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Mathematic Properties and their Chemical Applicabilities of Atom Valency Block Indices

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Abstract: The Atom Valency Block (AVB) Indices of an undirected, finite, simple, connected molecular graph/graph $G = (V, E)$ are defined as $\mathrm{AVB}_1(G) \sum_{u \in V}[d(u)b(u)]$ and $\mathrm{AVB}_2(G) = \sum_{u \in V}[d(u) \times b(u)]$, where the valency (or degree) $d(u)$ of an atom (or vertex) u is the number of atoms adjacent to u, and the block number $b(u)$ of an atom (vertex) u represents the number of blocks of G containing u (the maximal non-separable subgraph of a graph is said to be the block of that graph). In this article, we initiate these new molecular descriptors to compute exact values of separable and non-separable graph and found some inequalities in terms of the order, size, and minimum/maximum valency. Also, we have made comparisons concerning other pre-existing atom valency-based descriptors. In addition, we present the statistical analysis of some chemical trees via scatter plotted correlations between AVB indices and other well-known atom valency-based descriptors.

Keywords: graph; valency; molecular descriptors; AVB indices; chemical trees; correlation matrix.

1. Introduction

The structural formulas of covalently bonded compounds are molecular graphs or constitutional graphs, where each atom is a vertex, and each bond is an edge. In this article, all molecular graphs/graphs $G = (V, E)$ is nonempty, finite, undirected, simple graphs unless otherwise noted. The notation p denotes the cardinality of the set of atoms $V=V(G)$, and q denotes the cardinality of the set of bonds $E=E(G)$. A vertex whose removal results in a trivial or disconnected graph is said to be the cut vertex. A graph that is connected, non-trivial, and has no cut vertices is a non-separable graph. The maximal non-separable subgraph of a graph is said to be the block of that graph. The block number of graph G denoted by $b(G)$ represents the total number of blocks in graph G. Generally speaking, and we refer the reader to Harary [1] for basic graph-theoretic terminology and notation.

Topological indices are numeric quantities that transform the chemical structure into a real number, which are used in QSAR/QSPR/QSTR studies to correlate the bioactivity and physicochemical properties of the molecule. For their history, applications, and mathematical properties, see [2-8] and the references cited therein. Many topological indices have been introduced in theoretical chemistry to measure the topological properties of molecules. Especially in a chemical reaction, the atoms exchange the valency (or degree) electrons to stabilize their valence shell. Without a valence shell, the chemical reaction won't occur, and an

atom's number of valence electrons governs its bonding behavior. For these reasons, here we initiate the new valency-based topological molecular descriptors in atom blocks as follows.

Table 1. Valency-based topological indices.

Topological indices	Mathematical Representations
First Zagreb Index, [9,10]	$M_1(G) = \sum_{uv\in E}[d(u) + d(v)]$
Second Zagreb Index, [9,11]	$M_2(G) = \sum_{uv\in E}[d(u).d(v)]$
Randic Index, [12,13]	$R(G) = \sum_{uv\in E}\frac{1}{\sqrt{d(u).d(v)}}$
ABC Index, [14,15]	$ABC(G) = \sum_{uv\in E}\sqrt{\frac{d(u)+d(v)-2}{d(u).d(v)}}$
Sombor Index, [16-20]	$SO(G) = \sum_{uv\in E}\sqrt{d(u)^2 + d(v)^2}$
Forgotten Index, [21,22]	$F(G) = \sum_{uv\in E} d(u)^2 + d(v)^2$
First Banhatti Index, [23,24]	$B_1(G) = \sum_{ue}[d(u) + d(e)]$
Second Banhatti Index, [24]	$B_2(G) = \sum_{ue}[d(u).d(e)]$
Reformulated First Zagreb Index, [25]	$EM_1(G) = \sum_{uv\in E} d(uv)^2$
Hyper Zagreb Index, [26,27]	$HM_1(G) = \sum_{uv\in E}[d(u) + d(v)]^2$

The Atom Valency Block (AVB) indices of a connected graph G are defined by

$\mathrm{AVB}_1(G) = \sum_{u\in V}[d(u) + b(u)]$, and (1)

$\mathrm{AVB}_2(G) = \sum_{u\in V}[d(u) \times b(u)]$, (2)

where the valency $d(u)$ of an atom u is the number of atoms adjacent to u, and the block number $b(u)$ of an atom u represents the number of blocks of G containing u. Table 1 represents different Valency-based topological indices that are used for comparisons with AVB indices.

