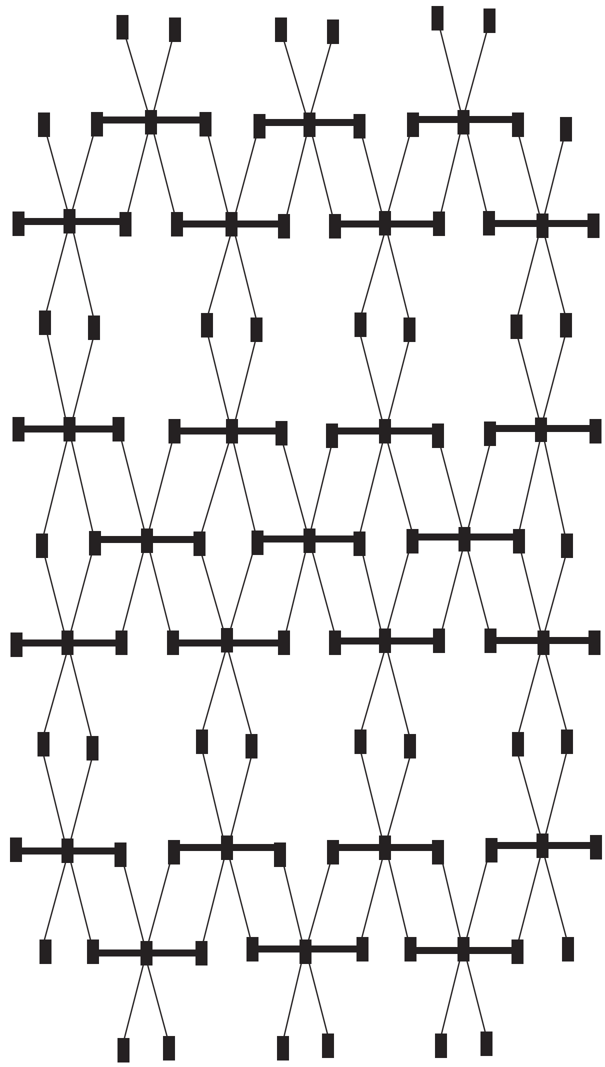

FIGURE 4: Sheet for $m = 2$ and $n = 3$ (bismuth tri-iodide).

TABLE 2: Partition of $E(BiI_3(m \times n))$.

(d_u, d_v)	Frequency
(1, 6)	$4(m+n+1)$
(2, 6)	$4(3mn+2m+2n-1)$
(3, 6)	$6n(m-1)$

(7) $IRA(BiI_3(m \times n)) = (1/3)[(33 - 4\sqrt{3} - 2\sqrt{2})mn + (10 - 4\sqrt{6} - 8\sqrt{3})m + (21 - 2\sqrt{6} + 8\sqrt{3} + 5\sqrt{2})n + (6 - 2\sqrt{6} + 2\sqrt{3})]$

(8) $IRB(BiI_3(m \times n)) = (150 - 48\sqrt{3} - 36\sqrt{2})mn + (92 - 8\sqrt{3} - 4\sqrt{6})m - (90 - 4\sqrt{2} - 8\sqrt{3} + 2\sqrt{6})n - (4 - 2\sqrt{3} + 2\sqrt{6})$

(9) $IRC(BiI_3(m \times n)) = (((18\sqrt{(2)} + 24\sqrt{(3)})mn + (2\sqrt{(6)} + 4\sqrt{(3)})m - (2\sqrt{(2)} + 4\sqrt{(3)} - \sqrt{(6)})n + \sqrt{(6)} - \sqrt{(3)})/(18mn + 12m + 6n)) - (2(18mn + 12m + 6n)/(11mn + 10m + 7n + 2))$

(10) $IRDIF(BiI_3(m \times n)) = (1/3)(123mn + 134m - 21n + 38)$

(11) $IRL(BiI_3(m \times n)) = 17.22mn + 15.88m - 5.70n + 2.80$

(12) $IRLU(BiI_3(m \times n)) = 30mn + 36m - 2n + 12$

(13) $IRLF(BiI_3(m \times n)) = (1/3)[(9\sqrt{2} + 24\sqrt{3})mn + (10\sqrt{6} + 16\sqrt{3})m + (10\sqrt{6} - 16\sqrt{3} - 9\sqrt{2})n + (10\sqrt{6} - 8\sqrt{3})]$

