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Theoretical study of benzene ring embedded in P-type surface in 2d network using some new degree based topological indices *via* M-polynomial

Sabir Hussain[a] |Farkhanda Afzal[b] |Deeba Afzal[a,*] |Mohammad Reza Farahani[c] |Murat Cancan[d] |Süleyman Ediz[d]

[a]Department of Mathematics and Statistics, The University of Lahore, Lahore, 54000, Pakistan

[b]MCS, National University of Sciences and Technology, Islamabad, Pakistan

[c]Department of Applied Mathematics, Iran University of Science and Technology, Tehran, Iran

[d]Faculty of Education, Van Yuzuncu Yıl University, Zeve Campus, Tuşba, 65080, Van, Turkey

***Corresponding Author:**
Deeba Afzal
Email: deebafzal@gmail.com
Tel.: +923351572532

Algebraic polynomials play an important role in theoretical chemistry because these can reflect the properties of the chemical compound. M-polynomial is also an algebraic polynomial that is used to find the expressions of several degree dependent topological indices. These topological indices have the ability to explore the information store in the chemical molecule. In this work, we computed the M-polynomial and then obtained the degree-based topological indices for the benzene ring embedded in P-type-surface in 2D network. We also explored the results graphically.

KEYWORDS

Benzene ring embedded in P-type surface in 2D network; graph polynomial; M-polynomial; chemical molecule; degree dependent topological indices.

Introduction

The combination of chemistry with graph theory is called chemical graph theory. This interdisciplinary solves the questions that arise in chemistry with the help of graph theory. So, this branch has influenced both mathematics and chemistry. A molecule represents with the graphical tools is known as a chemical graph. The chemical graphs explore the valuable information that presents insight into the molecule [15]. The basic definitions about graphs are explained in the following citations [4, 16-34].

One of the great interesting topics in chemical graph theory is topological indices. Topological indices are a solitary number that describes some property of the molecular compound and are deduced from the chemical graph. There are many types of topological indices but degree-based topological indices are the most important. Numerous degree dependent topological indices have been discovered so far with many applications in QSAR and QSPR studies [7, 10, 13]. For chemical graphs, we calculate the index using a specific function [9]. But these are aslo obtained by using some graphical polynomial [8]. For definitions of some important indices see the following citation [12].

E. Deutsch and S. Klavžar, for the graph G, introduced the concept of M-polynomial in 2015 [6] and this polynomial is defined as:

$$M(G;x,y)=\sum_{\psi\leq k\leq j\leq\Psi} m_{kj}(G)x^k y^j.$$

Here min $\{d_v|v\in V(G)\}=\psi$, max $\{d_v|v\in V(G)\}=\Psi$ and the $n(E_{vu}(G))=m_{kj}(G)$ where $vu\in E(G)$ with the relation $\{d_v,d_u\}=$

$\{k, j\}$. Normally topological indices are computed by using definitions, but these are also calculated by using the M-Polynomial of the graph. Closed formulas of topological indices [3] are given in Table 1. M-polynomial and topological indices of various graphs have been previously computed [1, 2, 5, 11,14].

TABLE 1 Topological indices derive from $M(G; x, y) = h(x, y)$

$ABC[G]$	=	$D_x^{\frac{1}{2}} Q_{-2} J S_x^{\frac{1}{2}} S_y^{\frac{1}{2}} [h(x,y)]_{x=1}$
$GA[G]$	=	$2 S_x J D_x^{\frac{1}{2}} D_y^{\frac{1}{2}} [h(x,y)]_{x=1}$
$B_1[G]$	=	$(D_x + D_y + 2D_x Q_{-2} J)[h(x,y)]_{x=y=1}$
$B_2[G]$	=	$D_x Q_{-2} J (D_x + D_y)[h(x,y)]_{x=1}$
$HB_1[G]$	=	$(D_x^2 + D_y^2 + 2D_x^2 Q_{-2} J$ $+2D_x Q_{-2} J (D_x + D_y))[h(x,y)]_{x=y=1}$
$HB_2[G]$	=	$D_x^2 Q_{-2} J (D_x^2 + D_y^2)[h(x,y)]_{x=1}$
${}^m B_1[G]$	=	$S_x Q_{-2} J (L_x + L_y)[h(x,y)]_{x=1}$
${}^m B_2[G]$	=	$S_x Q_{-2} J (S_x + S_y)[h(x,y)]_{x=1}$
$H_b[G]$	=	$2 S_x Q_{-2} J (L_x + L_y)[h(x,y)]_{x=1}$