2. Materials and Methods

2.1. Mathematical properties.

In this section, we have computed the exact values of separable and non-separable graphs and found some inequalities in order, size, and minimum/maximum valency. Also, we have made comparisons concerning other pre-existing atom valency-based descriptors.

2.1.1. Exact values of separable and non-separable graphs.

Let G be a non-separable graph. Then G does not have any cut-atoms, and the number of blocks in a graph remains one, which means $b(G) = 1$. Thus the number of blocks to which the atom u belongs is one, which means $b(u) = 1$ for each atom u in $V(G)$. By equations (1) and (2), we have

$\mathrm{AVB}_1(G) = 2q + p$, and (3)

$\mathrm{AVB}_2(G) = 2q$. (4)

Now, let G be a separable graph. Then G contains at least one cut atom. By equation (1), we have,

$$\begin{aligned}\mathrm{AVB}_1(G) &= \sum_{u\in V}[d(u) + b(u)]\\ &= \sum_{u\in V(C)}[d(u) + b(u)] + \sum_{u\in V-V(C)}[d(u) + b(u)]\\ &= \sum_{u\in V} d(u) + \sum_{u\in V(C)} b(u) + \sum_{u\in V-V(C)} b(u)\\ &= 2q + p - c(G) + \sum_{u\in V(C)} b(u). \quad (5)\end{aligned}$$

Similarly, from equation (2), we have

$$\mathrm{AVB}_2(G) = 2q - \sum_{u\in V(C)} d(u) + \sum_{u\in V(C)} [d(u) \times b(u)], \quad (6)$$

where $V(C)$ is the set of cut-atoms in a connected graph G with $|V(C)| = c(G)$.

2.1.2. Exact values of some specific families of graphs.

From equations (1) to (6), we have

(i) For any Complete graph K_p with $p \geq 1$ vertices,

$$AVB_1(K_p) = p^2 \text{ and } \mathrm{AVB}_2(K_p) = p^2 - p.$$

(ii) For any Cycle C_p with $p \geq 3$ vertices,

$$AVB_1(C_p) = 3p \text{ and } \mathrm{AVB}_2(C_p) = 2p.$$

(iii) For any Complete regular bipartite graph $K_{s,s}$, where s is the number of vertices in each partition,

$$\mathrm{AVB}_1(\mathrm{K}_{s,s}) = 2s(s+1) \text{ and } \mathrm{AVB}_2(\mathrm{K}_{s,s}) = 2s^2.$$

(iv) For any star graph S_p,

$$\mathrm{AVB}_1(\mathrm{S}_p) = 4(p-1) \text{ and } \mathrm{AVB}_2(\mathrm{S}_p) = p^2 - p.$$

(v) For any n-hypercube graph Q_n,

$$\mathrm{AVB}_1(\mathrm{Q}_n) = 2^n(n+1) \text{ and } \mathrm{AVB}_2(\mathrm{Q}_n) = n2^n.$$

(vi) For any generalized Petersen graph $GP(n, k)$,

$$\mathrm{AVB}_1(\mathrm{GP}(n,k)) = 8n \text{ and } \mathrm{AVB}_2(\mathrm{GP}(n,k)) = 6n,$$

where $\mathrm{GP}(n,k)$ for $n \geq 3$ and $1 \leq k \leq \lfloor (n-1)/2 \rfloor$ is a connected cubic graph consisting of an inner star polygon $\{n, k\}$ (circulant graph $\mathrm{Ci}_n(k)$) and an outer regular polygon n (cycle graph C_n) with corresponding vertices in the inner and outer polygons connected with edges.

(vii) For any m × n grid graph L(m,n) with (mn)-vertices and (2mn–m–n)-edges,

$$\mathrm{AVB}_1(\mathrm{L}(m,n)) = 5mn - 2m - 2n \text{ and } \mathrm{AVB}_2(\mathrm{L}(m,n)) = 4mn - 2m - 2n,$$

where the m×n grid graph L(m,n) can be represented as a cartesian product of $P_m \square P_n$ of a path of length m–1 and a path of length n–1.

