Multiplicative degree based topological indices of some chemical structures applied for the treatment of COVID-19 patients

Gowtham K. J.[1] and Mohamad Nazri Husin [2*]

[1]Department of Mathematics, University College of Science, Tumkur University, Tumakuru, Karnataka State, INDIA, Pin 572 103

[2]Special Interest Group on Modelling Data Analytics (SIGMDA), Faculty of Ocean Engineering Technology and Informatics Universiti Malaysia Terengganu, Malaysia.

nazri.husin@umt.edu.my

Abstract

The COVID-19 coronavirus pandemic defines the current global health crisis and is humanity's biggest challenge since World War Two. Remdesivir (GS-5734), chloroquine, hydroxychloroquine, and theaflavin are antiviral medications used to treat COVID-19, but they are ineffective for treating coronavirus patients who are hospitalized. By gathering information from the molecular graph, a topological index is a useful tool for predicting molecules' various physical and chemical properties. Additionally, employed to research the biological effects of chemical compounds. The antiviral medications investigated in this paper, we have found their multiplicative degree-based topological indices, and the findings can be used to develop new or better COVID-19 treatment options. For further analysis of how the parameters in play affected our computed results, we also plotted them.

Keywords: multiplicative degree based topological indices; chloroquine; COVID-19; hydroxychloroquine; molecular graph; remdesivir (GS-5734); theaflavin

Introduction

A global clinical trial (Solidarity) has been started by the World Health Organisation and its collaborators to aid in the search for a cure for COVID-19. It includes 12000 patients at 500 hospital sites across more than 30 countries, making it one of the biggest international randomized trials for COVID-19 treatments. In the Solidarity Trial, 3 crucial outcomes for COVID-19 patients are being examined: mortality, the requirement for assisted ventilation, and the length of hospital stay. The Solidarity Trial released its preliminary findings on October 15, 2020. Remdesivir, hydroxychloroquine, lopinavir/ritonavir, and interferon were all found to have little to no effect on overall mortality, the start of ventilation, or the length of hospital stay in patients who were hospitalized. In order to continue its search for potent COVID-19 therapeutics, the Solidarity Trial is thinking about evaluating additional therapies or making improvements. Millions of lives are saved annually by vaccines. The following antiviral agents have been tested by researchers:[1- 5] . Vaccinations train and prepare the immune system, the body's natural defense, to recognize and neutralize the viruses and bacteria they target.

Immediately after receiving a vaccination, the body is ready to obliterate the disease-causing microorganisms, preventing illness.

Chloroquine and hydroxy chloroquine will be FDA-approved for use in the treatment of coronavirus emergencies on March 30, 2020. Inhibiting T cell activation with hydroxychloroquine prevents the cytokine storm from increasing COVID-19 growth. a polyphenolic compound found in black tea For the health benefits of black tea, theaflavin was found to be responsible. Influenza A, B, and hepatitis C viruses are just a few of the viruses that theaflavin has been shown to have a wide range of antiviral activity [6,7]. It is extremely encouraging that so many vaccines are demonstrating efficacy and progressing into development because vaccines are a vital new tool in the war against COVID-19. The world's scientists are working together and innovating as quickly as they can to create tests, medicines, and vaccines that will enable us all to save lives and end this pandemic. The COVID-19 drugs have thus far been studied using degree-based topological indices and their reverse vertex degree-based topological indices [8-13]. Surprisingly, multiplicative degree-based topological indices received little attention. With this as our inspiration, we identified some chemical structures' multiplicative degree-based topological indices and investigated some of their properties in this paper.

Table: 1 Multiplicative topological index with their formula.