The operator used to find the degree based topological indices via M-polynomial are defined as:

$$D_x h(x,y) = x \frac{\partial}{\partial x} h(x,y), \quad D_y h(x,y) = y \frac{\partial}{\partial y} h(x,y),$$

$$S_x h(x,y) = \int_0^x \frac{h(t,y)}{t} dt, \quad S_y h(x,y) = \int_0^y \frac{h(x,t)}{t} dt,$$

$$L_x h(x,y) = h(x^2, y), \quad L_y h(x,y) = h(x, y^2),$$

$$J h(x,y) = h(x,x), \quad Q_\alpha h(x,y) = x^\alpha h(x,y),$$

$$D_x^{\frac{1}{2}} h(x,y) = \sqrt{x \frac{\partial}{\partial x} h(x,y)} \cdot \sqrt{h(x,y)},$$

$$D_y^{\frac{1}{2}} h(x,y) = \sqrt{y \frac{\partial}{\partial y} h(x,y)} \cdot \sqrt{h(x,y)},$$

$$S_x^{\frac{1}{2}} h(x,y) = \sqrt{\int_0^x \frac{g(t,y)}{t} dt} \cdot \sqrt{h(x,y)},$$

$$S_y^{\frac{1}{2}} h(x,y) = \sqrt{\int_0^y \frac{g(x,t)}{t} dt} \cdot \sqrt{h(x,y)}.$$

Benzene ring embedded in P-type surface in 2D network

Figure 1 shows the structure of benzene ring embedded in P-type surface in 2D network ($BP_{p,q}$), in which green and red dot represent the vertices of degree 2 and 3 respectively and brown, blue and red edges represent the edges having degree of end vertices (2,2), (2,3) and (3,3) respectively. In the present work, some degree based topological indices shown in Table 1 are computed by using the M-polynomial for the $BP_{p,q}$.

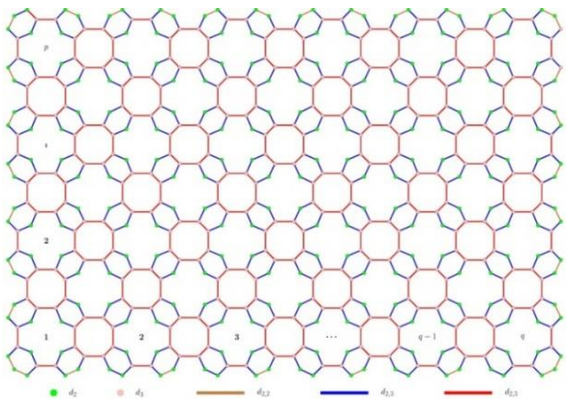


FIGURE 1 Benzene Ring Embedded in P-Type Surface in 2D Network $BP_{p,q}$

TABLE 2 Vertex partition of $BP_{p,q}$

d_v	2	3	Total vertices
Number of vertices	*4(2pq+9+q)*	*4(4pq-p-q)*	24pq

TABLE 3 Edge partition of $BP_{p,q}$

(d_v, d_u)	Number of edges
(2,2)	$4(p+q)$
(2,3)	$16pq$
(3,3)	$2(8pq-3p-3q)$
Total	$2(16pq-2p-2q)$

M-polynomial and topological indices of benzene ring embedded in P-type surface in 2D network

Theorem 3.1 *Let $BP_{p,q}$ be a benzene ring embedded in P-type surface in 2D network then M-polynomial of $BP_{p,q}$* [35] *is*

$$M[BP_{p,q};x,y] = 4(p+q)x^2y^2 + 16pqx^2y^3 + 2(8pq-3p-3q)x^3y^3.$$

Theorem 3.2 *Let $BP_{p,q}$ represents a benzene ring embedded in P-type surface in 2D network and $M[BP_{p,q};x,y] = 4(p+q)x^2y^2 + 16pqx^2y^3 + 2(8pq-3p-3q)x^3y^3$. Then*

