SAR and QSAR in Environmental Research, 1997, Vol. 7, pp. 63–87
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MOLECULAR GRAPH MATRICES AND DERIVED STRUCTURAL DESCRIPTORS

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(Received 13 March 1997; In final form 16 July 1997)

A number of recently graph matrices encoding in various ways the topological information is presented. Four graph operators are used to compute 19 topological indices for a set of 306 alkanes. The intercorrelation coefficients of the 19 topological indices are computed and used to identify highly intercorrelated indices.

Keywords: Graph matrix; graph operator; topological index

The graph theoretical characterization of molecular structure is realized by means of various matrices, polynomials, spectra, spectral moments, sequences counting distances, paths and walks. In order to perform Quantitative Structure-Activity Relationships (QSAR) and Quantitative Structure-Property Relationships (QSPR) analysis the structure of a molecule is represented by a number, called Topological Index (TI) [1–5]. A TI is a scalar numerical descriptor of the structure of a molecule, derived from the corresponding molecular graph. The topological description of a molecule is composed of information on the atom-atom connectivity in a molecule, which encodes the size, shape and branching. The description neglects information on bond lengths, bond angles, and torsion angles.

The high correlational ability of TIs with a wide range of physico-chemical and biological properties was theoretically interpreted by

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Klein [6]. He suggested that TIs are low-order cluster expansions of the chemical structure, with a rapid convergence.

As presented above, the molecular matrices represent an important source of structural descriptors. Usually, a small set of matrices is used to characterize the molecular topology, namely the adjacency, the distance and sometimes, the Laplacian matrix. Novel matrices were developed in recent years, encoding in various ways the topological information. The scope of the present paper is to review the molecular matrices used in the generation of molecular graph descriptors, and to explore the similarity of selected topological indices computed on the basis of graph matrices.

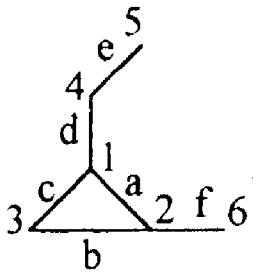
THE ADJACENCY MATRIX

The adjacency matrix $\mathbf{A} = \mathbf{A}(G)$ of a graph G with N vertices is the square $N \times N$ symmetric matrix whose entry in the ith row and jth column is defined as [7]:

$$[\mathbf{A}]_{ij} = \begin{cases} 1 & \text{if} \quad i \neq j \quad \text{and} \quad (i, j) \in \mathbf{E}(G) \\ 0 & \text{if} \quad i = j \quad \text{or} \quad (i, j) \notin \mathbf{E}(G) \end{cases} \tag{1}$$

where $\mathbf{E}(G)$ represents the set of edges of G. The sum of entries over row i or column i in $\mathbf{A}(G)$ is the degree of vertex i, $\mathbf{deg}_i$.

As an example, the molecular graph and the adjacency matrix of 1-ethyl-2-methylcyclopropane (**1**) are given below. The vertices and edges are labeled from 1 to 6 and from a to f, respectively. This graph represents the smallest identity cycloalkane because no vertices are topologically equivalent.



1

	1	2	3	4	5	6
1	0	1	1	1	0	0
2	1	0	1	0	0	1
3	1	1	0	0	0	0
4	1	0	0	0	1	0
5	0	0	0	1	0	0
6	0	1	0	0	0	0

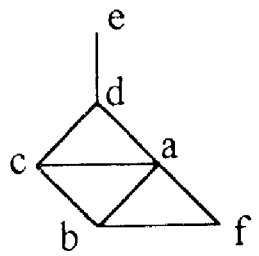
Molecules containing heteroatoms and/or multiple bonds are represented by vertex- and edge-weighted graphs [8, 9]. The adjacency matrix of vertex- and edge-weighted molecular graph is defined by:

$$[\mathbf{A}]_{ij} = \begin{cases} \mathbf{Vw}_i & \text{if} \quad i = j \\ \mathbf{Ew}_{ij} & \text{if} \quad (i, j) \in \mathbf{E}(G) \\ 0 & \text{if} \quad (i, j) \notin \mathbf{E}(G) \end{cases} \tag{2}$$

where $\mathbf{Vw}_i$ is the weight of the vertex i, and $\mathbf{Ew}_{ij}$ is the weight of the edge (i, j). $\mathbf{Vw}_i$ depends on the chemical nature of the corresponding atom in a molecule and is equal to zero if the vertex i represents a carbon atom. $\mathbf{Ew}_{ij}$ depends on the chemical nature of the atoms i and j as well as on the bond multiplicity.

THE EDGE-ADJACENCY MATRIX

The line graph of a graph G, denoted by $\mathbf{Li}(G)$, is obtained from G in such a way that edges in G are considered vertices in $\mathbf{Li}(G)$. Two vertices in $\mathbf{Li}(G)$ are connected if the corresponding edges in G are adjacent. The line graph of 1-ethyl-2-methylcyclopropane is represented by the graph **2**. The vertices in the graph **2** are labeled from **a** to **f**, and each vertex in **2** corresponds to the edge with the same label in **1**.