Multiplicative Topological index	Formula
Multiplicative Zagreb index$\left(\Pi_1^*(\mathcal{G})\right)$ [14]	$\prod_{\mu\nu\in E(\mathcal{G})}\left(d_{\mathcal{G}}(\mu)+d_{\mathcal{G}}(\nu)\right)$
Multiplicative first Zagreb index$\left(H\Pi_1(\mathcal{G})\right)$ [15]	$\prod_{\mu\nu\in E(\mathcal{G})}\left(d_{\mathcal{G}}(\mu)+d_{\mathcal{G}}(\nu)\right)^2$
Multiplicative second Zagreb index$\left(H\Pi_2(\mathcal{G})\right)$ [15]	$\prod_{\mu\nu\in E(\mathcal{G})}\left(d_{\mathcal{G}}(\mu)\cdot d_{\mathcal{G}}(\nu)\right)^2$
Fist generalized multiplicative Zagreb index$\left(MZ_1^a(\mathcal{G})\right)$ [16]	$\prod_{\mu\nu\in E(\mathcal{G})}\left(d_{\mathcal{G}}(\mu)+d_{\mathcal{G}}(\nu)\right)^a$
Second generalized multiplicative Zagreb index$MZ_2^a(\mathcal{G})$ [16]	$\prod_{\mu\nu\in E(\mathcal{G})}\left(d_{\mathcal{G}}(\mu)\cdot d_{\mathcal{G}}(\nu)\right)^a$
Multiplicative sum-connectivity index$\left(SC\Pi(\mathcal{G})\right)$ [17]	$\prod_{\mu\nu\in E(\mathcal{G})}\left(d_{\mathcal{G}}(\mu)+d_{\mathcal{G}}(\nu)\right)^{-\frac{1}{2}}$
Multiplicative Product connectivity index$\left(PC\Pi(\mathcal{G})\right)$ [17]	$\prod_{\mu\nu\in E(\mathcal{G})}\left(d_{\mathcal{G}}(\mu)\cdot d_{\mathcal{G}}(\nu)\right)^{-\frac{1}{2}}$
Multiplicative atomic bond connectivity index$\left(\mathcal{G}AH(\mathcal{G})\right)$ [18]	$\prod_{\mu\nu\in E(\mathcal{G})}\frac{2\sqrt{d_{\mathcal{G}}(\mu)\cdot d_{\mathcal{G}}(\nu)}}{d_{\mathcal{G}}(\mu)+d_{\mathcal{G}}(\nu)}$
Multiplicative Geometric arithmetic index$\left(ABC(\mathcal{G})\right)$ [18]	$\prod_{\mu\nu\in E(\mathcal{G})}\sqrt{\frac{d_{\mathcal{G}}(\mu)+d_{\mathcal{G}}(\nu)-2}{d_{\mathcal{G}}(\mu)\cdot d_{\mathcal{G}}(\nu)}}$

Here, we consider the simple connected graph $\mathcal{G}$ with the vertex set($V(\mathcal{G})$) and the edge set ($E(\mathcal{G})$). The degree of a vertex v is the number of edges incident to that vertex v and it is denoted by $d_{\mathcal{G}}(v)$. The multiplicative topological indices which are used in this paper are tabulated in the Table **1** Some of their properties are found in [19 - 30].

Main Result

We present our key findings in this section. Remdesivir, chloroquine, hydroxychloroquine, and theaflavin chemical structures were obtained from *pubchem.ncbi.nlm.nih.gov*. Since hydrogen atom vertices do not contribute to graph isomorphism, we consider hydrogen-available molecular graphs of compounds. To arrive at our conclusions, we employ combinatorial computation, the edge partition method, graph theoretical tools, analytical techniques, and the degree counting method. The degree and community degree sums of the end vertices are used to construct the edge partitions of the compounds' hydrogen-deleted molecular graph.

