AIMS Mathematics, 8(9): 21668–21682.
DOI: 10.3934/math.20231105
Received: 01 March 2023
Revised: 19 June 2023
Accepted: 25 June 2023
Published: 07 July 2023

http://www.aimspress.com/journal/Math

Research article

On *ABC* energy and its application to anticancer drugs

Alaa Altassan[1], **Muhammad Imran**[2] **and Bilal Ahmad Rather**[2,*]

[1] Department of Mathematics, Faculty of Science, King Abdulaziz University, P.O. Box 80203, Jeddah 21589, Saudi Arabia

[2] Department of Mathematical Sciences, College of Science, United Arab Emirates University, Al Ain 15551, Abu Dhabi, United Arab Emirates

* **Correspondence:** Email: bilalahmadrr@gmail.com.

Abstract: For a simple connected graph Γ with node set $V(\Gamma) = \{w_1, w_2, \ldots, w_n\}$ and degree sequence d_i, the atom-bond connectivity (ABC) matrix of Γ has an (ij)-th entry $\sqrt{\frac{d_i+d_j-2}{d_i d_j}}$ if w_i is adjacent to w_j and 0, otherwise. The multiset of all eigenvalues of ABC matrix is known as the ABC spectrum and their absolute sum is known as the ABC energy of Γ. Two graphs of same order are known as ABC equienergetic if they have the same ABC energy but share different ABC spectrum. We describe the ABC spectrum of some special graph operations and as an application, we construct the ABC equienergetic graphs. Further, we give linear regression analysis of ABC index/energy with the physical properties of anticancer drugs. We observe that they are better correlated with ABC-energy.

Keywords: adjacency matrix; ABC matrix; atom-bond connectivity; equienergetic graphs; correlation
Mathematics Subject Classification: 05C50, 05C92, 92E10, 15A18

1. Introduction

Throughout this paper all graphs will be assumed to be finite, connected and simple. A graph Γ consists of node set $V(\Gamma) = \{w_1, w_2, \ldots, w_n\}$ and edge set $E(\Gamma)$. Furthermore $|V(\Gamma)|$ is the *order* n and $|E(\Gamma)|$ is the *size* m of Γ. We write $w \sim u$ if w is adjacent to u. The neighbourhood of w denoted by $N(w)$ is the set of nodes adjacent to v. The notation $d_\Gamma(w_i)$ (d_{w_i} or d_i) denotes the degree of w_i. A graph Γ is *r-regular* if $d_w = r$, for every w. For other graph terminology and definitions we follow [3].

The adjacency matrix $A(\Gamma) = (a_{ij})$ of Γ is a square matrix of order n, with $a_{ij} = 1$, if $w_i \sim w_j$, and $a_{ij} = 0$, otherwise. The adjacency matrix $A(\Gamma)$ is real symmetric, so its eigenvalues are real, denoted by $\zeta_1(\Gamma) \geq \zeta_2(\Gamma) \geq \cdots \geq \zeta_n(\Gamma)$ and is known as the adjacency spectrum (or spectrum) of Γ. The energy

of Γ is defined as

$$\mathbb{E}(\Gamma) = \sum_{i=1}^{n} |\zeta_i(\Gamma)|.$$

The spectral parameter $\mathbb{E}(\Gamma)$ is widely studied parameter since it is related to the π-electron energy of hydrocarbons in mathematical chemistry. Two graphs with same order are known as equienergetic (or adjacency equienergetic) if they share the same energy but have the different adjacency spectrum. For more about the energy $\mathbb{E}(\Gamma)$ of Γ, we refer to [17]. If an eigenvalue θ of matrix M is repeated k times we say θ is the eigenvalue of M with multiplicity (order) k and denote it by $\theta^{[k]}$. Further readings about $A(\Gamma)$ can be seen in [2, 8].

The ABC index is a topological index defined in [10] as following

$$ABC = \sum_{w_i w_j \in E(\Gamma)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}.$$

In [10] the ABC index was shown to be correlated to the heat formation of alkanes. In [15] the authors proved that the ABC index can generate the heat of formation with sound accuracy comparable to that of high-level ab into and DFT (MP2, B3LYP) quantum chemical calculations. More mathematical literature of ABC index can be found in [4, 9, 12, 16]. The ABC matrix of graph Γ is a square matrix of order n and is defined as

$$ABC(\Gamma) = \begin{cases} \sqrt{\dfrac{d_i + d_j - 2}{d_i d_j}} & \text{if} \quad w_i \sim w_j, \\ 0 & \text{otherwise.} \end{cases}$$

Estrada [11] introduced an ABC matrix which is related to atom-bond connectivity (ABC index) of Γ.

Let $\theta_1 \geq \theta_2 \geq \cdots \geq \theta_n$ be the ABC eigenvalues of Γ, where θ_1 is the ABC spectral radius of Γ. The ABC energy $EABC$ [11] of Γ is defined as

$$EABC(\Gamma) = \sum_{i=1}^{n} |\theta_i|.$$

The graphs Γ_1 and Γ_2 of order n are said to be ABC equienergetic if $EABC(\Gamma_1) = EABC(\Gamma_2)$ while they share the distinct ABC spectrum. The ABC spectral parameters like energy were studied in [5], ABC spectral radius in [14] and other spectral properties in [6, 7, 13, 21, 22].

K_n is the complete graph, $K_{a,b}$ is the complete bipartite graph, $\mathcal{P}_n$ is the path graph and C_n is the cycle graph. For terminology and notations not defined here, we refer the readers to [8, 27].

Ramane et al. [26] established several results concerning the equienergetic graphs. Li et al. [22] introduced the ABC matrix index of graphs and related with the ABC energy. Gao et al. [13] characterized the extremal ABC energy of trees. Chen [5, 6] obtained results about distinct ABC eigenvalues and results about ABC spectral radius of trees.

The present report is organized as follows: In Section 2 we discuss the ABC spectrum of the Γ-join of regular graphs and the lexicographic product of graphs. In Section 3 we presents results on the ABC equienergetic graphs. In Section 4 we discusses applications of ABC energy/index to physical properties of anticancer drugs and gives their linear regression analysis.

2. The ABC eigenvalues of the Γ-join of regular graphs

The Γ-join $\Gamma[\Gamma_1, \Gamma_2, \ldots, \Gamma_n]$ of graphs $\Gamma_1, \Gamma_2, \ldots, \Gamma_n$ with underlying graph Γ is the graph $\bigcup_{i=1}^{n} \Gamma_i$ together with the edges from each node of Γ_i to every node of Γ_j when $w_i \sim w_j$ in Γ. Thus, the join of two graphs $\Gamma_1 \sqcup \Gamma_2$ is the Γ-join $K_2[\Gamma_1, \Gamma_2]$.