2

The edge-adjacency matrix of a graph G, $\mathbf{EA} = \mathbf{EA}(G)$, is equal to the adjacency matrix of the line graph of G: $\mathbf{EA}(G) = \mathbf{A}(\mathbf{Li}(G))$. A certain

number of structural descriptors were derived from the **EA** matrix [10–14]. The edge-adjacency matrix of the graph **1**, **EA(1)**, is:

	a	**b**	**c**	**d**	**e**	**f**
a	0	1	1	1	0	1
b	1	0	1	0	0	1
c	1	1	0	1	0	0
d	1	0	1	0	1	0
e	0	0	0	1	0	0
f	1	1	0	0	0	0

THE LAPLACIAN MATRIX

Let define for a graph G the diagonal matrix, $\mathbf{DEG} = \mathbf{DEG}(G)$, whose ii entry is equal to the degree (valency) of the vertex i, $\mathbf{deg}_i$. The Laplacian matrix of G, $\mathbf{L} = \mathbf{L}(G)$, is defined by the following Eq. [15]:

$$\mathbf{L}(G) = \mathbf{DEG}(G) - \mathbf{A}(G) \tag{3}$$

The elements of the Laplacian matrix are:

$$[\mathbf{L}]_{ij} = \begin{cases} \mathbf{deg}_i & \text{if } i = j \\ -1 & \text{if } (i, j) \in \mathbf{E}(G) \\ 0 & \text{if } (i, j) \notin \mathbf{E}(G) \end{cases} \tag{4}$$

The Laplacian matrix of the graph **1** corresponding to the carbon skeleton of 1-ethyl-2-methylcyclopropane is presented below:

	1	**2**	**3**	**4**	**5**	**6**
1	3	−1	−1	−1	0	0
2	−1	3	−1	0	0	−1
3	−1	−1	2	0	0	0
4	−1	0	0	2	−1	0
5	0	0	0	−1	1	0
6	0	−1	0	0	0	1

Let us mention that the Laplacian matrix is sometimes called the Kirchhoff matrix due to its role in the spanning tree theorem of Kirchhoff. The Laplacian matrix offers a new way to compute the Wiener index of trees, being the source of new graph invariants [16–19].

The χ Matrix

The χ matrix [20] can be considered as a weighted adjacency matrix whose elements are 0 and $(\mathbf{deg}_i\ \mathbf{deg}_j)^{-1/2}$:

$$[\chi]_{ij} = \begin{cases} (\mathbf{deg}_i\ \mathbf{deg}_j)^{-1/2} & \text{if} \quad (i, j) \in \mathbf{E}(G) \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

The matrix $\chi(\mathbf{1})$ is presented below:

	1	**2**	**3**	**4**	**5**	**6**
1	0	0.333	0.408	0.408	0	0
2	0.333	0	0.408	0	0	0.577
3	0.408	0.408	0	0	0	0
4	0.408	0	0	0	0.707	0
5	0	0	0	0.707	0	0
6	0	0.577	0	0	0	0

The χ-**EA** matrix of a graph G is the χ matrix of the line graph $\mathbf{Li}(G)$. As an example we present the matrix χ-**EA(1)**:

	a	**b**	**c**	**d**	**e**	**f**
a	0	0.289	0.289	0.289	0	0.354
b	0.289	0	0.333	0	0	0.408
c	0.289	0.333	0	0.333	0	0
d	0.289	0	0.333	0	0.577	0
e	0	0	0	0.577	0	0
f	0.354	0.408	0	0	0	0

THE DISTANCE MATRIX

The length of a path in a molecular graph is equal to the number of edges along the path. For a given pair of vertices (i, j) of G, let $\mathbf{d}_{ij}$ denote the topological distance – the length of the shortest path connecting the vertices. The topological distance has the following properties: $\mathbf{d}_{ij} \geq 0$ for all $i, j \in \mathbf{V}(G)$ (equality holds if and only if $i = j$); $\mathbf{d}_{ij} = \mathbf{d}_{ji}$ for all $i,\ j \in \mathbf{V}(G)$; $\mathbf{d}_{ik} + \mathbf{d}_{kj} \geq \mathbf{d}_{ij}$ for all $i, j, k \in \mathbf{V}(G)$, where $\mathbf{V}(G)$ is the set of vertices of G. The distance matrix, $\mathbf{D} = \mathbf{D}(G)$, of a connected graph G is a real symmetric matrix whose

elements $[\mathbf{D}]_{ij}$ are defined as [21–25]:

$$[\mathbf{D}]_{ij} = \begin{cases} \mathbf{d}_{ij} & \text{if} \quad i \neq j \\ 0 & \text{if} \quad i = j \end{cases} \tag{6}$$

As an example, the distance matrix of 1-ethyl-2-methylcyclopropane (graph **1**) is shown:

	1	**2**	**3**	**4**	**5**	**6**
1	0	1	1	1	2	2
2	1	0	1	2	3	1
3	1	1	0	2	3	2
4	1	2	2	0	1	3
5	2	3	3	1	0	4
6	2	1	2	3	4	0

The **D** matrix is the source of a large number of graph descriptors, and its computation can be performed with various algorithms [24–27]. The distance edge-adjacency matrix **DEA** of a graph G is the distance matrix of the line graph **Li**(G). This matrix was recently used to define the index MTI(E) [28]. The **DEA** of the molecular graph **1** is:

	a	**b**	**c**	**d**	**e**	**f**
a	0	1	1	1	2	1
b	1	0	1	2	3	1
c	1	1	0	1	2	2
d	1	2	1	0	1	2
e	2	3	2	1	0	3
f	1	1	2	2	3	0

THE RECIPROCAL DISTANCE MATRIX

The reciprocal distance, $\mathbf{rd}_{ij}$, for a pair of vertices (i, j) of a graph G, is defined as the reciprocal of the distance $\mathbf{d}_{ij}$ [29]. The reciprocal distance matrix of a graph G with N vertices, $\mathbf{RD} = \mathbf{RD}(G)$, is a square $N \times N$ symmetric matrix, whose entries $[\mathbf{RD}]_{ij}$ are equal to the reciprocal of the distance between vertices i and j, $1/\mathbf{d}_{ij}$, for non-diagonal elements, and is

equal to zero for the diagonal elements [30–32]:

$$[\mathbf{RD}]_{ij} = \begin{cases} 0 & \text{if } i = j \\ 1/\mathbf{d}_{ij} & \text{if } i \neq j \end{cases} \tag{7}$$

As an example, the **RD** matrix of the molecular graph **1** is:

	1	**2**	**3**	**4**	**5**	**6**
1	0	1	1	1	1/2	1/2
2	1	0	1	1/2	1/3	1
3	1	1	0	1/2	1/3	1/2
4	1	1/2	1/2	0	1	1/3
5	1/2	1/3	1/3	1	0	1/4
6	1/2	1	1/2	1/3	1/4	0

The **RD** matrix was successfully used to generate the new structural descriptors **Ch (RD)**, **Sp (RD)**, **Sum Ch (RD)**, **Min Sp (RD)**, and **Max Sp (RD)** [33] as well as in the computer generation of acyclic graphs based on local vertex invariants and topological indices [30].