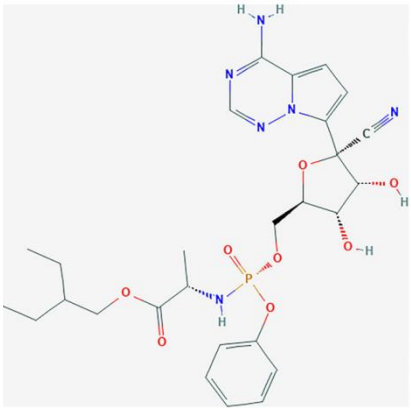


Figure 1: Molecular structure of Remdesivir

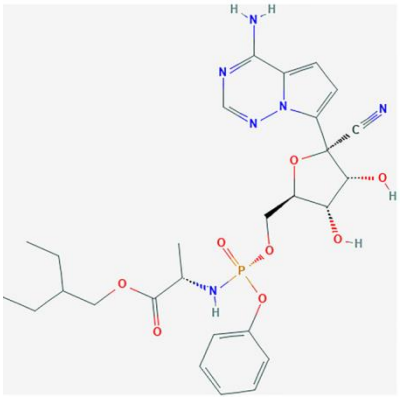
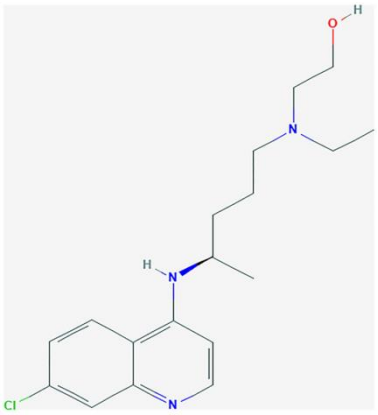


Figure 2: Molecular structure of Chloroquine



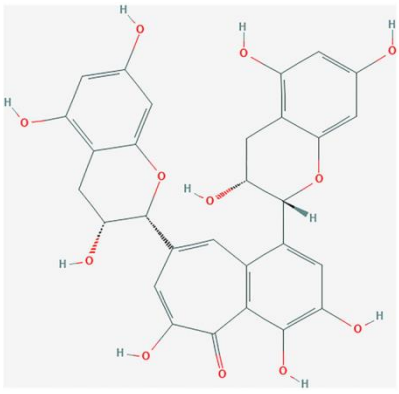


Figure 4: Molecular structure of Theaflavin

Figure 3: Molecular structure of Hydroxychloroquine

Table 2: An edge set of Remdesivir (GS-5734).

$\left(d_{\mathcal{G}}(\mu), d_{\mathcal{G}}(\nu)\right)$	(1,2)	(1,3)	(1,4)	(2,2)	(2,3)	(3,3)	(3,4)
Number of Bounds	2	5	2	9	14	6	2

Theorem 1. If Remdesivir (GS-5734) (see Figure 1) structure is denoted by $\mathcal{G}$, then

- $MZ_1^a(\mathcal{G}) = (3^{8a}) \cdot (2^{34a}) \cdot (5^{16a}) \cdot (7^{2a})$
- $MZ_2^a(\mathcal{G}) = (2^{42a}) \cdot (3^{33a})$
- $ABC(\mathcal{G}) = \left(\frac{15}{96}\right) \cdot \left(\frac{2}{3}\right)^{\frac{17}{2}} \cdot \left(\frac{1}{2}\right)^{\frac{23}{2}}$
- $\mathcal{G}AH(\mathcal{G}) = \left(\frac{3072}{11025}\right) \cdot \left(\frac{\sqrt{3}}{2}\right)^{5} \cdot \left(\frac{2\sqrt{6}}{5}\right)^{14}$

Proof. With the help of Table 2 and definitions in Table 1 we have,

$$
\begin{aligned}
MZ_1^a(\mathcal{G}) = & \prod \mu\nu \in E(\mathcal{G}) \left(d_{\mathcal{G}}(\mu) + d_{\mathcal{G}}(\nu)\right)^a \\
= & \prod \mu\nu \in E(\{1,2\}) \left(d_{\mathcal{G}}(\mu) + d_{\mathcal{G}}(\nu)\right)^a \cdot \prod \mu\nu \in E(\{1,3\}) \left(d_{\mathcal{G}}(\mu) + d_{\mathcal{G}}(\nu)\right)^a \cdot \prod \mu\nu \in E(\{1,4\}) \left(d_{\mathcal{G}}(\mu) + d_{\mathcal{G}}(\nu)\right)^a \cdot \\
& \prod \mu\nu \in E(\{2,2\}) \left(d_{\mathcal{G}}(\mu) + d_{\mathcal{G}}(\nu)\right)^a \cdot \prod \mu\nu \in E(\{2,3\}) \left(d_{\mathcal{G}}(\mu) + d_{\mathcal{G}}(\nu)\right)^a \cdot \prod \mu\nu \in E(\{3,3\}) \left(d_{\mathcal{G}}(\mu) + d_{\mathcal{G}}(\nu)\right)^a \cdot \\
& \prod \mu\nu \in E(\{3,4\}) \left(d_{\mathcal{G}}(\mu) + d_{\mathcal{G}}(\nu)\right)^a \\
= & (3^a)^2 \cdot (4^a)^5 \cdot (5^a)^2 \cdot (4^a)^9 \cdot (5^a)^{14} \cdot (6^a)^6 \cdot (7^a)^2 \\
= & (3^{8a}) \cdot (2^{34a}) \cdot (5^{16a}) \cdot (7^{2a})
\end{aligned}
$$