Let M be a partitioned block matrix and Q be the matrix with entries as the average row sums (column sums) of the blocks of M. Q is know as the quotient matrix and if the row sums (columns sums) of each block in M are some constants then the partition is regular (equitable) and we say Q is regular (equitable) quotient matrix (see [2]). The eigenvalue of M interlace the eigenvalues of Q. However, for regular partitions the spectrum (see [2, 8]) of Q is contained in the spectrum of M.

Our first result gives the ABC spectrum of $\Gamma[\Gamma_1, \Gamma_2, \ldots, \Gamma_n]$ where Γ_i are regular graphs in terms of the adjacency spectrum of Γ_i and the spectrum of an auxiliary matrix.

Theorem 2.1. *Let Γ be a connected graph with nodes $\{w_1, w_2, \ldots, w_n\}$ and let Γ_i be an r_i regular graphs of orders n_i having adjacency eigenvalues $\zeta_{i,1} = r_i \geq \zeta_{i,2} \geq \cdots \geq \zeta_{i,n_i}$. Then, the ABC spectrum of $\Gamma[\Gamma_1, \Gamma_2, \ldots, \Gamma_n]$ consists of the eigenvalues $\frac{\sqrt{2r_i'-2}}{r_i'}\zeta_{i,k}$ where $k = 2, 3, \ldots, n_i$ and $r_i' = r_i + \sum_{w_j \in N_\Gamma(w_i)} n_j$, for $i = 1, 2, \ldots, n$. The other ABC eigenvalues of $\Gamma[\Gamma_1, \Gamma_2, \ldots, \Gamma_n]$ are the eigenvalues of the following regular quotient matrix*

$$\begin{pmatrix} \frac{r_1}{r_1'}\sqrt{2r_1'-2} & n_2 q_{1,2} & \ldots & n_n q_{1,n} \\ n_1 q_{2,1} & \frac{r_2}{r_2'}\sqrt{2r_2'-2} & \ldots & n_n q_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ n_1 q_{n,1} & n_2 q_{n,2} & \ldots & \frac{r_n}{r_n'}\sqrt{2r_n'-2} \end{pmatrix}, \tag{2.1}$$

where $q_{ij} = q_{ji} = \sqrt{\frac{r_i'+r_j'-2}{r_i' r_j'}}$ if w_i is adjacent to w_j and 0 otherwise.

Proof. Let $V(\Gamma_i) = \{w_{i1}, \ldots, w_{in_i}\}$ be the node set of Γ_i, for $i = 1, 2, \ldots, n$. Let $\mathbb{H} = \Gamma[\Gamma_1, \ldots, \Gamma_n]$ be the Γ-join of r_i regular graphs Γ_i, where $i = 1, 2, \ldots, n$. Since Γ_i is r_i regular, the degree of nodes $w_{ij} \in V(\mathbb{H})$ for $1 \leq i \leq n$ and $1 \leq j \leq n_i$ is equal to the degree of j-th node in Γ_j plus the sum of order of Γ_j's in $\mathbb{H}$ which neighbours the node w_j in Γ, that is, $d_{\mathbb{H}}(w_{ij}) = r_i + \sum_{w_j \in N_\Gamma(w_i)} n_i$. Labelling the nodes of $\mathbb{H}$ from Γ_1 to Γ_n, the ABC matrix can be put as

$$ABC(\mathbb{H}) = \begin{pmatrix} \frac{\sqrt{2r_1'-2}}{r_1'}A(\Gamma_1) & a_{12} & \ldots & a_{1n} \\ a_{21} & \frac{\sqrt{2r_2'-2}}{r_2'}A(\Gamma_2) & \ldots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \ldots & \frac{\sqrt{2r_n'-2}}{r_n'}A(\Gamma_n) \end{pmatrix},$$

where $a_{ij} = \sqrt{\frac{r_i'+r_j'-2}{r_i' r_j'}} J_{n_i \times n_j}$ if w_i is adjacent to w_j in Γ and 0 otherwise. J is the matrix with all entries equal to 1 and $r_i' = r_i + \sum_{w_j \in N_\Gamma(w_i)} n_j$, for $i = 1, 2, \ldots, n$.

For a regular graph Γ_i, the vector $\mathcal{E}_{n_i} = (\underbrace{1, 1, \ldots, 1}_{n_i})^T$ is the eigenvector of the eigenvalue r_i of $A(\Gamma_i)$ and the remaining eigenvectors of $A(\Gamma_i)$ are orthogonal to it. Let ζ_{ik}, $2 \leq k \leq n_i$ be an arbitrary eigenvalue of $A(\Gamma_i)$ with the eigenvector $\mathcal{X} = (b_{i1}, b_{i2}, \ldots, b_{in_i})^T$ such that $\mathcal{E}_{n_i}^T X = 0$. Thus, $\mathcal{X}$ can be considered as a mapping defined on $V(\Gamma_i)$ relating w_{ij} to b_{ij}, that is, $\mathcal{X}(w_{ij}) = b_{ij}$ for $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, n_i$. Consider the new vector $\mathcal{Y} = (c_1, c_2, \ldots, c_n)^T$, where

$$c_j = \begin{cases} b_{ij} & \text{if } w_{ij} \in V(\Gamma_i), \\ 0 & \text{otherwise.} \end{cases}$$

Since $\mathcal{E}_{n_i}^T \mathcal{X} = 0$ the coordinates of $\mathcal{Y}$ related to nodes in $\bigcup_{j \neq i} w_j$ of $\mathbb{H}$ are zeros.

$$ABC(\mathbb{H})\mathcal{Y} = \begin{pmatrix} \sqrt{\frac{r_1'+r_i'-2}{r_1'r_i'}} J_{n_1 \times n_i}\mathcal{X} \\ \vdots \\ \sqrt{\frac{r_{i-1}'+r_i'-2}{r_{i-1}'r_i'}} J_{n_{i-1} \times n_i}\mathcal{X} \\ \frac{\sqrt{2r_i'-2}}{r_i'} A(\Gamma_i)X \\ \sqrt{\frac{r_{i+1}'+r_i'-2}{r_{i+1}'r_i'}} J_{n_{i+1} \times n_i}\mathcal{X} \\ \vdots \\ \sqrt{\frac{r_n'+r_i'-2}{r_n'r_i'}} J_{n_n \times n_i}\mathcal{X} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \frac{\sqrt{2r_i'-2}}{r_i'}\zeta_{ik}\mathcal{X} \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \left(\frac{\sqrt{2r_1'-2}}{r_1'}\zeta_{ik} \right) \mathcal{Y}.$$

