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HYPER DOWNHILL INDICES AND THEIR POLYNOMIALS OF CERTAIN CHEMICAL DRUGS

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ABSTRACT
In this paper, we introduce the first and second hyper downhill indices and their polynomials of a graph. Also we determine these newly defined the first and second hyper downhill indices and their polynomials for some important chemical drugs such as chloroquine, hydroxychloroquins and remdesivir.

KEYWORDS: hyper downhill indices, hyper downhill polynomials, chemical structure.
Mathematics Subject Classification: 05C10, 05C69

1. INTRODUCTION

In this paper, G denotes a finite, simple, connected graph, V(G) and E(G) denote the vertex set and edge set of G. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u. A u-v path P in G is a sequence of vertices in G, starting with u and ending at V, such that consecutive vertices in P are adjacent, and no vertex is repeated. A path $\pi = v_1, v_2, \ldots v_{k+1}$ in G is a downhill path if for every i, $1 \le i \le k$, $d_G(v_i) \ge d_G(v_{i+1})$.

A vertex v is downhill dominates a vertex u if there exists a dowmhill path originated from u to v. The downhill neighborhood of a vertex v is denoted by $N_{dn}(v)$ and defined as: $N_{dn}(v)$ = {u: v downhill dominates u}. The downhill degree $d_{dn}(v)$ of a vertex v is the number of downhill neighbors of v [1].

The first and second downhill Zagreb indices were introduced by Al-Ahmadi et al. in [1] and defined as

$$DWM_1(G) = \sum_{uv \in E(G)} \left(d_{dn}(u)\right)^2.$$

$$DWM_2(G) = \sum_{uv \in E(G)} d_{dn}(u) d_{dn}(v).$$

Recently, some downhill indices were studied in [2, 3, 4, 5].

A new version of the first downhill index is defined as

$$DWM_1^*(G) = \sum_{uv \in E(G)} \left[d_{dn}(u) + d_{dn}(v)\right].$$

We now define the first and second hyper downhill indices as

$$HDW_1(G) = \sum_{uv \in E(G)} \left[d_{dn}(u) + d_{dn}(v)\right]^2$$

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$$HDW_2(G)=\sum_{uv\in E(G)}\left[d_{dn}(u)d_{dn}(v)\right]^2.$$

Considering the first and second hyper downhill indices, we propose the first and second hyper downhill polynomials of G, defined respectively as

$$DWM_1^*(G,x)=\sum_{uv\in E(G)} x^{d_{dn}(u)+d_{dn}(v)}$$

$$HDW_1(G,x)=\sum_{uv\in E(G)} x^{\left[d_{dn}(u)+d_{dn}(v)\right]^2}$$

$$HDW_2(G,x)=\sum_{uv\in E(G)} x^{\left[d_{dn}(u)d_{dn}(v)\right]^2}.$$

Recently, some topological indices were studied in [6-11].

In this paper, we compute the first and second hyper downhill indices and their polynomials of chloroquine, hydroxychloroquine and remdesivir.

2. RESULTS AND DISCUSSION: CHLOROQUINE

Chloroquine is an antiviral compound (drug) which was discovered in 1934 by H.Andersag. This drug is medication primarily used to prevent and treat malaria.

Let G be the chemical structure of chloroqine. This structure has 21 vertices and 23 edges.

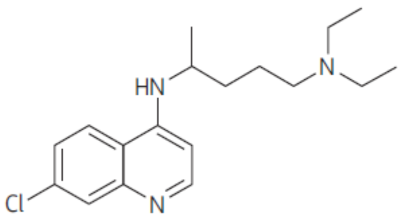

Figure 1. Chemical structure of chloroquine

From Figure 1, we obtain that

{($d_{dn}(u),d_{dn}(v)$) \ uv □ E(G)} has 13 edge set partitions.