Similarly, rest can be proved as above. □

Corollary 2. Different multiplicative degree-based indies of Remdersivir (GS-5734) are given by (putting $a = \frac{-1}{2}$ and 2),

- $SC\Pi(\mathcal{G}) = \left(\frac{1}{3}\right)^4 \cdot \left(\frac{1}{2}\right)^{17} \cdot \left(\frac{1}{5}\right)^8 \cdot \left(\frac{1}{7}\right)$
- $PC\Pi(\mathcal{G}) = \left(\frac{1}{2}\right)^{21} \cdot \left(\frac{1}{3}\right)^{\frac{33}{2}}$
- $H\Pi_1(\mathcal{G}) = (3^{16}) \cdot (2^{68}) \cdot (5^{32}) \cdot (7^{14})$
- $H\Pi_2(\mathcal{G}) = (2^{84}) \cdot (3^{66})$

Table 3: An edge set of Chloroquine.

$\left(d_{\mathcal{G}}(\mu), d_{\mathcal{G}}(\nu)\right)$	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Number of Bounds	2	2	5	12	2

Theorem 3. If Chloroquine structure (see Figure 2) is denoted by $\mathcal{G}$ then,

- $\mathrm{MZ}_1^{\mathrm{a}}(\mathcal{G}) = (2^{16\mathrm{a}}) \cdot (3^{4\mathrm{a}}) \cdot (5^{12\mathrm{a}})$
- $\mathrm{MZ}_2^{\mathrm{a}}(\mathcal{G}) = (2^{24\mathrm{a}}) \cdot (3^{18\mathrm{a}})$
- $\mathrm{ABC}(\mathcal{G}) = \left(\frac{1}{3}\right) \cdot \left(\frac{1}{2}\right)^{\frac{17}{2}}$
- $\mathcal{G}\mathrm{AH}(\mathcal{G}) = \left(\frac{2}{3}\right) \cdot \left(\frac{2\sqrt{6}}{5}\right)^{12}$

Proof. With help of Table 3 we can easily found the result like Theorem 1. □

Corollary 4. Different multiplicative degree-based indies of chloroquine are given by (putting a $= \frac{-1}{2}$ and 2),

- $\mathrm{SC\Pi}(\mathcal{G}) = \left(\frac{1}{2}\right)^8 \cdot \left(\frac{1}{3}\right)^2 \cdot \left(\frac{1}{5}\right)^6$
- $\mathrm{PC\Pi}(\mathcal{G}) = \left(\frac{1}{2}\right)^{12} \cdot \left(\frac{1}{3}\right)^9$
- $\mathrm{H\Pi}_1(\mathcal{G}) = (2^{32}) \cdot (3^8) \cdot (5^{24})$
- $\mathrm{H\Pi}_2(\mathcal{G}) = (2^{48}) \cdot (3^{36})$

Theorem 5. If Hydroxychloroquine (see Figure 3) structure is denoted by $\mathcal{G}$ then,

- $\mathrm{MZ}_1^{\mathrm{a}}(\mathcal{G}) = (2^{18\mathrm{a}}) \cdot (3^{4\mathrm{a}}) \cdot (5^{12\mathrm{a}})$
- $\mathrm{MZ}_2^{\mathrm{a}}(\mathcal{G}) = (2^{26\mathrm{a}}) \cdot (3^{6\mathrm{a}})$
- $\mathrm{ABC}(\mathcal{G}) = \left(\frac{4}{27}\right) \cdot \left(\frac{1}{2}\right)^9$
- $\mathcal{G}\mathrm{AH}(\mathcal{G}) = \left(\frac{2}{3}\right) \cdot \left(\frac{2\sqrt{6}}{5}\right)^{12}$

Proof. With help of Table 5, we can easily find the result like Theorem 1. □

Table 4: An edge set of Hydroxychloroquine.