This proves that $\mathcal{Y}$ is the eigenvector of $ABC(\mathbb{H})$ related to the eigenvalue $\frac{\sqrt{2r_1'-2}}{r_1'}\zeta_{ik}$ for each eigenvalue ζ_{ik}, $2 \leq k \leq n_i$, of $A(\Gamma_i)$. So, it implies that with $1 \leq i \leq n$ and $2 \leq k \leq n_i$, $\frac{\sqrt{2r_1'-2}}{r_1'}\zeta_{ik}$ is an eigenvalue of $ABC(\mathbb{H})$. Thus, we obtain $\sum_{i=1}^{n} n_i - n$ eigenvalues of $ABC(\mathbb{H})$. The other n, ABC eigenvalues of $\mathbb{H}$ are the eigenvalues of the following regular quotient matrix.

$$\begin{pmatrix} \frac{r_1}{r_1'}\sqrt{2r_1'-2} & n_2 q_{1,2} & \ldots & n_n q_{1,n} \\ n_1 q_{2,1} & \frac{r_2}{r_2'}\sqrt{2r_2'-2} & \ldots & n_n q_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ n_1 q_{n,1} & n_2 q_{n,2} & \ldots & \frac{r_n}{r_n'}\sqrt{2r_n'-2} \end{pmatrix}.$$

This completes the proof. □

The *lexicographic product* $\Gamma[H_1]$ of two graphs Γ and H_1 is the graph with node set $V(\Gamma) \times V(H_1)$ and $(c, x)(d, y) \in E(\Gamma[H_1])$ whenever $cd \in E(\Gamma)$ or $c = d$ and $xy \in E(H_1)$. Clearly, the lexicographic product $\Gamma[H_1]$ of Γ and H_1 is the Γ-join $\Gamma[H_1, H_1, \ldots, H_1]$. That is, $\Gamma[H_1] = \Gamma[H_1, H_1, \ldots, H_1]$. Taking, $\Gamma_i = H_1$ for all i in Theorem 2.1, we obtain the following result which gives the ABC spectrum of the lexicographic product $\Gamma[H_1]$.

Corollary 2.2. *Let Γ be a connected graph of order n and let H_1 be a connected r regular graph of order n_1. Let $\zeta_1(H_1) \geq \zeta_2(H_1) \geq \ldots \geq \zeta_{n_1}(H_1)$ be the eigenvalues of $A(H_1)$. The ABC spectrum*

of the lexicographic product $\Gamma[H_1] = \Gamma[H_1, \ldots, H_1]$ *consists of the eigenvalues* $\frac{\sqrt{2r_i'-2}}{r_i'}\zeta_k(H_1)$*, where* $r_i' = r + n_1 \sum_{v \in N_\Gamma(w_i)}$*, for* $i = 1, 2, \ldots, n$ *and* $k = 1, 2, \ldots, n_1 - 1$*. The other* n *eigenvalues of* $\Gamma[H_1]$ *are the eigenvalues of the following regular quotient matrix*

$$\begin{pmatrix} \frac{r}{r_1'}\sqrt{2r_2'-2} & n_2 q_{1,2} & \ldots & n_n q_{1,n} \\ n_1 q_{2,1} & \frac{r}{r_1'}\sqrt{2r_1'-2} & \ldots & n_n q_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ n_1 q_{n,1} & n_2 q_{n,2} & \ldots & \frac{r}{r_n'}\sqrt{2r_n'-2} \end{pmatrix}, \tag{2.2}$$

where $q_{ij} = q_{ji} = \sqrt{\frac{r_i'+r_j'-2}{r_i' r_j'}}$ *if* $w_i \sim w_j$ *and* 0 *otherwise.*

As an application of Theorem 2.1, we obtain the *ABC* eigenvalues of the join of regular graphs Γ_1 and Γ_2.

Corollary 2.3. *Let* Γ_1 *and* Γ_2 *be* r_1 *and* r_2 *regular graphs with orders* n_1 *and* n_2*, respectively. Let* $\zeta_1 = r_1, \zeta_2, \ldots, \zeta_{n_1}$ *and* $\mu_1 = r_2, \mu_2, \ldots, \mu_{n_2}$ *be the adjacency eigenvalues of* Γ_1 *and* Γ_2*, respectively. Then the ABC spectrum of* $\Gamma_1 \sqcup \Gamma_2$ *consists of eigenvalues* $\frac{\sqrt{2r_1'-2}}{r_1'}\zeta_i$ *and* $\frac{\sqrt{2r_2'-2}}{r_2'}\mu_j$ *with multiplicities* $n_1 - 1$ *and* $n_2 - 1$ *respectively, where* $r_1' = r_1 + n_2$ *and* $r_2' = r_2 + n_1$*. The remaining two ABC eigenvalues of* $\Gamma_1 \sqcup \Gamma_2$ *are the eigenvalues of the matrix given below*

$$\begin{pmatrix} \frac{r_1}{r_1'}\sqrt{2r_1'-2} & n_2\sqrt{\frac{r_1'+r_2'-2}{r_1' r_2'}} \\ n_1\sqrt{\frac{r_1'+r_2'-2}{r_1' r_2'}} & \frac{r_2}{r_2'}\sqrt{2r_2'-2} \end{pmatrix}. \tag{2.3}$$

From Corollary 2.3, we obtain the ABC spectrum of $K_{a,n-a} = \overline{K}_a \sqcup \overline{K}_{n-a}$, the complete split graph $CS_{\omega,n-\omega} = K_\omega \sqcup \overline{K}_{n-\omega}$, the graph $K_n - e = K_{n-2} \sqcup \overline{K}_2$ obtained from K_n by deleting an edge and many other graphs.

The double star $D(\alpha, \beta)$ is the tree of order $n = \alpha + \beta + 2$, obtained by adding an edge between the nodes of maximum degrees of the stars $K_{1,\alpha}$ and $K_{1,\beta}$. The complement of Γ is denoted by $\overline{\Gamma}$. As an application of Theorem 2.1, we can find the *ABC* spectrum of the double star and its complement.

Proposition 2.4. *Let* α, β *be the positive integers such that* $\alpha + \beta = n - 2$*. Then, the following holds.*

(i) *The ABC eigenvalues of* $D(\alpha, \beta)$ *are* 0 *with order* $n - 2$ *and the zeros of the following polynomial*

$$x^4 - x^2\left(\frac{\alpha^2}{\alpha+1} + \frac{\alpha}{(\alpha+1)(\beta+1)} + \frac{\beta}{(\alpha+1)(\beta+1)} + \frac{\beta^2}{\beta+1}\right) + \frac{\alpha^2\beta^2}{(\alpha+1)(\beta+1)}.$$

(ii) *The ABC eigenvalues of* $\overline{D}(\alpha, \beta)$ *are* $-\sqrt{\frac{2n-6}{n-2}}$ *with order* $n - 2$ *and the eigenvalues of matrix* (2.4).