$d_{dn}(u),d_{dn}(v)$ \ uv □ E(G)	(9,9)	(2,9)	(1,9)	(2,7)	(1,7)	(2,5)	(1,4)	(2,2)	(1,1)	(0,9)	(0,5)	(0,4)	(0,1)
Number of edges	2	2	1	1	2	1	1	4	1	2	2	2	2

We calculate the first downhill index and its polynomial of chloroquine as follows.

Theorem 1. Let G be the chemical structure of chloroquine. Then

(i) $DWM_1^*(G)=161$

(ii) $DWM_1^*(G,x)=2x^{18}+2x^{11}+1x^{10}+3x^9+2x^8+1x^7+3x^5+6x^4+1x^2+2x^1$

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Proof: By using the definitions and edge partition of G, we deduce

(i) $$DWM_1^*(G) = \sum_{uv \in E(G)} \left[d_{dn}(u) + d_{dn}(v)\right]$$

$$= (9+9)2 + (2+9)2 + (1+9)1 + (2+7)1 + (1+7)2 + (2+5)1 + (1+4)1$$
$$+ (2+2)4 + (1+1)1 + (0+9)2 + (0+5)2 + (0+4)2 + (0+1)2$$

By simplifying the above equation, we get desired result.

(ii) $$DWM_1^*(G,x) = \sum_{uv \in E(G)} x^{d_{dn}(u)+d_{dn}(v)}$$

$$= 2x^{9+9} + 2x^{2+9} + 1x^{1+9} + 1x^{2+7} + 2x^{1+7} + 1x^{2+5} + 1x^{1+4}$$
$$+4x^{2+2} + 1x^{1+1} + 2x^{0+9} + 2x^{0+5} + 2x^{0+4} + 2x^{0+1}$$

By simplifying the above equation, we get desired result.

We calculate the first hyper downhill index and its polynomial of chloroquine as follows.

Theorem 2. Let G be the chemical structure of chloroquine. Then

(i) $HDW_1(G) = 1587$

(ii) $HDW_1(G,x) = 2x^{324} + 2x^{121} + 1x^{100} + 3x^{81} + 2x^{64} + 1x^{49} + 3x^{25} + 6x^{16} + 1x^{4} + 2x^{1}$

Proof: By using the definitions and edge partition of G, we deduce

$$HDW_1(G) = \sum_{uv \in E(G)} \left[d_{dn}(u) + d_{dn}(v)\right]^2$$

$$= (9+9)^2 2 + (2+9)^2 2 + (1+9)^2 1 + (2+7)^2 1 + (1+7)^2 2 + (2+5)^2 1 + (1+4)^2 1$$
$$+ (2+2)^2 4 + (1+1)^2 1 + (0+9)^2 2 + (0+5)^2 2 + (0+4)^2 2 + (0+1)^2 2$$

By simplifying the above equation, we get desired result.

(ii) $$HDW_1(G,x) = \sum_{uv \in E(G)} x^{\left[d_{dn}(u)+d_{dn}(v)\right]^2}$$

$$= 2x^{(9+9)^2} + 2x^{(2+9)^2} + 1x^{(1+9)^2} + 1x^{(2+7)^2} + 2x^{(1+7)^2} + 1x^{(2+5)^2} + 1x^{(1+4)^2}$$
$$+4x^{(2+2)^2} + 1x^{(1+1)^2} + 2x^{(0+9)^2} + 2x^{(0+5)^2} + 2x^{(0+4)^2} + 2x^{(0+1)^2}$$

By simplifying the above equation, we get desired result.

We calculate the second hyper downhill index and its polynomial of chloroquine as follows.

Theorem 3. Let G be the chemical structure of chloroquine. Then

(i) $HDW_2(G) = 14326$

(ii) $HDW_2(G,x) = 2x^{6561} + 2x^{324} + 1x^{81} + 1x^{196} + 2x^{49} + 1x^{100} + 5x^{16} + 1x^{1} + 8$

Proof: By using the definitions and edge partition of G, we deduce

(i) $$HDW_2(G) = \sum_{uv \in E(G)} \left[d_{dn}(u) d_{dn}(v)\right]^2$$

$$= (9\times 9)^2 2 + (2\times 9)^2 2 + (1\times 9)^2 1 + (2\times 7)^2 1 + (1\times 7)^2 2 + (2\times 5)^2 1 + (1\times 4)^2 1$$
$$+ (2\times 2)^2 4 + (1\times 1)^2 1 + (0\times 9)^2 2 + (0\times 5)^2 2 + (0\times 4)^2 2 + (0\times 1)^2 2$$

By simplifying the above equation, we get desired result.