$\left(\mathrm{d}_{\mathcal{G}}(\mu), \mathrm{d}_{\mathcal{G}}(\nu)\right)$	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Number of Bounds	2	2	6	12	2

Corollary 6. Different multiplicative degree-based indies of chloroquine are given by (putting a $= \frac{-1}{2}$ and 2),

- $\mathrm{SC\Pi}(\mathcal{G}) = \left(\frac{1}{2}\right)^9 \cdot \left(\frac{1}{3}\right)^2 \cdot \left(\frac{1}{5}\right)^6$
- $\mathrm{PC\Pi}(\mathcal{G}) = \left(\frac{1}{2}\right)^{13} \cdot \left(\frac{1}{3}\right)^3$
- $\mathrm{H\Pi}_1(\mathcal{G}) = (2^{36}) \cdot (3^8) \cdot (5^{24})$

- $\mathrm{H\Pi}_2(\mathcal{G}) = (2^{52}) \cdot (3^{12})$

Theorem 7. If Theaflavin (zINC3978446) (see Figure 4) structure is denoted by $\mathcal{G}$ then,

- $\mathrm{MZ}_1^{\mathrm{a}}(\mathcal{G}) = (4^{10\mathrm{a}}) \cdot (5^{22\mathrm{a}}) \cdot (6^{14\mathrm{a}})$
- $\mathrm{MZ}_2^{\mathrm{a}}(\mathcal{G}) = (3^{60\mathrm{a}}) \cdot (2^{22\mathrm{a}})$
- $\mathrm{ABC}(\mathcal{G}) = \left(\frac{1}{2}\right)^{22} \cdot \left(\frac{2}{3}\right)^{19}$
- $\mathrm{GAH}(\mathcal{G}) = \left(\frac{\sqrt{3}}{2}\right)^{10} \cdot \left(\frac{2\sqrt{6}}{5}\right)^{22}$

Proof. Further, with the help of Table 5, we can easily find the result like Theorem 1. □

Table 5: An edge set of Theaflavin.

$\left(\mathrm{d}_{\mathcal{G}}(\mu), \mathrm{d}_{\mathcal{G}}(\nu)\right)$	(1,3)	(2,3)	(3,3)
Number of Bounds	10	22	14

Corollary 8. Different multiplicative degree-based indies of Theaflavin are given by (putting $\mathrm{a} = \frac{-1}{2}$ and 2),

- $\mathrm{SC\Pi}(\mathcal{G}) = \left(\frac{1}{4}\right)^5 \cdot \left(\frac{1}{5}\right)^{11} \cdot \left(\frac{1}{6}\right)^7$
- $\mathrm{PC\Pi}(\mathcal{G}) = \left(\frac{1}{3}\right)^{30} \cdot \left(\frac{1}{2}\right)^{11}$
- $\mathrm{H\Pi}_1(\mathcal{G}) = (4^{20}) \cdot (5^{44}) \cdot (6^{28})$
- $\mathrm{H\Pi}_2(\mathcal{G}) = (3^{120}) \cdot (2^{44})$

Conclusion

In this article, we looked at some topological aspects of some chemical structures that were used to slow the spread of COVID-19 and its epidemic. Remdesivir (GS-5734), chloroquine, hydroxychloroquine, and theaflavin are among the antiviral medications that are part of it. Our results can be used to develop new drugs and vaccines for the treatment of COVID-19, and the corresponding graphs of $\mathrm{MZ}_1\mathrm{a}(\mathcal{G})$ and $\mathrm{MZ}_2\mathrm{a}(\mathcal{G})$ are also plotted for study. The graphical repersentions are shown in the Figures 6,8,10, and 12. The calculated multiplicative degree-based topological can predict various properties and activities such as boiling point, entropy, enthalpy, acentric factor, critical pressure, and so on.