The reciprocal distance edge-adjacency matrix **RDEA** of a graph G is the reciprocal distance matrix of the line graph **Li**(G). The **RDEA** matrix of the molecular graph **1** is presented below:

	a	**b**	**c**	**d**	**e**	**f**
a	0	1	1	1	1/2	1
b	1	0	1	1/2	1/3	1
c	1	1	0	1	1/2	1/2
d	1	1/2	1	0	1	1/2
e	1/2	1/3	1/2	1	0	1/3
f	1	1	1/2	1/2	1/3	0

THE RESISTANCE DISTANCE MATRIX

Klein and Randić have recently introduced a new distance function on graphs named resistance distance [34]. The resistance distance is based on electrical network theory. A single bond between two carbon atoms from the molecular graph corresponds to a 1 ohm resistor, and the resistance distance between a given pair of vertices (i, j) is defined as the effective

electrical resistance between the vertices. We present the resistance matrix Ω of the molecular graph **1**, $\Omega(\mathbf{1})$:

	1	**2**	**3**	**4**	**5**	**6**
1	0.000	0.666	0.666	1.000	2.000	1.666
2	0.666	0.000	0.666	1.666	2.666	1.000
3	0.666	0.666	0.000	1.666	2.666	1.666
4	1.000	1.666	1.666	0.000	1.000	2.666
5	2.000	2.666	2.666	1.000	0.000	3.666
6	1.666	1.000	1.666	2.666	3.666	0.000

As an example, we present the computation of the resistance distance between vertices 3 and 4 from graph **1**. The resistance distance $[\Omega(\mathbf{1})]_{34}$ is the sum of the resistance distance between the vertices 3 and 1 and that between the vertices 1 and 4, namely $[\Omega(\mathbf{1})]_{34} = [\Omega(\mathbf{1})]_{31} + [\Omega(\mathbf{1})]_{14}$. From the definition, $[\Omega(\mathbf{1})]_{14}$ is equal to 1 ohm, while $1/[\Omega(\mathbf{1})]_{31} = 1/1 + 1/2 = 3/2$, giving $[\Omega(\mathbf{1})]_{31} = 2/3 = 0.666$. Overall, $[\Omega(\mathbf{1})]_{34} = 0.666 + 1 = 1.666$.

The resistance distance was used to generate rules to characterize molecular cyclicity and centricity [35].

THE DETOUR MATRIX Δ

The detour matrix (or the maximum path matrix **MP** [36]) element $[\Delta]_{ij}$ is defined as [36–39]:

$$[\mathbf{\Delta}]_{ij} = \begin{cases} \max\ (\mathbf{p}_{ij}) & \text{if} \quad i \neq j \\ 0 & \text{if} \quad i = j \end{cases} \tag{8}$$

where max ($\mathbf{p}_{ij}$) is the length of the longest path connecting the vertices i and j. As an example, the detour matrix $\Delta(\mathbf{1})$ is given:

	1	**2**	**3**	**4**	**5**	**6**
1	0	2	2	1	2	3
2	2	0	2	3	4	1
3	2	2	0	3	4	3
4	1	3	3	0	1	4
5	2	4	4	1	0	5
6	3	1	3	4	5	0

The detour-distance matrix Δ-**D** (originally called the maximum/minimum path matrix **MmP** [36]) collects in its upper triangle the elements

of the detour matrix while the lower triangle elements are identical to those in the distance matrix:

$$[\mathbf{\Delta} - \mathbf{D}]_{ij} = \begin{cases} [\mathbf{\Delta}]_{ij} & \text{if } i < j \\ [\mathbf{D}]_{ij} & \text{if } i \geq j \\ 0 & \text{if } i = j \end{cases} \tag{9}$$

We present here the Δ-**D** matrix of the graph **1**:

	1	**2**	**3**	**4**	**5**	**6**
1	0	2	2	1	2	3
2	1	0	2	3	4	1
3	1	1	0	3	4	3
4	1	2	2	0	1	4
5	2	3	3	1	0	5
6	2	1	2	3	4	0

THE WIENER MATRIX

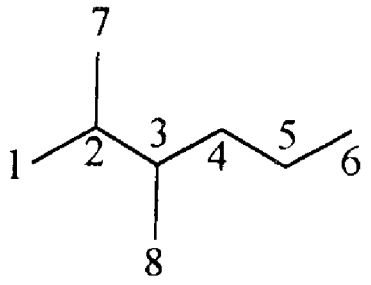
Randić [40] has recently proposed a new graph matrix, the Wiener matrix **W**, and exploited it as a source of new structural invariants. For trees, the Wiener matrix entries are defined as:

$$[\mathbf{W}_{\mathbf{e/p}}]_{ij} = \mathbf{N}_{i,\mathbf{e/p}} \cdot \mathbf{N}_{j,\mathbf{e/p}} \tag{10}$$

where $\mathbf{N}_i$ and $\mathbf{N}_j$ denote the number of vertices lying on the two sides of the edge/path **e**/**p** having vertices i and j as endpoints. This equation defines the "edge/path contributions" to a global descriptor that is identical to the Wiener index when it is defined on edges. The similar equation defined on molecular paths gives a molecular descriptor that is identical to the hyper-Wiener index R [40]. The Wiener matrices were used as the basis of new topological indices [40–42]. The matrix $\mathbf{W}_\Delta$ is defined by the following equation [43, 44]:

$$\mathbf{W}_\Delta = \mathbf{W}_\mathbf{p} - \mathbf{W}_\mathbf{e} \tag{11}$$

The three Wiener matrices are exemplified for the molecular graph of 2, 3-dimethylhexane, **3**:



3

The matrix $\mathbf{W}_e(\mathbf{3})$:

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
1	0	7	0	0	0	0	0	0
2	7	0	15	0	0	0	7	0
3	0	15	0	15	0	0	0	7
4	0	0	15	0	12	0	0	0
5	0	0	0	12	0	7	0	0
6	0	0	0	0	7	0	0	0
7	0	7	0	0	0	0	0	0
8	0	0	7	0	0	0	0	0

The matrix $\mathbf{W}_p(\mathbf{3})$:

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
1	0	7	5	3	2	1	1	1
2	7	0	15	9	6	3	7	3
3	5	15	0	15	10	5	5	7
4	3	9	15	0	12	6	3	3
5	2	6	10	12	0	7	2	2
6	1	3	5	6	7	0	1	1
7	1	7	5	3	2	1	0	1
8	1	3	7	3	2	1	1	0

The matrix $\mathbf{W}_\Delta(\mathbf{3})$:

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
1	0	0	5	3	2	1	1	1
2	0	0	0	9	6	3	0	3
3	5	0	0	0	10	5	5	0
4	3	9	0	0	0	6	3	3
5	2	6	10	0	0	0	2	2
6	1	3	5	6	0	0	1	1
7	1	0	5	3	2	1	0	1
8	1	3	0	3	2	1	1	0

COMBINATORIAL MATRICES

Diudea [43, 44] has recently proposed two matrices: the distance-delta matrix, $\mathbf{D}_\Delta$, and distance-path matrix, $\mathbf{D}_\mathbf{p}$, whose elements are calculated by a combinatorial algorithm from the classical distance matrix **D**:

$$[\mathbf{D}_\Delta]_{ij} = \binom{[\mathbf{D}]_{ij}}{2} \tag{12}$$

$$[\mathbf{D}_\mathbf{p}]_{ij} = \binom{[\mathbf{D}]_{ij}+1}{2} \tag{13}$$

The element $[\mathbf{D}_\Delta]_{ij}$ counts the number of "internal" paths (larger than unity) included in the shortest paths between vertices i and j; the element $[\mathbf{D}_\mathbf{p}]_{ij}$ counts all internal paths included in the shortest paths between vertices i and j in a graph. The matrix $\mathbf{D}_\mathbf{p}$ allows the direct computation of the hyper-Wiener index R, whereas the matrix $\mathbf{D}_\Delta$ gives an index related to the "non-Wiener" part of the hyper-Wiener index. Obviously, $\mathbf{D}_\Delta = \mathbf{D}_\mathbf{p} - \mathbf{D}$. From the matrix **D(3)**:

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
1	0	1	2	3	4	5	2	3
2	1	0	1	2	3	4	1	2
3	2	1	0	1	2	3	2	1
4	3	2	1	0	1	2	3	2
5	4	3	2	1	0	1	4	3
6	5	4	3	2	1	0	5	4
7	2	1	2	3	4	5	0	3
8	3	2	1	2	3	4	3	0

we obtain the combinatorial matrix $\mathbf{D}_\mathbf{p}$**(3)**:

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
1	0	1	3	6	10	15	3	6
2	1	0	1	3	6	10	1	3
3	3	1	0	1	3	6	3	1
4	6	3	1	0	1	3	6	3
5	10	6	3	1	0	1	10	6
6	15	10	6	3	1	0	15	10
7	3	1	3	6	10	15	0	6
8	6	3	1	3	6	10	6	0

and the matrix $\mathbf{D}_{\Delta}(\mathbf{3})$:

	1	2	3	4	5	6	7	8
1	0	0	1	3	6	10	1	3
2	0	0	0	1	3	6	0	1
3	1	0	0	0	1	3	1	0
4	3	1	0	0	0	1	3	1
5	6	3	1	0	0	0	6	3
6	10	6	3	1	0	0	10	6
7	1	0	1	3	6	10	0	3
8	3	1	0	1	3	6	3	0

SZEGED MATRICES

Gutman extended the meaning of the terms $\mathbf{N}_i$ and $\mathbf{N}_j$ from the definition of the hyper-Wiener index R in order to allow their computation for cycle-containing molecular graphs [45, 46]:

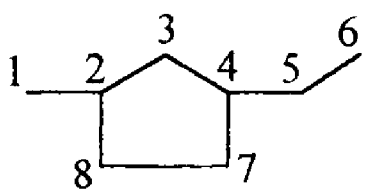
$$\mathbf{N}_{i,\mathbf{e/p}} = |\{v|v \in \mathbf{V}(\mathbf{G}); [\mathbf{D}]_{iv} \leq [\mathbf{D}]_{jv}\}| \tag{14}$$

$$\mathbf{N}_{j,\mathbf{e/p}} = |\{v|v \in \mathbf{V}(\mathbf{G}); [\mathbf{D}]_{jv} \leq [\mathbf{D}]_{iv}\}| \tag{15}$$

Thus, $\mathbf{N}_i$ and $\mathbf{N}_j$ denote the cardinality of the sets of vertices closer to the two vertices i and j, respectively; in this equation the vertices equidistant to i and j are not counted. The Szeged matrix is defined by the equation [47, 48]:

$$[\mathbf{SZ}_{\mathbf{e/p}}]_{ij} = \mathbf{N}_{i,\mathbf{e/p}} \cdot \mathbf{N}_{j,\mathbf{e/p}} \tag{16}$$