(14) $IRLA(BiI_3(m \times n)) = (1/7)(112mn + 64m - 76n - 20)$

(15) $IRD1(BiI_3(m \times n)) = 27.48mn + 19.96m - 13.92n + 0.76$

(16) $IRGA(BiI_3(m \times n)) = 1.86mn + 2.44m + 0.06n + 0.88$

Proof

$$\begin{aligned}
\mathrm{VAR}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{u\in V}\left(d_u-\frac{2m}{n}\right)^2=\frac{M_1\left(\mathrm{BiI}_3(m\times n)\right)}{n}-\left(\frac{2m}{n}\right)^2\\
&=\left(\frac{150mn+92m-90n-4}{11mn+10m+7n+2}\right)-\left(\frac{2(18mn+12m+6n)}{11mn+10m+7n+2}\right)^2\\
&=\frac{1}{(11mn+10m+7n+2)^2}\left(2\left(177m^2n^2+392m^2n-402mn^2\right.\right.\\
&\quad\left.\left.+172m^2-288mn-387n^2+72m-104n-4\right)\right),
\end{aligned}\tag{17}$$

$$\begin{aligned}
\mathrm{AL}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)}\left|d_u-d_v\right|\\
&=|1-6|(4m+4n+4)+|1-3|(1)+|2-6|(12mn+8m+8n-4)\\
&\quad+|3-6|(6mn-6n)=66mn+52m-30n+4,
\end{aligned}\tag{18}$$

$$\begin{aligned}
\mathrm{IR1}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{u\in V)}d_u^3-\frac{2m}{n}\sum_{u\in V)}d_u^2=F(G)-\frac{2m}{n}M_1\left(\mathrm{BiI}_3(m\times n)\right)\\
&=(750mn+468m-442n-12)\\
&\quad-\left(\frac{2(18mn+12m+6n)}{11mn+10m+7n+2}\right)(150mn+92m-90n-4)\\
&=\frac{1}{11mn+10m+7n+2}\left(2\left(1425m^2n^2+2868m^2n\right.\right.\\
&\quad\left.\left.+914mn^2+1236m^2+712mn-1007n^2+456m-460n-12\right)\right),
\end{aligned}\tag{19}$$

$$\begin{aligned}
\mathrm{IR2}\left(\mathrm{BiI}_3(m\times n)\right) &= \sqrt{\frac{\sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)}d_ud_v}{m}}-\frac{2m}{n}=\sqrt{\frac{M_2\left(\mathrm{BiI}_3(m\times n)\right)}{m}}-\frac{2m}{n}\\
&=\sqrt{\frac{252mn+120m+180n-24}{18mn+12m+6n}}-\frac{2(18mn+12m+6n)}{11mn+10m+7n+2}\\
&=\frac{1}{\left(\sqrt{18mn+12m+6n}\right)(11mn+10m+7n+2)}\\
&\quad\cdot\left[\left(\sqrt{252mn+468m-442n-12}\right)(11mn+10m+7n+2)\right.\\
&\quad\left.-2(18mn+12m+6n)\left(\sqrt{18mn+12m+6n}\right)\right],
\end{aligned}\tag{20}$$

$$\begin{aligned}
\mathrm{IRF}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)}\left(d_u-d_v\right)^2\\
&=(1-6)^2(4m+4n+4)+(2-6)^2\\
&\quad\cdot(12mn=8m+8n-4)+(3-6)^2(6mn-6n)\\
&=246mn+228m-82n+36,
\end{aligned}\tag{21}$$

$$\begin{aligned}
\mathrm{IRFW}\left(\mathrm{BiI}_3(m\times n)\right) &= \frac{(\mathrm{IRF}(m\times n))}{M_2\left(\mathrm{BiI}_3(m\times n)\right)}\\
&=\frac{246mn+228m-82n+36}{252mn+120m-180-24},
\end{aligned}\tag{22}$$

