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RESEARCH ARTICLE

Mathematical Modelling

Revan indices for the hexadentate-3-hydroxypyridinones-terminated dendrimers

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Abstract: Dendrimers are highly ordered, unimolecular, monodisperse, micellar nanostructures, applied in various fields such as drug delivery, nanotechnology, and biomedical applications. Hexadentate 3-hydroxypyridinones-terminated dendrimers are used in iron binding and anti-microbial activities. In the molecular graph, atoms are the vertices, and the bonds are the edges. A graph G consists of a pair of nonempty sets of vertices $V(G)$ and edges $E(G)$ and $d_G(u)$ is the degree of a vertex $u \in V(G)$. In this study, multiple bonds were modeled as multi-edges, and all hydrogen atoms were included in the molecular graph, thereby reducing the assumptions of traditional computational methods. Here, different Revan indices, which are topological descriptors derived from graph theory, were computed for hexadentate-3-hydroxypyridinones-terminated dendrimers. The Revan degree $r_G(u)$ of a vertex u is defined as $r_G(u) = \Delta(G) + \delta(G) - d_G(u)$, where $\Delta(G)$ is the maximum degree and $\delta(G)$ is the minimum degree among the vertices in G. In this paper, the first, second, and third Revan indices, forgotten Revan index, hyper Revan index, atom-bond connectivity Revan index, product connectivity Revan index, sum connectivity Revan index, harmonic Revan index, and geometric arithmetic Revan index were computed for different generations of hexadentate 3-hydroxypyridinones-terminated dendrimers. The results demonstrate that the complex topology in dendrimers can be accurately represented with the Revan indices, and as a result, their structural properties can be better understood. This study underlines the importance of these topological indices in directing design and development toward advanced applications with dendrimer-based systems.

Keywords: Dendrimers, hexadentate 3-hydroxypyridinones-terminated dendrimers, Revan degree, Revan Index, topological index.

INTRODUCTION

Dendrimers are synthetic polymeric macromolecules of nanometer dimensions with well-defined, homogeneous, and monodisperse structure, and their structure consists of tree-like arms or branches. They provide controlled release from the inner core, and the active compounds are incorporated in the interior as well as begin attached on the surface. Their unique architecture is highly useful in drug delivery, nanotechnology, and biomedical operations (Abbasi, 2014). The idea of the dendrimers was introduced first in 1978, and they are still laboriously delved into worldwide (Vogtle et al., 1978). Hexadentate 3-hydroxypyridinones-terminated dendrimers were synthesized for iron binding and implicit antibacterial operations (Zhou et al., 2018).

Chemical graph theory is a branch of mathematics that helps to study molecules in chemistry. This simplifies molecular structures, enabling quantitative analysis, property prediction, drug discovery, and the development of algorithms for efficient chemical research. A molecular graph is a simple graph that does not contain loops or

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multiple edges. A graph $G = (V, E)$ consists of a finite nonempty set of vertices $V = V(G)$ and a set of edges $E = E(G)$. Two vertices of G connected by an edge, are said to be adjacent. The degree $d_v(G)$ or d_v of a vertex v in $V(G)$ is the number of vertices of G, adjacent to the vertex v (Gutman, 2013).

A topological index is a numerical descriptor that is computed based on the molecular graph of a chemical compound and used to determine the chemical and physical properties of any chemical compound. These indices derive from the mathematical field of graph theory, which studies networks or graphs. Different aspects of the molecule structure are captured by each topological index (Babujee et al., 2013).

The Wiener index is the first distance-based topological index in chemical graph theory and has been studied the most. In 1947, Harold Wiener presented this index as the path number. It was defined as the total distance between each carbon atom in the molecules, expressed in terms of carbon-carbon bonds (Wiener, 1947).

The Zagreb indices are the first vertex-degree-based topological indices (Gutman & Trinajstić, 1972). The definitions of the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$ and $M_2(G) = \sum_{uv \in E(G)} d_u d_v$

Another popular and studied degree-based topological index is the Randić index. This is the first genuine degree-based topological index (Randić, 1975) and is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

In 2009, the sum connectivity index of a graph G (Zhou & Trinajstić, 2009) was introduced and defined as,

$$S(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u + d_v}}$$

In 1993, the harmonic index of a graph G (Favaron et al., 1993) was introduced and defined as,

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$$

In 2009, the geometric arithmetic index of a graph G (Vukičević & Furtula, 2009) was introduced and defined as,

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

The atom-bond connectivity index of a graph G (Estrada et al., 1998) was introduced and defined as,

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

The forgotten topological index of a graph G (Furtula & Gutman, 2015) was defined as,

$$F(G) = \sum_{uv \in E(G)} ({d_u}^2 + {d_v}^2)$$

In this study, the first, second, and third Revan indices, along with the forgotten Revan index, hyper Revan index, atom-bond connectivity Revan index, product connectivity Revan index, sum connectivity Revan index, harmonic Revan index, and geometric arithmetic Revan index, are computed for the hexadentate 3-hydroxypyridinone-terminated dendrimers. Connecting the Revan vertices u and v is the edge uv, which is a Revan edge. For any vertex v in G, the Revan vertex degree $r_G(v)$ is defined as

$$r_G(v) = \Delta(G) + \delta(G) - d_G(v).$$

Here $\Delta(G)$ is the maximum degree among the vertices in G and $\delta(G)$ is the minimum degree among the vertices in G (Kulli, 2017a).

MATERIALS AND METHODS

The molecular graph describes the dendrimeric structure in which the atoms and bonds are treated as vertices and edges, respectively. In this study, all the multi-bonds were treated as multi-edges, and all hydrogen atoms were included in a molecular graph. This is an enhanced method for computing topological indices to reduce the assumptions of traditional computing techniques (Gunawardhana et al., 2024). In this paper, we computed different versions of Revan indices for four types of hexadentate 3-hydroxypyridinones-terminated dendrimers using the following formulas.

The molecular structures considered in this study were adapted from Zhou et al. (2018). The analyzed structures correspond to compound 6b from Scheme 1 (Figure 1), structure 7 from Scheme 2 (Figure 2), compound 10 from Scheme 3 (Figure 3), and compound 13 from Scheme 4 (Figure 4) of Zhou et al. Each structure was treated as an independent molecular graph for the computation of Revan indices. Figure 2 represents the benzyl-protected dendron intermediate (structure 7), which was also independently analyzed in the present graph-theoretical study.