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(ii)
$$HDW_2(G,x) = \sum_{uv \in E(G)} x^{\left[d_{dn}(u) d_{dn}(v)\right]^2}$$
$$= 2x^{(9\times9)^2} + 2x^{(2\times9)^2} + 1x^{(1\times9)^2} + 1x^{(2\times7)^2} + 2x^{(1\times7)^2} + 1x^{(2\times5)^2} + 1x^{(1\times4)^2}$$
$$+4x^{(2\times2)^2} + 1x^{(1\times1)^2} + 2x^{(0\times9)^2} + 2x^{(0\times5)^2} + 2x^{(0\times4)^2} + 2x^{(0\times1)^2}$$

By simplifying the above equation, we get desired result.

3. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

Let H be the molecular structure of hydroxychloroquine. Clearly H has 22 vertices and 24 edges, see Figure 2.

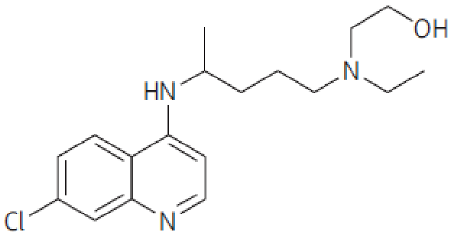

Figure 2

From Figure 2, we obtain that

{($d_{dn}(u), d_{dn}(v)$ \ uv □ E(H)} has 14 edge set partitions

$d_{dn}(u), d_{dn}(v)$ \ uv □ E(H)	Number of edges
(9,9)	2
(2,9)	2
(1,9)	1
(2,8)	2
(1,8)	1
(2,5)	1
(1,4)	1
(2,2)	5
(1,1)	1
(0,9)	2
(0,5)	2
(0,4)	2
(0,2)	1
(0,1)	1

We calculate the first downhill index and its polynomial of hydroxychloroquine as follows.

Theorem 4. Let H be the chemical structure of hydroxychloroquine. Then

(i) $DWM_1^*(H) = 170$

(ii) $DWM_1^*(H,x) = 2x^{18} + 2x^{11} + 3x^{10} + 3x^9 + 1x^7 + 3x^5 + 7x^4 + 2x^2 + 1x^1.$

Proof: By using the definitions and edge partition of H, we deduce

(i)
$$DWM_1^*(H) = \sum_{uv \in E(H)} \left[d_{dn}(u) + d_{dn}(v)\right]$$
$$= (9+9)2 + (2+9)2 + (1+9)1 + (2+8)2 + (1+8)1 + (2+5)1 + (1+4)1$$
$$+(2+2)5 + (1+1)1 + (0+9)2 + (0+5)2 + (0+4)2 + (0+2)1 + (0+1)1$$

By simplifying the above equation, we get desired result.

(ii)
$$DWM_1^*(H,x) = \sum_{uv \in E(H)} x^{d_{dn}(u) + d_{dn}(v)}$$

$$= 2x^{9+9} + 2x^{2+9} + 1x^{1+9} + 2x^{2+8} + 1x^{1+8} + 1x^{2+5} + 1x^{1+4}$$
$$+5x^{2+2} + 1x^{1+1} + 2x^{0+9} + 2x^{0+5} + 2x^{0+4} + 1x^{0+2} + 1x^{0+1}$$

By simplifying the above equation, we get desired result.

We calculate the first hyper downhill index and its polynomial of hydroxychloroquine as follows.