$$\begin{aligned}
\mathrm{IRA}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)} \left(d_u^{-1/2}-d_v^{-1/2}\right)^2 = n-2R(G) \\
&= (11mn+10m+7n+2)-\frac{2}{3}((\sqrt{2}+2\sqrt{3})mn \\
&\quad +(2\sqrt{6}+\sqrt{3})m-(2\sqrt{2}+4\sqrt{3}-\sqrt{6})n \\
&\quad +(\sqrt{6}-\sqrt{3})) = \frac{1}{3}((33-4\sqrt{3}-2\sqrt{2})mn \\
&\quad +(10-4\sqrt{6}-8\sqrt{3})m+(21-2\sqrt{6}+8\sqrt{3} \\
&\quad +5\sqrt{2})n+(6-2\sqrt{6}+2\sqrt{3})),
\end{aligned} \tag{23}$$

$$\begin{aligned}
\mathrm{IRB}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)} \left(d_u^{1/2}-d_v^{1/2}\right)^2 = M_1(G)-2\mathrm{RR}(G) \\
&= (252mn+120m-180n-24)-[(24\sqrt{3}+18\sqrt{2})mn \\
&\quad +(4\sqrt{6}+16\sqrt{3})m+(4\sqrt{6}-16\sqrt{3}-18\sqrt{2})n \\
&\quad +(4\sqrt{6}-8\sqrt{3})] = (150-48\sqrt{3}-36\sqrt{2})mn \\
&\quad +(92-8\sqrt{3}-4\sqrt{6})m-(90-4\sqrt{2}-8\sqrt{3} \\
&\quad +2\sqrt{6})n-(4-2\sqrt{3}+2\sqrt{6}),
\end{aligned} \tag{24}$$

$$\begin{aligned}
\mathrm{IRC}\left(\mathrm{BiI}_3(m\times n)\right) &= \frac{\sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)}\sqrt{d_u d_v}}{m}-\frac{2m}{n} \\
&= \frac{\mathrm{RR}\left(\mathrm{BiI}_3(m\times n)\right)}{m}-\frac{2m}{n} \\
&= \frac{1}{18mn+12m+6n}((24\sqrt{3}+18\sqrt{2})mn+(4\sqrt{6} \\
&\quad +16\sqrt{3})m+(4\sqrt{6}-16\sqrt{3}-18\sqrt{2})n \\
&\quad +(4\sqrt{6}-8\sqrt{3})-\frac{2(18mn+12m+6n)}{11mn+10m+7n+2}\Bigg),
\end{aligned} \tag{25}$$

$$\begin{aligned}
\mathrm{IRDIF}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)} \left|\frac{d_u}{d_v}-\frac{d_v}{d_u}\right| \\
&= \left|\frac{1}{6}-\frac{6}{1}\right|(4m+4n+4)+\left|\frac{2}{6}-\frac{6}{2}\right|(12mn \\
&\quad +8m+8n-4)+\left|\frac{3}{6}-\frac{6}{3}\right|(6mn \\
&\quad -6n) = \frac{1}{3}(123mn+134m-21n+38),
\end{aligned} \tag{26}$$

$$\begin{aligned}
\mathrm{IRL}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)} \left|\ln d_u-\ln d_v\right| \\
&= |\ln 1-\ln 6|(4m+4n+4)+|\ln 2-\ln 3| \\
&\quad \cdot (12mn+8m+8n-4)+|\ln 3-\ln 6|(6mn-6n) \\
&= 17.22mn+15.88m-5.70n+2.80,
\end{aligned} \tag{27}$$

$$\begin{aligned}
\mathrm{IRLU}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)} \frac{\left|d_u-d_v\right|}{\min\left(d_u,d_v\right)}\\
&= \left(\frac{|1-6|}{1}\right)(4m+4n+4)+\left(\frac{|2-6|}{2}\right)\\
&\quad\cdot(12mn+8m+8n-4)+\left(\frac{|3-6|}{3}\right)(6mn-6n)\\
&= 30mn+36m-2n+12,
\end{aligned} \tag{28}$$