In 2017, the first, second, and third Revan indices of a graph G (Kulli, 2017b) were introduced and defined as,

$$R_1(G) = \sum_{uv\in E(G)} r_G(u) + r_G(v) \quad ...(01)$$

$$R_2(G) = \sum_{uv\in E(G)} r_G(u)\, r_G(v) \quad ...(02)$$

$$R_3(G) = \sum_{uv\in E(G)} |r_G(u) - r_G(v)| \quad ...(03)$$

The F-Revan index (also called forgotten Revan index) of a graph G (Kulli, 2018b) was defined as,

$$FR(G) = \sum_{uv\in E(G)} r_G(u)^2 + r_G(v)^2 \quad ...(04)$$

The first hyper Revan index of a graph G (Kulli, 2018c) was defined as,

$$HR_1(G) = \sum_{uv\in E(G)} (r_G(u) + r_G(v))^2 \quad ...(05)$$

The atom bond connectivity Revan index of a graph G (Estrada, 1998) was defined as,

$$ABCR(G) = \sum_{uv\in E(G)} \sqrt{\frac{r_G(u) + r_G(v) - 2}{r_G(u) r_G(v)}} \quad ...(06)$$

The product connectivity Revan index (also called Randi`c Revan index) of a graph G (Kulli, 2017a) was defined as,

$$RR(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{r_G(u) r_G(v)}} \quad ...(07)$$

The sum connectivity Revan index of a graph G (Kulli, 2017c) was defined as,

$$SR(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{r_G(u) + r_G(v)}} \quad ...(08)$$

The harmonic Revan index of a graph G (Kulli, 2020) was defined as,

$$HMR(G) = \sum_{uv\in E(G)} \frac{2}{r_G(u) + r_G(v)} \quad ...(09)$$

The geometric-arithmetic Revan index of a graph G (Kulli, 2018a) was defined as,

$$GAR(G) = \sum_{uv\in E(G)} \frac{2\sqrt{r_G(u) r_G(v)}}{r_G(u) + r_G(v)} \quad ...(10)$$

The Revan indices were computed using respective formulas. Zhou et al. synthesized a range of novel hexadentate 3-hydroxypyridinone-terminated dendrimers which were shown as Figures in this paper (Zhou et al., 2018). As Figure 1 illustrates, first generation dendrimeric chelators that is consists of three hexadentate moieties. The structure of the second generation dendrimeric chelators is depicted in Figure 2. It was conjugated with tri-acid and di-acid, respectively, to form structures in Figures 3 and 4, which have nine and six hexadentate centres, respectively. In this study, the first, second, and third Revan indices, along with the forgotten Revan index, hyper Revan index, atom-bond connectivity Revan index, product connectivity Revan index, sum connectivity Revan index, harmonic Revan index, and geometric arithmetic Revan index are computed for the above-mentioned dendrimers. Thus far, these selected Revan indices have not been calculated for the above dendrimeric structures.

RESULTS AND DISCUSSION

Theorem 1.

Let G be the first generation dendrimeric chelators. Then the first Revan index $R_1(G)$, the second Revan index $R_2(G)$, the third Revan index $R_3(G)$, the forgotten Revan index $FR(G)$, the first Hyper Revan index $HR_1(G)$, the ABC Revan index $ABCR(G)$, the Randi`c Revan index $RR(G)$, the Sum connectivity Revan index $SR(G)$, the harmonic Revan index $HMR(G)$, and the GA Revan index $GAR(G)$ for G are

i. $R_1(G) = 1506$,

ii. $R_2(G) = 1266$,

iii. $R_3(G) = 618$,

iv. $FR(G) = 4068$,

v. $HR_1(G) = 6600$,

vi. $ABCR(G) = 9\sqrt{\frac{5}{3}} + 75\sqrt{\frac{1}{2}} + 63\sqrt{3} + 66\sqrt{\frac{2}{3}}$,

vii. $RR(G) = 171 + \frac{135}{2}\sqrt{\frac{1}{2}} + 75\sqrt{\frac{1}{3}}$,

viii. $SR(G) = 18\sqrt{\frac{1}{7}} + 15\sqrt{\frac{1}{6}} + 126\sqrt{\frac{1}{5}} + 108\sqrt{\frac{1}{2}} + 33 + 60\sqrt{\frac{1}{3}}$,

ix. $HMR(G) = \frac{15753}{70}$, and

x. $GAR(G) = \frac{1044}{5} + 50\sqrt{2} + \frac{303}{7}\sqrt{3}$.

Proof:

From the Figure 1, it is easy to see that the vertices of G have degree 1,2,3, or 4. Thus $\Delta(G) = 4$, $\delta(G) = 1$, and therefore $r_G(u) = 4 + 1 - d_G(u)$ is the Revan degree of any vertex u. According to the Revan vertex degree, there are six types of Revan edge sets in the structure of the first generation dendrimeric chelators G shown in Figure 1, as follows:

$E_1 = \{uv \in E(G) | r_G(u) = 4, r_G(v) = 3\}$, $|E_1| = 18$

$E_2 = \{uv \in E(G) | r_G(u) = 4, r_G(v) = 2\}$, $|E_2| = 15$

$E_3 = \{uv \in E(G) | r_G(u) = 4, r_G(v) = 1\}$, $|E_3| = 126$

$E_4 = \{uv \in E(G) | r_G(u) = r_G(v) = 1\}$, $|E_4| = 108$

$E_5 = \{uv \in E(G) | r_G(u) = 3, r_G(v) = 1\}$, $|E_5| = 66$

$E_6 = \{uv \in E(G) | r_G(u) = 1, r_G(v) = 2\}$, $|E_6| = 60$

By using the above Revan edge partitions,

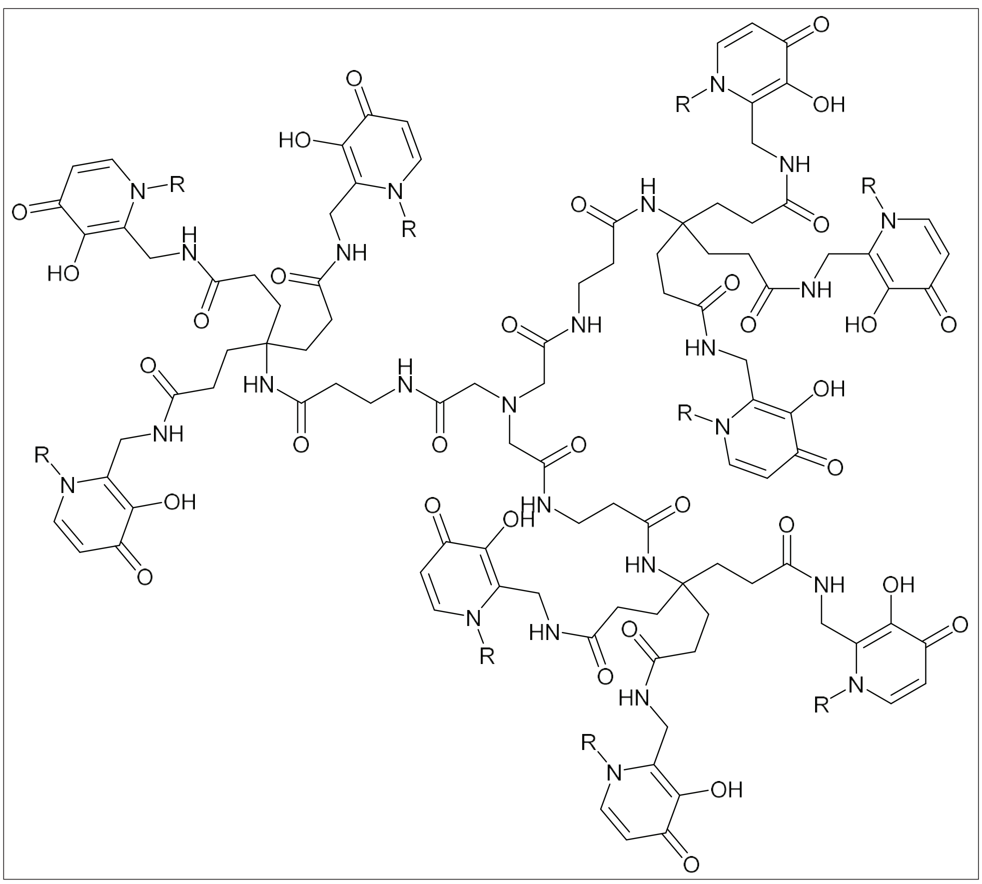

Figure 1: First-generation dendrimeric chelator corresponding to compound 6b in Scheme 1 of Zhou et al. (2018), containing three hexadentate chelating ligands and nine 3-hydroxypyridinone units (R = CH2CH2OH). Structure adapted from Zhou et al. (2018).

$$R_1(G) = \sum_{uv\in E(G)} r_G(u) + r_G(v)$$
$$= 18(4 + 3) + 15(4 + 2) + 126(4 + 1) + 108(1 + 1) + 66(3 + 1) + 60(1 + 2)$$
$$= 1506.$$

$$R_2(G) = \sum_{uv\in E(G)} r_G(u)\, r_G(v)$$
$$= 18(4\times 3) + 15(4\times 2) + 126(4\times 1) + 108(1\times 1) + 66(3\times 1) + 60(1\times 2)$$
$$= 1266.$$

$$R_3(G) = \sum_{uv\in E(G)} |r_G(u) - r_G(v)|$$
$$= 18|4-3| + 15|4-2| + 126|4-1| + 108|1-1| + 66|3-1| + 60|1-2|$$
$$= 618.$$

$$FR(G) = \sum_{uv\in E(G)} r_G(u)^2 + r_G(v)^2$$
$$= 18(4^2 + 3^2) + 15(4^2 + 2^2) + 126(4^2 + 1^2) + 108(1^2 + 1^2) + 66(3^2 + 1^2) + 60(1^2 + 2^2)$$
$$= 4068.$$

$$HR_1(G) = \sum_{uv\in E(G)} (r_G(u) + r_G(v))^2$$
$$= 18(4 + 3)^2 + 15(4 + 2)^2 + 126(4 + 1)^2 + 108(1 + 1)^2 + 66(3 + 1)^2 + 60(1+2)^2$$
$$= 6600.$$

$$ABCR(G) = \sum_{uv\in E(G)} \sqrt{\frac{r_G(u)+r_G(v)-2}{r_G(u)r_G(v)}}$$
$$= 18\sqrt{\frac{4+3-2}{4\times3}} + 15\sqrt{\frac{4+2-2}{4\times2}} + 126\sqrt{\frac{4+1-2}{4\times1}} + 108\sqrt{\frac{1+1-2}{1\times1}} + 66\sqrt{\frac{3+1-2}{3\times1}} + 60\sqrt{\frac{1+2-2}{1\times2}}$$
$$= 9\sqrt{\frac{5}{3}} + 75\sqrt{\frac{1}{2}} + 63\sqrt{3} + 66\sqrt{\frac{2}{3}}.$$

$$RR(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{r_G(u)r_G(v)}}$$
$$= 18\sqrt{\frac{1}{4\times3}} + 15\sqrt{\frac{1}{4\times2}} + 126\sqrt{\frac{1}{4\times1}} + 108\sqrt{\frac{1}{1\times1}} + 66\sqrt{\frac{1}{3\times1}} + 60\sqrt{\frac{1}{1\times2}}$$
$$= 171 + \frac{135}{2}\sqrt{\frac{1}{2}} + 75\sqrt{\frac{1}{3}}.$$

$$SR(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{r_G(u)+r_G(v)}}$$
$$= 18\sqrt{\frac{1}{4+3}} + 15\sqrt{\frac{1}{4+2}} + 126\sqrt{\frac{1}{4+1}} + 108\sqrt{\frac{1}{1+1}} + 66\sqrt{\frac{1}{3+1}} + 60\sqrt{\frac{1}{1+2}}$$
$$= 18\sqrt{\frac{1}{7}} + 15\sqrt{\frac{1}{6}} + 126\sqrt{\frac{1}{5}} + 108\sqrt{\frac{1}{2}} + 33 + 60\sqrt{\frac{1}{3}}.$$

$$HMR(G) = \sum_{uv\in E(G)} \frac{2}{r_G(u)+r_G(v)}$$
$$= 18\left(\frac{2}{4+3}\right) + 15\left(\frac{2}{4+2}\right) + 126\left(\frac{2}{4+1}\right) + 108\left(\frac{2}{1+1}\right) + 66\left(\frac{2}{3+1}\right) + 60\left(\frac{2}{1+2}\right)$$
$$= \frac{15753}{70}.$$

$$GAR(G) = \sum_{uv\in E(G)} \frac{2\sqrt{r_G(u)r_G(v)}}{r_G(u)+r_G(v)}$$
$$= 18\left(\frac{2\sqrt{4\times3}}{4+3}\right) + 15\left(\frac{2\sqrt{4\times2}}{4+2}\right) + 126\left(\frac{2\sqrt{4\times1}}{4+1}\right) + 108\left(\frac{2\sqrt{1\times1}}{1+1}\right) + 66\left(\frac{2\sqrt{3\times1}}{3+1}\right) + 60\left(\frac{2\sqrt{1\times2}}{1+2}\right)$$
$$= \frac{1044}{5} + 50\sqrt{2} + \frac{303}{7}\sqrt{3}.$$

Theorem 2.