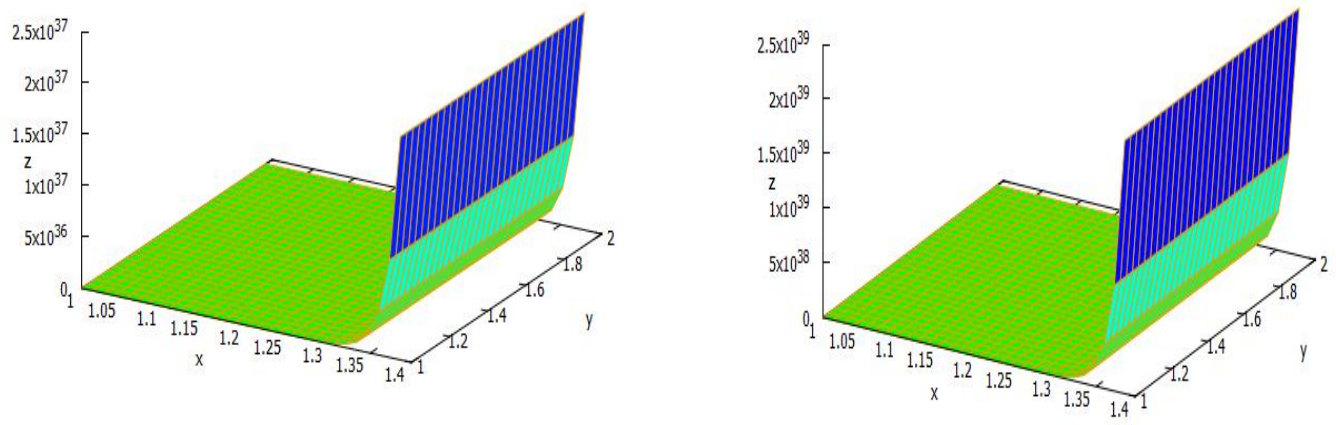


Figure 5: The graph of $MZ_1^a(\mathcal{G})$ and $MZ_2^a(\mathcal{G})$ for the antiviral drug remdesivir (GS-5734).

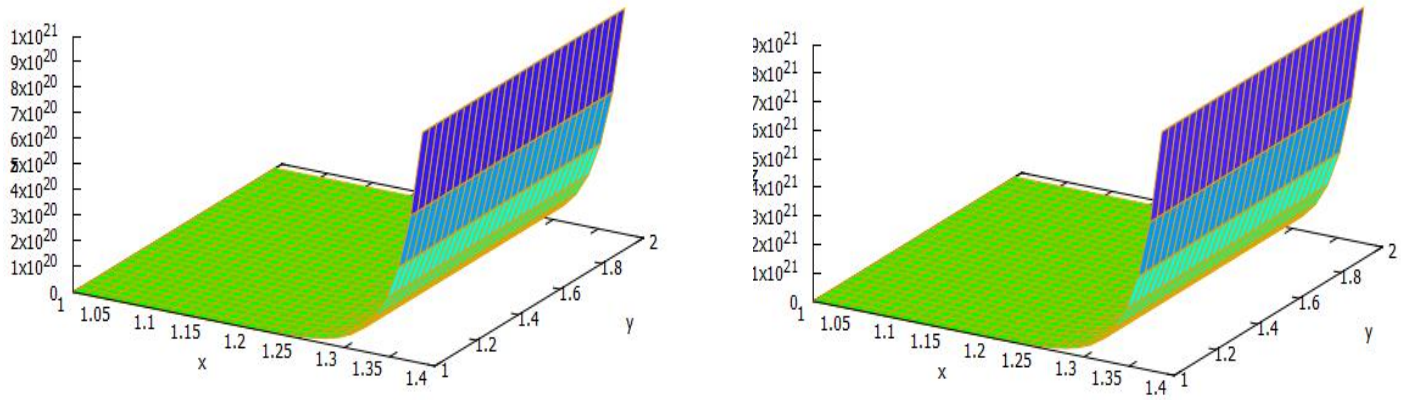


Figure 6: The graph of $MZ_1^a(\mathcal{G})$ and $MZ_2^a(\mathcal{G})$ for the antiviral drug chloroquine.