Proof. It is clear that $D(\alpha,\beta) = \mathcal{P}_4[K_1, \overline{K}_\alpha, \overline{K}_\beta, K_1]$. By using Theorem 2.1 and the adjacency spectrum of $\overline{K}_n$ is $\{0^n\}$ we obtain the *ABC* eigenvalue 0 with order $\alpha+\beta-2$. The other four *ABC* eigenvalues of $D(\alpha,\beta)$ are the eigenvalues of the following matrix

$$\begin{pmatrix} 0 & \sqrt{\frac{\alpha}{\alpha+1}} & 0 & 0 \\ \alpha\sqrt{\frac{\alpha}{\alpha+1}} & 0 & \sqrt{\frac{\alpha+\beta}{(\alpha+1)(\beta+1)}} & 0 \\ 0 & \sqrt{\frac{\alpha+\beta}{(\alpha+1)(\beta+1)}} & 0 & \beta\sqrt{\frac{\beta}{\beta+1}} \\ 0 & 0 & \sqrt{\frac{\beta}{\beta+1}} & 0 \end{pmatrix},$$

and its characteristic polynomial is

$$x^4 - x^2\left(\frac{\alpha^2}{\alpha+1} + \frac{\alpha}{(\alpha+1)(\beta+1)} + \frac{\beta}{(\alpha+1)(\beta+1)} + \frac{\beta^2}{\beta+1}\right) + \frac{\alpha^2\beta^2}{(\alpha+1)(\beta+1)}.$$

Similarly, $\overline{D}(\alpha,\beta)$ can be presented as $\overline{D}(\alpha,\beta) = \mathcal{P}_4[K_1, K_\alpha, K_\beta, K_1]$. Now by applying Theorem 2.1 and the spectrum of K_η is $\{\eta-1, (-1)^{[\eta-1]}\}$, the *ABC* eigenvalues of $\overline{D}(a,b)$ are the eigenvalue $-\frac{\sqrt{2(\alpha+\beta)-2}}{\alpha+\beta}$ with order $\alpha+\beta-2$ and the eigenvalues of the matrix presented below

$$\begin{pmatrix} 0 & \alpha\sqrt{\frac{2\alpha+\beta-2}{\alpha(\alpha+\beta)}} & 0 & 0 \\ \sqrt{\frac{2\alpha+\beta-2}{\alpha(\alpha+\beta)}} & \frac{(\alpha-1)\sqrt{2\alpha+2\beta-2}}{\alpha+\beta} & \frac{\beta\sqrt{2\alpha+2\beta-2}}{\alpha+\beta} & 0 \\ 0 & \frac{\alpha\sqrt{2\alpha+2\beta-2}}{\alpha+\beta} & \frac{(\beta-1)\sqrt{2\alpha+2\beta-2}}{\alpha+\beta} & \sqrt{\frac{\alpha+2\beta-2}{\beta(\alpha+\beta)}} \\ 0 & 0 & \beta\sqrt{\frac{\alpha+2\beta-2}{\beta(\alpha+\beta)}} & 0 \end{pmatrix}. \tag{2.4}$$

□

The graph operation Γ-join is known by several names in the literature, like generalized composition, generalized join graph operation and Γ-join graph operation. Among the graph operations, Γ-join is an interesting operation because almost all connected graphs can be written in terms of Γ-join. More interestingly, the graphs defined on algebraic structures like power graphs of finite groups, commuting graphs of finite groups, zero divisor graphs of finite rings (modules and lattices), unit graphs or rings and many other algebraic graphs can be written in terms of the Γ-join of graphs. For some applications of the spectrum of the Γ-join of graphs with different types of graph matrices the reader is referred to [18, 23, 25, 27–30] and the references therein.

3. *ABC* equienergetic graphs

In this section, we construct the *ABC* equienergetic graphs using Theorem 2.1 and the operation Γ-join of graphs.

Theorem 3.1. *Let* Γ *be a connected graph with nodes* $\{w_1, w_2, \ldots, w_n\}$ *and for* $i = 1, 2, \ldots, n$, *let* Γ_i *and* H_i *be* r_i *regular adjacency equienergetic graphs of orders* n_i *having adjacency eigenvalues* $\zeta_{i,1} = r_i \geq \zeta_{i,2} \geq \cdots \geq \zeta_{i,n_i}$. *Then,*

$$EABC(\Gamma[\Gamma_1, \Gamma_2, \ldots, \Gamma_n]) = EABC(\Gamma[H_1, H_2, \ldots, H_n]).$$

Proof. As Γ_i's and H_i's are of same order n_i (same degree r_i), for each $i = 1, 2, \ldots, n$. So, the regular quotient matrices of $\Gamma[\Gamma_1, \Gamma_2, \ldots, \Gamma_n]$ and $\Gamma[H_1, H_2, \ldots, H_n]$ are same

$$\begin{pmatrix} \frac{r_1}{r'_1}\sqrt{2r'_2-2} & n_2q_{1,2} & \ldots & n_nq_{1,n} \\ n_1q_{2,1} & \frac{r_1}{r'_1}\sqrt{2r'_1-2} & \ldots & n_nq_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ n_1q_{n,1} & n_2q_{n,2} & \ldots & \frac{r_n}{r'_n}\sqrt{2r'_n-2} \end{pmatrix},$$

where $q_{ij} = q_{ji} = \sqrt{\frac{r'_i+r'_j-2}{r'_ir'_j}}$, if w_i is adjacent to w_j and 0, otherwise. Thus, the spectrum of regular quotient matrix adds the same quantity say $\mathbb{E}_1$ to the *ABC* energy of Γ-joins. Now, for $i = 1, 2, \ldots, n$, using the fact that $\sum_{j=1}^{n_i} |\zeta_{i,j}(\Gamma_i)| = \mathbb{E}(\Gamma_i)$ and *ABC* spectrum of $\Gamma[\Gamma_1, \Gamma_2, \ldots, \Gamma_n]$ consists of the eigenvalues $\frac{\sqrt{2r'_i-2}}{r'_i}\zeta_{i,k}(\Gamma_i)$ we obtain

$$\sum_{i=1}^{n}\sum_{j=2}^{n_i}\frac{\sqrt{2r'_i-2}}{r'_i}|\zeta_{i,j}(\Gamma_i)| = \sum_{i=1}^{n}\frac{\sqrt{2r'_i-2}}{r'_i}\sum_{j=2}^{n_i}|\zeta_{i,j}(\Gamma_i)| = \sum_{i=1}^{n}\frac{\sqrt{2r'_i-2}}{r'_i}\Big(\mathbb{E}(\Gamma_i) - r_i\Big),$$

where $\mathbb{E}(\Gamma_i)$ is the energy of Γ_i, for $i = 1, 2, \ldots, n$.