The half sum of entries in the $\mathbf{SZ}_{\mathbf{e/p}}$ matrix gives the Szeged index $\mathbf{SZ}_{\mathbf{e}}$, and the hyper-Szeged index $\mathbf{SZ}_{\mathbf{p}}$, respectively. The difference between $\mathbf{SZ}_{\mathbf{p}}$ and $\mathbf{SZ}_{\mathbf{e}}$ gives the $\mathbf{SZ}_{\Delta}$ matrix: $\mathbf{SZ}_{\Delta} = \mathbf{SZ}_{\mathbf{p}} - \mathbf{SZ}_{\mathbf{e}}$. The three Szeged matrices are exemplified for the molecular graph of 1-ethyl-3-methylcyclopentane, **4**:



4

The matrix $\mathbf{SZ_e(4)}$:

	1	2	3	4	5	6	7	8
1	0	7	0	0	0	0	0	0
2	7	0	12	0	0	0	0	6
3	0	12	0	12	0	0	0	0
4	0	0	12	0	12	0	8	0
5	0	0	0	12	0	7	0	0
6	0	0	0	0	7	0	0	0
7	0	0	0	8	0	0	0	12
8	0	6	0	0	0	0	12	0

The matrix $\mathbf{SZ_p(4)}$:

	1	2	3	4	5	6	7	8
1	0	7	5	10	12	12	10	5
2	7	0	12	8	12	10	12	6
3	5	12	0	12	8	12	6	8
4	10	8	12	0	12	6	8	12
5	12	12	8	12	0	7	8	12
6	12	10	12	6	7	0	12	10
7	10	12	6	8	8	12	0	12
8	5	6	8	12	12	10	12	0

The matrix $\mathbf{SZ_\Delta(4)}$:

	1	2	3	4	5	6	7	8
1	0	0	5	10	12	12	10	5
2	0	0	0	8	12	10	12	0
3	5	0	0	0	8	12	6	8
4	10	8	0	0	0	6	0	12
5	12	12	8	0	0	0	8	12
6	12	10	12	6	0	0	12	10
7	10	12	6	0	8	12	0	0
8	5	0	8	12	12	10	0	0

CLUJ MATRICES

In the Wiener and Szeged matrices a path is characterized by its endpoint vertices i and j, namely by their associated numbers $\mathbf{N}_i$ and $\mathbf{N}_j$. If we

renounce to the characterization of the vertex j and define a square matrix with entries characterizing a single endpoint i we obtain a new matrix called the unsymmetric Cluj matrix, $\mathbf{CJ_u}$ [48, 49]:

$$[\mathbf{CJ_u}]_{ij} = \mathbf{N}_{i,(ij)} \tag{17}$$

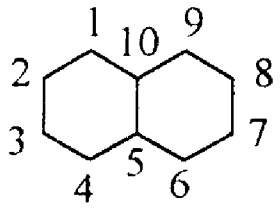
where

$$\mathbf{N}_{i,(ij)} = \mathbf{max}|\{v|v \in \mathbf{V(G)}; [\mathbf{D}]_{iv} \leq [\mathbf{D}]_{jv}; (i, v) \cap (i, j) = \mathbf{max}\{i\}; |(i, j)| = \mathbf{min}\}|.$$

The definition of the unsymmetric Cluj matrix holds both for acyclic and cycle-containing molecular graphs. The unsymmetric Cluj matrix allows the definition of symmetric Cluj matrices $\mathbf{CJ_{e/p}}$ with the relation:

$$[\mathbf{CJ_{e/p}}]_{ij} = [\mathbf{CJ_u}]_{ij}[\mathbf{CJ_u}]_{ji} \tag{18}$$

We have to note that in acyclic graphs the $\mathbf{CJ_{e/p}}$ matrices are identical to $\mathbf{W_{e/p}}$ matrices. For cycle-containing graphs $\mathbf{CJ_e}$ is equal to the $\mathbf{SZ_e}$ matrix, while $\mathbf{CJ_p}$ is different both from $\mathbf{W_p}$ and $\mathbf{SZ_p}$. The matrix $\mathbf{CJ_\Delta}$ is obtained in the same way as the $\mathbf{CJ_p}$ matrix, by defining it on paths larger than unity. The unsymmetric Cluj matrix $\mathbf{CJ_u}$ is exemplified for the molecular graph of tetraline, **5**:



The matrix $\mathbf{CJ_u}$ (**5**):

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
1	0	7	4	4	2	3	3	5	3	3
2	3	0	5	2	2	2	3	3	3	2
3	2	5	0	3	2	3	3	3	2	2
4	4	4	7	0	3	3	5	3	3	2
5	4	6	6	7	0	7	6	6	4	5
6	3	3	5	3	3	0	7	4	4	2
7	2	3	3	3	2	3	0	5	2	2
8	3	3	3	2	2	2	5	0	3	2
9	3	5	3	3	2	4	4	7	0	3
10	7	6	6	4	5	4	6	6	7	0

Using a similar definition, it was defined the unsymmetric Szeged matrix $\mathbf{SZ_u}$; the Szeged matrix $\mathbf{SZ_u(5)}$ is presented below:

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
1	0	7	4	5	2	5	4	6	3	3
2	3	0	5	2	3	3	5	4	4	2
3	2	5	0	3	2	4	4	5	3	3
4	5	4	7	0	3	3	6	4	5	2
5	4	7	6	7	0	7	6	7	4	5
6	5	4	6	3	3	0	7	4	5	2
7	3	5	4	4	2	3	0	5	2	3
8	4	4	5	3	3	2	5	0	3	2
9	3	6	4	5	2	5	4	7	0	3
10	7	6	7	4	5	4	7	6	7	0