Let G be the second generation dendrimeric chelators. Then the first Revan index $R_1(G)$, the second Revan index $R_2(G)$, the third Revan index $R_3(G)$, the forgotten Revan index $FR(G)$, the first Hyper Revan index $HR_1(G)$, the ABC Revan index $ABCR(G)$, the Randi`c Revan index $RR(G)$, the Sum connectivity Revan index $SR(G)$, the Harmonic Revan index $HMR(G)$, and the Geometric-Arithmatic Revan index $GAR(G)$ for G are

i. $R_1(G) = 2336$,

ii. $R_2(G) = 1749$,

iii. $R_3(G) = 1018$

iv. $FR(G) = 6260$,

v. $HR_1(G) = 9758$,

vi. $ABCR(G) = 39\sqrt{2} + 131\sqrt{3} + 68\sqrt{\frac{2}{3}}$,

vii. $RR(G) = 364 + 69\sqrt{\frac{1}{2}} + 68\sqrt{\frac{1}{3}}$.

viii. $SR(G) = 34 + 233\sqrt{\frac{1}{2}} + 60\sqrt{\frac{1}{3}} + 262\sqrt{\frac{1}{5}} + 18\sqrt{\frac{1}{6}}$.

ix. $HMR(G) = \frac{2089}{5}$, and

x. $GAR(G) = \frac{2213}{5} + 52\sqrt{2} + 34\sqrt{3}$.

Proof:
From the Figure 2, it is easy to see that the vertices of G have degree 1,2,3, or 4. Thus $\Delta(G) = 4$, $\delta(G) = 1$, and therefore $r_G(u) = 4 + 1 - d_G(u)$ is the Revan degree of any vertex u. According to the Revan vertex degree, there are five types of Revan edge sets in the structure of the second generation dendrimeric chelators G shown in Figure 2, as follows:

$E_1 = \{uv \in E(G) | r_G(u) = 4, r_G(v) = 2\}, \quad |E_1| = 18$

$E_2 = \{uv \in E(G) | r_G(u) = 4, r_G(v) = 1\}, \quad |E_2| = 262$

$E_3 = \{uv \in E(G) | r_G(u) = r_G(v) = 1\}, \quad |E_3| = 233$

$E_4 = \{uv \in E(G) | r_G(u) = 3, r_G(v) = 1\}, \quad |E_4| = 68$

$E_5 = \{uv \in E(G) | r_G(u) = 1, r_G(v) = 2\}, \quad |E_5| = 60$

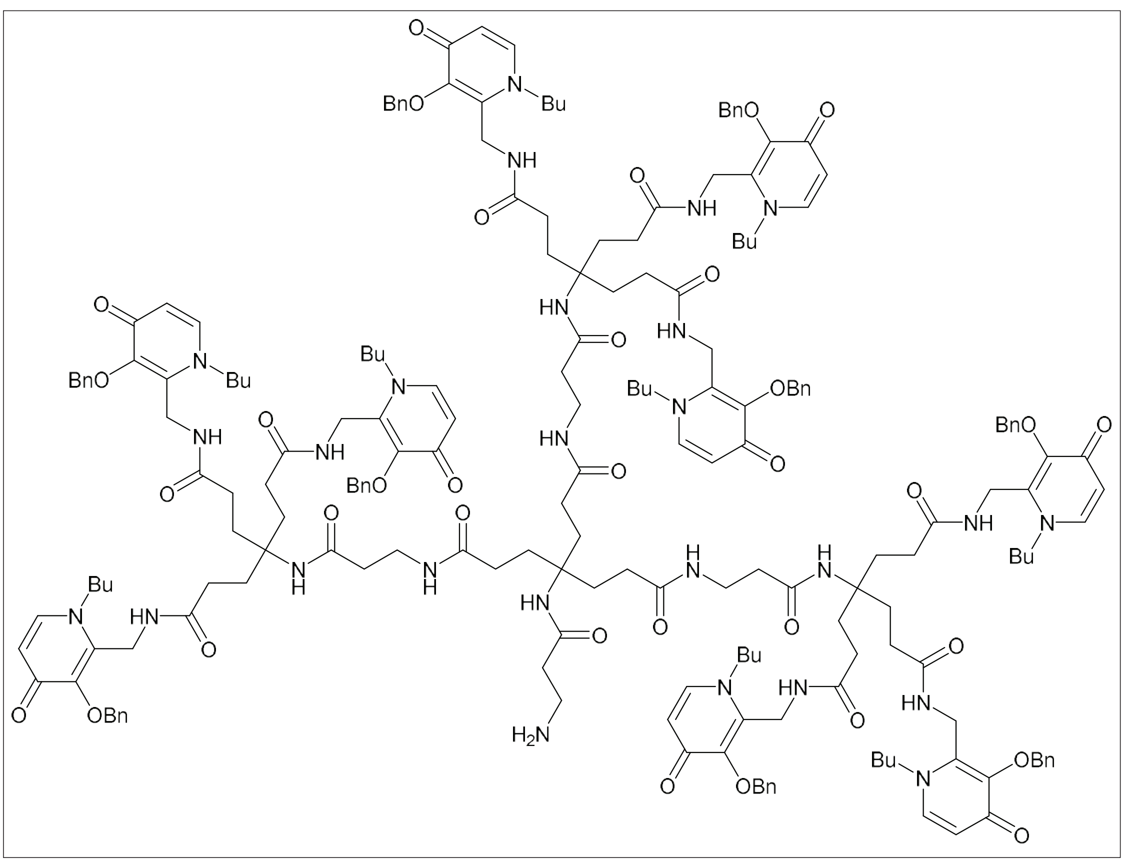

Figure 2: Benzyl-protected first-generation dendron intermediate corresponding to structure 7 in Scheme 2 of Zhou et al. (2018), containing three hexadentate chelating ligands and nine benzyl-protected 3-hydroxypyridinone units. Structure adapted from Zhou et al. (2018).