(viii) For any Harary graph,

$$\mathrm{AVB}_1(\mathrm{H}_{k,p}) = 2\left\lceil \frac{kp}{2} \right\rceil + p \text{ and } \mathrm{AVB}_2(\mathrm{H}_{k,p}) = 2\left\lceil \frac{kp}{2} \right\rceil,$$

where $H_{k,p}$, is a k-connected graph on p vertices of degree at least k with $\left\lceil \frac{kp}{2} \right\rceil$ edges.

2.1.3. Inequalities in terms of order and size.

Let G be a connected graph with p vertices. Then, $b(G) - 1 = \sum_{u\in V}[b(u) - 1]$ becomes

$$\sum_{u\in V} b(u) - \sum_{u\in V} 1 = b(G) - 1 \Rightarrow \sum_{u\in V} b(u) - p \leq p - 1 - 1 \Rightarrow \sum_{u\in V} b(u) \leq 2(p-1).$$

Since the non-trivial connected graph G has at least two vertices in G with minimum $b(u) = 1$, their summation will be at least 2.

Thus $2 \leq \sum_{u\in V(G)} b(u) \leq 2(p-1)$. (7)

From equations (1), (2), and (7) with $1 \leq b(u) \leq p-1$, we have

$$p + 2q \leq AVB_1(G) \leq p^2 - p + 2q, \text{ and} \quad (8)$$

$$2q \leq AVB_2(G) \leq 2q(p-1). \quad (9)$$

2.1.4. Inequalities in terms of order and minimum/maximum degree.

From equations (1) and (2) with $1 \le b(u) \le p-1$ and $\delta(G) \le d(u) \le \Delta(G)$, we have

$$p\delta(G) + 2 \le AVB_1(G) \le p\Delta(G) + 2(p-1), \text{ and} \quad (10)$$

$$2\delta(G) \le AVB_2(G) \le 2(p-1)\Delta(G). \quad (11)$$

$$p(\delta(G)+1) \le AVB_1(G) \le p(\Delta(G)+p-1), \text{ and} \quad (12)$$

$$p\delta(G) \le AVB_2(G) \le p(p-1)\Delta(G). \quad (13)$$

2.1.5. Inequalities in terms of diameter.

From equations (1) and (2) with$b(u) \le diam(G)$, we have

$$AVB_1(G) \le 2q + p\ diam(G), \text{ and} \quad (14)$$

$$AVB_2(G) \le 2q\ diam(G) \quad (15)$$

Equations (14) and (15) hold if and only if $G \cong K_p$.

2.1.6. Inequality among the AVB indices.

Let *G* be a graph with *p* vertices. We know that, $2d(u)b(u) \le \mathrm{d}(u)^2\mathrm{b}(u)^2$ becomes $d(u)b(u) \le \frac{1}{2}[\mathrm{d}(u)^2 + \mathrm{b}(u)^2] \Rightarrow d(u)b(u) \le \frac{1}{2}[d(u)+b(u)]^2 - d(u)b(u)$.

Taking summation over $u \in V$ and applying equations (1) and (2), we have

$$AVB_2(G) \le \frac{1}{2}(AVB_1(G))^2 - AVB_2(G) \Rightarrow 4AVB_2(G) \le (AVB_1(G))^2.$$

Thus $2\sqrt{AVB_2(G)} \le AVB_1(G)$.

Also, if $d(u)+b(u) = d(u)b(u)\left(\frac{1}{d(u)} + \frac{1}{b(u)}\right)$ then taking summation over $u \in V$ and applying equations (1) and (2), we have $AVB_1(G) \le AVB_2(G)\left(\frac{1}{\delta} + \frac{1}{2(p-1)}\right)$.

Hence $2\sqrt{AVB_2(G)} \le AVB_1(G) \le AVB_2(G)\left(\frac{1}{\delta} + \frac{1}{2(p-1)}\right)$. (16)

2.1.7. Inequality in terms of other topological indices.

(i) Let G be a non-trivial graph. If $d(u)+b(u) = \frac{[d(u)+b(u)]^2}{d(u)+b(u)} = \frac{d(u)^2+b(u)^2+2d(u)b(u)}{d(u)+b(u)}$.