EXPANDED DISTANCE MATRICES

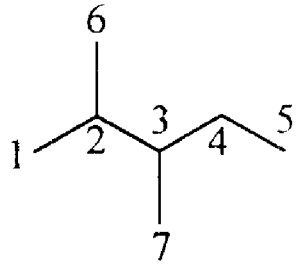
Tratch and coworkers [50] have recently proposed a new graph matrix, an expanded distance matrix $\tilde{\mathbf{D}}$, whose entries are the product of the elements of the distance matrix and a multiplier m_{ij} that is the number of paths containing the path $\mathbf{p}_{ij}$ as a subpath. In acyclic structures it equals the entries in the $\mathbf{W_p}$ matrix, and we will denote $\tilde{\mathbf{D}}$ as the expaned distance $\mathbf{W_p}$ matrix, $\mathbf{D\_W_p}$:

$$[\mathbf{D\_W_p}]_{ij} = [\mathbf{D}]_{ij} m_{ij} = [\mathbf{D}]_{ij}[\mathbf{W_p}]_{ij} \tag{19}$$

Similarly, Diudea defined a new unsymmetric matrix $\mathbf{D\_CJ_u}$ that offers a new definition of the hyper-Wiener number [49]:

$$[\mathbf{D\_CJ_u}]_{ij} = [\mathbf{D}]_{ij}[\mathbf{CJ_u}]_{ij} \tag{20}$$

The $\mathbf{D\_W}_p$ and $\mathbf{D\_CJ_u}$ matrices are exemplified for 2, 3-dimethylpentane, **6**:



6

The matrix $\mathbf{D\_W_p(6)}$:

	1	**2**	**3**	**4**	**5**	**6**	**7**
1	0	6	8	6	4	2	3
2	6	0	12	12	9	6	6
3	8	12	0	10	10	8	6
4	6	12	10	0	6	6	4
5	4	9	10	6	0	4	3
6	2	6	8	6	4	0	3
7	3	6	6	4	3	3	0

The matrix $\mathbf{D\_CJ_u(6)}$:

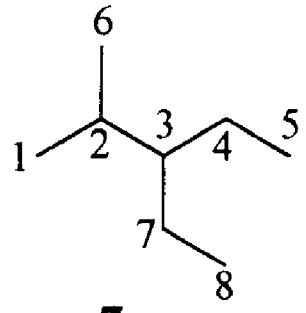
	1	**2**	**3**	**4**	**5**	**6**	**7**
1	0	1	2	3	4	2	3
2	6	0	3	6	9	6	6
3	8	4	0	5	10	8	6
4	6	4	2	0	6	6	4
5	4	3	2	1	0	4	3
6	2	1	2	3	4	0	3
7	3	2	1	2	3	3	0

WALK MATRIX

Diudea has recently proposed the walk matrix $\mathbf{W_{(M1, M2, M3)}}$, defined by the equation [43]:

$$[\mathbf{W_{(M1, M2, M3)}}]_{ij} = {}^{[\mathbf{M2}]_{ij}}\mathbf{W_{M1},}_{i}[\mathbf{M3}]_{ij} \tag{21}$$

where ${}^{[\mathbf{M2}]_{ij}}\mathbf{W_{M1},}_{i}$ is computed on the basis of the matrix **M1** and represents the number of walks with the length $[\mathbf{M2}]_{ij}$ starting at the vertex i, and the multiplier $[\mathbf{M3}]_{ij}$ is an element from a third square matrix. The matrices $\mathbf{W_{(M1, M2, M3)}}$ are exemplified for 3-ethyl-4-methylpentane, **7**:



7

The matrix $\mathbf{W}_{(A,\,D,\,1)}$ (7):

	1	2	3	4	5	6	7	8
1	0	1	3	5	13	3	5	13
2	3	0	3	5	13	3	5	13
3	7	3	0	3	7	7	3	7
4	9	4	2	0	2	9	4	9
5	9	4	2	1	0	9	4	9
6	3	1	3	5	13	0	5	13
7	9	4	2	4	9	9	0	2
8	9	4	2	4	9	9	1	0

The matrix $\mathbf{W}_{(A,\,D,\,D)}$ (7):

	1	2	3	4	5	6	7	8
1	0	1	6	15	52	6	15	52
2	3	0	3	10	39	3	10	39
3	14	3	0	3	14	14	3	14
4	27	8	2	0	2	27	8	27
5	36	12	4	1	0	36	12	36
6	6	1	6	15	52	0	15	52
7	27	8	2	8	27	27	0	2
8	36	12	4	12	36	36	1	0

The matrix $\mathbf{W}_{(A,\,1,\,D)}$ (7):

	1	2	3	4	5	6	7	8
1	0	1	2	3	4	2	3	4
2	3	0	3	6	9	3	6	9
3	6	3	0	3	6	6	3	6
4	6	4	2	0	2	6	4	6
5	4	3	2	1	0	4	3	4
6	2	1	2	3	4	0	3	4
7	6	4	2	4	6	6	0	2
8	4	3	2	3	4	4	1	0

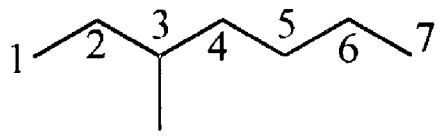
HOSOYA MATRIX

Randić has recently put forward a novel matrix, the Hosoya **Z** matrix, associated with acyclic molecular graphs as well as two molecular indices

path numbers $^1\mathbf{Z}$ and $^2\mathbf{Z}$ derived from it [51]. The $\mathbf{Z}$ matrix entry $[\mathbf{Z}]_{ij}$ corresponding to a pair of vertices (i, j) of a tree, T, is given by:

$$[\mathbf{Z}]_{ij} = \begin{cases} Z(T - \mathbf{p}_{ij}) & \text{if} \quad i \neq j \\ 0 & \text{if} \quad i = j \end{cases} \tag{22}$$

where $Z(T - \mathbf{p}_{ij})$ is the Z index [52–54] of the spanning subgraph $T - \mathbf{p}_{ij}$ obtained from T by the removal of all edges along the path $\mathbf{p}_{ij}$ connecting the vertices i and j. The Hosoya matrix is exemplified for 3-methylheptane, **8**:



8

The matrix **Z(8)**:

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
1	0	17	12	9	5	3	1	7
2	17	0	25	18	11	7	3	15
3	12	25	0	24	14	9	4	20
4	9	18	24	0	20	13	6	14
5	5	11	14	20	0	22	11	8
6	3	7	9	13	22	0	18	5
7	1	3	4	6	11	18	0	2
8	7	15	20	14	8	5	2	0

The $\mathbf{Z}$ matrix and the path numbers were generalized to be defined for all simple connected undirected graphs as well as edge-weighted graphs [55, 56].