By using the above Revan edge partitions,

$$R_1(G) = \sum_{uv\in E(G)} \quad r_G(u) + r_G(v)$$

$$= 18(4 + 2) + 262(4 + 1) + 233(1 + 1) + 68(3 + 1) + 60(1 + 2)$$

$$= 2336.$$

$$R_2(G) = \sum_{uv\in E(G)} \quad r_G(u)\, r_G(v)$$

$$= 18(4 \times 2) + 262(4 \times 1) + 233(1 \times 1) + 68(3 \times 1) + 60(1 \times 2)$$

$$= 1749.$$

$$R_3(G) = \sum_{uv\in E(G)} \quad |r_G(u) - r_G(v)|$$

$$= 18|4 - 2| + 262|4 - 1| + 233|1 - 1| + 68|3 - 1| + 60|1 - 2|$$

$$= 1018.$$

$$FR(G) = \sum_{uv\in E(G)} \quad r_G(u)^2 + r_G(v)^2$$

$$= 18(4^2 + 2^2) + 262(4^2 + 1^2) + 233(1^2 + 1^2) + 68(3^2 + 1^2) + 60(1^2 + 2^2)$$

$$= 6260.$$

$$HR_1(G) = \sum_{uv\in E(G)} \quad (r_G(u) + r_G(v))^2$$

$$= 18(4 + 2)^2 + 262(4 + 1)^2 + 233(1 + 1)^2 + 68(3 + 1)^2 + 60(1 + 2)^2$$

$$= 9758.$$

$$ABCR(G) = \sum_{uv\in E(G)} \quad \sqrt{\frac{r_G(u)+r_G(v)-2}{r_G(u)r_G(v)}}$$

$$= 18\sqrt{\frac{4+2-2}{4\times2}} + 262\sqrt{\frac{4+1-2}{4\times1}} + 233\sqrt{\frac{1+1-2}{1\times1}} + 68\sqrt{\frac{3+1-2}{3\times1}} + 60\sqrt{\frac{1+2-2}{1\times2}}$$

$$= 39\sqrt{2} + 131\sqrt{3} + 68\sqrt{\frac{2}{3}}.$$

$$RR(G) = \sum_{uv\in E(G)} \quad \frac{1}{\sqrt{r_G(u)r_G(v)}}$$

$$= 18\sqrt{\frac{1}{4\times2}} + 262\sqrt{\frac{1}{4\times1}} + 233\sqrt{\frac{1}{1\times1}} + 68\sqrt{\frac{1}{3\times1}} + 60\sqrt{\frac{1}{1\times2}}$$

$$= 364 + 69\sqrt{\frac{1}{2}} + 68\sqrt{\frac{1}{3}}.$$

$$HMR(G) = \sum_{uv\in E(G)} \frac{2}{r_G(u)+r_G(v)}$$

$$= 18\left(\frac{2}{4+2}\right) + 262\left(\frac{2}{4+1}\right) + 233\left(\frac{2}{1+1}\right) + 68\left(\frac{2}{3+1}\right) + 60\left(\frac{2}{1+2}\right)$$

$$= \frac{2089}{5}.$$

$$GAR(G) = \sum_{uv\in E(G)} \frac{2\sqrt{r_G(u)r_G(v)}}{r_G(u)+r_G(v)}$$

$$= 18\left(\frac{2\sqrt{4\times2}}{4+2}\right) + 262\left(\frac{2\sqrt{4\times1}}{4+1}\right) + 233\left(\frac{2\sqrt{1\times1}}{1+1}\right) + 68\left(\frac{2\sqrt{3\times1}}{3+1}\right) + 60\left(\frac{2\sqrt{1\times2}}{1+2}\right)$$

$$= \frac{2213}{5} + 52\sqrt{2} + 34\sqrt{3}.$$

Theorem 3.

Let G be the dendrimeric chelators contain six hexadentate centers. Then the first Revan index $R_1(G)$, the second Revan index $R_2(G)$, the third Revan index $R_3(G)$, the forgotten Revan index $FR(G)$, the first Hyper Revan index $HR_1(G)$, the ABC Revan index $ABCR(G)$, the Randi`c Revan index $RR(G)$, the Sum connectivity Revan index $SR(G)$, the Harmonic Revan index $HMR(G)$, and the Geometric-Arithmatic Revan index $GAR(G)$ for G are

i. $R_1(G) = 3876$,

ii. $R_2(G) = 3075$,

iii. $R_3(G) = 1698$,

iv. $FR(G) = 10632$,

v. $HR_1(G) = 16386$,

vi. $ABCR(G) = 81\sqrt{2} + 205\sqrt{3} + 126\sqrt{\frac{2}{3}} + 9\sqrt{\frac{5}{3}}$,

vii. $RR(G) = 506 + 72\sqrt{2} + 45\sqrt{3}$,

viii. $SR(G) = 63 + 301\sqrt{\frac{1}{2}} + 126\sqrt{\frac{1}{3}} + 410\sqrt{\frac{1}{5}}$

$+ 36\sqrt{\frac{1}{6}} + 18\sqrt{\frac{1}{7}}$,

ix. $HMR(G) = \frac{4404}{7}$, and

x. $GAR(G) = 629 + 108\sqrt{2} + \frac{513}{7}\sqrt{3}$.

Proof:
From the Figure 3, it is easy to see that the vertices of G have degree 1, 2, 3, or 4. Thus $\Delta(G) = 4$, $\delta(G) = 1$, and therefore $r_G(u) = 4 + 1 - d_G(u)$ is the Revan degree of any vertex *u*. According to the Revan vertex degree, there are six types of Revan edge sets in the structure of the dendrimeric chelators contain six hexadentate centres G shown in Figure 3, as follows:

$E_1 = \{uv \in E(G) | r_G(u) = 4, r_G(v) = 3\}$, $|E_1| = 18$

$E_2 = \{uv \in E(G) | r_G(u) = 4, r_G(v) = 2\}$, $|E_2| = 36$

$E_3 = \{uv \in E(G) | r_G(u) = 4, r_G(v) = 1\}$, $|E_3| = 410$

$E_4 = \{uv \in E(G) | r_G(u) = r_G(v) = 1\}$, $|E_4| = 301$

$E_5 = \{uv \in E(G) | r_G(u) = 3, r_G(v) = 1\}$, $|E_5| = 126$

$E_6 = \{uv \in E(G) | r_G(u) = 1, r_G(v) = 2\}$, $|E_6| = 126$

By using the above Revan edge partitions,

$$R_1(G) = \sum_{uv\in E(G)} r_G(u) + r_G(v)$$

$$= 18(4+3) + 36(4+2) + 410(4+1)$$

$$+ 301(1+1) + 126(3+1) + 126(1+2)$$

$$= 3876.$$

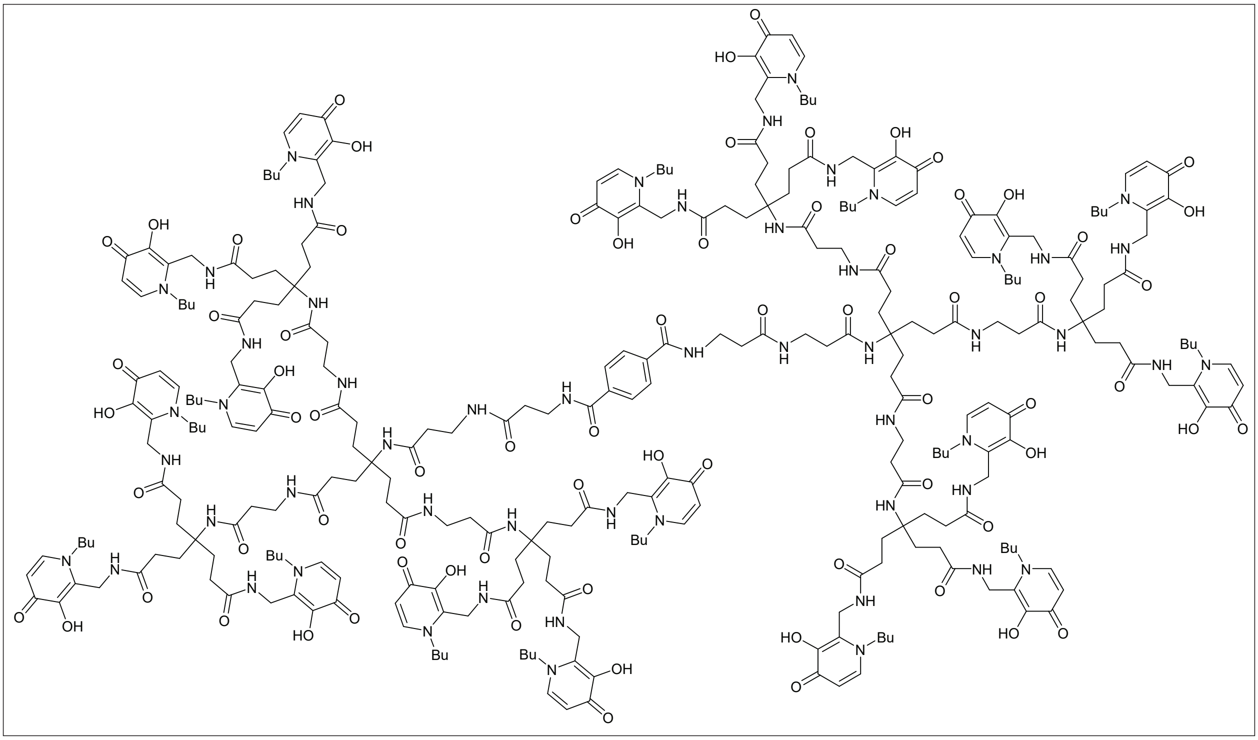

Figure 3: Second-generation dendrimeric chelator corresponding to compound 10 in Scheme 3 of Zhou et al. (2018), containing six hexadentate chelating ligands and eighteen 3-hydroxypyridinone units. Structure adapted from Zhou et al. (2018).

$$R_2(G) = \sum_{uv\in E(G)} r_G(u)\, r_G(v)$$

$$= 18(4\times 3) + 36(4\times 2) + 410(4\times 1) + 301(1\times 1) + 126(3\times 1) + 126(1\times 2)$$

$$= 3075.$$

$$R_3(G) = \sum_{uv\in E(G)} |r_G(u) - r_G(v)|$$

$$= 18|4-3| + 36|4-2| + 410|4-1| + 301|1-1| + 126|3-1| + 126|1-2|$$

$$= 1698.$$

$$FR(G) = \sum_{uv\in E(G)} r_G(u)^2 + r_G(v)^2$$

$$= 18(4^2+3^2) + 36(4^2+2^2) + 410(4^2+1^2) + 301(1^2+1^2) + 126(3^2+1^2) + 126(1^2+2^2)$$

$$= 10632.$$

$$HR_1(G) = \sum_{uv\in E(G)} (r_G(u) + r_G(v))^2$$

$$= 18(4+3)^2 + 36(4+2)^2 + 410(4+1)^2 + 301(1+1)^2 + 126(3+1)^2 + 126(1+2)^2$$

$$= 16386.$$

$$ABCR(G) = \sum_{uv\in E(G)} \sqrt{\frac{r_G(u)+r_G(v)-2}{r_G(u)r_G(v)}}$$

$$= 18\sqrt{\frac{4+3-2}{4\times3}} + 36\sqrt{\frac{4+2-2}{4\times2}} + 410\sqrt{\frac{4+1-2}{4\times1}} + 301\sqrt{\frac{1+1-2}{1\times1}} + 126\sqrt{\frac{3+1-2}{3\times1}} + 126\sqrt{\frac{1+2-2}{1\times2}}$$

$$= 81\sqrt{2} + 205\sqrt{3} + 126\sqrt{\frac{2}{3}} + 9\sqrt{\frac{5}{3}}.$$

$$RR(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{r_G(u)r_G(v)}}$$

$$= 18\sqrt{\frac{1}{4\times3}} + 36\sqrt{\frac{1}{4\times2}} + 410\sqrt{\frac{1}{4\times1}} + 301\sqrt{\frac{1}{1\times1}} + 126\sqrt{\frac{1}{3\times1}} + 126\sqrt{\frac{1}{1\times2}}$$

$$= 506 + 72\sqrt{2} + 45\sqrt{3}\,.$$

$$SR(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{r_G(u)+r_G(v)}}$$

$$= 18\sqrt{\frac{1}{4+3}} + 36\sqrt{\frac{1}{4+2}} + 410\sqrt{\frac{1}{4+1}} + 301\sqrt{\frac{1}{1+1}} + 126\sqrt{\frac{1}{3+1}} + 126\sqrt{\frac{1}{1+2}}$$

$$= 63 + 301\sqrt{\frac{1}{2}} + 126\sqrt{\frac{1}{3}} + 410\sqrt{\frac{1}{5}} + 36\sqrt{\frac{1}{6}} + 18\sqrt{\frac{1}{7}}.$$

$$HMR(G) = \sum_{uv\in E(G)} \frac{2}{r_G(u)+r_G(v)}$$

$$= 18\left(\frac{2}{4+3}\right) + 36\left(\frac{2}{4+2}\right) + 410\left(\frac{2}{4+1}\right) + 301\left(\frac{2}{1+1}\right) + 126\left(\frac{2}{3+1}\right) + 126\left(\frac{2}{1+2}\right)$$

$$= \frac{4404}{7}.$$

$$GAR(G) = \sum_{uv\in E(G)} \frac{2\sqrt{r_G(u)r_G(v)}}{r_G(u)+r_G(v)}$$

$$= 18\left(\frac{2\sqrt{4\times3}}{4+3}\right) + 36\left(\frac{2\sqrt{4\times2}}{4+2}\right) + 410\left(\frac{2\sqrt{4\times1}}{4+1}\right) + 301\left(\frac{2\sqrt{1\times1}}{1+1}\right) + 126\left(\frac{2\sqrt{3\times1}}{3+1}\right) + 126\left(\frac{2\sqrt{1\times2}}{1+2}\right)$$

$$= 629 + 108\sqrt{2} + \frac{513}{7}\sqrt{3}\,.$$

Theorem 4.