Taking summation over $u \in$V and applying equation (1), we have

$$AVB_1(G) \le \frac{\sum_{u\in V} d(u)^2 + [\sum_{u\in V} b(u)]^2 + 2\sum_{u\in V} d(u).b(u)}{\delta + 2(p-1)}.$$

$$\text{Hence} \quad AVB_1(G) \le \frac{M_1(G) + 4(p-1)^2 + 2AVB_2(G)}{\delta + 2(p-1)}. \quad (17)$$

From equation (13), we have $AVB_1(G) \le \frac{3M_1(G) + 4(p-1)^2}{\delta + 2(p-1)}$. (18)

(ii) Let *G* be a non-trivial graph with $b(u) \le d(u)$. Then multiplying *d*(*u*) to $b(u) \le d(u)$ and taking summation over $u \in V$and applying equation (2), we have

$$AVB_2(G) \le M_1(\mathrm{G}). \quad (19)$$

Further, let *T* be a non-trivial tree with *b*(*u*) = *d*(*u*). Then equation (2) becomes

$$AVB_2(T) = \sum_{u\in V(T)}[d(u).b(u)] = \sum_{u\in V(T)}[d(u)]^2 \le [\sum_{u\in V(T)} d(u)]^2 \le 4q^2.$$

Also, $AVB_2(T) = \sum_{u\in V(T)}[d(u).b(u)] = \sum_{u\in V(T)}[d(u)]^2 = \mathrm{M}_1(T)$. (20)

(iii) By equation (19), from [5], we have

$$AVB_2(G) \le \frac{B_1(G) + 4q}{3},$$

$$AVB_2(G) \leq HM_1(G) - EM_1(G) - B_1(G)\text{ , and}$$
$$AVB_2(G) \leq B_1(G) + B_2(G) - HM_1(G) + 4q.$$

3. Results and Discussion

3.1. Chemical applicability.

Correlation between Atom Valency Block (AVB) indices and other topological indices is obtained with the help of isomers of valency two to eight.

Here, we are finding the relationship between existing and newly introduced indices. The statistic which measures these relationships is said to be a correlation. The numerical value of that relationship is the correlation coefficient—the values of the correlation coefficient range from -1 to 1. For more details on correlation, refer to [28]. The correlation between Atom Valency Block (AVB) indices and other topological indices mentioned above was calculated for chemical trees of orders two to eight.

3.1.1. Chemical trees.

Table 2 shows the number of trees and chemical trees of different orders, where N_t represents several trees (without isomorphism), and N_{ct} represents several chemical trees. The total number of trees with isomorphism can be calculated using the formula $2^{\binom{p}{2}}$.

Table 2. The number of trees of different valences.

Order	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
N_t		1	2	3	6	11	23	47	106	235	551	1301	3159	7741	19320	48629	123867	317955	823065
Nct	1	1	2	3	5	9	18	35	75	159	355	802	1858	4347	10359	24894	60523	148284	366319

3.2. Computed values of Toloplogical Indices of some chemical trees.

The topological indices of all the isomers (chemical trees) of valency two to eight are calculated and have been listed in Table 3.

Table 3. Computed values of Toloplogical Indices of some chemical trees.

Compound Name	**M_2**	**R**	**ABC**	**SO**	**F**	**AVB_1**	**AVB_2/ M_1**
Ethane	1	1	0	1.4142	2	4	2
Propane	4	1.4142	1.4142	4.4721	10	8	6
Butane	8	1.9142	2.1213	7.3006	18	12	10
2-Methylpropane	9	1.7321	2.4495	9.4868	30	12	12
Pentane	12	2.4142	2.8284	10.1290	26	16	14
2-Methylbutane	14	2.2701	2.3570	12.1662	38	16	16
2,2-Dimethylpropane	16	2	3.4641	16.4924	68	16	20
Hexane	16	2.9142	3.5355	12.9574	34	20	18
2-Methylpentane	18	2.7701	3.0641	14.9946	46	20	20
3-Methylpentane	19	2.8081	3.6449	14.8455	46	20	20
2,3-Dimethylbutane	21	2.6427	3.9327	16.8918	58	20	22
2,2-Dimethylbutane	22	2.5607	4.0123	19.077	76	20	24
Heptane	20	3.4142	4.2426	15.7858	42	24	22
2-Methylhexane	22	3.2701	4.4614	17.8230	54	24	24
3-Methylhexane	23	3.3081	4.3520	17.6739	54	24	24
2,2-Dimethylpentane	26	3.0607	4.7194	21.9059	84	24	28
2,3-Dimethylpentane	26	3.1807	4.5304	19.5711	66	24	26
2,4-Dimethylpentane	24	3.1259	4.6802	19.8602	66	24	26
3,3-Dimethylpentane	28	3.1213	4.5605	17.5249	54	24	28
3-Ethylpentane	24	3.3461	4.2426	17.5249	54	24	24