1. $ABC[BP_{p,q}] = \frac{24\sqrt{2}+32}{3}pq + (2\sqrt{2}-4)(p+q)$.
2. $GA[BP_{p,q}] = \frac{32\sqrt{6}+80}{5}pq - 2(p+q)$.
3. $B_1[BP_{p,q}] = 400pq - 52(p+q)$.
4. $B_2[BP_{p,q}] = 624pq - 112(p+q)$.
5. $HB_1[BP_{p,q}] = 2544pq - 460(p+q)$.
6. $HB_2[BP_{p,q}] = 6480pq - 1600(p+q)$.
7. ${}^{m}B_1[BP_{p,q}] = \frac{1096}{105}pq + \frac{2}{7}(p+q)$.
8. ${}^{m}B_2[BP_{p,q}] = \frac{64}{9}pq + (p+q)$.
9. $H_b[BP_{p,q}] = \frac{2192}{105}ql + \frac{4}{7}(p+q)$.

Proof. Let $M[BP_{p,q};x,y] = g(x,y)$

The atom-bond connectivity index

$$S_y^{\frac{1}{2}}h(x,y) = \frac{4}{\sqrt{2}}(p+q)x^2y^2 + \frac{16}{\sqrt{3}}pqx^2y^3 + \frac{2}{\sqrt{3}}(8pq-3p-3q)x^3y^3,$$

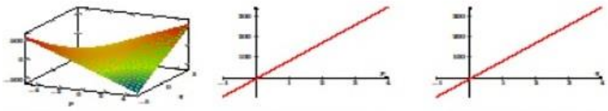
$$S_x^{\frac{1}{2}}S_y^{\frac{1}{2}}h(x,y) = 2(p+q)x^2y^2 + \frac{16}{\sqrt{6}}pqx^2y^3 + \frac{2}{3}(8pq-3p-3q)x^3y^3,$$

$$JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}h(x,y) = 2(p+q)x^4 + \frac{16}{\sqrt{6}}pqx^5 + \frac{2}{3}(8pq-3p-3q)x^6,$$

$$Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}h(x,y) = 2(p+q)x^2 + \frac{16}{\sqrt{6}}pqx^3 + \frac{2}{3}(8pq-3p-3q)x^4,$$

$$D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}h(x,y) = 2\sqrt{2}(p+q)x^2 + 8\sqrt{2}pqx^3 + \frac{4}{3}(8pq-3p-3q)x^4,$$

$$ABC[BP_{p,q}] = D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}[h(x,y)]_{x=1}, = \frac{24\sqrt{2}+32}{3}pq + (2\sqrt{2}-4)(p+q).$$



(a) 3D plot of $ABC(BP_{p,q})$ (b) Plot of $ABC(BP_{p,4})$ (c) Plot of $ABC(BP_{4,q})$

FIGURE 2 Graphs of atom-bond connectivity index of $BP_{p,q}$

The geometric arithmetic index

$$D_y^{\frac{1}{2}}h(x,y) = 4\sqrt{2}(p+q)x^2y^2 + 16\sqrt{3}pqx^2y^3 + 2\sqrt{3}(8pq-3p-3q)x^3y^3,$$

$$D_x^{\frac{1}{2}}D_y^{\frac{1}{2}}h(x,y) = 8(p+q)x^2y^2 + 16\sqrt{6}pqx^2y^3 + 6(8pq-3p-3q)x^3y^3,$$

$$JD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}h(x,y) = 8(p+q)x^4 + 16\sqrt{6}pqx^5 + 6(8pq-3p-3q)x^6,$$

$$S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}h(x,y) = 2(p+q)x^4 + \frac{16\sqrt{6}}{5}pqx^5 + (8pq-3p-3q)x^6,$$

$$2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}h(x,y) = 4(p+q)x^4 + \frac{32\sqrt{6}}{5}pqx^5 + 2(8pq-3p-3q)x^6,$$

$$GA[BP_{p,q}] = 2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}[h(x,y)]_{x=1}, = \frac{32\sqrt{6}+80}{5}pq - 2(p+q).$$