Theorem 5. Let H be the chemical structure of hydroxychloroquine. Then

(i) $HDW_1(H) = 1678$

(ii) $HDW_1(H,x) = 2x^{324} + 2x^{121} + 3x^{100} + 3x^{81} + 1x^{49} + 3x^{25} + 7x^{16} + 2x^{4} + 1x^{1}.$

Proof: By using the definitions and edge partition of H, we deduce

$$HDW_1(H) = \sum_{uv\in E(H)} \left[d_{dn}(u) + d_{dn}(v)\right]^2$$
$$= (9+9)^2 2 + (2+9)^2 2 + (1+9)^2 1 + (2+8)^2 2 + (1+8)^2 1 + (2+5)^2 1 + (1+4)^2 1$$
$$+(2+2)^2 5 + (1+1)^2 1 + (0+9)^2 2 + (0+5)^2 2 + (0+4)^2 2 + (0+2)^2 1 + (0+1)^2 1$$

By simplifying the above equation, we get desired result.

(ii)
$$HDW_1(H,x) = \sum_{uv\in E(H)} x^{\left[d_{dn}(u)+d_{dn}(v)\right]^2}$$
$$= 2x^{(9+9)^2} + 2x^{(2+9)^2} + 1x^{(1+9)^2} + 2x^{(2+8)^2} + 1x^{(1+8)^2} + 1x^{(2+5)^2} + 1x^{(1+4)^2}$$
$$+5x^{(2+2)^2} + 1x^{(1+1)^2} + 2x^{(0+9)^2} + 2x^{(0+5)^2} + 2x^{(0+4)^2} + 1x^{(0+2)^2} + 1x^{(0+1)^2}$$

By simplifying the above equation, we get desired result.

We calculate the second hyper downhill index and its polynomial of hydroxychloroquine as follows.

Theorem 6. Let H be the chemical structure of hydroxychloroquine. Then

(i) $HDW_2(H) = 14624$

(ii) $HDW_2(H,x) = 2x^{6561} + 2x^{324} + 1x^{81} + 2x^{256} + 1x^{64} + 1x^{100} + 6x^{16} + 1x^{1} + 8$

Proof: By using the definitions and edge partition of H, we deduce

(i)
$$HDW_2(H) = \sum_{uv\in E(H)} \left[d_{dn}(u) d_{dn}(v)\right]^2$$
$$= (9\times 9)^2 2 + (2\times 9)^2 2 + (1\times 9)^2 1 + (2\times 8)^2 2 + (1\times 8)^2 1 + (2\times 5)^2 1 + (1\times 4)^2 1$$
$$+(2\times 2)^2 5 + (1\times 1)^2 1 + (0\times 9)^2 2 + (0\times 5)^2 2 + (0\times 4)^2 2 + (0\times 2)^2 1 + (0\times 1)^2 1$$

By simplifying the above equation, we get desired result.

(ii)
$$HDW_2(H,x) = \sum_{uv\in E(H)} x^{\left[d_{dn}(u) d_{dn}(v)\right]^2}$$
$$= 2x^{(9\times 9)^2} + 2x^{(2\times 9)^2} + 1x^{(1\times 9)^2} + 2x^{(2\times 8)^2} + 1x^{(1\times 8)^2} + 1x^{(2\times 5)^2} + 1x^{(1\times 4)^2}$$
$$+5x^{(2\times 2)^2} + 1x^{(1\times 1)^2} + 2x^{(0\times 9)^2} + 2x^{(0\times 5)^2} + 2x^{(0\times 4)^2} + 1x^{(0\times 2)^2} + 1x^{(0\times 1)^2}$$

By simplifying the above equation, we get desired result.

4. RESULTS AND DISCUSSION: REMDESIVIR

Let R be the molecular structure of remdesivir. Clearly R has 41 vertices and 44 edges, see Figure 3.