$$\begin{aligned}
\mathrm{IRLF}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)} \frac{\left|d_u-d_v\right|}{\sqrt{d_u\cdot d_v}}\\
&= \left(\frac{|1-6|}{\sqrt{6}}\right)(4m+4n+4)+\left(\frac{|2-6|}{\sqrt{12}}\right)\\
&\quad\cdot(12mn+8m+8n-4)+\left(\frac{|3-6|}{\sqrt{18}}\right)(6mn-6n)\\
&= \frac{1}{3}\left[\left(9\sqrt{2}+24\sqrt{3}\right)mn+\left(10\sqrt{6}+16\sqrt{3}\right)m\right.\\
&\quad\left.+\left(10\sqrt{6}-16\sqrt{3}-9\sqrt{2}\right)n+\left(10\sqrt{6}-8\sqrt{3}\right)\right],
\end{aligned} \tag{29}$$

$$\begin{aligned}
\mathrm{IRLA}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)} 2\frac{\left|d_u-d_v\right|}{\left(d_u+d_v\right)}\\
&= 2\left(\frac{|1-6|}{1+6}\right)(4m+4n+4)+2\left(\frac{|2-6|}{2+6}\right)\\
&\quad\cdot(12mn+8m+8n-4)+2\left(\frac{|3-6|}{3+6}\right)(6mn-6n)\\
&= \frac{1}{7}(112mn+64m-76n-20),
\end{aligned} \tag{30}$$

$$\begin{aligned}
\mathrm{IRD1}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)} \ln\left\{1+\left|d_u-d_v\right|\right\}\\
&= \ln\{1+|1-6|\}(4m+4n+4)+\ln\{1+|2-6|\}\\
&\quad\cdot(12mn+8m+8n-4)+\ln\{1+|3-6|\}(6mn-6n)\\
&= 27.48mn+19.96m-13.92n+0.76,
\end{aligned} \tag{31}$$

$$\begin{aligned}
\mathrm{IRGA}\left(\mathrm{BiI}_3(m\times n)\right) &= \sum_{uv\in E\left(\mathrm{BiI}_3(m\times n)\right)} \ln\left(\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right)\\
&= \ln\left(\frac{1+6}{2\sqrt{1\times 6}}\right)(4m+4m+4)+\ln\left(\frac{2+6}{2\sqrt{2\times 6}}\right)\\
&\quad\cdot(12mn+8m+8n-4)+\ln\left(\frac{3+6}{2}\sqrt{3\times 6}\right)(6mn-6n)\\
&= 1.86mn+2.44m+0.06n+0.88.
\end{aligned} \tag{32}$$

□

4.1. Graphical Representation of Bismuth Tri-Iodide Sheet $BiI_3(m\times n)$. Here, we will graphically present results of irregularity indices for bismuth tri-iodide sheet $\mathrm{BiI}_3(m\times n)$. From these plots, one can observe the behavior of computed results on the involved parameters (Figure 5).