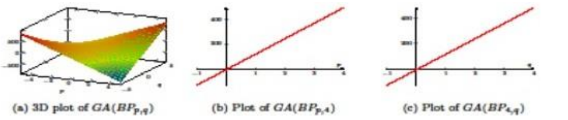


FIGURE 3 Graphs of GA index of $BP_{p,q}$

The first K Banhatti index

$$
\begin{aligned}
D_x h(x,y) &= 8(p+q)x^2y^2 + 32pqx^2y^3 \\
&\quad +6(8pq-3p-3q)x^3y^3, \\
D_y h(x,y) &= 8(p+q)x^2y^2 + 48pqx^2y^3 \\
&\quad +6(8pq-3p-3q)x^3y^3, \\
(D_x + D_y)h(x,y) &= 16(p+q)x^2y^2 + 80pqx^2y^3 \\
&\quad +12(8pq-3p-3q)x^3y^3, \\
Jh(x,y) &= 4(p+q)x^4 + 16pqx^5 \\
&\quad +2(8pq-3p-3q)x^6, \\
Q_{-2}Jh(x,y) &= 4(p+q)x^2 + 16pqx^3 \\
&\quad +2(8pq-3p-3q)x^4, \\
D_xQ_{-2}Jh(x,y) &= 8(p+q)x^2 + 48pqx^3 \\
&\quad +8(8pq-3p-3q)x^4, \\
2D_xQ_{-2}Jh(x,y) &= 16(p+q)x^2 + 96pqx^3 \\
&\quad +16(8pq-3p-3q)x^4, \\
(D_x + D_y + 2D_xQ_{-2}J)h(x,y) &= 32(p+q)x^2 + 176pqx^3 \\
&\quad +28(8pq-3p-3q)x^4, \\
B_1[BP_{p,q}] &= (D_x + D_y + 2D_xQ_{-2}J)[h(x,y)]_{x=y=1}, \\
B_1[BP_{p,q}] &= 400pq - 52(p+q).
\end{aligned}
$$

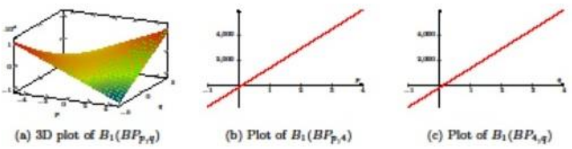


FIGURE 4 Graphs of first K Banhatti index of $BP_{p,q}$

The second K Banhatti index

$$
\begin{aligned}
J(D_x + D_y)h(x,y) &= 16(p+q)x^4 + 80pqx^5 \\
&\quad +12(8pq-3p-3q)x^6, \\
Q_{-2}J(D_x + D_y)h(x,y) &= 16(p+q)x^2 + 80pqx^3 \\
&\quad +12(8pq-3p-3q)x^4, \\
D_xQ_{-2}J(D_x + D_y)h(x,y) &= 32(p+q)x^2 + 240pqx^3 \\
&\quad +48(8pq-3p-3q)x^4, \\
B_2[BP_{p,q}] &= D_xQ_{-2}J(D_x + D_y)[h(x,y)]_{x=1}, \\
&= 624pq - 112(p+q).
\end{aligned}
$$

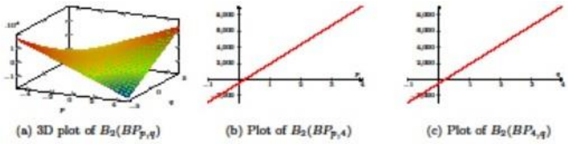
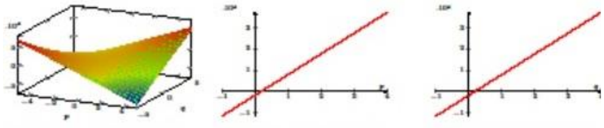