Similarly, using the fact that the *ABC* eigenvalues of $\Gamma[H_1, H_2, \ldots, H_n]$ are of the form $\frac{\sqrt{2r'_i-2}}{r'_i}\zeta_{i,k}(H_i)$ we have

$$\sum_{i=1}^{n}\sum_{j=2}^{n_i}\frac{\sqrt{2r'_i-2}}{r'_i}|\zeta_{i,j}(H_i)| = \sum_{i=1}^{n}\frac{\sqrt{2r'_i-2}}{r'_i}\sum_{j=2}^{n_i}|\zeta_{i,j}(H_i)| = \sum_{i=1}^{n}\frac{\sqrt{2r'_i-2}}{r'_i}\Big(\mathbb{E}(H_i) - r_i\Big),$$

where $\mathbb{E}(H_i) = \sum_{i=1}^{n}|\zeta_i(H_i)|$ is the energy of H_i, for $i = 1, 2, \ldots, n$. Therefore, by the equienergetic properties of Γ_i and H_i we have

$$\begin{aligned} EABC(\Gamma[\Gamma_1, \Gamma_2, \ldots, \Gamma_n]) &= \mathbb{E}_1 + \sum_{i=1}^{n}\frac{\sqrt{2r'_i-2}}{r'_i}\Big(\mathbb{E}(\Gamma_i) - r_i\Big) \\ &= \mathbb{E}_1 + \sum_{i=1}^{n}\frac{\sqrt{2r'_i-2}}{r'_i}\Big(\mathbb{E}(H_i) - r_i\Big) = EABC(\Gamma[H_1, H_2, \ldots, H_n]). \end{aligned}$$

□

We will illustrate Theorem 3.1 with the help of a example.

Example 3.2. *Let* $\Gamma = K_2[C_6, C_6]$ *and* $H = K_2[C_6, (K_3 \cup K_3)]$ *be the two graphs. We will show that* $EABC(\Gamma) = EABC(H)$. *Since the eigenvalues of* $A(C_6)$ *are* $\{2, -2, (-1)^2, 1^2\}$ *and by Theorem 2.1, the ABC eigenvalues of* Γ *are*

$$\{(0.46774)^4, (-0.46774)^4, (-0.93541)^2)\},$$

the remaining two ABC eigenvalues of Γ *are the eigenvalues of the following matrix*

$$\begin{pmatrix} \frac{1}{4}\sqrt{14} & \frac{3}{4}\sqrt{14} \\ \frac{3}{4}\sqrt{14} & \frac{3}{4}\sqrt{14} \end{pmatrix}, \tag{3.1}$$

and its eigenvalues are 3.74166 *and* −1.87083. *Thus, by using Theorem 3.1 the ABC energy of* Γ *is*

$$EABC(\Gamma) = 3.74166 + 1.87083 + 2(0.93541) + 8(0.46774) = 11.22497.$$

Similarly, noting that the adjacency spectrum of K_3 *is* $\{2, -1, -1\}$*, the ABC spectrum of H consists of the eigenvalues* $\{0.935414, -0.935414, (0.467707)^2, (-0.467707)^6\}$ *and the eigenvalues of* (3.1)*. Now, it is easy to verify that* $EABC(H) = 11.22497 = EABC(\Gamma)$.

From Theorem 3.1, we see that $\Gamma[\Gamma_1, \Gamma_2, \ldots, \Gamma_n]$ and $\Gamma[H_1, H_2, \ldots, H_n]$ share the same regular quotient matrix and have equal part in their *ABC* energy. Thus, it is necessary for *ABC* equienergetic graphs that the set of the union of adjacency spectra $A(\Gamma_i) - \{r_i\}$ is different from the set of the union of adjacency spectrum $A(H_i) - \{r_i\}$.

As in Example 3.2, we have the following collection of *ABC* equienergetic graphs.

$$\begin{aligned}
&\mathcal{P}_n[C_6, C_6, \ldots, C_6, C_6],\\
&\mathcal{P}_n[C_6, C_6, \ldots, C_6, C_3 \cup C_3],\\
&\mathcal{P}_n[C_6, C_6, \ldots, C_3 \cup C_3, C_3 \cup C_3],\\
&\vdots\\
&\mathcal{P}_n[C_6, C_3 \cup C_3, \ldots, C_3 \cup C_3, C_3 \cup C_3],\\
&\mathcal{P}_n[C_3 \cup C_3, C_3 \cup C_3, \ldots, C_3 \cup C_3, C_3 \cup C_3].
\end{aligned}$$

In the above manner, for any pair of adjacency equienergetic graphs say Γ_1 and Γ_2, we get at least three *ABC* equienergetic graphs $K_2[\Gamma_1, \Gamma_1], K_2[\Gamma_1, \Gamma_2]$ and $K_2[\Gamma_2, \Gamma_2]$. Therefore, we construct infinite class of *ABC* equienergetic graphs by using the graph operation Γ-join.

4. Anti-cancer drugs

Topological indices are numeric descriptors that are obtained from molecular graphs to describe their chemical system. Degree-based topological indices are of great importance and particularly in mathematical chemistry. The use of graph invariant in QSPR and QSAR studies has been of key interest in recent years. Topological indices have application in the non-empirical Quantitative Structure-Property Relationships (QSPR) and Quantitative Structure -Activity Relationships (QSAR) [1, 19, 20, 24, 31]. These psychochemical qualities are being studied because they have direct impact on bioactivity and drug transit in the human body and thereby help in designing better drugs. We compute *ABC* index and *ABC* energy of certain cancer drugs. We carry the linear regression and study their correlation and coefficient of determinations R^2. We consider the following drugs (see chemical structures Figure 1) for our QSPR study.