Compound Name	M_2	R	ABC	SO	F	AVB_1	AVB_2/M_1
2,2,3-Trimethylbutane	30	2.9434	4.8766	23.6939	96	24	30
Octane	24	3.9142	4.9497	18.6142	50	28	26
2-Methylheptane	26	3.7701	5.1685	20.6515	62	28	28
3-Methylheptane	27	3.8081	5.0591	20.5024	62	28	28
4-Methylheptane	27	3.8081	5.0591	20.5024	62	28	28
3-Ethylhexane	28	3.8461	4.9497	20.3533	62	28	28
2,2-Dimethylhexane	30	3.5607	5.4265	24.7344	92	28	32
2,3-Dimethylhexane	30	3.6807	5.2375	22.3995	74	28	30
2,2,4-Trimethylpentane	32	3.4165	5.6453	26.7716	103	28	34
2,3,3-Trimethylpentane	36	3.5040	5.4248	26.2790	104	28	34
2,3,4-Trimethylpentane	33	3.5534	5.4158	24.2967	86	28	32
2,2,3,3-Tetramethylbutane	40	3.25	5.8085	30.3955	134	28	38
2,4-Dimethylhexane	29	3.6639	5.2779	22.5396	74	28	30
2,5-Dimethylhexane	28	3.6259	5.3873	22.6886	74	28	30
3,3-Dimethylhexane	32	3.6213	5.2676	24.4910	92	28	32
3,4-Dimethylhexane	31	3.7187	5.1281	22.2504	74	28	30
3-Ethyl-2-Methylpentane	31	3.7187	5.1281	22.2504	74	28	30
3-Ethyl-3-Methylpentane	34	3.6820	5.1087	24.2477	92	28	32
2,2,3-Trimethylpentane	35	3.4814	5.4743	26.3732	104	28	34

3.2. Correlation Matrix of topological indices.

Table 4 represents the correlation matrix of topological indices. Since we are comparing more indices, we use the concept of correlation matrix than the Pearson correlation coefficient.

Table 4. Correlation Matrix of topological indices.

	M_1	M_2	R	ABC	SO	F	AVB_1	AVB_2
M_1	1.0000	0.9910	0.8662	0.9761	0.9951	0.9309	0.9495	1.0000
M_2	0.9910	1.0000	0.8532	0.9542	0.9849	0.9294	0.9341	0.9910
R	0.8662	0.8532	1.0000	0.9200	0.8137	0.6281	0.9783	0.8662
ABC	0.9761	0.9542	0.9200	1.0000	0.9582	0.8506	0.9768	0.9761
SO	0.9951	0.9849	0.8137	0.9582	1.0000	0.9609	0.9151	0.9951
F	0.9309	0.9294	0.6281	0.8506	0.9609	1.0000	0.7706	0.9309
AVB_1	0.9495	0.9341	0.9783	0.9768	0.9151	0.7706	1.0000	0.9495
AVB_2	1.0000	0.9910	0.8662	0.9761	0.9951	0.9309	0.9495	1.0000

3.2. Analysis.

A scatter plot is a mathematical diagram that depicts the values of two variables for a set of data. The pattern of dots indicates a positive correlation that slopes from the lower left to the upper right. A negative correlation is indicated by the pattern of dots that slopes from the upper right to the lower left. Figure 1 represents the correlation between the topological indices mentioned above scatter plot. We, at this moment, conclude that $AVB_1(G)$ is strongly positively correlated with Randic and ABC indices. $AVB_2(G)$ is strongly positively correlated with the first Zagreb index, second Zagreb index, ABC index, and Sombor index. Also, it is very clear that M_1 and $AVB_1(G)$ have the same correlation with all the other indices.