FIGURE 5 Graphs of second K Banhatti index of $BP_{p,q}$

The first K hyper Banhatti index

$$
\begin{aligned}
D_x^2 h(x,y) &= 16(p+q)x^2y^2 + 64pqx^2y^3 \\
&\quad +18(8pq-3p-3q)x^3y^3, \\
D_y^2 h(x,y) &= 16(p+q)x^2y^2 + 144pqx^2y^3 \\
&\quad +18(8pq-3p-3q)x^3y^3, \\
(D_x^2 + D_y^2)h(x,y) &= 32(p+q)x^2y^2 + 208pqx^2y^3 \\
&\quad +36(8pq-3p-3q)x^3y^3, \\
(D_x^2 + D_y^2)h(x,y)_{x=y=1} &= 496pq - 76(p+q), \\
D_x^2Q_{-2}Jh(x,y) &= 16(p+q)x^2 + 144pqx^3 \\
&\quad +32(8pq-3p-3q)x^4, \\
2D_x^2Q_{-2}Jh(x,y) &= 32(p+q)x^2 + 288pqx^3 \\
&\quad +64(8pq-3p-3q)x^4, \\
2D_x^2Q_{-2}Jh(x,y)_{x=1} &= 800pq - 160(p+q), \\
2D_xQ_{-2}J(D_x + D_y)h(x,y) &= 64(p+q)x^2 + 480pqx^3 \\
&\quad +96(8pq-3p-3q)x^4, \\
2D_xQ_{-2}J(D_x + D_y)[h(x,y)]_{x=1} &= 1248pq - 224(p+q), \\
HB_1[BP_{p,q}] &= (D_x^2 + D_y^2 + 2D_x^2Q_{-2}J + 2D_xQ_{-2}J(D_x + D_y))[h(x,y)]_{x=y=1}, \\
HB_1[BP_{p,q}] &= 2544pq - 460(p+q).
\end{aligned}
$$



(a) 3D plot of $HB_1(BP_{p,q})$ (b) Plot of $HB_1(BP_{p,4})$ (c) Plot of $HB_1(BP_{4,q})$

FIGURE 6 Graphs of first K hyper Banhatti index of $BP_{p,q}$

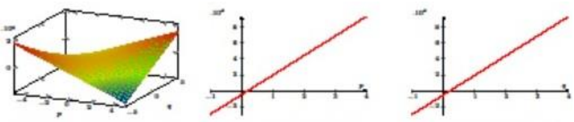
The second K hyper Banhatti index

$$J(D_x^2+D_y^2)h(x,y) = 32(p+q)x^4 + 208pqx^5 + 36(8pq-3p-3q)x^6,$$

$$Q_{-2}J(D_x^2+D_y^2)h(x,y) = 32(p+q)x^2 + 208pqx^3 + 36(8pq-3p-3q)x^4,$$

$$D_x^2Q_{-2}J(D_x^2+D_y^2)h(x,y) = 128(p+q)x^2 + 1872pqx^3 + 576(8pq-3p-3q)x^4,$$

$$HB_2[BP_{p,q}] = D_x^2Q_{-2}J(D_x^2+D_y^2)[h(x,y)]_{x=1},$$
$$= 6480-1600(p+q).$$



(a) 3D plot of $HB_2(BP_{p,q})$ (b) Plot of $HB_2(BP_{p,4})$ (c) Plot of $HB_2(BP_{4,q})$

FIGURE 7 Graphs of second K hyper Banhatti index of $BP_{p,q}$

Modified first K Banhatti index

$$L_xh(x,y) = 4(p+q)x^4y^2 + 16pqx^4y^3 + 2(8pq-3p-3q)x^6y^3,$$

$$L_yh(x,y) = 4(p+q)x^2y^4 + 16pqx^2y^6 + 2(8pq-3p-3q)x^3y^6,$$

$$(L_x+L_y)h(x,y) = 4(p+q)(x^4y^2+x^2y^4) + 16pq(x^4y^3+x^2y^6) + 2(8pq-3p-3q)(x^6y^3+x^3y^6),$$

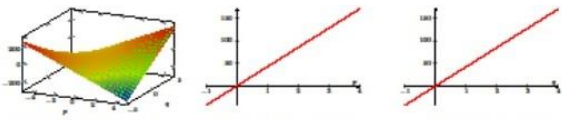
$$J(L_x+L_y)h(x,y) = 8(p+q)x^6 + 16pq(x^7+x^8) + 4(8pq-3p-3q)x^9,$$

$$Q_{-2}J(L_x+L_y)h(x,y) = 8(p+q)x^4 + 16pq(x^5+x^6) + 4(8pq-3p-3q)x^7,$$

$$S_xQ_{-2}J(L_x+L_y)h(x,y) = 2(p+q)x^4 + 16pq(\frac{x^5}{5}+\frac{x^6}{6}) + \frac{4}{7}(8pq-3p-3q)x^7,$$