THE PATH MATRIX P

The $\mathbf{P}$ matrix of a graph G, $\mathbf{P} = \mathbf{P}(G)$, is the square symmetric $N \times N$ matrix whose entry in the i th row and j th column is defined as [57, 58]:

$$[\mathbf{P}]_{ij} = \begin{cases} \mathbf{p}'_{ij}/\mathbf{p} & \text{if} \quad (i, j) \in \mathbf{E}(G) \\ 0 & \text{otherwise} \end{cases} \tag{23}$$

where $\mathbf{p}'_{ij}$ is the total number of paths in the subgraph G' obtained from the graph G by deleting the edge between vertices i and j, and $\mathbf{p}$ is the total number of paths in G. If G' is disjoint then the contributions of each

component are added. The **P** matrix is the source of novel graph invariants [59]. Using a similar algorithm Randić and coworkers defined the graphical bond order of the edge (i, j), $\mathbf{I}'(i, j)$, related to a certain graph invariant **I** and computed with the equation [60].

$$\mathbf{I}'(i, j) = \mathbf{I}(G') / \mathbf{I}(G) \tag{24}$$

where $\mathbf{I}(G)$ and $\mathbf{I}(G')$ represent the value of the graph invariant **I** for the graph G and for its subgraph G', respectively.

We have restricted the presentation of molecular matrices to graph matrices containing only the topological information of a molecule. In order to incorporate more information on the molecular structure new matrices were defined using the geometrical coordinates of the non-hydrogen atoms [61–64].

DEFINITIONS OF GRAPH OPERATORS

We define the molecular graph operators that will be used to compute some topological indices defined on the basis of molecular graph matrices.

The Wiener operator, $\mathbf{Wi}(\mathbf{M}, G)$, is defined by analogy with the Wiener index [65, 66]:

$$\mathbf{Wi}(\mathbf{M}, G) = \sum_{i=1}^{N} \sum_{j=i}^{N} [\mathbf{M}]_{ij} \tag{25}$$

where **M** represents the molecular matrix of G. If **M** is the distance matrix, the operator is identical with the Wiener index, while if **M** is the reciprocal distance matrix, this operator gives the Harary index [31, 32].

By analogy with the hyper-Wiener index [40] we define the Hyper-Wiener operator of a graph G, $\mathbf{HyWi}(\mathbf{M}, G)$:

$$\mathbf{HyWi}(\mathbf{M}, G) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=i}^{N} ([\mathbf{M}]_{ij}^2 + [\mathbf{M}]_{ij}) \tag{26}$$

If **M** is the distance matrix, the **HyWi** operator is identical with the hyper-Wiener index R [40].

The Vertex Sum operator for the vertex i in a graph G, $\mathbf{VS}(\mathbf{M}, G)_i$, is defined as the sum of the elements in the row i (or column i) of the

molecular matrix **M**:

$$\mathbf{VS}(\mathbf{M}, G) = \sum_{j=1}^{N} [\mathbf{M}]_{ij} \tag{27}$$

If **M** is the adjacency matrix, the operator gives the vertex degree **deg**; if **M** is the distance matrix, this operator gives the distance sum **DS** [67, 68]; if **M** is the **RΔ** matrix, the **VS** operator is identical with the reciprocal distance sum **RΔS** [29, 32].

By analogy with the **J** index [67, 68] we define the Ivanciuc-Balaban operator of a graph G, **IB**(**M**, G):

$$\mathbf{IB}(\mathbf{M}, G) = \frac{m}{\mu + 1} \sum_{\mathbf{E}(G)} (\mathbf{VS}_i \mathbf{VS}_j)^{-1/2} \tag{28}$$

where m is the number of edges in G, μ is the cyclomatic number of G (the number of cycles in G), and the summation goes over all edges from the edge set **E**(G). The **IB** operator gives the **J** index when **M** is the distance matrix.

INTERCORRELATION OF TOPOLOGICAL INDICES

Certain properties of a molecular graph encoded in an implicit form in the adjacency matrix, are explicitly expressed in the presented matrix. These matrices can be computed, using specific algorithms, on the basis of the adjacency matrix. Owing to the common source of the matrices, it is possible that the topological indices derived from the presented matrices express predominantly the same type of structural information. It is well known that the high degree of intercorrelation among topological indices used as predictor variables in a multiple linear regression model prevents the unambiguous interpretation of the model [69–71]. Hence, we studied the existence of linear relationships between pairs of topological indices by computing the intercorrelation matrix presented in Table I.