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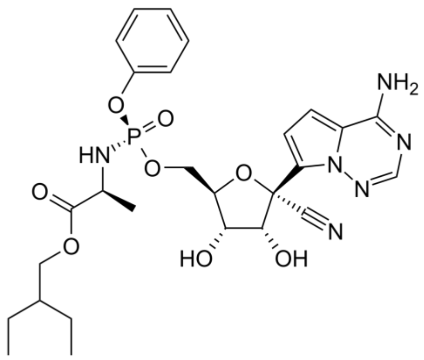

Figure 3

From Figure 3, we find that

{($d_{dn}(u), d_{dn}(v)$) \ uv □ E(R)} has 20 bond set partitions.

Table 3, Edge set partitions of remdesivir

$d_{dn}(u), d_{dn}(v)$ \uv∈E(R)	(9,19)	(7,19)	(9,9)	(2,9)	(1,9)	(7,7)	(1,7)	(6,6)
Number of edges	1	1	3	2	2	2	1	1
	(4,6)	(1,6)	(1,5)	(4,4)	(2,2)	(1,1)	(0,19)	(0,9)
	2	4	1	4	2	3	2	1
	(0,7)	(0,6)	(0,5)	(0,1)				
	3	4	3	2				

We calculate the first downhill index and its polynomial of remdesivir as follows.

Theorem 7. Let R be the chemical structure of remdesivir. Then

(i) $DWM_1^*(R) = 407$

(ii) $DWM_1^*(R,x) = 1x^{28} + 1x^{26} + 3x^{18} + 2x^{11} + 4x^{10} + 2x^{14} + 5x^{8} + 1x^{12} + 7x^{7}$
$+5x^{6} + 2x^{4} + 3x^{2} + 2x^{19} + 1x^{9} + 3x^{5} + 2x^{1}$

Proof: By using the definitions and edge partition of R, we deduce

(i) $$DWM_1^*(R) = \sum_{uv \in E(R)} \left[d_{dn}(u) + d_{dn}(v)\right]$$

$$= (9+19)1 + (7+19)1 + (9+9)3 + (2+9)2 + (1+9)2 + (7+7)2 + (1+7)1$$
$$+ (6+6)1 + (4+6)2 + (1+6)4 + (1+5)1 + (4+4)4 + (2+2)2 + (1+1)3$$
$$+ (0+19)2 + (0+9)1 + (0+7)3 + (0+6)4 + (0+5)3 + (0+1)2$$

By simplifying the above equation, we get desired result.

(ii) $$DWM_1^*(R,x) = \sum_{uv \in E(R)} x^{d_{dn}(u) + d_{dn}(v)}$$

$$= 1x^{9+19} + 1x^{7+19} + 3x^{9+9} + 2x^{2+9} + 2x^{1+9} + 2x^{7+7} + 1x^{1+7} + 1x^{6+6} + 2x^{4+6} + 4x^{1+6}$$
$$+ 1x^{1+5} + 4x^{4+4} + 2x^{2+2} + 3x^{1+1} + 2x^{0+19} + 1x^{0+9} + 3x^{0+7} + 4x^{0+6} + 3x^{0+5} + 2x^{0+1}$$

By simplifying the above equation, we get desired result.

We calculate the first hyper downhill index and its polynomial of remdesivir as follows.

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Theorem 8. Let R be the chemical structure of remdesivir. Then

(i) $HDW_1(R) = 5377$

(ii) $HDW_1(R,x) = 1x^{784} + 1x^{676} + 3x^{324} + 2x^{121} + 4x^{100} + 2x^{196} + 5x^{64} + 1x^{144} + 7x^{49}$
$+5x^{36} + 2x^{16} + 3x^{4} + 2x^{361} + 1x^{81} + 3x^{25} + 2x^{1}$

Proof: By using the definitions and edge partition of R, we deduce

(i) $HDW_1(R) = \sum_{uv \in E(R)} \left[d_{dn}(u) + d_{dn}(v)\right]^2$

$$= (9+19)^2 1 + (7+19)^2 1 + (9+9)^2 3 + (2+9)^2 2 + (1+9)^2 2 + (7+7)^2 2 + (1+7)^2 1$$
$$+ (6+6)^2 1 + (4+6)^2 2 + (1+6)^2 4 + (1+5)^2 1 + (4+4)^2 4 + (2+2)^2 2 + (1+1)^2 3$$
$$+ (0+19)^2 2 + (0+9)^2 1 + (0+7)^2 3 + (0+6)^2 4 + (0+5)^2 3 + (0+1)^2 2$$

By simplifying the above equation, we get desired result.