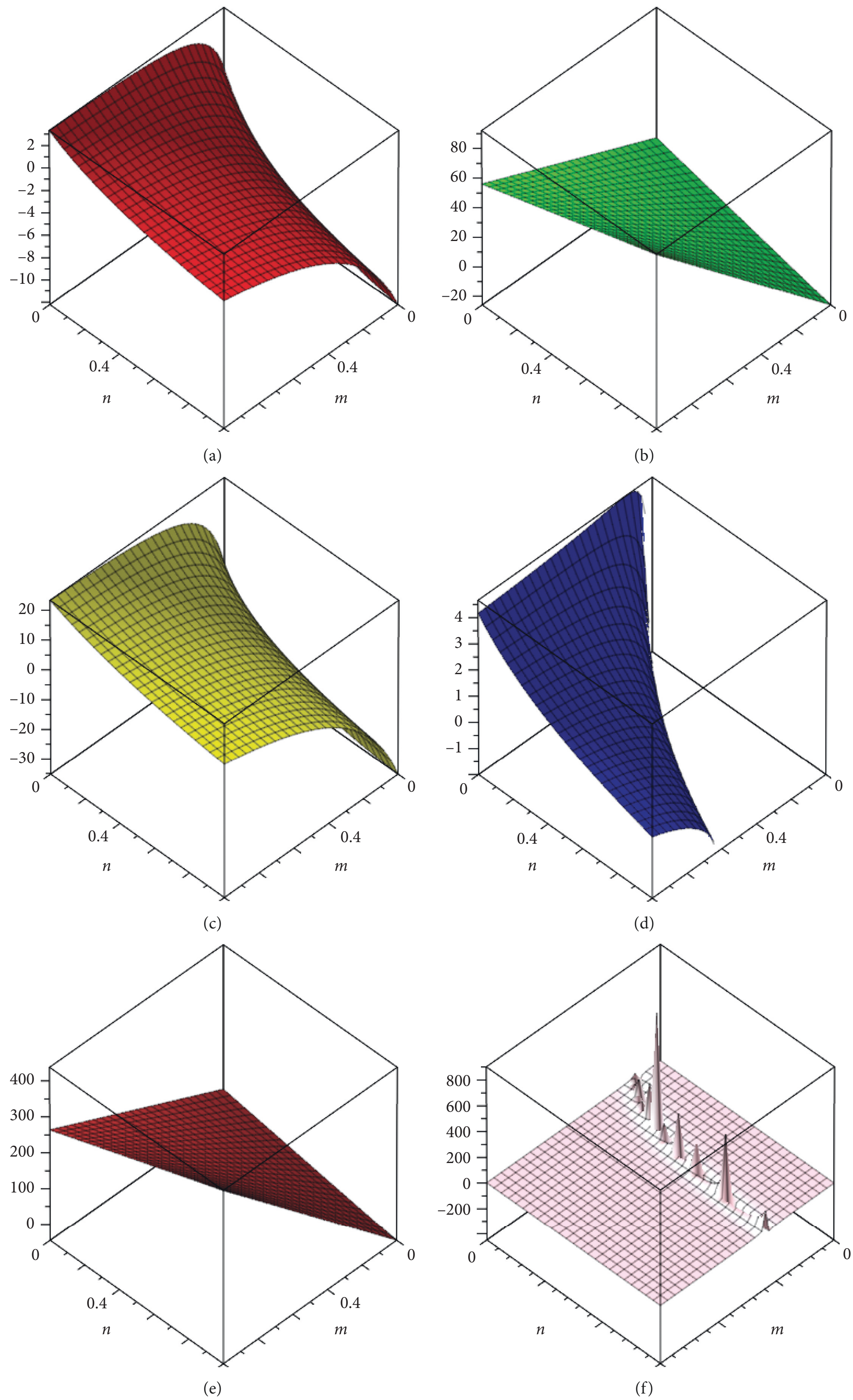

Figure 5: Continued.