The present study uses 19 structural descriptors, presented in the following list with their symbol and the number that identifies each descriptor in Table I: N (the number of carbon atoms), 1; ${}^{0}\chi$, 2; ${}^{1}\chi$, 3; ${}^{2}\chi$, 4; ${}^{3}\chi_{p}$, 5; ${}^{3}\chi_{c}$, 6; **Wi(D)**, 7; **Wi(RD)**, 8; **Wi(D**$_{\Delta}$**)**, 9; **Wi(D**$_{p}$**)**, 10; **Wi(RD**$_{p}$**)**, 11; **HyWi(RD)**, 12; **HyWi(D**$_{\Delta}$**)**, 13; **HyWi(D**$_{p}$**)**, 14; **HyWi(RD**$_{p}$**)**, 15; **IB(D)**, 16; **IB(RD)**, 17; **IB(D**$_{p}$**)**, 18; **IB(RD**$_{p}$**)**, 19. The connectivity indices χ [72, 73] are included because they represent the most used TIs in developing QSPR and

TABLE I The matrix of the intercorrelation coefficients of 19 topological descriptors for 306 alkanes containing from 4 up to 11 carbon atoms. Each topological descriptors is identified in this matrix with the number following its symbol in the list: N, 1; $^{0}\chi$, 2; $^{1}\chi$, 3; $^{2}\chi$, 4; $^{3}\chi$, 5; $^{3}\chi_{c}$, 6; **Wi(D)**, 7; **Wi(RD)**, 8; **Wi(D_{Δ})**, 9; **Wi(D_{p})**, 10; **Wi(RD_{p})**, 11; **HyWi(RD)**, 12; **HyWi(D_{Δ})**, 13; **HyWi(D_{p})**, 14; **HyWi(RD_{p})**, 15; **IB(D)**, 16; **IB(RD)**, 17; **IB(D_{p})**, 18; **IB(RD_{p})**, 19

	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	0.98	0.97	0.73	0.72	0.23	0.93	0.98	0.75	0.82	0.98	0.98	0.50	0.58	0.98	0.54	0.96	−0.03	0.95
2		0.91	0.82	0.76	0.38	0.88	0.99	0.65	0.74	1.00	1.00	0.39	0.47	1.00	0.66	0.90	0.11	0.89
3			0.53	0.67	−0.01	0.95	0.91	0.82	0.88	0.90	0.91	0.60	0.67	0.91	0.38	0.98	−0.19	0.99
4				0.48	0.82	0.58	0.79	0.36	0.44	0.80	0.79	0.15	0.21	0.80	0.67	0.58	0.29	0.55
5					0.19	0.53	0.79	0.26	0.36	0.80	0.79	0.04	0.10	0.79	0.79	0.58	0.46	0.58
6						0.05	0.35	−0.14	−0.08	0.38	0.35	−0.25	−0.23	0.36	0.60	0.03	0.53	0.00
7							0.87	0.93	0.97	0.85	0.87	0.75	0.81	0.87	0.25	0.99	−0.32	0.99
8								0.64	0.73	1.00	1.00	0.37	0.44	1.00	0.68	0.90	0.14	0.89
9									0.99	0.61	0.63	0.93	0.97	0.64	−0.10	0.89	−0.60	0.90
10										0.70	0.72	0.89	0.93	0.72	0.01	0.94	−0.52	0.94
11											1.00	0.34	0.42	1.00	0.70	0.88	0.18	0.87
12												0.36	0.44	1.00	0.68	0.90	0.15	0.89
13													0.99	0.37	−0.35	0.69	−0.71	0.70
14														0.45	−0.28	0.776	−0.69	0.76
15															0.68	0.90	0.14	0.89
16																0.30	0.82	0.29
17																	−0.28	1.00
18																		−0.29

QSAR models. The intercorrelation coefficients were calculated using the TIs values for 306 alkanes containing from 4 up to 11 carbon atoms.

The inspection of intercorrelation coefficients r from Table I shows that the linear relationship between the indices varies from strong ($r > 0.9$) to the complete lack of linear correlation (orthogonal indices, $r = 0$). This situation indicates that although all structural descriptors have a common source, they express in part or completely different structural information.

The number of carbon atoms N is highly intercorrlelated ($r > 0.9$) with nine indices: ${}^{0}\chi$, 0.98; ${}^{1}\chi$, 0.97; **Wi(D)**, 0.93; **Wi(RD)**, 0.98; **Wi(RD$_p$)**, 0.98; **HyWi(RD)**, 0.98; **HyWi(RD$_p$)**, 0.98; **IB(RD)**, 0.96; **IB(RD$_p$)**, 0.95. This finding shows that these indices express to a large extent the same type of structural information. On the other hand, there are some topological indices which have a low intercorrelation coefficient with N, namely: ${}^{3}\chi_c$, 0.23; **HyWi(D$_\Delta$)**, 0.50; **HyWi(D$_p$)**, 0.58; **IB(D)**, 0.54; **IB(D$_p$)**, −0.03.

The high values of the intercorrelation coefficients of some pairs of TIs indicate that the development of a multiple linear regression model with two or more TIs as independent variables requires a careful selection of TIs. For example, from the set presented above of nine topological indices highly intercorrelated with the number of carbon atoms no one can be used in a multiple linear regression model together with N. Also, the intercorrelation coefficient between **Wi(D)** and **Wi(D$_p$)** is $r = 0.97$, indicating that a multiple linear regression model cannot contain both topological indices. Other examples of highly intercorrelated TIs are **Wi(D$_\Delta$)** and **Wi(D$_p$)** with $r = 0.99$, **HyWi(D$_\Delta$)** and **HyWi(D$_p$)**, with $r = 0.99$, and **Wi(D$_\Delta$)** and **HyWi(D$_p$)** with $r = 0.97$.

The structural descriptors **Wi(D$_\Delta$)**, **Wi(D$_p$)**, **HyWi(D$_\Delta$)**, **HyWi(D$_p$)**, **IB(D$_p$)**, **IB(RD$_p$)**, based on the new matrices $\mathbf{D}_p$ and $\mathbf{D}_\Delta$, have low intercorrelation coefficients with the descriptors derived from other molecular matrices. This is an indication that these two new matrices express some structural information that is absent from other matrices, and the TIs derived from them are good candidates for developing structure-property models.

The obtained results suggest that novel molecular graph matrices could be a source of new and interesting topological indices for QSAR and QSPR studies.

Acknowledgement

We would like to thank the referees for their suggestions that greatly improved the paper. We acknowledge the partial financial support of this

research by the Ministry of Research and Technology under Grant 381 TA10 and by the Ministry of Education under Grant 5001 TB10.

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