(ii) $HDW_1(R,x) = \sum_{uv \in E(R)} x^{\left[d_{dn}(u) + d_{dn}(v)\right]^2}$

$$= 1x^{(9+19)^2} + 1x^{(7+19)^2} + 3x^{(9+9)^2} + 2x^{(2+9)^2} + 2x^{(1+9)^2} + 2x^{(7+7)^2} + 1x^{(1+7)^2} + 1x^{(6+6)^2} + 2x^{(4+6)^2} + 4x^{(1+6)^2}$$

$$+ 1x^{(1+5)^2} + 4x^{(4+4)^2} + 2x^{(2+2)^2} + 3x^{(1+1)^2} + 2x^{(0+19)^2} + 1x^{(0+9)^2} + 3x^{(0+7)^2} + 4x^{(0+6)^2} + 3x^{(0+5)^2} + 2x^{(0+1)^2}$$

By simplifying the above equation, we get desired result.

We calculate the second hyper downhill index and its polynomial of remdesivir as follows.

Theorem 9. Let R be the chemical structure of remdesivir. Then

(i) $HDW_2(R) = 75950$

(ii) $HDW_2(R,x) = 1x^{29241} + 1x^{17689} + 3x^{6561} + 2x^{324} + 2x^{81} + 2x^{2401} + 1x^{49} + 1x^{1296} + 2x^{576} + 4x^{36}$
$+1x^{25} + 4x^{256} + 2x^{16} + 3x^{1} + 15x^{0}$

Proof: By using the definitions and edge partition of R, we deduce

(i) $HDW_2(R) = \sum_{uv \in E(R)} \left[d_{dn}(u) d_{dn}(v)\right]^2$

$$= (9\times19)^2 1 + (7\times19)^2 1 + (9\times9)^2 3 + (2\times9)^2 2 + (1\times9)^2 2 + (7\times7)^2 2 + (1\times7)^2 1$$
$$+ (6\times6)^2 1 + (4\times6)^2 2 + (1\times6)^2 4 + (1\times5)^2 1 + (4\times4)^2 4 + (2\times2)^2 2 + (1\times1)^2 3$$
$$+ (0\times19)^2 2 + (0\times9)^2 1 + (0\times7)^2 3 + (0\times6)^2 4 + (0\times5)^2 3 + (0\times1)^2 2$$

By simplifying the above equation, we get desired result.

(ii) $HDW_2(R,x) = \sum_{uv \in E(R)} x^{\left[d_{dn}(u) d_{dn}(v)\right]^2}$

$$= 1x^{(9\times19)^2} + 1x^{(7\times19)^2} + 3x^{(9\times9)^2} + 2x^{(2\times9)^2} + 2x^{(1\times9)^2} + 2x^{(7\times7)^2} + 1x^{(1\times7)^2} + 1x^{(6\times6)^2} + 2x^{(4\times6)^2} + 4x^{(1\times6)^2}$$
$$+ 1x^{(1\times5)^2} + 4x^{(4\times4)^2} + 2x^{(2\times2)^2} + 3x^{(1\times1)^2} + 2x^{(0\times19)^2} + 1x^{(0\times9)^2} + 3x^{(0\times7)^2} + 4x^{(0\times6)^2} + 3x^{(0\times5)^2} + 2x^{(0\times1)^2}$$

By simplifying the above equation, we get desired result.

5. CONCLUSION

In this paper, we have introduced the first and second hyper downhill indices and their corresponding polynomials of a graph. Also these newly defined the first and second hyper downhill indices and their polynomials for some important chemical drugs such as chloroquine, hydroxychloroquine and remdesivir are computed.

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