Let G be the dendrimeric chelators contain nine hexadentate centers. Then the first Revan index $R_1(G)$, the second Revan index $R_2(G)$, the third Revan index $R_3(G)$, the forgotten Revan index $FR(G)$, the first Hyper Revan index $HR_1(G)$, the ABC Revan index $ABCR(G)$, the Randi`c Revan index $RR(G)$, the Sum connectivity Revan index $SR(G)$, the Harmonic Revan index $HMR(G)$, and the Geometric-Arithmatic Revan index $GAR(G)$ for G are

i. $R_1(G) = 5790$,

ii. $R_2(G) = 4596$,

iii. $R_3(G) = 2538$,

iv. $FR(G) = 15888$,

v. $HR_1(G) = 25080$,

vi. $ABCR(G) = 243\sqrt{\frac{1}{2}} + 306\sqrt{3} + 189\sqrt{\frac{2}{3}} + \frac{27}{2}\sqrt{\frac{5}{3}}$,

vii. $RR(G) = 753 + 108\sqrt{2} + \frac{405}{2}\sqrt{\frac{1}{3}}$,

viii. $SR(G) = \frac{189}{2} + 447\sqrt{\frac{1}{2}} + 189\sqrt{\frac{1}{3}} + 612\sqrt{\frac{1}{5}}$

$+ 54\sqrt{\frac{1}{6}} + 27\sqrt{\frac{1}{7}}$,

ix. $HMR(G) = \frac{65661}{70}$, and

x. $GAR(G) = \frac{4683}{5} + 162\sqrt{2} + \frac{1539}{14}\sqrt{3}$.

Proof:

From the Figure 4, it is easy to see that the vertices of G have degree 1, 2, 3, or 4. Thus $\Delta(G) = 4$, $\delta(G) = 1$, and therefore $r_G(u) = 4 + 1 - d_G(u)$ is the Revan degree of any vertex u. According to the Revan vertex degree, there are six types of Revan edge sets in the structure of the dendrimeric chelators contain nine hexadentate centres G shown in Figure 4, as follows:

$E_1 = \{uv \in E(G) | r_G(u) = 4, r_G(v) = 3\}$, $|E_1| = 27$

$E_2 = \{uv \in E(G) | r_G(u) = 4, r_G(v) = 2\}$, $|E_2| = 54$

$E_3 = \{uv \in E(G) | r_G(u) = 4, r_G(v) = 1\}$, $|E_3| = 612$

$E_4 = \{uv \in E(G) | r_G(u) = r_G(v) = 1\}$, $|E_4| = 447$

$E_5 = \{uv \in E(G) | r_G(u) = 3, r_G(v) = 1\}$, $|E_5| = 189$

$E_6 = \{uv \in E(G) | r_G(u) = 1, r_G(v) = 2\}$, $|E_6| = 189$

By using the above Revan edge partitions,

$$R_1(G) = \sum_{uv\in E(G)} r_G(u) + r_G(v)$$

$$= 27(4 + 3) + 54(4 + 2) + 612(4 + 1) + 447(1 + 1) + 189(3 + 1) + 189(1 + 2)$$

$$= 5790.$$

$$R_2(G) = \sum_{uv\in E(G)} r_G(u)\, r_G(v)$$

$$= 27(4 \times 3) + 54(4 \times 2) + 612(4 \times 1) + 447(1 \times 1) + 189(3 \times 1) + 189(1 \times 2)$$

$$= 4596.$$

$$R_3(G) = \sum_{uv\in E(G)} |r_G(u) - r_G(v)|$$

$$= 27|4 - 3| + 54|4 - 2| + 612|4 - 1| + 447|1 - 1| + 189|3 - 1| + 189|1 - 2|$$

$$= 2538.$$

$$FR(G) = \sum_{uv\in E(G)} r_G(u)^2 + r_G(v)^2$$

$$= 27(4^2 + 3^2) + 54(4^2 + 2^2) + 612(4^2 + 1^2) + 447(1^2 + 1^2) + 189(3^2 + 1^2) + 189(1^2 + 2^2)$$

$$= 15888.$$

$$HR_1(G) = \sum_{uv\in E(G)} (r_G(u) + r_G(v))^2$$

$$= 27 + 15(4 + 2)^2 + 54(4 + 1)^2 + 612(1 + 1)^2 + 447(3 + 1)^2 + 189(1 + 2)^2$$

$$= 25080.$$

$$ABCR(G) = \sum_{uv\in E(G)} \sqrt{\frac{r_G(u)+r_G(v)-2}{r_G(u)r_G(v)}}$$

$$= 27\sqrt{\frac{4+3-2}{4\times3}} + 54\sqrt{\frac{4+2-2}{4\times2}} + 612\sqrt{\frac{4+1-2}{4\times1}} + 447\sqrt{\frac{1+1-2}{1\times1}} + 189\sqrt{\frac{3+1-2}{3\times1}} + 189\sqrt{\frac{1+2-2}{1\times2}}$$

$$= 243\sqrt{\frac{1}{2}} + 306\sqrt{3} + 189\sqrt{\frac{2}{3}} + \frac{27}{2}\sqrt{\frac{5}{3}}.$$