$$^mB_1[BP_{p,q}] = S_xQ_{-2}J(L_x+L_y)[h(x,y)]_{x=1},$$

$$^mB_1[BP_{p,q}] = \frac{1096}{105}pq + \frac{2}{7}(p+q).$$



(a) 3D plot of $^mB_1(BP_{p,q})$ (b) Plot of $^mB_1(BP_{p,4})$ (c) Plot of $^mB_1(BP_{4,q})$

FIGURE 8 Graphs of modified first K Banhatti index of $BP_{p,q}$

Modified second K Banhatti index

$$S_xh(x,y) = 2(p+q)x^2y^2 + 2pqx^2y^3 + \frac{2}{3}(8pq-3p-3q)x^3y^3,$$

$$S_yh(x,y) = 2(p+q)x^2y^2 + \frac{16}{3}pqx^2y^3 + \frac{2}{3}(8pq-3p-3q)x^3y^3,$$

$$(S_x+S_y)h(x,y) = 4(p+q)x^2y^2 + \frac{40}{3}pqx^2y^3 + \frac{4}{3}(8pq-3p-3q)x^3y^3,$$

$$J(S_x+S_y)h(x,y) = 4(p+q)x^4 + \frac{40}{3}pqx^5, + \frac{4}{3}(8pq-3p-3q)x^6$$

$$Q_{-2}J(S_x+S_y)h(x,y) = 4(p+q)x^2 + \frac{40}{3}pqx^3 + \frac{4}{3}(8pq-3p-3q)x^4,$$

$$S_xQ_{-2}J(S_x+S_y)h(x,y) = 2(p+q)x^2 + \frac{40}{9}pqx^3 + \frac{1}{3}(8pq-3p-3q)x^4,$$

$$^mB_2[BP_{p,q}] = S_xQ_{-2}J(S_x+S_y)[h(x,y)]_{x=1},$$

$$^mB_2[BP_{p,q}] = \frac{64}{9}pq + (p+q).$$

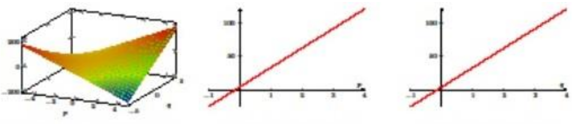


FIGURE 9 Graphs of modified second K Banhatti index of $BP_{p,q}$

Harmonic K Banhatti index

$$\begin{aligned} 2S_xQ_{-2}J(L_x + L_y)h(x,y) &= 4(p+q)x^4 + 32pq(\frac{x^5}{5} + \frac{x^6}{6}) \\ &+ \frac{8}{7}(8pq - 3p - 3q)x^7, \\ H_b[BP_{p,q}] &= 2S_xQ_{-2}J(L_x + L_y)[g(x,y)]_{x=1}, \\ &= \frac{2192}{105}pq + \frac{4}{7}(p+q). \end{aligned}$$

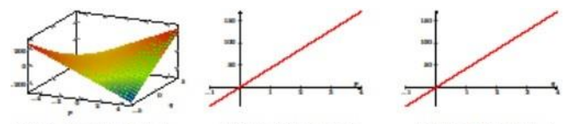


Figure 10 Graphs of Harmonic K Banhatti index of $BP_{p,q}$

Conclusion

$M(BP_{p,q}; x, y)$ and some degree dependent topological indices were computed in the present article. These indices have valuable information for the benzene ring embedded in P-type surface in 2D network and are the best predictor about the physical, chemical and biological behavior of the chemical molecule. Results obtained were also presented graphically.

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Orcid:

Sabir Hussain: https://orcid.org/0000-0002-2441-0077
Farkhanda Afzal: https://orcid.org/0000-0001-5396-7598
Deeba Afzal: https://orcid.org/0000-0001-5268-7260
Mohammad Reza Farahani: https://orcid.org/0000-0003-2969-4280
Murat Cancan: https://orcid.org/0000-0002-8606-2274
Süleyman Ediz: https://orcid.org/0000-0003-0625-3634

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