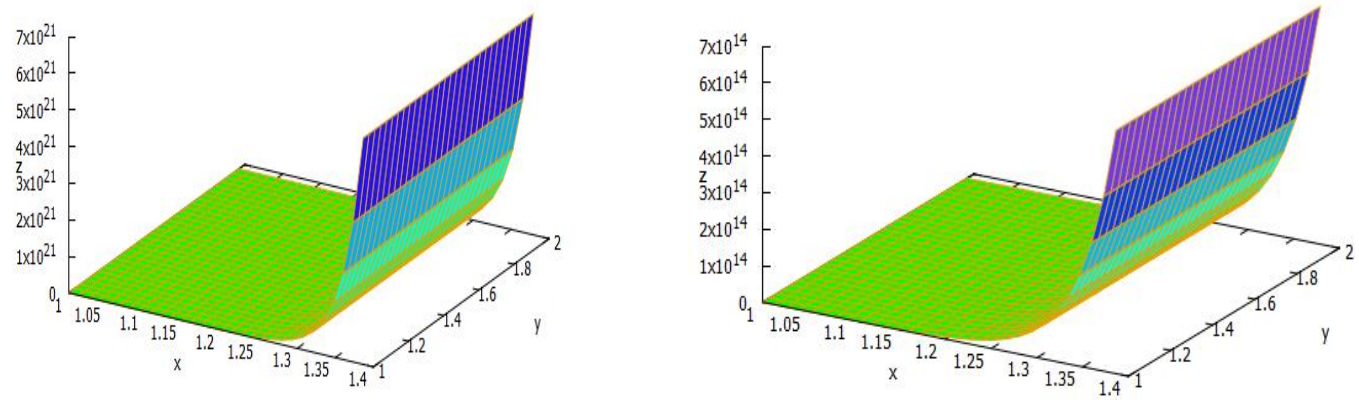


Figure 7: The graph of $MZ_1^a(\mathcal{G})$ and $MZ_2^a(\mathcal{G})$ for the antiviral drug hydroxychloroquine.

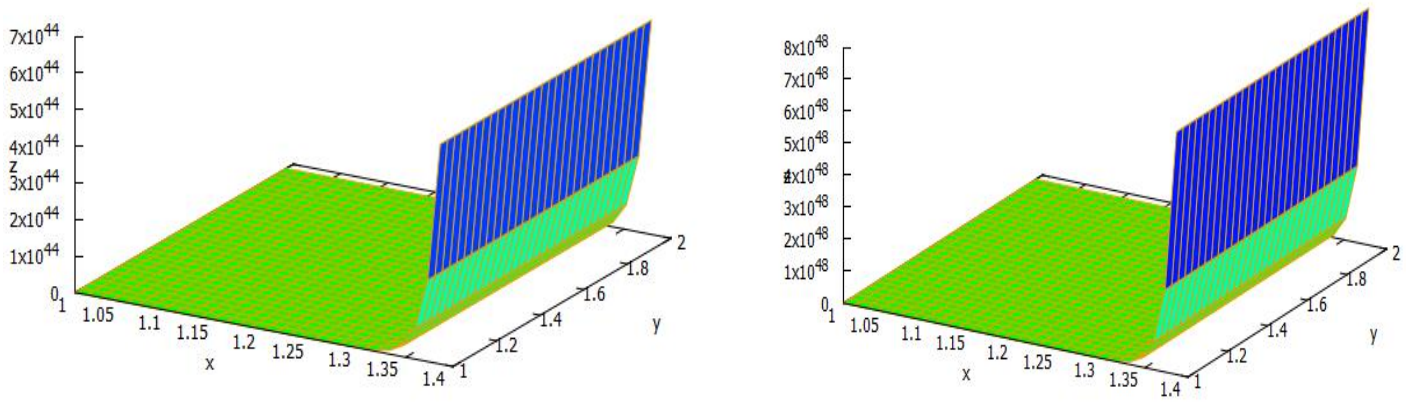


Figure 8: The graph of $\mathrm{MZ}_1^{\mathrm{a}}(\mathcal{G})$ and $\mathrm{MZ}_2^{\mathrm{a}}(\mathcal{G})$ for the antiviral drug theaflavin.

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Conflict of interest

The authors declare no conflict of interest.

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