4. Conclusions

The Atom Valency Block (AVB) indices are introduced, and the values are calculated for different classes of graphs. Also, some lower and upper bounds are being calculated. The correlation matrix is obtained to see the intensity of the relationship between existing indices with our indices. The scatter plot is well-plotted so that it picturizes the best-correlated indices

with our atom valency block indices and within the indices themselves. A line of best fit can be drawn in further extension.

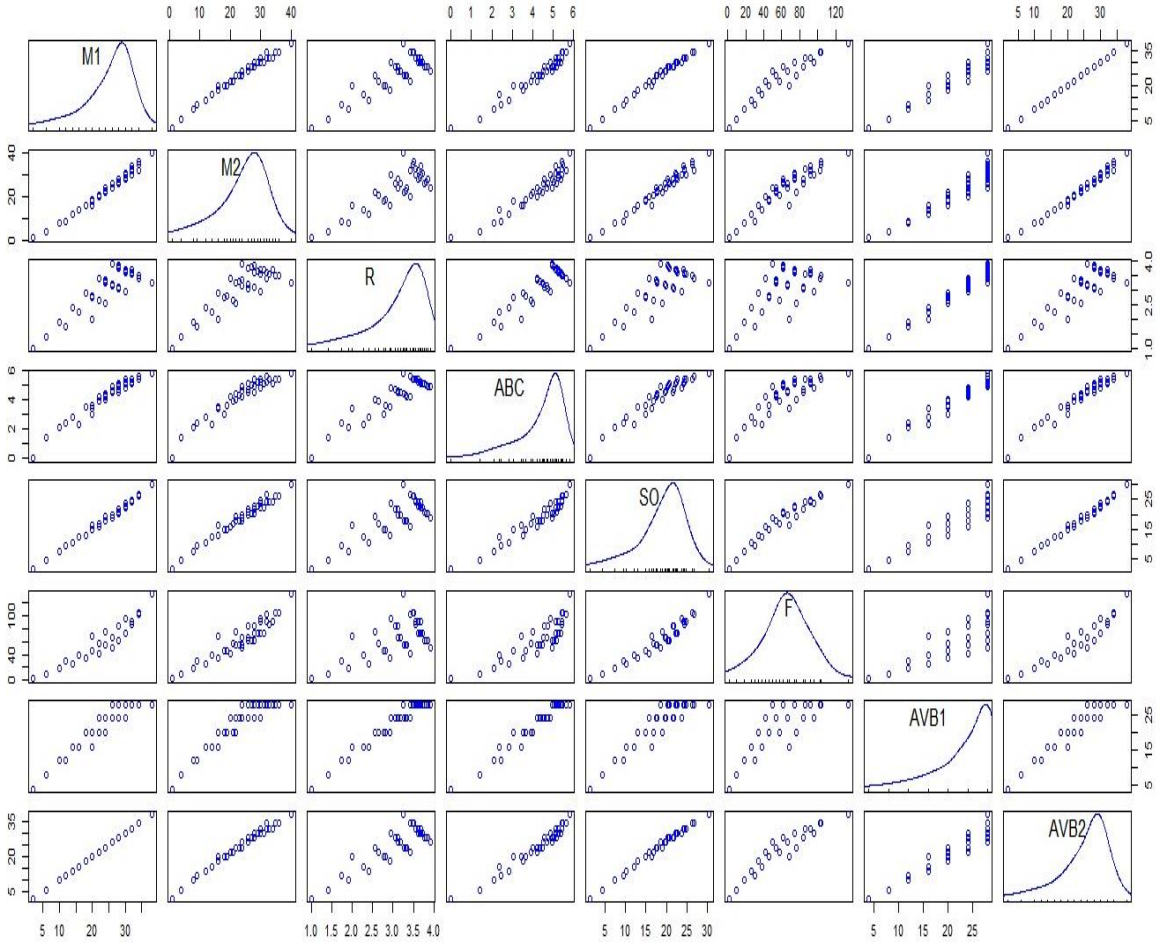

Figure 1. Scatterplot of Correlations.

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Conflicts of Interest

The authors declare no conflict of interest.

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