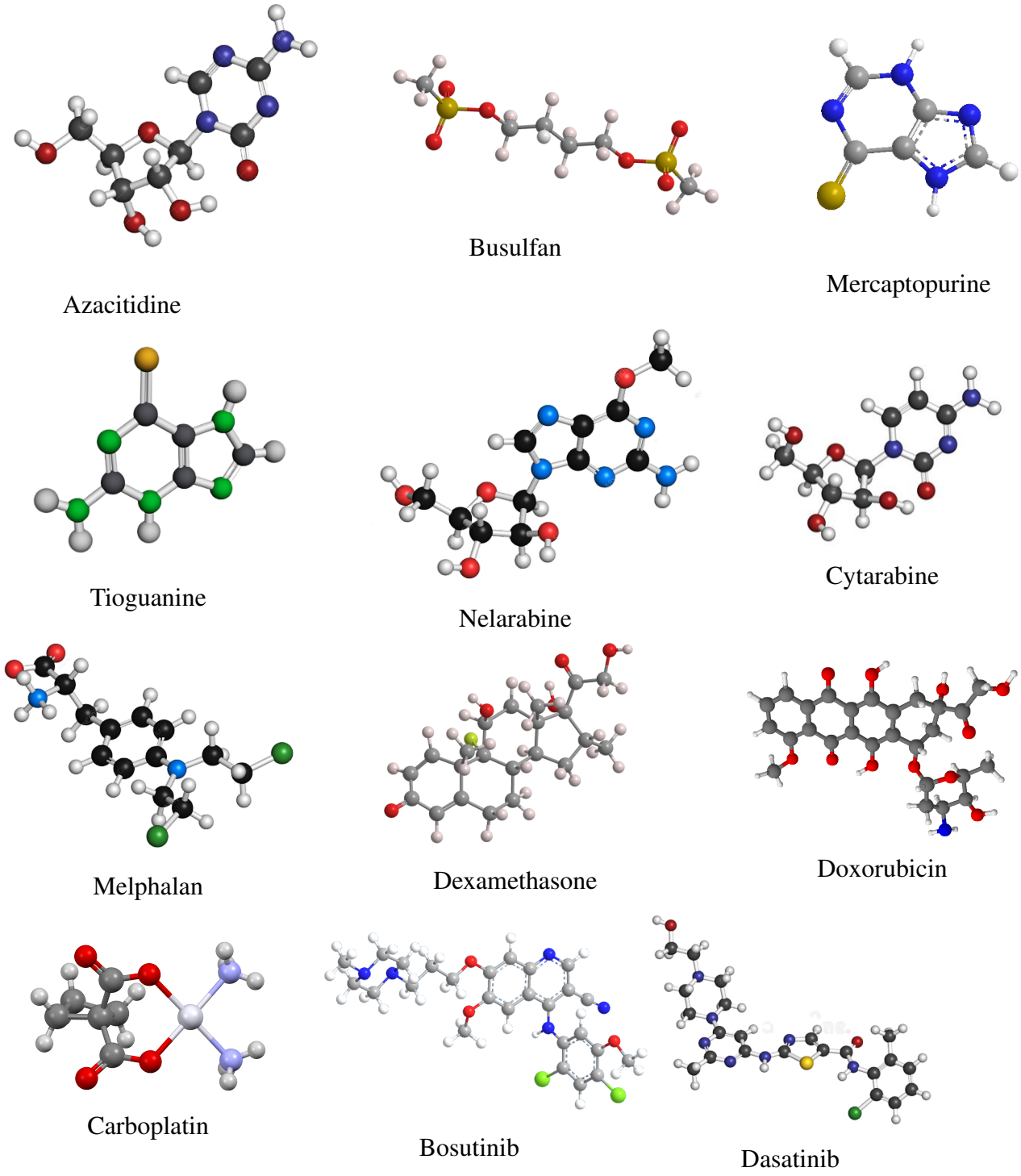


Figure 1. Molecular structure of certain drugs.

Azacytidine is used as an antineoplastic agent and its chemical formula is $C_8H_{12}N_4O_5$. Busulfan is an antineoplastic alkylating agent commonly used for several types of cancer. They prevent tumor development by cross linking guanine bases in DNA double-helix strands, directly attacking DNA. Thus strands are unable to separate and uncoil which is necessary in DNA replication and cells are

no longer divided. The molecular formula for bulasan is $C_8H_{14}N_6S_2$. Mercaptopurine ($C_5H_4N_4S$) is s series of purine analogues that interfere with nucleic acid biosynthesis and is active against human leukemias. Tioguanine ($C_5H_5N_5S$) is an antineoplastic compound which also has antimetabolite action and is used in the therapy of acute leukemia. Nelarabine ($C_{11}H_{15}N_5O_5$) is a purine nucleoside analog and antineoplastic agent used for the treatment of acute T-cell lymphoblastic leukemia and T cell lymphoblastic lymphoma with inadequate clinical response to prior chemotherapeutic treatments. Cytarabine ($C_9H_{13}N_3O_5$) is an antineoplastic antimetabolite used in the treatment of various forms of leukemia, including acute myelogenous leukemia and meningeal leukemia. Melphala is ($C_{13}H_{18}Cl_2N_2O_2$) is an antineoplastic alkylating agents and is used in the treatment of cancers. Alkylating agents are known for their ability to add alkyl groups to many electronegative groups under conditions present in cells. They stop tumor growth by crosslinking guanine bases in DNA. Dexamethasone ($C_{22}H_{29}FO_5$) is a glucocorticoid available in various modes of administration that is used to prevent various inflammatory conditions, including bronchial asthma, endocrine and rheumatic disorders. Doxorubicine ($C_{27}H_{29}NOD$) is an antineoplastic in the anthracycline class. Anthracyclines are the most important anti tumor drugs available. Carbopalatin ($C_6H_{12}N_2O_4Pt$) is a alkylating agent used to treat advanced ovarian cancer. Bosutinib ($C_{26}H_{29}Cl_2N_5O_5$) is used to treat chronic myeloid leukemia (a type of cancer of white blood cells). Dasatinib ($C_{22}H_{26}ClN_7S$) is a tyrosine kinase inhibitor used for the treatment of lymphoblastic or chronic myeloid leukemia.

The physical properties values of these anticancer drugs are taken from Chem Spider. Properties include molar volume (MV), refractive index (R), complexity (C) and flash point (FP). The ABC index and ABC energy are calculated by mathematical software. From Table 1, it is clear that these data values are normally distributed. So, linear regression model is most suitable to test and adopt an analysis for the same.

Table 1. Molar volume MV, refractive index RI, complicity C, flash point FP, ABC index and ABC energy of drugs given in Figure 1.

Drug	MV (cm^3)	RI (m^3 mol^{-1})	C	FP °C	ABC	$EABC$
Azacitidine	117.10	54.10	384.00	277.00	22.0424	25.7008
Busulfan	182.40	50.90		234.40	21.4787	22.8048
Mercaptopurine	94.20	41.00	19.00	250.50	10.9109	12.7935
Tioguanine	80.20	46.89	225.00	232.00	12.3941	14.5517
Nelarabine	149.90	65.80	377.00	389.90	27.9857	31.9586
Cytarabine	128.40	52.60	383.00	283.80	22.778	26.8256
Melphalan	231.20	78.23	265.00	239.00	28.4535	31.5644
Dexamethasone	296.20	100.20	805.00	298.00	43.9525	49.7114
Doxorubicin	336.60	134.59	977.00	443.80	53.0933	60.3944
Carboplatin		60.04	177.00		19.819	21.178
Bosutinib	388.30	142.12	734.00	346.70	51.1774	56.4559
Dasatinib	366.40	133.08	642.00		46.3232	52.3302

We carry the regression analysis for the drugs listed in Figure 1. Linear regression model is tested with the help of equation:

$$P = a + b \cdot *,$$

where P is a physicochemical property of a drug, $*$ is either ABC or ABC energy, a is a constant and b represents regression coefficient.

Table 2 gives the correlation coefficients of the physiochemical properties of drugs given in Figure 1 with the graph invariants ABC index and the ABC energy. From the table, we observe that RI is highly correlated with ABC index while FP is least related in both cases.