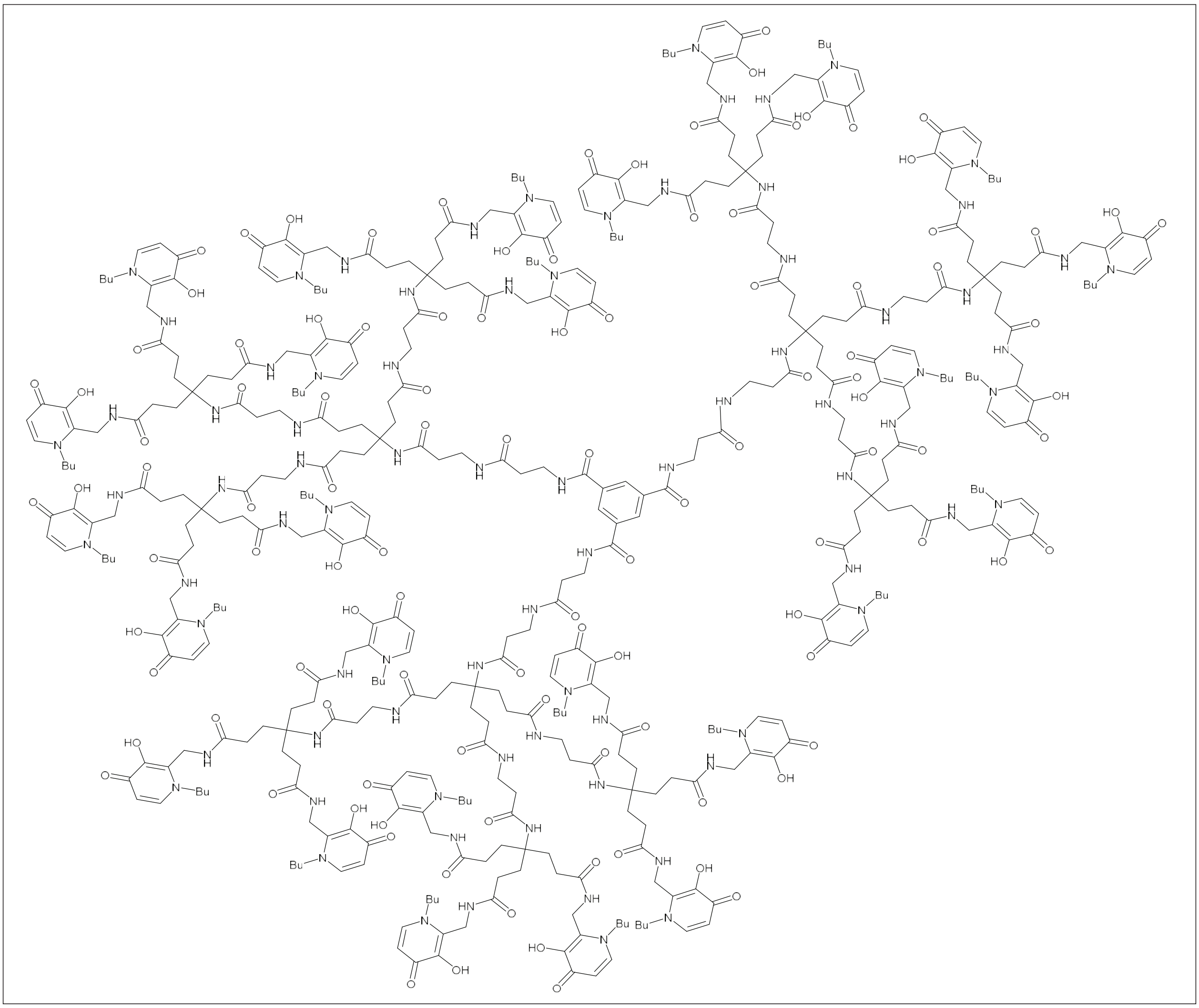

Figure 4: Second-generation dendrimeric chelator corresponding to compound 13 in Scheme 4 of Zhou et al. (2018), containing nine hexadentate chelating ligands and twenty-seven 3-hydroxypyridinone units. Structure adapted from Zhou et al. (2018).

$$RR(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{r_G(u)r_G(v)}}$$

$$= 27\sqrt{\frac{1}{4\times3}} + 54\sqrt{\frac{1}{4\times2}} + 612\sqrt{\frac{1}{4\times1}} + 447\sqrt{\frac{1}{1\times1}} + 189\sqrt{\frac{1}{3\times1}} + 189\sqrt{\frac{1}{1\times2}}$$

$$= 753 + 108\sqrt{2} + \frac{405}{2}\sqrt{\frac{1}{3}}.$$

$$SR(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{r_G(u)+r_G(v)}}$$

$$= 27\sqrt{\frac{1}{4+3}} + 54\sqrt{\frac{1}{4+2}} + 612\sqrt{\frac{1}{4+1}} + 447\sqrt{\frac{1}{1+1}} + 189\sqrt{\frac{1}{3+1}} + 189\sqrt{\frac{1}{1+2}}$$

$$= \frac{189}{2} + 447\sqrt{\frac{1}{2}} + 189\sqrt{\frac{1}{3}} + 612\sqrt{\frac{1}{5}} + 54\sqrt{\frac{1}{6}} + 27\sqrt{\frac{1}{7}}.$$

$$HMR(G) = \sum_{uv\in E(G)} \frac{2}{r_G(u)+r_G(v)}$$

$$= 27\left(\frac{2}{4+3}\right) + 54\left(\frac{2}{4+2}\right) + 612\left(\frac{2}{4+1}\right) + 447\left(\frac{2}{1+1}\right) + 189\left(\frac{2}{3+1}\right) + 189\left(\frac{2}{1+2}\right)$$

$$= \frac{65661}{70}.$$

$$GAR(G) = \sum_{uv\in E(G)} \frac{2\sqrt{r_G(u)r_G(v)}}{r_G(u)+r_G(v)}$$

$$= 27\left(\frac{2\sqrt{4\times3}}{4+3}\right) + 54\left(\frac{2\sqrt{4\times2}}{4+2}\right) + 612\left(\frac{2\sqrt{4\times1}}{4+1}\right) + 447\left(\frac{2\sqrt{1\times1}}{1+1}\right) + 189\left(\frac{2\sqrt{3\times1}}{3+1}\right) + 189\left(\frac{2\sqrt{1\times2}}{1+2}\right)$$

$$= \frac{4683}{5} + 162\sqrt{2} + \frac{1539}{14}\sqrt{3}.$$

CONCLUSION

In this work, four new hexadentate 3-hydroxypyridinone-terminated dendrimers were analyzed using different Revan indices. These indices, comprising the first, second, and third Revan indices, as well as the forgotten Revan index and others, offer important new perspectives on the topological properties of these dendrimeric structures. Using the Revan edge set partitions of the structures of dendrimers, these indices were calculated. The calculated indices reveal a strong correlation between the dendrimeric structures and its potential applications, thereby underscoring the utility of Revan indices in the study and development of advanced molecular systems. The results of this study, the computed values of Revan indices differ with various dendrimeric structures, and they assist in recognizing those structures' complexities. This study can be extended to study the physicochemical and biological properties of dendrimeric structures using the QSPR (quantitative structure-property relationship) and QSAR (quantitative structure- activity relationship) models as a future study.

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