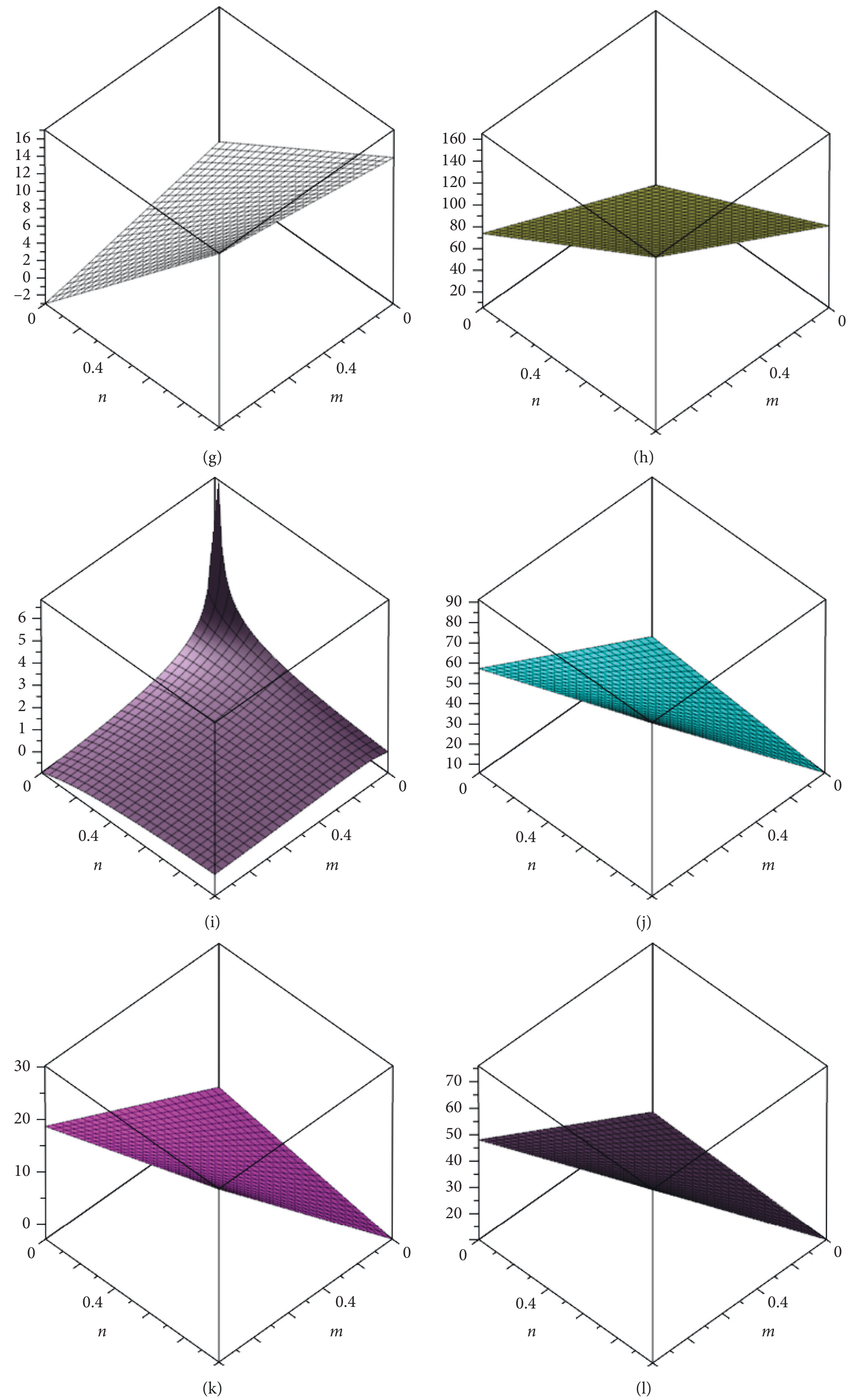

FIGURE 5: Continued.