Table 2. Correlation coefficients of MV, RI, C and FP with ABC index and ABC energy of drugs given in Figure 1.

Invariant	MV (cm^3)	RI (m^3 mol^{-1})	C	FP °C
ABC	0.957399	0.968961	0.940544	0.735575
$EABC$	0.949354	0.964731	0.950077	0.752718

Table 3 gives the coefficient of determinations R^2 of the physiochemical properties with ABC and $EABC$. We see that RI achieves maximum R^2 in both case of ABC and $EABC$.

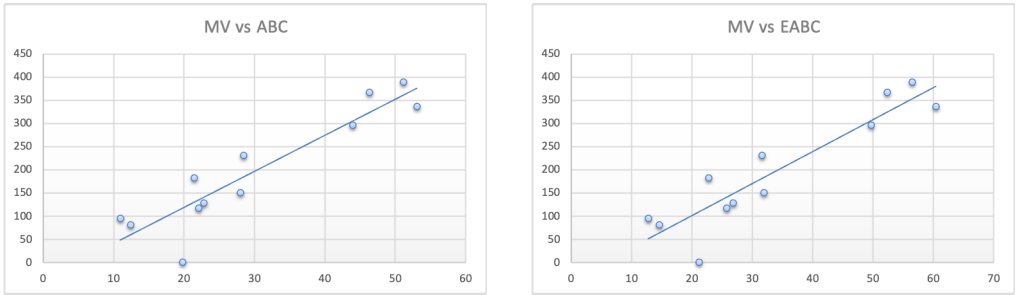
Table 3. R^2 of MV, RI, C and FP with ABC index and ABC energy of drugs given in Figure 1.

Invariant	MV (cm^3)	RI (m^3 mol^{-1})	C	FP °C
ABC	0.8442	0.9389	0.8385	0.0609
$EABC$	0.8405	0.9307	0.867	0.0.0699

Figure 2 shows the pictorial representation of linear regression of ABC and $EABC$ with MV. The approximated regression equations are:

$$MV = 7.7609 \cdot ABC - 35.517 \text{with } R^2 = 0.8442.$$

$$MV = 6.9126 \cdot EABC - 36.449 \text{with } R^2 = 0.8405.$$



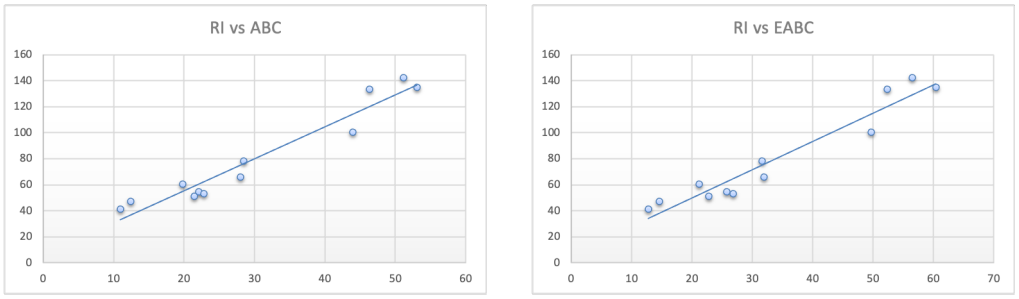
MV with ABC MV with $EABC$

Figure 2. Linear regression of ABC index and ABC energy with molar volume (MV).

Figure 3 shows the pictorial representation of linear regression of ABC and $EABC$ with RI. The approximated regression equations are:

$$RI = 2.4579 \cdot ABC + 6.158 \text{with } R^2 = 0.9389.$$

$$RI = 6.9126 \cdot EABC + 6.0212 \text{with } R^2 = 0.9307.$$



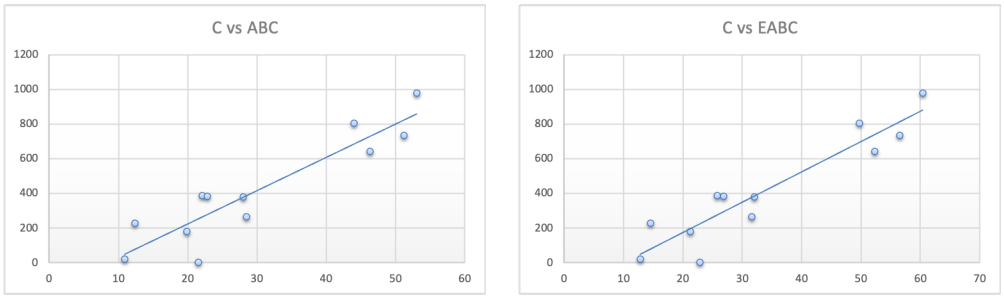
RI with ABC RI with $EABC$

Figure 3. Linear regression of ABC index and ABC energy with Refractive Index (RI).

Figure 4 shows the pictorial representation of linear regression of ABC and $EABC$ with C. The approximated regression equations are:

$$C = 19.264 \cdot ABC - 162.9 \text{with } R^2 = 0.8385.$$

$$C = 17.486 \cdot EABC - 176.31 \text{with } R^2 = 0.867.$$



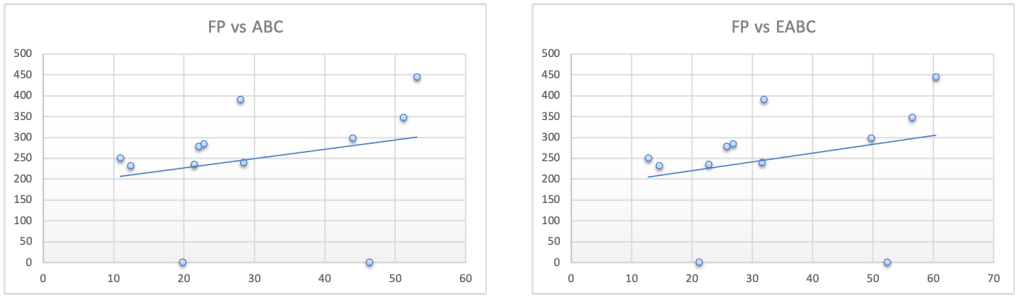
C with ABC C with $EABC$

Figure 4. Linear regression of ABC index and ABC energy with Complexity (C).

Figure 5 shows the linear regression of ABC and $EABC$ with FP. The approximated regression equations are:

$$FP = 2.2249 \cdot ABC + 182.77 \text{with } R^2 = 0.0609.$$

$$FP = 0.0699 \cdot EABC + 177.55 \text{with } R^2 = 0.0699.$$



FP with *ABC* FP with *EABC*

Figure 5. Linear regression of *ABC* index and *ABC* energy with Flash Point (FP).