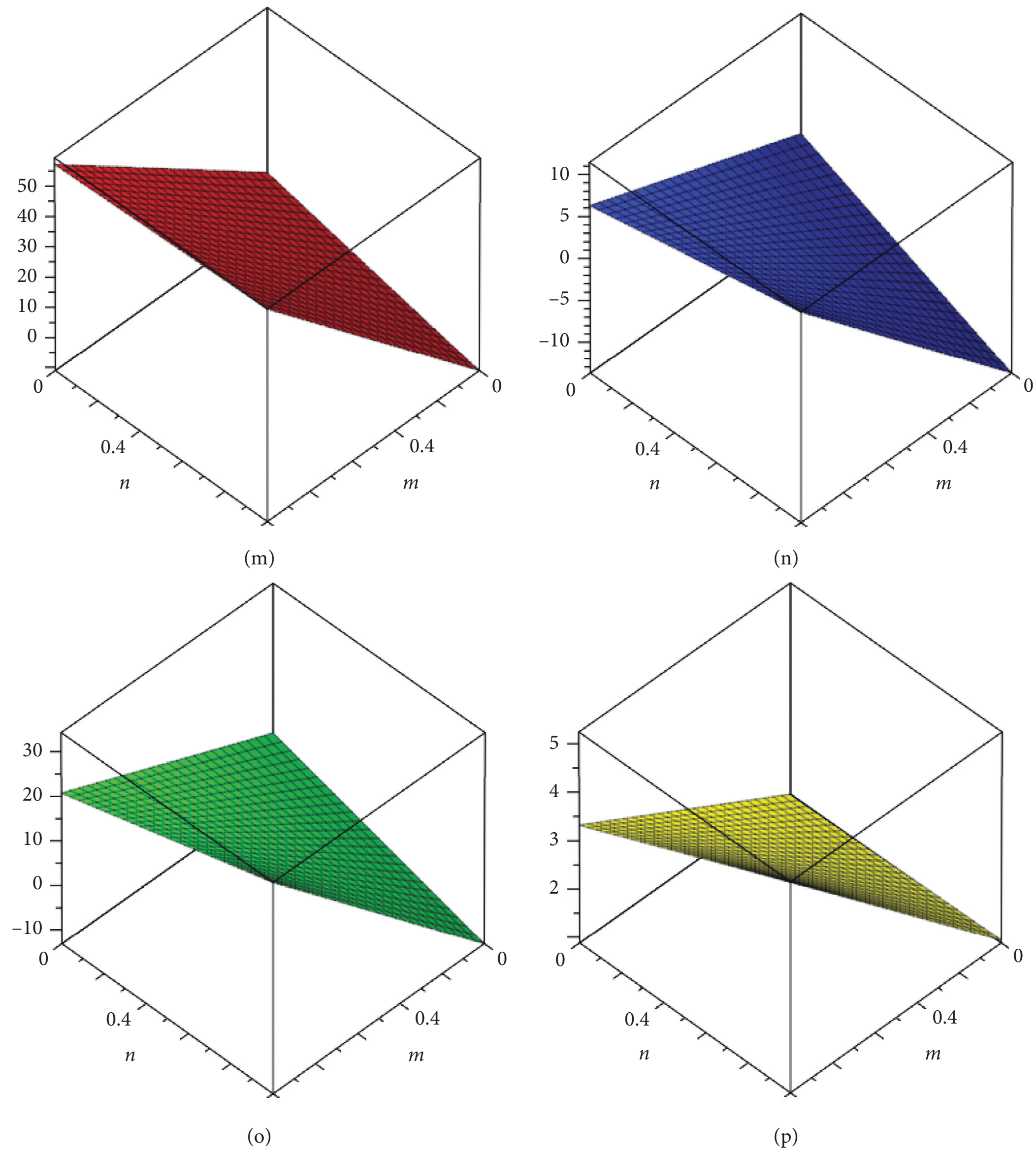

Figure 5: (a) VAR $(m-\mathrm{BiI}_3)$; (b) AL $(m-\mathrm{BiI}_3)$; (c) IR1 $(m-\mathrm{BiI}_3)$; (d) IR2 $(m-\mathrm{BiI}_3)$; (e) IRF $(m-\mathrm{BiI}_3)$; (f) IRFW $(m-\mathrm{BiI}_3)$; (g) IRA $(m-\mathrm{BiI}_3)$; (h) IRB $(m-\mathrm{BiI}_3)$; (i) IRC $(m-\mathrm{BiI}_3)$; (j) IRDIF $(m-\mathrm{BiI}_3)$; (k) IRL $(m-\mathrm{BiI}_3)$; (l) IRLU $(m-\mathrm{BiI}_3)$; (m) IRLF $(m-\mathrm{BiI}_3)$; (n) IRLA $(m-\mathrm{BiI}_3)$; (o) IRD1 $(m-\mathrm{BiI}_3)$; (p) IRGA $(m-\mathrm{BiI}_3)$.

5. Conclusion

TIs are used to see the properties of concerned compound without going to wet lab. In the present paper, we have computed several degree-based TIs. All these indices are useful in QSPR and QSAR. Our results can help to guess properties of bismuth tri-iodide chain and sheet. Computing distance-based TIs is an interesting problem.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

Authors' Contributions

All authors contributed equally in this paper.

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