The significant observation is that molar volume (MV), refractive index (R) and complexity (C) are better related with the *ABC* index and the *ABC* energy and thereby may help in designing better drugs. With this study, we can better understand the structure of these drugs and increase their efficiency against cancer related diseases.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

Acknowledgments

This research work was funded by Institutional Fund Projects under grant no. (IFPIP: 1293-247-1443). The authors gratefully acknowledge the technical and financial support provided by the Ministry of Education and King Abdulaziz University, DSR, Jeddah, Saudi Arabia.

Conflict of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Data availability

All data generated or analyzed during this study is included in this published article.

References

1. A. Altassan, B. A. Rather, M. Imran, Inverse sum indeg index (energy) with applications to anticancer drugs, *Mathematics*, **10** (2022), 4749. https://doi.org/10.3390/math10244749
2. A. E. Brouwer, W. H. Haemers, *Spectra of graphs*, New York: Springer 2011.
3. G. Chartrand, P. Zhang, *Introduction to graph theory*, Tata McGraw-Hill edition, New Delhi, 2006.
4. J. Chen, X. Gou, Extreme atom-bond connectivity index of graphs, *MATCH Commun. Math. Comput. Chem.*, **65** (2011), 713–722.

5. X. Chen, On *ABC* eigenvalues and *ABC* energy, *Linear Algebra Appl.*, **544** (2018), 141–157. https://doi.org/10.1016/j.laa.2018.01.011
6. X. Chen, On extremality of *ABC* spectral radius of a tree, *Linear Algebra Appl.*, **564** (2019), 159–169. https://doi.org/10.1016/j.laa.2018.12.003
7. X. Chen, A note on *ABC* spectral radius of graphs, *Linear Multilinear Algebra*, **70** (2022), 775–786. http://doi.org/10.1080/03081087.2020.1748849
8. D. M. Cvetković, M. Doob, H. Sachs, *Spectra of graphs: theory and applications*, Pure and Applied Mathematics, New York: Academic Press, 1980.
9. K. C. Das, Atom-bond connectivity index of graphs, *Discrete Appl. Math.*, **158** (2010), 1181–1188. https://doi.org/10.1016/j.dam.2010.03.006
10. E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, *Indian J. Chem.*, **37A** (1998), 849–855.
11. E. Estrada, The *ABC* matrix, *J. Math. Chem.*, **55** (2017), 1021–1033. https://doi.org/10.1007/s10910-016-0725-5
12. B. Furtula, A. Graovac, D. Vukičević, Atom-bond connectivity index of trees, *Discrete Appl. Math.*, **157** (2009), 2828–2835. https://doi.org/10.1016/j.dam.2009.03.004
13. Y. Gao, Y. Shao, The minimum *ABC* energy of trees, *Linear Algebra Appl.*, **577** (2019), 186–203. https://doi.org/10.1016/j.laa.2019.04.032
14. M. Ghorbani, X. Li, M. Hakimi-Nezhaad, J. Wang, Bounds on the *ABC* spectral radius and *ABC* energy of graphs, *Linear Algebra Appl.*, **598** (2020), 145–164. https://doi.org/10.1016/j.laa.2020.03.043
15. I. Gutman, J. Tošović, S. Radenković, S. Marković, On atom-bond connectivity index and its chemical applications, *Indian J. Chem.*, **51A** (2012), 690–694.
16. I. Gutman, B. Furtula, Trees with smallest atom-bond connectivity index, *MATCH Commun. Math. Comput. Chem.*, **68** (2012), 131–136.
17. I. Gutman, X. Li, Y. Shi, *Graph energy*, New York: Springer, 2009.
18. A. Hamzeh, A. R. Ashrafi, Spectrum and L-spectrum of the power graph and its main supergraph for certain finite groups, *Filomat*, **31** (2017), 5323–5334. https://doi.org/10.2298/FIL1716323H
19. S. M. Hosamani, B. B. Kulkarni, R. G. Boli, V. M. Gadag, QSPR analysis of certain graph theoratical matrices and their corresponding energy, *Appl. Math. Nonlinear Sci.*, **2** (2017), 131–150. https://doi.org/10.21042/AMNS.2017.1.00011
20. S. A. K. Kirmani, P. Ali, F. Azam, P. A. Alvi, On ve-degree and ev-degree topological properties of hyaluronic acid? Anticancer drug conjugates with QSPR, *J. Chem.*, **2021** (2021), 3860856. https://doi.org/10.1155/2021/3860856
21. X. Li, J. Wang, on the *ABC* spectral radius of unicyclic graphs, *Linear Algebra Appl.*, **596** (2020), 71–81. https://doi.org/10.1016/j.laa.2020.03.007
22. S. Li, L. Wang, H. Zhang, on *ABC* Estrada index of graphs, *Discrete Math.*, **344** (2021), 112586. https://doi.org/10.1016/j.disc.2021.112586

23. Z. Mehranian, A. Gholami, A. R. Ashrafi, The spectra of power graphs of certain finite groups, *Linear Multilinear Algebra*, **65** (2017), 1003–1010. https://doi.org/10.1080/03081087.2016.1221375

24. S. Nasir, N. ul Hassan Awan, F. B. Farooq, S. Parveen, Topological indices of novel drugs used in blood cancer treatment and its QSPR modelling, *AIMS Math.*, **7** (2022), 11829–11850. https://doi.org/10.3934/math.2022660

25. A. Patil, K. Shinde, Spectrum of the zero divisor graphs of von Neumann regular rings, *J. Algebra Appl.*, **21** (2021), 2250193. http://doi.org/10.1142/S0219498822501936

26. H. S. Ramane, H. B. Walikar, S. B. Rao, B. D. Acharya, P. R. Hampiholi, S. R. Jog, et al., Equienergetic graphs, *Kragujevac J. Math.*, **26** (2004), 5–13.

27. B. A. Rather, On distribution of Laplacian eigenvalues of graphs, *arXiv*, 2020. https://doi.org/10.48550/arXiv.2107.09161

28. B. A. Rather, S. Pirzada, G. F. Zhou, On distance Laplacian spectra of power graphs of certain finite groups, *Acta Math. Sin.*, **39** (2023), 603–617. https://doi.org/10.1007/s10114-022-0359-4

29. B. A. Rather, H. A. Ganie, S. Pirzada, On A_α-spectrum of joined union and its applications to power graphs of certain finite groups, *J. Algebra Appl.*, 2022, 2350257. https://doi.org/10.1142/S0219498823502572

30. B. A. Rather, M. Aouchiche, M. Imran, On Laplacian eigenvalues of comaximal graphs of commutative rings, *Indian J. Pure Appl. Math.*, 2023. https://doi.org/10.1007/s13226-023-00364-8

31. M. C. Shanmukha, N. S. Basavarajappa, K. C. Shilpa, A. Usha, Degree-based topological indices on anticancer drugs with QSPR analysis, *Heliyon*, **6** (2020), e04235. https://doi.org/10.1016/j.heliyon.2020.e04235

AIMS Press